

B. Structure elucidation of mutaxanthenes

ELECTRONIC SUPPLEMENTARY INFORMATION

Antimicrobial drug resistance affects broad changes in metabolomic phenotype in addition to secondary metabolism

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1. Putative mutaxanthene gene cluster

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A. Metabolomic analysis of microbial extracts

1. Mutational analysis of antibiotic resistant mutants. PCR of antibiotic resistance genes was performed using Taq DNA polymerase (Roche) and the primers listed in table S1. PCR products were purified and sequenced using BigDye Terminator chemistry and resolved on the ABI 3730xl or 3730 DNA analyzers. UPLC-IM-MS of mutants

Table S1. Primers used in this study.

Gene	Primer name	Sequence
<i>rpsL</i>	rpslf	5'-rtgccwacsatycagcag-3'
	rpslr	5'-yccytcttvgcgcgtar-3'
<i>rpoB</i>	rpobb1f	5'-ttggcagtctctcccgcaa-3'
	rpobb1r	5'-gacacgtccatgttagtcg-3'
	rpobb2f	5'-ccgttcggcttcatcgag-3'
	rpobb2r	5'-tgcacgacgtcgccaccga-3'

Table S1B. Mutations in rifampicin (R1-R5) and streptomycin (S1-S6) cohort

Organism	gene	mutation
R1	<i>rpoB</i>	G3280A
R2	<i>rpoB</i>	G3280A
R3	<i>rpoB</i>	G3280A
R4	<i>rpoB</i>	G3280A
R5	<i>rpoB</i>	G3280A
S1	<i>rpsl</i>	No mutation
S2	<i>rpsl</i>	No mutation
S3	<i>rpsl</i>	A43G, C9G, G10C
S4	<i>rpsl</i>	C9G, G10C, G129C
S5	<i>rpsl</i>	No mutation
S6	<i>rpsl</i>	C9G, G10C

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2. Liquid chromatography-ion mobility-mass spectrometry conditions. LC-IM-MS and LC-IM-MS^E analyses were performed on a SYNAPT G2 HDMS (Waters, Milford, MA) mass spectrometer equipped with a nanoAcuity UPLC and autosampler (Waters, Milford, MA). Metabolites were separated on a 1 mm X 100 mm HSS C18 (1.8 μ m particle size) column and 1 mm X 20 mm HSS C18 (5 μ m particle size) guard column. Column temperature was maintained at 40°C to minimize chromatographic drift, and the auto-injector sample tray held at 4°C to minimize sample degradation. A double-loop injection volume of 10 μ L was injected in a 5 μ L loop. Chromatographic separations were performed by using a 20 min gradient at a flow rate of 60 uL/min using a gradient mixer of 0.1% formic acid in H₂O (mobile phase A) and 0.1% formic acid in ACN (mobile phase B). Briefly, the mobile phase was held constant at 100% A for 1 min, then ramped linearly to 100% B over 11 minutes, held for 2 minutes at 100% B, then returned to 100% A over 0.1min for a 5.9 min reequilibration period. All analytes were analyzed using positive mode electrospray ionization. Typical parameters include a capillary voltage of 3.0kV, sampling cone setting of 30.0 and extraction cone setting of 2.0, source temperature of 110°C, desolvation gas (N₂) flow of 700 L/hr, and a cone gas flow of 10 L/hr. Data were acquired in MS^E mode, which acquires both a low energy spectrum and a high energy spectrum. Collision induced dissociation (CID) was performed post mobility separation with a ramped energy profile from 15-40 V in the high CID acquisition. Traveling wave velocity was held constant at 550 m/s and a height of 40.0 V. Data was acquired at a sampling rate of 2 Hz over the mass range 50-2000 m/z. Sodium formate (10 μ g/mL) in 90:10 propan-2-ol:water (v:v) was used to calibrate over this range with < 1 ppm mass accuracy. Leucine enkephalin in 50:50 H₂O:ACN with 0.1% formic acid (v:v) was used as a lock mass compound (accurate mass 278.1141, 556.2771 Da) at a flow rate of 7.0 μ L/min and a concentration of 2 ng/mL every 10 seconds, with data corrected during acquisition. Data acquisition was performed from 0 to 20 minutes of the liquid chromatography separation. Duplicate technical analysis was performed in a randomized fashion; with quality control samples analyzed every 5 injections. Quality control samples contained equal volume aliquots of each sample mixed together.

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3. Multivariate statistical analysis of microbial extracts from *Micrococcus luteus*, *Escherichia coli*, and *Bacillus subtilis*.

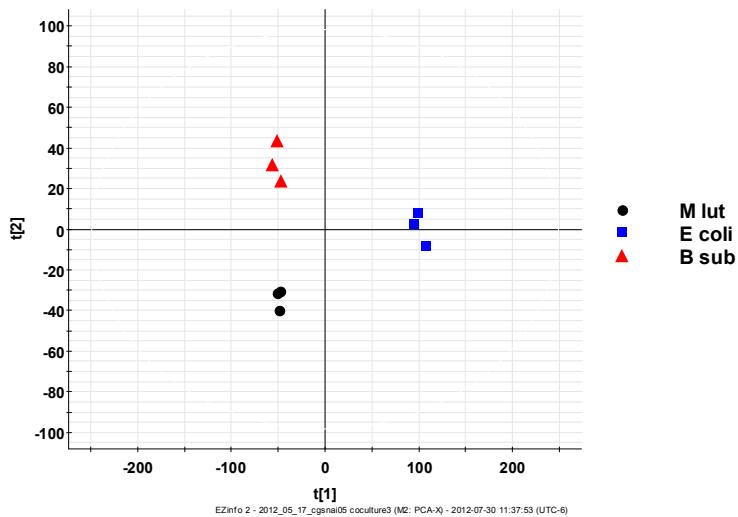


Figure S1. Principal component analysis of microbial extracts from *Micrococcus luteus*, *Escherichia coli*, and *Bacillus subtilis*. Symbols represent technical replicates. The clustering of technical replicates indicates instrument stability. The separation of groups indicates that the three organisms have sufficiently different metabolic profiles that the first two principal components are defined by these differences.

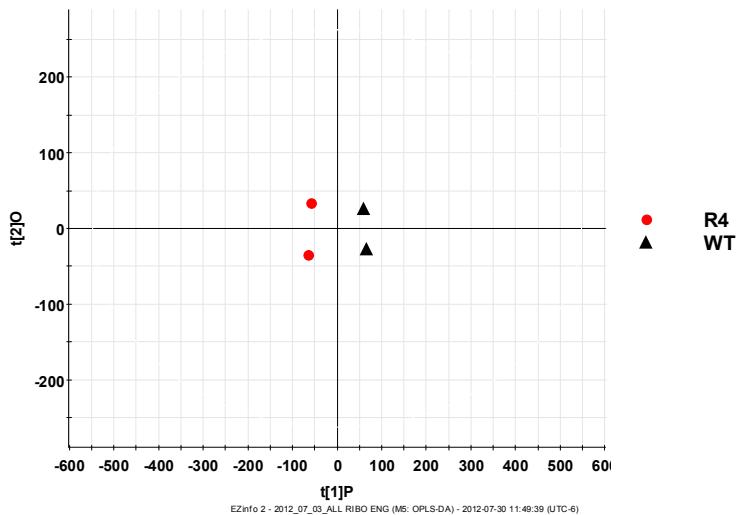


Figure S2. Orthogonal projection to latent structures-discriminant analysis (OPLS-DA) scores plot depicting R4 mutant vs. wild type in a binary fashion. OPLS-DA defines the first principal component as the eigenvector that with maximum eigenvalue of the covariance matrix between the two defined groups (R4 and wild type). The orthogonal vector describes the greatest intragroup differences.

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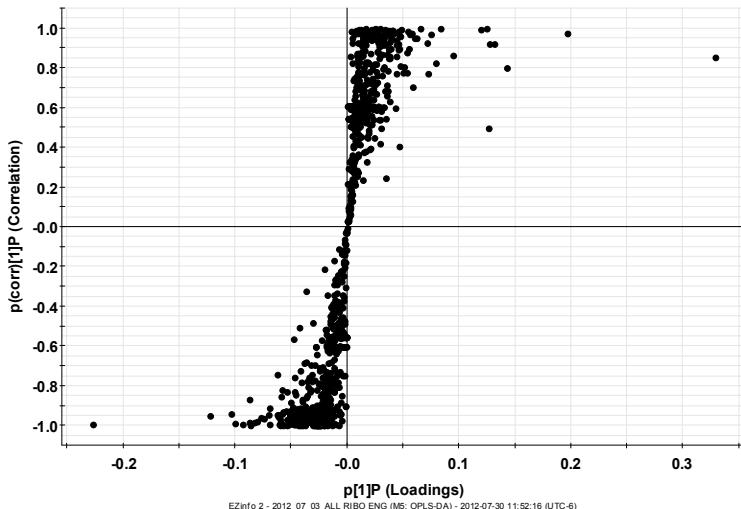


Figure S3. Representative S-plot of R4 mutant (-1) vs. wild type (+1). This S-plot corresponds to figure S2, and is a visualization of loadings contribution. The correlation describes how specific to a particular group in the OPLS-DA a feature is (represented by a black dot). A correlation of 1 is perfect group correlation. The loadings correspond to the contribution of that feature to the first principal component of the OPLS-DA. As a result, outliers in quadrant I and III correspond to high abundance and exclusive features in the wild type and R4 mutant extracts, respectively. For all analyses, a correlation cutoff of ≥ 0.9 was used.

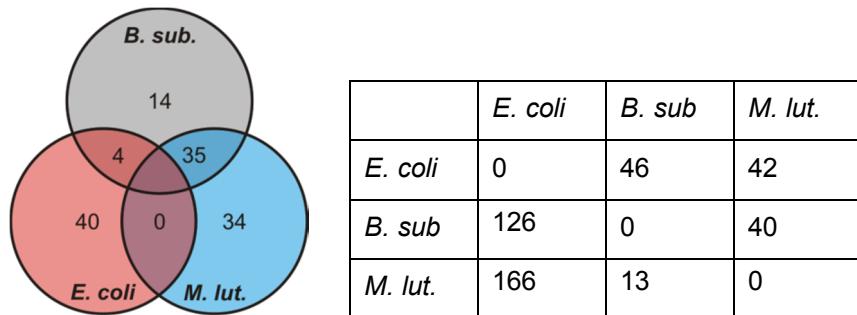


Figure S4. Left: Feature specificity diagram comparing *Bacillus subtilis*, *Escherichia coli*, *Micrococcus luteus*. Pareto scaled OPLS-DA was used, and features with a correlation coefficient ≥ 0.9 were considered specific to a group. There are 963 total features. Groups were permuted in a binary fashion, with two organisms compared against one at a given time. There are 838 shared features. **Right:** Feature specificity matrix comparing *Bacillus subtilis*, *Escherichia coli*, *Micrococcus luteus* in a binary fashion. Pareto scaled OPLS-DA was used and a correlation coefficient of ≥ 0.9 was used as a threshold for feature specific to an organism pair. The bottom half of the matrix corresponds to features specific to the organism indicated in the first column compared to the organism in the first row. The top half of the matrix corresponds to features specific to the organism in the first row when compared to the organism in the first column. There are 963 total features.

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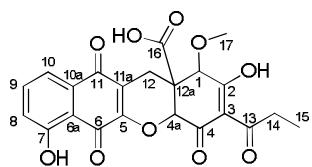
Feature 1 (Fig. 3B, Table S2) was isolated with UV spectrum showing absorption maxima at 225, 252, 279 and 409 nm. The high resolution mass spectrum yielded an apparent m/z of 443.101, $[M+H]^+$. Combining mass with 1H and ^{13}C NMR spectral data (Table S2) determined molecular formula of $C_{22}H_{18}O_{10}$ with 14 degrees of unsaturation. The ^{13}C NMR and HMBC spectra indicated the presence of 22 carbons including one methyl group, one methoxy, two methylene, five methine and thirteen quaternary carbons. The ten olefinic carbons and 5 carbonyls accounted for 10 degrees of unsaturation suggesting the presence of four rings. The 2D NMR spectral data allowed to establish partial structures (I - III) (Fig. 3A). The COSY, HSQC and HMBC NMR correlations indicated that the aromatic ring of fragment a is substituted with the hydroxyl group in C7 position. The chemical shifts of carbons C6 and C11 suggested that they are α,β -unsaturated carbonyls in a ring. The HMBC correlations from aromatic proton H10 to carbon C11 and from aromatic proton H8 to carbon C6 allowed to establish the positions of carbons C6 and C11 in the ring and suggested that they are adjacent to the aromatic ring. The structure of fragment a was confirmed by the feeding experiment with the 1,2- ^{13}C sodium acetate where the incorporation pattern allowed to unambiguously establish the carbon backbone of I. The partial structure II (Fig. 3A) was determined based on 1H and ^{13}C NMR chemical shifts, HMBC and 1,1-ADEQUATE correlations and confirmed with data from incorporation of labeled 1,2- ^{13}C sodium acetate experiment. The HMBC correlations from H12 methylene protons to the quaternary carbons C11a and C12a indicated the position of C12 in the fragment II. The 1,1-ADEQUATE experiment and labeled acetate incorporation pattern further confirmed that C12 is adjacent to C11a and C12a. The chemical shift of methine C1 indicated the presence of neighboring oxygen atom. The HMBC correlations from H1 proton to C17 carbon and from H17 protons to C1 carbon confirmed the presence of the methoxy group attached to the methine C1. The HMBC correlations from proton H1 to carbons C2 and C12a indicated that methine C1 is adjacent to C2 and C12a and this was confirmed by 1,1-ADEQUATE spectral data and labeled acetate incorporation pattern. The chemical shift of methine C4a also indicated the presence of neighboring oxygen. The HMBC correlations from proton C4a to carbons C4 and C12a suggested that they are adjacent and the position of carbon C3 was established based on labeled acetate incorporation pattern which indicated that carbons C2 and C3 are attached. Furthermore the HMBC correlation from proton H1 to carbon C3 allowed assembling another ring within fragment II. The crucial HMBC and 1,1-ADEQUATE correlations from protons H12 to carbon C11a and from proton C4a to carbon C5 determined the connectivity between fragments I and II and allowed to assemble the last ring which turned out to be unusual xanthene scaffold. Finally, the position of carboxylic acid moiety in fragment II was established based on HMBC correlations from H12 methylene protons, H4a methine proton and H1 methine proton to C16 carbon. The last partial structure III (Fig. 3A) was determined based on COSY correlations between methyl C15 and methylene C14 and HMBC from C14 protons to C13 ketone. Furthermore, the HMBC correlations from C14 methylene protons to C3 quaternary carbon allowed assembling fragment II with

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fragment **III** and as result we proposed the final structure (Fig 3B). Mutaxanthene B (**2**) was assigned to the molecular formula of $C_{23}H_{20}O_{10}$ by HR-MS (m/z 457.115, $[M + H]^+$). Comparison of 1H and ^{13}C NMR spectra of compounds **1** and **2** revealed the presence of the additional methoxy group (δ_H 3.96, δ_C 56.9) which showed the HMBC correlations to two olefinic carbons (C7 and C8) in the aromatic ring (Table S3). The molecular formula of mutaxanthene C (**3**) was established as $C_{21}H_{16}O_{10}$ by HR-MS of m/z 429.085, $[M + H]^+$. Comparison of 1H and ^{13}C NMR spectra revealed the absence of methylene C14 and significant downfield shift of C15 methyl suggesting replacement of ethyl group with methyl group. The HMBC correlations to C13 and C3 confirmed the structure of **3** (Table S4). Mutaxanthene D (**4**) was assigned to the molecular formula of $C_{22}H_{19}NO_9$. The 1H and ^{13}C NMR spectra of **1** and **4** were very similar with the most significant difference in chemical shift from 208.2 for **1** to 182.5 for **2** for carbon C13 indicating the replacement of ketone group with amino group in this position along with equilibrium shift from endocyclicenol as dominant tautomer for compound **1** and ketone as dominant tautomer for compound **4** (Table S5). The structure of mutaxanthene E (**5**) was established based on molecular formula of $C_{21}H_{17}NO_9$ and comparison of 1H and ^{13}C NMR spectra of **5** to compounds **3** and **4** indicating the presence of amino group in C13 position and methyl group adjacent to C13 carbon (Table S6).

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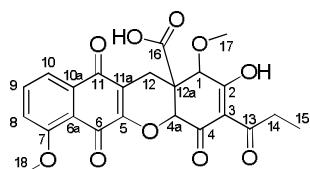
Table S2. NMR spectroscopic data for compound **1** in CD₃OD.



Pos.	¹³ C	¹ H	HMBC	<i>J</i> _{CC} /Hz
1	83.3	4.12, 1H, br	2,3,4a,12,12a, 16,17	br
2	190.2			48.3
3	109.1			60
4	190.8			br
4a	76.3	5.56, 1H, br	1,4,5,12,12a, 16	br
5	154.3			61.6
6	183.9			61.6
6a	114.6			64
7	162.3			64
8	124.7	7.0, 1H, d, 8.3 Hz	6, 6a, 7, 10	58.2
9	137.8	7.43, 1H, br dd, 8Hz	7, 10a	58.2
10	119.6	7.24, 1H, d, 7.2Hz	6a, 8, 11	62.5
10a	132.5			62.5
11	183.3			56.9
11a	120			56.9
12	23.1	2.38, 1H br d, 3.08, 1H, br d, 19Hz	1,4a,5,11,11a,12a,16	33.3
12a	48			33.3
13	208.2			
14	34.5	2.97, 2H, m	3, 13, 15	35.2
15	8.3	1.05, 3H, br t, 7.1Hz	13, 14	35.2
16	172.1			
17	60.9	3.5, 3H, br s	1	

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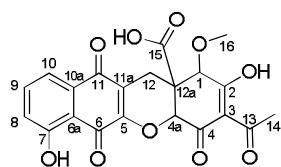
Table S3. NMR spectroscopic data for compound **2** in D₂O.



Pos.	¹³ C	¹ H	HMBC
1	86.0	3.77, 1H, br	2, 3, 4a, 12, 12a, 16, 17
2	188.6		
3	112.2		
4	189.5		
4a	76.5	5.44, 1H, br	4, 5, 12, 12a, 16
5	154.5		
6	179.1		
6a	116.9		
7	159.6		
8	118.5	7.23, 1H, d,	6, 6a, 7, 10
9	136.4	7.52, 1H, brdd,	7, 10a
10	119.0	7.34, 1H, d,	6a, 8, 11
10a	133.1		
11	184.8		
11a	117.6		
12	22.4	2.26, 1H br d, 2.96, 1H, br d,	1, 4a, 5, 11, 11a, 12a, 16
12a	48.2		
13	210.0		
14	35.8	2.55, 2H, m	13, 15
15	8.5	0.89, 3H, br t,	13, 14
16	176.5		
17	59.8	3.43, 3H, br s	1
18	56.2	3.83, 3H, s	7, 8

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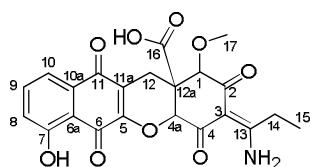
Table S4. NMR spectroscopic data for compound **3** in CD₃OD.



Pos.	¹³ C	¹ H	HMBC
1	82.9	4.17, 1H, br	
2	-		
3	109.6		
4	-		
4a	76.9	5.55, 1H, br	
5	154.4		
6	178.4		
6a	114.9		
7	162.6		
8	124.5	7.24, 1H, d,	6a, 7, 10
9	137.7	7.65, 1H, brdd,	7, 10a
10	119.4	7.56, 1H, d,	6a, 8,11
10a	132.9		
11	183.4		
11a	119.9		
12	23.0	2.50, 1H br d, 3.19, 1H, br d,	1, 4a, 5,6, 11, 11a, 12a, 16
12a	48.1		
13	203.7		
14	27.4	2.56, 3H, s	3, 13
15	172.0		
16	60.7	3.57, 3H, br s	

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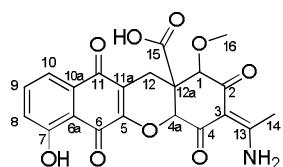
Table S5. NMR spectroscopic data for compound **4** in D₂O.



Pos.	¹³ C	¹ H	HMBC	<i>J_{CC}</i> /Hz
1	85.7	3.82, 1H, s	2, 3, 4a, 12, 12a, 16, 17	45.5
2	192.5			45.5
3	102.3			61.2
4	192.2			61.2
4a	77.2	5.43, 1H, d	1, 4, 5, 12, 12a, 16	
5	153.4			61.0
6	183.1			61.0
6a	113.3			64.5
7	160.0			64.5
8	123.8	7.0, 1H, d, 8.3 Hz	6, 6a, 7, 10	58.4
9	137.1	7.43, 1H, dd, 8Hz	7, 10a	58.4
10	119.2	7.22, 1H, d, 7.2Hz	6a, C8, 11	62.8
10a	131.1			62.8
11	183.9			57.6
11a	119.9			57.6
12	22.2	2.17, 1H dd, 2.94, 1H, dd, 19Hz	1, 4a, 5, 11, 11a, 12a, 16	34.4
12a	47.3			34.4
13	182.5			56
14	29.8	2.83, 2H, dq	3, 13, 15	-
15	11.3	1.09, 3H, t, 7.1Hz	13, 14	-
16	175.8			
17	59.9	3.42, 3H, s	1	

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Table S6. NMR spectroscopic data for compound **5** in D₂O.



Pos.	¹³ C	¹ H	HMBC
1	85.3	3.83, 1H, s	2, 3, 4a, 12, 12a, 16, 17
2	192.7		
3	103.3		
4	192.3		
4a	77.4	5.42, 1H, d	1, 4, 5, 12, 12a, 16
5	153.7		
6	183.3		
6a	113.6		
7	160.2		
8	123.8	7.15, 1H, d,	6, 6a, 7, 10
9	137.1	7.56, 1H, dd,	7, 10a
10	119.3	7.43, 1H, d,	6a, 8, 11
10a	131.4		
11	184.6		
11a	120.0		
12	22.3	2.26, 1H dd, 2.95, 1H, dd,	1, 4a, 5, 11, 11a, 12a, 16
12a	47.6		
13	177.8		
14	24.2	2.41, 3H, s	13, 3
15	175.9		
16	60.0	3.42, 3H, s	1

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Mutaxanthene A

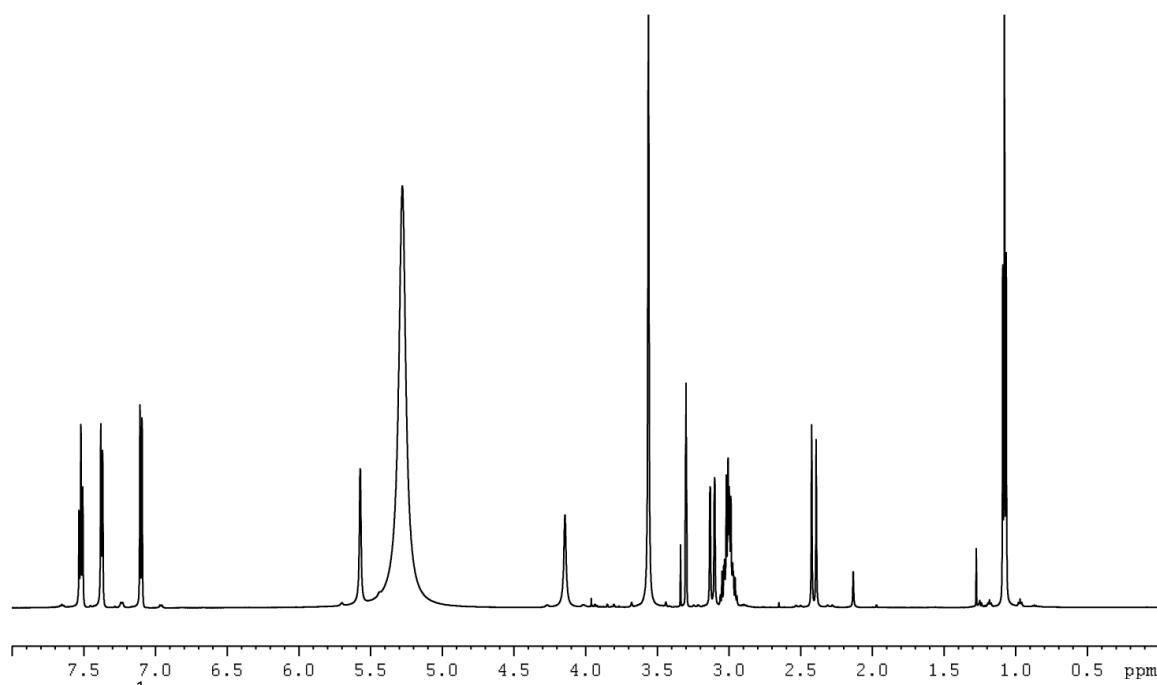


Figure S6. ^1H proton NMR of mutaxanthene A (1) in CD_3OD .

Mutaxanthene A

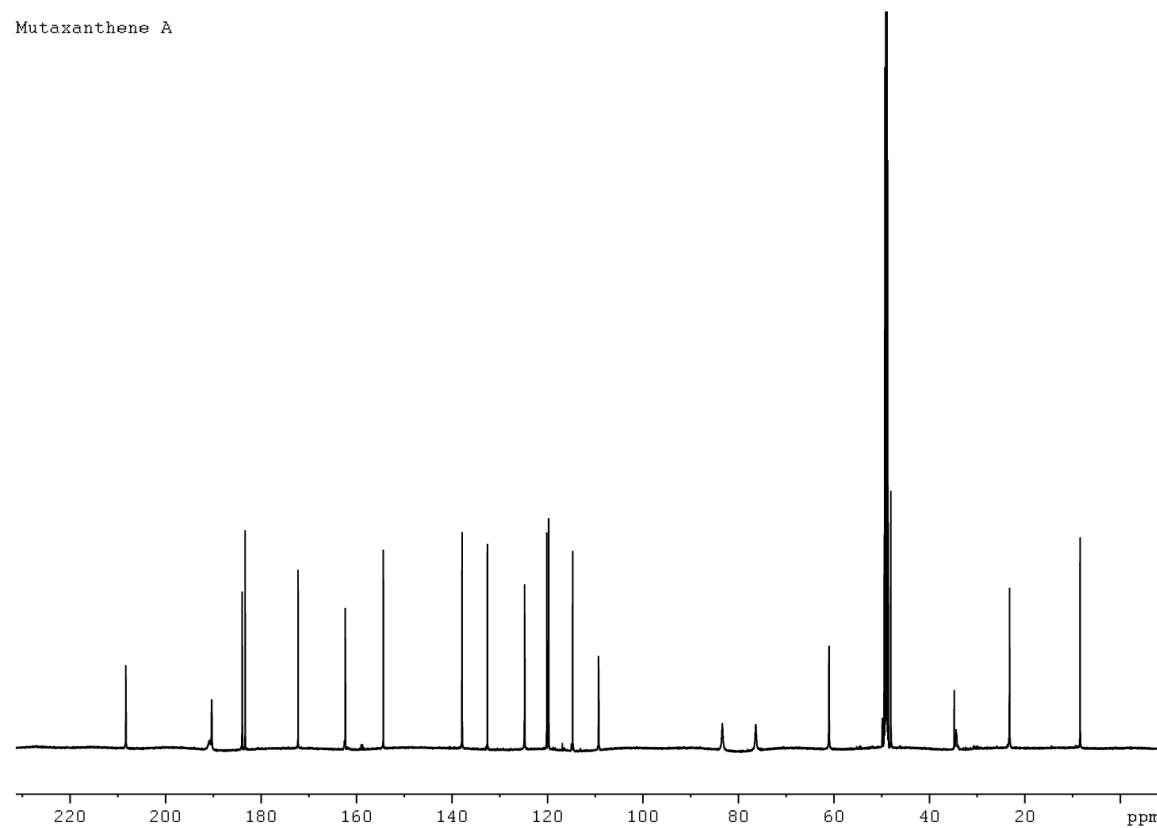


Figure S7. ^{13}C carbon NMR of mutaxanthene A (1) in CD_3OD .

B. Structure elucidation of mutaxanthenes

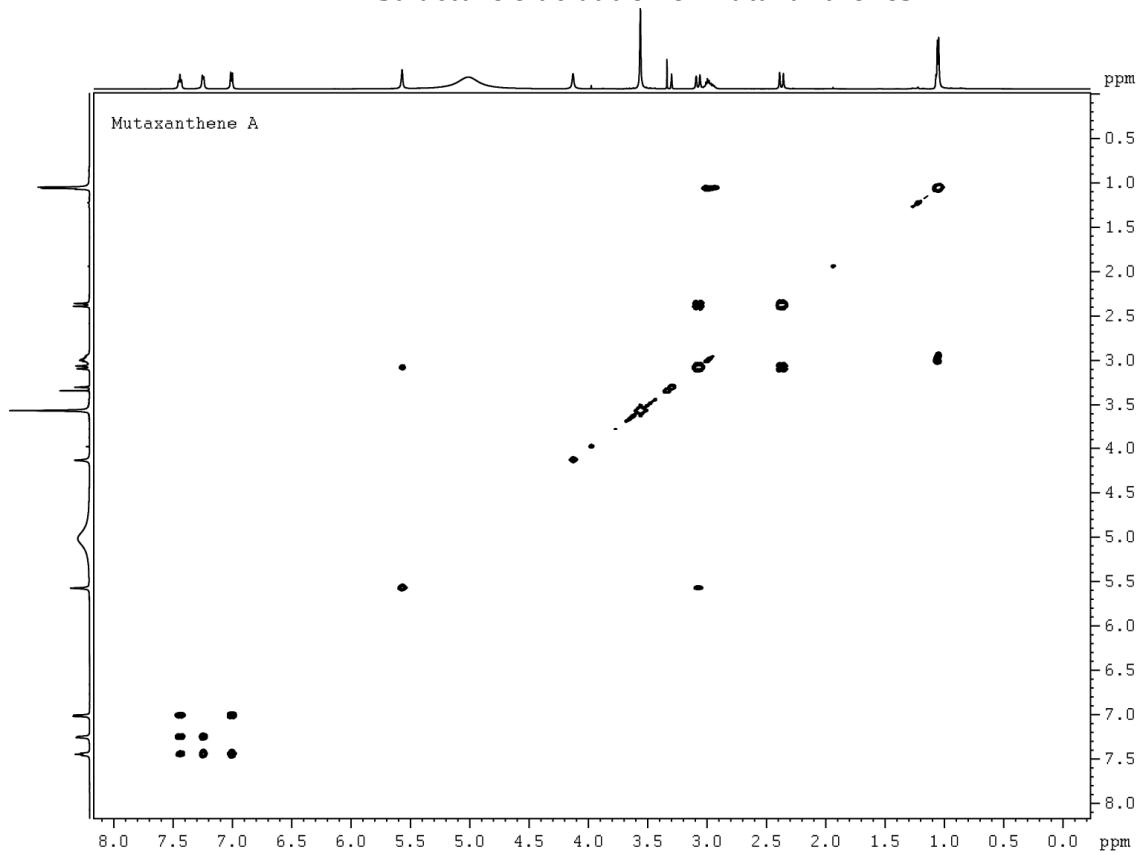


Figure S8. 2D COSY NMR of mutaxanthene A (**1**) in CD_3OD .

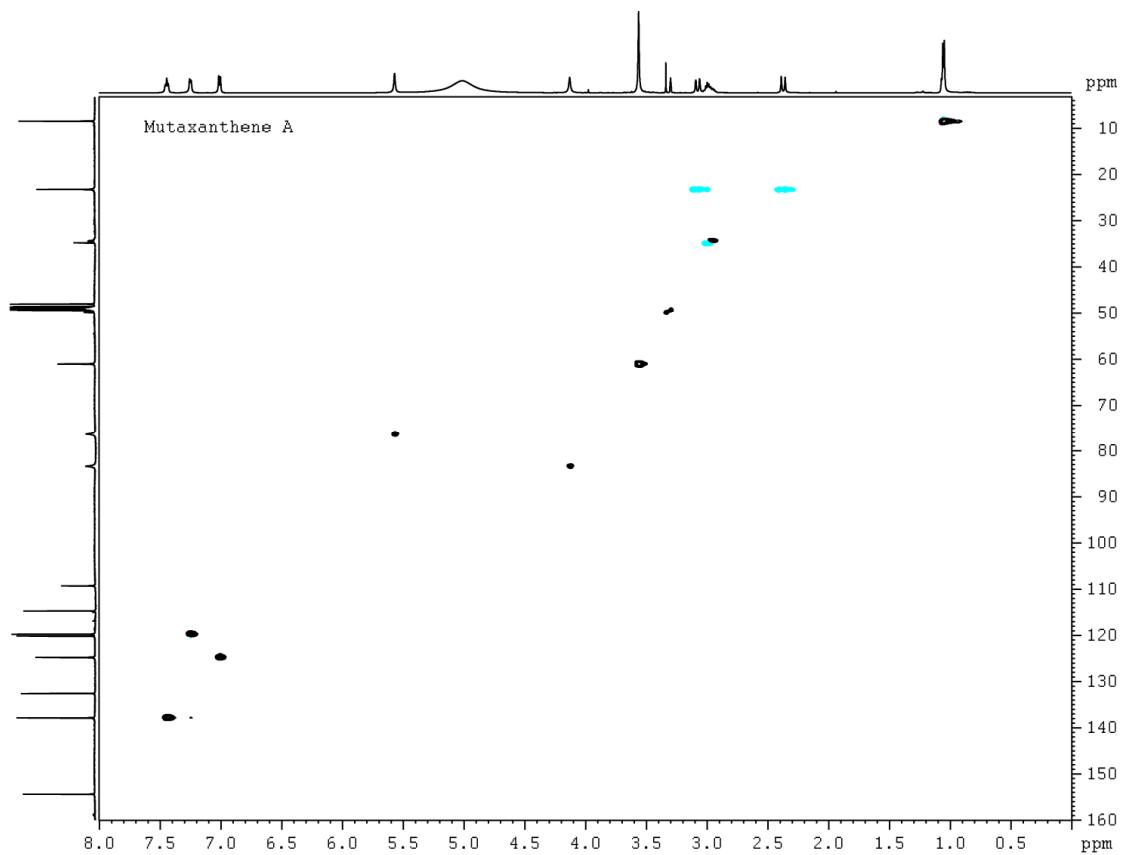


Figure S9. 2D HSQC NMR of mutaxanthene A (**1**) in CD_3OD .

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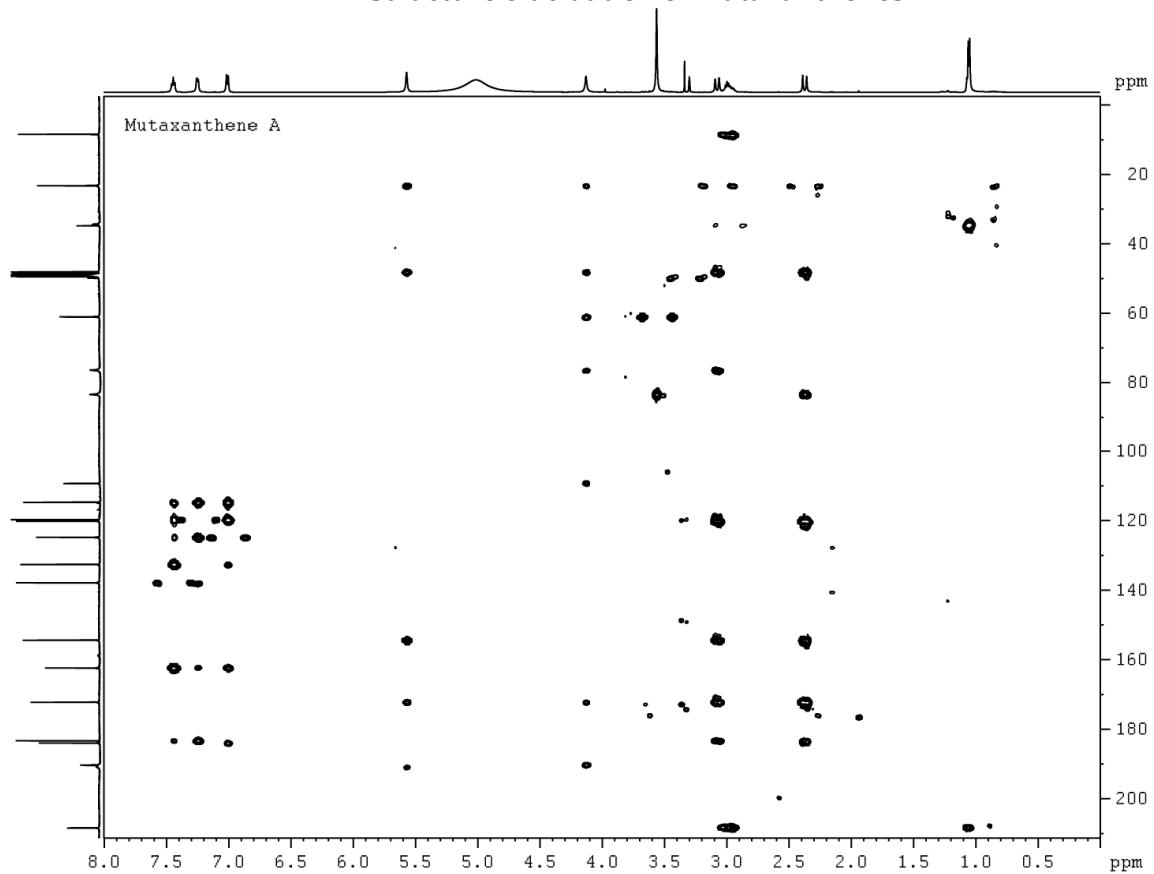


Figure S10. 2D HMBC NMR of mutaxanthene A (1) in CD₃OD.

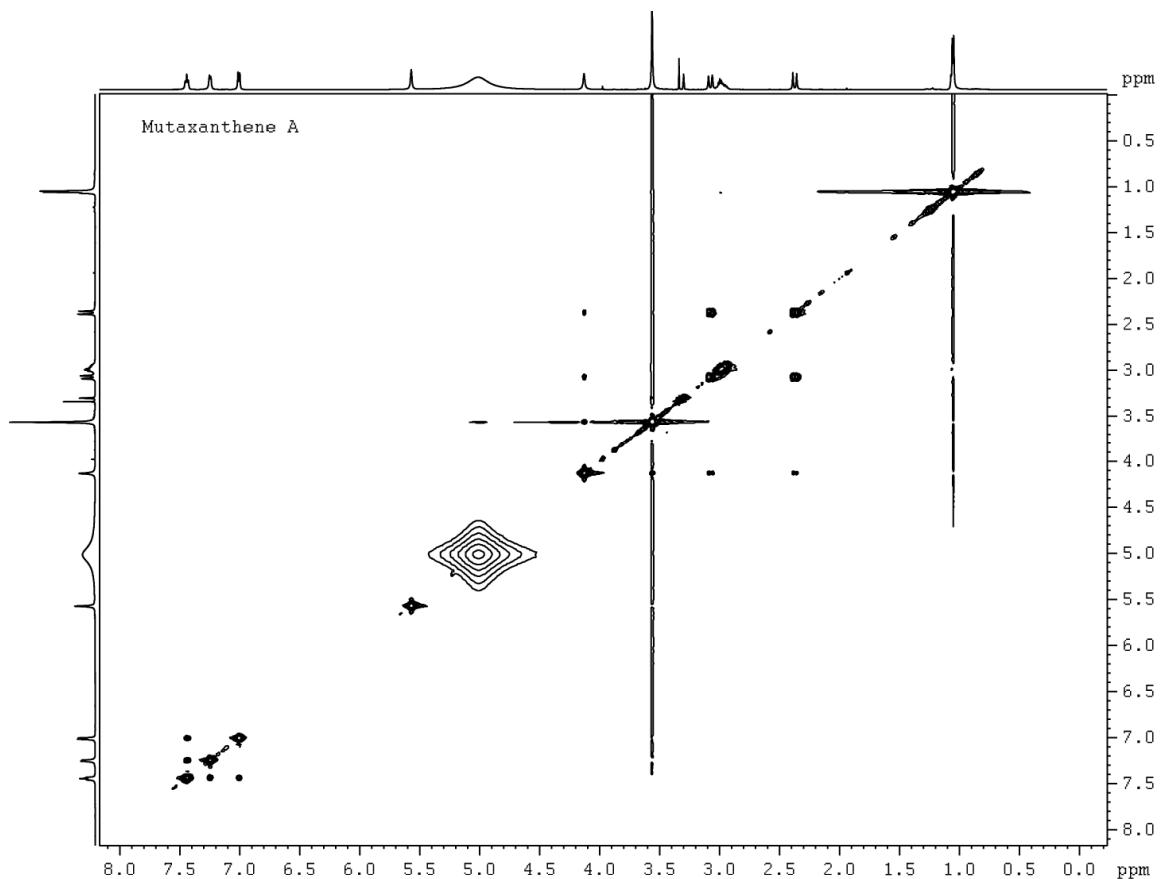


Figure S11. 2D NOESY NMR of mutaxanthene A (1) in CD₃OD.

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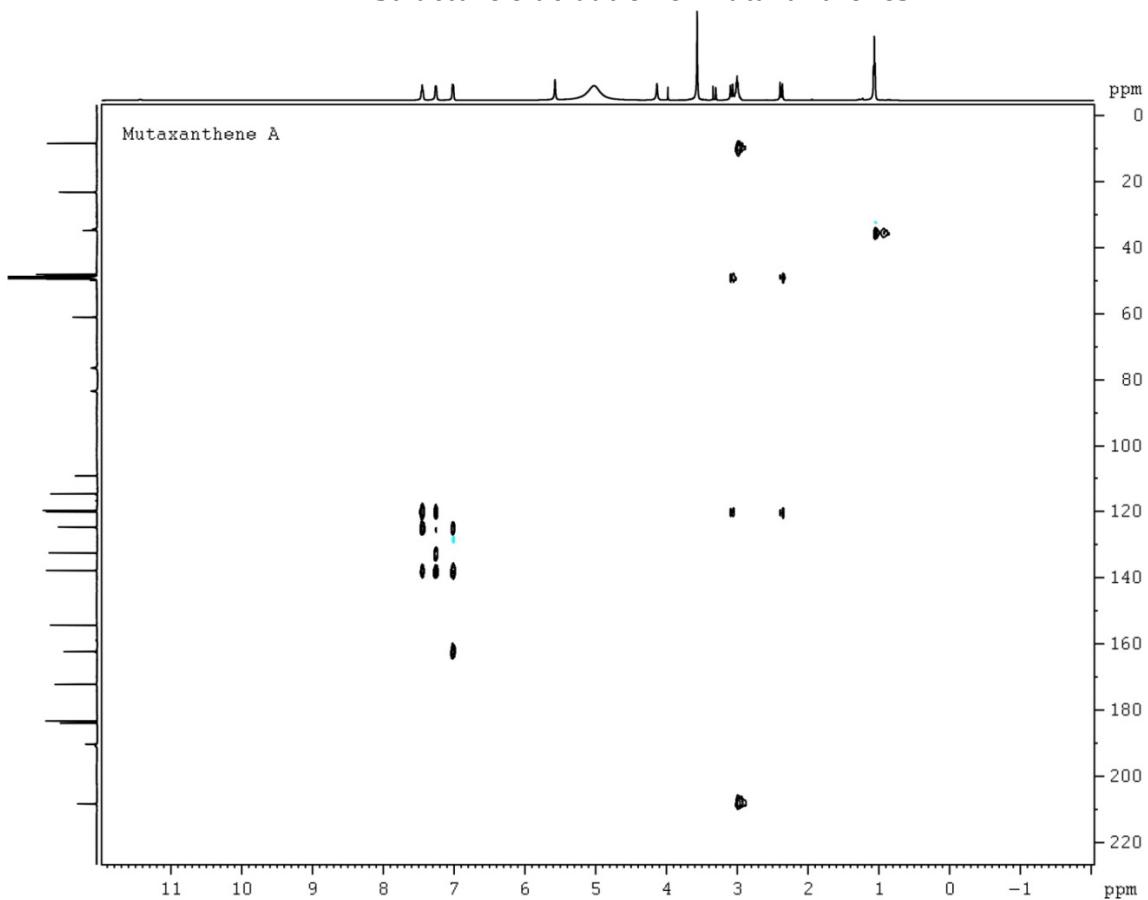


Figure S12. 2D 1,1-ADEQUATE NMR of mutaxanthene A (**1**) in CD_3OD .

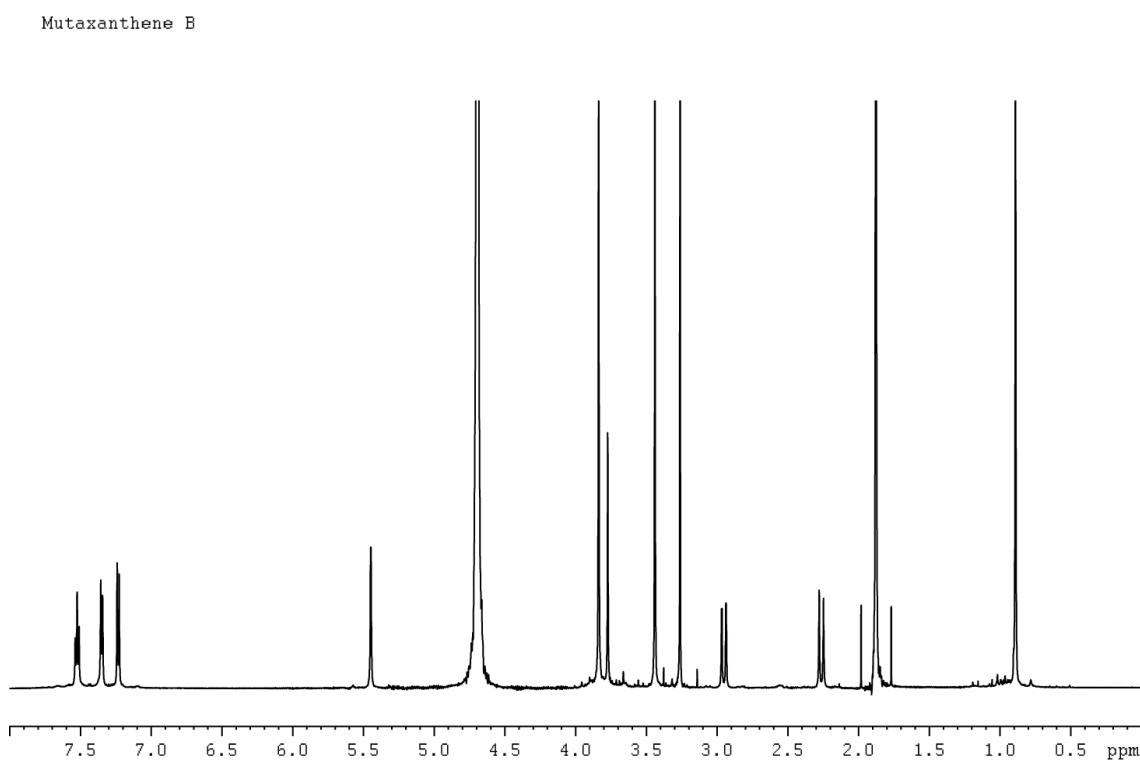


Figure S13. ^1H proton NMR of mutaxanthene B (**2**) in D_2O .

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Mutaxanthene B

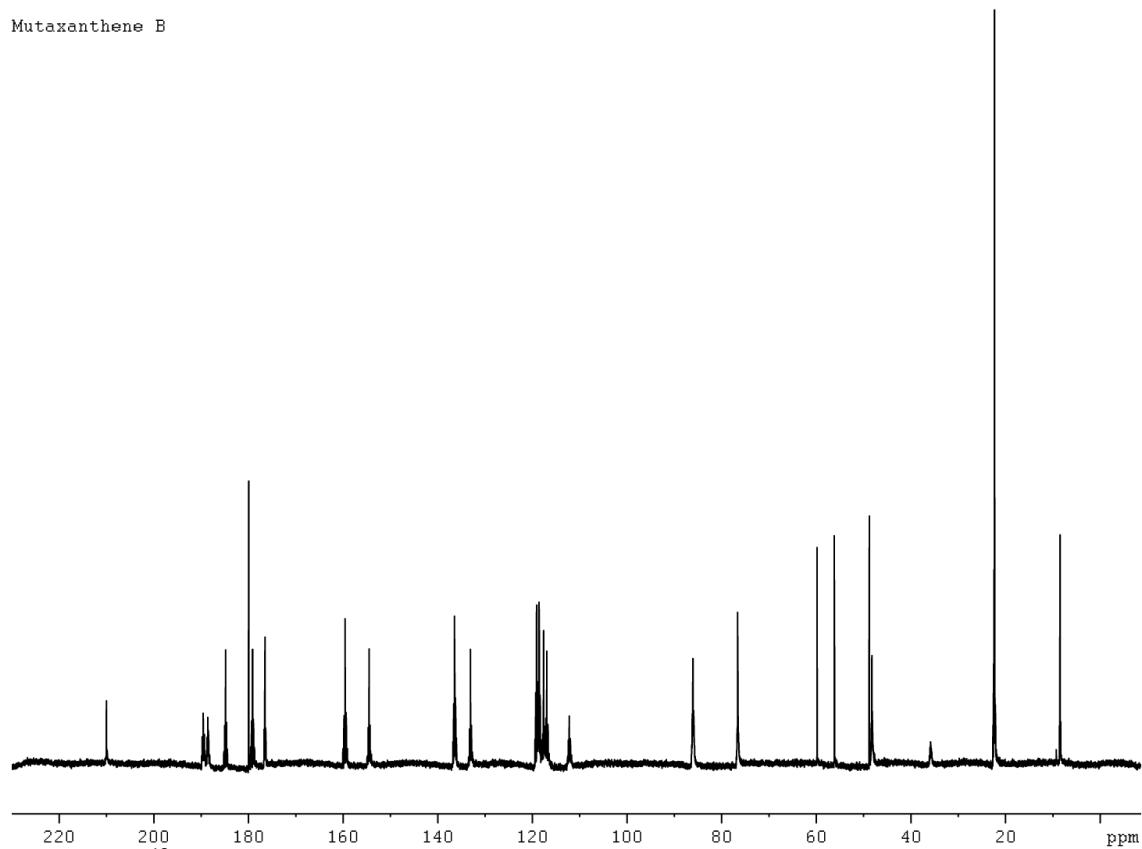


Figure S14. ^{13}C carbon NMR of mutaxanthene B (2) in D_2O .

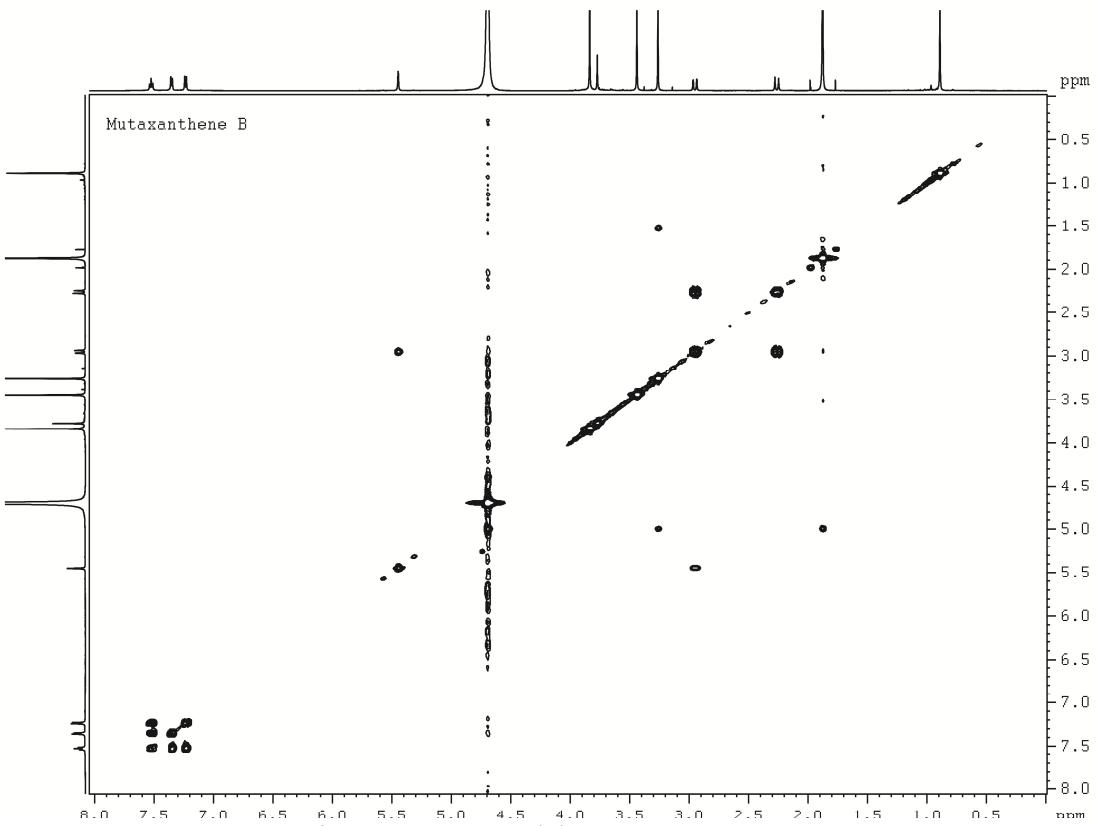


Figure S15. 2D COSY NMR of mutaxanthene B (2) in D_2O .

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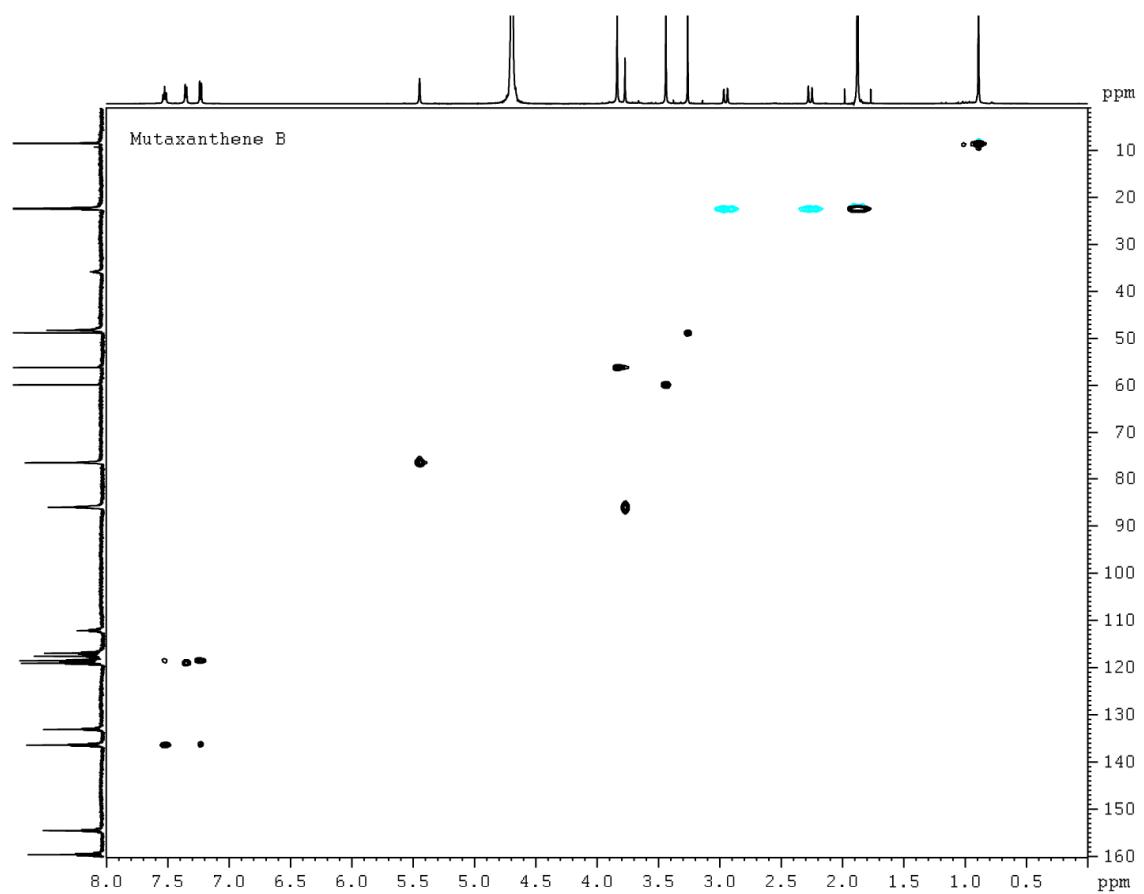


Figure S16. 2D HSQC NMR of mutaxanthene B (2) in D_2O .

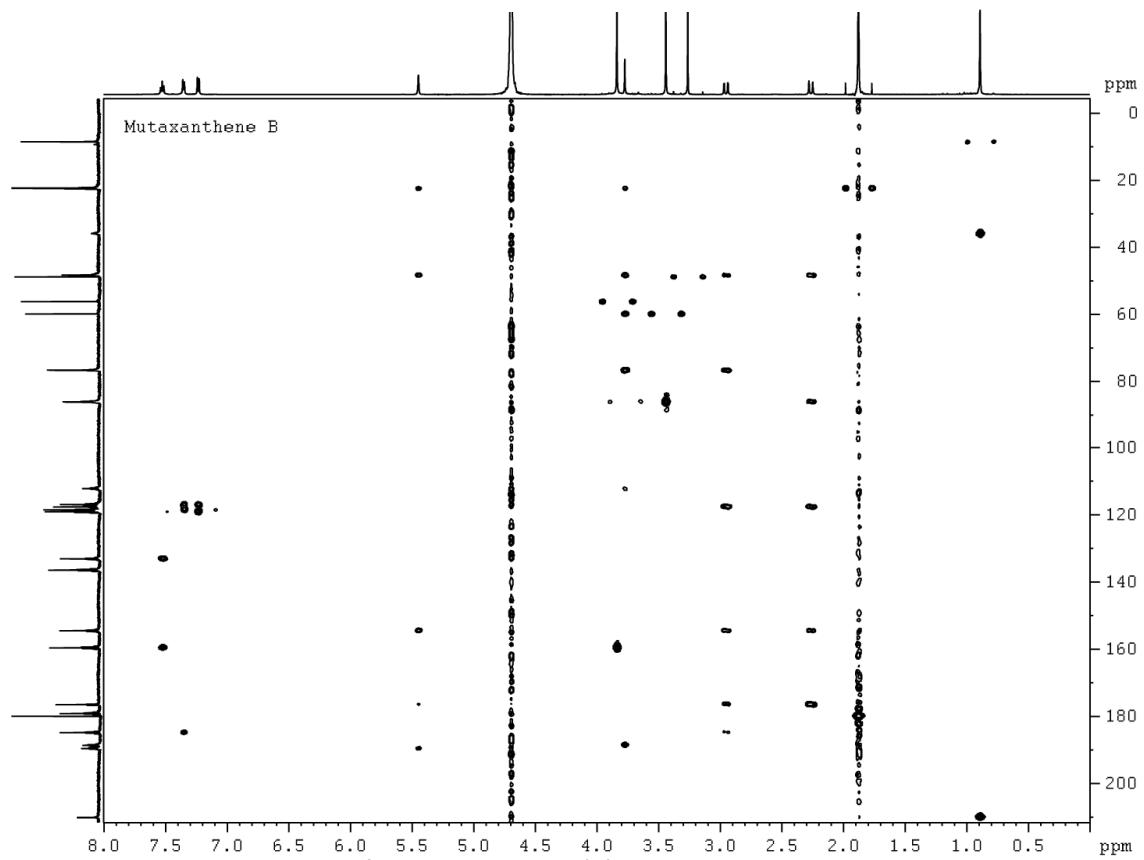


Figure S17. 2D HMBC NMR of mutaxanthene B (2) in D_2O .

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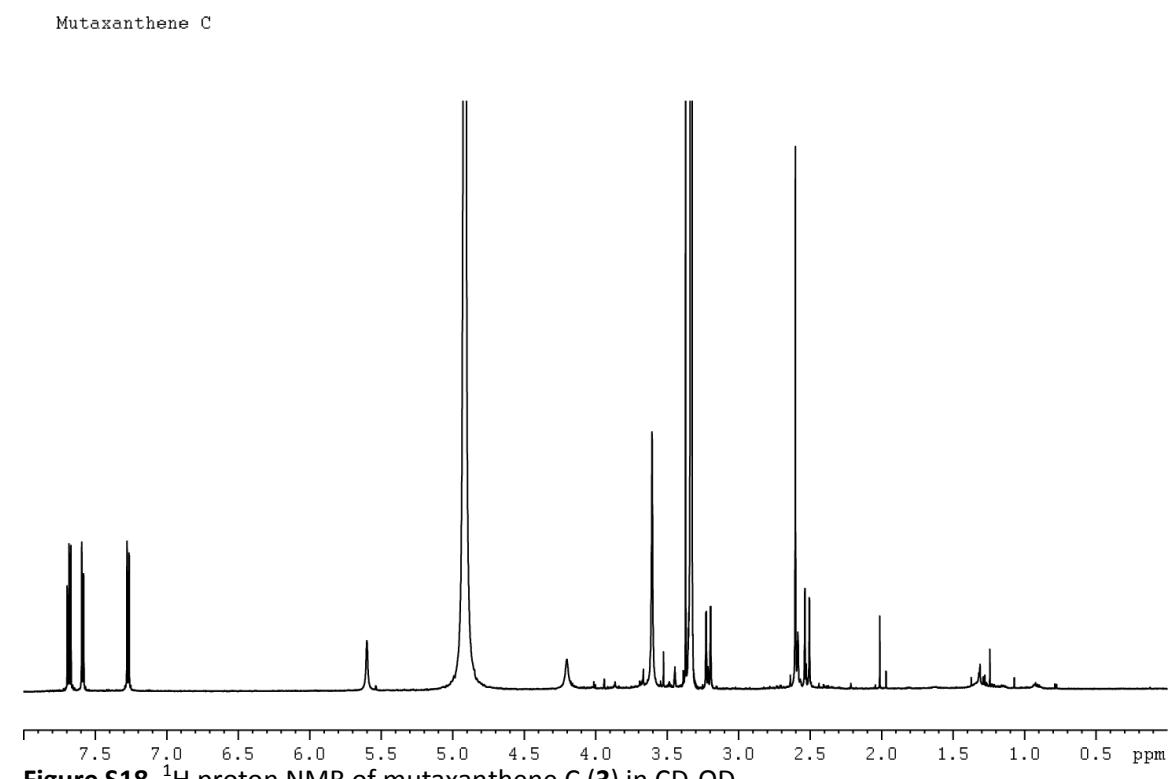


Figure S18. ^1H proton NMR of mutaxanthene C (**3**) in CD_3OD .

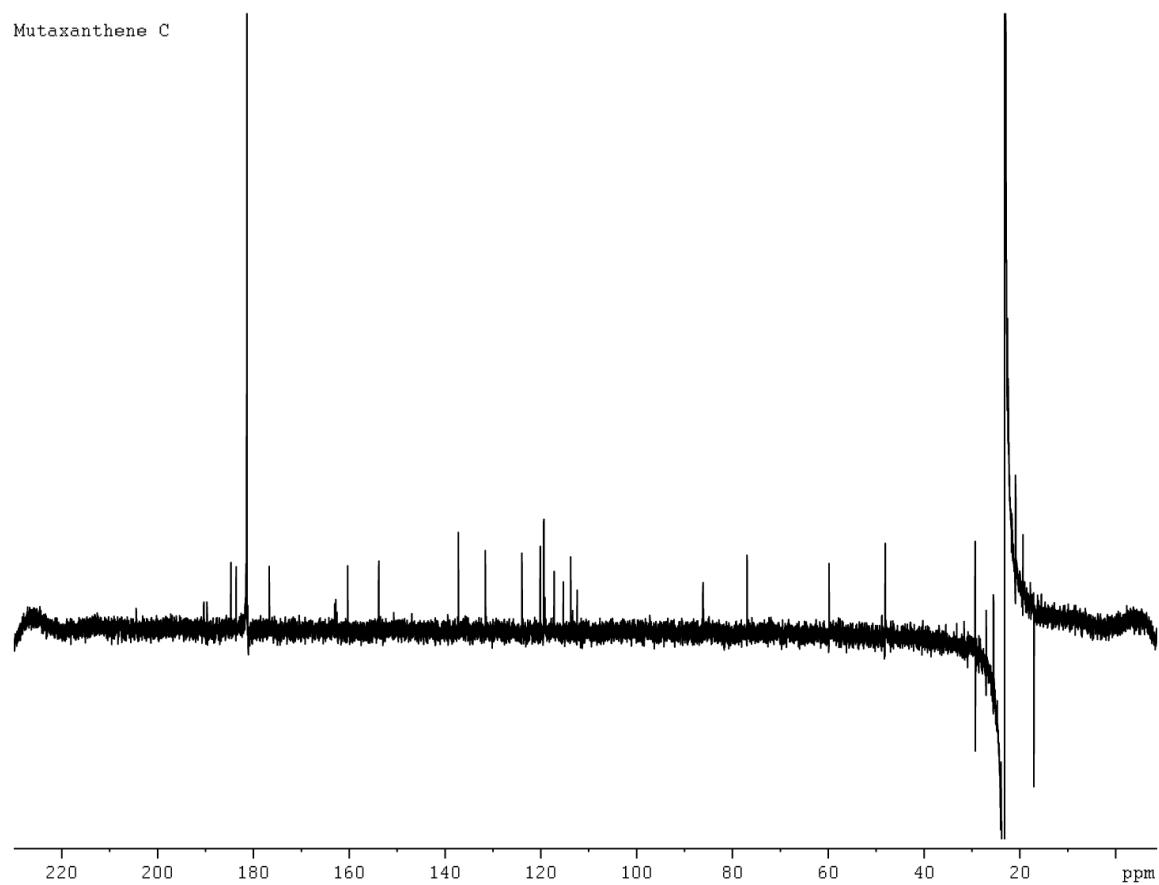


Figure S19. ^{13}C carbon NMR of mutaxanthene C (**2**) in D_2O .

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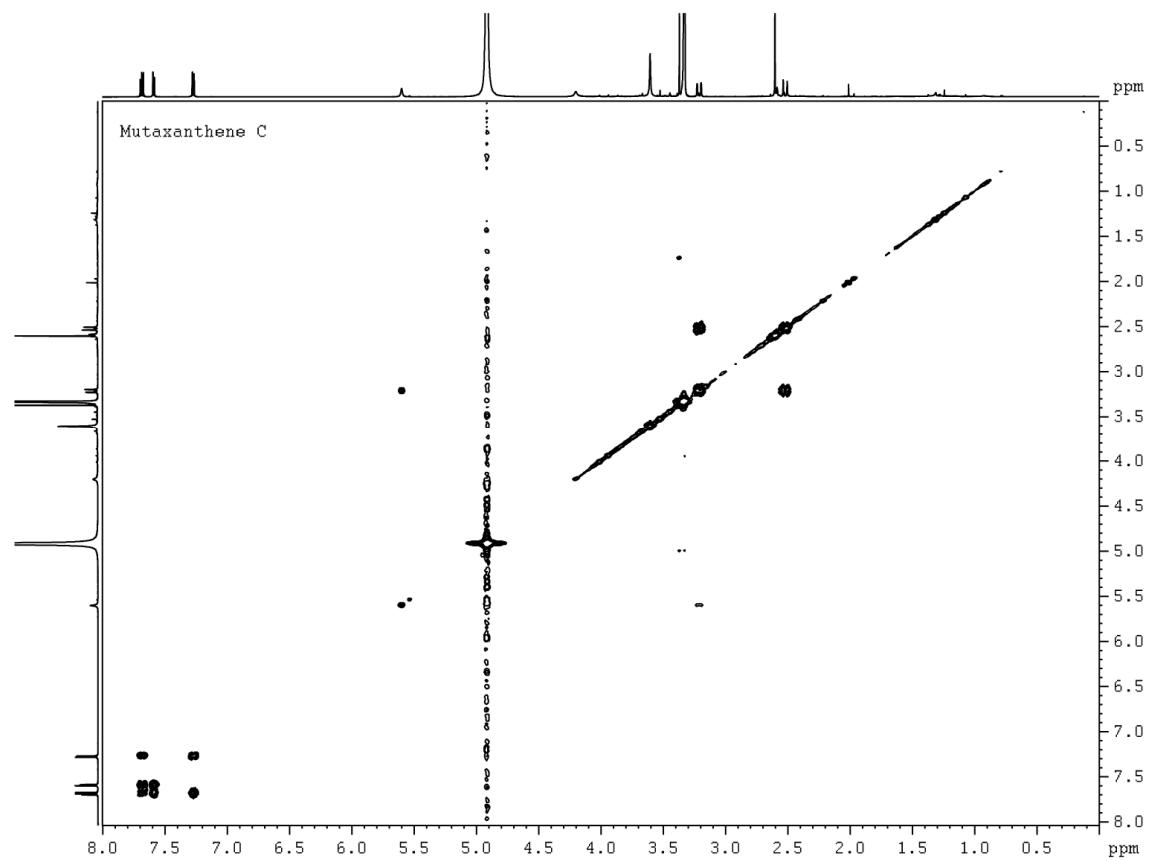


Figure S20. 2D COSY NMR of mutaxanthene C (3) in CD_3OD .

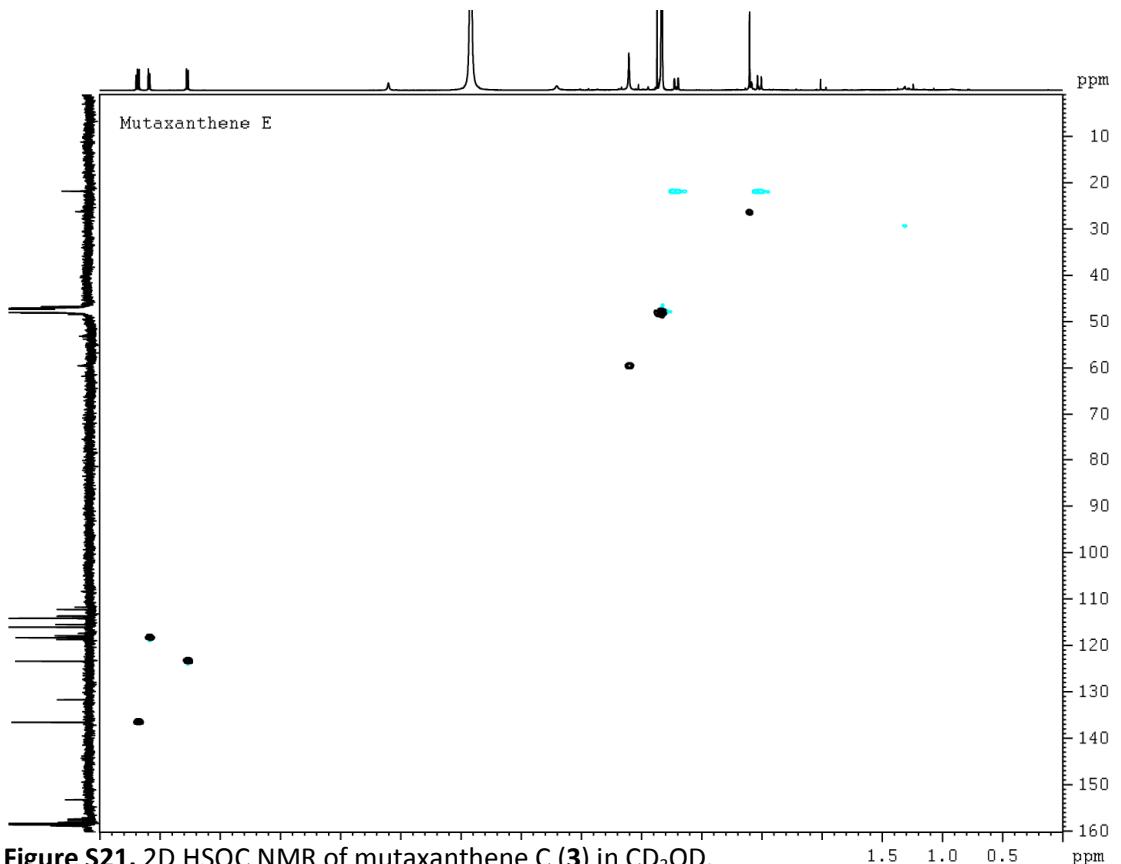


Figure S21. 2D HSQC NMR of mutaxanthene C (3) in CD_3OD .

B. Structure elucidation of mutaxanthenes

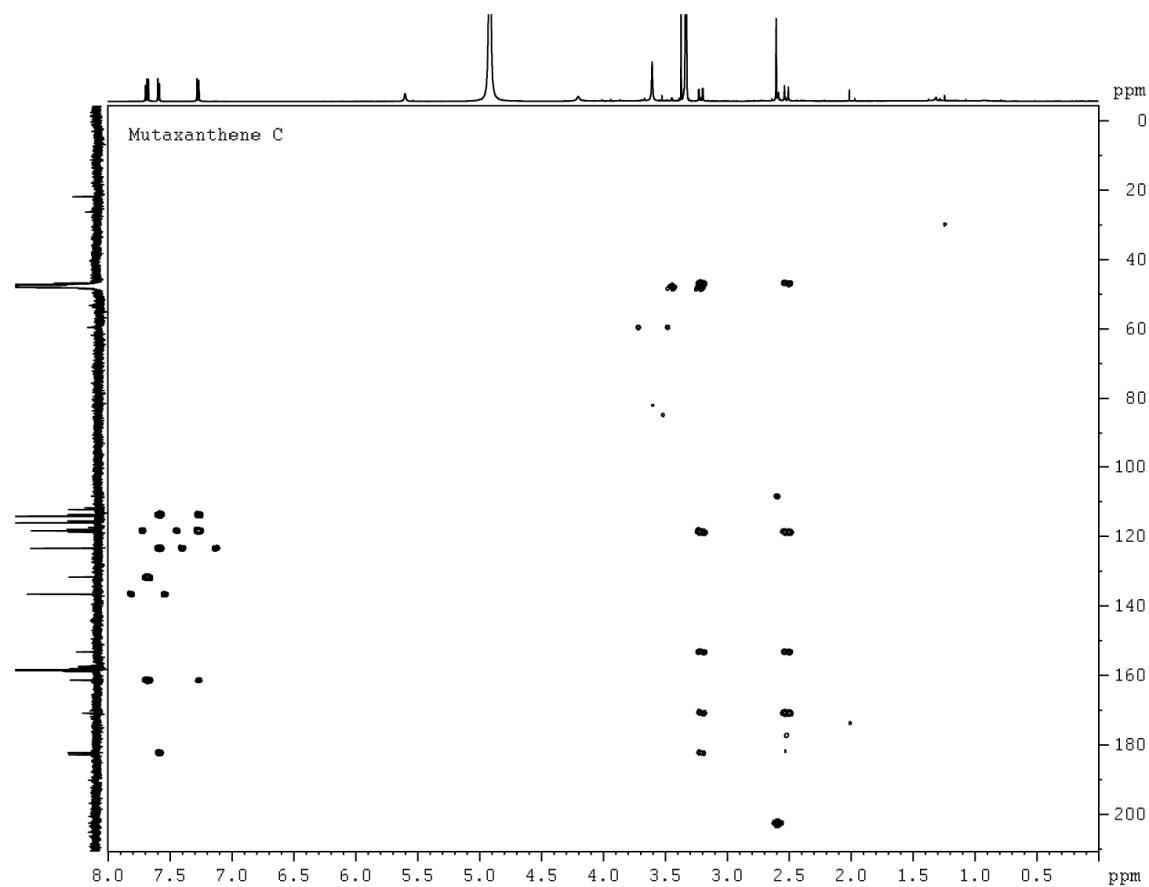


Figure S22. 2D HMBC NMR of mutaxanthene C (3) in CD₃OD.

