Supporting Information

Development of AIEE Active Fluorescent and Colorimetric Probe for Solid, Solution, and Vapor Phase Detection of Cyanide: Smartphone and Food Applications

Shumaila Majeed[a], Muhammad Tahir Waseem[a], Gul Shahzada Khan[b], Hafiz Muhammad Junaid[a], Muhammad Imran[c], Shamyla Nawazish[d], Tausif Ahmad Khan[a], Tariq Mahmood[a], Sohail Anjum Shahzad[a,*]

[a] Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, University Road, Abbottabad 22060, Pakistan

[b] Department of Chemistry, College of Science, University of Bahrain, Sakhir 32038, Bahrain

[c] Department of Chemistry, Faculty of Science, King Khalid University, P.O. Box 9004, Abha 61413, Saudi Arabia

[d] Department of Environmental Sciences, COMSATS University Islamabad, Abbottabad Campus, Abbottabad 22060, Pakistan

* **Corresponding Author**: Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, University Road, Abbottabad 22060, Pakistan (S.A. Shahzad). E-mail address: sashahzad@cuiatd.edu.pk (S.A. Shahzad).

TABLE OF CONTENTS

SI-1. Instruments and reagents

Proton nuclear magnetic resonance (^1H NMR) spectra of compounds **1** and **2** were recorded at Bruker Avance 400 and 500 MHz while ^{13}C NMR spectra were carried out at Bruker Avance 100 and 125 MHz. Photophysical properties and sensing studies of compound **2** were scanned through fluorescence spectroscopy (FluoroMax-Plus-P-C, Horiba Jobin Yvon Technology, USA). UV-Vis spectrophotometer (SPECORD 200 PLUS-223E2003C, Analytik Jena, Germany) was used to record absorption spectra. Used reagents and chemicals were acquired from Daejung Chemicals & Metals (Korea), Alfa Aesar (UK), and Sigma Aldrich (USA). The chemicals enlist 9*H*-fluorenone, aniline, 9,9-Bis(4-aminophenyl)fluorene, methanesulfonic acid, ethyl acetate, *n*-hexane, DMSO-d_6, salicylaldehyde, methanol, DMF, acetonitrile, THF, DCM, $CHCl_3$, DMSO, CN^-, I^-, NO_3^-, Cl^-, F^-, N_3^-, Br^-, $H_2PO_4^-$, ClO_4^-, CH_3COO^-, and NO_2^-.

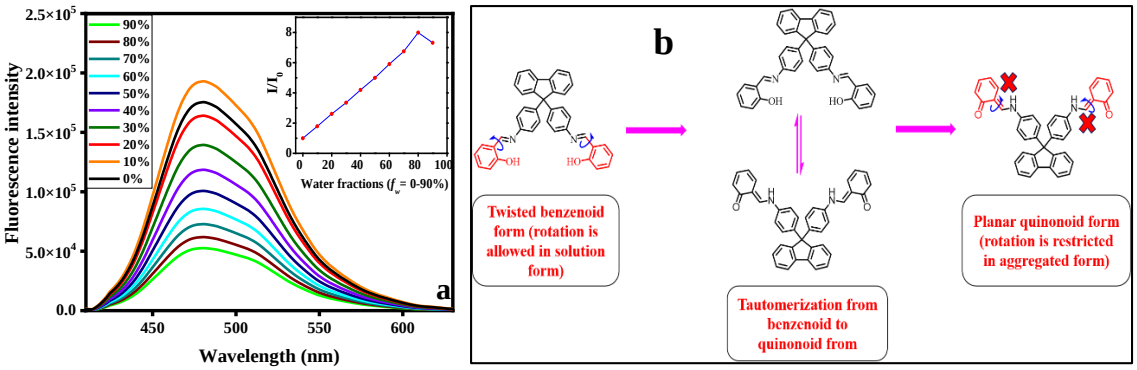


Fig. S1. The fluorescence spectral changes of probe **2** (10 μM) at various DMF/H_2O ratios (a) and plausible AIEE mechanism (b). Inset shows the general representation of AIEE pattern.

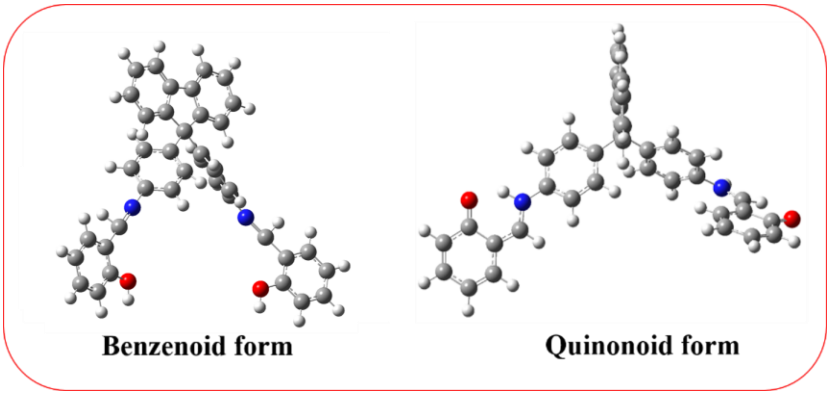


Fig. S2. Theoretical representation of the benzenoid and quinonoid form of probe **2** accomplished through Gaussian 09 package at B3LYP/6-31G (d).

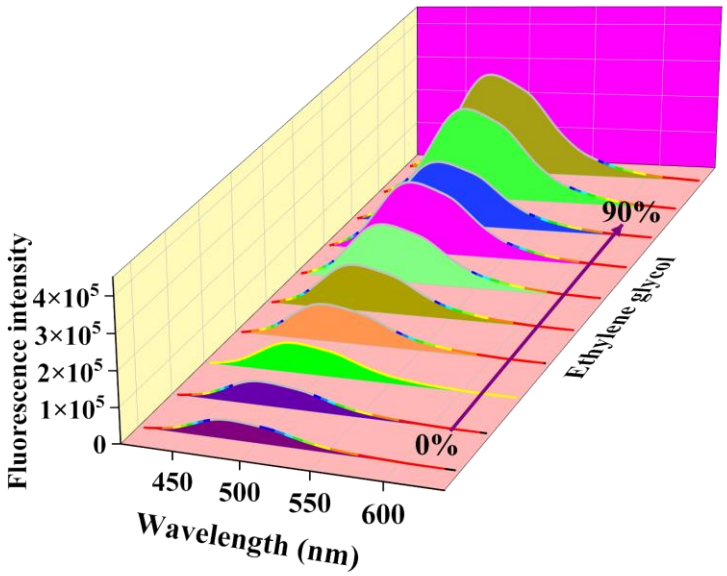


Fig. S3. The fluorescence spectral changes of probe **2** (10 µM) at various DMF/ethylene glycol ratios.

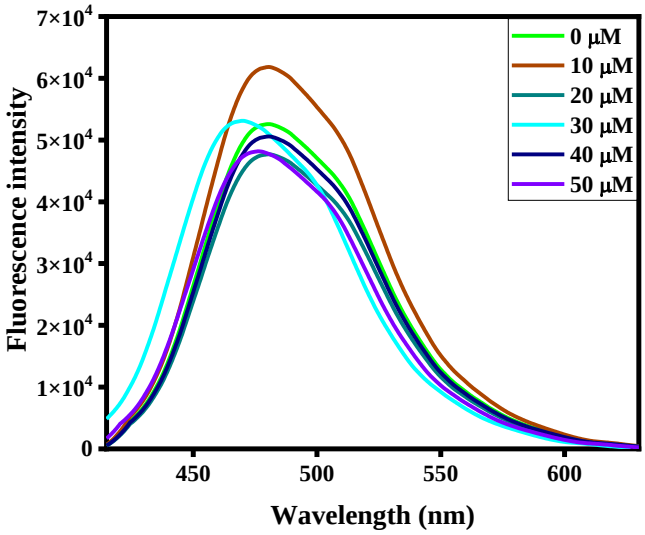


Fig. S4. The fluorescence spectral changes of probe **2** at its various concentrations (0–50 µM).

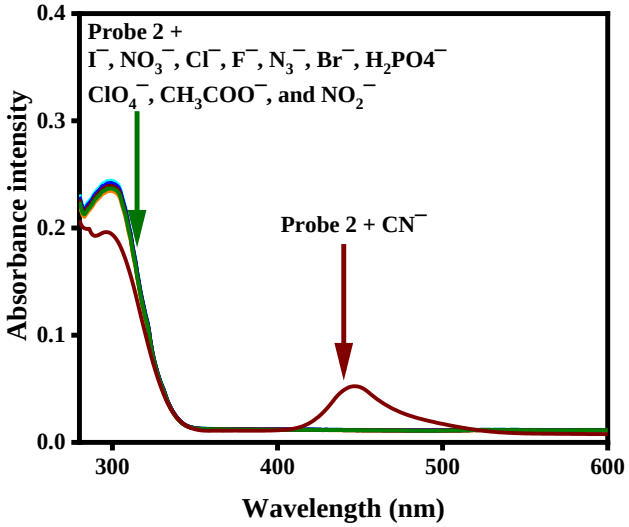


Fig. S5. The UV-vis spectral change of probe **2** (10 µM) in the presence of different anions.

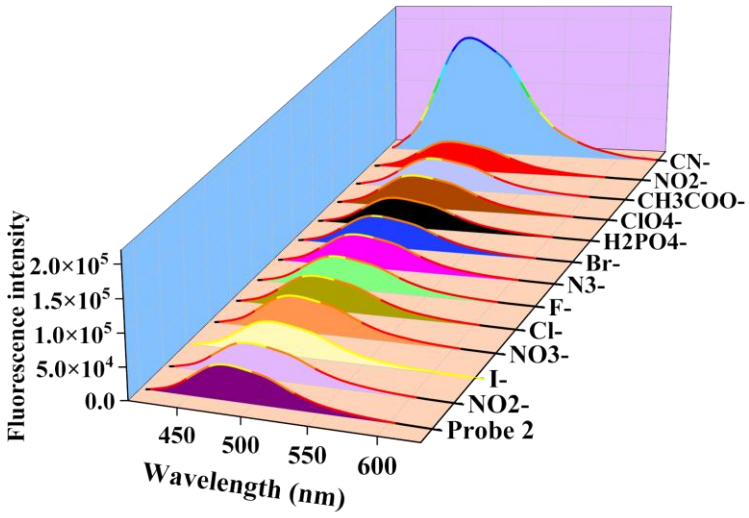


Fig. S6. The fluorescence spectral change of probe **2** (10 μM) in the presence of different anions (Excitation wavelength = 410 nm).

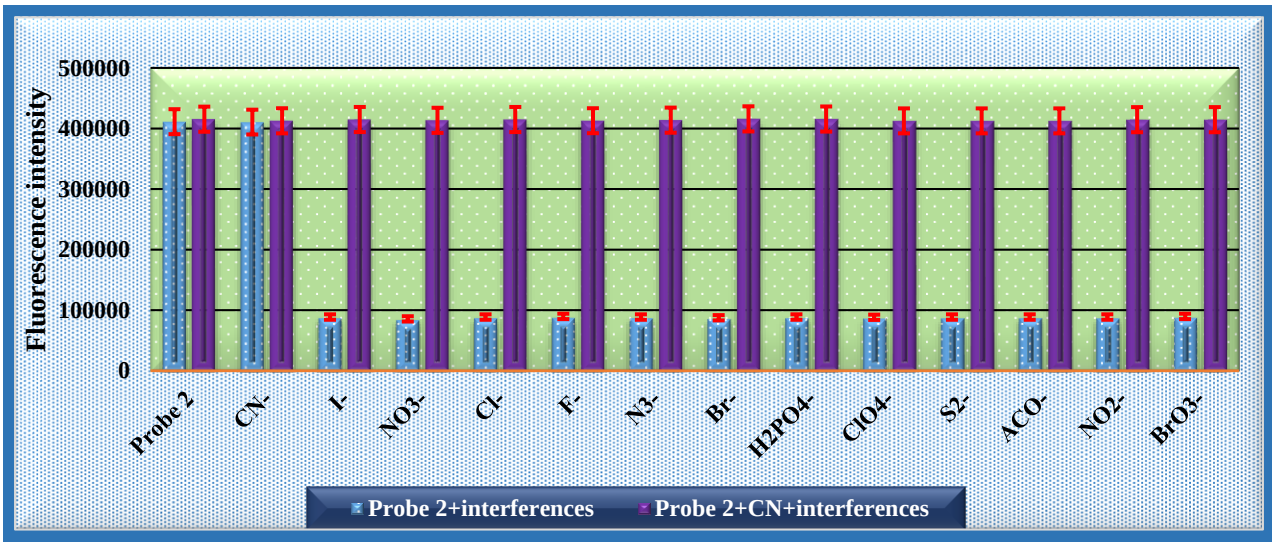


Fig. S7. The fluorescence change of probe **2** (10 μM) containing 50 nM of CN^- ions in the presence of interferences (100 equiv).

Table S1. The comparison of LOD for CN^- and other features of probe **2** with already reported CN^- probes.

