

**Lead Identification and Structure – Activity Relationships of Heteroarylpyrazole  
Arylsulfonamides as Allosteric CC-Chemokine Receptor 4 (CCR4) Antagonists.**

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## Supporting Information

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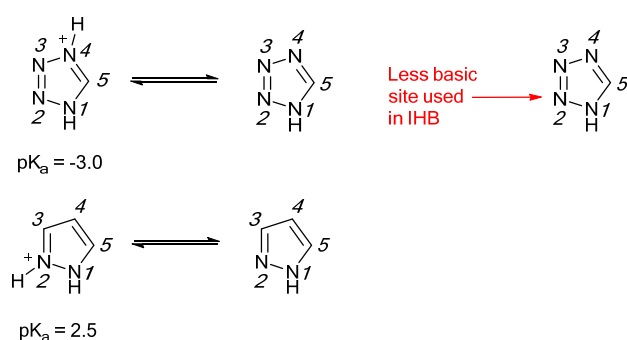
#### *Details of computational procedures*

Structures corresponding to **7**, **14** and **16** were built in Spartan'08<sup>S1</sup> and Monte Carlo conformational searching was carried out using the PM3 semi-empirical method. Relatively small sets of conformers (10 typically) were obtained and geometry optimisation calculations were carried out for all members of the sets using the B3LYP functional<sup>S2,S3</sup> and the 6-31G\* and 6-31+G\* basis sets, *in vacuo* and in water (Truhlar's SM8 model<sup>S4,S5</sup> was applied). Single point energy calculations were also carried out (*in vacuo*) with the larger 6-311+G\*\* basis set (using the dual basis set approximation implemented in Spartan'08). The solvation model was invoked using the ADDSOLVENT=WATER keyword. Full frequency calculations were carried out with the smaller 6-31G\* basis *in vacuo* and in water.

Calculations were carried out on a Dell Precision T1500 (Intel i7 Quad Core, 2.93 GHz) with 8GB RAM, Microsoft Windows 7 OS 64-bit, or a Dell Precision T7500 (2 x Intel E5530 processors, four cores each, 2.40 GHz) with 24 GB RAM Debian GNU/Linux 5.

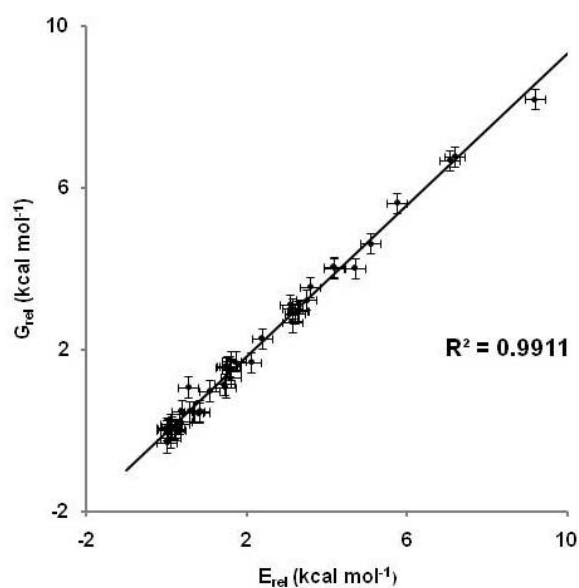
### Azole basicities

The comparison between the nitrogen atoms which act as hydrogen bond acceptor sites in the main text was based on the data presented below. In compounds **14** and **16**, *N*-1 was arylated; In **14**, the acceptor is *N*-2 which is the basic site in pyrazole; in **16**, the *N*-2 site is less basic than *N*-4.<sup>S6</sup> The difference of 5 pK<sub>a</sub> units referred to in the main text represents a minimum basicity difference.



- S1. Wavefunction, Irvine, CA, **2008**.
- S2. A. D. Becke, *J. Chem. Phys.*, **1993**, 98, 5648.
- S3. C. T. Lee, W. T. Yang and R. G. Parr, *Physical Rev. B*, **1988**, 37, 785.
- S4. A. C. Chamberlin, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, **2008**, 112, 8651.
- S5. C. J. Cramer and D. G. Truhlar, *Accounts Chem. Res.*, **2008**, 41, 760.
- S6. *The Chemistry of Heterocycles*, T. Eicher and S. Hauptman, Thieme, Stuttgart, **1995**, pp. 181, 212.

Correlation between  $E_{rel}$  and  $G_{rel}$  (test of conformer ordering by electronic energies)



Electronic energies and free energies (**Table SX**) calculated (B3LYP/6-31G\*) for all conformers obtained for **7**, **14** and **16** *in vacuo*, and selected conformers in water were included in the correlation. The congruence suggests very strongly that electronic energies calculated with the larger 6-31+G\* basis set in water can be used to order the conformers correctly. Error bars are set at  $\pm 0.25 \text{ kcal mol}^{-1}$  in the plotting.

| Molecule and conformer | E (au)      | E <sub>rel</sub> (kcal mol <sup>-1</sup> ) | G (au)      | G <sub>rel</sub> (kcal mol <sup>-1</sup> ) | # v <sub>i</sub> |
|------------------------|-------------|--------------------------------------------|-------------|--------------------------------------------|------------------|
| <b>7 in vacuo</b>      |             |                                            |             |                                            |                  |
| 1                      | -2287.83028 | 0.2                                        | -2287.60745 | 0.0                                        | 0                |
| 2                      | -2287.83047 | 0.1                                        | -2287.60776 | -0.2                                       | 0                |
| 3                      | -2287.82255 | 5.1                                        | -2287.60009 | 4.6                                        | 0                |
| 4                      | -2287.82314 | 4.7                                        | -2287.60106 | 4.0                                        | 0                |
| 5                      | -2287.82493 | 3.6                                        | -2287.60181 | 3.5                                        | 0                |
| 6                      | -2287.82565 | 3.1                                        | -2287.60264 | 3.0                                        | 0                |
| 7                      | -2287.82554 | 3.2                                        | -2287.60284 | 2.9                                        | 0                |
| 8                      | -2287.81601 | 9.2                                        | -2287.59441 | 8.2                                        | 0                |
| 9                      | -2287.82813 | 1.6                                        | -2287.60539 | 1.3                                        | 0                |
| 10                     | -2287.83064 | 0.0                                        | -2287.60792 | -0.3                                       | 0                |
| <b>7 water</b>         |             |                                            |             |                                            |                  |
| 2                      | -2287.85603 | 0.0                                        | -2287.63356 | 0.0                                        | 0                |
| 1                      | -2287.8559  | 0.1                                        | -2287.63329 | 0.2                                        | 0                |
| 10                     | -2287.85553 | 0.3                                        | -2287.6333  | 0.2                                        | 0                |
| 9                      | -2287.85346 | 1.6                                        | -2287.63082 | 1.7                                        | 0                |
| 5                      | -2287.85114 | 3.1                                        | -2287.62861 | 3.1                                        | 0                |
| <b>14 in vacuo</b>     |             |                                            |             |                                            |                  |
| 1                      | -2211.40233 | 0.0                                        | -2211.20417 | 0.0                                        | 0                |
| 2                      | -2211.40001 | 1.5                                        | -2211.20169 | 1.6                                        | 0                |
| 3                      | -2211.4023  | 0.0                                        | -2211.20413 | 0.0                                        | 0                |
| 4                      | -2211.40143 | 0.6                                        | -2211.20341 | 0.5                                        | 0                |
| 5                      | -2211.40128 | 0.7                                        | -2211.20345 | 0.5                                        | 0                |
| 6                      | -2211.39996 | 1.5                                        | -2211.20163 | 1.6                                        | 0                |
| 7                      | -2211.39961 | 1.7                                        | -2211.20146 | 1.7                                        | 0                |
| 8                      | -2211.39319 | 5.7                                        | -2211.1952  | 5.6                                        | 0                |
| 9                      | -2211.39566 | 4.2                                        | -2211.19778 | 4.0                                        | 0                |
| 10                     | -2211.39571 | 4.2                                        | -2211.19772 | 4.0                                        | 0                |
| 11                     | -2211.39087 | 7.2                                        | -2211.19338 | 6.8                                        | 0                |
| 12                     | -2211.40234 | 0.0                                        | -2211.20408 | 0.1                                        | 0                |
| <b>14 water</b>        |             |                                            |             |                                            |                  |
| 3                      | -2211.42267 | 0.0                                        | -2211.22476 | 0.0                                        | 0                |
| 4                      | -2211.42209 | 0.4                                        | -2211.22442 | 0.2                                        | 0                |
| 2                      | -2211.42019 | 1.6                                        | -2211.22225 | 1.6                                        | 0                |
| 7                      | -2211.4201  | 1.6                                        | -2211.22236 | 1.5                                        | 0                |
| <b>16 in vacuo</b>     |             |                                            |             |                                            |                  |
| 1                      | -2243.44612 | 3.5                                        | -2243.27251 | 3.2                                        | 0                |
| 2                      | -2243.44997 | 1.1                                        | -2243.27609 | 1.0                                        | 0                |
| 3                      | -2243.45146 | 0.1                                        | -2243.27752 | 0.1                                        | 0                |
| 4                      | -2243.45167 | 0.0                                        | -2243.27765 | 0.0                                        | 0                |
| 5                      | -2243.4467  | 3.1                                        | -2243.27338 | 2.7                                        | 0                |
| 6                      | -2243.45059 | 0.7                                        | -2243.27692 | 0.5                                        | 0                |
| 7                      | -2243.45155 | 0.1                                        | -2243.27764 | 0.0                                        | 0                |
| 8                      | -2243.45037 | 0.8                                        | -2243.27688 | 0.5                                        | 0                |
| 9                      | -2243.44939 | 1.4                                        | -2243.27584 | 1.1                                        | 0                |
| 10                     | -2243.44643 | 3.3                                        | -2243.27294 | 3.0                                        | 0                |
| 11                     | -2243.44042 | 7.1                                        | -2243.26701 | 6.7                                        | 0                |

|                 |             |     |             |     |   |
|-----------------|-------------|-----|-------------|-----|---|
| 12              | -2243.45041 | 0.8 | -2243.27696 | 0.4 | 0 |
| <b>16</b> water |             |     |             |     |   |
| 1               | -2243.47324 | 1.5 | -2243.30014 | 1.1 | 0 |
| 2               | -2243.47178 | 2.4 | -2243.2982  | 2.3 | 0 |
| 3               | -2243.4753  | 0.2 | -2243.30177 | 0.0 | 0 |
| 5               | -2243.47035 | 3.3 | -2243.29712 | 3.0 | 0 |
| 6               | -2243.47497 | 0.4 | -2243.30106 | 0.5 | 0 |
| 7               | -2243.47556 | 0.0 | -2243.30183 | 0.0 | 0 |
| 9               | -2243.47222 | 2.1 | -2243.29914 | 1.7 | 0 |
| 12              | -2243.47471 | 0.5 | -2243.30012 | 1.1 | 0 |

**Table S1.** Conformer energies (optimisation and full frequency calculation, B3LYP/6-31G\*)

with number of imaginary frequencies

*Coordinates of the three lowest energy species for 7, 14 and 16 (optimisation only, B3LYP/6-31+G\*, water [SM8])*

**7, Global minimum**  
-2287.894099 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | H  | H1  | -4.7211091 | -1.8929293 | 1.2191096  |
| 2  | C  | C1  | -3.9926246 | -1.3394366 | 0.6289573  |
| 3  | C  | C4  | -2.1239421 | 0.1084661  | -0.8391405 |
| 4  | C  | C2  | -3.8280361 | -1.5962070 | -0.7302408 |
| 5  | C  | C6  | -3.2160737 | -0.3605386 | 1.2588881  |
| 6  | C  | C5  | -2.2725605 | 0.3807365  | 0.5314570  |
| 7  | C  | C3  | -2.8901453 | -0.8753291 | -1.4665612 |
| 8  | H  | H2  | -4.4327645 | -2.3596376 | -1.2173833 |
| 9  | H  | H3  | -2.7418252 | -1.0619200 | -2.5236787 |
| 10 | Cl | Cl1 | -1.3119346 | 1.5907620  | 1.3400801  |
| 11 | Cl | Cl2 | -3.4530727 | -0.0811975 | 2.9647330  |
| 12 | S  | S1  | -1.0139942 | 1.0526194  | -1.9003978 |
| 13 | O  | O1  | -1.0500333 | 0.4213001  | -3.2265965 |
| 14 | O  | O2  | -1.3073997 | 2.4895153  | -1.7791934 |
| 15 | N  | N1  | 0.5444735  | 0.9102858  | -1.2925039 |
| 16 | C  | C8  | 1.1685411  | -0.2670439 | -0.8539237 |
| 17 | H  | H8  | 0.8264361  | 1.7324538  | -0.7651799 |
| 18 | N  | N2  | 0.7433324  | -1.4873501 | -1.1197822 |
| 19 | N  | N3  | 1.6411028  | -2.3330909 | -0.5181585 |
| 20 | C  | C7  | 2.6404238  | -1.6440518 | 0.1116983  |
| 21 | C  | C9  | 2.3645746  | -0.2734477 | -0.0874516 |
| 22 | C  | C10 | 1.4653420  | -3.7766064 | -0.5857384 |
| 23 | H  | H4  | 2.2646373  | -4.2462865 | -1.1752684 |
| 24 | H  | H6  | 0.5043521  | -3.9793192 | -1.0640147 |
| 25 | H  | H7  | 1.4591506  | -4.2089705 | 0.4245823  |
| 26 | C  | C11 | 3.2170675  | 0.7185713  | 0.4424935  |
| 27 | C  | C12 | 4.3339090  | 0.3084537  | 1.1564335  |
| 28 | H  | H10 | 5.0236737  | 1.0323598  | 1.5806875  |
| 29 | C  | C13 | 4.5910878  | -1.0758324 | 1.3456112  |
| 30 | H  | H12 | 5.4760621  | -1.3576960 | 1.9150957  |
| 31 | C  | C14 | 3.7687588  | -2.0718660 | 0.8409595  |
| 32 | H  | H13 | 3.9885462  | -3.1257058 | 0.9980230  |
| 33 | O  | O3  | 2.8407557  | 2.0160759  | 0.1929064  |
| 34 | C  | C15 | 3.6958807  | 3.0745732  | 0.6673786  |
| 35 | H  | H5  | 3.2157500  | 4.0033343  | 0.3512924  |
| 36 | H  | H9  | 4.6915682  | 3.0014584  | 0.2098047  |
| 37 | H  | H11 | 3.7723952  | 3.0516603  | 1.7627273  |

**7, Second conformer**  
-2287.893582 au

|   |   |    |            |           |           |
|---|---|----|------------|-----------|-----------|
| 1 | C | C1 | 0.3056402  | 2.1881155 | 1.8861381 |
| 2 | C | C4 | -0.2725463 | 0.0220979 | 3.6856615 |

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 3  | C  | C2  | 0.3768682  | 0.8459010  | 1.4453314  |
| 4  | C  | C6  | -0.0672609 | 2.4265087  | 3.2014023  |
| 5  | C  | C5  | -0.3490029 | 1.3476391  | 4.0803003  |
| 6  | C  | C3  | 0.0937542  | -0.2067951 | 2.3451321  |
| 7  | H  | H6  | -0.1446531 | 3.4404044  | 3.5828206  |
| 8  | H  | H5  | -0.6319678 | 1.5819384  | 5.1063232  |
| 9  | H  | H4  | -0.4845681 | -0.7928673 | 4.3752917  |
| 10 | C  | C7  | 0.6910630  | 0.1840196  | 0.2269275  |
| 11 | N  | N1  | 0.6220061  | -1.1338110 | 0.3541176  |
| 12 | N  | N2  | 0.2428111  | -1.3711558 | 1.6363244  |
| 13 | O  | O1  | 0.6322771  | 3.1436668  | 0.9560862  |
| 14 | C  | C8  | 0.5190201  | 4.5269023  | 1.3406924  |
| 15 | H  | H2  | 0.7886737  | 5.1013849  | 0.4521833  |
| 16 | H  | H3  | 1.2141194  | 4.7631620  | 2.1577989  |
| 17 | H  | H1  | -0.5119917 | 4.7664935  | 1.6329398  |
| 18 | N  | N3  | 1.0582864  | 0.7477341  | -1.0179713 |
| 19 | H  | H8  | 1.4902192  | 1.6657712  | -0.9242119 |
| 20 | S  | S1  | -0.1295630 | 0.8930140  | -2.2447726 |
| 21 | O  | O2  | -1.4449513 | 1.2480714  | -1.6836942 |
| 22 | O  | O3  | 0.4796980  | 1.7902917  | -3.2418204 |
| 23 | C  | C9  | -0.2713722 | -0.7870143 | -2.8794909 |
| 24 | C  | C10 | -0.7153995 | -3.3643527 | -3.8345098 |
| 25 | C  | C11 | 0.7824262  | -1.4666906 | -3.5186996 |
| 26 | C  | C12 | -1.5266466 | -1.3822366 | -2.7299145 |
| 27 | C  | C13 | -1.7483548 | -2.6712213 | -3.2098856 |
| 28 | C  | C14 | 0.5399243  | -2.7670859 | -3.9881483 |
| 29 | H  | H10 | -2.3150445 | -0.8241933 | -2.2376564 |
| 30 | H  | H11 | -2.7273529 | -3.1349186 | -3.0958112 |
| 31 | H  | H13 | -0.8687772 | -4.3728904 | -4.2155233 |
| 32 | C  | C15 | 0.0850727  | -2.7328266 | 2.1339304  |
| 33 | H  | H9  | 0.2385273  | -3.4180499 | 1.2972314  |
| 34 | H  | H14 | -0.9252931 | -2.8782664 | 2.5396707  |
| 35 | H  | H15 | 0.8256135  | -2.9479826 | 2.9163959  |
| 36 | Cl | Cl1 | 2.3541905  | -0.7516708 | -3.7425516 |
| 37 | Cl | Cl2 | 1.7945551  | -3.6790876 | -4.7880381 |

7, Third conformer  
-2287.891714 au

|    |   |    |            |            |           |
|----|---|----|------------|------------|-----------|
| 1  | C | C1 | 1.4177617  | 1.3674582  | 1.8328363 |
| 2  | C | C4 | -0.9151266 | 0.5737331  | 3.3195814 |
| 3  | C | C2 | 0.6827706  | 0.2145990  | 1.4498586 |
| 4  | C | C6 | 0.9553283  | 2.1099547  | 2.9128639 |
| 5  | C | C5 | -0.1969813 | 1.7134779  | 3.6372890 |
| 6  | C | C3 | -0.4496986 | -0.1639265 | 2.2142891 |
| 7  | H | H6 | 1.4851947  | 3.0029599  | 3.2301915 |
| 8  | H | H5 | -0.5132982 | 2.3282454  | 4.4795546 |
| 9  | H | H4 | -1.7876359 | 0.2654084  | 3.8921908 |
| 10 | C | C7 | 0.7671391  | -0.7947967 | 0.4480635 |
| 11 | N | N1 | -0.1941453 | -1.7003631 | 0.5875440 |
| 12 | N | N2 | -0.9261083 | -1.3235321 | 1.6597089 |



|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 13 | O  | O1  | 2.5455270  | 1.6427214  | 1.1171912  |
| 14 | C  | C8  | 3.2412045  | 2.8696760  | 1.3886616  |
| 15 | H  | H2  | 4.0477858  | 2.9166228  | 0.6543701  |
| 16 | H  | H3  | 3.6672925  | 2.8678822  | 2.4019182  |
| 17 | H  | H1  | 2.5781204  | 3.7358461  | 1.2572410  |
| 18 | N  | N3  | 1.7300551  | -0.9647039 | -0.5763535 |
| 19 | H  | H8  | 1.8831802  | -1.9489534 | -0.7963629 |
| 20 | S  | S1  | 1.5508479  | -0.1285628 | -2.0584739 |
| 21 | O  | O2  | 1.5213147  | 1.3050489  | -1.7529367 |
| 22 | O  | O3  | 2.6047653  | -0.6785235 | -2.9245074 |
| 23 | C  | C9  | -0.0710030 | -0.5425262 | -2.7434407 |
| 24 | C  | C10 | -2.5959277 | -0.9893398 | -3.8307995 |
| 25 | C  | C11 | -0.4327608 | -1.8484339 | -3.1190589 |
| 26 | C  | C12 | -0.9607208 | 0.5233908  | -2.9053648 |
| 27 | C  | C13 | -2.2217470 | 0.2977790  | -3.4553498 |
| 28 | C  | C14 | -1.7089881 | -2.0575970 | -3.6616444 |
| 29 | H  | H10 | -0.6492378 | 1.5196344  | -2.6096355 |
| 30 | H  | H11 | -2.9132668 | 1.1281642  | -3.5912394 |
| 31 | H  | H13 | -3.5768329 | -1.1839894 | -4.2609907 |
| 32 | C  | C15 | -2.0368466 | -2.1417279 | 2.1354015  |
| 33 | H  | H9  | -2.1788399 | -2.9613055 | 1.4266985  |
| 34 | H  | H14 | -2.9568611 | -1.5442475 | 2.1852880  |
| 35 | H  | H15 | -1.8163187 | -2.5556283 | 3.1288027  |
| 36 | Cl | Cl1 | 0.6546919  | -3.2023806 | -2.9290408 |
| 37 | Cl | Cl2 | -2.2306346 | -3.6520647 | -4.1443454 |

**14**, Global minimum  
-2211.460397 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | 0.2934067  | -1.7459607 | -1.8775833 |
| 2  | O  | O1  | 1.5892481  | -2.4058232 | -2.1051791 |
| 3  | O  | O2  | -0.7732889 | -1.9141408 | -2.8827056 |
| 4  | C  | C1  | -0.2760847 | -2.2854584 | -0.2518523 |
| 5  | C  | C4  | -1.0053016 | -3.2396681 | 2.2629939  |
| 6  | C  | C2  | 0.5290441  | -3.2231337 | 0.4036594  |
| 7  | C  | C6  | -1.4650826 | -1.8192192 | 0.3408240  |
| 8  | C  | C5  | -1.8147631 | -2.3042427 | 1.6112258  |
| 9  | C  | C3  | 0.1599813  | -3.7019766 | 1.6587515  |
| 10 | H  | H1  | 1.4363428  | -3.5666564 | -0.0808352 |
| 11 | H  | H3  | 0.7844832  | -4.4338087 | 2.1687957  |
| 12 | H  | H4  | -1.3060658 | -3.5982726 | 3.2460747  |
| 13 | Cl | Cl1 | -3.2657345 | -1.7583102 | 2.4116088  |
| 14 | Cl | Cl2 | -2.5029873 | -0.6594308 | -0.4503363 |
| 15 | N  | N1  | 0.5522616  | -0.0902683 | -1.8116811 |
| 16 | H  | H5  | -0.2243651 | 0.4510901  | -2.1967299 |
| 17 | C  | C7  | 1.2004624  | 0.5479104  | -0.7217737 |
| 18 | C  | C8  | 2.4725591  | 1.8310382  | 1.4331110  |
| 19 | C  | C9  | 0.6798763  | 1.7538053  | -0.2028047 |
| 20 | C  | C10 | 2.3702532  | 0.0170398  | -0.1616134 |
| 21 | C  | C11 | 2.9891724  | 0.6386903  | 0.9216928  |
| 22 | C  | C12 | 1.3384994  | 2.3948162  | 0.8529462  |

|    |   |     |            |            |            |
|----|---|-----|------------|------------|------------|
| 23 | H | H6  | 2.7857417  | -0.8905810 | -0.5837218 |
| 24 | H | H7  | 3.8880095  | 0.1970093  | 1.3493955  |
| 25 | H | H8  | 0.9595254  | 3.3493919  | 1.2136682  |
| 26 | H | H9  | 2.9639317  | 2.3375064  | 2.2627562  |
| 27 | N | N2  | -0.5108542 | 2.3342891  | -0.7261230 |
| 28 | N | N3  | -0.8216918 | 2.2541250  | -2.0571831 |
| 29 | C | C13 | -1.4625144 | 3.0324187  | -0.0342783 |
| 30 | H | H14 | -1.4029627 | 3.1710753  | 1.0402087  |
| 31 | C | C14 | -1.9761957 | 2.9124993  | -2.1815578 |
| 32 | H | H2  | -2.4408357 | 2.9872552  | -3.1572069 |
| 33 | C | C15 | -2.4220397 | 3.4282854  | -0.9472814 |
| 34 | H | H12 | -3.3220506 | 3.9987055  | -0.7472653 |

