Supporting Information

Total Syntheses of Fimsbactin A and B and Their Stereoisomers to Probe the Stereoselectivity of the Fimsbactin Uptake Machinery in *Acinetobacter baumannii*

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SUPPLEMENTAL FIGURES

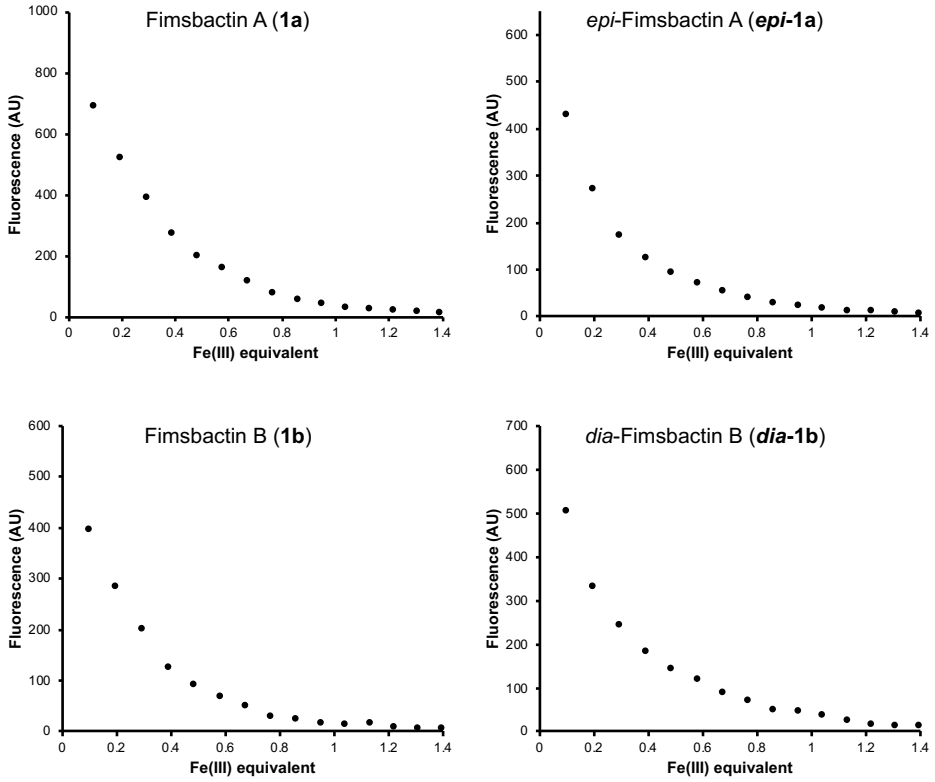


Figure S1. Fluorescence titration of each 500 μM fimsbactin in ethanol with $FeCl_3$ (λ_{ex} = 320 nm, λ_{em} = 400 nm). The plot of fluorescence versus Fe(III) equivalent for each fimsbactin was very close to the one previously presented by Bohac et al.[S5], which shows that all fimsbactin isomers are likely bind with Fe(III) at the 1:1 stoichiometry. Since *epi*-fimsbactin B (***epi*-1b**) and *ent*-fimsbactin B (***ent*-1b**) were enantiomers of ***dia*-1b** and **1b**, respectively, they were not included in this experiment.

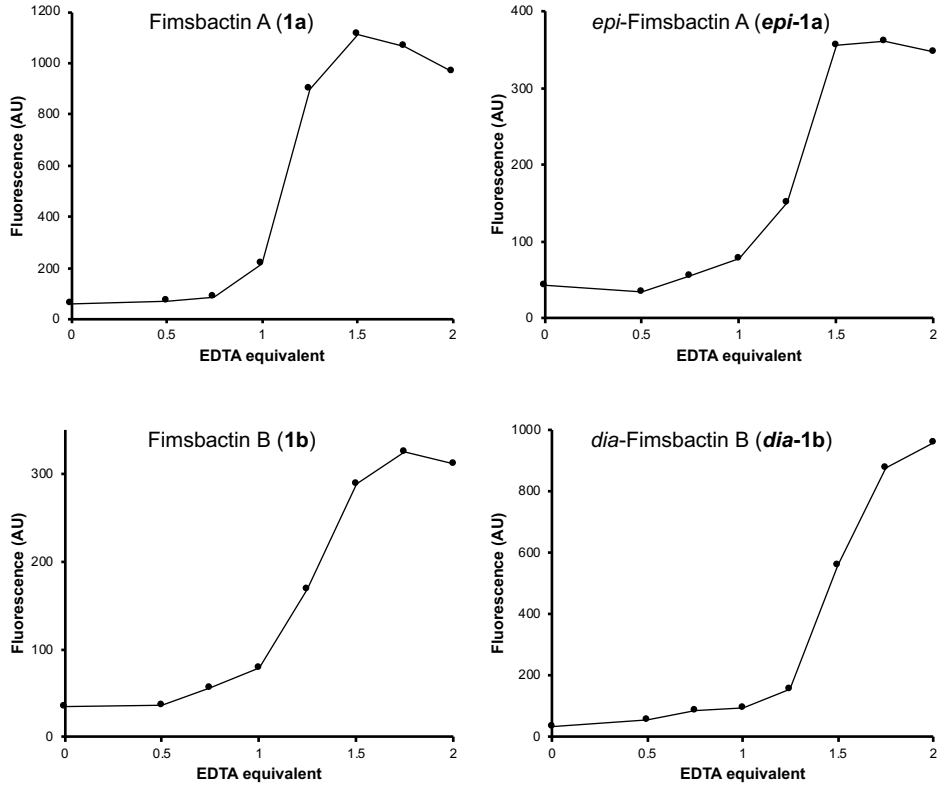


Figure S2. Fluorescence titration of each 500 μM Fe(III)-fimsbactin complex in ethanol with EDTA (λ_{ex} = 320 nm, λ_{em} = 400 nm). Upon a series of additions of EDTA, gradual recovery of the fluorescence corresponding to the release of *apo*-fimsbactin caused by competition of EDTA was observed. In all cases, discernible fluorescence recovery became visible right after addition of 1 equivalent of EDTA to the similar extent, which indicates that the Fe(III) affinities of all tested fimsbactin isomers would be comparable to each other. Since *epi*-fimsbactin B (***epi*-1b**) and *ent*-fimsbactin B (***ent*-1b**) were enantiomers of ***dia*-1b** and **1b**, respectively, they were not included in this experiment.

SUPPLEMENTAL TABLE

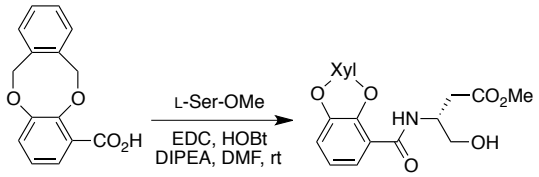
	^{15}N-labeled Fimsbactin A (reported)[S3]			**Fimsbactin A (1a)**			***epi*-Fimsbactin A (*epi*-1a)**		
Position	^{13}C, ppm	^{1}H, ppm	*J* (Hz)	^{13}C, ppm	^{1}H, ppm	*J* (Hz)	^{13}C, ppm	^{1}H, ppm	*J* (Hz)
1	148.2			148.3			146.8		
2	145.7			145.8			145.8		
3	119.3	6.968	dd, 1H (8.0, 1.5)	119.5	6.96	*app* t, 1H (8.0)	119.4	6.97	*br* d, 1H (7.4)
4	118.6	6.74	t, 1H (8.0)	118.7	6.74	*app* t, 1H (7.6)	118.7	6.74	*app* t, 1H (7.8)
5	117.7	7.08	dd, 1H (8.0, 1.5)	117.9	7.09	d, 1H (7.7)	117.9	7.08	d, 1H (7.8)
6	110.1			110.1			110.1		
7	166.3			166.5			166.6		
9	69.1	4.52	dd, 1H (8.0, 7.5)	69.3	4.52	*app* t, 1H (7.7)	69.4	4.46	m, 1H
		4.61	dd, 1H (10.0, 8.5)		4.61	*br* m, 1H		4.60	*br* m, 1H
10	66.9	5.06	dd, 1H (10.0, 7.5)	67.2	5.07	dd, 1H (10.0, 7.5)	67.1	5.07	dd, 1H (10.0, 7.5)
11									
12	169.9			170.1			170.0		
13		8.72	dd, 1H (93.0, 8.0)		8.80	*br* s, 1H		8.74	*br* s, 1H
14	51.5	4.72	m, 1H	51.7	4.71	m, 1H	51.6	4.73	m, 1H
15	64.3	4.39	m, 1H	64.4	4.39	m, 1H	64.2	4.46	m, 1H
		4.61	m, 1H		4.57	dd, 1H (11, 4.7)		4.46	m, 1H
17	168.7			168.9			168.8		
18	112.8			112.7			112.6		
19	149.5			148.3			148.3		
20	146.0			146.2			146.4		
21	120.7	6.97	dd, 1H (8.0, 1.5)	120.4	6.96	*app* t, 1H (8.0)	119.9	6.97	*br* d, 1H (7.4)
22	118.6	6.59	t, 1H (8.0)	118.7	6.55	*app* t, 1H (7.6)	118.7	6.64	*app* t, 1H, (7.8)
23	119.6	7.15	dd, 1H (8.0, 1.5)	119.8	7.14	d, 1H (7.7)	118.8	7.18	d,1H (7.9)
24	167.7			167.9			168.0		
25		8.23	dt, 1H (92.0, 5.5)		8.31	*br* s, 1H		8.39	*br* s, 1H
26	38.3	3.10	m, 2H	38.5	3.12	m, 2H	38.5	3.11	m, 2H
27	25.9	1.38	m, 2H	26.1	1.38	m, 2H	26.0	1.37	m, 2H
28	23.5	1.49	m, 2H	23.7	1.49	m, 2H	23.7	1.48	m, 2H
29	46.3	3.45	t, 2H (7.0)	46.5	3.45	m, 2H	46.4	3.44	t, 2H (6.5)
30									
31	170.1			170.2			170.2		
32	20.1	1.96	s, 3H	20.4	1.96	s, 3H	20.4	1.95	s, 3H

Table S1. Comparison of the NMR spectral data of fimsbactin A (1a) and *epi*-fimsbactinA (*epi*-1a).

SUPPLEMENTAL METHODS

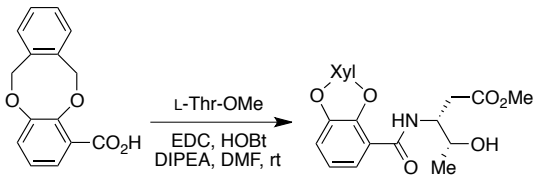
A. PROCEDURES FOR CHEMICAL SYNTHESIS

All reactions were conducted in oven-dried glassware under nitrogen atmosphere with anhydrous solvents, unless otherwise noted. All reactions were monitored by analytical thin-layer chromatography (TLC) using pre-coated silica aluminum plate with F254 indicators, and the product profiles were visualized by UV irradiation (254 nm, 365 nm) and/or staining with a phosphomolybdic acid, ninhydrin, or potassium permanganate solution. The solvents, dichloromethane, toluene, tetrahydrofuran (THF), and *N*,*N*-dimethylformate (DMF) were dried by being passed through activated alumina column. Other anhydrous solvents were purchased from Sigma-Aldrich (Missouri, USA) or Acros Organics (Belgium). All chemical reagents used in the reactions were purchased from Sigma-Aldrich, Acros Organics, TCI Chemicals (Japan), Alfa-Aesar (Massachusettes, USA), AK Scientific (California, USA), or Daejung Chemicals & Metals (Republic of Korea), and they were used as received unless otherwise noted. ^{1}H-NMR and ^{13}C-NMR data were recorded using Varian Unity 400 (400/100 MHz) or Bruker Advance 500 (500/125 MHz). Chemical shifts were reported in parts per million (ppm) relative to chloroform (^{1}H: 7.26 ppm, ^{13}C: 77.0 ppm), methanol (^{1}H: 3.31 ppm, ^{13}C: 49.05 ppm), D_2O (^{1}H: 4.65 ppm), or tetramethylsilane (TMS, 0.00 ppm), and the coupling constants were reported in Herz (Hz). High-resolution mass spectra were collected using Bruker Compact QTOF, where the electrospray ionization method was employed for ionization.

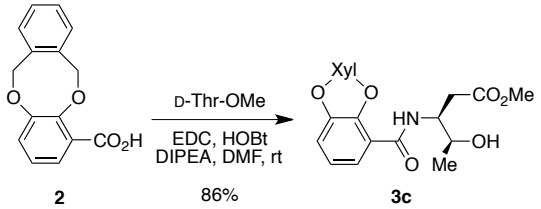


Compound 3a. To a solution of acid **2** [S1] (2.170 g, 8.468 mmol), L-Ser-OMe•HCl (1.970 g, 12.70 mmol), and *N*,*N*-diisopropylethylamine (DIPEA, 4.4 ml, 25.40 mmol) in *N*,*N*-dimethylformamide (DMF, 42 mL) was added *N*-(3-dimethylaminopropyl)-*N*′-ethylcarbodiimide (EDC, 3.25 g, 16.93 mmol) and 1-hydroxybenzotriazole hydrate (HOBt, 2.59 g, 16.93 mmol) at 0 ºC. After the temperature was elevated to room temperature, the stirring continued for 3 hr. Upon confirmation of complete consumption of **2**, the solvent was removed under reduced pressure, and the resulting residue was diluted with ethyl acetate (250 mL). The organic phase was sequentially washed with 1 M HCl solution, saturated sodium bicarbonate solution, and brine. The solution was dried over anhydrous magnesium sulfate and concentrated under reduced pressure to afford the crude product in a solid form. After washed with petroleum ether, the solid was resuspended in dichloromethane, and the resulting solution was washed with 1 M HCl solution and saturated sodium bicarbonate solution in sequence. After concentration under reduced pressure, the desired amide **3a** (2.768 g, 7.282 mmol) was obtained in 86% yield with no further purification. ^{1}H NMR (500

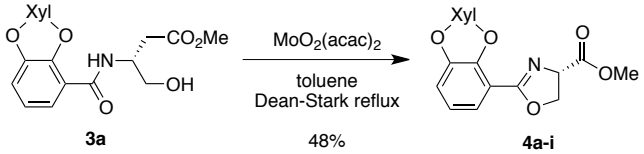
MHz, $CDCl_3$) δ 9.14 (d, *J* = 6.7 Hz, 1H), 7.78 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.28 – 7.25 (m, 2H), 7.20 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.12 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.98 (*app* t, *J* = 7.9 Hz, 1H), 5.68 (d, *J* = 12.3 Hz, 1H), 5.58 (d, *J* = 12.3 Hz, 1H), 5.40 (d, *J* = 13.7 Hz, 1H), 5.31 (d, *J* = 13.7 Hz, 1H), 4.86 (dt, *J* = 7.2, 3.7 Hz, 1H), 4.05 – 4.03 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 165.4, 150.2, 149.6, 136.5, 133.9, 130.3, 129.3, 128.8, 128.0, 126.7, 126.3, 124.7, 123.1, 76.5, 75.2, 63.8, 55.6, 55.9. HR-MS (ESI-TOF) *m/z* for $[C_{19}H_{19}NNaO_6]^+$ ($[M + Na]^+$): calculated 380.1110, found 380.1107.



Compound 3b. Amide **3b** was prepared by following the previously established synthetic method[S1] from acid **2** using L-Thr-OMe in 89% yield. The ^{1}H-, ^{13}C-NMR and HR-MS spectra of compound **3b** were reported in Ref. S1.

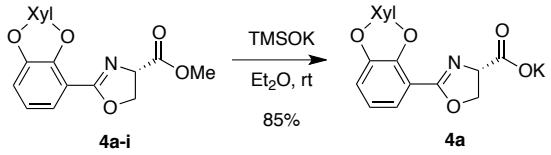


Compound 3c. Amide **3c** was prepared following the method used for synthesis of amide **3b**[S1] except for the use of D-Thr-OMe instead of L-Thr-OMe, and the yield was 86%. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **3c** were identical to those of its enantiomer, compound **3b**.

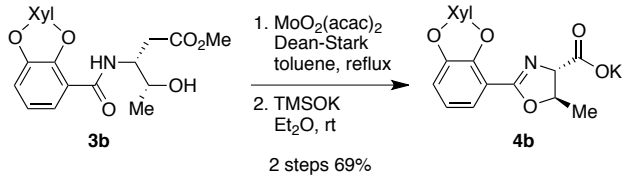


Compound 4a-i. The reaction was carried out in a flask fitted with a pressure-equalized addition funnel (containing a cotton plug and molecular sieves to function as a Soxhlet extractor) surmounted with a reflux condenser. A solution of amide **3a** (0.512 g, 1.491 mmol) and bis(acetylacetonato)dioxomolybdenum(VI) ($MoO_2(acac)_2$, 48.6 mg, 10 mol%) in toluene (150 mL) was heated with an oil bath under azeotropic reflux. After 8 h, the reaction mixture was cooled to the ambient temperature and concentrated under reduced pressure. The crude product was subjected to flash column chromatography (SiO_2, hexanes:etheyl acetate = 9:1) to yield the desired ester **4a-i** (0.242 g, 0.710 mmol) in 48% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.8, 1.7 Hz, 1H). 7.26 – 7.24 (m, 2H), 7.20 – 7.19

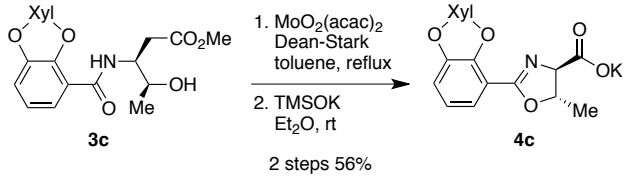
(m, 1H), 7.17 – 7.15 (m, 1H), 7.10 (dd, *J* = 8, 1.7 Hz, 1H), 6.93 (t, 7.9 Hz, 1H), 5.45 (d, *J* = 12.4 Hz, 1H), 5.44 (d, *J* = 5.1 Hz, 2H), 5.38 (d, *J* = 12.8 Hz, 1H), 4.97 (dd, *J* = 10.6, 7.9 Hz, 1H), 4.66 (t, *J* = 8.3 Hz, 1H), 4.58 (dd, *J* = 10.7, 8.7 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.9, 165.2, 151.5, 149.6, 136.0, 135.4, 129.3, 128.7, 128.6, 128.5, 125.2, 124.9, 123.5, 121.5, 76.0, 74.9, 69.5, 68.8, 52.7. HR-MS (ESI-TOF) *m/z* for $[C_{19}H_{18}NO_5]^+$ ($[M + H]^+$): calculated 340.1185, found 340.1192.



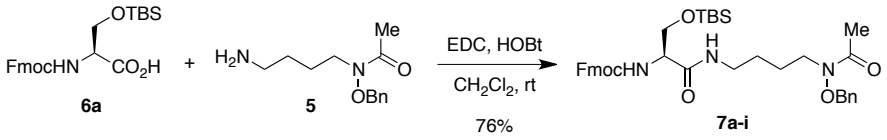
Compound 4a. Ester **4a-i** (0.242 g, 0.710 mmol) was dissolved in ethyl ether (20 mL) and treated with potassium trimethylsilanolate (0.288 g, 0.852 mmol) at room temperature. After stirred for 3 hr, the resulting solid was collected by filtration and washed with hexane/ethyl ether (1:1). The crude product was dried under reduced pressure to afford the desired potassium carboxylate **4a** (0.199 g, 0.61 mmol) in 85% yield. The product was used in the next step without further purification. ^{1}H NMR (500 MHz, methanol-d^4) δ 7.38 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.28 – 7.25 (m, 2H), 7.27 – 7.22 (m, 2H), 7.08 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.94 (*app* t, *J* = 7.9 Hz, 1H), 5.49 (d, *J* = 13.2 Hz, 1H), 5.44 (d, *J* = 13.2 Hz, 1H), 5.43 (d, *J* = 2.3 Hz, 2H), 4.77 (dd, *J* = 10.6, 8.5 Hz, 1H), 4.62 (dd, *J* = 10.6, 8.2 Hz, 1H), 4.52 (t, *J* = 8.4 Hz, 1H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, methanol-d^4) δ 180.4, 178.8, 165.2, 152.3, 150.3, 137.2, 136.9, 130.4, 130.0, 129.8, 129.7, 126.2, 125.8, 124.4, 123.4, 76.2, 75.7, 72.4, 72.2. HR-MS (ESI-TOF) *m/z* for $[C_{18}H_{16}NO_5]^+$ ($[M + H]^+$): calculated 326.1028, found 326.1023.



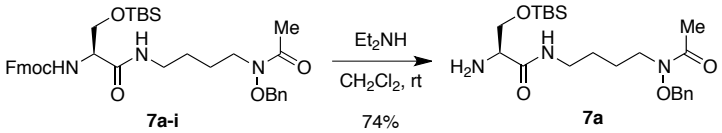
Compound 4b. The synthesis of compound **4b** from **3b** was previously reported in Ref S1.



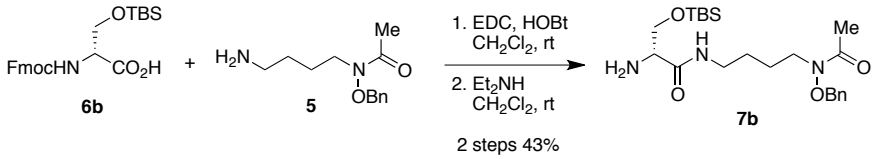
Compound 4c. Potassium carboxylate **4c** was prepared from **3c** following the method used for synthesis of amide **4a**, and the two-step yield was 56%. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **4c** were identical to those of its enantiomer, compound **4b** reported in Ref S1.



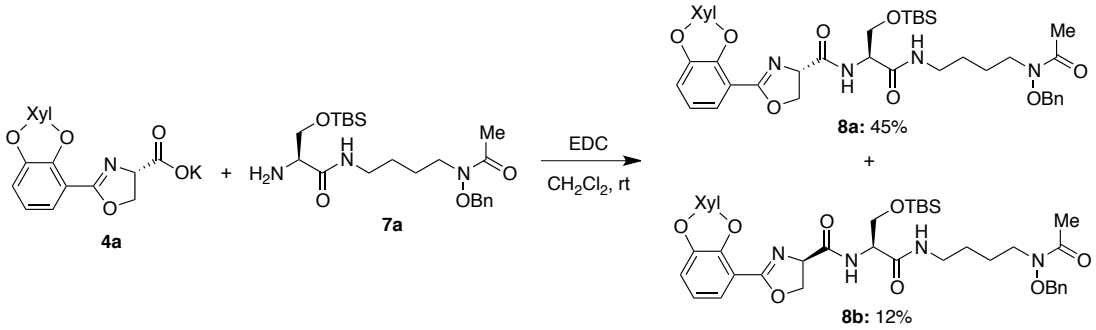
Compound 7a-i. To a solution of the amine **5**[S2] (3.00 g, 10.2 mmol) and Fmoc-L-Ser(TBS)-OH **6a** (4.60 g, 12.2 mmol) in dichloromethane (60 mL) was added EDC (2.33 g, 12.2 mmol) and HOBt (1.65 g, 12.2 mmol) at 0 ºC. After stirred for 3 hr at room temperature, the reaction mixture was diluted with ethyl acetate (50 mL) and poured into 1 N HCl solution (100 mL). After collecting the organic layer, the aqueous layer was further extracted with ethyl acetate (100 mL × 2). The combined organic layers were washed with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. The crude residue was subjected to flash column chromatography (SiO_2, 2% methanol in dichloromethane) to afford the desired Fmoc-amine intermediate **7a-i** (5.12 g, 7.75 mmol) in 76% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.5 Hz, 2H), 7.59 (*br* t, *J* = 6.5 Hz, 2H), 7.42 – 7.34 (m, 7H), 7.31 (td, *J* = 7.5, 1.0 Hz, 2H), 6.66 (*br* s, 1H), 5.77 (*br* s, 1H), 4.79 (s, 2H), 4.40 (d, *J* = 7.4 Hz, 2H), 4.22 (t, *J* = 7.1 Hz, 1H), 4.16 (*br* s, 1H), 4.02 (dd, *J* = 9.8, 3.9 Hz, 1H), 3.68 – 3.60 (m, 3H), 3.35 – 3.24 (m, 2H), 2.08 (s, 3H), 1.70 – 1.63 (m, 2H), 1.55 – 1.47 (m, 2H), 0.89 (s, 9H), 0.08 (s, 3H), 0.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.4, 170.1, 156.1, 143.9, 143.8, 141.37, 141.36, 134.4, 129.3, 129.1, 128.8, 127.8, 127.1, 125.18, 125.16, 120.1, 76.4, 67.2, 63.3, 55.8, 47.2, 44.8, 39.3, 26.6, 25.9, 24.4, 20.5, 18.2, –5.4, –5.5. HR-MS (ESI-TOF) *m/z* for $[C_{37}H_{49}N_3NaO_6Si]^+$ ($[M + Na]^+$): calculated 682.3288, found 682.3286.



Compound 7a. A solution of **7a-i** (5.12 g, 7.75 mmol) in dichloromethane (40 mL) was treated with diethylamine (20 mL) at room temperature. After stirred for 6 hr, the crude product was dried under reduced pressure. The crude product was subjected to flash column chromatography (SiO_2, 10% methanol in dichloromethane) to afford the desired amine **7a** (2.50 g, 5.71 mmol) in 74% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (*br* t, *J* = 4.6 Hz, 1H), 7.40 – 7.34 (m, 4H), 4.80 (s, 2H), 3.82 (dd, *J* = 9.9, 4.6 Hz, 1H), 3.77 (dd, *J* = 9.9, 6.1 Hz, 1H), 3.68 – 3.63 (*br* m, 2H), 3.46 (dd, *J* = 5.9, 4.7 Hz, 1H), 3.25 (q, *J* = 6.9 Hz, 2H), 2.09 (s, 3H), 1.69 – 1.63 (m, 2H), 1.54 – 1.48 (m, 2H), 0.87 (s, 9H), 0.06 (s, 3H), 0.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.9, 172.2, 134.3, 129.1, 128.9, 128.6, 76.2, 65.3, 56.5, 50.1, 44.7, 38.5, 26.7, 25.7, 24.2, 20.4, 18.1, –5.5, –5.6. HR-MS (ESI-TOF) *m/z* for $[C_{22}H_{40}N_3O_4Si]^+$ ($[M + H]^+$): calculated 438.2788, found 438.2788.

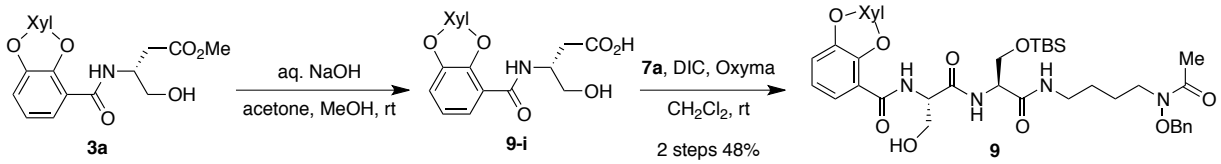


Compound 7b. Compound **7b** was synthesized analogously to preparation of compound **7a** from amine **5** using Fmoc-D-Ser(TBS)-OH. The two-step yield was 43%, and the ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **7b** were identical to those of its enantiomer, compound **7a**.



