Supporting Information for

Rationalizing Hydrogen Bond Solvation with Kamlet-Taft LSER and Molecular Torsion Balances

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General Experimental

All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware with magnetic stirring unless otherwise indicated. Reagents were purchased from commercial sources and used without further purification. Solvents for chemical reactions were dried. Purification of the reaction products was carried out by flash chromatography using silica gel 40-63 μm (230-400 mesh) unless otherwise stated. Reactions were monitored by ^{1}H NMR and/or thin-layer chromatography. Visualization was accomplished with UV light, staining with 5% KMnO4 followed by heating or with p-anisaldehyde in EtOH solution. NMR was recorded using a 400 MHz Bruker spectrometer. Data are reported as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet; integration; coupling constant(s) in Hz). Melting points were measured with a Gallenkamp melting point apparatus.

Measurement of interaction energies (ΔG) and error analysis

The folded/unfolded ratios were measured by proton NMR spectra at room temperature (~ 25°C). The peak areas corresponding to the ortho methyl proton in the folded and unfolded states were integrated. The folding energies were estimated from the equation: $\Delta G = -RT\ln K = -RT\ln[\text{folded}]/[\text{unfolded}]$.

The error in the folding energies was estimated to be 0.03 kcal/mol based on a conservative estimate of the NMR measured folded/unfolded ratio of ±5%. Multiple linear regression was performed with Excel, and the result (with errors included) are as follows:[1]

$\delta(\ln K) = \delta K/K = 0.05$

$\delta(\Delta G) = RT[\delta(\ln K)] = 0.03$ kcal/mol

Synthesis of Balance 1

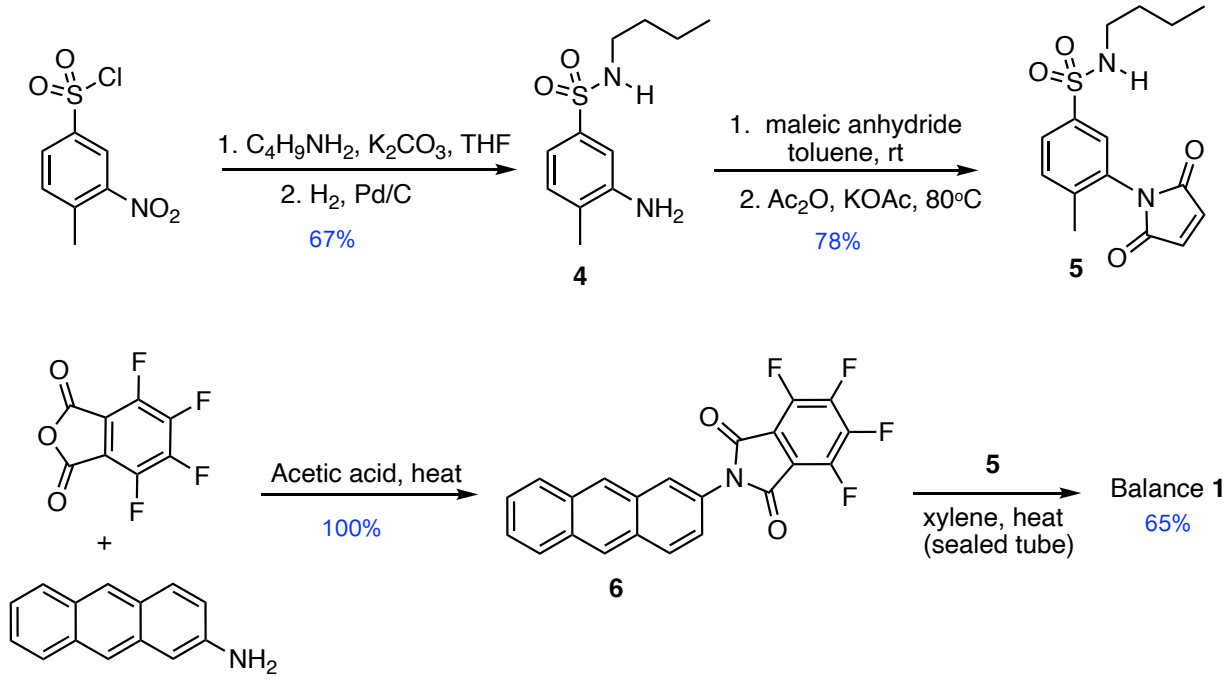


Figure S1. Synthetic scheme

Preparation and characterization of 3-amino-N-butyl-4-methylbenzenesulfonamide (4)

In a 100 ml round-bottom flask, 4-methyl-3-nitrobenzenesulfonyl chloride (1.5 g, 6.38 mmol) was dissolved in 20 ml of 50% (v/v) aqueous THF. To the mixture, K_2CO_3 (1.32g, 9.57 mmol) and butylamine (0.7g, 9.57 mmol) were added sequentially at room temperature. The reaction flask was then heated to reflux for 2 hours, and the reaction progress was monitored by TLC. After completion, the reaction was cooled to room temperature and the volume was reduced to half by removing solvent under reduced pressure. Next, 20 ml of water was added, and the mixture was extracted three times using 20 mL portions of ethyl acetate. The combined organic layers were washed with brine and water, dried over anhydrous $MgSO_4$, and concentrated to yield the crude intermediate. The crude intermediate (dissolved in 15 mL ethyl acetate) was then added to 150 mg of 10% Pd/C and the reaction was stirred overnight under normal atmospheric pressure of hydrogen gas. The reaction mixture was filtered, and the concentrated product was purified by flash column chromatography using mixtures of ethyl acetate and hexane to yield 1.04 g of 3-amino-*N*-butyl-4-methylbenzenesulfonamide (**4**).

Proton NMR:
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (t, *J* = 8.4 Hz, 3H), 4.96 (t, *J* = 6.1 Hz, 1H), 3.97 (s, 2H), 2.88 (q, *J* = 6.8 Hz, 2H), 2.18 (d, *J* = 3.4 Hz, 3H), 1.42 (m, 2H), 1.26 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H)
Carbon NMR:
^{13}C{1H} NMR (101 MHz, $CDCl_3$) δ 145.5, 137.9, 130.8, 127.1, 116.6, 112.6, 42.9, 31.5, 19.7, 17.5, 13.6
Mass spec: ESI(MS) for $C_{11}H_{18}N_2O_2S$ $(M+Na)^+$; calcd 265.0987, found 265.0980

Preparation and characterization of N-butyl-3-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)-4-methylbenzenesulfonamide (5)

A mixture of 3-amino-*N*-butyl-4-methylbenzenesulfonamide (1.2 g, 4.95 mmol) and maleic anhydride (0.5 g, 5.1 mmol) was prepared in 10 ml of toluene and was stirred overnight at room temperature. The toluene was removed by decantation, and acetic anhydride (20 ml) and potassium acetate (0.15 g) were added to the mixture. The reaction was heated for 30 mins, and progress was monitored by TLC. The acetic anhydride was removed under reduced pressure, and 20 ml of water was carefully added. The aqueous mixture was extracted three times using 15 ml portions of diethyl ether, and the combined extracts were washed with brine and water before being dried with anhydrous $MgSO_4$. The product was purified by column chromatography to yield 1.24 g (78%) of N-butyl-3-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)-4-methylbenzenesulfonamide (**5**).

Proton NMR:
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (q, *J* = 3.3, 1H), 7.66 (d, *J* = 1.9 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 6.92 (s, 2H), 4.79 (t, *J* = 6.1 Hz, 1H), 2.97 (q, *J* = 6.8 Hz, 2H), 2.25 (s, 3H), 1.46 (m, *J* = 4.9 Hz, 2H), 1.32 (m, *J* = 7.4 Hz, 2H), 0.87 (t, *J* = 7.3, 3H)
Carbon NMR:
^{13}C{1H} NMR (101 MHz, $CDCl_3$) δ 168.9, 142.0, 138.7, 134.6, 131.9, 130.8, 127.8, 127.6, 43.0, 31.6, 19.7, 18.3, 13.5
Mass spec: ESI(MS) for $C_{15}H_{18}N_2O_4S$ $(M+Na)^+$; calcd 345.0885, found 345.0880

Preparation and characterization of 2-(anthracen-2-yl)-4,5,6,7-tetrafluoroisoindoline-1,3-dione (6).

A mixture containing 2-aminoanthracene (0.386 g, 2mmol) and pentafluorophthalic anhydride (0.44 g, 2mmol) in 15 ml acetic acid was then heated and refluxed overnight. The reaction was cooled, and water was added to it. The desired product was isolated by filtration. The filtrate was washed several times, first with water, then with a small amount of cold acetone, and finally with hexane. The resulting dried product was found to be pure and was used without further purification. The yield of the product (**6**) was 0.78 g.

Proton NMR:

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.43 (m, 3H), 8.04 (m, 3H), 8.40 (m, 3H)

Carbon NMR:

^{13}C{1H} NMR (101 MHz, DMSO-d_6) δ 169.9, 136.4, 132.1, 131.9, 130.9, 129.3, 128.3, 128.9, 128.9, 128.5, 128.1, 126.3, 126.2, 125.5, 125.4, 121.4, 114.4

Mass spec: CI(MS) for $C_{22}H_9NO_2F_4$ $(M)^+$; calcd 395.0569, found 395.0574

Diels-Alder: Preparation and characterization of Balance 1

A mixture of **5** (0.2 g, 0.85 mmol) and **6** (0.28 g, 0.71 mmol) in 1 ml xylene was heated in a sealed reaction tube for two days. The cooled reaction was then purified by column chromatography to yield 0.33g of balance **1**.

Proton NMR:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (q, *J* = 3.3 Hz, 1H), 7.53 (d, *J* = 1.9 Hz), 7.49 (m, *J* = 2.7 Hz, 3H), 7.39 (q, *J* = 3.3 Hz, 1H), 7.33 (d, 2H), 6.14 (d, *J* = 1.8 Hz, 1H), 5.27 (q, *J* = 4.0 Hz, 1H), 4.99 (d, *J* = 1.7 Hz, 2H), 3.50 (t, *J* = 1.5 Hz, 2H), 2.98 (m, *J* = 6.6 Hz, 1H), 2.79 (m, *J* = 6.1 Hz, 1H), 1.49 (m, *J* = 6.3 Hz, 2H), 1.37 (q, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H)

Carbon NMR:

^{13}C{1H} NMR (101 MHz, $CDCl_3$) δ 175.4, 174.9, 162.3, 142.5, 140.7, 140.3, 140.2, 139.6, 139.3, 138.7, 131.6, 130.9, 129.3, 128.4, 127.7, 127.4, 127.3, 126.3, 126.2, 125.6, 124.6, 122.8, 113.4, 47.1, 47.1, 46.0, 45.6, 45.3, 45.1, 43.0, 31.6, 31.3, 19.7, 18.0, 17.0, 13.6, 13.5

Mass spec: ESI(MS) for $C_{37}H_{27}N_3O_6SF_4$ $(M+Na)^+$; calcd 740.1449, found 740.1450

Melting point: 239 – 241°C

Preparation and characterization of Balance 2

A mixture of anthracene (0.18g, 1 mmol) and **5** (0.282 g, 1.2 mmol) in 1 ml xylene was heated in a sealed reaction tube overnight. The cooled reaction was then purified by column chromatography to yield 0.395g (96%) of balance **2**.

Proton NMR:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (m, *J* = 2.5 Hz, 1H), 7.33 (m, 9H), 5.94 (d, *J* = 1.8 Hz, 1H), 4.92 (s, 2H), 4.36 (dt, *J* = 5.8, 1H), 3.45 (q, *J* = 1.7, 2H), 2.91 (m, *J* = 6.7 Hz, 1.5H), 2.15 (s, 2H), 1.37 (m, 4H), 1.14 (s, 1.7H), 0.93 (t, *J* = 7.3 Hz, 1.5 H), 0.87 (t, *J* = 7.3 Hz, 1.5H)

Carbon NMR:

^{13}C{1H} NMR (101 MHz, $CDCl_3$) δ 175.6, 175.5, 141.7, 141.1, 141.0, 139.3, 138.6, 138.6, 138.3, 131.7, 131.5, 131.3, 127.6, 127.4, 127.1, 126.9, 126.9, 126.8, 125.5, 125.2, 124.3, 47.3, 45.9, 45.3, 43.0, 31.6, 31.5, 19.8, 19.7, 17.9, 16.7, 13.6, 13.6

Mass spec: ESI(MS) for $C_{29}H_{28}N_2O_4S$ $(M+Na)^+$; calcd 523.1, found 523.2

Melting point: 122 – 124 °C

Table 1. **Summary of solvent parameters**

	Kamlet-Taft parameters				solvent polarity			Hunter parameters	
solvents	α	β	π*	δ	$E_T(30)$	μ	ε	α_s	β_s
CCl_4	0	0.1	0.58	0.5	32.4	0	2.2	1.4	0.6
toluene	0	0.11	0.54	1	33.9	0.31	2.4	1	2.1
benzene	0	0.1	0.59	1	34.3	0	2.3	1.1	1.6
chloroform	0.2	0.1	0.58	0.5	39.1	1.15	4.8	2.2	1.3
CH_2Cl_2	0.13	0.1	0.82	0.5	40.7	1.14	8.9	1.7	1.1
acetic acid	1.12	0.45	0.64	0	55.2	1.78	6.2	3.7	4.9
acetone	0.08	0.43	0.71	0	42.2	2.69	21	1.2	5.7
acetonitrile	0.19	0.4	0.75	0	45.6	3.5	36.6	1.5	5.1
methanol	0.98	0.66	0.6	0	55.4	2.87	32.6	2.8	4.8
pyridine	0	0.64	0.87	1	40.5	2.37	12.3	1.2	7.2
ethanol	0.86	0.75	0.54	0	51.9	1.66	24.6	2.7	5.2
DMF	0	0.69	0.88	0	43.8	3.9	36.7	2.2	7.4
DMSO	0	0.76	1	0	45.1	4.1	47	0.8	8.9
t-butanol	0.42	0.93	0.41	0	43.7	1.31	10.9	2.7	5.7

Symbols and definition:

α = Kamlet-Taft parameter describing hydrogen bond donor ability

β = Kamlet-Taft parameter describing hydrogen bond acceptor ability
π* = Kamlet-Taft parameter describing dipolarity-polarizability
δ = correction factor: 0.5 for chlorinated solvent, 1.0 for aromatic solvents
$E_T(30)$ = Reichardt's solvent-polarity parameter
μ = solvent dipole moment in Debye
ε = relative permittivity (dielectric constant)
α_s = Hunter solvent hydrogen-bond donor parameter
β_s = Hunter hydrogen-bond acceptor parameter

Table 2. **Summary of experimental measurements and predicted values**

	% folded		equilibrium constants		folding energy (kcal/mol)		H-bond energy (kcal/mol)		
solvents	**1**	**2**	K_{eq}(**1**)	K_{eq}(**2**)	ΔG(**1**)	ΔG(**2**)	expt.	(Kamlet-Taft)	(Hunter)
CCl_4	82	46	4.56	0.85	-0.90	0.09	-0.99	-0.87	-1.02
toluene	84	52	5.25	1.08	-0.98	-0.05	-0.93	-1.02	-0.85
benzene	85	53	5.67	1.13	-1.03	-0.07	-0.96	-1.01	-0.96
chloroform	83	50	4.88	1.00	-0.94	0.00	-0.94	-0.90	-0.84
CH_2Cl_2	82	53	4.56	1.13	-0.90	-0.07	-0.83	-0.71	-0.92
acetic acid	50	49	1.00	0.96	0.00	0.02	-0.02	-0.11	0.17
acetone	34	40	0.52	0.67	0.39	0.24	0.15	0.05	0.29
acetonitrile	39	42	0.64	0.72	0.26	0.19	0.07	0.00	0.16
methanol	39	51	0.64	1.04	0.26	-0.02	0.29	0.32	0.13
pyridine	31	44	0.45	0.79	0.47	0.14	0.33	0.34	0.30
ethanol	35	51	0.54	1.04	0.37	-0.02	0.39	0.48	0.22
DMF	19	42	0.23	0.72	0.86	0.19	0.67	0.73	0.69
DMSO	9	35	0.10	0.54	1.37	0.37	1.00	0.97	0.99
t-butanol	64	39	1.78	0.64	-0.34	0.26	-0.61	0.85	0.37

Plots of experimental H-bond ($\Delta G_{H\text{-}bond}$ in kcal/mol) with solvent polarity parameters

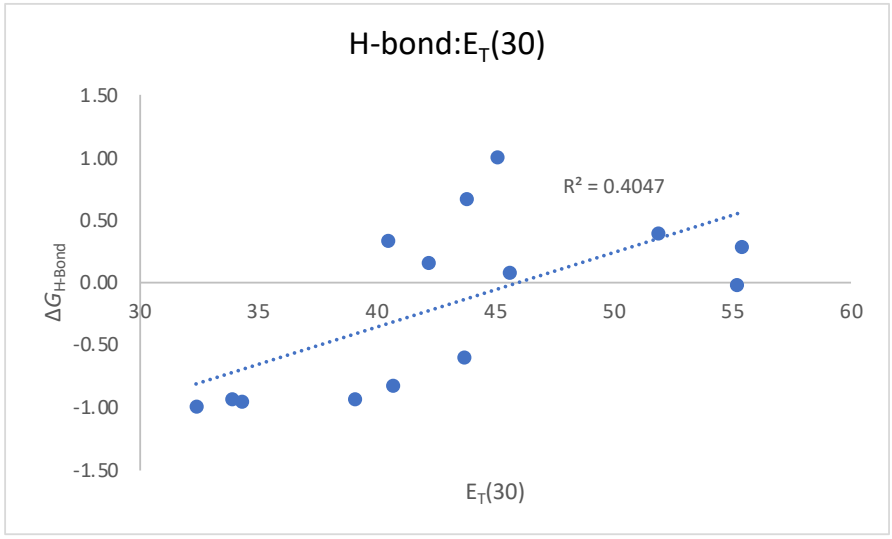


Figure S2 A plot of ΔGH-bond in kcal/mol against ET(30) solvent polarity parameter

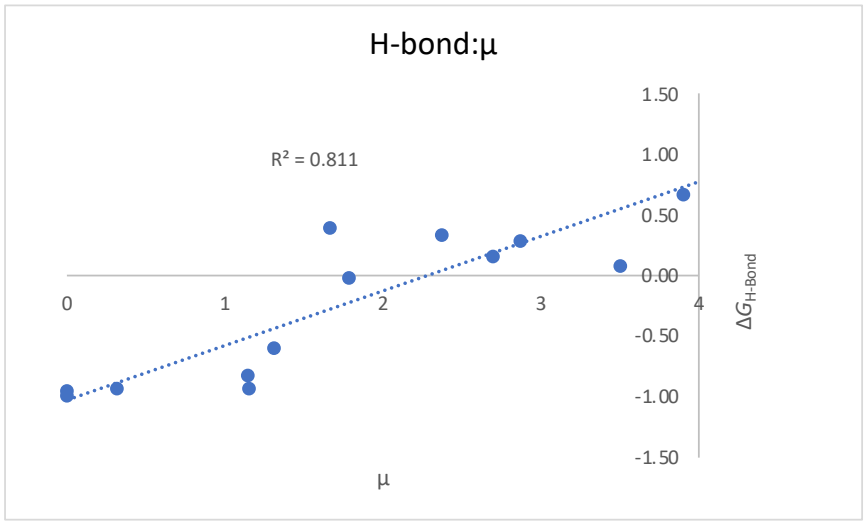


Figure S3 A plot of $\Delta G_{H\text{-}bond}$ in kcal/mol against solvents' dipole moment (in Debye)

