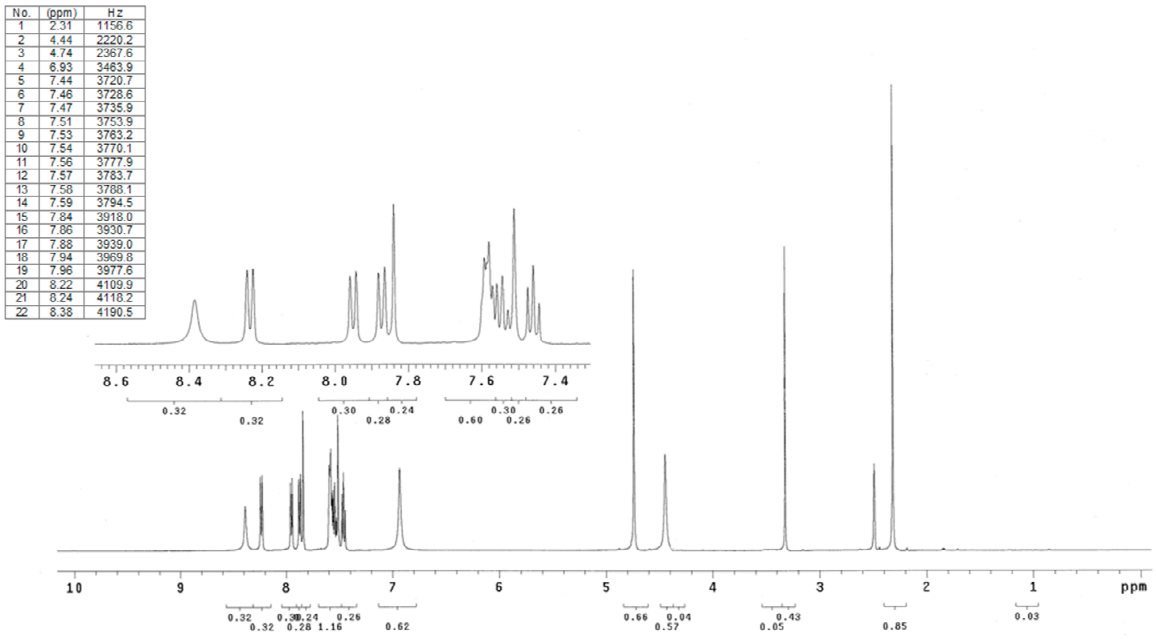
# Supplementary Materials: Novel 5-Substituted 2-(Aylmethylthio)-4-chloro-*N*-(5-aryl-1,2,4-triazin-3-yl)benzenesulfonamides: Synthesis, Molecular Structure, Anticancer Activity, Apoptosis-Inducing Activity and Metabolic Stability

**Beata Żołnowska, Jarosław Sławiński, Aneta Pogorzelska, Krzysztof Szafrański, Anna Kawiak, Grzegorz Stasiłojć, Mariusz Belka, Szymon Ulenberg, Tomasz Bączek and Jarosław Chojnacki**



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.31 | 1156.6 |
| 2 | 4.44 | 2220.2 |
| 3 | 4.74 | 2367.6 |
| 4 | 6.93 | 3463.9 |
| 5 | 7.44 | 3720.7 |
| 6 | 7.46 | 3728.6 |
| 7 | 7.47 | 3735.9 |
| 8 | 7.51 | 3753.9 |
| 9 | 7.53 | 3763.2 |
| 10 | 7.54 | 3770.1 |
| 11 | 7.56 | 3777.9 |
| 12 | 7.57 | 3783.7 |
| 13 | 7.58 | 3788.1 |
| 14 | 7.59 | 3794.5 |
| 15 | 7.84 | 3918.0 |
| 16 | 7.86 | 3930.7 |
| 17 | 7.88 | 3939.0 |
| 18 | 7.94 | 3969.8 |
| 19 | 7.96 | 3977.6 |
| 20 | 8.22 | 4109.9 |
| 21 | 8.24 | 4118.2 |
| 22 | 8.38 | 4190.5 |

**Figure S1.** $^{1}$H-NMR of compd **21** (500 MHz, DMSO-$d_6$).

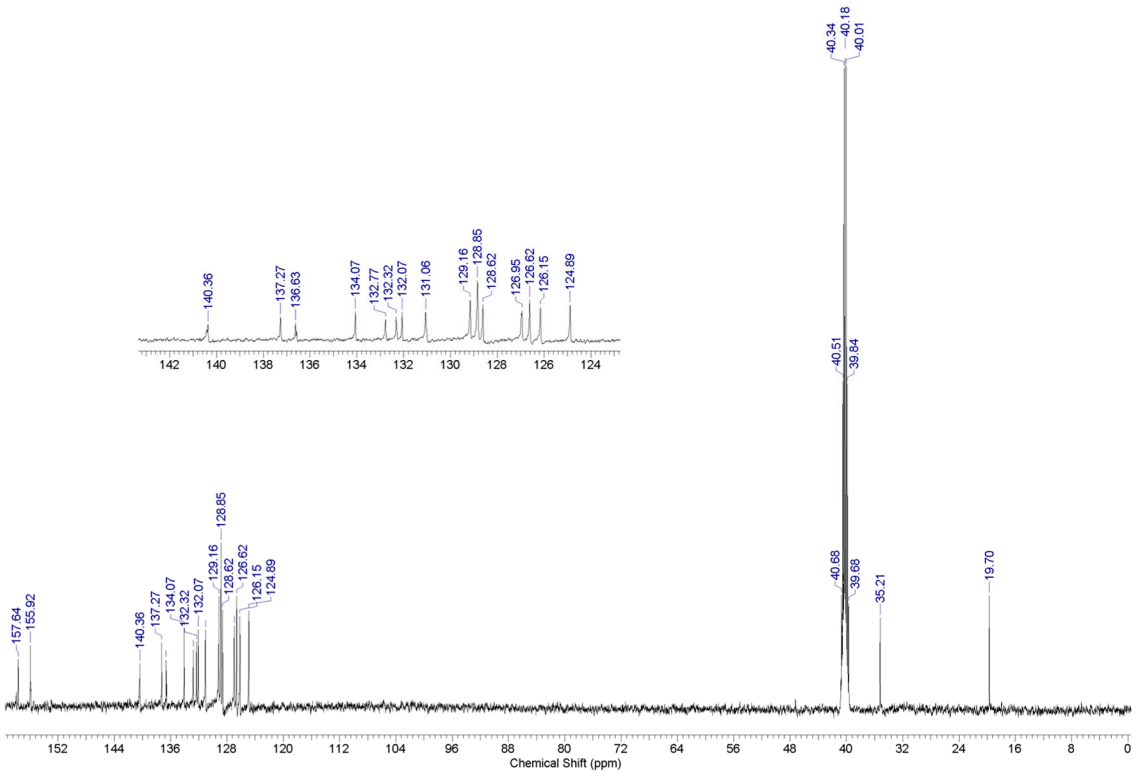



**Figure S2.** $^{13}$C-NMR of compd **21** (125 MHz, DMSO-$d_6$).

| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 2.21 | 1104.3 |
| 2 | 2.30 | 1149.7 |
| 3 | 2.31 | 1153.1 |
| 4 | 4.08 | 2037.4 |
| 5 | 4.49 | 2245.0 |
| 6 | 6.97 | 3483.3 |
| 7 | 7.43 | 3713.8 |
| 8 | 7.82 | 3906.2 |
| 9 | 8.38 | 4190.9 |

