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Novel A-seco-nortriterpenoids from Ganoderma cochlear inhibiting Tau pathology by activating AMPK-ULK1-mediated autophagy†

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Ten structurally diverse *Ganoderma* triterpenoids, including one unprecedented highly degraded A-seconortriterpenoid, ganolearin A (**1**) with a 6/6/5-tricyclo structure containing a unique benzene ring, three new rearranged nortriterpenoids, ganolearin B (**2**) and ganolearin C (**3**) with a rare 3/5/6/5-fused skeleton, and ganolearin D (**4**) featuring a $3 \rightarrow 10 \gamma$ -lactone ring and a five-membered carbon ring, and six analogues, ganolearates E–G and J (**5–7**, **10**), and ganolearic acids H (**8**) and I (**9**), were isolated from the fruiting bodies of *Ganoderma cochlear*. Their structures were elucidated by extensive 1D and 2D NMR spectroscopy, HRESIMS, X-ray crystallography and ECD calculation analysis. A plausible biosynthetic pathway for **1–4** was proposed. Furthermore, compounds **1–4** significantly inhibited Tau pathology by inducing autophagy mediated by the AMPK-ULK1 pathway, suggesting their potential against Alzheimer's disease (AD).

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Introduction

Ganoderma has attracted significant attention from pharmacologists, chemists, and phytochemists because it has long been used as a traditional medicine in many countries^{1,2} and is also an important source of meroterpenoids and lanostane triterpenoids with significant bioactivities and captivating structures.^{3–9} In particular, *Ganoderma* triterpenoids (GTs) have been widely studied as the main active constituents of *Ganoderma* for their anti-tumor, anti-aging, liver-protective, and neuroprotective activities. Notably, previous studies have confirmed that GTs can reverse cognitive impairment,¹⁰ attenuate LPS-induced inflammation and apoptosis,¹¹ promote amyloid- β clearance and inhibit Tau pathology through activating autophagy,^{6,12} suggesting that GTs exhibit huge potential in the treatment of neurodegenerative diseases.

Alzheimer's disease (AD), the most pervasive neurodegenerative disease associated with aging, seriously threatens people's lives.^{13,14} The extracellular amyloid plaques (which are composed of amyloid beta (A β) peptides) and the intraneuronal neurofibrillary tangles (NFTs) composed of the Tau (MAPT/Tau) protein are two hallmarks of AD pathology. Autophagy is a key process wherein cellular components such as corrupted organelles or unwanted protein materials aggregate in intracellular autophagosomes and undergo degradation or/and recycling in lysosomes.¹⁵ Various studies prove that autophagy is the main route to remove A β or/and MAPT/ Tau aggregates.^{16,17} Thus, activation of autophagy might be a vital strategy for AD treatment.^{18–22}

Therefore, we continue isolating structurally diverse GTs from the fruiting bodies of *Ganoderma cochlear* in order to provide more possibilities for the development of anti-AD drugs. Interestingly, ten new A-*seco*-norlanostane triterpenoids with five different skeletons were found (Fig. 1 and Fig. S1†). Their structures were confirmed by using 1D and 2D NMR spectroscopic data, X-ray single crystollography, and electronic circular dichroism (ECD) calculation methods. The further cellular assay indicated that compounds **1–4** induced autophagy by activating the AMPK-ULK1 signaling pathway (mTOR-independent

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5

pathway). Overall, the current data demonstrated that 1–4 could be potential compounds for AD therapy by inducing autophagy.

Results and discussion

Ganolearin A (1) has a molecular formula of $C_{24}H_{32}O_5$, as determined by HRESIMS at m/z 401.2322 [M + H]⁺ (calcd 401.2323), indicating 9 degrees of unsaturation. The ¹H NMR spectroscopic data (Table S1[†]) of 1 showed four singlet methyls at δ_H 0.74, 1.21, 2.55, and 2.57, one doublet methyl at δ_H 0.90 (d, J = 6.4 Hz), one methoxyl at δ_H 3.68 (s), two aromatic methines at δ_H 7.47 (d, J = 7.9 Hz) and δ_H 7.54 (d, J = 7.9Hz), and one oxygenated methine at δ_H 5.60 (dd, J = 5.1 and 9.5 Hz). In the ¹³C-DEPT spectra of 1, twenty-four carbon resonances were observed, comprising five methyls, one methoxyl, four methylenes, five methines, and nine quaternary carbons (two ketones, one ester carbonyl, and four aromatic quaternary carbons). The above data showed that compound 1 could be a norlanostane triterpenoid.

The HMBC correlations (Fig. 2) of H₃-18 with C-12, C-13, C-14, and C-17; of H₂-12 with C-11 ($\delta_{\rm C}$ 200.4) and C-9 ($\delta_{\rm C}$ 140.7); of H₃-21 with C-17, C-20, and C-22; and of H₂-22 and OMe ($\delta_{\rm H}$ 3.68, s) with C-24 ($\delta_{\rm c}$ 174.2), as well as a series of ¹H-¹H COSY correlations (Fig. 2) of H-15/H₂-16/H-17/H-20/H₂-22/H₂-23, indicated that compound **1** had similar C and D

rings and side chains to those of fornicatin E.²³ Further analysis of the HMBC spectrum (Fig. 2) showed that H₃-30 correlated with C-13, C-14, C-15 ($\delta_{\rm C}$ 74.1), and C-8 ($\delta_{\rm C}$ 152.8); simultaneously, H-15 showed correlations with C-13, C-8, and C-17. The aforementioned information illustrated that the hydroxyl group was linked to C-15. These functionalities accounted for five degrees of unsaturation.

Except for a ketone carbonyl, the remaining 4 degrees of unsaturation were representative of another benzene ring, which was consistent with the observation of six aromatic signals at $\delta_{\rm H}$ 7.47 (d, J = 7.9 Hz), $\delta_{\rm C}$ 122.6; $\delta_{\rm H}$ 7.54 (d, J = 7.9 Hz), $\delta_{\rm C}$ 131.2; $\delta_{\rm C}$ 131.2; $\delta_{\rm C}$ 138.1; $\delta_{\rm C}$ 140.7 and $\delta_{\rm C}$ 152.8. The HMBC correlations (Fig. 2) of H₃-19 with C-5 ($\delta_{\rm C}$ 131.2), C-9 ($\delta_{\rm C}$ 140.7), and C-10 ($\delta_{\rm C}$ 138.1), of H₃-29 with C-5 and C-4 ($\delta_{\rm C}$ 203.9), of H-6 ($\delta_{\rm H}$ 7.54, d, J = 7.9 Hz) with C-4, C-10, and C-8 ($\delta_{\rm C}$ 152.8), and of H-7 ($\delta_{\rm H}$ 7.47, d, J = 7.9 Hz) with C-5, C-9 ($\delta_{\rm C}$ 140.7), and C-14 ($\delta_{\rm C}$ 52.3) further confirmed that C-1, C-2, C-3, and C-28 were degraded and the B ring was aromatized. In the ROESY spectrum (Fig. 3) of 1, H-15 correlated with H₃-18, indicating that 15-OH was α -oriented. Therefore, the structure of compound 1 was finally established.

The molecular formula of ganolearin B (2) was determined to be $C_{26}H_{38}O_6$ based on the positive HRESIMS at m/z469.2564 [M + Na]⁺ (calcd 469.2561), which indicated 8 degrees of unsaturation. The 1D NMR spectroscopic data (Table S1[†]) of 2 showed that the structure of 2 resembles that of ganolearic acid A,²⁴ except for the presence of an additional methoxyl and an oxymethine, and the absence of one methylene. The detailed comparison of the 1D NMR spectra of 2 and ganolearic acid A showed the replacement of the carboxyl at C-24 by a methyl ester carbonyl, which was confirmed by the HMBC correlations (Fig. 2) of OCH₃ ($\delta_{\rm H}$ 3.71, s) with C-24 ($\delta_{\rm C}$ 176.2) in 2. Furthermore, the oxymethine proton ($\delta_{\rm H}$ 4.71, dd, *J* = 12.9 and 5.9 Hz) showed HMBC correlations with C-13 ($\delta_{\rm C}$ 48.1), C-14 ($\delta_{\rm C}$ 48.2), C-15 ($\delta_{\rm C}$ 40.9), and C-17 ($\delta_{\rm C}$ 54.7), as well as $^1{\rm H}{-}^1{\rm H}$ COSY correlations (Fig. 2) of H₂-15/H-16/H-17/H-20/H₃-21, suggesting that C-15 was connected to a hydroxyl group. Thus, the planar structure of 2 was established.

The ROESY spectrum of 2 showed the correlations of H-16/ $H_3\mathchar`-30$, indicating that 16-OH was $\beta\mathchar`-01\mathchar`-31\m$



Fig. 2 Selected HMBC (H \rightarrow C) and $^{1}\text{H}-^{1}\text{H}$ COSY (H–H) correlations of compounds 1–4.



Fig. 3 Key ROESY (x · · · ·) correlations of compounds 1-4.

addition, the ROESY correlations of H₃-19/H-5/H-7/H-6a and of H-6b/H₃-30 were observed, indicating that the relative configurations of H-5 and H-7 were β , opposite to 5 α and 7 α of ganolearic acid A.²⁴ Furthermore, the X-ray crystallographic data (Fig. 4A) proved that the absolute configuration of 2 was 5*S*,7*R*,10*S*,13*R*,14*R*,16*S*,17*R*,20*R*. Thus, the structure of compound 2 including the stereostructure was finally determined.

The HRESIMS of ganolearin C (3) showed an $[M - H]^-$ peak at m/z 457.2602 $[M - H]^-$ (calcd 457.2596), indicating a molecular formula of $C_{27}H_{38}O_6$ for 3 and 9 degrees of unsaturation. Its 1D NMR spectroscopic data (Table S1†) were similar to those of ganolearic acid A,²⁴ suggesting that compound 3 was also a norlanostane triterpenoid with a 3/4/6/4-tetracyclic skel-



Fig. 4 (A) X-ray crystallographic structures of compounds **2** and **4**. (B) Calculated and experimental CD curves of compound **3**.

eton. However, an additional methyl group ($\delta_{\rm H}$ 2.25, s; $\delta_{\rm C}$ 30.5) and a ketone group ($\delta_{\rm C}$ 205.4) were present in 3; meanwhile, one methylene in ganolearic acid A was replaced by a methine $(\delta_{\rm H} 1.62, {\rm m}; \delta_{\rm C} 35.7)$ in 3. Furthermore, the HMBC spectrum (Fig. 2) of 3 showed the correlations of the methyl protons ($\delta_{\rm H}$ 2.25, s) with the ketone carbonyl ($\delta_{\rm C}$ 205.4) and methine ($\delta_{\rm C}$ 35.7), of the methine proton ($\delta_{\rm H}$ 1.62, m) with C-6 ($\delta_{\rm C}$ 39.2), C-10 ($\delta_{\rm C}$ 49.7), and C-8 ($\delta_{\rm C}$ 171.8), of H-6 ($\delta_{\rm H}$ 2.04, m) with C-10 $(\delta_{\rm C}$ 49.7), C-9 $(\delta_{\rm C}$ 135.6), and C-19 $(\delta_{\rm C}$ 22.5), and of H-7 $(\delta_{\rm H}$ 2.47, m) with C-9 and C-14 ($\delta_{\rm C}$ 49.7). Meanwhile, the ¹H-¹H COSY correlations (Fig. 2) of H-5/H-6/H-7 illustrated that C-5 was linked with an acetyl group. The ROESY correlations (Fig. 3) of H-5/H₃-18/H₃-19 and H-6/H-7/H₃-30 indicated that H-5 was β -oriented; in contrast, H-6 and H-7 were α -oriented. Furthermore, the ECD calculation method was used to confirm its absolute configuration. As shown in Fig. 4B, the ECD curve of 5R,6S,7R,10S,13R,14R,17R,20R-3 corresponds to the experimental CD curve. Therefore, the structure of 3 was established.

Ganolearin D (4) has a molecular formula of $C_{25}H_{36}O_6$, which was determined using HRESIMS at m/z 471.2143 [M + K]⁺ (calcd 471.2143) with 8 degrees of unsaturation. It had similar 1D NMR spectroscopic data to those of ganocochlearic acid A²⁵ except that an oxymethine replaced the methylene in 4. Furthermore, the oxymethine proton (δ_H 5.36, t, J = 7.3 Hz) showed the HMBC correlations of C-5 (δ_C 48.5), C-6 (δ_C 38.5), C-8 (δ_C 174.1), C-9 (δ_C 133.7), and C-14 (δ_C 49.8), which indicated that the hydroxyl group was located at C-7. The ROESY correlation of H-7/H₃-30 proved the β -configuration of 7-OH. The X-ray crystallographic data (Fig. 4A) further confirmed that the absolute configuration of 4 was 5*S*,7*S*,10*R*,13*R*,14*R*,17*R*,20*R*. Finally, the structure of 4 was determined.

Compounds 1–4 were highly degraded and rearranged lanostane-triterpenoids, in which major changes were present in the B ring. Biosynthetically, fornicatin A^{23} was deduced to be a plausible biosynthetic precursor, which was further oxidized to a 4-oxo derivative (intermediate I). Subsequently, the



Scheme 1 A plausible biosynthetic pathway for 1-4.



Fig. 5 Inhibition effects of compounds 1–4 on Tau pathology by activating autophagy in SH-SY5Y MAPT cells. (A–H) Western blotting assays showing the protein levels of autophagy markers LC3-II/LC3-I and SQSTM1, and Tau P301S in the SH-SY5Y MAPT cells treated with or without the compounds. (I, K) Western blotting analyses of autophagy markers LC3-II/LC3-I and SQSTM1, and Tau P301S in cell lysates from SH-SY5Y MAPT cells treated with BAFA1 (bafilomycin A1, 20 nM), 1–4 (20 μ M) or both (BAFA1 and 1, BAFA1 and 2, BAFA1 and 3, or BAFA1 and 4). (A–L) A representative western blotting result (A, C, E, G, I and K) and quantification of the respective protein levels (B, D, F, H, J and L) based on 3 independent experiments. DMSO (dimethyl sulfoxide), used as a solvent for the compounds, served as the control. Rapamycin (Rapa) was used as a positive control. Relative protein abundance was normalized to GAPDH. ns, not significant; *, *P* < 0.05; **, *P* < 0.01; ***, *P* < 0.001; ****, *P* < 0.0001; one-way ANOVA with Tukey's *post-hoc* test. Bars represent mean <u>+</u> SD.

dehydration of 7-OH and H-6 happened, forming **II** containing a long-range unsaturated fraction (C-6/C-7/C-8/C-9/C-11). The allylic oxidation at C-5 led to the formation of **III**, which was dehydrated to form a carbocation (**IV**). The further aromatization of ring B occurred by losing the C-1/C-2/C-3 moiety. The oxidation of C-15 and the esterification of 24-COOH finally resulted in the formation of compound **1**. In addition, **II** can also be transformed to **V** *via* a 1,2-alkyl shift under acidic conditions. The cyclization between C-7 and C-5 and esterification at C-3 resulted in the formation of **3**.

VI was obtained from **I** through a Baeyer–Villiger reaction. Then, the hydrolyzation of **VI** led to the formation of **VII** and the carbocation at C-5 was obtained as **VIII** through the dehydration of 5-OH because of the acid. Meanwhile, the cleavage of C-10/C-9 and the linkage of C-9/C-5 resulted in the formation of a carbocation at C-10. Simultaneously, 3-COOH attacked C-10 to form $3 \rightarrow 10 \gamma$ -lactone (compound 4). Additionally, the dehydration of 7-OH occurred under the acidic conditions, forming a carbocation (C-7). C-5 further attacked C-7, resulting in the formation of a unique threemembered ring accompanied by the deacetyloxy group. Both 3-COOH and 24-COOH were finally esterified to obtain compound **2** (Scheme 1).

It is well known that autophagy is a promising therapeutic strategy against tauopathy for promoting the clearance of Tau.²⁶ In our present study, compounds 1–4 could significantly induce autophagy and show no toxicities in SH-SY5Y mCherry-GFP-LC3 cells, at concentrations of 5 and 20 μ M (Fig. S4 and S5†). Then, the human MAPT mutant MAPT-p.P301S was stably expressed in SH-SY5Y cells (named SH-SY5Y MAPT cells).⁶ In the SH-SY5Y MAPT cells treated with 1–4, an increased protein level of the lipidated (PE-conjugated) form of MAP1LC3/LC3 (microtubule-associated protein 1 light chain 3; LC3-II/LC3-I) and a decreased protein level of SQSTM1 (sequestosome 1) in a dose-dependent manner were observed (Fig. 5A–H).

Meanwhile, compounds 1–4 reduced the Tau P301S level in SH-SY5Y MAPT cells (Fig. 5A–H). Furthermore, BAFA1 (bafilo-



Fig. 6 Compounds 1–4 activate the AMPK-ULK1 pathway. (A–H) Western blotting assays showing the protein levels of pAMPK α , AMPK α , pAMPK β 1, AMPK β 1, AMPK β 2, pULK1ser777, pULK1ser757, pULK1ser555 and ULK1 in the SH-SY5Y MAPT cells treated with or without the compounds. (A–H) A representative western blotting result (A, C, E and G) and quantification of the respective protein levels (B, D, F and H) based on 3 independent experiments. Relative protein abundance was normalized to ACTB. ns, not significant; *, *P* < 0.05; **, *P* < 0.01; ***, *P* < 0.001; one-way ANOVA with Tukey's *post-hoc* test. Bars represent mean \pm SD.



Fig. 7 The molecular docking results of compounds 1–4 with AMPK (PDB: 4CFH).

mycin A1), an inhibitor of the vacuolar(v)-type ATPase resulting in the blockage of autophagosome–lysosome fusion and accumulation of LC3-II,²⁷ was further used to demonstrate the role of autophagy induced by **1–4** in MAPT/Tau clearance in SH-SY5Y MAPT cells. Treatment with BAFA1 (20 nM) alone raised LC3-II/LC3-I, but with no significant effect on Tau P301S. BAFA1 could reverse the decreased levels of Tau P301S induced by compounds **1–4** (Fig. 5I–L). These results illustrated that compounds **1–4** reduce Tau P301S by activating autophagy.

Furthermore, we investigated the mechanism by which compounds 1–4 regulate autophagy. First, we checked whether these compounds would affect the mTOR activity. Rapamycin (an inhibitor of mTOR) is used as a positive control. Our results show that the activity of mTOR is not influenced by compounds 1–4 because of no significant changes in the protein levels of mTOR, pmTOR2448 and pmTOR2481 in SH-SY5Y MAPT cells (Fig. S6†).

As AMPK activation is one of the critical pathways involved in autophagy induction,²⁸ recent studies have reported that the inactivation of mTOR is not always necessary for autophagy.²⁹ AMPK can also directly phosphorylate and activate ULK1 at Ser317, Ser555, and Ser777 to initiate autophagy.³⁰ In the present study, compounds 1-4 significantly increased the protein levels of pAMPKα, pAMPKβ1, pULKser777, pULKser317, and pULKser555, whereas the protein levels of AMPKa, AMPKβ1, AMPKβ2, ULK1 and pULKser757 did not significantly change after treatment with compounds 1-4 in SH-SH5Y MAPT cells (Fig. 6). The further molecular docking revealed the interaction mode of compounds 1-4 with AMPK, and their binding energy ranged from -7.7 to -8.2 kcal mol⁻¹. Compounds 1-4 bound the key domain of AMPK containing ARG263 (Fig. 7), which affects AMPK phosphorylation. These results suggest that compounds 1-4 induce autophagy by activating the AMPK-ULK1 pathway rather than the mTOR-dependent signaling pathway.

Conclusions

In summary, we isolated ten A-seco-nortriterpenoids with six different types of skeletons from *G. cochlear*, of which com-

pound 1 is the first example of a 6/6/5-tricyclic-hexanortriterpenoid containing a unique aromatic ring. Although 2 and 3 have similar skeletons, combined analysis of their detailed structures and stereochemistry suggests that they could be derived via different biosynthetic pathways. The autophagy process is mainly regulated through mTOR-dependent and mTOR-independent signaling pathways.28 Previous research studies showed that GTs reverse cognitive impairment by suppressing PI3K/AKT/mTOR expression.¹⁰ However, in our study, compounds 1-4 could significantly reduce Tau pathology by activating autophagy mediated by the AMPK-ULK1 pathway rather than the mTOR-dependent pathway, indicating that GTs with different skeletons can exhibit anti-neurodegeneration via multiple targets and signaling pathways. Meanwhile, these results also provide scientific evidence for the application of Ganoderma in anti-neurodegenerative diseases.

Experimental section

General experimental procedures

Silica gel (200-300 mesh, Qingdao Marine Chemical, Inc.), Lichroprep RP-18 (40-63 µm, Fuji) and Sephadex LH-20 (20-150 µm, Pharmacia) were used for column chromatography. Methanol, chloroform, ethyl acetate, acetone, petroleum ether, n-hexane and 2-propanol were purchased from Tianjin Chemical Reagents Co. (Tianjin, China). A Shimadzu UV-2401PC spectrometer was used for recording ultraviolet (UV) spectra. A Horiba SEPA-300 polarimeter was used for optical rotations. A Chirascan instrument was used for recording CD spectra. A Bruker AV-600 MHz spectrometer (Bruker, Zurich, Switzerland) was used for recording nuclear magnetic resonance (NMR) spectra and tetramethyl chlorosilane (TMS) was used as an internal standard for chemical shifts. Electrospray ionization mass spectrometry (ESIMS) and HRTOF-ESIMS spectra were recorded using an API QSTAR Pulsar spectrometer. A Bruker Tensor-27 instrument with KBr pellets was used for recording IR spectra. An Agilent 1100 series instrument equipped with an Agilent ZORBAX SB-C18 column (5 µm, 9.6 mm × 250 mm) was used for high-performance liquid chromatography (HPLC) separation.

Fungal materials

Ganoderma cochlear samples (44 kg) were purchased in December 2020 from the Traditional Chinese Medicine Market in Kunming, Yunnan, China, which was identified by Prof. Yang Zhuliang, Kunming Institute of Botany, Chinese Academy of Sciences (voucher no. 20202501).

Extraction and isolation

G. cochlear samples (44 kg) were extracted three times with 95% ethanol (EtOH) (80 L × 3) under reflux (3 h per extraction). The combined ethanol extracts were evaporated under reduced pressure. The residue (4 kg) was suspended in H_2O and extracted with ethyl acetate (EtOAc). The volume of the combined EtOAc extracts (1.5 kg) was reduced to one-third under

reduced pressure. The residue was fractionated by using a silica gel column (CH₂Cl₂-MeOH, 100:0, 80:1, 50:1, 20:1, 10:1, and 5:1, v/v): fractions I-VI.

Fraction III (523 g) was further fractioned by using a silica gel column with CH2Cl2-acetone as the mobile phase (100:0 \rightarrow 10:1), yielding five subfractions (Fr. III-1 \rightarrow Fr. III-5). Fr. III-3 (37 g) was further subjected to an Rp-18 column (MeOH-H₂O = $35\% \rightarrow 100\%$, v/v) to afford eight subfractions. Furthermore, Fr. III-3-1 (304 mg) was separated by using a silica gel column (petroleum ether-ethyl acetate) to obtain five parts (1a-1e). Then, Fr. III-3-1a (42 mg) was purified by semipreparative HPLC (CH₃CN-H₂O = 41%, v/v, flow rate: 3 mL min^{-1}) to yield compound 9 (11.8 mg, $t_{\rm R}$ = 36.5 min). Fr. III-3-1b (54 mg) was subjected to semi-preparative HPLC (CH₃CN- $H_2O = 36\%$, v/v, flow rate: 3 mL min⁻¹) to obtain compound 7 (7.2 mg, $t_{\rm R}$ = 32.6 min). Similarly, compounds 6 (5.7 mg, $t_{\rm R}$ = 23.9 min) and 4 (7.8 mg, $t_{\rm R}$ = 33.3 min) were respectively obtained from Fr. III-3-1c (93 mg) and Fr. III-3-1d (35 mg) by semi-preparative HPLC (CH₃CN-H₂O = 55% and 53%, v/v, flow rate: 3 mL min⁻¹). Fr. III-3-2 (502 mg) was further subjected to LH-20 (MeOH) to afford six subfractions (2a-2f), of which Fr. III-3-2c was purified to yield compound 10 (8.2 mg, $t_{\rm R}$ = 43.8 min, $t_{\rm R}$ = 43.8 min) by semi-preparative HPLC (CH₃CN- $H_2O = 40\%$, v/v, flow rate: 3 mL min⁻¹). Additionally, Fr. III-3-2d was subjected to semi-preparative HPLC (CH₃CN-H₂O = 40%, v/v, flow rate: 3 mL min⁻¹) to obtain compound 1 (5.8 mg, $t_{\rm R}$ = 34.5 min). Compound 5 (6.1 mg, $t_{\rm R}$ = 43.8 min) was isolated from Fr. III-3-2e by semi-preparative HPLC $(CH_3CN-H_2O = 40\%, v/v, flow rate: 3 mL min^{-1}).$

Fr. III-4 (35 g) was subjected to a silica gel column (CH₂Cl₂-MeOH = 80 : 1, 50 : 1, 20 : 1, 10 : 1, 5 : 1, v/v) to obtain five fractions: Fr. III-4a–Fr. III-4e. Fr. III-4b was subjected to LH-20 (MeOH) to obtain five subfractions (4b-1–4b-5). Fr. III-4b-3 was purified by semi-preparative HPLC (CH₃CN–H₂O = 55%, v/v, flow rate: 3 mL min⁻¹) to obtain compound 2 (5.4 mg, t_R = 33.8 min). Similarly, 4b-4 and 4b-5 were respectively subjected to semi-preparative HPLC (CH₃CN–H₂O = 42%, v/v, flow rate: 3 mL min⁻¹) to yield compounds 8 (31.7 mg, t_R = 36.5 min) and 3 (13.2 mg, t_R = 49.3 min).

Ganolearin A (1). White powder (MeOH); $[\alpha]_D^{24}$ 22.75 (*c* 0.16, MeOH); UV (MeOH); λ_{max} (log ε): 201 (3.72), 234 (3.88), and 297 (2.87); ¹H NMR and ¹³C NMR data: see Table S1;[†] HRMS (ESI-TOF) *m/z*: 401.2322 [M + H]⁺ (calcd for C₂₄H₃₃O₅, 401.2323).

Ganolearin B (2). White powder (MeOH); $[\alpha]_D^{20}$ + 51.13 (*c* 0.13, MeOH); UV (MeOH) λ_{max} (log ε): 277 (2.09), 195 (2.03); ¹H NMR and ¹³C NMR data: see Table S1;† HRMS (ESI-TOF) *m/z*: 469.2564 [M + Na]⁺ (calcd for C₂₆H₃₈O₆Na, 469.2561).

Ganolearin C (3). White powder (MeOH); $[\alpha]_D^{24}$ -53.39 (*c* 0.23, MeOH); UV (MeOH); λ_{max} (log ε): 202 (3.68), and 273 (3.80); ¹H NMR and ¹³C NMR data: see Table S1;† HRMS (ESI-TOF) *m/z*: 457.2602 [M – H]⁻ (calcd for C₂₇H₃₇O₆, 457.2596).

Ganolearin D (4). White powder (MeOH); $[\alpha]_D^{24}$ 12.67 (*c* 0.18, MeOH); UV (MeOH); λ_{max} (log ε): 202 (3.25), and 256 (3.33); ¹H NMR and ¹³C NMR data: see Table S1;[†] HRMS (ESI-TOF) *m*/*z*: 471.2143 [M + K]⁺ (calcd for C₂₅H₃₆O₆K, 471.2143).

Ganolearate E (5). White powder (MeOH); $[\alpha]_{D}^{24}$ 97.07 (*c* 0.13, MeOH); UV (MeOH); λ_{max} (log ε): 202 (3.72), and 257 (3.77); ¹H NMR and ¹³C NMR data: see Table S1;[†] HRMS (ESI-TOF) *m/z*: 490.3162 [M + NH₄]⁺ (calcd for C₂₈H₄₀O₆NH₄, 490.3163).

Ganolearate F (6). White powder (MeOH); $[\alpha]_D^{23}$ 7.61 (*c* 0.16, MeOH); UV (MeOH); λ_{max} (log ε): 201 (3.72), 234 (3.88), and 297 (2.87); ¹H NMR and ¹³C NMR data: see Table S1;† HRMS (ESI-TOF) *m/z*: 497.2511 [M + Na]⁺ (calcd for C₂₇H₃₈O₇Na, 497.2510).

Ganolearate G (7). White powder (MeOH); $[\alpha]_D^{23} + 17.74$ (*c* 0.10, MeOH); UV (MeOH); λ_{max} (log ε): 258 (2.98), 201 (2.77); ¹H NMR and ¹³C NMR data: see Table S1;[†] HRMS (ESI-TOF) *m*/*z*: 513.2821 [M + Na]⁺ (calcd for C₂₈H₄₂O₇Na, 513.2823).

Ganolearic aicd H (8). White powder (MeOH); $[\alpha]_D^{23.9} 20.56$ (*c* 0.25, MeOH); UV (MeOH); λ_{max} (log ε): 203 (3.58), 254 (3.58), and 270 (3.57); ¹H NMR and ¹³C NMR data: see Table S2;[†] HRMS (ESI-TOF) *m/z*: 473.2550 [M – H]⁻ (calcd for C₂₇H₃₇O₇, 473.2545).

Ganolearic acid I (9). White powder (MeOH); $[\alpha]_D^{22} 8.95$ (*c* 0.05, MeOH); UV (MeOH); λ_{max} (log ε): 260 (2.57), 202 (2.78); ¹H NMR and ¹³C NMR data: see Table S2;[†] HRMS (ESI-TOF) *m/z*: 445.2586 [M + H]⁺ (calcd for C₂₆H₃₇O₆, 445.2585).

Ganolearate J (10). White powder (MeOH); $[\alpha]_D^{24}$ 14.59 (*c* 0.17, MeOH); UV (MeOH); λ_{max} (log ε): 202 (3.29), and 260 (3.54); ¹H NMR and ¹³C NMR data: see Table S2;† HRMS (ESI-TOF) *m*/*z*: 511.2673 [M + Na]⁺ (calcd for C₂₈H₄₀O₇Na, 511.2666).

The crystallographic data (excluding structure factor tables) for the reported structures have been deposited at the Cambridge Crystallographic Data Center (CCDC) as supplementary publication no. CCDC 2258231 for 2 and CCDC 2201713 for 4, and CCDC 2258230 for 5. Copies of the data can be obtained free of charge from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: + 44(0)1223 336 033; e-mail: deposit@ccdc.cam.ac.uk).‡

Crystal data for 4: $C_{25}H_{36}O_6$, M = 432.54, a = 7.7089(3) Å, b = 8.1588(3) Å, c = 36.7130(13) Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, V = 2309.08(15) Å³, T = 150.(2) K, space group *P*212121, Z = 4, μ (Cu K α) = 0.709 mm⁻¹, 16444 reflections measured, 4355 independent reflections ($R_{int} = 0.0890$). The final R_1 value was 0.0449 ($I > 2\sigma(I)$). The final $wR(F^2)$ value was 0.1142 ($I > 2\sigma(I)$). The final R_1 value was 0.0600 (all data). The final $wR(F^2)$ value was 0.1190 (all data). The goodness of fit on F^2 was 1.146. Flack parameter = 0.07(8).

Crystal data for 5: C₂₈H₄₀O₆, *M* = 472.60, *a* = 8.1802(3) Å, *b* = 13.5202(4) Å, *c* = 11.2870(4) Å, *α* = 90°, *β* = 92.6960(10)°, *γ* = 90°, *V* = 1246.94(7) Å³, *T* = 150.(2) K, space group *P*1211, *Z* = 2, μ (Cu Kα) = 0.701 mm⁻¹, 22359 reflections measured, 4854 independent reflections ($R_{int} = 0.0348$). The final R_1 value was 0.0311 (*I* > 2 σ (*I*)). The final w*R*(F^2) value was 0.1015 (*I* > 2 σ (*I*)). The final R_1 value was 0.0312 (all data). The final w*R*(F^2) value was 0.1017 (all data). The goodness of fit on F^2 was 0.978. Flack parameter = -0.09(3).

[‡] **Crystal data for 2**: C₂₆H₃₈O₆, *M* = 446.56, *a* = 10.8614(3) Å, *b* = 36.7053(9) Å, *c* = 6.0922(2) Å, *α* = 90°, *β* = 90°, *γ* = 90°, *V* = 2428.78(12) Å³, *T* = 150.(2) K, space group *P*21212, *Z* = 4, μ (Cu Kα) = 0.689 mm⁻¹, 15579 reflections measured, 4402 independent reflections ($R_{int} = 0.0887$). The final R_1 value was 0.0335 ($I > 2\sigma(I)$). The final *w*(F^2) value was 0.0856 ($I > 2\sigma(I)$). The final R_1 value was 0.0597 (all data). The final *w*(F^2) value was 0.0960 (all data). The goodness of fit on F^2 was 1.099. Flack parameter = -0.05(6).