#### 14, Second conformer

-2211.458434 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | 0.7498527  | -1.8674008 | -1.6250549 |
| 2  | O  | O1  | 1.1447618  | -3.2285897 | -1.2135096 |
| 3  | O  | O2  | 0.8715786  | -1.4684958 | -3.0318441 |
| 4  | C  | C1  | -0.9540814 | -1.6446914 | -1.0481903 |
| 5  | C  | C4  | -3.5276416 | -1.4761883 | 0.0245328  |
| 6  | C  | C2  | -1.4246491 | -2.6374542 | -0.1809219 |
| 7  | C  | C6  | -1.7733785 | -0.5525046 | -1.4006106 |
| 8  | C  | C5  | -3.0639954 | -0.4870067 | -0.8481113 |
| 9  | C  | C3  | -2.7093936 | -2.5532110 | 0.3526452  |
| 10 | H  | H1  | -0.7820332 | -3.4756369 | 0.0586628  |
| 11 | H  | H3  | -3.0701677 | -3.3301751 | 1.0243620  |
| 12 | H  | H4  | -4.5322361 | -1.3898614 | 0.4352312  |
| 13 | Cl | Cl1 | -4.1347468 | 0.8377193  | -1.2302230 |
| 14 | Cl | Cl2 | -1.2538876 | 0.7062759  | -2.4839254 |
| 15 | N  | N1  | 1.7758508  | -0.8805755 | -0.7071879 |
| 16 | H  | H5  | 1.7754940  | -1.2004994 | 0.2659080  |
| 17 | C  | C7  | 1.7615798  | 0.5438283  | -0.7869040 |
| 18 | C  | C8  | 1.8029002  | 3.3445352  | -0.9277147 |
| 19 | C  | C9  | 1.3464182  | 1.3165075  | 0.3160590  |
| 20 | C  | C10 | 2.2153819  | 1.1889844  | -1.9417476 |
| 21 | C  | C11 | 2.2166853  | 2.5802377  | -2.0224188 |
| 22 | C  | C12 | 1.3906097  | 2.7125248  | 0.2453456  |
| 23 | H  | H6  | 2.5435756  | 0.5825178  | -2.7763910 |
| 24 | H  | H7  | 2.5602375  | 3.0647497  | -2.9347353 |
| 25 | H  | H8  | 1.1096508  | 3.3003616  | 1.1176562  |
| 26 | H  | H9  | 1.8254415  | 4.4327992  | -0.9749871 |
| 27 | N  | N2  | 0.8730396  | 0.6962093  | 1.5086648  |
| 28 | N  | N3  | 1.4813827  | -0.4181034 | 2.0195932  |
| 29 | C  | C13 | -0.1643906 | 1.1079133  | 2.3007753  |
| 30 | H  | H14 | -0.7775844 | 1.9640329  | 2.0370705  |
| 31 | C  | C14 | 0.8047566  | -0.6966094 | 3.1374358  |
| 32 | H  | H2  | 1.0955770  | -1.5527899 | 3.7347321  |
| 33 | C  | C15 | -0.2343688 | 0.2300865  | 3.3671177  |
| 34 | H  | H12 | -0.9422197 | 0.2505097  | 4.1886852  |

**14, Third conformer**  
-2211.457096 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | -1.7241071 | -0.6883716 | -0.3490095 |
| 2  | O  | O1  | -2.0759354 | 0.7376706  | -0.2153165 |
| 3  | O  | O2  | -2.7588795 | -1.6934843 | -0.0352288 |
| 4  | C  | C1  | -1.1040310 | -0.9182545 | -2.0236783 |
| 5  | C  | C4  | -0.2129338 | -1.0458732 | -4.6596567 |
| 6  | C  | C2  | -1.0629276 | 0.2390179  | -2.8081978 |
| 7  | C  | C6  | -0.7107744 | -2.1640926 | -2.5509937 |
| 8  | C  | C5  | -0.2596462 | -2.2059997 | -3.8801838 |
| 9  | C  | C3  | -0.6175300 | 0.1739642  | -4.1263417 |
| 10 | H  | H1  | -1.3824612 | 1.1801689  | -2.3737205 |
| 11 | H  | H3  | -0.5829643 | 1.0759534  | -4.7357592 |
| 12 | H  | H4  | 0.1424821  | -1.1177698 | -5.6865109 |
| 13 | Cl | Cl1 | 0.2534894  | -3.7088262 | -4.6032839 |
| 14 | Cl | Cl2 | -0.7563738 | -3.6399271 | -1.6206159 |
| 15 | N  | N1  | -0.3958471 | -1.1106919 | 0.6304308  |
| 16 | H  | H5  | -0.7697912 | -1.2928156 | 1.5675094  |
| 17 | C  | C7  | 0.7200152  | -0.2079214 | 0.6976519  |
| 18 | C  | C8  | 2.9515276  | 1.4950488  | 0.7876793  |
| 19 | C  | C9  | 0.8820350  | 0.6948234  | 1.7686534  |
| 20 | C  | C10 | 1.7008880  | -0.2609328 | -0.2993320 |
| 21 | C  | C11 | 2.8009820  | 0.5970416  | -0.2716502 |
| 22 | C  | C12 | 2.0082056  | 1.5236842  | 1.8140861  |
| 23 | H  | H6  | 1.5963015  | -0.9968535 | -1.0899230 |
| 24 | H  | H7  | 3.5496276  | 0.5415941  | -1.0610346 |
| 25 | H  | H8  | 2.1514155  | 2.1818500  | 2.6694393  |
| 26 | H  | H9  | 3.8195841  | 2.1519801  | 0.8356523  |
| 27 | N  | N2  | -0.0736468 | 0.7827217  | 2.8219766  |
| 28 | N  | N3  | -0.7093477 | -0.3296329 | 3.3028036  |
| 29 | C  | C13 | -0.4524834 | 1.9085426  | 3.5021363  |
| 30 | H  | H14 | -0.0806986 | 2.8911707  | 3.2326285  |
| 31 | C  | C14 | -1.4870428 | 0.1199086  | 4.2906920  |
| 32 | H  | H2  | -2.1088621 | -0.5780172 | 4.8377568  |
| 33 | C  | C15 | -1.3664864 | 1.5152014  | 4.4601958  |
| 34 | H  | H12 | -1.8837833 | 2.1491218  | 5.1711451  |

**16, Global minimum**  
-2243.513948 au

|    |   |    |            |            |            |
|----|---|----|------------|------------|------------|
| 1  | S | S1 | -1.4285988 | 0.8383942  | 1.7738983  |
| 2  | O | O1 | -1.7933417 | 2.2277014  | 1.4824103  |
| 3  | O | O2 | -1.7896611 | 0.2386798  | 3.0722599  |
| 4  | C | C1 | -2.0808440 | -0.2715877 | 0.5065812  |
| 5  | C | C4 | -3.1616520 | -2.1261940 | -1.2747610 |
| 6  | C | C2 | -2.6335516 | -1.4659720 | 0.9834914  |
| 7  | C | C6 | -2.0636511 | 0.0150885  | -0.8741662 |
| 8  | C | C5 | -2.6120877 | -0.9333367 | -1.7540691 |
| 9  | C | C3 | -3.1734178 | -2.3898102 | 0.0916101  |
| 10 | H | H1 | -2.6480142 | -1.6539311 | 2.0491839  |

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 11 | H  | H3  | -3.6059823 | -3.3144607 | 0.4664313  |
| 12 | H  | H4  | -3.5785455 | -2.8377452 | -1.9842897 |
| 13 | C1 | C11 | -2.6267289 | -0.6542278 | -3.4761562 |
| 14 | C1 | C12 | -1.3941766 | 1.4841277  | -1.5159908 |
| 15 | N  | N1  | 0.2694247  | 0.7408500  | 1.7848645  |
| 16 | H  | H5  | 0.5617889  | -0.1733067 | 2.1210114  |
| 17 | C  | C7  | 1.1229331  | 1.3059314  | 0.7973304  |
| 18 | C  | C8  | 2.8417717  | 2.4479021  | -1.1200964 |
| 19 | C  | C9  | 1.9938066  | 0.5026619  | 0.0328236  |
| 20 | C  | C10 | 1.1500520  | 2.6910189  | 0.5984834  |
| 21 | C  | C11 | 1.9835772  | 3.2539467  | -0.3662597 |
| 22 | C  | C12 | 2.8628306  | 1.0702532  | -0.9034978 |
| 23 | H  | H6  | 0.4936687  | 3.3111995  | 1.1944982  |
| 24 | H  | H7  | 1.9741269  | 4.3323350  | -0.5134880 |
| 25 | H  | H8  | 3.5558593  | 0.4322665  | -1.4529399 |
| 26 | H  | H9  | 3.5098945  | 2.8892156  | -1.8583543 |
| 27 | N  | N2  | 2.0017976  | -0.9227226 | 0.1943407  |
| 28 | N  | N3  | 1.9710756  | -1.5256689 | 1.4147955  |
| 29 | N  | N4  | 2.0221855  | -2.8015523 | 1.2026676  |
| 30 | N  | N5  | 2.0977086  | -3.0737256 | -0.1199918 |
| 31 | C  | C13 | 2.0788936  | -1.8998825 | -0.7378913 |
| 32 | H  | H14 | 2.0988585  | -1.7374487 | -1.8147296 |

**16, Second conformer**  
-2243.513283 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | -1.1491307 | -1.5972555 | -1.3341302 |
| 2  | O  | O1  | -2.0467219 | -2.7137508 | -0.9803462 |
| 3  | O  | O2  | -0.6272661 | -1.4763560 | -2.6968826 |
| 4  | C  | C1  | -2.0306223 | -0.0900827 | -0.8680602 |
| 5  | C  | C4  | -3.5782904 | 2.1124944  | -0.1369526 |
| 6  | C  | C2  | -3.2650217 | -0.2773714 | -0.2376571 |
| 7  | C  | C6  | -1.5487061 | 1.2061776  | -1.1373556 |
| 8  | C  | C5  | -2.3434056 | 2.3023019  | -0.7645140 |
| 9  | C  | C3  | -4.0355882 | 0.8249376  | 0.1268234  |
| 10 | H  | H1  | -3.6152419 | -1.2841744 | -0.0517872 |
| 11 | H  | H3  | -4.9970873 | 0.6763583  | 0.6127536  |
| 12 | H  | H4  | -4.1705070 | 2.9821900  | 0.1389017  |
| 13 | C1 | C11 | -1.8164092 | 3.9374143  | -1.0699739 |
| 14 | C1 | C12 | -0.0124320 | 1.4832505  | -1.9005943 |
| 15 | N  | N1  | 0.1640298  | -1.8264964 | -0.2903438 |
| 16 | H  | H5  | -0.1547615 | -2.0136328 | 0.6572907  |
| 17 | C  | C7  | 1.4363887  | -1.1964635 | -0.3804284 |
| 18 | C  | C8  | 3.9945527  | -0.0225972 | -0.5322227 |
| 19 | C  | C9  | 1.9631677  | -0.4586077 | 0.7003346  |
| 20 | C  | C10 | 2.2235269  | -1.3454448 | -1.5284310 |
| 21 | C  | C11 | 3.4790983  | -0.7442993 | -1.6126115 |
| 22 | C  | C12 | 3.2421800  | 0.1028459  | 0.6352524  |
| 23 | H  | H6  | 1.8296292  | -1.9233733 | -2.3547206 |
| 24 | H  | H7  | 4.0652922  | -0.8634296 | -2.5221414 |
| 25 | H  | H8  | 3.6440512  | 0.6316768  | 1.4997669  |

|    |   |     |            |            |            |
|----|---|-----|------------|------------|------------|
| 26 | H | H9  | 4.9859164  | 0.4248447  | -0.5868350 |
| 27 | N | N2  | 1.1879539  | -0.2439646 | 1.8889322  |
| 28 | N | N3  | 0.4444271  | -1.2199876 | 2.4765395  |
| 29 | N | N4  | -0.1006838 | -0.6943314 | 3.5274093  |
| 30 | N | N5  | 0.2611494  | 0.6013649  | 3.6670468  |
| 31 | C | C13 | 1.0569695  | 0.8721882  | 2.6407479  |
| 32 | H | H14 | 1.5135423  | 1.8335742  | 2.4141890  |

16, Third conformer  
-2243.512889 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | -2.2655084 | -0.7414764 | 0.8848814  |
| 2  | O  | O1  | -2.9992765 | 0.2236473  | 1.7139104  |
| 3  | O  | O2  | -2.7968399 | -2.1096047 | 0.7368909  |
| 4  | C  | C1  | -2.0122979 | 0.0409980  | -0.7199477 |
| 5  | C  | C4  | -1.7268770 | 1.4129841  | -3.1265975 |
| 6  | C  | C2  | -2.6463937 | 1.2748790  | -0.9025763 |
| 7  | C  | C6  | -1.2382218 | -0.5298695 | -1.7488499 |
| 8  | C  | C5  | -1.0952796 | 0.1779158  | -2.9523834 |
| 9  | C  | C3  | -2.5052260 | 1.9550423  | -2.1087819 |
| 10 | H  | H1  | -3.2403756 | 1.6907195  | -0.0952612 |
| 11 | H  | H3  | -2.9982437 | 2.9147716  | -2.2542551 |
| 12 | H  | H4  | -1.5977130 | 1.9381915  | -4.0712051 |
| 13 | C1 | C11 | -0.1282960 | -0.4572985 | -4.2593144 |
| 14 | C1 | C12 | -0.4516543 | -2.0862574 | -1.5720239 |
| 15 | N  | N1  | -0.7361453 | -0.9654691 | 1.5708237  |
| 16 | H  | H5  | -0.4515886 | -1.9378863 | 1.5345625  |
| 17 | C  | C7  | 0.2985752  | -0.0090691 | 1.4515299  |
| 18 | C  | C8  | 2.3479046  | 1.9048386  | 1.1534615  |
| 19 | C  | C9  | 1.6286121  | -0.4045348 | 1.1910360  |
| 20 | C  | C10 | 0.0281769  | 1.3602458  | 1.5873807  |
| 21 | C  | C11 | 1.0354553  | 2.3062178  | 1.4143498  |
| 22 | C  | C12 | 2.6476133  | 0.5478114  | 1.0711072  |
| 23 | H  | H6  | -0.9832085 | 1.6709992  | 1.8229237  |
| 24 | H  | H7  | 0.7934793  | 3.3638703  | 1.5081294  |
| 25 | H  | H8  | 3.6743244  | 0.2153586  | 0.9169329  |
| 26 | H  | H9  | 3.1424367  | 2.6415199  | 1.0431186  |
| 27 | N  | N2  | 1.9596189  | -1.7899526 | 1.0358371  |
| 28 | N  | N3  | 1.4018629  | -2.7710715 | 1.7972415  |
| 29 | N  | N4  | 1.9143903  | -3.8912989 | 1.3977485  |
| 30 | N  | N5  | 2.8007290  | -3.6917682 | 0.3963178  |
| 31 | C  | C13 | 2.8123108  | -2.3844879 | 0.1733444  |
| 32 | H  | H14 | 3.3907509  | -1.8699651 | -0.5903316 |

*Coordinates of IHB-opened structure for 16 (optimisation only, B3LYP/6-31+G\*, water*

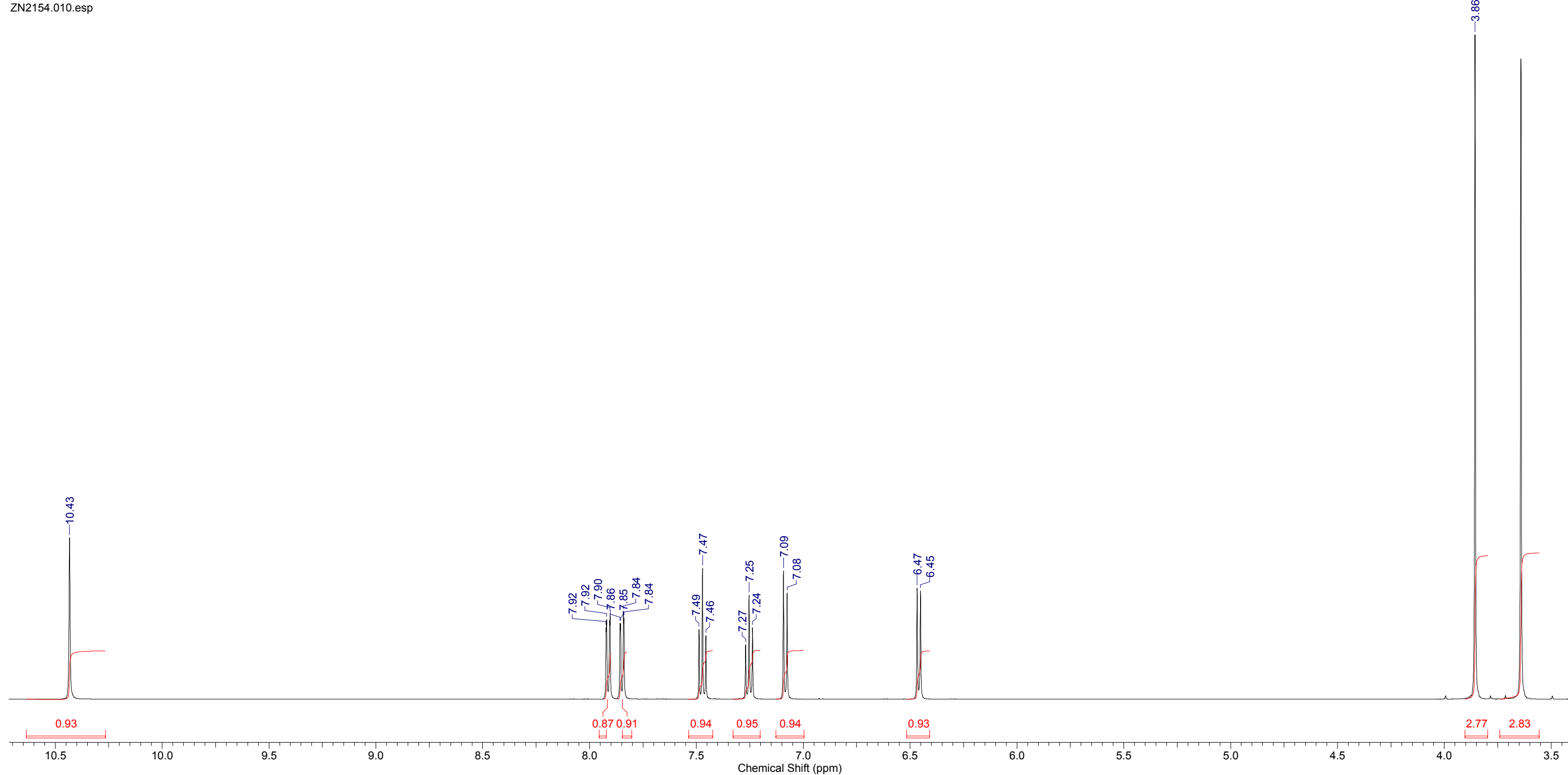
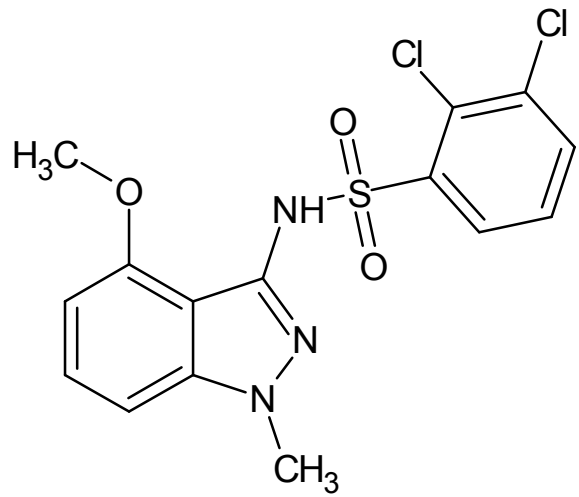
*[SM8])*