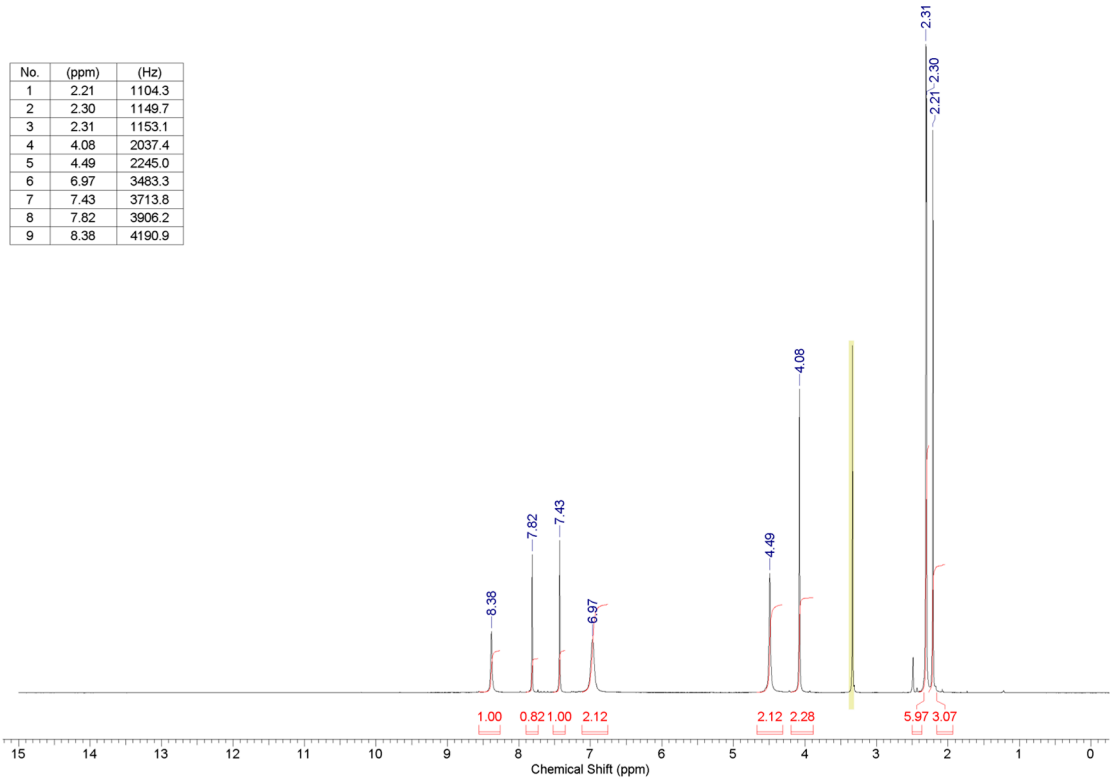



**Figure S3.** $^{1}$H-NMR of compd **22** (500 MHz, DMSO-$d_6$).

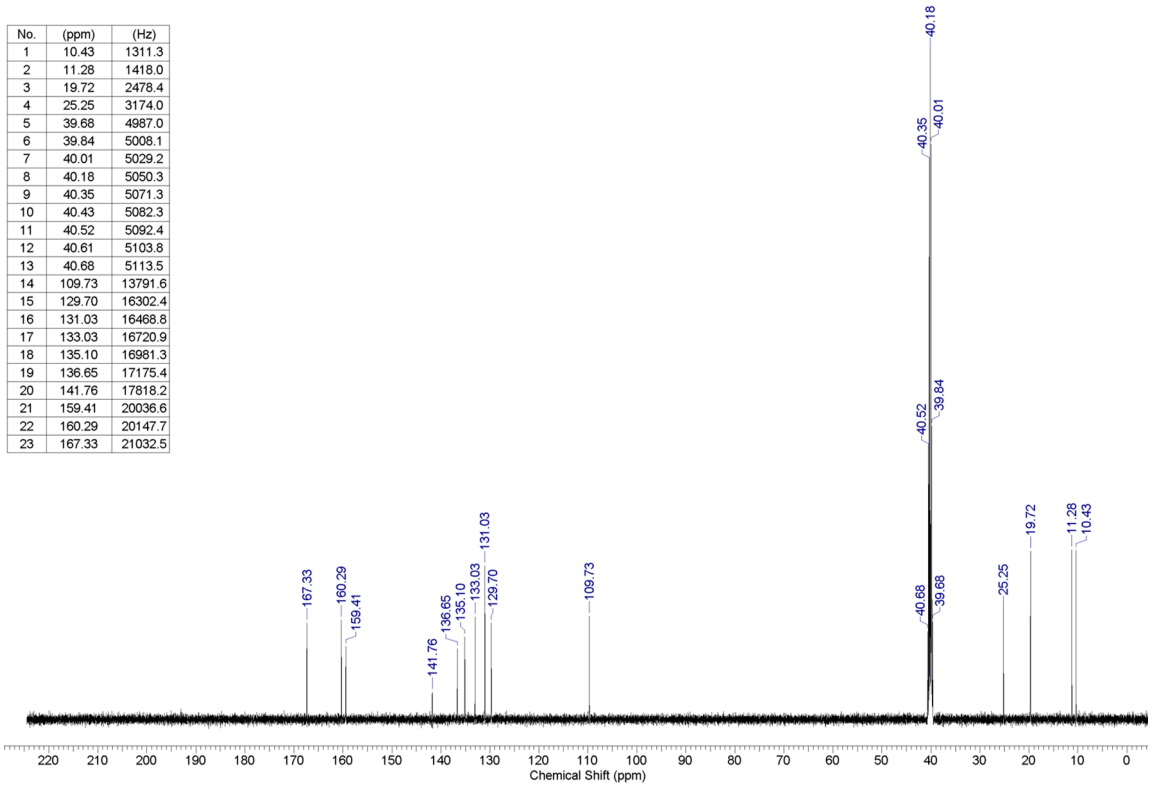



**Figure S4.** $^{13}$C-NMR of compd **22** (125 MHz, DMSO-$d_6$).

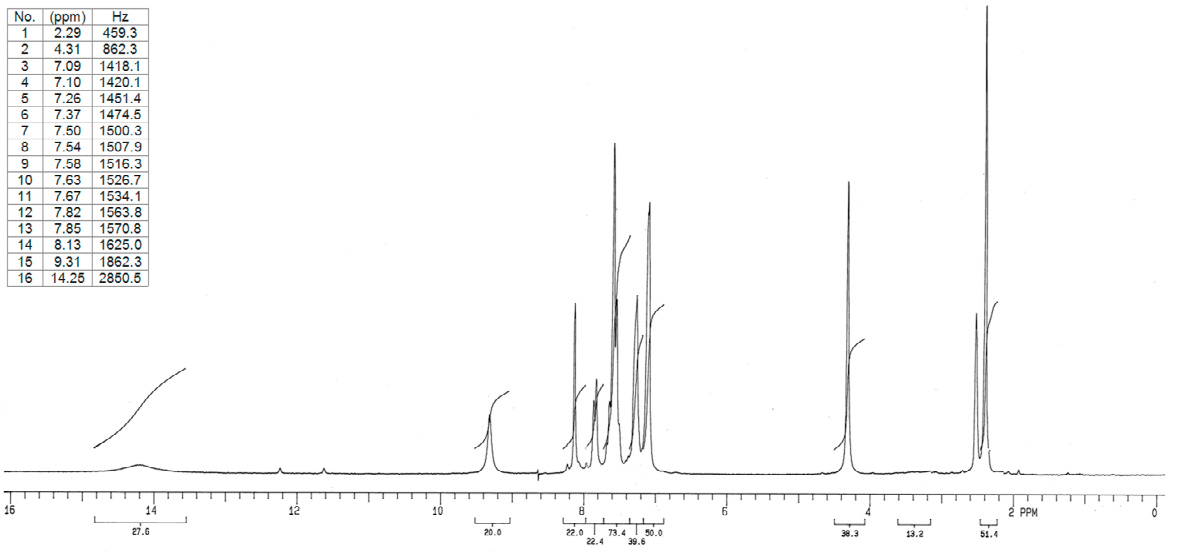
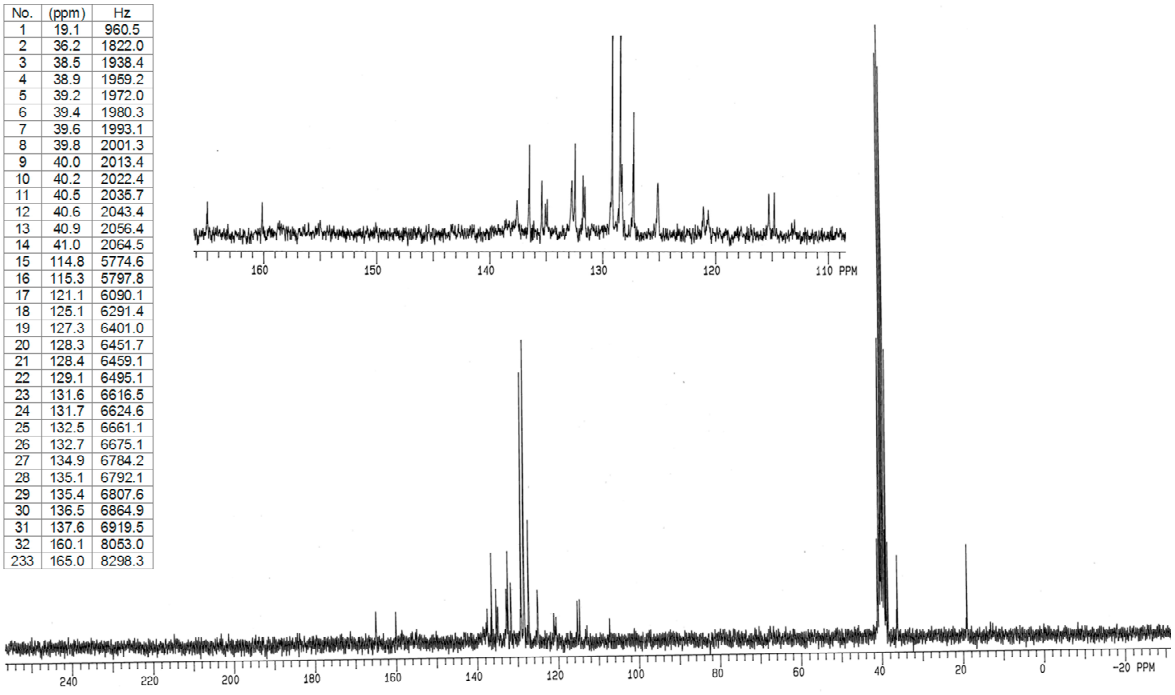
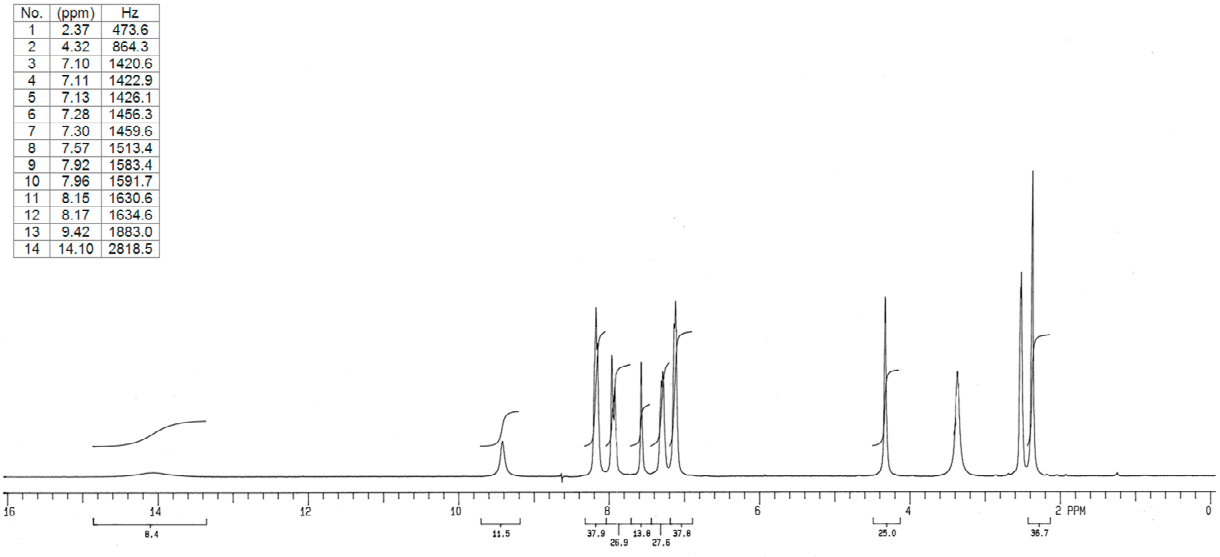



**Figure S5.** $^{1}$H-NMR of compd **27** (200 MHz, DMSO-$d_6$).



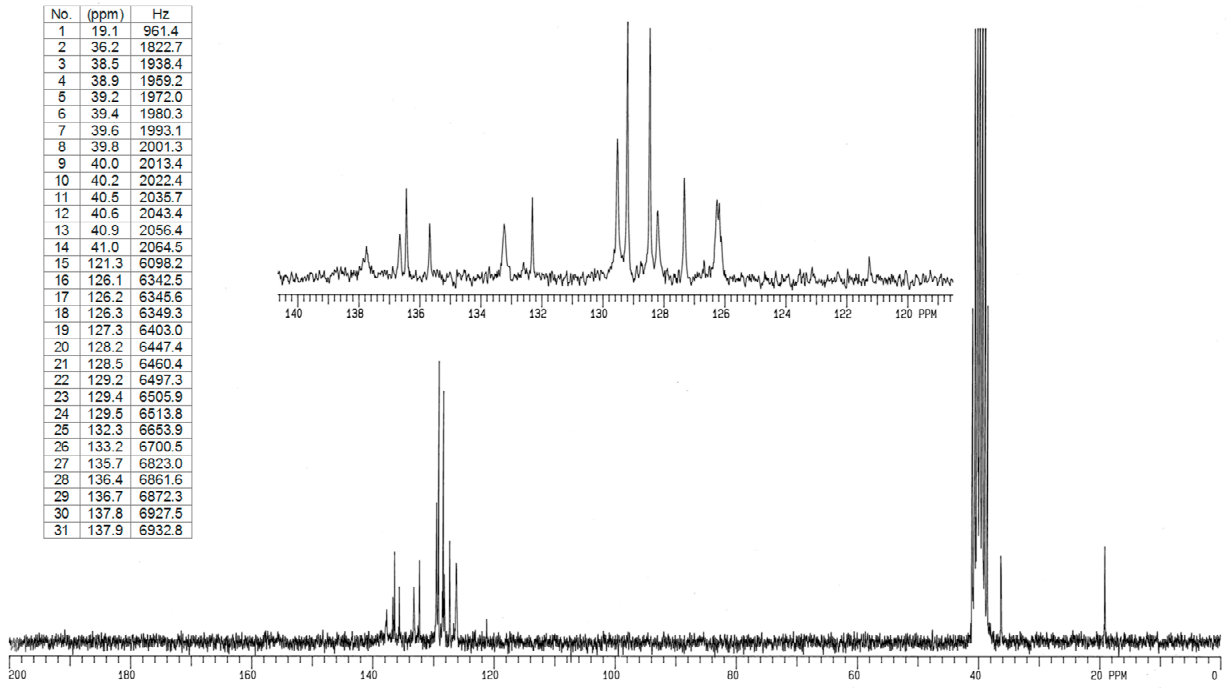
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 19.1 | 960.5 |
| 2 | 36.2 | 1822.0 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 114.8 | 5774.6 |
| 16 | 115.3 | 5797.8 |
| 17 | 121.1 | 6090.1 |
| 18 | 125.1 | 6291.4 |
| 19 | 127.3 | 6401.0 |
| 20 | 128.3 | 6451.7 |
| 21 | 128.4 | 6459.1 |
| 22 | 129.1 | 6495.1 |
| 23 | 131.6 | 6616.5 |
| 24 | 131.7 | 6624.6 |
| 25 | 132.5 | 6661.1 |
| 26 | 132.7 | 6675.1 |
| 27 | 134.9 | 6784.2 |
| 28 | 135.1 | 6792.1 |
| 29 | 135.4 | 6807.6 |
| 30 | 136.5 | 6864.9 |
| 31 | 137.6 | 6919.5 |
| 32 | 160.1 | 8053.0 |
| 233 | 165.0 | 8298.3 |

**Figure S6.** $^{13}$C-NMR of compd **27** (50 MHz, DMSO-$d_6$).



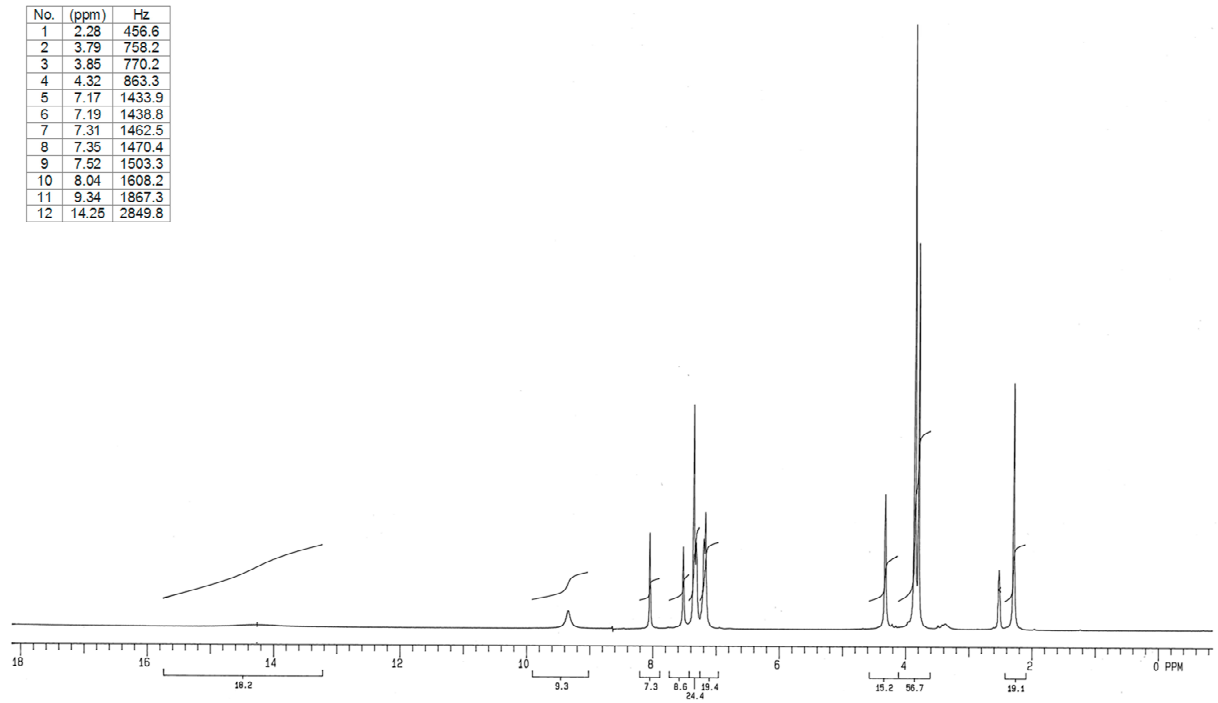
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.37 | 473.6 |
| 2 | 4.32 | 864.3 |
| 3 | 7.10 | 1420.6 |
| 4 | 7.11 | 1422.9 |
| 5 | 7.13 | 1426.1 |
| 6 | 7.28 | 1456.3 |
| 7 | 7.30 | 1459.6 |
| 8 | 7.57 | 1513.4 |
| 9 | 7.92 | 1583.4 |
| 10 | 7.96 | 1591.7 |
| 11 | 8.15 | 1630.6 |
| 12 | 8.17 | 1634.6 |
| 13 | 9.42 | 1883.0 |
| 14 | 14.10 | 2818.5 |

**Figure S7.** $^{1}$H-NMR of compd **28** (200 MHz, DMSO-$d_6$).



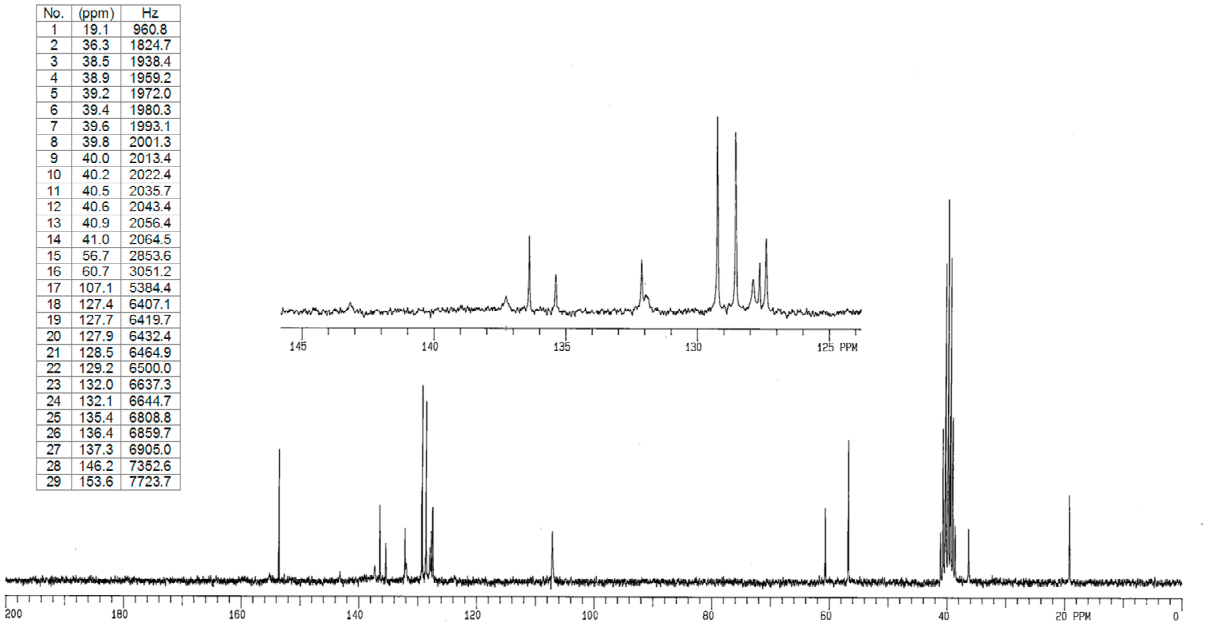
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 19.1 | 961.4 |
| 2 | 36.2 | 1822.7 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 121.3 | 6098.2 |
| 16 | 126.1 | 6342.5 |
| 17 | 126.2 | 6345.6 |
| 18 | 126.3 | 6349.3 |
| 19 | 127.3 | 6403.0 |
| 20 | 128.2 | 6447.4 |
| 21 | 128.5 | 6460.4 |
| 22 | 129.2 | 6497.3 |
| 23 | 129.4 | 6505.9 |
| 24 | 129.5 | 6513.8 |
| 25 | 132.3 | 6653.9 |
| 26 | 133.2 | 6700.5 |
| 27 | 135.7 | 6823.0 |
| 28 | 136.4 | 6861.6 |
| 29 | 136.7 | 6872.3 |
| 30 | 137.8 | 6927.5 |
| 31 | 137.9 | 6932.8 |