ECD calculation method for 3

The theoretical calculations of compound 3 were performed using Gaussian 16.³¹ Conformational analysis was carried out. The optimized conformation geometries and thermodynamic parameters of all conformations are provided. The conformers were optimized at the B3LYP/6-311G (d,p) level. The theoretical calculation of ECD was performed using time-dependent density functional theory (TDDFT) at the B3LYP/6-311G(d,p) level in MeOH with the PCM model. The ECD spectra of compound 3 were obtained by weighing the Boltzmann distribution rate of each geometric conformation.

Cell culture and treatment

The SH-SY5Y mCherry-GFP-LC3 and SH-SY5Y MAPT cells generated in our previous study were used.⁶ These cells were maintained in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% fetal bovine serum (FBS), $1 \times MEM$ nonessential amino acid solution (Gibco, 11140050), 100 U ml⁻¹ penicillin and 100 mg ml⁻¹ streptomycin at 37 °C in a humidified atmosphere incubator with 5% CO₂ and 95% humidity, as described in our previous studies.^{6,32} Cells were seeded in prewarmed growth medium in 6-well plates or 12-well plates. Rapamycin (InvivoGen, trl-rap) or bafilomycin A1 (tlrl-baf) was used as a positive control. Drugs were applied directly to the culture medium for treatment, and cells were harvested at 24 h after treatment for further analysis.

Cell counting kit-8 (CCK-8) cell viability assay

For cell viability assays, the CCK-8 kit was used as described by the manufacturer (Beyotime, C0038). Briefly, the SH-SY5Y mCherry-GFP-LC3 cells were plated at 4×10^3 cells per well in 96-well culture plates. Twenty-four hours after treatment with compounds **1–10**, the CCK-8 reagent was added into each well. Cell viability was evaluated by gauging the optical density at 450 nm.

Flow cytometry analysis

SH-SY5Y mCherry-GFP-LC3 cells, that is, the SH-SY5Y cells stably expressing a triple fusion protein (red fluorescent protein (mCherry), green fluorescent protein (GFP) and the autophagosome marker LC3),^{33,34} which can directly reflect the strength of autophagic flux, were used in detecting the bioactivities of compounds 1-10. These cells show yellow fluorescence due to the co-expression of red mCherry and green GFP in the absence of autophagy. When the autophagy process goes well, autophagosomes and lysosomes fuse to form autolysosomes, and the acidic lysosomal environment quenches the fluorescence of acid-sensitive GFP, while mCherry is not affected, and then the autolysosomes show red fluorescence. Therefore, red fluorescence in the cells can indicate the formation of autolysosomes.³⁴⁻³⁶ A higher red fluorescence and a lower green fluorescence indicate a smoother flux from autophagosomes to autolysosomes. SH-SY5Y mCherry-GFP-LC3 cells were cultured in DMEM supplemented with 10% fetal bovine serum (Gibco-BRL, 10099-141) at 37 °C in an incubator with

5% CO_2 and 95% humidity. These cells were cultured in 12-well plates for 24 h, and the compound was added directly to the culture medium (5 μ M and 20 μ M). Twenty-four hours after the treatment, the cells were harvested and fixed using 4% paraformaldehyde. The fixed cells were then subjected to a flow cytometry test to check the autophagic flux. Data were analyzed using FlowJo software (FLOWJO, LLC).

Western blot analysis

For western blotting, the method described in our previous studies was used.^{22,32,37} In brief, the SH-SY5Y and SH-SY5Y MAPT cells were lysed with RIPA lysis buffer (Beyotime, P0013). The protein concentration was determined using the BCA protein assay kit (Beyotime, P0012). A total of 20 µg of protein was separated by 12% or 8% (vol/vol) SDS-polyacrylamide gel and electrophoretically transferred onto a polyvinylidene difluoride membrane (Bio-Rad, L1620177 Rev D). The membrane was soaked with 5% (wt/vol.) skim milk for 2 h at room temperature. The membrane was incubated with primary antibodies (ACTB [Beijing Zhong Shan-Golden Bridge Biological Technology Co., Ltd, TA-09], GAPDH, glyceraldehyde-3-phosphate dehydrogenase [Proteintech, 60004-1-Ig], LC3 [Proteintech, 14600-1-AP], phospho-AMPKβ1 (ser108) (E8N3N) [Cell Signaling Technology, 23021], AMPKα (D63G4) [Cell Signaling Technology, 5832], phospho-AMPKa (thr172) (D4D6D) [Cell Signaling Technology, 50081], AMPKβ1/2 (57C12) [Cell Signaling Technology, 4150], mTOR (7C10) [Cell Signaling Technology, 2983], phospho-mTOR (ser2448) (D9C2) [Cell Signaling Technology, 5536], phospho-mTOR (ser2481) [Cell Signaling Technology, 2974], phospho-ULK1 (ser757) (D7O6U) [Cell Signaling Technology, 14202], phospho-ULK1 (ser317) [Cell Signaling Technology, 37762], ULK1 (D8H5) [Cell Signaling Technology, 8054], phospho-ULK1 (ser555) [Cell Signaling Technology, 5869], phospho-ULK1 (ser777) [Sigma-Aldrich, ABC213], SQSTM1, sequestosome 1 [Elabscience, EAP3350] and Tau (D1M9X) [Cell Signaling Technology, 46687S]) overnight at 4 °C. After three washes with TBST (Trisbuffered saline [Cell Signaling Technology, 9997] with Tween 20 [0.1%; Sigma, P1379]), each lasting 5 min, the membranes were incubated for 1 h with the peroxidase-conjugated antimouse (474-1806) or antirabbit (474-1516) IgG (1:5000; KPL) at room temperature. The epitope was visualized using an ECL western blot detection kit (Millipore, WBKLS0500). ImageJ software (National Institutes of Health, Bethesda, Maryland, USA) was used for densitometric analysis. GAPDH or ACTB was used as a loading control for the densitometric analysis of the target protein.

Confocal laser scanning assay

The SH-SY5Y mCherry-GFP-LC3 cells were cultured overnight in DMEM supplemented with 10% FBS, $1 \times MEM$ nonessential amino acid solution (Gibco, 11140050), 100 U ml⁻¹ penicillin and 100 mg ml⁻¹ streptomycin in a glass-bottom cell culture dish (NEST, 801001). For evaluating tandem fluorescent LC3 puncta, 24 h after treatment with rapamycin and compounds 1, 2, 3 or 4, the cells were washed three times with PBS and fixed with 4% paraformaldehyde. The fixed intact cells were observed using a FluoView 1000 confocal microscope (Olympus, America).

Statistics

Statistical analysis was performed using GraphPad Prism 8 software. The one-way ANOVA (analysis of variance) was performed using Tukey's *post hoc* test for comparison between the treated group and the control group, and the values were expressed as mean \pm standard deviation (SD). A *P*-value <0.05 was considered statistically significant throughout the study.

Molecular docking

The crystal structure of the AMPK complex (PDB code: 4CFH) was used for preparing new docking templates through the Swiss-model server. The best configuration of small molecules was refined through energy minimization and molecular docking was performed using Autodock Vina with a center box: x = -14.105, y = 38.735, z = -12.962 and the dimensions: $72 \times 82 \times 64$ Å. The docking results were analyzed and shown using Discovery Studio® Visualizer (BIOVIA, San Diego, USA) and PyMOL software (Schrödinger, LLC: NY, USA).⁵

Author contributions

M. H. Q. and X. R. P. designed this study. X. R. P. supervised the project. Y. L. and D. S. F. performed the isolation and structural analysis. X. R. P. performed the ECD calculation. X. R. P. and R. C. L. wrote the paper. R. C. L. performed cell assays and statistical analysis. Y. G. Y. and M. H. Q. revised the whole manuscript. All authors contributed to the discussion and interpretation of the results.

Conflicts of interest

There are no conflicts to declare.

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Novel A-*seco*-nortriterpenoids from *Ganoderma cochlear* inhibiting Tau pathology by activating AMPK-ULK1-mediated autophagy

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Table of Content

Structural elucidation of compounds 5–10	3
NMR spectra of new compounds 1–10	13
HRESIMS spectra of new compounds	43
X-ray crystallographic data of compounds 2, 4, and 5	53
Calculated ECD data of compound 3	56
Uncropped images of western blot	64
References	67

1. Structural elucidation of compounds 5–10

The molecular formula of ganolearate E (5) (Figure S1) was determined to be $C_{28}H_{40}O_6$ on the basis of HRESIMS ion peak *m/z*: 490.3162 [M + NH₄]⁺ (calcd. 490.3163). Its 1D NMR spectroscopic data (Table S1) showed similarity with those of cochlearic acid A with the only difference in the presence of an additional methoxyl at C-3, which was confirmed by the HMBC correlations (Figure S2) of OMe (δ_H 3.63, s) with C-3 (δ_C 174.1), of H₂-1 and H₂-2 with C-3, and of H₃-19 with C-1, C-5, and C-10. The further X-ray crystallographic analysis (Figure S3) proved that the absolute configuration of 5 was 5*S*,7*S*,10*S*,13*R*,14*R*,17*S*,20*S*. Thus, the structure of compound 5 was determined.

Comparison of molecular weight and 1D NMR spectroscopic data (**Table S1**) between **6** and **5** showed that compound **6** had a similar structure with **5**, except for the absence of the terminal double bond at C-4 and C-28 and the presence of an additional ketone carbonyl (δ_C 214.0). The HMBC correlations of H₃-29 with the ketone carbonyl and C-5 (δ_C 52.5), and of H₃-19 with C-1, C-5, and C-9 (δ_C 137.3) confirmed that C-4 was the ketone carbonyl. Subsequently, the ROESY correlation of H-7/H₃-30 proved that 7-OH was β -oriented. Finally, the structure of **6** (ganolearate F) was established.

Ganolearate G (7) had a molecular formula of $C_{28}H_{42}O_7$ determined by the HRESIMS *m/z*: 513.2821 [M + Na]⁺ (calcd. 513.2823). Meanwhile, compound 7 showed similar 1D NMR spectra with those of compound 6. However, an additional methoxyl group (δ_H 3.67, s; δ_C 51.4) was observed in 1D NMR spectra of 7, rather than an oxygenated quaternary carbon in 6. Furthermore, the methoxyl group showed HMBC correlation (**Figure S2**) with C-24 (δ_C 174.4), simultaneously, H₃-21 exhibited a doublet methyl signals at δ_H 0.89 (d, *J* = 6.4 Hz) in the ¹H NMR spectrum of 7. Thus, we speculated that the methoxyl was connected to C-24 and the oxygenated quaternary carbon at C-20 was transformed into a methine. Therefore, the structure of 7 was confirmed.

According to the 1D NMR spectra (**Table S2**) of **8**, the structure of **8** resembled that of **7** except for the absence of a methoxyl at C-24 and a ketone carbonyl instead of the hydroxyl at C-7. The HMBC correlations of H₃-19 ($\delta_{\rm H}$ 1.31, s) with C-5 ($\delta_{\rm C}$ 52.5) and C-9 ($\delta_{\rm C}$ 145.6), of H-5 ($\delta_{\rm H}$ 3.05, t, J = 4.5 Hz) with C-10 ($\delta_{\rm C}$ 39.2) and C-7 ($\delta_{\rm C}$ 196.7), of H₃-21 ($\delta_{\rm H}$ 0.88, d, J = 6.4 Hz) with C-20 ($\delta_{\rm C}$ 35.6), C-17 ($\delta_{\rm C}$ 49.0), and C-22 ($\delta_{\rm C}$ 30.6), and of H₂-22 ($\delta_{\rm H}$ 2.20, m; 2.46, m) with C-24 ($\delta_{\rm C}$ 178.8) confirmed above deduction. Thus, the structure of **8** was determined and name as ganoclearic acid

The molecular formula of compound 9 was determined to be $C_{26}H_{36}O_6$ based on the HRESIMS m/z: 445.2586 [M + H]⁺ (calcd. 445.2585) with 9 degrees of unsaturation. Its ¹H NMR spectrum (Table S2) showed that three singlet methyl proton signals at $\delta_{\rm H}$ 0.91 (s), $\delta_{\rm H}$ 1.25 (s), $\delta_{\rm H}$ 1.77 (s), one doublet methyl proton signal at $\delta_{\rm H}$ 0.88 (d, J = 6.4 Hz), one methoxyl proton signal at $\delta_{\rm H}$ 3.63 (s), one oxymethine proton signal at $\delta_{\rm H}$ 4.59 (d, J = 5.2 Hz), and two terminal double bond proton signals at $\delta_{\rm H}$ 4.84 (s) and $\delta_{\rm H}$ 4.94 (s). except for the methoxyl, ¹³C-DEPT NMR spectra of **9** showed 25 carbon resonances, which were assigned as four methyls, eight methylenes (one terminal double bond), four methines (one oxymethine), and nine quaternary carbons (one ester carbonyl, one carboxyl, one ketone, three olefiniccarbons, and one oxygenated carbon). These data suggested that compound 9 was a highly degraded lanostane triterpenoid and had a similar 7/6/5-tricyclo skeleton with that of cochlate B, which was confirmed by the HMBC correlations (Figure S2) of H₃-29 with C-4 ($\delta_{\rm C}$ 145.8), C-28 ($\delta_{\rm C}$ 114.7), and C-5 ($\delta_{\rm C}$ 54.8), of H-5 ($\delta_{\rm H}$ 2.75, m) with C-1 ($\delta_{\rm C}$ 31.8), C-10 ($\delta_{\rm C}$ 83.5), C-7 ($\delta_{\rm C}$ 75.0), and C-19 ($\delta_{\rm C}$ 36.0), of H-7 ($\delta_{\rm H}$ 4.50, d, J = 5.2 Hz) with C-5, C-9, and C-10, C-14 ($\delta_{\rm C}$ 50.8), and of H₂-19 with C-1, C-8 ($\delta_{\rm C}$ 167.9), and C-11 ($\delta_{\rm C}$ 201.2). However, combination the absence of two methylenes and the HMBC correlations (Figure S2) of H₃-21 ($\delta_{\rm H}$ 1.16, d, J = 6.5 Hz) with C-17 ($\delta_{\rm C}$ 47.7), C-20 ($\delta_{\rm C}$ 45.1), and C-22 ($\delta_{\rm C}$ 181.7), indicating that C-23 and C-24 were degraded. The ROESY correlations (Figure S2) of H-5/H₃-30/H-7, which demonstrated that H-7 was α -oriented. Therefore, the structure of **9** was established and named as ganoclearic acid I.

Ganolearate J (10) had a molecular formula of $C_{28}H_{40}O_7$ based on the HRESIMS *m/z*: 511.2673 $[M + Na]^+$ (calcd. 511.2666). Its 1D NMR spectroscopic data (**Table S2**) were similar with those of cochlate A with the difference in the absence of double bond at C-4 and C-28 and the presence of one oxygenated methylene ($\delta_H 3.77$, d, J = 12.0 Hz, 4.21, d, J = 12.0 Hz; $\delta_C 64.9$) and one quaternary carbon containing oxygen ($\delta_C 86.0$). The detailed analysis of HMBC spectrum (**Figure S2**) of **10** showed the correlations of H₃-29 ($\delta_H 1.39$, s) and H-5 ($\delta_H 2.36$, d, J = 7.6 Hz) with the oxygenated methylene and quaternary carbons, suggesting that C-4 and C-28 were linked to hydroxyl group, respectively. Considering the molecular weight of **10** and the chemical shift of C-3 ($\delta_C 175.8$), an ester bond between C-4 and C-3 was deduced. Finally, the structure of **10** was determined.

	1 ^{<i>a</i>}		2 ^{<i>a</i>}		3 ^a		4 <i>a</i>		5 ^{<i>a</i>}		6 ^b		7 ^b	
position	$\delta_{ m H}$	δ_{C}	$\delta_{ m H}$	$\delta_{\rm C}$	$\delta_{ m H}$	$\delta_{ m C}$	$\delta_{ m H}$	$\delta_{\rm C}$	$\delta_{ m H}$	$\delta_{\rm C}$	$\delta_{ m H}$	δ_{C}	$\delta_{ m H}$	$\delta_{\rm C}$
1			1.59	31.7	1.86	34.8	2.60, m;	31.7	1.04	33.1	1.80	35.1	1.70, m;	33.6
1			1.38, m	CH_2	1.80, m; 2.19, m	CH_2	1.84, m	CH_2	1.94, m; 2.10, m	CH_2	1.89, m; 2.13, m	CH_2	2.31, m	CH_2
2			2.49 m	31.2	2.26 m· 2.46 m	29.3	2.10, m;	29.0	1.97, m;	29.4	2 20 m· 2 33 m	30.2	2.54, m;	29.4
2			2.49, 11	CH_2	2.20, 11, 2.40, 11	CH_2	1.46, m	CH_2	2.21, m	CH_2	2.20, 11, 2.55, 11	CH_2	1.36, m	CH_2
3				174.8		174.0		176.7		174.1		175.9		173.8
				С		С		С		С		С		С
4		203.9				205.4				147.0		214.0		217.1
		С				С		40.5		С		C		C
5		131.2	1.44, m	27.2	1.62, m	35.7 CH	3.15, d	48.5	2.13, m	44.7 CU	2.83, m	52.5	2.92, m	50.9
		121.2	1.00 11 (7.9.4.2)	CH		CH 20.2	(8.8)	CH 29.5		CH 22.4		CH 22.1		CH 20.0
6	7.54, d (7.9)	131.2 CU	1.09, dd, (7.8, 4.3);	17.3 CU	2.04, m	39.2 CH	1.78, m	38.5 CH	2.06, m; 2.14, m	32.4 CH	2.49, m; 2.67, m	32.1 CU	2.10, m	28.8 CU
		122.6	0.29, dd, (7.2, 4.3)	CH ₂		24.0	2.52, m	CH ₂		CH2		CH ₂	4.02 44	CH ₂
7	7.47, d (7.9)	122.0 CH	1.85, m	22.5 CH	2.47, m	54.0 CH	(7.2)	//.2 CH	4.29, t (6.0)	00.8 CH	4.23, t (6.0)	04.3 CH	(10.4, 4.0)	62.5 CH
		152.9		СП 174.5		СП 171.9	(7.3)	СП 174.1		СП 1607		160 5	(10.4, 4.0)	СП 158.6
8		152.8 C		1/4.5 C		1/1.0 C		1/4.1 C		100.7		100.5 C		138.0 C
		140.7		1377		135.6		133.7		137.2		1373		135.1
9		C		157.7 C		155.0 C		135.7 C		137.2 C		137.5 C		155.1 C
		138.1		48.8		C		C		C		C		C
10		С		CH		49.7 C		89.3 C		39.1 C		38.6 C		37.4 C
		200.4		197.5		196.3		198.9		199.1		202.0		200.1
11		C 200.1		С		C		C		C		C 202.0		200.1 C
							2.58, d						2.43. d	
	2.58, d (18.8);	52.3		50.1	2.38, d (17.6);	49.2	(16.6)	49.6	2.62, d (17.4);	51.1	2.51, d (18.0);	52.3	(18.8)	51.4
12	2.91, d (18.8)	CH_2	2.43, d, (7.4)	CH_2	2.54, d (17.6)	CH_2	2.69, d	CH_2	2.74, d (17.4)	CH_2	2.77, d (18.0)	CH_2	2.59, d	CH_2
	,						(16.6)						(18.8)	
13		45.2 C		48.1 C		48.0 C		49.7 C		45.6 C		46.5 C		44.1 C
14		52.3 C		48.2 C		49.7 C		49.8 C		51.9 C		52.8 C		51.2 C
15	5.60, dd (9.5,	74.1	2.27, dd, (12.8, 7.9);	40.9	1.52 m 1.72 m	29.5	1.25, m;	29.3	1 47 m 2 56 m	30.2	1.42 m; 2.20 m	30.7	1.25, m;	29.5
15	5.1)	CH	1.88, dd, (12.8, 4.8)	CH_2	1.32, 111, 1.72, 111	CH_2	2.15, m	CH_2	1.47, 111, 2.30, 111	CH_2	1.43, 111, 2.20, 111	CH_2	2.15, m	CH_2
16	2.20 m 1.04 m	39.0	471 44 (120 50)	72.0	2.12 m 1.51 m	27.4	1.45, m;	27.8	171 m 180 m	21.7	1.05 m 1.65 m	22.8	1.45, m;	27.3
10	2.20, 111, 1.94, 111	CH_2	4.71, dd, (12.9, 5.9)	CH	2.12, 11, 1.31, 11	CH_2	2.05, m	CH_2	1./1, 11, 1.69, 11	CH_2	1.95, 11, 1.05, 11	CH_2	2.03, m	CH_2
17	1.00 m	49.0	173 m	54.7	1.76 m	1.76 m 49.2	1.72 m	48.9	2 10 m	52.9	234 m	54.3	1.63 m	50.5
1 /	1.70 III	CH	1.73, 111	CH	1.70, 111	CH	1.72,111	CH	2.17 111	CH	2.34, 111	CH	1.05, 11	CH
18	0.74 s	18.5	1.05 s	17.7	0.77 s	17.4	0.87 s	17.2	111 s	19.2	1 15 s	19.7	1 10 s	17.7
10	0.77, 5	CH_3	1.00, 5	CH_3	0.77, 5	CH_3	0.07, 5	CH_3	1.11, 5	CH_3	1.15, 5	CH_3	1.10, 5	CH_3
19	2.57, s	18.3	1.21, s	24.5	1.30, s	22.5	1.50, s	27.7	1.25 s	22.4	1.23, s	22.4	1.17, s	21.2

Table S1.¹H and ¹³C-DEPT NMR spectroscopic data of 1-7 (600/150 MHz, δ in *ppm*, *J* in Hz).

		CH_3		CH ₃		CH_3		CH ₃		CH_3		CH_3		CH_3
20	1.40 m	35.4	1.75 m	29.5	1.46 m	35.7	1.45 m	35.5		877C		00.1 C	1.42 m	35.6
20	1.40, m	CH	1./3, m	CH	1.40, m	CH	1.43, m	CH		87.7 C		90.1 C	1.45, m	CH
21	0.00 + (6.4)	17.7	0.04 + (5.6)	18.0	$0.90 \pm (6.2)$	17.8	0.91, d	18.1	1.45 -	26.0	1.46 -	26.3	0.90 1(6.4)	17.7
21	0.90, 0 (0.4)	CH_3	0.94, d (3.0)	CH ₃	0.89, 0 (0.5)	CH_3	(6.4)	CH_3	1.45, 8	CH_3	1.40, 8	CH_3	0.89, 0 (0.4)	CH_3
22	1.21 m 1.02 m	30.7	2.46 m	30.3	1.22 m 1.02 m	30.7	1.84, m;	31.0	2.02 mi 2.17 m	32.4	1.09 m 2.22 m	34.5	1.84, m;	30.8
22	1.51, 11, 1.62, 11	CH_2	2.40, 111	CH_2	1.55, 111, 1.65, 111	CH_2	1.34, m	CH_2	2.05, 111, 2.17, 111	CH_2	1.96, 111, 2.25, 111	CH_2	1.34, m	CH_2
22	2.27		1.07 m	30.7	2.27 mi 2.40 m	31.0	2.24, m;	31.1	2.40 m	27.9	2.45 m; 2.60 m	28.6	2.24, m;	31.1
25	2.27, 111,		1.97, 111	CH_2	2.27, 111, 2.40, 111	CH_2	2.48, m	CH_2	2.49, III	CH_2	2.45, 111, 2.09, 111	CH_2	2.48, m	CH_2
24	2.20 m	31.0		176.2		178.7		174.4		177.1		180.1		174.4
24	2.39, 111	CH_2		С		С		С		С		С		С
28		174.2							1.82 - 5.05 -	114.9				
28		С							4.62, 8, 5.05, 8	CH				
20					2.25	30.5			1.82 .	24.0	2.21 6	31.3	2.28	33.5
29					2.23, 8	CH_3			1.65, 8	CH_3	2.21, 8	CH_3	2.20, 5	CH_3
20	2.55	30.9	1 11 g	26.3 24.7 113 24.4 117 25	25.7	7 1.12 a	26.6	0.00 5	26.1					
50	2.55, 8	CH_3	1.11, 5	CH_3	1.10, 8	CH_3	1.15, 8	CH_3	1.17, 5	CH_3	1.15, 8	CH_3	0.99, 8	CH_3
3 OCH	1.21 s	19.3	266 5	51.8	3 63 5	51.6	267 5	51.5	2.62 5	51.5	2.62 5	52.1	367 5	51.7
3-0CH3	1.21, 8	CH_3	5.00, 8	CH_3	5.05, 8	CH_3	5.07, 8	CH_3	5.05, 8	CH_3	5.05, 8	CH_3	5.07, 8	CH_3
24-	2.68 5	2 68 - 51.6	2 71 s	52.3									367 5	51.4
OCH ₃	5.00, 8	CH ₃	5.71,8	CH ₃									5.07, 8	CH_3

^{*a*}: CDCl₃; ^{*b*}: CD₃OD

position -	8^{b}		9 ^b		10 ^{<i>a</i>}		
	$\delta_{ m H}$	$\delta_{ m C}$	$\delta_{ m H}$	$\delta_{ m C}$	$\delta_{ m H}$	$\delta_{ m C}$	
1	2.07, m; 2.38, m	33.4 CH ₂	1.83, m	31.8 CH ₂	1.86, m	32.6 CH ₂	
2	2.29, m; 2.38, m	29.4 CH ₂	2.40, m; 2.45, m	29.5 CH ₂	2.47, m; 2.84, m	27.7 CH ₂	
3		173.7 C		175.9 C		175.8 C	
4		20.9 C		145.8 C		86.0 C	
5	3.05, t (4.5)	52.5 CH	2.75, m	54.8 CH	2.36, d (7.6)	54.6 CH	
6	2.52, m; 2.66, m	36.8 CH ₂	2.28, m	42.1 CH ₂	1.67, m 2.72, m	36.2 CH ₂	
7		196.7 C	4.59, d (5.2)	75.0 CH	4.64, t (8.9)	74.4 CH	
8		152.3 C		167.9 C		168.8 C	
9		145.6 C		126.5 C		127.3 C	
10		39.2 C		83.5 C		86.3 C	
11		202.3 C		201.2 C		199.1 C	
12	2.50, d (18.0); 2.63, d (18.0)	51.1 CH ₂	2.44, d (17.6); 2.78, d (17.6)	49.9 CH ₂	2.56, d (18.8)	48.4 CH ₂	
13		45.2 C		48.8 C		45.8 C	
14		48.4 C		50.8 C		51.0 C	
15	2.18, m; 2.07, m	$31.7 \ \mathrm{CH_2}$	1.27, m; 1.90, m	$30.8 \ \mathrm{CH_2}$	1.51, m; 1.91, m	$31.0 \ \mathrm{CH_2}$	
16	1.43, m; 2.05, m	$27.6 \ \mathrm{CH_2}$	1.53, m; 2.07, m	$27.7 \ \mathrm{CH_2}$	1.51, m; 2.07, m	$26.6 \ \mathrm{CH_2}$	
17	1.62 m	49.0 CH	2.32, m	47.7 CH	1.73, m	49.6 CH	
18	0.95, s	17.7 CH ₃	0.91, s	17.8 CH ₃	0.87, s	17.2 CH ₃	
19	1.31 s	22.0 CH ₃	2.06, m; 2.32, m	36.0 CH ₂	3.09, d (14.8); 3.24, d (14.8)	29.6 CH ₃	
20	1.45, m	35.6 CH	2.42, m	45.1 CH	1.45, m	35.7 CH	
21	0.88, d (6.4)	17.6 CH ₃	1.16, d (6.5)	17.8 CH ₃	0.89, d (6.5)	17.5 CH ₃	
22	2.20, m; 2.46, m	$30.6 \ \mathrm{CH}_2$		181.7 C	2.24, m; 2.48, m	$30.7 \ \mathrm{CH_2}$	
23	1.89, m;2.08, m	31.1 CH ₂			1.84, m; 1.34, m	$31.1 \ \mathrm{CH}_2$	
24		178.8 C				174.4 C	
28			4.84, s; 4.94, s	114.7 CH2	3.77, d (12.0); 4.21, d	64.9 CH ₂	
29	2.23, s	32.6 CH ₃	1.77, s	22.4 CH ₃	1.39, s	24.9 CH ₃	
30	1.08, s	24.4 CH ₃	1.25, s	26.5 CH ₃	1.11, s	25.7 CH ₃	
OCH ₃	3.67, s	51.8 CH ₃	3.63, s	52.1 CH ₃	3.67, s	51.5 CH ₃	

Fable S2 . ¹ H and ¹³ C-DEPT NM	spectroscopic data of 8–10	$(600/150 \text{ MHz}, \delta \text{ in ppm})$	J in Hz).
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Figure S1. Structures of compounds 5–10.



Figure S2. Selected HMBC (H \rightarrow C), ¹H-¹H COSY (H-H) correlations of compounds 5, 6, 9, 10, and ROESY (\checkmark) correlations of compounds 5 and 9.



Figure S3. X-ray crystallographic structure of compound 5.

2. Autophagy activation of compounds 1–10

In order to test whether compounds1–10 would affect autophagy, we used the SH-SY5Y mCherry-GFP-LC3 cell line, which contains thetandem monomeric mCherry-GFP-tagged LC3 (mCherry-GFP-LC3) reporter and was reported in our previous study.^[1] The mCherry-GFP-LC3 in autolysosomes displayed more stable red mCherry fluorescence in the acidic lysosome while the GFP signal was sensitive to the acidic condition.^[2] DMSO (dimethyl sulfoxide) and rapamycin were respectively as blank and positive controls.^[3] The flow cytometry analysis results showed that compounds 1–10 significantly increased the autophagic flux (FigureS4A–B). Moreover, all of them displayed no toxicities in SH-SY5Y mCherry-GFP-LC3 cells by using the CCK-8 assay (FigureS5A). Compounds 1–4 with diverse rearranged skeleton were further investigated for their effect on autophagy and anti-ADs. Treatment with compounds 1–4 can increase autophagic flux in the SH-SY5Y mCherry-GFP-LC3 cells, similar as rapamycin (Figure S5B–C). Collectively, these results demonstrated that compounds 1–4 can activate autophagy.



Figure S4.Compounds 1-10 induced autophagy in SH-SY5Y mCherry-GFP-LC3 cells by flow cytometry analysis. (A) Flow cytometry of SH-SY5Y mCherry-GFP-LC3 cells with or without drug treatment. The percentage of 10,000 cells expressing GFP or/and mCherry were counted. The Q1 area represents the proportion of cells with green fluorescence; the Q2 area represents the proportion of cells with yellow fluorescence; the Q3 area represents the proportion of cells with only red fluorescence; the Q4 area represents the proportion of cells showing no red and green fluorescence. (B) Quantification of the Q3 area in (A) based on 3 independent experiments. Record the proportion cells of that only emit red fluorescence in Q3 area under each treatment.



Figure S5. Increase of autophagic flux by compound **1–10** in SH-SY5Y mCherry-GFP-LC3 cells. (A) The CCK-8 assay showing the effects of compound **1–10** on cell viability. (B-C) Increased autophagic flux in response to **1–4** or Rapamycin (Rapa) treatment in SH-SY5Y mCherry-GFP-LC3 cells. (B) **1–4** treatment increased the maturation of autolysosomes as shown by the increased red puncta of mRFP-GFP-LC3 in cells, and this effect was similar to that of Rapamycin. (C) Quantification of LC3 puncta in (B) based on 3 independent experiments. ns, not significant; *, P < 0.05; **, P < 0.01; ***, P < 0.001; ****, P < 0.0001; one-way ANOVA with the Tukey's post-hoc test. Bars represent mean ± SD.



Figure S6. No inhibition effect of compounds 1–4 on mTOR. (A-H) Western blotting assays showing the protein levels of mTOR, pmTOR2448 and pmTOR2481 in the SH-SY5Y MAPT cells treated with or without compounds. Rapamycin (Rapa) as a positive control. (A-H) A representative Western blotting result (A, C, E, G) and quantification of respective protein levels (B, D, F, H) based on 3 independent experiments were presented. Relative protein abundance was normalized to ACTB. ns, not significant; **, P < 0.01; ***, P < 0.001; one-way ANOVA with the Tukey's posthoc test. Bars represent mean ± SD.



Figure S7. The molecular docking results of compounds 1–4 with AMPK (PDB: 4CFH).

NMR spectra of new compounds 1-10





Figure S10. HSQC spectrum (600/150 MH, CDCl₃) of compound 1.





