

Controlling Pd-catalyzed *N*-arylation and Dimroth rearrangement in the synthesis of *N*,1-diaryl-1*H*-tetrazol-5-amines

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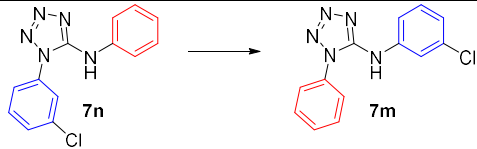
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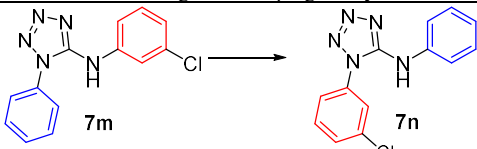
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Table S1. Monitoring reaction progress by ¹H NMR



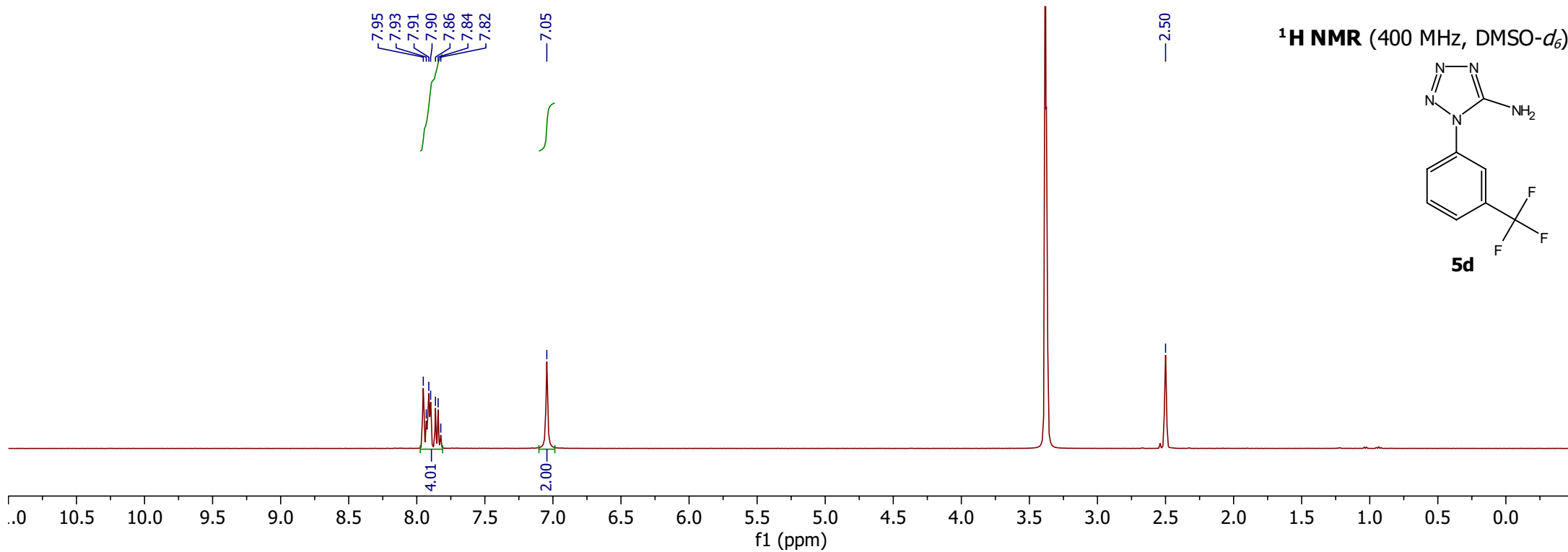
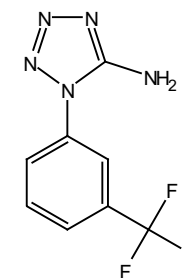
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6	29	0
11	34	0
16	40	0
21	45	0
26	50	0
31	56	0
36	60	0
41	65	0
46	70	0
51	75	0
56	80	<5
61	85	5
71	86	9
72	90	10
73	90	11
75	90	12
79	90	15
86	90	20
92	90	23

Table S2. Monitoring reactions progress by ¹H NMR

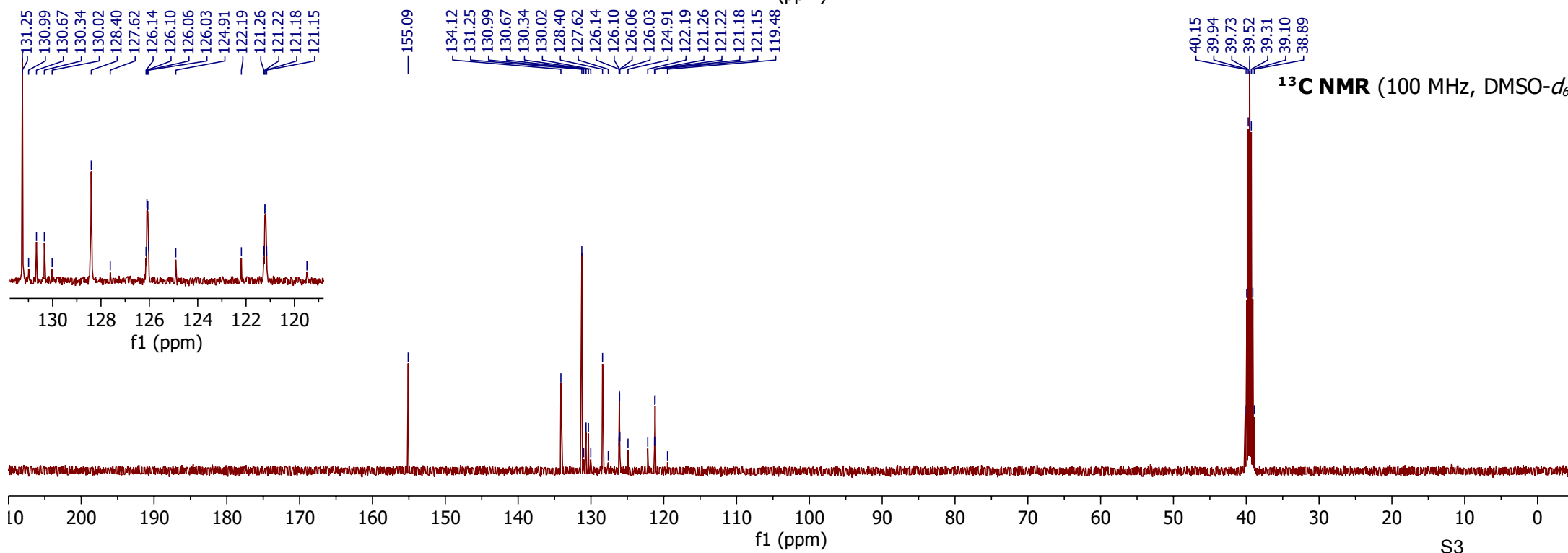


time (min.)	temperature (C°)	Yield (%) of 7n
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11	35	0
17	40	0
21	45	0
26	50	0
31	55	0
37	60	0
42	65	0
48	70	0
50	73	0
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74	99	5
75	100	6
80	100	7

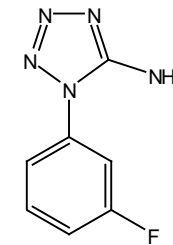
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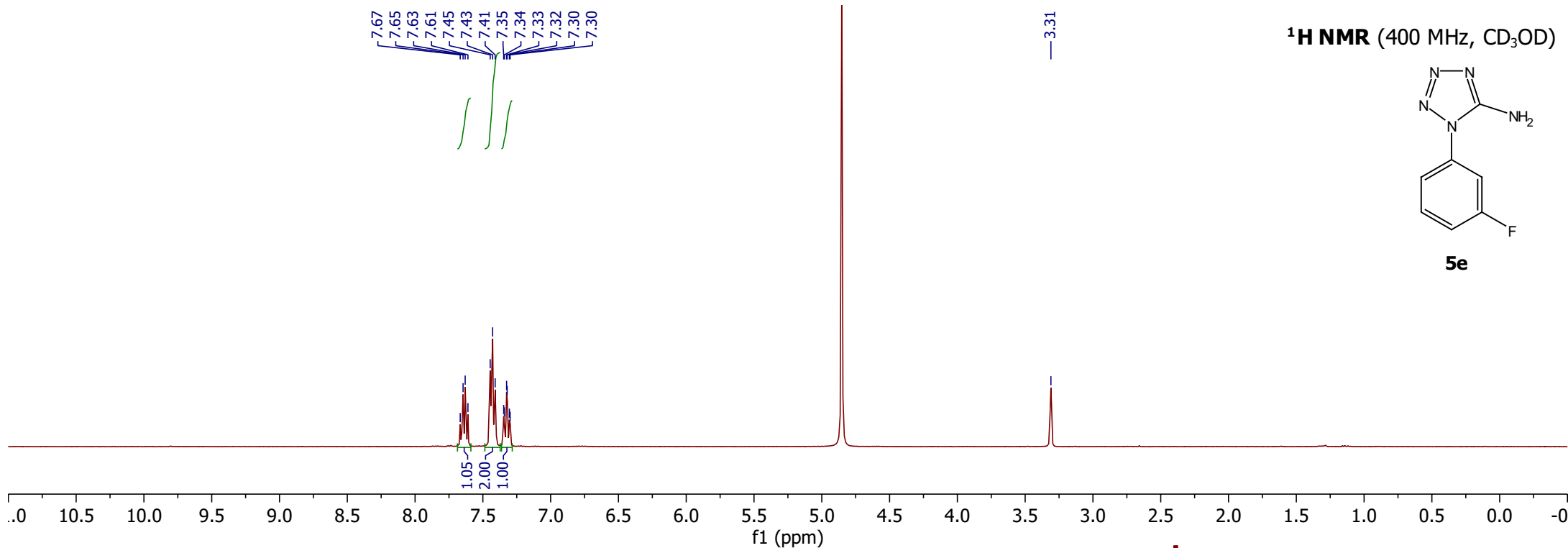
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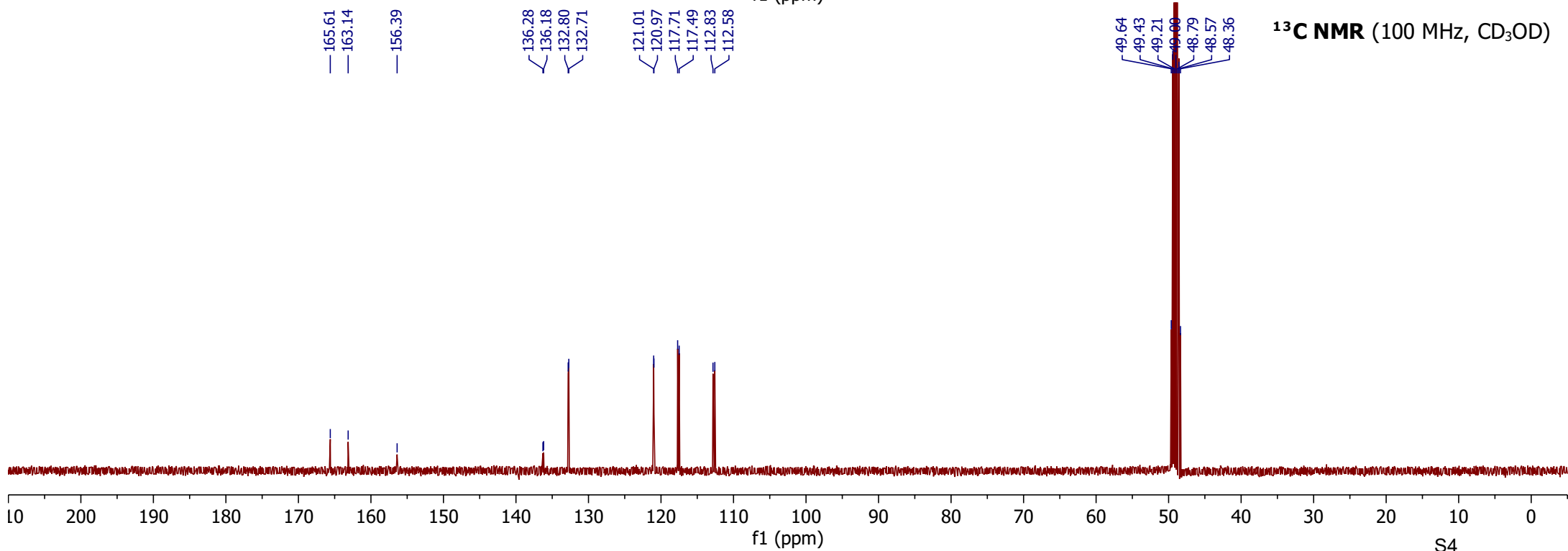
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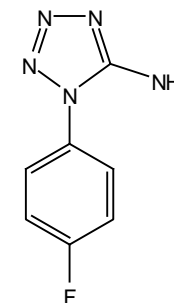
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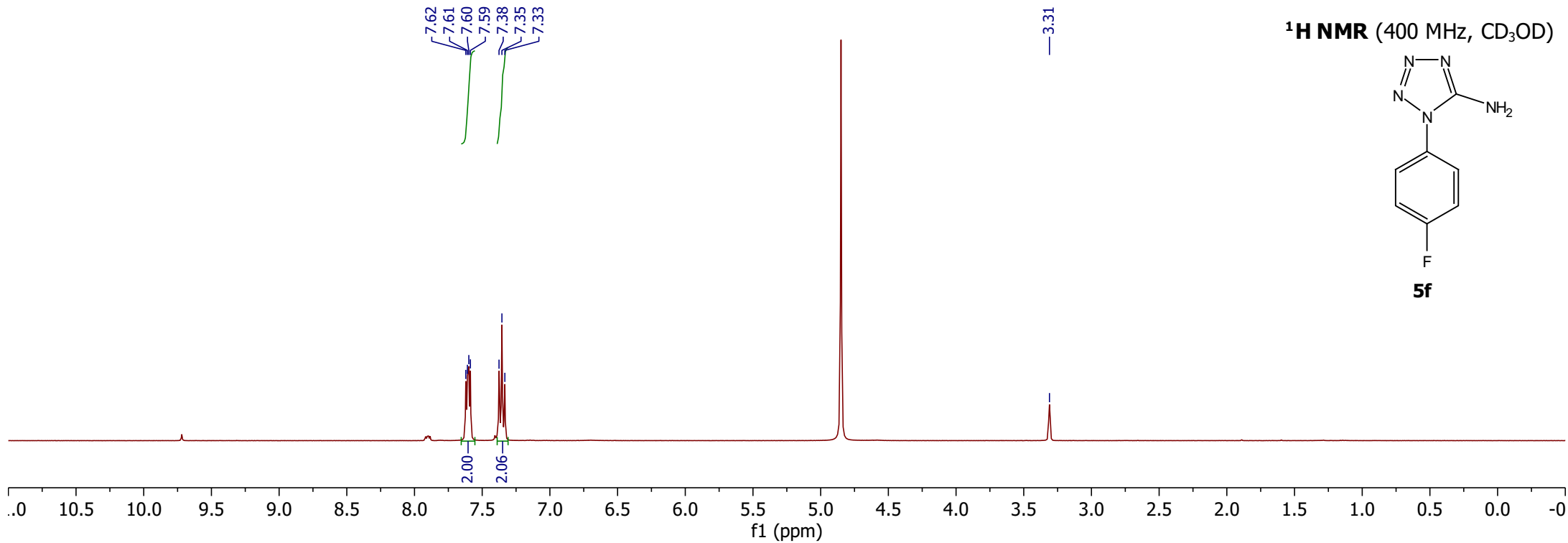
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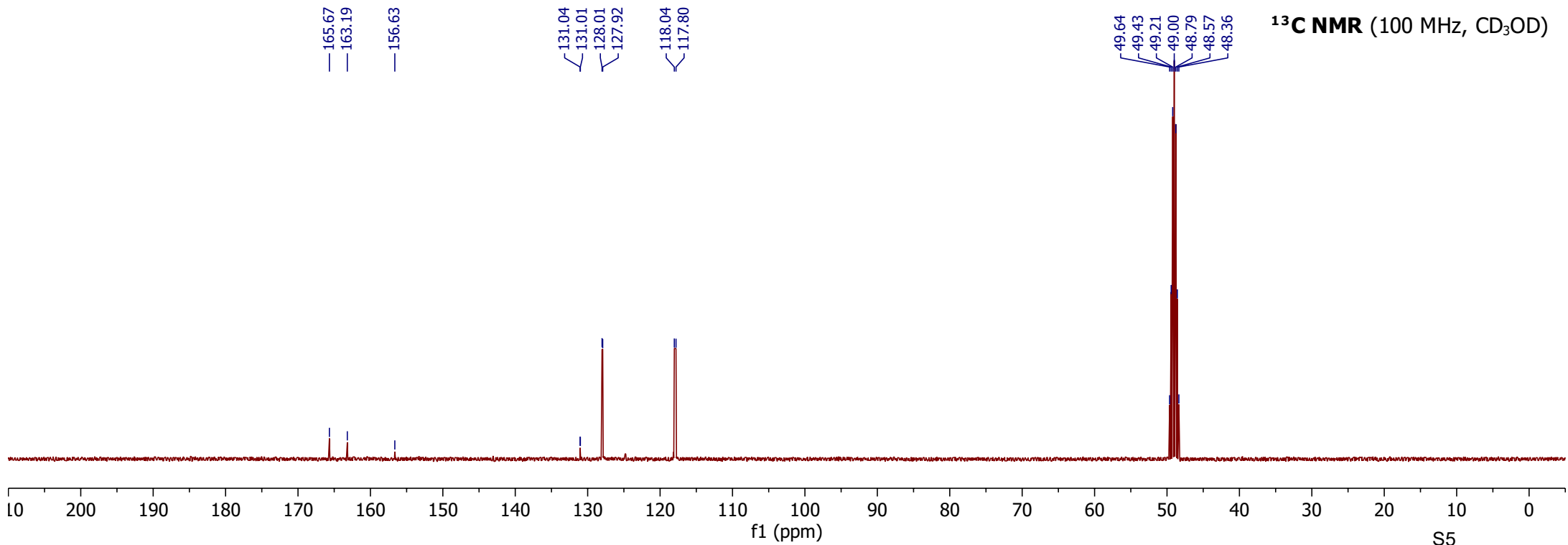
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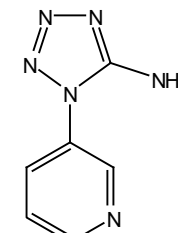
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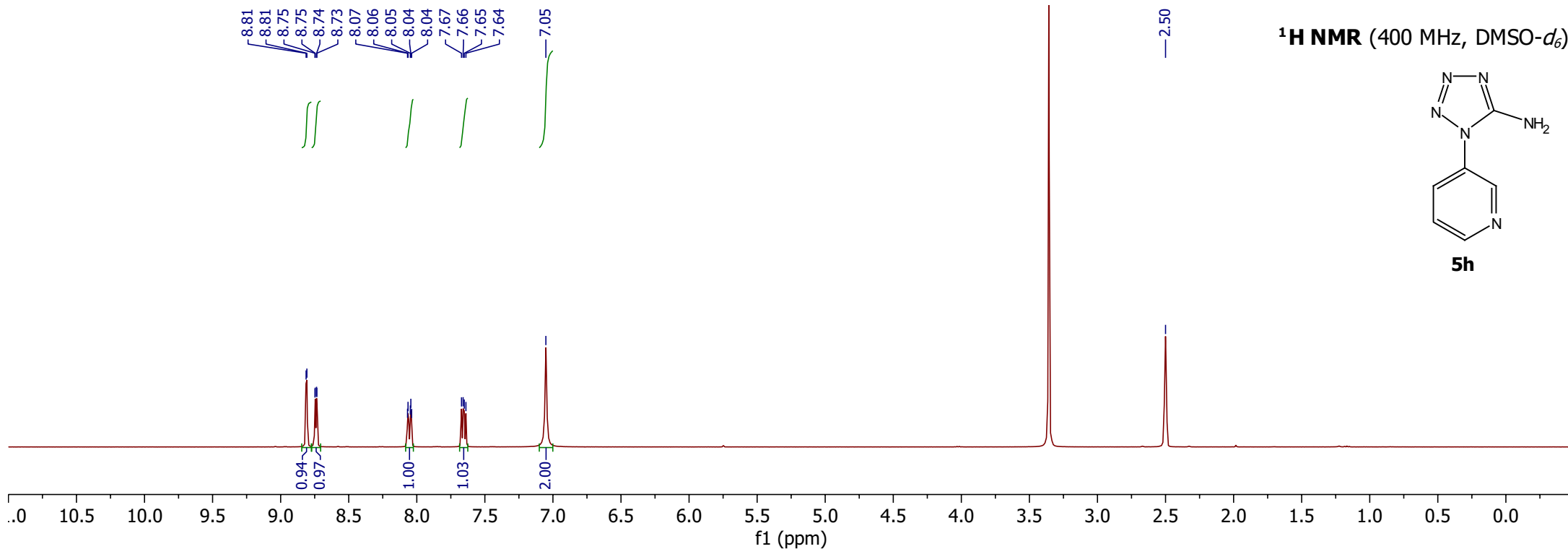
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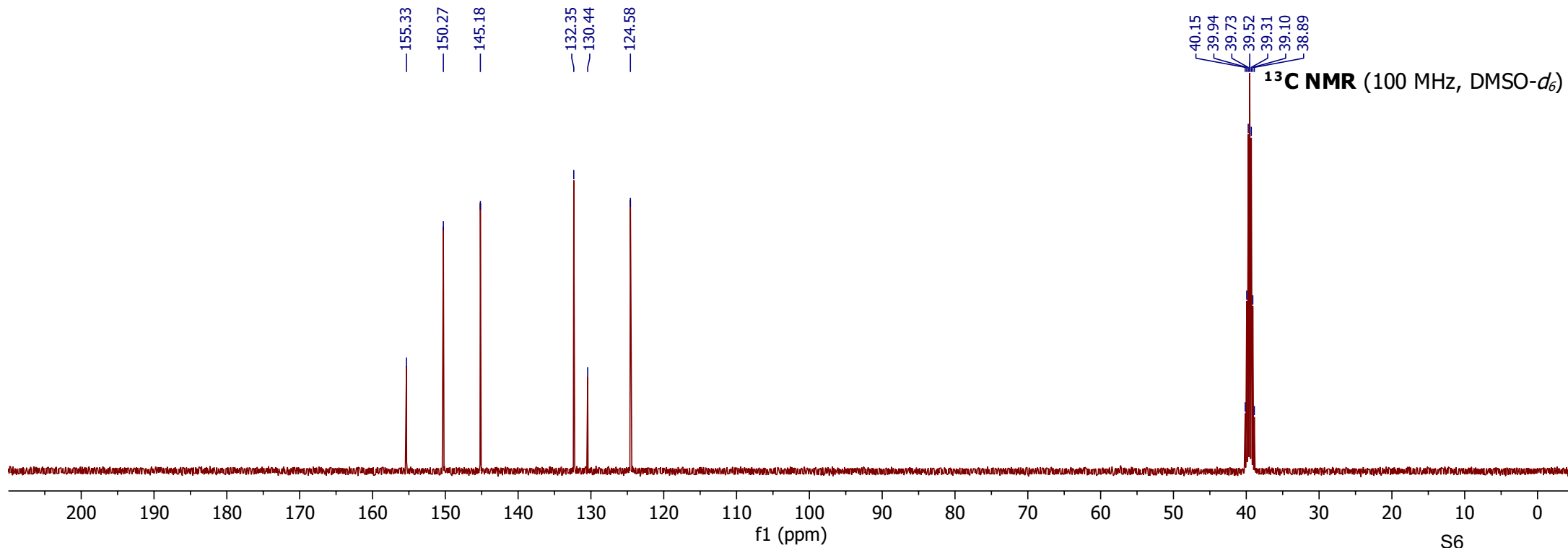
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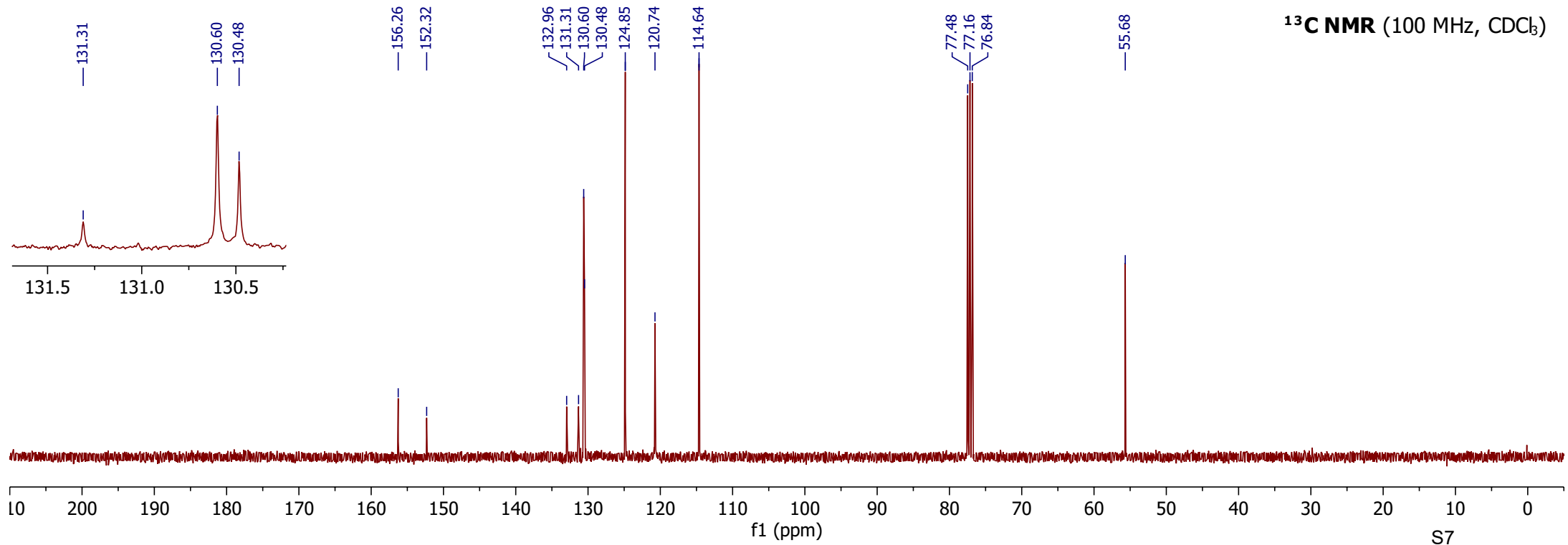
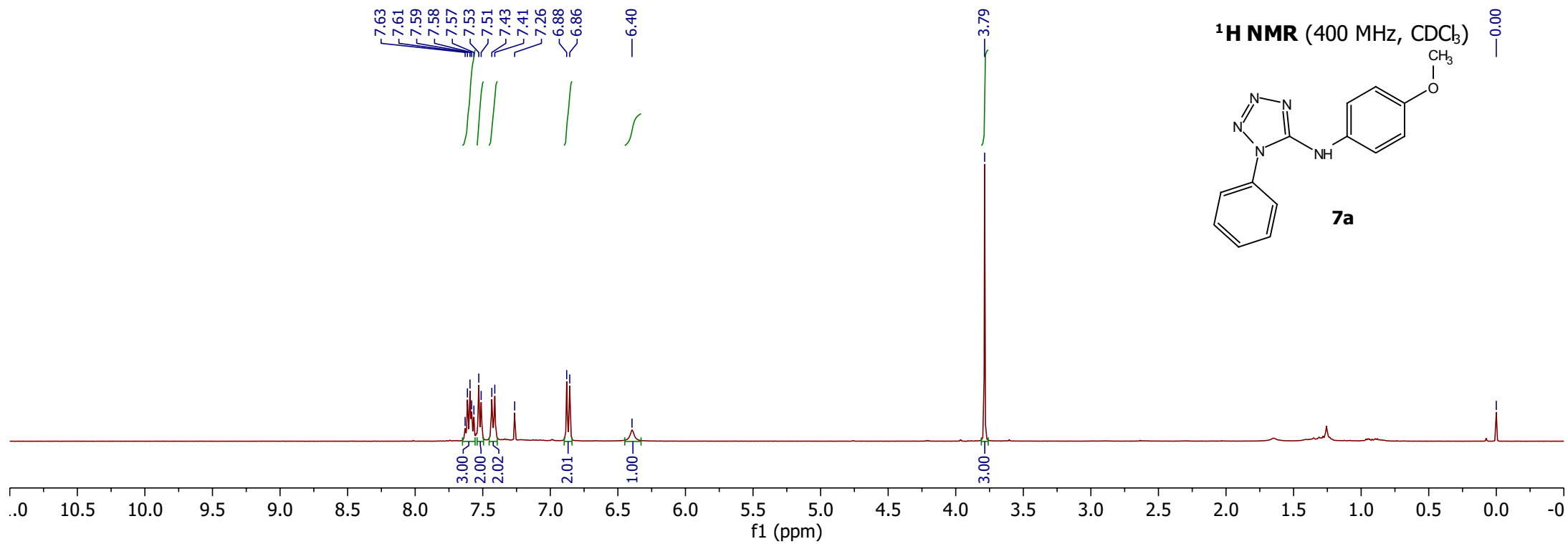


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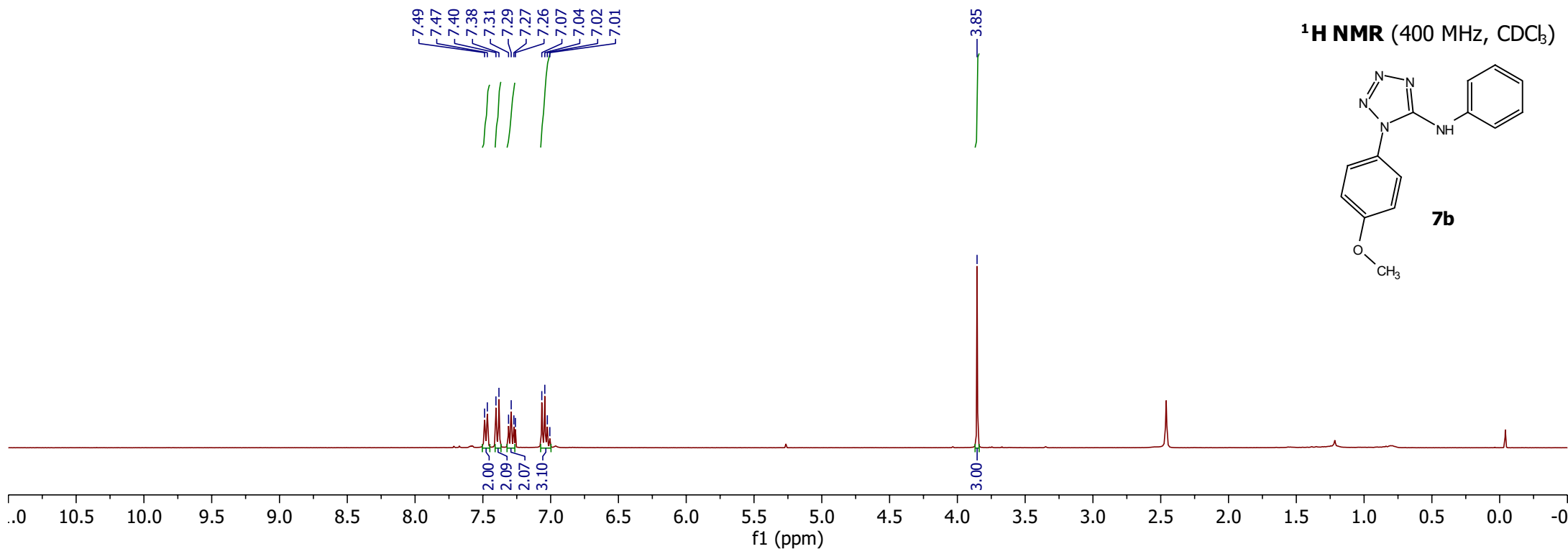
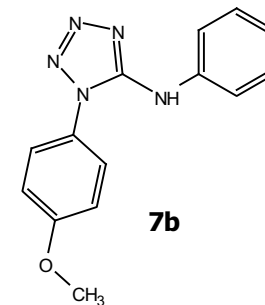


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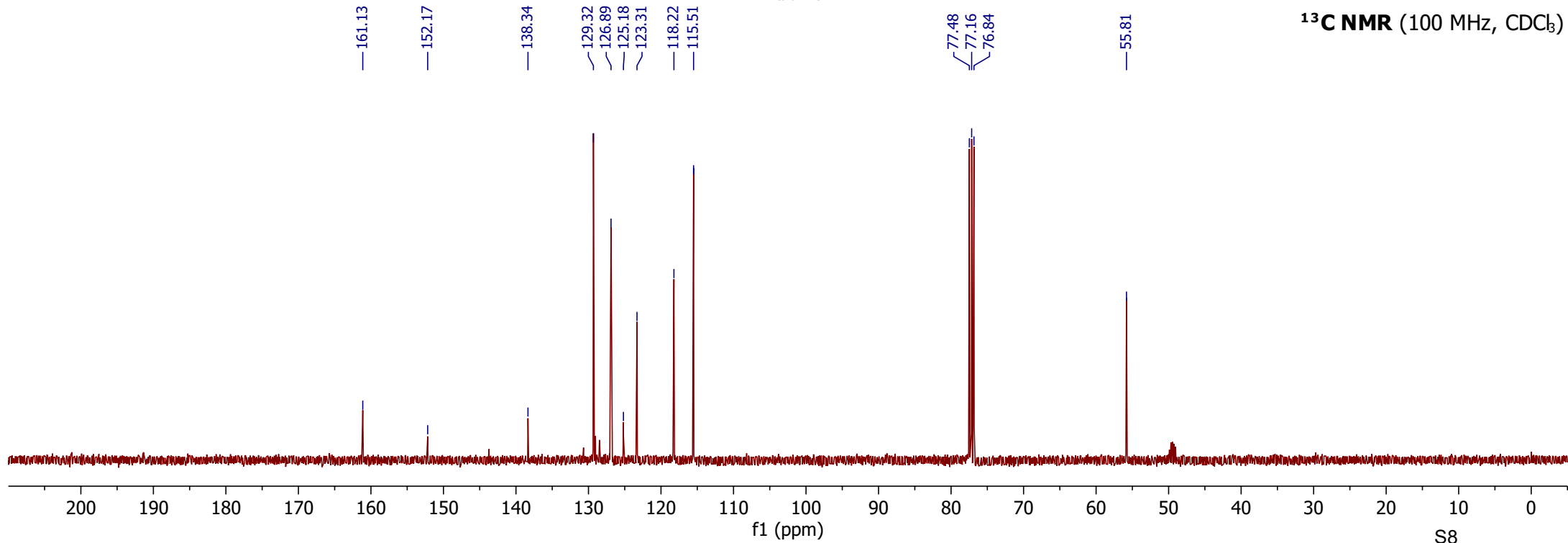