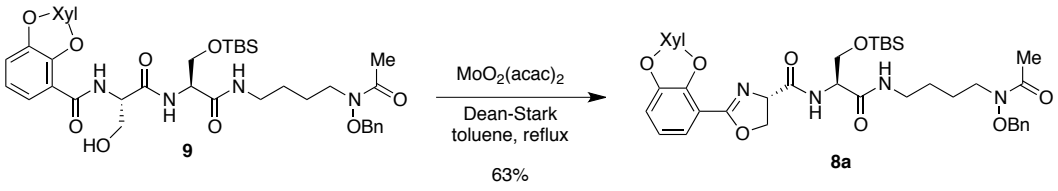
Compound 8a/**8b** (the condition in which epimerization was observed)**.** To a solution of amine **7a** (0.310 g, 0.711 mmol) and potassium carboxylate **4a** (0.387 g, 1.07 mmol) in dichloromethane (10 mL) was added EDC (0.204 g, 1.07 mmol) at 0 ºC. The reaction mixture was stirred at room temperature for 5 hr, and then it was diluted with dichloromethane (25 mL) and 1 N HCl solution (25 mL). After collection of the organic layer, the aqueous layer was extracted with dichloromethane (20 mL × 2). The combined organic layers were then washed with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. In the crude residue, two discernible spots suspected to be diastereomers were detected at R_f = 0.28 and 0.31 based on the thin layer chromatography analysis (5% methanol in dichloromethane). This mixture was separated by flash column chromatography (SiO_2, 3% methanol in dichloromethane) to give the desired amide **8a** (0.258 g, 0.320 mmol) and its diastereomer **8b** (0.0.63 g, 0.085 mmol) in 45% and 12% yields, respectively. **8a:** ^{1}H NMR (500 MHz, methanol-d^4) δ 7.44 – 7.35 (m, 6H), 7.31 – 7.27 (m, 3H), 7.23 (d, J = 7.0 Hz, 1H), 7.17 (d, J = 8.0 Hz, 1H), 6.96 (t, J = 7.9 Hz, 1H), 5.53 (s, 1H), 5.48 (s, 2H), 5.43 (d, J = 13.1 Hz, 1H), 5.39 (d, J = 13.0 Hz, 1H), 4.96 (dd, J = 10.6, 8.0 Hz, 2H), 4.88 (s, 2H), 4.64 (*app* t, J = 9.9 Hz, 1H), 4.50 (*app* t, J = 8.2 Hz, 1H), 4.44 (*br* t, J = 4.2 Hz, 1H), 3.93 (dd, J = 10.0, 3.9 Hz, 1H), 3.81 (dd, J = 10.0, 4.6 Hz, 2H), 3.73 – 3.65 (m, 2H), 3.25 (*br* t, J = 6.0 Hz, 2H) 2.04 (s, 3H), 1.70 – 1.63 (m, 2H), 1.55 – 1.48 (m, 2H), 0.76 (s, 9H), –0.04 (s, 3H), –0.06 (s, 3H). ^{13}C NMR (125 MHz, methanol-d^4) δ 173.8, 171.7, 171.6, 166.6, 152.5, 151.2, 137.1, 136.9, 136.0, 130.7, 130.3, 130.0, 129.9, 129.8, 129.7, 129.7, 126.7, 126.3, 124.2, 122.0, 77.1, 76.33, 76.25, 71.1, 70.3, 64.4, 56.3, 40.1, 27.6, 26.2, 25.2, 20.4, 19.0, –5.39, –5.44. HR-MS (ESI-TOF) *m/z* for $[C_{40}H_{53}N_4O_8Si]^+$ ($[M + H]^+$): calculated 745.3633, found 745.3630. **8b:** ^{1}H NMR (500 MHz, methanol-d^4) δ 7.43 – 7.35 (m, 6H), 7.30 – 7.22 (m, 4H), 7.15 (dd, J = 8.1, 1.7 Hz, 1H), 6.97 (t, J = 7.9 Hz, 1H), 5.54 (d, J = 13.1 Hz, 1H), 5.49 (d, J = 13.1 Hz, 1H), 5.44 (d, J = 13.0 Hz, 1H),

5.41 (d, *J* = 13.0 Hz, 1H), 4.96 (dd, *J* = 10.9, 8.0 Hz, 1H), 4.84 (s, 2H), 4.65 (dd, *J* = 10.9, 8.6 Hz, 1H), 4.55 (*app* t, *J* = 8.3 Hz, 1H), 4.45 (*app* t, *J* = 4.9 Hz, 1H), 3.96 (dd, *J* = 10.1, 4.6 Hz, 1H), 3.89 (dd, *J* = 10.1, 5.3 Hz, 1H), 3.21 (t, *J* = 6.9 Hz, 2H), 2.00 (s, 3H), 1.66 – 1.58 (m, 2H), 1.51 – 1.44 (m, 2H), 0.88 (s, 9H), 0.07 (s, 3H), 0.06 (s, 3H). ^{13}C NMR (125 MHz, methanol-d^4) δ 173.7, 171.62, 171.58, 166.6, 152.5, 150.9, 137.07, 137.02, 136.1, 130.7, 130.3, 130.1, 130.00, 129.81, 129.79, 129.7, 126.6, 126.3, 124.3, 122.3, 77.1, 76.4, 76.1, 70.8, 70.3, 64.4, 56.5, 40.1, 27.5, 26.3, 25.3, 20.4, 19.1, –5.33, –5.35. HR-MS (ESI-TOF) *m/z* for $[C_{40}H_{53}N_4O_8Si]^+$ ([M + H]$^+$): calculated 745.3633, found 745.3630.

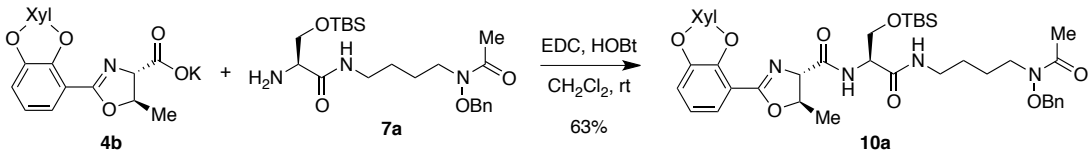


Compound 9. To a solution of **3a** (2.27 g, 6.36 mmol) in acetone (15 mL) and methanol (15 mL) was added an aqueous solution of sodium hydroxide (1.0 M, 15 mL) at 0 °C, and the mixture was stirred for 30 min at 0 °C. After stirred for 1 hr at room temperature, the reaction mixture was cooled to 0 °C and acidified to pH 2 with concentrated hydrochloric acid. Then, acetone and methanol were removed under reduced pressure, and the resulting aqueous layer was diluted with water followed by extraction with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine, dried over magnesium sulfate, and concentrated under reduced pressure. The resulting acid **9-i** (crude 249 mg, 0.686 mmol) was used in the next step without further purification. Acid **9-i** was mixed with amine **7a** (250 mg, 0.572 mmol) in dichloromethane (10 mL), and this mixture was treated with diisopropylcarbodiimide (DIC, 144 mg, 1.14 mmol), and Oxyma® (163 mg, 1.14 mmol) at room temperature. After stirred for 3 hr, the reaction mixture was diluted with dichloromethane (30 mL). The organic layer was washed with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. The crude residue was subjected to flash column chromatography (SiO_2, 2% methanol in dichloromethane) to afford the desired product **9** (567 mg, 1.06 mmol) in two steps 48% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (d, *J* = 6.6 Hz, 1H), 7.79 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.47 (*br* s, 1H), 7.41 – 7.32 (m, 6H), 7.28 – 7.25 (m, 1H), 7.21 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.12 – 7.10 (m, 1H), 6.99 (t, *J* = 7.9 Hz, 1H), 6.96 (*br* d, *J* = 8.5 Hz, 1H), 5.65 (d, *J* = 12.2 Hz, 1H), 5.61 (d, *J* = 12.3 Hz, 1H), 5.38 (d, *J* = 13.8 Hz, 1H), 5.33 (d, *J* = 13.8 Hz, 1H), 4.80 (s, 2H), 4.79 – 4.74 (m, 1H), 4.52 – 4.50 (m, 1H), 4.22 (dd, *J* = 9.8, 2.1 Hz, 1H), 4.17 (dd, *J* = 10.4, 4.8 Hz, 1H), 3.75 (dd, *J* = 10.4, 7.7 Hz, 1H), 3.71 (dd, *J* = 9.9, 4.3 Hz, 1H), 3.70 – 3.63 (m, 1H), 3.57 – 3.51 (m, 1H), 3.34 – 3.28 (m, 1H), 3.23 – 3.17 (m, 1H), 2.04 (s, 3H), 1.69 – 1.63 (m, 2H), 1.57 – 1.47 (m, 2H), 0.80 (s, 9H), 0.02 (s, 3H), 0.00 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.9, 170.4, 170.0, 165.2, 150.2, 149.7, 136.5, 134.3, 133.8, 130.5, 129.3, 129.3, 129.2, 128.9, 128.8, 127.8, 126.8, 126.4, 124.6, 123.0, 76.6, 76.6, 75.1, 63.0, 62.9, 55.3, 55.1, 38.9, 26.1, 25.8, 24.1, 20.5, 18.2, 14.3, –5.4, –5.5. HR-MS (ESI-TOF) *m/z* for $[C_{40}H_{54}N_4NaO_9Si]^+$ ([M + Na]$^+$): calculated

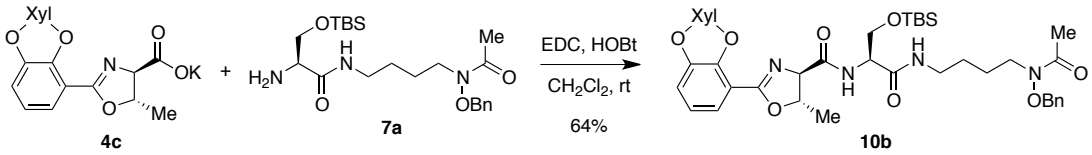
785.3558, found 785.3555.



Compound 8a (stereoselective condition)**.** The reaction was carried out in a flask fitted with a pressure-equalized addition funnel (containing a cotton plug and molecular sieves to function as a Soxhlet extractor) surmounted with a reflux condenser. A solution of **9** (0.882 g, 1.16 mmol) and $MoO_2(acac)_2$ (75 mg, 20 mol%) in toluene (230 mL) was heated with an oil bath under azeotropic reflux. After stirred for 8 h, the reaction mixture was cooled to room temperature and concentrated under reduced pressure. The crude residue was then subjected to flash column chromatography (SiO_2, 2% methanol in dichloromethane) to afford the desired amide **8a** (0.545 g, 0.730 mmol) in 63 % yield without formation of its diastereomer **8b**.

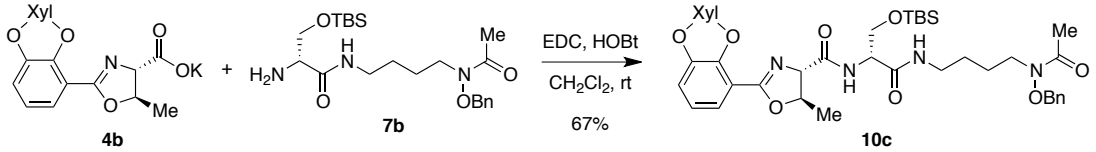


Compound 10a. The synthesis of compound **10a** from **4b** and **7a** was previously reported in Ref. S2.

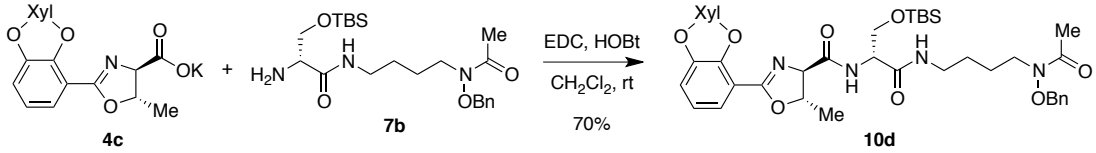


Compound 10b. To a solution of amine **7a** (0.220 g, 0.502 mmol) and potassium carboxylate **4c** (0.236 g, 0.625 mmol) in dichloromethane (3 mL) was added EDC (0.120 g, 0.781 mmol) and HOBt (0.140 g, 0.781 mmol) at 0 ºC. The reaction mixture was stirred at room temperature for 5 hr, and then it was diluted with dichloromethane (25 mL) and 1 N HCl solution (25 mL). After collection of the organic layer, the aqueous layer was extracted with dichloromethane (20 mL × 2). The combined organic layers were then washed with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. The crude residue was subjected to flash column chromatography (SiO_2, 3% methanol in dichloromethane) to afford the desired amide **10b** (244 mg, 0.322 mmol) in 64% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 6.7 Hz, 1H), 7.44 (dd, J = 7.8, 1.7 Hz, 1H), 7.39 – 7.36 (m, 3H), 7.35 – 7.31 (m, 2H), 7.27 – 7.25 (m, 1H), 7.22 – 7.18 (m, 1H), 7.13 (dd, J = 8.0, 1.7 Hz, 1H), 6.95 (t, J = 7.9 Hz, 1H), 6.57 (*br* t, J = 5.5 Hz, 1H), 5.64 (d, J = 13.5 Hz, 1H), 5.50 (d, J = 11.4 Hz, 1H), 5.47 (d, J = 11.9 Hz, 1H), 5.34 (d, J = 13.0 Hz, 1H), 4.89 – 4.83 (m, 1H), 4.76 (s, 2H), , 4.38

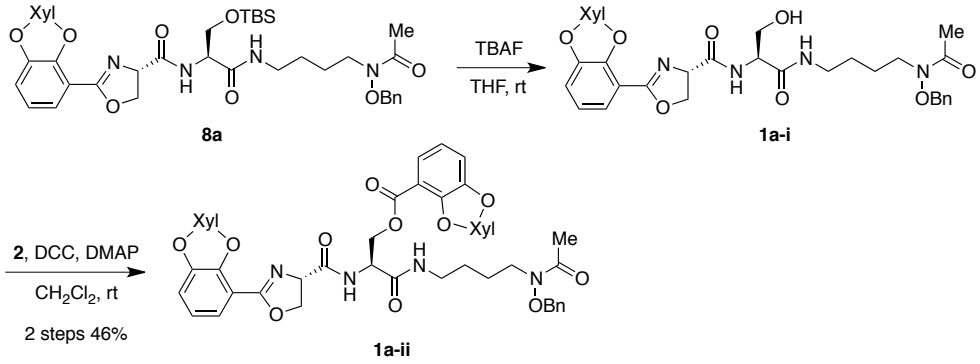
– 4.34 (m, 1H), 4.06 (dd, J = 9.7, 4.2 Hz, 1H), 3.63 – 3.58 (m, 2H), 3.27 (q, J = 6.9 Hz, 2H), 2.05 (s, 3H), 1.68 – 1.58 (m, 2H), 1.59 (d, J = 6.2 Hz, 3H), 1.51 – 1.45 (m, 2H), 0.88 (s, 9H), 0.11 (s, 3H), 0.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.3, 171.8, 169.8, 163.9, 151.5, 149.9, 136.0, 135.4, 134.4, 129.2, 129.01, 128.97, 128.9, 128.8, 128.6, 128.4, 125.0, 123.3, 121.6, 78.9, 76.3, 76.0, 75.9, 75.1, 62.7, 53.9, 44.8, 39.2, 26.7, 25.8, 24.4, 22.0, 20.5, 18.1, –5.41, –5.49. HR-MS (ESI-TOF) *m/z* for $[C_{41}H_{55}N_4O_8Si]^+$ ($[M + H]^+$): calculated 759.3789, found 759.3787.



Compound 10c. Compound **10c** was synthesized analogously to preparation of compound **10b**, in which the reaction between amine **7b** (0.476 g, 0.721 mmol) and potassium carboxylate **4b** (0.326 g, 1.87 mmol) led to formation of the desired product **10c** (0.360 g, 0.483 mmol) in 67% yield. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **10c** were were identical to those of its enantiomer, compound **10b**.

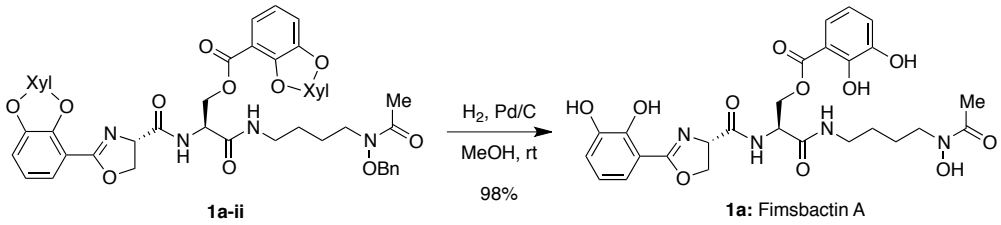


Compound 10d. Compound **10d** was synthesized analogously to preparation of compound **10b**, in which the reaction between amine **7b** (1.07 g, 2.45 mmol) and potassium carboxylate **4c** (1.01 g, 2.70 mmol) led to formation of the desired product **10d** (1.30 g, 1.72 mmol) in 70% yield. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **10d** were identical to those of its enantiomer, compound **10a**.



Compound 1a-ii. To a solution of **8a** (0.248 g, 0.323 mmol) in tetrahydrofuran (THF, 2 mL) was added tetrabutylammonium fluoride (TBAF, 1 M in THF, 0.485 mL, 0.485 mmol) at 0 ºC, and the resulting mixture was stirred at room temperature for 5 hr. After the substrate was completely consumed, the solvent was removed under reduced pressure. The resulting crude product **1a-i** was used in the next step without further purification. To a

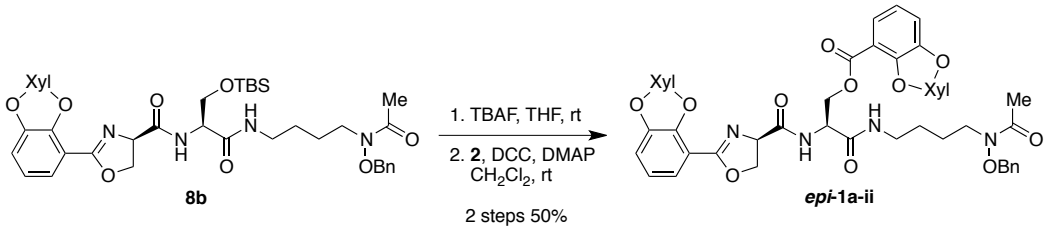
solution of crude **1a-i** and acid **2** (0.165 g, 0.646 mmol) in dichloromethane (2 mL) was added dicyclohexylcarbodiimide (DCC, 0.199 g, 0.969 mmol) and 4-(dimethylamino)pyridine (DMAP, 11.8 mg, 0.0969 mmol) at room temperature. After stirred for 3 hr, the reaction mixture was diluted with dichloromethane (10 mL) and 1 N hydrochloric acid solution (10 mL). After collecting the organic layer, the aqueous layer was extracted with dichloromethane (2 × 20 mL). The combined organic layers were washed with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and concentrated under the reduced pressure. The crude residue was purified by flash column chromatography (SiO_2, 3% methanol in dichloromethane) to afford the ester intermediate **1a-ii** (0.129 g, 0.149 mmol) in a two-step 46% yield. ^{1}H NMR (500 MHz, methanol-d^4) δ 7.38 (dd, J = 7.8, 1.7 Hz, 1H), 7.37 – 7.33 (m, 6H), 7.26 – 7.19 (m, 8H), 7.16 – 7.11 (*app* t, *J* = 1.5 Hz, 1H), 7.12 (*app* t, *J* = 1.5 Hz, 1H), 6.94 (t, *J* = 7.9 Hz, 1H), 6.88 (t, *J* = 7.9 Hz, 1H), 5.48 (d, *J* = 12.9 Hz, 1H), 5.45 (s, 2H), 5.42 (d, *J* = 12.9 Hz, 1H), 5.38 (d, *J* = 12.9 Hz, 1H), 5.35 (s, 2H), 5.34 (d, *J* = 12.9 Hz, 1H), 4.95 (dd, *J* = 10.7, 8.1 Hz, 1H), 4.82 (t, *J* = 4.8 Hz, 1H), 4.78 (s, 2H), 4.64 (dd, *J* = 4.8, 2.1 Hz, 2H), 4.60 – 4.52 (m, 2H), 3.58 (*br* m, 2H), 3.29 – 3.24 (m, 1H), 3.21 – 3.15 (m, 1H), 1.95 (s, 3H), 1.61 – 1.55 (m, 2H), 1.49 – 1.43 (m, 2H). ^{13}C NMR (125 MHz, methanol-d^4) δ 173.9, 170.3, 166.9, 166.6, 152.5, 152.4, 151.1, 150.9, 137.0, 137.0, 136.92, 136.89, 136.0, 130.7, 130.3, 130.2, 130.1, 130.0, 129.9, 129.8, 129.73, 129.71, 129.69, 127.1, 126.5, 126.5, 126.2, 125.7, 124.2, 124.2, 122.1, 77.1, 76.6, 76.3, 76.1, 75.8, 70.8, 70.4, 65.1, 54.8, 53.9, 40.1, 29.5, 27.5, 20.4. HR-MS (ESI-TOF) *m/z* for $[C_{49}H_{49}N_4O_{11}]^+$ ([M + H]$^+$): calculated 869.3398, found 869.3395.



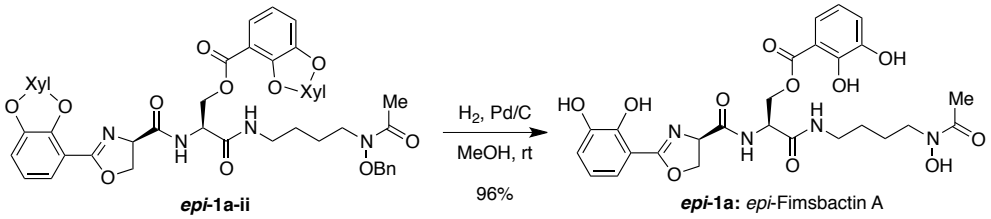
1a-ii **1a:** Fimsbactin A

Fimsbactin A (1a). For the hydrogenolytic global deprotection, a catalytic amount of palladium on activated carbon (10 wt%, 15.9 mg, 0.015mmol) was suspended in a solution of ester **1a-ii** (26.3 mg, 0.0303 mmol) in methanol (1 mL) at room temperature, and the reaction was initiated by charging the reaction flask with hydrogen gas in a balloon (1 atm). After 3 hr, the reaction mixture was filtered through a pad of celite to remove the palladium catalyst, and the filtrate was concentrated under reduced pressure to afford the desired product **1a** (Fimsbactin A, 17.7 mg, 0.0297 mmol) in 98% yield without further purification. ^{1}H NMR (500 MHz, DMSO-d^6) δ 8.80 (*br* s, 1H), 8.31 (*br* s, 1H), 7.14 (d, *J* = 7.7 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 6.96 (*app* t, *J* = 8.0 Hz, 2H), 6.74 (*app* t, *J* = 7.6 Hz, 1H), 6.55 (*app* t, *J* = 7.6 Hz, 1H), 5.07 (dd, *J* = 10.0, 7.5 Hz, 1H), 4.73–4.68 (m, 1H), 4.63–4.58 (*br* m, 1H), 4.57 (dd, *J* = 11, 4.7 Hz, 1H), 4.52 (*app* t, *J* = 7.7 Hz, 1H), 4.42–4.37 (m, 1H), 3.47–3.43 (m, 2H), 3.13–3.07 (m, 2H), 1.96 (s, 3H), 1.53–1.46 (m, 2H), 1.43–1.35 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 170.2, 170.1, 168.9, 167.9, 166.5,

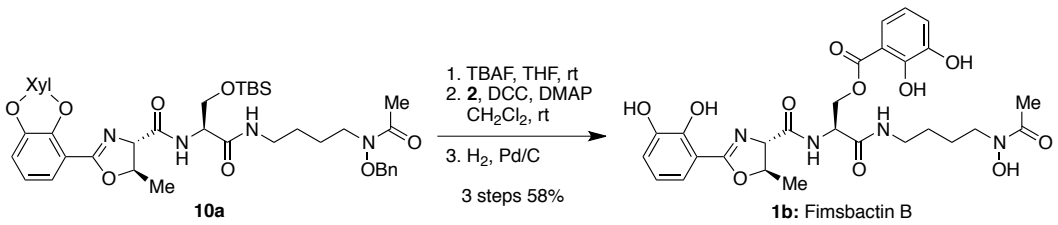
148.3, 146.2, 145.8, 120.4, 119.8, 119.5, 118.7, 117.9, 112.7, 110.1, 69.3, 67.2, 64.4, 51.7, 46.5, 38.5, 26.1, 23.7, 20.4. HR-MS (ESI-TOF) *m/z* for $[C_{26}H_{30}N_4NaO_{11}]^+$ ($[M + Na]^+$): calculated 597.1809, found 597.1807.



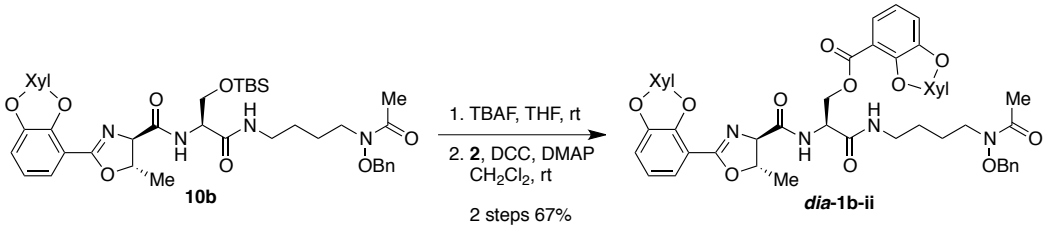
Compound *epi*-1a-ii. Compound ***epi*-1a-ii** was synthesized analogously to preparation of compound **1a-ii**, in which a two-reaction sequence from **8b** (30 mg, 0.035 mmol) led to formation of the desired product ***epi*-1a-ii** (15.3 mg, 0.0175 mmol) in two step 50% yield. ^{1}H NMR (500 MHz, methanol-d^4) δ 7.39 – 7.32 (m, 5H), 7.24 – 7.12 (m, 10H), 7.07 (dd, J = 8.1, 1.7 Hz, 1H), 7.00 (dd, J = 8.0, 1.7 Hz, 1H), 6.81 (t, J = 7.9 Hz, 1H), 6.64 (t, J = 7.9 Hz, 1H), 5.44 (d, J = 13.1 Hz, 1H), 5.36 (d, J = 13.0 Hz, 1H), 5.33 (s, 2H), 5.32 (d, J = 12.9 Hz, 1H), 5.28 (s 1H), 5.26 (s, 1H), 5.23 (d, J = 12.9 Hz, 1H), 4.94 (dd, J = 10.9, 7.8 Hz, 1H), 4.81 (s, 2H), 4.72 (dd, J = 11.4, 4.0 Hz, 1H), 4.60 – 4.49 (m, 3H), 3.67 – 3.60 (*br* m, 2H), 3.35 – 3.29 (m, 2H), 3.24 – 3.19 (m, 2H), 1.98 (s, 3H), 1.85 – 1.59 (m, 2H), 1.53 – 1.47 (m, 2H). ^{13}C NMR (125 MHz, methanol-d^4) δ 173.8, 170.3, 167.0, 166.5, 152.6, 152.5, 151.3, 150.9, 137.1, 136.99, 136.95, 130.7, 130.30, 130.28, 130.1, 129.98, 129.97, 129.82, 129.79, 129.76, 129.7, 127.3, 126.6, 126.5, 126.2, 125.8, 124.4, 124.3, 122.3, 77.10, 77.05, 76.5, 76.3, 76.0, 70.7, 70.4, 65.4, 54.8, 53.8, 40.1, 34.6, 27.5, 20.3. HR-MS (ESI-TOF) *m/z* for $[C_{49}H_{49}N_4O_{11}]^+$ ($[M + H]^+$): calculated 869.3398, found 869.3396.



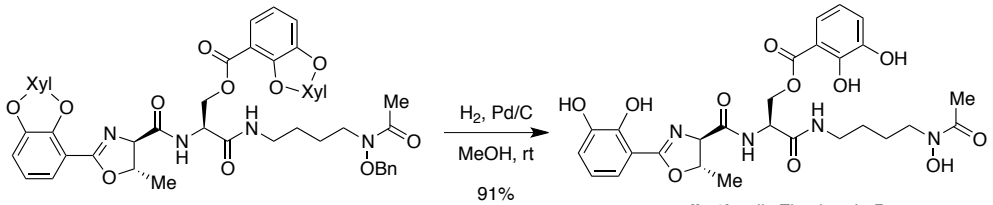
epi*-Fimsbactin A (*epi*-1a).** *epi*-Fimsbactin A (epi*-1a**) was synthesized analogously to preparation of fimsbactin A (**1a**), in which ***epi*-1a-ii** (15.3 mg, 0.0175 mmol) was subjected to hydrogenolysis to afford *epi*-fimsbactin A (***epi*-1a**, 9.3 mg, 0.016 mmol) in 96% yield. ^{1}H NMR (500 MHz, DMSO-d^6) δ 8.74 (*br* s, 1H), 8.39 (*br* s, 1H), 7.18 (d, J = 7.9 Hz, 1H), 7.08 (d, J = 7.8 Hz, 1H), 6.97 (*br* d, J = 7.4 Hz, 2H), 6.74 (*app* t, J = 7.8 Hz, 1H), 6.64 (*app* t, J = 7.8 Hz, 1H), 5.07 (dd, J = 10.0, 7.5 Hz, 1H), 4.76–4.71 (m, 1H), 4.63–4.57 (*br* m, 1H), 4.49–4.42 (m, 3H), 3.44 (t, J = 6.5 Hz, 2H), 3.16–3.02 (m, 2H), 1.95 (s, 3H), 1.52–1.44 (m, 2H), 1.45–1.32 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 170.2, 170.0, 168.8, 168.0, 166.6, 148.3, 146.8, 146.4, 145.8, 119.9, 119.4, 118.8, 118.7, 117.9, 112.6, 110.1, 69.4, 67.1, 64.2, 51.6, 46.4, 38.5, 26.0, 23.7, 20.4. HR-MS (ESI-TOF) *m/z* for $[C_{26}H_{30}N_4NaO_{11}]^+$ ($[M + Na]^+$): calculated 597.1809, found 597.1806.



Fimsbactin B (1b). Compound **1b** was synthesized analogously to preparation of compound **1a**, in which a three-reaction sequence from **10a** (0.291 g, 0.391 mmol) led to formation of the desired product **1b** (0.133 g, 0.227 mmol) in three step 58% yield. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound **1b** were previously reported in Ref. S2.

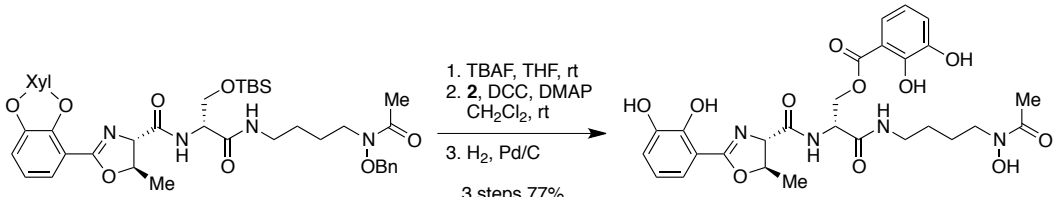


Compound *dia*-1b-ii. Compound ***dia*-1b-ii** was synthesized analogously to preparation of compound **1a-ii**, in which a two-reaction sequence from **10b** (0.092 g, 0.140 mmol) led to formation of the desired product ***dia*-1b-ii** (63.3 mg, 0.094 mmol) in two step 67% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.4 Hz, 1H), 7.44 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.42 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.38 – 7.33 (m, 3H), 7.32 – 7.28 (m, 2H), 7.27 – 7.13 (m, 9H), 7.11 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.91 (t, *J* = 7.9 Hz, 1H), 6.84 (*br* t, *J* = 5.3 Hz, 1H), 5.58 (d, *J* = 13.4 Hz, 1H), 5.49 – 5.42 (m, 4H), 5.37 – 5.29 (m, 3H), 4.90 – 4.85 (m, 1H), 4.83 – 4.79 (m, 1H), 4.74 – 4.71 (m, 1H), 4.71 (s, 2H), 3.51 (*br* t, *J* = 7.2 Hz, 2H), 3.25 – 3.18 (m, 1H), 3.15 – 3.09 (m, 1H), 2.01 (s, 3H), 1.56 (d, *J* = 6.2 Hz, 3H), 1.54 – 1.48 (m, 2H), 1.38 – 1.32 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.1, 168.5, 165.5, 163.9, 151.6, 151.5, 150.3, 150.0, 136.0, 135.6, 135.5, 135.4, 129.3, 129.13, 129.06, 129.0, 128.9, 128.9, 128.8, 128.7, 128.5, 126.3, 125.9, 125.1, 125.1, 124.4, 123.4, 121.6, 78.8, 76.4, 76.0, 75.9, 75.4, 75.2, 64.1, 52.0, 39.5, 26.2, 24.5, 22.0, 20.5. HR-MS (ESI-TOF) *m/z* for $[C_{50}H_{51}N_4O_{11}]^+$ ($[M + H]^+$): calculated 883.3554, found 883.3552.



