Supporting Information

Passive membrane permeability in cyclic peptomer scaffolds is robust to extensive variation in side chain functionality and backbone geometry.

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1 Library Design and Synthesis

1.1 Calculated molecular properties of Library 1

Molecular properties of Library 1 were calculated by using Discovery Studio 4.0. This library covered a wide range of AlogP (-0.56 ~ 7.54) and molecular weight (608.8 ~ 944.2).

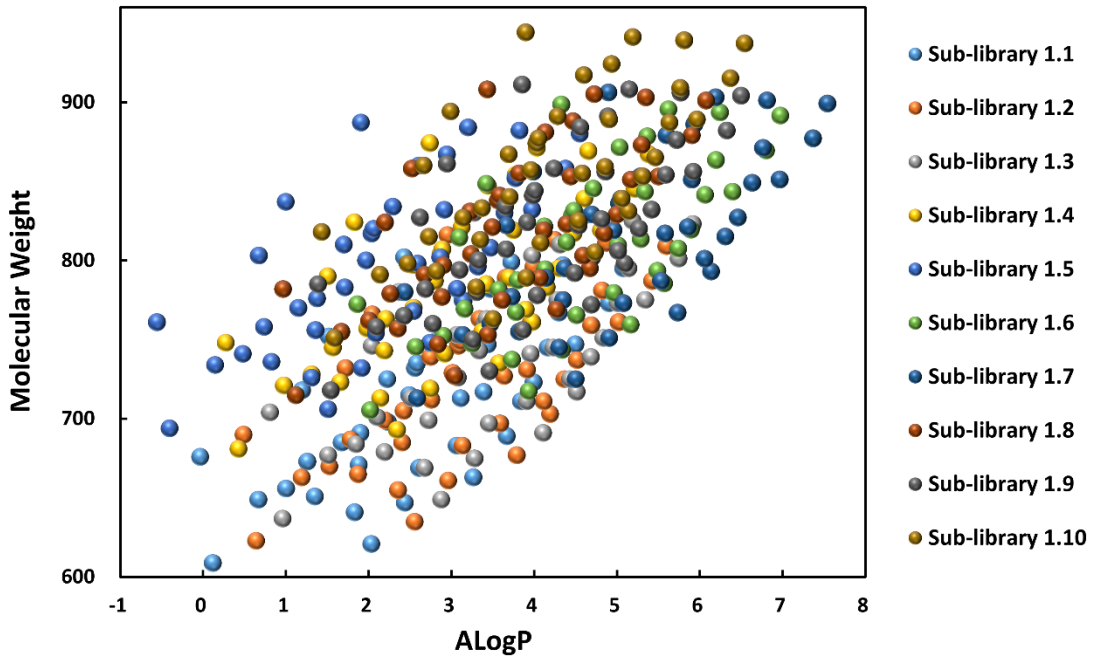


Figure S1. ALogP vs MW of Library 1

1.2 Synthetic procedures

Library 1 of hexameric cyclic peptomers was synthesized in ten sub-libraries using split-pool techniques (Scheme S1) and standard Fmoc-based solid phase peptide synthesis (SPPS), starting with Fmoc-L-norleucine linked to 2-chlorotrityl resin (approximately 0.3 mmol/g) prepared by the following procedure. 1.55 g of 2-chlorotrityl chloride resin (200-400 mesh, 1%DVB) was

added to a fritted solid phase extraction (SPE) tube and swelled in DCM. 0.46 mmol of Fmoc-L-norleucine and 4 eq. of DIPEA (0.32 mL) were dissolved in 30 mL of DCM and transferred to the SPE tube. The SPE tube was sealed and agitated gently at room temperature. After 1.5 h, the resin was drained and treated with a solution of DCM, MeOH, and DIPEA (17:2:1, 30min, 2×20 mL), then washed with DCM (3×20 mL), DMF (3×20 mL), and again DCM (3×20 mL).

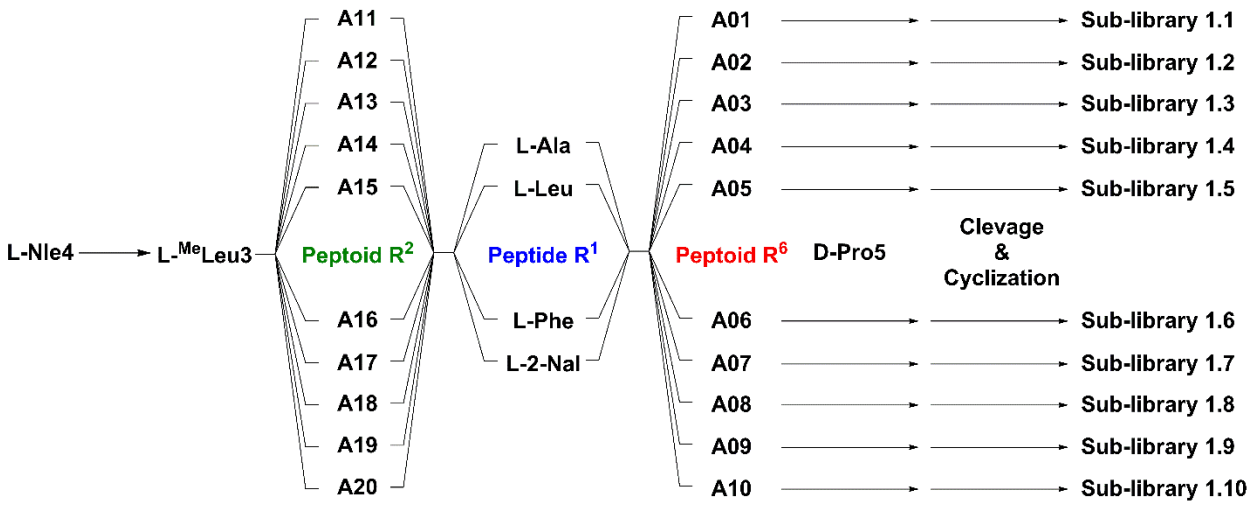
Standard Fmoc-based SPPS synthesis methods were as follows. For Fmoc deprotection, a solution (15 mL per gram of resin) of 2% of piperidine and 2% DBU in DMF was added to the resin, and the mixture was agitated for 10 min. After the resin was drained, the process was repeated. Then, the resin was washed with DMF (3×20 mL per gram of resin), DCM (3×20 mL per gram of resin), and again DMF (3×20 mL per gram of resin). To couple Fmoc amino acids, a solution (15 mL per gram of resin) of 0.2 mol/L Fmoc amino acid, 0.2 mol/L HATU, and 0.4 mol/L of DIPEA was added to the resin, and then the mixture was agitated for 1.5 h. The resin was drained and washed with DMF (3×20 mL per gram of resin), DCM (3×20 mL per gram of resin), and again DMF (3×20 mL per gram of resin).

For peptoid synthesis, a solution (15 mL per gram of resin) of 0.6 mol/L bromoacetic acid and 0.55 mol/L of DIC was added to the resin, and then the mixture was agitated for 30 min. After the resin was drained and washed with DCM (3×20 mL per gram of resin) and DMF (3×20 mL per gram of resin), a solution (15 mL per gram of resin) of 1.0 mol/L primary amine in NMP was

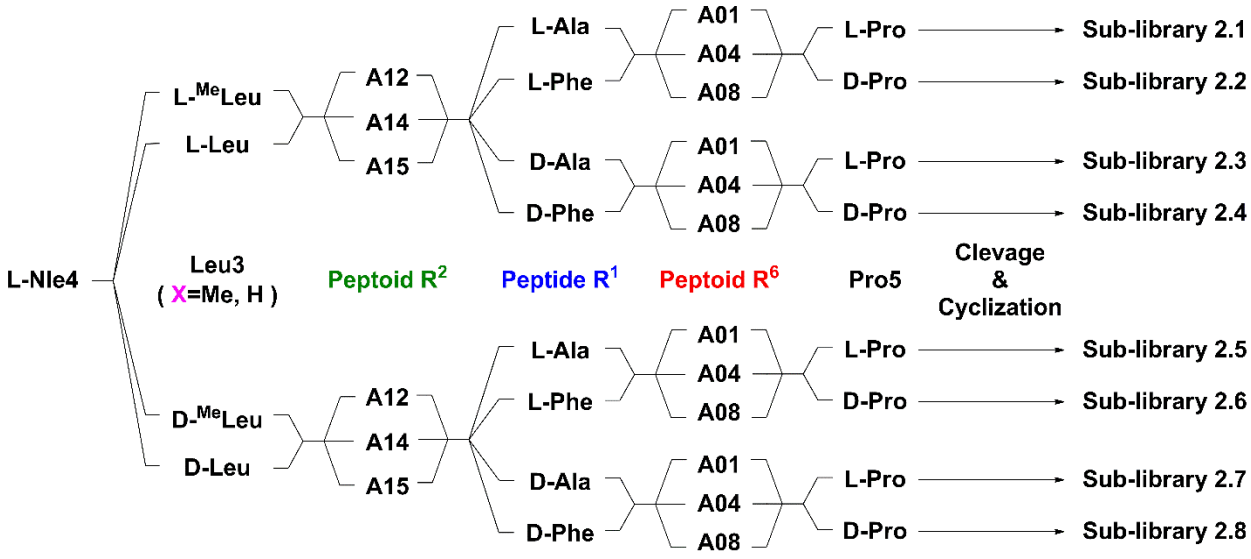
added to the resin, and then the mixture was agitated for 1.5 h. In the case of **A01**, a mixture of **A01** 2.0 mol/L in THF and NMP (1:3) was used. The resin was drained and washed with DMF (3×20 mL per gram of resin), DCM (3×20 mL per gram of resin), and again DMF (3×20 mL per gram of resin).

After assembling fifth monomers, the resin was kept separate in ten sub-libraries. Then, the last proline was incorporated and Fmoc was deprotected. The linear peptomers in each sub-library were cleaved from the resin by treating with a solution (40 mL per gram of resin) of 30% 1,1,1,3,3,3-hexafluoroisopropanol in DCM for 2 h. The filtrates were collected and concentrated. One-quarter amount of compound in each sub-library (approximately 0.012 mmol) was used for cyclization; the linear peptomers were dissolved in 9 mL of ACN and THF (1:1), then 1 mL of a solution of 0.02 mol/L COMU and 0.04 mol/L DIPEA was added to the solution. After stirring for 20 h, 0.1 mL of water was added to each reaction, and then the reactions were concentrated. The cyclic peptomers were roughly purified by the following SPE procedure. 10 mL of 20% ACN in water was added to the residue. The resulting suspension was loaded onto an Isolute 103 SPE cartridge (200mg/6mL, Biotage) and allowed to drain under gravity. The column was washed with 4 mL of water, and then the organic compounds were eluted with 6 mL of ACN. The eluted materials were concentrated.

Library 2 was also synthesized in eight sub-libraries by the same method. (Scheme S2)



Scheme S1. Split-pool synthesis of Library 1



Scheme S2. Split-pool synthesis of Library 2

1.3 LCMS analyses of the Library 1

The production of all peptomers in each sub-library were confirmed by LCMS analyses performed on HPLC (UltiMate 3000, Dionex) with attached mass spectrometer (Orbitrap Velos Pro, Thermo Scientific). The samples were injected on a 1.9 μm C18 column (Hypersil GOLD 30×2.1 mm, Thermo Scientific) then eluted by the mixture of 0.1% formic acid in water (solvent A) and 0.1% formic acid in acetonitrile (solvent B) with a 0.6 mL/min flow rate (0-0.5 min, B: 10%, 0.5-3.5 min, B: 10%-100% linear gradient, 3.5-5.0 min, B: 100%, 5.0-6.5 min, B: 10%).

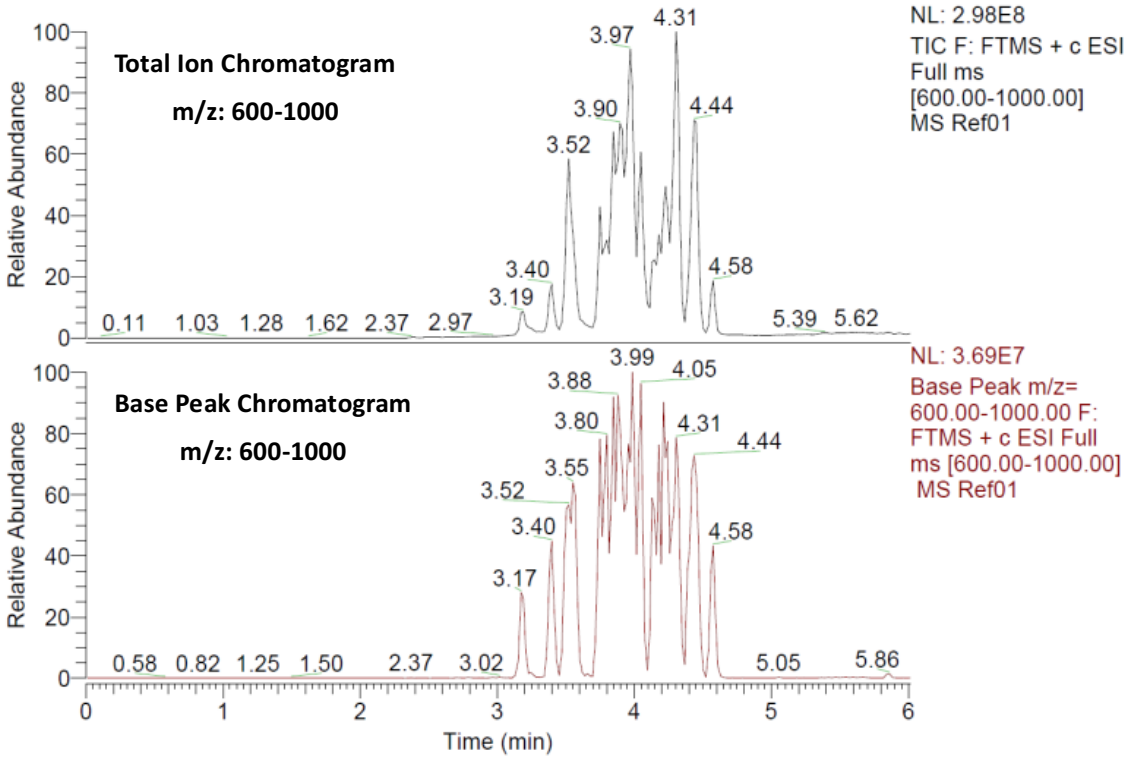


Figure S2.1. LCMS analysis of Sub-library 1.1

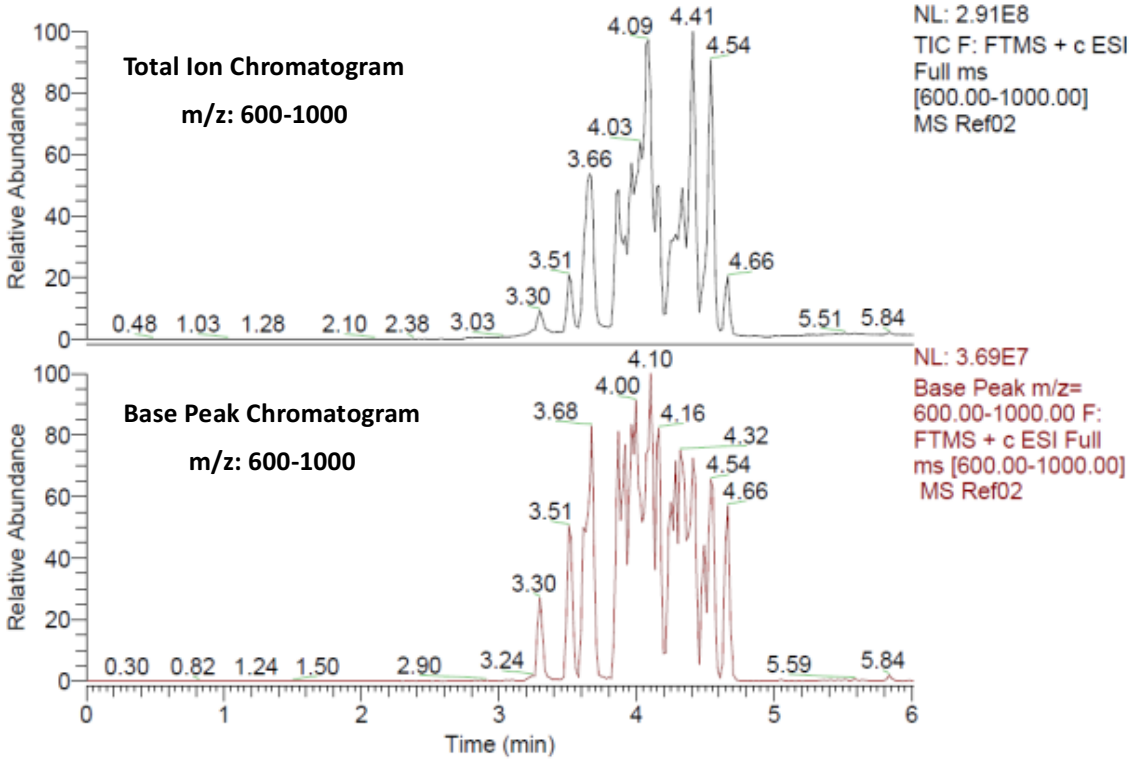


Figure S2.2. LCMS analysis of Sub-library 1.2

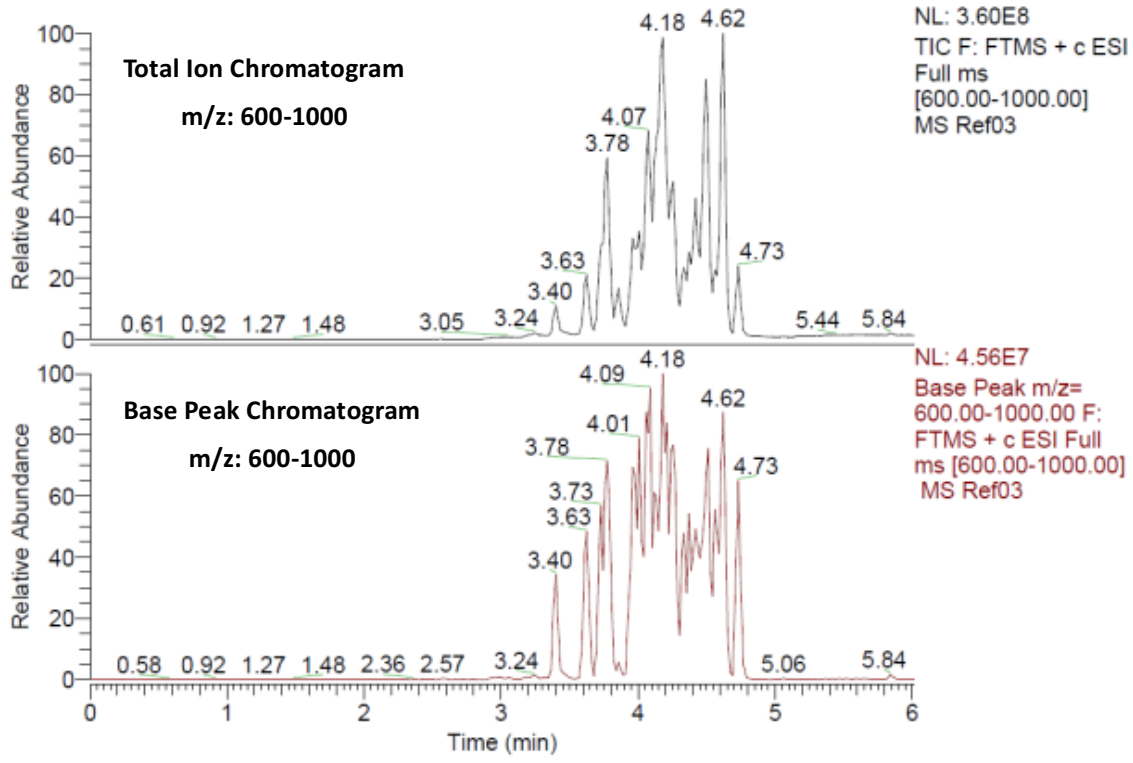


Figure S2.3. LCMS analysis of Sub-library 1.3

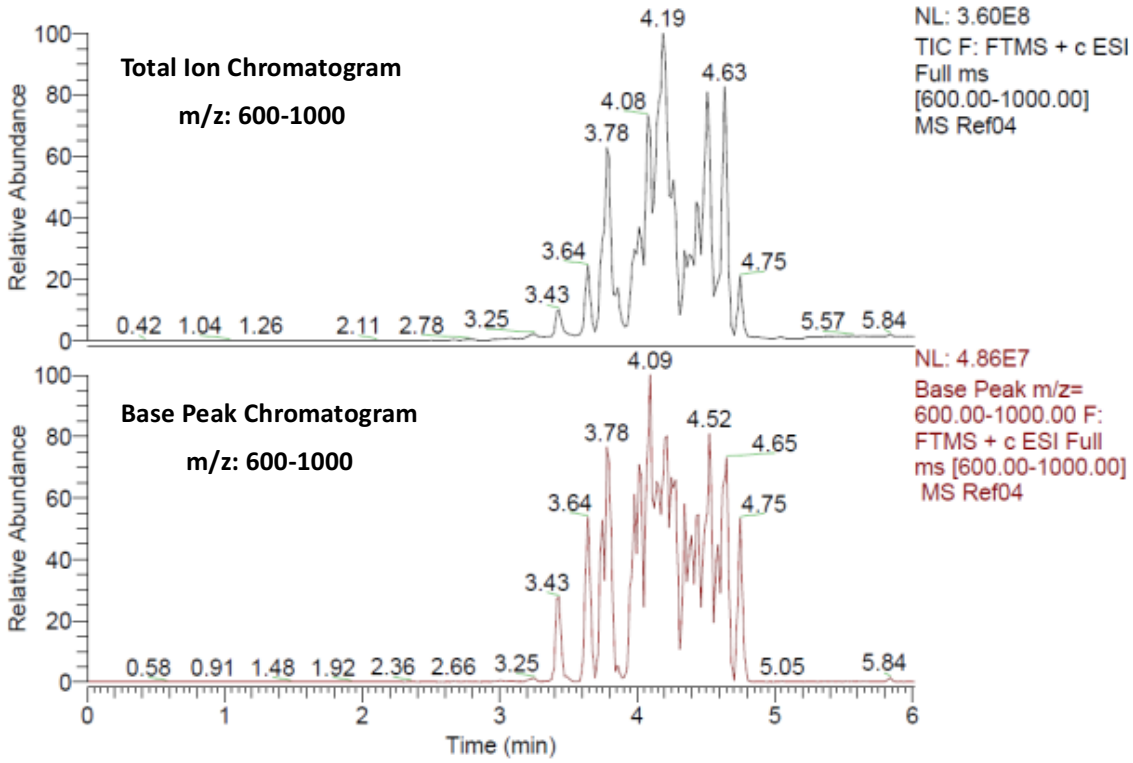
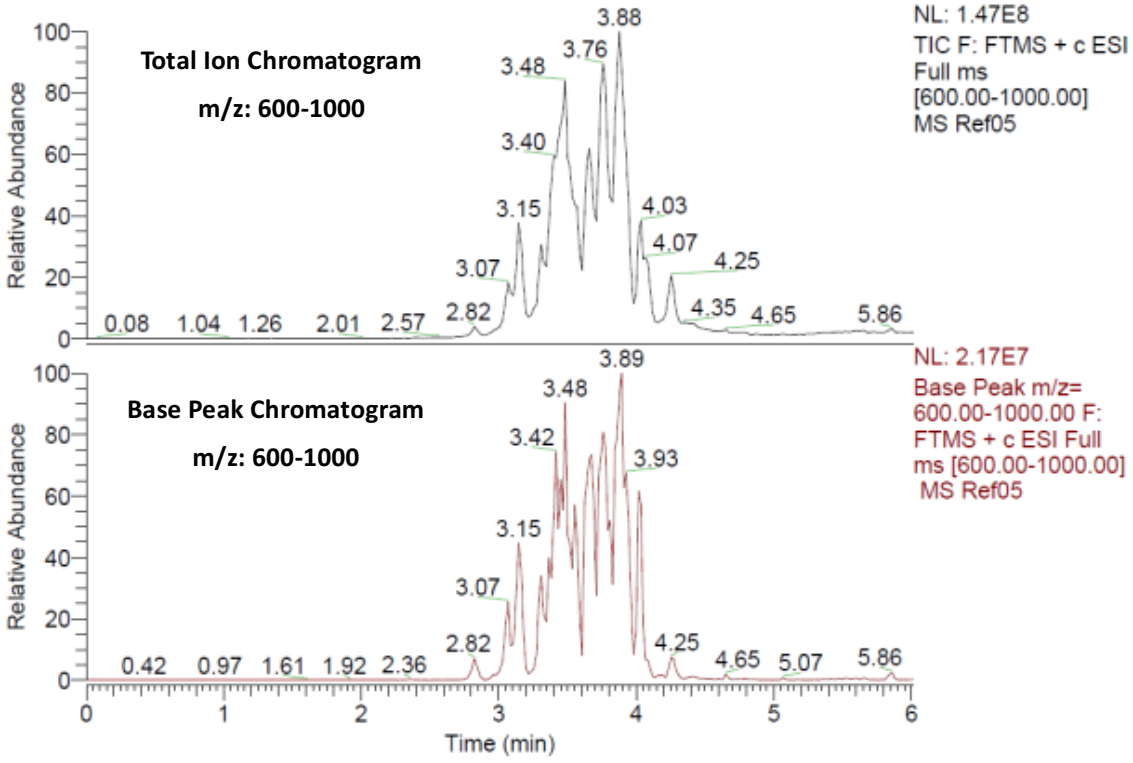


Figure S2.4. LCMS analysis of Sub-library 1.4



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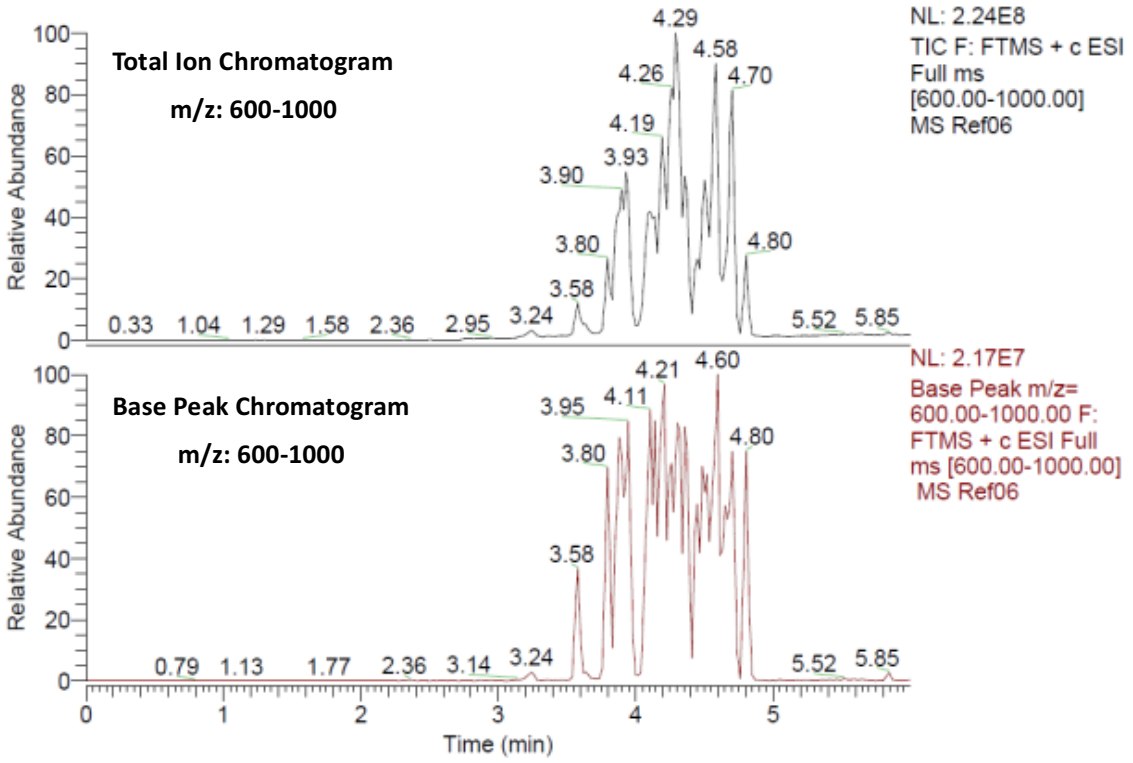

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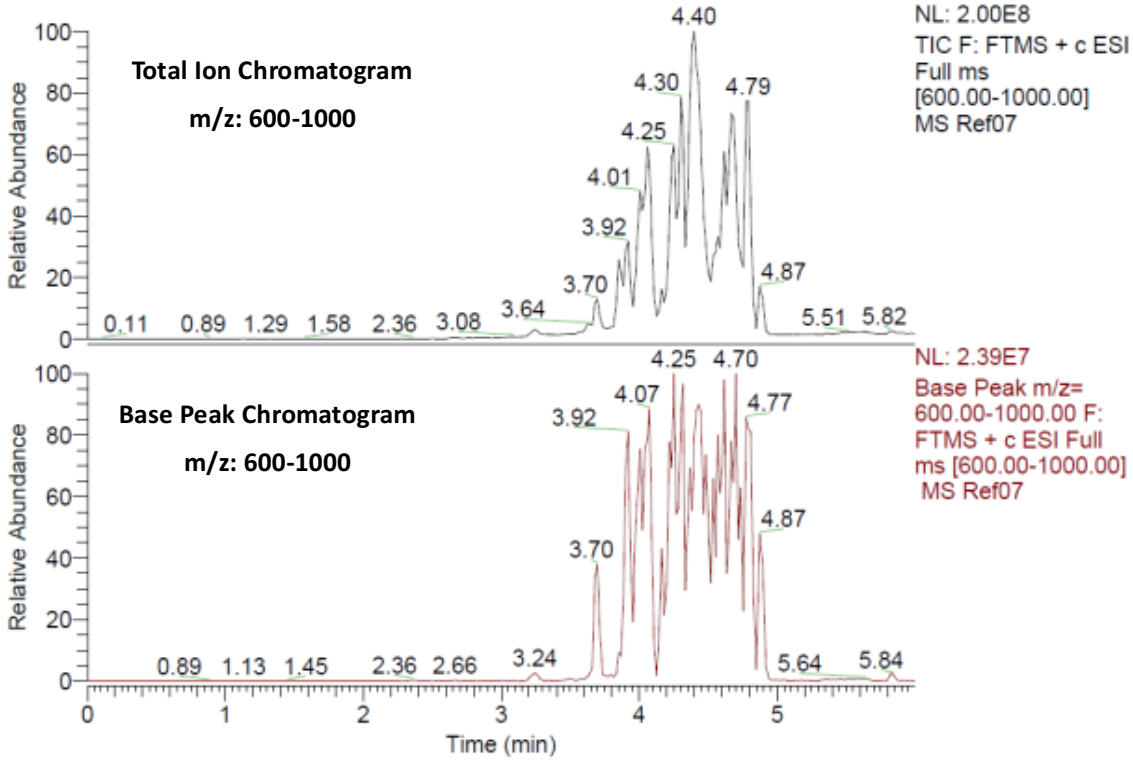
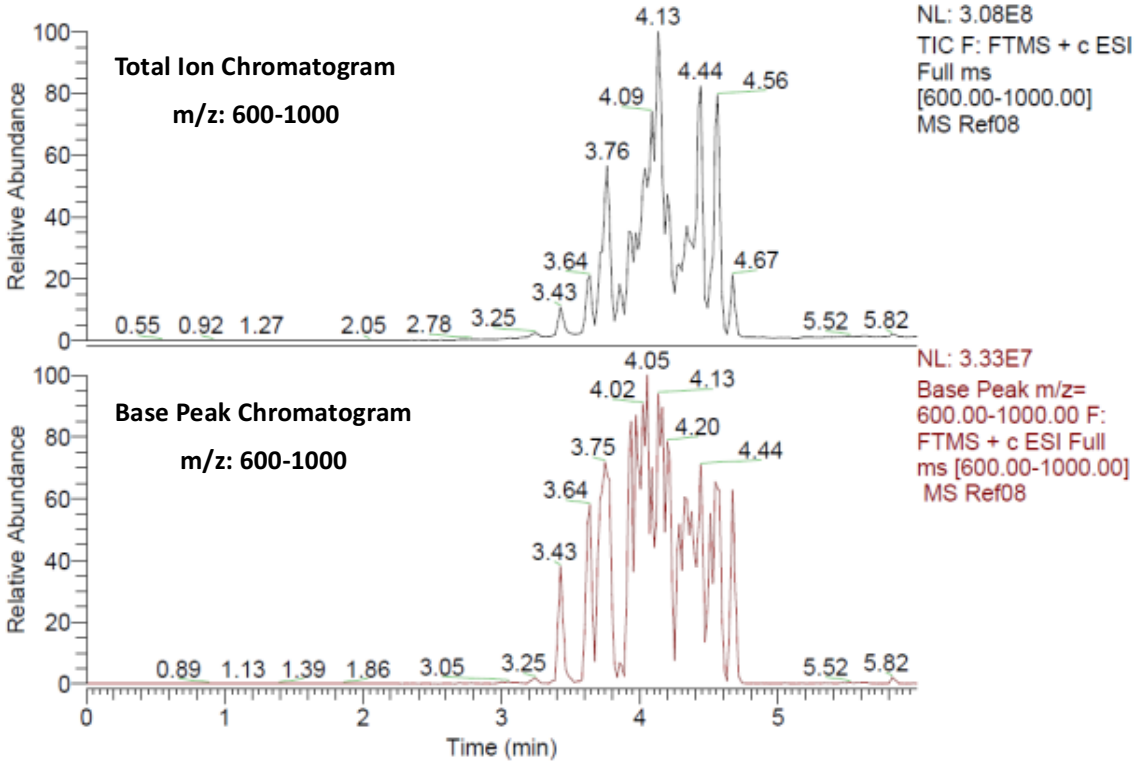


Figure S2.7. LCMS analysis of Sub-library 1.7



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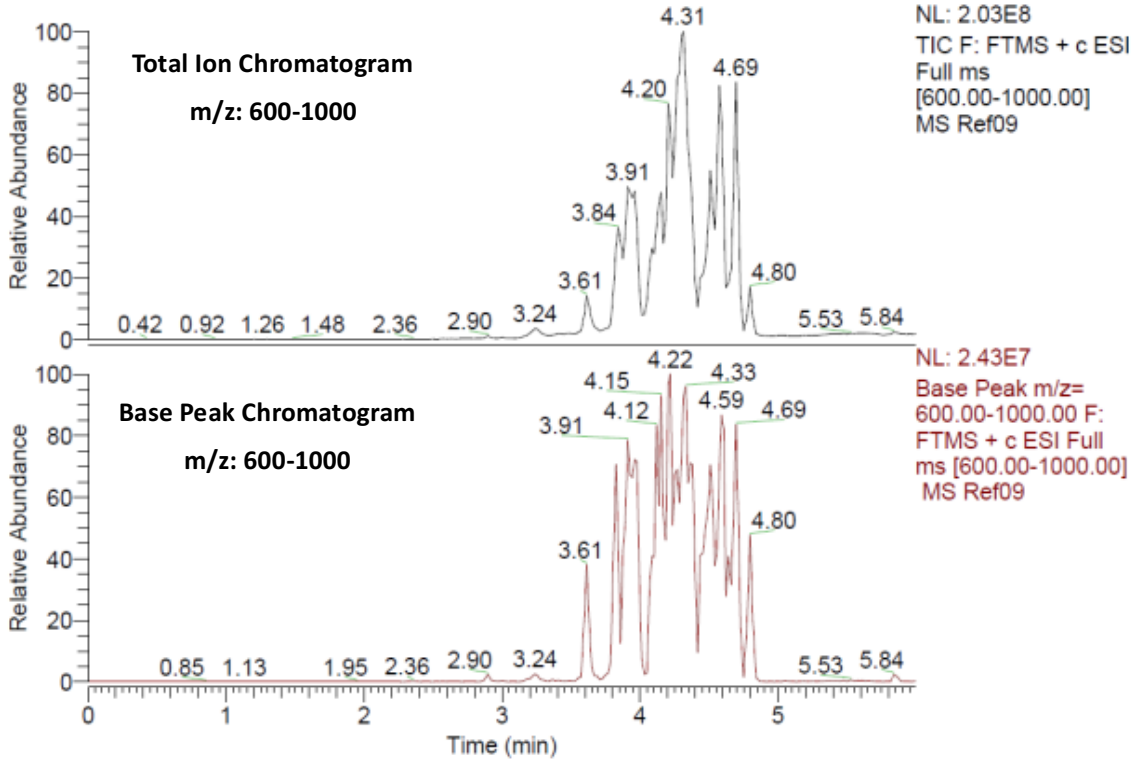