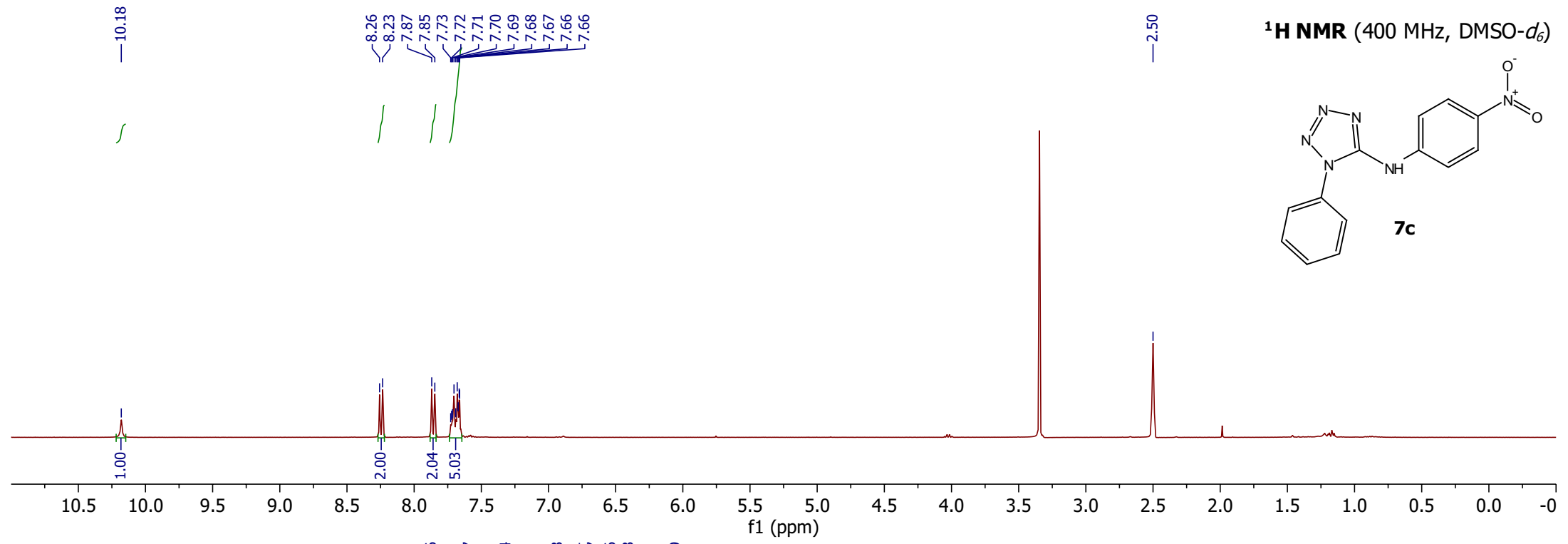
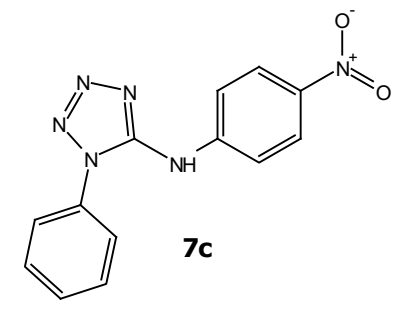
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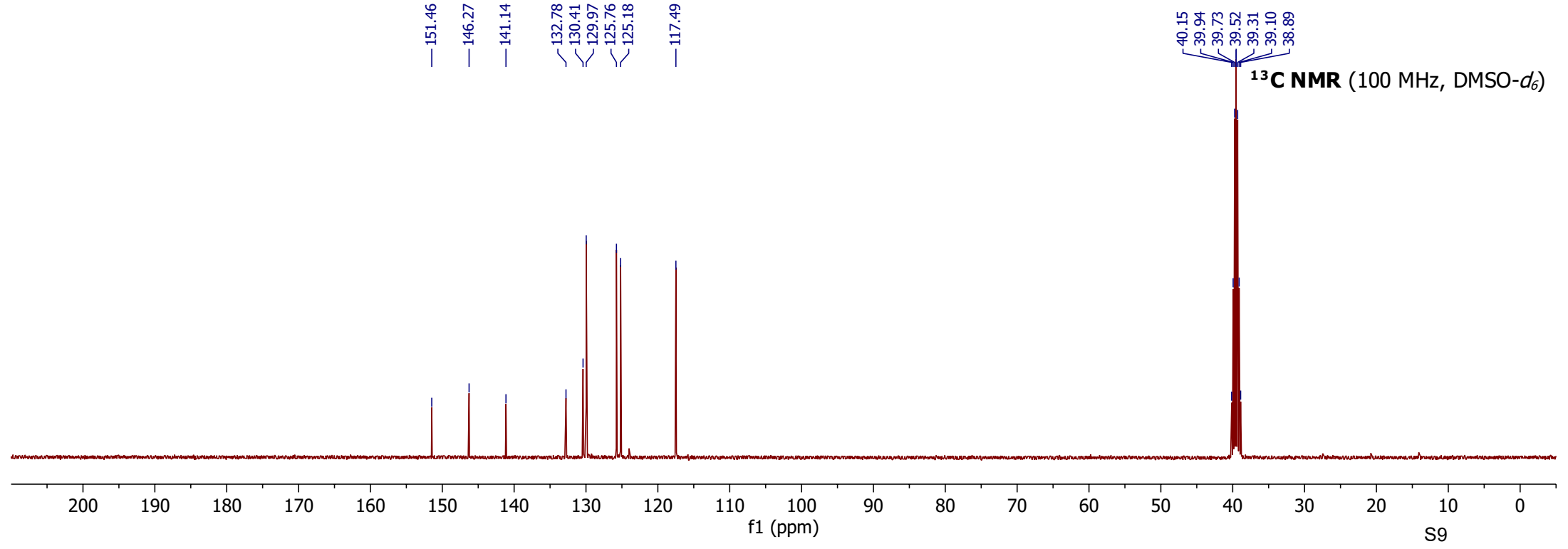
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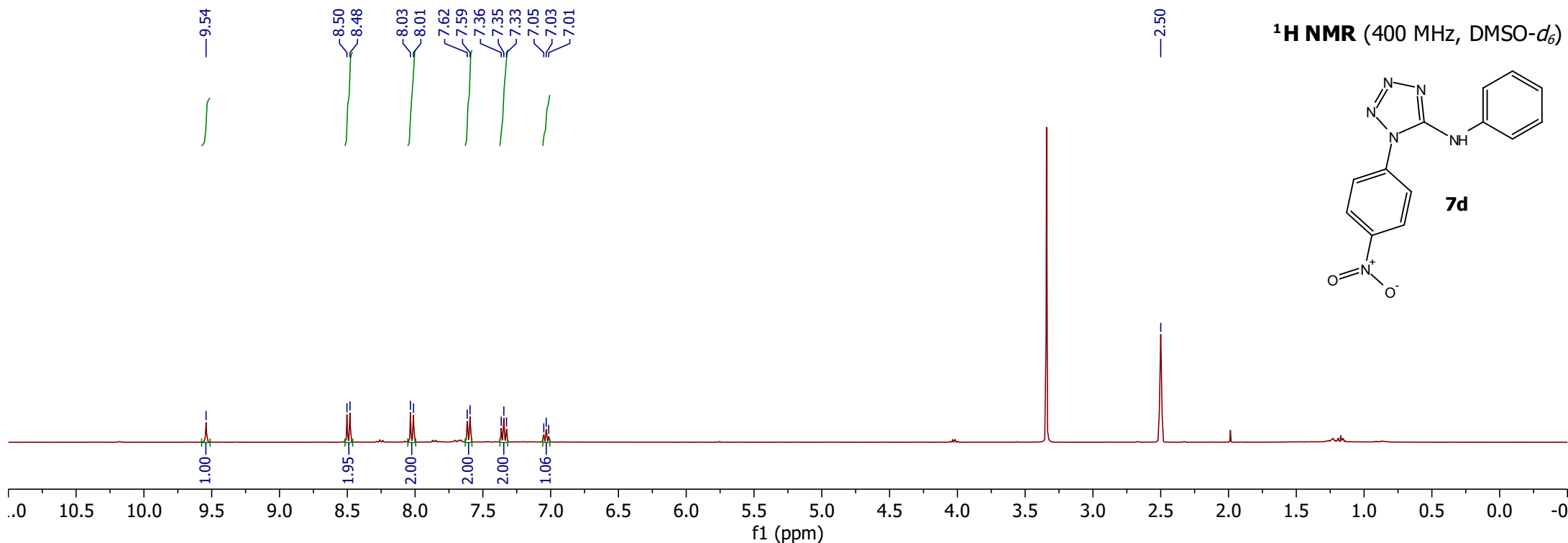
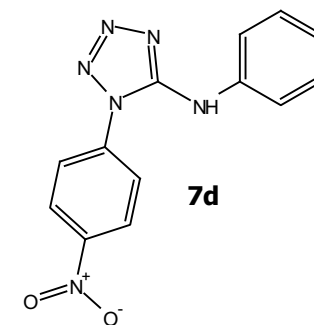
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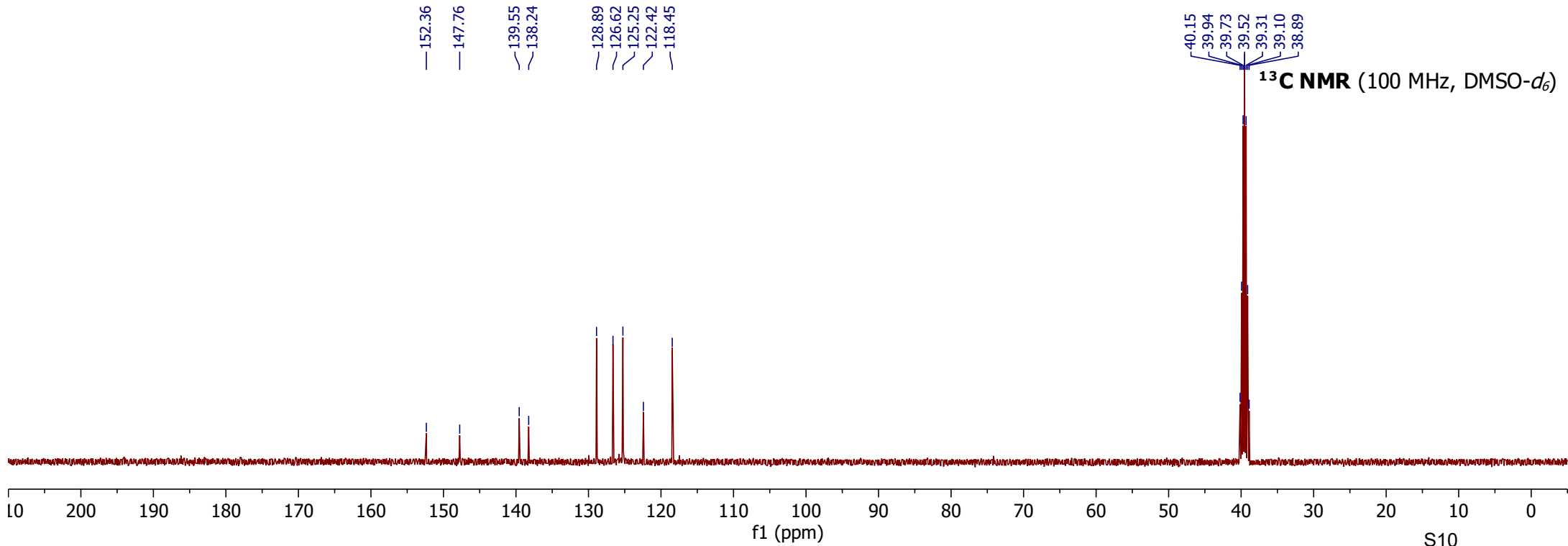
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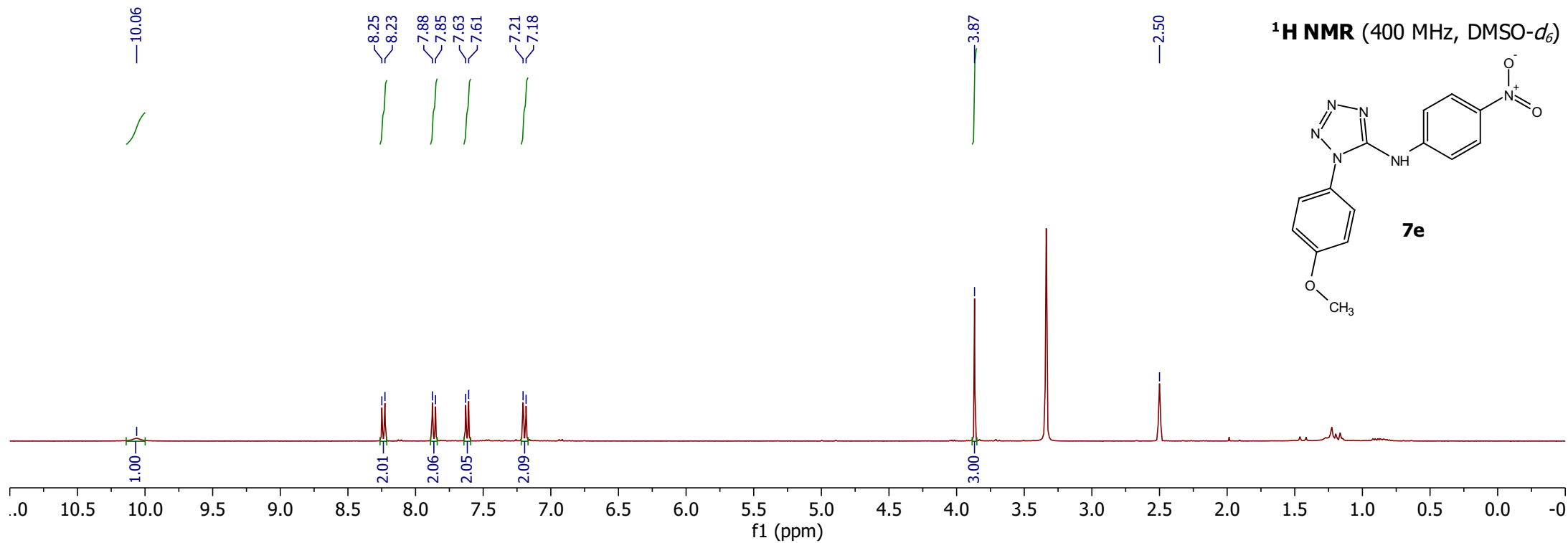
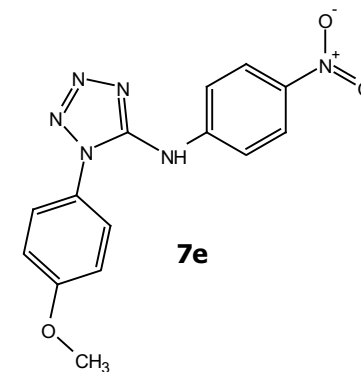
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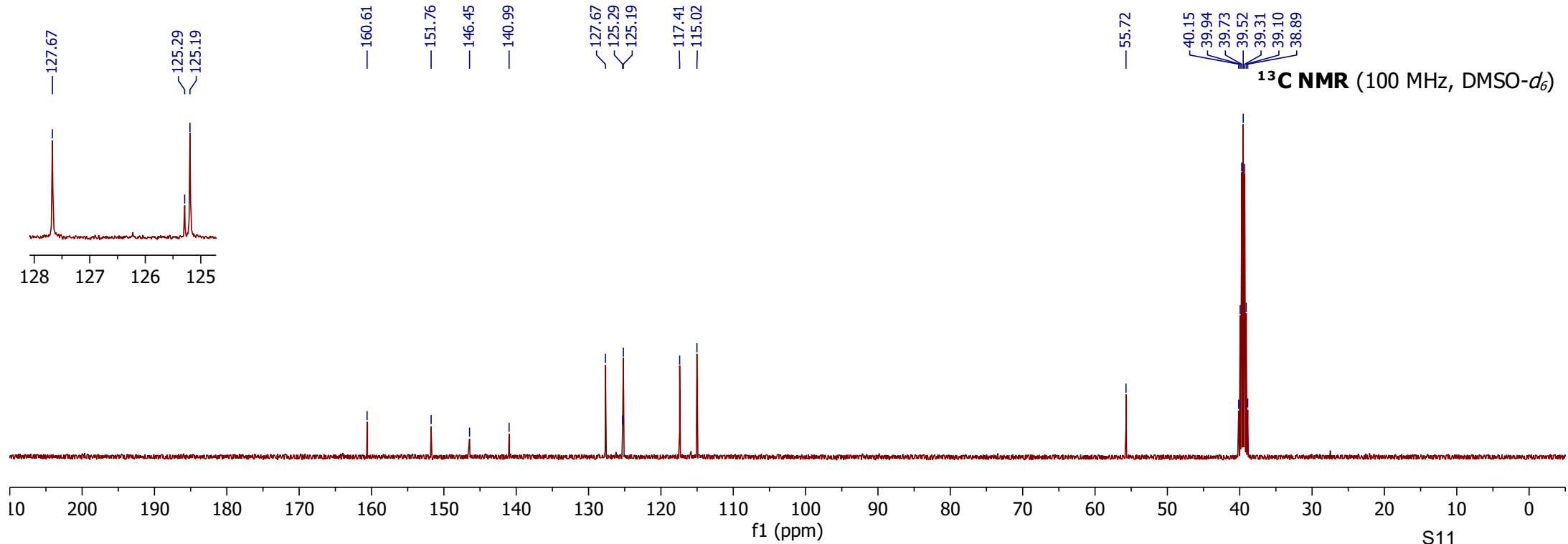
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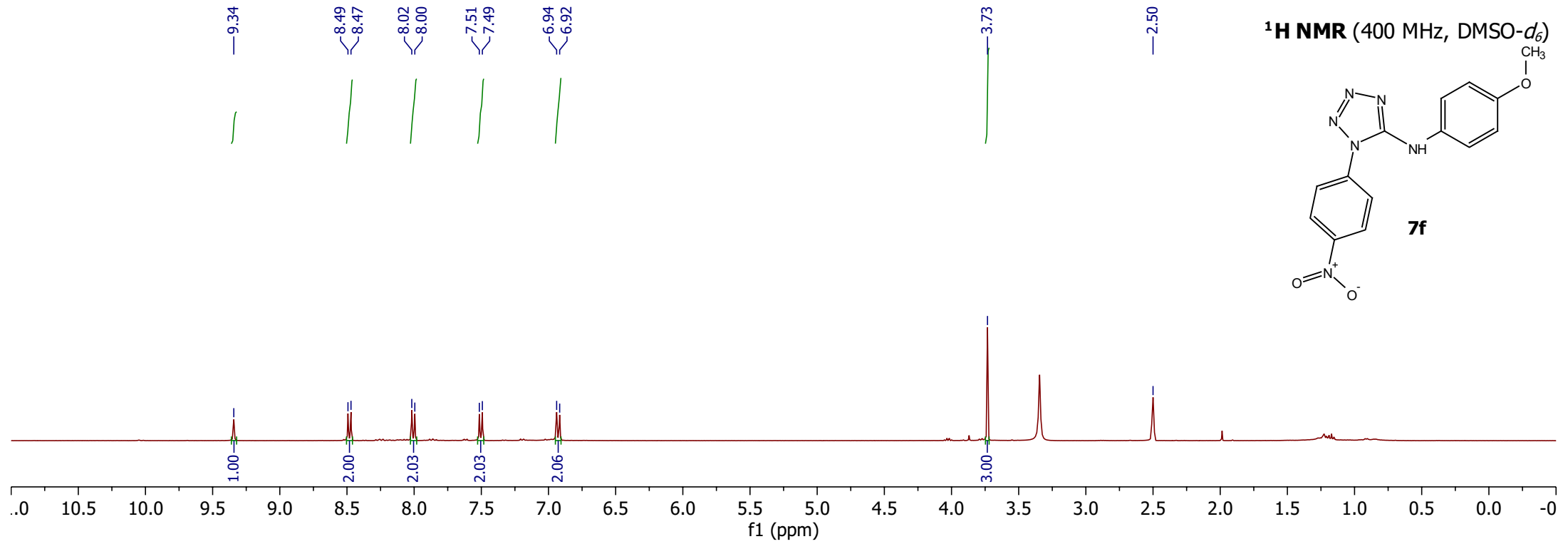
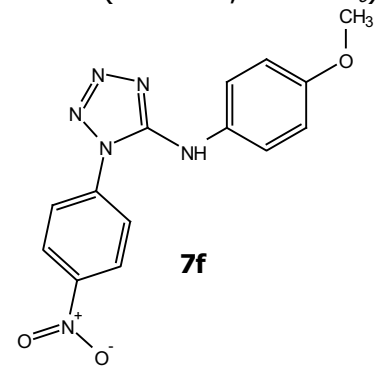
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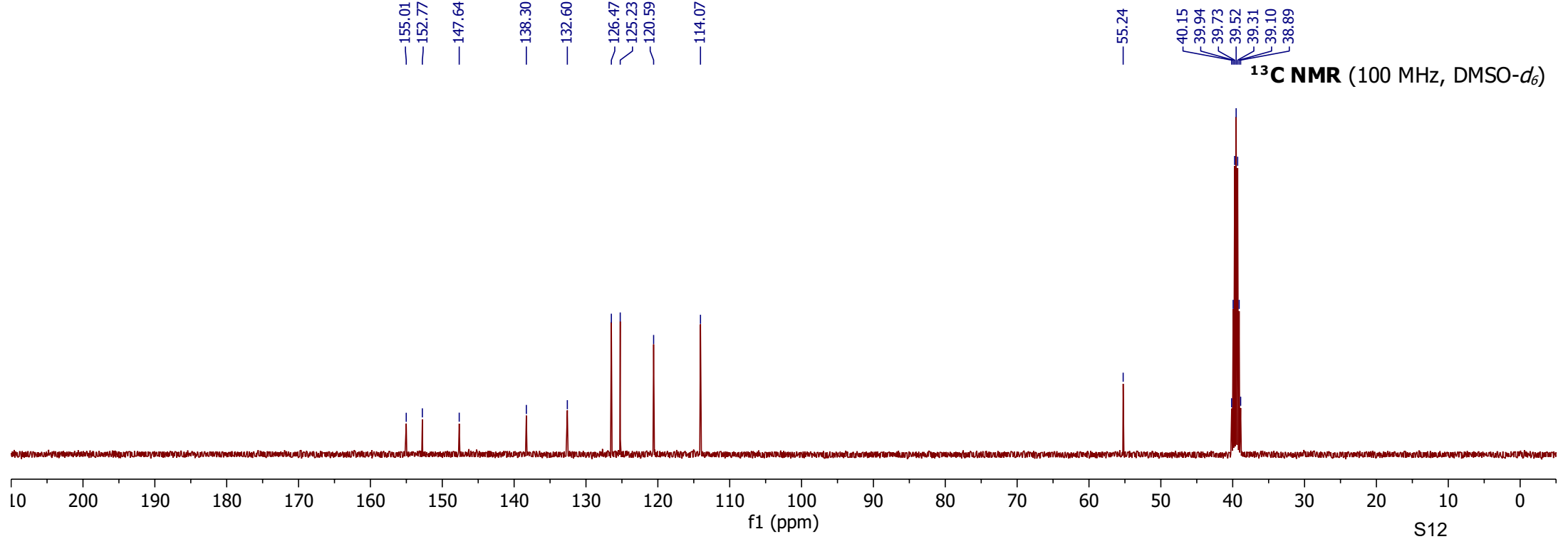
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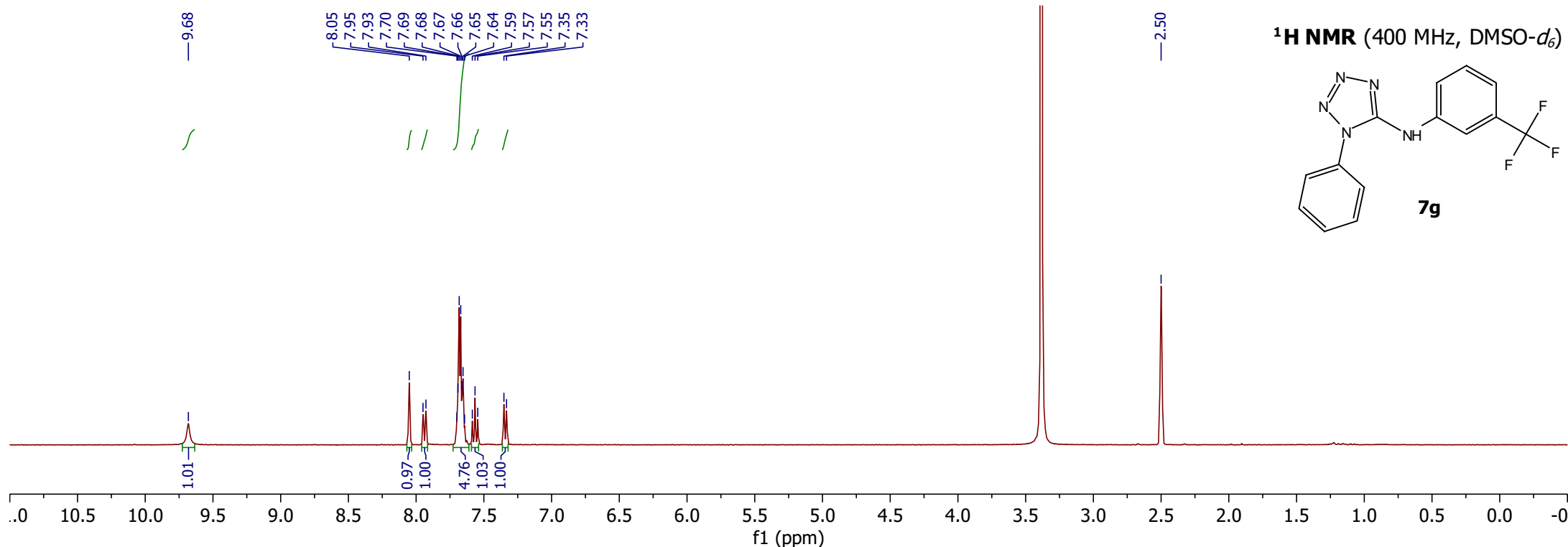
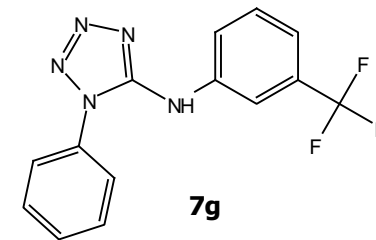
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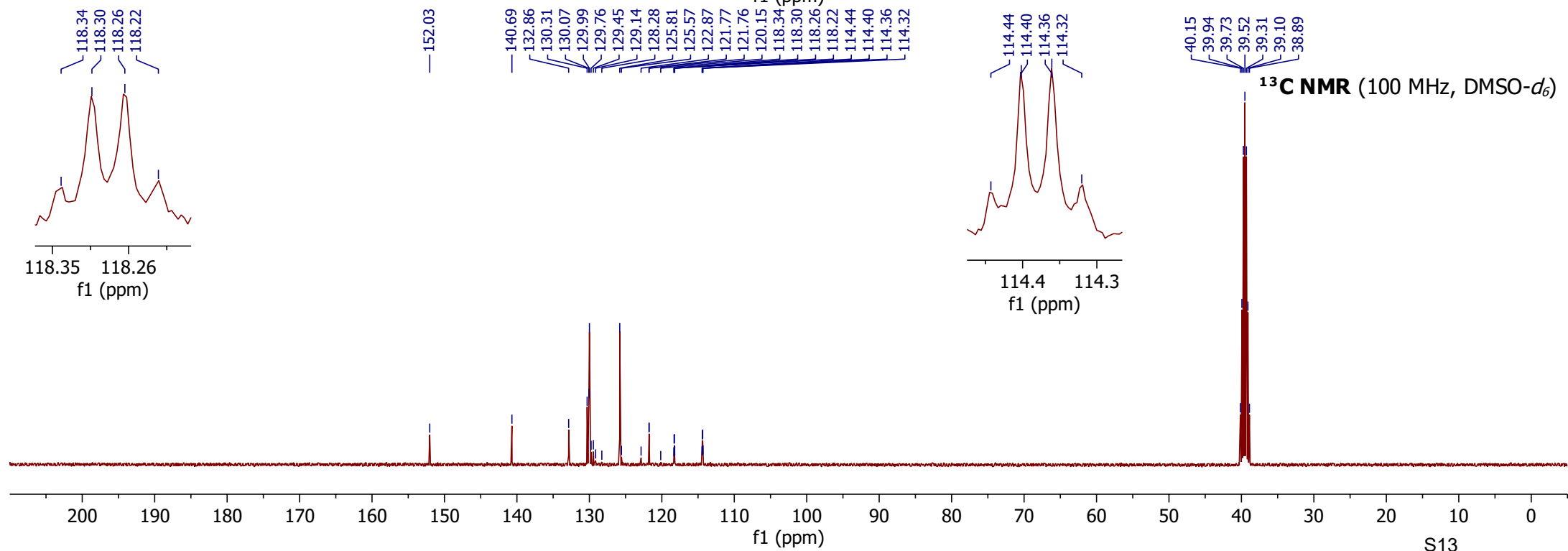
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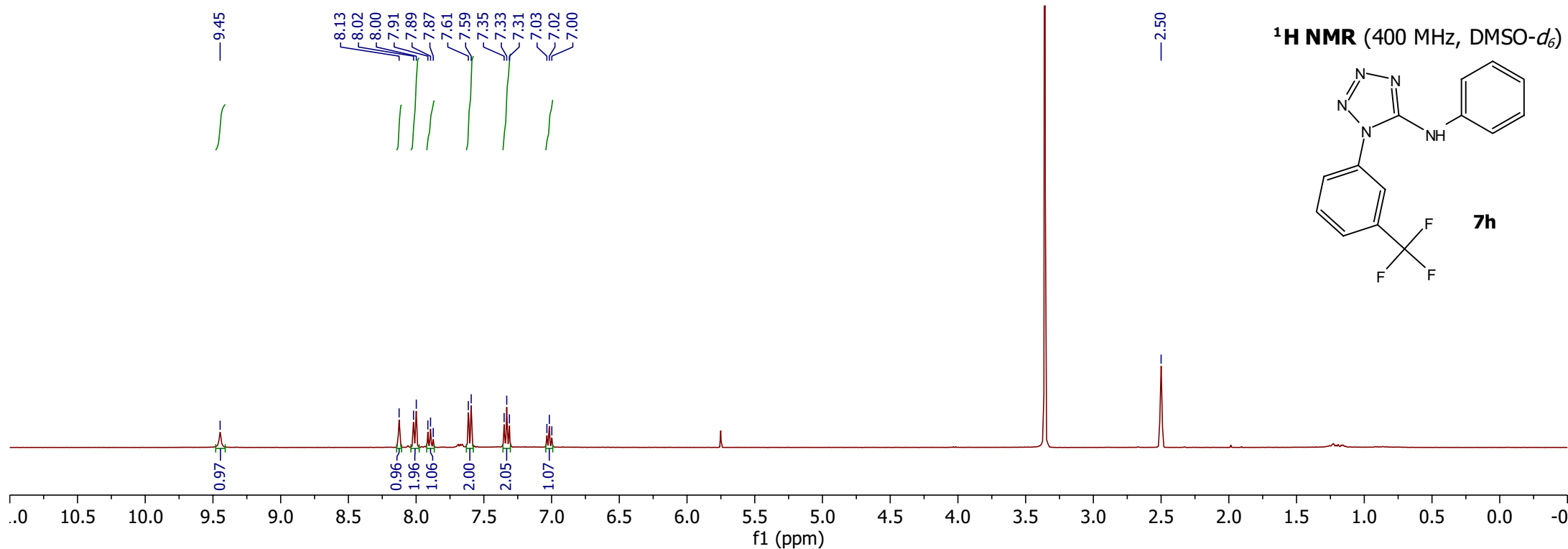
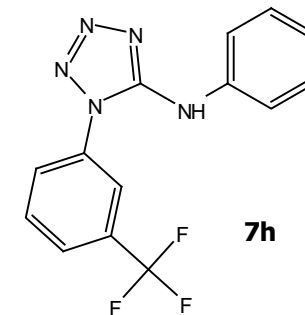
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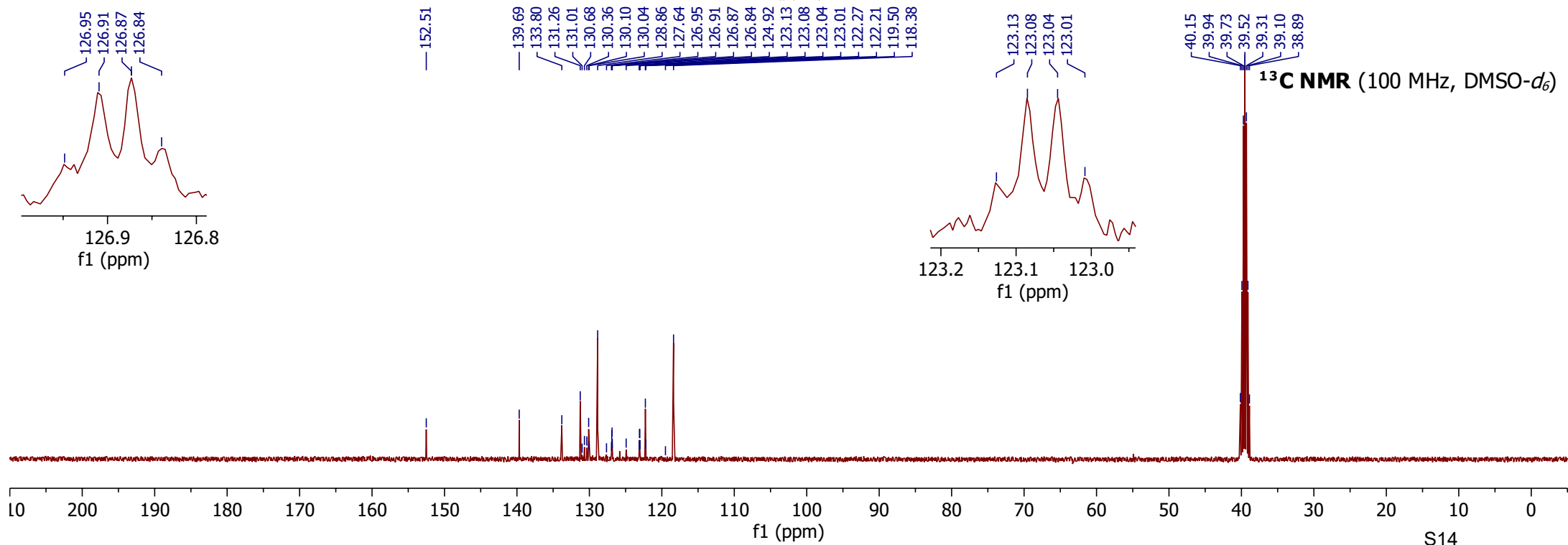
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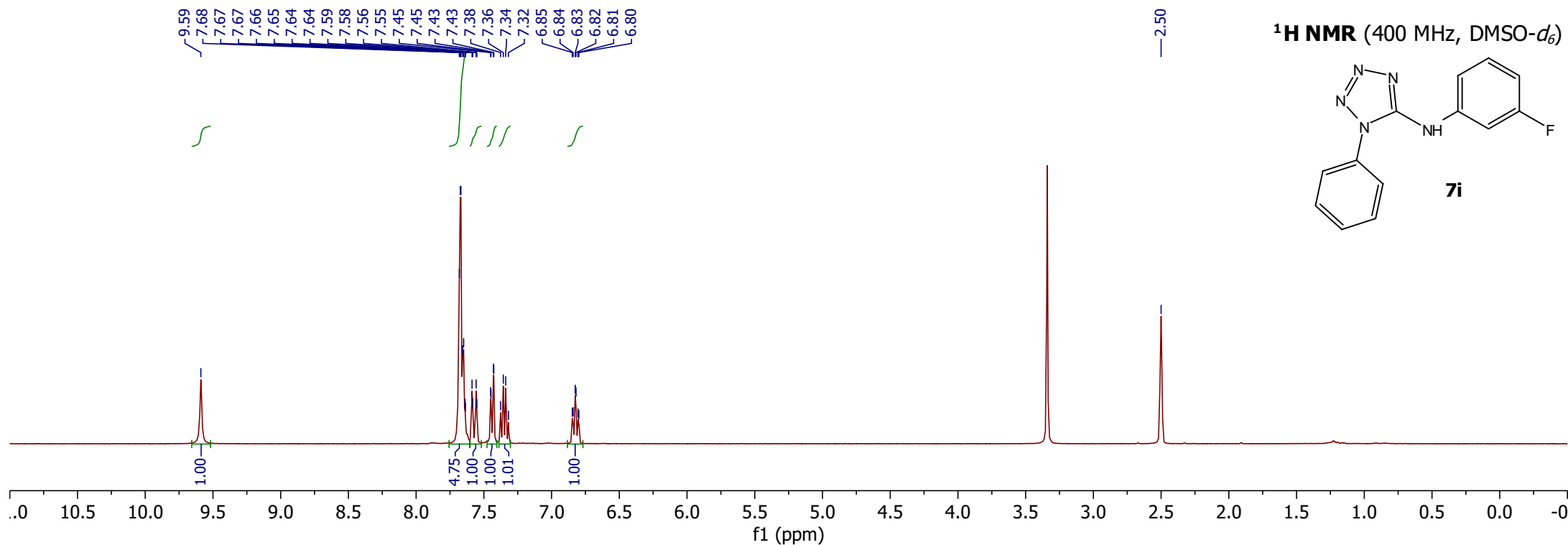
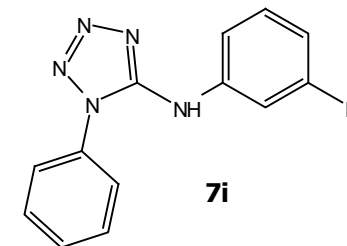
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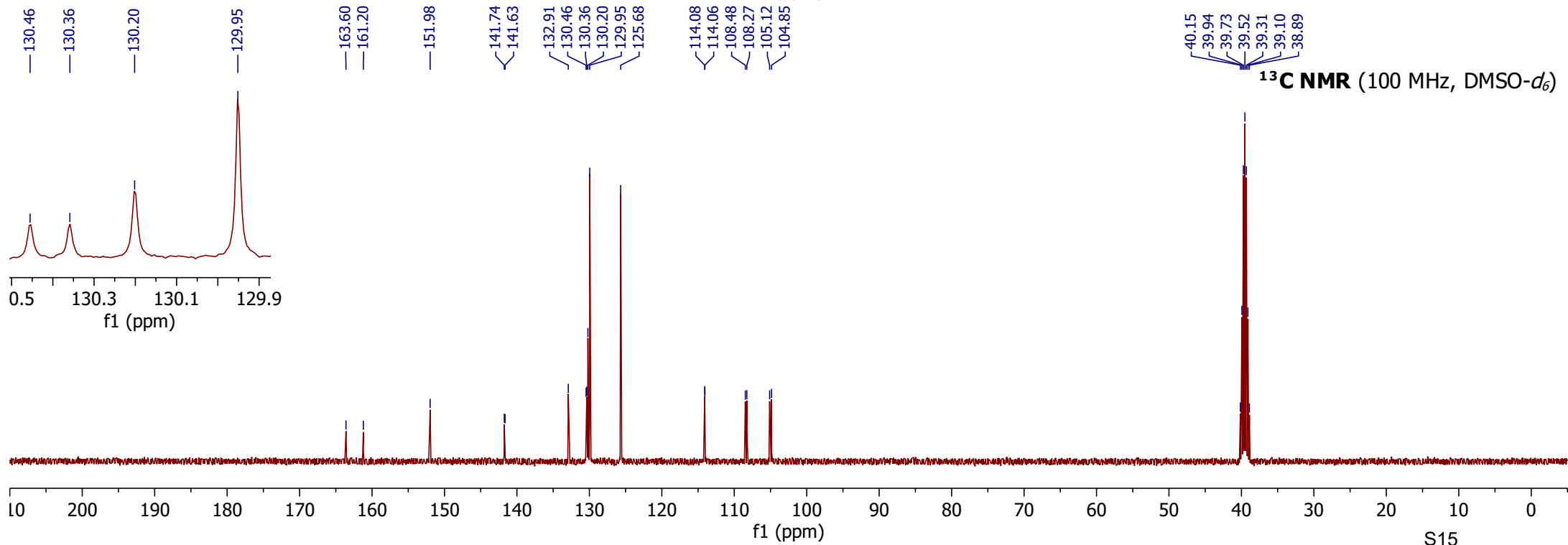
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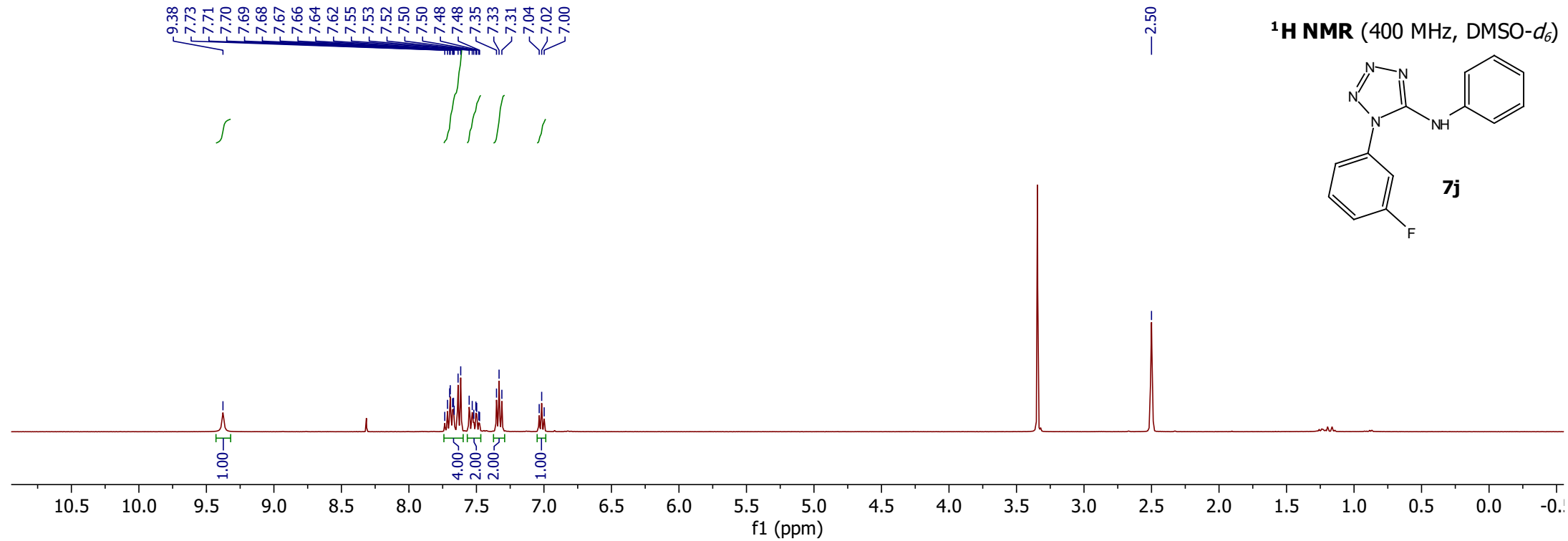
