

Supplementary Material

Alkaloids from a Hawaiian fungal strain *Aspergillus felis* FM324

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Cartesian coordinates of all compounds under study

Figure S1. HRESIMS spectrum of compound **1**

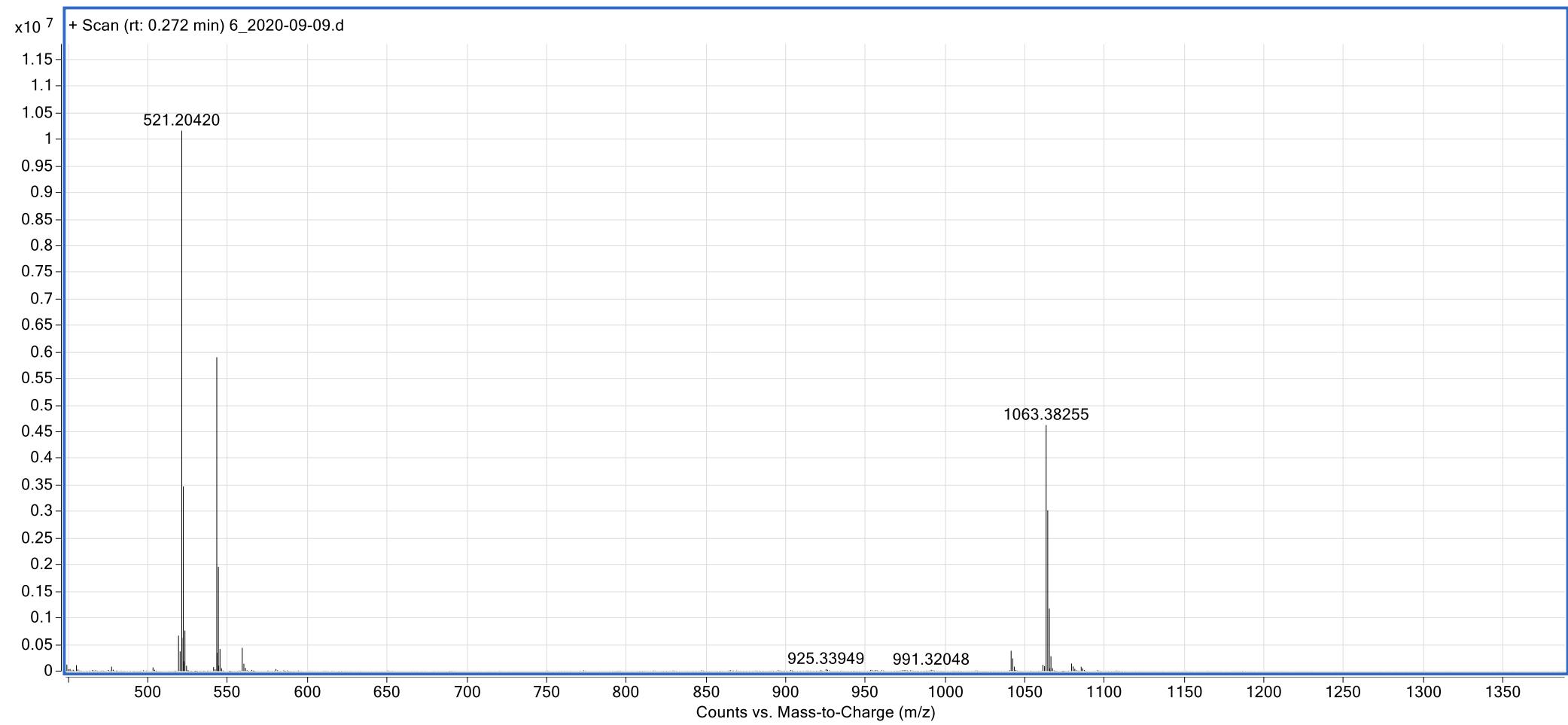


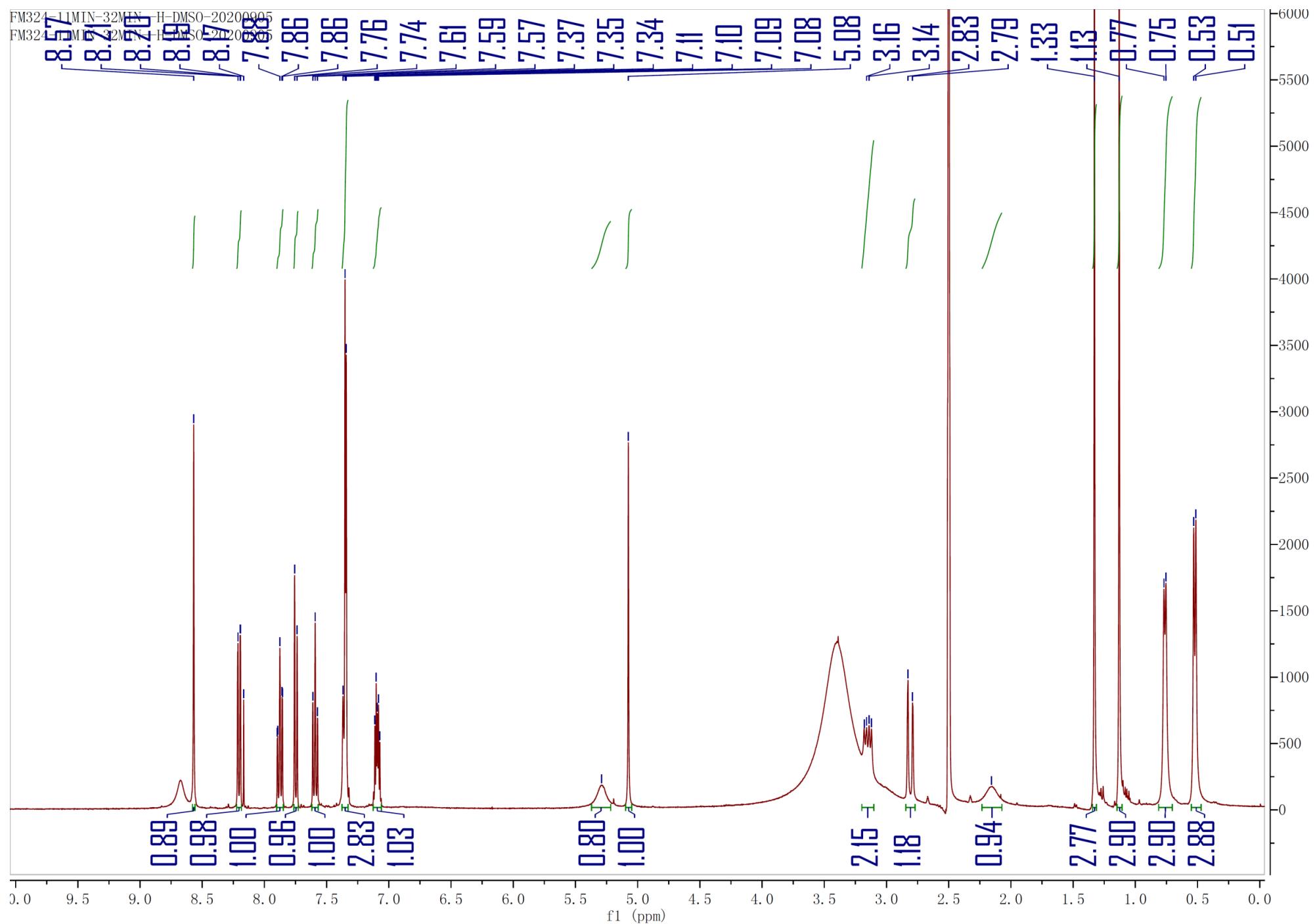
Figure S2. The ^1H -NMR spectrum of compound **1** in $\text{DMSO}-d_6$ 

Figure S3. ^{13}C -NMR spectrum of compound **1** in $\text{DMSO}-d_6$

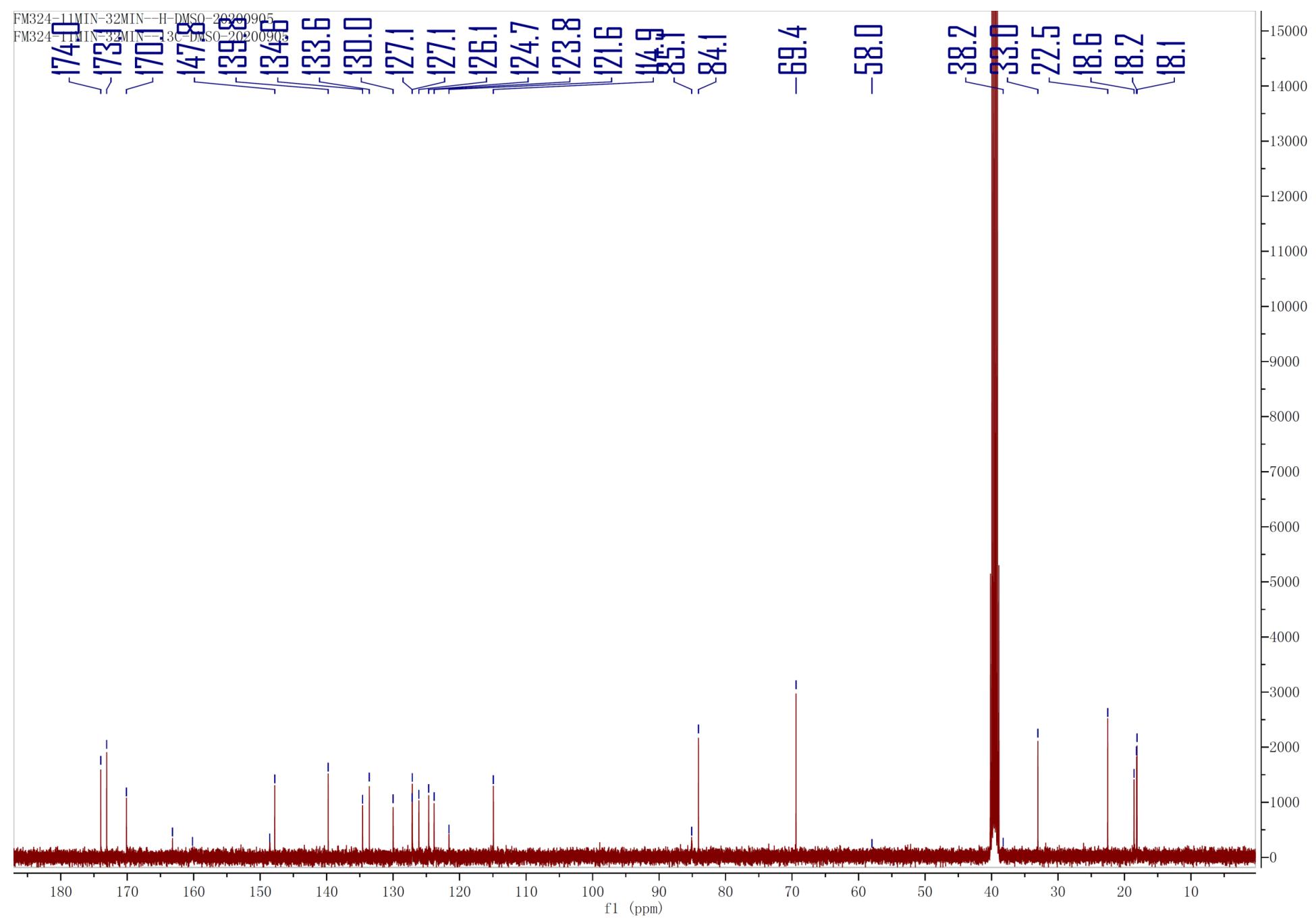


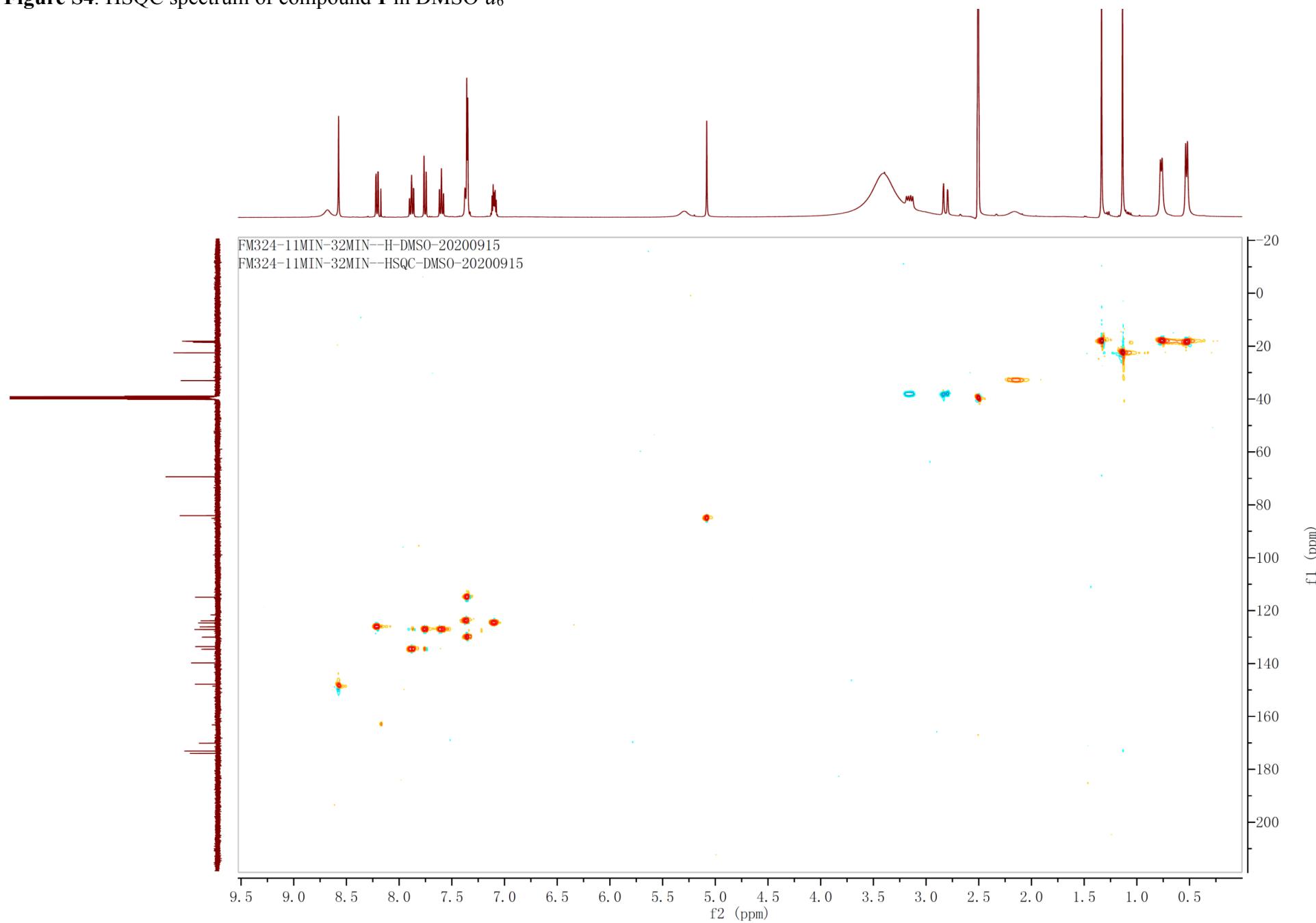
Figure S4. HSQC spectrum of compound **1** in DMSO-*d*₆