Figure S2.9. LCMS analysis of Sub-library 1.9

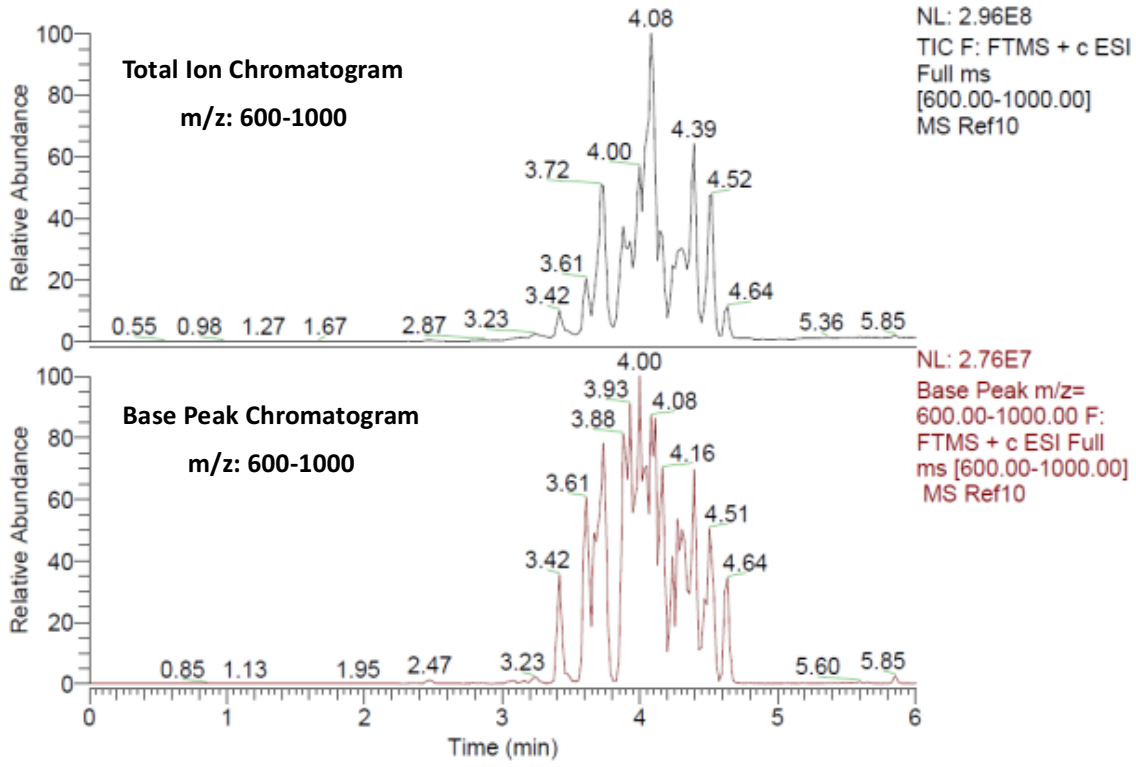


Figure S2.10. LCMS analysis of Sub-library 1.10

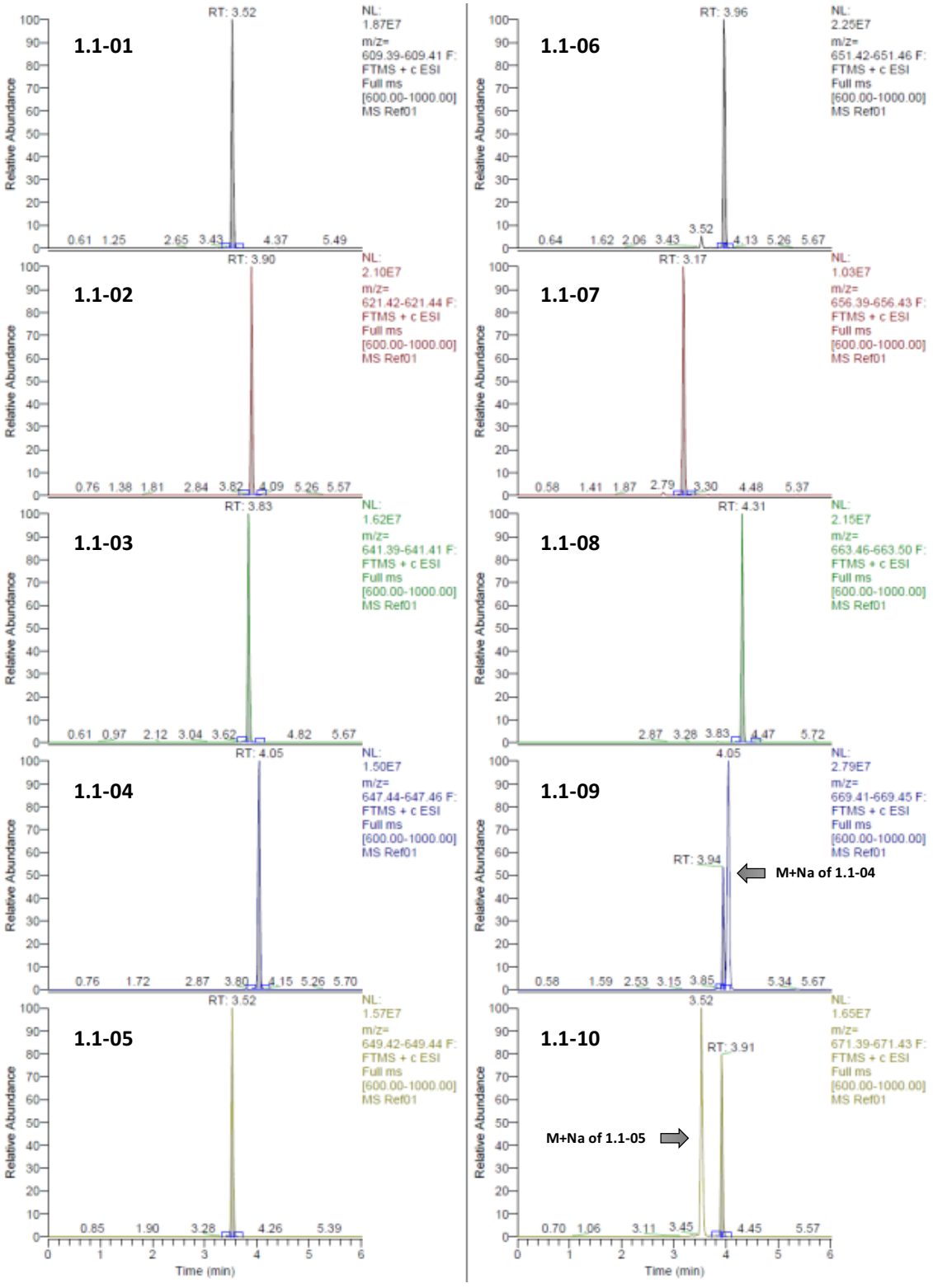


Figure S3.1a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.1

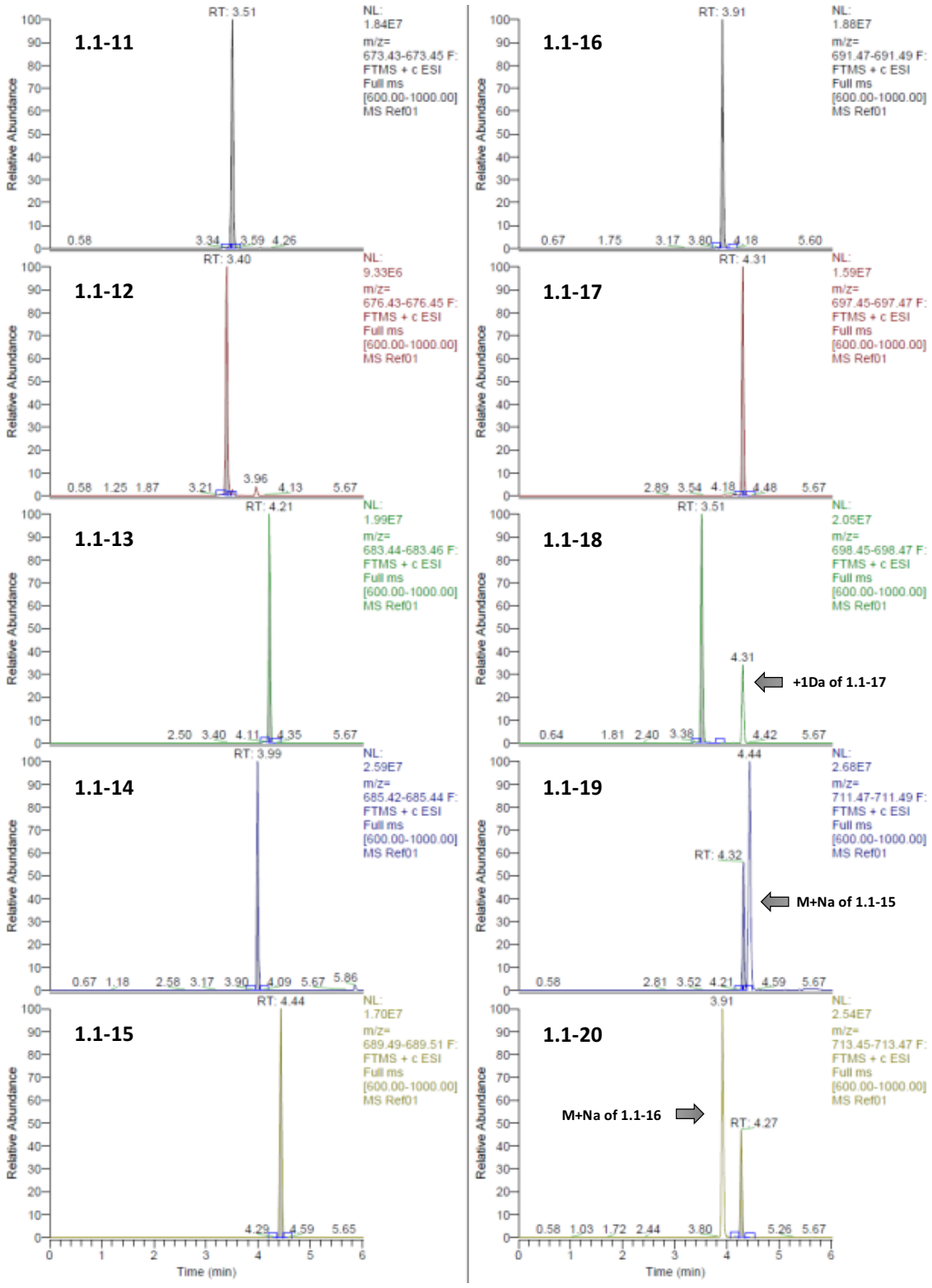


Figure S3.1b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.1

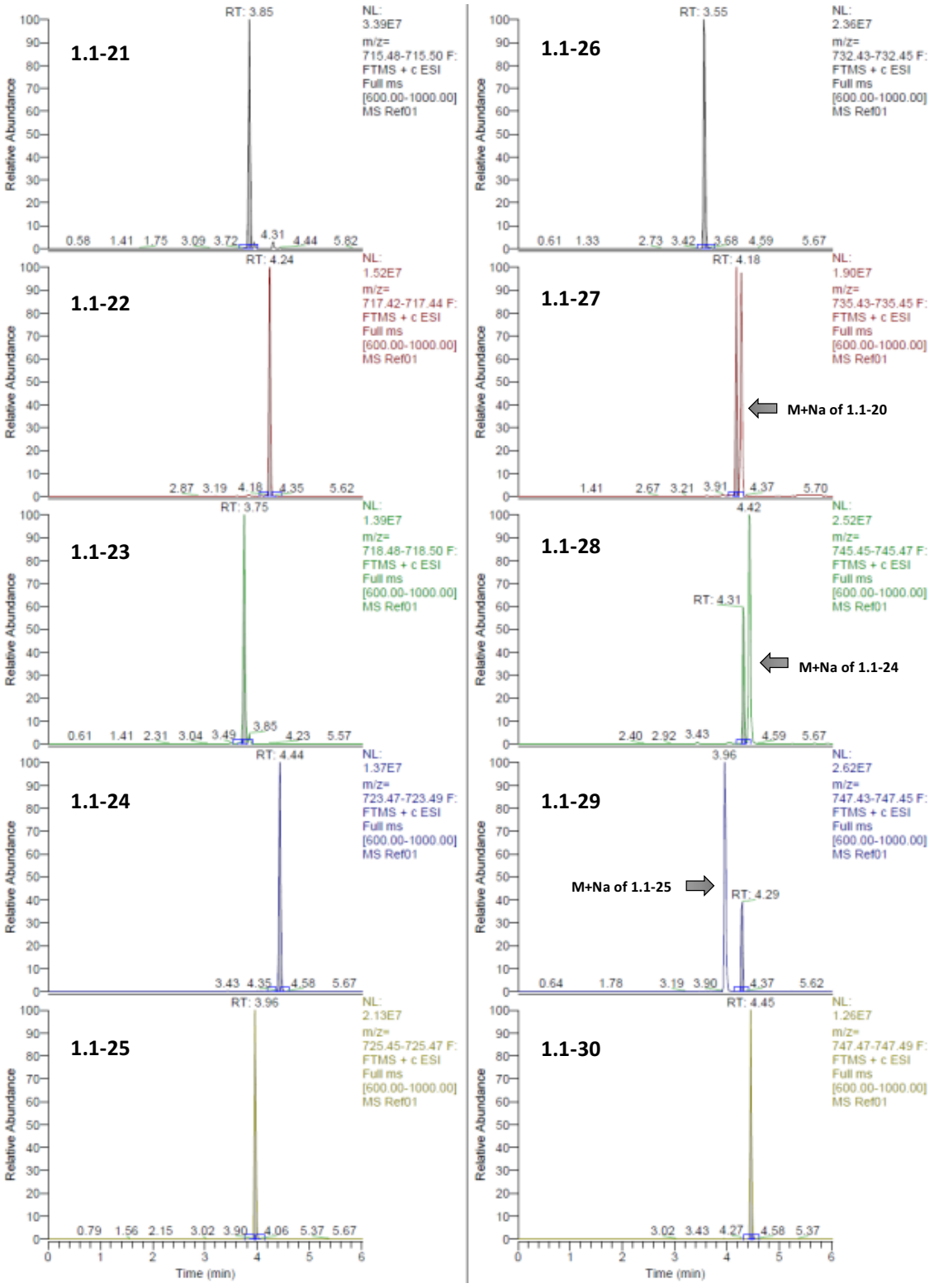


Figure S3.1c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.1

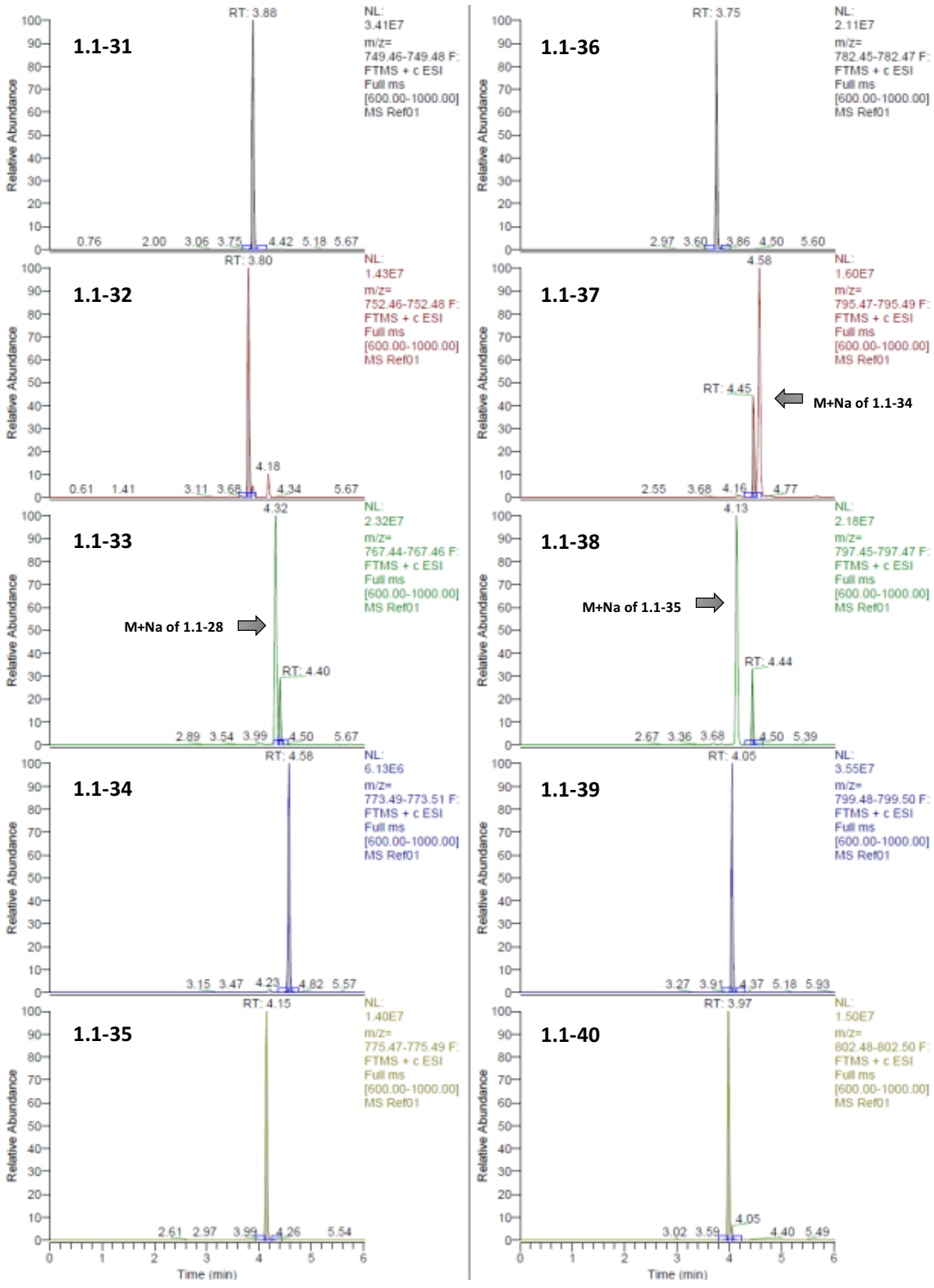


Figure S3.1d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.1

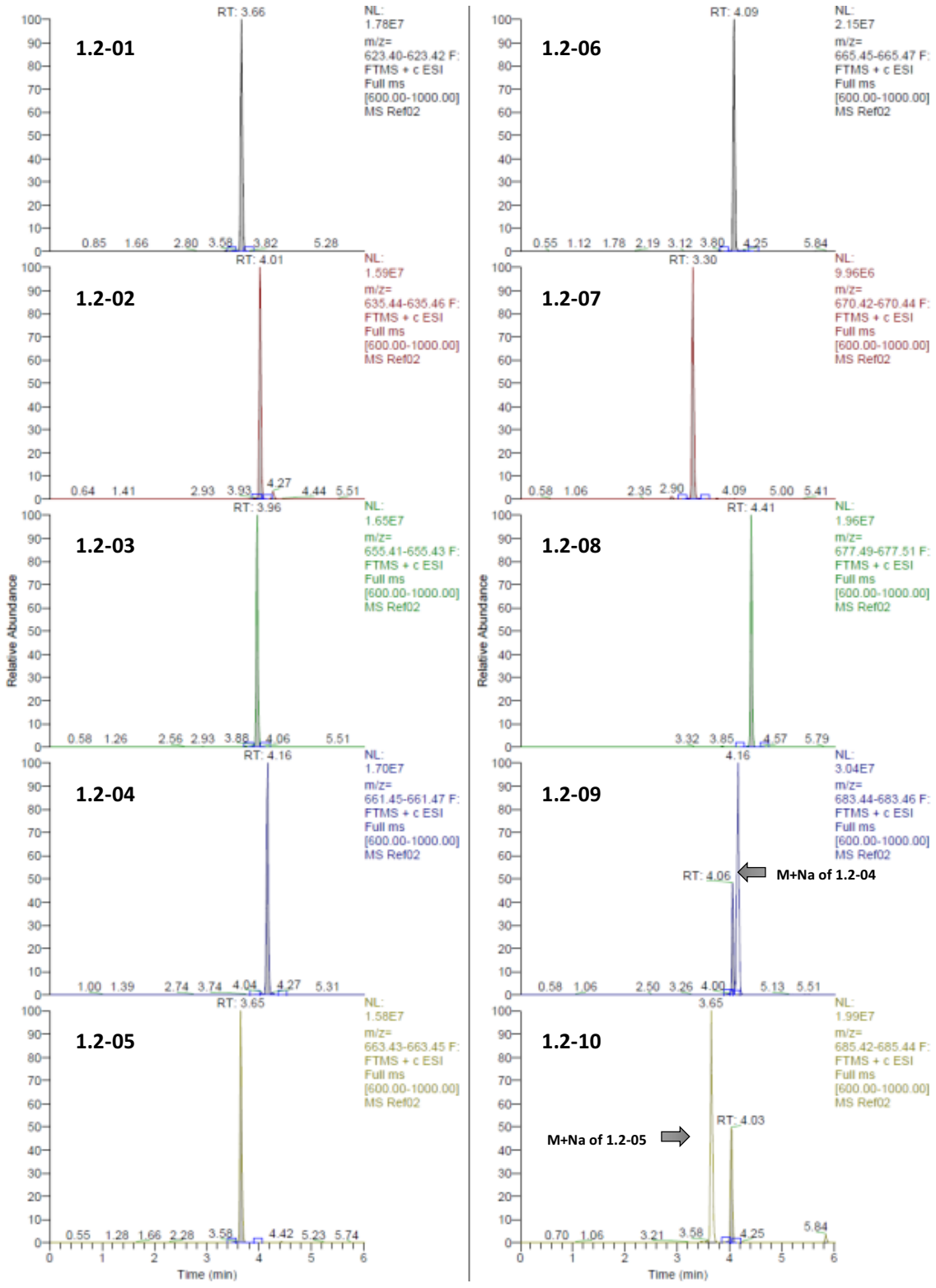


Figure S3.2a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.2

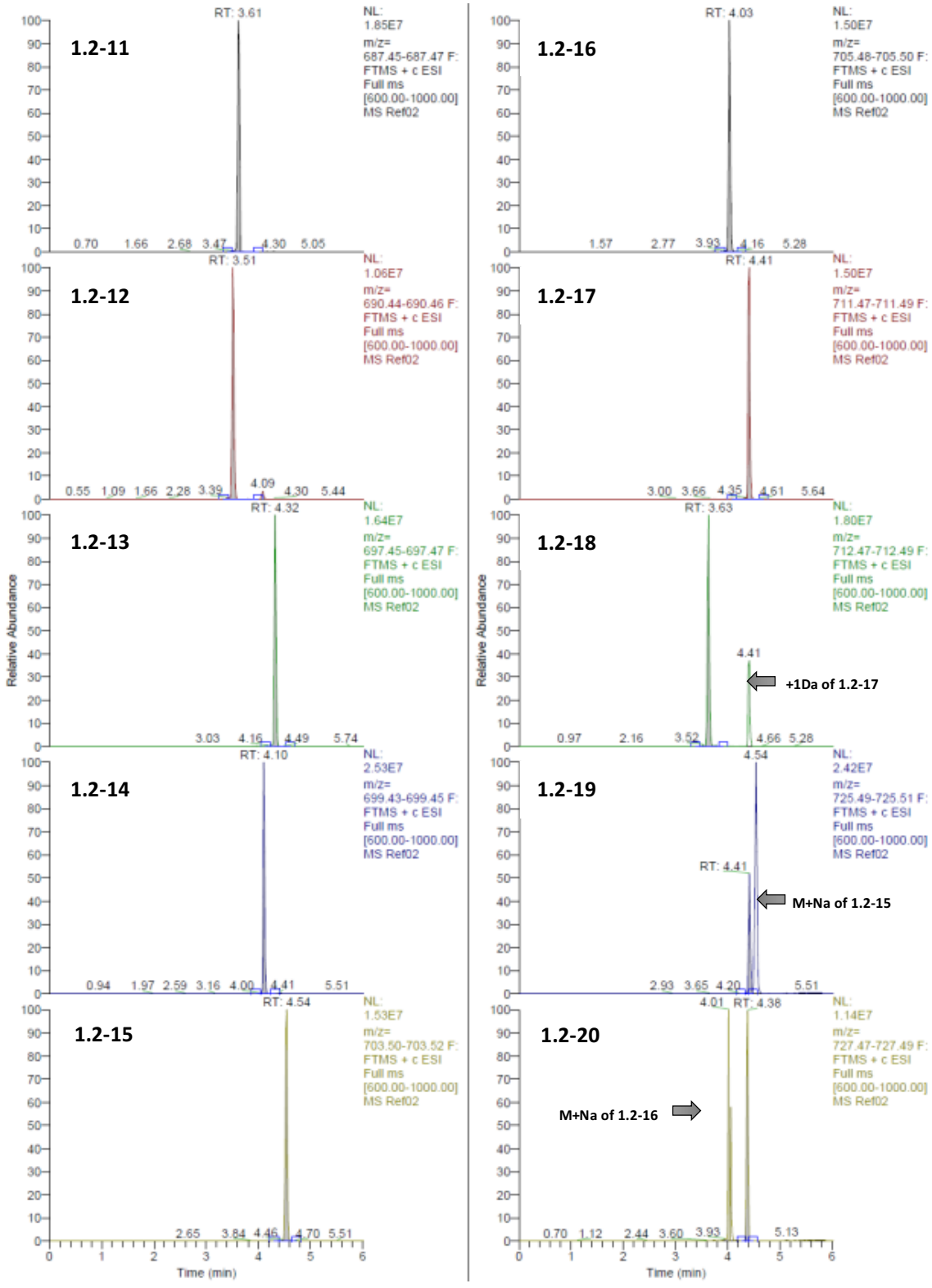


Figure S3.2b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.2

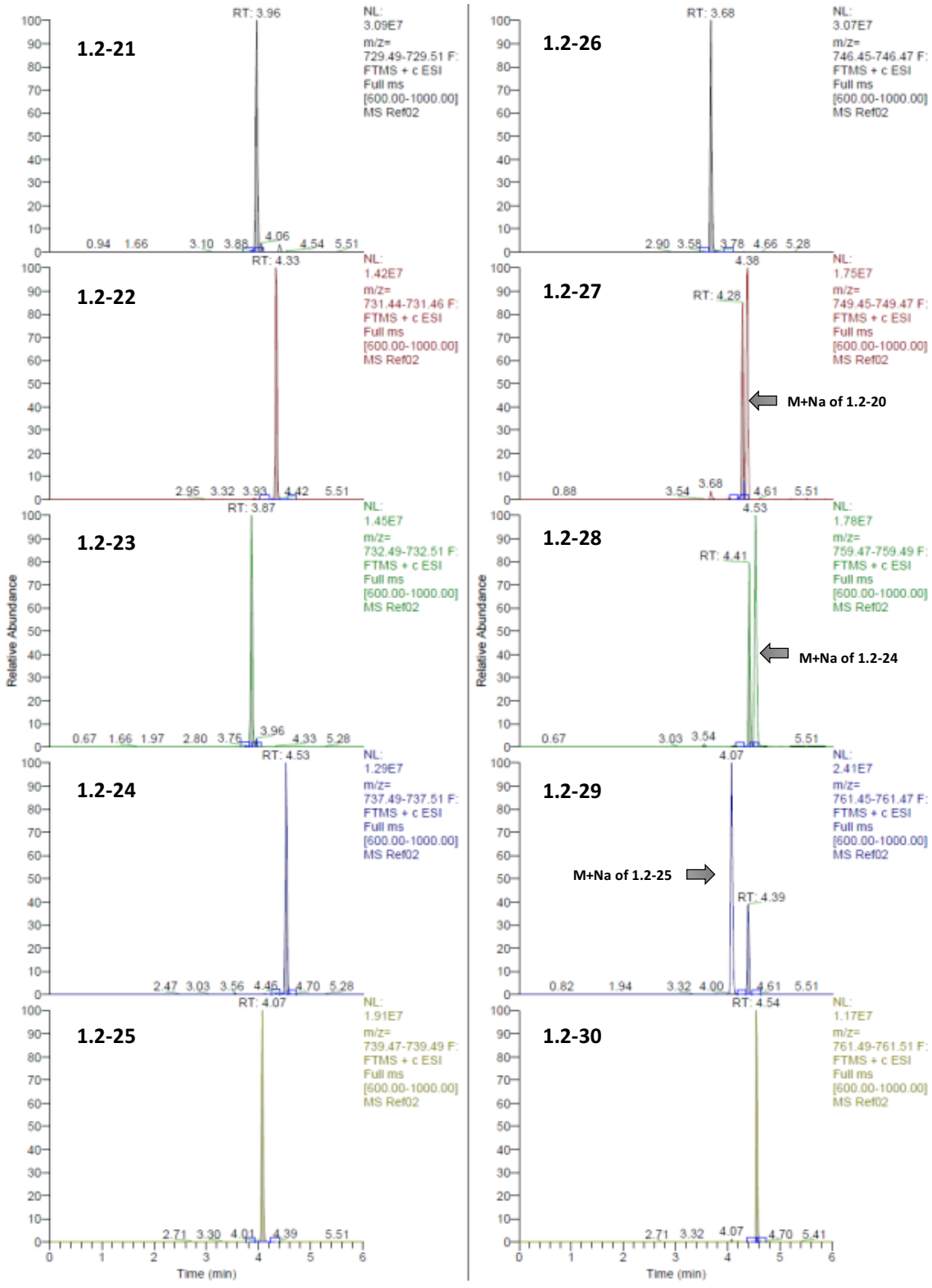


Figure S3.2c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.2

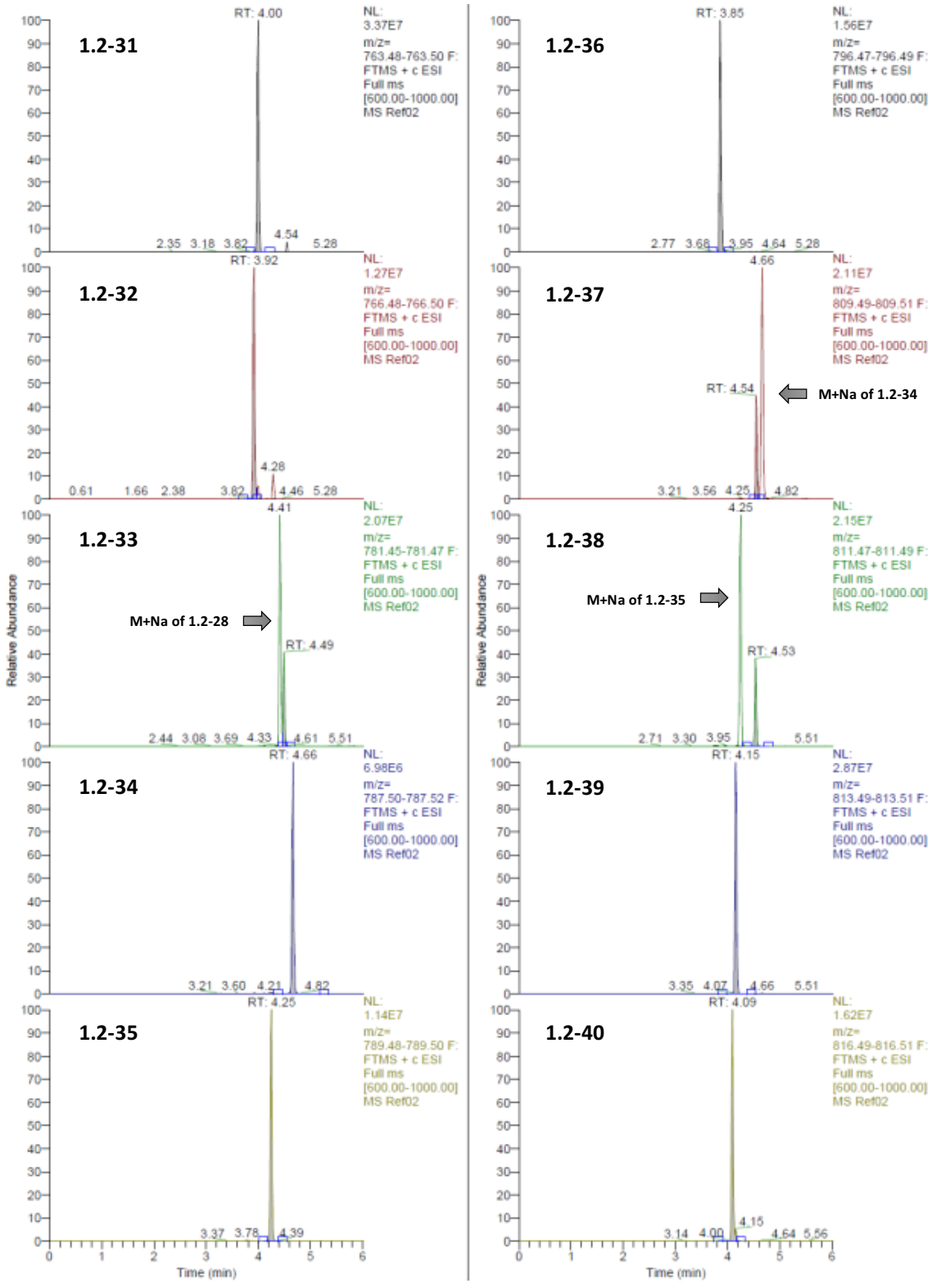


Figure S3.2d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.2

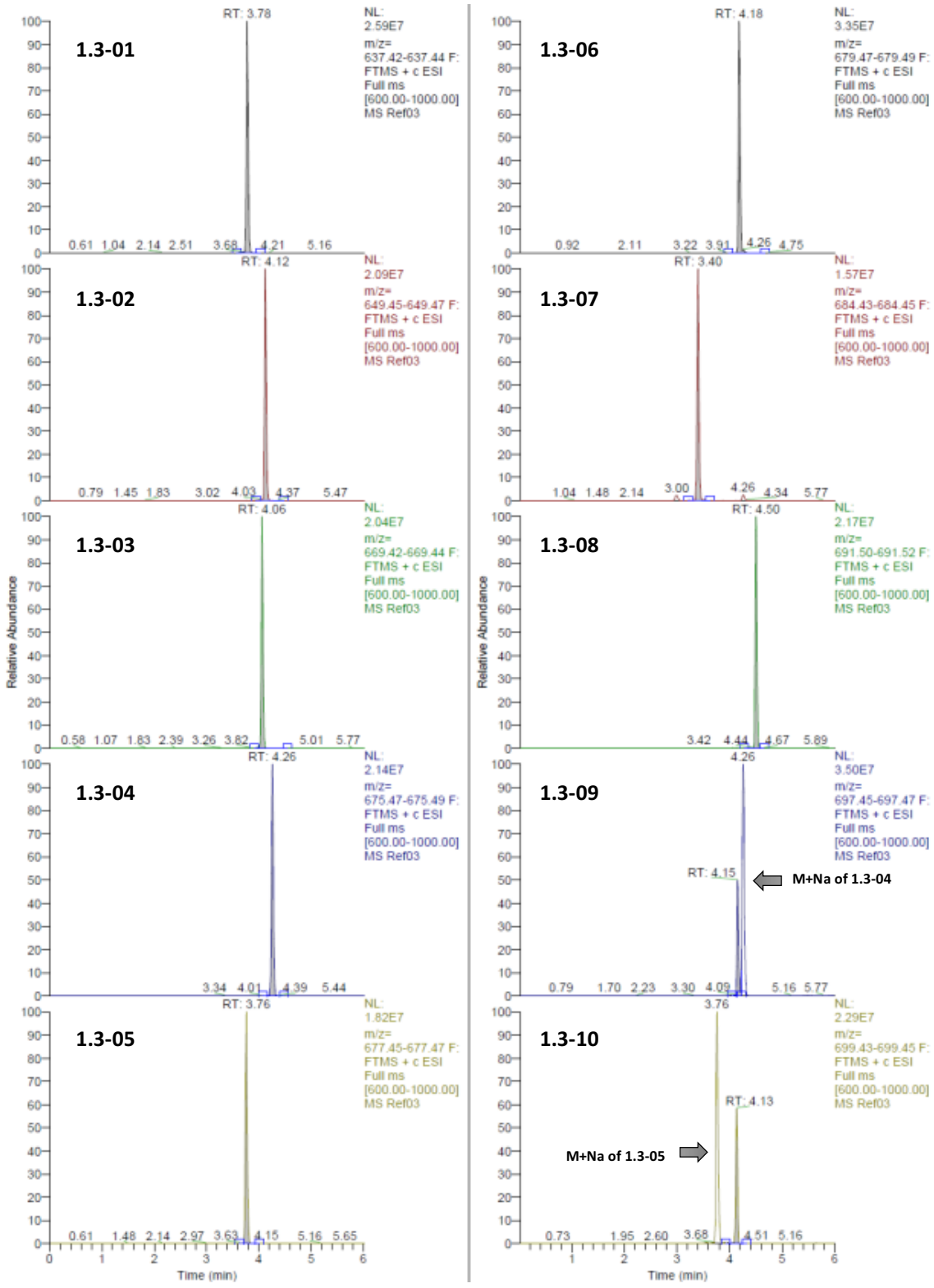


Figure S3.3a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.3

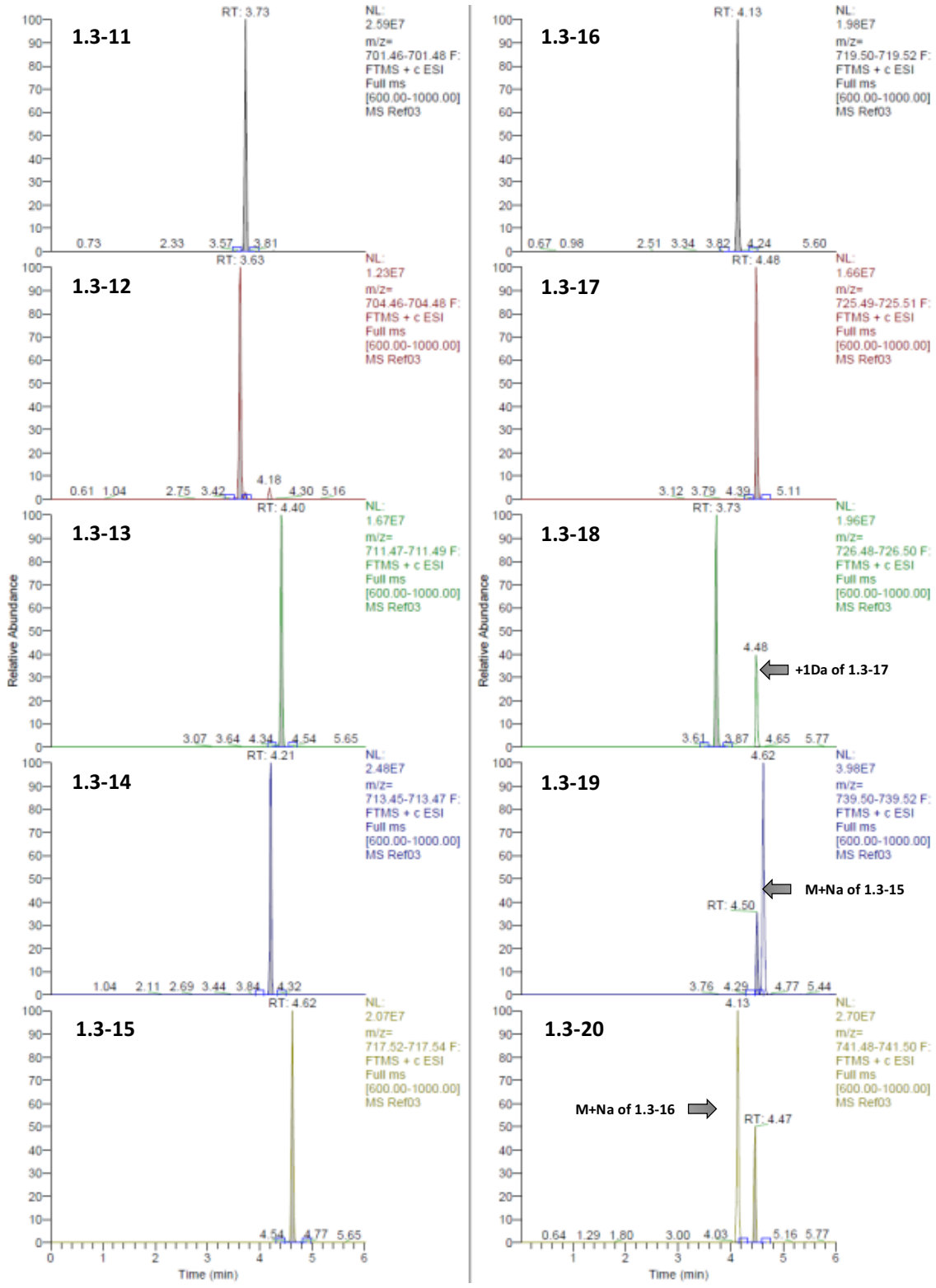


Figure S3.3b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.3

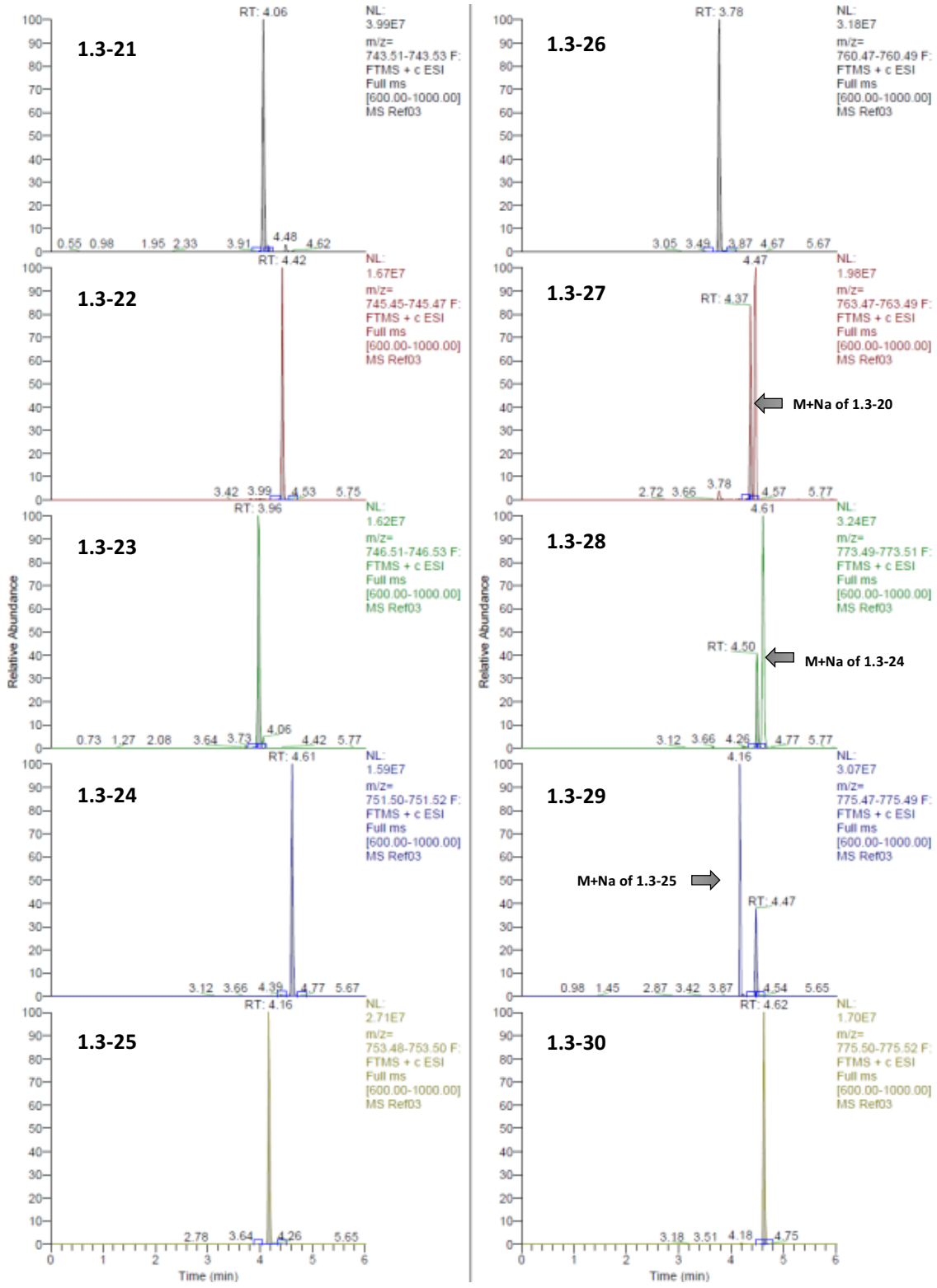


Figure S3.3c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.3

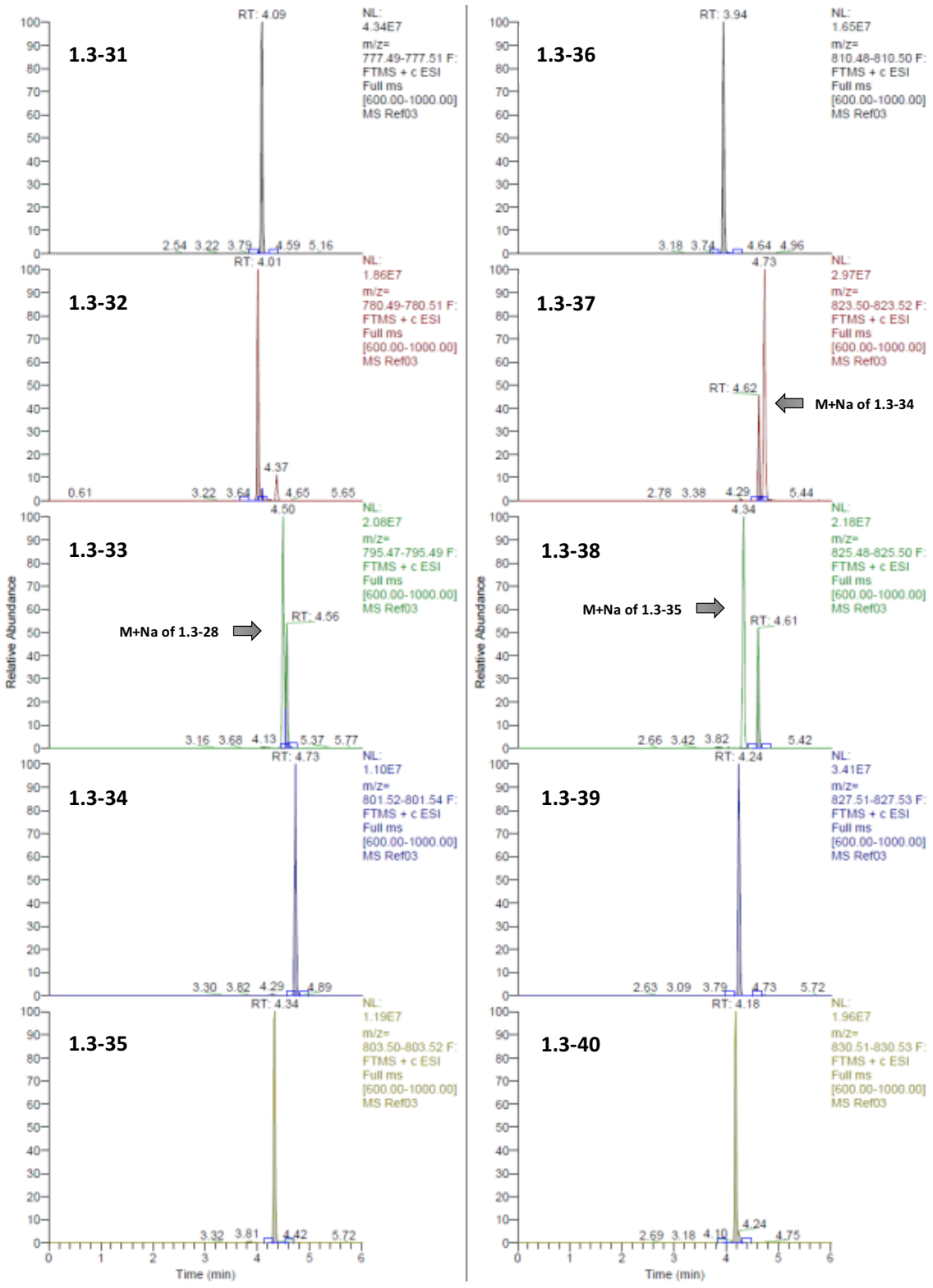


Figure S3.3d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.3

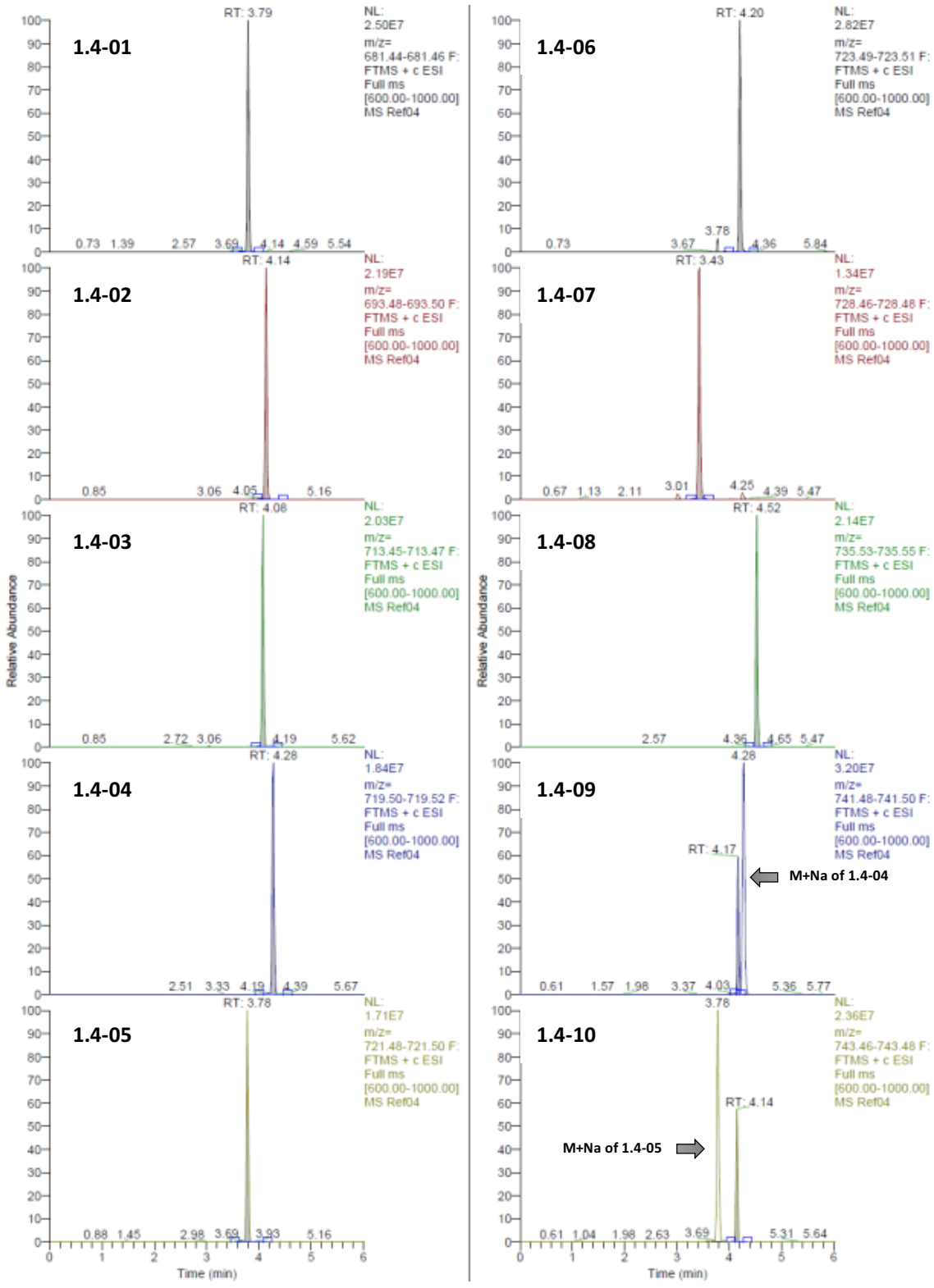
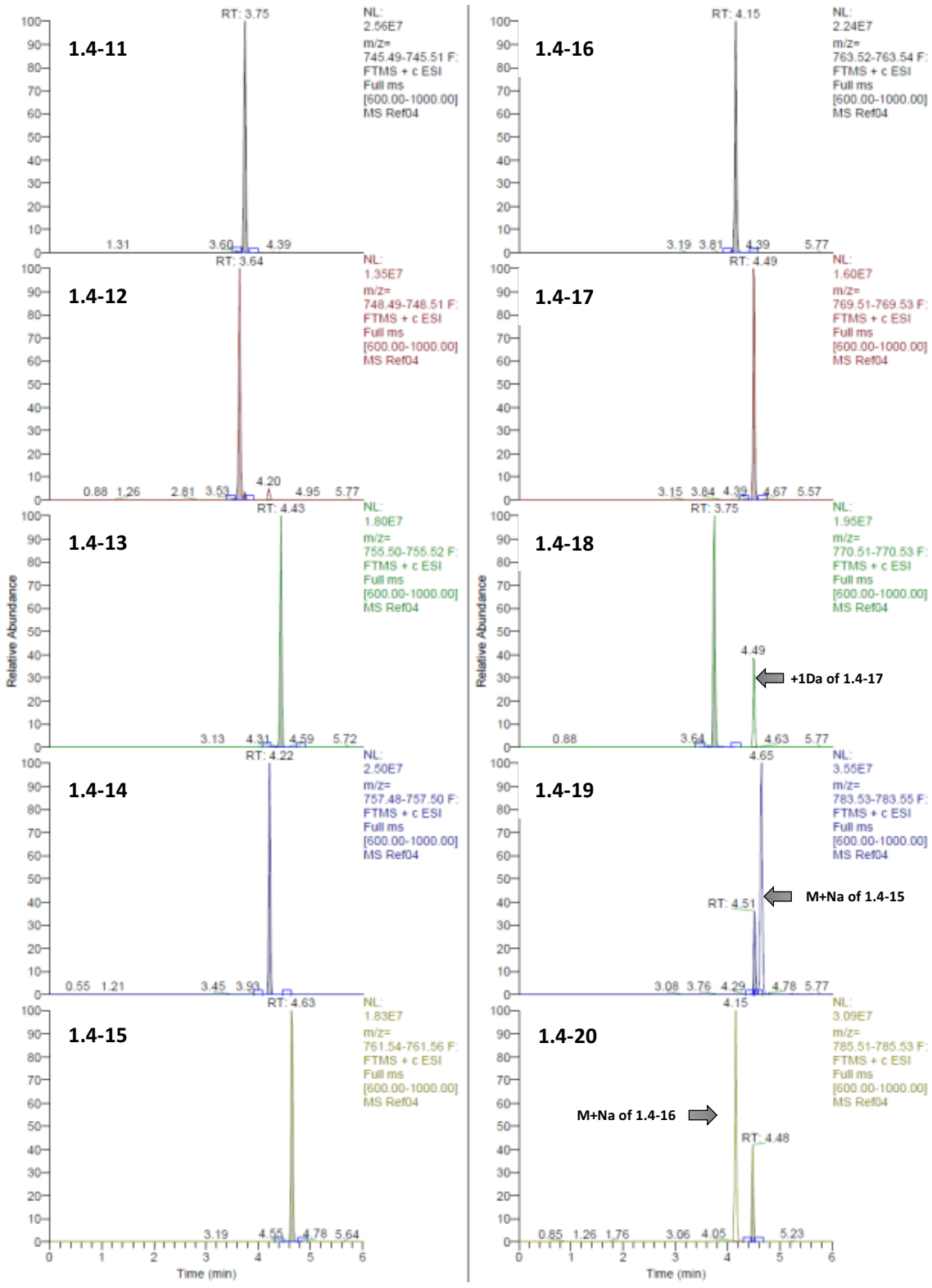


Figure S3.4a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.4



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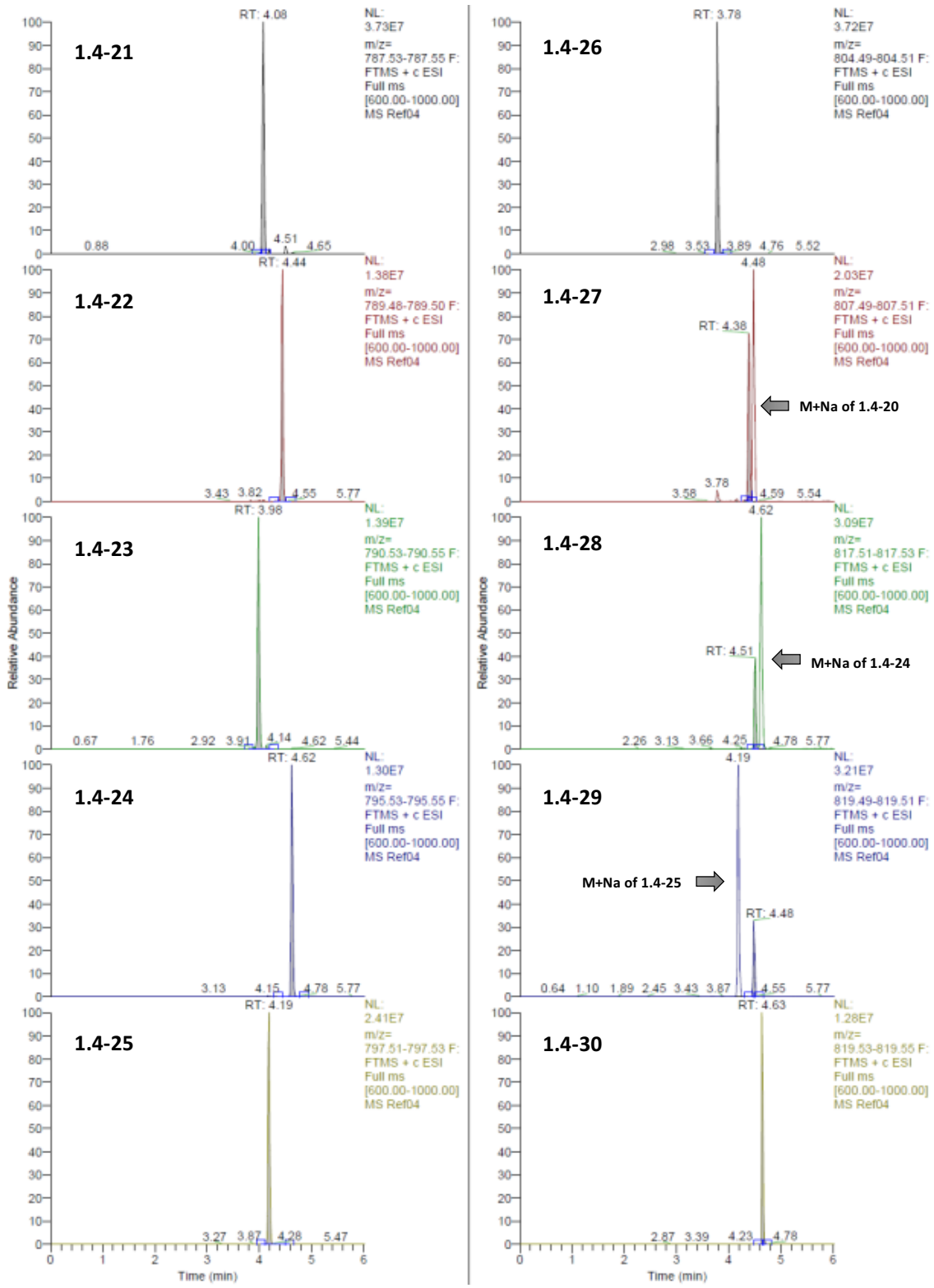
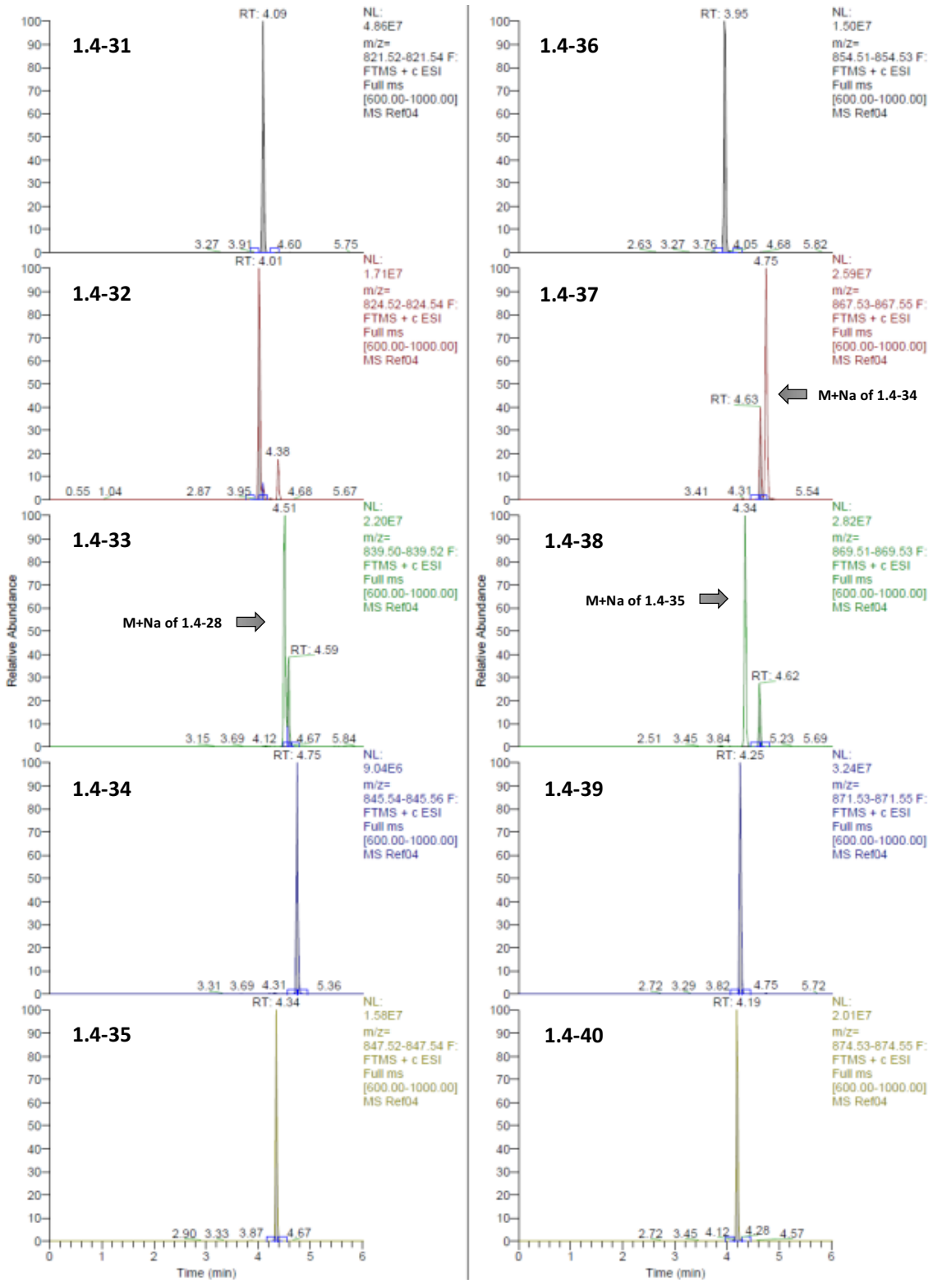


Figure S3.4c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.4



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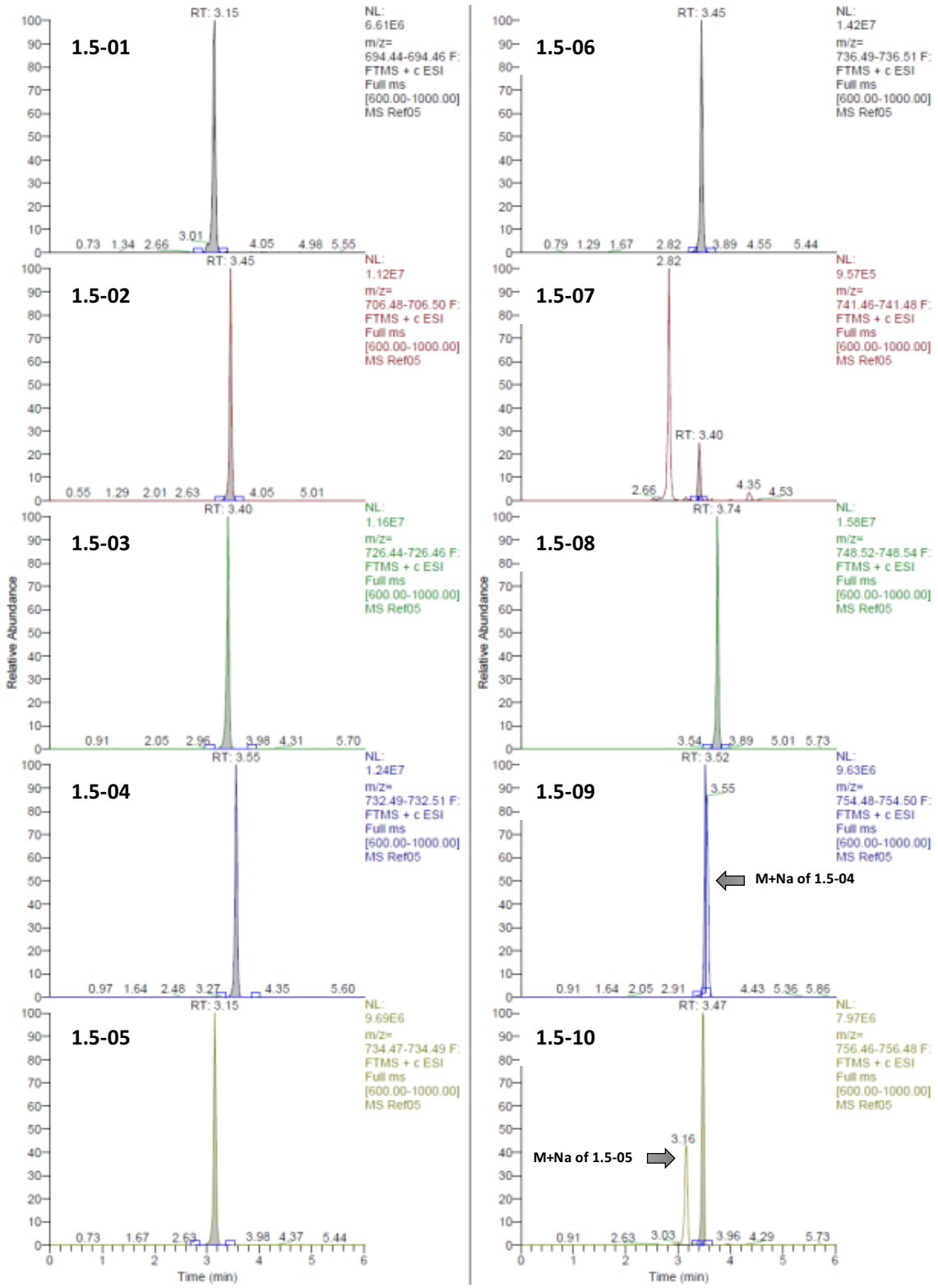
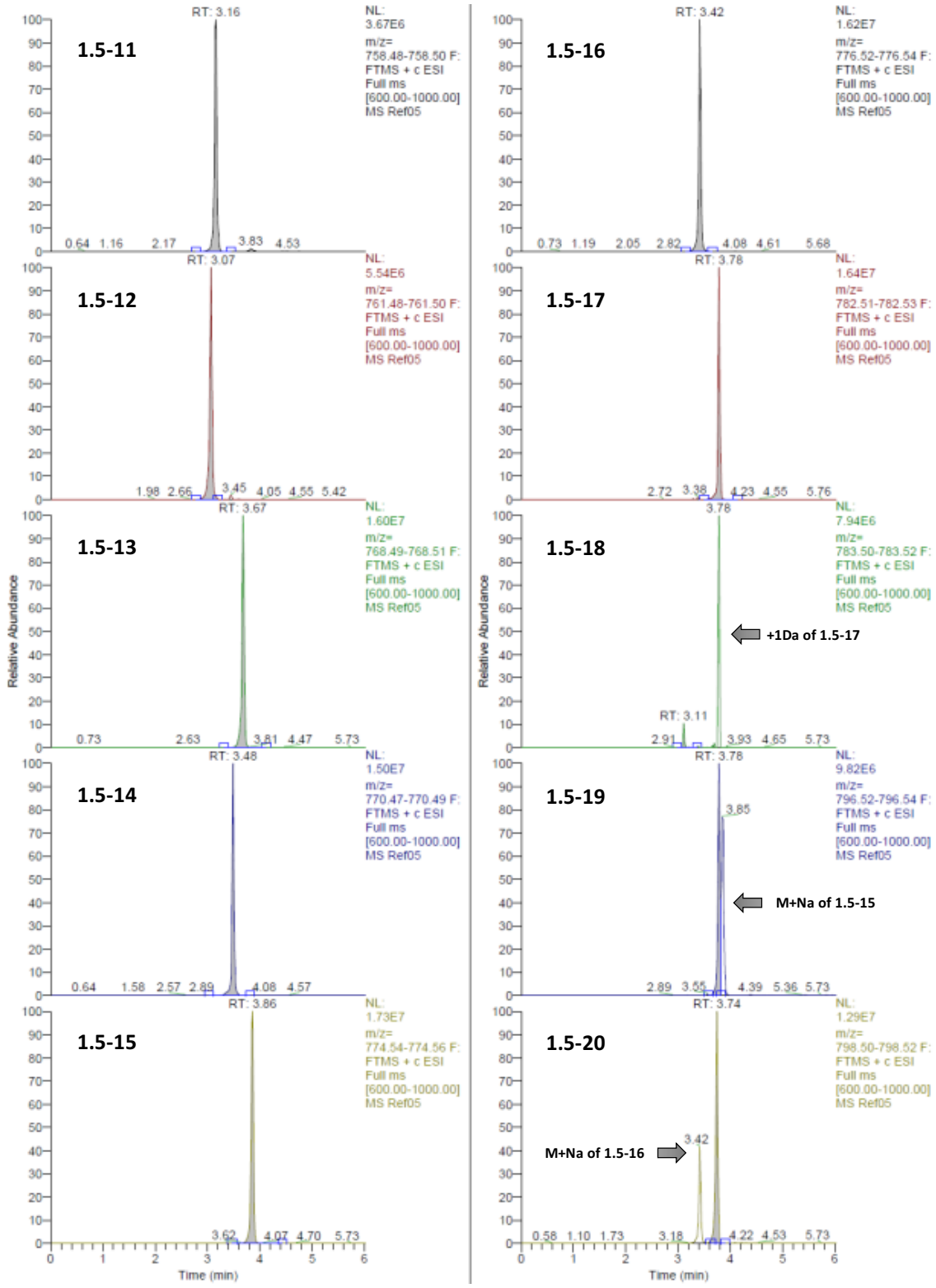


Figure S3.5a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.5



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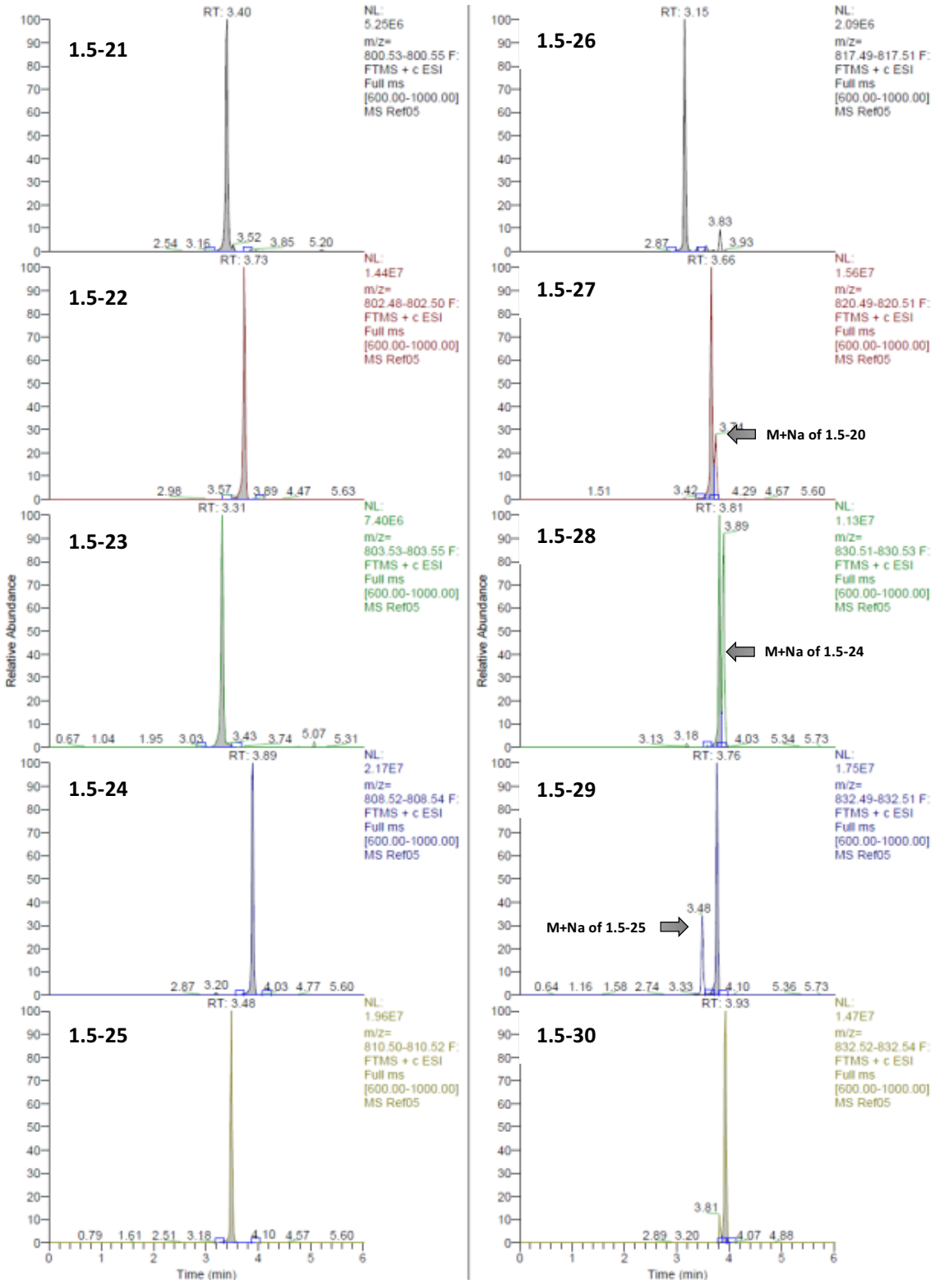
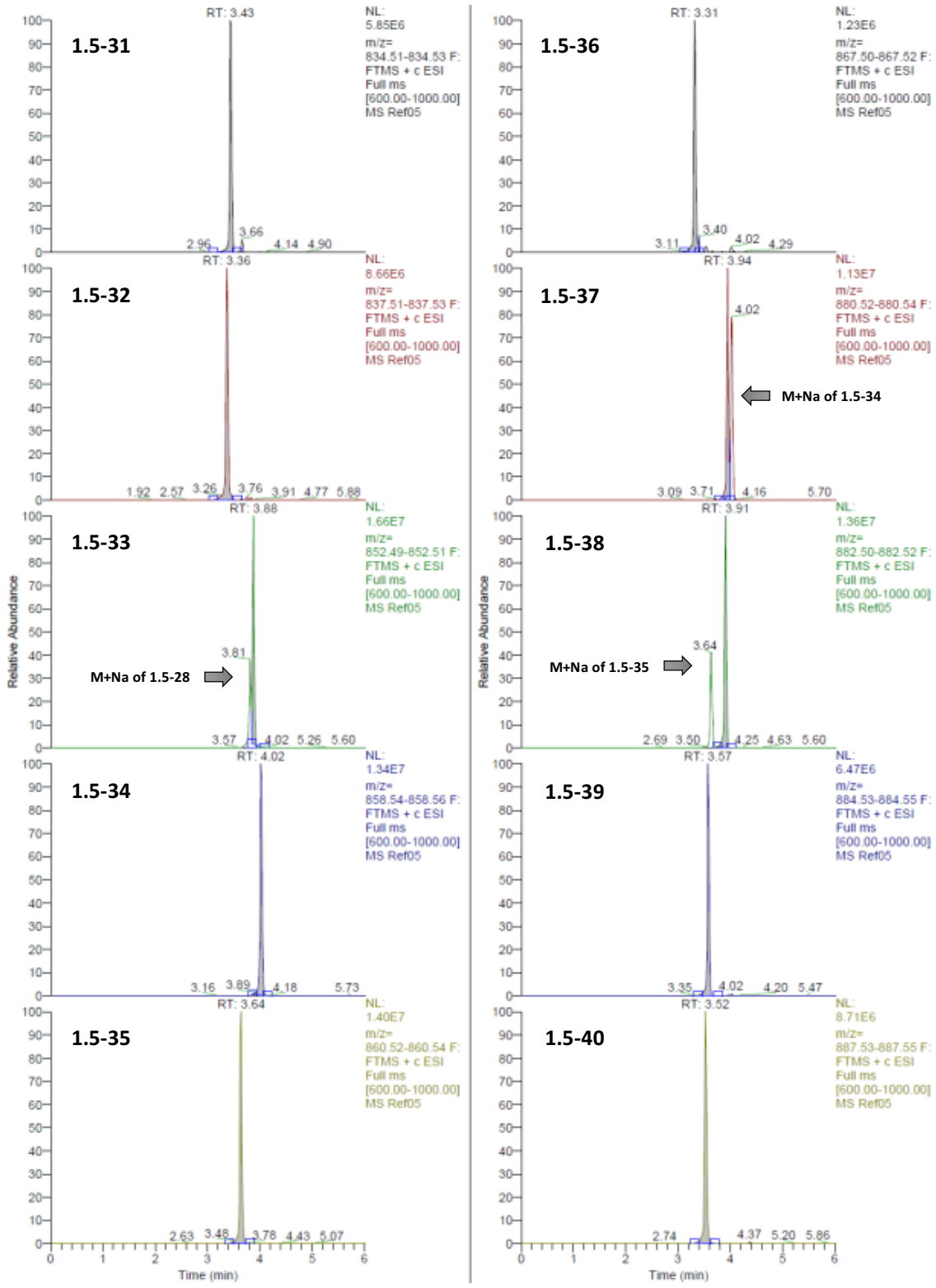


Figure S3.5c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.5



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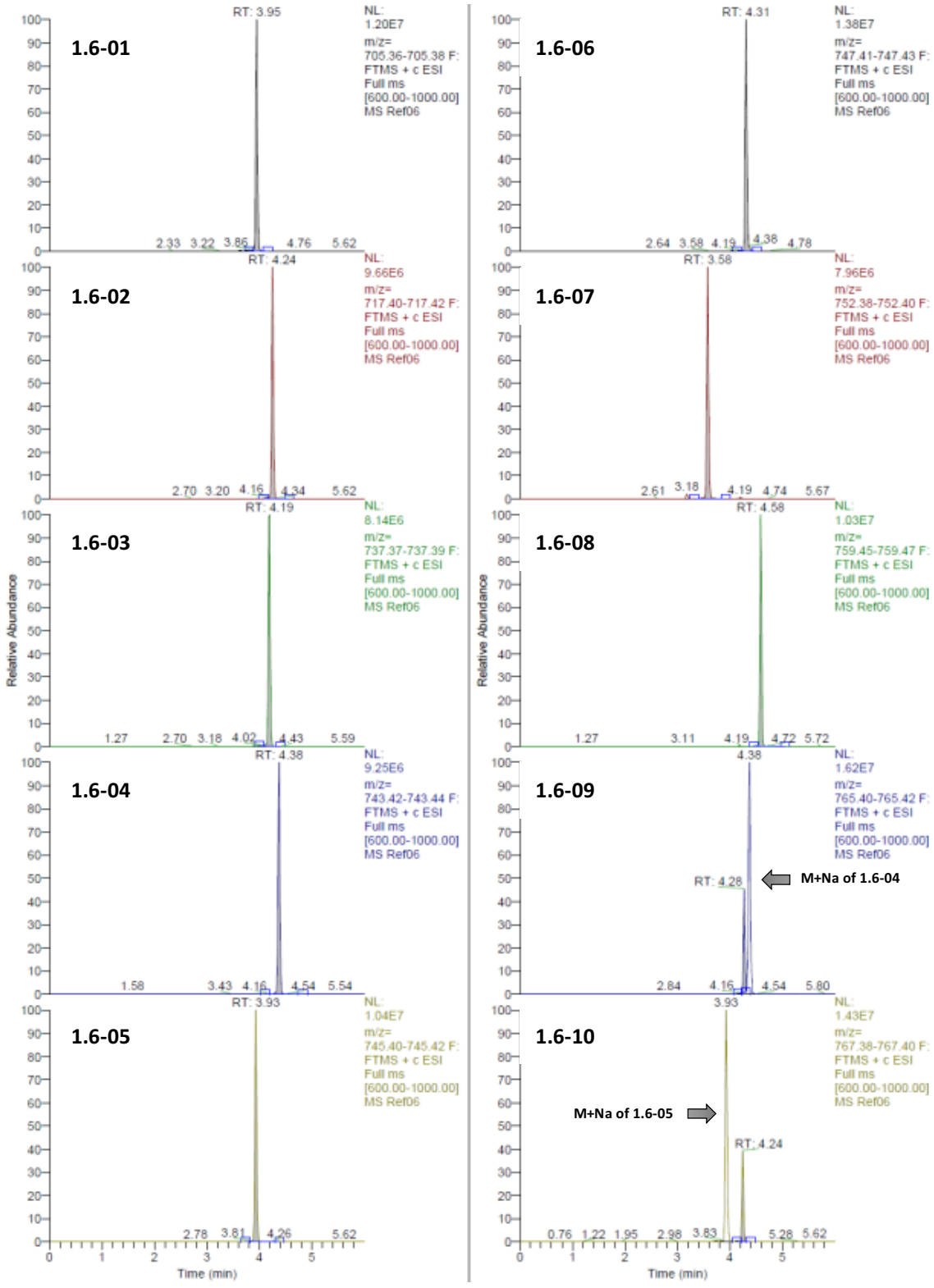


Figure S3.6a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.6

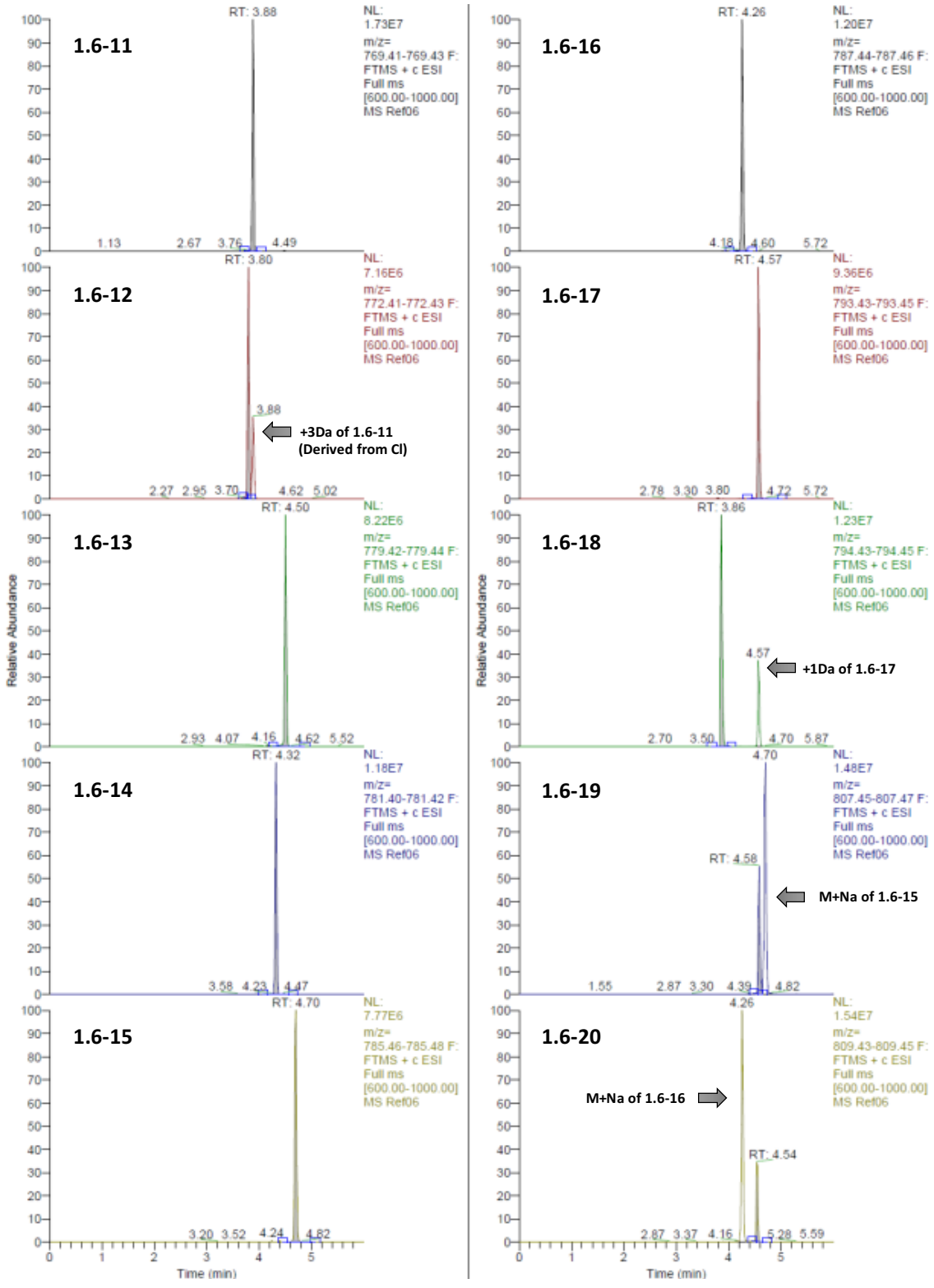


Figure S3.6b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.6

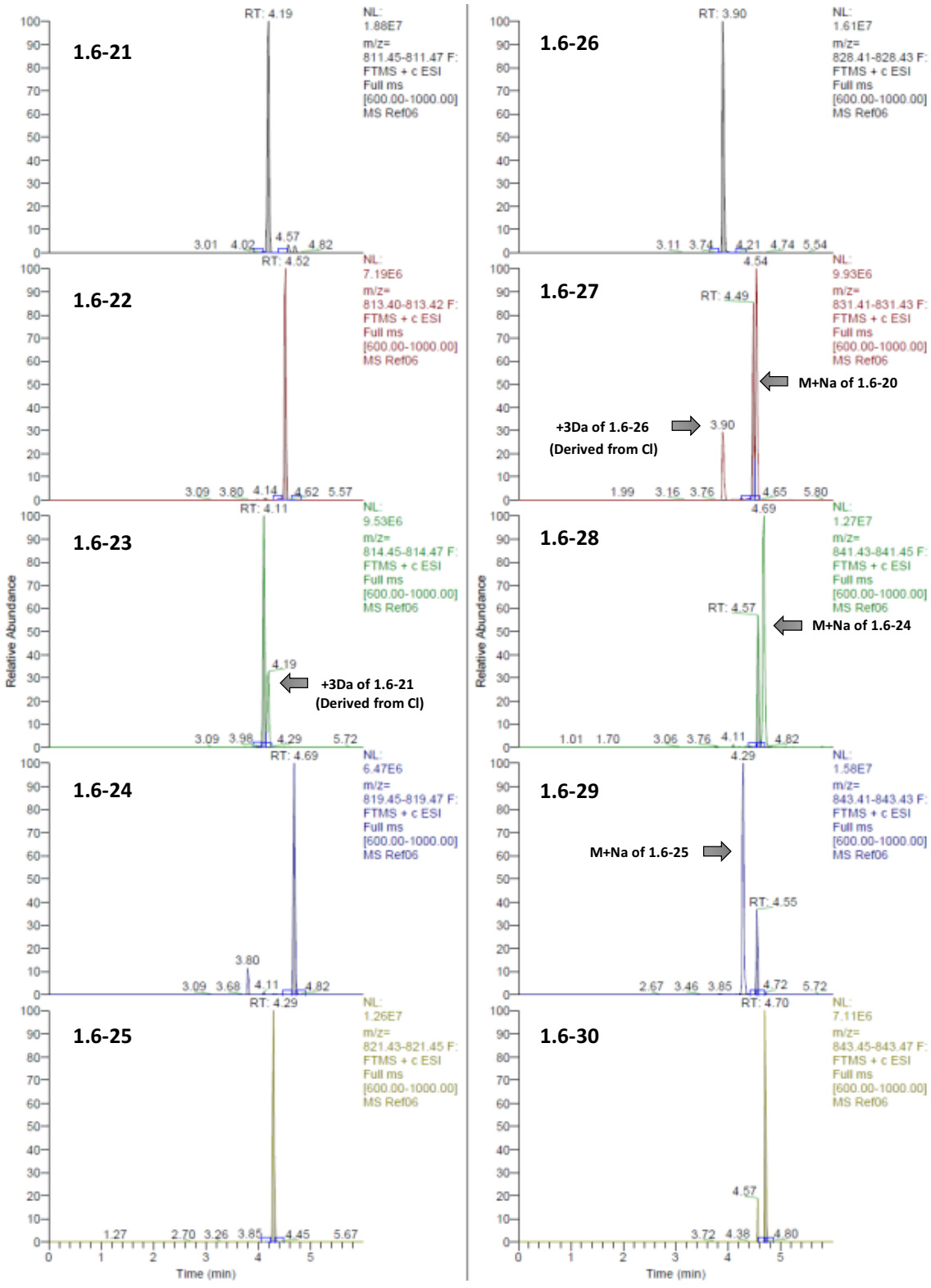


Figure S3.6c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.6

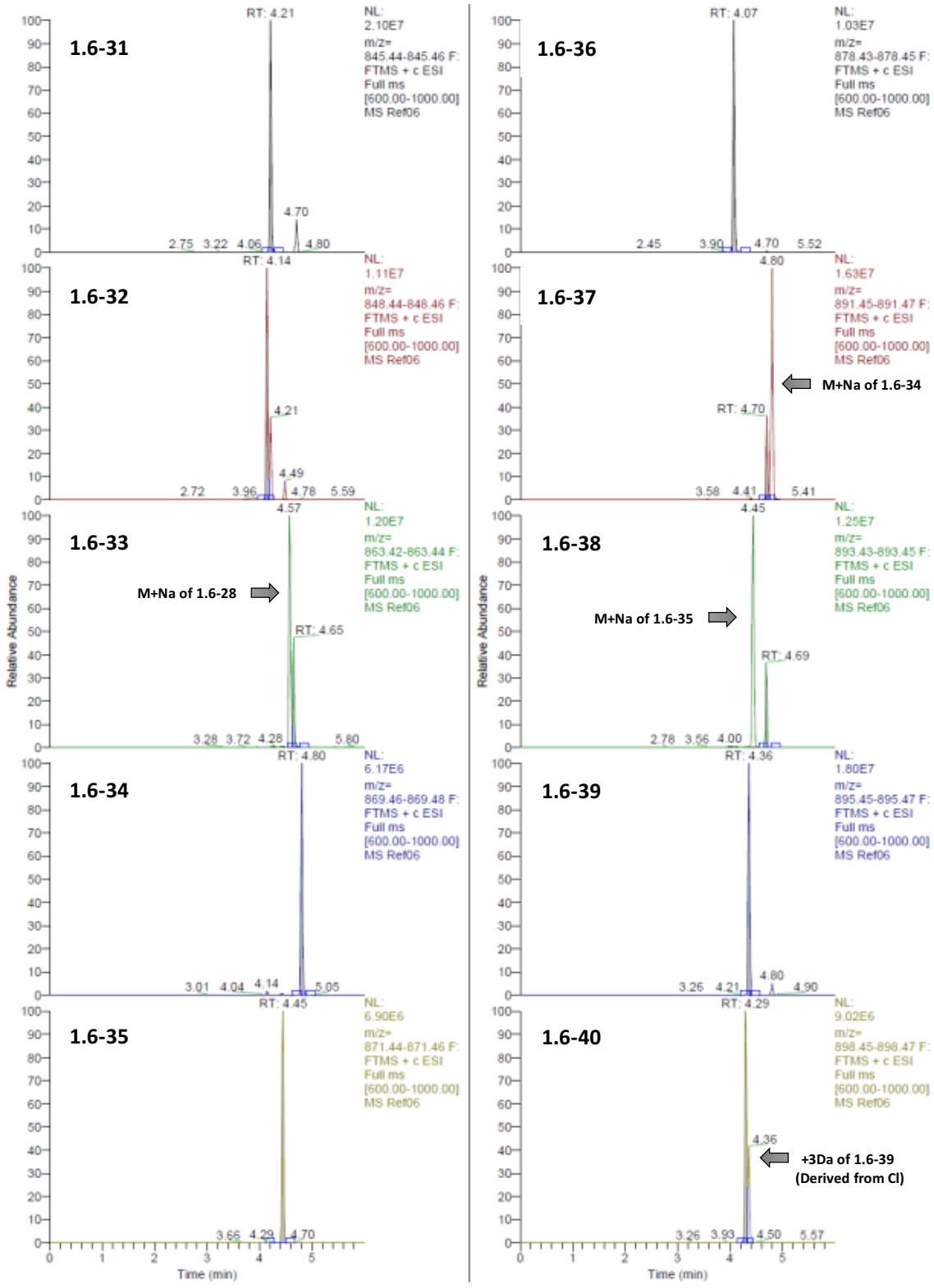


Figure S3.6d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.6

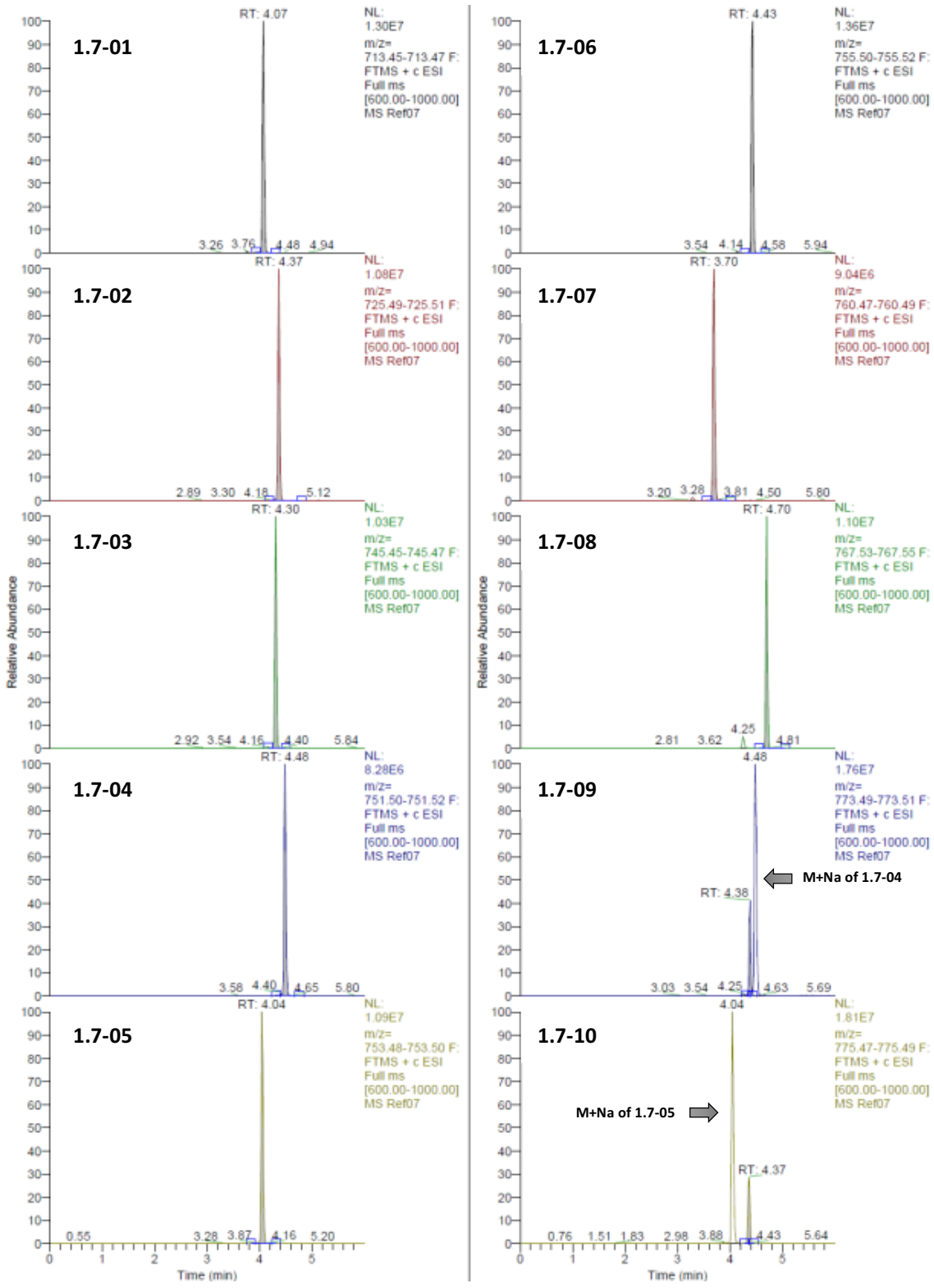
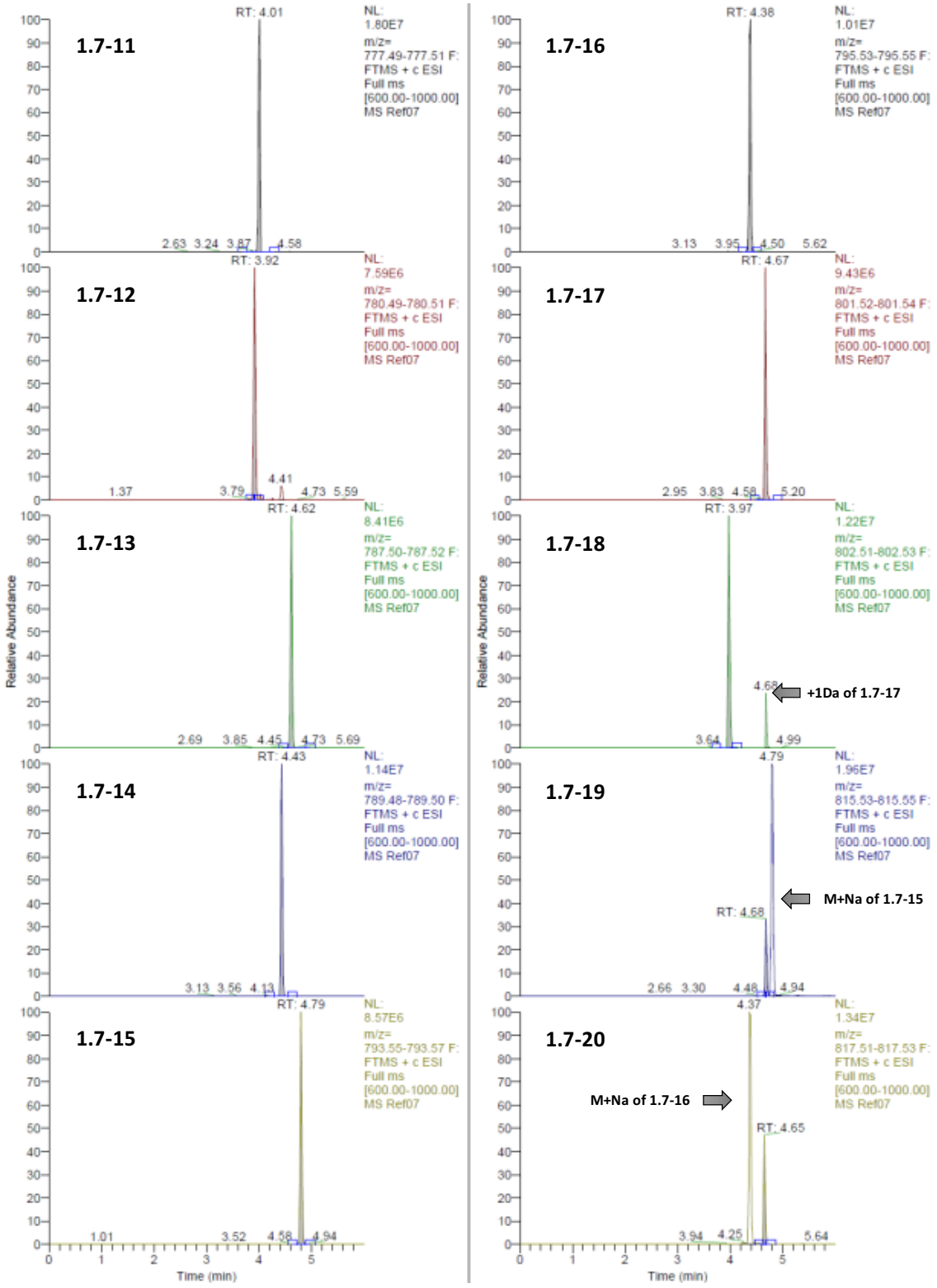