**Figure S8.** $^{13}$C-NMR of compd **28** (50 MHz, DMSO-$d_6$).



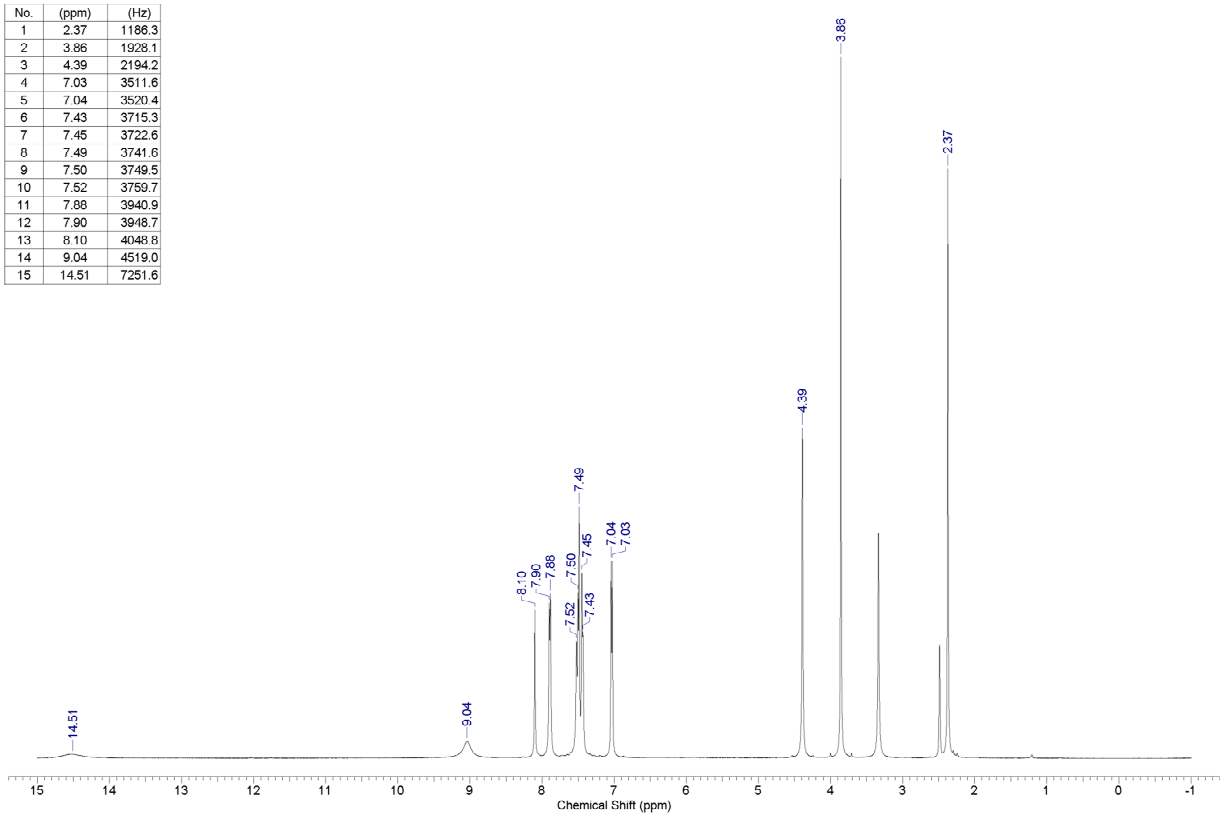
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.28 | 456.6 |
| 2 | 3.79 | 758.2 |
| 3 | 3.85 | 770.2 |
| 4 | 4.32 | 863.3 |
| 5 | 7.17 | 1433.9 |
| 6 | 7.19 | 1438.8 |
| 7 | 7.31 | 1462.5 |
| 8 | 7.35 | 1470.4 |
| 9 | 7.52 | 1503.3 |
| 10 | 8.04 | 1608.2 |
| 11 | 9.34 | 1867.3 |
| 12 | 14.25 | 2849.8 |

**Figure S9.** $^{1}$H-NMR of compd **32** (200 MHz, DMSO-$d_6$).



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 19.1 | 960.8 |
| 2 | 36.3 | 1824.7 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 56.7 | 2853.6 |
| 16 | 60.7 | 3051.2 |
| 17 | 107.1 | 5384.4 |
| 18 | 127.4 | 6407.1 |
| 19 | 127.7 | 6419.7 |
| 20 | 127.9 | 6432.4 |
| 21 | 128.5 | 6464.9 |
| 22 | 129.2 | 6500.0 |
| 23 | 132.0 | 6637.3 |
| 24 | 132.1 | 6644.7 |
| 25 | 135.4 | 6808.8 |
| 26 | 136.4 | 6859.7 |
| 27 | 137.3 | 6905.0 |
| 28 | 146.2 | 7352.6 |
| 29 | 153.6 | 7723.7 |

**Figure S10.** $^{13}$C-NMR of compd **32** (50 MHz, DMSO-$d_6$).



| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 2.37 | 1186.3 |
| 2 | 3.86 | 1928.1 |
| 3 | 4.39 | 2194.2 |
| 4 | 7.03 | 3511.6 |
| 5 | 7.04 | 3520.4 |
| 6 | 7.43 | 3715.3 |
| 7 | 7.45 | 3722.6 |
| 8 | 7.49 | 3741.6 |
| 9 | 7.50 | 3749.5 |
| 10 | 7.52 | 3759.7 |
| 11 | 7.88 | 3940.9 |
| 12 | 7.90 | 3948.7 |
| 13 | 8.10 | 4048.8 |
| 14 | 9.04 | 4519.0 |
| 15 | 14.51 | 7251.6 |

**Figure S11.** $^{1}$H-NMR of compd **35** (500 MHz, DMSO-$d_6$).

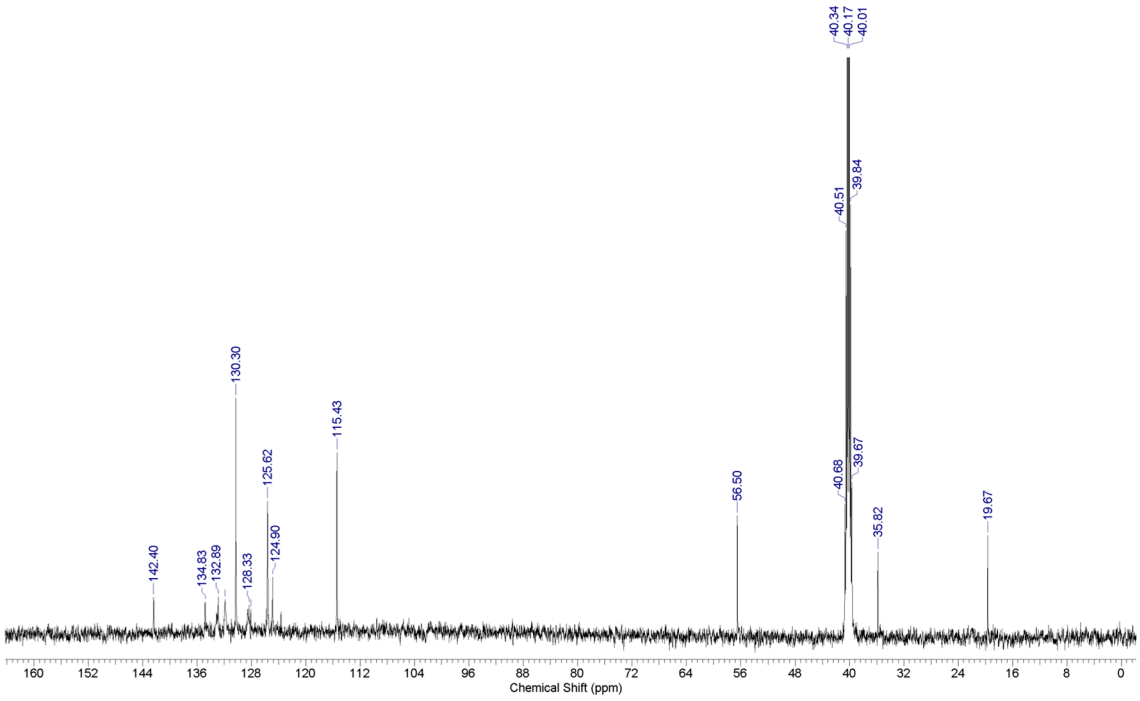



**Figure S12.** $^{13}$C-NMR of compd **35** (125 MHz, DMSO-$d_6$).

| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 2.38 | 1188.8 |
| 2 | 2.49 | 1243.4 |
| 3 | 4.76 | 2380.2 |
| 4 | 7.27 | 3634.2 |
| 5 | 7.29 | 3641.5 |
| 6 | 7.30 | 3649.4 |
| 7 | 7.47 | 3734.8 |
| 8 | 7.67 | 3832.5 |
| 9 | 7.75 | 3875.9 |
| 10 | 7.77 | 3883.7 |
| 11 | 7.86 | 3926.7 |
| 12 | 7.87 | 3932.1 |
| 13 | 7.87 | 3935.5 |
| 14 | 7.90 | 3947.7 |
| 15 | 7.91 | 3955.5 |
| 16 | 8.12 | 4056.1 |
| 17 | 8.17 | 4083.5 |
| 18 | 9.33 | 4662.6 |

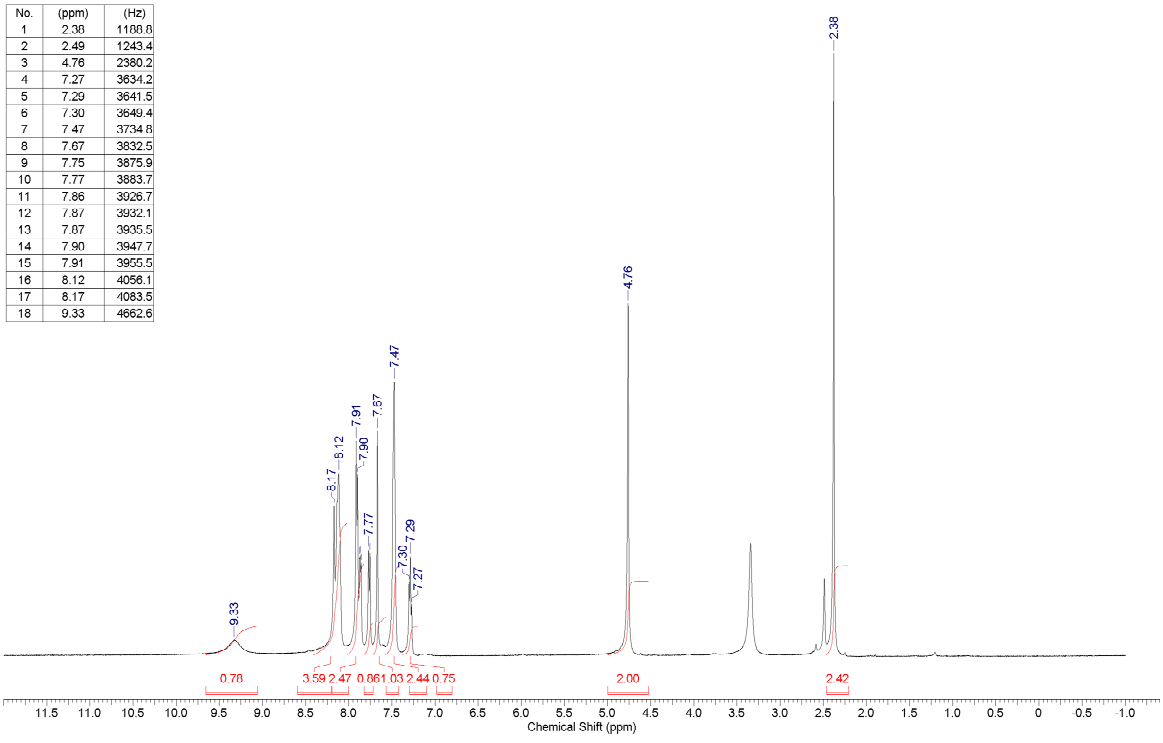



**Figure S13.** $^{1}$H-NMR of compd **37** (500 MHz, DMSO-$d_6$).

| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 19.57 | 2460.0 |
| 2 | 34.87 | 4383.3 |
| 3 | 39.68 | 4987.0 |
| 4 | 39.84 | 5007.7 |
| 5 | 40.01 | 5028.7 |
| 6 | 40.18 | 5049.8 |
| 7 | 40.34 | 5070.9 |
| 8 | 40.51 | 5092.0 |
| 9 | 40.68 | 5112.6 |
| 10 | 124.85 | 15692.1 |
| 11 | 125.98 | 15835.2 |
| 12 | 126.62 | 15914.7 |
| 13 | 126.95 | 15956.4 |
| 14 | 128.63 | 16167.6 |
| 15 | 128.84 | 16194.0 |
| 16 | 129.14 | 16231.3 |
| 17 | 130.00 | 16340.2 |
| 18 | 131.92 | 16581.3 |
| 19 | 132.22 | 16619.5 |
| 20 | 132.71 | 16680.5 |
| 21 | 133.52 | 16781.9 |
| 22 | 133.97 | 16839.0 |
| 23 | 137.01 | 17220.6 |