Figure S5. COSY spectrum of compound **1** in DMSO-*d*₆

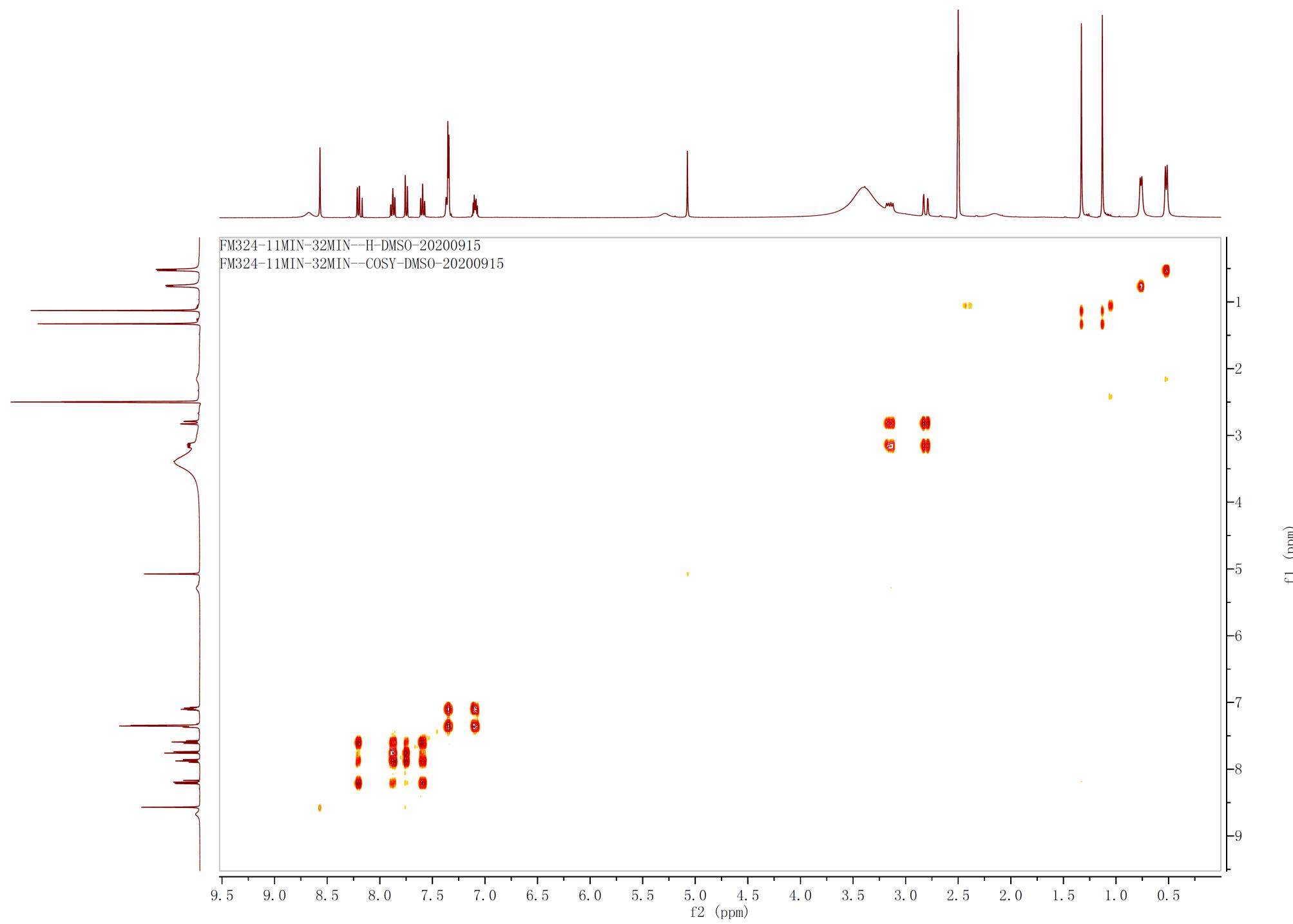


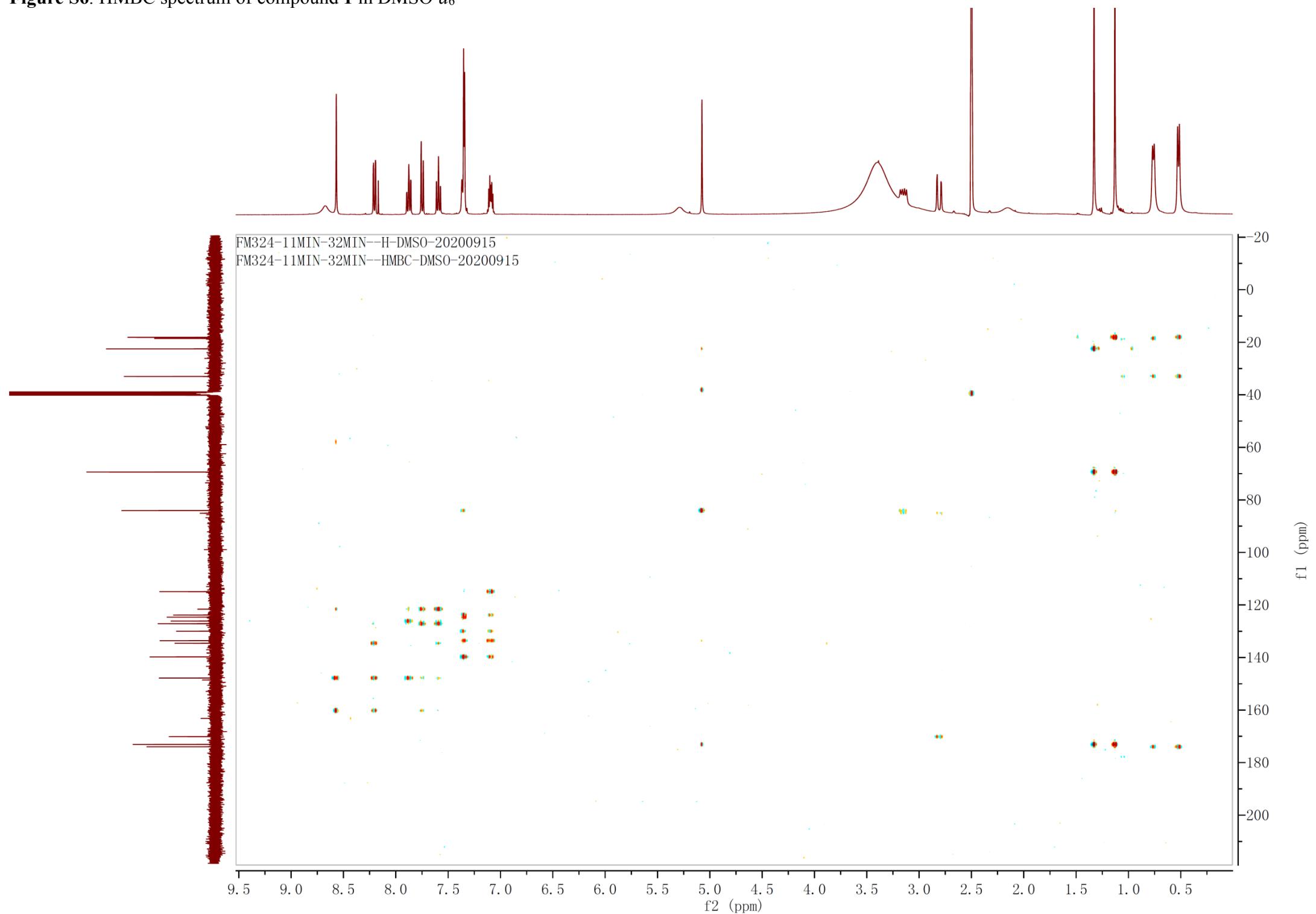
Figure S6. HMBC spectrum of compound **1** in DMSO-*d*₆

Figure S7. ROESY spectrum of compound **1** in $\text{DMSO}-d_6$

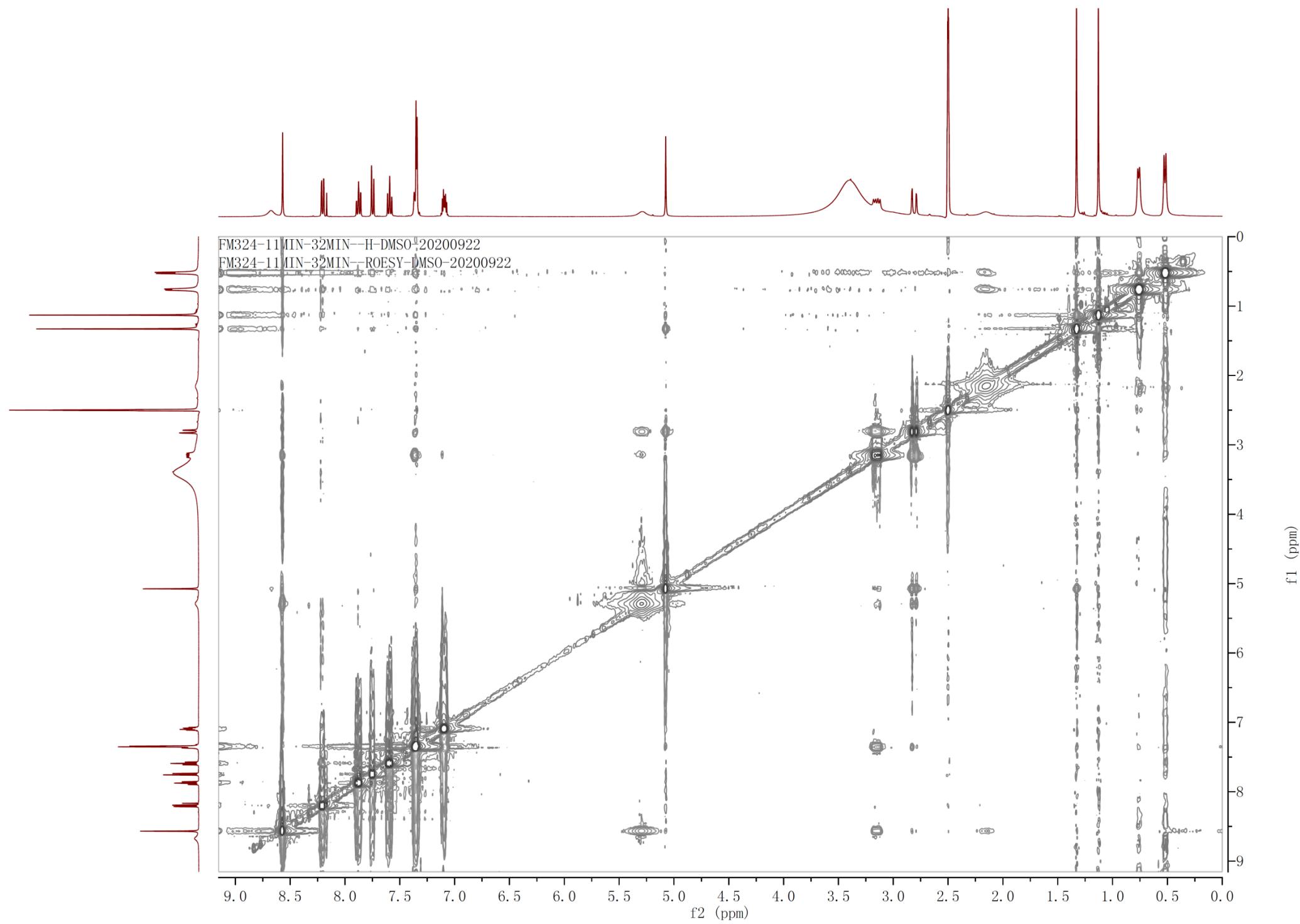


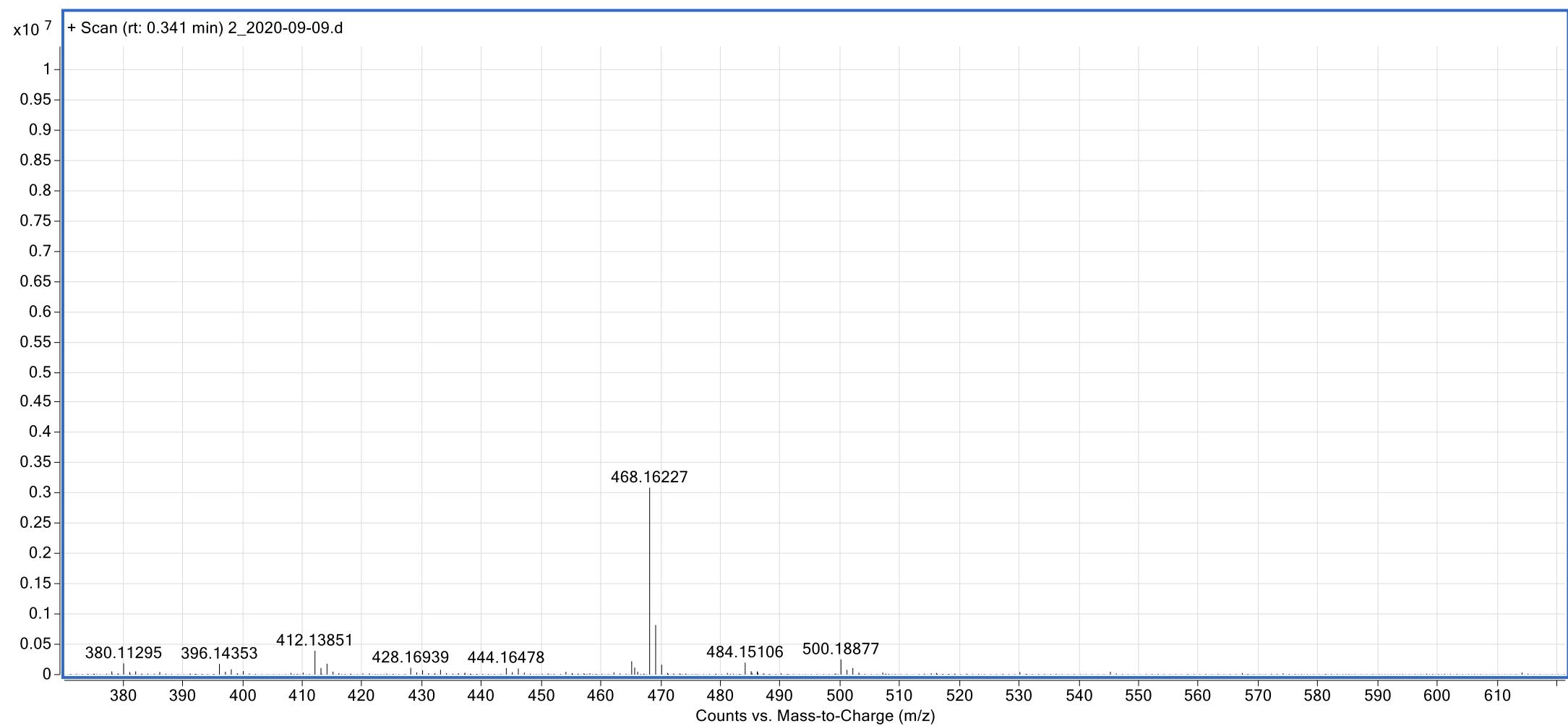
Figure S8. HRESIMS spectrum of compound 2

Figure S9. ^1H -NMR spectrum of compound **2** in $\text{DMSO}-d_6$

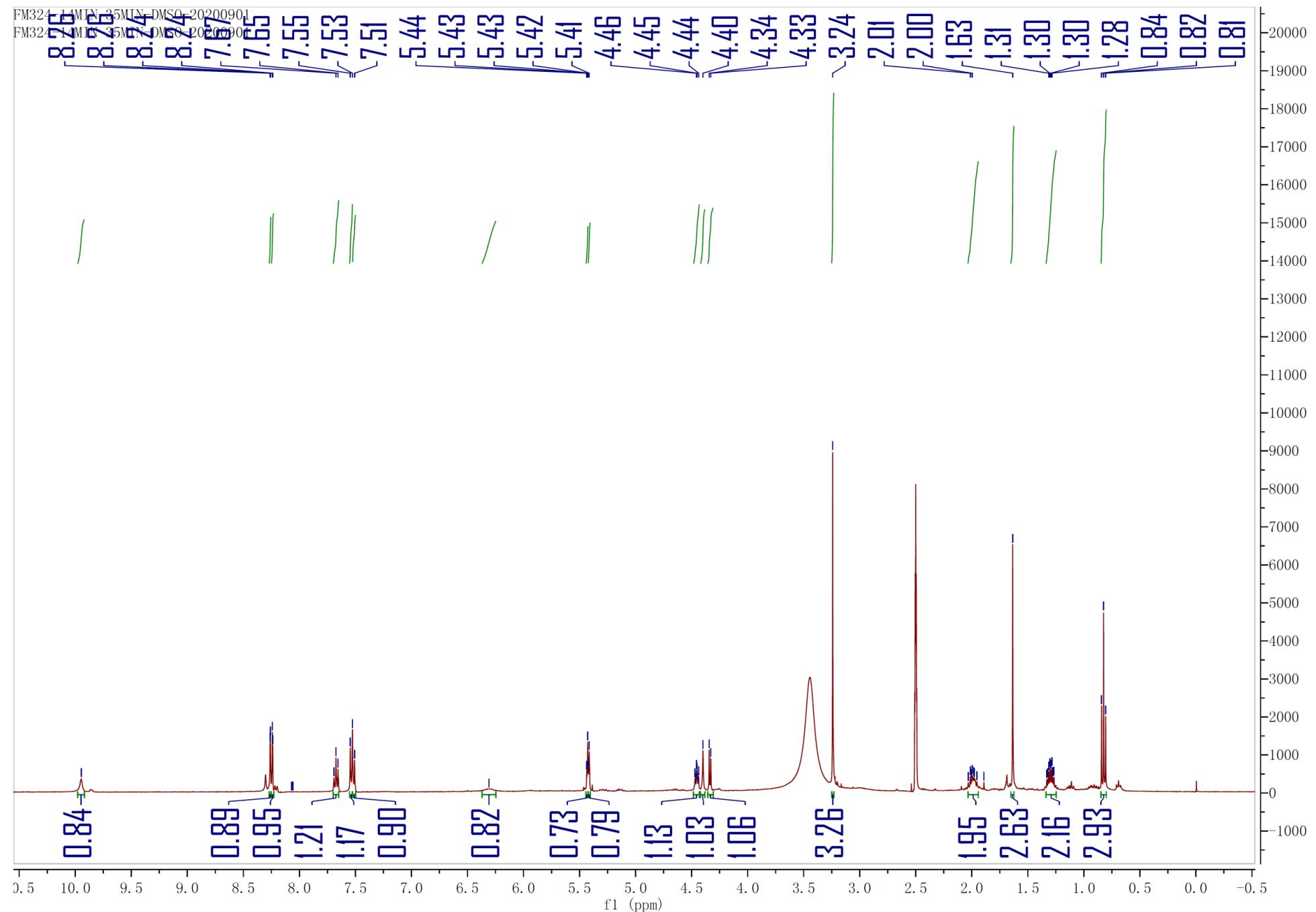


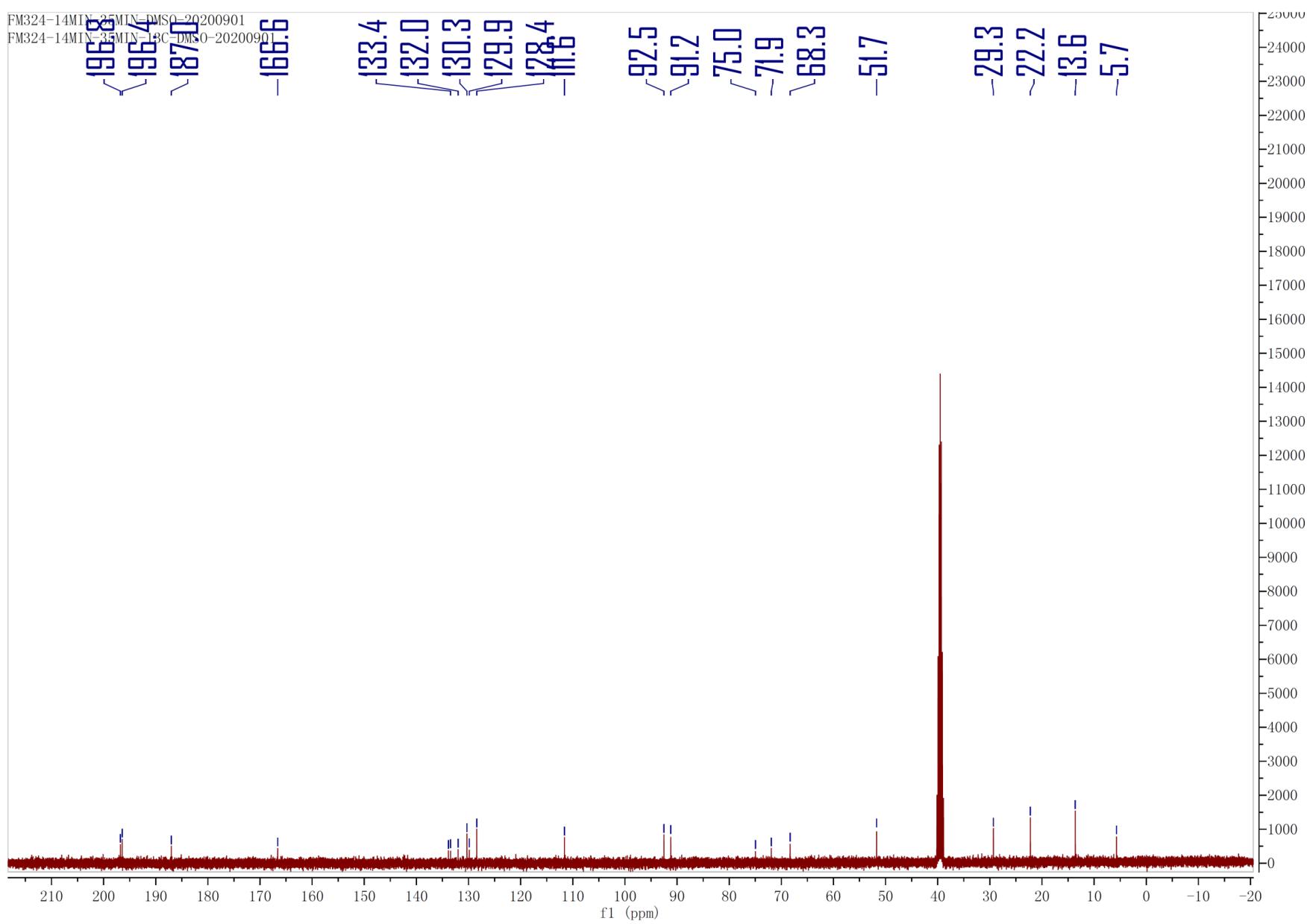
Figure S10. ^{13}C -NMR spectrum of compound **2** in $\text{DMSO}-d_6$ 