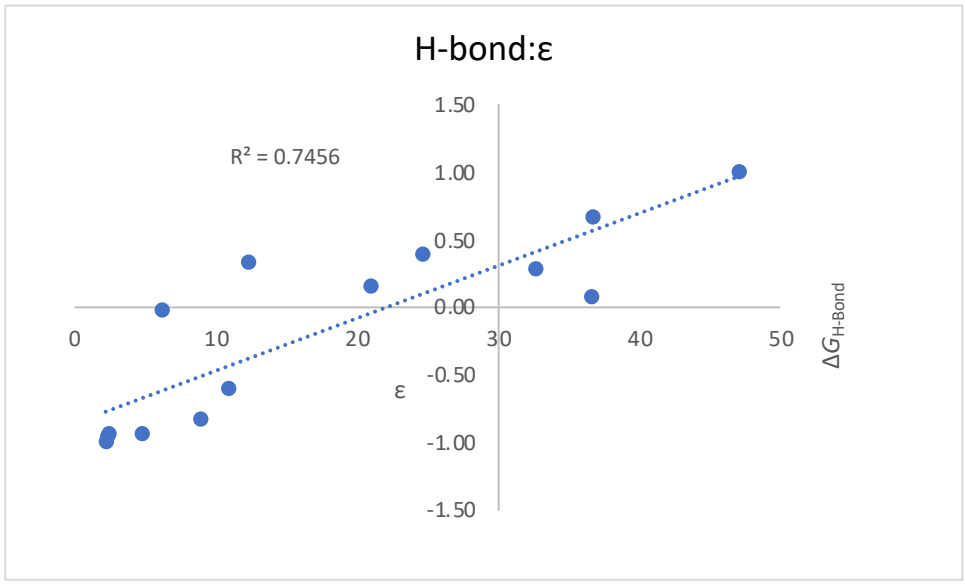


Figure S4 A plot of $\Delta G_{H\text{-}bond}$ (in kcal/mol) against solvents' dielectric constant solvent

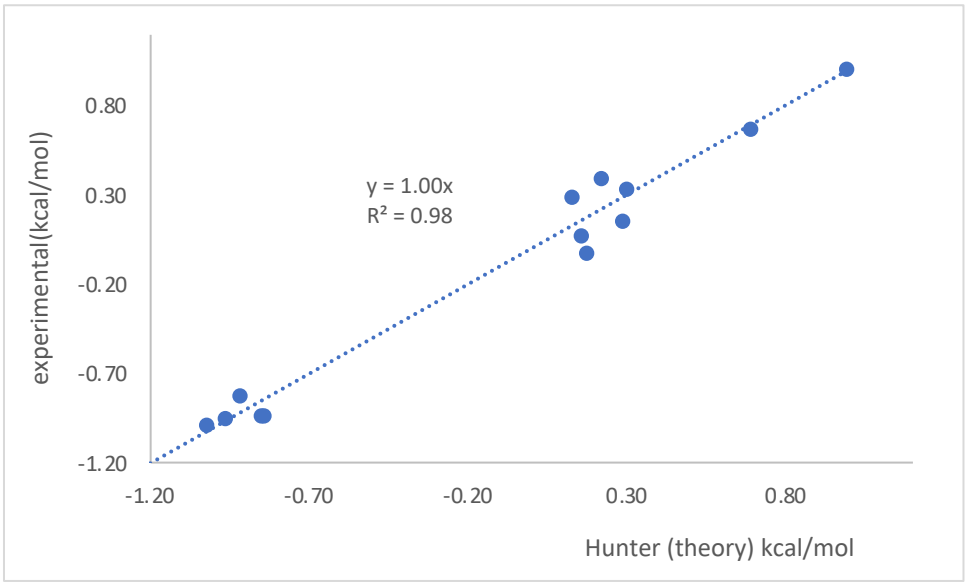


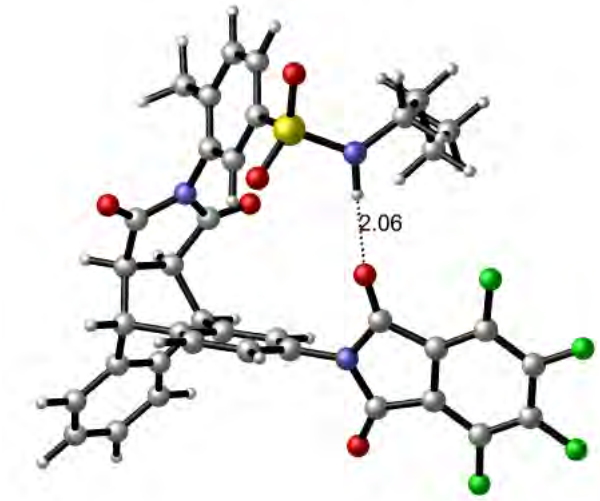
Figure S5. Correlating the experimental $\Delta G_{H\text{-}bond}$ (in kcal/mol) with Hunter solvation parameters (including π* dipolarity-polarization term)

$$\Delta G_{H\text{-}Bond} = -1.0 + 0.03\alpha_s + 0.28\beta_s - 0.06\pi^* - 0.32\delta$$

Summary of computational single-point calculations performed at the M06-2X/6-31+G* using conformers optimized at the B3LYP/6-31G+* level

		Total Energy		Relative Energies		Imaginary
Model System	Conformer	(a.u)	(kcal/mol)	(a.u)	(kcal/mol)	Frequency
1	folded	-2838.454735	-1781158.73	-0.005403	-3.39	0
1	unfolded	-2838.449332	-1781155.34	0	0.00	0
2	folded	-1929.919842	-1211044.00	-0.00071	-0.45	0
2	unfolded	-1929.919132	-1211043.55	0	0.00	0

The cartesian coordinates for the optimized conformer at the B3LYP/6-31+G* level: Balance 1 folded conformer

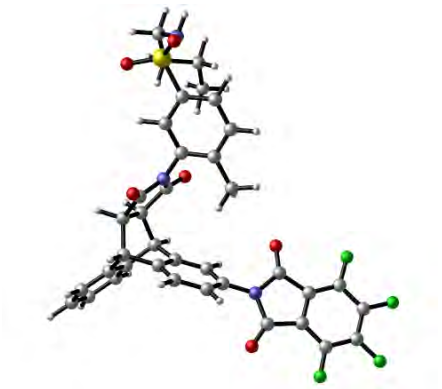


C-C_R	2.11643	-0.14443	4.79692
C-C_R	1.88722	1.19886	4.44644
C-C_3	1.3801	-1.13306	3.90498
H-H_	1.56594	-2.17578	4.17346
C-C_3	0.96519	1.35808	3.24639

C-C_R	1.75722	-0.82154	2.4669
C-C_R	2.36443	0.06371	-0.094
C-C_R	2.25629	-1.72246	1.52871
C-C_R	1.54546	0.52488	2.11649
C-C_R	1.84227	0.97218	0.83384
C-C_R	2.56997	-1.27558	0.24056
H-H_	2.40241	-2.76721	1.78983
H-H_	1.67839	2.00776	0.54928
H-H_	2.96407	-1.96493	-0.49971
C-C_3	-0.14356	-0.78554	4.07396
H-H_	-0.43237	-0.98649	5.11033
C-C_3	-0.39262	0.68309	3.66051
H-H_	-0.84283	1.27292	4.46565
C-C_R	-1.03791	-1.61507	3.1617
C-C_R	-1.39106	0.60824	2.50883
O-O_R	-1.15784	-2.82092	3.16388
O-O_R	-1.84013	1.54225	1.87548
N-N_R	-1.7186	-0.73833	2.29461
C-C_R	-2.58762	-1.19684	1.24597
C-C_R	-4.21132	-2.18153	-0.79068
C-C_R	-3.9781	-1.01191	1.34384
C-C_R	-2.00888	-1.85545	0.16191
C-C_R	-2.82707	-2.33991	-0.85745
C-C_R	-4.76917	-1.5178	0.30264
H-H_	-4.84117	-2.59414	-1.57227
N-N_R	2.69999	0.52412	-1.41112
C-C_R	3.80046	1.36967	-1.68835
C-C_R	1.98426	0.18345	-2.56856
O-O_R	4.57211	1.81731	-0.87239
O-O_R	0.99215	-0.51518	-2.60777
C-C_R	3.77948	1.57254	-3.16982
C-C_R	3.27214	1.61323	-5.89502
C-C_R	4.61687	2.30456	-3.99221
C-C_R	2.69215	0.86039	-3.69737
C-C_R	2.42782	0.87226	-5.05541
C-C_R	4.35361	2.32096	-5.36981
H-H_	0.8067	2.40094	2.96195
S-S_3+4	-2.06869	-3.18734	-2.26395

O-O_2	-3.13958	-3.95283	-2.91442
O-O_2	-0.8506	-3.8169	-1.74236
N-N_3	-1.56143	-2.05423	-3.35601
H-H_	-0.69151	-1.59198	-3.10163
C-C_3	-2.41327	-1.46468	-4.39271
C-C_R	2.48332	2.22612	5.17361
H-H_	2.30987	3.26498	4.90098
C-C_R	3.31659	1.90926	6.25543
H-H_	3.79059	2.70636	6.82218
C-C_R	3.545	0.5756	6.60262
H-H_	4.19538	0.33662	7.43997
C-C_R	2.94119	-0.4587	5.87396
H-H_	3.12067	-1.49722	6.14389
H-H_	-3.12705	-2.23606	-4.69504
H-H_	-1.75962	-1.28002	-5.25531
C-C_3	-3.14901	-0.16898	-4.01528
H-H_	-3.81912	0.07886	-4.85261
H-H_	-3.7948	-0.34972	-3.14557
C-C_3	-2.22912	1.02663	-3.73511
H-H_	-1.57348	1.18616	-4.6044
H-H_	-1.56938	0.79255	-2.88952
C-C_3	-3.00269	2.31564	-3.43169
H-H_	-3.64325	2.60316	-4.27565
H-H_	-2.32334	3.15264	-3.22929
H-H_	-3.64627	2.19202	-2.55186
F-F_	1.40309	0.21193	-5.60076
F-F_	3.04401	1.64773	-7.20962
F-F_	5.13836	3.02218	-6.1904
F-F_	5.66091	2.99503	-3.53071
H-H_	-0.93537	-2.00849	0.12413
H-H_	-5.84862	-1.40185	0.35966
C-C_3	-4.606	-0.30878	2.52096
H-H_	-5.69532	-0.40711	2.49489
H-H_	-4.36055	0.75987	2.5163
H-H_	-4.25379	-0.72574	3.47216

The cartesian coordinates for the optimized conformer at the B3LYP/6-31G+* level: Balance 1 unfolded conformer



C-C_R	-2.81235	3.70679	-0.20028
C-C_R	-2.32589	3.46543	1.09893
C-C_3	-2.36908	2.65871	-1.21426
H-H_	-2.76417	2.83653	-2.21716
C-C_3	-1.46268	2.21367	1.19474
C-C_R	-2.77058	1.30285	-0.66068
C-C_R	-3.40222	-1.06649	0.65875
C-C_R	-3.55635	0.34657	-1.29926
C-C_R	-2.28558	1.06372	0.63803
C-C_R	-2.60051	-0.11503	1.30573
C-C_R	-3.87228	-0.84516	-0.63895
H-H_	-3.92767	0.52199	-2.30567
H-H_	-2.23069	-0.29952	2.30903
H-H_	-4.49368	-1.58931	-1.12464
C-C_3	-0.80261	2.72603	-1.21403
H-H_	-0.5003	3.70473	-1.60256
C-C_3	-0.2662	2.47784	0.21448
H-H_	0.30052	3.33217	0.599
C-C_R	-0.12961	1.66814	-2.08323
C-C_R	0.71124	1.31591	0.07809
O-O_R	-0.29415	1.48667	-3.27032
O-O_R	1.36969	0.81004	0.96353
N-N_R	0.75439	0.93202	-1.27189
C-C_R	1.68742	-0.03439	-1.78431

C-C_R	3.57869	-1.8269	-2.77348
C-C_R	2.8127	0.45006	-2.45338
C-C_R	1.47595	-1.41019	-1.59714
C-C_R	2.44472	-2.28776	-2.11018
C-C_R	3.75632	-0.45189	-2.93481
H-H_	2.94986	1.51568	-2.6038
H-H_	4.31129	-2.52342	-3.16891
N-N_R	-3.74638	-2.27919	1.33742
C-C_R	-5.06296	-2.79006	1.42672
C-C_R	-2.81022	-3.11015	1.99208
O-O_R	-6.05771	-2.28477	0.95768
O-O_R	-1.61691	-2.91682	2.06817
C-C_R	-4.94821	-4.05848	2.20882
C-C_R	-4.17507	-6.28209	3.67361
C-C_R	-5.91453	-4.97115	2.5945
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H-H_	0.27086	-1.65661	0.18088
H-H_	0.22905	-3.03091	-0.92983
H-H_	-0.66144	-1.54918	-1.3172
H-H_	2.30063	-3.35772	-1.98442
S-S_3+4	5.22845	0.16336	-3.76188
O-O_2	5.01844	1.59691	-4.00751
O-O_2	5.55727	-0.77048	-4.84829
N-N_3	6.46413	-0.0512	-2.62328
H-H_	7.21107	-0.55189	-3.09915
C-C_3	6.92357	1.09794	-1.80969
C-C_R	-2.6301	4.34086	2.13744
H-H_	-2.25271	4.15483	3.14079
C-C_R	-3.43096	5.46268	1.88023
H-H_	-3.67681	6.14625	2.68865
C-C_R	-3.9135	5.70314	0.59171
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H-H_	-3.97863	5.01357	-1.4591

H-H_	6.90527	2.0183	-2.40545
H-H_	7.97049	0.88102	-1.56616
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H-H_	6.50136	2.2049	-0.03742
H-H_	5.07284	1.48738	-0.76191
C-C_3	6.21283	0.11891	0.4717
H-H_	7.27096	-0.07531	0.7054
H-H_	5.82979	-0.79027	-0.00812
C-C_3	5.44136	0.38301	1.77079
H-H_	5.82406	1.27561	2.28305
H-H_	5.5314	-0.46209	2.46375
H-H_	4.37337	0.53979	1.57597
F-F_	-1.9304	-5.57319	3.62419
F-F_	-3.82531	-7.3595	4.38032
F-F_	-6.42078	-6.9932	3.72527
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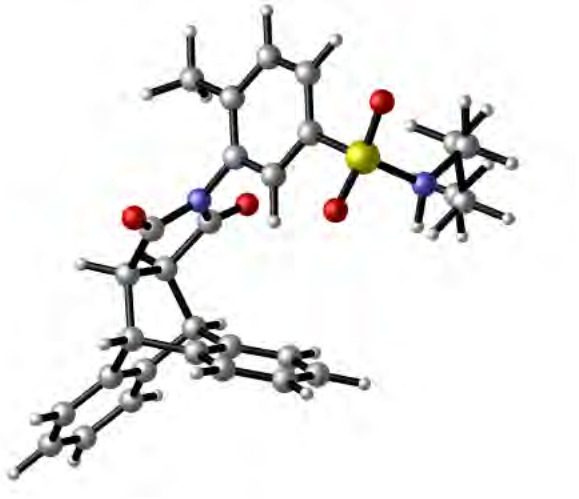
The cartesian coordinates for the optimized conformer at the B3LYP/6-31G+* level: Balance 2 folded conformer



C-C_R	2.80322	0.28408	3.75049
C-C_R	2.51264	1.60568	3.36364
C-C_3	2.0954	-0.7601	2.90056
H-H_	2.32974	-1.78548	3.19743
C-C_3	1.56408	1.68953	2.17717

C-C_R	2.43278	-0.47687	1.44604
C-C_R	2.95248	0.35403	-1.16531
C-C_R	2.95909	-1.38412	0.52822
C-C_R	2.1527	0.84626	1.05765
C-C_R	2.40883	1.26267	-0.24707
C-C_R	3.22294	-0.96272	-0.78207
H-H_	3.16194	-2.41029	0.82541
H-H_	2.19053	2.28436	-0.55026
H-H_	3.63647	-1.66494	-1.50091
C-C_3	0.56105	-0.47182	3.08917
H-H_	0.29541	-0.66002	4.13437
C-C_3	0.24458	0.97634	2.64774
H-H_	-0.20503	1.56883	3.45144
C-C_R	-0.31286	-1.35778	2.21173
C-C_R	-0.78051	0.837	1.52817
O-O_R	-0.38282	-2.56747	2.23501
O-O_R	-1.29205	1.73573	0.89061
N-N_R	-1.05212	-0.52722	1.34586
C-C_R	-1.91825	-1.03412	0.32034
C-C_R	-3.53698	-2.0683	-1.69834
C-C_R	-3.31321	-0.89231	0.43317
C-C_R	-1.3325	-1.67964	-0.76793
C-C_R	-2.14901	-2.18835	-1.7768
C-C_R	-4.10122	-1.42188	-0.59857
H-H_	-4.16219	-2.4927	-2.47734
H-H_	1.35557	2.71633	1.86679
S-S_3+4	-1.39007	-2.98823	-3.20462
O-O_2	-2.45041	-3.75836	-3.86197
O-O_2	-0.13578	-3.59035	-2.7418
N-N_3	-0.91603	-1.81007	-4.28944
H-H_	-0.04941	-1.36553	-4.00185
C-C_3	-1.86689	-0.99785	-5.0617
C-C_R	3.07514	2.6779	4.05165
H-H_	2.85195	3.70006	3.75272
C-C_R	3.93708	2.42964	5.12919
H-H_	4.38376	3.26294	5.66548
C-C_R	4.22743	1.11779	5.51146
H-H_	4.8994	0.93118	6.34515

C-C_R	3.65634	0.03797	4.82317
H-H_	3.88349	-0.98367	5.12065
H-H_	-2.76699	-1.60603	-5.18859
H-H_	-1.4332	-0.87218	-6.06293
C-C_3	-2.20926	0.37704	-4.46652
H-H_	-2.99882	0.8163	-5.09434
H-H_	-2.64053	0.25232	-3.46482
C-C_3	-1.0243	1.35157	-4.40389
H-H_	-0.58485	1.45238	-5.40755
H-H_	-0.23424	0.94156	-3.75781
C-C_3	-1.41946	2.73593	-3.87473
H-H_	-2.17535	3.2038	-4.51846
H-H_	-0.55467	3.40871	-3.83383
H-H_	-1.83642	2.66743	-2.86261
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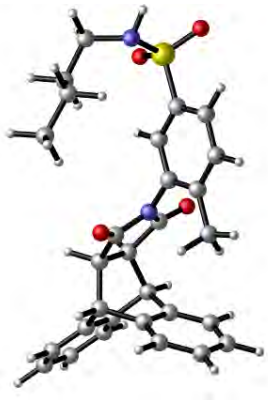
H-H_	-5.18277	-1.33619	-0.53037
C-C_3	-3.94997	-0.20728	1.61585
H-H_	-5.03569	-0.34114	1.60218
H-H_	-3.73919	0.86865	1.60552
H-H_	-3.57282	-0.61	2.56338
H-H_	3.1666	0.67845	-2.18067

The cartesian coordinates for the optimized conformer at the B3LYP/6-31G+* level: Balance 2 unfolded conformer