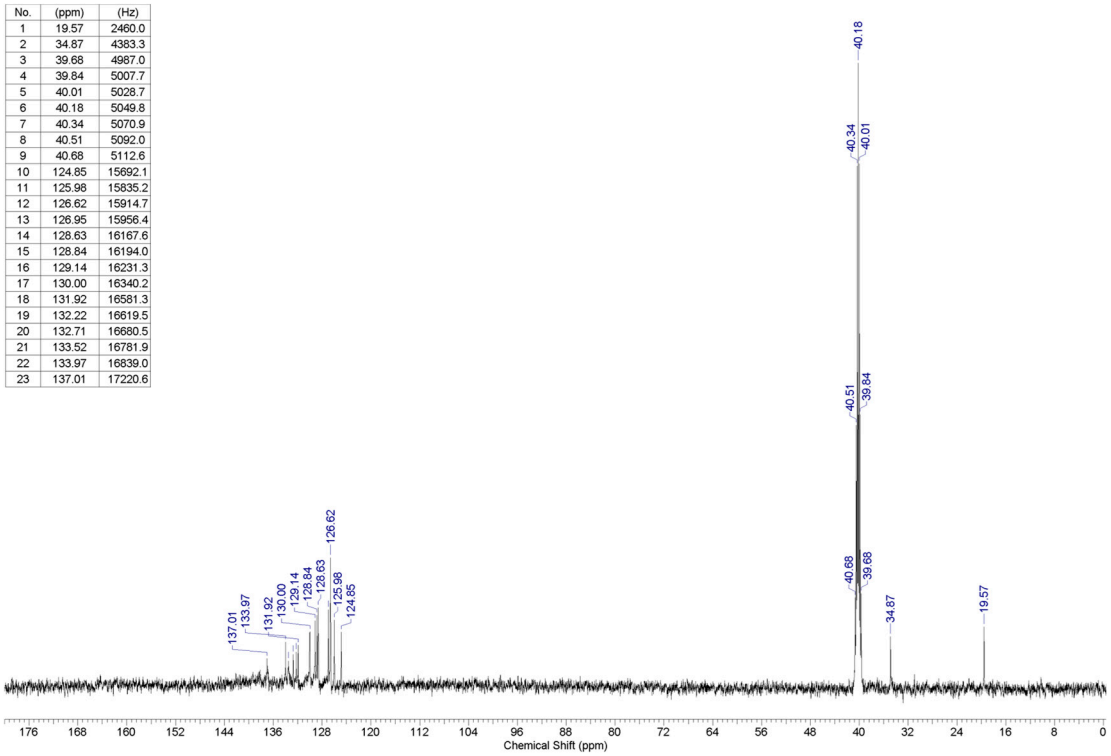



**Figure S14.** $^{13}$C-NMR of compd **37** (125 MHz, DMSO-$d_6$).

| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 2.42 | 1211.2 |
| 2 | 3.88 | 1938.3 |
| 3 | 4.73 | 2361.7 |
| 4 | 7.05 | 3525.8 |
| 5 | 7.07 | 3534.6 |
| 6 | 7.28 | 3637.6 |
| 7 | 7.29 | 3644.5 |
| 8 | 7.31 | 3652.8 |
| 9 | 7.46 | 3729.4 |
| 10 | 7.47 | 3735.3 |
| 11 | 7.49 | 3742.1 |
| 12 | 7.50 | 3748.5 |
| 13 | 7.51 | 3755.3 |
| 14 | 7.60 | 3799.7 |
| 15 | 7.77 | 3884.2 |
| 16 | 7.79 | 3892.5 |
| 17 | 7.88 | 3937.9 |
| 18 | 7.89 | 3945.8 |
| 19 | 7.93 | 3963.3 |
| 20 | 7.94 | 3970.7 |
| 21 | 8.08 | 4040.0 |
| 22 | 8.10 | 4047.8 |
| 23 | 8.13 | 4065.4 |
| 24 | 9.00 | 4496.5 |
| 25 | 14.39 | 7191.6 |

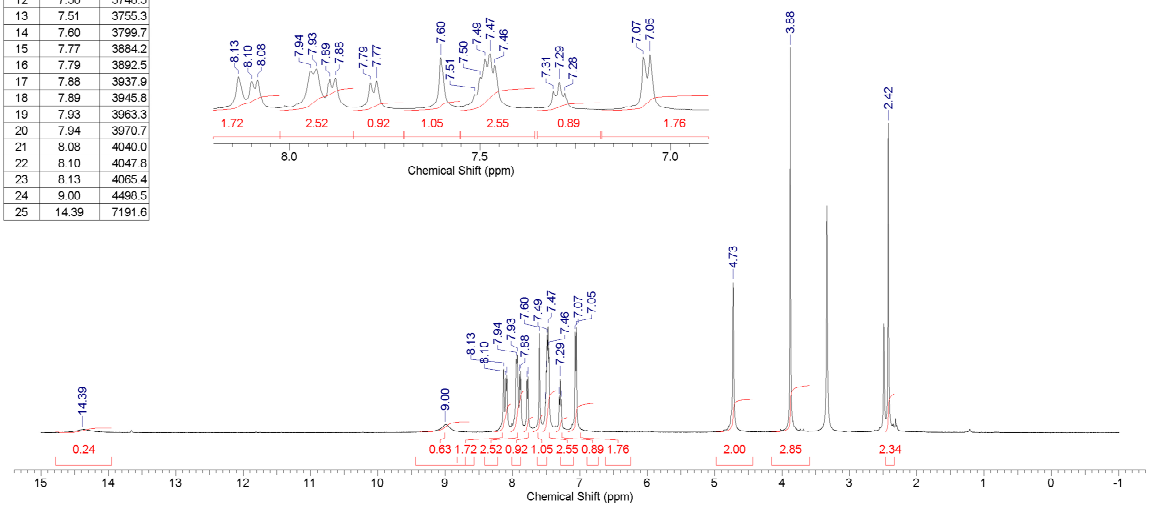



**Figure S15.** $^{1}$H-NMR of compd **38** (500 MHz, DMSO-$d_6$).

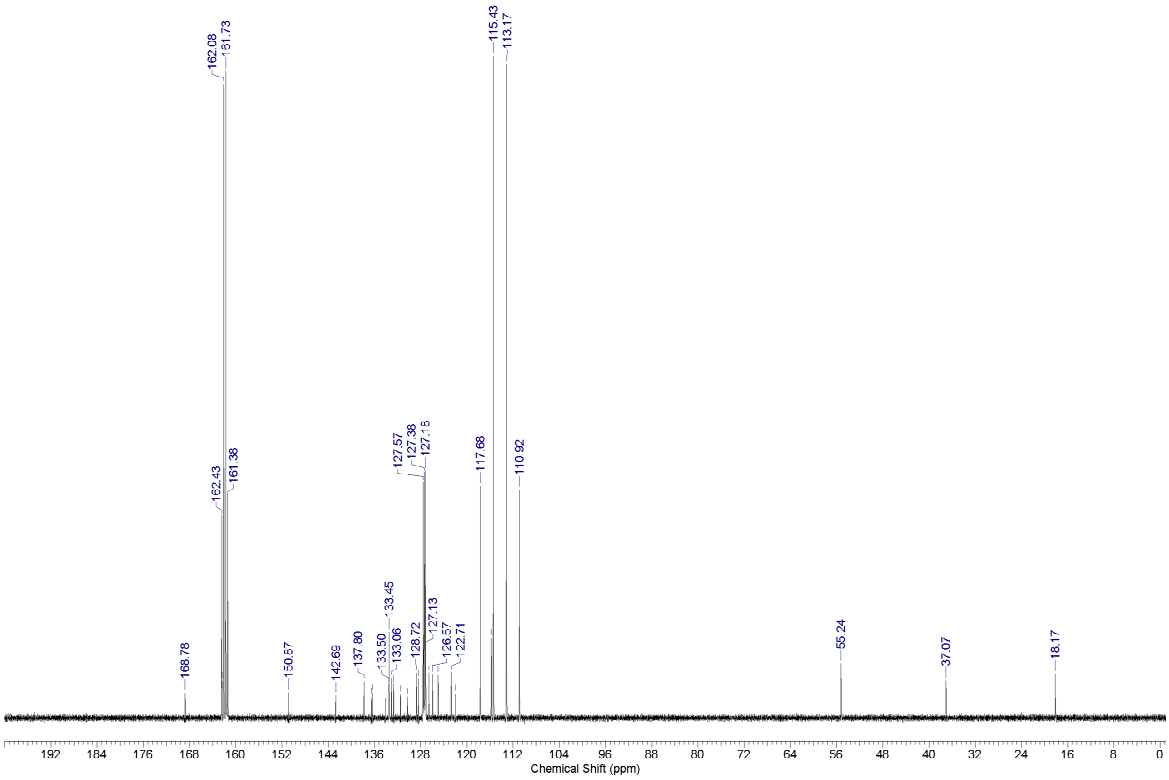



**Figure S16.** $^{13}$C-NMR of compd **38** (125 MHz, TFA).

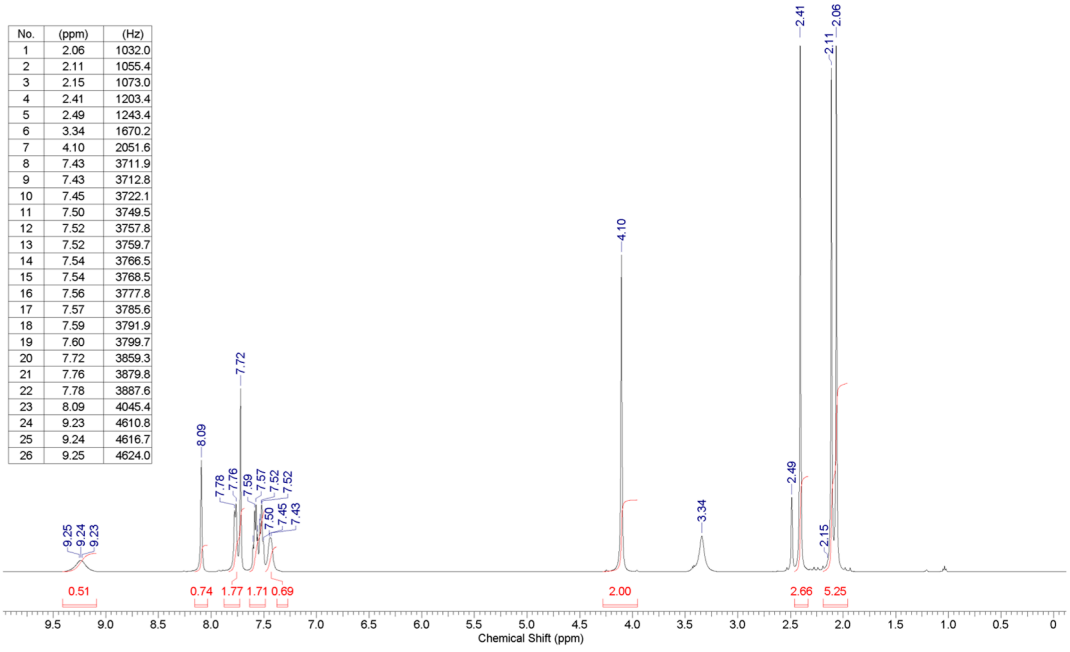



**Figure S17.** $^{1}$H-NMR of compd **39** (500 MHz, DMSO-*d*$_6$).

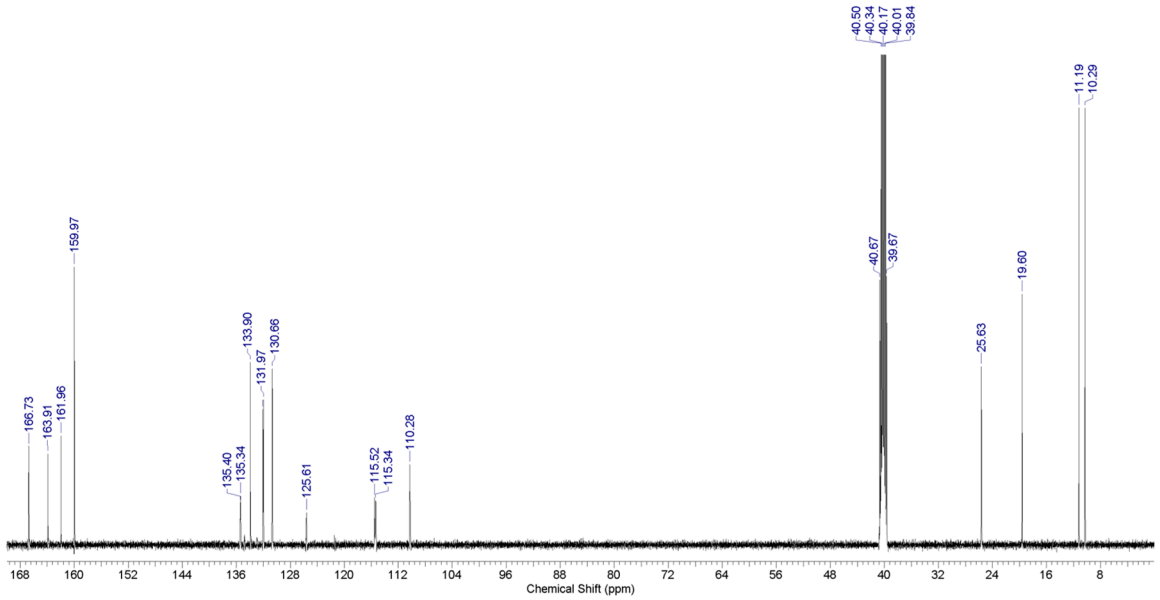



**Figure S18.** $^{13}$C-NMR of compd **39** (125 MHz, DMSO-$d_6$).

| No. | (ppm) | (Hz) |
|---|---|---|
| 1 | 2.08 | 1040.3 |
| 2 | 2.14 | 1072.0 |
| 3 | 2.39 | 1196.6 |
| 4 | 4.11 | 2054.0 |
| 5 | 7.66 | 3831.0 |
| 6 | 7.89 | 3944.8 |
| 7 | 7.91 | 3953.1 |
| 8 | 8.10 | 4049.8 |
| 9 | 8.12 | 4056.6 |
| 10 | 8.15 | 4075.6 |
| 11 | 9.36 | 4676.8 |

