

Fragment-based Drug Discovery from a Natural Product Library

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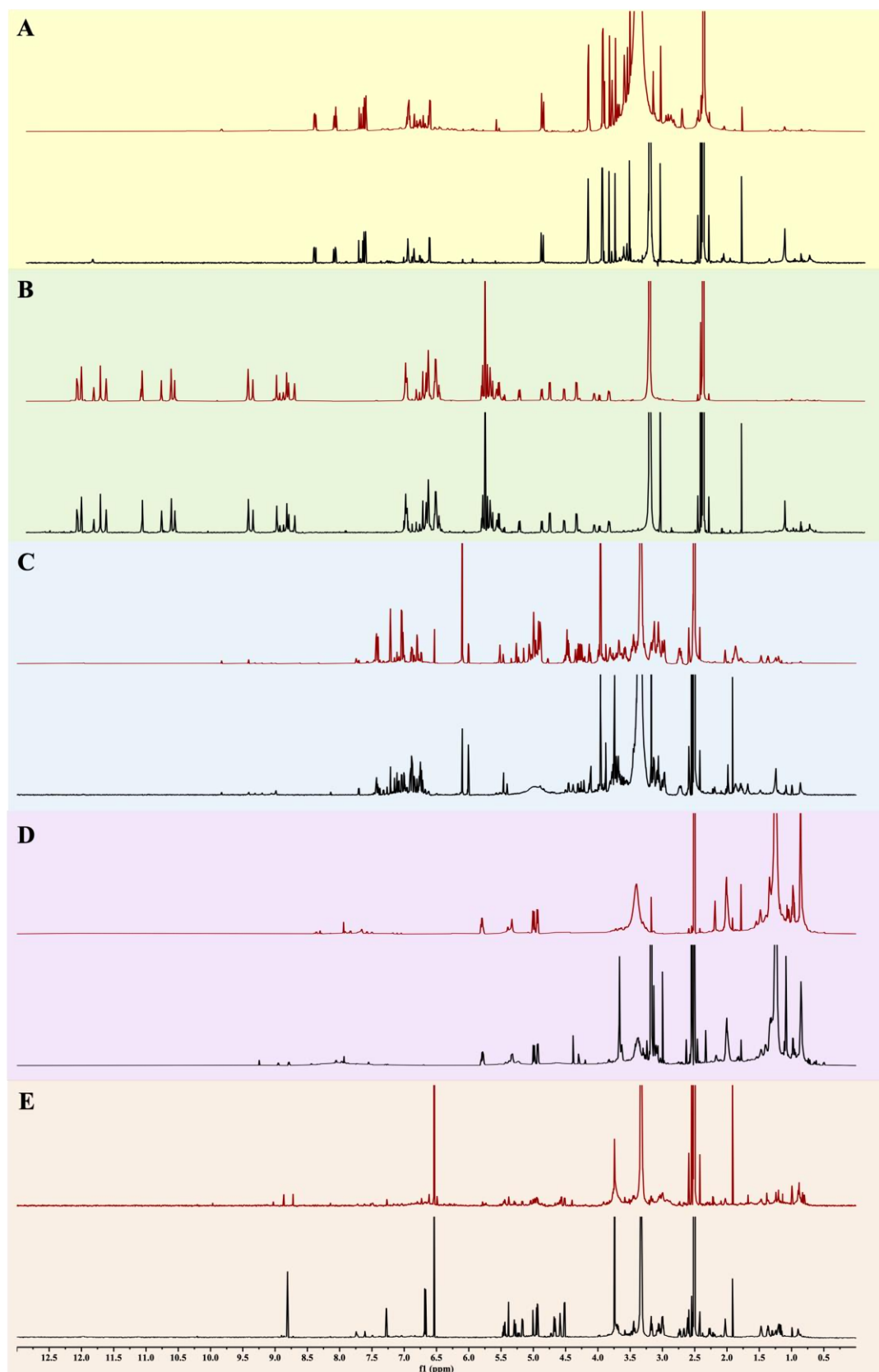


Figure S1: Comparison of ^1H NMR fingerprints between extraction procedures using DCM-MeOH-SPE (top spectra) and 95% ethanol (bottom spectra) for A). plant *Doryphora aromatica* NB024954; B). plant *Garcinia* sp. NB028261; C). plant *Styrax faberi* perk NB101030, D). marine *Haliclona chrysa* NB019667 E). marine *Endotricha docilisalis* NB003781.

