Supporting Information

Genome Mining and Molecular Networking Targeted Discovery of Siderophores with Plant Growth-promoting Activities from the marine-derived *Streptomonospora nanhaiensis* 12A09^{T}

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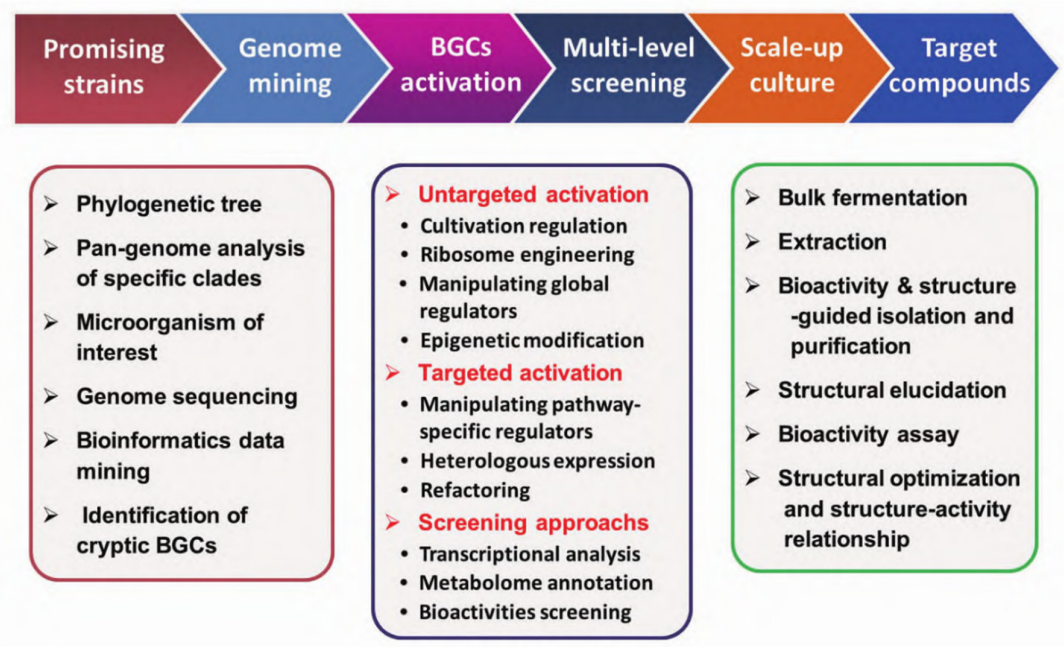

Figure S1. The systematic pipeline for efficient lead structure discovery from microbial natural products by promising strain selection and multi-omics mining (SPLSD) [1] (Cited from the literature: Pan, H.Q. Design and prospects of an efficient mining pipeline for microbial natural products in the post-genome era. Journal of Microbiology. (Chinese), 2022, 42 (3), 1−14. http://wswx.cnjournals.com/ch/reader/view_abstract.aspx?file_no=20220301&flag=1).