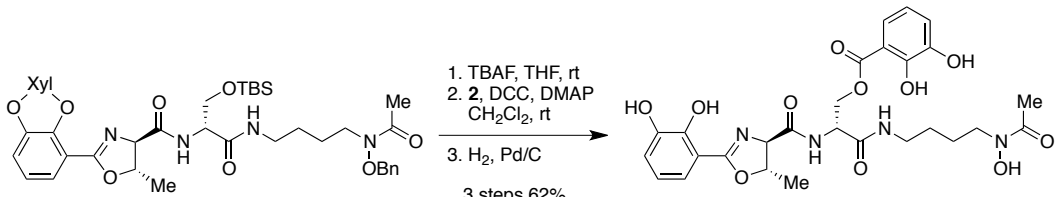
***dia*-1b-ii** ***dia*-1b:** *dia*-Fimsbactin B

dia*-Fimsbactin B (*dia*-1b).** *dia*-Fimsbactin B (dia*-1b**, 50.9 mg, 0.086 mmol) was synthesized from ***dia*-1b-ii** (63.3 mg, 0.094 mmol) by hydrogenolytic global deprotection, analogously to preparation of fimsbactin A (**1a**), and the yield was 91%. ^{1}H NMR (500 MHz, DMSO-d^6) δ 11.81 (s, 1H), 10.26 (s, 1H), 9.66 (s, 1H), 9.45 (s, 1H), 9.26 (s, 1H), 8.64 (d, J = 8.2 Hz, 1H), 8.29 (t, J = 5.5 Hz, 1H), 7.22 (dd, J = 8.0, 1.5 Hz, 1H), 7.06 (dd, J = 7.9, 1.5 Hz, 1H), 7.04 (dd, J = 7.8, 1.5 Hz, 1H), 6.97 (dd, J = 7.9, 1.5 Hz, 1H), 6.75 (*app* q, J = 8.0 Hz, 2H), 4.82 – 4.74 (m, 2H), 4.60 (d, J = 7.0 Hz, 1H), 4.54 (dd, J = 10.9, 5.1 Hz, 1H), 4.46 (dd, J = 10.9, 6.7 Hz, 1H), 3.43 (t, J = 6.7 Hz, 2H), 3.13 (dq, J = 12.6, 6.6 Hz, 1H), 3.05 (dq, J = 12.5, 6.6 Hz, 1H), 1.95 (s, 3H), 1.52 – 1.43 (m, 2H), 1.41 (d, J = 6.3 Hz, 3H), 1.39 – 1.33 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 170.2, 169.8, 168.9, 167.8, 166.0, 149.5, 148.3, 146.1, 145.8, 120.9, 119.8, 119.5, 118.9, 118.7, 117.9, 112.9, 110.2, 79.0, 73.2, 64.4, 51.5, 46.4, 38.5, 26.1, 23.7, 20.5, 20.3. HR-MS (ESI-TOF) *m/z* for $[C_{27}H_{32}N_4NaO_{11}]^+$ ([M + Na]$^+$): calculated 611.1965, found 611.1963.



10c ***epi*-1b:** Fimsbactin B

epi*-Fimsbactin B (*epi*-1b).** Compound ***epi*-1b** was synthesized analogously to preparation of compound **1a**, in which a three-reaction sequence from **10c** (74.3 mg, 0.1 mmol) led to formation of the desired product ***epi*-1b** (45.3 mg, 0.077mmol) in three step 77% yield. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound ***epi*-1b** were identical to those of its enantiomer, *dia*-fimsbactin B (dia*-1b**).



10d ***ent*-1b:** *ent*-Fimsbactin B

***ent*-Fimsbactin B (*ent*-1b).** Compound ***ent*-1b** was synthesized analogously to preparation of compound **1a**, in which a three-reaction sequence from **10d** (0.446 g, 0.599 mmol) led to formation of the desired product ***ent*-1b** (0.218 g, 0.371 mmol) in three step 62% yield. The ^{1}H-, ^{13}C-NMR, and HR-MS spectra of compound ***ent*-1b** were identical to those of its enantiomer, fimsbactin B (**1b**).

B. Procedures for Biological/biochemical Experiments

Growth promotion activity assay

A single colony was picked from a fresh Luria-Bertani (LB) agar-plate overlaid with the *A. baumannii* strain of interest and was then used to inoculate 5 mL of LB media. After incubation at 37 °C overnight in a shaking incubator (200 rpm), the culture solution was diluted with LB broth for an $OD_{600} \approx 1$. This solution was further diluted 1:100 with LB media containing the designated concentration of 2,2′-bipyridyl (DP) (275 μM for *A. baumannii* ATCC 17978, 175 μM for *A. baumannii* ATCC 19606 wild-type or Δ*bauA* mutant). An aliquot (198 μL) of the diluted culture was mixed with a 2-μL aliquot of fimsbactin or fimsbactin stereoisomer DMSO stock solution whose concentrations were adjusted to make the intended final concentrations indicated in Figure 2 in a sterile Greiner Bio-One 96-well microplate (Kremsmünster, Austria). The microplate was then covered with a Breathe-Easy® sealing tape (Sigma-Aldrich) for efficient aeration, and it was incubated at 37 ºC with shaking at 200 rpm. The OD600 values were recorded every hour using Epoch 2 microplate reader (Biotek, Vermont, USA). All measurements were made using duplicate or quadruplicate biological samples, and the mean values were used for plotting the results, in which the error bars indicate the standard deviation (Figure 2A and 2B) or the standard error (Figure 2C). *A. baumannii* ATCC 19606 and 17978 were obtained from ATCC (Virginia, USA) or KCTC (Korean Collection for Type Cultures, Jeollabuk-do, Republic of Korea), and the preparation of *A. baumannii* ATCC 19606 Δ*bauA* was reported previously.[S4]

Determination of the Fe(III) binding stoichiometry of a fimsbactin

The fluorescence titration-based determination of the Fe(III) binding stoichiometry of a fimsbactin was conducted by following the procedure described in Ref S5. Briefly, to a 600 μL solution of 500 μM fimsbactin in ethanol was added 3 μL aliquots of 10 mM $FeCl_3$ in ethanol, and emission at 400 nm (λ_{ex} = 320 nm) was recorded after each addition. The emission signal was plotted against the equivalents of Fe(III) as shown in Figure S1. This set of experiments was conducted using a Hitachi F-7000 fluorescence spectrophotometer, in which the slit sizes for excitation and emission were 5 nm and 10 nm, respectively.

EDTA competition assay

To qualitatively compare the Fe(III) binding affinity of various fimsbactin isomers, the fluorescence recovery of the corresponding Fe(III) complexes upon addition of a competing Fe(III) chelator, ethylenediaminetetraacetic acid (EDTA), was monitored. The Fe(III)-fimsbactin complex was prepared by dissolving 30 μL of 10 mM fimsbactin and 30 μL of 10 mM $FeCl_3$ in 540 μL ethanol, in which the final concentration of the resulting Fe(III)-fimsbactin complex was 500 μM. To this solution, aliquots of 10 mM Na_4EDTA in water were added one after the other to adjust the equivalents of EDTA with respect to Fe(III)-fimsbactin complex to be 0.5, 0.75, 1, 1.25, 1.5, 1.75, and 2.

The fluorescence emission at 400 nm (λ_{ex} = 320 nm) was recorded after each addition. The emission signal versus the equivalent of EDTA was plotted in Figure S2. The experimental setup was identical to the binding stoichiometry determination experiment.

Parallel artificial membrane permeability assay (PAMPA)

A parallel artificial membrane permeability assay was conducted by following the instruction provided in a Corning Gentest Pre-coated PAMPA Plate System (Cat. No. 353015, Corning, New York, USA). Initially, Fe(III)-preloaded fimsbactin A and B (*holo*-**1a** and *holo*-**1b**) were prepared by mixing each of these compounds with 1.1 eq. iron(III) acetylacetonate, $Fe(acac)_3$, in methanol, and the mixture was incubated at room temperature overnight for complete complexation. Then, methanol was completely removed by using a spinvac, and the resulting residue was triturated and washed with cold ether several times to afford pure *holo*-fimsbactins. To the wells of a Receiver plate ("donor wells"), 300 µL of a solution of *holo*-fimsbactin A or B (200 µM) in 100 mM Tris•HCl buffer (pH 7) was added, and the wells of a Filter plate ("acceptor wells") were filled with the buffer alone (200 µL). Then, these two plates were coupled, and the resulting assembly was incubated at room temperature for 4 hr without agitation. At the end of the incubation, the plates were separated, and 150 µL solutions from each well of both plates were aliquoted and transferred to a Greiner UV-star® 96-well microplate. The final concentrations of compounds in both donor and acceptor wells were analyzed by measuring the absorption with Epoch 2 microplate reader (the standard concentration plot for each *holo*-fimsbactin was created beforehand). Finally, the permeability of each *holo*-fimsbactin was calculated using the following formula:

Permeability (cm/s): $P_e = \{-\ln[1 - C_A(t)/C_{eq}]\}/[A \times (1/V_D + 1/V_A) \times t]$

A = Filter area (0.3 cm^2)
V_D = Donor well volume (0.3 mL)
V_A = Acceptor well volume (0.2 mL)
$C_A(t)$ = compound concentration in acceptor well at time t
$C_D(t)$ = compound concentration in donor well at time t
$C_{eq} = [C_D(t) \times V_D + C_A(t) \times V_A] / (V_D + V_A)$

SUPPLEMENTAL REFERENCES

S1. Kim, J.; Lee, J. E.; Ree, H.; Kim, H. J. *Bull. Kor. Chem. Soc.* **2015**, *36*, 439.

S2. Ree, H.; Kim, J.; Song, W. Y.; Lee, J. E.; Kim, H. J. *Bull. Kor. Chem. Soc.* **2015**, *36*, 1520.

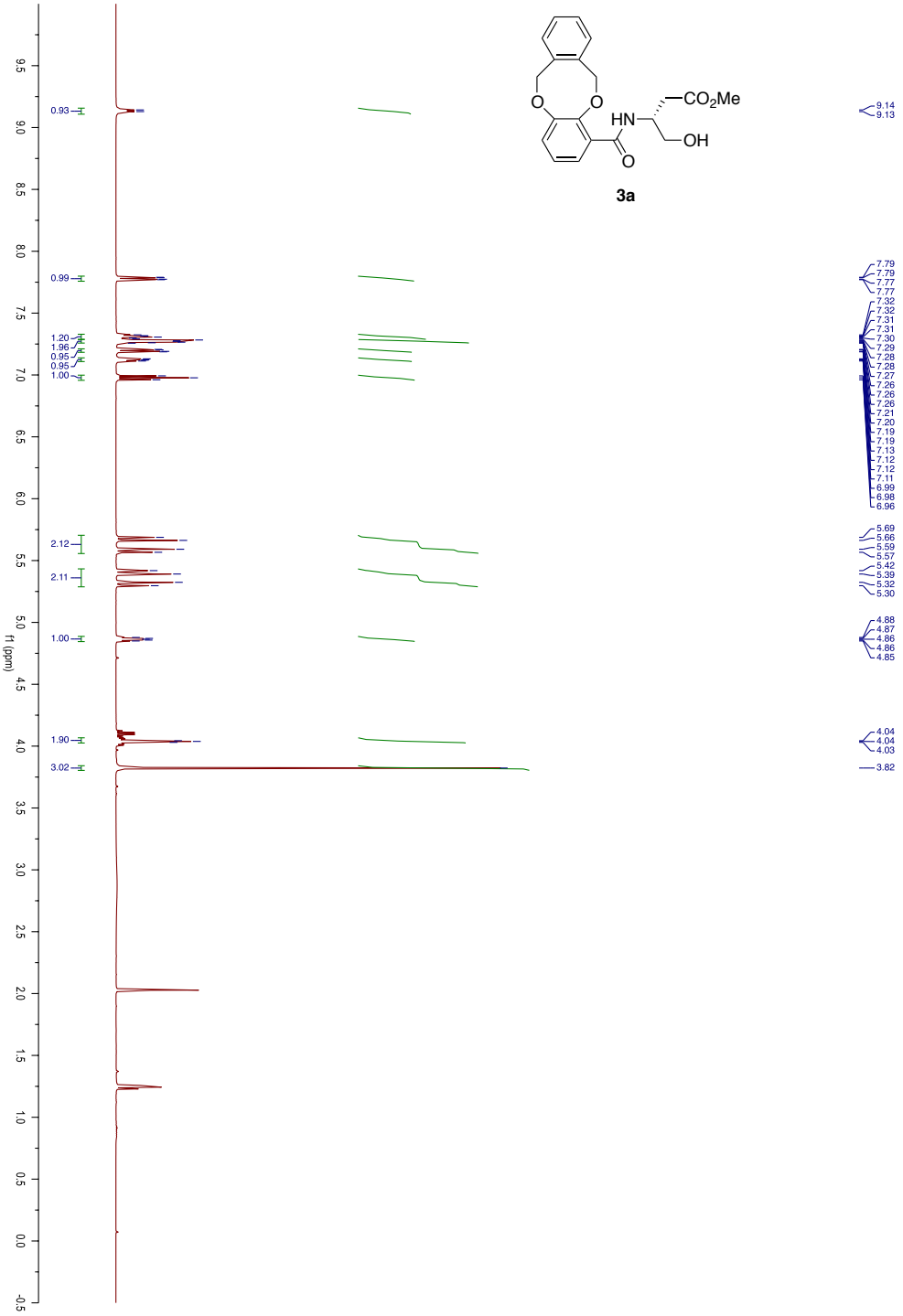
S3. Proschak, A.; Lubuta, P.; Grün, P.; Löhr, F.; Wilharm, G.; De Berardinis, V.; Bode, H. B. *Chembiochem* **2013**, *14*, 633.

S4. Oh, M. H.; Lee, J. C.; Kim, J.; Choi, C. H.; Han, K. *Appl. Environ. Microbiol.* **2015**, *81*, 3357.

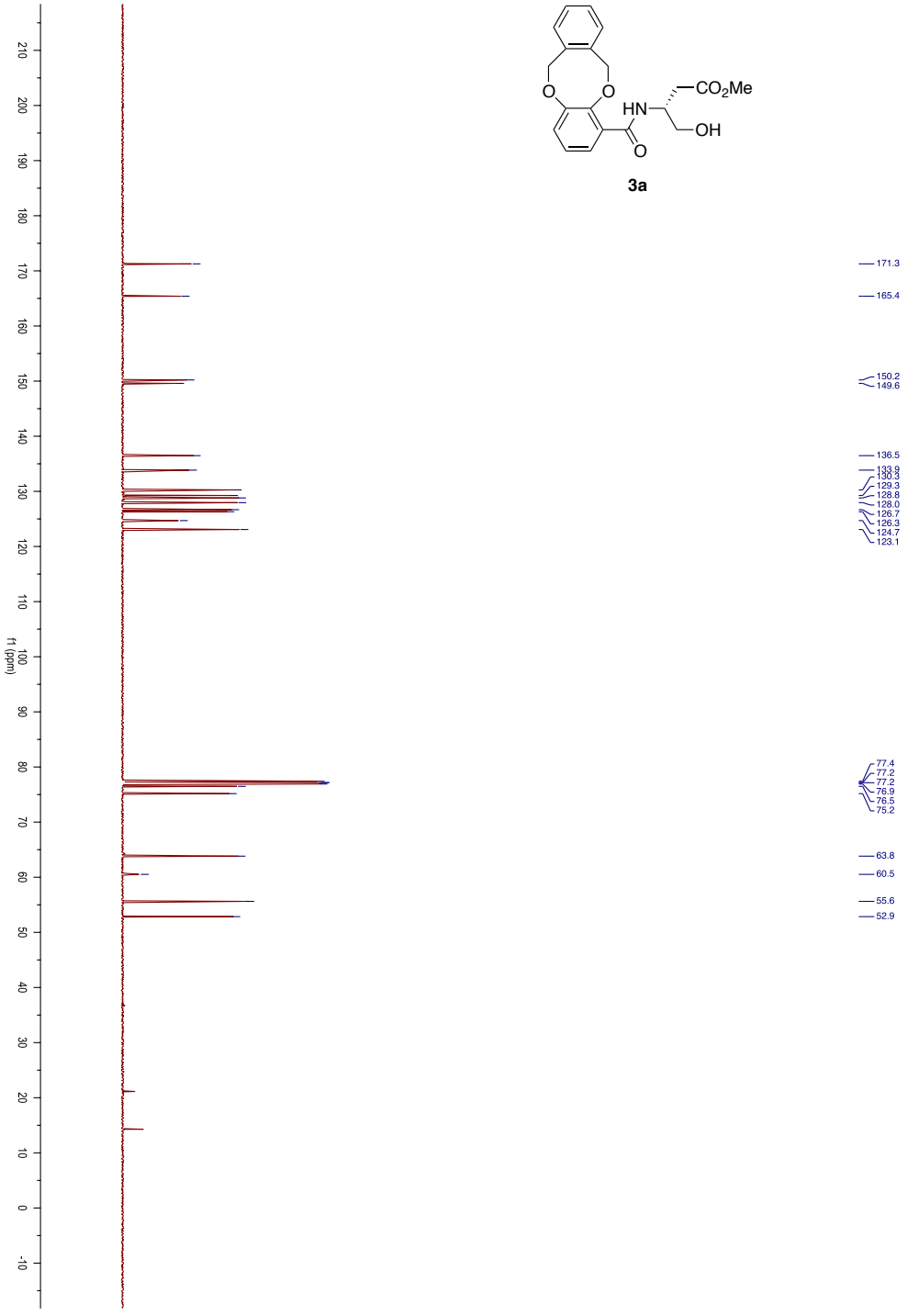
S5. Bohac, T. J.; Fang, L.; Giblin, D. E.; Wencewicz, T. A. *ACS Chem. Biol.* **2019**, *14*, 674.

SPECTRAL DATA

^{1}H-NMR of Compound 3a (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 3a (125 MHz, $CDCl_3$)



HR-MS of Compound 3a

Compound Spectrum SmartFormula Report

Analysis Info

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Method	Tune_pos_Standard_100_600_190102.d.m	Operator	lee
Sample Name	KSJ01_3a	Instrument	compact 8255754.10024
Comment			

Acquisition Parameter

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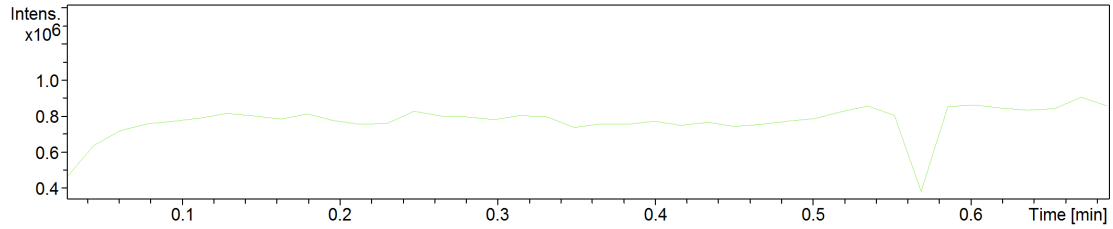
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
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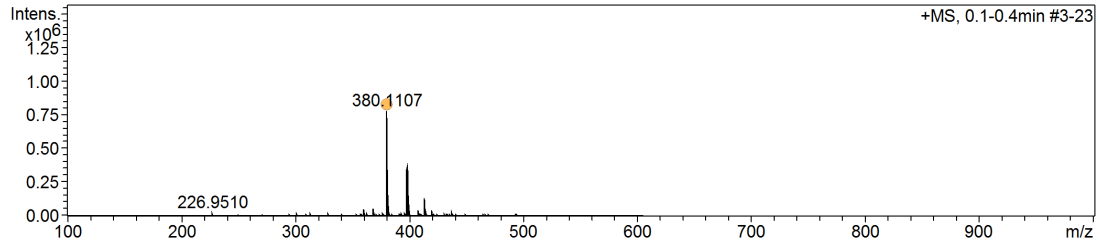
+MS, 0.1-0.4min #3-23



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
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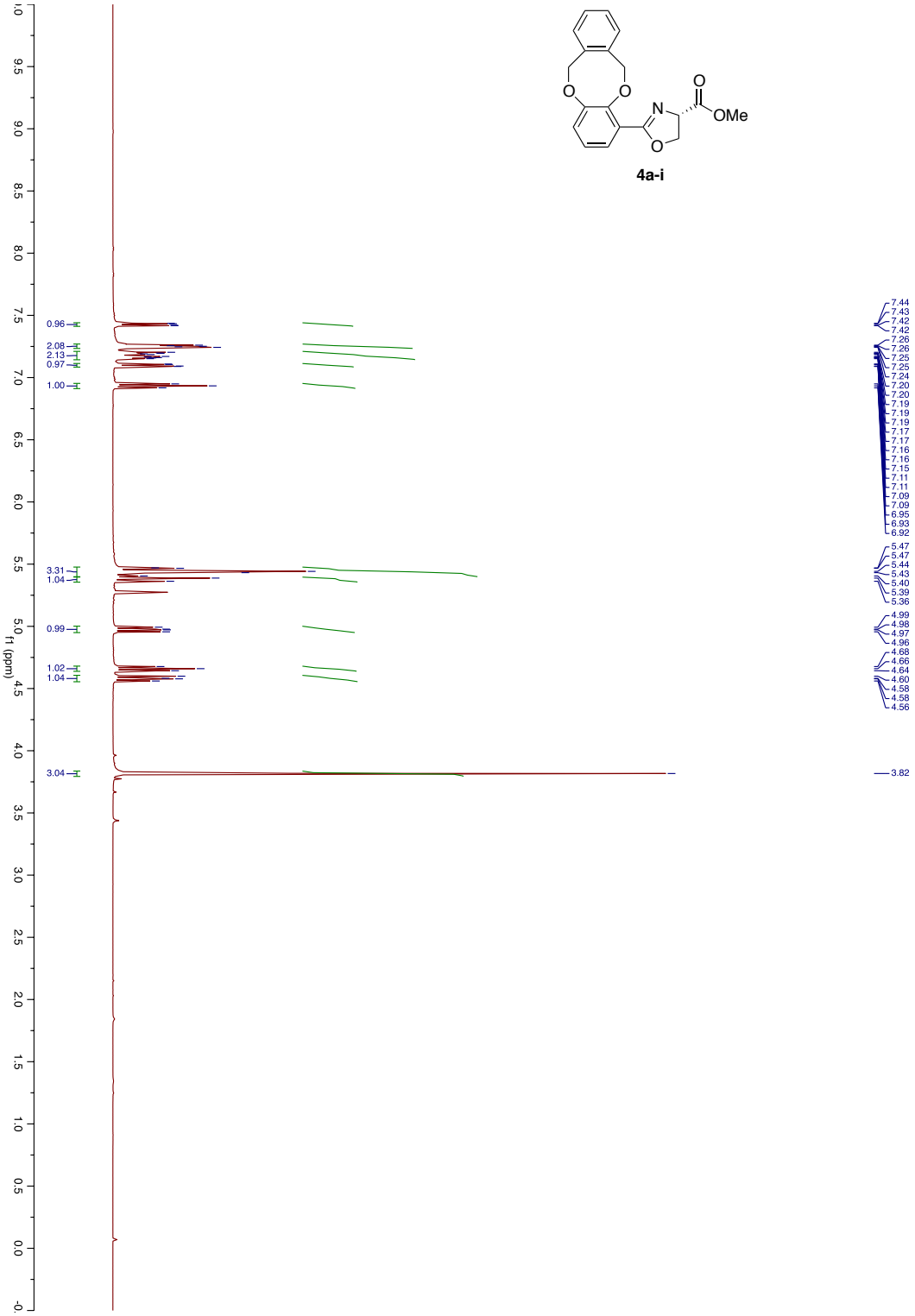
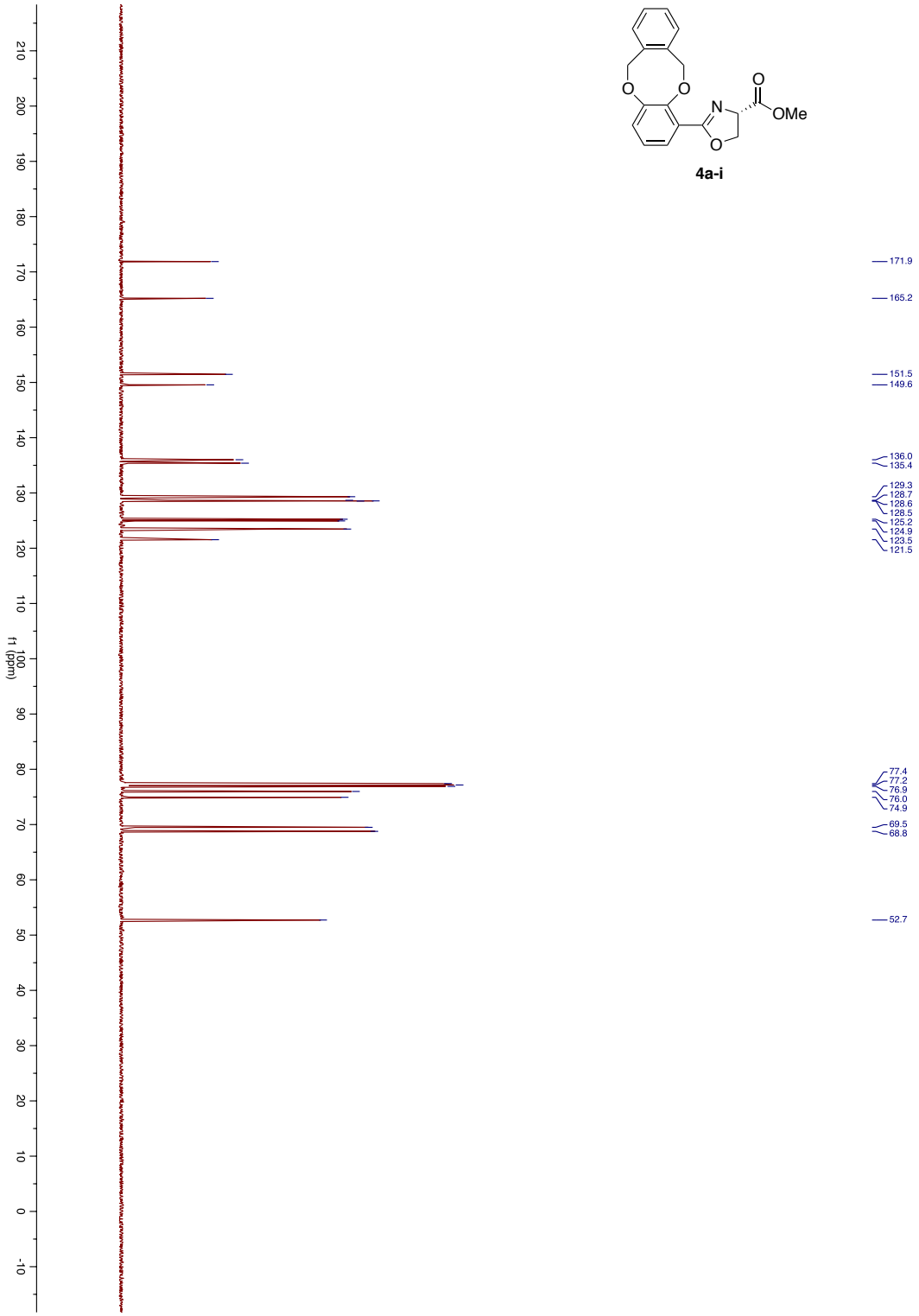
	2	C16H18N3O8	380.1088	4.9	10.0	2	51.62	9.5	even	ok
	3	C13H10N13O2	380.1075	8.5	12.5	3	11.35	15.5	even	ok
	4	C21H18NO6	380.1129	5.7	13.5	4	38.91	13.5	even	ok
	5	C18H10N11	380.1115	-2.1	15.9	5	67.94	19.5	even	ok
	6	C22H14N5O2	380.1142	-9.2	24.9	6	8.79	18.5	even	ok
	7	C28H14NO	380.1070	9.8	50.4	7	3.46	22.5	even	ok
	1	C19H19NNaO6	380.1105	0.7	2.6	1	100.00	10.5	even	ok
	2	C16H11N11Na	380.1091	-4.2	6.5	2	33.03	16.5	even	ok
	3	C15H15N7NaO4	380.1078	7.7	11.0	3	10.18	11.5	even	ok
	4	C20H15N5NaO2	380.1118	-2.9	16.2	4	38.14	15.5	even	ok

^{1}H-NMR of Compound 4a-i (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 4a-i (125 MHz, $CDCl_3$)



HR-MS of Compound 4a-i

Compound Spectrum SmartFormula Report

Analysis Info

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Sample Name	KSJ02_3a-1	Instrument	compact 8255754.10024
Comment			