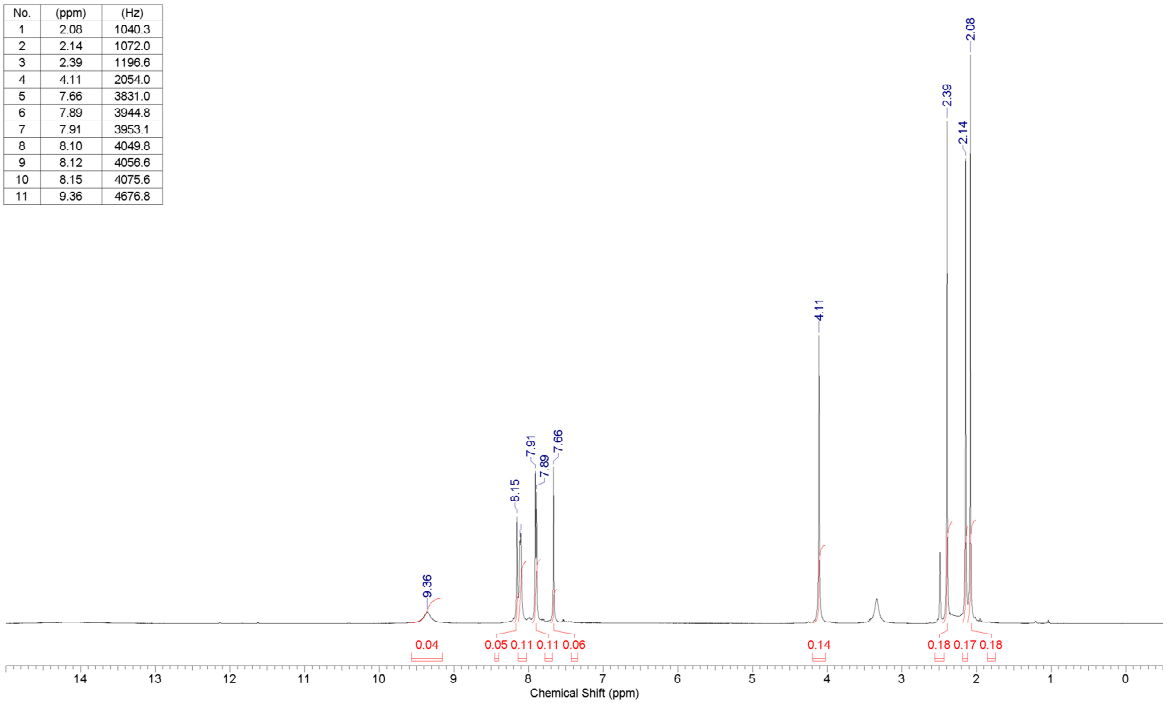



**Figure S19.** $^{1}$H-NMR of compd **40** (500 MHz, DMSO-$d_6$).

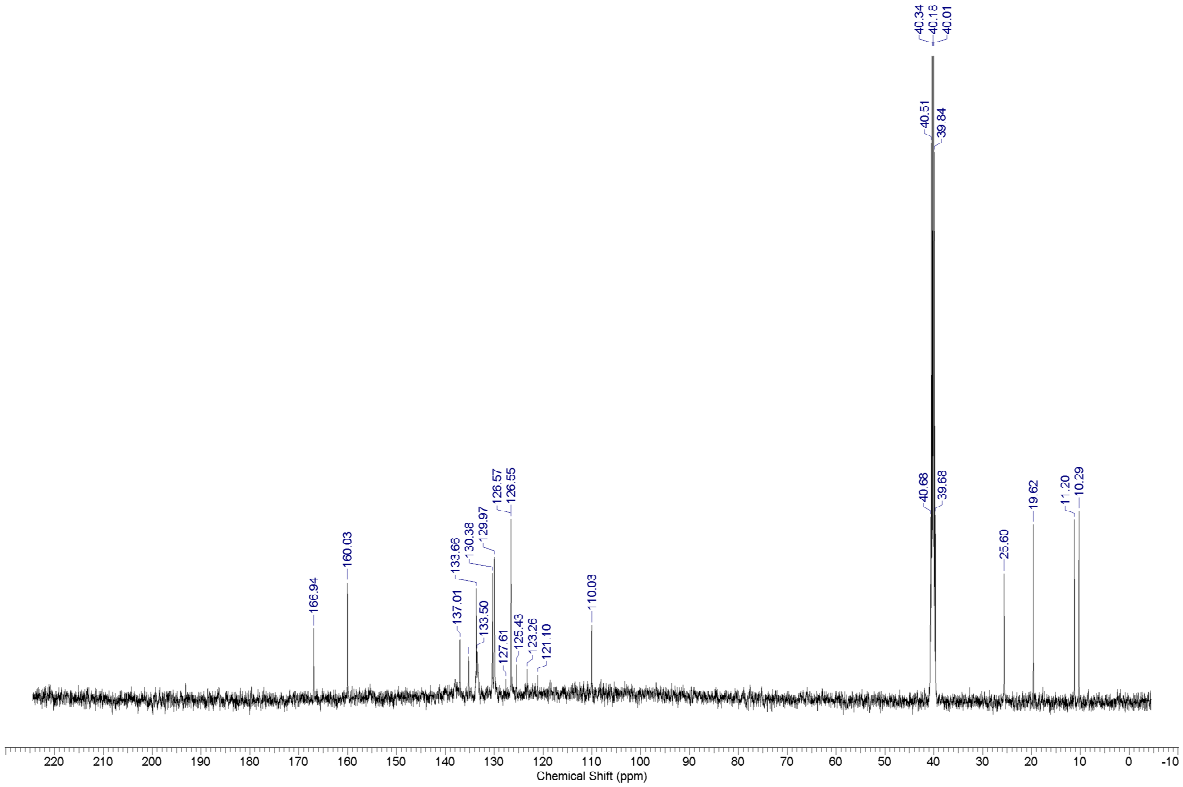



**Figure S20.** $^{13}$C-NMR of compd **40** (125 MHz, DMSO-$d_6$).

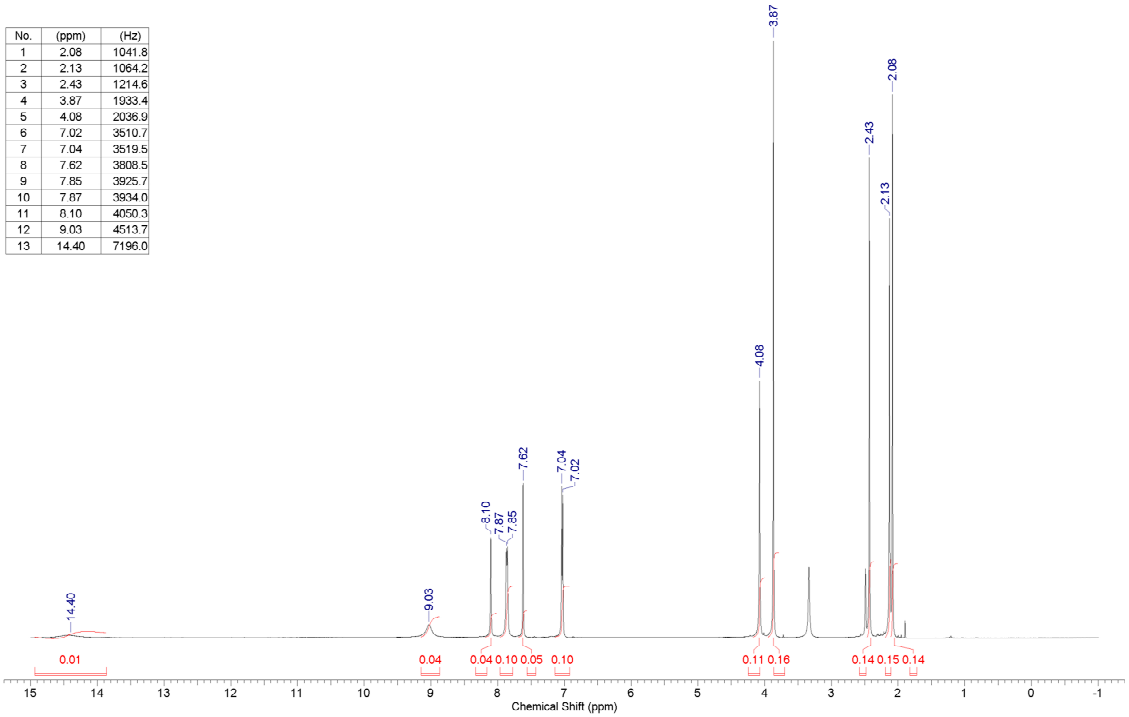



**Figure S21.** $^{1}$H-NMR of compd **41** (500 MHz, DMSO-$d_6$).

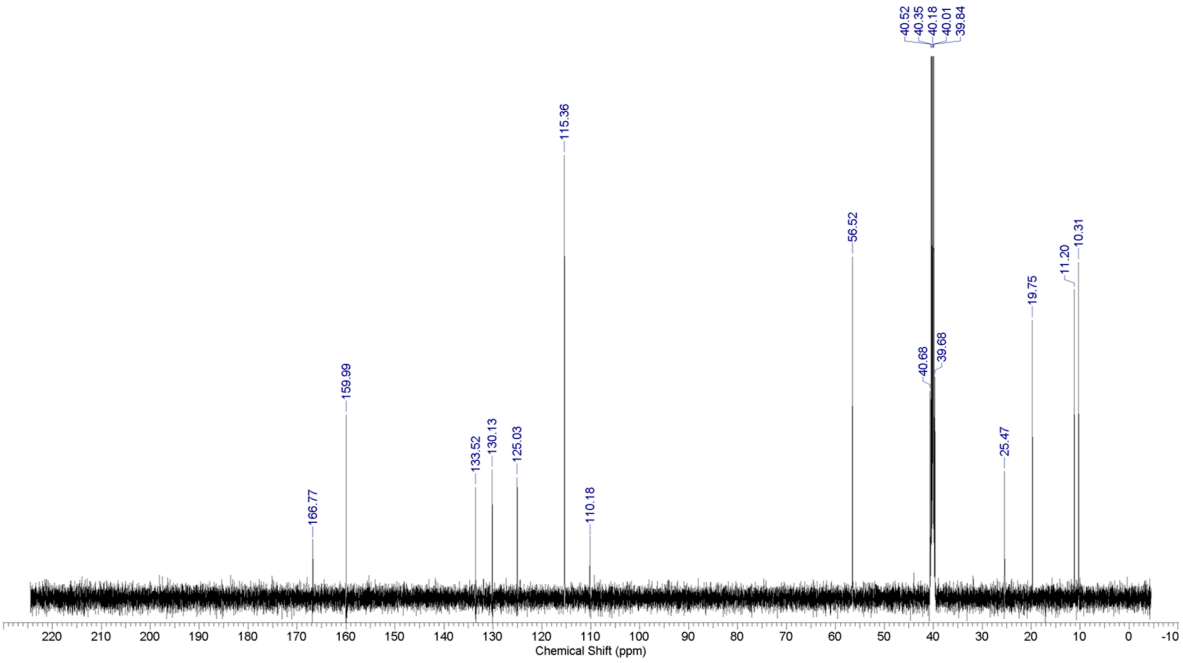



**Figure S22.** $^{13}$C-NMR of compd **41** (125 MHz, DMSO-$d_6$).

| No. | (ppm) | Hz |
|---|---|---|
| 1 | 4.43 | 886.5 |
| 2 | 7.16 | 1432.6 |
| 3 | 7.28 | 1455.0 |
| 4 | 7.34 | 1467.8 |
| 5 | 7.35 | 1470.1 |
| 6 | 7.42 | 1483.6 |
| 7 | 7.46 | 1492.2 |
| 8 | 7.73 | 1545.5 |
| 9 | 7.77 | 1553.4 |
| 10 | 7.85 | 1569.6 |
| 11 | 7.89 | 1577.2 |
| 12 | 8.09 | 1618.1 |
| 13 | 8.13 | 1625.5 |
| 14 | 8.30 | 1660.6 |
| 15 | 9.36 | 1871.0 |
| 16 | 10.80 | 2158.7 |

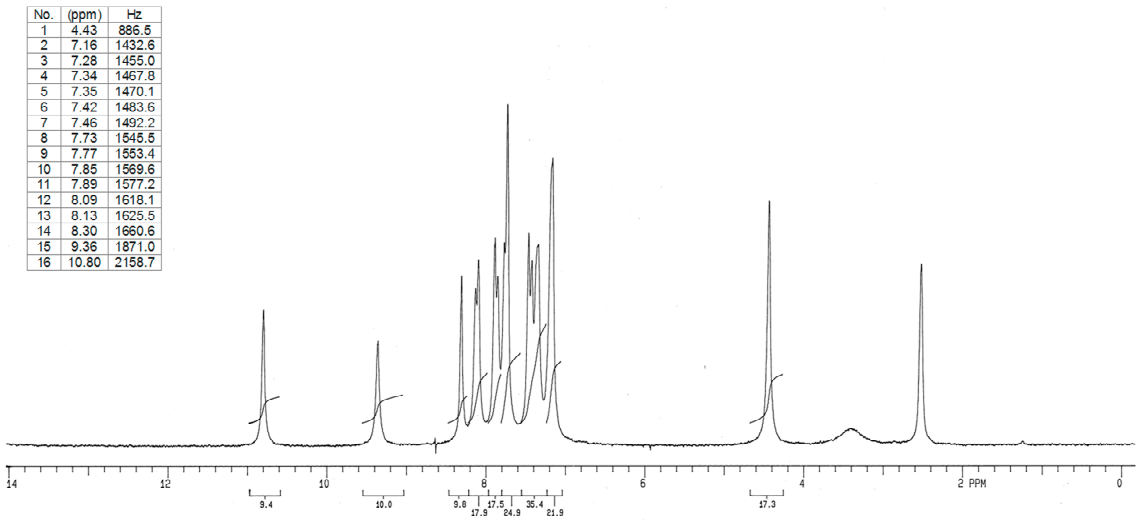
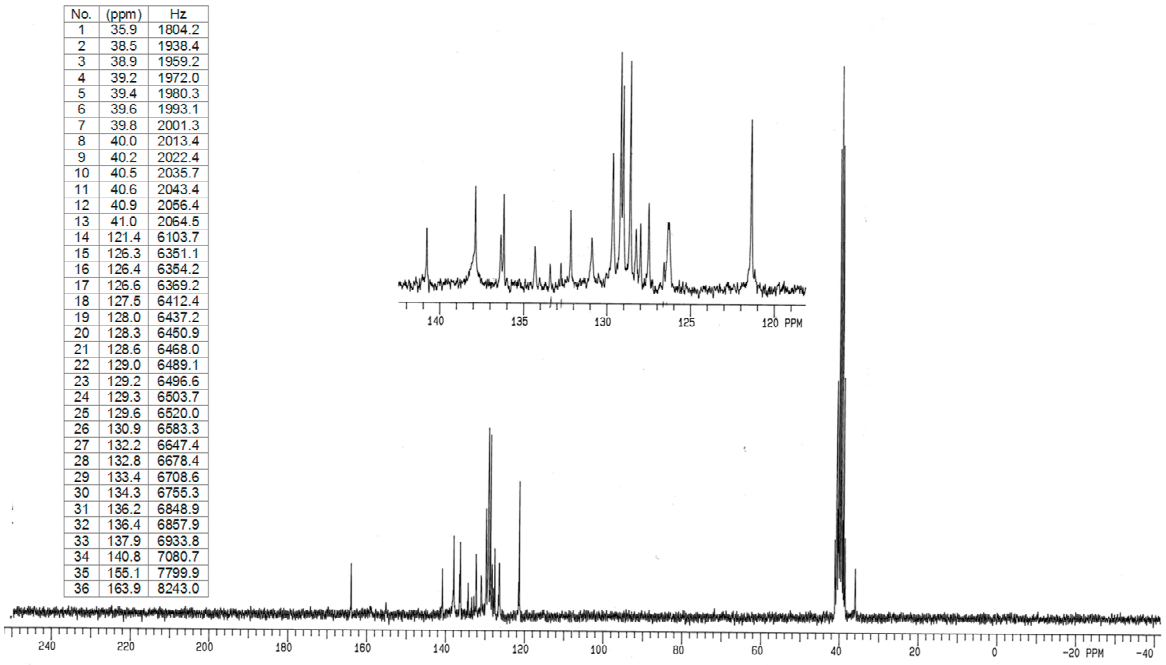
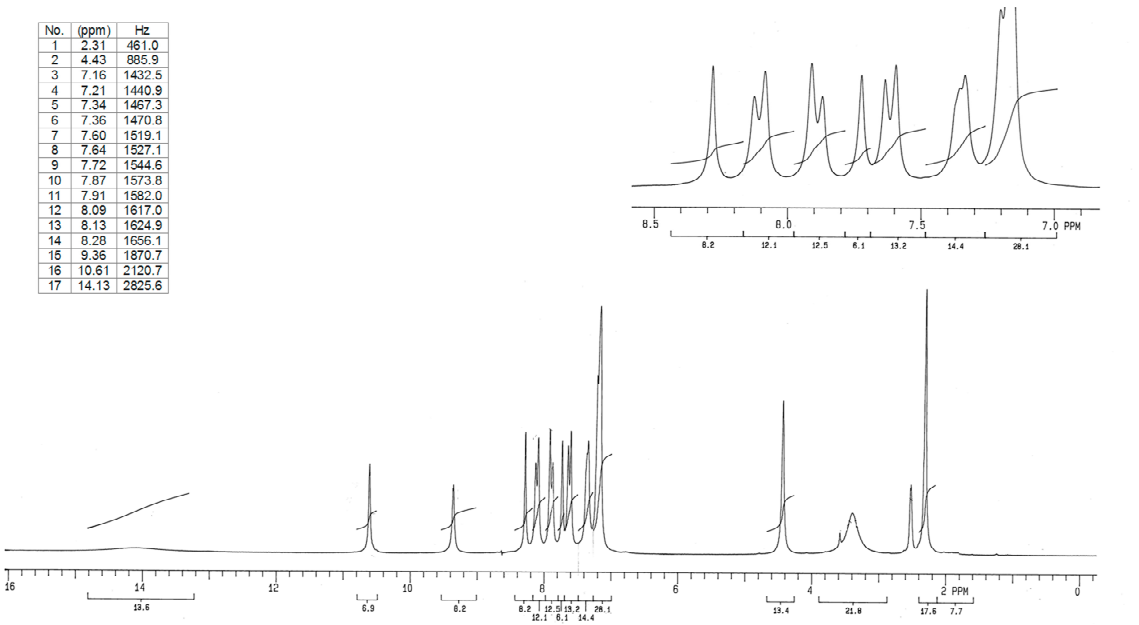