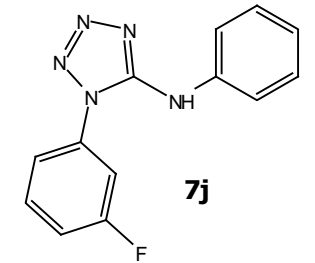
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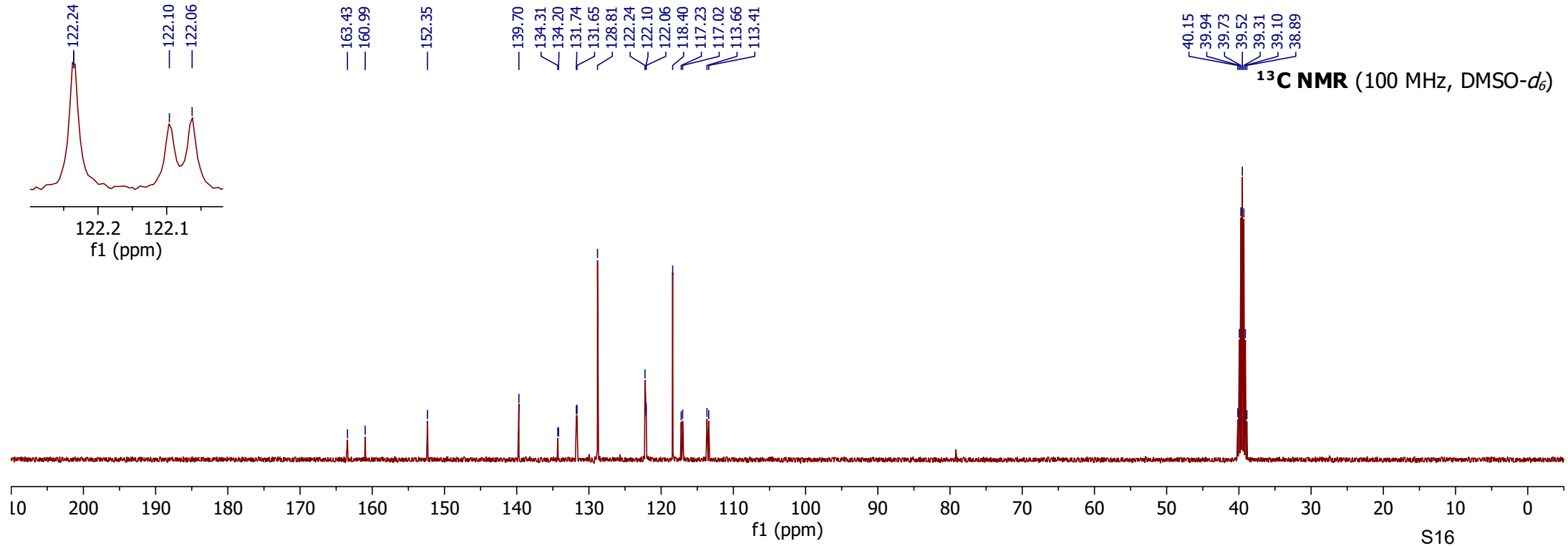
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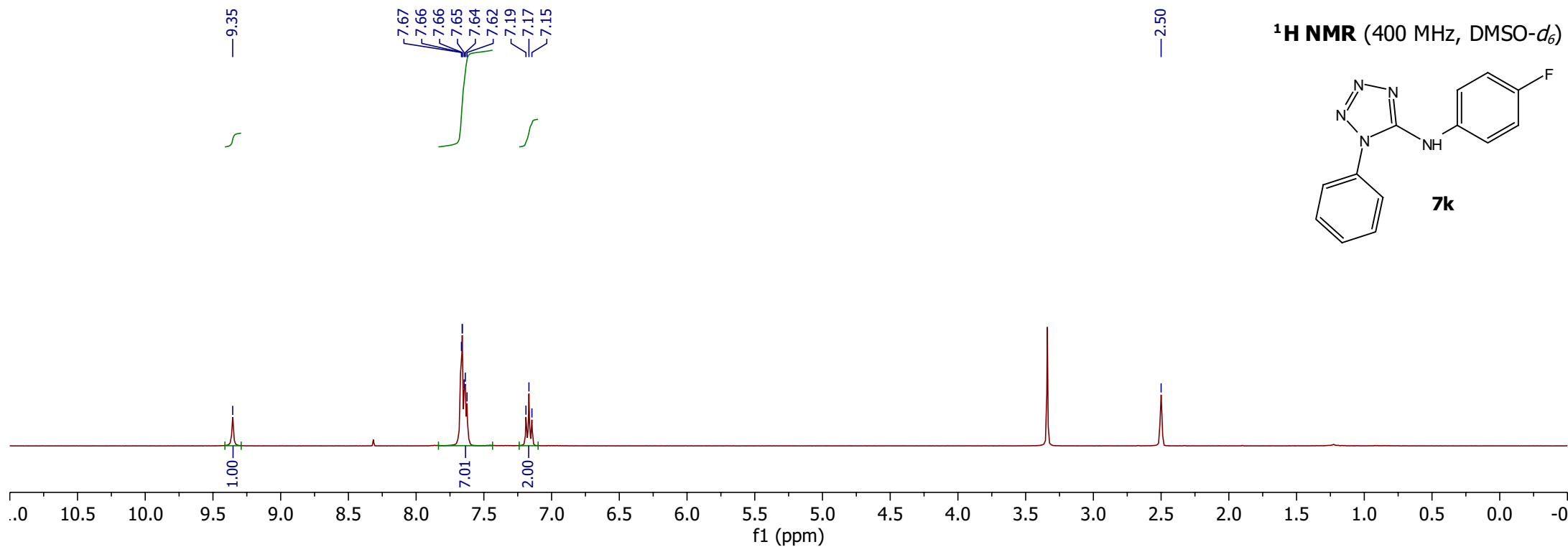
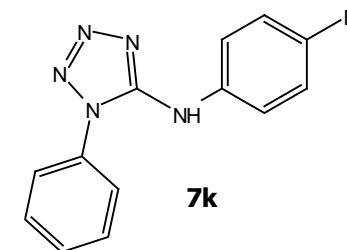
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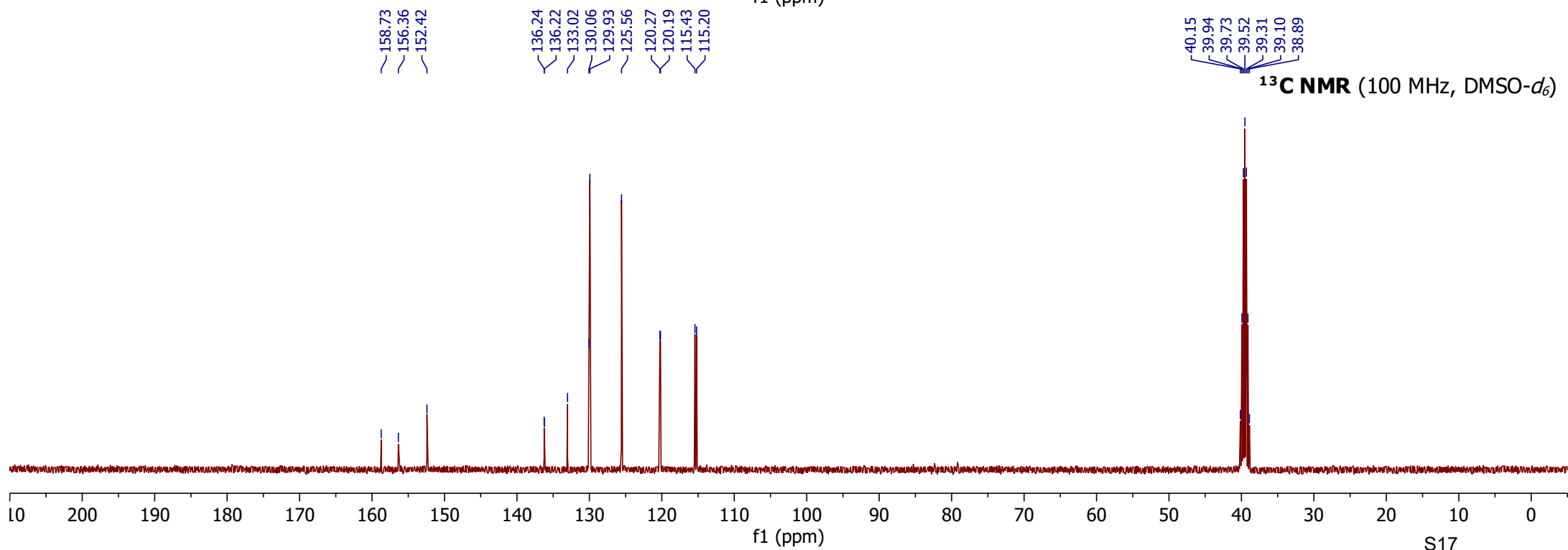
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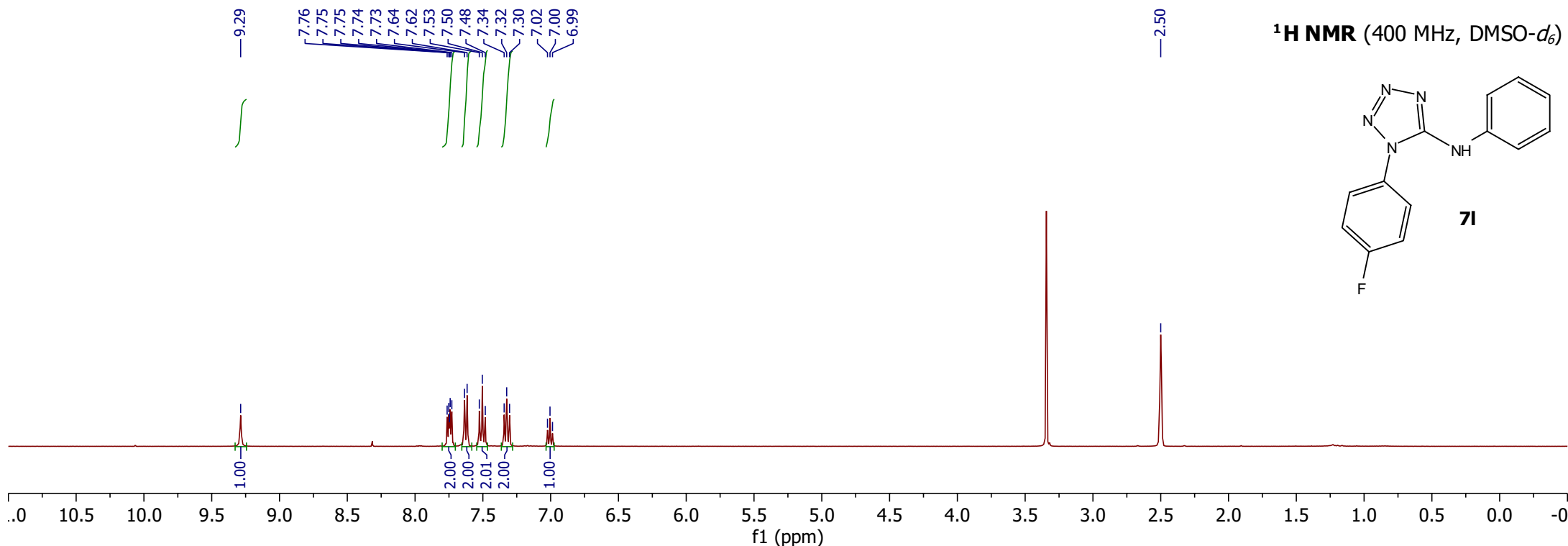
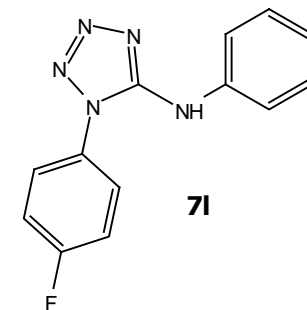
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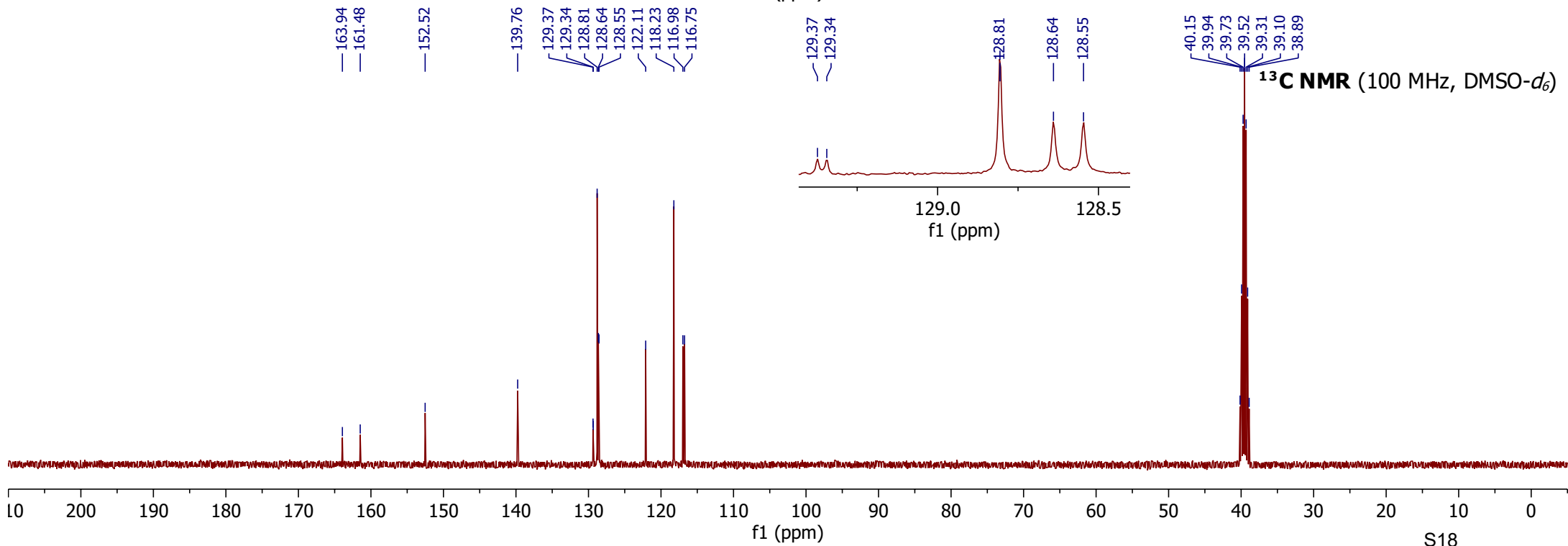
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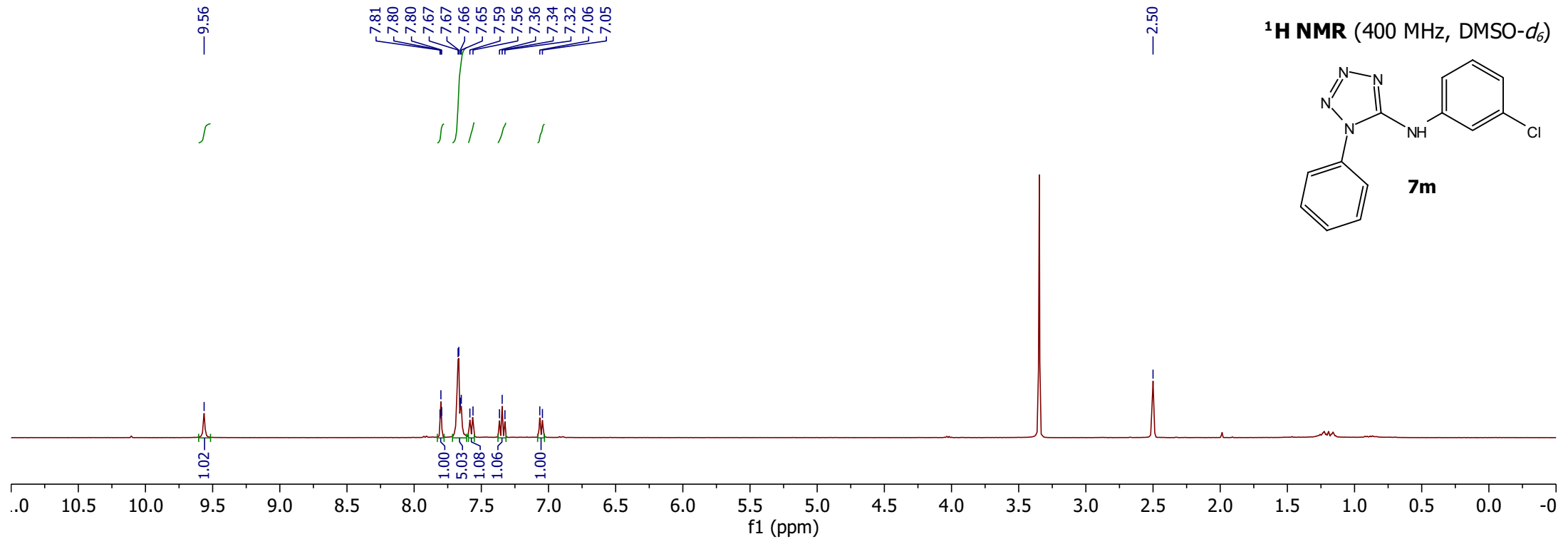
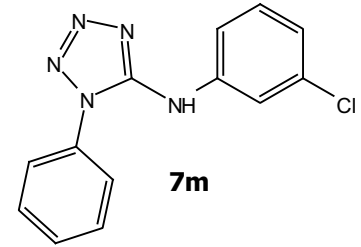
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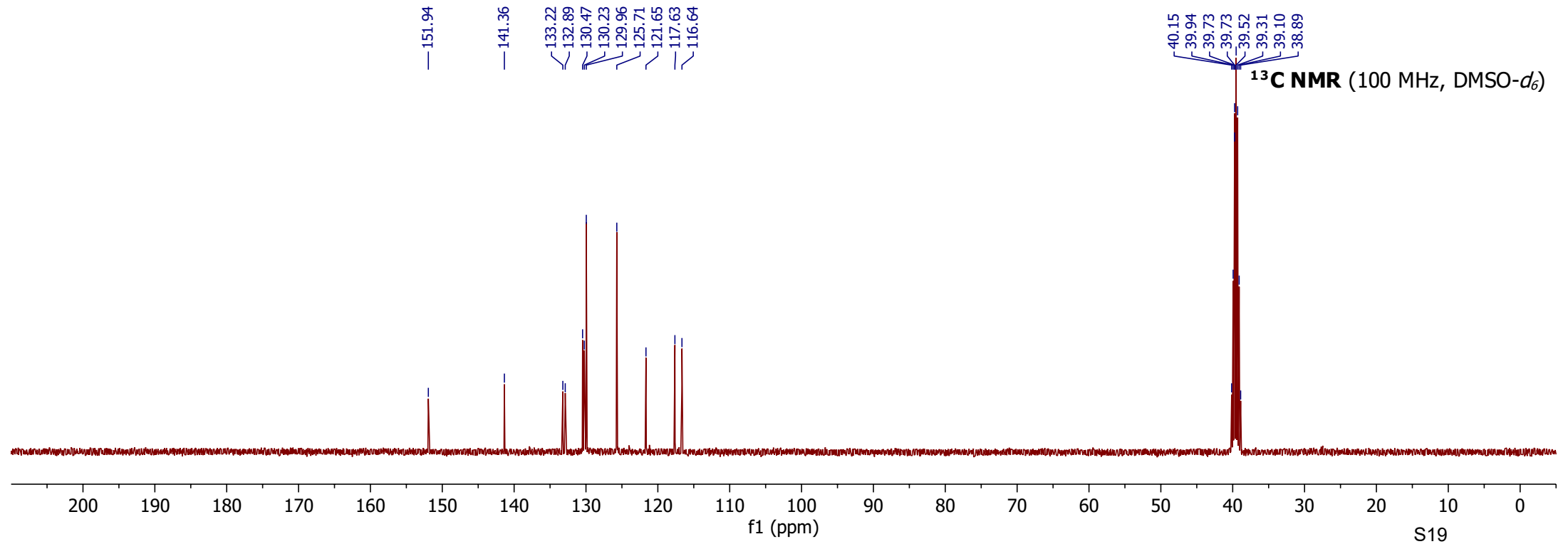
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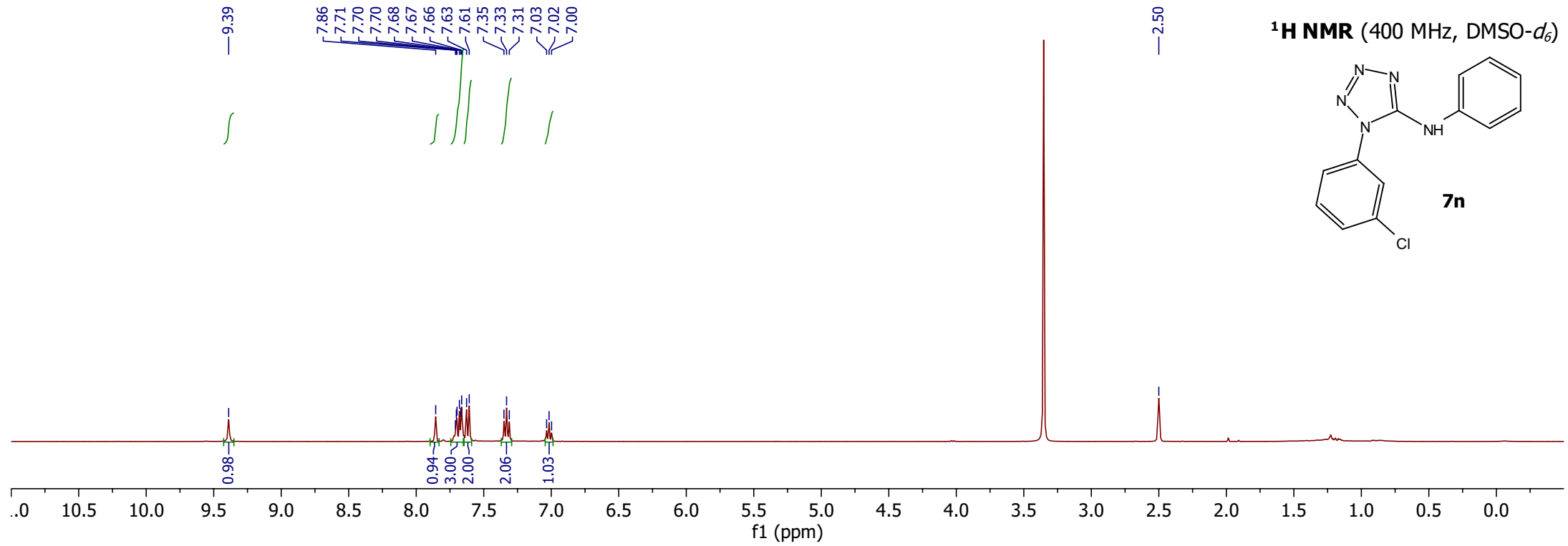
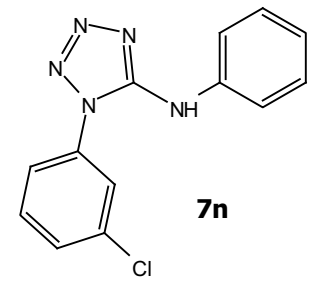
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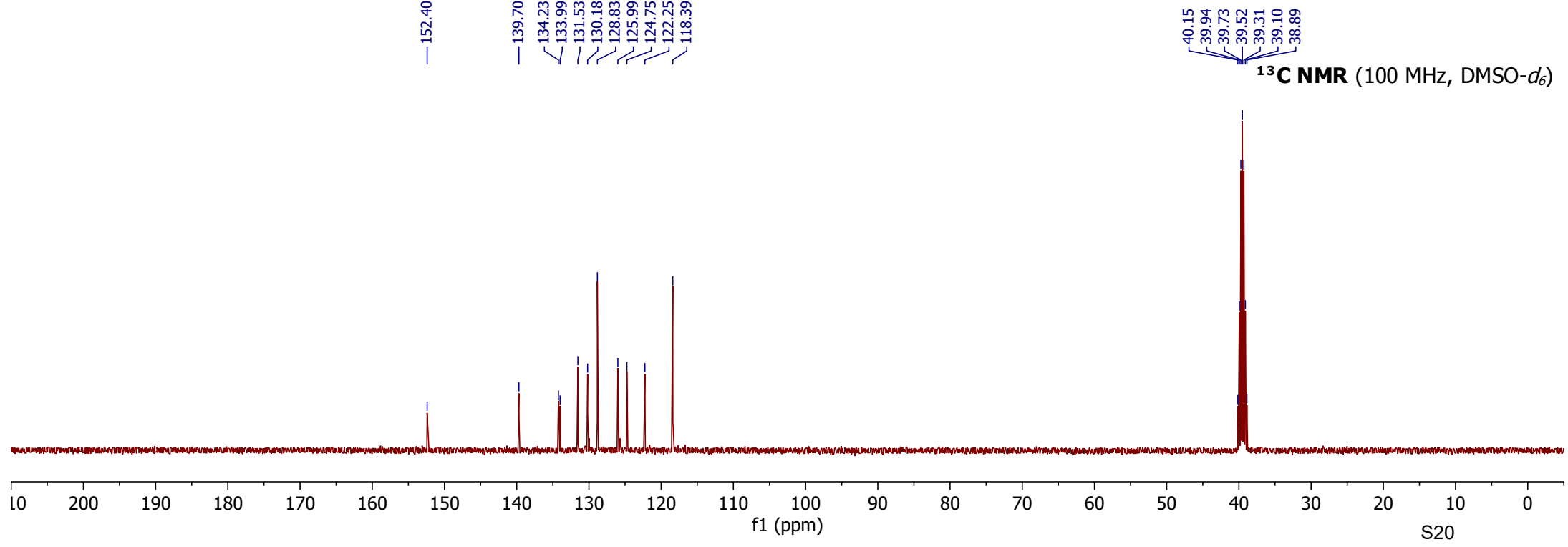
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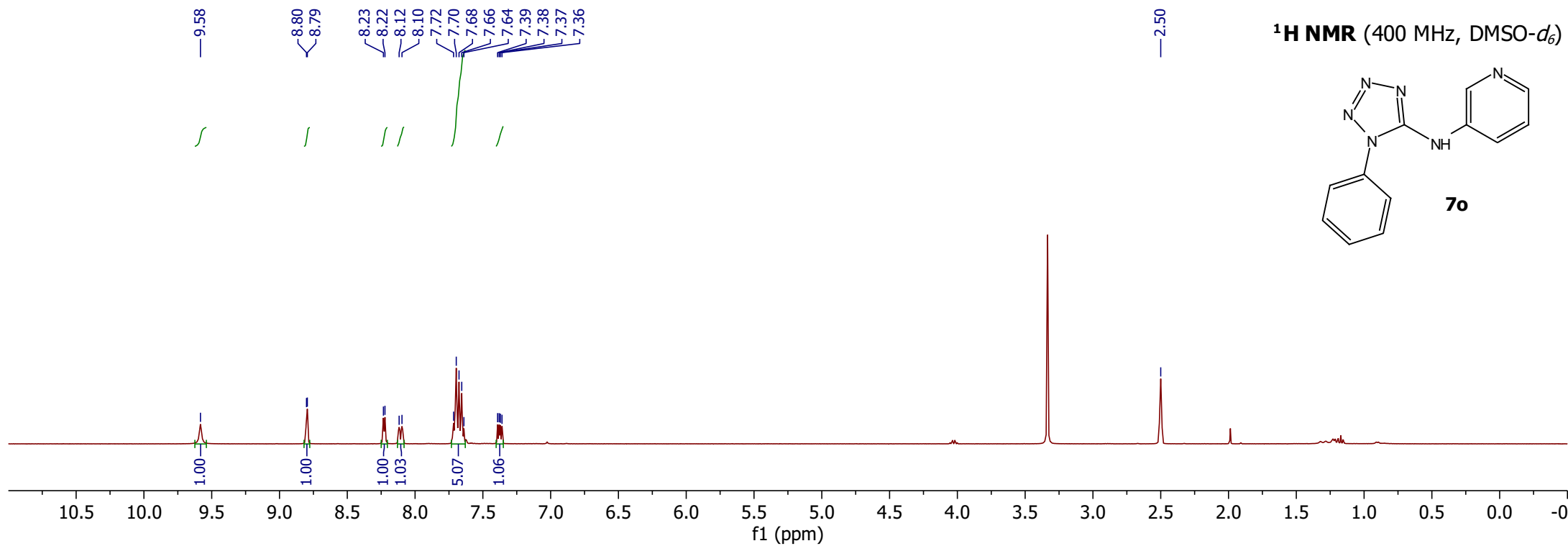
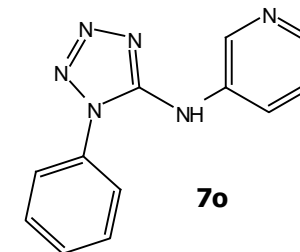
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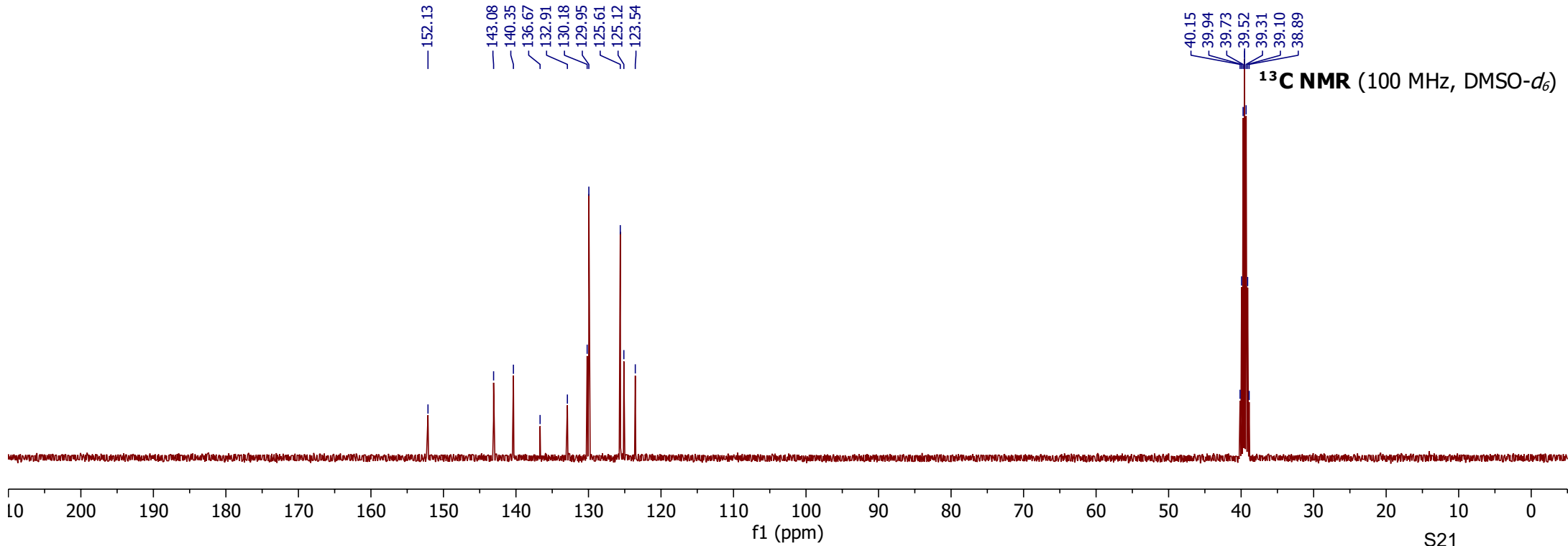
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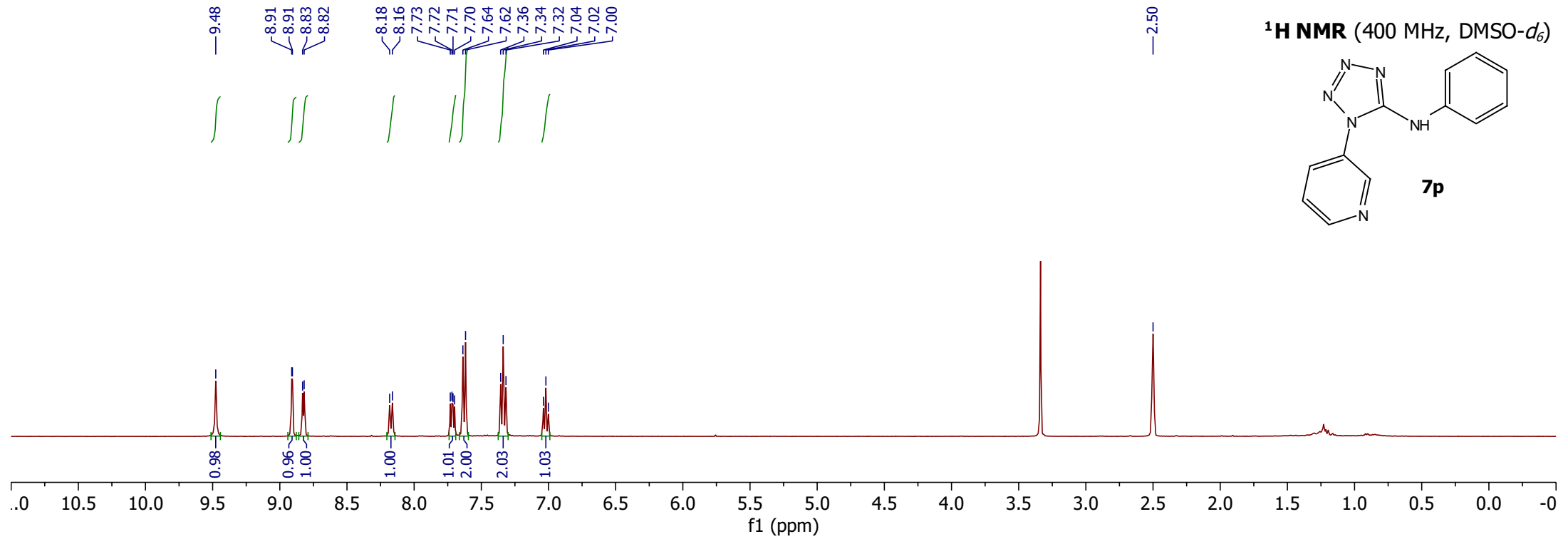
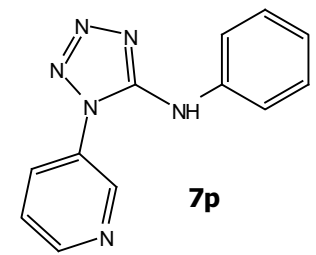
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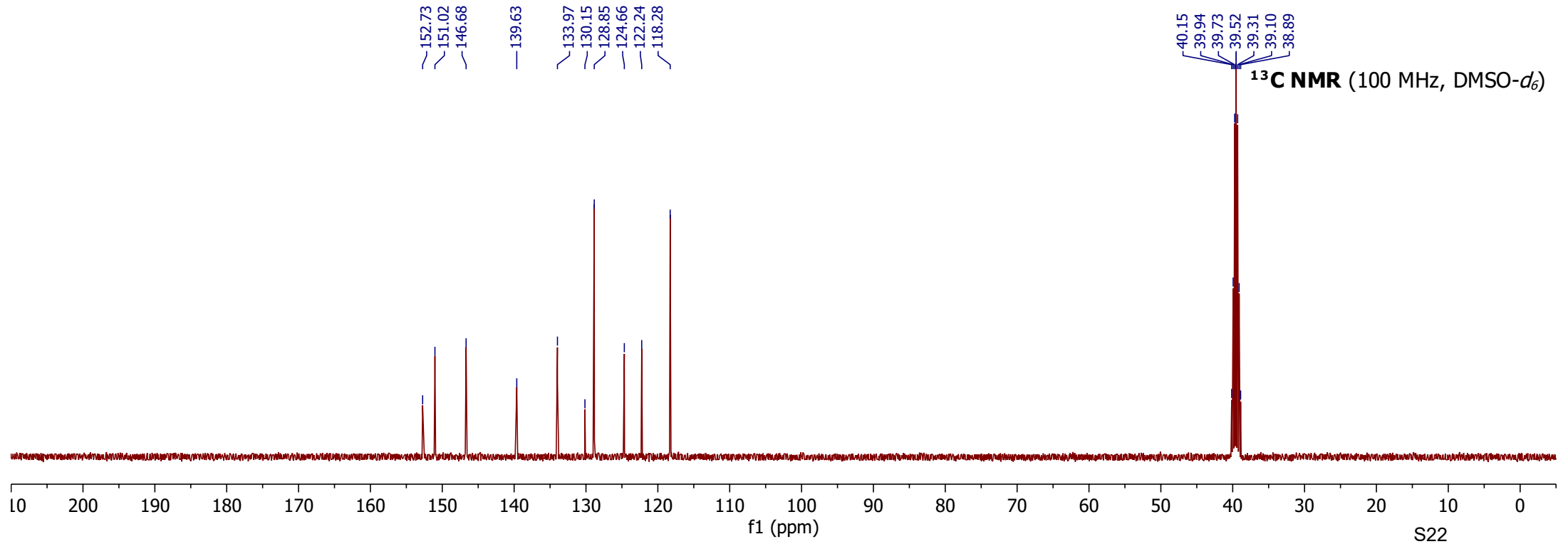
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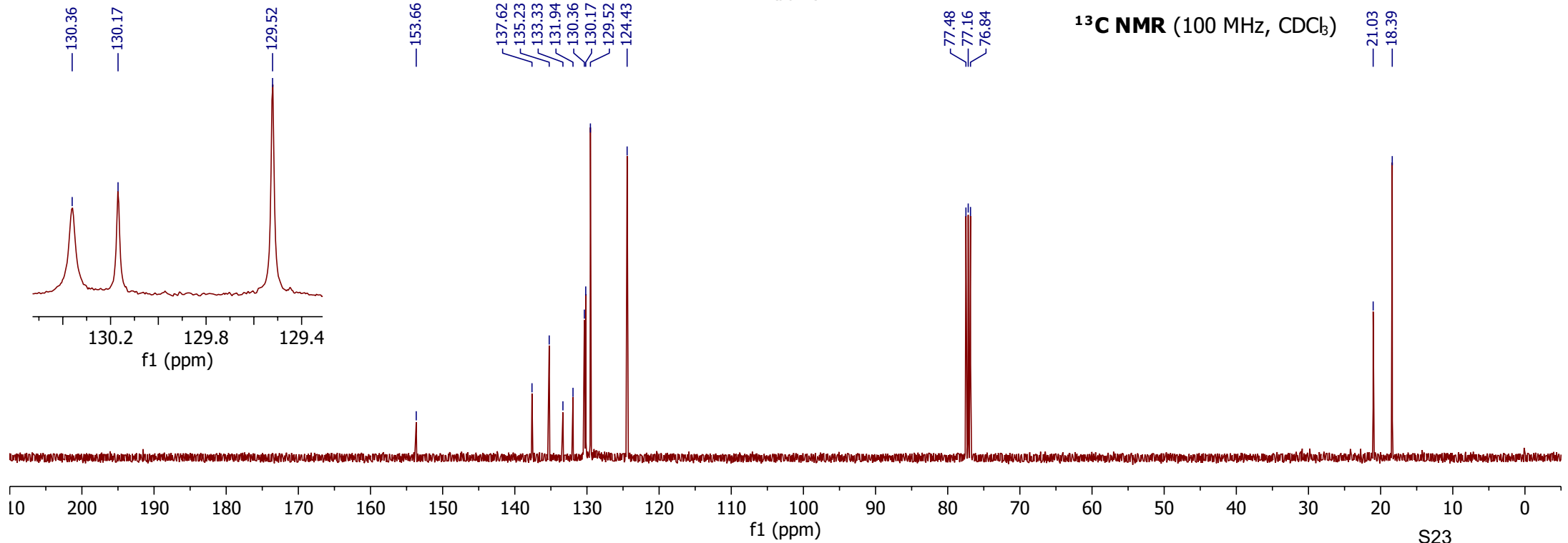
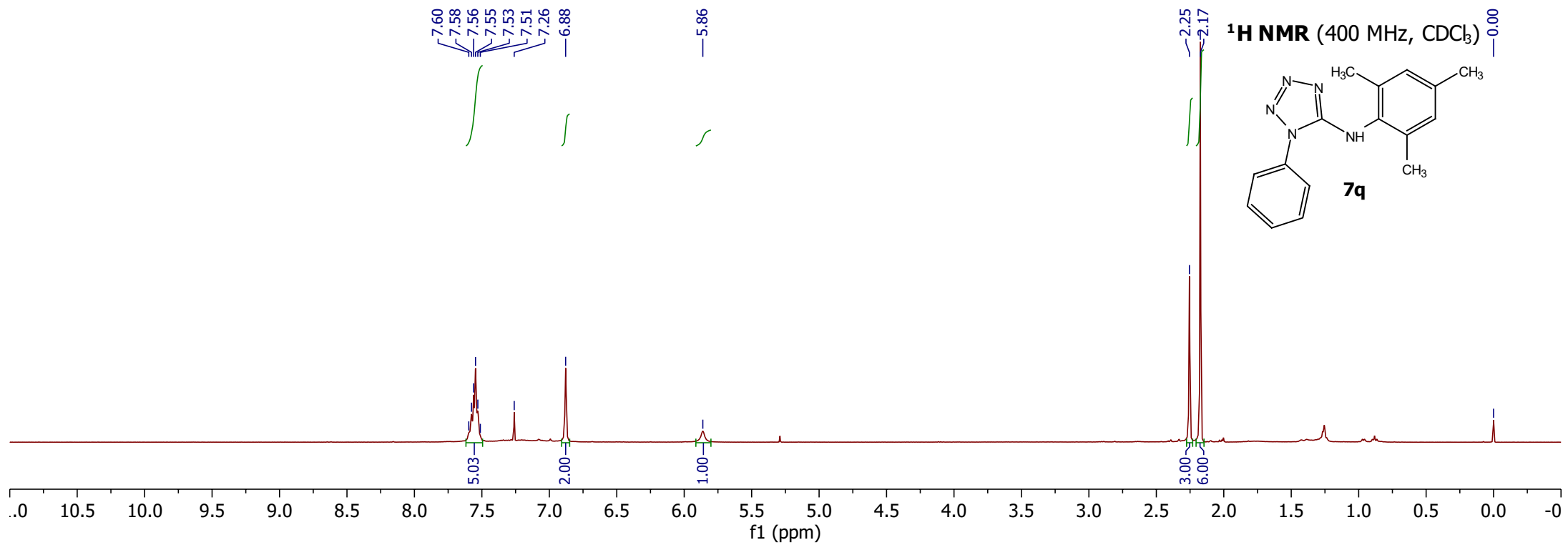