Figure S14. ¹H NMR spectrum (600 MH, CDCl₃) of compound 2.





Figure S16. HSQC spectrum (600/150 MH, CDCl₃) of compound 2.









Figure S18. ¹H-¹H COSY spectrum (150 MH, CDCl₃) of compound 2.





Figure S20. ¹H NMR spectrum (600 MH, CDCl₃) of compound 3.

の 1.1.1.2.2.2.1.1.2.2.2.0.4 1.1.2.2.0.4 1.1.2.2.0.4 1.1.2.4 1.1.2.4





Figure S22. HSQC spectrum (600/150 MH, CDCl₃) of compound 3.









Figure S27. ¹³C NMR spectrum (150 MH, CDCl₃) of compound 4.











Figure S30. ¹H-¹H COSY spectrum (600 MH, CDCl₃) of compound 4.





Figure S32. ¹H NMR spectrum (600 MH, CDCl₃) of compound 5.



Figure S33. ¹³C NMR spectrum (150 MH, CDCl₃) of compound 5.








Figure S36. ¹H-¹H COSY spectrum (600 MH, CDCl₃) of compound 5.



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Figure S39. ¹³C NMR spectrum (150 MH, CD₃OD) of compound 6.











Figure S42. ¹H-¹H COSY spectrum (600 MH, CD₃OD) of compound 6.







Figure S44. ¹³C NMR spectrum (150 MH, CDCl₃) of compound 7.







 Figure S49. ¹H NMR spectrum (600 MH, CDCl₃) of compound 8.

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Figure S52. HMBC spectrum (600/150 MH, CDCl₃) of compound 8.

Figure S53.¹H-¹H COSY spectrum (600 MH, CDCl₃) of compound 8.

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Figure S54. ROESY spectrum (600 MH, CDCl₃) of compound 8.



Figure S55. ¹H NMR spectrum (600 MH, CDCl₃) of compound 9.









Figure S58. HMBC spectrum (600/150 MH, CDCl₃) of compound 9.

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Figure S62. ¹³C NMR spectrum (150 MH, CDCl₃) of compound 10.



Figure S64. HMBC spectrum (600/150 MH, CDCl₃) of compound 10.



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Figure S66. ROESY spectrum (600 MH, CDCl₃) of compound 10.

HRESIMS spectra of new compounds

Figure S67. HRESIMS spectrum of compound 1.

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(C24 H32 OS)+H)+
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OS)+H)+
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Q-TOF B.0.5.01 (B5125.2) r Spectra Fragmentor Voltage Collision Energy Ionization Mode
Est 04 +ESi Scan (0.13-0.14 min. 2 Scans) Frag=135.0V Md8-12-5+.d. Subtract (2)
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401.2322
((C24 H32 C5)+H)+
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(C24 H32 C5)+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Ister Track Tom 746 1 49620.82 Tom 747 1 21394.35 1 21394.35 748 1 21394.35 1 21394.35</th> <th>Info. asistion SW
ion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) r Spectra Fragmentor Voltage Collision Energy Ionization Mode
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(C24 H32 OS)+H)+ Coll 2323
(C24 H32 OS)+H)+ Coll 2325
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2323
(C24 H32 OS)+H)+ Coll 2363
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(C24 H32 OS)+H)+ Coll 2323
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2324
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2325
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(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2325
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(C24 H32 OS)+H)+ Co</th><th>Info. Info. uisition SW 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Q-TOF B.05.01 (B5125.2) Prespectra Info. 104 0 Info. 105 0 Info. 104 0 Info. 105 0 Info. 106 0 Info. 107 0 Info. 108 0 Info. 104 +ESI 0 105 0 Info. 106 -105 Info. 107 +ESI -105 108 -101 -1012322 109 -1012322 -1014401640184018402 -1012440224024402240244026402840340324034403.6403.8 -1033974 -101244022 -1012401640164016401640164016401640164028 -10124402240224024402640284034034403.6403.8403.8403.8403.8403.8403.8403.8403.8</th><th>Info. aistion SW 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) r Spectra Fragmentor Voltage Collision Energy Ionization Mode
ESI 0⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V McB-12-54-d. Subtract (2)
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401.2322
((C24 H32 C05]+H)+
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(C24 H32 C05]+H)+
400.5 400.8 401 4012 4014 4015 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 tist Trace Toning Trace Toning 100 Toning
Toning 101 4012 4014 4015 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 101 Toning Toning 101 Toning Toning 102 Toning Toning 103 1 46747.81 Toning 103 1 41733.164 Toning 103 1 41733.164 Toning 103 1 47733.164 Toning 103 1 41733.164 Toning 102 1 1 3773.64 Toning</th><th>Info. uisition SW
sion 6200 series TOF/6500 series
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Counts vis. Massito-Charge (m/z) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0<!--</th--><th>Info. Info. guistion SW
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sion 6200 series TOF/6500 series
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(C24 H32 OS]+H)+
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rsion 6200 series TOF/6500 series
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rsion 6200 series TOF/6500 series
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(1024 H32 OS)+H)+
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rsion 6200 series TOF/6500 series
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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(IC24 H32 OS)+H)+
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Q-TOF B.05.01 (B5125.2) Ser Spectra Tragmentor Voltage Collision Energy Ionization Mode
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(1224 H32 OS)+H)+ 401
402 402 2363
(1C24 H32 OS)+H)+ 402 2363
(1C24 H32 OS)+H)+ 403 3974
(1C24 H32 OS)+H)+ 402 2363
400.6 400.8 401 401.2 401.4 401.6 401.8 402
402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403 403.6 403.8 403.6 403.8 at List X X Abunda formula formula formula form
12322 1 19914.69 C24 H32 OS (H1+H)+ Ton 42322 1 19914.69 C24 H32 OS (M+H)+ 103 100 formula form 100 formula form</th><th>Info. Gaussition SW
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Q-TOF B.05.01 (85125.2) Ser Spectra Fragmentor Voltage Collision Energy Ionization Mode
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(122 H32 OS)+H)+ 404 402 2363
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401-2322
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4002-363
((C24 H32 OS)+H)+
4

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Counts vs. Mass-to-Charge (m/z) Ionization discontered
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((C24 H32 OS)+H)+
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((C24 H32 OS)+H)+
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Counts vs. Mass-to-Charge (m/z) 400 500 1 49620.82
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(IC24 H32 OS]+H)+
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(IC24 H32 OS]+H)+
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(IC24 H32 OS]+H)+
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(IC24 H32 OS]+H)+
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(IC24 H32 OS]+H)+
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(IC24 H32 OS]+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 401.4 403.6 403.8 403.4 403.6 403.8
(IC24 H32 OS]+H)+
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rsion 6200 series TOF/6500 series
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Q-TOF B.0.5.01 (B5125.2) r Spectra Fragmentor Voltage Collision Energy Ionization Mode
Est 04 +ESi Scan (0.13-0.14 min. 2 Scans) Frag=135.0V Md8-12-5+.d. Subtract (2)
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401.2322
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(C24 H32 C5)+H)+
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ion 6200 series TOF/6500 series
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squisition SW Collosition Exp(5500 series
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(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2323
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(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2363
(C24 H32 OS)+H)+ Coll 2324
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Q-TOF B.05.01 (B5125.2) r Spectra Fragmentor Voltage Collision Energy Ionization Mode
ESI 0⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V McB-12-54-d. Subtract (2)
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401.2322
((C24 H32 C05]+H)+
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(C24 H32 C05]+H)+
400.5 400.8 401 4012 4014 4015 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 tist Trace Toning Trace Toning 100 Toning Toning 101 4012 4014 4015 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 101 Toning Toning 101 Toning Toning 102 Toning Toning 103 1 46747.81 Toning 103 1 41733.164 Toning 103 1 41733.164 Toning 103 1 47733.164 Toning 103 1 41733.164 Toning 102 1 1 3773.64 Toning</th> <th>Info. uisition SW
sion 6200 series TOF/6500 series
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strion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) er Spectra Pragmentor Voltage
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sion 6200 series TOF/6500 series
Q-TOF B.05.01 (85125.2) Presentor Collision Energy
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(C24 H32 O5]+H)+ 403.3974 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 K Lst 107 2746 1 402.05 103 107 109 103 107 109 103 101 101 101 202 1 1 1994.35 1 103 1 1094.35 1 103 1 1094.35 1 103 1 1094.35 1 103 1 1094.35 1 103 1 1094.35 1 103 1 1094.35 1 103 1 1094.35 1 1094.35 </th><th>Info. Info. puisition SW
sion 6200 series TOF/6500 series
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135 101 1232 (C24 H32 C5]+H)+ 4012322
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requisition SW G200 series TOF/6500 series
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(C24 H32 OS)+H)+ 13/2 Collision Energy
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rsion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) Ser Spectra Tragmentor Voltage Collision Energy
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juisition SW
sion E200 series TOF/6500 series
Q-TOF B.05.01 (85125.2) er Spectra Pragmentor Voltage
135 Collision Energy
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sion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) Presentation Collision Energy
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Est Ionization Mode
Est Image: Spectra Collision Energy
(IC24 H32 C5)(H1)+
400.5 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403</th><th>Info. Info. uisition SW
sion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) er Spectra Tragmentor Voltage Collision Energy
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uisition SW
sion E200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) Prespectra Pragmentor Voltage
135 Collision Energy
0 Ionization Mode
Esi 14 4012322
((C24 H32 OS)+H)+
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sion 6200 series TOF/6500 series
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sion 6200 series TOF/6500 series
Q-TOF B.05.01 (85125.2) er Spectra Pragmentor Voltage Collision Energy
0 Ionization Mode
Esi 100 135 100 135 100 135 100 130 101 1232 (IC24 H32 C05]+H)+ 4012322
(IC24 H32 C05]+H)+ 100 12322
(IC24 H32 C05]+H)+ 100 12322
(IC24 H32 C05]+H)+ 100 4002 2363
(IC24 H32 C05]+H)+ 100 4002 2363
(IC24 H32 C05]+H)+ 100 4002 2363
(IC24 H32 C05]+H)+ 101 4012 4014 4016 4018 402 4022 4024 402.6 402.8 403 4032 403.4 403.6 403.8 101 202 1002 402.2 402.6 402.8 403 403.2 403.4 403.6 403.8 101 202 1001 4012 4014 4016 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 101 10194.69 12 41432 05 101 1194.69 12 41432 05 11996.1 1 21394.35 1 1194.30 5 11996.1 1 21394.37 1 1194.43 05</th><th>Info. guisition SW
rsion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) Ser Spectra Tragmentor Voltage
0 Collision Energy
0 Ionization Mode
ESI x10⁴
1451 Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2)
401.2222
((C24 H32 OS]+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 x10⁴
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 x10⁴
402.2363
(C24 H32 OS]+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 x1 X X2746
3.3008 1 46747.81
(2394.35 1 21394.35 1 21394.35 1 21394.35 1 21394.35 1 224 122 05 (M+H)+
13350 1 2 1394.35 1 22394.35 1 21394.35 1 224 123 05 (M+H)+</th><th>Info. guisition SW
rsion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) ere Spectra Transmitter Voltage Collision Energy Ionization Mode
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4012322 Collision Energy Ionization Mode
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4012322 (C24 H32 OS)(H)+ 4012323
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rsion 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2) are Spectra Transmitter State (0.13-0.14 min, 2 scans) frage 135.0V McB-12-5+.d. Subtract (2)
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(1024 H32 OS)+H)+
4012322
(1024 H32 OS)+H)+
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(1024 H32 OS)+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
(1024 H32 OS)+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
(1024 H32 OS)+H)+
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
(1024 H32
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402.2363
(C24 H32 OS]+H)+
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rsion 6200 series TOF/6500 series
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Counts vs. Mass-to-Charge (m/z) At List Y 1396 1 49520.82 1 19914.69 C24 H32 O5 11936 1 19708.68</th> <th>Pagmentor Voltage
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0 (C24 H32 OSI+H)+
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Counts vs. Mass-to-Charge (m/z)
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1 46747.81
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((C24 H32 OS)+H)+ -400.6 400.8 401.4 401.6 -400.6 400.8 401.2 401.8 -400.6 400.8 401.2 401.8 -400.6 400.8 401.8 402.2 -400.6 400.8 401.8 402.2 -400.6 400.8 401.4 401.6 -400.6 400.8 401.2 402.2 -400.6 400.8 401.2 402.2 -400.6 400.8 401.8 402.2 -400.6 400.8 401.8 402.4 -400.8 403.4 403.6</th> <th>Pragmentor Voltage
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Counts vs. Mass-to-Charge (m/z)
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Counts vs. Mass-to-Charge (m/z)
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Counts vs. Mass-to-Charge (mv2)
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((C24 H32 OS)+H)+
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((C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 4022 402.4 402.6 402.8 403 403.2 403.4 403.5 403.8
Counts vs. Mass-to-Charge (m/z)
K List
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1 19914.69 C24 H32 OS
1 46747.81
2322 1 19914.69 C24 H32 OS
402 205 (M+H)+
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((C24 H32 O5]+H)+
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16 | See Spectra Fragmentor Voltage Collision Energy Ionization Mode 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d. Subtract (2) 401.2322 1404 -ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d. Subtract (2) 401.2322 156 -40.2 2363 ((C24 H32 OS)+H)+ 166 -40.2 2363 ((C24 H32 OS)+H)+ 166 -40.0 8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 006 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 2746 1 49620.82
 | See Spectra Pragmentor Voltage
135 Collision Energy
0 Ionization Mode
Est 135 0 Est 136 0 Est 104 +Est Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2)
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((C24 H32 O5)+H)+ 401.2322
((C24 H32 O5)+H)+ 146 402.2363
((C24 H32 O5)+H)+ 403.3974
403.3974 104 401.2 401.4 401.6 401.8 402 4022 4022 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) At List Y 1396 1 49520.82 1 19914.69 C24 H32 O5 11936 1 19708.68 | Pagmentor Voltage
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135 Collision Energy Lonization Mode ESI
145 Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2)
145 Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2)
145 (C24 H32 O5]+H)+
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1401.2322
0 (C24 H32 OSI+H)+
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 | Pragmentor Voltage 0 Ionization Mode ESI
135 0 Olision Energy ESI
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1451 Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2)
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1451 Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2)
1052 (IC24 H32 OS]+H)+
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1052 (IC24 H32 OS]+H)+
1052 (IC24 H32 OS]+H)+ | Pragmentor Voltage
135 0 1012a20
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135 0 1012a20
1014 451 Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/68-12-5+.d Subtract (2)
4012322
((C24 H32 OS)+H)+
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402 2363
((C24 H32 OS)+H)+
403.3974
400.6 400.8 401 401.2 401.4 401.6 401.8 402 4022 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
K List
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1 19914.69 C24 H32 OS
1 46747.81
2322 1 19914.69 C24 H32 OS
402 205 (M+H)+
1 33674.77
1 2394.35
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 | Seer Spectra Fragmentor Voltage Collision Energy Inization Mode
ESI 135 0 ESI x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V McB-12-5+.d Subtract (2)
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((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 14 -40.6 400.2363
((C24 H32 OS)+H)+ 403.3974
403.3974 0 -40.0 401.2 401.2 400.6 400.8 401.2 402.2363
((C24 H32 OS)+H)+ -400.6 400.8 401.4 401.6 -400.6 400.8 401.2 401.8 -400.6 400.8 401.2 401.8 -400.6 400.8 401.8 402.2 -400.6 400.8 401.8 402.2 -400.6 400.8 401.4 401.6 -400.6 400.8 401.2 402.2 -400.6 400.8 401.2 402.2 -400.6 400.8 401.8 402.2 -400.6 400.8 401.8 402.4 -400.8 403.4 403.6 | Pragmentor Voltage
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(IC24 H32 OS)+H)+
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Counts vs. Mass-to-Charge (m/z)
K List
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1996
1 46747.81
1 49620.82
1 19914.69
C24 H32 OS
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(IC24 H32 OS)+H)+
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Counts vs. Mass-to-Charge (m/z)
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((C24 H32 O5)+H)+
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((C24 H32 O5)+H)+
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102 | Pragmentor Voltage
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Collision Energy
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(IC24 H32 O5)+H)+
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Counts vs. Mass-to-Charge (mv2)
Counts vs. Mass | Pragmentor Voltage
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1014 4ESI Scan (0.13-0.14 min, 2 Scans) Fragr 135.0V kt/c8-12-5+.d. Subtract (2)
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((C24 H32 OS)+H)+
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((C24 H32 OS)+H)+
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1014 451 Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/ds.12-5t+.d Subtract (2)
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((C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 4022 402.4 402.6 402.8 403 403.2 403.4 403.5 403.8
Counts vs. Mass-to-Charge (m/z)
K List
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Progreen Voltage 0 Inization Mode
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((C24 H32 OS)+H)+ 0.4 403.3974 0.4 400.6 0.4 401.2 400.6 400.8 400.6 400.8 401.4 401.6 402.2363 (IC24 H32 OS)+H)+ 402.2 400.6 400.6 400.6 400.6 400.6 400.6 400.8 401.4 401.2 401.4 401.6 402.2 400.6 400.8 401.4 401.8 402.2 402.2 1 402.2 1 402.4 402.4 402.4 402.4 402.7 402.7 401 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401,2322 2 (IC24 H32 OS)+H)+ 402,2363 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 2.0 - - 400.6 401.4 401.6 2.0 - - 400.6 401.4 401.6 2.0 - - 4.0 - - 2.0 - - 4.0 - - 2.0 - - 2.0 - - 2.0 - - 2.2 1 401.4 2.2 1 1 </th <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kdc8-12-5+.d Subtract (2) 401.2322 1 401.2322 ((C24 H32 205)+H)+ 1.8 1.4 1.4 1.4 1.5 1 V/2 1 1.4 1.401.4 1.2 1 1.336.1 1 1.4 1.5 1.1 1.20782.95 1.1 1.40747.81 1.1 1.401.4 1.1 1.401.4 1.1 1.401.4 1.1 1.40747.81</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012 322 ([C24 H32 05]+H)+ 4012 2363 1.4 ([C24 H32 05]+H)+ 1.4 ([C24 H32 05]+H)+ 1.5 402 2363 0.6 ([C24 H32 05]+H)+ 1.6 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ceak List VZ 74.2746 1 1.9914.69 C24 H32 05 (M+H)+ 7.1936 1 21394.35 1 8.4422 1 1.9918.68 1 8.4422 1 1.9708.68 1 8.4251 1 1.42411.8 1 9.4277 1 20782.95 1.42812.4</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 22 (C24 H32 OS]+H)+ 402.2363 14 14 14 14 14 14 15 14 14 16 14 14 17 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 18 14 14 14 14 14 15 1400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 16 Counts vs. Mass-to-Charge (m/z) eak List 17 14 12.322 1 19914.69 C24 H32 OS 11.2322 1 19914.69 C24 H32 OS 14 19008.68 8.4422 1 13674.77 1 144211.8 1 9.4321 1 14231 1 142411.8 1</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
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(Counts vs. Mass-to-Charge (m/z)) rak List Z Abund 4.2746 1 4.602.72 1 4.2746 1 4.602.71 1 4.2746 1 4.2746 1 4.2746 1 4.2776 1 4.2776 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 94227 1 20782.95 </th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 101.2322 ((C24 H32 OS)+H)+ 402.2363 14 400.2363 ((C24 H32 OS)+H)+ 14 400.2463 ((C24 H32 OS)+H)+ 14 400.2403.4 403.6 403.8 403.3974 14 400.4 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 49620.82 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12321 1 19916.68 12322 1 19914.69 12411.8 401.4411.8 144211.8 401.4411.8 14422 1 1442411.8 401.4411.8 1442411.8 401.4411.8</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401.2322 22 (IC24 H32 OS)+H)+ 402.2363 14 </th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
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ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 02)+H)+ 4012322 18 </th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 403.3974 0.8 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 do3.4 do3.6 403.8 0.4 (C24 H32 OS) (M+H)+ 1.2746 1 49620.82 1.3008 1 46747.81 1.3008 1 46747.81 1.3026 1 21394.35 1.4422 1 53674.77 1.44251 1 19708.68 1.44277 1 20782.95 1.44277 1 20782.95</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 C5)+H)+ 1.4 - 2.4 - 2.4 - 2.4 - 2.5 - 2.6 - 2.7 - 2.8 403 2.9 - 2.7 - 2.7 - 2.2 1</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th> <th>135 0 ESI 136 0 ESI 137 1 1 14 1 1 15 1 1 16 1 1 17 1 18 1 18 1 19 1 104 1 105 1 106 1 107 1 108 1 109 1 100 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 102 1 103 1 104 1 105 1 106 1 107 1 108 1 109 1 109 1 109 1 109 1 109 1 109 <t< th=""><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 O5)+H)+ 1.4 (C24 H32 O5)+H)+ 1.5 (C24 H32 O5)+H)+ 1.6 (C24 H32 O5)+H)+ 1.7 (C24 H32 O5)+H)+ 1.9 (H+H)+ 1.936 1 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 <th>135 0 ESI $x104 +ESi Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt08-12-5+.d Subtract (2) 401.2322 ((C24 H32 OS)+H)+ 401.2322 ((C24 H32 OS)+H)+ 402.2363 ((C24 H32 OS)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 10 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 402.2 402.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 20.8 10 10 10 10 10 10 10 10 10 10 10 10 10$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 2-2 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 (C24 H32 O5)+H)+ 16 (C24 H32 O5)+H)+ 17 (C24 H32 O5)+H)+ 18 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 1936 1 13 (C24 H32 O5)+H)+ 13 (C24 H32 O5)+H)+ 133008 1 14 (C24 H32 O5)+ 14</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 101 401.2322 ((C24 H32 O5)+H)+ 108 ((C24 H32 O5)+H)+ 109 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 402.2363 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 104 105 1 107 1 108 1 109 1 119916.69 C24 H32 05 119916.69 C24 H32 05 119916.69 C24 H32 05 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 14 12 (C24 H32 OS)+H)+ 0.8 ((C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 doi: 0.4 Counts vs. Mass-to-Charge (m/z) ak List 7 Z 12300 1 13000 1 14222 1 13036 1 21394.35 (M+H)+ 1336 1 14422 1 1 19708.68</th><th>$135 0 ESI$ $x10^{4} + ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 (1C24 H32 OS]+H)+ 401.2322 (1C24 H32 OS]+H)+ 402.2363 (1C24 H32 OS]+H)+ 403.3974 403.6 403.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4 403.2 403.4 403.6 403.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 2 ((C24 H32 OS)+H)+ 402.2363 14 - - 18 - - 0.4 - - 0.5 400.6 401.4 0.6 - - 0.7 - - 1.4 - - 1.2746 1 49620.82 1.27394.35 -</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 16 (C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 18 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 402.3363 14 (C24 H32 OS)+H)+ 403.3974 14 (C24 H32 OS)+H)+ 403.403.6 403.8 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 46747.81 322 1 19914.69 14 46747.81 1 322 1 19914.69 22 1 53674.77 14 12 1394.35 1</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 12- (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 18- (C24 H32 O5)+H)+ 403.3974 10- 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) x List 2746 1 1222 1 135008 1 146747.81 13501 136 13724 138 1422 1 1396 1
123674.77</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 14 </th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 O5)+H)+ 4012322 18 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 15 - - 16 - - 17 - - 18 - - 20 - - 21 1 59674.77 108 - - 211 1 19708.68 222 1 19708.64</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 14 -401.2322 ((C24 H32 O5)+H)+ 18 -402.2363 ((C24 H32 O5)+H)+ 14 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 04 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ctist -400.6 400.82 -400.7 10.1 10.1 10.1 10.1 10.1 10.1 10.1</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th><th>135 0 ESI $135 0 ESI$ $105 0 ESI$ 105</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012332 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 ((C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.403.2 403.4 403.6 403.8 1.4 (Counts vs. Mass-to-Charge (m/z)) 403.2 403.4 403.6 403.8 2746 1 49620.82 1 3008 1 46747.81 1 2322 1 19914.69 C24 H32 O5 4422 1 53674.77 1 4422 1 13204.86 1</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H)+ (0.12322 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.24 H32 OS)+H)+ (0.25 H32 OS)+H)$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 22 (1224 H32 OS)+H)+ 401.2323 14 (1224 H32 OS)+H)+ 402.2363 14 (1224 H32 OS)+H)+ 403.3974 0.4 (1224 H32 OS)+H)+ 403.4 403.6 403.8 0.4 (202 H32 OS)+H)+ 403.2 403.4 403.6 403.8 1 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.8 403 403.2 403.4 403.6 403.8 1 (200 H) (114 H)+ 1 4102 H32 OS (114 H)+ 1 4102 H32 OS (114 H)+ 1 4104 H1 (114 H1)+ 1 1 4104 H1 1 1<th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 1 401.2322 ((C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.746 1 49620.82 1.4 - - 2.3008 1 40747.81 1.2322 1 19914.69 1.21394.35 - 1.4422 1 53674.77<</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th><th>135 0 ESI $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) + 0.12322 (12-4H32.0S)+H)+ 0.12322 (12-2H32.0S)+H)+ 0.12323 + 0.12323 + 0.12323 + 0.1233$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 104 403.3974 105 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 104 Counts vs. Mass-to-Charge (m/z) 105 1 10746 1 11 407.2363 105 1 105 1 106 1 10746 1 10746 1 108 1 10914.69 C24 H32 O5 11 1914.69 12 1 135674.77 1 135674.77 1</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktG8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H) + (0.12322 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.124 H32 OS)+H$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 18 402.2363
(IC24 H32 OS]+H)+ 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 15 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 403.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7 2 1 4.2746 1 4.9620.82 1 3.3008 1 1 46747.81 1.2322 1 1 19914.69 1 121394.35 1 121394.35</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401,2322 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 - 402,2363 0.4 - ((C24 H32 O5)+H)+ 400.6 401.2 401.4 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.7 1 401.2 1.3 - - 2.2 1 19914.69 1.2 1 - 1.3008 1 46747.81 1.3005 1 21394.35 </th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d. Subtract (2) 401,2322 22 ((C24 H32 C5)+H)+ ((C24 H32 C5)+H)+ 1.4 12 ((C24 H32 C5)+H)+ 0.8 ((C24 H32 C5)+H)+ 403,3974 0.4 ((C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ (C24 H32 C5)+H)+ 1.2322 1 19914.69 C24 H32 C5 1.3304 1 46747.81 (M+H)+ 1.336 1 21394.35 (M+H)+</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d. Subtract (2) 401,2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 1.4
 - - 1.4 - - 1.5 - - 2.2 1 1914.69 1.4 1205 - 1.1 21394.35 -</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 138 (C24 H32 O5)+H)+ 403.3974 141 (C24 H32 O5)+H)+ 403.3974 140 (C24 H32 O5)+H)+ 403.3974 140 400.6 400.8 401 140 401.2 401.4 401.6 140 401.4 401.6 401.8 140 402.2363 (C24 H32 O5)+H)+ 140 401.4 401.6 401.8 140 401.4 401.6 401.8 402.2 140 401.4 401.6 401.8 402.4 135 Counts vs. Mass-to-Charge (m/z) 403.4 403.6 141 401.6 101.8 402.4 402.8 403.4 142 402.8 101.4 101.6 101.8 142 149620.82 1491.4 1491.4 1491.4 12322 1 19914.69 C24 H32 O5 (M+H)+ 11936 1 21394.35 1 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 401.2322 ((C24 H32 O5)+H)+ 403.3974 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 14 - - 15 - - 26 - - 16 - - 17 - - 18 - - 18 - - 18 - - 19 - - 100 - - 11 - - 12 19014.69 C24 H32 O5 11</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 184 402.2363
((C24 H32 OS)+H)+ 403.3974 104 403.3974 403.3974 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7z Abund 1 46747.81 1 46747.81 1 21394.335</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401,2322
(IC24 H32 OS]+H)+ 401,2322
(IC24 H32 OS]+H)+ 184 402,2363
(IC24 H32 OS]+H)+ 403,3974 194 401,401,6 401,6 194 401,401,2 401,401,6 194 403,3974 403,2974 194 401,401,6 401,6 194 401,401,6 401,6 194 401,401,6 401,6 194 403,201,403,4 403,6 199 14,692 C24 H32 O5 1,12322 1 19914.69 1914.69 C24 H32 O5 1,12394.35 1 1,12324 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 4 401.2322 ((C24 H32 OS)+H)+ 1.4 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401,2322 401,2322 ((C24 H32 OS)+H)+ 18 402,2363 14 12 14 12 14 12 14 12 14 12 14 12 15 402,2363 ((C24 H32 OS)+H)+ 15 403,3974 16 401,401.6 17 400.6 400.6 400.8 401 401.6 16 401.8 17 1 18 1 17.222 1 19314.69 C24 H32 OS 141924.69 C24 H32 OS 142746 1 12322 1 13914.69 C24 H32 OS 142745 1 13914.69 C24 H32 OS 1421394.35 <t< th=""><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc</th></t<></th></th></th></t<></th> | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kdc8-12-5+.d Subtract (2) 401.2322 1 401.2322 ((C24 H32 205)+H)+ 1.8 1.4 1.4 1.4 1.5 1 V/2 1 1.4 1.401.4 1.2 1 1.336.1 1 1.4 1.5 1.1 1.20782.95 1.1 1.40747.81 1.1 1.401.4 1.1 1.401.4 1.1 1.401.4 1.1 1.40747.81 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012 322 ([C24 H32 05]+H)+ 4012 2363 1.4 ([C24 H32 05]+H)+ 1.4 ([C24 H32 05]+H)+ 1.5 402 2363 0.6 ([C24 H32 05]+H)+ 1.6 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ceak List VZ
 74.2746 1 1.9914.69 C24 H32 05 (M+H)+ 7.1936 1 21394.35 1 8.4422 1 1.9918.68 1 8.4422 1 1.9708.68 1 8.4251 1 1.42411.8 1 9.4277 1 20782.95 1.42812.4 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 22 (C24 H32 OS]+H)+ 402.2363 14 14 14 14 14 14 15 14 14 16 14 14 17 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 18 14 14 14 14 14 15 1400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 16 Counts vs. Mass-to-Charge (m/z) eak List 17 14 12.322 1 19914.69 C24 H32 OS 11.2322 1 19914.69 C24 H32 OS 14 19008.68 8.4422 1 13674.77 1 144211.8 1 9.4321 1 14231 1 142411.8 1 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OS]+H)+ 401.2322
(1C24 H32 OS]+H)+ 4 402.2363
(1C24 H32 OS]+H)+ 403.3974 0.4
0.4
0.4
0.4
0.4
0.4
0.4
0.4
0.4
0.4 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt08-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 OS)+H)+ ((C24 H32 OS)+H)+ 18 402.2363 0.4 ((C24 H32 OS)+H)+ 0.4 (UC24 H32 OS)+H)+ 100 (UC24 H32 OS)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) ak List Z X Abund Formula 1 199014.69 12 21394.35 1 12 1394.35 1 12 1394.35 1 12 1294.35 1 12 407.7 1 24221 1 3674.777 1 24251 1 4277.1 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2)
401.2322
(1C24 H32 OS]+H)+ 401.2322
(1C24 H32 OS]+H)+ 4 402.2363
(1C24 H32 OS]+H)+ 403.3974 4 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
(Counts vs. Mass-to-Charge (m/z)) rak List Z Abund 4.2746 1 4.602.72 1 4.2746 1 4.602.71 1 4.2746 1 4.2746 1 4.2746 1 4.2776 1 4.2776 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1 4.2774 1
4.2774 1 94227 1 20782.95 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 101.2322 ((C24 H32 OS)+H)+ 402.2363 14 400.2363 ((C24 H32 OS)+H)+ 14 400.2463 ((C24 H32 OS)+H)+ 14 400.2403.4 403.6 403.8 403.3974 14 400.4 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 49620.82 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12321 1 19916.68 12322 1 19914.69 12411.8 401.4411.8 144211.8 401.4411.8 14422 1 1442411.8 401.4411.8 1442411.8 401.4411.8 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401.2322 22 (IC24 H32 OS)+H)+ 402.2363 14 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 402.2363
((C24 H32 OS)+H)+ 14 | 135 0 ESI *104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012322 4012 4012322 ((C24 H32 OS)+H)+ 18- 4012 4012 104 4012 4014 105 402 402 105 402 402 105 402 402 106 400 401 107 400 401 108 402 402 109 401 401.6 109 401 401.6 107 400 401 108 401 401.6 109 401 401.6 109 401.6 401.8 1100 401.2 401.4 112322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12322 1 19914.69 12324 1 19708.68 18.4422 1 19708.68 18.4251 1 42411.8 194277 1 20782.95 194277
 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 02)+H)+ 4012322 18 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 403.3974 0.8 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 do3.4 do3.6 403.8 0.4 (C24 H32 OS) (M+H)+ 1.2746 1 49620.82 1.3008 1 46747.81 1.3008 1 46747.81 1.3026 1 21394.35 1.4422 1 53674.77 1.44251 1 19708.68 1.44277 1 20782.95 1.44277 1 20782.95 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 C5)+H)+ 1.4 - 2.4 - 2.4 - 2.4 - 2.5 - 2.6 - 2.7 - 2.8 403 2.9 - 2.7 - 2.7 - 2.2 1 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 | 135 0 ESI 136 0 ESI 137 1 1 14 1 1 15 1 1 16 1 1 17 1 18 1 18 1 19 1 104 1 105 1 106 1 107 1 108 1 109 1 100 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 101 1 102 1 103 1 104 1 105 1 106 1 107 1 108 1 109 1 109 1 109 1 109 1 109 1 109 <t< th=""><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 O5)+H)+ 1.4 (C24 H32 O5)+H)+ 1.5 (C24 H32 O5)+H)+ 1.6 (C24 H32 O5)+H)+ 1.7 (C24 H32 O5)+H)+ 1.9 (H+H)+ 1.936 1 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 <th>135 0 ESI $x104 +ESi Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt08-12-5+.d Subtract (2) 401.2322 ((C24 H32 OS)+H)+ 401.2322 ((C24 H32 OS)+H)+ 402.2363 ((C24 H32 OS)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
counts vs. Mass-to-Charge (m/z) 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 10 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 402.2 402.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 20.8 10 10 10 10 10 10 10 10 10 10 10 10 10$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 2-2 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 (C24 H32 O5)+H)+ 16 (C24 H32 O5)+H)+ 17 (C24 H32 O5)+H)+ 18 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 1936 1 13 (C24 H32 O5)+H)+ 13 (C24 H32 O5)+H)+ 133008 1 14 (C24 H32 O5)+ 14</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 101 401.2322 ((C24 H32 O5)+H)+ 108 ((C24 H32 O5)+H)+ 109 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 402.2363 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 104 105 1 107 1 108 1 109 1 119916.69 C24 H32 05 119916.69 C24 H32 05 119916.69 C24 H32 05 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 14 12 (C24 H32 OS)+H)+ 0.8 ((C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 doi: 0.4 Counts vs. Mass-to-Charge (m/z) ak List 7 Z 12300 1 13000 1 14222 1 13036 1 21394.35 (M+H)+ 1336 1 14422 1 1 19708.68</th><th>$135 0 ESI$ $x10^{4} + ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 (1C24 H32 OS]+H)+ 401.2322 (1C24 H32 OS]+H)+ 402.2363 (1C24 H32 OS]+H)+ 403.3974 403.6 403.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4 403.2 403.4 403.6 403.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 2 ((C24 H32 OS)+H)+ 402.2363 14 - - 18 - - 0.4 - - 0.5 400.6 401.4 0.6 - - 0.7 - - 1.4 - - 1.2746 1 49620.82 1.27394.35 -</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 16 (C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 18 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 402.3363 14 (C24 H32 OS)+H)+ 403.3974 14 (C24 H32 OS)+H)+ 403.403.6 403.8 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 46747.81 322 1 19914.69 14 46747.81 1 322 1 19914.69 22 1 53674.77 14 12 1394.35 1</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 12- (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 18- (C24 H32 O5)+H)+ 403.3974 10- 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) x List 2746 1 1222 1 135008 1 146747.81 13501 136 13724 138 1422 1 1396 1 123674.77</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 14 </th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 O5)+H)+ 4012322 18 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 15 - - 16 - - 17 - - 18 - - 20 - - 21 1 59674.77 108 - - 211 1 19708.68 222 1 19708.64</th><th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 14 -401.2322 ((C24 H32 O5)+H)+ 18 -402.2363 ((C24 H32 O5)+H)+ 14 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 04 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ctist -400.6 400.82 -400.7 10.1 10.1 10.1 10.1 10.1 10.1 10.1</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th><th>135 0 ESI $135 0 ESI$ $105 0 ESI$ 105</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012332 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 ((C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.403.2 403.4 403.6 403.8 1.4 (Counts vs. Mass-to-Charge (m/z)) 403.2 403.4 403.6 403.8 2746 1 49620.82 1 3008 1 46747.81 1 2322 1 19914.69 C24 H32 O5 4422 1 53674.77 1 4422 1 13204.86 1</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H)+ (0.12322 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.24 H32 OS)+H)+ (0.25 H32 OS)+H)$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 22 (1224 H32 OS)+H)+ 401.2323 14 (1224 H32 OS)+H)+ 402.2363 14 (1224 H32 OS)+H)+ 403.3974 0.4 (1224 H32 OS)+H)+ 403.4 403.6 403.8 0.4 (202 H32 OS)+H)+ 403.2 403.4 403.6 403.8 1 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.8 403 403.2 403.4 403.6 403.8 1 (200 H) (114 H)+ 1 4102 H32 OS (114 H)+ 1 4102 H32 OS (114 H)+ 1 4104 H1 (114 H1)+ 1
 1 4104 H1 1 1<th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 1 401.2322 ((C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.746 1 49620.82 1.4 - - 2.3008 1 40747.81 1.2322 1 19914.69 1.21394.35 - 1.4422 1 53674.77<</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th><th>135 0 ESI $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) + 0.12322 (12-4H32.0S)+H)+ 0.12322 (12-2H32.0S)+H)+ 0.12323 + 0.12323 + 0.12323 + 0.1233$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 104 403.3974 105 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 104 Counts vs. Mass-to-Charge (m/z) 105 1 10746 1 11 407.2363 105 1 105 1 106 1 10746 1 10746 1 108 1 10914.69 C24 H32 O5 11 1914.69 12 1 135674.77 1 135674.77 1</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktG8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H) + (0.12322 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.124 H32 OS)+H$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 18 402.2363
(IC24 H32 OS]+H)+ 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 15 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 403.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7 2 1 4.2746 1 4.9620.82 1 3.3008 1 1 46747.81 1.2322 1 1 19914.69 1 121394.35 1 121394.35</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401,2322 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 - 402,2363 0.4 - ((C24 H32 O5)+H)+ 400.6 401.2 401.4 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.7 1 401.2 1.3 - - 2.2 1 19914.69 1.2 1 - 1.3008 1 46747.81 1.3005 1 21394.35 </th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d. Subtract (2) 401,2322 22 ((C24 H32 C5)+H)+ ((C24 H32 C5)+H)+ 1.4 12 ((C24 H32 C5)+H)+ 0.8 ((C24 H32 C5)+H)+ 403,3974 0.4 ((C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ (C24 H32 C5)+H)+ 1.2322 1 19914.69 C24 H32 C5 1.3304 1 46747.81 (M+H)+ 1.336 1 21394.35 (M+H)+</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d. Subtract (2) 401,2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.2 1 1914.69 1.4 1205 - 1.1 21394.35 -</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 138 (C24 H32 O5)+H)+ 403.3974 141 (C24 H32 O5)+H)+ 403.3974 140 (C24 H32 O5)+H)+ 403.3974 140 400.6 400.8 401 140 401.2 401.4 401.6 140 401.4 401.6 401.8 140 402.2363 (C24 H32 O5)+H)+ 140 401.4 401.6 401.8 140 401.4 401.6 401.8 402.2 140 401.4 401.6 401.8 402.4 135 Counts vs. Mass-to-Charge (m/z) 403.4 403.6 141 401.6 101.8 402.4 402.8 403.4 142 402.8 101.4 101.6 101.8 142 149620.82 1491.4 1491.4 1491.4 12322 1 19914.69 C24 H32 O5 (M+H)+ 11936 1 21394.35 1 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 401.2322 ((C24 H32 O5)+H)+ 403.3974 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 14 - - 15 - - 26 - - 16 - - 17 - - 18 - - 18 - - 18 - - 19 - - 100 - - 11 - - 12 19014.69 C24 H32 O5 11</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 184 402.2363
((C24 H32 OS)+H)+ 403.3974 104 403.3974 403.3974 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7z Abund 1 46747.81 1 46747.81 1 21394.335</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401,2322
(IC24 H32 OS]+H)+ 401,2322
(IC24 H32 OS]+H)+ 184 402,2363
(IC24 H32 OS]+H)+ 403,3974 194 401,401,6 401,6 194 401,401,2 401,401,6 194 403,3974 403,2974 194 401,401,6 401,6 194
 401,401,6 401,6 194 401,401,6 401,6 194 403,201,403,4 403,6 199 14,692 C24 H32 O5 1,12322 1 19914.69 1914.69 C24 H32 O5 1,12394.35 1 1,12324 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 4 401.2322 ((C24 H32 OS)+H)+ 1.4 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401,2322 401,2322 ((C24 H32 OS)+H)+ 18 402,2363 14 12 14 12 14 12 14 12 14 12 14 12 15 402,2363 ((C24 H32 OS)+H)+ 15 403,3974 16 401,401.6 17 400.6 400.6 400.8 401 401.6 16 401.8 17 1 18 1 17.222 1 19314.69 C24 H32 OS 141924.69 C24 H32 OS 142746 1 12322 1 13914.69 C24 H32 OS 142745 1 13914.69 C24 H32 OS 1421394.35 <t< th=""><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc</th></t<></th></th></th></t<> | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 2 ((C24 H32 O5)+H)+ 1.4 (C24 H32 O5)+H)+ 1.5 (C24 H32 O5)+H)+ 1.6 (C24 H32 O5)+H)+ 1.7 (C24 H32 O5)+H)+ 1.9 (H+H)+ 1.936 1 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 1.1 19708.68 <th>135 0 ESI $x104 +ESi Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt08-12-5+.d Subtract (2) 401.2322 ((C24 H32 OS)+H)+ 401.2322 ((C24 H32 OS)+H)+ 402.2363 ((C24 H32 OS)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 10 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 402.2 402.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 20.8 10 10 10 10 10 10 10 10 10 10 10 10 10$</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 2-2 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 (C24 H32 O5)+H)+ 16 (C24 H32 O5)+H)+ 17 (C24 H32 O5)+H)+ 18 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 1936 1 13 (C24 H32 O5)+H)+ 13 (C24 H32 O5)+H)+ 133008 1 14 (C24 H32 O5)+ 14</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 101 401.2322 ((C24 H32 O5)+H)+ 108 ((C24 H32 O5)+H)+ 109 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 402.2363 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 104 105 1 107 1 108 1 109 1 119916.69 C24 H32 05 119916.69 C24 H32 05 119916.69 C24 H32 05 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 14 12 (C24 H32 OS)+H)+ 0.8 ((C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 doi: 0.4 Counts vs. Mass-to-Charge (m/z) ak List 7 Z 12300 1 13000 1 14222 1 13036 1 21394.35 (M+H)+ 1336 1 14422 1 1 19708.68</th> <th>$135 0 ESI$ $x10^{4} + ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 (1C24 H32 OS]+H)+ 401.2322 (1C24 H32 OS]+H)+ 402.2363 (1C24 H32 OS]+H)+ 403.3974 403.6 403.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4 403.2 403.4 403.6 403.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4$</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 2 ((C24 H32 OS)+H)+ 402.2363 14 - - 18 - - 0.4 - - 0.5 400.6 401.4 0.6 - - 0.7 - - 1.4 -
- 1.2746 1 49620.82 1.27394.35 -</th> <th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 16 (C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 18 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 402.3363 14 (C24 H32 OS)+H)+ 403.3974 14 (C24 H32 OS)+H)+ 403.403.6 403.8 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 46747.81 322 1 19914.69 14 46747.81 1 322 1 19914.69 22 1 53674.77 14 12 1394.35 1</th> <th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 12- (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 18- (C24 H32 O5)+H)+ 403.3974 10- 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) x List 2746 1 1222 1 135008 1 146747.81 13501 136 13724 138 1422 1 1396 1 123674.77</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 14 </th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 O5)+H)+ 4012322 18 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 15 - - 16 - - 17 - - 18 - - 20 - - 21 1 59674.77 108 - - 211 1 19708.68 222 1 19708.64</th> <th>135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 14 -401.2322 ((C24 H32 O5)+H)+ 18 -402.2363 ((C24 H32 O5)+H)+ 14 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 04 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ctist -400.6 400.82 -400.7 10.1 10.1 10.1 10.1 10.1 10.1 10.1</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th> <th>135 0 ESI $135 0 ESI$ $105 0 ESI$ 105</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012332 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 ((C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.403.2 403.4 403.6 403.8 1.4 (Counts vs. Mass-to-Charge (m/z)) 403.2 403.4 403.6 403.8 2746 1 49620.82 1 3008 1 46747.81 1 2322 1 19914.69 C24 H32 O5 4422 1 53674.77 1 4422 1 13204.86 1</th> <th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H)+ (0.12322 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.24 H32 OS)+H)+ (0.25 H32 OS)+H)$</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 22 (1224 H32 OS)+H)+ 401.2323 14 (1224 H32 OS)+H)+ 402.2363 14 (1224 H32 OS)+H)+ 403.3974 0.4 (1224 H32 OS)+H)+ 403.4 403.6 403.8 0.4 (202 H32 OS)+H)+ 403.2 403.4 403.6 403.8 1 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.8 403 403.2 403.4 403.6 403.8 1 (200 H) (114 H)+ 1 4102 H32 OS (114 H)+ 1 4102 H32 OS (114 H)+ 1 4104 H1 (114 H1)+ 1 1 4104 H1 1 1<th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 1 401.2322 ((C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.746 1 49620.82 1.4 - - 2.3008 1 40747.81 1.2322 1 19914.69 1.21394.35 - 1.4422 1 53674.77<</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th><th>135 0 ESI $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) + 0.12322 (12-4H32.0S)+H)+ 0.12322 (12-2H32.0S)+H)+ 0.12323 + 0.12323 + 0.12323 + 0.1233$</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 104 403.3974 105 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 104 Counts vs. Mass-to-Charge (m/z) 105 1 10746 1 11 407.2363 105 1 105 1 106 1 10746 1 10746 1 108 1 10914.69 C24 H32 O5 11 1914.69 12 1 135674.77 1 135674.77 1</th><th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktG8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H) + (0.12322 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.124 H32 OS)+H$</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 18 402.2363
(IC24 H32 OS]+H)+ 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 15 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 403.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7 2 1 4.2746 1 4.9620.82 1 3.3008 1 1 46747.81 1.2322 1 1 19914.69 1 121394.35 1 121394.35</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401,2322 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 - 402,2363 0.4 - ((C24 H32 O5)+H)+ 400.6 401.2 401.4 1.4 - -
1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.7 1 401.2 1.3 - - 2.2 1 19914.69 1.2 1 - 1.3008 1 46747.81 1.3005 1 21394.35 </th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d. Subtract (2) 401,2322 22 ((C24 H32 C5)+H)+ ((C24 H32 C5)+H)+ 1.4 12 ((C24 H32 C5)+H)+ 0.8 ((C24 H32 C5)+H)+ 403,3974 0.4 ((C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ (C24 H32 C5)+H)+ 1.2322 1 19914.69 C24 H32 C5 1.3304 1 46747.81 (M+H)+ 1.336 1 21394.35 (M+H)+</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d. Subtract (2) 401,2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.2 1 1914.69 1.4 1205 - 1.1 21394.35 -</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 138 (C24 H32 O5)+H)+ 403.3974 141 (C24 H32 O5)+H)+ 403.3974 140 (C24 H32 O5)+H)+ 403.3974 140 400.6 400.8 401 140 401.2 401.4 401.6 140 401.4 401.6 401.8 140 402.2363 (C24 H32 O5)+H)+ 140 401.4 401.6 401.8 140 401.4 401.6 401.8 402.2 140 401.4 401.6 401.8 402.4 135 Counts vs. Mass-to-Charge (m/z) 403.4 403.6 141 401.6 101.8 402.4 402.8 403.4 142 402.8 101.4 101.6 101.8 142 149620.82 1491.4 1491.4 1491.4 12322 1 19914.69 C24 H32 O5 (M+H)+ 11936 1 21394.35 1 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 401.2322 ((C24 H32 O5)+H)+ 403.3974 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 14 - - 15 - - 26 - - 16 - - 17 - - 18 - - 18 - - 18 - - 19 - - 100 - - 11 - - 12 19014.69 C24 H32 O5 11</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 184 402.2363
((C24 H32 OS)+H)+ 403.3974 104 403.3974 403.3974 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7z Abund 1 46747.81 1 46747.81 1 21394.335</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401,2322
(IC24 H32 OS]+H)+ 401,2322
(IC24 H32 OS]+H)+ 184 402,2363
(IC24 H32 OS]+H)+ 403,3974 194 401,401,6 401,6 194 401,401,2 401,401,6 194 403,3974 403,2974 194 401,401,6 401,6 194 401,401,6 401,6 194 401,401,6 401,6 194 403,201,403,4 403,6 199 14,692 C24 H32 O5 1,12322 1 19914.69 1914.69 C24 H32 O5 1,12394.35 1 1,12324 1</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 4 401.2322 ((C24 H32 OS)+H)+ 1.4 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401,2322 401,2322 ((C24 H32 OS)+H)+ 18 402,2363 14 12 14 12 14 12 14 12 14 12 14 12 15 402,2363 ((C24 H32 OS)+H)+ 15 403,3974 16 401,401.6 17 400.6 400.6 400.8 401 401.6 16 401.8 17 1 18 1 17.222 1 19314.69 C24 H32 OS 141924.69 C24 H32 OS 142746 1 12322 1 13914.69 C24 H32 OS 142745 1 13914.69 C24 H32 OS 1421394.35 <t< th=""><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc</th></t<></th></th>
 | 135 0 ESI $x104 +ESi Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt08-12-5+.d Subtract (2) 401.2322 ((C24 H32 OS)+H)+ 401.2322 ((C24 H32 OS)+H)+ 402.2363 ((C24 H32 OS)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 400.8 10 1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 10 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 402.2 402.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) 400.6 11 407.4 11 407.6 20.8 10 10 10 10 10 10 10 10 10 10 10 10 10$ | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 2-2 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 (C24 H32 O5)+H)+ 16 (C24 H32 O5)+H)+ 17 (C24 H32 O5)+H)+ 18 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 19 (C24 H32 O5)+H)+ 1936 1 13 (C24 H32 O5)+H)+ 13 (C24 H32 O5)+H)+ 133008 1 14 (C24 H32 O5)+ 14