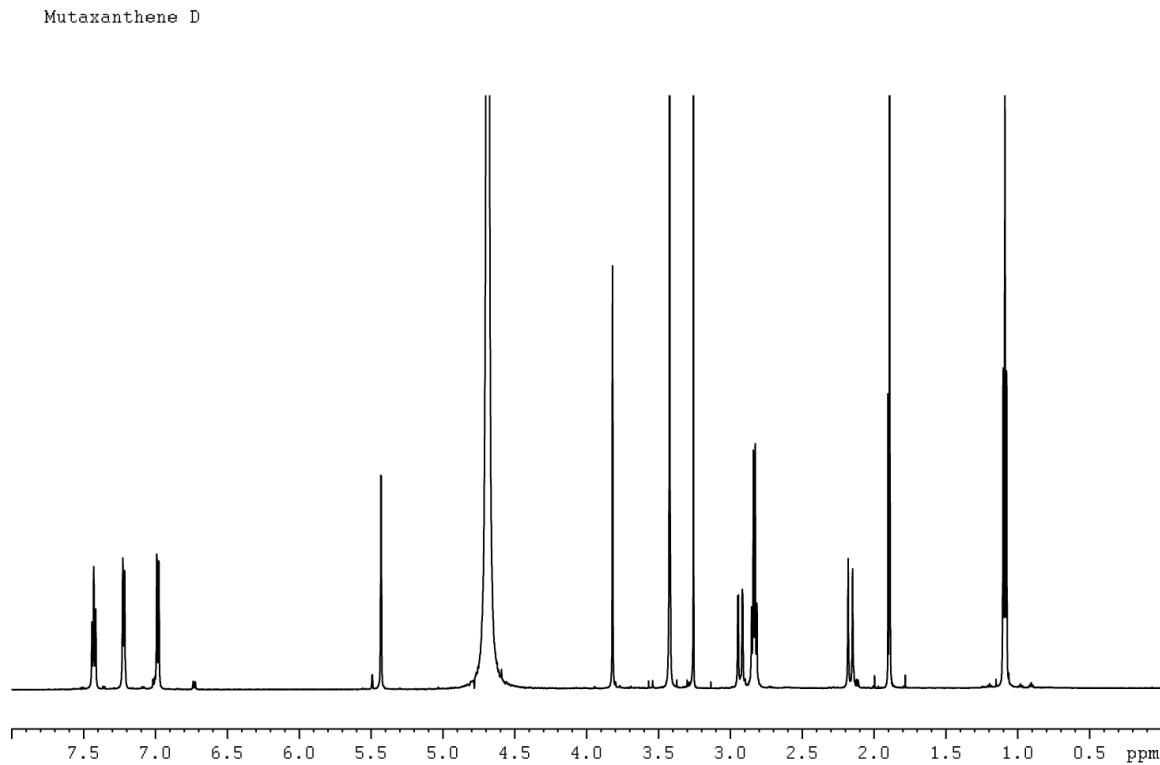


Figure S23. ¹H proton NMR of mutaxanthene D (4) in D₂O.

B. Structure elucidation of mutaxanthenes

Mutaxanthene D

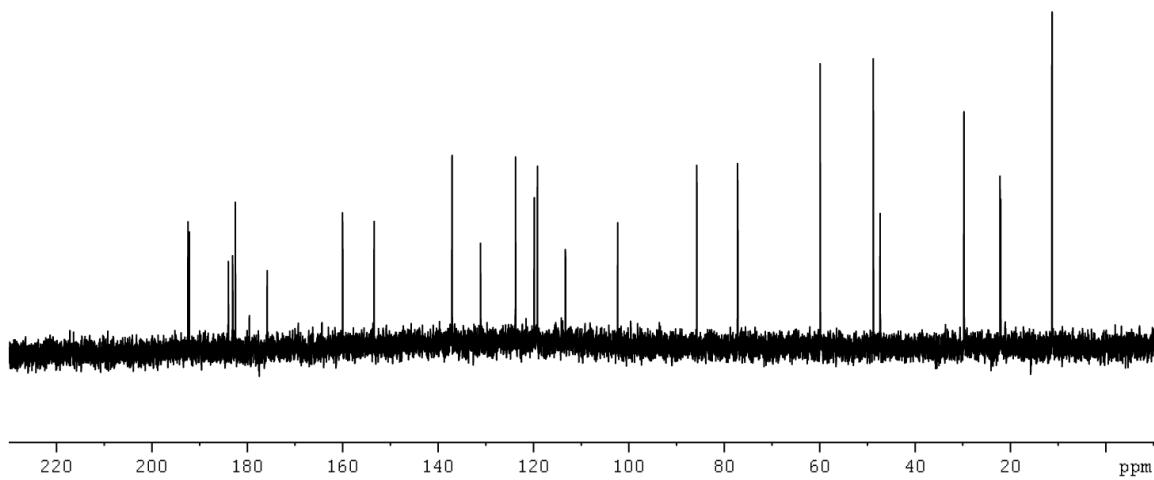


Figure S24. ¹³C carbon NMR of mutaxanthene D (**4**) in D_2O .

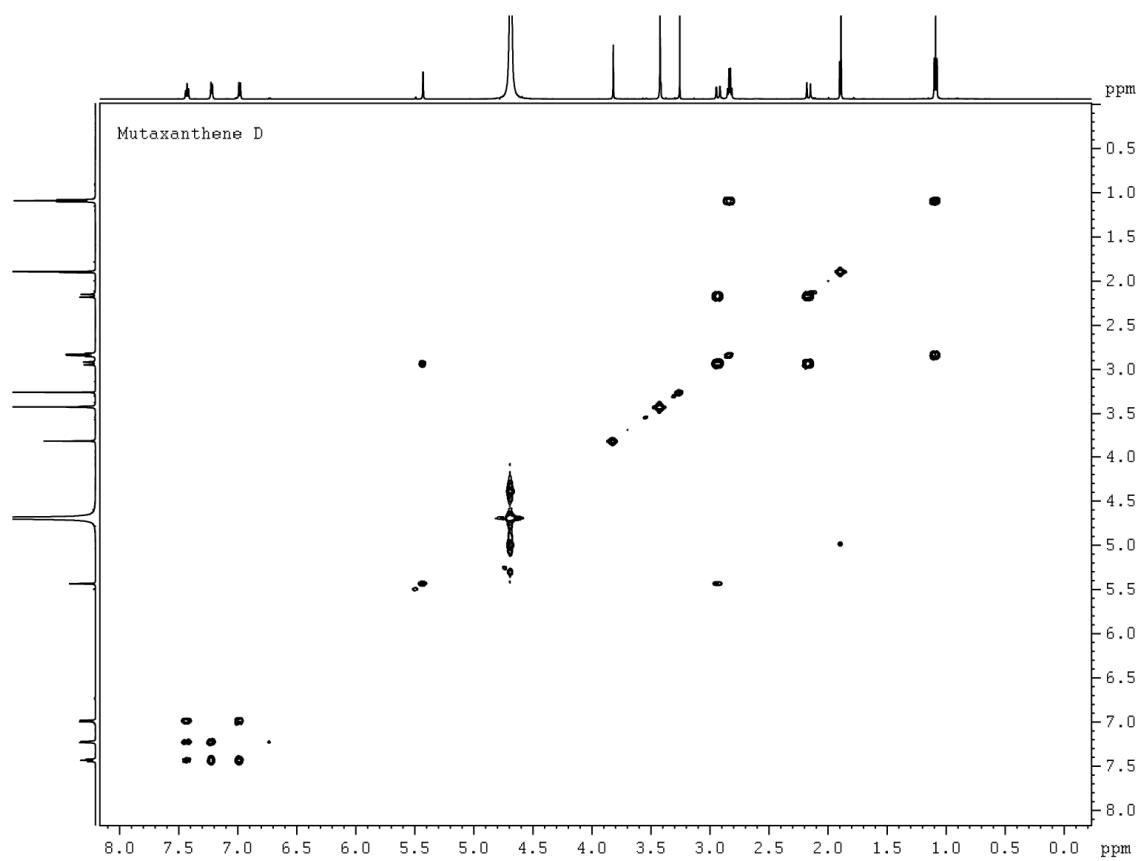


Figure S25. 2D COSY NMR of mutaxanthene D (**4**) in D_2O .

B. Structure elucidation of mutaxanthenes

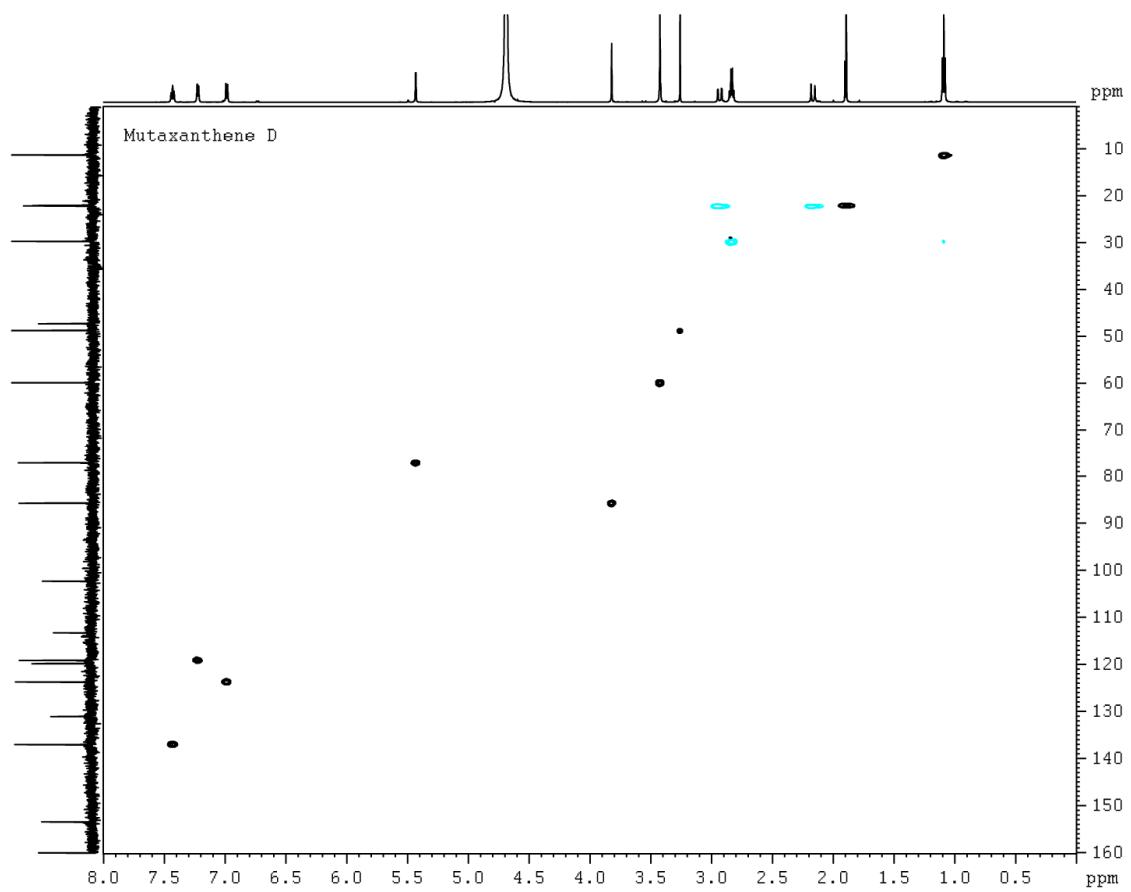


Figure S26. 2D HSQC NMR of mutaxanthene D (4) in D_2O .

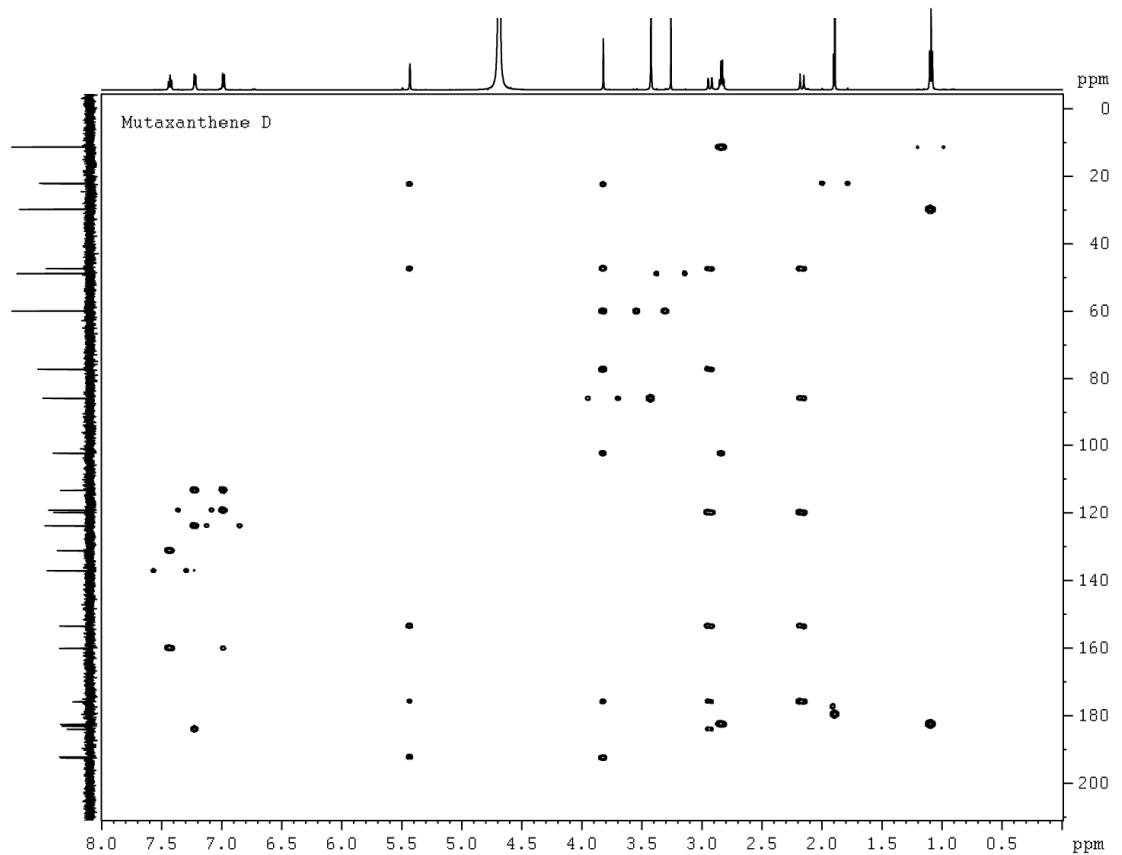


Figure S27. 2D HMBC NMR of mutaxanthene D (4) in D_2O .

B. Structure elucidation of mutaxanthenes

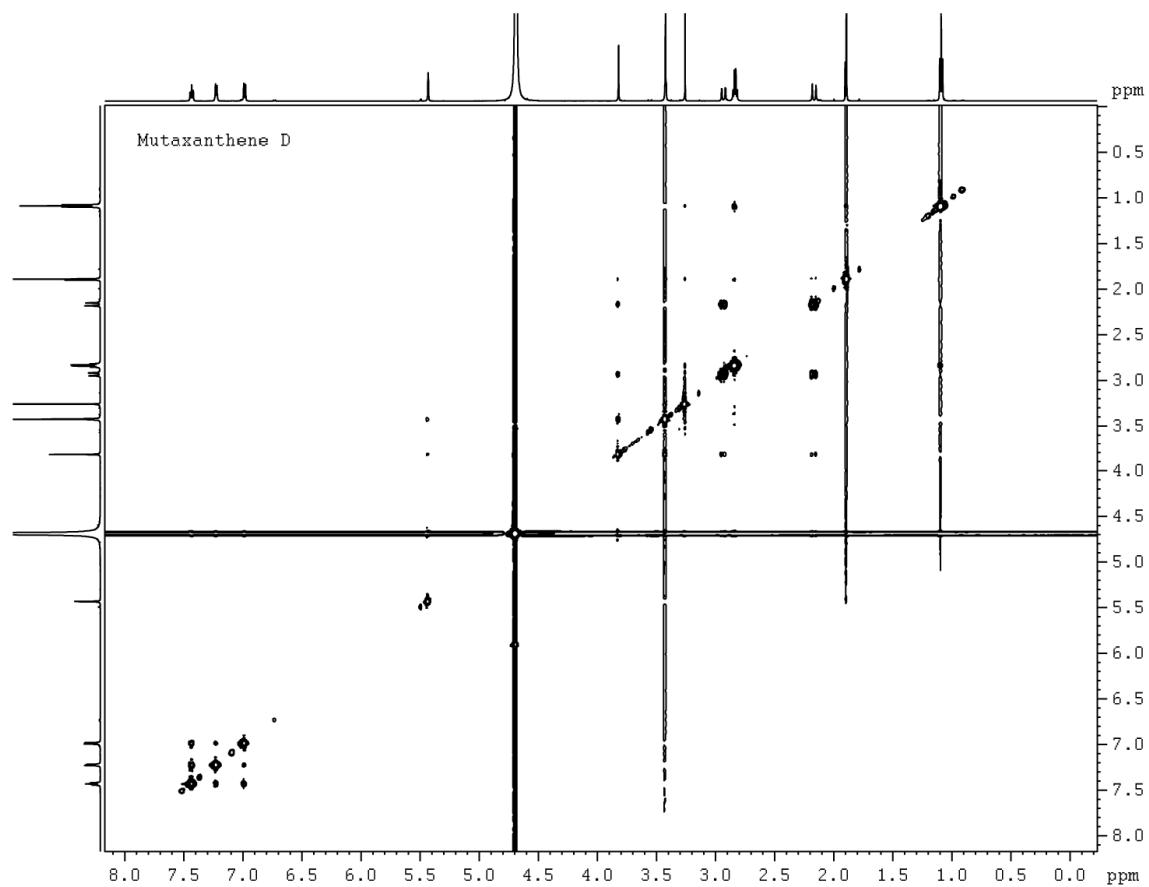


Figure S28. 2D NOESY NMR of mutaxanthene D (**4**) in D_2O .

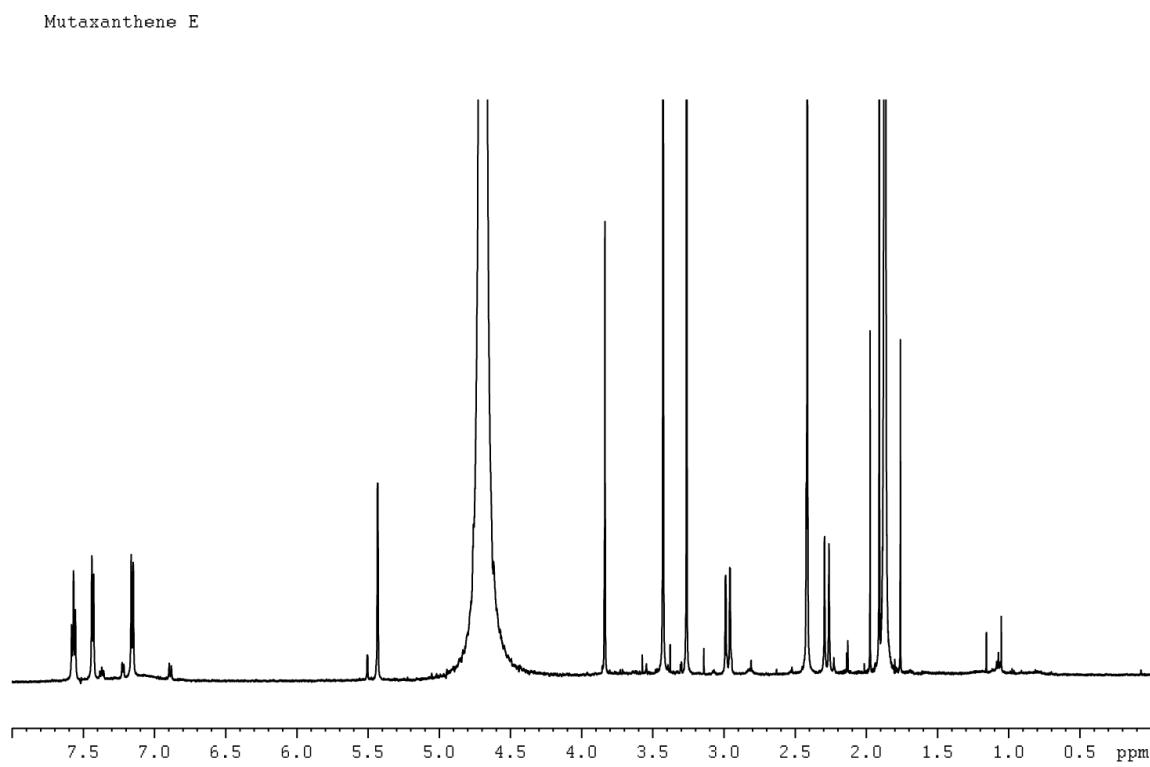


Figure S29. ^1H proton NMR of mutaxanthene E (**5**) in D_2O .

B. Structure elucidation of mutaxanthenes

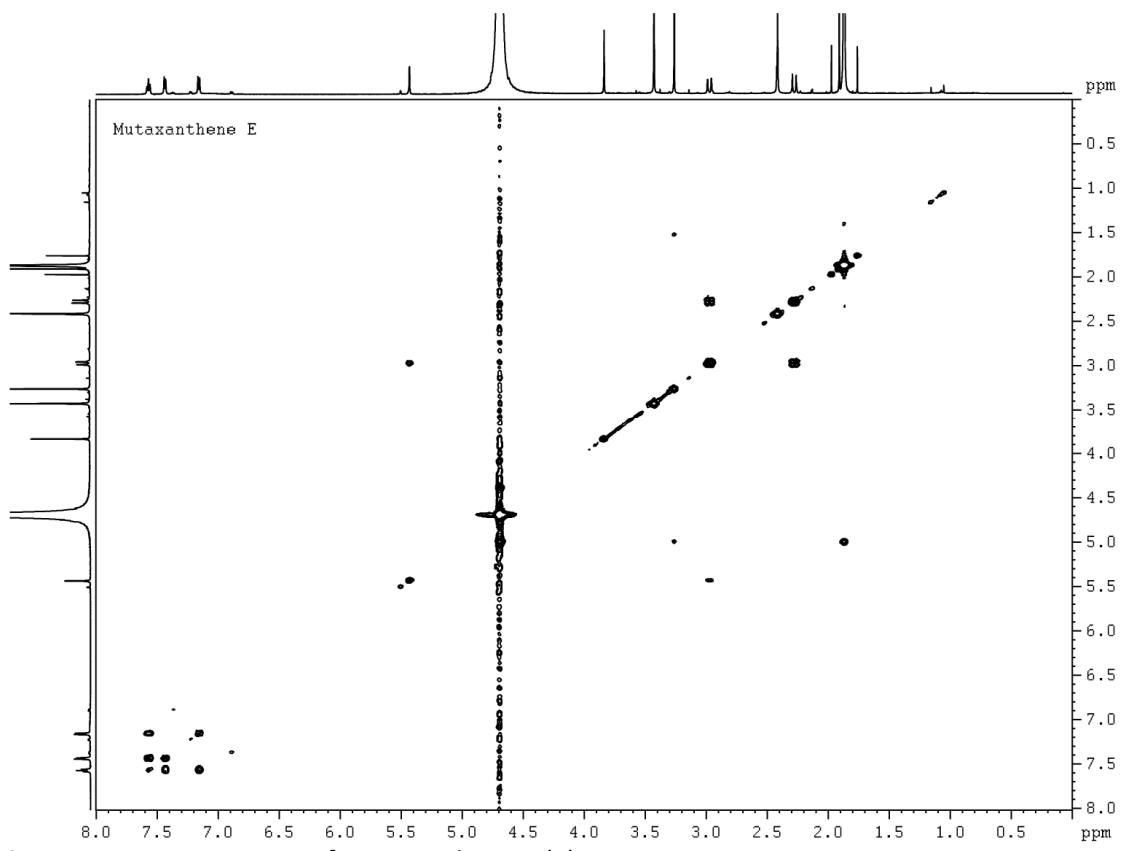


Figure S30. 2D COSY NMR of mutaxanthene E (5) in D_2O .

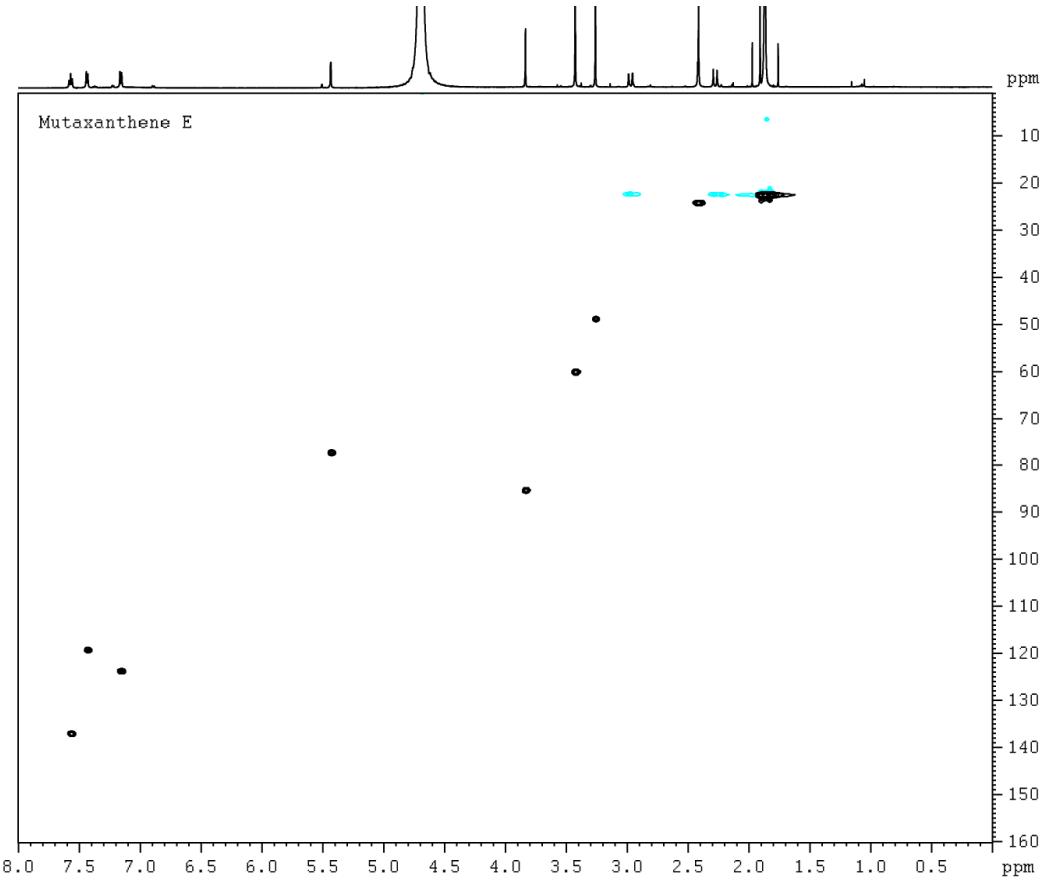


Figure S31. 2D HSQC NMR of mutaxanthene E (5) in D_2O .

B. Structure elucidation of mutaxanthenes

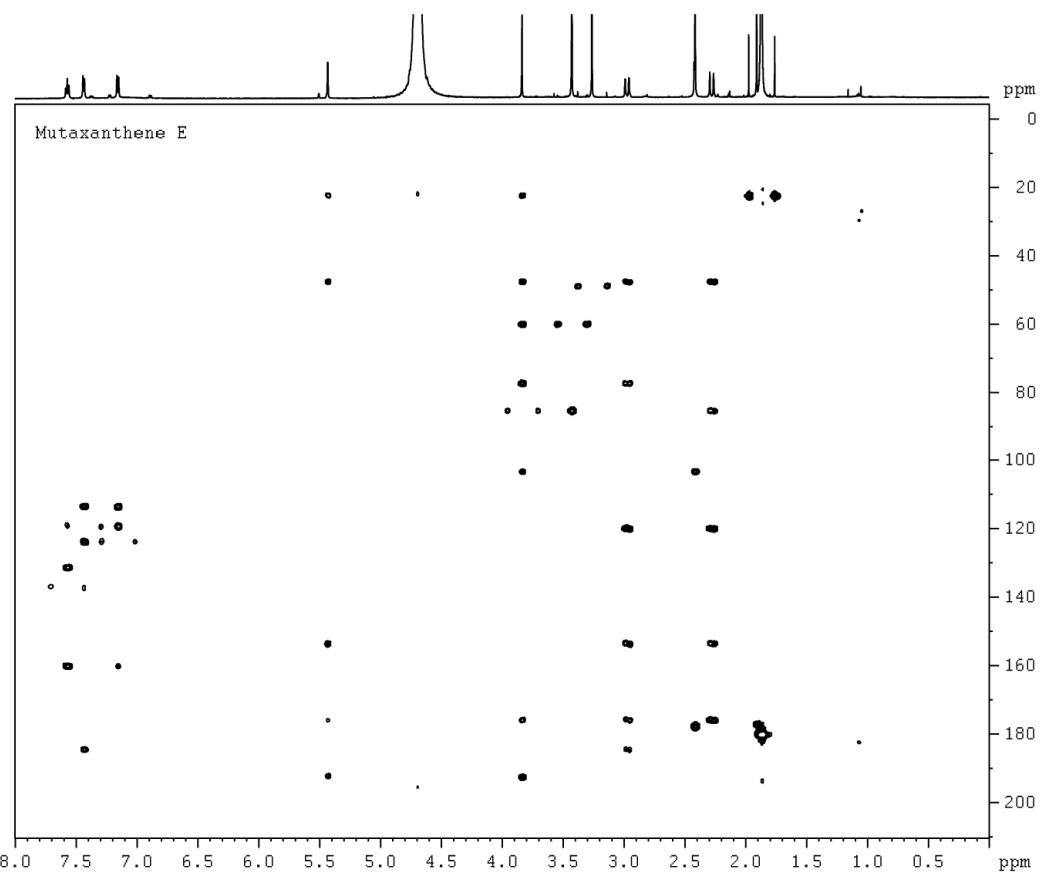


Figure S32. 2D HMBC NMR of mutaxanthene E (5) in D₂O.

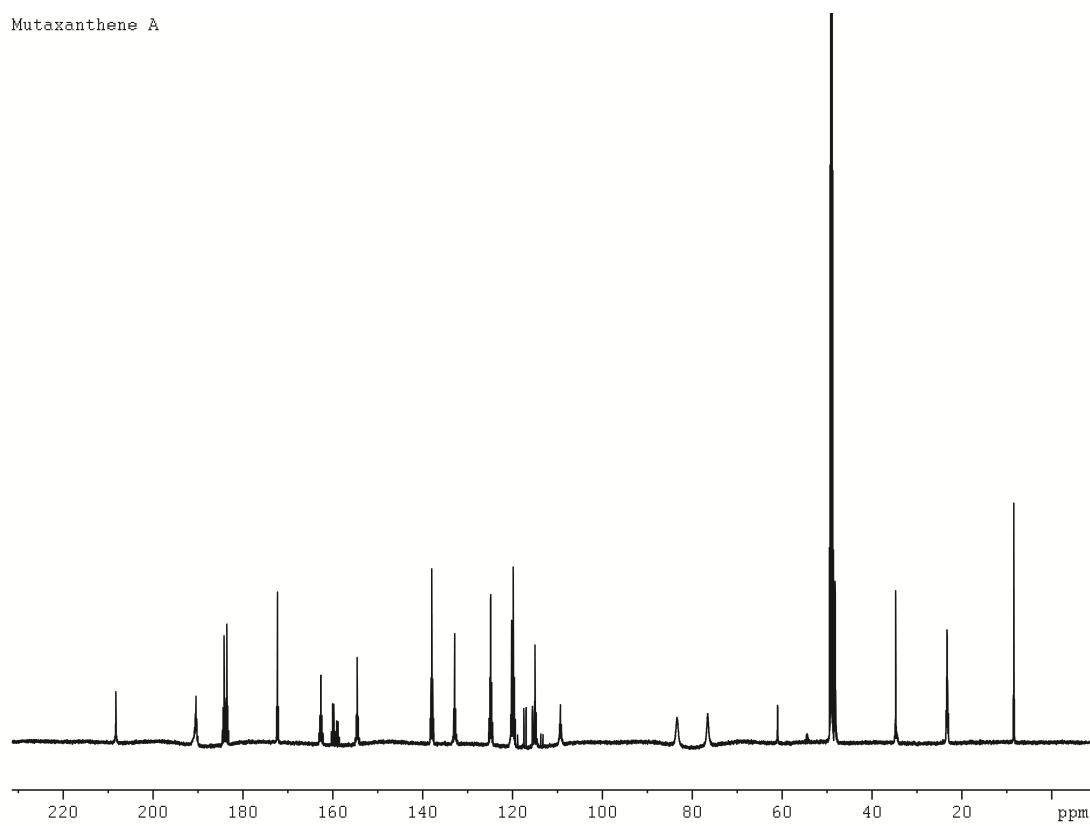


Figure S33. ¹³C carbon NMR of mutaxanthene A (4) enriched with 1,2-¹³C sodium acetate in CD₃OD.

B. Structure elucidation of mutaxanthenes

Mutaxanthene A

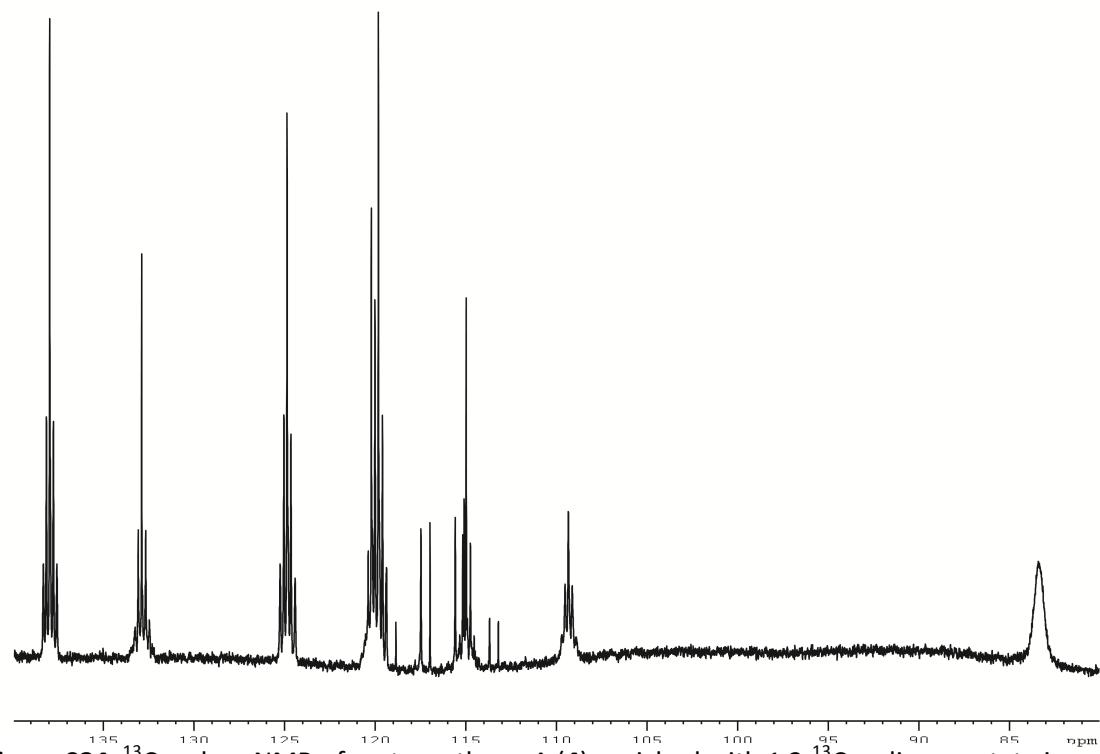


Figure S34. ¹³C carbon NMR of mutaxanthene A (**4**) enriched with 1,2-¹³C sodium acetate in CD₃OD.

Mutaxanthene D

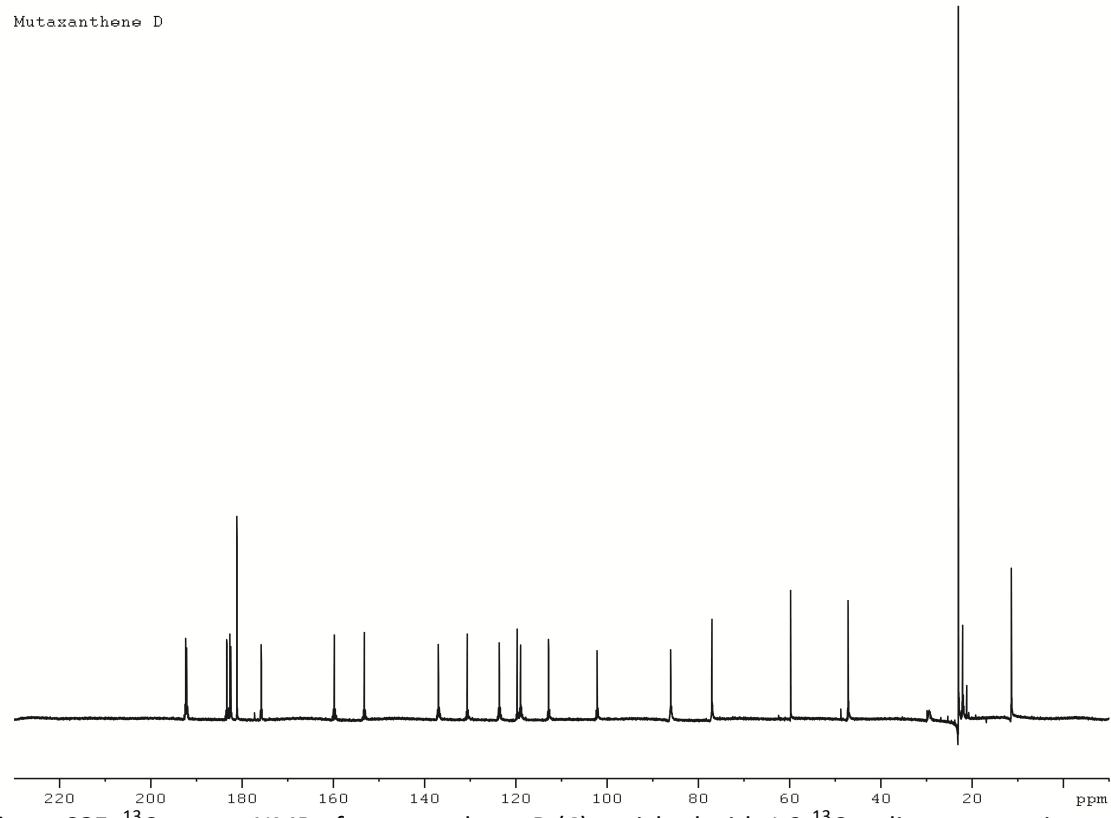


Figure S35. ¹³C proton NMR of mutaxanthene D (**4**) enriched with 1,2-¹³C sodium acetate in CD₃OD.

B. Structure elucidation of mutaxanthenes

Mutaxanthene D

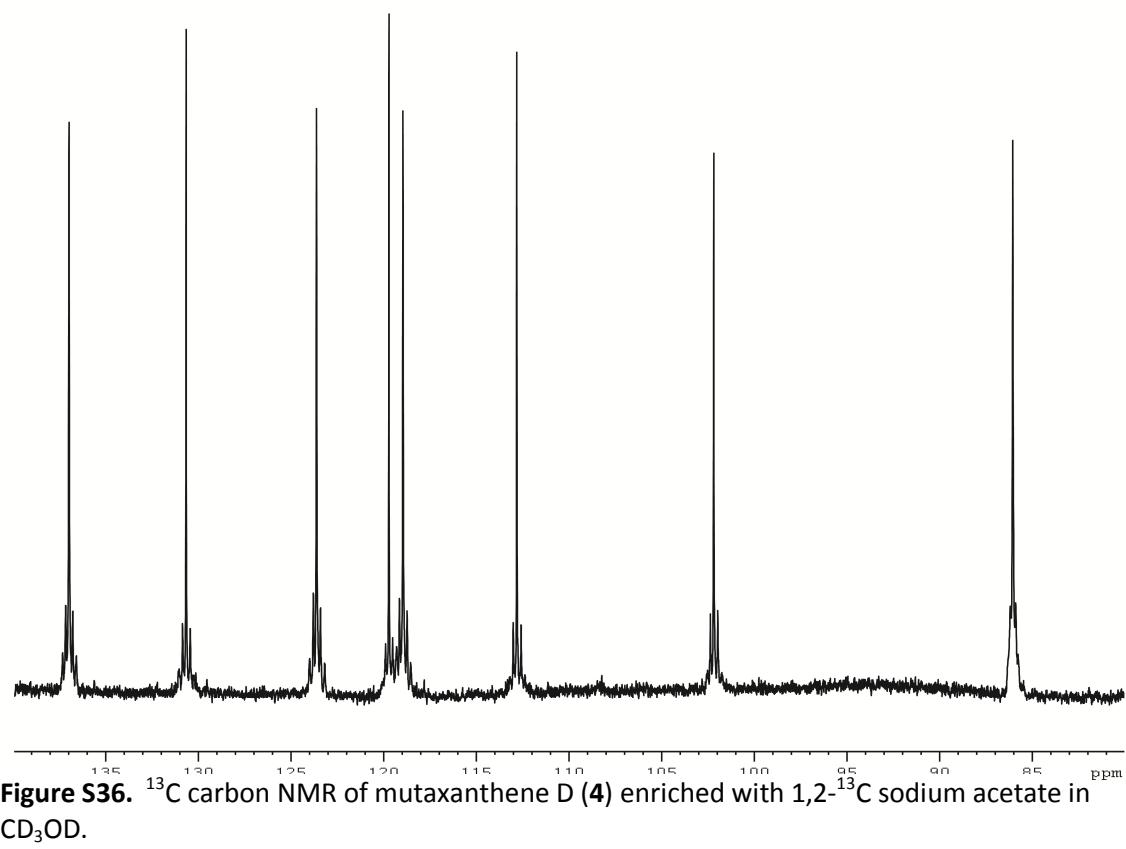
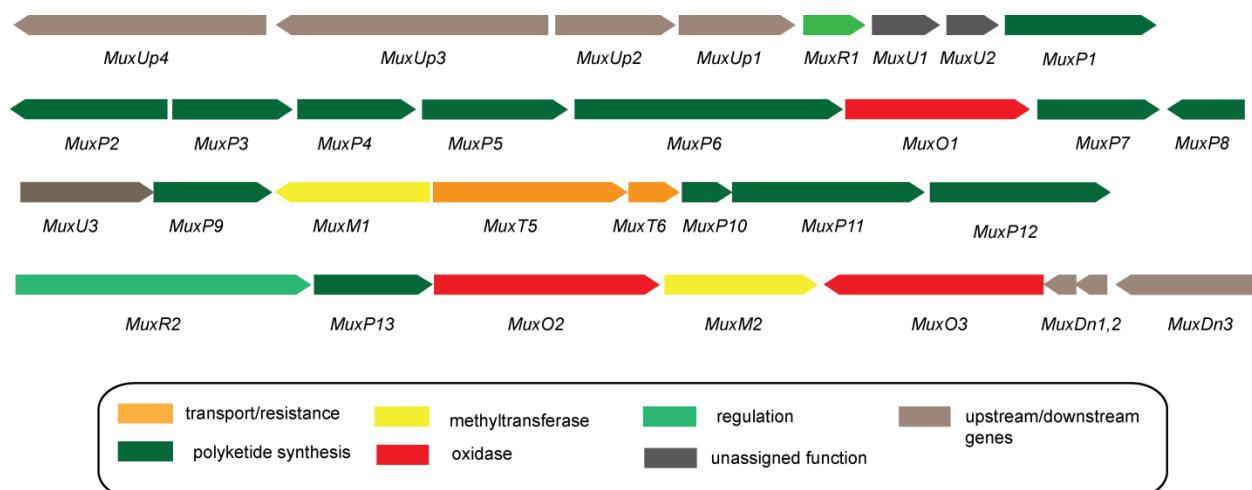


Figure S36. ^{13}C carbon NMR of mutaxanthene D (4) enriched with 1,2- ^{13}C sodium acetate in CD_3OD .

C. Genetic Analysis of putative mutaxanthene gene cluster

Table S7. Deduced functions of ORFs in the mutaxanthene biosynthetic gene cluster



gene	size (aa)	similar protein	GeneBank accession numbers	Identity(%) /similarity(%)	proposed function
<i>MuxUp4</i>	-577	SSMG_06347, Streptomyces sp. AA4	ZP_07282307	99/99	ABC transporter
<i>MuxUp3</i>	-627	SSMG_06347, Streptomyces sp. AA4	ZP_07282307.1	99/98	ABC transporter
<i>MuxUp2</i>	254	SSMG_06348, Streptomyces sp. AA4	ZP_07282308	96/98	ABC transporter
<i>MuxUp1</i>	247	SSMG_06349, Streptomyces sp. AA4	ZP_07282309	96/98	ABC transporter
<i>MuxR2</i>	114	SSMG_06351, Streptomyces sp. AA4	ZP_07282311	97/96	PadR fam.transcriptional repressor
<i>MuxU1</i>	128	SSMG_06350	ZP_07282310	94/98	hypothetical protein
<i>MuxU2</i>	91	SSMG_06352	ZP_07282312.1	97/94	hypothetical protein
<i>MuxP1</i>	332	AlkNF, Streptomyces galilaeus	BAB72049	69/55	type II acyl transferase (AT)
<i>MuxP2</i>	-345	CosE, Streptomyces olindensis	ABC00733	56/69	type II ketosynthase (KS) for starter
<i>MuxP3</i>	258	PokC2, Streptomyces diastatochromogenes	ACN64846	78/65	type II polyketide cyclase
<i>MuxP4</i>	250	PokT1, Streptomyces diastatochromogenes	ACN64844.1	64/50	type II ketoreductase (KR)
<i>MuxP5</i>	320	orf6, Streptomyces echinatus	ABL09954	69/57	type II cyclase/dehydratase
<i>MuxP6</i>	618	Sfla_5326,Streptomyces flavogriseus	YP_004926240	60/47	acyl CoA ligase
<i>MuxO1</i>	412	Sfla_5326,Streptomyces flavogriseus	YP_004926243.1	70/55	flavin-dependent oxidase
<i>MuxD1</i>	262	simA6, Streptomyces antibioticus	AF324838_6	86/75	type II ketoreductase
<i>MuxP7</i>	-154	SnoaL_4, uncultured bacterium (expressed)	AEM44306.1	60/51	type II cyclase/dehydratase
<i>MuxU3</i>	288	none	--	--	hypothetical protein
<i>MuxD2</i>	253	Strvi_4376, Streptomyces violaceusniger Tu 4113	YP_004814300	61/42	type II ketoreductase (KR)
<i>MuxM1</i>	-341	phzM, Saccharopolyspora erythraea	YP_001106227	57/43	O-methyltransferase
<i>MuxT4</i>	438	SAV_5944,Streptomyces avermitilis	NP_827121	63/47	transport efflux
<i>MuxT5</i>	84	Sros_2592, Streptosporangium roseum	YP_003338305	72/50	transport efflux
<i>MuxP8</i>	86	ChaC, Streptomyces chartreusis	CAH10163	69/51	type II acyl carrier protein (ACP)
<i>MuxP9</i>	431	ORF32, uncultured bacterium (expressed)	AEM44309	85/74	type II beta-ketoacyl synthase (KS)
<i>MuxP10</i>	402	ORF2, uncultured bacterium (expressed)	AEM44279.1	66/53	type II beta-ketoacyl synthase (KS)
<i>MuxR3</i>	681	RubS, Streptomyces collinus	AAM97369.1	55/41	SARP type transcriptional activator
<i>MuxD3</i>	252	ORF2, uncultured bacterium (expressed)	AEM44279	66/53	type II ketoreductase (KR)
<i>MuxO2</i>	511	ORF20, uncultured bacterium (expressed)	AEM44297	71/61	flavin-dependent oxidase
<i>MuxM2</i>	335	SsfM1, Streptomyces sp. SF2575	ADE34508.1	72/89	O-methyltransferase
<i>MuxO3</i>	-500	ovmOl, Streptomyces antibioticus	CAG14963.1	63/50	flavin-dependent oxidase

D. Mass Spectral Data for Selected Features

Figure 1 Banned Energy Spectrum
100
2690239

4.36e5

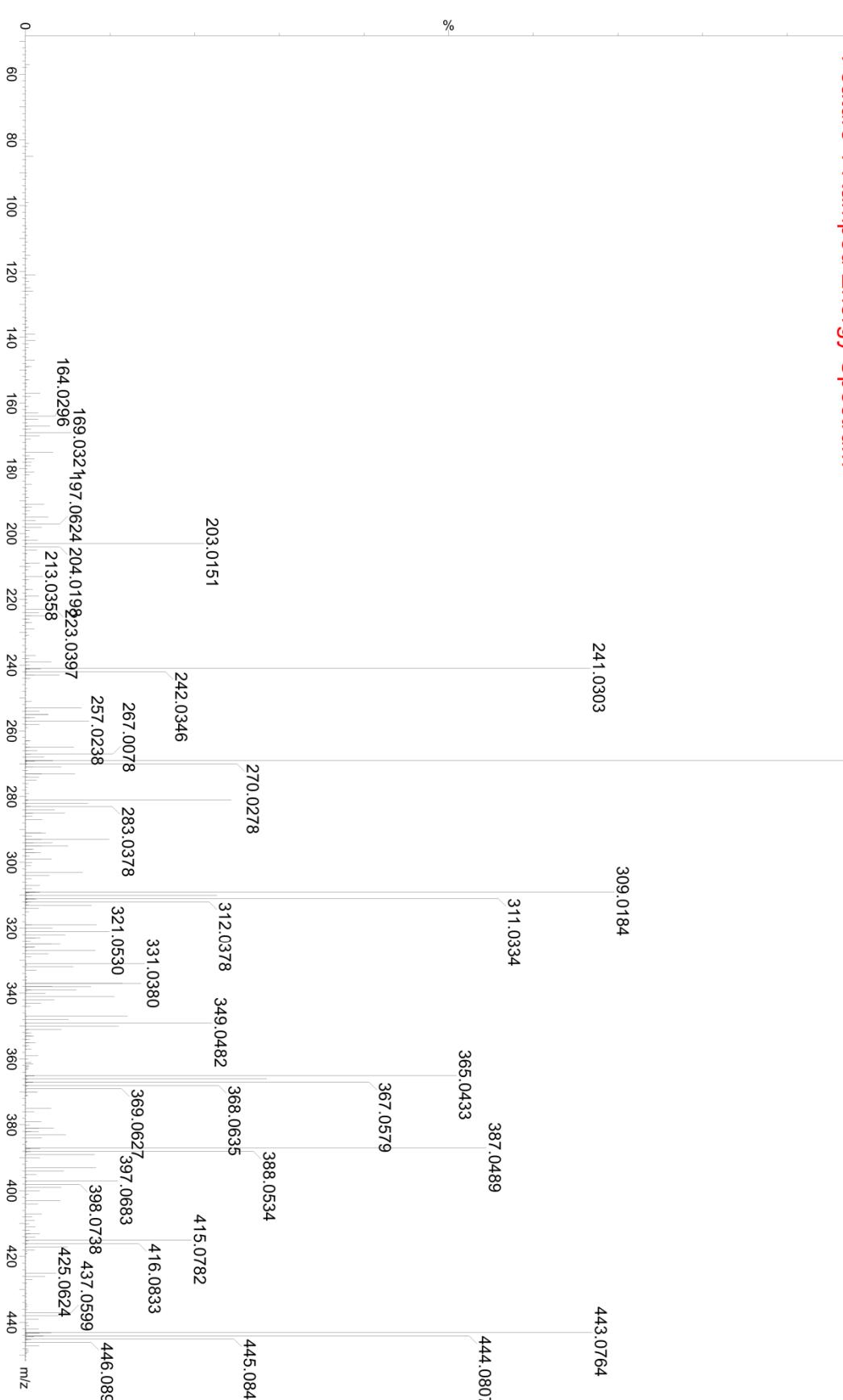


Figure S37. Mobility separated ramped energy mass spectrum for feature 1, Mutaxanthene A.

D. Mass Spectral Data for Selected Features

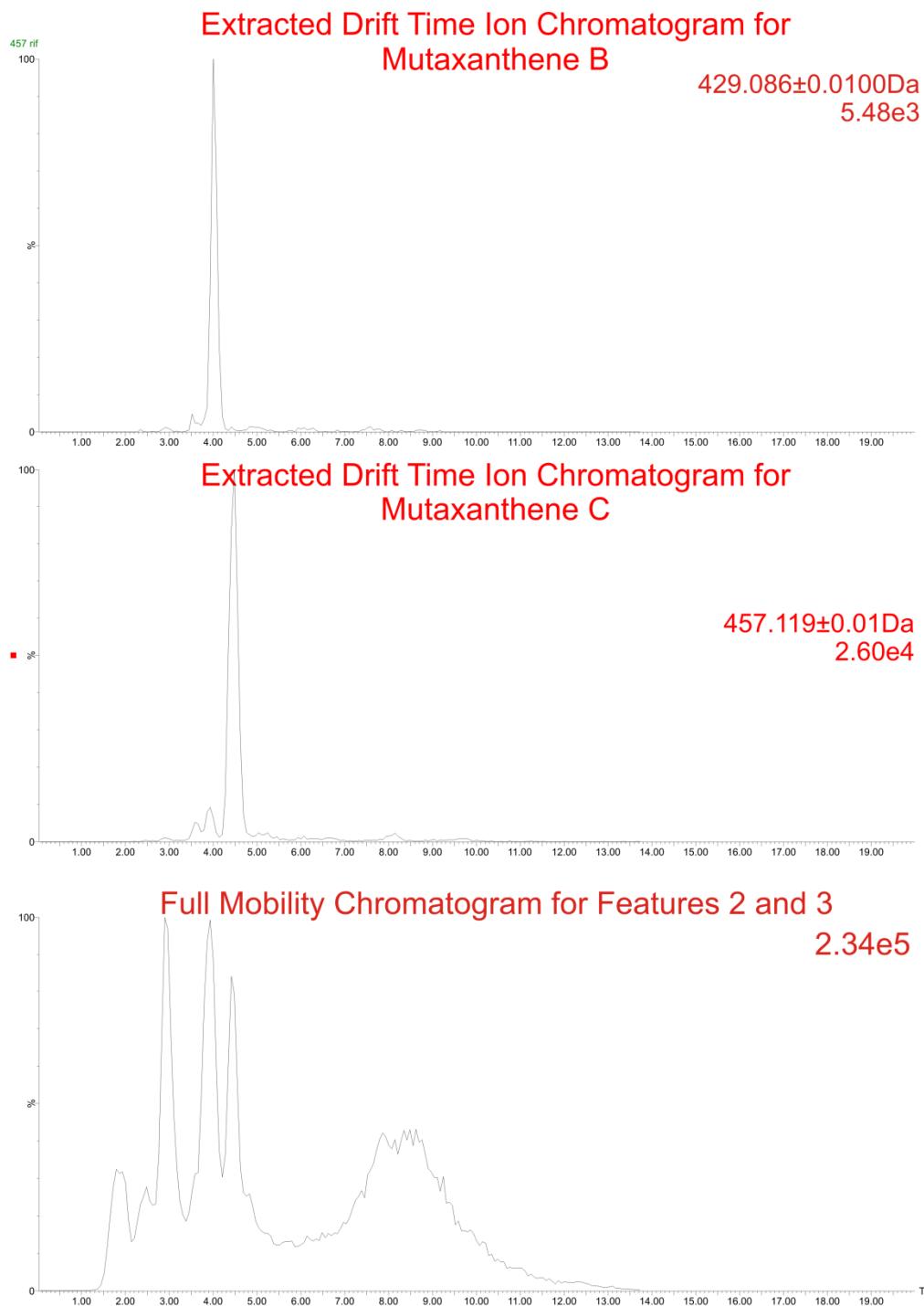


Figure S38. Retention time selected drift time chromatograms and extracted drift time ion chromatograms for coeluting mutaxantenes B and C. Using mobility separation, fragmentation profiles for each were extracted.

D. Mass Spectral Data for Selected Features



Figure S39. Mobility separated ramped energy mass spectrum for feature 2, Mutaxanthene C.

Feature 3 Ramped Energy Spectrum

2.56e4

429.0819

269.0447

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D. Mass Spectral Data for Selected Features

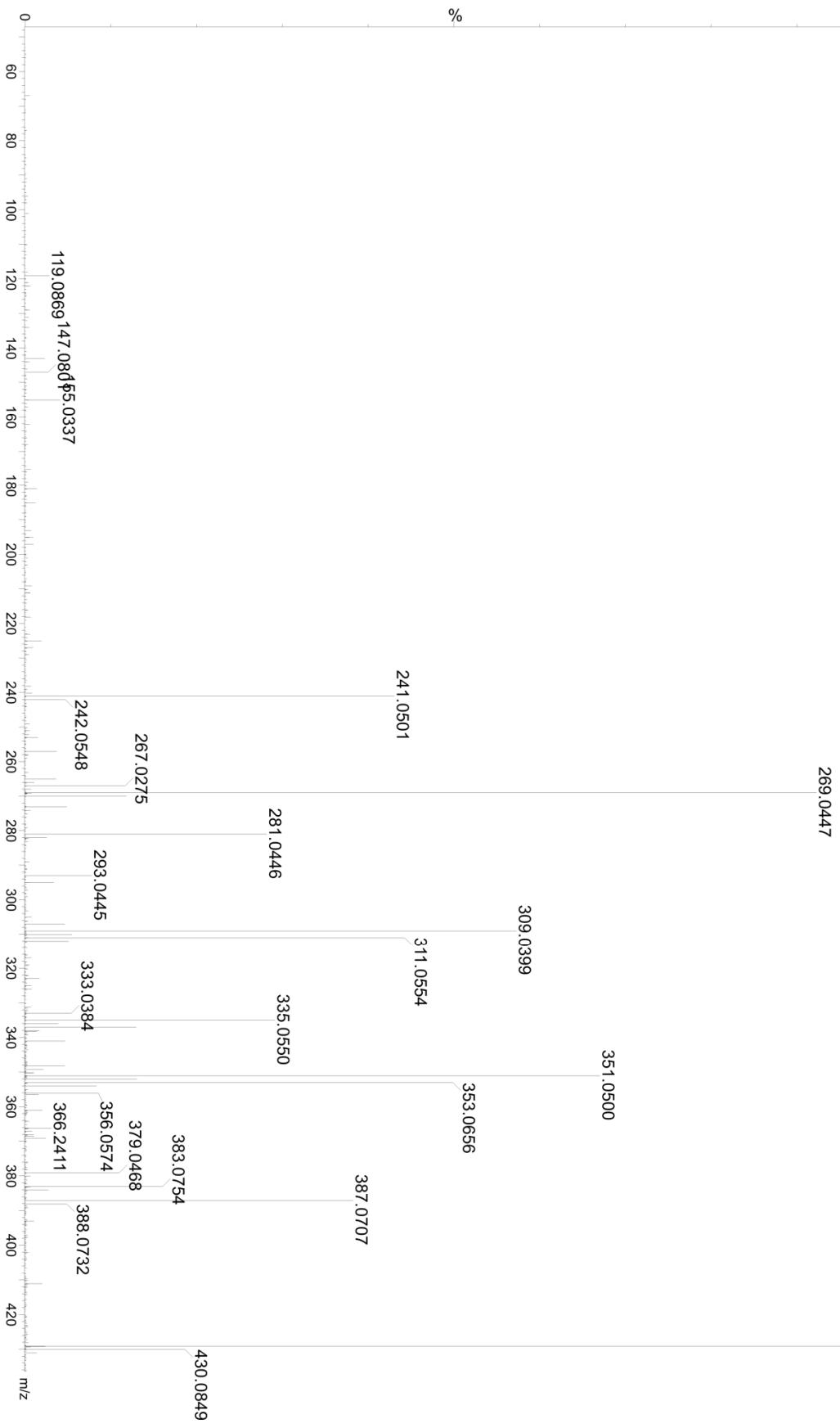


Figure S40. Mobility separated ramped energy mass spectrum for feature 3, Mutaxanthene B.

D. Mass Spectral Data for Selected Features

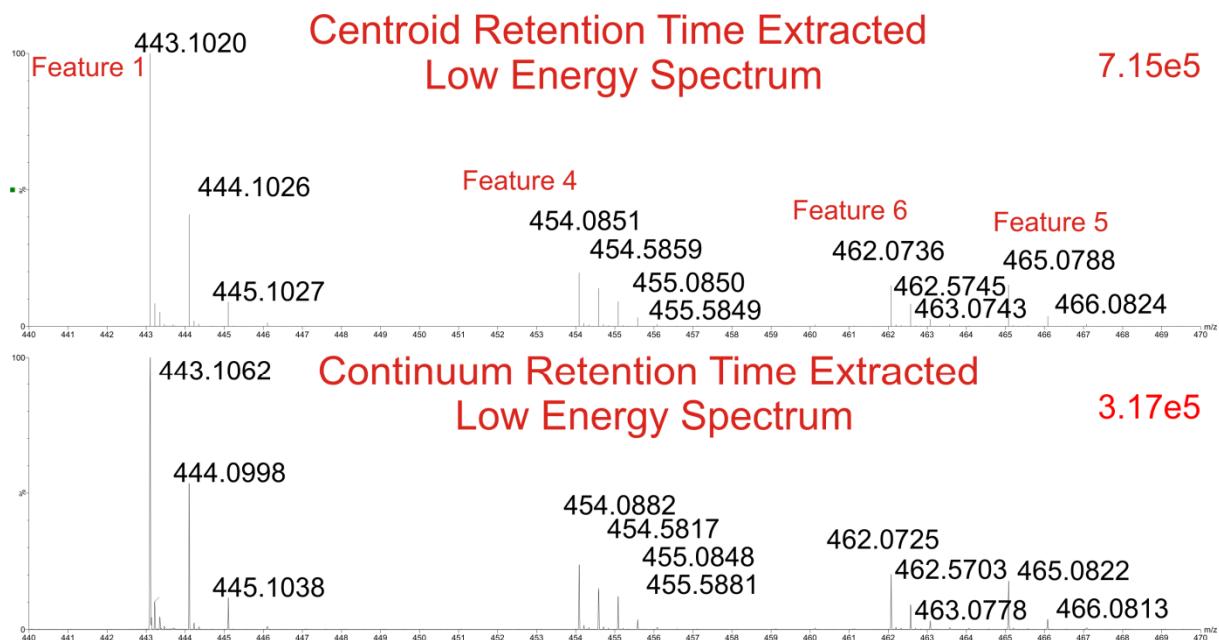


Figure S41. Retention time extracted low energy spectrum demonstrating Mutaxanthene A adducts.

D. Mass Spectral Data for Selected Features

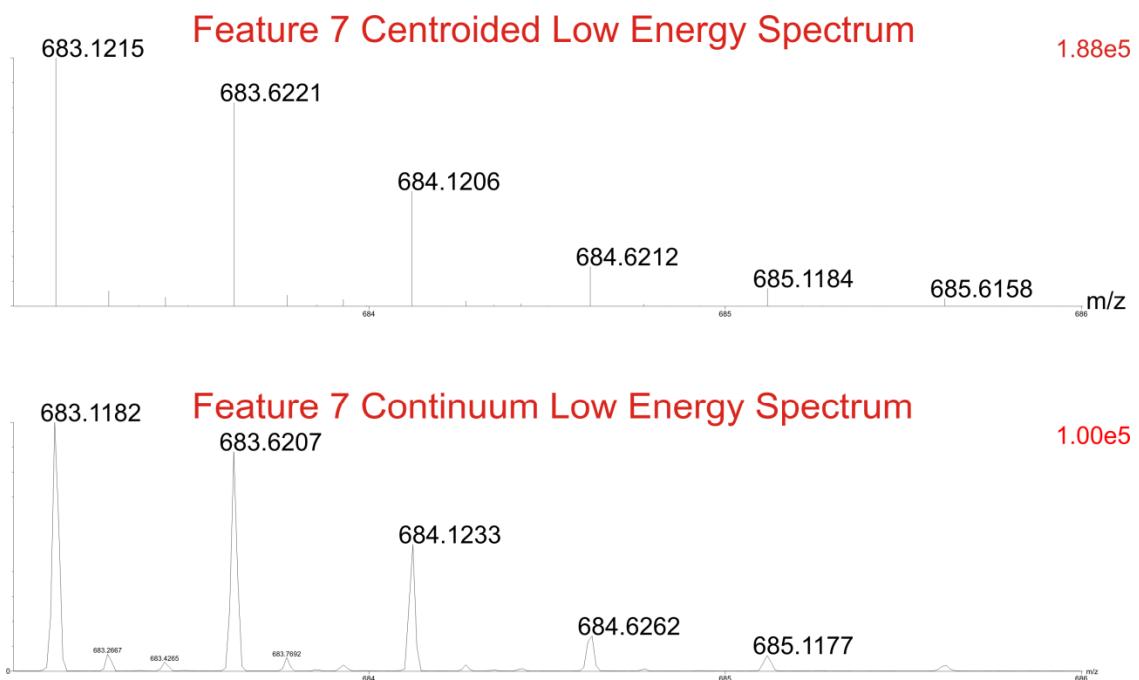
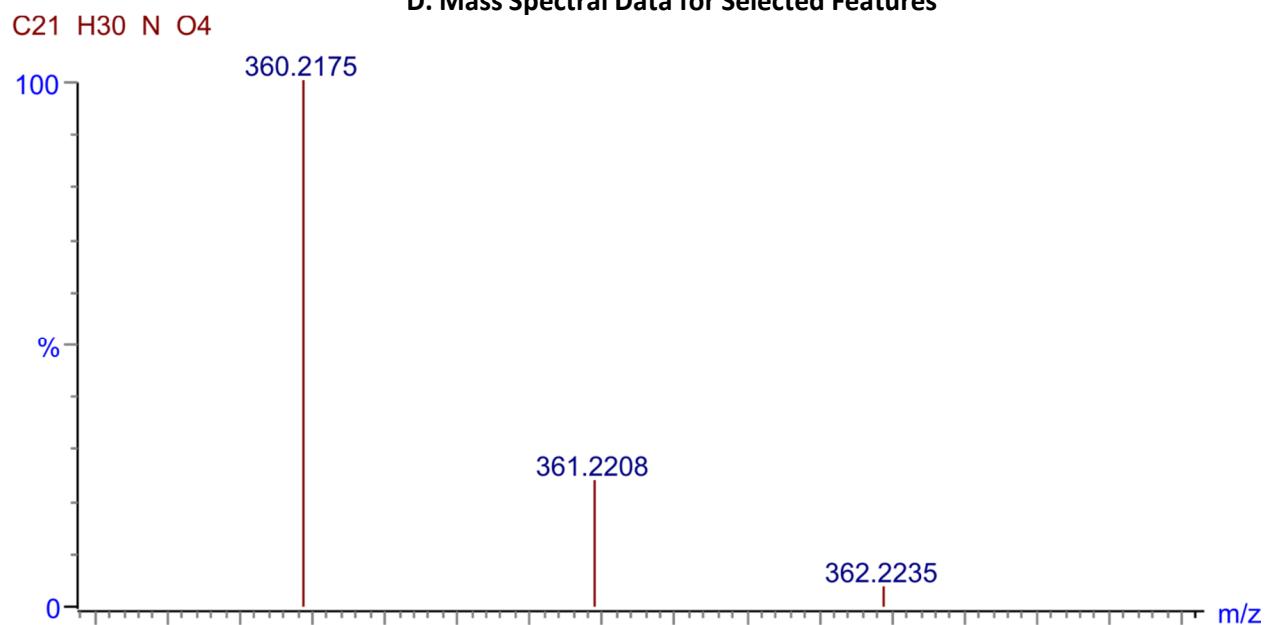


Figure S42. Retention time extracted low energy spectrum displaying feature 7 isotopic envelope.

D. Mass Spectral Data for Selected Features



Feature 8 $[M+H]^+$

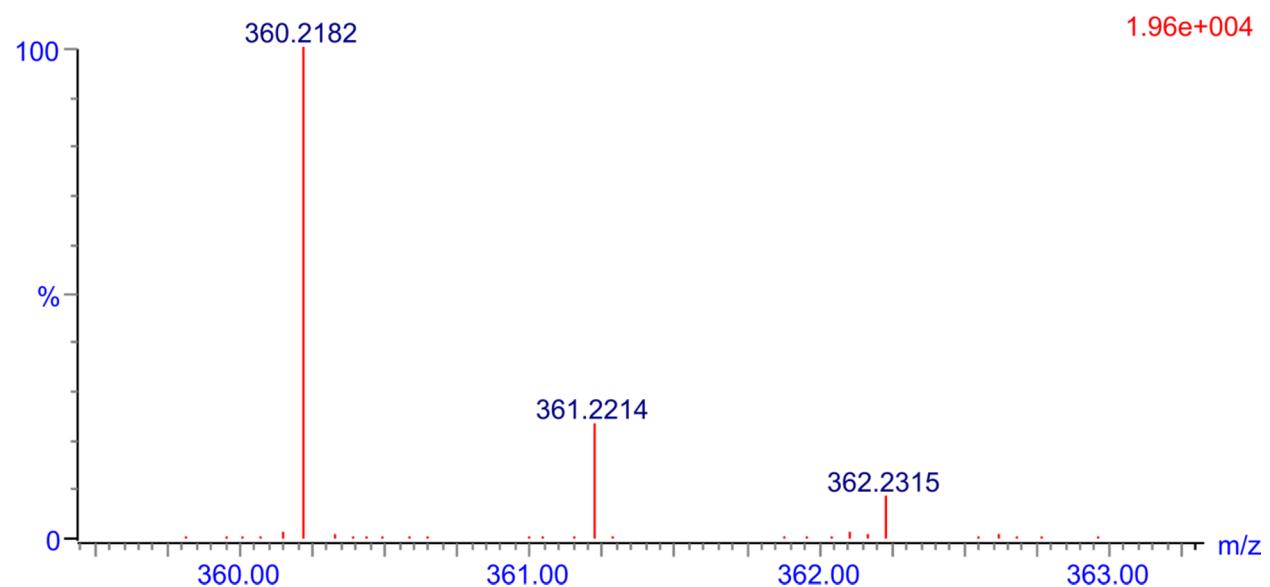


Figure S43. (Above) Theoretical isotopic profile for $[C_{21}H_{29}NO_4 + H]^+$. **(Below)** Accurate mass isotopic envelope of feature 8, as specified in Table 1.

D. Mass Spectral Data for Selected Features

Feature 8 Ramped Energy Spectrum
9.03e3

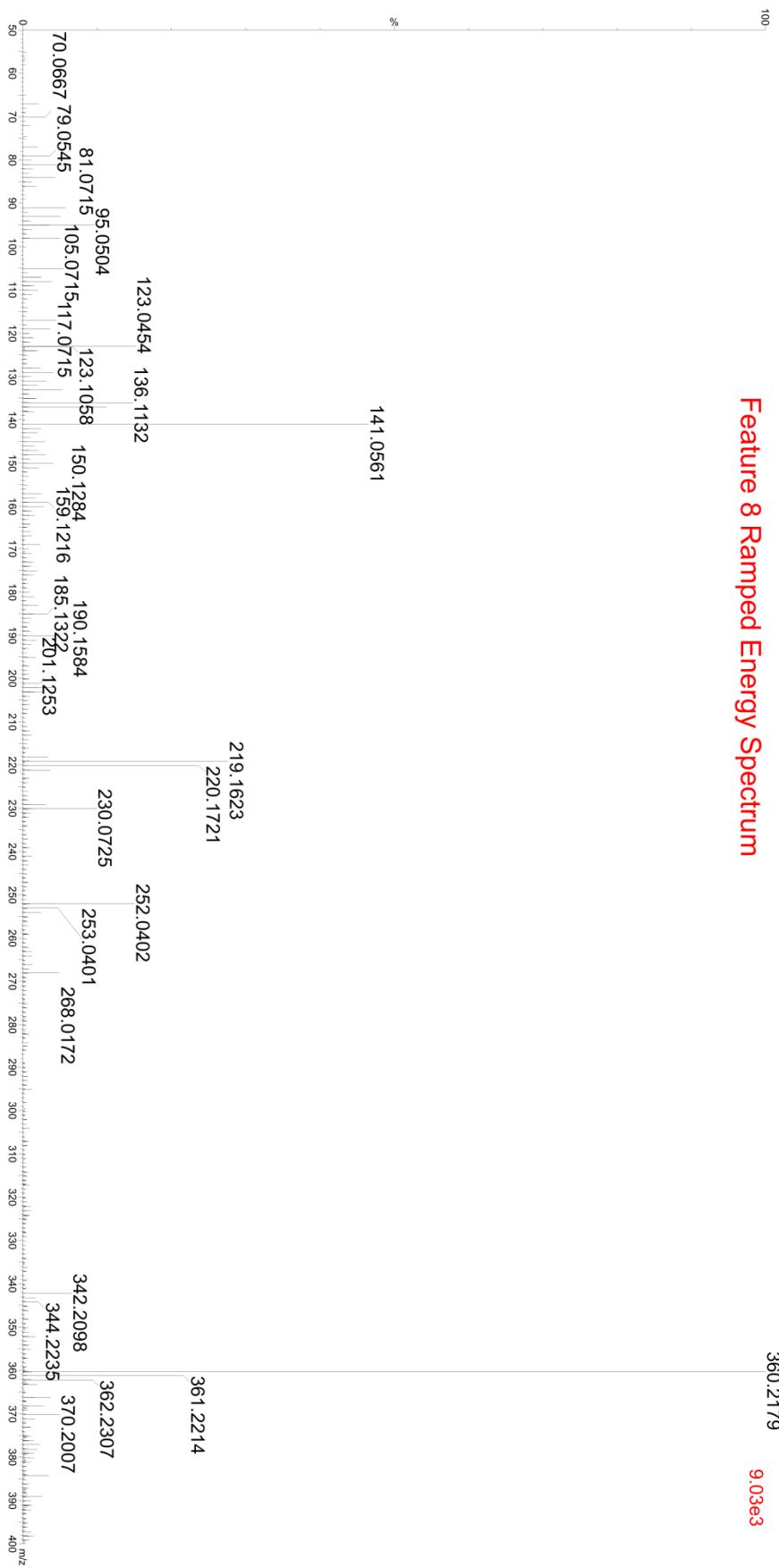


Figure S44. Mobility separated ramped energy mass spectrum for feature 8.

