

**Supporting Information:** *Thalassosamide, a Siderophore Discovered from the Marine-Derived Bacterium *Thalassospira profundimaris**

**Thalassosamide, a Siderophore Discovered from the Marine-Derived Bacterium *Thalassospira profundimaris***

Fan Zhang,<sup>†</sup> Kenneth Barns,<sup>‡</sup> F. Michael Hoffmann,<sup>‡</sup> Doug R. Braun,<sup>†</sup> David R. Andes,<sup>§</sup> and Tim S. Bugni<sup>\*,†</sup>

<sup>†</sup>Pharmaceutical Sciences Division, University of Wisconsin–Madison, Madison, Wisconsin 53705, United States

<sup>‡</sup>Small Molecule Screening & Synthesis Facility, UW Carbone Cancer Center, Madison, Wisconsin, United States

<sup>§</sup>Department of Medicine, University of Wisconsin–Madison, Madison, Wisconsin 53705, United States

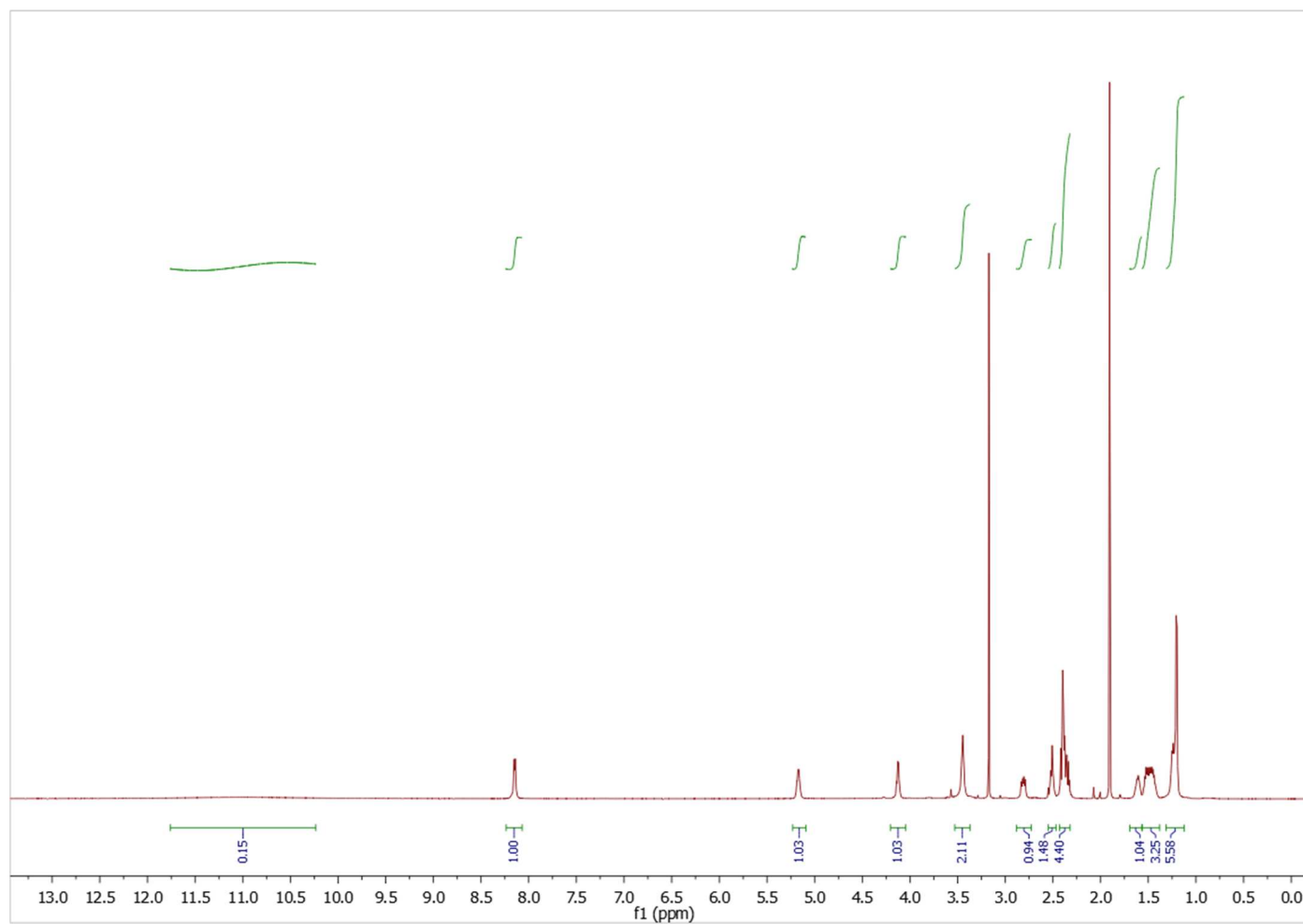
\* To whom correspondence should be addressed. Tel.: 1-608-263-2519. E-mail:

[tim.bugni@wisc.edu](mailto:tim.bugni@wisc.edu).