Figure S11. HSQC spectrum of compound **2** in DMSO-*d*₆

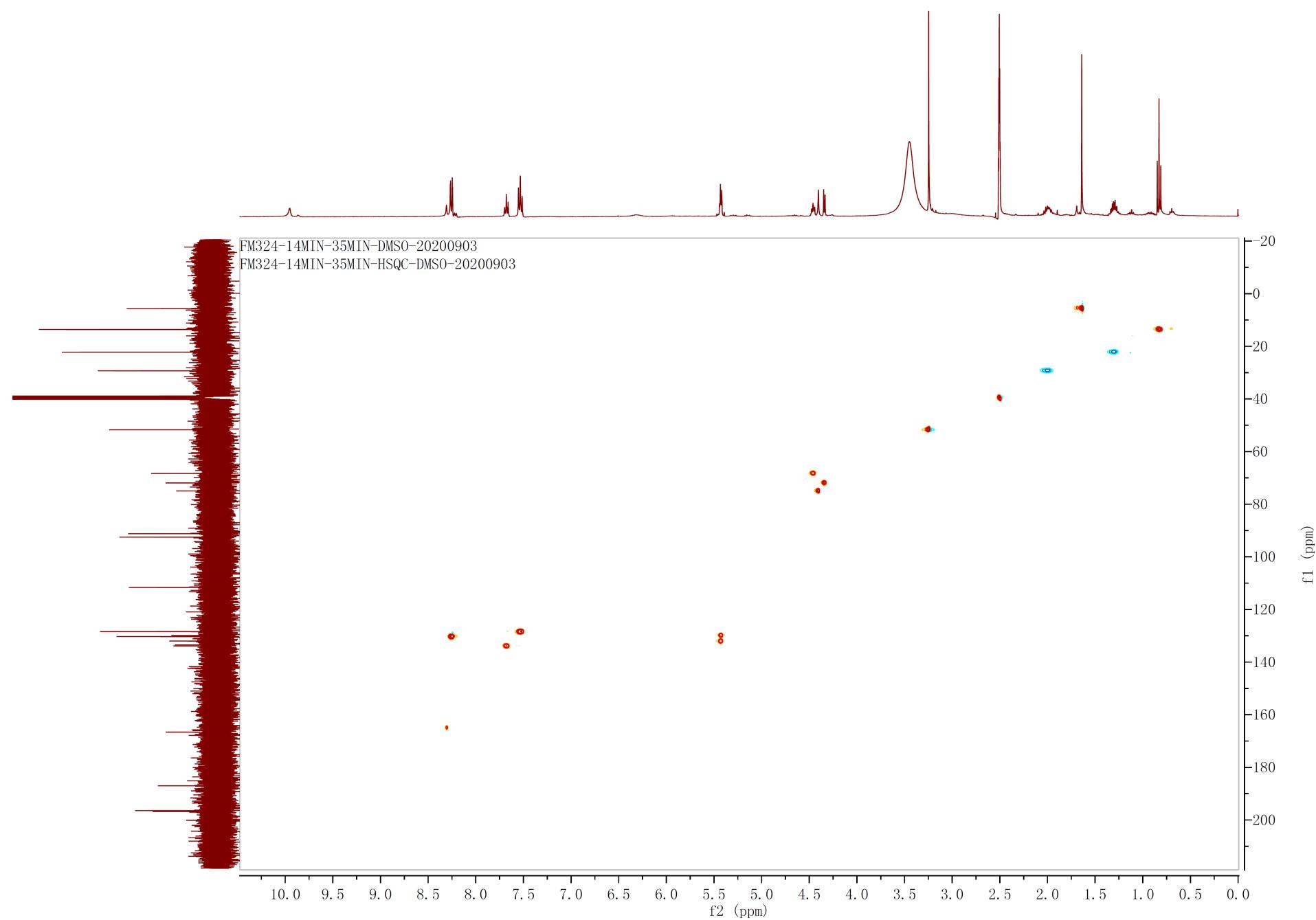


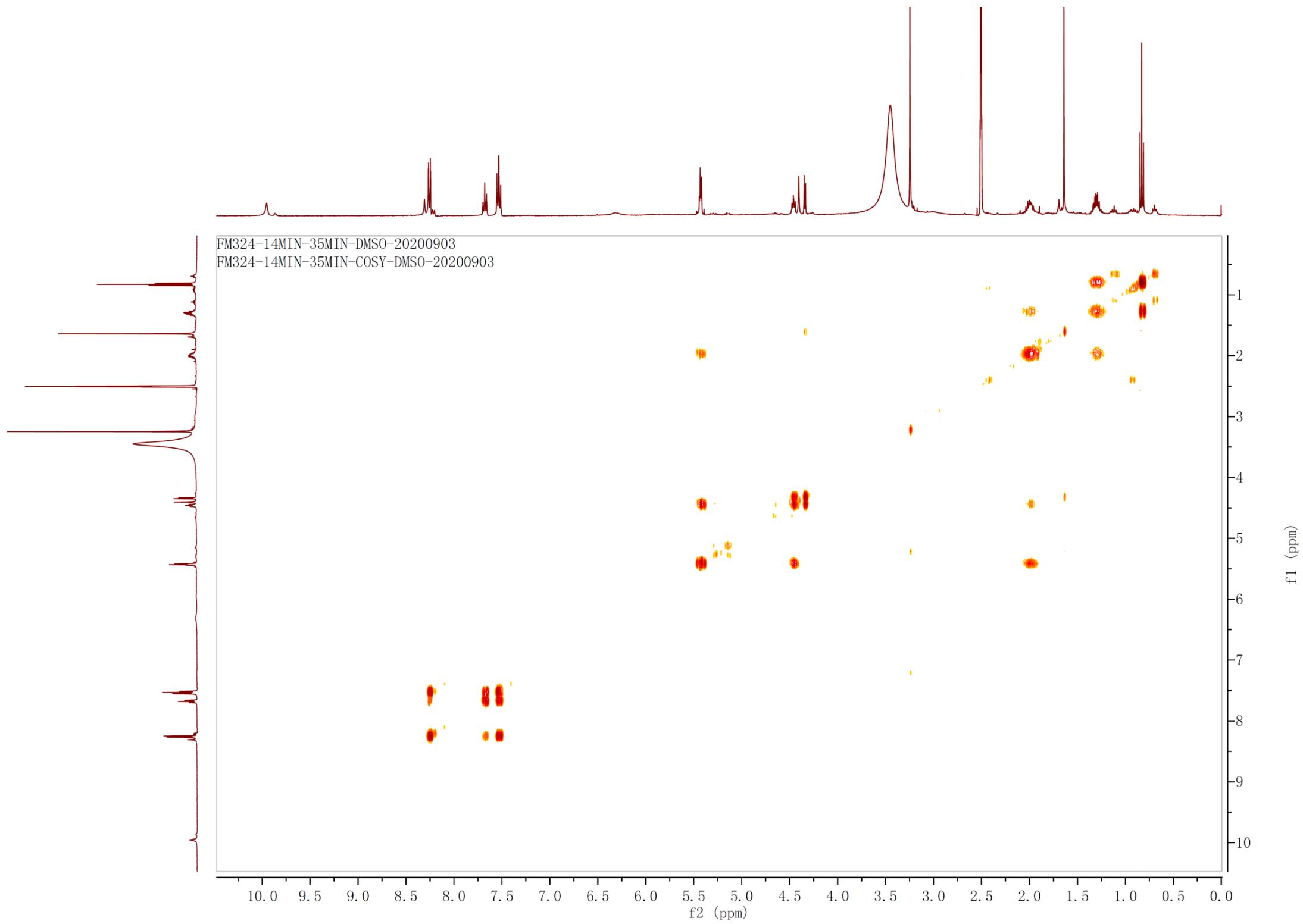
Figure S12. COSY spectrum of compound **2** in DMSO-*d*₆

Figure S13. HMBC spectrum of compound **2** in DMSO-*d*₆

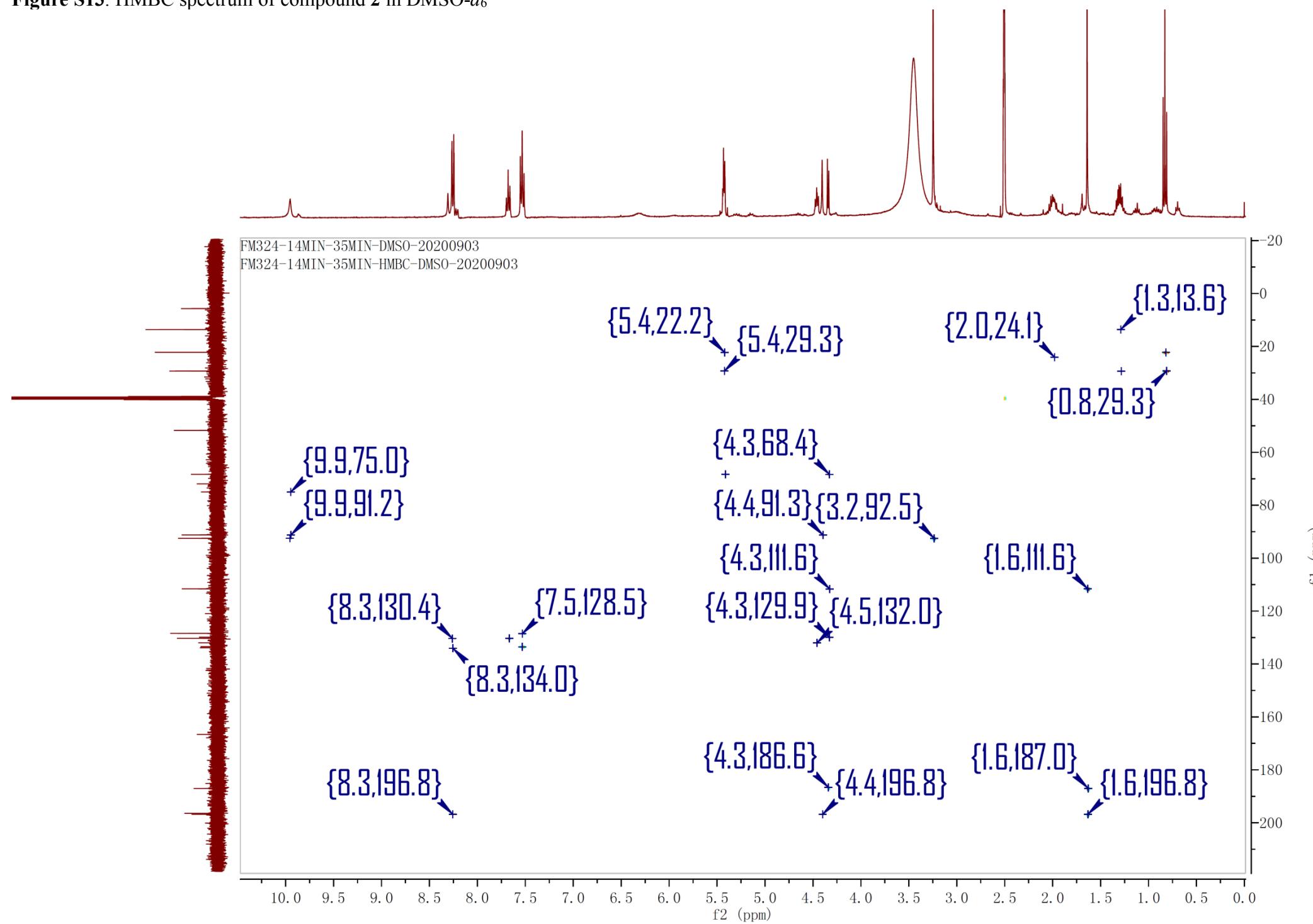


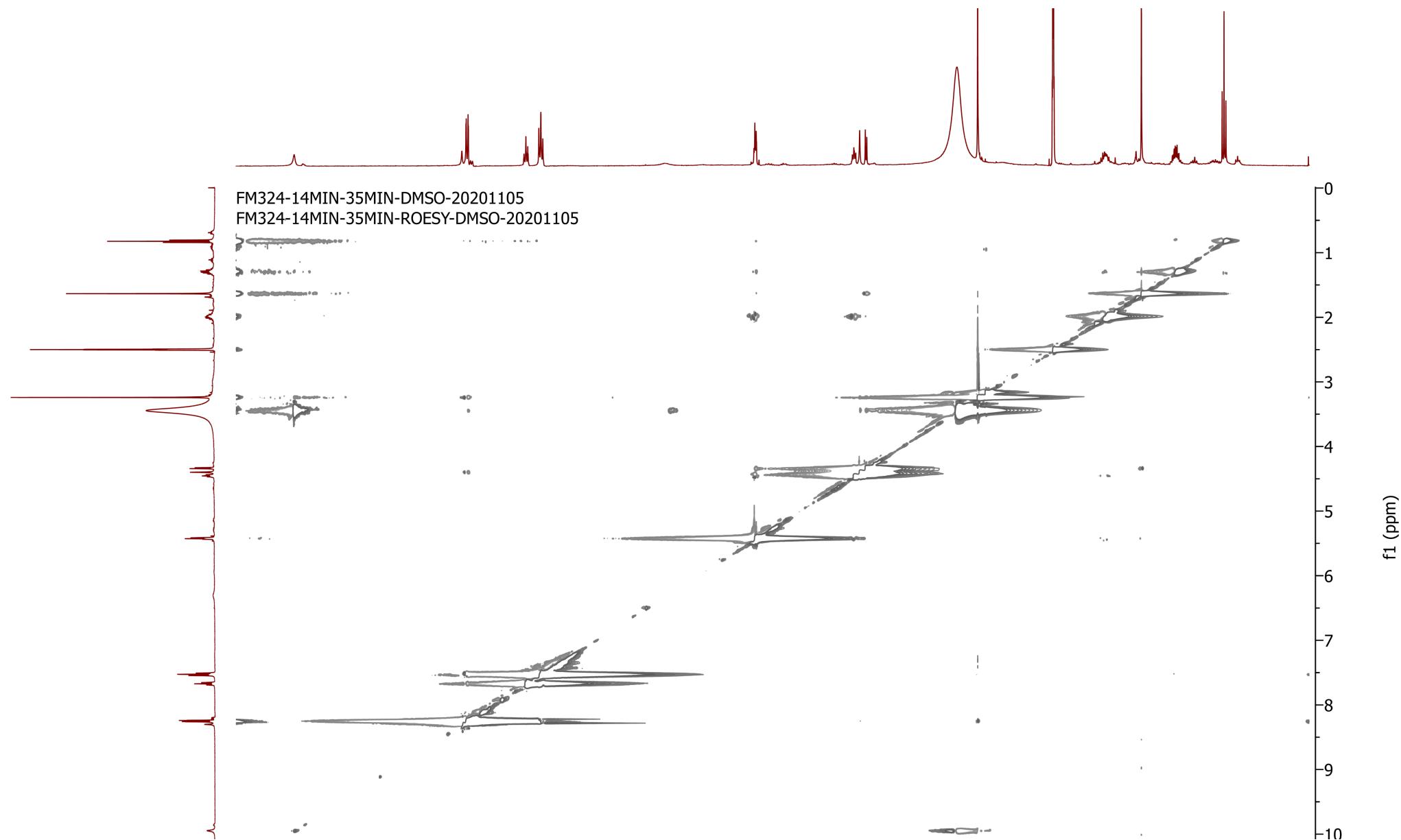
Figure S14. The ROESY spectrum of compound **2** in DMSO-*d*₆