Acquisition Parameter

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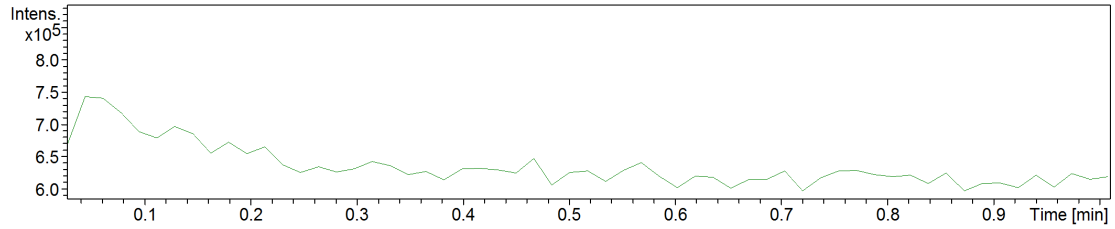
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



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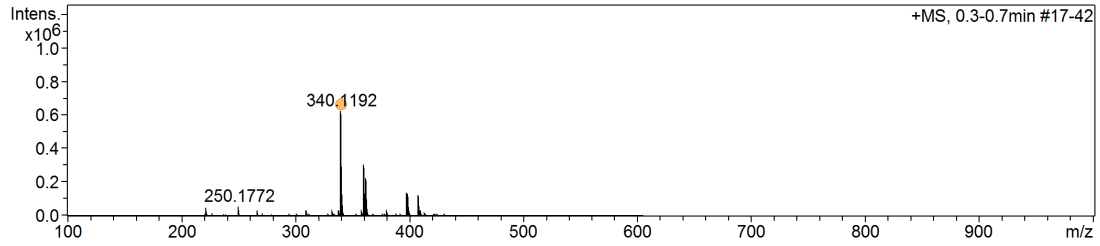
+MS, 0.3-0.7min #17-42



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
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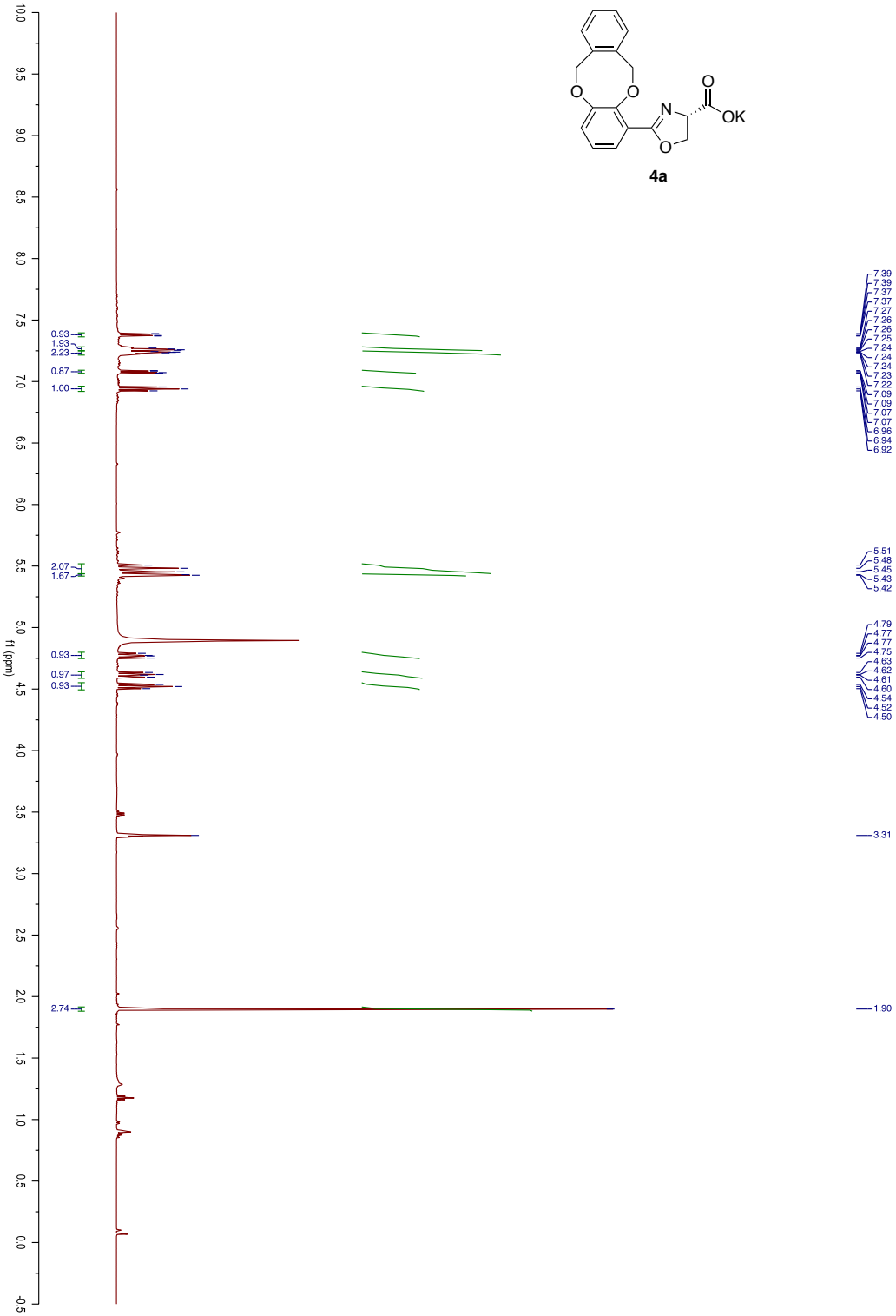
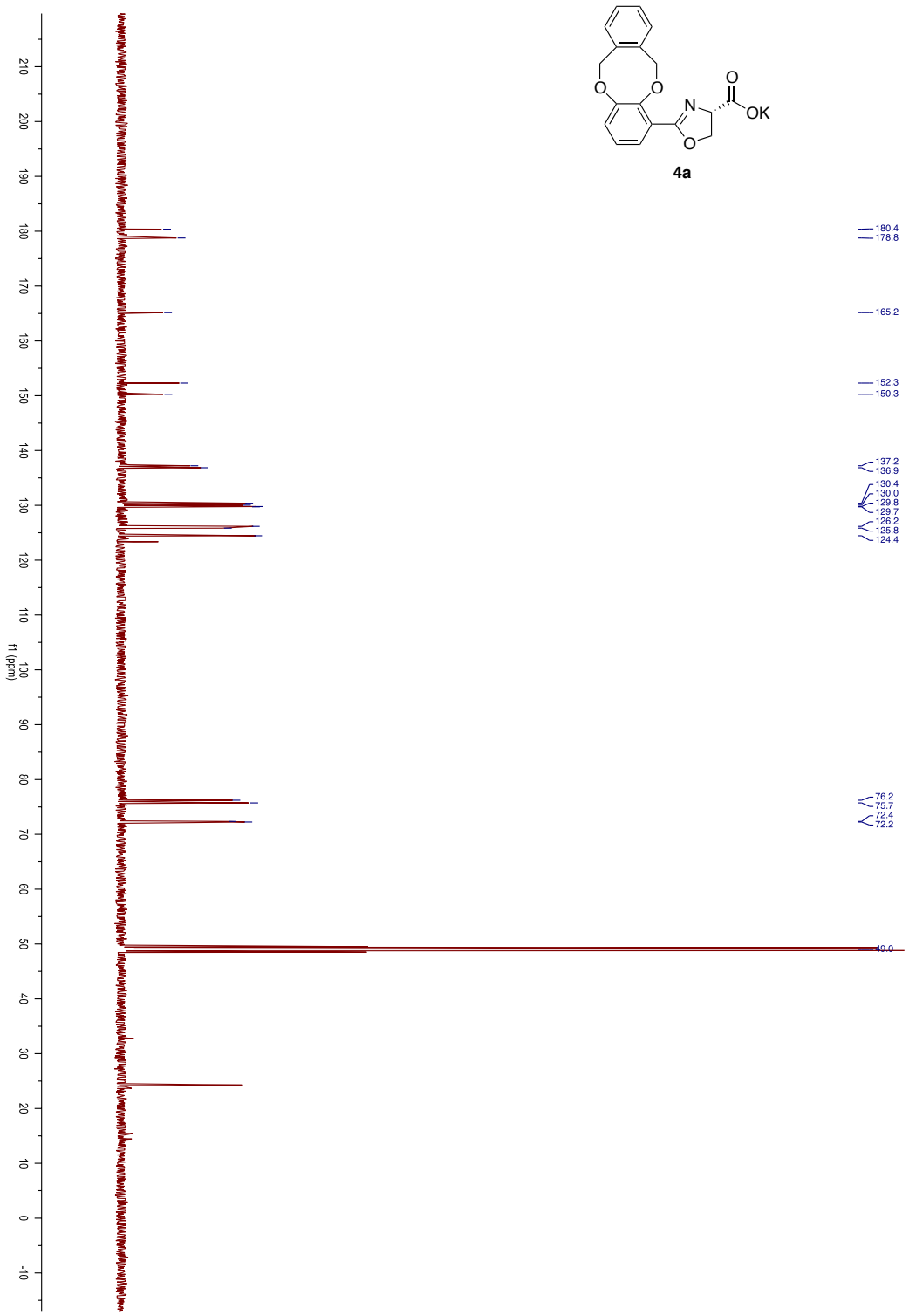
	2	C15H14N7O3	340.1153	-11.6	12.1	2	5.46	12.5	even	ok
	3	C20H14N5O	340.1193	0.3	15.7	3	100.00	16.5	even	ok
	1	C18H15N5NaO	340.1169	-6.8	5.6	1	100.00	13.5	even	ok
	2	C17H19NNaO5	340.1155	10.7	10.7	2	24.99	8.5	even	ok
	3	C11H19N5NaO6	340.1228	-10.5	39.7	3	14.37	4.5	even	ok
	4	C10H23NNaO10	340.1214	6.5	52.8	4	34.63	-0.5	even	ok

^{1}H-NMR of Compound 4a (500 MHz, CD_3OD)



^{13}C-NMR of Compound 4a (125 MHz, CD_3OD)



HR-MS of Compound 4a

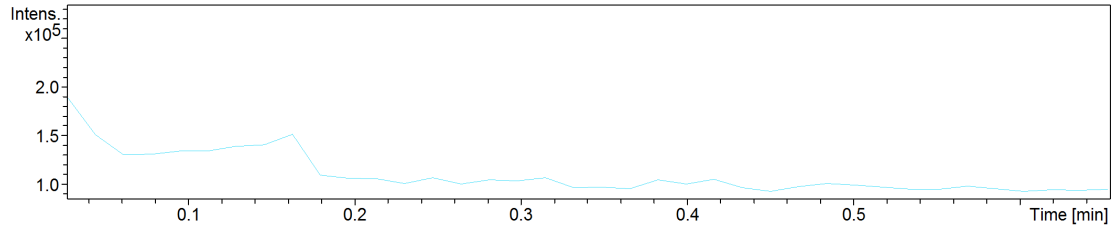
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ003.d	Acquisition Date	7/9/2019 5:20:01 PM
Method	Tune_pos_Standard_100_600_190102.d.m	Operator	lee
Sample Name	KSJ03_4a	Instrument	compact 8255754.10024
Comment			

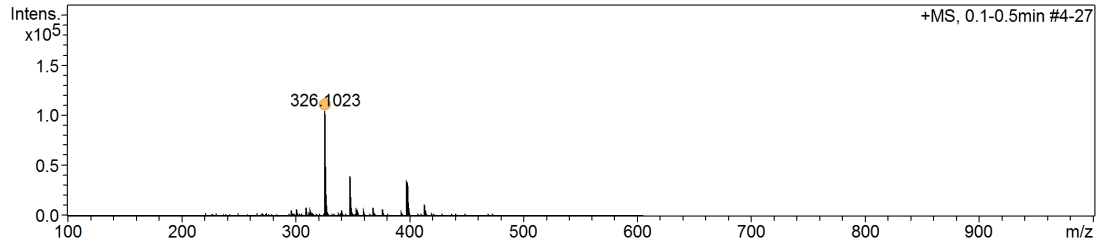
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



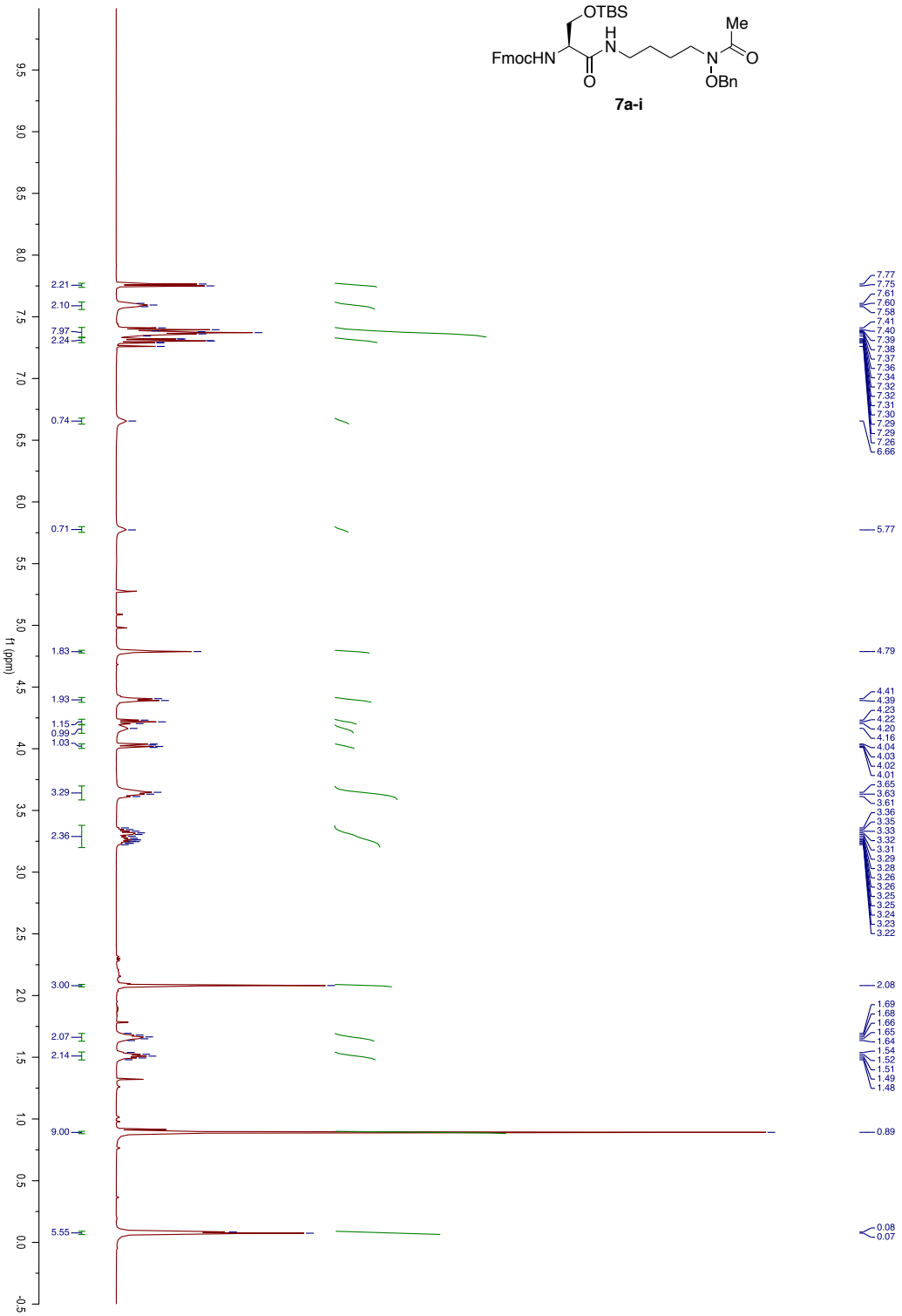
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	326.1023	n.a.

+MS, 0.1-0.5min #4-27

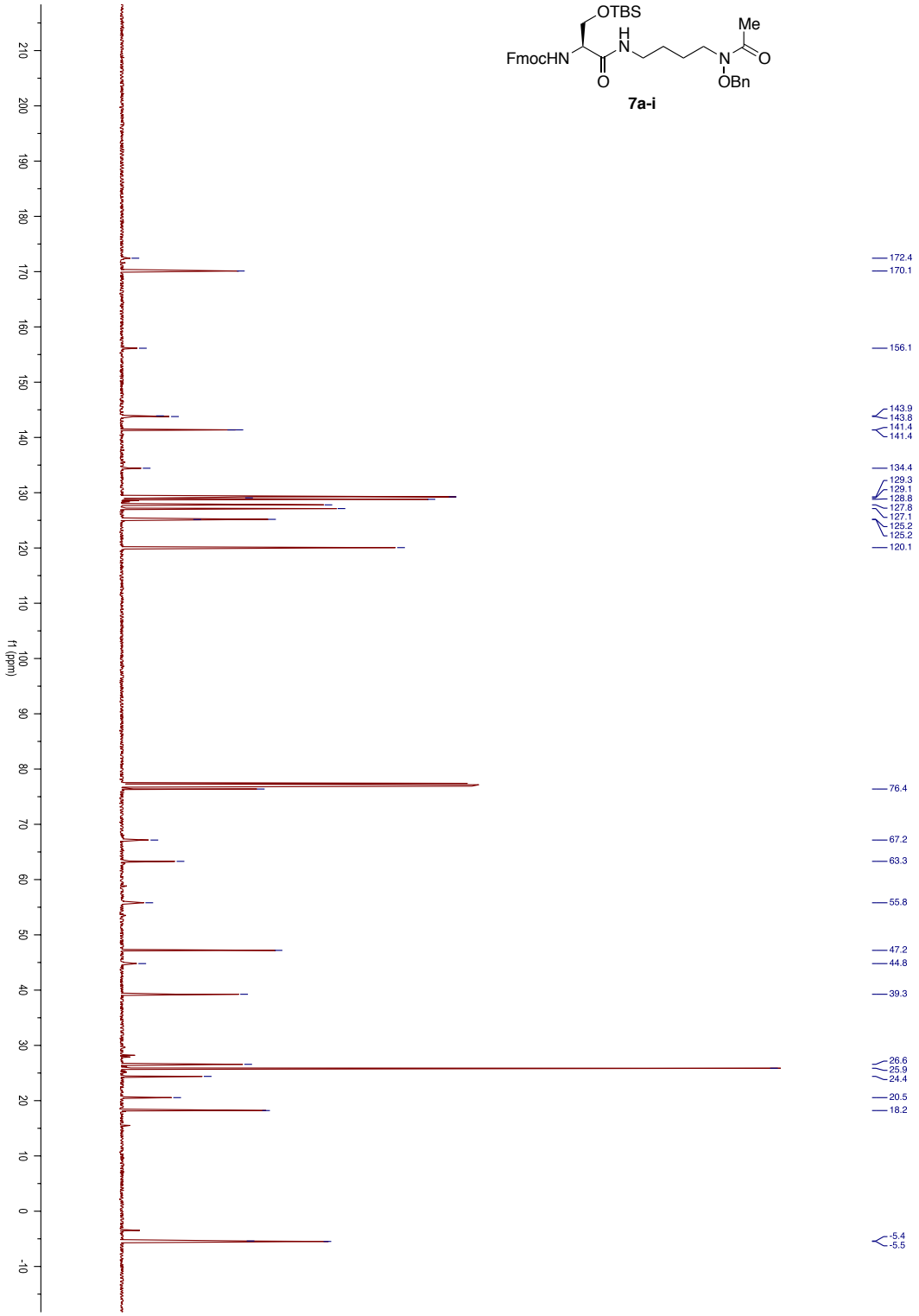


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
326.1023	1	C19H17KN3	326.1054	9.5	33.1	1	20.38	12.5	even	ok
	2	C14H17KN5O2	326.1014	2.9	35.7	2	100.00	8.5	even	ok
	3	C10H13KN11	326.0987	11.1	40.0	3	9.78	9.5	even	ok
	4	C13H21KNO6	326.1000	7.0	44.6	4	31.33	3.5	even	ok
	5	C14H22K2N3O	326.1032	-2.6	61.6	5	48.22	4.5	even	ok
	6	C9H22K2N5O3	326.0991	-9.8	69.9	6	5.91	0.5	even	ok
	7	C14H27K3N	326.1049	8.0	92.7	7	4.03	0.5	even	ok
	1	C17H18KN3Na	326.1030	2.1	31.2	1	100.00	9.5	even	ok
	2	C12H18KN5NaO2	326.0990	-10.2	41.1	2	10.03	5.5	even	ok
	3	C12H23K2N3NaO	326.1007	4.8	63.9	3	22.33	1.5	even	ok

^{1}H-NMR of Compound 7a-i (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 7a-i (125 MHz, CDCl3)



HR-MS of Compound 7a-i

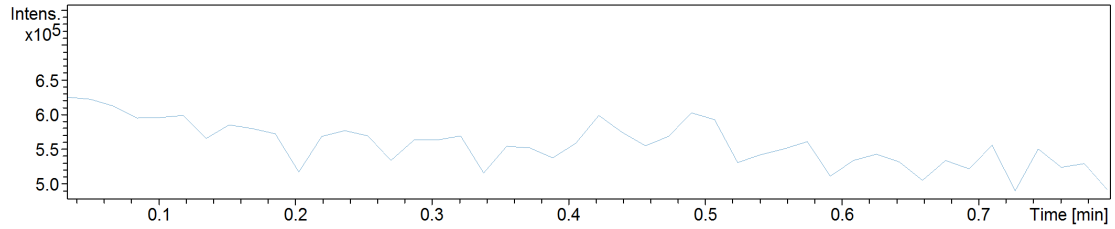
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ004.d	Acquisition Date	7/10/2019 5:09:58 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ04_6a-1	Instrument	compact 8255754.10024
Comment			

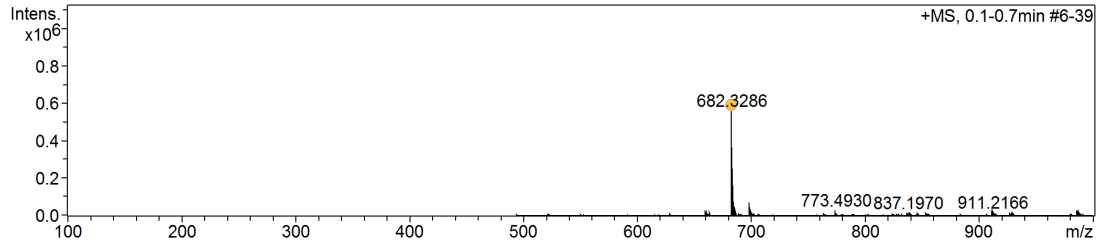
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



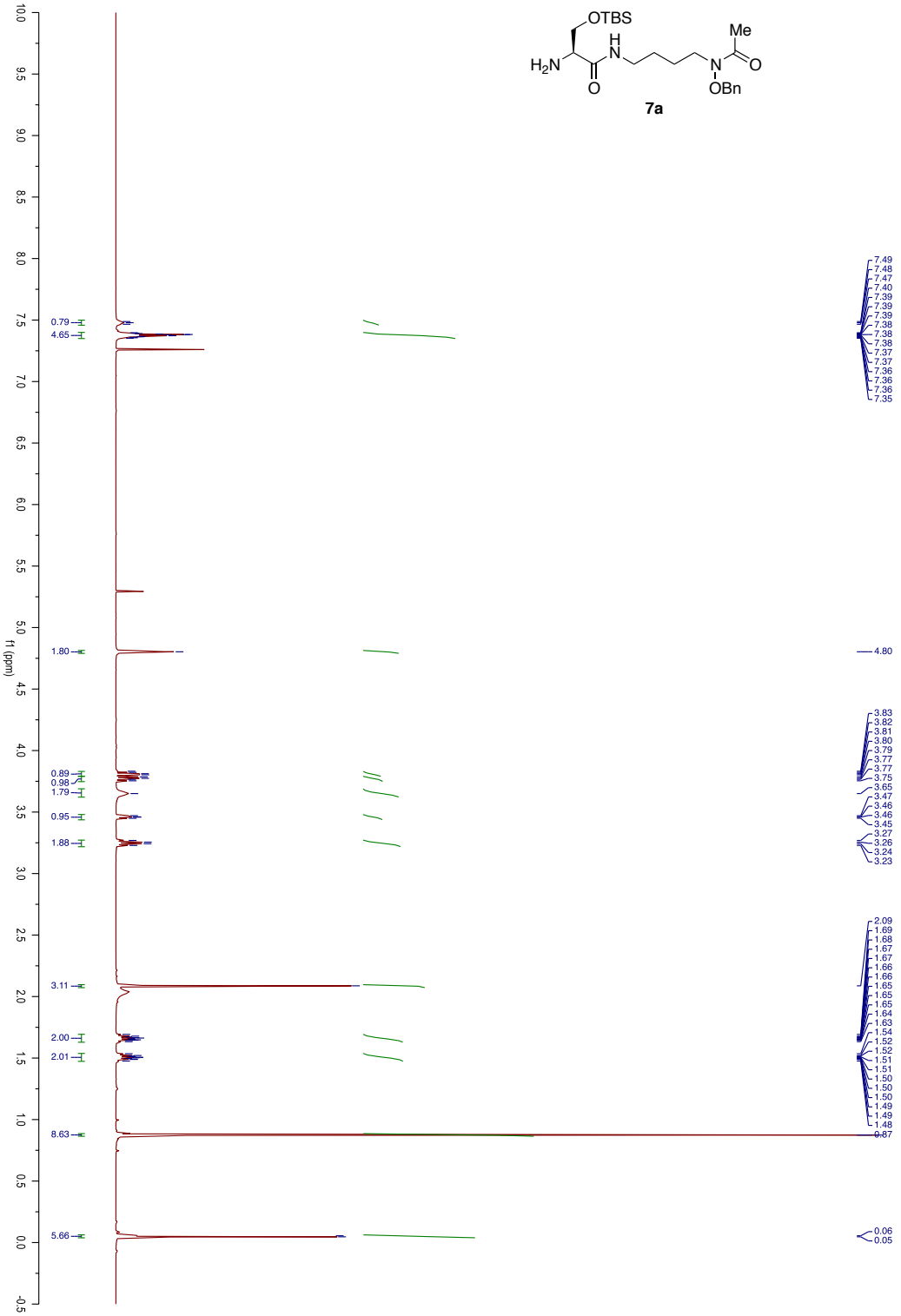
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	682.3286	n.a.