Sensors	Aggregation induced emission enhancement (AIEE)	Piezofluorochromic behavior	Vapor phase detection	Detection in actual food Samples	Smartphone based detection	LOD (nM)	Ref.

Schiff base based probe **2**	Described in detail	Excellent piezofluorochromic character	Yes	Yes	Yes	6.17	**This work**
Spiropyran and spironaphthoxazine based sensor	Didn't display	Didn't display	Not described	Not described	Not described	91	[1]
Naphthopyranbenzothiazole core sensor	Didn't display	Didn't display	Not described	Not described	Not described	330	[2]
aldehyde-appended salamo-type sensor	Didn't display	Didn't display	Not described	Not described	Not described	80	[3]
Indoleoxazine functionalized compound	Didn't display	Didn't display	Not described	Explored	Not described	100	[4]
D-π-A organic fluorophore	Didn't display	Didn't display	Not described	Not described	Not described	380	[5]
Pyridine based nanoparticles as cyanide ion sensor	Explored	Didn't display	Not described	Not described	Not described	8.2	[6]
Naphthopyran functionalized sensor	Explored	Didn't display	Not described	Not described	Not described	427	[7]
Oligothiophene-benzothiazole based sensor	Didn't display	Didn't display	Not described	Explored	Not described	15×10^3	[8]
Triphenylamine based probe	Explored	Didn't display	Not described	Explored	Not described	2×10^4	[9]
Carbazole based sensor	Explored	Didn't display	Not described	Not described	Not described	67.4	[10]

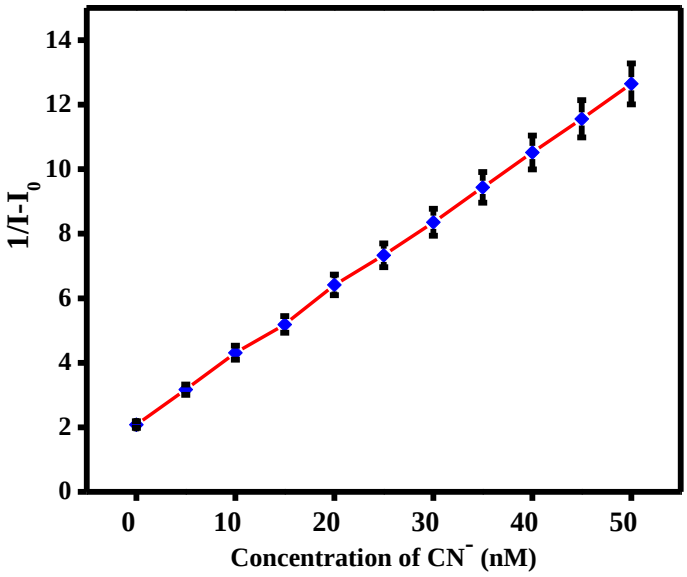


Fig. S8. The Benesi–Hildebrand plot of probe **2** (10 μM) between fluorescence response vs increasing concentrations of CN^-.

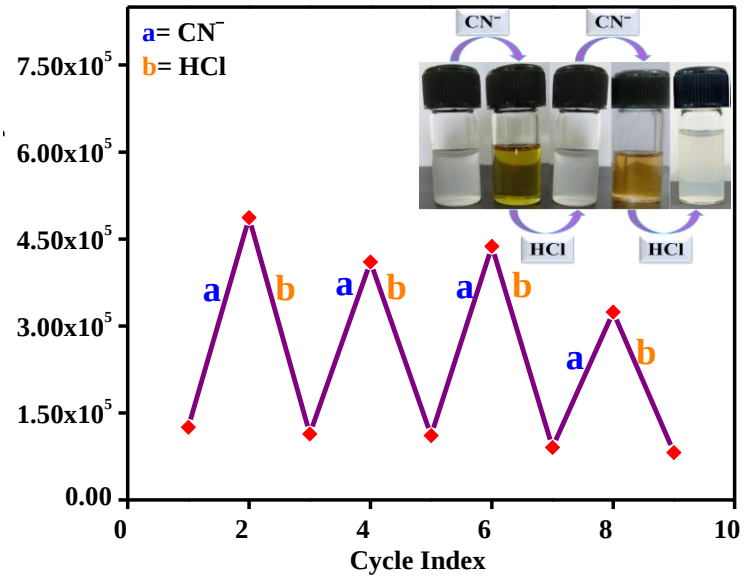


Fig. S9. The switchable fluorescence and colorimetric response of probe **2**.

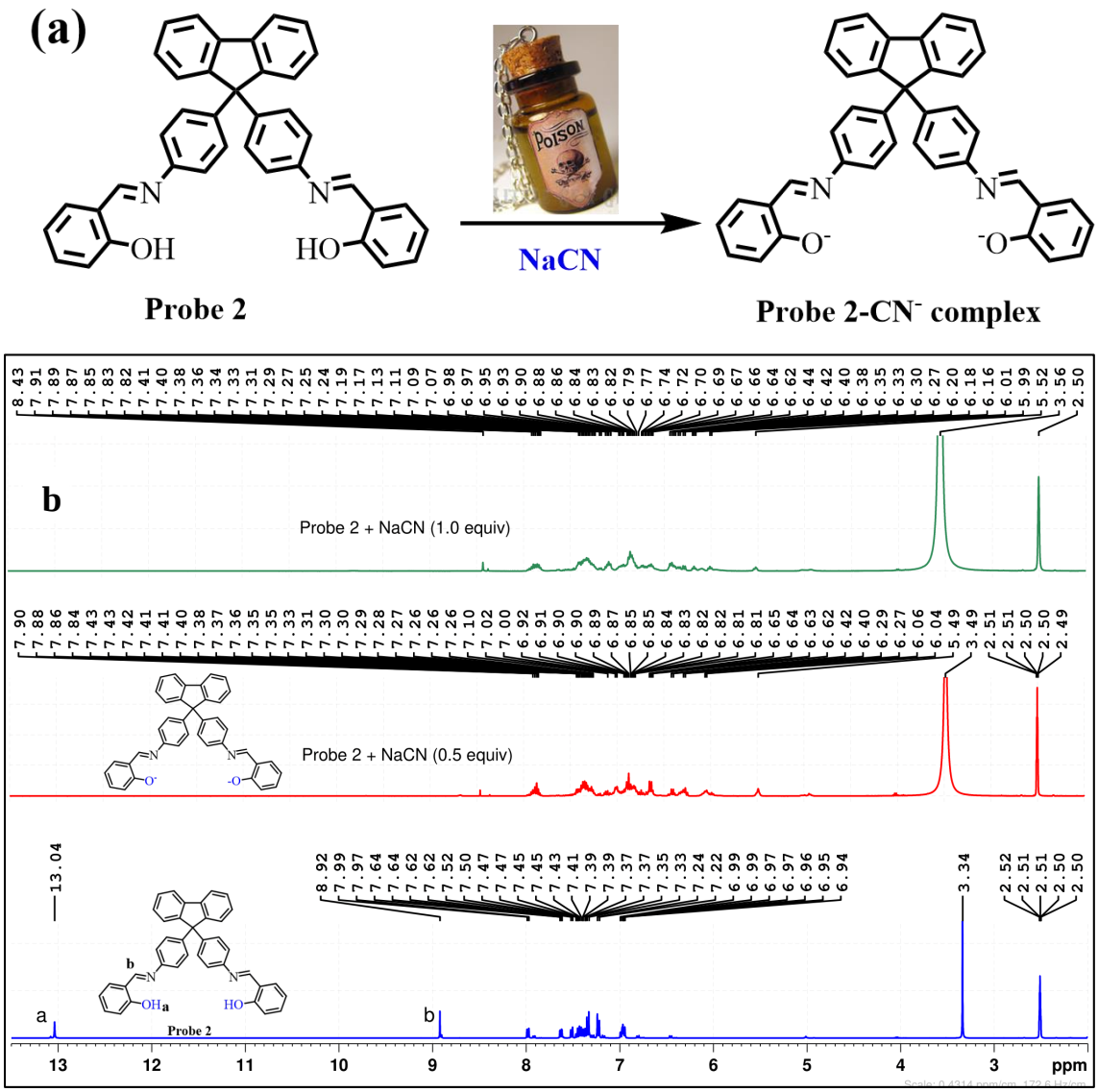


Fig. S10. The putative sensing mechanism (a) and ^{1}H NMR titration of probe **2** (b) upon addition of increasing amounts of CN^{-}.

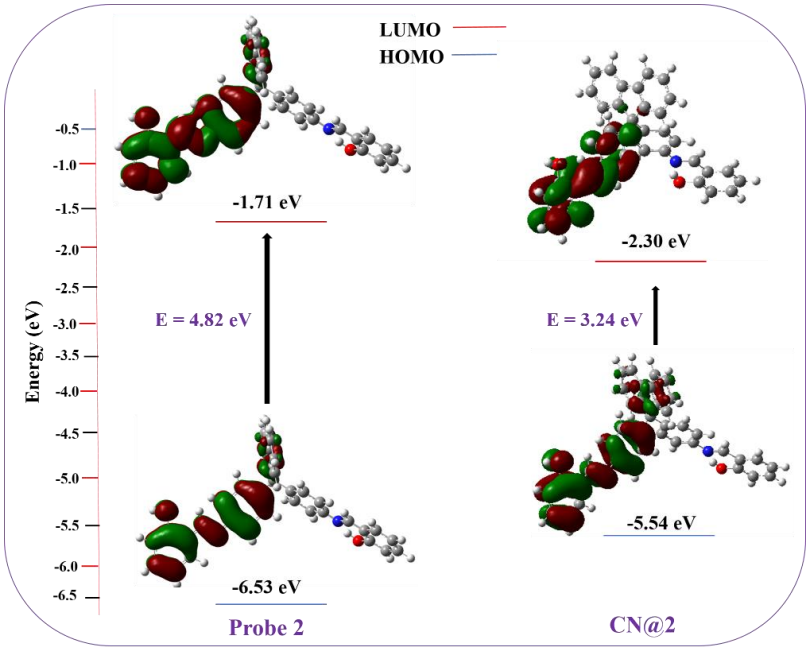


Fig. S11. Frontier molecular orbital (FMO) plots of probe **2** and its probe– CN^- complex (achieved through Gaussian 09 program).

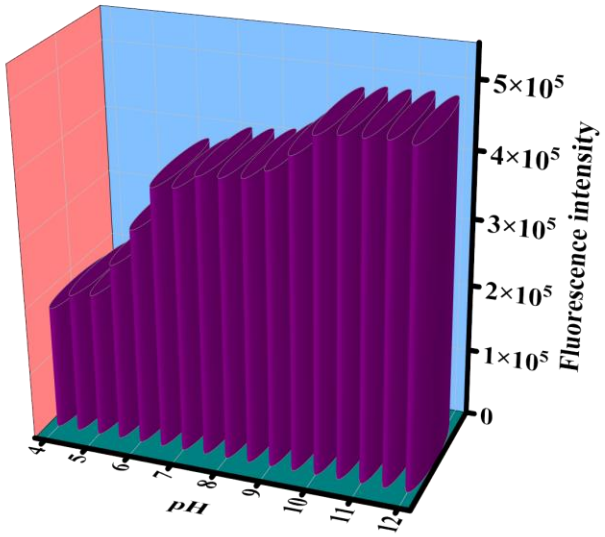


Fig. S12. Effect of pH on the enhanced fluorescence emission response of probe **2** towards CN^-.

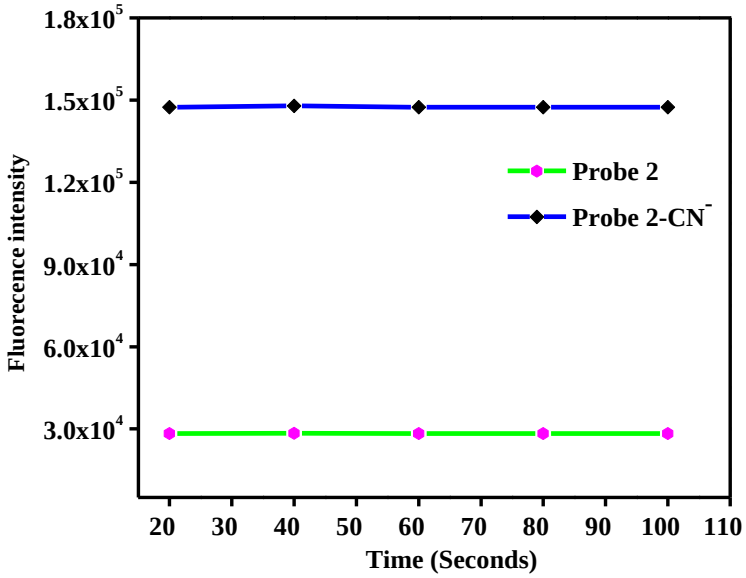
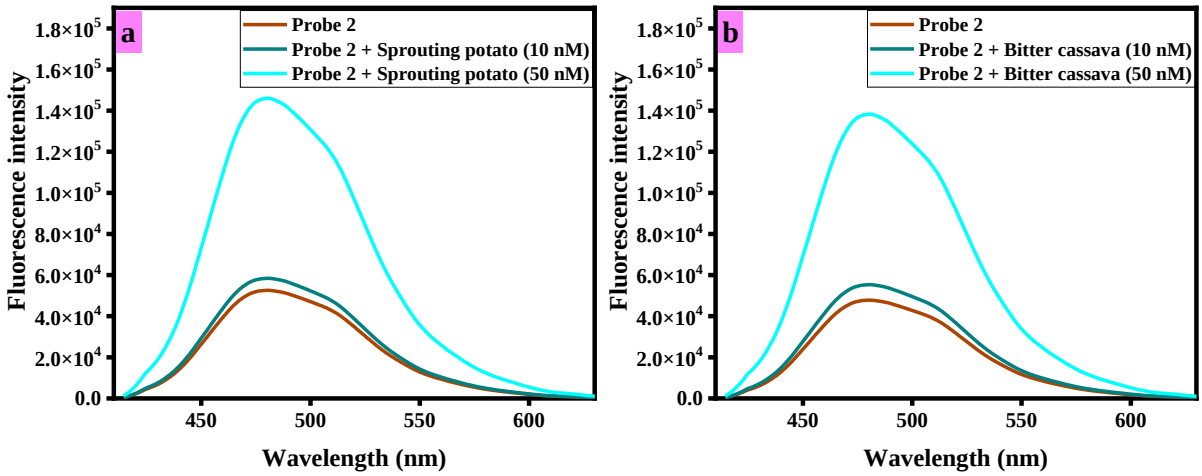


Fig. **S13**. Photostability analysis of probe **2** and **2**–CN^{-} complex.