Figure S3.7a. Extracted Ion Chromatograms (M+H± 0.01Da) of Sub-library 1.7



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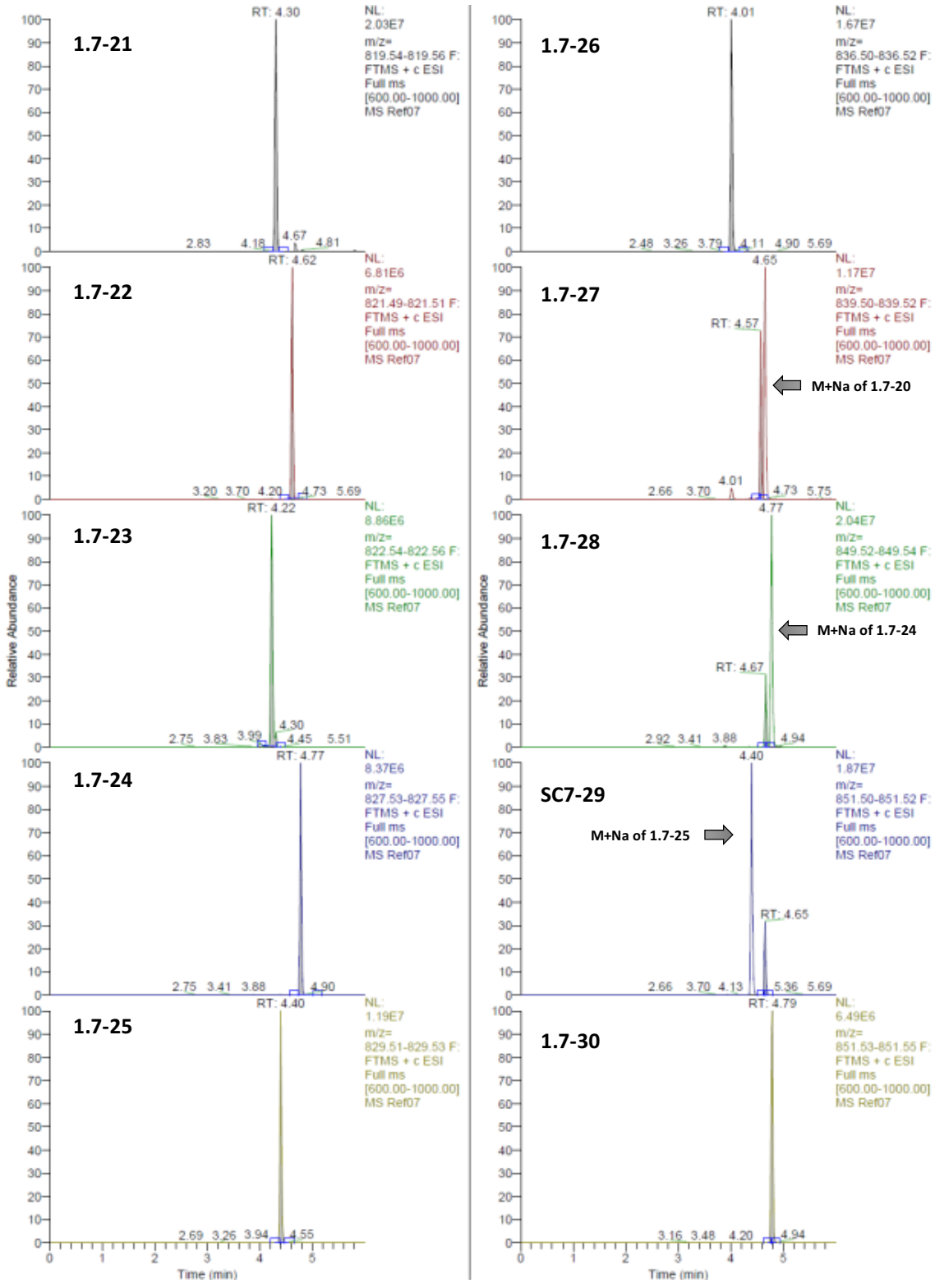