Figure S15. Experimental ECD spectra of **2** and **8**

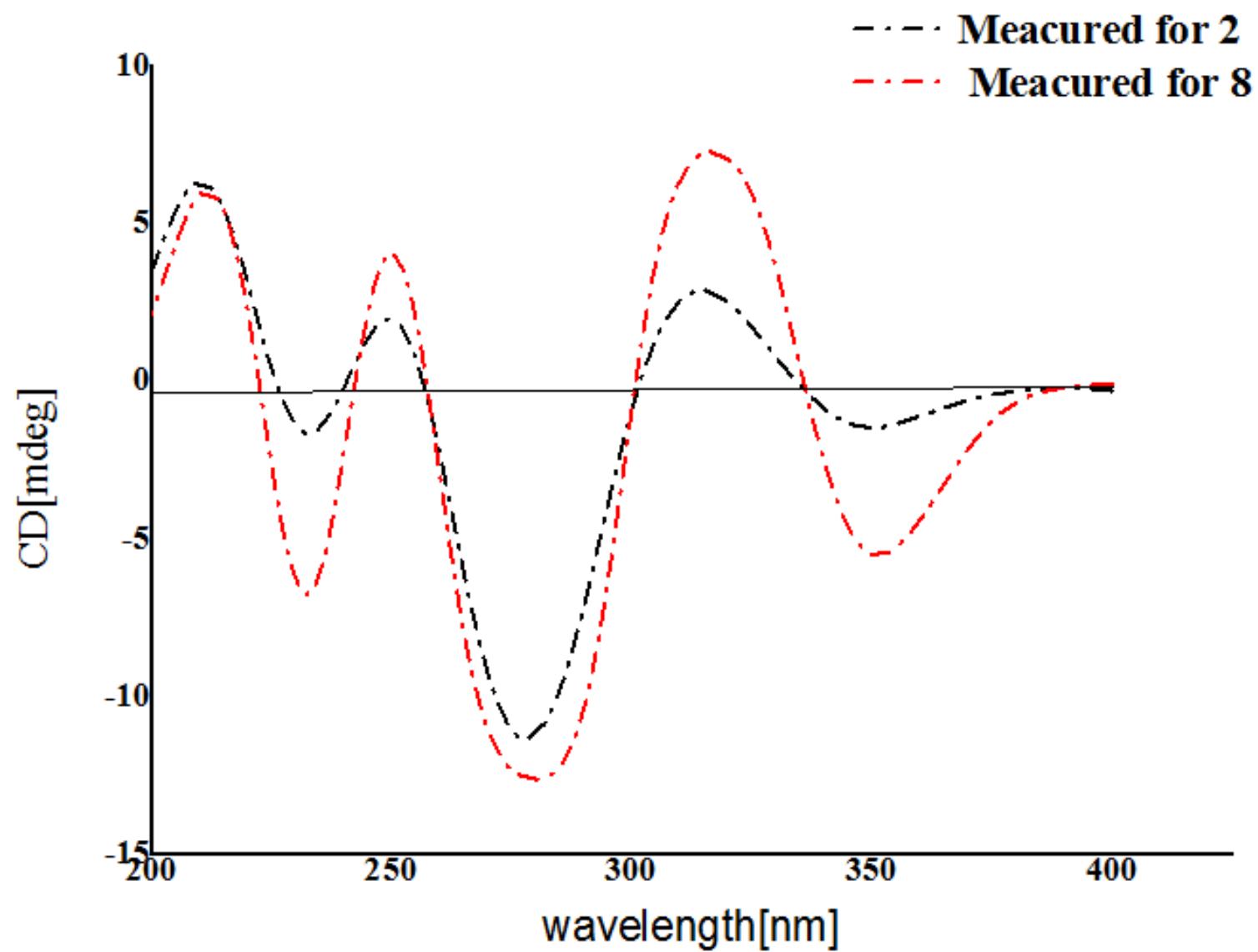


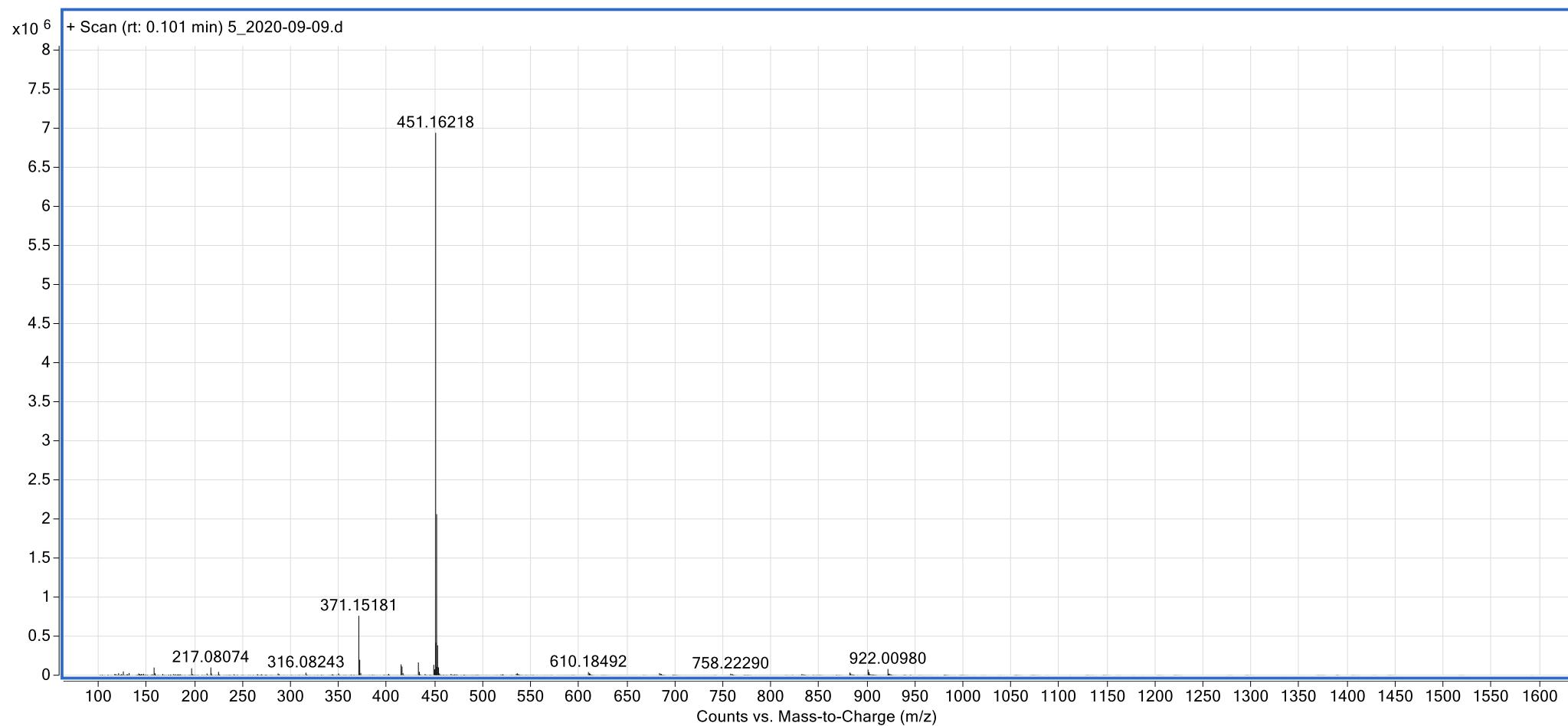
Figure S16. HRESIMS spectrum of compound 3

Figure S17. ^1H -NMR spectrum of compound **3** in $\text{DMSO}-d_6$

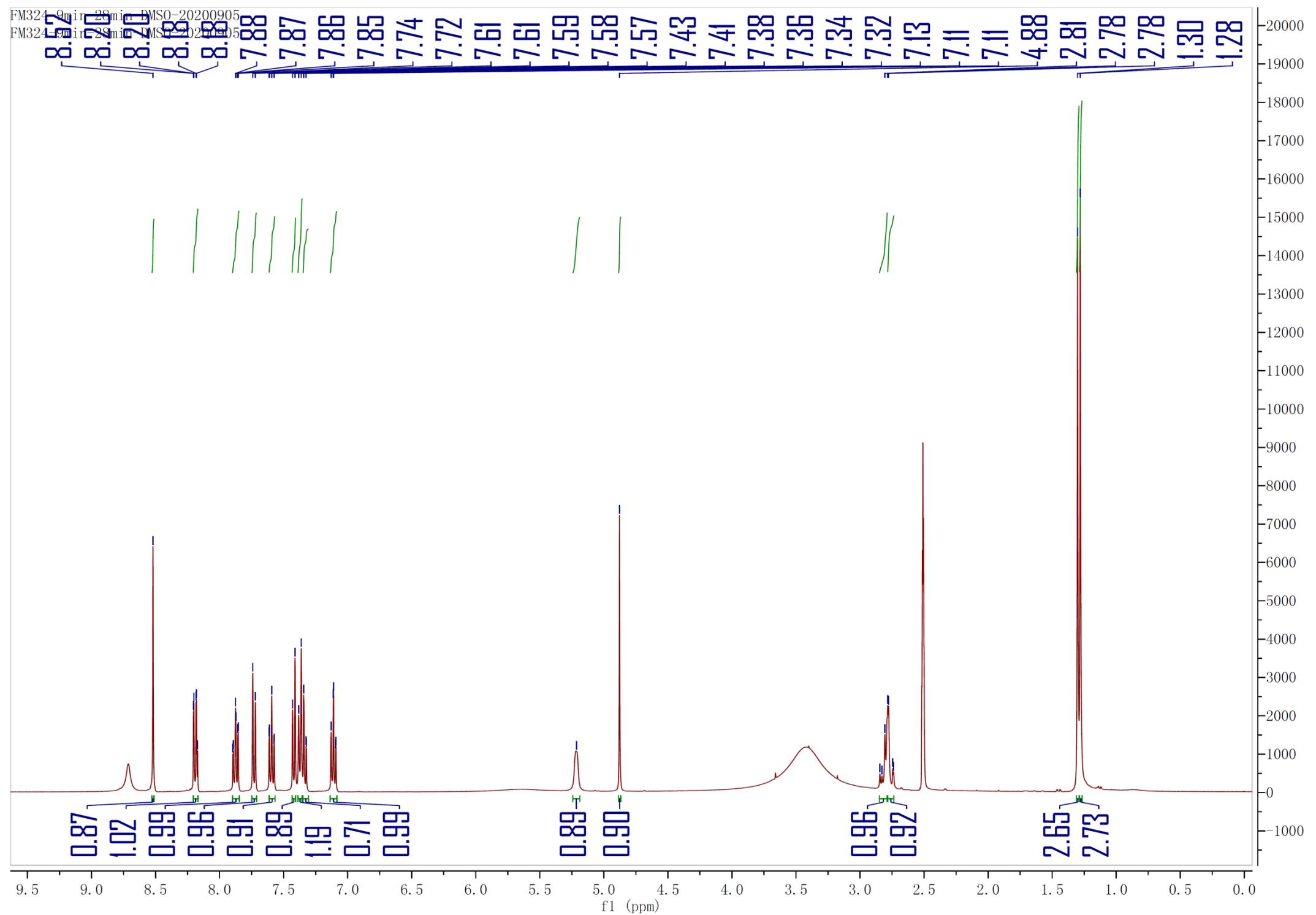


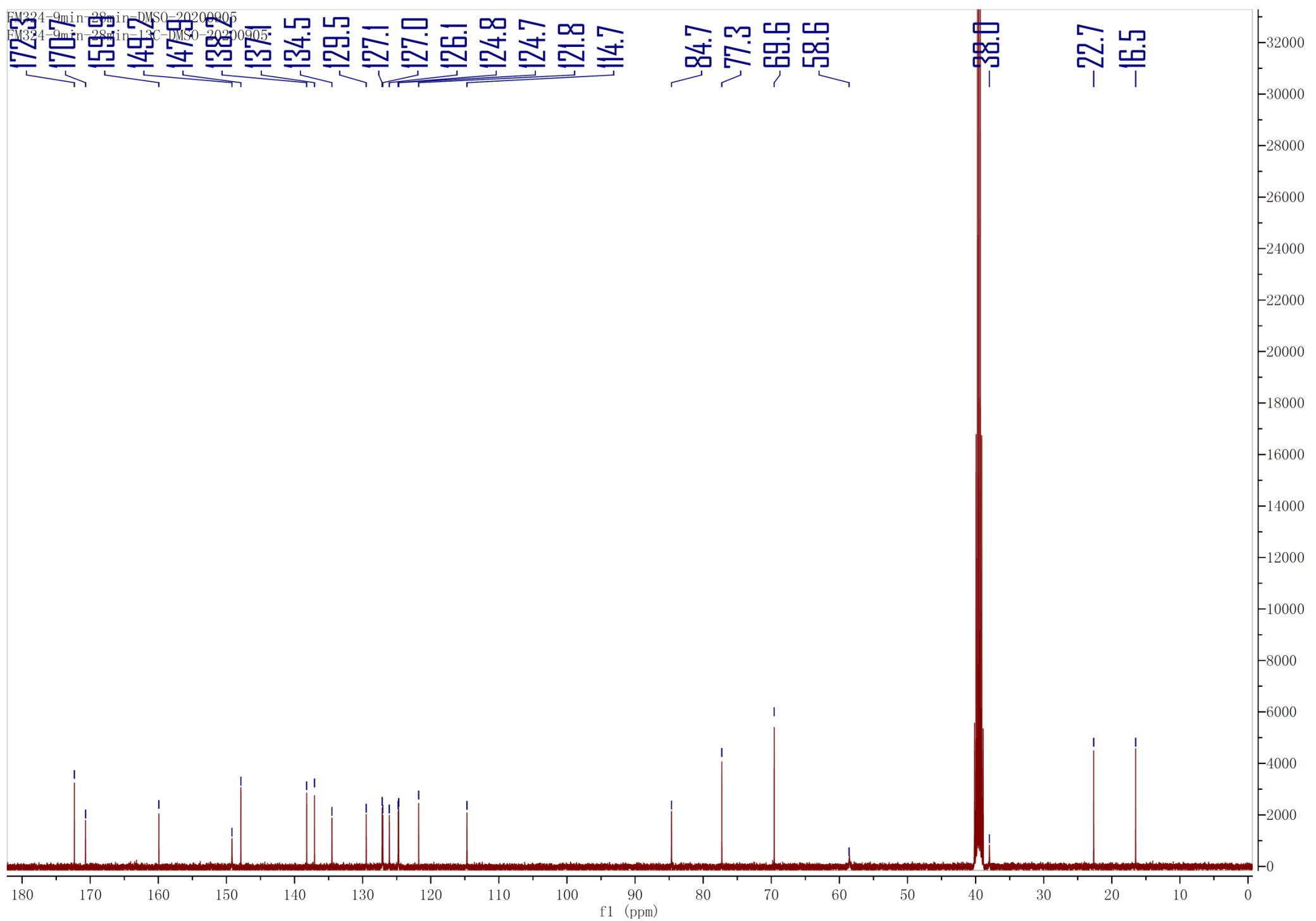
Figure S18. ^{13}C -NMR spectrum of compound 3 in $\text{DMSO}-d_6$ 