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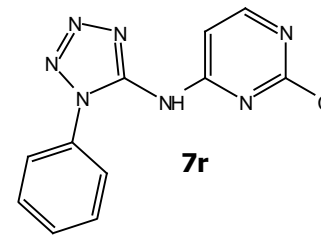


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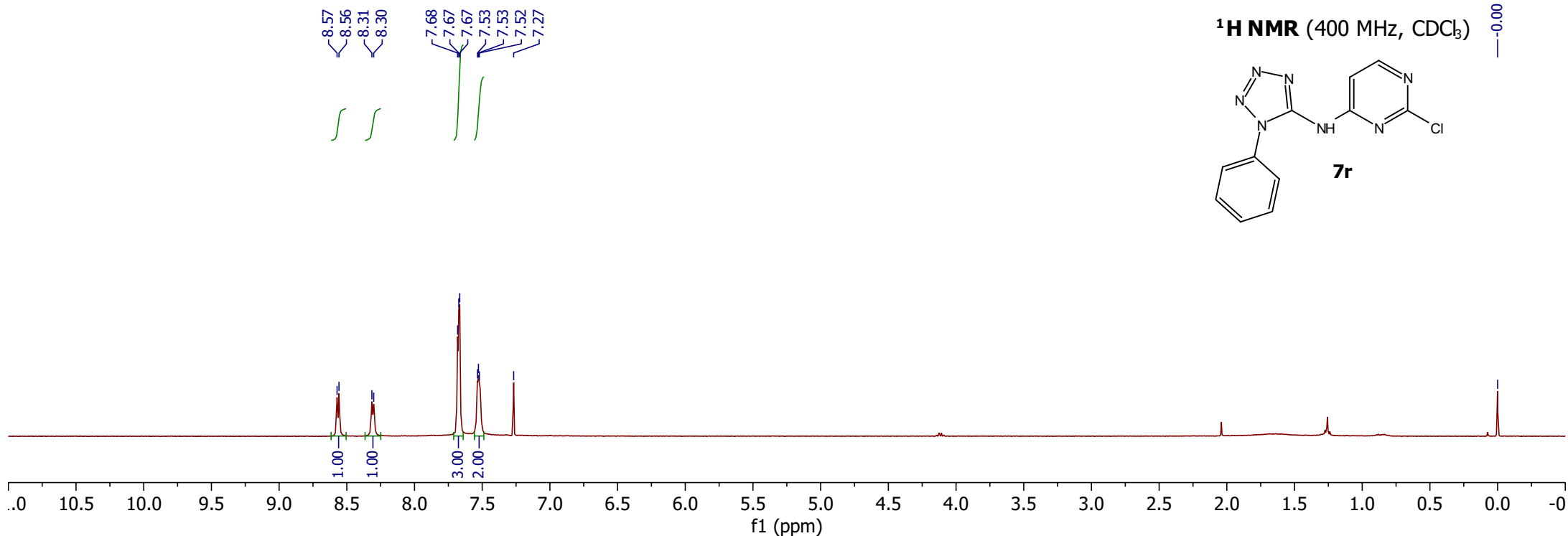




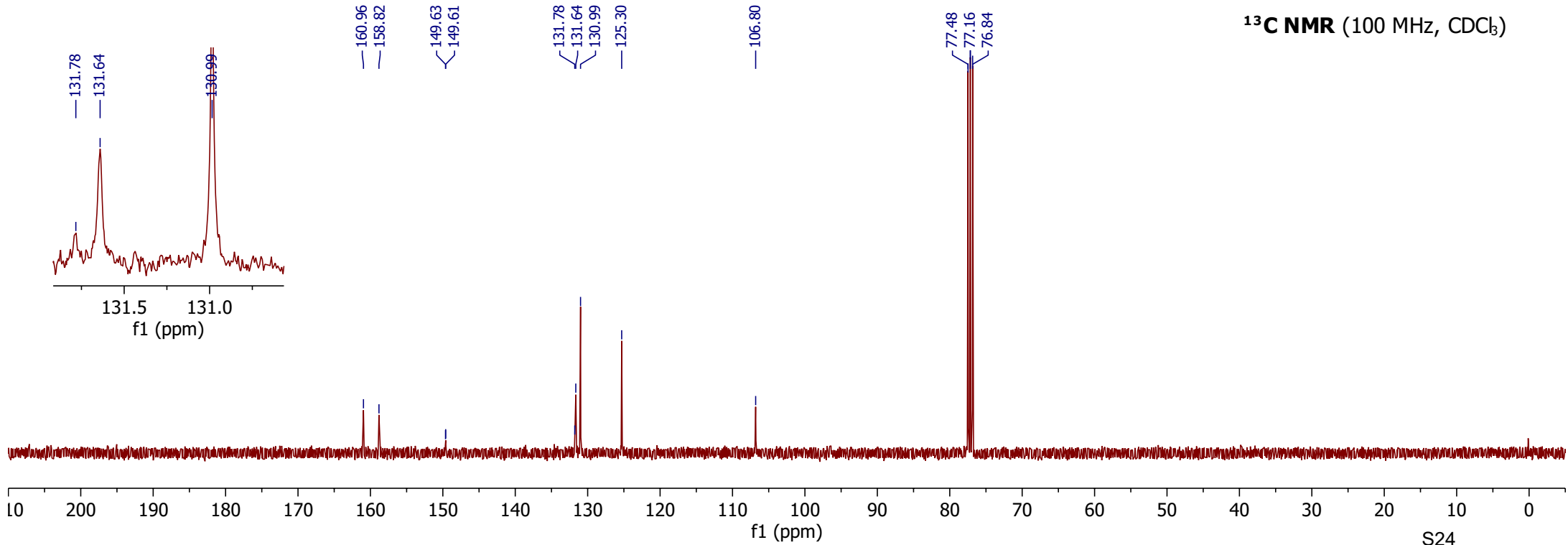
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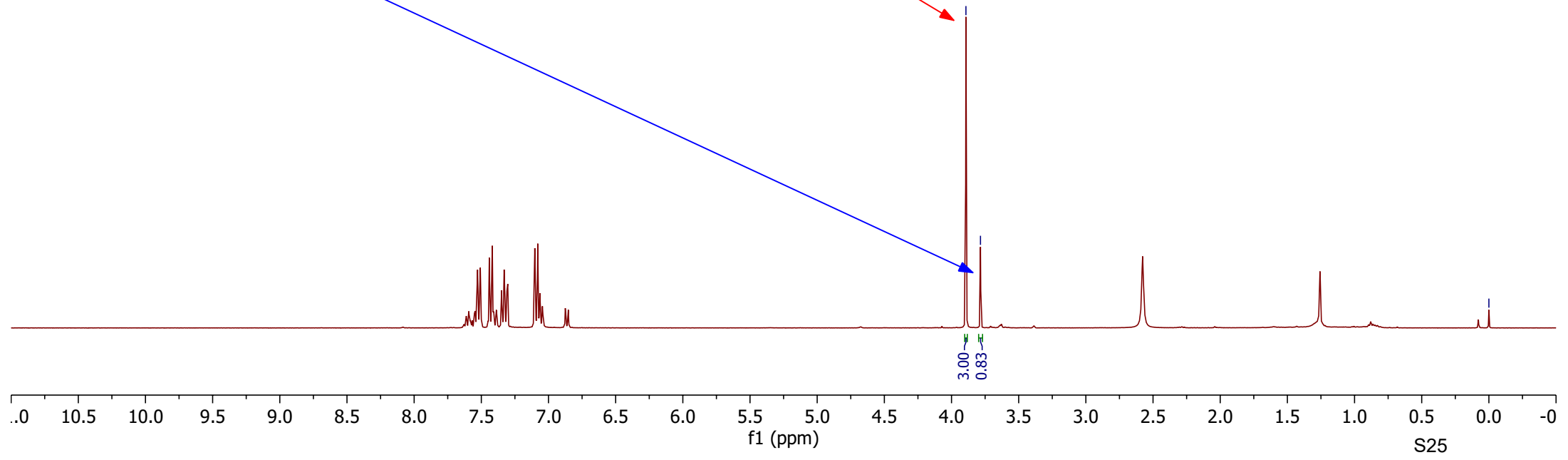
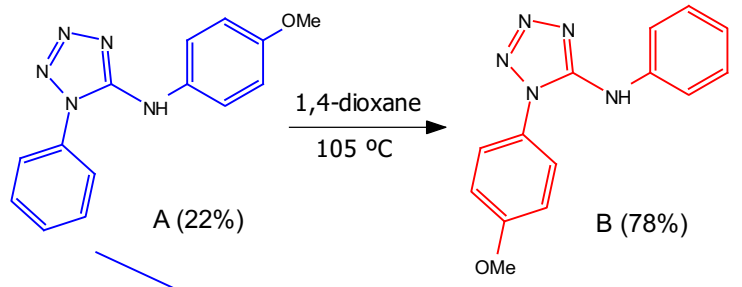
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¹H NMR (400 MHz, CDCl₃)

0.00

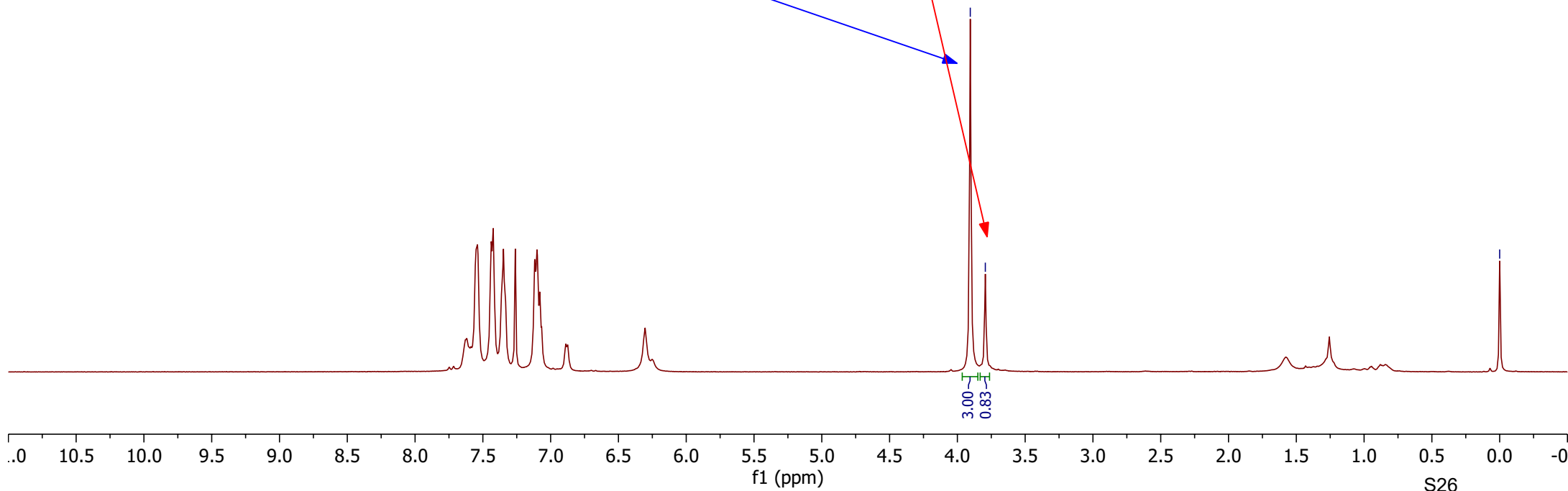
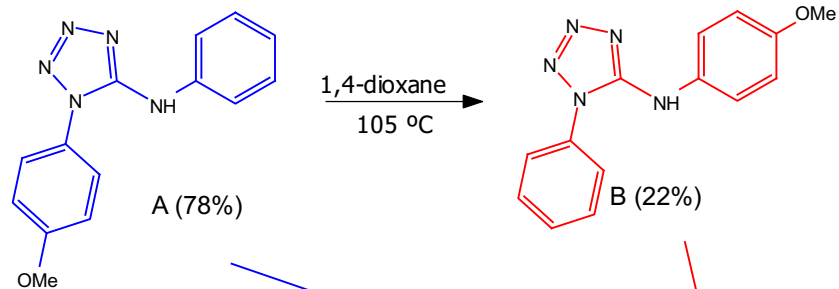
3.89
3.78



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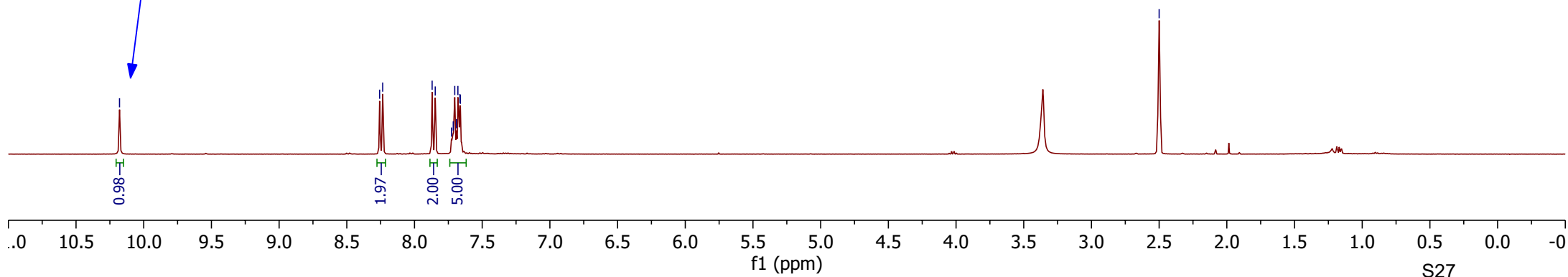
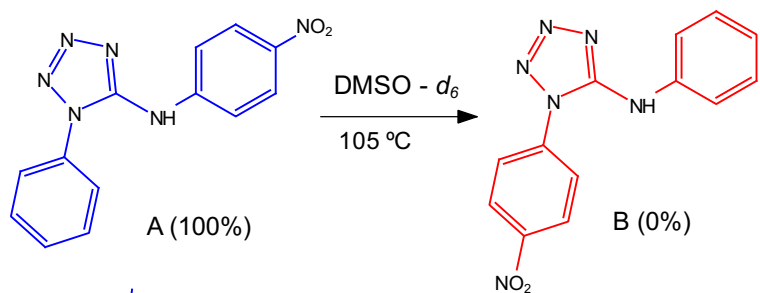
3.90
3.79