Figure S3.7c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.7

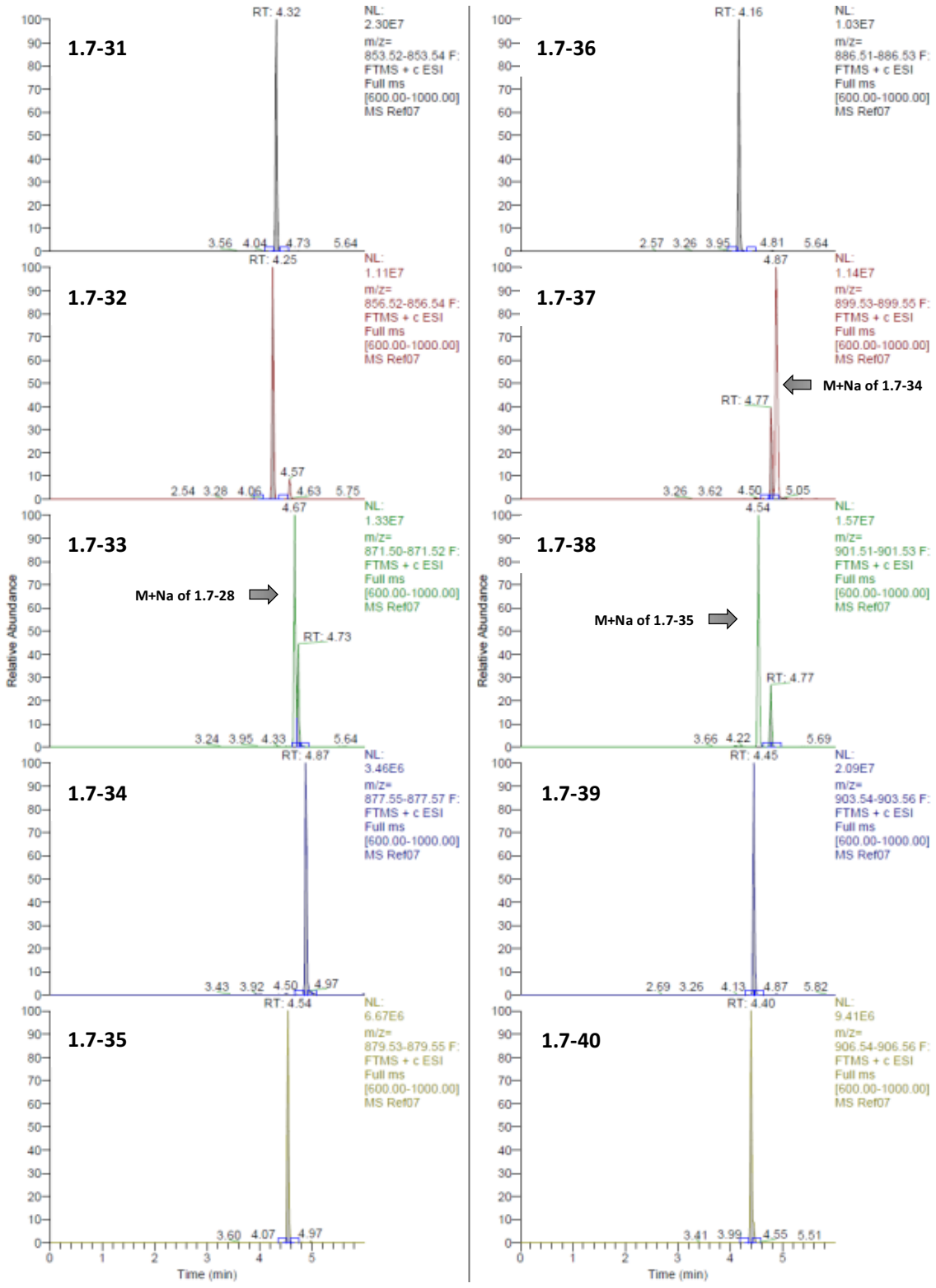


Figure S3.7d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.7

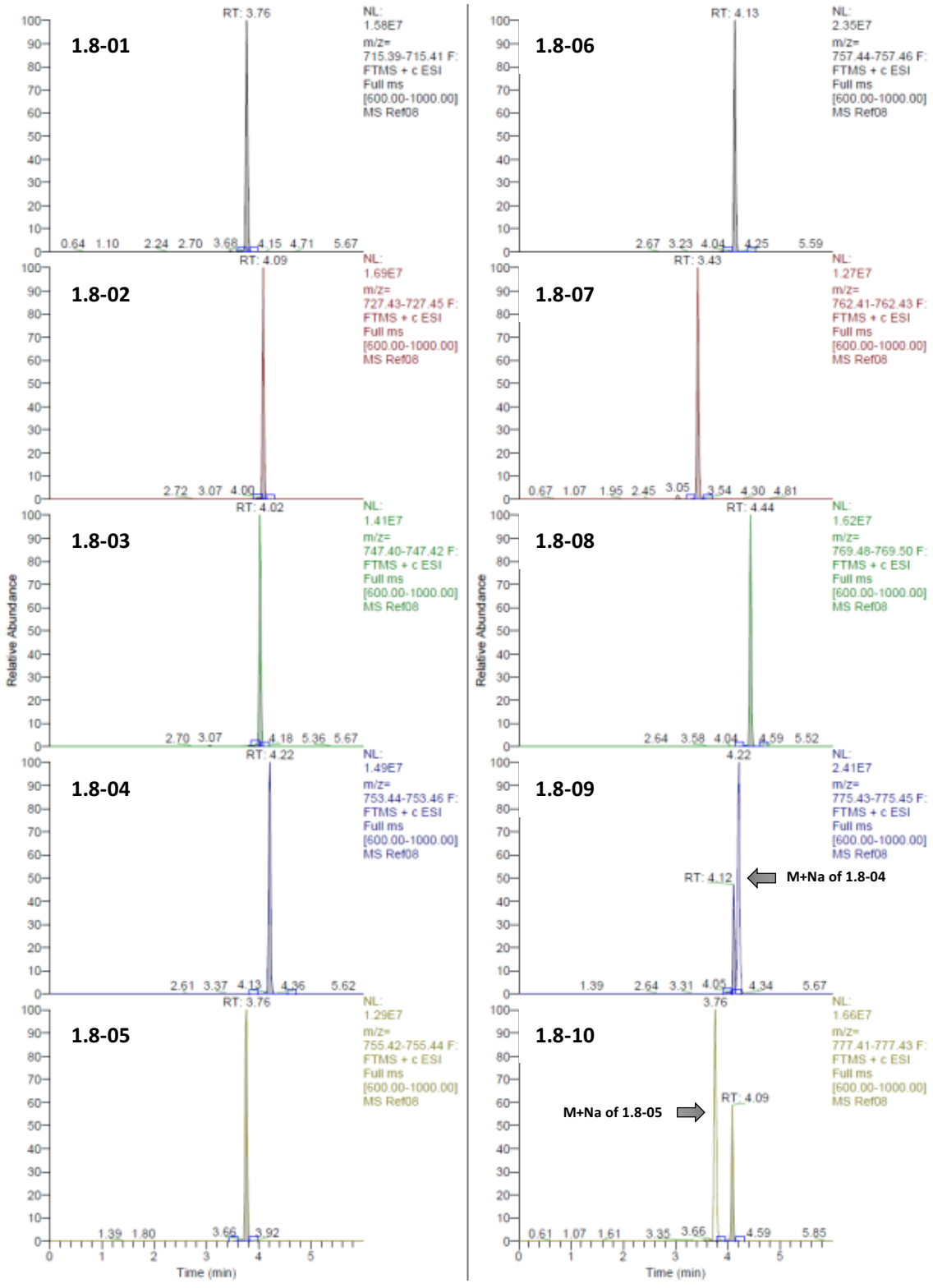


Figure S3.8a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.8

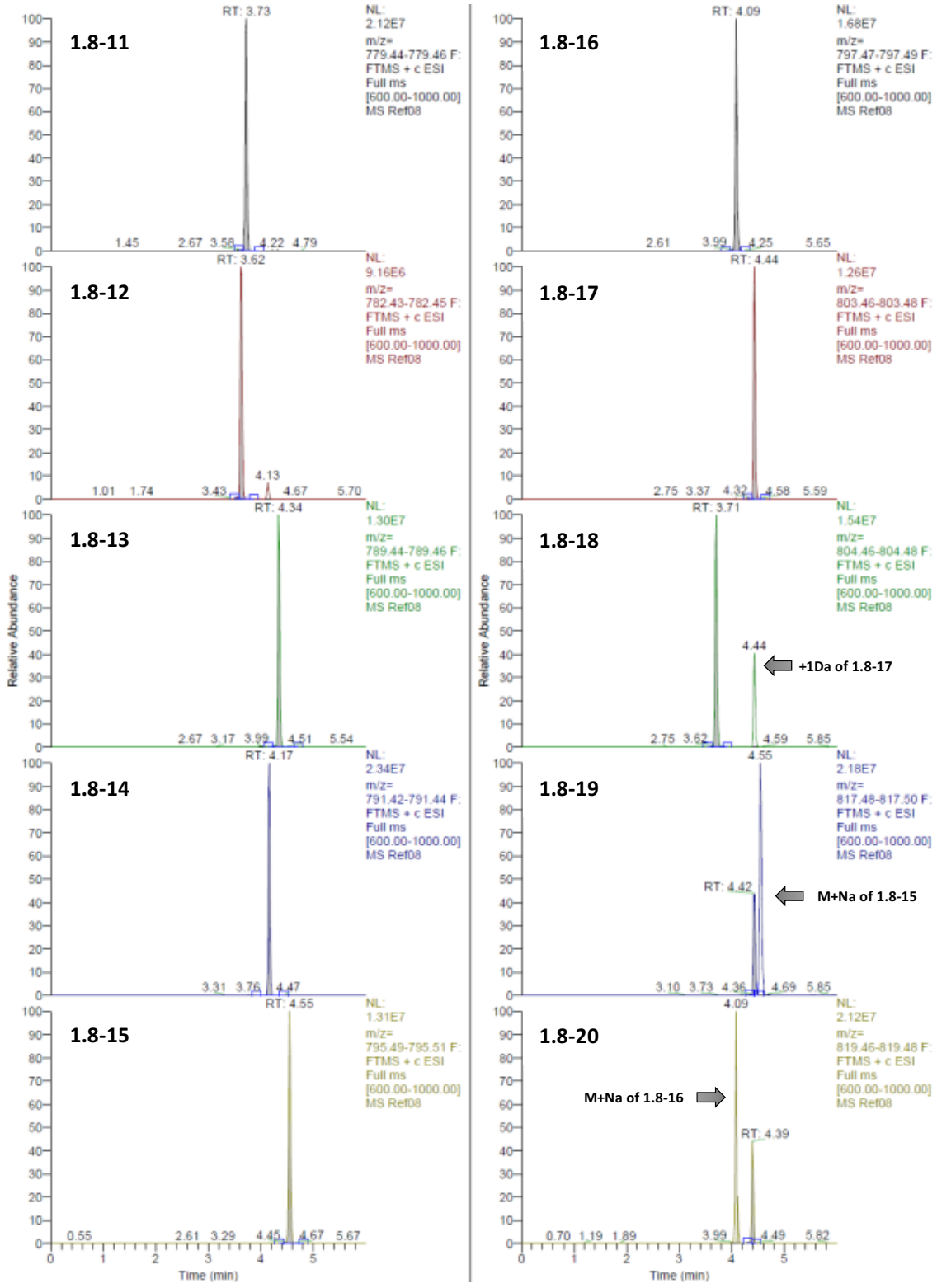


Figure S3.8b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.8

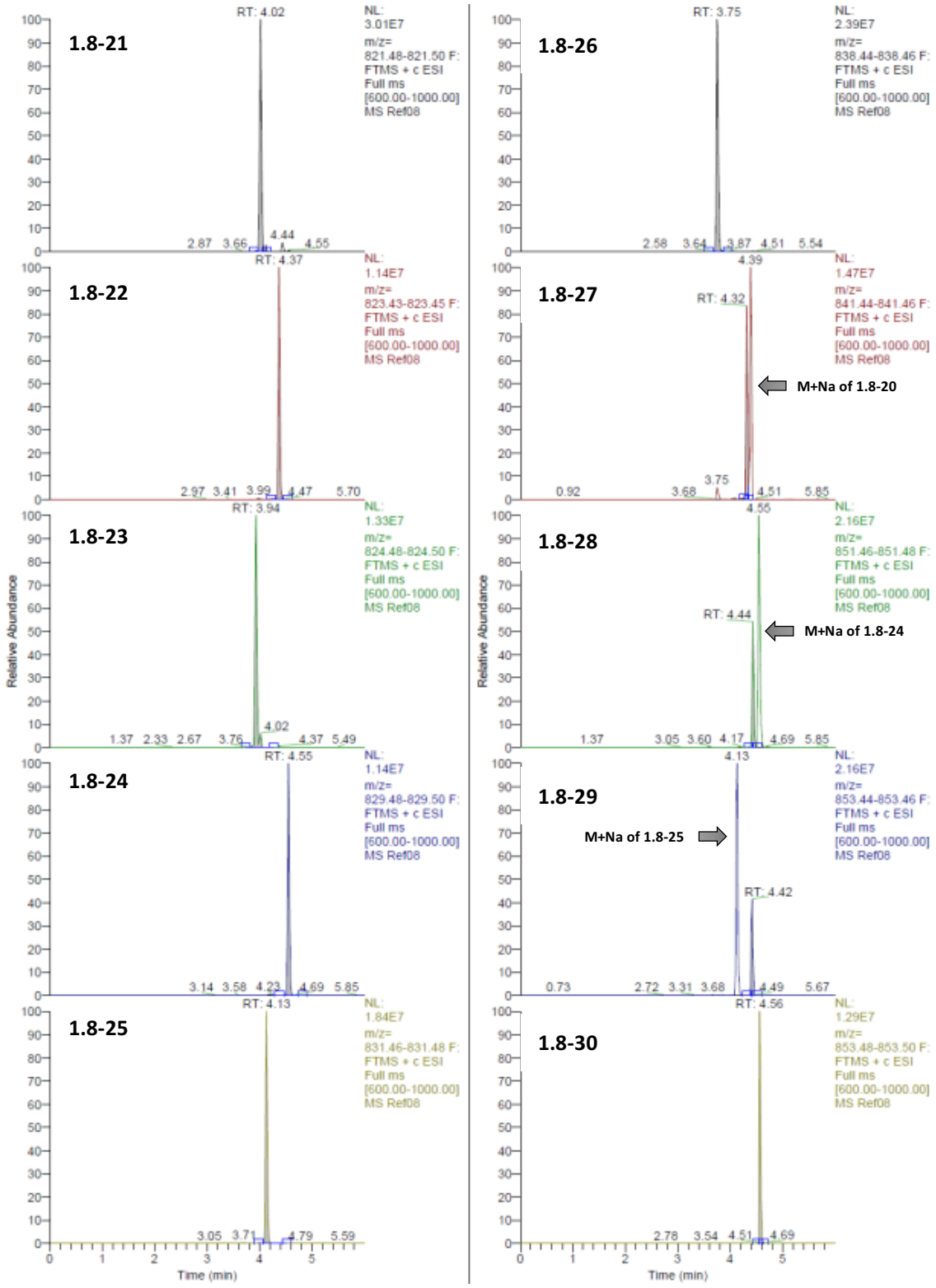


Figure S3.8c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.8

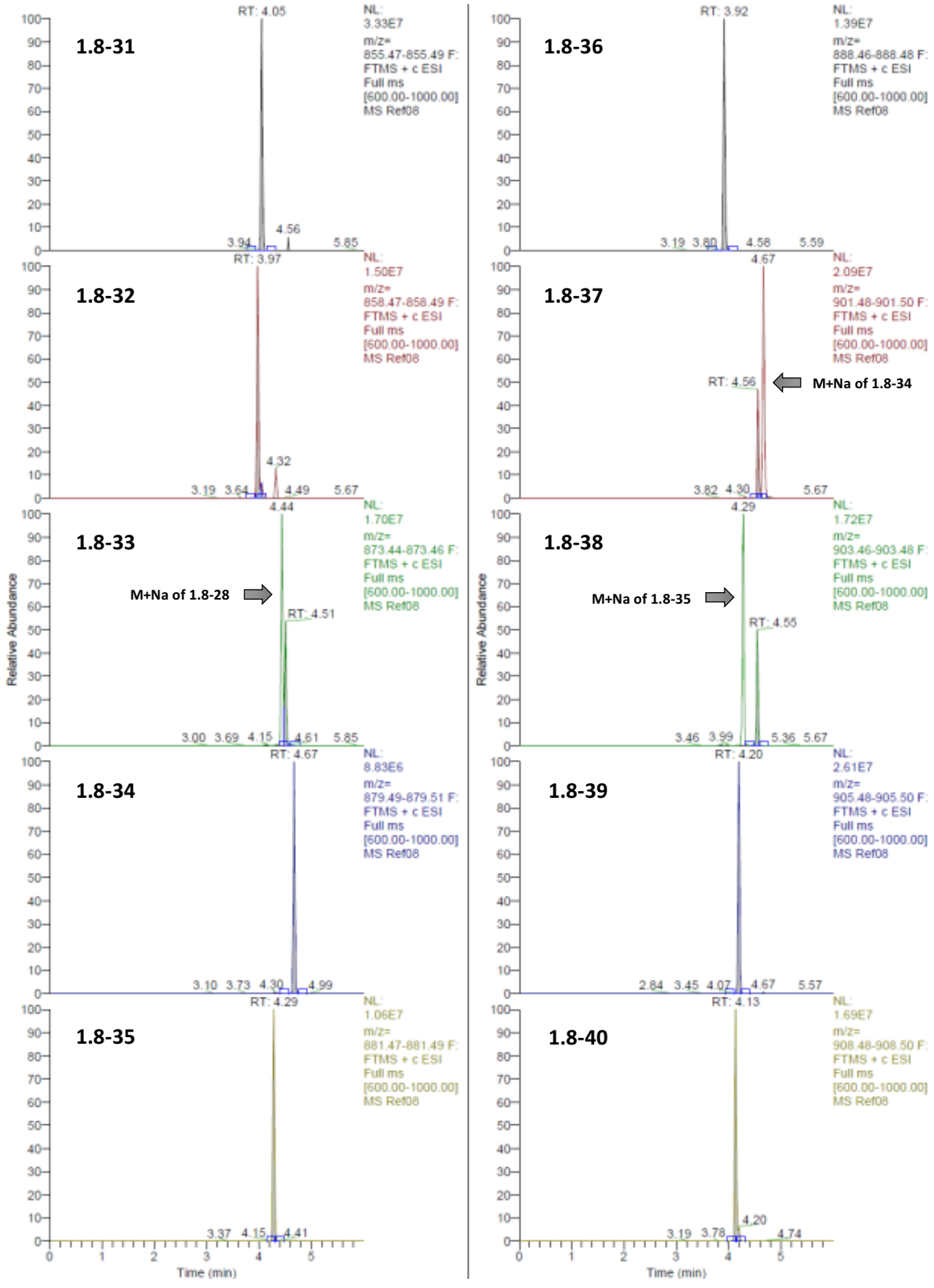


Figure S3.8d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.8

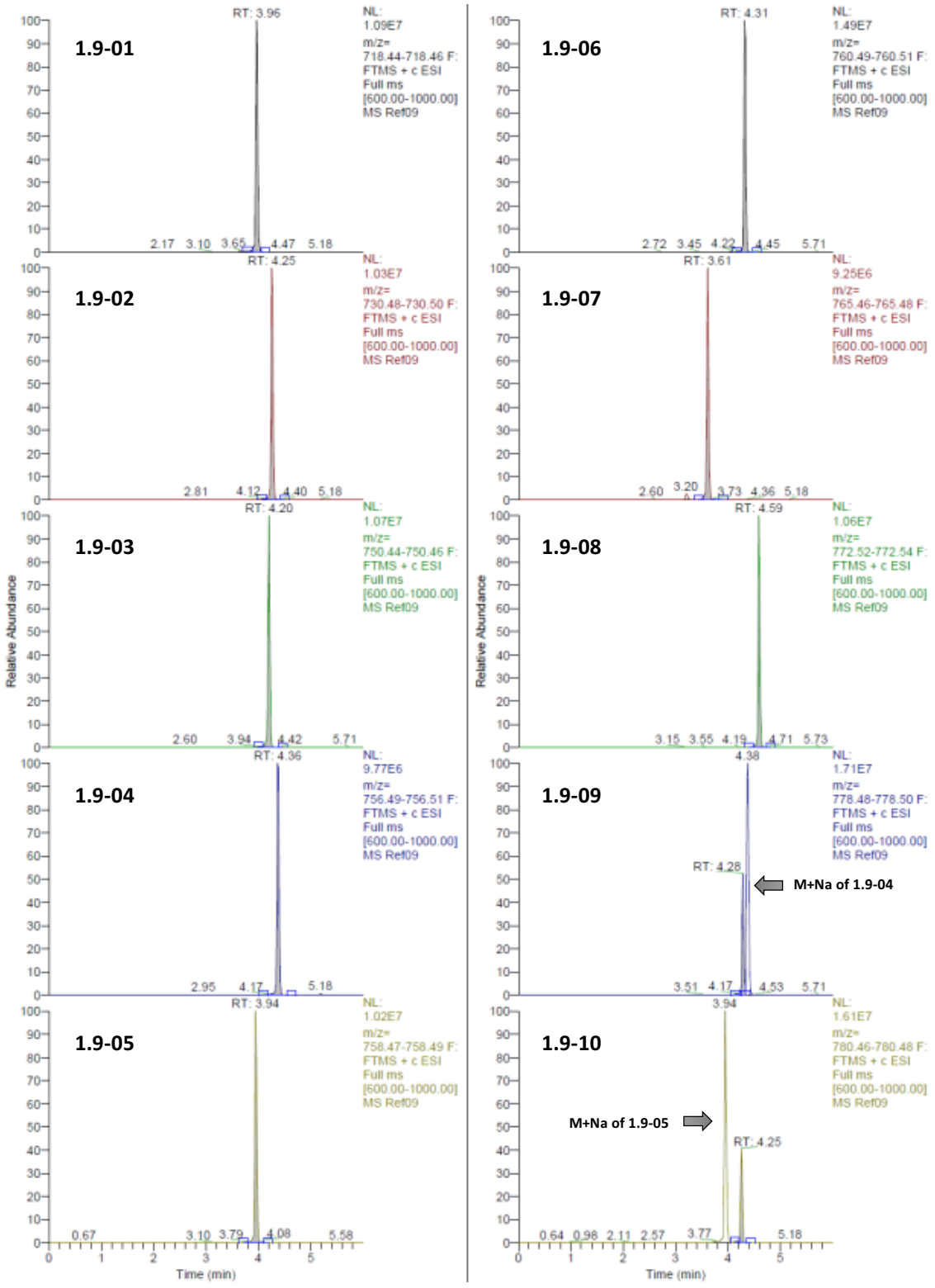


Figure S3.9a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.9

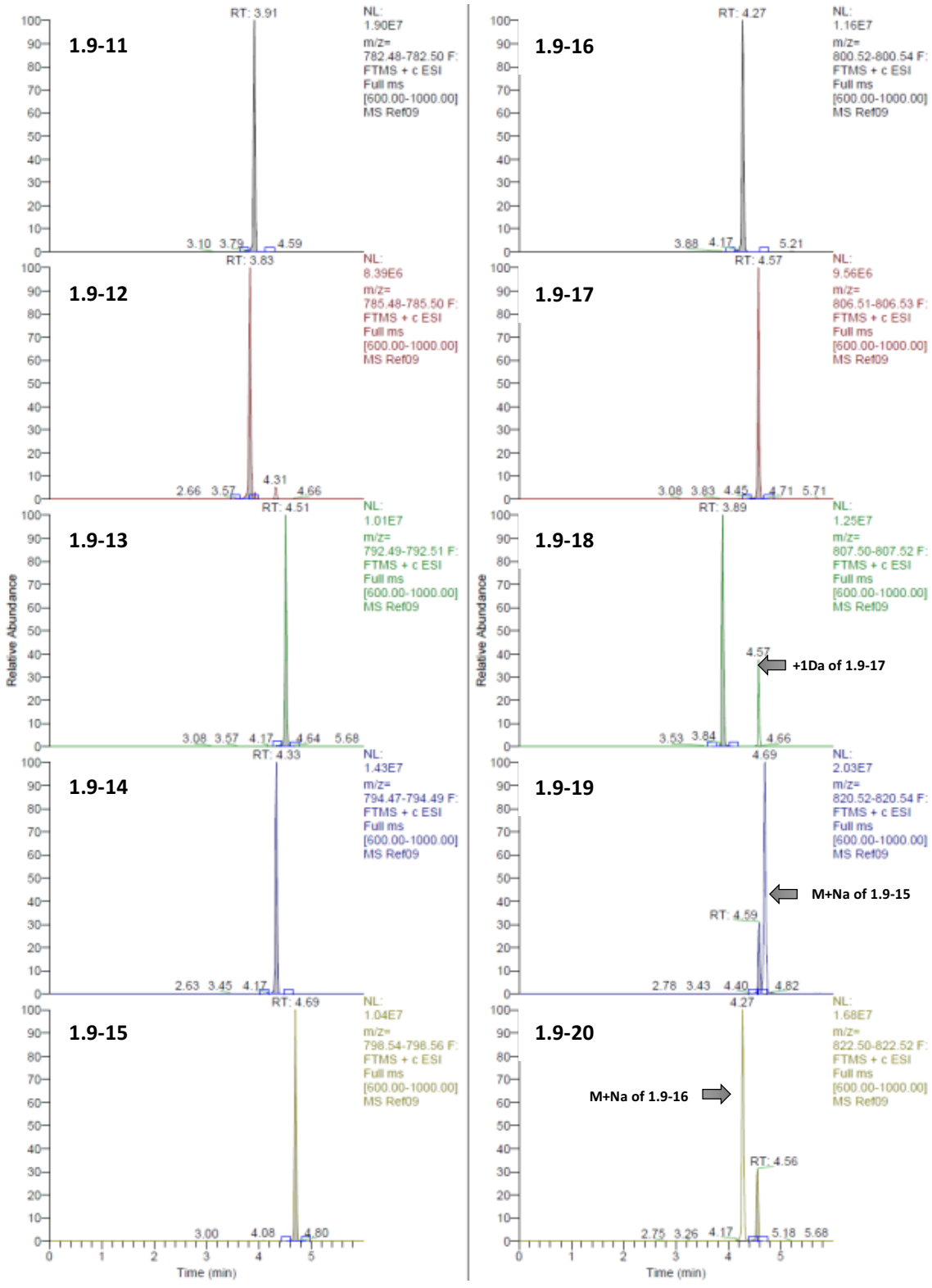


Figure S3.9b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.9

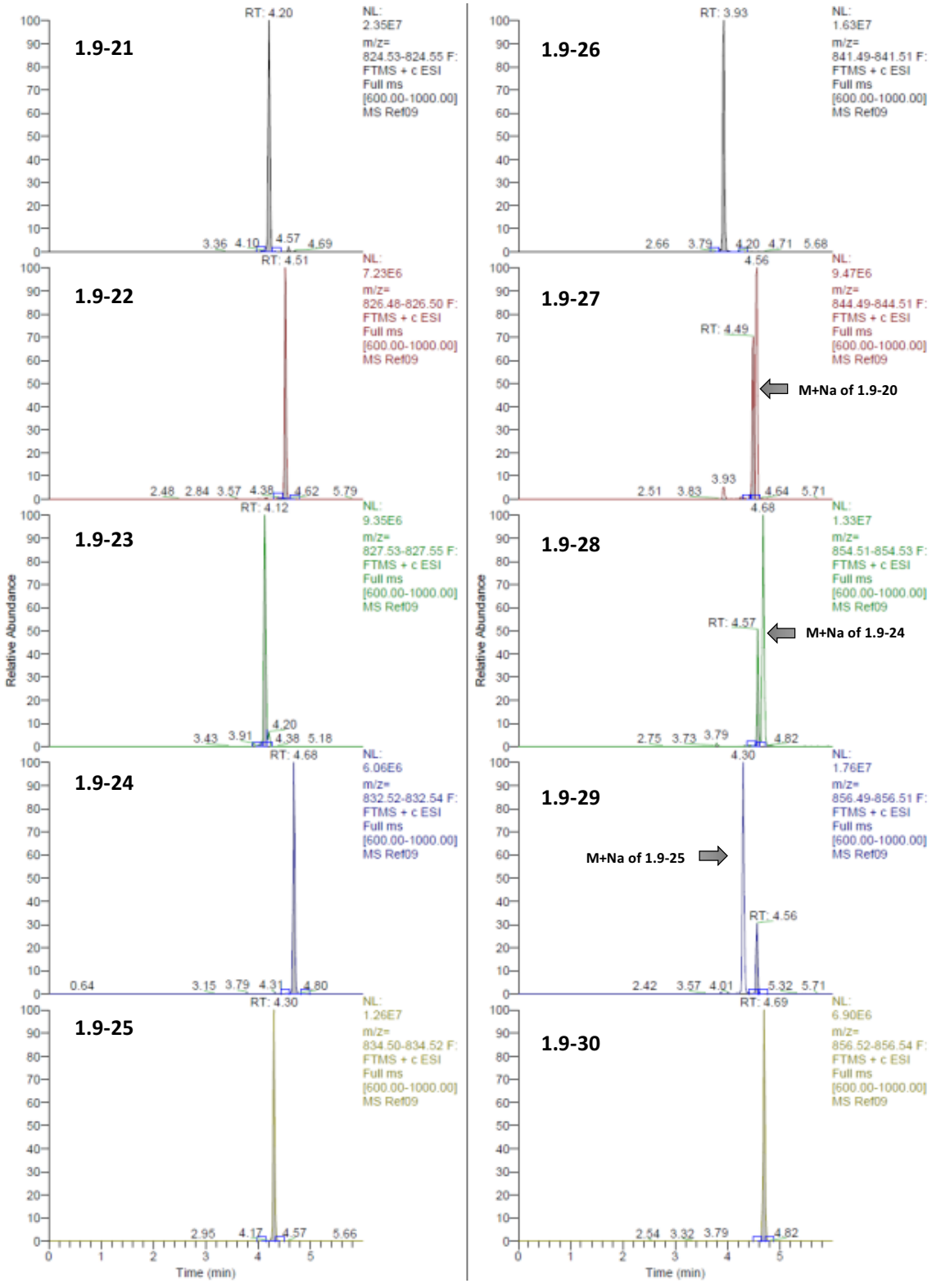


Figure S3.9c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.9

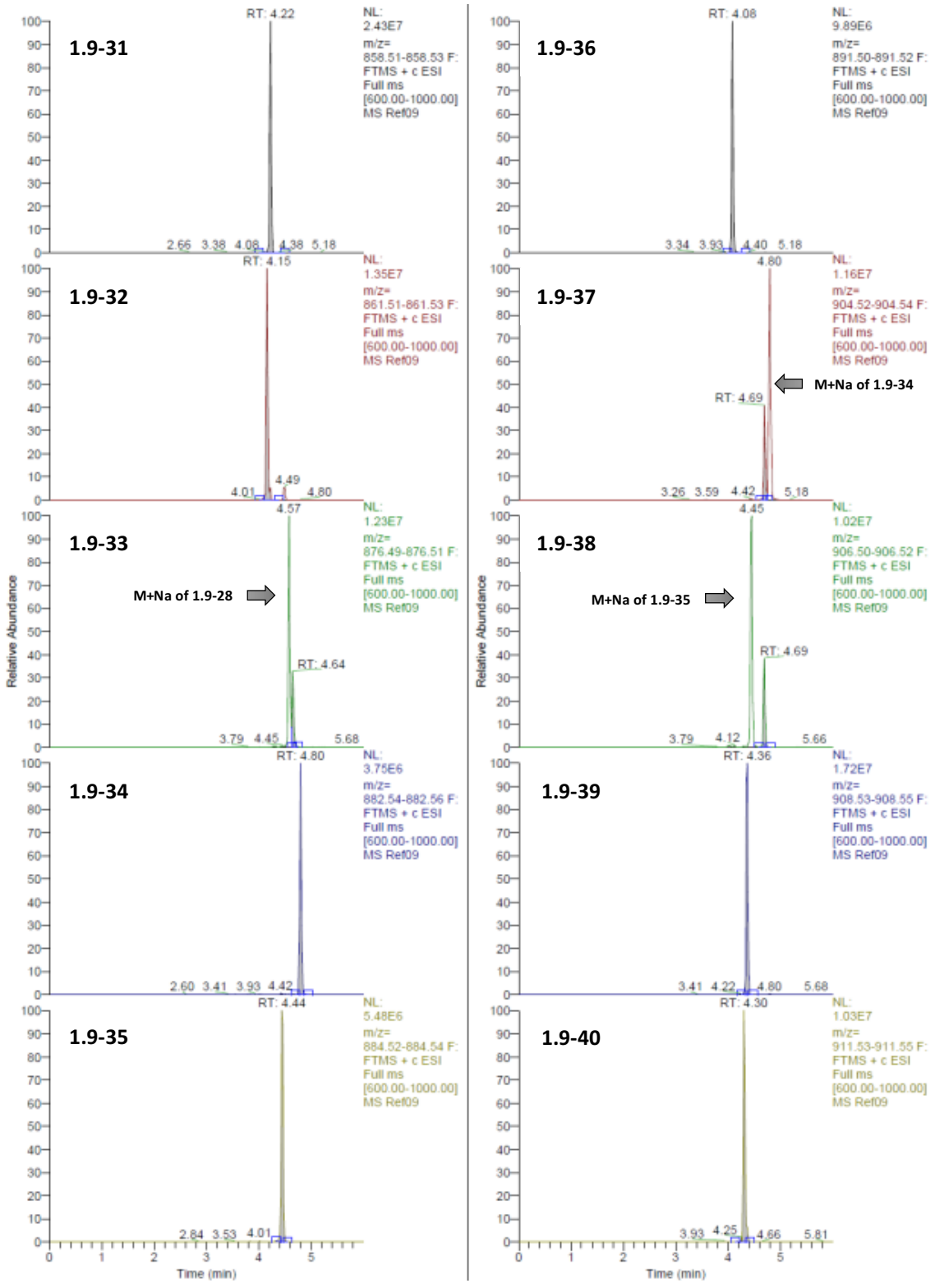


Figure S3.9d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.9

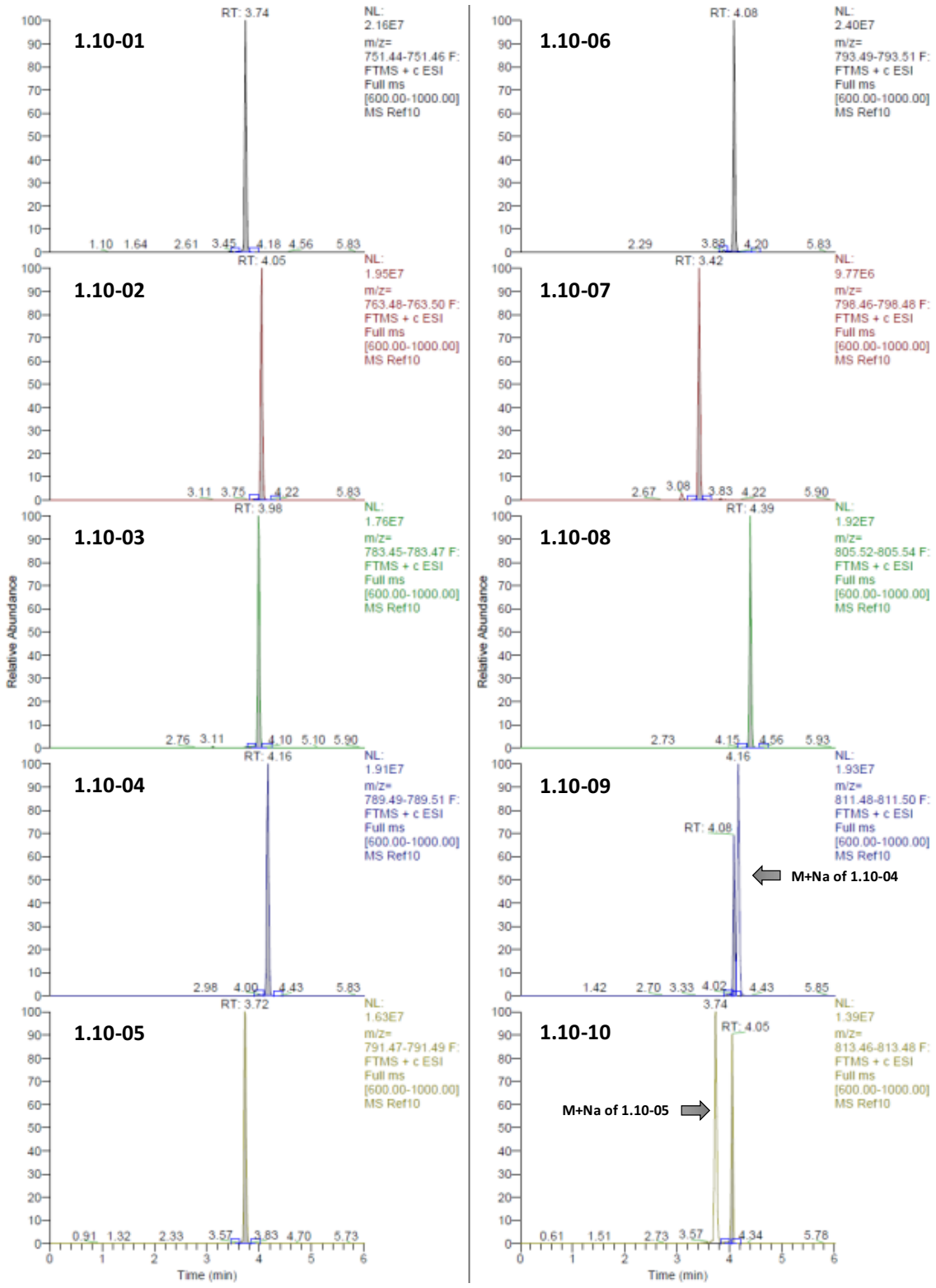


Figure S3.10a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.10

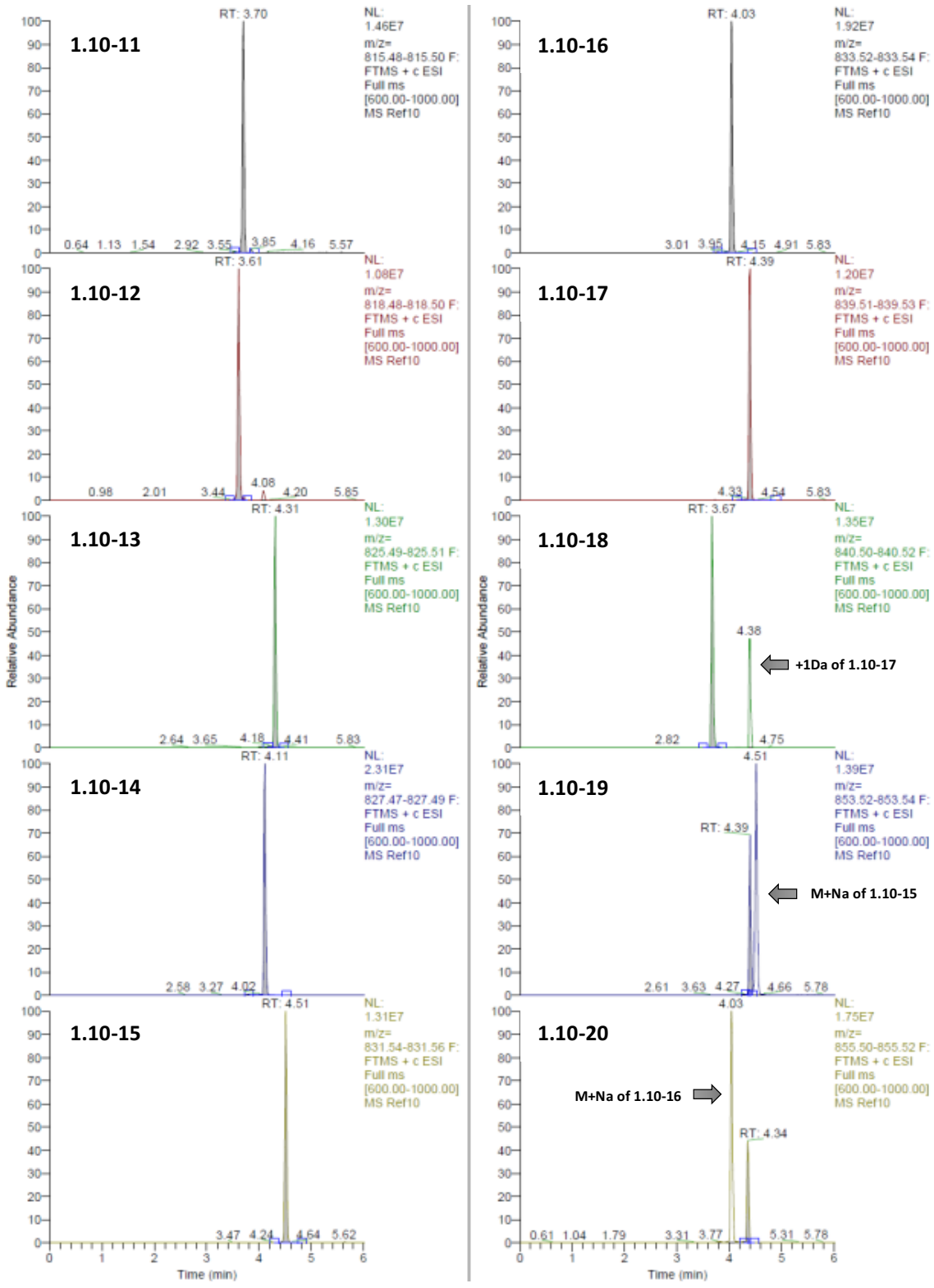


Figure S3.10b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.10

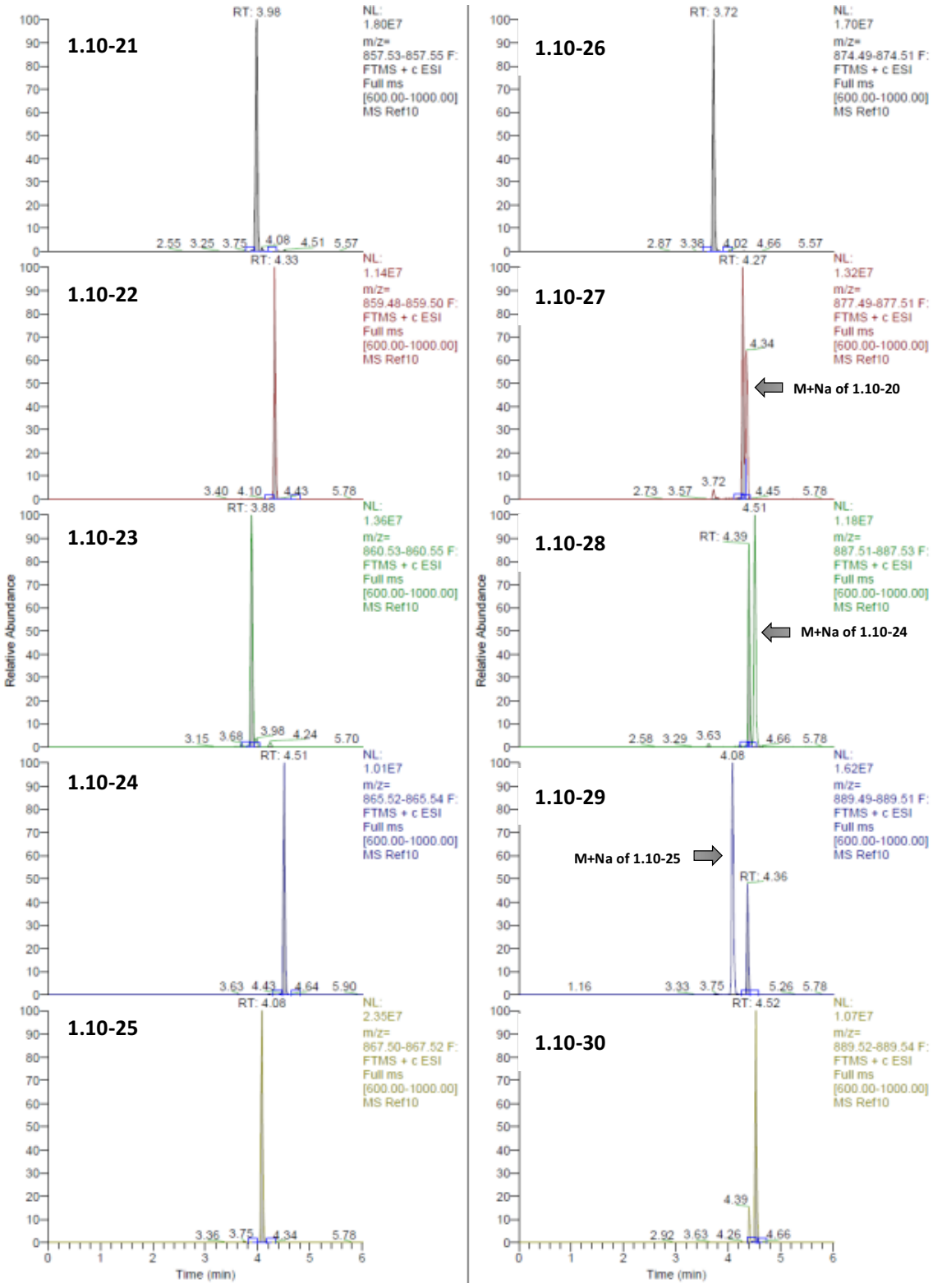


Figure S3.10c. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.10

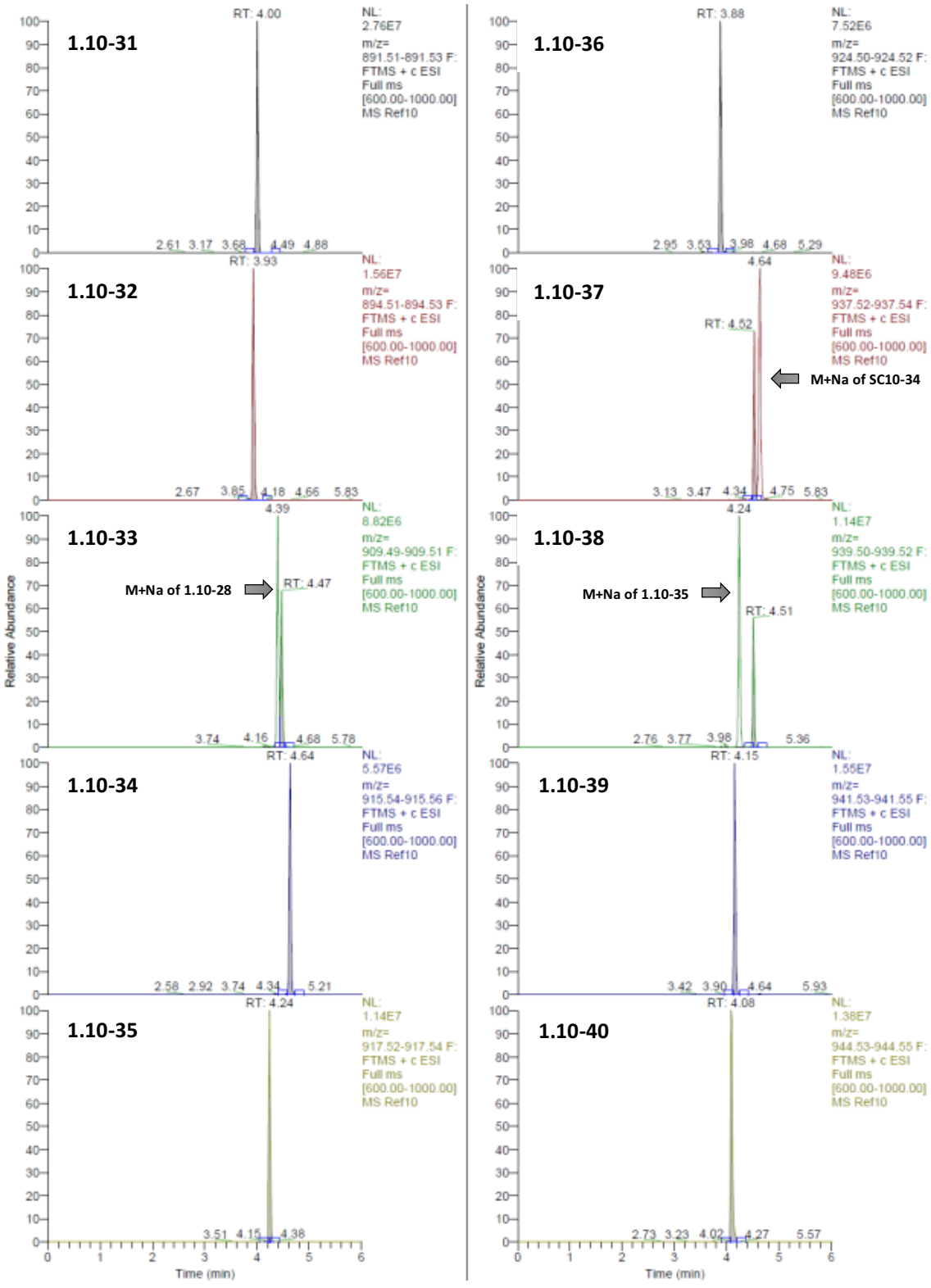


Figure S3.10d. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 1.10

1.4 LCMS analyses of **Library 2**

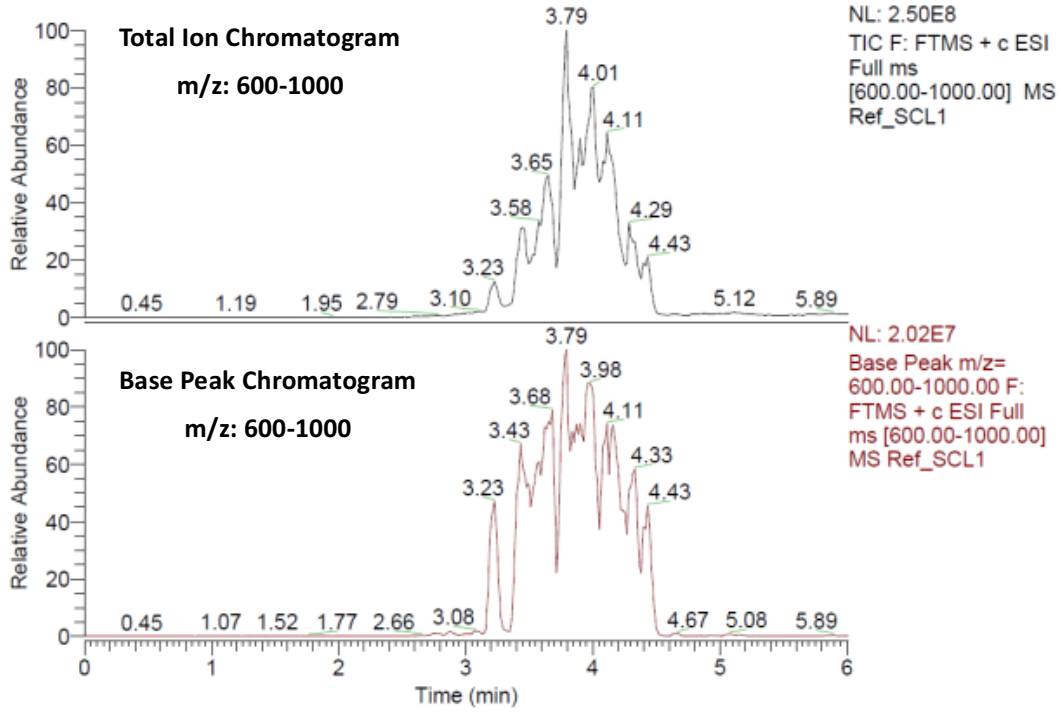


Figure S4.1. LCMS analysis of Sub-library 2.1

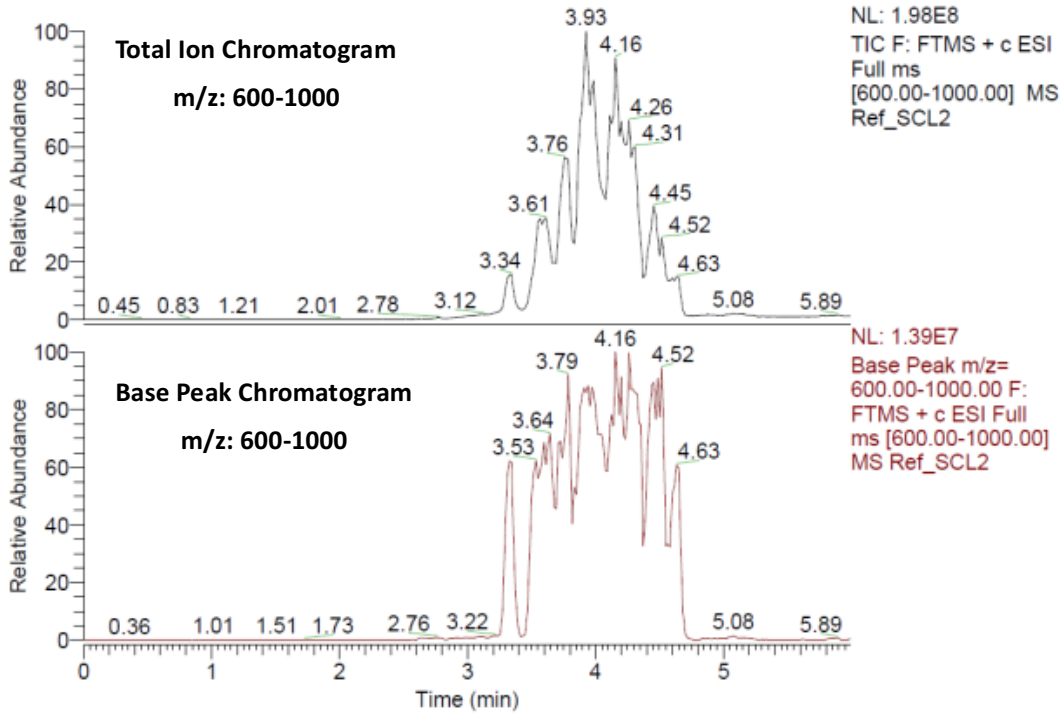


Figure S4.2. LCMS analysis of Sub-library 2.2

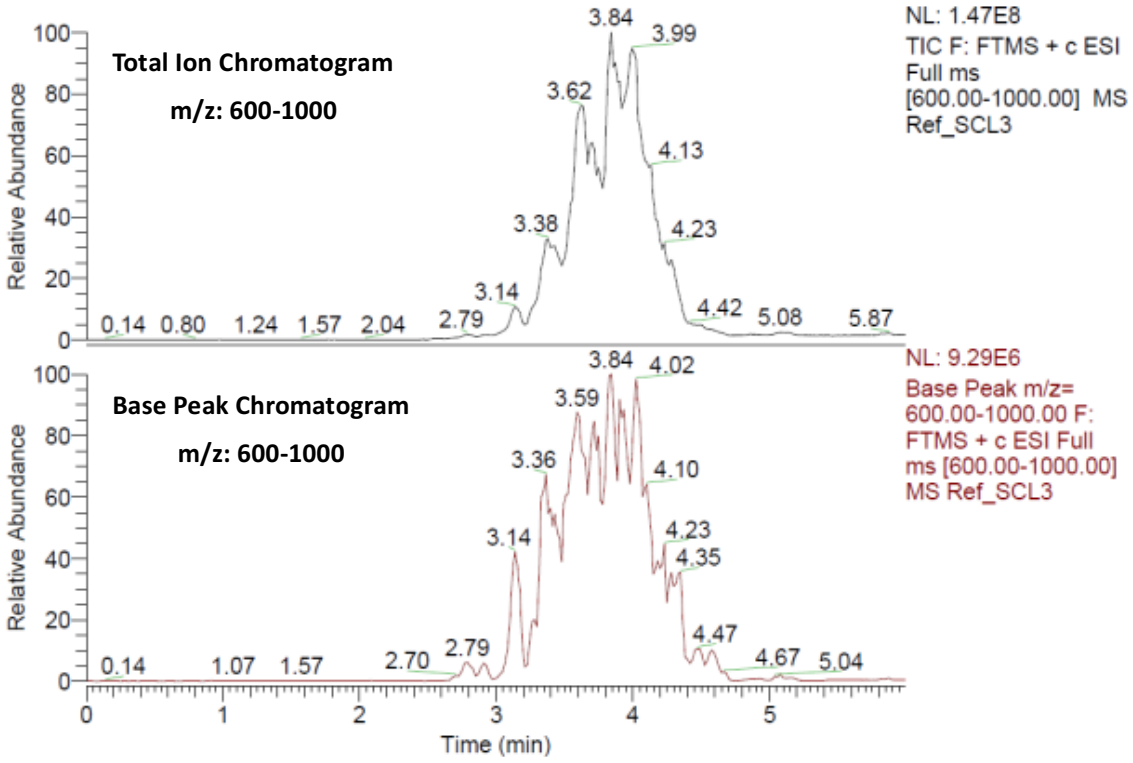


Figure S4.3. LCMS analysis of Sub-library 2.3

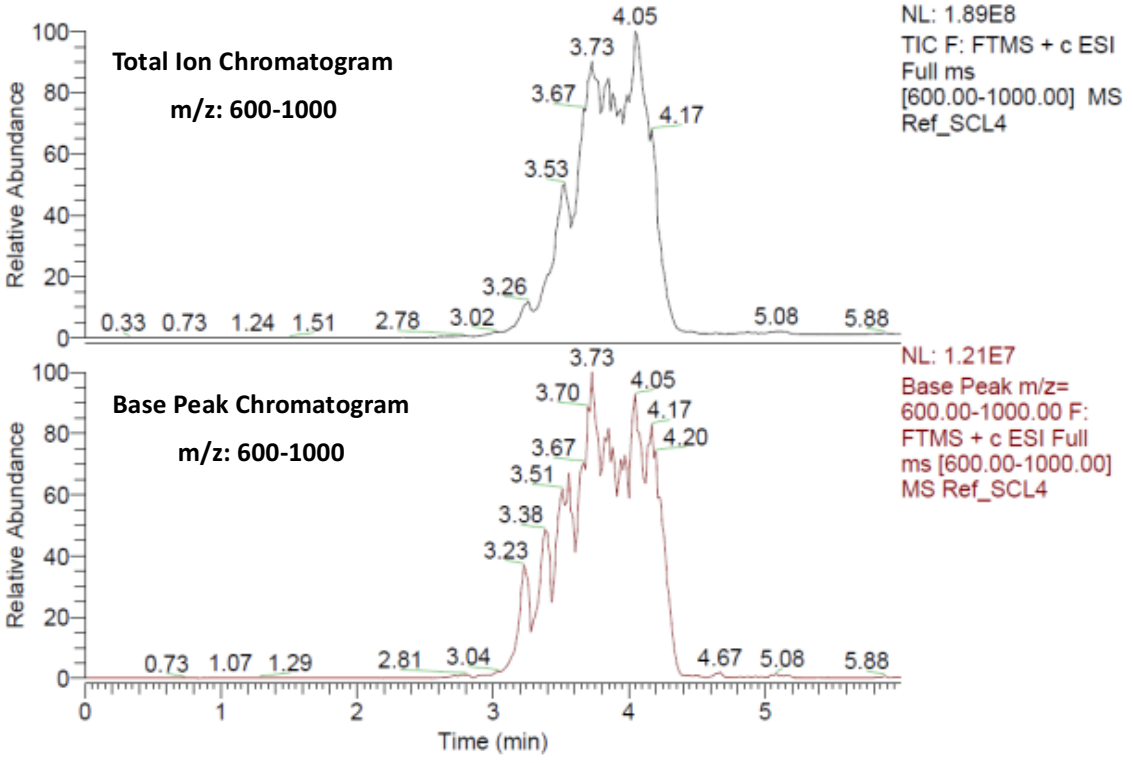


Figure S4.4. LCMS analysis of Sub-library 2.4

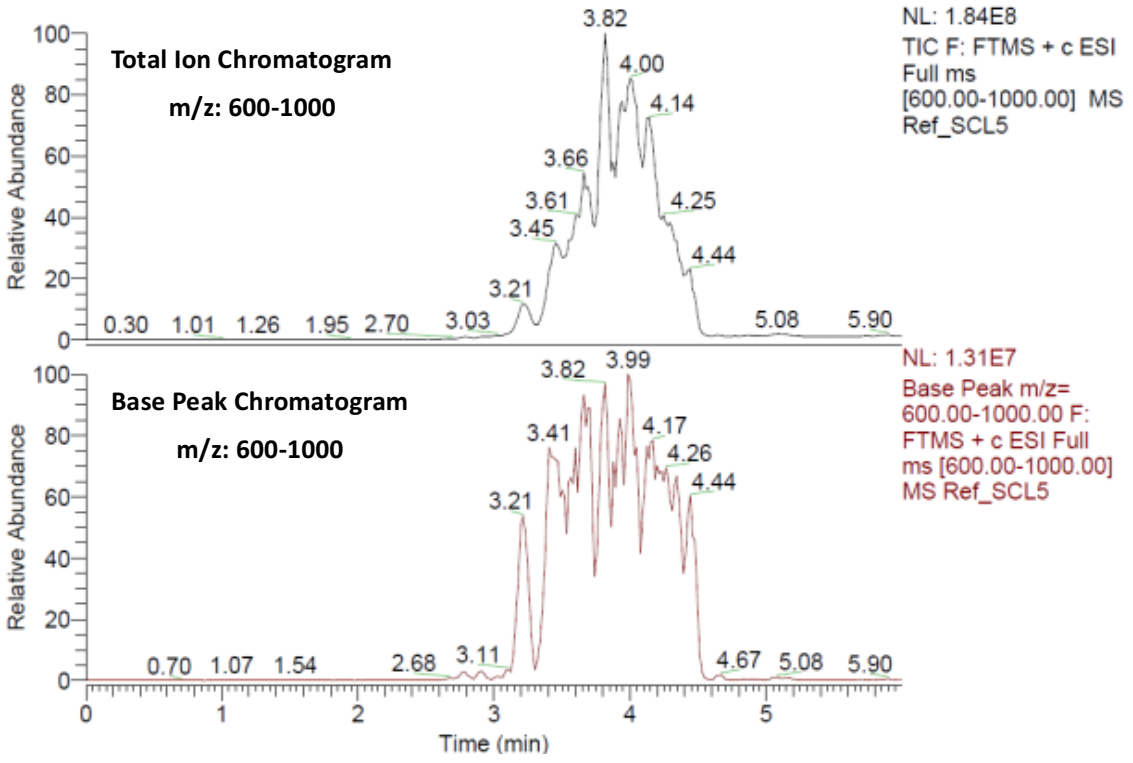


Figure S4.5. LCMS analysis of Sub-library 2.5

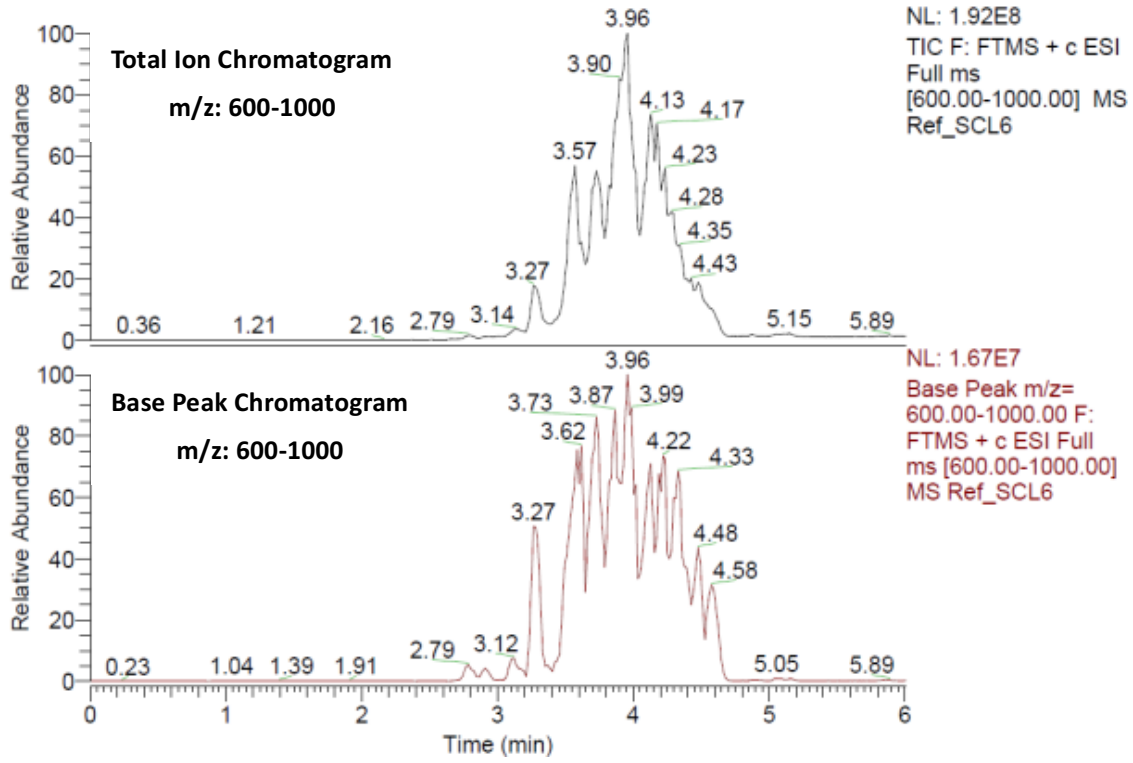


Figure S4.6. LCMS analysis of Sub-library 2.6

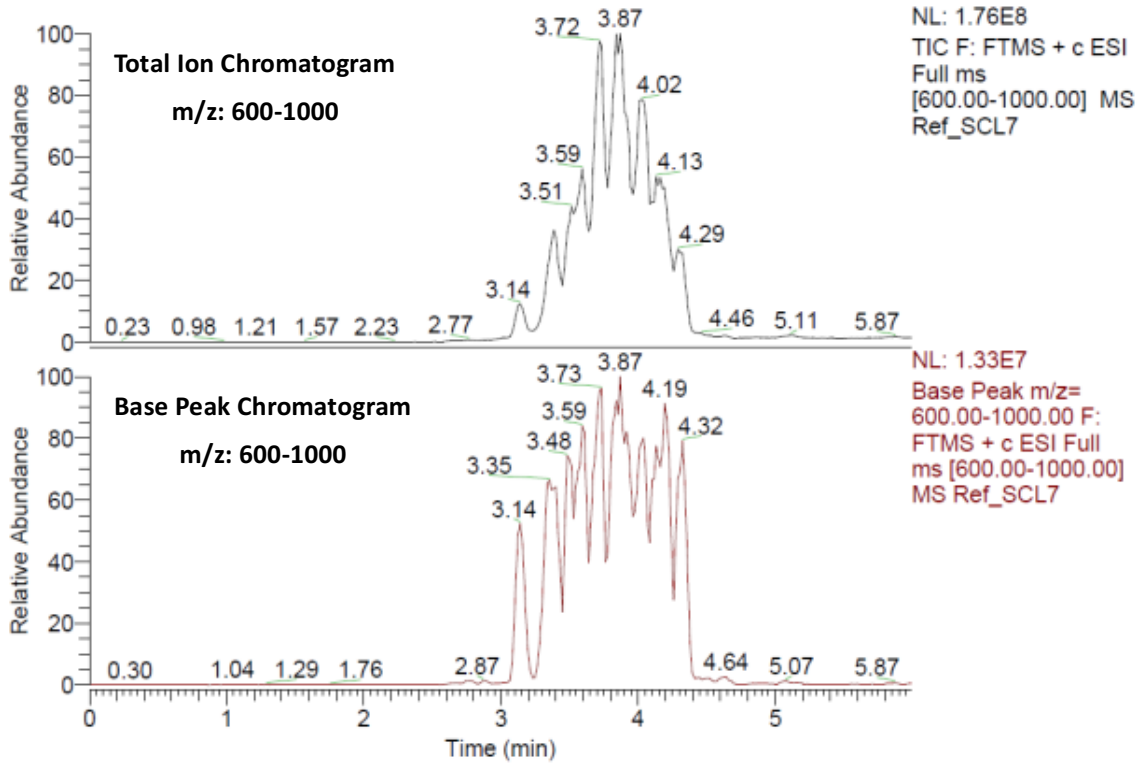


Figure S4.7. LCMS analysis of Sub-library 2.7

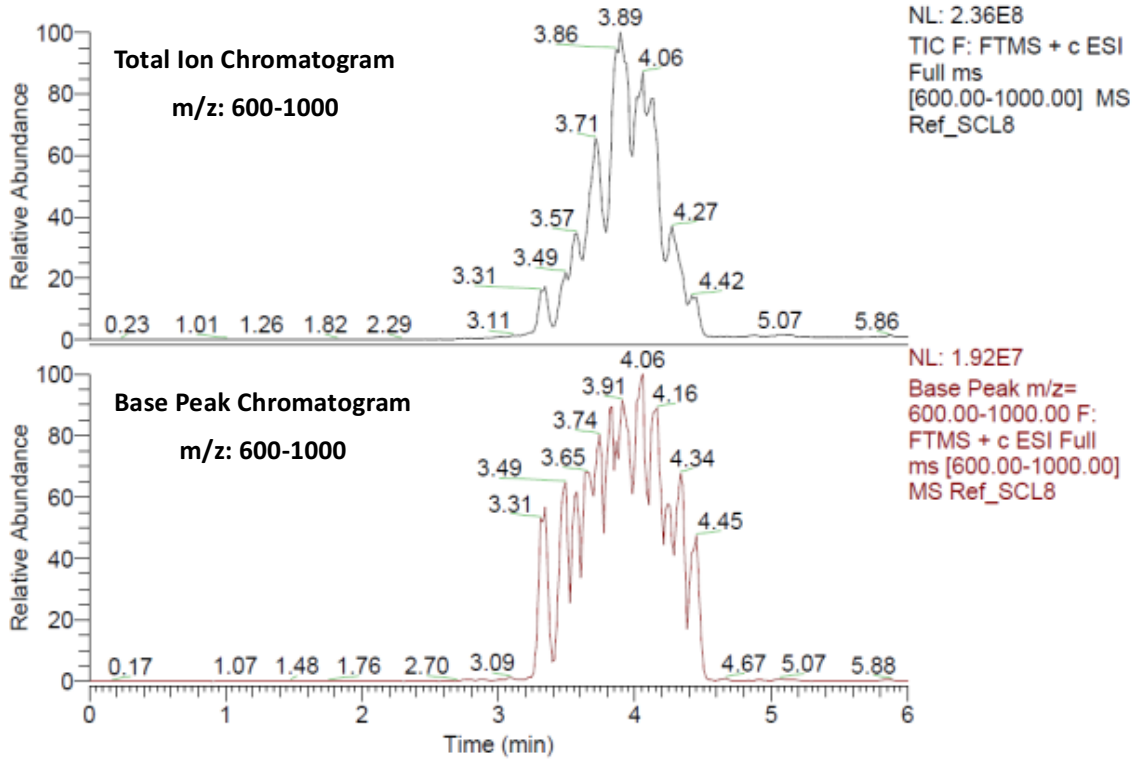


Figure S4.8. LCMS analysis of Sub-library 2.8

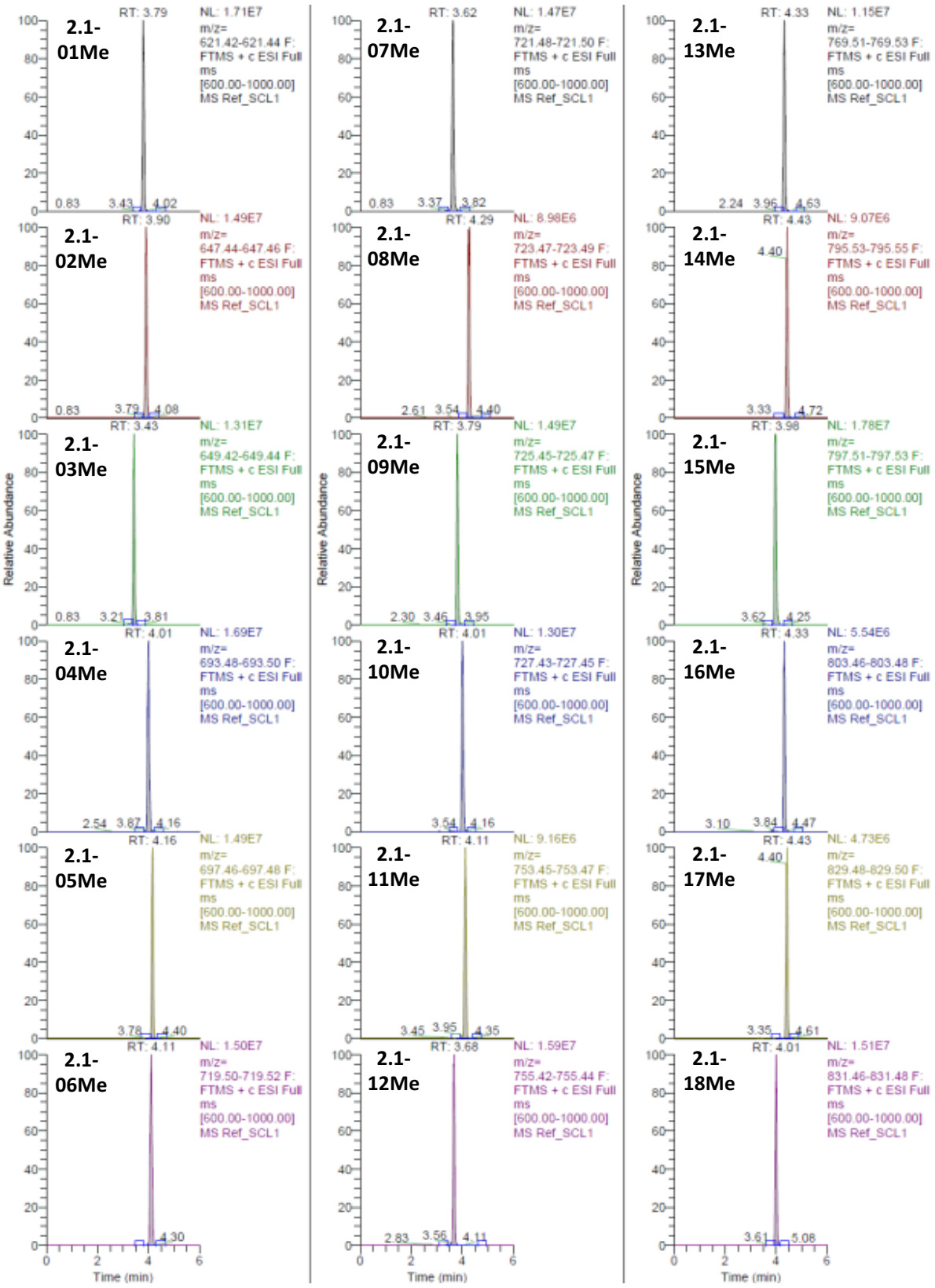


Figure S5.1a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.1

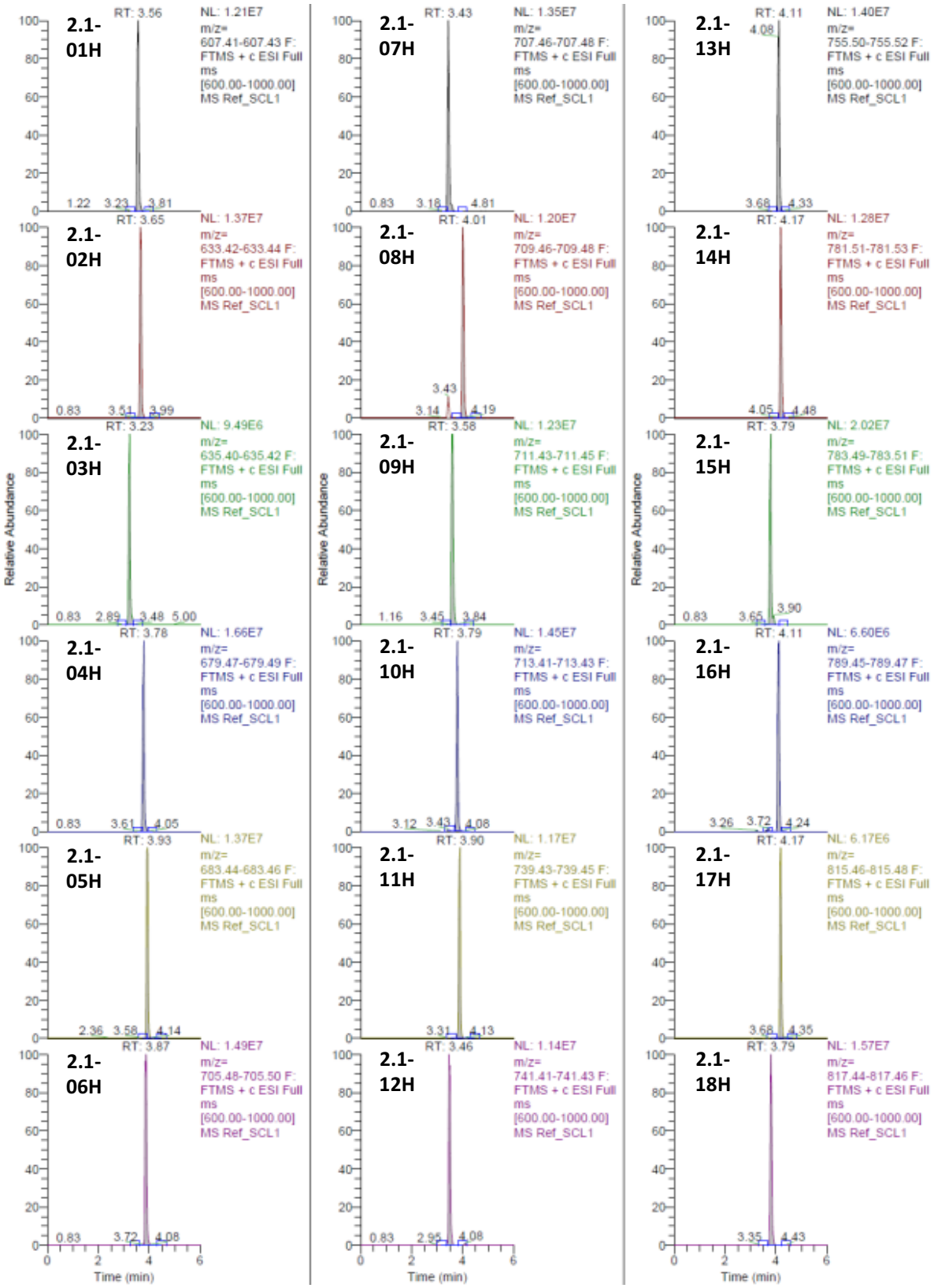


Figure S5.1b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.1

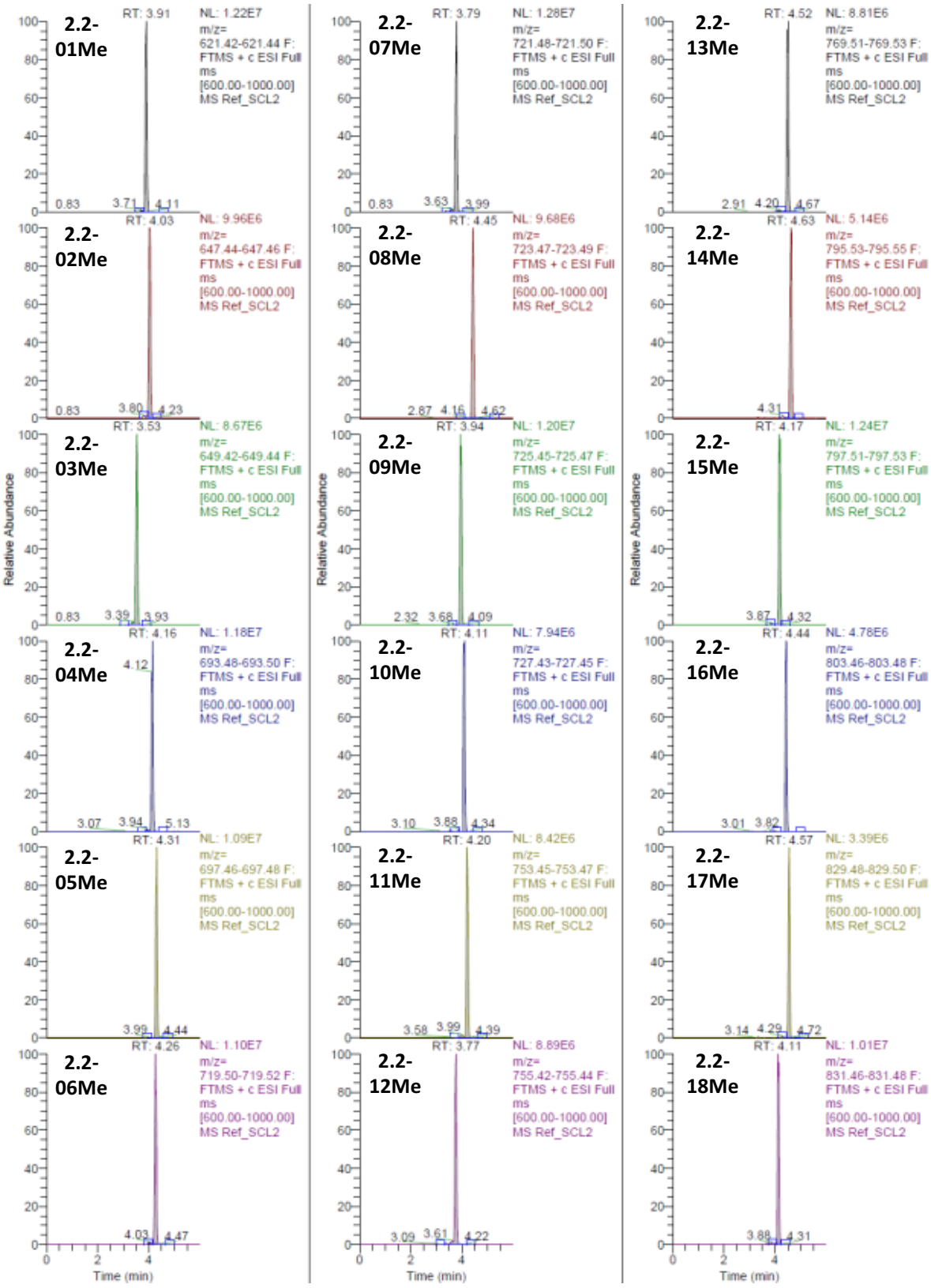


Figure S5.2a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.2

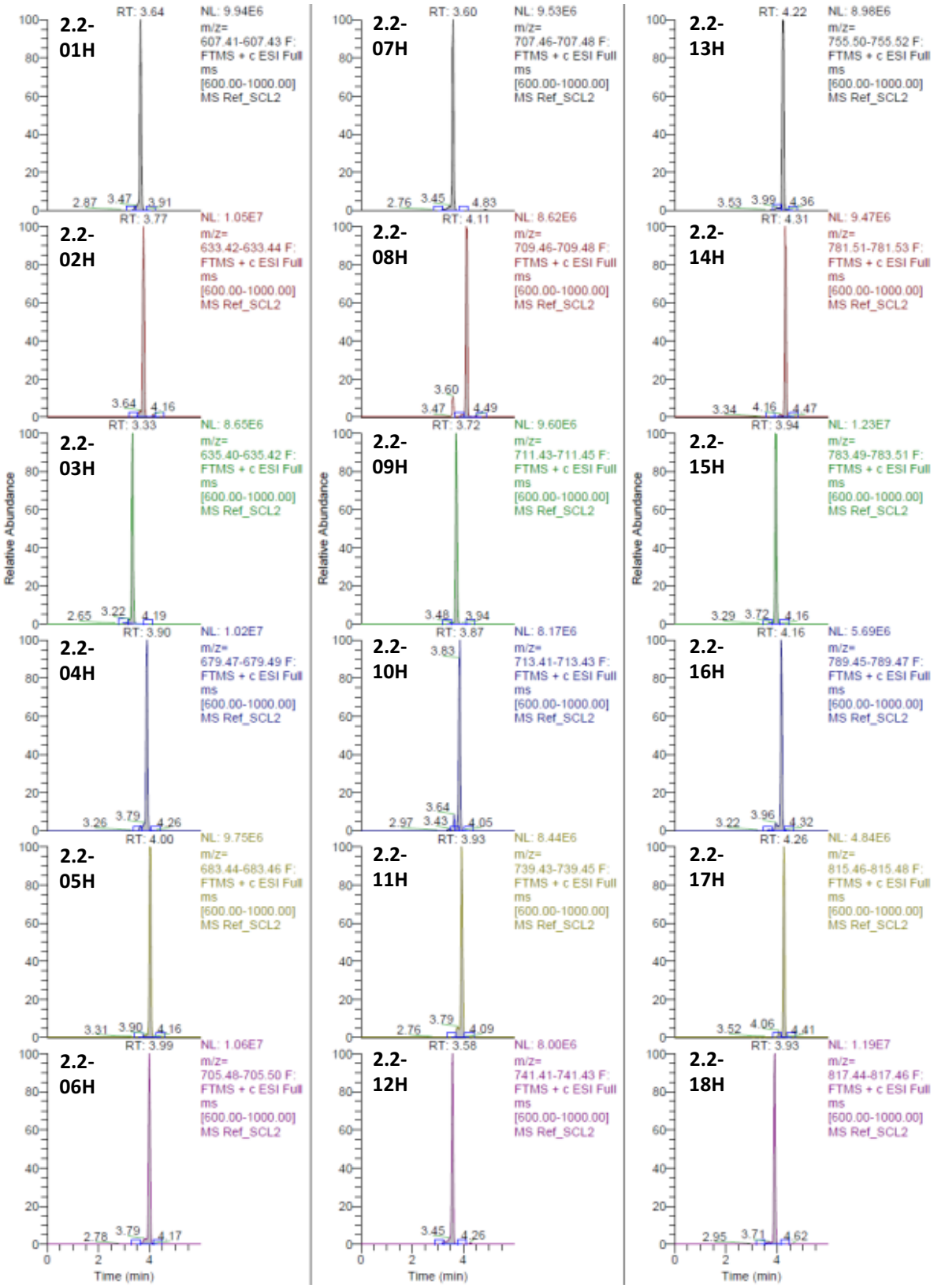


Figure S5.2b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.2

★ epimer at Nle4: enantiomeric isomer of corresponding compound in sub-library 2.6

▼ conformational isomer

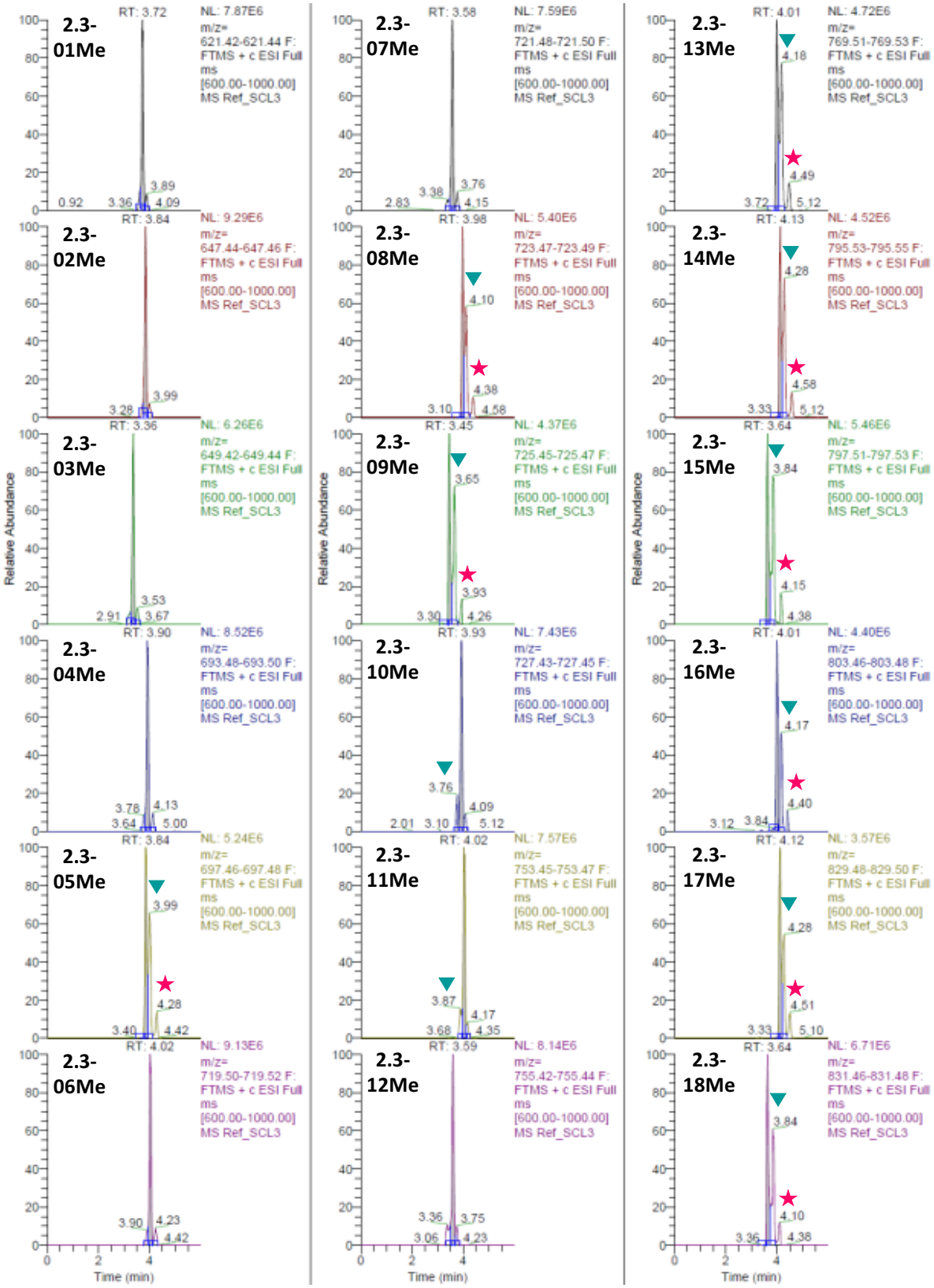


Figure S5.3a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.3

★ epimer at Nle4: enantiomeric isomer of corresponding compound in sub-library 2.6

▼ conformational isomer

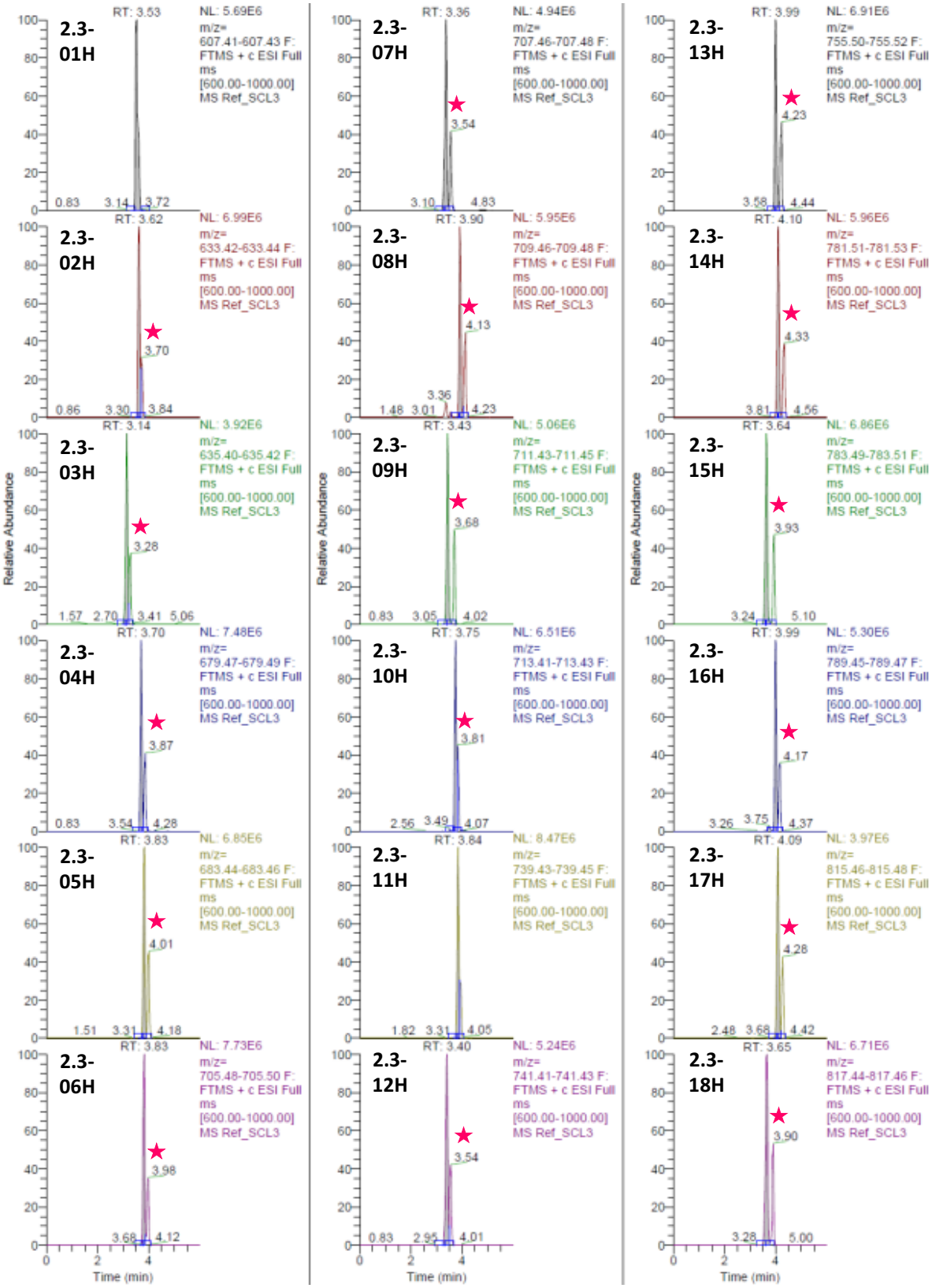


Figure S5.3b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.3

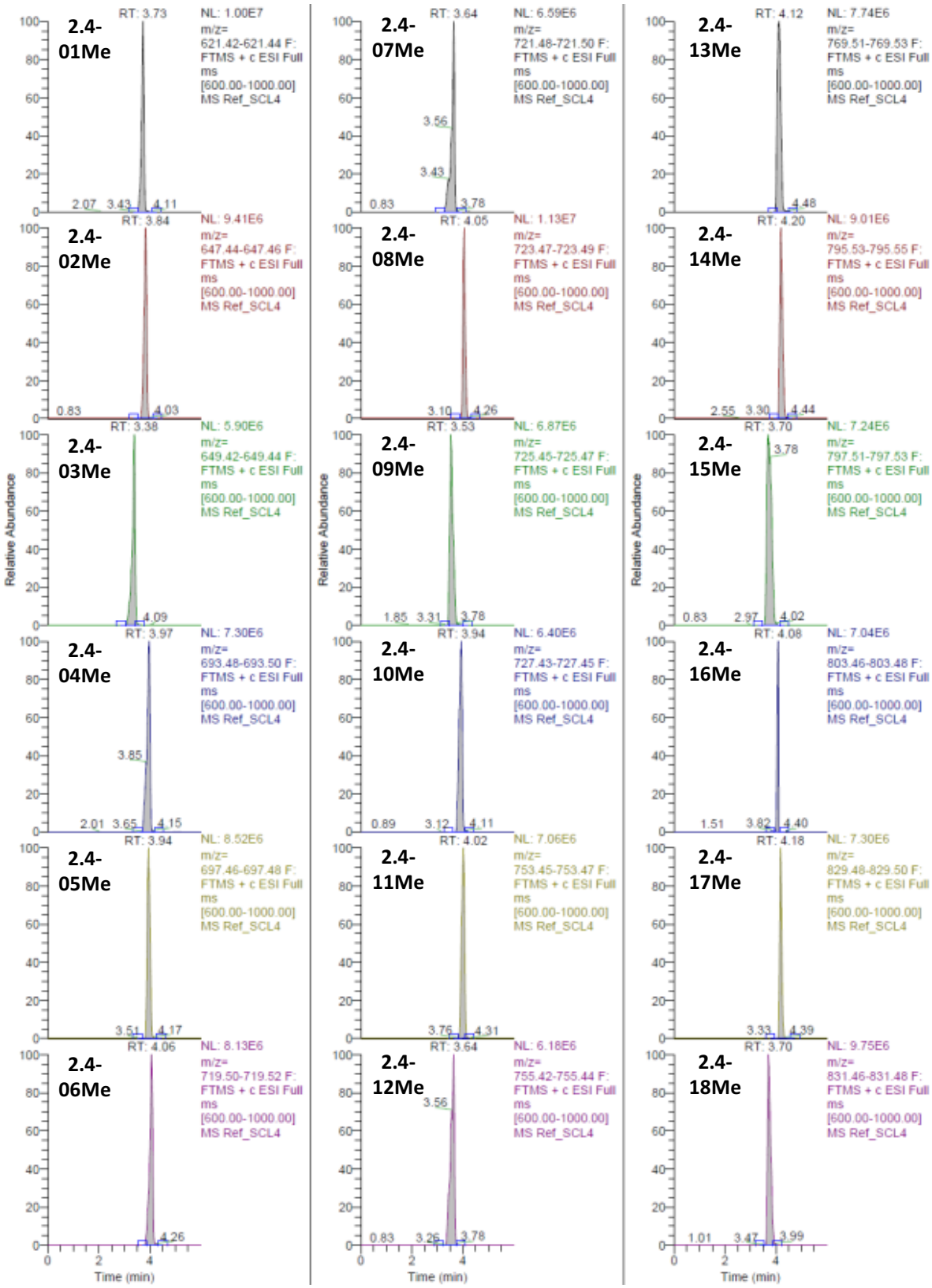


Figure S5.4a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.4

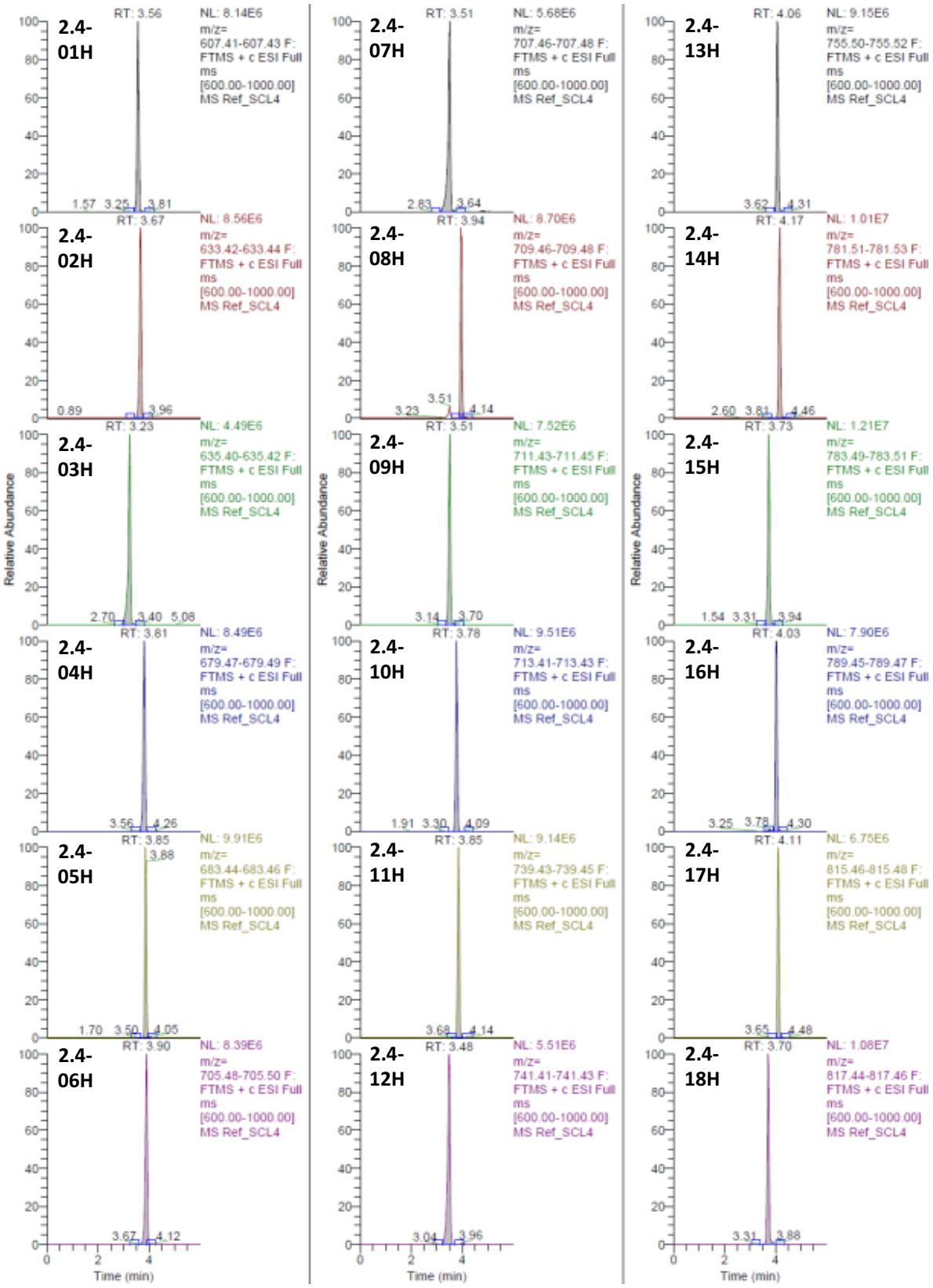


Figure S5.4b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.4

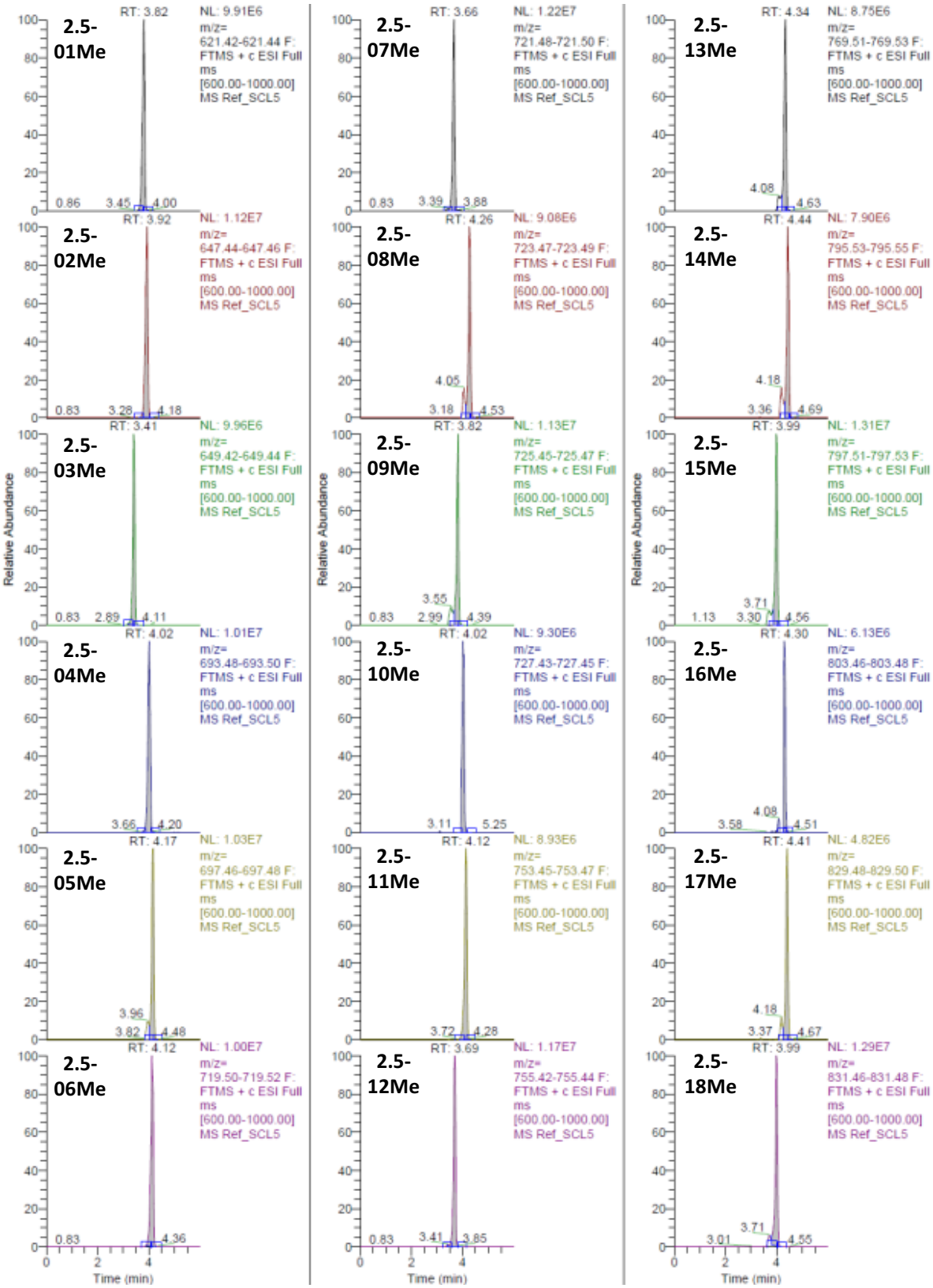


Figure S5.5a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.5

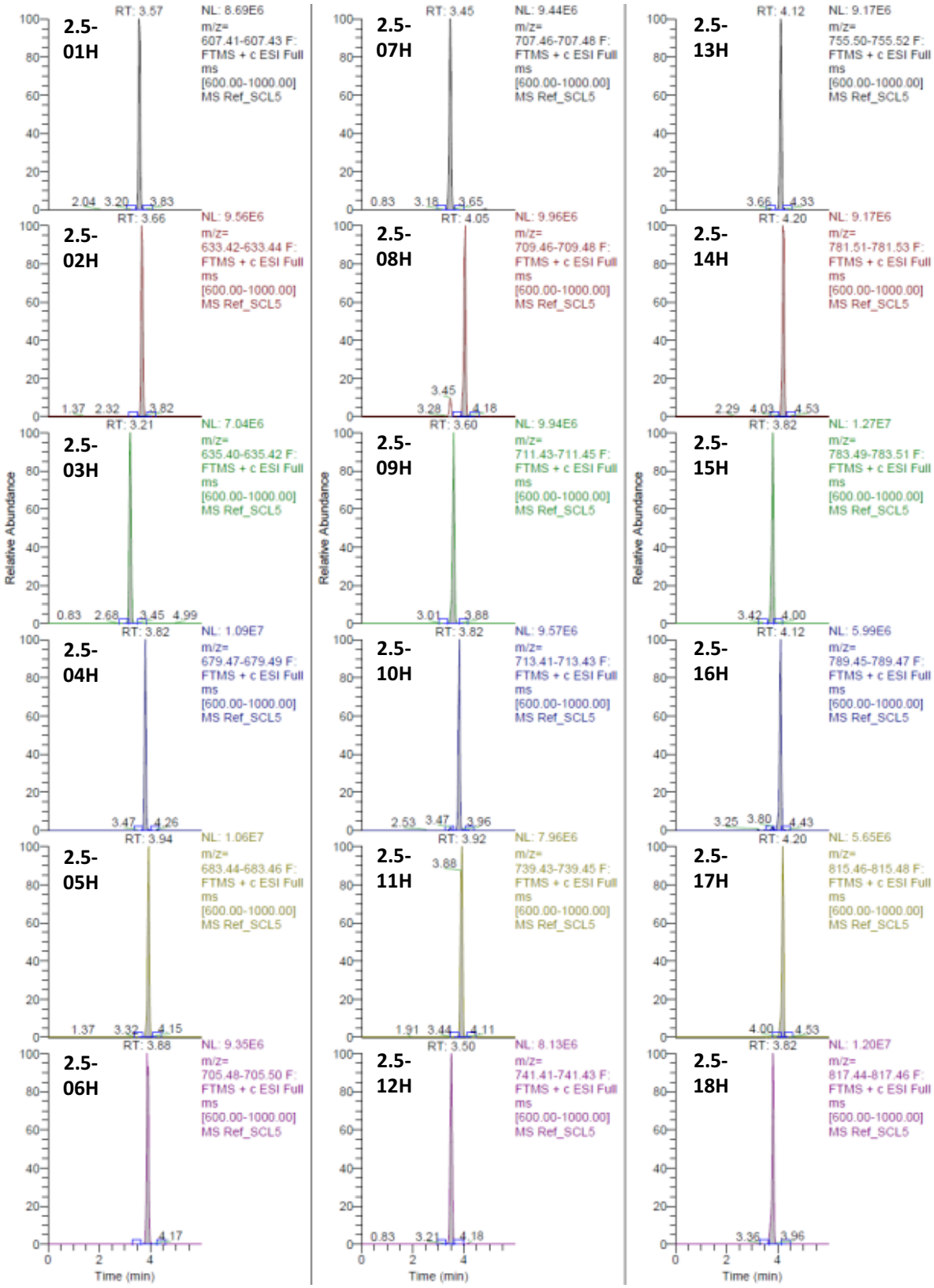


Figure S5.5b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.5

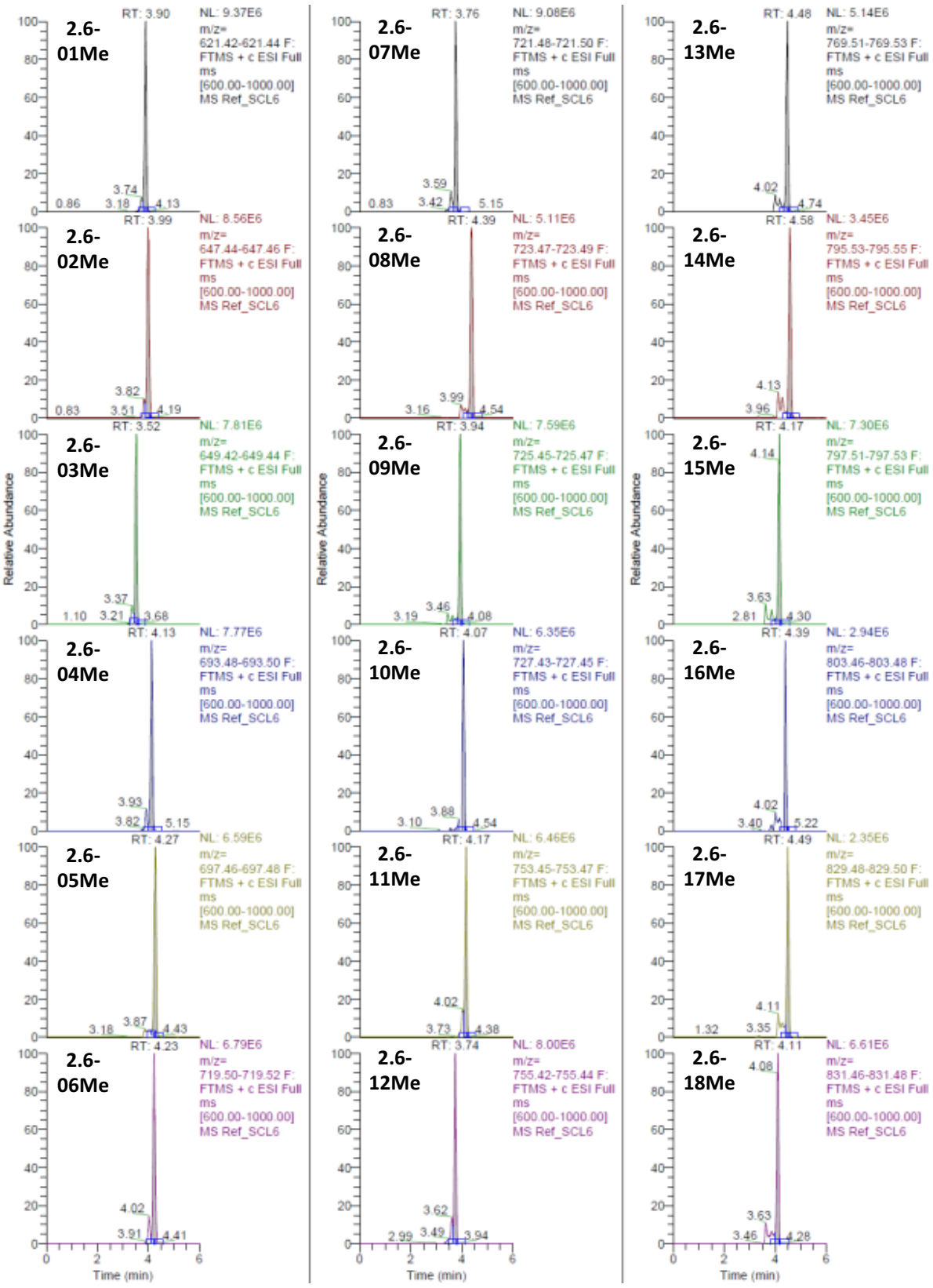


Figure S5.6a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.6

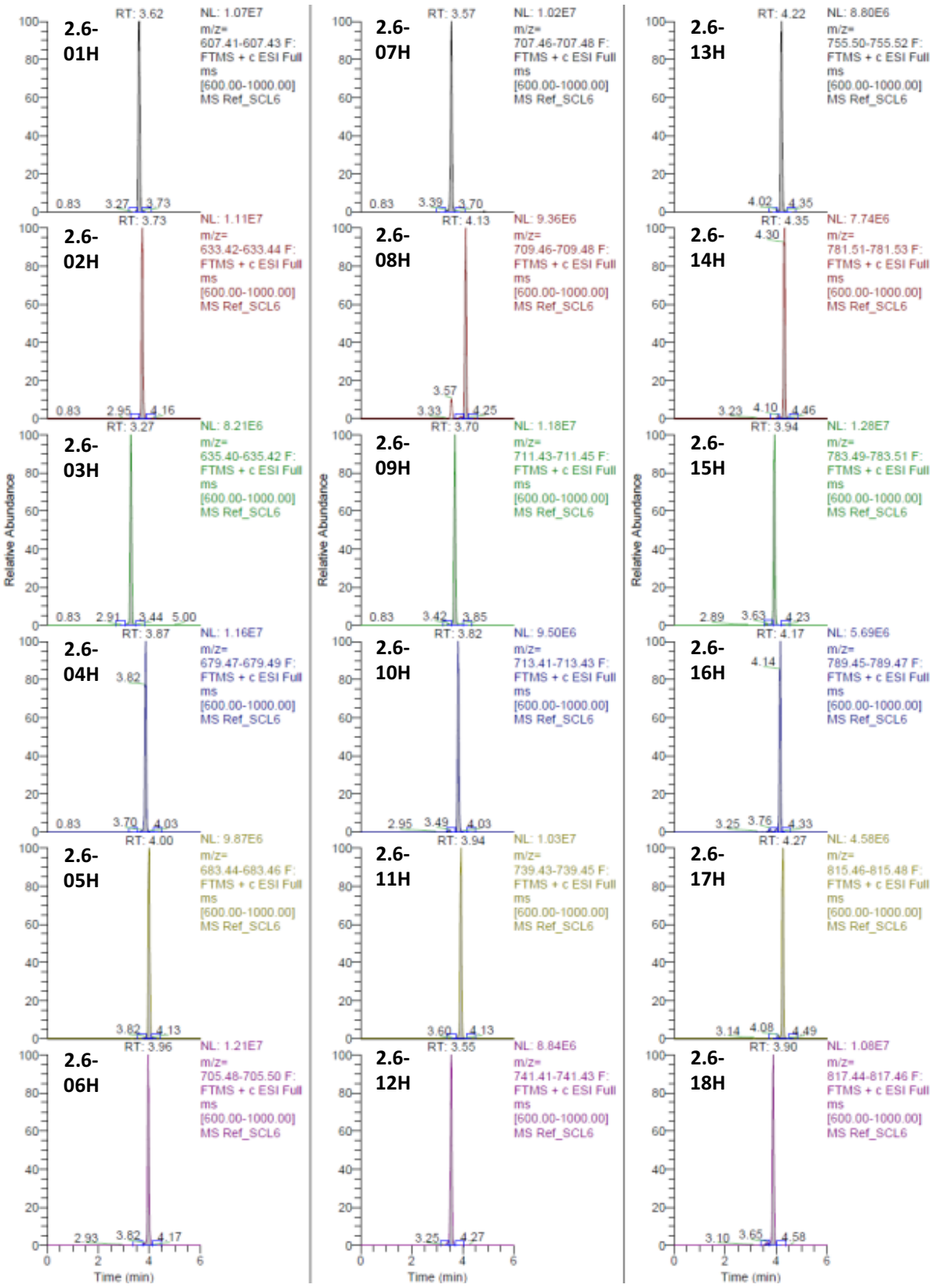


Figure S5.6b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.6

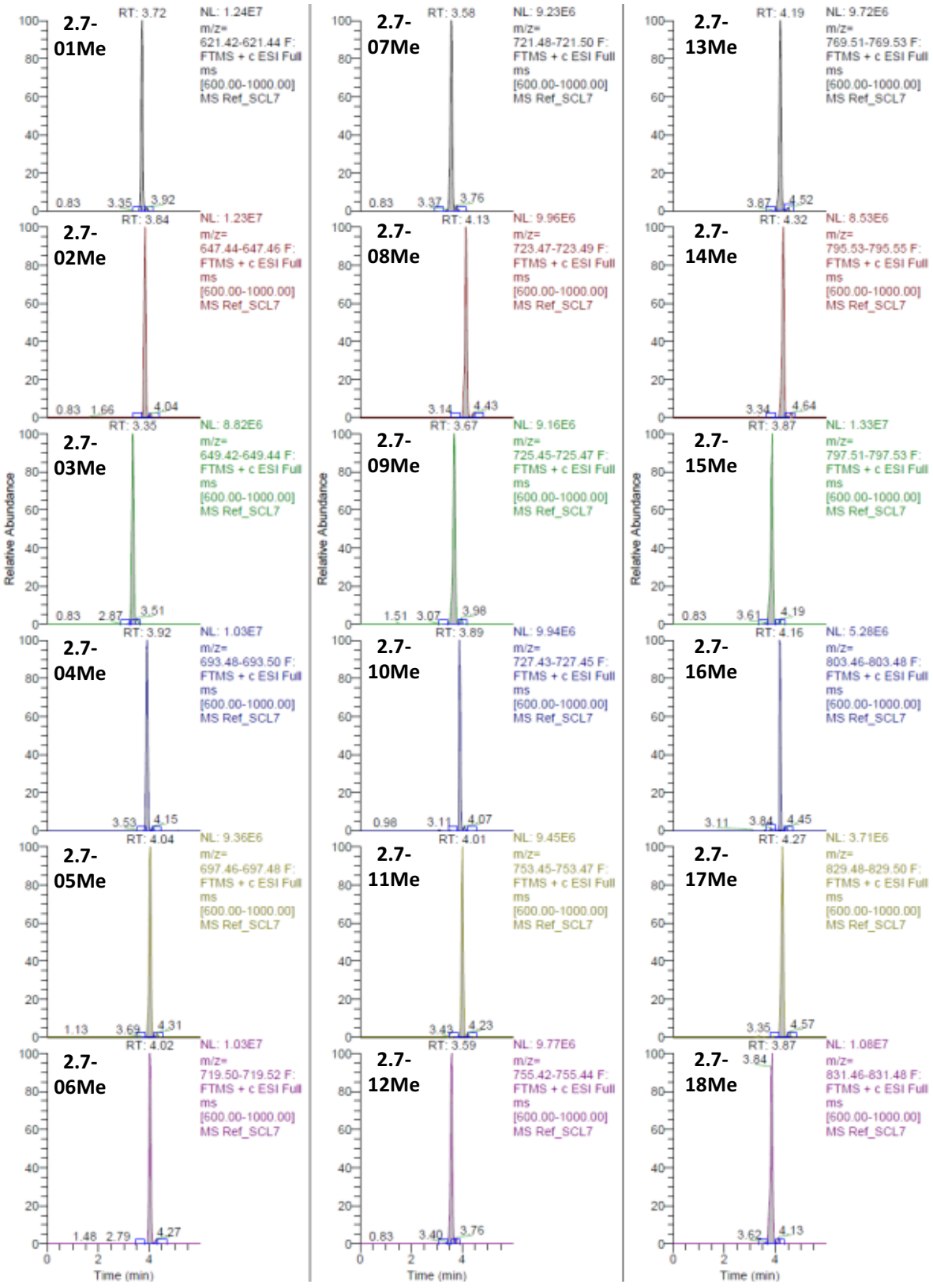


Figure S5.7a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.7

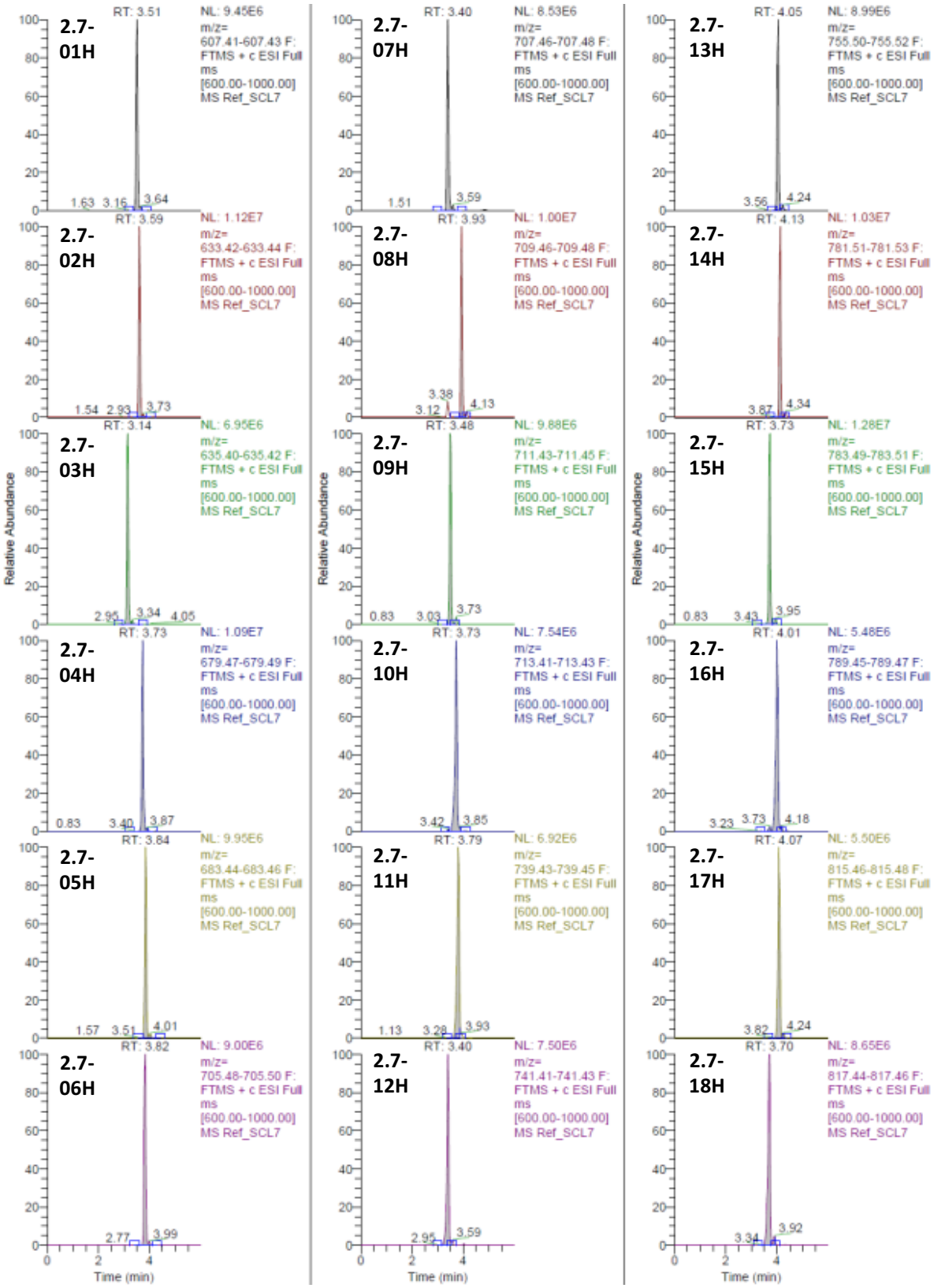


Figure S5.7b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.7

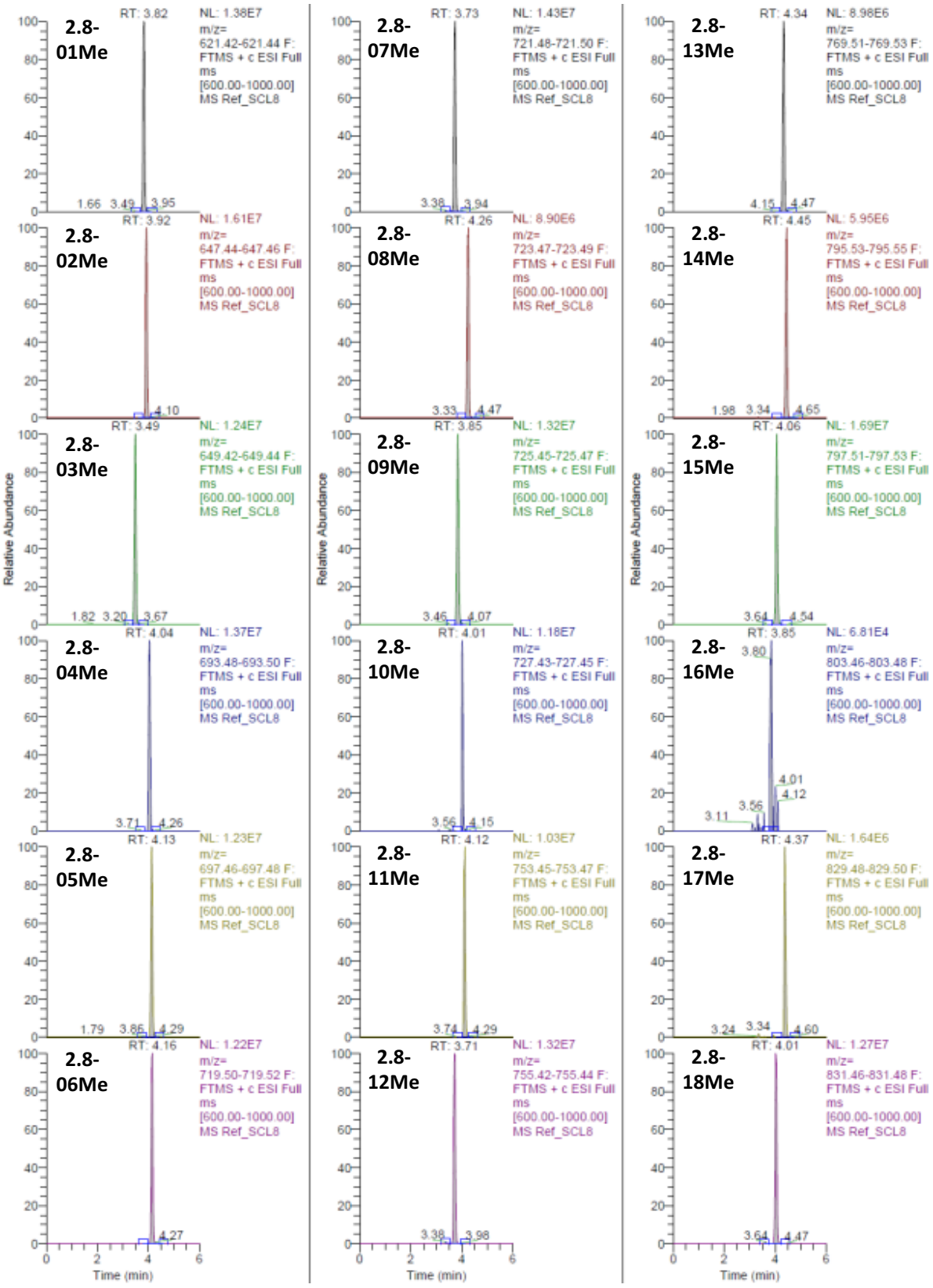


Figure S5.8a. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.8

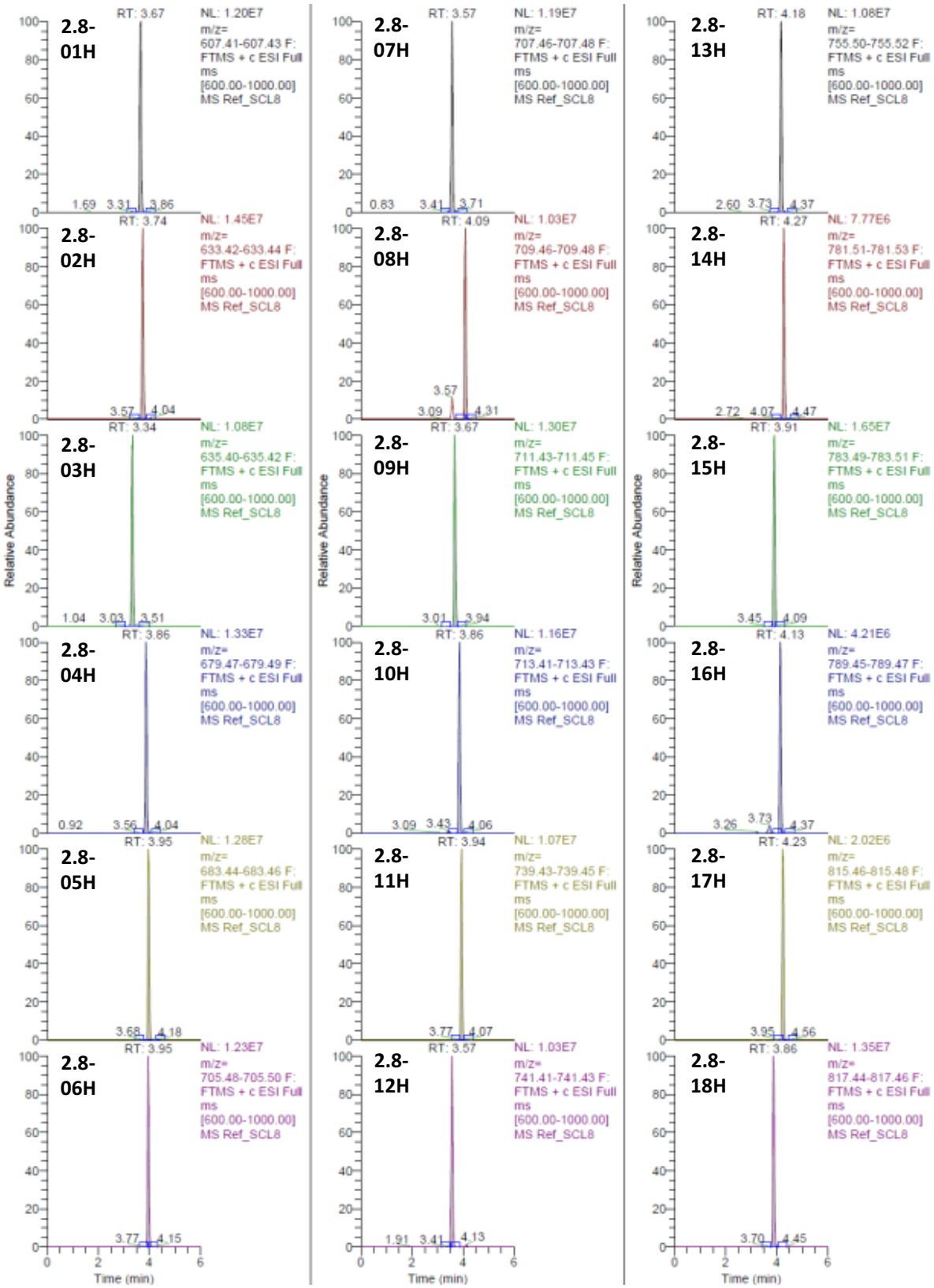


Figure S5.8b. Extracted Ion Chromatograms (M+H ± 0.01Da) of Sub-library 2.8

2 PAMPA

2.1 Experimental procedures of PAMPA

PAMPA was conducted using a 96-well donor plate with 0.45 μm hydrophobic Immobilon-P membrane supports (Millipore), and a 96-well Teflon acceptor plate. 160 μM (theoretical concentration) solutions of the sub-libraries (4 μM for each compound) for Library 1 and 180 μM (theoretical concentration) solutions of the sub-libraries (5 μM for each compound) for Library 2 were prepared in 5% DMSO/PBS buffer. 5 μL of a 1% (w/v) solution of lecithin in *n*-dodecane was carefully applied to the membrane supports in the wells of the donor plate. Without allowing this solution to evaporate, 150 μL of test compounds solutions were added to the donor wells. Each sub-library was prepared in triplicate. The acceptor plate was prepared by adding 300 μL of 5% DMSO/PBS to each well. The donor plate was then placed on top of the acceptor plate so that the artificial membrane was in contact with the buffer solution below. A lid was put on the donor well, and the system was placed in a chamber with wet paper towels to prevent evaporation for approximately 14h (the actual elapsed time was recorded).

