Supporting Information

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The Theoretical and Experimental Study of Diazomethane- Styrene [3+2]-Cycloadditions

Sergey P. Ivonin[1], Serhii Shuvakin[1,2]

[1] *Institute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Akademik Kuhar str., 02660 Kyiv, Ukraine*

[2] *Enamine Ltd, 78 Winston Churchill str., 02094 Kyiv, Ukraine*

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Computed Energies, Thermochemical Parameters, and Frequencies for Model Reactions

Table S1. Calculated (RI-BP86/TZVP) total energy values (E), total energy values (E), total correction (TC) – total thermal correction + zero point energy (ZPE), corrected energy (E+TC), enthalpy (H) – E+TC+RT; entropy term (ET); Gibbs free energy (G = H-ET), relative energy, enthalpy and Gibbs free energy values (ΔE, ΔH and ΔG, respectively) and lowest vibration frequencies (ν, cm^{-1}) for model reactions (Figure 1).

Struc-ture*	X	E, a.u.	TEC, a.u.	E+TEC, a.u.	ΔE kcal/mol^{-1}	RT, a.u.	H, a.u.	ΔH, kcal/mol^{-1}	ET, a.u.	G, a.u.	ΔG, kcal·mol^{-1}	ν (cm^{-1})
CH_2N_2	-	-148.814289	0.03441306	-148.779876		0.000944	-148.778932		0.027664	-148.806596		367.4
1h	CH	-309.752616	0.136126	-309.616491		0.000944	-309.615546		0.038879	-309.654426		46.5
1h-TS	CH	-458.546364	0.172900	-458.373465	14.37	0.000944	-458.372520	13.78	0.046239	-458.418759	26.52	-422.9
2h	CH	-458.605501	0.177305	-458.428196	-19.97	0.000944	-458.427251	-20.57	0.044349	-458.471601	-6.64	29.9
1f	CMe	-349.081967	0.163535	-348.918432		0.000944	-348.917488		0.041281	-348.958769		46.3
1f-TS	CMe	-497.875294	0.201242	-497.674052	15.22	0.000944	-497.673107	14.63	0.050696	-497.723804	26.08	-423.3
2f	CMe	-497.934772	0.204719	-497.730053	-19.92	0.000944	-497.729109	-20.51	0.046629	-497.775738	-6.51	30.7
1a	CF	-409.039134	0.128975	-408.910159		0.000944	-408.909215		0.040947	-408.950162		46.2
1a-TS	CF	-557.832689	0.165758	-557.666931	14.50	0.000944	-557.665987	13.91	0.048232	-557.714218	26.69	-424.3
2a	CF	-557.891792	0.170140	-557.721652	-19.84	0.000944	-557.720707	-20.43	0.046311	-557.767019	-6.44	26.8
1b	CCOOMe	-537.734892	0.182069	-537.552822		0.000944	-537.551878		0.049572	-537.601450		39.8
1b-TS	CCOOMe	-686.530416	0.218894	-686.311522	13.29	0.000944	-686.310578	12.70	0.056655	-686.367232	25.61	-417.6
2b	CCOOMe	-686.587323	0.223212	-686.364111	-19.71	0.000944	-686.363167	-20.30	0.054800	-686.417967	-6.23	24.4
1g	N	-325.801194	0.124629	-325.676565		0.000944	-325.675621		0.038715	-325.714336		45.9
1g_TS	N	-474.597241	0.161488	-474.435753	12.98	0.000944	-474.434809	12.39	0.046023	-474.480832	25.16	-412.9
2g	N	-474.653902	0.165759	-474.488143	-19.89	0.000944	-474.487199	-20.49	0.044260	-474.531459	-6.61	26.6

*) Denoted in accord with Fig. 1

Table S2. Calculated (RICOSX-M06-2X/def2-TZVP) total energy values (E), total correction (TC) – total thermal correction + zero point energy (ZPE), corrected energy (E+TC), enthalpy (H) – E+TC+RT; entropy term (ET); Gibbs free energy (G = H-ET), relative energy, enthalpy and Gibbs free energy values (ΔE, ΔH and ΔG, respectively) and lowest vibration frequencies (ν, cm^{-1}) for model reactions (Figure 1).

Struc-ture*	X*	E, a.u.	TEC, a.u.	E+TEC, a.u.	ΔE kcal/mol^{-1}	RT, a.u.	H, a.u.	ΔH, kcal/mol^{-1}	ET, a.u.	G, a.u.	ΔG, kcal·mol^{-1}	ν (cm^{-1})
CH_2N_2	-	-148.735197	0.03587424	-148.699323		0.000944	-148.698379		0.027387	-148.725766		447.9
1h	CH	-309.617500	0.141396	-309.476105		0.000944	-309.475160		0.038326	-309.513487		61.6
1h-TS	CH	-458.328704	0.179827	-458.148877	16.66	0.000944	-458.147933	16.07	0.045014	-458.192946	29.06	-520.4
2h	CH	-458.406436	0.184785	-458.221651	-29.01	0.000944	-458.220707	-29.60	0.043667	-458.264374	-15.76	29.9
1f	CMe	-348.928260	0.171022	-348.757238		0.000944	-348.756294		0.042059	-348.798353		69.7
1f-TS	CMe	-497.638821	0.209284	-497.429537	16.96	0.000944	-497.428593	16.37	0.048638	-497.477231	29.42	-526.5
2f	CMe	-497.716528	0.213519	-497.503010	-29.15	0.000944	-497.502066	-29.74	0.048074	-497.550139	-16.33	16.4
1a	CF	-408.871273	0.134140	-408.737133		0.000944	-408.736189		0.040266	-408.776455		67.3
1a-TS	CF	-557.582222	0.172587	-557.409635	16.83	0.000944	-557.408691	16.24	0.047014	-557.455705	29.19	-524.2
2a	CF	-557.660121	0.177373	-557.482748	-29.05	0.000944	-557.481804	-29.64	0.045526	-557.527331	-15.76	26.8
1b	CCOOMe	-537.507202	0.189859	-537.317343		0.000944	-537.316399		0.048060	-537.364459		59.9
1b-TS	CCOOMe	-686.220129	0.228134	-685.991995	15.48	0.000944	-685.991051	14.89	0.055183	-686.046234	27.60	-513.5
2b	CCOOMe	-686.295910	0.232889	-686.063021	-29.09	0.000944	-686.062077	-29.68	0.053279	-686.115356	-15.77	31.6
1g	N	-325.658983	0.129684	-325.529300		0.000944	-325.528355		0.038715	-325.567071		52.7
1g_TS	N	-474.372653	0.168168	-474.204486	15.15	0.000944	-474.203541	14.55	0.044806	-474.248348	27.92	-508.7
2g	N	-474.447757	0.172964	-474.274793	-28.97	0.000944	-474.273849	-29.56	0.043392	-474.317241	-15.31	39.7

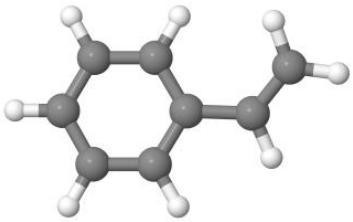
*) Denoted in accord with Fig. 1

Table S3. Calculated (CPCM(CH_2Cl_2)//RICOSX-M06-2X/def2-TZVP) total energy values (E), total correction (TC) – total thermal correction + zero point energy (ZPE), corrected energy (E+TC), enthalpy (H) – E+TC+RT; entropy term (ET); Gibbs free energy (G = H-ET), relative energy, enthalpy and Gibbs free energy values (ΔE, ΔH and ΔG, respectively) and lowest vibration frequencies (ν, cm^{-1}) for model reactions (Figure 1).