Figure S19. HSQC spectrum of compound **3** in DMSO-*d*₆

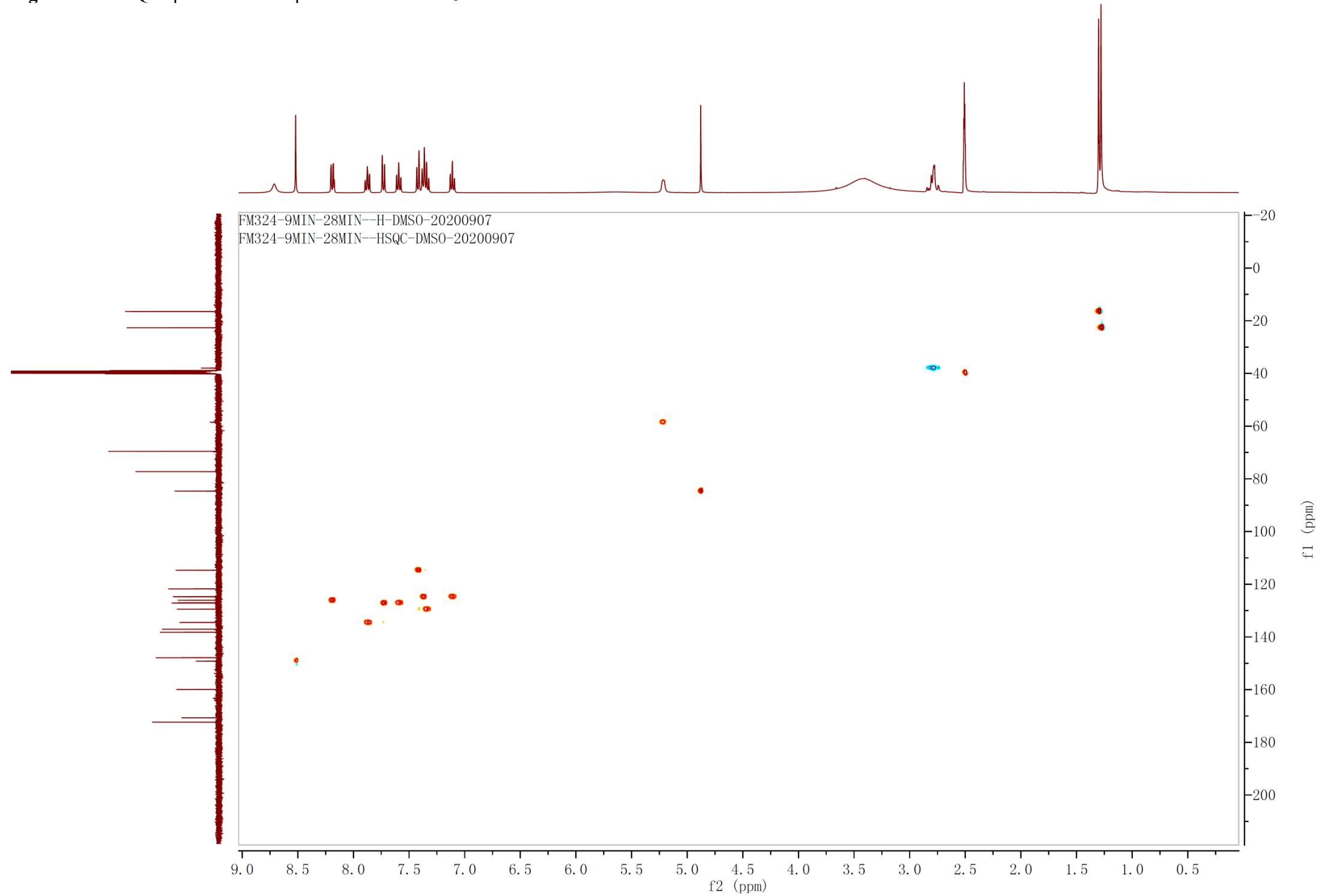


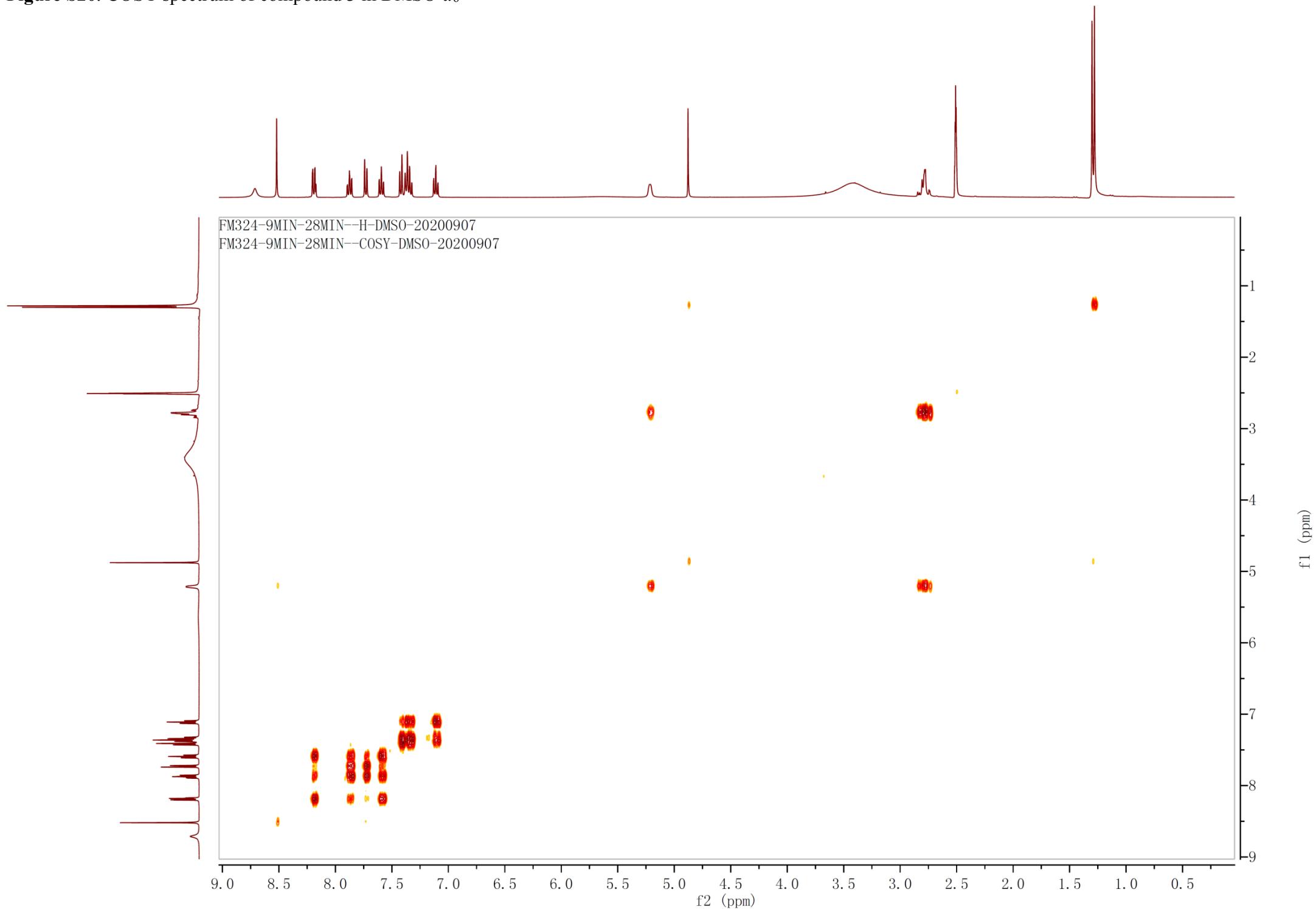
Figure S20. COSY spectrum of compound **3** in DMSO-*d*₆

Figure S21. HMBC spectrum of compound **3** in DMSO-*d*₆

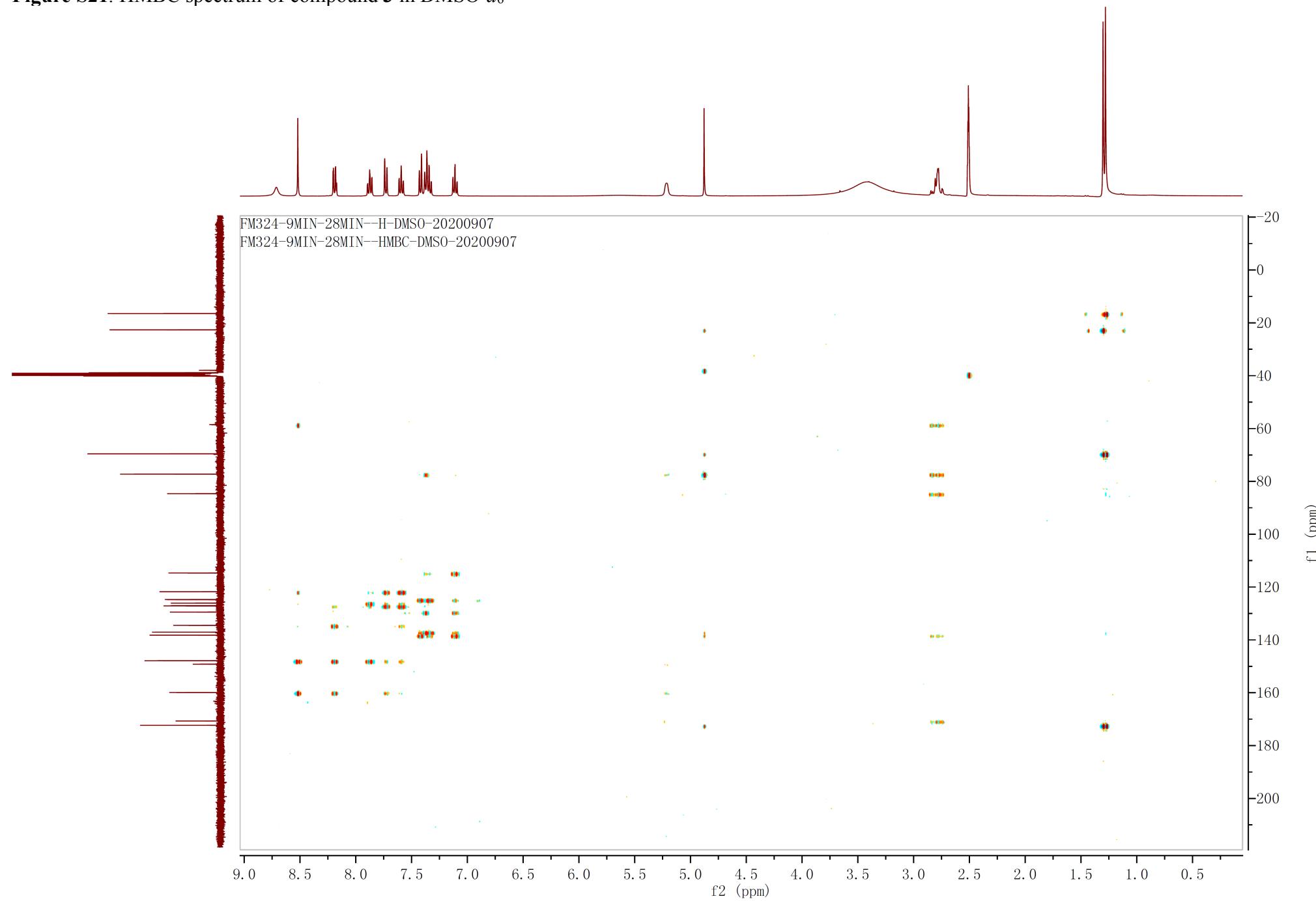
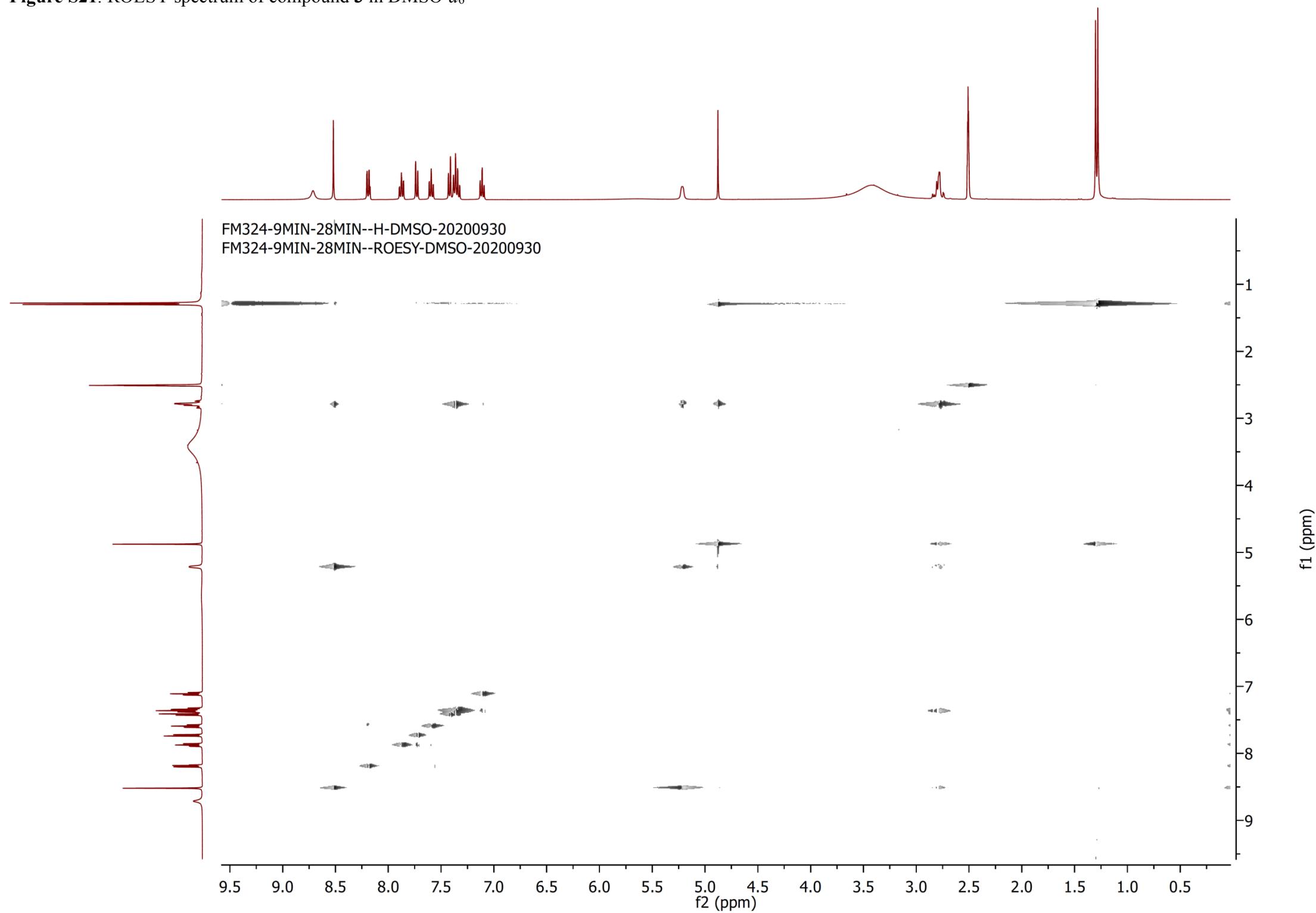


Figure S21. ROESY spectrum of compound **3** in DMSO-*d*₆

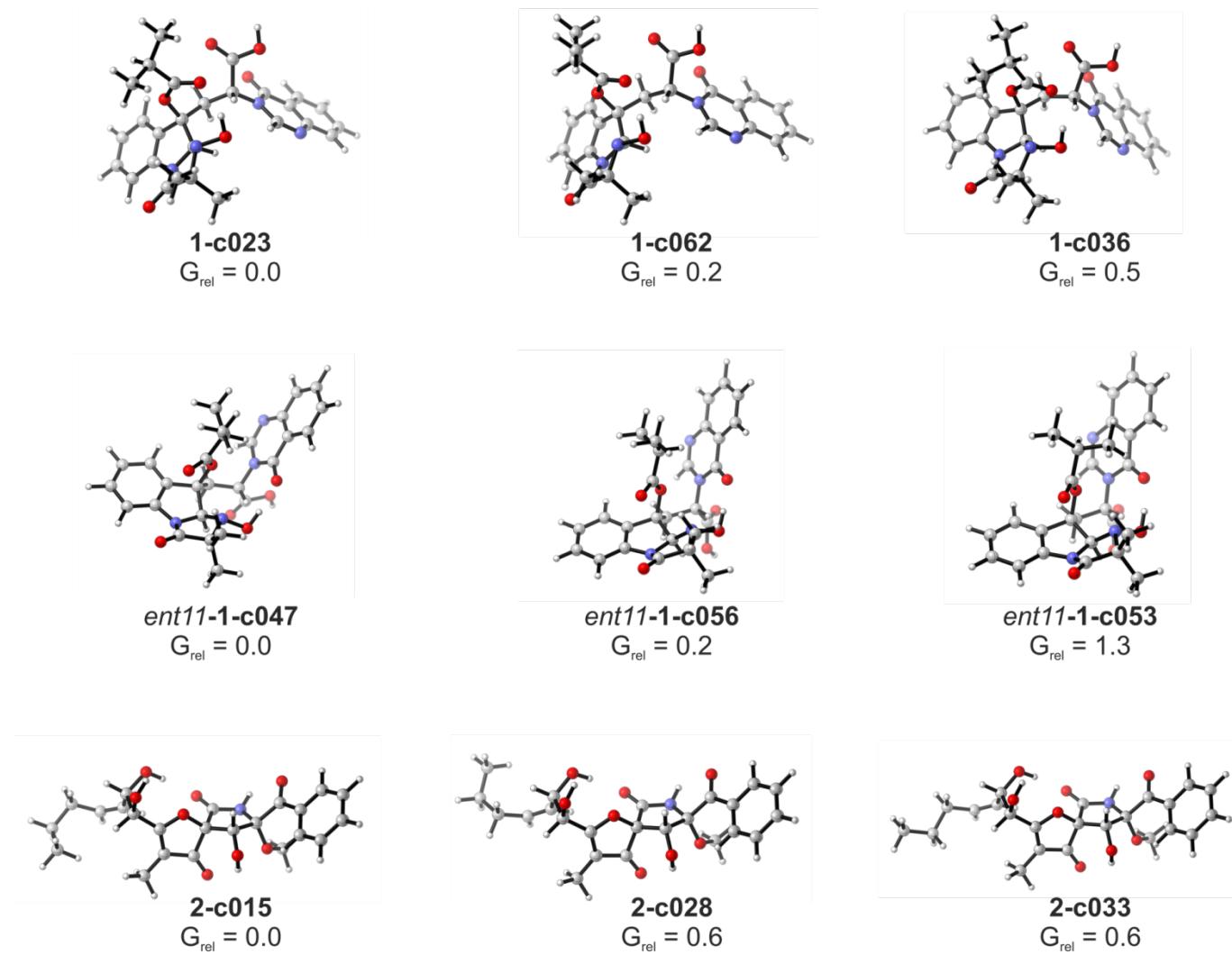


Figure S23. B3LYP/6-31G* optimized geometries of the most stable conformers found for **1**, *IIepi-1* and **2**, with relative Gibbs free energies (in kcal/mol) computed at the SMD/M06-2X/6-31G* level (solvent: methanol).