Each 50 μL of donor well solution, acceptor well solution, and initial test sub-library solution were mixed with 50 μL of the internal standard (10 μM Tyr(tBu) in MeOH). Then, the relative concentrations were analyzed by LCMS analyses performed on HPLC (UltiMate 3000, Dionex) with attached mass spectrometer (Orbitrap Velos Pro, Thermo Scientific). The 10 μL of samples

were injected on a 1.9 μm C18 column (Hypersil GOLD 30×2.1 mm, Thermo Scientific) then eluted by the mixture of 0.1% formic acid in water (solvent A) and 0.1% formic acid in acetonitrile (solvent B) with a 0.6 mL/min flow rate (0-0.5 min, B: 10%, 0.5-3.5 min, B: 10%-100% linear gradient, 3.5-5.0 min, B: 100%, 5.0-6.5 min, B: 10%). PAMPA parameters were obtained by automatic analysis of the LCMS data using a python program developed in-house. The program extracted single-ion chromatograms for each mass of interest and found the bounds of the peak at the appropriate retention time for that compound. The ion counts between the peak bounds were then summed and used to calculate the PAMPA parameters. In the case of unknown retention time and multiple peaks in the reference spectrum, the highest peak in the reference spectrum was chosen and its retention time was used for peak-finding in the donor and acceptor wells. All peak-picking and integration bounds were reviewed visually and corrected when necessary. In cases where a contaminant peak overlapped the correct peak, integration bounds were adjusted to split the peaks vertically. The ion counts in for each compound were corrected using the ion count of an internal standard to compensate for instrument injection error.

PAMPA permeability parameters were calculated by the following formulae:

$$C_{equilibrium} = (C_D \times V_D + C_A \times V_A)/(V_D + V_A)$$

$$\%T = \frac{C_A}{C_{equilibrium}} \times 100$$

$$P_{app} = \frac{-\ln\left(1 - C_A/C_{equilibrium}\right)}{(1/V_A + 1/V_D) \times \text{Area} \times \text{Time}}$$

$$\%\text{recovery} = \frac{(C_D \times V_D + C_A \times V_A)}{C_0 \times V_D} \times 100$$

C_D: relative concentration in donor well, C_A: relative concentration in acceptor well, C_0: relative concentration of initial test solution added to donor well, V_D: volume of donor well (0.15 cm^3), V_A: volume of acceptor well (0.30 cm^3), Area: membrane area (0.24 cm^2), Time: actual elapsed time in second (51480 sec for side chain library, 51120 sec for diverse scaffold library).

2.2 PAMPA results of Library 1

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave LogP_{app}
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.1-01	609.397	0.12	A01	Ala	A11	211	0.9	87.9	0.08	0.8	98.1	0.07	1.0	88.7	0.08	91.58	5.66	0.07	0.01	-7.13
1.1-02	621.433	2.03	A01	Ala	A12	234	44.9	82.8	4.82	41.4	95.6	4.32	47.1	89.1	5.16	89.21	6.40	4.77	0.42	-5.32
1.1-03	641.402	1.83	A01	Ala	A13	230	35.9	78.1	3.61	33.5	88.9	3.30	36.8	85.4	3.71	84.14	5.47	3.54	0.21	-5.45
1.1-04	647.449	2.44	A01	Ala	A14	243	68.2	68.6	9.26	62.3	75.6	7.89	71.0	75.4	10.02	73.19	4.00	9.06	1.08	-5.04
1.1-05	649.428	0.67	A01	Ala	A15	211	0.7	87.5	0.06	0.6	96.2	0.05	0.7	88.2	0.06	90.63	4.82	0.05	0.01	-7.27
1.1-06	651.444	1.35	A01	Leu	A11	238	29.9	82.8	2.88	27.1	91.1	2.56	31.1	86.2	3.01	86.70	4.16	2.81	0.23	-5.55
1.1-07	656.413	1.00	A01	Ala	A16	190	0.6	90.6	0.05	0.4	103.4	0.03	0.5	97.0	0.04	96.99	6.42	0.04	0.01	-7.40
1.1-08	663.480	3.26	A01	Leu	A12	259	76.4	26.1	11.69	74.4	29.7	11.02	76.7	30.2	11.78	28.68	2.22	11.50	0.41	-4.94
1.1-09	669.433	2.61	A01	Ala	A17	236	58.0	70.9	7.03	56.2	79.8	6.69	58.1	80.6	7.03	77.10	5.36	6.92	0.20	-5.16
1.1-10	671.413	1.88	A01	Ala	A18	235	37.8	65.9	3.85	31.3	78.4	3.04	35.8	75.3	3.59	73.21	6.52	3.49	0.41	-5.46
1.1-11	673.440	1.26	A01	Ala	A19	211	0.7	85.2	0.06	0.4	96.0	0.03	0.6	90.2	0.05	90.45	5.40	0.05	0.01	-7.33
1.1-12	676.439	-0.04	A01	Ala	A20	204	0.1	91.3	0.01	0.0	104.7	0.00	0.1	99.0	0.01	98.34	6.71	0.01	0.00	-8.28
1.1-13	683.449	3.06	A01	Leu	A13	253	72.2	22.5	10.35	68.9	25.7	9.45	72.9	25.9	10.56	24.72	1.92	10.12	0.59	-4.99
1.1-14	685.428	1.67	A01	Phe	A11	239	40.0	69.8	4.14	35.5	83.1	3.55	40.1	78.1	4.15	77.03	6.73	3.95	0.34	-5.40
1.1-15	689.496	3.67	A01	Leu	A14	266	58.9	11.8	7.20	54.8	11.9	6.43	56.7	12.4	6.77	12.04	0.29	6.80	0.39	-5.17
1.1-16	691.475	1.90	A01	Leu	A15	235	21.2	80.2	1.93	17.9	95.7	1.59	20.1	90.1	1.81	88.67	7.83	1.78	0.17	-5.75
1.1-17	697.465	3.59	A01	Phe	A12	259	63.7	14.9	8.21	61.2	16.1	7.67	62.5	16.4	7.93	15.80	0.78	7.94	0.27	-5.10
1.1-18	698.460	2.23	A01	Leu	A16	211	9.3	81.5	0.79	7.4	92.6	0.63	9.1	85.7	0.77	86.62	5.57	0.73	0.09	-6.14
1.1-19	711.480	3.84	A01	Leu	A17	259	63.1	13.4	8.08	60.7	14.3	7.57	61.0	15.0	7.62	14.25	0.78	7.75	0.28	-5.11
1.1-20	713.460	3.11	A01	Leu	A18	256	57.2	15.9	6.87	53.5	17.0	6.19	55.4	16.6	6.53	16.52	0.53	6.53	0.34	-5.19
1.1-21	715.487	2.49	A01	Leu	A19	231	12.3	84.0	1.06	10.3	94.8	0.88	12.5	91.1	1.08	89.96	5.52	1.01	0.11	-6.00
1.1-22	717.433	3.39	A01	Phe	A13	254	55.9	12.5	6.62	56.2	12.7	6.69	59.1	13.4	7.25	12.89	0.44	6.85	0.34	-5.16
1.1-23	718.486	1.20	A01	Leu	A20	225	1.4	84.4	0.11	0.9	90.6	0.08	1.2	95.8	0.10	90.26	5.71	0.10	0.02	-7.02
1.1-24	723.480	3.99	A01	Phe	A14	266	30.0	7.7	2.88	30.7	7.0	2.97	29.4	7.6	2.82	7.45	0.37	2.89	0.07	-5.54
1.1-25	725.460	2.22	A01	Phe	A15	238	33.2	71.6	3.27	29.3	81.3	2.80	34.8	76.5	3.46	76.46	4.83	3.18	0.34	-5.50
1.1-26	732.444	2.56	A01	Phe	A16	213	16.6	77.1	1.47	13.2	89.1	1.14	16.7	83.6	1.48	83.28	6.00	1.36	0.19	-5.87
1.1-27	735.444	2.58	A01	2-Nal	A11	251	59.2	21.0	7.25	54.6	23.7	6.40	56.7	23.2	6.77	22.62	1.46	6.80	0.43	-5.17
1.1-28	745.465	4.16	A01	Phe	A17	259	41.4	8.9	4.32	39.4	8.8	4.05	38.9	9.6	3.99	9.09	0.44	4.12	0.17	-5.38
1.1-29	747.444	3.44	A01	Phe	A18	257	37.9	10.1	3.85	30.6	10.3	2.96	33.2	10.9	3.27	10.42	0.42	3.36	0.45	-5.47
1.1-30	747.480	4.50	A01	2-Nal	A12	267	2.9	5.6	0.24	3.2	7.4	0.26	5.6	7.3	0.47	6.79	1.00	0.32	0.13	-6.49
1.1-31	749.471	2.81	A01	Phe	A19	233	22.9	76.9	2.10	19.1	90.5	1.71	23.9	83.9	2.21	83.75	6.81	2.01	0.26	-5.70
1.1-32	752.471	1.52	A01	Phe	A20	228	3.6	77.8	0.30	2.4	89.4	0.20	3.2	89.5	0.26	85.58	6.72	0.25	0.05	-6.60
1.1-33	767.449	4.30	A01	2-Nal	A13	264	8.3	10.6	0.70	12.4	11.6	1.07	8.4	10.6	0.71	10.92	0.59	0.83	0.21	-6.08
1.1-34	773.496	4.90	A01	2-Nal	A14	275	3.0	10.2	0.25	2.9	11.5	0.24	3.6	10.5	0.30	10.74	0.67	0.26	0.03	-6.58
1.1-35	775.475	3.13	A01	2-Nal	A15	249	53.7	25.6	6.23	48.4	29.0	5.35	52.2	27.6	5.98	27.37	1.70	5.85	0.45	-5.23
1.1-36	782.460	3.47	A01	2-Nal	A16	225	35.2	28.0	3.51	29.3	30.9	2.81	31.1	31.9	3.02	30.28	2.02	3.11	0.36	-5.51
1.1-37	795.480	5.07	A01	2-Nal	A17	267	0.0	8.4	0.00	0.0	9.4	0.00	3.0	9.1	0.25	8.97	0.50	0.08	0.14	-7.08
1.1-38	797.460	4.34	A01	2-Nal	A18	266	6.3	8.3	0.53	4.2	9.9	0.35	6.8	8.7	0.57	8.96	0.85	0.48	0.12	-6.32
1.1-39	799.487	3.72	A01	2-Nal	A19	243	37.2	28.3	3.77	29.8	32.7	2.87	36.1	30.6	3.63	30.53	2.24	3.42	0.49	-5.47
1.1-40	802.486	2.43	A01	2-Nal	A20	238	17.9	61.1	1.60	12.5	73.2	1.08	17.4	68.6	1.54	67.60	6.12	1.41	0.28	-5.85

Table S1.1. PAMPA parameters of Sub-library 1.1

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.2-01	623.413	0.64	A02	Ala	A11	220	3.1	97.4	0.25	3.4	90.5	0.28	3.7	90.4	0.30	92.77	4.02	0.28	0.02	-6.56
1.2-02	635.449	2.56	A02	Ala	A12	241	67.1	83.5	8.99	66.6	81.3	8.89	66.6	84.4	8.88	83.08	1.57	8.92	0.06	-5.05
1.2-03	655.418	2.36	A02	Ala	A13	238	59.7	77.0	7.36	61.1	76.2	7.65	60.4	79.9	7.49	77.69	1.92	7.50	0.14	-5.12
1.2-04	661.465	2.96	A02	Ala	A14	250	76.6	53.5	11.77	74.6	53.8	11.08	77.4	54.3	12.03	53.89	0.42	11.63	0.49	-4.93
1.2-05	663.444	1.19	A02	Ala	A15	219	2.3	94.5	0.19	2.5	88.8	0.21	2.7	88.7	0.22	90.63	3.33	0.21	0.02	-6.69
1.2-06	665.460	1.87	A02	Leu	A11	245	56.4	85.5	6.72	57.2	83.8	6.86	58.7	84.3	7.15	84.57	0.88	6.91	0.22	-5.16
1.2-07	670.429	1.53	A02	Ala	A16	198	1.3	109.1	0.10	1.4	97.1	0.12	1.5	101.4	0.12	102.53	6.10	0.11	0.01	-6.94
1.2-08	677.496	3.79	A02	Leu	A12	265	55.2	15.6	6.50	52.1	15.8	5.95	46.8	16.6	5.10	16.02	0.52	5.85	0.70	-5.23
1.2-09	683.449	3.13	A02	Ala	A17	244	74.3	66.0	10.99	71.8	68.1	10.25	75.4	68.9	11.36	67.65	1.50	10.87	0.57	-4.96
1.2-10	685.428	2.40	A02	Ala	A18	242	54.3	61.8	6.34	50.6	61.1	5.71	53.1	62.1	6.13	61.64	0.53	6.06	0.32	-5.22
1.2-11	687.455	1.78	A02	Ala	A19	217	1.6	93.5	0.13	1.6	90.8	0.13	1.9	91.4	0.15	91.92	1.44	0.14	0.01	-6.86
1.2-12	690.455	0.49	A02	Ala	A20	211	0.1	98.7	0.01	0.1	96.2	0.01	0.1	95.8	0.01	96.89	1.58	0.01	0.00	-7.96
1.2-13	697.465	3.59	A02	Leu	A13	259	57.7	16.7	6.97	54.2	16.4	6.32	50.3	16.9	5.65	16.65	0.22	6.31	0.66	-5.20
1.2-14	699.444	2.20	A02	Phe	A11	246	60.0	61.7	7.41	61.1	59.9	7.64	61.2	61.6	7.66	61.08	1.00	7.57	0.14	-5.12
1.2-15	703.512	4.19	A02	Leu	A14	272	24.3	10.9	2.26	23.7	10.7	2.18	17.6	11.2	1.57	10.93	0.24	2.00	0.38	-5.70
1.2-16	705.491	2.42	A02	Leu	A15	242	43.6	88.4	4.63	42.1	88.1	4.42	43.4	89.1	4.61	88.56	0.53	4.55	0.12	-5.34
1.2-17	711.480	4.11	A02	Phe	A12	265	31.9	10.4	3.11	29.6	10.5	2.85	24.6	11.5	2.29	10.80	0.58	2.75	0.42	-5.56
1.2-18	712.476	2.76	A02	Leu	A16	218	24.9	84.9	2.32	24.8	85.0	2.31	26.6	85.0	2.50	84.97	0.06	2.38	0.11	-5.62
1.2-19	725.496	4.36	A02	Leu	A17	265	32.2	10.5	3.15	29.3	10.5	2.80	23.8	11.3	2.20	10.75	0.47	2.72	0.48	-5.57
1.2-20	727.475	3.64	A02	Leu	A18	263	31.0	9.7	3.00	28.0	10.2	2.66	23.1	11.2	2.12	10.39	0.77	2.60	0.44	-5.59
1.2-21	729.502	3.01	A02	Leu	A19	238	26.7	83.7	2.51	27.4	80.7	2.59	27.7	86.7	2.62	83.70	3.04	2.57	0.06	-5.59
1.2-22	731.449	3.91	A02	Phe	A13	260	28.5	10.2	2.71	25.4	10.3	2.37	21.9	11.0	2.00	10.50	0.41	2.36	0.36	-5.63
1.2-23	732.502	1.72	A02	Leu	A20	232	3.7	90.3	0.30	2.8	85.5	0.23	4.0	90.6	0.33	88.79	2.84	0.29	0.05	-6.54
1.2-24	737.496	4.52	A02	Phe	A14	272	7.7	10.4	0.65	8.0	10.3	0.67	5.5	10.8	0.46	10.54	0.26	0.59	0.12	-6.23
1.2-25	739.475	2.75	A02	Phe	A15	244	54.4	63.2	6.36	53.7	63.7	6.23	55.8	62.6	6.61	63.18	0.56	6.40	0.19	-5.19
1.2-26	746.460	3.08	A02	Phe	A16	221	26.5	68.1	2.49	27.2	66.7	2.57	29.0	67.1	2.77	67.28	0.71	2.61	0.15	-5.58
1.2-27	749.460	3.11	A02	2-Nal	A11	257	45.8	15.3	4.95	45.2	15.0	4.87	39.0	15.2	4.00	15.17	0.13	4.61	0.53	-5.34
1.2-28	759.480	4.69	A02	Phe	A17	265	12.4	9.7	1.07	11.4	9.7	0.98	8.1	10.5	0.68	9.96	0.47	0.91	0.20	-6.04
1.2-29	761.460	3.96	A02	Phe	A18	263	11.9	9.5	1.03	10.9	10.0	0.94	8.3	10.6	0.70	10.02	0.57	0.89	0.17	-6.05
1.2-30	761.496	5.02	A02	2-Nal	A12	272	0.4	11.1	0.03	1.4	9.7	0.11	0.6	12.3	0.05	11.03	1.26	0.06	0.04	-7.20
1.2-31	763.487	3.34	A02	Phe	A19	240	37.3	69.0	3.78	35.7	67.3	3.58	36.9	68.4	3.73	68.24	0.87	3.69	0.10	-5.43
1.2-32	766.486	2.04	A02	Phe	A20	235	6.5	97.7	0.54	6.4	92.6	0.53	7.9	97.5	0.67	95.94	2.88	0.58	0.07	-6.24
1.2-33	781.465	4.82	A02	2-Nal	A13	269	3.0	18.3	0.24	2.3	20.1	0.19	1.4	17.8	0.11	18.71	1.19	0.18	0.06	-6.74
1.2-34	787.512	5.42	A02	2-Nal	A14	280	0.7	21.5	0.06	0.9	19.5	0.07	0.5	22.5	0.04	21.14	1.54	0.06	0.01	-7.24
1.2-35	789.491	3.66	A02	2-Nal	A15	255	44.5	16.8	4.77	41.5	16.6	4.34	37.4	16.8	3.80	16.73	0.10	4.30	0.49	-5.37
1.2-36	796.476	3.99	A02	2-Nal	A16	231	40.7	21.3	4.23	36.7	20.7	3.70	32.3	22.2	3.16	21.37	0.74	3.70	0.53	-5.43
1.2-37	809.496	5.60	A02	2-Nal	A17	272	0.6	19.2	0.05	0.5	18.7	0.04	0.3	19.4	0.02	19.10	0.36	0.04	0.01	-7.44
1.2-38	811.475	4.87	A02	2-Nal	A18	272	0.9	20.2	0.07	0.6	22.3	0.05	0.4	20.2	0.04	20.86	1.21	0.05	0.02	-7.29
1.2-39	813.502	4.25	A02	2-Nal	A19	249	33.3	18.3	3.28	29.8	18.3	2.86	28.9	18.8	2.76	18.46	0.28	2.97	0.28	-5.53
1.2-40	816.502	2.95	A02	2-Nal	A20	245	19.9	50.0	1.79	18.4	48.3	1.65	20.2	49.8	1.83	49.35	0.96	1.76	0.09	-5.76

Table S1.2. PAMPA parameters of Sub-library 1.2

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.3-01	637.428	0.96	A03	Ala	A11	227	9.3	92.9	0.79	10.7	97.0	0.92	9.6	90.8	0.82	93.59	3.16	0.84	0.07	-6.08
1.3-02	649.465	2.88	A03	Ala	A12	247	75.2	68.7	11.30	79.4	73.8	12.80	81.3	70.5	13.56	70.99	2.62	12.55	1.15	-4.90
1.3-03	669.433	2.67	A03	Ala	A13	244	67.9	62.1	9.19	75.3	68.3	11.31	73.6	66.1	10.78	65.49	3.12	10.42	1.10	-4.98
1.3-04	675.480	3.28	A03	Ala	A14	256	69.2	34.8	9.54	75.3	38.2	11.33	77.7	37.3	12.14	36.77	1.79	11.00	1.33	-4.96
1.3-05	677.460	1.51	A03	Ala	A15	226	5.9	95.1	0.50	7.2	99.3	0.61	6.5	89.6	0.55	94.70	4.86	0.55	0.06	-6.26
1.3-06	679.475	2.19	A03	Leu	A11	251	66.4	55.2	8.83	71.1	62.4	10.04	72.5	61.3	10.45	59.62	3.91	9.77	0.84	-5.01
1.3-07	684.444	1.85	A03	Ala	A16	204	3.3	87.3	0.27	4.1	95.7	0.34	3.2	93.3	0.27	92.07	4.31	0.29	0.04	-6.54
1.3-08	691.512	4.11	A03	Leu	A12	270	25.6	12.0	2.40	30.0	11.8	2.89	33.9	10.9	3.35	11.57	0.56	2.88	0.48	-5.54
1.3-09	697.465	3.45	A03	Ala	A17	249	69.9	43.0	9.71	74.2	47.7	10.95	78.5	48.7	12.45	46.49	3.02	11.04	1.37	-4.96
1.3-10	699.444	2.72	A03	Ala	A18	248	66.4	44.1	8.82	65.0	44.9	8.50	68.1	44.8	9.25	44.59	0.42	8.85	0.38	-5.05
1.3-11	701.471	2.10	A03	Ala	A19	224	4.0	95.6	0.33	5.3	99.6	0.44	4.3	90.1	0.36	95.11	4.79	0.38	0.06	-6.43
1.3-12	704.471	0.81	A03	Ala	A20	218	0.2	102.0	0.02	0.4	94.4	0.03	0.2	100.7	0.02	99.01	4.06	0.02	0.01	-7.62
1.3-13	711.480	3.91	A03	Leu	A13	264	29.3	12.2	2.81	35.9	12.0	3.60	42.8	11.0	4.52	11.72	0.62	3.65	0.86	-5.44
1.3-14	713.460	2.52	A03	Phe	A11	253	61.7	34.0	7.76	66.6	36.6	8.87	70.2	38.3	9.79	36.29	2.19	8.81	1.02	-5.06
1.3-15	717.527	4.51	A03	Leu	A14	277	6.4	11.5	0.53	7.7	11.5	0.65	8.6	10.5	0.73	11.18	0.56	0.64	0.10	-6.20
1.3-16	719.507	2.74	A03	Leu	A15	248	61.6	73.8	7.75	66.9	80.3	8.94	67.3	76.4	9.04	76.81	3.30	8.58	0.72	-5.07
1.3-17	725.496	4.43	A03	Phe	A12	269	13.7	12.1	1.19	10.6	11.3	0.91	12.5	10.3	1.08	11.24	0.94	1.06	0.14	-5.97
1.3-18	726.491	3.08	A03	Leu	A16	224	43.4	75.2	4.61	48.9	85.1	5.44	48.1	79.0	5.30	79.75	4.98	5.12	0.45	-5.29
1.3-19	739.512	4.68	A03	Leu	A17	270	9.3	11.5	0.79	11.4	10.8	0.98	12.8	9.8	1.11	10.71	0.83	0.96	0.16	-6.02
1.3-20	741.491	3.95	A03	Leu	A18	268	12.3	10.8	1.06	14.8	10.5	1.30	17.3	8.5	1.54	9.93	1.24	1.30	0.24	-5.89
1.3-21	743.518	3.33	A03	Leu	A19	244	42.3	76.5	4.45	50.4	81.9	5.67	46.7	79.7	5.09	79.37	2.74	5.07	0.61	-5.30
1.3-22	745.465	4.23	A03	Phe	A13	265	7.7	12.9	0.65	10.7	11.4	0.92	12.1	10.1	1.04	11.44	1.38	0.87	0.20	-6.06
1.3-23	746.517	2.04	A03	Leu	A20	238	5.4	85.9	0.45	8.0	87.4	0.67	5.7	81.5	0.48	84.94	3.07	0.53	0.12	-6.27
1.3-24	751.512	4.84	A03	Phe	A14	277	1.7	15.6	0.14	1.9	15.7	0.16	1.9	15.2	0.16	15.53	0.27	0.15	0.01	-6.82
1.3-25	753.491	3.07	A03	Phe	A15	250	60.1	40.9	7.43	66.3	45.1	8.80	68.1	46.1	9.24	44.02	2.73	8.49	0.94	-5.07
1.3-26	760.476	3.40	A03	Phe	A16	227	38.2	49.3	3.90	44.1	54.0	4.71	44.1	51.8	4.71	51.69	2.31	4.44	0.47	-5.35
1.3-27	763.475	3.42	A03	2-Nal	A11	262	19.5	12.0	1.76	24.3	12.1	2.25	28.5	10.1	2.72	11.39	1.08	2.24	0.48	-5.65
1.3-28	773.496	5.01	A03	Phe	A17	270	2.8	14.4	0.23	3.2	14.0	0.26	3.7	13.0	0.31	13.80	0.73	0.27	0.04	-6.57
1.3-29	775.475	4.28	A03	Phe	A18	268	4.9	14.6	0.41	5.7	14.6	0.47	6.4	12.7	0.54	13.97	1.09	0.47	0.07	-6.33
1.3-30	775.512	5.34	A03	2-Nal	A12	277	0.1	25.3	0.01	0.0	27.2	0.00	0.0	22.7	0.00	25.05	2.24	0.00	0.00	-8.59
1.3-31	777.502	3.66	A03	Phe	A19	245	47.9	51.0	5.28	54.7	55.3	6.41	55.7	53.9	6.58	53.43	2.19	6.09	0.71	-5.22
1.3-32	780.502	2.36	A03	Phe	A20	241	9.2	83.2	0.79	13.4	88.6	1.17	9.9	81.0	0.84	84.26	3.94	0.93	0.21	-6.03
1.3-33	795.480	5.14	A03	2-Nal	A13	274	0.2	33.9	0.02	0.2	33.3	0.01	0.3	30.0	0.02	32.39	2.10	0.02	0.01	-7.78
1.3-34	801.527	5.74	A03	2-Nal	A14	284	0.0	40.4	0.00	0.0	45.0	0.00	0.1	39.6	0.01	41.64	2.92	0.00	0.00	-8.71
1.3-35	803.507	3.97	A03	2-Nal	A15	260	26.1	13.3	2.45	31.0	13.2	3.00	35.1	12.0	3.50	12.84	0.70	2.99	0.53	-5.53
1.3-36	810.491	4.31	A03	2-Nal	A16	236	26.0	17.0	2.44	33.4	16.8	3.29	32.8	15.2	3.22	16.34	0.98	2.98	0.47	-5.53
1.3-37	823.512	5.92	A03	2-Nal	A17	277	0.0	38.4	0.00	0.0	43.9	0.00	0.0	35.6	0.00	39.30	4.20	0.00	0.00	-8.95
1.3-38	825.491	5.19	A03	2-Nal	A18	277	0.1	37.4	0.01	0.1	42.8	0.01	0.2	35.2	0.01	38.45	3.90	0.01	0.00	-7.97
1.3-39	827.518	4.57	A03	2-Nal	A19	254	19.4	13.4	1.75	26.2	12.9	2.46	26.2	11.2	2.46	12.50	1.16	2.22	0.41	-5.65
1.3-40	830.517	3.27	A03	2-Nal	A20	251	19.8	31.3	1.78	26.7	32.2	2.52	20.5	33.3	1.86	32.25	1.01	2.05	0.40	-5.69

Table S1.3. PAMPA parameters of Sub-library 1.3

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.4-01	681.455	0.43	A04	Ala	A11	227	5.9	92.2	0.49	5.9	91.1	0.49	5.3	96.7	0.44	93.34	2.98	0.48	0.03	-6.32
1.4-02	693.491	2.34	A04	Ala	A12	248	82.6	71.3	14.15	78.9	71.0	12.59	78.6	72.4	12.49	71.59	0.75	13.07	0.93	-4.88
1.4-03	713.460	2.14	A04	Ala	A13	245	73.8	66.8	10.85	73.0	69.5	10.61	72.3	70.0	10.38	68.77	1.69	10.61	0.23	-4.97
1.4-04	719.507	2.75	A04	Ala	A14	257	87.0	44.3	16.53	84.3	47.6	15.00	84.0	48.0	14.83	46.62	2.01	15.46	0.94	-4.81
1.4-05	721.486	0.98	A04	Ala	A15	227	4.3	91.6	0.35	4.3	90.7	0.35	3.8	96.6	0.31	92.99	3.20	0.34	0.02	-6.47
1.4-06	723.501	1.66	A04	Leu	A11	252	69.1	66.9	9.49	66.1	72.5	8.75	64.2	72.2	8.32	70.55	3.17	8.85	0.60	-5.05
1.4-07	728.471	1.31	A04	Ala	A16	206	2.4	97.4	0.20	2.2	93.4	0.18	2.0	101.2	0.16	97.31	3.87	0.18	0.02	-6.74
1.4-08	735.538	3.57	A04	Leu	A12	271	49.2	9.1	5.48	54.0	9.8	6.28	49.4	11.3	5.51	10.05	1.15	5.76	0.46	-5.24
1.4-09	741.491	2.92	A04	Ala	A17	250	81.2	50.6	13.54	80.4	50.9	13.19	79.2	54.7	12.70	52.06	2.25	13.14	0.42	-4.88
1.4-10	743.470	2.19	A04	Ala	A18	248	67.9	46.2	9.19	64.9	48.7	8.47	65.2	49.9	8.55	48.27	1.93	8.74	0.39	-5.06
1.4-11	745.497	1.57	A04	Ala	A19	225	2.7	97.3	0.22	2.7	93.9	0.22	2.4	99.5	0.20	96.90	2.82	0.21	0.02	-6.67
1.4-12	748.497	0.27	A04	Ala	A20	218	0.3	96.6	0.02	0.2	90.4	0.02	0.2	99.8	0.02	95.59	4.79	0.02	0.00	-7.72
1.4-13	755.507	3.37	A04	Leu	A13	266	53.2	10.5	6.14	59.0	10.8	7.22	56.4	12.1	6.72	11.12	0.85	6.69	0.54	-5.17
1.4-14	757.486	1.98	A04	Phe	A11	253	66.3	45.6	8.80	64.9	52.1	8.47	61.4	52.5	7.69	50.09	3.89	8.32	0.57	-5.08
1.4-15	761.554	3.98	A04	Leu	A14	278	16.3	6.6	1.44	23.4	6.5	2.16	17.6	8.4	1.56	7.18	1.02	1.72	0.39	-5.76
1.4-16	763.533	2.21	A04	Leu	A15	249	61.1	75.4	7.64	58.2	75.6	7.07	57.3	78.9	6.89	76.64	1.98	7.20	0.40	-5.14
1.4-17	769.522	3.90	A04	Phe	A12	269	30.8	7.0	2.98	38.5	7.2	3.94	32.2	8.9	3.14	7.69	1.04	3.35	0.51	-5.47
1.4-18	770.517	2.54	A04	Leu	A16	225	34.5	82.3	3.42	34.8	85.1	3.46	32.1	87.3	3.13	84.92	2.53	3.34	0.18	-5.48
1.4-19	783.538	4.15	A04	Leu	A17	271	25.1	6.6	2.34	30.6	6.7	2.95	24.4	8.5	2.26	7.30	1.08	2.52	0.38	-5.60
1.4-20	785.517	3.42	A04	Leu	A18	269	31.4	5.9	3.04	36.5	6.8	3.68	29.5	7.9	2.83	6.91	1.00	3.18	0.44	-5.50
1.4-21	787.544	2.80	A04	Leu	A19	245	37.7	72.8	3.83	36.0	78.2	3.62	35.8	78.5	3.59	76.50	3.20	3.68	0.13	-5.43
1.4-22	789.491	3.70	A04	Phe	A13	266	28.0	7.2	2.66	34.3	7.2	3.41	30.3	8.7	2.92	7.71	0.87	2.99	0.38	-5.52
1.4-23	790.544	1.50	A04	Leu	A20	239	4.7	85.0	0.39	4.0	85.9	0.33	3.6	90.8	0.30	87.24	3.15	0.34	0.05	-6.47
1.4-24	795.538	4.30	A04	Phe	A14	277	8.0	8.2	0.67	12.4	7.1	1.07	7.2	10.3	0.60	8.53	1.67	0.78	0.25	-6.11
1.4-25	797.517	2.53	A04	Phe	A15	251	62.7	48.9	7.98	60.8	51.9	7.57	60.9	54.1	7.61	51.62	2.63	7.72	0.23	-5.11
1.4-26	804.502	2.87	A04	Phe	A16	227	33.3	57.1	3.28	32.1	61.6	3.13	30.0	65.3	2.89	61.33	4.10	3.10	0.20	-5.51
1.4-27	807.501	2.89	A04	2-Nal	A11	263	48.5	10.7	5.37	49.6	12.1	5.54	49.1	13.6	5.46	12.14	1.46	5.46	0.09	-5.26
1.4-28	817.522	4.47	A04	Phe	A17	271	13.8	6.6	1.20	20.0	6.5	1.81	13.3	8.2	1.16	7.09	1.00	1.39	0.36	-5.86
1.4-29	819.501	3.75	A04	Phe	A18	269	16.7	6.6	1.48	26.0	7.5	2.44	16.5	8.5	1.46	7.53	0.97	1.79	0.56	-5.75
1.4-30	819.538	4.81	A04	2-Nal	A12	278	0.4	8.9	0.03	1.2	4.7	0.10	0.8	9.8	0.06	7.78	2.70	0.06	0.03	-7.19
1.4-31	821.528	3.12	A04	Phe	A19	245	46.0	55.1	4.99	42.5	62.1	4.47	42.5	63.8	4.48	60.33	4.60	4.65	0.29	-5.33
1.4-32	824.528	1.83	A04	Phe	A20	241	7.7	83.7	0.65	7.1	85.9	0.59	6.3	87.3	0.52	85.64	1.82	0.59	0.06	-6.23
1.4-33	839.507	4.60	A04	2-Nal	A13	275	2.5	12.3	0.20	4.9	10.5	0.40	2.9	15.2	0.24	12.68	2.34	0.28	0.11	-6.55
1.4-34	845.554	5.21	A04	2-Nal	A14	285	0.7	16.0	0.06	2.3	11.8	0.19	0.8	18.7	0.07	15.50	3.44	0.10	0.07	-6.98
1.4-35	847.533	3.44	A04	2-Nal	A15	260	47.6	11.2	5.23	48.0	12.9	5.29	48.4	14.0	5.36	12.70	1.38	5.29	0.06	-5.28
1.4-36	854.517	3.78	A04	2-Nal	A16	237	43.4	17.5	4.60	46.5	18.6	5.06	44.4	21.3	4.75	19.12	1.95	4.80	0.24	-5.32
1.4-37	867.538	5.38	A04	2-Nal	A17	278	1.0	13.8	0.08	1.9	12.9	0.15	0.9	17.3	0.07	14.69	2.30	0.10	0.05	-7.00
1.4-38	869.517	4.65	A04	2-Nal	A18	277	1.7	13.8	0.14	2.8	15.1	0.23	1.4	18.0	0.11	15.62	2.13	0.16	0.06	-6.80
1.4-39	871.544	4.03	A04	2-Nal	A19	255	35.4	13.3	3.53	37.3	14.8	3.77	36.5	16.3	3.67	14.76	1.50	3.66	0.12	-5.44
1.4-40	874.544	2.74	A04	2-Nal	A20	251	18.3	35.8	1.63	16.3	41.5	1.44	16.2	42.1	1.43	39.80	3.47	1.50	0.12	-5.82

Table S1.4. PAMPA parameters of Sub-library 1.4

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.5-01	694.450	-0.41	A05	Ala	A11	189	0.1	104.8	0.01	0.1	120.4	0.01	0.1	122.3	0.01	115.84	9.59	0.01	0.00	-8.12
1.5-02	706.486	1.51	A05	Ala	A12	207	5.1	96.3	0.42	4.5	105.2	0.37	4.1	107.5	0.34	102.99	5.89	0.38	0.04	-6.42
1.5-03	726.455	1.31	A05	Ala	A13	204	4.6	92.2	0.38	3.7	107.2	0.30	3.4	108.6	0.28	102.66	9.09	0.32	0.05	-6.49
1.5-04	732.502	1.91	A05	Ala	A14	213	16.0	83.1	1.41	13.0	97.9	1.13	12.0	100.4	1.03	93.80	9.38	1.19	0.20	-5.92
1.5-05	734.481	0.14	A05	Ala	A15	189	0.1	101.7	0.01	0.1	119.8	0.01	0.0	120.8	0.00	114.10	10.78	0.01	0.00	-8.28
1.5-06	736.497	0.83	A05	Leu	A11	207	3.3	95.3	0.27	2.7	107.2	0.22	2.4	109.6	0.20	104.04	7.64	0.23	0.04	-6.64
1.5-07	741.466	0.48	A05	Ala	A16	169	0.5	99.5	0.04	0.3	112.1	0.03	0.4	114.3	0.04	108.63	7.99	0.03	0.01	-7.48
1.5-08	748.533	2.74	A05	Leu	A12	224	53.0	47.0	6.12	45.4	53.4	4.90	46.1	57.4	5.00	52.60	5.22	5.34	0.68	-5.27
1.5-09	754.486	2.09	A05	Ala	A17	211	18.1	95.1	1.61	15.1	108.3	1.33	13.9	111.0	1.21	104.78	8.51	1.39	0.21	-5.86
1.5-10	756.465	1.36	A05	Ala	A18	208	8.7	88.6	0.73	7.3	98.0	0.61	5.8	103.3	0.49	96.64	7.42	0.61	0.12	-6.21
1.5-11	758.492	0.74	A05	Ala	A19	190	0.1	100.8	0.01	0.1	119.4	0.00	0.1	120.3	0.01	113.51	10.99	0.01	0.00	-8.20
1.5-12	761.492	-0.56	A05	Ala	A20	184	0.0	104.1	0.00	0.0	116.4	0.00	0.0	116.8	0.00	112.41	7.20	0.00	0.00	-9.00
1.5-13	768.502	2.54	A05	Leu	A13	220	43.5	49.0	4.62	36.1	57.1	3.63	36.3	61.0	3.65	55.72	6.11	3.97	0.56	-5.40
1.5-14	770.481	1.15	A05	Phe	A11	209	6.0	91.2	0.50	5.0	102.0	0.41	4.0	107.1	0.33	100.10	8.11	0.42	0.08	-6.38
1.5-15	774.549	3.15	A05	Leu	A14	232	60.0	32.0	7.41	53.7	33.9	6.23	54.7	37.1	6.40	34.34	2.61	6.68	0.64	-5.18
1.5-16	776.528	1.38	A05	Leu	A15	205	2.0	97.9	0.16	1.6	111.3	0.13	1.4	111.0	0.11	106.73	7.66	0.14	0.02	-6.87
1.5-17	782.517	3.07	A05	Phe	A12	227	51.7	29.2	5.90	45.9	33.7	4.97	45.4	35.9	4.91	32.90	3.41	5.26	0.55	-5.28
1.5-18	783.513	1.71	A05	Leu	A16	187	2.1	243.0	0.17	3.7	126.9	0.30	3.8	100.8	0.31	156.91	75.70	0.26	0.08	-6.58
1.5-19	796.533	3.32	A05	Leu	A17	227	49.6	30.6	5.54	45.4	34.3	4.90	41.8	41.6	4.38	35.50	5.59	4.94	0.58	-5.31
1.5-20	798.512	2.59	A05	Leu	A18	224	29.6	31.5	2.84	25.9	37.3	2.43	25.0	39.3	2.33	36.02	4.07	2.53	0.27	-5.60
1.5-21	800.539	1.97	A05	Leu	A19	204	1.5	91.1	0.12	1.1	109.3	0.09	0.7	110.2	0.06	103.52	10.78	0.09	0.03	-7.04
1.5-22	802.486	2.87	A05	Phe	A13	224	41.2	25.9	4.29	36.1	30.0	3.62	34.3	32.1	3.40	29.32	3.15	3.77	0.46	-5.42
1.5-23	803.539	0.67	A05	Leu	A20	199	0.3	97.4	0.02	0.2	116.8	0.02	0.2	114.0	0.01	109.40	10.46	0.02	0.00	-7.77
1.5-24	808.533	3.47	A05	Phe	A14	233	49.5	13.8	5.53	42.9	15.9	4.53	41.7	16.7	4.37	15.47	1.51	4.81	0.63	-5.32
1.5-25	810.512	1.70	A05	Phe	A15	209	5.2	88.4	0.44	4.1	101.8	0.34	3.4	105.7	0.28	98.63	9.07	0.35	0.08	-6.45
1.5-26	817.497	2.04	A05	Phe	A16	189	3.5	93.9	0.29	2.6	116.1	0.21	2.2	117.7	0.18	109.26	13.29	0.22	0.06	-6.65
1.5-27	820.497	2.06	A05	2-Nal	A11	220	24.3	43.0	2.25	19.9	52.5	1.80	17.3	55.1	1.54	50.20	6.35	1.86	0.36	-5.73
1.5-28	830.517	3.64	A05	Phe	A17	229	35.4	15.6	3.54	32.4	18.9	3.16	31.2	20.3	3.02	18.27	2.38	3.24	0.27	-5.49
1.5-29	832.497	2.91	A05	Phe	A18	226	20.9	15.4	1.90	19.7	18.4	1.77	17.0	20.9	1.51	18.23	2.78	1.73	0.20	-5.76
1.5-30	832.533	3.97	A05	2-Nal	A12	236	18.7	6.8	1.68	18.1	7.3	1.62	17.3	8.7	1.54	7.62	0.99	1.61	0.07	-5.79
1.5-31	834.524	2.29	A05	Phe	A19	206	3.6	93.9	0.29	2.7	105.6	0.22	2.3	107.5	0.19	102.35	7.35	0.23	0.05	-6.63
1.5-32	837.523	1.00	A05	Phe	A20	202	0.7	94.5	0.06	0.5	114.1	0.04	0.4	114.2	0.04	107.61	11.32	0.04	0.01	-7.35
1.5-33	852.502	3.77	A05	2-Nal	A13	233	15.9	8.1	1.40	14.0	9.4	1.22	11.0	10.5	0.95	9.36	1.21	1.19	0.23	-5.92
1.5-34	858.549	4.38	A05	2-Nal	A14	241	5.4	8.2	0.45	4.8	9.3	0.39	3.6	10.5	0.30	9.34	1.13	0.38	0.08	-6.42
1.5-35	860.528	2.61	A05	2-Nal	A15	218	19.2	48.4	1.72	15.5	59.7	1.36	14.8	62.4	1.29	56.86	7.42	1.46	0.23	-5.84
1.5-36	867.513	2.94	A05	2-Nal	A16	199	13.3	59.6	1.16	10.1	73.6	0.86	9.8	75.0	0.83	69.40	8.50	0.95	0.18	-6.02
1.5-37	880.533	4.55	A05	2-Nal	A17	236	6.1	7.2	0.51	5.7	8.4	0.47	3.8	10.5	0.31	8.70	1.68	0.43	0.11	-6.37
1.5-38	882.512	3.82	A05	2-Nal	A18	235	3.9	8.1	0.32	5.4	9.0	0.45	2.2	10.9	0.18	9.30	1.43	0.32	0.13	-6.50
1.5-39	884.539	3.20	A05	2-Nal	A19	214	12.4	50.5	1.07	9.9	59.9	0.84	8.9	64.7	0.76	58.38	7.25	0.89	0.16	-6.05
1.5-40	887.539	1.91	A05	2-Nal	A20	211	5.2	85.8	0.43	3.8	101.9	0.32	3.3	105.6	0.27	97.74	10.54	0.34	0.08	-6.47

Table S1.5. PAMPA parameters of Sub-library 1.5

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.6-01	705.374	2.02	A06	Ala	A11	237	51.6	64.0	5.88	51.2	70.3	5.81	46.9	65.0	5.13	66.43	3.39	5.61	0.41	-5.25
1.6-02	717.410	3.93	A06	Ala	A12	254	46.4	13.8	5.05	51.2	14.0	5.80	47.3	12.3	5.18	13.34	0.93	5.35	0.40	-5.27
1.6-03	737.379	3.73	A06	Ala	A13	251	32.9	15.8	3.23	35.2	15.5	3.51	31.7	14.6	3.09	15.27	0.63	3.27	0.21	-5.48
1.6-04	743.426	4.34	A06	Ala	A14	263	10.8	16.2	0.93	12.9	14.1	1.12	10.5	12.5	0.90	14.26	1.82	0.98	0.12	-6.01
1.6-05	745.405	2.57	A06	Ala	A15	236	41.2	64.1	4.30	41.1	71.4	4.29	36.8	68.8	3.71	68.10	3.71	4.10	0.34	-5.39
1.6-06	747.421	3.25	A06	Leu	A11	259	40.9	13.0	4.26	46.9	13.5	5.13	41.0	11.7	4.28	12.71	0.92	4.56	0.49	-5.34
1.6-07	752.390	2.90	A06	Ala	A16	215	26.0	74.5	2.43	24.6	84.0	2.28	21.8	84.6	1.99	81.02	5.66	2.23	0.23	-5.65
1.6-08	759.457	5.16	A06	Leu	A12	275	0.7	27.0	0.06	0.6	21.2	0.04	0.3	25.6	0.02	24.58	3.04	0.04	0.02	-7.39
1.6-09	765.410	4.51	A06	Ala	A17	257	11.1	18.1	0.95	14.0	16.2	1.22	9.8	15.2	0.83	16.51	1.45	1.00	0.20	-6.00
1.6-10	767.389	3.78	A06	Ala	A18	254	6.1	17.1	0.51	7.3	15.5	0.61	4.8	14.8	0.40	15.81	1.20	0.51	0.11	-6.30
1.6-11	769.416	3.16	A06	Ala	A19	233	29.7	74.0	2.85	29.0	79.5	2.77	27.7	70.5	2.63	74.66	4.52	2.75	0.11	-5.56
1.6-12	772.416	1.86	A06	Ala	A20	228	4.7	92.1	0.39	4.8	96.9	0.40	3.7	99.6	0.30	96.20	3.79	0.36	0.05	-6.44
1.6-13	779.426	4.96	A06	Leu	A13	270	2.8	35.4	0.23	3.2	30.5	0.26	2.6	34.0	0.21	33.31	2.53	0.23	0.03	-6.63
1.6-14	781.405	3.57	A06	Phe	A11	259	12.6	14.3	1.09	15.8	13.8	1.39	11.0	12.6	0.94	13.57	0.92	1.14	0.23	-5.94
1.6-15	785.473	5.57	A06	Leu	A14	282	0.7	45.9	0.05	1.1	40.7	0.09	1.2	43.3	0.10	43.28	2.61	0.08	0.02	-7.10
1.6-16	787.452	3.80	A06	Leu	A15	256	51.3	17.2	5.83	56.8	18.1	6.80	49.3	15.5	5.50	16.94	1.29	6.04	0.67	-5.22
1.6-17	793.441	5.49	A06	Phe	A12	274	0.2	50.4	0.01	0.1	43.0	0.01	0.1	47.2	0.01	46.88	3.72	0.01	0.00	-8.04
1.6-18	794.437	4.13	A06	Leu	A16	232	40.1	22.0	4.14	47.7	21.4	5.25	36.0	20.7	3.61	21.39	0.66	4.33	0.84	-5.36
1.6-19	807.457	5.74	A06	Leu	A17	275	0.2	49.3	0.02	0.1	42.7	0.01	0.1	46.9	0.01	46.31	3.31	0.01	0.00	-7.97
1.6-20	809.436	5.01	A06	Leu	A18	272	0.4	48.4	0.03	0.3	43.8	0.02	0.3	42.2	0.03	44.80	3.24	0.03	0.00	-7.56
1.6-21	811.463	4.39	A06	Leu	A19	251	30.9	16.8	2.99	34.3	17.8	3.41	28.2	16.4	2.68	17.00	0.72	3.02	0.36	-5.52
1.6-22	813.410	5.29	A06	Phe	A13	271	0.1	57.7	0.01	0.1	51.0	0.01	0.1	53.5	0.00	54.06	3.36	0.01	0.00	-8.11
1.6-23	814.463	3.09	A06	Leu	A20	247	22.9	46.2	2.11	24.7	48.8	2.30	20.9	46.0	1.89	47.00	1.53	2.10	0.20	-5.68
1.6-24	819.457	5.89	A06	Phe	A14	281	0.1	67.5	0.00	0.0	65.9	0.00	0.0	62.4	0.00	65.29	2.61	0.00	0.00	-8.61
1.6-25	821.436	4.12	A06	Phe	A15	257	11.7	15.6	1.01	13.6	14.5	1.18	9.5	13.1	0.80	14.40	1.25	1.00	0.19	-6.00
1.6-26	828.421	4.46	A06	Phe	A16	234	9.2	21.6	0.78	10.6	21.3	0.90	7.3	20.1	0.61	21.02	0.78	0.77	0.15	-6.12
1.6-27	831.421	4.48	A06	2-Nal	A11	269	0.2	42.8	0.02	0.2	41.3	0.02	0.2	36.5	0.01	40.18	3.31	0.02	0.00	-7.82
1.6-28	841.441	6.06	A06	Phe	A17	274	0.1	60.8	0.01	0.0	53.3	0.00	0.0	58.1	0.00	57.41	3.79	0.00	0.00	-8.47
1.6-29	843.421	5.34	A06	Phe	A18	273	0.1	62.2	0.00	0.1	58.8	0.00	0.0	51.1	0.00	57.39	5.70	0.00	0.00	-8.36
1.6-30	843.457	6.40	A06	2-Nal	A12	282	0.0	80.3	0.00	0.0	74.7	0.00	0.0	77.5	0.00	77.49	2.81	0.00	0.00	—
1.6-31	845.448	4.71	A06	Phe	A19	253	9.4	17.5	0.80	11.0	16.6	0.94	7.2	16.1	0.60	16.73	0.71	0.78	0.17	-6.11
1.6-32	848.447	3.42	A06	Phe	A20	248	18.8	30.2	1.68	21.9	31.3	2.01	15.1	30.8	1.33	30.78	0.59	1.67	0.34	-5.78
1.6-33	863.426	6.19	A06	2-Nal	A13	279	0.0	69.0	0.00	0.0	63.5	0.00	0.0	65.3	0.00	65.94	2.84	0.00	0.00	-9.46
1.6-34	869.473	6.80	A06	2-Nal	A14	288	0.0	65.5	0.00	0.0	66.0	0.00	0.0	70.4	0.00	67.32	2.72	0.00	0.00	—
1.6-35	871.452	5.03	A06	2-Nal	A15	267	0.3	44.2	0.02	0.2	39.9	0.01	0.1	41.8	0.01	41.94	2.17	0.02	0.01	-7.82
1.6-36	878.437	5.37	A06	2-Nal	A16	244	0.1	55.8	0.01	0.0	51.7	0.00	0.0	52.8	0.00	53.45	2.10	0.00	0.00	-8.45
1.6-37	891.457	6.97	A06	2-Nal	A17	282	0.0	72.4	0.00	0.0	70.3	0.00	0.0	69.2	0.00	70.62	1.65	0.00	0.00	—
1.6-38	893.436	6.24	A06	2-Nal	A18	281	0.0	69.9	0.00	0.0	69.6	0.00	0.0	66.7	0.00	68.77	1.76	0.00	0.00	-9.41
1.6-39	895.463	5.62	A06	2-Nal	A19	262	0.2	43.5	0.01	0.1	40.2	0.01	0.1	39.1	0.01	40.89	2.30	0.01	0.00	-7.99
1.6-40	898.463	4.33	A06	2-Nal	A20	257	1.0	19.2	0.08	1.2	18.1	0.10	0.6	18.5	0.05	18.63	0.56	0.08	0.02	-7.11

Table S1.6. PAMPA parameters of Sub-library 1.6

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.7-01	713.460	2.59	A07	Ala	A11	244	59.9	45.8	7.39	52.3	49.9	5.98	53.3	53.5	6.17	49.73	3.85	6.51	0.76	-5.19
1.7-02	725.496	4.50	A07	Ala	A12	262	25.5	7.4	2.38	24.8	7.2	2.31	29.4	7.3	2.82	7.29	0.12	2.50	0.28	-5.60
1.7-03	745.465	4.30	A07	Ala	A13	258	17.5	7.9	1.56	17.7	7.7	1.57	21.5	7.7	1.95	7.77	0.11	1.70	0.22	-5.77
1.7-04	751.512	4.91	A07	Ala	A14	269	7.2	8.7	0.60	6.3	8.2	0.53	6.9	8.0	0.58	8.33	0.33	0.57	0.04	-6.24
1.7-05	753.491	3.14	A07	Ala	A15	242	51.5	48.1	5.86	42.6	52.9	4.49	44.7	56.3	4.79	52.45	4.13	5.05	0.72	-5.30
1.7-06	755.507	3.82	A07	Leu	A11	266	17.2	6.1	1.53	19.4	6.0	1.75	22.1	5.7	2.02	5.91	0.19	1.76	0.25	-5.75
1.7-07	760.476	3.47	A07	Ala	A16	222	33.8	54.4	3.33	25.1	60.9	2.34	26.2	66.0	2.46	60.44	5.82	2.71	0.54	-5.57
1.7-08	767.543	5.73	A07	Leu	A12	282	2.1	14.3	0.17	3.1	12.1	0.26	1.9	13.2	0.16	13.19	1.08	0.20	0.05	-6.71
1.7-09	773.496	5.08	A07	Ala	A17	263	8.6	10.6	0.73	8.9	10.1	0.76	9.0	9.8	0.77	10.17	0.41	0.75	0.02	-6.12
1.7-10	775.475	4.35	A07	Ala	A18	262	6.0	11.4	0.50	7.5	10.8	0.63	6.2	10.3	0.52	10.84	0.59	0.55	0.07	-6.26
1.7-11	777.502	3.73	A07	Ala	A19	241	30.3	39.5	2.92	22.3	44.9	2.05	23.5	48.7	2.17	44.35	4.63	2.38	0.47	-5.62
1.7-12	780.502	2.43	A07	Ala	A20	235	9.5	76.2	0.81	5.7	93.5	0.48	6.1	94.5	0.51	88.06	10.24	0.60	0.18	-6.22
1.7-13	787.512	5.53	A07	Leu	A13	277	0.2	22.2	0.02	0.6	20.2	0.05	0.2	20.8	0.02	21.11	1.02	0.03	0.02	-7.53
1.7-14	789.491	4.14	A07	Phe	A11	266	4.9	7.9	0.41	6.6	7.4	0.55	6.4	6.8	0.54	7.36	0.57	0.50	0.08	-6.30
1.7-15	793.559	6.14	A07	Leu	A14	287	0.0	28.3	0.00	0.3	25.7	0.02	0.0	27.2	0.00	27.07	1.28	0.01	0.01	-8.15
1.7-16	795.538	4.37	A07	Leu	A15	263	40.7	8.7	4.23	42.5	8.7	4.48	42.7	8.6	4.50	8.67	0.07	4.41	0.15	-5.36
1.7-17	801.527	6.06	A07	Phe	A12	280	0.0	32.7	0.00	0.1	28.7	0.01	0.0	30.2	0.00	30.55	2.02	0.00	0.01	-8.51
1.7-18	802.523	4.70	A07	Leu	A16	238	18.3	10.0	1.64	21.5	9.4	1.96	28.3	7.5	2.69	8.96	1.31	2.10	0.54	-5.68
1.7-19	815.543	6.31	A07	Leu	A17	281	0.0	34.3	0.00	0.0	31.9	0.00	0.0	32.1	0.00	32.77	1.34	0.00	0.00	—
1.7-20	817.522	5.58	A07	Leu	A18	279	0.3	34.7	0.03	0.7	33.0	0.06	0.4	33.4	0.04	33.71	0.87	0.04	0.02	-7.39
1.7-21	819.549	4.96	A07	Leu	A19	258	15.7	8.9	1.39	17.0	8.8	1.51	17.6	9.0	1.57	8.87	0.11	1.49	0.09	-5.83
1.7-22	821.496	5.86	A07	Phe	A13	277	0.0	39.3	0.00	0.1	39.1	0.01	0.0	38.3	0.00	38.92	0.52	0.00	0.01	-8.45
1.7-23	822.549	3.66	A07	Leu	A20	253	17.2	23.7	1.53	13.0	24.9	1.13	13.3	28.5	1.16	25.68	2.50	1.27	0.22	-5.90
1.7-24	827.543	6.46	A07	Phe	A14	286	0.0	44.3	0.00	0.1	42.3	0.00	0.0	43.5	0.00	43.34	1.01	0.00	0.00	-8.53
1.7-25	829.522	4.69	A07	Phe	A15	264	14.8	8.7	1.30	18.8	8.3	1.68	16.3	7.7	1.44	8.27	0.52	1.48	0.20	-5.83
1.7-26	836.507	5.03	A07	Phe	A16	241	4.1	10.6	0.34	5.9	9.9	0.49	4.4	9.7	0.36	10.06	0.46	0.40	0.08	-6.40
1.7-27	839.507	5.05	A07	2-Nal	A11	274	0.1	28.8	0.01	0.4	25.7	0.03	0.1	27.7	0.01	27.42	1.54	0.02	0.01	-7.74
1.7-28	849.527	6.63	A07	Phe	A17	280	0.0	47.5	0.00	0.1	45.2	0.01	0.0	45.4	0.00	46.02	1.26	0.00	0.00	-8.51
1.7-29	851.507	5.90	A07	Phe	A18	279	0.0	44.1	0.00	0.1	45.5	0.01	0.0	44.1	0.00	44.58	0.80	0.00	0.00	-8.56
1.7-30	851.543	6.97	A07	2-Nal	A12	287	0.1	51.9	0.01	0.1	54.8	0.01	0.1	53.1	0.01	53.26	1.46	0.01	0.00	-8.11
1.7-31	853.533	5.28	A07	Phe	A19	259	4.9	10.4	0.41	7.0	9.6	0.58	5.2	9.5	0.44	9.83	0.52	0.48	0.10	-6.32
1.7-32	856.533	3.99	A07	Phe	A20	255	9.8	13.9	0.84	8.4	15.2	0.71	8.4	15.6	0.71	14.91	0.87	0.75	0.08	-6.12
1.7-33	871.512	6.76	A07	2-Nal	A13	284	0.0	41.9	0.00	0.0	42.7	0.00	0.0	44.3	0.00	42.97	1.20	0.00	0.00	-8.95
1.7-34	877.559	7.37	A07	2-Nal	A14	292	0.1	54.6	0.00	0.0	58.6	0.00	0.0	54.2	0.00	55.80	2.42	0.00	0.00	-8.84
1.7-35	879.538	5.60	A07	2-Nal	A15	272	0.1	27.9	0.01	0.7	26.4	0.05	0.2	27.6	0.01	27.33	0.80	0.02	0.02	-7.61
1.7-36	886.523	5.93	A07	2-Nal	A16	250	0.1	37.9	0.01	0.7	36.4	0.05	0.1	38.2	0.01	37.50	0.95	0.02	0.02	-7.62
1.7-37	899.543	7.54	A07	2-Nal	A17	286	0.0	52.6	0.00	0.0	53.8	0.00	0.0	54.8	0.00	53.73	1.12	0.00	0.00	-9.27
1.7-38	901.522	6.81	A07	2-Nal	A18	286	0.2	50.1	0.01	0.1	53.0	0.01	0.2	52.6	0.01	51.86	1.58	0.01	0.00	-7.95
1.7-39	903.549	6.19	A07	2-Nal	A19	267	0.0	27.2	0.00	0.4	25.7	0.03	0.0	26.0	0.00	26.27	0.81	0.01	0.02	-8.00
1.7-40	906.549	4.90	A07	2-Nal	A20	264	0.3	11.0	0.02	1.3	10.5	0.10	0.4	9.7	0.03	10.39	0.68	0.05	0.05	-7.28

Table S1.7. PAMPA parameters of Sub-library 1.7

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.8-01	715.403	1.12	A08	Ala	A11	226	12.4	75.9	1.07	13.8	80.7	1.20	14.2	82.7	1.24	79.78	3.46	1.17	0.09	-5.93
1.8-02	727.439	3.04	A08	Ala	A12	245	83.7	33.6	14.70	84.9	34.7	15.29	74.7	34.3	11.12	34.20	0.59	13.70	2.26	-4.86
1.8-03	747.408	2.83	A08	Ala	A13	241	65.4	27.8	8.59	63.9	28.7	8.25	55.1	29.3	6.48	28.60	0.75	7.77	1.13	-5.11
1.8-04	753.455	3.44	A08	Ala	A14	253	52.6	14.9	6.05	54.8	15.6	6.43	42.3	15.5	4.45	15.32	0.35	5.64	1.05	-5.25
1.8-05	755.434	1.67	A08	Ala	A15	226	8.5	76.5	0.72	9.5	81.2	0.81	10.0	81.7	0.85	79.80	2.83	0.79	0.06	-6.10
1.8-06	757.449	2.35	A08	Leu	A11	248	68.7	26.4	9.39	71.7	27.0	10.22	61.4	27.8	7.71	27.05	0.67	9.11	1.28	-5.04
1.8-07	762.418	2.00	A08	Ala	A16	206	5.5	83.2	0.46	6.7	87.1	0.56	7.1	88.8	0.60	86.38	2.85	0.54	0.07	-6.27
1.8-08	769.486	4.27	A08	Leu	A12	266	3.4	14.3	0.28	3.6	14.3	0.30	3.0	16.4	0.25	14.99	1.20	0.28	0.03	-6.56
1.8-09	775.439	3.61	A08	Ala	A17	247	49.8	19.5	5.58	54.0	19.6	6.28	40.5	19.6	4.20	19.55	0.05	5.35	1.06	-5.27
1.8-10	777.418	2.88	A08	Ala	A18	245	28.7	18.1	2.74	31.9	17.8	3.11	25.6	19.0	2.39	18.26	0.62	2.75	0.36	-5.56
1.8-11	779.445	2.26	A08	Ala	A19	224	5.8	73.4	0.49	7.1	74.3	0.59	8.1	78.6	0.69	75.43	2.78	0.59	0.10	-6.23
1.8-12	782.445	0.97	A08	Ala	A20	217	0.9	93.7	0.07	1.2	91.4	0.09	1.3	95.6	0.11	93.55	2.07	0.09	0.02	-7.04
1.8-13	789.455	4.07	A08	Leu	A13	260	2.9	20.4	0.24	2.3	21.3	0.19	2.7	21.8	0.22	21.20	0.71	0.21	0.02	-6.67
1.8-14	791.434	2.68	A08	Phe	A11	250	39.6	14.9	4.08	46.6	15.1	5.08	37.4	15.7	3.79	15.26	0.45	4.32	0.68	-5.36
1.8-15	795.501	4.67	A08	Leu	A14	273	0.7	26.2	0.06	0.2	26.3	0.02	0.3	27.9	0.02	26.79	0.93	0.03	0.02	-7.50
1.8-16	797.481	2.90	A08	Leu	A15	245	69.3	37.5	9.55	73.3	38.7	10.70	63.2	39.9	8.10	38.71	1.16	9.45	1.30	-5.02
1.8-17	803.470	4.59	A08	Phe	A12	266	0.6	29.3	0.05	0.4	30.0	0.03	0.4	32.3	0.04	30.52	1.58	0.04	0.01	-7.41
1.8-18	804.465	3.24	A08	Leu	A16	223	43.3	39.1	4.60	49.6	37.4	5.55	44.6	39.8	4.78	38.78	1.24	4.98	0.50	-5.30
1.8-19	817.486	4.84	A08	Leu	A17	265	0.7	30.3	0.05	0.2	30.6	0.02	0.5	33.3	0.04	31.43	1.65	0.04	0.02	-7.44
1.8-20	819.465	4.11	A08	Leu	A18	263	1.4	30.5	0.11	0.9	29.4	0.07	0.9	31.2	0.08	30.34	0.89	0.09	0.02	-7.06
1.8-21	821.492	3.49	A08	Leu	A19	241	35.6	32.8	3.57	38.2	34.8	3.89	34.7	36.8	3.45	34.80	1.96	3.64	0.23	-5.44
1.8-22	823.439	4.39	A08	Phe	A13	262	0.5	40.6	0.04	0.2	39.3	0.02	0.4	41.1	0.03	40.32	0.95	0.03	0.01	-7.51
1.8-23	824.492	2.20	A08	Leu	A20	236	9.8	68.1	0.84	12.3	69.4	1.06	13.5	75.5	1.18	71.01	3.96	1.03	0.17	-5.99
1.8-24	829.486	5.00	A08	Phe	A14	273	0.5	46.6	0.04	0.3	45.5	0.02	0.3	50.1	0.02	47.40	2.40	0.03	0.01	-7.54
1.8-25	831.465	3.23	A08	Phe	A15	248	33.3	15.9	3.28	39.8	16.1	4.10	31.1	17.2	3.02	16.41	0.70	3.47	0.57	-5.46
1.8-26	838.450	3.56	A08	Phe	A16	225	16.1	23.3	1.42	19.6	25.1	1.77	18.0	25.4	1.61	24.61	1.15	1.60	0.17	-5.80
1.8-27	841.449	3.58	A08	2-Nal	A11	259	1.1	28.9	0.09	0.7	29.9	0.05	1.0	31.4	0.08	30.06	1.26	0.07	0.02	-7.13
1.8-28	851.470	5.17	A08	Phe	A17	266	0.2	42.7	0.02	0.0	43.2	0.00	0.1	46.8	0.01	44.25	2.25	0.01	0.01	-8.01
1.8-29	853.449	4.44	A08	Phe	A18	265	0.4	42.8	0.03	0.1	42.0	0.01	0.1	46.2	0.01	43.66	2.22	0.02	0.01	-7.76
1.8-30	853.486	5.50	A08	2-Nal	A12	274	0.0	56.1	0.00	0.0	52.8	0.00	0.0	58.9	0.00	55.93	3.04	0.00	0.00	-8.89
1.8-31	855.476	3.82	A08	Phe	A19	243	18.7	19.9	1.68	22.6	20.9	2.08	20.8	22.0	1.89	20.95	1.01	1.88	0.20	-5.73
1.8-32	858.476	2.52	A08	Phe	A20	238	13.3	45.4	1.16	16.7	46.7	1.48	17.3	52.2	1.53	48.11	3.64	1.39	0.20	-5.86
1.8-33	873.455	5.30	A08	2-Nal	A13	271	0.1	58.8	0.01	0.0	64.1	0.00	0.0	68.9	0.00	63.97	5.04	0.00	0.00	-8.53
1.8-34	879.501	5.90	A08	2-Nal	A14	280	0.0	61.2	0.00	0.0	55.9	0.00	0.0	61.1	0.00	59.38	3.01	0.00	0.00	-9.12
1.8-35	881.481	4.13	A08	2-Nal	A15	257	0.9	33.0	0.08	0.7	32.0	0.06	0.9	35.1	0.07	33.37	1.57	0.07	0.01	-7.16
1.8-36	888.465	4.47	A08	2-Nal	A16	235	0.6	38.4	0.05	0.3	37.4	0.02	0.6	41.5	0.05	39.11	2.13	0.04	0.02	-7.42
1.8-37	901.486	6.08	A08	2-Nal	A17	274	0.0	58.1	0.00	0.0	55.2	0.00	0.0	61.1	0.00	58.15	2.92	0.00	0.00	-9.29
1.8-38	903.465	5.35	A08	2-Nal	A18	273	0.0	57.8	0.00	0.0	55.8	0.00	0.0	60.1	0.00	57.91	2.16	0.00	0.00	-8.88
1.8-39	905.492	4.73	A08	2-Nal	A19	252	0.4	28.3	0.03	0.1	28.4	0.01	0.4	30.0	0.03	28.89	0.97	0.02	0.01	-7.60
1.8-40	908.492	3.43	A08	2-Nal	A20	248	3.1	16.9	0.26	3.9	16.2	0.33	4.4	18.3	0.36	17.13	1.09	0.32	0.05	-6.50