 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 101 401.2322 ((C24 H32 O5)+H)+ 108 ((C24 H32 O5)+H)+ 109 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 402.2363 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 104 104 105 1 107 1 108 1 109 1 119916.69 C24 H32 05 119916.69 C24 H32 05 119916.69 C24 H32 05 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 119908.68 1 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 14 12 (C24 H32 OS)+H)+ 0.8 ((C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.3974 0.4 (C24 H32 OS)+H)+ 403.403.6 403.8 doi: 0.4 Counts vs. Mass-to-Charge (m/z) ak List 7 Z 12300 1 13000 1 14222 1 13036 1 21394.35 (M+H)+ 1336 1 14422 1 1 19708.68 | $135 0 ESI$ $x10^{4} + ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 (1C24 H32 OS]+H)+ 401.2322 (1C24 H32 OS]+H)+ 402.2363 (1C24 H32 OS]+H)+ 403.3974 403.6 403.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4 403.2 403.4 403.6 403.8 403 403.2 403.4 403.6 403.8 403 403.2 403.4$ | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 2 ((C24 H32 OS)+H)+ 402.2363 14 - - 18 - - 0.4 - - 0.5 400.6 401.4 0.6 - - 0.7 - - 1.4 - - 1.2746 1 49620.82 1.27394.35 - | 135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 22 (C24 H32 OS)+H)+ 402.2363 16 (C24 H32 OS)+H)+ (C24 H32 OS)+H)+ 18 (C24 H32 OS)+H)+ 402.2363 14 (C24 H32 OS)+H)+ 402.3363 14 (C24 H32 OS)+H)+ 403.3974 14 (C24 H32 OS)+H)+ 403.403.6 403.8 403.4 403.6 403.8 15 Counts vs. Mass-to-Charge (m/z) 15 1 46747.81 322 1 19914.69 14 46747.81
 1 322 1 19914.69 22 1 53674.77 14 12 1394.35 1 | 135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 12- (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 18- (C24 H32 O5)+H)+ 403.3974 10- 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) x List 2746 1 1222 1 135008 1 146747.81 13501 136 13724 138 1422 1 1396 1 123674.77

 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 14 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 4012322 22 ((C24 H32 O5)+H)+ 4012322 18 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 15 - - 16 - - 17 - - 18 - - 20 - - 21 1 59674.77 108 - - 211 1 19708.68 222 1 19708.64 | 135 0 ESI 04 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 14 -401.2322 ((C24 H32 O5)+H)+ 18 -402.2363 ((C24 H32 O5)+H)+ 14 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 04 -400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ctist -400.6 400.82 -400.7 10.1 10.1 10.1 10.1 10.1 10.1 10.1
 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18

 | 135 0 ESI $135 0 ESI$ $105 0 ESI$ 105 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 4012332 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 ((C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.3974 1.4 (C24 H32 O5)+H)+ 403.403.2 403.4 403.6 403.8 1.4
 (Counts vs. Mass-to-Charge (m/z)) 403.2 403.4 403.6 403.8 2746 1 49620.82 1 3008 1 46747.81 1 2322 1 19914.69 C24 H32 O5 4422 1 53674.77 1 4422 1 13204.86 1 | 135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H)+ (0.12322 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.2363 + (0.124 H32 OS)+H)+ (0.24 H32 OS)+H)+ (0.25 H32 OS)+H)$

 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2) 401.2322 22 (1224 H32 OS)+H)+ 401.2323 14 (1224 H32 OS)+H)+ 402.2363 14 (1224 H32 OS)+H)+ 403.3974 0.4 (1224 H32 OS)+H)+ 403.4 403.6 403.8 0.4 (202 H32 OS)+H)+ 403.2 403.4 403.6 403.8 1 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.8 403 403.2 403.4 403.6 403.8 1 (200 H) (114 H)+ 1 4102 H32 OS (114 H)+ 1 4102 H32 OS (114 H)+ 1 4104 H1 (114 H1)+ 1 1 4104 H1 1 1 <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 1 401.2322 ((C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.746 1 49620.82 1.4 - - 2.3008 1 40747.81 1.2322 1 19914.69 1.21394.35 - 1.4422 1 53674.77<</th> <th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th> <th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th> <th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 </th> <th>135 0 ESI $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) + 0.12322 (12-4H32.0S)+H)+ 0.12322 (12-2H32.0S)+H)+ 0.12323 + 0.12323 + 0.12323 + 0.1233$</th> <th>135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 104 403.3974 105 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 104 Counts vs. Mass-to-Charge (m/z) 105 1 10746 1 11 407.2363 105 1 105 1 106 1 10746 1 10746 1 108 1 10914.69 C24 H32 O5 11 1914.69 12 1 135674.77 1 135674.77 1</th> <th>135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktG8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H) + (0.12322 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.124 H32 OS)+H$</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 18 402.2363
(IC24 H32 OS]+H)+ 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 15 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 403.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7 2 1 4.2746 1 4.9620.82 1 3.3008 1 1 46747.81 1.2322 1 1 19914.69 1 121394.35 1 121394.35</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401,2322 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 - 402,2363 0.4 - ((C24 H32 O5)+H)+ 400.6 401.2 401.4 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.7 1 401.2 1.3 - - 2.2 1 19914.69 1.2 1 - 1.3008 1 46747.81 1.3005 1 21394.35 </th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d. Subtract (2) 401,2322 22 ((C24 H32 C5)+H)+ ((C24 H32 C5)+H)+ 1.4 12 ((C24 H32 C5)+H)+ 0.8 ((C24 H32 C5)+H)+ 403,3974 0.4 ((C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ (C24 H32 C5)+H)+ 1.2322 1 19914.69 C24 H32 C5 1.3304 1 46747.81 (M+H)+ 1.336 1 21394.35 (M+H)+</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d. Subtract (2) 401,2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.2 1 1914.69 1.4 1205 - 1.1 21394.35 -</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 138 (C24 H32 O5)+H)+ 403.3974 141 (C24 H32 O5)+H)+ 403.3974 140 (C24 H32 O5)+H)+ 403.3974 140 400.6 400.8 401 140 401.2 401.4 401.6 140 401.4 401.6 401.8 140 402.2363 (C24 H32 O5)+H)+ 140 401.4 401.6 401.8 140 401.4 401.6 401.8 402.2 140 401.4 401.6 401.8 402.4 135 Counts vs. Mass-to-Charge (m/z) 403.4 403.6 141 401.6 101.8 402.4 402.8 403.4 142 402.8 101.4 101.6 101.8 142 149620.82 1491.4 1491.4 1491.4 12322 1 19914.69 C24 H32 O5 (M+H)+ 11936 1 21394.35 1 1</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 401.2322 ((C24 H32 O5)+H)+ 403.3974 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 14 - - 14 - -
14 - - 14 - - 14 - - 15 - - 14 - - 14 - - 15 - - 26 - - 16 - - 17 - - 18 - - 18 - - 18 - - 19 - - 100 - - 11 - - 12 19014.69 C24 H32 O5 11</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 184 402.2363
((C24 H32 OS)+H)+ 403.3974 104 403.3974 403.3974 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7z Abund 1 46747.81 1 46747.81 1 21394.335</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401,2322
(IC24 H32 OS]+H)+ 401,2322
(IC24 H32 OS]+H)+ 184 402,2363
(IC24 H32 OS]+H)+ 403,3974 194 401,401,6 401,6 194 401,401,2 401,401,6 194 403,3974 403,2974 194 401,401,6 401,6 194 401,401,6 401,6 194 401,401,6 401,6 194 403,201,403,4 403,6 199 14,692 C24 H32 O5 1,12322 1 19914.69 1914.69 C24 H32 O5 1,12394.35 1 1,12324 1</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 4 401.2322 ((C24 H32 OS)+H)+ 1.4 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2<</th> <th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401,2322 401,2322 ((C24 H32 OS)+H)+ 18 402,2363 14 12 14 12 14 12 14 12 14 12 14 12 15 402,2363 ((C24 H32 OS)+H)+ 15 403,3974 16 401,401.6 17 400.6 400.6 400.8 401 401.6 16 401.8 17 1 18 1 17.222 1 19314.69 C24 H32 OS 141924.69 C24 H32 OS 142746 1 12322 1 13914.69 C24 H32 OS 142745 1 13914.69 C24 H32 OS 1421394.35 <t< th=""><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc</th></t<></th> | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 1 401.2322 ((C24 H32 O5)+H)+ 1.4 - - 1.5 - - 2.746 1 49620.82 1.4 - - 2.3008 1 40747.81 1.2322 1 19914.69 1.21394.35 - 1.4422 1 53674.77< | 135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$ | 135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kt/c8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$
 | 135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ (C24 H32 H32 H32 H32 H32 H32 H32 H32 H32 H32$ | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktds-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 | 135 0 ESI $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktd8-12-5+.d Subtract (2) + 0.12322 (12-4H32.0S)+H)+ 0.12322 (12-2H32.0S)+H)+ 0.12323 + 0.12323 + 0.12323 + 0.1233$ | 135 0 ESI 104 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401.2322 104 401.2322 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 104 403.3974 105 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 104 Counts vs. Mass-to-Charge (m/z) 105 1 10746 1 11 407.2363 105 1 105 1 106 1 10746 1 10746 1 108 1 10914.69 C24 H32 O5 11 1914.69 12 1 135674.77 1 135674.77 1 | 135 0 ESI $135 0 ESI$ $104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V ktG8-12-5+.d Subtract (2) + (0.12322 + (0.124 H32 OS)+H) + (0.12322 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.12323 + (0.124 H32 OS)+H) + (0.124 H32 OS)+H$
 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 18 402.2363
(IC24 H32 OS]+H)+ 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 14 403.3974 15 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 403.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7 2 1 4.2746 1 4.9620.82 1 3.3008 1 1 46747.81 1.2322 1 1 19914.69 1 121394.35 1 121394.35 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d Subtract (2) 401,2322 22 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 1.4 - 402,2363 0.4 - ((C24 H32 O5)+H)+ 400.6 401.2 401.4 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.7 1 401.2 1.3 - - 2.2 1 19914.69 1.2 1 - 1.3008 1 46747.81 1.3005 1 21394.35 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d. Subtract (2) 401,2322 22 ((C24 H32 C5)+H)+ ((C24 H32 C5)+H)+ 1.4 12 ((C24 H32 C5)+H)+ 0.8 ((C24 H32 C5)+H)+ 403,3974 0.4 ((C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ 403,3974 0.4 (C24 H32 C5)+H)+ (C24 H32 C5)+H)+ 1.2322 1 19914.69 C24 H32 C5 1.3304 1 46747.81 (M+H)+ 1.336 1 21394.35 (M+H)+ | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d. Subtract (2) 401,2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 - - 1.4 -
 - 1.4 - - 1.4 - - 1.4 - - 1.5 - - 2.2 1 1914.69 1.4 1205 - 1.1 21394.35 - | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s8-12-5+.d. Subtract (2) 401.2322 2 (C24 H32 O5)+H)+ (C24 H32 O5)+H)+ 138 (C24 H32 O5)+H)+ 403.3974 141 (C24 H32 O5)+H)+ 403.3974 140 (C24 H32 O5)+H)+ 403.3974 140 400.6 400.8 401 140 401.2 401.4 401.6 140 401.4 401.6 401.8 140 402.2363 (C24 H32 O5)+H)+ 140 401.4 401.6 401.8 140 401.4 401.6 401.8 402.2 140 401.4 401.6 401.8 402.4 135 Counts vs. Mass-to-Charge (m/z) 403.4 403.6 141 401.6 101.8 402.4 402.8 403.4 142 402.8 101.4 101.6 101.8 142 149620.82 1491.4 1491.4 1491.4 12322 1 19914.69 C24 H32 O5 (M+H)+ 11936 1 21394.35 1 1 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401.2322 401.2322 ((C24 H32 O5)+H)+ 403.3974 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 14 - - 15 - - 14 - - 14 - - 15 - - 26 - - 16 - - 17 - - 18 - - 18 - - 18 - - 19 - - 100 - - 11 - - 12 19014.69 C24 H32 O5 11 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
((C24 H32 OS)+H)+ 401.2322
((C24 H32 OS)+H)+ 184 402.2363
((C24 H32 OS)+H)+ 403.3974 104 403.3974 403.3974 105 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) ak List 7z Abund 1 46747.81 1 46747.81 1 21394.335 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401,2322
(IC24 H32 OS]+H)+ 401,2322
(IC24 H32 OS]+H)+ 184 402,2363
(IC24 H32 OS]+H)+ 403,3974 194 401,401,6 401,6 194 401,401,2 401,401,6 194 403,3974 403,2974 194 401,401,6 401,6 194 401,401,6 401,6 194 401,401,6 401,6 194 403,201,403,4 403,6 199 14,692 C24 H32 O5 1,12322 1 19914.69
 1914.69 C24 H32 O5 1,12394.35 1 1,12324 1 | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401.2322 4 401.2322 ((C24 H32 OS)+H)+ 1.4 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2 - - 2.2< | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2) 401,2322 401,2322 ((C24 H32 OS)+H)+ 18 402,2363 14 12 14 12 14 12 14 12 14 12 14 12 15 402,2363 ((C24 H32 OS)+H)+ 15 403,3974 16 401,401.6 17 400.6 400.6 400.8 401 401.6 16 401.8 17 1 18 1 17.222 1 19314.69 C24 H32 OS 141924.69 C24 H32 OS 142746 1 12322 1 13914.69 C24 H32 OS 142745 1 13914.69 C24 H32 OS 1421394.35 <t< th=""><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68</th><th>135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -<</th><th>135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc</th></t<> | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 401.2322 22 ((C24 H32 O5)+H)+ 18 ((C24 H32 O5)+H)+ 14 ((C24 H32 O5)+H)+ 15 ((C24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 14 (UC24 H32 O5)+H)+ 15 (UC24 H32 O5) 13008 1 1 46747.81 13008 1 1 19914.69 121394.35 (MH+H)+ 11936.68 1 14222 1 1 1306.68 | 135 0 ESI 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktd8-12-5+.d Subtract (2) 4012322 2 (IC24 H32 02)+H)+ (IC24 H32 05)+H)+ 18 - - 14 - - 15 - - 16 - - 17 - - 18 - - 14 - - 14 - - 14 - - 16 - - 16 - - 17 - - 18 - - 19 - - 14 - - 14 - - 15 - - 16 - - 17 - - 18 - - 19 - - 100 - - 22 - - 400.2 363 - - 14 - - 14 - - 14 - - 27 - - 27 -< | 135 0 ESI x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d. Subtract (2)
401.2322
(IC24 H32 OS]+H)+ 401.2322
(IC24 H32 OS]+H)+ 184 402.2363
(IC24 H32 OS]+H)+ 403.3974 104 403.401.4 do1.5 401.8 402 402.2 402.4 do2.6 402.8 403 403.2 403.4 do3.6 403.8
Counts vs. Mass-to-Charge (m/z) rak List Zz Abund 12322 1 19914.69 C24 H32 OS 1 205 1.2322 1 1 21394.35 3.4422 1 21 1 22 1 1 10200 cc
 |
| x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401.2322
(C24 H32 O3)+H)+
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14 | x10 ⁴ +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1024 H32 03)+H)+
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 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2)
401.2322
((C24 H32 205)+H)+
401.2322
((C24 H32 205)+H)+
402.2363
((C24 H32 205)+H)+
402.2363
((C24 H32 205)+H)+
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403.4403.6403.8
8.3008
1 46747.81
8.3008
1 46747.81 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kId8-12-5+.d Subtract (2)
401 2322
([C24 H32 OS]+H)+
401 2322
([C24 H32 OS]+H)+
402 2363
([C24 H32 OS]+H)+
402 2363
([C24 H32 OS]+H)+
403.3974
400.6 400.8 401 4012 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z) eak List YZ X Abund Formula Ion
Counts vs. Mass-to-Charge (m/z) YZ X Abund Formula Ion
Counts vs. Mass-to-Charge (m/z) eak List YZ X Abund Formula Ion
Counts vs. Mass-to-Charge (m/z) YZ X Abund Formula Ion
Counts vs. Mass-to-Charge (m/z) eak List YZ X Abund Formula Ion
Counts vs. Mass-to-Charge (m/z) Y4.2746 1 49620.82 Ion
Counts vs. Mass-to-Charge (m/z) Ion
Counts vs. Mass-to-Charge (m/z) 9.4452 1 19914.69 C24 H32 OS (M+H)+ 7.1936 1 21394.35 Ion
Counts vs. Mass-to-Charge (m/z) 9.44271 1 20782.95 Ion
Counts vs. Mass-to-Charge (m/z) 9.4277 1 20782.95 Ion
Counts vs. Mass-to-Charge (m/z)
 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(IC24 H32 O5]+H)+
401.2322
(IC24 H32 O5]+H)+
402.2363
(IC24 H32 O5]+H)+
402.2363
(IC24 H32 O5]+H)+
403.3974
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
eak List
V/Z z Abund Formula Ion
42.2746 1 49620.82
8.3008 1 46747.81
1.2322 1 19914.69 C24 H32 O5 (M+H)+
7.1936 1 21394.35
8.4422 1 53674.77
9.44574 1 19708.68
8.4422 1 1 47733.64
9.4277 1 20782.95
6.4351 1 42411.8 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OSI+H)+
402.2463
(1C24 H32 OSI+H)+
403.3974
400.5 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
eak List
7 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
((C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
((C24 H32 OS)+H)+
403.3974
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403.3974
403.3008
1 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
Z
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402 21
1 49620.82
1 19914.69
C24 H32 O5
(M+H)+
1 21394.35
1 21394.35
1 21394.35
1 47773.64
2 402.4 118
1 47733.64
1 4773 | x104 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/s=12-5+.d Subtract (2) 401_2322 (1024 H32 OS)+H)+ 14 (1C24 H32 OS)+H)+ 15 (1C24 H32 OS)+H)+ 16 (1C24 H32 OS)+H)+ 16 (1C24 H32 OS)+H)+ 17 (1C24 H32 OS)+H)+ 18 (1C24 H32 OS)+H)+ 19 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 counts vs. Mass-to-Charge (m/z) rak List 2 1 4.2746 1 1 49620.82 8.3008 1 1 46747.81 1.2322 1 1 19914.69 12 13674.77 2.44521 1 3.6422 1 3.674.77 1 2.44521 1 4.2774 1 1 4773.64 9.4277 1 2.775 1 4.4721.18 1 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scan) Frag=135.0V ktoB-12-54 d Subtract (2)
401_2322
(1C24 H32 OSI+H)+
402_263
(1C24 H32 OSI+H)+
403_3974
400.5 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
sak List
7
 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktoB=12-54 d Subtract (2)
401_2322
(1C24 H32 OS]+H)+
402_263
(1C24 H32 OS]+H)+
403.3974
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
sak List
// | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
((C24 H32 OS)+H)+
403.3974
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
/z x Abund Formula Ion
4.2746 1 49620.82
8.3008 1 46747.81
1.2322 1 19914.69 C24 H32 OS (M+H)+
7.1936 1 21394.35
8.4422 1 53674.77
9.4454 1 19708.68
8.4251 1 47733.64
9.4277 1 20782.95
6.4351 1 4211.8
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1.421 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfc8-12-5+.d Subtract (2) 4012322 ((C24 H32 OS)+H)+ 18- 402.2363 14- ((C24 H32 OS)+H)+ 14- 402.2363 0.4- ((C24 H32 OS)+H)+ 0.4- 403.3974 0.4- ((C24 H32 OS)+H)+ 0.4- ((C24 H32 OS)+H)+ 0.4- (C24 H32 OS)+ 0.4- (C24 H32 OS)+ 0.4- (C24 H32 OS)+ 1.2322 1 19914.69 1.4308 1 1.2322 1 19914.69 1.46747.81 1 1.2322 1 19914.69 1.4374 1 1.4421 1 1.53674.777 1 2.94554 1 1.47733.64 1 2.4277 1 2.42785 1 | x10 ⁴ +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
(IC24 H32 O3)+H)+
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 | x10 ⁴ +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
1.4
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1.4
1.4
1.4 | 104 +ESI Scan (0.13-0.14 min, 2 Scana) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
18-
14-
12-
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12-
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14-
14-
14-
14-
14-
14-
14 | HESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kto8-12-5+.d Subtract (2) 4012322 (IC24 H32 O5)+H)+ 4012363 (IC24 H32 O5)+H)+ 402.2363 (IC24 H32 O5)+H)+ 403.3974 400.5 400.8 401 4012 4014 4015 4018 402 4022 4024 4026 4028 403 4032 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 401 4012 4014 4015 4018 402 4022 4024 4026 4028 403 4032 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 401 4012 4014 4015 018 402 402 4024 4026 4028 403 4032 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 401 4012 4014 4015 018 402 402 402 402 402 402 6 402 8 403 403 2 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 101 4012 4014 4015 018 402 402 402 402 402 6 402 8 403 403 2 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 101 4012 4014 4015 018 402 402 402 402 402 6 402 8 403 403 2 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 101 4012 4014 4015 018 402 402 402 402 402 6 402 8 403 403 2 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 400.8 101 4012 4014 4015 018 402 402 402 402 402 402 6 402 8 403 403 2 403.4 403.6 403.8 (IC24 H32 O5)+H)+ 400.5 101 4012 4014 4015 018 402 402 402 402 402 402 402 6 402 8 403 403 2 403 403 2 403 403 6 403 8 (IC24 H32 O5)+H)+ (IC24 H | 104 +ESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kfc8-12-5+.d Subtract (2) 22 4012322 ([C24 H32 O5]+H)+ 18 4022363 14 12 14 12 14 12 14 12 14 12 14 12 14 12 14 12 14 12 14 12 15 ((C24 H32 O5]+H)+ 16 402.2363 17 403.3974 18 402.2363 19 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) 403.3974 2746 1 49620.82 3008 1 46747.81 1222 1 19914.69 C24 H32 O5 121 19394.35 1 4422 1 53674.77 19306.41 1 19708.68 1251 1 47733.64