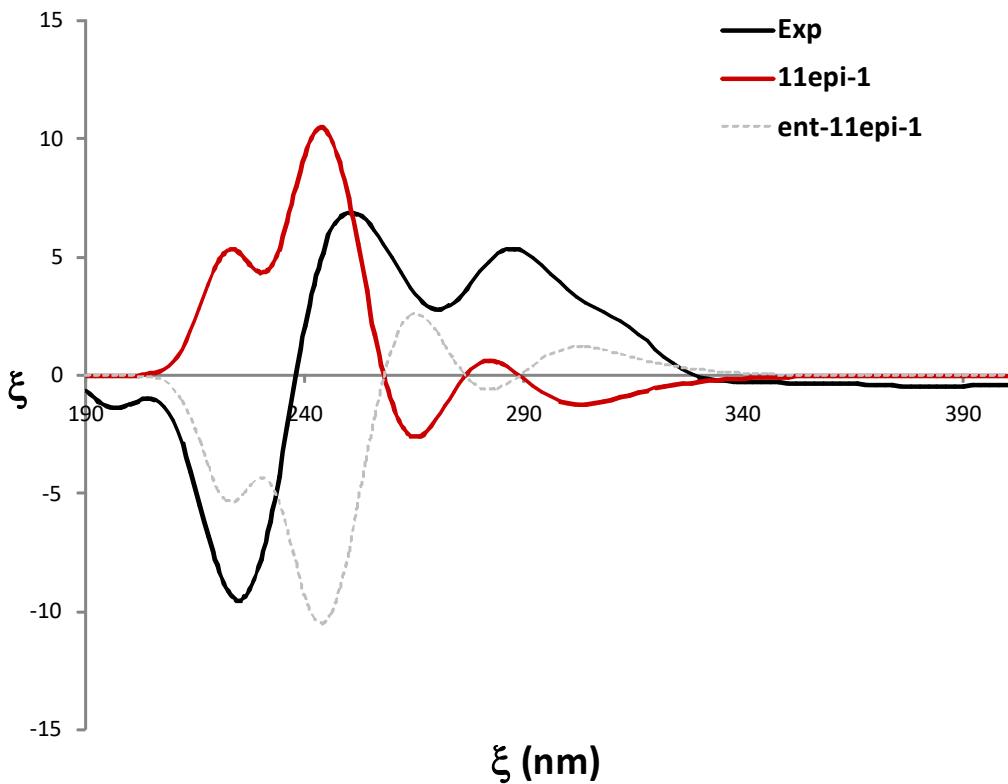


Figure S24. Experimental ECD of **1** and calculated ECD of *11epi-1*

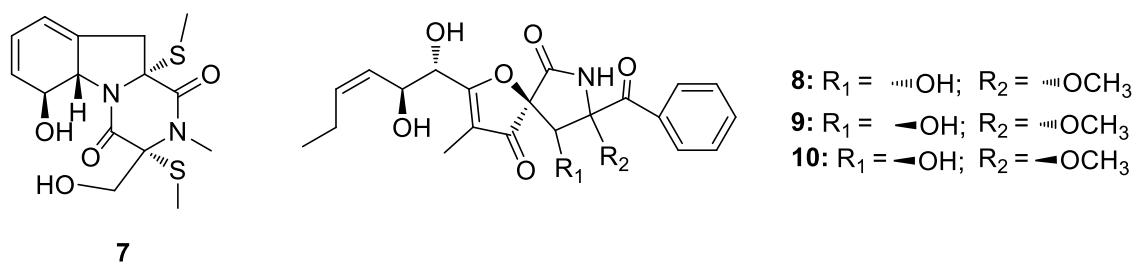
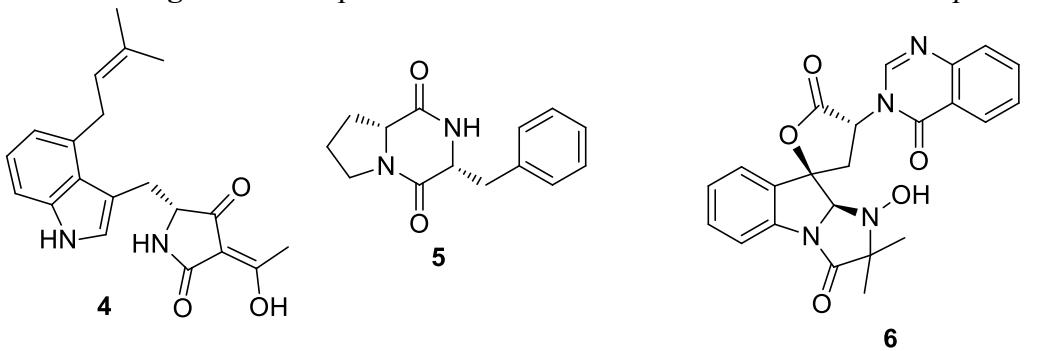


Figure S25. Structures of compounds **4-10**

Cartesian coordinates of all compounds under study

11epi-1_c0002
B3LYP/6-31G* Geometry

C 2.360101 2.538478 1.671104
C 4.710708 1.611064 0.381443
C 3.532763 3.303357 1.678241
C 2.363661 1.306815 1.022163
C 3.542186 0.856259 0.404318
C 4.685114 2.849254 1.029624
N 3.331955 -0.424671 -0.124543
C 2.054349 -0.961274 0.325507
C 1.228448 0.307323 0.769416
N 1.606274 -1.740245 -0.822646
C 2.831233 -2.202797 -1.545438
C 3.794313 -1.030993 -1.270985
O 4.777827 -0.711803 -1.912022
C 3.442855 -3.494510 -0.966295
C 2.541254 -2.346107 -3.038272
O 0.835371 -2.853249 -0.365476
O 0.469213 0.704073 -0.412774
C -0.248723 1.853325 -0.432690
O -0.453417 2.552041 0.538975
C -0.752652 2.139770 -1.841656
C -1.821489 3.235997 -1.824017
C 0.439723 2.501024 -2.752586
C 0.339622 0.046152 1.993444
C -0.789537 -0.988961 1.804714
C -1.149052 -1.645805 3.144468
O -0.377436 -1.777954 4.066488
O -2.411924 -2.121799 3.162162
N -1.988986 -0.478072 1.115666
N -3.832033 1.026887 1.256662
C -3.656969 -0.539999 -0.617583
C -4.321244 0.502298 0.069238
C -2.419932 -1.095413 -0.069932
C -2.732420 0.530227 1.703918
O -1.796792 -2.024519 -0.587306
C -5.515390 1.022673 -0.465617
C -6.024018 0.513516 -1.650050
C -5.360326 -0.524978 -2.329947
C -4.185155 -1.049579 -1.816824
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H 5.581877 3.462880 1.034873

H 2.194173 -1.602647 1.210890
H 4.385459 -3.709824 -1.479236
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H -2.666110 2.963128 -1.184262
H -2.198098 3.408416 -2.838058
H 1.177044 1.694166 -2.777884
H 0.086802 2.680957 -3.773615
H 0.935972 3.413244 -2.401525
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H -0.069603 0.993553 2.348201
H -0.423704 -1.812151 1.182514
H -2.524955 -2.567347 4.023389
H -2.319572 0.917784 2.631367
H -6.012790 1.821606 0.074670
H -6.945617 0.919542 -2.058219
H -5.771205 -0.914560 -3.256715
H -3.653452 -1.851849 -2.317454
SCF Energy (B3LYP/6-31G*)= -1791.33199853

11epi-1_c0020
B3LYP/6-31G* Geometry
C 2.353793 2.580640 1.607835
C 4.691678 1.638319 0.306261
C 3.524748 3.347925 1.590102
C 2.352766 1.338773 0.978241
C 3.525430 0.881058 0.354426
C 4.670686 2.886348 0.935383
N 3.312886 -0.408383 -0.151893
C 2.043170 -0.942450 0.322829
C 1.217461 0.332180 0.752528
N 1.583341 -1.746053 -0.803416
C 2.799105 -2.205839 -1.543696
C 3.759704 -1.026264 -1.298838
O 4.731801 -0.709719 -1.958156
C 3.430873 -3.487155 -0.962856
C 2.483162 -2.366745 -3.029525
O 0.838013 -2.861345 -0.312511
O 0.442527 0.705440 -0.423922
C -0.276657 1.855154 -0.452645
O -0.460543 2.571492 0.509964

C -0.810558 2.113085 -1.855469
C -1.875615 3.213065 -1.837057
C 0.361262 2.449624 -2.801820
C 0.343107 0.089299 1.993533
C -0.788412 -0.960241 1.832133
C -1.196777 -1.548799 3.187003
O -2.297039 -1.497843 3.683728
O -0.145480 -2.165126 3.771914
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C -2.424652 -1.138298 -0.020858
C -2.727525 0.563115 1.685052
O -1.806166 -2.092696 -0.498615
C -5.515479 0.966281 -0.498708
C -6.030028 0.406070 -1.656904
C -5.371742 -0.663688 -2.292853
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H 5.570857 1.262908 -0.203741
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H 5.565808 3.502189 0.920252
H 2.195190 -1.566890 1.218195
H 4.366645 -3.699504 -1.489377
H 2.748913 -4.331441 -1.086483
H 3.654041 -3.382605 0.104442
H 2.020578 -1.457483 -3.424211
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H -0.471984 -2.529666 4.616432
H -2.315574 0.987283 2.593860
H -6.009224 1.789171 0.007934
H -6.952582 0.795565 -2.078915
H -5.787510 -1.093228 -3.199584
H -3.668273 -1.993050 -2.227497
SCF Energy (B3LYP/6-31G*)= -1791.33244423

11epi-1_c0045
B3LYP/6-31G* Geometry
C -2.145088 1.173543 2.944467
C -4.625577 0.543288 1.727541
C -3.323463 1.147564 3.699578
C -2.212157 0.891949 1.585321
C -3.445607 0.586709 0.992839
C -4.543127 0.828749 3.094077
N -3.267027 0.330685 -0.376343
C -1.903081 0.646213 -0.782252
C -1.088987 0.790948 0.561839
N -1.534374 -0.428000 -1.698728
C -2.806410 -0.961819 -2.280709
C -3.808352 -0.688525 -1.140467
O -4.882051 -1.226015 -0.962123
C -3.273637 -0.202811 -3.538809
C -2.680527 -2.461224 -2.546392
O -0.689856 0.112849 -2.721678
O -0.175160 -0.310839 0.827856
C -0.624334 -1.588629 0.983094
O -1.783076 -1.925136 0.908719
C 0.532708 -2.540291 1.258759
C 0.172340 -3.472871 2.424466
C 0.843729 -3.333093 -0.026295
C -0.185998 2.032030 0.552374
C 0.939262 2.024272 -0.507436
C 1.258128 3.448343 -0.981516
O 0.467703 4.363747 -0.965751
O 2.506294 3.555829 -1.483234
N 2.156063 1.305828 -0.095027
N 3.976121 1.270519 1.441879
C 3.801411 -0.434310 -0.309235
C 4.459739 0.136109 0.805277
C 2.566692 0.170478 -0.809226
C 2.891873 1.781053 0.972127
O 1.927048 -0.261482 -1.771142
C 5.644334 -0.458142 1.279986
C 6.153780 -1.584868 0.654313
C 5.499688 -2.146108 -0.458384
C 4.331879 -1.574832 -0.937579
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H -5.561606 0.277252 1.251373
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H -1.876671 1.614812 -1.304283
H -4.260312 -0.573373 -3.833710

H -2.570256 -0.361346 -4.359540
H -3.351140 0.874980 -3.359707
H -2.363177 -2.980470 -1.638597
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H -0.737486 -4.035337 2.194306
H -0.002581 -2.911956 3.349308
H 0.986790 -4.182733 2.606073
H 1.101206 -2.664430 -0.853334
H 1.688327 -4.008807 0.148351
H -0.022506 -3.933859 -0.323086
H -0.809915 2.907882 0.358800
H 0.243072 2.164813 1.551336
H 0.587369 1.505858 -1.406208
H 2.592435 4.471427 -1.810947
H 2.490430 2.678645 1.437188
H 6.135690 -0.007719 2.136338
H 7.069044 -2.038693 1.024533
H 5.912320 -3.026804 -0.941691
H 3.809313 -1.984155 -1.795457
SCF Energy (B3LYP/6-31G*)= -1791.33226994

11epi-1_c0047
B3LYP/6-31G* Geometry
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C -4.597816 0.275568 1.836250
C -3.249661 0.554624 3.849360
C -2.183584 0.621811 1.697433
C -3.432478 0.422986 1.091881
C -4.484874 0.344369 3.228522
N -3.285458 0.381916 -0.304380
C -1.926246 0.744093 -0.686652
C -1.083083 0.677384 0.645936
N -1.588007 -0.189088 -1.755975
C -2.875891 -0.605738 -2.394146
C -3.854589 -0.501075 -1.206166
O -4.931748 -1.048790 -1.091400
C -3.348266 0.348565 -3.509199
C -2.777060 -2.045846 -2.895140
O -0.739879 0.477927 -2.697521
O -0.171359 -0.453177 0.702214
C -0.625721 -1.739921 0.669688
O -1.790454 -2.054070 0.604334
C 0.544527 -2.711946 0.764848
C 1.192350 -2.626510 2.162248
C 0.087678 -4.134978 0.431412

C -0.173785 1.902957 0.809969
C 0.928061 2.055167 -0.263145
C 1.231403 3.533838 -0.537233
O 0.439840 4.433170 -0.370869
O 2.465366 3.718684 -1.051443
N 2.155990 1.293511 0.018595
N 4.018424 1.064405 1.487486
C 3.793479 -0.399790 -0.463459
C 4.485402 0.025308 0.694222
C 2.543886 0.258508 -0.845657
C 2.921044 1.627581 1.118624
O 1.876249 -0.053013 -1.833267
C 5.685091 -0.619061 1.050901
C 6.175180 -1.653671 0.269569
C 5.485271 -2.072058 -0.883582
C 4.302276 -1.449423 -1.248029
H -1.123533 0.826530 3.567390
H -5.546254 0.095020 1.344754
H -3.191015 0.610377 4.932446
H -5.378123 0.233630 3.837241
H -1.900002 1.778569 -1.062328
H -4.344299 0.042030 -3.843469
H -2.658519 0.312158 -4.355667
H -3.407056 1.385566 -3.161417
H -2.454826 -2.706917 -2.086478
H -2.052475 -2.104445 -3.714660
H -3.751448 -2.385827 -3.258557
H 0.134413 0.065913 -2.538296
H 1.285063 -2.382907 0.024844
H 0.476866 -2.918233 2.940125
H 1.544646 -1.614364 2.380951
H 2.048630 -3.306911 2.220483
H -0.341031 -4.190063 -0.573851
H 0.937528 -4.824451 0.482151
H -0.677997 -4.473626 1.136160
H -0.797685 2.799127 0.770361
H 0.278881 1.877273 1.807133
H 0.559549 1.667262 -1.219556
H 2.540732 4.671952 -1.248194
H 2.532061 2.454514 1.708761
H 6.202980 -0.280319 1.942365
H 7.102446 -2.146324 0.549226
H 5.882021 -2.882699 -1.487649
H 3.750935 -1.748925 -2.133149
SCF Energy (B3LYP/6-31G*)= -1791.33195089

11epi-1_c0053

B3LYP/6-31G* Geometry

C -2.116413 1.200653 2.939328
C -4.599952 0.529379 1.750683
C -3.289348 1.178264 3.703020
C -2.190829 0.895461 1.585591
C -3.425593 0.569934 1.006746
C -4.510433 0.839116 3.111502
N -3.254346 0.290754 -0.358767
C -1.895931 0.610015 -0.780829
C -1.074226 0.787147 0.555607
N -1.522350 -0.478728 -1.678061
C -2.792873 -1.040868 -2.236439
C -3.790045 -0.751543 -1.096537
O -4.857184 -1.294822 -0.898228
C -3.278182 -0.317929 -3.508998
C -2.651738 -2.544703 -2.467480
O -0.696675 0.050704 -2.721308
O -0.144075 -0.294746 0.832653
C -0.577025 -1.575954 1.013900
O -1.733256 -1.924240 0.960415
C 0.594444 -2.509751 1.287254
C 0.255533 -3.440338 2.460834
C 0.907501 -3.305697 0.004368
C -0.188656 2.042511 0.518877
C 0.936733 2.027629 -0.553849
C 1.290619 3.444470 -1.015914
O 2.370441 3.978773 -0.923569
O 0.211155 4.039592 -1.570373
N 2.154613 1.324712 -0.133842
N 3.967248 1.290047 1.411384
C 3.810549 -0.405835 -0.349370
C 4.460749 0.163906 0.770027
C 2.572888 0.191575 -0.847684
C 2.884906 1.802787 0.938451
O 1.935796 -0.244964 -1.810622
C 5.647755 -0.425837 1.245561
C 6.166800 -1.545475 0.615656
C 5.520348 -2.105742 -0.502381
C 4.350375 -1.540063 -0.982004
H -1.163233 1.437470 3.405897
H -5.536848 0.246526 1.286057
H -3.249331 1.420234 4.761052
H -5.411132 0.816111 3.718874
H -1.880023 1.567408 -1.323220
H -4.262877 -0.706635 -3.786617
H -2.579224 -0.488719 -4.330950
H -3.366083 0.763047 -3.355664
H -2.325218 -3.039304 -1.549270

H -1.914666 -2.731745 -3.255881
H -3.612640 -2.970194 -2.772033
H 0.194167 -0.290913 -2.498168
H 1.465131 -1.896198 1.541768
H -0.647616 -4.017319 2.240572
H 0.079148 -2.876571 3.383645
H 1.081488 -4.137159 2.640656
H 1.145857 -2.638792 -0.829691
H 1.765574 -3.964830 0.176104
H 0.049437 -3.923872 -0.280169
H -0.840167 2.897842 0.323306
H 0.248780 2.197204 1.510597
H 0.573080 1.503047 -1.441149
H 0.498062 4.926897 -1.858647
H 2.482837 2.697735 1.401858
H 6.133500 0.023966 2.105417
H 7.084231 -1.994700 0.986268
H 5.940945 -2.980790 -0.989100
H 3.833293 -1.948279 -1.843755
SCF Energy (B3LYP/6-31G*)= -1791.33280638

11epi-1_c0056
B3LYP/6-31G* Geometry
C -2.054359 0.732921 3.074445
C -4.568822 0.260517 1.856419
C -3.210335 0.602079 3.853103
C -2.160682 0.634641 1.692387
C -3.410813 0.406088 1.100138
C -4.447026 0.362292 3.245945
N -3.273075 0.333624 -0.295728
C -1.920976 0.703230 -0.697193
C -1.068463 0.680179 0.631812
N -1.576383 -0.251494 -1.745437
C -2.862410 -0.709060 -2.358855
C -3.833760 -0.585567 -1.167372
O -4.901215 -1.146077 -1.027698
C -3.361083 0.203781 -3.497169
C -2.742846 -2.161235 -2.818846
O -0.753603 0.406699 -2.714256
O -0.136607 -0.429305 0.709851
C -0.569507 -1.724803 0.714807
O -1.729664 -2.057729 0.665686
C 0.617436 -2.674006 0.827187
C 1.291611 -2.522666 2.206455
C 0.177014 -4.115999 0.559494
C -0.180168 1.927431 0.762450
C 0.922995 2.068595 -0.323751