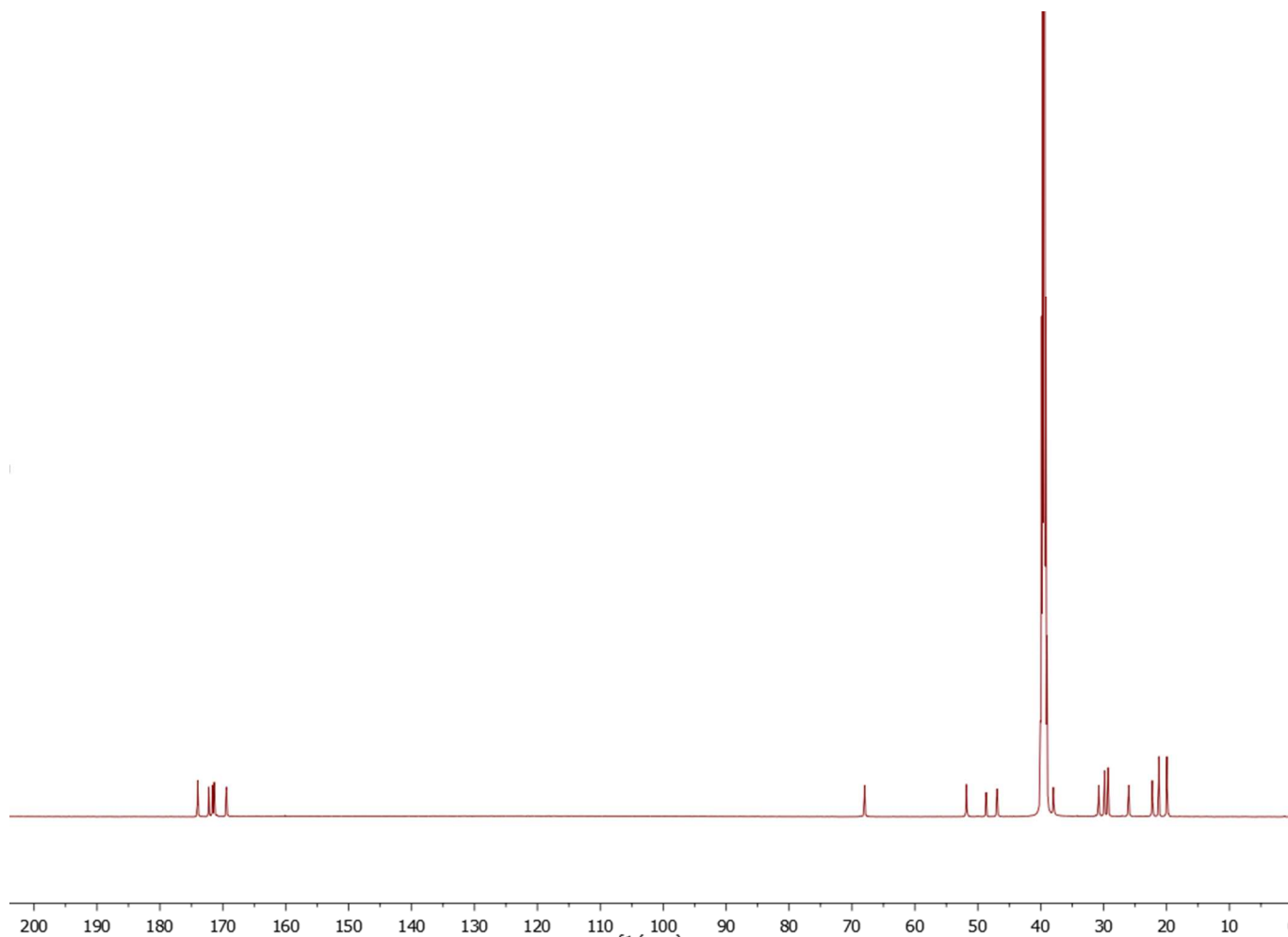
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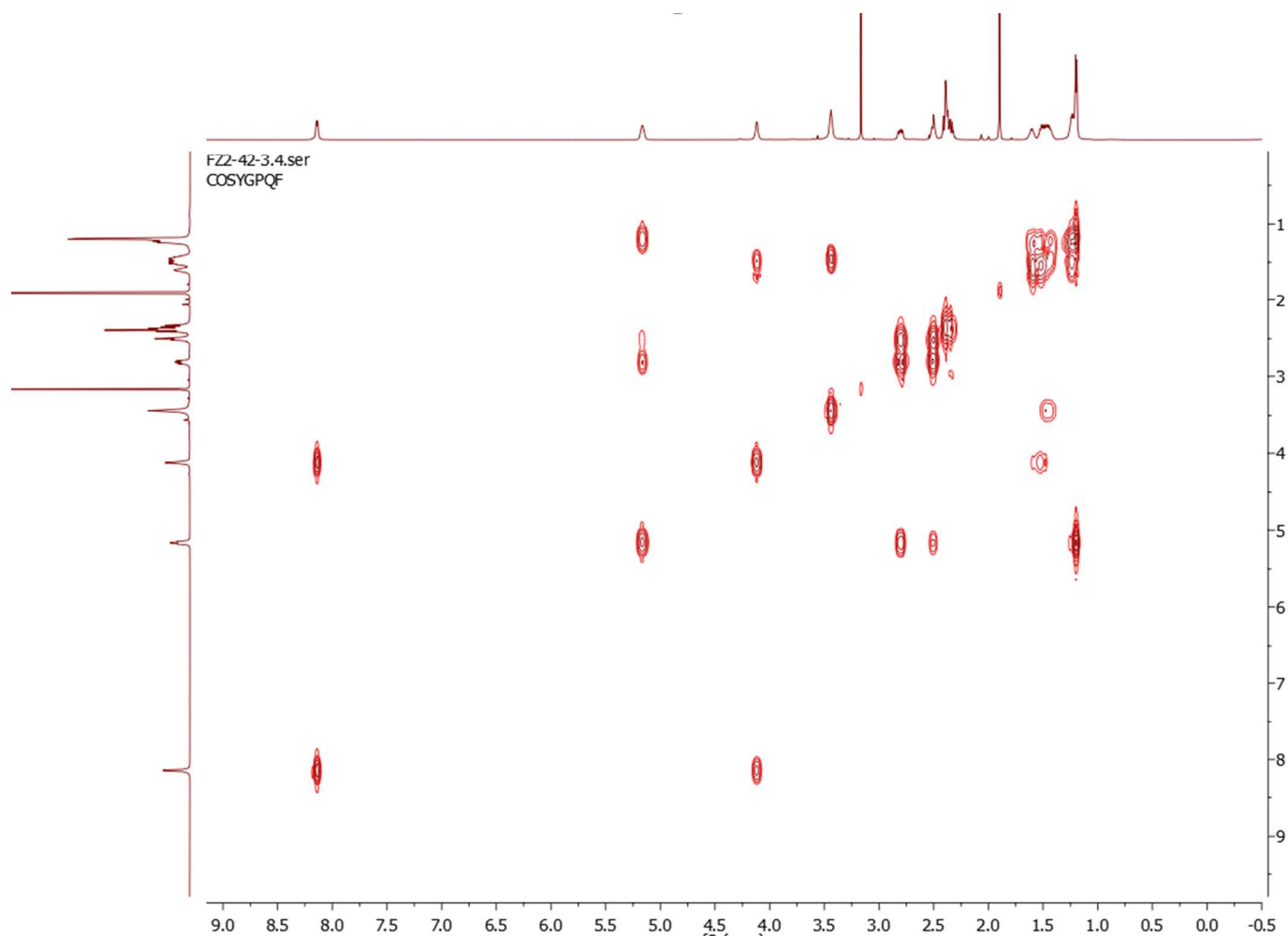
**Figure S1.**  $^1\text{H}$  NMR Spectrum of Thalassosamide (**1**; 600 MHz,  $\text{DMSO-}d_6$ )



