NMR Characterization of Rearranged Staurosporine Aglycone Analogues from the Marine Sponge *Damiria* sp.

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SUPPORTING INFORMATION

Figure S11. COSY Spectrum of **2** in DMSO-d_6

Figure S12. HMBC (J = 8 Hz) Spectrum of **2** in DMSO-d_6

Figure S13. HMBC (J = 3 Hz) Spectrum of **2** in DMSO-d_6

Figure S14. LR-HSQMBC (J = 2 Hz) Spectrum of **2** in DMSO-d_6

Figure S15. ROESY Spectrum of **2** in DMSO-d_6

Figure S16. ^{1}H-^{15}N HSQC Spectrum of **2** in DMSO-d_6

Figure S17. Underwater Photograph of *Damiria* sp.

Figure S18. NCI-60 Cell Line Anticancer Screening Data

Figure S19. GIAO nuclear magnetic shielding tensors for damirines A (**1**) in DMSO

TABLE S1. Calculated ^{13}C and ^{1}H chemical shifts in DMSO-d_6 using TMS or benzene as a standard reference and their statistical parameters.

Figure S1. ^{1}H Spectrum of **1** in DMSO-d_6

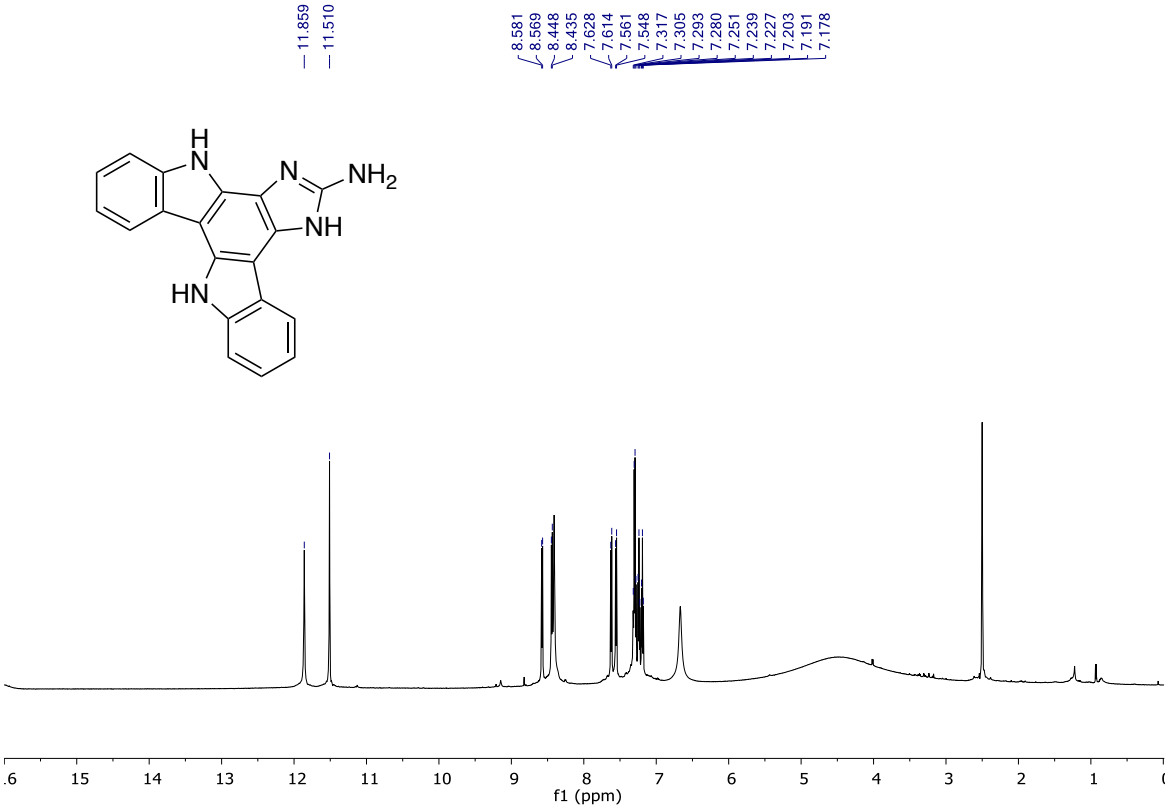