**16**, IHB-opened structure matching crystal structure

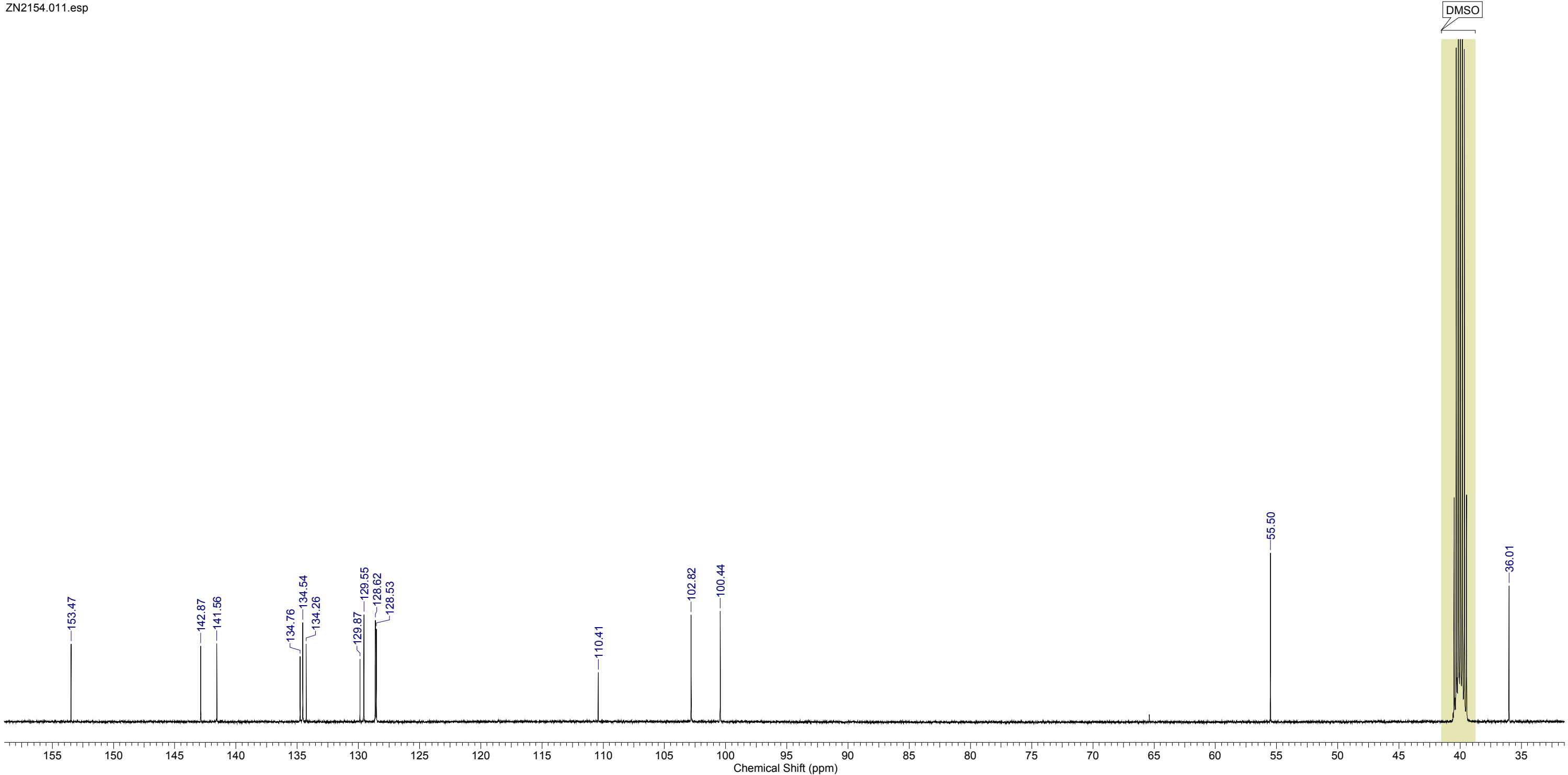
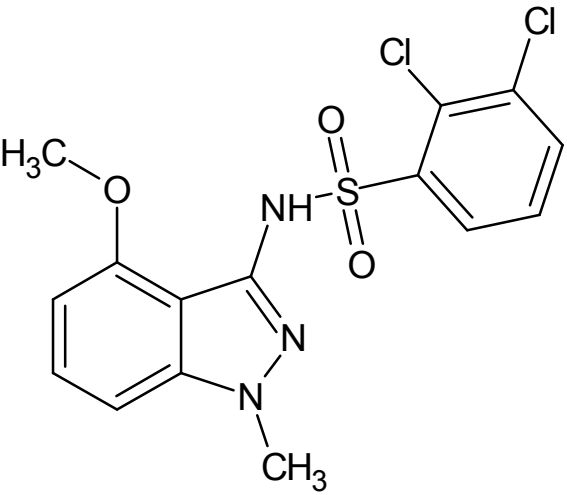
-2243.505858 au

|    |    |     |            |            |            |
|----|----|-----|------------|------------|------------|
| 1  | S  | S1  | -1.8385762 | -1.2825371 | 0.3286990  |
| 2  | O  | O1  | -2.5751222 | -0.1456646 | 0.9015988  |
| 3  | O  | O2  | -2.4629714 | -2.6127360 | 0.3081430  |
| 4  | C  | C1  | -1.2971448 | -0.7857480 | -1.3140061 |
| 5  | C  | C4  | -0.4885568 | 0.1690560  | -3.7945118 |
| 6  | C  | C2  | -1.5572137 | 0.5410470  | -1.6670449 |
| 7  | C  | C6  | -0.6262515 | -1.6562421 | -2.1926771 |
| 8  | C  | C5  | -0.2262847 | -1.1588235 | -3.4429425 |
| 9  | C  | C3  | -1.1523737 | 1.0149222  | -2.9111915 |
| 10 | H  | H1  | -2.0722650 | 1.1829990  | -0.9642379 |
| 11 | H  | H3  | -1.3524772 | 2.0461307  | -3.1923894 |
| 12 | H  | H4  | -0.1643206 | 0.5264575  | -4.7698992 |
| 13 | Cl | Cl1 | 0.6099974  | -2.1763131 | -4.5875176 |
| 14 | Cl | Cl2 | -0.2717589 | -3.3117475 | -1.7693230 |
| 15 | N  | N1  | -0.4112262 | -1.4794765 | 1.2766346  |
| 16 | H  | H5  | -0.1275036 | -2.4575970 | 1.1898068  |
| 17 | C  | C7  | 0.7038325  | -0.5946025 | 1.0815543  |
| 18 | C  | C8  | 2.9168623  | 1.0931344  | 0.6434849  |
| 19 | C  | C9  | 0.7409192  | 0.7043672  | 1.6258744  |
| 20 | C  | C10 | 1.8166231  | -1.0383888 | 0.3537243  |
| 21 | C  | C11 | 2.9202389  | -0.2112265 | 0.1441771  |
| 22 | C  | C12 | 1.8319042  | 1.5462381  | 1.3908642  |
| 23 | H  | H6  | 1.8059757  | -2.0466244 | -0.0581315 |
| 24 | H  | H7  | 3.7719385  | -0.5852309 | -0.4223494 |
| 25 | H  | H8  | 1.8217270  | 2.5467380  | 1.8125535  |
| 26 | H  | H9  | 3.7648395  | 1.7534244  | 0.4709912  |
| 27 | N  | N2  | -0.3130220 | 1.2139441  | 2.4579192  |
| 28 | N  | N3  | -0.8300871 | 2.4540845  | 2.2511466  |
| 29 | N  | N4  | -1.6676941 | 2.6711409  | 3.2117974  |
| 30 | N  | N5  | -1.7278688 | 1.6118430  | 4.0591879  |
| 31 | C  | C13 | -0.8803435 | 0.7191402  | 3.5772433  |
| 32 | H  | H14 | -0.6617961 | -0.2517086 | 4.0008213  |

2,3-Dichloro-N-[1-methyl-4-(methoxy)-1H-indazol-3-yl]benzenesulfonamide (7)

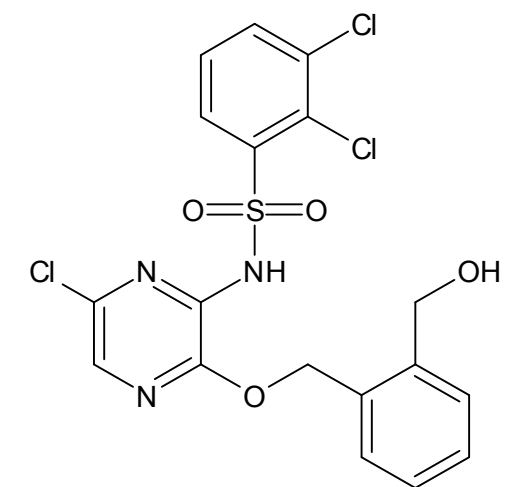


2,3-Dichloro-N-[1-methyl-4-(methoxy)-1H-indazol-3-yl]benzenesulfonamide (7)

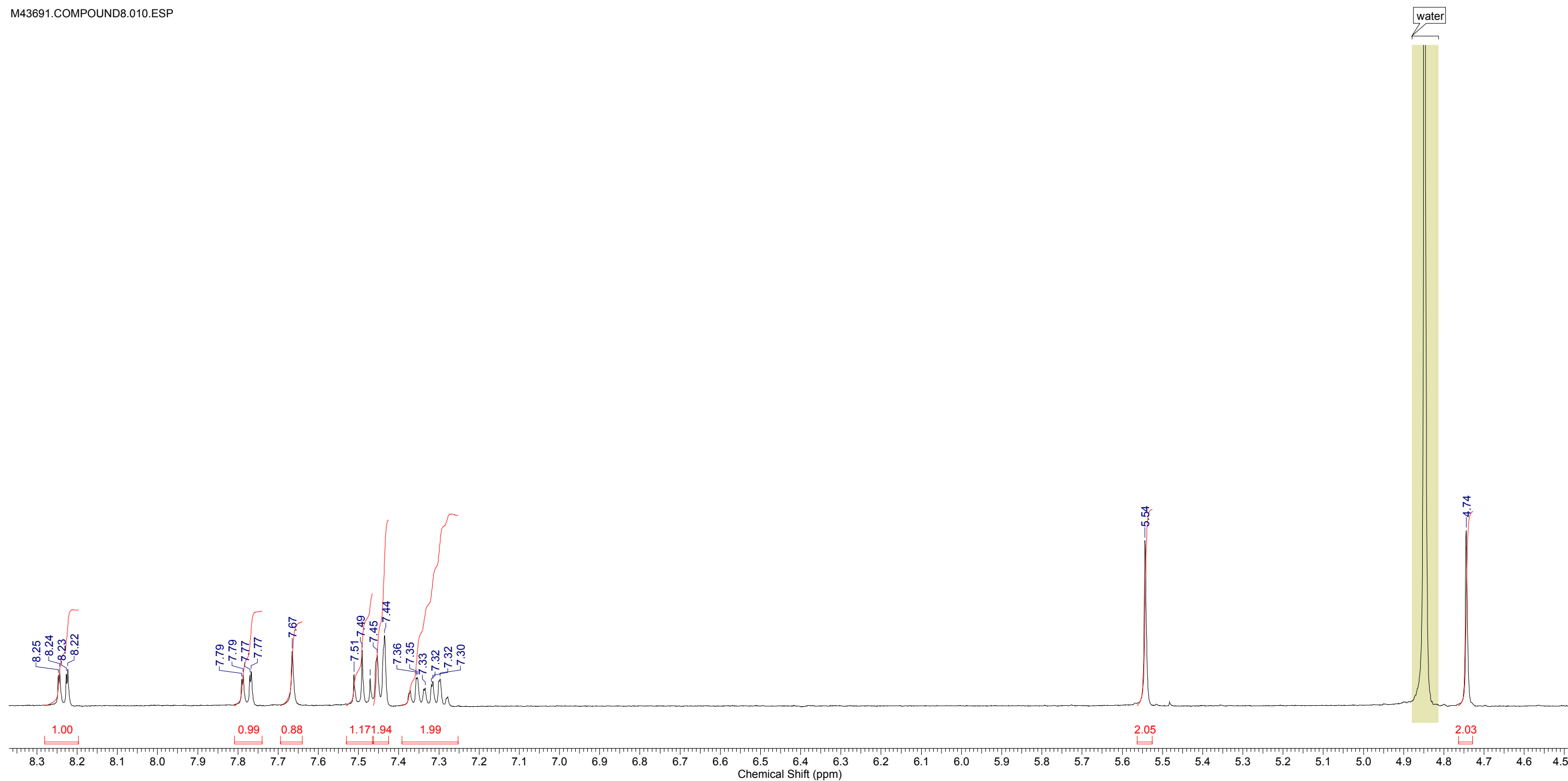




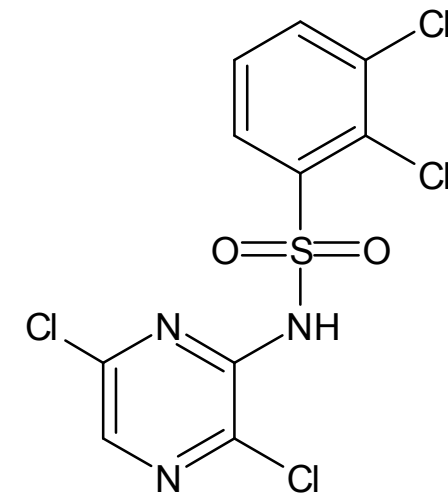
2,3-Dichloro-N-(6-chloro-3-((2-(hydroxymethyl)benzyl)oxy)pyrazin-2-yl)benzenesulfonamide (8)



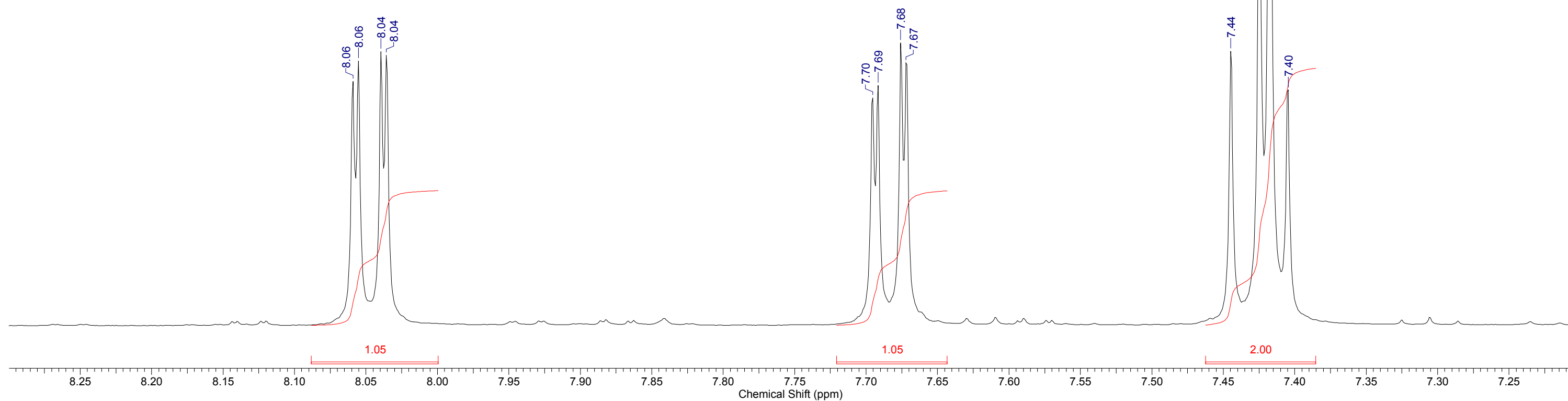
M43691.COMPOUND8.010.ESP



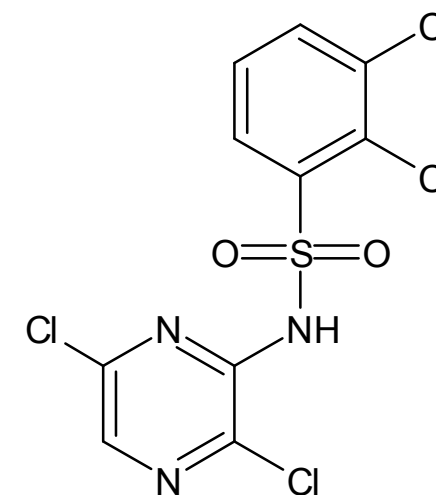
2,3-D2,3-Dichloro-N-(3,6-dichloropyrazin-2-yl)benzenesulfonamide (9)



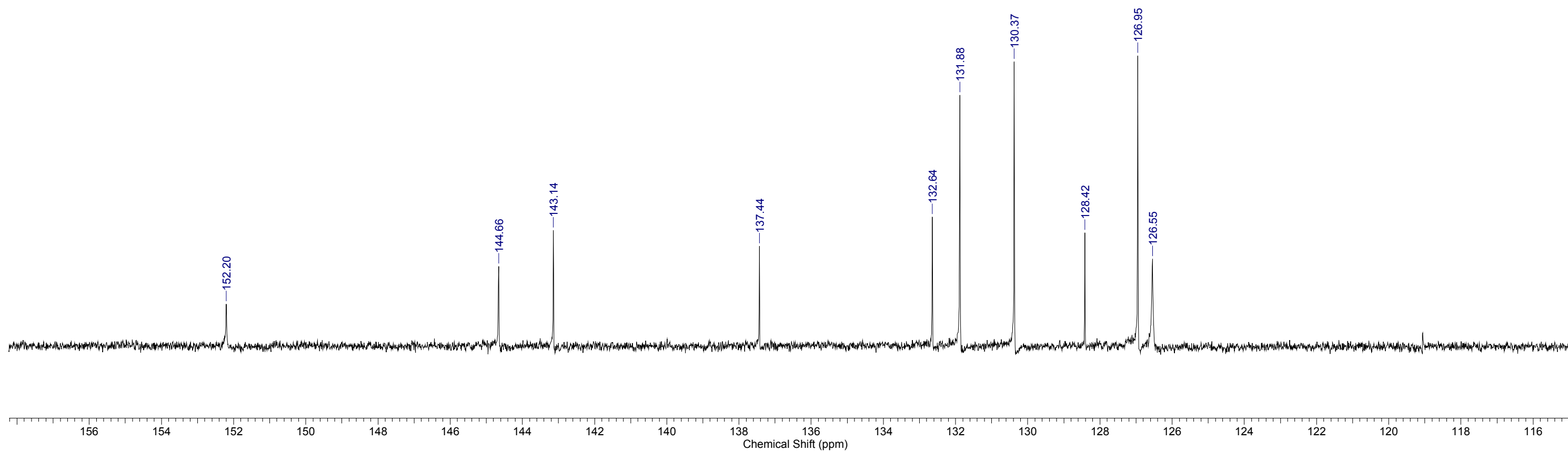
X183692.010.esp



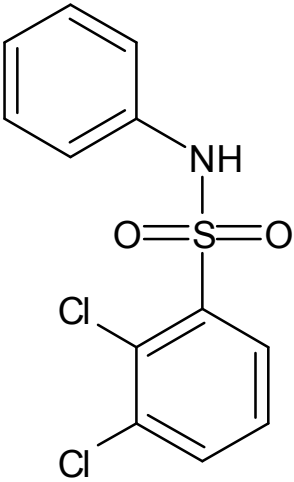
2,3-D2,3-Dichloro-N-(3,6-dichloropyrazin-2-yl)benzenesulfonamide (9)



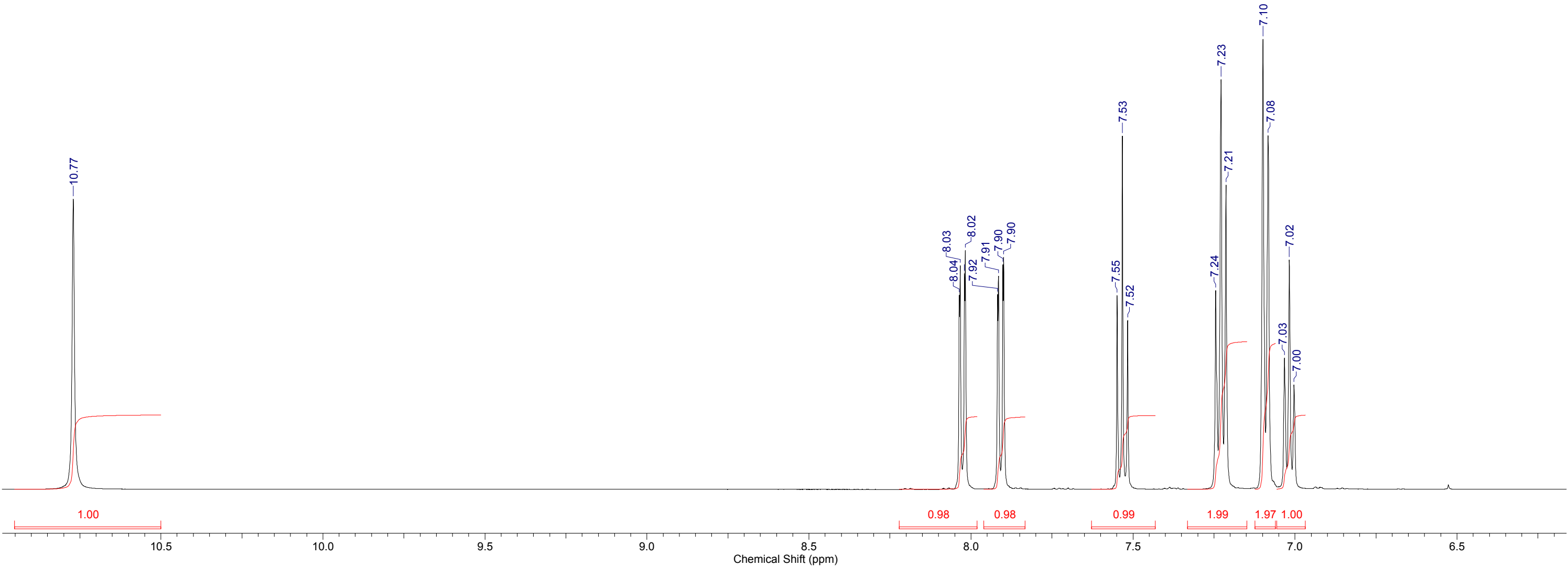
X183692.011.esp



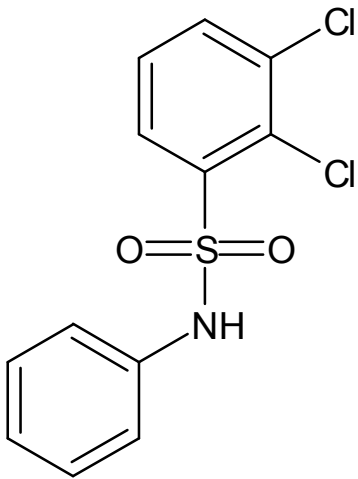
2,3-Dichloro-N-phenylbenzenesulfonamide (10)



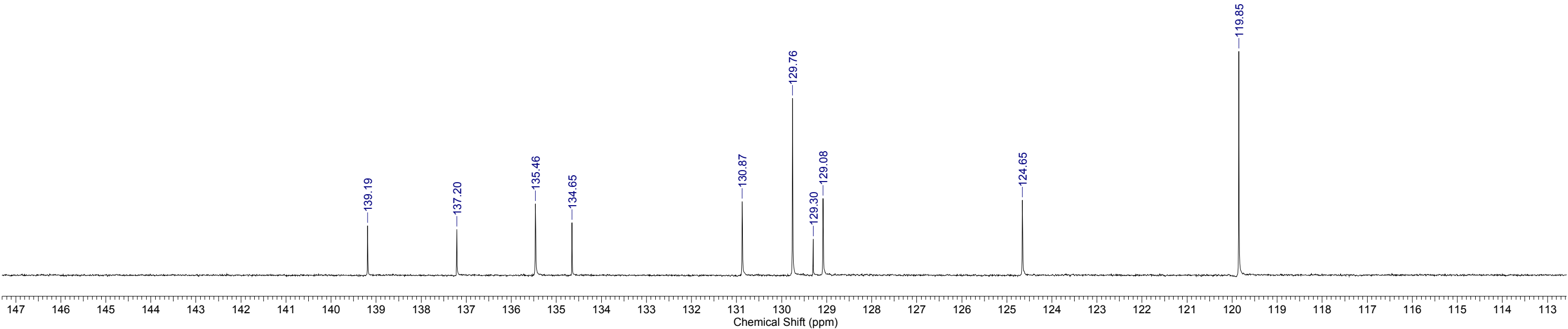
ZN2124, GSK1689233A.010.ESP



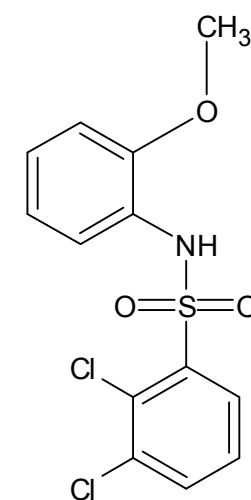
2,3-Dichloro-N-phenylbenzenesulfonamide (10)