D. Mass Spectral Data for Selected Features

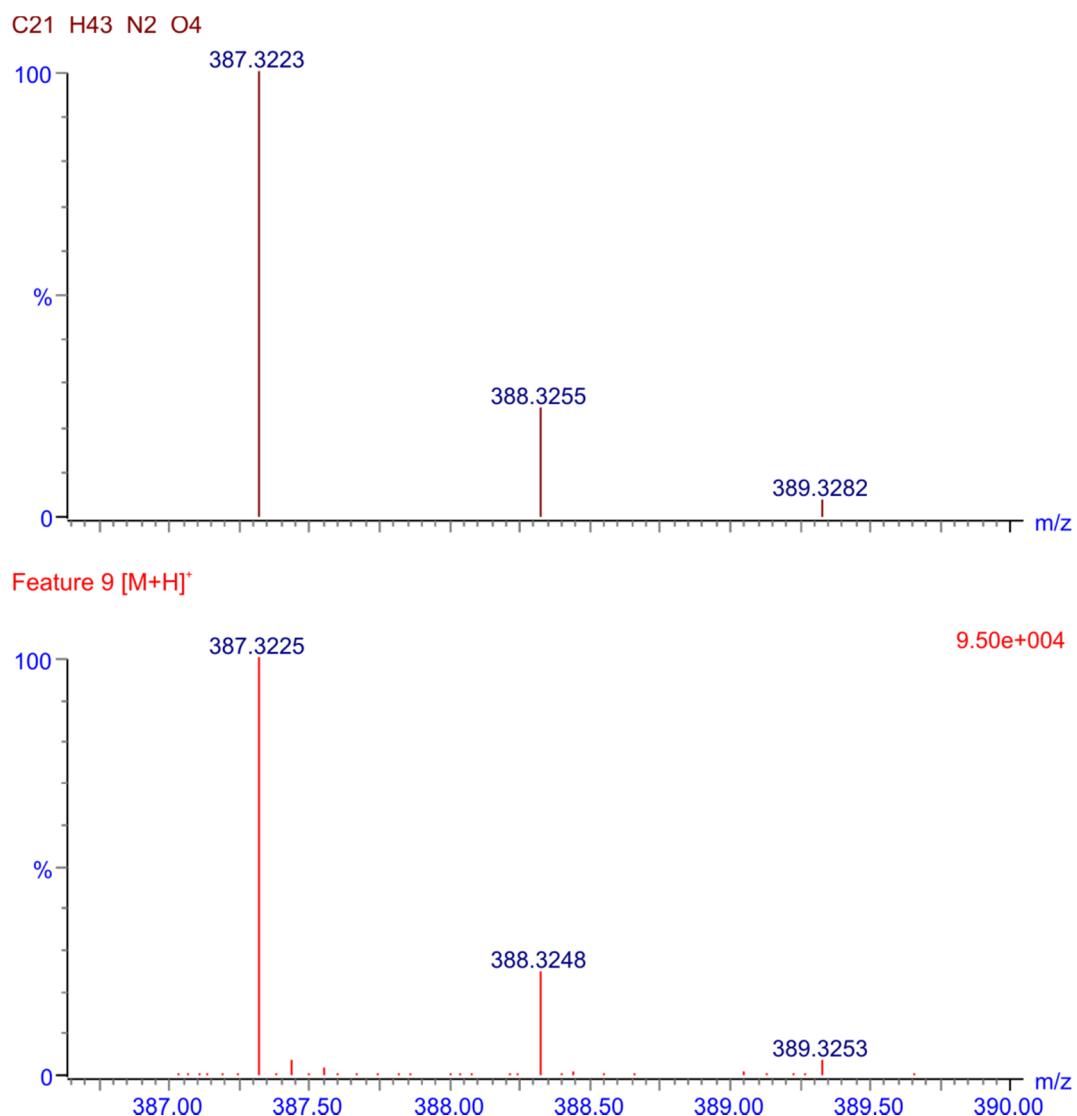


Figure S45. (Above) Theoretical isotopic profile for $[C_{21}H_{42}N_2O_4+H]^+$. **(Below)** Accurate mass isotopic envelope of feature 9, as specified in Table 1.

Feature 9 ramped energy spectrum



Figure S46. Mobility separated ramped energy mass spectrum for feature 9, indicating neutral losses. These neutral losses corroborate the chemical formula determination.

D. Mass Spectral Data for Selected Features

Feature 9 Ramped Energy Spectrum

9.57e4
387.33225

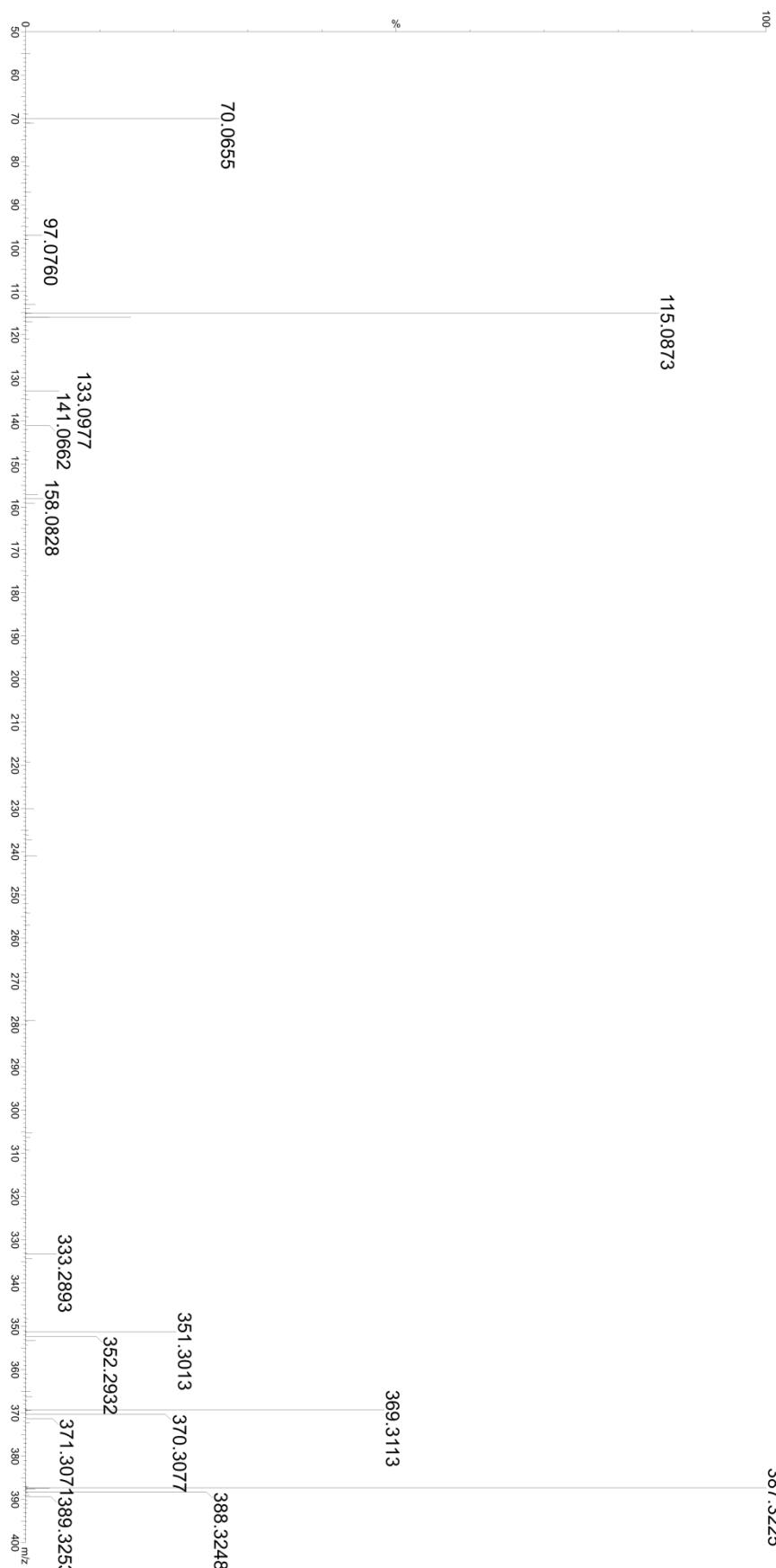


Figure S47. Mobility separated ramped energy mass spectrum for feature 9.

D. Mass Spectral Data for Selected Features

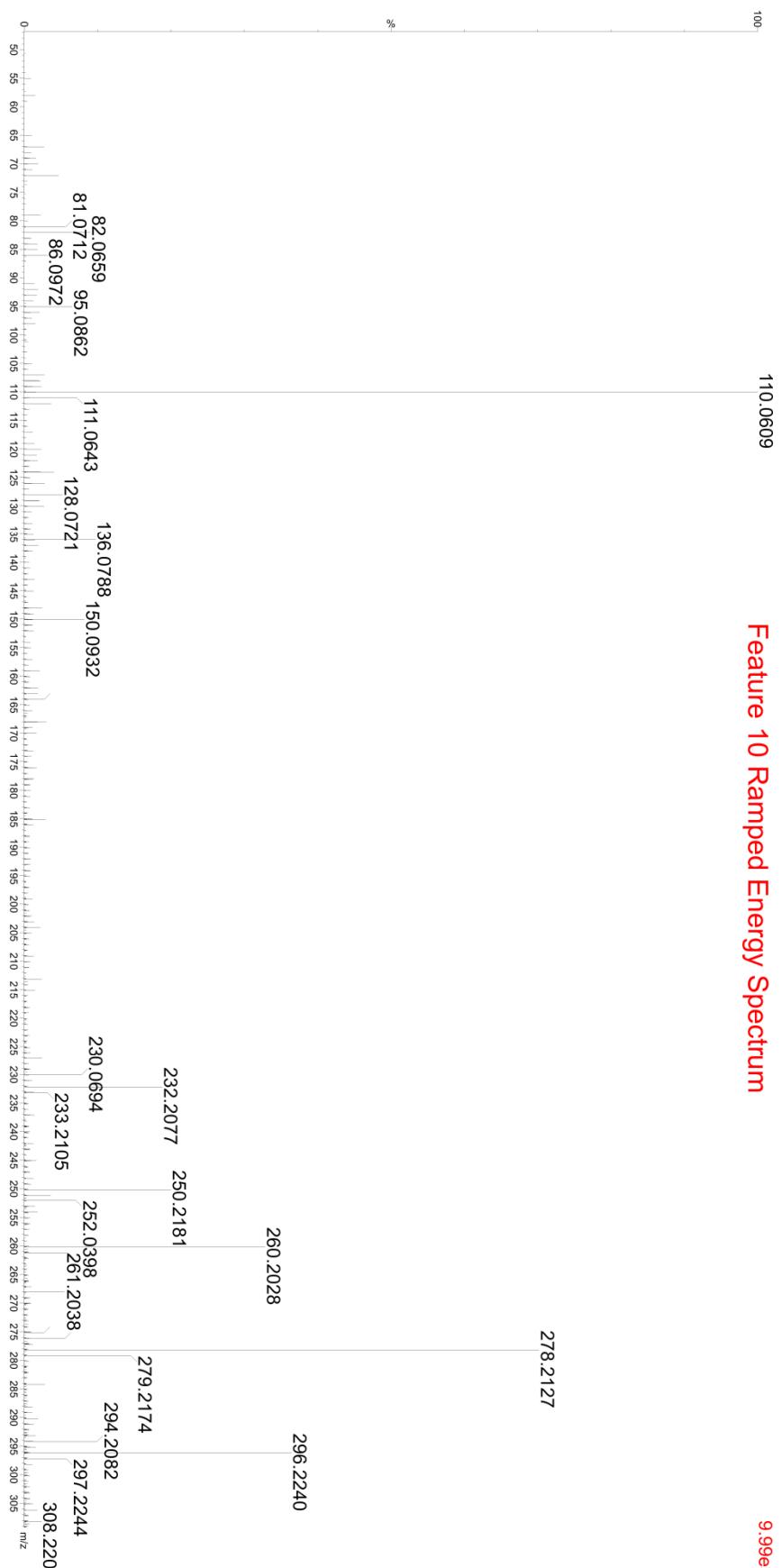


Figure S48. Mobility separated ramped energy mass spectrum for feature 10.

Feature 11 Ramped Energy Spectrum 4.10e3

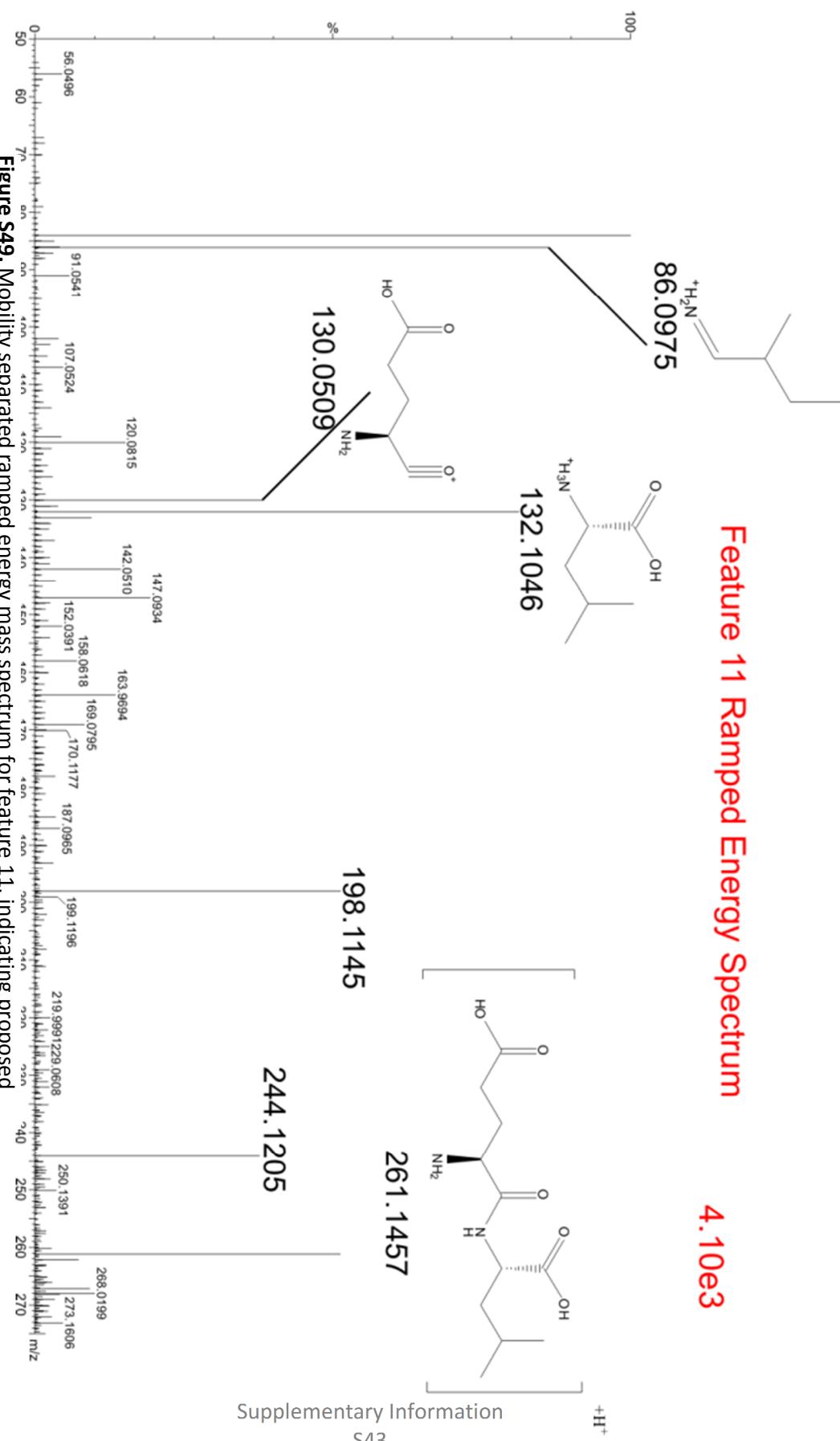
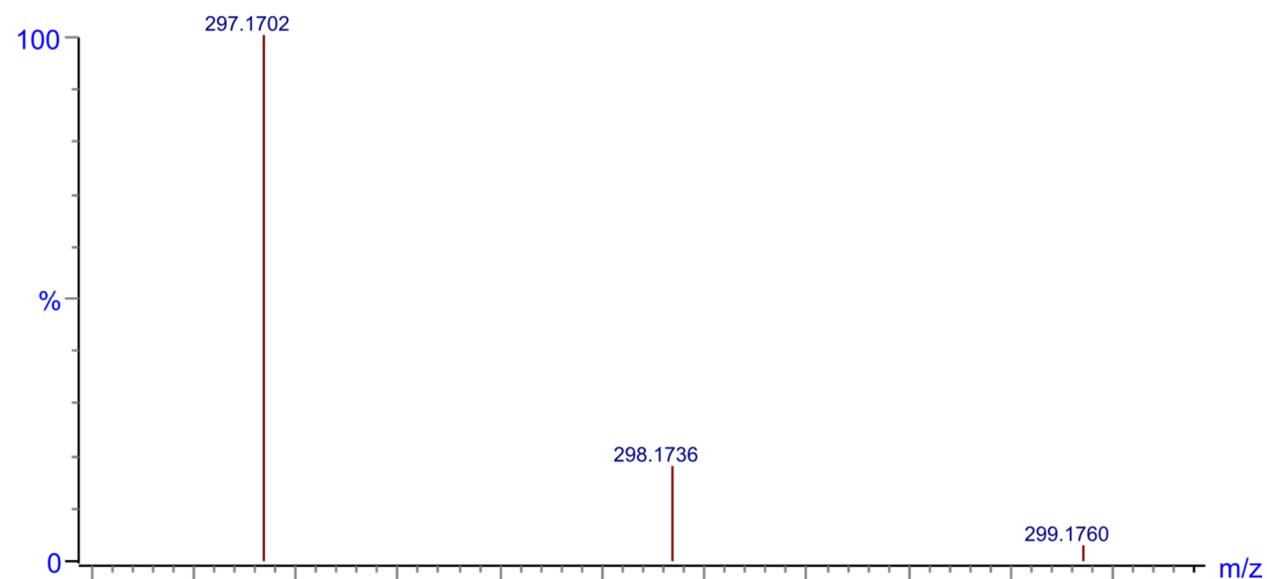


Figure S49. Mobility separated ramped energy mass spectrum for feature 11, indicating proposed fragment identities.

D. Mass Spectral Data for Selected Features

C16 H25 O5



Feature 12 $[M+H]^+$

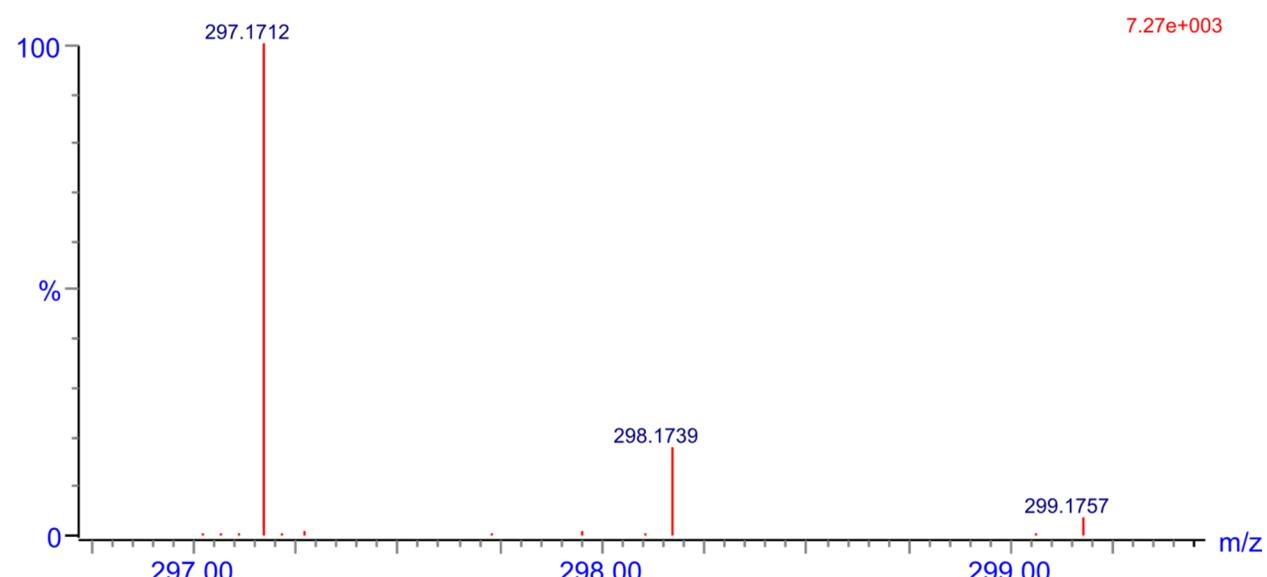


Figure S50. (Above) Theoretical isotopic profile for $[C_{16}H_{24}O_5 + H]^+$. **(Below)** Accurate mass isotopic envelope of feature 12, as specified in Table 1.

D. Mass Spectral Data for Selected Features

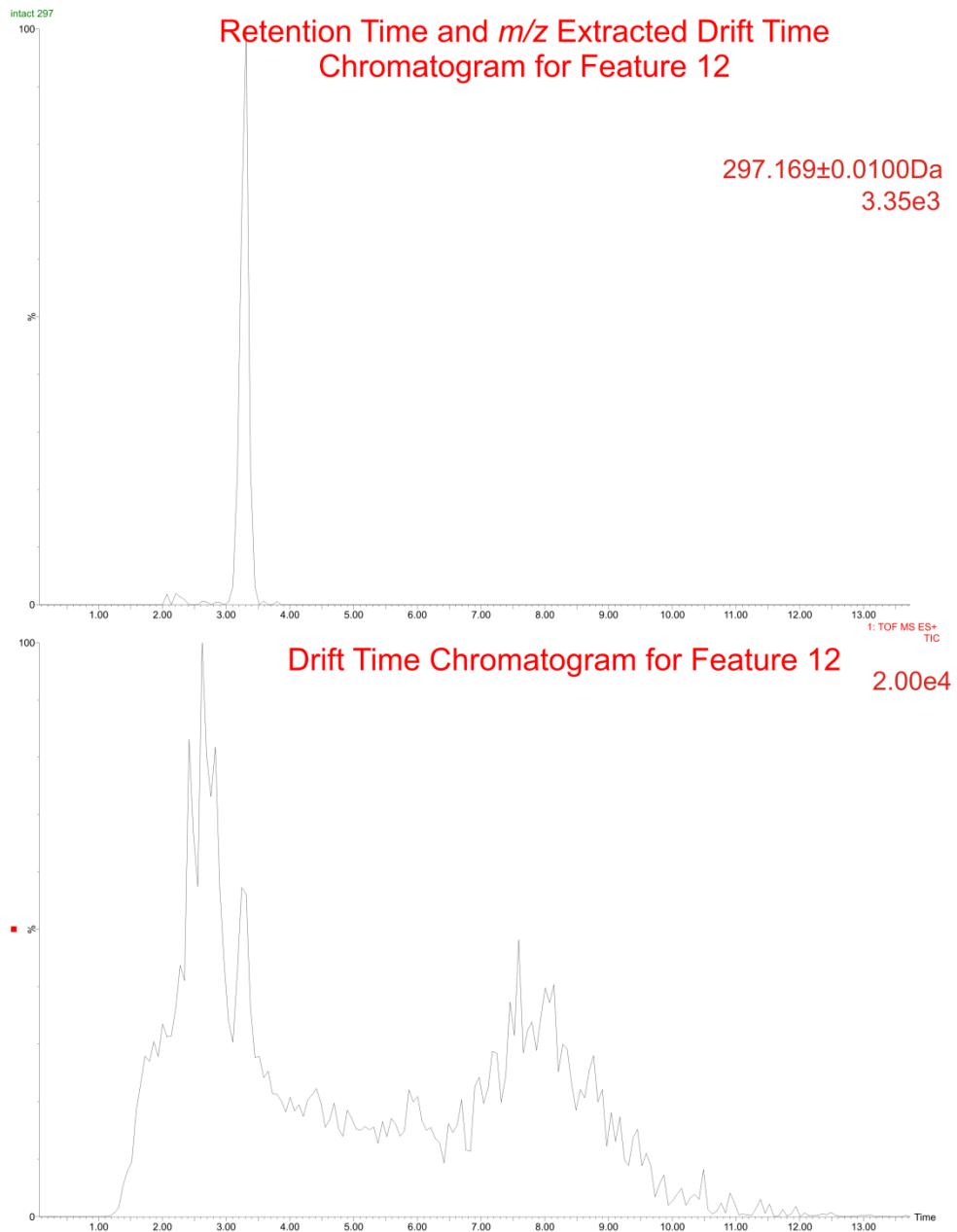


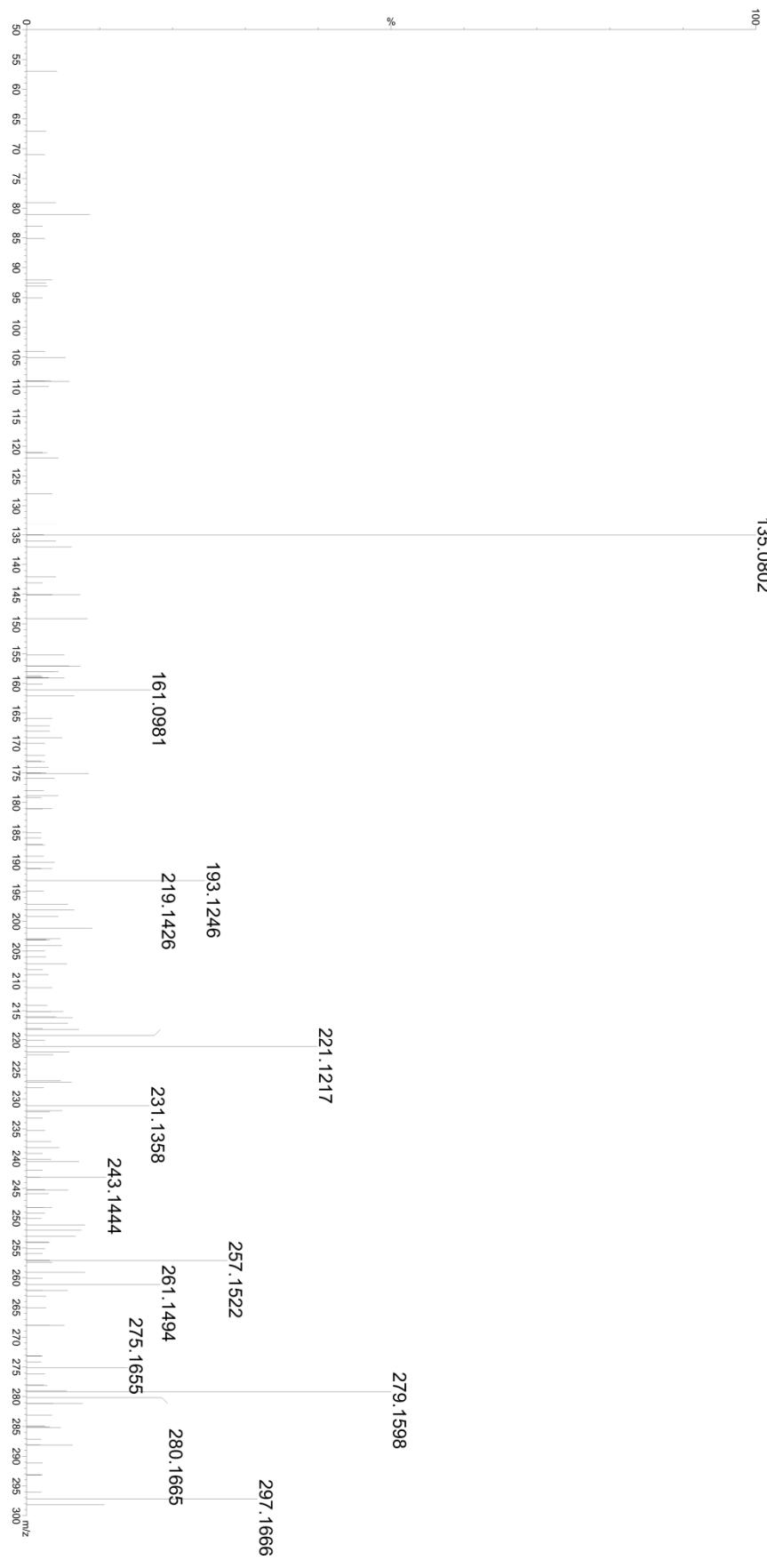
Figure S51. Retention time selected drift time chromatograms and extracted drift time ion chromatogram for feature 12. This drift time was used to select the proper drift time for high energy data interrogation.

D. Mass Spectral Data for Selected Features

Feature 12 Ramped Energy Spectrum

135.0802

600



Supplementary Information
S46

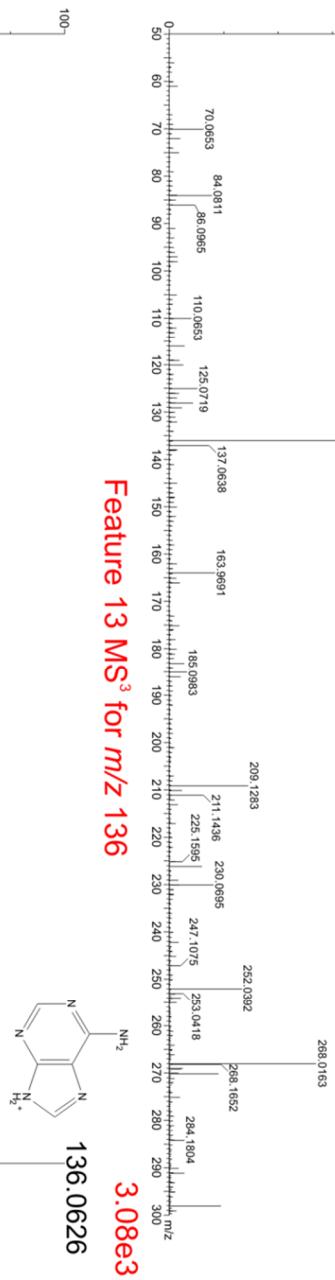
Figure S52. Mobility separated ramped energy mass spectrum for feature 12.

Feature 13 Ramped Energy Spectrum

4.03e4



Feature 13 MS³ for m/z 136



[M-NH₃+H]⁺

137.0241

138.0266

119.0352

107.0128

105.0727

109.0239

117.0566

120.0807

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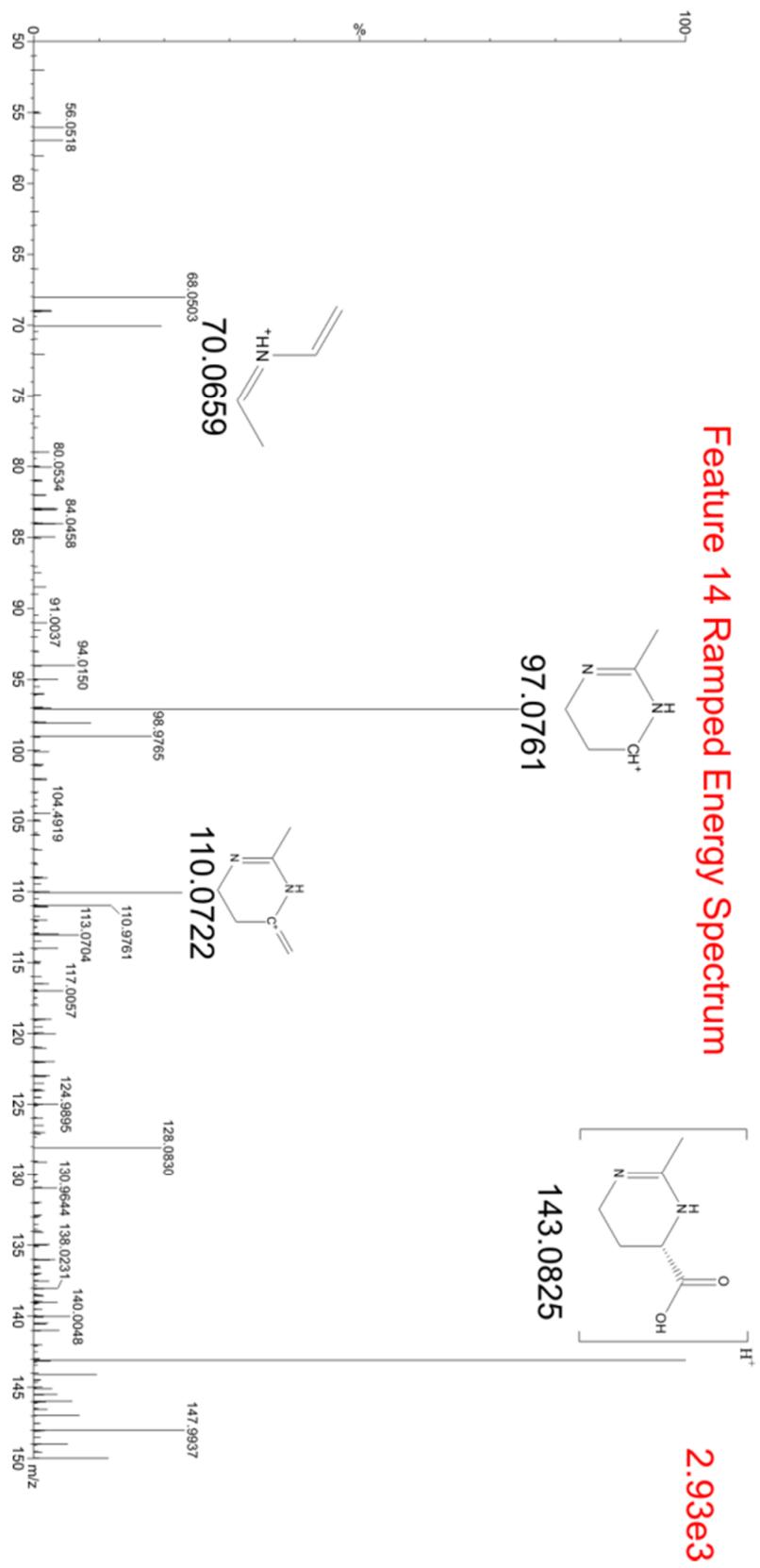
645.0670

646.0670

647.0670

648

D. Mass Spectral Data for Selected Features



Feature 15 Ramped Energy Spectrum

$[M-H_2O+H]^+$
162.0920
 $1.14e4$

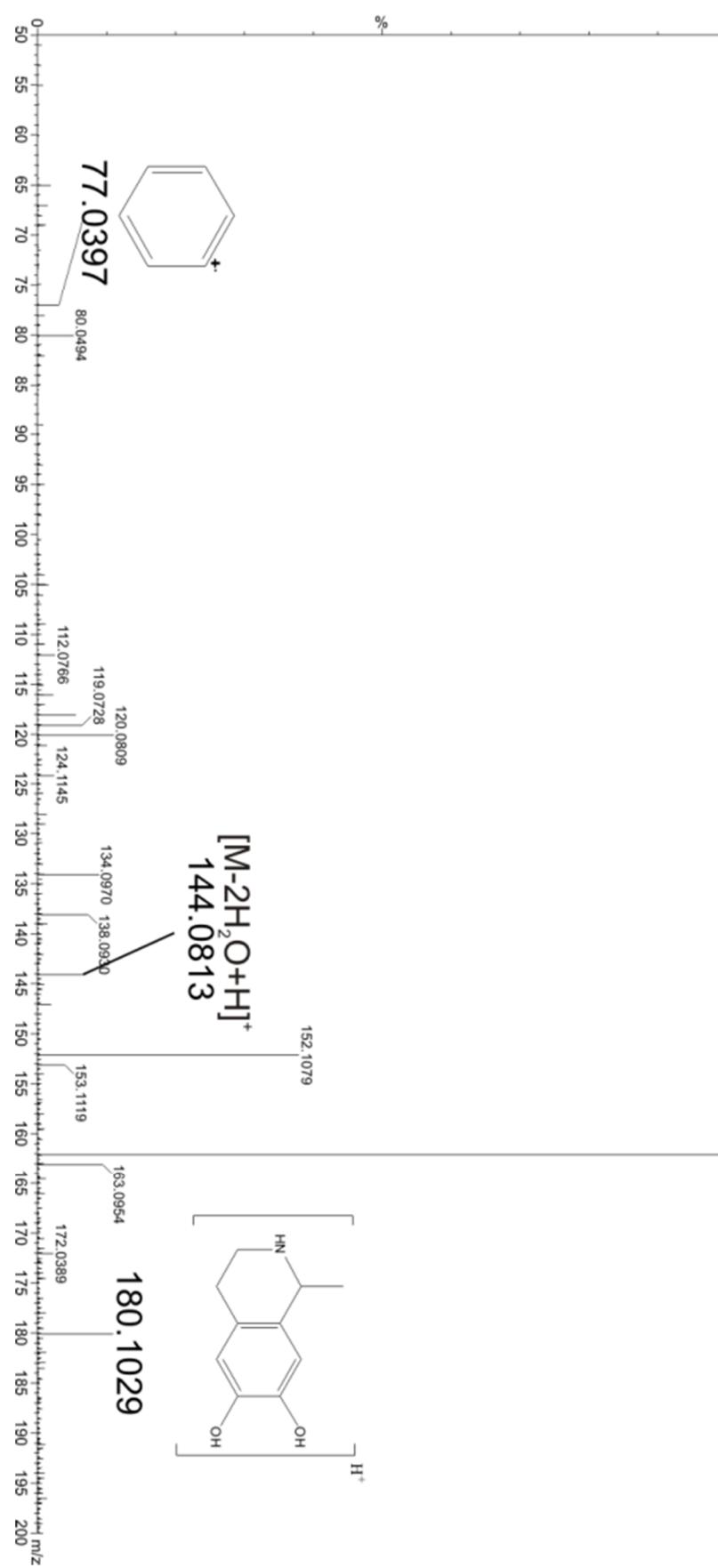


Figure S55. (Above) Mobility separated ramped energy mass spectrum for feature 15, indicating proposed fragment identities. Feature 15 is the result of the in-source neutral loss of water.

D. Mass Spectral Data for Selected Features

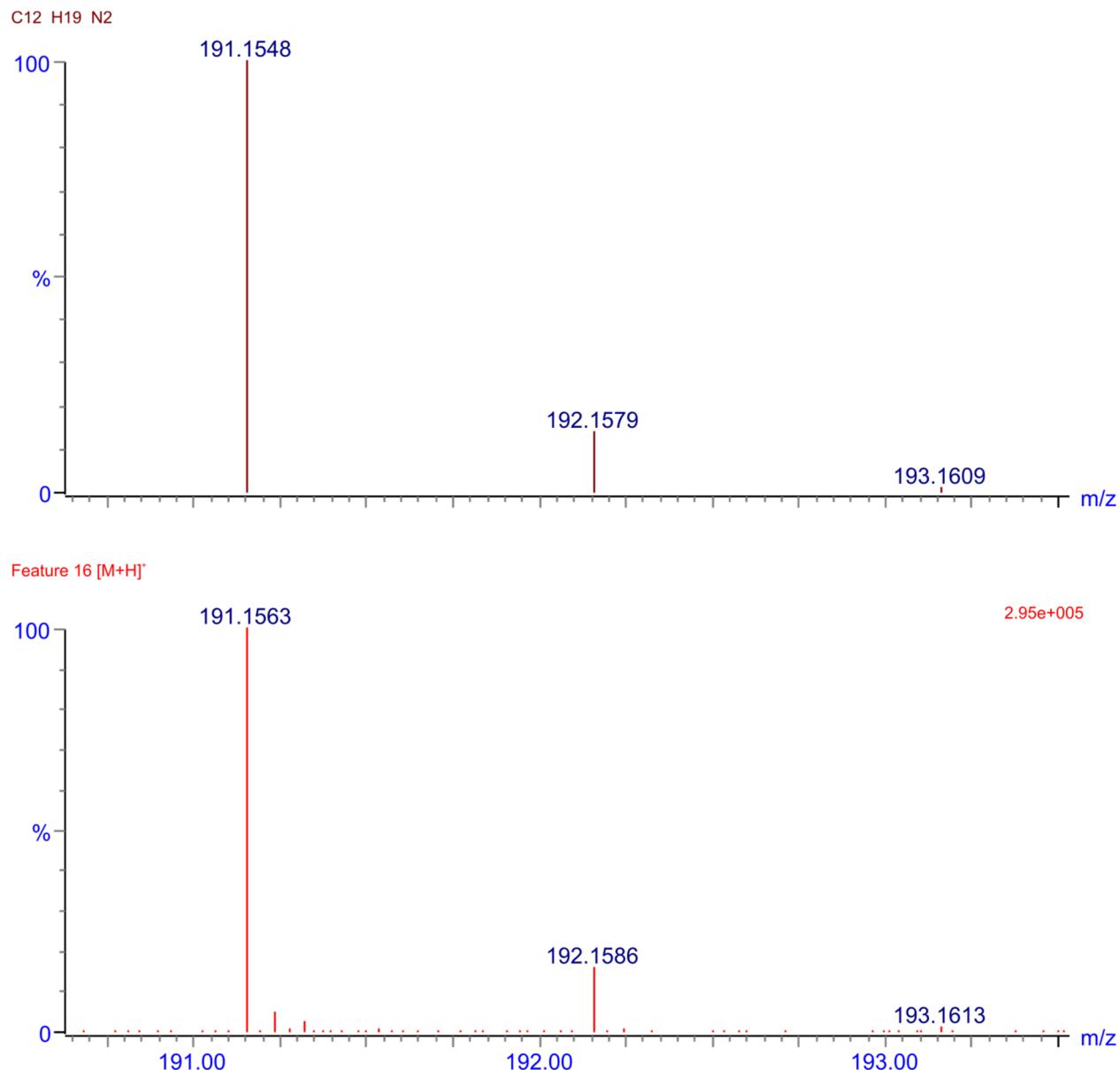


Figure S56. (Above) Theoretical isotopic profile for [C₁₂H₁₈N₂+H]⁺. **(Below)** Accurate mass isotopic envelope of feature 16, as specified in Table 1.

D. Mass Spectral Data for Selected Features

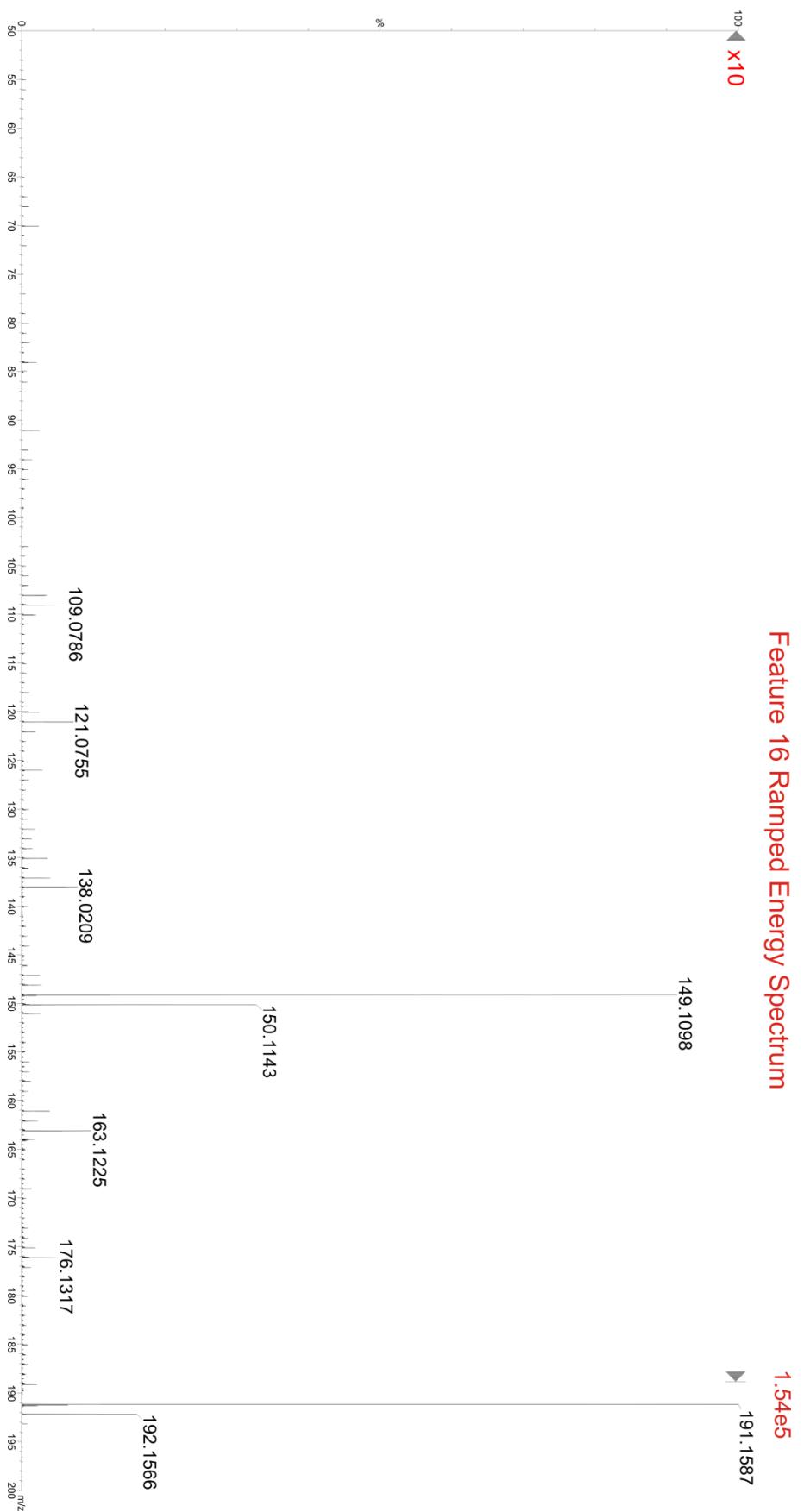


Figure S57. Mobility separated ramped energy mass spectrum for feature 16. The region from 50-190Da is magnified 10x.

D. Mass Spectral Data for Selected Features

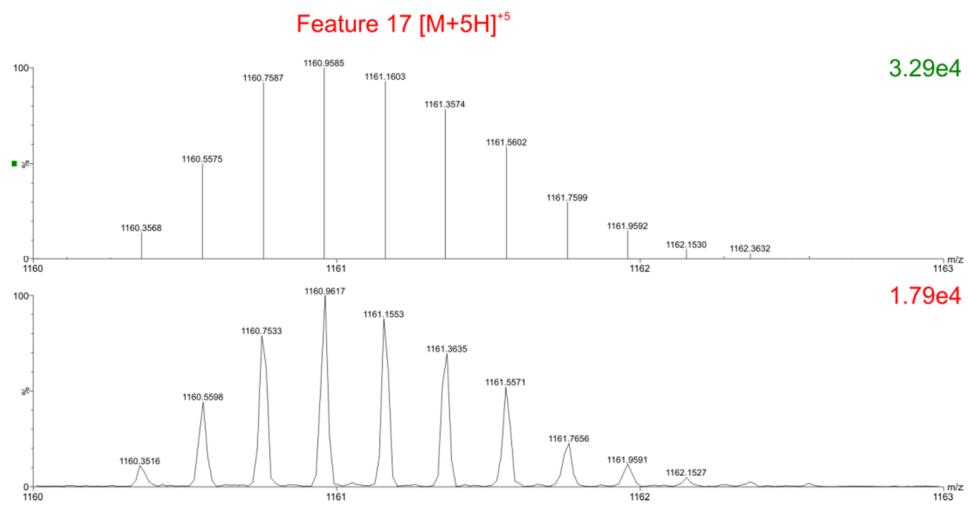


Figure S58. (Above) Centroded accurate mass isotopic envelope for feature 17 . **(Below)** Continuum accurate mass isotopic envelope of feature 17, as specified in Table 1.

D. Mass Spectral Data for Selected Features

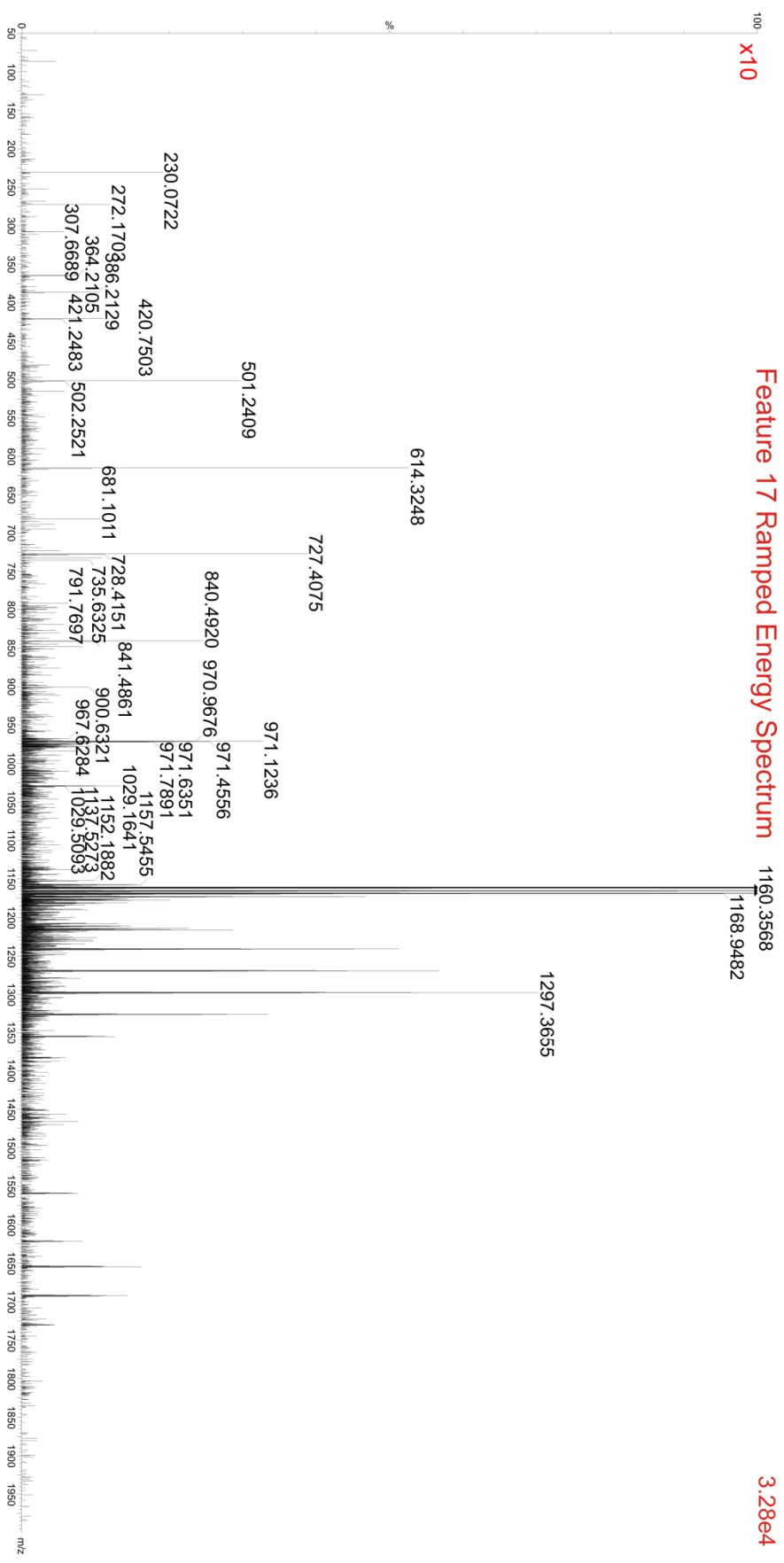
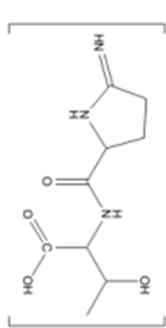


Figure S59. Mobility separated ramped energy mass spectrum for feature 17. Spectrum is magnified 10x.

Feature 18 Ramped Energy Spectrum

230.1140 2.28e4



%

D. Mass Spectral Data for Selected Features

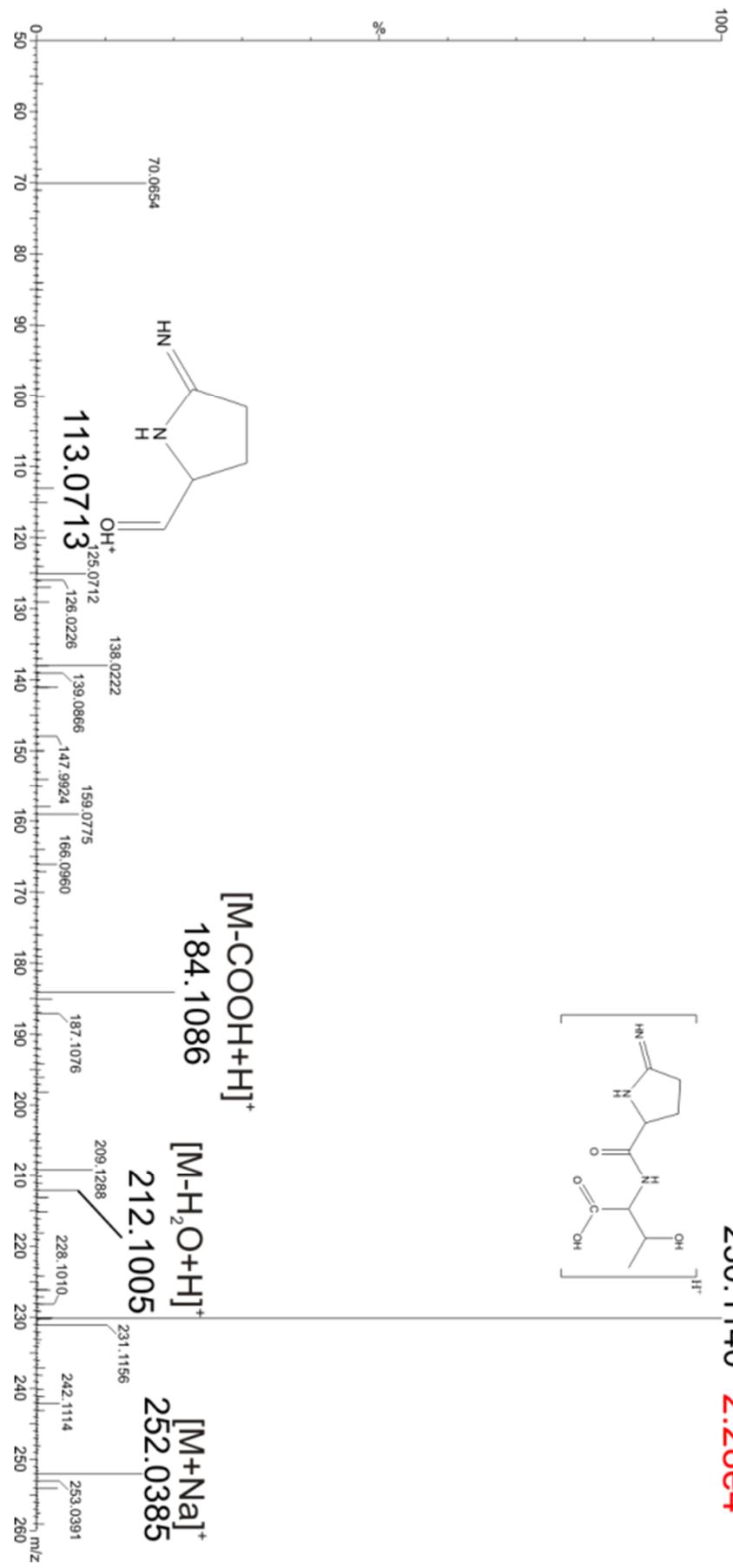


Figure S60. (Above) Mobility separated ramped energy mass spectrum for feature 18, indicating proposed fragment identities.

Features 19 and 20 Ramped Energy Spectrum

$[M-C_5H_9NO_3+H]^+$
384.2171
 $2.34e4$

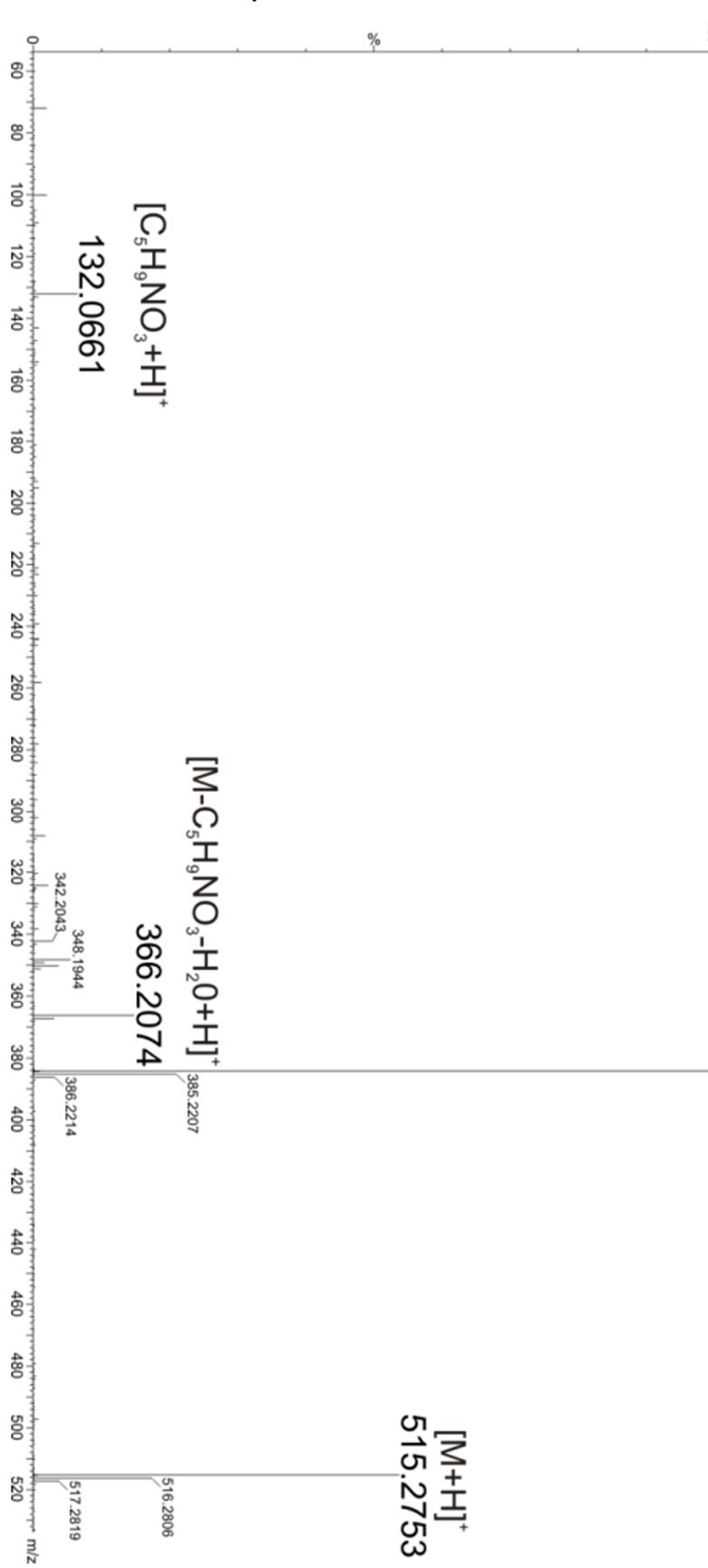


Figure S61. (Above) Mobility separated ramped energy mass spectrum for feature 18 and 19, indicating proposed fragment identities.

Feature 21 Ramped Energy Spectrum

9.03e3

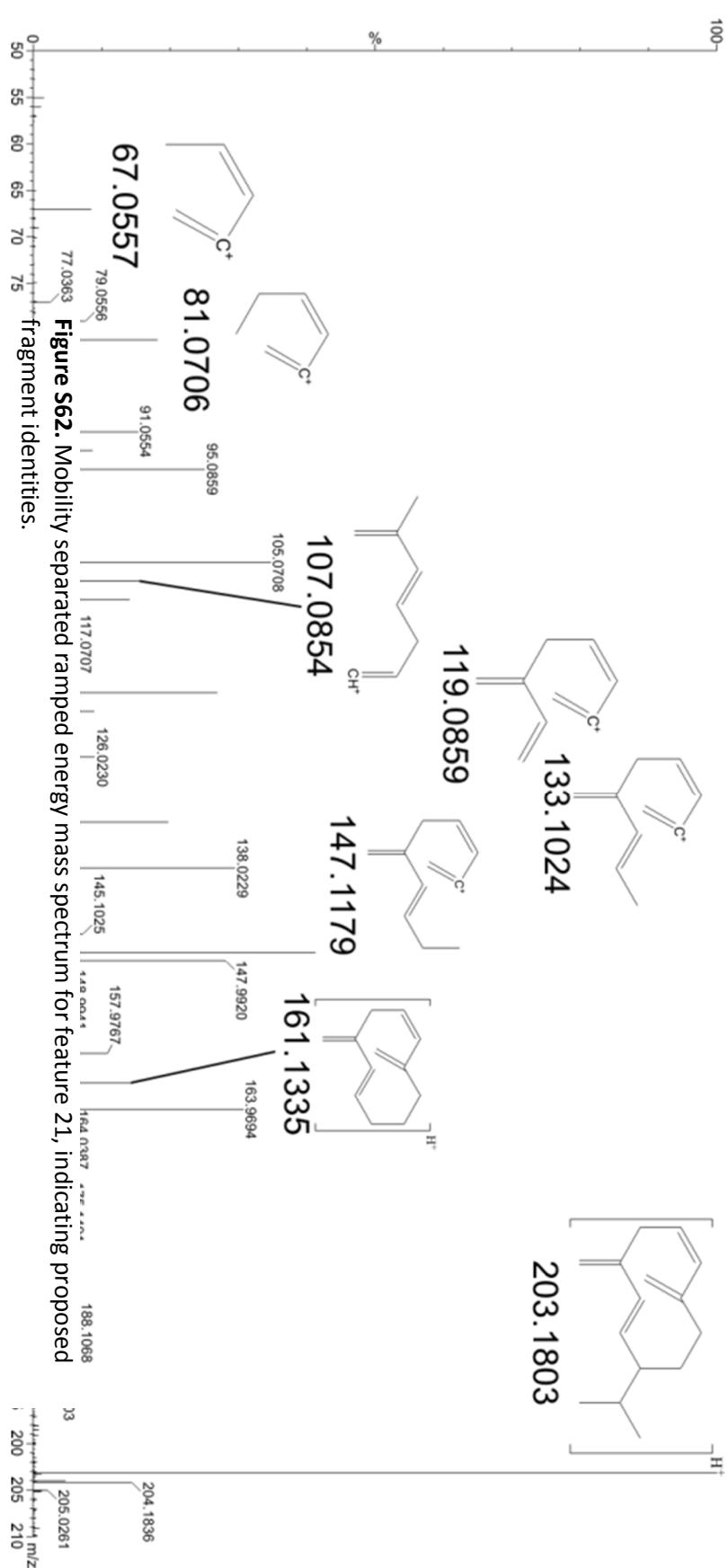


Figure S62. Mobility separated ramped energy mass spectrum for feature 21, indicating proposed

D. Mass Spectral Data for Selected Features

Feature 22 Ramped Energy Spectrum

1.99e3

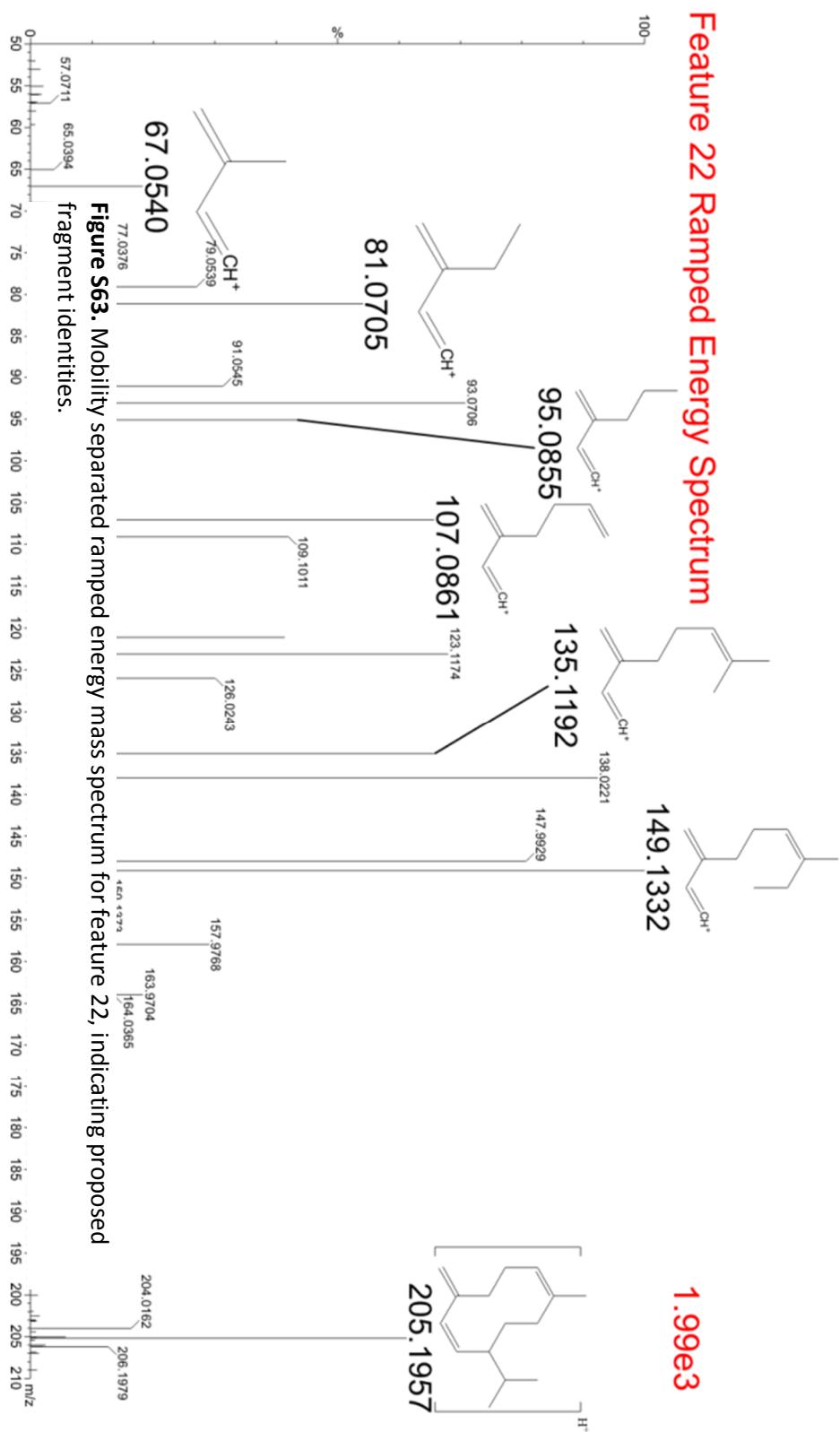


Figure S63. Mobility separated ramped energy mass spectrum for feature 22, indicating proposed fragment identities.

D. Mass Spectral Data for Selected Features

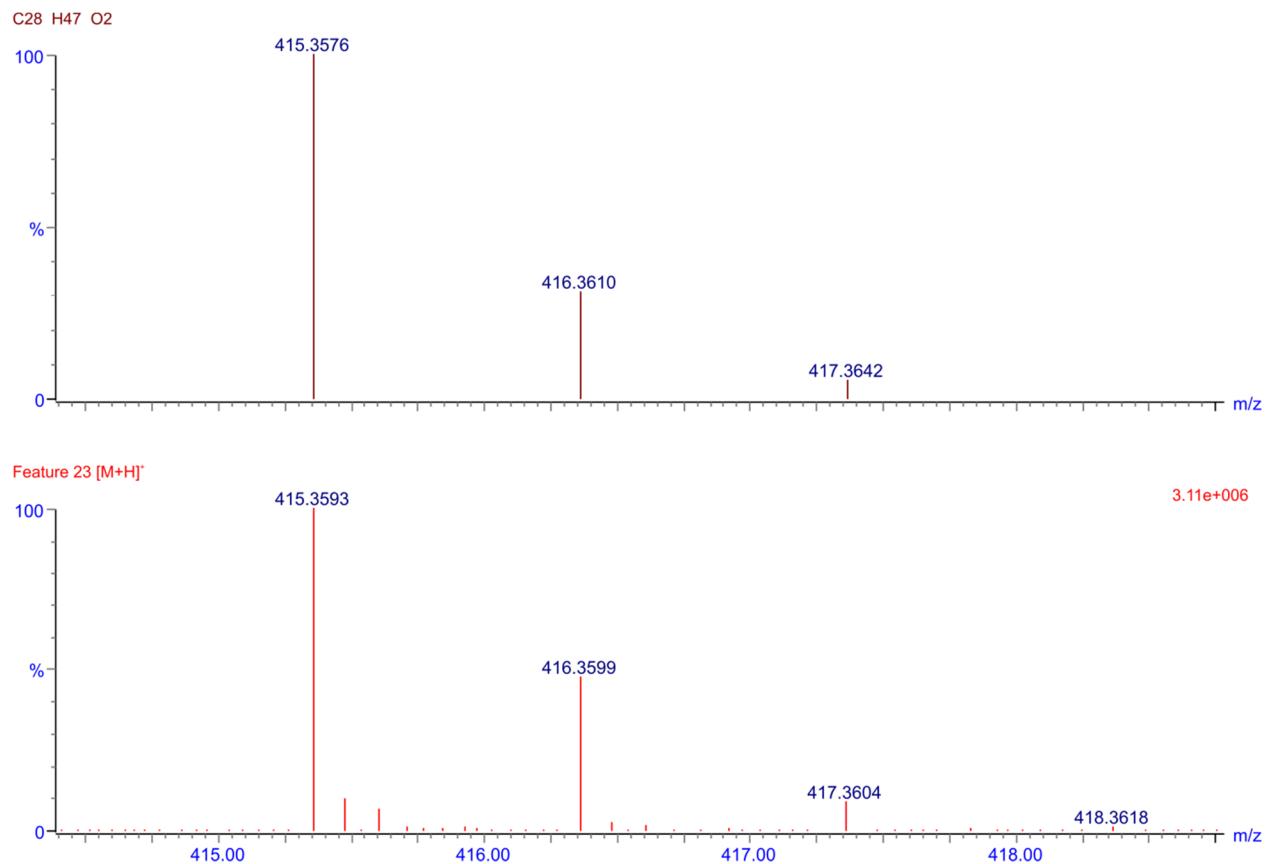


Figure S64. (Above) Theoretical isotopic profile for $[C_{28}H_{46}O_2 + H]^+$. **(Below)** Accurate mass isotopic envelope of feature 23, as specified in Table 1.

D. Mass Spectral Data for Selected Features

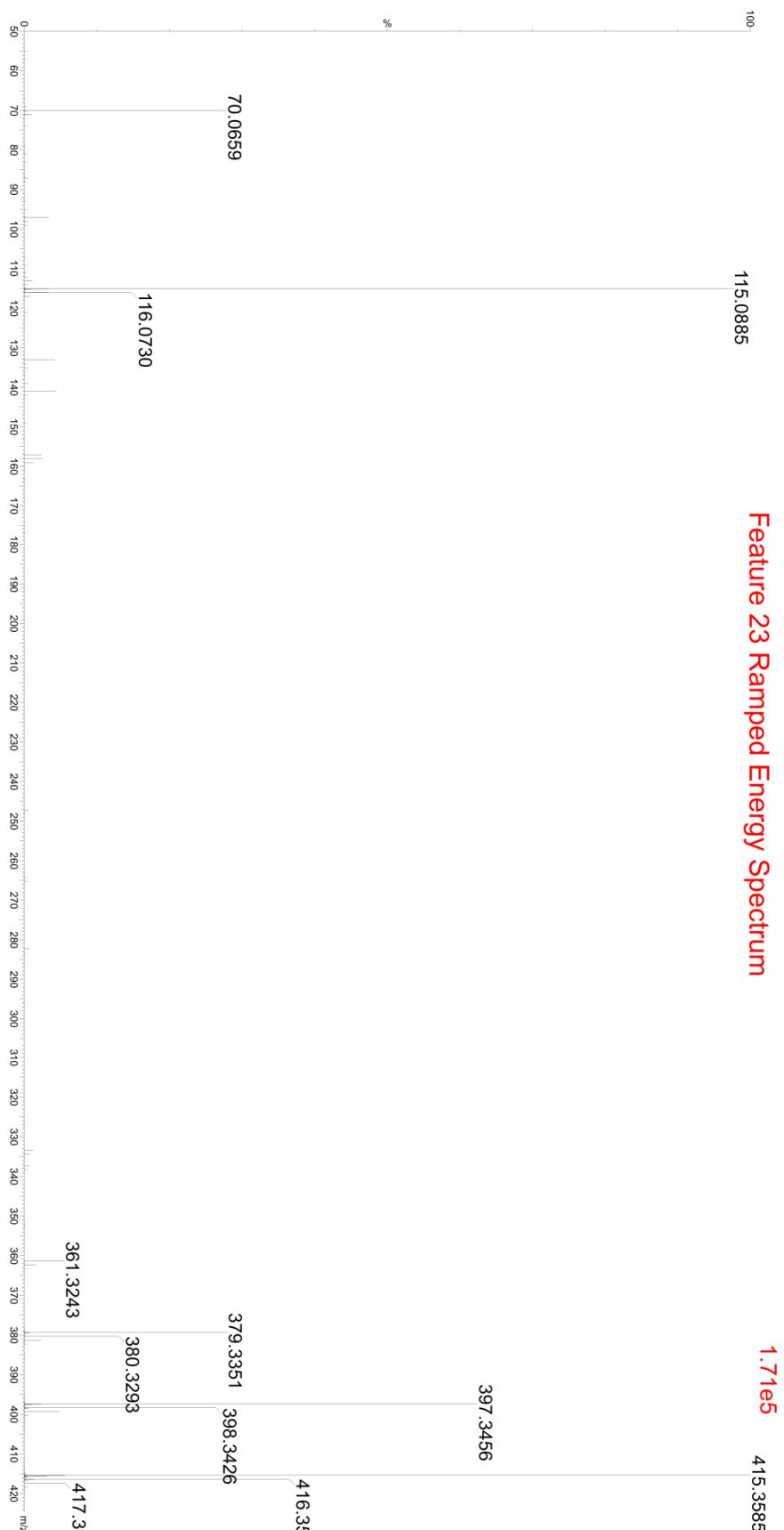


Figure S65. Mobility separated ramped energy mass spectrum for feature 23.