**Figure S2.**  $^{13}\text{C}$  NMR Spectrum of Thalassosamide (**1**; 125 MHz,  $\text{DMSO-}d_6$ ).



**Figure S3.** gCOSY Spectrum of Thalassosamide (**1**; 600 MHz, DMSO- $d_6$ ).



**Figure S4.** gHSQC Spectrum of Thalassosamide (**1**; 600 MHz, DMSO- $d_6$ ).

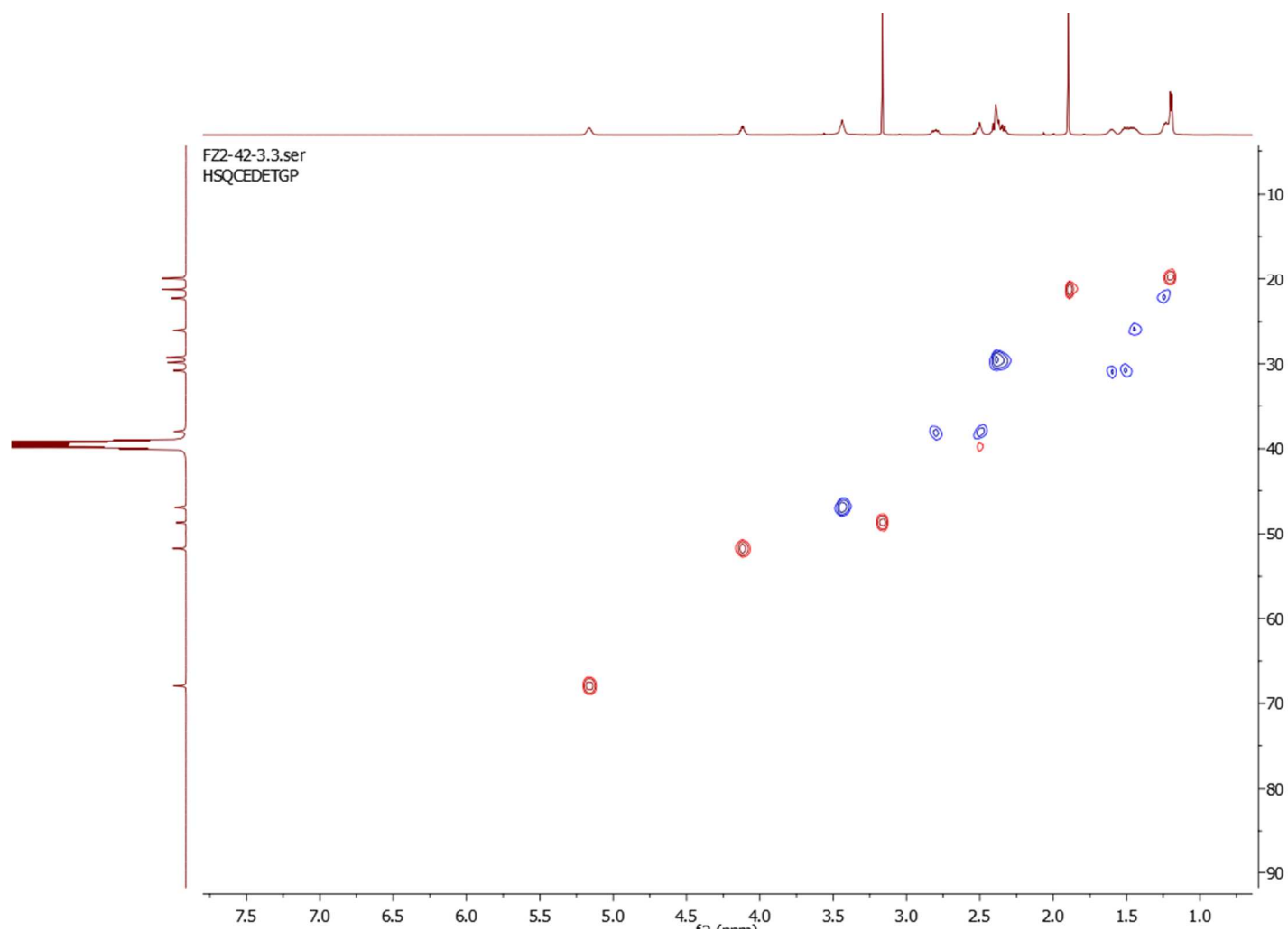


Figure S5. gHMBC Spectrum of Thalassosamide (1; 600 MHz, DMSO- $d_6$ ).

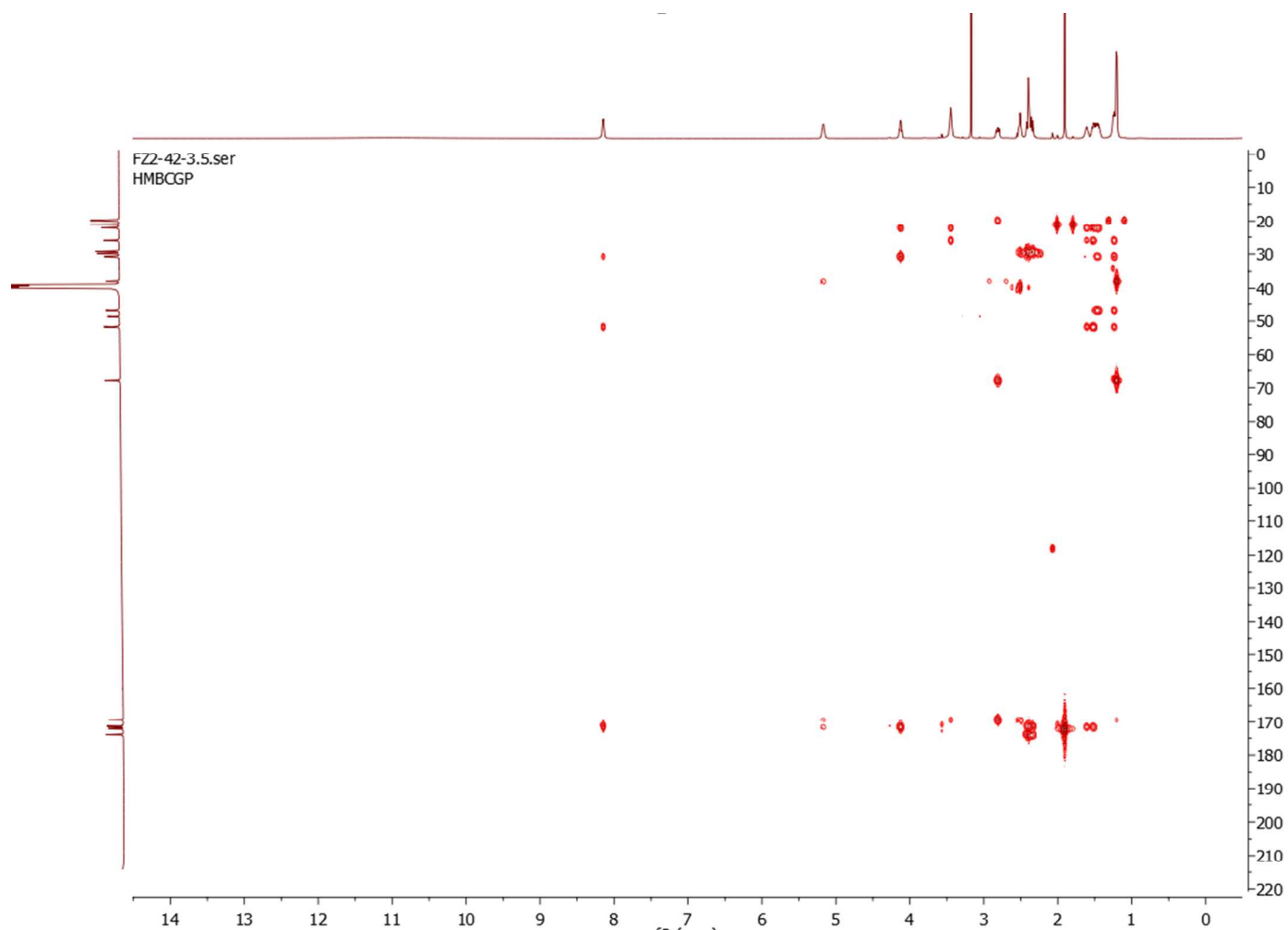
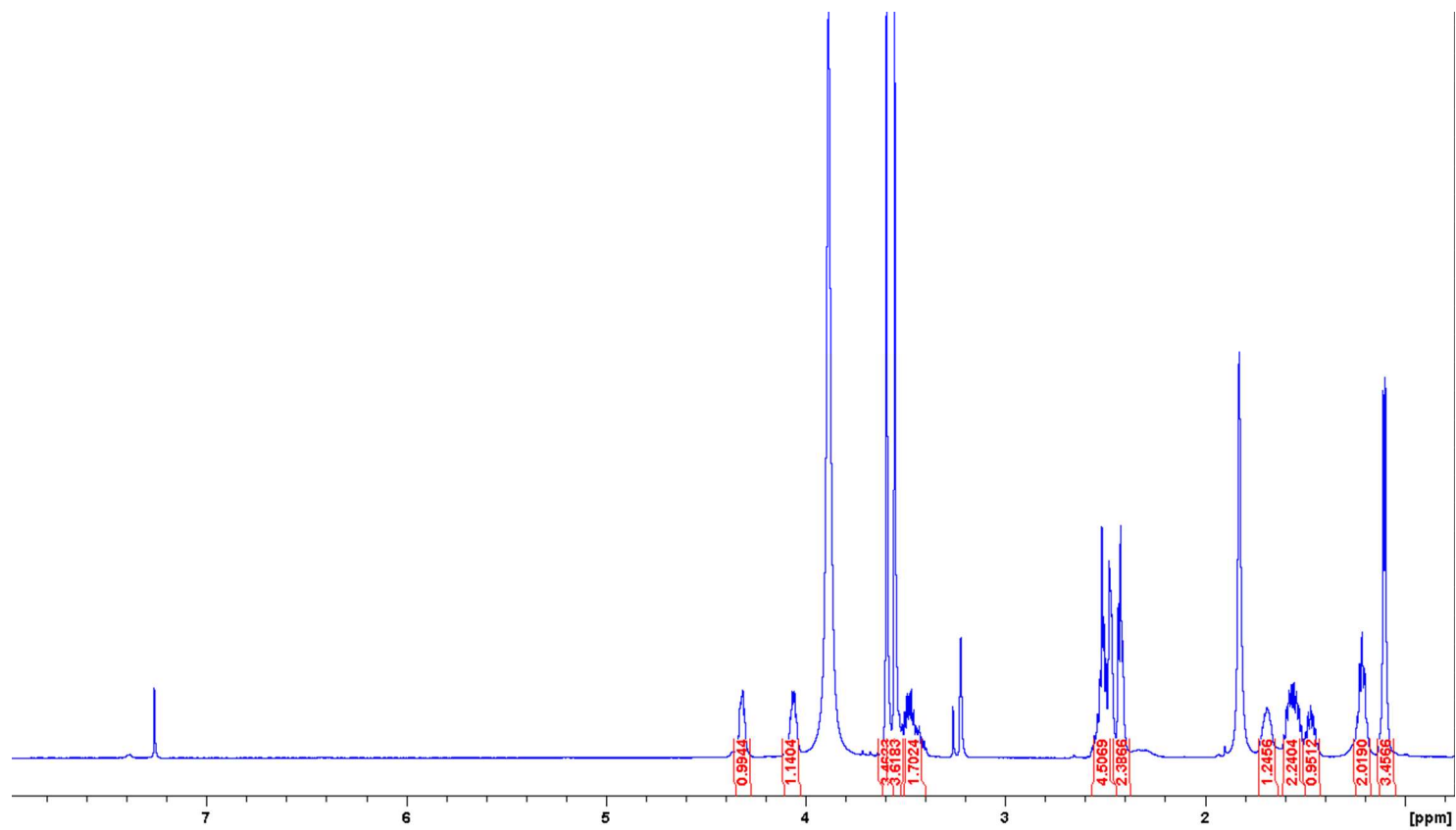
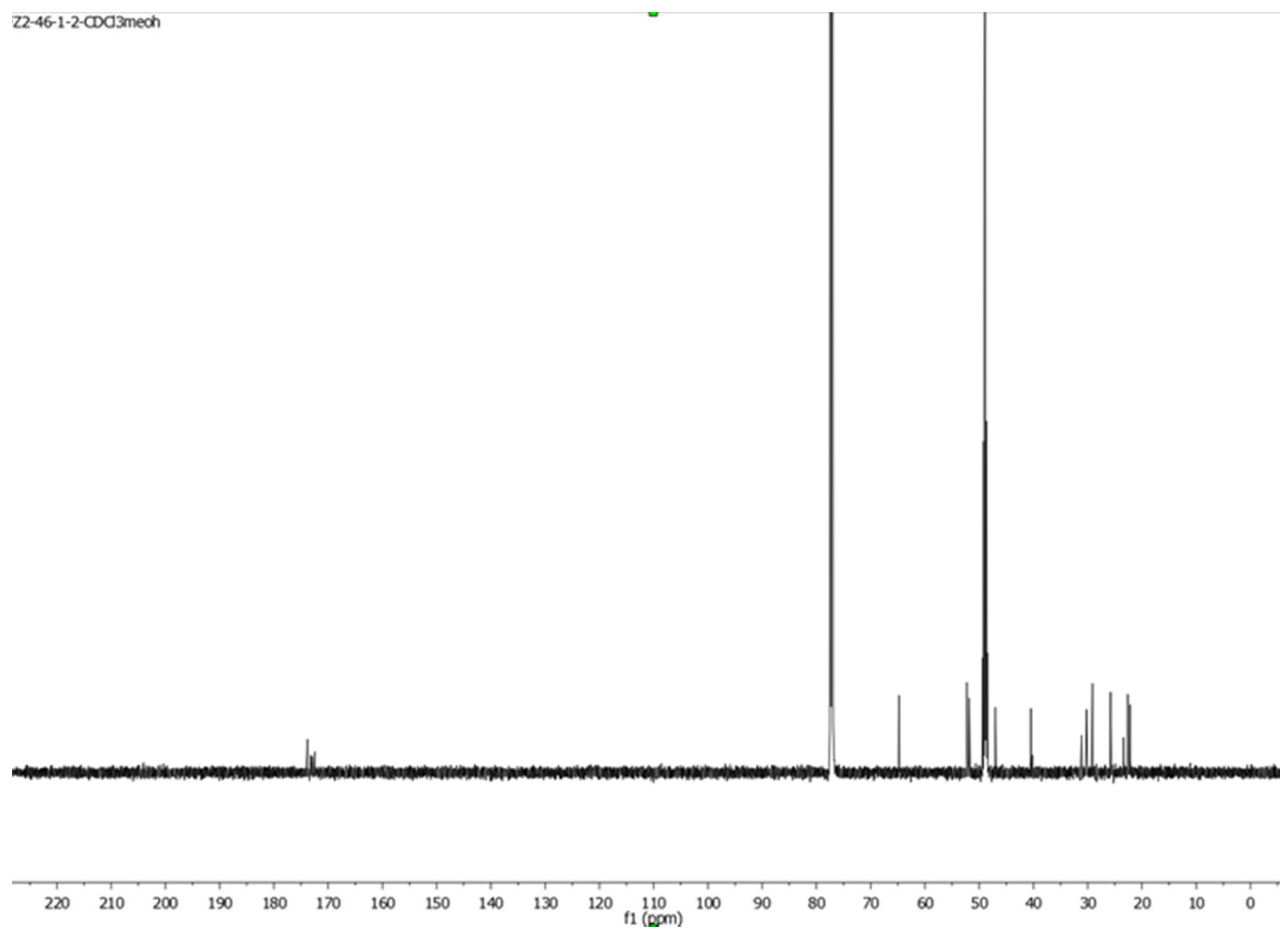