+MS, 0.1-0.7min #6-39

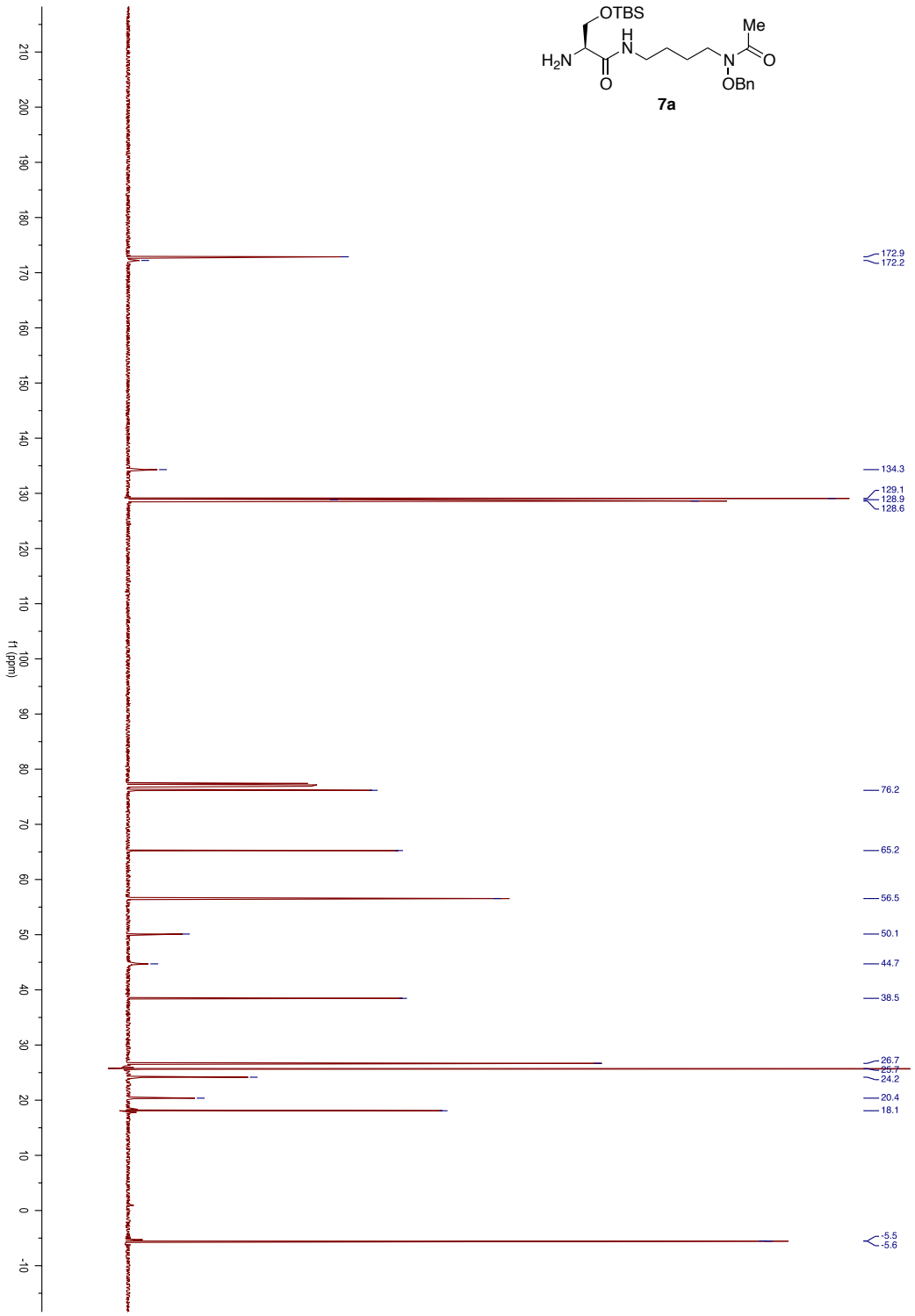


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
682.3286	1	C34H48N5O8Si	682.3267	2.8	3.0	1	49.39	14.5	even	ok
	2	C35H44N9O4Si	682.3280	-0.9	10.1	2	100.00	19.5	even	ok
	3	C33H52NO12Si	682.3253	4.8	11.8	3	12.90	9.5	even	ok
	4	C39H48N3O6Si	682.3307	3.1	22.1	4	30.42	18.5	even	ok
	5	C33H52N5O5Si3	682.3271	-2.2	59.6	5	19.45	13.5	even	ok
	6	C38H52N3O3Si3	682.3311	-3.7	79.0	6	4.51	17.5	even	ok
	1	C33H45N9NaO4Si	682.3256	4.4	2.7	1	17.81	16.5	even	ok
	2	C37H49N3NaO6Si	682.3283	0.5	11.4	2	100.00	15.5	even	ok
	3	C33H53N3NaO7Si2	682.3314	4.1	27.7	3	12.79	10.5	even	ok
	4	C42H49NNaO4Si	682.3323	5.4	33.5	4	4.49	19.5	even	ok
	5	C36H53N3NaO3Si3	682.3287	0.1	69.0	5	27.00	14.5	even	ok

^{1}H-NMR of Compound 7a (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 7a (125 MHz, $CDCl_3$)



HR-MS of Compound 7a

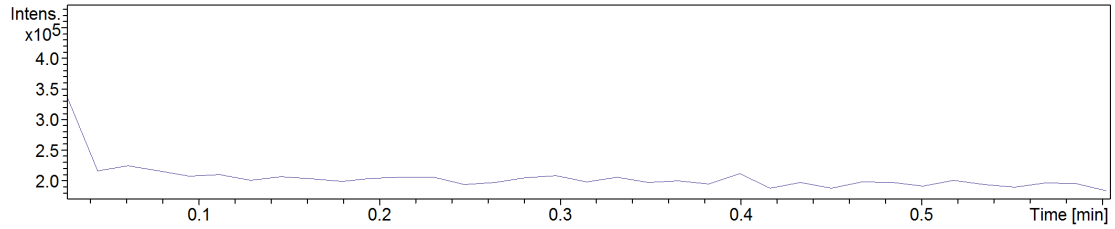
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ005.d	Acquisition Date	7/9/2019 5:23:05 PM
Method	Tune_pos_Standard_100_600_190102.d.m	Operator	lee
Sample Name	KSJ05_7a	Instrument	compact 8255754.10024
Comment			

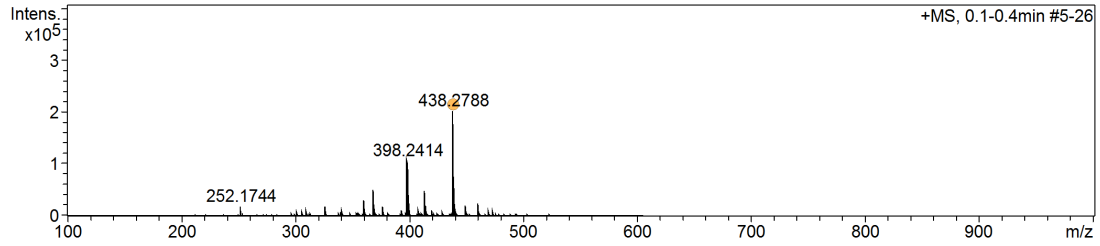
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



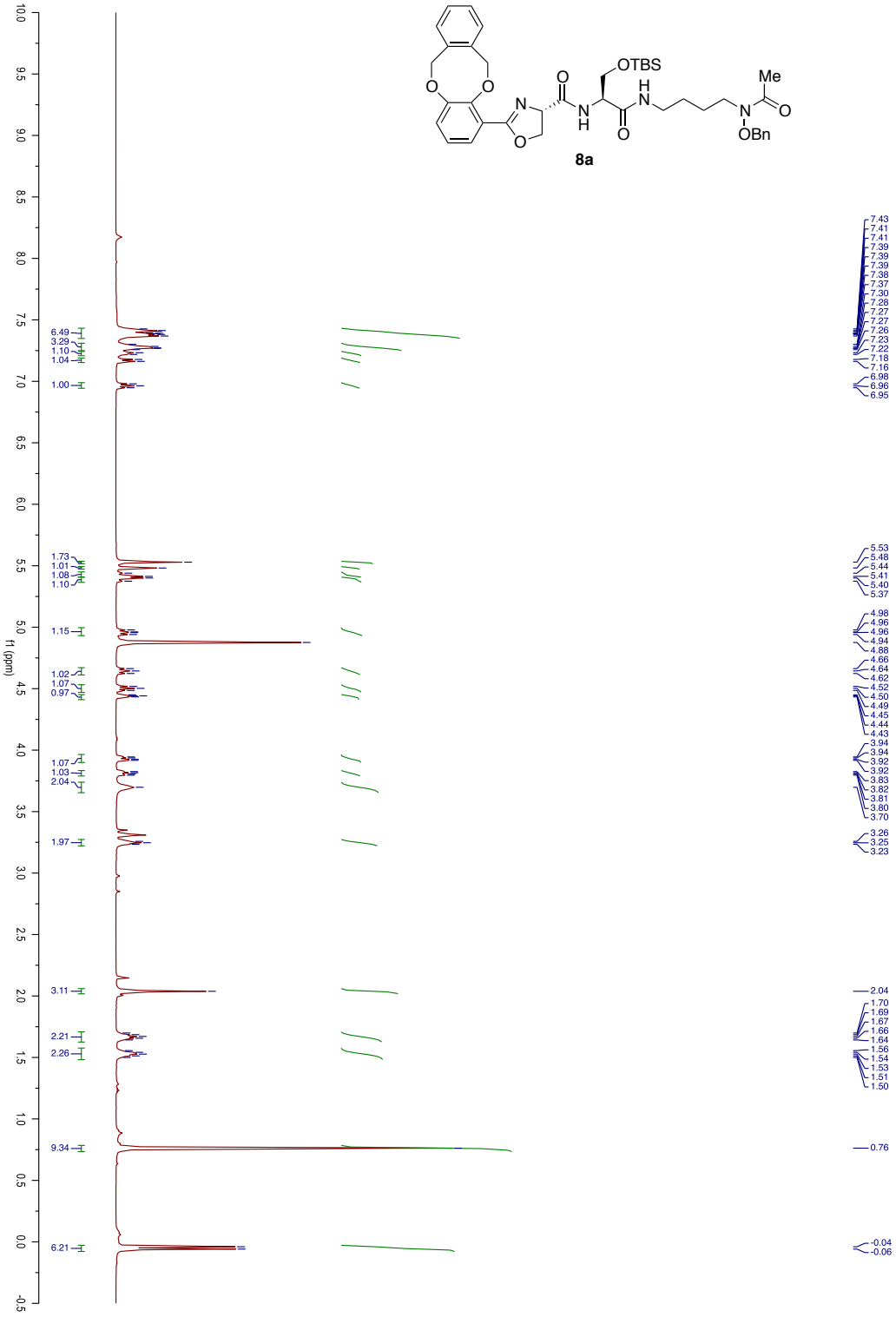
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	438.2788	n.a.

+MS, 0.1-0.4min #5-26

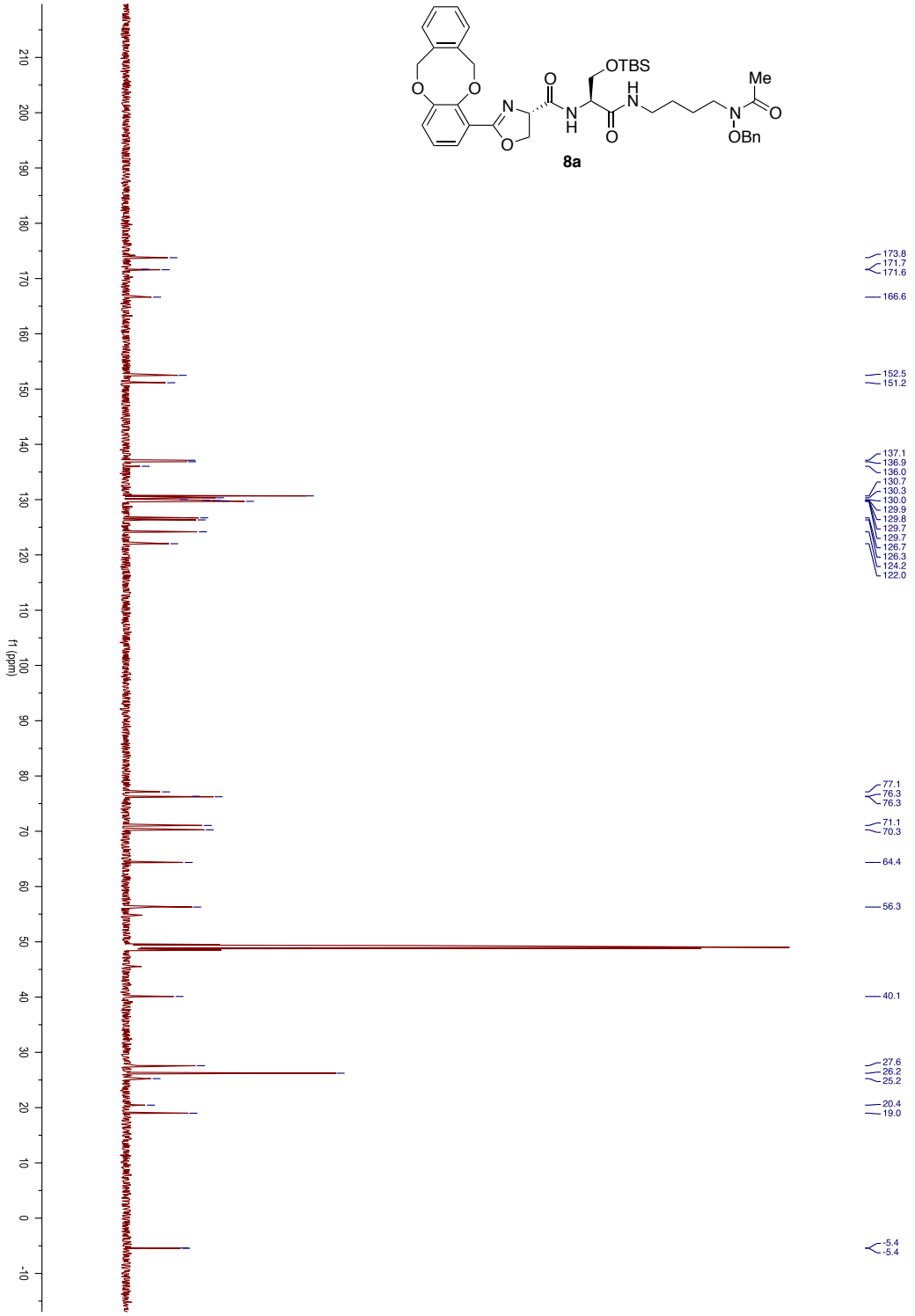


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
438.2788	1	C22H40N3O4Si	438.2783	1.3	8.9	1	100.00	5.5	even	ok
	2	C18H36N9O2Si	438.2756	7.4	15.7	2	11.73	6.5	even	ok
	3	C18H44N3O5Si2	438.2814	5.9	18.1	3	26.62	0.5	even	ok
	4	C19H40N7OSi2	438.2827	-8.9	22.7	4	6.16	5.5	even	ok
	5	C27H40NO2Si	438.2823	7.9	25.3	5	7.73	9.5	even	ok
	6	C21H44N3OSi3	438.2787	0.4	57.9	6	43.38	4.5	even	ok
	7	C17H48N3O2Si4	438.2818	-6.8	73.8	7	3.56	-0.5	even	ok
	1	C20H41N3NaO4Si	438.2759	-6.8	14.4	1	23.29	2.5	even	ok
	2	C25H41NNaO2Si	438.2799	2.4	15.4	2	100.00	6.5	even	ok
	3	C17H41N7NaOSi2	438.2803	3.4	15.5	3	93.87	2.5	even	ok
	4	C19H45N3NaOSi3	438.2763	-5.9	48.6	4	18.19	1.5	even	ok

^{1}H-NMR of Compound 8a (500 MHz, CD_3OD)



^{13}C-NMR of Compound 8a (125 MHz, CD_3OD)



HR-MS of Compound 8a

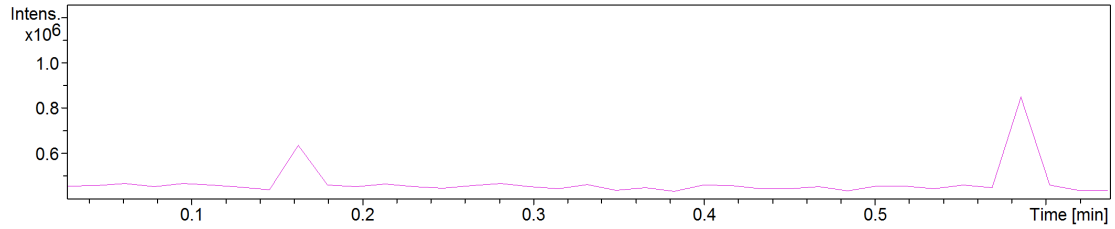
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ016.d	Acquisition Date	9/3/2019 3:29:58 PM
Method	Tune_pos_Standard_100_1000_190902.d.m	Operator	lee
Sample Name	KSJ-8a	Instrument	compact 8255754.10024
Comment			

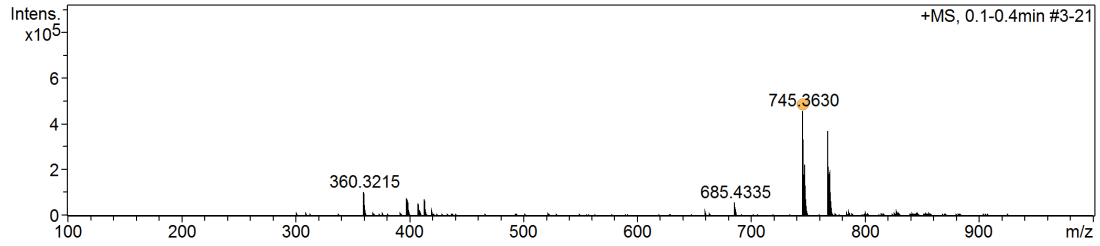
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



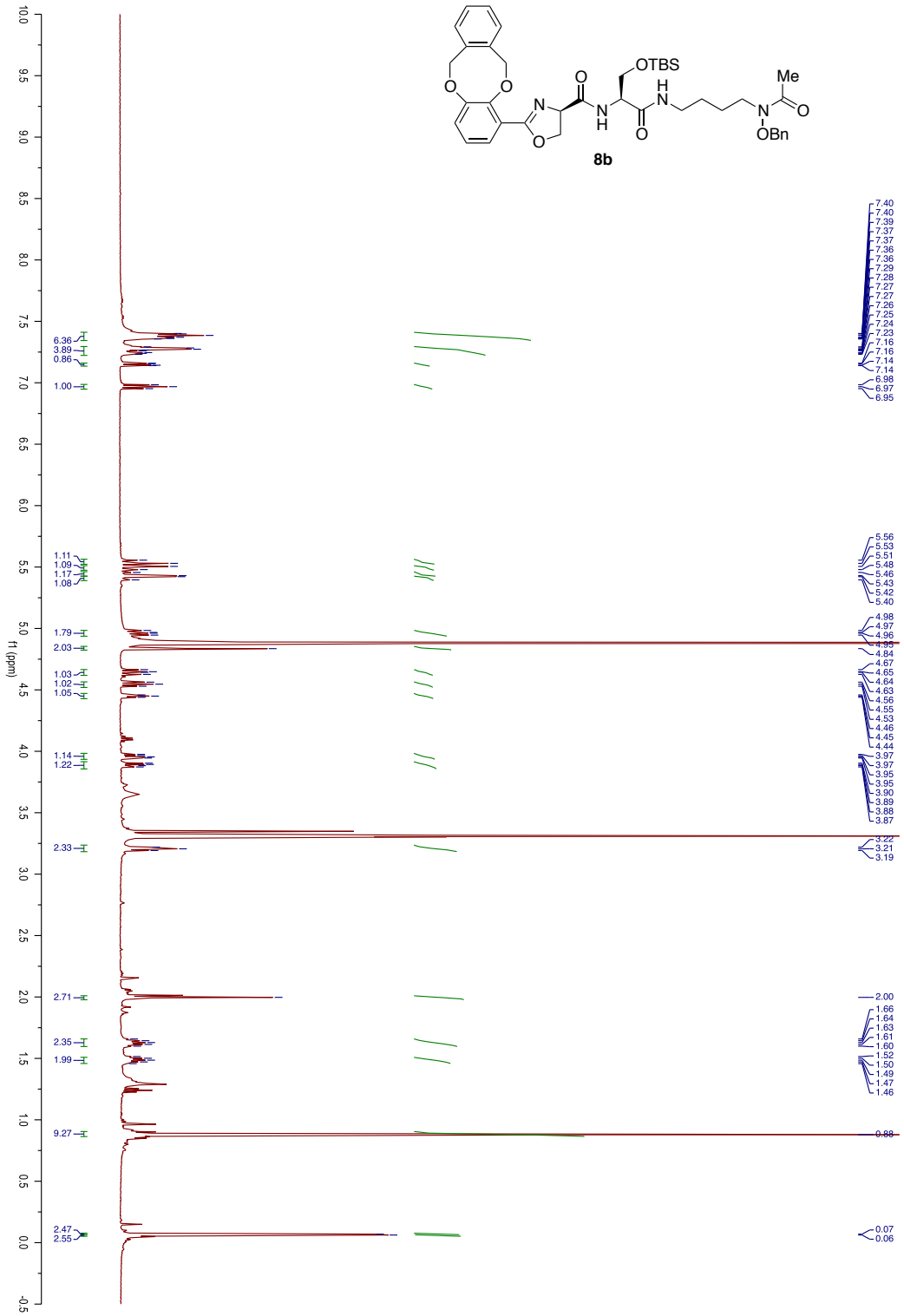
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	745.3630	n.a.

+MS, 0.1-0.4min #3-21

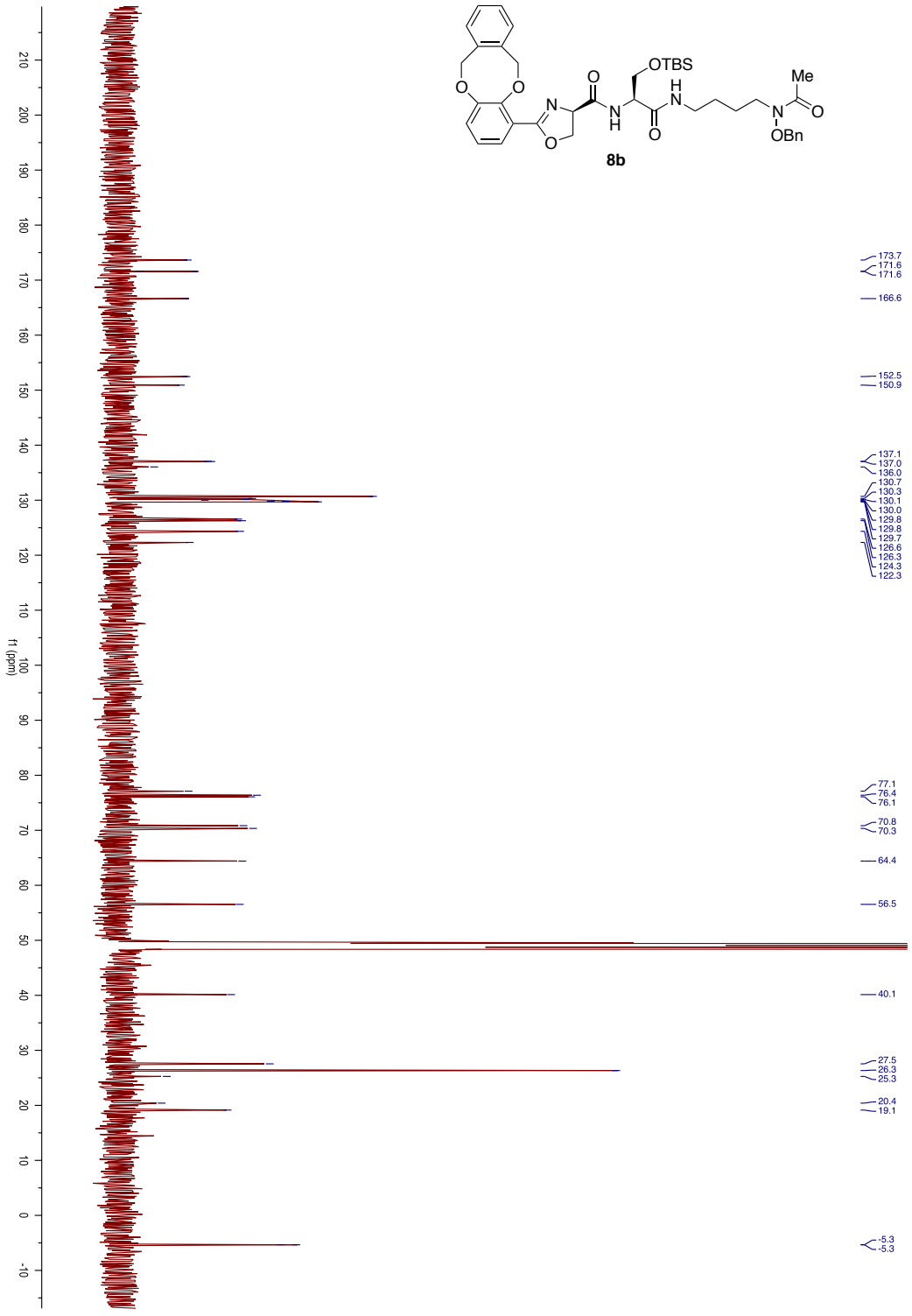


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
745.3630	1	C36H49N10O6Si	745.3600	3.9	3.7	1	17.62	18.5	even	ok
	2	C40H53N4O8Si	745.3627	-0.3	9.8	2	100.00	17.5	even	ok
	3	C41H49N8O4Si	745.3641	1.5	20.3	3	52.81	22.5	even	ok
	4	C36H57N4O9Si2	745.3659	-3.9	26.4	4	11.64	12.5	even	ok
	5	C45H53N2O6Si	745.3667	-5.1	32.4	5	4.02	21.5	even	ok
	6	C43H53N4O4Si2	745.3600	-4.0	58.8	6	4.28	21.5	even	ok
	7	C39H57N4O5Si3	745.3631	-0.2	69.1	7	24.62	16.5	even	ok
	1	C38H54N4NaO8Si	745.3603	3.6	1.5	1	41.87	14.5	even	ok
	2	C39H50N8NaO4Si	745.3616	-1.8	9.9	2	100.00	19.5	even	ok
	3	C43H54N2NaO6Si	745.3643	-1.8	21.4	3	76.79	18.5	even	ok
	4	C37H58N4NaO5Si3	745.3607	3.0	59.2	4	17.28	13.5	even	ok

^{1}H-NMR of Compound 8b (500 MHz, CD_3OD)



^{13}C-NMR of Compound 8b (125 MHz, CD_3OD)



HR-MS of Compound 8b

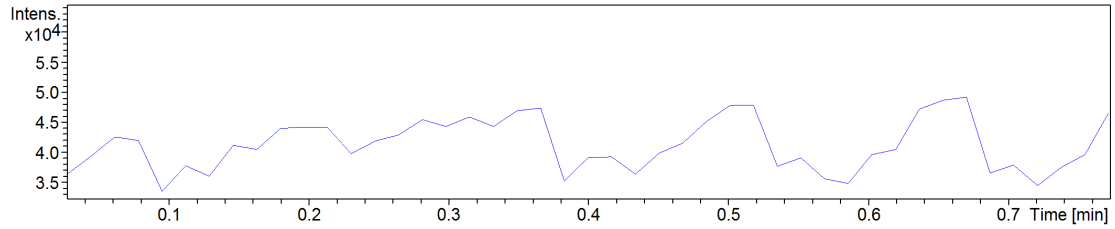
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ009.d	Acquisition Date	7/10/2019 5:22:01 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ09_8b	Instrument	compact 8255754.10024
Comment			

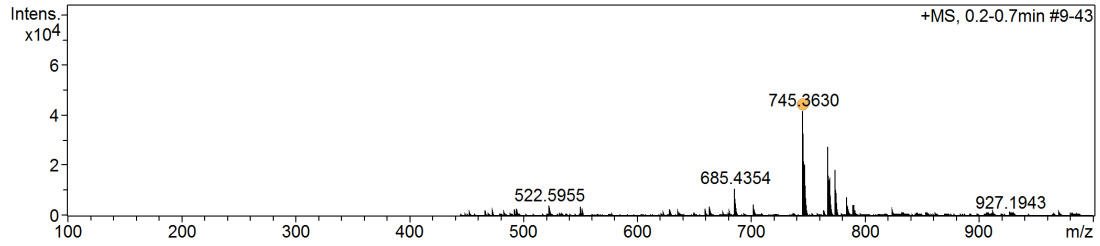
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	450 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



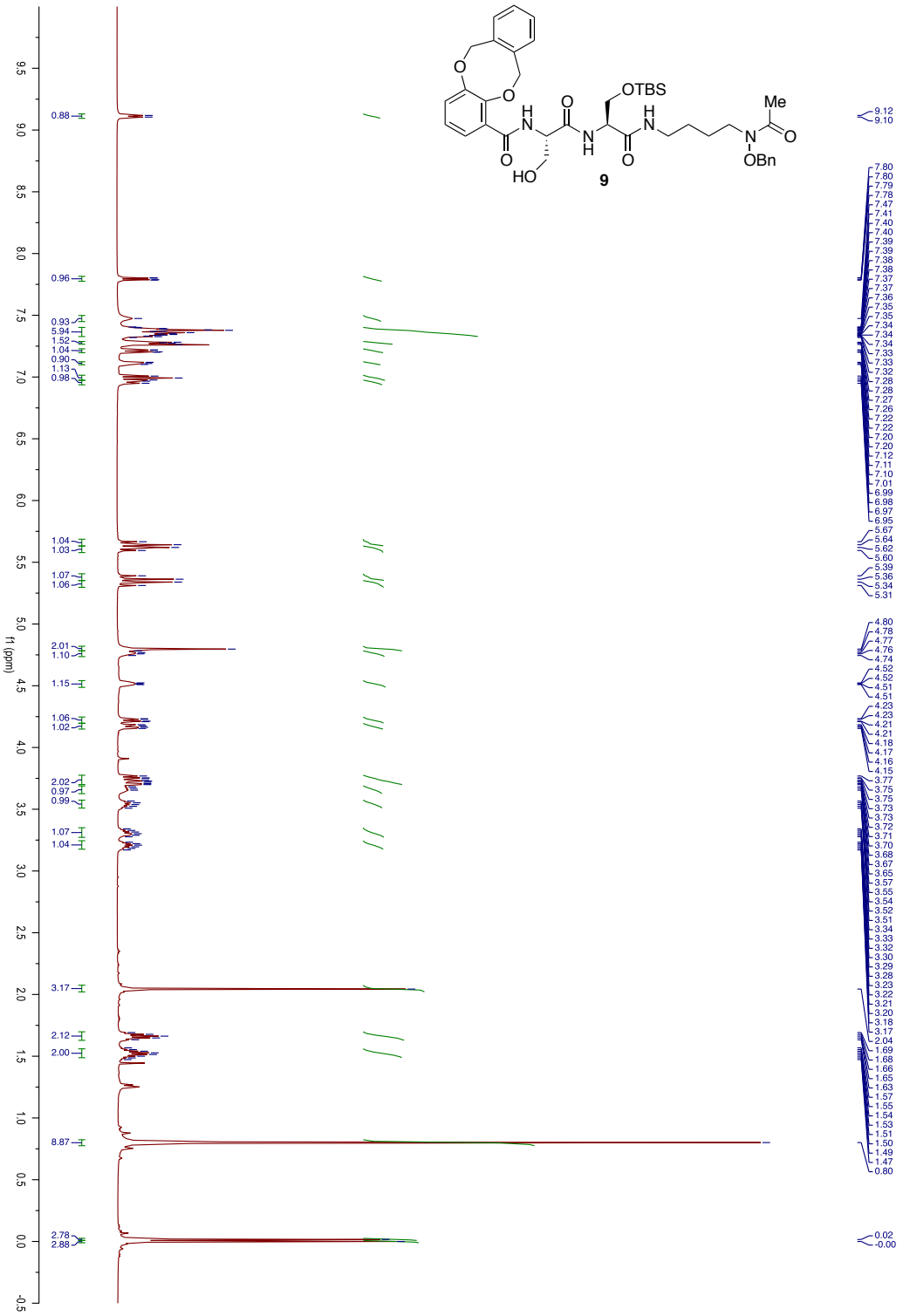
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.5	n.a.	Average spectrum	n.a.	n.a.	n.a.	745.3630	n.a.