Figure S66. Mobility separated ramped energy mass spectrum for feature 24.

D. Mass Spectral Data for Selected Features

D. Mass Spectral Data for Selected Features



Figure S67. Mobility separated ramped energy mass spectrum for features 25 and 26.

D. Mass Spectral Data for Selected Features



Figure S68. Mobility separated ramped energy mass spectrum for feature 27.

D. Mass Spectral Data for Selected Features

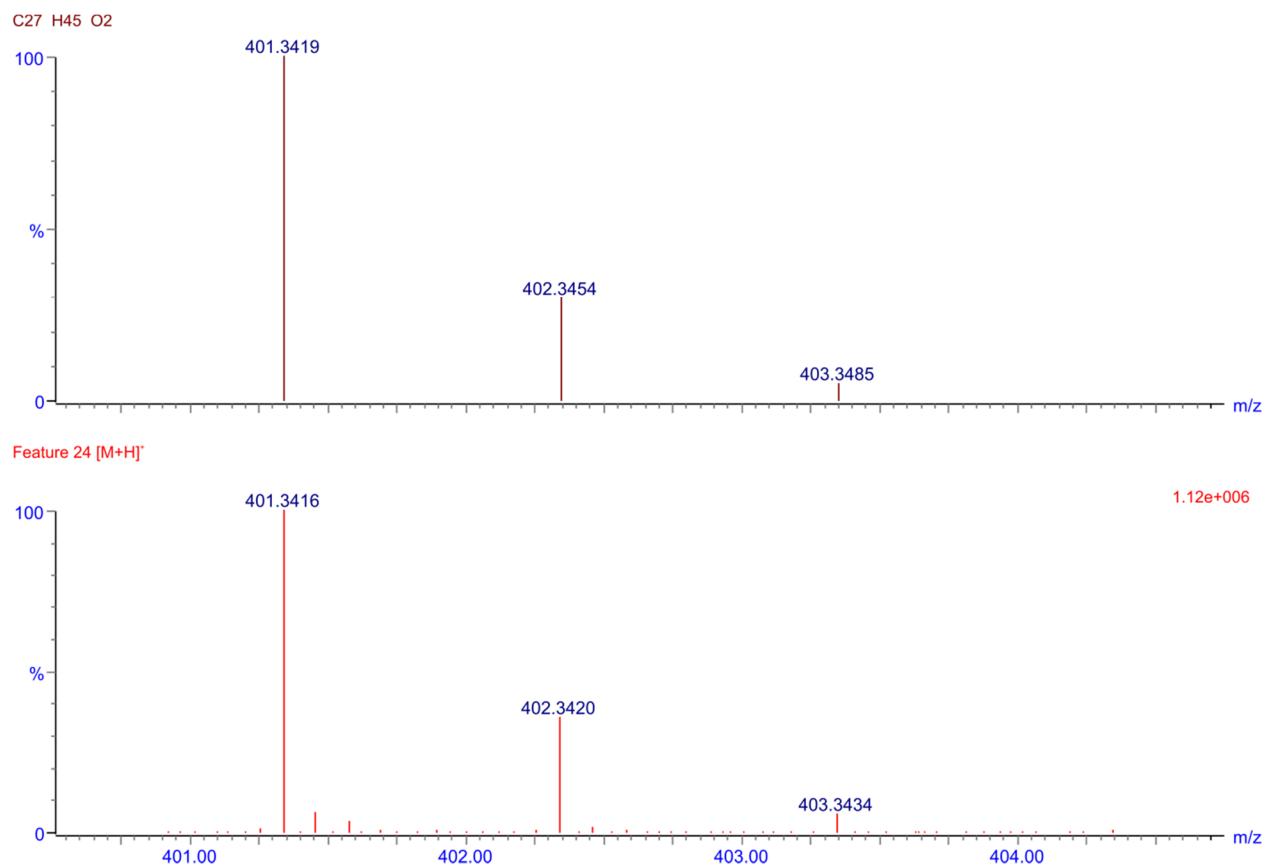


Figure S69. (Above) Theoretical isotopic profile for $[C_{27}H_{44}O_2 + H]^+$. **(Below)** Accurate mass isotopic envelope of feature 24, as specified in Table 1.

D. Mass Spectral Data for Selected Features

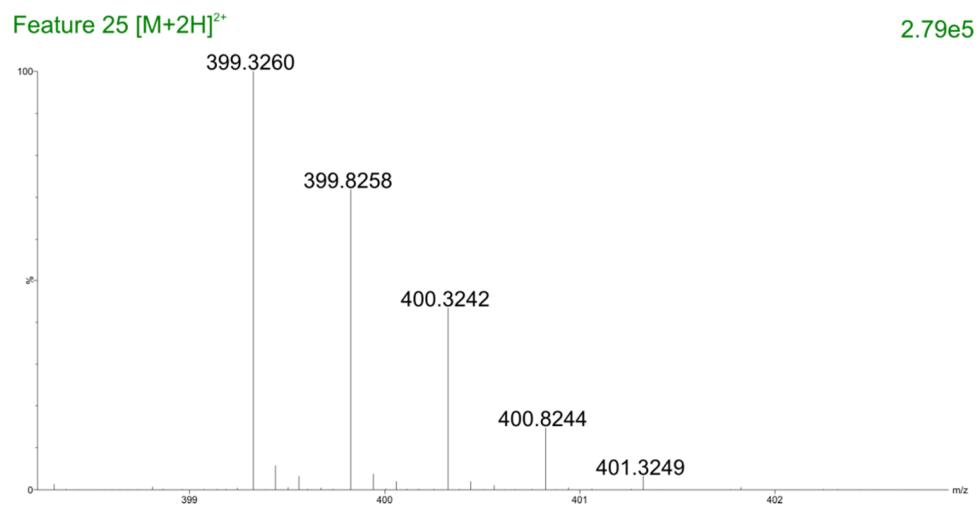


Figure S70. Accurate mass isotopic envelope of feature 25, as specified in Table 1.

D. Mass Spectral Data for Selected Features

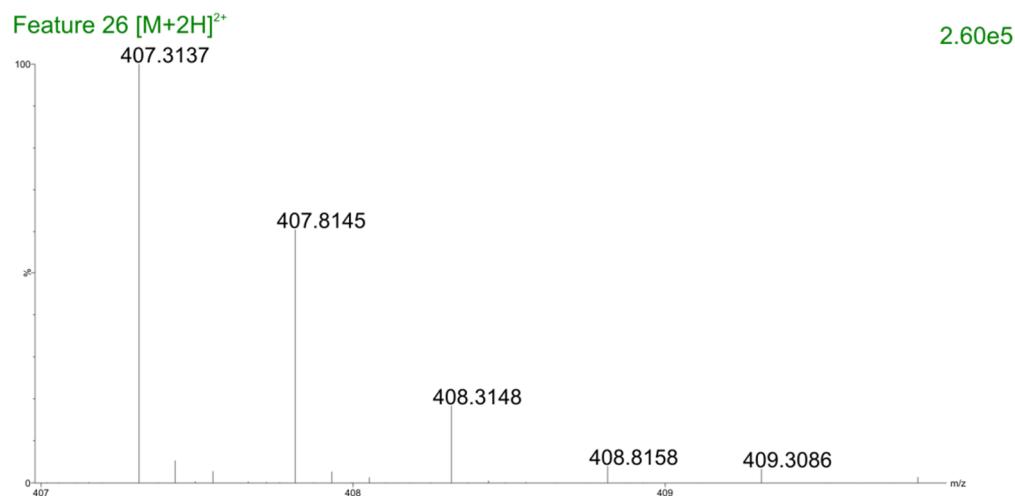


Figure S71. Accurate mass isotopic envelope of feature 26, as specified in Table 1.

D. Mass Spectral Data for Selected Features

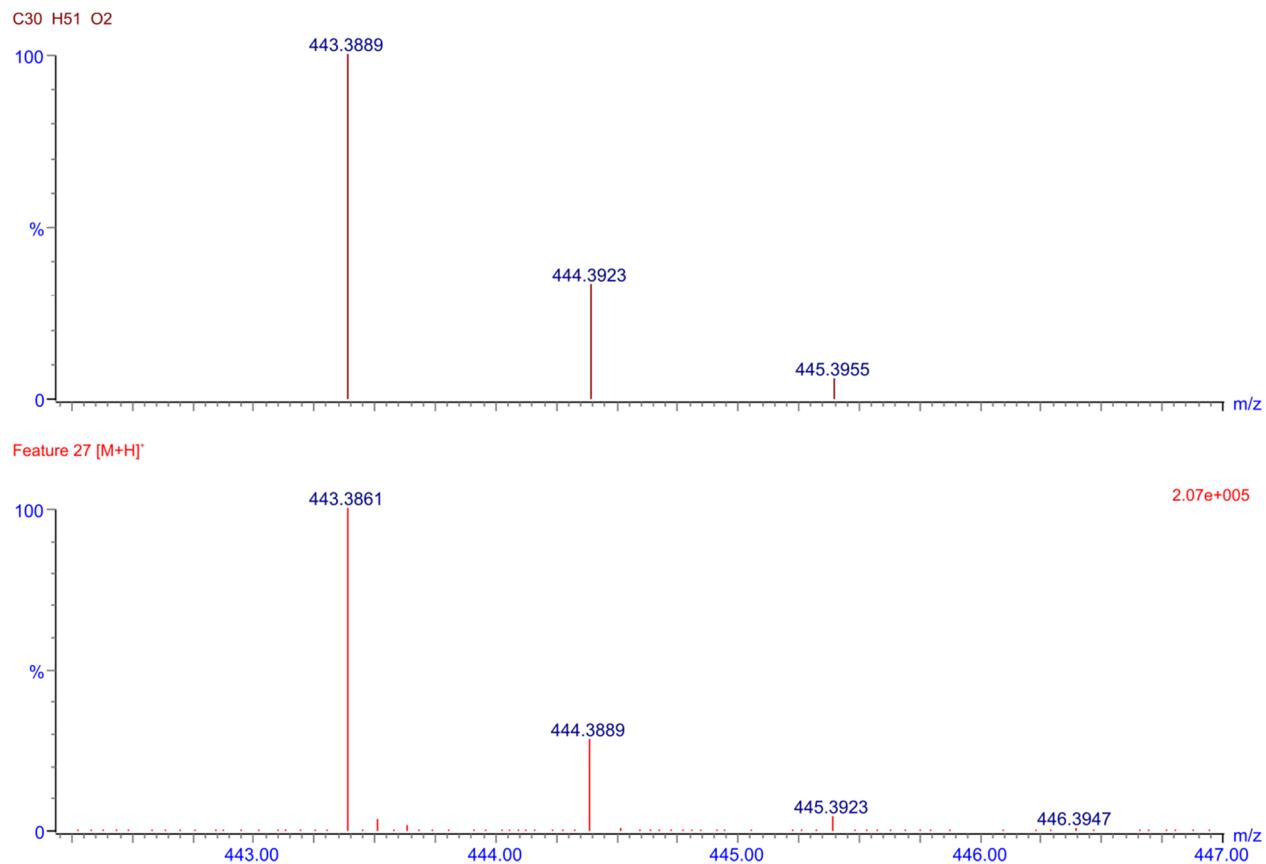


Figure S72. (Above) Theoretical isotopic profile for $[C_{30}H_{50}O_2 + H]^+$. **(Below)** Accurate mass isotopic envelope of feature 27, as specified in Table 1.

D. Mass Spectral Data for Selected Features

Feature 1 EIC ($\pm 0.01\text{Da}$)

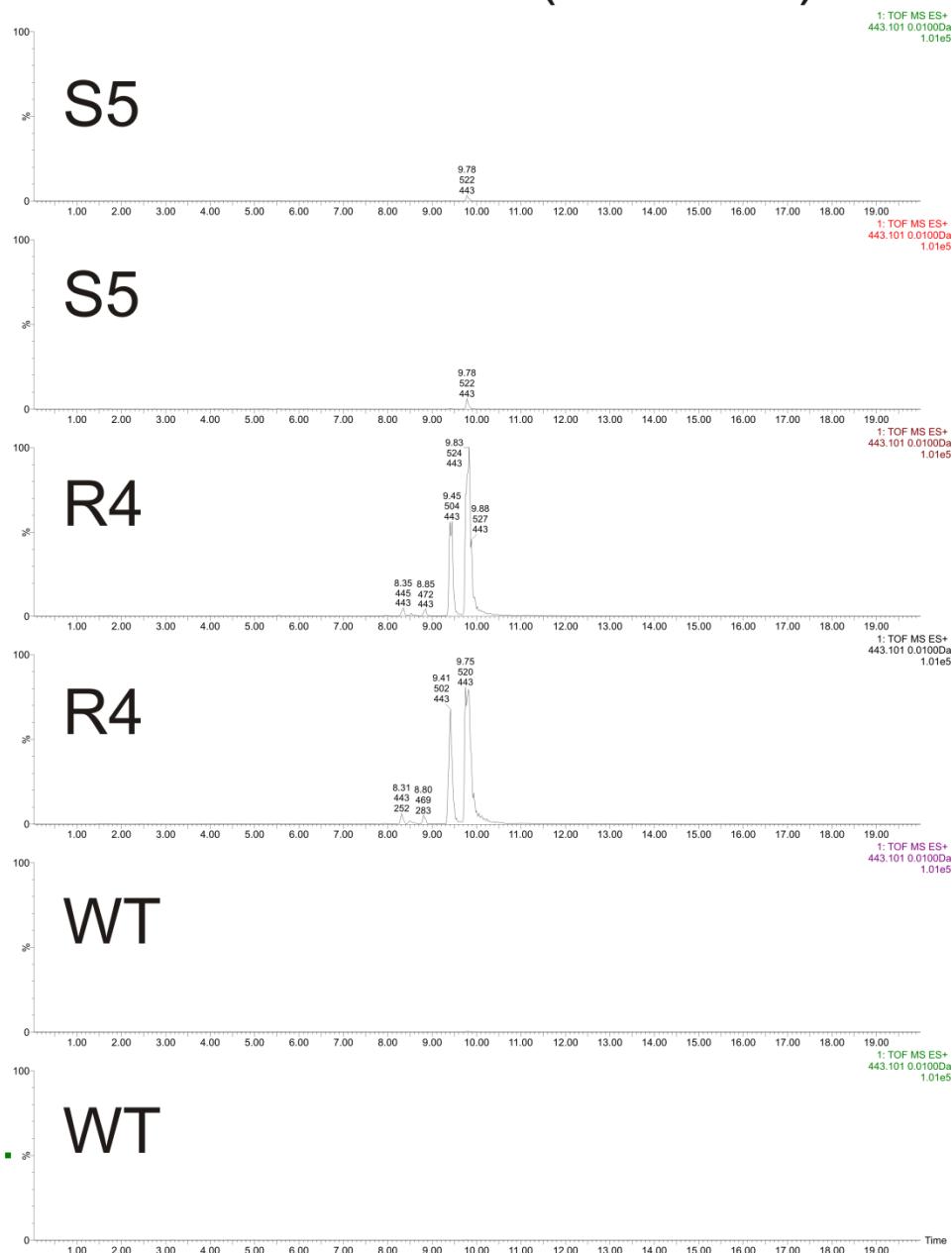


Figure S73. Extracted ion chromatograms for feature 1 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 2 EIC ($\pm 0.01\text{Da}$)

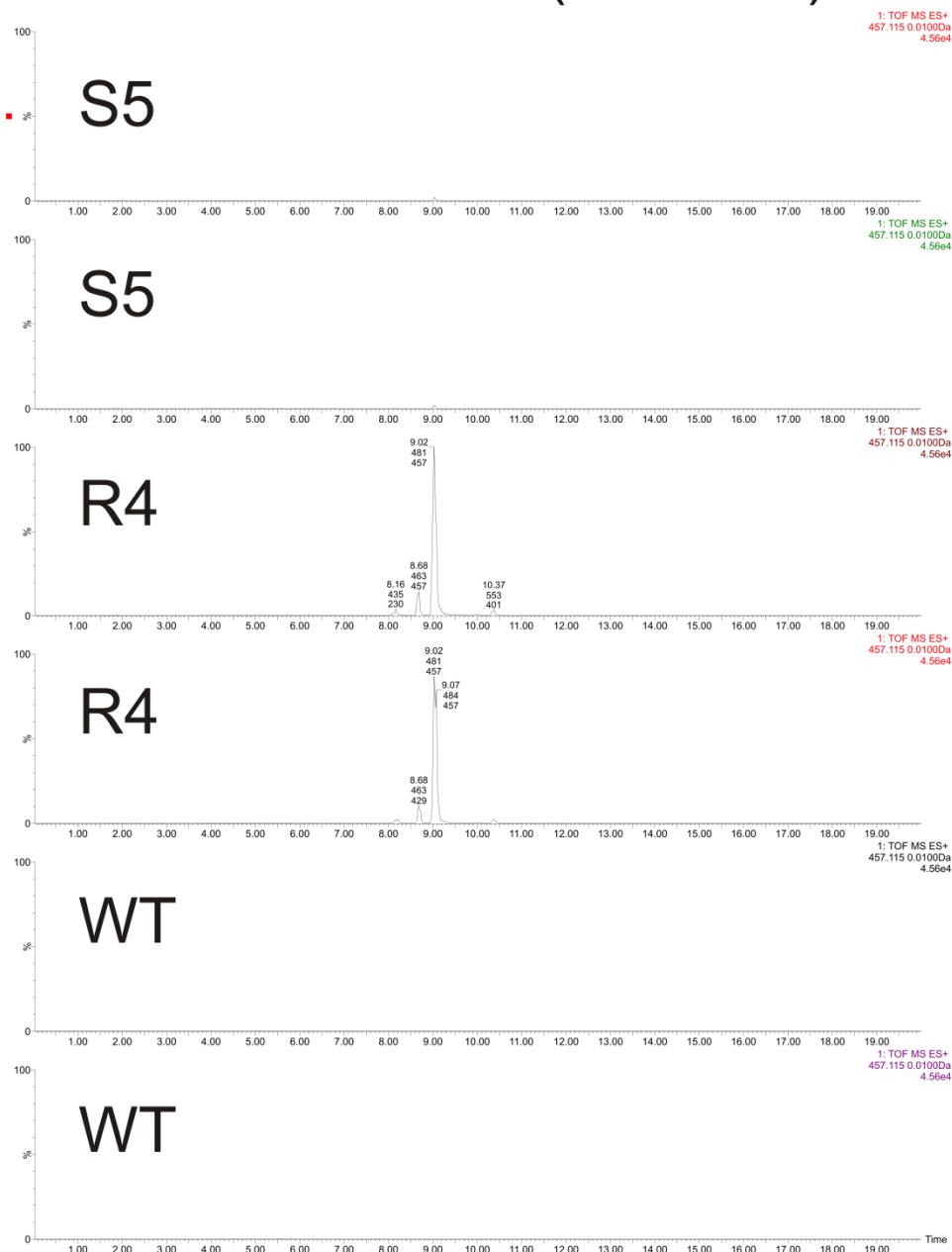


Figure S74. Extracted ion chromatograms for feature 2 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 3 EIC ($\pm 0.01\text{Da}$)

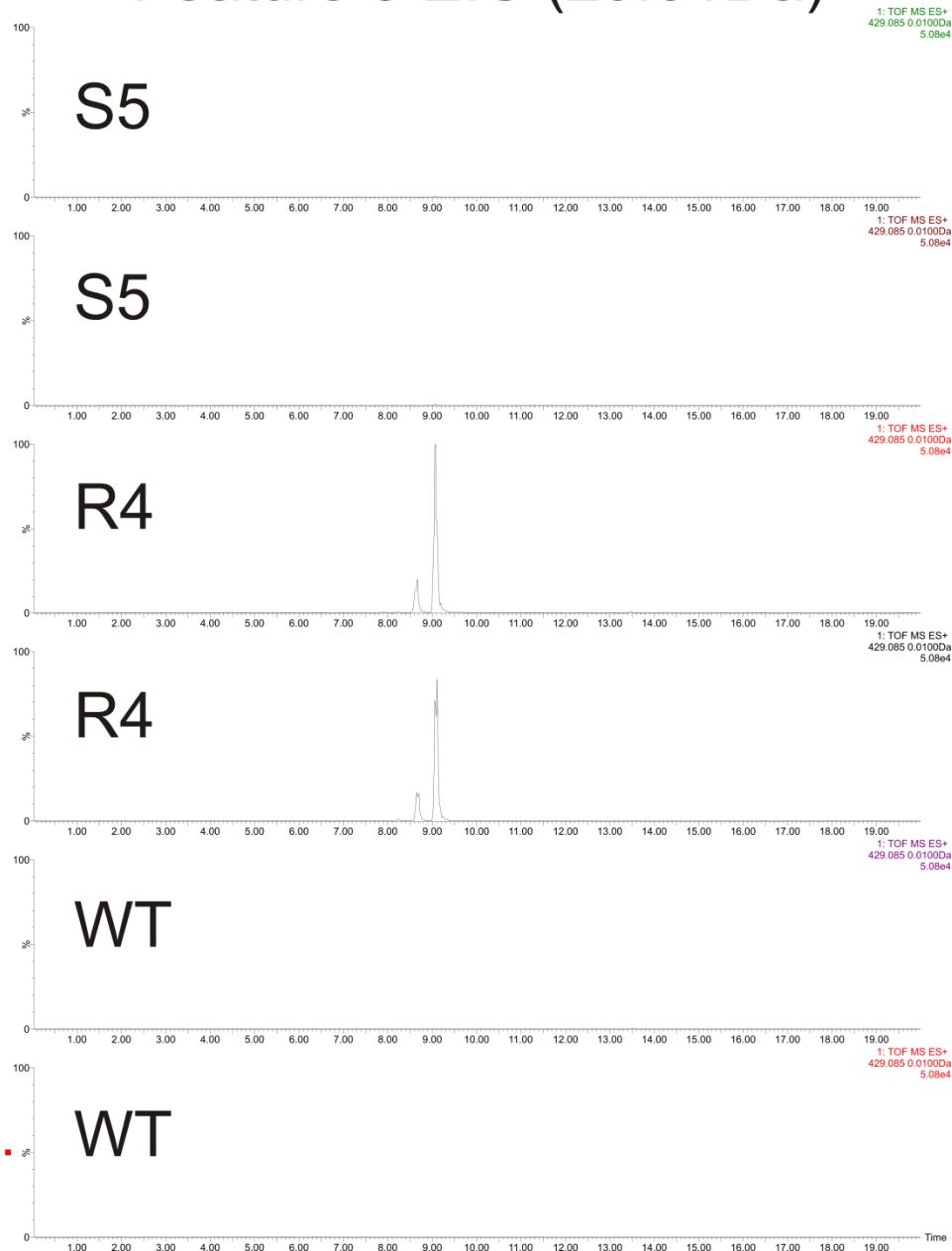


Figure S75. Extracted ion chromatograms for feature 3 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 4 EIC ($\pm 0.01\text{Da}$)

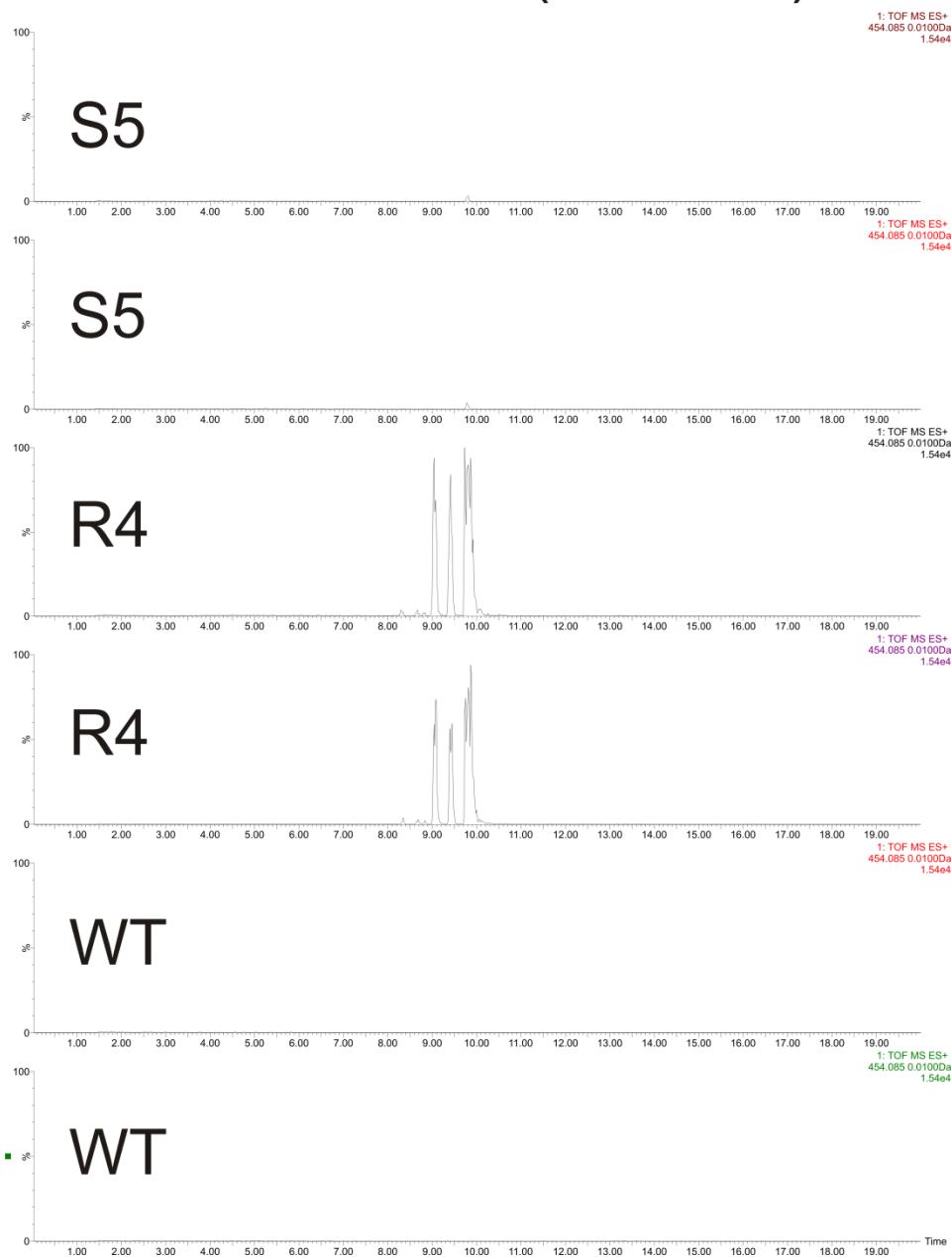


Figure S76. Extracted ion chromatograms for feature 4 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 5 EIC ($\pm 0.01\text{Da}$)

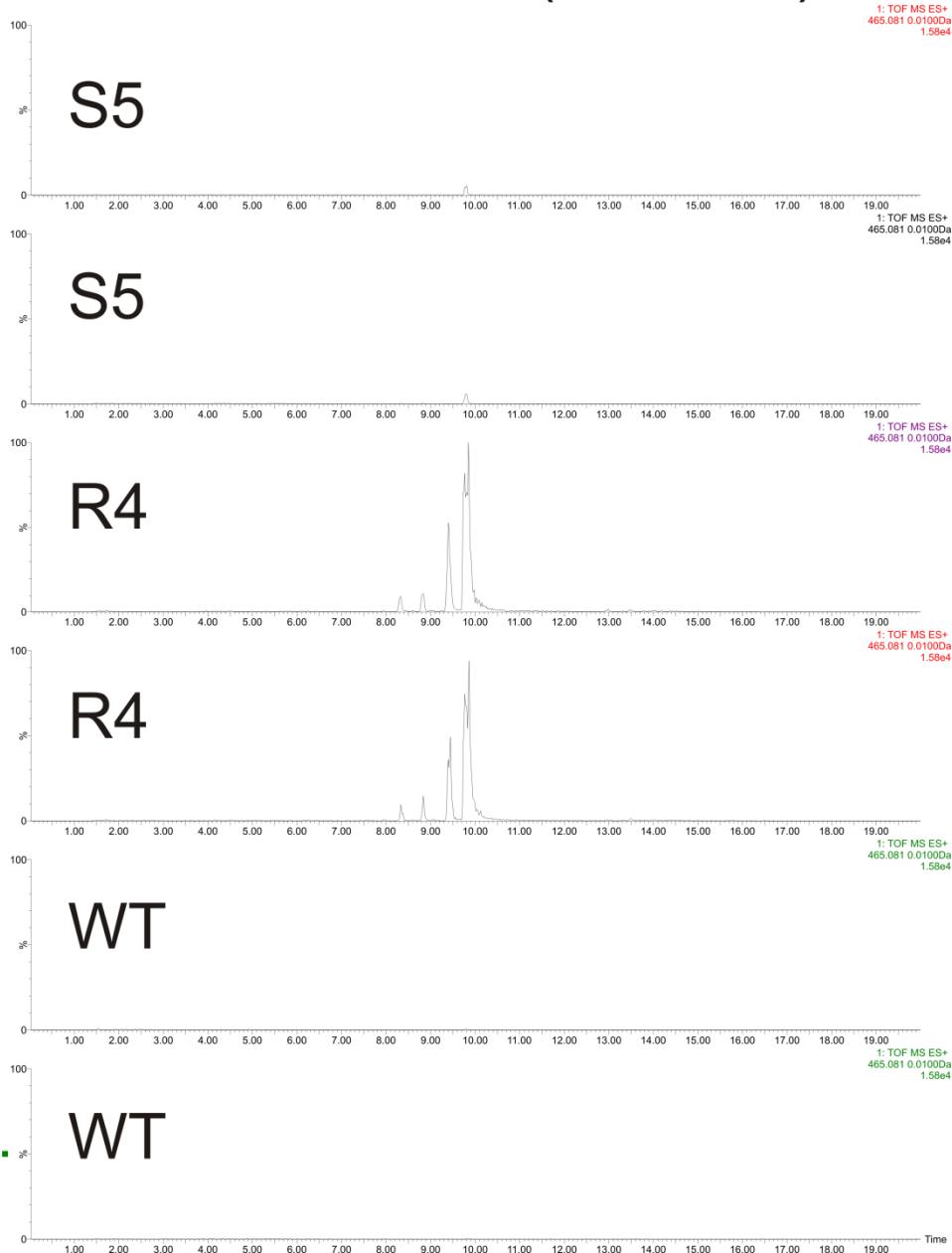


Figure S77. Extracted ion chromatograms for feature 5 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 6 EIC ($\pm 0.01\text{Da}$)

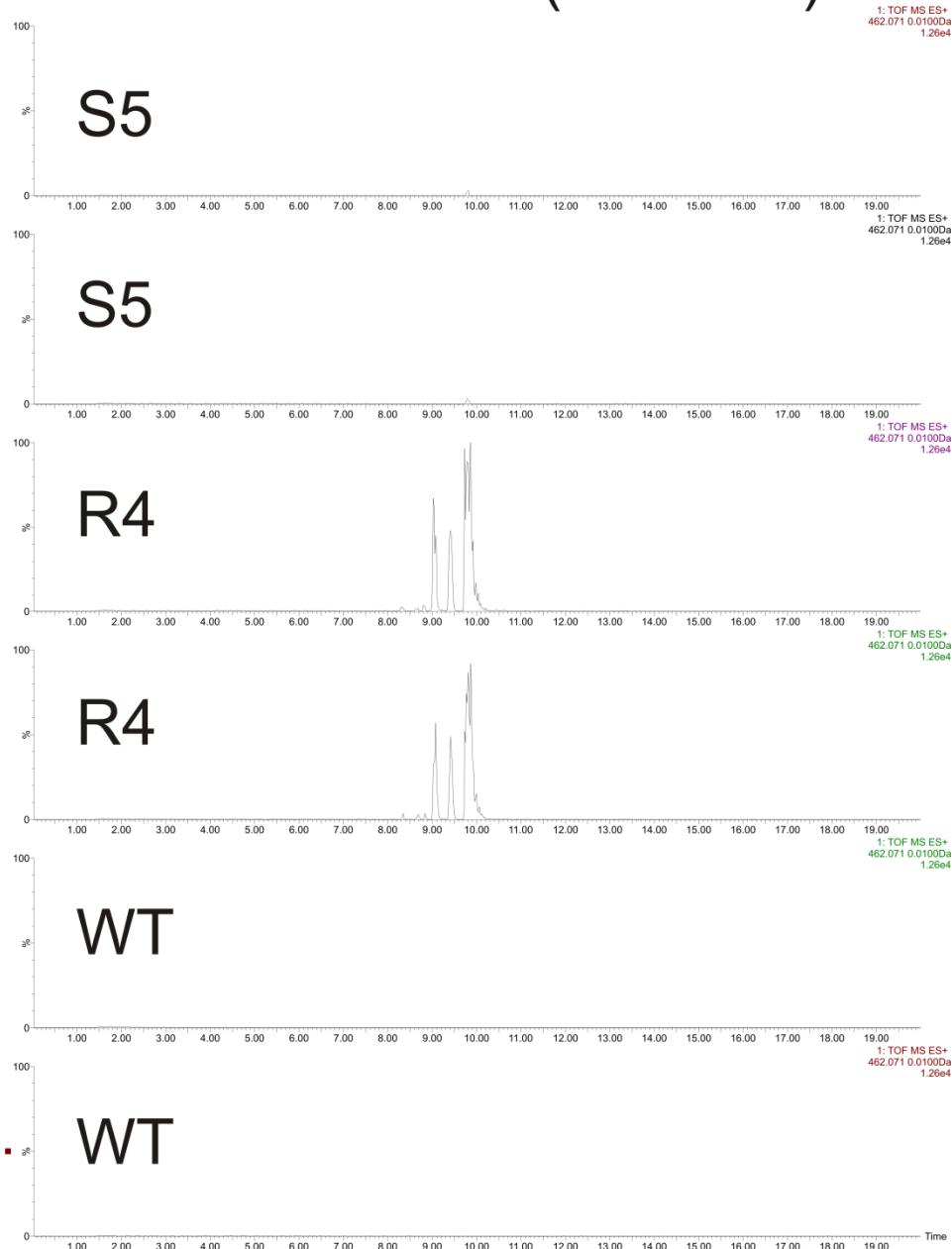


Figure S78. Extracted ion chromatograms for feature 6 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

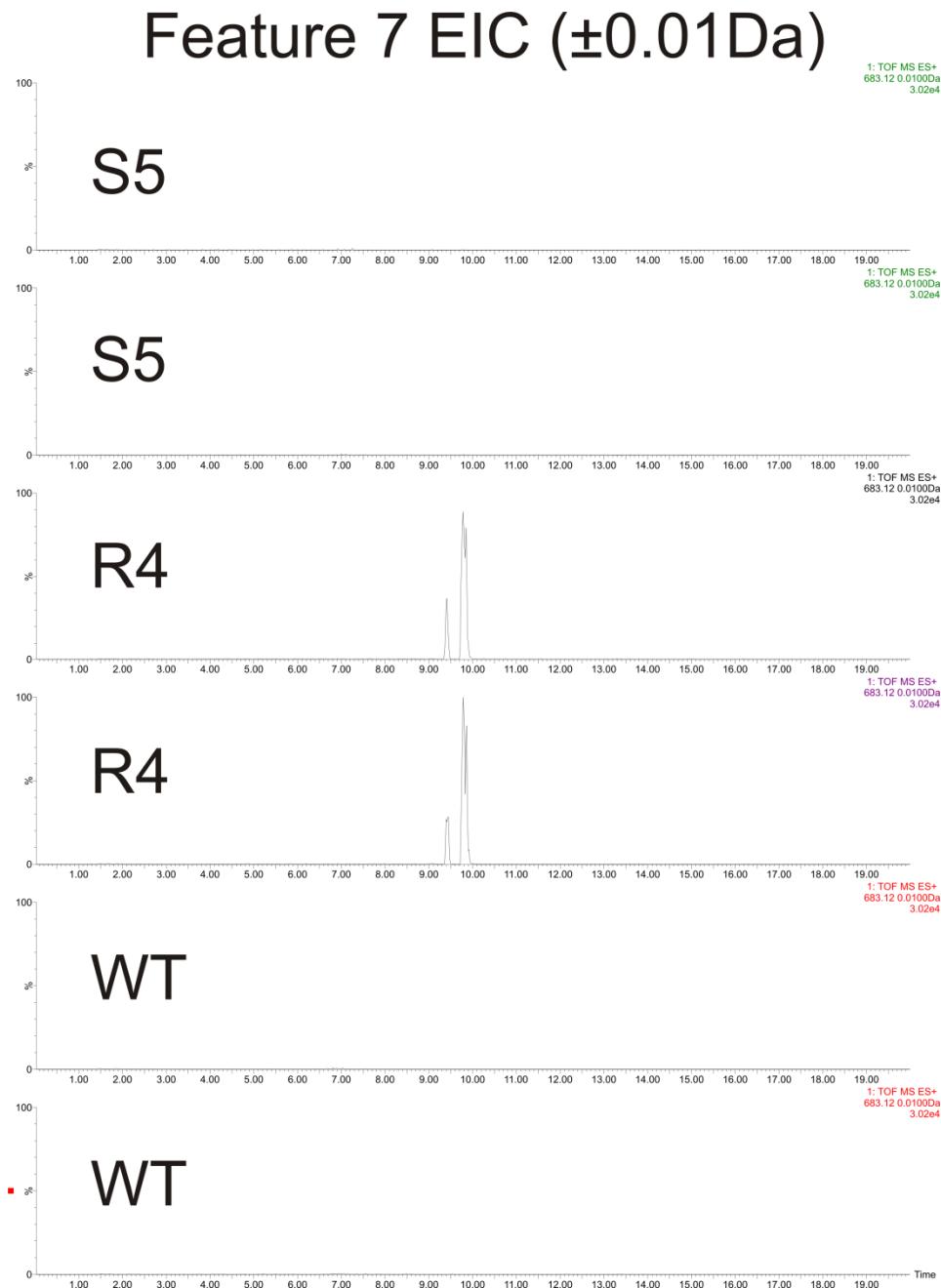


Figure S79. Extracted ion chromatograms for feature 7 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 8 EIC ($\pm 0.01\text{Da}$)

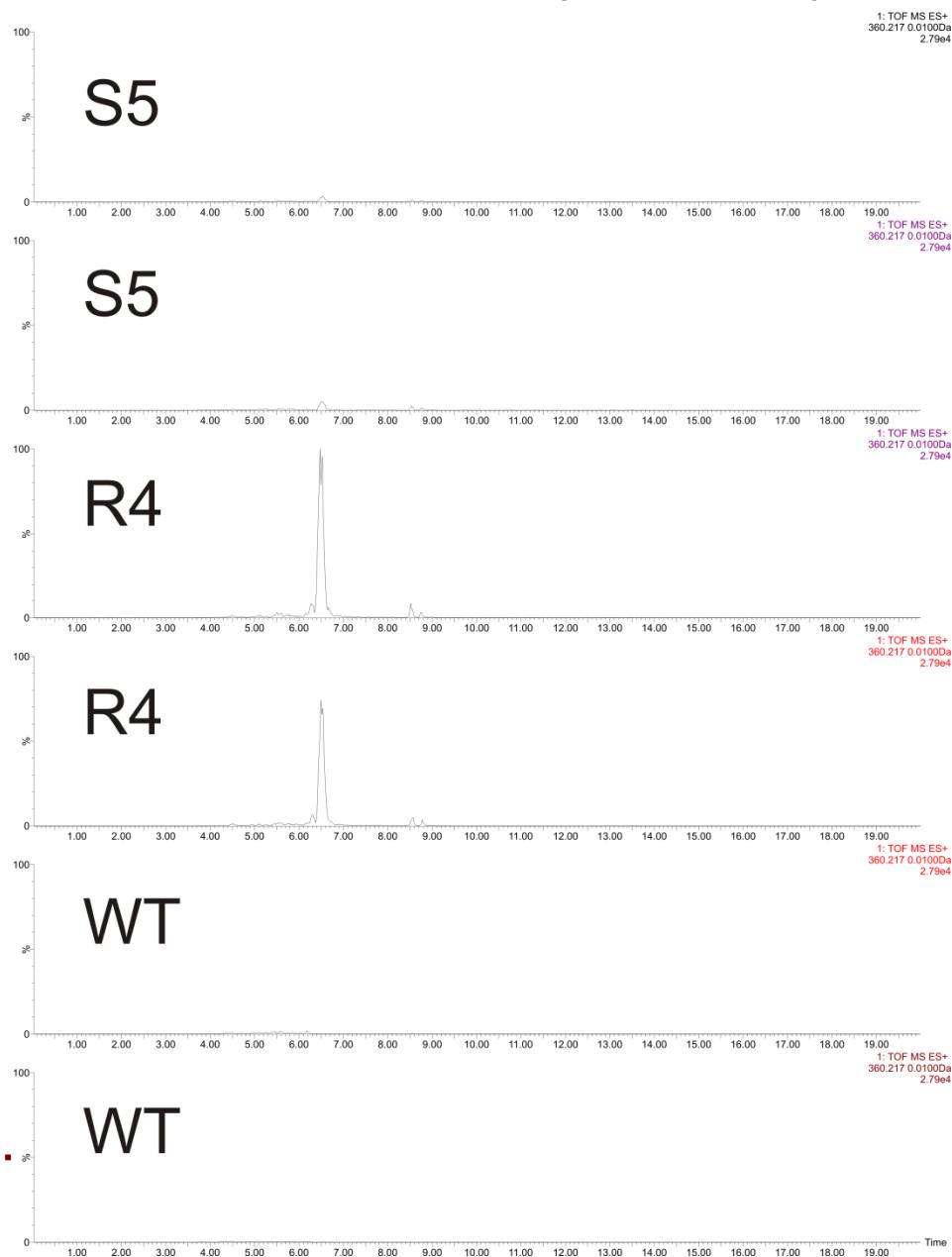


Figure S80. Extracted ion chromatograms for feature 8 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 9 EIC ($\pm 0.01\text{Da}$)

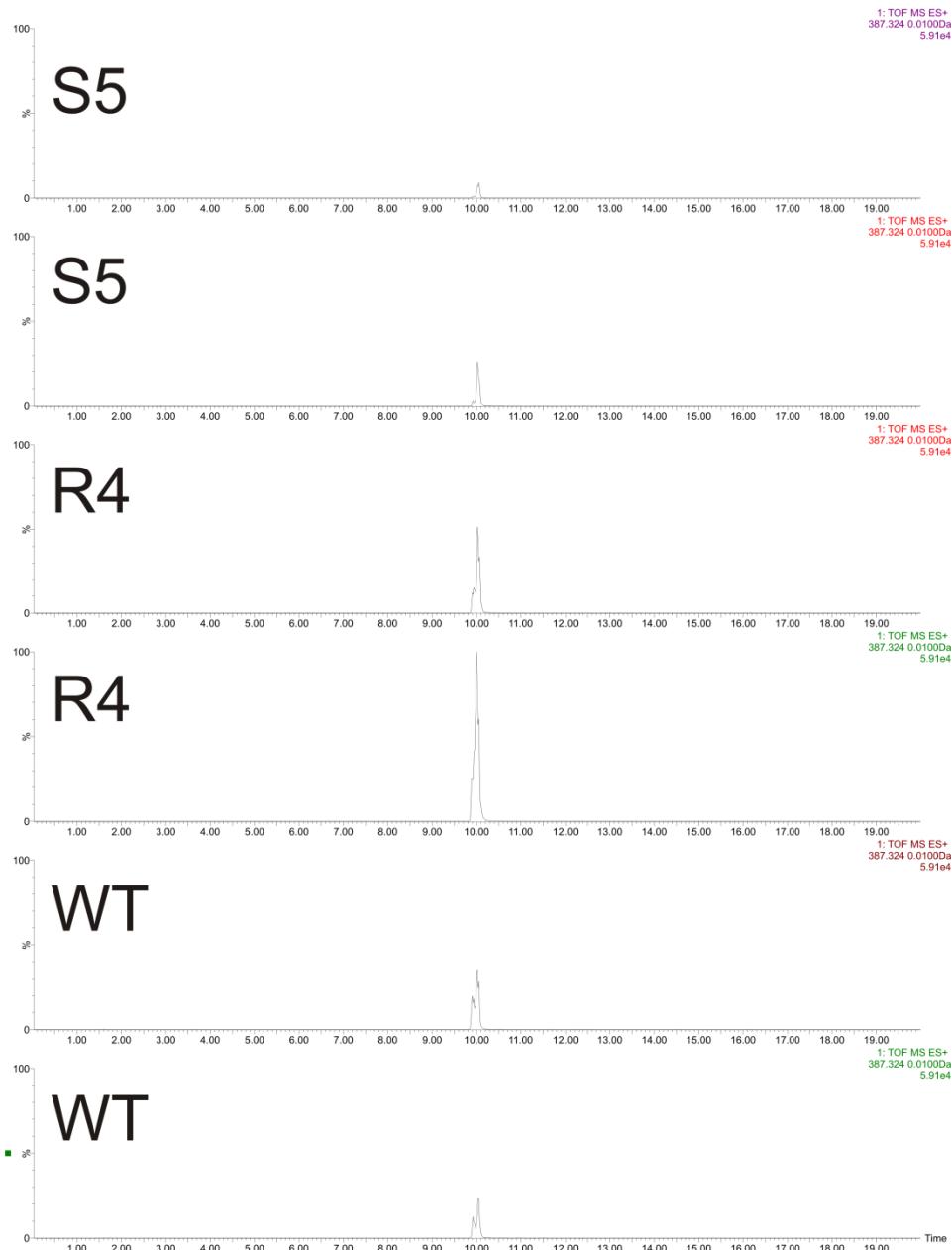


Figure S81. Extracted ion chromatograms for feature 9 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 10 EIC ($\pm 0.01\text{Da}$)

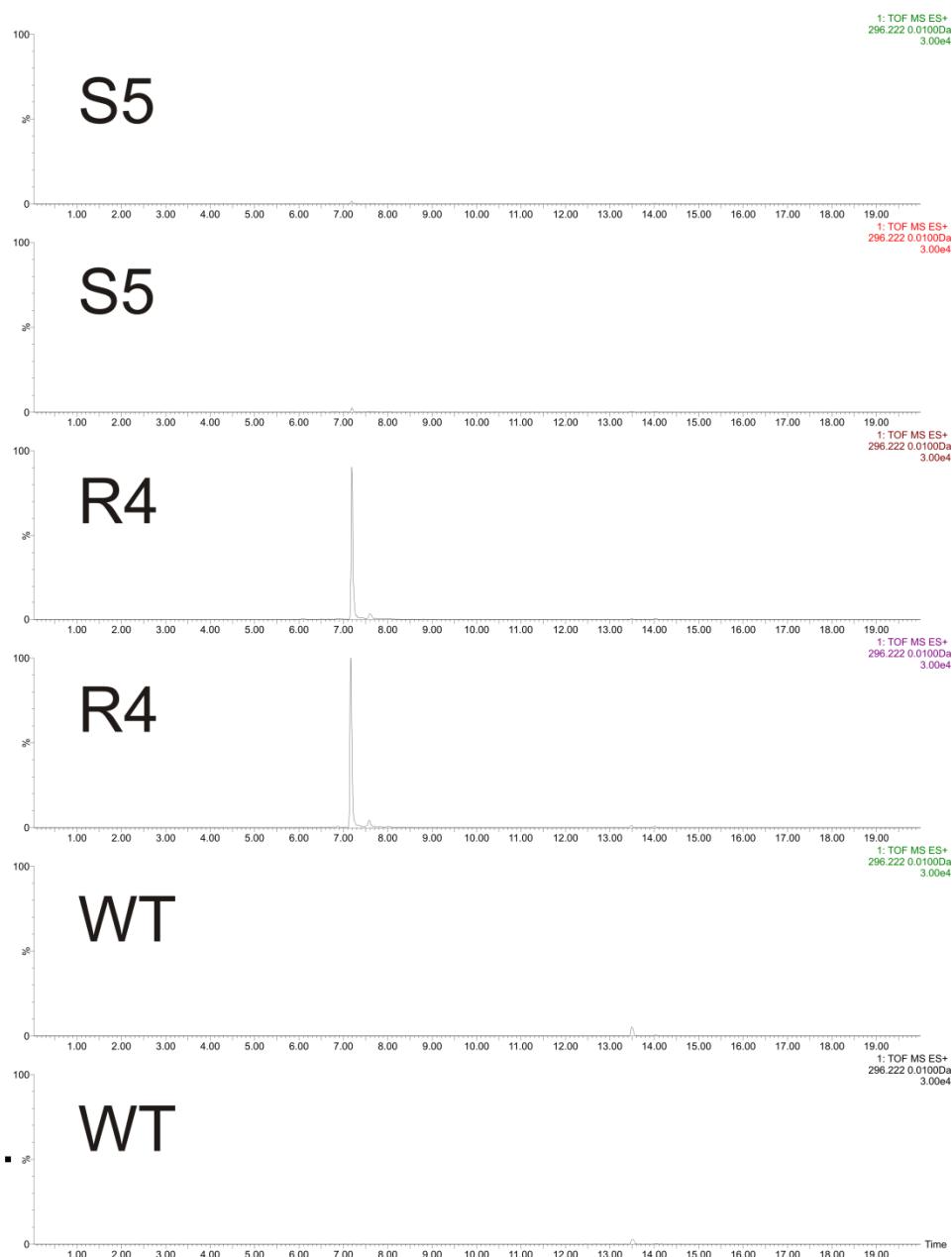


Figure S82. Extracted ion chromatograms for feature 10 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 11 EIC ($\pm 0.01\text{Da}$)

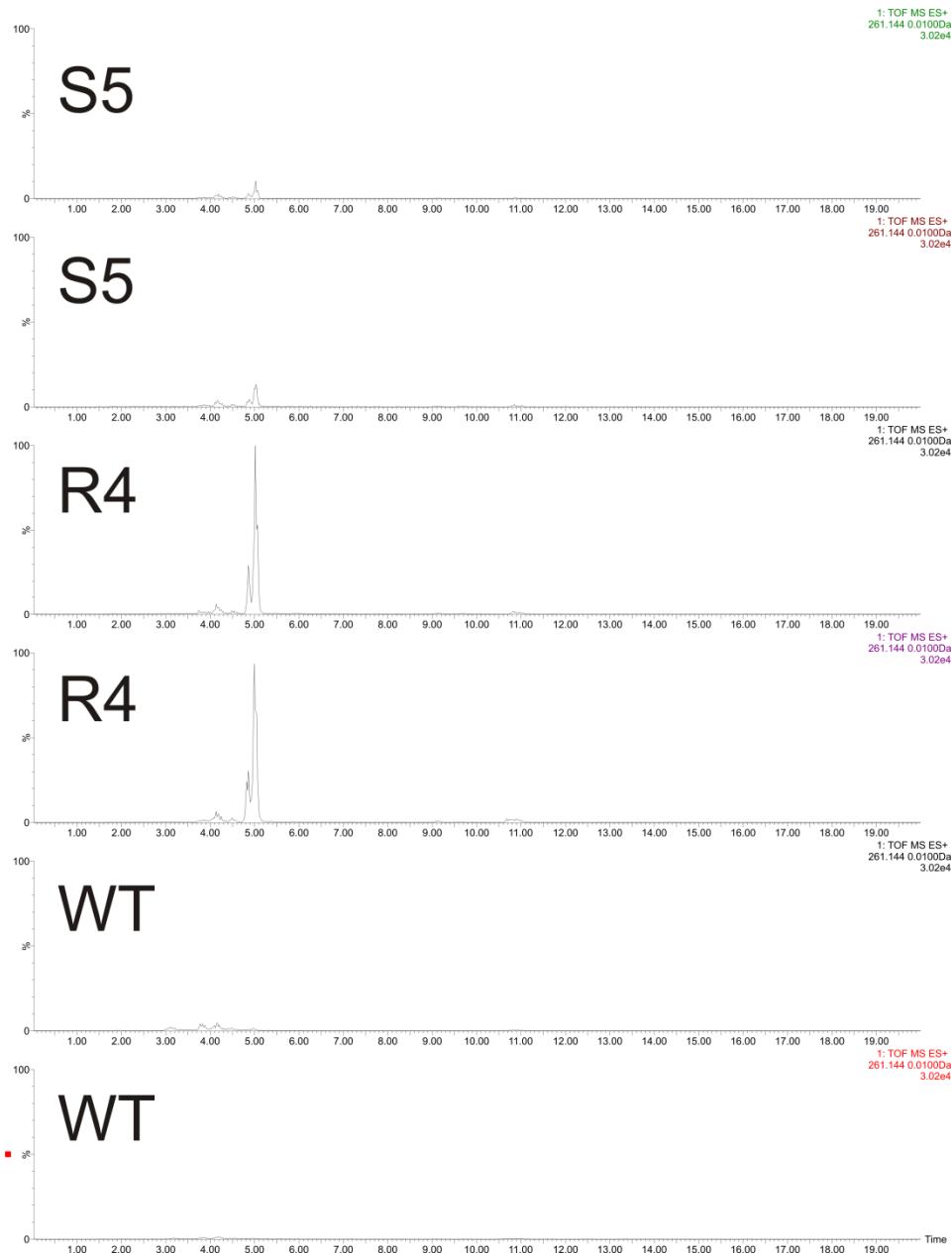


Figure S83. Extracted ion chromatograms for feature 11 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 12 EIC ($\pm 0.01\text{Da}$)

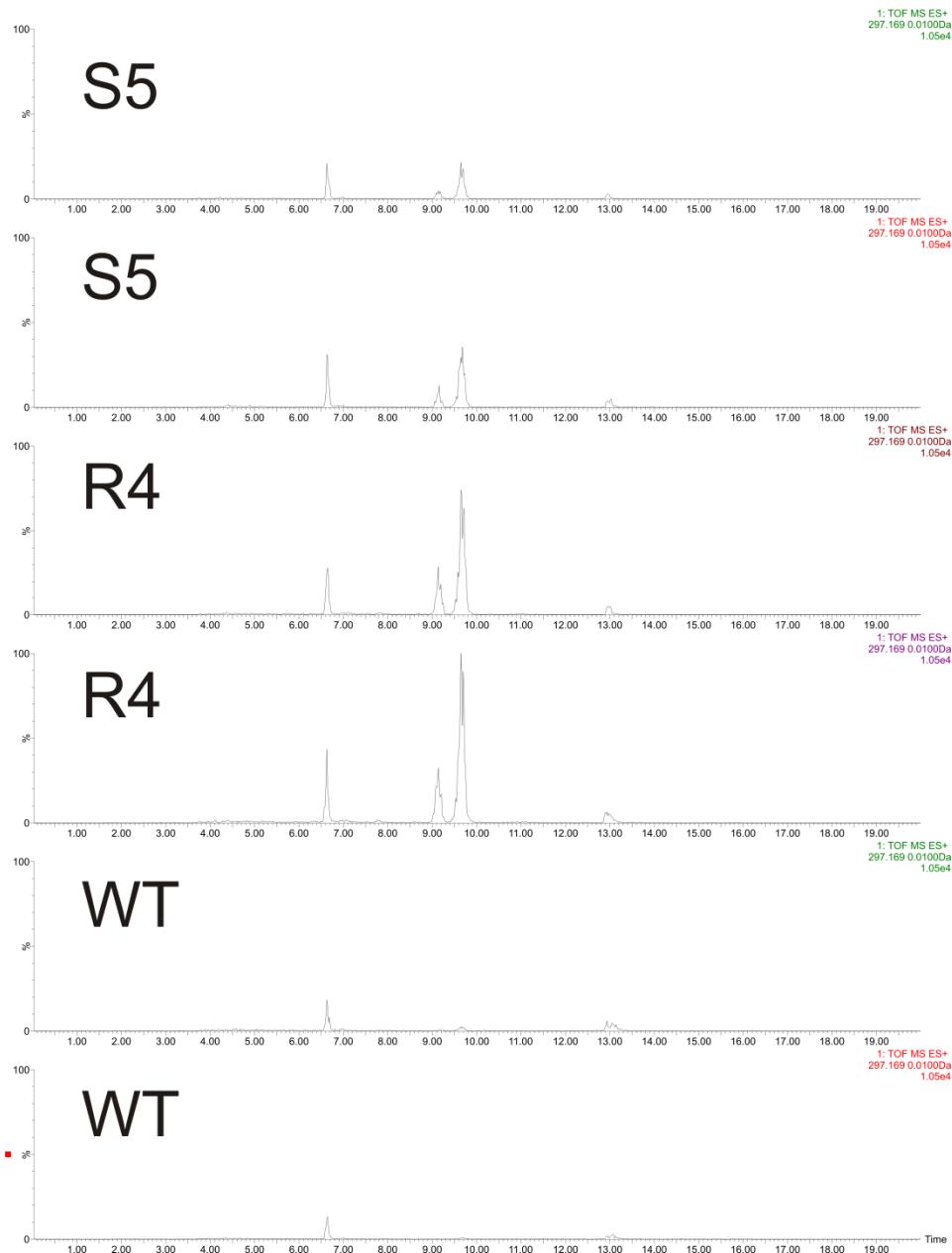


Figure S84. Extracted ion chromatograms for feature 12 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 13 EIC ($\pm 0.01\text{Da}$)

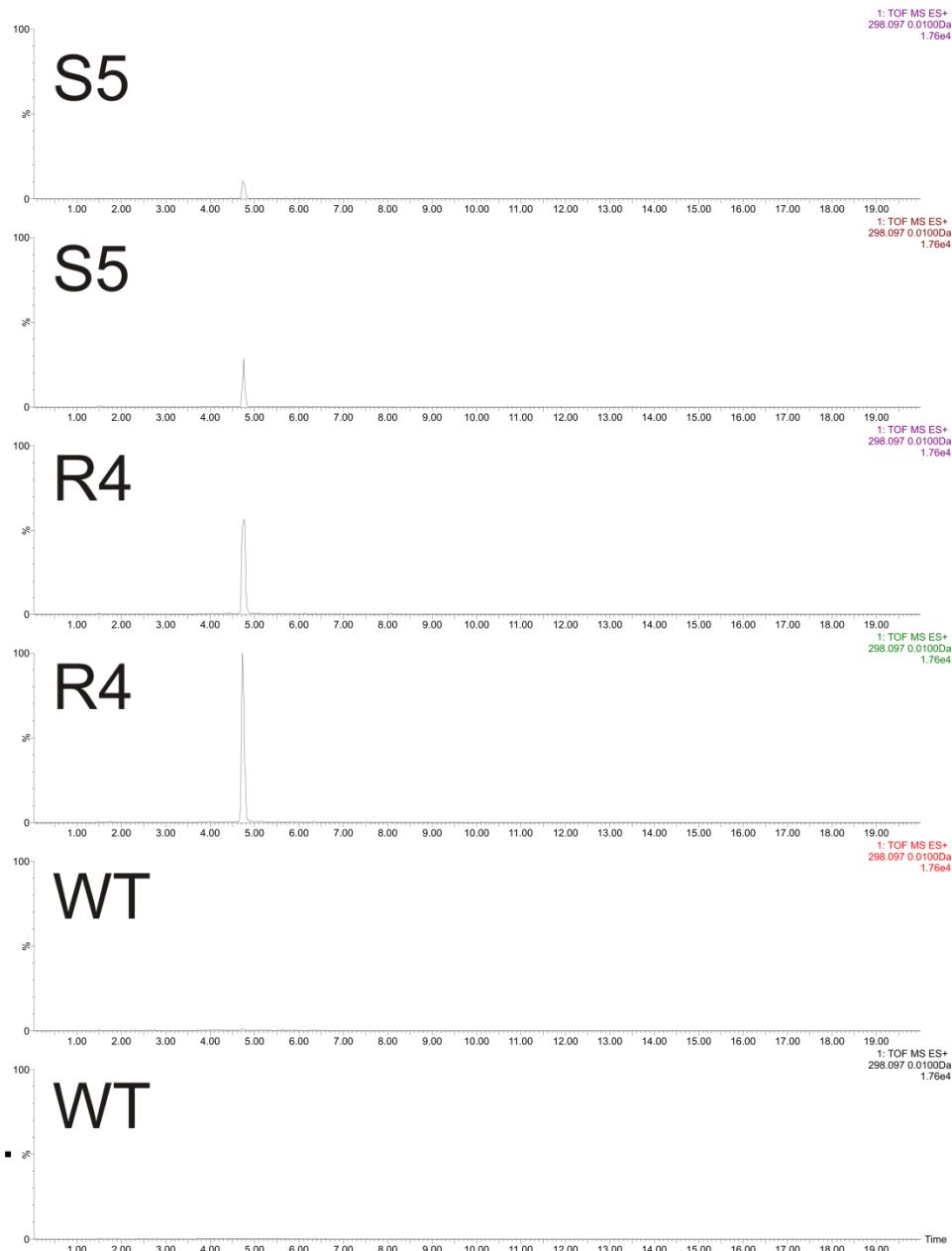


Figure S85. Extracted ion chromatograms for feature 13 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 14 EIC ($\pm 0.01\text{Da}$)

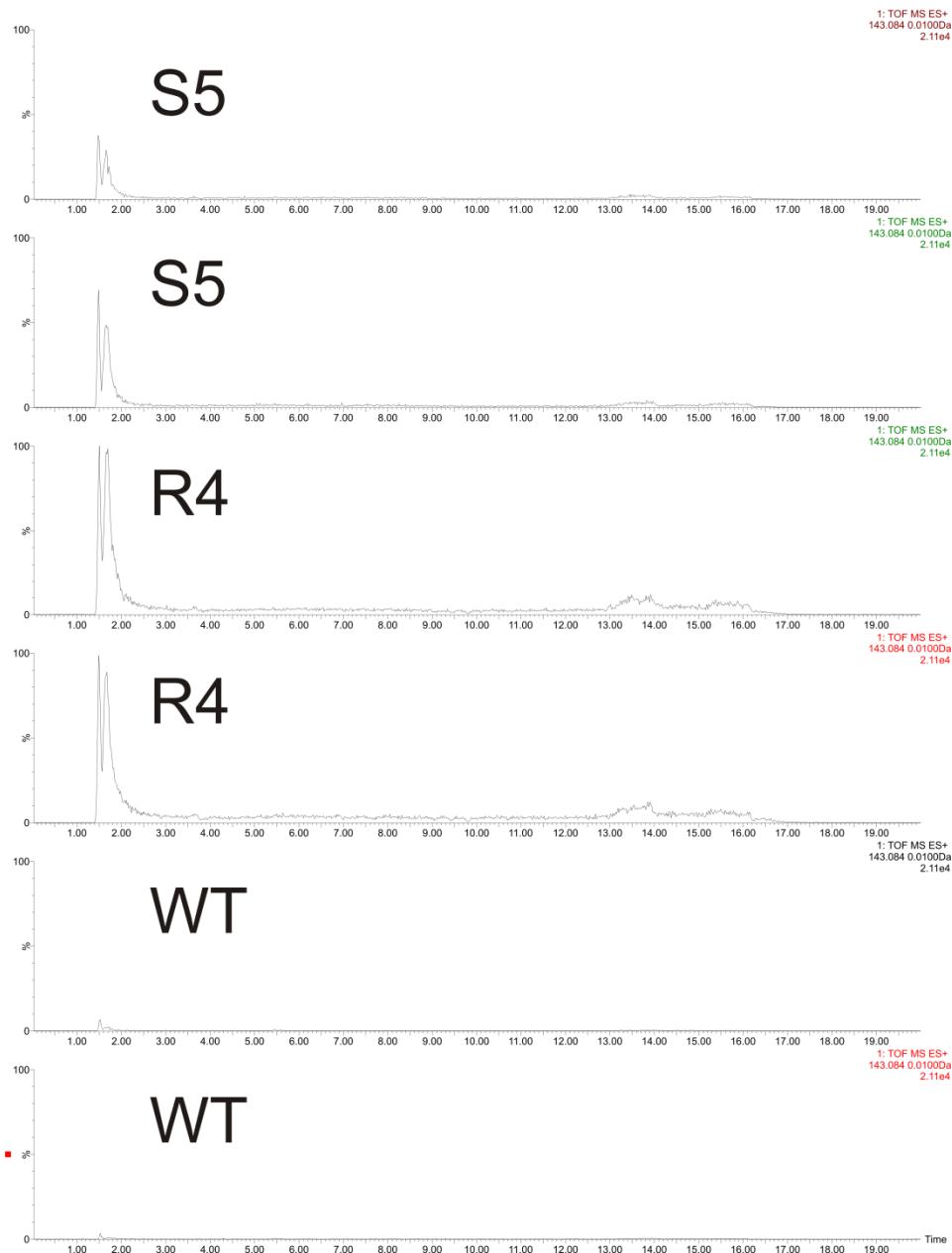


Figure S86. Extracted ion chromatograms for feature 14 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 15 EIC ($\pm 0.01\text{Da}$)

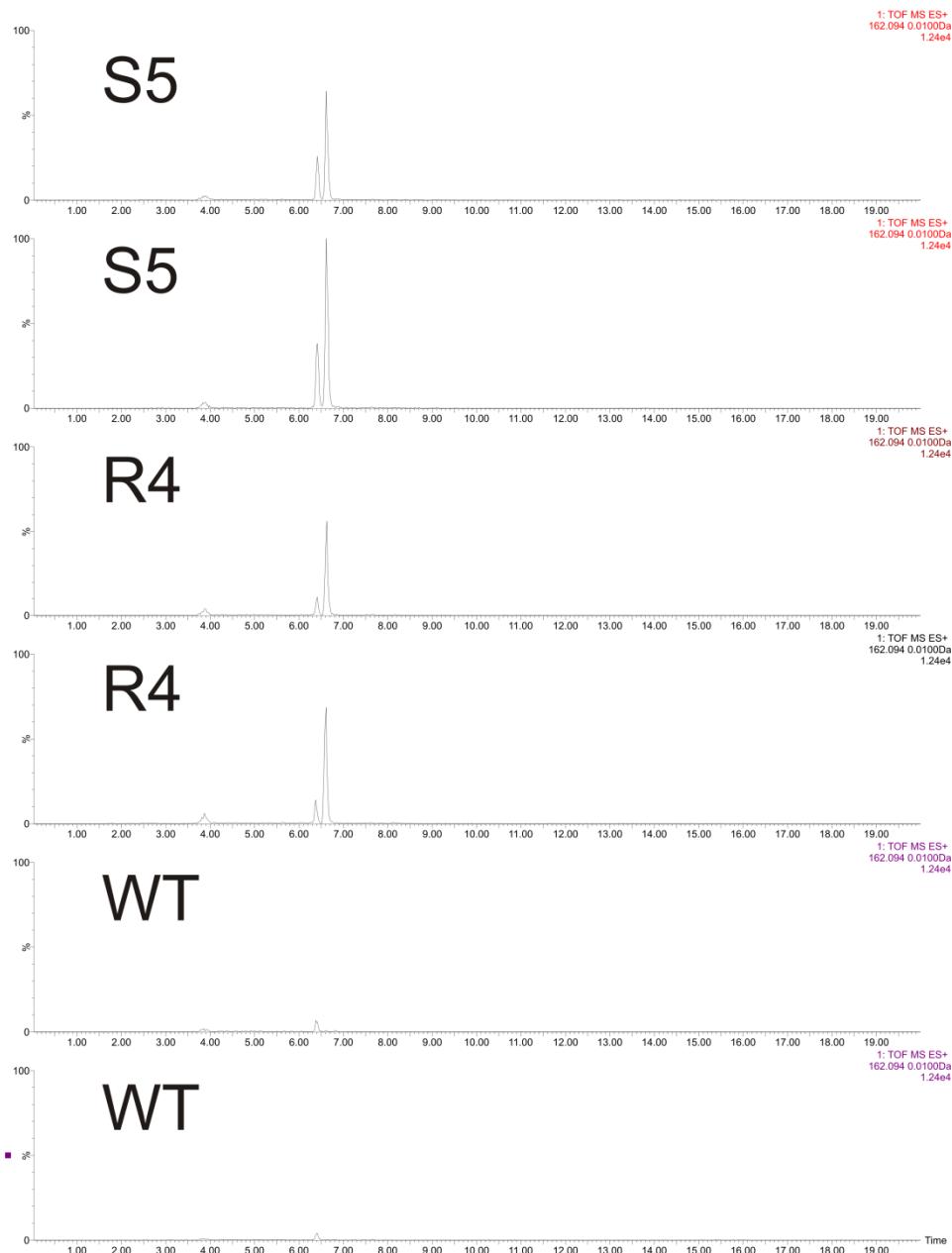


Figure S87. Extracted ion chromatograms for feature 15 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 16 EIC ($\pm 0.01\text{Da}$)

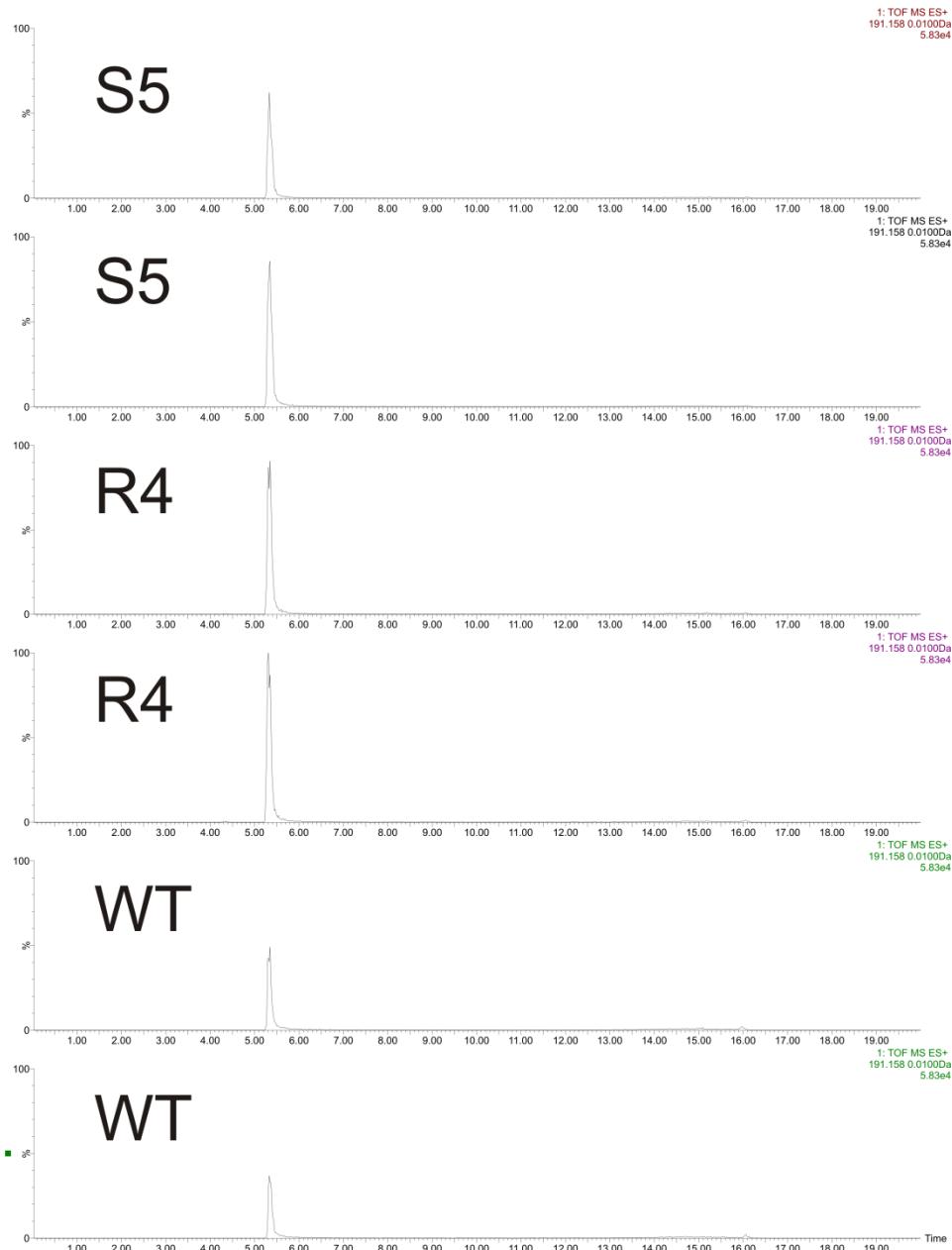


Figure S88. Extracted ion chromatograms for feature 16 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 17 EIC ($\pm 0.01\text{Da}$)