Figure S6.  $^1\text{H}$  NMR Spectrum of Compound **2** (600 MHz,  $\text{CDCl}_3:\text{CD}_3\text{OD}$  4:1)

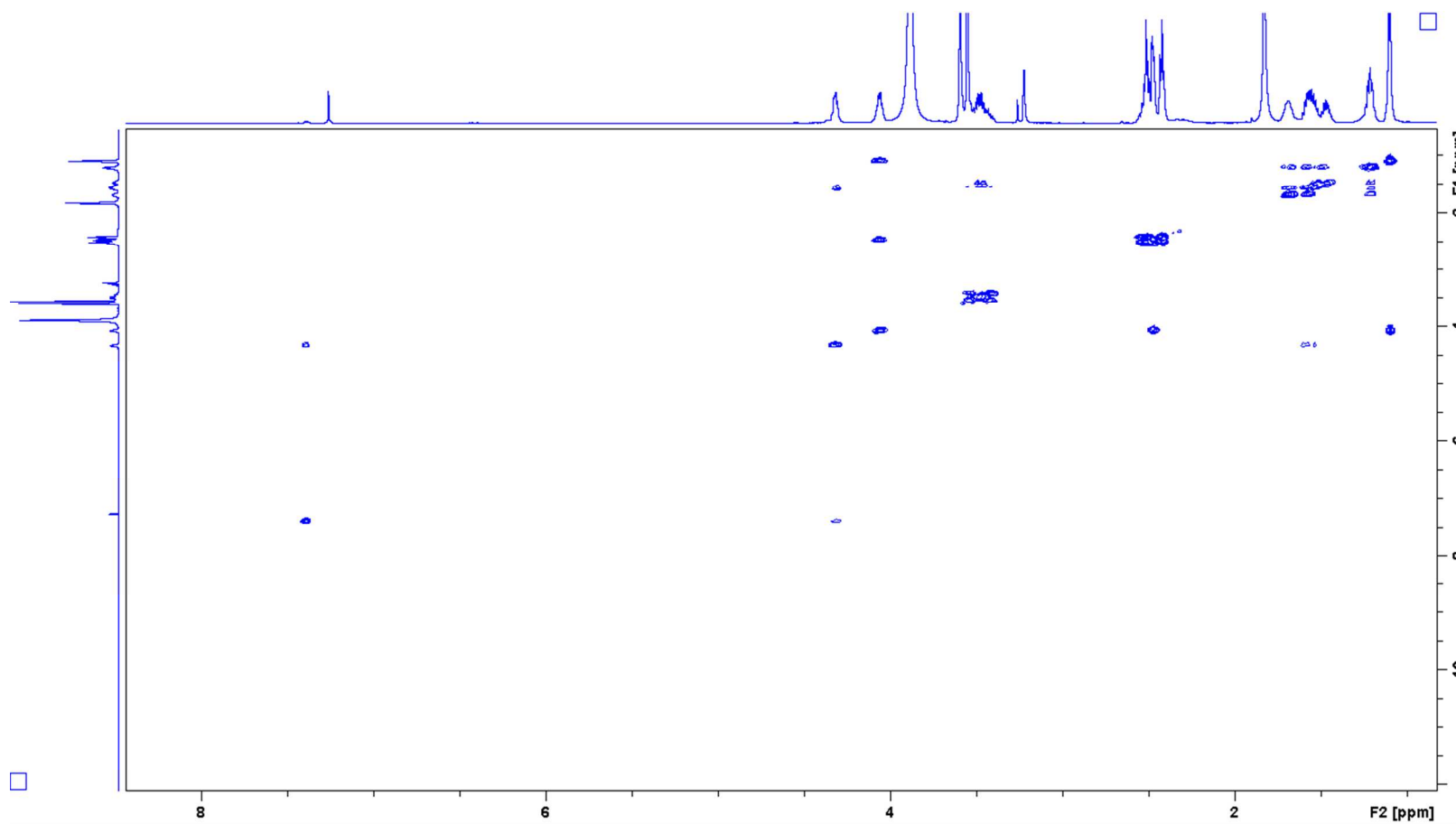




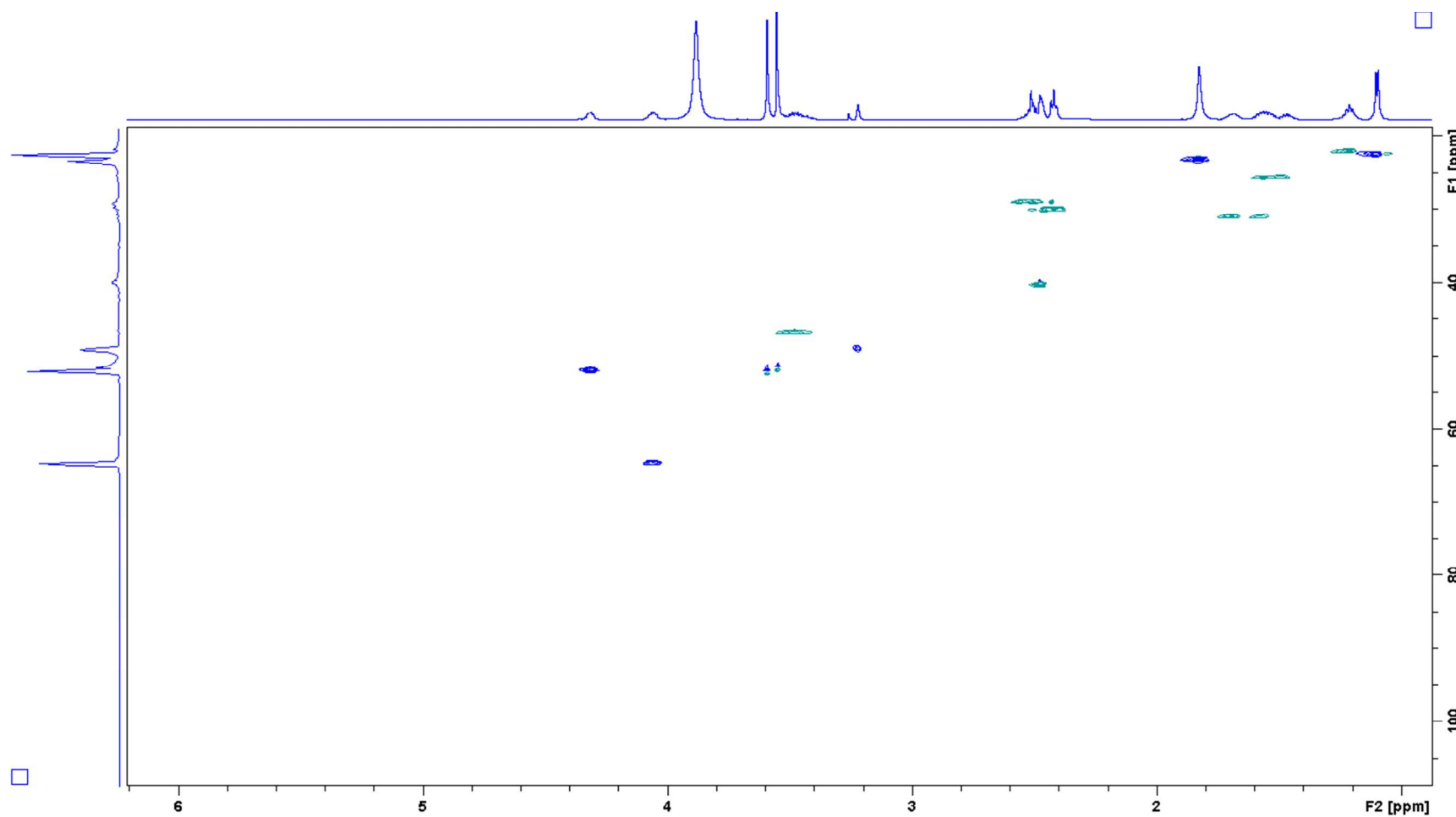
**Figure S7.**  $^{13}\text{C}$  NMR Spectrum of Compound **2** (150 MHz,  $\text{CDCl}_3:\text{CD}_3\text{OD}$  4:1).