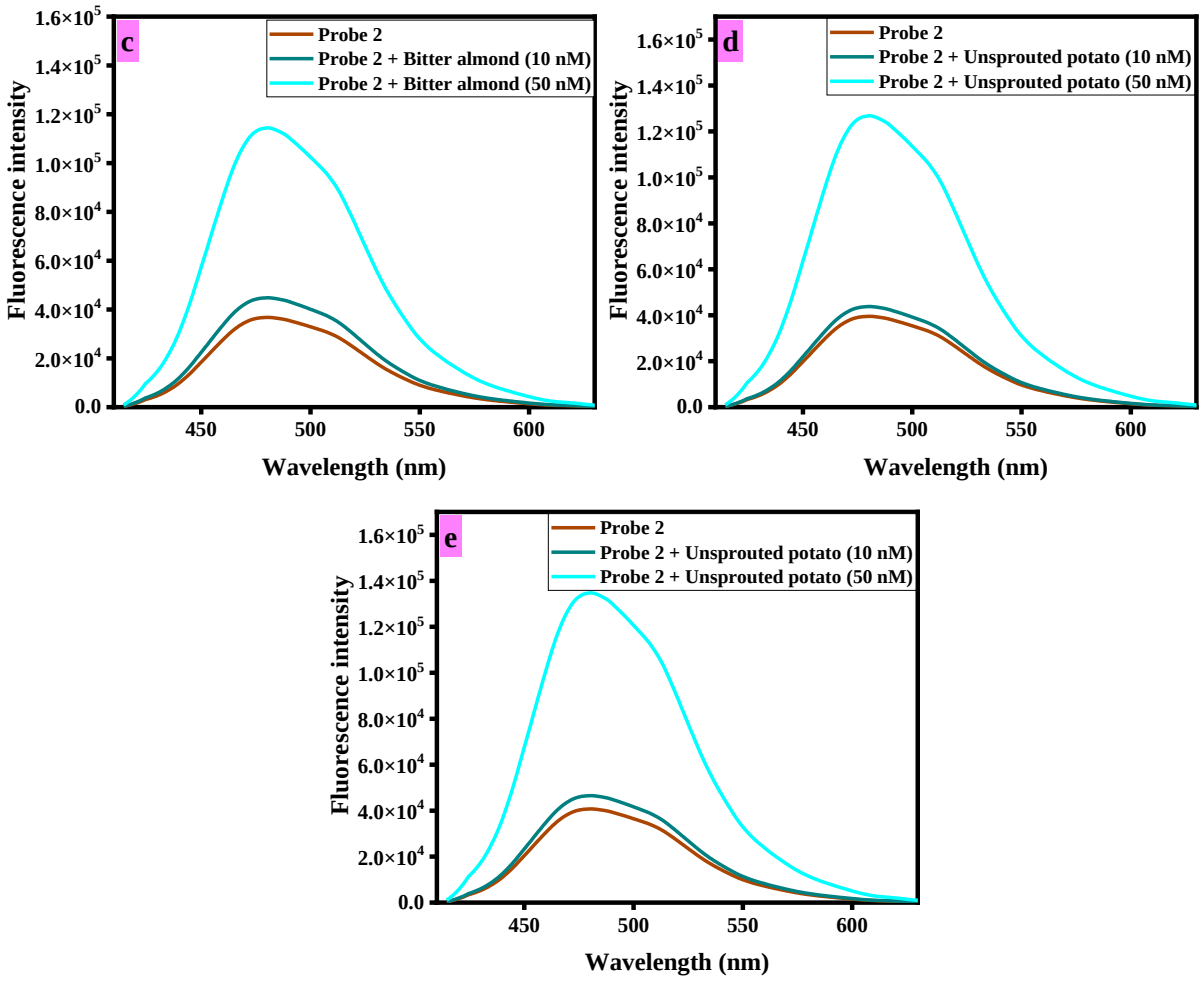


Fig. S14. The fluorescence spectral changes of probe **2** (10 µM) towards endogenous cyanide in food samples (sprouting potato (a), bitter cassava (b), bitter almond (c), un-sprouted potatoes (d), and sweet almond (e)).

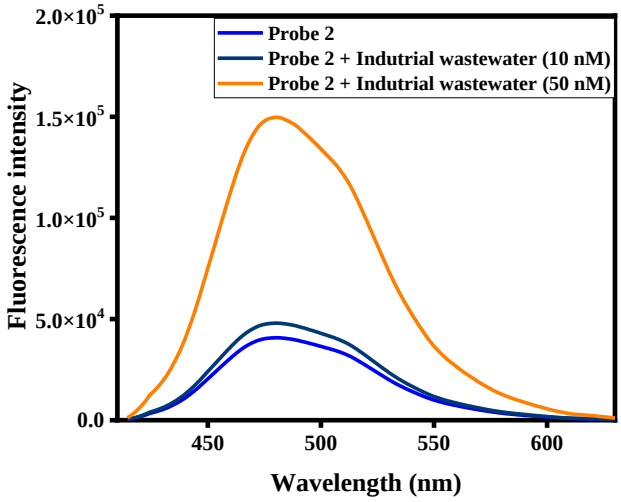


Fig. S15. The fluorescence spectra changes of probe **2** (10 μM) towards CN^- spiked industrial wastewater.

References

1 S. Sanjabi, J. K. Rad and A. R. Mahdavian, *J. Photochem. Photobiol. A: Chem.*, 2022, **424**, 113626.

2 Q. Li, J. Chang, H. Shi, T. Niu, H. Dong and H. Mu, *Supramol. Chem.*, 2022, 1-7.

3 L.-M. Pu, R.-Y. Li, Z.-Z. Chen, W.-B. Xu, H.-T. Long and W.-K. Dong, *J. Photochem. Photobiol. A: Chem.*, 2022, 113883.

4 Z. Zhang, G. Chen, W. Pan, Y. Bi, S. Shen, X. Cao, X. Pang and Y. Zhu, *J. Mol. Struct.*, 2022, **1251**, 131893.

5 C. Liu, D. Zhang, S. Ye, T. Chen and R. Liu, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 2022, **267**, 120593.

6. R. Nazarian, H. R. Darabi, K. Aghapoor, R. Firouzi and H. Sayahi, *Chem. Comm.*, 2020, **56**, 8992-8995.

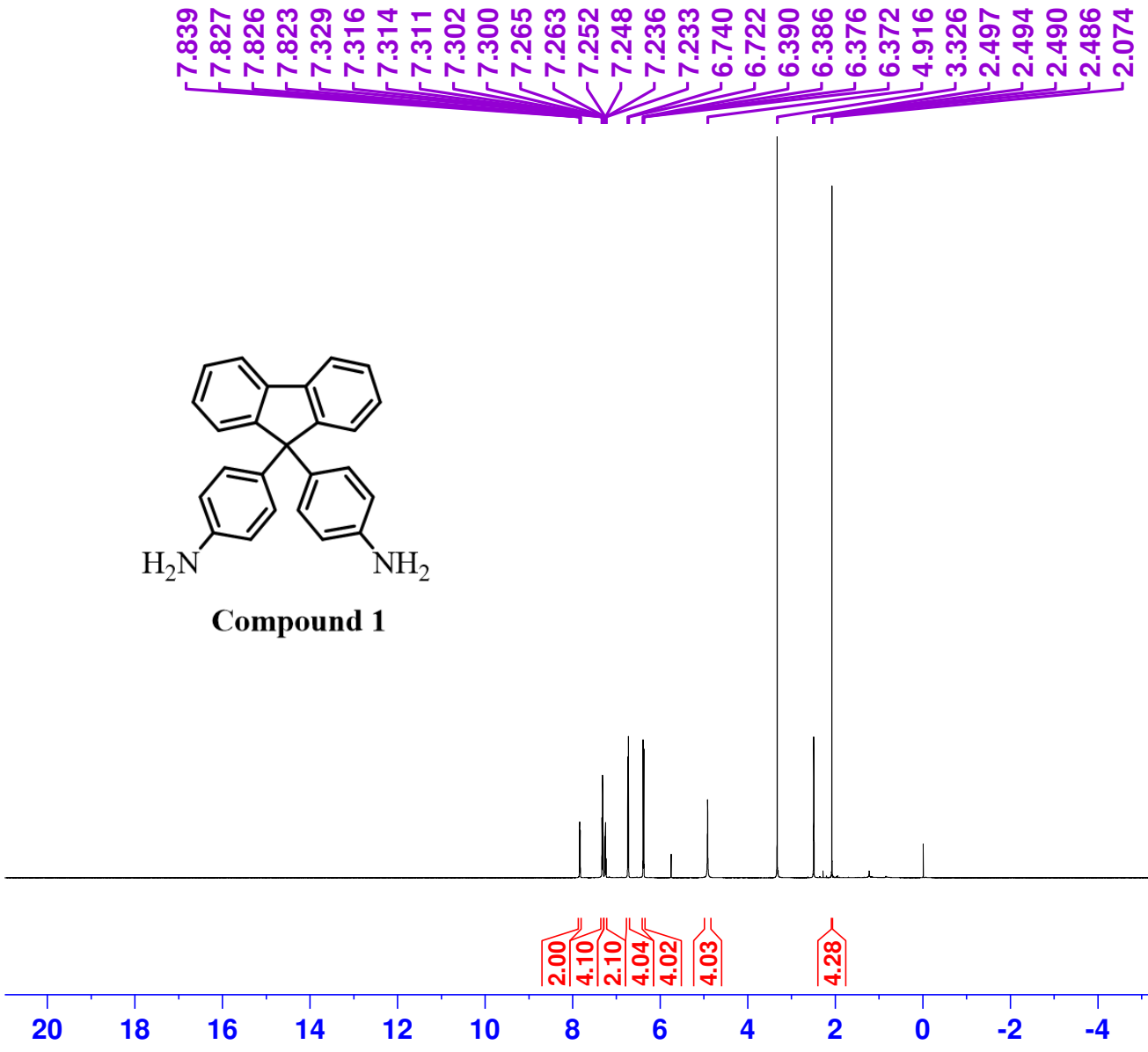
7 Z. M. Dong, H. Ren, J. N. Wang and Y. Wang, *Microchem. J.*, 2020, **155**, 104676.