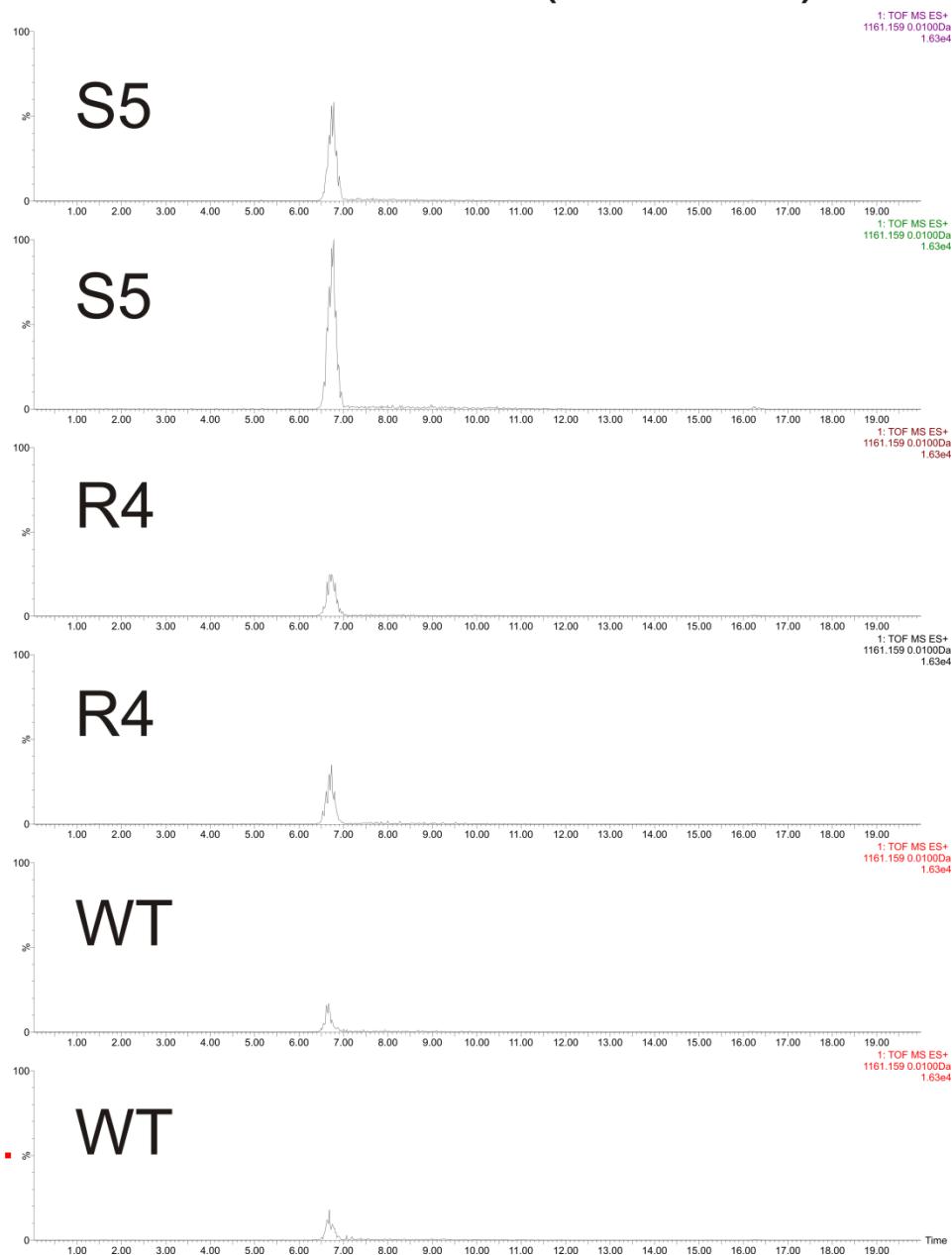


Figure S89. Extracted ion chromatograms for feature 17 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 18 EIC ($\pm 0.01\text{Da}$)

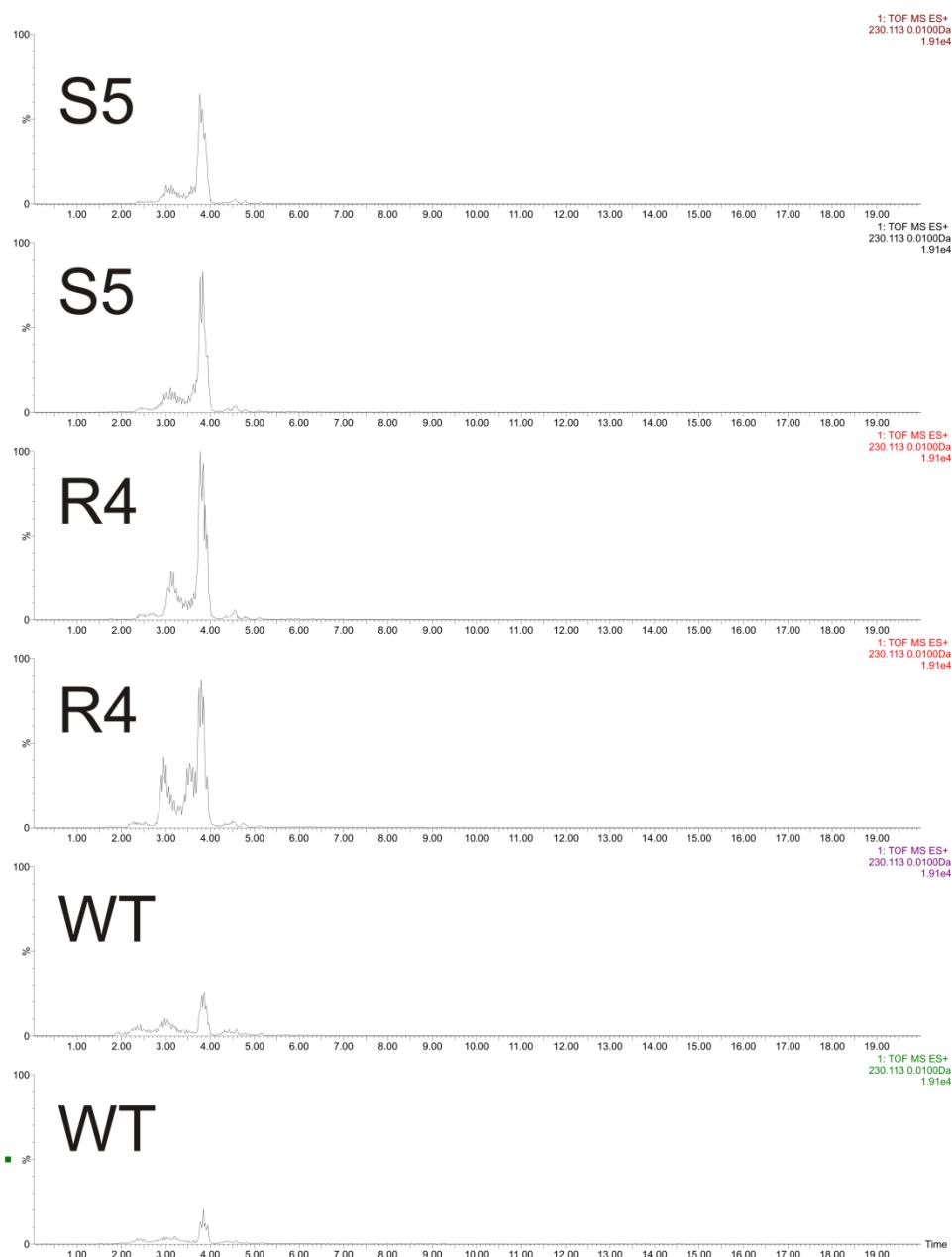


Figure S90. Extracted ion chromatograms for feature 18 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 19 EIC ($\pm 0.01\text{Da}$)

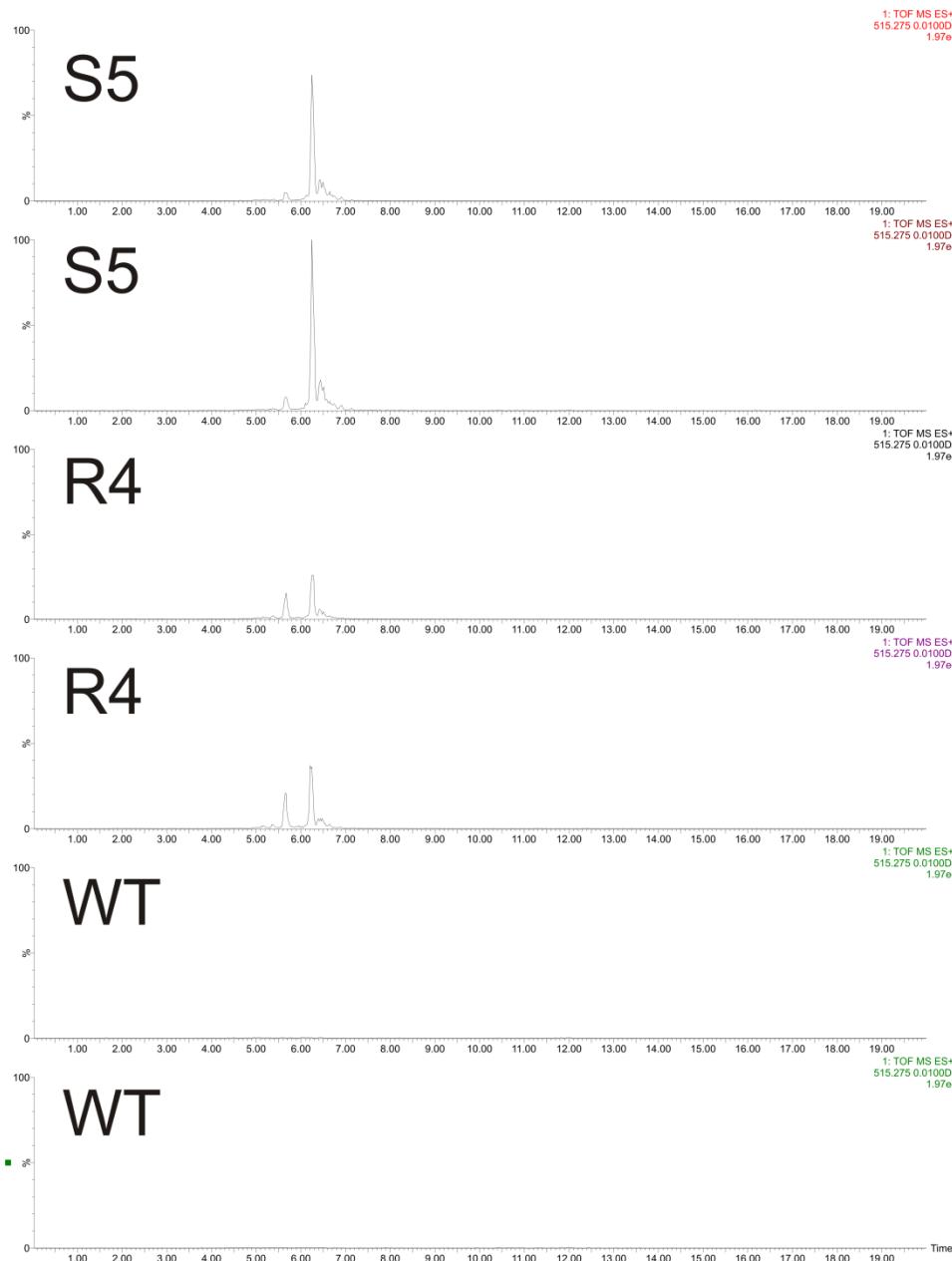


Figure S91. Extracted ion chromatograms for feature 19 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 20 EIC ($\pm 0.01\text{Da}$)

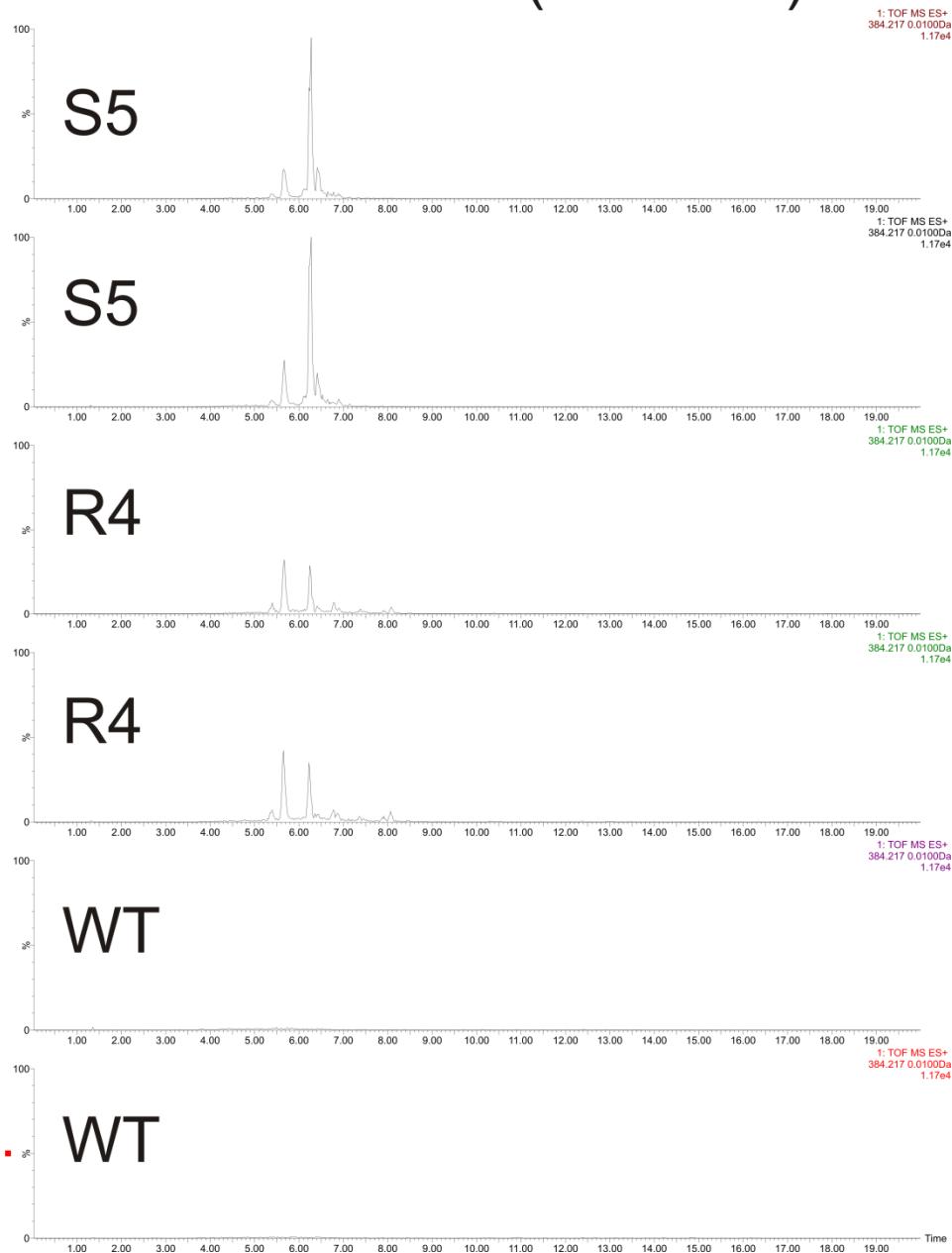


Figure S92. Extracted ion chromatograms for feature 20 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 21 EIC ($\pm 0.01\text{Da}$)

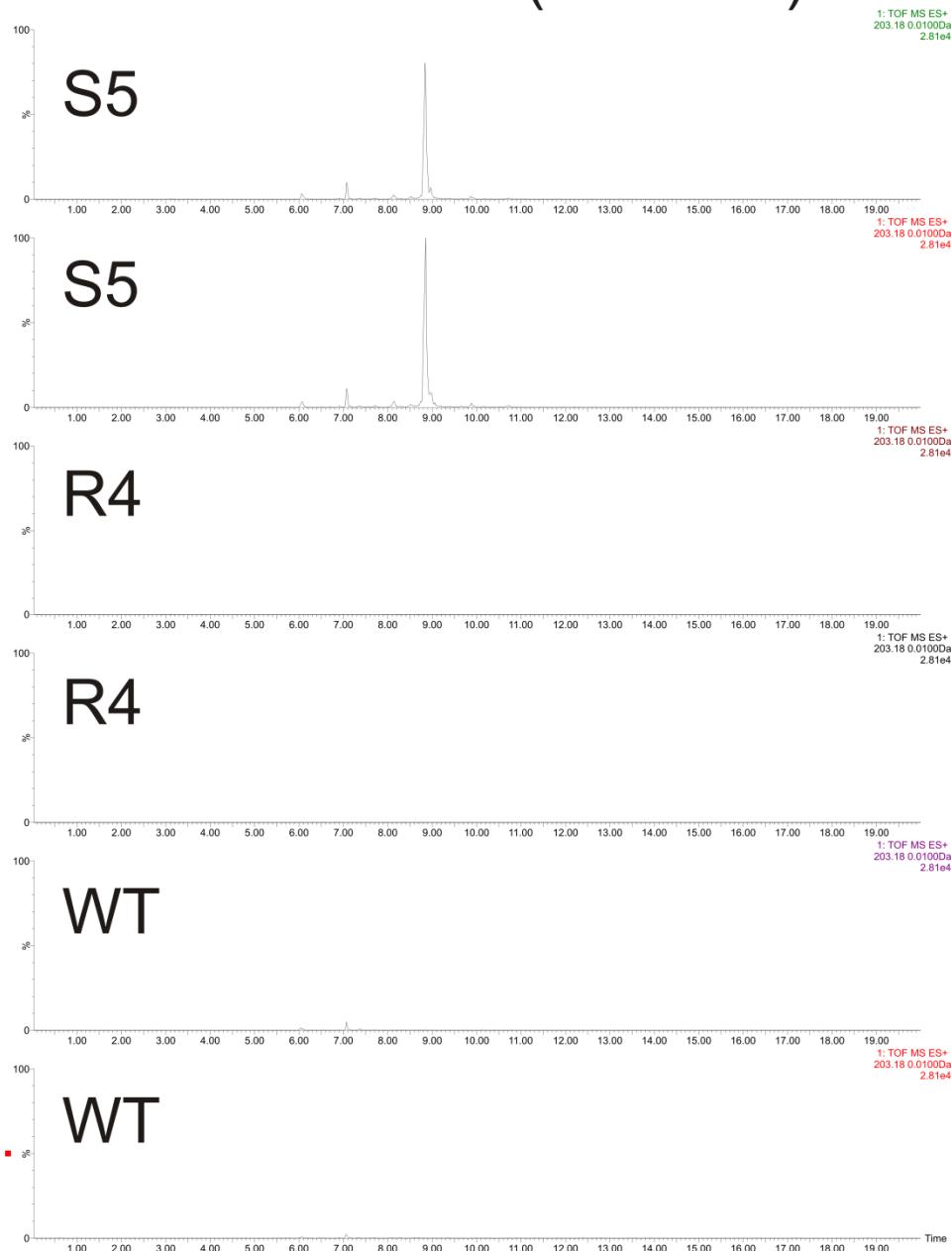


Figure S93. Extracted ion chromatograms for feature 21 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 22 EIC ($\pm 0.01\text{Da}$)

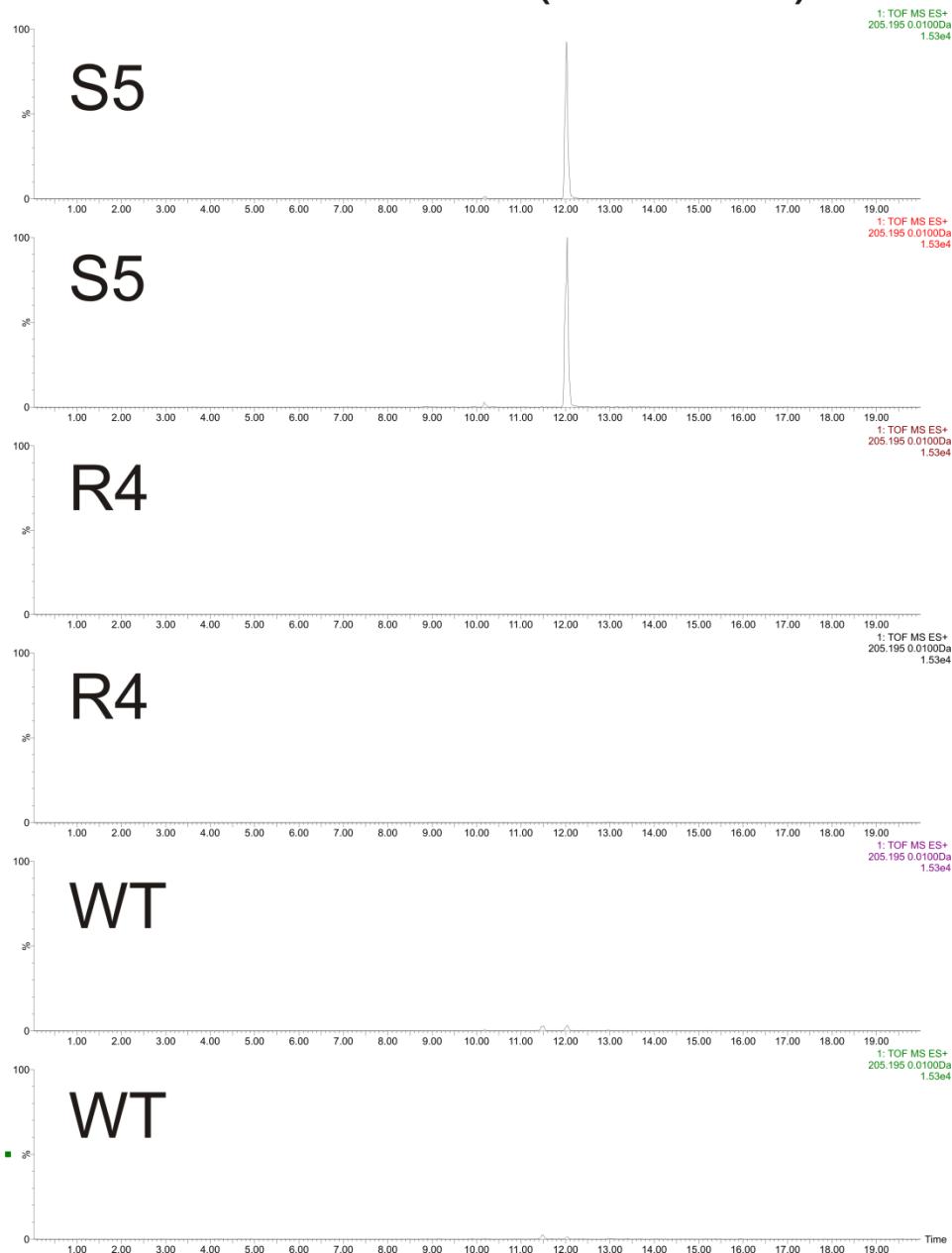


Figure S94. Extracted ion chromatograms for feature 22 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 23 EIC ($\pm 0.01\text{Da}$)

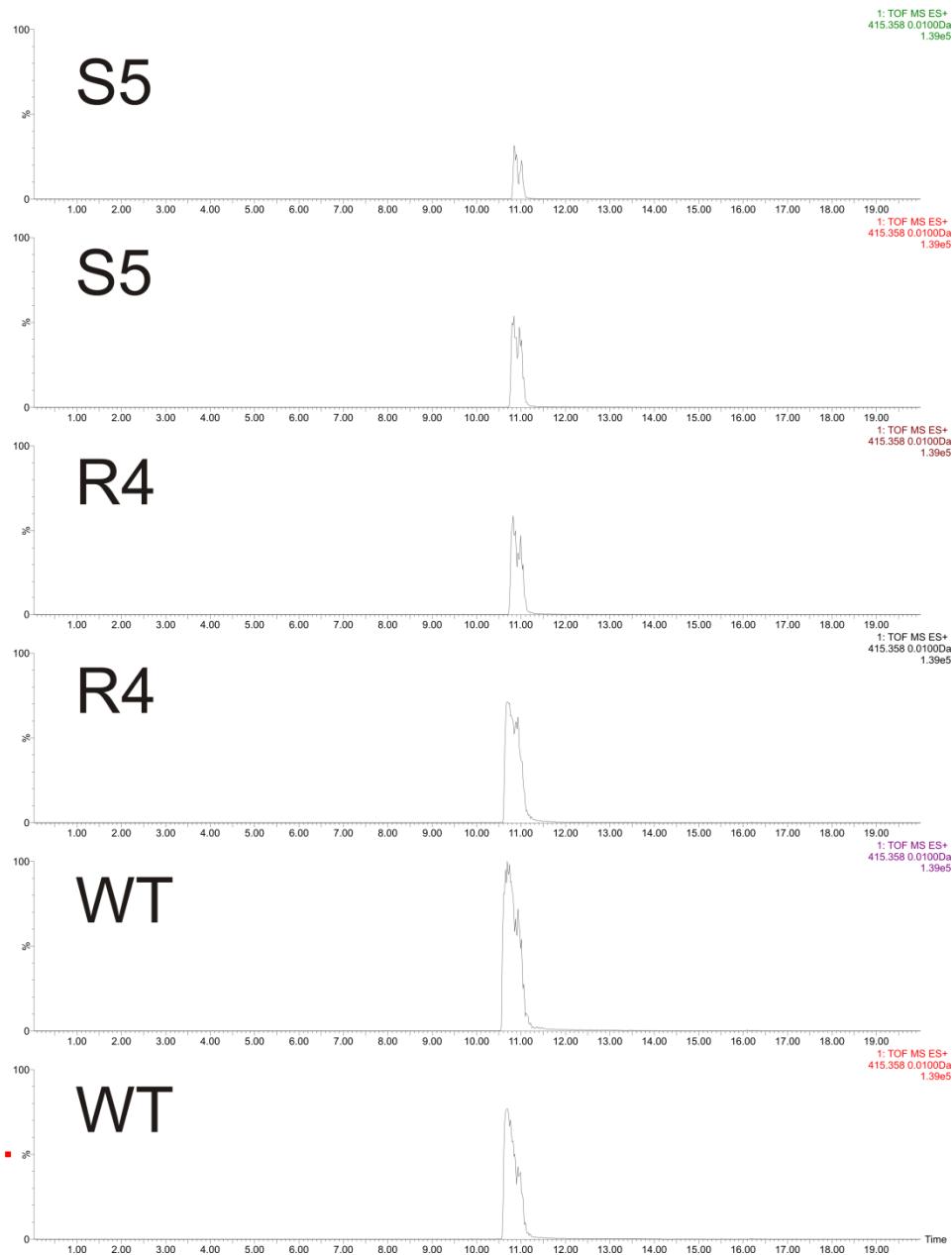


Figure S95. Extracted ion chromatograms for feature 23 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 24 EIC ($\pm 0.01\text{Da}$)

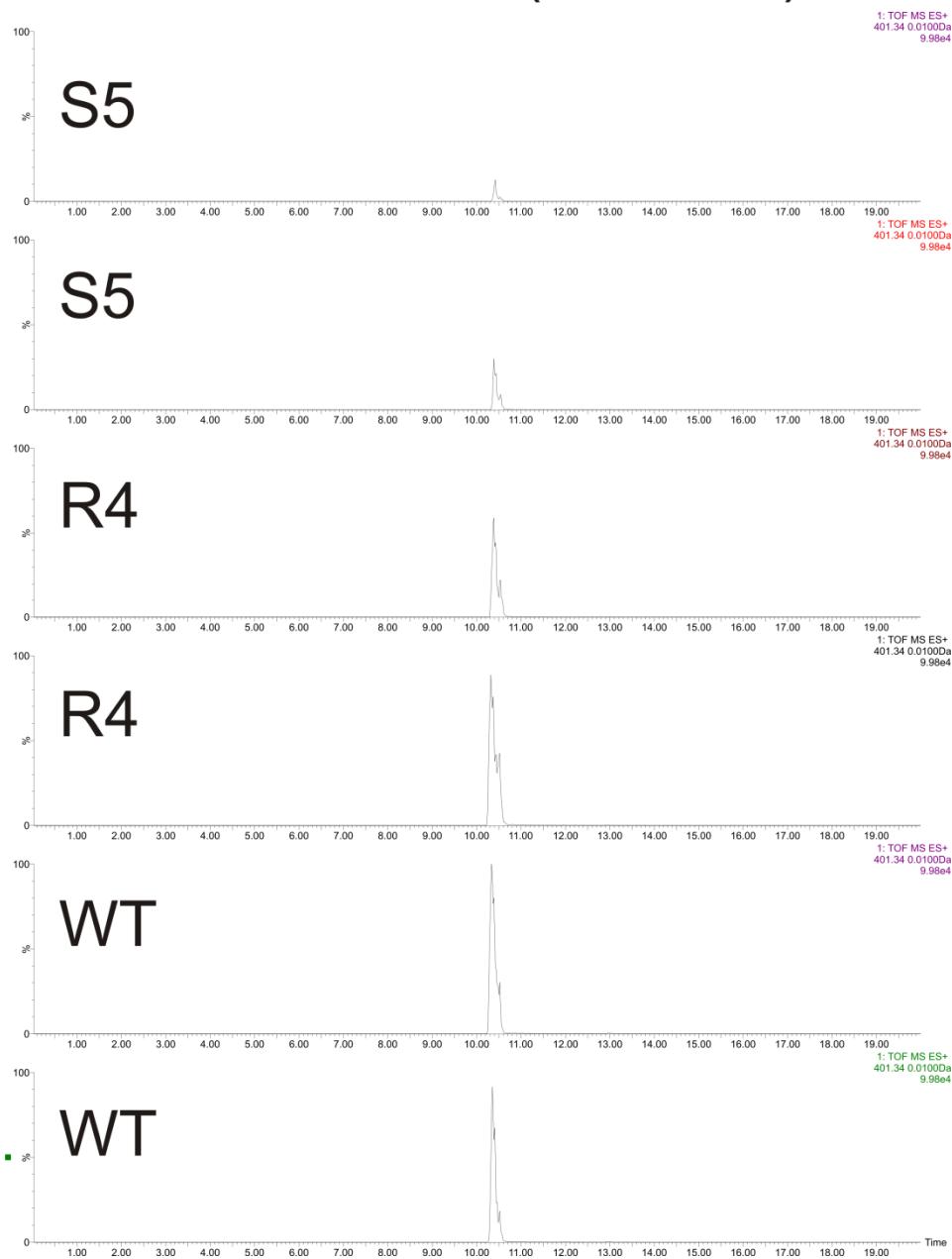


Figure S96. Extracted ion chromatograms for feature 24 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 25 EIC ($\pm 0.01\text{Da}$)

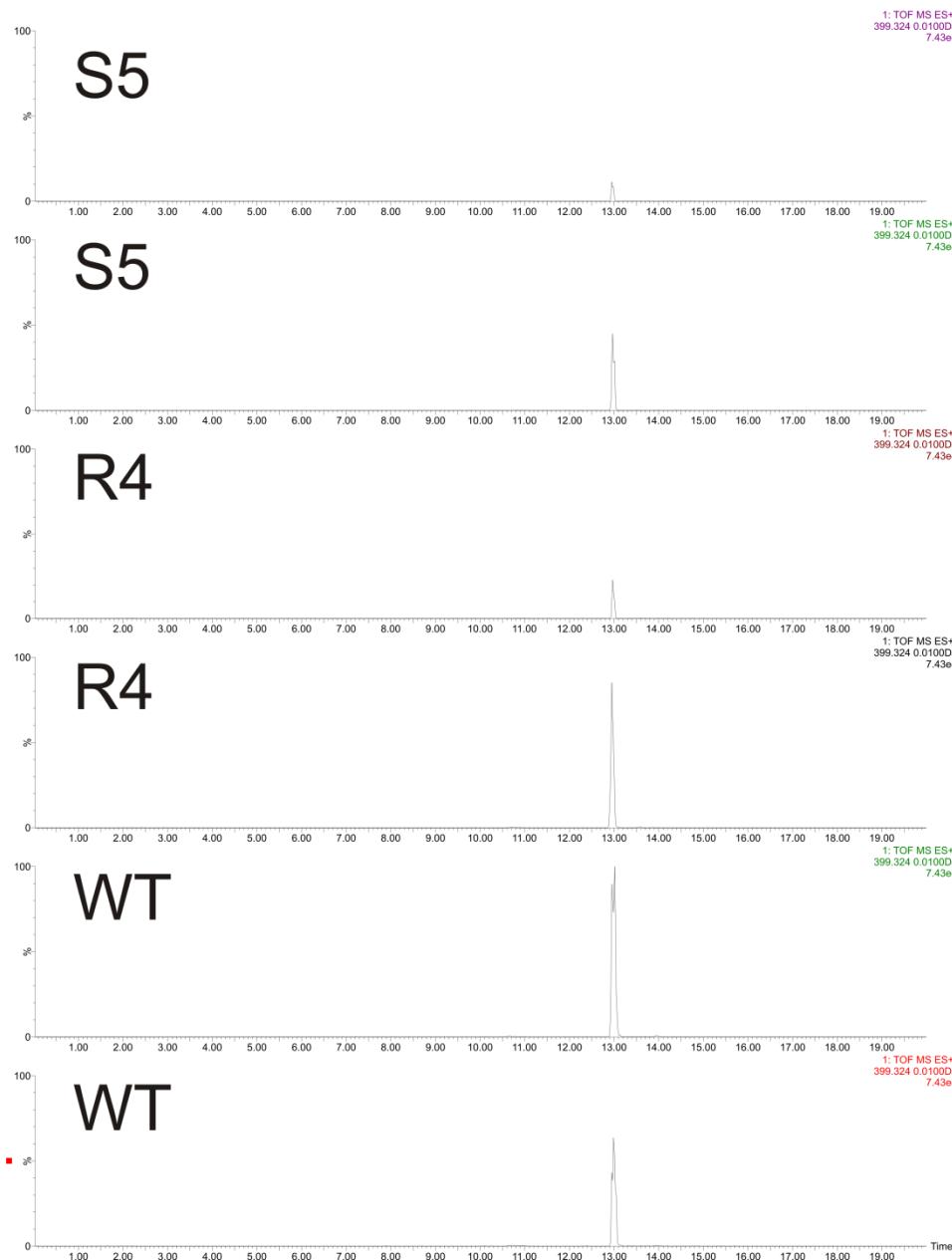


Figure S97. Extracted ion chromatograms for feature 25 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 26 EIC ($\pm 0.01\text{Da}$)

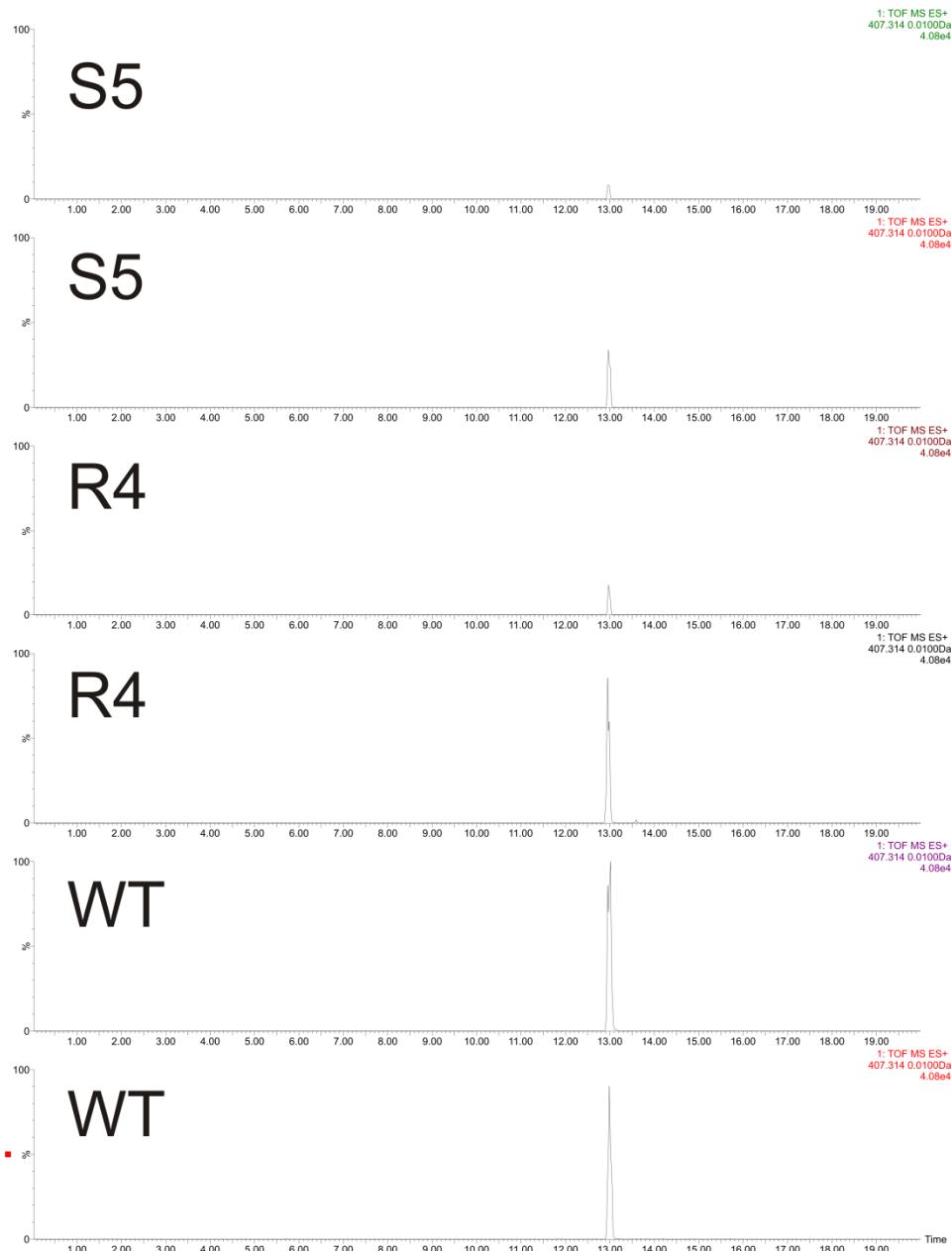


Figure S98. Extracted ion chromatograms for feature 26 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Feature 27 EIC ($\pm 0.01\text{Da}$)

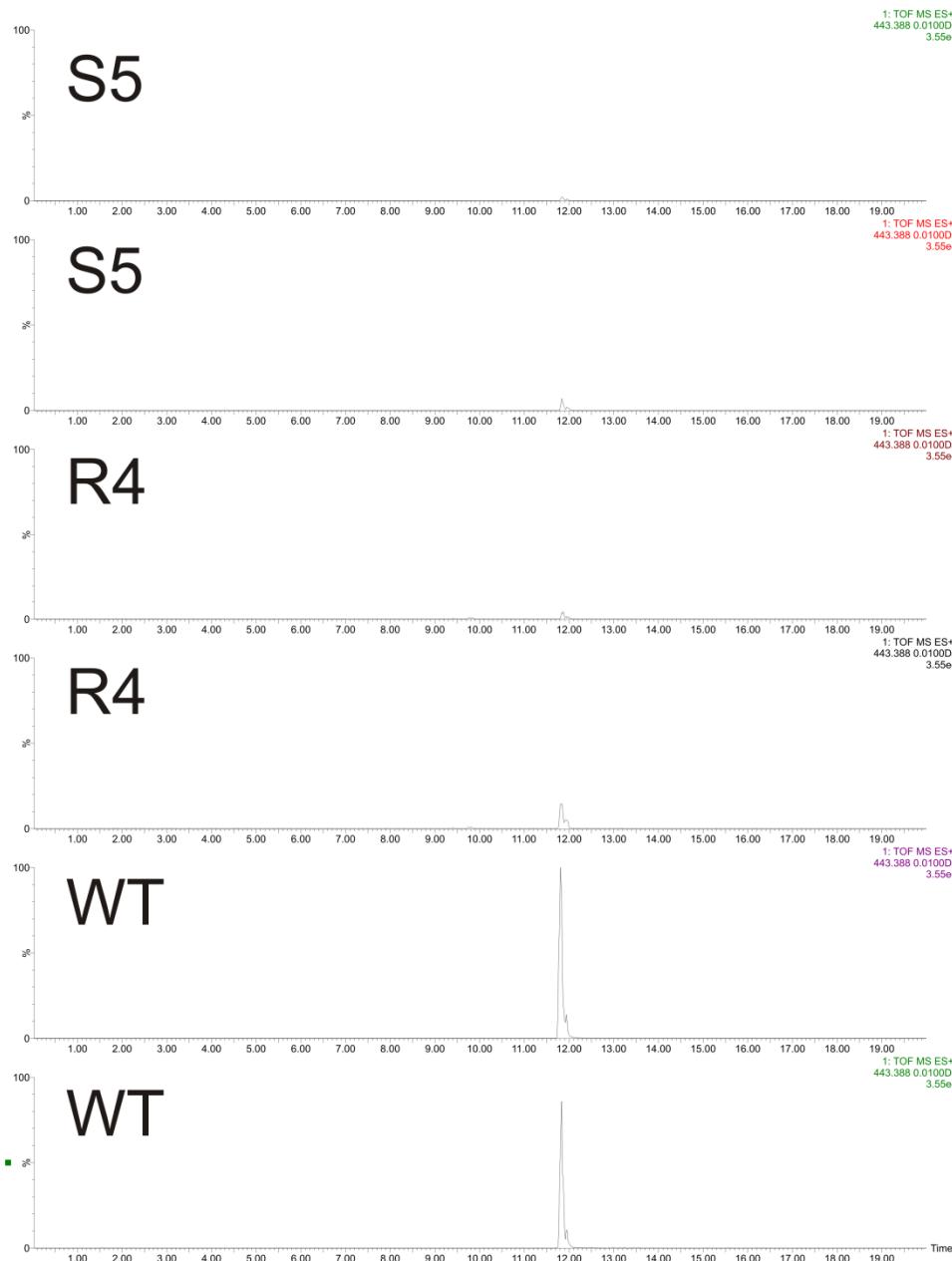


Figure S99. Extracted ion chromatograms for feature 27 w/ $\pm 0.01\text{Da}$ tolerance.

D. Mass Spectral Data for Selected Features

Table S7. Normalized heat map of features described as unique in figure S4 when comparing *Bacillus subtilis* and *Micrococcus luteus* to *Escherichia coli* extracts using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	B sub	B sub	B sub	E coli	E coli	E coli	M lut	M lut	M lut
1.59_136.0628	0.00	0.04	0.07	0.36	1.00	0.87	0.00	0.06	0.03
1.18_203.0538	0.00	0.22	0.00	1.00	0.71	0.75	0.00	0.01	0.00
8.87_225.1991	0.00	0.00	0.00	0.86	1.00	0.78	0.00	0.00	0.00
8.87_226.1249	0.00	0.00	0.00	1.00	0.95	0.88	0.00	0.00	0.00
6.33_243.0892	0.00	0.16	0.13	0.87	0.78	1.00	0.00	0.00	0.00
3.58_246.1339	0.00	0.00	0.02	0.68	0.79	1.00	0.00	0.02	0.00
1.23_258.1102	0.00	0.00	0.00	0.80	1.00	0.76	0.00	0.01	0.01
3.47_276.1486	0.00	0.00	0.00	0.95	1.00	0.64	0.00	0.00	0.00
1.16_280.0940	0.00	0.00	0.00	0.61	1.00	0.88	0.00	0.00	0.00
7.38_364.1685	0.00	0.00	0.00	1.00	0.79	0.52	0.00	0.01	0.00
8.87_392.1643	0.00	0.00	0.00	0.93	1.00	0.66	0.00	0.00	0.00
2.45_424.1838	0.00	0.00	0.00	0.74	1.00	0.64	0.00	0.00	0.00
3.59_438.1989	0.00	0.00	0.00	1.00	0.66	0.87	0.00	0.00	0.00
10.27_452.2766	0.00	0.00	0.00	0.50	0.81	1.00	0.00	0.00	0.00
2.41_442.1934	0.00	0.00	0.00	1.00	0.50	0.72	0.00	0.00	0.00
3.58_456.2096	0.00	0.00	0.01	1.00	0.69	0.88	0.00	0.00	0.00
10.91_466.2961	0.00	0.00	0.00	0.61	0.62	1.00	0.00	0.00	0.00
3.40_488.1789	0.00	0.00	0.00	1.00	0.40	0.69	0.02	0.00	0.02
11.83_494.3263	0.00	0.00	0.00	0.52	0.62	1.00	0.00	0.00	0.00
5.04_542.3153	0.00	0.00	0.00	1.00	0.91	0.92	0.01	0.00	0.00
3.37_604.2482	0.00	0.00	0.00	0.91	0.58	1.00	0.00	0.00	0.01
3.63_600.2512	0.00	0.00	0.00	0.56	0.57	1.00	0.01	0.00	0.02
1.19_723.1992	0.00	0.00	0.00	0.57	0.98	1.00	0.00	0.00	0.00
1.22_707.2229	0.00	0.00	0.00	1.00	0.80	0.93	0.00	0.00	0.00
14.78_742.5100	0.00	0.00	0.01	0.90	0.60	1.00	0.00	0.08	0.00
11.13_454.2957	0.00	0.00	0.00	0.56	0.91	1.00	0.00	0.00	0.00
10.68_466.2947	0.00	0.00	0.00	0.55	0.56	1.00	0.00	0.00	0.00
1.33_428.1800	0.00	0.01	0.00	0.93	0.82	1.00	0.00	0.00	0.00
7.37_226.1255	0.00	0.00	0.00	0.92	0.94	1.00	0.00	0.00	0.00
1.21_365.1089	0.00	0.00	0.00	0.77	1.00	0.89	0.00	0.00	0.00
4.33_260.1502	0.00	0.00	0.00	1.00	0.60	0.86	0.01	0.14	0.06
1.20_381.0798	0.01	0.00	0.00	1.00	0.83	0.94	0.00	0.00	0.00
1.13_380.0978	0.01	0.01	0.02	0.78	0.92	1.00	0.00	0.00	0.01
4.15_260.1506	0.02	0.00	0.00	1.00	0.51	0.99	0.00	0.01	0.00
3.50_230.1384	0.02	0.07	0.00	0.66	1.00	0.60	0.00	0.03	0.00
1.23_446.1908	0.03	0.00	0.00	0.99	0.85	1.00	0.00	0.00	0.00
4.29_447.2276	0.05	0.00	0.00	1.00	0.40	0.96	0.00	0.00	0.00
3.95_328.1408	0.06	0.09	0.00	0.83	1.00	0.63	0.01	0.07	0.08
5.25_164.0700	0.11	0.18	0.08	0.88	1.00	0.71	0.45	0.14	0.22
5.57_277.1177	0.16	0.12	0.11	0.86	0.98	1.00	0.07	0.01	0.12
6.91_233.0782	0.30	0.27	0.35	1.00	0.98	0.93	0.37	0.45	0.39
1.32_247.1405	0.38	0.77	1.00	0.04	0.00	0.00	0.67	0.77	0.84
5.24_374.2291	0.49	0.89	0.96	0.00	0.00	0.00	1.00	0.72	0.91
6.71_514.3211	0.52	0.77	0.64	0.00	0.00	0.00	1.00	0.65	0.80
5.31_489.2739	0.55	0.60	0.59	0.00	0.00	0.00	0.85	0.89	1.00
5.97_441.3089	0.56	0.52	0.53	0.05	0.05	0.02	1.00	0.81	0.86
6.93_527.2267	0.58	0.76	1.00	0.00	0.00	0.00	0.83	0.78	0.48
3.65_248.1052	0.62	0.76	0.66	0.00	0.00	0.08	0.89	1.00	0.51
7.20_340.2507	0.63	0.73	0.89	0.00	0.00	0.00	0.95	0.97	1.00
8.43_384.2770	0.64	0.47	0.60	0.00	0.00	0.00	0.88	1.00	0.71
8.74_340.2520	0.66	0.52	0.71	0.00	0.00	0.00	0.86	0.76	1.00
8.15_368.2806	0.66	0.47	0.57	0.00	0.00	0.00	0.87	1.00	0.91
5.48_287.1006	0.69	0.72	1.00	0.00	0.00	0.05	0.77	0.69	0.61
7.14_120.0804	0.69	0.84	0.88	0.01	0.01	0.02	1.00	0.88	0.81
8.16_386.2928	0.70	0.70	0.69	0.00	0.00	0.00	0.69	1.00	0.90
1.26_246.1797	0.70	0.99	0.82	0.02	0.00	0.00	0.89	0.99	1.00
7.49_358.2600	0.71	0.66	0.72	0.00	0.00	0.00	0.90	0.96	1.00
6.73_224.1250	0.71	0.83	0.75	0.02	0.00	0.00	1.00	0.67	0.97
5.17_188.0713	0.72	1.00	0.93	0.00	0.04	0.00	0.77	0.85	0.69

D. Mass Spectral Data for Selected Features

6.72_406.2313	0.72	0.80	0.81	0.00	0.00	0.00	0.98	0.81	1.00
1.24_369.1533	0.77	1.00	0.86	0.00	0.00	0.00	0.66	0.71	0.87
7.59_517.3020	0.77	0.77	0.99	0.00	0.00	0.01	1.00	0.91	0.92
7.90_328.2507	0.77	0.54	0.61	0.00	0.00	0.00	0.98	1.00	0.75
1.05_341.1557	0.80	0.90	0.46	0.00	0.00	0.00	0.86	0.75	1.00
6.97_326.2351	0.81	0.64	0.75	0.00	0.01	0.00	0.87	1.00	1.00
1.05_323.1483	0.81	0.81	0.88	0.00	0.00	0.00	0.80	1.00	0.79
1.20_257.1491	0.81	0.44	0.64	0.05	0.04	0.00	0.96	1.00	0.74
7.13_236.1285	0.81	0.78	0.87	0.01	0.00	0.00	0.80	1.00	0.95
7.14_396.2770	0.81	0.69	0.85	0.00	0.00	0.00	0.98	1.00	0.79
7.20_358.2601	0.87	0.65	0.72	0.00	0.00	0.00	0.85	0.92	1.00
7.59_263.1407	0.87	0.64	0.88	0.00	0.00	0.00	1.00	0.89	0.73
6.07_159.0926	0.87	0.56	0.85	0.00	0.01	0.00	0.72	1.00	0.56
6.45_341.1501	0.90	0.63	0.86	0.02	0.02	0.03	0.80	0.99	1.00
6.94_227.1782	0.90	0.84	1.00	0.00	0.00	0.03	0.75	0.72	0.69
6.07_299.1768	0.90	0.83	1.00	0.00	0.00	0.00	0.81	0.62	0.67
6.96_300.1824	0.91	0.63	1.00	0.00	0.00	0.00	0.86	0.89	0.70
4.93_265.1574	0.92	0.66	0.89	0.01	0.00	0.00	0.86	0.80	1.00
5.09_245.1881	0.96	0.77	0.82	0.00	0.00	0.00	0.95	1.00	0.99
6.96_382.2573	0.96	0.78	0.73	0.00	0.00	0.00	0.76	0.96	1.00
6.08_201.1028	0.97	0.97	1.00	0.00	0.00	0.02	1.00	0.76	0.94
6.96_282.1702	0.99	0.70	0.94	0.00	0.00	0.00	0.86	0.99	1.00
7.14_258.1102	1.00	0.62	0.88	0.00	0.00	0.00	0.94	1.00	0.97
6.08_188.0708	1.00	0.80	0.58	0.01	0.02	0.00	0.54	1.00	0.99
3.90_186.0783	1.00	0.70	0.58	0.00	0.02	0.00	0.61	0.92	0.84
3.98_215.1417	1.00	0.60	0.80	0.00	0.00	0.00	0.57	0.88	0.62
5.42_245.1308	1.00	0.74	0.80	0.00	0.00	0.03	0.68	0.68	0.65
4.69_302.2081	1.00	0.95	0.90	0.02	0.00	0.00	0.93	0.87	0.75
6.71_327.0330	1.00	0.72	0.98	0.00	0.01	0.03	0.82	0.87	0.64
6.68_356.1087	1.00	0.86	0.92	0.00	0.00	0.00	0.95	0.92	0.76
6.76_393.1819	1.00	0.67	0.89	0.01	0.01	0.02	0.66	0.73	0.77
5.66_522.2907	1.00	0.62	0.92	0.00	0.00	0.00	0.93	0.98	0.92
5.40_613.3562	1.00	0.58	0.73	0.00	0.00	0.01	0.86	0.81	0.94
6.96_913.9555	1.00	0.81	0.92	0.00	0.00	0.00	0.55	0.91	0.98

D. Mass Spectral Data for Selected Features

Table S8. Normalized heat map of features described as unique in figure S4 when comparing *Bacillus subtilis* and *Escherichia coli* to *Micrococcus luteus* extracts using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	B sub	B sub	B sub	E coli	E coli	E coli	M lut	M lut	M lut
3.85_239.1416	0.00	0.09	0.00	0.00	0.00	0.01	1.00	0.59	0.88
5.44_316.2237	0.00	0.20	0.00	0.00	0.00	0.03	0.81	1.00	0.63
1.31_324.1312	0.00	0.10	0.21	0.00	0.00	0.00	0.98	1.00	0.54
5.57_322.1904	0.00	0.19	0.21	0.00	0.00	0.00	0.62	1.00	0.88
5.04_334.1767	0.00	0.00	0.00	0.00	0.00	0.50	1.00	0.80	0.77
5.69_349.7333	0.00	0.08	0.09	0.00	0.00	0.00	1.00	0.78	0.72
5.31_368.1632	0.00	0.00	0.00	0.30	0.00	0.00	0.73	1.00	0.57
9.55_400.1299	0.00	0.00	0.00	0.00	0.00	0.00	0.61	1.00	0.45
5.16_408.2509	0.00	0.00	0.00	0.13	0.00	0.03	0.80	1.00	0.86
5.02_407.2347	0.00	0.00	0.05	0.00	0.00	0.00	0.69	1.00	0.78
6.75_431.2681	0.00	0.00	0.31	0.00	0.00	0.00	0.90	0.96	1.00
5.75_749.3707	0.00	0.24	0.01	0.00	0.00	0.00	1.00	0.97	0.84
5.88_473.2311	0.01	0.03	0.03	0.00	0.00	0.00	0.96	1.00	0.75
5.45_764.4128	0.03	0.00	0.02	0.00	0.00	0.00	0.92	1.00	0.87
6.02_378.2402	0.04	0.36	0.25	0.00	0.00	0.02	1.00	0.73	0.70
5.58_291.6759	0.06	0.30	0.18	0.00	0.00	0.00	1.00	0.83	0.85
5.64_507.2827	0.06	0.00	0.16	0.00	0.00	0.01	0.84	0.81	1.00
10.32_317.2674	0.07	0.03	0.08	0.00	0.00	0.00	1.00	0.97	0.80
5.06_471.2746	0.10	0.04	0.04	0.00	0.00	0.00	1.00	0.47	0.82
5.64_360.2149	0.10	0.20	0.21	0.00	0.00	0.14	0.95	1.00	0.87
10.32_299.2598	0.12	0.05	0.10	0.00	0.00	0.00	1.00	0.63	0.66
5.18_423.2211	0.14	0.16	0.26	0.00	0.09	0.00	1.00	0.60	0.72
4.50_493.2325	0.15	0.28	0.28	0.00	0.13	0.00	1.00	0.82	0.86
5.58_582.3392	0.17	0.00	0.23	0.01	0.00	0.01	1.00	0.69	0.69
6.17_557.3688	0.18	0.10	0.19	0.00	0.00	0.01	1.00	0.80	0.96
6.11_734.3731	0.22	0.15	0.07	0.00	0.00	0.00	0.49	1.00	0.79
4.74_284.1566	0.23	0.38	0.12	0.14	0.19	0.04	0.69	1.00	0.65
5.88_378.2396	0.23	0.00	0.00	0.06	0.00	0.00	0.59	1.00	0.81
6.80_857.4155	0.28	0.00	0.26	0.00	0.00	0.00	0.98	0.86	1.00
8.64_342.2650	0.35	0.00	0.03	0.00	0.00	0.00	0.78	1.00	0.81
6.15_608.3295	0.39	0.35	0.18	0.00	0.00	0.01	1.00	0.87	0.98
6.00_288.0498	0.42	0.17	0.15	0.00	0.00	0.00	0.98	1.00	0.61
6.26_475.2939	0.42	0.09	0.37	0.08	0.00	0.00	0.90	0.90	1.00
5.50_374.2277	0.45	0.36	0.17	0.00	0.00	0.12	1.00	0.75	0.87

D. Mass Spectral Data for Selected Features

Table S9. Normalized heat map of features described as unique in figure S4 when comparing *Bacillus subtilis* to *Micrococcus luteus* and *Escherichia coli* extracts using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	B sub	B sub	B sub	E coli	E coli	E coli	M lut	M lut	M lut
4.42_357.1859	0.40	0.32	0.26	1.00	0.67	0.94	0.73	0.84	0.75
2.31_289.1405	0.62	1.00	0.56	0.02	0.00	0.00	0.33	0.12	0.00
3.38_271.1408	0.65	1.00	0.51	0.00	0.00	0.00	0.00	0.00	0.29
4.62_190.0525	0.67	1.00	0.69	0.00	0.00	0.08	0.03	0.24	0.17
5.71_441.7064	0.71	0.62	1.00	0.32	0.00	0.00	0.00	0.18	0.00
2.28_259.1292	0.74	1.00	0.59	0.00	0.00	0.05	0.22	0.00	0.08
4.49_201.1581	0.79	1.00	0.74	0.00	0.00	0.00	0.08	0.14	0.04
5.68_512.3435	0.88	1.00	0.98	0.00	0.00	0.01	0.02	0.15	0.19
8.21_272.1420	0.94	0.77	1.00	0.00	0.00	0.00	0.06	0.01	0.02
1.79_124.0404	1.00	0.85	0.84	0.07	0.10	0.00	0.28	0.50	0.18
8.29_223.1446	1.00	0.82	0.79	0.00	0.00	0.00	0.03	0.00	0.02
1.32_221.1124	1.00	0.69	0.94	0.02	0.00	0.00	0.46	0.00	0.08
6.22_246.1732	1.00	0.80	0.72	0.00	0.00	0.00	0.35	0.31	0.31
4.78_374.2088	1.00	0.88	0.91	0.00	0.00	0.00	0.42	0.43	0.00
4.69_431.2509	1.00	0.98	0.57	0.00	0.03	0.00	0.31	0.35	0.10

D. Mass Spectral Data for Selected Features

Table S10. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R1 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	R1	R1
12.03_135.1163	0.00	0.11	0.93	1.00
12.03_123.1165	0.00	0.00	1.00	0.99
4.87_118.0679	0.00	0.20	0.64	1.00
1.50_103.5345	0.00	0.00	1.00	0.69
13.61_149.0907	0.00	0.00	1.00	0.97
1.50_165.0624	0.00	0.00	1.00	0.78
6.56_162.0938	0.00	0.00	0.73	1.00
4.31_160.1140	0.00	0.00	0.63	1.00
5.78_170.1204	0.00	0.00	0.80	1.00
7.08_169.0882	0.00	0.06	1.00	0.83
2.44_166.0747	0.00	0.20	0.81	1.00
6.60_180.1017	0.00	0.03	0.76	1.00
5.02_180.1014	0.00	0.00	0.88	1.00
10.70_179.1435	0.00	0.00	0.97	1.00
4.95_177.1399	0.00	0.29	0.67	1.00
4.39_192.1130	0.00	0.21	0.90	1.00
9.12_191.0134	0.00	0.00	0.76	1.00
4.02_198.1143	0.00	0.00	0.71	1.00
8.84_203.1804	0.00	0.00	0.75	1.00
6.22_203.0786	0.00	0.10	1.00	1.00
9.80_203.0277	0.00	0.00	0.70	1.00
7.49_207.0994	0.00	0.07	0.71	1.00
1.30_205.9283	0.00	0.00	1.00	1.00
4.84_205.1323	0.00	0.00	0.68	1.00
9.81_205.1237	0.00	0.00	0.92	1.00
10.22_205.1232	0.00	0.00	0.92	1.00
1.32_211.8786	0.00	0.00	1.00	0.60
9.81_210.0363	0.00	0.00	0.77	1.00
5.35_210.0350	0.00	0.00	0.64	1.00
10.24_222.1533	0.00	0.00	1.00	0.96
9.81_222.1504	0.00	0.00	0.87	1.00
8.84_221.1903	0.00	0.00	0.73	1.00
7.99_225.1125	0.00	0.07	0.95	1.00
5.48_229.0656	0.00	0.00	0.73	1.00
4.61_230.0715	0.00	0.38	1.00	0.94
10.62_236.1643	0.00	0.00	1.00	0.83
5.11_236.1306	0.00	0.25	1.00	0.86
8.54_235.1344	0.00	0.00	0.80	1.00
11.28_233.1548	0.00	0.00	0.95	1.00
9.80_241.0261	0.00	0.00	0.70	1.00
11.75_239.1663	0.00	0.01	1.00	0.90
10.69_238.1826	0.00	0.00	1.00	1.00
5.81_248.1281	0.00	0.32	0.77	1.00
11.16_252.0381	0.00	0.00	1.00	0.60
13.78_251.2405	0.00	0.00	0.48	1.00
11.26_250.1814	0.00	0.00	1.00	0.91
4.56_252.0394	0.00	0.18	0.72	1.00
8.66_252.0394	0.00	0.00	0.47	1.00
7.48_252.0388	0.00	0.00	1.00	0.65
6.82_252.0384	0.00	0.00	1.00	0.57
3.87_257.1146	0.00	0.29	0.97	1.00
12.02_263.1978	0.00	0.09	0.94	1.00
1.78_262.1278	0.00	0.00	1.00	0.73
5.86_262.1048	0.00	0.32	0.66	1.00
10.71_261.1779	0.00	0.01	0.77	1.00
10.68_260.1641	0.00	0.00	0.98	1.00
5.43_268.0192	0.00	0.12	0.61	1.00
5.18_266.1406	0.00	0.33	0.76	1.00
5.27_264.2082	0.00	0.00	0.79	1.00
5.84_281.1328	0.00	0.00	0.63	1.00
9.12_279.1585	0.00	0.00	1.00	0.84
7.18_278.2110	0.00	0.00	0.60	1.00
13.60_278.2028	0.00	0.00	0.93	1.00
7.50_283.1523	0.00	0.04	0.65	1.00

D. Mass Spectral Data for Selected Features

1.73_282.0649	0.00	0.03	1.00	0.92
7.72_281.1420	0.00	0.00	1.00	0.91
7.82_294.2085	0.00	0.00	0.75	1.00
7.15_293.2251	0.00	0.00	0.71	1.00
3.76_299.1387	0.00	0.05	0.68	1.00
4.74_298.0969	0.00	0.08	0.90	1.00
9.60_297.1694	0.00	0.01	0.46	1.00
7.19_296.2224	0.00	0.00	0.82	1.00
3.78_300.1386	0.00	0.33	0.74	1.00
14.29_307.2281	0.00	0.00	1.00	0.82
8.43_314.1381	0.00	0.29	1.00	0.89
7.24_312.2197	0.00	0.00	0.98	1.00
5.82_322.1007	0.00	0.00	0.78	1.00
1.74_322.0446	0.00	0.03	1.00	0.72
14.63_321.2420	0.00	0.00	1.00	0.89
9.13_319.1539	0.00	0.00	1.00	0.68
6.08_324.1828	0.00	0.42	0.79	1.00
10.73_340.1475	0.00	0.19	1.00	1.00
14.63_339.2533	0.00	0.00	1.00	0.90
14.31_347.2205	0.00	0.00	1.00	0.82
5.26_354.0787	0.00	0.16	0.69	1.00
8.24_352.2057	0.00	0.00	1.00	0.84
6.95_350.2147	0.00	0.05	1.00	0.93
8.53_359.2035	0.00	0.25	0.80	1.00
9.80_367.0822	0.00	0.00	0.60	1.00
6.22_366.2068	0.00	0.36	0.76	1.00
14.32_379.2817	0.00	0.00	1.00	0.61
9.80_387.0731	0.00	0.00	0.72	1.00
6.24_384.2171	0.00	0.00	0.75	1.00
13.61_399.3201	0.00	0.00	1.00	0.57
1.49_394.1142	0.00	0.00	1.00	0.58
14.57_393.2988	0.00	0.00	0.76	1.00
13.61_407.3140	0.00	0.00	1.00	0.69
3.75_414.2692	0.00	0.00	0.64	1.00
9.08_429.0845	0.00	0.00	1.00	0.92
14.04_428.3345	0.00	0.07	0.79	1.00
14.04_420.3477	0.00	0.05	0.78	1.00
6.99_443.3240	0.00	0.12	0.66	1.00
9.73_443.1014	0.00	0.00	0.83	1.00
10.02_459.0960	0.00	0.00	0.57	1.00
11.52_456.3791	0.00	0.00	1.00	0.88
9.81_454.0847	0.00	0.00	0.86	1.00
9.78_481.0499	0.00	0.00	1.00	0.98
6.98_499.2793	0.00	0.00	1.00	0.74
4.37_494.2617	0.00	0.00	0.82	1.00
9.09_512.3013	0.00	0.00	0.91	1.00
13.62_510.2556	0.00	0.03	1.00	0.94
12.00_515.2832	0.00	0.00	1.00	1.00
1.76_515.1445	0.00	0.00	0.84	1.00
1.49_527.1567	0.00	0.00	1.00	0.64
10.06_526.3139	0.00	0.00	0.84	1.00
7.20_544.2918	0.00	0.00	1.00	0.66
12.03_565.3746	0.00	0.04	1.00	0.99
1.72_551.1035	0.00	0.00	1.00	0.66
5.52_601.2501	0.00	0.00	0.53	1.00
1.76_588.1814	0.00	0.00	0.54	1.00
9.79_576.6021	0.00	0.00	0.60	1.00
7.01_1221.4414	0.00	0.00	0.67	1.00
7.00_1216.1209	0.00	0.43	0.97	1.00
14.64_361.2361	0.00	0.00	1.00	0.86
7.48_177.0877	0.01	0.00	0.55	1.00
9.79_218.0234	0.01	0.08	0.72	1.00
1.82_228.1004	0.01	0.00	1.00	0.70
1.29_203.9309	0.01	0.00	1.00	0.96
1.75_507.1572	0.02	0.00	0.70	1.00
9.66_279.1583	0.02	0.00	0.72	1.00
9.78_465.0808	0.02	0.06	0.88	1.00
9.81_269.0437	0.03	0.00	0.73	1.00
6.95_368.2220	0.03	0.05	0.97	1.00
13.79_531.4249	0.03	0.10	0.80	1.00

D. Mass Spectral Data for Selected Features

16.15_710.1773	0.03	0.01	1.00	0.90
12.02_205.1953	0.04	0.00	0.94	1.00
5.43_377.1482	0.04	0.00	0.67	1.00
14.31_325.2414	0.04	0.03	1.00	0.81
9.41_281.1770	0.04	0.08	0.81	1.00
9.67_319.1539	0.04	0.06	1.00	0.93
6.24_515.2753	0.04	0.02	0.78	1.00
4.75_136.0625	0.05	0.00	0.68	1.00
13.79_365.2675	0.05	0.06	1.00	0.67
8.60_236.1631	0.05	0.11	0.69	1.00
1.74_150.0789	0.06	0.00	1.00	0.95
8.53_283.1523	0.06	0.13	0.72	1.00
9.14_239.1284	0.06	0.06	1.00	0.73
14.78_323.2583	0.07	0.13	1.00	0.83
1.73_338.0231	0.07	0.00	1.00	0.66
8.53_177.0880	0.07	0.07	0.66	1.00
3.86_150.0940	0.07	0.13	0.61	1.00
6.95_218.1203	0.07	0.15	0.69	1.00
8.53_207.1002	0.07	0.09	0.69	1.00
14.04_295.2283	0.08	0.15	1.00	0.86
1.70_260.1135	0.10	0.00	1.00	0.70
7.42_280.1237	0.11	0.31	0.64	1.00
11.43_466.2973	0.12	0.35	1.00	0.78
6.27_207.0660	0.12	0.22	0.74	1.00
7.89_192.1015	0.13	0.22	0.69	1.00
3.07_230.1126	0.13	0.31	1.00	0.81
6.41_165.0905	0.13	0.09	0.72	1.00
8.29_401.1993	0.14	0.00	0.73	1.00
4.87_329.1844	0.14	0.00	0.72	1.00
4.88_188.0708	0.15	0.26	0.68	1.00
14.41_309.2409	0.16	0.29	1.00	0.85
3.83_198.1623	0.17	0.12	0.62	1.00
3.85_276.1433	0.18	0.10	0.67	1.00
7.42_196.0651	0.18	0.09	0.69	1.00
4.30_310.1305	0.19	0.04	0.73	1.00
9.47_211.0868	0.19	0.33	0.69	1.00
5.27_685.1761	0.20	0.00	0.84	1.00
3.82_230.1126	0.21	0.13	0.61	1.00
13.84_397.2963	0.22	0.00	1.00	0.86
8.08_219.1411	0.22	0.32	0.75	1.00
6.78_176.0714	0.22	0.37	0.69	1.00
16.18_335.9929	0.28	0.00	0.83	1.00
13.50_409.7445	0.30	0.38	0.84	1.00
6.15_485.2027	0.37	0.39	0.67	1.00
12.62_416.2462	0.37	0.45	1.00	0.88
9.69_220.1127	0.40	0.47	0.98	1.00
16.15_481.1090	0.42	0.00	0.89	1.00
14.82_332.2940	0.43	0.28	1.00	0.85
4.29_244.1199	0.45	0.46	0.78	1.00
5.16_210.1137	0.45	0.44	0.70	1.00
12.40_251.2372	0.47	0.00	1.00	0.98
11.97_299.2600	0.49	0.61	1.00	0.91
10.60_346.3091	0.51	1.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.00	0.00
10.70_288.2557	0.52	1.00	0.00	0.00
6.40_439.1986	0.52	0.52	0.90	1.00
9.48_225.1993	0.53	1.00	0.01	0.02
6.81_807.1918	0.54	1.00	0.00	0.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.00	0.00
4.09_573.1785	0.58	1.00	0.00	0.00
4.37_663.2850	0.59	1.00	0.00	0.00
5.20_239.1759	0.62	1.00	0.10	0.12
4.64_412.2067	0.62	1.00	0.00	0.14
6.19_181.1351	0.63	1.00	0.05	0.05
1.50_432.0982	0.66	1.00	0.13	0.00
4.27_647.2871	0.67	1.00	0.04	0.00
1.50_448.0831	0.67	1.00	0.14	0.00
11.44_223.2060	0.67	1.00	0.00	0.00
7.62_970.6124	0.70	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

6.85_824.9348	0.70	1.00	0.00	0.00
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
3.89_518.1743	0.73	1.00	0.03	0.00
11.18_473.3585	0.75	1.00	0.52	0.41
1.53_143.0837	0.76	1.00	0.00	0.00
12.74_443.3505	0.77	1.00	0.00	0.07
12.98_282.2118	0.82	1.00	0.00	0.14
3.86_242.1126	0.82	0.90	1.00	1.00
9.26_219.1735	0.88	1.00	0.00	0.00
4.50_359.1197	0.89	1.00	0.24	0.28
1.49_594.1582	0.91	1.00	0.66	0.45
15.94_338.3442	0.91	1.00	0.78	0.80
13.48_341.2200	0.91	1.00	0.00	0.00
13.49_295.2258	0.91	1.00	0.14	0.08
1.47_508.0657	0.91	1.00	0.47	0.19
1.50_260.0296	0.92	1.00	0.12	0.06
1.47_748.1127	0.94	1.00	0.66	0.51
12.73_320.2010	0.94	1.00	0.00	0.30
1.48_481.1031	0.96	1.00	0.70	0.43
4.49_225.1597	0.97	1.00	0.20	0.23
13.95_270.2746	1.00	1.00	0.52	0.66
3.99_164.0936	1.00	0.90	0.39	0.60
1.50_230.0720	1.00	0.75	0.52	0.27
9.27_240.2315	1.00	0.88	0.17	0.15
10.39_268.2627	1.00	0.83	0.00	0.00
6.59_273.1670	1.00	0.84	0.00	0.21
13.97_282.2786	1.00	0.85	0.67	0.58
3.80_288.1929	1.00	0.87	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
15.49_338.3442	1.00	0.86	0.18	0.00
1.55_385.5441	1.00	0.65	0.22	0.05
1.50_401.0693	1.00	0.93	0.73	0.51
12.86_485.3471	1.00	0.86	0.66	0.44
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.30
7.66_916.7249	1.00	0.76	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S11. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R2 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT _m/z)	WT	WT	R2	R2
12.03_135.1163	0.00	0.31	0.69	1.00
12.03_123.1165	0.00	0.00	1.00	0.65
4.87_118.0679	0.00	0.18	1.00	1.00
12.03_149.1327	0.00	0.00	1.00	0.61
13.61_149.0907	0.00	0.00	1.00	0.91
1.50_165.0624	0.00	0.00	1.00	0.98
10.69_163.6058	0.00	0.00	1.00	0.67
6.56_162.0938	0.00	0.00	0.66	1.00
5.78_170.1204	0.00	0.00	1.00	1.00
7.08_169.0882	0.00	0.01	0.62	1.00
6.60_180.1017	0.00	0.03	1.00	0.91
5.02_180.1014	0.00	0.00	1.00	0.86
4.95_177.1399	0.00	0.38	1.00	0.94
4.39_192.1130	0.00	0.26	0.80	1.00
9.26_191.1250	0.00	0.00	1.00	0.74
9.12_191.0134	0.00	0.00	1.00	0.88
6.97_190.1257	0.00	0.00	1.00	0.80
4.14_186.1168	0.00	0.00	0.95	1.00
9.08_196.0187	0.00	0.00	1.00	0.68
8.84_203.1804	0.00	0.00	1.00	0.90
8.12_203.1781	0.00	0.00	1.00	0.94
9.08_203.0278	0.00	0.00	1.00	0.72
9.80_203.0277	0.00	0.00	1.00	0.72
9.42_202.0393	0.00	0.00	0.75	1.00
4.35_209.0956	0.00	0.00	0.82	1.00
5.44_208.0539	0.00	0.01	1.00	0.97
7.49_207.0994	0.00	0.10	1.00	0.75
1.30_205.9283	0.00	0.00	1.00	1.00
4.84_205.1323	0.00	0.00	1.00	0.91
1.32_211.8786	0.00	0.00	1.00	0.98
9.25_211.0284	0.00	0.04	1.00	0.81
8.31_210.0369	0.00	0.00	1.00	0.59
9.81_210.0363	0.00	0.00	1.00	0.76
9.07_210.0305	0.00	0.00	1.00	0.86
9.41_219.0312	0.00	0.00	1.00	0.77
9.03_217.0413	0.00	0.00	1.00	0.82
16.16_223.9875	0.00	0.00	1.00	0.84
8.84_221.1903	0.00	0.00	1.00	0.93
6.51_220.1710	0.00	0.07	0.97	1.00
5.15_226.5984	0.00	0.03	1.00	0.86
7.35_225.1140	0.00	0.00	1.00	0.89
7.99_225.1125	0.00	0.02	1.00	0.94
9.04_225.0298	0.00	0.01	1.00	0.79
9.77_224.0325	0.00	0.00	1.00	0.83
5.48_229.0656	0.00	0.00	0.97	1.00
5.11_227.1386	0.00	0.00	1.00	0.99
9.19_230.0719	0.00	0.00	1.00	0.69
9.82_230.0718	0.00	0.03	0.79	1.00
8.41_230.0715	0.00	0.00	1.00	0.90
10.62_236.1643	0.00	0.00	1.00	0.82
5.11_236.1306	0.00	0.17	1.00	0.92
8.54_235.1344	0.00	0.00	1.00	0.88
9.80_241.0261	0.00	0.00	1.00	0.85
8.82_241.0249	0.00	0.00	0.72	1.00
5.81_248.1281	0.00	0.36	0.99	1.00
9.03_248.0351	0.00	0.00	1.00	0.83
8.44_247.1345	0.00	0.00	0.75	1.00
4.04_247.1287	0.00	0.00	1.00	0.88
7.33_247.0943	0.00	0.11	1.00	0.94
9.07_246.5440	0.00	0.00	1.00	0.83
5.04_244.1219	0.00	0.00	1.00	0.91
11.26_250.1814	0.00	0.00	1.00	0.82
4.94_250.1290	0.00	0.00	1.00	0.93
8.52_250.0297	0.00	0.00	1.00	0.94