 | 10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
4012322
((C24 H32 O5)+H)+
18-
16-
14-
12-
14-
12-
14-
14-
12-
14-
14-
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12-
14-
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14-
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14-
14

 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2) 401,2322 (1024 H32 05]+H)+ 18 16 18 18 18 18 18 18 18 18 18 18 18 19 1936 1 1936 1 1936 1 1936 1 1936.88 | x10 ⁴ +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
((C24 H32 O5)+H)+
((C24 H32 O5)+H)+
403.3974
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
7 	 x 	 Abund 	 Formula 	 Ion
4.2746 	 1 	 49620.82

 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(C24 H32 03)+H)+
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16
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14 | x10 4 HESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktG8-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
1.4
1.2
1.4
1.2
1.4
1.2
1.4
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
7 2 Abund Formula Ion
1.2746 1 49620.82 10
3.000 1 46747.81 10
2.2222 1 19914.69 C24 H32 O5 (M+H)+
1.936 1 21394.35 10
1.4422 1 53674.77 10
1.4454 1 19708.68 10
1.4454 10
1.4454 1 19708.68 10
1.4454 10
1.4454 1 19708.68 10
1.4454 10 | x10 4 HESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
1.4
1.2
1.4
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1.4
1.2
1.4
1.2
1.4
1.2
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1.4
 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
(IC24 H32 OS]+H)+
14
12
14
08
06
04
02
04
02
04
00.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
<u>x x Abund Formula</u>
12746 1 49620.82
13008 1 46747.81
12746 1 49620.82
13008 1 46747.81
12746 1 219914.69 C24 H32 O5 (M+H)+
1936 1 21394.35
402 25
10
10
10
10
10
10
10
10
10
10 | 0.4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktc8-12-5+.d Subtract (2) 401.2322 401.2322 2 ((C24 H32 OS)+H)+ 18 ((C24 H32 OS)+H)+ 18 ((C24 H32 OS)+H)+ 14 ((C24 H32 OS)+H)+ 15 ((C24 H32 OS)+H)+ 16 ((C24 H32 OS)+H)+ 17 (H) 18 ((C24 H32 OS)+H)+ 19 (H) 19 (H) 11 401.2 12 (H) 13 (H) 14 (H) 15 (H) 16 (H) 17 (H) 18 (H) 19 (H) 19 (H) 108 (H) 11 (H) 122 (H) 12394.35 (H) 14 (H) 15 (H) | 0.4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfc8-12-5+.d Subtract (2) 401.2322 401.2322 1 (C24 H32 O5]+H)+ 18 4 16 (C24 H32 O5]+H)+ 18 (C24 H32 O5]+H)+ 14 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 14 Counts vs. Mass-to-Charge (m/z) 14 Counts vs. Mass-to-Charge (m/z) 15 1 16 1 17 1 18 1 19914.69 C24 H32 O5 1936 1 1222 1 13674.777 1

 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfc8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
1.4
1.4
1.2
1.4
1.4
1.2
1.4
1.4
1.4
1.4
1.4
1.4
1.4
1.4 | 10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfc8-12-5+.d Subtract (2)
401.2322
((C24 H32
O5)+H)+
18
16
14
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14
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14
14
14
14 | 0.4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfc8-12-5+.d Subtract (2) 22-
401.2322
((C24 H32 O5]+H)+ 4012.2363
((C24 H32 O5]+H)+ 18-
14-
12-
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12-
14-
12-
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14-
14 | 10 4 +ESI Scan (0.13-0.14 min, 2 Scana) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
1.8
1.6
1.4
1.4
1.4
1.4
1.4
1.4
1.4
1.4

 | 4 4ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2) 401,2322 ((C24 H32 OS)+H)+ 18 16 17 18 19 19 10 10 10 10 10 11 10 11 10 12 11 10 12 11 10 12 12 12 12 12 12 13 14 15 16 16 17 18 | 104 +ESI Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
18-
16-
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12-
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14 | 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401 2322 (1/22 H32 OS)+H)+ 14- 12- 14- 12- 14- 12- 14- 12- 14- 14- 12- 14- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 14- 12- 12- 14- 12- 14- 12- 14- 14- 14- 12- 14- 12- 12- 14- 12- 12- 12- 12- 12- 12- 12- 12- 12- </th <th>x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
(1C24 H32 OSI+H)+
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04
04</th> <th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
((C24 H32 OS)+H)+
18
16
14
12-
1
400.6 400.8 401 401.2 401.4 401.5 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
72 z Abund Formula Ion
1.2726 1 49620.82
1 4962</th> <th>10⁴ +ESI Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
1.8
1.6
1.4
1.2
1.4
1.2
1.4
1.2
1.4
1.4
1.2
1.4
1.4
1.2
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1.4
1.4
1.4
1.4
1.4</th> <th>HeSi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5t.d Subtract (2) 401.2322 ((C24 H32 O5)+H)+ 401.2323 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+</th> <th>Hesi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2) 401.2322 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 402.2363 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 K List K List X Abund Formula Ion 2746 1 49620.82 1 19914.69 C24 H32 O5 (M+H)+ 1336 1 21394.35 1 19914.69 C24 H32 O5 (M+H)+ 136 1 21394.35 1 121394.35 1
 1 1</th> <th>HeSi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ ((C24 H32 05)+H)+ 402.2363 ((C24 H32 05)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 101 401.2 401.4 401.6 401.8 102 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 11 401.2 401.4 401.6 401.8 402 402.2 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 11 401.2 401.4 401.6 401.8 402 402.2 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ ((M+H)+ (C24 H32 05)+H)+ ((M+H)+ ((M+H)+ (M+H)+ ((M+H)+ ((M+H)+</th> <th>10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
(1C24 H32 O5)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
tk List
2746 1 49620.82 10
2746 1 49620.82 10
3008 1 46747.81 10
2322 1 19914.69 C24 H32 O5 (M+H)+
1936 1 21394.35 10
4422 1 53674.77 10
402.367
402.367
402.2363
(IC24 H32 O5)+H)+
403.3974
403.3974
403.3974
403.4 403.6 403.8
403 403.2 403.4 403.6 403.8
403 403.2 403.4 403.6 403.8
404 405.6 405.8 405
405.2 405.6 405.8 4</th> <th>HESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kto8-12-5+.d Subtract (2) 4012322 (IC24 H32 O5)+H)+ 4012323 (IC24 H32 O5)+H)+ 403.3974 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) kList z</th> <th>4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401 2322 (1224 H32 02) (122 H32 05) (1232) 14- (122 H32 05) 15 (123 H32 05) 16 (124 H32 05) 17 (129 H32 H14) 18 (129 H14) 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 <td< th=""><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OSI+H)+
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18</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
1.4
1.2
1.4
1.4
1.2
1.4
402.2363
(1C24 H32 05]+H)+
403.3974
403.3974
403.3974
403.3974
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403.3974
403.3974
403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2746 1 49520.82
1.3008 1 46747.81
1.2322 1 19914.69 C24 H32 05 (M+H)+
1.1936 1 2 1394.35</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(C24 H32 OS)+H)+
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16
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12
1.
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
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7</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
1.4
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1.2
1.4
1.2
1.4
1.2
1.4
1.2
1.4
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1.4</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(IC24 H32 03]+H)+
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14</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 03]+H)+
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14</th><th>x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 O3]+H)+
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101.8 402
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101.8 402
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14
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101.8 402
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101.5 401.8 402
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102</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OS]+H)+
18
16
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12-
10-
400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2322 1 19914.69 C24 H32 OS
(M+H)+
1.2322 1 19914.69 C24 H32 OS
(M+H)+</th><th>x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
(1C24 H32 O5]+H)+
402.2363
(1C24 H32 O5]+H)+
402.2363
(1C24 H32 O5]+H)+
403.3974
403.3974
403.3974
403.3974
403.3974
403.3974
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403.3974
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403.4 403.6 403.8
counts vs. Mass-to-Charge (m/z)
stak List
<u>7</u> z Abund Formula Ion
4.2746 1 49620.82
8.3008 1 46747.81
1.2322 1 19914.69 C24 H32 O5 (M+H)+
7.1936 1 21394.35
4.427 7 1</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
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400.6 400.8 401 4012 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
rak List
/z z Abund Formula Ion
4.2746 1 49620.82
1 49747.81
1 49620.82
1 19914.69 C24 H32 OS (M+H)+
7.1936 1 21394.35
8.4422 1 53674.77</th><th>x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag-135.0V kt/sl-12-5t-d Subtract (2) 4012322 4012322 (IC24 H32 O5)+H)+ 18 14 12-1 18 14 12-1 14 12-1 14 14 14 12-1 14 14 14 12-1
 14 14 14 15 16 16 16 17 18 18 19 19 12 13008 1 12394.35 13008 1 12394.35 1 1306.1 12394.35 1 1306.1 1306.8 1 1306.8 1 1306.8 1 1306.8 1 1 1 1 1 1 1 1 1 1 <th>10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401 2322
(IC24 H32 D3)+H)+
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14</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS]+H)+
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10</th></th></td<></th> | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
(1C24 H32 OSI+H)+
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 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
((C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.5 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
ak List
72 z Abund Formula Ion
1.2726 1 49620.82
1 4962 | 10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
((C24 H32 O5)+H)+
1.8
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1.4
1.2
1.4
1.2
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1.4
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1.4
1.4 | HeSi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5t.d Subtract (2) 401.2322 ((C24 H32 O5)+H)+ 401.2323 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 O5)+H)+
 | Hesi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2) 401.2322 ((C24 H32 O5)+H)+ ((C24 H32 O5)+H)+ 402.2363 ((C24 H32 O5)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 K List K List X Abund Formula Ion 2746 1 49620.82 1 19914.69 C24 H32 O5 (M+H)+ 1336 1 21394.35 1 19914.69 C24 H32 O5 (M+H)+ 136 1 21394.35 1 121394.35 1 | HeSi Scan (0.13-0.14 min, 2 Scan) Frag=135.0V kt68-12-5+.d Subtract (2) 401.2322 ((C24 H32 05)+H)+ ((C24 H32 05)+H)+ 402.2363 ((C24 H32 05)+H)+ 403.3974 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 400.8 101 401.2 401.4 401.6 401.8 102 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 11 401.2 401.4 401.6 401.8 402 402.2 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ 400.6 11 401.2 401.4 401.6 401.8 402 402.2 402.4 102.6 402.8 403 403.2 403.4 403.6 403.8 ((C24 H32 05)+H)+ ((M+H)+ (C24 H32 05)+H)+ ((M+H)+ ((M+H)+ (M+H)+ ((M+H)+ | 10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401.2322
(1C24 H32 O5)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
tk List
2746 1 49620.82 10
2746 1 49620.82 10
3008 1 46747.81 10
2322 1 19914.69 C24 H32 O5 (M+H)+
1936 1 21394.35 10
4422 1 53674.77 10
402.367
402.367
402.2363
(IC24 H32 O5)+H)+
403.3974
403.3974
403.3974
403.4 403.6 403.8
403 403.2 403.4 403.6 403.8
403 403.2 403.4 403.6 403.8
404 405.6 405.8 405
405.2 405.6 405.8 4 | HESI Scan (0.13-0.14 min, 2 Scans) Frage 135.0V kto8-12-5+.d Subtract (2) 4012322 (IC24 H32 O5)+H)+ 4012323 (IC24 H32 O5)+H)+ 403.3974 400.6 400.8 401 4012 4014 4016 4018 402 4022 4024 4026 402.8 403 4032 403.4 403.6 403.8 Counts vs. Mass-to-Charge (m/z) kList z | 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt/c8-12-5+.d Subtract (2) 401 2322 (1224 H32 02) (122 H32 05) (1232) 14- (122 H32 05) 15 (123 H32 05) 16 (124 H32 05) 17 (129 H32 H14) 18 (129 H14) 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 1 1936 <td< th=""><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OSI+H)+
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18</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
1.4
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402.2363
(1C24 H32 05]+H)+
403.3974
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403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2746 1 49520.82
1.3008 1 46747.81
1.2322 1 19914.69 C24 H32 05 (M+H)+
1.1936 1 2 1394.35</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
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7</th><th>x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
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1.4</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(IC24 H32 03]+H)+
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401 2322
(1C24 H32
03]+H)+
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401.2322
(1C24 H32 O3]+H)+
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102</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OS]+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2322 1 19914.69 C24 H32 OS
(M+H)+
1.2322 1 19914.69 C24 H32 OS
(M+H)+</th><th>x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
(1C24 H32 O5]+H)+
402.2363
(1C24 H32 O5]+H)+
402.2363
(1C24 H32 O5]+H)+
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counts vs. Mass-to-Charge (m/z)
stak List
<u>7</u> z Abund Formula Ion
4.2746 1 49620.82
8.3008 1 46747.81
1.2322 1 19914.69 C24 H32 O5 (M+H)+
7.1936 1 21394.35
4.427 7 1</th><th>x10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
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400.6 400.8 401 4012 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
rak List
/z z Abund Formula Ion
4.2746 1 49620.82
1 49747.81
1 49620.82
1 19914.69 C24 H32 OS (M+H)+
7.1936 1 21394.35
8.4422 1 53674.77</th><th>x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag-135.0V kt/sl-12-5t-d Subtract (2) 4012322 4012322 (IC24 H32 O5)+H)+ 18 14 12-1 18 14 12-1 14 12-1 14 14 14 12-1 14 14 14 12-1 14 14 14 15 16 16 16 17 18 18 19 19 12 13008 1 12394.35 13008 1 12394.35 1 1306.1 12394.35 1 1306.1 1306.8 1 1306.8 1 1306.8 1 1306.8 1 1 1 1 1 1 1 1 1 1 <th>10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
401 2322
(IC24 H32 D3)+H)+
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401.2322
((C24 H32 OS]+H)+
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401.2322
(1C24 H32 OSI+H)+
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18 | x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
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402.2363
(1C24 H32 05]+H)+
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403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2746 1 49520.82
1.3008 1 46747.81
1.2322 1 19914.69 C24 H32 05 (M+H)+
1.1936 1 2 1394.35 | x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(C24 H32 OS)+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
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 | x10 4 +ESI Scan (0.13-0.14 min. 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 05]+H)+
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1.4 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(IC24 H32 03]+H)+
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14 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kto8-12-5+.d Subtract (2)
401 2322
(1C24 H32 03]+H)+
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14 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 O3]+H)+
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 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V ktds-12-5+.d Subtract (2)
401.2322
(1C24 H32 OS]+H)+
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400.6 400.8 401 401.2 401.4 401.6 401.8 402 402.2 402.4 402.6 402.8 403 403.2 403.4 403.6 403.8
Counts vs. Mass-to-Charge (m/z)
3008 1 46747.81
1.2322 1 19914.69 C24 H32 OS
(M+H)+
1.2322 1 19914.69 C24 H32 OS
(M+H)+ | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
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(1C24 H32 O5]+H)+
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<u>7</u> z Abund Formula Ion
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8.3008 1 46747.81
1.2322 1 19914.69 C24 H32 O5 (M+H)+
7.1936 1 21394.35
4.427 7 1 | x10 ⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kfd8-12-5+.d Subtract (2)
401.2322
((C24 H32 OS)+H)+
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Counts vs. Mass-to-Charge (m/z)
rak List
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1 49747.81
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1 19914.69 C24 H32 OS (M+H)+
7.1936 1 21394.35
8.4422 1 53674.77 | x10 4 +ESI Scan (0.13-0.14 min, 2 Scans) Frag-135.0V kt/sl-12-5t-d Subtract (2) 4012322 4012322 (IC24 H32 O5)+H)+ 18 14 12-1 18 14 12-1 14 12-1 14 14 14 12-1 14 14 14 12-1 14 14 14 15 16 16 16 17 18 18 19 19 12 13008 1 12394.35 13008 1 12394.35 1 1306.1 12394.35 1 1306.1 1306.8 1 1306.8 1 1306.8 1 1306.8 1 1 1 1 1 1 1 1 1 1 <th>10⁴ +ESI Scan (0.13-0.14 min, 2 Scans) Frag=135.0V kt68-12-5+.d Subtract (2)
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 | 9.4277 1 20782.95 | 12// 1 20/02.95 | 1 20/02.23 | 92/7 1 20/82.95

 | 4277 1 20782.95
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 | 8.4251 1 47733.64
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 | 0.4351 1 42411.8 | 0.4351 1 42411.8 | 7.4383 1 18953 54 | 20.4351 1 42411.8
 | 0.4351 1 42411.8 | 3.4.51 | 1254 1 12344.0 | | 12// 1 20/02.95

 | .4277 1 20782.95

 | 1.4277 1 20782.95
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 | 9.4277 1 20782.95 | 3.4277 1 20782.95 | 3.4277 1 20782.95 | 1.4277 1 20782.95 | 1 47733.64 277 1 20782.95
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 | 9.4277 1 20782.95 | 12// 1 20/62.95 | 1 20/02.73 | 42/7 1 20/82.95

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 | 8.4251 1 47733.64
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 | 0.4331 1 42411.8 | 17 4202 1 10022 54
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 | 7.4292 1 10052.54 | 0.4393 1 19052 54 | 7.4383 1 18953.54 |
 | 0.4351 1 42411.8 | | 4254 1 42444.0 | | 1 20/02.95

 | .4277 1 20782.95

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 | 9.4277 1 20782.95 | 9.4277 1 20782.95 | A4277 1 20782.95 | 1.4277 1 20782.95 | 1 47733.64 1277 1 20782.95
 | 4251 1 47733.64 4277 1 20782.95

 | 9.4277 1 20782.95 | 12// 1 20/02.95 | 1 20/02.73 | 42// 1 20/82.95

 | 4277 1 20782.95
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 | | 17 4292 1 19052 54
 | 17.4202 1 (0002.54 | 7.4202 4 10002.54 | 1 12/11.0 |
 | 7.4292 1 (2002) 2.4 | 7 4393 1 19052 54 | 7,4383 1 18953.54 |
 | V. 7331 1 Y2Y11.0 | | 4254 1 124410 | | 1 20/02/35

 | .4277 1 20782.95

 | 1.4277 1 20782.95
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 | 9.4277 1 20782.95 | 9.4277 1 20782.95 | 3.4277 1 20782.95 | 1.4277 1 20782.95 | 1 47733.64 1277 1 20782.95
 | 4251 1 47733.64 4277 1 20782.95

 | 9.4277 1 20782.95 | 1 20/02.95 | 1 20/02.33 | 42// 1 20/82.95

 | 4277 1 20782.95
 | 4277 1 20782.95 | 4251 1 47733.64 4277 1 20782.95

 | 8.4251 1 47733.64 9.4277 1 20782.95

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 | | 7/2022 1 10022 64
 | | 7.4292 4 10522 54 | 1 4003 4 (6050 54) |
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 | | 47444 1 197911.0 | 4251 1 42444.0 | | 1 20/02/35

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 | 9.4277 1 20782.95 | 1 20/02/35 | 1 20/02.55 | 42// 1 20/82.95

 | 14277 1 20782.95
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 | 8.4251 1 47733.64 9.4277 1 20782.95

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 | 3.4251 1 47733.64 9.4277 1 20782.95 | 9.4954 1 19708.68 3.4251 1 47733.64 3.4277 1 20782.95 | 9.4454 1 19708.68 3.4251 1 4773.64 1.4277 1 20782.95 | 9.4454 1 19708.68
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| 0.11737 1 4001.0 |

 | | 17 4292 1 19052 54
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 | 4277 1 20782.95

 | 0.4277 1 20782.95
 | 9.4277 1 20782.95

 | 9.4277 1 20782.95 | 9.4277 1 20782.95 | 0.4277 1 20782.95 | 3.4277 1 20782.95 | 1 47733.64 1277 1 20782.95
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 | 4277 1 20782.95
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 | 8.4251 1 4773.64 9.4277 1 20782.95

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 | .4251 1 47733.64 .4277 1 20782.95 | 4251 1 47733.64 4277 1 20782.95 421 1 4010 | .4251 1 47733.64 .4277 1 20782.95
 | 3.4251 1 4773.64 9.4277 1 20782.95 | 9.4454 1 19708.68 3.4251 1 47733.64 4.4277 1 20782.95 | 9.4454 1 19708.68 3.4251 1 47733.64 4.4277 1 20782.95 3.425 - - | 9.4454 1 19708.68 3.4251 1 47733.64 9.4277 1 20782.95 1.427 1 20782.95
 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 1.4274 1 20782.95 | 9.4454 1 19708.68 3.4251 1 47733.64 9.4277 1 20782.95 1 4714.0 1 | 9.4454 1 19708.68
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 | 1 19708.08 8.4251 1 47733.64 9.4277 1 20782.95 1 4100.000 1000.000 | 8.4251 1 47733.64
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 |
| 7.4383 1 18953.54 | (4303 1 118353.54

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 | | 2,4383 1 18953.54 | 4383 1 18953.54 | 4351 1 42411.8 4383 1 18953.54 | 4277 1 20702.95 4351 1 42411.8 4383 1 18953.54

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 | 9.4277 1 20782.95
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 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54

 | 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54 | 4351 1 42411.8 4383 1 18953.54 | 1351 1 42411.8
1383 1 1895.54 | 4277 1 20/82.95 4351 1 42411.8 4383 1
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 | 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 1895.54

 | 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 7.4383 1 18953.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54
 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54
 | .4251 1 4773.64 .4277 1 20782.95 .4351 1 42411.8 .4383 1 1.8953.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4383 1 18953.54
 | 1 19708.08 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54 | 9.4454 1 19708.68 3.4251 1 47733.64 9.4277 1 20782.95 3.4351 1 42411.8 4.4383 1 18953.54 | 0.4454 1 19708.68 0.4251 1 47733.64 0.4277 1 20782.95 0.4351 1 42411.8 1.4383 1 18953.54 | 9.4454 1 19708.68 3.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 7.4383 1 18953.54
 | 9.4454 1 19708.68 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 7.4383 1 18953.54 | 9.4454 1 19708.68 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54 | 9.4454 1 19708.68 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 1895.54
 | 9.4757 1 19708.08 8.4251 1 47773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 1895.54 | 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54 | 0.4277 1 20782.95 0.4351 1 42411.8 1 4983 1 1 19953.54 1 | 4277 1 20782.95 44351 1 42411.8 1 18953.54 1 | 0.4251 1 4/733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4383 1 18953.54
 |
| 7 4292 1 10052 54 |

 | 7,700 1 110955,54 | 27,7303 1 10933.54
 | 1,10953.54 | 1,10953.54 | 1,10935.54 | 7.303 1 10333.54
 | 1,10953.54 | 1,105 1 10535,34 | * ******* | 2/.7303 1 10753.54
 | (1200) 1 1 1 10000 5 56 | 14292 1 10052 54 | 4292 1 19953 54 | 4351 1 42411.8 | 427 1 20762.93 4351 1 42411.8 4292 1 10072.54

 | 4277 1 20782.95 4351 1 42411.8 4382 1 1982.54

 | 3.4277 1 20782.95 5.4351 1 42411.8 1.4282 1 1965.8.4
 | 9.4277 1 20782.95
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1 4922 1 19052.54 | 9.4277 1 20782.95 5.4351 1 42411.8 1.4282 1 19852.64 | 9.4277 1 20782.95 5.4351 1 42411.8 4.4392 1 10952.64 | 3.4277 1 20782.95 5.4351 1 42411.8 4382 1 1802.2 fc | 4251 1 47733.64 4277 1 20782.95 1351 1 42411.8 1292 1 19952.64
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 | 4277 1 20782.95 4351 1 42411.8 4282 1 1985.5.6
 | 4277 1 20782.95 4351 1 42411.8 | .4251 1 4773.64 .4277 1 20782.95 .4351 1 42411.8 .4282 1 1985.54

 | 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8

 | 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 42822 1 18052.64 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4282 1 1095.54
 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1282 1 1005.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1282 1 1905.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4282 1 1905.54
 | .4251 1 4773.64 .4277 1 20782.95 .4351 1 42411.8 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1 1005.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1282 1 1985.54
 | 3.137 1 15708.08 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 | 9.4454 1 19708.68 3.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 1.4282 1 19672.64 | 0.4454 1 19708.68 0.4251 1 4773.64 0.4277 1 20782.95 0.4351 1 42411.8 1 19972.64 | 9.4454 1 19708.68 3.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 1 1992.64
 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 4.4892 1 1907.5 f. | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 1 1907.64 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4392 1 1902.54 | 9.4454 1 19708.68 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4392 1 19073.64
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1 1995 54 | 0.4251 1 14773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4392 1 1092.5 €
 |
| 7 4292 1 10052 54 |

 | 7,4303 1 118953,54 | 27,7303 1 10933.54
 | 1/1000 1 10003.54 | 7.4303 1 18953.54 | 7.4303 1 118953.54 | /.4303 1 10953.54
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 | (9303 1111895354 | 14292 1 10052 54 | 4302 1 1052 5 | 4351 1 42411.8 | 4277 1 20762.93 4351 1 4241.8 4282 4 4007.54

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1007.57

 | 4277 1 20782.95 4351 1 42411.8 4282 1 1005.05
 | 4277 1 20782.95 4351 1 42411.8 | .4251 1 4773.64 .4277 1 20782.95 .4351 1 42411.8 .4277 1 10767.64

 | 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8

 | 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8
 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1282 1 4005.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 4282 1 1005.54 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8
 | .4251 1 47733.64 .4277 1 20782.95 .4351 1 42411.8 .4277 1 10767.64 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8 1282 1 10075.64 | 4251 1 47733.64 4277 1 20782.95 4351 1 42411.8
 | 3.137 1 15708.08 8.4251 1 47733.64 9.4277 1 20782.95 5.4351 1 42411.8 | 9.4454 1 19708.68 3.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 1.4382 1 10972.64 | 9.4454 1 19708.68 9.4454 1 19708.68 9.4251 1 4773.64 9.4277 1 20782.95 9.4351 1 42411.8 1.4392 1 10972.64 | 9.4454 1 19708.68 3.4251 1 4773.64 9.4477 1 20782.95 5.4351 1 42411.8 1 4020 4
 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 4.4992 4 9 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 5.4351 1 42411.8 1 42902.56 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 1 4292.5 1 | 9.4454 1 19708.68 8.4251 1 4773.64 9.4277 1 20782.95 6.4351 1 42411.8 4.4992 4 4000.5 (c)
 | 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4322 4 4000.5 f. | 8.4251 1 47733.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4392 4 4092.54 | 1 1773.04 2,4277 1 2,751 1 4,752 1 4,753 1 4,753 1 4,753 1 4,753 1 1 1,057.04 | 14277 1 20782.95
(4351 1 42411.8
1 1075.54 | 0.4251 1 14773.64 9.4277 1 20782.95 6.4351 1 42411.8 7.4392 4 4002.54
 |

Figure S68. HRESIMS spectrum of compound 2.