Struc-ture*	X*	E, a.u.	TEC, a.u.	E+TEC, a.u.	ΔE kcal/mol^{-1}	RT, a.u.	H, a.u.	ΔH, kcal/mol^{-1}	ET, a.u.	G, a.u.	ΔG, kcal·mol^{-1}	ν (cm^{-1})
CH_2N_2	-	-148.738974	0.03587424	-148.703100		0.000944	-148.702156		0.027387	-148.729543		447.9
1h	CH	-309.623004	0.141396	-309.481609		0.000944	-309.480664		0.038326	-309.518991		61.6
1h-TS	CH	-458.338165	0.179827	-458.158338	14.18	0.000944	-458.157394	13.59	0.045014	-458.202408	26.57	-520.4
2h	CH	-458.418100	0.184785	-458.233315	-32.87	0.000944	-458.232371	-33.46	0.043667	-458.276037	-19.63	29.9
1f	CMe	-348.933996	0.171022	-348.762974		0.000944	-348.762030		0.042059	-348.804088		69.7
1f-TS	CMe	-497.648227	0.209284	-497.438943	14.65	0.000944	-497.437999	14.06	0.048638	-497.486637	27.12	-526.5
2f	CMe	-497.728915	0.213519	-497.515397	-33.32	0.000944	-497.514452	-33.91	0.048074	-497.562526	-20.50	16.4
1a	CF	-408.877148	0.134140	-408.743008		0.000944	-408.742064		0.040266	-408.782330		67.3
1a-TS	CF	-557.591989	0.172587	-557.419402	14.39	0.000944	-557.418458	13.80	0.047014	-557.465473	26.75	-524.2
2a	CF	-557.672374	0.177373	-557.495001	-33.05	0.000944	-557.494057	-33.64	0.045526	-557.539584	-19.76	26.8
1b	CCOOMe	-537.516797	0.189859	-537.326938		0.000944	-537.325993		0.048060	-537.374053		59.9
1b-TS	CCOOMe	-686.234487	0.228134	-686.006353	12.49	0.000944	-686.005409	11.90	0.055183	-686.060592	24.62	-513.5
2b	CCOOMe	-686.311851	0.232889	-686.078962	-33.07	0.000944	-686.078018	-33.66	0.053279	-686.131297	-19.75	31.6
1g	N	-325.667187	0.129684	-325.537503		0.000944	-325.536559		0.038715	-325.575275		52.7
1g_TS	N	-474.385802	0.168168	-474.217634	12.04	0.000944	-474.216690	11.45	0.044806	-474.261496	24.81	-508.7
2g	N	-474.462254	0.172964	-474.289290	-32.92	0.000944	-474.288346	-33.51	0.043392	-474.331738	-19.26	39.7

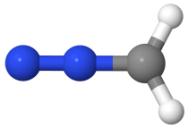
*) Denoted in accord with Fig. 1

Cartesian coordinates corresponding to the equilibrium local minima structures and transition states (RICOSX-M06-2X/def2-TZVP)



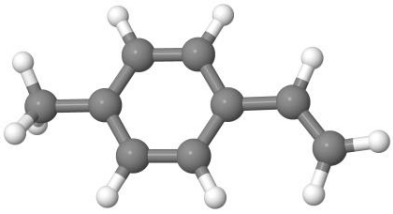
1h

C	-2.09987	0.54764	0.31261
C	-2.06574	-0.83949	0.39951
C	-0.86359	-1.50725	0.22159
C	0.29524	-0.78931	-0.03582
C	0.27839	0.60313	-0.11170
C	-0.94163	1.26147	0.05767
C	1.53814	1.32056	-0.36658
C	1.75119	2.62208	-0.21000
H	-3.03795	1.07323	0.43694
H	-2.97357	-1.39381	0.59825
H	-0.82679	-2.58730	0.28167
H	1.23442	-1.31222	-0.17376
H	-0.98787	2.33965	-0.02633
H	2.36280	0.69517	-0.69614
H	2.71943	3.05490	-0.42151
H	0.98144	3.29722	0.14239



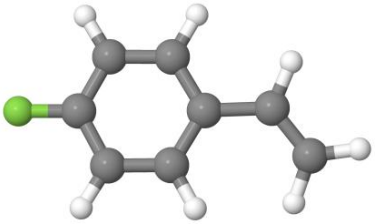
CH_2N_2

C	-0.00000	0.00000	-1.21110
N	-0.00000	0.00000	0.08014
N	0.00000	-0.00000	1.20426
H	-0.95290	-0.00000	-1.70866
H	0.95290	-0.00000	-1.70866



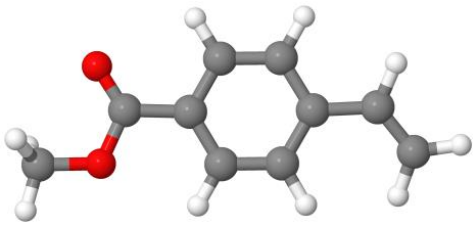
1f

C	-2.09987	0.54764	0.31261
C	-2.06574	-0.83949	0.39951
C	-0.86359	-1.50725	0.22159
C	0.29524	-0.78931	-0.03582
C	0.27839	0.60313	-0.11170
C	-0.94163	1.26147	0.05767
C	1.53814	1.32056	-0.36658
C	1.75119	2.62208	-0.21000
H	-3.03795	1.07323	0.43694
H	-2.97357	-1.39381	0.59825
H	-0.82679	-2.58730	0.28167
H	1.23442	-1.31222	-0.17376
H	-0.98787	2.33965	-0.02633
H	2.36280	0.69517	-0.69614
H	2.71943	3.05490	-0.42151
H	0.98144	3.29722	0.14239



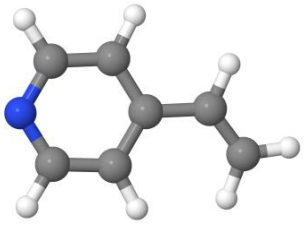
1a

C	-1.99711	0.53863	0.45158
C	-1.99745	-0.84189	0.35771
C	-0.85516	-1.55733	0.06668
C	0.32719	-0.85932	-0.12279
C	0.37911	0.53010	-0.01589
C	-0.80577	1.21643	0.26182
C	1.67119	1.20988	-0.19373
C	1.95209	2.47134	0.11231
F	-3.14387	-1.50815	0.55024
H	-2.92089	1.05955	0.66389
H	-0.90504	-2.63482	-0.00749
H	1.23388	-1.40613	-0.35101
H	-0.80221	2.29713	0.31980
H	2.46170	0.58539	-0.59934
H	2.94186	2.87424	-0.05304
H	1.21922	3.14144	0.54434