D. Mass Spectral Data for Selected Features

4.31_249.0807	0.00	0.00	1.00	0.87
8.16_249.0423	0.00	0.00	1.00	0.80
4.56_252.0394	0.00	0.13	0.90	1.00
6.01_252.0391	0.00	0.00	1.00	0.84
6.82_252.0384	0.00	0.00	1.00	0.82
6.23_258.1449	0.00	0.00	1.00	0.86
6.94_256.2241	0.00	0.00	1.00	0.89
4.75_255.5956	0.00	0.28	1.00	0.83
6.97_254.2139	0.00	0.00	1.00	0.86
9.81_253.5524	0.00	0.01	1.00	0.86
4.75_263.0841	0.00	0.16	1.00	0.81
1.78_262.1278	0.00	0.00	1.00	0.73
9.91_261.5430	0.00	0.00	0.52	1.00
5.01_261.1438	0.00	0.06	1.00	0.94
9.03_260.5527	0.00	0.00	1.00	0.64
8.32_268.0180	0.00	0.00	1.00	0.94
10.77_267.1616	0.00	0.06	0.55	1.00
5.18_266.1406	0.00	0.37	1.00	0.82
5.27_264.2082	0.00	0.00	1.00	0.80
7.49_268.0200	0.00	0.00	1.00	0.68
9.67_268.0195	0.00	0.00	1.00	0.74
7.61_273.1085	0.00	0.00	1.00	0.84
5.84_281.1328	0.00	0.00	1.00	0.97
7.18_278.2110	0.00	0.00	1.00	0.88
6.07_276.1943	0.00	0.00	1.00	0.79
5.71_286.2118	0.00	0.00	1.00	0.83
7.19_284.2219	0.00	0.00	0.86	1.00
12.79_284.1681	0.00	0.05	1.00	0.98
7.50_283.1523	0.00	0.05	1.00	0.92
1.73_282.0649	0.00	0.03	1.00	0.94
7.72_281.1420	0.00	0.00	0.83	1.00
3.93_291.1653	0.00	0.00	1.00	0.83
9.72_290.1445	0.00	0.00	0.99	1.00
7.06_287.2336	0.00	0.00	0.93	1.00
5.22_295.1312	0.00	0.03	0.87	1.00
6.82_294.2084	0.00	0.00	1.00	0.82
7.15_293.2251	0.00	0.00	1.00	0.65
4.87_293.1612	0.00	0.35	1.00	0.91
6.49_292.1923	0.00	0.01	0.96	1.00
3.76_299.1387	0.00	0.00	0.54	1.00
2.95_299.1385	0.00	0.00	1.00	0.90
12.77_298.1902	0.00	0.00	0.95	1.00
4.74_298.0969	0.00	0.06	0.99	1.00
7.19_296.2224	0.00	0.00	1.00	0.92
5.83_303.1558	0.00	0.04	0.65	1.00
7.70_303.1206	0.00	0.04	1.00	0.99
3.78_300.1386	0.00	0.05	1.00	0.78
12.02_309.1921	0.00	0.06	1.00	0.80
6.00_308.2238	0.00	0.00	1.00	0.83
8.43_314.1381	0.00	0.21	1.00	0.60
6.06_312.2197	0.00	0.00	0.92	1.00
6.84_312.2197	0.00	0.00	1.00	0.91
7.24_312.2197	0.00	0.00	1.00	0.81
9.72_312.1580	0.00	0.00	1.00	0.77
10.59_311.1859	0.00	0.00	1.00	0.72
9.79_311.0549	0.00	0.00	1.00	0.92
7.47_310.2026	0.00	0.00	0.84	1.00
5.82_322.1007	0.00	0.00	1.00	0.87
1.74_322.0446	0.00	0.03	1.00	0.96
9.13_319.1539	0.00	0.00	1.00	0.83
6.92_318.2094	0.00	0.00	1.00	0.93
6.00_328.7423	0.00	0.13	1.00	0.93
5.91_328.5999	0.00	0.00	1.00	0.92
6.01_326.2353	0.00	0.00	0.95	1.00
4.97_326.0999	0.00	0.34	1.00	0.77
6.08_324.1828	0.00	0.23	1.00	0.93
6.31_335.7452	0.00	0.00	1.00	0.80
6.62_334.2005	0.00	0.00	1.00	0.80
9.73_334.1684	0.00	0.00	1.00	0.77
8.76_329.1942	0.00	0.19	0.99	1.00

D. Mass Spectral Data for Selected Features

12.72_342.2152	0.00	0.10	1.00	0.86
5.99_338.1374	0.00	0.00	0.88	1.00
9.08_348.2310	0.00	0.00	1.00	0.77
6.22_346.2031	0.00	0.00	0.71	1.00
7.48_345.1875	0.00	0.00	1.00	0.85
7.37_344.2218	0.00	0.00	1.00	0.84
9.69_356.1867	0.00	0.00	1.00	0.85
5.26_354.0787	0.00	0.28	0.97	1.00
8.24_352.2057	0.00	0.00	1.00	0.88
12.66_364.2323	0.00	0.28	1.00	0.74
6.67_362.2335	0.00	0.00	0.97	1.00
6.51_360.2165	0.00	0.00	1.00	0.89
8.53_359.2035	0.00	0.18	1.00	0.87
8.77_368.2219	0.00	0.00	1.00	0.92
7.52_368.2211	0.00	0.00	1.00	0.87
9.80_367.0822	0.00	0.00	1.00	0.96
10.08_366.2455	0.00	0.00	1.00	0.72
9.04_366.2404	0.00	0.00	1.00	0.83
6.22_366.2068	0.00	0.12	0.76	1.00
5.64_366.2063	0.00	0.00	0.91	1.00
8.47_382.2398	0.00	0.00	1.00	0.75
9.68_378.2012	0.00	0.00	1.00	0.72
7.43_374.2181	0.00	0.00	0.61	1.00
7.83_387.1861	0.00	0.00	1.00	0.94
9.80_387.0731	0.00	0.00	1.00	0.86
6.88_386.2329	0.00	0.01	1.00	0.90
6.24_384.2171	0.00	0.00	1.00	0.85
8.63_398.2317	0.00	0.00	1.00	1.00
1.49_394.1142	0.00	0.00	1.00	0.92
12.60_408.2538	0.00	0.15	1.00	0.67
7.68_401.3048	0.00	0.00	1.00	0.86
9.40_418.0851	0.00	0.00	1.00	0.97
8.66_429.0854	0.00	0.00	1.00	0.77
9.08_429.0845	0.00	0.00	1.00	0.82
4.02_423.1940	0.00	0.00	0.98	1.00
1.48_431.0890	0.00	0.45	1.00	0.91
9.07_451.0615	0.00	0.00	1.00	0.97
9.09_448.0576	0.00	0.00	1.00	0.71
6.99_443.3240	0.00	0.08	1.00	0.95
9.73_443.1014	0.00	0.00	1.00	0.87
8.33_443.0954	0.00	0.00	1.00	0.90
6.90_461.2902	0.00	0.00	1.00	0.96
5.90_459.3212	0.00	0.13	1.00	0.76
10.02_459.0960	0.00	0.00	1.00	0.77
9.03_457.1145	0.00	0.00	1.00	0.79
8.67_457.1133	0.00	0.00	1.00	0.95
11.52_456.3791	0.00	0.00	0.70	1.00
6.21_455.1906	0.00	0.19	1.00	0.85
9.81_454.0847	0.00	0.00	1.00	0.88
9.05_454.0819	0.00	0.00	1.00	0.72
5.01_452.1838	0.00	0.00	0.99	1.00
6.42_472.2832	0.00	0.00	0.56	1.00
6.46_471.2466	0.00	0.01	1.00	0.90
10.02_470.0758	0.00	0.00	1.00	0.82
9.02_468.1011	0.00	0.00	1.00	0.83
8.31_465.0807	0.00	0.00	1.00	0.79
8.82_465.0807	0.00	0.00	1.00	0.70
9.79_462.0710	0.00	0.00	1.00	0.81
9.04_462.0699	0.00	0.00	1.00	0.73
9.78_481.0499	0.00	0.00	0.74	1.00
9.02_479.0963	0.00	0.00	1.00	0.88
10.01_478.0692	0.00	0.00	1.00	0.66
4.15_476.2404	0.00	0.00	1.00	0.84
9.02_476.0877	0.00	0.00	1.00	0.79
7.51_499.2782	0.00	0.06	1.00	0.92
9.02_495.0687	0.00	0.00	1.00	0.95
4.37_494.2617	0.00	0.00	0.50	1.00
9.74_493.2809	0.00	0.01	1.00	0.93
5.37_493.1709	0.00	0.00	1.00	0.80
9.79_513.1525	0.00	0.00	1.00	0.62

D. Mass Spectral Data for Selected Features

6.65_512.8485	0.00	0.00	0.95	1.00
5.76_512.6875	0.00	0.00	1.00	1.00
9.09_512.3013	0.00	0.00	1.00	0.82
13.62_510.2556	0.00	0.37	1.00	0.85
5.65_504.2609	0.00	0.00	1.00	0.99
5.64_515.2738	0.00	0.00	1.00	0.91
9.71_537.3041	0.00	0.00	0.95	1.00
10.06_526.3139	0.00	0.00	1.00	0.86
7.21_526.2839	0.00	0.02	0.97	1.00
7.20_544.2918	0.00	0.00	1.00	0.93
7.57_542.3960	0.00	0.15	1.00	0.65
12.03_565.3746	0.00	0.08	0.73	1.00
7.14_560.1805	0.00	0.00	0.75	1.00
6.90_555.3068	0.00	0.00	1.00	0.92
5.52_601.2501	0.00	0.00	1.00	0.87
9.02_590.6205	0.00	0.00	1.00	0.79
9.74_581.3322	0.00	0.00	0.96	1.00
9.79_576.6021	0.00	0.00	0.82	1.00
9.06_576.6005	0.00	0.00	0.97	1.00
1.25_639.8836	0.00	0.00	1.00	0.83
12.72_634.4531	0.00	0.00	1.00	0.73
9.71_625.3598	0.00	0.00	1.00	0.84
9.73_669.3835	0.00	0.00	1.00	0.90
9.02_704.1451	0.00	0.00	1.00	0.61
9.03_696.1548	0.00	0.00	1.00	0.81
9.71_694.1152	0.00	0.00	0.77	1.00
9.03_690.1259	0.00	0.00	1.00	0.54
9.79_683.1204	0.00	0.00	1.00	0.77
9.06_676.1101	0.00	0.00	1.00	0.87
9.74_713.4076	0.00	0.00	0.65	1.00
9.78_885.1896	0.00	0.00	1.00	0.69
9.07_879.1306	0.00	0.00	0.96	1.00
9.02_935.1961	0.00	0.00	1.00	0.77
7.20_920.0962	0.00	0.00	0.77	1.00
7.21_916.0943	0.00	0.00	0.54	1.00
9.80_907.1678	0.00	0.00	1.00	0.88
9.04_907.1662	0.00	0.00	1.00	0.53
7.65_1000.0444	0.00	0.00	0.87	1.00
7.63_942.9948	0.00	0.00	1.00	0.83
7.01_1221.4414	0.00	0.00	0.92	1.00
6.97_357.2762	0.00	0.00	1.00	0.85
9.79_218.0234	0.00	0.01	1.00	0.89
7.07_184.1710	0.00	0.00	1.00	0.83
9.78_465.0808	0.00	0.01	1.00	0.94
8.21_315.2621	0.00	0.01	1.00	0.83
8.21_212.2021	0.00	0.00	1.00	0.84
5.66_384.2168	0.00	0.00	1.00	0.87
9.79_1349.2480	0.01	0.00	1.00	0.88
9.27_343.2981	0.01	0.03	1.00	0.92
8.34_150.0928	0.01	0.09	0.90	1.00
10.70_288.2557	0.01	0.01	1.00	0.74
1.64_174.0879	0.01	0.00	1.00	1.00
6.76_310.2021	0.01	0.00	1.00	1.00
1.82_228.1004	0.01	0.00	1.00	0.82
6.06_294.2084	0.01	0.00	1.00	0.80
6.24_515.2753	0.01	0.00	1.00	0.97
8.74_542.3146	0.01	0.00	0.89	1.00
1.29_203.9309	0.01	0.00	0.96	1.00
1.64_246.1172	0.01	0.00	1.00	0.96
9.71_757.4327	0.01	0.00	0.92	1.00
6.65_282.2073	0.02	0.11	1.00	0.75
7.48_177.0877	0.02	0.00	1.00	0.86
1.75_507.1572	0.02	0.00	1.00	0.62
8.10_301.1534	0.02	0.10	1.00	0.95
8.29_401.1993	0.03	0.00	1.00	0.82
4.82_393.2208	0.03	0.00	1.00	0.74
16.15_710.1773	0.03	0.01	0.61	1.00
1.53_143.0837	0.04	0.05	0.82	1.00
9.27_240.2315	0.04	0.03	1.00	0.81
5.43_377.1482	0.04	0.00	1.00	0.99

D. Mass Spectral Data for Selected Features

12.62_416.2462	0.04	0.05	1.00	0.74
3.22_235.1201	0.05	0.00	0.91	1.00
7.06_325.1861	0.05	0.31	1.00	0.78
9.66_279.1583	0.06	0.00	1.00	0.80
12.02_205.1953	0.07	0.00	1.00	0.62
9.14_239.1284	0.07	0.06	1.00	0.88
1.74_150.0789	0.07	0.00	1.00	0.87
4.75_136.0625	0.07	0.00	0.85	1.00
1.73_338.0231	0.07	0.00	0.97	1.00
6.39_336.2172	0.08	0.06	1.00	0.68
12.57_815.5173	0.08	0.25	1.00	0.86
10.40_371.3275	0.08	0.15	1.00	0.80
12.73_328.1928	0.08	0.00	1.00	0.86
6.72_1450.6973	0.08	0.02	0.72	1.00
8.53_283.1523	0.08	0.18	0.82	1.00
1.70_260.1135	0.08	0.00	1.00	0.97
6.66_264.1980	0.08	0.04	1.00	0.88
6.95_218.1203	0.09	0.19	1.00	0.87
12.66_372.2164	0.10	0.24	1.00	0.80
12.70_350.2054	0.10	0.19	1.00	0.86
16.22_252.0441	0.11	0.19	0.60	1.00
1.77_218.1042	0.11	0.03	1.00	1.00
3.86_150.0940	0.11	0.21	1.00	0.92
7.25_371.1508	0.12	0.00	1.00	0.87
6.71_1160.7578	0.12	0.00	0.81	1.00
12.78_306.1796	0.13	0.22	1.00	0.89
12.63_394.2284	0.13	0.10	1.00	0.73
7.06_221.1900	0.14	0.44	1.00	0.97
7.62_970.6124	0.15	0.21	0.74	1.00
8.53_207.1002	0.15	0.19	0.85	1.00
7.42_280.1237	0.15	0.42	1.00	0.93
12.55_438.2596	0.16	0.26	1.00	0.68
3.80_288.1929	0.17	0.15	1.00	0.93
12.73_320.2010	0.17	0.18	1.00	0.90
12.62_787.4580	0.18	0.31	1.00	0.92
7.06_203.1787	0.19	0.35	1.00	0.91
8.53_177.0880	0.19	0.18	1.00	0.85
10.98_442.3651	0.20	0.16	1.00	0.77
4.88_188.0708	0.20	0.35	1.00	0.92
12.70_699.4109	0.20	0.23	1.00	0.96
6.41_165.0905	0.21	0.14	0.89	1.00
6.06_203.1781	0.21	0.37	1.00	0.92
4.87_329.1844	0.22	0.00	1.00	0.87
16.18_335.9929	0.22	0.00	0.66	1.00
12.78_611.3565	0.22	0.25	1.00	0.98
1.51_393.5330	0.23	0.58	1.00	0.98
5.84_299.0939	0.23	0.11	0.69	1.00
12.61_771.4862	0.24	0.30	1.00	0.83
12.73_655.3845	0.24	0.29	1.00	1.00
4.31_265.0552	0.24	0.00	1.00	0.82
12.67_743.4367	0.24	0.27	1.00	0.95
12.70_683.4373	0.24	0.32	1.00	0.83
5.97_286.6247	0.24	0.04	0.82	1.00
12.79_595.3829	0.25	0.34	1.00	0.84
12.67_727.4605	0.25	0.34	1.00	0.81
2.84_200.1047	0.25	0.00	1.00	0.99
12.74_639.4067	0.26	0.31	1.00	0.84
6.95_368.2220	0.27	0.47	1.00	0.85
12.86_523.3040	0.27	0.18	0.94	1.00
12.80_567.3292	0.27	0.32	0.97	1.00
3.85_276.1433	0.28	0.16	0.98	1.00
1.65_159.0768	0.28	0.00	0.65	1.00
12.86_507.3281	0.28	0.43	1.00	0.74
4.30_310.1305	0.28	0.06	1.00	0.96
4.12_413.1243	0.32	0.58	1.00	0.99
7.91_389.2523	0.33	0.15	1.00	0.93
3.83_198.1623	0.33	0.23	1.00	0.89
7.65_970.5389	0.33	0.00	1.00	0.95
12.82_551.3593	0.34	0.50	0.86	1.00
12.87_262.1528	0.35	0.15	1.00	0.94

D. Mass Spectral Data for Selected Features

6.78_176.0714	0.36	0.62	1.00	0.87
12.70_678.4764	0.37	0.21	1.00	0.72
12.86_502.3745	0.37	0.45	1.00	0.72
12.86_463.2998	0.37	0.49	1.00	0.79
3.76_347.1589	0.38	0.00	1.00	0.75
12.56_441.2657	0.39	0.56	0.84	1.00
6.73_1160.5609	0.39	0.00	0.82	1.00
12.67_722.5060	0.41	0.20	1.00	0.73
5.61_343.2002	0.43	0.10	1.00	0.85
4.29_244.1199	0.47	0.49	0.93	1.00
4.00_320.1711	0.49	0.06	1.00	0.99
14.78_323.2583	0.50	1.00	0.00	0.03
13.49_420.3478	0.51	1.00	0.01	0.00
10.60_346.3091	0.51	1.00	0.00	0.00
13.00_413.3095	0.52	1.00	0.05	0.00
5.16_210.1137	0.52	0.51	0.96	1.00
9.48_225.1993	0.53	1.00	0.01	0.00
6.81_807.1918	0.54	1.00	0.00	0.00
6.15_485.2027	0.55	0.59	1.00	0.88
7.42_196.0651	0.55	0.29	1.00	0.92
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.04	0.00
10.15_739.4618	0.56	1.00	0.03	0.02
14.41_309.2409	0.56	1.00	0.04	0.03
10.53_531.4000	0.57	1.00	0.00	0.00
4.86_372.1909	0.57	0.29	1.00	0.89
12.97_407.3144	0.58	1.00	0.01	0.00
12.98_399.3242	0.58	1.00	0.01	0.00
4.09_573.1785	0.58	1.00	0.00	0.00
3.79_359.1699	0.59	0.29	1.00	0.92
4.64_137.0376	0.59	0.61	1.00	0.87
4.37_663.2850	0.59	1.00	0.05	0.00
13.98_433.3418	0.61	1.00	0.01	0.00
4.64_412.2067	0.62	1.00	0.10	0.08
6.19_181.1351	0.63	1.00	0.00	0.07
10.97_401.2525	0.63	1.00	0.00	0.00
11.58_415.2745	0.65	1.00	0.00	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.97_290.7254	0.66	1.00	0.15	0.05
4.27_647.2871	0.67	1.00	0.01	0.06
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.36	0.28
6.40_263.1761	0.70	0.75	1.00	0.88
6.85_824.9348	0.70	1.00	0.19	0.00
4.81_506.2950	0.71	1.00	0.39	0.33
16.15_442.8736	0.71	1.00	0.15	0.06
4.40_158.0302	0.72	0.53	0.99	1.00
4.34_266.1408	0.72	0.56	0.98	1.00
4.37_150.0945	0.72	1.00	0.00	0.00
5.94_213.1018	0.73	0.55	0.97	1.00
3.89_518.1743	0.73	1.00	0.00	0.00
11.18_473.3585	0.75	1.00	0.02	0.02
16.18_214.9181	0.76	1.00	0.43	0.27
12.74_443.3505	0.77	1.00	0.00	0.00
12.97_547.4060	0.77	1.00	0.07	0.00
13.86_425.2896	0.78	1.00	0.22	0.14
5.26_147.0936	0.79	1.00	0.33	0.30
13.50_409.7445	0.80	1.00	0.34	0.09
4.28_227.1066	0.80	1.00	0.59	0.57
11.97_299.2600	0.80	1.00	0.00	0.00
13.50_524.2740	0.81	1.00	0.22	0.15
15.06_413.2647	0.81	1.00	0.27	0.14
4.55_279.1361	0.81	1.00	0.65	0.60
1.50_710.1736	0.81	0.82	0.96	1.00
11.84_443.3878	0.82	1.00	0.09	0.06
11.03_354.1608	0.82	1.00	0.11	0.09
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.00
13.79_365.2675	0.84	1.00	0.00	0.00
9.69_220.1127	0.87	1.00	0.19	0.44

D. Mass Spectral Data for Selected Features

10.38_401.3397	0.88	1.00	0.18	0.13
9.26_219.1735	0.88	1.00	0.00	0.00
14.79_310.3109	0.90	1.00	0.55	0.67
15.94_338.3442	0.91	1.00	0.44	0.37
13.48_341.2200	0.91	1.00	0.34	0.19
13.49_295.2258	0.91	1.00	0.00	0.00
1.47_508.0657	0.91	1.00	0.76	0.71
1.47_748.1127	0.94	1.00	0.84	0.83
4.58_336.1924	0.95	1.00	0.68	0.54
1.48_481.1031	0.96	1.00	0.73	0.71
4.49_225.1597	0.97	1.00	0.52	0.50
13.95_270.2746	1.00	1.00	0.33	0.27
6.34_150.0787	1.00	0.95	0.88	0.81
10.36_211.6353	1.00	0.89	0.20	0.00
3.82_209.1275	1.00	0.90	0.72	0.65
11.31_225.6512	1.00	0.95	0.17	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
5.53_306.1782	1.00	0.69	0.37	0.26
12.62_313.2746	1.00	0.83	0.00	0.00
14.31_325.2414	1.00	0.74	0.00	0.08
14.82_332.2940	1.00	0.65	0.00	0.10
15.49_338.3442	1.00	0.86	0.00	0.00
4.26_356.1796	1.00	0.84	0.64	0.56
15.92_360.3229	1.00	0.71	0.26	0.20
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.18	0.15
13.95_411.3586	1.00	0.78	0.00	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.21	0.00
12.97_555.3910	1.00	0.94	0.19	0.09
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.20	0.23
6.87_807.0837	1.00	0.57	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S12. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R2 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT _m/z)	WT	WT	R3	R3
12.03_135.1163	0.00	0.13	1.00	0.81
1.52_129.5659	0.00	0.00	1.00	0.65
12.03_123.1165	0.00	0.00	1.00	0.81
4.87_118.0679	0.00	0.13	0.60	1.00
4.95_114.0908	0.00	0.00	0.84	1.00
1.50_165.0624	0.00	0.00	1.00	0.83
6.56_162.0938	0.00	0.00	1.00	0.86
4.31_160.1140	0.00	0.00	1.00	0.88
5.78_170.1204	0.00	0.00	1.00	0.92
7.08_169.0882	0.00	0.02	0.64	1.00
2.44_166.0747	0.00	0.12	1.00	0.85
6.60_180.1017	0.00	0.02	1.00	0.77
4.95_177.1399	0.00	0.43	1.00	0.94
9.12_191.0134	0.00	0.00	1.00	0.78
6.97_190.1257	0.00	0.00	1.00	0.82
4.99_198.1134	0.00	0.00	0.68	1.00
9.08_196.0187	0.00	0.00	1.00	0.99
8.84_203.1804	0.00	0.00	1.00	0.93
9.08_203.0278	0.00	0.00	0.89	1.00
9.80_203.0277	0.00	0.00	1.00	0.82
9.42_202.0393	0.00	0.00	1.00	0.87
4.35_209.0956	0.00	0.00	0.65	1.00
4.54_208.1355	0.00	0.00	0.95	1.00
5.44_208.0539	0.00	0.00	0.95	1.00
7.49_207.0994	0.00	0.07	1.00	0.63
1.30_205.9283	0.00	0.00	1.00	0.75
4.84_205.1323	0.00	0.00	1.00	0.94
8.67_212.0251	0.00	0.00	1.00	0.87
1.32_211.8786	0.00	0.00	1.00	0.84
9.81_210.0363	0.00	0.00	0.85	1.00
9.07_210.0305	0.00	0.00	0.58	1.00
9.41_219.0312	0.00	0.00	0.69	1.00
3.69_218.1136	0.00	0.30	1.00	0.83
8.67_218.0490	0.00	0.00	0.92	1.00
9.03_217.0413	0.00	0.00	1.00	0.99
8.84_221.1903	0.00	0.00	1.00	0.85
6.51_220.1710	0.00	0.03	0.59	1.00
4.58_226.1445	0.00	0.00	0.91	1.00
5.11_226.1427	0.00	0.03	0.67	1.00
9.04_225.0298	0.00	0.01	1.00	0.97
9.77_224.0325	0.00	0.00	0.95	1.00
5.11_227.1386	0.00	0.00	0.91	1.00
9.82_230.0718	0.00	0.04	1.00	1.00
6.24_230.0717	0.00	0.34	1.00	0.88
8.41_230.0715	0.00	0.00	1.00	0.75
5.11_236.1306	0.00	0.12	0.68	1.00
4.89_235.1441	0.00	0.00	1.00	0.98
9.80_241.0261	0.00	0.00	1.00	0.63
5.81_248.1281	0.00	0.25	0.76	1.00
9.03_248.0351	0.00	0.00	1.00	0.51
4.04_247.1287	0.00	0.00	1.00	0.91
5.04_244.1219	0.00	0.00	0.87	1.00
2.62_252.0382	0.00	0.29	0.96	1.00
11.26_250.1814	0.00	0.00	1.00	0.73
14.09_252.0478	0.00	0.00	0.56	1.00
8.66_252.0394	0.00	0.00	0.67	1.00
12.02_263.1978	0.00	0.10	1.00	0.79
1.78_262.1278	0.00	0.00	0.87	1.00
5.86_262.1048	0.00	0.26	0.68	1.00
10.71_261.1779	0.00	0.03	1.00	0.87
5.01_261.1438	0.00	0.03	1.00	0.79
5.43_268.0192	0.00	0.06	1.00	0.52
8.32_268.0180	0.00	0.00	0.97	1.00
10.77_267.1616	0.00	0.12	1.00	0.81

D. Mass Spectral Data for Selected Features

2.47_276.1033	0.00	0.00	0.81	1.00
9.12_279.1585	0.00	0.00	1.00	0.94
7.18_278.2110	0.00	0.00	1.00	0.97
7.19_284.2219	0.00	0.00	0.95	1.00
7.50_283.1523	0.00	0.05	1.00	0.81
9.01_283.1521	0.00	0.13	0.70	1.00
1.73_282.0649	0.00	0.03	0.98	1.00
7.72_281.1420	0.00	0.00	0.95	1.00
5.22_295.1312	0.00	0.02	1.00	0.82
7.82_294.2085	0.00	0.00	1.00	0.80
6.82_294.2084	0.00	0.00	0.68	1.00
7.15_293.2251	0.00	0.00	1.00	0.96
4.87_293.1612	0.00	0.25	0.79	1.00
3.76_299.1387	0.00	0.00	1.00	0.57
4.74_298.0969	0.00	0.07	1.00	0.85
9.60_297.1694	0.00	0.01	1.00	0.84
7.19_296.2224	0.00	0.00	0.97	1.00
3.78_300.1386	0.00	0.03	1.00	0.68
12.02_309.1921	0.00	0.03	1.00	0.66
6.00_308.2238	0.00	0.00	1.00	0.97
6.06_312.2197	0.00	0.00	1.00	0.87
6.84_312.2197	0.00	0.00	0.95	1.00
7.24_312.2197	0.00	0.00	0.96	1.00
9.79_311.0549	0.00	0.00	0.75	1.00
1.74_322.0446	0.00	0.02	0.91	1.00
9.13_319.1539	0.00	0.00	1.00	0.92
6.92_318.2094	0.00	0.00	1.00	0.85
6.00_328.7423	0.00	0.09	1.00	0.56
5.91_328.5999	0.00	0.00	0.62	1.00
7.34_326.2353	0.00	0.00	1.00	0.89
6.01_326.2353	0.00	0.00	1.00	0.87
4.97_326.0999	0.00	0.27	1.00	0.90
12.03_325.1706	0.00	0.00	1.00	0.66
6.08_324.1828	0.00	0.23	0.81	1.00
6.62_334.2005	0.00	0.00	1.00	1.00
8.76_329.1942	0.00	0.09	0.92	1.00
5.84_341.1007	0.00	0.00	0.85	1.00
7.48_345.1875	0.00	0.00	0.89	1.00
7.37_344.2218	0.00	0.00	1.00	0.75
6.06_359.1205	0.00	0.00	0.58	1.00
8.24_352.2057	0.00	0.00	0.71	1.00
4.01_351.5992	0.00	0.00	0.81	1.00
6.67_362.2335	0.00	0.00	0.99	1.00
6.51_360.2165	0.00	0.00	1.00	0.75
8.53_359.2035	0.00	0.12	1.00	0.70
8.77_368.2219	0.00	0.00	1.00	0.66
6.02_368.2219	0.00	0.07	0.95	1.00
7.52_368.2211	0.00	0.00	1.00	0.73
9.80_367.0822	0.00	0.00	1.00	0.99
9.04_366.2404	0.00	0.00	1.00	0.66
5.64_366.2063	0.00	0.00	0.75	1.00
9.80_387.0731	0.00	0.00	0.98	1.00
6.88_386.2329	0.00	0.00	1.00	0.76
6.89_384.2172	0.00	0.00	0.86	1.00
6.24_384.2171	0.00	0.00	0.54	1.00
8.63_398.2317	0.00	0.00	0.97	1.00
1.49_394.1142	0.00	0.00	0.53	1.00
8.66_429.0854	0.00	0.00	0.94	1.00
9.08_429.0845	0.00	0.00	1.00	0.92
9.42_432.0873	0.00	0.00	1.00	1.00
9.07_451.0615	0.00	0.00	1.00	0.69
9.09_448.0576	0.00	0.00	1.00	0.66
6.99_443.3240	0.00	0.06	1.00	0.61
9.73_443.1014	0.00	0.00	1.00	0.99
8.33_443.0954	0.00	0.00	1.00	0.82
6.90_461.2902	0.00	0.00	0.96	1.00
5.90_459.3212	0.00	0.09	1.00	0.68
10.02_459.0960	0.00	0.00	1.00	0.76
9.03_457.1145	0.00	0.00	1.00	0.91
8.67_457.1133	0.00	0.00	1.00	0.75

D. Mass Spectral Data for Selected Features

11.52_456.3791	0.00	0.00	1.00	0.50
6.21_455.1906	0.00	0.16	0.99	1.00
9.81_454.0847	0.00	0.00	1.00	0.70
6.46_471.2466	0.00	0.01	1.00	0.67
9.02_468.1011	0.00	0.00	1.00	0.61
9.08_467.0388	0.00	0.00	1.00	0.68
9.79_462.0710	0.00	0.00	1.00	0.67
9.78_481.0499	0.00	0.00	0.57	1.00
9.02_479.0963	0.00	0.00	1.00	0.84
10.01_478.0692	0.00	0.00	1.00	0.76
4.15_476.2404	0.00	0.00	1.00	0.80
9.02_476.0877	0.00	0.00	1.00	0.78
6.98_499.2793	0.00	0.00	1.00	0.62
7.51_499.2782	0.00	0.05	0.81	1.00
9.02_495.0687	0.00	0.00	1.00	0.61
4.37_494.2617	0.00	0.00	0.98	1.00
5.37_493.1709	0.00	0.00	0.71	1.00
9.79_513.1525	0.00	0.00	1.00	0.59
9.09_512.3013	0.00	0.00	1.00	0.54
5.65_504.2609	0.00	0.00	0.83	1.00
5.64_515.2738	0.00	0.01	1.00	0.79
10.06_526.3139	0.00	0.00	1.00	0.57
7.21_526.2839	0.00	0.02	1.00	0.98
5.90_546.1391	0.00	0.00	0.76	1.00
7.20_544.2918	0.00	0.00	1.00	0.69
7.57_542.3960	0.00	0.09	1.00	0.59
9.00_540.1495	0.00	0.00	1.00	0.72
6.63_570.3104	0.00	0.00	1.00	0.84
12.03_565.3746	0.00	0.04	1.00	0.90
6.90_555.3068	0.00	0.00	1.00	0.77
5.52_601.2501	0.00	0.00	0.95	1.00
9.79_576.6021	0.00	0.00	1.00	0.56
1.25_639.8836	0.00	0.00	1.00	0.72
9.07_662.0928	0.00	0.00	1.00	0.90
9.02_704.1451	0.00	0.00	1.00	0.95
9.79_683.1204	0.00	0.00	1.00	0.66
9.06_676.1101	0.00	0.00	1.00	1.00
9.78_885.1896	0.00	0.00	1.00	0.56
7.60_846.3434	0.00	0.00	0.75	1.00
9.02_935.1961	0.00	0.00	1.00	0.55
9.80_907.1678	0.00	0.00	1.00	0.66
7.69_1031.1674	0.00	0.09	0.61	1.00
7.63_942.9948	0.00	0.00	0.57	1.00
7.01_1221.4414	0.00	0.00	1.00	0.76
9.79_218.0234	0.00	0.01	1.00	0.86
9.78_465.0808	0.00	0.01	1.00	0.81
8.74_542.3146	0.00	0.00	0.66	1.00
9.79_1349.2480	0.00	0.00	1.00	0.51
8.34_150.0928	0.00	0.07	1.00	0.93
1.64_174.0879	0.01	0.00	0.88	1.00
9.81_269.0437	0.01	0.00	0.62	1.00
6.76_310.2021	0.01	0.00	1.00	0.84
1.82_228.1004	0.01	0.00	0.88	1.00
5.66_384.2168	0.01	0.00	1.00	0.77
6.06_294.2084	0.01	0.00	0.81	1.00
1.29_203.9309	0.01	0.00	1.00	0.80
1.64_246.1172	0.01	0.00	1.00	0.94
6.24_515.2753	0.01	0.01	0.93	1.00
7.48_177.0877	0.02	0.00	0.94	1.00
8.10_301.1534	0.02	0.07	1.00	0.75
1.53_143.0837	0.03	0.03	0.93	1.00
1.75_507.1572	0.03	0.00	0.68	1.00
3.22_235.1201	0.03	0.00	1.00	0.87
16.15_710.1773	0.03	0.01	0.77	1.00
12.02_205.1953	0.04	0.00	1.00	0.79
5.43_377.1482	0.05	0.00	1.00	0.86
1.73_338.0231	0.05	0.00	0.98	1.00
7.06_325.1861	0.05	0.29	1.00	0.91
8.29_401.1993	0.05	0.00	1.00	0.92
4.37_326.1802	0.05	0.32	0.66	1.00

D. Mass Spectral Data for Selected Features

6.39_336.2172	0.05	0.04	1.00	0.91
9.66_279.1583	0.06	0.00	0.69	1.00
6.66_264.1980	0.06	0.03	0.66	1.00
3.07_230.1126	0.06	0.15	0.85	1.00
1.77_218.1042	0.06	0.02	1.00	0.83
9.67_319.1539	0.07	0.09	0.83	1.00
4.75_136.0625	0.07	0.00	1.00	0.84
8.53_283.1523	0.07	0.14	1.00	0.90
7.62_970.6124	0.07	0.10	0.54	1.00
1.74_150.0789	0.07	0.00	1.00	0.81
1.70_260.1135	0.07	0.00	1.00	0.93
6.95_218.1203	0.08	0.16	1.00	0.83
9.14_239.1284	0.10	0.09	1.00	0.62
16.24_268.0194	0.10	0.20	0.72	1.00
8.53_207.1002	0.10	0.12	0.61	1.00
3.83_292.1654	0.11	0.00	0.56	1.00
6.72_1450.6973	0.12	0.03	1.00	0.69
3.80_288.1929	0.12	0.11	0.88	1.00
3.86_150.0940	0.13	0.23	1.00	0.92
1.65_159.0768	0.13	0.00	0.83	1.00
6.95_368.2220	0.13	0.22	1.00	0.95
7.06_221.1900	0.13	0.39	1.00	0.74
8.53_177.0880	0.13	0.13	1.00	0.98
7.25_371.1508	0.13	0.00	0.58	1.00
10.52_673.3745	0.14	0.22	1.00	0.70
16.22_252.0441	0.14	0.25	0.77	1.00
7.42_280.1237	0.16	0.43	1.00	0.84
1.76_596.1679	0.16	0.00	0.74	1.00
13.77_459.1339	0.16	0.35	0.67	1.00
6.71_1160.7578	0.17	0.00	1.00	0.69
7.06_203.1787	0.17	0.33	1.00	0.91
5.97_286.6247	0.18	0.03	1.00	1.00
3.82_230.1126	0.20	0.12	0.78	1.00
6.41_165.0905	0.21	0.14	1.00	0.85
4.87_329.1844	0.22	0.00	1.00	0.97
4.31_265.0552	0.23	0.00	0.85	1.00
4.88_188.0708	0.23	0.40	0.92	1.00
9.41_281.1770	0.26	0.48	1.00	0.84
3.85_276.1433	0.26	0.15	1.00	0.83
4.30_284.1098	0.27	0.08	0.68	1.00
4.30_310.1305	0.28	0.06	0.94	1.00
4.12_413.1243	0.28	0.50	0.76	1.00
16.18_335.9929	0.28	0.00	1.00	0.67
6.06_203.1781	0.29	0.51	1.00	0.99
5.11_307.1591	0.31	0.00	0.74	1.00
4.81_464.2611	0.34	0.41	1.00	0.92
3.76_347.1589	0.38	0.00	1.00	0.78
6.78_176.0714	0.39	0.66	1.00	0.96
3.80_194.0821	0.43	0.00	0.92	1.00
4.29_244.1199	0.44	0.45	1.00	0.93
4.64_137.0376	0.44	0.45	1.00	0.86
5.61_343.2002	0.49	0.11	1.00	0.96
4.86_372.1909	0.49	0.25	1.00	0.86
12.43_386.2820	0.50	1.00	0.00	0.00
3.79_359.1699	0.51	0.25	1.00	0.93
10.60_346.3091	0.51	1.00	0.00	0.00
9.48_225.1993	0.53	1.00	0.01	0.01
6.81_807.1918	0.54	1.00	0.00	0.00
6.15_485.2027	0.55	0.59	0.86	1.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.00	0.00
10.15_739.4618	0.56	1.00	0.03	0.02
14.41_309.2409	0.56	1.00	0.00	0.09
6.27_207.0660	0.57	1.00	0.00	0.00
10.53_531.4000	0.57	1.00	0.00	0.00
12.97_407.3144	0.58	1.00	0.05	0.02
12.98_399.3242	0.58	1.00	0.05	0.02
7.42_196.0651	0.59	0.30	0.97	1.00
4.37_663.2850	0.59	1.00	0.05	0.03
13.98_433.3418	0.61	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

6.90_166.0720	0.61	1.00	0.00	0.00
4.64_412.2067	0.62	1.00	0.00	0.06
6.19_181.1351	0.63	1.00	0.03	0.00
10.97_401.2525	0.63	1.00	0.00	0.00
11.58_415.2745	0.65	1.00	0.00	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.86_507.3281	0.66	1.00	0.20	0.14
12.97_290.7254	0.66	1.00	0.31	0.16
4.27_647.2871	0.67	1.00	0.02	0.01
12.82_551.3593	0.67	1.00	0.21	0.16
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.14	0.17
12.56_441.2657	0.70	1.00	0.28	0.26
6.40_263.1761	0.70	0.75	1.00	0.89
6.85_824.9348	0.70	1.00	0.00	0.00
4.81_506.2950	0.71	1.00	0.12	0.10
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
12.79_595.3829	0.73	1.00	0.25	0.17
3.89_518.1743	0.73	1.00	0.03	0.00
12.67_727.4605	0.74	1.00	0.33	0.21
11.18_473.3585	0.75	1.00	0.02	0.00
12.70_683.4373	0.77	1.00	0.28	0.21
12.86_463.2998	0.77	1.00	0.07	0.18
12.74_443.3505	0.77	1.00	0.00	0.00
12.97_547.4060	0.77	1.00	0.00	0.04
13.86_425.2896	0.78	1.00	0.27	0.23
1.50_401.0693	0.79	0.73	0.95	1.00
5.26_147.0936	0.79	1.00	0.29	0.30
3.75_267.1417	0.80	1.00	0.58	0.43
12.61_771.4862	0.80	1.00	0.32	0.24
11.97_299.2600	0.80	1.00	0.00	0.00
15.06_413.2647	0.81	1.00	0.27	0.26
12.86_502.3745	0.82	1.00	0.18	0.12
11.84_443.3878	0.82	1.00	0.09	0.04
11.03_354.1608	0.82	1.00	0.05	0.05
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.00
12.73_655.3845	0.83	1.00	0.00	0.22
12.74_639.4067	0.83	1.00	0.31	0.22
13.79_365.2675	0.84	1.00	0.00	0.00
12.80_567.3292	0.85	1.00	0.30	0.19
12.83_546.4021	0.86	1.00	0.19	0.13
10.38_401.3397	0.88	1.00	0.24	0.16
9.26_219.1735	0.88	1.00	0.00	0.00
12.67_743.4367	0.88	1.00	0.37	0.24
4.50_359.1197	0.89	1.00	0.63	0.50
12.70_699.4109	0.89	1.00	0.20	0.00
5.43_241.1546	0.91	0.93	0.98	1.00
12.78_611.3565	0.91	1.00	0.33	0.07
15.94_338.3442	0.91	1.00	0.41	0.39
13.49_295.2258	0.91	1.00	0.04	0.02
12.73_320.2010	0.94	1.00	0.00	0.20
1.48_481.1031	0.96	1.00	0.88	0.83
4.49_225.1597	0.97	1.00	0.45	0.40
12.89_441.3208	0.99	1.00	0.15	0.13
12.78_590.4295	1.00	1.00	0.20	0.14
13.95_270.2746	1.00	1.00	0.35	0.33
3.99_164.0936	1.00	0.90	0.63	0.69
10.36_211.6353	1.00	0.89	0.25	0.00
3.82_209.1275	1.00	0.90	0.51	0.39
11.31_225.6512	1.00	0.95	0.00	0.00
9.27_240.2315	1.00	0.88	0.16	0.16
10.39_268.2627	1.00	0.83	0.00	0.03
6.59_273.1670	1.00	0.84	0.66	0.53
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.01	0.00
14.31_325.2414	1.00	0.74	0.00	0.00

D. Mass Spectral Data for Selected Features

14.82_332.2940	1.00	0.65	0.16	0.00
15.49_338.3442	1.00	0.86	0.00	0.06
4.26_356.1796	1.00	0.84	0.59	0.52
15.92_360.3229	1.00	0.71	0.32	0.13
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.22	0.15
13.95_411.3586	1.00	0.78	0.00	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.18	0.00
12.86_485.3471	1.00	0.86	0.13	0.09
12.86_523.3040	1.00	0.66	0.25	0.24
12.81_529.3766	1.00	0.77	0.13	0.12
12.97_555.3910	1.00	0.94	0.00	0.12
12.79_573.4039	1.00	0.73	0.11	0.15
12.75_617.4294	1.00	0.84	0.16	0.15
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.00
12.67_705.4810	1.00	0.93	0.25	0.15
6.87_807.0837	1.00	0.57	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S13. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R4 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_ m/z)	WT	WT	R4	R4
1.51_137.5554	0.00	0.00	1.00	0.52
1.52_129.5659	0.00	0.00	1.00	0.52
1.50_103.5345	0.00	0.00	0.50	1.00
13.61_149.0907	0.00	0.00	1.00	0.75
6.56_162.0938	0.00	0.00	0.80	1.00
4.31_160.1140	0.00	0.00	0.67	1.00
5.78_170.1204	0.00	0.00	0.64	1.00
6.60_180.1017	0.00	0.03	0.58	1.00
5.02_180.1014	0.00	0.00	0.58	1.00
9.12_191.0134	0.00	0.00	0.60	1.00
4.14_186.1168	0.00	0.00	0.93	1.00
9.08_196.0187	0.00	0.00	0.79	1.00
8.68_204.0325	0.00	0.00	0.72	1.00
9.08_203.0278	0.00	0.00	0.76	1.00
9.42_202.0393	0.00	0.00	0.68	1.00
1.42_201.0074	0.00	0.00	0.79	1.00
4.35_209.0956	0.00	0.00	0.51	1.00
4.54_208.1355	0.00	0.00	0.90	1.00
5.44_208.0539	0.00	0.00	0.78	1.00
7.49_207.0994	0.00	0.11	0.55	1.00
1.30_205.9283	0.00	0.00	0.53	1.00
4.84_205.1323	0.00	0.00	0.86	1.00
8.67_212.0251	0.00	0.00	0.63	1.00
1.49_211.0584	0.00	0.19	0.65	1.00
9.25_211.0284	0.00	0.01	1.00	0.92
8.31_210.0369	0.00	0.00	0.81	1.00
9.81_210.0363	0.00	0.00	1.00	0.66
9.07_210.0305	0.00	0.00	0.77	1.00
9.41_219.0312	0.00	0.00	1.00	0.86
8.67_218.0490	0.00	0.00	0.82	1.00
9.03_217.0413	0.00	0.00	0.70	1.00
2.51_216.0981	0.00	0.02	0.49	1.00
16.16_223.9875	0.00	0.00	0.90	1.00
6.51_220.1710	0.00	0.04	1.00	0.99
4.58_226.1445	0.00	0.00	1.00	0.82
5.11_226.1427	0.00	0.02	0.53	1.00
8.67_226.0395	0.00	0.00	0.61	1.00
9.04_225.0298	0.00	0.01	0.74	1.00
9.77_224.0325	0.00	0.00	0.63	1.00
5.11_227.1386	0.00	0.00	0.56	1.00
9.19_230.0719	0.00	0.00	1.00	0.54
9.82_230.0718	0.00	0.03	0.91	1.00
8.41_230.0715	0.00	0.00	0.96	1.00
10.62_236.1643	0.00	0.00	1.00	0.76
5.11_236.1306	0.00	0.18	0.96	1.00
4.89_235.1441	0.00	0.00	0.93	1.00
8.54_235.1344	0.00	0.00	0.60	1.00
9.80_241.0261	0.00	0.00	1.00	0.78
8.82_241.0249	0.00	0.00	1.00	0.94
4.13_237.1268	0.00	0.35	1.00	0.96
5.81_248.1281	0.00	0.35	1.00	0.99
9.03_248.0351	0.00	0.00	0.80	1.00
4.04_247.1287	0.00	0.00	0.50	1.00
9.07_246.5440	0.00	0.00	0.71	1.00
5.63_245.1880	0.00	0.00	1.00	0.83
5.04_244.1219	0.00	0.00	0.85	1.00
4.70_243.1326	0.00	0.00	0.55	1.00

D. Mass Spectral Data for Selected Features

8.52_250.0297	0.00	0.00	0.76	1.00
4.31_249.0807	0.00	0.00	0.72	1.00
8.08_252.0397	0.00	0.00	1.00	0.84
4.56_252.0394	0.00	0.16	1.00	0.63
8.66_252.0394	0.00	0.00	1.00	0.58
6.82_252.0384	0.00	0.00	0.83	1.00
6.23_258.1449	0.00	0.00	1.00	0.75
9.81_253.5524	0.00	0.02	0.91	1.00
1.78_262.1278	0.00	0.00	0.75	1.00
5.86_262.1048	0.00	0.41	0.85	1.00
9.91_261.5430	0.00	0.00	1.00	0.65
5.01_261.1438	0.00	0.08	0.80	1.00
9.03_260.5527	0.00	0.00	0.72	1.00
8.32_268.0180	0.00	0.00	1.00	0.55
10.77_267.1616	0.00	0.02	1.00	1.00
5.27_264.2082	0.00	0.00	0.79	1.00
9.67_268.0195	0.00	0.00	1.00	0.94
2.47_276.1033	0.00	0.00	0.83	1.00
9.12_279.1585	0.00	0.00	0.56	1.00
7.18_278.2110	0.00	0.00	0.62	1.00
6.07_276.1943	0.00	0.00	0.57	1.00
5.71_286.2118	0.00	0.00	0.84	1.00
7.19_284.2219	0.00	0.00	0.63	1.00
12.79_284.1681	0.00	0.22	1.00	0.68
7.50_283.1523	0.00	0.06	0.78	1.00
1.73_282.0649	0.00	0.03	0.61	1.00
5.22_295.1312	0.00	0.05	0.70	1.00
7.48_294.2085	0.00	0.00	1.00	0.58
7.82_294.2085	0.00	0.00	0.56	1.00
6.82_294.2084	0.00	0.00	0.63	1.00
7.15_293.2251	0.00	0.00	0.92	1.00
4.87_293.1612	0.00	0.39	1.00	0.83
6.49_292.1923	0.00	0.01	0.80	1.00
3.76_299.1387	0.00	0.08	0.64	1.00
7.73_298.2024	0.00	0.00	0.60	1.00
4.74_298.0969	0.00	0.05	0.68	1.00
9.60_297.1694	0.00	0.01	0.61	1.00
7.19_296.2224	0.00	0.00	0.58	1.00
6.00_308.2238	0.00	0.00	0.64	1.00
6.92_313.1550	0.00	0.00	0.55	1.00
6.06_312.2197	0.00	0.00	0.84	1.00
6.84_312.2197	0.00	0.00	0.52	1.00
7.24_312.2197	0.00	0.00	0.62	1.00
10.59_311.1859	0.00	0.00	0.65	1.00
9.79_311.0549	0.00	0.00	0.57	1.00
7.47_310.2026	0.00	0.00	1.00	0.56
5.82_322.1007	0.00	0.00	0.89	1.00
1.74_322.0446	0.00	0.03	0.90	1.00
3.86_320.0995	0.00	0.00	0.64	1.00
9.13_319.1539	0.00	0.00	0.60	1.00
6.92_318.2094	0.00	0.00	0.76	1.00
5.91_328.5999	0.00	0.00	0.65	1.00
7.34_326.2353	0.00	0.00	0.58	1.00
6.01_326.2353	0.00	0.00	0.79	1.00
4.97_326.0999	0.00	0.23	0.83	1.00
6.08_324.1828	0.00	0.09	0.64	1.00
6.31_335.7452	0.00	0.00	1.00	0.52
6.62_334.2005	0.00	0.00	0.50	1.00
5.84_341.1007	0.00	0.00	0.59	1.00
5.99_338.1374	0.00	0.00	1.00	0.77
6.22_346.2031	0.00	0.00	1.00	0.86
7.48_345.1875	0.00	0.00	0.84	1.00
7.37_344.2218	0.00	0.00	0.66	1.00
5.26_354.0787	0.00	0.32	1.00	0.94
8.24_352.2057	0.00	0.00	0.54	1.00

D. Mass Spectral Data for Selected Features

6.67_362.2335	0.00	0.00	1.00	0.86
6.51_360.2165	0.00	0.00	1.00	0.81
8.53_359.2035	0.00	0.11	0.90	1.00
8.77_368.2219	0.00	0.00	0.73	1.00
6.02_368.2219	0.00	0.04	0.72	1.00
7.52_368.2211	0.00	0.00	0.90	1.00
9.80_367.0822	0.00	0.00	0.66	1.00
5.64_366.2063	0.00	0.00	0.71	1.00
8.47_382.2398	0.00	0.00	0.89	1.00
7.30_389.1593	0.00	0.00	1.00	0.89
9.80_387.0731	0.00	0.00	0.56	1.00
6.88_386.2329	0.00	0.00	0.66	1.00
6.24_384.2171	0.00	0.00	0.70	1.00
8.63_398.2317	0.00	0.00	0.65	1.00
1.49_394.1142	0.00	0.00	0.61	1.00
9.40_418.0851	0.00	0.00	0.59	1.00
8.66_429.0854	0.00	0.00	0.56	1.00
9.08_429.0845	0.00	0.00	0.57	1.00
4.02_423.1940	0.00	0.00	0.61	1.00
9.15_440.0708	0.00	0.00	0.59	1.00
9.42_432.0873	0.00	0.00	0.65	1.00
1.48_431.0890	0.00	0.41	0.98	1.00
9.09_448.0576	0.00	0.00	0.61	1.00
9.73_443.1014	0.00	0.00	0.82	1.00
8.33_443.0954	0.00	0.00	0.93	1.00
8.80_443.0945	0.00	0.00	0.61	1.00
6.90_461.2902	0.00	0.00	0.90	1.00
10.02_459.0960	0.00	0.00	0.58	1.00
9.03_457.1145	0.00	0.00	0.60	1.00
8.67_457.1133	0.00	0.00	0.66	1.00
6.21_455.1906	0.00	0.16	0.86	1.00
9.81_454.0847	0.00	0.00	0.78	1.00
9.05_454.0819	0.00	0.00	0.57	1.00
6.42_472.2832	0.00	0.00	0.75	1.00
6.46_471.2466	0.00	0.01	0.64	1.00
10.02_470.0758	0.00	0.00	0.62	1.00
9.02_468.1011	0.00	0.00	0.58	1.00
9.08_467.0388	0.00	0.00	0.79	1.00
8.31_465.0807	0.00	0.00	0.70	1.00
8.82_465.0807	0.00	0.00	0.67	1.00
9.79_462.0710	0.00	0.00	0.72	1.00
9.04_462.0699	0.00	0.00	0.61	1.00
7.03_483.0939	0.00	0.00	0.72	1.00
9.78_481.0499	0.00	0.00	1.00	0.75
9.02_479.0963	0.00	0.00	0.62	1.00
10.01_478.0692	0.00	0.00	0.53	1.00
4.15_476.2404	0.00	0.00	0.56	1.00
9.02_476.0877	0.00	0.00	0.55	1.00
7.06_475.1057	0.00	0.00	0.61	1.00
9.02_495.0687	0.00	0.00	0.70	1.00
4.37_494.2617	0.00	0.00	0.68	1.00
5.37_493.1709	0.00	0.00	1.00	0.69
9.79_513.1525	0.00	0.00	0.48	1.00
5.64_515.2738	0.00	0.01	0.65	1.00
1.76_515.1445	0.00	0.00	0.74	1.00
10.06_526.3139	0.00	0.00	1.00	0.54
7.21_526.2839	0.00	0.06	0.58	1.00
7.20_544.2918	0.00	0.00	0.61	1.00
9.00_540.1495	0.00	0.00	0.63	1.00
6.63_570.3104	0.00	0.00	0.91	1.00
9.67_563.3802	0.00	0.00	0.59	1.00
9.08_562.5875	0.00	0.00	0.62	1.00
7.14_560.1805	0.00	0.00	0.64	1.00
6.90_555.3068	0.00	0.00	0.53	1.00
1.72_551.1035	0.00	0.00	0.96	1.00

D. Mass Spectral Data for Selected Features

5.52_601.2501	0.00	0.00	0.73	1.00
9.02_590.6205	0.00	0.00	0.63	1.00
9.79_576.6021	0.00	0.00	1.00	0.60
9.06_576.6005	0.00	0.00	0.60	1.00
1.25_639.8836	0.00	0.00	0.63	1.00
9.07_662.0928	0.00	0.00	0.48	1.00
9.02_704.1451	0.00	0.00	0.54	1.00
9.03_696.1548	0.00	0.00	0.49	1.00
9.71_694.1152	0.00	0.00	0.66	1.00
9.03_690.1259	0.00	0.00	0.54	1.00
9.79_683.1204	0.00	0.00	1.00	0.68
9.06_676.1101	0.00	0.00	0.53	1.00
9.41_675.1324	0.00	0.00	0.54	1.00
9.78_885.1896	0.00	0.00	0.47	1.00
9.07_879.1306	0.00	0.00	0.69	1.00
7.69_868.6024	0.00	0.00	1.00	0.57
9.02_935.1961	0.00	0.00	0.53	1.00
7.21_916.0943	0.00	0.00	1.00	0.78
9.80_907.1678	0.00	0.00	0.82	1.00
9.04_907.1662	0.00	0.00	0.51	1.00
9.41_904.1590	0.00	0.00	0.53	1.00
7.67_1031.2480	0.00	0.14	0.97	1.00
7.69_1031.1674	0.00	0.10	1.00	0.91
7.67_1031.0798	0.00	0.00	0.91	1.00
7.69_1000.1273	0.00	0.00	0.49	1.00
7.65_1000.0444	0.00	0.00	0.92	1.00
7.63_942.9948	0.00	0.00	1.00	0.90
7.01_1221.4414	0.00	0.00	0.55	1.00
9.41_1125.2062	0.00	0.00	0.48	1.00
9.78_465.0808	0.00	0.00	0.87	1.00
9.79_1349.2480	0.00	0.00	0.51	1.00
6.06_294.2084	0.00	0.00	0.59	1.00
9.81_269.0437	0.00	0.00	0.61	1.00
8.34_150.0928	0.00	0.07	0.56	1.00
6.65_282.2073	0.01	0.04	0.76	1.00
6.76_310.2021	0.01	0.00	1.00	0.90
8.74_542.3146	0.01	0.00	1.00	0.73
1.75_507.1572	0.01	0.00	0.69	1.00
1.29_203.9309	0.01	0.00	0.50	1.00
5.66_384.2168	0.01	0.00	0.71	1.00
1.64_246.1172	0.02	0.00	0.74	1.00
7.48_177.0877	0.02	0.00	0.60	1.00
1.64_174.0879	0.02	0.01	1.00	0.56
6.66_264.1980	0.03	0.01	0.63	1.00
8.10_301.1534	0.03	0.11	0.90	1.00
5.43_377.1482	0.03	0.00	0.68	1.00
16.15_710.1773	0.04	0.01	0.70	1.00
9.14_239.1284	0.04	0.04	0.59	1.00
6.24_515.2753	0.04	0.02	0.84	1.00
9.66_279.1583	0.05	0.00	0.65	1.00
9.67_319.1539	0.05	0.06	0.64	1.00
1.74_150.0789	0.05	0.00	0.59	1.00
3.22_235.1201	0.05	0.00	1.00	0.67
6.95_368.2220	0.05	0.09	1.00	0.59
8.53_283.1523	0.05	0.12	0.85	1.00
8.29_401.1993	0.06	0.00	0.56	1.00
3.07_230.1126	0.06	0.14	0.82	1.00
4.75_136.0625	0.06	0.00	0.78	1.00
1.73_338.0231	0.06	0.00	0.84	1.00
1.70_260.1135	0.08	0.00	0.75	1.00
8.53_207.1002	0.09	0.11	0.81	1.00
6.95_218.1203	0.09	0.18	0.63	1.00
8.53_177.0880	0.09	0.09	0.84	1.00
7.25_371.1508	0.09	0.00	0.67	1.00
9.41_281.1770	0.10	0.19	0.65	1.00

D. Mass Spectral Data for Selected Features

10.52_673.3745	0.12	0.19	0.63	1.00
10.18_621.4210	0.13	0.00	0.59	1.00
3.86_150.0940	0.14	0.25	0.68	1.00
3.83_198.1623	0.14	0.10	0.57	1.00
1.77_218.1042	0.14	0.03	0.70	1.00
3.80_288.1929	0.15	0.13	1.00	0.77
6.41_165.0905	0.17	0.11	0.78	1.00
3.86_338.1113	0.19	0.00	0.65	1.00
4.31_265.0552	0.19	0.00	0.80	1.00
1.65_159.0768	0.21	0.00	1.00	0.65
1.73_288.1454	0.21	0.00	0.85	1.00
5.97_286.6247	0.22	0.04	1.00	0.66
4.30_478.1379	0.22	0.05	0.76	1.00
3.85_276.1433	0.22	0.13	0.58	1.00
4.87_329.1844	0.23	0.00	0.80	1.00
7.91_389.2523	0.23	0.10	0.63	1.00
7.89_192.1015	0.23	0.40	0.74	1.00
6.72_1450.6973	0.25	0.06	0.68	1.00
3.76_347.1589	0.28	0.00	0.76	1.00
16.18_335.9929	0.29	0.00	0.69	1.00
1.60_229.1318	0.29	0.06	0.78	1.00
4.30_310.1305	0.29	0.06	0.71	1.00
5.97_278.6345	0.30	0.08	1.00	0.95
9.11_505.3321	0.33	0.00	0.70	1.00
9.47_211.0868	0.34	0.59	1.00	0.98
3.82_230.1126	0.34	0.22	1.00	0.80
4.00_320.1711	0.43	0.05	0.99	1.00
5.11_307.1591	0.44	0.00	1.00	0.92
4.81_464.2611	0.44	0.52	1.00	0.80
4.86_372.1909	0.49	0.25	0.81	1.00
10.60_346.3091	0.51	1.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.00	0.00
10.70_288.2557	0.52	1.00	0.00	0.00
4.64_137.0376	0.53	0.55	0.84	1.00
9.48_225.1993	0.53	1.00	0.01	0.02
7.06_203.1787	0.53	1.00	0.01	0.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.00	0.04
10.15_739.4618	0.56	1.00	0.06	0.05
14.41_309.2409	0.56	1.00	0.14	0.13
10.53_531.4000	0.57	1.00	0.00	0.00
12.97_407.3144	0.58	1.00	0.20	0.09
12.98_399.3242	0.58	1.00	0.19	0.09
4.09_573.1785	0.58	1.00	0.00	0.00
4.37_663.2850	0.59	1.00	0.01	0.00
5.45_144.0814	0.60	1.00	0.13	0.21
13.98_433.3418	0.61	1.00	0.02	0.01
4.64_412.2067	0.62	1.00	0.08	0.10
6.19_181.1351	0.63	1.00	0.09	0.11
10.97_401.2525	0.63	1.00	0.00	0.00
11.58_415.2745	0.65	1.00	0.00	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.86_507.3281	0.66	1.00	0.37	0.22
4.27_647.2871	0.67	1.00	0.00	0.01
12.82_551.3593	0.67	1.00	0.38	0.32
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.00	0.00
12.56_441.2657	0.70	1.00	0.24	0.35
6.85_824.9348	0.70	1.00	0.00	0.00
4.81_506.2950	0.71	1.00	0.24	0.26
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
12.79_595.3829	0.73	1.00	0.46	0.37
12.67_727.4605	0.74	1.00	0.22	0.33

D. Mass Spectral Data for Selected Features

11.18_473.3585	0.75	1.00	0.04	0.01
4.34_266.1408	0.75	0.59	0.98	1.00
12.70_683.4373	0.77	1.00	0.48	0.36
12.86_463.2998	0.77	1.00	0.48	0.31
12.74_443.3505	0.77	1.00	0.00	0.00
12.97_547.4060	0.77	1.00	0.38	0.19
13.86_425.2896	0.78	1.00	0.30	0.28
5.26_147.0936	0.79	1.00	0.25	0.37
12.61_771.4862	0.80	1.00	0.47	0.38
11.97_299.2600	0.80	1.00	0.00	0.00
12.86_502.3745	0.82	1.00	0.34	0.33
11.84_443.3878	0.82	1.00	0.09	0.05
11.03_354.1608	0.82	1.00	0.00	0.04
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.14	0.03
12.73_655.3845	0.83	1.00	0.56	0.44
12.74_639.4067	0.83	1.00	0.51	0.39
13.79_365.2675	0.84	1.00	0.05	0.00
12.80_567.3292	0.85	1.00	0.55	0.36
12.83_546.4021	0.86	1.00	0.00	0.24
5.16_237.1592	0.87	1.00	0.21	0.29
10.38_401.3397	0.88	1.00	0.50	0.32
9.26_219.1735	0.88	1.00	0.00	0.00
12.67_743.4367	0.88	1.00	0.54	0.53
4.50_359.1197	0.89	1.00	0.00	0.00
14.79_310.3109	0.90	1.00	0.51	0.53
12.78_611.3565	0.91	1.00	0.63	0.53
15.94_338.3442	0.91	1.00	0.32	0.34
13.49_295.2258	0.91	1.00	0.08	0.03
1.47_508.0657	0.91	1.00	0.60	0.39
1.50_260.0296	0.92	1.00	0.58	0.26
1.47_748.1127	0.94	1.00	0.76	0.59
4.29_244.1199	0.97	1.00	0.42	0.49
4.49_225.1597	0.97	1.00	0.49	0.50
12.89_441.3208	0.99	1.00	0.40	0.25
12.78_590.4295	1.00	1.00	0.40	0.33
13.95_270.2746	1.00	1.00	0.31	0.41
3.99_164.0936	1.00	0.90	0.41	0.45
10.36_211.6353	1.00	0.89	0.60	0.50
11.31_225.6512	1.00	0.95	0.26	0.18
9.27_240.2315	1.00	0.88	0.00	0.11
4.59_251.1399	1.00	0.99	0.81	0.84
10.39_268.2627	1.00	0.83	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00
14.31_325.2414	1.00	0.74	0.00	0.00
14.82_332.2940	1.00	0.65	0.00	0.20
4.25_343.1235	1.00	0.70	0.01	0.00
15.49_338.3442	1.00	0.86	0.00	0.03
4.42_351.1212	1.00	0.79	0.09	0.14
4.39_362.1069	1.00	0.88	0.00	0.08
15.92_360.3229	1.00	0.71	0.22	0.13
13.48_397.3392	1.00	0.75	0.00	0.01
10.78_415.3581	1.00	0.61	0.36	0.19
13.95_411.3586	1.00	0.78	0.00	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
12.86_485.3471	1.00	0.86	0.31	0.23
1.45_519.0543	1.00	0.72	0.41	0.18
12.81_529.3766	1.00	0.77	0.31	0.19
12.97_555.3910	1.00	0.94	0.56	0.33
12.79_573.4039	1.00	0.73	0.29	0.21
12.75_617.4294	1.00	0.84	0.00	0.25
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.00

D. Mass Spectral Data for Selected Features

12.67_705.4810	1.00	0.93	0.15	0.26
6.87_807.0837	1.00	0.57	0.08	0.00

D. Mass Spectral Data for Selected Features

Table S14. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R5 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT _m/z)	WT	WT	R5	R5
12.03_135.1163	0.00	0.07	1.00	0.65
12.03_123.1165	0.00	0.00	1.00	0.99
1.50_103.5345	0.00	0.00	1.00	0.70
6.56_162.0938	0.00	0.00	1.00	0.88
16.16_174.0876	0.00	0.00	0.70	1.00
5.78_170.1204	0.00	0.00	1.00	0.77
7.08_169.0882	0.00	0.02	1.00	0.84
6.60_180.1017	0.00	0.01	0.84	1.00
5.02_180.1014	0.00	0.00	1.00	0.74
4.95_177.1399	0.00	0.21	0.98	1.00
4.39_192.1130	0.00	0.14	1.00	0.80
9.12_191.0134	0.00	0.00	0.93	1.00
4.14_186.1168	0.00	0.00	1.00	0.54
9.08_196.0187	0.00	0.00	1.00	0.74
8.84_203.1804	0.00	0.00	1.00	0.91
8.12_203.1781	0.00	0.00	0.96	1.00
9.08_203.0278	0.00	0.00	0.99	1.00
9.80_203.0277	0.00	0.00	1.00	0.84
9.42_202.0393	0.00	0.00	1.00	0.83
5.44_208.0539	0.00	0.01	0.66	1.00
7.49_207.0994	0.00	0.05	1.00	0.74
1.30_205.9283	0.00	0.00	1.00	0.91
4.84_205.1323	0.00	0.00	1.00	0.96
1.32_211.8786	0.00	0.00	0.81	1.00
1.49_211.0584	0.00	0.15	0.98	1.00
9.81_210.0363	0.00	0.00	1.00	0.85
9.07_210.0305	0.00	0.00	1.00	0.67
9.41_219.0312	0.00	0.00	0.67	1.00
3.69_218.1136	0.00	0.32	1.00	0.78
8.84_221.1903	0.00	0.00	1.00	0.98
7.35_225.1140	0.00	0.00	0.67	1.00
7.99_225.1125	0.00	0.03	1.00	0.60
7.49_230.0712	0.00	0.00	0.82	1.00
5.48_229.0656	0.00	0.00	1.00	0.91
9.82_230.0718	0.00	0.09	1.00	0.74
5.11_236.1306	0.00	0.13	1.00	0.67
4.89_235.1441	0.00	0.00	1.00	0.71
8.54_235.1344	0.00	0.00	0.83	1.00
4.13_237.1268	0.00	0.17	1.00	0.82
7.33_247.0943	0.00	0.25	1.00	0.90
5.04_244.1219	0.00	0.00	1.00	0.62
4.31_249.0807	0.00	0.00	0.96	1.00
8.08_252.0397	0.00	0.00	1.00	0.86
4.56_252.0394	0.00	0.21	0.86	1.00
6.01_252.0391	0.00	0.00	1.00	0.87
5.12_252.0389	0.00	0.00	0.90	1.00
7.48_252.0388	0.00	0.00	1.00	0.91
6.23_258.1449	0.00	0.00	1.00	0.57
12.02_263.1978	0.00	0.03	1.00	0.93
1.78_262.1278	0.00	0.00	0.63	1.00
5.86_262.1048	0.00	0.17	1.00	0.77
5.01_261.1438	0.00	0.03	0.85	1.00
7.18_278.2110	0.00	0.00	1.00	0.75
6.07_276.1943	0.00	0.00	0.85	1.00
7.50_283.1523	0.00	0.03	0.83	1.00
7.72_281.1420	0.00	0.00	0.90	1.00
5.22_295.1312	0.00	0.01	0.56	1.00
7.48_294.2085	0.00	0.00	0.58	1.00
7.82_294.2085	0.00	0.00	1.00	1.00
1.50_294.0959	0.00	0.44	1.00	0.85
7.15_293.2251	0.00	0.00	1.00	0.51
4.87_293.1612	0.00	0.19	0.73	1.00
7.73_298.2024	0.00	0.00	0.75	1.00
7.19_296.2224	0.00	0.00	1.00	0.93

D. Mass Spectral Data for Selected Features

5.83_303.1558	0.00	0.01	1.00	0.88
7.70_303.1206	0.00	0.09	1.00	0.65
3.78_300.1386	0.00	0.03	1.00	0.51
12.02_309.1921	0.00	0.01	0.89	1.00
6.00_308.2238	0.00	0.00	1.00	0.86
6.84_312.2197	0.00	0.00	1.00	0.97
7.24_312.2197	0.00	0.00	1.00	0.93
7.47_310.2026	0.00	0.00	0.99	1.00
1.74_322.0446	0.00	0.03	0.56	1.00
6.92_318.2094	0.00	0.00	0.58	1.00
7.34_326.2353	0.00	0.00	0.84	1.00
6.01_326.2353	0.00	0.00	0.99	1.00
12.03_325.1706	0.00	0.00	1.00	0.93
6.08_324.1828	0.00	0.31	0.99	1.00
5.99_338.1374	0.00	0.00	0.92	1.00
6.07_337.1394	0.00	0.03	0.55	1.00
10.06_348.2310	0.00	0.00	0.79	1.00
5.19_344.6196	0.00	0.23	0.89	1.00
6.06_359.1205	0.00	0.00	0.98	1.00
5.26_354.0787	0.00	0.13	0.78	1.00
8.24_352.2057	0.00	0.00	0.92	1.00
4.01_351.5992	0.00	0.00	0.64	1.00
6.51_360.2165	0.00	0.00	0.56	1.00
8.77_368.2219	0.00	0.00	0.60	1.00
7.52_368.2211	0.00	0.00	1.00	0.74
7.83_387.1861	0.00	0.00	1.00	0.55
6.88_386.2329	0.00	0.02	0.60	1.00
6.89_384.2172	0.00	0.01	1.00	0.84
6.24_384.2171	0.00	0.00	1.00	0.64
1.49_394.1142	0.00	0.00	1.00	0.99
3.74_416.1928	0.00	0.01	1.00	0.70
3.75_414.2692	0.00	0.00	1.00	0.76
8.66_429.0854	0.00	0.00	0.93	1.00
9.08_429.0845	0.00	0.00	0.52	1.00
9.07_451.0615	0.00	0.00	1.00	0.76
9.09_448.0576	0.00	0.00	1.00	0.77
9.73_443.1014	0.00	0.00	0.77	1.00
8.33_443.0954	0.00	0.00	0.81	1.00
5.90_459.3212	0.00	0.02	0.69	1.00
9.03_457.1145	0.00	0.01	0.76	1.00
8.67_457.1133	0.00	0.00	1.00	0.97
11.52_456.3791	0.00	0.00	0.86	1.00
6.21_455.1906	0.00	0.11	1.00	0.75
9.81_454.0847	0.00	0.00	0.67	1.00
9.05_454.0819	0.00	0.00	0.79	1.00
6.42_472.2832	0.00	0.00	1.00	0.67
9.08_467.0388	0.00	0.00	0.94	1.00
8.82_465.0807	0.00	0.00	1.00	0.90
9.79_462.0710	0.00	0.00	0.79	1.00
9.04_462.0699	0.00	0.00	1.00	0.86
9.78_481.0499	0.00	0.00	1.00	1.00
4.15_476.2404	0.00	0.00	1.00	0.57
7.51_499.2782	0.00	0.02	0.93	1.00
5.37_493.1709	0.00	0.00	1.00	0.81
6.65_512.8485	0.00	0.00	1.00	0.82
5.65_504.2609	0.00	0.00	1.00	0.90
5.64_515.2738	0.00	0.03	1.00	1.00
1.76_515.1445	0.00	0.00	1.00	0.96
10.06_526.3139	0.00	0.00	0.60	1.00
7.21_526.2839	0.00	0.06	1.00	0.82
6.79_549.3505	0.00	0.00	1.00	0.52
7.20_544.2918	0.00	0.00	0.56	1.00
7.57_542.3960	0.00	0.01	1.00	0.67
6.63_570.3104	0.00	0.00	1.00	0.87
12.03_565.3746	0.00	0.00	1.00	0.87
9.67_563.3802	0.00	0.00	1.00	0.88
6.90_555.3068	0.00	0.00	0.84	1.00
5.52_601.2501	0.00	0.00	1.00	0.77
9.79_576.6021	0.00	0.00	0.51	1.00
9.06_576.6005	0.00	0.00	0.51	1.00