+MS, 0.2-0.7min #9-43

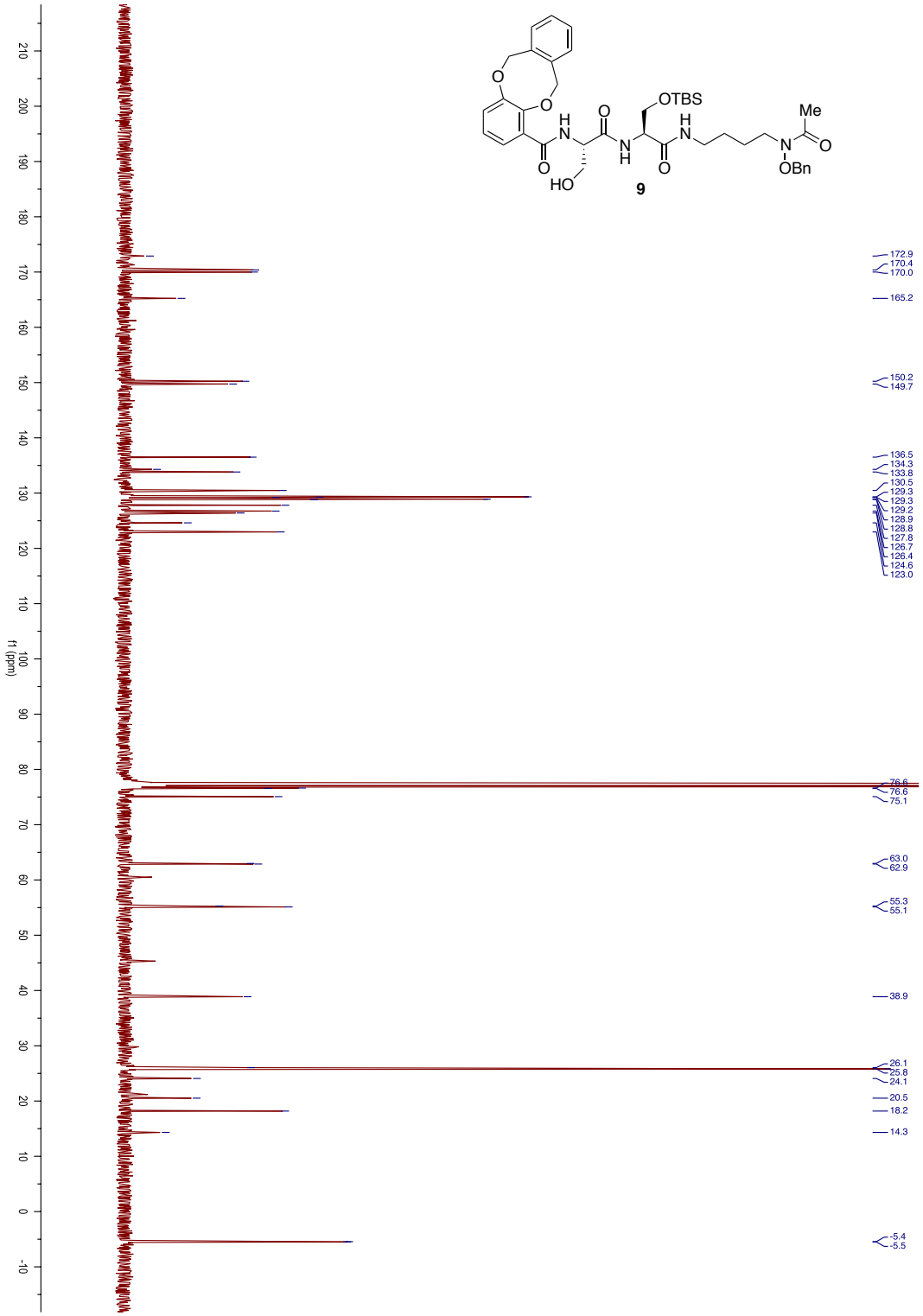


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
745.3630	1	C36H49N10O6Si	745.3600	-4.0	7.4	1	16.06	18.5	even	ok
	2	C40H53N4O8Si	745.3627	-0.4	10.4	2	100.00	17.5	even	ok
	3	C37H45N14O2Si	745.3614	-2.2	12.4	3	44.61	23.5	even	ok
	4	C41H49N8O4Si	745.3641	-1.4	20.9	4	56.96	22.5	even	ok
	5	C36H57N4O9Si2	745.3659	-3.8	24.0	5	13.83	12.5	even	ok
	6	C45H53N2O6Si	745.3667	5.0	32.3	6	4.60	21.5	even	ok
	7	C43H53N4O4Si2	745.3600	-4.1	57.6	7	4.33	21.5	even	ok
	8	C39H57N4O5Si3	745.3631	0.1	67.4	8	28.39	16.5	even	ok
	9	C52H49N2OSi	745.3609	-2.9	68.3	9	6.54	30.5	even	ok
	10	C48H53N2O2Si2	745.3640	1.3	74.0	10	14.46	25.5	even	ok
	11	C40H53N8OSi3	745.3645	-1.9	75.9	11	10.17	21.5	even	ok
	12	C42H57N4OSi4	745.3604	3.6	116.1	12	0.62	20.5	even	ok
	13	C38H61N4O2Si5	745.3635	0.7	133.3	13	1.02	15.5	even	ok
	1	C38H54N4NaO8Si	745.3603	3.7	5.3	1	39.93	14.5	even	ok
	2	C39H50N8NaO4Si	745.3616	1.9	11.9	2	100.00	19.5	even	ok
	3	C43H54N2NaO6Si	745.3643	1.7	21.7	3	87.27	18.5	even	ok
	4	C36H50N12NaOSi2	745.3661	-4.1	30.8	4	16.74	19.5	even	ok
	5	C44H50N6NaO2Si	745.3657	3.5	32.4	5	24.75	23.5	even	ok
	6	C37H58N4NaO5Si3	745.3607	-3.1	57.3	6	18.83	13.5	even	ok

^{1}H-NMR of Compound 9 (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 9 (125 MHz, $CDCl_3$)



HR-MS of Compound 9

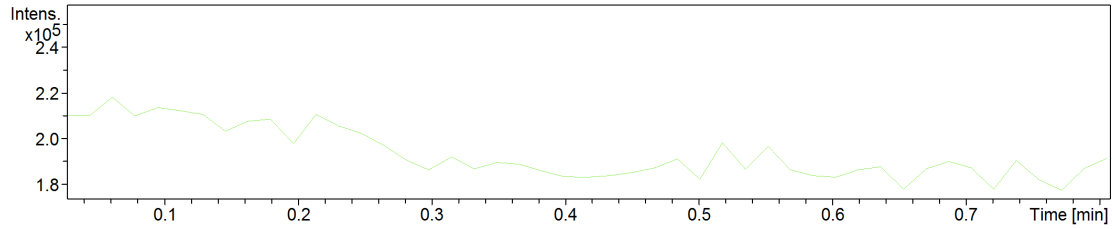
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ012-1.d	Acquisition Date	7/10/2019 5:39:24 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ12_9	Instrument	compact 8255754.10024
Comment			

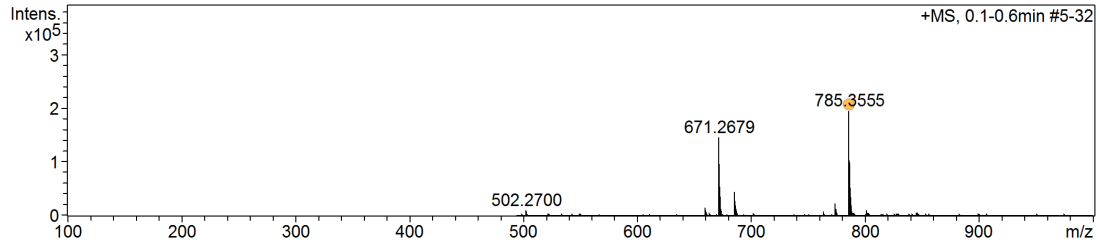
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



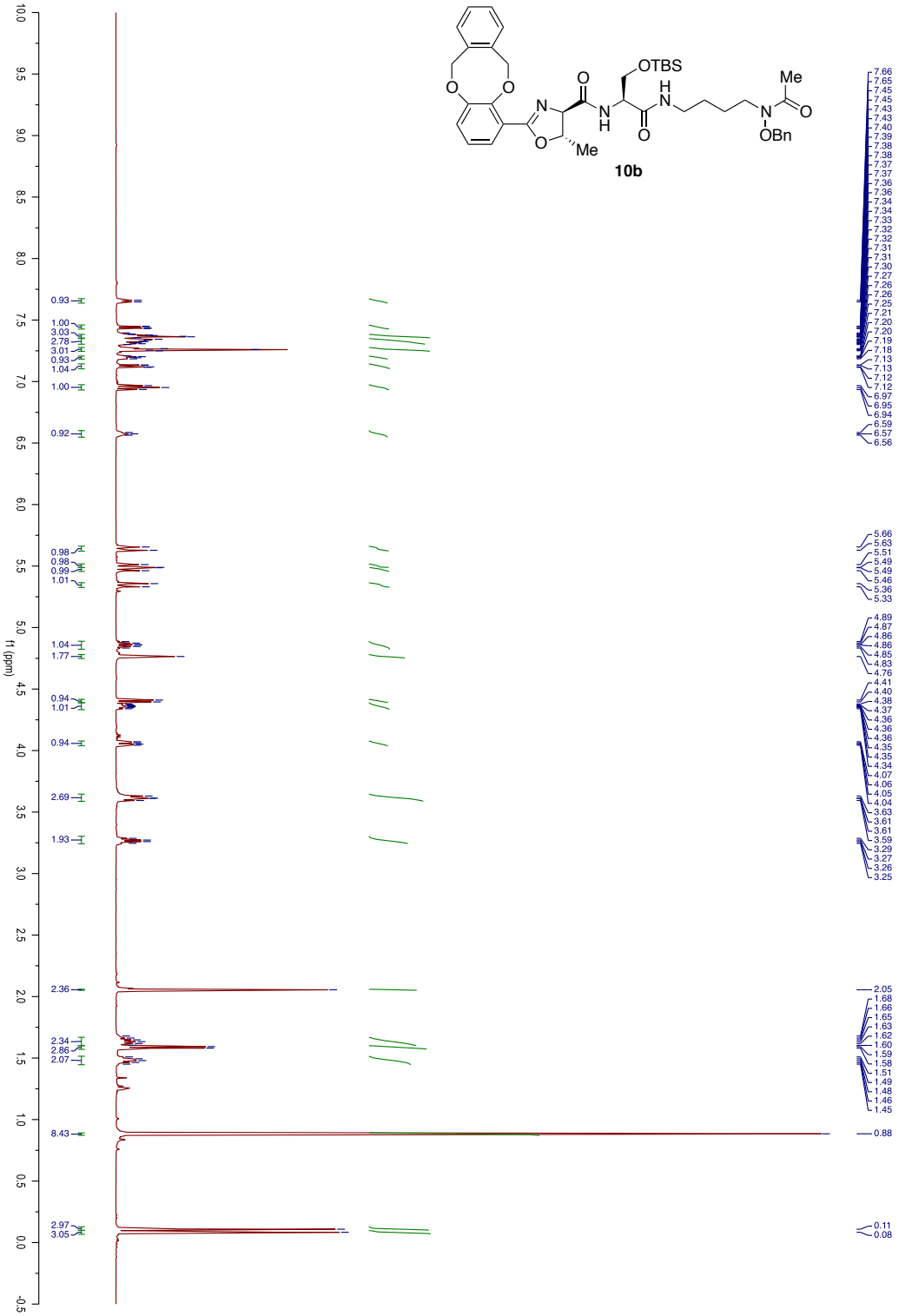
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	785.3555	n.a.

+MS, 0.1-0.6min #5-32

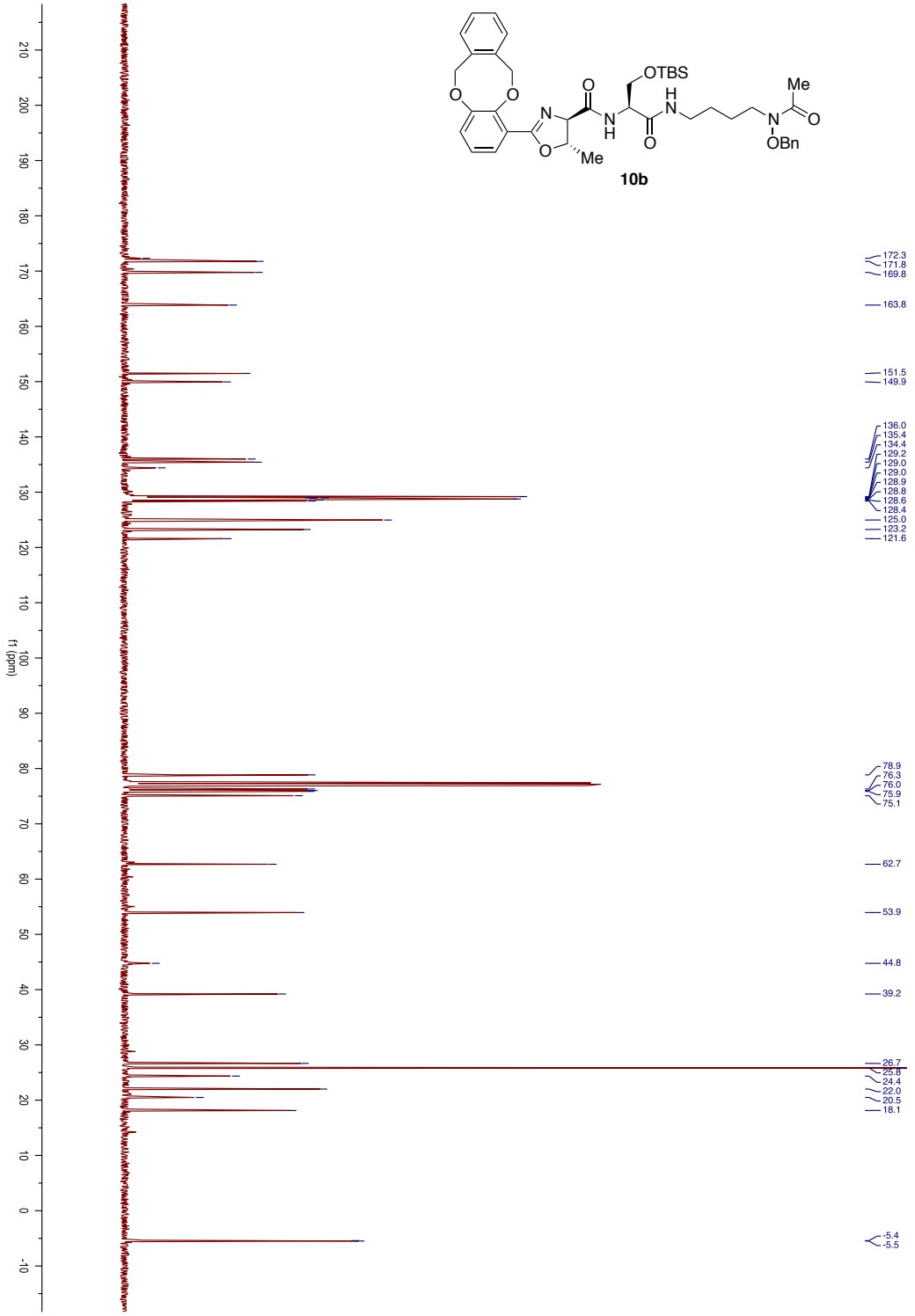


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
785.3555	1	C38H49N10O7Si	785.3549	-0.7	4.1	1	100.00	20.5	even	ok
	2	C42H53N4O9Si	785.3576	2.7	10.8	2	31.40	19.5	even	ok
	3	C39H45N14O3Si	785.3563	-1.0	11.0	3	76.44	25.5	even	ok
	4	C43H49N8O5Si	785.3590	-4.5	21.4	4	7.26	24.5	even	ok
	5	C49H49N4O4Si	785.3518	4.7	46.5	5	3.01	28.5	even	ok
	6	C41H49N10O3Si2	785.3522	4.1	46.9	6	4.86	24.5	even	ok
	7	C45H53N4O5Si2	785.3549	0.7	54.9	7	34.14	23.5	even	ok
	8	C54H49N2O2Si	785.3558	-0.4	70.0	8	19.14	32.5	even	ok
	9	C46H49N8OSi2	785.3562	1.0	70.2	9	15.20	28.5	even	ok
	10	C41H57N4O6Si3	785.3580	-3.3	70.5	10	5.11	18.5	even	ok
	11	C50H53N2O3Si2	785.3589	-4.4	76.5	11	1.73	27.5	even	ok
	12	C42H53N8O2Si3	785.3594	5.0	79.0	12	0.94	23.5	even	ok
	13	C48H53N4OSi3	785.3522	4.2	103.4	13	0.62	27.5	even	ok
	14	C44H57N4O2Si4	785.3553	-0.2	120.0	14	2.48	22.5	even	ok
	15	C40H61N4O3Si5	785.3585	-3.8	127.7	15	0.28	17.5	even	ok
	16	C38H61N6OSi6	785.3517	-4.8	155.9	16	0.02	17.5	even	ok
	1	C40H54N4NaO9Si	785.3552	-0.3	1.9	1	100.00	16.5	even	ok
	2	C41H50N8NaO5Si	785.3566	1.4	11.1	2	55.18	21.5	even	ok
	3	C42H46N12NaOSi	785.3579	-3.1	21.7	3	17.07	26.5	even	ok

^{1}H-NMR of Compound 10b (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound 10b (125 MHz, $CDCl_3$)



HR-MS of Compound 10b

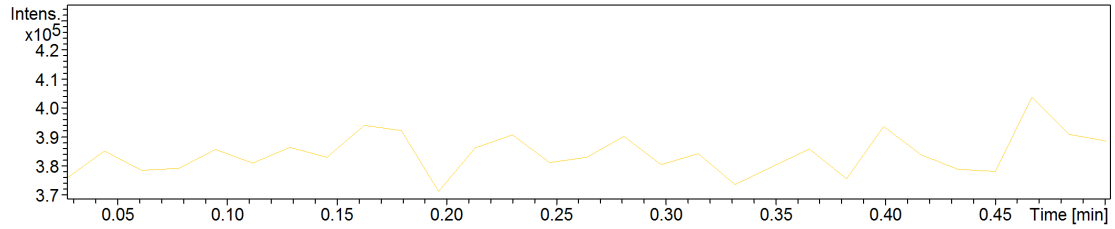
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ013.d	Acquisition Date	7/10/2019 5:43:49 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ13_10b	Instrument	compact 8255754.10024
Comment			

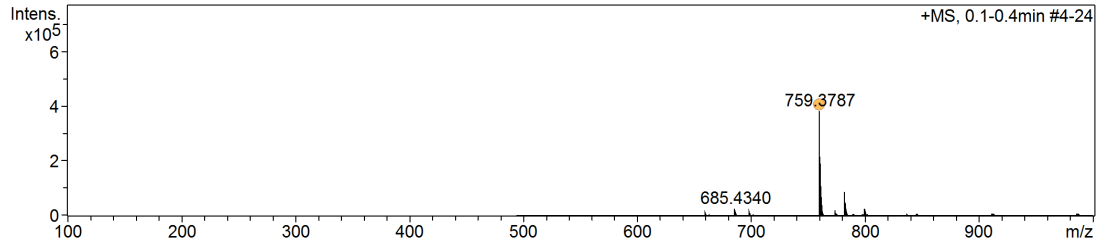
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



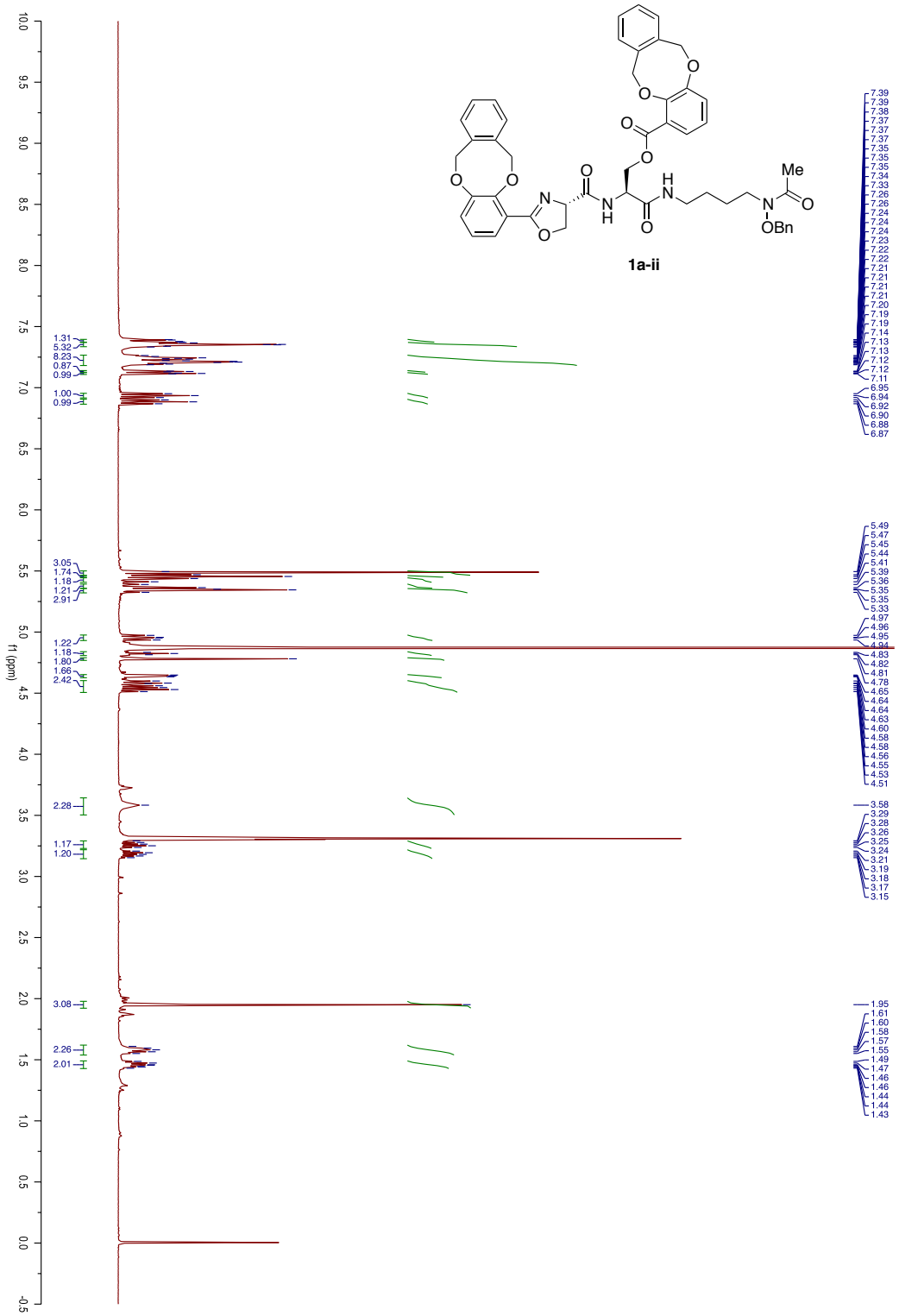
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	759.3787	n.a.

+MS, 0.1-0.4min #4-24

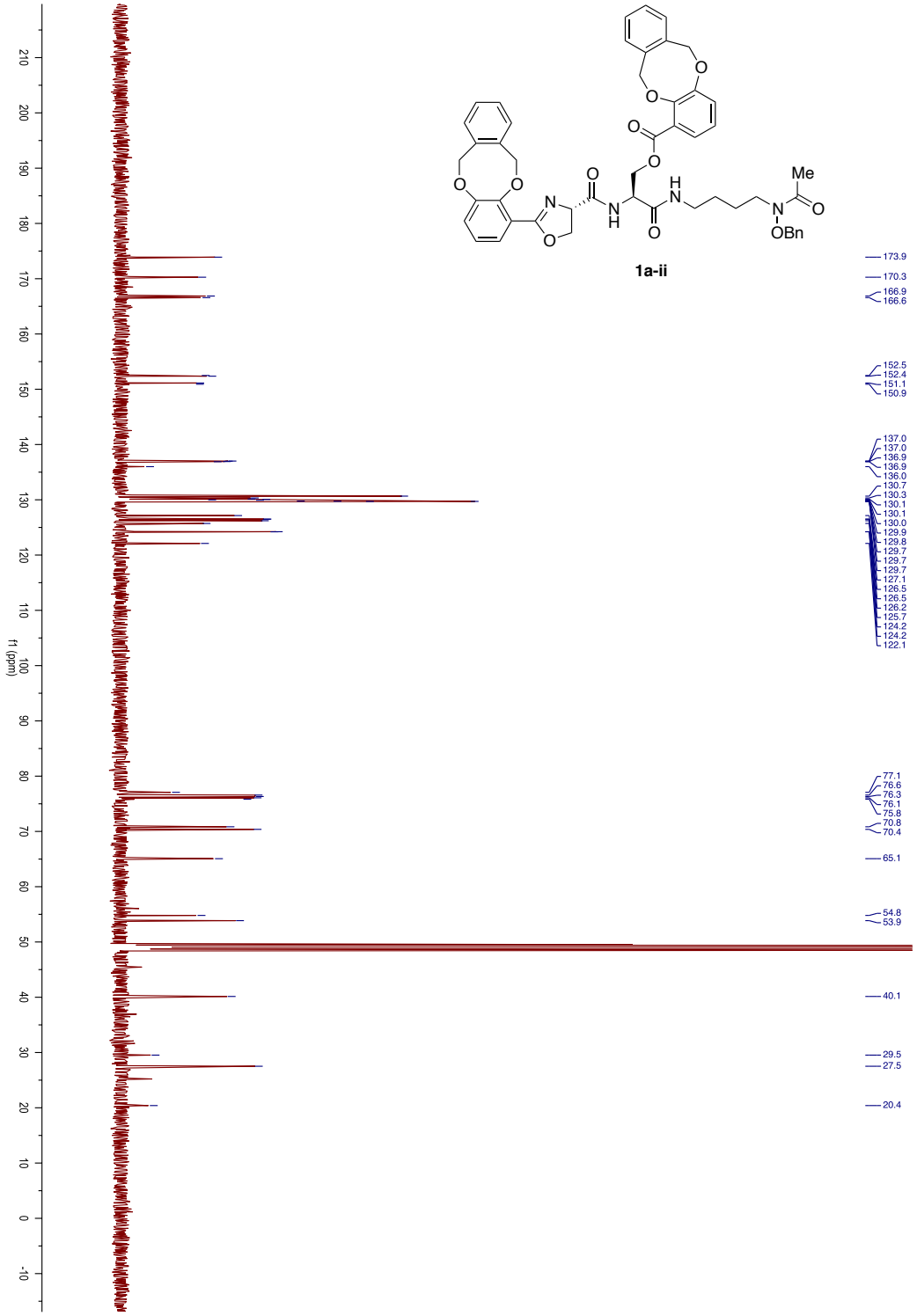


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
759.3787	1	C37H51N10O6Si	759.3757	-4.0	8.0	1	15.20	18.5	even	ok
	2	C41H55N4O8Si	759.3784	-0.4	8.5	2	100.00	17.5	even	ok
	3	C38H47N14O2Si	759.3770	2.2	11.0	3	44.03	23.5	even	ok
	4	C42H51N8O4Si	759.3797	1.3	19.0	4	58.20	22.5	even	ok
	5	C37H59N4O9Si2	759.3815	3.7	22.6	5	14.09	12.5	even	ok
	6	C46H55N2O6Si	759.3824	4.8	30.5	6	4.76	21.5	even	ok
	7	C44H55N4O4Si2	759.3756	-4.0	56.2	7	4.35	21.5	even	ok
	8	C40H59N4O5Si3	759.3788	-0.1	66.4	8	23.94	16.5	even	ok
	9	C53H51N2OSi	759.3765	2.9	66.6	9	6.67	30.5	even	ok
	10	C49H55N2O2Si2	759.3797	1.3	72.8	10	12.37	25.5	even	ok
	11	C41H55N8OSi3	759.3801	-1.9	75.0	11	8.64	21.5	even	ok
	12	C43H59N4OSi4	759.3760	3.5	115.6	12	0.51	20.5	even	ok
	13	C39H63N4O2Si5	759.3792	0.6	123.3	13	1.48	15.5	even	ok
	1	C39H56N4NaO8Si	759.3760	3.6	5.7	1	38.27	14.5	even	ok
	2	C40H52N8NaO4Si	759.3773	-1.9	10.3	2	100.00	19.5	even	ok
	3	C44H56N2NaO6Si	759.3800	-1.7	19.8	3	89.97	18.5	even	ok
	4	C37H52N12NaOSi2	759.3818	-4.0	29.1	4	17.36	19.5	even	ok
	5	C45H52N6NaO2Si	759.3813	-3.4	30.5	5	25.76	23.5	even	ok
	6	C38H60N4NaO5Si3	759.3764	-3.1	56.3	6	15.66	13.5	even	ok

^{1}H-NMR of Compound 1a-ii (500 MHz, CD_3OD)



^{13}C-NMR of Compound 1a-ii (CD_3OD)



HR-MS of Compound 1a-ii

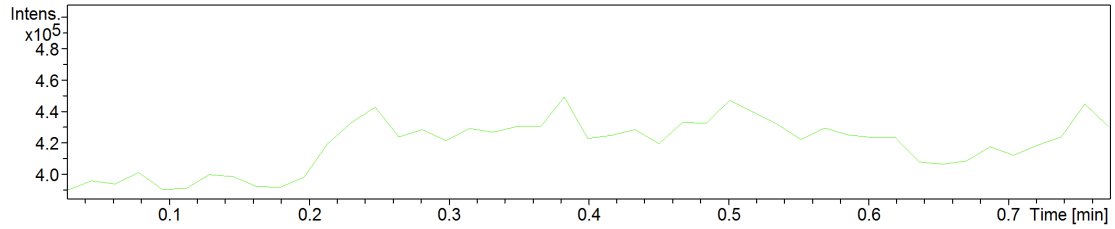
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ007.d	Acquisition Date	7/10/2019 5:13:40 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ07_8a-1	Instrument	compact 8255754.10024
Comment			