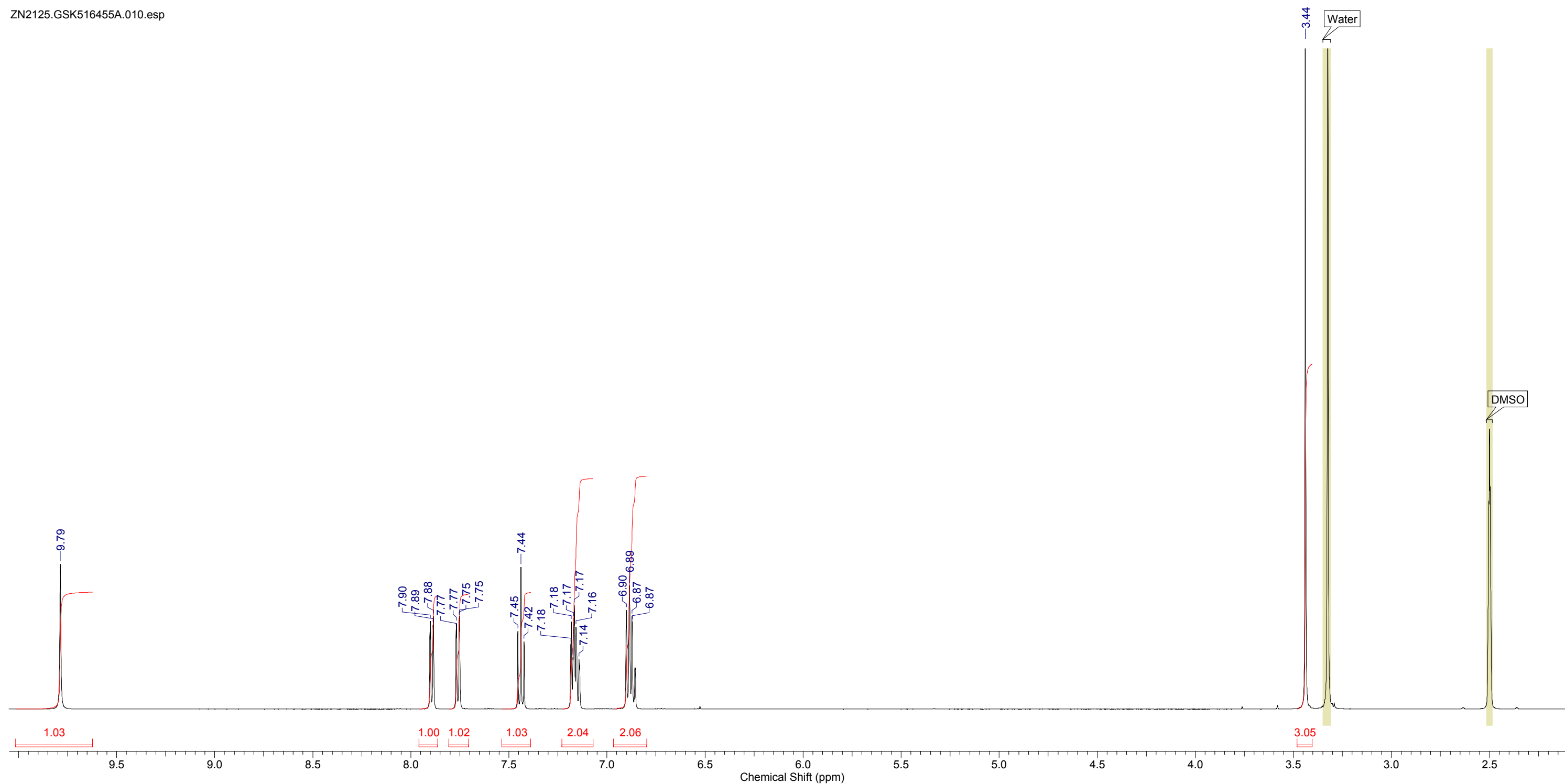
ZN2124.011.esp



# 2,3-Dichloro-N-(2-methoxyphenyl)benzenesulfonamide (11)

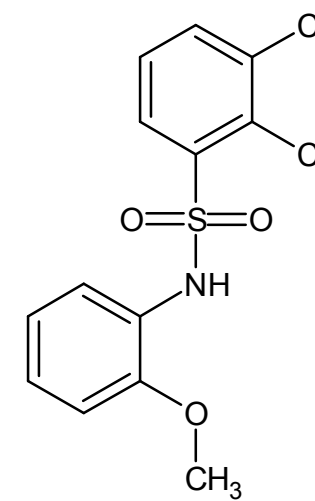


ZN2125.GSK516455A.010.esp

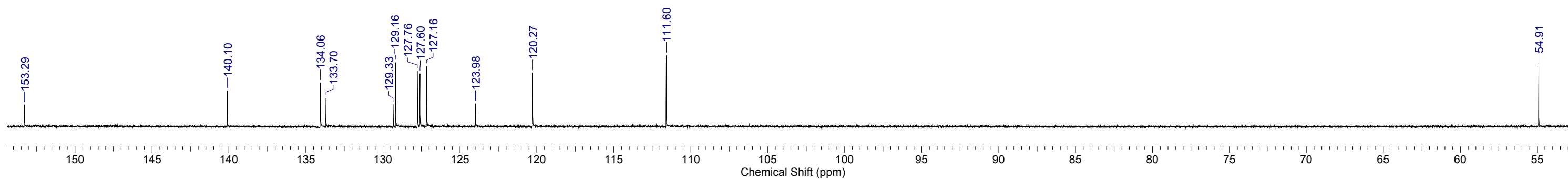




2,3-Dichloro-N-(2-methoxyphenyl)benzenesulfonamide (11)

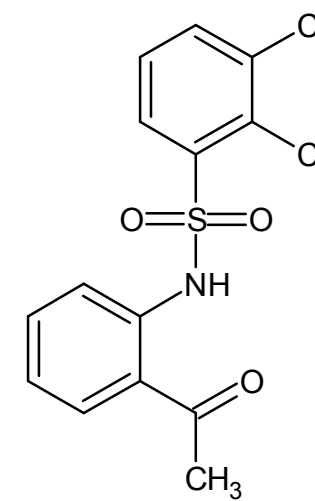


ZN2125.011.esp

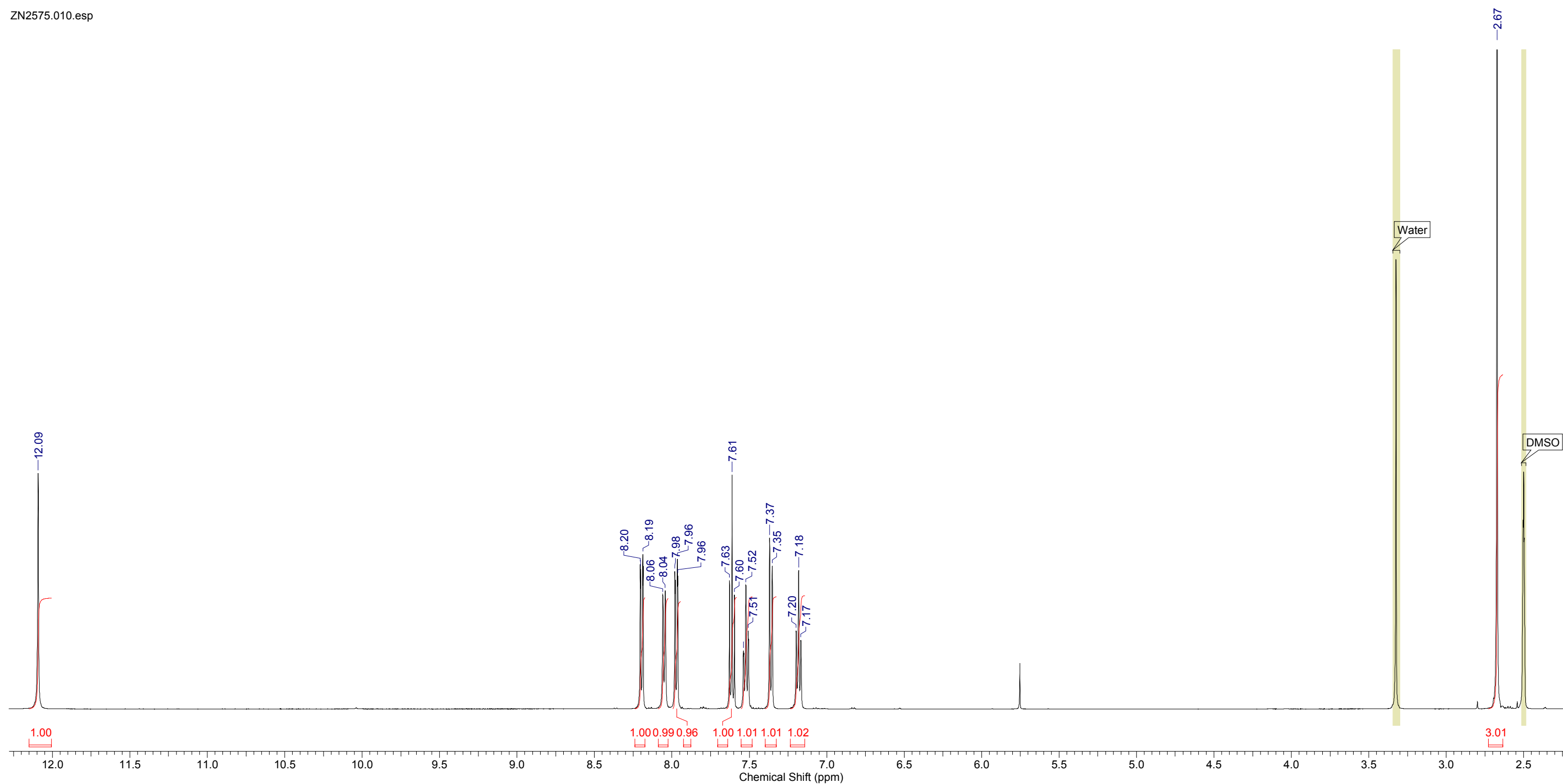


S22

# N-(2-Acetylphenyl)-2,3-dichlorobenzenesulfonamide (12)



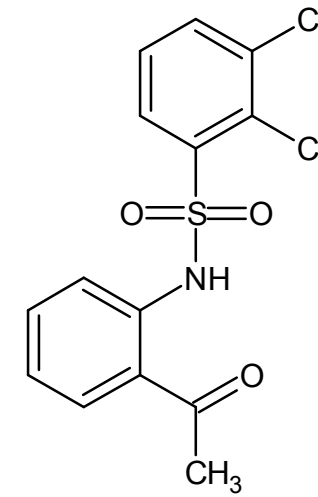
ZN2575.010.esp



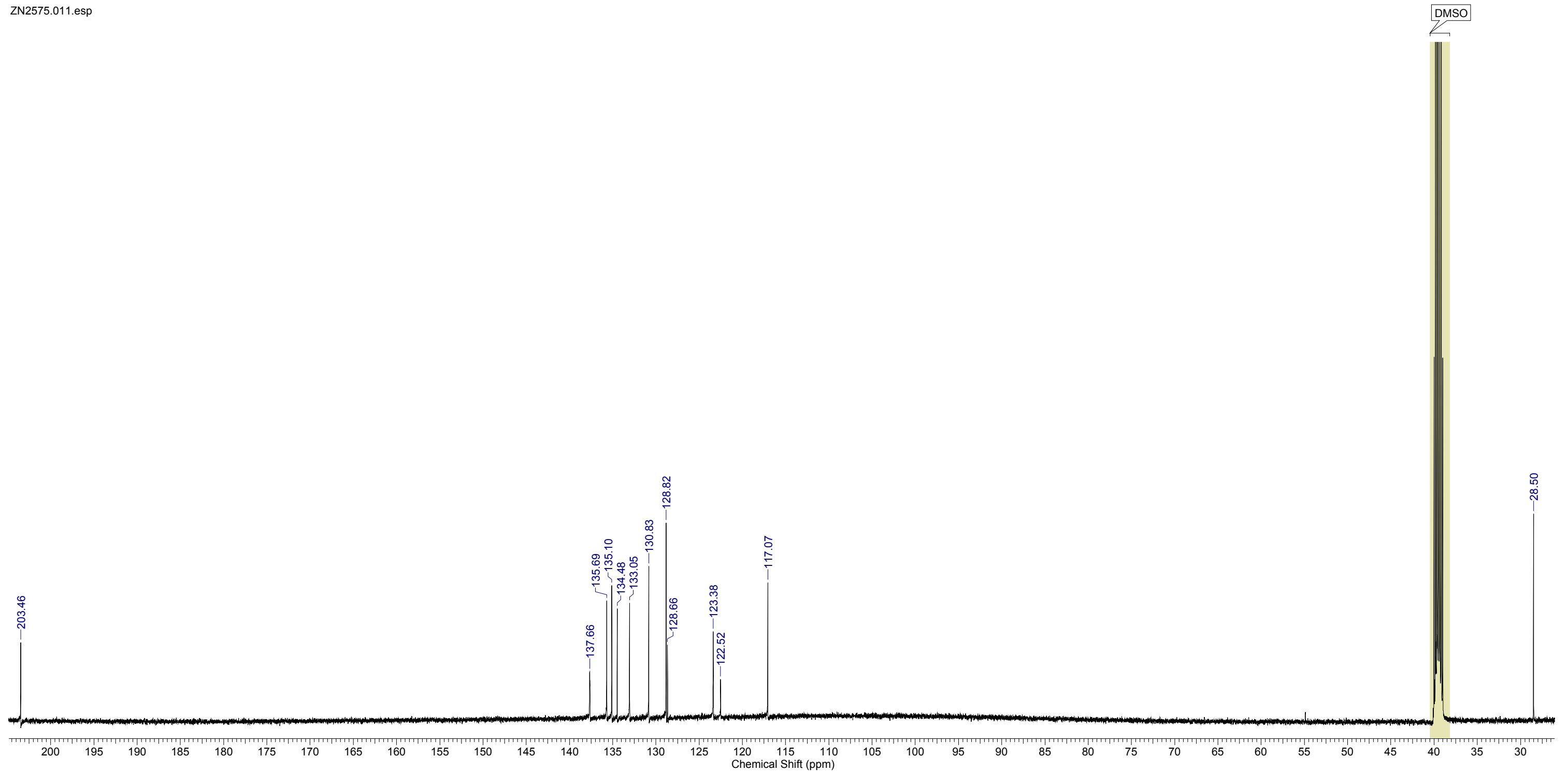
S23



# N-(2-Acetylphenyl)-2,3-dichlorobenzenesulfonamide (12)

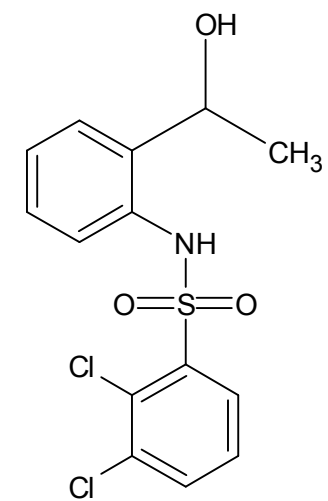


ZN2575.011.esp

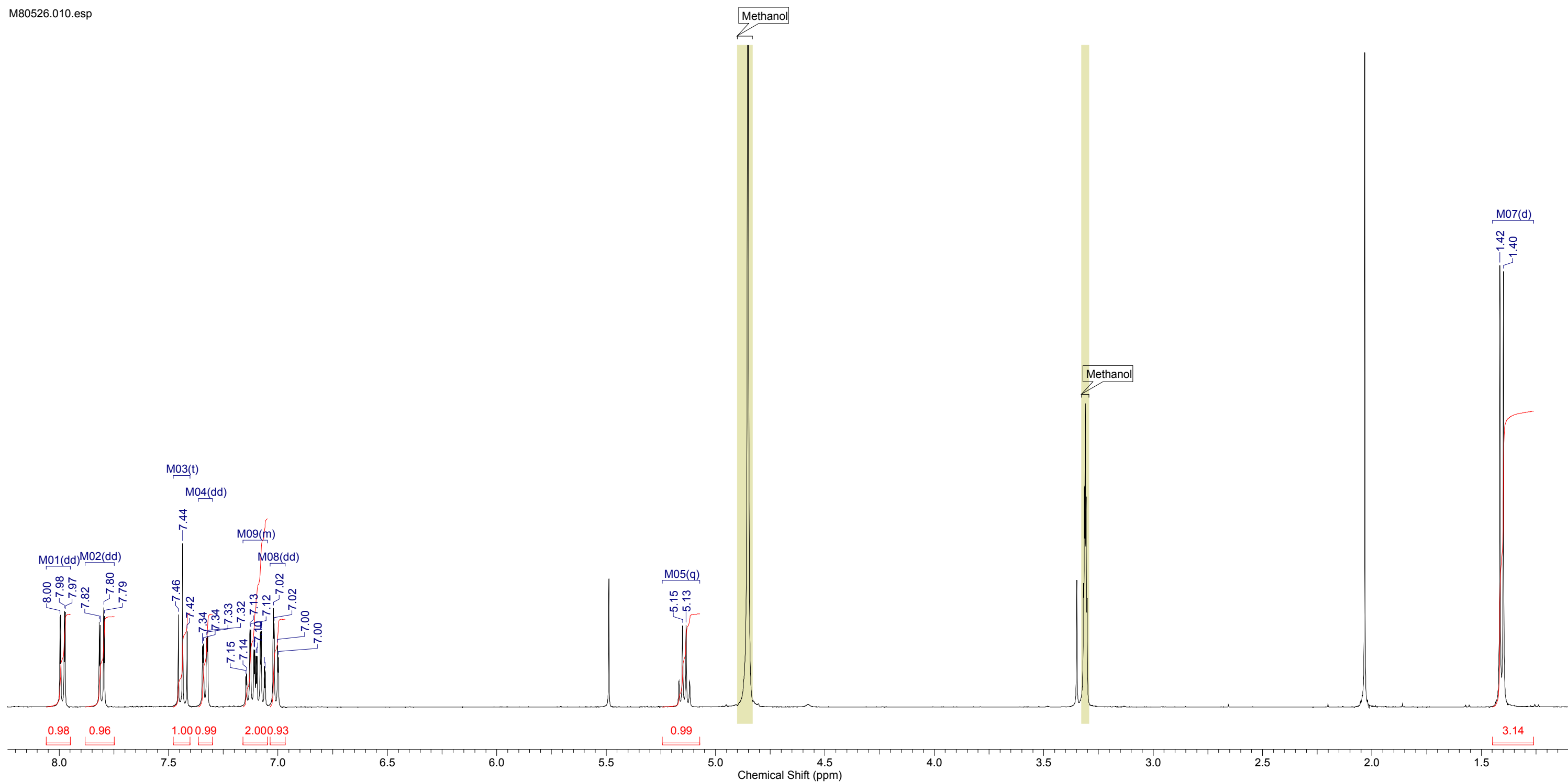


S24

(the2,3-Dichloro-N-(2-(1-hydroxyethyl)phenyl)benzenesulfonamide (13)

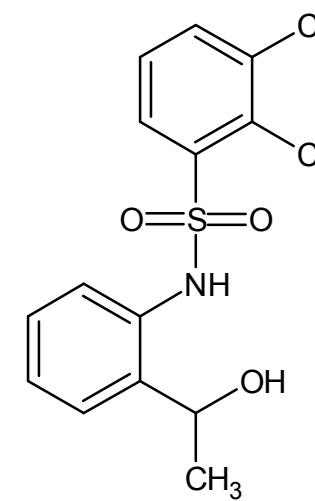


M80526.010.esp

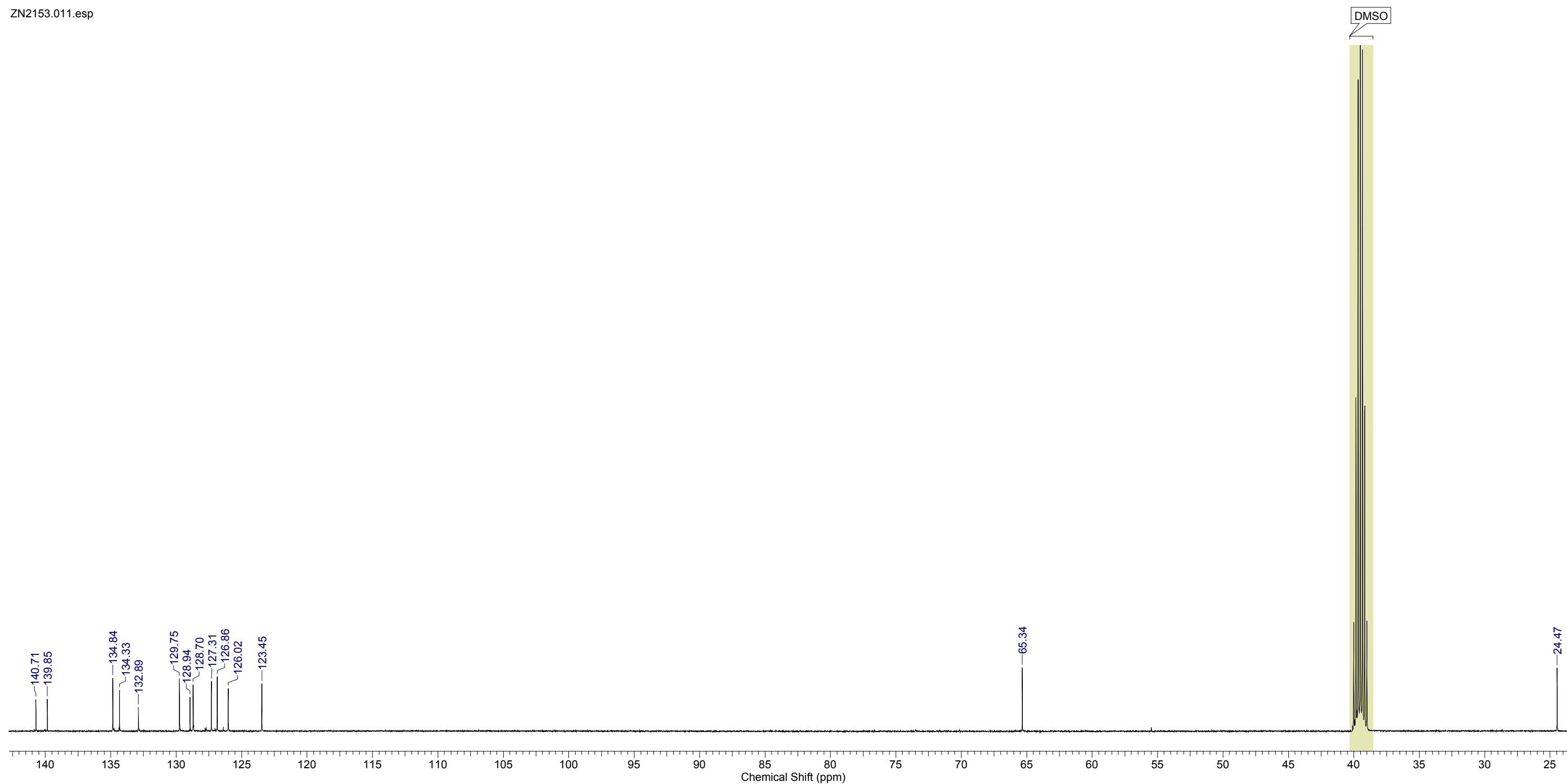


S25

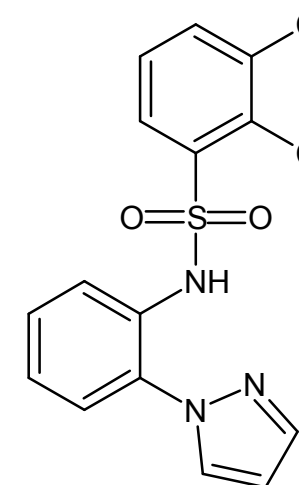
2,3-Dichloro-N-(2-(1-hydroxyethyl)phenyl)benzenesulfonamide (13)