D. Mass Spectral Data for Selected Features

1.25_639.8836	0.00	0.00	1.00	0.75
6.02_637.3187	0.00	0.00	1.00	0.97
5.79_646.1977	0.00	0.00	0.82	1.00
9.79_683.1204	0.00	0.00	0.81	1.00
9.80_907.1678	0.00	0.00	0.84	1.00
7.01_1221.4414	0.00	0.00	0.65	1.00
7.00_1216.1209	0.00	0.37	0.79	1.00
9.79_218.0234	0.00	0.02	0.98	1.00
8.34_150.0928	0.00	0.04	0.66	1.00
9.78_465.0808	0.00	0.01	1.00	0.94
6.76_310.2021	0.01	0.00	1.00	0.98
7.48_177.0877	0.01	0.00	1.00	0.72
8.10_301.1534	0.01	0.03	1.00	0.87
1.75_507.1572	0.01	0.00	0.61	1.00
1.82_228.1004	0.01	0.00	0.88	1.00
6.06_294.2084	0.02	0.00	1.00	0.70
6.24_515.2753	0.02	0.01	0.83	1.00
8.74_542.3146	0.02	0.00	0.73	1.00
7.06_325.1861	0.02	0.14	1.00	0.86
6.65_282.2073	0.03	0.15	1.00	0.69
5.43_377.1482	0.03	0.00	1.00	0.87
8.29_401.1993	0.03	0.00	0.83	1.00
1.64_174.0879	0.03	0.02	0.97	1.00
4.75_136.0625	0.03	0.00	1.00	0.69
9.66_279.1583	0.04	0.00	1.00	0.61
1.53_143.0837	0.04	0.05	1.00	0.81
5.66_384.2168	0.04	0.00	1.00	0.86
6.95_218.1203	0.04	0.09	0.92	1.00
3.22_235.1201	0.05	0.00	1.00	0.97
1.73_338.0231	0.05	0.00	1.00	0.76
7.06_221.1900	0.06	0.17	0.71	1.00
7.42_280.1237	0.06	0.16	0.65	1.00
8.53_283.1523	0.06	0.13	0.91	1.00
3.86_150.0940	0.06	0.11	1.00	0.97
6.66_264.1980	0.06	0.03	1.00	0.75
8.53_177.0880	0.06	0.06	1.00	0.58
7.80_291.1290	0.06	0.23	1.00	0.93
10.52_673.3745	0.07	0.10	0.94	1.00
8.53_207.1002	0.07	0.08	1.00	0.70
3.75_289.1389	0.07	0.31	1.00	0.93
9.67_319.1539	0.07	0.10	0.74	1.00
1.77_218.1042	0.07	0.02	1.00	0.92
3.83_198.1623	0.08	0.06	0.84	1.00
4.88_188.0708	0.08	0.14	1.00	0.91
7.06_203.1787	0.08	0.15	1.00	0.89
4.37_326.1802	0.08	0.50	1.00	0.91
6.72_1450.6973	0.09	0.02	1.00	0.94
6.06_203.1781	0.10	0.18	1.00	0.98
4.30_310.1305	0.11	0.02	1.00	0.55
4.87_329.1844	0.12	0.00	1.00	0.85
6.41_165.0905	0.14	0.09	1.00	0.83
9.47_211.0868	0.15	0.25	1.00	0.91
9.14_239.1284	0.16	0.15	1.00	0.77
5.27_685.1761	0.17	0.00	1.00	0.82
5.83_325.1311	0.17	0.00	1.00	0.98
4.26_450.2439	0.19	0.01	0.78	1.00
1.65_159.0768	0.19	0.00	0.78	1.00
7.89_192.1015	0.20	0.35	1.00	0.96
16.18_335.9929	0.22	0.00	0.93	1.00
4.30_284.1098	0.24	0.07	1.00	0.94
5.20_239.1759	0.24	0.39	1.00	0.97
3.85_258.1333	0.24	0.00	1.00	0.62
4.86_372.1909	0.25	0.13	1.00	0.74
6.60_152.1087	0.25	0.46	1.00	0.93
4.63_149.1104	0.26	0.41	1.00	0.94
5.34_191.1575	0.26	0.37	1.00	0.71
5.19_249.1604	0.27	0.43	1.00	0.87
1.73_288.1454	0.27	0.00	1.00	0.81
4.00_320.1711	0.28	0.03	1.00	0.79
3.80_194.0821	0.29	0.00	1.00	0.95

D. Mass Spectral Data for Selected Features

9.41_281.1770	0.29	0.54	0.95	1.00
7.15_504.8508	0.30	0.59	1.00	0.91
16.22_252.0441	0.30	0.53	1.00	0.96
6.74_1160.9454	0.31	0.26	0.83	1.00
4.34_266.1408	0.31	0.24	1.00	0.72
5.00_152.1079	0.33	0.50	1.00	0.84
6.78_176.0714	0.33	0.56	1.00	0.97
6.62_297.1617	0.33	0.59	1.00	0.88
5.16_237.1592	0.33	0.38	1.00	0.79
16.15_365.1085	0.34	0.00	1.00	0.82
3.82_230.1126	0.34	0.21	1.00	0.74
8.22_220.1332	0.34	0.49	0.95	1.00
4.53_236.1764	0.34	0.44	1.00	0.95
5.78_164.0706	0.34	0.46	0.98	1.00
4.77_179.0472	0.34	0.62	1.00	1.00
4.64_137.0376	0.35	0.36	0.95	1.00
4.40_158.0302	0.36	0.27	1.00	0.94
5.71_249.1598	0.38	0.52	1.00	0.89
6.15_485.2027	0.38	0.41	1.00	0.84
5.81_605.2195	0.39	0.55	1.00	0.88
4.70_221.1315	0.39	0.58	0.99	1.00
3.81_136.0628	0.40	0.64	1.00	0.86
4.16_256.1718	0.40	0.55	1.00	0.87
4.66_304.1776	0.42	0.62	1.00	0.90
5.16_210.1137	0.43	0.42	1.00	0.82
16.17_188.9130	0.43	0.00	1.00	0.88
16.18_204.8884	0.44	0.00	0.99	1.00
4.67_270.1917	0.44	0.60	1.00	0.97
3.94_254.1629	0.45	0.17	1.00	0.90
6.34_469.2088	0.49	0.63	1.00	0.87
4.39_362.1069	0.49	0.43	0.99	1.00
6.23_251.1781	0.49	0.54	1.00	0.87
12.43_386.2820	0.50	1.00	0.00	0.00
14.79_323.2583	0.50	1.00	0.00	0.00
13.49_420.3478	0.51	1.00	0.00	0.00
10.60_346.3091	0.51	1.00	0.00	0.00
13.00_413.3095	0.52	1.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.00	0.03
10.70_288.2557	0.52	1.00	0.00	0.00
9.48_225.1993	0.53	1.00	0.00	0.02
6.81_807.1918	0.54	1.00	0.00	0.00
13.53_339.2529	0.55	1.00	0.00	0.00
4.26_669.2631	0.56	1.00	0.00	0.13
11.80_235.1712	0.56	1.00	0.06	0.07
10.15_739.4618	0.56	1.00	0.06	0.04
14.41_309.2409	0.56	1.00	0.00	0.00
12.99_526.2341	0.56	1.00	0.00	0.06
10.53_531.4000	0.57	1.00	0.00	0.00
4.81_415.2090	0.57	0.40	1.00	0.89
12.97_407.3144	0.58	1.00	0.00	0.00
6.02_274.1066	0.58	0.40	1.00	0.86
12.98_399.3242	0.58	1.00	0.00	0.00
4.09_573.1785	0.58	1.00	0.00	0.00
12.98_510.2581	0.59	1.00	0.00	0.11
4.37_663.2850	0.59	1.00	0.00	0.20
4.59_251.1399	0.60	0.60	1.00	0.90
13.98_433.3418	0.61	1.00	0.00	0.00
6.90_166.0720	0.61	1.00	0.00	0.00
4.64_412.2067	0.62	1.00	0.00	0.16
6.19_181.1351	0.63	1.00	0.00	0.07
10.97_401.2525	0.63	1.00	0.08	0.08
16.14_274.0340	0.63	0.45	1.00	0.97
11.58_415.2745	0.65	1.00	0.00	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.86_507.3281	0.66	1.00	0.21	0.02
12.97_290.7254	0.66	1.00	0.00	0.00
4.27_647.2871	0.67	1.00	0.00	0.14
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.22	0.18
4.44_178.1088	0.70	0.60	0.99	1.00

D. Mass Spectral Data for Selected Features

6.85_824.9348	0.70	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
3.89_518.1743	0.73	1.00	0.00	0.00
11.18_473.3585	0.75	1.00	0.00	0.03
12.86_463.2998	0.77	1.00	0.00	0.08
12.74_443.3505	0.77	1.00	0.00	0.01
12.97_547.4060	0.77	1.00	0.00	0.00
13.86_425.2896	0.78	1.00	0.48	0.46
13.50_409.7445	0.80	1.00	0.00	0.04
4.28_227.1066	0.80	1.00	0.41	0.47
12.61_771.4862	0.80	1.00	0.00	0.37
11.97_299.2600	0.80	1.00	0.03	0.00
13.50_524.2740	0.81	1.00	0.01	0.10
15.06_413.2647	0.81	1.00	0.42	0.42
12.86_502.3745	0.82	1.00	0.36	0.00
11.84_443.3878	0.82	1.00	0.06	0.06
11.03_354.1608	0.82	1.00	0.00	0.03
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.00
13.79_365.2675	0.84	1.00	0.00	0.00
12.80_567.3292	0.85	1.00	0.00	0.00
10.38_401.3397	0.88	1.00	0.29	0.27
14.79_310.3109	0.90	1.00	0.18	0.00
12.78_611.3565	0.91	1.00	0.21	0.57
13.48_341.2200	0.91	1.00	0.00	0.20
13.49_295.2258	0.91	1.00	0.00	0.00
1.50_260.0296	0.92	1.00	0.30	0.47
4.49_225.1597	0.97	1.00	0.51	0.49
12.89_441.3208	0.99	1.00	0.46	0.31
12.78_590.4295	1.00	1.00	0.25	0.00
3.99_164.0936	1.00	0.90	0.58	0.61
10.36_211.6353	1.00	0.89	0.00	0.34
11.31_225.6512	1.00	0.95	0.00	0.00
5.40_230.0720	1.00	0.81	0.58	0.47
9.27_240.2315	1.00	0.88	0.25	0.00
10.39_268.2627	1.00	0.83	0.00	0.00
12.97_278.2028	1.00	0.62	0.00	0.04
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00
14.31_325.2414	1.00	0.74	0.00	0.00
14.82_332.2940	1.00	0.65	0.27	0.10
15.49_338.3442	1.00	0.86	0.00	0.03
15.92_360.3229	1.00	0.71	0.37	0.20
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.20	0.19
13.95_411.3586	1.00	0.78	0.00	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.00	0.16
10.98_442.3651	1.00	0.78	0.00	0.00
12.86_485.3471	1.00	0.86	0.19	0.41
12.81_529.3766	1.00	0.77	0.00	0.31
12.97_555.3910	1.00	0.94	0.00	0.00
12.75_617.4294	1.00	0.84	0.20	0.41
13.92_641.5490	1.00	0.85	0.00	0.00
12.67_705.4810	1.00	0.93	0.15	0.50
6.87_807.0837	1.00	0.57	0.19	0.00

D. Mass Spectral Data for Selected Features

Table S15. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S1 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	S1	S1
12.03_135.1163	0.00	0.04	0.67	1.00
12.03_123.1165	0.00	0.00	0.66	1.00
4.95_114.0908	0.00	0.00	0.50	1.00
1.50_103.5345	0.00	0.00	0.76	1.00
12.03_149.1327	0.00	0.00	0.66	1.00
13.61_149.0907	0.00	0.00	0.87	1.00
6.56_162.0938	0.00	0.00	1.00	0.94
5.78_170.1204	0.00	0.00	0.73	1.00
4.29_169.0959	0.00	0.00	1.00	0.76
2.44_166.0747	0.00	0.13	0.99	1.00
6.60_180.1017	0.00	0.03	0.85	1.00
9.12_191.0134	0.00	0.00	0.60	1.00
4.14_186.1168	0.00	0.00	1.00	0.79
4.02_198.1143	0.00	0.00	0.72	1.00
8.84_203.1804	0.00	0.00	0.69	1.00
6.22_203.0786	0.00	0.03	0.84	1.00
7.49_207.0994	0.00	0.08	0.88	1.00
1.30_205.9283	0.00	0.00	0.73	1.00
4.84_205.1323	0.00	0.00	0.53	1.00
10.22_205.1232	0.00	0.00	0.91	1.00
1.32_211.8786	0.00	0.00	0.85	1.00
9.81_210.0363	0.00	0.00	0.51	1.00
9.03_217.0413	0.00	0.00	1.00	0.82
16.16_223.9875	0.00	0.00	0.92	1.00
10.24_222.1533	0.00	0.06	0.72	1.00
8.84_221.1903	0.00	0.00	0.78	1.00
5.48_229.0656	0.00	0.00	0.78	1.00
5.11_236.1306	0.00	0.14	0.83	1.00
8.54_235.1344	0.00	0.00	0.81	1.00
11.28_233.1548	0.00	0.01	0.51	1.00
11.16_252.0381	0.00	0.00	0.52	1.00
13.78_251.2405	0.00	0.00	0.96	1.00
11.26_250.1814	0.00	0.00	0.78	1.00
8.08_252.0397	0.00	0.00	1.00	0.65
4.56_252.0394	0.00	0.17	0.90	1.00
5.12_252.0389	0.00	0.00	0.91	1.00
7.48_252.0388	0.00	0.00	0.98	1.00
12.02_263.1978	0.00	0.03	0.71	1.00
5.86_262.1048	0.00	0.37	0.81	1.00
10.71_261.1779	0.00	0.01	0.72	1.00
11.95_266.1298	0.00	0.00	0.66	1.00
5.27_264.2082	0.00	0.00	1.00	0.99
7.50_283.1523	0.00	0.06	0.95	1.00
9.01_283.1521	0.00	0.09	0.88	1.00
1.73_282.0649	0.00	0.03	0.80	1.00
7.15_293.2251	0.00	0.00	0.75	1.00
4.87_293.1612	0.00	0.33	0.74	1.00
6.49_292.1923	0.00	0.14	1.00	0.82
3.78_300.1386	0.00	0.42	0.90	1.00
12.02_309.1921	0.00	0.01	0.61	1.00
14.29_307.2281	0.00	0.00	0.89	1.00
1.74_322.0446	0.00	0.03	0.45	1.00
14.63_321.2420	0.00	0.00	1.00	0.91
12.03_325.1706	0.00	0.00	0.66	1.00
13.85_333.2427	0.00	0.00	1.00	0.79
10.73_340.1475	0.00	0.10	0.81	1.00
14.63_339.2533	0.00	0.00	1.00	0.75
15.50_349.2615	0.00	0.00	1.00	0.89
14.31_347.2205	0.00	0.00	0.78	1.00
7.48_345.1875	0.00	0.00	1.00	0.94
4.01_351.5992	0.00	0.00	1.00	0.79
6.95_350.2147	0.00	0.02	1.00	1.00
12.59_361.1697	0.00	0.15	1.00	0.92
6.51_360.2165	0.00	0.00	0.52	1.00

D. Mass Spectral Data for Selected Features

7.52_368.2211	0.00	0.00	0.58	1.00
9.80_367.0822	0.00	0.00	0.51	1.00
14.32_379.2817	0.00	0.00	1.00	0.80
7.43_374.2181	0.00	0.00	0.76	1.00
6.24_384.2171	0.00	0.00	0.66	1.00
13.61_399.3201	0.00	0.00	1.00	0.94
1.49_394.1142	0.00	0.00	0.48	1.00
14.57_393.2988	0.00	0.00	1.00	0.89
14.04_420.3477	0.00	0.07	0.68	1.00
8.04_432.2606	0.00	0.00	1.00	0.83
9.03_457.1145	0.00	0.15	0.53	1.00
11.52_456.3791	0.00	0.00	0.46	1.00
6.21_455.1906	0.00	0.17	0.88	1.00
11.66_454.2954	0.00	0.23	1.00	0.89
9.81_454.0847	0.00	0.00	0.43	1.00
9.79_462.0710	0.00	0.00	0.51	1.00
9.78_481.0499	0.00	0.00	0.49	1.00
7.51_499.2782	0.00	0.06	0.86	1.00
4.37_494.2617	0.00	0.00	0.75	1.00
8.58_490.2972	0.00	0.00	0.67	1.00
12.00_515.2832	0.00	0.00	0.84	1.00
1.76_515.1445	0.00	0.00	0.63	1.00
9.11_548.3433	0.00	0.06	0.65	1.00
12.03_565.3746	0.00	0.00	0.77	1.00
6.90_555.3068	0.00	0.00	0.91	1.00
12.03_549.4012	0.00	0.00	0.74	1.00
9.02_549.3610	0.00	0.02	1.00	0.81
5.52_601.2501	0.00	0.00	0.82	1.00
7.20_920.0962	0.00	0.00	1.00	0.74
7.21_916.0943	0.00	0.00	1.00	0.92
7.01_1221.4414	0.00	0.00	1.00	0.93
8.34_150.0928	0.00	0.06	0.69	1.00
14.64_361.2361	0.01	0.00	1.00	0.90
7.48_177.0877	0.01	0.00	0.82	1.00
6.95_368.2220	0.01	0.02	0.86	1.00
8.10_301.1534	0.01	0.05	0.53	1.00
8.54_447.2904	0.02	0.13	0.57	1.00
3.22_235.1201	0.02	0.00	0.84	1.00
12.02_205.1953	0.02	0.00	0.72	1.00
10.18_621.4210	0.02	0.00	0.53	1.00
1.29_203.9309	0.02	0.00	0.65	1.00
13.79_365.2675	0.02	0.02	1.00	0.93
14.31_335.2563	0.03	0.00	1.00	0.60
11.43_466.2973	0.03	0.08	0.95	1.00
6.92_332.1986	0.03	0.01	1.00	0.97
6.24_515.2753	0.03	0.01	1.00	0.83
1.75_507.1572	0.04	0.00	0.92	1.00
9.11_505.3321	0.05	0.00	0.63	1.00
8.52_491.3179	0.06	0.00	0.63	1.00
1.74_150.0789	0.06	0.00	0.64	1.00
3.07_230.1126	0.06	0.15	0.84	1.00
13.79_531.4249	0.06	0.19	0.69	1.00
9.78_465.0808	0.06	0.18	0.55	1.00
1.73_338.0231	0.06	0.00	1.00	0.95
8.53_177.0880	0.07	0.06	0.73	1.00
10.52_673.3745	0.07	0.11	0.49	1.00
12.39_279.1366	0.07	0.19	0.99	1.00
3.86_150.0940	0.08	0.14	0.60	1.00
8.53_283.1523	0.08	0.17	1.00	0.96
8.53_207.1002	0.08	0.10	0.84	1.00
5.97_286.6247	0.09	0.01	0.94	1.00
7.95_433.2783	0.09	0.24	0.65	1.00
11.73_360.1653	0.10	0.23	0.78	1.00
6.95_218.1203	0.10	0.21	0.61	1.00
14.78_323.2583	0.11	0.21	1.00	0.83
11.33_299.2599	0.11	0.08	0.97	1.00
5.43_377.1482	0.11	0.00	0.63	1.00
12.40_251.2372	0.11	0.00	0.94	1.00
11.73_352.1729	0.11	0.48	1.00	1.00
11.97_299.2600	0.11	0.14	0.67	1.00

D. Mass Spectral Data for Selected Features

13.53_339.2529	0.12	0.21	1.00	0.85
1.82_228.1004	0.13	0.01	0.57	1.00
7.42_280.1237	0.13	0.36	0.64	1.00
7.89_192.1015	0.13	0.23	0.88	1.00
5.97_278.6345	0.14	0.03	1.00	0.88
6.41_165.0905	0.15	0.10	0.89	1.00
14.31_325.2414	0.16	0.12	1.00	0.87
7.91_389.2523	0.17	0.08	0.64	1.00
14.04_295.2283	0.17	0.32	1.00	0.95
4.87_329.1844	0.18	0.00	0.68	1.00
12.39_401.2333	0.19	0.47	1.00	0.96
12.62_313.2746	0.19	0.16	0.89	1.00
4.31_265.0552	0.20	0.00	0.73	1.00
7.06_203.1787	0.21	0.38	0.66	1.00
12.62_273.1378	0.21	0.32	0.83	1.00
6.06_203.1781	0.22	0.39	0.71	1.00
6.87_807.0837	0.22	0.13	1.00	0.80
9.69_220.1127	0.23	0.26	0.73	1.00
4.30_310.1305	0.23	0.05	0.75	1.00
4.75_136.0625	0.24	0.00	1.00	0.85
1.73_288.1454	0.24	0.00	0.71	1.00
3.82_230.1126	0.25	0.15	0.71	1.00
3.83_198.1623	0.25	0.18	0.77	1.00
14.41_309.2409	0.26	0.46	1.00	0.94
3.85_276.1433	0.28	0.16	0.76	1.00
5.96_534.2942	0.32	0.07	1.00	0.95
16.18_335.9929	0.33	0.00	0.68	1.00
4.88_188.0708	0.34	0.58	0.80	1.00
5.61_343.2002	0.35	0.08	0.67	1.00
13.84_397.2963	0.38	0.00	1.00	0.82
12.70_699.4109	0.39	0.43	0.78	1.00
12.62_787.4580	0.39	0.66	0.91	1.00
14.79_310.3109	0.41	0.46	1.00	0.78
12.79_611.3565	0.43	0.47	0.73	1.00
3.80_194.0821	0.43	0.00	0.97	1.00
12.86_523.3040	0.43	0.29	0.94	1.00
12.63_394.2284	0.47	0.36	1.00	0.93
12.67_743.4367	0.48	0.54	0.81	1.00
12.73_655.3845	0.48	0.58	0.85	1.00
13.50_409.7445	0.48	0.60	0.84	1.00
12.74_639.4067	0.48	0.58	0.77	1.00
15.06_413.2647	0.49	0.60	1.00	0.85
12.61_771.4862	0.49	0.62	0.80	1.00
6.15_485.2027	0.50	0.53	0.75	1.00
12.86_463.2998	0.50	0.66	1.00	0.99
10.60_346.3091	0.51	1.00	0.00	0.00
9.48_225.1993	0.53	1.00	0.02	0.02
5.18_364.0987	0.54	1.00	0.07	0.07
12.78_590.4295	0.55	0.56	0.90	1.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.00	0.05
3.80_119.0369	0.56	1.00	0.11	0.00
12.83_546.4021	0.58	0.67	0.85	1.00
1.28_188.9112	0.59	1.00	0.24	0.00
4.37_663.2850	0.59	1.00	0.01	0.00
13.92_641.5490	0.61	0.52	1.00	0.83
12.70_678.4764	0.61	0.35	0.93	1.00
6.90_166.0720	0.61	1.00	0.00	0.00
4.64_412.2067	0.62	1.00	0.00	0.11
5.19_249.1604	0.63	1.00	0.20	0.27
6.19_181.1351	0.63	1.00	0.03	0.00
6.39_336.2172	0.66	0.54	1.00	0.89
4.27_647.2871	0.67	1.00	0.00	0.00
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.00	0.10
1.28_172.9358	0.69	1.00	0.28	0.39
7.62_970.6124	0.70	1.00	0.10	0.00
4.81_506.2950	0.71	1.00	0.29	0.33
4.37_150.0945	0.72	1.00	0.00	0.00
3.89_518.1743	0.73	1.00	0.00	0.02

D. Mass Spectral Data for Selected Features

11.18_473.3585	0.75	1.00	0.29	0.35
12.89_441.3208	0.75	0.76	0.92	1.00
12.74_443.3505	0.77	1.00	0.00	0.03
4.28_227.1066	0.80	1.00	0.35	0.50
4.55_279.1361	0.81	1.00	0.47	0.53
11.28_440.3462	0.82	1.00	0.55	0.36
12.98_282.2118	0.82	1.00	0.21	0.15
4.27_302.2070	0.86	1.00	0.70	0.59
5.16_237.1592	0.87	1.00	0.36	0.32
9.26_219.1735	0.88	1.00	0.00	0.00
4.50_359.1197	0.89	1.00	0.00	0.00
10.84_227.1557	0.90	1.00	0.15	0.00
13.49_295.2258	0.91	1.00	0.22	0.18
1.47_508.0657	0.91	1.00	0.40	0.00
1.50_260.0296	0.92	1.00	0.05	0.14
1.47_748.1127	0.94	1.00	0.61	0.76
4.58_336.1924	0.95	1.00	0.76	0.57
1.48_481.1031	0.96	1.00	0.62	0.69
4.29_244.1199	0.97	1.00	0.28	0.00
4.49_225.1597	0.97	1.00	0.12	0.18
1.50_710.1736	0.99	1.00	0.73	0.82
13.95_270.2746	1.00	1.00	0.34	0.39
4.44_178.1088	1.00	0.86	0.33	0.50
3.80_288.1929	1.00	0.87	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
4.25_343.1235	1.00	0.70	0.08	0.00
15.49_338.3442	1.00	0.86	0.00	0.00
4.26_356.1796	1.00	0.84	0.42	0.58
4.42_351.1212	1.00	0.79	0.18	0.20
4.39_362.1069	1.00	0.88	0.18	0.00
1.55_385.5441	1.00	0.65	0.12	0.00
13.95_411.3586	1.00	0.78	0.60	0.53
10.98_442.3651	1.00	0.78	0.12	0.33
4.37_685.2548	1.00	0.86	0.00	0.00
7.66_916.7249	1.00	0.76	0.00	0.00
7.00_916.3325	1.00	0.59	0.07	0.17
7.00_913.0933	1.00	0.71	0.00	0.10

D. Mass Spectral Data for Selected Features

Table S16. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S2 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_ m/z)	WT	WT	S2	S2
12.03_135.1163	0.00	0.07	1.00	0.69
12.03_123.1165	0.00	0.00	1.00	0.72
1.50_103.5345	0.00	0.00	1.00	0.81
12.03_149.1327	0.00	0.00	1.00	0.70
13.61_149.0907	0.00	0.00	0.76	1.00
1.50_165.0624	0.00	0.00	1.00	0.85
6.56_162.0938	0.00	0.00	0.58	1.00
2.01_158.0950	0.00	0.30	1.00	0.88
5.78_170.1204	0.00	0.00	1.00	0.91
4.29_169.0959	0.00	0.00	0.66	1.00
6.60_180.1017	0.00	0.02	0.99	1.00
5.02_180.1014	0.00	0.00	0.91	1.00
10.70_179.1435	0.00	0.00	1.00	0.66
4.95_177.1399	0.00	0.28	1.00	0.96
4.39_192.1130	0.00	0.30	1.00	0.94
9.12_191.0134	0.00	0.00	1.00	0.84
4.02_198.1143	0.00	0.00	0.95	1.00
4.99_198.1134	0.00	0.00	0.76	1.00
9.08_196.0187	0.00	0.00	0.55	1.00
8.84_203.1804	0.00	0.00	1.00	0.82
8.12_203.1781	0.00	0.00	1.00	0.78
9.08_203.0278	0.00	0.00	1.00	0.72
9.80_203.0277	0.00	0.00	1.00	0.86
4.35_209.0956	0.00	0.00	1.00	0.91
5.44_208.0539	0.00	0.00	1.00	0.80
7.49_207.0994	0.00	0.12	1.00	0.85
1.30_205.9283	0.00	0.00	1.00	0.96
4.84_205.1323	0.00	0.00	1.00	0.98
1.32_211.8786	0.00	0.00	1.00	0.91
1.49_211.0584	0.00	0.24	1.00	0.85
9.81_210.0363	0.00	0.00	1.00	0.77
9.41_219.0312	0.00	0.00	1.00	0.70
9.03_217.0413	0.00	0.00	1.00	0.90
1.85_216.1242	0.00	0.05	0.98	1.00
16.16_223.9875	0.00	0.00	0.63	1.00
10.24_222.1533	0.00	0.08	1.00	0.70
9.81_222.1504	0.00	0.05	1.00	0.80
8.84_221.1903	0.00	0.00	1.00	0.79
9.04_225.0298	0.00	0.04	1.00	0.86
9.77_224.0325	0.00	0.00	1.00	0.80
5.48_229.0656	0.00	0.00	1.00	0.94
9.19_230.0719	0.00	0.00	1.00	0.98
9.82_230.0718	0.00	0.05	0.84	1.00
8.41_230.0715	0.00	0.00	1.00	0.63
10.62_236.1643	0.00	0.00	0.93	1.00
5.11_236.1306	0.00	0.13	0.79	1.00
8.54_235.1344	0.00	0.00	1.00	0.69
9.80_241.0261	0.00	0.00	1.00	0.91
10.69_238.1826	0.00	0.00	1.00	0.65
4.13_237.1268	0.00	0.31	1.00	0.81
5.81_248.1281	0.00	0.27	1.00	0.85
9.03_248.0351	0.00	0.00	0.80	1.00
8.44_247.1345	0.00	0.00	1.00	0.95
4.04_247.1287	0.00	0.00	0.74	1.00
9.07_246.5440	0.00	0.00	1.00	0.75
5.04_244.1219	0.00	0.00	1.00	0.94
4.31_249.0807	0.00	0.00	1.00	0.87
8.08_252.0397	0.00	0.00	0.91	1.00
9.63_252.0395	0.00	0.00	0.88	1.00
8.66_252.0394	0.00	0.00	1.00	0.55
5.12_252.0389	0.00	0.00	0.55	1.00
7.48_252.0388	0.00	0.00	0.79	1.00

D. Mass Spectral Data for Selected Features

6.23_258.1449	0.00	0.00	1.00	0.69
3.87_257.1146	0.00	0.30	1.00	0.95
9.81_253.5524	0.00	0.03	1.00	0.97
12.02_263.1978	0.00	0.08	1.00	0.84
1.78_262.1278	0.00	0.00	0.96	1.00
5.86_262.1048	0.00	0.27	0.97	1.00
5.01_261.1438	0.00	0.06	0.77	1.00
9.03_260.5527	0.00	0.00	0.94	1.00
10.52_268.0194	0.00	0.21	0.89	1.00
5.43_268.0192	0.00	0.06	0.96	1.00
6.28_268.0191	0.00	0.10	1.00	0.96
8.32_268.0180	0.00	0.00	1.00	0.55
5.18_266.1406	0.00	0.27	1.00	0.91
5.27_264.2082	0.00	0.00	1.00	0.88
7.49_268.0200	0.00	0.00	0.51	1.00
4.60_268.0196	0.00	0.00	1.00	0.82
11.39_268.0195	0.00	0.00	0.93	1.00
5.84_281.1328	0.00	0.00	0.91	1.00
9.12_279.1585	0.00	0.00	1.00	0.67
7.18_278.2110	0.00	0.00	1.00	0.80
6.07_276.1943	0.00	0.00	1.00	0.97
4.52_276.1726	0.00	0.00	0.97	1.00
5.71_286.2118	0.00	0.00	1.00	0.70
7.19_284.2219	0.00	0.00	1.00	0.68
7.50_283.1523	0.00	0.05	1.00	0.74
1.73_282.0649	0.00	0.02	1.00	0.87
7.72_281.1420	0.00	0.00	1.00	0.80
5.22_295.1312	0.00	0.04	1.00	0.81
7.82_294.2085	0.00	0.00	1.00	0.84
6.82_294.2084	0.00	0.00	1.00	0.56
3.86_294.1559	0.00	0.40	1.00	0.86
7.15_293.2251	0.00	0.00	1.00	0.67
4.87_293.1612	0.00	0.22	0.87	1.00
6.49_292.1923	0.00	0.03	0.65	1.00
3.76_299.1387	0.00	0.00	1.00	0.71
7.73_298.2024	0.00	0.00	1.00	0.87
4.74_298.0969	0.00	0.06	1.00	0.84
9.60_297.1694	0.00	0.00	1.00	0.64
7.19_296.2224	0.00	0.00	1.00	0.89
5.83_303.1558	0.00	0.01	0.95	1.00
3.78_300.1386	0.00	0.04	1.00	0.81
12.02_309.1921	0.00	0.02	1.00	0.90
6.00_308.2238	0.00	0.00	1.00	0.92
6.06_312.2197	0.00	0.00	0.99	1.00
6.84_312.2197	0.00	0.00	1.00	0.78
7.24_312.2197	0.00	0.00	1.00	0.70
10.59_311.1859	0.00	0.00	1.00	0.67
7.47_310.2026	0.00	0.00	0.97	1.00
5.82_322.1007	0.00	0.00	1.00	0.89
1.74_322.0446	0.00	0.02	1.00	0.91
14.63_321.2420	0.00	0.00	0.64	1.00
9.13_319.1539	0.00	0.00	1.00	0.71
6.92_318.2094	0.00	0.00	0.94	1.00
6.00_328.7423	0.00	0.24	1.00	0.83
7.34_326.2353	0.00	0.00	1.00	0.84
12.03_325.1706	0.00	0.00	1.00	0.92
6.08_324.1828	0.00	0.30	1.00	0.84
6.31_335.7452	0.00	0.00	1.00	0.82
6.62_334.2005	0.00	0.00	0.51	1.00
8.76_329.1942	0.00	0.10	1.00	0.76
5.84_341.1007	0.00	0.00	1.00	0.86
14.63_339.2533	0.00	0.00	1.00	0.89
7.48_345.1875	0.00	0.00	1.00	0.78
5.26_354.0787	0.00	0.16	0.98	1.00
8.24_352.2057	0.00	0.00	1.00	0.96
4.01_351.5992	0.00	0.00	1.00	0.87
6.95_350.2147	0.00	0.10	1.00	0.72
6.51_360.2165	0.00	0.00	1.00	0.82
8.53_359.2035	0.00	0.09	1.00	0.74
7.52_368.2211	0.00	0.00	0.92	1.00

D. Mass Spectral Data for Selected Features

9.80_367.0822	0.00	0.00	1.00	0.84
10.08_366.2455	0.00	0.00	1.00	0.73
6.22_366.2068	0.00	0.15	1.00	0.92
5.64_366.2063	0.00	0.00	0.75	1.00
7.83_387.1861	0.00	0.00	1.00	0.96
9.80_387.0731	0.00	0.00	1.00	0.77
6.88_386.2329	0.00	0.03	0.95	1.00
6.24_384.2171	0.00	0.00	1.00	0.96
8.63_398.2317	0.00	0.00	1.00	0.69
9.08_429.0845	0.00	0.00	1.00	0.75
7.98_431.2698	0.00	0.05	1.00	0.80
9.07_451.0615	0.00	0.00	1.00	0.78
6.99_443.3240	0.00	0.06	1.00	0.92
9.73_443.1014	0.00	0.00	1.00	0.83
6.90_461.2902	0.00	0.00	0.88	1.00
5.90_459.3212	0.00	0.14	1.00	0.88
10.02_459.0960	0.00	0.00	1.00	0.67
9.03_457.1145	0.00	0.01	1.00	0.77
11.52_456.3791	0.00	0.00	1.00	0.64
6.21_455.1906	0.00	0.15	1.00	0.82
9.81_454.0847	0.00	0.00	1.00	0.73
9.79_462.0710	0.00	0.00	1.00	0.67
9.78_481.0499	0.00	0.00	1.00	0.79
9.02_479.0963	0.00	0.00	1.00	0.87
4.15_476.2404	0.00	0.00	1.00	0.74
6.98_499.2793	0.00	0.00	1.00	0.75
7.51_499.2782	0.00	0.04	1.00	0.91
9.02_495.0687	0.00	0.00	1.00	0.78
5.37_493.1709	0.00	0.00	1.00	0.85
9.09_512.3013	0.00	0.00	1.00	0.78
13.62_510.2556	0.00	0.28	1.00	0.73
5.65_504.2609	0.00	0.00	1.00	0.98
5.64_515.2738	0.00	0.01	1.00	0.74
6.62_515.2737	0.00	0.00	0.86	1.00
1.76_515.1445	0.00	0.00	0.92	1.00
10.06_526.3139	0.00	0.00	1.00	0.65
7.21_526.2839	0.00	0.03	0.97	1.00
6.79_549.3505	0.00	0.00	1.00	0.60
7.20_544.2918	0.00	0.00	1.00	0.85
7.57_542.3960	0.00	0.20	1.00	0.78
12.03_565.3746	0.00	0.02	1.00	0.85
7.14_560.1805	0.00	0.00	0.76	1.00
6.90_555.3068	0.00	0.00	1.00	0.82
1.72_551.1035	0.00	0.00	1.00	0.87
12.03_549.4012	0.00	0.00	1.00	0.84
5.52_601.2501	0.00	0.00	0.60	1.00
1.25_639.8836	0.00	0.00	1.00	0.61
6.02_637.3187	0.00	0.00	1.00	0.84
9.79_683.1204	0.00	0.00	1.00	0.51
7.60_846.3434	0.00	0.00	1.00	0.91
7.20_920.0962	0.00	0.00	0.89	1.00
7.21_916.0943	0.00	0.00	0.86	1.00
9.80_907.1678	0.00	0.00	1.00	0.79
7.67_1031.2480	0.00	0.22	1.00	0.77
7.69_1031.1674	0.00	0.27	1.00	0.93
7.67_1031.0798	0.00	0.00	1.00	0.59
7.63_970.6960	0.00	0.00	1.00	0.53
7.01_1221.4414	0.00	0.00	1.00	0.93
7.00_1216.1209	0.00	0.36	1.00	0.85
7.70_1064.5448	0.00	0.13	0.60	1.00
8.34_150.0928	0.00	0.03	1.00	0.86
9.79_218.0234	0.00	0.02	0.96	1.00
1.64_174.0879	0.00	0.00	0.59	1.00
9.78_465.0808	0.01	0.02	1.00	0.61
6.76_310.2021	0.01	0.00	0.99	1.00
6.24_515.2753	0.01	0.00	1.00	0.79
1.82_228.1004	0.01	0.00	0.89	1.00
1.29_203.9309	0.01	0.00	1.00	0.90
8.10_301.1534	0.01	0.04	1.00	0.77
5.66_384.2168	0.01	0.00	1.00	0.96

D. Mass Spectral Data for Selected Features

1.64_246.1172	0.01	0.00	0.93	1.00
3.22_235.1201	0.01	0.00	0.84	1.00
9.81_269.0437	0.02	0.00	1.00	0.73
6.06_294.2084	0.02	0.00	1.00	0.78
7.48_177.0877	0.02	0.00	1.00	0.89
9.66_279.1583	0.02	0.00	1.00	0.69
8.74_542.3146	0.02	0.00	0.90	1.00
12.02_205.1953	0.02	0.00	1.00	0.71
9.14_239.1284	0.03	0.02	1.00	0.75
5.43_377.1482	0.03	0.00	1.00	0.74
9.67_319.1539	0.03	0.05	0.64	1.00
1.73_338.0231	0.04	0.00	1.00	0.99
7.06_325.1861	0.04	0.23	1.00	1.00
8.53_283.1523	0.04	0.09	0.88	1.00
1.74_150.0789	0.04	0.00	1.00	0.77
6.95_218.1203	0.05	0.10	1.00	0.90
6.95_368.2220	0.05	0.09	1.00	0.76
3.07_230.1126	0.05	0.12	0.96	1.00
10.52_673.3745	0.06	0.10	1.00	0.69
1.70_260.1135	0.06	0.00	0.91	1.00
7.42_280.1237	0.07	0.19	1.00	0.88
4.75_136.0625	0.07	0.00	0.80	1.00
10.98_442.3651	0.07	0.05	1.00	0.65
4.61_247.1287	0.07	0.00	0.81	1.00
3.83_198.1623	0.07	0.05	1.00	0.89
3.86_150.0940	0.07	0.13	1.00	0.90
1.76_596.1679	0.07	0.00	0.64	1.00
4.37_326.1802	0.07	0.44	0.97	1.00
8.53_207.1002	0.07	0.09	0.97	1.00
5.97_286.6247	0.08	0.01	0.84	1.00
8.53_177.0880	0.08	0.07	1.00	0.95
7.80_291.1290	0.08	0.30	1.00	0.91
14.64_361.2361	0.09	0.00	0.95	1.00
5.84_299.0939	0.11	0.05	0.99	1.00
7.25_371.1508	0.11	0.00	0.89	1.00
5.83_325.1311	0.12	0.00	0.92	1.00
9.41_281.1770	0.13	0.24	1.00	0.77
7.06_221.1900	0.13	0.40	1.00	0.79
6.41_165.0905	0.14	0.09	1.00	0.72
1.65_159.0768	0.16	0.00	0.75	1.00
9.79_1349.2480	0.16	0.00	0.89	1.00
4.87_329.1844	0.17	0.00	1.00	0.86
4.30_310.1305	0.17	0.04	1.00	0.86
3.85_276.1433	0.17	0.10	1.00	0.86
6.71_1160.7578	0.17	0.00	1.00	0.77
7.06_203.1787	0.17	0.32	1.00	0.90
6.06_203.1781	0.18	0.32	1.00	0.79
1.78_217.1296	0.18	0.37	0.78	1.00
9.47_211.0868	0.18	0.32	1.00	0.72
1.73_288.1454	0.20	0.00	1.00	0.86
4.31_265.0552	0.20	0.00	1.00	0.92
4.81_464.2611	0.21	0.25	1.00	0.82
8.29_401.1993	0.21	0.00	1.00	0.92
3.82_230.1126	0.22	0.14	0.93	1.00
4.30_478.1379	0.23	0.05	1.00	0.89
5.81_222.1598	0.24	0.46	1.00	0.85
16.18_335.9929	0.24	0.00	1.00	0.83
4.12_413.1243	0.25	0.45	1.00	0.89
7.42_196.0651	0.25	0.13	1.00	0.87
4.09_573.1785	0.27	0.46	1.00	0.90
6.39_336.2172	0.28	0.23	1.00	0.95
4.88_188.0708	0.29	0.50	0.99	1.00
12.62_416.2462	0.30	0.36	1.00	0.90
4.26_450.2439	0.30	0.01	1.00	0.92
4.86_372.1909	0.30	0.16	1.00	0.91
6.27_207.0660	0.32	0.57	1.00	1.00
4.64_137.0376	0.33	0.34	1.00	0.98
5.27_685.1761	0.33	0.00	1.00	0.89
3.80_194.0821	0.34	0.00	0.77	1.00
5.96_534.2942	0.35	0.08	1.00	0.90

D. Mass Spectral Data for Selected Features

16.15_459.1339	0.35	0.00	0.74	1.00
5.81_605.2195	0.36	0.51	1.00	0.81
4.63_149.1104	0.38	0.61	1.00	0.89
6.78_176.0714	0.38	0.65	1.00	0.93
5.16_210.1137	0.40	0.39	1.00	0.83
8.22_220.1332	0.40	0.59	1.00	0.81
5.34_191.1575	0.44	0.63	1.00	0.90
4.32_308.1712	0.46	0.16	1.00	0.89
4.34_266.1408	0.46	0.36	0.90	1.00
12.43_386.2820	0.50	1.00	0.00	0.00
13.49_420.3478	0.51	1.00	0.03	0.04
10.60_346.3091	0.51	1.00	0.00	0.00
3.93_438.1964	0.51	0.19	1.00	0.89
13.00_413.3095	0.52	1.00	0.06	0.04
10.40_371.3275	0.52	1.00	0.00	0.00
6.40_263.1761	0.53	0.57	1.00	0.92
9.48_225.1993	0.53	1.00	0.02	0.01
6.81_807.1918	0.54	1.00	0.00	0.00
4.40_158.0302	0.54	0.40	1.00	0.88
13.53_339.2529	0.55	1.00	0.00	0.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.07	0.00
10.15_739.4618	0.56	1.00	0.01	0.02
14.41_309.2409	0.56	1.00	0.05	0.17
6.15_485.2027	0.57	0.61	1.00	0.81
10.53_531.4000	0.57	1.00	0.00	0.00
1.94_252.0411	0.57	0.43	0.95	1.00
12.97_407.3144	0.58	1.00	0.04	0.03
12.98_399.3242	0.58	1.00	0.05	0.03
4.37_663.2850	0.59	1.00	0.00	0.00
4.29_244.1199	0.61	0.63	1.00	0.87
13.98_433.3418	0.61	1.00	0.00	0.00
6.90_166.0720	0.61	1.00	0.00	0.00
5.20_239.1759	0.62	1.00	0.23	0.19
4.64_412.2067	0.62	1.00	0.13	0.12
3.86_242.1126	0.63	0.68	0.91	1.00
6.19_181.1351	0.63	1.00	0.06	0.06
10.97_401.2525	0.63	1.00	0.12	0.04
3.87_166.0522	0.65	0.38	0.96	1.00
6.40_439.1986	0.65	0.65	1.00	0.84
11.58_415.2745	0.65	1.00	0.02	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.86_507.3281	0.66	1.00	0.29	0.25
12.97_290.7254	0.66	1.00	0.31	0.24
4.27_647.2871	0.67	1.00	0.01	0.01
12.82_551.3593	0.67	1.00	0.37	0.26
11.44_223.2060	0.67	1.00	0.00	0.00
5.72_240.1231	0.68	0.47	0.88	1.00
6.85_824.9348	0.70	1.00	0.00	0.00
4.81_506.2950	0.71	1.00	0.10	0.00
16.15_442.8736	0.71	1.00	0.00	0.00
4.50_359.1197	0.71	0.79	0.97	1.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
12.79_595.3829	0.73	1.00	0.43	0.35
3.89_518.1743	0.73	1.00	0.05	0.00
12.67_727.4605	0.74	1.00	0.45	0.40
4.81_415.2090	0.74	0.52	1.00	0.95
11.18_473.3585	0.75	1.00	0.00	0.01
3.75_245.1607	0.75	1.00	0.13	0.15
6.23_251.1781	0.76	0.84	1.00	0.94
5.43_241.1546	0.76	0.78	0.98	1.00
12.70_683.4373	0.77	1.00	0.52	0.40
12.86_463.2998	0.77	1.00	0.00	0.23
12.74_443.3505	0.77	1.00	0.01	0.02
6.34_150.0787	0.77	0.73	0.91	1.00
12.97_547.4060	0.77	1.00	0.10	0.13
13.86_425.2896	0.78	1.00	0.32	0.26
5.26_147.0936	0.79	1.00	0.38	0.32
11.97_299.2600	0.80	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

13.50_524.2740	0.81	1.00	0.54	0.42
15.06_413.2647	0.81	1.00	0.09	0.34
12.86_502.3745	0.82	1.00	0.52	0.35
11.84_443.3878	0.82	1.00	0.21	0.13
11.03_354.1608	0.82	1.00	0.10	0.10
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.04
12.73_655.3845	0.83	1.00	0.22	0.42
12.74_639.4067	0.83	1.00	0.46	0.40
13.79_365.2675	0.84	1.00	0.00	0.00
12.80_567.3292	0.85	1.00	0.00	0.37
12.83_546.4021	0.86	1.00	0.46	0.30
10.38_401.3397	0.88	1.00	0.29	0.21
9.26_219.1735	0.88	1.00	0.00	0.00
12.67_743.4367	0.88	1.00	0.59	0.51
12.70_699.4109	0.89	1.00	0.34	0.24
14.79_310.3109	0.90	1.00	0.67	0.66
12.78_611.3565	0.91	1.00	0.19	0.49
15.94_338.3442	0.91	1.00	0.59	0.48
13.49_295.2258	0.91	1.00	0.01	0.00
1.47_508.0657	0.91	1.00	0.44	0.17
12.73_320.2010	0.94	1.00	0.13	0.00
4.49_225.1597	0.97	1.00	0.36	0.32
12.89_441.3208	0.99	1.00	0.38	0.19
12.78_590.4295	1.00	1.00	0.58	0.46
10.36_211.6353	1.00	0.89	0.31	0.00
3.82_209.1275	1.00	0.90	0.62	0.56
11.31_225.6512	1.00	0.95	0.38	0.31
9.27_240.2315	1.00	0.88	0.10	0.00
10.39_268.2627	1.00	0.83	0.00	0.00
6.59_273.1670	1.00	0.84	0.62	0.67
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00
14.82_332.2940	1.00	0.65	0.21	0.23
4.25_343.1235	1.00	0.70	0.34	0.08
15.49_338.3442	1.00	0.86	0.00	0.00
15.92_360.3229	1.00	0.71	0.09	0.32
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.11	0.22
13.95_411.3586	1.00	0.78	0.01	0.02
13.27_419.3131	1.00	0.81	0.00	0.00
12.86_485.3471	1.00	0.86	0.32	0.24
12.81_529.3766	1.00	0.77	0.35	0.14
12.97_555.3910	1.00	0.94	0.00	0.23
12.79_573.4039	1.00	0.73	0.34	0.24
12.75_617.4294	1.00	0.84	0.39	0.25
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.00
12.67_705.4810	1.00	0.93	0.57	0.33
6.87_807.0837	1.00	0.57	0.11	0.00

D. Mass Spectral Data for Selected Features

Table S17. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S3 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT _m/z)	WT	WT	S3	S3
12.03_135.1163	0.00	0.05	0.98	1.00
12.03_123.1165	0.00	0.00	0.93	1.00
4.87_118.0679	0.00	0.14	0.81	1.00
12.03_149.1327	0.00	0.00	0.98	1.00
6.56_162.0938	0.00	0.00	0.88	1.00
2.01_158.0950	0.00	0.27	1.00	0.67
5.78_170.1204	0.00	0.00	1.00	0.97
7.08_169.0882	0.00	0.01	1.00	0.70
2.44_166.0747	0.00	0.10	0.94	1.00
6.60_180.1017	0.00	0.02	1.00	0.98
5.02_180.1014	0.00	0.00	0.66	1.00
4.95_177.1399	0.00	0.31	0.92	1.00
4.39_192.1130	0.00	0.16	1.00	0.98
9.12_191.0134	0.00	0.00	0.83	1.00
4.14_186.1168	0.00	0.00	1.00	0.60
4.02_198.1143	0.00	0.00	1.00	0.96
4.99_198.1134	0.00	0.00	1.00	0.97
9.08_196.0187	0.00	0.00	1.00	0.97
8.84_203.1804	0.00	0.00	0.96	1.00
8.12_203.1781	0.00	0.00	0.97	1.00
9.08_203.0278	0.00	0.00	1.00	0.98
9.80_203.0277	0.00	0.00	0.95	1.00
1.42_201.0074	0.00	0.00	0.99	1.00
4.35_209.0956	0.00	0.00	0.86	1.00
4.54_208.1355	0.00	0.00	0.72	1.00
5.44_208.0539	0.00	0.00	1.00	0.76
7.49_207.0994	0.00	0.08	1.00	0.83
1.30_205.9283	0.00	0.00	1.00	0.94
4.84_205.1323	0.00	0.00	0.92	1.00
9.81_205.1237	0.00	0.00	1.00	1.00
10.22_205.1232	0.00	0.00	1.00	0.51
1.32_211.8786	0.00	0.00	0.80	1.00
1.49_211.0584	0.00	0.18	0.74	1.00
9.81_210.0363	0.00	0.00	0.94	1.00
9.07_210.0305	0.00	0.00	0.76	1.00
9.41_219.0312	0.00	0.00	0.99	1.00
3.69_218.1136	0.00	0.39	1.00	0.78
9.03_217.0413	0.00	0.00	1.00	1.00
8.84_221.1903	0.00	0.00	1.00	0.98
6.51_220.1710	0.00	0.13	1.00	0.86
5.15_226.5984	0.00	0.08	1.00	0.85
7.35_225.1140	0.00	0.00	1.00	0.73
7.99_225.1125	0.00	0.02	1.00	0.97
9.04_225.0298	0.00	0.02	0.93	1.00
9.77_224.0325	0.00	0.00	1.00	0.92
5.48_229.0656	0.00	0.00	0.97	1.00
4.02_228.1701	0.00	0.00	0.91	1.00
9.82_230.0718	0.00	0.04	1.00	0.58
8.41_230.0715	0.00	0.00	1.00	0.50
5.11_236.1306	0.00	0.16	0.98	1.00
8.54_235.1344	0.00	0.00	1.00	0.92
9.80_241.0261	0.00	0.00	1.00	0.99
8.82_241.0249	0.00	0.00	1.00	0.85
10.69_238.1826	0.00	0.00	1.00	0.74
5.81_248.1281	0.00	0.23	1.00	0.85
9.03_248.0351	0.00	0.00	1.00	0.90
4.04_247.1287	0.00	0.00	1.00	0.99
7.33_247.0943	0.00	0.18	0.96	1.00
9.07_246.5440	0.00	0.00	1.00	0.72
5.04_244.1219	0.00	0.00	0.84	1.00
4.31_249.0807	0.00	0.00	1.00	0.94
4.56_252.0394	0.00	0.11	1.00	0.57
6.01_252.0391	0.00	0.00	0.63	1.00
7.48_252.0388	0.00	0.00	0.92	1.00

D. Mass Spectral Data for Selected Features

3.87_257.1146	0.00	0.33	0.88	1.00
9.81_253.5524	0.00	0.03	0.89	1.00
12.02_263.1978	0.00	0.03	0.87	1.00
1.78_262.1278	0.00	0.00	1.00	0.89
5.86_262.1048	0.00	0.27	1.00	0.82
10.71_261.1779	0.00	0.01	0.79	1.00
5.01_261.1438	0.00	0.03	0.99	1.00
9.03_260.5527	0.00	0.00	1.00	0.75
10.68_260.1641	0.00	0.00	0.98	1.00
6.81_268.0194	0.00	0.00	1.00	0.67
5.18_266.1406	0.00	0.25	0.71	1.00
5.27_264.2082	0.00	0.00	1.00	0.83
9.67_268.0195	0.00	0.00	0.87	1.00
5.84_281.1328	0.00	0.00	1.00	0.78
7.18_278.2110	0.00	0.00	0.93	1.00
6.07_276.1943	0.00	0.00	0.64	1.00
5.71_286.2118	0.00	0.00	1.00	0.93
9.01_283.1521	0.00	0.07	0.97	1.00
1.73_282.0649	0.00	0.02	0.91	1.00
7.72_281.1420	0.00	0.00	1.00	0.72
5.10_288.1525	0.00	0.05	0.97	1.00
5.22_295.1312	0.00	0.01	1.00	0.86
7.82_294.2085	0.00	0.00	0.89	1.00
4.87_293.1612	0.00	0.29	0.69	1.00
6.49_292.1923	0.00	0.02	1.00	0.68
3.76_299.1387	0.00	0.00	0.70	1.00
2.95_299.1385	0.00	0.00	0.87	1.00
4.74_298.0969	0.00	0.08	1.00	0.91
9.60_297.1694	0.00	0.01	1.00	1.00
7.19_296.2224	0.00	0.00	0.83	1.00
5.83_303.1558	0.00	0.01	1.00	0.98
7.70_303.1206	0.00	0.05	1.00	0.73
12.02_309.1921	0.00	0.01	0.91	1.00
3.90_307.1446	0.00	0.00	0.93	1.00
6.84_312.2197	0.00	0.00	0.85	1.00
10.59_311.1859	0.00	0.00	0.51	1.00
9.79_311.0549	0.00	0.00	0.82	1.00
7.47_310.2026	0.00	0.00	0.81	1.00
1.74_322.0446	0.00	0.02	0.94	1.00
9.13_319.1539	0.00	0.00	0.82	1.00
6.92_318.2094	0.00	0.00	1.00	0.98
6.00_328.7423	0.00	0.09	1.00	0.83
5.91_328.5999	0.00	0.00	0.60	1.00
7.34_326.2353	0.00	0.00	0.84	1.00
6.01_326.2353	0.00	0.00	0.99	1.00
4.97_326.0999	0.00	0.15	0.94	1.00
12.03_325.1706	0.00	0.00	0.99	1.00
6.31_335.7452	0.00	0.00	1.00	0.77
5.84_341.1007	0.00	0.00	0.99	1.00
6.07_337.1394	0.00	0.03	0.91	1.00
10.06_348.2310	0.00	0.00	1.00	0.76
7.48_345.1875	0.00	0.00	0.73	1.00
5.19_344.6196	0.00	0.04	1.00	0.77
7.37_344.2218	0.00	0.00	0.93	1.00
6.06_359.1205	0.00	0.00	1.00	0.82
4.84_357.1855	0.00	0.16	1.00	0.72
5.26_354.0787	0.00	0.16	1.00	0.97
8.24_352.2057	0.00	0.00	0.60	1.00
6.67_362.2335	0.00	0.00	0.62	1.00
6.51_360.2165	0.00	0.00	0.89	1.00
8.53_359.2035	0.00	0.09	1.00	0.90
8.77_368.2219	0.00	0.00	1.00	0.67
7.52_368.2211	0.00	0.00	0.98	1.00
9.80_367.0822	0.00	0.00	0.75	1.00
5.64_366.2063	0.00	0.00	0.90	1.00
7.43_374.2181	0.00	0.00	0.95	1.00
7.83_387.1861	0.00	0.00	0.93	1.00
9.80_387.0731	0.00	0.00	0.74	1.00
6.89_384.2172	0.00	0.01	1.00	0.92
6.24_384.2171	0.00	0.00	0.93	1.00

D. Mass Spectral Data for Selected Features

8.63_398.2317	0.00	0.00	1.00	0.84
1.49_394.1142	0.00	0.00	1.00	0.97
9.40_418.0851	0.00	0.00	0.88	1.00
3.74_416.1928	0.00	0.04	0.77	1.00
8.66_429.0854	0.00	0.00	0.91	1.00
9.08_429.0845	0.00	0.00	0.97	1.00
8.04_432.2606	0.00	0.00	1.00	0.95
1.48_431.0890	0.00	0.37	1.00	0.90
9.07_451.0615	0.00	0.00	0.86	1.00
6.99_443.3240	0.00	0.08	0.84	1.00
9.73_443.1014	0.00	0.00	0.96	1.00
8.33_443.0954	0.00	0.00	1.00	0.99
8.80_443.0945	0.00	0.00	0.88	1.00
6.90_461.2902	0.00	0.00	1.00	0.96
5.90_459.3212	0.00	0.03	1.00	0.95
10.02_459.0960	0.00	0.00	1.00	0.98
9.03_457.1145	0.00	0.01	0.92	1.00
8.67_457.1133	0.00	0.00	0.94	1.00
11.52_456.3791	0.00	0.00	1.00	0.93
6.21_455.1906	0.00	0.15	0.85	1.00
9.81_454.0847	0.00	0.00	0.86	1.00
9.05_454.0819	0.00	0.00	0.97	1.00
6.42_472.2832	0.00	0.00	1.00	0.99
6.46_471.2466	0.00	0.03	1.00	0.83
9.02_468.1011	0.00	0.00	0.91	1.00
8.82_465.0807	0.00	0.00	0.68	1.00
9.79_462.0710	0.00	0.00	0.98	1.00
9.78_481.0499	0.00	0.00	0.92	1.00
4.15_476.2404	0.00	0.00	1.00	0.83
9.02_476.0877	0.00	0.00	1.00	0.85
7.51_499.2782	0.00	0.06	1.00	0.94
9.02_495.0687	0.00	0.00	1.00	0.99
4.37_494.2617	0.00	0.00	0.98	1.00
5.37_493.1709	0.00	0.00	0.91	1.00
1.49_491.1254	0.00	0.17	1.00	0.74
8.58_490.2972	0.00	0.00	0.89	1.00
9.79_513.1525	0.00	0.00	0.94	1.00
6.65_512.8485	0.00	0.00	1.00	0.95
9.09_512.3013	0.00	0.00	0.90	1.00
5.65_504.2609	0.00	0.00	1.00	0.55
5.64_515.2738	0.00	0.02	1.00	0.90
1.76_515.1445	0.00	0.00	0.74	1.00
10.06_526.3139	0.00	0.00	0.69	1.00
7.21_526.2839	0.00	0.08	1.00	1.00
6.79_549.3505	0.00	0.00	1.00	0.90
9.11_548.3433	0.00	0.02	0.83	1.00
7.20_544.2918	0.00	0.00	1.00	0.71
7.57_542.3960	0.00	0.34	0.86	1.00
12.03_565.3746	0.00	0.00	0.94	1.00
9.67_563.3802	0.00	0.00	0.86	1.00
6.90_555.3068	0.00	0.00	1.00	0.95
12.03_549.4012	0.00	0.00	1.00	0.93
9.02_549.3610	0.00	0.01	0.84	1.00
5.52_601.2501	0.00	0.00	1.00	0.97
9.79_576.6021	0.00	0.00	1.00	0.96
9.06_576.6005	0.00	0.00	1.00	0.87
1.25_639.8836	0.00	0.00	1.00	0.94
9.79_683.1204	0.00	0.00	1.00	0.92
9.78_885.1896	0.00	0.00	0.66	1.00
7.69_868.6024	0.00	0.00	1.00	0.84
7.60_846.3434	0.00	0.00	1.00	0.50
7.20_920.0962	0.00	0.00	1.00	0.94
9.80_907.1678	0.00	0.00	0.83	1.00
7.69_1031.1674	0.00	0.20	1.00	0.90
7.65_1000.0444	0.00	0.00	0.89	1.00
7.63_970.6960	0.00	0.00	0.61	1.00
7.63_942.9948	0.00	0.00	0.74	1.00
7.01_1221.4414	0.00	0.00	1.00	0.56
7.00_1216.1209	0.00	0.29	1.00	0.68
9.79_218.0234	0.00	0.02	0.79	1.00

D. Mass Spectral Data for Selected Features

8.34_150.0928	0.00	0.04	0.96	1.00
9.78_465.0808	0.00	0.01	1.00	0.99
6.76_310.2021	0.00	0.00	1.00	0.93
1.64_174.0879	0.01	0.00	1.00	0.96
10.18_621.4210	0.01	0.00	0.87	1.00
8.54_447.2904	0.01	0.05	0.90	1.00
1.82_228.1004	0.01	0.00	1.00	0.93
9.81_269.0437	0.01	0.00	0.81	1.00
1.29_203.9309	0.01	0.00	0.92	1.00
1.64_246.1172	0.01	0.00	0.98	1.00
8.10_301.1534	0.01	0.05	1.00	0.98
7.48_177.0877	0.02	0.00	1.00	0.83
12.02_205.1953	0.02	0.00	0.96	1.00
8.74_542.3146	0.02	0.00	1.00	0.68
9.11_505.3321	0.02	0.00	0.91	1.00
3.22_235.1201	0.02	0.00	1.00	0.97
9.79_1349.2480	0.02	0.00	0.88	1.00
5.66_384.2168	0.02	0.00	1.00	0.89
8.52_491.3179	0.02	0.00	0.86	1.00
6.24_515.2753	0.02	0.01	1.00	0.79
4.82_393.2208	0.02	0.00	1.00	0.79
6.06_294.2084	0.02	0.00	0.89	1.00
8.29_401.1993	0.02	0.00	0.89	1.00
7.06_325.1861	0.02	0.14	1.00	0.99
10.18_223.2085	0.03	0.21	1.00	1.00
1.73_338.0231	0.04	0.00	1.00	0.98
6.65_282.2073	0.04	0.24	0.85	1.00
7.95_433.2783	0.04	0.10	0.90	1.00
5.43_377.1482	0.04	0.00	0.94	1.00
3.07_230.1126	0.05	0.12	1.00	0.79
16.15_710.1773	0.05	0.01	1.00	0.97
1.74_150.0789	0.05	0.00	0.87	1.00
1.70_260.1135	0.05	0.00	0.92	1.00
9.66_279.1583	0.06	0.00	0.85	1.00
6.95_218.1203	0.06	0.12	0.96	1.00
8.53_283.1523	0.06	0.14	0.91	1.00
7.06_221.1900	0.07	0.20	1.00	0.99
5.84_299.0939	0.07	0.03	1.00	0.95
8.53_207.1002	0.07	0.09	0.86	1.00
4.37_326.1802	0.07	0.42	1.00	0.93
8.53_177.0880	0.07	0.07	0.81	1.00
6.71_1160.7578	0.07	0.00	1.00	0.97
3.86_150.0940	0.08	0.14	0.97	1.00
5.83_325.1311	0.08	0.00	1.00	0.92
7.06_203.1787	0.08	0.15	0.98	1.00
9.67_319.1539	0.09	0.12	1.00	0.64
4.75_136.0625	0.09	0.00	0.92	1.00
3.83_198.1623	0.10	0.07	0.94	1.00
7.42_280.1237	0.11	0.29	0.92	1.00
5.97_286.6247	0.11	0.02	1.00	0.82
6.06_203.1781	0.11	0.19	0.86	1.00
3.80_288.1929	0.11	0.10	0.95	1.00
7.91_389.2523	0.12	0.05	0.86	1.00
1.65_159.0768	0.12	0.00	0.96	1.00
9.14_239.1284	0.12	0.11	0.89	1.00
1.73_288.1454	0.14	0.00	1.00	0.56
5.97_278.6345	0.14	0.04	1.00	0.88
5.11_231.1676	0.14	0.51	0.95	1.00
4.88_188.0708	0.15	0.26	0.80	1.00
6.39_336.2172	0.16	0.13	1.00	0.85
6.41_165.0905	0.17	0.11	0.94	1.00
3.85_276.1433	0.19	0.11	0.93	1.00
4.30_310.1305	0.19	0.04	0.95	1.00
6.66_264.1980	0.19	0.08	1.00	0.84
3.82_230.1126	0.20	0.12	0.86	1.00
4.87_329.1844	0.20	0.00	0.89	1.00
4.31_265.0552	0.20	0.00	1.00	0.82
4.64_137.0376	0.21	0.22	1.00	0.97
4.30_478.1379	0.22	0.05	1.00	0.75
7.25_371.1508	0.22	0.00	1.00	0.88

D. Mass Spectral Data for Selected Features

4.12_413.1243	0.24	0.43	1.00	0.82
4.77_179.0472	0.28	0.51	0.90	1.00
7.64_999.9779	0.28	0.00	0.74	1.00
5.27_685.1761	0.29	0.00	1.00	0.91
4.81_464.2611	0.29	0.34	0.99	1.00
16.18_335.9929	0.30	0.00	1.00	0.84
4.86_372.1909	0.30	0.15	1.00	0.91
7.42_196.0651	0.33	0.17	0.85	1.00
9.41_281.1770	0.34	0.65	0.93	1.00
9.47_211.0868	0.34	0.60	0.93	1.00
5.11_307.1591	0.35	0.00	0.97	1.00
5.61_343.2002	0.37	0.08	0.90	1.00
3.80_194.0821	0.38	0.00	0.91	1.00
4.63_149.1104	0.40	0.65	0.88	1.00
12.62_416.2462	0.42	0.52	1.00	0.94
5.16_210.1137	0.44	0.44	0.96	1.00
3.85_258.1333	0.45	0.00	1.00	0.98
4.34_266.1408	0.46	0.36	0.98	1.00
5.34_191.1575	0.48	0.68	0.90	1.00
7.29_331.2114	0.50	0.72	0.94	1.00
12.43_386.2820	0.50	1.00	0.00	0.00
4.32_308.1712	0.50	0.18	1.00	0.91
14.78_323.2583	0.50	1.00	0.00	0.00
13.49_420.3478	0.51	1.00	0.00	0.00
10.60_346.3091	0.51	1.00	0.00	0.00
3.94_180.0961	0.51	0.23	0.88	1.00
13.00_413.3095	0.52	1.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.04	0.00
9.48_225.1993	0.53	1.00	0.01	0.01
14.04_295.2283	0.54	1.00	0.00	0.00
6.81_807.1918	0.54	1.00	0.00	0.00
3.86_242.1126	0.55	0.60	0.90	1.00
13.53_339.2529	0.55	1.00	0.00	0.00
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.00	0.00
10.15_739.4618	0.56	1.00	0.00	0.00
14.41_309.2409	0.56	1.00	0.00	0.00
12.99_526.2341	0.56	1.00	0.08	0.03
10.53_531.4000	0.57	1.00	0.00	0.00
4.29_244.1199	0.57	0.59	1.00	0.98
4.40_158.0302	0.57	0.42	0.92	1.00
12.97_407.3144	0.58	1.00	0.00	0.00
12.98_399.3242	0.58	1.00	0.00	0.00
12.98_510.2581	0.59	1.00	0.12	0.00
6.40_263.1761	0.59	0.63	0.89	1.00
4.37_663.2850	0.59	1.00	0.00	0.00
13.98_433.3418	0.61	1.00	0.00	0.00
6.90_166.0720	0.61	1.00	0.00	0.00
5.72_240.1231	0.62	0.43	1.00	0.88
4.64_412.2067	0.62	1.00	0.11	0.05
6.19_181.1351	0.63	1.00	0.00	0.00
4.39_362.1069	0.63	0.55	1.00	0.89
10.97_401.2525	0.63	1.00	0.00	0.00
4.50_359.1197	0.64	0.72	1.00	0.99
6.15_485.2027	0.65	0.69	0.91	1.00
11.58_415.2745	0.65	1.00	0.00	0.00
12.62_273.1378	0.66	1.00	0.00	0.00
12.86_507.3281	0.66	1.00	0.29	0.26
12.97_290.7254	0.66	1.00	0.05	0.00
4.27_647.2871	0.67	1.00	0.04	0.00
12.82_551.3593	0.67	1.00	0.23	0.23
1.49_594.1582	0.67	0.74	1.00	0.92
11.44_223.2060	0.67	1.00	0.00	0.00
1.50_401.0693	0.67	0.62	1.00	0.90
6.40_439.1986	0.68	0.69	0.94	1.00
12.56_441.2657	0.70	1.00	0.37	0.29
4.59_251.1399	0.70	0.70	1.00	0.86
6.85_824.9348	0.70	1.00	0.00	0.00
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

4.37_150.0945	0.72	1.00	0.00	0.00
12.79_595.3829	0.73	1.00	0.32	0.31
13.98_292.2624	0.73	1.00	0.22	0.21
3.89_518.1743	0.73	1.00	0.00	0.05
12.67_727.4605	0.74	1.00	0.37	0.34
11.18_473.3585	0.75	1.00	0.01	0.01
6.23_251.1781	0.75	0.82	0.94	1.00
12.70_683.4373	0.77	1.00	0.38	0.38
12.86_463.2998	0.77	1.00	0.31	0.00
12.74_443.3505	0.77	1.00	0.00	0.00
10.84_227.1557	0.77	0.85	1.00	0.99
12.97_547.4060	0.77	1.00	0.13	0.08
13.86_425.2896	0.78	1.00	0.17	0.23
5.26_147.0936	0.79	1.00	0.28	0.35
13.50_409.7445	0.80	1.00	0.06	0.00
12.61_771.4862	0.80	1.00	0.38	0.00
11.97_299.2600	0.80	1.00	0.00	0.00
13.50_524.2740	0.81	1.00	0.10	0.04
15.06_413.2647	0.81	1.00	0.19	0.19
12.86_502.3745	0.82	1.00	0.28	0.00
11.84_443.3878	0.82	1.00	0.03	0.00
11.03_354.1608	0.82	1.00	0.00	0.02
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.00
12.73_655.3845	0.83	1.00	0.53	0.47
12.74_639.4067	0.83	1.00	0.44	0.40
13.79_365.2675	0.84	1.00	0.00	0.00
12.80_567.3292	0.85	1.00	0.45	0.00
12.83_546.4021	0.86	1.00	0.28	0.12
10.38_401.3397	0.88	1.00	0.18	0.19
12.67_743.4367	0.88	1.00	0.53	0.47
12.70_699.4109	0.89	1.00	0.61	0.62
14.79_310.3109	0.90	1.00	0.57	0.67
12.79_611.3565	0.91	1.00	0.53	0.41
15.94_338.3442	0.91	1.00	0.41	0.48
13.48_341.2200	0.91	1.00	0.17	0.00
13.49_295.2258	0.91	1.00	0.00	0.00
1.47_508.0657	0.91	1.00	0.73	0.79
12.73_320.2010	0.94	1.00	0.52	0.24
4.49_225.1597	0.97	1.00	0.26	0.27
12.89_441.3208	0.99	1.00	0.18	0.20
12.78_590.4295	1.00	1.00	0.38	0.36
13.95_270.2746	1.00	1.00	0.40	0.47
10.36_211.6353	1.00	0.89	0.22	0.26
3.82_209.1275	1.00	0.90	0.55	0.58
11.31_225.6512	1.00	0.95	0.00	0.00
9.27_240.2315	1.00	0.88	0.00	0.00
10.39_268.2627	1.00	0.83	0.00	0.00
12.97_278.2028	1.00	0.62	0.09	0.02
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00
14.31_325.2414	1.00	0.74	0.00	0.00
14.82_332.2940	1.00	0.65	0.11	0.00
15.49_338.3442	1.00	0.86	0.00	0.23
15.92_360.3229	1.00	0.71	0.26	0.32
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.14	0.15
13.95_411.3586	1.00	0.78	0.00	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.00	0.00
12.86_485.3471	1.00	0.86	0.14	0.29
12.81_529.3766	1.00	0.77	0.39	0.00
12.97_555.3910	1.00	0.94	0.14	0.00
12.79_573.4039	1.00	0.73	0.21	0.24
12.75_617.4294	1.00	0.84	0.10	0.27
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.42	0.21
6.87_807.0837	1.00	0.57	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S18. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S4 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	S4	S4
1.50_165.0624	0.00	0.00	1.00	1.00
6.56_162.0938	0.00	0.00	0.63	1.00
5.78_170.1204	0.00	0.00	0.55	1.00
5.02_180.1014	0.00	0.00	0.73	1.00
4.95_177.1399	0.00	0.17	0.57	1.00
4.14_186.1168	0.00	0.00	1.00	0.70
4.02_198.1143	0.00	0.00	0.81	1.00
9.08_196.0187	0.00	0.00	0.85	1.00
9.80_203.0277	0.00	0.00	0.57	1.00
7.49_207.0994	0.00	0.05	0.62	1.00
4.84_205.1323	0.00	0.00	0.63	1.00
5.48_229.0656	0.00	0.00	0.51	1.00
4.61_230.0715	0.00	0.18	0.90	1.00
4.27_237.0717	0.00	0.26	1.00	0.73
9.80_241.0261	0.00	0.00	1.00	0.67
5.81_248.1281	0.00	0.15	0.83	1.00
5.04_244.1219	0.00	0.00	1.00	0.60
13.78_251.2405	0.00	0.00	0.96	1.00
4.31_249.0807	0.00	0.00	0.78	1.00
8.08_252.0397	0.00	0.00	0.67	1.00
6.01_252.0391	0.00	0.00	0.93	1.00
1.78_262.1278	0.00	0.00	0.87	1.00
5.01_261.1438	0.00	0.17	0.72	1.00
5.18_266.1406	0.00	0.19	1.00	0.90
11.95_266.1298	0.00	0.00	0.74	1.00
7.50_283.1523	0.00	0.03	0.63	1.00
1.73_282.0649	0.00	0.01	0.67	1.00
4.87_293.1612	0.00	0.11	1.00	0.86
4.74_298.0969	0.00	0.15	1.00	0.99
6.00_308.2238	0.00	0.00	1.00	0.90
5.82_322.1007	0.00	0.00	1.00	0.69
1.74_322.0446	0.00	0.01	0.99	1.00
8.76_329.1942	0.00	0.14	1.00	1.00
10.73_340.1475	0.00	0.10	0.65	1.00
14.63_339.2533	0.00	0.00	1.00	0.84
6.07_337.1394	0.00	0.13	0.86	1.00
5.19_344.6196	0.00	0.07	1.00	0.85
5.26_354.0787	0.00	0.14	1.00	0.98
4.01_351.5992	0.00	0.00	0.59	1.00
8.53_359.2035	0.00	0.10	0.54	1.00
5.64_366.2063	0.00	0.00	1.00	0.72
1.49_394.1142	0.00	0.00	0.78	1.00
14.04_420.3477	0.00	0.23	1.00	0.79
11.52_456.3791	0.00	0.00	1.00	0.97
6.21_455.1906	0.00	0.09	0.55	1.00
6.98_499.2793	0.00	0.00	0.78	1.00
5.64_515.2738	0.00	0.02	0.68	1.00
1.49_527.1567	0.00	0.00	1.00	0.53
5.52_601.2501	0.00	0.00	0.57	1.00
1.25_639.8836	0.00	0.00	0.78	1.00
12.72_634.4531	0.00	0.00	1.00	0.79
7.21_916.0943	0.00	0.00	0.69	1.00
3.22_235.1201	0.01	0.00	1.00	0.79
16.15_710.1773	0.02	0.00	0.84	1.00
1.73_338.0231	0.02	0.00	0.93	1.00
1.74_150.0789	0.03	0.00	0.67	1.00
3.86_150.0940	0.04	0.07	0.64	1.00
5.43_377.1482	0.04	0.00	0.57	1.00
6.24_515.2753	0.05	0.02	0.69	1.00
1.82_228.1004	0.05	0.01	1.00	0.68
1.70_260.1135	0.05	0.00	1.00	0.98
4.87_329.1844	0.07	0.00	0.55	1.00
11.79_304.1184	0.08	0.42	0.97	1.00
6.41_165.0905	0.08	0.05	0.87	1.00