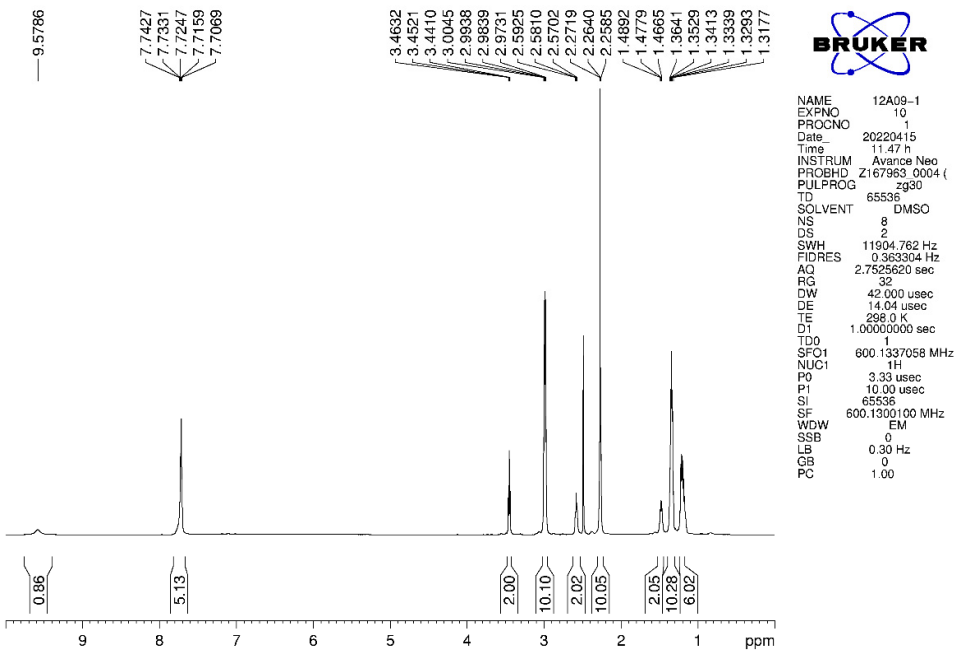

Figure S2. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **1**

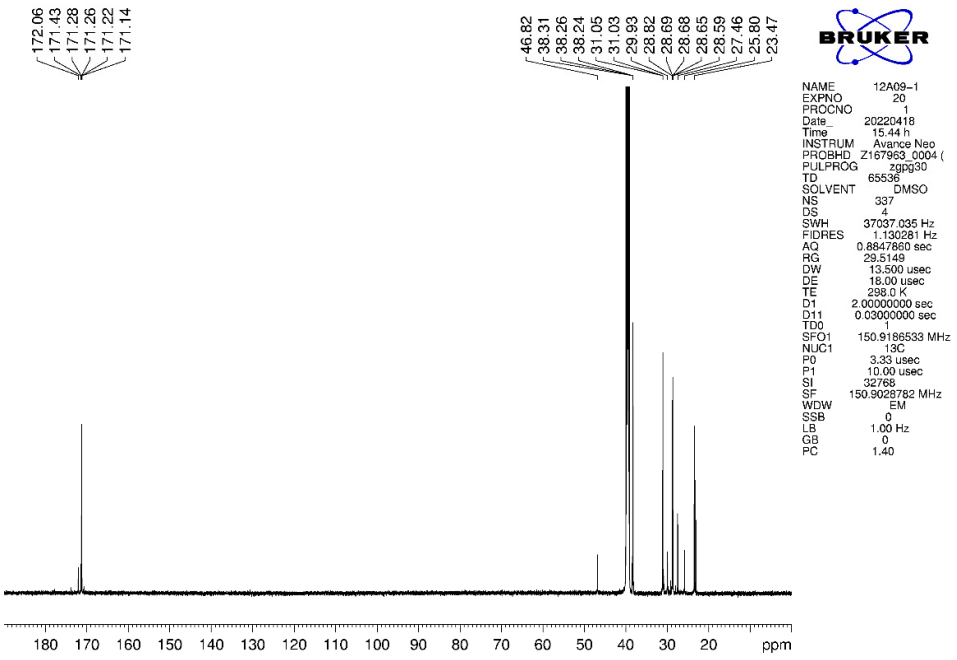

Figure S3. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **1**

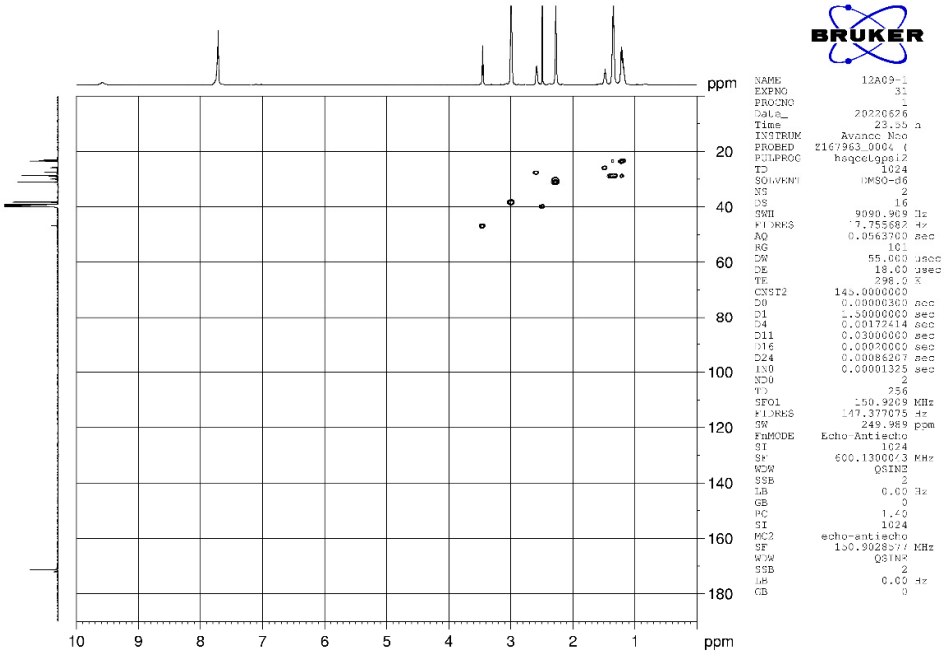

Figure S4. HSQC spectrum of **1**

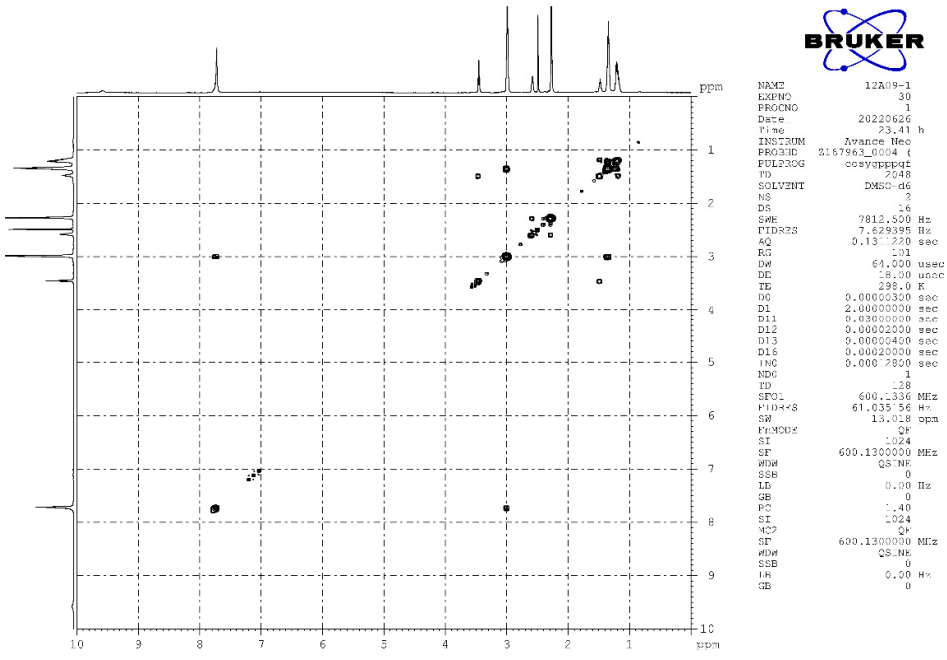

Figure S5. ^{1}H-^{1}H COSY spectrum of **1**