—2.50

8.26
8.23
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7.66
7.66

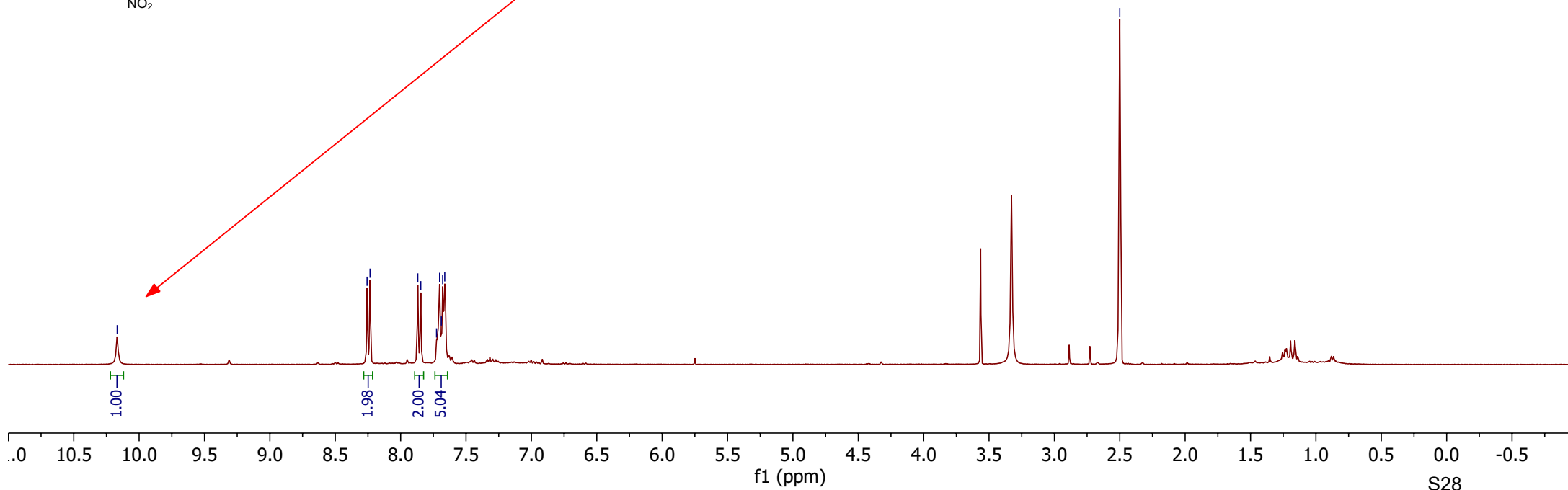
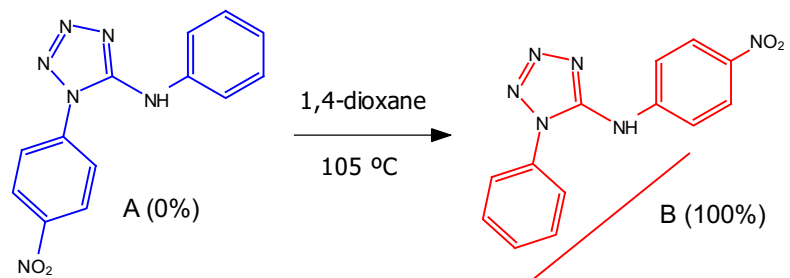
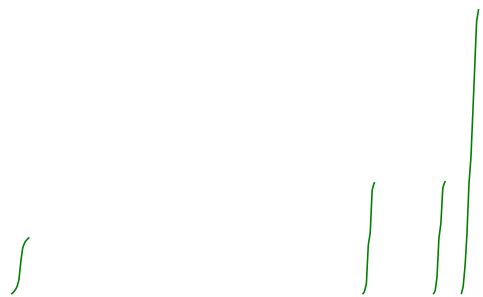
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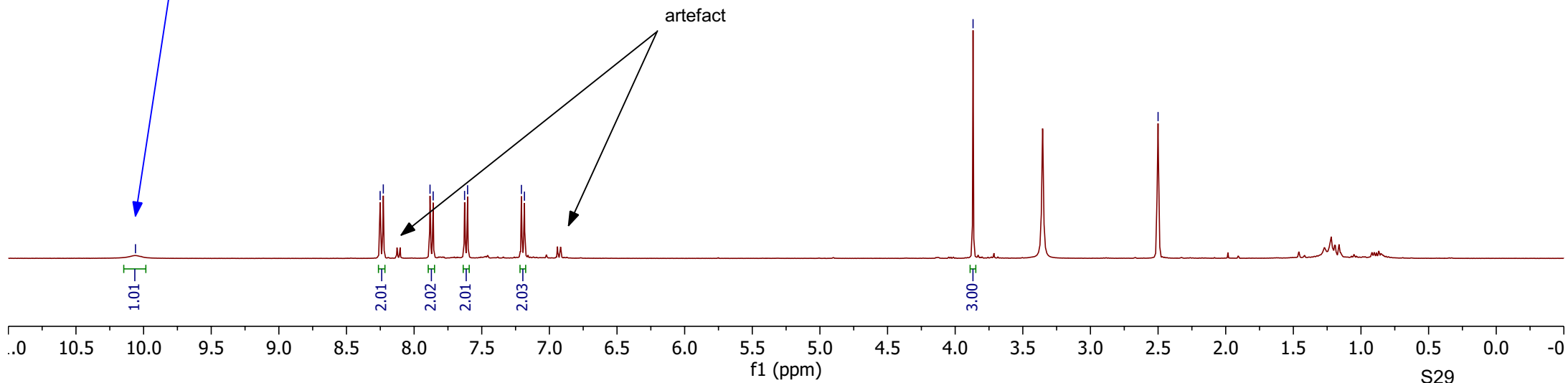
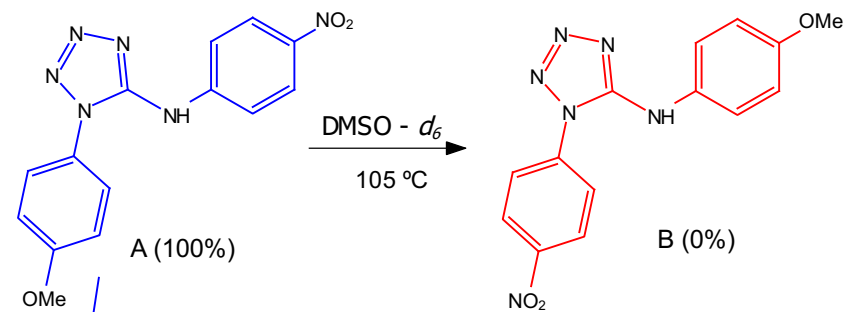
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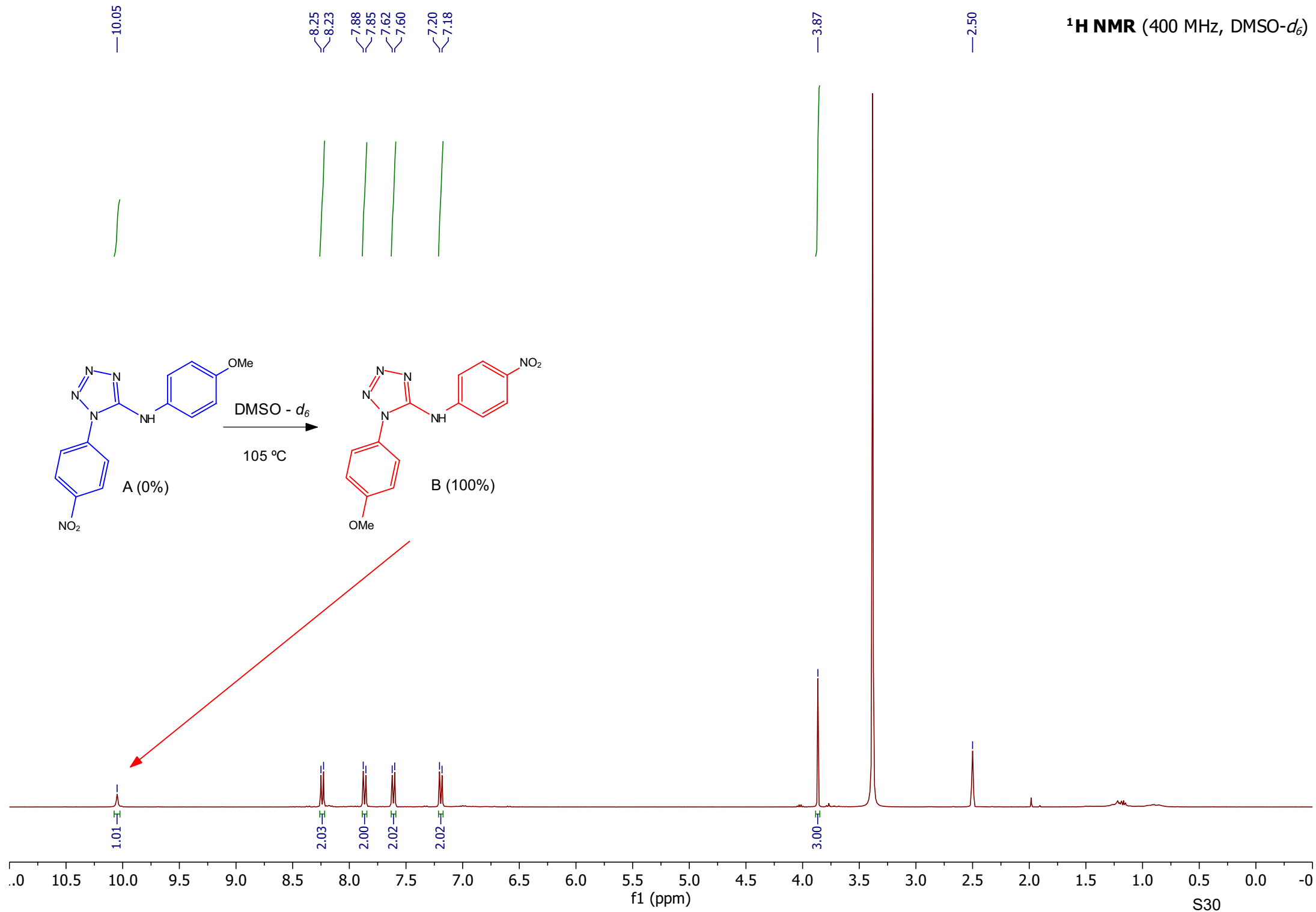
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7.85
7.73
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7.66

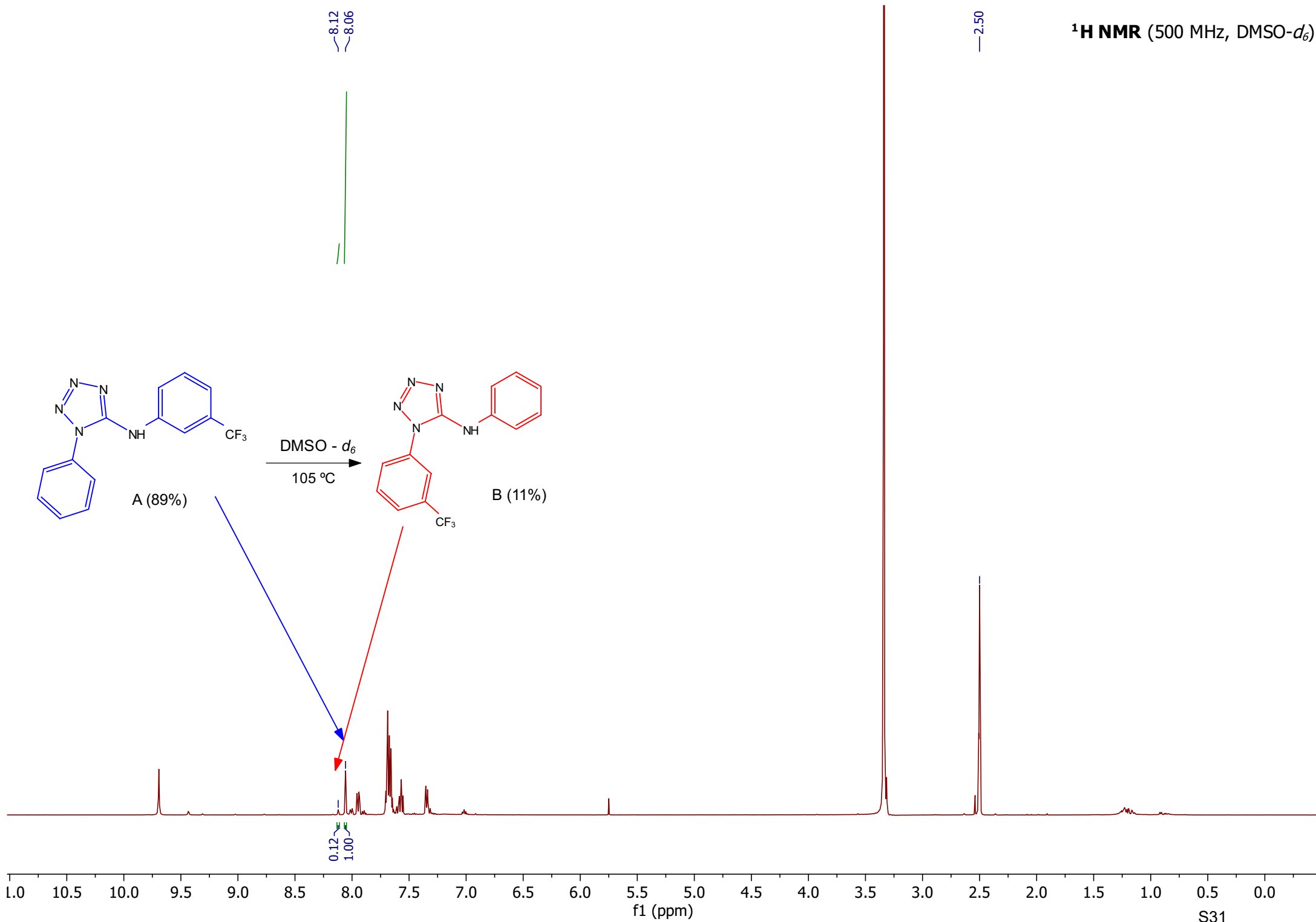
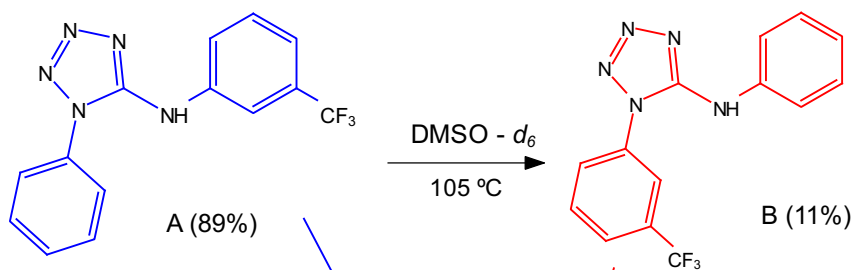
2.50



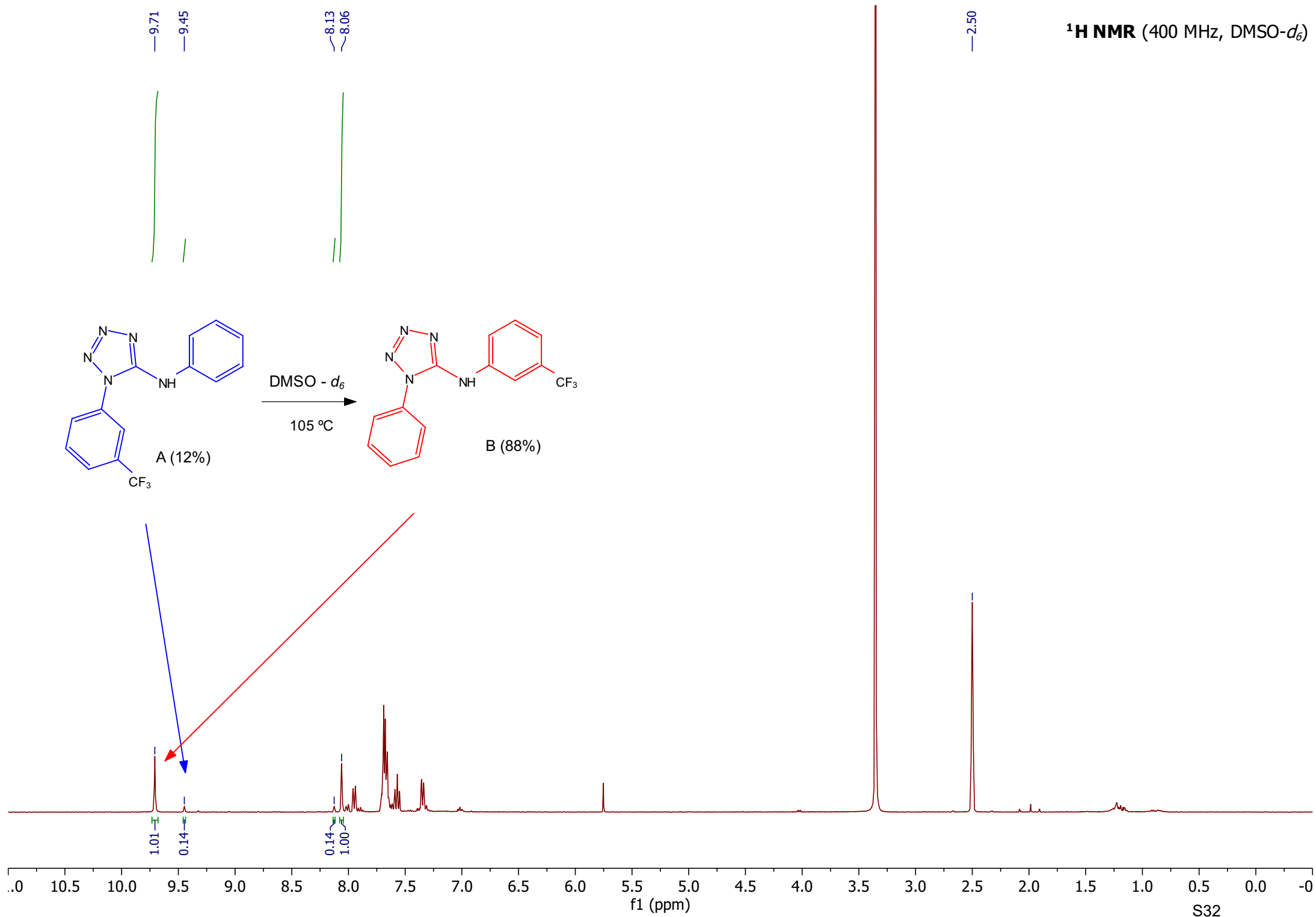
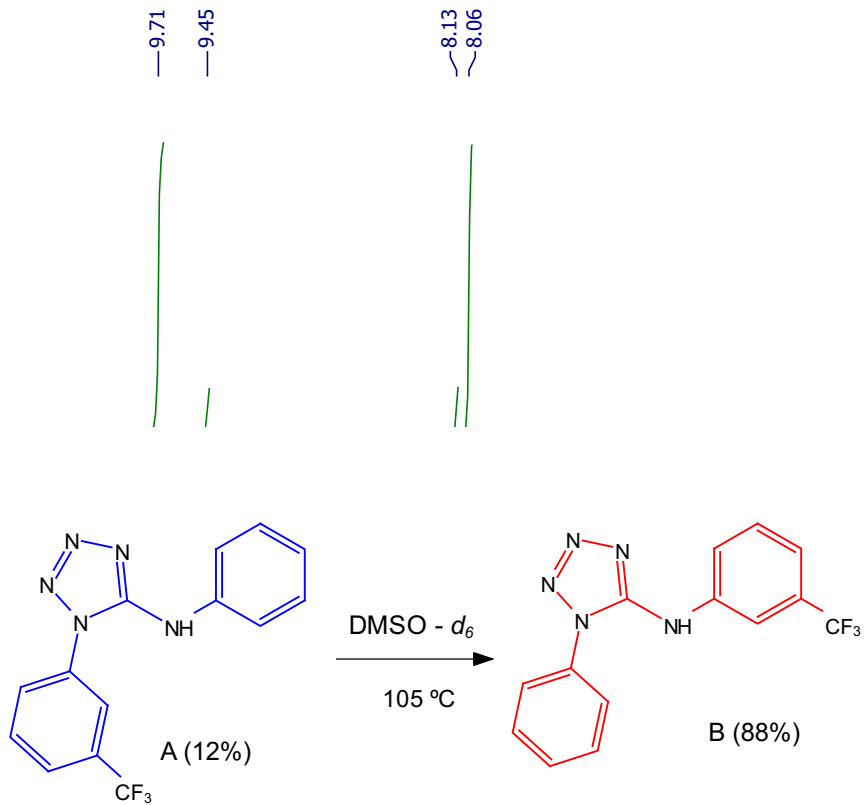
—10.06
8.25
8.23
7.88
7.86
7.63
7.60
7.21
7.18
—3.87
—2.50





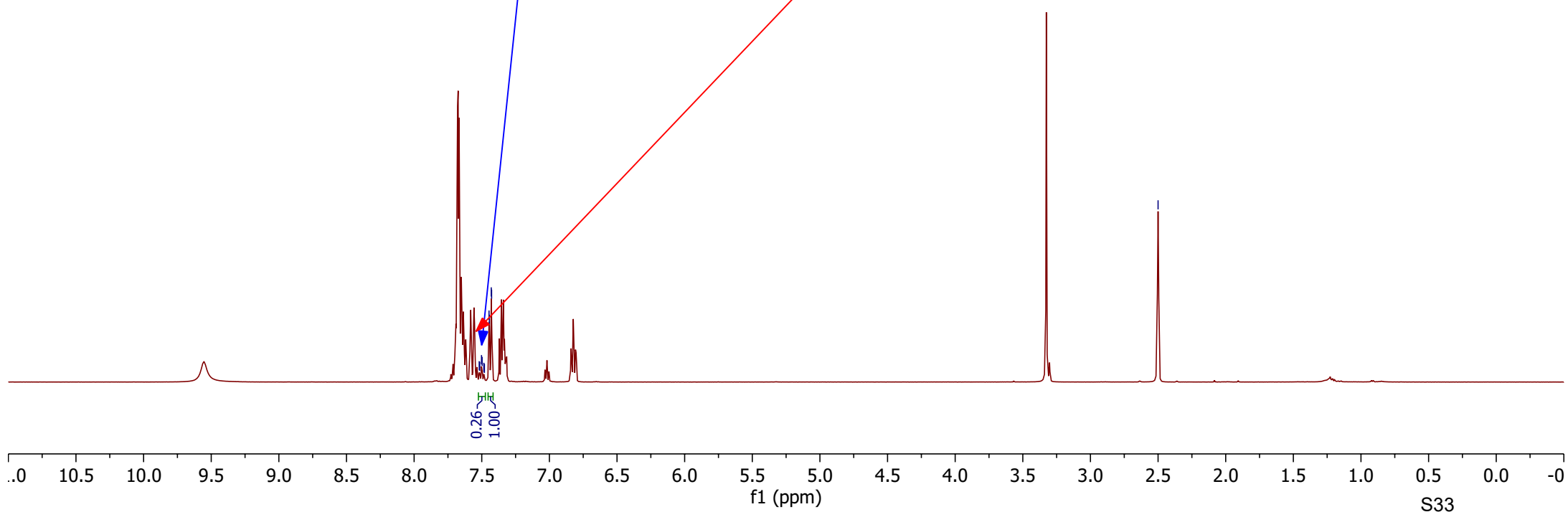
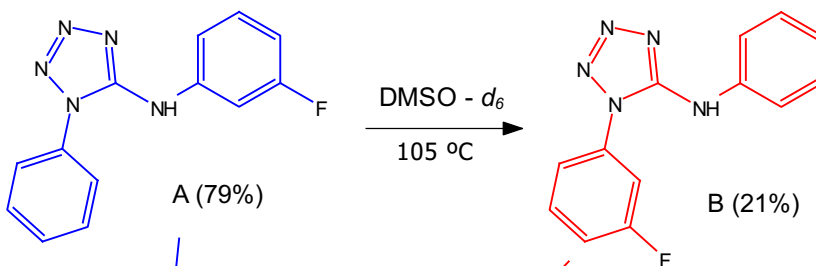


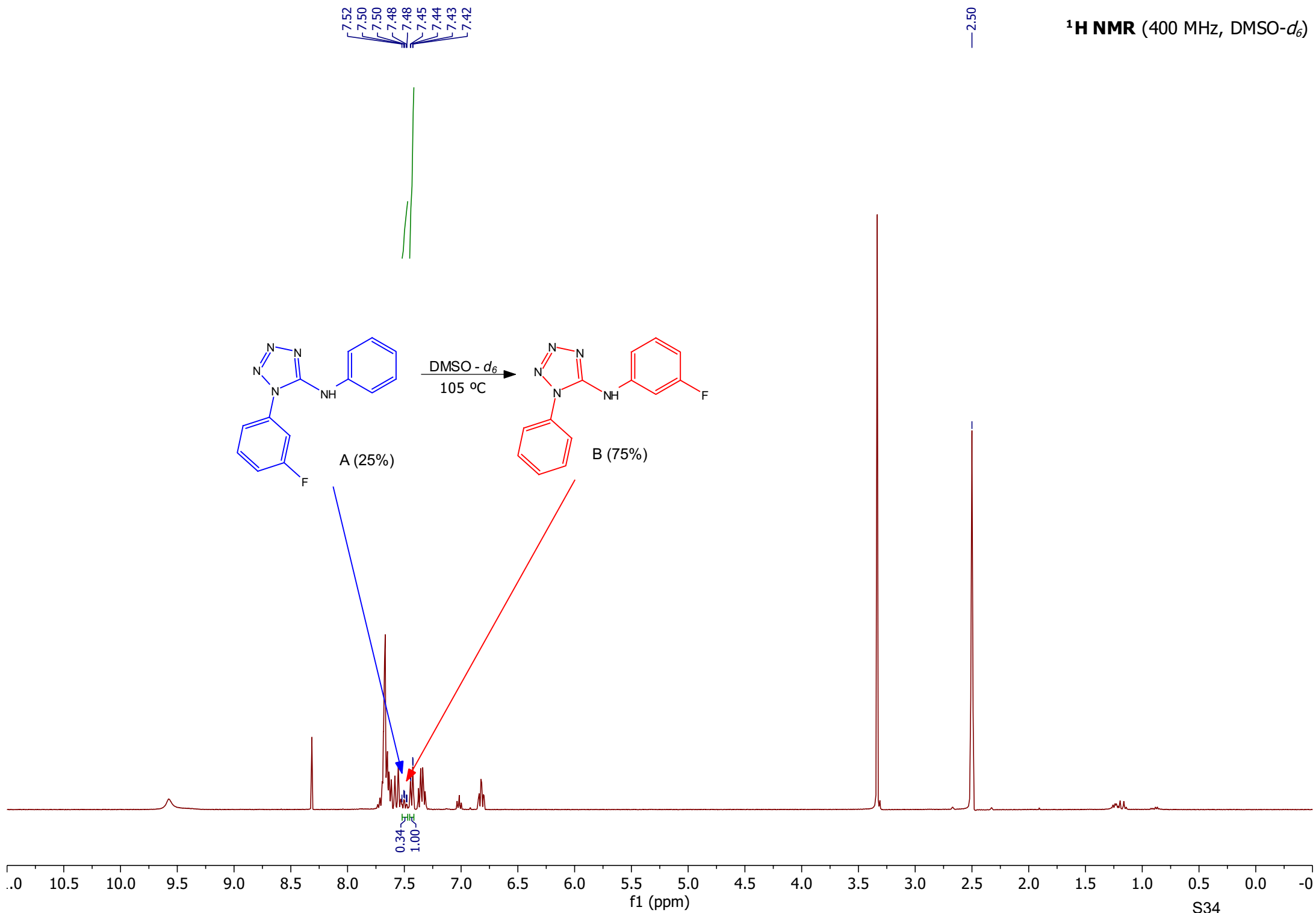
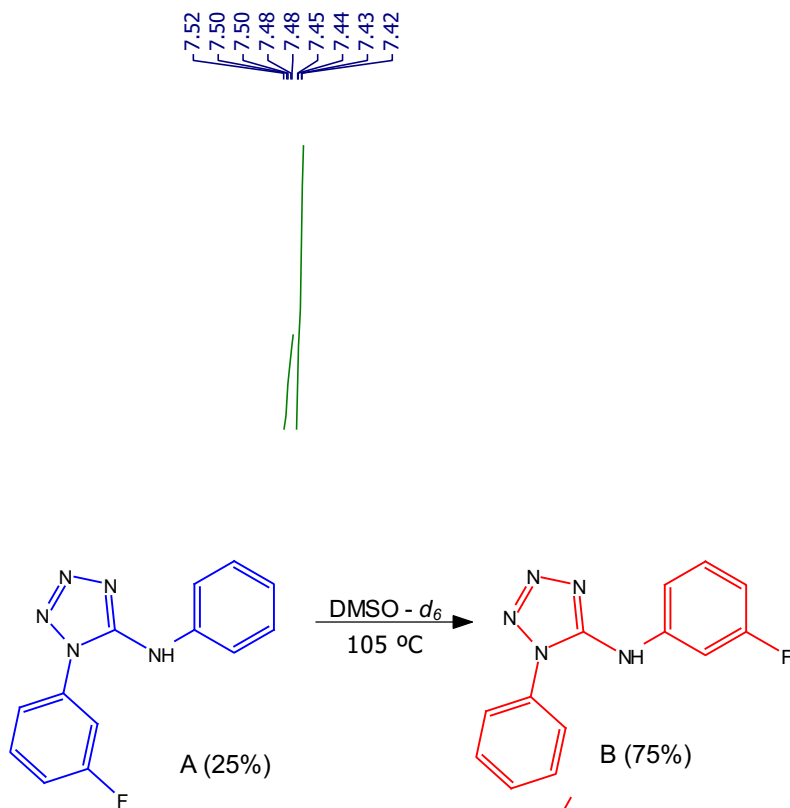
¹H NMR (400 MHz, DMSO-*d*₆)