D. Mass Spectral Data for Selected Features

11.43_466.2973	0.09	0.27	0.98	1.00
4.30_310.1305	0.10	0.02	0.65	1.00
6.89_843.7588	0.11	0.00	1.00	0.69
15.37_230.0721	0.11	0.37	1.00	0.84
16.24_268.0194	0.11	0.22	1.00	0.94
3.83_198.1623	0.12	0.09	0.63	1.00
16.22_252.0441	0.13	0.23	1.00	0.71
4.30_478.1379	0.14	0.03	0.79	1.00
5.27_685.1761	0.17	0.00	0.60	1.00
4.12_413.1243	0.18	0.31	0.99	1.00
4.34_266.1408	0.21	0.16	1.00	0.65
5.16_210.1137	0.22	0.21	0.63	1.00
3.85_276.1433	0.22	0.13	1.00	0.99
3.80_194.0821	0.23	0.00	1.00	0.91
4.26_450.2439	0.24	0.01	0.78	1.00
13.79_365.2675	0.25	0.29	1.00	0.85
4.38_242.1131	0.26	0.47	1.00	0.76
5.61_343.2002	0.26	0.06	0.84	1.00
16.15_365.1085	0.28	0.00	0.67	1.00
12.73_328.1928	0.28	0.00	0.76	1.00
3.85_258.1333	0.28	0.00	0.69	1.00
5.71_249.1598	0.29	0.40	0.83	1.00
4.32_308.1712	0.29	0.10	1.00	0.79
4.88_188.0708	0.29	0.50	0.78	1.00
4.70_221.1315	0.31	0.45	0.74	1.00
1.50_423.1007	0.33	0.49	1.00	0.76
4.86_372.1909	0.35	0.18	0.71	1.00
4.59_251.1399	0.38	0.37	1.00	0.91
3.82_209.1275	0.38	0.34	0.91	1.00
6.10_320.1966	0.40	0.00	0.77	1.00
6.34_150.0787	0.41	0.39	0.71	1.00
4.60_303.1563	0.43	0.30	1.00	0.71
6.02_274.1066	0.44	0.31	0.85	1.00
12.43_386.2820	0.50	1.00	0.00	0.00
13.97_282.2786	0.50	0.43	0.75	1.00
13.49_420.3478	0.51	1.00	0.04	0.02
10.60_346.3091	0.51	1.00	0.00	0.00
3.86_242.1126	0.51	0.56	0.78	1.00
10.70_288.2557	0.52	1.00	0.00	0.00
3.94_180.0961	0.53	0.24	0.94	1.00
9.48_225.1993	0.53	1.00	0.01	0.00
13.53_339.2529	0.55	1.00	0.00	0.00
4.26_669.2631	0.56	1.00	0.00	0.01
11.80_235.1712	0.56	1.00	0.02	0.10
3.80_119.0369	0.56	1.00	0.14	0.00
10.15_739.4618	0.56	1.00	0.03	0.04
10.53_531.4000	0.57	1.00	0.00	0.00
6.95_368.2220	0.57	1.00	0.00	0.00
12.97_407.3144	0.58	1.00	0.13	0.08
12.98_399.3242	0.58	1.00	0.13	0.08
4.09_573.1785	0.58	1.00	0.00	0.00
4.37_663.2850	0.59	1.00	0.00	0.00
3.79_359.1699	0.60	0.30	1.00	0.89
13.98_433.3418	0.61	1.00	0.00	0.02
6.90_166.0720	0.61	1.00	0.00	0.00
4.64_412.2067	0.62	1.00	0.22	0.25
6.19_181.1351	0.63	1.00	0.00	0.00
11.58_415.2745	0.65	1.00	0.06	0.12
4.27_647.2871	0.67	1.00	0.05	0.09
11.44_223.2060	0.67	1.00	0.00	0.00
1.48_497.0811	0.68	0.39	1.00	0.99
8.08_219.1411	0.68	1.00	0.00	0.00
7.62_970.6124	0.70	1.00	0.00	0.00
4.81_506.2950	0.71	1.00	0.00	0.00
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.38	0.28
4.37_150.0945	0.72	1.00	0.00	0.01
3.89_518.1743	0.73	1.00	0.05	0.01
11.18_473.3585	0.75	1.00	0.03	0.02
12.74_443.3505	0.77	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

12.97_547.4060	0.77	1.00	0.34	0.23
15.06_413.2647	0.81	1.00	0.59	0.55
11.84_443.3878	0.82	1.00	0.04	0.04
11.03_354.1608	0.82	1.00	0.00	0.00
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.07	0.00
5.16_237.1592	0.87	1.00	0.00	0.00
10.38_401.3397	0.88	1.00	0.18	0.23
9.26_219.1735	0.88	1.00	0.00	0.00
13.49_295.2258	0.91	1.00	0.00	0.00
4.49_225.1597	0.97	1.00	0.18	0.14
5.94_213.1018	1.00	0.76	0.00	0.00
10.36_211.6353	1.00	0.89	0.06	0.01
11.31_225.6512	1.00	0.95	0.00	0.00
9.27_240.2315	1.00	0.88	0.16	0.50
10.39_268.2627	1.00	0.83	0.00	0.07
6.59_273.1670	1.00	0.84	0.46	0.23
11.44_291.1951	1.00	0.75	0.00	0.00
12.62_313.2746	1.00	0.83	0.43	0.46
6.39_336.2172	1.00	0.82	0.00	0.00
14.82_332.2940	1.00	0.65	0.08	0.00
15.49_338.3442	1.00	0.86	0.10	0.00
13.48_397.3392	1.00	0.75	0.00	0.00
10.78_415.3581	1.00	0.61	0.24	0.18
13.95_411.3586	1.00	0.78	0.06	0.08
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.00	0.00
10.98_442.3651	1.00	0.78	0.16	0.14
12.97_555.3910	1.00	0.94	0.52	0.61
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.10	0.00
7.66_916.7249	1.00	0.76	0.00	0.26
7.00_916.3325	1.00	0.59	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S19. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S5 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	S5	S5
12.03_135.1163	0.00	0.04	0.79	1.00
12.03_123.1165	0.00	0.00	0.84	1.00
4.95_114.0908	0.00	0.00	0.96	1.00
1.50_103.5345	0.00	0.00	0.92	1.00
12.03_149.1327	0.00	0.00	0.88	1.00
1.50_165.0624	0.00	0.00	1.00	0.96
6.56_162.0938	0.00	0.00	0.82	1.00
16.16_174.0876	0.00	0.00	0.60	1.00
5.78_170.1204	0.00	0.00	0.97	1.00
2.44_166.0747	0.00	0.24	1.00	0.91
6.60_180.1017	0.00	0.01	0.89	1.00
5.02_180.1014	0.00	0.00	0.90	1.00
4.95_177.1399	0.00	0.27	0.99	1.00
9.26_191.1250	0.00	0.00	0.89	1.00
9.12_191.0134	0.00	0.00	0.88	1.00
4.14_186.1168	0.00	0.00	0.81	1.00
4.02_198.1143	0.00	0.00	1.00	0.61
8.84_203.1804	0.00	0.00	0.85	1.00
8.12_203.1781	0.00	0.00	0.96	1.00
6.22_203.0786	0.00	0.02	1.00	0.92
9.80_203.0277	0.00	0.00	0.93	1.00
7.49_207.0994	0.00	0.06	0.86	1.00
1.30_205.9283	0.00	0.00	1.00	0.89
4.84_205.1323	0.00	0.00	1.00	0.89
1.32_211.8786	0.00	0.00	1.00	0.92
1.49_211.0584	0.00	0.25	1.00	0.88
9.81_210.0363	0.00	0.00	1.00	0.65
9.41_219.0312	0.00	0.00	1.00	0.77
8.84_221.1903	0.00	0.00	0.98	1.00
4.61_230.0715	0.00	0.25	1.00	0.81
10.62_236.1643	0.00	0.00	1.00	0.97
5.11_236.1306	0.00	0.11	0.88	1.00
8.54_235.1344	0.00	0.00	0.96	1.00
7.38_246.1513	0.00	0.00	0.62	1.00
2.62_252.0382	0.00	0.47	0.96	1.00
4.31_249.0807	0.00	0.00	0.73	1.00
10.50_252.0400	0.00	0.11	0.52	1.00
8.08_252.0397	0.00	0.00	1.00	0.97
4.56_252.0394	0.00	0.09	0.81	1.00
6.01_252.0391	0.00	0.00	0.56	1.00
7.48_252.0388	0.00	0.00	0.82	1.00
3.58_252.0387	0.00	0.35	1.00	1.00
3.87_257.1146	0.00	0.34	0.72	1.00
9.81_253.5524	0.00	0.12	1.00	0.57
12.02_263.1978	0.00	0.03	0.93	1.00
1.78_262.1278	0.00	0.00	0.74	1.00
5.86_262.1048	0.00	0.22	0.91	1.00
10.71_261.1779	0.00	0.01	0.90	1.00
5.01_261.1438	0.00	0.16	1.00	0.98
9.03_260.5527	0.00	0.00	1.00	0.76
6.81_268.0194	0.00	0.00	0.64	1.00
6.28_268.0191	0.00	0.13	1.00	0.72
10.77_267.1616	0.00	0.05	0.99	1.00
5.18_266.1406	0.00	0.28	1.00	0.89
5.27_264.2082	0.00	0.00	0.97	1.00
4.60_268.0196	0.00	0.00	0.83	1.00
9.12_279.1585	0.00	0.00	0.54	1.00
7.18_278.2110	0.00	0.00	0.79	1.00
6.07_276.1943	0.00	0.00	1.00	0.74
7.50_283.1523	0.00	0.03	0.93	1.00
1.73_282.0649	0.00	0.01	0.74	1.00
7.72_281.1420	0.00	0.00	1.00	0.98
3.86_294.1559	0.00	0.44	0.98	1.00
7.15_293.2251	0.00	0.00	0.69	1.00

D. Mass Spectral Data for Selected Features

4.87_293.1612	0.00	0.19	1.00	0.61
6.49_292.1923	0.00	0.03	0.89	1.00
3.76_299.1387	0.00	0.04	0.68	1.00
7.73_298.2024	0.00	0.00	0.88	1.00
4.74_298.0969	0.00	0.09	1.00	0.92
9.60_297.1694	0.00	0.01	1.00	1.00
7.19_296.2224	0.00	0.00	0.85	1.00
12.02_309.1921	0.00	0.01	0.90	1.00
6.00_308.2238	0.00	0.00	1.00	0.57
6.06_312.2197	0.00	0.00	1.00	0.83
7.24_312.2197	0.00	0.00	0.97	1.00
10.59_311.1859	0.00	0.00	0.80	1.00
5.82_322.1007	0.00	0.00	1.00	0.99
1.74_322.0446	0.00	0.01	0.78	1.00
9.13_319.1539	0.00	0.00	0.91	1.00
6.92_318.2094	0.00	0.00	1.00	0.94
12.03_325.1706	0.00	0.00	0.84	1.00
8.76_329.1942	0.00	0.09	0.81	1.00
10.73_340.1475	0.00	0.14	1.00	0.71
5.99_338.1374	0.00	0.00	1.00	0.97
6.22_346.2031	0.00	0.00	0.95	1.00
7.48_345.1875	0.00	0.00	1.00	0.72
7.37_344.2218	0.00	0.00	0.73	1.00
5.26_354.0787	0.00	0.18	0.81	1.00
4.01_351.5992	0.00	0.00	1.00	0.57
6.67_362.2335	0.00	0.00	1.00	0.74
6.51_360.2165	0.00	0.00	0.96	1.00
8.53_359.2035	0.00	0.13	1.00	0.80
7.52_368.2211	0.00	0.00	0.71	1.00
9.80_367.0822	0.00	0.00	1.00	1.00
7.83_387.1861	0.00	0.00	1.00	1.00
9.80_387.0731	0.00	0.00	0.59	1.00
6.24_384.2171	0.00	0.00	0.71	1.00
1.49_394.1142	0.00	0.00	0.69	1.00
9.08_429.0845	0.00	0.00	1.00	0.88
4.02_423.1940	0.00	0.00	0.75	1.00
7.98_431.2698	0.00	0.06	0.90	1.00
1.48_431.0890	0.00	0.30	0.88	1.00
9.07_451.0615	0.00	0.00	0.68	1.00
6.99_443.3240	0.00	0.23	0.87	1.00
9.73_443.1014	0.00	0.00	1.00	0.95
10.02_459.0960	0.00	0.00	0.87	1.00
9.03_457.1145	0.00	0.02	0.69	1.00
6.21_455.1906	0.00	0.09	0.66	1.00
6.46_471.2466	0.00	0.03	0.93	1.00
9.79_462.0710	0.00	0.00	0.89	1.00
9.78_481.0499	0.00	0.00	0.92	1.00
9.02_479.0963	0.00	0.00	0.83	1.00
7.51_499.2782	0.00	0.02	1.00	0.97
4.37_494.2617	0.00	0.00	0.78	1.00
1.49_527.1567	0.00	0.00	0.55	1.00
7.21_526.2839	0.00	0.15	0.70	1.00
7.20_544.2918	0.00	0.00	1.00	0.80
12.03_549.4012	0.00	0.00	0.87	1.00
5.52_601.2501	0.00	0.00	0.86	1.00
5.18_599.2879	0.00	0.00	1.00	0.78
1.76_588.1814	0.00	0.00	0.69	1.00
1.25_639.8836	0.00	0.00	1.00	0.77
9.79_683.1204	0.00	0.00	1.00	0.63
9.80_907.1678	0.00	0.00	1.00	1.00
7.62_891.8938	0.00	0.00	1.00	0.76
8.34_150.0928	0.00	0.05	1.00	0.94
9.79_218.0234	0.01	0.05	0.92	1.00
6.24_515.2753	0.01	0.00	0.77	1.00
1.29_203.9309	0.01	0.00	1.00	0.72
7.48_177.0877	0.01	0.00	0.69	1.00
8.10_301.1534	0.01	0.03	0.81	1.00
5.66_384.2168	0.01	0.00	0.81	1.00
12.02_205.1953	0.01	0.00	0.84	1.00
9.78_465.0808	0.02	0.04	0.81	1.00

D. Mass Spectral Data for Selected Features

6.76_310.2021	0.02	0.00	0.93	1.00
8.29_401.1993	0.02	0.00	0.93	1.00
6.06_294.2084	0.02	0.00	0.75	1.00
3.22_235.1201	0.03	0.00	1.00	0.84
16.15_710.1773	0.03	0.01	1.00	0.97
9.66_279.1583	0.03	0.00	0.73	1.00
1.73_338.0231	0.04	0.00	0.82	1.00
1.74_150.0789	0.04	0.00	1.00	0.99
10.18_223.2085	0.04	0.25	1.00	0.79
3.07_230.1126	0.05	0.11	0.79	1.00
5.97_286.6247	0.05	0.01	0.92	1.00
8.53_283.1523	0.05	0.10	0.92	1.00
4.37_326.1802	0.05	0.29	0.77	1.00
6.95_218.1203	0.05	0.10	0.89	1.00
9.14_239.1284	0.05	0.05	1.00	0.70
7.42_280.1237	0.06	0.16	0.95	1.00
8.53_177.0880	0.06	0.06	0.72	1.00
3.86_150.0940	0.06	0.11	0.92	1.00
10.52_673.3745	0.06	0.09	0.87	1.00
8.53_207.1002	0.06	0.07	0.84	1.00
5.43_377.1482	0.06	0.00	0.86	1.00
5.97_278.6345	0.06	0.02	1.00	0.96
4.75_136.0625	0.07	0.00	0.66	1.00
1.53_143.0837	0.08	0.10	0.93	1.00
6.72_1450.6973	0.08	0.02	1.00	0.92
6.41_165.0905	0.09	0.06	0.83	1.00
1.77_218.1042	0.09	0.02	0.92	1.00
7.89_192.1015	0.10	0.17	0.80	1.00
7.42_196.0651	0.10	0.05	0.58	1.00
7.06_221.1900	0.12	0.36	1.00	0.97
15.37_230.0721	0.12	0.40	0.82	1.00
4.30_478.1379	0.13	0.03	0.66	1.00
9.47_211.0868	0.13	0.23	0.82	1.00
3.83_198.1623	0.13	0.09	0.86	1.00
4.87_329.1844	0.13	0.00	0.95	1.00
3.82_230.1126	0.14	0.09	0.81	1.00
6.06_203.1781	0.15	0.26	0.83	1.00
7.06_203.1787	0.15	0.28	0.88	1.00
4.30_310.1305	0.15	0.03	0.80	1.00
3.85_276.1433	0.16	0.09	0.78	1.00
6.73_1161.1593	0.16	0.04	0.85	1.00
5.96_534.2942	0.16	0.04	0.97	1.00
6.78_176.0714	0.17	0.28	0.81	1.00
6.71_1160.7578	0.17	0.00	1.00	0.86
9.41_281.1770	0.19	0.36	0.99	1.00
6.73_1160.5609	0.20	0.00	1.00	1.00
1.60_229.1318	0.21	0.04	0.91	1.00
5.27_685.1761	0.22	0.00	0.72	1.00
4.88_188.0708	0.23	0.39	0.94	1.00
5.61_343.2002	0.23	0.05	0.84	1.00
4.81_464.2611	0.24	0.29	0.94	1.00
3.80_194.0821	0.26	0.00	0.66	1.00
9.11_505.3321	0.27	0.00	0.93	1.00
16.22_252.0441	0.28	0.50	0.80	1.00
5.81_605.2195	0.28	0.40	0.77	1.00
16.18_335.9929	0.28	0.00	0.95	1.00
4.32_308.1712	0.29	0.11	0.73	1.00
4.26_450.2439	0.31	0.02	0.69	1.00
6.60_152.1087	0.31	0.58	0.95	1.00
6.74_1160.9454	0.32	0.26	1.00	0.79
4.63_149.1104	0.32	0.51	0.98	1.00
5.34_191.1575	0.32	0.46	0.91	1.00
4.86_372.1909	0.32	0.17	0.79	1.00
4.00_320.1711	0.33	0.04	0.80	1.00
5.16_210.1137	0.33	0.33	0.91	1.00
6.10_320.1966	0.33	0.00	0.70	1.00
1.49_365.1079	0.35	0.48	0.78	1.00
16.15_481.1090	0.35	0.00	0.73	1.00
6.15_485.2027	0.36	0.38	0.68	1.00
7.25_371.1508	0.36	0.00	1.00	0.98

D. Mass Spectral Data for Selected Features

6.40_263.1761	0.36	0.38	0.81	1.00
3.85_258.1333	0.36	0.00	0.73	1.00
4.53_236.1764	0.37	0.48	0.94	1.00
7.29_331.2114	0.38	0.55	0.91	1.00
5.78_164.0706	0.39	0.52	1.00	0.96
8.22_220.1332	0.39	0.57	0.94	1.00
3.75_267.1417	0.40	0.50	0.78	1.00
9.69_220.1127	0.41	0.48	1.00	0.98
5.71_249.1598	0.41	0.57	0.84	1.00
4.40_158.0302	0.42	0.31	1.00	0.98
5.20_239.1759	0.42	0.69	0.98	1.00
4.67_270.1917	0.43	0.59	0.81	1.00
3.79_359.1699	0.45	0.22	0.72	1.00
4.34_266.1408	0.45	0.35	0.75	1.00
3.94_254.1629	0.45	0.17	0.91	1.00
4.70_221.1315	0.45	0.67	0.96	1.00
4.16_256.1718	0.46	0.62	0.88	1.00
12.73_328.1928	0.46	0.00	0.98	1.00
6.40_439.1986	0.47	0.47	0.81	1.00
8.66_655.2795	0.48	1.00	0.00	0.00
6.23_251.1781	0.49	0.54	0.87	1.00
3.93_438.1964	0.49	0.18	0.91	1.00
1.48_610.1314	0.50	0.23	0.82	1.00
10.60_346.3091	0.51	1.00	0.00	0.00
3.86_242.1126	0.51	0.56	0.83	1.00
10.40_371.3275	0.52	1.00	0.02	0.02
9.48_225.1993	0.53	1.00	0.02	0.02
1.50_401.0693	0.54	0.50	1.00	0.98
4.26_669.2631	0.56	1.00	0.00	0.08
11.80_235.1712	0.56	1.00	0.00	0.09
10.15_739.4618	0.56	1.00	0.11	0.07
5.72_240.1231	0.56	0.39	0.89	1.00
10.53_531.4000	0.57	1.00	0.00	0.00
4.37_663.2850	0.59	1.00	0.00	0.00
12.63_394.2284	0.59	0.45	1.00	0.87
6.59_273.1670	0.60	0.51	0.84	1.00
13.48_341.2200	0.60	0.66	1.00	0.86
13.98_433.3418	0.61	1.00	0.05	0.00
5.43_241.1546	0.61	0.63	0.93	1.00
4.64_412.2067	0.62	1.00	0.15	0.20
6.19_181.1351	0.63	1.00	0.08	0.10
10.97_401.2525	0.63	1.00	0.08	0.21
4.64_137.0376	0.64	0.67	0.83	1.00
3.99_164.0936	0.65	0.59	0.89	1.00
11.58_415.2745	0.65	1.00	0.07	0.02
12.62_273.1378	0.66	1.00	0.00	0.00
4.27_647.2871	0.67	1.00	0.09	0.00
11.44_223.2060	0.67	1.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.30	0.24
6.85_824.9348	0.70	1.00	0.00	0.23
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
3.89_518.1743	0.73	1.00	0.06	0.00
11.18_473.3585	0.75	1.00	0.08	0.04
12.74_443.3505	0.77	1.00	0.01	0.00
1.50_230.0720	0.77	0.58	1.00	0.98
11.97_299.2600	0.80	1.00	0.31	0.21
15.06_413.2647	0.81	1.00	0.42	0.57
11.84_443.3878	0.82	1.00	0.11	0.06
11.03_354.1608	0.82	1.00	0.09	0.25
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.15	0.10
5.16_237.1592	0.87	1.00	0.66	0.73
10.38_401.3397	0.88	1.00	0.27	0.16
9.26_219.1735	0.88	1.00	0.00	0.00
4.50_359.1197	0.89	1.00	0.00	0.00
15.94_338.3442	0.91	1.00	0.74	0.68
13.49_295.2258	0.91	1.00	0.06	0.00
1.47_508.0657	0.91	1.00	0.37	0.00

D. Mass Spectral Data for Selected Features

4.49_225.1597	0.97	1.00	0.54	0.56
12.89_441.3208	0.99	1.00	0.49	0.58
10.36_211.6353	1.00	0.89	0.03	0.00
11.31_225.6512	1.00	0.95	0.00	0.00
9.27_240.2315	1.00	0.88	0.00	0.00
10.39_268.2627	1.00	0.83	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
12.62_313.2746	1.00	0.83	0.12	0.11
14.31_325.2414	1.00	0.74	0.00	0.00
15.49_338.3442	1.00	0.86	0.00	0.00
13.48_397.3392	1.00	0.75	0.00	0.00
13.95_411.3586	1.00	0.78	0.06	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.98_442.3651	1.00	0.78	0.00	0.29
12.97_555.3910	1.00	0.94	0.77	0.59
12.75_617.4294	1.00	0.84	0.36	0.00
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.12	0.23
7.00_916.3325	1.00	0.59	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S20. Normalized heat map of features described as unique in figure 2b and c when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the S6 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	S6	S6
12.03_135.1163	0.00	0.04	0.52	1.00
12.03_123.1165	0.00	0.00	0.83	1.00
1.50_103.5345	0.00	0.00	0.90	1.00
12.03_149.1327	0.00	0.00	0.77	1.00
13.61_149.0907	0.00	0.00	1.00	0.65
1.50_165.0624	0.00	0.00	0.96	1.00
6.56_162.0938	0.00	0.00	0.91	1.00
4.31_160.1140	0.00	0.00	0.71	1.00
16.16_174.0876	0.00	0.00	0.77	1.00
5.78_170.1204	0.00	0.00	0.84	1.00
7.08_169.0882	0.00	0.05	0.72	1.00
6.60_180.1017	0.00	0.02	1.00	0.97
5.02_180.1014	0.00	0.00	0.73	1.00
10.70_179.1435	0.00	0.00	1.00	0.89
4.95_177.1399	0.00	0.17	0.64	1.00
4.39_192.1130	0.00	0.27	0.80	1.00
9.12_191.0134	0.00	0.00	0.86	1.00
4.14_186.1168	0.00	0.00	0.86	1.00
4.02_198.1143	0.00	0.00	0.97	1.00
9.08_196.0187	0.00	0.00	0.64	1.00
8.84_203.1804	0.00	0.00	0.95	1.00
8.12_203.1781	0.00	0.00	0.91	1.00
6.22_203.0786	0.00	0.08	1.00	0.92
9.08_203.0278	0.00	0.00	0.77	1.00
9.80_203.0277	0.00	0.00	0.61	1.00
9.42_202.0393	0.00	0.00	0.61	1.00
5.44_208.0539	0.00	0.01	0.91	1.00
7.49_207.0994	0.00	0.07	0.89	1.00
1.30_205.9283	0.00	0.00	0.96	1.00
4.84_205.1323	0.00	0.00	0.62	1.00
10.22_205.1232	0.00	0.00	0.61	1.00
8.67_212.0251	0.00	0.00	1.00	0.81
1.32_211.8786	0.00	0.00	0.94	1.00
1.49_211.0584	0.00	0.14	0.92	1.00
9.81_210.0363	0.00	0.00	0.60	1.00
5.35_210.0350	0.00	0.00	0.84	1.00
9.41_219.0312	0.00	0.00	0.93	1.00
10.24_222.1533	0.00	0.14	1.00	0.98
8.84_221.1903	0.00	0.00	1.00	0.94
6.51_220.1710	0.00	0.04	1.00	0.60
8.67_226.0395	0.00	0.00	1.00	0.94
7.99_225.1125	0.00	0.09	0.76	1.00
9.04_225.0298	0.00	0.02	0.56	1.00
9.77_224.0325	0.00	0.00	0.95	1.00
5.48_229.0656	0.00	0.00	0.95	1.00
9.82_230.0718	0.00	0.05	1.00	0.75
5.11_236.1306	0.00	0.11	0.76	1.00
9.80_241.0261	0.00	0.00	1.00	0.83
8.82_241.0249	0.00	0.00	0.97	1.00
5.04_244.1219	0.00	0.00	0.71	1.00
11.26_250.1814	0.00	0.00	1.00	0.69
8.08_252.0397	0.00	0.00	1.00	0.69
9.63_252.0395	0.00	0.00	0.48	1.00
6.01_252.0391	0.00	0.00	0.79	1.00
5.12_252.0389	0.00	0.00	1.00	0.84
7.48_252.0388	0.00	0.00	0.62	1.00
3.87_257.1146	0.00	0.30	0.82	1.00
12.02_263.1978	0.00	0.03	0.77	1.00
1.78_262.1278	0.00	0.00	0.86	1.00
5.86_262.1048	0.00	0.22	0.90	1.00
10.71_261.1779	0.00	0.00	0.71	1.00
5.01_261.1438	0.00	0.12	0.78	1.00
10.77_267.1616	0.00	0.21	0.58	1.00
5.18_266.1406	0.00	0.18	0.78	1.00

D. Mass Spectral Data for Selected Features

5.27_264.2082	0.00	0.00	1.00	0.78
7.18_278.2110	0.00	0.00	0.83	1.00
6.07_276.1943	0.00	0.00	0.83	1.00
12.79_284.1681	0.00	0.20	0.88	1.00
7.50_283.1523	0.00	0.05	1.00	0.82
1.73_282.0649	0.00	0.01	0.63	1.00
7.82_294.2085	0.00	0.00	1.00	1.00
4.87_293.1612	0.00	0.21	0.98	1.00
6.49_292.1923	0.00	0.03	1.00	0.96
4.74_298.0969	0.00	0.07	1.00	0.84
9.60_297.1694	0.00	0.05	0.66	1.00
7.19_296.2224	0.00	0.00	0.94	1.00
3.78_300.1386	0.00	0.10	0.69	1.00
12.02_309.1921	0.00	0.01	0.99	1.00
6.00_308.2238	0.00	0.00	0.80	1.00
6.06_312.2197	0.00	0.00	1.00	0.91
6.84_312.2197	0.00	0.00	0.91	1.00
7.24_312.2197	0.00	0.00	1.00	0.78
5.82_322.1007	0.00	0.00	1.00	0.98
6.92_318.2094	0.00	0.00	1.00	0.76
7.34_326.2353	0.00	0.00	1.00	0.82
6.01_326.2353	0.00	0.00	0.80	1.00
12.03_325.1706	0.00	0.00	0.78	1.00
8.76_329.1942	0.00	0.06	0.98	1.00
5.84_341.1007	0.00	0.00	1.00	0.70
5.19_344.6196	0.00	0.18	0.77	1.00
7.37_344.2218	0.00	0.00	0.98	1.00
5.26_354.0787	0.00	0.13	1.00	0.83
8.24_352.2057	0.00	0.00	0.91	1.00
4.01_351.5992	0.00	0.00	1.00	1.00
6.67_362.2335	0.00	0.00	0.67	1.00
6.51_360.2165	0.00	0.00	1.00	0.75
9.80_367.0822	0.00	0.00	0.61	1.00
9.80_387.0731	0.00	0.00	0.64	1.00
6.88_386.2329	0.00	0.01	1.00	0.82
6.89_384.2172	0.00	0.00	0.57	1.00
6.24_384.2171	0.00	0.00	0.92	1.00
8.63_398.2317	0.00	0.00	0.87	1.00
1.49_394.1142	0.00	0.00	0.83	1.00
3.74_416.1928	0.00	0.07	0.72	1.00
9.08_429.0845	0.00	0.00	1.00	0.92
4.02_423.1940	0.00	0.00	0.55	1.00
9.07_451.0615	0.00	0.00	0.78	1.00
6.99_443.3240	0.00	0.15	1.00	0.61
9.73_443.1014	0.00	0.00	1.00	0.99
8.80_443.0945	0.00	0.00	0.95	1.00
10.02_459.0960	0.00	0.00	1.00	0.93
9.03_457.1145	0.00	0.01	1.00	0.98
6.21_455.1906	0.00	0.10	0.95	1.00
9.81_454.0847	0.00	0.00	0.80	1.00
9.05_454.0819	0.00	0.00	1.00	0.98
6.46_471.2466	0.00	0.01	0.76	1.00
8.82_465.0807	0.00	0.00	0.84	1.00
9.79_462.0710	0.00	0.00	0.68	1.00
9.04_462.0699	0.00	0.00	0.59	1.00
9.78_481.0499	0.00	0.00	0.87	1.00
9.02_479.0963	0.00	0.00	0.79	1.00
7.37_478.2069	0.00	0.12	0.69	1.00
4.15_476.2404	0.00	0.00	1.00	0.96
7.51_499.2782	0.00	0.05	1.00	0.83
8.58_490.2972	0.00	0.00	1.00	0.76
9.79_513.1525	0.00	0.00	0.79	1.00
5.64_515.2738	0.00	0.01	0.57	1.00
6.62_515.2737	0.00	0.00	1.00	0.61
1.76_515.1445	0.00	0.00	0.60	1.00
7.21_526.2839	0.00	0.02	1.00	0.95
7.20_544.2918	0.00	0.00	1.00	0.68
6.63_570.3104	0.00	0.00	0.95	1.00
12.03_565.3746	0.00	0.00	0.96	1.00
9.67_563.3802	0.00	0.00	0.86	1.00

D. Mass Spectral Data for Selected Features

6.90_555.3068	0.00	0.00	0.84	1.00
1.72_551.1035	0.00	0.00	0.72	1.00
12.03_549.4012	0.00	0.00	1.00	0.86
9.02_590.6205	0.00	0.00	0.87	1.00
9.79_576.6021	0.00	0.00	0.77	1.00
1.25_639.8836	0.00	0.00	0.63	1.00
12.72_634.4531	0.00	0.00	1.00	0.53
9.79_683.1204	0.00	0.00	0.84	1.00
7.20_920.0962	0.00	0.00	1.00	0.83
9.80_907.1678	0.00	0.00	1.00	1.00
7.01_1221.4414	0.00	0.00	0.91	1.00
9.79_218.0234	0.00	0.01	0.64	1.00
8.34_150.0928	0.00	0.03	0.85	1.00
9.78_465.0808	0.00	0.01	0.78	1.00
9.81_269.0437	0.00	0.00	0.57	1.00
6.76_310.2021	0.00	0.00	0.99	1.00
6.24_515.2753	0.01	0.00	1.00	0.78
8.10_301.1534	0.01	0.03	1.00	0.92
5.66_384.2168	0.01	0.00	0.95	1.00
1.29_203.9309	0.01	0.00	0.99	1.00
7.48_177.0877	0.01	0.00	0.81	1.00
8.74_542.3146	0.01	0.00	1.00	0.77
12.02_205.1953	0.01	0.00	0.89	1.00
3.22_235.1201	0.02	0.00	0.59	1.00
6.65_282.2073	0.02	0.11	1.00	0.97
16.15_710.1773	0.02	0.01	1.00	0.63
5.43_377.1482	0.02	0.00	0.85	1.00
8.54_447.2904	0.02	0.21	1.00	1.00
1.74_150.0789	0.03	0.00	0.69	1.00
8.53_177.0880	0.03	0.03	0.81	1.00
4.75_136.0625	0.03	0.00	0.83	1.00
8.53_283.1523	0.03	0.07	1.00	0.92
6.95_218.1203	0.03	0.07	0.71	1.00
8.53_207.1002	0.04	0.04	0.97	1.00
9.79_1349.2480	0.04	0.00	0.82	1.00
7.06_325.1861	0.04	0.21	1.00	0.95
1.73_338.0231	0.04	0.00	1.00	0.98
3.86_150.0940	0.04	0.08	0.83	1.00
10.52_673.3745	0.05	0.08	0.97	1.00
3.07_230.1126	0.06	0.14	1.00	0.79
1.70_260.1135	0.06	0.00	0.83	1.00
1.82_228.1004	0.06	0.01	0.92	1.00
10.18_223.2085	0.06	0.39	1.00	0.81
1.53_143.0837	0.07	0.09	0.75	1.00
7.42_196.0651	0.07	0.04	0.55	1.00
4.82_393.2208	0.07	0.00	1.00	0.93
6.66_264.1980	0.08	0.03	0.99	1.00
6.41_165.0905	0.08	0.06	0.80	1.00
7.42_280.1237	0.09	0.26	1.00	0.96
4.87_329.1844	0.10	0.00	0.91	1.00
5.27_685.1761	0.10	0.00	0.77	1.00
6.78_176.0714	0.11	0.18	0.79	1.00
7.06_221.1900	0.11	0.34	0.90	1.00
7.89_192.1015	0.11	0.20	0.74	1.00
5.97_286.6247	0.12	0.02	0.83	1.00
4.30_310.1305	0.12	0.03	0.95	1.00
7.06_203.1787	0.12	0.23	0.87	1.00
5.97_278.6345	0.12	0.03	0.61	1.00
6.06_203.1781	0.13	0.22	0.92	1.00
1.77_218.1042	0.13	0.03	0.92	1.00
9.47_211.0868	0.13	0.23	0.78	1.00
16.18_335.9929	0.14	0.00	1.00	0.75
5.81_605.2195	0.14	0.20	0.97	1.00
3.82_230.1126	0.16	0.10	1.00	0.92
4.63_149.1104	0.21	0.35	0.81	1.00
4.88_188.0708	0.22	0.37	1.00	1.00
7.29_331.2114	0.22	0.32	0.81	1.00
4.31_265.0552	0.22	0.00	0.66	1.00
1.60_229.1318	0.23	0.05	0.90	1.00
8.29_401.1993	0.24	0.00	0.86	1.00

D. Mass Spectral Data for Selected Features

1.73_288.1454	0.24	0.00	1.00	0.94
5.81_222.1598	0.25	0.48	0.91	1.00
6.60_152.1087	0.26	0.47	0.83	1.00
4.64_137.0376	0.26	0.27	0.75	1.00
16.15_365.1085	0.28	0.00	1.00	0.86
6.15_485.2027	0.29	0.31	0.98	1.00
4.77_179.0472	0.29	0.54	0.96	1.00
6.34_150.0787	0.31	0.29	0.81	1.00
4.34_266.1408	0.31	0.24	0.72	1.00
16.18_204.8884	0.32	0.00	1.00	0.98
8.22_220.1332	0.33	0.49	0.84	1.00
5.78_164.0706	0.34	0.46	0.95	1.00
6.62_297.1617	0.34	0.61	0.90	1.00
5.71_249.1598	0.35	0.49	0.88	1.00
4.40_158.0302	0.36	0.26	0.83	1.00
4.70_268.1679	0.36	0.65	1.00	0.99
3.80_288.1929	0.37	0.32	1.00	0.77
4.67_270.1917	0.38	0.52	0.97	1.00
4.16_256.1718	0.38	0.51	0.99	1.00
4.00_320.1711	0.38	0.04	1.00	0.73
3.94_254.1629	0.39	0.15	1.00	0.94
6.34_469.2088	0.39	0.51	1.00	0.92
5.16_210.1137	0.41	0.40	0.80	1.00
16.17_188.9130	0.42	0.00	1.00	1.00
6.23_251.1781	0.42	0.46	0.81	1.00
6.40_263.1761	0.43	0.46	0.91	1.00
3.75_267.1417	0.44	0.55	0.98	1.00
6.10_320.1966	0.44	0.00	0.94	1.00
3.82_209.1275	0.44	0.40	0.78	1.00
4.66_304.1776	0.45	0.67	1.00	0.97
6.40_439.1986	0.46	0.46	1.00	1.00
11.27_448.3444	0.48	1.00	0.00	0.00
12.43_386.2820	0.50	1.00	0.00	0.00
3.75_245.1607	0.50	0.67	1.00	0.91
16.14_274.0340	0.51	0.36	1.00	0.77
10.60_346.3091	0.51	1.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.00	0.00
10.70_288.2557	0.52	1.00	0.00	0.00
3.86_242.1126	0.52	0.57	0.82	1.00
9.48_225.1993	0.53	1.00	0.00	0.02
3.94_180.0961	0.54	0.24	0.90	1.00
6.74_1160.9454	0.54	0.45	0.89	1.00
3.79_359.1699	0.55	0.27	0.90	1.00
13.53_339.2529	0.55	1.00	0.00	0.00
7.22_541.3491	0.56	1.00	0.00	0.10
4.26_669.2631	0.56	1.00	0.00	0.00
11.80_235.1712	0.56	1.00	0.06	0.07
10.15_739.4618	0.56	1.00	0.08	0.07
14.41_309.2409	0.56	1.00	0.22	0.09
5.95_273.1788	0.56	1.00	0.23	0.00
10.53_531.4000	0.57	1.00	0.00	0.00
4.59_251.1399	0.57	0.57	0.85	1.00
12.97_407.3144	0.58	1.00	0.24	0.02
5.72_240.1231	0.58	0.40	0.95	1.00
6.02_274.1066	0.58	0.40	0.86	1.00
12.98_399.3242	0.58	1.00	0.22	0.02
4.37_663.2850	0.59	1.00	0.00	0.00
13.98_433.3418	0.61	1.00	0.04	0.00
6.90_166.0720	0.61	1.00	0.00	0.00
5.20_239.1759	0.62	1.00	0.25	0.31
9.69_220.1127	0.62	0.72	0.88	1.00
4.64_412.2067	0.62	1.00	0.07	0.20
6.19_181.1351	0.63	1.00	0.06	0.11
10.97_401.2525	0.63	1.00	0.00	0.09
11.58_415.2745	0.65	1.00	0.00	0.03
12.62_273.1378	0.66	1.00	0.00	0.00
4.27_647.2871	0.67	1.00	0.00	0.07
1.50_448.0831	0.67	1.00	0.19	0.00
11.44_223.2060	0.67	1.00	0.00	0.00
1.50_423.1007	0.67	1.00	0.00	0.20

D. Mass Spectral Data for Selected Features

8.08_219.1411	0.68	1.00	0.00	0.00
4.81_415.2090	0.69	0.48	0.91	1.00
16.15_442.8736	0.71	1.00	0.00	0.00
7.07_184.1710	0.72	1.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00
3.89_518.1743	0.73	1.00	0.00	0.02
11.18_473.3585	0.75	1.00	0.04	0.02
12.86_463.2998	0.77	1.00	0.31	0.33
12.74_443.3505	0.77	1.00	0.00	0.00
12.97_547.4060	0.77	1.00	0.46	0.06
13.86_425.2896	0.78	1.00	0.55	0.40
11.97_299.2600	0.80	1.00	0.05	0.00
15.06_413.2647	0.81	1.00	0.53	0.42
11.84_443.3878	0.82	1.00	0.14	0.07
11.03_354.1608	0.82	1.00	0.06	0.05
11.28_440.3462	0.82	1.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.00	0.00
13.79_365.2675	0.84	1.00	0.00	0.00
4.81_464.2611	0.84	1.00	0.48	0.21
12.83_546.4021	0.86	1.00	0.71	0.59
10.38_401.3397	0.88	1.00	0.41	0.26
9.26_219.1735	0.88	1.00	0.00	0.00
10.84_227.1557	0.90	1.00	0.62	0.43
15.94_338.3442	0.91	1.00	0.58	0.52
13.49_295.2258	0.91	1.00	0.05	0.01
1.47_508.0657	0.91	1.00	0.53	0.67
1.50_260.0296	0.92	1.00	0.28	0.12
12.73_320.2010	0.94	1.00	0.00	0.37
4.49_225.1597	0.97	1.00	0.22	0.24
5.43_241.1546	0.98	1.00	0.00	0.00
12.89_441.3208	0.99	1.00	0.65	0.48
3.99_164.0936	1.00	0.90	0.67	0.59
1.64_174.0879	1.00	0.59	0.00	0.00
5.94_213.1018	1.00	0.76	0.00	0.00
10.36_211.6353	1.00	0.89	0.00	0.00
11.31_225.6512	1.00	0.95	0.03	0.00
9.27_240.2315	1.00	0.88	0.00	0.30
10.39_268.2627	1.00	0.83	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00
11.33_299.2599	1.00	0.77	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00
14.31_325.2414	1.00	0.74	0.00	0.24
4.25_343.1235	1.00	0.70	0.00	0.00
15.49_338.3442	1.00	0.86	0.00	0.00
13.48_397.3392	1.00	0.75	0.03	0.00
13.95_411.3586	1.00	0.78	0.06	0.00
13.27_419.3131	1.00	0.81	0.00	0.00
10.77_434.3251	1.00	0.58	0.00	0.00
12.86_485.3471	1.00	0.86	0.57	0.49
1.61_539.0459	1.00	0.57	0.00	0.00
13.92_641.5490	1.00	0.85	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.00
7.66_916.7249	1.00	0.76	0.00	0.25

D. Mass Spectral Data for Selected Features

Table S21. Normalized heat map of features described as unique in figure 2a when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* and S5 streptomycin resistant mutant to the R4 rifampicin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	R4	R4	S5	S5
1.51_137.5554	0.00	0.00	1.00	0.52	0.00	0.00
1.52_129.5659	0.00	0.00	1.00	0.52	0.00	0.00
4.95_114.0908	0.00	0.00	0.45	1.00	0.12	0.13
4.31_160.1140	0.00	0.00	0.67	1.00	0.00	0.00
9.08_196.0187	0.00	0.00	0.79	1.00	0.00	0.00
8.68_204.0325	0.00	0.00	0.72	1.00	0.00	0.00
9.08_203.0278	0.00	0.00	0.76	1.00	0.00	0.05
9.42_202.0393	0.00	0.00	0.68	1.00	0.00	0.00
1.42_201.0074	0.00	0.00	0.79	1.00	0.00	0.00
4.54_208.1355	0.00	0.00	0.90	1.00	0.02	0.00
8.67_212.0251	0.00	0.00	0.63	1.00	0.00	0.01
9.25_211.0284	0.00	0.01	1.00	0.92	0.00	0.00
8.31_210.0369	0.00	0.00	0.81	1.00	0.00	0.00
9.81_210.0363	0.00	0.00	1.00	0.66	0.23	0.15
9.07_210.0305	0.00	0.00	0.77	1.00	0.00	0.00
9.41_219.0312	0.00	0.00	1.00	0.86	0.04	0.03
8.67_218.0490	0.00	0.00	0.82	1.00	0.00	0.00
9.03_217.0413	0.00	0.00	0.70	1.00	0.05	0.02
2.51_216.0981	0.00	0.02	0.49	1.00	0.05	0.08
16.16_223.9875	0.00	0.00	0.90	1.00	0.00	0.00
6.51_220.1710	0.00	0.04	1.00	0.99	0.00	0.00
4.58_226.1445	0.00	0.00	1.00	0.82	0.00	0.00
5.11_226.1427	0.00	0.02	0.53	1.00	0.00	0.00
8.67_226.0395	0.00	0.00	0.61	1.00	0.15	0.00
9.04_225.0298	0.00	0.01	0.74	1.00	0.04	0.00
9.77_224.0325	0.00	0.00	0.63	1.00	0.32	0.09
5.11_227.1386	0.00	0.00	0.56	1.00	0.00	0.00
9.19_230.0719	0.00	0.00	1.00	0.54	0.00	0.00
9.82_230.0718	0.00	0.03	0.91	1.00	0.16	0.50
4.89_235.1441	0.00	0.00	0.93	1.00	0.00	0.00
9.80_241.0261	0.00	0.00	1.00	0.78	0.00	0.09
8.82_241.0249	0.00	0.00	1.00	0.94	0.00	0.00
9.03_248.0351	0.00	0.00	0.80	1.00	0.00	0.00
4.04_247.1287	0.00	0.00	0.50	1.00	0.00	0.05
9.07_246.5440	0.00	0.00	0.71	1.00	0.03	0.01
5.63_245.1880	0.00	0.00	1.00	0.83	0.00	0.00
5.04_244.1219	0.00	0.00	0.85	1.00	0.13	0.00
4.70_243.1326	0.00	0.00	0.55	1.00	0.00	0.10
8.52_250.0297	0.00	0.00	0.76	1.00	0.00	0.00
9.81_253.5524	0.00	0.02	0.91	1.00	0.13	0.07
9.91_261.5430	0.00	0.00	1.00	0.65	0.00	0.00
9.03_260.5527	0.00	0.00	0.72	1.00	0.05	0.04
10.77_267.1616	0.00	0.02	1.00	1.00	0.31	0.32
9.67_268.0195	0.00	0.00	1.00	0.94	0.49	0.00
7.18_278.2110	0.00	0.00	0.62	1.00	0.05	0.06
6.07_276.1943	0.00	0.00	0.57	1.00	0.19	0.14
5.71_286.2118	0.00	0.00	0.84	1.00	0.08	0.32
7.19_284.2219	0.00	0.00	0.63	1.00	0.00	0.08
5.22_295.1312	0.00	0.05	0.70	1.00	0.10	0.00
7.48_294.2085	0.00	0.00	1.00	0.58	0.00	0.03
7.82_294.2085	0.00	0.00	0.56	1.00	0.00	0.08
6.82_294.2084	0.00	0.00	0.63	1.00	0.18	0.00
7.73_298.2024	0.00	0.00	0.60	1.00	0.09	0.10
7.19_296.2224	0.00	0.00	0.58	1.00	0.05	0.06
6.00_308.2238	0.00	0.00	0.64	1.00	0.07	0.04
6.92_313.1550	0.00	0.00	0.55	1.00	0.09	0.00
6.06_312.2197	0.00	0.00	0.84	1.00	0.10	0.09
6.84_312.2197	0.00	0.00	0.52	1.00	0.06	0.00
9.79_311.0549	0.00	0.00	0.57	1.00	0.00	0.22
3.86_320.0995	0.00	0.00	0.64	1.00	0.00	0.01
6.92_318.2094	0.00	0.00	0.76	1.00	0.11	0.10
5.91_328.5999	0.00	0.00	0.65	1.00	0.06	0.00

D. Mass Spectral Data for Selected Features

7.34_326.2353	0.00	0.00	0.58	1.00	0.03	0.06
6.01_326.2353	0.00	0.00	0.79	1.00	0.12	0.03
4.97_326.0999	0.00	0.23	0.83	1.00	0.00	0.00
6.08_324.1828	0.00	0.09	0.64	1.00	0.08	0.21
6.62_334.2005	0.00	0.00	0.50	1.00	0.00	0.00
5.84_341.1007	0.00	0.00	0.59	1.00	0.00	0.00
6.22_346.2031	0.00	0.00	1.00	0.86	0.26	0.27
7.37_344.2218	0.00	0.00	0.66	1.00	0.03	0.04
8.24_352.2057	0.00	0.00	0.54	1.00	0.07	0.00
6.67_362.2335	0.00	0.00	1.00	0.86	0.07	0.05
6.51_360.2165	0.00	0.00	1.00	0.81	0.20	0.21
8.77_368.2219	0.00	0.00	0.73	1.00	0.09	0.00
6.02_368.2219	0.00	0.04	0.72	1.00	0.00	0.00
9.80_367.0822	0.00	0.00	0.66	1.00	0.13	0.13
5.64_366.2063	0.00	0.00	0.71	1.00	0.00	0.00
8.47_382.2398	0.00	0.00	0.89	1.00	0.05	0.00
7.30_389.1593	0.00	0.00	1.00	0.89	0.16	0.00
9.80_387.0731	0.00	0.00	0.56	1.00	0.08	0.13
6.88_386.2329	0.00	0.00	0.66	1.00	0.11	0.00
8.63_398.2317	0.00	0.00	0.65	1.00	0.00	0.00
9.40_418.0851	0.00	0.00	0.59	1.00	0.00	0.00
8.66_429.0854	0.00	0.00	0.56	1.00	0.00	0.00
9.08_429.0845	0.00	0.00	0.57	1.00	0.02	0.02
9.15_440.0708	0.00	0.00	0.59	1.00	0.00	0.00
9.42_432.0873	0.00	0.00	0.65	1.00	0.00	0.00
9.09_448.0576	0.00	0.00	0.61	1.00	0.00	0.00
9.73_443.1014	0.00	0.00	0.82	1.00	0.06	0.06
8.33_443.0954	0.00	0.00	0.93	1.00	0.03	0.00
8.80_443.0945	0.00	0.00	0.61	1.00	0.00	0.00
6.90_461.2902	0.00	0.00	0.90	1.00	0.29	0.00
10.02_459.0960	0.00	0.00	0.58	1.00	0.07	0.09
9.03_457.1145	0.00	0.00	0.60	1.00	0.03	0.04
8.67_457.1133	0.00	0.00	0.66	1.00	0.00	0.00
3.92_456.2075	0.00	0.32	0.61	1.00	0.00	0.00
9.81_454.0847	0.00	0.00	0.78	1.00	0.00	0.03
9.05_454.0819	0.00	0.00	0.57	1.00	0.00	0.00
6.42_472.2832	0.00	0.00	0.75	1.00	0.00	0.02
6.46_471.2466	0.00	0.01	0.64	1.00	0.19	0.21
10.02_470.0758	0.00	0.00	0.62	1.00	0.00	0.00
9.02_468.1011	0.00	0.00	0.58	1.00	0.00	0.00
9.08_467.0388	0.00	0.00	0.79	1.00	0.00	0.00
8.31_465.0807	0.00	0.00	0.70	1.00	0.00	0.00
8.82_465.0807	0.00	0.00	0.67	1.00	0.00	0.00
9.79_462.0710	0.00	0.00	0.72	1.00	0.03	0.03
9.04_462.0699	0.00	0.00	0.61	1.00	0.00	0.00
7.03_483.0939	0.00	0.00	0.72	1.00	0.00	0.00
9.78_481.0499	0.00	0.00	1.00	0.75	0.07	0.08
9.02_479.0963	0.00	0.00	0.62	1.00	0.04	0.04
10.01_478.0692	0.00	0.00	0.53	1.00	0.00	0.00
4.15_476.2404	0.00	0.00	0.56	1.00	0.00	0.03
9.02_476.0877	0.00	0.00	0.55	1.00	0.00	0.00
7.06_475.1057	0.00	0.00	0.61	1.00	0.00	0.01
9.02_495.0687	0.00	0.00	0.70	1.00	0.00	0.03
5.37_493.1709	0.00	0.00	1.00	0.69	0.00	0.14
9.79_513.1525	0.00	0.00	0.48	1.00	0.00	0.00
1.76_515.1445	0.00	0.00	0.74	1.00	0.00	0.00
10.06_526.3139	0.00	0.00	1.00	0.54	0.02	0.00
7.20_544.2918	0.00	0.00	0.61	1.00	0.20	0.16
9.00_540.1495	0.00	0.00	0.63	1.00	0.00	0.00
6.63_570.3104	0.00	0.00	0.91	1.00	0.00	0.00
9.08_562.5875	0.00	0.00	0.62	1.00	0.00	0.00
7.14_560.1805	0.00	0.00	0.64	1.00	0.13	0.00
9.02_590.6205	0.00	0.00	0.63	1.00	0.00	0.00
9.79_576.6021	0.00	0.00	1.00	0.60	0.03	0.00
9.06_576.6005	0.00	0.00	0.60	1.00	0.00	0.00
9.07_662.0928	0.00	0.00	0.48	1.00	0.00	0.00
9.02_704.1451	0.00	0.00	0.54	1.00	0.00	0.00
9.03_696.1548	0.00	0.00	0.49	1.00	0.00	0.00
9.71_694.1152	0.00	0.00	0.66	1.00	0.00	0.00
9.03_690.1259	0.00	0.00	0.54	1.00	0.00	0.00

D. Mass Spectral Data for Selected Features

9.79_683.1204	0.00	0.00	1.00	0.68	0.00	0.00
9.06_676.1101	0.00	0.00	0.53	1.00	0.00	0.00
9.41_675.1324	0.00	0.00	0.54	1.00	0.00	0.00
9.78_885.1896	0.00	0.00	0.47	1.00	0.00	0.00
9.07_879.1306	0.00	0.00	0.69	1.00	0.00	0.00
9.02_935.1961	0.00	0.00	0.53	1.00	0.00	0.00
7.21_916.0943	0.00	0.00	1.00	0.78	0.13	0.00
9.80_907.1678	0.00	0.00	0.82	1.00	0.01	0.01
9.04_907.1662	0.00	0.00	0.51	1.00	0.02	0.00
9.41_904.1590	0.00	0.00	0.53	1.00	0.00	0.00
7.67_1031.2480	0.00	0.14	0.97	1.00	0.47	0.00
7.69_1031.1674	0.00	0.10	1.00	0.91	0.13	0.22
7.67_1031.0798	0.00	0.00	0.91	1.00	0.00	0.00
7.69_1000.1273	0.00	0.00	0.49	1.00	0.00	0.07
7.63_942.9948	0.00	0.00	1.00	0.90	0.00	0.00
7.01_1221.4414	0.00	0.00	0.55	1.00	0.00	0.00
9.41_1125.2062	0.00	0.00	0.48	1.00	0.00	0.00
9.78_465.0808	0.00	0.00	0.87	1.00	0.09	0.11
9.79_1349.2480	0.00	0.00	0.51	1.00	0.00	0.00
6.06_294.2084	0.00	0.00	0.59	1.00	0.11	0.14
9.81_269.0437	0.00	0.00	0.61	1.00	0.17	0.00
6.65_282.2073	0.01	0.04	0.76	1.00	0.00	0.14
8.74_542.3146	0.01	0.00	1.00	0.73	0.00	0.00
1.64_246.1172	0.02	0.00	0.74	1.00	0.19	0.00
1.64_174.0879	0.02	0.01	1.00	0.56	0.12	0.01
6.66_264.1980	0.03	0.01	0.63	1.00	0.00	0.02
1.70_260.1135	0.08	0.00	0.75	1.00	0.49	0.00
7.25_371.1508	0.09	0.00	0.67	1.00	0.26	0.25
10.18_621.4210	0.13	0.00	0.59	1.00	0.00	0.00
3.80_288.1929	0.15	0.13	1.00	0.77	0.13	0.00
3.86_338.1113	0.19	0.00	0.65	1.00	0.00	0.18
7.91_389.2523	0.23	0.10	0.63	1.00	0.34	0.00
4.39_362.1069	0.62	0.54	0.00	0.05	0.64	1.00
12.61_771.4862	0.68	0.85	0.40	0.33	0.86	1.00
12.67_727.4605	0.69	0.94	0.21	0.30	0.86	1.00
12.79_595.3829	0.73	1.00	0.46	0.37	0.79	0.83
12.70_683.4373	0.77	1.00	0.48	0.36	0.89	0.90
12.78_590.4295	0.78	0.78	0.32	0.26	0.79	1.00
12.73_655.3845	0.83	1.00	0.56	0.44	0.82	1.00
12.80_567.3292	0.85	1.00	0.55	0.36	0.75	0.92
14.79_310.3109	0.85	0.95	0.48	0.50	0.72	1.00
12.83_546.4021	0.86	1.00	0.00	0.24	0.76	0.84
5.16_237.1592	0.87	1.00	0.21	0.29	0.66	0.73
15.94_338.3442	0.91	1.00	0.32	0.34	0.74	0.68
11.33_299.2599	1.00	0.77	0.00	0.00	0.69	0.51
4.42_351.1212	1.00	0.79	0.09	0.14	0.79	0.66
15.92_360.3229	1.00	0.71	0.22	0.13	0.66	0.88

D. Mass Spectral Data for Selected Features

Table S22. Normalized heat map of features described as unique in figure 2a when comparing wild type *Nocardiopsis sp. FU40* Δ ApoS8 and R4 rifampicin resistant mutant to the S5 streptomycin resistant mutant extract using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	R4	R4	S5	S5
12.03_135.1163	0.00	0.04	0.00	0.00	0.79	1.00
12.03_123.1165	0.00	0.00	0.00	0.00	0.84	1.00
12.03_149.1327	0.00	0.00	0.00	0.00	0.88	1.00
6.56_162.0938	0.00	0.00	0.28	0.35	0.82	1.00
16.16_174.0876	0.00	0.00	0.00	0.00	0.60	1.00
6.60_180.1017	0.00	0.01	0.23	0.40	0.89	1.00
8.84_203.1804	0.00	0.00	0.00	0.00	0.85	1.00
8.12_203.1781	0.00	0.00	0.00	0.00	0.96	1.00
6.22_203.0786	0.00	0.02	0.00	0.00	1.00	0.92
7.49_207.0994	0.00	0.06	0.28	0.52	0.86	1.00
8.84_221.1903	0.00	0.00	0.00	0.00	0.98	1.00
10.62_236.1643	0.00	0.00	0.39	0.30	1.00	0.97
8.54_235.1344	0.00	0.00	0.30	0.51	0.96	1.00
7.38_246.1513	0.00	0.00	0.00	0.00	0.62	1.00
3.58_252.0387	0.00	0.35	0.11	0.52	1.00	1.00
12.02_263.1978	0.00	0.03	0.00	0.00	0.93	1.00
10.71_261.1779	0.00	0.01	0.00	0.00	0.90	1.00
6.28_268.0191	0.00	0.13	0.17	0.16	1.00	0.72
5.27_264.2082	0.00	0.00	0.36	0.46	0.97	1.00
4.60_268.0196	0.00	0.00	0.44	0.18	0.83	1.00
7.15_293.2251	0.00	0.00	0.27	0.29	0.69	1.00
12.02_309.1921	0.00	0.01	0.00	0.00	0.90	1.00
12.03_325.1706	0.00	0.00	0.00	0.00	0.84	1.00
10.73_340.1475	0.00	0.14	0.00	0.00	1.00	0.71
5.99_338.1374	0.00	0.00	0.30	0.24	1.00	0.97
4.01_351.5992	0.00	0.00	0.00	0.00	1.00	0.57
7.52_368.2211	0.00	0.00	0.31	0.34	0.71	1.00
7.83_387.1861	0.00	0.00	0.50	0.00	1.00	1.00
6.24_384.2171	0.00	0.00	0.07	0.11	0.71	1.00
7.98_431.2698	0.00	0.06	0.00	0.11	0.90	1.00
6.99_443.3240	0.00	0.23	0.00	0.00	0.87	1.00
7.51_499.2782	0.00	0.02	0.07	0.49	1.00	0.97
4.37_494.2617	0.00	0.00	0.06	0.09	0.78	1.00
7.57_542.3960	0.00	0.42	0.00	0.00	0.79	1.00
12.03_549.4012	0.00	0.00	0.00	0.00	0.87	1.00
5.18_599.2879	0.00	0.00	0.00	0.00	1.00	0.78
6.02_637.3187	0.00	0.00	0.00	0.00	0.38	1.00
6.24_515.2753	0.01	0.00	0.15	0.18	0.77	1.00
8.10_301.1534	0.01	0.03	0.28	0.31	0.81	1.00
12.02_205.1953	0.01	0.00	0.00	0.00	0.84	1.00
8.29_401.1993	0.02	0.00	0.20	0.36	0.93	1.00
10.18_223.2085	0.04	0.25	0.00	0.00	1.00	0.79
5.97_286.6247	0.05	0.01	0.21	0.14	0.92	1.00
7.42_280.1237	0.06	0.16	0.21	0.37	0.95	1.00
3.86_150.0940	0.06	0.11	0.29	0.43	0.92	1.00
10.52_673.3745	0.06	0.09	0.32	0.51	0.87	1.00
5.97_278.6345	0.06	0.02	0.21	0.20	1.00	0.96
6.72_1450.6973	0.08	0.02	0.22	0.32	1.00	0.92
7.89_192.1015	0.10	0.17	0.31	0.42	0.80	1.00
7.42_196.0651	0.10	0.05	0.11	0.19	0.58	1.00
7.06_221.1900	0.12	0.36	0.01	0.00	1.00	0.97
15.37_230.0721	0.12	0.40	0.20	0.45	0.82	1.00
9.47_211.0868	0.13	0.23	0.39	0.38	0.82	1.00
3.82_230.1126	0.14	0.09	0.41	0.33	0.81	1.00
6.06_203.1781	0.15	0.26	0.00	0.13	0.83	1.00
7.06_203.1787	0.15	0.28	0.00	0.00	0.88	1.00
6.73_1161.1593	0.16	0.04	0.12	0.07	0.85	1.00
5.96_534.2942	0.16	0.04	0.16	0.16	0.97	1.00
6.71_1160.7578	0.17	0.00	0.31	0.00	1.00	0.86
6.73_1160.5609	0.20	0.00	0.05	0.17	1.00	1.00
5.61_343.2002	0.23	0.05	0.22	0.32	0.84	1.00
4.81_464.2611	0.24	0.29	0.55	0.44	0.94	1.00
5.81_605.2195	0.28	0.40	0.38	0.62	0.77	1.00
4.32_308.1712	0.29	0.11	0.32	0.50	0.73	1.00

D. Mass Spectral Data for Selected Features

6.74_1160.9454	0.32	0.26	0.22	0.14	1.00	0.79
4.63_149.1104	0.32	0.51	0.38	0.66	0.98	1.00
5.34_191.1575	0.32	0.46	0.31	0.56	0.91	1.00
1.49_365.1079	0.35	0.48	0.31	0.35	0.78	1.00
6.40_263.1761	0.36	0.38	0.37	0.56	0.81	1.00
13.98_292.2624	0.36	0.49	0.29	0.40	0.66	1.00
4.53_236.1764	0.37	0.48	0.36	0.57	0.94	1.00
5.78_164.0706	0.39	0.52	0.39	0.60	1.00	0.96
8.22_220.1332	0.39	0.57	0.44	0.73	0.94	1.00
3.75_267.1417	0.40	0.50	0.35	0.62	0.78	1.00
9.69_220.1127	0.41	0.48	0.29	0.00	1.00	0.98
5.71_249.1598	0.41	0.57	0.38	0.61	0.84	1.00
4.67_270.1917	0.43	0.59	0.44	0.57	0.81	1.00
4.70_221.1315	0.45	0.67	0.43	0.63	0.96	1.00
6.23_251.1781	0.49	0.54	0.37	0.61	0.87	1.00
1.50_401.0693	0.54	0.50	0.60	0.33	1.00	0.98
5.72_240.1231	0.56	0.39	0.47	0.51	0.89	1.00
6.59_273.1670	0.60	0.51	0.53	0.67	0.84	1.00
5.43_241.1546	0.61	0.63	0.59	0.79	0.93	1.00
7.00_916.3325	1.00	0.59	0.55	0.66	0.00	0.00

D. Mass Spectral Data for Selected Features

Table S23. Normalized heat map of features described as unique in figure 2a when comparing wild type *Nocardiopsis sp. FU40 ΔApoS8* to the R4 rifampicin resistant and S5 streptomycin resistant mutant extracts using OPLS-DA and extracting features from the generated S-plot with correlation coefficients ≥ 0.9 . Features are normalized to maximum intensity for that feature.

Feature ID (RT_m/z)	WT	WT	R4	R4	S5	S5
1.50_103.5345	0.00	0.00	0.50	1.00	0.83	0.90
4.14_186.1168	0.00	0.00	0.76	0.81	0.81	1.00
4.84_205.1323	0.00	0.00	0.74	0.86	1.00	0.89
1.32_211.8786	0.00	0.00	0.42	0.94	1.00	0.92
1.49_211.0584	0.00	0.19	0.65	1.00	0.77	0.68
5.11_236.1306	0.00	0.11	0.59	0.61	0.88	1.00
8.08_252.0397	0.00	0.00	0.72	0.60	1.00	0.97
1.78_262.1278	0.00	0.00	0.61	0.81	0.74	1.00
9.60_297.1694	0.00	0.01	0.61	1.00	0.71	0.71
5.82_322.1007	0.00	0.00	0.87	0.97	1.00	0.99
9.13_319.1539	0.00	0.00	0.60	1.00	0.63	0.70
7.48_345.1875	0.00	0.00	0.77	0.91	1.00	0.72
8.53_359.2035	0.00	0.11	0.90	1.00	0.78	0.62
1.49_394.1142	0.00	0.00	0.61	1.00	0.63	0.92
4.02_423.1940	0.00	0.00	0.53	0.86	0.75	1.00
1.48_431.0890	0.00	0.30	0.72	0.73	0.88	1.00
5.52_601.2501	0.00	0.00	0.53	0.73	0.86	1.00
1.25_639.8836	0.00	0.00	0.48	0.77	1.00	0.77
5.66_384.2168	0.01	0.00	0.45	0.64	0.81	1.00
16.15_710.1773	0.03	0.01	0.60	0.86	1.00	0.97
9.66_279.1583	0.03	0.00	0.46	0.71	0.73	1.00
5.43_377.1482	0.03	0.00	0.68	1.00	0.50	0.58
1.73_338.0231	0.04	0.00	0.50	0.59	0.82	1.00
9.14_239.1284	0.04	0.04	0.59	1.00	0.80	0.56
1.74_150.0789	0.04	0.00	0.47	0.80	1.00	0.99
3.07_230.1126	0.05	0.11	0.65	0.79	0.79	1.00
8.53_283.1523	0.05	0.10	0.73	0.86	0.92	1.00
8.53_177.0880	0.06	0.06	0.53	0.63	0.72	1.00
4.75_136.0625	0.06	0.00	0.78	1.00	0.56	0.85
8.53_207.1002	0.06	0.07	0.56	0.69	0.84	1.00
3.83_198.1623	0.13	0.09	0.54	0.95	0.86	1.00
1.73_288.1454	0.16	0.00	0.62	0.73	1.00	0.56
1.60_229.1318	0.21	0.04	0.54	0.70	0.91	1.00
9.11_505.3321	0.27	0.00	0.59	0.84	0.93	1.00
16.18_335.9929	0.28	0.00	0.67	0.98	0.95	1.00
4.00_320.1711	0.33	0.04	0.76	0.77	0.80	1.00
12.11_316.2860	0.41	1.00	0.00	0.01	0.00	0.00
11.78_354.1615	0.44	1.00	0.00	0.00	0.00	0.00
11.49_251.2052	0.45	1.00	0.00	0.00	0.00	0.00
11.27_448.3444	0.48	1.00	0.09	0.00	0.00	0.00
12.43_386.2820	0.50	1.00	0.15	0.00	0.18	0.00
10.60_346.3091	0.51	1.00	0.00	0.00	0.00	0.00
10.40_371.3275	0.52	1.00	0.00	0.00	0.02	0.02
10.70_288.2557	0.52	1.00	0.00	0.00	0.00	0.20
9.48_225.1993	0.53	1.00	0.01	0.02	0.02	0.02
4.26_669.2631	0.56	1.00	0.00	0.00	0.00	0.08
11.80_235.1712	0.56	1.00	0.00	0.04	0.00	0.09
10.15_739.4618	0.56	1.00	0.06	0.05	0.11	0.07
14.41_309.2409	0.56	1.00	0.14	0.13	0.32	0.23
10.53_531.4000	0.57	1.00	0.00	0.00	0.00	0.00
12.97_407.3144	0.58	1.00	0.20	0.09	0.30	0.12
12.98_399.3242	0.58	1.00	0.19	0.09	0.31	0.12
4.37_663.2850	0.59	1.00	0.01	0.00	0.00	0.00
13.98_433.3418	0.61	1.00	0.02	0.01	0.05	0.00
4.64_412.2067	0.62	1.00	0.08	0.10	0.15	0.20
6.19_181.1351	0.63	1.00	0.09	0.11	0.08	0.10
10.97_401.2525	0.63	1.00	0.00	0.00	0.08	0.21
11.58_415.2745	0.65	1.00	0.00	0.00	0.07	0.02
12.62_273.1378	0.66	1.00	0.00	0.00	0.00	0.00
4.27_647.2871	0.67	1.00	0.00	0.01	0.09	0.00
11.44_223.2060	0.67	1.00	0.00	0.00	0.00	0.00
8.08_219.1411	0.68	1.00	0.00	0.00	0.30	0.24
6.85_824.9348	0.70	1.00	0.00	0.00	0.00	0.23
16.15_442.8736	0.71	1.00	0.00	0.00	0.00	0.00

D. Mass Spectral Data for Selected Features

7.07_184.1710	0.72	1.00	0.00	0.00	0.00	0.00
4.37_150.0945	0.72	1.00	0.00	0.00	0.00	0.00
11.18_473.3585	0.75	1.00	0.04	0.01	0.08	0.04
12.74_443.3505	0.77	1.00	0.00	0.00	0.01	0.00
11.97_299.2600	0.80	1.00	0.00	0.00	0.31	0.21
11.84_443.3878	0.82	1.00	0.09	0.05	0.11	0.06
11.03_354.1608	0.82	1.00	0.00	0.04	0.09	0.25
11.28_440.3462	0.82	1.00	0.00	0.00	0.00	0.00
12.98_282.2118	0.82	1.00	0.14	0.03	0.15	0.10
10.38_401.3397	0.88	1.00	0.50	0.32	0.27	0.16
9.26_219.1735	0.88	1.00	0.00	0.00	0.00	0.00
4.50_359.1197	0.89	1.00	0.00	0.00	0.00	0.00
13.49_295.2258	0.91	1.00	0.08	0.03	0.06	0.00
4.49_225.1597	0.97	1.00	0.49	0.50	0.54	0.56
12.89_441.3208	0.99	1.00	0.40	0.25	0.49	0.58
11.31_225.6512	1.00	0.95	0.26	0.18	0.00	0.00
9.27_240.2315	1.00	0.88	0.00	0.11	0.00	0.00
10.39_268.2627	1.00	0.83	0.00	0.00	0.00	0.00
11.44_291.1951	1.00	0.75	0.00	0.00	0.00	0.00
12.62_313.2746	1.00	0.83	0.00	0.00	0.12	0.11
14.31_325.2414	1.00	0.74	0.00	0.00	0.00	0.00
15.49_338.3442	1.00	0.86	0.00	0.03	0.00	0.00
13.48_397.3392	1.00	0.75	0.00	0.01	0.00	0.00
13.95_411.3586	1.00	0.78	0.00	0.00	0.06	0.00
13.27_419.3131	1.00	0.81	0.00	0.00	0.00	0.00
12.75_617.4294	1.00	0.84	0.00	0.25	0.36	0.00
13.92_641.5490	1.00	0.85	0.00	0.00	0.00	0.00
4.37_685.2548	1.00	0.86	0.00	0.00	0.12	0.23