Figure S2. ^{13}C Spectrum of **1** in DMSO-d_6

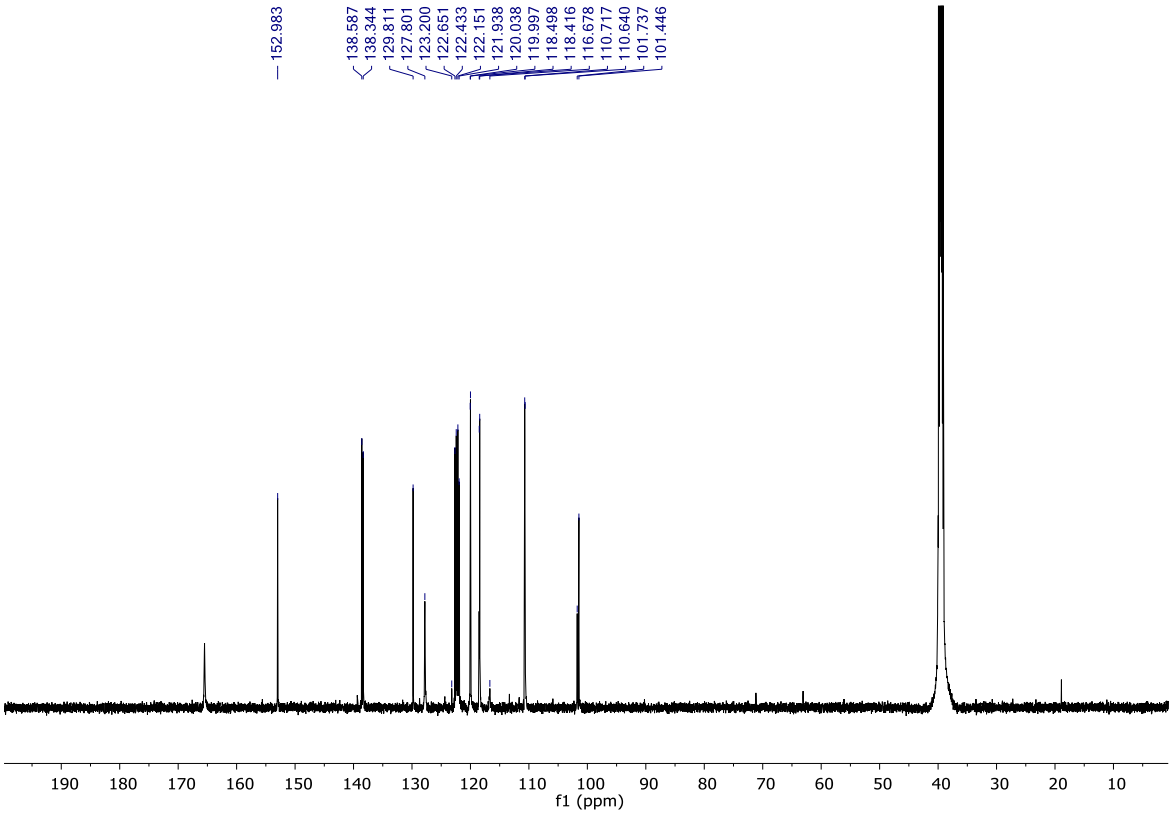

Figure S3. HSQC Spectrum of **1** in DMSO-d_6

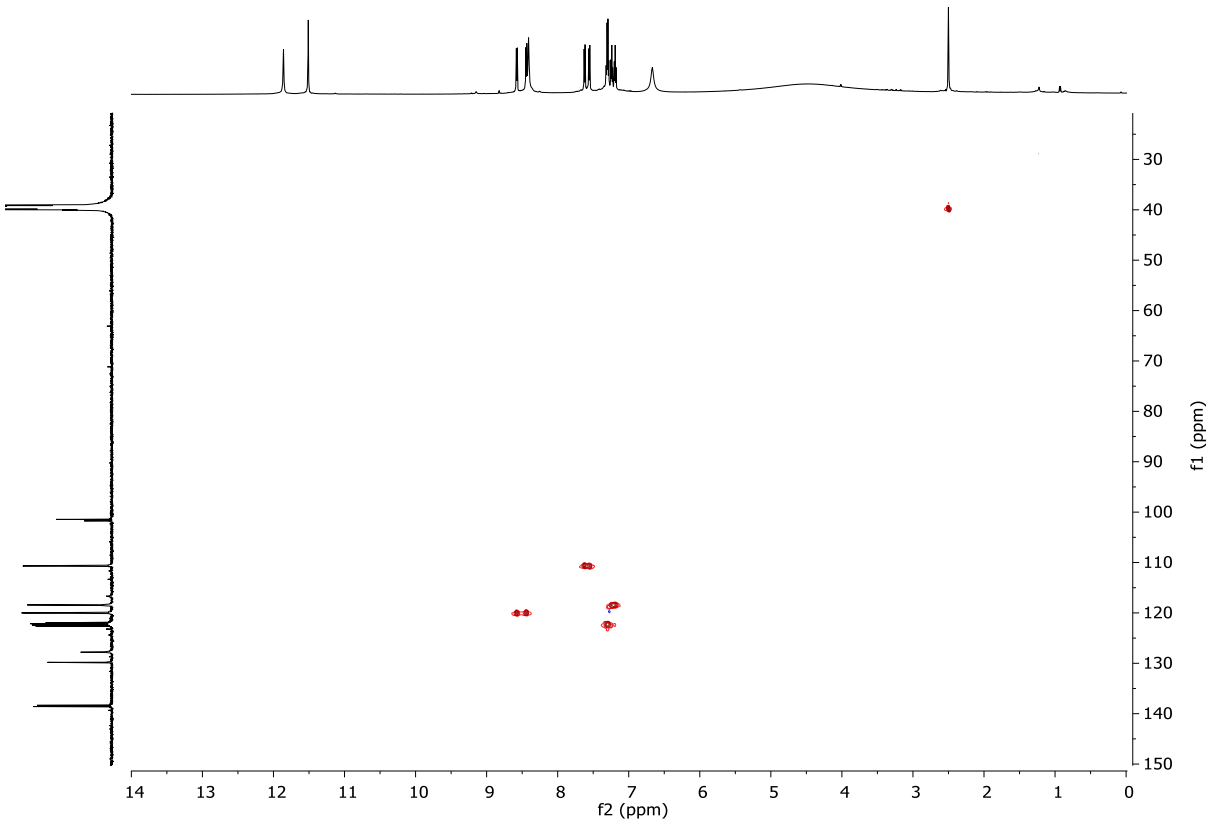

Figure S4. COSY Spectrum of **1** in DMSO-d_6

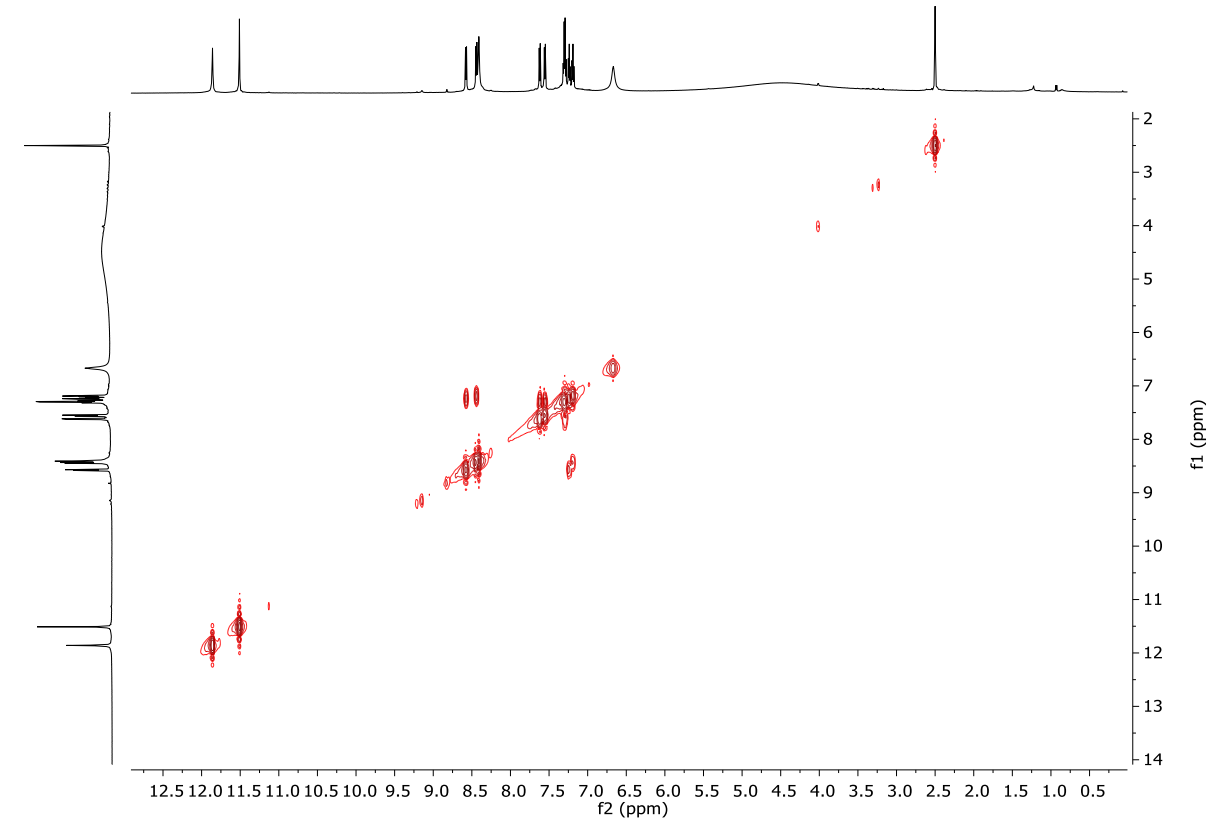

Figure S5. HMBC (J = 8 Hz) Spectrum of **1** in DMSO-d_6

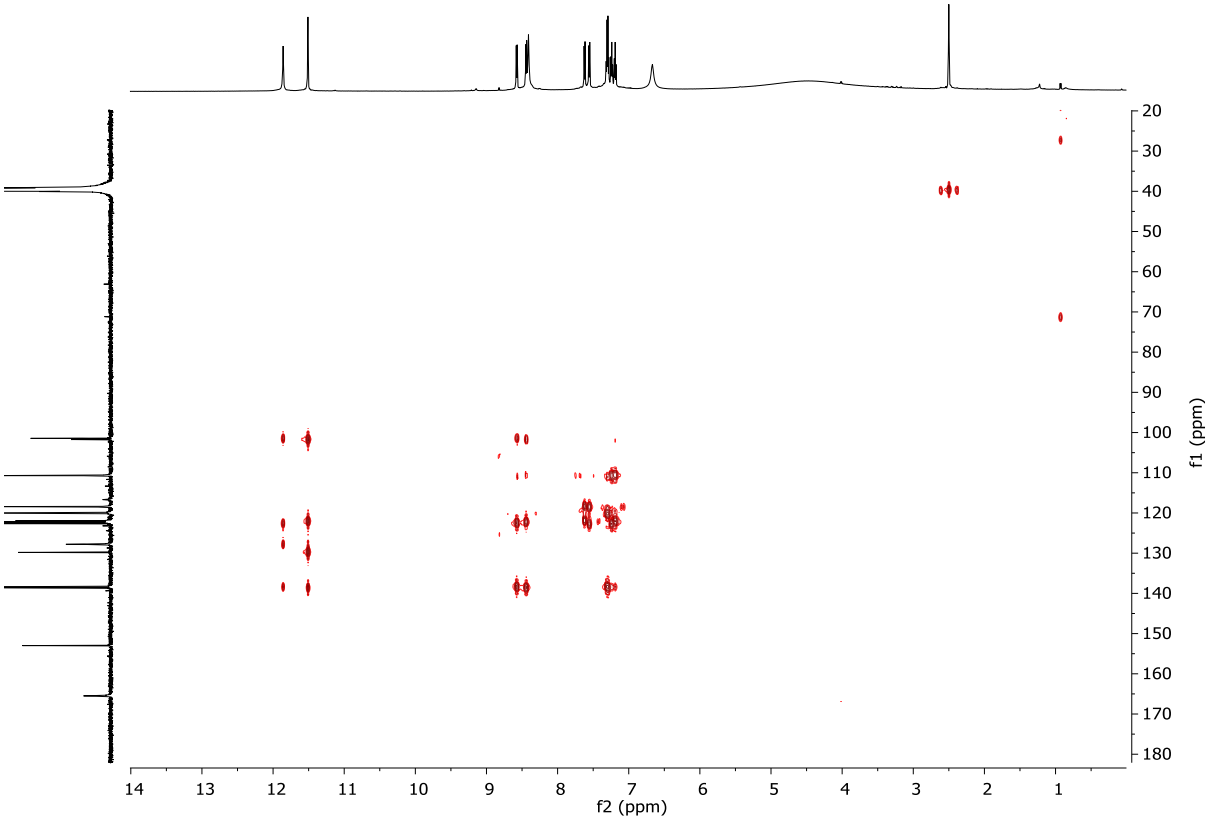

Figure S6. HMBC (J = 3 Hz) Spectrum of **1** in DMSO-d_6

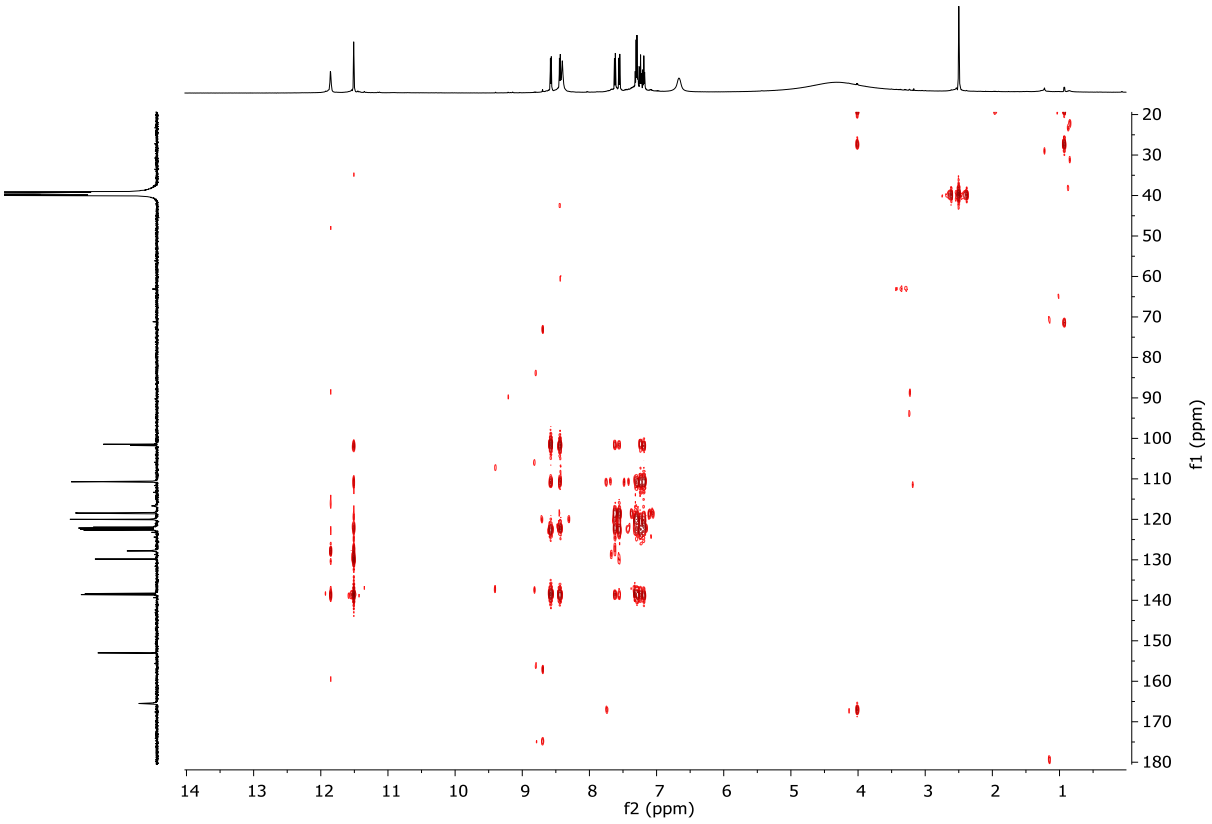

Figure S7. ROESY Spectrum of **1** in DMSO-d_6