C-C_R	-3.79856	2.6579	0.39431
C-C_R	-3.30906	2.42857	1.69468
C-C_3	-3.34528	1.60867	-0.61284

H-H_	-3.74057	1.77859	-1.61726
C-C_3	-2.43649	1.18467	1.79735
C-C_R	-3.73018	0.24856	-0.05432
C-C_R	-4.31831	-2.13989	1.26672
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H-H_	-4.86534	-0.54786	-1.70542
H-H_	-3.15818	-1.34469	2.91296
H-H_	-5.39993	-2.67368	-0.52177
C-C_3	-1.77885	1.69677	-0.61264
H-H_	-1.48853	2.68042	-0.99762
C-C_3	-1.24089	1.44878	0.81596
H-H_	-0.66914	2.30177	1.19683
C-C_R	-1.09534	0.65004	-1.48512
C-C_R	-0.27054	0.28138	0.68
O-O_R	-1.24376	0.47937	-2.67578
O-O_R	0.37793	-0.23682	1.56707
N-N_R	-0.22021	-0.09588	-0.67086
C-C_R	0.70722	-1.06602	-1.18397
C-C_R	2.5861	-2.86829	-2.18177
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C-C_R	0.48756	-2.44136	-1.0018
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H-H_	-0.75974	-4.05698	-0.32198
H-H_	-1.65371	-2.58081	-0.72161
H-H_	1.29817	-4.39346	-1.39835
S-S_3+4	4.24793	-0.88457	-3.16401
O-O_2	4.04676	0.55127	-3.40278
O-O_2	4.57012	-1.81542	-4.25493
N-N_3	5.48376	-1.11247	-2.02721

H-H_	6.22822	-1.61226	-2.508
C-C_3	5.94969	0.03064	-1.2087
C-C_R	-3.62268	3.30683	2.72812
H-H_	-3.24402	3.1297	3.73268
C-C_R	-4.43504	4.4192	2.46539
H-H_	-4.68797	5.10433	3.27039
C-C_R	-4.91981	4.64793	1.17559
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C-C_R	-4.59975	3.76648	0.133
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H-H_	4.84941	-1.86074	0.58427
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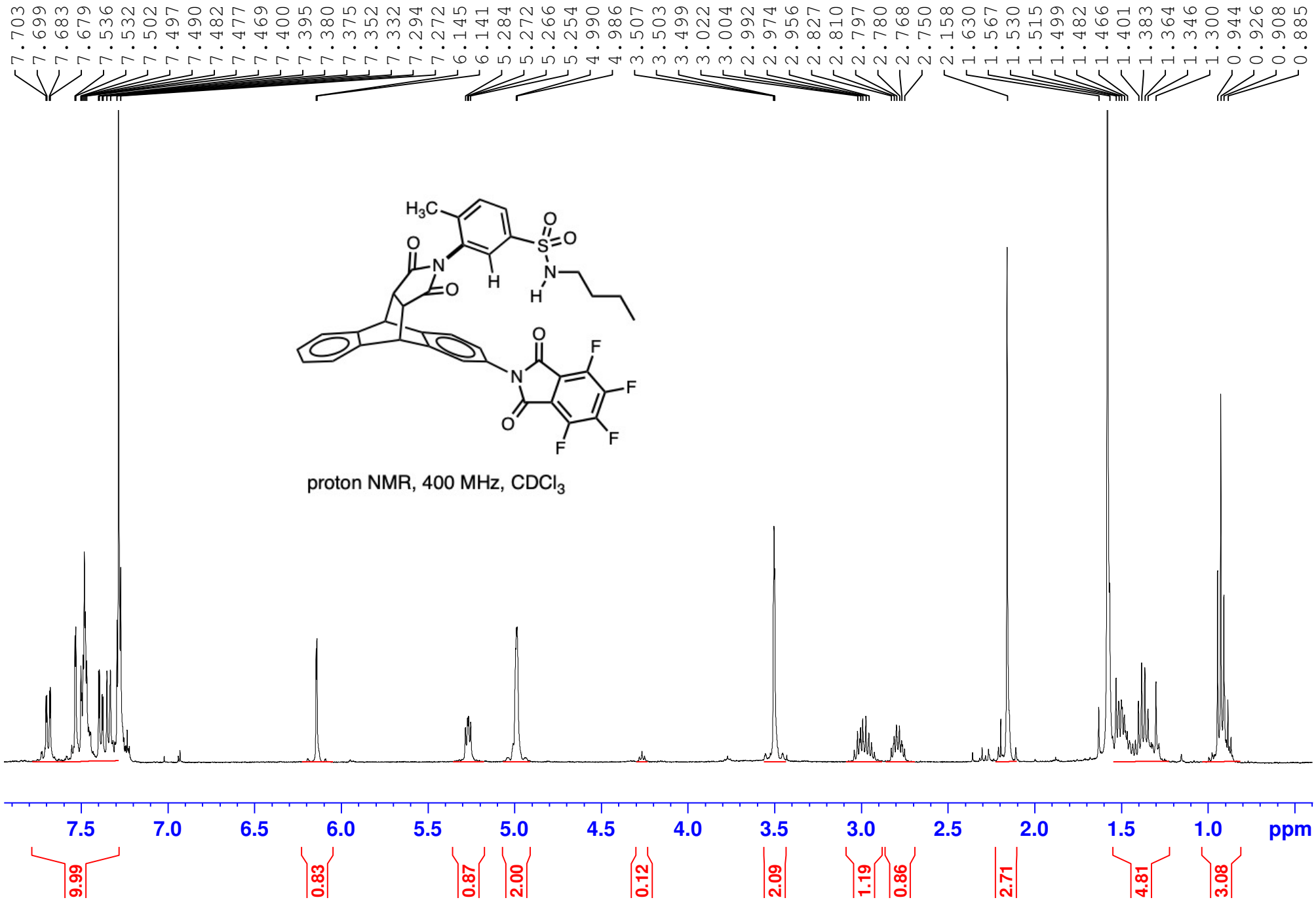
H-H_	3.39805	-0.53253	2.17484
H-H_	-4.55665	-3.06766	1.78017

References

1. Gardarsson, H.; Schweizer, W. B.; Trapp, N.; Diederich, F., Structures and Properties of Molecular Torsion Balances to Decipher the Nature of Substituent Effects on the Aromatic Edge-to-Face Interaction. *Chemistry – A European Journal* **2014,** *20* (16), 4608-4616.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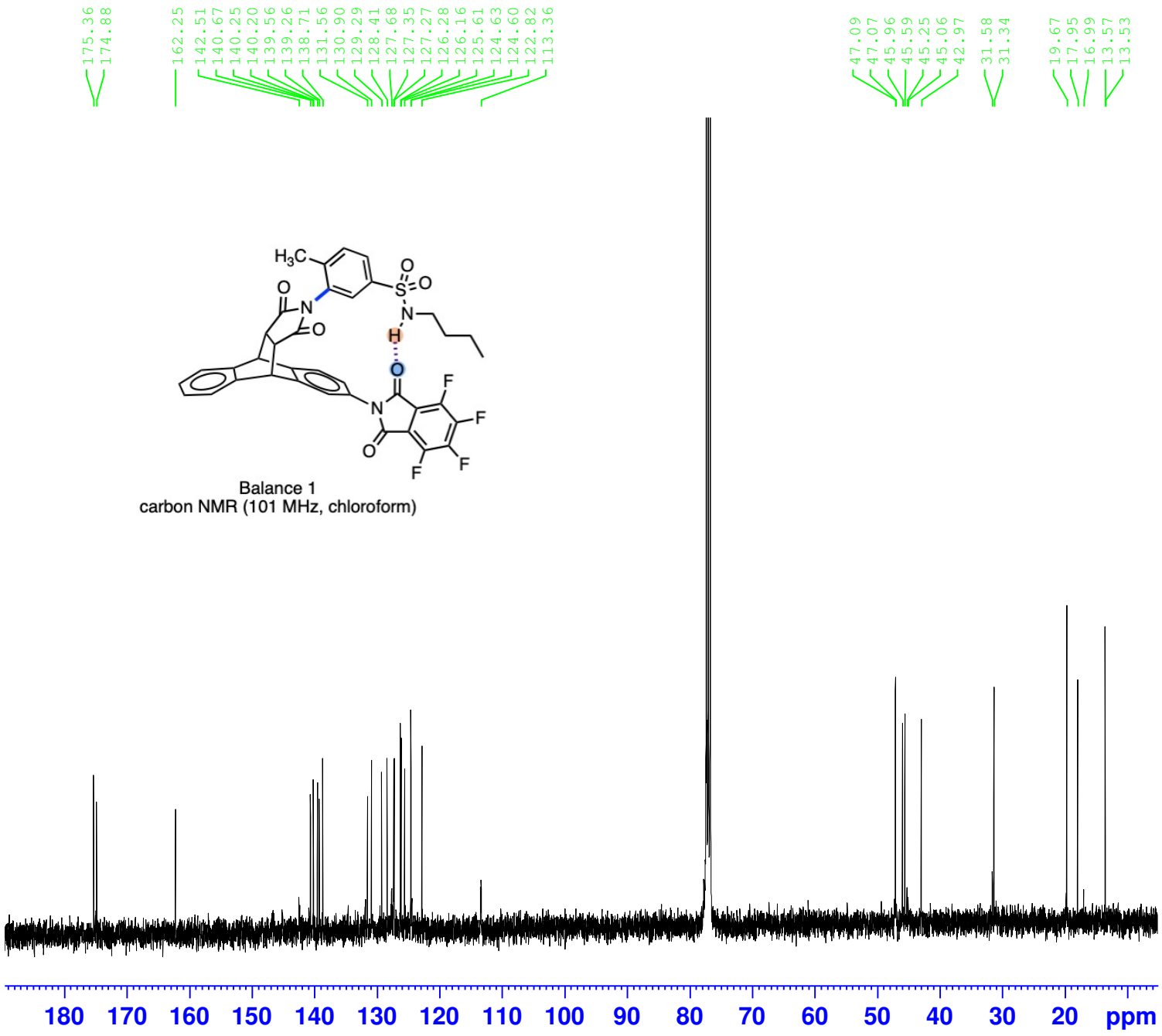


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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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Time                19.48
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2883
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                13C
P1                 7.50 usec
PLW1         75.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         18.00000000 W
PLW12         0.19220001 W
PLW13         0.09667500 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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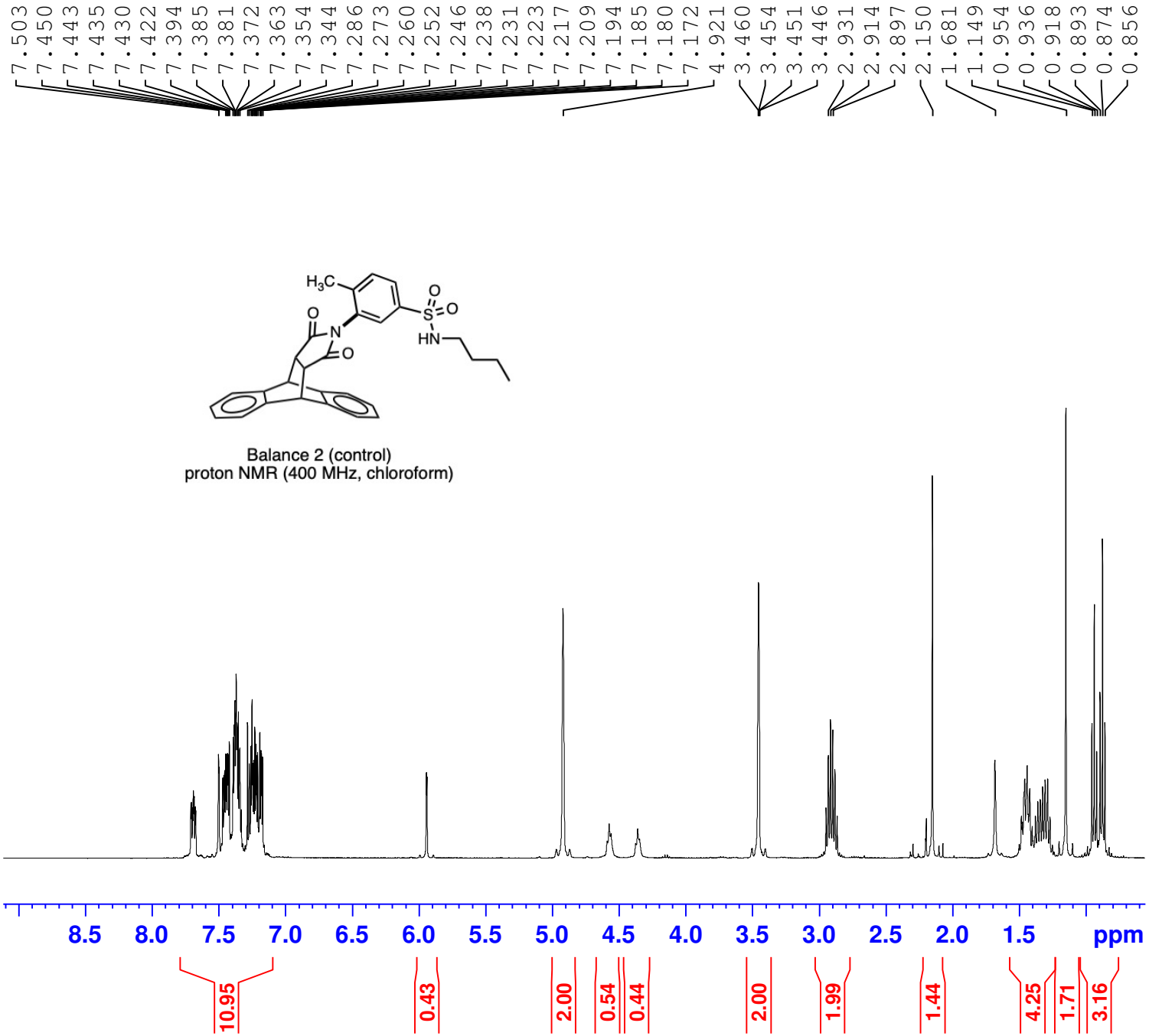


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EXPNO                          1
PROCNO                         1

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Time                   15.40
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                       144
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                      1H
P1                     9.30 usec
PLW1           18.00000000 W

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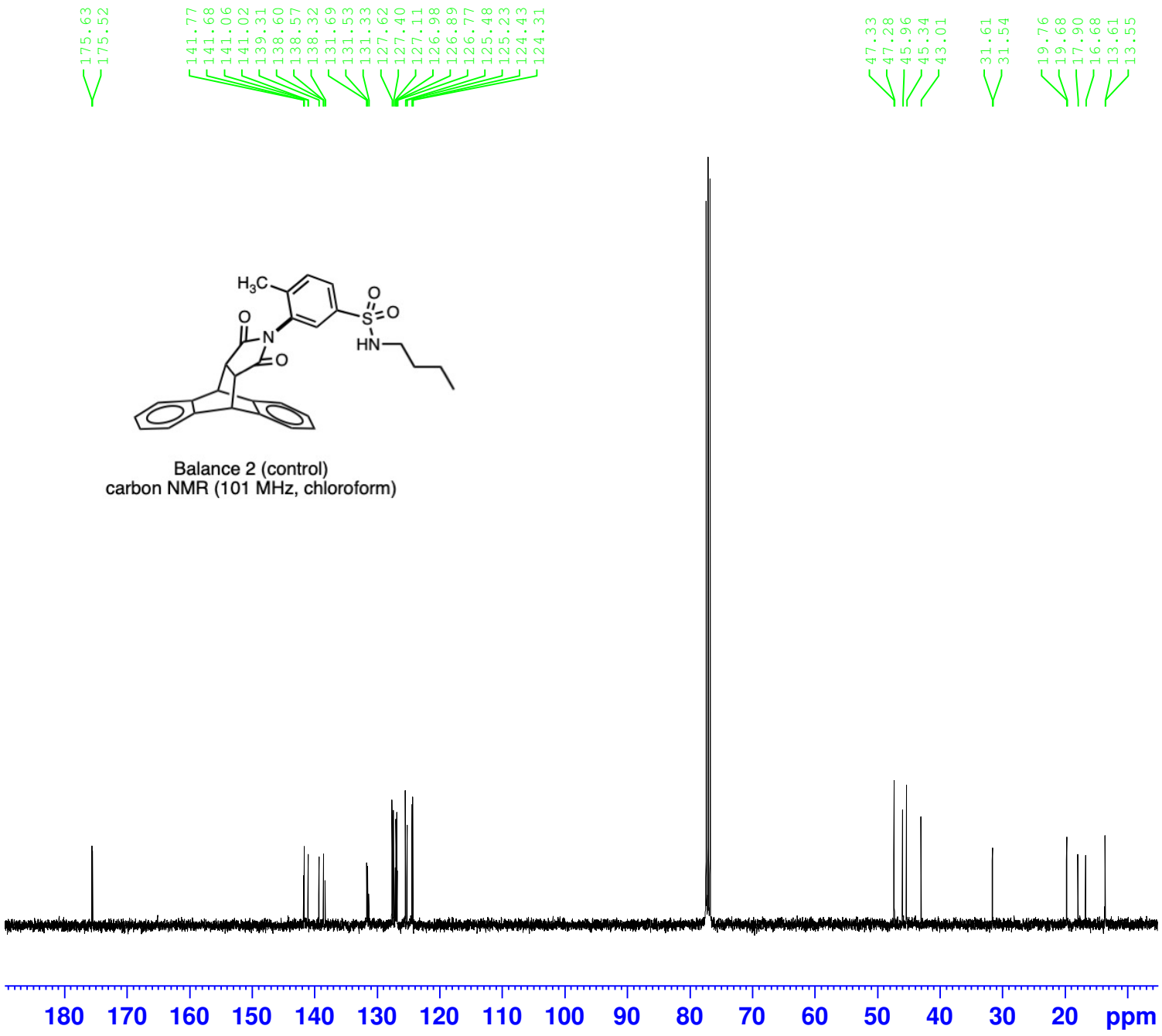


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EXPNO                          1
PROCNO                         1

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Time                   16.04
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       383
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                      2050
DW                    20.800 usec
DE                     6.50 usec
TE                     300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                    13C
P1                     7.50 usec
PLW1             75.00000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             18.00000000 W
PLW12             0.19220001 W
PLW13             0.09667500 W