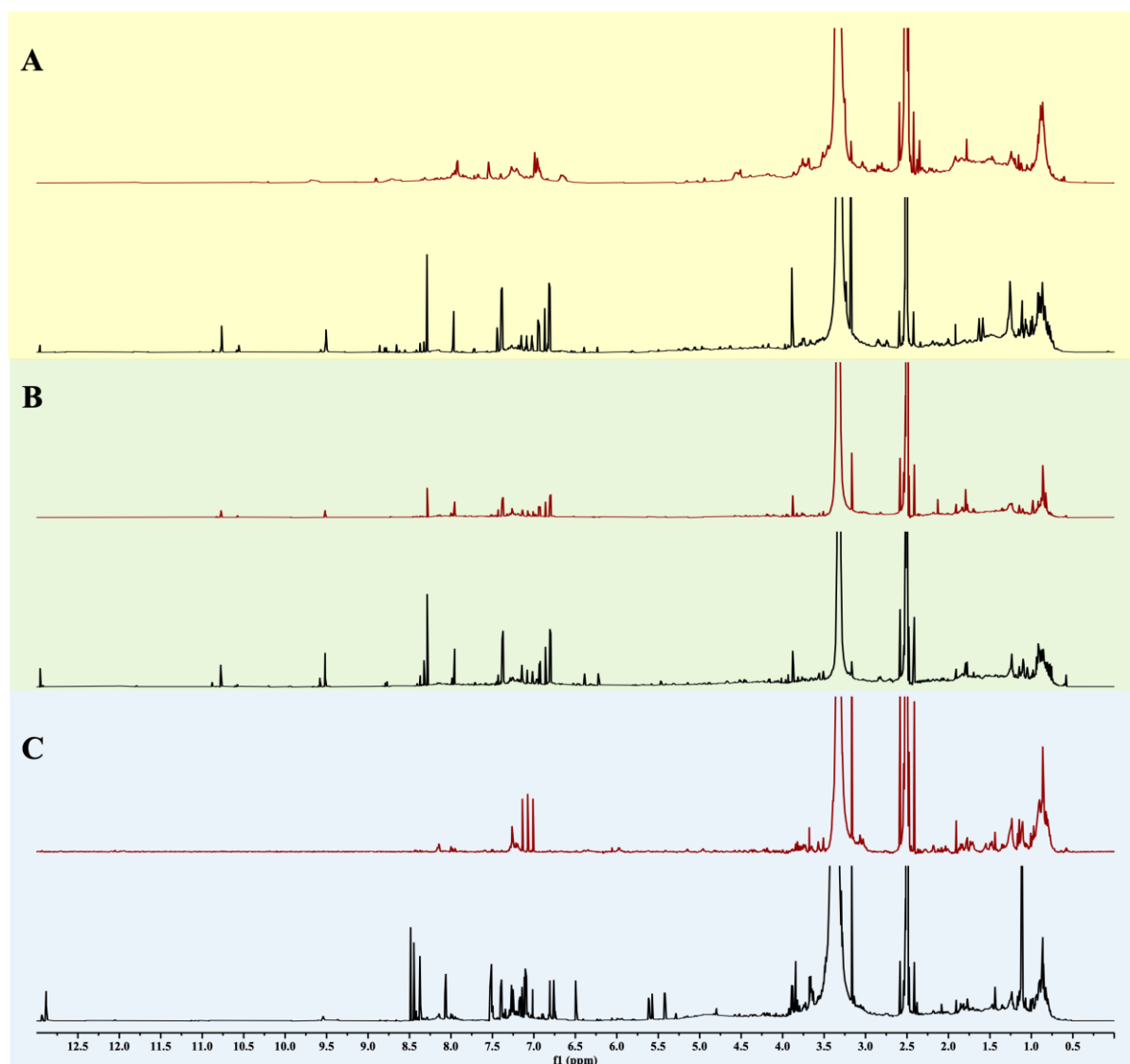


Figure S2: Comparison of ^1H NMR fingerprints between extraction procedures using DCM-MeOH-SPE (top spectra) and n-butanol (bottom spectra) for A). marine strain *Streptomyces* sp. MS120045; B). desert strain *Streptomyces* sp. LS120167; C). endophyte strain *Streptomyces* sp ES120055.