Table S1.8. PAMPA parameters of Sub-library 1.8

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.9-01	718.450	1.54	A09	Ala	A11	238	28.2	81.0	2.68	33.3	83.3	3.28	31.2	86.2	3.02	83.53	2.60	2.99	0.30	-5.52
1.9-02	730.486	3.46	A09	Ala	A12	255	65.8	15.5	8.67	78.1	17.5	12.29	67.9	18.4	9.20	17.14	1.48	10.05	1.96	-5.00
1.9-03	750.455	3.26	A09	Ala	A13	252	55.8	14.0	6.62	69.5	15.4	9.62	61.0	16.5	7.63	15.30	1.26	7.95	1.53	-5.10
1.9-04	756.502	3.86	A09	Ala	A14	262	34.1	8.1	3.37	44.6	7.5	4.78	40.3	8.5	4.18	8.03	0.50	4.11	0.71	-5.39
1.9-05	758.481	2.09	A09	Ala	A15	236	21.5	82.2	1.96	25.0	86.0	2.33	24.1	86.2	2.23	84.83	2.25	2.17	0.19	-5.66
1.9-06	760.497	2.77	A09	Leu	A11	259	56.4	13.0	6.72	67.5	14.1	9.10	60.3	15.2	7.49	14.09	1.09	7.77	1.22	-5.11
1.9-07	765.466	2.43	A09	Ala	A16	217	15.2	87.7	1.34	18.6	90.1	1.66	14.9	94.0	1.30	90.60	3.19	1.43	0.20	-5.84
1.9-08	772.533	4.69	A09	Leu	A12	275	3.4	8.1	0.28	3.0	6.3	0.25	3.1	7.8	0.26	7.42	0.94	0.26	0.02	-6.58
1.9-09	778.486	4.03	A09	Ala	A17	257	41.5	8.9	4.34	49.6	9.1	5.54	41.6	10.4	4.36	9.44	0.85	4.75	0.69	-5.32
1.9-10	780.465	3.30	A09	Ala	A18	255	27.9	9.0	2.65	29.2	8.2	2.80	26.8	9.3	2.52	8.85	0.57	2.66	0.14	-5.58
1.9-11	782.492	2.68	A09	Ala	A19	235	17.1	73.4	1.52	20.5	74.0	1.85	17.0	81.3	1.51	76.25	4.40	1.63	0.20	-5.79
1.9-12	785.492	1.39	A09	Ala	A20	230	3.2	102.3	0.26	3.6	100.3	0.30	2.6	104.7	0.22	102.41	2.19	0.26	0.04	-6.59
1.9-13	792.502	4.49	A09	Leu	A13	271	4.4	9.8	0.36	3.6	7.4	0.29	3.7	9.7	0.31	8.96	1.31	0.32	0.04	-6.49
1.9-14	794.481	3.10	A09	Phe	A11	260	36.0	7.4	3.61	45.4	7.1	4.90	39.9	7.9	4.12	7.47	0.42	4.21	0.65	-5.38
1.9-15	798.549	5.09	A09	Leu	A14	281	1.8	13.1	0.14	1.4	9.6	0.12	1.1	12.7	0.09	11.80	1.88	0.12	0.03	-6.93
1.9-16	800.528	3.32	A09	Leu	A15	256	61.8	20.3	7.80	72.6	22.5	10.49	64.3	24.8	8.35	22.54	2.21	8.88	1.42	-5.05
1.9-17	806.517	5.01	A09	Phe	A12	274	1.7	13.1	0.14	1.0	11.1	0.08	1.1	14.5	0.09	12.87	1.71	0.10	0.03	-6.99
1.9-18	807.513	3.66	A09	Leu	A16	233	53.0	26.3	6.10	62.5	27.7	7.95	55.1	33.6	6.48	29.19	3.88	6.84	0.97	-5.16
1.9-19	820.533	5.26	A09	Leu	A17	275	1.9	15.4	0.16	1.0	13.2	0.08	1.0	16.7	0.08	15.13	1.76	0.11	0.05	-6.97
1.9-20	822.512	4.54	A09	Leu	A18	274	3.8	15.6	0.32	2.3	14.1	0.19	2.3	17.7	0.19	15.77	1.82	0.23	0.07	-6.64
1.9-21	824.539	3.91	A09	Leu	A19	252	39.5	17.6	4.06	48.9	18.2	5.44	42.3	20.5	4.45	18.80	1.53	4.65	0.71	-5.33
1.9-22	826.486	4.81	A09	Phe	A13	271	1.7	18.8	0.14	1.1	15.7	0.09	1.1	20.3	0.09	18.25	2.37	0.11	0.03	-6.97
1.9-23	827.539	2.62	A09	Leu	A20	247	18.1	57.6	1.62	25.3	58.7	2.36	21.1	65.9	1.91	60.72	4.51	1.96	0.37	-5.71
1.9-24	832.533	5.42	A09	Phe	A14	281	0.7	27.9	0.06	0.5	23.9	0.04	0.4	30.8	0.03	27.54	3.47	0.04	0.01	-7.35
1.9-25	834.512	3.65	A09	Phe	A15	258	32.7	7.9	3.21	39.6	7.6	4.08	34.5	8.8	3.43	8.13	0.60	3.57	0.45	-5.45
1.9-26	841.497	3.98	A09	Phe	A16	236	25.9	11.7	2.42	29.9	11.1	2.88	28.7	13.0	2.74	11.95	0.97	2.68	0.23	-5.57
1.9-27	844.497	4.01	A09	2-Nal	A11	269	3.0	12.2	0.24	0.9	10.3	0.07	0.7	13.3	0.06	11.95	1.50	0.13	0.10	-6.90
1.9-28	854.517	5.59	A09	Phe	A17	274	0.8	26.3	0.07	0.4	23.2	0.03	0.5	29.0	0.04	26.17	2.86	0.05	0.02	-7.34
1.9-29	856.497	4.86	A09	Phe	A18	274	1.4	24.5	0.11	0.6	23.2	0.05	0.7	29.3	0.05	25.66	3.21	0.07	0.03	-7.14
1.9-30	856.533	5.92	A09	2-Nal	A12	281	0.2	37.1	0.02	0.1	36.7	0.01	0.1	41.5	0.01	38.44	2.69	0.01	0.01	-7.96
1.9-31	858.524	4.24	A09	Phe	A19	253	23.0	9.2	2.12	26.9	8.9	2.54	24.2	10.1	2.24	9.41	0.65	2.30	0.22	-5.64
1.9-32	861.523	2.94	A09	Phe	A20	249	17.9	35.2	1.59	24.9	34.0	2.32	20.8	41.1	1.89	36.76	3.78	1.93	0.36	-5.71
1.9-33	876.502	5.72	A09	2-Nal	A13	278	0.2	52.2	0.02	0.1	44.9	0.01	0.1	48.5	0.01	48.53	3.68	0.01	0.01	-7.88
1.9-34	882.549	6.33	A09	2-Nal	A14	288	0.0	61.7	0.00	0.0	52.7	0.00	0.0	62.4	0.00	58.92	5.44	0.00	0.00	—
1.9-35	884.528	4.56	A09	2-Nal	A15	266	4.2	15.4	0.35	2.1	13.0	0.17	1.9	15.7	0.16	14.69	1.48	0.23	0.11	-6.64
1.9-36	891.513	4.89	A09	2-Nal	A16	245	3.1	19.8	0.25	0.4	17.1	0.03	0.8	20.3	0.07	19.06	1.71	0.12	0.12	-6.93
1.9-37	904.533	6.50	A09	2-Nal	A17	281	0.0	48.4	0.00	0.0	41.5	0.00	0.0	48.9	0.00	46.27	4.12	0.00	0.00	—
1.9-38	906.512	5.77	A09	2-Nal	A18	281	0.1	47.1	0.01	0.0	40.3	0.00	0.1	47.0	0.00	44.79	3.91	0.01	0.00	-8.27
1.9-39	908.539	5.15	A09	2-Nal	A19	262	3.0	14.2	0.25	1.1	12.3	0.09	1.1	14.5	0.09	13.65	1.19	0.14	0.09	-6.85
1.9-40	911.539	3.85	A09	2-Nal	A20	258	6.8	8.5	0.57	4.5	7.8	0.37	4.3	8.3	0.36	8.20	0.35	0.43	0.12	-6.36

Table S1.9. PAMPA parameters of Sub-library 1.9

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
1.10-01	751.450	1.59	A10	Ala	A11	224	3.6	93.9	0.29	4.0	94.8	0.33	3.8	94.9	0.31	94.55	0.58	0.31	0.02	-6.51
1.10-02	763.487	3.50	A10	Ala	A12	243	60.7	67.2	7.57	65.0	72.2	8.50	66.1	74.8	8.76	71.43	3.86	8.28	0.63	-5.08
1.10-03	783.455	3.30	A10	Ala	A13	239	47.3	57.9	5.19	50.0	61.0	5.61	51.6	61.9	5.88	60.27	2.14	5.56	0.35	-5.26
1.10-04	789.502	3.90	A10	Ala	A14	250	69.6	35.8	9.64	72.7	39.0	10.51	74.1	41.5	10.93	38.75	2.83	10.36	0.66	-4.98
1.10-05	791.481	2.14	A10	Ala	A15	223	2.5	94.9	0.20	2.8	96.8	0.23	2.7	97.0	0.22	96.22	1.11	0.22	0.01	-6.67
1.10-06	793.497	2.82	A10	Leu	A11	245	48.6	62.7	5.39	53.8	68.1	6.25	53.7	71.4	6.23	67.41	4.40	5.96	0.49	-5.23
1.10-07	798.466	2.47	A10	Ala	A16	205	1.9	99.3	0.16	2.3	104.5	0.19	2.0	105.7	0.16	103.19	3.40	0.17	0.01	-6.77
1.10-08	805.533	4.73	A10	Leu	A12	263	25.6	9.2	2.39	27.6	9.4	2.62	28.8	9.6	2.75	9.38	0.21	2.59	0.18	-5.59
1.10-09	811.487	4.08	A10	Ala	A17	245	59.5	42.7	7.31	66.1	45.7	8.76	67.7	49.8	9.15	46.08	3.55	8.41	0.97	-5.08
1.10-10	813.466	3.35	A10	Ala	A18	243	36.2	38.4	3.64	40.9	39.4	4.26	42.4	42.3	4.46	40.04	1.98	4.12	0.43	-5.38
1.10-11	815.493	2.73	A10	Ala	A19	222	2.4	94.1	0.20	3.1	94.8	0.25	2.5	95.0	0.21	94.65	0.49	0.22	0.03	-6.66
1.10-12	818.492	1.43	A10	Ala	A20	217	0.4	98.4	0.03	0.5	105.3	0.04	0.4	109.3	0.03	104.30	5.52	0.04	0.00	-7.45
1.10-13	825.502	4.53	A10	Leu	A13	259	22.9	13.2	2.11	23.4	13.4	2.16	25.0	14.2	2.33	13.62	0.54	2.20	0.12	-5.66
1.10-14	827.481	3.14	A10	Phe	A11	247	45.4	36.0	4.89	51.1	36.7	5.79	52.2	39.5	5.97	37.39	1.89	5.55	0.58	-5.26
1.10-15	831.549	5.14	A10	Leu	A14	271	5.3	13.4	0.44	6.2	13.3	0.52	6.2	13.4	0.52	13.38	0.07	0.49	0.05	-6.31
1.10-16	833.528	3.37	A10	Leu	A15	242	37.9	65.9	3.85	42.1	71.1	4.43	41.3	73.1	4.31	70.02	3.72	4.20	0.30	-5.38
1.10-17	839.518	5.06	A10	Phe	A12	263	0.0	14.5	0.00	0.0	13.9	0.00	4.5	14.7	0.37	14.37	0.40	0.12	0.22	-6.90
1.10-18	840.513	3.70	A10	Leu	A16	220	24.5	73.6	2.28	29.5	75.0	2.83	27.8	77.0	2.64	75.19	1.74	2.58	0.28	-5.59
1.10-19	853.533	5.31	A10	Leu	A17	263	5.7	15.8	0.48	7.5	15.4	0.63	7.2	16.0	0.61	15.73	0.30	0.57	0.08	-6.24
1.10-20	855.513	4.58	A10	Leu	A18	260	5.9	18.7	0.50	8.8	17.8	0.74	6.5	19.1	0.54	18.53	0.64	0.59	0.13	-6.23
1.10-21	857.540	3.96	A10	Leu	A19	239	18.2	66.1	1.63	21.7	68.9	1.98	20.5	70.2	1.86	68.40	2.09	1.82	0.18	-5.74
1.10-22	859.487	4.86	A10	Phe	A13	260	3.7	24.0	0.31	4.6	23.0	0.38	4.4	24.5	0.36	23.83	0.78	0.35	0.04	-6.46
1.10-23	860.539	2.66	A10	Leu	A20	233	5.2	96.0	0.43	7.0	98.6	0.59	5.8	102.3	0.49	98.94	3.13	0.50	0.08	-6.30
1.10-24	865.533	5.46	A10	Phe	A14	271	1.0	27.8	0.08	1.7	26.5	0.14	1.5	27.2	0.12	27.17	0.64	0.11	0.03	-6.95
1.10-25	867.513	3.69	A10	Phe	A15	245	36.2	36.8	3.64	40.7	38.8	4.23	40.5	42.1	4.21	39.23	2.71	4.03	0.34	-5.40
1.10-26	874.497	4.03	A10	Phe	A16	223	20.3	44.7	1.84	23.4	46.7	2.16	23.5	47.1	2.16	46.17	1.31	2.05	0.19	-5.69
1.10-27	877.497	4.05	A10	2-Nal	A11	256	7.0	17.4	0.58	8.3	18.3	0.70	8.6	19.2	0.73	18.30	0.92	0.67	0.08	-6.17
1.10-28	887.518	5.63	A10	Phe	A17	263	0.0	25.3	0.00	0.0	25.0	0.00	0.0	25.4	0.00	25.22	0.19	0.00	0.00	—
1.10-29	889.497	4.90	A10	Phe	A18	262	1.5	28.4	0.12	2.7	28.7	0.22	1.7	29.0	0.14	28.69	0.33	0.16	0.05	-6.79
1.10-30	889.533	5.97	A10	2-Nal	A12	271	0.1	39.6	0.01	0.3	38.4	0.03	0.1	38.4	0.01	38.78	0.67	0.02	0.01	-7.80
1.10-31	891.524	4.28	A10	Phe	A19	240	20.8	39.0	1.89	24.3	39.9	2.26	23.7	41.1	2.19	39.98	1.01	2.11	0.20	-5.68
1.10-32	894.524	2.99	A10	Phe	A20	236	10.2	80.3	0.87	12.6	86.5	1.09	11.3	88.3	0.97	85.00	4.18	0.98	0.11	-6.01
1.10-33	909.502	5.76	A10	2-Nal	A13	268	0.4	50.7	0.04	0.8	49.5	0.07	0.4	48.9	0.03	49.68	0.90	0.05	0.02	-7.34
1.10-34	915.549	6.37	A10	2-Nal	A14	278	0.2	53.9	0.01	0.2	53.5	0.02	0.1	51.7	0.01	53.04	1.20	0.01	0.00	-7.83
1.10-35	917.528	4.60	A10	2-Nal	A15	254	5.1	18.8	0.42	6.8	18.0	0.57	6.5	19.9	0.54	18.88	0.91	0.51	0.08	-6.29
1.10-36	924.513	4.93	A10	2-Nal	A16	233	4.3	21.1	0.36	5.1	20.5	0.42	4.7	22.9	0.39	21.50	1.23	0.39	0.03	-6.41
1.10-37	937.533	6.54	A10	2-Nal	A17	271	0.2	48.4	0.01	0.3	45.9	0.02	0.2	46.2	0.01	46.79	1.36	0.02	0.00	-7.80
1.10-38	939.513	5.81	A10	2-Nal	A18	271	0.2	46.7	0.02	0.4	44.7	0.03	0.2	46.4	0.02	45.93	1.06	0.02	0.01	-7.68
1.10-39	941.540	5.19	A10	2-Nal	A19	249	2.6	18.8	0.21	3.9	17.8	0.32	3.0	19.4	0.25	18.65	0.80	0.26	0.06	-6.58
1.10-40	944.539	3.90	A10	2-Nal	A20	245	9.2	27.5	0.78	11.3	27.4	0.97	9.9	29.2	0.85	28.02	0.98	0.87	0.10	-6.06

Table S1.10. PAMPA parameters of Sub-library 1.10

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

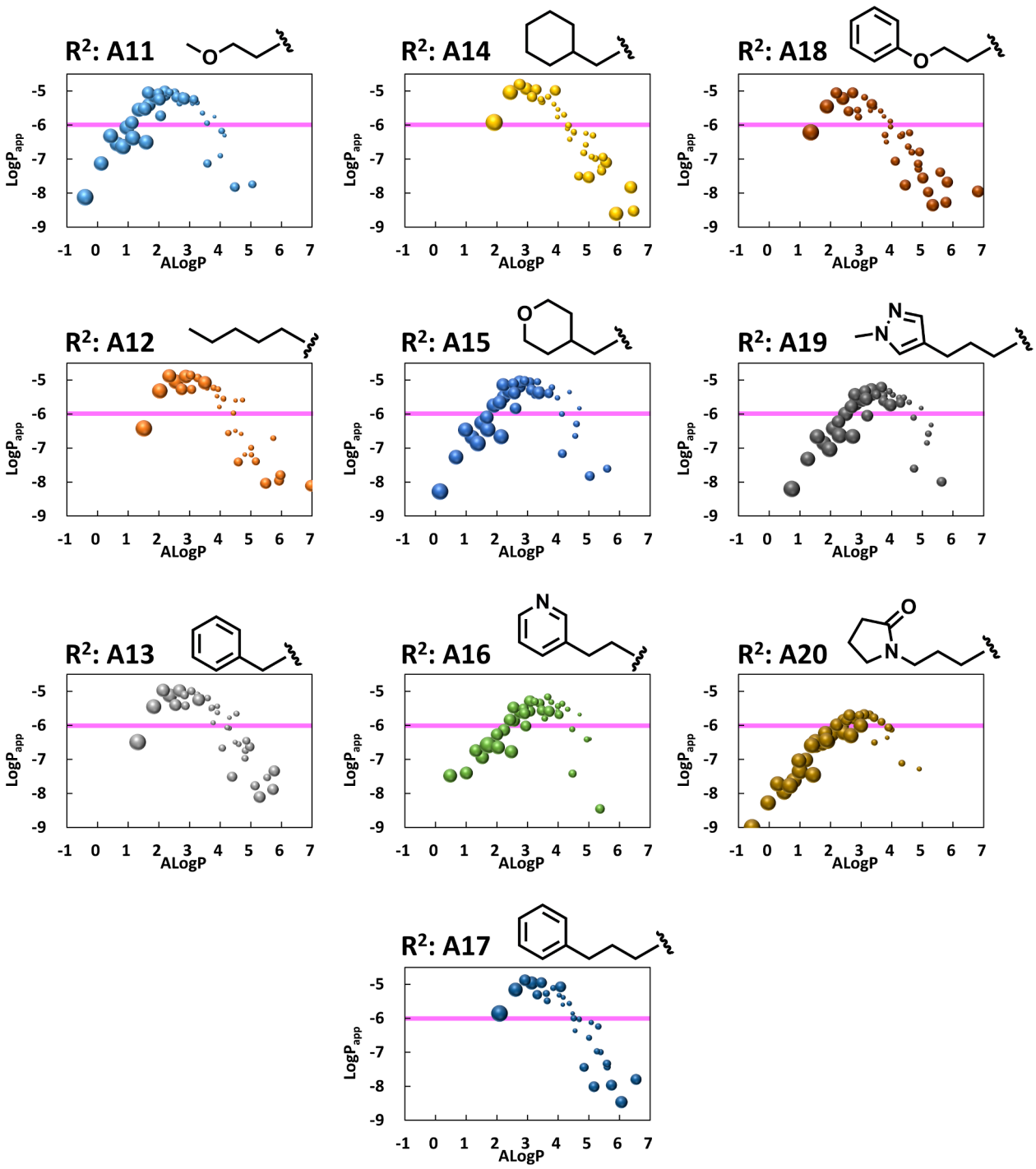


Figure S6. Scatter plot of Library 1 grouped by **R**^{2} structures

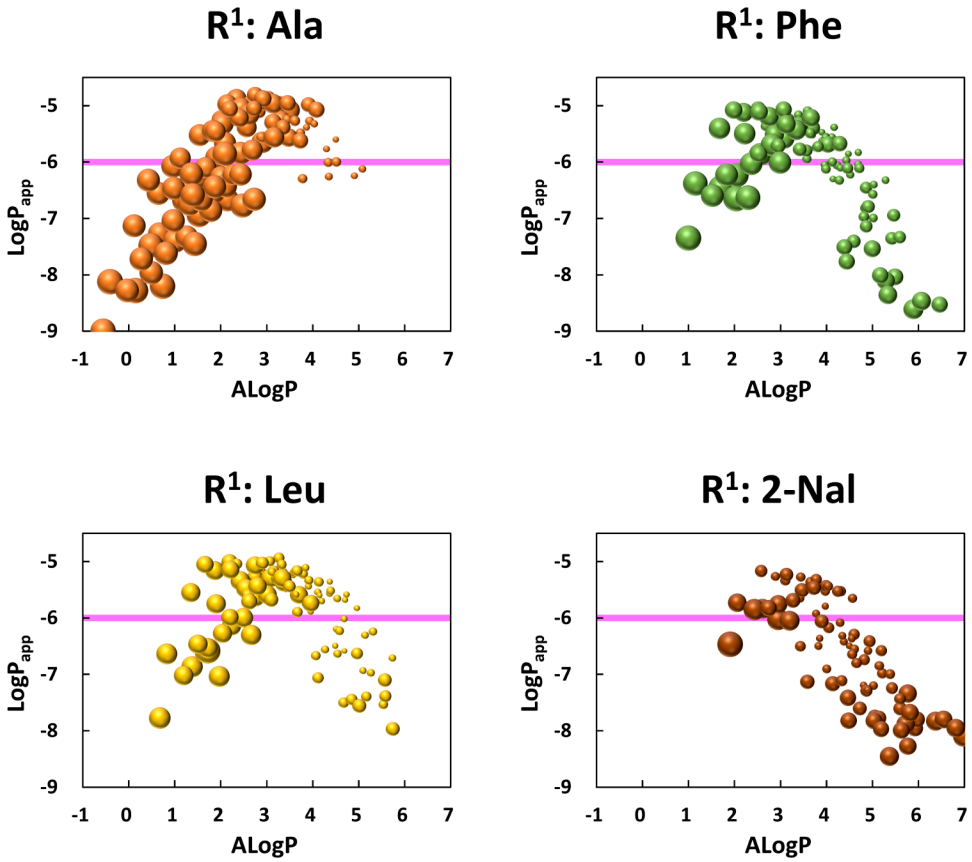


Figure S7. Scatter plot of Library 1 grouped by R^1 structures

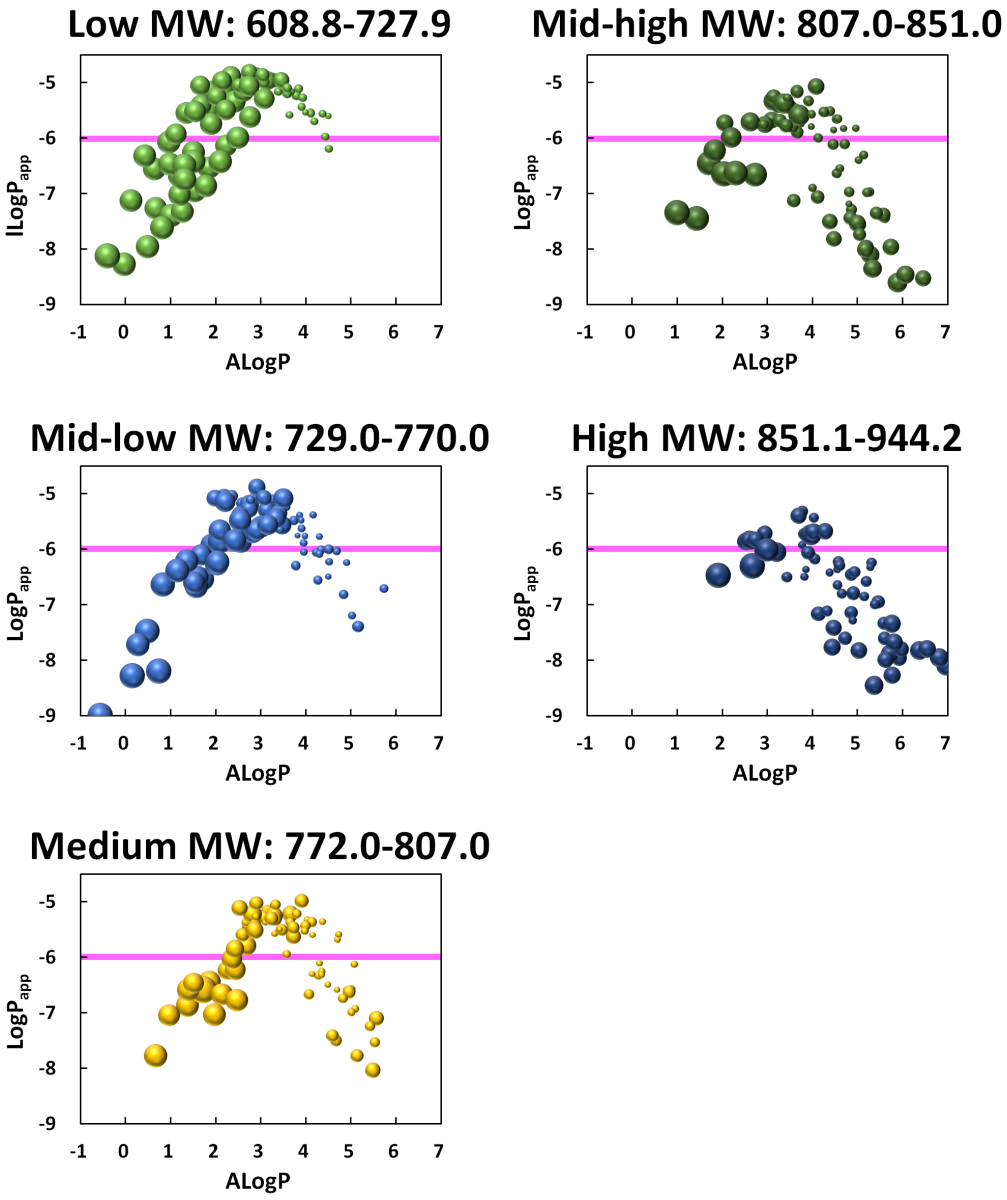


Figure S8. Scatter plot of Library 1 grouped by MW

2.3 PAMPA results of Library-2

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.1-01Me	621.433	2.03	A01	Ala	A12	228	29.7	78.6	2.87	28.9	75.4	2.78	30.1	73.8	2.92	75.9	2.5	2.85	0.07	-5.54
2.1-02Me	647.449	2.44	A01	Ala	A14	234	58.9	67.4	7.26	56.3	68.7	6.74	58.8	66.6	7.22	67.6	1.0	7.07	0.29	-5.15
2.1-03Me	649.428	0.67	A01	Ala	A15	206	0.9	80.8	0.08	0.8	79.5	0.06	0.8	79.7	0.06	80.0	0.7	0.07	0.01	-7.17
2.1-04Me	693.491	2.34	A04	Ala	A12	240	72.5	63.5	10.52	69.9	63.5	9.79	71.6	63.4	10.25	63.4	0.0	10.19	0.37	-4.99
2.1-05Me	697.465	3.59	A01	Phe	A12	250	76.2	23.4	11.71	80.5	26.1	13.32	81.9	27.4	13.94	25.6	2.0	12.99	1.15	-4.89
2.1-06Me	719.507	2.75	A04	Ala	A14	247	83.6	57.2	14.73	81.7	59.7	13.83	85.3	61.1	15.65	59.4	2.0	14.74	0.91	-4.83
2.1-07Me	721.486	0.98	A04	Ala	A15	217	3.3	77.8	0.27	2.7	80.5	0.23	2.8	80.9	0.23	79.7	1.7	0.25	0.03	-6.61
2.1-08Me	723.480	3.99	A01	Phe	A14	257	56.9	14.7	6.86	68.8	17.2	9.50	67.7	18.3	9.22	16.7	1.9	8.53	1.45	-5.07
2.1-09Me	725.460	2.22	A01	Phe	A15	228	34.7	72.6	3.47	33.0	71.4	3.26	35.2	69.5	3.54	71.1	1.5	3.42	0.14	-5.47
2.1-10Me	727.439	3.04	A08	Ala	A12	240	80.1	39.1	13.15	79.0	40.1	12.72	79.8	40.9	13.06	40.0	0.9	12.98	0.22	-4.89
2.1-11Me	753.455	3.44	A08	Ala	A14	247	75.9	23.9	11.60	75.1	25.7	11.34	78.6	26.9	12.56	25.5	1.5	11.83	0.64	-4.93
2.1-12Me	755.434	1.67	A08	Ala	A15	221	14.5	74.3	1.28	12.3	75.4	1.07	13.1	74.1	1.15	74.6	0.7	1.17	0.11	-5.93
2.1-13Me	769.522	3.90	A04	Phe	A12	260	55.5	14.6	6.61	68.1	17.3	9.32	67.8	18.9	9.24	16.9	2.2	8.39	1.54	-5.08
2.1-14Me	795.538	4.30	A04	Phe	A14	266	26.9	10.4	2.55	42.0	11.7	4.44	47.3	11.6	5.22	11.2	0.7	4.07	1.37	-5.39
2.1-15Me	797.517	2.53	A04	Phe	A15	239	66.4	56.9	8.89	63.0	58.4	8.09	65.5	57.9	8.68	57.8	0.7	8.55	0.41	-5.07
2.1-16Me	803.470	4.59	A08	Phe	A12	260	5.8	8.5	0.48	11.2	9.0	0.97	13.1	8.5	1.14	8.7	0.3	0.87	0.34	-6.06
2.1-17Me	829.486	5.00	A08	Phe	A14	266	0.8	12.0	0.07	2.9	11.8	0.24	4.4	10.9	0.36	11.6	0.6	0.22	0.15	-6.65
2.1-18Me	831.465	3.23	A08	Phe	A15	240	68.1	25.1	9.32	66.7	26.7	8.96	69.4	27.3	9.66	26.4	1.2	9.31	0.35	-5.03
2.1-01H	607.418	1.83	A01	Ala	A12	214	2.4	76.6	0.20	2.0	79.0	0.17	2.0	77.9	0.16	77.8	1.2	0.18	0.02	-6.76
2.1-02H	633.433	2.23	A01	Ala	A14	219	5.3	79.1	0.45	4.6	79.9	0.38	4.8	78.7	0.40	79.2	0.6	0.41	0.03	-6.39
2.1-03H	635.413	0.46	A01	Ala	A15	194	0.1	80.1	0.01	0.1	78.3	0.01	0.1	80.3	0.01	79.6	1.1	0.01	0.00	-8.00
2.1-04H	679.475	2.14	A04	Ala	A12	227	9.2	81.7	0.79	8.6	79.7	0.74	9.2	79.0	0.78	80.1	1.4	0.77	0.03	-6.11
2.1-05H	683.449	3.38	A01	Phe	A12	236	52.8	64.1	6.11	49.2	68.5	5.52	52.7	65.5	6.10	66.0	2.3	5.91	0.34	-5.23
2.1-06H	705.491	2.54	A04	Ala	A14	232	21.2	79.3	1.94	20.5	77.4	1.87	22.8	74.0	2.11	76.9	2.7	1.97	0.12	-5.70
2.1-07H	707.470	0.77	A04	Ala	A15	206	0.4	83.1	0.03	0.3	80.1	0.02	0.3	81.2	0.03	81.5	1.5	0.03	0.00	-7.57
2.1-08H	709.465	3.79	A01	Phe	A14	240	70.9	53.2	10.05	70.1	55.7	9.84	72.0	56.7	10.37	55.2	1.8	10.09	0.27	-5.00
2.1-09H	711.444	2.02	A01	Phe	A15	215	6.0	76.8	0.50	4.5	80.6	0.38	4.9	78.7	0.41	78.7	1.9	0.43	0.07	-6.37
2.1-10H	713.423	2.83	A08	Ala	A12	228	33.2	76.1	3.29	31.2	74.9	3.05	32.7	73.2	3.23	74.7	1.5	3.19	0.12	-5.50
2.1-11H	739.439	3.23	A08	Ala	A14	234	55.1	65.3	6.52	52.9	65.7	6.14	56.2	64.0	6.73	65.0	0.9	6.47	0.30	-5.19
2.1-12H	741.418	1.46	A08	Ala	A15	208	3.9	82.1	0.33	3.1	78.8	0.26	3.3	83.4	0.27	81.4	2.4	0.29	0.04	-6.54
2.1-13H	755.507	3.69	A04	Phe	A12	247	75.6	53.4	11.49	75.9	58.0	11.59	80.2	60.1	13.21	57.2	3.4	12.10	0.96	-4.92
2.1-14H	781.522	4.10	A04	Phe	A14	250	75.0	38.4	11.31	82.9	42.9	14.40	84.4	43.5	15.14	41.6	2.8	13.62	2.04	-4.87
2.1-15H	783.501	2.33	A04	Phe	A15	228	11.4	80.8	0.98	10.0	78.8	0.86	10.6	77.8	0.91	79.2	1.5	0.92	0.06	-6.04
2.1-16H	789.455	4.39	A08	Phe	A12	247	58.3	23.0	7.13	62.2	25.5	7.94	67.8	27.2	9.22	25.2	2.1	8.10	1.06	-5.09
2.1-17H	815.470	4.79	A08	Phe	A14	250	29.2	14.0	2.81	40.1	15.6	4.18	43.8	16.1	4.70	15.2	1.1	3.90	0.97	-5.41
2.1-18H	817.449	3.02	A08	Phe	A15	228	44.2	62.9	4.76	41.0	63.2	4.31	44.0	62.5	4.72	62.9	0.3	4.60	0.25	-5.34

Table S2.1. PAMPA parameters of Sub-library 2.1

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.2-01Me	621.433	2.03	A01	Ala	A12	235	39.0	84.5	4.03	39.7	82.5	4.12	37.4	80.0	3.82	82.3	2.3	3.99	0.16	-5.40
2.2-02Me	647.449	2.44	A01	Ala	A14	242	67.0	75.4	9.05	66.3	78.1	8.87	65.3	75.2	8.62	76.2	1.6	8.85	0.21	-5.05
2.2-03Me	649.428	0.67	A01	Ala	A15	212	2.1	103.6	0.17	2.2	101.6	0.18	2.0	100.9	0.16	102.0	1.4	0.17	0.01	-6.76
2.2-04Me	693.491	2.34	A04	Ala	A12	249	74.7	62.0	11.21	72.6	64.4	10.55	71.0	62.5	10.09	63.0	1.2	10.62	0.56	-4.97
2.2-05Me	697.465	3.59	A01	Phe	A12	259	68.0	18.6	9.29	67.9	18.8	9.26	65.9	19.0	8.77	18.8	0.2	9.11	0.29	-5.04
2.2-06Me	719.507	2.75	A04	Ala	A14	256	81.2	45.3	13.60	79.4	46.8	12.87	79.1	46.6	12.77	46.2	0.8	13.08	0.46	-4.88
2.2-07Me	721.486	0.98	A04	Ala	A15	227	7.7	99.8	0.66	7.7	99.2	0.65	7.5	95.4	0.64	98.1	2.4	0.65	0.01	-6.19
2.2-08Me	723.480	3.99	A01	Phe	A14	267	44.2	9.0	4.76	39.1	9.6	4.04	38.6	9.4	3.98	9.3	0.3	4.26	0.44	-5.37
2.2-09Me	725.460	2.22	A01	Phe	A15	236	56.2	70.0	6.73	56.1	73.6	6.70	53.8	72.1	6.29	71.9	1.8	6.58	0.24	-5.18
2.2-10Me	727.439	3.04	A08	Ala	A12	247	77.2	39.2	12.05	77.9	38.9	12.31	77.6	37.5	12.18	38.6	0.9	12.18	0.13	-4.91
2.2-11Me	753.455	3.44	A08	Ala	A14	252	62.6	16.6	8.03	61.1	17.1	7.69	58.6	17.2	7.19	17.0	0.3	7.64	0.42	-5.12
2.2-12Me	755.434	1.67	A08	Ala	A15	226	30.2	91.2	2.93	30.0	91.6	2.90	28.7	89.5	2.75	90.8	1.1	2.86	0.10	-5.54
2.2-13Me	769.522	3.90	A04	Phe	A12	271	36.6	9.4	3.71	34.1	9.9	3.40	29.4	9.7	2.84	9.7	0.3	3.32	0.44	-5.48
2.2-14Me	795.538	4.30	A04	Phe	A14	278	18.5	7.6	1.67	16.1	8.6	1.43	12.0	8.4	1.04	8.2	0.6	1.38	0.32	-5.86
2.2-15Me	797.517	2.53	A04	Phe	A15	250	73.6	46.9	10.86	71.4	49.1	10.20	67.9	48.0	9.26	48.0	1.1	10.11	0.80	-5.00
2.2-16Me	803.470	4.59	A08	Phe	A12	266	3.9	6.5	0.33	2.1	8.4	0.17	1.8	7.8	0.15	7.5	1.0	0.21	0.10	-6.67
2.2-17Me	829.486	5.00	A08	Phe	A14	274	1.2	14.9	0.09	0.3	16.1	0.02	0.4	16.6	0.03	15.9	0.9	0.05	0.04	-7.31
2.2-18Me	831.465	3.23	A08	Phe	A15	247	56.9	16.3	6.87	54.7	17.3	6.46	51.8	17.0	5.95	16.9	0.5	6.43	0.46	-5.19
2.2-02H	607.418	1.83	A01	Ala	A12	219	3.6	99.0	0.30	3.7	100.2	0.30	3.6	94.8	0.30	98.0	2.8	0.30	0.00	-6.52
2.2-03H	633.433	2.23	A01	Ala	A14	226	9.4	98.2	0.81	9.3	98.8	0.80	8.6	97.4	0.73	98.1	0.7	0.78	0.04	-6.11
2.2-04H	635.413	0.46	A01	Ala	A15	200	0.3	98.9	0.02	0.3	104.7	0.02	0.3	96.4	0.02	100.0	4.3	0.02	0.00	-7.62
2.2-05H	679.475	2.14	A04	Ala	A12	234	16.7	88.4	1.49	16.8	86.0	1.50	15.2	83.4	1.35	86.0	2.5	1.45	0.09	-5.84
2.2-06H	683.449	3.38	A01	Phe	A12	240	61.1	75.9	7.70	60.7	78.7	7.61	58.4	75.1	7.15	76.6	1.9	7.48	0.30	-5.13
2.2-07H	705.491	2.54	A04	Ala	A14	239	33.2	84.7	3.29	33.7	85.6	3.35	31.7	83.7	3.10	84.7	1.0	3.25	0.13	-5.49
2.2-08H	707.470	0.77	A04	Ala	A15	216	1.2	105.1	0.10	1.2	105.1	0.10	1.1	101.4	0.09	103.9	2.1	0.10	0.00	-7.00
2.2-09H	709.465	3.79	A01	Phe	A14	247	75.6	52.4	11.50	73.7	55.2	10.88	71.7	53.2	10.30	53.6	1.5	10.89	0.60	-4.96
2.2-10H	711.444	2.02	A01	Phe	A15	223	13.9	99.0	1.22	13.0	102.9	1.13	12.1	100.8	1.05	100.9	1.9	1.13	0.08	-5.95
2.2-11H	713.423	2.83	A08	Ala	A12	232	45.6	85.0	4.96	45.9	82.2	5.00	42.4	78.4	4.50	81.9	3.3	4.82	0.28	-5.32
2.2-12H	739.439	3.23	A08	Ala	A14	236	63.0	67.5	8.09	62.8	70.3	8.07	60.2	68.5	7.52	68.8	1.4	7.89	0.33	-5.10
2.2-13H	741.418	1.46	A08	Ala	A15	215	5.7	104.5	0.48	5.7	105.3	0.47	5.0	102.9	0.42	104.2	1.2	0.46	0.03	-6.34
2.2-14H	755.507	3.69	A04	Phe	A12	253	76.6	45.1	11.86	74.5	47.5	11.13	72.1	46.5	10.41	46.4	1.2	11.13	0.72	-4.95
2.2-15H	781.522	4.10	A04	Phe	A14	259	70.3	27.2	9.89	68.9	27.3	9.51	65.8	27.0	8.73	27.2	0.1	9.38	0.59	-5.03
2.2-16H	783.501	2.33	A04	Phe	A15	236	36.8	79.7	3.74	37.2	82.7	3.79	34.8	80.7	3.49	81.0	1.5	3.67	0.16	-5.44
2.2-17H	789.455	4.39	A08	Phe	A12	249	54.6	20.0	6.44	50.0	20.5	5.66	47.3	20.4	5.22	20.3	0.3	5.77	0.61	-5.24
2.2-18H	815.470	4.79	A08	Phe	A14	256	24.7	13.4	2.32	20.7	15.1	1.89	17.7	14.8	1.58	14.4	1.0	1.93	0.37	-5.71
2.2-19H	817.449	3.02	A08	Phe	A15	236	63.1	61.2	8.13	63.2	61.9	8.15	59.4	59.3	7.34	60.8	1.4	7.87	0.46	-5.10

Table S2.2. PAMPA parameters of Sub-library 2.2

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.3-01Me	621.433	2.03	A01	Ala	A12	223	19.1	80.6	1.73	18.6	80.3	1.68	19.8	82.5	1.80	81.1	1.2	1.74	0.06	-5.76
2.3-02Me	647.449	2.44	A01	Ala	A14	230	45.7	70.7	4.98	43.5	72.0	4.66	45.0	75.3	4.87	72.7	2.4	4.84	0.16	-5.32
2.3-03Me	649.428	0.67	A01	Ala	A15	202	0.4	86.7	0.03	0.3	84.0	0.03	0.3	94.2	0.03	88.3	5.3	0.03	0.00	-7.56
2.3-04Me	693.491	2.34	A04	Ala	A12	234	52.4	71.9	6.04	50.0	74.3	5.65	52.7	77.4	6.10	74.5	2.7	5.93	0.24	-5.23
2.3-05Me	697.465	3.59	A01	Phe	A12	230	53.6	56.0	6.25	50.9	59.7	5.80	51.8	62.6	5.95	59.4	3.3	6.00	0.23	-5.22
2.3-06Me	719.507	2.75	A04	Ala	A14	241	74.3	59.1	11.08	70.5	61.1	9.94	74.0	64.0	10.96	61.4	2.5	10.66	0.63	-4.97
2.3-07Me	721.486	0.98	A04	Ala	A15	215	1.1	85.3	0.09	1.0	85.6	0.08	1.2	83.9	0.10	84.9	0.9	0.09	0.01	-7.04
2.3-08Me	723.480	3.99	A01	Phe	A14	239	62.7	41.4	8.04	60.5	43.3	7.57	64.4	47.2	8.41	44.0	3.0	8.00	0.42	-5.10
2.3-09Me	725.460	2.22	A01	Phe	A15	207	2.2	84.6	0.18	2.2	80.2	0.19	2.3	81.9	0.19	82.2	2.2	0.19	0.01	-6.73
2.3-10Me	727.439	3.04	A08	Ala	A12	236	58.7	49.2	7.21	56.5	52.1	6.79	61.2	53.2	7.72	51.5	2.1	7.24	0.47	-5.14
2.3-11Me	753.455	3.44	A08	Ala	A14	241	64.1	30.8	8.36	59.2	32.9	7.31	66.1	35.5	8.82	33.1	2.4	8.17	0.78	-5.09
2.3-12Me	755.434	1.67	A08	Ala	A15	215	3.6	77.9	0.30	3.2	79.3	0.27	3.7	82.9	0.31	80.0	2.6	0.29	0.02	-6.54
2.3-13Me	769.522	3.90	A04	Phe	A12	241	63.1	36.9	8.12	55.8	39.1	6.65	68.5	41.7	9.42	39.2	2.4	8.06	1.38	-5.09
2.3-14Me	795.538	4.30	A04	Phe	A14	248	61.2	24.5	7.72	56.3	24.4	6.76	67.5	27.7	9.17	25.5	1.9	7.88	1.21	-5.10
2.3-15Me	797.517	2.53	A04	Phe	A15	218	6.5	80.0	0.55	6.2	81.9	0.52	6.5	85.9	0.55	82.6	3.0	0.54	0.02	-6.27
2.3-16Me	803.470	4.59	A08	Phe	A12	241	32.9	14.7	3.25	27.4	15.0	2.60	35.5	16.9	3.57	15.5	1.2	3.14	0.49	-5.50
2.3-17Me	829.486	5.00	A08	Phe	A14	247	13.0	16.3	1.13	9.6	16.9	0.82	15.6	17.6	1.38	16.9	0.6	1.11	0.28	-5.95
2.3-18Me	831.465	3.23	A08	Phe	A15	218	7.8	68.9	0.66	7.9	67.7	0.67	8.3	71.5	0.71	69.4	2.0	0.68	0.02	-6.17
2.3-01H	607.418	1.83	A01	Ala	A12	212	3.9	83.7	0.33	3.7	87.0	0.31	4.1	84.8	0.35	85.1	1.7	0.33	0.02	-6.48
2.3-02H	633.433	2.23	A01	Ala	A14	217	4.2	84.7	0.35	3.5	85.7	0.29	4.1	87.4	0.34	85.9	1.3	0.33	0.03	-6.48
2.3-03H	635.413	0.46	A01	Ala	A15	188	0.0	87.8	0.00	0.0	87.3	0.00	0.0	90.4	0.00	88.5	1.7	0.00	0.00	-8.88
2.3-04H	679.475	2.14	A04	Ala	A12	222	4.3	82.2	0.36	4.0	83.2	0.33	4.4	84.7	0.37	83.4	1.3	0.35	0.02	-6.45
2.3-05H	683.449	3.38	A01	Phe	A12	230	32.7	66.1	3.23	28.0	70.3	2.68	30.4	73.9	2.95	70.1	3.9	2.95	0.28	-5.53
2.3-06H	705.491	2.54	A04	Ala	A14	230	13.7	74.3	1.20	11.3	78.2	0.98	12.7	82.2	1.10	78.2	4.0	1.10	0.11	-5.96
2.3-07H	707.470	0.77	A04	Ala	A15	202	0.2	87.4	0.01	0.1	84.9	0.01	0.2	92.5	0.01	88.3	3.9	0.01	0.00	-7.92
2.3-08H	709.465	3.79	A01	Phe	A14	234	48.9	59.6	5.48	43.9	62.8	4.71	49.8	66.5	5.61	63.0	3.5	5.27	0.48	-5.28
2.3-09H	711.444	2.02	A01	Phe	A15	206	0.7	88.1	0.06	0.6	86.2	0.05	0.7	90.9	0.06	88.4	2.3	0.06	0.00	-7.24
2.3-10H	713.423	2.83	A08	Ala	A12	225	21.9	73.9	2.02	21.7	76.7	2.00	23.7	76.0	2.21	75.5	1.5	2.07	0.12	-5.68
2.3-11H	739.439	3.23	A08	Ala	A14	230	41.9	48.6	4.43	34.4	51.1	3.44	40.7	53.9	4.26	51.2	2.7	4.04	0.53	-5.39
2.3-12H	741.418	1.46	A08	Ala	A15	204	1.2	87.3	0.10	1.0	84.9	0.08	1.2	90.4	0.10	87.5	2.7	0.09	0.01	-7.03
2.3-13H	755.507	3.69	A04	Phe	A12	240	49.2	50.6	5.51	42.4	52.4	4.50	49.2	56.5	5.51	53.2	3.0	5.18	0.59	-5.29
2.3-14H	781.522	4.10	A04	Phe	A14	246	59.3	38.2	7.32	54.0	38.8	6.32	62.1	43.4	7.92	40.1	2.9	7.19	0.80	-5.14
2.3-15H	783.501	2.33	A04	Phe	A15	218	1.8	84.5	0.15	1.6	86.1	0.13	1.8	86.6	0.15	85.8	1.1	0.14	0.01	-6.85
2.3-16H	789.455	4.39	A08	Phe	A12	240	40.5	19.6	4.24	32.8	20.6	3.24	43.5	23.0	4.65	21.1	1.7	4.04	0.73	-5.39
2.3-17H	815.470	4.79	A08	Phe	A14	245	25.5	17.3	2.40	19.1	18.6	1.73	28.8	20.3	2.77	18.7	1.5	2.30	0.53	-5.64
2.3-18H	817.449	3.02	A08	Phe	A15	219	8.4	73.1	0.71	7.2	76.8	0.61	8.5	77.5	0.72	75.8	2.4	0.68	0.06	-6.17

Table S2.3. PAMPA parameters of Sub-library 2.3

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.4-01Me	621.433	2.03	A01	Ala	A12	224	3.6	104.3	0.30	5.3	90.7	0.44	4.5	87.1	0.37	94.0	9.1	0.37	0.07	-6.43
2.4-02Me	647.449	2.44	A01	Ala	A14	230	9.9	100.1	0.85	14.2	87.7	1.25	11.9	83.5	1.03	90.4	8.6	1.04	0.20	-5.98
2.4-03Me	649.428	0.67	A01	Ala	A15	203	0.1	107.4	0.01	0.2	86.7	0.02	0.1	89.0	0.01	94.4	11.3	0.01	0.00	-7.92
2.4-04Me	693.491	2.34	A04	Ala	A12	238	14.9	99.0	1.31	20.6	84.1	1.88	18.4	80.8	1.66	88.0	9.7	1.62	0.28	-5.79
2.4-05Me	697.465	3.59	A01	Phe	A12	236	38.0	73.3	3.90	46.0	69.0	5.02	44.6	68.5	4.81	70.2	2.6	4.58	0.60	-5.34
2.4-06Me	719.507	2.75	A04	Ala	A14	244	28.6	82.2	2.75	37.3	71.3	3.81	35.8	71.6	3.61	75.0	6.2	3.39	0.56	-5.47
2.4-07Me	721.486	0.98	A04	Ala	A15	218	0.5	111.3	0.04	0.7	94.7	0.06	0.6	94.1	0.04	100.0	9.8	0.05	0.01	-7.33
2.4-08Me	723.480	3.99	A01	Phe	A14	243	52.8	50.1	6.12	56.9	45.1	6.86	61.5	50.6	7.77	48.6	3.1	6.92	0.83	-5.16
2.4-09Me	725.460	2.22	A01	Phe	A15	212	1.3	102.9	0.11	1.7	92.0	0.14	1.4	90.8	0.11	95.2	6.6	0.12	0.02	-6.92
2.4-10Me	727.439	3.04	A08	Ala	A12	236	32.8	67.1	3.25	35.9	66.8	3.62	37.6	62.2	3.84	65.4	2.7	3.57	0.30	-5.45
2.4-11Me	753.455	3.44	A08	Ala	A14	241	41.4	49.0	4.35	44.8	43.6	4.85	49.5	48.0	5.56	46.9	2.9	4.92	0.61	-5.31
2.4-12Me	755.434	1.67	A08	Ala	A15	218	2.3	104.0	0.19	3.1	92.8	0.26	2.5	92.3	0.21	96.4	6.6	0.22	0.03	-6.66
2.4-13Me	769.522	3.90	A04	Phe	A12	247	52.4	47.2	6.04	55.5	41.4	6.59	63.1	45.8	8.12	44.8	3.0	6.92	1.07	-5.16
2.4-14Me	795.538	4.30	A04	Phe	A14	252	59.2	28.8	7.30	44.3	23.3	4.76	67.3	30.1	9.11	27.4	3.6	7.06	2.18	-5.15
2.4-15Me	797.517	2.53	A04	Phe	A15	222	3.0	99.6	0.25	4.2	89.3	0.35	3.7	86.7	0.30	91.9	6.8	0.30	0.05	-6.52
2.4-16Me	803.470	4.59	A08	Phe	A12	245	37.4	17.7	3.82	28.3	16.1	2.71	39.4	18.1	4.08	17.3	1.0	3.53	0.73	-5.45
2.4-17Me	829.486	5.00	A08	Phe	A14	251	20.3	14.4	1.85	9.6	13.5	0.83	22.0	15.8	2.03	14.6	1.1	1.57	0.65	-5.80
2.4-18Me	831.465	3.23	A08	Phe	A15	222	5.6	80.2	0.47	7.1	77.3	0.60	6.4	75.6	0.54	77.7	2.3	0.54	0.07	-6.27
2.4-01H	607.418	1.83	A01	Ala	A12	214	1.5	113.0	0.12	2.1	94.5	0.17	1.7	92.4	0.14	100.0	11.3	0.14	0.03	-6.84
2.4-02H	633.433	2.23	A01	Ala	A14	220	2.3	105.6	0.19	3.2	93.5	0.26	2.6	92.3	0.22	97.1	7.4	0.22	0.04	-6.65
2.4-03H	635.413	0.46	A01	Ala	A15	194	0.0	103.0	0.00	0.0	89.3	0.00	0.0	87.9	0.00	93.4	8.4	0.00	0.00	-8.80
2.4-04H	679.475	2.14	A04	Ala	A12	228	10.3	102.1	0.88	14.8	87.2	1.30	12.2	83.7	1.06	91.0	9.7	1.08	0.21	-5.97
2.4-05H	683.449	3.38	A01	Phe	A12	231	34.9	80.5	3.49	40.3	75.0	4.20	37.9	74.5	3.89	76.7	3.3	3.86	0.36	-5.41
2.4-06H	705.491	2.54	A04	Ala	A14	234	13.8	102.2	1.21	17.7	89.4	1.59	15.2	87.6	1.35	93.1	8.0	1.38	0.19	-5.86
2.4-07H	707.470	0.77	A04	Ala	A15	211	0.1	105.1	0.01	0.2	88.3	0.02	0.1	90.1	0.01	94.5	9.2	0.01	0.00	-7.84
2.4-08H	709.465	3.79	A01	Phe	A14	236	43.1	69.6	4.60	46.8	63.6	5.15	47.7	66.4	5.28	66.5	3.0	5.01	0.36	-5.30
2.4-09H	711.444	2.02	A01	Phe	A15	211	1.1	100.4	0.09	1.4	88.8	0.12	1.2	89.2	0.10	92.8	6.6	0.10	0.01	-6.99
2.4-10H	713.423	2.83	A08	Ala	A12	227	20.2	84.2	1.83	25.8	78.0	2.43	23.4	75.7	2.17	79.3	4.4	2.15	0.30	-5.67
2.4-11H	739.439	3.23	A08	Ala	A14	231	26.1	79.9	2.47	30.4	74.4	2.95	28.9	74.9	2.78	76.4	3.0	2.73	0.25	-5.56
2.4-12H	741.418	1.46	A08	Ala	A15	209	0.6	101.2	0.05	0.9	88.9	0.07	0.7	90.1	0.05	93.4	6.8	0.06	0.01	-7.23
2.4-13H	755.507	3.69	A04	Phe	A12	244	53.0	40.3	6.16	45.8	30.6	5.00	63.1	40.2	8.13	37.0	5.6	6.43	1.59	-5.19
2.4-14H	781.522	4.10	A04	Phe	A14	250	54.0	34.4	6.34	36.9	26.2	3.75	61.6	35.4	7.80	32.0	5.1	5.96	2.05	-5.22
2.4-15H	783.501	2.33	A04	Phe	A15	224	4.7	100.3	0.39	6.5	89.6	0.55	5.7	85.3	0.47	91.7	7.8	0.47	0.08	-6.33
2.4-16H	789.455	4.39	A08	Phe	A12	242	39.3	18.3	4.06	27.5	14.4	2.62	42.8	19.9	4.56	17.5	2.8	3.75	1.01	-5.43
2.4-17H	815.470	4.79	A08	Phe	A14	246	29.0	18.9	2.79	14.3	15.6	1.26	32.3	20.0	3.17	18.2	2.3	2.41	1.02	-5.62
2.4-18H	817.449	3.02	A08	Phe	A15	222	13.1	83.4	1.15	15.2	80.2	1.35	14.4	78.0	1.27	80.5	2.7	1.25	0.10	-5.90

Table S2.4. PAMPA parameters of Sub-library 2.4

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.5-01Me	621.433	2.03	A01	Ala	A12	229	45.3	85.3	4.92	43.6	85.0	4.67	48.7	94.7	5.44	88.3	5.5	5.01	0.39	-5.30
2.5-02Me	647.449	2.44	A01	Ala	A14	235	68.7	79.5	9.46	66.1	79.4	8.82	73.6	89.2	10.85	82.7	5.6	9.71	1.04	-5.01
2.5-03Me	649.428	0.67	A01	Ala	A15	204	1.4	91.5	0.11	1.3	89.1	0.11	1.6	96.4	0.13	92.4	3.7	0.12	0.01	-6.93
2.5-04Me	693.491	2.34	A04	Ala	A12	241	78.7	73.0	12.60	74.2	74.3	11.05	80.3	81.3	13.23	76.2	4.4	12.29	1.12	-4.91
2.5-05Me	697.465	3.59	A01	Phe	A12	250	83.5	38.0	14.70	81.6	38.9	13.79	81.3	39.4	13.66	38.7	0.7	14.05	0.57	-4.85
2.5-06Me	719.507	2.75	A04	Ala	A14	247	84.8	64.0	15.36	81.5	65.2	13.74	85.6	69.4	15.78	66.2	2.9	14.96	1.07	-4.83
2.5-07Me	721.486	0.98	A04	Ala	A15	220	6.2	93.3	0.52	6.0	95.0	0.50	6.9	96.7	0.59	95.0	1.7	0.54	0.04	-6.27
2.5-08Me	723.480	3.99	A01	Phe	A14	256	72.9	22.6	10.63	73.1	22.9	10.70	62.1	20.5	7.90	22.0	1.3	9.75	1.60	-5.01
2.5-09Me	725.460	2.22	A01	Phe	A15	229	34.0	87.4	3.39	32.8	88.9	3.24	36.5	96.7	3.71	91.0	5.0	3.44	0.24	-5.46
2.5-10Me	727.439	3.04	A08	Ala	A12	241	86.1	42.9	16.10	82.1	44.2	14.01	81.2	44.2	13.61	43.7	0.7	14.57	1.34	-4.84
2.5-11Me	753.455	3.44	A08	Ala	A14	247	74.5	26.7	11.15	71.5	27.0	10.22	69.1	26.6	9.56	26.8	0.2	10.31	0.80	-4.99
2.5-12Me	755.434	1.67	A08	Ala	A15	222	28.5	86.7	2.74	28.9	87.8	2.78	31.5	91.0	3.08	88.5	2.2	2.86	0.19	-5.54
2.5-13Me	769.522	3.90	A04	Phe	A12	261	69.3	21.7	9.61	68.3	22.5	9.35	51.4	18.9	5.87	21.0	1.9	8.28	2.09	-5.08
2.5-14Me	795.538	4.30	A04	Phe	A14	267	49.6	13.0	5.58	49.3	14.3	5.53	25.9	10.7	2.44	12.6	1.8	4.52	1.80	-5.35
2.5-15Me	797.517	2.53	A04	Phe	A15	239	64.1	69.9	8.34	60.5	71.9	7.58	66.0	76.6	8.80	72.8	3.5	8.24	0.62	-5.08
2.5-16Me	803.470	4.59	A08	Phe	A12	258	21.0	9.7	1.92	23.1	9.2	2.14	6.5	8.6	0.55	9.2	0.6	1.54	0.86	-5.81
2.5-17Me	829.486	5.00	A08	Phe	A14	265	6.6	12.0	0.55	7.4	12.4	0.63	1.3	11.3	0.10	11.9	0.6	0.43	0.28	-6.37
2.5-18Me	831.465	3.23	A08	Phe	A15	239	72.6	40.7	10.56	69.8	42.3	9.75	69.1	42.5	9.56	41.9	1.0	9.96	0.53	-5.00
2.5-01H	607.418	1.83	A01	Ala	A12	214	6.4	91.3	0.54	6.2	95.0	0.52	7.6	95.5	0.65	93.9	2.3	0.57	0.07	-6.25
2.5-02H	633.433	2.23	A01	Ala	A14	220	13.5	90.9	1.18	13.5	92.4	1.18	16.3	95.3	1.45	92.9	2.3	1.27	0.16	-5.90
2.5-03H	635.413	0.46	A01	Ala	A15	193	0.4	93.7	0.03	0.3	97.6	0.03	0.5	93.6	0.04	94.9	2.3	0.03	0.01	-7.48
2.5-04H	679.475	2.14	A04	Ala	A12	229	25.8	85.4	2.43	25.5	84.2	2.40	31.0	93.4	3.02	87.7	5.0	2.62	0.35	-5.58
2.5-05H	683.449	3.38	A01	Phe	A12	236	64.8	68.6	8.51	63.9	69.6	8.30	69.4	75.7	9.66	71.3	3.8	8.82	0.73	-5.05
2.5-06H	705.491	2.54	A04	Ala	A14	233	45.2	82.0	4.90	43.2	82.6	4.62	51.3	89.9	5.87	84.9	4.4	5.13	0.66	-5.29
2.5-07H	707.470	0.77	A04	Ala	A15	207	1.7	90.3	0.14	1.7	91.7	0.14	2.2	93.7	0.18	91.9	1.7	0.15	0.02	-6.81
2.5-08H	709.465	3.79	A01	Phe	A14	243	75.6	54.0	11.48	72.3	56.0	10.46	73.8	57.3	10.91	55.8	1.7	10.95	0.51	-4.96
2.5-09H	711.444	2.02	A01	Phe	A15	216	10.1	90.4	0.87	9.8	93.9	0.84	12.0	95.0	1.04	93.1	2.4	0.92	0.11	-6.04
2.5-10H	713.423	2.83	A08	Ala	A12	229	63.6	66.4	8.23	62.1	66.1	7.91	67.3	72.8	9.12	68.4	3.8	8.42	0.63	-5.07
2.5-11H	739.439	3.23	A08	Ala	A14	235	69.2	50.8	9.61	68.5	51.7	9.40	72.0	54.4	10.36	52.3	1.9	9.79	0.51	-5.01
2.5-12H	741.418	1.46	A08	Ala	A15	210	13.9	87.6	1.22	13.9	91.5	1.22	15.9	91.6	1.41	90.2	2.3	1.28	0.11	-5.89
2.5-13H	755.507	3.69	A04	Phe	A12	247	78.1	45.8	12.39	74.8	47.1	11.23	73.8	45.7	10.91	46.2	0.8	11.51	0.78	-4.94
2.5-14H	781.522	4.10	A04	Phe	A14	252	72.1	30.1	10.40	73.2	31.8	10.73	61.0	27.0	7.67	29.6	2.5	9.60	1.68	-5.02
2.5-15H	783.501	2.33	A04	Phe	A15	229	26.9	84.0	2.55	27.2	83.9	2.58	32.5	92.0	3.20	86.7	4.6	2.78	0.37	-5.56
2.5-16H	789.455	4.39	A08	Phe	A12	247	54.4	17.9	6.41	51.1	18.4	5.83	41.0	15.3	4.30	17.2	1.6	5.51	1.09	-5.26
2.5-17H	815.470	4.79	A08	Phe	A14	252	29.0	13.4	2.79	32.7	13.4	3.22	16.2	11.3	1.44	12.7	1.2	2.48	0.93	-5.61
2.5-18H	817.449	3.02	A08	Phe	A15	229	57.3	64.4	6.94	56.8	65.4	6.84	59.9	70.3	7.46	66.7	3.1	7.08	0.33	-5.15

Table S2.5. PAMPA parameters of Sub-library 2.5

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.6-01Me	621.433	2.03	A01	Ala	A12	234	58.9	69.1	7.25	59.3	70.9	7.34	59.8	67.2	7.42	69.1	1.8	7.33	0.08	-5.13
2.6-02Me	647.449	2.44	A01	Ala	A14	239	77.8	62.1	12.28	77.0	64.3	11.98	78.3	60.4	12.45	62.3	1.9	12.24	0.24	-4.91
2.6-03Me	649.428	0.67	A01	Ala	A15	211	2.9	83.8	0.24	2.8	89.9	0.24	3.4	83.6	0.28	85.8	3.6	0.25	0.02	-6.60
2.6-04Me	693.491	2.34	A04	Ala	A12	248	84.6	50.6	15.23	81.4	53.3	13.73	80.8	50.5	13.45	51.5	1.6	14.14	0.96	-4.85
2.6-05Me	697.465	3.59	A01	Phe	A12	256	63.1	16.0	8.12	60.1	17.3	7.48	60.1	16.5	7.49	16.6	0.6	7.70	0.36	-5.11
2.6-06Me	719.507	2.75	A04	Ala	A14	254	83.3	36.4	14.57	80.0	38.8	13.13	81.8	37.5	13.88	37.6	1.2	13.86	0.72	-4.86
2.6-07Me	721.486	0.98	A04	Ala	A15	225	12.4	76.9	1.08	12.0	86.3	1.05	14.2	77.3	1.25	80.2	5.3	1.12	0.11	-5.95
2.6-08Me	723.480	3.99	A01	Phe	A14	264	40.0	8.1	4.16	34.8	9.2	3.48	34.2	8.5	3.41	8.6	0.6	3.68	0.41	-5.43
2.6-09Me	725.460	2.22	A01	Phe	A15	237	54.5	64.1	6.41	55.7	65.8	6.64	58.3	61.6	7.13	63.8	2.1	6.73	0.36	-5.17
2.6-10Me	727.439	3.04	A08	Ala	A12	244	74.0	26.0	10.99	72.3	28.0	10.46	70.3	26.1	9.89	26.7	1.1	10.44	0.55	-4.98
2.6-11Me	753.455	3.44	A08	Ala	A14	250	60.7	14.6	7.61	54.6	16.2	6.44	53.9	15.2	6.30	15.4	0.8	6.79	0.72	-5.17
2.6-12Me	755.434	1.67	A08	Ala	A15	225	32.6	71.9	3.21	32.1	79.0	3.16	36.6	71.9	3.71	74.3	4.1	3.36	0.30	-5.47
2.6-13Me	769.522	3.90	A04	Phe	A12	269	31.3	7.9	3.05	25.8	8.9	2.43	25.1	8.4	2.36	8.4	0.5	2.61	0.38	-5.58
2.6-14Me	795.538	4.30	A04	Phe	A14	275	14.5	6.3	1.28	12.8	7.7	1.12	28.7	7.3	2.75	7.1	0.7	1.72	0.90	-5.77
2.6-15Me	797.517	2.53	A04	Phe	A15	250	70.7	41.1	10.01	67.1	44.5	9.06	67.8	42.6	9.24	42.7	1.7	9.44	0.50	-5.03
2.6-16Me	803.470	4.59	A08	Phe	A12	264	0.2	6.5	0.02	0.0	8.4	0.00	0.0	7.0	0.00	7.3	1.0	0.01	0.01	-8.26
2.6-17Me	829.486	5.00	A08	Phe	A14	270	1.3	14.1	0.11	0.9	15.7	0.07	0.3	13.8	0.02	14.6	1.0	0.07	0.04	-7.17
2.6-18Me	831.465	3.23	A08	Phe	A15	247	35.4	22.0	3.56	33.5	23.9	3.33	31.7	22.4	3.11	22.8	1.0	3.33	0.22	-5.48
2.6-01H	607.418	1.83	A01	Ala	A12	217	11.4	86.9	0.99	11.7	89.9	1.02	12.2	85.9	1.06	87.5	2.1	1.02	0.04	-5.99
2.6-02H	633.433	2.23	A01	Ala	A14	224	28.2	77.3	2.71	26.2	85.6	2.47	28.5	80.1	2.73	81.0	4.2	2.64	0.14	-5.58
2.6-03H	635.413	0.46	A01	Ala	A15	196	0.5	89.2	0.04	0.4	92.7	0.04	0.6	88.5	0.05	90.1	2.3	0.04	0.01	-7.39
2.6-04H	679.475	2.14	A04	Ala	A12	232	49.0	78.5	5.49	49.0	80.5	5.49	49.7	75.6	5.60	78.2	2.5	5.53	0.06	-5.26
2.6-05H	683.449	3.38	A01	Phe	A12	240	85.2	69.1	15.55	84.0	70.7	14.93	85.5	66.9	15.75	68.9	1.9	15.41	0.43	-4.81
2.6-06H	705.491	2.54	A04	Ala	A14	237	68.5	76.3	9.42	69.2	76.5	9.61	70.5	72.6	9.95	75.1	2.2	9.66	0.27	-5.02
2.6-07H	707.470	0.77	A04	Ala	A15	214	2.0	84.4	0.17	2.0	90.1	0.17	2.4	85.9	0.19	86.8	3.0	0.18	0.02	-6.75
2.6-08H	709.465	3.79	A01	Phe	A14	248	90.7	48.7	19.40	87.0	50.9	16.61	86.2	48.5	16.15	49.3	1.4	17.39	1.76	-4.76
2.6-09H	711.444	2.02	A01	Phe	A15	222	14.5	79.6	1.27	13.6	88.4	1.19	15.5	82.3	1.38	83.5	4.5	1.28	0.09	-5.89
2.6-10H	713.423	2.83	A08	Ala	A12	229	71.1	72.6	10.11	69.0	76.9	9.56	73.0	70.5	10.69	73.3	3.2	10.12	0.57	-4.99
2.6-11H	739.439	3.23	A08	Ala	A14	237	77.9	55.0	12.30	78.7	56.7	12.61	79.0	53.7	12.70	55.1	1.5	12.54	0.21	-4.90
2.6-12H	741.418	1.46	A08	Ala	A15	213	9.7	83.0	0.83	9.8	87.9	0.84	11.5	83.8	1.00	84.9	2.6	0.89	0.09	-6.05
2.6-13H	755.507	3.69	A04	Phe	A12	253	87.2	43.6	16.79	83.2	46.1	14.55	85.1	44.5	15.53	44.7	1.3	15.62	1.12	-4.81
2.6-14H	781.522	4.10	A04	Phe	A14	261	75.6	25.6	11.51	71.3	26.4	10.18	72.5	25.9	10.51	26.0	0.4	10.73	0.69	-4.97
2.6-15H	783.501	2.33	A04	Phe	A15	237	41.4	72.8	4.36	43.0	75.0	4.58	44.9	70.5	4.86	72.8	2.3	4.60	0.25	-5.34
2.6-16H	789.455	4.39	A08	Phe	A12	250	56.2	20.2	6.74	48.5	21.7	5.41	48.2	20.6	5.36	20.9	0.8	5.83	0.78	-5.23
2.6-17H	815.470	4.79	A08	Phe	A14	256	15.8	18.8	1.40	14.1	21.4	1.24	13.6	19.0	1.19	19.7	1.4	1.28	0.11	-5.89
2.6-18H	817.449	3.02	A08	Phe	A15	234	64.9	56.4	8.53	65.8	59.1	8.75	67.2	56.5	9.08	57.4	1.5	8.79	0.28	-5.06