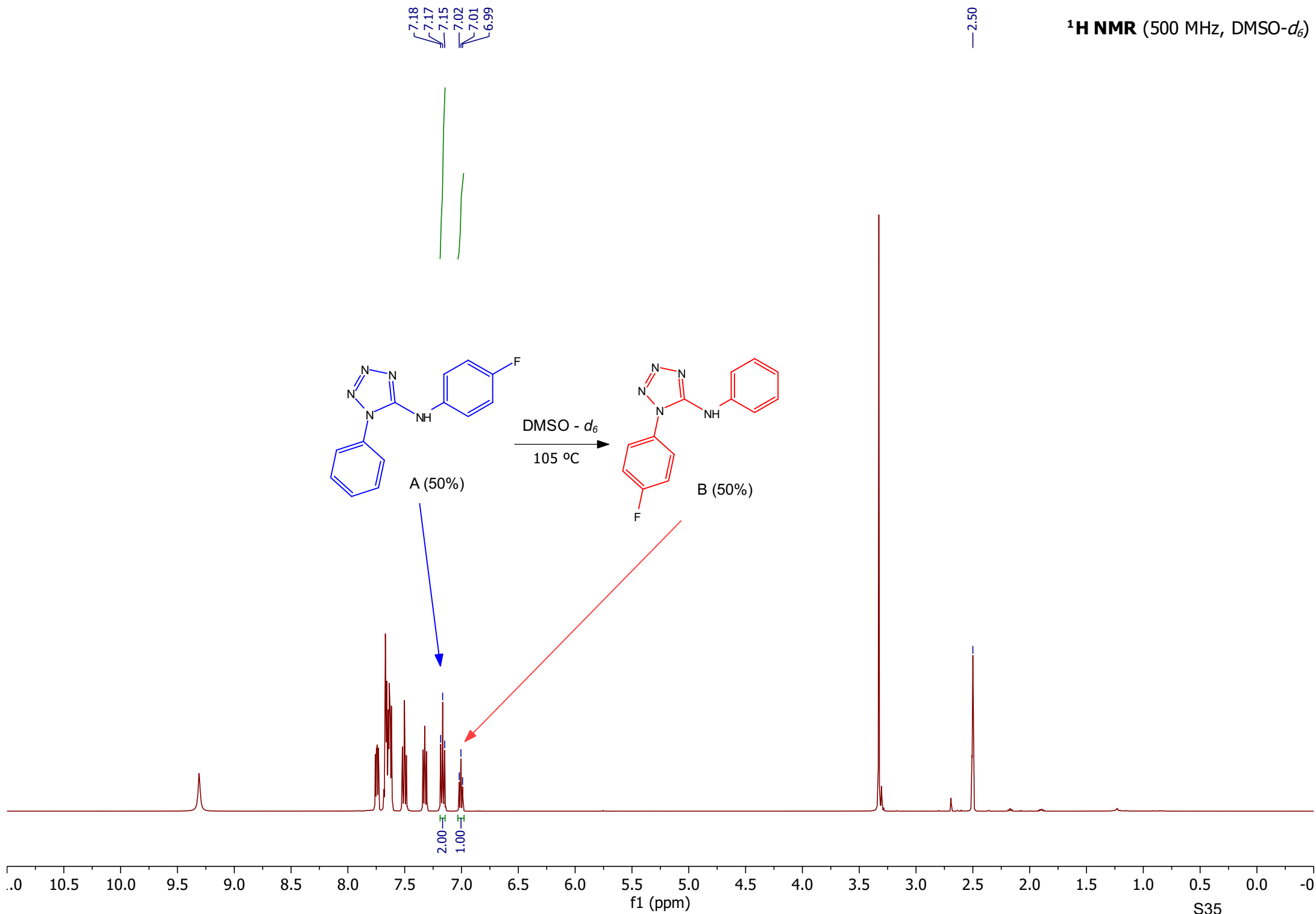


7.52
7.51
7.50
7.48
7.48
7.45
7.44
7.43

2.50

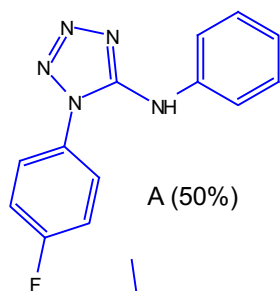




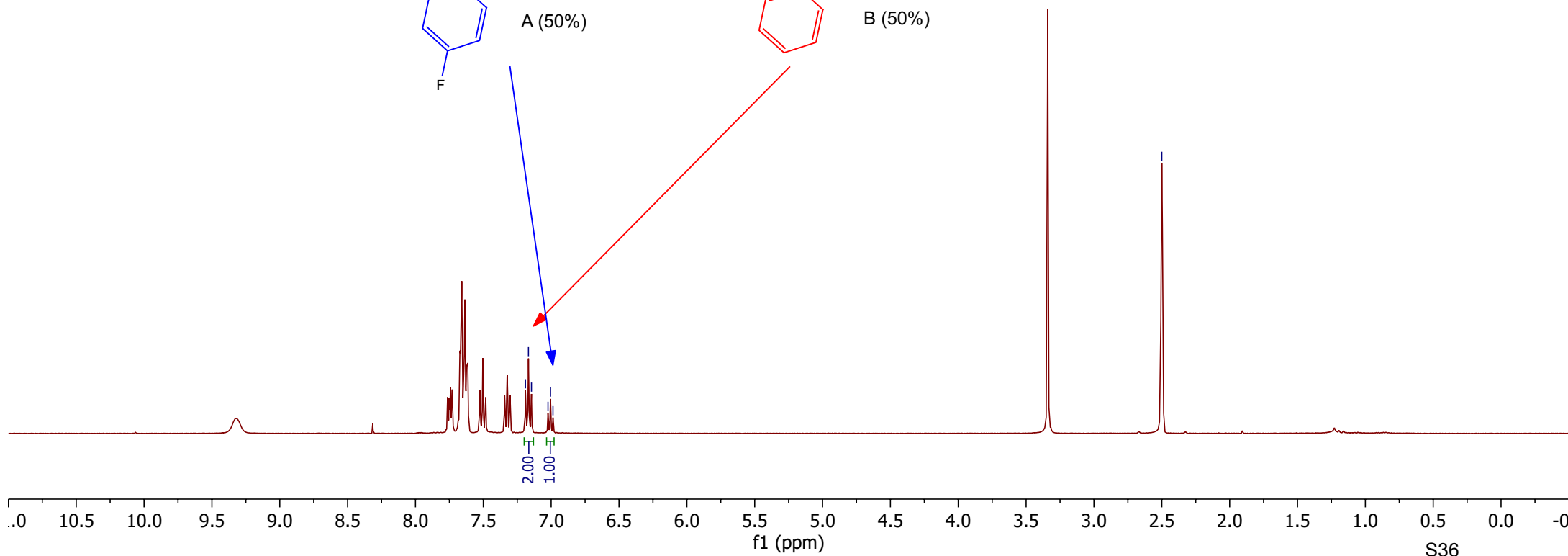
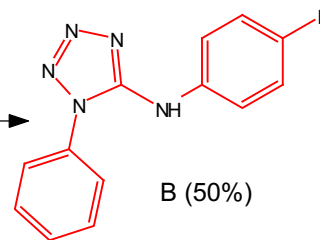


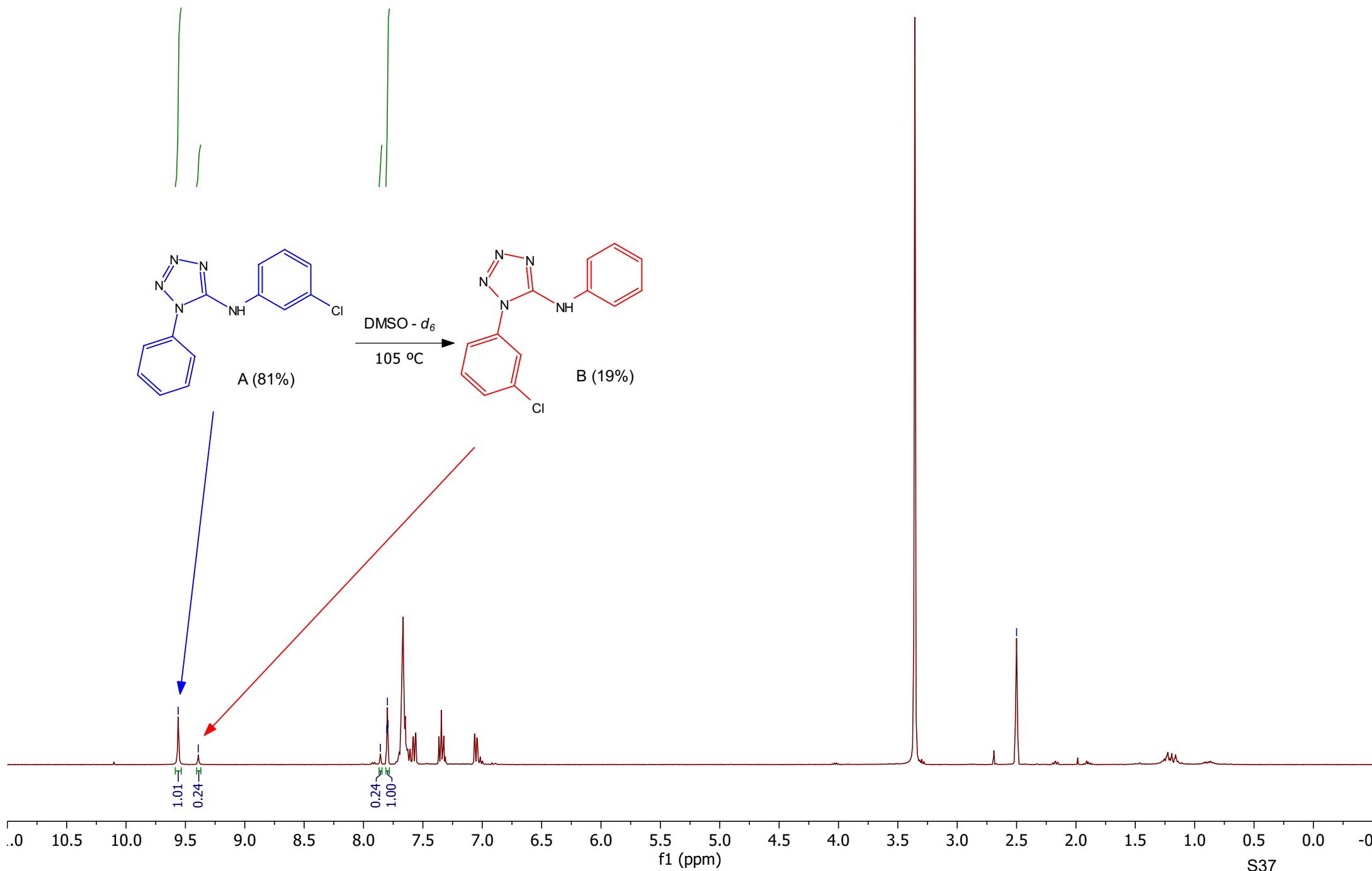
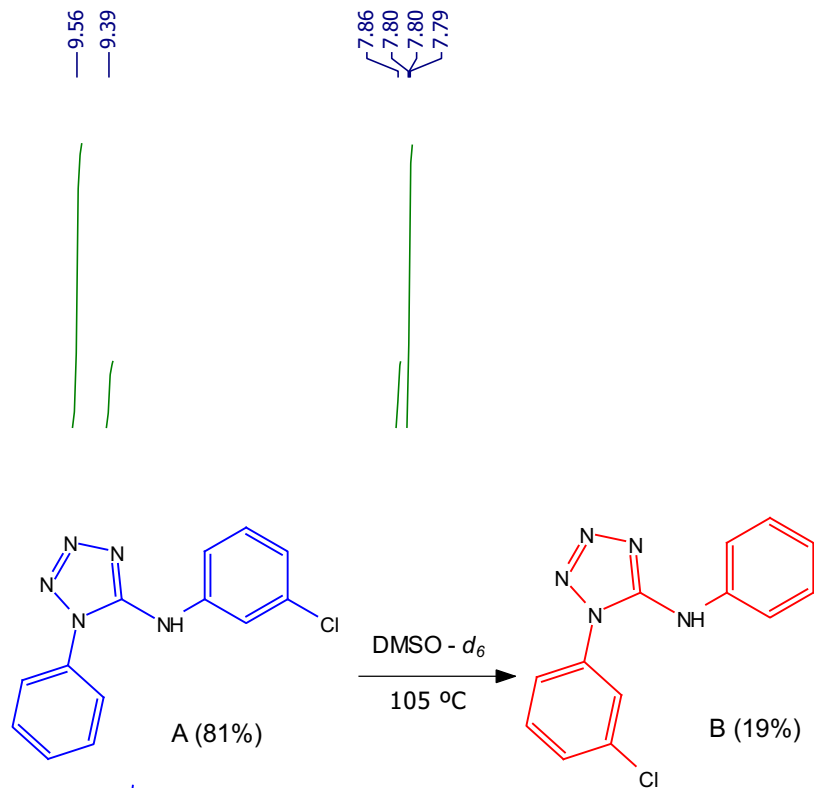
7.19
7.17
7.15
7.02
6.99

2.50



DMSO - d₆
105 °C

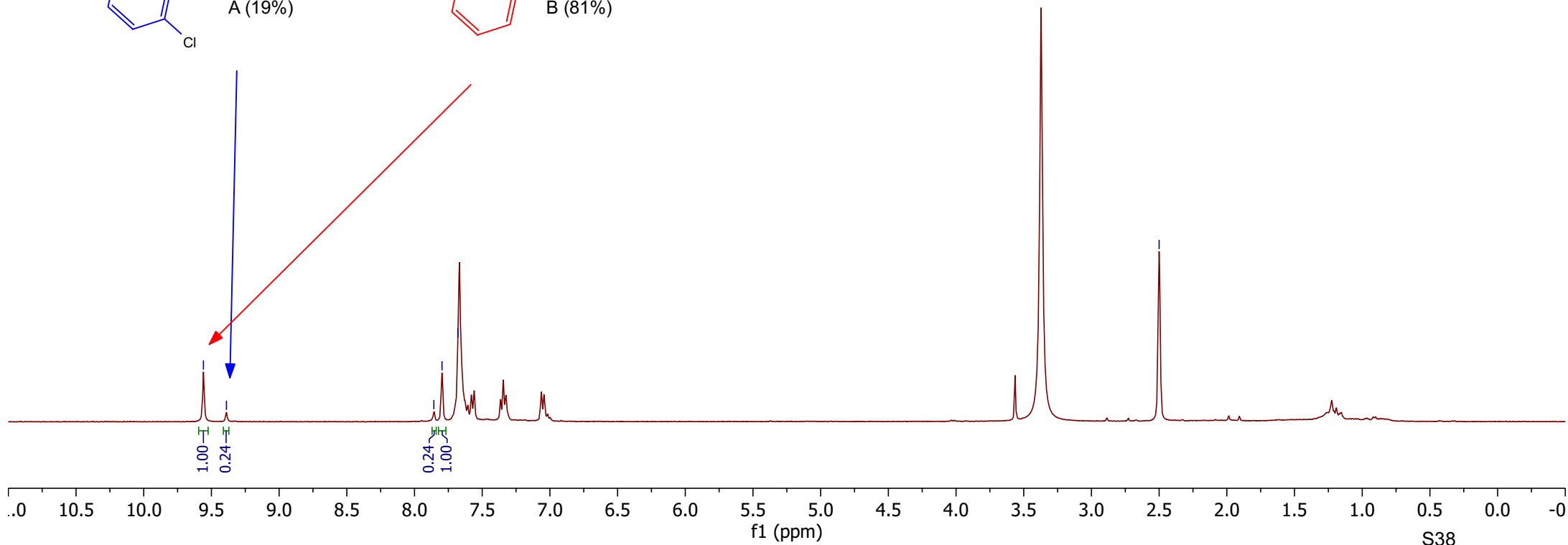
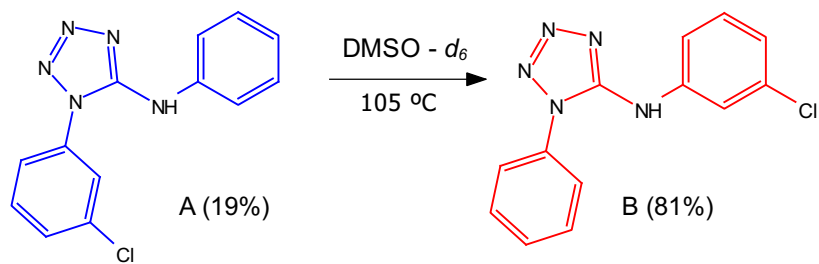


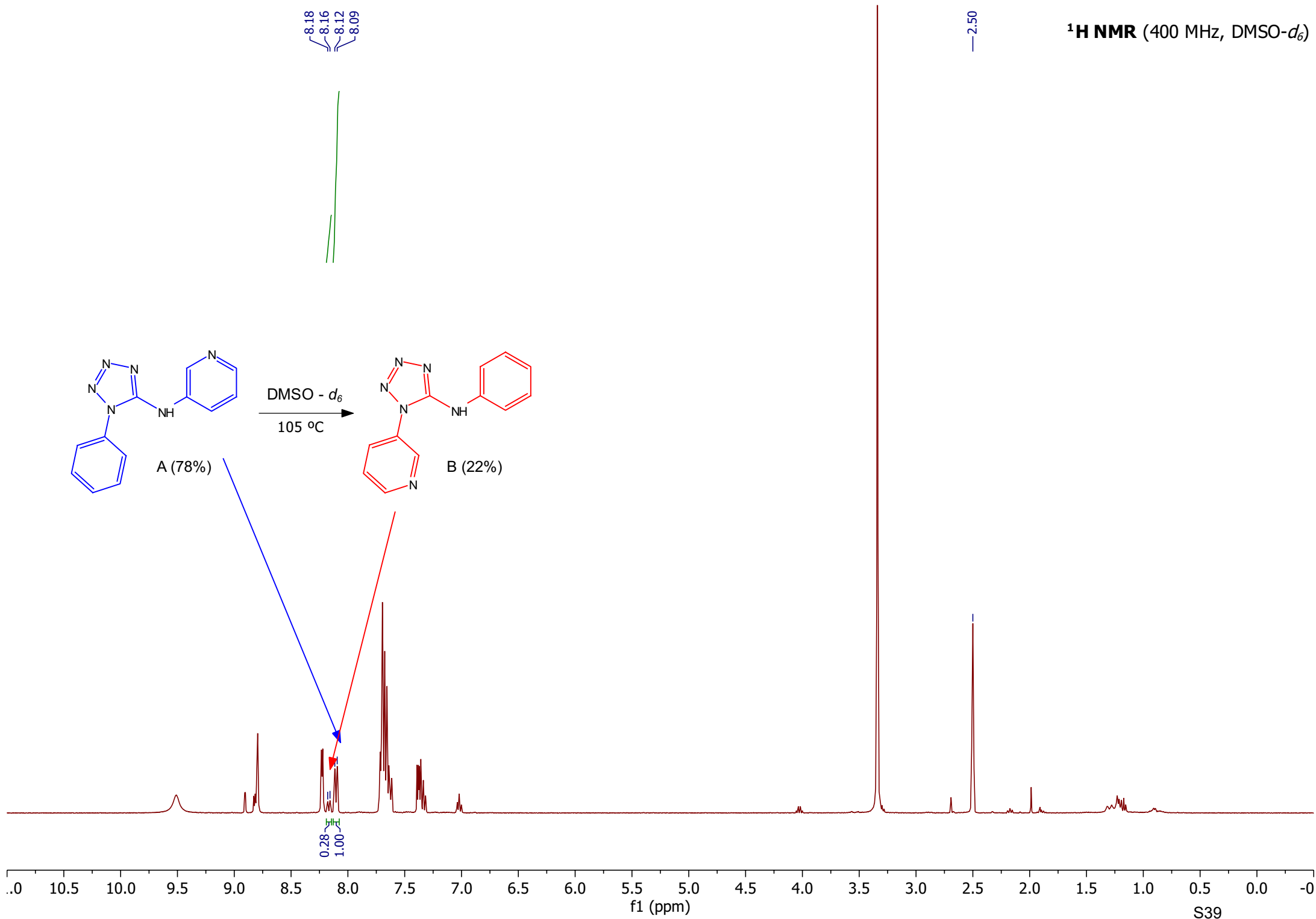


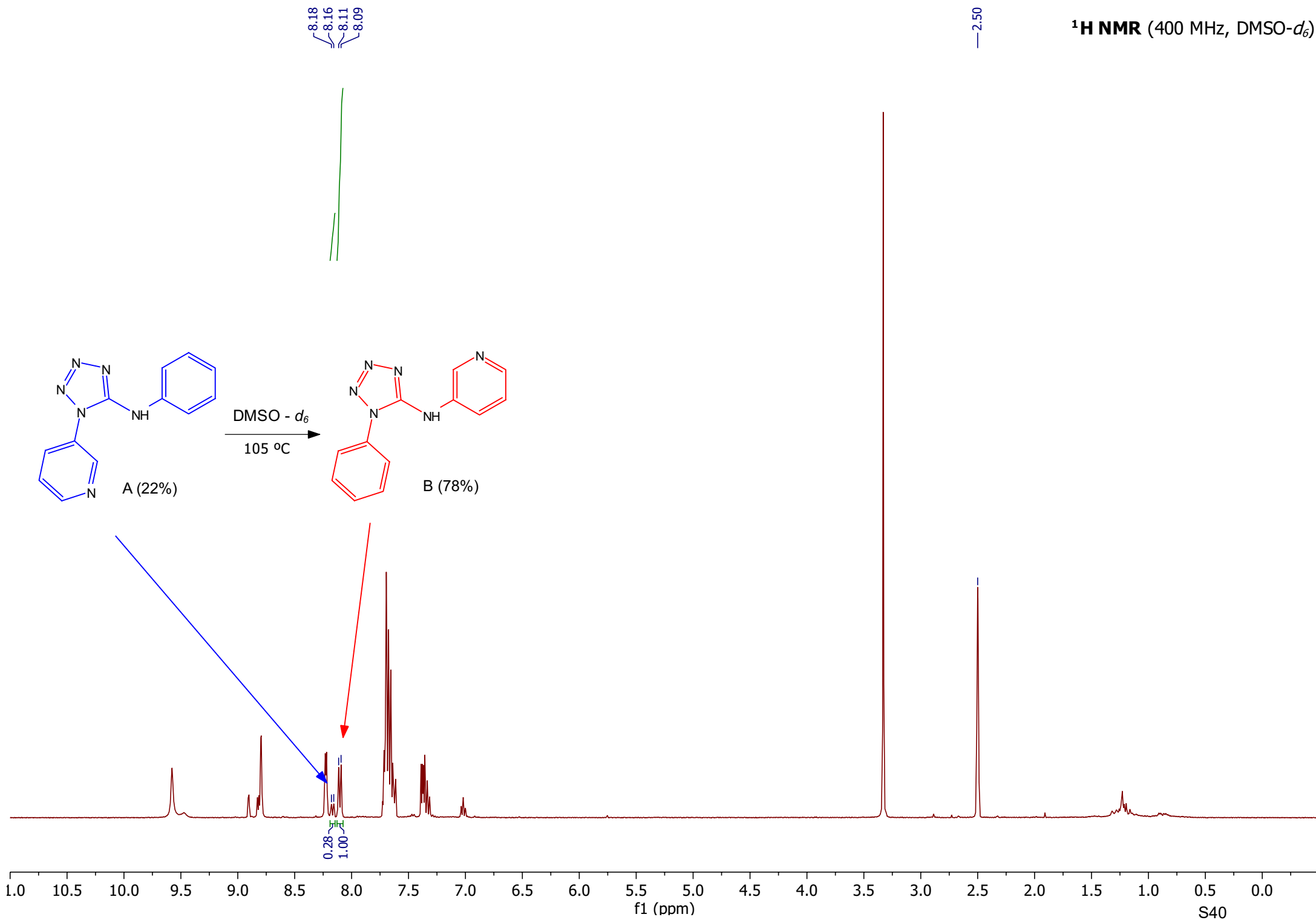
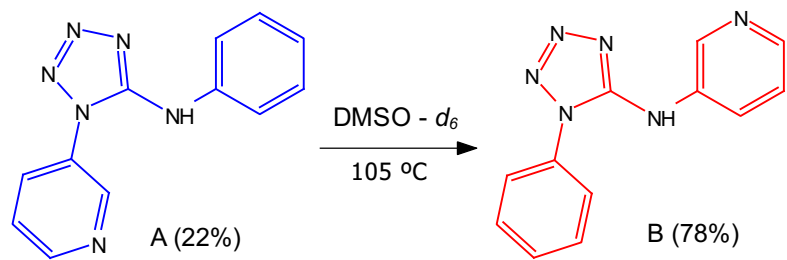
9.56
9.39

7.86
7.80
7.68

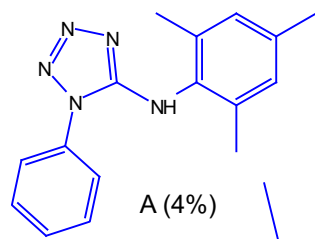
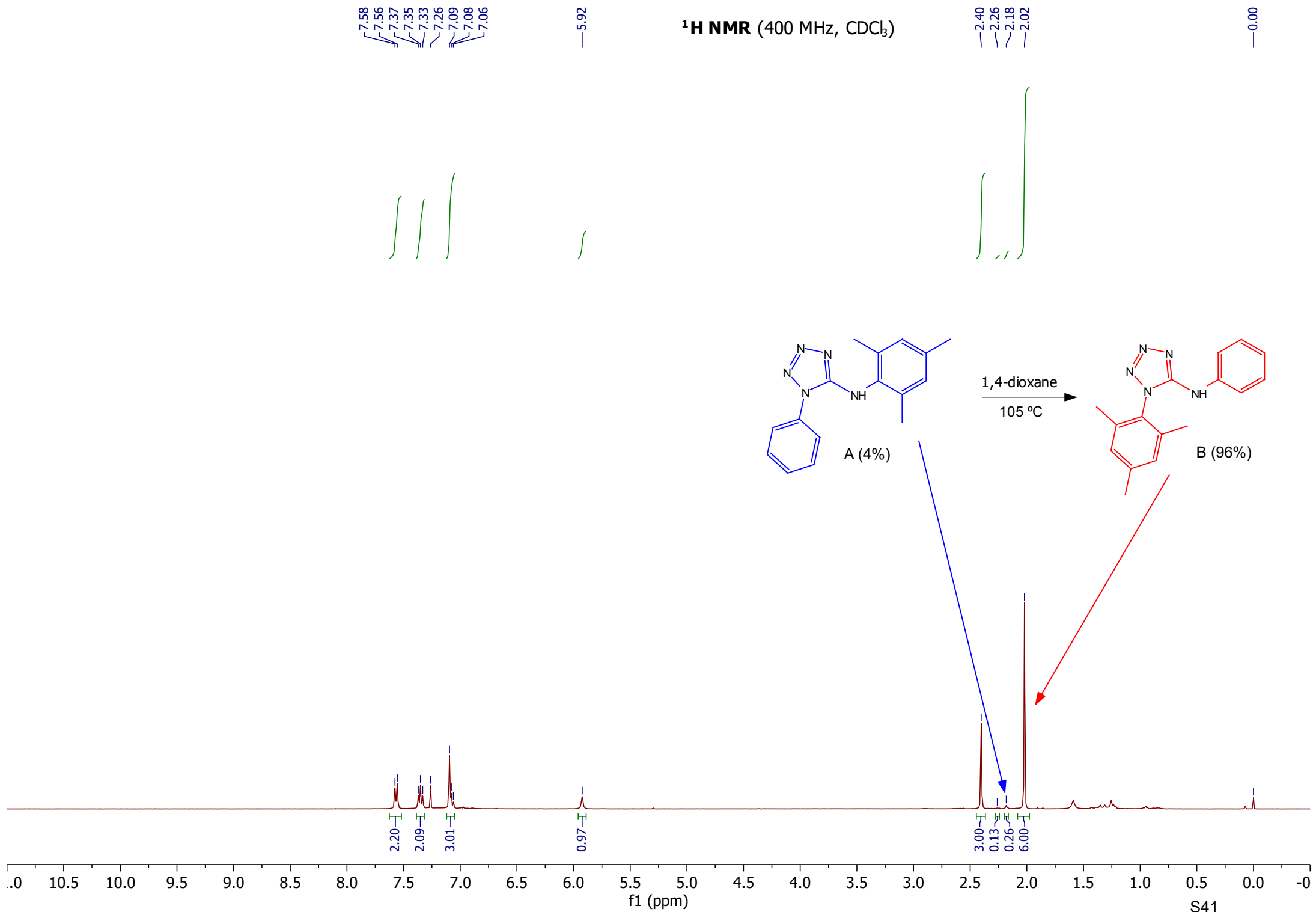
2.50



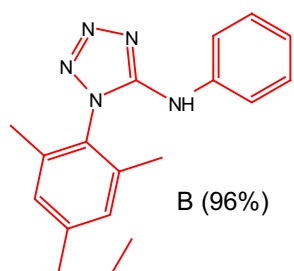




¹H NMR (400 MHz, CDCl₃)



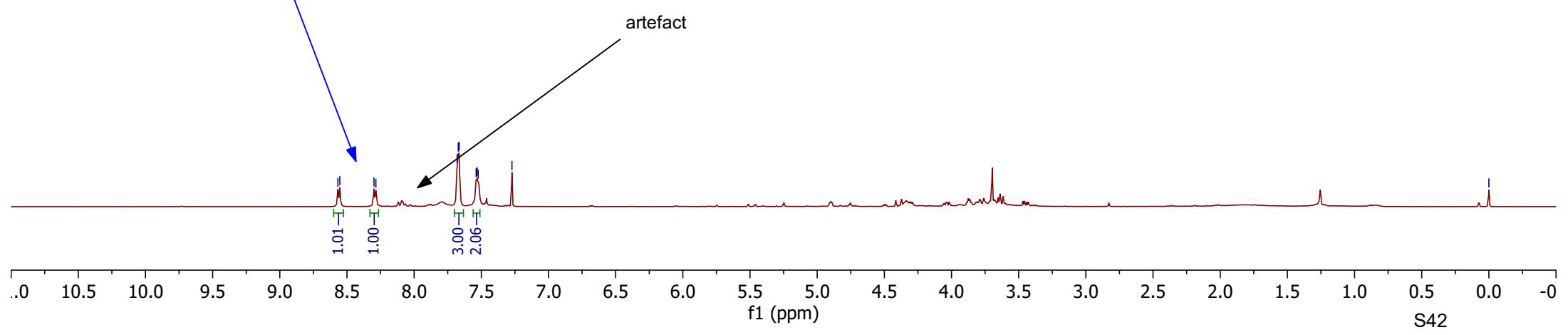
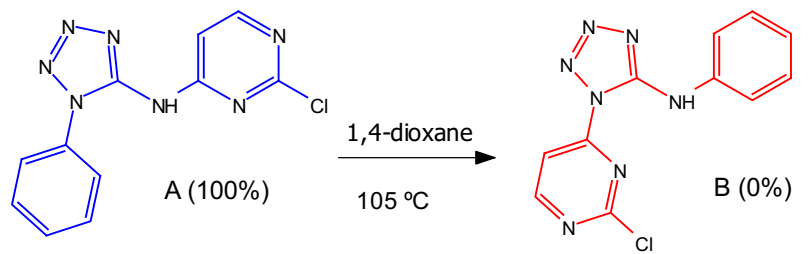
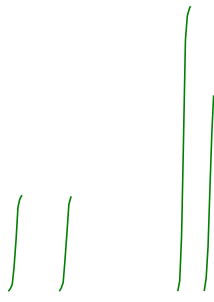
1,4-dioxane
105 °C



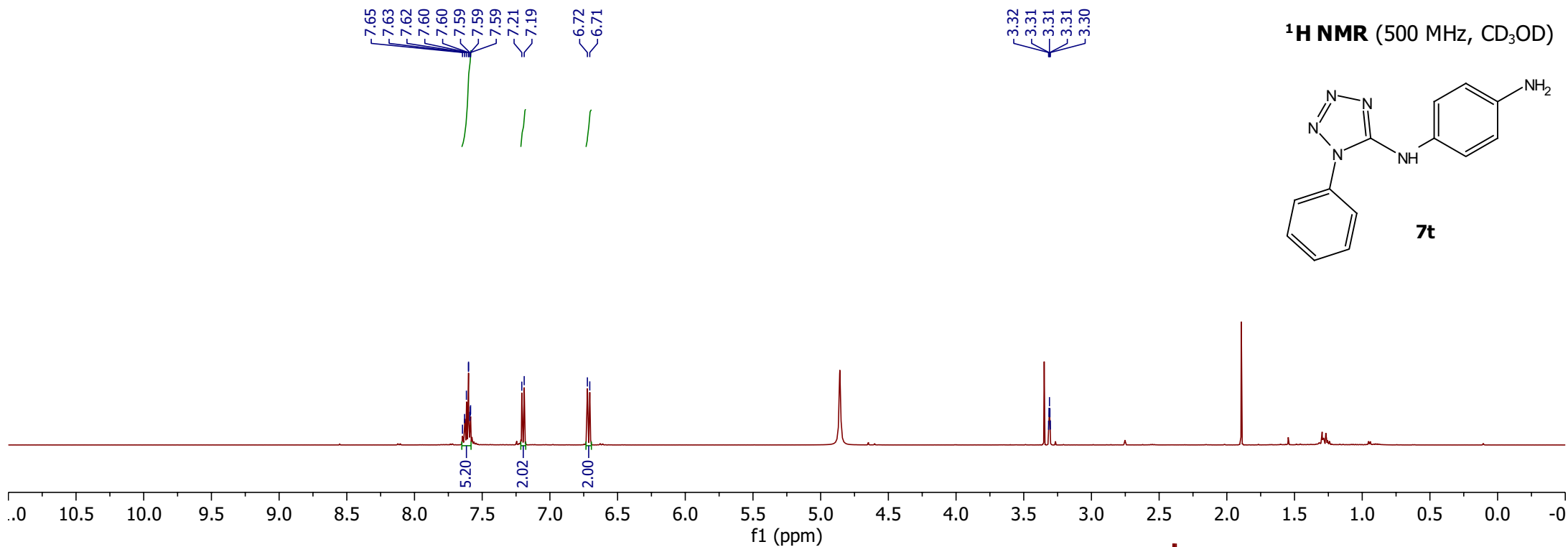
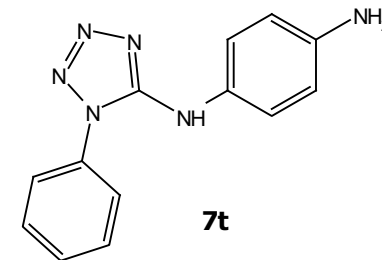
¹H NMR (400 MHz, CDCl₃)

0.00

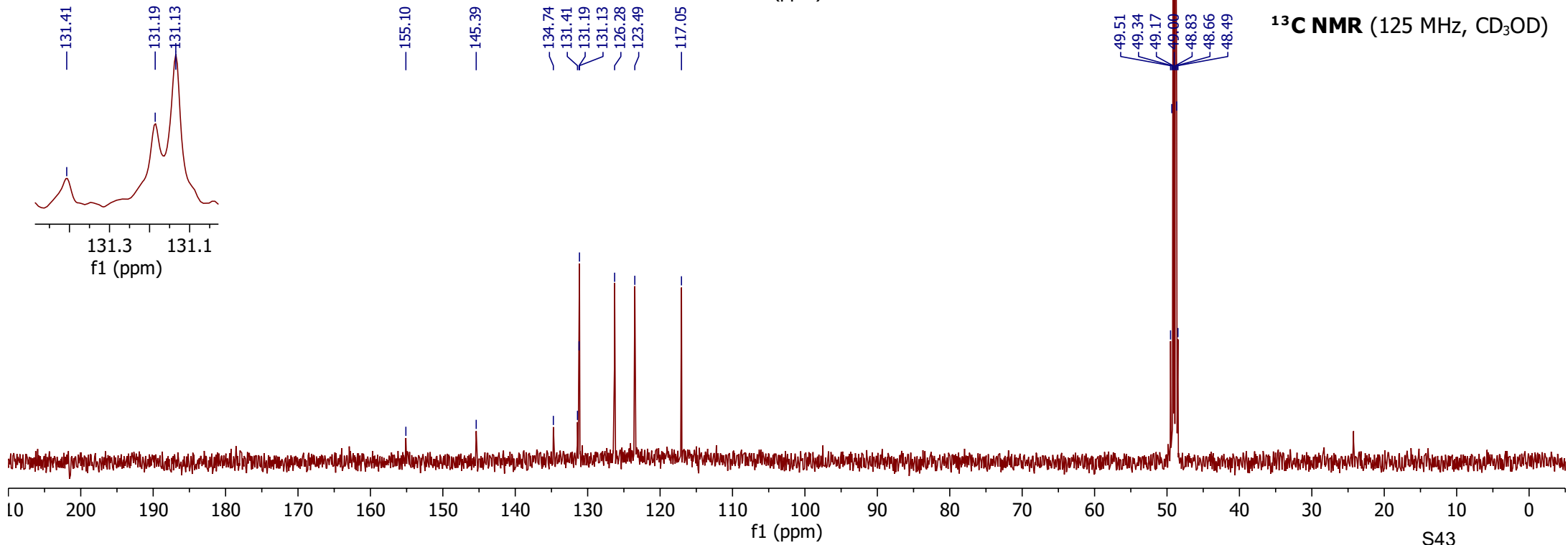
8.57
8.55
8.30
8.28
7.68
7.67
7.66
7.54
7.53
7.52
7.27