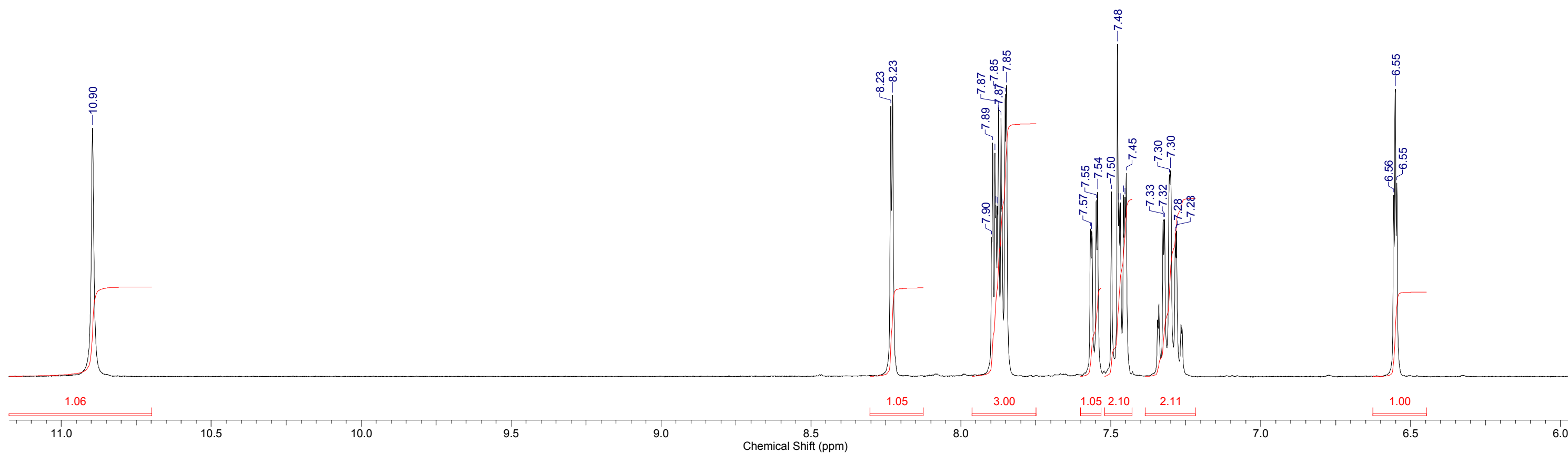
ZN2153.011.esp



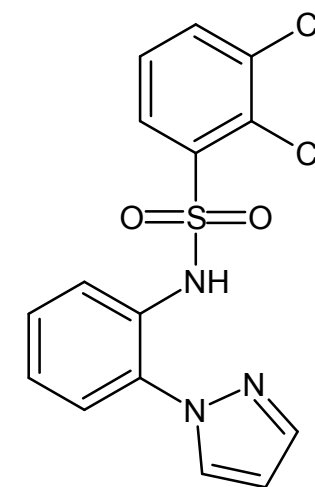
N-(2-(1H-Pyrazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (14)



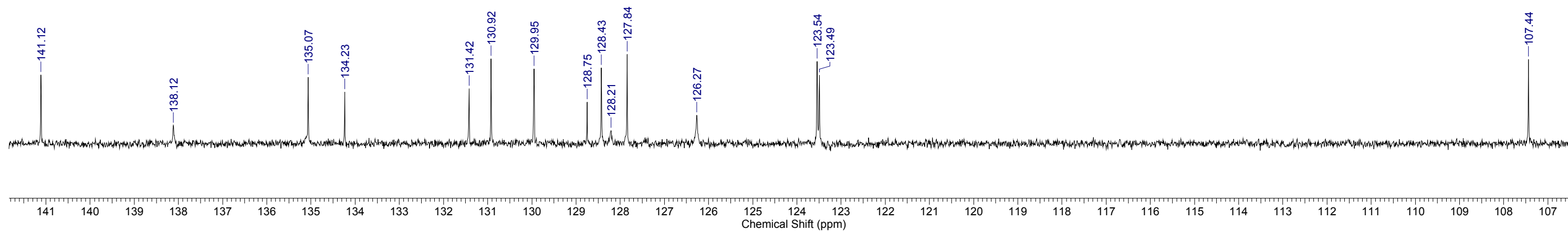
M82505, GSK2694130A.010.esp



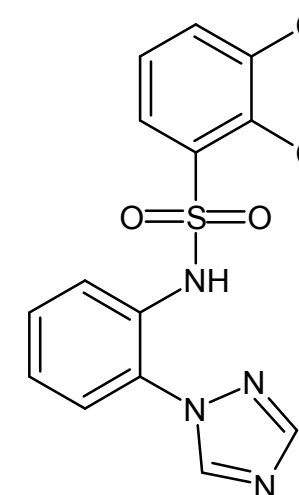
# N-(2-(1H-Pyrazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (14)



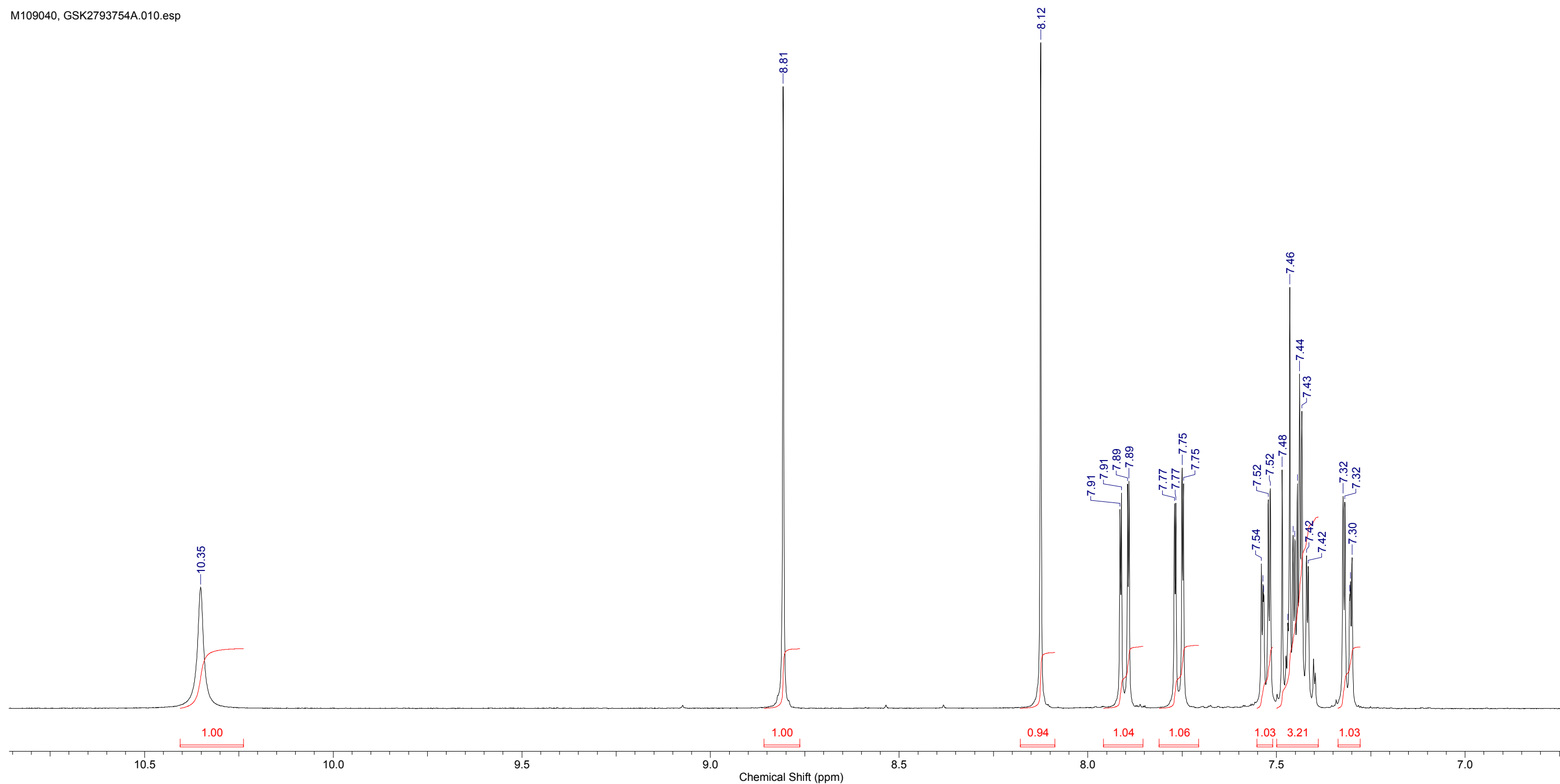
M82505.012.esp



N-(2-(1H-1,2,4-Triazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (15)



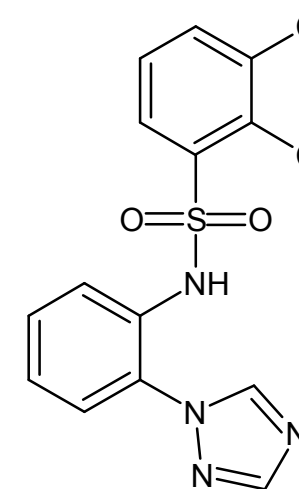
M109040, GSK2793754A.010.esp



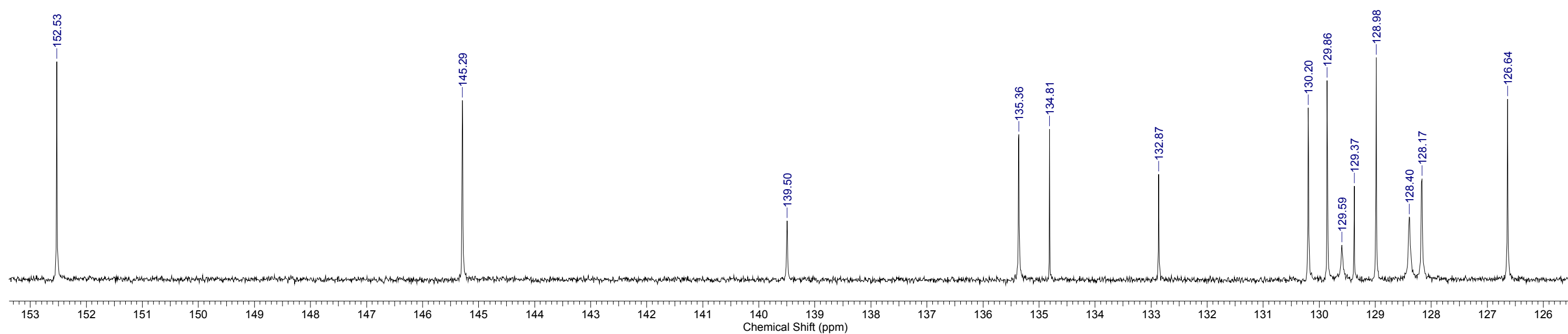
S29



# N-(2-(1H-1,2,4-Triazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (15)

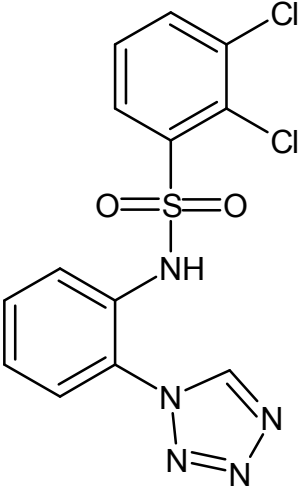


ZN2117.011.esp

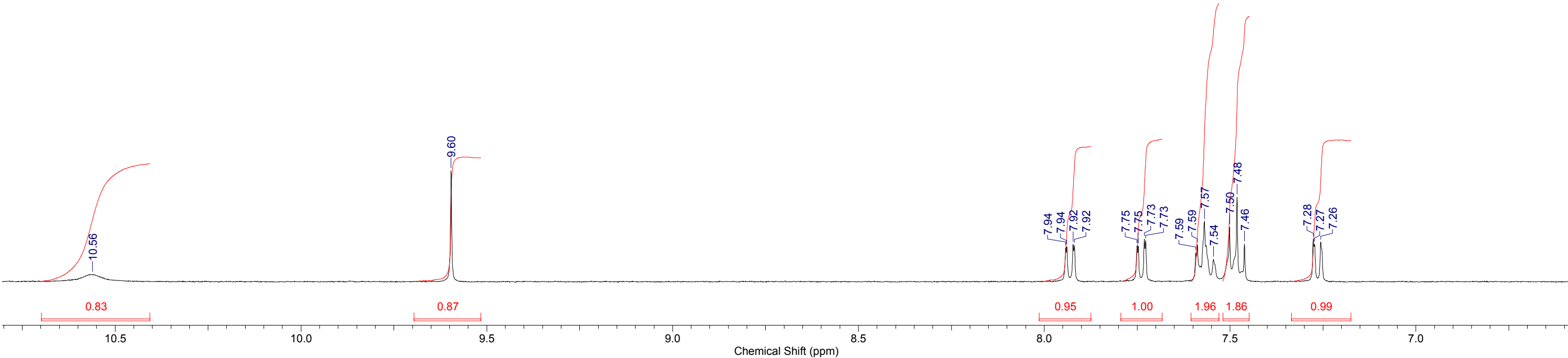


S30

N-(2-(1H-Tetrazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (16)

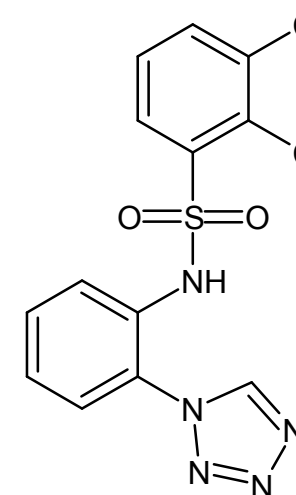


M82125.GSK2794897A.010.ESP

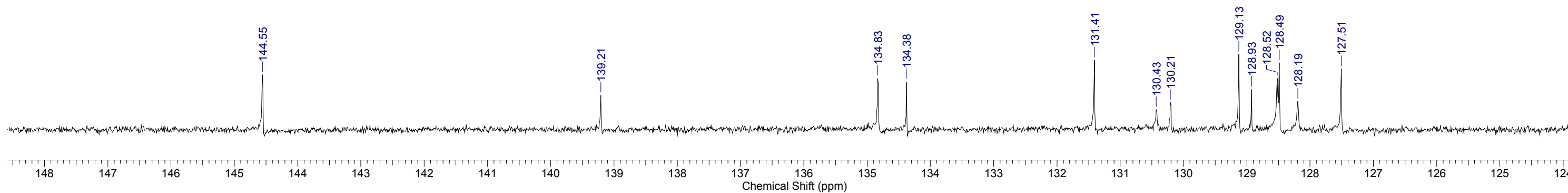




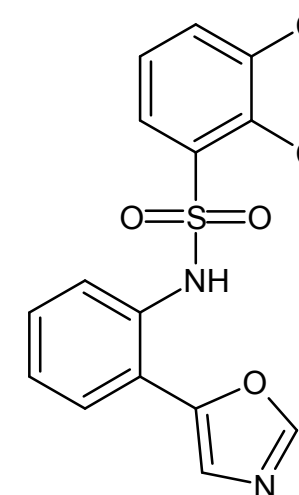
N-(2-(1H-Tetrazol-1-yl)phenyl)-2,3-dichlorobenzenesulfonamide (16)



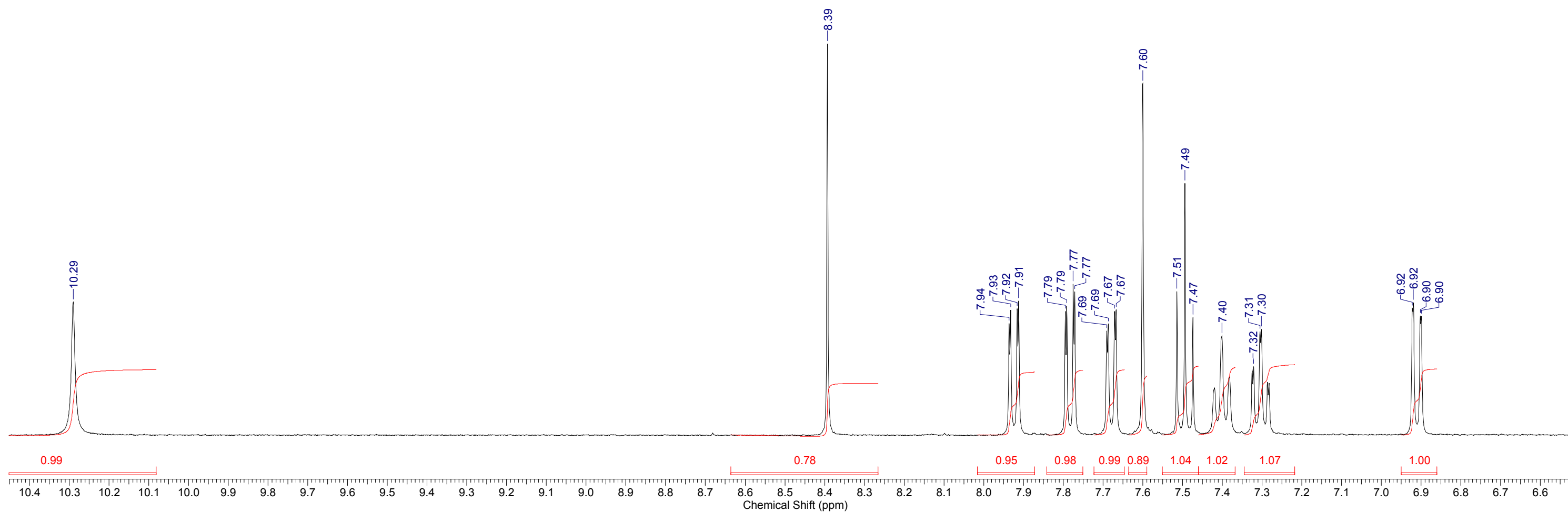
13C.X169564.COMPOUND16.011.ESP



2,3-Dichloro-N-(2-(oxazol-5-yl)phenyl)benzenesulfonamide (17)