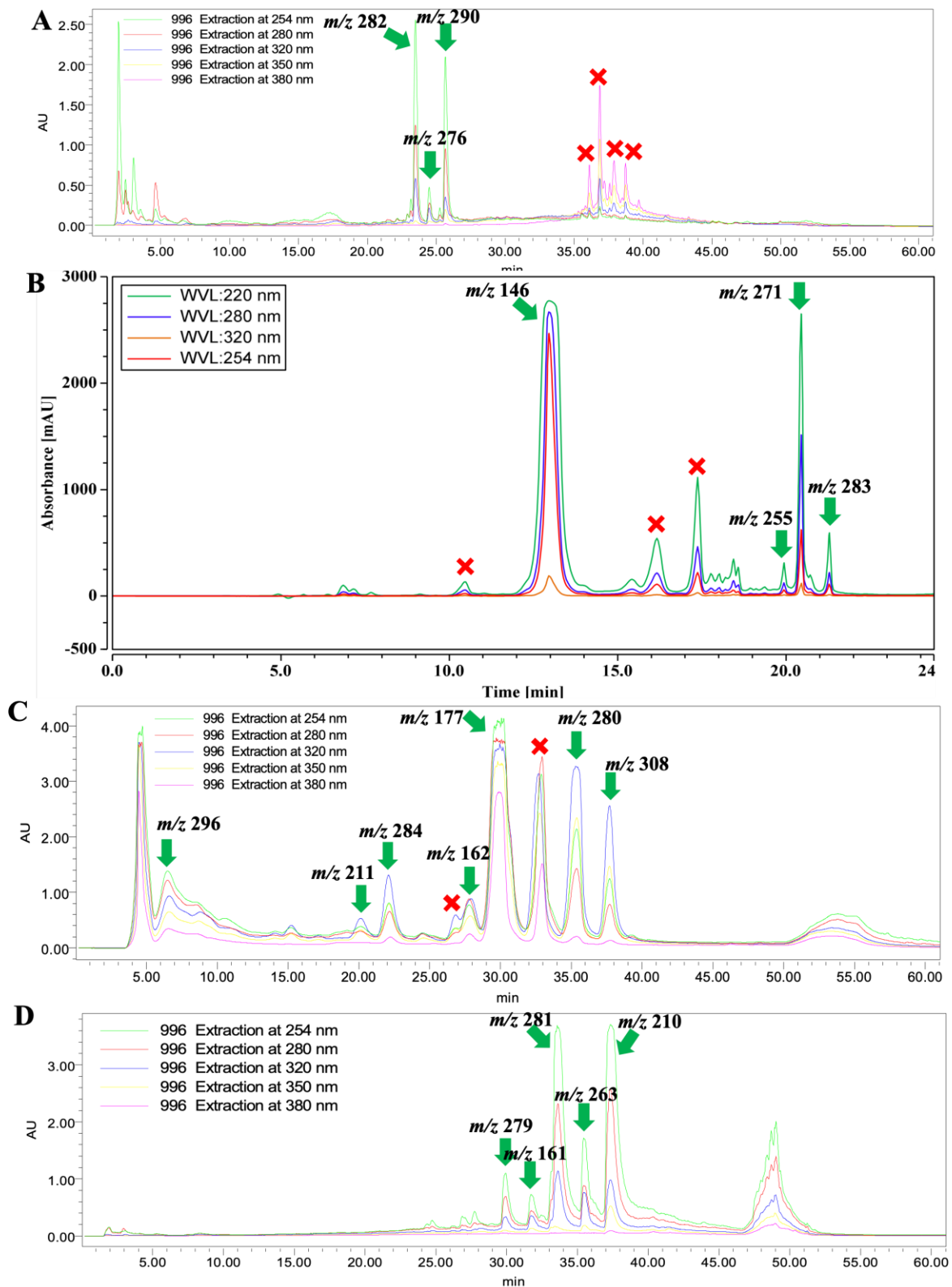


Figure S3. HPLC chromatograms of sephadex fractions from A). a marine strain *Streptomyces* sp. MS11010, B). an endophyte strain *Streptomyces* sp. ES120055, C). an endophyte strain *Streptomyces* sp. ES130127 and D). a desert strain *Streptomyces* sp. LS120194.