**Figure S23.** $^{1}$H-NMR of compd **46** (200 MHz, DMSO-$d_6$).



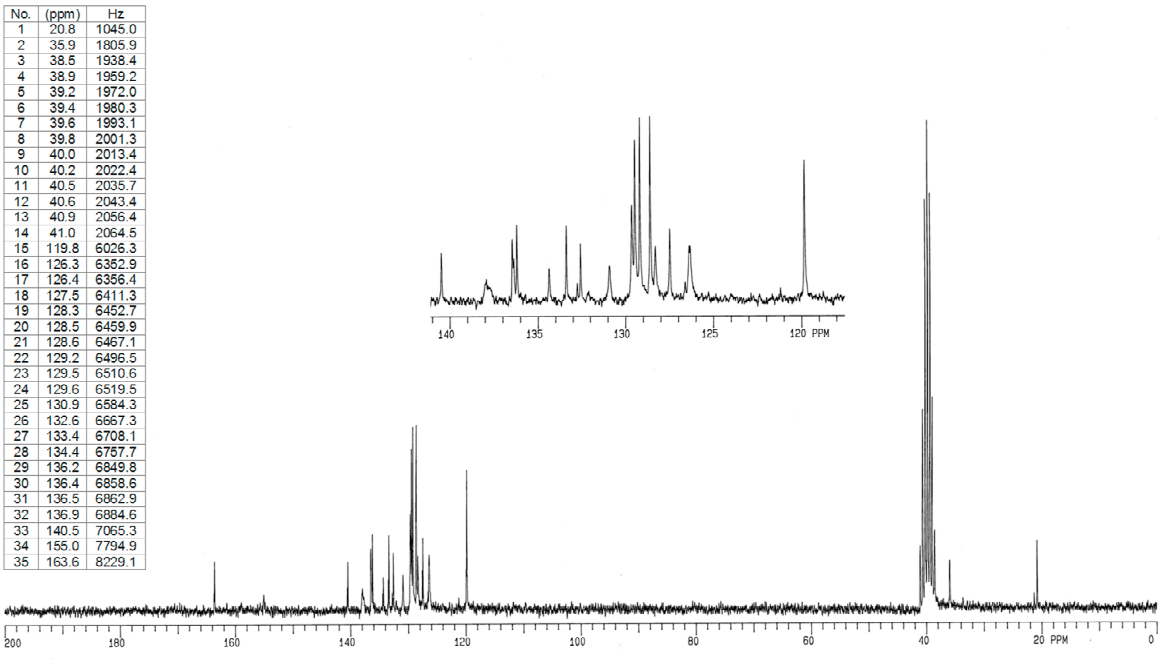
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 35.9 | 1804.2 |
| 2 | 38.5 | 1938.4 |
| 3 | 38.9 | 1959.2 |
| 4 | 39.2 | 1972.0 |
| 5 | 39.4 | 1980.3 |
| 6 | 39.6 | 1993.1 |
| 7 | 39.8 | 2001.3 |
| 8 | 40.0 | 2013.4 |
| 9 | 40.2 | 2022.4 |
| 10 | 40.5 | 2035.7 |
| 11 | 40.6 | 2043.4 |
| 12 | 40.9 | 2056.4 |
| 13 | 41.0 | 2064.5 |
| 14 | 121.4 | 6103.7 |
| 15 | 126.3 | 6351.1 |
| 16 | 126.4 | 6354.2 |
| 17 | 126.6 | 6369.2 |
| 18 | 127.5 | 6412.4 |
| 19 | 128.0 | 6437.2 |
| 20 | 128.3 | 6450.9 |
| 21 | 128.6 | 6468.0 |
| 22 | 129.0 | 6489.1 |
| 23 | 129.2 | 6496.6 |
| 24 | 129.3 | 6503.7 |
| 25 | 129.6 | 6520.0 |
| 26 | 130.9 | 6583.3 |
| 27 | 132.2 | 6647.4 |
| 28 | 132.8 | 6678.4 |
| 29 | 133.4 | 6708.6 |
| 30 | 134.3 | 6755.3 |
| 31 | 136.2 | 6848.9 |
| 32 | 136.4 | 6857.9 |
| 33 | 137.9 | 6933.8 |
| 34 | 140.8 | 7080.7 |
| 35 | 155.1 | 7799.9 |
| 36 | 163.9 | 8243.0 |

**Figure S24.** $^{13}$C-NMR of compd **46** (50 MHz, DMSO-$d_6$).



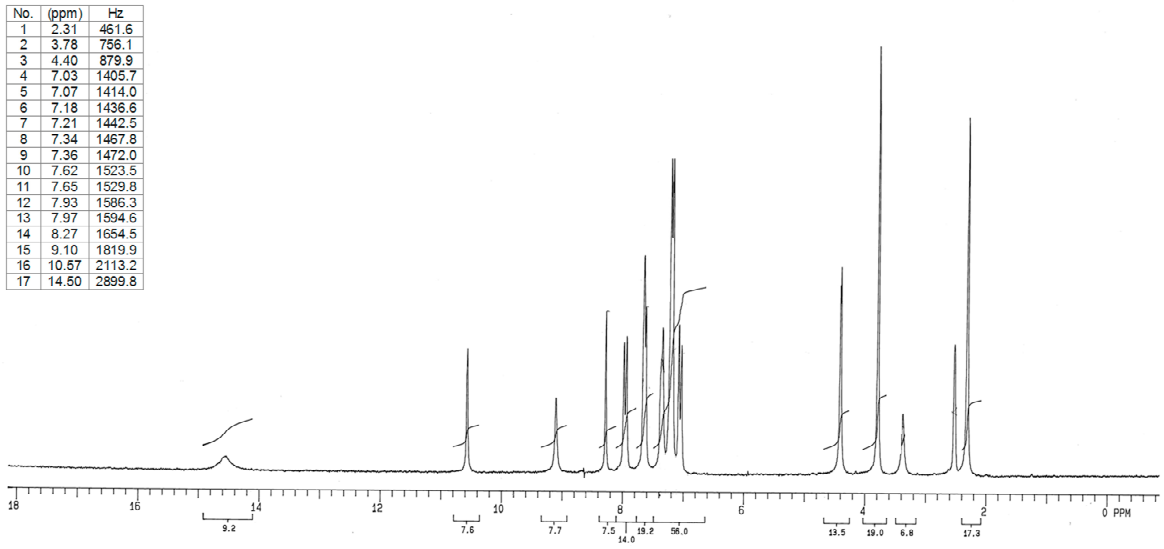
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.31 | 461.0 |
| 2 | 4.43 | 885.9 |
| 3 | 7.16 | 1432.5 |
| 4 | 7.21 | 1440.9 |
| 5 | 7.34 | 1467.3 |
| 6 | 7.36 | 1470.8 |
| 7 | 7.60 | 1519.1 |
| 8 | 7.64 | 1527.1 |
| 9 | 7.72 | 1544.6 |
| 10 | 7.87 | 1573.8 |
| 11 | 7.91 | 1582.0 |
| 12 | 8.09 | 1617.0 |
| 13 | 8.13 | 1624.9 |
| 14 | 8.28 | 1656.1 |
| 15 | 9.36 | 1870.7 |
| 16 | 10.61 | 2120.7 |
| 17 | 14.13 | 2825.6 |

**Figure S25.** $^{1}$H-NMR of compd **52** (200 MHz, DMSO-$d_6$).



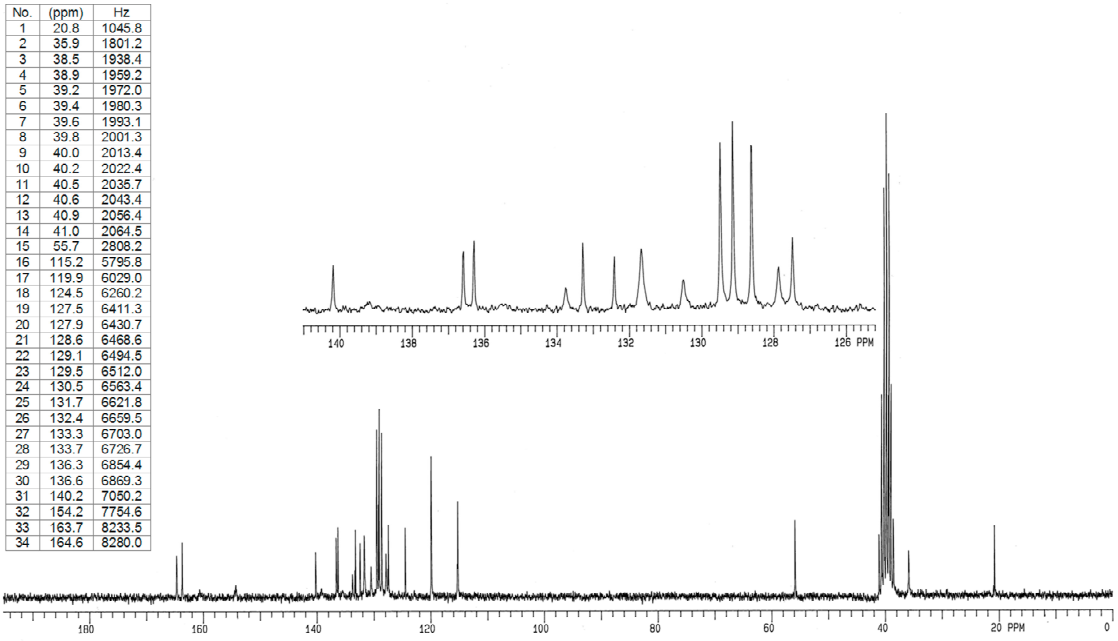
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 20.8 | 1045.0 |
| 2 | 35.9 | 1805.9 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 119.8 | 6026.3 |
| 16 | 126.3 | 6352.9 |
| 17 | 126.4 | 6356.4 |
| 18 | 127.5 | 6411.3 |
| 19 | 128.3 | 6452.7 |
| 20 | 128.5 | 6459.9 |
| 21 | 128.6 | 6467.1 |
| 22 | 129.2 | 6496.5 |
| 23 | 129.5 | 6510.6 |
| 24 | 129.6 | 6519.5 |
| 25 | 130.9 | 6584.3 |
| 26 | 132.6 | 6667.3 |
| 27 | 133.4 | 6708.1 |
| 28 | 134.4 | 6757.7 |
| 29 | 136.2 | 6849.8 |
| 30 | 136.4 | 6858.6 |
| 31 | 136.5 | 6862.9 |
| 32 | 136.9 | 6884.6 |
| 33 | 140.5 | 7065.3 |
| 34 | 155.0 | 7794.9 |
| 35 | 163.6 | 8229.1 |

**Figure S26.** $^{13}$C-NMR of compd **52** (50 MHz, DMSO-$d_6$).



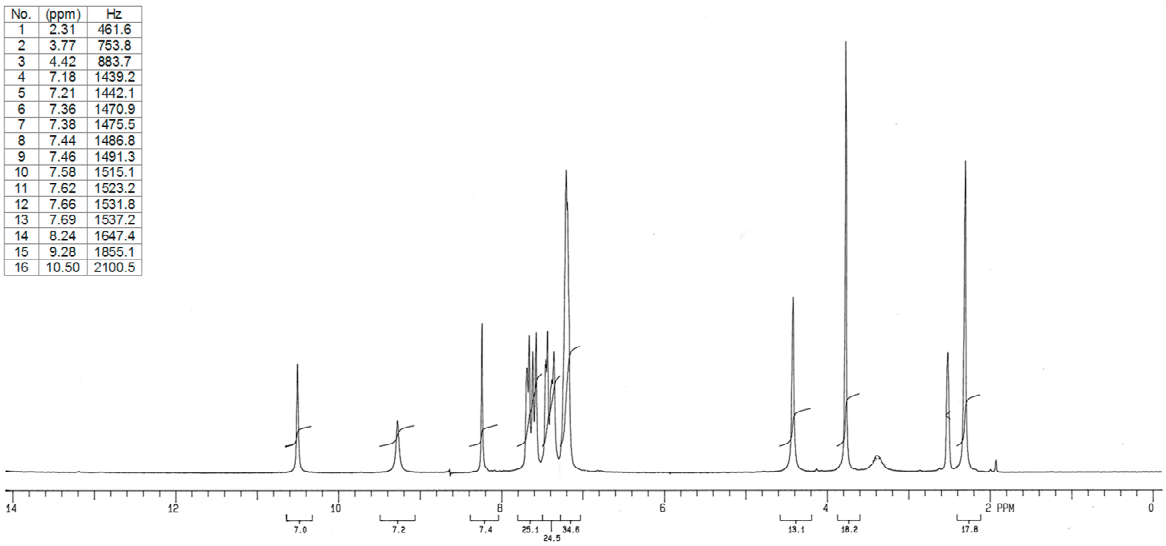
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.31 | 461.6 |
| 2 | 3.78 | 756.1 |
| 3 | 4.40 | 879.9 |
| 4 | 7.03 | 1405.7 |
| 5 | 7.07 | 1414.0 |
| 6 | 7.18 | 1436.6 |
| 7 | 7.21 | 1442.5 |
| 8 | 7.34 | 1467.8 |
| 9 | 7.36 | 1472.0 |
| 10 | 7.62 | 1523.5 |
| 11 | 7.65 | 1529.8 |
| 12 | 7.93 | 1586.3 |
| 13 | 7.97 | 1594.6 |
| 14 | 8.27 | 1654.5 |
| 15 | 9.10 | 1819.9 |
| 16 | 10.57 | 2113.2 |
| 17 | 14.50 | 2899.8 |