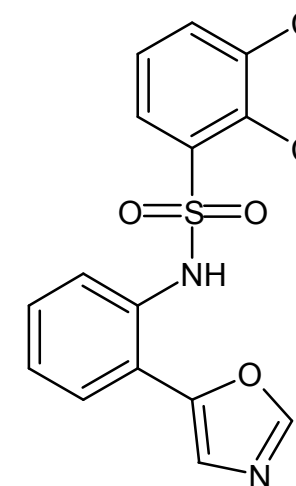
M81636.GSK2793530A.010.esp



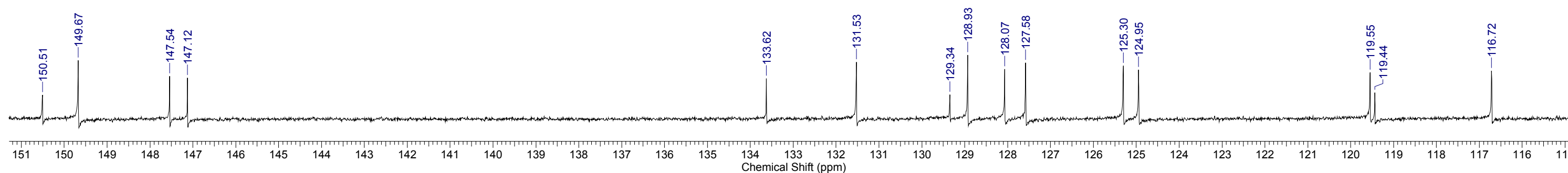
S33

# 2,3-Dichloro-N-(2-(oxazol-5-yl)phenyl)benzenesulfonamide (17)

DMSO-d6 + NaHCO3

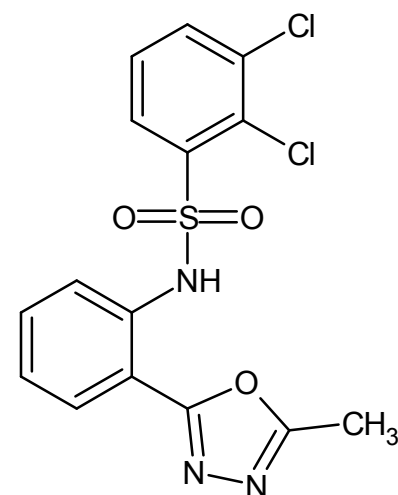


ZN2144.011.esp

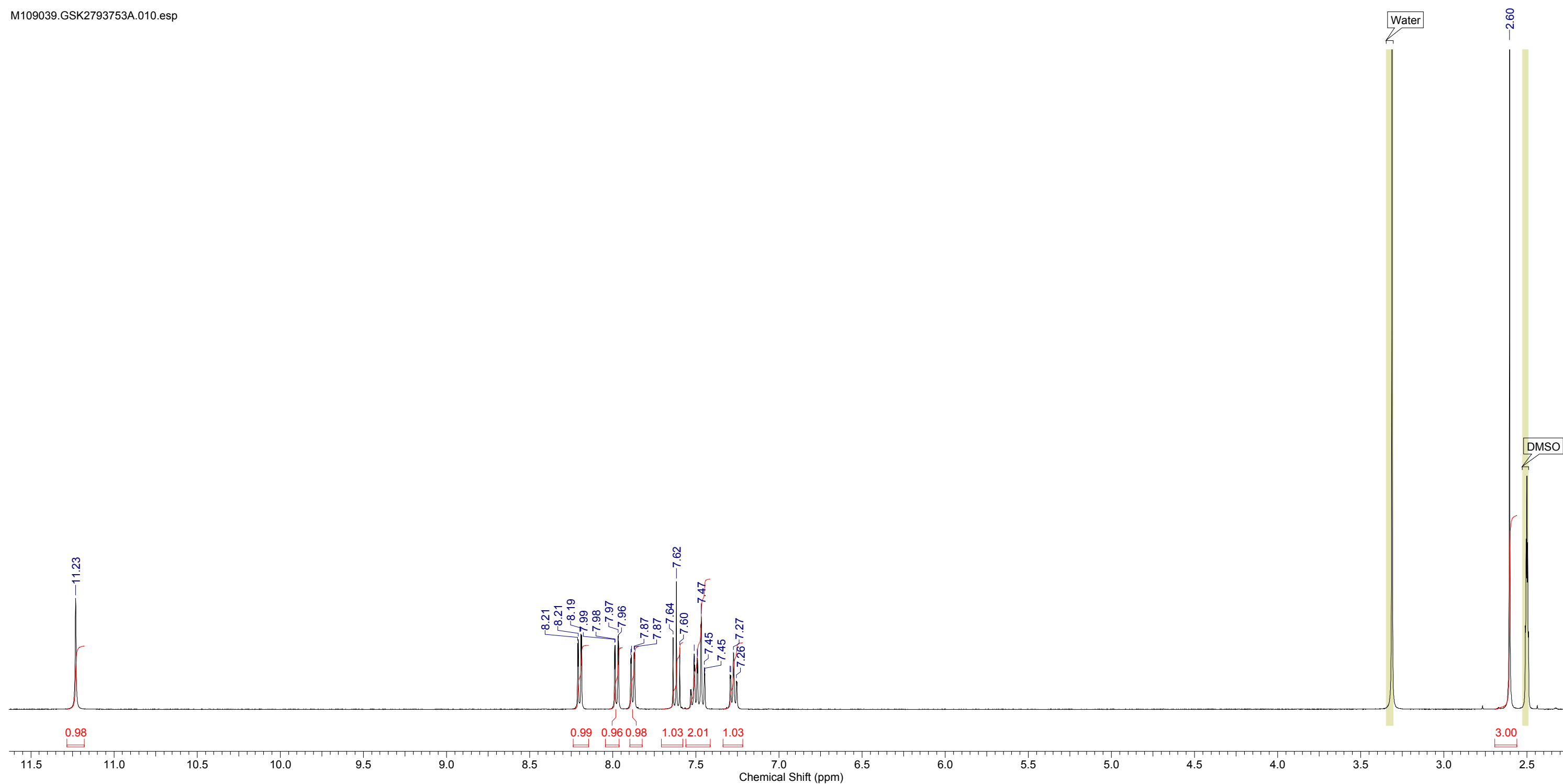


S34

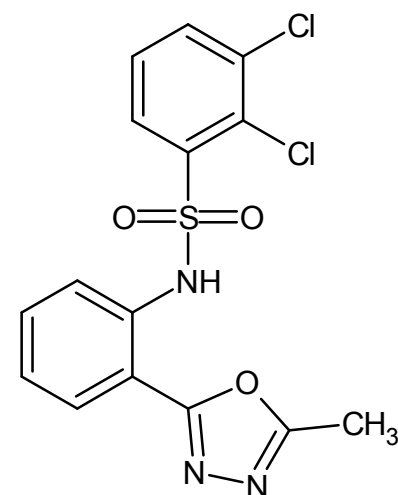
2,3-Dichloro-N-(2-(5-methyl-1,3,4-oxadiazol-2-yl)phenyl)benzenesulfonamide (18)



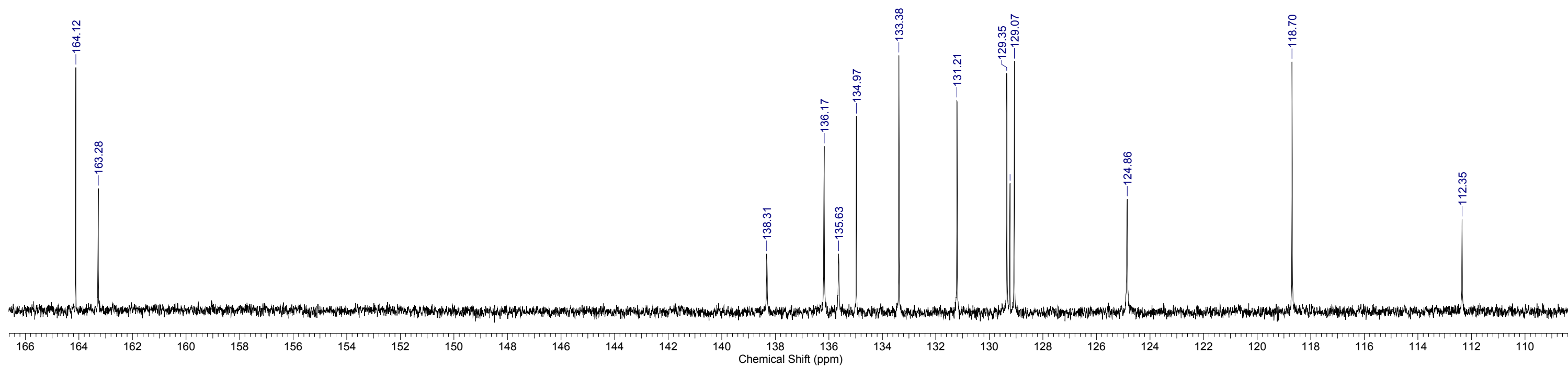
M109039.GSK2793753A.010.esp



2,3-Dichloro-N-(2-(5-methyl-1,3,4-oxadiazol-2-yl)phenyl)benzenesulfonamide (18)

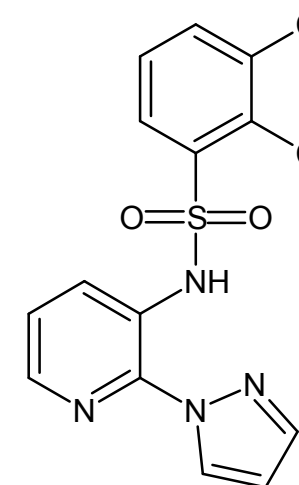


ZN2121.011.esp

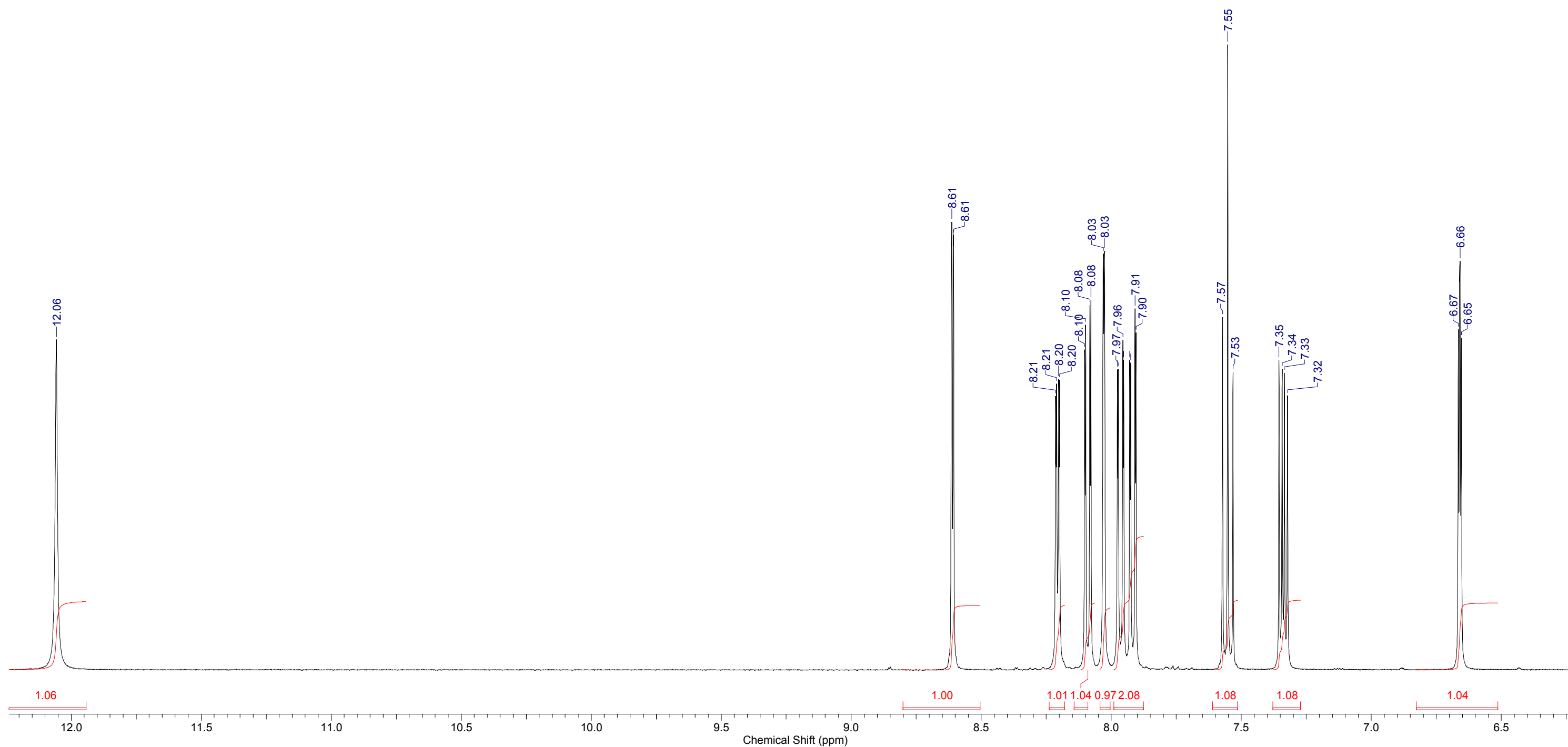


S36

2,3-Dichloro-N-[2-(1H-pyrazol-1-yl)-3-pyridinyl]benzenesulfonamide (19)

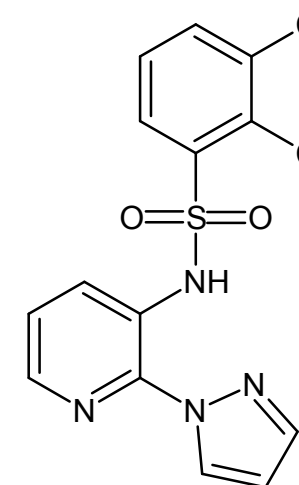


X169565.compound 19.010.esp

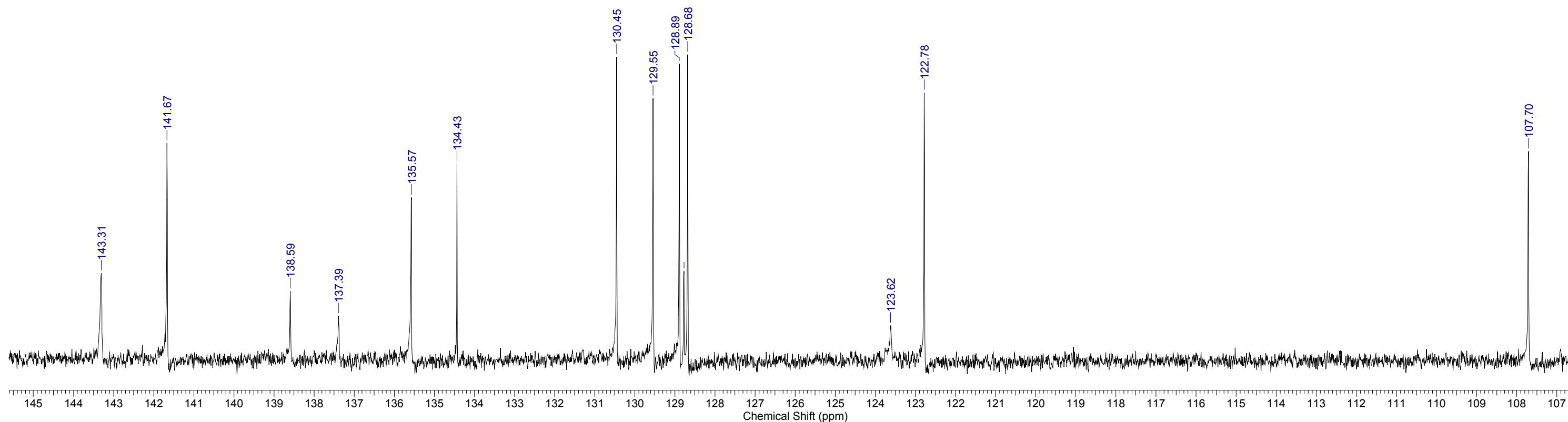




2,3-Dichloro-N-[2-(1H-pyrazol-1-yl)-3-pyridinyl]benzenesulfonamide (19)