8 Q. Niu, L. Lan, T. Li, Z. Guo, T. Jiang, Z. Zhao, Z. Feng and J. Xi, *Sens. Actuators B Chem.*, 2018, **276**, 13-22.

9 X. Wen, L. Yan and Z. Fan, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 2020, **241**, 118664.

10 L. Tang, L. Zhou, A. Liu, X. Yan, K. Zhong, X. Liu, X. Gao and J. Li, *Dyes Pigm.*, 2021, **186**, 109034.

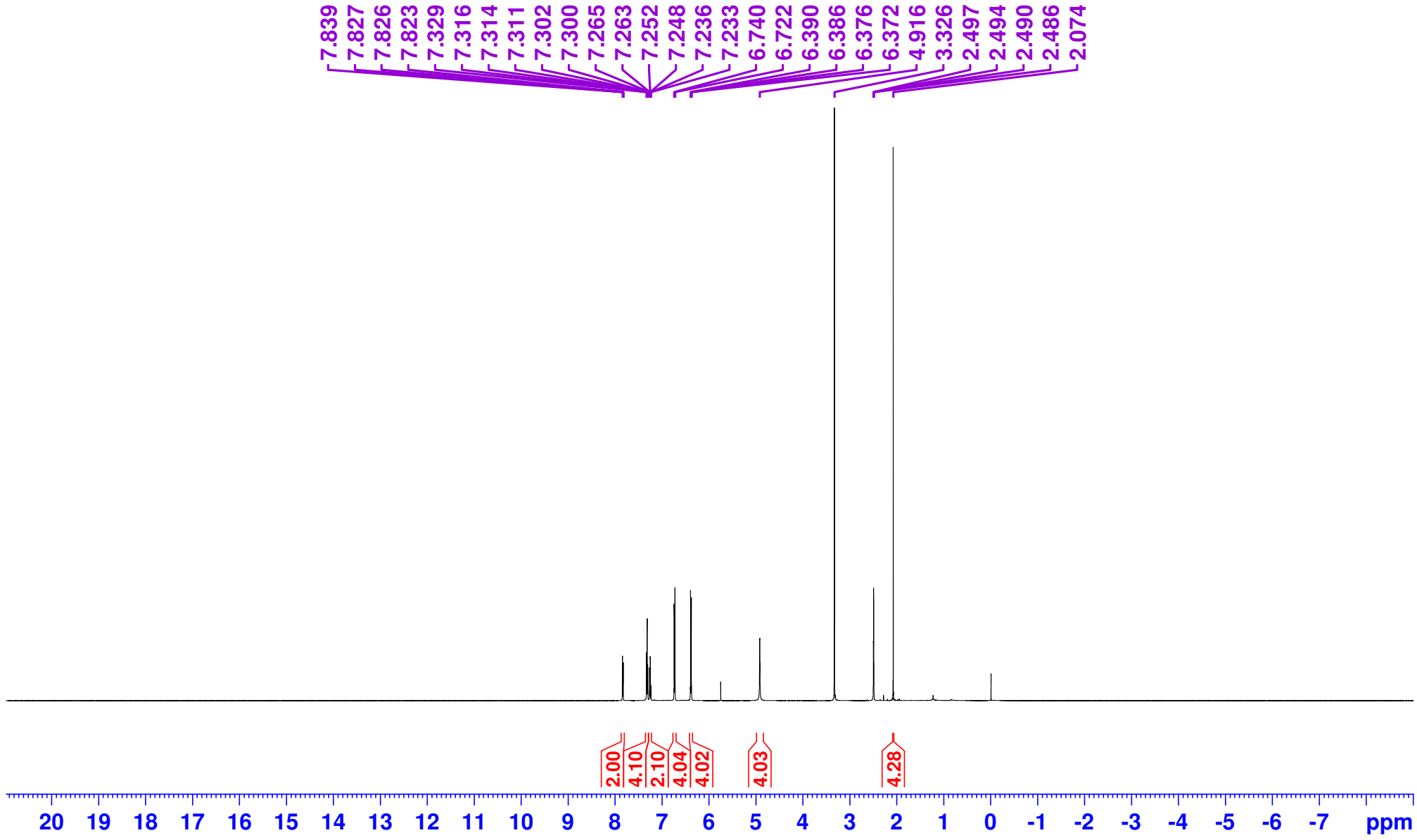
Compound 1 (1H NMR, 500 MHz, DMSO-d6)