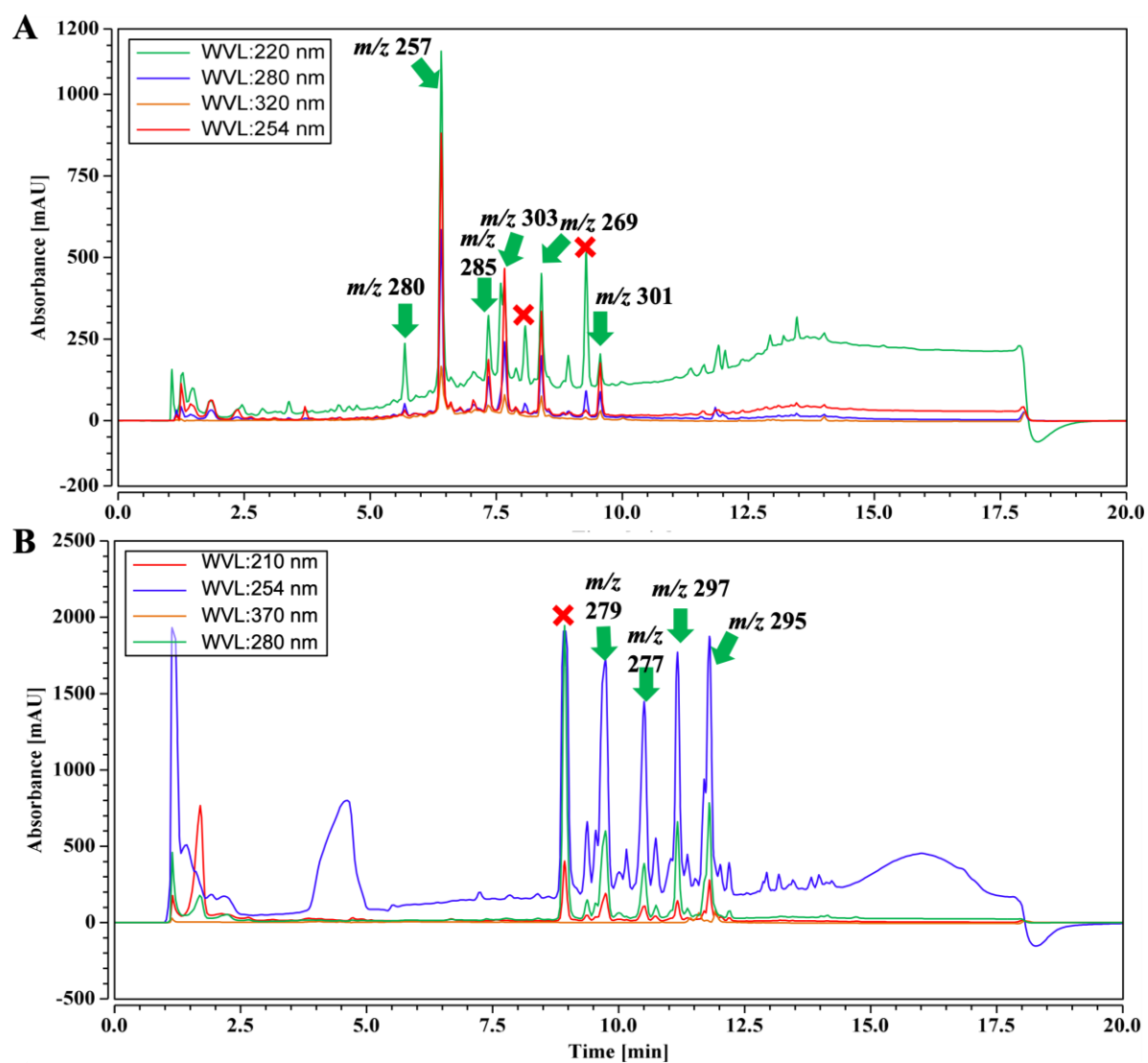


Figure S4. HPLC chromatograms of sephadex fractions from TCMs A). Huangqi B). Danshen.