**Figure S27.** $^{1}$H-NMR of compd **53** (200 MHz, DMSO-$d_6$).



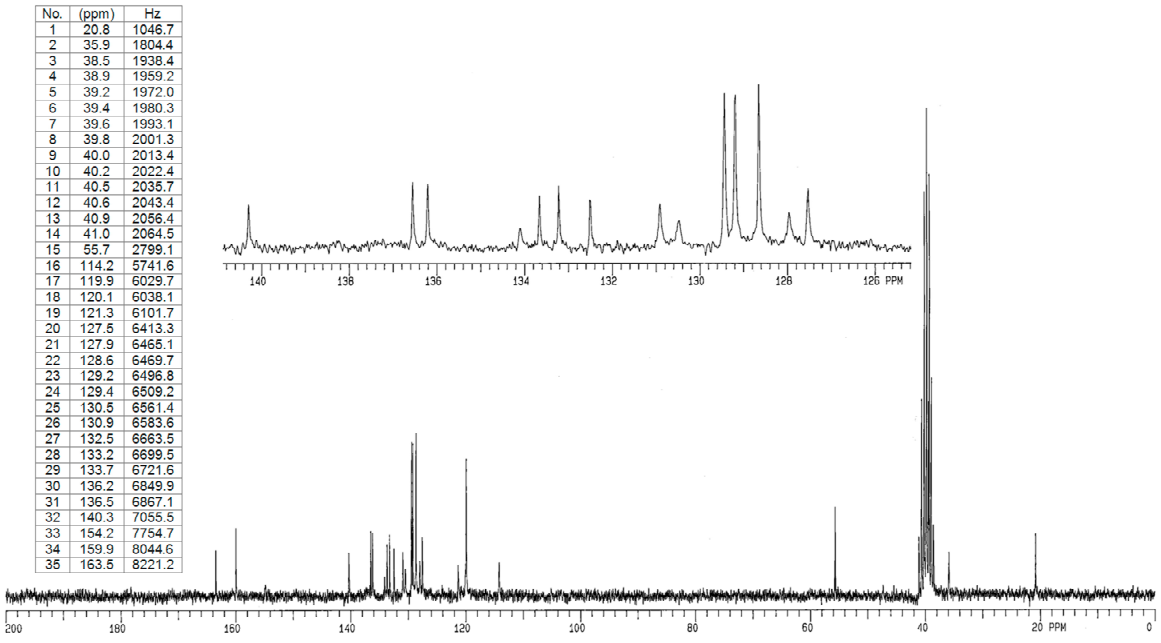
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 20.8 | 1045.8 |
| 2 | 35.9 | 1801.2 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 55.7 | 2808.2 |
| 16 | 115.2 | 5795.8 |
| 17 | 119.9 | 6029.0 |
| 18 | 124.5 | 6260.2 |
| 19 | 127.5 | 6411.3 |
| 20 | 127.9 | 6430.7 |
| 21 | 128.6 | 6468.6 |
| 22 | 129.1 | 6494.5 |
| 23 | 129.5 | 6512.0 |
| 24 | 130.5 | 6563.4 |
| 25 | 131.7 | 6621.8 |
| 26 | 132.4 | 6659.5 |
| 27 | 133.3 | 6703.0 |
| 28 | 133.7 | 6726.7 |
| 29 | 136.3 | 6854.4 |
| 30 | 136.6 | 6869.3 |
| 31 | 140.2 | 7050.2 |
| 32 | 154.2 | 7754.6 |
| 33 | 163.7 | 8233.5 |
| 34 | 164.6 | 8280.0 |

**Figure S28.** $^{13}$C-NMR of compd **53** (50 MHz, DMSO-$d_6$).



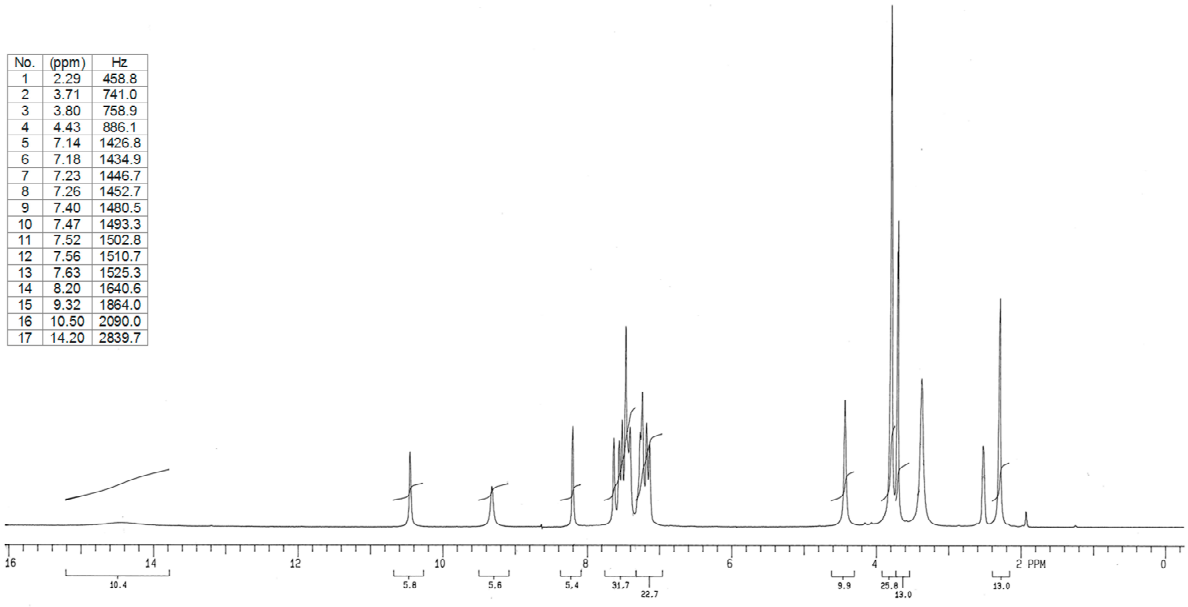
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.31 | 461.6 |
| 2 | 3.77 | 753.8 |
| 3 | 4.42 | 883.7 |
| 4 | 7.18 | 1439.2 |
| 5 | 7.21 | 1442.1 |
| 6 | 7.36 | 1470.9 |
| 7 | 7.38 | 1475.5 |
| 8 | 7.44 | 1486.8 |
| 9 | 7.46 | 1491.3 |
| 10 | 7.58 | 1515.1 |
| 11 | 7.62 | 1523.2 |
| 12 | 7.66 | 1531.8 |
| 13 | 7.69 | 1537.2 |
| 14 | 8.24 | 1647.4 |
| 15 | 9.28 | 1855.1 |
| 16 | 10.50 | 2100.5 |

**Figure S29.** $^{1}$H-NMR of compd **54** (200 MHz, DMSO-$d_6$).



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 20.8 | 1046.7 |
| 2 | 35.9 | 1804.4 |
| 3 | 38.5 | 1938.4 |
| 4 | 38.9 | 1959.2 |
| 5 | 39.2 | 1972.0 |
| 6 | 39.4 | 1980.3 |
| 7 | 39.6 | 1993.1 |
| 8 | 39.8 | 2001.3 |
| 9 | 40.0 | 2013.4 |
| 10 | 40.2 | 2022.4 |
| 11 | 40.5 | 2035.7 |
| 12 | 40.6 | 2043.4 |
| 13 | 40.9 | 2056.4 |
| 14 | 41.0 | 2064.5 |
| 15 | 55.7 | 2799.1 |
| 16 | 114.2 | 5741.6 |
| 17 | 119.9 | 6029.7 |
| 18 | 120.1 | 6038.1 |
| 19 | 121.3 | 6101.7 |
| 20 | 127.5 | 6413.3 |
| 21 | 127.9 | 6465.1 |
| 22 | 128.6 | 6469.7 |
| 23 | 129.2 | 6496.8 |
| 24 | 129.4 | 6509.2 |
| 25 | 130.5 | 6561.4 |
| 26 | 130.9 | 6583.6 |
| 27 | 132.5 | 6663.5 |
| 28 | 133.2 | 6699.5 |
| 29 | 133.7 | 6721.6 |
| 30 | 136.2 | 6849.9 |
| 31 | 136.5 | 6867.1 |
| 32 | 140.3 | 7055.5 |
| 33 | 154.2 | 7754.7 |
| 34 | 159.9 | 8044.6 |
| 35 | 163.5 | 8221.2 |

**Figure S30.** $^{13}$C-NMR of compd **54** (50 MHz, DMSO-$d_6$).



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 2.29 | 458.8 |
| 2 | 3.71 | 741.0 |
| 3 | 3.80 | 758.9 |
| 4 | 4.43 | 886.1 |
| 5 | 7.14 | 1426.8 |
| 6 | 7.18 | 1434.9 |
| 7 | 7.23 | 1446.7 |
| 8 | 7.26 | 1452.7 |
| 9 | 7.40 | 1480.5 |
| 10 | 7.47 | 1493.3 |
| 11 | 7.52 | 1502.8 |
| 12 | 7.56 | 1510.7 |
| 13 | 7.63 | 1525.3 |
| 14 | 8.20 | 1640.6 |
| 15 | 9.32 | 1864.0 |
| 16 | 10.50 | 2090.0 |
| 17 | 14.20 | 2839.7 |