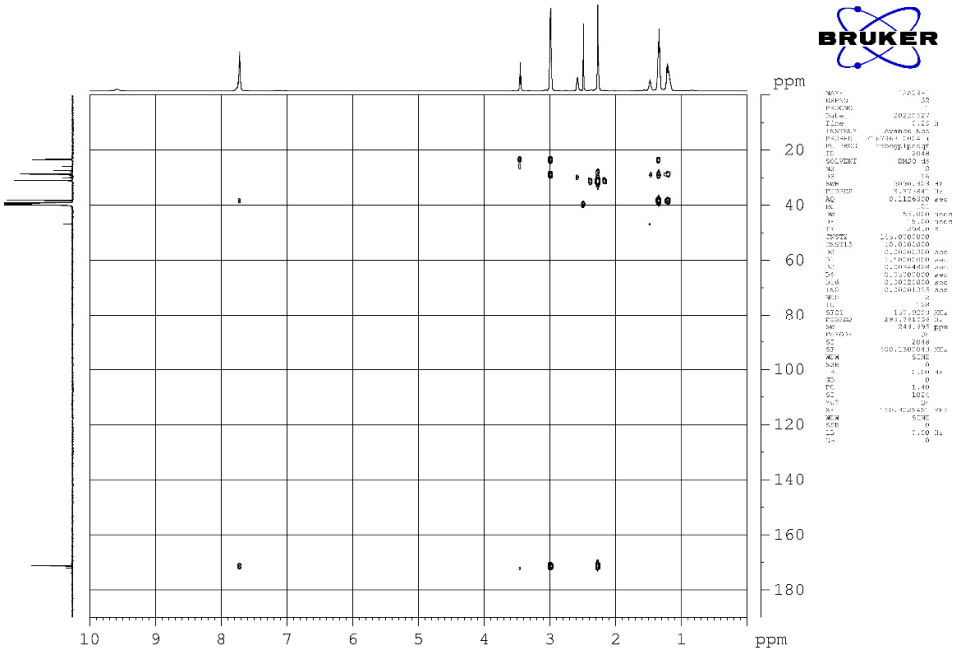

Figure S6. HMBC spectrum of **1**

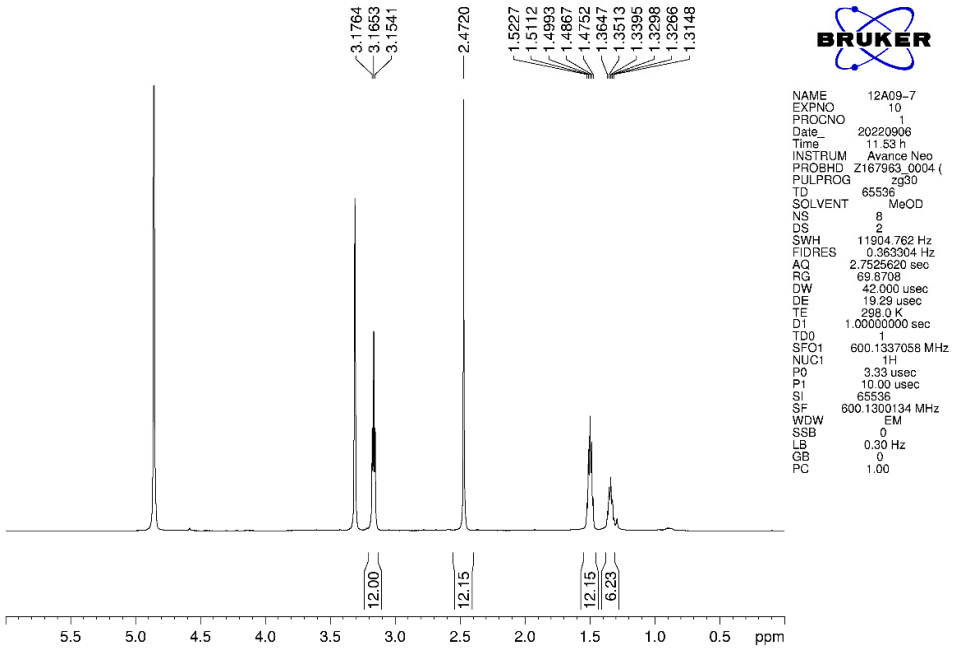

Figure S7. ^{1}H NMR (600 MHz, CD_3OD-d_4) spectrum of **2**

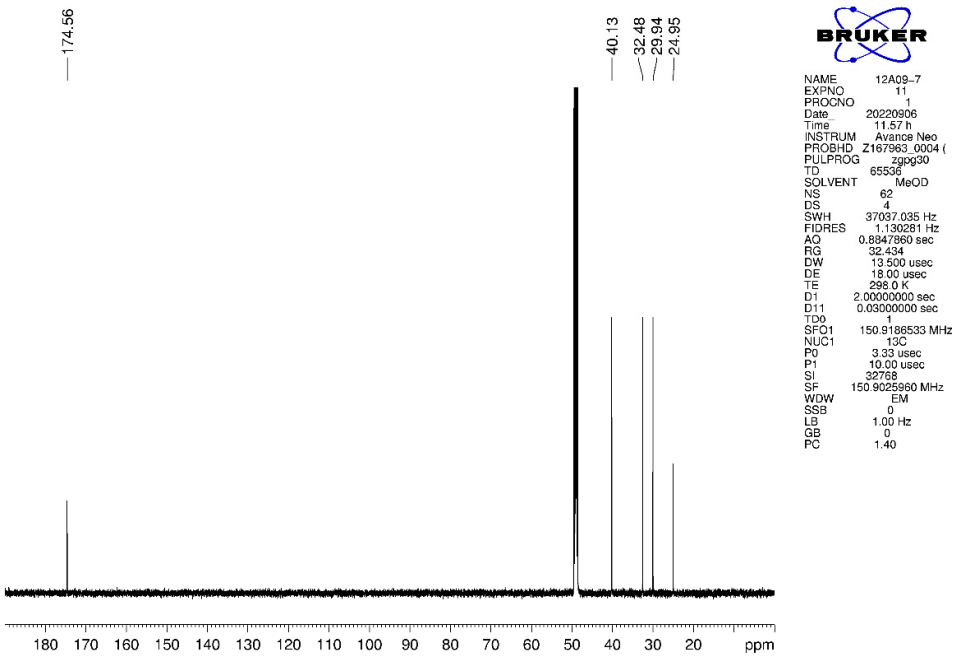

Figure S8. ^{13}C NMR (150 MHz, CD_3OD-d_4) spectrum of **2**

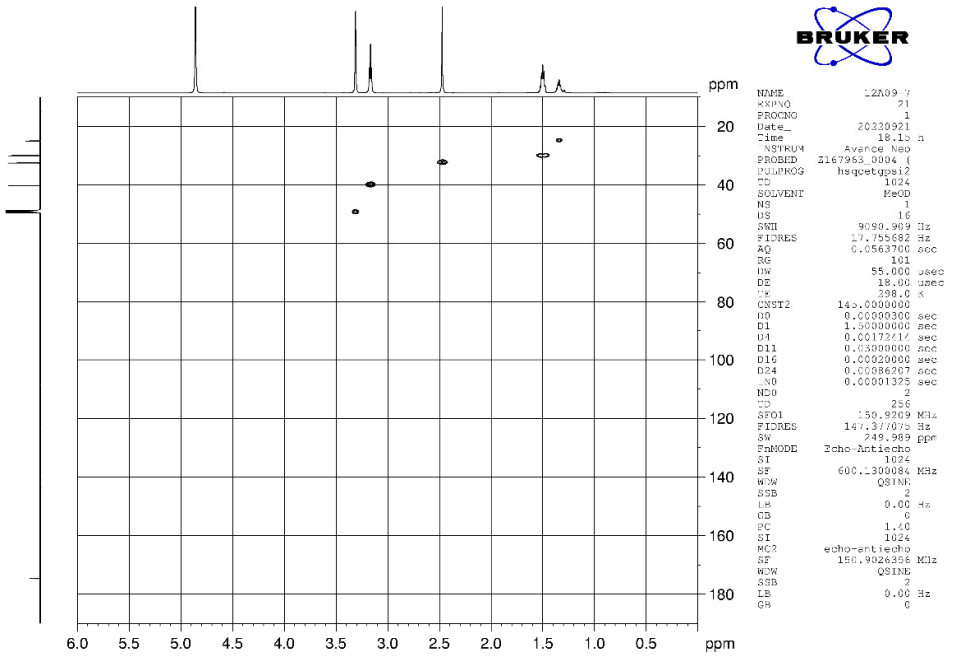

Figure S9. HSQC spectrum of **2**