F2 - Processing parameters
SI                     32768
SF               100.6127690 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
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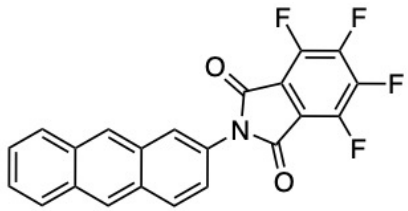
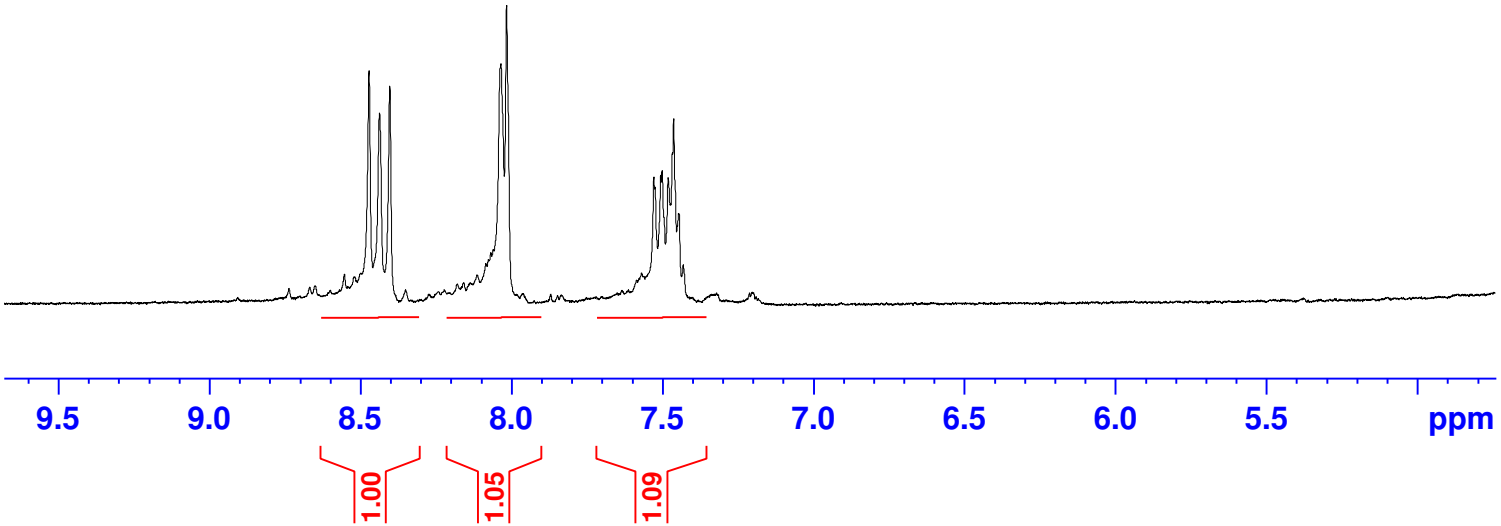


6

proton NMR (400 MHz, DMSO-d6)

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EXPNO                  1
PROCNO                 1

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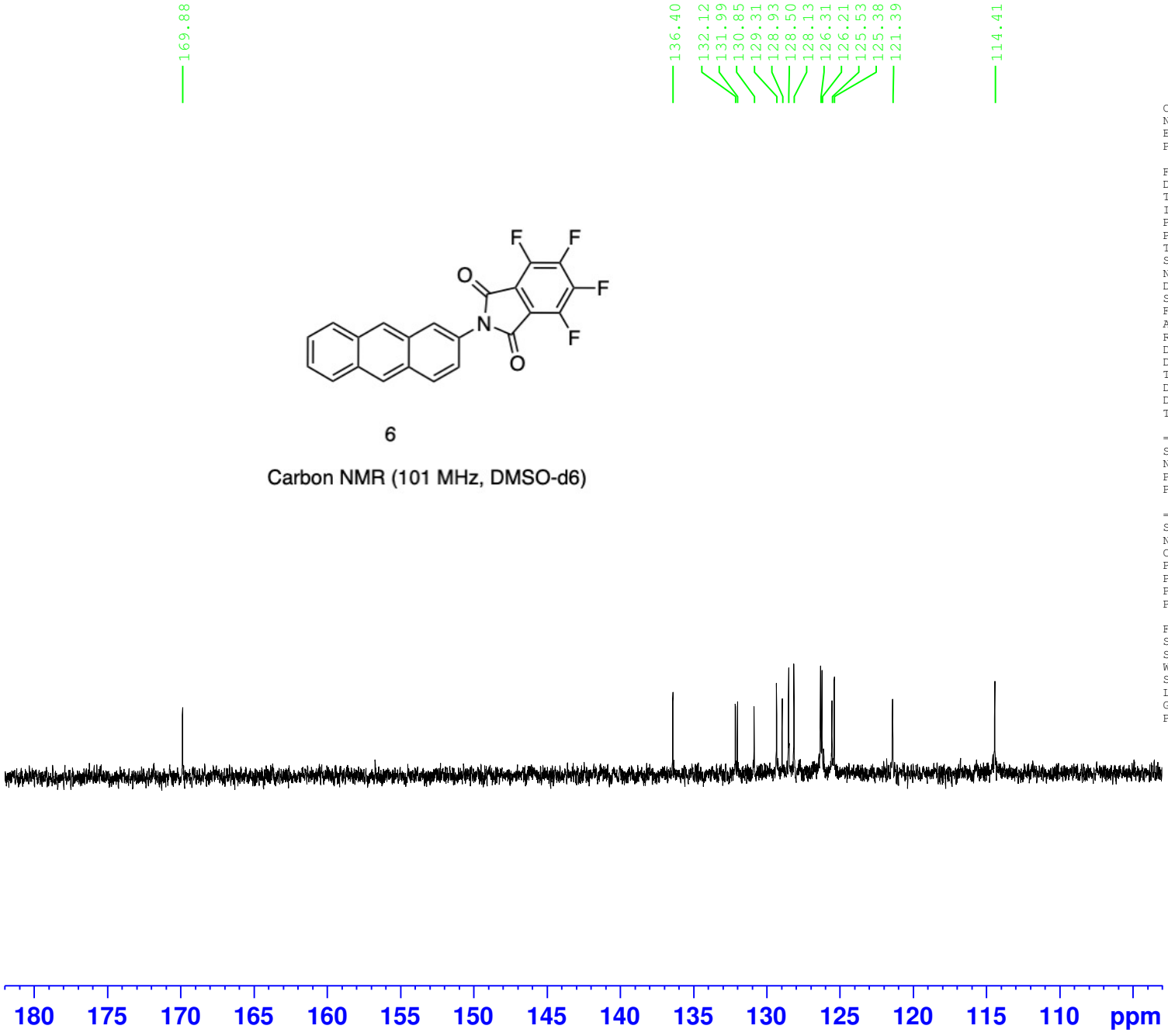
PULPROG            zg30
TD                65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                    32
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1         18.00000000 W

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



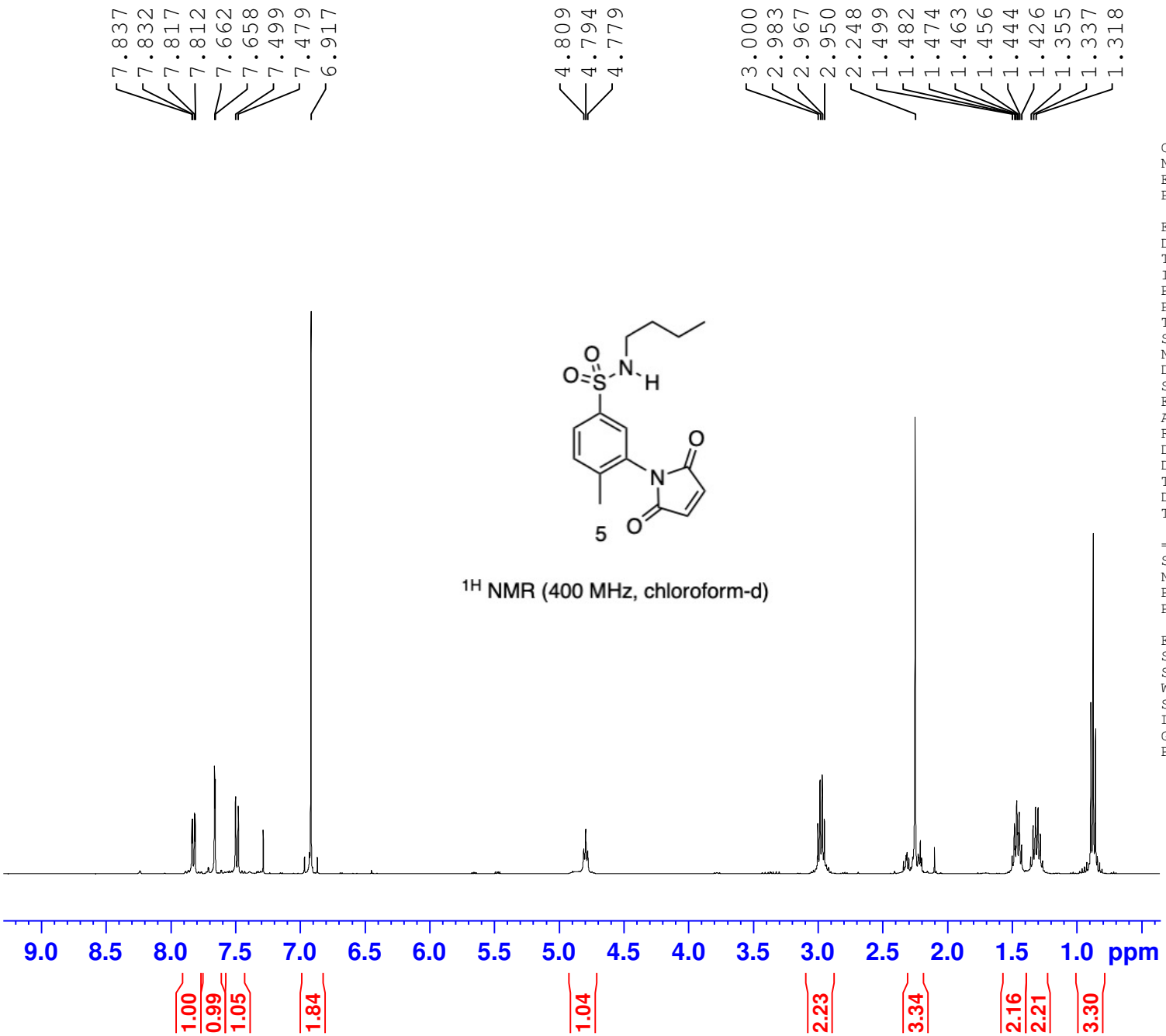

```
Current Data Parameters
NAME      controljan1162023balance1CARBON
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230116
Time               19.18
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2782
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1                13C
P1                 7.50 usec
PLW1        75.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        18.00000000 W
PLW12        0.19220001 W
PLW13        0.09667500 W

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

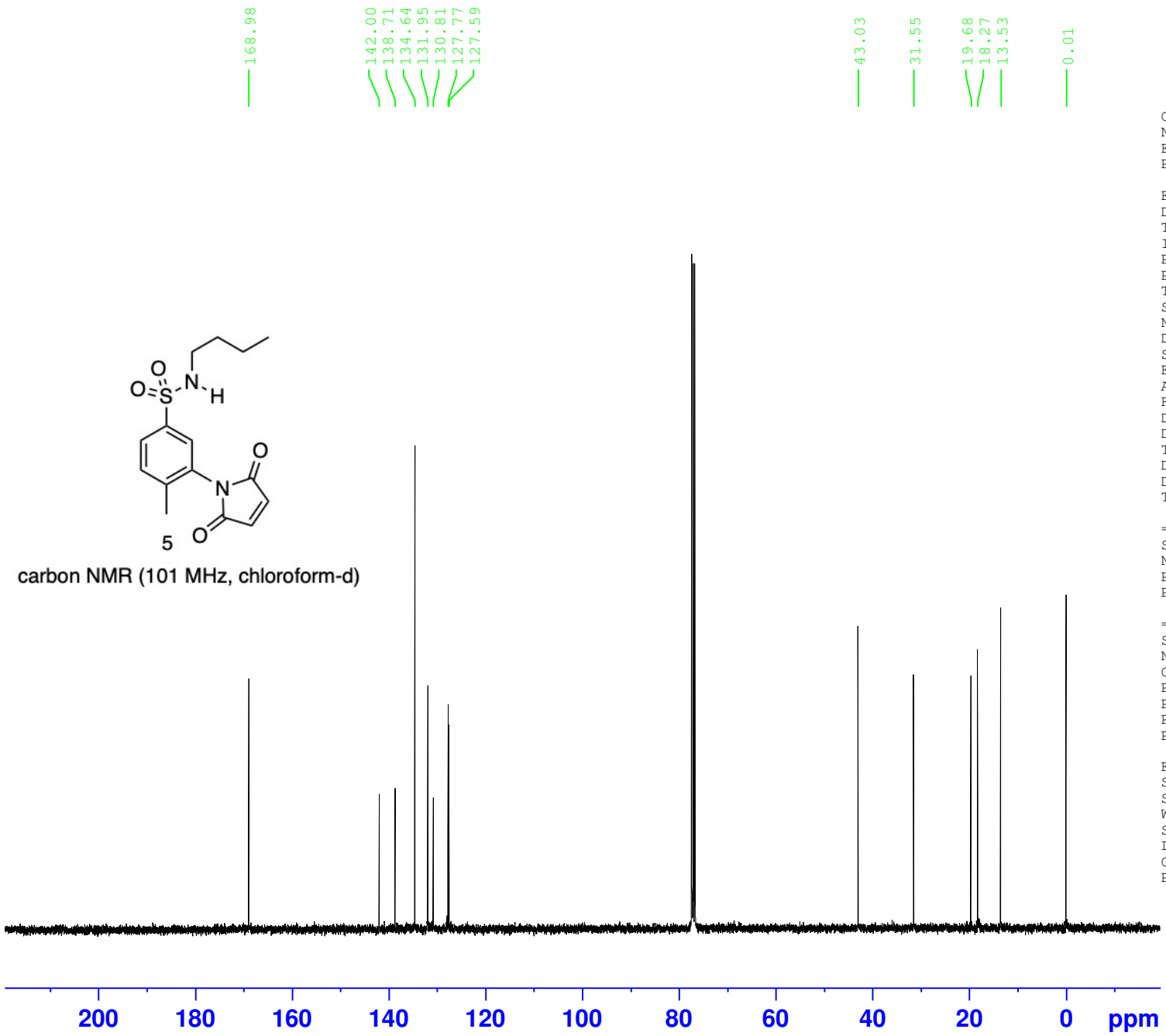



```
Current Data Parameters
NAME      controljan142023proton2
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230114
Time              16.14
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  114
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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




```
Current Data Parameters
NAME      controljan142023carbon2
EXPNO                           1
PROCNO                          1

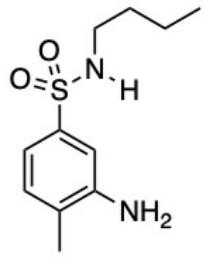
F2 - Acquisition Parameters
Date_                    20230114
Time                        16.50
INSTRUM                     spect
PROBHD    5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                     CDCl3
NS                            561
DS                              4
SWH                     24038.461 Hz
FIDRES                   0.366798 Hz
AQ                       1.3631488 sec
RG                           2050
DW                         20.800 usec
DE                          6.50 usec
TE                         300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                             1

======== CHANNEL f1 ========
SFO1                100.6228293 MHz
NUC1                        13C
P1                         7.50 usec
PLW1                75.00000000 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                18.00000000 W
PLW12                0.19220001 W
PLW13                0.09667500 W

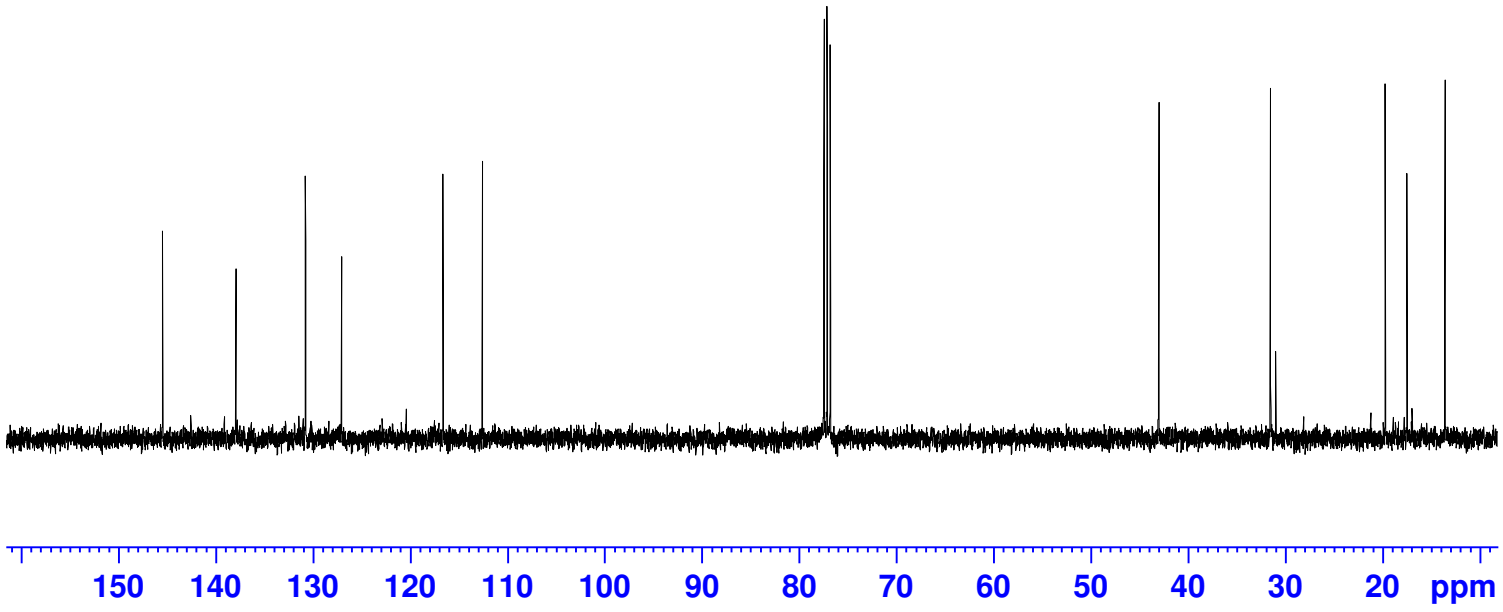
F2 - Processing parameters
SI                          32768
SF                  100.6127690 MHz
WDW                            EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```

145.48
137.94
130.78
127.07
116.64
112.59
42.99
31.50
19.72
17.47
13.56



4

carbon NMR (101 MHz, chloroform-d)



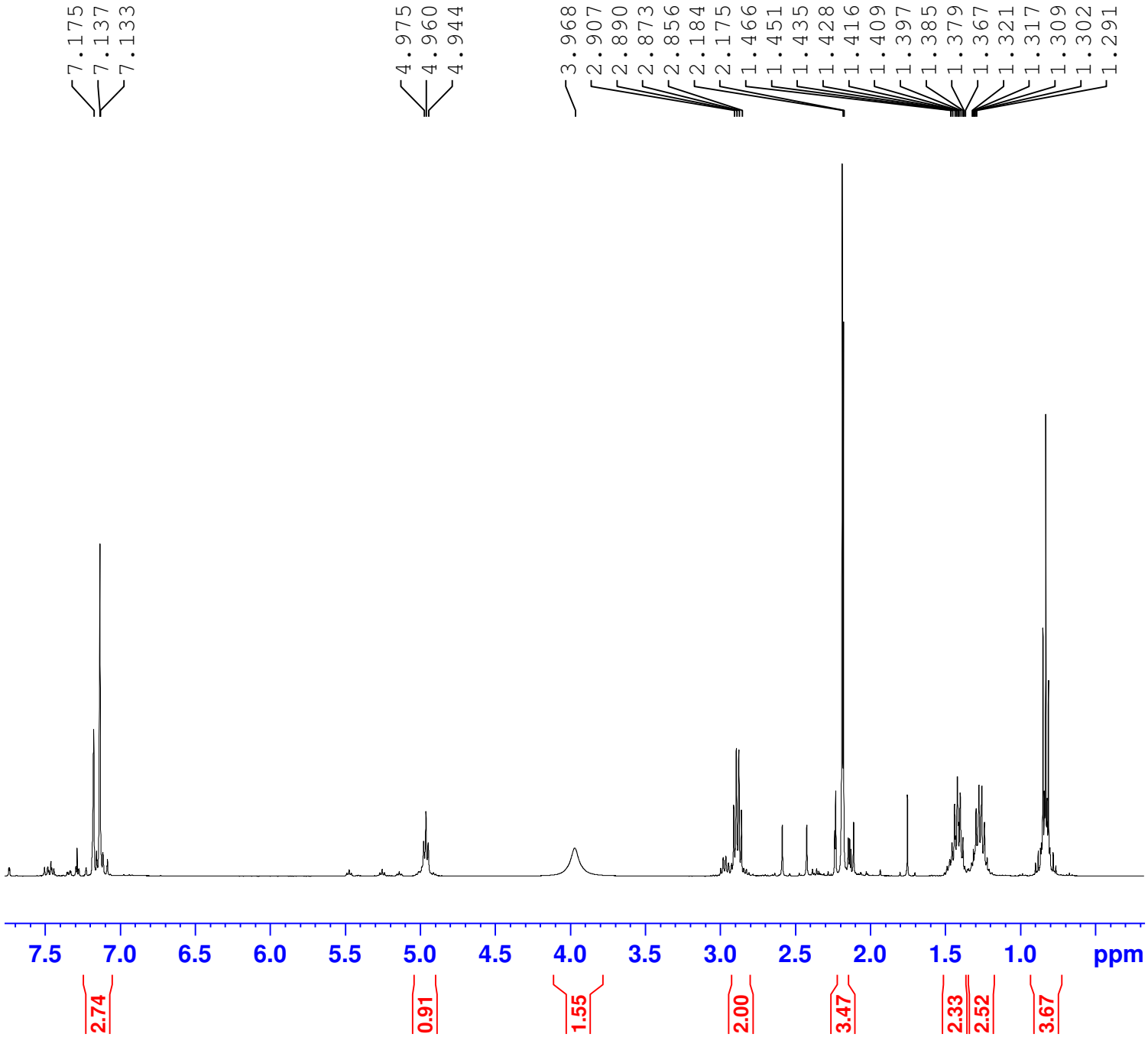