**Figure S8.** gCOSY Spectrum of Compound **2** (600 MHz, CDCl<sub>3</sub>:CD<sub>3</sub>OD 4:1).

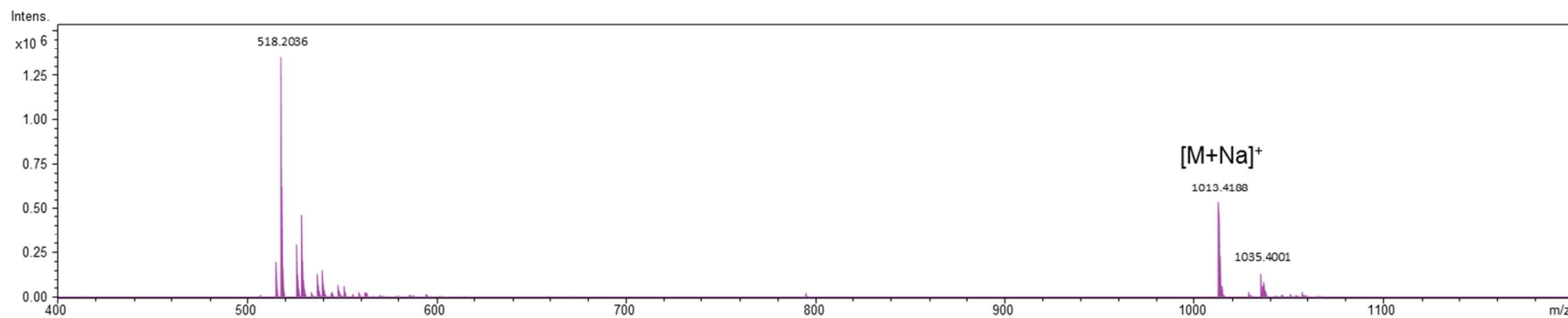


**Figure S9.** gHSQC Spectrum of Compound **2** (600 MHz, CDCl<sub>3</sub>:CD<sub>3</sub>OD 4:1).

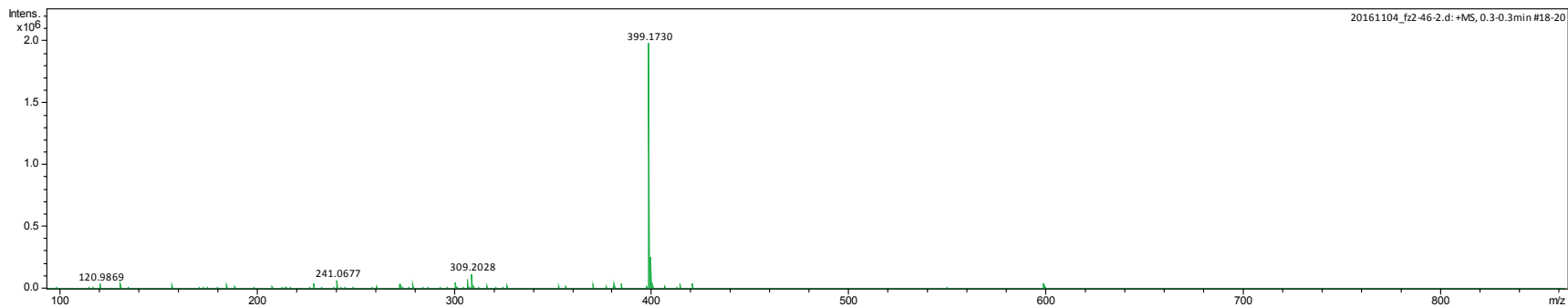




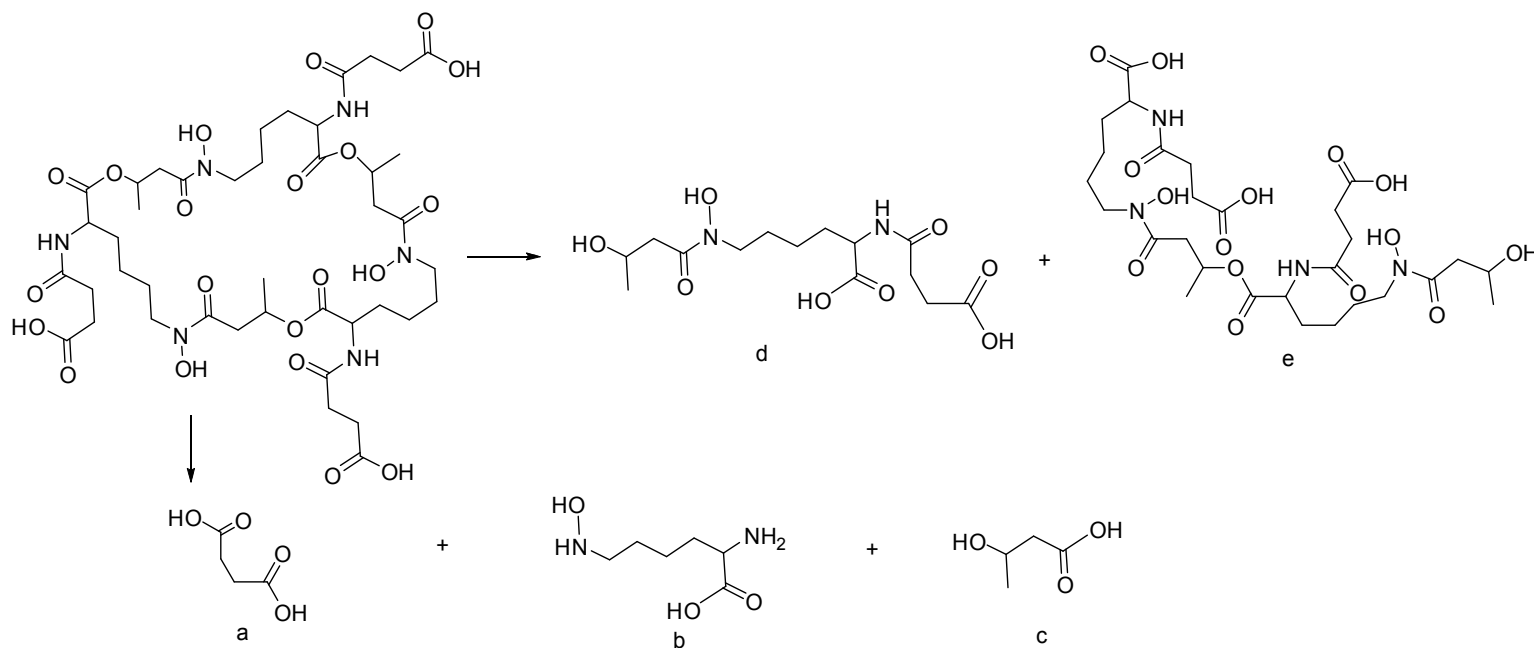
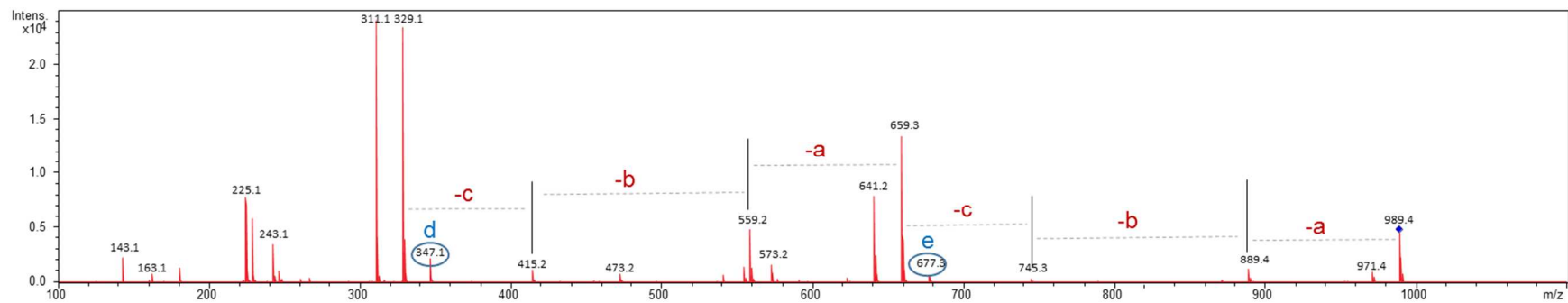
**Figure S11.** Positive Ion HRESIMS of Thalassosamide (1).