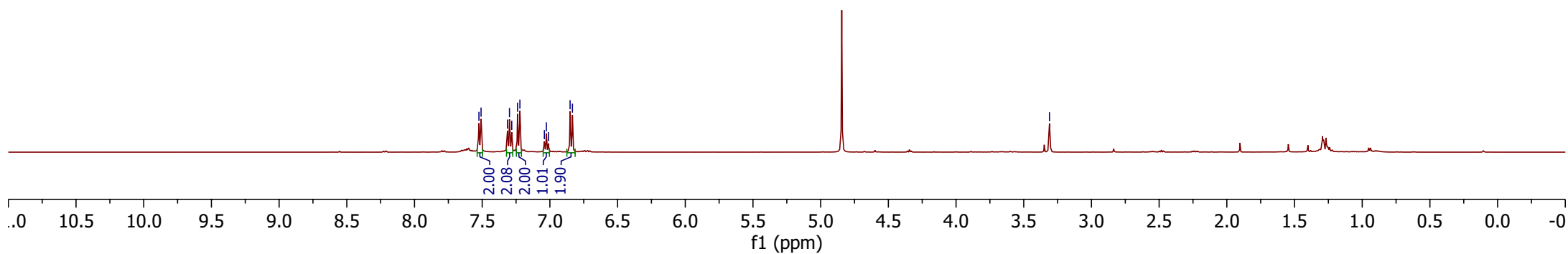
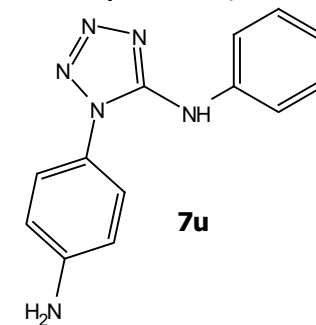
¹H NMR (500 MHz, CD₃OD)



¹³C NMR (125 MHz, CD₃OD)



¹H NMR (500 MHz, CD₃OD)



¹³C NMR (125 MHz, CD₃OD)

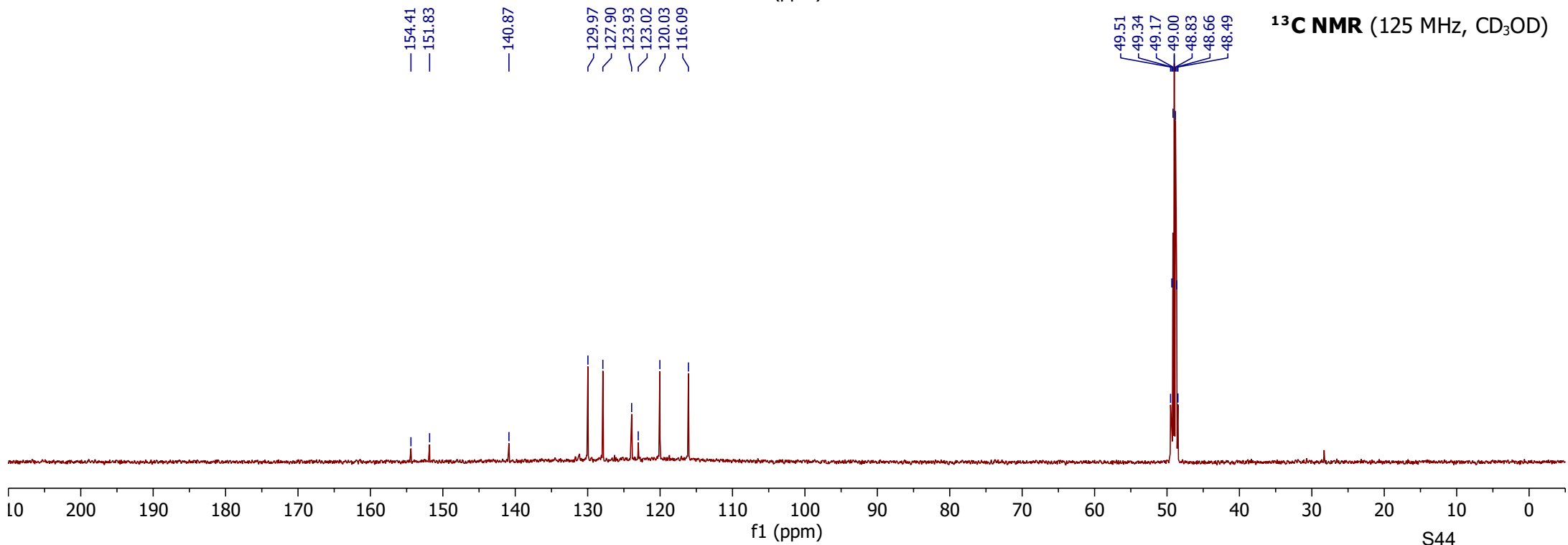
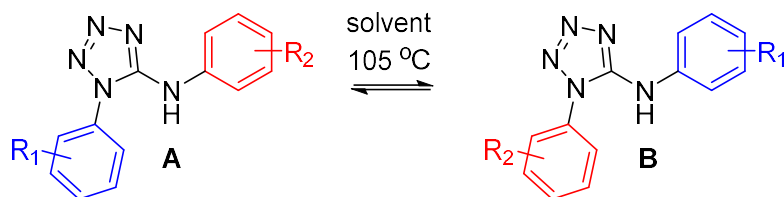


Table S3. DFT calculated energetics of Dimroth rearrangement

entry	R ₁	R ₂	BLYP-D4/def2-TZVP(-f) SMD (dioxane)			B3LYP-D4/ def2-TZVP(-f) SMD (dioxane)//BLYP-D4/ def2-TZVP(-f) SMD (dioxane)		
			ΔE^a	$\Delta_r G^{298.15b}$ (ratio A:B) ^d	$\Delta_r G^{378.15c}$ (ratio A:B) ^d	ΔE^a	$\Delta_r G^{298.15b}$ (ratio A:B) ^d	$\Delta_r G^{378.15c}$ (ratio A:B) ^d
1	H	4-OMe	-1.48	-1.42 (8:92)	-1.42 (13:87)	-1.51	-1.46 (8:92)	-1.46 (13:87)
2	H	4-NO ₂	3.49	3.49 (100:0)	3.50 (99:1)	3.60	3.59 (100:0)	3.61 (99:1)
3	4-OMe	4-NO ₂	4.97	4.86 (100:0)	4.87 (100:0)	5.13	5.03 (100:0)	5.03 (100:0)
4	H	3-CF ₃	1.21	1.46 (92:8)	1.50 (88:12)	1.25	1.50 (93:7)	1.53 (88:12)
5	H	3-F	0.80	1.00 (84:16)	1.04 (80:20)	1.07	1.27 (90:10)	1.30 (85:15)
6	H	4-F	-0.12	0.02 (51:49)	0.04 (51:49)	-0.12	0.01 (50:50)	0.03 (51:49)
7	H	3-Cl	0.98	1.28 (90:10)	1.33 (85:15)	1.17	1.47 (92:8)	1.51 (88:12)
8	H	3-Pyr	1.64	1.69 (95:5)	1.69 (90:10)	1.63	1.68 (94:6)	1.68 (90:10)
9	H	Mes	-3.87	-4.10 (0:100)	-4.18 (0:100)	-3.97	-4.20 (0:100)	-4.28 (0:100)
10	H	3-Cl-pyrimidine	0.67	0.81 (80:20)	0.87 (76:24)	1.45	1.59 (94:6)	1.65 (90:10)
11	H	4-NH ₂	-2.58	-2.47 (2:98)	-2.44 (4:96)	-2.66	-2.56 (1:99)	-2.53 (3:97)

^aDifference in electronic energies (kcal/mol) between isomers; ^bDifference in Gibbs free energies of isomers (kcal/mol, T=298.15 K); ^cDifference in Gibbs free energies of isomers (kcal/mol, T=378.15 K); ^dRatio of isomers given in brackets

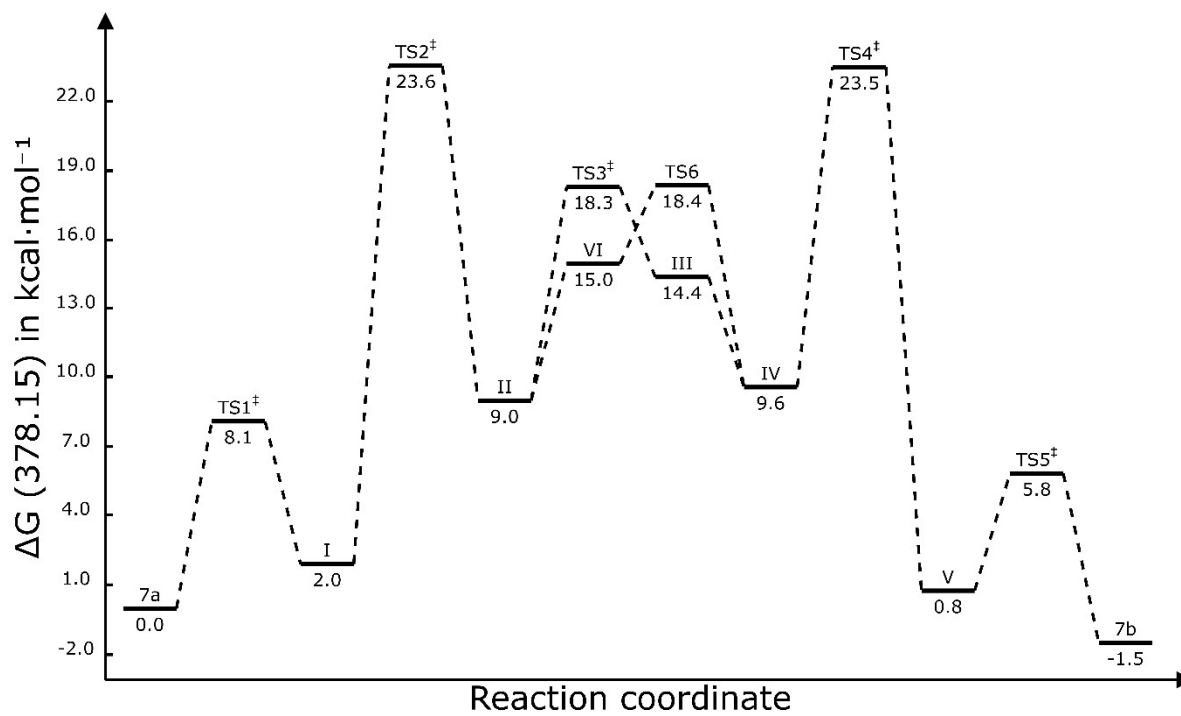


Figure S1. Calculated reaction profile for the Dimroth rearrangement of **7a** and **7b**. Gibbs free energies (in kcal/mol relative to **7a**) at 378.15 K, obtained using the B3LYP-D4/ def2-TZVP(-f)-SMD (dioxane)//BLYP-D4/ def2-TZVP(-f)-SMD (dioxane) level of theory.

Table S4. Total electronic energies and number of imaginary frequencies for all DFT optimized structures ^a			
Molecule	E(BLYP-D4/def2-TZVP(-f) SMD (dioxane)) ^b	E(B3LYP-D4/ def2-TZVP(-f) SMD (dioxane) // BLYP-D4/ def2-TZVP(-f) SMD (dioxane)) ^b	No. imag. freq.
7a	-890.3671498	-890.1145736	0
7b	-890.3695010	-890.1169859	0
7c	-980.4184211	-980.1088933	0
7d	-980.4128577	-980.1031559	0
7e	-1094.966570	-1094.625180	0
7f	-1094.95865	-1094.616997	0
7g	-1112.995136	-1112.671155	0
7h	-1112.993205	-1112.669166	0
7i	-875.1034199	-874.8491230	0
7j	-875.1021410	-874.8477264	0
7k	-875.1023830	-874.8479996	0
7l	-875.1025668	-874.8481976	0
7m	-1235.440926	-1235.1659440	0
7n	-1235.439359	-1235.1640867	0
7o	-791.8725128	-791.6394104	0
7p	-791.8698988	-791.6368141	0
7q_A ^c	-893.7528176	-893.5189077	0
7q_B ^d	-893.7589911	-893.5252407	0
7r_A ^c	-1267.561945	-1267.2635064	0
7r_B ^d	-1267.560882	-1267.2611996	0
7t	-831.1915115	-830.9546023	0
7u	-831.1956185	-830.9588478	0
I	-890.3651062	-890.1123561	0
II	-890.3560030	-890.0968986	0
III	-890.3486362	-890.0880130	0
IV	-890.3554548	-890.0961817	0
V	-890.3666959	-890.1139739	0
VI	-890.3486431	-890.0879838	0
TS1	-890.3541191	-890.1022152	1 (-40.24) ^e
TS2	-890.3376585	-890.0744767	1 (-225.35) ^e
TS3	-890.3435079	-890.0830720	1 (-56.31) ^e
TS4	-890.3554548	-890.0743605	1 (-219.42) ^e
TS5	-890.3578027	-890.1058223	1 (-52.85) ^e
TS6	-890.3436385	-890.0832605	1 (-63.17) ^e

^a All structures optimized at BLYP-D4/def2-TZVP(-f) SMD (dioxane) level of theory; ^b energies in Hartrees; ^c isomer A; ^d isomer B; ^e value of imaginary frequency given in brackets as negative cm⁻¹

Table S5. Cartesian coordinates of all DFT optimized structures

33			
Coordinates 7a			
H	0.30907622917978	-0.58682890820555	0.23385915427022
N	0.51672353873190	-0.75613593868353	-0.74531645205386
C	1.76310453070795	-0.40045295894785	-1.15330475491458
N	2.27209795009268	-0.41253065366599	-2.39128593039139
N	3.55835384018847	0.06169628152465	-2.26641226827737
N	3.85352001539840	0.35872993816750	-1.04366416881579
N	2.72195358294915	0.06222832740485	-0.28729259826416
C	2.66647898374703	0.31162095489283	1.11362815889539
C	2.15120558648579	-0.66216643533132	1.98010577784344
C	2.09204834784218	-0.39425928592098	3.35086896379350
C	2.56192154742395	0.82354068744493	3.85239627510695
H	2.52113038054190	1.02426675005141	4.92102839005772
C	3.09237506893987	1.78075814143283	2.97903422166143
C	3.13920368111690	1.53472252450732	1.60596963615069
C	-0.56937925888264	-1.23054844789141	-1.52170060058295
C	-0.49097067502067	-1.49537375990207	-2.89438094304414
C	-1.61242954477461	-1.97670751138916	-3.58266590660446
C	-2.82139364896531	-2.19742222706842	-2.91022077548629
C	-2.89767954606435	-1.93011440133605	-1.53195443359984
C	-1.78659301631278	-1.45395181736584	-0.84892452129650
H	1.83153492386218	-1.62750098690228	1.59499044114513
H	1.69457618312298	-1.14859244687984	4.02681210408983
H	3.46332902369036	2.72764246974767	3.36601342823531
H	3.53776980213688	2.27174416568773	0.91407052226910
H	0.43763951111667	-1.32651393747884	-3.42824588414962
H	-1.52079267484801	-2.17260613924227	-4.64648956429183
O	-3.97525093117391	-2.66647018139132	-3.49670239432538
H	-3.83701572950730	-2.10114028463580	-1.01051430296510
H	-1.85871671200975	-1.25111307490531	0.21952804617102
C	-3.92882916975351	-2.95401475356228	-4.90828720990096
H	-4.92820865249437	-3.31502929872495	-5.16854385598260
H	-3.70299912165046	-2.05054733208726	-5.49340645832897
H	-3.18808404581733	-3.73522945934340	-5.13269209641394
33			
Coordinates 7b			
N	-1.75792911086251	1.27115995871199	0.24170676563815
C	-0.49385051863997	1.52987100007925	0.70065646906584
N	-0.49078902668580	2.71710010426636	1.31535845666624
N	-1.78690273324452	3.17651151539321	1.23315113301073
N	-2.55931778822254	2.34595811402689	0.61045312884614
N	0.53525321530515	0.65605554753253	0.51507604716717
C	1.86948804768623	0.74953104911934	0.96647839475113
C	2.38790002658496	1.88008172232803	1.62056034548947
C	3.72813039072674	1.88466346163723	2.01948986129308
C	4.56050081740237	0.78755822760403	1.77913085197358
C	4.03750676060752	-0.33561771973091	1.12639627911586
C	2.70405211126568	-0.35780637314417	0.72194903109968
C	-2.27940632123436	0.12060227168014	-0.41862418399179
C	-3.38496671858996	-0.54655591428845	0.13065120114961
C	-3.90295760238470	-1.66416020962410	-0.50927925500622
C	-3.31359466485966	-2.14148369750496	-1.69635096853064
O	-3.89288809808400	-3.25468370744600	-2.24137207418019
C	-3.33257446584166	-3.77281356235550	-3.46867641672233
C	-2.20443187124857	-1.47402972683023	-2.24136169542785
C	-1.69824155711139	-0.33668226972355	-1.60431382180318

H	1.74918415058587	2.73495250751086	1.81325846140678
H	4.12084314045134	2.76439254525033	2.52661759005663
H	5.60113847629820	0.80460476400730	2.09603007725899
H	4.66910365724452	-1.20051781271259	0.93131893175789
H	2.29968533560160	-1.23415774396631	0.21549116318380
H	-3.83121284467584	-0.17836497100050	1.05081375158612
H	-4.76286536857903	-2.19021452686732	-0.10087447736807
H	-3.93656645505810	-4.64963319388824	-3.71756815872921
H	-3.40564025490763	-3.03512032557833	-4.27984074591739
H	-2.28551869239179	-4.07625133637205	-3.32968382736502
H	-1.74208627306557	-1.81310127532304	-3.16251149003499
H	-0.86593024559699	0.20324355534442	-2.05024197924074
H	0.28148448152439	-0.22769197813578	0.08251115380071

31

Coordinates 7c

H	0.30982014771195	-0.55313213588281	0.22886069286719
N	0.50379541773338	-0.73239427211473	-0.75282576401370
C	1.76461137575360	-0.40361431342817	-1.17001263014319
N	2.27032169021291	-0.43178931144413	-2.40386603438957
N	3.56523109333480	0.01959209413648	-2.27942155444996
N	3.86019199982393	0.31497380287571	-1.05456786871715
N	2.72395298384322	0.04426127619332	-0.30367227184606
C	2.66188457735418	0.29481786175431	1.10022987255244
C	2.18479170039665	-0.69835869813741	1.96536827655200
C	2.11435028824160	-0.42973693310871	3.33550462132845
C	2.53536728913154	0.80737636325815	3.83340103018339
H	2.48651198715790	1.00850182302082	4.90153050820517
C	3.02792401776775	1.78381355734719	2.95909232265454
C	3.08593150781240	1.53692922200419	1.58656857160728
C	-0.57340726961069	-1.20922735524779	-1.50626357277939
C	-0.49078169294100	-1.49423108671541	-2.88436694167735
C	-1.61052615348213	-1.97646838312258	-3.55275122094594
C	-2.80761683876853	-2.17464442320779	-2.85808850809521
C	-2.90447036617825	-1.89471476701123	-1.48913698856060
C	-1.79078603386363	-1.41466351484236	-0.81950496883440
H	1.90494067679073	-1.67628298701234	1.58075897398472
H	1.74770318364723	-1.19727680564968	4.01381712160877
H	3.36081077897781	2.74497875023215	3.34511746845492
H	3.45521337974283	2.28734923737670	0.89268509213789
H	0.43969409940349	-1.33483071961123	-3.41718362713771
H	-1.56335804247001	-2.20020048408422	-4.61371387280797
N	-3.98386689935522	-2.68398573548442	-3.57237083264686
H	-3.84349321710730	-2.05476876435643	-0.96953900256892
H	-1.85282071319766	-1.19300245222564	0.24493715764567
O	-5.03934511401408	-2.84871939964899	-2.92336250069138
O	-3.87227585384940	-2.92875144586295	-4.79192354947708

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Coordinates 7d

N	-1.76783475271673	1.15118210339106	0.32494728055664
C	-0.49369507361963	1.43156363030457	0.76345575169053
N	-0.51443772521915	2.59675319136079	1.41822157853238
N	-1.82234995369654	3.02099789863827	1.38310686696467
N	-2.59136959538556	2.19332330272732	0.76141552457570
N	0.56065175457297	0.60093238106201	0.55132996749802
C	1.90662449849525	0.75051081215486	0.96500971383731
C	2.40152952725344	1.90338048007703	1.59551279122563
C	3.75259565616456	1.95826666900148	1.95227293355424
C	4.61469998747659	0.88907233642249	1.69297283398765

C	4.11342281377195	-0.25698502586247	1.06387687645298
C	2.76991289061536	-0.32895510642969	0.70084986062773
C	-2.29950322484618	0.04197670318572	-0.37559232661692
C	-3.54461655656464	-0.47337677121024	0.01825656188871
C	-4.08350562835708	-1.55915735092189	-0.66227502424426
C	-3.36401549046620	-2.12415548620140	-1.71923410300686
C	-2.12915243767254	-1.61610562099507	-2.12590527838336
C	-1.59708045693770	-0.51811916880875	-1.45525542810659
H	1.73993348695823	2.73631404592303	1.80415144645501
H	4.12939056532614	2.85468929542573	2.44155361069923
H	5.66317785349245	0.94525403660307	1.97767137747591
H	4.76924123200948	-1.10004630542859	0.85468896216284
H	2.38189919785957	-1.22268385762611	0.21232045857052
H	-4.07428285224071	-0.02148336470107	0.85136718667398
H	-5.04253524952014	-1.97827052132871	-0.37594122566514
H	-1.60934815061761	-2.06274970201278	-2.96713210211331
H	-0.66564533093311	-0.07726237245614	-1.79960089115787
H	0.34095395803571	-0.29754563417444	0.13288135035281
N	-3.93029279197726	-3.29041174744948	-2.43381864607401
O	-3.25256994570155	-3.79594564324332	-3.34846295613313
O	-5.05129820555938	-3.70036320742728	-2.08014495228106

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Coordinates 7e

H	0.36711837119556	-0.49894878567439	0.20439836371563
N	0.54299355768774	-0.71221769207609	-0.77410876000974
C	1.81023667245409	-0.43397578147962	-1.21094157253348
N	2.31060347982114	-0.51581185356612	-2.44455948665215
N	3.61931505708019	-0.10008720936458	-2.33514963546493
N	3.92630185467121	0.21829807458365	-1.11780986292360
N	2.78342075625066	0.00783167535200	-0.35937178410969
C	2.71927651494338	0.29673867812966	1.03679792392770
C	2.29918038203631	-0.69100899044432	1.94148585190627
C	2.22516251811181	-0.39482318741178	3.29742739442353
C	2.59049207304085	0.88138440196759	3.76645061117679
O	2.48940638451090	1.06778672890036	5.11612153942682
C	3.02863479682724	1.86027185992436	2.85662481822801
C	3.08188413607349	1.56573105015358	1.49328683534146
C	-0.55121923501998	-1.18788110120172	-1.50063600490171
C	-0.48741508602713	-1.51863300428402	-2.86987783742269
C	-1.62345489651766	-1.99566371428167	-3.51369251021312
C	-2.81909514998496	-2.14400593058771	-2.80378431815586
C	-2.89715346552377	-1.81844101139568	-1.44352513777774
C	-1.76741064339523	-1.34326555198425	-0.79807871645433
H	2.05758678277316	-1.69156950746505	1.59032178320729
H	1.90703577481476	-1.14810567227857	4.01440262299647
H	3.32066691607223	2.84911474424832	3.19446472439248
H	3.41062176909542	2.31866788784721	0.78145620358290
H	0.44218707759292	-1.39818834750692	-3.41456732011014
H	-1.58987067502225	-2.25399486358955	-4.56728335127949
N	-4.01217761942750	-2.64802262733928	-3.49162392985458
H	-3.83512400125664	-1.94036427429567	-0.91174489440231
H	-1.81535202590857	-1.08671277145333	0.25920628548704
O	-5.06571933985930	-2.76857758005885	-2.82928879463972
O	-3.91772078379386	-2.93240559491761	-4.70434857015471
C	2.87658173831142	2.35483267215369	5.65154287055976
H	2.72210221605866	2.27862939545030	6.73119434180662
H	3.93493884194970	2.56575781539657	5.44608131654879
H	2.24586525036396	3.15796006854951	5.24622900033243

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Coordinates 7f

N	-1.82240948435688	1.13592070904685	0.31394199311168
C	-0.55697106229525	1.42114582380826	0.77898909958466
N	-0.59752373134755	2.58599228046898	1.43691428152086
N	-1.90611577586822	3.00289215577729	1.37742412744765
N	-2.65969347363889	2.17377953951718	0.73951479718947
N	0.50680994139684	0.60235275653132	0.58824234874865
C	1.84244394243713	0.76177594000336	1.04231200604986
C	2.31449622634034	1.90510780456926	1.69727029809003
C	3.65517015866964	1.98242953021468	2.09554172504363
C	4.53552571827472	0.92115568399660	1.84489670701101
C	4.05713456737154	-0.22660823170635	1.18737483901487
C	2.72907471675011	-0.30337505834058	0.79174591609412
C	-2.33658937720643	0.02894447939152	-0.39964848424843
C	-3.60278033522327	-0.47130736444786	-0.05400242785851
C	-4.12500195408701	-1.55645329156377	-0.74784274699883
C	-3.37015439863056	-2.13724919890062	-1.77153850179445
C	-2.11471354068871	-1.64387321074694	-2.13156875536457
C	-1.59813440823896	-0.54732011097219	-1.44713289976682
H	1.64390882202510	2.73243664284028	1.90014569468887
H	3.99141395945220	2.88161285713659	2.60190894449536
O	5.86482441955375	0.90145438428113	2.19480314855301
H	4.74152470341137	-1.04992904487200	0.99487514518374
H	2.37056966278719	-1.19821449927028	0.28335553429668
H	-4.16073657352313	-0.00813825043513	0.75397381003348
H	-5.09890651458633	-1.96382089923673	-0.49694924742898
H	-1.56668272775878	-2.10195348361995	-2.94834997063387
H	-0.65002481656486	-0.11796932243775	-1.75884783496555
H	0.30663614519961	-0.29630312803412	0.16138678356428
N	-3.91913740689334	-3.30182231746907	-2.49962235034264
O	-3.21103796032648	-3.82150125201946	-3.38338660406960
O	-5.058030225000520	-3.69811660048940	-2.18858129481076
C	6.39032442390453	2.06143076918044	2.87303260871487
H	7.44662883174365	1.84290417920888	3.05414764807373
H	6.30483828059884	2.96143550266978	2.24741190779854
H	5.88111927132331	2.22588422591977	3.83346175397397

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Coordinates 7g

H	0.29652049353397	-0.54617121415011	0.23010151907347
N	0.49998694656850	-0.72546815924195	-0.74870083530589
C	1.75327659198965	-0.38133871388573	-1.16358014055799
N	2.25557784808762	-0.39821067148037	-2.40067115422947
N	3.54692061551100	0.06497045323382	-2.27945153670253
N	3.84608490739098	0.35642995359770	-1.05578019064416
N	2.71412250821413	0.07091945944275	-0.29926073473260
C	2.66132625830876	0.30907066806745	1.10570433903831
C	2.17239896911729	-0.68377203873448	1.96500301760628
C	2.11428670506730	-0.42813106158360	3.33821820773437
C	2.55916459789659	0.79639971947666	3.84674763102056
C	3.06317553457748	1.77275690035371	2.97880247434979
C	3.10883573172636	1.53872379296642	1.60354117417404
C	-0.57945531052210	-1.20262148205760	-1.51574446222040
C	-0.48447062821024	-1.48907145910899	-2.88454587210353
C	-1.61265526296663	-1.97804784981778	-3.55657004592209
C	-2.82792894777810	-2.18276541506463	-2.89868501868377
C	-2.90935372572492	-1.89039794704749	-1.53215056913561
C	-1.80160336138144	-1.40708732683385	-0.84407363783761

H	1.87299929881945	-1.65268596302241	1.57255093176159
H	1.73831236014172	-1.19634773363372	4.01068927574400
H	3.41478411811991	2.72436691372088	3.37184280710794
H	3.48722502388100	2.28963200227686	0.91517682039867
H	0.45136755506395	-1.33194915592645	-3.40958143520791
C	-1.47112938404320	-2.28111879901182	-5.02674520596404
H	-1.87354533696425	-1.18354299600211	0.21986656287413
H	2.52003499864724	0.98771487479447	4.91706703928568
H	-3.69186044900335	-2.56097355948054	-3.43582977211480
H	-3.84628757951702	-2.04230048307965	-1.00072405253177
F	-2.61958156739343	-2.77731763702352	-5.58173105024365
F	-1.13105721059065	-1.16426925908537	-5.75461829412465
F	-0.48337229856757	-3.20859581265854	-5.26726779190634

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Coordinates 7h

N	-1.78047655351118	1.21578750036644	0.31980698702609
C	-0.51010061808095	1.47155601977689	0.77359710779034
N	-0.51995490729284	2.62851838644489	1.44368898611434
N	-1.82238464813285	3.07093036583127	1.40113281825498
N	-2.59402718950505	2.26048053330942	0.75666067839036
N	0.53336554929521	0.62797694237605	0.54852989856247
C	1.88120539500771	0.75261428469457	0.96030316149288
C	2.38705915975337	1.87974062201905	1.62804518330723
C	3.73972456360003	1.91299913820647	1.98177595705440
C	4.59344086868837	0.84720977093425	1.68354156136764
C	4.08153121635438	-0.27284242391041	1.01714966198334
C	2.73649360257504	-0.32287467696841	0.65616272111120
C	-2.31155314692274	0.10835926091580	-0.39510786274997
C	-3.50758714118256	-0.47481020517215	0.03990193339983
C	-4.03650676083724	-1.55676740607135	-0.66554548360167
C	-3.37171137806419	-2.06880194729198	-1.78166702096771
C	-2.17576399580049	-1.47488066148969	-2.20539204496166
C	-1.64409816366425	-0.37573733109843	-1.52686161679120
H	1.73207392493637	2.71010115314723	1.86625452221136
H	4.12461054508217	2.78974654386861	2.49972108655208
H	4.73074691820181	-1.11252486603463	0.77595497451092
H	2.34130858967288	-1.19544046454496	0.13604482554682
H	-4.00924334972871	-0.07624743756205	0.91722137050913
H	-4.96766455156667	-2.01089833192800	-0.33496040190843
C	-1.47367147441302	-2.03722952394120	-3.41606007385876
H	-0.74764318352803	0.11442236976911	-1.89333206771797
H	0.29748615343183	-0.25961519605391	0.11554940295111
H	5.64334356104429	0.88618003892664	1.96596234782639
H	-3.78039580056987	-2.91942667947402	-2.32139704015193
F	-0.35071172839373	-1.33262535233440	-3.75293720683267
F	-1.08011057973475	-3.33993489209367	-3.21395243379301
F	-2.28668487671435	-2.04876553461744	-4.52249193262791

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Coordinates 7i

H	0.31352806558721	-0.57538500421395	0.23107577681534
N	0.51626658094027	-0.75215200248554	-0.74824760704152
C	1.76886691033905	-0.40484874978523	-1.16021318690826
N	2.27946030409063	-0.42421020389520	-2.39480881288229
N	3.56810686438709	0.04405622642409	-2.26756018722887
N	3.85948092954709	0.34208706792695	-1.04372776810466
N	2.72425614447092	0.05478272749504	-0.29234233027518
C	2.66302365757555	0.30637280495716	1.10949651395833
C	2.16359904687043	-0.67484666611998	1.97626428126812

C	2.09711874295648	-0.40428962828532	3.34626812376155
C	2.54428384701505	0.82321830053114	3.84505972510328
C	3.05914534138790	1.78778998061328	2.97035941793392
C	3.11309447758838	1.53909730790548	1.59806952605010
C	-0.56638306756501	-1.22463612569575	-1.51737802224044
C	-0.48285868497636	-1.49446883355420	-2.89456506927930
C	-1.61169948199149	-1.97279165058520	-3.56608428174625
C	-2.82528068091982	-2.19136416248967	-2.90642846293294
C	-2.86809512969203	-1.91251574216283	-1.54422333975225
C	-1.77826801127359	-1.43722469678634	-0.83164657341543
H	1.86232541481717	-1.64678900719296	1.59287322830163
H	1.71202960288984	-1.16364296158850	4.02364265359200
H	3.41226210316336	2.74183833042383	3.35614741332352
H	3.49951642834198	2.28141420685940	0.90487798062435
H	0.44759696333266	-1.32871547430926	-3.42463702777072
H	-1.87085117129667	-1.23646633355451	0.23377258006478
H	2.49799601962927	1.02580399918659	4.91303582246211
H	-3.70691135099695	-2.56195700169560	-3.42204209198785
F	-4.04512134110905	-2.11509622352088	-0.86141872371017
H	-1.54148852510936	-2.17886048440203	-4.63221955798292