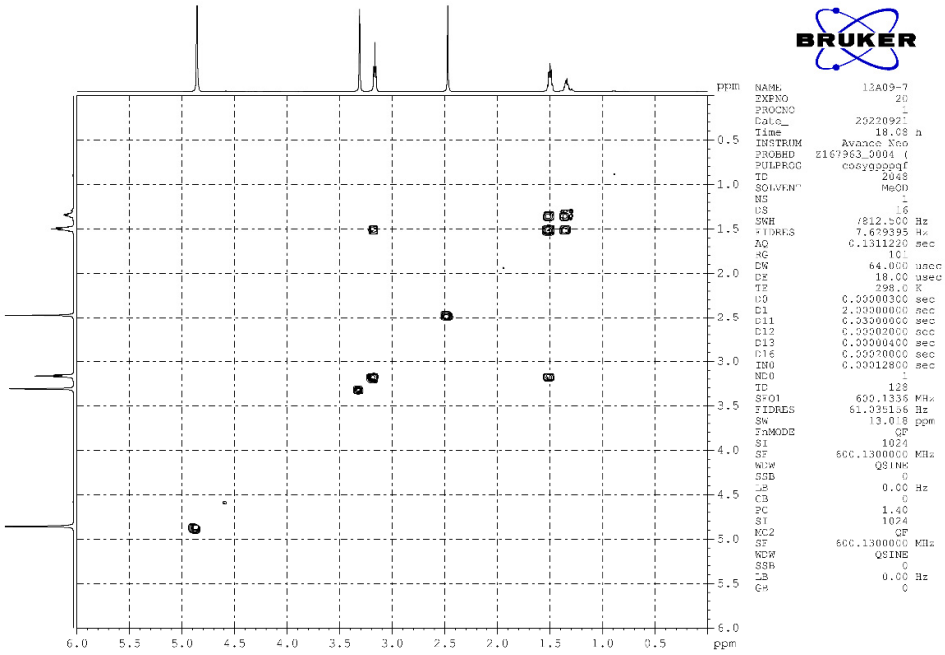

Figure S10. ^{1}H-^{1}H COSY spectrum of **2**

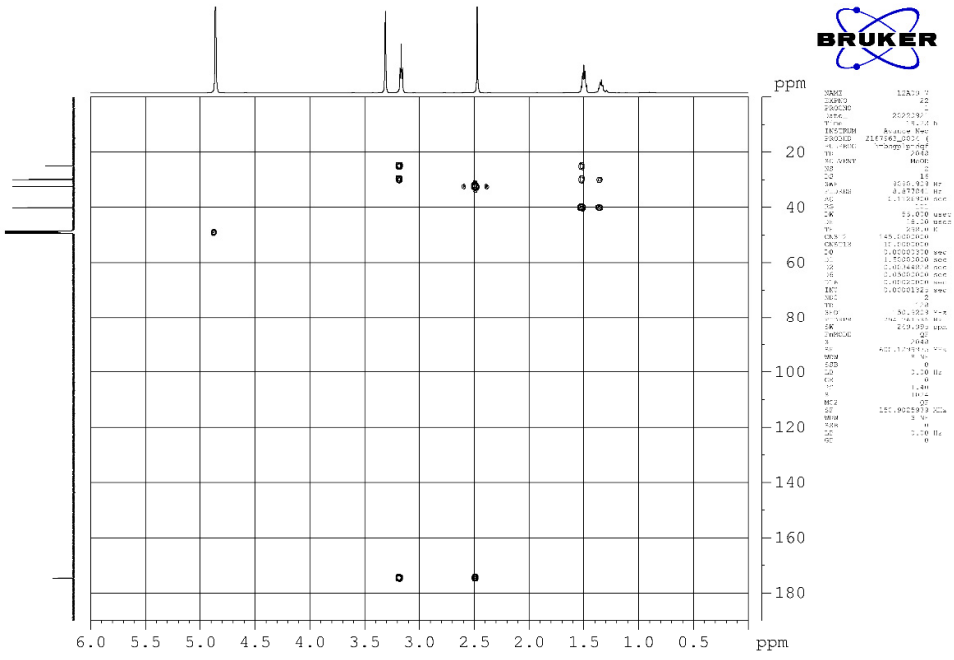

Figure S11. HMBC spectrum of **2**

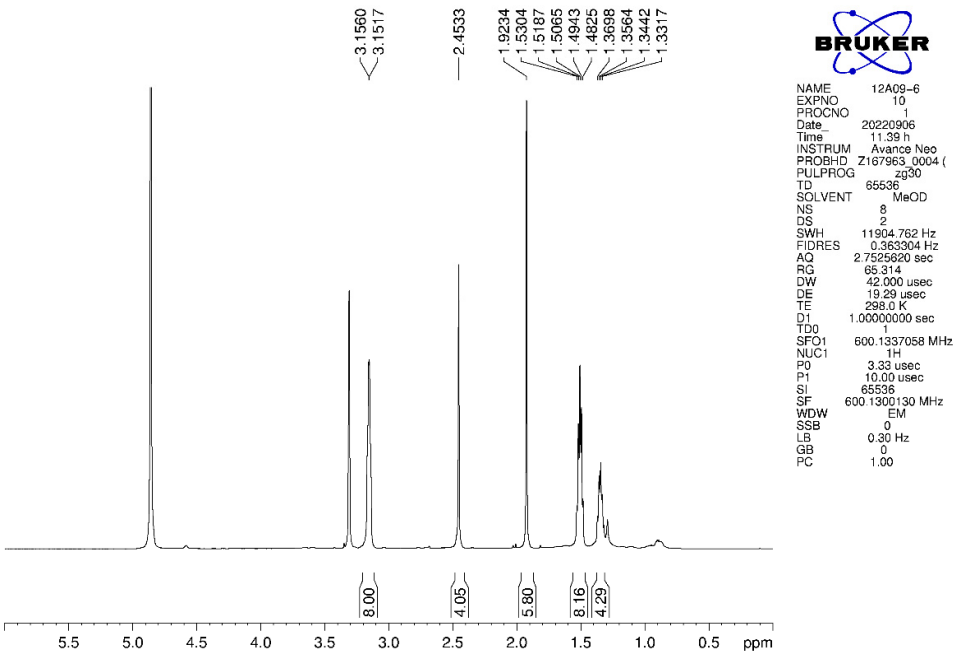

Figure S12. ^{1}H NMR (600 MHz, CD_3OD-d_4) spectrum of **3**

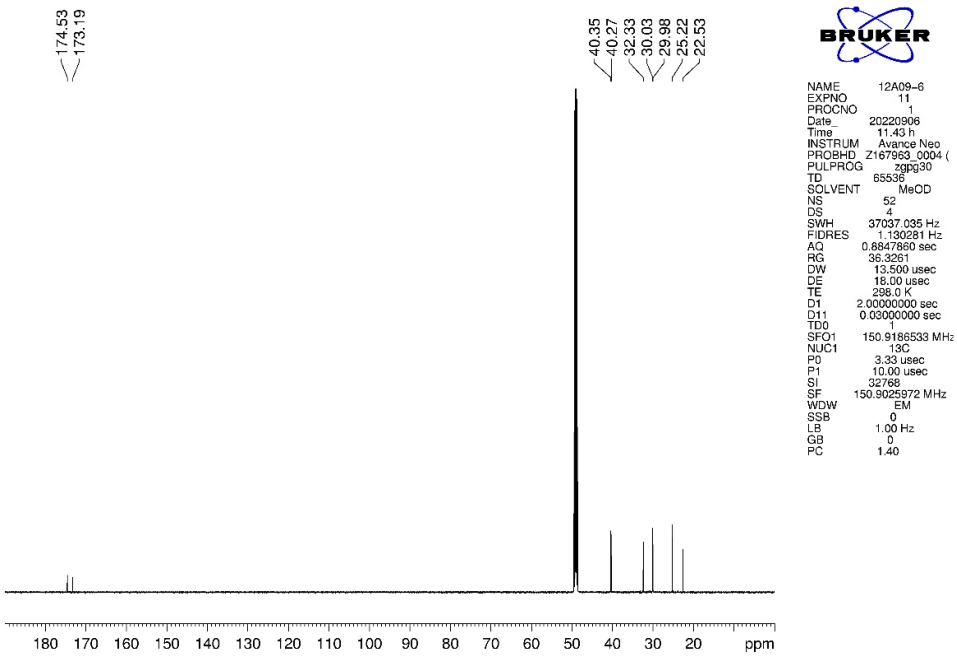

Figure S13. ^{13}C NMR (150 MHz, CD_3OD-d_4) spectrum of **3**

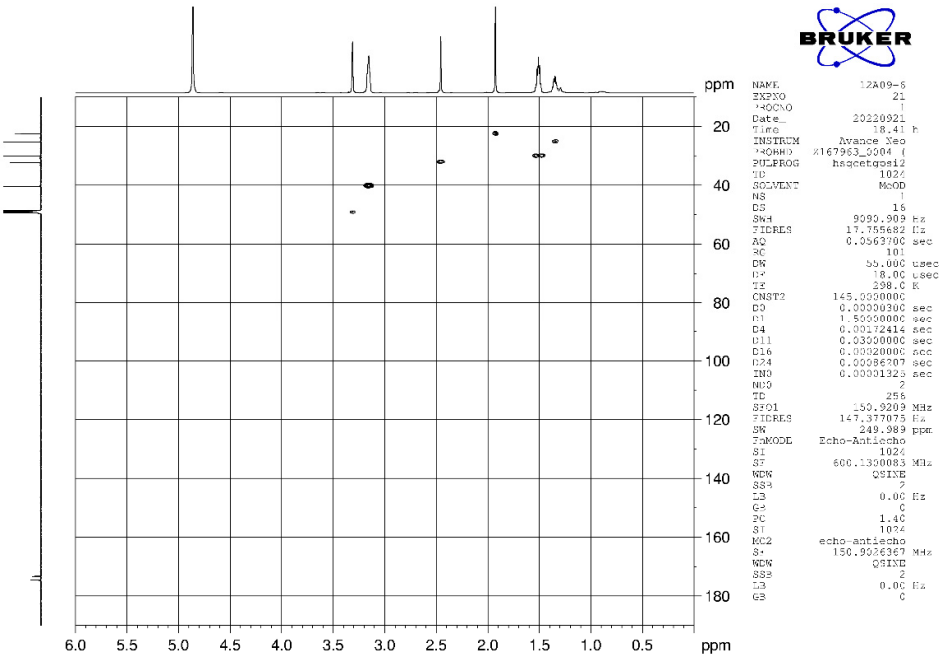