**Figure S31.** $^{1}$H-NMR of compd **56** (200 MHz, DMSO-$d_6$).

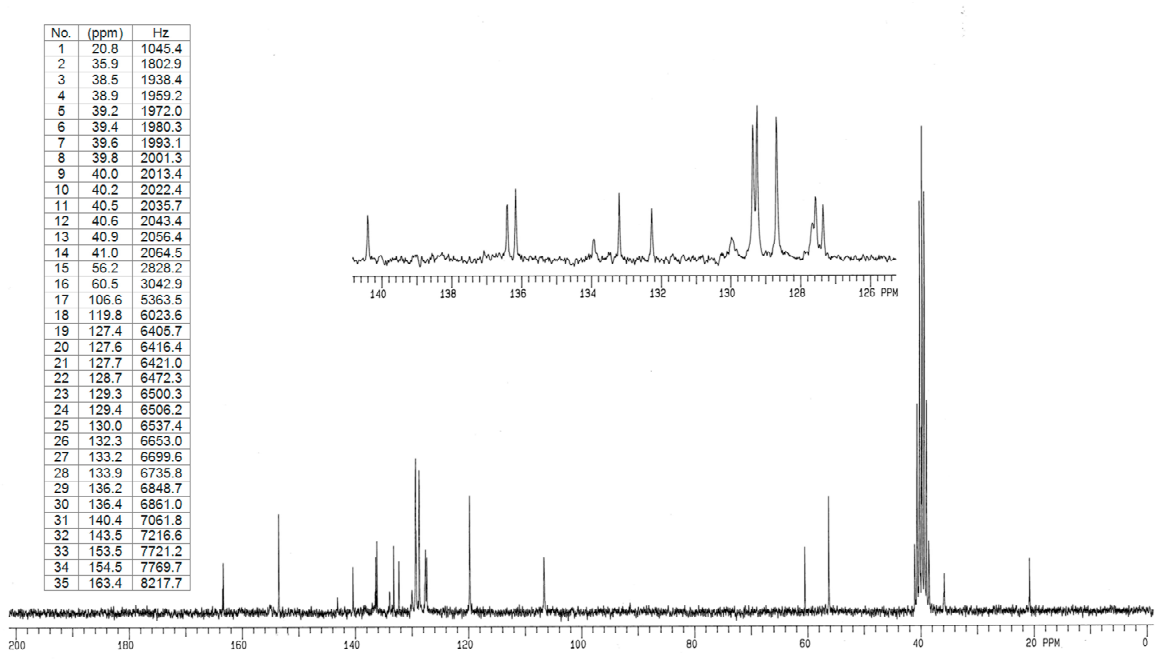



**Figure S32.** $^{13}$C-NMR of compd **56** (50 MHz, DMSO-$d_6$).

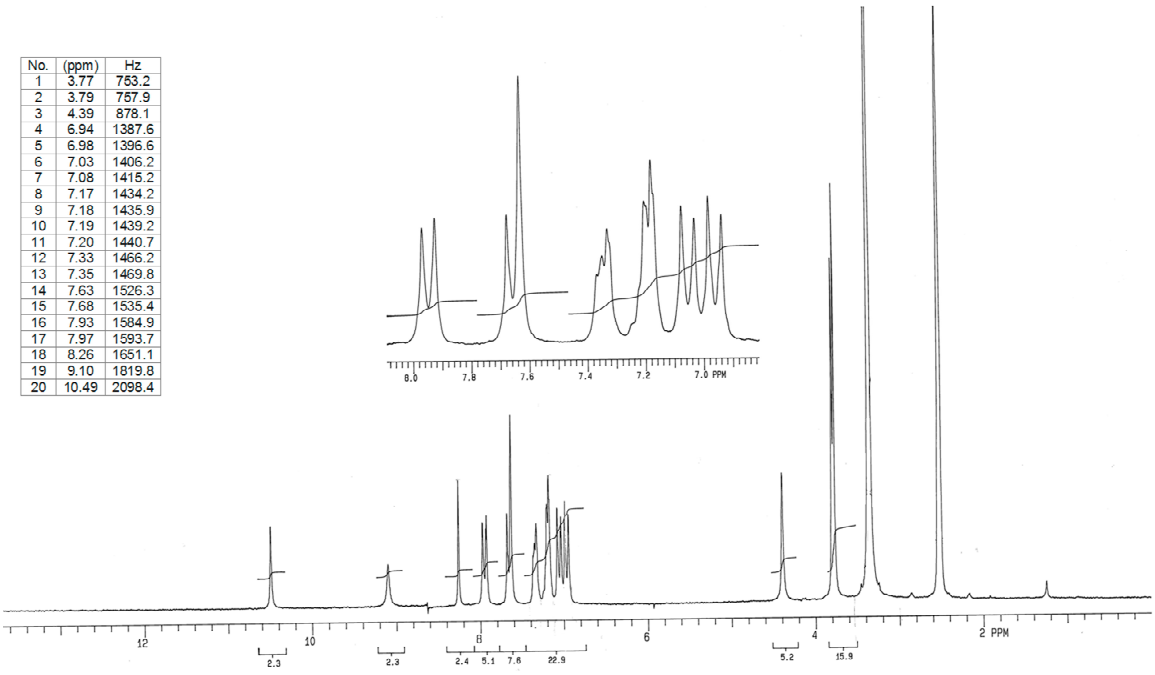



**Figure S33.** $^{1}$H-NMR of compd **57** (200 MHz, DMSO-$d_6$).

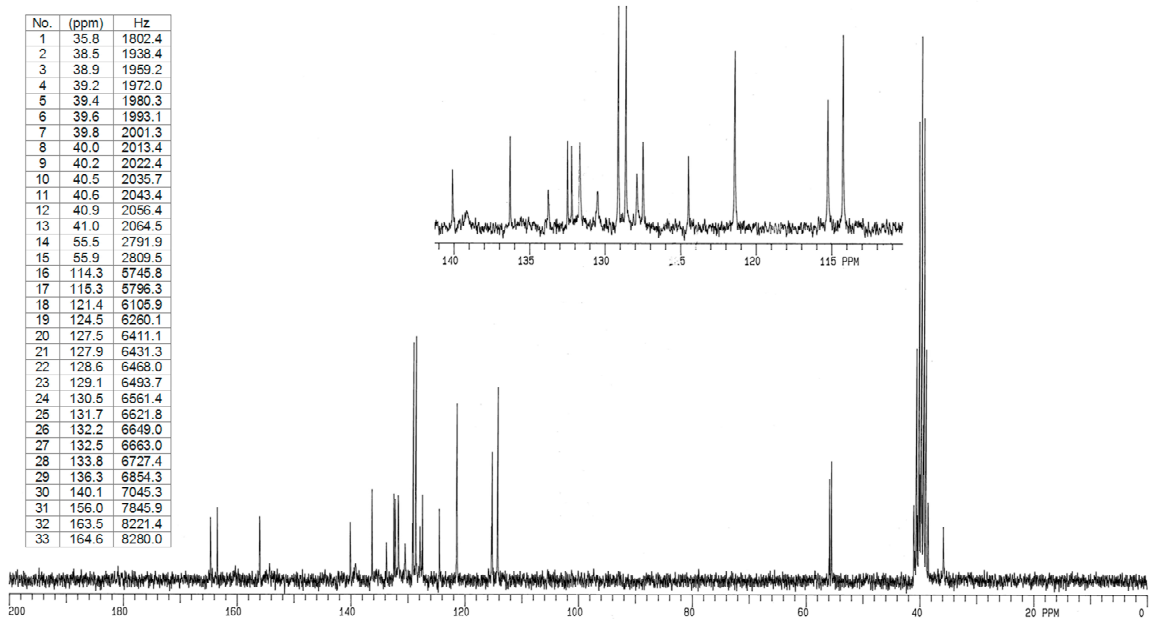



**Figure S34.** $^{13}$C-NMR of compd **57** (50 MHz, DMSO-$d_6$).

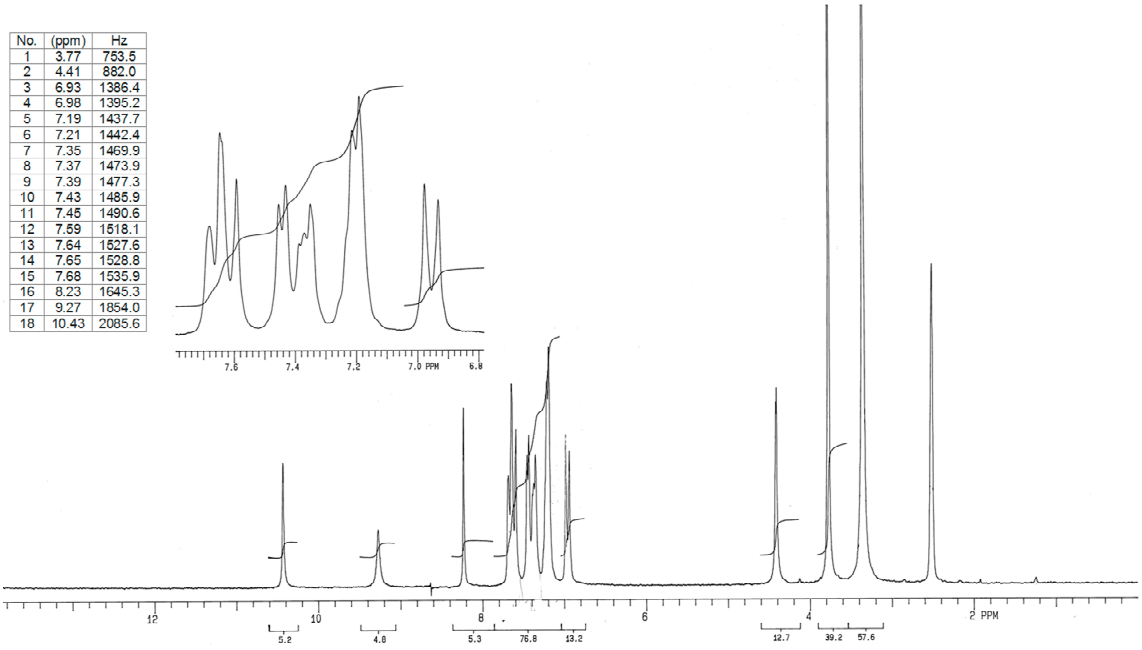
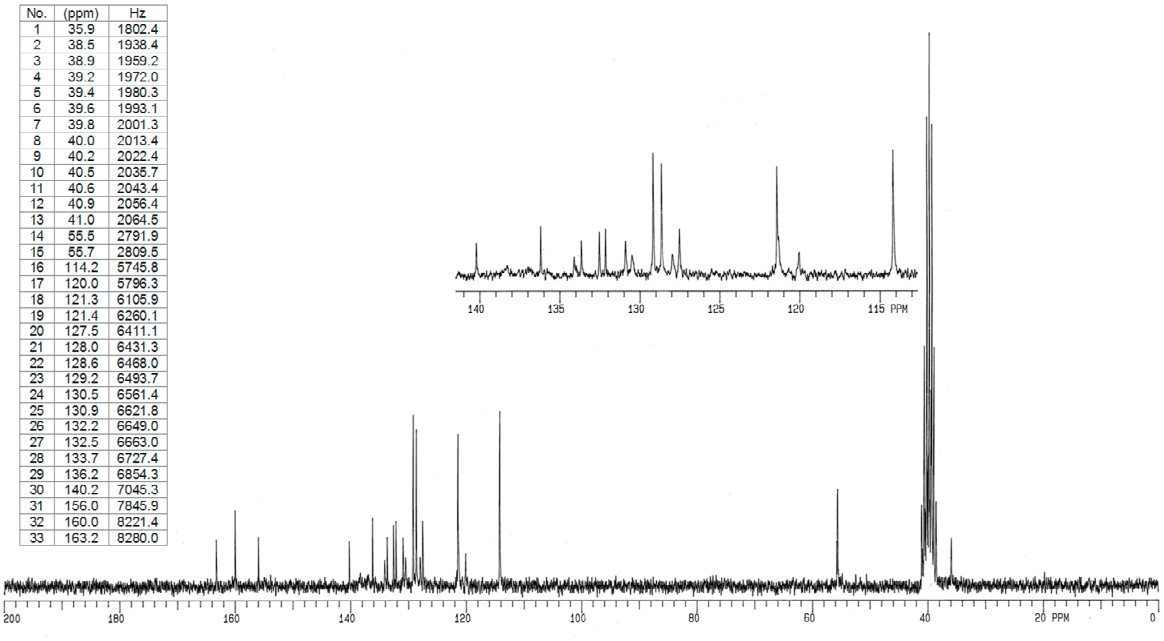
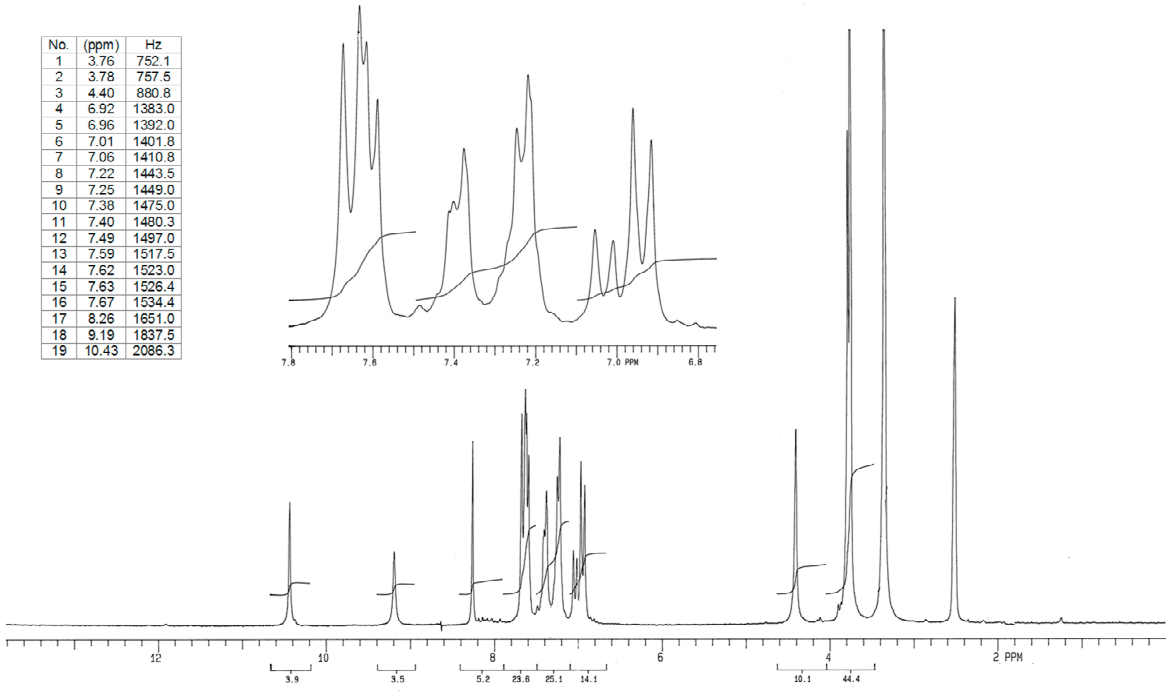



**Figure S35.** $^{1}$H-NMR of compd **58** (200 MHz, DMSO-$d_6$).



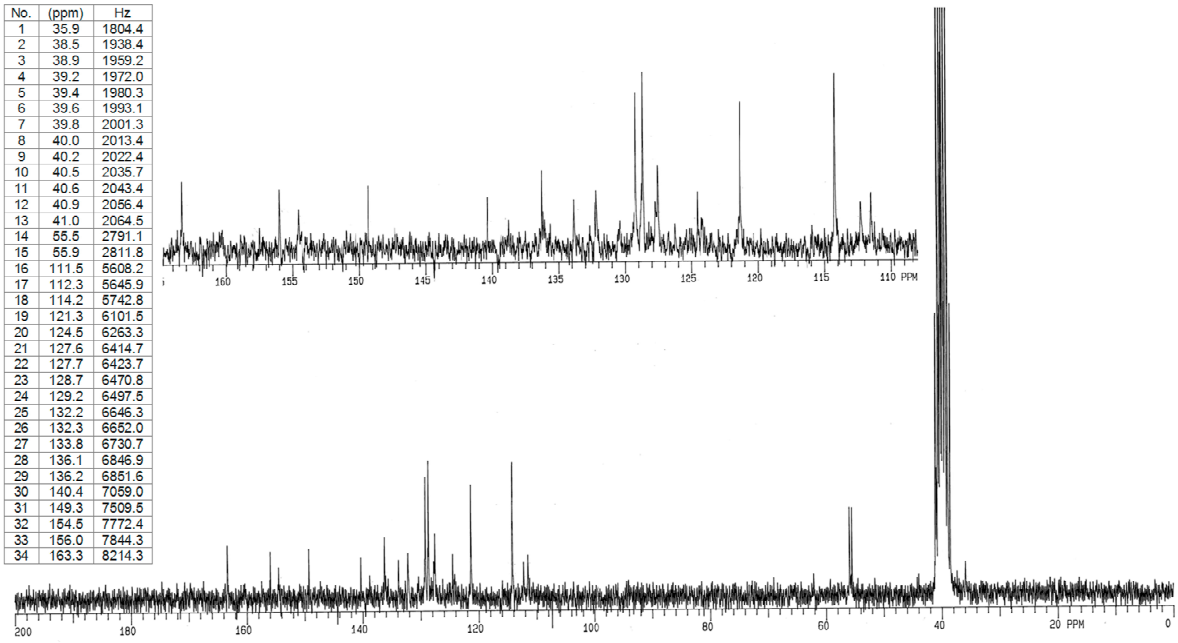
| No. | (ppm) | Hz |
|---|---|---|
| 1 | 35.9 | 1802.4 |
| 2 | 38.5 | 1938.4 |
| 3 | 38.9 | 1959.2 |
| 4 | 39.2 | 1972.0 |
| 5 | 39.4 | 1980.3 |
| 6 | 39.6 | 1993.1 |
| 7 | 39.8 | 2001.3 |
| 8 | 40.0 | 2013.4 |
| 9 | 40.2 | 2022.4 |
| 10 | 40.5 | 2035.7 |
| 11 | 40.6 | 2043.4 |
| 12 | 40.9 | 2056.4 |
| 13 | 41.0 | 2064.5 |
| 14 | 55.5 | 2791.9 |
| 15 | 55.7 | 2809.5 |
| 16 | 114.2 | 5745.8 |
| 17 | 120.0 | 5796.3 |
| 18 | 121.3 | 6105.9 |
| 19 | 121.4 | 6260.1 |
| 20 | 127.5 | 6411.1 |
| 21 | 128.0 | 6431.3 |
| 22 | 128.6 | 6468.0 |
| 23 | 129.2 | 6493.7 |
| 24 | 130.5 | 6561.4 |
| 25 | 130.9 | 6621.8 |
| 26 | 132.2 | 6649.0 |
| 27 | 132.5 | 6663.0 |
| 28 | 133.7 | 6727.4 |
| 29 | 136.2 | 6854.3 |
| 30 | 140.2 | 7045.3 |
| 31 | 156.0 | 7845.9 |
| 32 | 160.0 | 8221.4 |
| 33 | 163.2 | 8280.0 |

**Figure S36.** $^{13}$C-NMR of compd **58** (50 MHz, DMSO-$d_6$).



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 3.76 | 752.1 |
| 2 | 3.78 | 757.5 |
| 3 | 4.40 | 880.8 |
| 4 | 6.92 | 1383.0 |
| 5 | 6.96 | 1392.0 |
| 6 | 7.01 | 1401.8 |
| 7 | 7.06 | 1410.8 |
| 8 | 7.22 | 1443.5 |
| 9 | 7.25 | 1449.0 |
| 10 | 7.38 | 1475.0 |
| 11 | 7.40 | 1480.3 |
| 12 | 7.49 | 1497.0 |
| 13 | 7.59 | 1517.5 |
| 14 | 7.62 | 1523.0 |
| 15 | 7.63 | 1526.4 |
| 16 | 7.67 | 1534.4 |
| 17 | 8.26 | 1651.0 |
| 18 | 9.19 | 1837.5 |
| 19 | 10.43 | 2086.3 |

**Figure S37.** $^{1}$H-NMR of compd **59** (200 MHz, DMSO-$d_6$).



| No. | (ppm) | Hz |
|---|---|---|
| 1 | 35.9 | 1804.4 |
| 2 | 38.5 | 1938.4 |
| 3 | 38.9 | 1959.2 |
| 4 | 39.2 | 1972.0 |
| 5 | 39.4 | 1980.3 |
| 6 | 39.6 | 1993.1 |
| 7 | 39.8 | 2001.3 |
| 8 | 40.0 | 2013.4 |
| 9 | 40.2 | 2022.4 |
| 10 | 40.5 | 2035.7 |
| 11 | 40.6 | 2043.4 |
| 12 | 40.9 | 2056.4 |
| 13 | 41.0 | 2064.5 |
| 14 | 55.5 | 2791.1 |
| 15 | 55.9 | 2811.8 |
| 16 | 111.5 | 5608.2 |
| 17 | 112.3 | 5645.9 |
| 18 | 114.2 | 5742.8 |
| 19 | 121.3 | 6101.5 |
| 20 | 124.5 | 6263.3 |
| 21 | 127.6 | 6414.7 |
| 22 | 127.7 | 6423.7 |
| 23 | 128.7 | 6470.8 |
| 24 | 129.2 | 6497.5 |
| 25 | 132.2 | 6646.3 |
| 26 | 132.3 | 6652.0 |
| 27 | 133.8 | 6730.7 |
| 28 | 136.1 | 6846.9 |
| 29 | 136.2 | 6851.6 |
| 30 | 140.4 | 7059.0 |
| 31 | 149.3 | 7509.5 |
| 32 | 154.5 | 7772.4 |
| 33 | 156.0 | 7844.3 |
| 34 | 163.3 | 8214.3 |

**Figure S38.** $^{13}$C-NMR of compd **59** (50 MHz, DMSO-$d_6$).