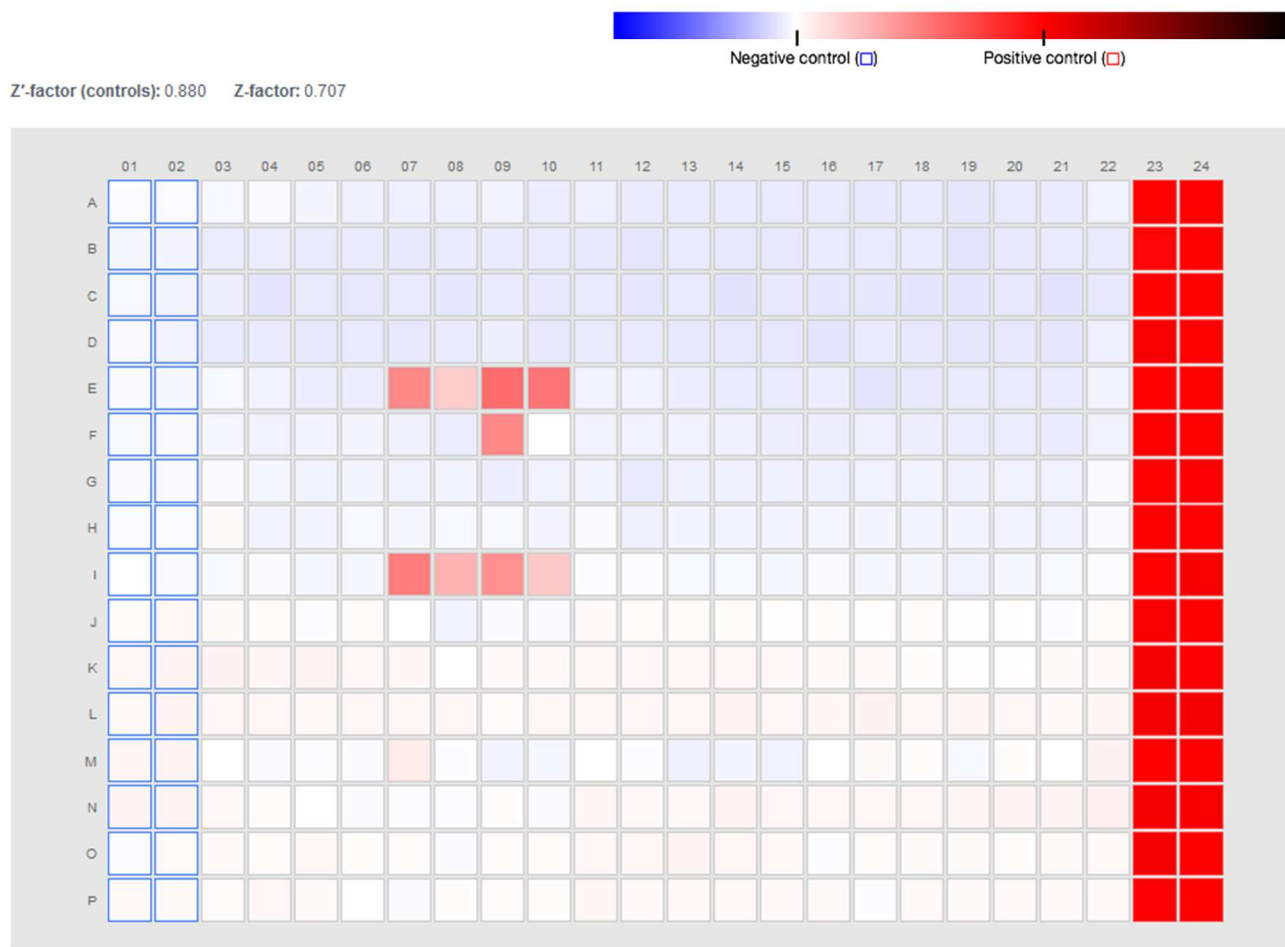
**Figure S12.** Positive Ion HRESIMS of Compound **2**.



**Figure S13.** Negative Ion ESI-MS/MS spectrum of Thalassosamide (1).

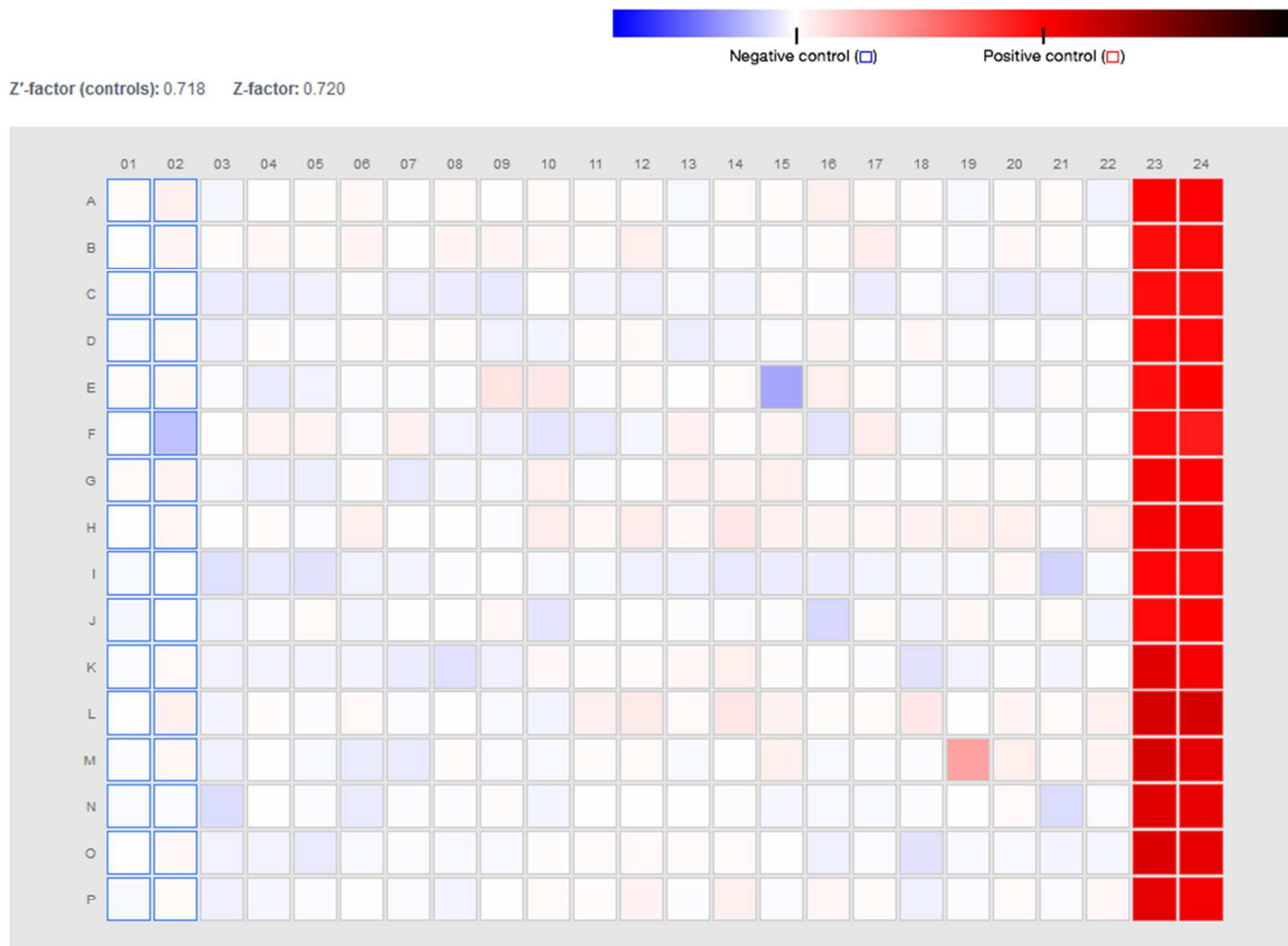


**Figure S14.** A heat map to display high throughput screening results of WMMC 317 against *Pseudomonas auruginosa* (ATCC # 275853).