Table S2.6. PAMPA parameters of Sub-library 2.6

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.7-01Me	621.433	2.03	A01	Ala	A12	223	6.5	91.1	0.55	6.4	90.6	0.54	6.8	91.1	0.57	90.9	0.3	0.55	0.02	-6.26
2.7-02Me	647.449	2.44	A01	Ala	A14	230	20.3	85.9	1.85	18.8	88.1	1.70	20.1	88.2	1.83	87.4	1.3	1.79	0.08	-5.75
2.7-03Me	649.428	0.67	A01	Ala	A15	201	0.3	99.8	0.02	0.2	97.8	0.02	0.3	99.6	0.02	99.1	1.1	0.02	0.00	-7.68
2.7-04Me	693.491	2.34	A04	Ala	A12	235	22.1	86.4	2.04	19.9	88.4	1.81	20.8	89.8	1.91	88.2	1.7	1.92	0.12	-5.72
2.7-05Me	697.465	3.59	A01	Phe	A12	242	73.5	60.4	10.82	72.7	59.9	10.58	75.1	61.8	11.34	60.7	1.0	10.92	0.39	-4.96
2.7-06Me	719.507	2.75	A04	Ala	A14	241	46.2	80.5	5.05	45.5	79.6	4.94	47.1	79.1	5.20	79.7	0.7	5.06	0.13	-5.30
2.7-07Me	721.486	0.98	A04	Ala	A15	215	0.5	95.6	0.04	0.4	95.6	0.03	0.5	93.7	0.04	95.0	1.1	0.04	0.00	-7.42
2.7-08Me	723.480	3.99	A01	Phe	A14	248	77.7	36.5	12.23	77.4	35.6	12.13	80.2	38.5	13.21	36.9	1.5	12.52	0.60	-4.90
2.7-09Me	725.460	2.22	A01	Phe	A15	220	7.1	90.7	0.60	6.8	92.6	0.58	7.5	90.4	0.63	91.2	1.2	0.60	0.03	-6.22
2.7-10Me	727.439	3.04	A08	Ala	A12	233	45.1	70.3	4.88	40.4	73.0	4.21	45.1	73.6	4.88	72.3	1.8	4.66	0.39	-5.33
2.7-11Me	753.455	3.44	A08	Ala	A14	240	63.0	52.1	8.11	60.8	51.9	7.64	64.0	53.9	8.33	52.6	1.1	8.03	0.36	-5.10
2.7-12Me	755.434	1.67	A08	Ala	A15	216	2.7	93.7	0.22	2.7	92.9	0.22	3.0	91.3	0.25	92.6	1.2	0.23	0.01	-6.64
2.7-13Me	769.522	3.90	A04	Phe	A12	252	80.8	41.0	13.46	81.1	40.2	13.56	82.4	43.6	14.18	41.6	1.8	13.73	0.39	-4.86
2.7-14Me	795.538	4.30	A04	Phe	A14	259	71.7	25.0	10.29	67.3	23.9	9.10	70.9	26.3	10.06	25.1	1.2	9.82	0.63	-5.01
2.7-15Me	797.517	2.53	A04	Phe	A15	232	17.9	83.5	1.61	16.1	87.7	1.43	17.4	87.7	1.55	86.3	2.5	1.53	0.09	-5.81
2.7-16Me	803.470	4.59	A08	Phe	A12	250	41.6	11.4	4.38	34.5	11.1	3.45	33.7	11.1	3.35	11.2	0.2	3.73	0.57	-5.43
2.7-17Me	829.486	5.00	A08	Phe	A14	256	14.5	13.9	1.28	10.9	13.9	0.94	13.5	13.5	1.19	13.8	0.2	1.14	0.18	-5.94
2.7-18Me	831.465	3.23	A08	Phe	A15	232	38.1	59.4	3.91	34.6	62.6	3.46	37.7	62.7	3.85	61.6	1.9	3.74	0.24	-5.43
2.7-01H	607.418	1.83	A01	Ala	A12	211	2.4	98.8	0.19	2.3	98.0	0.19	2.5	96.4	0.20	97.7	1.3	0.19	0.01	-6.71
2.7-02H	633.433	2.23	A01	Ala	A14	216	5.4	91.9	0.45	5.2	92.0	0.43	5.7	91.3	0.47	91.7	0.4	0.45	0.02	-6.34
2.7-03H	635.413	0.46	A01	Ala	A15	188	0.1	96.1	0.01	0.1	95.3	0.01	0.1	98.0	0.01	96.5	1.4	0.01	0.00	-8.00
2.7-04H	679.475	2.14	A04	Ala	A12	224	7.9	90.6	0.67	7.7	89.0	0.66	7.9	90.9	0.67	90.2	1.0	0.67	0.01	-6.18
2.7-05H	683.449	3.38	A01	Phe	A12	230	53.0	80.0	6.16	48.8	82.7	5.46	51.3	84.6	5.86	82.4	2.3	5.83	0.35	-5.23
2.7-06H	705.491	2.54	A04	Ala	A14	229	17.7	89.0	1.59	16.7	90.2	1.49	17.9	89.5	1.61	89.6	0.6	1.56	0.06	-5.81
2.7-07H	707.470	0.77	A04	Ala	A15	204	0.4	102.8	0.03	0.4	98.0	0.03	0.4	101.6	0.03	100.8	2.5	0.03	0.00	-7.50
2.7-08H	709.465	3.79	A01	Phe	A14	236	68.9	72.9	9.53	65.7	73.5	8.72	68.1	76.0	9.31	74.2	1.6	9.19	0.42	-5.04
2.7-09H	711.444	2.02	A01	Phe	A15	209	1.4	99.9	0.11	1.3	98.6	0.10	1.5	97.7	0.12	98.7	1.1	0.11	0.01	-6.95
2.7-10H	713.423	2.83	A08	Ala	A12	224	22.7	80.9	2.10	22.1	80.3	2.04	23.4	81.1	2.17	80.8	0.4	2.10	0.07	-5.68
2.7-11H	739.439	3.23	A08	Ala	A14	228	37.6	70.9	3.85	35.8	72.4	3.61	38.2	72.2	3.92	71.8	0.9	3.79	0.16	-5.42
2.7-12H	741.418	1.46	A08	Ala	A15	204	2.7	101.2	0.22	2.6	95.5	0.22	2.9	99.0	0.24	98.6	2.9	0.23	0.01	-6.64
2.7-13H	755.507	3.69	A04	Phe	A12	243	76.2	69.0	11.71	75.5	69.2	11.48	77.6	69.9	12.19	69.4	0.5	11.79	0.36	-4.93
2.7-14H	781.522	4.10	A04	Phe	A14	248	79.9	54.2	13.06	80.8	53.7	13.45	82.1	57.5	14.04	55.1	2.1	13.52	0.49	-4.87
2.7-15H	783.501	2.33	A04	Phe	A15	224	3.3	92.3	0.27	3.2	91.5	0.27	3.4	92.4	0.29	92.0	0.5	0.28	0.01	-6.56
2.7-16H	789.455	4.39	A08	Phe	A12	240	61.1	27.3	7.69	58.4	26.8	7.14	61.2	28.1	7.71	27.4	0.7	7.51	0.32	-5.12
2.7-17H	815.470	4.79	A08	Phe	A14	244	46.3	18.9	5.06	41.1	18.0	4.32	44.5	18.1	4.80	18.3	0.5	4.73	0.38	-5.33
2.7-18H	817.449	3.02	A08	Phe	A15	222	11.5	77.9	1.00	11.0	79.6	0.95	12.0	79.5	1.04	79.0	1.0	1.00	0.05	-6.00

Table S2.7. PAMPA parameters of Sub-library 2.7

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

Comp	Target MS	ALogP	R^6	R^1	R^2	RT (sec)	Well_1			Well_2			Well_3			Ave_%R	SD_%R	Ave_P_{app} $\times10^{-6}$cm/s	SD_P_{app} $\times10^{-6}$cm/s	Ave $LogP_{app}$
							%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s	%T	%R	P_{app} $\times10^{-6}$ cm/s					
2.8-01Me	621.433	2.03	A01	Ala	A12	229	13.3	85.4	1.16	12.5	83.4	1.09	9.6	107.8	0.83	92.2	13.6	1.03	0.18	-5.99
2.8-02Me	647.449	2.44	A01	Ala	A14	235	31.3	76.6	3.06	28.9	77.2	2.78	24.4	95.3	2.28	83.0	10.6	2.71	0.40	-5.57
2.8-03Me	649.428	0.67	A01	Ala	A15	210	1.0	94.9	0.08	0.8	91.9	0.06	0.6	118.5	0.05	101.8	14.6	0.06	0.01	-7.19
2.8-04Me	693.491	2.34	A04	Ala	A12	243	43.6	64.0	4.67	40.7	68.5	4.26	34.5	83.7	3.45	72.0	10.3	4.13	0.62	-5.38
2.8-05Me	697.465	3.59	A01	Phe	A12	248	71.7	30.4	10.29	72.8	32.4	10.62	62.8	37.1	8.07	33.3	3.4	9.66	1.39	-5.01
2.8-06Me	719.507	2.75	A04	Ala	A14	250	65.9	55.4	8.76	65.9	57.7	8.76	56.2	68.2	6.73	60.5	6.8	8.09	1.17	-5.09
2.8-07Me	721.486	0.98	A04	Ala	A15	224	3.2	95.4	0.26	2.7	93.9	0.22	2.2	116.6	0.18	102.0	12.7	0.22	0.04	-6.66
2.8-08Me	723.480	3.99	A01	Phe	A14	255	63.8	15.7	8.29	69.8	16.7	9.77	57.2	19.3	6.92	17.3	1.9	8.33	1.43	-5.08
2.8-09Me	725.460	2.22	A01	Phe	A15	231	23.6	79.7	2.19	22.0	78.7	2.03	19.5	92.8	1.76	83.7	7.9	1.99	0.22	-5.70
2.8-10Me	727.439	3.04	A08	Ala	A12	241	60.3	36.7	7.53	65.5	43.8	8.67	61.1	45.7	7.70	42.1	4.8	7.97	0.62	-5.10
2.8-11Me	753.455	3.44	A08	Ala	A14	247	63.4	23.7	8.18	62.4	25.9	7.97	52.0	30.3	5.98	26.7	3.3	7.38	1.21	-5.13
2.8-12Me	755.434	1.67	A08	Ala	A15	223	12.3	88.7	1.07	10.2	88.9	0.87	8.9	105.0	0.76	94.2	9.4	0.90	0.16	-6.05
2.8-13Me	769.522	3.90	A04	Phe	A12	260	54.0	12.4	6.33	57.7	13.4	7.02	45.9	16.1	5.00	14.0	1.9	6.12	1.03	-5.21
2.8-14Me	795.538	4.30	A04	Phe	A14	267	37.1	9.1	3.77	36.4	9.9	3.69	26.4	13.2	2.50	10.7	2.2	3.32	0.71	-5.48
2.8-15Me	797.517	2.53	A04	Phe	A15	244	53.1	49.8	6.17	48.3	55.0	5.38	44.1	63.0	4.75	55.9	6.7	5.43	0.71	-5.26
2.8-16Me	803.470	4.59	A08	Phe	A12	231	0.0	97.7	0.00	0.0	96.5	0.00	0.0	117.5	0.00	103.9	11.8	0.00	0.00	—
2.8-17Me	829.486	5.00	A08	Phe	A14	262	1.2	8.4	0.10	1.9	10.1	0.15	1.8	12.3	0.14	10.2	2.0	0.13	0.03	-6.88
2.8-18Me	831.465	3.23	A08	Phe	A15	241	50.6	18.7	5.74	47.2	20.5	5.21	42.5	23.3	4.51	20.8	2.3	5.16	0.62	-5.29
2.8-01H	607.418	1.83	A01	Ala	A12	220	6.1	96.6	0.52	5.3	89.9	0.45	4.2	118.3	0.35	101.6	14.8	0.44	0.08	-6.36
2.8-02H	633.433	2.23	A01	Ala	A14	225	13.2	88.8	1.15	11.6	88.4	1.01	9.5	106.3	0.81	94.5	10.2	0.99	0.17	-6.00
2.8-03H	635.413	0.46	A01	Ala	A15	201	1.1	91.7	0.09	0.9	89.1	0.07	0.7	116.3	0.06	99.0	15.0	0.07	0.01	-7.14
2.8-04H	679.475	2.14	A04	Ala	A12	232	19.8	81.4	1.80	17.7	79.1	1.59	14.7	102.2	1.30	87.6	12.8	1.56	0.25	-5.81
2.8-05H	683.449	3.38	A01	Phe	A12	237	56.1	56.6	6.71	53.3	59.4	6.20	46.7	68.4	5.13	61.5	6.1	6.01	0.81	-5.22
2.8-06H	705.491	2.54	A04	Ala	A14	237	40.1	72.5	4.18	36.1	73.6	3.65	30.5	90.1	2.97	78.7	9.8	3.60	0.61	-5.44
2.8-07H	707.470	0.77	A04	Ala	A15	214	3.8	91.9	0.32	2.9	90.5	0.24	2.5	116.7	0.20	99.7	14.7	0.25	0.06	-6.60
2.8-08H	709.465	3.79	A01	Phe	A14	245	71.4	35.4	10.21	70.1	38.8	9.83	62.1	43.4	7.91	39.2	4.1	9.32	1.23	-5.03
2.8-09H	711.444	2.02	A01	Phe	A15	220	9.6	94.1	0.83	8.2	90.5	0.70	7.0	110.3	0.59	98.3	10.5	0.71	0.12	-6.15
2.8-10H	713.423	2.83	A08	Ala	A12	232	48.6	57.9	5.42	46.6	59.6	5.12	40.6	70.8	4.25	62.8	7.0	4.93	0.61	-5.31
2.8-11H	739.439	3.23	A08	Ala	A14	236	58.7	43.5	7.21	55.4	45.4	6.59	48.8	52.5	5.46	47.1	4.8	6.42	0.89	-5.19
2.8-12H	741.418	1.46	A08	Ala	A15	214	17.3	85.7	1.55	14.1	85.5	1.24	12.4	105.5	1.08	92.2	11.5	1.29	0.24	-5.89
2.8-13H	755.507	3.69	A04	Phe	A12	251	69.3	30.6	9.64	72.1	31.9	10.40	62.2	37.3	7.93	33.3	3.6	9.32	1.26	-5.03
2.8-14H	781.522	4.10	A04	Phe	A14	256	57.7	16.2	7.01	60.9	18.1	7.66	52.2	20.8	6.02	18.3	2.3	6.90	0.83	-5.16
2.8-15H	783.501	2.33	A04	Phe	A15	235	30.9	76.4	3.01	27.1	76.9	2.58	24.1	91.9	2.25	81.7	8.8	2.61	0.38	-5.58
2.8-16H	789.455	4.39	A08	Phe	A12	248	38.1	10.6	3.91	39.1	11.3	4.04	30.6	14.2	2.98	12.0	1.9	3.64	0.58	-5.44
2.8-17H	815.470	4.79	A08	Phe	A14	254	0.0	8.1	0.00	0.0	8.9	0.00	0.2	11.2	0.02	9.4	1.6	0.01	0.01	-8.27
2.8-18H	817.449	3.02	A08	Phe	A15	232	51.2	47.7	5.85	47.7	50.1	5.29	44.6	56.0	4.81	51.3	4.3	5.32	0.52	-5.27

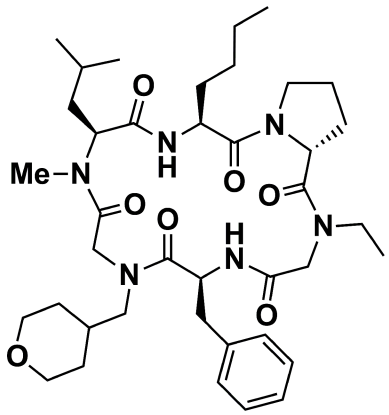
Table S2.8. PAMPA parameters of Sub-library 2.8

RT: retention time, %R: %-recovery, Ave: Average, SD: Standard deviation

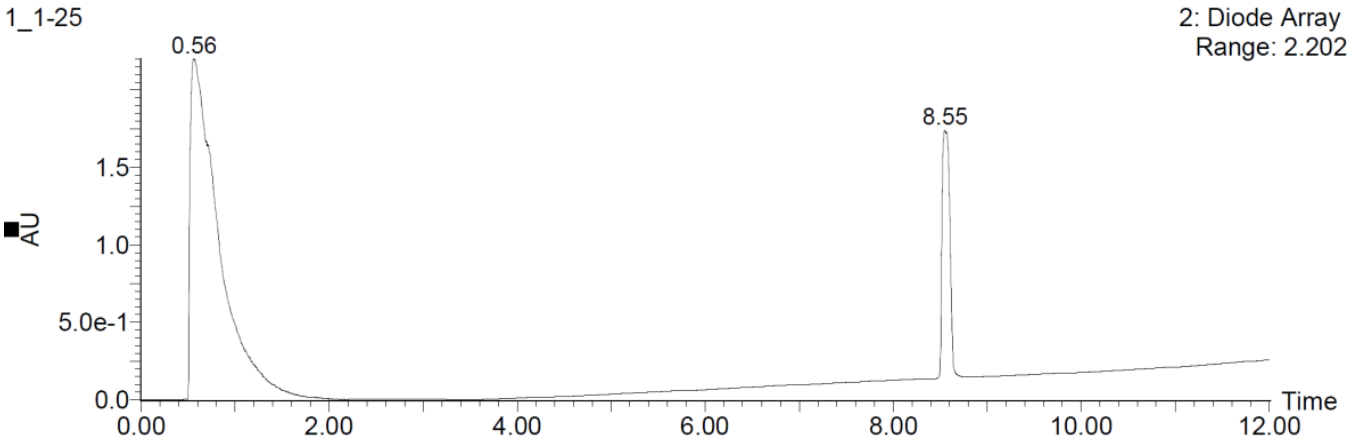
3 Characterization of individually synthesized compounds (LCMS and NMR in $CDCl_3$)

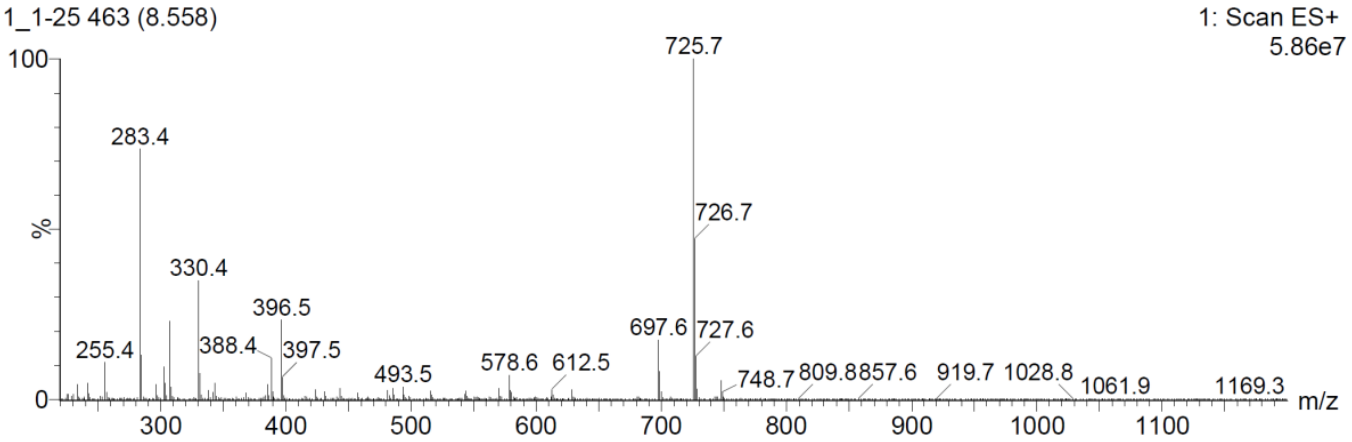
Micromass ZQ and Waters 2998 PDA detector were used for this purpose.

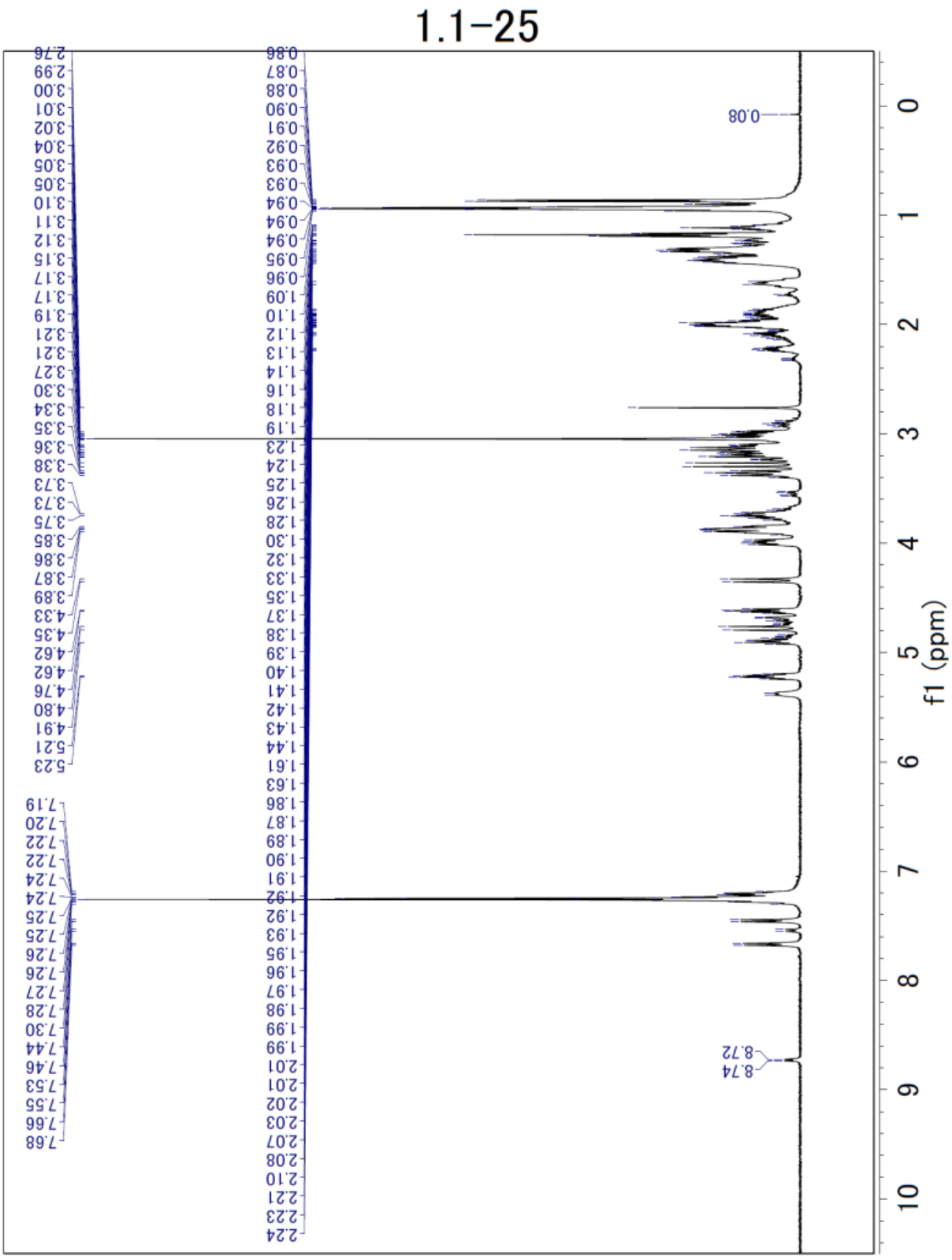
3.1 Compound **3** (1.1-25)



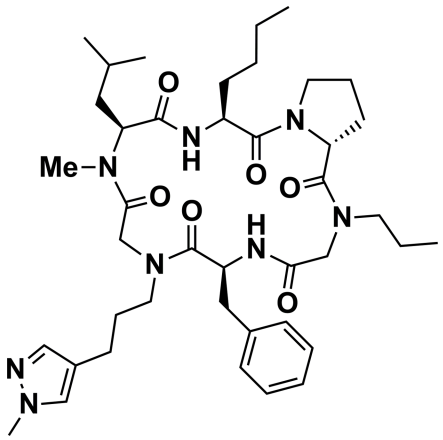
Chemical Formula: $C_{39}H_{60}N_6O_7$
Molecular Weight: 724.93
M+H: 725.460



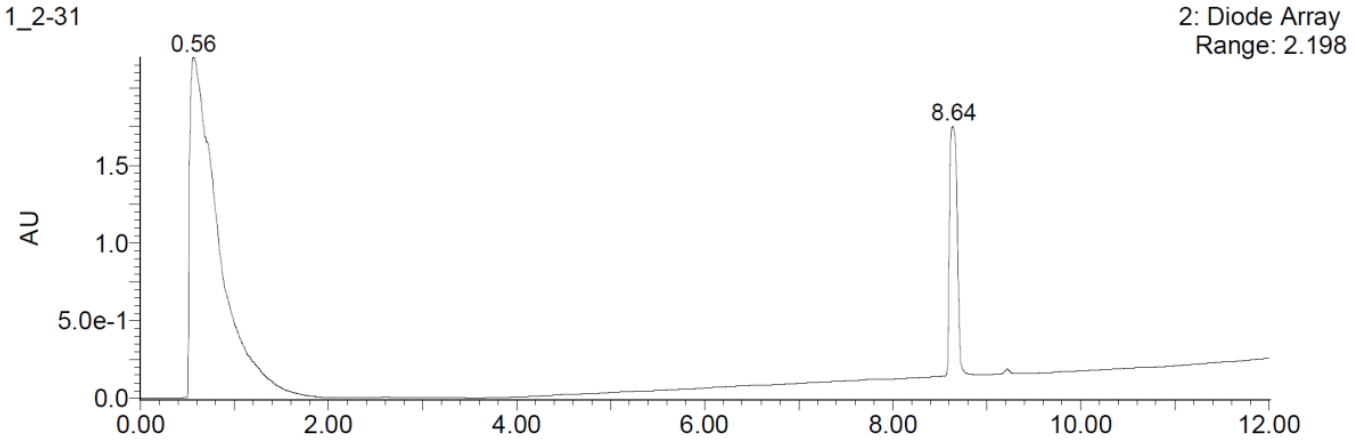


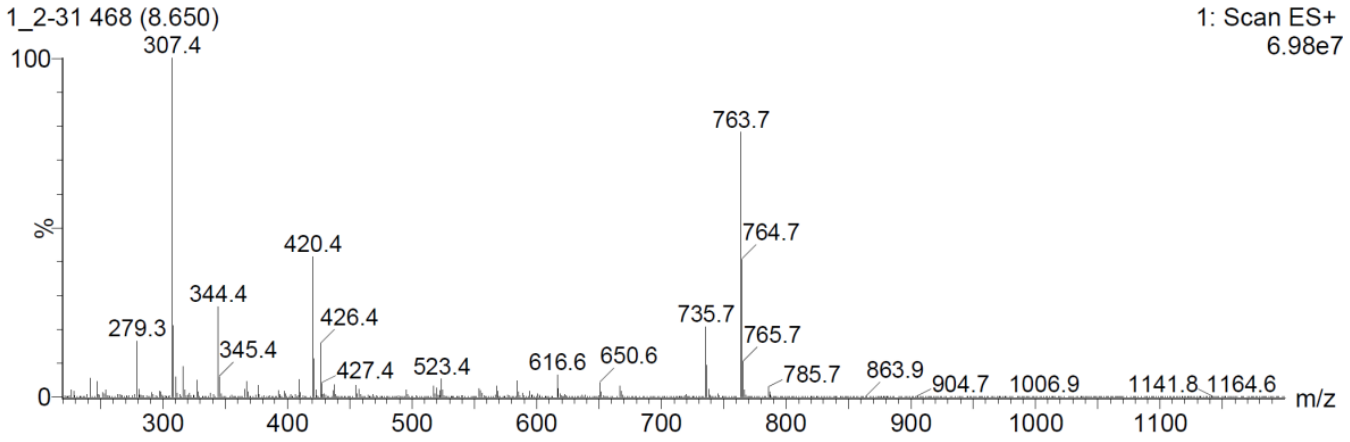

1.1-25
f1 (ppm)

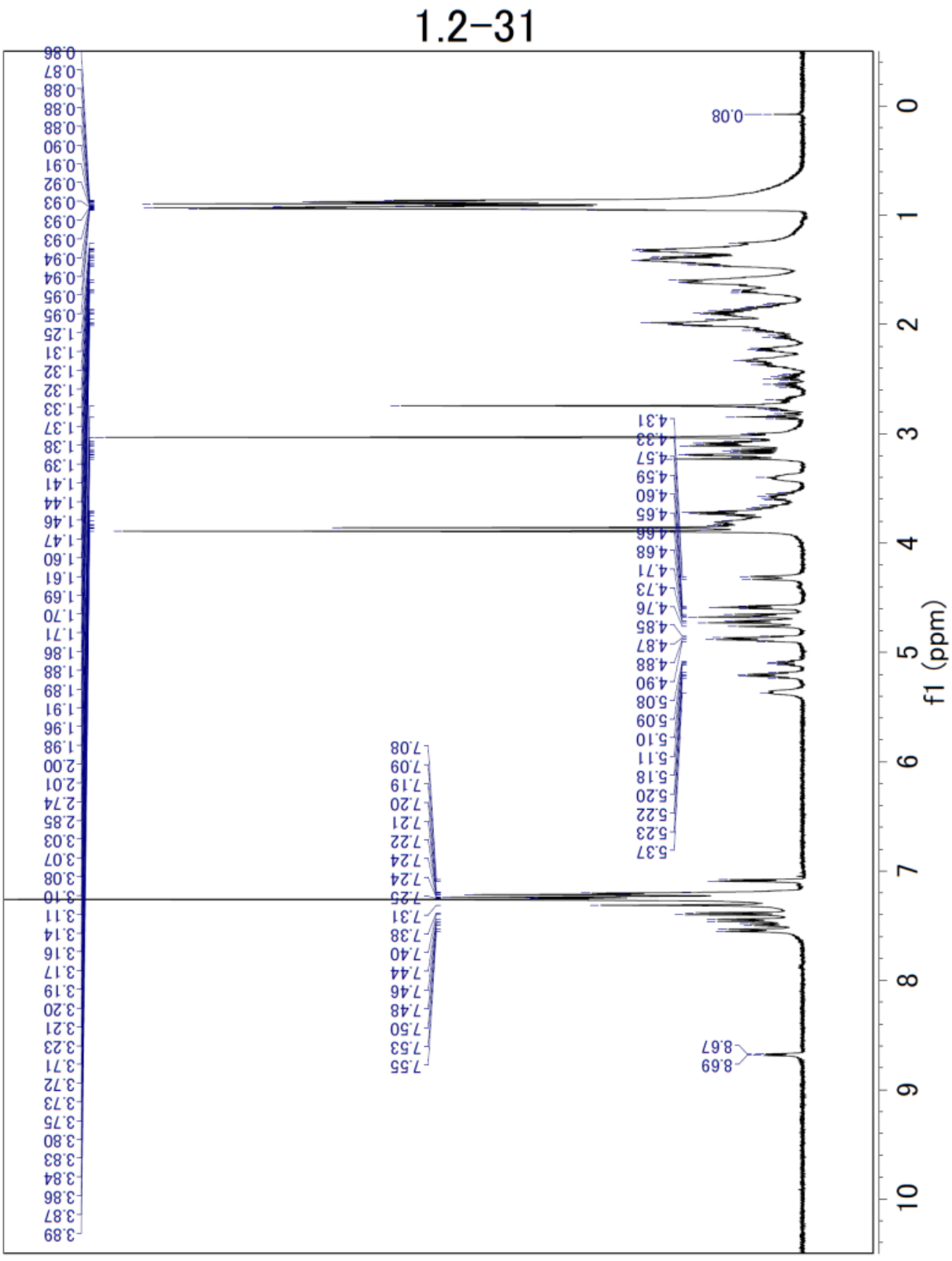
3.2 Compound **4** (1.2-31)



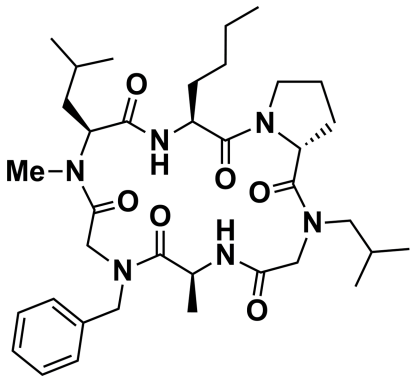
Chemical Formula: $C_{41}H_{62}N_8O_6$
Molecular Weight: 762.98
M+H: 763.487



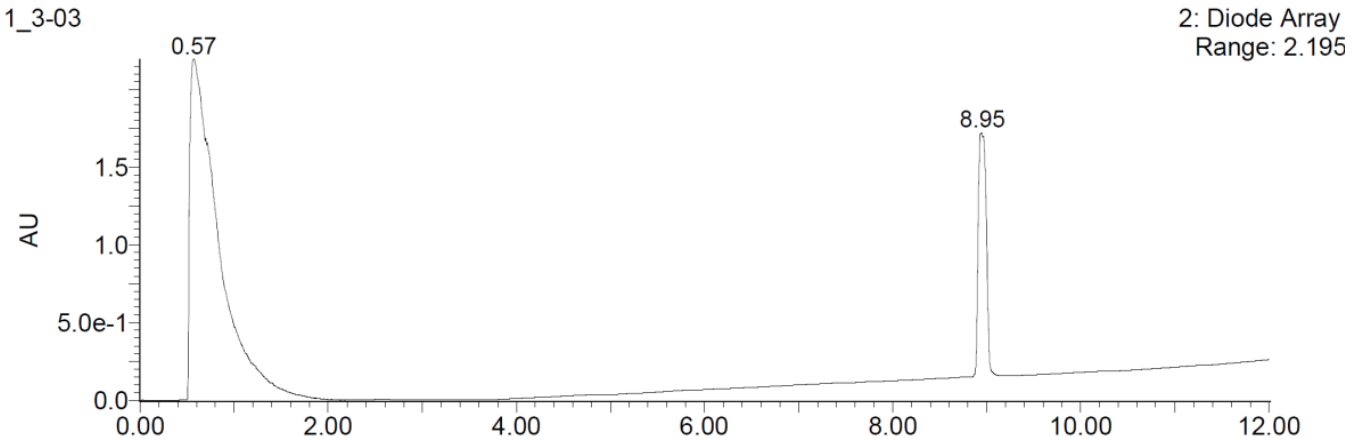


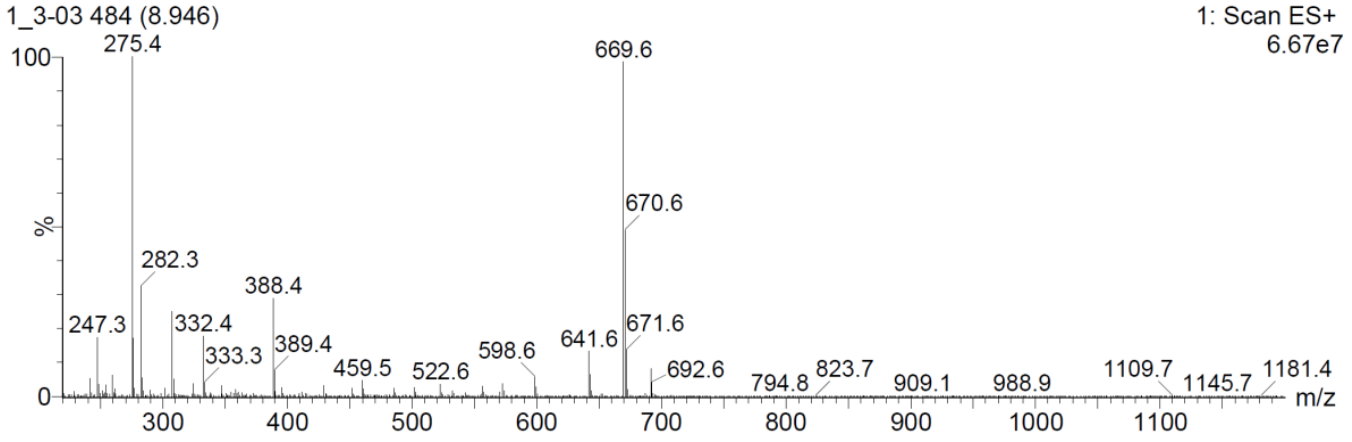

1.2-31
f1 (ppm)

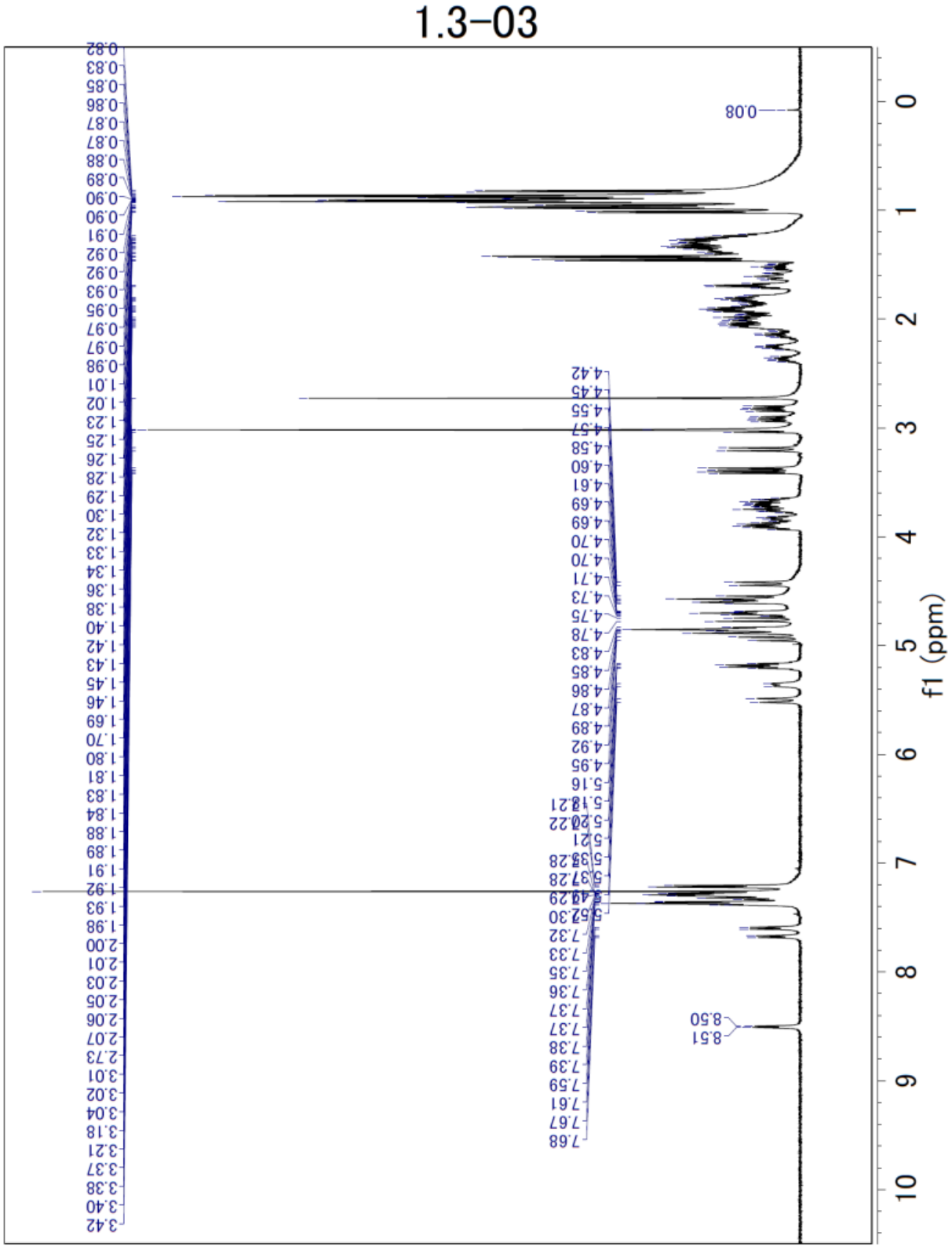
3.3 Compound **5** (1.3-03)



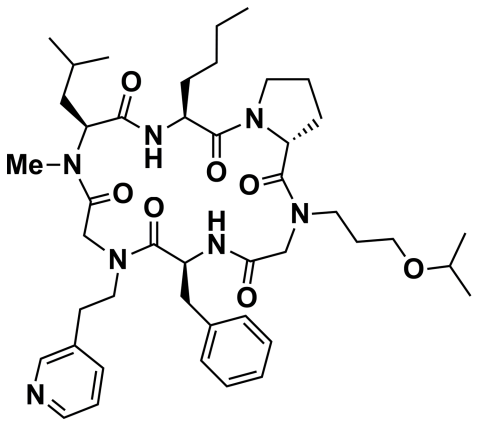
Chemical Formula: $C_{36}H_{56}N_6O_6$
Molecular Weight: 668.87
M+H: 669.433



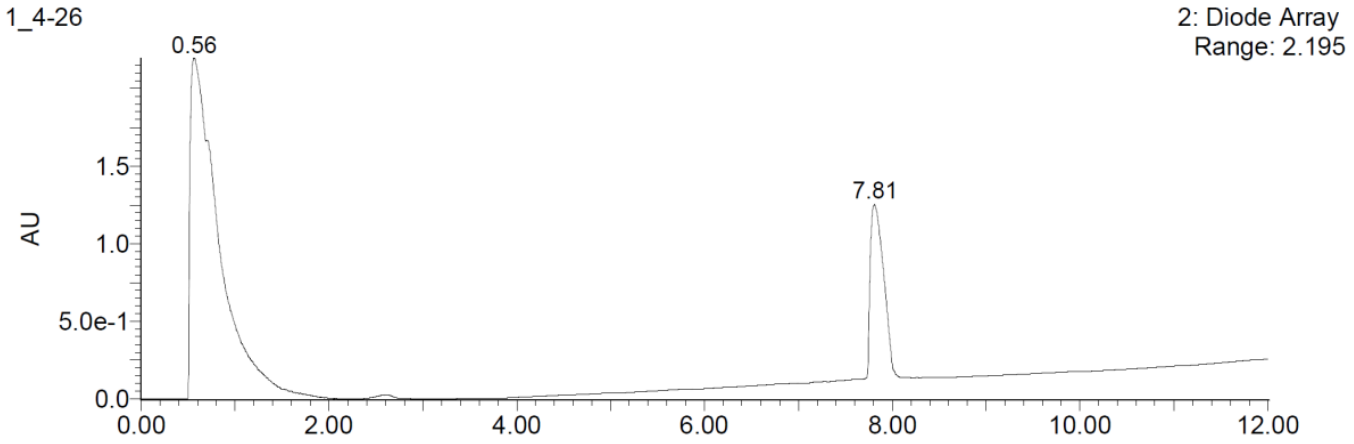


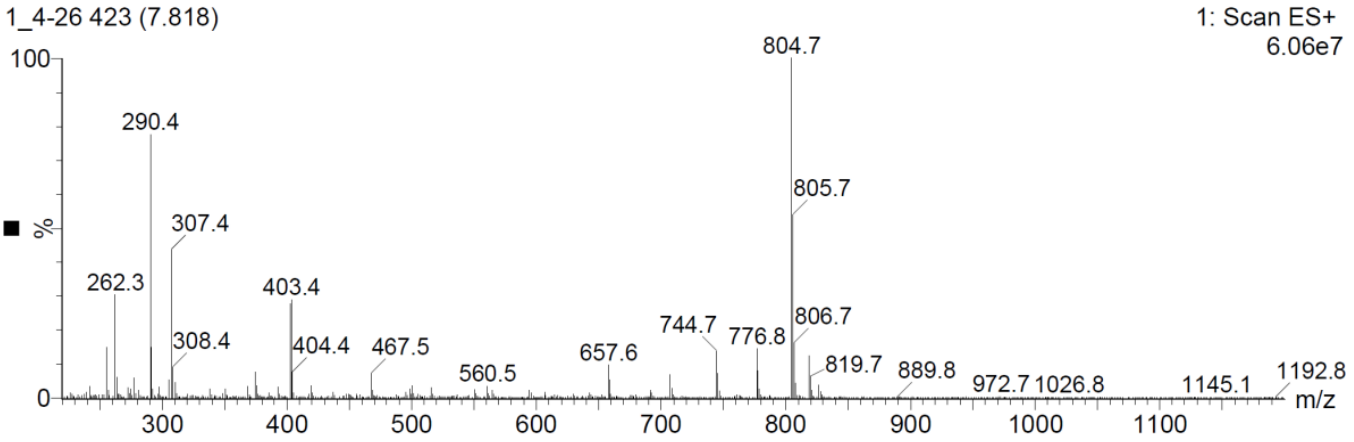

1.3-03
f1 (ppm)

3.4 Compound **6** (1.4-26)

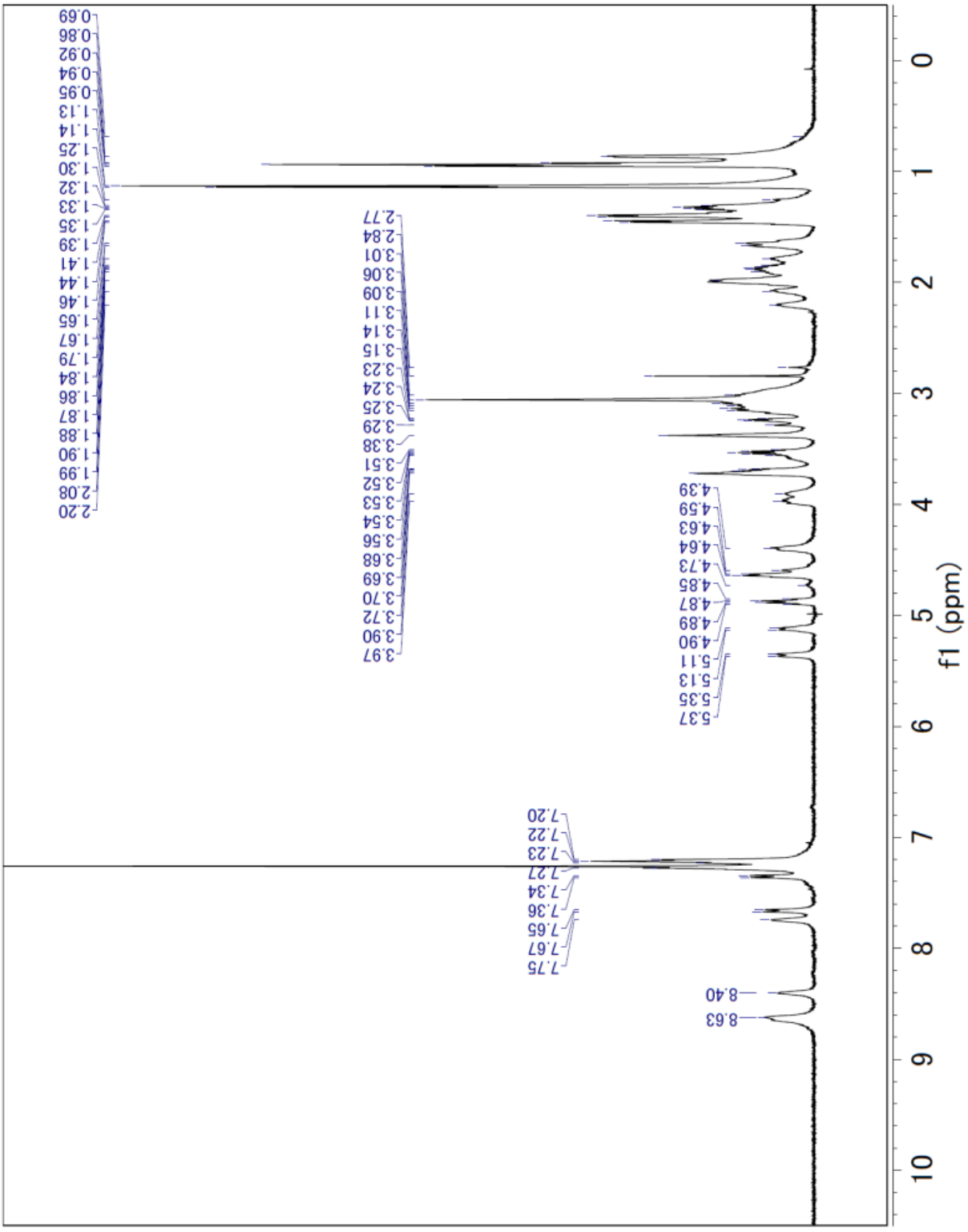


Chemical Formula: $C_{44}H_{65}N_7O_7$
Molecular Weight: 804.03
M+H: 804.502





1.4-26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5.37
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7.22
7.23
7.27
7.34
7.36
7.65
7.67
7.75
8.40
8.63
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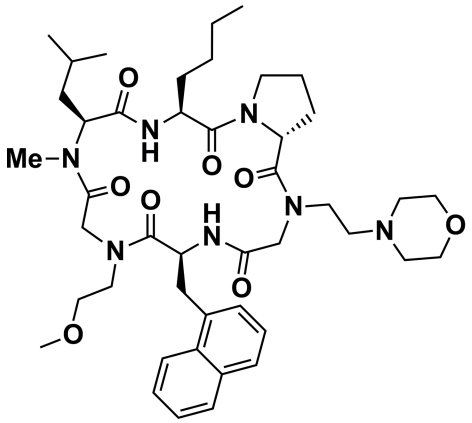
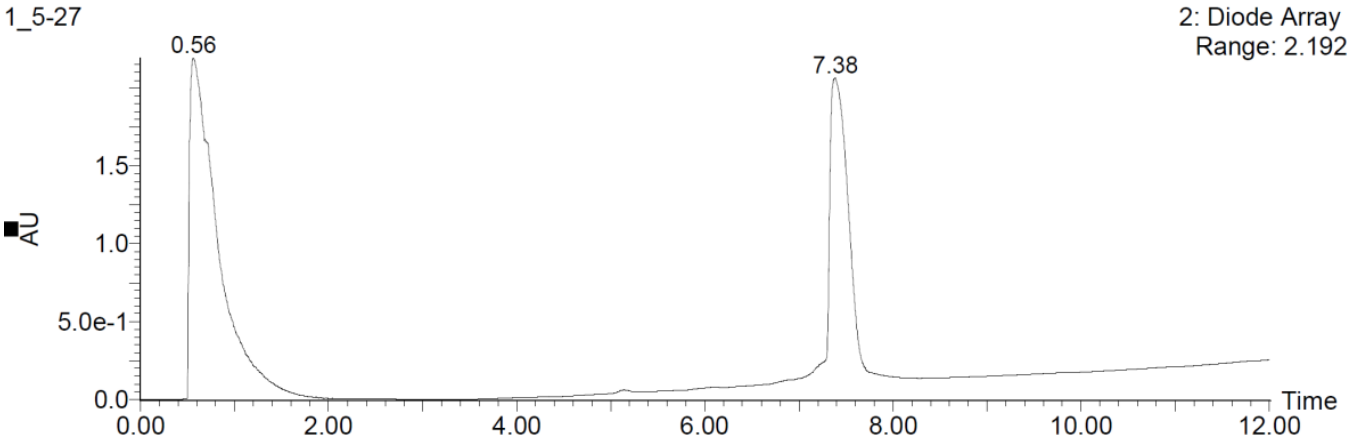
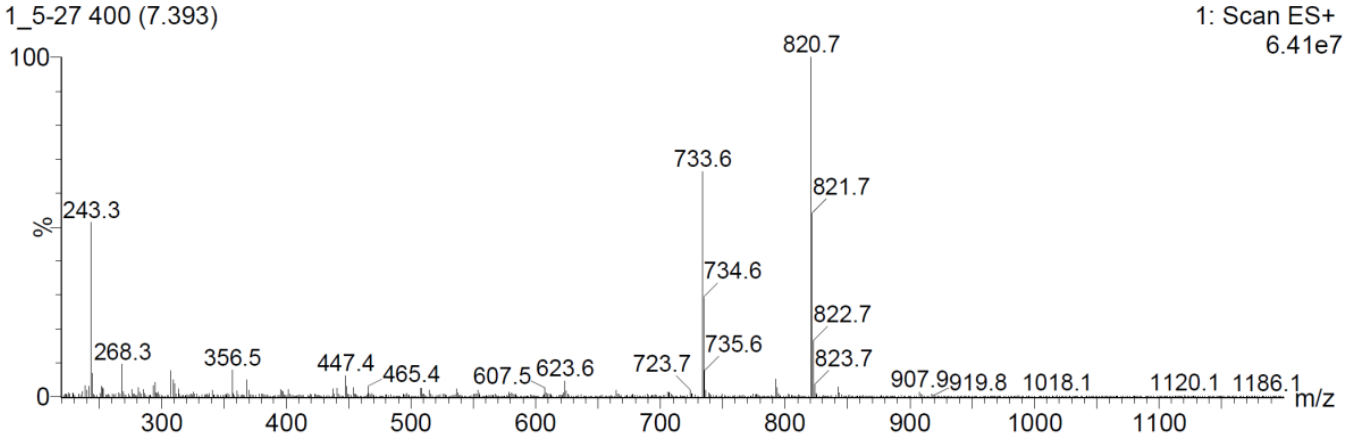
2
3
4
5
6
7
8
9
10
f1 (ppm)

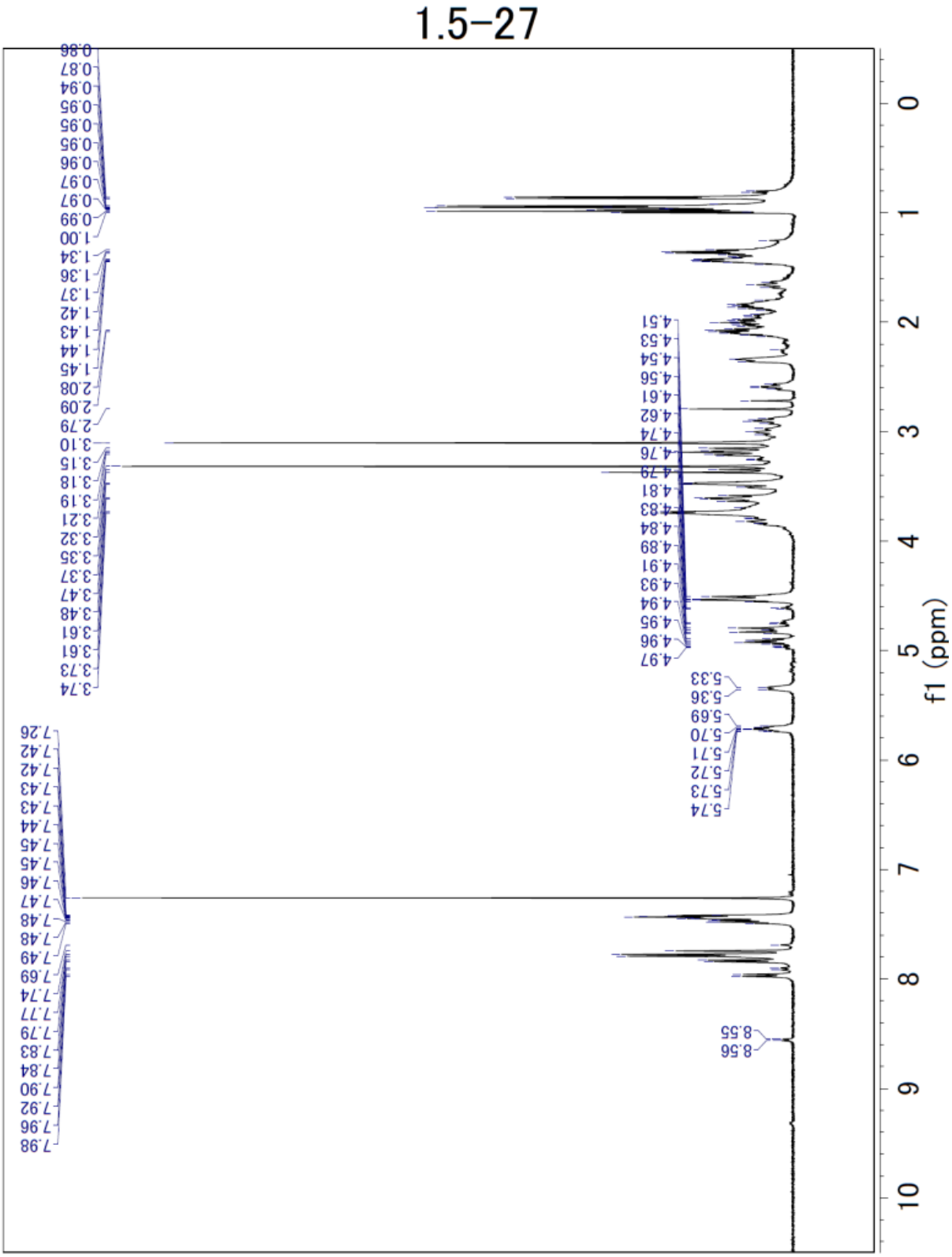
3.5 Compound **7** (1.5-27)



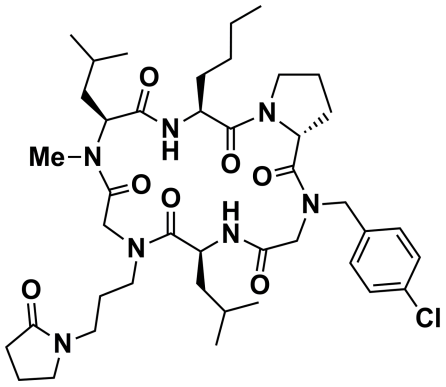
Chemical Formula: $C_{44}H_{65}N_7O_8$
Molecular Weight: 820.03
M+H: 820.497



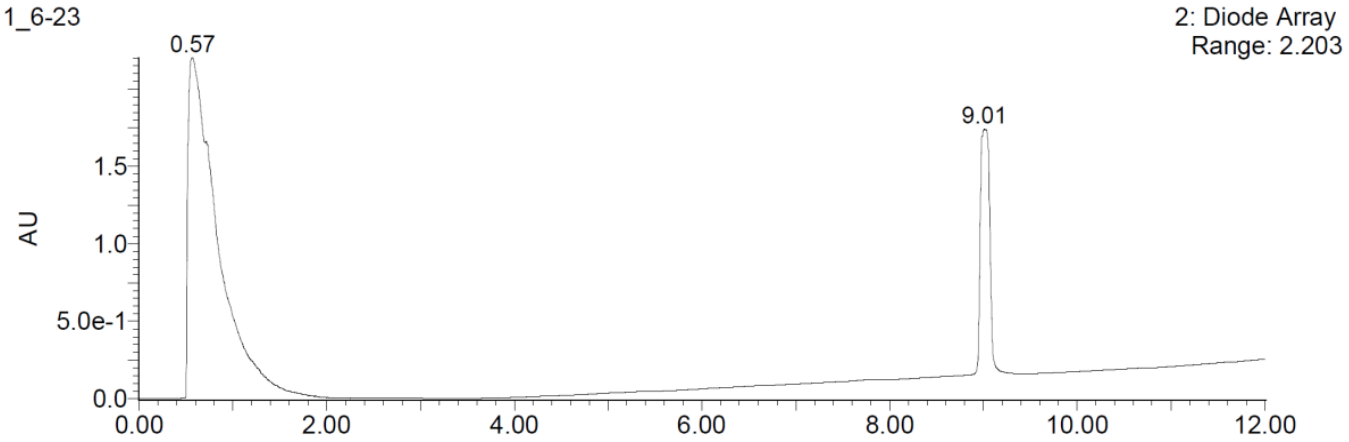


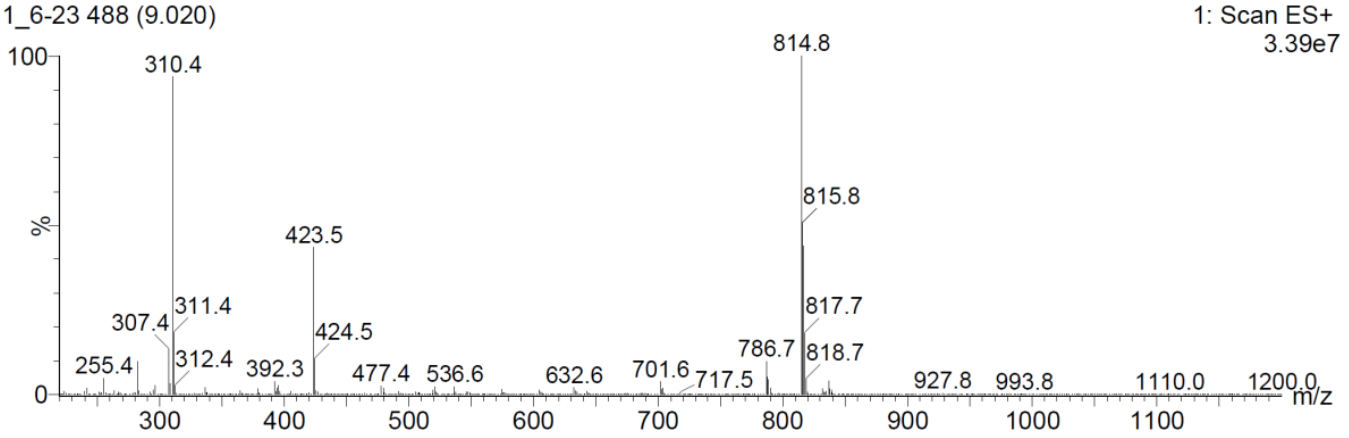

1.5-27
f1 (ppm)

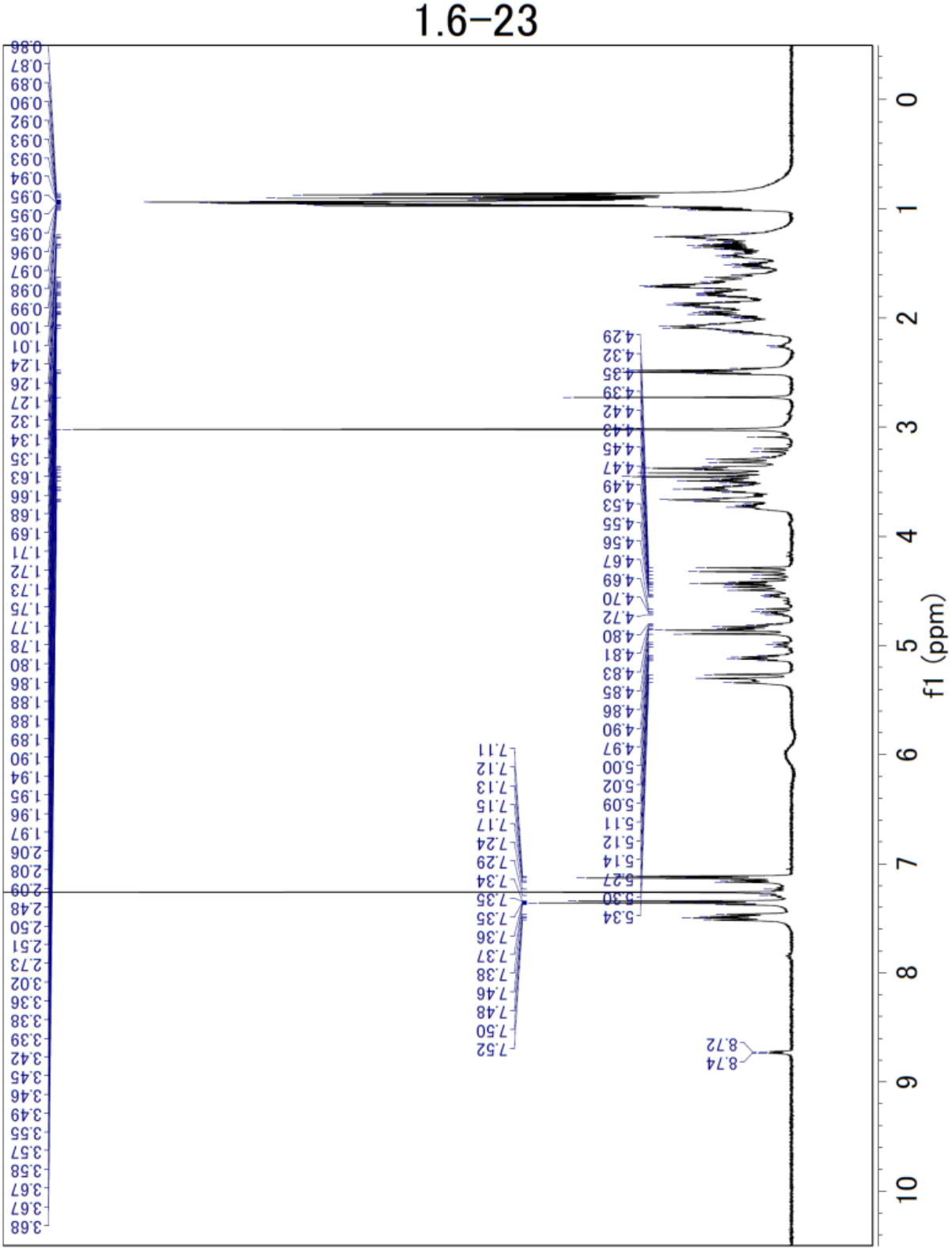
3.6 Compound **8** (1.6-23)



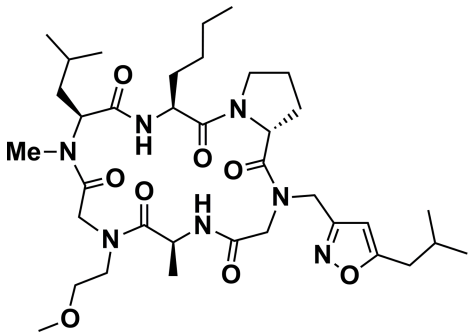
Chemical Formula: $C_{42}H_{64}ClN_7O_7$
Molecular Weight: 814.45
M+H: 814.463