C 1.264621 3.537476 -0.590788
O 2.345168 4.059101 -0.447826
O 0.172122 4.199175 -1.033140
N 2.149982 1.318846 -0.029419
N 3.999132 1.081150 1.454328
C 3.793599 -0.370633 -0.507361
C 4.475308 0.050240 0.657665
C 2.544615 0.284657 -0.892368
C 2.906804 1.651256 1.079176
O 1.881468 -0.028488 -1.883677
C 5.674391 -0.593648 1.018827
C 6.172979 -1.621836 0.234855
C 5.492428 -2.036104 -0.925714
C 4.310310 -1.415069 -1.294443
H -1.089523 0.892386 3.549711
H -5.518086 0.055617 1.376233
H -3.144736 0.681922 4.934264
H -5.334394 0.253303 3.863501
H -1.908503 1.727578 -1.099622
H -4.354677 -0.129302 -3.812797
H -2.678232 0.154313 -4.348457
H -3.434081 1.249344 -3.179003
H -2.403254 -2.793145 -1.994216
H -2.023215 -2.230786 -3.641793
H -3.713851 -2.528060 -3.164824
H 0.134234 0.026246 -2.548954
H 1.338496 -2.363830 0.060070
H 0.595464 -2.789940 3.010300
H 1.636999 -1.498824 2.375702
H 2.156688 -3.190756 2.274854
H -0.270591 -4.217781 -0.433755
H 1.038931 -4.789380 0.620244
H -0.568806 -4.438336 1.292691
H -0.833460 2.801956 0.709932
H 0.279254 1.934371 1.756382
H 0.542814 1.670621 -1.268445
H 0.451065 5.119361 -1.200929
H 2.518095 2.476560 1.666736
H 6.185245 -0.258029 1.915503
H 7.100121 -2.112953 0.517801
H 5.896145 -2.841858 -1.531729
H 3.765745 -1.711001 -2.184963
SCF Energy (B3LYP/6-31G*)= -1791.33248473

1_c0023
B3LYP/6-31G* Geometry
C 1.657843 -0.478847 3.329765
C 3.008092 -2.773166 2.352549

C 2.318716 -1.346861 4.206041
C 1.666558 -0.765484 1.969506
C 2.333421 -1.902961 1.500747
C 2.989605 -2.473186 3.717663
N 2.200725 -1.979685 0.105682
C 1.283149 -0.956787 -0.389942
C 1.105298 0.056780 0.808307
N 1.945219 -0.519375 -1.613870
C 2.671301 -1.703892 -2.164168
C 3.102301 -2.392096 -0.854211
O 4.034749 -3.154046 -0.688107
C 1.772843 -2.663145 -2.970944
C 3.879138 -1.253247 -2.982158
O 0.973881 -0.042215 -2.548630
O 2.018395 1.203188 0.755040
C 2.034733 2.171392 -0.176213
O 1.296617 2.251645 -1.145077
C 3.135359 3.177359 0.126824
C 4.450316 2.683989 -0.513477
C 2.738088 4.572562 -0.368095
C -0.352237 0.469568 1.090574
C -1.177842 1.095767 -0.059792
C -1.423389 2.590717 0.179538
O -0.780571 3.282247 0.934899
O -2.387219 3.072699 -0.631017
N -2.436344 0.378533 -0.316633
N -3.684108 -0.959619 -1.832413
C -4.660016 -0.282625 0.316532
C -4.733224 -0.963282 -0.922078
C -3.443696 0.452956 0.662220
C -2.622934 -0.306451 -1.500992
O -3.252515 1.093547 1.692161
C -5.910281 -1.666520 -1.243410
C -6.973771 -1.685413 -0.354571
C -6.895437 -1.005718 0.875277
C -5.745415 -0.307873 1.208057
H 1.157898 0.408115 3.708138
H 3.531697 -3.635924 1.958679
H 2.315096 -1.140439 5.272185
H 3.505049 -3.132413 4.410626
H 0.298676 -1.399501 -0.607296
H 2.348848 -3.552104 -3.246109
H 1.419563 -2.171240 -3.880413
H 0.899726 -2.989128 -2.395481
H 4.503714 -0.567291 -2.402665
H 3.542880 -0.740072 -3.888994
H 4.484219 -2.118804 -3.267289

H 1.090740 0.924483 -2.448629
 H 3.267755 3.191647 1.213945
 H 4.352217 2.622253 -1.603094
 H 4.731275 1.696240 -0.134790
 H 5.260871 3.383614 -0.283340
 H 1.806366 4.905943 0.099911
 H 3.525672 5.294254 -0.126002
 H 2.589355 4.570833 -1.452176
 H -0.866847 -0.436670 1.420762
 H -0.352254 1.155167 1.939764
 H -0.615188 1.047532 -0.991941
 H -2.458134 4.025251 -0.432891
 H -1.772776 -0.282658 -2.180322
 H -5.953085 -2.183503 -2.196708
 H -7.878439 -2.230649 -0.610234
 H -7.736882 -1.028785 1.561692
 H -5.654232 0.227126 2.147845
 SCF Energy (B3LYP/6-31G*)= -1791.32909567

1_c0029

B3LYP/6-31G* Geometry

C 0.690419 2.446802 -1.630772
 C 3.497778 2.337937 -2.006841
 C 1.316093 3.228383 -2.609384
 C 1.473938 1.634457 -0.812417
 C 2.859306 1.579066 -1.030629
 C 2.700586 3.174807 -2.791515
 N 3.445045 0.642673 -0.164291
 C 2.477934 0.159369 0.809444
 C 1.060157 0.618274 0.255392
 N 2.777281 -1.266796 0.895715
 C 4.233866 -1.421599 0.595382
 C 4.442266 -0.279558 -0.416722
 O 5.312353 -0.188142 -1.260691
 C 5.144774 -1.179707 1.816986
 C 4.509031 -2.784224 -0.036550
 O 2.497002 -1.730248 2.217508
 O 0.392260 -0.435615 -0.504803
 C -0.025201 -1.596092 0.039091
 O -0.038387 -1.843420 1.234473
 C -0.529366 -2.542059 -1.042663
 C 0.638333 -2.980040 -1.950852
 C -1.264484 -3.734981 -0.424730
 C 0.228756 1.149795 1.441385
 C -1.165856 1.748458 1.184868
 C -1.594551 2.593477 2.394420
 O -0.824516 3.152113 3.141513
 O -2.935717 2.695725 2.502020

N -2.214200 0.794832 0.790155
N -3.579541 -1.037243 1.456919
C -3.959249 0.062752 -0.701921
C -4.271487 -0.928108 0.257581
C -2.885069 1.019305 -0.431513
C -2.622329 -0.199357 1.658678
O -2.564832 1.945053 -1.172324
C -5.317570 -1.831802 -0.009868
C -6.023590 -1.744258 -1.199697
C -5.709365 -0.756234 -2.151175
C -4.685054 0.143470 -1.902629
H -0.391991 2.449581 -1.556243
H 4.567498 2.253868 -2.155081
H 0.711691 3.870941 -3.242917
H 3.167083 3.782377 -3.562197
H 2.631690 0.639922 1.786139
H 6.190480 -1.198650 1.494301
H 4.985869 -1.959635 2.565180
H 4.949806 -0.210212 2.287389
H 3.870435 -2.941313 -0.910444
H 4.309397 -3.576991 0.691764
H 5.553749 -2.847708 -0.354617
H 1.598469 -2.099589 2.103847
H -1.227779 -1.957470 -1.656611
H 1.132804 -2.117666 -2.405504
H 0.262527 -3.627101 -2.750448
H 1.383458 -3.543769 -1.378797
H -2.086295 -3.409233 0.219309
H -1.673257 -4.370597 -1.217398
H -0.584115 -4.339700 0.183718
H 0.165990 0.359405 2.193556
H 0.810833 1.958792 1.891382
H -1.122190 2.459111 0.354730
H -3.105507 3.287945 3.259334
H -2.056754 -0.259787 2.584178
H -5.547206 -2.584926 0.737084
H -6.829379 -2.445457 -1.399594
H -6.271349 -0.699057 -3.078793
H -4.421739 0.918934 -2.614415
SCF Energy (B3LYP/6-31G*)= -1791.32731530

1_c0036
B3LYP/6-31G* Geometry
C 1.775842 0.599432 3.164033
C 3.047881 -1.924146 2.926021
C 2.459575 0.038278 4.248403
C 1.723238 -0.106618 1.967483

C 2.351725 -1.352656 1.864550
C 3.091572 -1.203583 4.123033
N 2.159543 -1.867365 0.572702
C 1.237386 -1.031378 -0.191938
C 1.125939 0.316116 0.624646
N 1.857156 -1.019048 -1.512749
C 2.551545 -2.331042 -1.682382
C 3.021299 -2.580655 -0.235983
O 3.950483 -3.271644 0.133393
C 1.616481 -3.477342 -2.118291
C 3.735550 -2.184931 -2.635404
O 0.857273 -0.841733 -2.519197
O 2.059638 1.349695 0.167711
C 2.044490 1.974830 -1.021719
O 1.249706 1.776176 -1.926720
C 3.149209 3.018532 -1.094647
C 2.891219 4.140503 -0.070848
C 4.538130 2.382674 -0.911977
C -0.309198 0.845355 0.811385
C -1.183603 1.070191 -0.446454
C -1.448992 2.562433 -0.681351
O -0.792063 3.462344 -0.211365
O -2.451104 2.757009 -1.562303
N -2.435791 0.298695 -0.420847
N -3.708133 -1.453383 -1.398686
C -4.626911 -0.145425 0.465264
C -4.727658 -1.179101 -0.496167
C -3.412802 0.668761 0.520873
C -2.647991 -0.723035 -1.325414
O -3.200007 1.600558 1.291855
C -5.902355 -1.954577 -0.540561
C -6.936697 -1.701753 0.346912
C -6.831044 -0.671792 1.300172
C -5.682976 0.102080 1.358030
H 1.304362 1.573595 3.256401
H 3.540955 -2.881884 2.811059
H 2.503838 0.573988 5.191987
H 3.625286 -1.621410 4.972172
H 0.238845 -1.493644 -0.225008
H 2.173819 -4.419216 -2.114670
H 1.237194 -3.290815 -3.125912
H 0.760182 -3.586685 -1.444082
H 4.387886 -1.366344 -2.317249
H 3.374885 -1.972366 -3.647070
H 4.320726 -3.108960 -2.653222
H 0.986442 0.104142 -2.735656
H 3.071228 3.432810 -2.105299
H 2.990331 3.760882 0.950934

H 1.886326 4.559711 -0.183807
H 3.621667 4.944771 -0.211549
H 4.713555 1.584937 -1.642263
H 5.315089 3.143032 -1.047383
H 4.643775 1.957208 0.090467
H -0.820836 0.124918 1.454733
H -0.253480 1.778939 1.374437
H -0.649000 0.738074 -1.336132
H -2.531780 3.722765 -1.673743
H -1.819922 -0.907697 -2.007278
H -5.966659 -2.743443 -1.283156
H -7.839685 -2.305101 0.305921
H -7.649825 -0.484765 1.988895
H -5.571175 0.904132 2.080529
SCF Energy (B3LYP/6-31G*)= -1791.32872869

1_c0062
B3LYP/6-31G* Geometry
C 1.711344 -0.170062 3.309861
C 2.991826 -2.588569 2.565654
C 2.359361 -0.959740 4.266303
C 1.698577 -0.596146 1.986802
C 2.330328 -1.793901 1.633605
C 2.996114 -2.148009 3.892322
N 2.179836 -2.012011 0.255068
C 1.280289 -1.024225 -0.335217
C 1.148983 0.115930 0.749713
N 1.937643 -0.730410 -1.604087
C 2.639248 -1.976778 -2.034570
C 3.063718 -2.539910 -0.663995
O 3.979676 -3.303155 -0.427543
C 1.721271 -2.994793 -2.741181
C 3.853512 -1.632949 -2.894393
O 0.967814 -0.331439 -2.576071
O 2.109011 1.206784 0.555075
C 2.127228 2.075737 -0.470342
O 1.349895 2.090567 -1.411064
C 3.239301 3.096265 -0.273169
C 3.554431 3.821318 -1.584808
C 2.833279 4.075865 0.849748
C -0.288359 0.612131 1.001075
C -1.129662 1.091162 -0.207242
C -1.381187 2.603197 -0.145638
O -0.739999 3.383650 0.518812
O -2.352333 2.980277 -1.002198
N -2.388722 0.345203 -0.361651
N -3.653644 -1.156979 -1.699132

C -4.603772 -0.239137 0.370632
 C -4.691081 -1.056918 -0.781127
 C -3.384950 0.532631 0.613610
 C -2.589423 -0.470115 -1.457789
 O -3.183241 1.289774 1.559012
 C -5.871242 -1.791882 -1.005453
 C -6.923583 -1.708699 -0.107123
 C -6.831135 -0.893081 1.036070
 C -5.677955 -0.161986 1.272707
 H 1.236683 0.763505 3.598380
 H 3.488753 -3.501022 2.258905
 H 2.372078 -0.644132 5.305312
 H 3.501975 -2.745156 4.645948
 H 0.282558 -1.462085 -0.494418
 H 2.281922 -3.915331 -2.930816
 H 1.371048 -2.587907 -3.692937
 H 0.845784 -3.249488 -2.134197
 H 4.489271 -0.900887 -2.388071
 H 3.526182 -1.211304 -3.850346
 H 4.444195 -2.533291 -3.086484
 H 1.107532 0.637276 -2.581491
 H 4.122026 2.539626 0.065062
 H 2.682391 4.377456 -1.942098
 H 3.847812 3.118336 -2.371160
 H 4.377352 4.527715 -1.432554
 H 2.675948 3.549049 1.794932
 H 3.624200 4.819446 0.995460
 H 1.906513 4.599755 0.593463
 H -0.819372 -0.217578 1.474639
 H -0.244604 1.414520 1.739952
 H -0.578110 0.932686 -1.133778
 H -2.429010 3.949003 -0.917103
 H -1.748269 -0.522714 -2.146486
 H -5.925436 -2.414365 -1.892825
 H -7.830747 -2.279257 -0.287689
 H -7.664124 -0.837517 1.730867
 H -5.575690 0.477354 2.143628
 SCF Energy (B3LYP/6-31G*)= -1791.32912769

1_c0063
 B3LYP/6-31G* Geometry
 C 1.474862 1.795332 2.599623
 C 3.787328 0.211771 3.045736
 C 2.352061 2.084538 3.651634
 C 1.751925 0.710250 1.772805
 C 2.891737 -0.073514 2.019994
 C 3.498227 1.310981 3.859402
 N 2.932335 -1.140728 1.111086

C 1.686784 -1.219557 0.363387
C 1.045293 0.213175 0.506875
N 2.125219 -1.670874 -0.950406
C 3.360639 -2.484769 -0.747232
C 3.978092 -1.772730 0.474820
O 5.141394 -1.780778 0.829196
C 3.082413 -3.956525 -0.379078
C 4.270293 -2.381218 -1.969911
O 1.093740 -2.444859 -1.566807
O 1.497176 0.956232 -0.659977
C 1.236528 2.284285 -0.807709
O 0.571157 2.940400 -0.035172
C 1.911305 2.807328 -2.066224
C 1.229215 4.089482 -2.551173
C 3.415243 3.012171 -1.785499
C -0.489601 0.184510 0.598671
C -1.201616 -0.491036 -0.600839
C -0.955007 0.172416 -1.982200
O -0.335269 -0.414804 -2.850241
O -1.423670 1.397519 -2.176273
N -2.650069 -0.686328 -0.314219
N -4.321634 -2.340894 0.088690
C -4.849975 0.034176 0.346758
C -5.218061 -1.330681 0.401539
C -3.497048 0.395831 -0.054547
C -3.128162 -1.988908 -0.237331
O -3.098220 1.565987 -0.166093
C -6.529617 -1.672469 0.781279
C -7.439041 -0.675807 1.096782
C -7.069103 0.681833 1.039651
C -5.784290 1.036683 0.664575
H 0.612369 2.424302 2.414182
H 4.668816 -0.400934 3.192833
H 2.144583 2.927348 4.304445
H 4.174921 1.560546 4.672130
H 1.003687 -1.948929 0.832180
H 4.027940 -4.456651 -0.147473
H 2.602259 -4.468403 -1.216489
H 2.428403 -4.042616 0.495778
H 4.445335 -1.333589 -2.230453
H 3.801504 -2.878878 -2.825244
H 5.233437 -2.857798 -1.764625
H 0.750313 -1.833624 -2.256167
H 1.810016 2.022306 -2.824806
H 1.278755 4.870796 -1.786348
H 0.175141 3.907940 -2.782170
H 1.722690 4.457234 -3.457335

H 3.888524 2.082024 -1.456663
H 3.920496 3.352064 -2.695872
H 3.567903 3.771612 -1.009855
H -0.754378 -0.394936 1.491310
H -0.860934 1.197822 0.744018
H -0.796439 -1.496213 -0.717506
H -1.970169 1.683520 -1.390932
H -2.394738 -2.753512 -0.481878
H -6.796137 -2.723670 0.816855
H -8.450296 -0.943976 1.389904
H -7.794607 1.450708 1.287886
H -5.473365 2.074405 0.608435
SCF Energy (B3LYP/6-31G*)= -1791.33437468

1_c0085
B3LYP/6-31G* Geometry
C 1.597272 -0.601493 3.332302
C 2.859350 -2.902007 2.257211
C 2.222001 -1.531627 4.170552
C 1.598475 -0.828386 1.960827
C 2.220938 -1.970126 1.443562
C 2.850016 -2.660727 3.634024
N 2.086675 -1.982250 0.046503
C 1.209517 -0.904958 -0.404546
C 1.075533 0.065065 0.834927
N 1.889835 -0.441695 -1.610719
C 2.568870 -1.631414 -2.210486
C 2.972570 -2.388718 -0.930444
O 3.875637 -3.191160 -0.796462
C 1.632433 -2.520341 -3.053693
C 3.793240 -1.197291 -3.012646
O 0.939849 0.110001 -2.525861
O 2.054285 1.158190 0.814979
C 2.128059 2.139106 -0.100596
O 1.338953 2.330557 -1.011374
C 3.356094 3.002629 0.154813
C 4.614117 2.251341 -0.331436
C 3.207506 4.373307 -0.511436
C -0.361342 0.536657 1.135133
C -1.179366 1.188303 -0.011103
C -1.533601 2.670485 0.183858
O -2.396997 3.238373 -0.440218
O -0.728416 3.297664 1.069934
N -2.419109 0.455574 -0.303876
N -3.671728 -0.774526 -1.903544
C -4.638140 -0.253002 0.292622
C -4.714903 -0.847183 -0.989465
C -3.423126 0.462043 0.681679