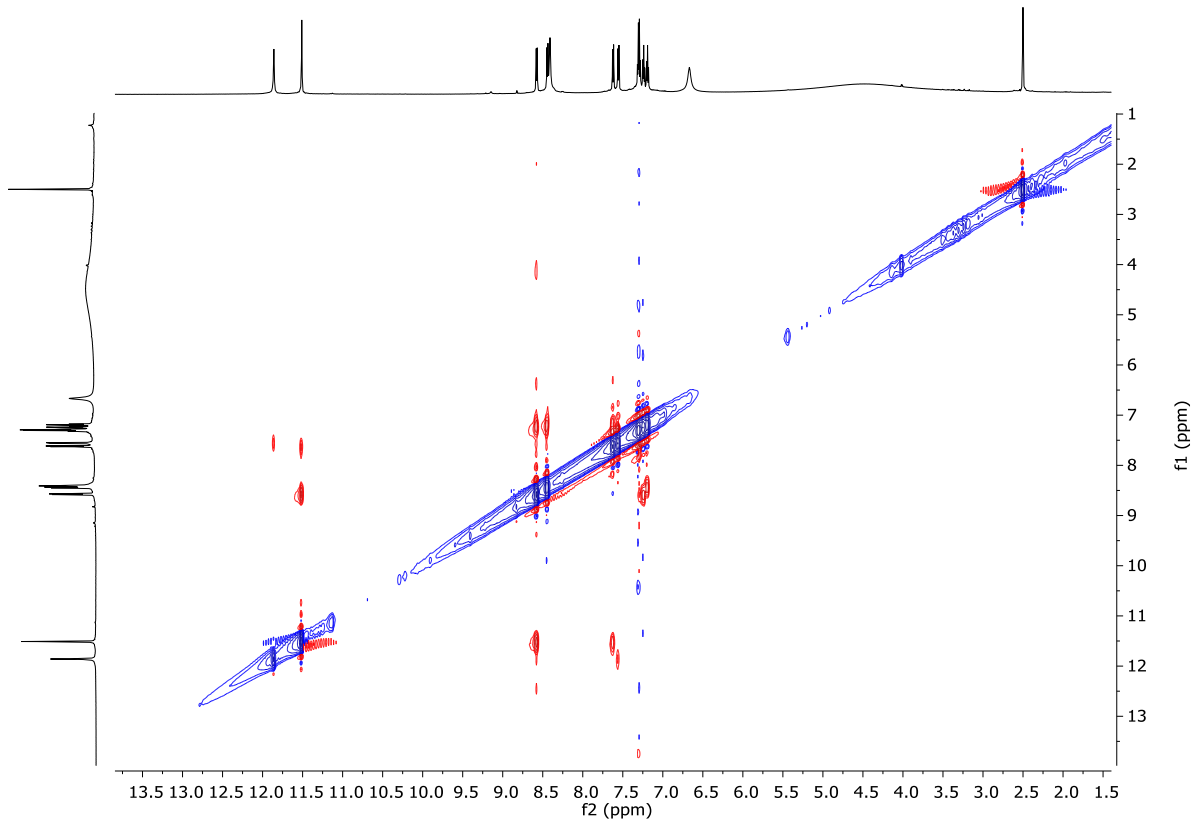

Figure S8. ^{1}H Spectrum of **2** in DMSO-d_6

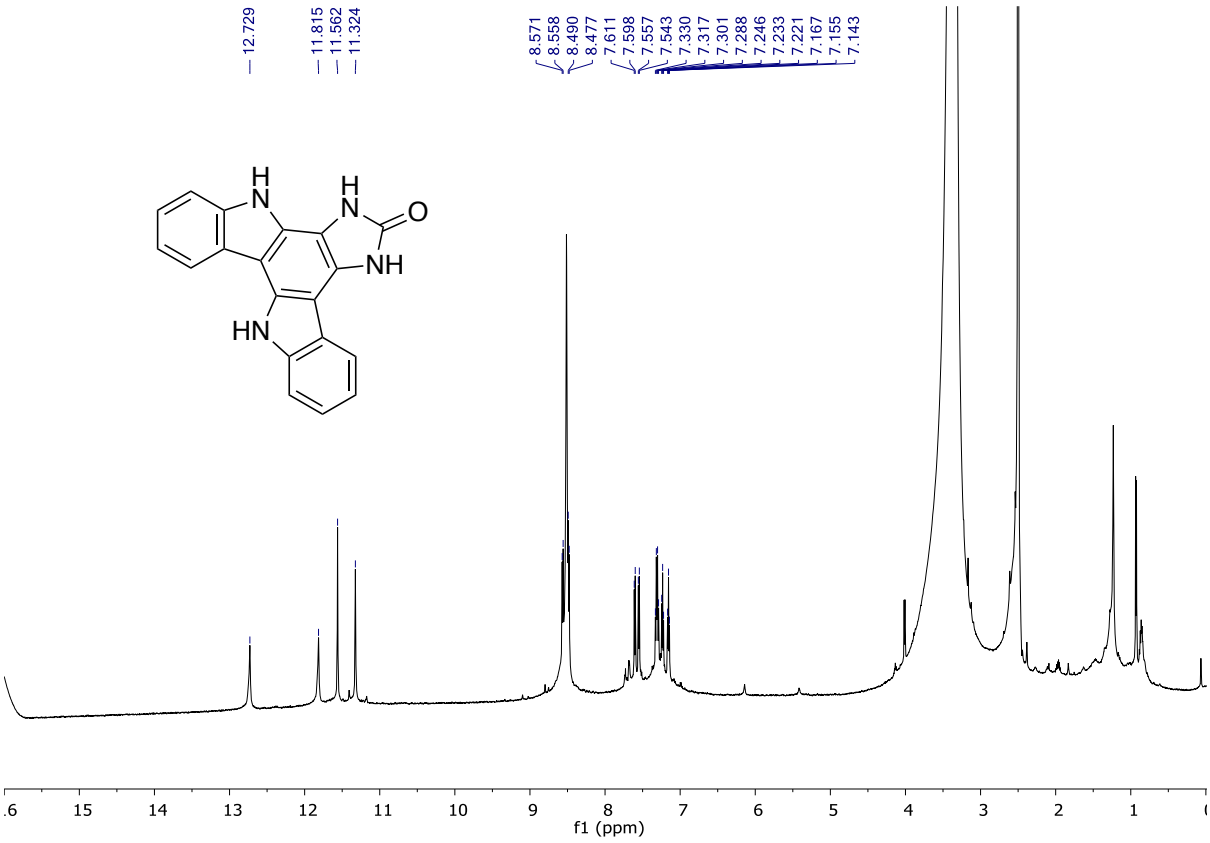

Figure S9. ^{13}C Spectrum of **2** in DMSO-d_6

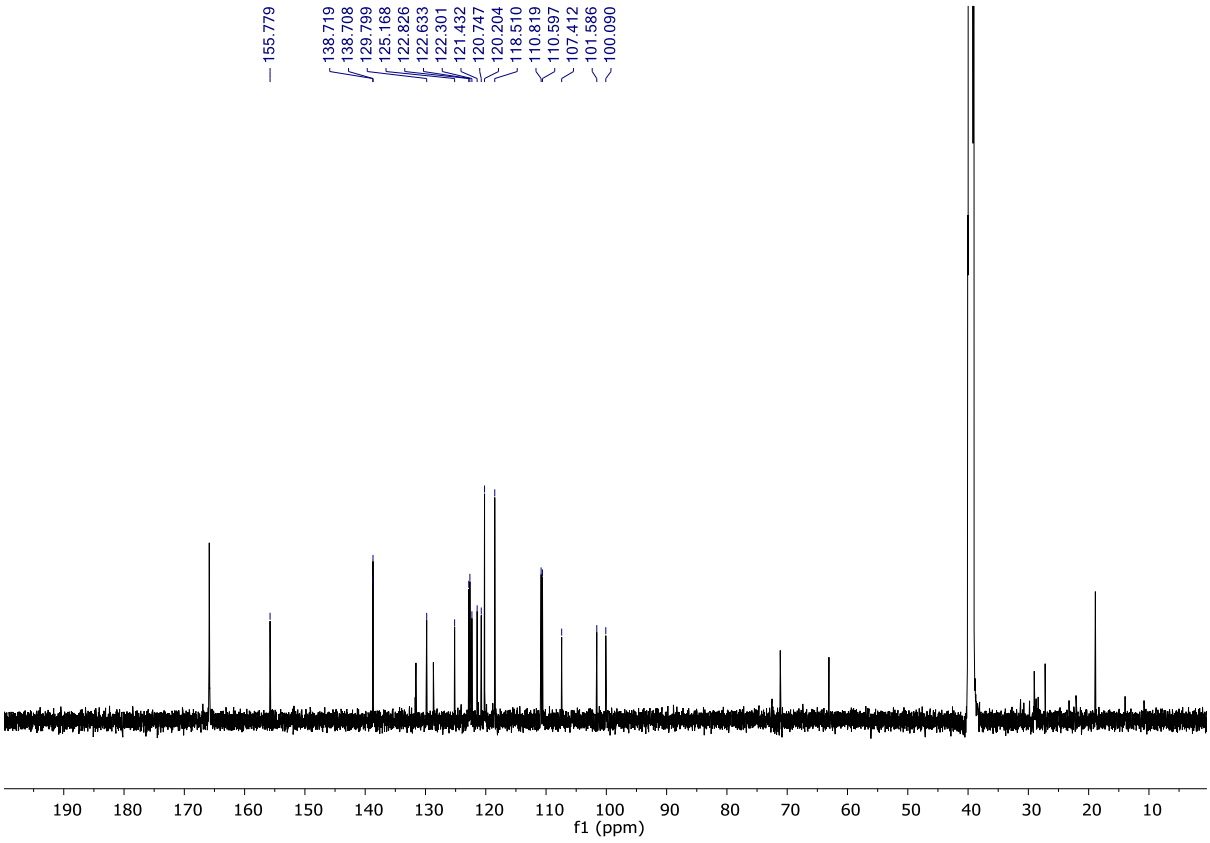

Figure S10. HSQC Spectrum of **2** in DMSO-d_6

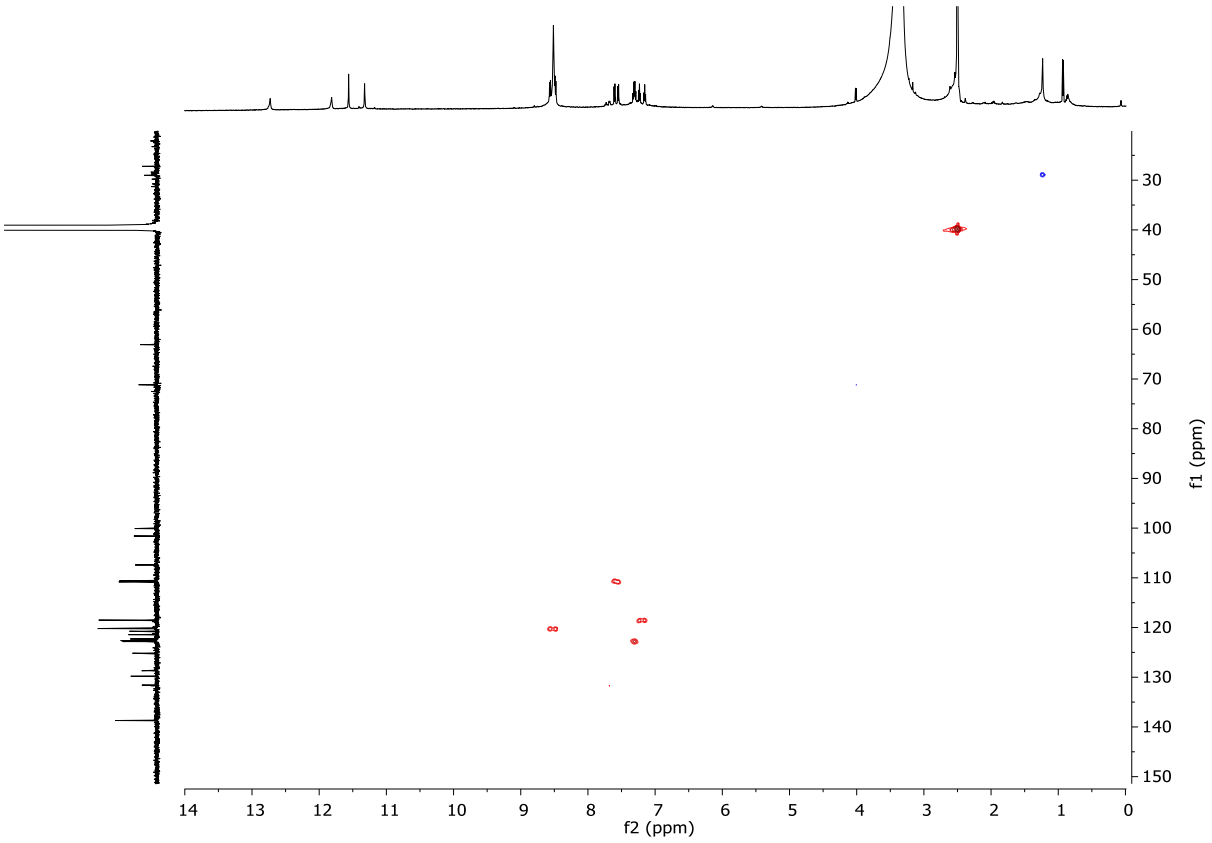

Figure S11. COSY Spectrum of **2** in DMSO-d_6

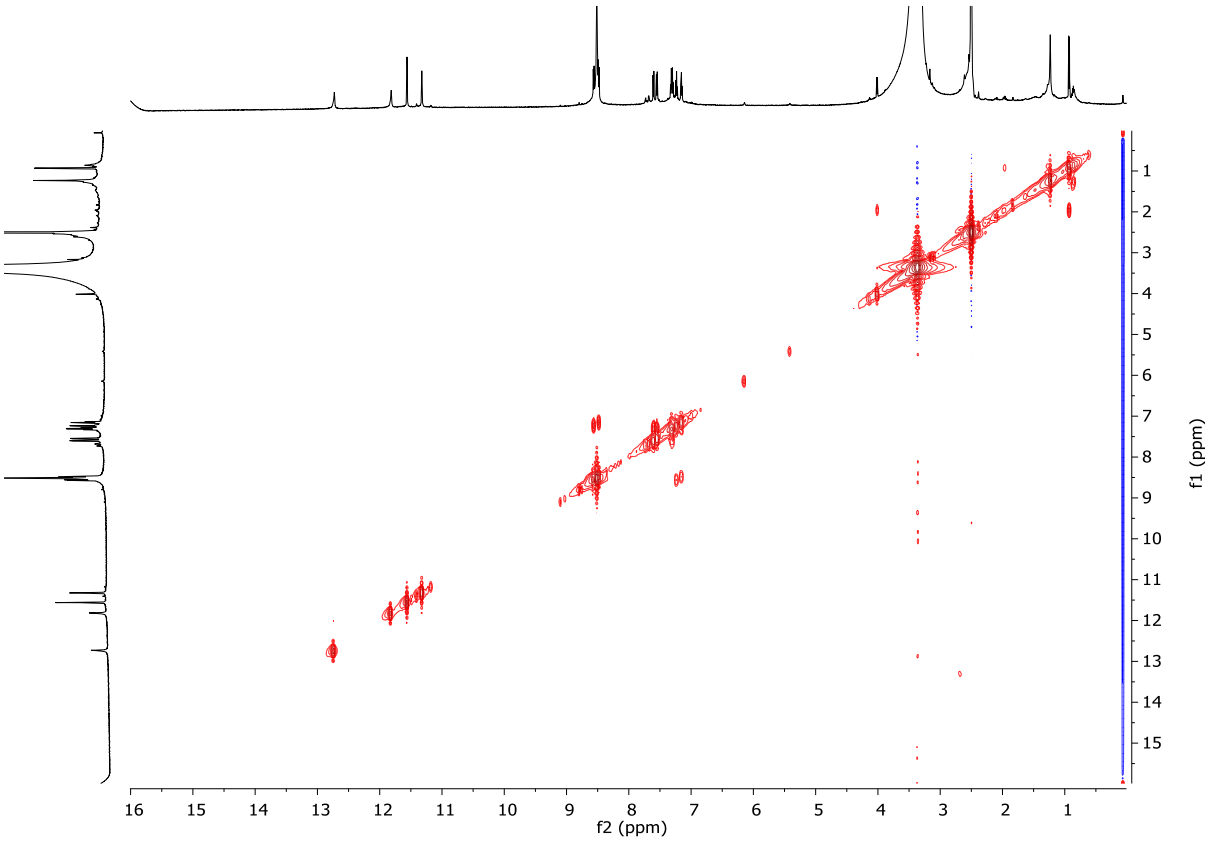

Figure S12. HMBC (J = 8 Hz) Spectrum of **2** in DMSO-d_6