```
Current Data Parameters
NAME      N-butyl(3-methyl-4-amino)benezenesulfanamide-carbon
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230124
Time              19.37
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   25
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.363488 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1               13C
P1                7.50 usec
PLW1         75.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.19220001 W
PLW13         0.09667500 W

F2 - Processing parameters
SI                32768
SF           100.6127690 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

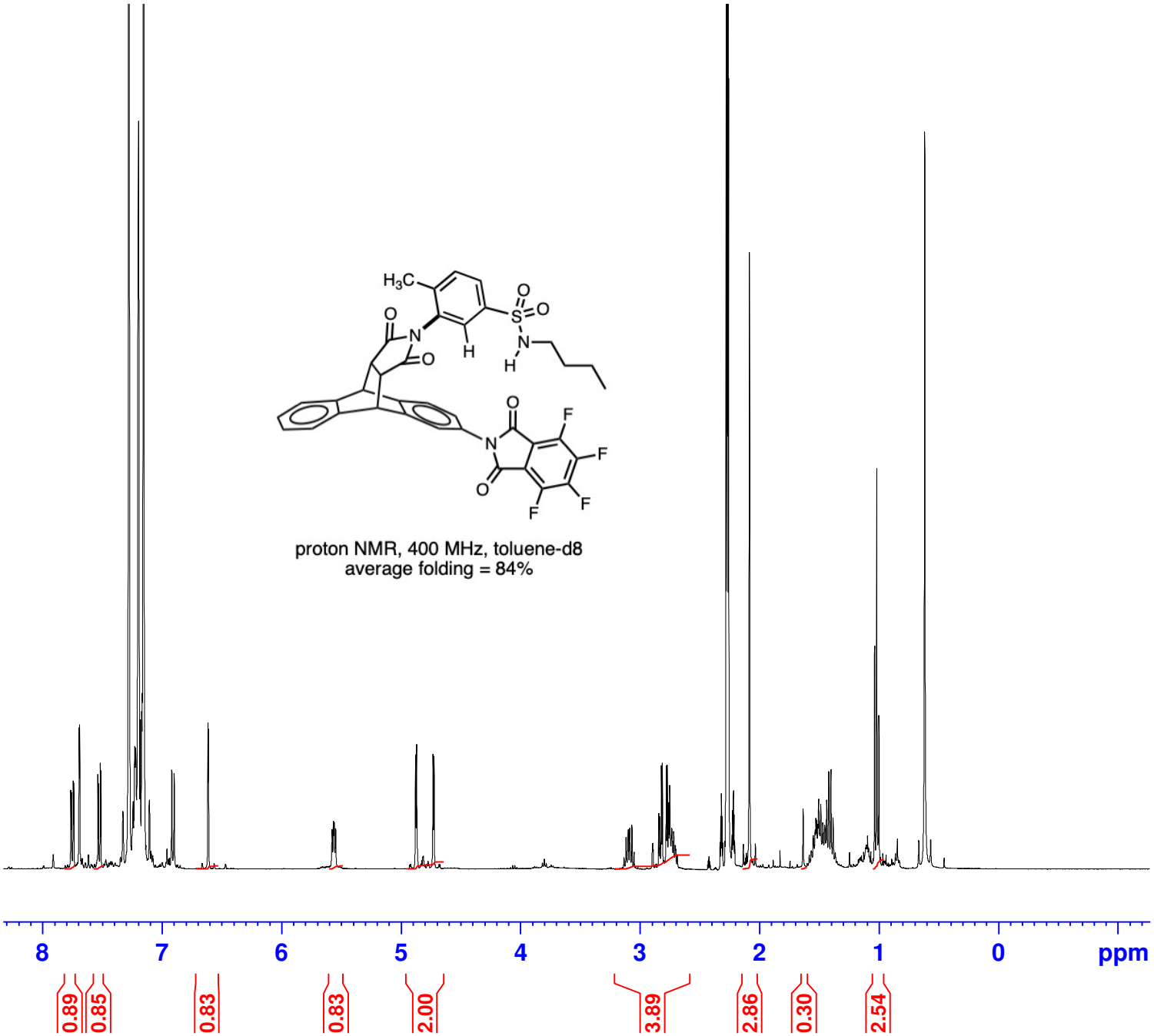



```
Current Data Parameters
NAME      N-butyl(3-methyl-4-amino)benezenesulfanamide-prot
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230124
Time               19.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                  71.8
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                 9.30 usec
PLW1        18.00000000 W

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

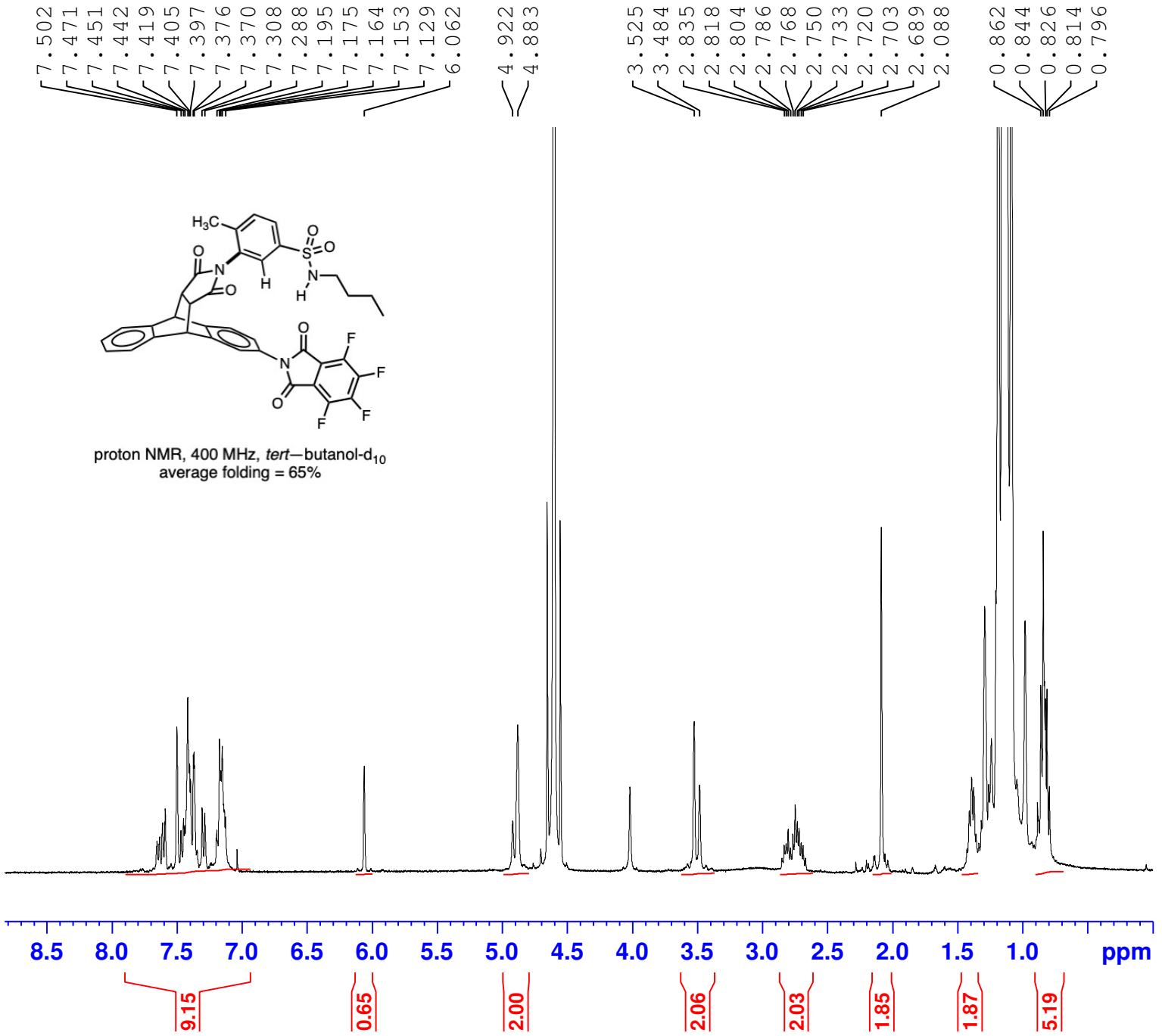



```
Current Data Parameters
NAME      conc-study~9.9mMOLAR-toluene
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211013
Time              18.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT            Tol
NS                 800
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                 512
DW               62.400 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                65536
SF          400.1299439 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



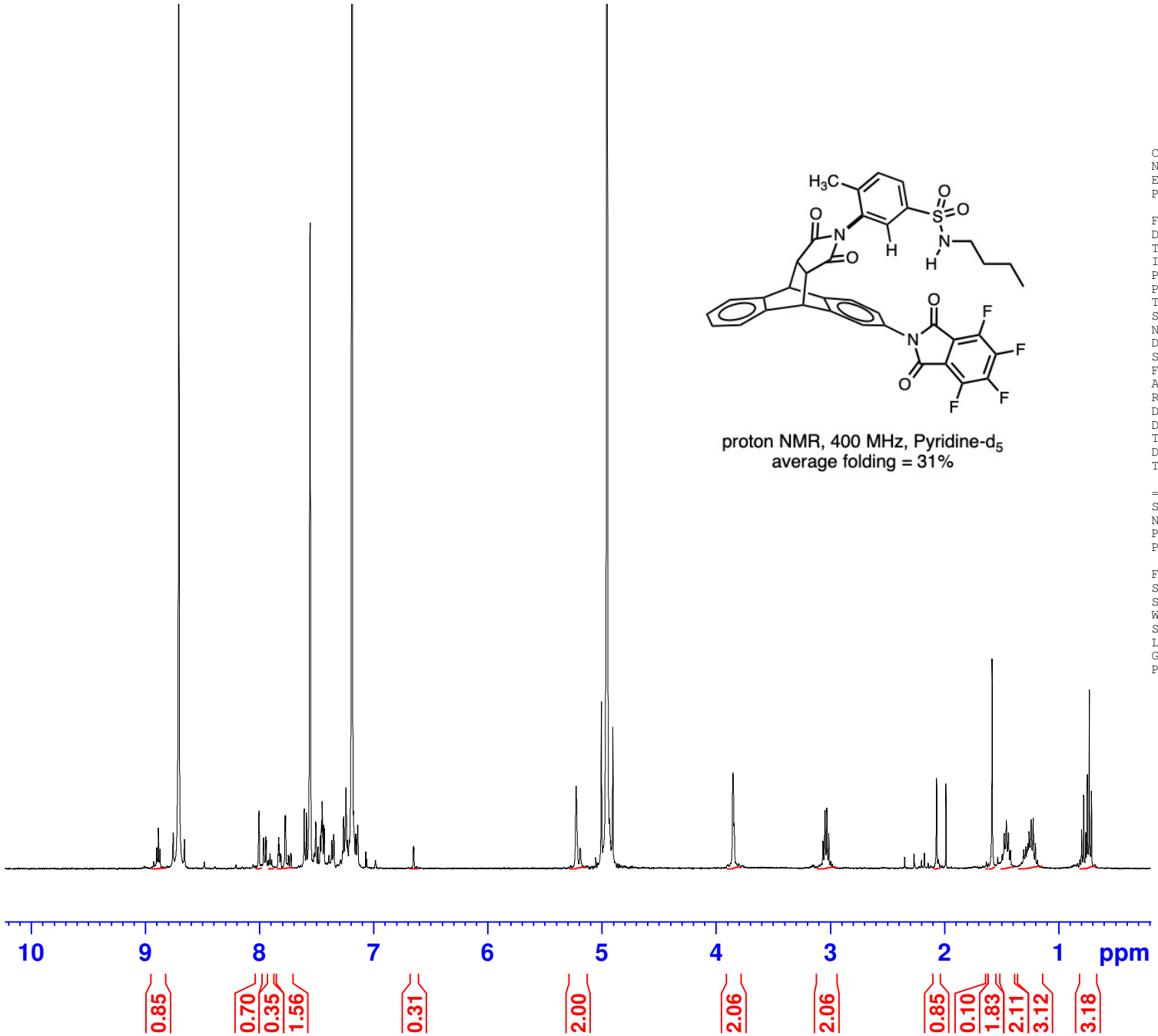
proton NMR, 400 MHz, *tert*—butanol-d_{10}
average folding = 65%

```
Current Data Parameters
NAME      conc-study~9.9mMOLAR-tertbutanol1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20221107
Time              15.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT             EtOD
NS                  320
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                  256
DW               62.400 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1         18.00000000 W

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



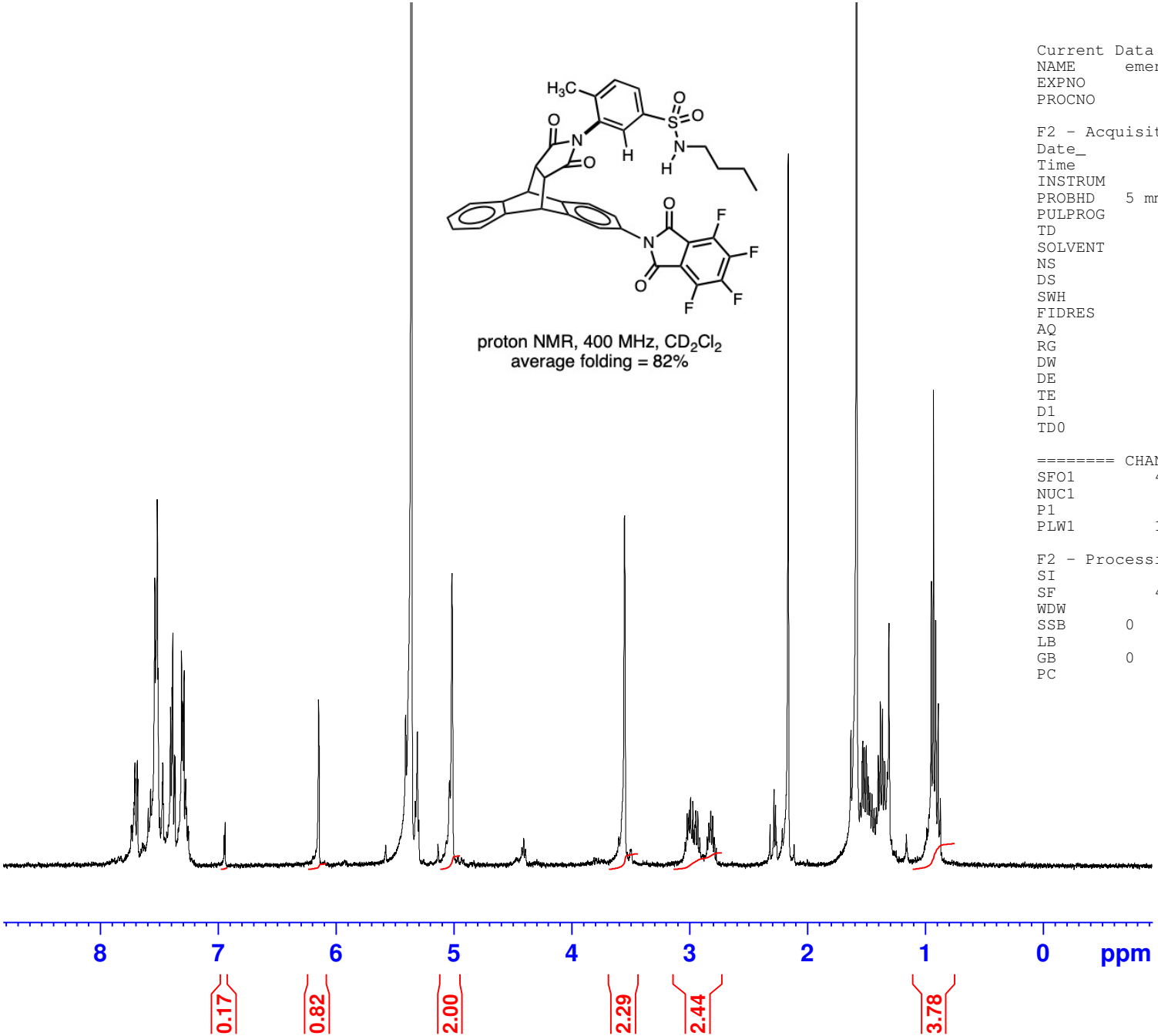
proton NMR, 400 MHz, Pyridine-d_5
average folding = 31%

```
Current Data Parameters
NAME      emenikemodel1a-inpyridine3mg
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221031
Time              17.43
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT            Pyr
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                 287
DW               62.400 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1         18.00000000 W