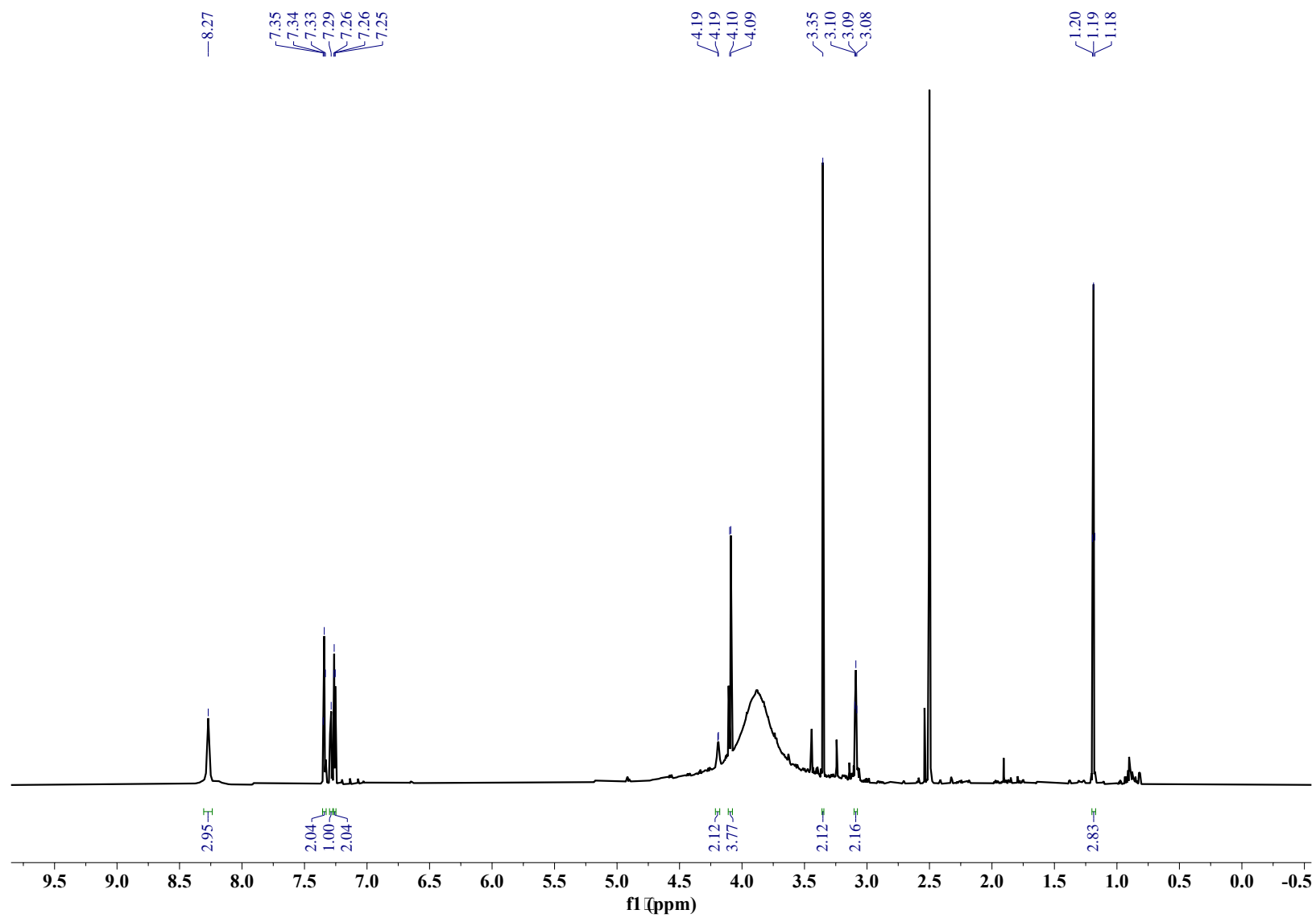


Figure S5. ¹H NMR spectrum of **20**.