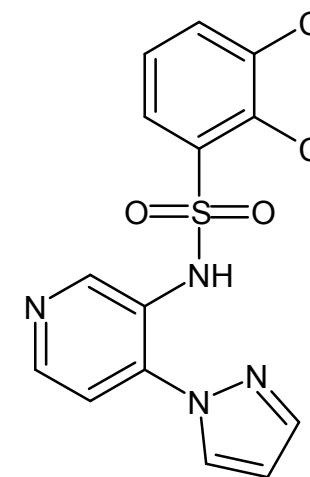
X169565.011.esp



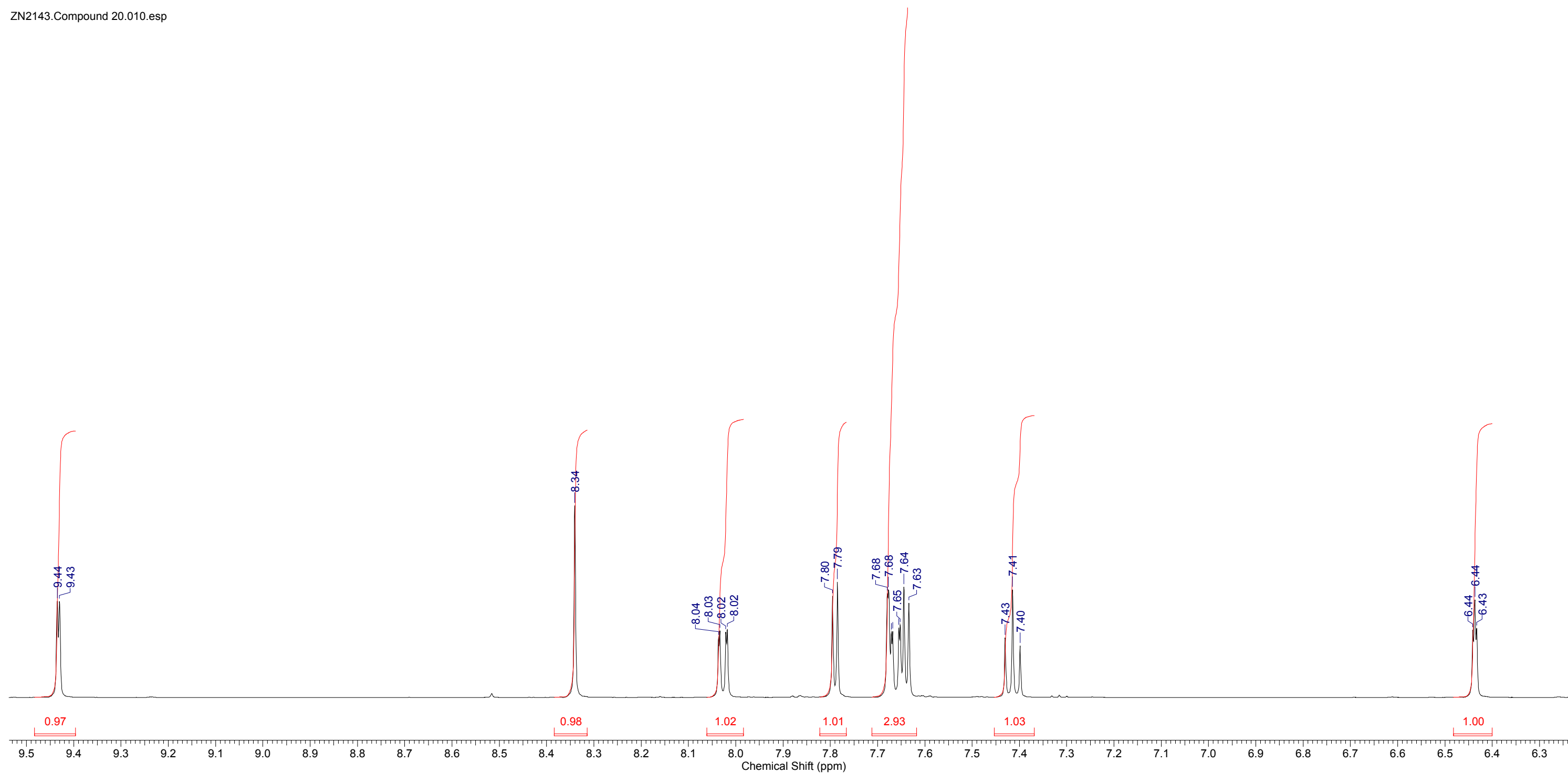
S38

# N-(4-(1H-Pyrazol-1-yl)pyridin-3-yl)-2,3-dichlorobenzenesulfonamide (20)

DMSO + NaHCO<sub>3</sub>



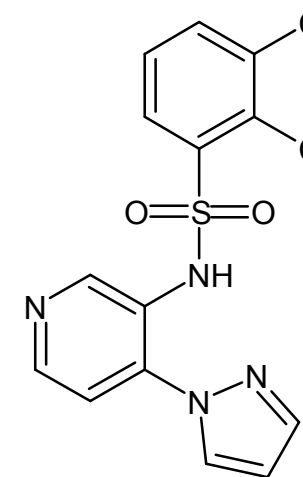
ZN2143.Compound 20.010.esp



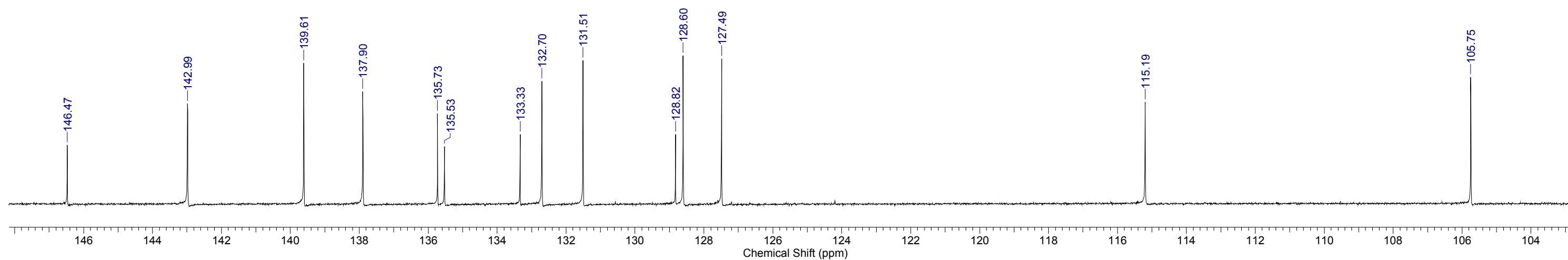


# N-(4-(1H-Pyrazol-1-yl)pyridin-3-yl)-2,3-dichlorobenzenesulfonamide (20)

DMSO-d6 + NaHCO3



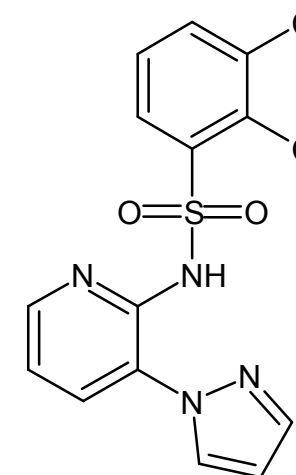
ZN2143.011.esp



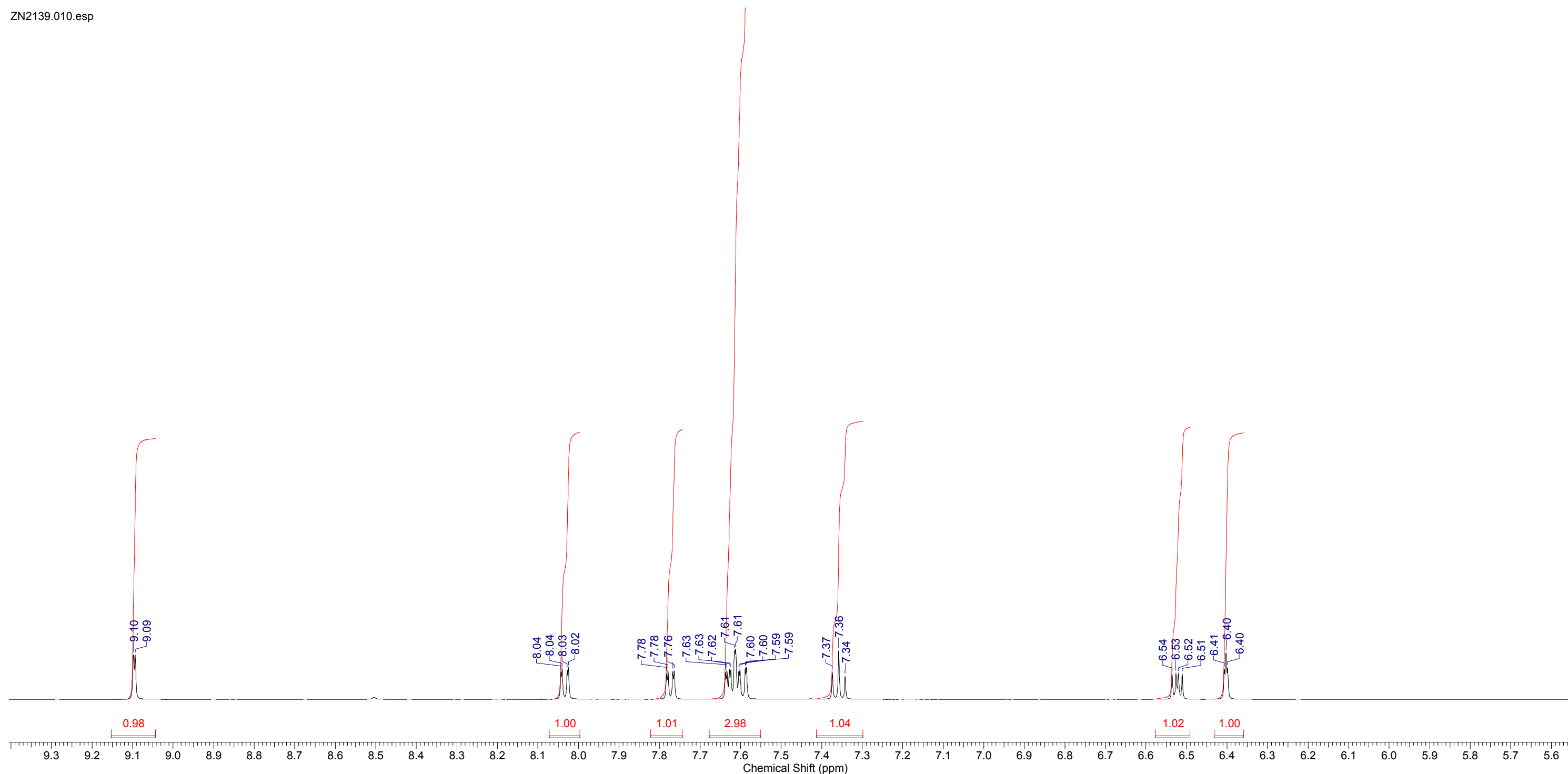
S40

# N-(3-(1H-Pyrazol-1-yl)pyridin-2-yl)-2,3-dichlorobenzenesulfonamide (23)

DMSO-d6 + NaHCO3



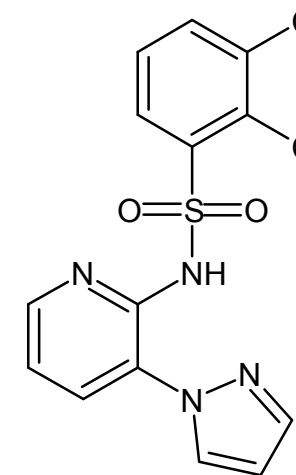
ZN2139.010.esp



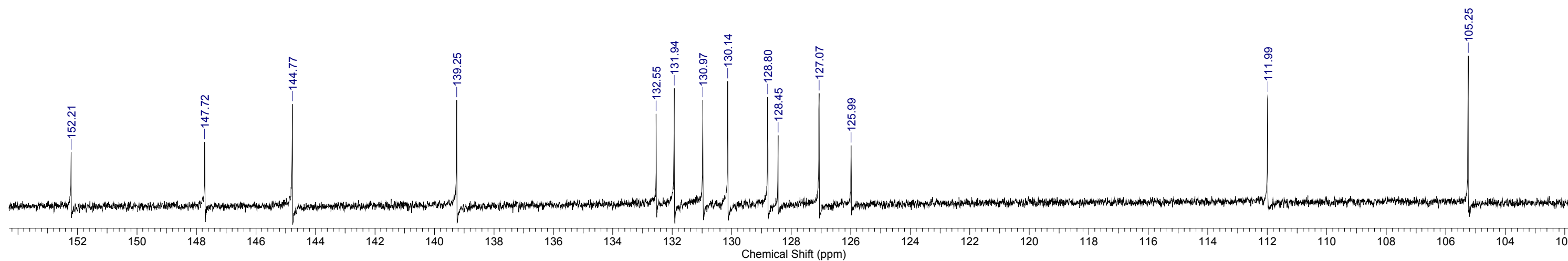
S41

# N-(3-(1H-Pyrazol-1-yl)pyridin-2-yl)-2,3-dichlorobenzenesulfonamide (23)

DMSO-d6 + NaHCO3

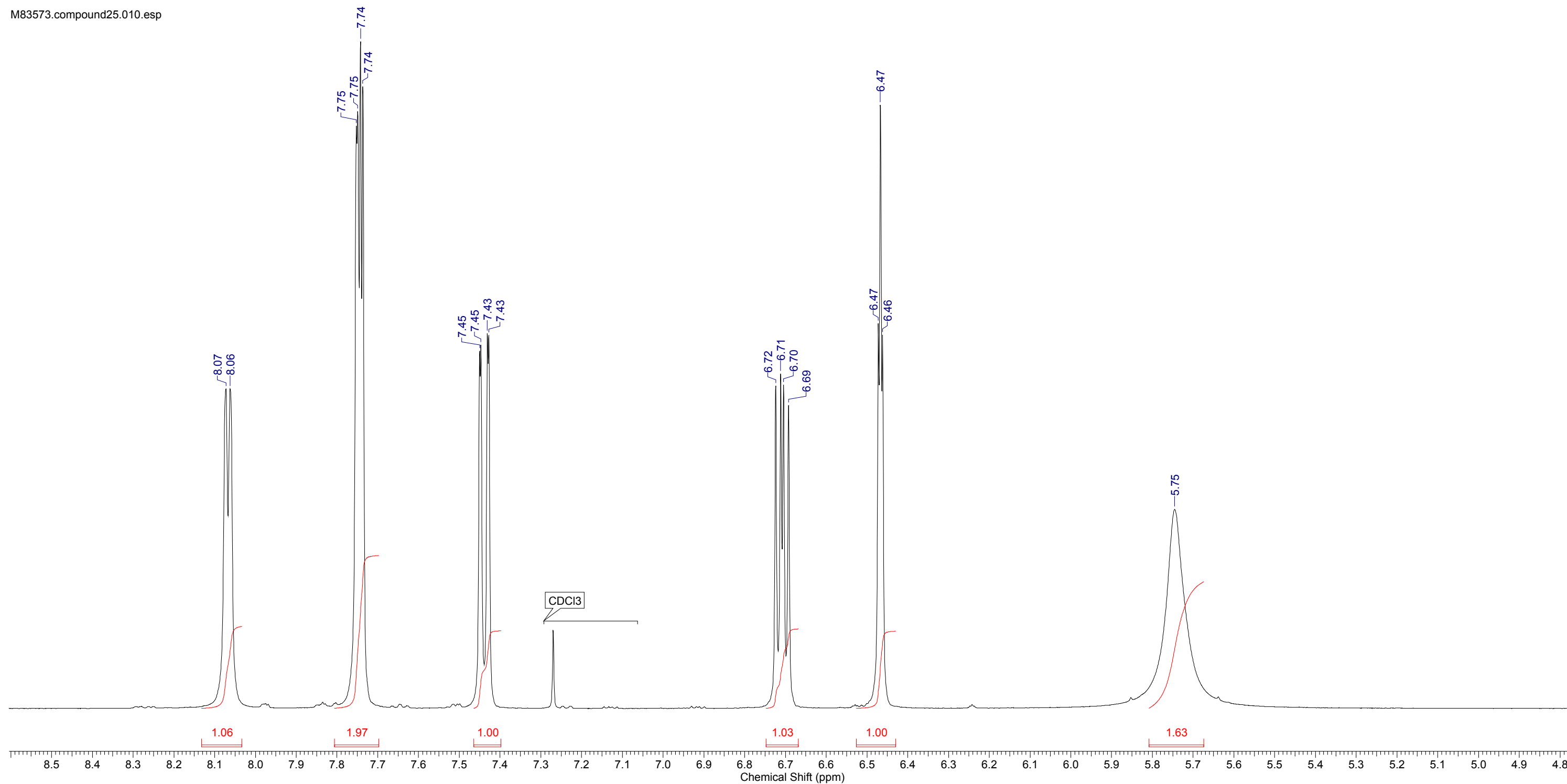
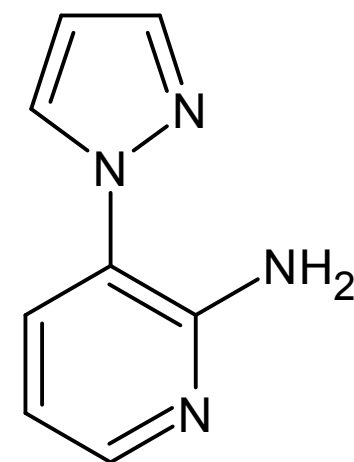


ZN2139.011.esp

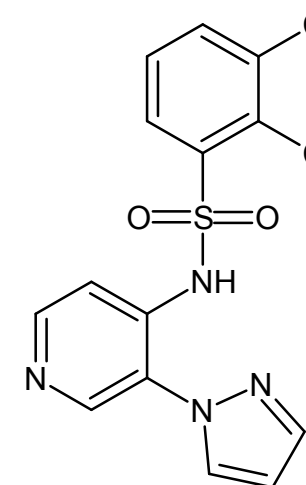


S42

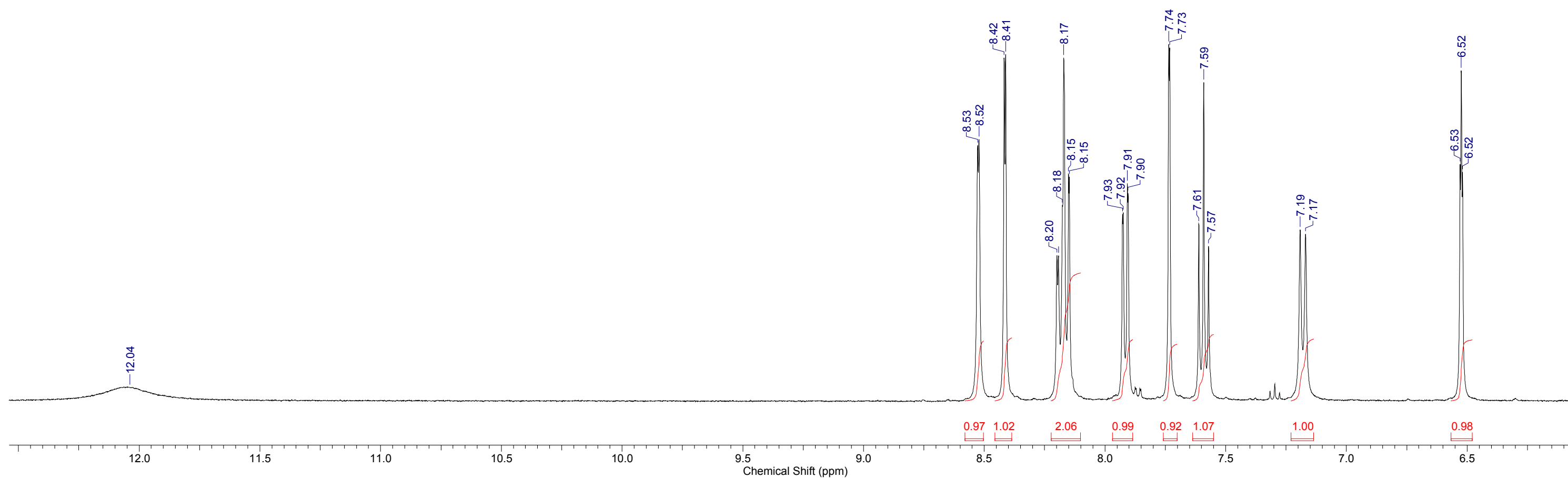
3-(1H-Pyrazol-1-yl)pyridin-2-amine (25)



N-(3-(1H-Pyrazol-1-yl)pyridin-4-yl)-2,3-dichlorobenzenesulfonamide (26)

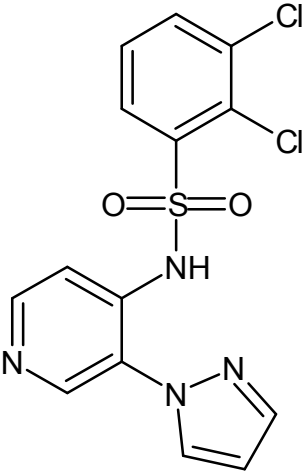


M95913.COMPOUND 26.010.ESP

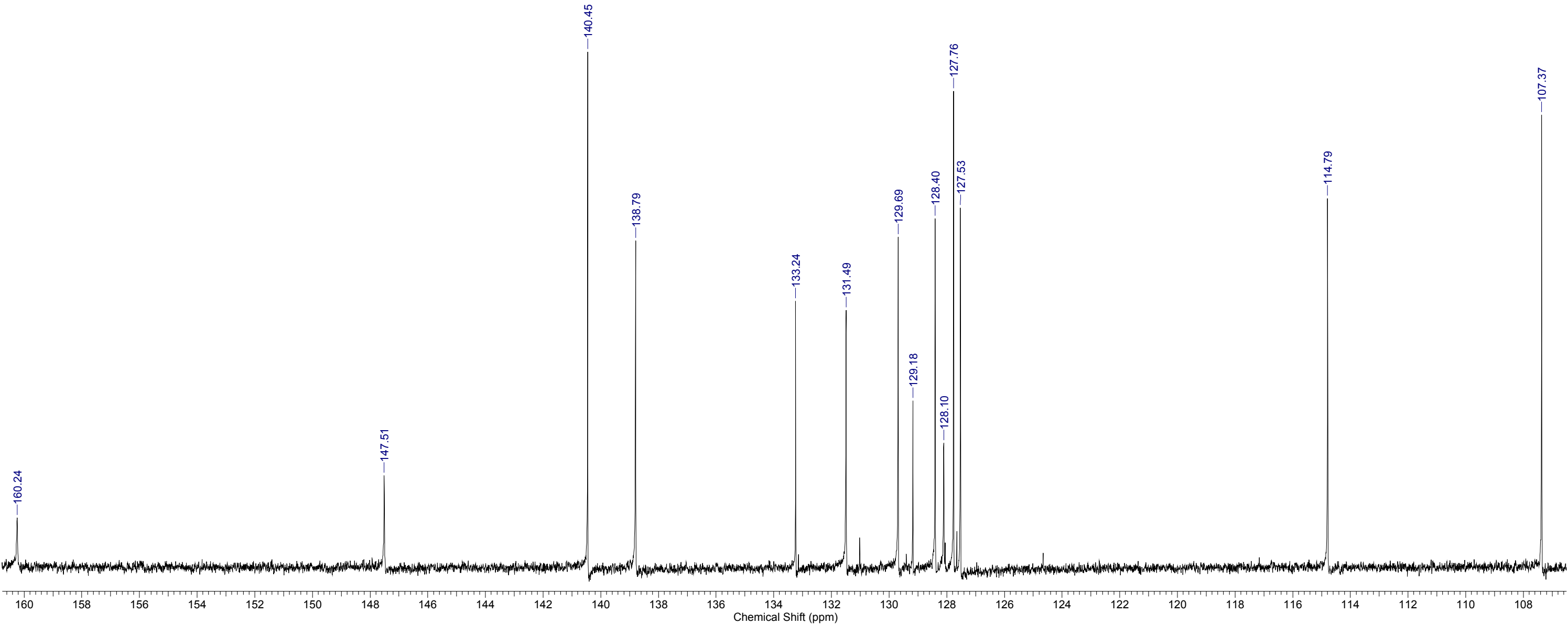


N-(3-(1H-Pyrazol-1-yl)pyridin-4-yl)-2,3-dichlorobenzenesulfonamide (26)

DMSO-d6 + NaHCO3

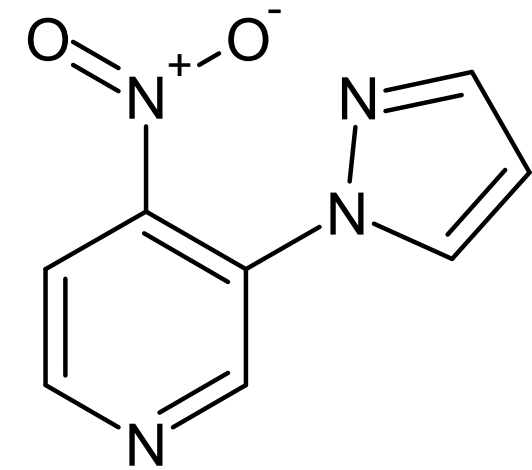


13C.ZN2145.Compound 26.011.esp

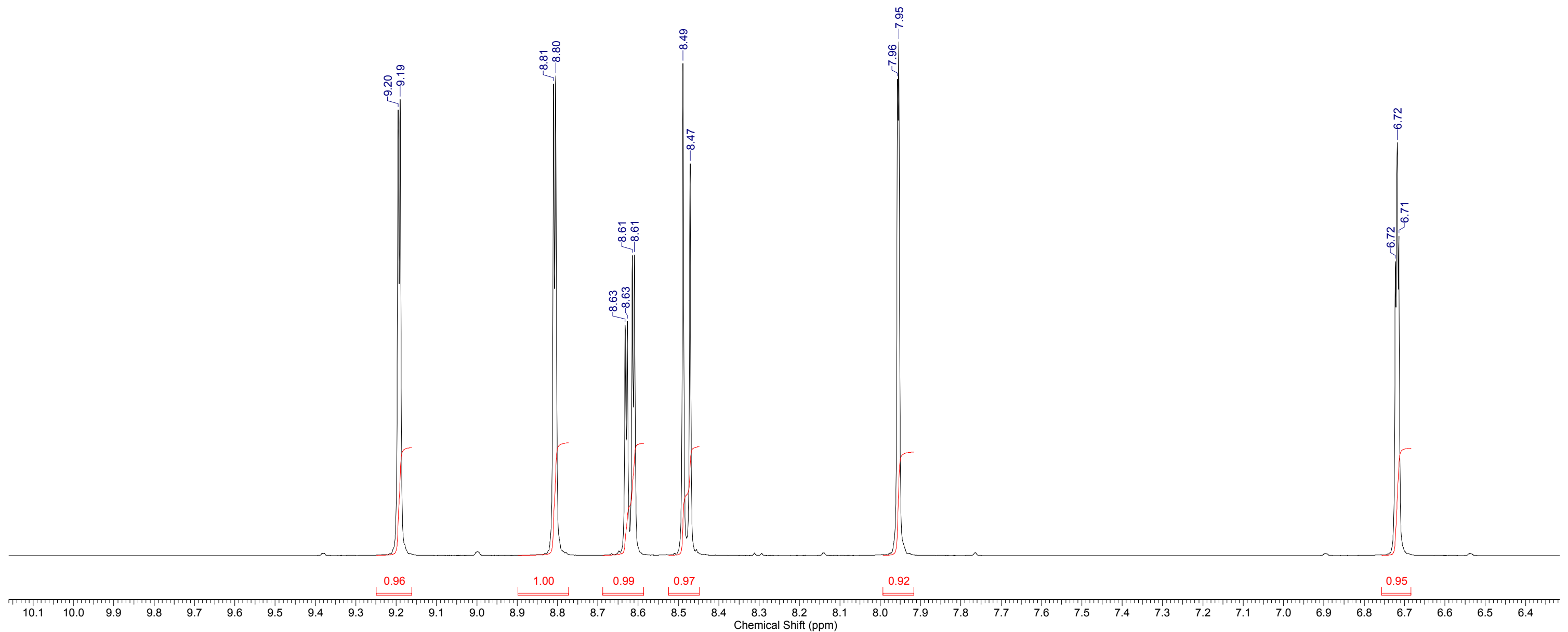




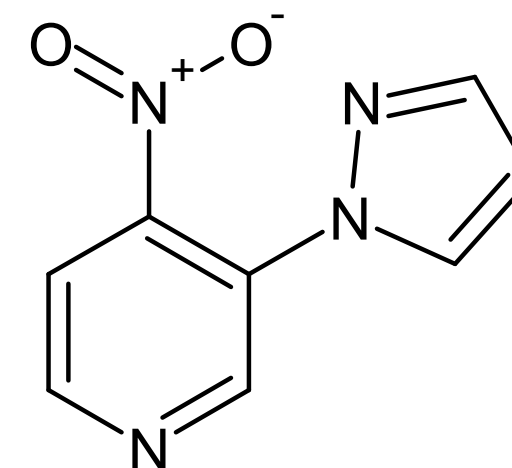
4-Nitro-3-(1H-pyrazol-1-yl)pyridine (28)