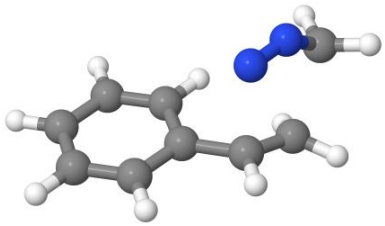
1b

C	-0.54647	0.62720	0.07638
C	-0.59938	-0.75961	-0.04723
C	0.54826	-1.46413	-0.39106
C	1.73453	-0.78617	-0.60922
C	1.80652	0.60160	-0.47685
C	0.64307	1.29769	-0.13695
C	3.09739	1.27039	-0.70082
C	3.39136	2.53438	-0.41719
C	-1.85224	-1.52979	0.17928
O	-1.92740	-2.72907	0.13891
O	-2.90557	-0.74199	0.43691
C	-4.13035	-1.43090	0.67190
H	-1.44186	1.17404	0.33707
H	0.49161	-2.54043	-0.48507
H	2.62664	-1.33768	-0.88095
H	0.66508	2.37587	-0.04964
H	3.87180	0.63812	-1.12451
H	4.37748	2.93156	-0.61587
H	2.67398	3.21328	0.02633
H	-4.87591	-0.66157	0.84864
H	-4.03757	-2.08310	1.53906
H	-4.39780	-2.03341	-0.19492



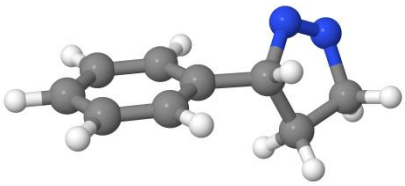
1g

C	-1.95790	0.21199	0.85563
N	-1.94201	-1.13329	0.85622
C	-0.75077	-1.71549	0.65348
C	0.43470	-1.00786	0.44867
C	0.41804	0.39747	0.44821
C	-0.83190	1.00765	0.66076
C	1.66717	1.13945	0.23265
C	1.81905	2.47219	0.20537
H	-2.93399	0.67777	1.02165
H	-0.74371	-2.80977	0.65491
H	1.37201	-1.54552	0.28938
H	-0.93306	2.09371	0.67515
H	2.55127	0.51150	0.08134
H	2.79801	2.92039	0.03661
H	0.98575	3.16223	0.34818



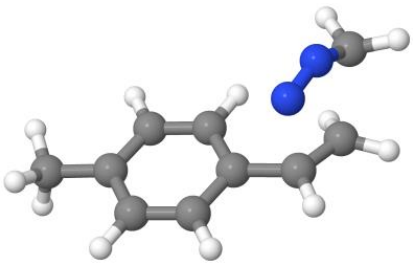
1h-TS

C	-1.76823	0.34024	1.40395
C	-0.83901	-0.58869	0.98924
C	0.49192	-0.23712	0.48418
C	0.80132	1.04900	0.02926
C	2.06674	1.35390	-0.44743
C	3.05578	0.38015	-0.48988
C	2.76036	-0.90513	-0.05426
C	1.49536	-1.20830	0.42254
H	-2.58915	0.01380	2.02878
H	-1.47309	1.37178	1.54965
H	-0.99281	-1.63095	1.23829
H	0.04238	1.82238	0.04322
H	2.28129	2.35804	-0.79121
H	4.04312	0.61900	-0.86233
H	3.51945	-1.67622	-0.08840
H	1.27218	-2.21444	0.75779
N	-1.71669	-1.00872	-1.14147
N	-2.47552	-0.16752	-1.07931
C	-2.98551	0.79921	-0.30035
H	-2.74481	1.79618	-0.65162
H	-4.02275	0.63166	-0.03477



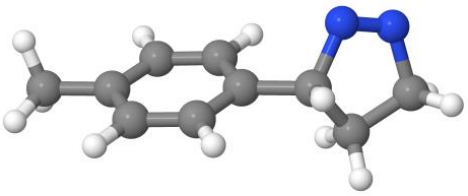
2h

C	1.61388	-1.00289	0.89539
C	0.27752	-0.35568	1.26537
C	-0.67272	-0.13427	0.12306
C	-0.53537	0.97434	-0.70729
C	-1.38499	1.14936	-1.79009
C	-2.37735	0.21543	-2.05735
C	-2.52022	-0.89179	-1.23310
C	-1.67465	-1.06052	-0.14535
N	0.68029	0.92796	1.91979
N	1.85877	0.93230	2.25105
C	2.54544	-0.33795	1.89815
H	1.59118	-2.08726	0.97339
H	1.88336	-0.73206	-0.12632
H	-0.22969	-0.92594	2.05098
H	0.23101	1.70978	-0.49301
H	-1.27605	2.02057	-2.42304
H	-3.04057	0.35439	-2.90115
H	-3.29557	-1.62061	-1.43132
H	-1.79402	-1.92067	0.50371
H	3.54369	-0.11016	1.53059
H	2.64850	-0.90237	2.82878



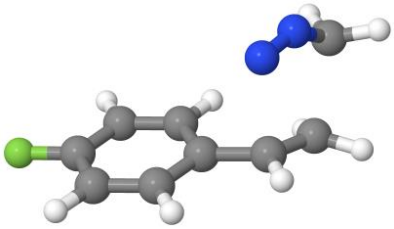
1f-TS

C	-1.76823	0.34024	1.40395
C	-0.83901	-0.58869	0.98924
C	0.49192	-0.23712	0.48418
C	0.80132	1.04900	0.02926
C	2.06674	1.35390	-0.44743
C	3.05578	0.38015	-0.48988
C	2.76036	-0.90513	-0.05426
C	1.49536	-1.20830	0.42254
H	-2.58915	0.01380	2.02878
H	-1.47309	1.37178	1.54965
H	-0.99281	-1.63095	1.23829
H	0.04238	1.82238	0.04322
H	2.28129	2.35804	-0.79121
H	4.04312	0.61900	-0.86233
H	3.51945	-1.67622	-0.08840
H	1.27218	-2.21444	0.75779
N	-1.71669	-1.00872	-1.14147
N	-2.47552	-0.16752	-1.07931
C	-2.98551	0.79921	-0.30035
H	-2.74481	1.79618	-0.65162
H	-4.02275	0.63166	-0.03477



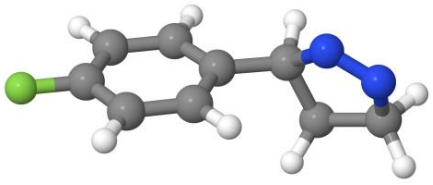
2f

C	1.61388	-1.00289	0.89539
C	0.27752	-0.35568	1.26537
C	-0.67272	-0.13427	0.12306
C	-0.53537	0.97434	-0.70729
C	-1.38499	1.14936	-1.79009
C	-2.37735	0.21543	-2.05735
C	-2.52022	-0.89179	-1.23310
C	-1.67465	-1.06052	-0.14535
N	0.68029	0.92796	1.91979
N	1.85877	0.93230	2.25105
C	2.54544	-0.33795	1.89815
H	1.59118	-2.08726	0.97339
H	1.88336	-0.73206	-0.12632
H	-0.22969	-0.92594	2.05098
H	0.23101	1.70978	-0.49301
H	-1.27605	2.02057	-2.42304
H	-3.04057	0.35439	-2.90115
H	-3.29557	-1.62061	-1.43132
H	-1.79402	-1.92067	0.50371
H	3.54369	-0.11016	1.53059
H	2.64850	-0.90237	2.82878