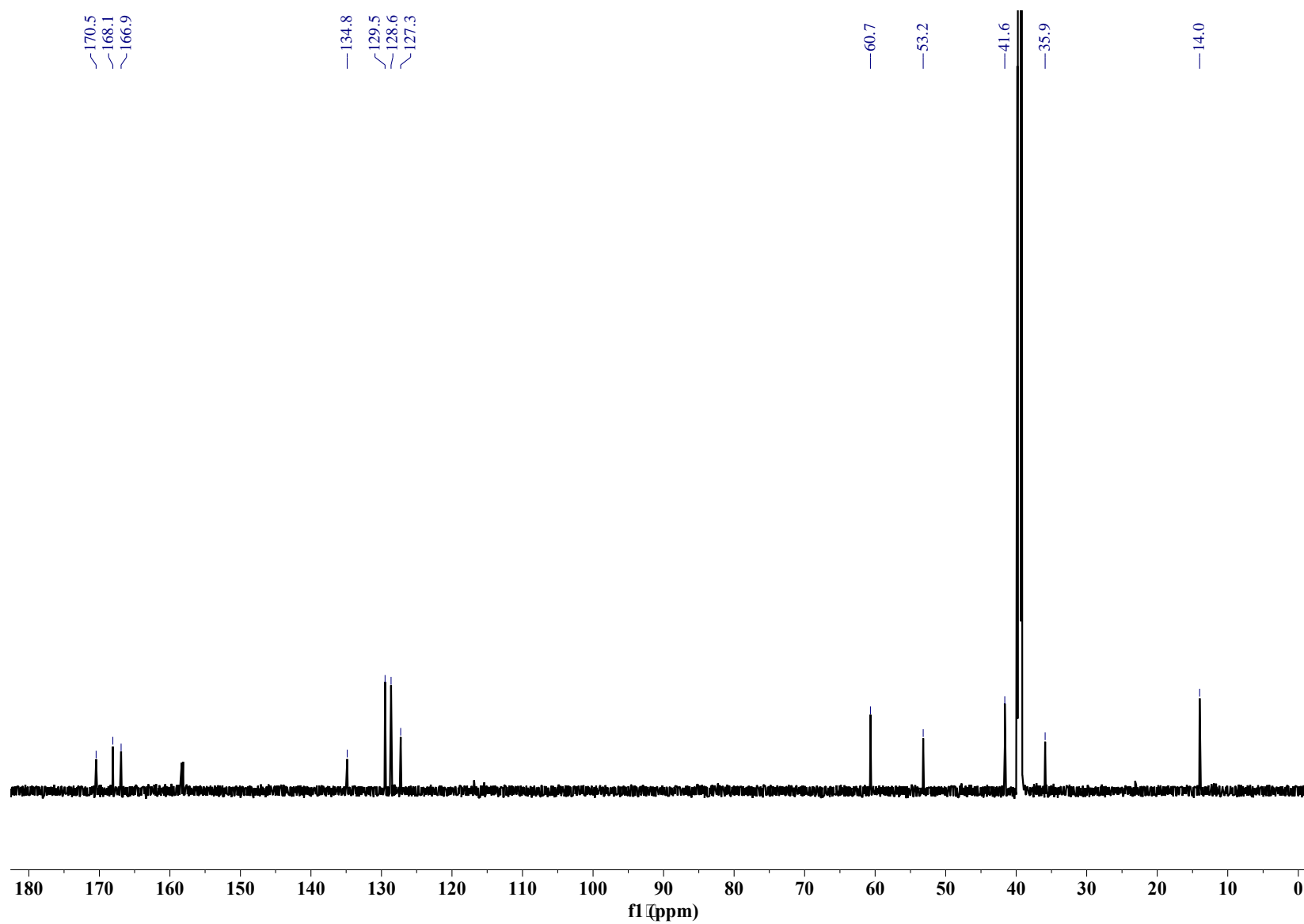


Figure S6. ^{13}C NMR spectrum of **20**

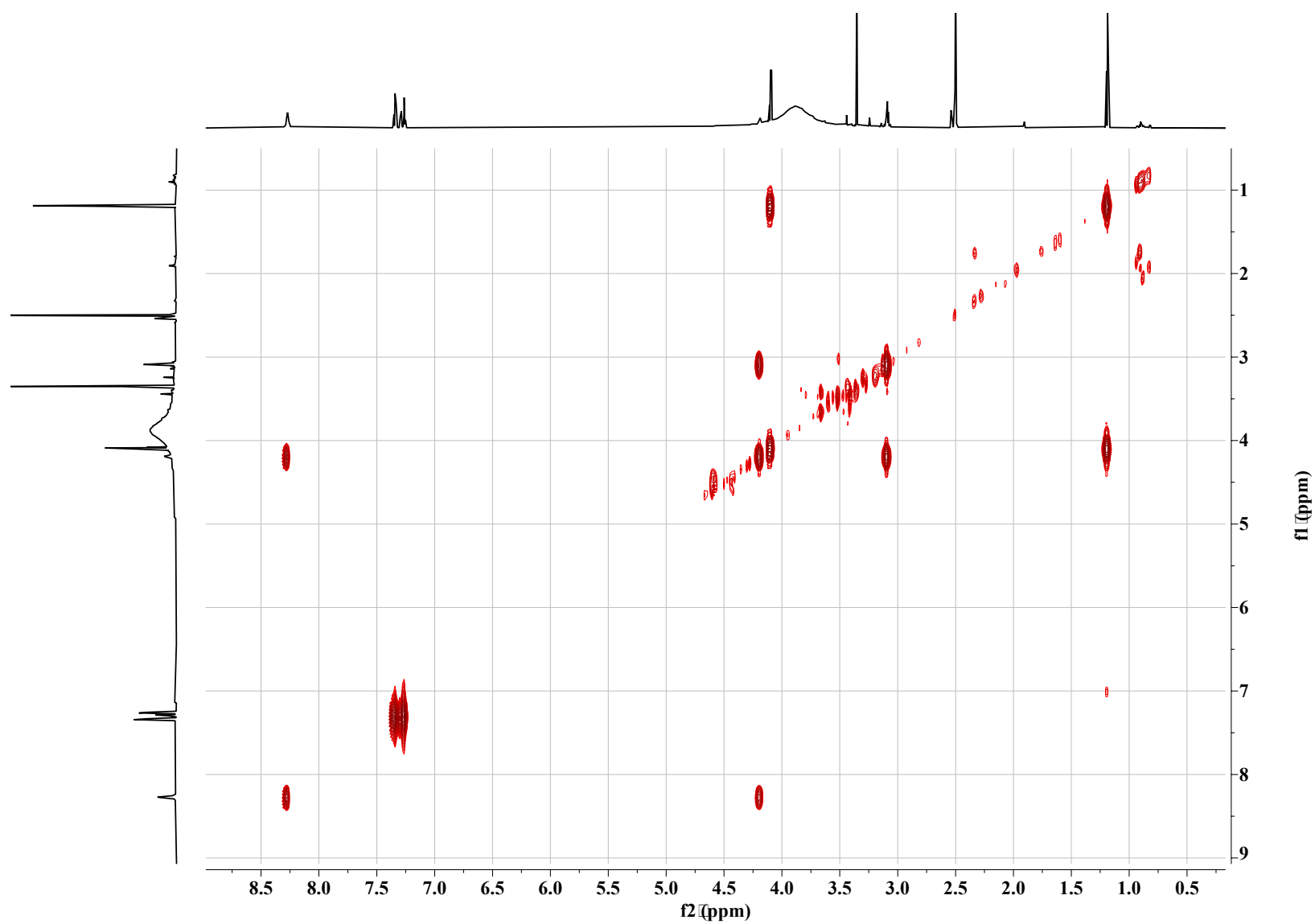


Figure S7. COSY NMR spectrum of **20**

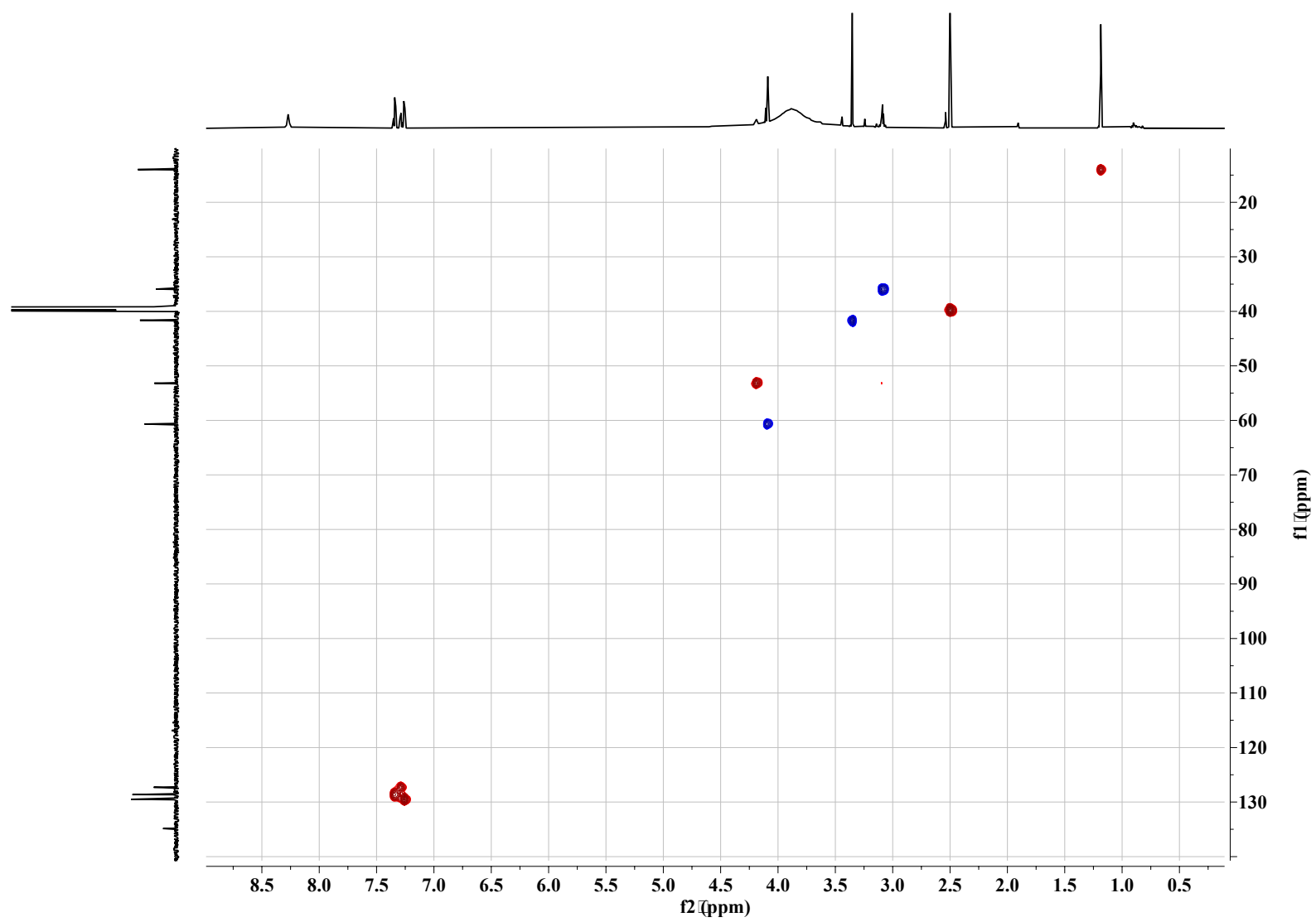


Figure S8. HSQC NMR spectrum of **20**

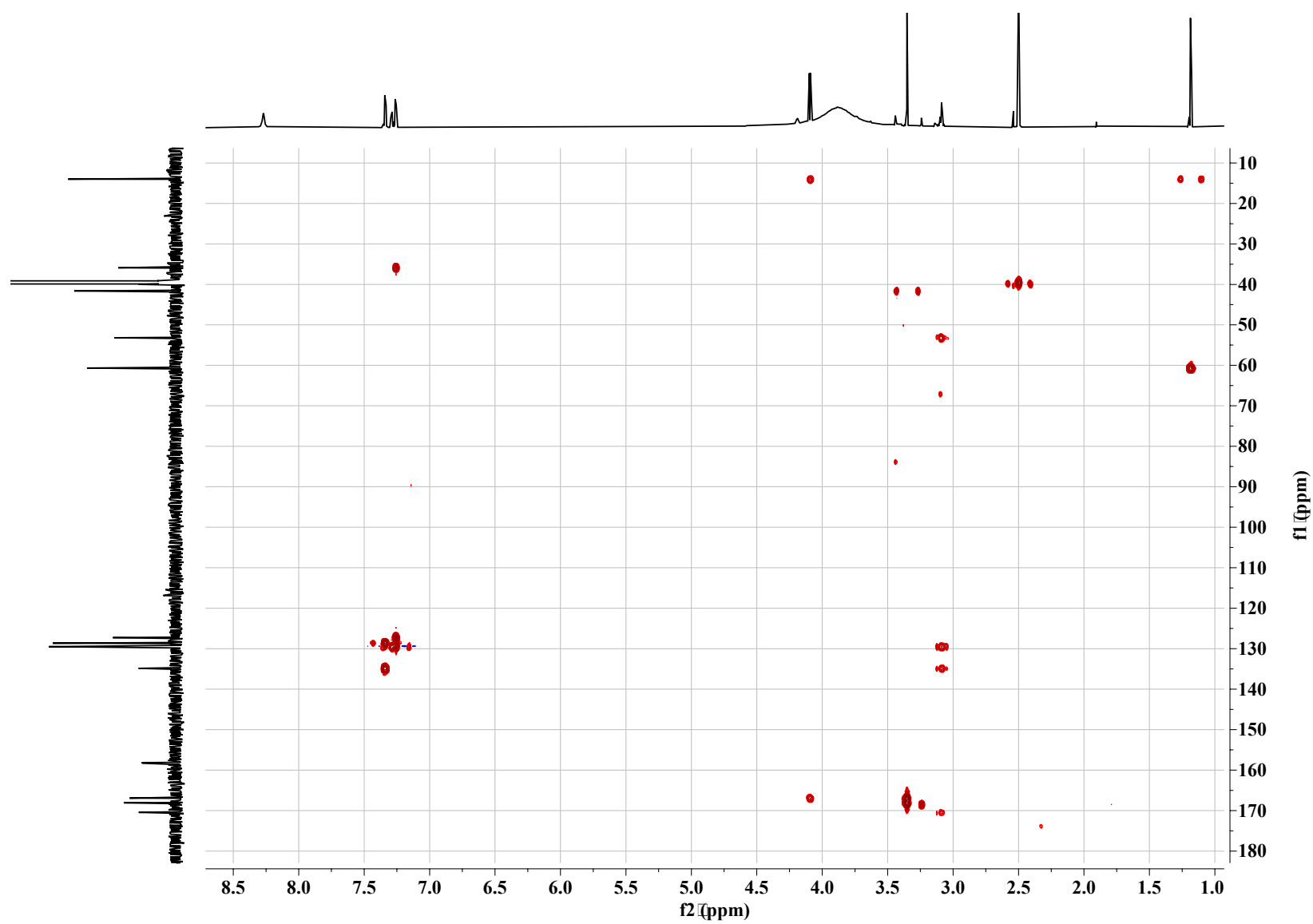


Figure S9. HMBC NMR spectrum of **20**

Table S1. Chemical diversity scores PC1 – PC8 for fragments 1 – 29 predicted by ChemGPS-NP

Fragments	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8
1	-2.150124	-1.28709	-0.651986	-0.304733	0.340312	0.204419	0.206539	-0.447454
2	-1.860493	0.896436	-0.565803	0.043809	0.569	-0.0617	0.219748	-0.380994
3	-1.459496	0.751982	-1.149619	-0.025329	0.417833	-0.100937	0.227197	-0.235763
4	-3.770376	2.782328	-0.597432	-0.034644	0.970668	0.203923	-0.272828	1.075707
5	-1.876056	3.182317	-0.642445	-0.360838	0.18282	0.308813	0.049806	-0.128127