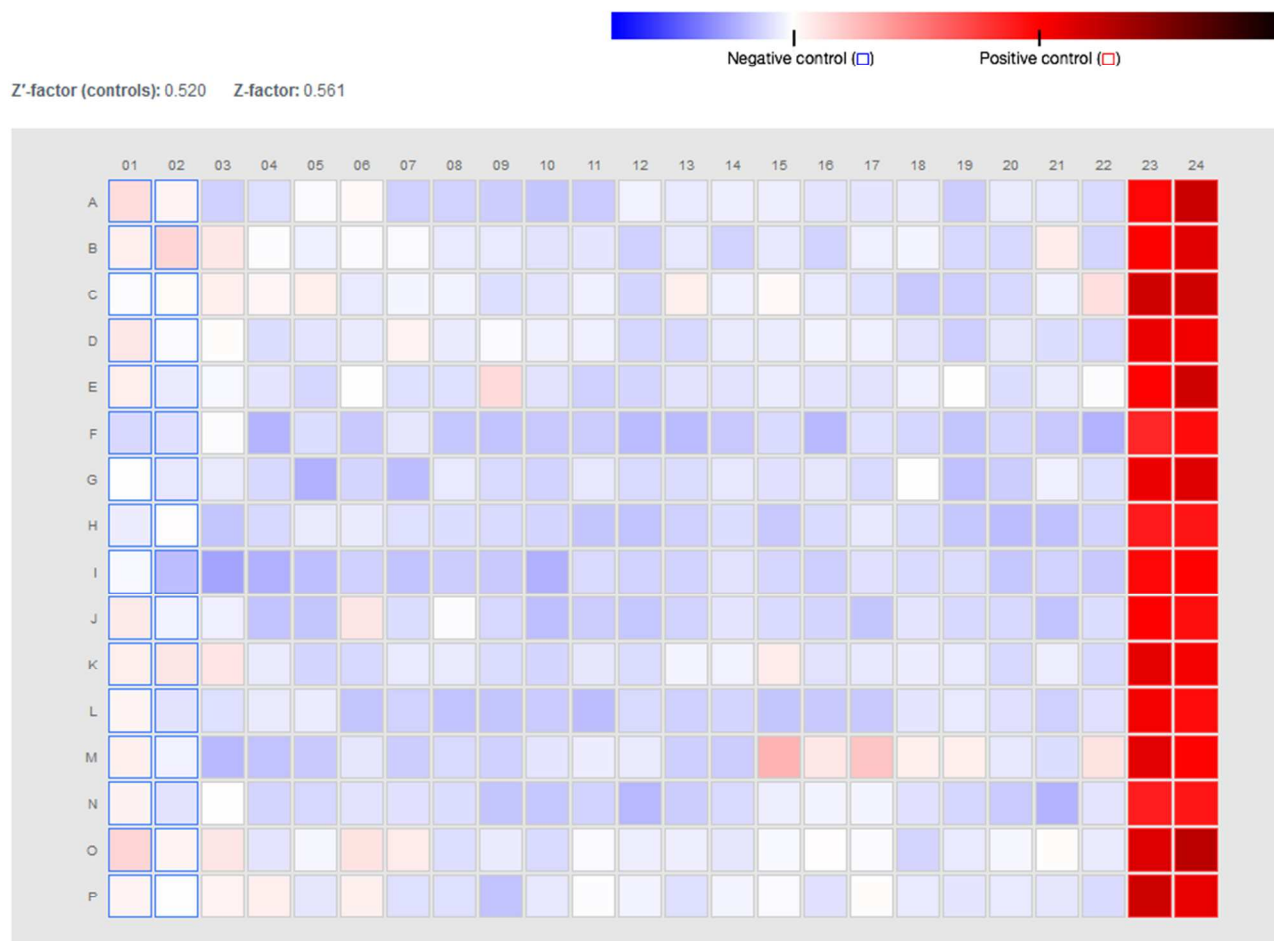




**Figure S15.** A heat map to display high throughput screening results of WMMC 317 against *Staphylococcus aureus*.



**Figure S16.** A heat map to display high throughput screening results of WMMC 317 against *Candida albicans*.



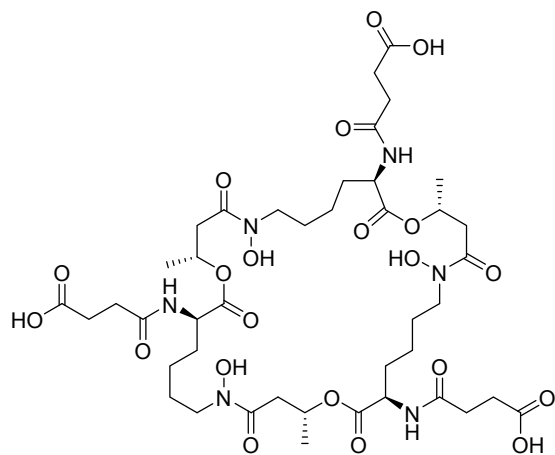


**Table S1.** DFT calculated  $^{13}\text{C}$  NMR chemical shifts for thalassosamide stereoisomer models.

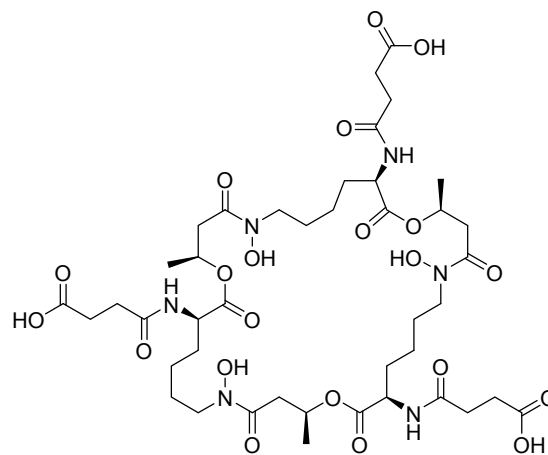
Position	Exp. (ppm)	Model 1		Model 2	
		Calcd. (ppm)	Delta (ppm)	Calcd. (ppm)	Delta (ppm)
1	171.7	166.595	5.105	168.417	3.283
2	51.8	54.447	2.647	61.153	9.353
3	30.8	33.669	2.869	30.956	0.156
4	22.3	24.364	2.064	26.156	3.856
5	26.0	29.095	3.095	28.557	2.557
6	46.9	52.225	5.325	45.924	0.976
7	169.3	168.673	0.627	165.287	4.013
8	38.0	42.980	4.980	38.227	0.227
9	68.0	70.508	2.508	70.828	2.828
10	171.4	163.679	7.721	163.597	7.803
11	29.9	32.397	2.497	31.747	1.847
12	29.3	32.149	2.849	28.365	0.935
13	174.0	171.147	2.853	164.911	9.089
14	20.0	21.072	1.072	18.463	1.537
1'	171.7	166.595	5.105	168.417	3.283
2'	51.8	54.447	2.647	61.153	9.353
3'	30.8	33.669	2.869	30.956	0.156
4'	22.3	24.364	2.064	26.156	3.856
5'	26.0	29.095	3.095	28.557	2.557
6'	46.9	52.225	5.325	45.924	0.976
7'	169.3	168.673	0.627	165.287	4.013
8'	38.0	42.980	4.980	38.227	0.227
9'	68.0	70.508	2.508	70.828	2.828
10'	171.4	163.679	7.721	163.597	7.803
11'	29.9	32.397	2.497	31.747	1.847
12'	29.3	32.149	2.849	28.365	0.935
13'	174.0	171.147	2.853	164.911	9.089

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14'	20.0	21.072	1.072	18.463	1.537
1"	171.7	166.595	5.105	168.417	3.283
2"	51.8	54.447	2.647	61.153	9.353
3"	30.8	33.669	2.869	30.956	0.156
4"	22.3	24.364	2.064	26.156	3.856
5"	26.0	29.095	3.095	28.557	2.557
6"	46.9	52.225	5.325	45.924	0.976
7"	169.3	168.673	0.627	165.287	4.013
8"	38.0	42.980	4.980	38.227	0.227
9"	68.0	70.508	2.508	70.828	2.828
10"	171.4	163.679	7.721	163.597	7.803
11"	29.9	32.397	2.497	31.747	1.847
12"	29.3	32.149	2.849	28.365	0.935
13"	174.0	171.147	2.853	164.911	9.089
14"	20.0	21.072	1.072	18.463	1.537
Total:			138.636		145.38



Model 1



Model 2

**Table S2.** DP4 probability calculation for thalassosamide stereoisomer models

Model	Configuration	DP4 Probability
1	2 <i>R</i> , 2' <i>R</i> , 2'' <i>R</i> , 9 <i>R</i> , 9' <i>R</i> , 9'' <i>R</i>	100%
2	2 <i>R</i> , 2' <i>R</i> , 2'' <i>R</i> , 9 <i>S</i> , 9' <i>S</i> , 9'' <i>S</i>	0%