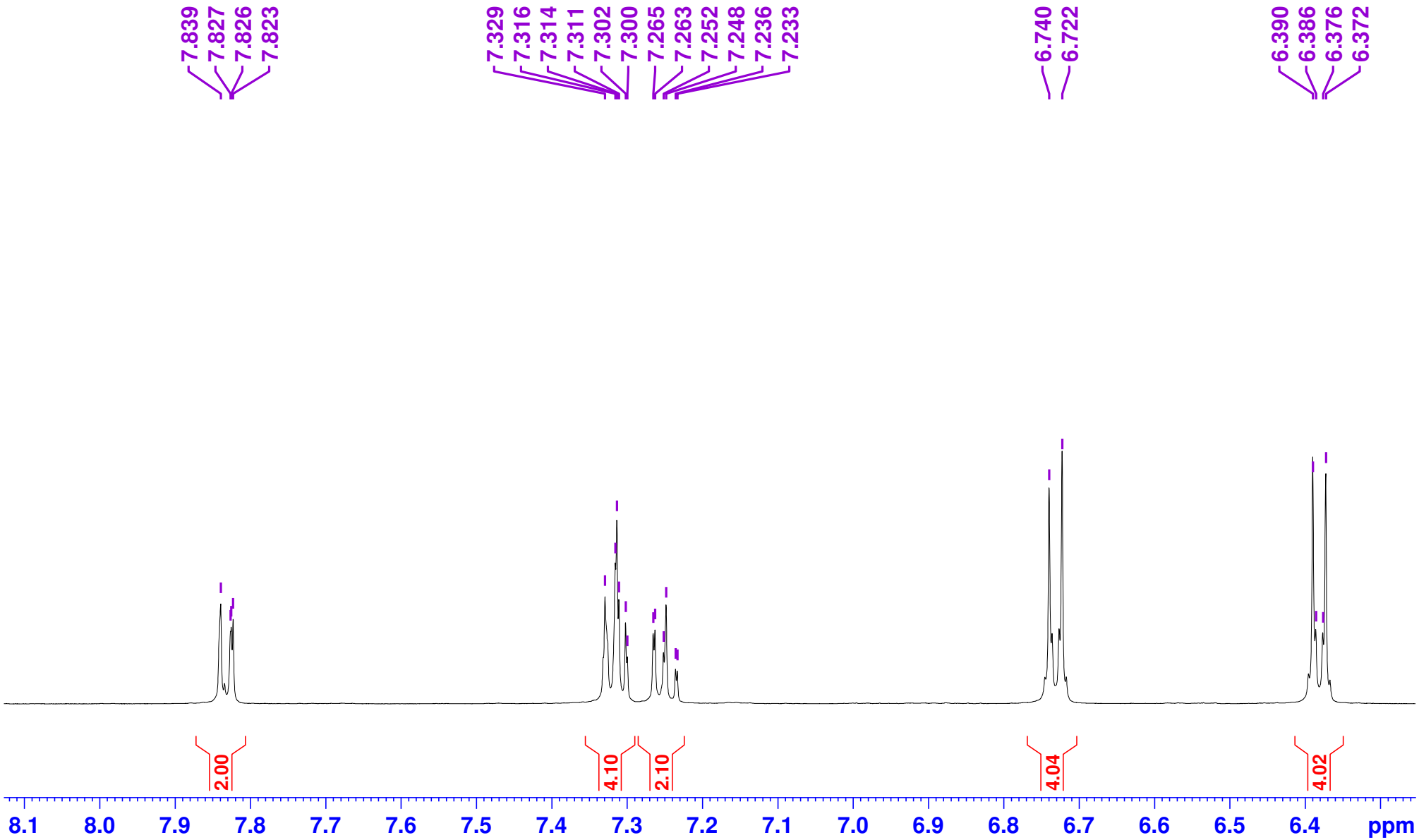
Compound 1

```
Current Data Parameters
NAME                  Shumaila Majeed
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_               20181120
Time                   11.56 h
INSTRUM                spect
PROBHD    Z119470_0109
PULPROG                  zg
TD                    65536
SOLVENT                DMSO
NS                       23
DS                        0
SWH               15000.000 Hz
FIDRES             0.457764 Hz
AQ                 2.1845334 sec
RG                     52.58
DW                    33.333 usec
DE                     6.50 usec
TE                    294.4 K
D1                3.00000000 sec
TD0                       1
SFO1           500.1830011 MHz
NUC1                     1H
P1                    11.60 usec
PLW1           14.00000000 W

F2 - Processing parameters
SI                     131072
SF             500.1800093 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```

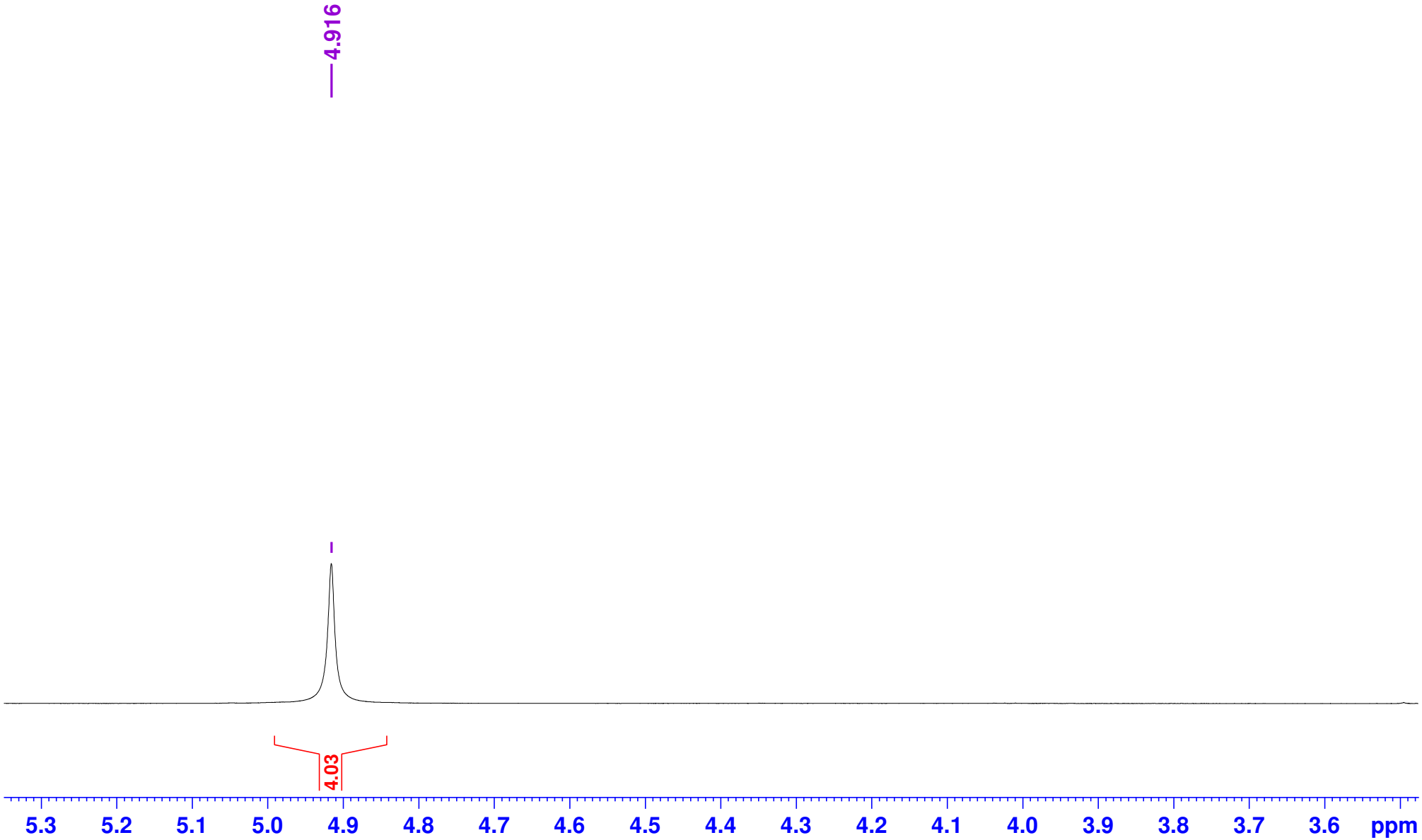
Compound 1 (1H NMR, 500 MHz, DMSO-d6)



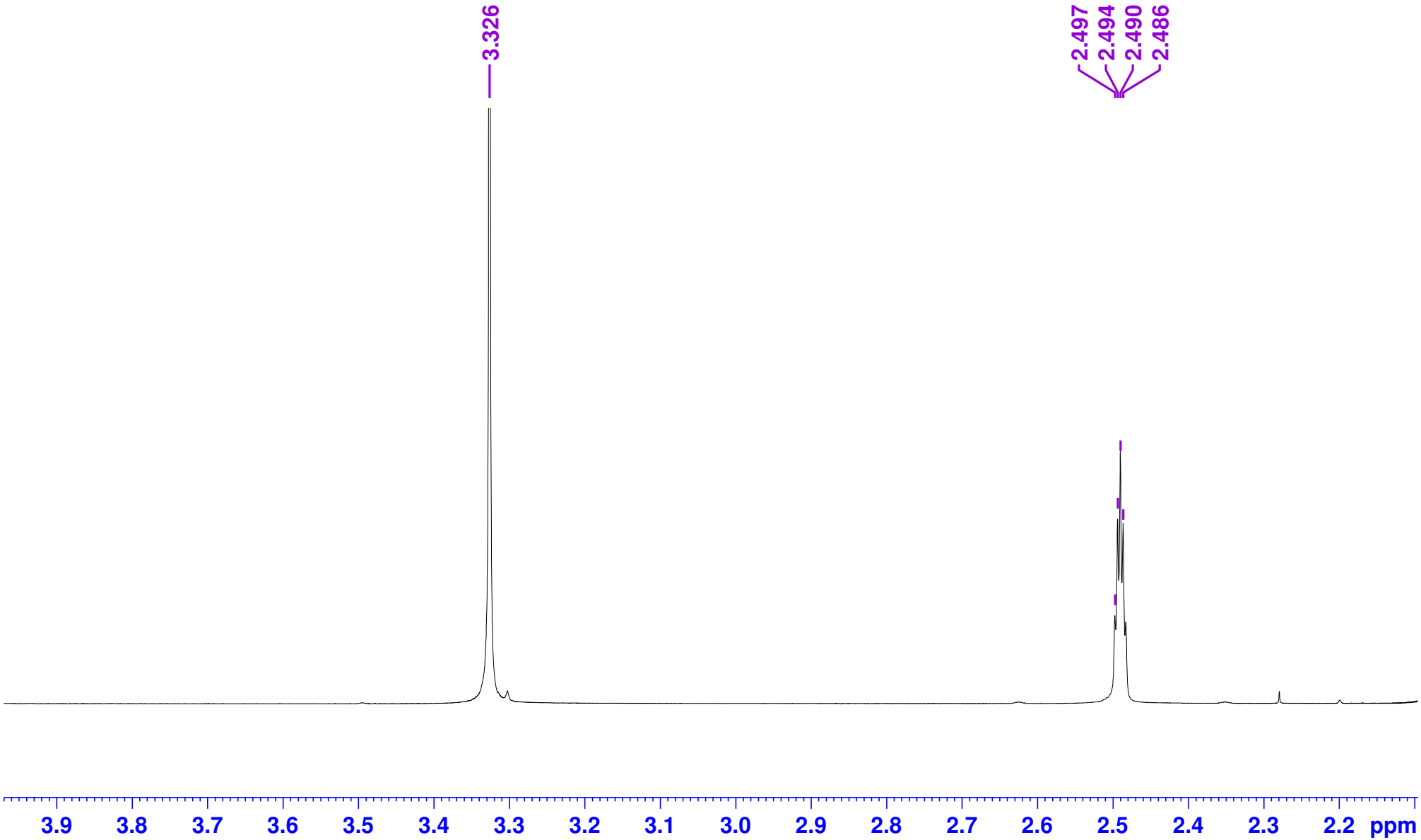
Compound 1 (1H NMR, 500 MHz, DMSO-d6)



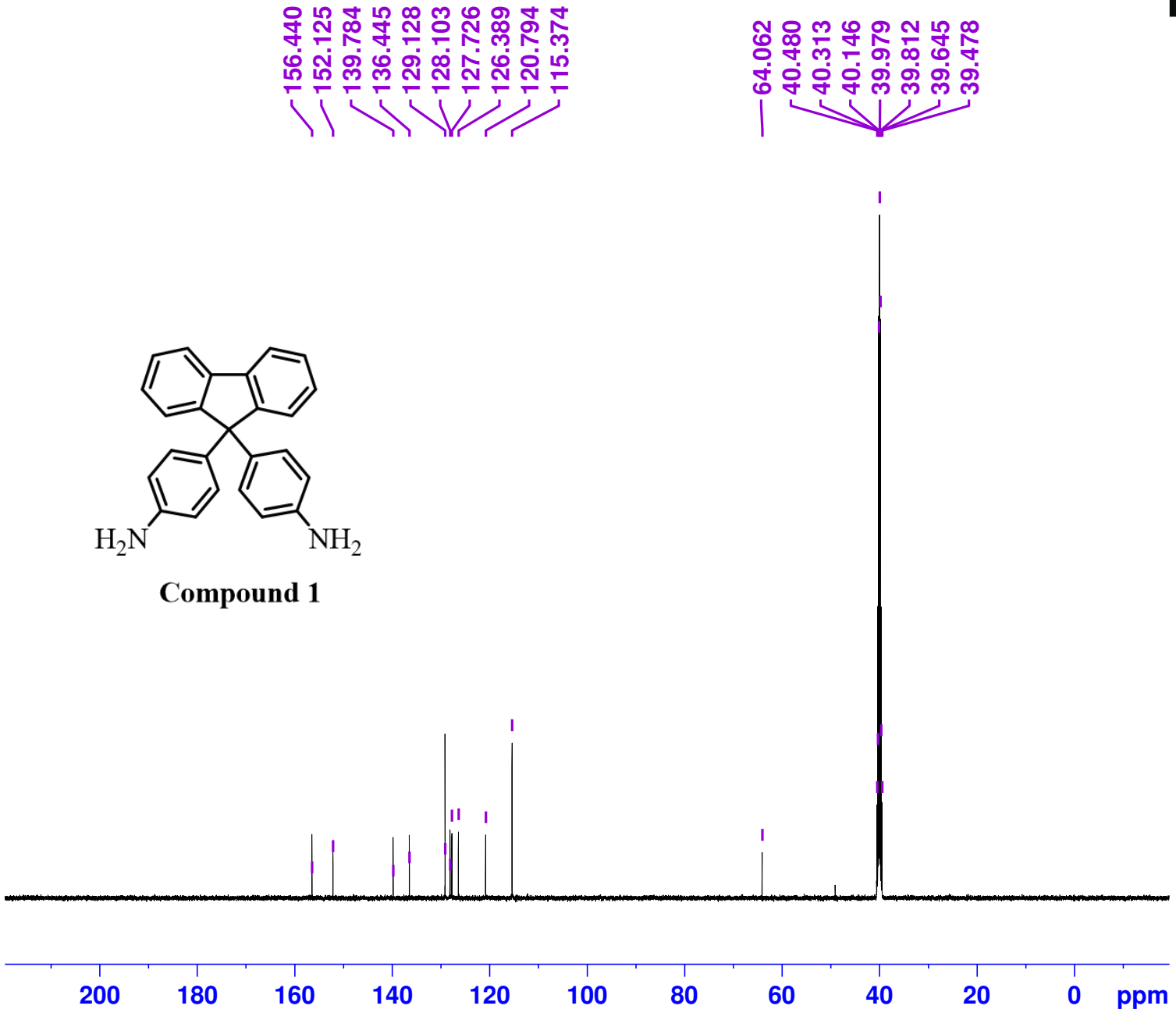
Compound 1 (1H NMR, 500 MHz, DMSO-d6)



Compound 1 (1H NMR, 500 MHz, DMSO-d6)

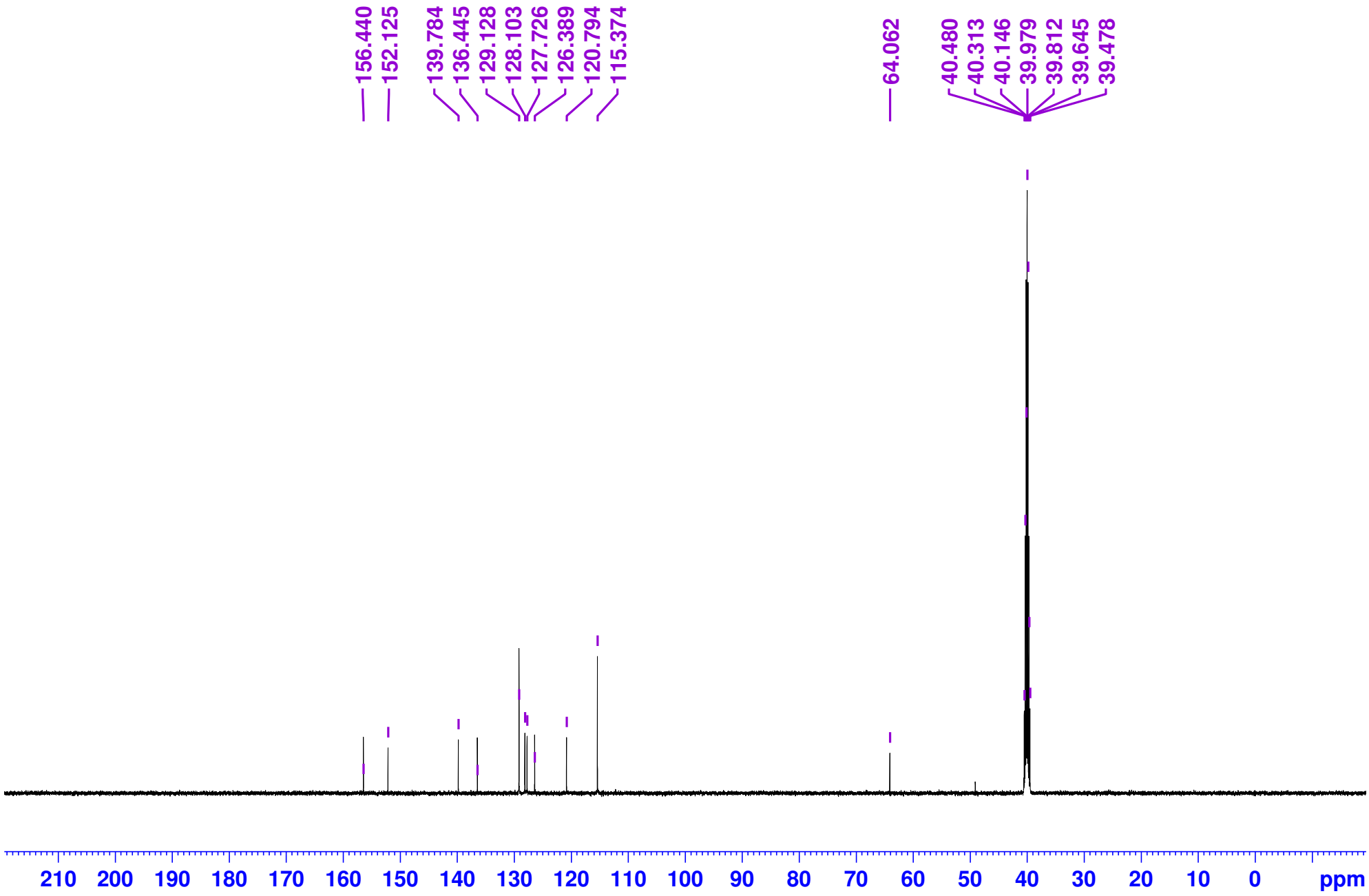


Compound 1 (13C NMR, 125 MHz, DMSO-d6)

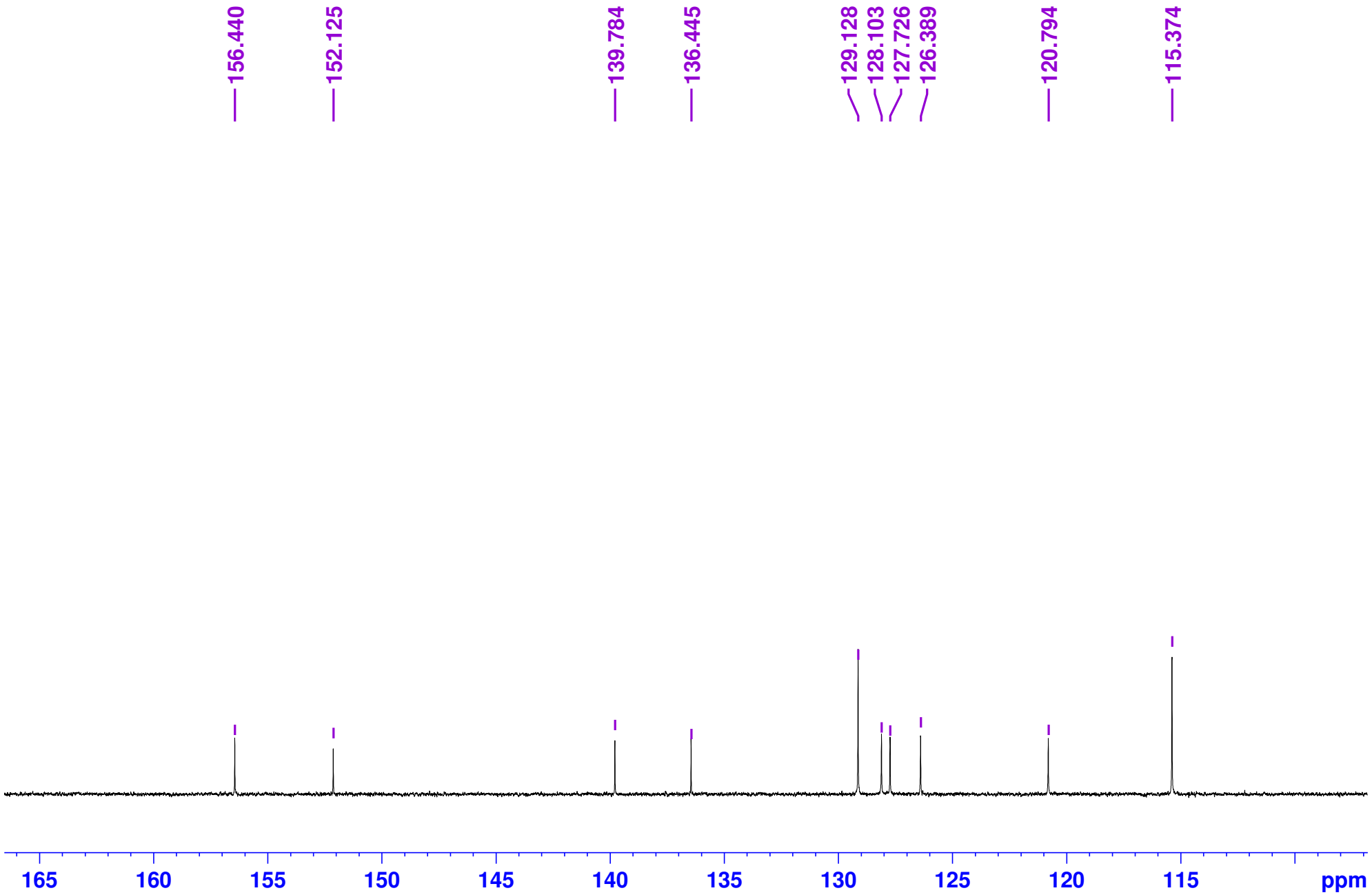