Data Filenar Sample Type Instrument Acq Method IRM Calibra Comment	ne e Name tion S	e Status	kfc8-13-13.d Sample Instrument 1 s.m Success	Sample Name Position User Name Acquired Time DA Method	kfc8-13-13 P1-A5 10/27/2022 3:38:48 PM PCDL.m
Sample Grou Acquisition Version	up SW	6200 si Q-TOF	eries TOF/6500 series B.05.01 (B5125.2)	Info.	
Fragmen	tor Vo	oltage	Collision Energy	Ionization Mode	
6- 5- 4- 3- 2- 1- 0- 4	68.6		50 (10) 10) 10) 100	470.2603 ([C26 H38 06]+Na)+	471.2631 ((C26 H38 O6)+Na)+
Peak List	00.0, -	400 4	Count	s vs. Mass-to-Charge (m/z)	8 4/1 4/1.2 471.4 471.6 471.8
m/z	Z	Abund	Formula	Ion	
77.038	1	715.02			
115.054	1	891.82			
128.0618	1	1282.71			
165.0692	1	483.91			
167.0841	1	501.32	626 1120 06	(11.11.2)	
470.2603	1	1448.57	C26 H38 06	(M+Na)+ (M+Na)+	
485.2298	1	1013.63	520110000	(irrita)+	
922.0098	1	594.93			
Formula Cal	Min	or Element Max	Limits		
С		3 60			
Н		0 150			
O Formula Cal	culat	0 30			
Formula		Calculated	Mass Calculat	edMz Mz	Diff. (mDa) Diff. (ppm) DBE
C26 H38 O6	_		446.2668	469.2561 469.256	4 -0.30 -0.64 8.0000
C26 H38 O6	port	-	446.2668	469.2561 469.256	4 -0.30 -0.64 8.000
- Agilent	Techr	iologies		Page 1 of 1	Printed at: 3:45 PM on: 10/27/2

Figure S69. HRESIMS spectrum of compound 3.



Figure S70. HRESIMS spectrum of compound 4.

s tatus 6200 se	Kfc8-10C-3.d Sample Instrument 1 s.m Success	Sample Name Position User Name Acquired Time DA Method	Kfc8-10C-3 P1-A1 6/8/2022 3:00:32 PM PCDL.m
Q-TOP B	.us.u1 (B5125.2)		
ltage	Collision Energy	Ionization Mode	
470.5 4	([C25 71 471.5 472 Counts	172.2171 H36 O6]+K)+ ([C25 H36 O6] (C25 H36	+K)+ 474.2173 ([C25 H36 O6]+K)+ 473.5 474 474.5
Abund	Formula	Ion	
26849.74			
15758.02	1		
13477.12			
29819.38			
68919.59	C25 H36 O6	(M+K)+	
18331.95	C25 H36 O6	(M+K)+	
15487.79			
13589.02			
or Element L	imits		
3 200	-		
0 500			
0 20			
0 30			
or Results	lass Calculate	dMz Mz	Diff (mDa)
	6200 ser Q-TOF B Itage 10-0.12 min, 2 S ((C2 470.5 4 Abund 26849.74 15758.02 13477.12 10989.4 29819.38 68919.59 18331.95 15487.79 11676.07 13589.02 or Element L Max 3 200	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)	Info. G200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Jage Collision Energy Ionization Mode Est 0 2 Est 1:0-0.12 min, 2 Scana) Frag=135.0V K/c8-10C-3.d Subtract 471.213 471.213 ([C25 H36 O6]+K)+ 470.5 471 471.5 472 470.5 471 471.213 ([C25 H36 O6]+K)+ 470.5 471 471.5 472 472.2171 ([C25 H36 O6] ([C25 H36 O6]+K)+ ([C25 H36 O6] 470.5 471 471.2 100 26849.74 100 13477.12 100 10989.4 100 29819.38 68919.59 68919.59 C25 H36 O6 (M+K)+ 13381.95 C25 H36 O6 (M+K)+ 13589.02 100 100 13589.02 100 100 13589.02 100 100 13589.02 100 100 13589.02 100 100

Figure S71. HRESIMS spectrum of compound 5.

hastrument Name Instrument I Mark Instrument I Mark Instrument I User Name Acquired Time 8/3/2022 2:25:06 PM DA Method S.m. Acquired Time 8/3/2022 2:25:06 PM DA Method PCDLm PC METHOD PCDLM	Answer Sample Position P1.42 Nethod Sim Acquired Time 8/3/2022 2:25:06 PM Mailbration Status Success DA Method PCDL Somment Success DA Method PCDL Somment Success DA Method PCDL Sample Group Info. Scousition SW S200 series TOF/6500 series Ser Spectra Gotto Status Success Success Jate Status Gotto Status Gotto Status Success Jate Status Gotto Status Gotto Status Gotto Status Ser Spectra Gotto Status Gotto Status Gotto Status Jate Status (C28 H40 OG) NH4)+ Gotto Status Gotto Status Gotto Status Gotto Status Substatuct Gotto Status Gotto Status Status Gotto Status Gotto Status Gotto Status Gotto Status Gotto Status Status Gotto Status Gotto Status Gotto Status Gotto Status Gotto Status Status Gott	Instrument Name Jainpie Position PI-A2 Instrument Name Instrument I User Name 8/3/2022 2:25:06 PM Kin Method Sm Acquired Time 8/3/2022 2:25:06 PM Somment Success DA Method PCDL Somment Success DA Method PCDL Sample Group Info. Success PCDL Sample Group Collision Energy Ionization Mode ES Jeer Spectra Collision Energy Ionization Mode ES 101 State 0 ES Collision Energy Ionization Mode 11 Collision Energy Ionization Mode ES Collision Energy Ionization Mode 11 12 0 Collision Energy Ionization Mode ES 110 Collision Energy Ionization Mode Ionization Mode Ionization Mode 12 (1228 H40 OB(HVH)+ (1228 H40 OB(HVH)+ (1228 H40 OB(HVH)+ Ionization Mode 12 Ionization Mode Ionization Mode Ionization Mode	$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Instrument Name Instrument I User Name Position P1-A2 Acq Method S.m Acquired Time 8/3/2022 2:25:06 PM Acq Method S.m Acquired Time 8/3/2022 2:25:06 PM Comment Buccess DA Method PCDL.m Sample Group Info. Acquisition Status G200 series Comment G200 series TOF/6500 series Comment EST User Spectra User Spectra (C28 H40 OP)=N14()+ 490.3162 (C28 H40 OP)=N14()+ 490.3162 (C28 H40 OP)=N14()+ 492.3222 493.3162 (C28 H40 OP)=N14()+ 492.3222 (C28 H40 OP)=N14()+ 492.3162 493.3162 Counts vs. Masses-Charge (m2) Counts vs. Masses-Charge (m2) 600.3162 1 1 Ca	Instrument Nan		kfc8-12-4.d	Sample Name	kfc8-12-4
Key Method S.m. Ocean RM Calibration Status Docess DA Method PCDL.m Sample Group Info. Counser Time 8/3/2022 2:25:06 PM Sample Group DA Method PCDL.m Sample Group G200 series Q-TOF B.05.01 (BS125.2) Jeer Spectra Sample Group Collision Energy Ionization Mode 315 0 ESI Sample Group Info. 410 15 Collision Energy Ionization Mode ESI 51 1 Fission (0:19-0.20 min, 2 Scana Frage=135.0V ktds-124.4d Subtract 493.312 (C28 H40 OB)+NH4)+ 492.322 40 495.5 490.02 490.25 490.75 491.4912 (C28 H40 OB)+NH4)+ 40 (C28 H40 OB)+NH4)+ (C28 H40 OB)+NH4)+ 492.352.492.55 493.3 52 1 1.3277.55 Counts vs. Mass-to-Churge (m2) 492.25 492.25 492.55 493.3 53 1 1.7277.55 C28 H40 O6 (M+NH4)+ 1.92.3 493.15 1.93.2 493.15 1.93.2	King Method S.m. Acquired Time 8/3/2022 2:25:06 PM RM Calibration Status Buces DA Method PCDLm ample Group Info. Counsered Time 8/3/2022 2:25:06 PM ample Group Counsered Time 8/3/2022 2:25:06 PM asymple Group Info. Counsered Time 9/3/2022 2:25:00 PM Joint Counsered Time Counsered Time 9/3/2022 2:25:00 PM 0 Joint Counsered Time Counsered Time 9/3/2022 2:25:00 PM 0 Joint Counsered Time Counsered Time PCDLm 0	Key Method S.m. Acquired Time 8/3/2022 2:25:06 PM RM Calibration Status Docess DA Method PCDL.m Sample Group Info. Counsent PCDL.m Sample Group Counsers OA Method PCDL.m Sample Group Counsers Counsers Counsers Sample Group Counsers Counsers Counsers Status Q-TOF B.05.01 (BS125.2) DA Method PCDL.m	Acq Method Smith Acquired Time 8/3/2022 2:25:06 PM IRM Calibration Status Dicess DA Method PCDL.m Sample Group Info. Acquired Time 8/3/2022 2:25:06 PM User Spectra Q-10F B.05.01 (BS125.2) Info. User Spectra (C28 H40 06) ESI *10	Acq Method S.m. Acquired Time B/J/2022 2:25:06 PM IRM Calibration Status Docess DA Method PCDL.m Sample Group Info. Acquisition SW 6200 series O.TOF B.05.01 (BS125.2) User Spectra Transmitter Voltage Collision Energy Info. Acquisition You Collision Energy Onization Mode EST Collision Energy Info. Acquisition You Collision Energy Info. Cols		ie	Instrument 1	Position	P1-A2
RM Calibration Status Dices DA Method PCDLm Comment Info. Sample Group (cupuistion Status) Collision Energy Q-TOF B.05.01 (B5125.2) Info. Ster Spectra Est Collision Energy 0 Lonization Mode Est Store Spectra (C28 H40 OC)+NH4)+ 492.3222 (C28 H40 OC)+NH4)+ 468:5 489:75 490 490:25 490:5 490:75 491 491:3192 (C28 H40 OC)+NH4)+ Vical H40 CO Counts vs. Mass-to-Churge (m2) Counts vs. Mass-to-Churge (m2) Vical H40 CO Counts vs. Mass-to-Churge (m2) 492:3222 (C28 H40 OC)+NH4)+ 1 Counts vs. Mass-to-Churge (m2) 492:322 (C28 H40 OC)+NH4)+ 1 Counts vs. Mass-to-Churge (m2) 492:492:5 492:5 492:5 492:5 493:7 493 viait 1 1 1 1 1 90:3162 1 6:26633.81 C28 H40 O6 (M+NH4)+ 1	RM Calibration Status Dicess DA Method PCDLm Somment Info. sample Group Collision Energy Info. counters Q-TOF B.05.01 (B5125.2)	RM Calibration Status Dicess DA Method PCDL/m Somment Info. sample Group Collision Energy Lnfo. scussion SW 6200 series TOF/6500 series Jeser Spectra Status 0 Voltage 0 1 1 490 - 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Comment DX Method PCDLm Sample Group Info. Acquisition SW 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)	TRM Calibration Status Data Method PODUL PODUL Sample Group Acquisition SW 6200 series TOF/6500 series Version Info. Acquisition SW 6200 series TOF/6500 series Version Collision Energy Info. User Spectra Fragmentor Voltage 0 Est Version Collision Energy Info. x10 ⁶ 13 Collision Energy Info. x10 ⁶ Est Collision Energy Info. x10 ⁶ Issatus 490.3162 Issatus x10 ⁶ Est Scan (0.19-0.20 min, 2 Scans) Frage-115.0V Mc8-124.d. Subtract 490.3162 x10 ⁶ Issatus (IC28 H40 O6]+NH4)+ (IC28 H40 O6]+NH4)+ 492.3222 0	Acq Method		s.m	Acquired Time	8/3/2022 2:25:06 PM
$\frac{1000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ $\frac{10000}{1000}$ 1	Zomment Info. Sample Group tension 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Jac 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Jer Spectra Image: Comparison of the series of the s	Somment Info. Sample Group Kersion 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Jate Spectra Jer Spectra 1^{451} Scan (0.19-0.20 min, 2 Scans) Frage=135.07 ktGs12.4.4 Subtract 490.3102 (C28 H40 06]+NH4)+ (C28 H40	Info. Sample Group Acquisition SW G-TOF B.05.01 (B5125.2) Info. Segmentor Voltage 0 Collision Energy 0 Info. Segmentor Voltage 0 Collision Energy 0 Info. Colspan: 2 Colspan= 2 <t< th=""><th>Comment Info. Sample Group Acquisition SW 5200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra 135 Collision Energy 135 Tonization Mode ESI 135 Collision Energy 135 Tonization Mode ESI 135 Collision Energy (C28 H40 Og!NH4)+ ESI 140 135 Collision Energy (C28 H40 Og!NH4)+ 490.3102 (C28 H40 Og!NH4)+ 140 (C28 H40 Og!NH4)+ 492.3222 (C28 H40 Og!NH4)+ 492.3222 (C28 H40 Og!NH4)+ 140 1/32/277.5 Counts vs. Mass-to-Charge (m/2) 492.492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.75 493 Minits in the set of th</th><th>IRM Calibration</th><th>Status</th><th>Success</th><th>DA Method</th><th>PCDL.m</th></t<>	Comment Info. Sample Group Acquisition SW 5200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra 135 Collision Energy 135 Tonization Mode ESI 135 Collision Energy 135 Tonization Mode ESI 135 Collision Energy (C28 H40 Og!NH4)+ ESI 140 135 Collision Energy (C28 H40 Og!NH4)+ 490.3102 (C28 H40 Og!NH4)+ 140 (C28 H40 Og!NH4)+ 492.3222 (C28 H40 Og!NH4)+ 492.3222 (C28 H40 Og!NH4)+ 140 1/32/277.5 Counts vs. Mass-to-Charge (m/2) 492.492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.5 492.75 493 Minits in the set of th	IRM Calibration	Status	Success	DA Method	PCDL.m
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Spectra Ser Spectra Violation SW Collision Energy 0 Ionization Mode ESI 135 0 0 ESI 140 0 19-020 min, 2 Scamp Frag=135.0V ktdsh12.4.d Subtract 490.3182 (IC28 H40 06]+NH4)+ 491.25 490.25 490.25 490.25 490.25 490.25 490.25 492.5</th> <th>Sample Group Acquisition SW Enfo. 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Ser Spectra Ser Spectra Ser Spectra (C28 H40 C6) HM47 Subscription Mode ESI Subscription Mode ESI Collision Energy 105 O Inization Mode ESI Collision Energy 105 A00 119-020 min, 2 Scams Fing=135.0V Mc8-12-4.d Subtract 400.3162 (C28 H40 C6]+NH47+ (C28 H40 C6]+NH47+</th> <th>Sample Group Acquisition SW 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra Vision Collision Emergy 0 Ionization Mode ESI 100 135 Collision Emergy 0 Ionization Mode ESI 100 135 Collision Emergy 0 Ionization Mode ESI 100 1400 CB(HH4)+ 491 3192 (C28 H40 OB(HH4)+ 492 3222 (C28 H40 OB(HH4)+ 489.5 489.75 490.405 490.75 491.491.25 491.75 492 3222 (C28 H40 OB(HH4)+ 72.2897 1 173277.75 Formula Counts vs. Masses-Ohung (m2) 100 492.322 492.5 492.75 493.302 101 173277.75 Formula 173.2897.71 195.15.15 C28 H40 O6 (M+NH4)+ 193.3102 1 1755.15 C28 H40 O6 (M+NH4)+ 193.3122 1 195.914.55 1 101 102 107 0.00 193.3122 1 195.914.55 1 100.61 (M+NH4)+ 103.45 100.61 101 102 107 <th< th=""><th>Sample Group Acquisition SW Callo series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra Vision Collision Energy 0 Donization Mode Est User Spectra Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Collision Energy 0 Donization Est 0 Donization Est 0 Donization Est 0 <t< th=""><th>Comment</th><th></th><th>The second s</th><th></th><th></th></t<></th></th<></th>	Bandbel Group Locquisition SW 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Ser Spectra Ser Spectra Violation SW Collision Energy 0 Ionization Mode ESI 135 0 0 ESI 140 0 19-020 min, 2 Scamp Frag=135.0V ktdsh12.4.d Subtract 490.3182 (IC28 H40 06]+NH4)+ 491.25 490.25 490.25 490.25 490.25 490.25 490.25 492.5	Sample Group Acquisition SW Enfo. 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) Ser Spectra Ser Spectra Ser Spectra (C28 H40 C6) HM47 Subscription Mode ESI Subscription Mode ESI Collision Energy 105 O Inization Mode ESI Collision Energy 105 A00 119-020 min, 2 Scams Fing=135.0V Mc8-12-4.d Subtract 400.3162 (C28 H40 C6]+NH47+ (C28 H40 C6]+NH47+	Sample Group Acquisition SW 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra Vision Collision Emergy 0 Ionization Mode ESI 100 135 Collision Emergy 0 Ionization Mode ESI 100 135 Collision Emergy 0 Ionization Mode ESI 100 1400 CB(HH4)+ 491 3192 (C28 H40 OB(HH4)+ 492 3222 (C28 H40 OB(HH4)+ 489.5 489.75 490.405 490.75 491.491.25 491.75 492 3222 (C28 H40 OB(HH4)+ 72.2897 1 173277.75 Formula Counts vs. Masses-Ohung (m2) 100 492.322 492.5 492.75 493.302 101 173277.75 Formula 173.2897.71 195.15.15 C28 H40 O6 (M+NH4)+ 193.3102 1 1755.15 C28 H40 O6 (M+NH4)+ 193.3122 1 195.914.55 1 101 102 107 0.00 193.3122 1 195.914.55 1 100.61 (M+NH4)+ 103.45 100.61 101 102 107 <th< th=""><th>Sample Group Acquisition SW Callo series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra Vision Collision Energy 0 Donization Mode Est User Spectra Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Collision Energy 0 Donization Est 0 Donization Est 0 Donization Est 0 <t< th=""><th>Comment</th><th></th><th>The second s</th><th></th><th></th></t<></th></th<>	Sample Group Acquisition SW Callo series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra User Spectra Vision Collision Energy 0 Donization Mode Est User Spectra Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Collision Energy 0 Donization Mode Est Collision Energy 0 Donization Mode Est Vision Collision Energy 0 Donization Mode Collision Energy 0 Donization Est 0 Donization Est 0 Donization Est 0 <t< th=""><th>Comment</th><th></th><th>The second s</th><th></th><th></th></t<>	Comment		The second s		
Year Spectra Fragmentor Voltaging Collision Energy 0 Disization Mode Est 10 490.3162 490.3162 10 (C28 H40 06]+NH4)+ 492.3227 10 490.5 490.75 490.490.25 490.5 491.5 491.5 491.5 491.5 492	Pragmentor Voltag Collision Energy Dirization Mode Est x10 ⁵ 4501 Scan (0.19-0.20 min, 2 Scans) Frag=135.0V ktGe.12.4.d. Subtract 490.3102 (IC28 H40 Oc]+NH4)+ 490.3162 (IC28 H40 Oc]+NH4)+ 492.3222 (IC28 H40 Oc]+NH4)+ 495.5 490.75 490.490.25 490.75 495.5 490.75 490.490.25 490.75 491.3192 (IC28 H40 Oc]+NH4)+ 492.3222 (IC28 H40 Oc]+NH4)+ 492.3222 (IC28 H40 Oc]+NH4)+ 493.5 490.25 490.25 490.5 490.75 492.492.25 492.25 492.55 492.75 492 ***********************************	Pragmentor Voltage (1) Collision Energy 0 Dirization Mode Esi x10 ⁴ +ESI Scan (0.19-0.20 min, 2 Scans) Frage=135.0V kIc8-12.4.d Subtract 490.3162 (IC28 H40 OG]+NH4)+ 490.3162 (IC28 H40 OG]+NH4)+ 490.5 489.75 490 490.25 490.5 490.15 491.51 491.225 491.5 492.2222 (IC28 H40 OG]+NH4)+ 489.5 489.75 490 490.25 490.55 490.15 491.55 491.57 492 492.25 492.25 492.5 492.55 492. Variation of the state	Yard Spectra Program Collision Collision Energy Collision Collision <thcolision< th=""> <thcolision< th=""> <thco< th=""><th>Yard Spectra Prignetiz Collision Energy Doization Mode 10 0 Second 10 9 (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ 492.3222 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 489.5 489.75 490.499.25 490.5 490.75 491.491.25 491.5 491.5 492.5 492.5 492.5 492.5 492.75 492. Particity 10 200.25 100.25 490.5 490.75 491.491.25 491.5 491.5 492.5 492.5 492.5 492.5 492.75 492. 10 173277.55 Counts vs. MassatorChange (mz) Particity 11 173277.55 Counts vs. MassatorChange (mz) 11 173277.55 Counts vs. MassatorChange (mz) 11 173277.55 Counts vs. MassatorChange (mz) 11 119163.45 Counts vs. MassatorChange (mz)</th><th>Acquisition SW Version</th><th>e</th><th>5200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)</th><th>Info.</th><th></th></thco<></thcolision<></thcolision<>	Yard Spectra Prignetiz Collision Energy Doization Mode 10 0 Second 10 9 (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ 492.3222 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 (C28 H40 06)+NH4)+ (C28 H40 06)+NH4)+ 10 489.5 489.75 490.499.25 490.5 490.75 491.491.25 491.5 491.5 492.5 492.5 492.5 492.5 492.75 492. Particity 10 200.25 100.25 490.5 490.75 491.491.25 491.5 491.5 492.5 492.5 492.5 492.5 492.75 492. 10 173277.55 Counts vs. MassatorChange (mz) Particity 11 173277.55 Counts vs. MassatorChange (mz) 11 173277.55 Counts vs. MassatorChange (mz) 11 173277.55 Counts vs. MassatorChange (mz) 11 119163.45 Counts vs. MassatorChange (mz)	Acquisition SW Version	e	5200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)	Info.	
Fragmentor Voltage 135 Collision Energy 0 Ionization Mode Esi x10 ⁵ +Esi Scan (0.19-0.20 min, 2 Scans) Frag=135.0V kt/s8-12-4.d Subtract 490.3182 ((C28 H40 06)+NH4)+ 490.3192 ((C28 H40 06)+NH4)+ 4 -4	Fragmentor Voltage 135 Collision Energy 0 Ionization Mode Esi x10 ⁵ + ESI Scan (0.19-0.20 min, 2 Scans) Frag=135.0V McB-12-4.d. Subtract 490.3152 ((C28 H40 OG)+NH4)+ 490.3192 ((C28 H40 OG)+NH4)+ 4 491.3192 ((C28 H40 OG)+NH4)+ 492.3222 ((C28 H40 OG)+NH4)+ 4 495.5 489.75 490 490.25 490.5 490.15 491.25 491.5 491.75 492 492.5 492.5 492.5 492.5 492. Value to the second seco	Fragmentor Voltage 135 Collision Energy 0 Ionization Mode Esi x10 ⁵ + ESI Scan (0.19-0.20 min, 2 Scans) Frag=135.0V McB-12-4.d Subtract 403.3182 (C28 H40 06]+NH4)+ 403.3192 (C28 H40 06]+NH4)+ 493.3192 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 489.5 489.75 490.490.25 490.5 490.25 492.3222 (C28 H40 06]+NH4)+ 489.5 489.75 490.490.25 490.5 491.3192 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 489.5 489.75 490.490.25 490.5 491.5 492.3225 492.5 492.5 reak List 7.2 Z Abund Formula Ion 73.2897 1 173277.55 Ion 90.3162 1 626633.81 C28 H40 06 (M+NH4)+ 91.3192 1 175515 C28 H40 06 (M+NH4)+ 95.2714 1 19163.45 Ion Ion 62.5977 1 99214.55 Ion Ion Ion 63.5001 1 6490.95.99 Ion	Fragmemeter Voltage 133 Collision Energy 0 Ionization Mode ESI x10 ⁵ +ESI Scan (0.19-0.20 min, 2 Scans J Frage 135.0V ktBe-124.d. Subtract 490.3162 ((228 H40 OC)+NH4)+ 490.3162 ((228 H40 OC)+NH4)+ 4 491.3192 ((228 H40 OC)+NH4)+ 492.3222 ((C28 H40 OC)+NH4)+ 492.3222 ((C28 H40 OC)+NH4)+ 4 495.5 490.490.25 490.75 491.491.25 491.5 492.3225 (C28 H40 OC)+NH4)+ 4 495.5 490.490.25 490.75 491.491.25 491.5 492.3225 492.75 493 T/Z X Max Non Counts vs. Mass-to-Charge (m2) 492.255 492.75 493 Tor 773.2897 1 173277.55 Counts vs. Mass-to-Charge (m2) 492.255 492.75 493 Tor 73.2897 1 173277.55 C28 H40 O6 (M+NH4)+ 195.2714 1 5499.09.1 1 565.559 1 90104.38 163.569 1 300.00 300 3 60 1 62.775.43 1 1 <th>Fragmentor Voltage 135 Collision Energy 0 Lonization Mode Est x10³ -Est Scan (0.19-0.20 min, 2 Scans) Frag=133.0V Mc8-12-4.d Subtract 490.3162 (C28 H40 O6]+NH4)+ -490.3162 (C28 H40 O6]+NH4)+ 4 -491.3192 (C28 H40 O6]+NH4)+ -492.3222 (C28 H40 O6]+NH4)+ 4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.7 490.222 -489.5 490.25 492.25 -495.2714 1 173277.55 -495.3472 1 19163.45 -967.5539 1 490.406 -11 4977.43 -4977.543 -11 -10975.43 -10977.643 -11 -10977.543 -10</th> <th>User Spectra</th> <th></th> <th></th> <th></th> <th></th>	Fragmentor Voltage 135 Collision Energy 0 Lonization Mode Est x10 ³ -Est Scan (0.19-0.20 min, 2 Scans) Frag=133.0V Mc8-12-4.d Subtract 490.3162 (C28 H40 O6]+NH4)+ -490.3162 (C28 H40 O6]+NH4)+ 4 -491.3192 (C28 H40 O6]+NH4)+ -492.3222 (C28 H40 O6]+NH4)+ 4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.5 490.75 -4 -495.7 490.222 -489.5 490.25 492.25 -495.2714 1 173277.55 -495.3472 1 19163.45 -967.5539 1 490.406 -11 4977.43 -4977.543 -11 -10975.43 -10977.643 -11 -10977.543 -10	User Spectra				
*+ESI Scan (0.19-0.20 min, 2 Scans) Frag=135.0V ktc8-12-4.d Subtract 490.3162 (C28 H40 C6]+NH4)+ 490.3192 (C28 H40 C6]+NH4)+ 490.3222 (C28 H40 C6]+NH4)+ 490.3222 (C28 H40 C6]+NH4)+ 489.5 489.75 490 490.25 490.75 491 5 491.75 492 492.25 492.5 492.75 493 teak List 7/2 73.2897 1 1 173277.55 C28 H40 O6 (M+NH4)+ 91.3192 1 1 173277.55 C28 H40 O6 (M+NH4)+ 91.3192 1 1 175215 C28 H40 O6 (M+NH4)+ 91.3192 1 1 154990.91 18.3472 1 1 19514.55 63.601 1 62.59977 1 1 99514.55 63.5559 1 1 199014.38 63.5559 1 1 98724.64 1 1 1	HESI Scan (0.19-0.20 min, 2 Scans) Frage 135.0V ktcB-12-4.d Subtract 490.3162 ((C28 H40 O6]+NH4)+ 491.3192 ((C28 H40 O6]+NH4)+ 492.3222 ((C28 H40 O6]+NH4)+ 499.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 491.75 492 492.25 492.5 492.75 493 eak List 7/2 z Abund Formula Tor 73.2897 1 173277.55 Caunts vs. Mass-to-Charge (mz) romals 2 Calculator Element Limits ement Limits eme	Hest Scan (0.19-0.20 min, 2 Scans) Frag=135.0V ktc8-12-4.d Subtract 490.3162 ((C28 H40 O6)+NH4)+ ((C28 H40 O6)+NH4)+ 492.3222 ((C28 H40 O6)+NH4)+ 499.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 491.75 492 492.25 492.5 492.75 493 (C28 H40 O6)+NH4)+ 489.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 491.75 492 492.25 492.5 492.75 493 (C28 H40 O6)+NH4)+ (228 H40 O6)+NH4)+ (228 H40 O6)+NH4)+ (228 H40 O6)+NH4)+ (128 H40 O6)+NH4)+ (228 H40 O6)+NH4)+ (128 H40 O6)+ (M+NH4)+ (131 H2) (1175151 C28 H40 O6)+ ((M+NH4)+ (131 H2) (119163.45 ((M+NH4)+ (131 H2) (119163.45 ((M+NH4)+ (131 H2) (119163.45 ((M+NH4)+ (131 H2) (119163.45 (28 H40 O6)+ ((M+NH4)+ (131 H2) (119163.45 ((M+NH4)+ (131 H2) (119163.45 (28 H40 O6)+ ((M+NH4)+ (131 H2) (119163.45 (119163 (119163.45 (119163.45 (119163	10 +ESI Scan (0.19-0.20 min, 2 Scans) Frag=135.0V ktGs-12-4.d Subtract 490.3162 490.3162 (C28 H40 OG)+NH4)+ 492.3222 499.3162 (C28 H40 OG)+NH4)+ 499.3162 (C28 H40 OG)+NH4)+ 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 489.5 489.5.75 490.3162 1 1 173277.55 1 173277.55 1 173277.55 190.3162 1 1 626633.81 C28 H40 O6 (M+NH4)+ 193.3162 1 1 1549990.91 11.62.75.74.3 1 62.5977 1 99724.64 1 99724.64 1 99724.64 1 1 0 1 10 0 0 1<	$ \frac{1}{90,3162} + \frac{515 \text{ Scan} (0.19-0.20 \text{ min}, 2 \text{ Scans}) \text{ Frag-135.0V kt68-12-4.d Subtract}}{(C28 H40 O6]+NH4)+} \\ \frac{490,3162}{(C28 H40 O6]+NH4)+} \\ \frac{490,3192}{(C28 H40 O6]+NH4)+} \\ \frac{492,3222}{(C24 H40 O6]+NH4)+} \\ \frac{492,3222}{(C24 H40 O6]+NH4)+} \\ \frac{492,3222}{(C24 H40 O6]+NH4)+} \\ \frac{492,322}{(C24 H40 O6]+NH4)+} \\ \frac{73,2897}{1,173,277,55} \\ \frac{1}{200} \\ \frac{73,2897}{1,173,277,55} \\ \frac{1}{200} \\ \frac{1}{200,3162} \\ \frac{1}{2$	Fragmentor V 135	oltage	Collision Energy	Ionization Mode	
40.3162 (C28 H40 O6]+NH4)+ 491.3192 (C28 H40 O6]+NH4)+ 4 491.3192 (C28 H40 O6]+NH4)+ 4 492.3222 (C28 H40 O6]+NH4)+ 4 489.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 491.75 492 492.25 492.5 492.75 493 Counts vs. Mass-to-Charge (m/z) Value Value 73.2897 1 1 1.755.15 C28 H40 O6 (M+NH4)+ 90.3162 1 1 1.755.15 C28 H40 O6 (M+NH4)+ 95.2714 1 1 15499.91 1 1.626633.81 C28 H40 O6 (M+NH4)+ 95.2714 1 1 15499.91 18.3472 1 1 19514.55 03.601 1 62.5977 1 1 99514.55 03.601 1 1 192.75.99 1 193.495 1 100.0338 63.5569 1 1 98724.64 0 300 </td <td>490.3162 491.3192 1 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 7/2 2 4 490.25 90.3162 1 1 173277.55 90.3162 1 1 173277.55 90.3162 1 1 1626633.81 C28 H40 O6 (M+NH4)+ 91.3192 1 1 175515 C28 H40 O6 (M+NH4)+ 95.2714 1 1 154990.91 18.3472 1 1 199514.55 62.5977 1 1 99514.55 63.601 1 1 162775.43 66.5559 1 3 60 0 300</td> <td>490.3162 (C28 H40 06]+NH4)+ 491.3192 (C28 H40 06]+NH4)+ 491.5 491.3192 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 499.5 499.75 499.5 490.25 490.21 1732277.55 21 1626633.81 22 175515 22.8 H40 O6 (M+NH4)+ 95.271.4 1 1951.455 1 63.501 1</td> <td>40.3162 490.3162 1 (C2B H40 O6]+NH4)+ 4 (C2B H40 O6]+NH4)+ 1 (C2B H40 O6]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 490.3162 1 1 1.732277.55 2 Counts vs. Mass-to-Charge (m/z) 190.3162 1 1 1.73277.55 2 Abund 1 1.73277.55 1 1.753515 1 1.753515 1 1.75375.43 462.5977 1 1 1.62775.43 499.3163 490.104.38 490.5599 1 1 1.62775.43 1 1.62775.43 1 1.6300 0 3.00 0</td> <td>40.3162 (C28 H40 O6]+NH4)+ 491.3192 (C28 H40 O6]+NH4)+ 4 491.3192 (C28 H40 O6]+NH4)+ 4 492.3222 (C28 H40 O6]+NH4)+ 4 492.3222 (C28 H40 O6]+NH4)+ 4 492.3224 (C28 H40 O6]+NH4)+ 4 492.3224 (C28 H40 O6]+NH4)+ 4 492.3225 492.5 492.5 492.75 493 4 492.322 492.25 492.5 492.75 493 9 9 73.2897 1 1 173277.55 490.3162 1 6 26633.81 C28 H40 O6 (M+NH4)+ 491.3192 1 1 175515 C28 H40 O6 (M+NH4)+ 495.2714 1 1 16490.91 562.5977 1 963.601 1 62775.43 1 963.556 1 963.556 1 963.556 1 963.595 1 963.595 1 963.595 1 963.595 1 963.595 1 963.595 1</td> <td>x10 5 +ESI Scan</td> <td>(0.19-0.20</td> <td>min, 2 Scans) Frag=135 0V Mos</td> <td>12-4 d Subtract</td> <td></td>	490.3162 491.3192 1 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 4 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 1 (C28 H40 O6]+NH4)+ 7/2 2 4 490.25 90.3162 1 1 173277.55 90.3162 1 1 173277.55 90.3162 1 1 1626633.81 C28 H40 O6 (M+NH4)+ 91.3192 1 1 175515 C28 H40 O6 (M+NH4)+ 95.2714 1 1 154990.91 18.3472 1 1 199514.55 62.5977 1 1 99514.55 63.601 1 1 162775.43 66.5559 1 3 60 0 300	490.3162 (C28 H40 06]+NH4)+ 491.3192 (C28 H40 06]+NH4)+ 491.5 491.3192 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 492.3222 (C28 H40 06]+NH4)+ 499.5 499.75 499.5 490.25 490.21 1732277.55 21 1626633.81 22 175515 22.8 H40 O6 (M+NH4)+ 95.271.4 1 1951.455 1 63.501 1	40.3162 490.3162 1 (C2B H40 O6]+NH4)+ 4 (C2B H40 O6]+NH4)+ 1 (C2B H40 O6]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 490.3162 1 1 1.732277.55 2 Counts vs. Mass-to-Charge (m/z) 190.3162 1 1 1.73277.55 2 Abund 1 1.73277.55 1 1.753515 1 1.753515 1 1.75375.43 462.5977 1 1 1.62775.43 499.3163 490.104.38 490.5599 1 1 1.62775.43 1 1.62775.43 1 1.6300 0 3.00 0	40.3162 (C28 H40 O6]+NH4)+ 491.3192 (C28 H40 O6]+NH4)+ 4 491.3192 (C28 H40 O6]+NH4)+ 4 492.3222 (C28 H40 O6]+NH4)+ 4 492.3222 (C28 H40 O6]+NH4)+ 4 492.3224 (C28 H40 O6]+NH4)+ 4 492.3224 (C28 H40 O6]+NH4)+ 4 492.3225 492.5 492.5 492.75 493 4 492.322 492.25 492.5 492.75 493 9 9 73.2897 1 1 173277.55 490.3162 1 6 26633.81 C28 H40 O6 (M+NH4)+ 491.3192 1 1 175515 C28 H40 O6 (M+NH4)+ 495.2714 1 1 16490.91 562.5977 1 963.601 1 62775.43 1 963.556 1 963.556 1 963.556 1 963.595 1 963.595 1 963.595 1 963.595 1 963.595 1 963.595 1	x10 5 +ESI Scan	(0.19-0.20	min, 2 Scans) Frag=135 0V Mos	12-4 d Subtract	
$ \frac{491.3192}{([C28 H40 O6]+NH4)+} $ $ \frac{492.3222}{([C28 H40 O6]+NH4)+} $ $ \frac{492.3222}{(IC28 H40 O6]+NH4)+} $ $ \frac{492.3222}{(IC28 H40 O6]+NH4)+} $ $ \frac{492.3222}{(IC28 H40 O6]+NH4)+} $ $ \frac{492.322}{(IC28 H40 O6]+NH4)+} $ $ \frac{1}{(IC28 H40 O6]} $ $ \frac{1}{(IC28 H40 O6]+NH4)+} $ $ \frac{1}{(IC28 H40 O6]+NH4)+} $ $ \frac{1}{(IC28 H40 O6]} $ $ \frac{1}{(IC28 H40 O6]+NH4)+} $ $ \frac{1}{(IC28 H40 O6]} $ $ \frac$	6- 5- 4- 3- 2- 4 (C28 H40 06]+NH4)+ (C28 H40 06]+NH4)+ 489.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 492.75 492 492.25 492.75 493 (C28 H40 06]+NH4)+ 489.5 489.75 490 490.25 490.5 490.75 491 491.25 491.5 492 492.25 492.5 492.75 493 veak List 7/2 veak veak veak veak veak veak veak veak	6-5-4-3-2-1 491,3192 1 ([C28 H40 O6]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 490.25 490.25 490.55 491.3192 ([C28 H40 O6]+NH4)+ 492.3222 ([C28 H40 O6]+NH4)+ 72.2897 1 1 1732277.55 90.3162 1 2 1 1 1732277.55 2897 1 1 1732277.55 1 154990.91 1 175515 C28 H40 O6 ((M+NH4)+ 91.3192 1 1 154990.91 18.3472 1 1 194990.91 18.3472 1 1 900.3162 68.5569 1 3 90.30 963.595 1 1 196724	6 491.3192 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.352 1 491.25 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1 1.73277.55 1.17515 C.28 H40 O.6 (M+NH4)+ 195.2714 1.154990.91 1.18.3472 1.119163.45 1.1963.45 1.10 665.5569 1.304059.59 1.9872.464 1.9872.464 0 3.00 1.0 3.00 1.0 3.00 1.0 3.00 <t< th=""><th>6 491.3192 1 (C28 H40 06]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 490.25 489.5 490.25 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.7 490.255 489.7 490.255 490.3162 1 626633.81 C28 H40 06 (M+NH4)+ 491.3192 1 1 175215 C28 H40 06 (M+NH4)+ 495.27214 1 1 154990.91 518.3472 1 1 199524.55 50 50 5063.601 1 6275.77 1 9955.95 1 99724.64 60</th><th>7-</th><th></th><th>490.3162</th><th></th><th></th></t<>	6 491.3192 1 (C28 H40 06]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 490.25 489.5 490.25 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.7 490.255 489.7 490.255 490.3162 1 626633.81 C28 H40 06 (M+NH4)+ 491.3192 1 1 175215 C28 H40 06 (M+NH4)+ 495.27214 1 1 154990.91 518.3472 1 1 199524.55 50 50 5063.601 1 6275.77 1 9955.95 1 99724.64 60	7-		490.3162		
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491.3192 ([C28 H40 O6]+NH4)+ 492.3222 ((C28 H40 O6]+NH4)+ 489.5 489.75 490.490.25 490.75 491.491.25 491.3192 ((C28 H40 O6]+NH4)+ 489.5 489.75 490.490.25 490.75 491.491.25 491.315 492.3222 ((C28 H40 O6]+NH4)+ eak List 73.2897 1 173277.55 C28 H40 O6 (M+NH4)+ 91.3192 1 175515 C28 H40 O6 (M+NH4)+ 95.2714 1 19403.45 - - 62.5977 1 99214.55 - - 63.501 1 62775.43 - - 68.5569 1 304059.59 - - 68.5569 1 304059.59 - - 69.5595 1 98724.64 - - 1 1304059.59 - - -	491.3192 ((C28 H40 O6]+NH4)+ 492.3222 ((C28 H40 O6]+NH4)+ 489.5 489.75 490 490.25 490.75 491.491.25 492.3222 492.5 492.75 493 eak List 72.2897 1 173277.55 Counts vs. Mass-to-Charge (m/z) 491.25 492.492.25 492.5 492.75 493 90.3162 1 626633.81 C28 H40 O6 (M+NH4)+ 491.25 492.492.25 492.5 492.75 493 90.3162 1 626633.81 C28 H40 O6 (M+NH4)+ 491.25 492.492.25 492.55 492.55 492.75 493 90.3162 1 626633.81 C28 H40 O6 (M+NH4)+ 491.25 491.25 492.492.25 492.55	$\frac{491.3192}{([C28 H40 O6]+NH4)+}$ $\frac{492.3222}{([C28 H40 O6]+NH4)+}$ $\frac{492.3222}{([C28 H40 O6]+NH4)+}$ $\frac{492.3222}{([C28 H40 O6]+NH4)+}$ $\frac{492.3222}{(IC28 H40 O6]+NH4)+}$ $\frac{492.322}{(IC28 H40 O6]+NH4)+}$ $\frac{72.2897}{1}$ $\frac{1}{173277.55}$ $\frac{1}{173277.55}$ $\frac{1}{173277.55}$ $\frac{1}{173277.55}$ $\frac{1}{173277.55}$ $\frac{1}{173277.55}$ $\frac{1}{119163.45}$ \frac	491.3192 1 492.3222 (C28 H40 O6]+NH4)+ 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.5 489.75 489.75 490.490.25 491.3192 (C28 H40 O6]+NH4)+ 173.2897 1 173.2897 1 190.3162 1 1 123277.55 190.3162 1 1 123277.55 1173515 C28 H40 O6 (M+NH4)+ 195.2714 1 1 1491.45.5 462.5997 1 463.5509 1 304059.59 1 463.5569 1 304059.59 1 463.5569 1 304059.59 1 463.5569 1 30400 <	$ \frac{491,3192}{(C28,H40,06]+NH4)+} \frac{492,3222}{(C28,H40,06]+NH4)+} \frac{492,3222}{(C28,H40,06]+NH4)+} \frac{492,3222}{(C28,H40,06]+NH4)+} \frac{492,322}{C20,015,00} \frac{495,5,5,490,75,491,491,25,491,55,491,75,492,492,25,492,25,492,75,493}{C00,015,02,01,$	6-				
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\\ & \end{array}{} \\ & \end{array}{} \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ & \end{array}{} \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ & \end{array}{} \\ & \end{array}{} \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ & \end{array}{} \\ & \begin{array}{c} & \begin{array}{c} & \end{array}{} \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ & \end{array}{} \\ & \begin{array}{c} & \begin{array}{c} & \begin{array}{c} & \end{array}{} \\ & \begin{array}{c} & \begin{array}{c} & \begin{array}{c} & \begin{array}{c} & \end{array}{} \\ \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ \\ & \end{array}{} \\ \\ & \begin{array}{c} & \end{array}{} \\ & \end{array}{} \\ \\ & \end{array}{} \\ \\ & \begin{array}{c} & \end{array}{} \\ \\ & \end{array}{} \\ \\ & \end{array}{} \\ \\ \\ & \begin{array}{c} & \end{array}{} \\ \\ & \end{array}{} \\ \\ & \end{array}{} \\ \\ & \end{array}{} \\ \\ \\ & \end{array}{} \\ \\ \\ \\ & \end{array}{} 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33.601 1 62775.43 Image: Constraint of the second s	33.601 1 62775.43 77.5539 1 490104.38 8.5569 1 304059.59 9.5595 1 98724.64 rmula Calculator Element Limits ement Min 3 60 0 300	33.601 1 62775.43 Image: Constraint of the second s	33.601 1 62775.43	33.601 1 62775.43 77.5539 1 490104.38 88.5569 1 304059.59 99.5595 1 98724.64 Immula Calculator Element Limits ement Min 0 300 0 300 0 300 0 300 Immula Calculator Results	8.3472 1	99514	.55		
667.5539 1 490104.38	67.5539 1 490104.38 68.5569 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits Iement Min 3 60 0 300	667.5539 1 490104.38 668.5569 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits Iement Min Min Max 0 300 0 30	1 490104.38 068.5569 1 304059.59 1 98724.64 formula Calculator Element Limits Isement Min Min Max 3 60 4 0 300 0 0 300 0 0 2 3 60 472.2825 490.3163 490.3162 0,10 0,20 9,0000	1 490104.38 968.5569 1 304059.59 1 98724.64 formula Calculator Element Limits Icement Min Max 3 60 1 0 300 0 300 0 300 0 300 0 300 0 300 0 300	18.3472162.59771		.43		
07.5357 1 190104.38 668.5569 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits Iement Min Max 3 60 0 300	07.3537 1 #90104.38 68.5569 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits Iement Min 3 60 0 300	1 1 <td>007.3327 1 190104,38 068.5569 1 304059.59 069.5595 1 98724.64 0commula Calculator Element Limits Element Min Max 0 300 00 300 0 0 0 300 0 300 0 300 0 0 0 300 0 0 0 300 0 300 0 0 0 300 0 0 0 300 0 0 0 0 0 300 0 0 0 300 0 0 0 300 0 300 0 0 0 300 0 10 0 10 0 10 0 10 0 10<!--</td--><td>1 1 1901/04.38 068.5569 1 304059.59 069.5595 1 98724.64 0formula Calculator Element Limits Element Min Max 2 3 60 1 0 300 0 300 0 0 30 60 1 1 0 300 0 300 0 300 0 300 0 300 0 300 0 300</td><td>18.3472 1 962.5977 1 963.601 1</td><td>62775</td><td>4.20</td><td></td><td></td></td>	007.3327 1 190104,38 068.5569 1 304059.59 069.5595 1 98724.64 0commula Calculator Element Limits Element Min Max 0 300 00 300 0 0 0 300 0 300 0 300 0 0 0 300 0 0 0 300 0 300 0 0 0 300 0 0 0 300 0 0 0 0 0 300 0 0 0 300 0 0 0 300 0 300 0 0 0 300 0 10 0 10 0 10 0 10 0 10 </td <td>1 1 1901/04.38 068.5569 1 304059.59 069.5595 1 98724.64 0formula Calculator Element Limits Element Min Max 2 3 60 1 0 300 0 300 0 0 30 60 1 1 0 300 0 300 0 300 0 300 0 300 0 300 0 300</td> <td>18.3472 1 962.5977 1 963.601 1</td> <td>62775</td> <td>4.20</td> <td></td> <td></td>	1 1 1901/04.38 068.5569 1 304059.59 069.5595 1 98724.64 0formula Calculator Element Limits Element Min Max 2 3 60 1 0 300 0 300 0 0 30 60 1 1 0 300 0 300 0 300 0 300 0 300 0 300 0 300	18.3472 1 962.5977 1 963.601 1	62775	4.20		
1 304059.59 1 304059.59 1 98724.64 ormula Calculator Element Limits Imment Max 1 3 0 300	685.5599 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits lement Min 3 60 0 300	1 304059.59 1 304059.59 69.5595 1 98724.64 ormula Calculator Element Limits Iement Min 3 60 1 0 300 0 300	104059.599 1 304059.59 1069.55595 1 98724.64 ormula Calculator Element Limits Element Min Max Calculator Results 3 Formula CalculatedMass CalculatedMz Mz C28 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9 0000	ve8.5569 1 304059.59 of09.5595 1 ormula Calculator Element Limits Element Min Min Max C 3 60 1 0 300 0 300 0 300 0 300 0 300 0 300 0 300 0 300	18.3472 1 062.5977 1 063.601 1 067.5539 1	62775			
69.5595 1 198724.64 formula Calculator Element Limits iement Min 3 60 0 300	69.5595 1 98724.64 ormula Calculator Element Limits lement Min Max 3 60 0 300	669.5595 1 198724.64 Formula Calculator Element Limits Iement Min Max 3 60 1 0 300 0 300	b69.5595 1 198724.64 Formula Calculator Element Limits Element Min Max C 3 60 1 0 300 0 300 0 300 0 300 Cormula Calculator Results Formula CalculatedMass CalculatedMz CalculatedMass CalculatedMz 228 H40 06 472.2825 490.3163 490.3162 0.10 0.20	b69.5595 1 98724.64 Formula Calculator Element Limits Element Min Max C 3 60 1 0 300 C 300 C 0 300 Comula Calculator Results Formula Calculated Mass ICalculated Mass	518.3472 1 962.5977 1 963.601 1 967.5539 1 968.5569 1	62775 49010	0.50		
ormula Calculator Element Limits lement Min Max 3 60 0 300	ormula Calculator Element Limits Min Max 3 60 0 300	ormula Calculator Element Limits Element Min Max 3 60 0 300 0 0 30	Formula Calculator Element Limits Element Min Max C 3 60 1 0 300 0 30	Formula Calculator Element Limits Element Min Max C 3 60 1 0 300 C 0 30 Formula Calculator Results Formula CalculatedMass (CalculatedMass)	518.3472 1 962.5977 1 963.601 1 967.5539 1 968.5569 1	62775 49010 30405	9.59		
Min Max 3 60 0 300	Image: Min Max 3 60 0 300	Min Max 2 3 60 4 0 300 5 0 30	Min Max C 3 60 1 0 300 0 0 30 formula Calculated Mass Calculated Mz Calculated Mass Calculated Mz Diff. (mDa) Diff. (ppm) DBE 228 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	Element Min Max C 3 60 H 0 300 D 0 30 Formula Calculator Results Formula [CalculatedMass [CalculatedMass]	518.3472 1 962.5977 1 963.601 1 967.5539 1 968.5569 1 969.5595 1	62775 49010 30405 98724	9.59		
3 60 0 300	3 60 0 300 0 30	3 60 4 0 300 0 30 0 30	3 60 H 0 300 O 0 30 Formula Calculator Results Formula CalculatedMass CalculatedMz C28 H40 O6 472.2825 490.3163 490.3162 0.10 0.20 9.0000	3 60 4 0 300 5 0 30 6 300 0 6 300 0 7 0 30 6 0 30 6 0 30 6 0 30 7 0 30 6 0 30 6 0 30 7 0 30 6 0 30 7 0 30 7 0 30 7 0 30 8 0 0 9 0 30 9 0 30 9 0 30 9 0 30 9 0 30 9 0 30 9 0 30 9 0 30 9 0	518.3472 1 962.5977 1 963.601 1 967.5539 1 968.5569 1 969.5595 1 969.5595 1 969.5595 1	62775 49010 30405 98724 tor Eler	9.59 .64 nent Limits		
0 300			Image: second state state Solution Solu	1 0 300 0 0 300 0 cormula Calculator Results Formula CalculatedMass ICalculatedMass	i18.3472 1 i62.5977 1 i63.601 1 i67.5539 1 i68.5569 1 i69.5595 1 cornula Calcula Calcula clement Mi	62775 49010 30405 98724 tor Eler	9.59 .64 nent Limits Max		
0 300			1 0 300 0 0 30 ormula Calculator Results CalculatedMass CalculatedMz C28 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	1 0 300 0 30 5 ormula Calculator Results 5 ormula Calculated Mass ICalculated Mass ID (Calculated Mass ID)	118.3472 1 162.5977 1 163.601 1 167.5539 1 168.5569 1 169.5595 1 <td>62775 49010 30405 98724 tor Eler n</td> <td>9.59 nent Limits Max 60</td> <td></td> <td></td>	62775 49010 30405 98724 tor Eler n	9.59 nent Limits Max 60		
			O 0 30 Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 28 H40 O6 472.2825 490.3163 490.3162 0.10 0.20 9.0000	ormula Calculator Results	18.3472 1 62.5977 1 63.601 1 67.5539 1 68.5569 1 69.5595 1 ormula Calcula Image: Calcula ement Mi	62775 49010 30405 98724 tor Eler n 1 3	19.59 .64 ment Limits 60		
	0 30	0 30	0 30 Formula Calculator Results CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 28 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	ormula Calculator Results	118.3472 1 62.5977 1 63.601 1 67.5539 1 68.5569 1 69.5595 1 ormula Calcula lement Mi	62775 49010 30405 98724 tor Eler n 1 3	9.59 		
	0 30	0 30	O 30 Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 228 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	ormula Calculator Results ormula Calculated Mass I Calculated Mass I Mass I Diff (2000)	i18.3472 1 i62.5977 1 i63.601 1 i67.5539 1 i68.5569 1 i69.5595 1 iormula Calcula iement Mi	62775 49010 30405 98724 tor Eler n 3	9.59 9.64 nent Limits 60 300		
		0 30	U 30 Formula Calculator Results Formula CalculatedMass CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 28 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	ormula Calculator Results ormula Calculated Mass I Calculated Mass I Mass I Diff (m. D.) 1917 (m. D.)	i18.3472 1 i62.5977 1 i63.601 1 i67.5539 1 i68.5569 1 i69.5595 1 i69.5595 1 iement Mi	62775 49010 30405 98724 tor Eler n 1 3 0	19.59 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.64 10.59 10		
			Ormula Calculator Results CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 228 H40 06 472.2825 490.3163 490.3162 0.10 0.20 9.0000	ormula Calculator Results	i18.3472 1 i62.5977 1 i63.601 1 i67.5539 1 i68.5569 1 i69.5595 1 iormula Calcula I iement Mi	62775 49010 30405 98724 tor Eler n 1 3 0	9.59 .64 ment Limits 60 300		
ormula Calculator Results	ormula calculator Results		28 H40 O6 472.2825 490.3163 490.3162 0.10 0.20 9 0000		i18.3472 1 i62.5977 1 i63.601 1 i67.5539 1 i68.5569 1 iomula Calcula 1	62775 49010 30405 98724 tor Eler 3 0 0 0 tor Res	64 60 300 30 30 30 30 30 30 30 30		
ormula Calculator Results	ormula calculator Results		C28 H40 O6 472.2825 490.3163 490.3162 0.10 0.20 9 0000	DBE	518.3472 1 562.5977 1 563.601 1 467.5539 1 568.5569 1 50mula Calcula 1 50mula Calcula 1 50mula Calcula 1	62775 49010 30405 98724 tor Eler n 1 3 0 0 0 tor Res	64 66 60 300 30 01 15 15 15 15 15 15 15 15 15 1		
ormula Calculator Results ormula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBF	ormula Calculator Results ormula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBF	ormula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBF	490,3163 490,3162 0,10 0,20 9,0000	228 H40 O6 473 2925 400 2162 400 2162	518.3472 1 962.5977 1 963.601 1 967.5539 1 969.5595 1 969.5595 1 967.40 Calcula Element Mi 1 - 2 - 3 - 3 - 4 - 5 - 6 - 7 - 8 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 - 9 -	62775 49010 30405 98724 tor Eler n N 3 0 0 tor Res Calcu	64 66 60 300 30 Ults Calcula	tedMz Mz	Diff. (mDa) IDiff. (ppm) IDBE
ormula Calculator Results ormula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 28 H40 O6 473 2935 400 216 210 216 216 216 216 216 216 216 216 216 216	ormula Calculated Mass Calculated Mz Diff. (mDa) Diff. (ppm) DBE	ormula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE 28 H40 06 472 3935 400 3163 400 3163 400 3163 400 3163		490.3163 490.3162 0.10 0.20 9.000	518.3472 1 962.5977 1 963.601 1 967.5539 1 968.5569 1 969.5595 1 Formula Calcula Element Mi C	62775 49010 30405 98724 tor Eler 3 0 0 0 tor Res Calcu	64 nent Limits 60 300 300 1atedMass Calcula	tedMz Mz	Diff. (mDa) Diff. (ppm) DBE