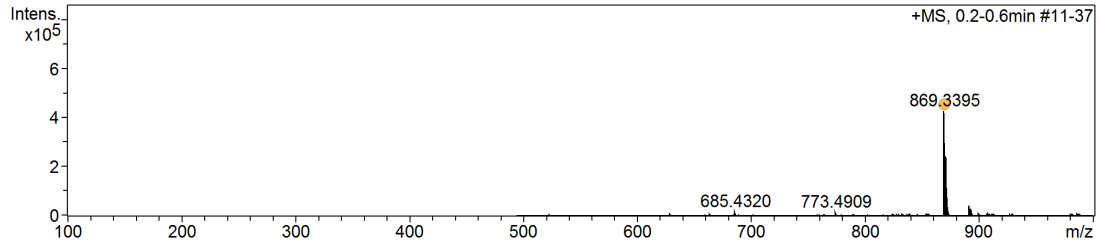
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



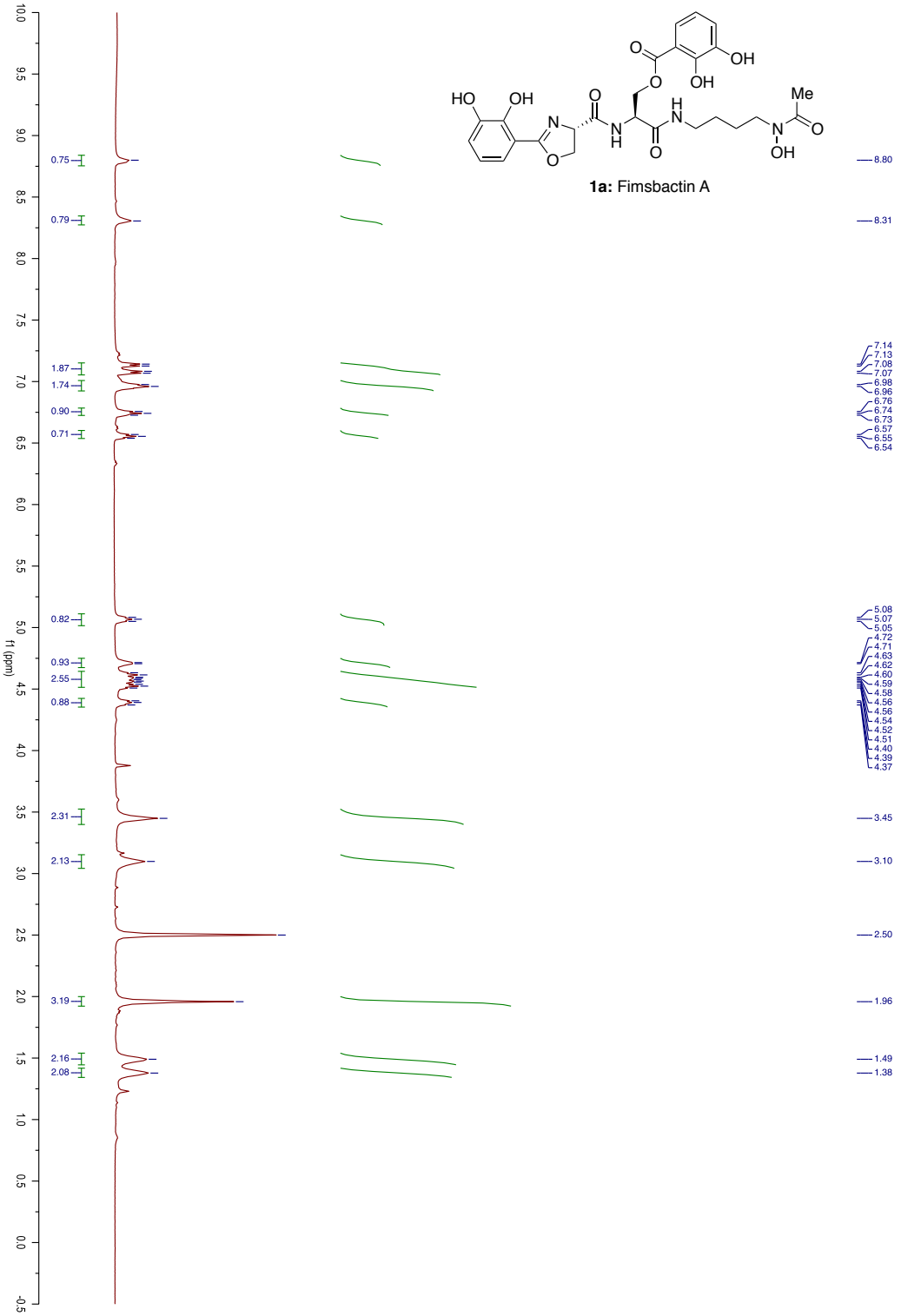
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	869.3395	n.a.

+MS, 0.2-0.6min #11-37

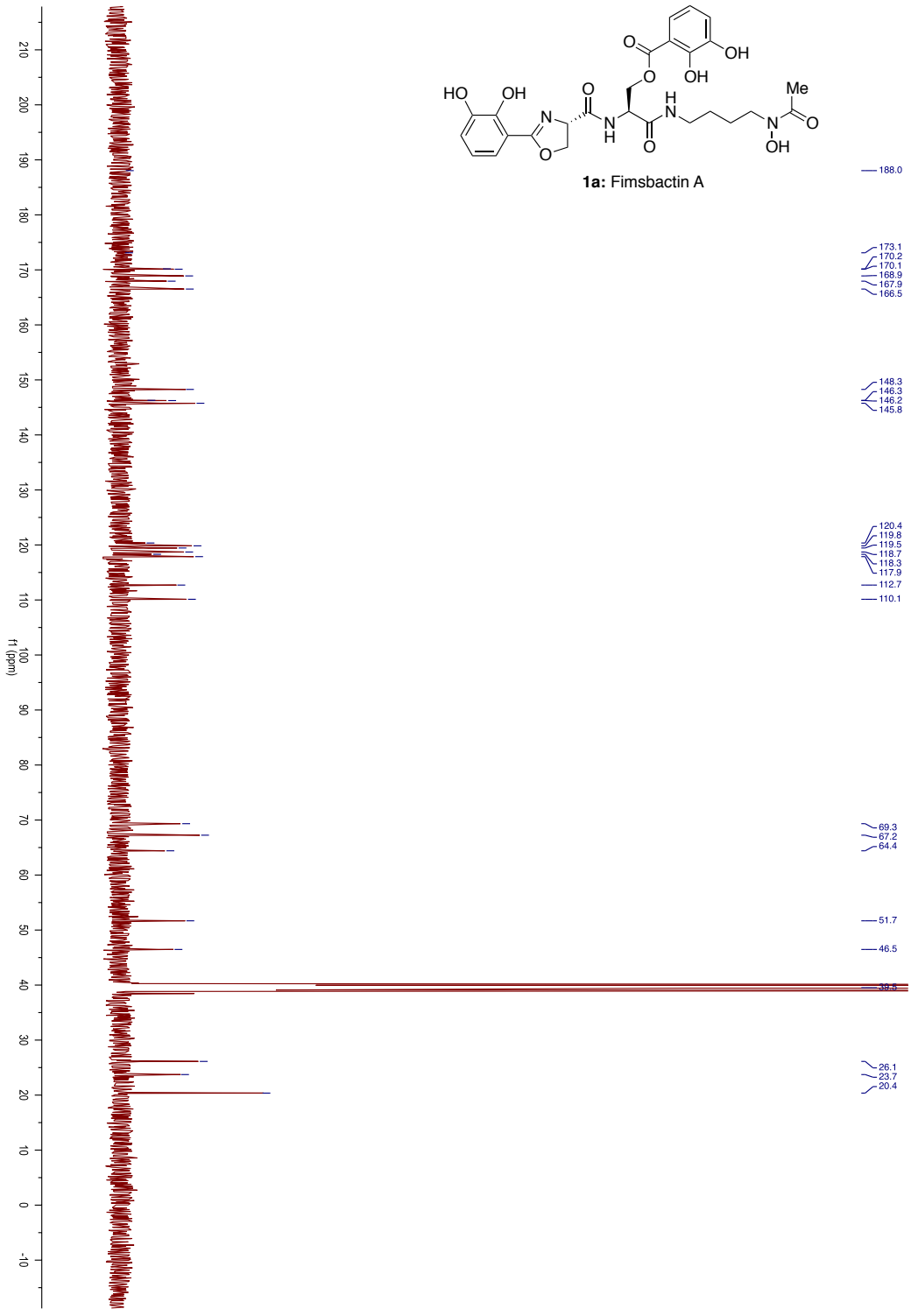


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
869.3395	1	C49H49N4O11	869.3392	-0.3	5.7	1	100.00	27.5	even	ok
	2	C50H45N8O7	869.3406	1.3	6.4	2	62.67	32.5	even	ok
	3	C47H37N18O	869.3392	0.3	10.3	3	91.54	38.5	even	ok
	4	C46H41N14O5	869.3379	1.8	10.5	4	43.48	33.5	even	ok
	5	C51H41N12O3	869.3419	-2.8	16.8	5	19.65	37.5	even	ok
	6	C54H49N2O9	869.3433	4.4	17.5	6	5.05	31.5	even	ok
	7	C45H45N10O9	869.3365	-3.3	18.4	7	12.54	28.5	even	ok
	1	C52H50N2NaO9	869.3409	-1.6	6.7	1	51.64	28.5	even	ok
	2	C48H46N8NaO7	869.3382	-1.5	8.2	2	53.54	29.5	even	ok
	3	C49H42N12NaO3	869.3395	-0.1	9.0	3	100.00	34.5	even	ok
	4	C45H38N18NaO	869.3368	-3.0	13.8	4	17.35	35.5	even	ok
	5	C47H50N4NaO11	869.3368	3.0	16.7	5	16.53	24.5	even	ok
	6	C53H46N6NaO5	869.3422	-3.1	17.4	6	14.89	33.5	even	ok
	7	C44H42N14NaO5	869.3355	-4.6	20.3	7	3.80	30.5	even	ok

^{1}H-NMR of Compound 1a (Fimsbactin A, 500 MHz, DMSO-d^{6})



^{13}C-NMR of Compound 1a (Fimsbactin A, 125 MHz, DMSO-d^{6})



HR-MS of Compound 1a (Fimsbactin A)

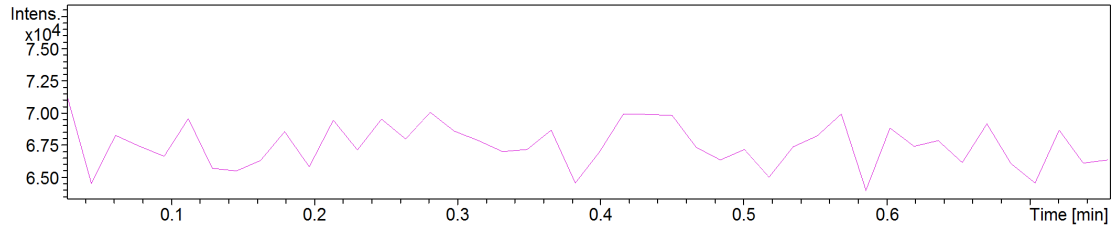
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ008.d	Acquisition Date	7/10/2019 5:19:01 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ08_1a	Instrument	compact 8255754.10024
Comment			

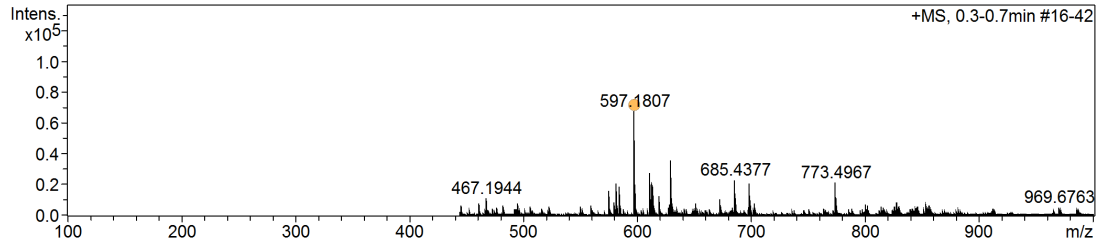
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	450 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



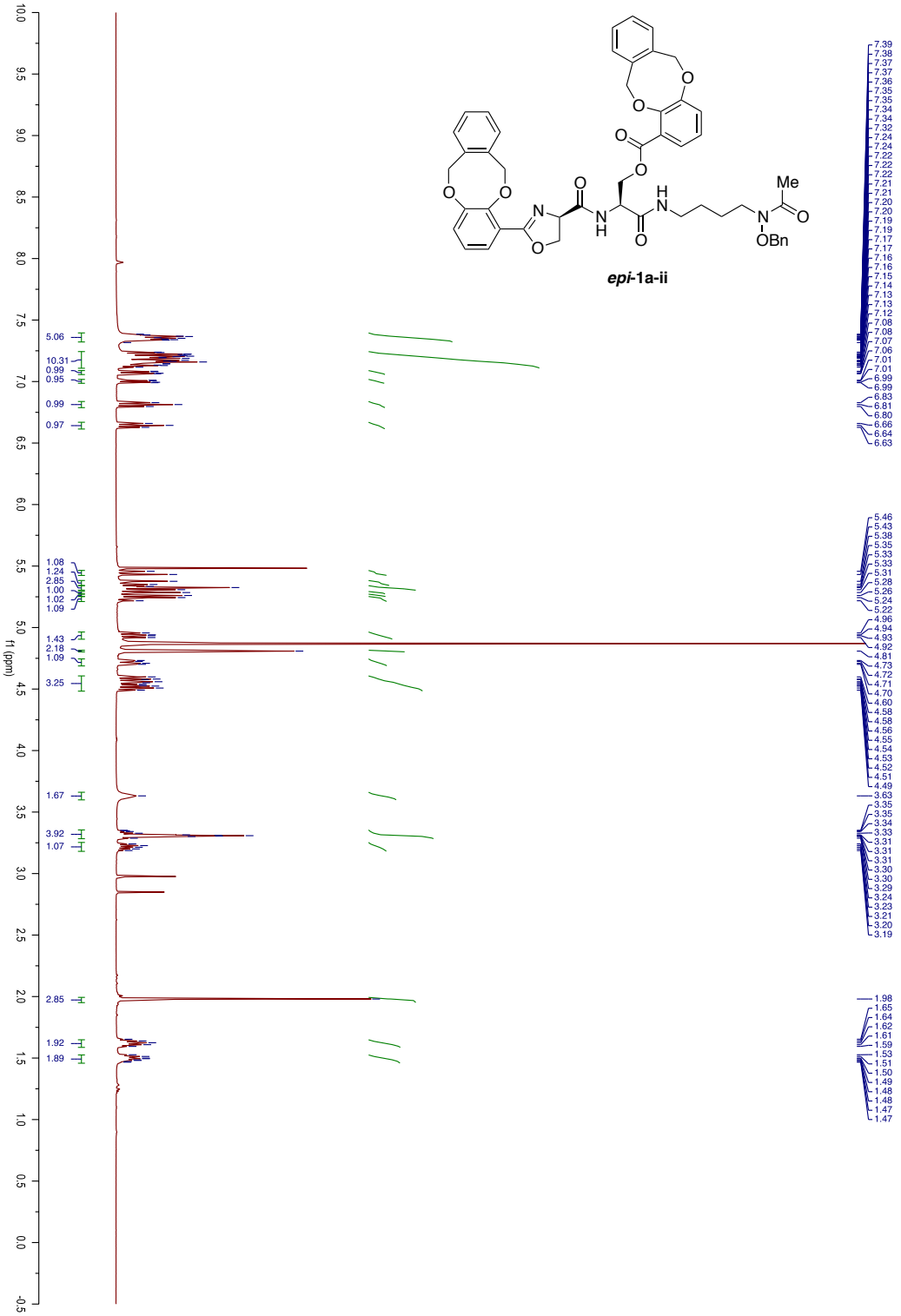
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.5	n.a.	Average spectrum	n.a.	n.a.	n.a.	597.1807	n.a.

+MS, 0.3-0.7min #16-42

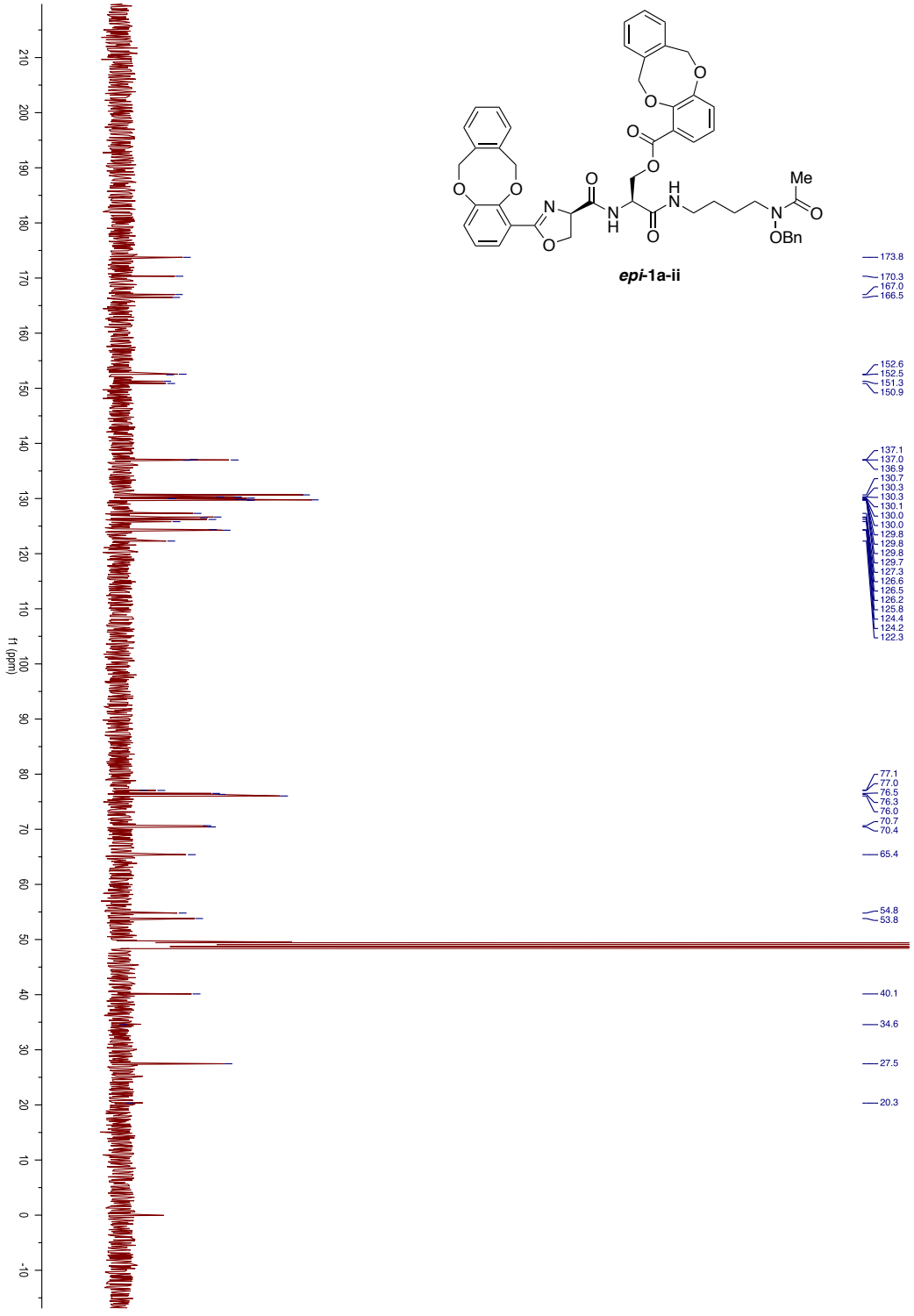


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
597.1807	1	C24H25N10O9	597.1800	1.0	12.8	1	100.00	17.5	even	ok
	2	C23H29N6O13	597.1787	-3.3	15.5	2	41.21	12.5	even	ok
	3	C28H29N4O11	597.1827	3.5	16.4	3	36.52	16.5	even	ok
	4	C21H17N20O3	597.1787	3.3	17.8	4	39.01	23.5	even	ok
	5	C25H21N14O5	597.1814	1.2	19.0	5	82.69	22.5	even	ok
	6	C20H21N16O7	597.1774	5.5	19.2	6	11.51	18.5	even	ok
	7	C22H33N2O17	597.1774	5.5	24.3	7	10.39	7.5	even	ok
	8	C29H25N8O7	597.1841	5.7	26.9	8	8.51	21.5	even	ok
	9	C26H17N18O	597.1827	3.5	28.9	9	27.88	27.5	even	ok
	10	C35H25N4O6	597.1769	6.4	51.1	10	2.92	25.5	even	ok
	11	C36H21N8O2	597.1782	4.1	62.7	11	7.56	30.5	even	ok
	12	C40H25N2O4	597.1809	-0.4	74.7	12	20.23	29.5	even	ok
	1	C26H30N4NaO11	597.1803	-0.5	11.4	1	100.00	13.5	even	ok
	2	C23H22N14NaO5	597.1790	-2.8	16.0	2	42.29	19.5	even	ok
	3	C22H26N10NaO9	597.1776	-5.0	17.3	3	13.50	14.5	even	ok
	4	C27H26N8NaO7	597.1817	1.7	18.4	4	61.35	18.5	even	ok
	5	C24H18N18NaO	597.1803	0.6	22.0	5	80.16	24.5	even	ok
	6	C31H30N2NaO9	597.1844	6.2	27.1	6	5.32	17.5	even	ok
	7	C28H22N12NaO3	597.1830	-3.9	28.7	7	19.10	23.5	even	ok

^{1}H-NMR of Compound *epi*-1a-ii (500 MHz, CD_3OD)



^{13}C-NMR of Compound *epi*-1a-ii



***epi*-1a-ii**

HR-MS of Compound *epi*-1a-ii

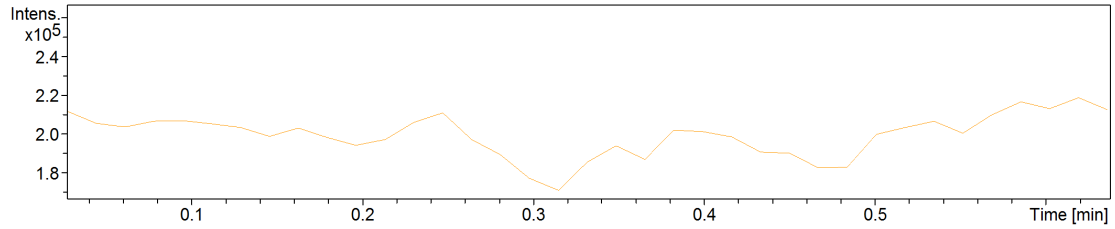
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ010.d	Acquisition Date	7/10/2019 5:24:28 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ10_8b-1	Instrument	compact 8255754.10024
Comment			

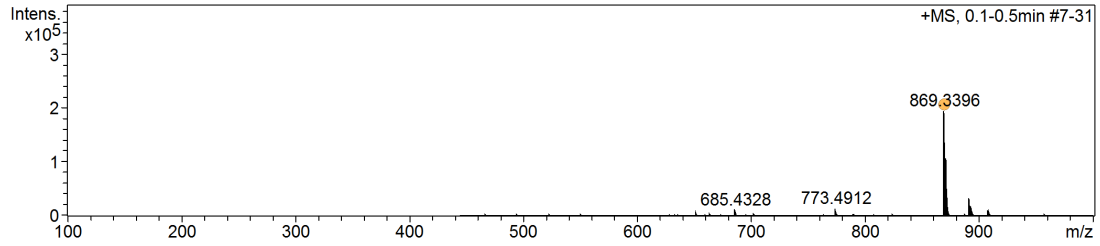
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	450 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



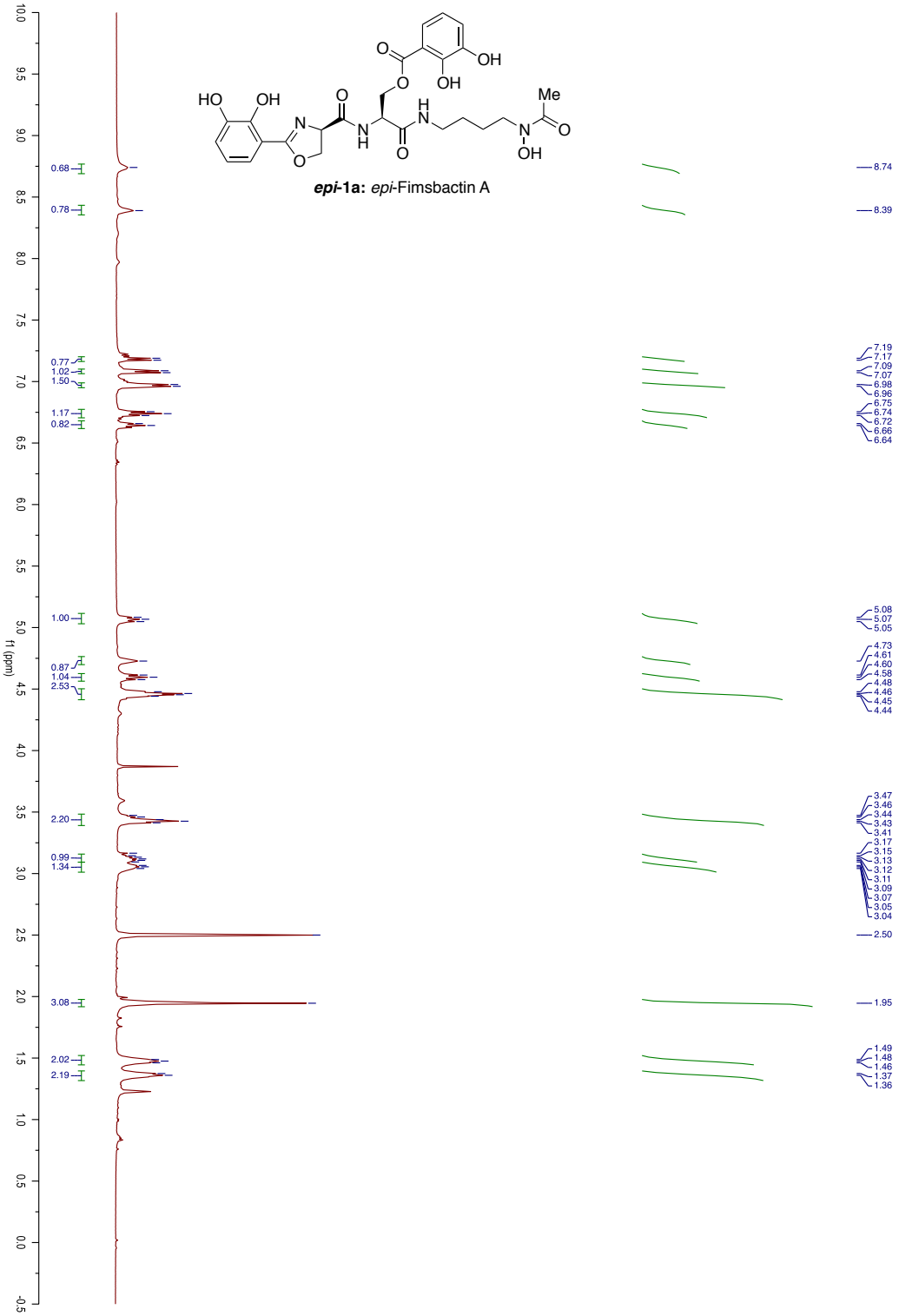
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	869.3396	n.a.