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

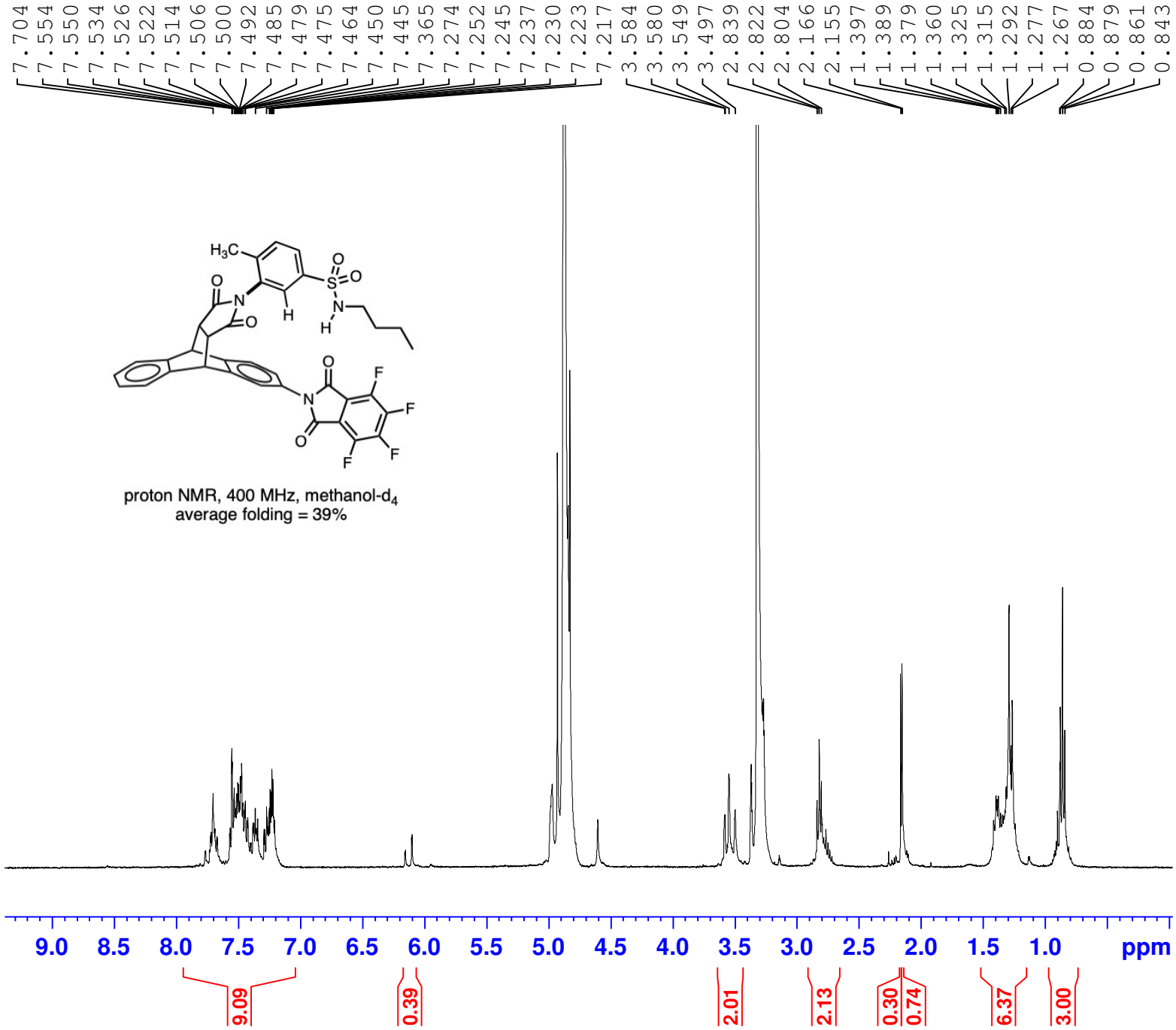



```
Current Data Parameters
NAME      emenikemodel1a-indichloromethane3mg
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221031
Time              16.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT          CD2Cl2
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  575
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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

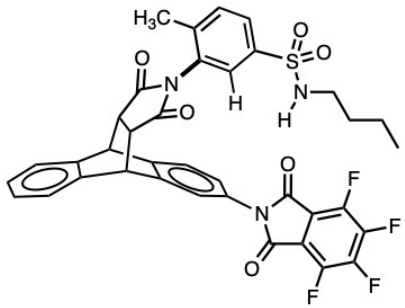



```
Current Data Parameters
NAME      conc-study~9.9mMOLAR-MeOH-1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211009
Time               17.48
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                   103
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   512
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300033 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



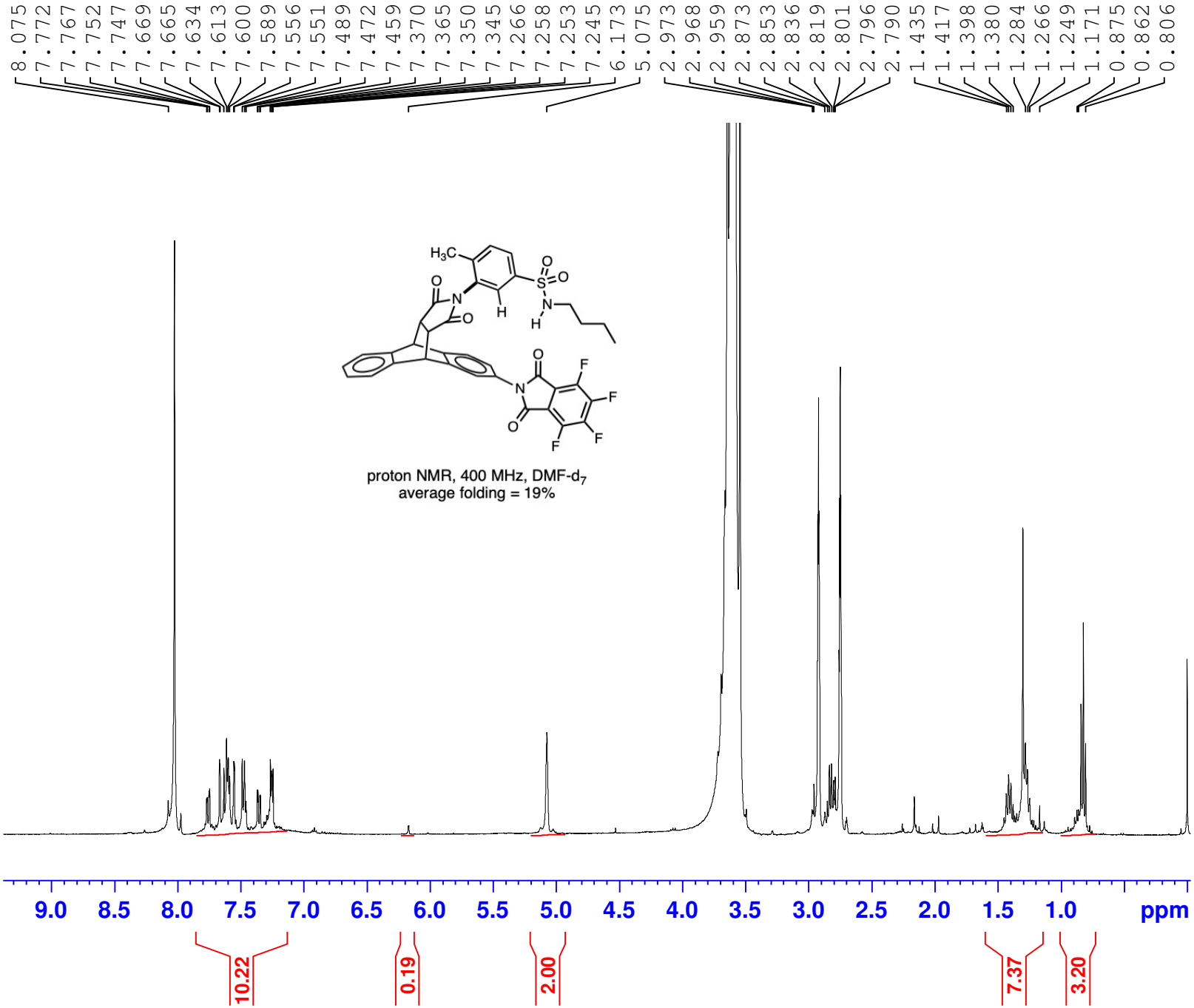
proton NMR, 400 MHz, DMSO-d_6
average folding = 9%


```
Current Data Parameters
NAME      emenikemodel1a-indmso3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221031
Time              16.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  322
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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

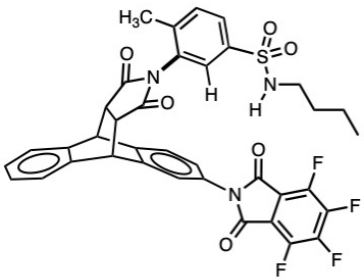



```
Current Data Parameters
NAME      conc-study~9.9mMOLAR-dmf-1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211006
Time              17.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT            DMF
NS                 220
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                 203
DW               62.400 usec
DE                6.50 usec
TE               298.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                65536
SF          400.1300033 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



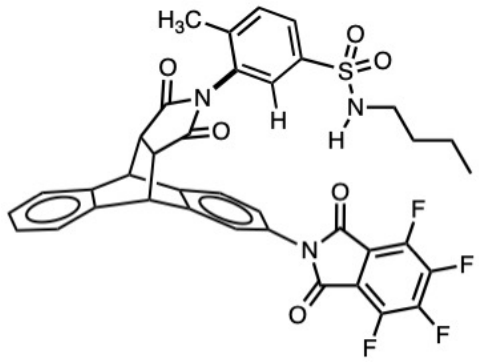
proton NMR, 400 MHz, CCl_4 (locked in $CDCl_3$ via insert)
average folding = 82%


```
Current Data Parameters
NAME     balance-sulfanamide-CCl4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221224
Time               15.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    48
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   322
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1        18.00000000 W

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



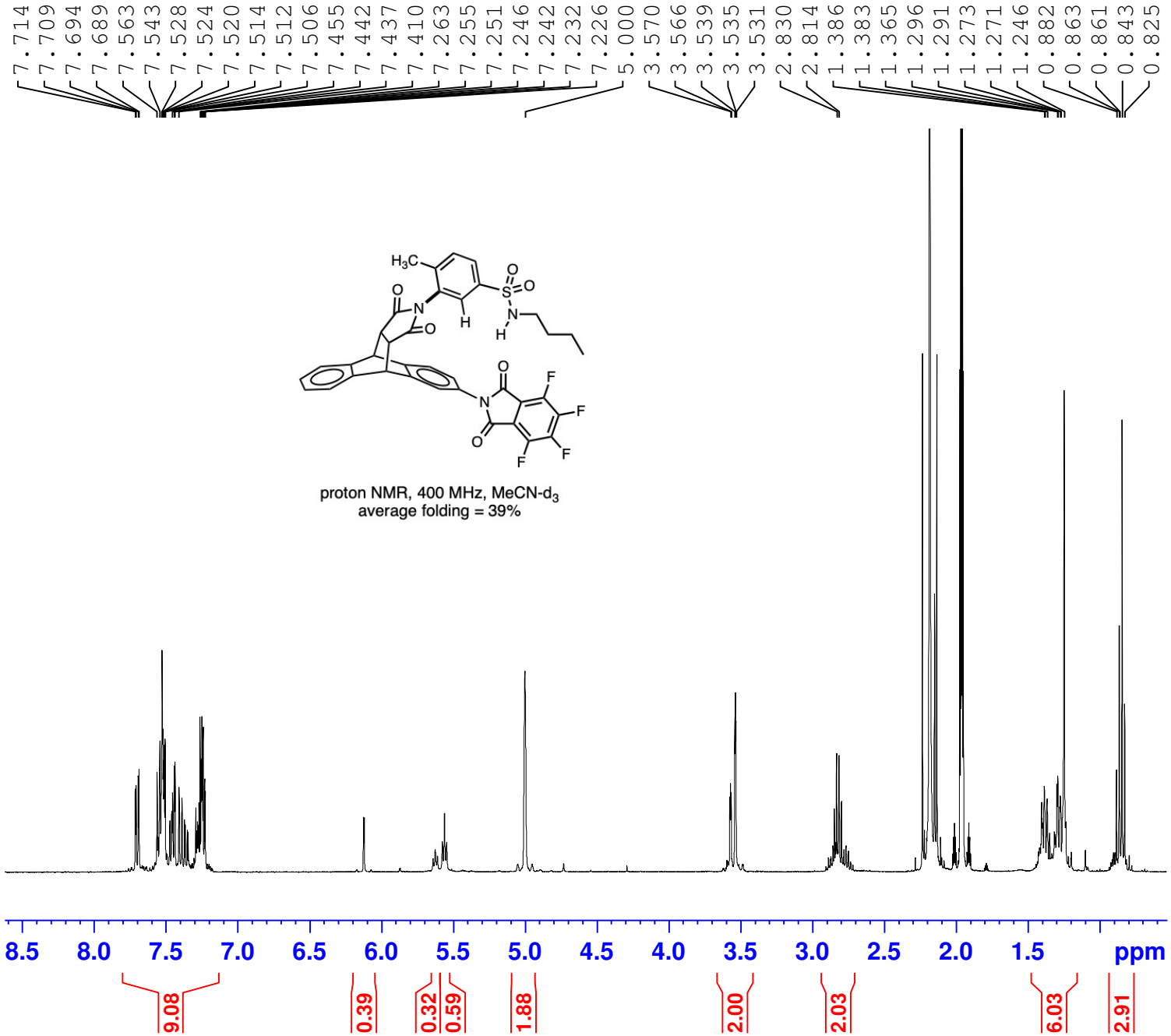
proton NMR, 400 MHz, Benzene-d6
average folding = 85%


```
Current Data Parameters
NAME      balance-sulfanamide-benzene
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221224
Time               15.25
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                    69
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                   256
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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

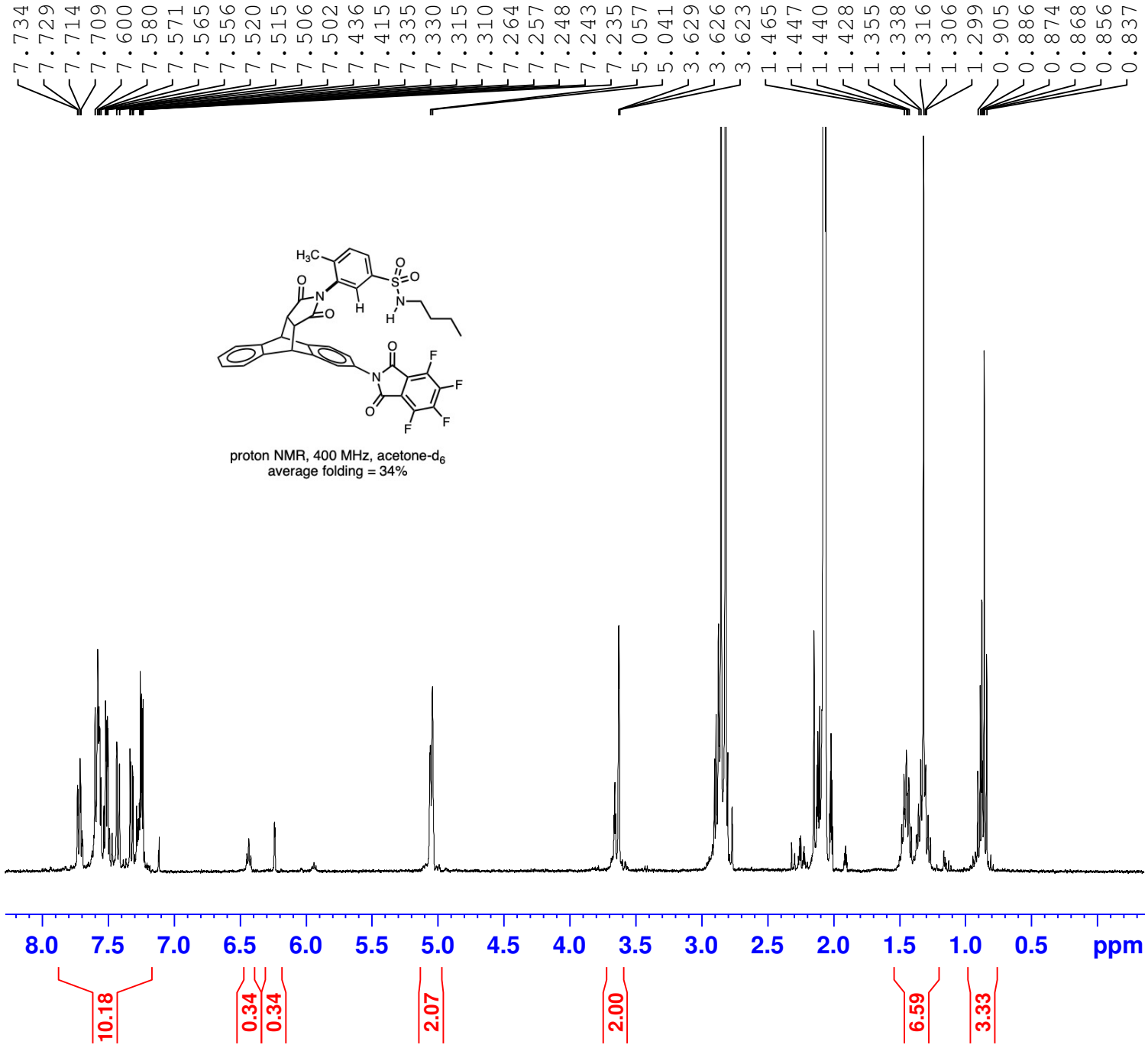



```
Current Data Parameters
NAME      conc-study-9.9mMOLAR-MECN
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210925
Time               15.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CD3CN
NS                   120
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   512
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300033 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

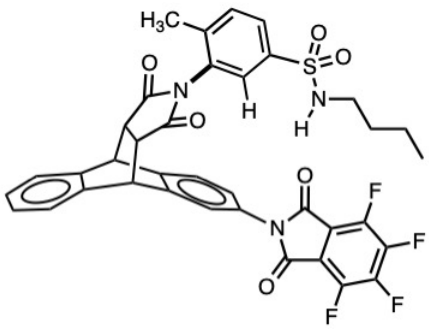



```
Current Data Parameters
NAME      emenikemodel1a-inacetone3mg
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221031
Time               15.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   362
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1         18.00000000 W

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



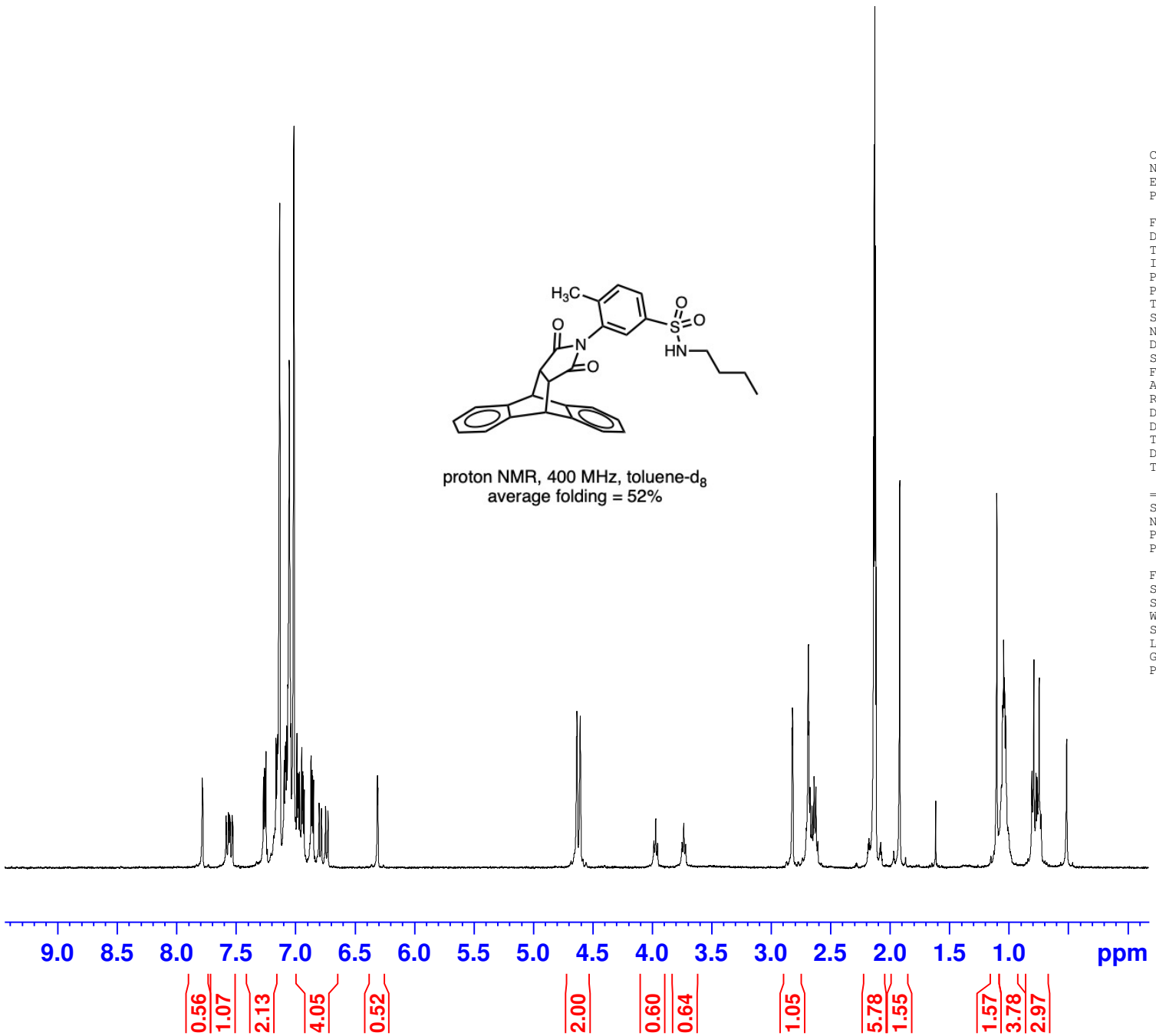
proton NMR, 400 MHz, acetic acid-d_4
average folding = 50%


```
Current Data Parameters
NAME      conc-study~9.9mMOLAR-aceticacid
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211009
Time              13.13
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           Acetic
NS                   150
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                   575
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300033 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

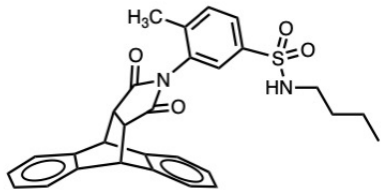