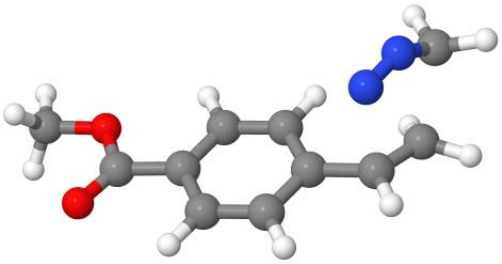
1a-TS

C	2.26746	-0.23607	1.37989
C	1.34280	0.68778	0.94541
C	-0.03286	0.35197	0.56440
C	-0.44878	-0.96339	0.33463
C	-1.74925	-1.25508	-0.04654
C	-2.64402	-0.21535	-0.20453
C	-2.27770	1.09901	0.00882
C	-0.97434	1.37085	0.38883
F	-3.90424	-0.48834	-0.58140
H	3.14655	0.11561	1.90366
H	1.95104	-1.23455	1.65345
H	1.55360	1.74152	1.07404
H	0.25279	-1.78047	0.45010
H	-2.07439	-2.27108	-0.22611
H	-3.00853	1.88481	-0.12665
H	-0.67355	2.39842	0.55364
N	2.07868	0.87252	-1.27373
N	2.79245	-0.00558	-1.18951
C	3.31286	-0.92185	-0.35780
H	2.99671	-1.93245	-0.59042
H	4.37503	-0.78961	-0.18839



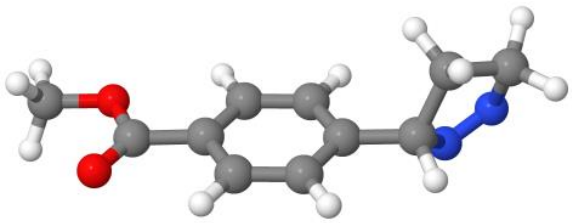
2a

C	-0.48320	-0.29682	1.87086
C	-0.29563	-1.66361	1.78710
C	-0.14631	-2.31221	0.57781
C	-0.19219	-1.55687	-0.58615
C	-0.37613	-0.17987	-0.54052
C	-0.51990	0.43990	0.69788
C	-0.38872	0.64052	-1.79931
C	0.89786	1.41241	-2.10735
F	-0.26697	-2.38208	2.91949
C	0.34043	2.69015	-2.72024
N	-1.05374	2.76914	-2.21452
N	-1.43720	1.70855	-1.73965
H	-0.60592	0.16583	2.84057
H	-0.00665	-3.38430	0.55783
H	-0.08637	-2.05132	-1.54469
H	-0.68122	1.51023	0.74418
H	-0.67941	0.00461	-2.64165
H	1.56272	0.86691	-2.77265
H	1.43236	1.62502	-1.18113
H	0.27093	2.65340	-3.81034
H	0.86504	3.60396	-2.44908



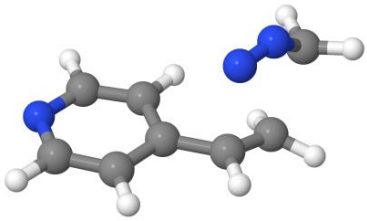
1b-TS

C	-3.44951	-0.16331	-1.29385
C	-2.61618	0.78497	-0.73815
C	-1.18004	0.59893	-0.54541
C	-0.57112	-0.66143	-0.60912
C	0.78809	-0.80977	-0.40353
C	1.57936	0.30072	-0.12107
C	0.98847	1.56020	-0.04828
C	-0.36851	1.70369	-0.25485
C	3.03755	0.19221	0.12271
O	3.75704	1.11712	0.39640
O	3.49011	-1.06776	0.01068
C	4.88124	-1.23178	0.26489
H	-4.41614	0.15364	-1.66251
H	-3.02927	-1.01666	-1.81112
H	-2.98663	1.79309	-0.60310
H	-1.16902	-1.54004	-0.81821
H	1.24438	-1.78873	-0.45534
H	1.61360	2.41435	0.17748
H	-0.82270	2.68515	-0.19093
H	5.11929	-0.92386	1.28241
H	5.46905	-0.63258	-0.42890
H	5.08689	-2.28920	0.12797
N	-3.10981	0.33852	1.54069
N	-3.71930	-0.58044	1.28378
C	-4.21165	-1.34658	0.29708
H	-3.75306	-2.32812	0.25862
H	-5.29388	-1.33113	0.24467



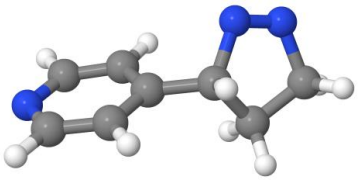
2b

C	-0.45201	-0.11450	-0.08377
C	-0.35797	-1.50195	-0.02091
C	0.47605	-2.18135	-0.90076
C	1.21222	-1.47614	-1.83851
C	1.12700	-0.08947	-1.90656
C	0.28790	0.58406	-1.02235
C	1.94569	0.68561	-2.89899
C	3.13999	1.44748	-2.32003
C	-1.14151	-2.30456	0.95877
O	-1.12351	-3.50490	1.02000
O	-1.88118	-1.54250	1.77561
C	-2.66585	-2.26011	2.72473
C	3.14567	2.69727	-3.19125
N	1.75888	2.79339	-3.71357
N	1.13084	1.75480	-3.56168
H	-1.10887	0.40863	0.59679
H	0.53082	-3.26016	-0.83927
H	1.85591	-2.00813	-2.52896
H	0.20303	1.66258	-1.08416
H	2.25448	0.01995	-3.71103
H	4.06479	0.87807	-2.37123
H	2.94591	1.70116	-1.27732
H	-3.19553	-1.50799	3.30133
H	-2.02530	-2.86096	3.36864
H	-3.36705	-2.91768	2.21296
H	3.79957	2.61523	-4.06295
H	3.39087	3.62249	-2.67388



1g-TS

C	-1.76936	0.42448	1.38396
C	-0.83018	-0.52532	1.04266
C	0.48958	-0.19984	0.50812
C	0.82025	1.06100	0.00262
C	2.09251	1.28520	-0.49714
N	3.05109	0.36345	-0.54024
C	2.73561	-0.84099	-0.06749
C	1.49582	-1.16706	0.45394
H	-2.58426	0.13771	2.03553