```
Current Data Parameters
NAME            Shumaila Maj
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_          20190122
Time               7.02 h
INSTRUM           spect
PROBHD   Z119470_0109
PULPROG          zgdc30
TD                65536
SOLVENT            DMSO
NS                   300
DS                     0
SWH            37878.789 Hz
FIDRES          1.155969 Hz
AQ             0.8650752 sec
RG                188.37
DW                13.200 usec
DE                 6.50 usec
TE                294.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7829380 MHz
NUC1                13C
P0                 3.10 usec
P1                 9.30 usec
PLW1         80.00000000 W
SFO2         500.1820007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         14.00000000 W
PLW12         0.29435000 W

F2 - Processing parameters
SI                131072
SF         125.7703616 MHz
WDW                 EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

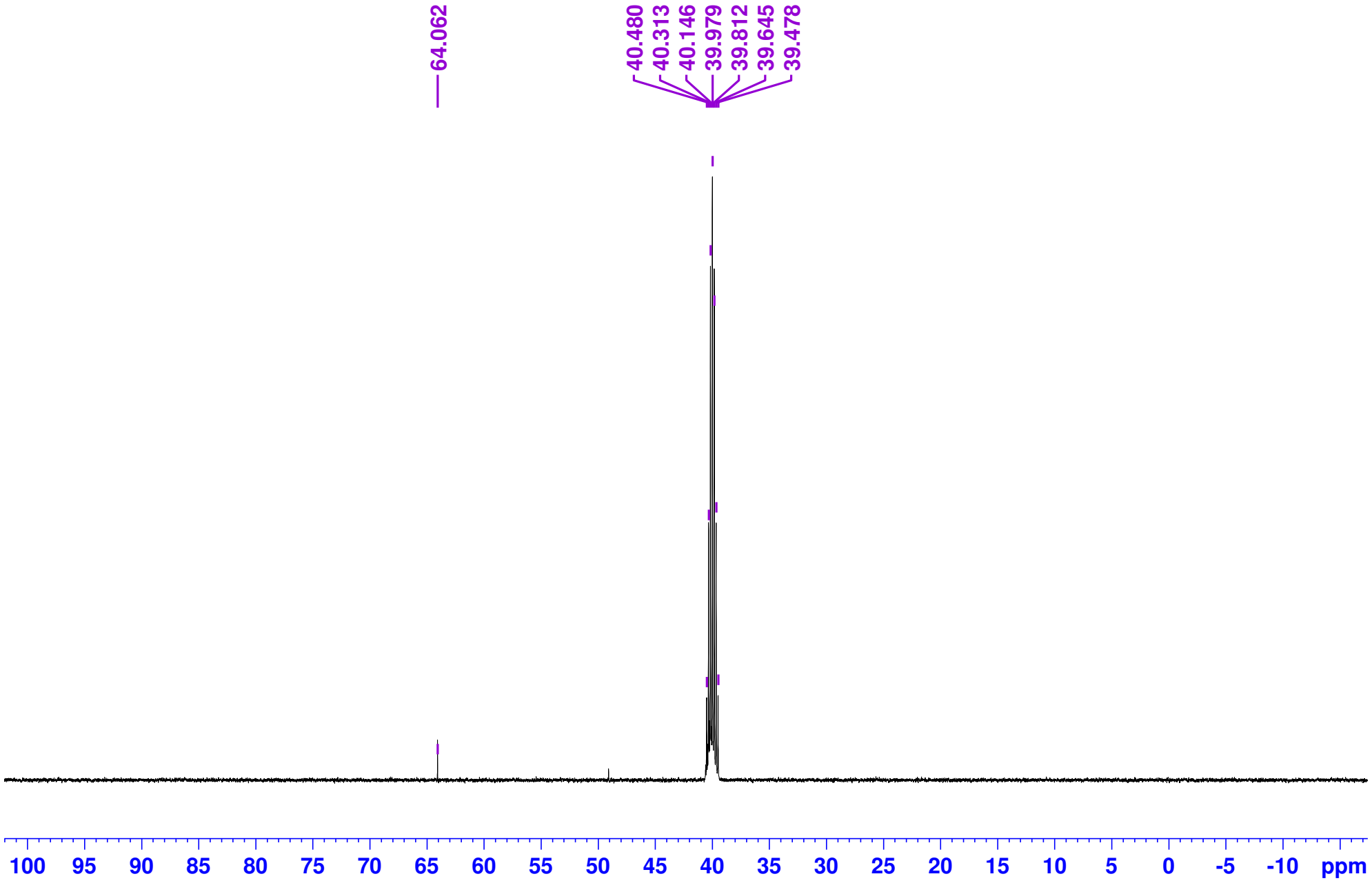
Compound 1 (13C NMR, 125 MHz, DMSO-d6)



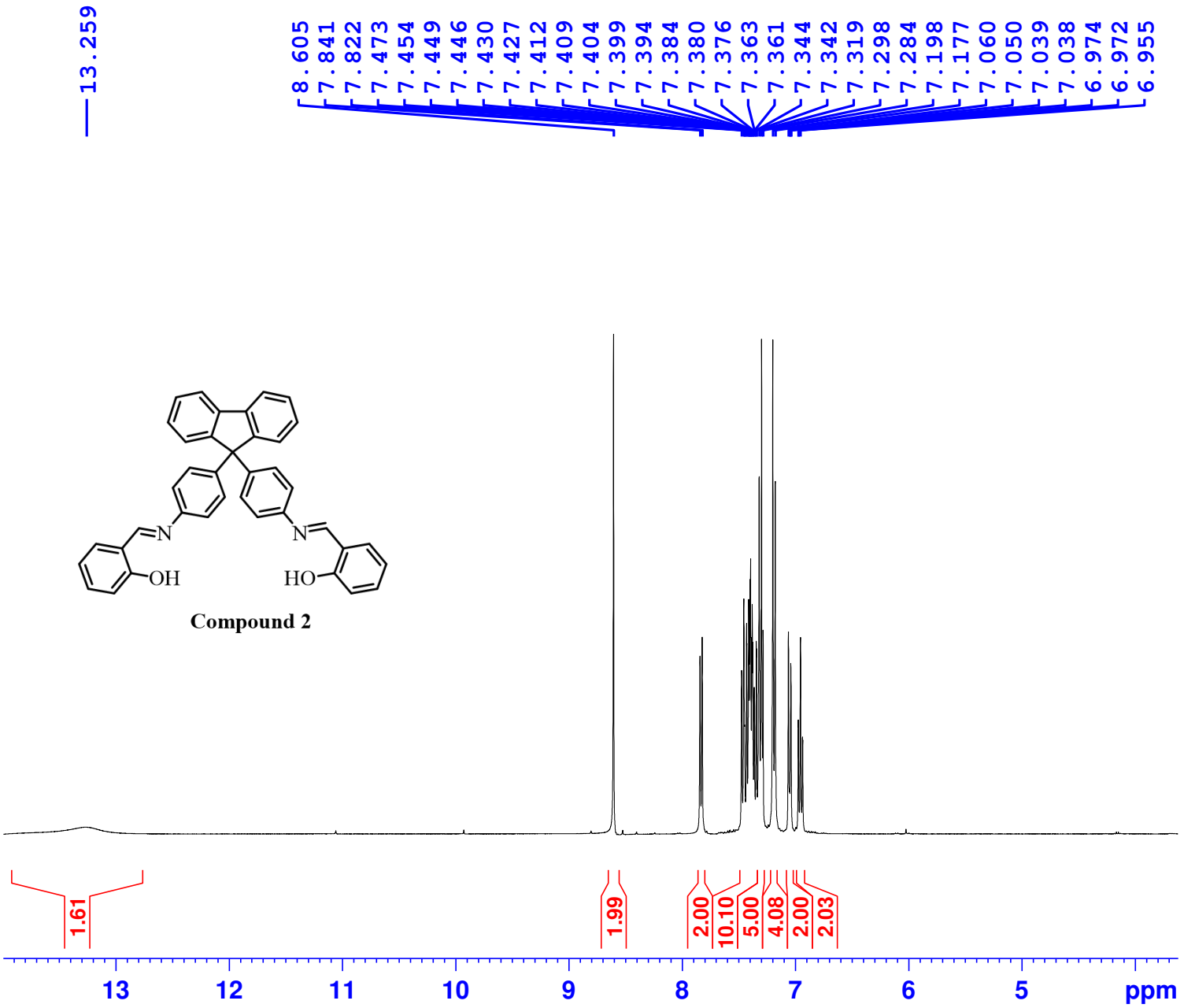
Compound 1 (13C NMR, 125 MHz, DMSO-d6)



Compound 1 (13C NMR, 125 MHz, DMSO-d6)



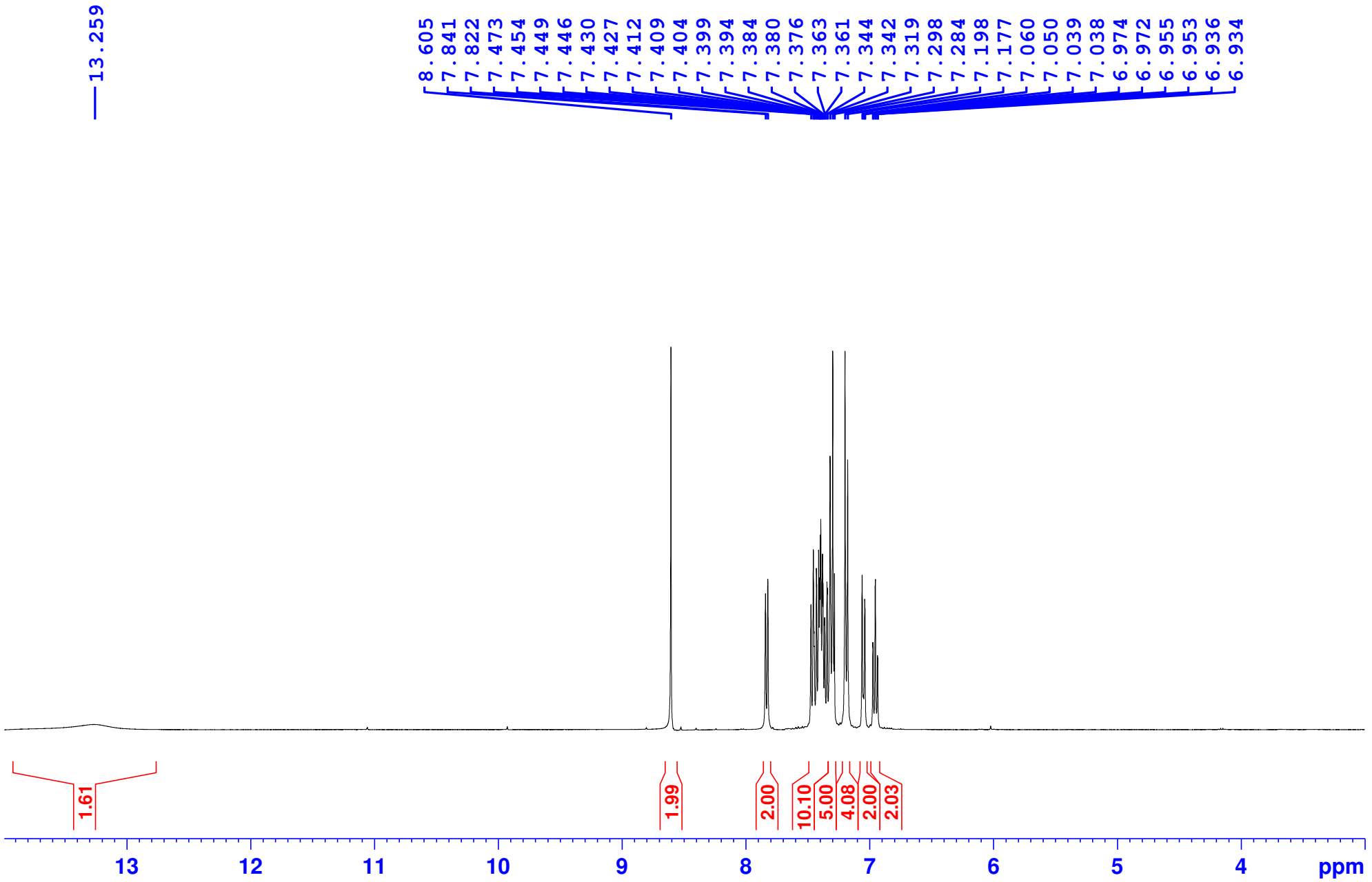
Compound 2 (1H NMR, 400 MHz, CDCl3)