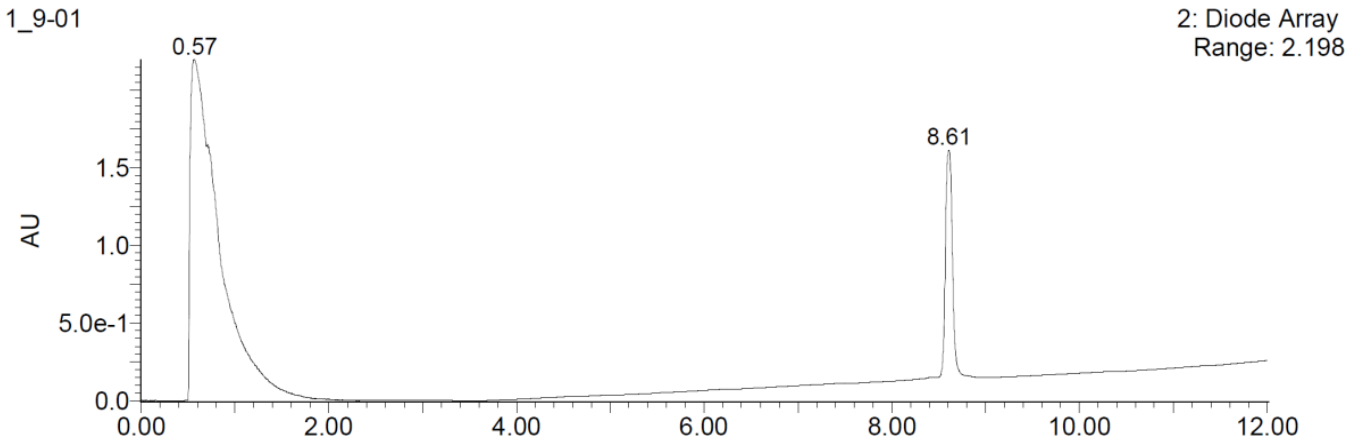


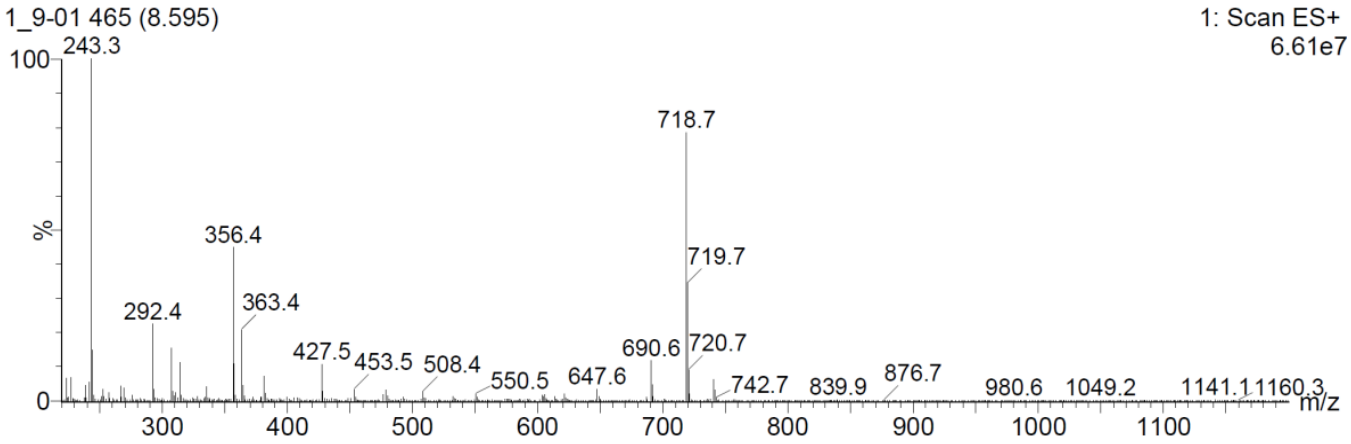

1.6-23
f1 (ppm)

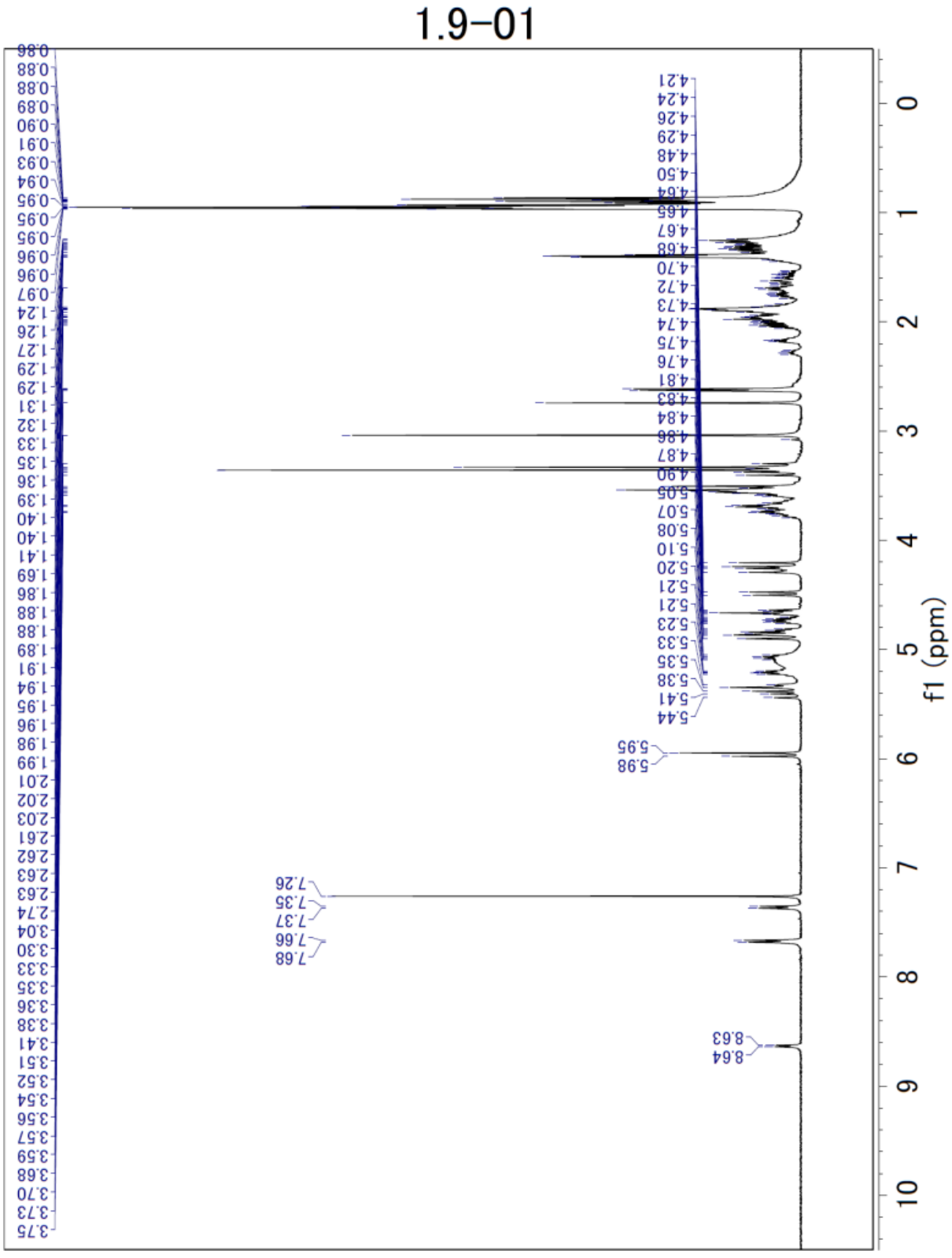
3.7 Compound **9** (1.9-01)



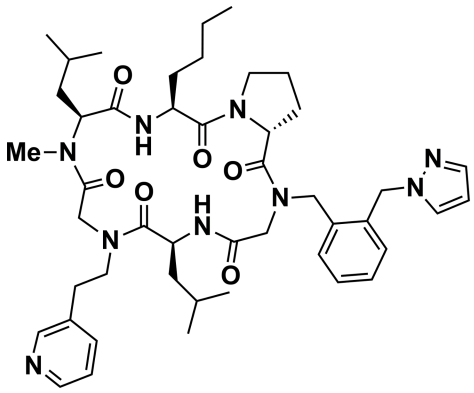
Chemical Formula: $C_{36}H_{59}N_7O_8$
Molecular Weight: 717.90
M+H: 718.450



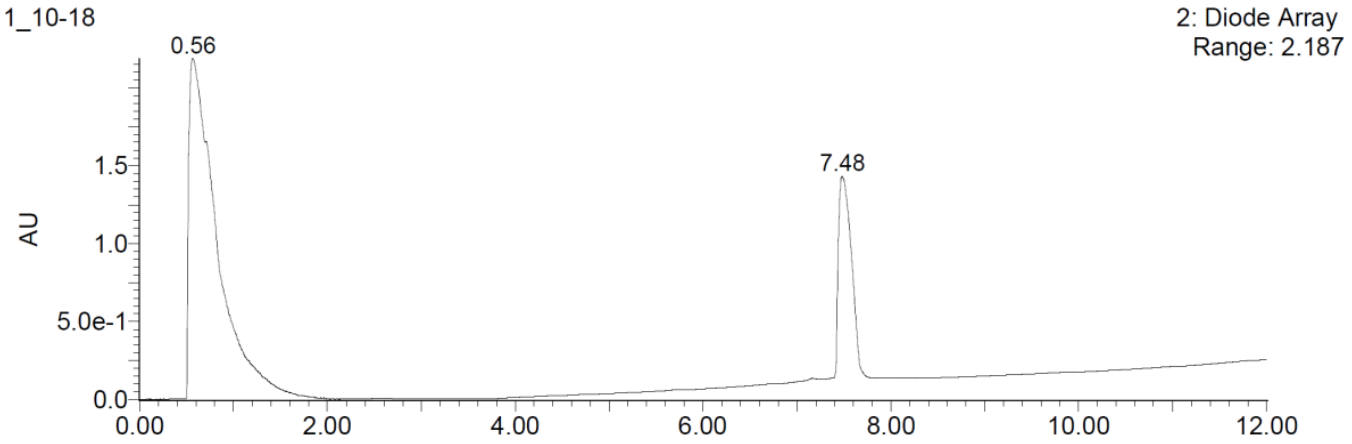


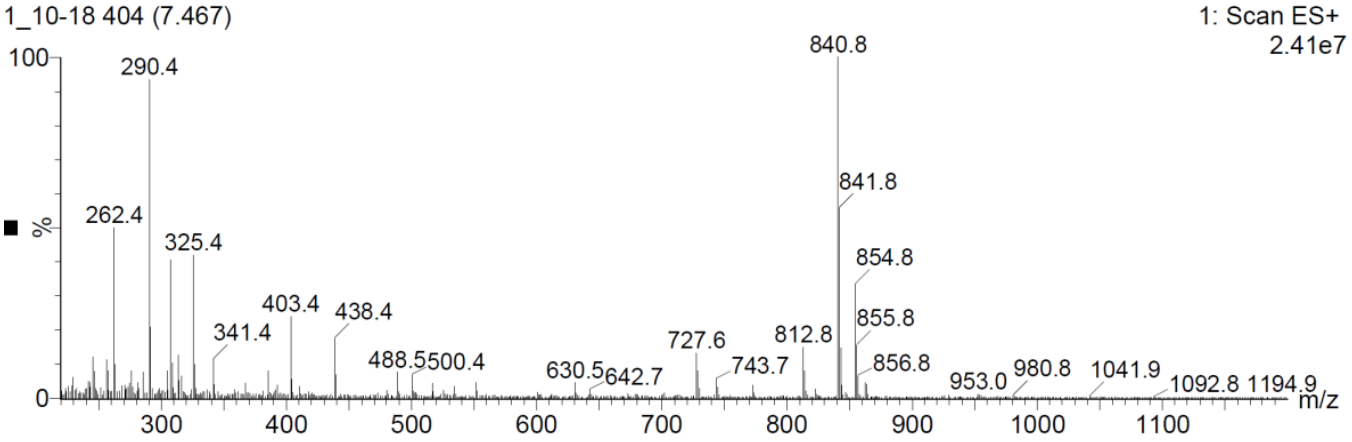

1.9-01
f1 (ppm)

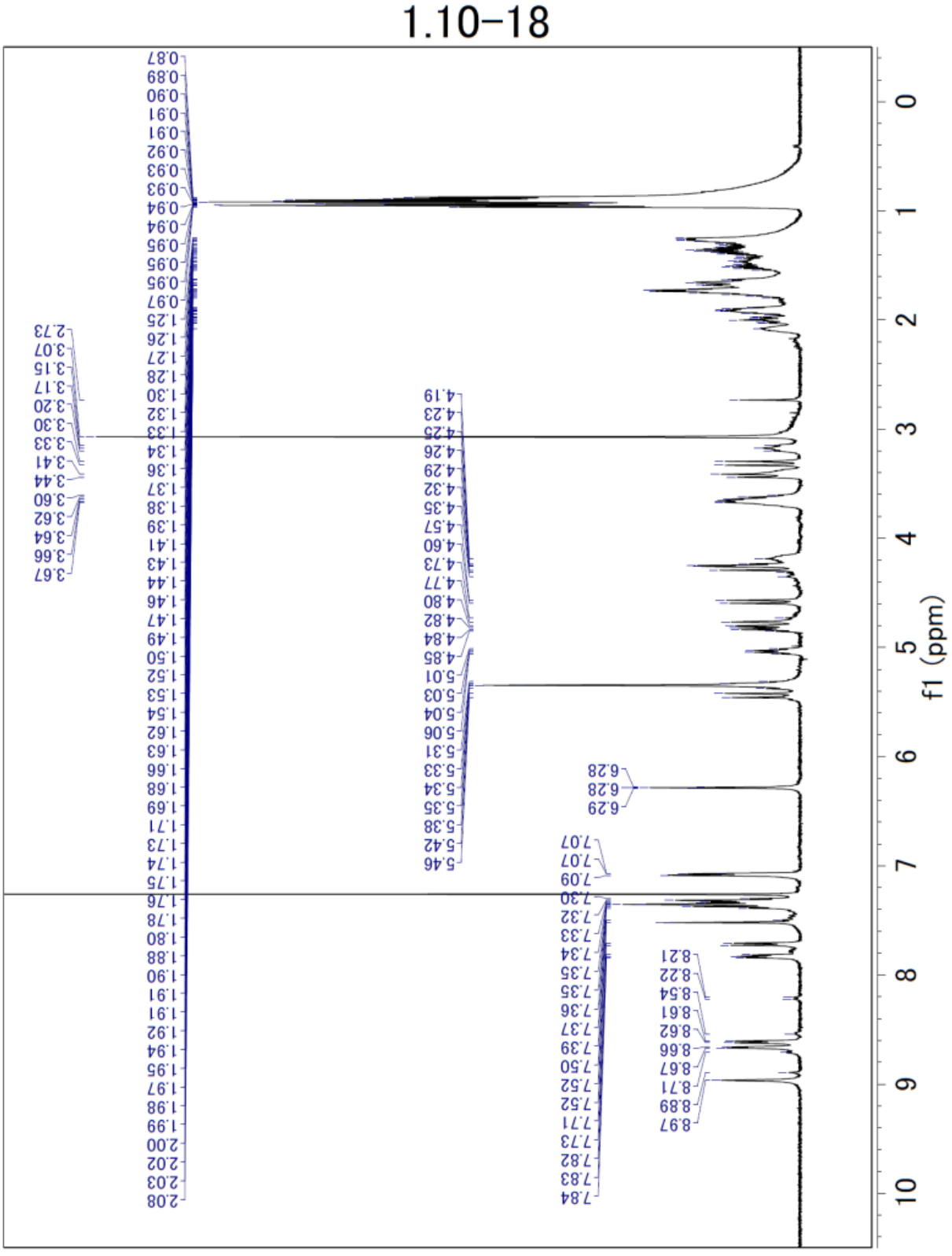
3.8 Compound **10** (1.10-18)



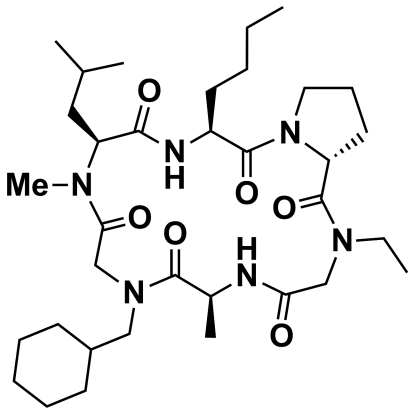
Chemical Formula: $C_{46}H_{65}N_9O_6$
Molecular Weight: 840.07
M+H: 840.513



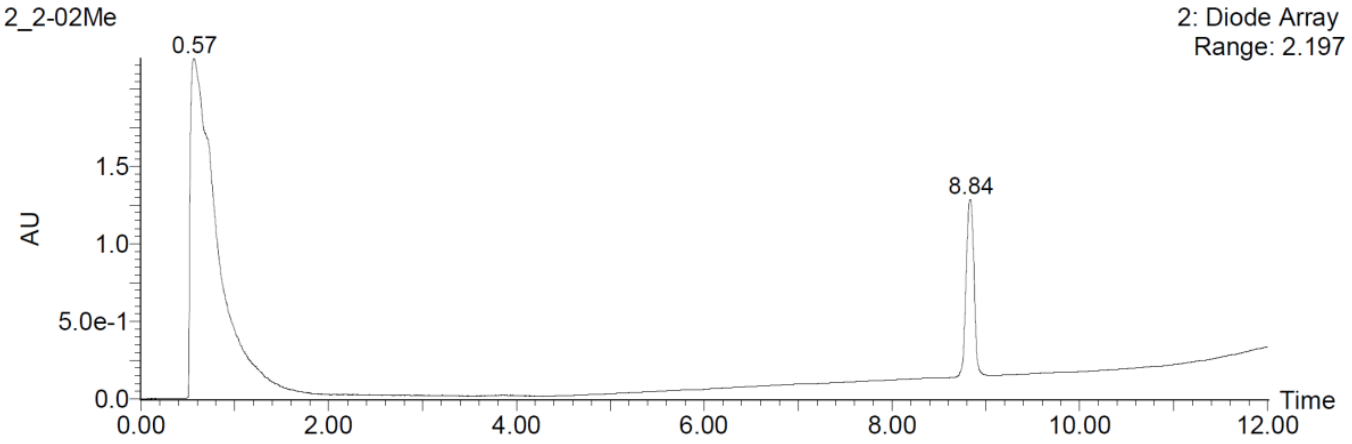


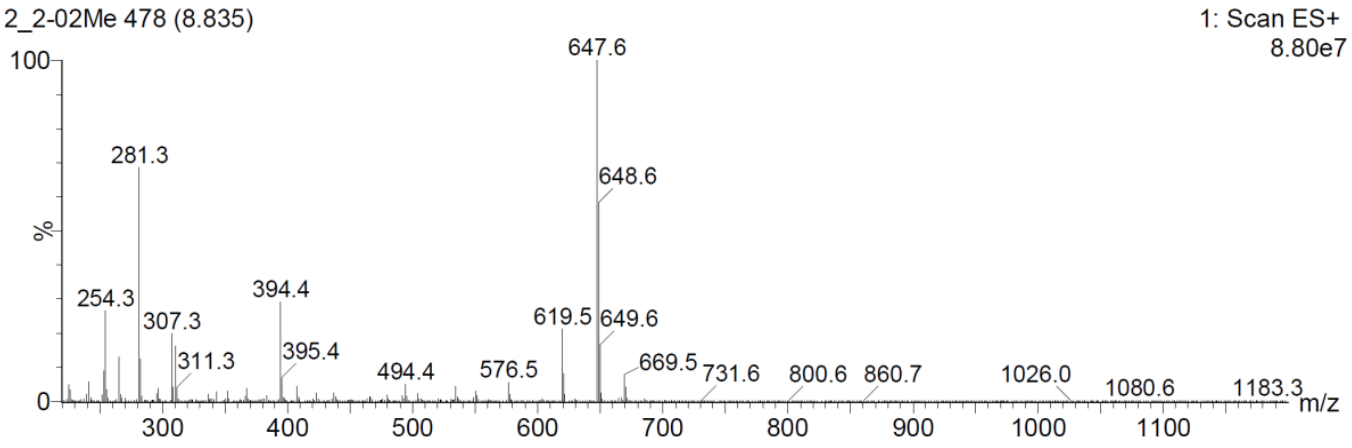

1.10-18
f1 (ppm)

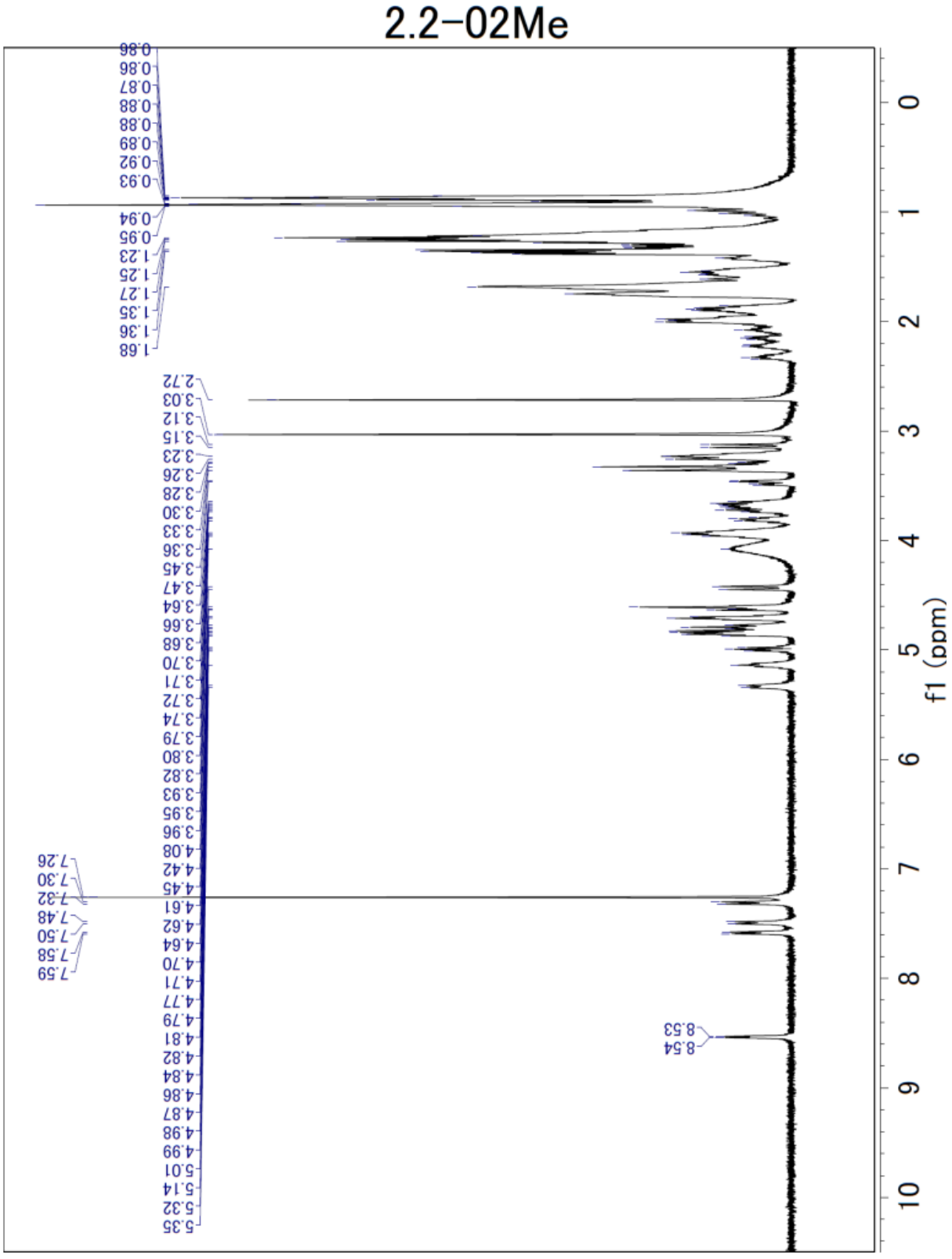
3.9 Compound **11a** (2.2-02Me)



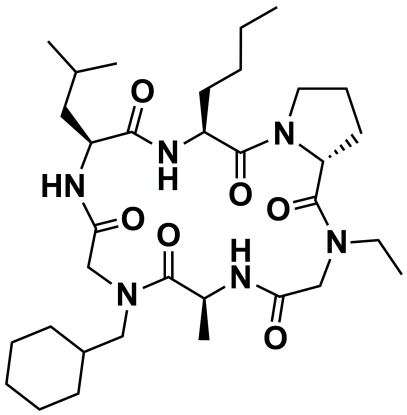
Chemical Formula: $C_{34}H_{58}N_6O_6$
Molecular Weight: 646.86
M+H: 647.449



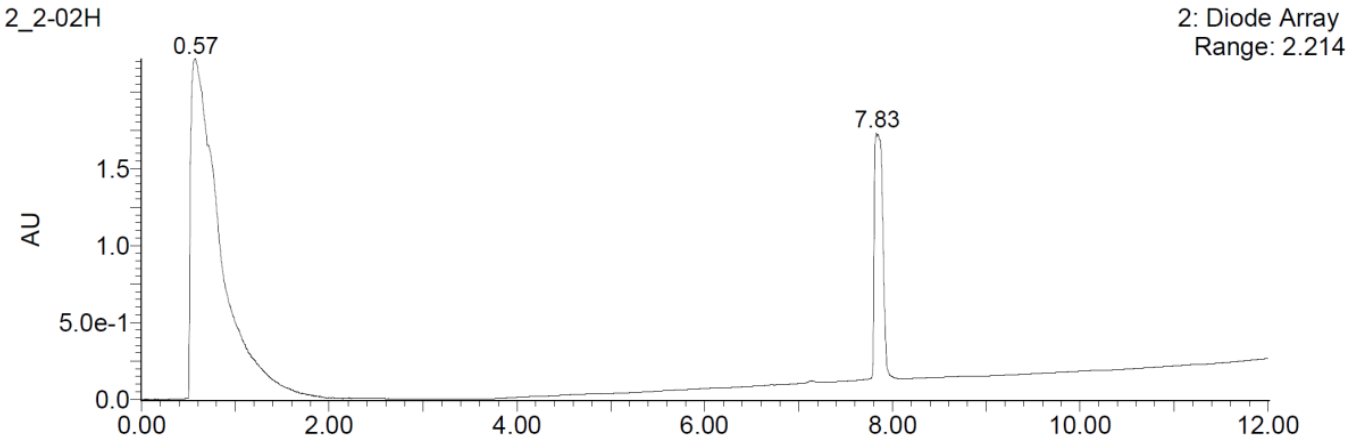


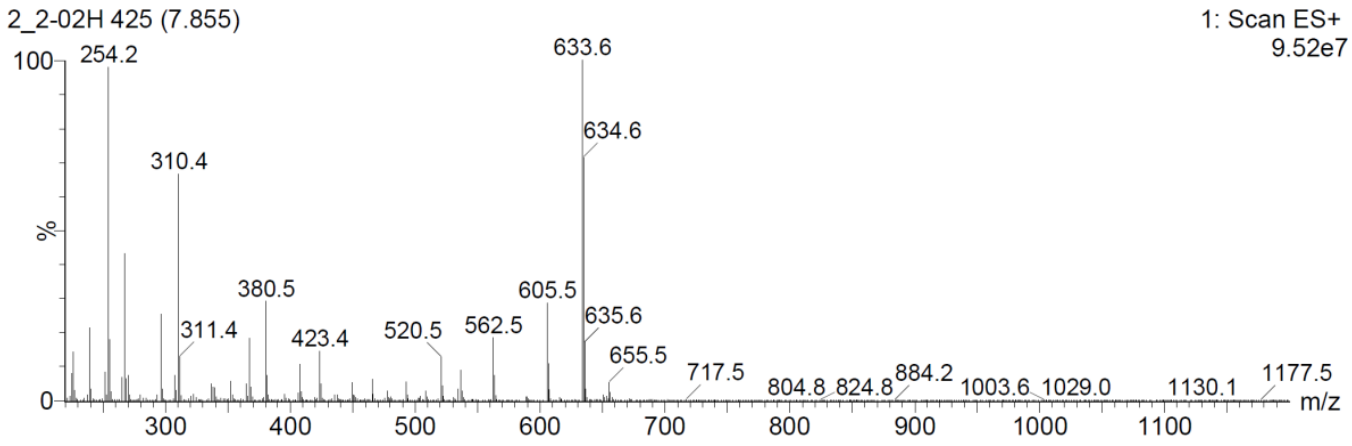

2.2-02Me
f1 (ppm)

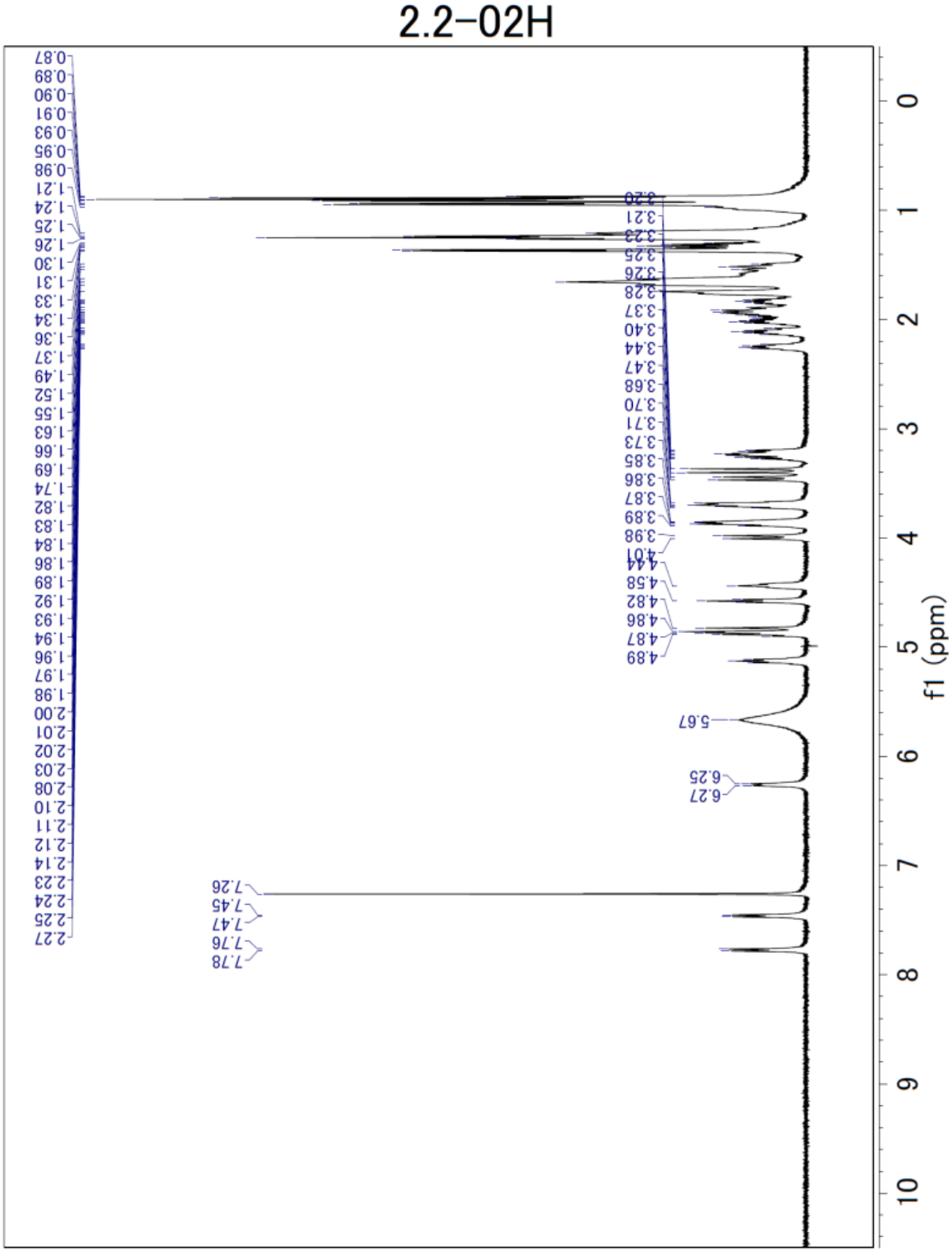
3.10 Compound **11b** (2.2-02H)



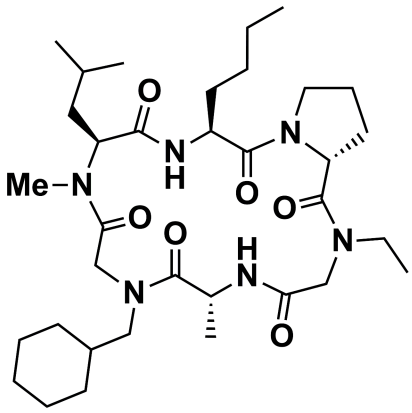
Chemical Formula: $C_{33}H_{56}N_6O_6$
Molecular Weight: 632.83
M+H: 633.433



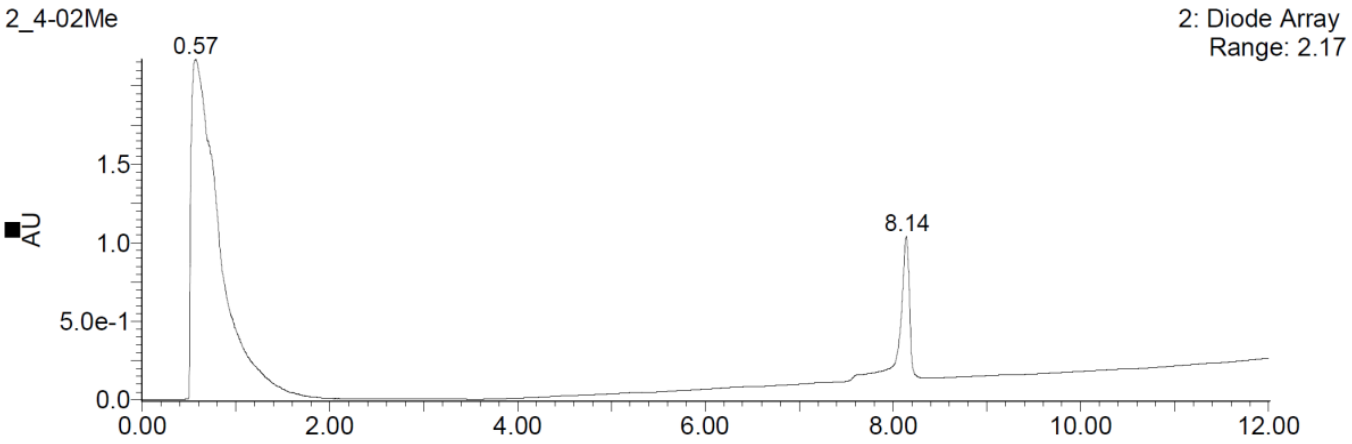


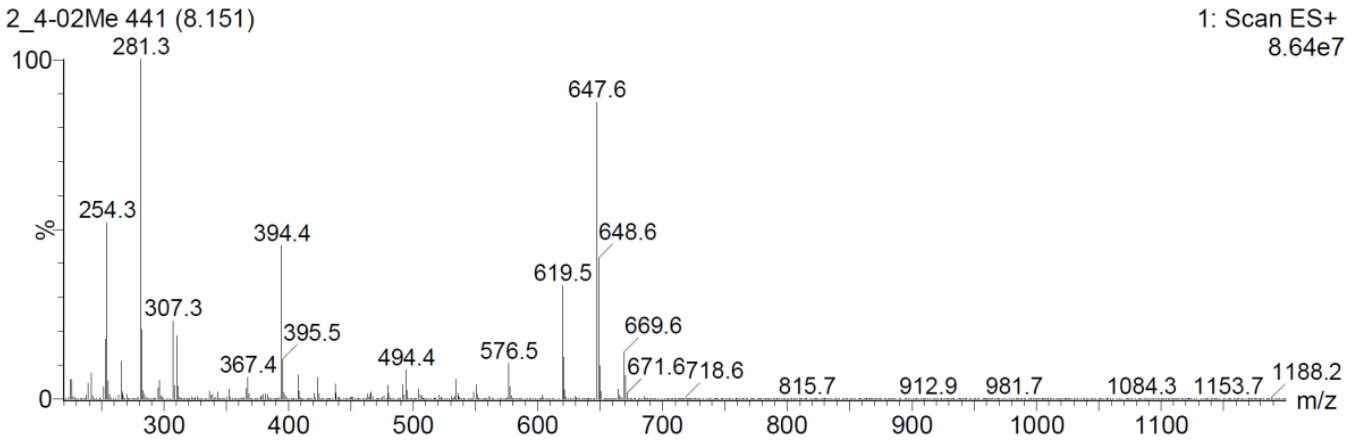

2.2-02H
f1 (ppm)

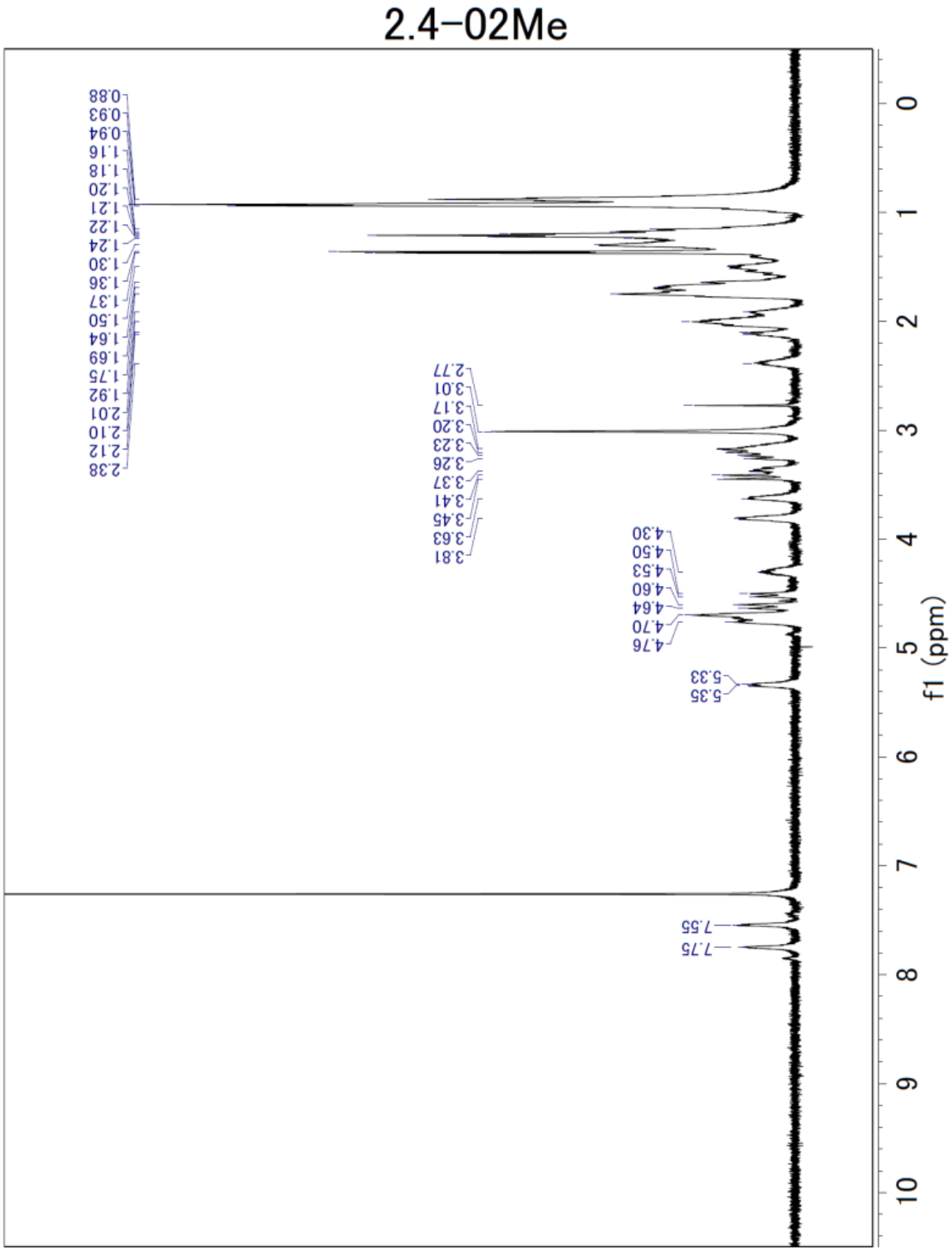
3.11 Compound **12a** (2.4-02Me)



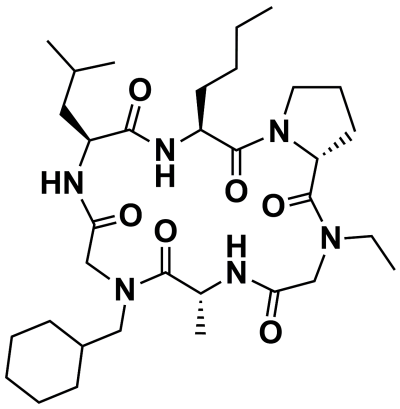
Chemical Formula: $C_{34}H_{58}N_6O_6$
Molecular Weight: 646.86
M+H: 647.449



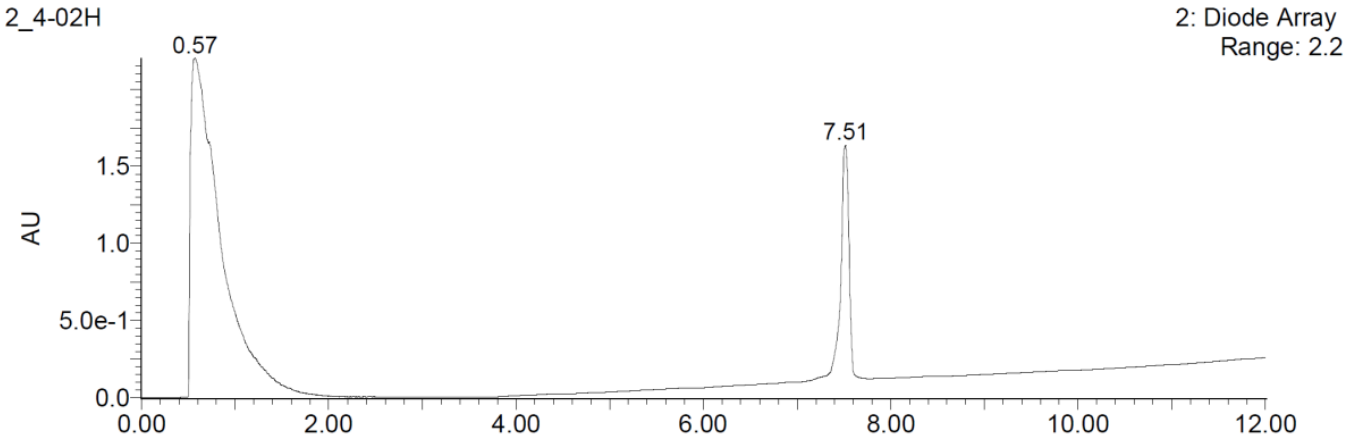


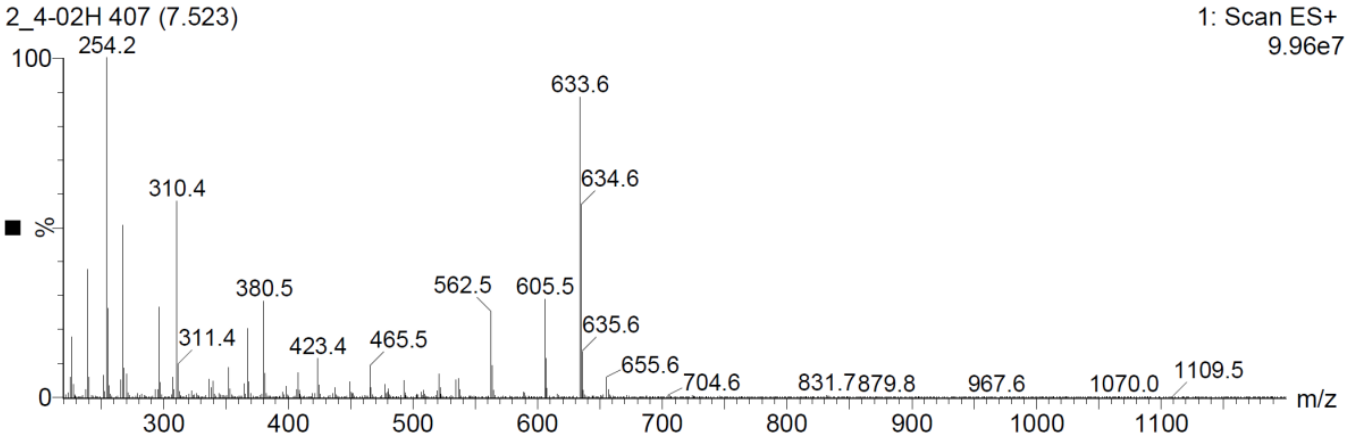

2.4-02Me
0.88
0.93
0.94
1.16
1.18
1.20
1.21
1.22
1.24
1.30
1.36
1.37
1.50
1.64
1.69
1.75
1.92
2.01
2.10
2.12
2.38
2.77
3.01
3.17
3.20
3.23
3.26
3.37
3.41
3.45
3.63
3.81
4.30
4.50
4.53
4.60
4.64
4.70
4.76
5.33
5.35
7.55
7.75
f1 (ppm)

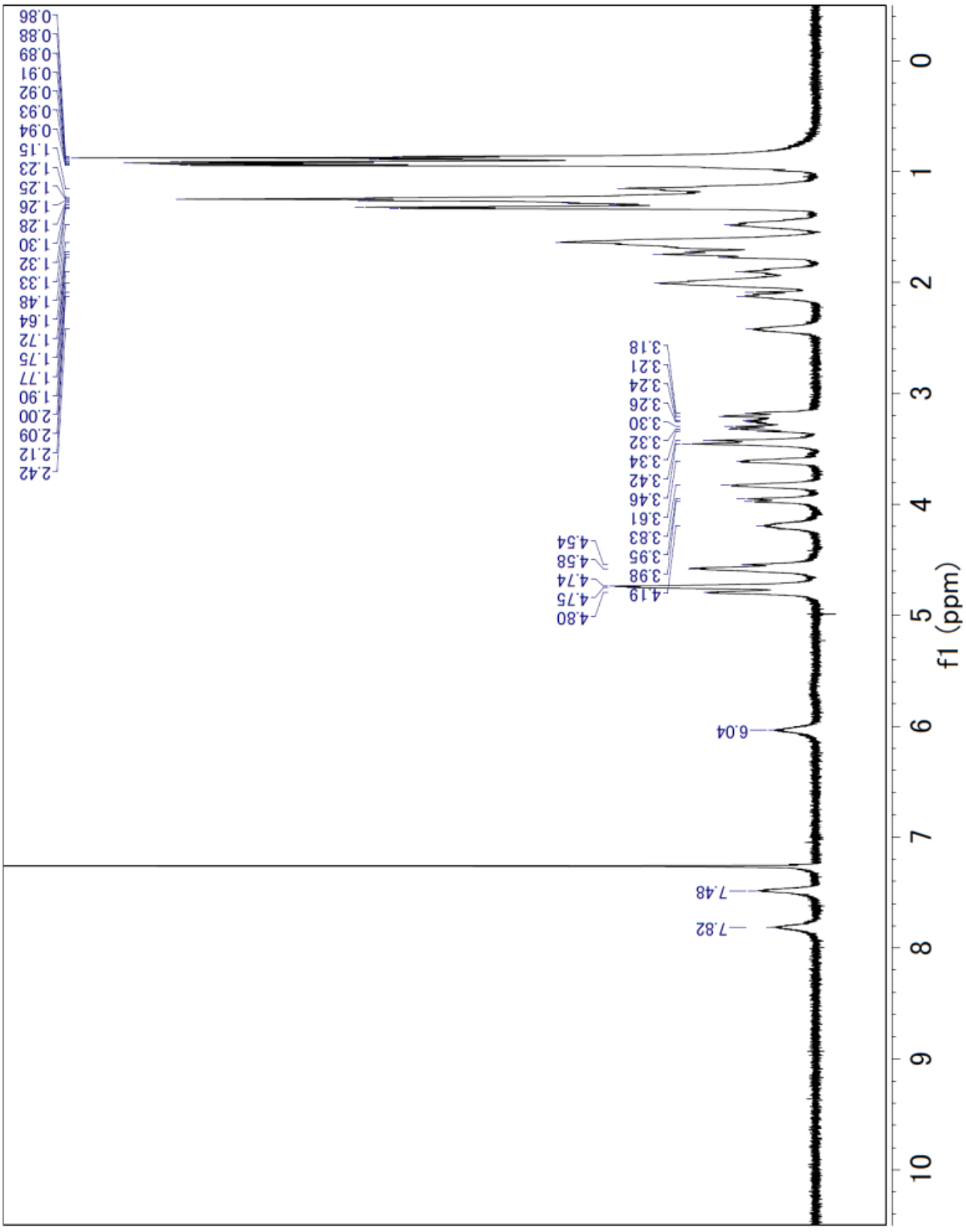
3.12 Compound **12b** (2.4-02H)



Chemical Formula: $C_{33}H_{56}N_6O_6$
Molecular Weight: 632.83
M+H: 633.433





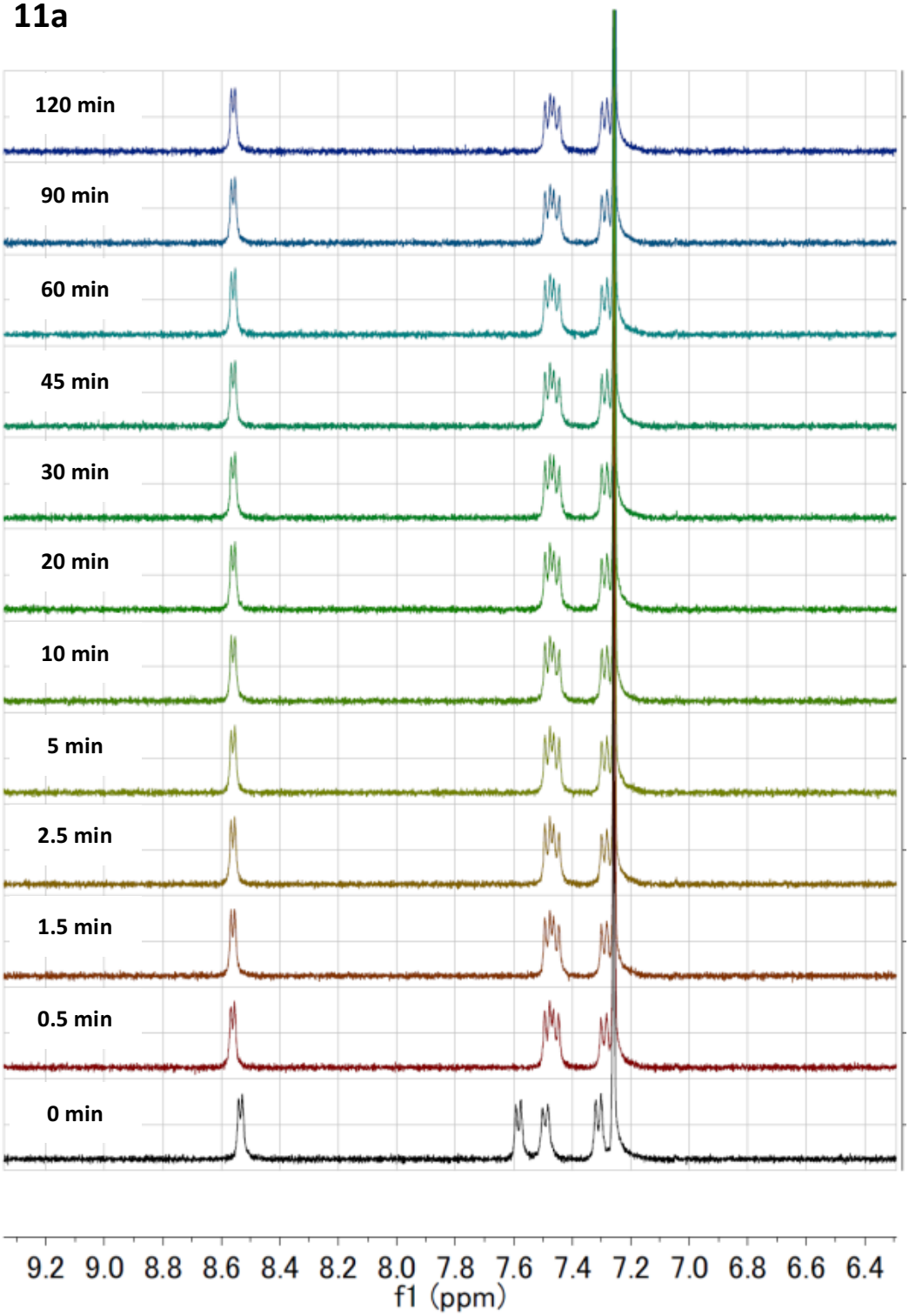

2.4-02H
0.86
0.88
0.89
0.91
0.92
0.93
0.94
1.15
1.23
1.25
1.26
1.28
1.30
1.32
1.33
1.48
1.64
1.72
1.75
1.77
1.90
2.00
2.09
2.12
2.42
3.18
3.21
3.24
3.26
3.30
3.32
3.34
3.42
3.46
3.61
3.83
3.95
3.98
4.19
4.54
4.58
4.74
4.75
4.80
6.04
7.48
7.82
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)

4 H-D exchange experiments

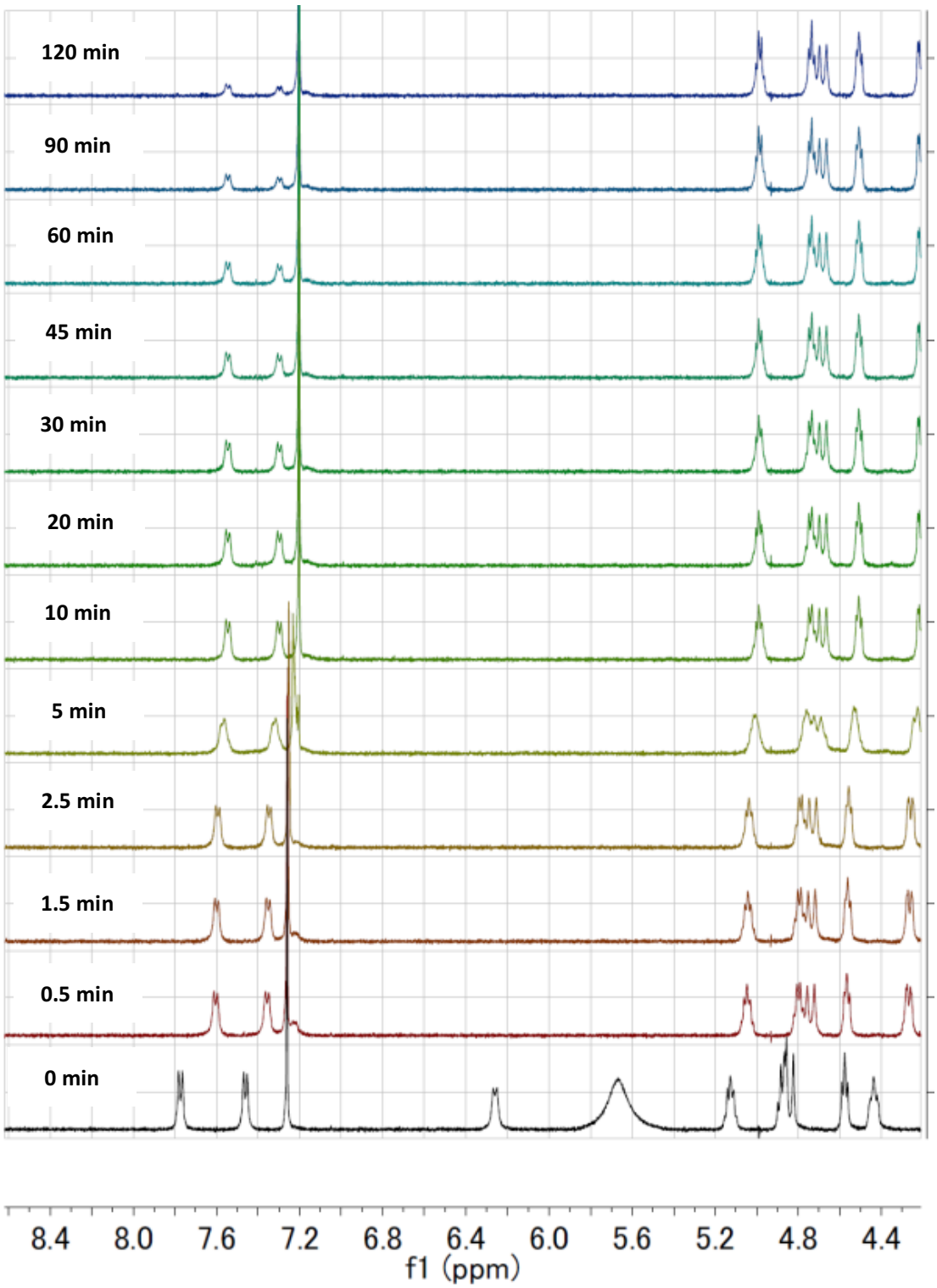
All NMR spectra were recorded in $CDCl_3$ on a Varian 500 MHz NMR instrument with Unity Plus console and 5 mm broadband probe at 25°C. Chemical Shifts were referenced to residual solvent proton signals (1H 7.26ppm for chloroform).

H-D exchange experiments were executed as follows. 5.0 mg of compounds were dissolved in 750 μL of chloroform-d. Before the H-D exchange reaction was initiated, a spectrum was recorded (t=0). The NMR tube was removed from the instrument, and a solution of 39 μL methanol-d_4 containing 10% acetic acid-d_4 was added by syringe to a final concentration of 4.5% (v/v) methanol- d_4 and 0.5% (v/v) acetic acid-d_4. Upon addition of the deuterated solvents and quick agitation, the NMR tube was returned to the spectrometer. Spectra were recorded using sixteen free induction decay transients for each time point at increasing intervals over a period of 2 h. H-D exchange rates were measured by integrating each exchangeable amide resonance separately and recording the ratio of its peak area versus the peak area for downfield nonexchangeable N-methyl protons or α protons.

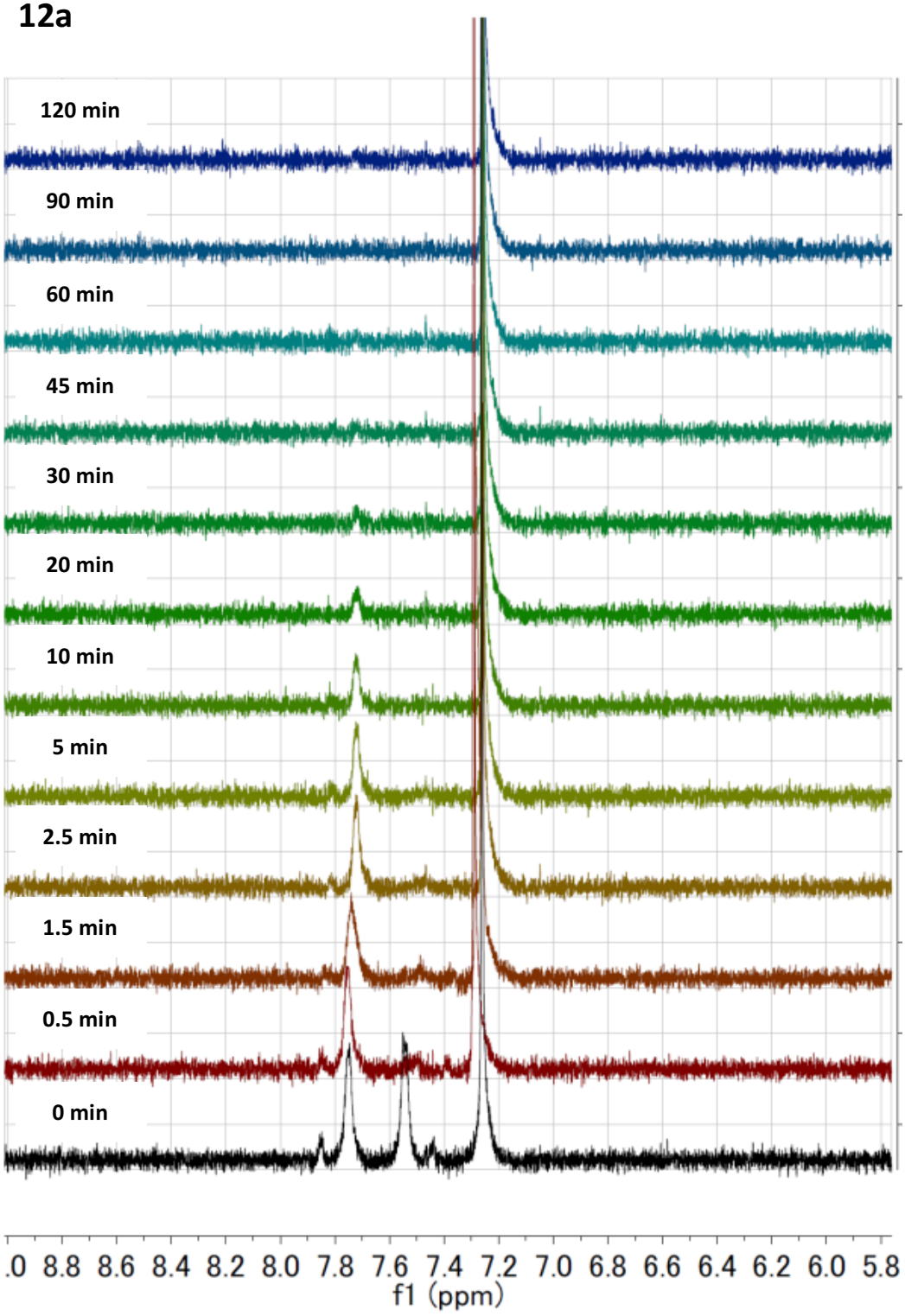
11a


120 min
90 min
60 min
45 min
30 min
20 min
10 min
5 min
2.5 min
1.5 min
0.5 min
0 min
9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)

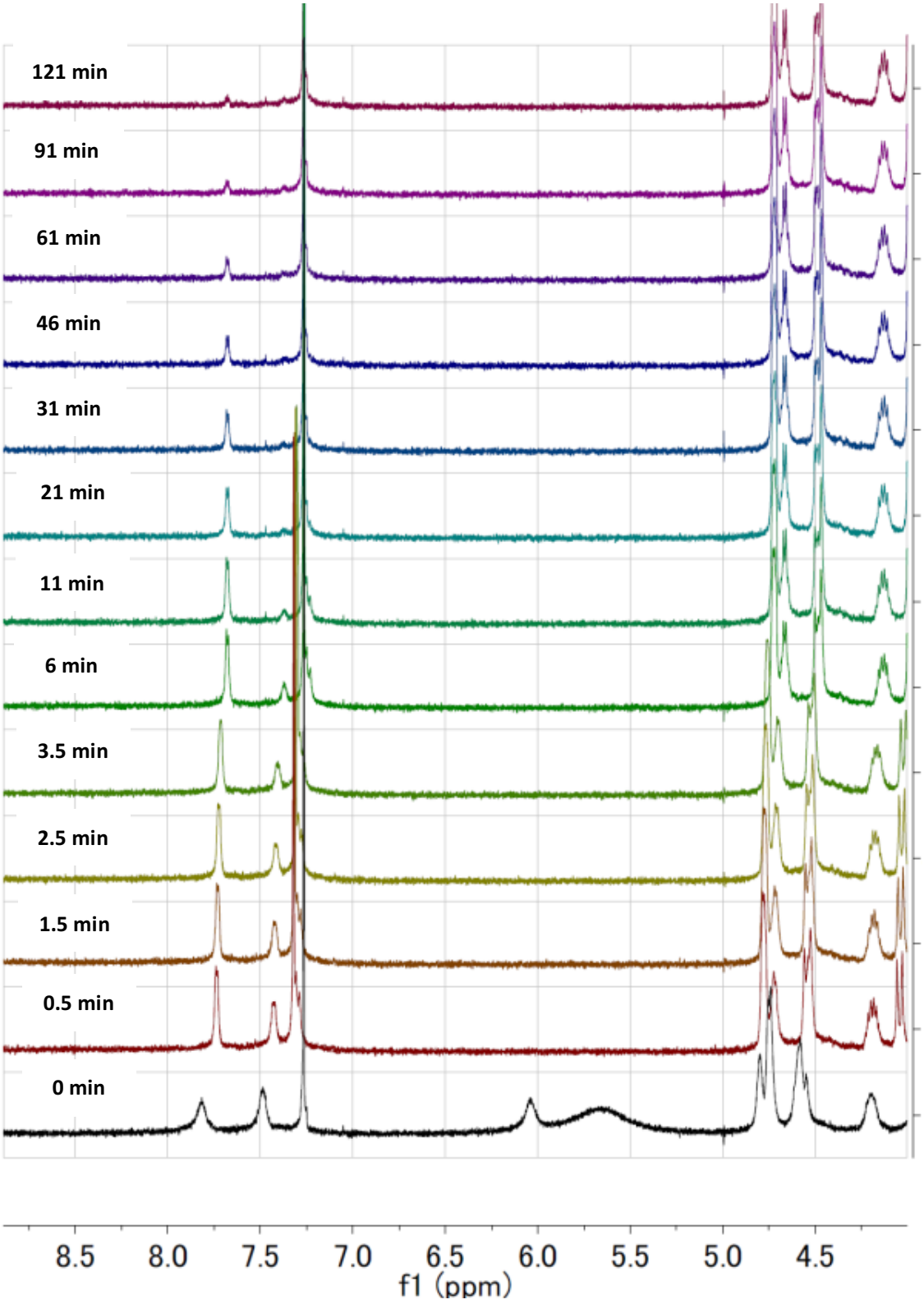
11b


120 min
90 min
60 min
45 min
30 min
20 min
10 min
5 min
2.5 min
1.5 min
0.5 min
0 min
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
f1 (ppm)

12a


120 min
90 min
60 min
45 min
30 min
20 min
10 min
5 min
2.5 min
1.5 min
0.5 min
0 min
.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8
f1 (ppm)

12b


121 min
91 min
61 min
46 min
31 min
21 min
11 min
6 min
3.5 min
2.5 min
1.5 min
0.5 min
0 min
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
f1 (ppm)

5 Caco-2 cell permeability

Caco-2 cell permeability assays was outsourced to Cyprotex PLC. In general, after a 20-day cell culture of Caco-2 cells, individual compounds were incubated at 10 μM for 2h at 37 °C. Then, the concentrations in apical and basolateral compartments were quantified by LC-MS/MS to calculate compound flux in apical to basolateral direction. Lucifer Yellow was used to validate membrane integrity of the Caco-2 cell monolayer. Three reference compounds, atenolol (paracellular transport), propranolol (passive transcellular transport), and talinolol (P-glycoprotein, P-gp, substrate) were screened alongside the test compounds. The same experiments were also conducted in the presence of verapamil as a P-gp inhibitor.

Compound	Direction=AtoB					Direction=AtoB, Inhibitor: verapamil				
	P_{app} ($\times10^{-6}$ cm/s)		Mean P_{app} ($\times10^{-6}$ cm/s)	SD	Mean % Recovery	Papp ($\times10^{-6}$ cm/s)		Mean P_{app} ($\times10^{-6}$ cm/s)	SD	Mean % Recovery
	Replicate 1	Replicate 2				Replicate 1	Replicate 2			
3	**1.03**	**1.04**	**1.04**	**0.01**	**92.6**	**9.32**	**11.1**	**10.2**	**1.25**	**87.7**
4	**1.24**	**1.34**	**1.29**	**0.07**	**77.9**	**11.9**	**12.9**	**12.4**	**0.71**	**79.9**
5	**3.66**	**4.10**	**3.88**	**0.31**	**85.4**	**20.1**	**22.0**	**21.1**	**1.33**	**87.6**
6	**1.02**	**1.55**	**1.29**	**0.38**	**83.1**	**13.6**	**15.9**	**14.8**	**1.66**	**92.7**
7	**0.84**	**0.72**	**0.78**	**0.08**	**81.6**	**8.96**	**10.4**	**9.67**	**1.00**	**82.3**
8	**0.63**	**0.70**	**0.67**	**0.05**	**62.7**	**4.90**	**7.97**	**6.43**	**2.17**	**67.6**
9	**0.64**	**0.78**	**0.71**	**0.10**	**74.8**	**7.67**	**9.84**	**8.75**	**1.53**	**80.3**
10	**0.92**	**0.99**	**0.96**	**0.05**	**75.5**	**5.59**	**8.16**	**6.87**	**1.82**	**77.5**
atenolol	**0.19**	**0.25**	**0.22**	**0.04**	**94.2**	**0.29**	**0.22**	**0.25**	**0.05**	**91.0**
propranolol	**27.3**	**26.6**	**27.0**	**0.48**	**68.8**	**37.8**	**31.1**	**34.5**	**4.79**	**80.4**
talinolol	**0.26**	**0.28**	**0.27**	**0.01**	**88.1**	**1.22**	**0.87**	**1.04**	**0.25**	**94.0**

Table S3. Caco-2 cell permeability