```
Current Data Parameters
NAME      controlnov19balanceintoluene
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20221119
Time              16.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT            Tol
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                 322
DW              62.400 usec
DE               6.50 usec
TE              298.0 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1       18.00000000 W

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



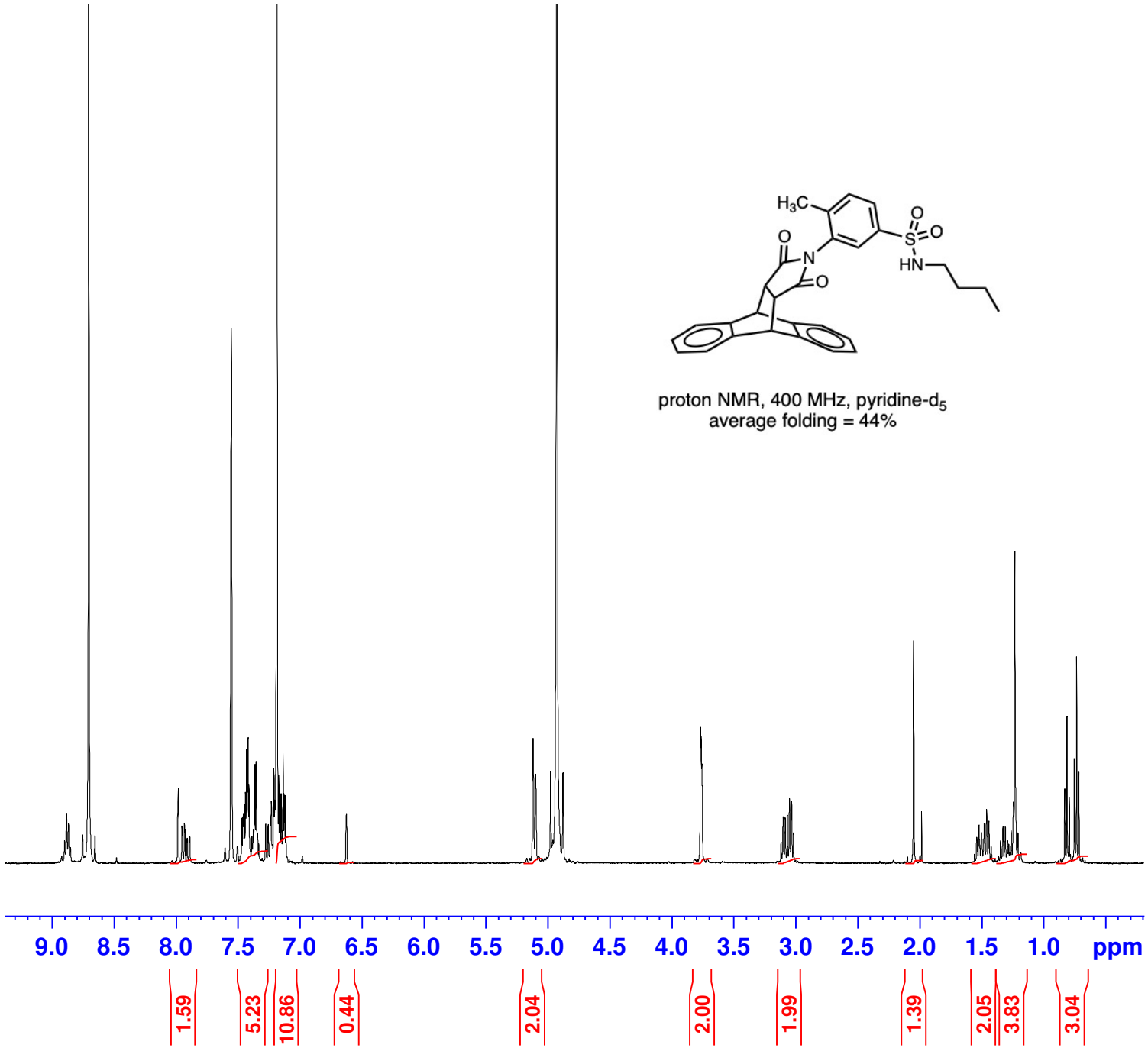
proton NMR, 400 MHz, *tert*—butanol-d_{10}
average folding = 39%


```
Current Data Parameters
NAME      controlnov19balancein-tertbutanol
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20221119
Time              18.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             EtOD
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   228
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1         18.00000000 W

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



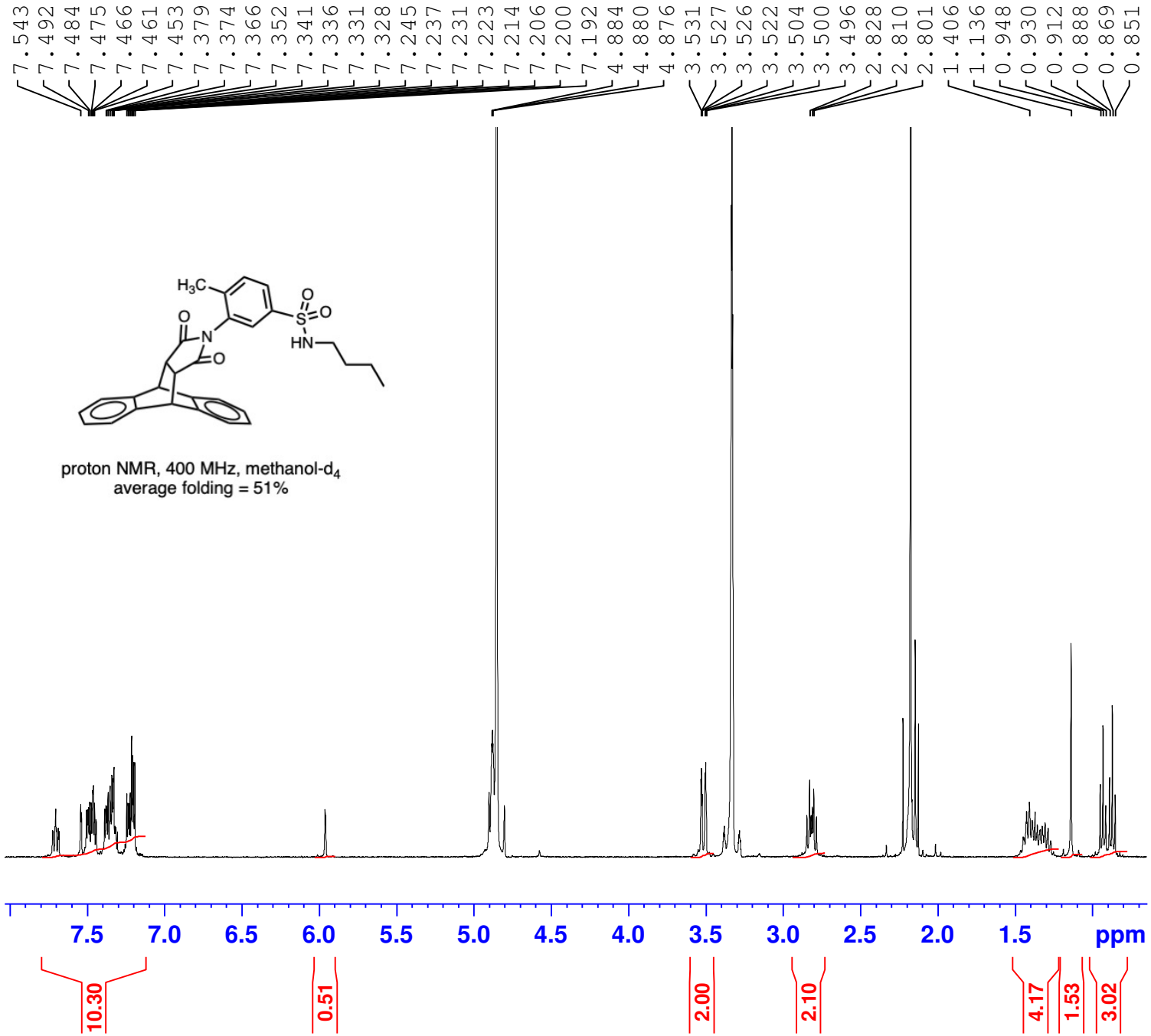
proton NMR, 400 MHz, pyridine-d_5
average folding = 44%

```
Current Data Parameters
NAME      controlnov19balanceinpyridine
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221119
Time               15.40
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT              Pyr
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   287
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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

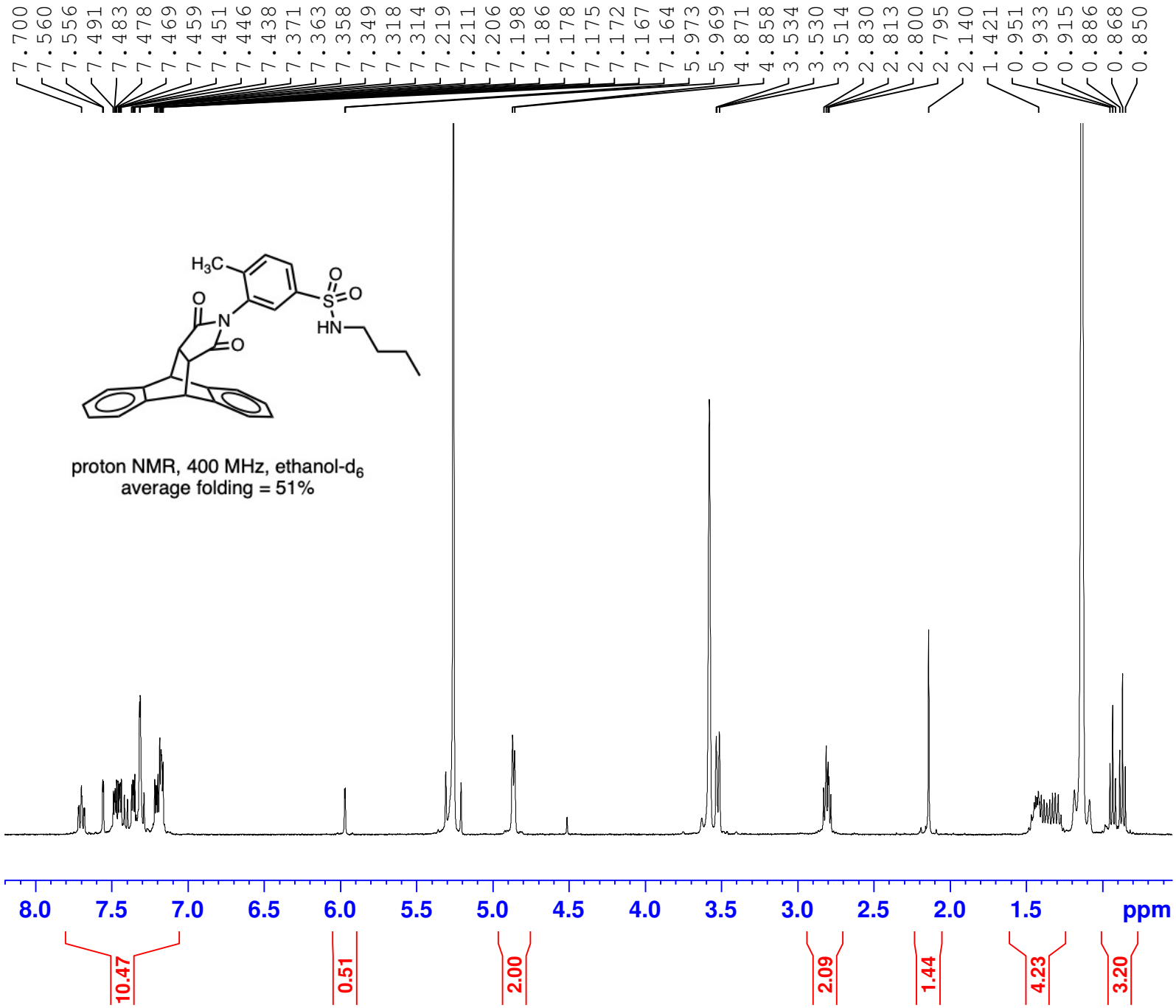



```
Current Data Parameters
NAME      controlnov19balanceinmethanol
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221119
Time              16.39
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            MeOD
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  322
DW               62.400 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1         18.00000000 W

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

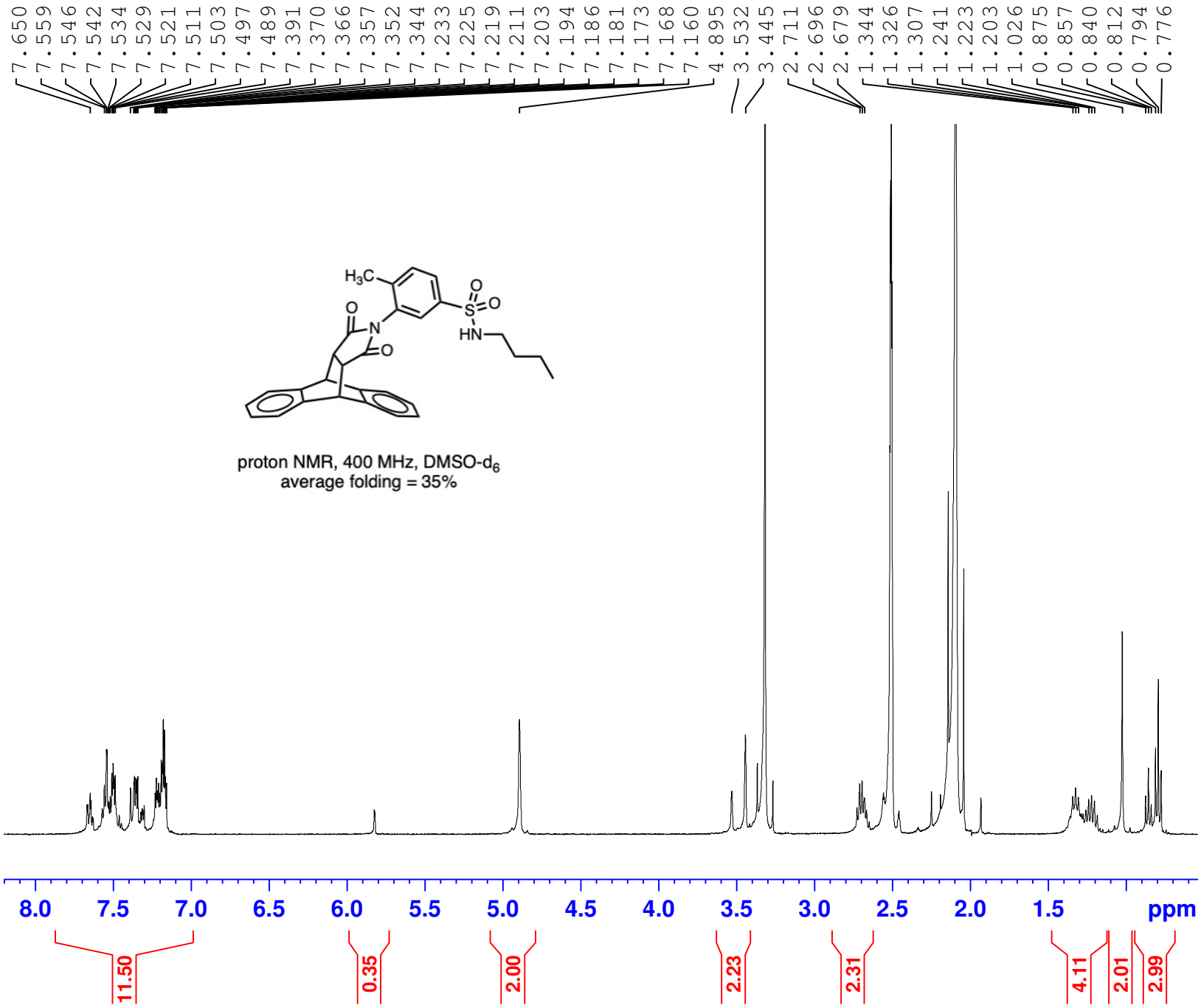



```
Current Data Parameters
NAME      controlnov19balancein-ethanol
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20221119
Time              18.52
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            EtOD
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                  322
DW               62.400 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1        18.00000000 W