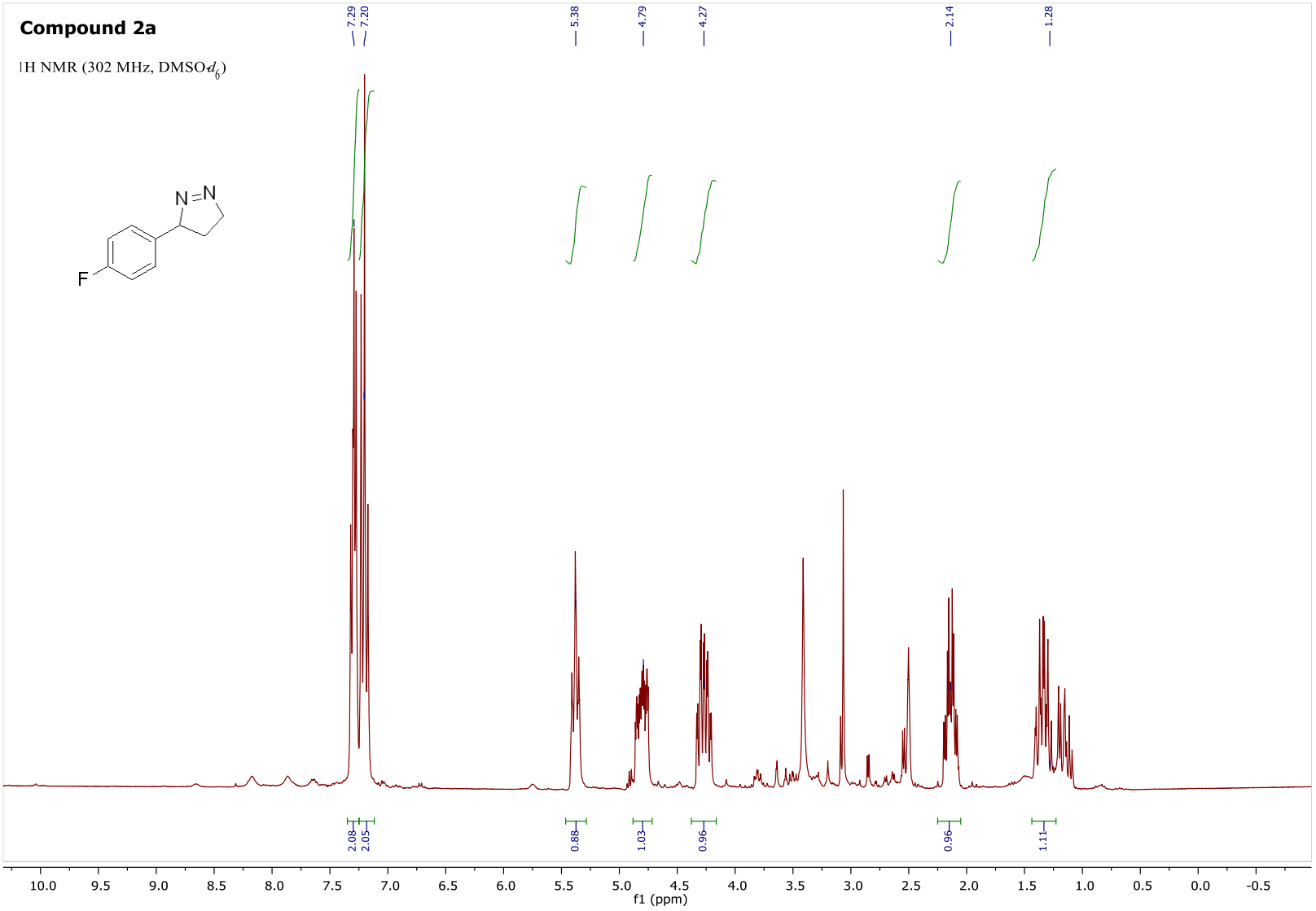


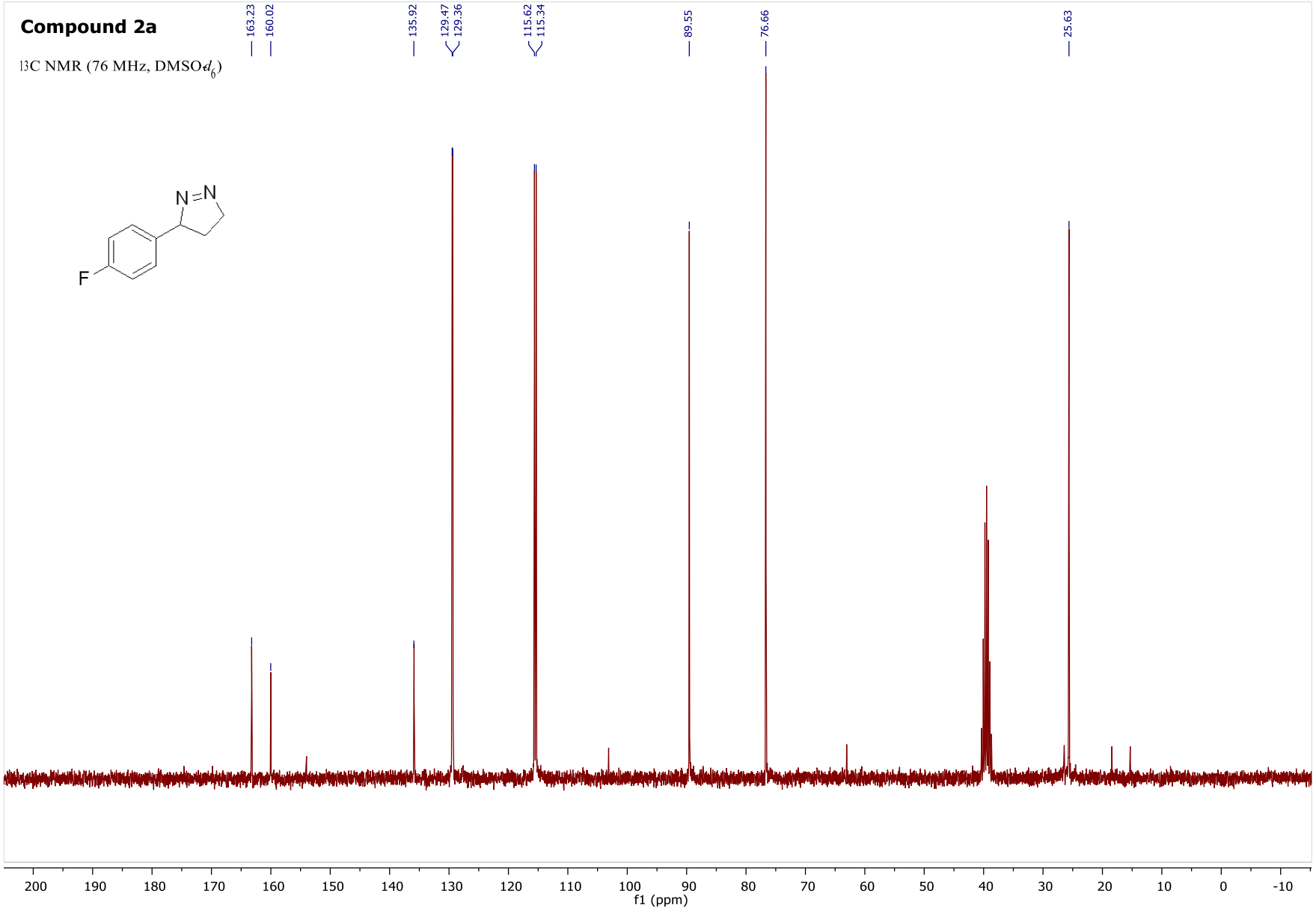
2g

C	1.75274	-0.76887	0.31414
C	0.39879	-0.24551	0.79884
C	-0.62474	-0.01000	-0.27339
C	-0.53920	1.09221	-1.11562
C	-1.48969	1.24862	-2.11333
N	-2.49101	0.39610	-2.31990
C	-2.56842	-0.65483	-1.51073
C	-1.67122	-0.89779	-0.47920
N	0.74576	1.02335	1.51556

H	-1.48096	1.46567	1.45596
H	-0.97838	-1.55103	1.35495
H	0.09885	1.86835	-0.00912
H	2.35414	2.26344	-0.88747
H	3.51940	-1.58986	-0.11102
H	1.30789	-2.16926	0.81871
N	-1.68850	-1.07830	-1.09181
N	-2.45724	-0.24814	-1.05728
C	-2.98456	0.75055	-0.33141
H	-2.76631	1.72983	-0.74225
H	-4.01806	0.57653	-0.05573
N	1.93921	1.09855	1.77455
C	2.69641	-0.08566	1.29590
H	1.81509	-1.85406	0.33552
H	1.93820	-0.42951	-0.70550
H	-0.02682	-0.90078	1.56544
H	0.24439	1.82883	-0.98682
H	-1.44772	2.10703	-2.77495
H	-3.39056	-1.33930	-1.69023
H	-1.79202	-1.76838	0.15359
H	3.64317	0.24930	0.87740
H	2.91424	-0.69256	2.17844