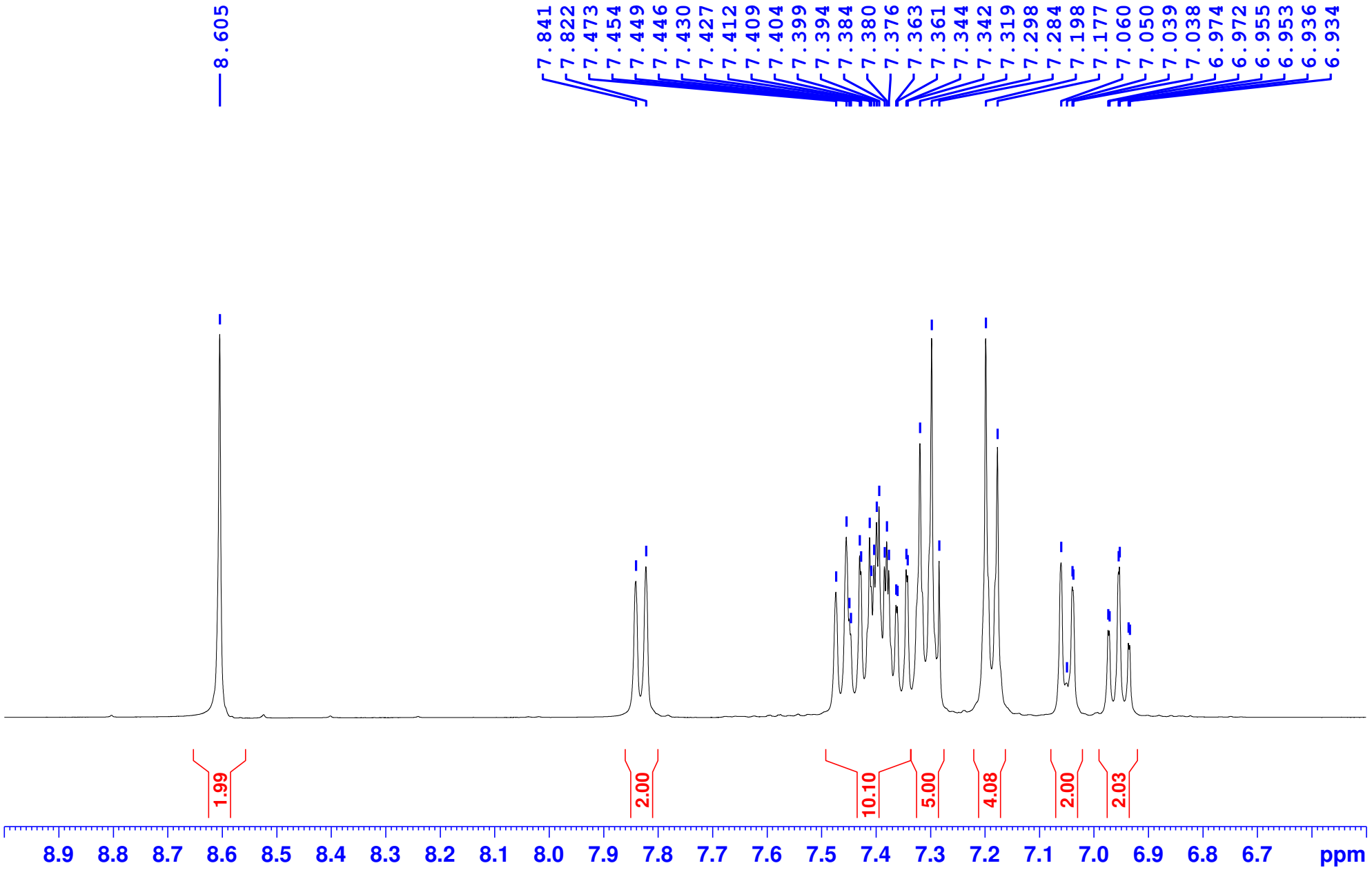
Compound 2

```
Current Data Parameters
NAME          Shumaila Majeed
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_           20190718
Time              16.33 h
INSTRUM           spect
PROBHD   Z116098_0621
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            5597.015 Hz
FIDRES         0.170807 Hz
AQ             5.8545494 sec
RG                78.01
DW               89.333 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1
SFO1         400.1328009 MHz
NUC1                 1H
P1                10.00 usec
PLW1         16.68099976 W

F2 - Processing parameters
SI               65536
SF         400.1300000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

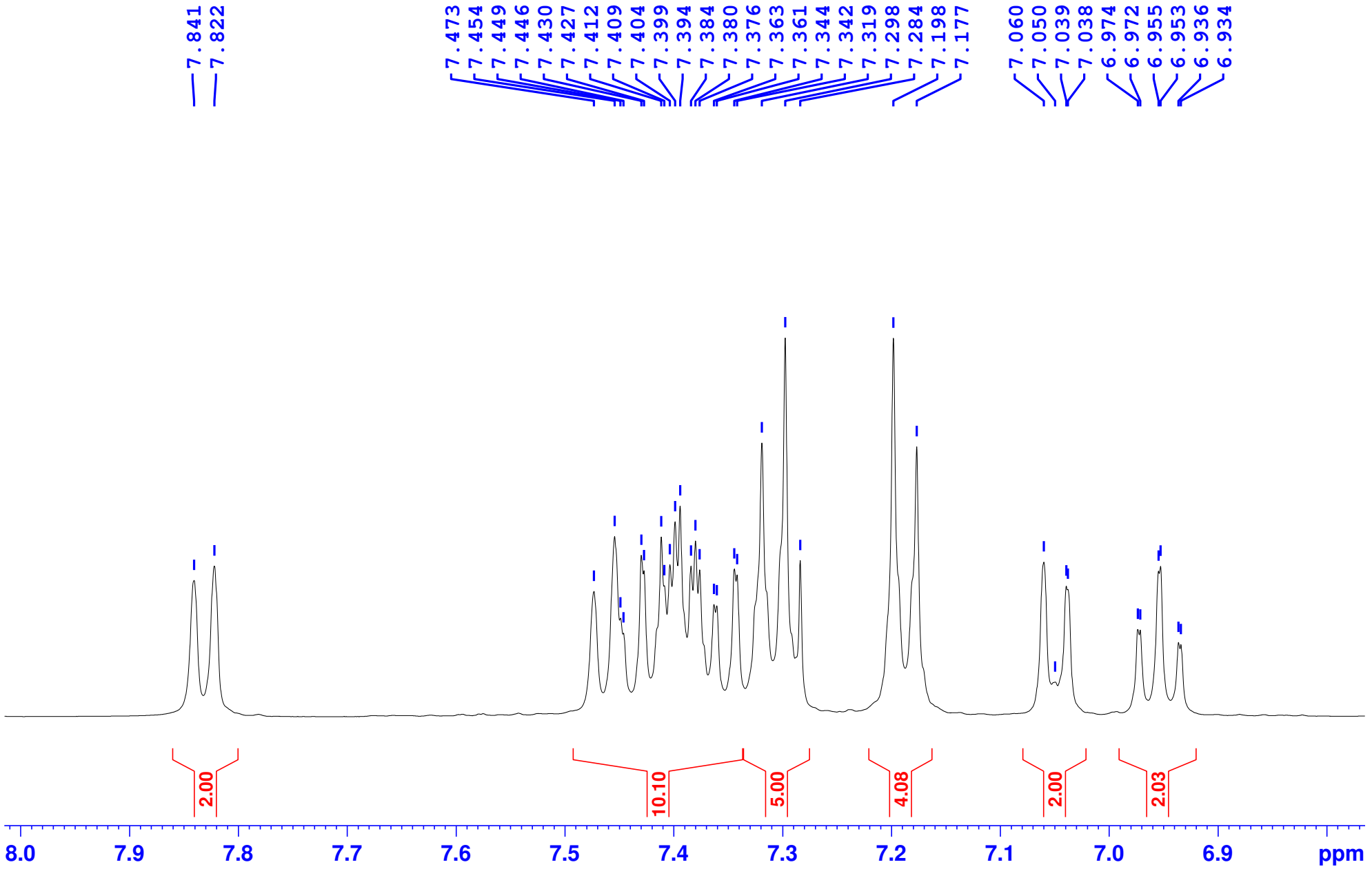
Compound 2 (1H NMR, 400 MHz, CDCl3)



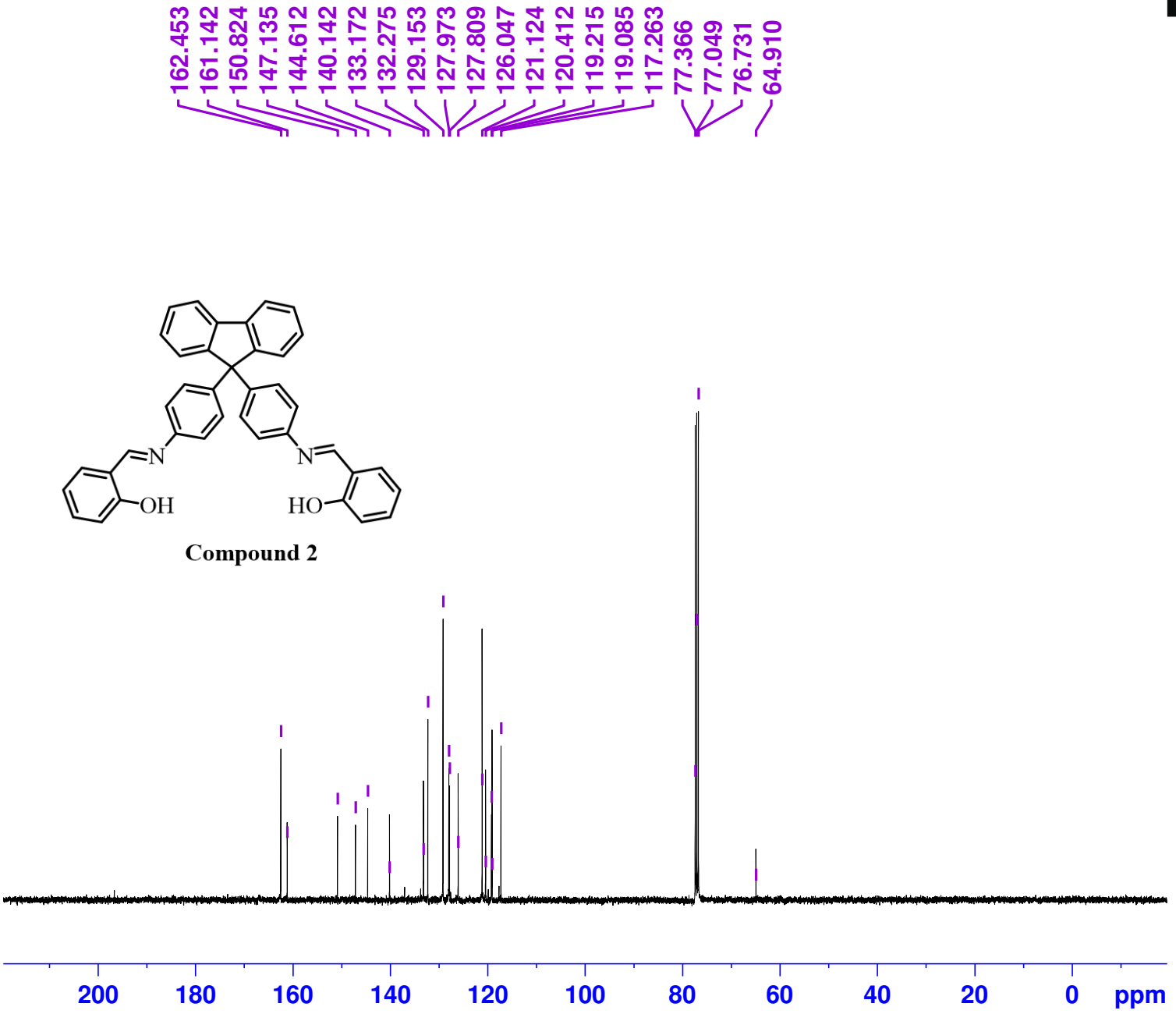
Compound 2 (1H NMR, 400 MHz, CDCl3)



Compound 2 (1H NMR, 400 MHz, CDCl3)



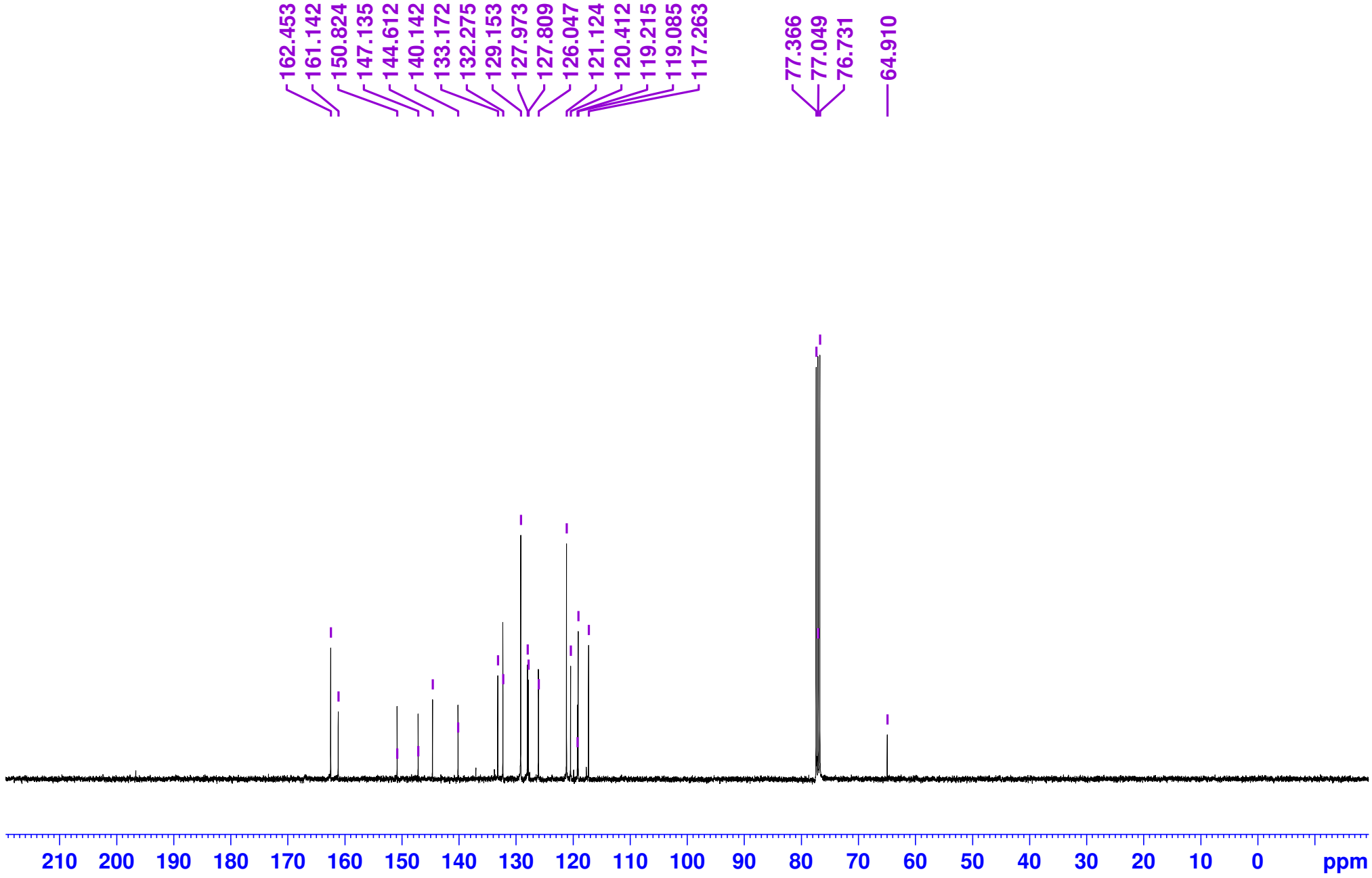
Compound 2 (13C NMR, 400 MHz, CDCl3)



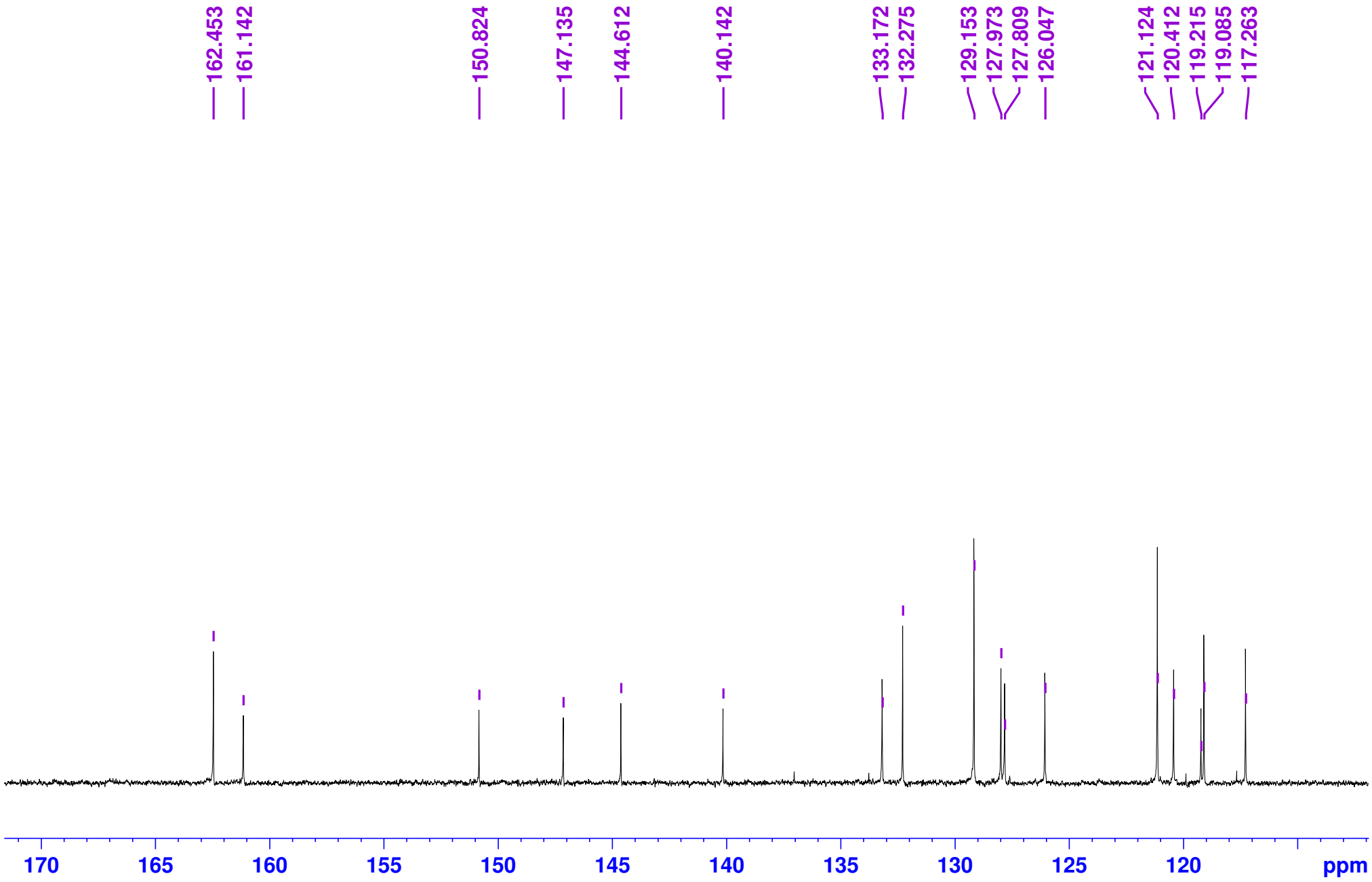
Compound 2