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

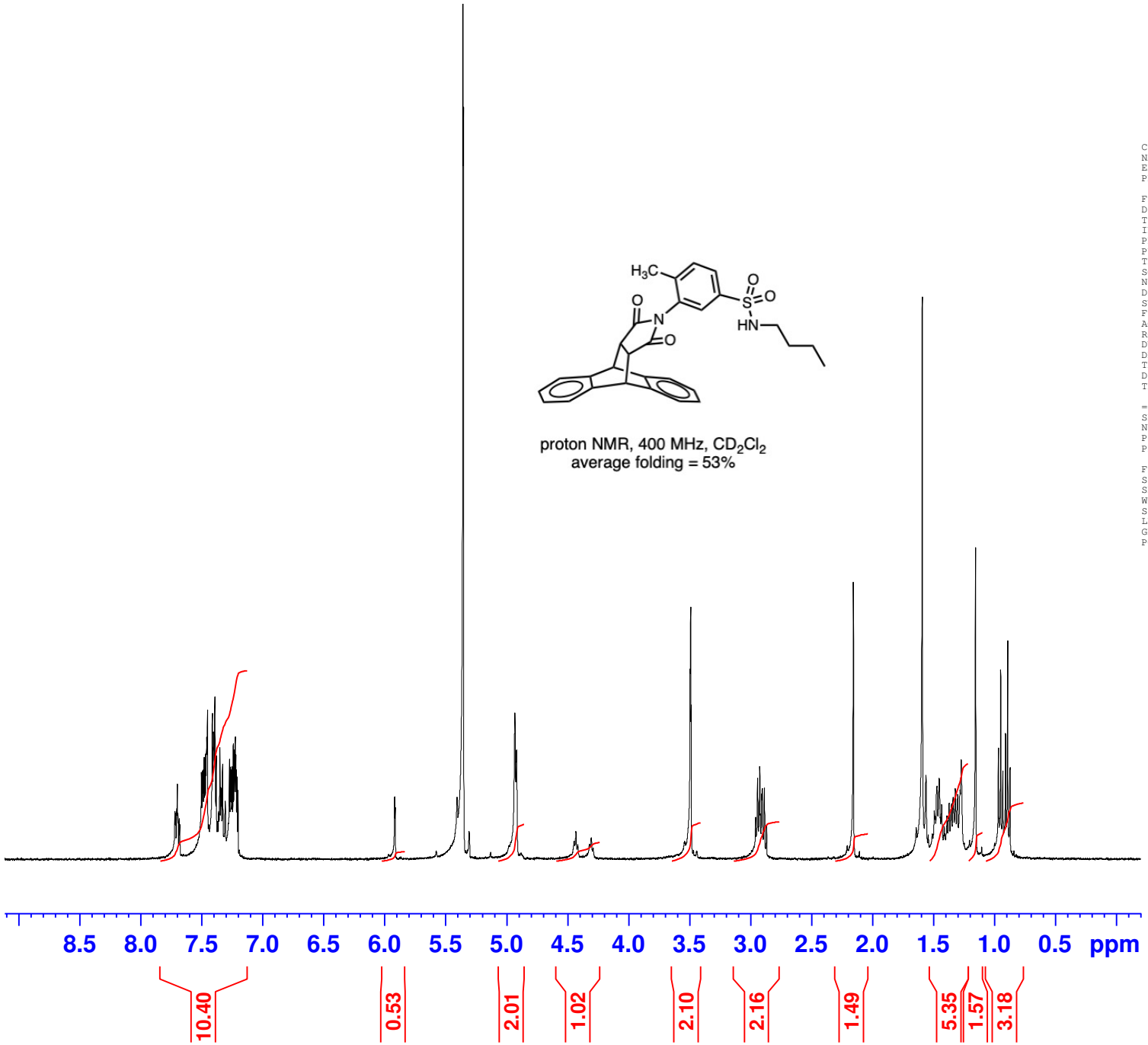



```
Current Data Parameters
NAME      controlnov19balanceindmso
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20221119
Time              14.33
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                 256
DW              62.400 usec
DE               6.50 usec
TE              298.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1               9.30 usec
PLW1        18.00000000 W

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



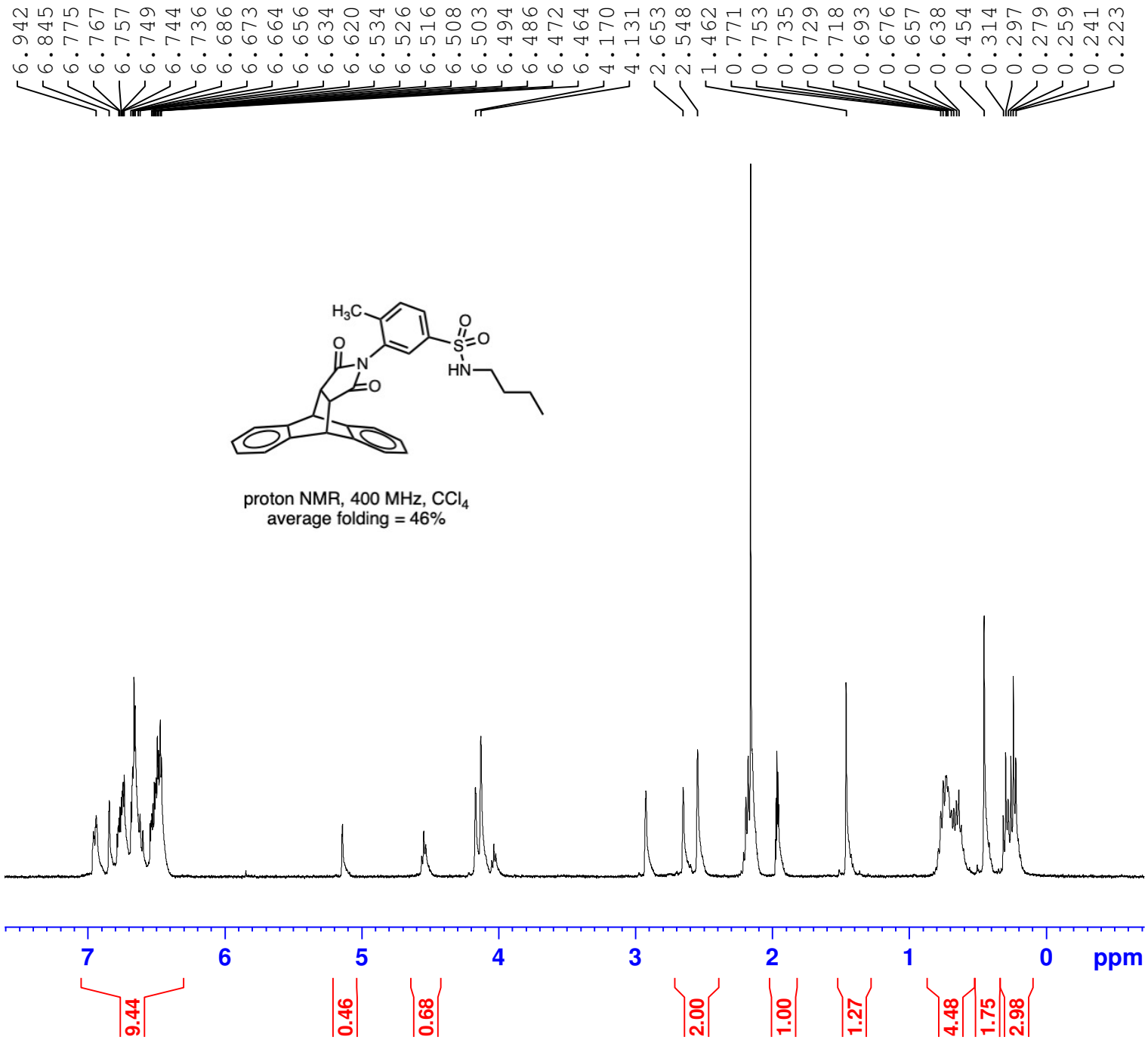
proton NMR, 400 MHz, CD_2Cl_2
average folding = 53%

```
Current Data Parameters
NAME      controlnov19balancein-methylenechloride
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221119
Time               19.00
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   575
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1         18.00000000 W

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

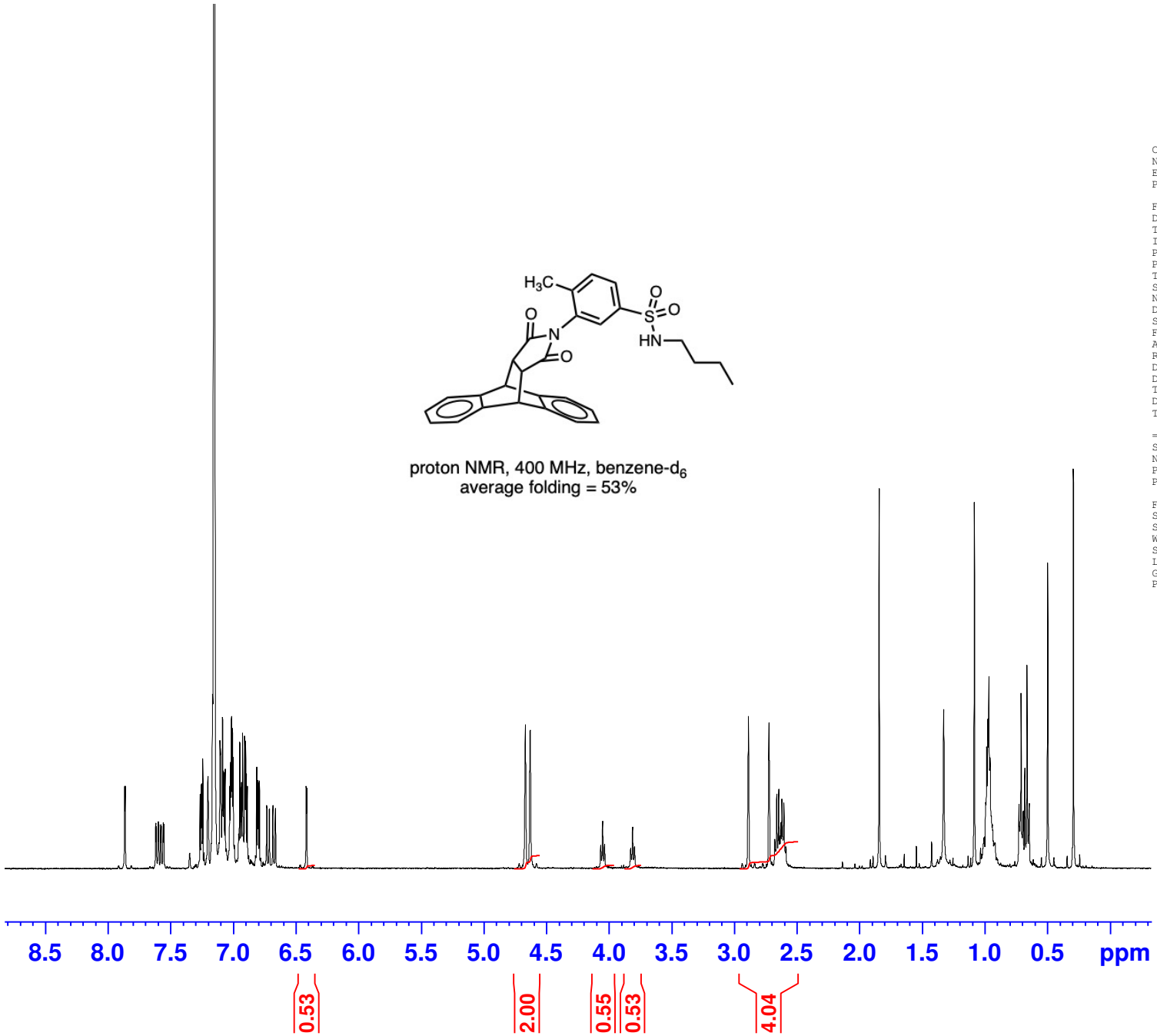



```
Current Data Parameters
NAME      controlnov19balancein-CC14
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20221119
Time              19.43
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CD3CN
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  645
DW               62.400 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                9.30 usec
PLW1         18.00000000 W

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

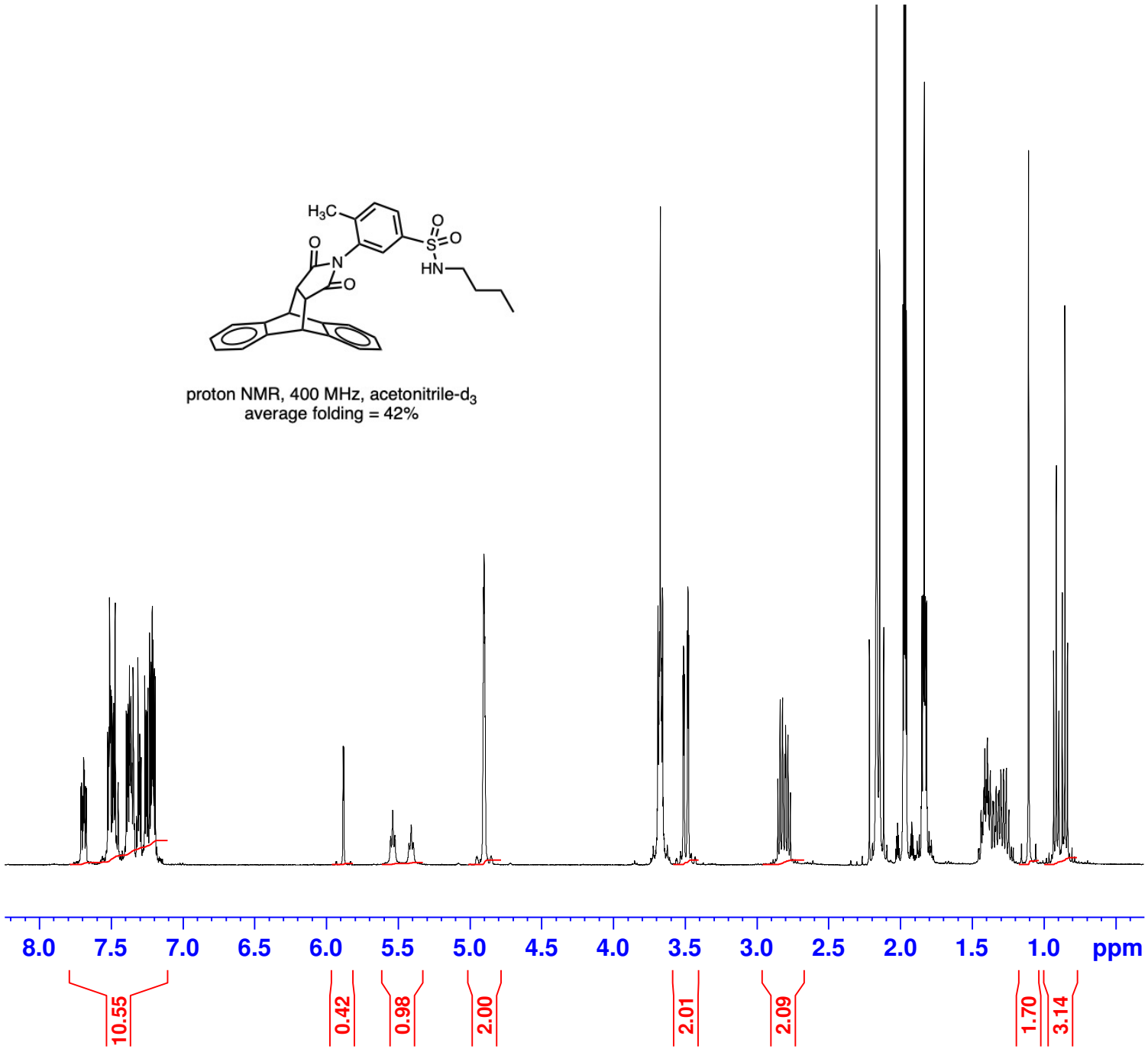



```
Current Data Parameters
NAME     balance-sulfanamide-control-benzene
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20221224
Time              15.31
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            C6D6
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  256
DW               62.400 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                9.30 usec
PLW1         18.00000000 W

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

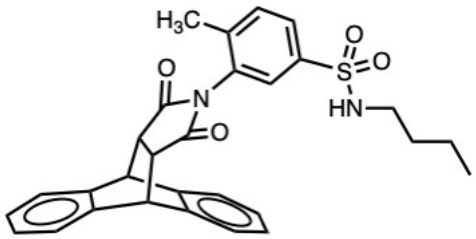



```
Current Data Parameters
NAME      controlnov19balancein-
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20221122
Time                   13.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CD3CN
NS                      160
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                      512
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                      1H
P1                     9.30 usec
PLW1            18.00000000 W

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



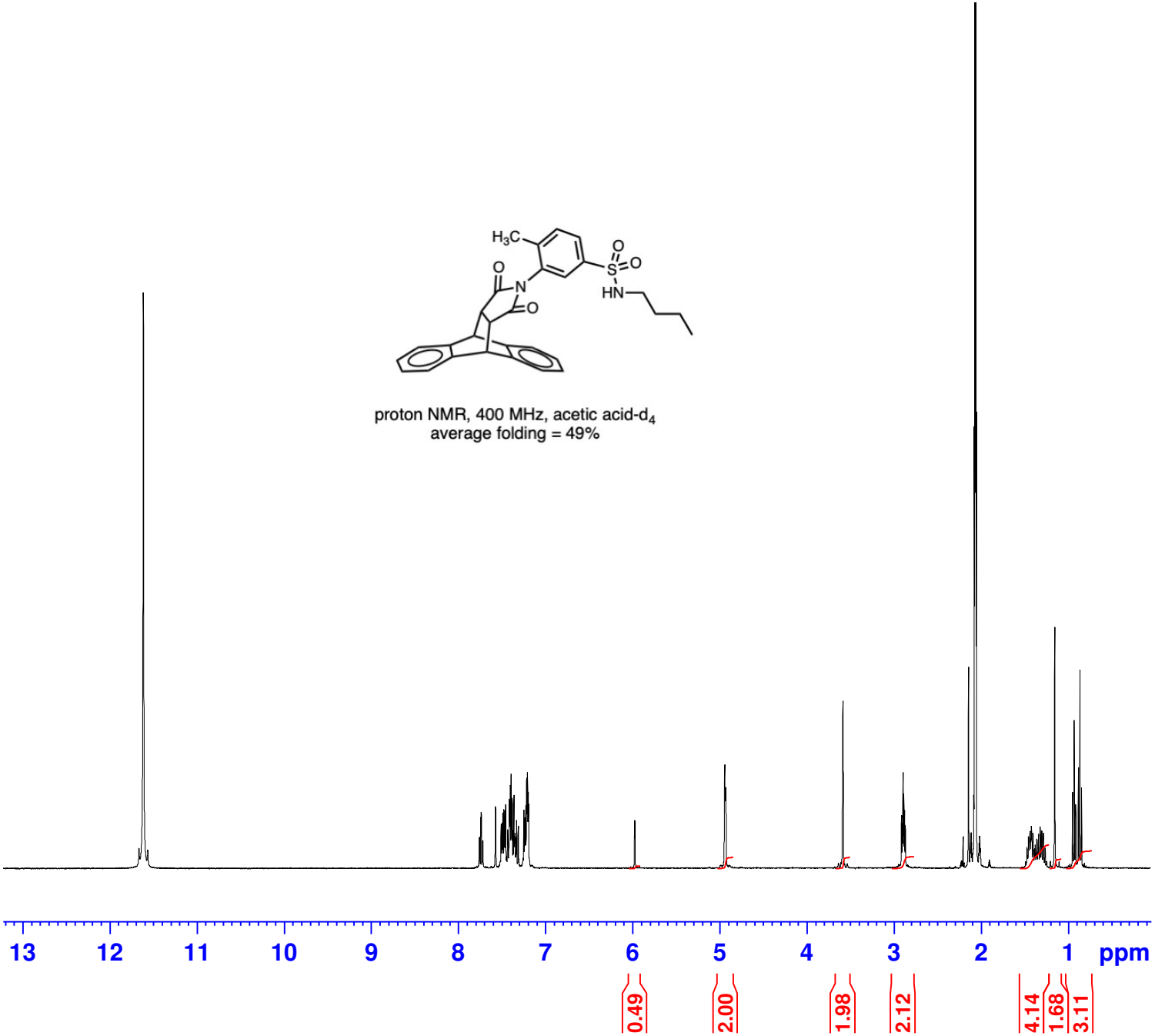
proton NMR, 400 MHz, acetone-d_6
average folding = 40%

```
Current Data Parameters
NAME      controlnov19balanceinacetone
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221119
Time              15.27
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                  512
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 9.30 usec
PLW1        18.00000000 W

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




```
Current Data Parameters
NAME      controlnov19balanceinaceticacid
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221119
Time              16.32
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT           Acetic
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                    322
DW                 62.400 usec
DE                  6.50 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.30 usec
PLW1         18.00000000 W

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