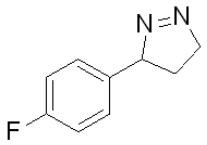
NMR spectra


Compound 2a
1H NMR (302 MHz, DMSO-d_6)
N=N
F
7.29
7.20
5.38
4.79
4.27
2.14
1.28
2.08
2.05
0.88
1.03
0.96
0.96
1.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Compound 2a
13C NMR (76 MHz, DMSO-d6)
163.23
160.02
135.92
129.47
129.36
115.62
115.34
89.55
76.66
25.63
N=N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

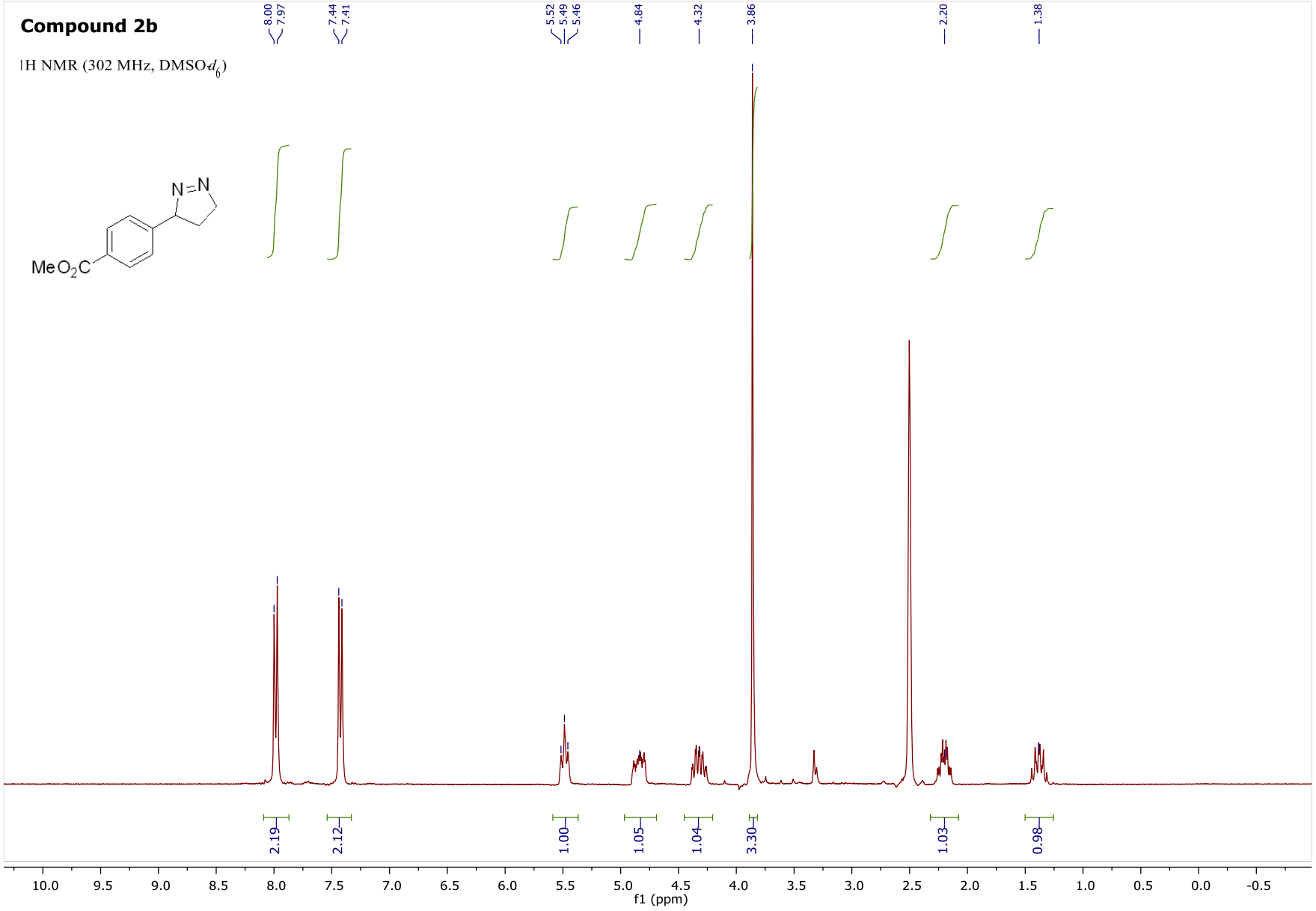
Compound 2a

^{19}F NMR (188 MHz, DMSOd_6)



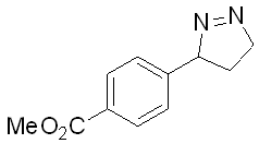
Compound 2b

^{1}H NMR (302 MHz, DMSO-d_6)