Figure S72. HRESIMS spectrum of compound 6.

Acquisition S Version	W 620 Q-T		User Name Acquired Time DA Method	3/7/2022 4:59:27 PM PCDL.m
		0 series TOF/6500 series OF B.05.01 (B5125.2)	Into.	
User Spect	tra	Collision Energy	Ionization Mode	
1	35	0	ESI	
x10 4 +ESI S	Scan (0.08-0.10 min	n, 2 Scans) Frag=135.0V KFD2	2-3-1.d Subtract	
3.5-		497.2511 ([C27 H38 O7]+Na)+		
3-				
2.5-				
2-				
1.5-			498.2548	
1-			([C27 H38 O7]+Na)+	
0.5-				499.2566
0.5-	6.4 496.6 496.8	497 497.2 497.4 497.6 49	7.8 498 498.2 498.4 498.6 498	499.2566 ([C27 H38 O7]+Na)+
0.5 0 490 Peak List <i>m/z</i>	6.4 496.6 496.8	497 497.2 497.4 497.6 49 Count	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 490 Peak List <i>m/z</i> 202.1893	6.4 496.6 496.8 z Abund 1 31287.2	497 497.2 497.4 497.6 49 Count	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0 490 Peak List m/z 202.1893 202.6902	z Abund 1 31287.2 1 10662.86	497 497.2 497.4 497.6 49 Count	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0 490 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 403.3687	z Abund 1 31287.2 1 10662.86 1 13301.61	497 497.2 497.4 497.6 49 Count	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5 0 491 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 403.2511	z Abund 1 31287.2 1 10662.86 1 13301.61 1 10997.82 1 31287.2	497 497.2 497.4 497.6 49 Count	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0 499 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 10233.24	497 497.2 497.4 497.6 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0 499 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302	z Abund 1 31287.2 1 10662.86 1 13301.61 1 10997.82 1 1023.24 1 32193.59	497 497.2 497.4 497.6 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0.5- 0.49 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335	z Abund 1 31287.2 1 10662.86 1 13301.61 1 10997.82 1 1023.24 1 32193.59 1 18944.55	497 497.2 497.4 497.6 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0.499 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128	z Abund 1 31287.2 1 10662.86 1 13301.61 1 10997.82 1 31826.124 1 0233.24 1 10233.24 1 32193.59 1 13644.55 1 36642.16	497 497.2 497.4 497.6 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/2)	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0.491 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164	z Abund 1 31287.2 1 10662.86 1 13301.61 1 10997.82 1 31826.12 1 10233.24 1 32193.59 1 36642.16 1 21769.71	497 497.2 497.4 497.5 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499.2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0.491 Peak List <i>m/z</i> 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calc Element	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 31826.12 1 0233.24 1 32193.59 1 13644.55 1 36642.16 1 21769.71 ulator Element Image: Manual Manua	497 497.2 497.4 497.5 49 Count Formula	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ((C27 H38 07)+Na)+ 3.8 499 499,2 499,4 499,6 499,8
0.5- 0.491 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calc Element C	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 31826.12 1 10233.24 1 32193.59 1 18944.55 1 36642.16 1 21769.71 ulator Element Min Max	497 497.2 497.4 497.6 49 Count Formula 5 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ((C27 H38 07)+Na)+ 3.8 499 4992 499.4 499.6 499.8
0.5- 0 499 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calco Element C H	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 31826.12 1 10233.24 1 3193.59 1 3642.16 1 21769.71 ulator Element Min 3 6 0 1	497 497.2 497.4 497.6 49 Count Formula 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ((C27 H38 07)+Na)+ 3.8 499 499,2 499,4 499,6 499,8
0.5- 0 499 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calc Element C H O	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 31826.12 1 10233.24 1 3193.59 1 8944.55 1 3642.16 1 21769.71 ulator Element Min Mag 0 1 0 1	497 497.2 497.4 497.6 49 Count Formula 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ((C27 H38 07)+Na)+ 3.8 499 499,2 499,4 499,6 499,8
0.5- 0 499 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calc Element C H 0 Formula Calc Formula Calc	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 1033.24 1 32193.59 1 18944.55 1 3642.16 1 21769.71 ulator Elemer Min Ma 3 0 1 0 3 0 1 0 2	497 497.2 497.4 497.6 49 Count Formula 5 2 2 2 2 2 3 5 5 5 5 5 5 5 5 5 5 5 5 5	7.8 498 498.2 498.4 498.6 498 s vs. Mass-to-Charge (m/z)	499,2566 ((C27 H38 07)+Na)+ 3.8 499 499.2 499.4 499.6 499.8
0.5- 0 49 Peak List m/z 202.1893 202.6902 403.3687 439.3191 497.2511 520.3275 877.6302 878.6335 971.5128 972.5164 Formula Calc Element C H O Formula Calc Formula Calc C C 202.72 H 0 C C C C C C C C C C O C O C C C C C C C O C C C O C O C	z Abund 1 31287.2 1 10662.86 1 1301.61 1 10997.82 1 31826.12 1 31287.2 1 10997.82 1 31826.12 1 32193.59 1 3642.16 1 21769.71 valor Element Min Max 6 0 1 0 1 0 1 0 3 0 1 0 1 0 1 0 1	497 497.2 497.4 497.6 49 Count Formula Formula 2 2 2 2 2 2 3 3 5 5 5 5 5 5 5 5 5 5 5 5	7.8 498.2 498.6 498.6 498.6 s vs. Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ 407.2510 407.2510	499,2566 ([C27 H38 07]+Na)+ 3.8 499 499.2 499.4 499.6 499.8 Diff. (mDa) Diff. (ppm) DBE

Figure S73. HRESIMS spectrum of compound 7.

Sample Group Acquisition SW Version User Spectra Fragmentor Voll 135	6200 seri Q-TOF B.	ies TOF/6500 series .05.01 (B5125.2)	Info.	
User Spectra Fragmentor Volt				
135	age	Collision Energy	Ionization Mode	
NTO 5 45010	(9 min) Error	0	ESI	
*10 • *ESI Scan (0. 1.6 - 1.4 - 1.2 - 1-	([C28	513.2821 1 H42 O7]+Na)+		
0.8-			514.2854	
0.4 -			([C28 H42 O7]+Na)+	
0.2-				515.2883 ([C28 H42 O7]+Na)+
m/z z 473.2898 1 474.293 1	Abund 221814.97 55384.8	Formula	Ion	
513.2821 1 527.2981 1	151907.83 91747	C28 H42 O7	(M+Na)+	
1003.5762 1	225621.08			
1004.5796 1	137058.69			
1017.5915 1	143907 52			
1019.5972 1	52641.04			
1031.6069 1 Formula Calculato	63325.15 r Element I	imits		
Element Min	Max	-		
C	3 60	-		
0	0 30			
	0 3			
N	Decision Iter		odMz Mz	Diff (mDa) Diff (nom)
N Formula Calculato	Calculated	1ass Calculat	Curiz Intz	
1019.5972 1 1031.6069 1 Formula Calculato Element Min C H	52641.04 63325.15 r Element L 3 60 0 120 0 30 0 30	imits	adMz Mz	[Diff (mDa) [Diff (mm)]

Figure S74. HRESIMS spectrum of compound 8.



Figure S75. HRESIMS spectrum of compound 9.

Instrument Acq Method IRM Calibra Comment Sample Gro	me Nam I Ition :	e Statı	15	kfD2-3B-3A.d Sample Instrument 1 s.m Success	Info.	Sample Name Position User Name Acquired Time DA Method	kfD2-3B-3A P1-A2 5/25/2022 2:32:01 PM PCDL.m
Acquisition Version	sw		6200 ser Q-TOF B	ies TOF/6500 series .05.01 (B5125.2)			
Fragmer	tor Vo	oltage	,	Collision Energy	Ioniza	tion Mode	
×10 4 +ESI	Scan (0.08 m	in) Frag=17	5.0V kfD2-3B-3A d Subtr	act	C31	
				445.2586			
3.5-			,				
2.5-							
2-							
1.5-					44	5,2620	
1-					([C26 H	36 O6]+H)+	
0.5-							447.2663 ([C26 H36 O6]+H)+
0		444.5	4	45 445.5 Counts	446 vs. Mass-to-	446.5 Charge (m/z)	447 447.5 448
Peak List	1.	Abu	nd	Cormula			
445.2586	1	345	22.68	C26 H36 O6		10n (M+H)+	
446.262	1	965	5.79	C26 H36 O6		(M+H)+	
459.2742	1	184	89.57				
461.2902	1	2349	93.76				
467.2408	1	275	59.51				
481.2564	1	982	3.39				
483.2716	1	1844	43.33				
490.3166	1	2097	75.84				
FOC 2470	culat	or El	ement Li	mits			
506.3478 Formula Cal	Min		Max]			
506.3478 Formula Cal Element	-	3	60	-			
506.3478 Formula Cal Element C		0	30	1			
506.3478 Formula Cal Element C H O	1		sults				
506.3478 Formula Cal Element C H O Formula Cal	culat	or Re	and the second	ass Calculate	edMz	Mz	Diff. (mDa) Diff. (ppm) DBE
506.3478 Formula Cal Element C H O Formula Cal Formula C26 H36 O6	culat	Cale	culatedM	444.2512	445.2	585 445 258	6 -0.10 -0.221 9.00001
506.3478 Formula Cal Element C H O Formula Cal Formula C26 H36 O6 End Of Rej	culat	Cald	culatedM	444.2512	445.2	445.258	6 -0.10 -0.22 9.0000

Figure S76. HRESIMS spectrum of compound 10.