```
Current Data Parameters
NAME          Shumaila Majeed
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_           20190719
Time              15.53 h
INSTRUM             spect
PROBHD    Z116098_0621
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                199.48
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        72.56700134 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        16.68099976 W
PLW12        0.20593999 W
PLW13        0.10342000 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

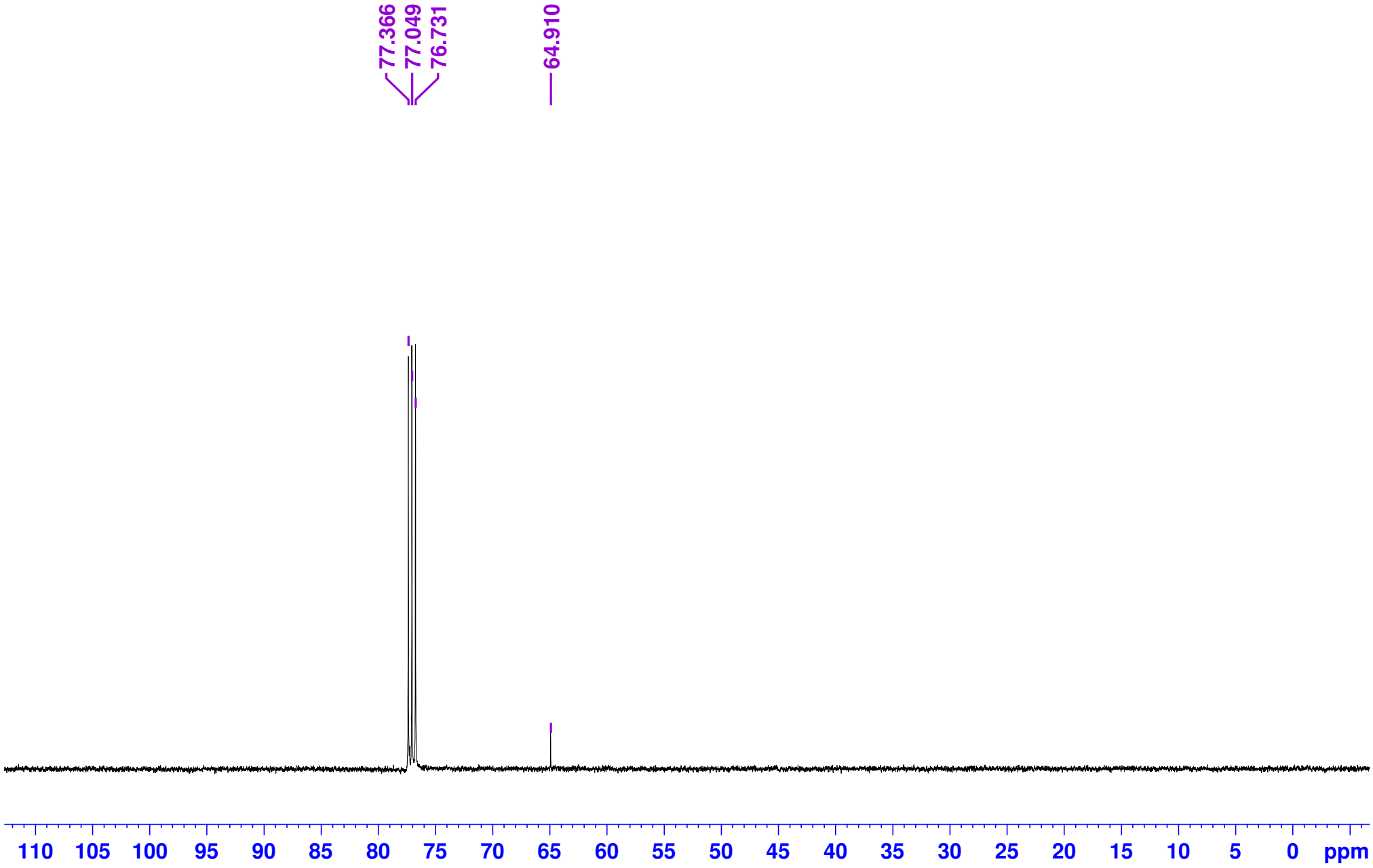
Compound 2 (13C NMR, 400 MHz, CDCl3)



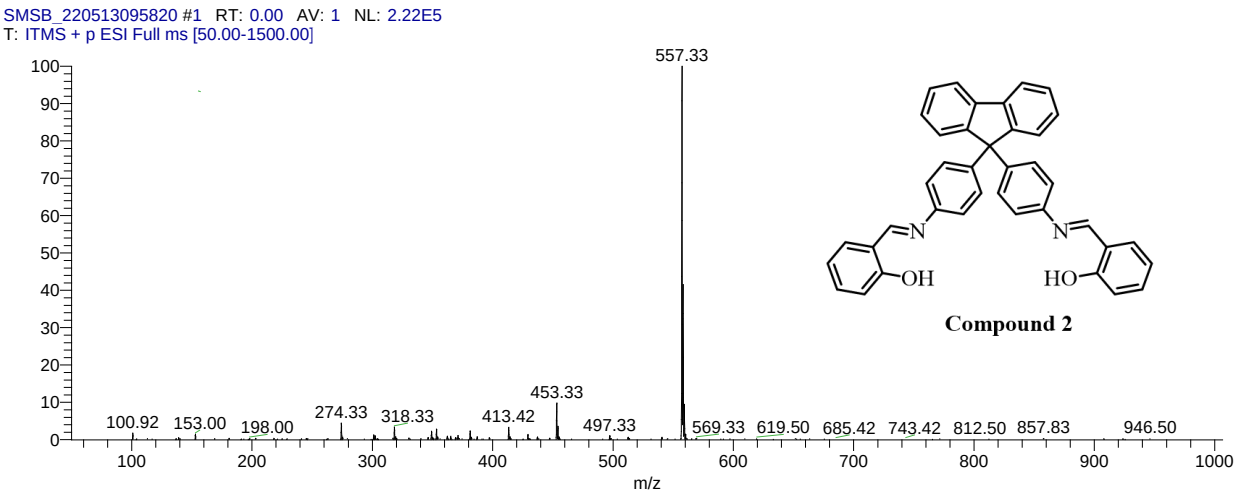
Compound 2 (13C NMR, 400 MHz, CDCl3)



Compound 2 (13C NMR, 400 MHz, CDCl3)



Compound 2 (Mass spectrum)



Compound 2