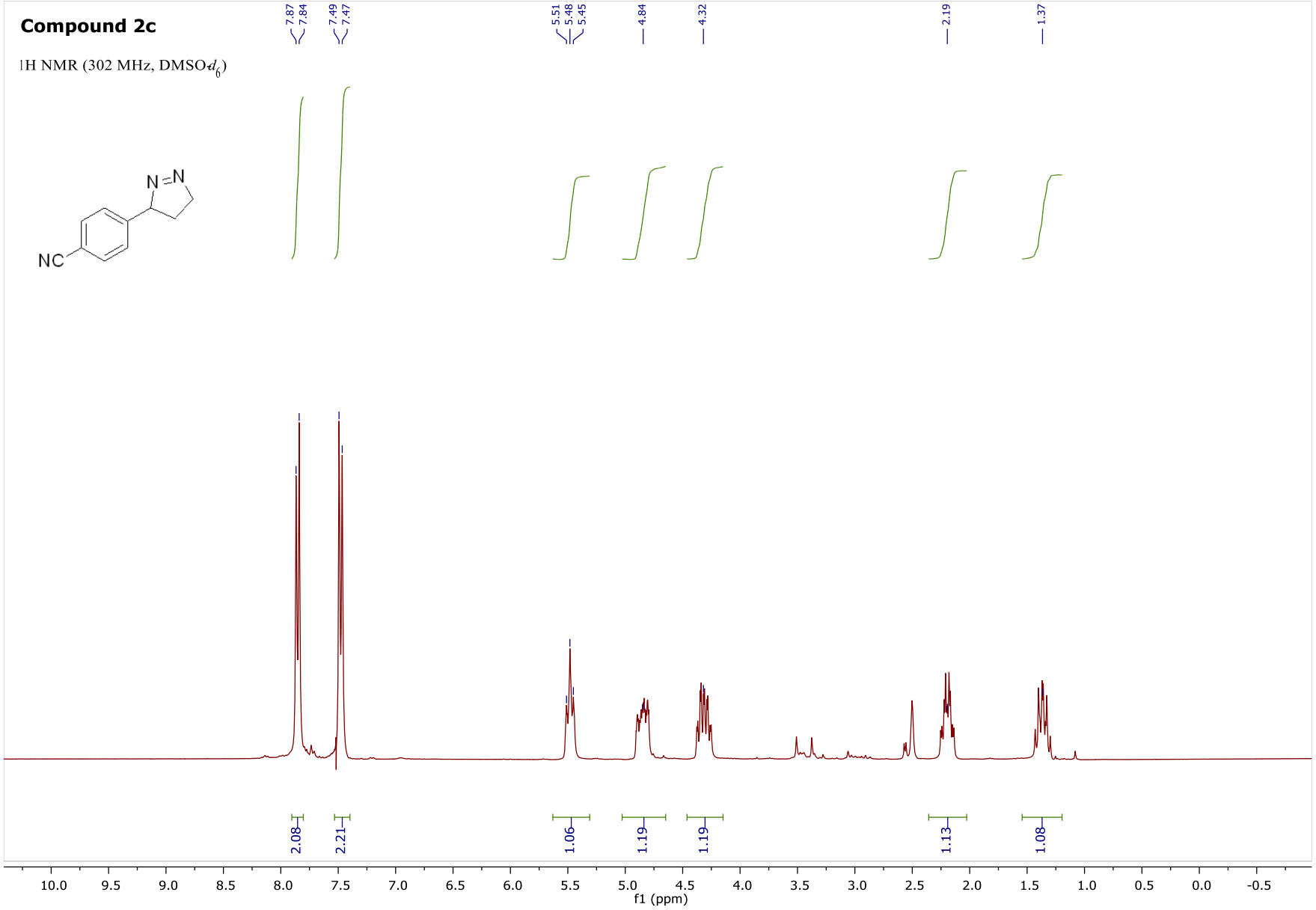
Compound 2b

^{13}C NMR (76 MHz, DMSO-d_6)



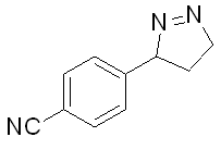
Compound 2c

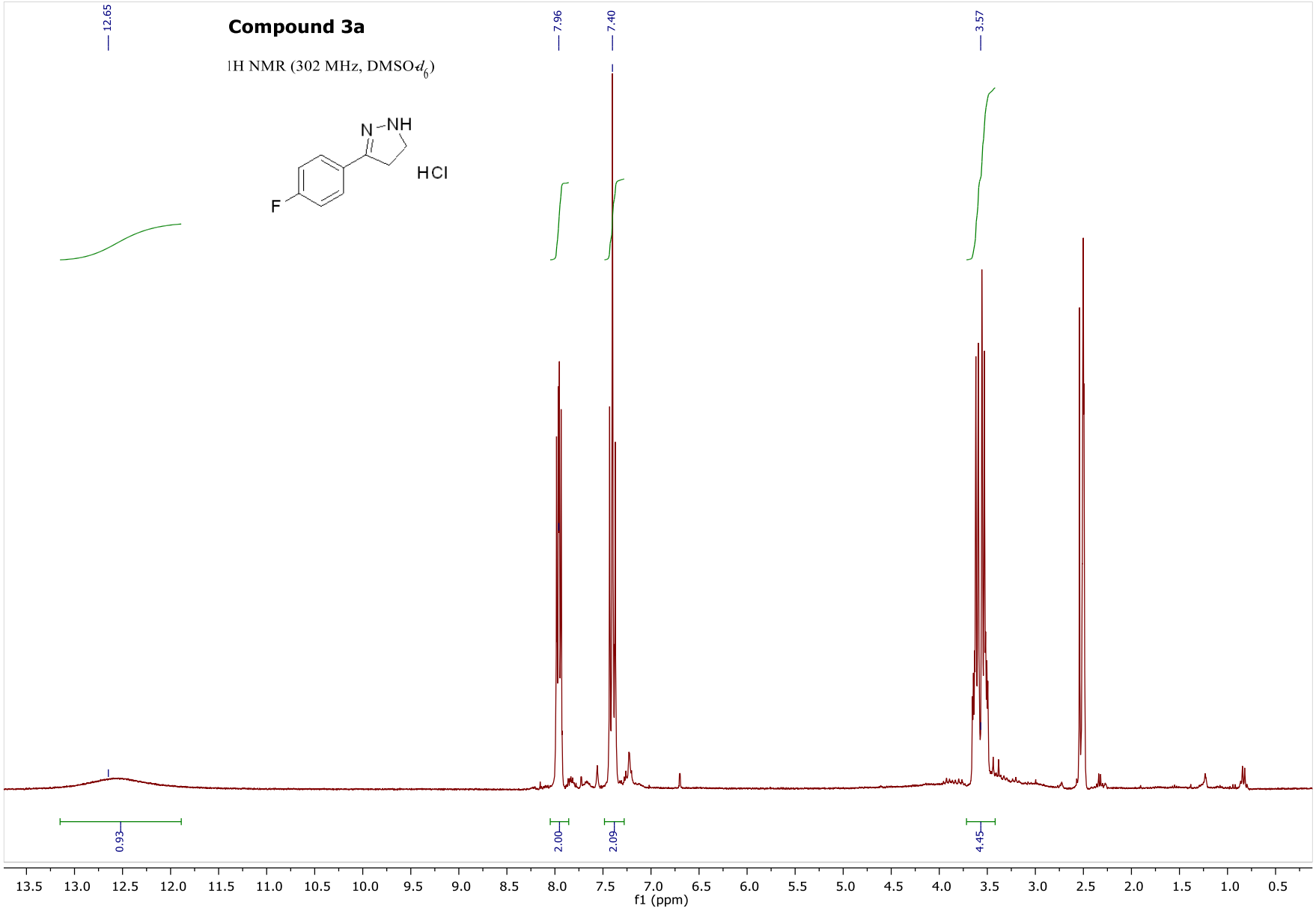
^{1}H NMR (302 MHz, DMSO-d_6)