6	-1.46761	3.218243	-1.141665	-0.379234	0.03008	0.206119	-0.011753	-0.546892
7	-1.68052	2.73256	0.13361	-0.291607	0.273609	0.102723	0.022945	0.138922
8	-1.340306	0.612659	-2.043614	0.046394	0.82841	0.418726	-0.498667	1.410431
9	-3.232833	-1.113922	-0.962454	-1.104781	-0.033566	0.616494	-0.149273	-0.368984
10	-1.669696	1.589626	-0.215517	-0.262092	1.005539	0.798158	-0.166931	0.510817
11	-3.36614	2.604083	-1.120641	-0.000008	0.680858	0.190406	-0.27119	1.081211
12	-3.101163	2.982375	-1.279064	-0.282328	0.606725	0.512638	-0.765777	0.280198
13	-1.358721	4.095818	-0.555538	-0.638868	0.128392	1.054567	-0.108945	0.570617
14	-0.927505	4.037337	-0.640855	-0.48617	0.072844	1.164936	0.273738	0.389587
15	-1.716733	0.932441	-1.76997	-0.342898	0.25125	0.721216	0.118128	-0.035312
16	-3.663007	1.671019	-0.958124	-0.226487	0.835319	0.990455	0.059215	0.364241
17	-1.405149	0.649834	-1.678473	0.703728	0.790487	-0.795198	0.100875	-0.114284