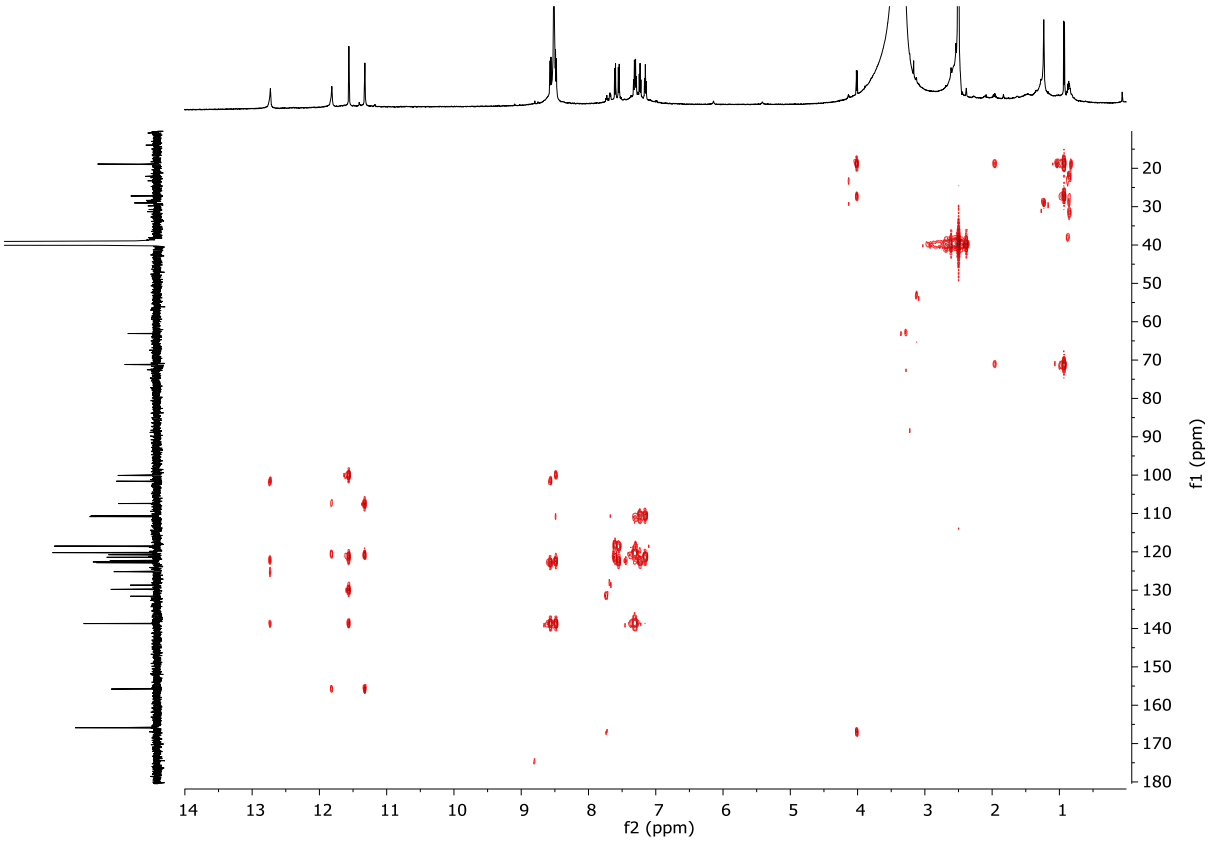

Figure S13. HMBC (J = 3 Hz) Spectrum of **2** in DMSO-d_6

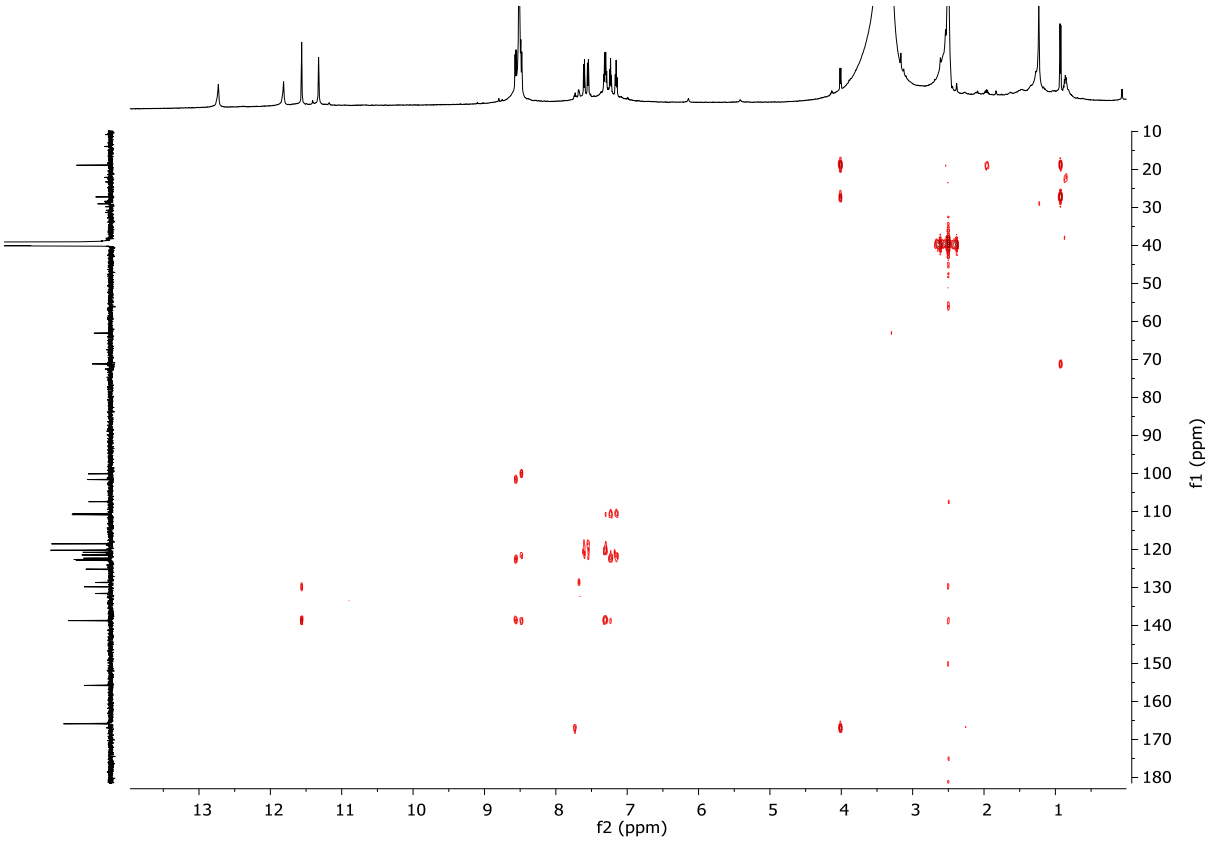

Figure S14. LR-HSQMBC (J = 2 Hz) Spectrum of **2** in DMSO-d_6

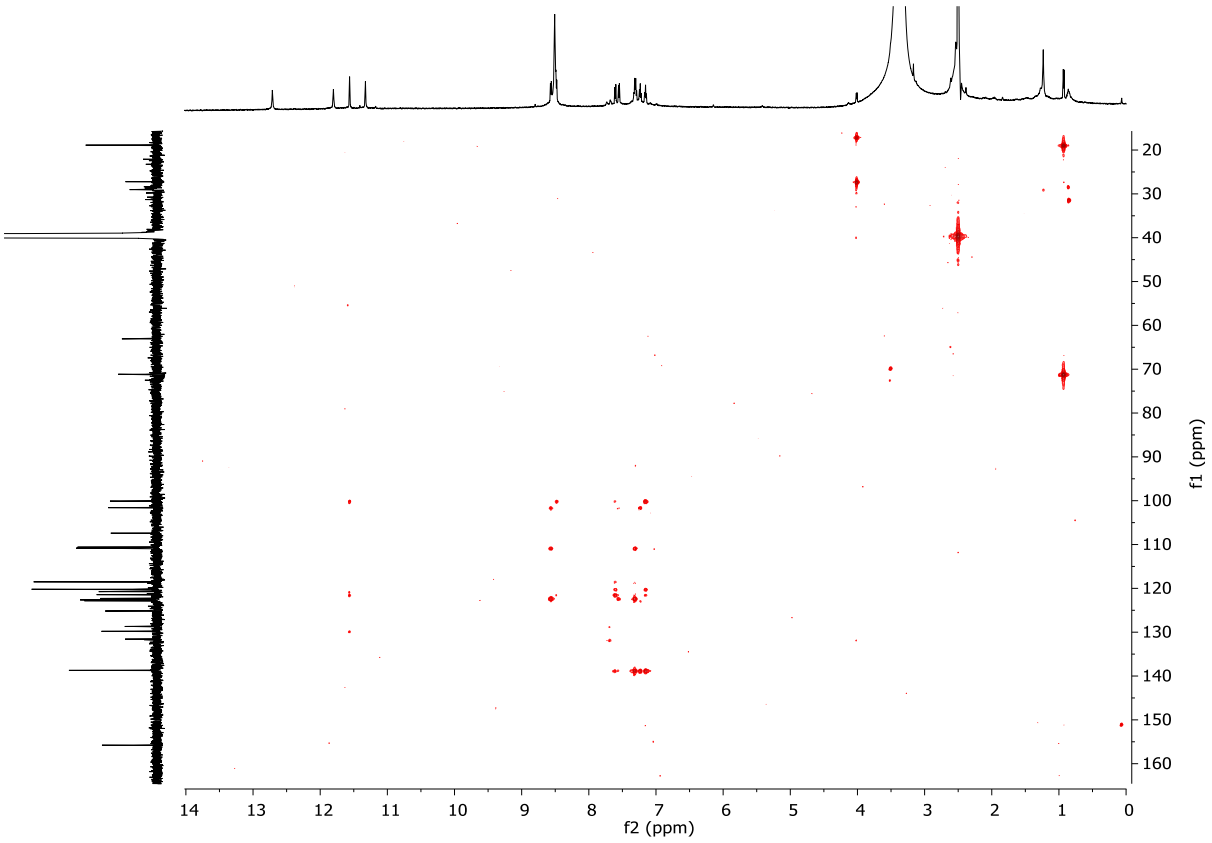

Figure S15. ROESY Spectrum of **2** in DMSO-d_6

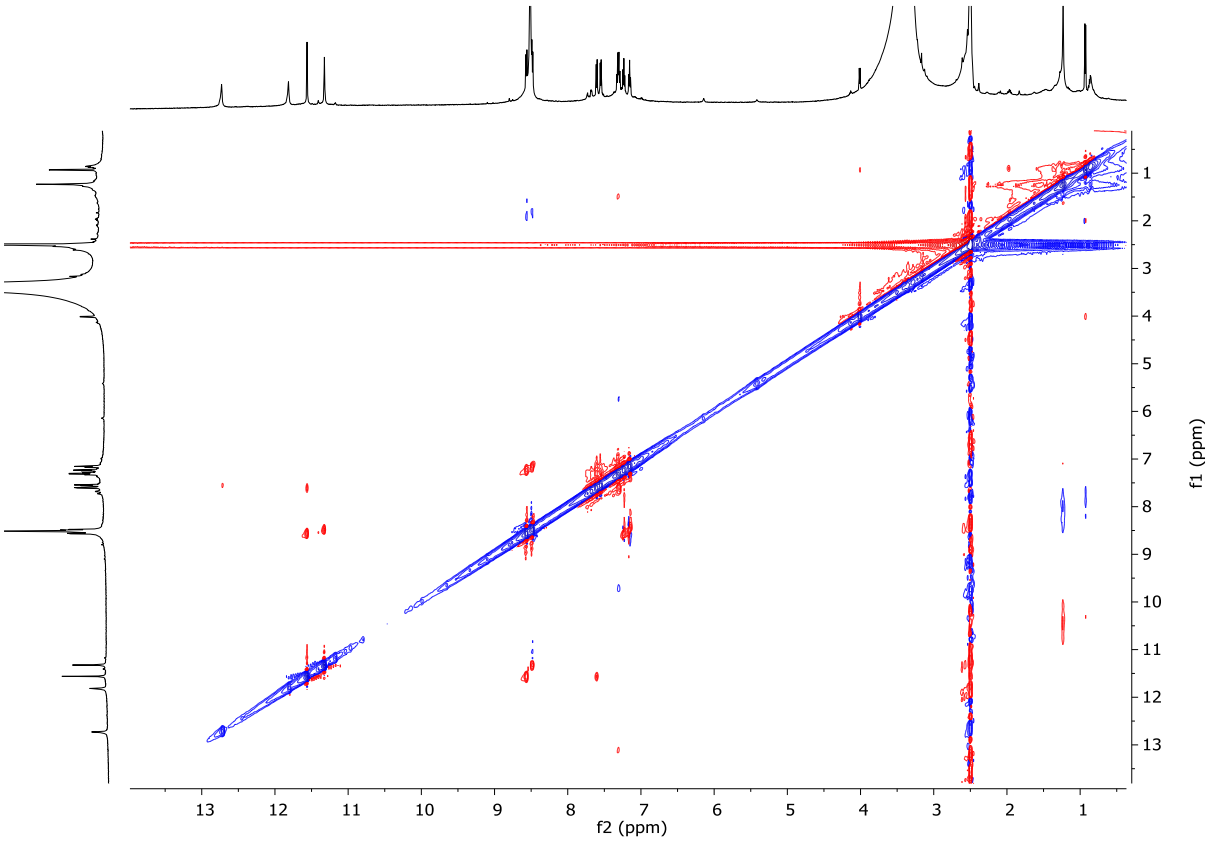

Figure S16. ^{1}H-^{15}N HSQC Spectrum of **2** in DMSO-d_6

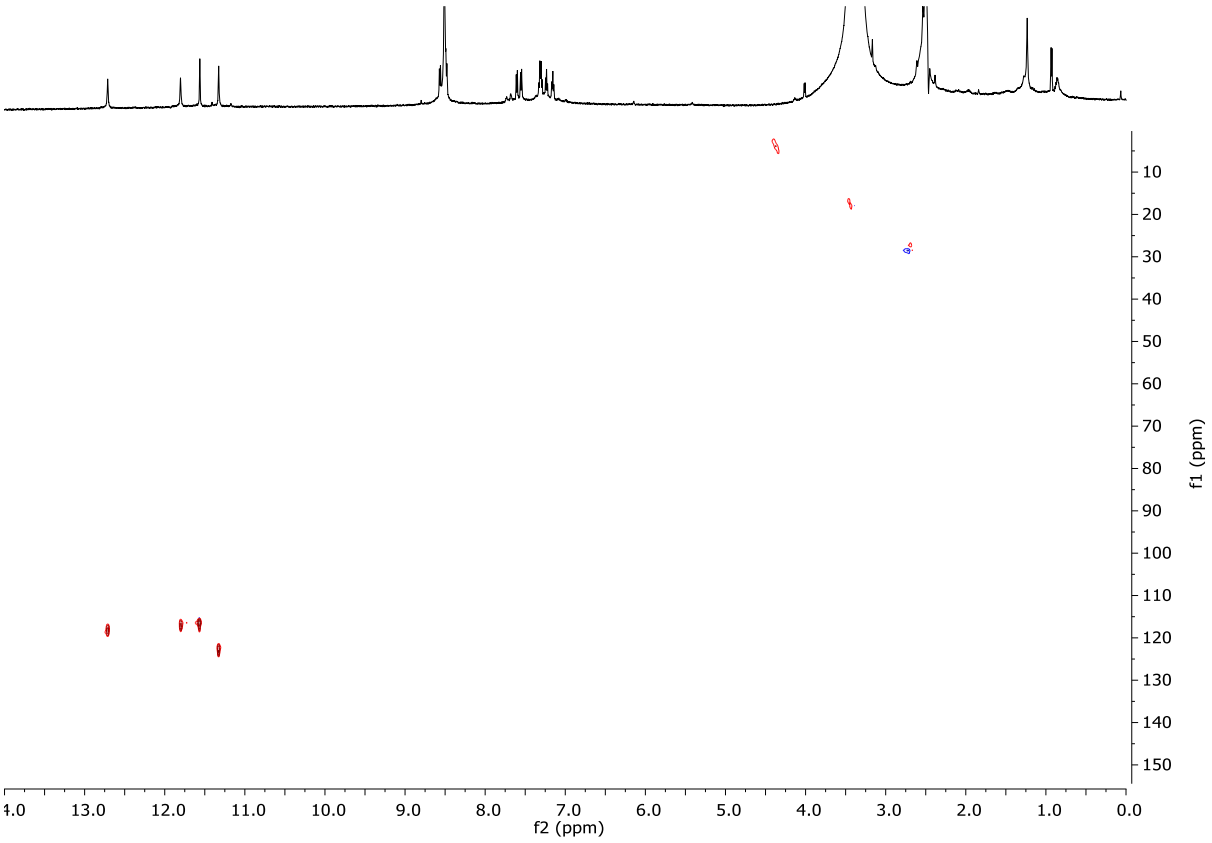

Figure S17. Underwater Photograph of *Damiria* sp.