Figure S14. HSQC spectrum of **3**

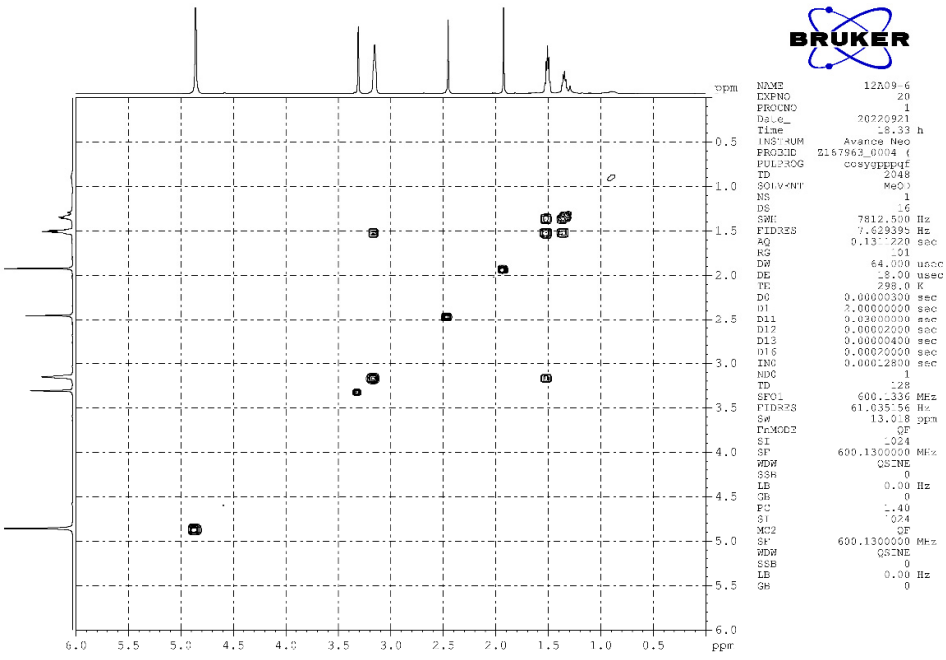

Figure S15. ^{1}H-^{1}H COSY spectrum of **3**

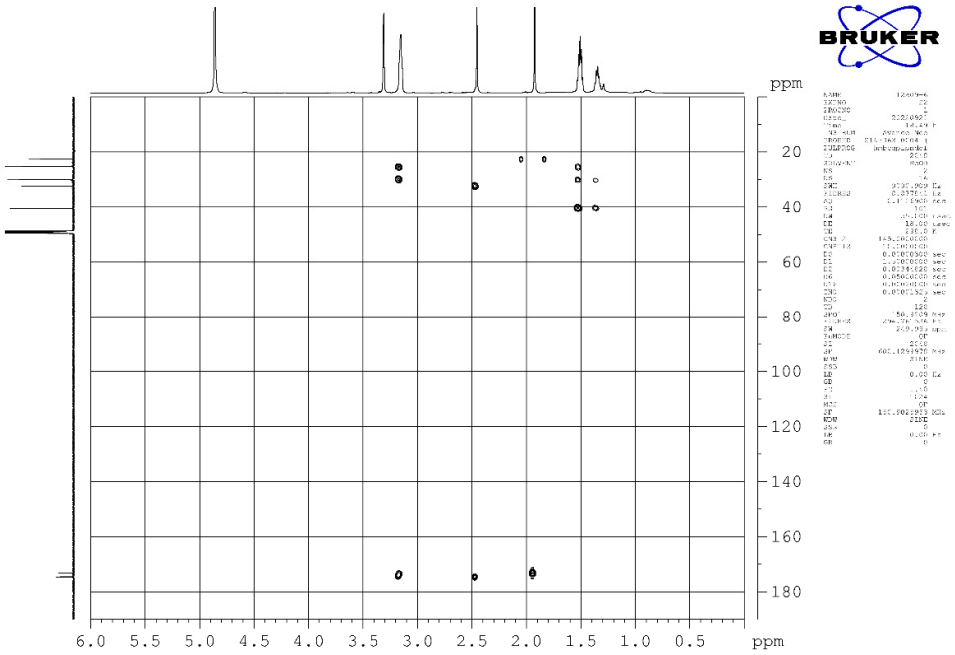

Figure S16. HMBC spectrum of **3**

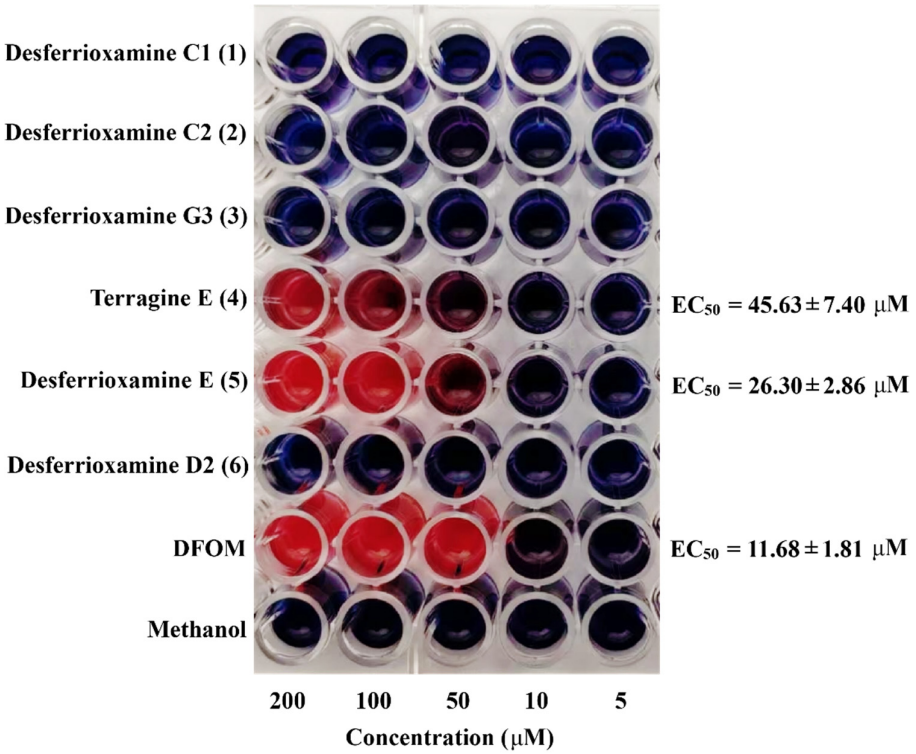

Figure S17. CAS assay results of **1-6** and DFOM. Concentration-dependent CAS liquid well-plate assay and EC_{50} values