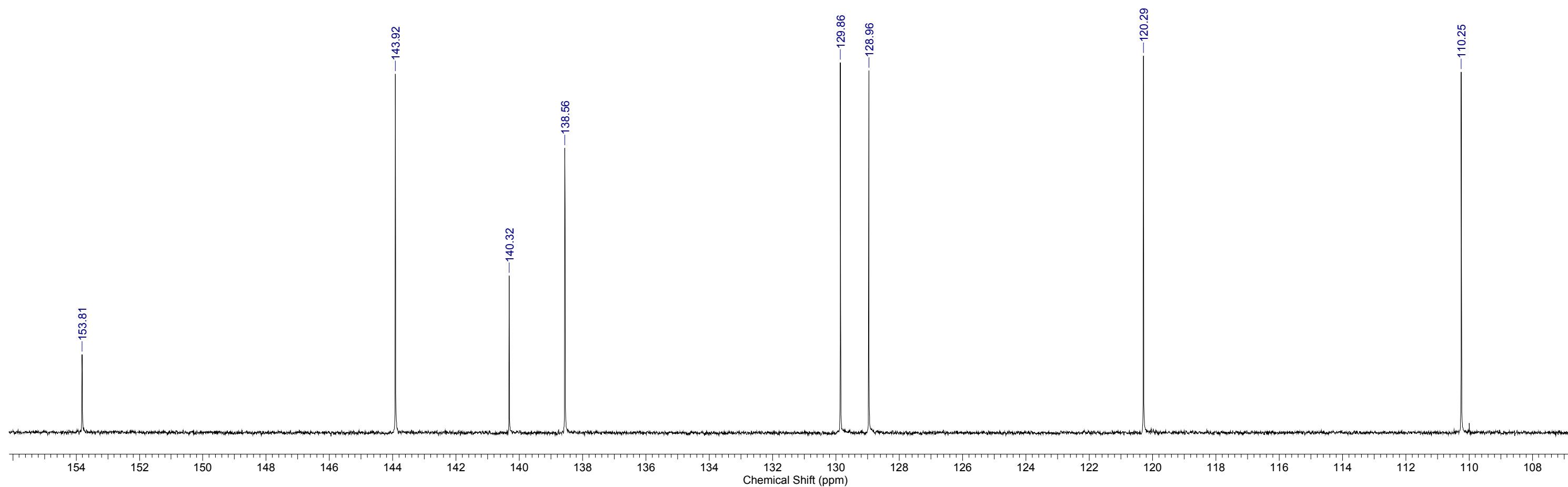
ZN2123.010.esp



# 4-Nitro-3-(1H-pyrazol-1-yl)pyridine (28)



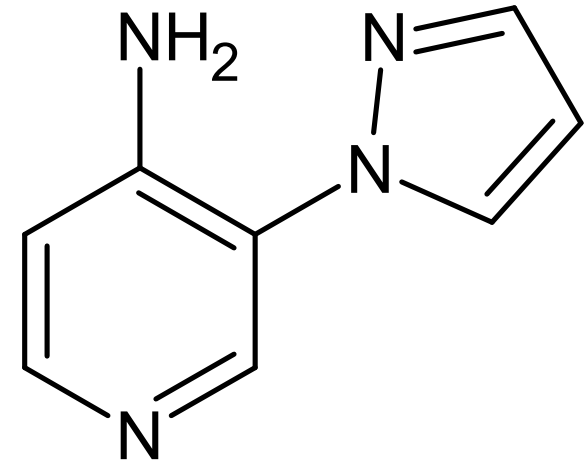
ZN2123.011.esp



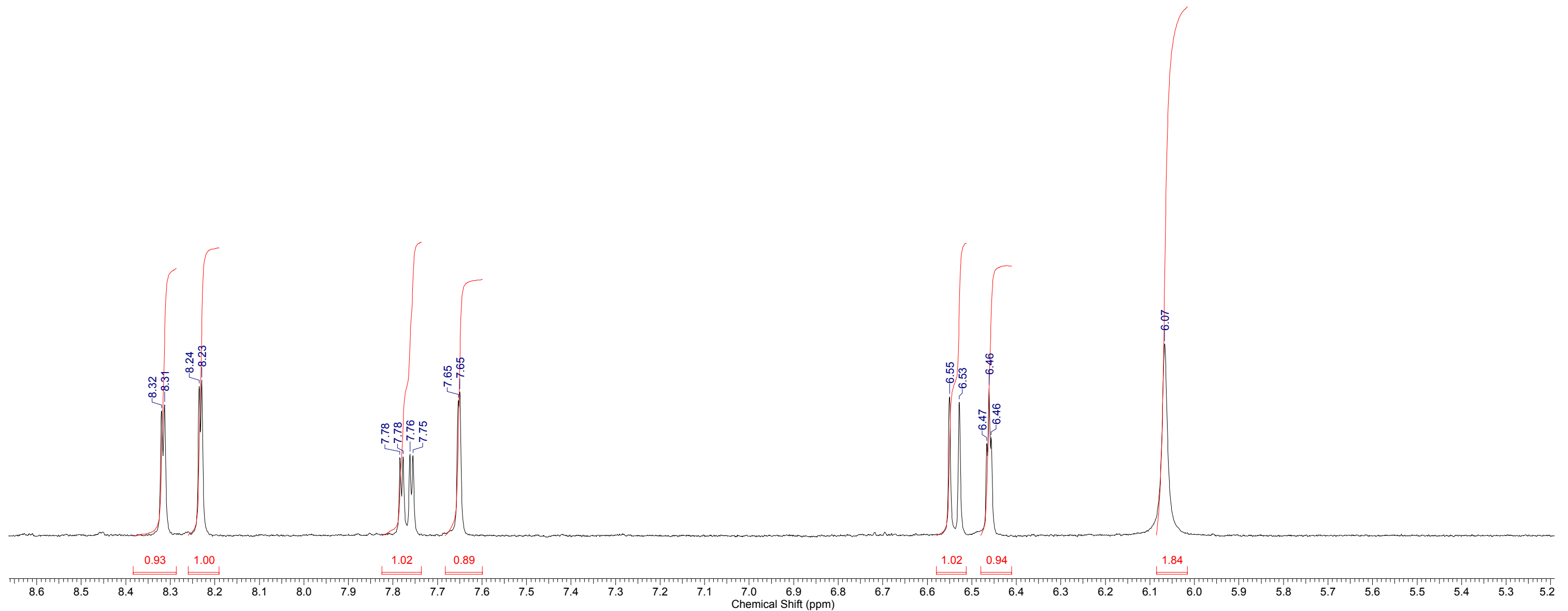
S47



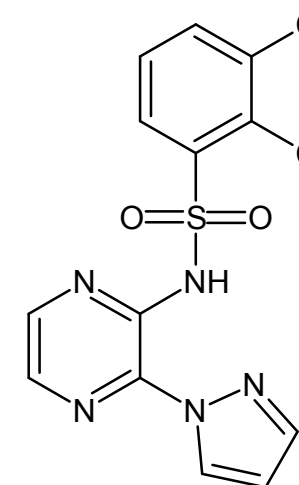
3-(1H-Pyrazol-1-yl)pyridin-4-amine (29)



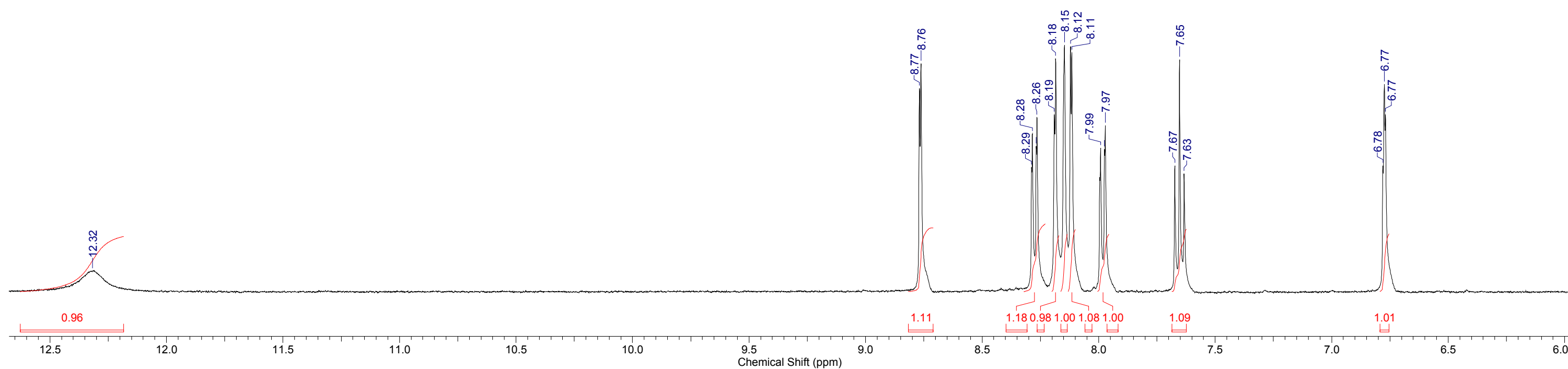
M83448.010.esp



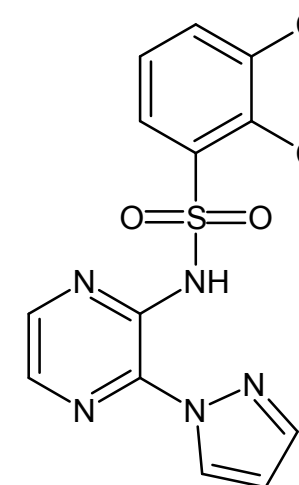
# N-(3-(1H-Pyrazol-1-yl)pyrazin-2-yl)-2,3-dichlorobenzenesulfonamide (30)



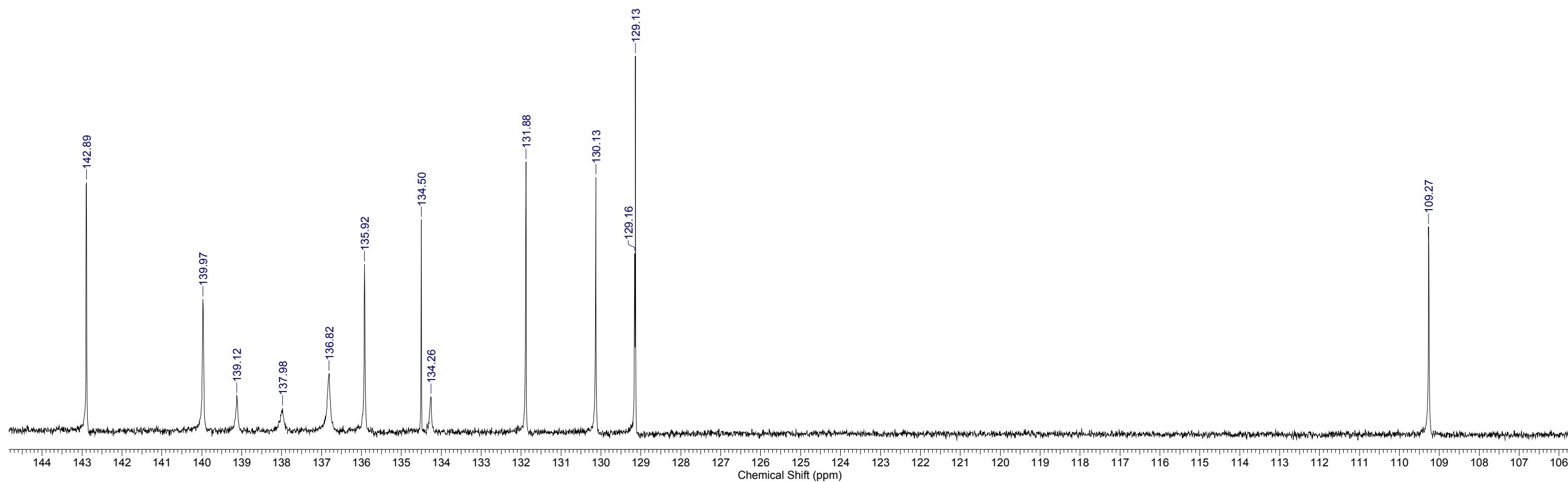
M82357.010.esp



N-(3-(1H-Pyrazol-1-yl)pyrazin-2-yl)-2,3-dichlorobenzenesulfonamide (30)

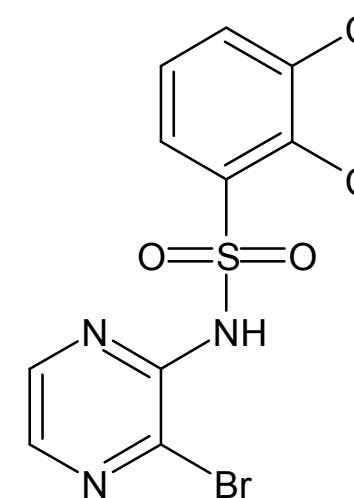


13C.PT11383.compound 30.014.esp

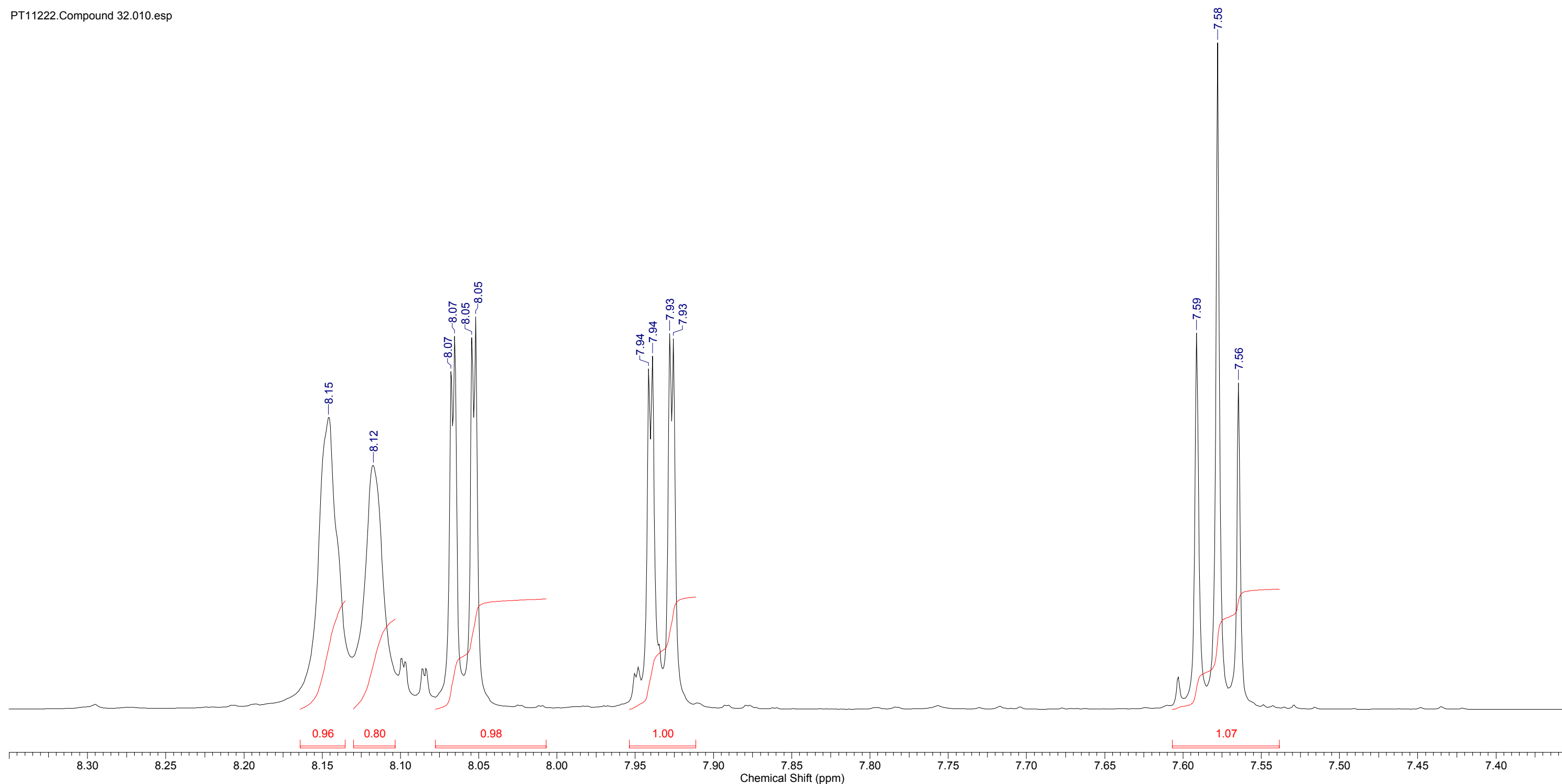


S50

# N-(3-Bromopyrazin-2-yl)-2,3-dichlorobenzenesulfonamide (32)



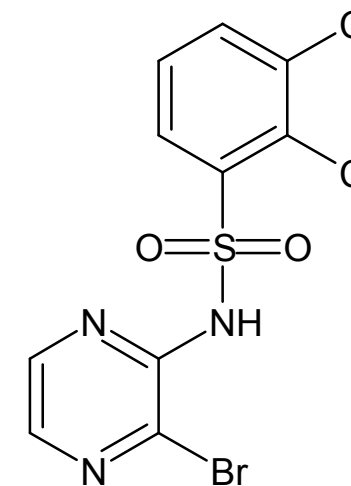
PT11222.Compound 32.010.esp



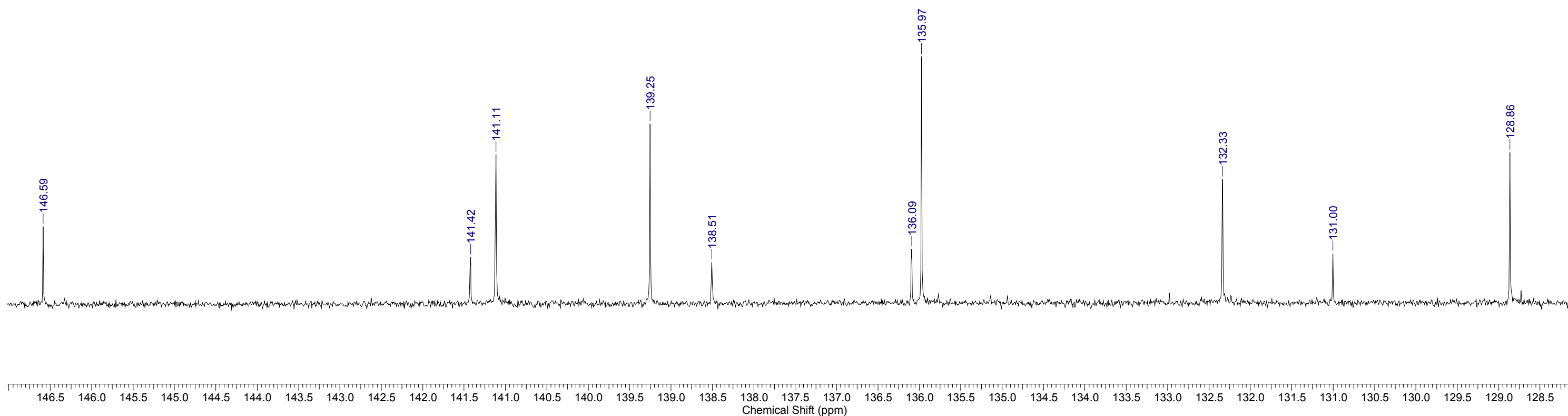
S51

# N-(3-Bromopyrazin-2-yl)-2,3-dichlorobenzenesulfonamide (32)

MeOD + DCI

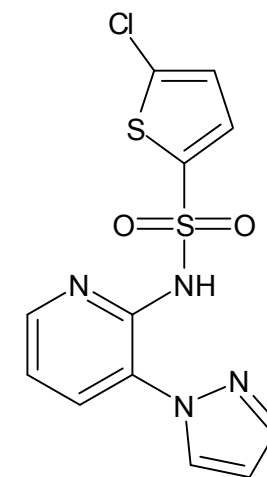


PT11241.017.esp

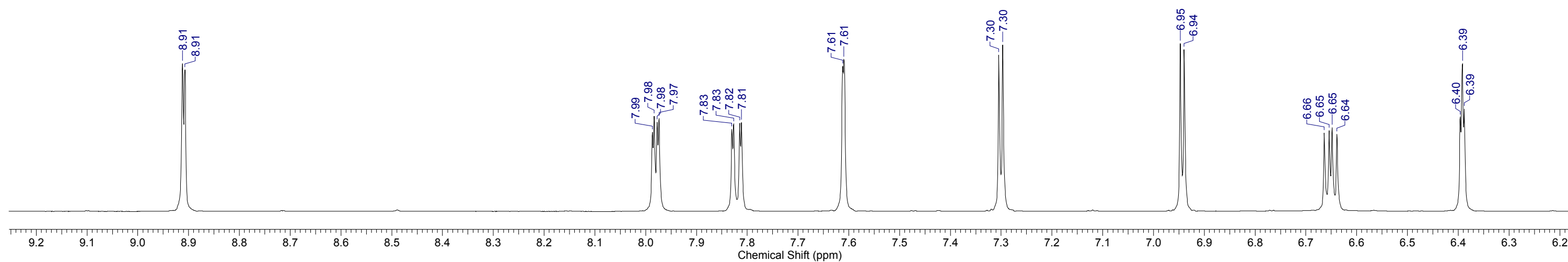


# N-(3-(1H-Pyrazol-1-yl)pyridin-2-yl)-5-chlorothiophene-2-sulfonamide (33)

DMSO-d6 + NaHCO3



ZN2278.010.esp

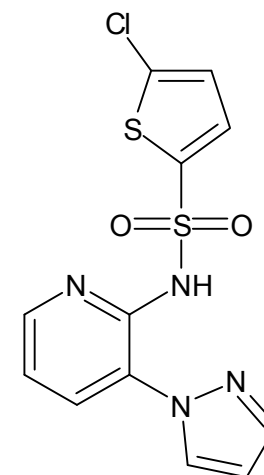


S53

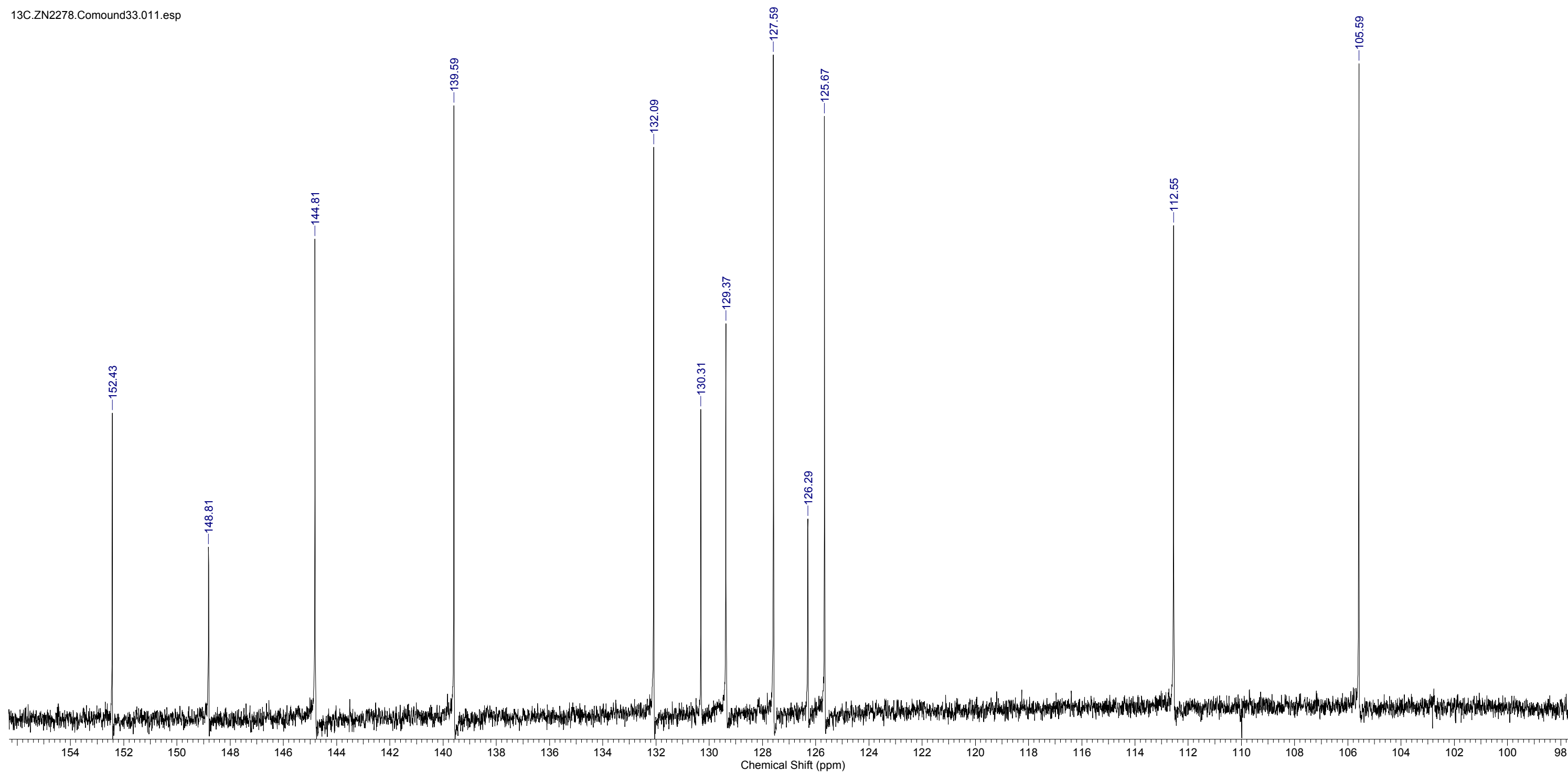


# N-(3-(1H-Pyrazol-1-yl)pyridin-2-yl)-5-chlorothiophene-2-sulfonamide (33)

DMSO-d6 + NaHCO3



13C.ZN2278.Comound33.011.esp



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