Figure S18. NCI-60 Cell Line Anticancer Screening Data

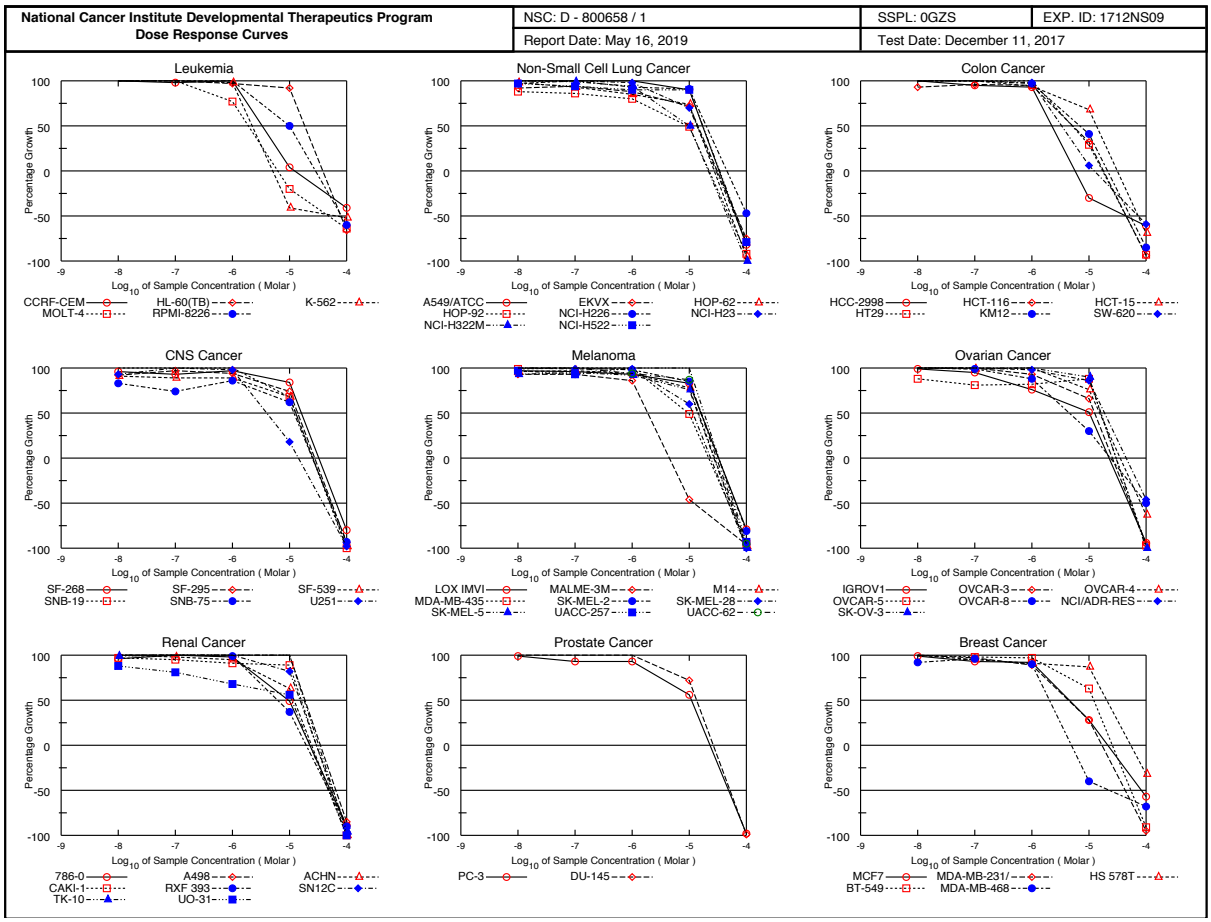

Figure S19. GIAO nuclear magnetic shielding tensors for damirines A (1) in DMSO

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SCF GIAO Magnetic shielding tensor (ppm):
      1  N    Isotropic =   199.3256   Anisotropy =   101.1541
   XX=   162.3543   YX=   -39.3419   ZX=    -0.0043
   XY=   -27.4900   YY=   256.0668   ZY=     0.0134
   XZ=     0.0075   YZ=    -0.0177   ZZ=   179.5558
   Eigenvalues:   151.6594   179.5558   266.7617
      2  C    Isotropic =    28.2395   Anisotropy =    84.3976
   XX=    29.9983   YX=   -10.2442   ZX=     0.0010
   XY=   -32.2576   YY=   -29.7845   ZY=    -0.0045
   XZ=     0.0002   YZ=     0.0008   ZZ=    84.5045
   Eigenvalues:   -36.5686    36.7825    84.5045
      3  N    Isotropic =    54.1688   Anisotropy =   258.4352
   XX=     8.5044   YX=    42.8055   ZX=    -0.0001
   XY=    45.4120   YY=   -72.4570   ZY=     0.0019
   XZ=    -0.0097   YZ=     0.0065   ZZ=   226.4589
   Eigenvalues:   -91.8450    27.8925   226.4589
      4  C    Isotropic =    55.4805   Anisotropy =   101.1711
   XX=    26.2413   YX=    -4.6475   ZX=    -0.0004
   XY=    15.6935   YY=    17.2724   ZY=     0.0007
   XZ=    -0.0037   YZ=     0.0001   ZZ=   122.9279
   Eigenvalues:    14.6425    28.8712   122.9279
      5  C    Isotropic =    52.3425   Anisotropy =   116.0975
   XX=    23.2456   YX=    24.4976   ZX=    -0.0006
   XY=    22.8027   YY=     4.0410   ZY=     0.0009
   XZ=    -0.0001   YZ=     0.0018   ZZ=   129.7408
   Eigenvalues:   -11.8819    39.1685   129.7408
      6  N    Isotropic =   120.4556   Anisotropy =    49.0421
   XX=    67.2897   YX=    23.4698   ZX=    -0.0012
   XY=     7.7364   YY=   140.9268   ZY=     0.0013
   XZ=    -0.0021   YZ=     0.0022   ZZ=   153.1504
   Eigenvalues:    64.1200   144.0965   153.1504
      7  C    Isotropic =    78.5027   Anisotropy =   113.1487
   XX=    39.8100   YX=   -10.4030   ZX=    -0.0006
   XY=    -1.8366   YY=    41.7629   ZY=     0.0003
   XZ=    -0.0009   YZ=    -0.0006   ZZ=   153.9352
   Eigenvalues:    34.5892    46.9837   153.9352
      8  C    Isotropic =    48.2181   Anisotropy =   119.7792
   XX=    25.6623   YX=    -8.6792   ZX=    -0.0005
   XY=   -14.6172   YY=    -9.0788   ZY=     0.0004
   XZ=    -0.0045   YZ=    -0.0002   ZZ=   128.0709
   Eigenvalues:   -12.6228    29.2062   128.0709
      9  N    Isotropic =   125.0515   Anisotropy =    54.7981
   XX=   119.4071   YX=    29.0842   ZX=    -0.0012
   XY=    28.0514   YY=    94.1639   ZY=     0.0019
   XZ=    -0.0010   YZ=     0.0000   ZZ=   161.5836
   Eigenvalues:    75.5537   138.0173   161.5836
     10  C    Isotropic =    40.1714   Anisotropy =   142.6695
   XX=   -34.0717   YX=    14.4677   ZX=    -0.0004
   XY=    17.7044   YY=    19.3016   ZY=     0.0010
   XZ=    -0.0001   YZ=     0.0043   ZZ=   135.2844
   Eigenvalues:   -38.5450    23.7748   135.2844
     11  C    Isotropic =    56.9383   Anisotropy =   154.9175
   XX=    17.7924   YX=   -15.3318   ZX=    -0.0005
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XY=   -20.8836   YY=    -7.1941   ZY=     0.0006
XZ=     0.0005   YZ=     0.0003   ZZ=   160.2167
Eigenvalues:   -16.7002    27.2985   160.2167
  12  C    Isotropic =    59.1155   Anisotropy =   164.8311
XX=    27.8758   YX=    33.2778   ZX=    -0.0006
XY=    35.7577   YY=   -19.5322   ZY=     0.0013
XZ=    -0.0005   YZ=     0.0011   ZZ=   169.0028
Eigenvalues:   -37.7013    46.0449   169.0028
  13  C    Isotropic =    59.5606   Anisotropy =   169.5692
XX=   -43.8721   YX=    17.3729   ZX=    -0.0006
XY=    20.1289   YY=    49.9471   ZY=     0.0010
XZ=    -0.0007   YZ=     0.0009   ZZ=   172.6067
Eigenvalues:   -47.4808    53.5559   172.6067
  14  C    Isotropic =    55.7181   Anisotropy =   175.8003
XX=    11.0130   YX=   -44.3879   ZX=     0.0000
XY=   -49.2016   YY=   -16.7770   ZY=     0.0013
XZ=     0.0001   YZ=     0.0009   ZZ=   172.9183
Eigenvalues:   -51.6961    45.9321   172.9183
  15  C    Isotropic =    69.1971   Anisotropy =   149.7041
XX=    50.6184   YX=    21.0312   ZX=    -0.0002
XY=    17.9605   YY=   -12.0270   ZY=     0.0015
XZ=     0.0002   YZ=     0.0006   ZZ=   168.9998
Eigenvalues:   -17.5987    56.1901   168.9998
  16  C    Isotropic =    77.8363   Anisotropy =   114.1172
XX=    36.5293   YX=     3.0363   ZX=     0.0000
XY=     9.7955   YY=    43.0651   ZY=    -0.0001
XZ=     0.0010   YZ=    -0.0010   ZZ=   153.9145
Eigenvalues:    32.5970    46.9974   153.9145
  17  C    Isotropic =    49.1332   Anisotropy =   122.4210
XX=    -5.4427   YX=    -1.5154   ZX=    -0.0001
XY=   -13.4917   YY=    22.0951   ZY=     0.0005
XZ=     0.0009   YZ=     0.0023   ZZ=   130.7472
Eigenvalues:    -7.3546    24.0069   130.7472
  18  N    Isotropic =   127.2444   Anisotropy =    58.5206
XX=   127.2833   YX=   -25.5663   ZX=     0.0003
XY=   -25.6880   YY=    88.1917   ZY=     0.0008
XZ=     0.0004   YZ=     0.0004   ZZ=   166.2581
Eigenvalues:    75.5073   139.9677   166.2581
  19  C    Isotropic =    39.8890   Anisotropy =   142.9454
XX=    20.2462   YX=    14.1376   ZX=     0.0002
XY=    17.0164   YY=   -35.7651   ZY=     0.0000
XZ=     0.0019   YZ=     0.0006   ZZ=   135.1860
Eigenvalues:   -39.8057    24.2868   135.1860
  20  C    Isotropic =    55.0875   Anisotropy =   154.3055
XX=   -18.2292   YX=     0.0610   ZX=     0.0005
XY=    -4.6943   YY=    25.5339   ZY=     0.0000
XZ=    -0.0001   YZ=    -0.0005   ZZ=   157.9578
Eigenvalues:   -18.3515    25.6562   157.9578
  21  C    Isotropic =    59.0117   Anisotropy =   164.0005
XX=    22.3283   YX=   -38.9256   ZX=     0.0003
XY=   -36.6444   YY=   -13.6386   ZY=    -0.0001
XZ=     0.0005   YZ=     0.0003   ZZ=   168.3454
Eigenvalues:   -37.5015    46.1912   168.3454
  22  C    Isotropic =    59.2725   Anisotropy =   169.5688
XX=    42.0245   YX=    30.4610   ZX=     0.0004
XY=    33.1254   YY=   -36.5255   ZY=    -0.0002
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XZ=     0.0004   YZ=    -0.0003   ZZ=   172.3184
Eigenvalues:   -47.7810    53.2800   172.3184
  23  C    Isotropic =    55.4654   Anisotropy =   176.6037
XX=   -50.7622   YX=    13.5527   ZX=     0.0006
XY=     8.8610   YY=    43.9573   ZY=    -0.0001
XZ=     0.0005   YZ=    -0.0002   ZZ=   173.2012
Eigenvalues:   -52.0701    45.2652   173.2012
  24  C    Isotropic =    69.0863   Anisotropy =   150.2300
XX=    20.8356   YX=   -35.2773   ZX=     0.0004
XY=   -38.3624   YY=    17.1836   ZY=     0.0000
XZ=     0.0002   YZ=    -0.0004   ZZ=   169.2396
Eigenvalues:   -17.8555    55.8747   169.2396
  25  H    Isotropic =    27.5397   Anisotropy =    14.1316
XX=    27.3019   YX=     1.9046   ZX=     0.0007
XY=     6.1958   YY=    35.2624   ZY=     0.0038
XZ=     0.0013   YZ=     0.0050   ZZ=    20.0548
Eigenvalues:    20.0548    25.6035    36.9608
  26  H    Isotropic =    27.5410   Anisotropy =    13.1402
XX=    34.2463   YX=    -2.7581   ZX=    -0.0039
XY=    -5.1370   YY=    28.7174   ZY=     0.0024
XZ=    -0.0056   YZ=     0.0030   ZZ=    19.6593
Eigenvalues:    19.6593    26.6626    36.3011
  27  H    Isotropic =    23.5509   Anisotropy =     9.6397
XX=    29.7068   YX=     0.9907   ZX=     0.0000
XY=     0.6904   YY=    27.3656   ZY=     0.0001