+MS, 0.1-0.5min #7-31

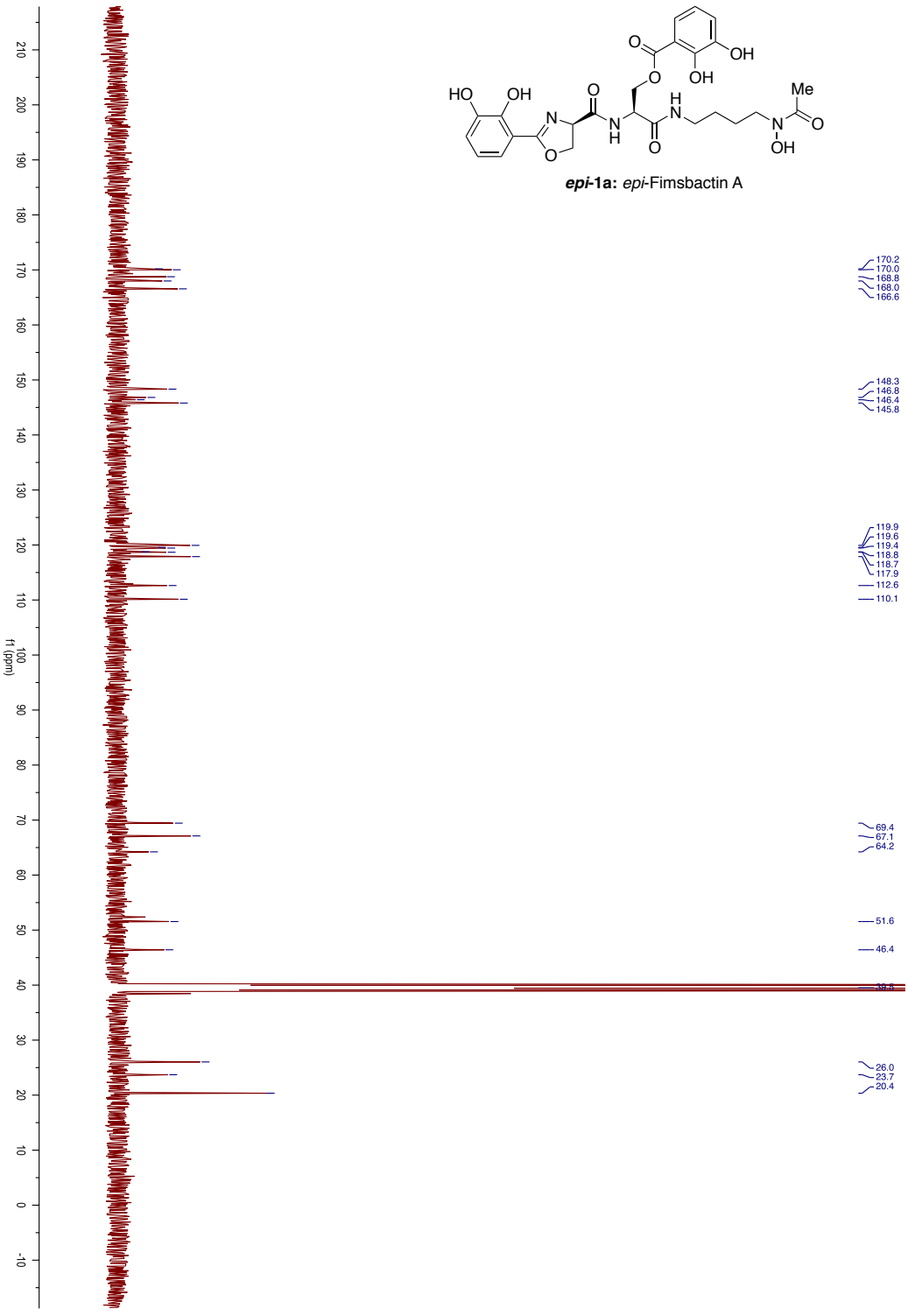


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
869.3396	1	C49H49N4O11	869.3392	-0.4	4.6	1	100.00	27.5	even	ok
	2	C46H41N14O5	869.3379	1.9	9.7	2	42.38	33.5	even	ok
	3	C45H45N10O9	869.3365	-3.5	12.3	3	13.25	28.5	even	ok
	4	C50H45N8O7	869.3406	1.2	14.2	4	58.64	32.5	even	ok
	5	C47H37N18O	869.3392	-0.4	16.1	5	80.30	38.5	even	ok
	6	C51H41N12O3	869.3419	-2.7	24.7	6	18.33	37.5	even	ok
	7	C54H49N2O9	869.3433	4.3	25.4	7	4.84	31.5	even	ok
	1	C48H46N8NaO7	869.3382	1.6	7.9	1	57.81	29.5	even	ok
	2	C47H50N4NaO11	869.3368	3.1	10.2	2	19.66	24.5	even	ok
	3	C45H38N18NaO	869.3368	3.1	13.4	3	18.31	35.5	even	ok
	4	C52H50N2NaO9	869.3409	-1.5	14.7	4	53.72	28.5	even	ok
	5	C49H42N12NaO3	869.3395	0.1	15.7	5	100.00	34.5	even	ok
	6	C53H46N6NaO5	869.3422	-3.0	25.4	6	15.52	33.5	even	ok
	7	C54H42N10NaO	869.3435	-4.6	36.2	7	2.98	38.5	even	ok

^{1}H-NMR of Compound *epi*-1a (*epi*-Fimsbactin A, 500 MHz, DMSO-d^{6})



^{13}C-NMR of Compound *epi*-1a (*epi*-Fimsbactin A, 125 MHz, DMSO-d^{6})



***epi*-1a:** *epi*-Fimsbactin A

HR-MS of Compound *epi*-1a (*epi*-Fimsbactin A)

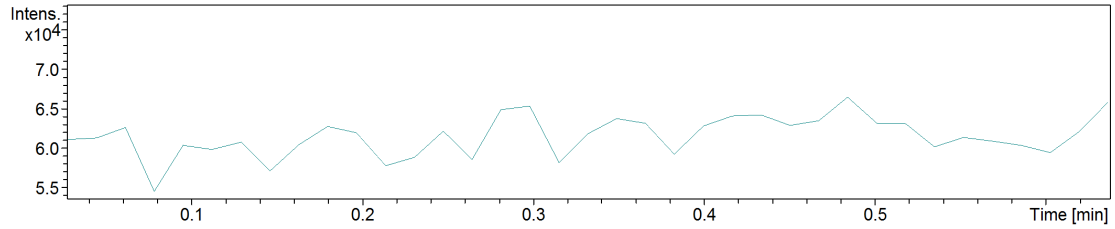
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ011.d	Acquisition Date	7/10/2019 5:30:11 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ11_epi-1a	Instrument	compact 8255754.10024
Comment			

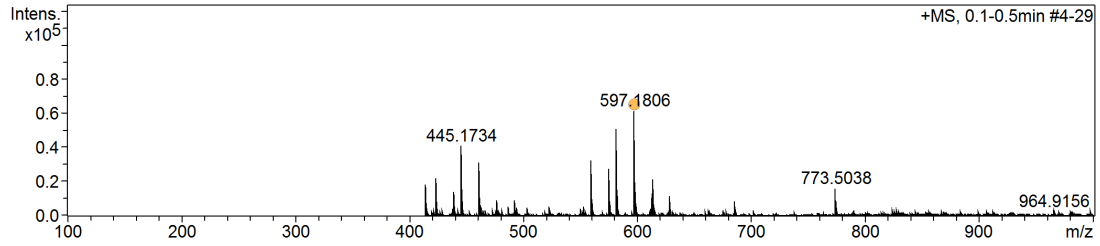
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	420 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



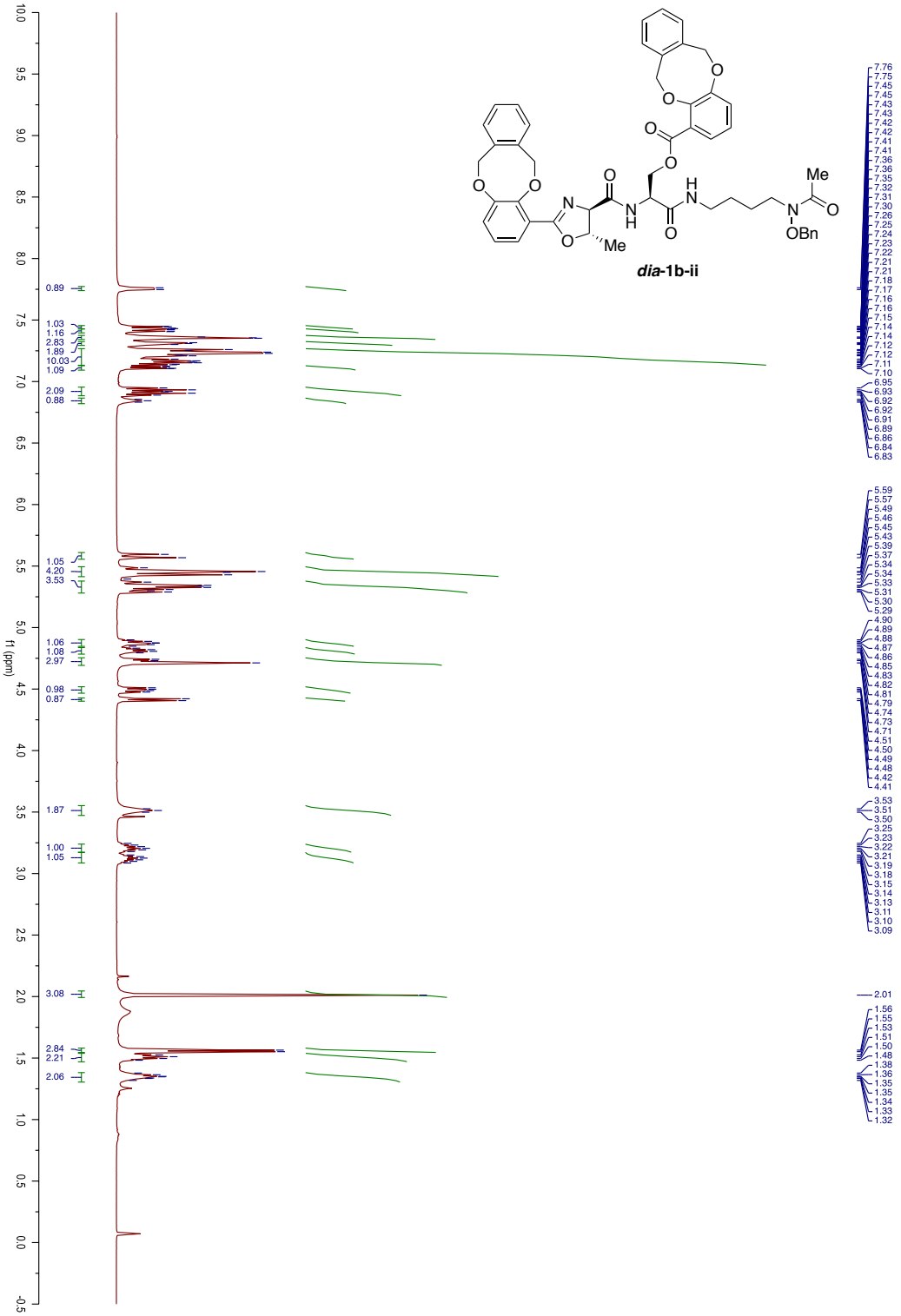
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	597.1806	n.a.

+MS, 0.1-0.5min #4-29

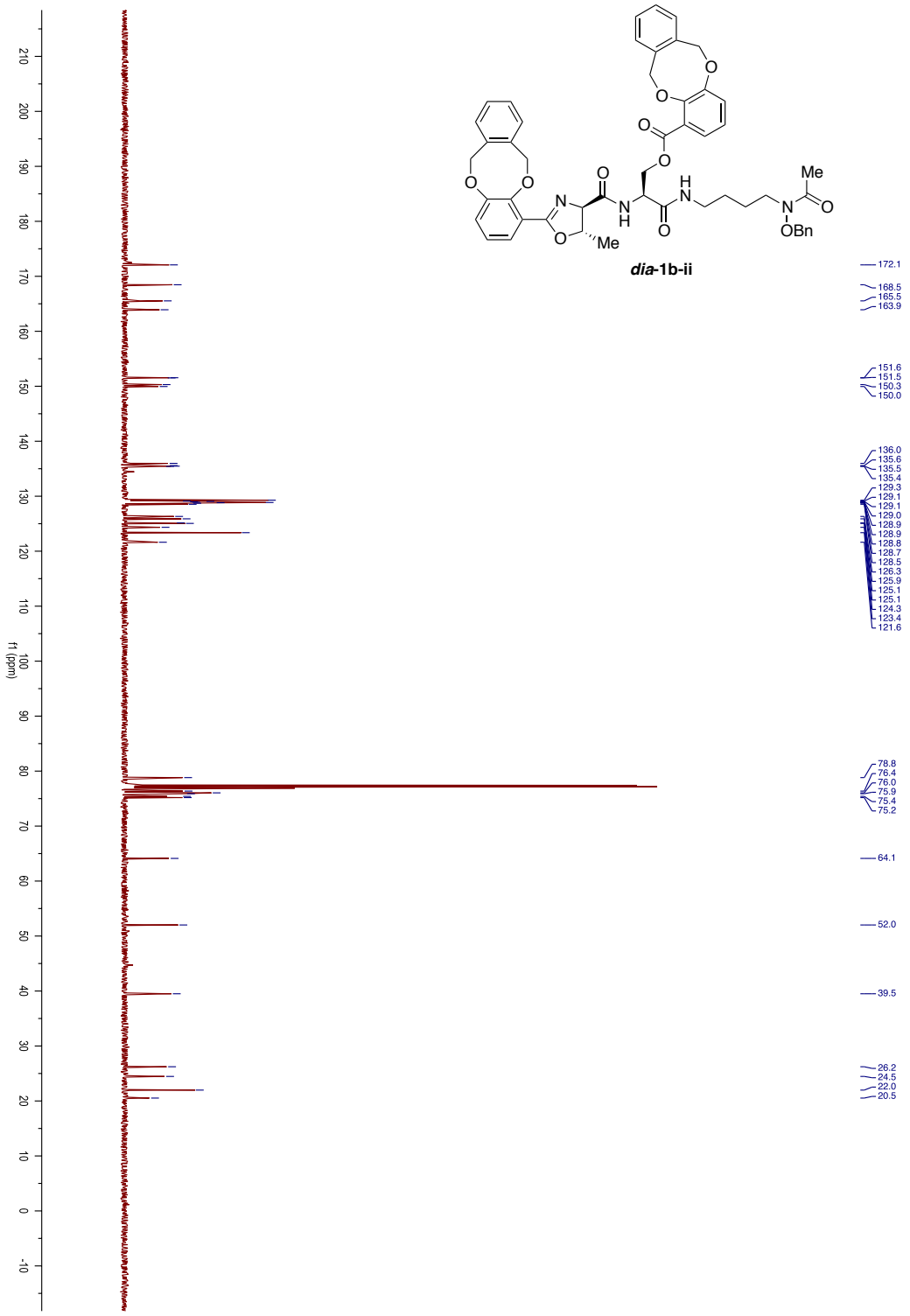


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
597.1806	1	C28H29N4O11	597.1827	-3.6	22.9	1	41.36	16.5	even	ok
	2	C29H25N8O7	597.1841	5.9	26.9	2	10.82	21.5	even	ok
	3	C25H21N14O5	597.1814	1.4	29.2	3	87.55	22.5	even	ok
	4	C24H25N10O9	597.1800	0.9	30.0	4	100.00	17.5	even	ok
	5	C26H17N18O	597.1827	-3.6	32.7	5	33.11	27.5	even	ok
	6	C23H29N6O13	597.1787	3.1	34.8	6	39.38	12.5	even	ok
	7	C35H25N4O6	597.1769	-6.2	41.4	7	5.96	25.5	even	ok
	8	C22H33N2O17	597.1774	-5.3	42.3	8	10.05	7.5	even	ok
	9	C36H21N8O2	597.1782	4.0	52.4	9	15.94	30.5	even	ok
	10	C40H25N2O4	597.1809	-0.5	62.1	10	43.00	29.5	even	ok
	1	C31H30N2NaO9	597.1844	-6.3	25.2	1	6.86	17.5	even	ok
	2	C27H26N8NaO7	597.1817	-1.8	26.9	2	65.59	18.5	even	ok
	3	C26H30N4NaO11	597.1803	-0.4	27.7	3	100.00	13.5	even	ok
	4	C28H22N12NaO3	597.1830	-4.1	30.8	4	22.90	23.5	even	ok
	5	C24H18N18NaO	597.1803	0.4	33.2	5	86.91	24.5	even	ok
	6	C23H22N14NaO5	597.1790	2.7	33.5	6	40.94	19.5	even	ok
	7	C22H26N10NaO9	597.1776	4.9	37.5	7	12.41	14.5	even	ok
	8	C38H26N2NaO4	597.1785	-3.5	52.3	8	16.68	26.5	even	ok

^{1}H-NMR of Compound *dia*-1b-ii (500 MHz, $CDCl_3$)



^{13}C-NMR of Compound *dia*-1b-ii (125 MHz, $CDCl_3$)



HR-MS of Compound *dia*-1b-ii

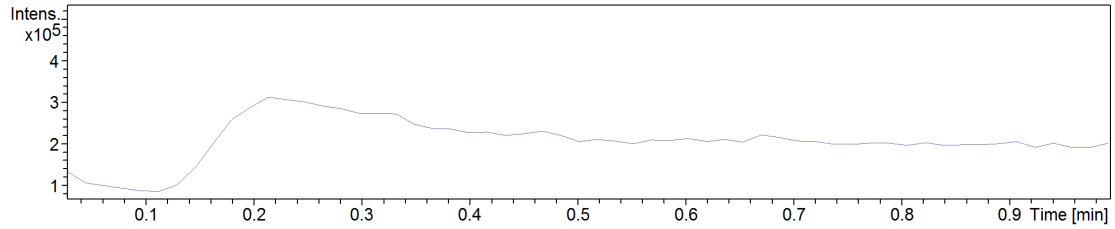
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ014.d	Acquisition Date	7/10/2019 5:47:27 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ14_10b-1	Instrument	compact 8255754.10024
Comment			

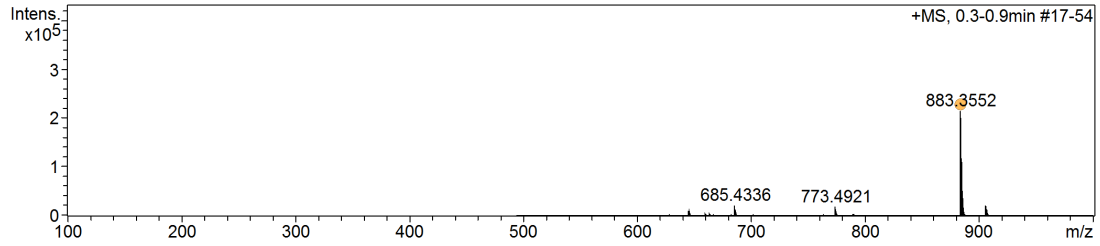
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



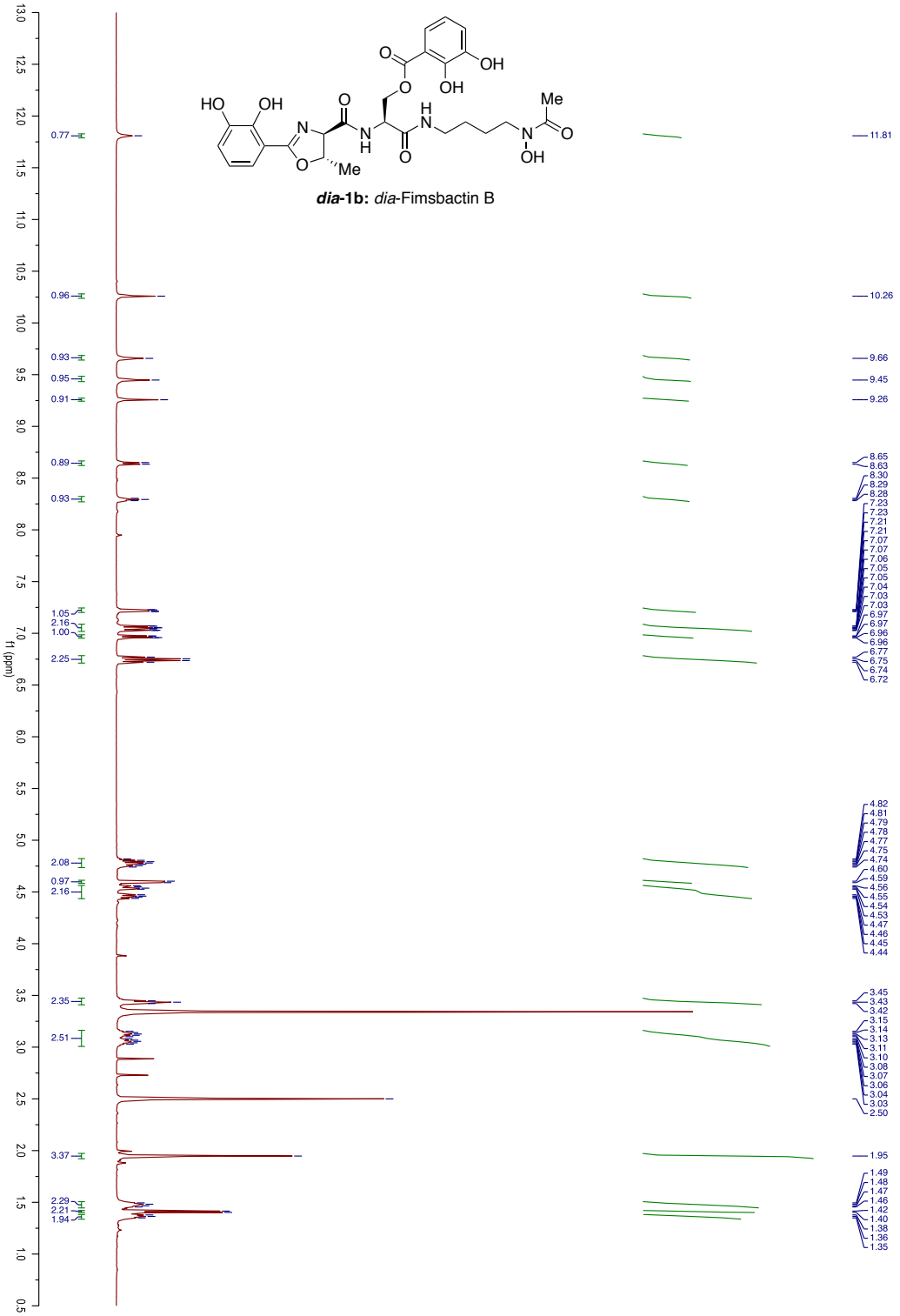
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.6	n.a.	Average spectrum	n.a.	n.a.	n.a.	883.3552	n.a.

+MS, 0.3-0.9min #17-54

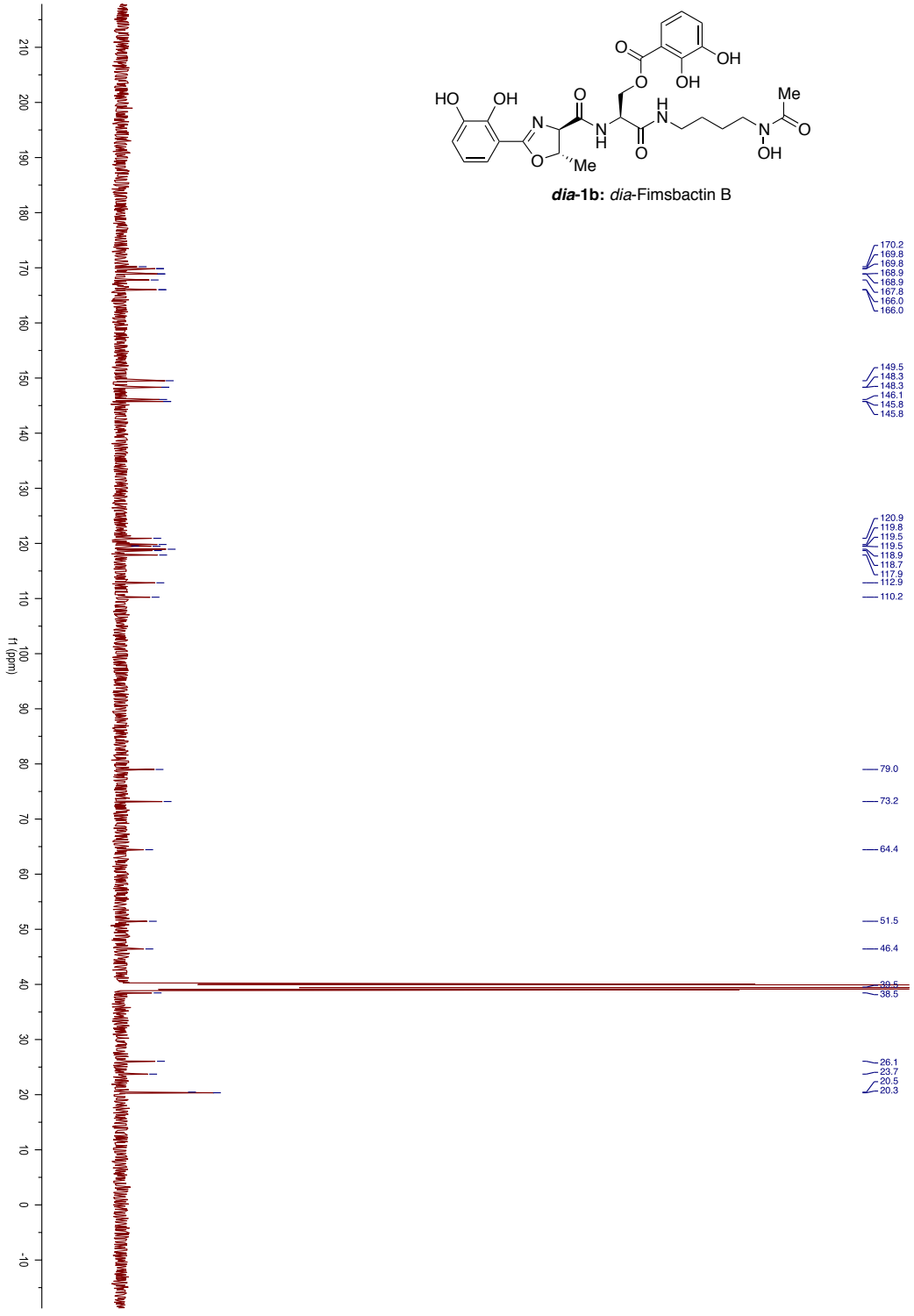


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
883.3552	1	C50H51N4O11	883.3549	-0.4	7.4	1	100.00	27.5	even	ok
	2	C46H47N10O9	883.3522	3.4	11.0	2	14.10	28.5	even	ok
	3	C47H43N14O5	883.3535	1.9	11.4	3	42.84	33.5	even	ok
	4	C51H47N8O7	883.3562	1.1	17.3	4	58.83	32.5	even	ok
	5	C55H51N2O9	883.3589	-4.2	28.5	5	4.87	31.5	even	ok
	1	C48H52N4NaO11	883.3525	-3.1	8.7	1	36.14	24.5	even	ok
	2	C49H48N8NaO7	883.3538	1.6	10.0	2	100.00	29.5	even	ok
	3	C53H52N2NaO9	883.3565	-1.4	17.9	3	92.86	28.5	even	ok
	4	C54H48N6NaO5	883.3578	3.0	28.6	4	26.69	33.5	even	ok
	5	C41H56N4NaO16	883.3584	3.5	41.0	5	11.95	15.5	even	ok

^{1}H-NMR of Compound *dia*-1b (*dia*-Fimsbactin B, 500 MHz, DMSO-d^{6})



^{13}C-NMR of Compound *dia*-1b (*dia*-Fimsbactin B, 125 MHz, DMSO-d^{6})



***dia*-1b:** *dia*-Fimsbactin B

HR-MS of Compound *dia*-1b (*dia*-Fimsbactin B)

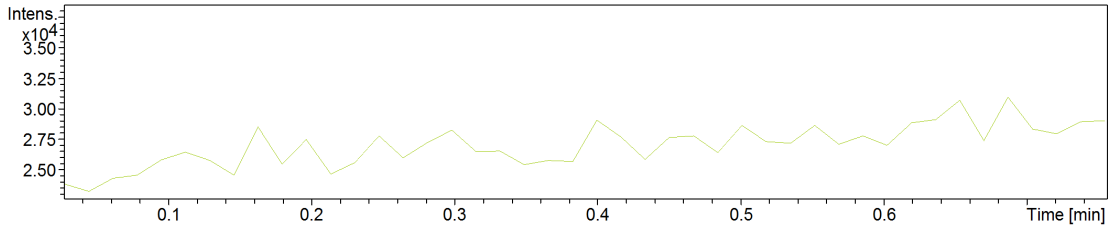
Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Data\2019\KU\KHJ\KSJ\KSJ015.d	Acquisition Date	7/10/2019 5:52:49 PM
Method	Tune_pos_Standard_100_1000_190102.d.m	Operator	lee
Sample Name	KSJ15_epi-1b	Instrument	compact 8255754.10024
Comment			

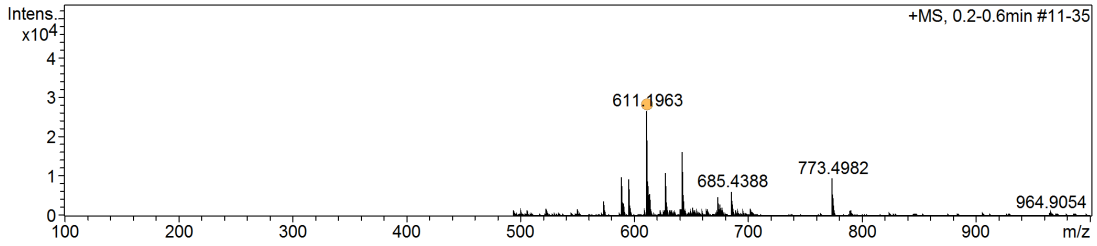
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	611.1963	n.a.

+MS, 0.2-0.6min #11-35



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
611.1963	1	C29H31N4O11	611.1984	-3.5	73.4	1	48.12	16.5	even	ok
	2	C30H27N8O7	611.1997	-5.7	74.7	2	13.29	21.5	even	ok
	3	C36H27N4O6	611.1925	-6.1	75.1	3	9.40	25.5	even	ok
	4	C26H23N14O5	611.1970	-1.3	79.7	4	90.84	22.5	even	ok
	5	C25H27N10O9	611.1957	0.9	79.9	5	100.00	17.5	even	ok
	6	C24H31N6O13	611.1944	-3.1	81.6	6	40.99	12.5	even	ok
	7	C41H27N2O4	611.1965	0.4	83.3	7	99.92	29.5	even	ok
	8	C23H35N2O17	611.1930	-5.3	84.7	8	11.11	7.5	even	ok
	1	C32H32N2NaO9	611.2000	-6.1	72.5	1	8.50	17.5	even	ok
	2	C28H28N8NaO7	611.1973	1.7	77.4	2	68.13	18.5	even	ok
	3	C27H32N4NaO11	611.1960	0.5	77.6	3	100.00	13.5	even	ok
	4	C39H28N2NaO4	611.1941	-3.5	79.6	4	29.68	26.5	even	ok
	5	C24H24N14NaO5	611.1946	2.7	83.7	5	36.33	19.5	even	ok
	6	C23H28N10NaO9	611.1933	4.9	85.2	6	11.35	14.5	even	ok