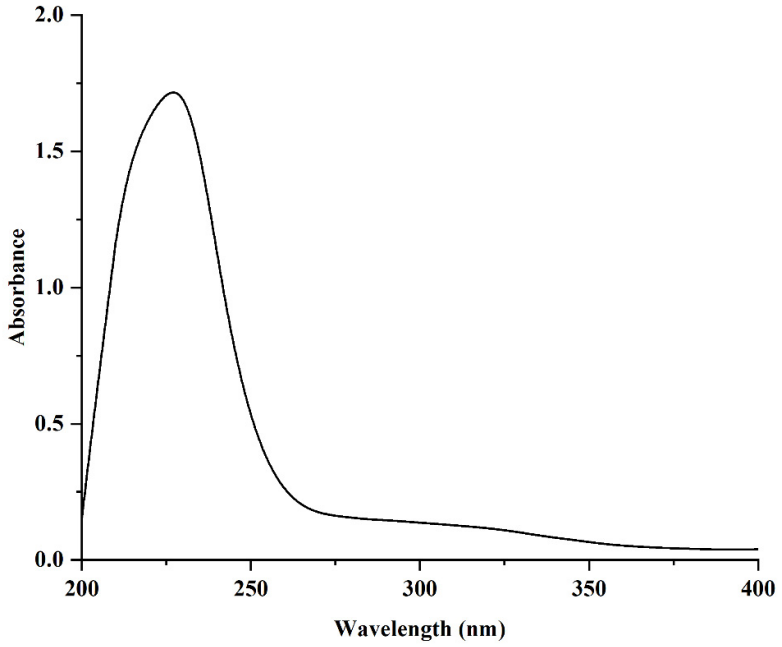

Figure S18. UV spectrum of **1**

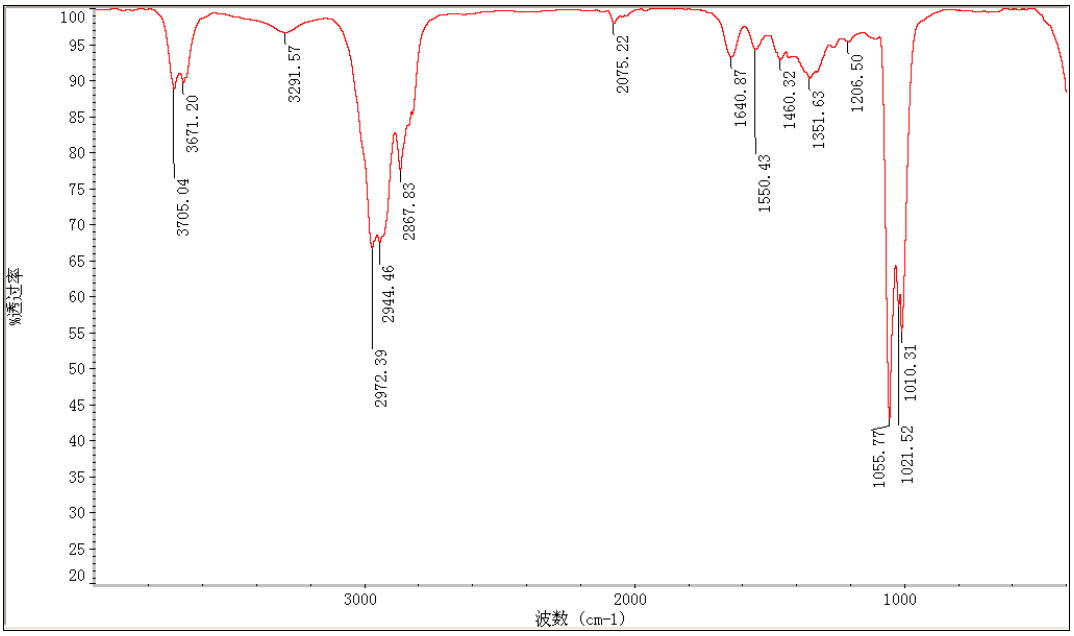

Figure S19. IR spectrum of **1**

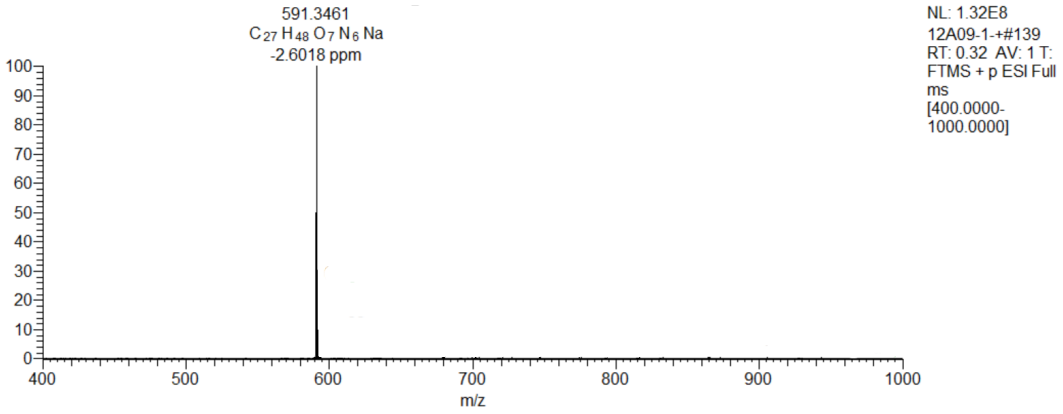

Figure S20. (+)-HRESIMS spectrum of **1**

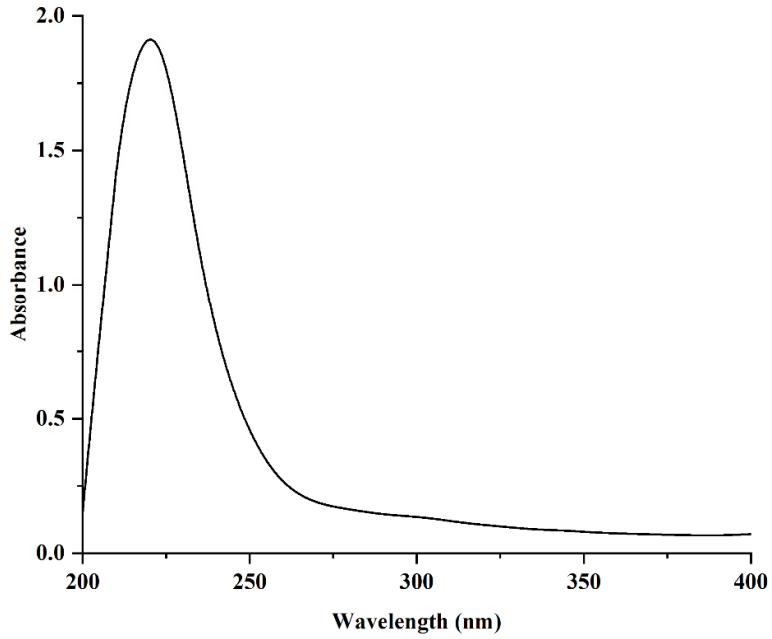

Figure S21. UV spectrum of **2**

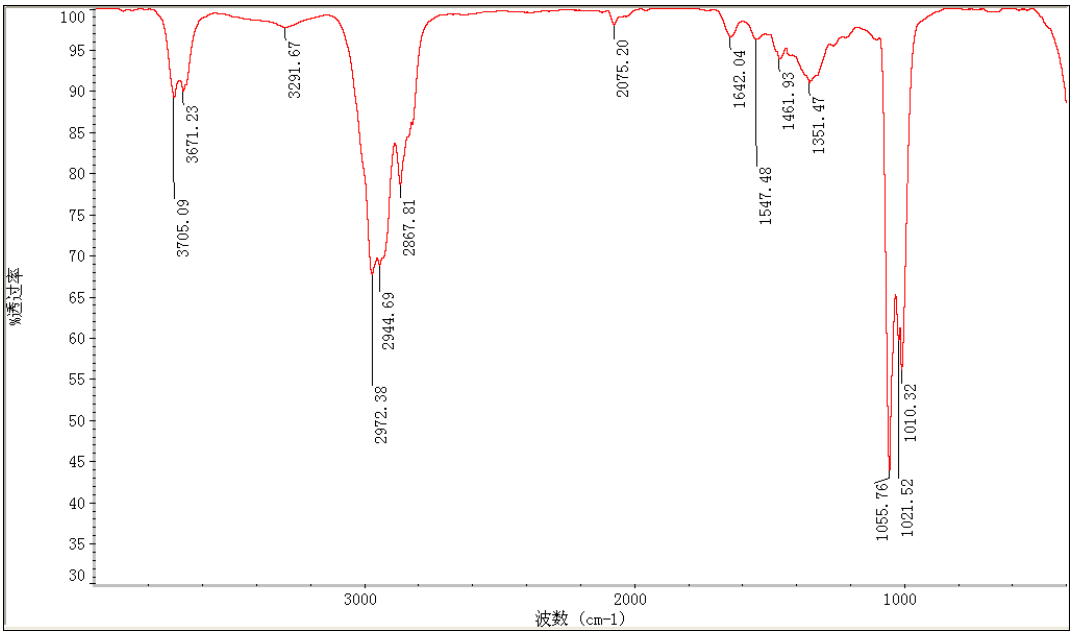

Figure S22. IR spectrum of **2**

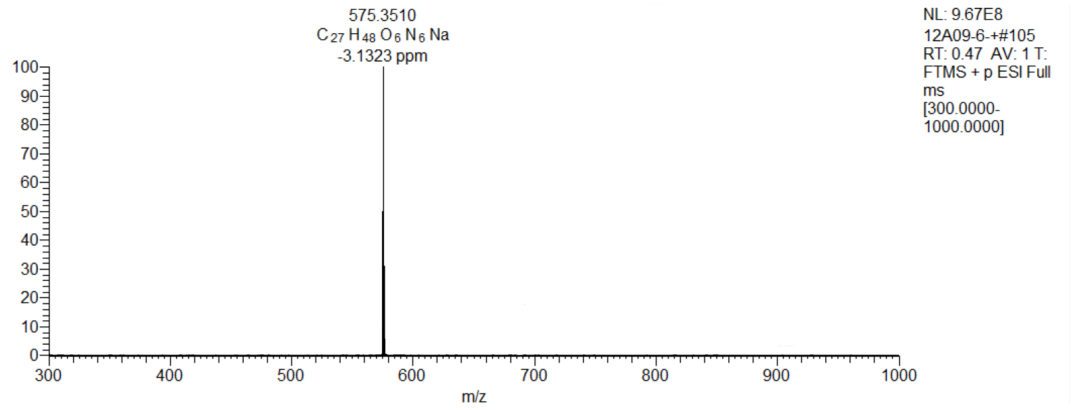

Figure S23. (+)-HRESIMS spectrum of **2**

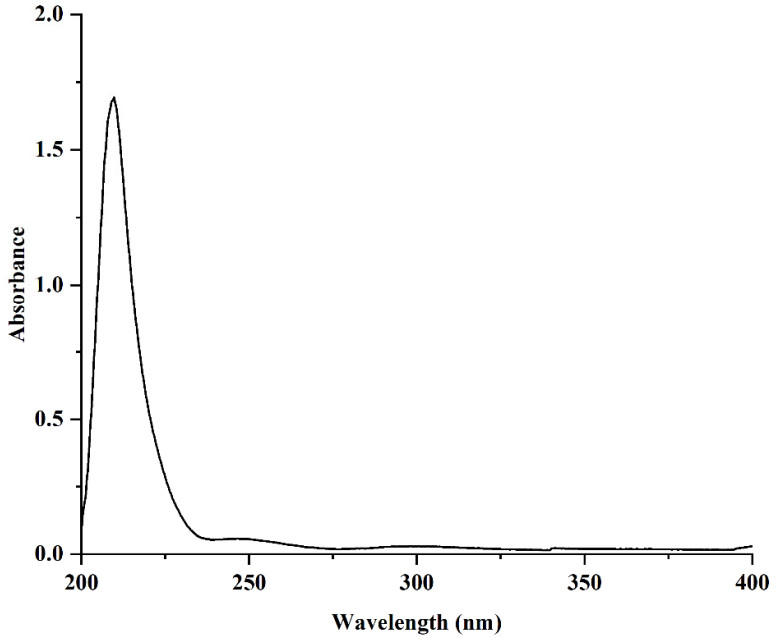

Figure S24. UV spectrum of **3**

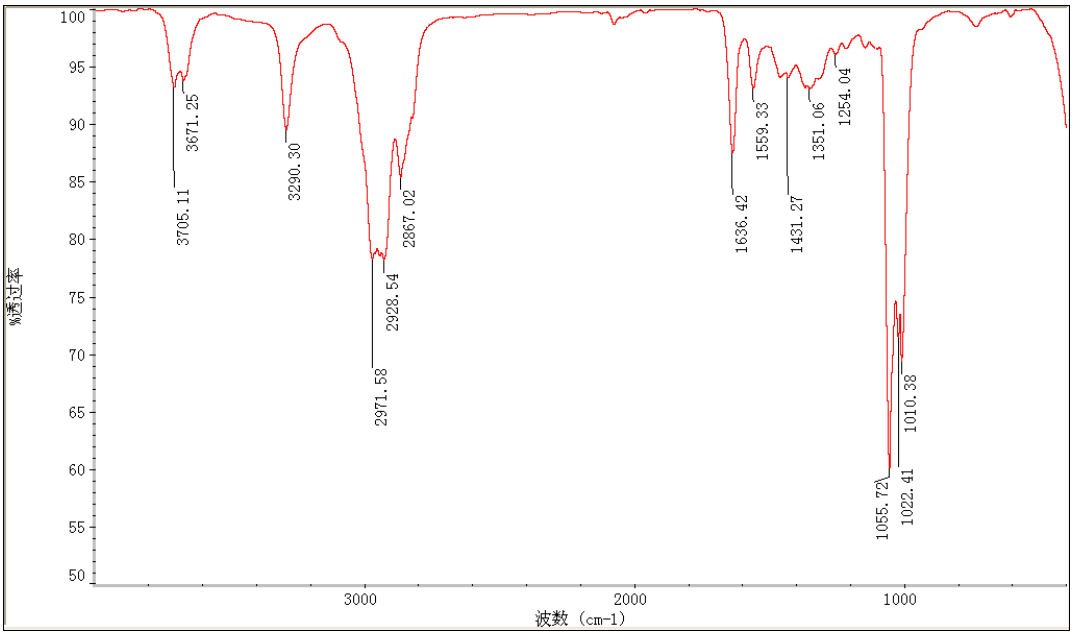

Figure S25. IR spectrum of **3**

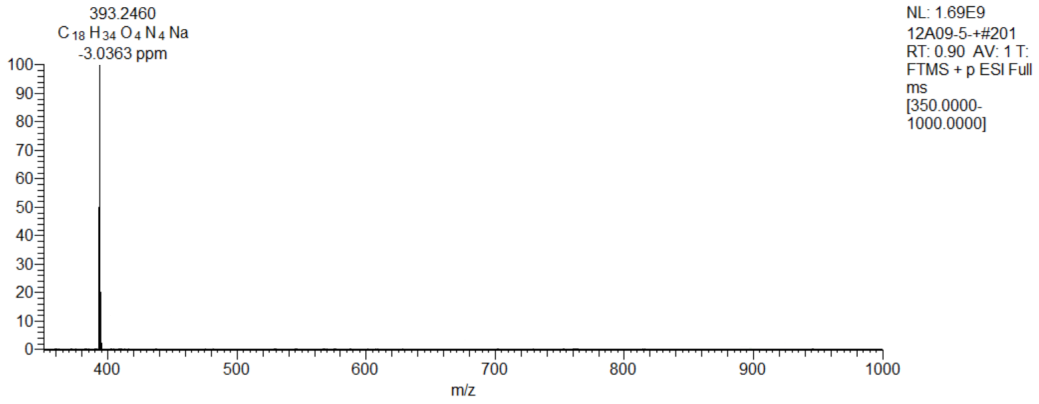

Figure S26. (+)-HRESIMS spectrum of **3**

Table S1 Number of genes associated with the 19 general COG functional categories

Type	Description of functional categories	Code	Value	Ratio
Information storage and processing	Translation, ribosomal structure and biogenesis	J	185	2.98%
	Transcription	K	609	9.82%
	Replication, recombination and repair	L	185	2.98%
Cellular processes and signaling	Cell cycle control, cell division, chromosome partitioning	D	32	0.52%
	Cell wall/membrane/envelope biogenesis	M	193	3.11%
	Cell motility	N	1	0.02%
	Posttranslational modification, protein turnover, chaperones	O	127	2.05%
	Intracellular trafficking, secretion, and vesicular transport	U	37	0.60%
Metabolism	Energy production and conversion	C	283	4.56%
	Amino acid transport and metabolism	E	315	5.08%
	Nucleotide transport and metabolism	F	102	1.65%