XZ=    -0.0002   YZ=     0.0000   ZZ=    13.5803
Eigenvalues:    13.5803    27.0951    29.9773
  28  H    Isotropic =    23.2328   Anisotropy =    11.3122
XX=    29.2774   YX=    -1.6613   ZX=     0.0002
XY=    -1.3051   YY=    29.3045   ZY=    -0.0002
XZ=     0.0004   YZ=    -0.0007   ZZ=    11.1164
Eigenvalues:    11.1164    27.8077    30.7742
  29  H    Isotropic =    23.6030   Anisotropy =     9.3235
XX=    28.5900   YX=     2.0968   ZX=     0.0000
XY=     2.4716   YY=    25.5720   ZY=     0.0000
XZ=     0.0000   YZ=     0.0000   ZZ=    16.6470
Eigenvalues:    16.6470    24.3434    29.8187
  30  H    Isotropic =    24.3326   Anisotropy =     5.3820
XX=    25.8357   YX=     0.8118   ZX=     0.0000
XY=     0.9201   YY=    27.5610   ZY=     0.0000
XZ=     0.0000   YZ=     0.0000   ZZ=    19.6012
Eigenvalues:    19.6012    25.4761    27.9206
  31  H    Isotropic =    24.2599   Anisotropy =     4.8907
XX=    27.1063   YX=    -0.7772   ZX=     0.0000
XY=    -0.8266   YY=    25.9673   ZY=     0.0000
XZ=     0.0000   YZ=    -0.0001   ZZ=    19.7061
Eigenvalues:    19.7061    25.5533    27.5204
  32  H    Isotropic =    24.0666   Anisotropy =     7.0470
XX=    27.8846   YX=     1.5526   ZX=     0.0000
XY=     1.5222   YY=    26.0788   ZY=     0.0000
XZ=     0.0000   YZ=    -0.0001   ZZ=    18.2364
Eigenvalues:    18.2364    25.1988    28.7646
  33  H    Isotropic =    23.5552   Anisotropy =    10.7047
XX=    27.8873   YX=     1.0149   ZX=     0.0000
XY=     1.7136   YY=    30.0280   ZY=    -0.0001
XZ=    -0.0002   YZ=    -0.0003   ZZ=    12.7503
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   Eigenvalues:    12.7503    27.2237    30.6917
     34  H    Isotropic =    23.4932   Anisotropy =     9.7743
   XX=    28.5419   YX=    -2.7638   ZX=     0.0000
   XY=    -2.2343   YY=    25.7539   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=    16.1840
   Eigenvalues:    16.1840    24.2863    30.0094
     35  H    Isotropic =    24.3208   Anisotropy =     5.4594
   XX=    27.9140   YX=     0.2840   ZX=     0.0000
   XY=     0.3927   YY=    25.4886   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=    19.5596
   Eigenvalues:    19.5596    25.4423    27.9604
     36  H    Isotropic =    24.2536   Anisotropy =     4.8349
   XX=    25.5478   YX=    -0.0366   ZX=     0.0000
   XY=    -0.0821   YY=    27.4751   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=    19.7381
   Eigenvalues:    19.7381    25.5460    27.4769
     37  H    Isotropic =    24.1187   Anisotropy =     6.8107
   XX=    27.8812   YX=    -1.4309   ZX=     0.0000
   XY=    -1.4203   YY=    26.0466   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=    18.4281
   Eigenvalues:    18.4281    25.2687    28.6591
```

Calculating GIAO nuclear magnetic shielding tensors for TMS in DMSO.

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  C    Isotropic =   184.7055   Anisotropy =    10.1581
   XX=   184.6788   YX=    -0.8392   ZX=    -4.7131
   XY=    -0.8277   YY=   181.5183   ZY=     1.1055
   XZ=    -4.7132   YZ=     1.1249   ZZ=   187.9194
   Eigenvalues:   181.2889   181.3501   191.4776
      2  Si   Isotropic =   339.7811   Anisotropy =     0.2642
   XX=   339.6943   YX=     0.0547   ZX=     0.1194
   XY=    -0.0101   YY=   339.7450   ZY=    -0.1055
   XZ=    -0.0329   YZ=    -0.0987   ZZ=   339.9040
   Eigenvalues:   339.6542   339.7318   339.9572
      3  C    Isotropic =   184.7097   Anisotropy =    10.0531
   XX=   181.9032   YX=     2.0294   ZX=    -0.9879
   XY=     2.0897   YY=   189.2537   ZY=    -3.5612
   XZ=    -0.9896   YZ=    -3.5661   ZZ=   182.9720
   Eigenvalues:   181.3065   181.4107   191.4117
      4  C    Isotropic =   184.6954   Anisotropy =    10.1004
   XX=   188.4201   YX=    -4.0398   ZX=     2.2476
   XY=    -4.0060   YY=   183.5983   ZY=    -1.3258
   XZ=     2.2504   YZ=    -1.3390   ZZ=   182.0677
   Eigenvalues:   181.2789   181.3783   191.4289
      5  C    Isotropic =   184.6900   Anisotropy =    10.0010
   XX=   183.8138   YX=     2.7164   ZX=     3.3481
   XY=     2.6923   YY=   184.3525   ZY=     3.7258
   XZ=     3.2866   YZ=     3.7162   ZZ=   185.9035
   Eigenvalues:   181.3267   181.3859   191.3573
      6  H    Isotropic =    31.9458   Anisotropy =     9.2668
   XX=    29.9046   YX=     2.3567   ZX=    -2.6912
   XY=     2.1649   YY=    33.7443   ZY=    -3.4860
```

```
XZ=    -2.6758   YZ=    -3.7575   ZZ=    32.1885
Eigenvalues:    28.1251    29.5886    38.1236
   7  H    Isotropic =    31.9458   Anisotropy =     9.2749
XX=    29.8036   YX=     1.3382   ZX=     1.2120
XY=     1.4792   YY=    30.7716   ZY=     4.0477
XZ=     1.4953   YZ=     4.1760   ZZ=    35.2621
Eigenvalues:    28.1247    29.5836    38.1291
   8  H    Isotropic =    31.9450   Anisotropy =     9.2633
XX=    36.1271   YX=    -4.0003   ZX=    -0.2527
XY=    -3.9420   YY=    30.1464   ZY=    -0.1463
XZ=    -0.5531   YZ=     0.0087   ZZ=    29.5616
Eigenvalues:    28.1247    29.5897    38.1206
   9  H    Isotropic =    31.9469   Anisotropy =     9.2749
XX=    31.3300   YX=     0.6991   ZX=    -4.5670
XY=     0.8952   YY=    29.8518   ZY=    -1.3960
XZ=    -4.5807   YZ=    -1.1265   ZZ=    34.6590
Eigenvalues:    28.1239    29.5868    38.1302
  10  H    Isotropic =    31.9442   Anisotropy =     9.2690
XX=    32.9298   YX=    -3.5091   ZX=     1.9228
XY=    -3.8177   YY=    33.4157   ZY=    -2.6902
XZ=     2.0618   YZ=    -2.6772   ZZ=    29.4871
Eigenvalues:    28.1192    29.5899    38.1235
  11  H    Isotropic =    31.9458   Anisotropy =     9.2640
XX=    30.5391   YX=     3.5830   ZX=     2.2989
XY=     3.6935   YY=    34.2519   ZY=     2.7688
XZ=     2.1706   YZ=     2.4706   ZZ=    31.0465
Eigenvalues:    28.1232    29.5925    38.1219
  12  H    Isotropic =    31.9463   Anisotropy =     9.2731
XX=    34.2671   YX=    -2.3309   ZX=    -4.0758
XY=    -2.3871   YY=    29.0997   ZY=     1.2333
XZ=    -3.7743   YZ=     1.0822   ZZ=    32.4721
Eigenvalues:    28.1267    29.5839    38.1284
  13  H    Isotropic =    31.9448   Anisotropy =     9.2660
XX=    33.3027   YX=     1.5855   ZX=     4.4800
XY=     1.3364   YY=    30.0759   ZY=     2.1150
XZ=     4.3265   YZ=     2.2848   ZZ=    32.4559
Eigenvalues:    28.1198    29.5925    38.1221
  14  H    Isotropic =    31.9474   Anisotropy =     9.2651
XX=    29.6446   YX=    -0.7392   ZX=     0.4317
XY=    -0.4338   YY=    36.2621   ZY=    -3.8227
XZ=     0.2865   YZ=    -3.8445   ZZ=    29.9355
Eigenvalues:    28.1248    29.5933    38.1241
  15  H    Isotropic =    31.9479   Anisotropy =     9.2702
XX=    30.2733   YX=    -0.2942   ZX=    -2.5505
XY=    -0.4351   YY=    29.3342   ZY=     2.8522
XZ=    -2.8372   YZ=     2.7272   ZZ=    36.2362
Eigenvalues:    28.1235    29.5921    38.1281
  16  H    Isotropic =    31.9470   Anisotropy =     9.2588
XX=    29.5864   YX=     3.3674   ZX=     0.0051
XY=     3.2579   YY=    36.7050   ZY=    -1.2248
XZ=     0.1348   YZ=    -0.9292   ZZ=    29.5498
Eigenvalues:    28.1246    29.5970    38.1196
  17  H    Isotropic =    31.9462   Anisotropy =     9.2655
XX=    35.6398   YX=    -2.0640   ZX=     3.7795
XY=    -1.8137   YY=    29.6852   ZY=    -0.2496
XZ=     3.9373   YZ=    -0.4142   ZZ=    30.5137
```

```
   Eigenvalues:    28.1208    29.5946    38.1232
```