18	-2.116181	1.093981	-1.101308	-0.265951	0.387556	0.758768	0.07773	-0.219955
19	-2.595757	1.13588	-1.674768	0.449238	0.503952	-0.647507	-0.023841	0.055944
20	-1.683061	0.404238	-0.654629	1.209954	0.723496	-1.56396	0.409826	0.349757
21	-1.915636	3.013092	-0.528402	-0.558598	0.128689	0.159971	-0.338905	-0.078911
22	-1.459574	2.910621	-0.571865	-0.207914	0.114283	0.020804	0.080236	-0.188827
23	-1.343498	2.435074	-0.09873	-0.495413	0.015196	-0.447184	-0.743592	-0.096262
24	-1.860057	2.869591	-0.091964	-0.181447	0.26415	0.116877	0.133258	0.223543
25	-1.559577	2.482695	0.056169	-0.631531	-0.131458	0.158617	-0.435855	0.286196
26	-1.917554	2.527714	0.526191	-0.738009	0.317687	1.046427	0.405827	0.283791
27	-1.77818	3.668818	0.663293	-0.635074	0.338621	0.915263	0.114424	0.699087
28	-1.969033	0.916955	0.827527	-0.93947	0.164447	1.097695	0.253892	-0.244043
29	-1.823761	2.031206	0.95448	-0.866523	0.21517	0.935115	-0.032151	0.17312