	Carbohydrate transport and metabolism	G	348	5.61%
	Coenzyme transport and metabolism	H	176	2.84%
	Lipid transport and metabolism	I	152	2.45%
	Inorganic ion transport and metabolism	P	297	4.79%
	Secondary metabolites biosynthesis, transport and catabolism	Q	129	2.08%
	Signal transduction mechanisms	T	271	4.37%
	Defense mechanisms	V	122	1.97%
Poorly characterized	Function unknown	S	1819	29.34%

Table S2 ^{1}H and ^{13}C NMR Data for 1 and 5 in DMSO-d_6 (600/150 MHz, δ in ppm)

Position	**1**		**5**	
	δ_H (J inHz)	δ_C,Type	δ_H (J inHz)	δ_C,Type
1		171.1 C		171.5 C
2	2.26 m	29.9 CH_2	2.27 m	30.0 CH_2
3	2.58 m	27.5 CH_2	2.57 m	27.5 CH_2
4		172.1 C		172.0 C
5	3.45 m	46.8 CH_2	3.45 m	46.8 CH_2
6	1.48 m	25.8 CH_2	1.48 m	25.8 CH_2
7	1.20 m	23.1 CH_2	1.19 m	23.2 CH_2
8	1.34 m	28.7 CH_2	1.36 m	28.6 CH_2
9	2.98 m	38.2 CH_2	2.98 m	38.3 CH_2
10		171.2 C		171.5 C
11	2.26 m	31.0 CH_2	2.27 m	30.0 CH_2
12	2.26 m	31.0 CH_2	2.57 m	27.5 CH_2
13		171.4 C		172.0 C
14	2.98 m	38.3 CH_2	3.45 m	46.8 CH_2
15	1.34 m	28.7 CH_2	1.48 m	25.8 CH_2
16	1.20 m	23.5 CH_2	1.19 m	23.2 CH_2
17	1.34 m	28.7 CH_2	1.36 m	28.6 CH_2
18	2.98 m	38.2 CH_2	2.98 m	38.3 CH_2
19		171.3 C		171.5 C
20	2.26 m	31.0 CH_2	2.27 m	30.0 CH_2
21	2.26 m	31.0 CH_2	2.57 m	27.5 CH_2
22		171.3 C		172.0 C
23	2.98 m	38.3 CH_2	3.45 m	46.8 CH_2
24	1.34 m	28.7 CH_2	1.48 m	25.8 CH_2
25	1.20 m	23.5 CH_2	1.19 m	23.2 CH_2
26	1.34 m	28.7 CH_2	1.36 m	28.6 CH_2
27	2.98 m	38.2 CH_2	2.98 m	38.3 CH_2
-NH	7.72 s		7.71 s	
N-OH	9.58 s		9.59 s	