Calculated GIAO nuclear magnetic shielding tensors for benzene in DMSO.

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  C    Isotropic =    49.3770   Anisotropy =   187.0180
   XX=   -20.8367   YX=    50.2295   ZX=    -0.0126
   XY=    50.2263   YY=    -5.0880   ZY=     0.0001
   XZ=    -0.0034   YZ=     0.0073   ZZ=   174.0557
   Eigenvalues:   -63.8037    37.8791   174.0557
      2  C    Isotropic =    49.3755   Anisotropy =   187.0164
   XX=    34.4553   YX=   -18.3091   ZX=     0.0019
   XY=   -18.3080   YY=   -60.3820   ZY=    -0.0115
   XZ=     0.0002   YZ=     0.0070   ZZ=   174.0531
   Eigenvalues:   -63.7938    37.8670   174.0531
      3  C    Isotropic =    49.3756   Anisotropy =   187.0105
   XX=   -52.5268   YX=   -31.9208   ZX=     0.0232
   XY=   -31.9282   YY=    26.6042   ZY=     0.0039
   XZ=     0.0150   YZ=     0.0069   ZZ=   174.0492
   Eigenvalues:   -63.8002    37.8777   174.0492
      4  C    Isotropic =    49.3779   Anisotropy =   187.0182
   XX=   -20.8183   YX=    50.2236   ZX=     0.0054
   XY=    50.2389   YY=    -5.1046   ZY=     0.0058
   XZ=     0.0085   YZ=    -0.0102   ZZ=   174.0567
   Eigenvalues:   -63.8034    37.8805   174.0567
      5  C    Isotropic =    49.3769   Anisotropy =   187.0166
   XX=    34.4627   YX=   -18.2814   ZX=    -0.0034
   XY=   -18.2985   YY=   -60.3867   ZY=     0.0044
   XZ=     0.0019   YZ=     0.0006   ZZ=   174.0546
   Eigenvalues:   -63.7914    37.8674   174.0546
      6  C    Isotropic =    49.3758   Anisotropy =   187.0089
   XX=   -52.5374   YX=   -31.9152   ZX=    -0.0118
   XY=   -31.9038   YY=    26.6164   ZY=    -0.0000
   XZ=    -0.0179   YZ=    -0.0075   ZZ=   174.0484
   Eigenvalues:   -63.7989    37.8780   174.0484
      7  H    Isotropic =    24.2620   Anisotropy =     4.8431
   XX=    25.4855   YX=     1.7154   ZX=    -0.0003
   XY=     1.7157   YY=    26.0229   ZY=     0.0001
   XZ=     0.0002   YZ=     0.0001   ZZ=    21.2776
   Eigenvalues:    21.2776    24.0178    27.4907
      8  H    Isotropic =    24.2625   Anisotropy =     4.8428
   XX=    27.3748   YX=    -0.6244   ZX=     0.0001
   XY=    -0.6248   YY=    24.1361   ZY=     0.0001
   XZ=     0.0000   YZ=     0.0004   ZZ=    21.2768
   Eigenvalues:    21.2768    24.0198    27.4911
      9  H    Isotropic =    24.2637   Anisotropy =     4.8428
   XX=    24.4041   YX=    -1.0892   ZX=     0.0003
   XY=    -1.0891   YY=    27.1081   ZY=     0.0000
   XZ=    -0.0005   YZ=    -0.0001   ZZ=    21.2789
   Eigenvalues:    21.2789    24.0199    27.4922
     10  H    Isotropic =    24.2621   Anisotropy =     4.8432
   XX=    25.4844   YX=     1.7152   ZX=     0.0000
   XY=     1.7157   YY=    26.0243   ZY=     0.0001
   XZ=     0.0000   YZ=    -0.0001   ZZ=    21.2777
```

```
Eigenvalues:    21.2777    24.0178    27.4909
  11  H    Isotropic =    24.2627   Anisotropy =     4.8428
XX=    27.3746   YX=    -0.6253   ZX=    -0.0001
XY=    -0.6259   YY=    24.1366   ZY=    -0.0003
XZ=     0.0001   YZ=    -0.0003   ZZ=    21.2769
Eigenvalues:    21.2769    24.0200    27.4912
  12  H    Isotropic =    24.2636   Anisotropy =     4.8427
XX=    24.4048   YX=    -1.0901   ZX=     0.0002
XY=    -1.0898   YY=    27.1072   ZY=     0.0001
XZ=     0.0002   YZ=     0.0000   ZZ=    21.2787
Eigenvalues:    21.2787    24.0200    27.4920
```

TABLE S1. Calculated ^{13}C and ^{1}H chemical shifts in DMSO-d_6 using TMS or benzene as a standard reference and their statistical parameters.

Position	δ^{C}_{exp}	TMS[a]		Benzene[b]		δ^{H}_{exp}	TMS[a]		Benzene[b]	
		δ^{C}_{calc}	δ^{C}_{calc*}	δ^{C}_{calc}	δ^{C}_{calc*}		δ^{H}_{calc}	δ^{H}_{calc*}	δ^{H}_{calc}	δ^{H}_{calc*}
1	110.6	115.5	108.9	108.5	108.9	7.62	7.88	7.63	7.57	7.63
2	122.2	129.0	122.5	122.0	122.5	7.29	7.69	7.31	7.37	7.31
3	118.4	125.1	118.6	118.1	118.6	7.19	7.61	7.19	7.30	7.19
4	120.0	125.6	119.1	118.6	119.1	8.44	8.34	8.41	8.03	8.41
4a	121.9	127.8	121.3	120.7	121.3					
4b	101.7	106.2	99.5	99.2	99.5					
4c	123.2	132.4	125.9	125.3	125.9					
6	153.0	156.5	150.2	149.4	150.2					
7a	116.7	129.2	122.7	122.2	122.7					
7b	127.8	135.6	129.1	128.5	129.1					
8a	138.3	144.8	138.5	137.8	138.5					
9	110.7	115.6	109.0	108.6	109.0	7.55	7.83	7.55	7.51	7.55
10	122.4	129.2	122.8	122.2	122.8	7.30	7.69	7.32	7.38	7.32
11	118.5	125.4	118.9	118.4	118.9	7.24	7.63	7.21	7.31	7.21
12	120.0	125.7	119.2	118.7	119.2	8.57	8.45	8.59	8.14	8.59
12a	122.7	129.6	123.1	122.6	123.1					
12b	101.4	106.9	100.2	99.8	100.2					
12c	129.8	136.5	130.1	129.5	130.1					
13a	138.6	144.5	138.2	137.5	138.2					
a		0.9914		0.9914			0.5965		0.5965	
b		7.5309		0.5072			3.3265		3.0132	
R^2		0.9759		0.9759			0.9983		0.9983	
MAE		6.5		1.4			0.29		0.16	
CMAE			1.3		1.3			0.02		0.02

[a] Calculated chemical shifts using TMS as a standard reference.

[b] Calculated chemical shifts using benzene as a standard reference.

$\delta_{calc*} = (\delta_{calc} - b)/a$; where the slope (a), the intercept (b) and the correlation coefficient (R^2) were determined from a plot of δ_{calc} against δ_{exp}.