C -2.612447 -0.138683 -1.534544
O -3.227131 1.028162 1.753856
C -5.890664 -1.532320 -1.352204
C -6.949502 -1.616647 -0.461678
C -6.867986 -1.021813 0.811185
C -5.719156 -0.343334 1.185226
H 1.129433 0.285656 3.749378
H 3.348931 -3.767195 1.826642
H 2.223215 -1.372190 5.244721
H 3.337673 -3.369087 4.297973
H 0.208585 -1.298460 -0.638427
H 2.173162 -3.418846 -3.366629
H 1.298035 -1.977876 -3.941248
H 0.747578 -2.835695 -2.490447
H 4.448871 -0.565055 -2.406880
H 3.477810 -0.632279 -3.895813
H 4.359779 -2.075097 -3.336770
H 1.095227 1.067656 -2.398468
H 3.436144 3.123186 1.241960
H 4.565079 2.069679 -1.410988
H 4.721463 1.288515 0.176075
H 5.507033 2.851742 -0.127780
H 2.317868 4.898257 -0.149020
H 4.084720 4.992358 -0.295500
H 3.113670 4.271153 -1.596786
H -0.905820 -0.350215 1.468268
H -0.326835 1.205417 1.995743
H -0.595788 1.167443 -0.930968
H -1.019004 4.229176 1.074680
H -1.768209 -0.059870 -2.216609
H -5.936683 -1.982083 -2.338857
H -7.853452 -2.146663 -0.749941
H -7.706282 -1.094561 1.498016
H -5.625896 0.127732 2.158422
SCF Energy (B3LYP/6-31G*)= -1791.32593082

2_c0015
B3LYP/6-31G* Geometry
O -0.744771 -0.497368 -0.864057
C 0.131480 0.263267 -0.029626
C -0.558611 1.640370 0.102133
C -1.885445 1.452220 -0.451514
C -1.921984 0.186626 -0.953581
C 0.206518 -0.491988 1.308256
C 1.597544 0.319821 -0.516300
C 2.441854 0.158046 0.818141
N 1.487908 -0.406259 1.750590

O -0.713320 -1.098866 1.835520
C 3.668421 -0.815395 0.762687
O 3.651102 -1.781678 1.515944
C 4.833276 -0.552906 -0.123472
C 7.105436 -0.211104 -1.724546
C 5.894307 -1.477573 -0.065576
C 4.925004 0.547080 -0.993621
C 6.058448 0.709002 -1.790175
C 7.021420 -1.307563 -0.859474
O 2.871097 1.461368 1.156839
C 3.365550 1.640074 2.481319
O 1.913952 1.468378 -1.243554
O -0.030453 2.638003 0.576953
C -2.940666 2.515414 -0.450848
C -3.059976 -0.642678 -1.479462
C -3.694442 -1.497295 -0.324011
C -4.196357 -0.700293 0.849420
O -2.638132 -1.516921 -2.503981
O -2.752678 -2.494790 0.064157
C -5.472867 -0.478807 1.189216
C -6.729751 -0.946304 0.503580
C -7.679256 0.206888 0.112641
C -7.114735 1.133344 -0.968123
H 1.775895 -0.540145 -1.168939
H 1.820192 -1.054812 2.457474
H 7.986391 -0.077138 -2.346861
H 5.807982 -2.321488 0.610376
H 4.113772 1.260890 -1.060754
H 6.121576 1.558640 -2.464084
H 7.834473 -2.026306 -0.808445
H 4.247361 1.014670 2.675883
H 3.647961 2.691576 2.553177
H 2.591119 1.421979 3.225467
H 1.781834 2.218641 -0.630985
H -2.462790 3.499427 -0.493286
H -3.618352 2.421728 -1.305432
H -3.547705 2.484374 0.461931
H -3.828533 0.018167 -1.892854
H -4.508025 -2.044727 -0.807629
H -3.412351 -0.295157 1.488577
H -2.219313 -2.261156 -2.030401
H -2.100060 -2.086964 0.669783
H -5.649060 0.110698 2.091510
H -7.267609 -1.613310 1.193920
H -6.500361 -1.543402 -0.386624
H -8.626230 -0.226233 -0.234470
H -7.921113 0.792890 1.010427
H -6.897320 0.578019 -1.889471

H -7.826066 1.927863 -1.220035
H -6.184403 1.608615 -0.637329
SCF Energy (B3LYP/6-31G*)= -1549.19872544

2_c0028
B3LYP/6-31G* Geometry
O -0.696234 -0.057028 -1.065763
C 0.193304 0.456104 -0.071744
C -0.375918 1.852043 0.273273
C -1.679269 1.895380 -0.360801
C -1.798727 0.746462 -1.082245
C 0.118076 -0.523213 1.112007
C 1.685085 0.447900 -0.476200
C 2.428593 -0.025954 0.843776
N 1.372440 -0.643816 1.618691
O -0.882712 -1.118539 1.481667
C 3.563394 -1.092891 0.672761
O 3.413229 -2.166634 1.243769
C 4.799876 -0.799773 -0.099393
C 7.189125 -0.414722 -1.509050
C 5.771910 -1.817911 -0.150377
C 5.040164 0.415520 -0.763234
C 6.230929 0.598740 -1.466067
C 6.957135 -1.626471 -0.849114
O 2.952613 1.149732 1.426963
C 3.379871 1.048071 2.782670
O 2.148458 1.667034 -0.973318
O 0.212472 2.694801 0.939168
C -2.637673 3.038227 -0.215354
C -2.973932 0.140533 -1.796833
C -3.751396 -0.830665 -0.837161
C -4.240931 -0.196654 0.437202
O -2.574280 -0.581233 -2.941596
O -2.933844 -1.971623 -0.593844
C -5.486702 0.214795 0.706199
C -6.707997 0.157267 -0.173498
C -7.896224 -0.564119 0.497551
C -7.651127 -2.057464 0.733643
H 1.823009 -0.300061 -1.262902
H 1.600968 -1.435889 2.211318
H 8.115674 -0.263655 -2.056748
H 5.571499 -2.750384 0.366277
H 4.298955 1.204520 -0.745308
H 6.408710 1.538534 -1.981073
H 7.700745 -2.417757 -0.883068
H 4.194726 0.320984 2.900992
H 3.742463 2.040720 3.054232

H 2.547187 0.774926 3.440746
H 2.049160 2.309614 -0.243314
H -3.179198 3.240328 -1.145659
H -3.381465 2.847391 0.567102
H -2.082138 3.938518 0.064870
H -3.651438 0.938361 -2.118026
H -4.585474 -1.199196 -1.441406
H -3.476268 -0.077170 1.204130
H -2.253798 -1.434289 -2.590847
H -2.279213 -1.743470 0.097774
H -5.664536 0.646515 1.693372
H -6.484200 -0.324705 -1.132880
H -7.016800 1.186454 -0.411749
H -8.120624 -0.070185 1.453581
H -8.785771 -0.430883 -0.131830
H -6.774120 -2.221810 1.369297
H -8.513735 -2.527636 1.219157
H -7.474413 -2.582383 -0.213303
SCF Energy (B3LYP/6-31G*)= -1549.19911056

2_c0033
B3LYP/6-31G* Geometry
O -0.695422 -0.644678 -0.721105
C 0.189466 0.276086 -0.078991
C -0.493204 1.652847 -0.251245
C -1.824850 1.355407 -0.741434
C -1.869441 0.010398 -0.951530
C 0.268101 -0.165955 1.392016
C 1.652725 0.213806 -0.572312
C 2.503929 0.344912 0.760835
N 1.551533 0.010765 1.800241
O -0.650495 -0.640202 2.043054
C 3.721904 -0.627918 0.918040
O 3.707552 -1.393791 1.874476
C 4.873830 -0.592491 -0.021271
C 7.117842 -0.661899 -1.695785
C 4.972755 0.294612 -1.107019
C 5.914127 -1.512344 0.215138
C 7.026643 -1.546981 -0.615947
C 6.092102 0.252515 -1.938070
O 2.945999 1.686488 0.800169
C 3.456233 2.148091 2.048303
O 1.970762 1.170268 -1.537879
O 0.043925 2.726719 -0.009733
C -2.881295 2.394982 -0.969061
C -3.016836 -0.904760 -1.276878
C -3.644484 -1.481831 0.042937
C -4.126783 -0.442469 1.019497

O -2.610601 -1.983347 -2.091180
O -2.706630 -2.379660 0.630027
C -5.394370 -0.074316 1.246890
C -6.649334 -0.572268 0.581622
C -7.381568 0.529607 -0.210963
C -8.702611 0.047267 -0.817487
H 1.822578 -0.770583 -1.018959
H 1.884312 -0.469593 2.630606
H 7.987690 -0.687948 -2.346935
H 4.177328 0.999958 -1.311464
H 5.823572 -2.190669 1.056761
H 7.823108 -2.261199 -0.426771
H 6.160685 0.938069 -2.777922
H 2.690006 2.101940 2.830488
H 4.338914 1.576456 2.365483
H 3.741724 3.188528 1.885257
H 1.840626 2.039012 -1.108935
H -2.422323 3.386192 -0.906251
H -3.349741 2.295451 -1.954920
H -3.675381 2.339243 -0.215978
H -3.783782 -0.341418 -1.818278
H -4.467896 -2.113866 -0.301984
H -3.336320 0.031521 1.600541
H -2.190537 -2.610622 -1.471865
H -2.041287 -1.855726 1.121631
H -5.558952 0.693542 2.005082
H -7.331451 -0.952330 1.357501
H -6.439696 -1.416970 -0.084888
H -7.569983 1.386097 0.451033
H -6.719147 0.898578 -1.005467
H -9.197856 0.847045 -1.379426
H -8.541217 -0.792413 -1.504511
H -9.395737 -0.291802 -0.037851
SCF Energy (B3LYP/6-31G*)= -1549.19923447

2_c0036

B3LYP/6-31G* Geometry

O -0.652779 -0.434630 -0.900748
C 0.241231 0.388353 -0.148039
C -0.358226 1.809731 -0.255963
C -1.673462 1.621964 -0.836895
C -1.775763 0.299728 -1.146622
C 0.214616 -0.160498 1.288404
C 1.724179 0.278998 -0.569100
C 2.507272 0.259311 0.811754
N 1.481460 -0.090027 1.773558
O -0.763325 -0.624518 1.854994

C 3.655451 -0.796730 0.952895
O 3.543401 -1.631309 1.843043
C 4.858618 -0.760849 0.080071
C 7.187825 -0.839505 -1.473714
C 5.833437 -1.753147 0.302482
C 5.066390 0.193841 -0.930465
C 6.227509 0.146760 -1.701811
C 6.988296 -1.792079 -0.468458
O 3.022959 1.564291 0.976055
C 3.506354 1.894643 2.275262
O 2.146749 1.285441 -1.438830
O 0.220211 2.832737 0.088653
C -2.658953 2.732121 -1.043808
C -2.947337 -0.526031 -1.599020
C -3.680298 -1.154690 -0.359996
C -4.165963 -0.156993 0.657732
O -2.549938 -1.567470 -2.464432
O -2.828182 -2.141139 0.214066
C -5.414661 0.305560 0.798975
C -6.640403 -0.050350 0.000897
C -7.788143 -0.574022 0.886301
C -9.063340 -0.871571 0.092087
H 1.865166 -0.677039 -1.082424
H 1.739861 -0.648545 2.581124
H 8.090848 -0.868995 -2.077840
H 5.659013 -2.482841 1.085916
H 4.323247 0.956866 -1.124818
H 6.380111 0.885015 -2.483945
H 7.733673 -2.562105 -0.290295
H 4.348924 1.255520 2.572116
H 3.846203 2.929529 2.210966
H 2.709896 1.822105 3.024643
H 2.039919 2.125448 -0.950336
H -3.410757 2.761056 -0.246681
H -2.126884 3.688349 -1.037920
H -3.189661 2.637161 -1.997373
H -3.651726 0.114012 -2.140158
H -4.514642 -1.714051 -0.793444
H -3.396372 0.204467 1.339012
H -2.199327 -2.257637 -1.869384
H -2.165917 -1.690110 0.776985
H -5.591403 1.022482 1.603052
H -6.410247 -0.791965 -0.773399
H -6.993410 0.846822 -0.531802
H -7.451945 -1.480195 1.406570
H -8.004639 0.166103 1.669174
H -9.860337 -1.244630 0.744961
H -9.437480 0.029023 -0.410393

H -8.882894 -1.630136 -0.679425
SCF Energy (B3LYP/6-31G*)= -1549.19953177

2_c0043
B3LYP/6-31G* Geometry
O -0.694039 -0.758055 -0.751195
C 0.148282 0.209363 -0.120981
C -0.573995 1.557996 -0.348167
C -1.885760 1.202822 -0.853931
C -1.883406 -0.148388 -1.024101
C 0.212315 -0.184313 1.364444
C 1.622246 0.178513 -0.584626
C 2.442082 0.381040 0.759143
N 1.480951 0.047854 1.790804
O -0.702961 -0.668311 2.013013
C 3.688814 -0.544056 0.971705
O 3.678837 -1.280734 1.950831
C 4.860895 -0.496073 0.058126
C 7.147025 -0.534609 -1.559628
C 5.933744 -1.358717 0.356706
C 4.948447 0.349346 -1.061342
C 6.088804 0.322429 -1.863996
C 7.067334 -1.377803 -0.445922
O 2.836751 1.737850 0.762141
C 3.313106 2.255670 2.001525
O 1.929051 1.113124 -1.574937
O -0.076356 2.655513 -0.130371
C -2.969306 2.200754 -1.133331
C -2.993438 -1.110152 -1.344481
C -3.629667 -1.668126 -0.020667
C -4.171584 -0.618374 0.913242
O -2.534622 -2.198475 -2.116858
O -2.674761 -2.512935 0.614779
C -5.454657 -0.272024 1.084616
C -6.666528 -0.819380 0.376932
C -7.354460 0.194218 -0.566568
C -7.931201 1.425659 0.140205
H 1.832135 -0.813875 -0.995019
H 1.812951 -0.395403 2.641838
H 8.033197 -0.548641 -2.188765
H 5.851446 -2.005620 1.223532
H 4.128712 1.009837 -1.314191
H 6.148404 0.975015 -2.730388
H 7.889036 -2.047576 -0.208322
H 3.559286 3.301449 1.810932
H 2.540032 2.202019 2.776489
H 4.213755 1.728881 2.344658

H 1.771262 1.990531 -1.173955
H -3.444535 2.029800 -2.105897
H -3.754795 2.172165 -0.369674
H -2.535086 3.205077 -1.135018
H -3.766433 -0.589346 -1.918805
H -4.421892 -2.339873 -0.363959
H -3.413902 -0.115768 1.513796
H -2.105626 -2.791472 -1.470564
H -2.037604 -1.950573 1.101355
H -5.659384 0.501851 1.824733
H -7.399575 -1.138738 1.133091
H -6.406499 -1.714207 -0.199102
H -6.635516 0.512565 -1.333424
H -8.162168 -0.327352 -1.096892
H -8.451115 2.077415 -0.570872
H -8.653229 1.135221 0.913785
H -7.149265 2.023046 0.622365
SCF Energy (B3LYP/6-31G*)= -1549.19786495

2_c0045
B3LYP/6-31G* Geometry
O -0.639519 -0.546262 -0.967291
C 0.211111 0.328063 -0.222079
C -0.417368 1.728978 -0.406964
C -1.708162 1.485903 -1.021328
C -1.770442 0.150124 -1.278853
C 0.153047 -0.163662 1.233996
C 1.708851 0.238628 -0.593400
C 2.447994 0.297773 0.810172
N 1.402471 -0.043291 1.753281
O -0.830805 -0.628250 1.789877
C 3.620963 -0.717072 1.029550
O 3.498669 -1.526268 1.941486
C 4.856959 -0.670711 0.204108
C 7.250898 -0.722948 -1.248955
C 5.857913 -1.613917 0.508671
C 5.070910 0.247899 -0.838122
C 6.264427 0.213872 -1.559129
C 7.045127 -1.639569 -0.212069
O 2.919548 1.623678 0.936153
C 3.349647 2.021042 2.235272
O 2.134309 1.217673 -1.492393
O 0.125451 2.779168 -0.087384
C -2.709084 2.563770 -1.306523
C -2.907795 -0.722174 -1.731379
C -3.666872 -1.312438 -0.489211
C -4.206631 -0.280077 0.465053
O -2.459259 -1.790919 -2.536267

O -2.812915 -2.252146 0.155693
C -5.467032 0.166605 0.543803
C -6.653979 -0.251275 -0.283882
C -7.821938 -0.827344 0.549396
C -8.479356 0.178281 1.500985
H 1.888405 -0.734595 -1.060290
H 1.649574 -0.562358 2.590101
H 8.179192 -0.742002 -1.813945
H 5.677776 -2.316339 1.315367
H 4.308191 0.971779 -1.095683
H 6.421918 0.923574 -2.366324
H 7.810877 -2.371278 0.029766
H 3.660780 3.062473 2.139256
H 2.531263 1.954176 2.961184
H 4.200371 1.420537 2.584768
H 1.994510 2.074358 -1.042738
H -3.281034 2.360786 -2.217942
H -3.424695 2.681023 -0.484297
H -2.186277 3.517393 -1.430080
H -3.608511 -0.123375 -2.322109
H -4.473640 -1.910546 -0.922909
H -3.466895 0.127264 1.153685
H -2.115315 -2.446775 -1.899925
H -2.178143 -1.761615 0.717263
H -5.674246 0.920655 1.303281
H -6.359528 -0.988772 -1.038689
H -7.025459 0.623729 -0.840187
H -8.580125 -1.208443 -0.147454
H -7.460378 -1.693706 1.118263
H -7.782874 0.532380 2.269078
H -8.849547 1.055683 0.955603
H -9.332446 -0.274857 2.018326
SCF Energy (B3LYP/6-31G*)= -1549.19795818