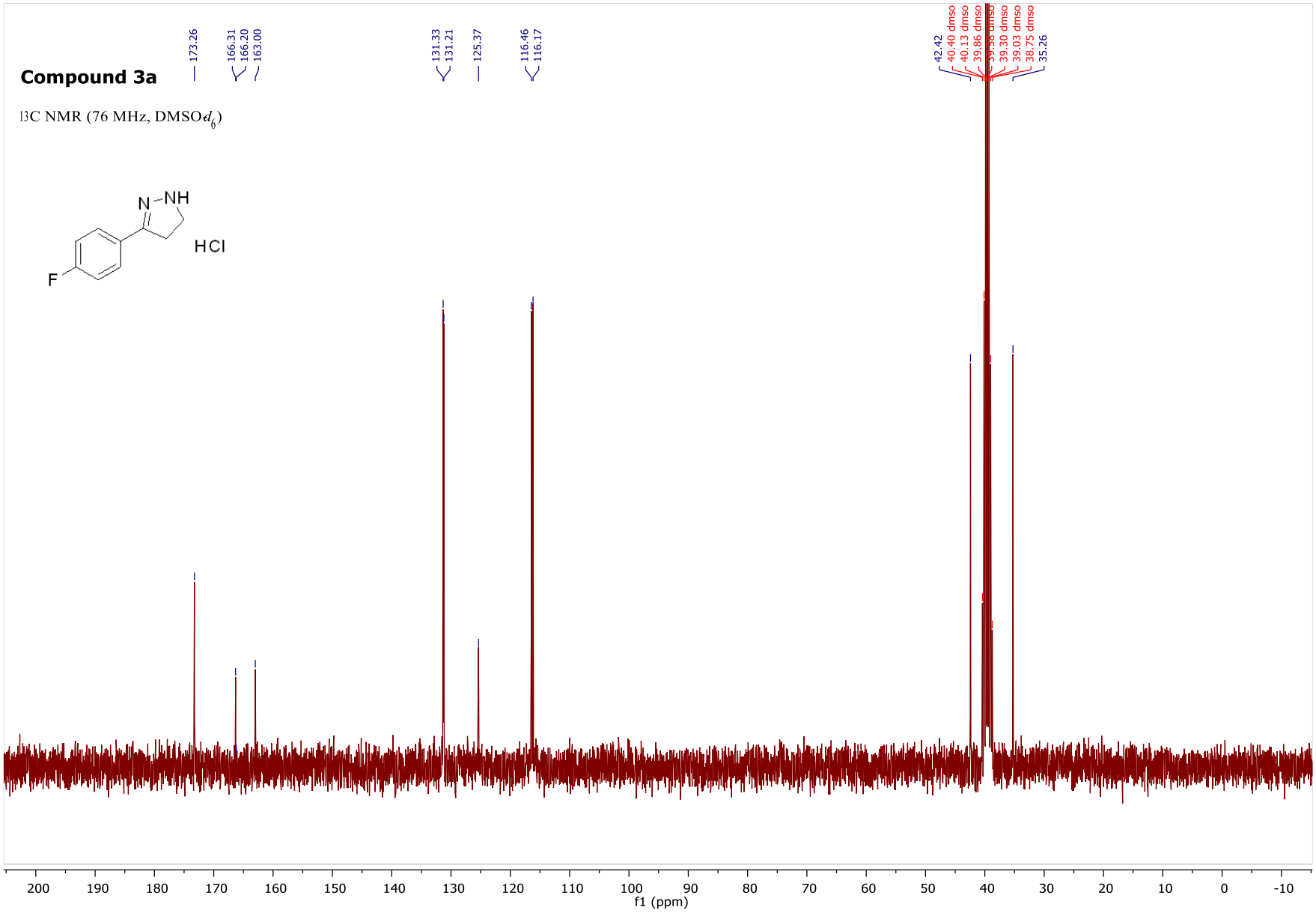


Compound 2c

^{13}C NMR (76 MHz, DMSO-d_6)

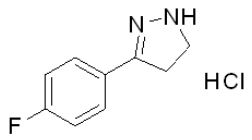



Compound 3a
1H NMR (302 MHz, DMSO-d_6)
N
NH
HCl
F
12.65
7.96
7.40
3.57
0.93
2.00
2.09
4.45
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


Compound 3a
13C NMR (76 MHz, DMSO-d_6)
173.26
166.31
166.20
163.00
131.33
131.21
125.37
116.46
116.17
42.42
40.40 dmso
40.13 dmso
39.86 dmso
39.30 dmso
39.03 dmso
38.75 dmso
35.26
N
NH
HCl
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

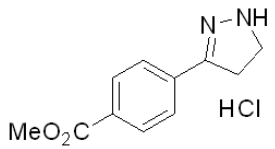
Compound 3a

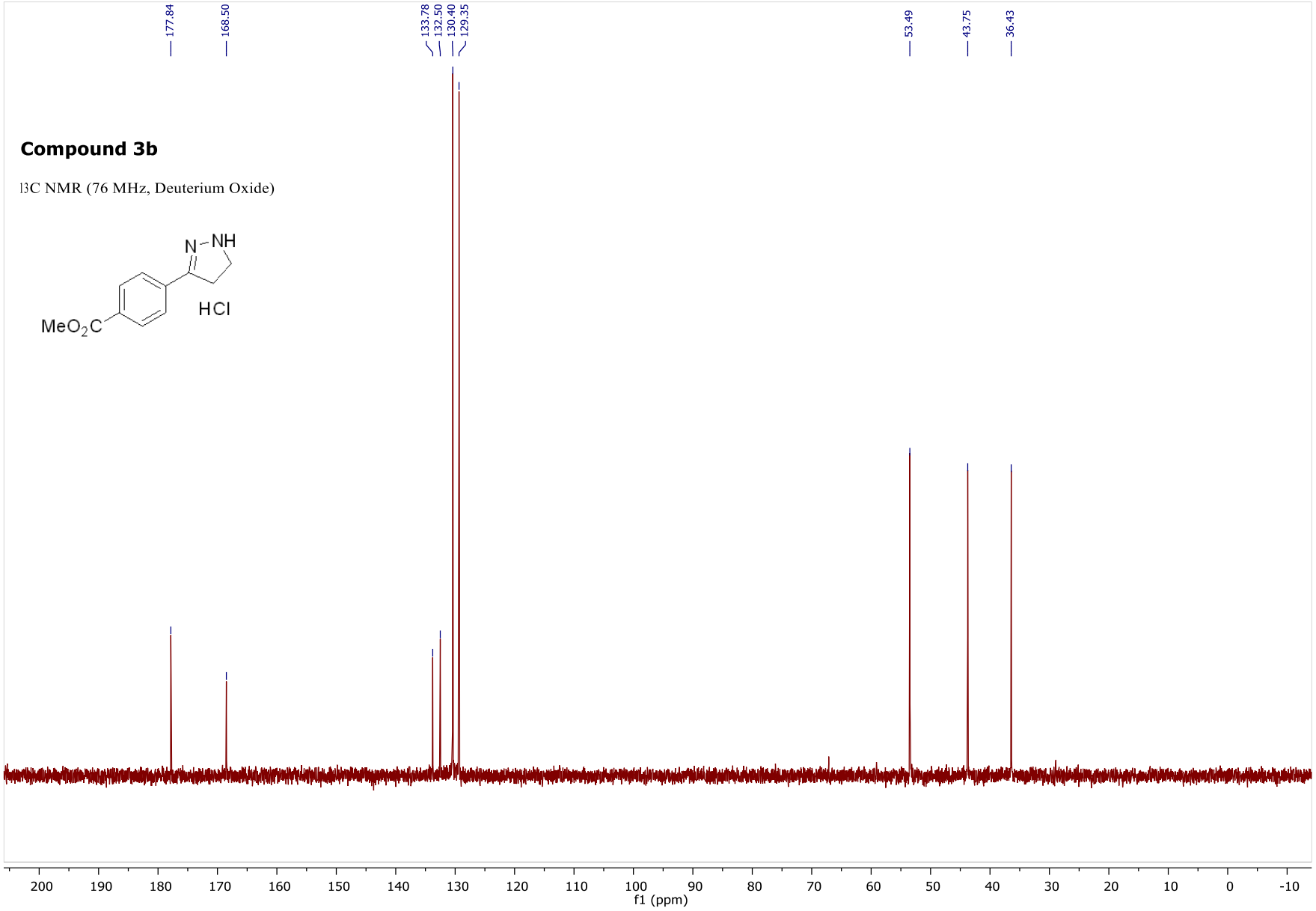
^{19}F NMR (188 MHz, DMSOd_6)



Compound 3b

1H NMR (302 MHz, Deuterium Oxide)




177.84
168.50
133.78
132.50
130.40
129.35
53.49
43.75
36.43
Compound 3b
13C NMR (76 MHz, Deuterium Oxide)
N
NH
HCl
MeO2C
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)