6200 se Q-TOF B	ries TOF/6500 series 3.05.01 (B5125.2)	Info.	
age	Collision Energy	Ionization Mode ESI	
		512.2697 ([C28 H40 O7]+Na)+	
			513.2784 ([C28 H40 O7]+Na)+
0.8 511 511	.2 511.4 511.6 511.8 Counts	512 512.2 512.4 512.6 512.8 s vs. Mass-to-Charge (m/z)	513.2784 ([C28 H40 O7]+Na)+ 8 513 513.2 513.4 513.6 513.8
0.8 511 511	2 511.4 511.6 511.8 Counts	512 512.2 512.4 512.6 512.8 s vs. Mass-to-Charge (m/z)	(1028 H40 07)+Na)+ 8 513 5132 5134 5136 5138
0.8 511 511	2 511.4 511.6 511.8 Counts	512 512.2 512.4 512.6 512.8 s vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 7710.53 1426.33	2 511.4 511.6 511.8 Counts	512 5122 5124 5126 512.6 s vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 1426.33 683.01	2 511.4 511.6 511.8 Counts	512 512 5124 5126 512.6 s vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 511 511 5710.53 5426.33 683.01 1055.67 55.67 567	E 511.4 511.6 511.8 Count Formula	512 5122 5124 5126 512.6 s vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 4426.33 1683.01 1055.67 427.04	Formula	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 1426.33 1683.01 2055.67 1427.04 945.35 5692.55	Formula	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/z)	((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 1426.33 1683.01 2055.67 1427.04 945.35 1683.55 1683.55	Formula	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/2)	((C28 H40 O7)+Na)+ ((C28 H40 O7)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 1426.33 1683.01 2055.67 7427.04 1945.35 1683.55 1324.01 1780.68	Formula	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/2)	((22 H40 07)+Na)+ 8 513 5132 5134 513.6 513.8
Abund 3710.53 1426.33 1683.01 2055.67 7427.04 1945.35 3683.55 324.01 7780.68 383.68	C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+	(1228H40 07]+Na)+ 8 513 5132 5134 5136 5138
Abund 7710.53 1426.33 1683.01 2055.67 1427.04 1945.35 1683.55 1324.01 1780.68 1383.68 Telement U	C28 H40 07 C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/z) Ion (m+Na)+ (M+Na)+	513.2784 ((C28.H40 O7]+Na)+ 8 513 513.2 513.4 513.6 513.8
Abund 7710.53 1426.33 1683.01 2055.67 1427.04 1945.35 1683.55 1224.01 1780.68 1383.68 • Element Li Max 3 120	C28 H40 07 C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/2) Ion (m+Na)+ (M+Na)+	513278 ((C28H40O7]+Na)+ 8 513 5132 5134 5136 5138
Abund 5710.53 1426.33 1683.01 2055.67 7427.04 1945.35 5683.55 2324.01 5780.68 383.68 • Element Li Max 3 120 0 200	C28 H40 07 C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/z) Ion (m+Na)+ (M+Na)+	513.2784 ((C28.H40.07]+Na)+ 8 513 513.2 513.4 513.6 513.8
Abund 5710.53 1426.33 1683.01 1055.67 7427.04 1945.35 5683.55 1324.01 5780.68 780.68 780.68 3 120 0 200 0 30	C28 H40 07 C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 s vs. Mass-to-Charge (m/z)	513.2784 ((C28.H40.07]+Na)+ 8 513 513.2 513.4 513.6 513.8
Abund 5710.53 1426.33 1683.01 2055.67 7427.04 1945.35 5683.55 1324.01 5780.68 1383.68 TElement Li Max 3 120 0 200 0 30 0 3	C28 H40 07 C28 H40 07 C28 H40 07	512 5122 5124 5126 512.6 vs. Mass-to-Charge (m/2)	513.2784 ((C28.H40.07]+Na)+ 8 513 5132 5134 513.6 513.8
Abund 5710.53 1426.33 1683.01 2055.67 7427.04 1945.35 5683.55 1324.01 5780.68 13283.68 Felement L1 Max 3 120 0 200 0 30 0 3 Results 500 120 120 120 120 120 120 120 1	C28 H40 07 C	512 5122 5124 5126 512.6 s vs. Mass-to-Charge (m/2)	513.2784 ((C28.H40 O7]+Na)+ 8 513 5132 5134 5136 513.8
	tage 08-0.09 min, 2 1 51 ([C28 H4	tage Collision Energy 0 08-0.09 min, 2 Scans) Frag=135.0V kfc8- 511.2673 ([C28 H40 07]+Na)+	Collision Energy Ionization Mode 0 ESI 08-0.09 min, 2 Scans) Frag=135.0V kfc8-11-5.d Subtract (3) 511.2573 511.2573 ([C28 H40 07]+Na)+ 512.2697 ([C28 H40 07]+Na)+

X-ray crystallographic data of compounds 2, 4, and 5



Figure S77. View of a molecule of compound 2 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

	F	
Identification code	global	
Empirical formula	C ₂₆ H ₃₈ O ₆	
Formula weight	446.56	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P21212	
Unit cell dimensions	a = 10.8614(3) Å	<i>α</i> = 90°.
	b = 36.7053(9) Å	β= 90°.
	c = 6.0922(2) Å	$\gamma = 90^{\circ}$.
Volume	2428.78(12) Å3	
Z	4	
Density (calculated)	1.221 mg/m ³	
Absorption coefficient	0.689 mm ⁻¹	
F(000)	968	
Crystal size	$0.250 \times 0.120 \times 0.070 \text{ mm}^3$	
Theta range for data collection	2.41 to 68.32°.	
Index ranges	-13<=h<=12, -44<=k<=34, -7<=l<=6	
Reflections collected	15579	
Independent reflections	4402 [R(int) = 0.0887]	
Completeness to theta = 68.32°	99.80%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.95 and 0.79	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4402 / 0 / 296	
Goodness-of-fit on F2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0335, WR2 = 0.0856	
R indices (all data)	R1 = 0.0597, wR2 = 0.0960	
Absolute structure parameter	-0.05(6)	

Table S3. Crystal data and structure refinement for compound 2.



Figure S78. View of a molecule of compound 4 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

¥	-	
Identification code	global	
Empirical formula	C ₂₅ H ₃₆ O ₆	
Formula weight	432.54	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 7.7089(3) Å	$\alpha = 90^{\circ}$.
	b = 8.1588(3) Å	$\beta = 90^{\circ}$.
	c = 36.7130(13) Å	$\gamma = 90^{\circ}$.
Volume	2309.08(15) Å3	
Z	4	
Density (calculated)	1.244 mg/m ³	
Absorption coefficient	0.709 mm ⁻¹	
F(000)	936	
Crystal size	$0.680 \times 0.190 \times 0.040 \text{ mm}^3$	
Theta range for data collection	2.41 to 69.95°.	
Index ranges	-9<=h<=9, -7<=k<=9, -44<=l<=44	
Reflections collected	16444	
Independent reflections	4355 [R(int) = 0.0890]	
Completeness to theta = 69.95°	99.90%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.97 and 0.78	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4355 / 0 / 286	
Goodness-of-fit on F2	1.146	
Final R indices [I>2sigma(I)]	R1 = 0.0449, WR2 = 0.1142	
R indices (all data)	R1 = 0.0600, wR2 = 0.1190	
Absolute structure parameter	0.07(8)	
Largest diff. peak and hole	0.482 and -0.454 e.Å-3	

Table S4. Crystal data and structure refinement for compound 4.



Figure S79. View of a molecule of compound 5 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

	1	
Identification code	global	
Empirical formula	$C_{28} H_{40}O_6$	
Formula weight	472.6	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 8.1802(3) Å	$\alpha = 90^{\circ}$.
	b = 13.5202(4) Å	$\beta = 90^{\circ}$.
	c = 11.2870(4) Å	$\gamma = 90^{\circ}$.
Volume	1246.94(7) Å3	
Z	2	
Density (calculated)	1.259 mg/m ³	
Absorption coefficient	0.701 mm ⁻¹	
F(000)	512	
Crystal size	$0.540 \times 0.450 \times 0.280 \text{ mm}^3$	
Theta range for data collection	3.92 to 72.31°.	
Index ranges	-8<=h<=10, -16<=k<=16, -13<=l<=13	
Reflections collected	22359	
Independent reflections	4854 [R(int) = 0.0348]	
Completeness to theta = 69.95°	99.00%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.83 and 0.69	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4854 / 1 / 314	
Goodness-of-fit on F2	0.978	
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.1015	
R indices (all data)	R1 = 0.0312, wR2 = 0.1017	
Absolute structure parameter	-0.09(3)	
Largest diff. peak and hole	0.213 and -0.214 e.Å-3	

Table 55. Crystal uata and structure remember for compound.

Calculated ECD data of compound 3



File: compound 2-1mm (195-400) 22090803.dsx

ProBinaryX

Attributes :

- Time Stamp: Thu Sep 08 13:38:16 2022

```
- File ID : F361B51F-DFB3-4086-8AA1-5D9E05E7A180
```

```
- Is CFR Compliant: false
```

```
- Original data has not been modified.
```

Remarks:

```
- User: CD
```

```
- Date: 2022/09/08
```

```
- Instrument: 0547
```

- DetectorType: LAAPD
- DichOS Calibration Correction Curve: 0547/2
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.4600 mg/mL MeOH
- Pathlength: 1 mm

```
- Temperature: 20°C
```

Settings:

```
- Time-per-point: 1s (25us x 40000)
```

- SE

```
- Wavelength: 195nm - 400nm
```

- Step Size: 1nm
- Bandwidth: 1nm

Figure	S80.	The	CD	spectrum	of	compound	3.
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Figure S81. Six optimized conformers of 3.

Table S6. Conformational analysis of the six optimized conformers of 3 in the gas phase (T = 298.15 K)

Conformer	E (Hartree)	C (Hartree)	G (kcal/mol)	ΔG (kcal/mol)	Population
3-1	-1502.963528	0.537406	-942787.415691	0	50.38%
3-2	-1502.961835	0.536663	-942786.819782	0.595908597	18.42%
3-3	-1502.961967	0.537037	-942786.667542	0.748148798	14.24%
3-4	-1502.961837	0.537663	-942786.193728	1.221962773	6.40%
3-5	-1502.962021	0.537875	-942786.175875	1.239815433	6.21%
3-6	-1502.963046	0.539234	-942785.965986	1.449704978	4.35%

Electronic energy obtained at M062X/6-311+G(2d,p) EmpiricalDispersion=GD3 of theory; Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) Scale=0.9813 SCRF=(IEFPCM,Solvent=Methanol) EmpiricalDispersion=GD3BJ of theory; Gibbs free energy (E + C); The relative Gibbs free energy; The Boltzmann distribution of each conformer.

С	-3.23512	0.526145	-0.56739	Η	0.119621	-2.313954	0.32708
С	-2.122056	2.896378	-0.333574	Н	0.932854	1.843407	2.580452
С	-1.13449	0.773697	0.569663	Н	1.159912	2.32409	0.903301
С	-1.824834	-0.010336	-0.300388	Н	3.317207	1.374559	1.078659
С	0.19691	0.375992	1.122447	Н	2.906236	0.525473	2.556464
С	1.018129	-0.352274	-0.001508	Н	2.240756	-1.418372	1.42333
С	0.207584	-1.568463	-0.473631	Н	1.875098	1.435588	-0.975986
С	-1.219404	-1.201115	-0.89923	Н	1.752793	0.019954	-2.016593
С	1.178004	1.466868	1.582592	Н	0.308422	0.950923	-1.62946
С	2.5539	0.744099	1.544493	Н	-0.729933	-1.391108	2.084626
С	2.37444	-0.581764	0.725174	Н	0.786959	-0.862865	2.855399
С	1.24866	0.574155	-1.219442	Н	-0.695622	0.065459	3.074908
С	-0.12209	-0.524864	2.351256	Н	3.808412	-0.068877	-0.792381
0	-1.811074	-1.911788	-1.716835	Н	3.074056	-3.015872	-0.36453
С	-1.894902	1.997591	0.899677	Н	4.370407	-2.489437	-1.446797
С	3.615907	-0.918382	-0.125625	Н	2.708263	-2.027755	-1.78732
С	3.428958	-2.179904	-0.980128	Н	4.840201	-0.320261	1.575478
С	4.850734	-1.078924	0.789155	Н	4.800665	-2.054169	1.290153
С	6.187484	-0.969472	0.053952	Н	7.015565	-1.257482	0.715448
С	6.485584	0.434647	-0.422474	Н	6.250334	-1.643829	-0.806332
0	7.5108	0.453524	-1.303706	Н	7.666171	1.387841	-1.542075
0	5.917714	1.449686	-0.0675	Н	-4.587147	1.070781	-2.180456
С	-3.585291	0.643382	-2.058433	Н	-3.554387	-0.332164	-2.546478
С	-4.320083	-0.278333	0.203834	Н	-2.872753	1.295602	-2.573463
С	-3.173286	1.904277	0.119222	Н	-4.073245	-0.255477	1.270618
С	-2.38695	4.33414	-0.060752	Н	-5.263685	0.2677	0.081917
С	-1.86563	5.315466	-1.085307	Н	-2.123343	6.336742	-0.798902
0	-2.990992	4.69569	0.942761	Н	-0.776564	5.21837	-1.174124
С	-4.562293	-1.732381	-0.210113	Н	-2.285984	5.088097	-2.072495
С	-3.570128	-2.718017	0.366447	Н	-5.550165	-2.046474	0.15403
0	-3.611285	-3.887548	-0.295365	Н	-4.58428	-1.858993	-1.294175
0	-2.850457	-2.523466	1.329283	Н	-1.651088	-4.534083	-0.035085
С	-2.671157	-4.884598	0.141134	Н	-2.804144	-5.10518	1.202588
Н	-4.086743	2.334432	0.517025	Н	-2.878612	-5.767613	-0.462583
Н	-1.809333	2.499346	1.857341				
Н	-1.539323	2.667968	-1.220473				
Н	0.663282	-2.079206	-1.324518				

Table S7. Atomic coordinates (Å) of 3-1 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.

C	2.79563	-0.680457	1.390819	H	-0.971786	-2.854745	0.019287
С	2.253769	1.860815	0.967764	Н	-0.512386	1.333837	-2.353118
С	0.992294	-0.055739	-0.061568	Н	-0.853291	1.911142	-0.726491
C	1.375258	-0.941184	0.894516	Н	-3.119431	1.416268	-1.174525
C	-0.299256	-0.200235	-0.799252	Н	-2.70924	0.467029	-2.589887
C	-1.396287	-0.716837	0.201496	Н	-2.598587	-1.545554	-1.387277
C	-0.933739	-2.064621	0.779735	Н	-2.328413	-0.135438	2.0802
C	0.501252	-2.030152	1.332218	Н	-0.66748	0.431175	1.933556
C	-0.961535	1.0526	-1.395634	Н	-1.961149	1.24348	1.047634
C	-2.450815	0.631029	-1.540007	Н	0.237855	-2.187098	-1.617189
C	-2.657523	-0.683452	-0.709736	Н	-0.860791	-1.257846	-2.654587
С	-1.593906	0.268625	1.377489	Н	0.851171	-0.819779	-2.537107
C	-0.011174	-1.183595	-1.970829	Н	-4.152325	0.141132	0.596154
0	0.880276	-2.912542	2.106212	Н	-3.984226	-2.902256	0.252736
C	2.02811	0.980112	-0.272846	Н	-5.279195	-2.099291	1.151181
С	-4.046809	-0.74386	-0.043294	Н	-3.619491	-1.979677	1.719159
C	-4.239964	-1.998527	0.819845	Н	-4.87735	0.052342	-1.894535
C	-5.15073	-0.67031	-1.121889	Н	-5.233152	-1.6464	-1.616907
C	-6.524701	-0.274218	-0.579214	Н	-7.295821	-0.403862	-1.3504
С	-6.591822	1.171867	-0.14129	Н	-6.84135	-0.901106	0.260874
0	-7.711346	1.422968	0.573971	Н	-7.702476	2.374237	0.795008
0	-5.777991	2.038676	-0.396402	H	2.250285	0.219608	3.305303
C	2.896829	-0.575603	2.921481	H	3.927143	-0.350532	3.219686
C	3.765093	-1.793494	0.908793	H	2.594346	-1.517018	3.386211
C	3.128508	0.65176	0.697344	H	4.78745	-1.502312	1.174859
C	2.874484	3.188217	0.708724	Н	3.529027	-2.701568	1.471526
C	2.429324	4.322631	1.601415	Н	1.346039	4.467469	1.507354
0	3.69805	3.346568	-0.186403	Н	2.626073	4.073882	2.651334
C	3.710207	-2.156426	-0.586911	Н	2.949992	5.244066	1.334669
C	4.115498	-1.061826	-1.549684	Н	4.392114	-2.999647	-0.754726
0	5.314822	-0.535429	-1.22911	Н	2.709619	-2.483114	-0.87513
0	3.46957	-0.699432	-2.515736	Н	5.104361	1.451901	-1.812029
C	5.742739	0.589136	-2.022653	Н	6.767096	0.791887	-1.711836
Η	4.160319	0.87564	0.45736	Н	5.702501	0.347191	-3.086178
Η	2.199825	1.43578	-1.240555				
Η	1.51023	1.812324	1.756957				
Η	-1.568952	-2.407157	1.600183				

Table S8. Atomic coordinates (Å) of 3-2 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.

C	-2.830567	-0.689934	-1.430543	H	0.892765	-2.84227	0.038079
С	-2.302268	1.857478	-1.056942	Н	0.475589	1.427938	2.257021
С	-1.026725	-0.032334	0.008477	Н	0.837853	1.941083	0.613658
С	-1.409647	-0.939055	-0.9275	Н	3.094428	1.438762	1.105227
С	0.259729	-0.160121	0.75781	Н	2.658246	0.54156	2.546426
С	1.359086	-0.721254	-0.214889	Н	2.541277	-1.508739	1.410107
С	0.885565	-2.081511	-0.75289	Н	1.959183	1.201644	-1.121502
С	-0.537057	-2.041249	-1.335537	Н	2.30721	-0.215726	-2.107291
С	0.930152	1.106682	1.314781	Н	0.655339	0.383143	-1.986073
С	2.413026	0.673549	1.488895	Н	0.801507	-1.168878	2.647426
С	2.613471	-0.670252	0.704768	Н	-0.894316	-0.685517	2.523304
С	1.576829	0.222927	-1.421219	Н	-0.326404	-2.103802	1.647033
С	-0.047804	-1.095721	1.963396	Н	4.126295	0.096507	-0.615448
0	-0.908871	-2.930915	-2.104524	Н	3.924386	-2.932033	-0.174169
С	-2.063206	1.004648	0.199524	Н	5.236512	-2.172262	-1.085105
С	4.007236	-0.765801	0.051932	Н	3.58383	-2.054028	-1.673538
С	4.195208	-2.050011	-0.767817	Н	4.829794	0.081772	1.884029
С	5.103201	-0.66705	1.136663	Н	5.17363	-1.627662	1.662826
С	6.484558	-0.299443	0.592714	Н	7.248947	-0.412112	1.373189
С	6.56757	1.131867	0.111187	Н	6.801732	-0.954421	-0.225498
0	7.696778	1.352557	-0.598797	Н	7.697539	2.296544	-0.849313
0	5.757537	2.012038	0.330116	Н	-2.275607	0.182588	-3.356375
С	-2.925414	-0.605223	-2.963213	Н	-3.954124	-0.382581	-3.268373
С	-3.789251	-1.809396	-0.942614	Н	-2.622826	-1.55372	-3.413265
С	-3.171356	0.651513	-0.754291	Н	-4.810628	-1.556317	-1.250216
С	-2.921677	3.189853	-0.819688	Н	-3.508477	-2.729734	-1.462069
С	-2.517259	4.295465	-1.766348	Н	-3.039765	5.220695	-1.516836
0	-3.713059	3.371713	0.09921	Н	-1.433296	4.454845	-1.710918
С	-3.783964	-2.096906	0.568704	Н	-2.742998	4.006658	-2.800061
С	-4.448425	-1.006365	1.377907	Н	-4.359488	-3.013382	0.746868
0	-3.676955	-0.585561	2.398672	Н	-2.771429	-2.2675	0.937886
0	-5.553022	-0.549193	1.146986	Н	-5.166096	0.246913	3.60922
С	-4.205163	0.514614	3.164959	Н	-3.464761	0.711762	3.939163
Н	-4.201736	0.87365	-0.504086	Н	-4.330334	1.389366	2.521302
Η	-2.221685	1.492172	1.153875				
Η	-1.567647	1.79206	-1.853187				
Η	1.531188	-2.465897	-1.545966				

Table S9. Atomic coordinates (Å) of 3-3 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.

C	-3.153679	0.39634	-0.869514	H	0.165579	-2.356128	0.316631
С	-2.25723	2.804436	-0.325539	Н	0.830543	1.911184	2.428515
С	-1.158136	0.670856	0.445269	Н	1.080915	2.31793	0.734748
С	-1.761872	-0.109811	-0.48915	Н	3.265316	1.451443	1.011653
С	0.179718	0.347103	1.029811	Н	2.840126	0.650505	2.511939
С	1.049861	-0.390264	-0.051639	Н	2.271354	-1.360721	1.441925
С	0.288462	-1.64443	-0.509325	Н	1.811142	-0.068956	-2.065501
С	-1.118181	-1.312966	-1.019991	Н	0.354146	0.862516	-1.730203
С	1.110818	1.495965	1.455701	Н	1.905356	1.377159	-1.06596
С	2.509419	0.816122	1.482791	Н	-0.679563	-1.409939	2.073545
С	2.394537	-0.548252	0.714271	Н	0.801346	-0.770312	2.830548
С	1.289163	0.504273	-1.29344	Н	-0.723667	0.097268	2.983656
С	-0.115457	-0.504606	2.298342	Н	3.8517	-0.045797	-0.785604
0	-1.68584	-2.065692	-1.816335	Н	2.843399	-2.075192	-1.732524
С	-2.023106	1.81157	0.823414	Н	3.201572	-2.997333	-0.263967
С	3.668281	-0.875044	-0.091571	Н	4.509399	-2.468324	-1.331091
С	3.545924	-2.173363	-0.901354	Н	4.826084	-0.170164	1.61498
С	4.881967	-0.959133	0.860964	Н	4.8481	-1.914488	1.400225
С	6.234886	-0.836928	0.158195	Н	7.052452	-1.071784	0.852909
С	6.503581	0.555165	-0.36826	Н	6.342683	-1.54323	-0.671542
0	7.560356	0.572171	-1.211447	Н	7.69287	1.500197	-1.485466
0	5.889047	1.564056	-0.079616	Н	-2.551874	1.402438	-2.7229
С	-3.288561	0.670662	-2.379223	Н	-4.287406	1.061137	-2.605877
С	-4.291388	-0.578107	-0.46373	Н	-3.139199	-0.25503	-2.940208
C	-3.248552	1.690496	-0.035022	H	-5.227998	-0.008896	-0.472972
C	-2.660002	4.18243	0.065526	Н	-4.385492	-1.350624	-1.229766
C	-2.175078	5.300231	-0.828482	Н	-1.078728	5.300353	-0.864459
0	-3.345229	4.390386	1.060187	Н	-2.526118	5.139874	-1.85516
С	-4.133573	-1.265266	0.908692	Н	-2.532815	6.263637	-0.460703
С	-3.354691	-2.56227	0.841358	Н	-3.645224	-0.615372	1.637995
0	-3.914723	-3.421221	-0.028025	Н	-5.128533	-1.513837	1.296576
0	-2.359121	-2.834459	1.488555	Н	-2.223254	-4.406064	-0.71987
С	-3.186715	-4.64079	-0.262524	Н	-3.035051	-5.184615	0.672293
Η	-4.214811	2.010564	0.341484	Н	-3.804209	-5.221139	-0.947476
Η	-2.032011	2.219882	1.82853				
Η	-1.612736	2.715253	-1.193926				
Η	0.796317	-2.181827	-1.312937				

Table S10. Atomic coordinates (Å) of 3-4 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.

С	-2.741717	-0.666045	-1.438733	Η	1.083615	-2.745604	-0.062543
С	-2.310669	1.87572	-0.90264	Н	0.395446	1.312848	2.470357
C	-0.999385	-0.030994	0.081966	H	0.737608	1.979672	0.878608
С	-1.324888	-0.89213	-0.916478	Н	3.006452	1.569902	1.327184
С	0.279491	-0.155577	0.845111	Н	2.636284	0.557557	2.710401
С	1.41992	-0.585294	-0.149408	Н	2.612853	-1.422983	1.440584
С	1.025244	-1.926744	-0.790438	Н	1.91184	1.431506	-0.904371
С	-0.399133	-1.929626	-1.371615	Н	2.377547	0.112321	-1.974998
С	0.873213	1.096836	1.509957	Н	0.687019	0.591959	-1.859498
C	2.377934	0.738412	1.663529	Н	-0.19585	-2.195056	1.567657
C	2.656637	-0.536561	0.794611	Н	0.840718	-1.267746	2.668805
C	1.60352	0.453107	-1.28106	Н	-0.883948	-0.892243	2.527304
C	0.004806	-1.198242	1.967806	Н	4.159559	0.394443	-0.429606
0	-0.725929	-2.7986	-2.183496	Н	5.365385	-1.69536	-1.130387
C	-2.079717	0.955225	0.307519	Н	3.675929	-1.738039	-1.603678
C	4.068473	-0.52065	0.172456	Н	4.212697	-2.665695	-0.195065
C	4.343733	-1.722454	-0.739982	Н	4.888145	0.404642	1.956324
C	5.116664	-0.44118	1.302619	Н	5.051538	-1.346039	1.920661
С	6.575923	-0.292119	0.825455	Н	7.217864	-0.115102	1.695808
С	6.737985	0.861437	-0.133408	Н	6.933734	-1.191238	0.321529
0	6.443674	2.047028	0.449834	Н	6.540002	2.735044	-0.236373
0	7.063249	0.775866	-1.301526	Н	-3.839492	-0.30849	-3.282996
С	-2.808691	-0.504198	-2.966383	Н	-2.456885	-1.41385	-3.458944
C	-3.678603	-1.833706	-1.026834	Н	-2.185505	0.330404	-3.302092
С	-3.143063	0.623687	-0.702258	Н	-4.705085	-1.569566	-1.304961
С	-2.991121	3.166097	-0.608185	Н	-3.395517	-2.707482	-1.621169
С	-2.577908	4.350426	-1.449973	Н	-2.744731	4.132727	-2.511908
0	-3.837808	3.256555	0.274664	Н	-3.142208	5.238674	-1.160352
С	-3.643038	-2.257679	0.453223	Н	-1.503682	4.537042	-1.329234
С	-4.109555	-1.220394	1.450908	Н	-4.296604	-3.13141	0.569828
0	-5.320633	-0.725182	1.12529	Н	-2.637562	-2.559784	0.751013
0	-3.498354	-0.875867	2.445665	Н	-6.831169	0.527228	1.628665
C	-5.807599	0.347491	1.955771	Н	-5.783328	0.060354	3.008489
Н	-4.188245	0.79773	-0.479434	Н	-5.196455	1.24079	1.798604
Η	-2.292345	1.364392	1.287827				
Η	-1.547505	1.887842	-1.674279				
Η	1.687545	-2.208879	-1.612406				

Table S11. Atomic coordinates (Å) of 3-5 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.
C	2.632342	0.016763	1.567426	Н	-1.761599	-1.181504	1.800101
C	2.698618	1.835883	-0.334578	H	-0.71321	0.401955	-2.644578
С	0.806003	0.219608	0.026269	Η	-0.549544	1.893254	-1.725449
C	1.124582	-0.005684	1.327335	H	-2.894586	2.031481	-1.740309
C	-0.596642	0.101818	-0.475209	Н	-3.073982	0.382005	-2.311087
C	-1.572921	0.654939	0.62704	Н	-3.183504	-0.521043	-0.139376
C	-1.372519	-0.161866	1.914092	Н	-0.260255	2.286415	1.305477
С	0.101333	-0.278745	2.337009	Н	-1.431554	2.790969	0.084368
C	-1.014466	0.903143	-1.719614	Н	-1.955947	2.485149	1.738368
С	-2.559618	1.001834	-1.574575	Н	-0.785573	-2.031133	0.09727
C	-2.929411	0.543835	-0.124816	Н	-1.75713	-1.578605	-1.317405
С	-1.282621	2.139077	0.948554	Н	-0.000112	-1.748233	-1.450244
С	-0.809911	-1.406451	-0.799109	Н	-3.935299	2.365038	0.403628
0	0.382492	-0.60771	3.491964	Н	-4.505179	-0.164055	2.038412
C	2.013701	0.530053	-0.771187	Н	-5.45518	1.323647	2.185781
С	-4.156318	1.289563	0.435815	Η	-3.73716	1.328079	2.584778
C	-4.478244	0.921686	1.892078	Н	-6.16959	1.809769	-0.119322
C	-5.405761	1.100053	-0.457809	Н	-5.174905	1.361496	-1.49529
C	-6.054249	-0.298982	-0.437171	Н	-6.25544	-0.632422	0.58258
С	-5.258063	-1.352915	-1.169386	Н	-7.018797	-0.236619	-0.955518
0	-4.99811	-2.435169	-0.400371	Н	-4.495177	-3.064962	-0.953017
0	-4.88875	-1.276093	-2.326124	H	4.144859	0.962676	2.812782
C	3.053854	0.956603	2.70902	H	2.613184	0.627326	3.653049
C	3.166174	-1.407249	1.880625	H	2.724968	1.982328	2.515982
С	3.158131	0.494013	0.202944	Н	4.26072	-1.367633	1.915157
С	3.583628	2.46848	-1.349988	Н	2.818941	-1.675514	2.882828
C	3.643132	3.97784	-1.34129	Н	3.974697	4.334405	-0.358455
0	4.224699	1.794395	-2.14951	Н	4.324074	4.336772	-2.115132
C	2.72485	-2.534305	0.928602	Н	2.640815	4.391348	-1.507168
С	3.197285	-2.415902	-0.503909	Н	3.120035	-3.480435	1.319551
0	4.529886	-2.223934	-0.575717	Н	1.637299	-2.620913	0.901155
0	2.486571	-2.504569	-1.488215	Н	4.722579	-1.017811	-2.261367
С	5.063223	-1.990228	-1.894334	Н	6.146142	-1.991055	-1.774798
Η	4.1451	0.184396	-0.116784	Н	4.74969	-2.778242	-2.581287
Η	2.105256	0.248467	-1.813297				
Η	2.137062	2.502906	0.311882				
Η	-1.902682	0.267764	2.767534				

Table S12. Atomic coordinates (Å) of 3-6 obtained at the Cam-B3LYP/6-311+G(d,p) level of theory in the MeOH.

Uncropped images of western blot



Figure S82. Uncropped images of western blot in figure 5 of paper.

Figure S83. Uncropped images of western blot in figure S6 of Supplementary information.



Figure S84. Uncropped images of western blot in figure 6 of paper.



References:

- [1] X. Peng, R. Luo, X. Ran, Y. Guo, Y. G. Yao, M. Qiu, Bioorg. Chem. 2023, 132, 106375.
- [2] L. Feng, Y. Ma, J. Sun, Q. Shen, L. Liu, H. Lu, F. Wang, Y. Yue, J. Li, S. Zhang, X. Lin, J. Chu, W. Han, X. Wang, H. Jin, *Autophagy* 2014, *10*, 1442-1453.
- B. Ravikumar, C. Vacher, Z. Berger, J. E. Davies, S. Luo, L. G. Oroz, F. Scaravilli, D. F. Easton, R. Duden, C. J. O'Kane, D. C. Rubinsztein, *Nat. Genet.* 2004, *36*, 585-595.