Table S3 ^{1}H and ^{13}C NMR Data for **4** and terragine E in DMSO-d_6 (600/150 MHz, δ in ppm) [22]

Position	**4**		terragine E	
	δ_H (J inHz)	δ_C,Type	δ_H (J inHz)	δ_C,Type
1		171.3 C		171.3 C
2	2.26 m	30.0 CH_2	2.26 t (7.0)	29.9 CH_2
3	2.58 m	27.5 CH_2	2.57 t (7.0)	27.5 CH_2
4		172.0 C		172.0 C
5	3.45 m	46.8 CH_2	3.45 t (7.0)	46.8 CH_2
6	1.48 m	25.8 CH_2	1.47 p (7.0)	25.8 CH_2
7	1.20 m	23.1 CH_2	1.20 p (7.0)	23.1 CH_2
8	1.34 m	28.7 CH_2	1.34 p (7.0)	28.5 CH_2
9	2.98 m	38.3 CH_2	2.98 dt (6.0, 7.0)	38.2 CH_2
10		171.3 C		171.3 C
11	2.26 m	30.0 CH_2	2.26 t (7.0)	29.9 CH_2
12	2.58 m	27.5 CH_2	2.57 t (7.0)	27.5 CH_2
13		172.0 C		172.0 C
14	3.45 m	46.8 CH_2	3.45 t (7.0)	46.8 CH_2
15	1.48 m	25.8 CH_2	1.47 p (7.0)	25.8 CH_2
16	1.20 m	23.1 CH_2	1.20 p (7.0)	23.1 CH_2
17	1.34 m	28.7 CH_2	1.34 p (7.0)	28.5 CH_2
18	2.98 m	38.3 CH_2	2.98 dt (6.0, 7.0)	38.2 CH_2
19		171.4 C		171.4 C
20	2.26 m	31.1 CH_2	2.26 s	31.0 CH_2
21	2.26 m	31.1 CH_2	2.26 s	31.0 CH_2
22		171.4 C		171.4 C
23	2.98 m	38.3 CH_2	2.98 dt (6.0, 7.0)	38.2 CH_2
24	1.34 m	28.7 CH_2	1.34 p (7.0)	28.5 CH_2
25	1.20 m	23.5 CH_2	1.20 p (7.0)	23.4 CH_2
26	1.34 m	28.7 CH_2	1.34 p (7.0)	28.5 CH_2
27	2.98 m	38.3 CH_2	2.98 dt (6.0, 7.0)	38.2 CH_2
-NH	7.72 s		7.73 s	
N-OH	9.58 s		9.61 s	

Table S4 ^{1}H and ^{13}C NMR Data for **5** and desferrioxamine E in DMSO-d_6 (600/150 MHz, δ in ppm) [21]

Position	**5**		desferrioxamine E	
	δ_H (J inHz)	δ_C,Type	δ_H (J inHz)	δ_C,Type
1		171.5 C		171.8 C
2	2.27 m	30.0 CH_2	2.27 m	31.3 CH_2
3	2.57 m	27.5 CH_2	2.57 m	27.8 CH_2
4		172.0 C		172.3 C
5	3.45 m	46.8 CH_2	3.46 m	47.1 CH_2
6	1.48 m	25.8 CH_2	1.46 m	26.0 CH_2
7	1.19 m	23.2 CH_2	1.19 m	23.4 CH_2
8	1.36 m	28.6 CH_2	1.36 m	28.8 CH_2
9	2.98 m	38.3 CH_2	2.98 m	38.6 CH_2
10		171.5 C		171.8 C
11	2.27 m	30.0 CH_2	2.27 m	31.3 CH_2
12	2.57 m	27.5 CH_2	2.57 m	27.8 CH_2
13		172.0 C		172.3 C
14	3.45 m	46.8 CH_2	3.46 m	47.1 CH_2
15	1.48 m	25.8 CH_2	1.46 m	26.0 CH_2
16	1.19 m	23.2 CH_2	1.19 m	23.4 CH_2
17	1.36 m	28.6 CH_2	1.36 m	28.8 CH_2
18	2.98 m	38.3 CH_2	2.98 m	38.6 CH_2
19		171.5 C		171.8 C
20	2.27 m	30.0 CH_2	2.27 m	31.3 CH_2
21	2.57 m	27.5 CH_2	2.57 m	27.8 CH_2
22		172.0 C		172.3 C
23	3.45 m	46.8 CH_2	3.46 m	47.1 CH_2
24	1.48 m	25.8 CH_2	1.46 m	26.0 CH_2
25	1.19 m	23.2 CH_2	1.19 m	23.4 CH_2
26	1.36 m	28.6 CH_2	1.36 m	28.8 CH_2
27	2.98 m	38.3 CH_2	2.98 m	38.6 CH_2
-NH	7.71 s		7.70 s	
N-OH	9.59 s		9.73 s	

Table S5 ^{1}H and ^{13}C NMR Data for **6** and desferrioxamine D2 [23]

Position	**6***		desferrioxamine D2#	
	δ_H (*J* inHz)	δ_C,Type	δ_H (*J* inHz)	δ_C,Type
1		171.5 C		174.6 C
2	2.27 m	30.0 CH_2	2.46 t (6.8)	31.7 CH_2
3	2.57 m	27.5 CH_2	2.77 t (6.8)	29.0 CH_2
4		172.0 C		175.0 C
5	3.45 m	46.8 CH_2	3.60 t (6.3)	48.6 CH_2
6	1.48 m	25.8 CH_2	1.63 tt (7.3, 6.3)	27.2 CH_2
7	1.19 m	23.1 CH_2	1.32 m	24.5 CH_2
8	1.36 m	28.6 CH_2	1.51 m	29.7 CH_2
9	2.98 m	38.3 CH_2	3.17 t (6.3)	40.0 CH_2
10		171.5 C		174.6 C
11	2.27 m	30.0 CH_2	2.46 t (6.8)	31.7 CH_2
12	2.57 m	27.5 CH_2	2.77 t (6.8)	29.0 CH_2
13		172.0 C		175.0 C
14	3.45 m	46.8 CH_2	3.60 t (6.3)	48.6 CH_2
15	1.48 m	25.8 CH_2	1.63 tt (7.3, 6.3)	27.2 CH_2
16	1.19 m	23.1 CH_2	1.32 m	24.5 CH_2
17	1.36 m	28.6 CH_2	1.51 m	29.7 CH_2
18	2.98 m	38.3 CH_2	3.17 t (6.3)	40.0 CH_2
19		171.5 C		174.6 C
20	2.27 m	30.0 CH_2	2.46 t (6.8)	31.7 CH_2
21	2.57 m	27.5 CH_2	2.77 t (6.8)	29.0 CH_2
22		172.0 C		175.0 C
23	3.45 m	46.8 CH_2	3.60 t (6.3)	48.6 CH_2
24	1.48 m	25.8 CH_2	1.63 tt (7.3, 6.3)	25.0 CH_2
25	1.36 m	28.6 CH_2	1.51 m	27.4 CH_2
26	2.98 m	38.3 CH_2	3.17 t (6.3)	40.0 CH_2
-NH	7.71 s			
N-OH	9.59 s			

* Measured in DMSO-d_6. # Measured in CD_3OD-d_4.

References

1. Pan, H.Q. Design and prospects of an efficient mining pipeline for microbial natural products in the post-genome era. *J. Microbiol.* **2022**, *42*, 1–14.