29

Coordinates 7j

N	-1.76528587887347	1.22313937166694	0.27243837784595
C	-0.49764073692025	1.48510355326763	0.72892629214900
N	-0.50649272525822	2.65932217027711	1.36845938207891
N	-1.80652795348501	3.10665300781600	1.30363499513819
N	-2.57662798560206	2.28275449378653	0.67377252239053
N	0.54282422001859	0.63018711798376	0.53381053865389
C	1.88386879008017	0.75099548771214	0.96565207410861
C	2.38551230021642	1.88133380711482	1.63170136736450
C	3.73177717662311	1.90963401563456	2.00944511330512
C	4.58420031666273	0.83610023559770	1.73640407204969
C	4.07695490364275	-0.28709230077136	1.07161498637336
C	2.73819010418188	-0.33257041803623	0.68747988107137
C	-2.29670142722051	0.09065514856359	-0.40386362942982
C	-3.48346950553808	-0.48814969378787	0.06316951196538
C	-4.00910375842852	-1.59629874033733	-0.60345923282598
C	-3.35656059641263	-2.14387721430071	-1.71385987968295
C	-2.18018206855634	-1.54077974440369	-2.14455467783185
C	-1.63093698059992	-0.42271977185348	-1.52603749421613
H	1.73147397202044	2.71795956505954	1.84996738367204
H	4.11241491793495	2.78903362876961	2.52610146491686
H	4.72517125909658	-1.13307566317152	0.85035879259628
H	2.34621923030621	-1.20820613338787	0.17019760868999
H	-3.97891423268152	-0.06721273716314	0.93293244648592
H	-0.74225231133027	0.04724139196700	-1.93803049301379
H	0.30907289902530	-0.25530516586322	0.09468017390850
H	5.62915000225927	0.87122249902175	2.03717555764101
H	-3.74611972966823	-3.01236940585266	-2.23859004992022
F	-1.53579084280732	-2.05289149640884	-3.24012658694841
H	-4.93232335868608	-2.04858700890077	-0.24860049853597

29

Coordinates 7k

H	0.31516563444045	-0.59467447836776	0.23764083684496
N	0.51893425810405	-0.76728355210400	-0.74202553158891
C	1.76776766825075	-0.41458510091649	-1.15399534280893
N	2.27610194282371	-0.43299223507896	-2.39050250286593
N	3.56337728825941	0.03997631508476	-2.26695223126035

N	3.85712625478067	0.34074369135940	-1.04466670198028
N	2.72455841867775	0.05006385648769	-0.28922577479557
C	2.66477484370625	0.30612494570628	1.11139477429507
C	2.16609263282240	-0.67224435395583	1.98194245995732
C	2.10016672788337	-0.39717256654028	3.35100199386223
C	2.54711114443729	0.83208426743938	3.84567835874469
C	3.06139996477403	1.79374735829582	2.96746547277008
C	3.11473657993625	1.54049296332484	1.59600050158996
C	-0.56842740460182	-1.23365075714869	-1.51483009555893
C	-0.48499723165968	-1.49007859653001	-2.89393031998195
C	-1.60859305258745	-1.96066024320503	-3.58071988566154
C	-2.79336707442329	-2.16780384791966	-2.88650013353044
C	-2.90300330670913	-1.92282177017404	-1.52132488383705
C	-1.78240992560552	-1.45413512842086	-0.83743267332757
H	1.86507157272200	-1.64552090553862	1.60164922670969
H	1.71584850977023	-1.15432932322412	4.03135325669999
H	3.41456302648359	2.74928077448891	3.34973726418607
H	3.50061391866800	2.28044176084904	0.90000315528806
H	0.44573796926228	-1.32079922575715	-3.42356070422125
H	-1.84975240272385	-1.25652166851118	0.23175098810127
H	2.50127494408551	1.03838947458549	4.91298919733155
F	-3.89735161714676	-2.62825338590585	-3.56844575711729
H	-3.84526999723866	-2.09468146877467	-1.00713321109841
H	-1.56065128719184	-2.16203679954842	-4.64816173674652

29			
Coordinates 7l			
N	-1.76135320439349	1.24270551547690	0.24856955502231
C	-0.49763364936900	1.50247436974823	0.71204355031395
N	-0.50278618079596	2.68520957034772	1.33579285552178
N	-1.79993915360911	3.13948369943588	1.25505252835633
N	-2.56897488099442	2.31180643047762	0.62692692211354
N	0.53708183651298	0.63643476316257	0.52991969697317
C	1.87541854929278	0.74795762525037	0.96997918523594
C	2.3825527470356	1.88070584343276	1.62809646863258
C	3.72587147296852	1.90094354830778	2.01601171131077
C	4.57097919253239	0.81713141642670	1.76074720402806
C	4.05861995204717	-0.30843340448123	1.10397651600908
C	2.72228621985867	-0.34603297483897	0.71012532972210
C	-2.28715151947075	0.09904124747922	-0.41746421457088
C	-3.43011841402608	-0.52329635172737	0.10088188910591
C	-3.96180934068890	-1.63876496141435	-0.54549727463130
C	-3.32133360346214	-2.11477212258552	-1.68680696834736
C	-2.18438010189005	-1.51431048231085	-2.21756777890568
C	-1.66834322760480	-0.38446256767112	-1.57821119490784
H	1.73406823923093	2.72524821320016	1.83259767552305
H	4.11065696861830	2.78214988638207	2.52654513225561
H	4.70049864919846	-1.16283559132641	0.89690447669885
H	2.32625969432530	-1.22404218499635	0.19998781473077
H	-3.89645658239951	-0.12924363149451	0.99953989750702
H	-0.80768932526585	0.13001457445188	-1.99845634607637
H	0.29619578979539	-0.24817009987610	0.09270611113491
H	5.61379920545536	0.84647584642614	2.06944116579884
F	-3.83565618760043	-3.21790403126384	-2.31504183682275
H	-1.72803964668402	-1.91011306101589	-3.12115564122529
H	-4.85012349728532	-2.14030108500349	-0.17014443050708

29			
Coordinates 7m			
H	0.31413998854777	-0.57856737379513	0.23075378235868

N	0.51745198935491	-0.75414884473141	-0.74877279681260
C	1.77009851094399	-0.40650366992366	-1.16032147752039
N	2.28051650102643	-0.42612023239720	-2.39489039709272
N	3.56894615852818	0.04302446030680	-2.26782962053352
N	3.86051626501830	0.34012187120907	-1.04376988897509
N	2.72525330418178	0.05328997509166	-0.29250526265687
C	2.66305210612161	0.30559430252735	1.10925400810779
C	2.16281810461652	-0.67522958959099	1.97598451402691
C	2.09452472353262	-0.40378790980947	3.34572416630989
C	2.54075215910189	0.82417280832109	3.84420389432263
C	3.05653474335985	1.78831913242897	2.96957375459540
C	3.11227322455807	1.53875293841414	1.59750421499815
C	-0.56454184485503	-1.22559371317953	-1.51880907490015
C	-0.48197670504897	-1.49227891967577	-2.89606518094894
C	-1.61233692407368	-1.96910271661819	-3.56458701964875
C	-2.82344637081590	-2.18836663182915	-2.90246247356884
C	-2.87698787319105	-1.91512750781191	-1.53479554097024
C	-1.77545652388854	-1.44010629771404	-0.83282857076473
H	1.86218172062922	-1.64747392850327	1.59283969385780
H	1.70866163827669	-1.16266656574056	4.02317419141173
H	3.40889473246796	2.74274395294200	3.35507473453991
H	3.49925747432599	2.28070971913751	0.90423851208728
H	0.44778548640476	-1.32553936169016	-3.42738706773077
H	-1.84932126738223	-1.23690669118456	0.23313082430632
H	2.49298682021227	1.02759304449759	4.91195318789938
Cl	-4.39486045790317	-2.17913198003468	-0.65367513088233
H	-1.54641414661547	-2.17392023663068	-4.63143080011383
H	-3.69780353743479	-2.55825003401582	-3.42947917570211

29

Coordinates 7n

N	-1.76761118888617	1.22703287494513	0.27312829144358
C	-0.50016336297945	1.48731635993513	0.73104864396035
N	-0.50833577102021	2.66135764446191	1.37079919873977
N	-1.80780186689161	3.11035435036105	1.30442117509751
N	-2.57829614694564	2.28751237314934	0.67364771635311
N	0.53917580938293	0.63101177776466	0.53658419928630
C	1.88120845909776	0.75041027606678	0.96595314552824
C	2.38430985806519	1.87849684738622	1.63442302454167
C	3.73127457930601	1.90538953911701	2.00943903221036
C	4.58287723139629	0.83246755348017	1.73140284857007
C	4.07412117790402	-0.28857303815231	1.06402685760776
C	2.73457238665892	-0.33244358140031	0.68239204406097
C	-2.29866950209745	0.09493386066884	-0.40379598800957
C	-3.48277566713523	-0.48749576941409	0.06383799851575
C	-4.00211355613705	-1.59655069610137	-0.60421634752853
C	-3.34582220572219	-2.13988100624857	-1.71404562997936
C	-2.16780765840934	-1.53838565972917	-2.15726443249223
C	-1.63397583008788	-0.41418182904997	-1.52747980407694
H	1.73094549388050	2.71472389637184	1.85633414183230
H	4.11309762903227	2.78321299427555	2.52789850519981
H	4.72179563180859	-1.13384744099203	0.83860875009370
H	2.34169049854815	-1.20596047519954	0.16214283396427
H	-3.97951508653602	-0.06939705841866	0.93444676888537
H	-0.74768417037627	0.07160899618538	-1.92440142592354
H	0.30423324032957	-0.25395236896677	0.09725590866542
H	5.62847121856275	0.86642409592697	2.03005045758588
Cl	-1.33168098369441	-2.19751292813820	-3.56957300955005
H	-4.92333039991983	-2.05522142391787	-0.25186520954241

H	-3.74358981713423	-3.01105016436710	-2.22679969503955
28			
Coordinates 7o			
H	0.30880781098366	-0.58919708577581	0.21902960729580
N	0.52458177048437	-0.75886711079517	-0.75953663509367
C	1.77930816599995	-0.40760257387352	-1.16102070239644
N	2.29229410818629	-0.42719888202557	-2.39448152481006
N	3.58048085876356	0.04189180194555	-2.26414875885557
N	3.86780315199106	0.34102578683047	-1.03947835367239
N	2.73093076310694	0.05334531105329	-0.29093535236941
C	2.66377575115187	0.30588366814938	1.11069668119201
C	2.15997853532639	-0.67489188854913	1.97524469291252
C	2.08614091137268	-0.40323127750270	3.34457111741876
C	2.53044006427649	0.82474197587289	3.84456051539772
C	3.04980874462446	1.78883200715649	2.97203078037220
C	3.11112586320998	1.53910943978040	1.60024692140176
C	-0.54403527479613	-1.22642886279858	-1.54453975081608
C	-0.46708917724222	-1.49027621516995	-2.92041426616149
C	-1.61479734841865	-1.96319539280967	-3.55878108046001
C	-2.78760554194121	-2.15810545418273	-2.82710707721973
N	-2.86818764425732	-1.90622925399361	-1.50479080691946
C	-1.77211071222629	-1.45329184252423	-0.88971330873204
H	1.86056688042541	-1.64709635225948	1.59087706316582
H	1.69727278868444	-1.16173769981641	4.02072168413412
H	3.40054878510371	2.74343979192466	3.35867430072761
H	3.50076360326278	2.28087069604213	0.90825247167042
H	0.45761977040313	-1.32717384543596	-3.46314103313002
H	-1.85536031525738	-1.25417681594021	0.18234520567437
H	2.47831013999342	1.02851057668877	4.91206108025750
H	-3.69383186506226	-2.52627748618870	-3.30752610823819
H	-1.59404058814913	-2.17817301580263	-4.62529736274605
28			
Coordinates 7p			
N	-1.76601324665406	1.21609883292519	0.27566962618223
C	-0.49567553434422	1.48109642445703	0.72466221107027
N	-0.49993939490879	2.66555902548283	1.34567839972202
N	-1.79814739146297	3.11596281995558	1.27824158230882
N	-2.57321073181148	2.28600607462741	0.66357702825248
N	0.54281397199769	0.62190354528541	0.54248091121147
C	1.88513165480643	0.74718129958888	0.97082924085863
C	2.38810297695047	1.88372055751888	1.62476297947446
C	3.73479526903985	1.91479991593073	2.00067482887691
C	4.58602048163616	0.83798070445954	1.73737739767853
C	4.07727171127333	-0.29149751221792	1.08424816446881
C	2.73799182392979	-0.33983573981089	0.70216034156356
C	-2.30869627472316	0.07946610474280	-0.37904521045917
C	-3.50425620126339	-0.48411898492388	0.07970251939040
C	-4.00231478773309	-1.59470202484590	-0.59575929057548
C	-3.28333018986112	-2.10649492952440	-1.68237916095068
N	-2.13694981113796	-1.56429568476739	-2.13024658153904
C	-1.66824712740326	-0.47922385554588	-1.49405414127935
H	1.73521257306965	2.72332048370030	1.83479351091550
H	4.11607104985357	2.79945509589447	2.50778907777375
H	4.72487657622517	-1.13983695215197	0.87054547407227
H	2.34474211387218	-1.21999232739384	0.19364877517257
H	-4.01669990255447	-0.05407108949262	0.93610211073157
H	-0.76242912217916	-0.02703194955041	-1.89886571066454
H	0.31263432405989	-0.26559972493495	0.10614134781144

H	5.63141456208919	0.87527344317836	2.03630859970503
H	-3.64405958030392	-2.98310486156236	-2.22040353516465
H	-4.93020979246232	-2.06671869102502	-0.28084049660781

38

Coordinates 7q

H	0.35419491053923	-0.89474153786932	0.32621178461548
N	0.49257097627771	-0.84358343665164	-0.67913783788523
C	1.42249167533028	0.06949347522697	-1.08569330470073
N	1.55662662564198	0.59588641906432	-2.30606605816967
N	2.63484174076156	1.44638636510293	-2.22427152443360
N	3.15079475638707	1.46947863278512	-1.03858450641129
N	2.39910836473694	0.57817108961847	-0.27209756696620
C	2.64507694634079	0.39145680250599	1.11776426049567
C	2.60194377800873	-0.89420751699717	1.67432134611474
C	2.83663205774802	-1.05375193763767	3.04287883800533
C	3.13053875904482	0.05417073491146	3.84355800232464
C	3.18851770378240	1.33114507332524	3.27251136030224
C	2.93810288624238	1.50851330781017	1.91106893243472
C	-0.62373703034390	-1.25556142521346	-1.48407666090718
C	-0.41285283765342	-2.00336325644090	-2.66063699416011
C	-1.53659941731871	-2.39188178985924	-3.40030199756374
C	-2.84279685416857	-2.09161401324125	-2.99212107507759
C	-3.01379541464893	-1.38453043178364	-1.79659286451050
C	-1.92284583239969	-0.95201926581712	-1.03139661269988
H	2.41433955665381	-1.76043863686742	1.04525579072716
H	2.80494344135325	-2.05080148137079	3.47759161633730
H	3.42117677649535	2.19593278885355	3.89072745101514
H	2.97090087829317	2.49446887868637	1.45574342405018
C	0.96831067711785	-2.40585700005198	-3.11204409249591
C	-2.14649036043578	-0.18169486511330	0.25007323325970
H	3.31867560547116	-0.07641766390695	4.90729169225955
C	-4.02927673598567	-2.53230027175094	-3.81984352958578
H	-4.02091848467997	-1.15055674041481	-1.45203033617341
H	-1.38288017362616	-2.96452148957902	-4.31530755489639
H	-3.21804863944056	-0.05286605622399	0.43853171640303
H	-1.72422516421471	-0.69846797213047	1.12592855479354
H	-1.69119042521777	0.81762955707683	0.21376124539943
H	0.90993241906630	-3.18209369106394	-3.88326656658026
H	1.51895120381064	-1.54941442209161	-3.52275160735338
H	1.56021035040813	-2.79881944728925	-2.27414400039807
H	-4.97577602134729	-2.24266994517711	-3.34794863670942
H	-4.00263601362666	-2.08431838854612	-4.82345916289912
H	-4.03941268440377	-3.62314044187832	-3.95564675796040

38

Coordinates 7q isomer B

N	-1.72790807778990	1.35818731812464	0.06315202937083
C	-0.49436295097999	1.58874289540680	0.60581901673120
N	-0.44102227104405	2.84844352818208	1.05051878479206
N	-1.67851465257205	3.38615470294322	0.76942456215716
N	-2.46006667034670	2.53353023825814	0.18859103838262
N	0.46485385458366	0.62115871714712	0.62014229944181
C	1.78992565681817	0.69112815613886	1.10032392459845
C	2.34851338910492	1.85478998093080	1.65541136198481
C	3.67498290897775	1.83248486675682	2.09714853573793
C	4.45336502699543	0.67546331193544	1.99770674297316
C	3.88967807909302	-0.48094520061638	1.44441445047939
C	2.56934711782722	-0.47666624133199	0.99796350447256
C	-2.25079815385087	0.16493284702592	-0.53603878032479

C	-3.18815505801784	-0.60401054091306	0.18376839262854
C	-3.67325989394165	-1.76571715275919	-0.42399800327864
C	-3.24942756573231	-2.17056363899968	-1.69974695781637
C	-2.32166071924020	-1.37348894658602	-2.38040853191665
C	-1.81155488179046	-0.19202345192846	-1.82383861050702
H	1.75104326659193	2.75618312441586	1.73830032151303
H	4.10011989513011	2.73818581661611	2.52631935803881
H	4.47904111933664	-1.39210088700183	1.35849736660138
H	2.13377136831915	-1.37793833910914	0.56681143366418
C	-3.65707365592445	-0.19112544591204	1.55817809778936
C	-0.84108855824429	0.67169470627209	-2.59360286789270
H	0.16703291304934	-0.28760511233162	0.27670553457229
H	5.48382625602436	0.67256736866930	2.34656764170372
C	-3.79889014051602	-3.43320081499581	-2.32153606295477
H	-1.99645482457150	-1.66450275929100	-3.37864514919041
H	-4.40383485352272	-2.37115617266041	0.11222072926540
H	-0.77894583537951	0.34188050550541	-3.63622803258199
H	-1.14873811756622	1.72499246734883	-2.58470930454069
H	0.17222392697212	0.62677086039396	-2.17016589212996
H	-3.36204358432532	-3.61634940501557	-3.30994863163016
H	-3.59136752970855	-4.30867920666186	-1.69038055800965
H	-4.89007847190031	-3.37348771199341	-2.43878698814807
H	-4.46627993159725	-0.84606280556691	1.89901483887249
H	-2.84643688350324	-0.25229184282345	2.29762523093649
H	-4.02186149675840	0.84292426442642	1.56670917421416

27

Coordinates 7r

H	0.25516814842744	-0.56469033507002	0.20106160739286
N	0.50230416260554	-0.73089662911891	-0.77321888565575
C	1.76970094325955	-0.39610256205339	-1.17246577676708
N	2.28248015993316	-0.42567352187271	-2.40167638448222
N	3.57606261927429	0.02686692849926	-2.26802165888531
N	3.86068401779702	0.32091108205543	-1.04009853630269
N	2.71821335377347	0.05203443268514	-0.29864679738497
C	2.64789611919446	0.30040046340135	1.10647193653984
C	2.14412283287444	-0.68500919292241	1.96444666582466
C	2.06803555805463	-0.41771852066932	3.33434119239074
C	2.50979779087459	0.80952840499410	3.83835915590418
C	3.02834623104844	1.77807265405531	2.97039088426185
C	3.09256917826940	1.53302448361180	1.59789704839340
C	-0.54527555997287	-1.21065244399476	-1.54605407571753
C	-0.47281550993017	-1.49298870316382	-2.92194938512961
C	-1.63837409973923	-1.97500156977869	-3.50303889515723
N	-2.78813537872337	-2.17227330606628	-2.81829824958279
C	-2.71535290260245	-1.86529340239975	-1.52855337142197
N	-1.68230411284420	-1.39954954021095	-0.84115376372741
H	1.84381748027180	-1.65513996245457	1.57604277849462
H	1.67771620235845	-1.17833592912807	4.00707034788885
H	3.37619836149623	2.73203909073320	3.36104017341528
H	3.48130809117402	2.27780087939438	0.90865388739151
H	2.45525672766748	1.00964781526897	4.90639709606896
Cl	-4.20253773669705	-2.10951829197921	-0.58819410114357
H	-1.66633550879534	-2.21678153226069	-4.56498670011985
H	0.43635283095028	-1.33950079155538	-3.49071619248875

27

Coordinates 7r isomer B

N	-1.83104025256066	1.04484874091849	0.58159422864296
C	-0.52916884039415	1.34565265766510	0.96248260071907

N	-0.55691788254638	2.46800553911418	1.68999610548481
N	-1.87839924606029	2.84717911428942	1.74963559518486
N	-2.65894729402437	2.04403012249055	1.11611778449920
N	0.52643212528797	0.58199646930469	0.61181517622286
C	1.89310295017487	0.75422518204326	0.92681532979583
C	2.39004016765352	1.82520980150300	1.68774255468911
C	3.76296328576773	1.90236528023672	1.94084604498188
C	4.64441574756885	0.93450640480806	1.45025409407794
C	4.14128016031279	-0.13021339177183	0.69244441707310
C	2.77609084571901	-0.22320848650555	0.43034406657732
C	-2.35211483253029	-0.00737580367905	-0.17377525668131
C	-3.72562010437147	-0.11927617716055	-0.43857631148454
C	-4.10437641652618	-1.21429022784572	-1.20276973119622
N	-3.22382358283041	-2.12925315118737	-1.67384336558877
C	-1.96018194216921	-1.90487348231868	-1.35187558408357
N	-1.45889664447566	-0.90279186858268	-0.63111623014813
H	1.71386039191629	2.58031168804685	2.07239293483116
H	4.14224637090444	2.73496067760989	2.53069358311577
H	4.81352752104166	-0.89257383179819	0.30328782083382
H	2.38533794987295	-1.05239028796225	-0.15846977344023
H	0.26856010375442	-0.23409888732431	0.04794263577627
H	5.71051846705839	1.00677343185981	1.65498000641533
Cl	-0.77023951246203	-3.07047922867260	-1.94309308833548
H	-5.14999096428194	-1.38045399819265	-1.45768943794199
H	-4.44005857179985	0.60621371311142	-0.06737620002105

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Coordinates 7t

H	0.30453168504157	-0.59727929790382	0.25817559893863
N	0.50403780975296	-0.77090071149420	-0.72189679682194
C	1.73891096800213	-0.39824198481874	-1.14563005893164
N	2.23285825018873	-0.40407043341777	-2.39065881703310
N	3.51325986870671	0.08867323757866	-2.28265538258396
N	3.82103287551117	0.39061437231612	-1.06434225692958
N	2.70340278561264	0.07829557769662	-0.29232351434717
C	2.66564469776716	0.32415118987504	1.10915732047418
C	2.16645357538018	-0.65358247352907	1.98090506166240
C	2.12560658866074	-0.38903486807453	3.35290571196870
C	2.59748970444932	0.82938962876526	3.85116795862235
H	2.57092651245405	1.02742496876256	4.92072505636714
C	3.11182932310185	1.79054925827903	2.97239683401533
C	3.14037621526995	1.54800086388275	1.59830768350282
C	-0.58861278823759	-1.25866538827815	-1.48410122088472
C	-0.51751295333832	-1.54926500091233	-2.85543384485363
C	-1.64065617225306	-2.04195113274468	-3.52122382190620
C	-2.85893971596181	-2.25869462428137	-2.85219842661662
C	-2.91811727031512	-1.96152793098852	-1.47653751208129
C	-1.80159828340167	-1.46993063854775	-0.80645758804932
H	1.84543322803216	-1.61937361207040	1.59812076338921
H	1.74082256869833	-1.14653126219656	4.03272035643776
H	3.48439164363258	2.73796318560299	3.35665317229189
H	3.52648266487279	2.28812211044503	0.90268466778415
H	0.40755556150278	-1.38639922303259	-3.39748460824025
H	-1.56838539652107	-2.26337859314728	-4.58569352879385
N	-3.96128832533268	-2.82277143934078	-3.51687676968034
H	-3.84630148132894	-2.11965935386550	-0.92856865010354
H	-1.87198126190226	-1.24458367435810	0.25782870629828
H	-4.86467923386292	-2.59203720906427	-3.11061363930447
H	-3.96687364418237	-2.67640554113764	-4.52335245459121

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Coordinates 7u

N	-1.75422430632455	1.27381691273934	0.22517584450473
C	-0.49732588123386	1.53118161059764	0.70166777395429
N	-0.49417859900028	2.72889949536456	1.29598335013465
N	-1.78573006233263	3.19621540746669	1.18409041853230
N	-2.55315813605009	2.36096372165140	0.56020891154527
N	0.52406148996775	0.64123623319942	0.55131878890752
C	1.86159636022965	0.74334570453903	0.98718269579966
C	2.38095890922619	1.87954976278805	1.63102096572699
C	3.72413351742089	1.89146410311519	2.01973358043735
C	4.55873369017311	0.79586785759064	1.78000925759988
C	4.03477240543206	-0.33314999989815	1.13808375596816
C	2.69857083231890	-0.36264375517842	0.74346256008466
C	-2.26422456799280	0.11244575112374	-0.42583821735800
C	-3.34290572314321	-0.58071009282983	0.13890054474692
C	-3.84959798362552	-1.71088901790987	-0.49222745750246
C	-3.27783033791163	-2.18506142494848	-1.69409334901350
N	-3.73704873534766	-3.35773722716739	-2.28519464571686
C	-2.19064966404373	-1.47636730034356	-2.24869435305012
C	-1.69568867252627	-0.33318094030323	-1.62666579212638
H	1.74031970674711	2.73321431757090	1.82310810314057
H	4.11741676001012	2.77566999528781	2.51861761250159
H	5.60165230008913	0.81858918642617	2.08900691317809
H	4.66811143429146	-1.19685228497020	0.94317090272367
H	2.29371259390749	-1.24323774186092	0.24489467623018
H	-3.78280879574459	-0.22238437284142	1.06635520768393
H	-4.69081525460240	-2.24417291134307	-0.05183576301351
H	-1.74650053295535	-1.81798326169324	-3.18249305177552
H	-0.88371363854558	0.22561317682616	-2.08701827675385
H	0.26905124859942	-0.24018578097388	0.11461904007182
H	-3.52616186938466	-3.47490205670085	-3.27186720217335
H	-4.68562848764846	-3.63581506732422	-2.05188279498867

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Coordinates I

H	0.53884195868221	2.37511569697963	-2.56168608305223
N	0.76302652126099	1.57481425960900	-1.97556067227057
C	2.10621417950001	1.39982852765557	-1.79955300236793
N	3.04931536588775	2.09495067940228	-2.44852465065898
N	4.24745285307727	1.65036730087627	-1.95479259259580
N	4.09334893085768	0.72468655668934	-1.06323314888515
N	2.71440893221061	0.54519857516220	-0.92229541578754
C	2.19162951611862	-0.35987238285720	0.04910959827076
C	2.73312542032594	-1.64685807427346	0.13025015600866
C	2.20652084192842	-2.55028704905930	1.05536451871705
C	1.13951439805677	-2.17439292673441	1.87904000258177
H	0.72399487952193	-2.88500118690172	2.59083441474923
C	0.61147368174216	-0.88192321948683	1.79132120488512
C	1.14130571236893	0.03591253413806	0.88318484524665
C	-0.24159458297958	0.56776759215580	-1.84626044941504
C	0.01600712424097	-0.78277220737907	-2.09642102654727
C	-0.97503676926318	-1.74750890001995	-1.89371784665297
C	-2.25291058918231	-1.35885084491348	-1.46586176211137
C	-2.52340744773817	0.00349806376936	-1.24647408336314
C	-1.52326044595260	0.95278669664347	-1.42159602721481
H	3.54924867585898	-1.92786180686716	-0.53016367996640
H	2.62391584619401	-3.55297575260145	1.12343969511460
H	-0.21315827272838	-0.58276949434817	2.43491321467702

H	0.73863141899360	1.04200980198407	0.81682874524542
H	0.99639772673096	-1.10036105402711	-2.43982369576869
H	-0.73813799337389	-2.79009605991896	-2.07928909963146
O	-3.29678547512136	-2.22237625824829	-1.23578945393703
H	-3.51803936191051	0.29795121233152	-0.91839939202064
H	-1.72642016548910	2.00210475722020	-1.21445920123777
C	-3.05614004775689	-3.62841072714330	-1.45031182574498
H	-3.99821627475876	-4.12830940177057	-1.20732025517512
H	-2.79357491713409	-3.83228504890908	-2.49830723312274
H	-2.26199164016901	-4.00237985915725	-0.78814579796861

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Coordinates II

H	-2.91196268699546	2.36849451204708	0.07170962699152
N	-2.02261912625551	1.89409041567036	-0.05558701449220
C	-0.91246395201749	2.70126395159675	0.03275144057371
N	-1.34969064388568	4.07323045717943	-0.00945441244353
N	-0.45762375076729	4.92458019431612	0.14845603723768
N	0.26934958259094	5.79161906488369	0.27645531156318
N	0.34434304147388	2.43397606514722	0.10953184405907
C	0.87905831679285	1.16148834080929	0.36799971359894
C	0.42941420861715	0.33403296143686	1.41703491633582
C	1.00323600349363	-0.92035785868200	1.62227893282060
C	2.03885539346149	-1.37441073901829	0.79699507183446
C	2.51456276139288	-0.54347396745915	-0.22367330209712
C	1.95069491876704	0.71662164928651	-0.42942512803651
C	-2.05640624535803	0.49903801994929	-0.32722996770178
C	-2.91004459620888	-0.32067054141918	0.42799989619084
C	-2.93725128879512	-1.69433333055790	0.21668078715990
C	-2.08992220061124	-2.27814930747311	-0.74106891674169
O	-2.15933842965912	-3.64665008948079	-0.84832929352991
C	-1.28227016389972	-4.28438099622165	-1.79942795641095
C	-1.24977947166138	-1.46015468299414	-1.51117072919603
C	-1.24974948348235	-0.07813858606019	-1.31215620279691
H	-0.37988420490912	0.67074686539779	2.05974153928632
H	0.63155187999186	-1.55206742087908	2.42770647601777
H	2.47857885467546	-2.35699162163641	0.95752542511984
H	3.33128418622481	-0.87689070015183	-0.86253255192168
H	2.31376045686857	1.36710288432466	-1.22314659885874
H	-3.53639720463138	0.12291975877513	1.20021735319199
H	-3.59259633835351	-2.33520262890546	0.80271045053253
H	-1.47705780799554	-5.35665466688733	-1.70535122166554
H	-1.50486601323482	-3.96232376375002	-2.82691332456119
H	-0.22718191965441	-4.08201103516170	-1.56637676964412
H	-0.59275048352207	-1.88111726945027	-2.26479711051355
H	-0.59783259245242	0.54477406536830	-1.91615832190271

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Coordinates III

H	1.99115386318990	0.29469455326504	-3.31432863037874
N	1.66002004356712	0.44603802108462	-2.36581936919548
C	2.54094125433402	1.05157870010640	-1.48244346689189
N	3.50711858478132	1.91950432959730	-2.09780053536708
N	3.34263970417558	2.25132696652503	-3.28337061939087
N	3.33012205494190	2.63169464234058	-4.36241478282019
N	2.61518096135833	0.99670236543721	-0.20039881420705
C	1.94935072355671	0.05107629279639	0.59430369176911
C	1.94262423425788	-1.33048309792394	0.31283184577892
C	1.26072338870916	-2.21589130457032	1.14691116761676
C	0.57961629320085	-1.74980173782916	2.27751861271349

H	0.04134902244979	-2.44439603609230	2.91959416123204
C	0.61318590681429	-0.38447697678944	2.58276907064627
C	1.30264720034869	0.50610925242239	1.75921219957974
C	0.43850746792750	-0.20368636251544	-2.03510127063611
C	0.13216146772401	-1.43209759023006	-2.62594870848005
C	-1.05272175664035	-2.10483144135806	-2.31022406307341
C	-1.93383092457545	-1.55175908416555	-1.36962227413611
C	-1.63147350198221	-0.30942845011560	-0.78541145873090
C	-0.46746552727753	0.36547379818663	-1.12564067980910
H	2.46223527387840	-1.70314031519217	-0.56592711322748
H	1.25471165442992	-3.27812548013827	0.90686141331143
H	0.10213370881428	-0.01063658833365	3.46885607257779
H	1.33228463440679	1.56975609012701	1.98806155672338
H	0.83405259182353	-1.88428730363239	-3.32536310871455
H	-1.26271288537475	-3.05773718311727	-2.78561100968337
O	-3.10993891615432	-2.13438736150739	-0.96148173899012
H	-2.32571462479864	0.11655767753885	-0.06471783773322
H	-0.25166785515886	1.32690816409343	-0.67039924010855
C	-3.45267156495999	-3.41243670601560	-1.53349032481668
H	-4.40794569697421	-3.69160579349582	-1.07954509190367
H	-3.57374734805359	-3.34269282089460	-2.62426692144632
H	-2.69716943274017	-4.17381921960382	-1.29129273220796

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Coordinates IV			
N	-1.70204631493303	2.01048503696073	0.07317745478893
C	-0.60175739835918	2.67191317960898	0.00083479791163
N	-0.62405445691932	4.11043990427694	0.04642311808501
N	-1.75293991562427	4.63202907677648	0.01900026125326
N	-2.72713808902397	5.22149705640503	0.00383547625230
N	0.71380026006045	2.26424475476689	-0.11163517085763
C	1.27575258779941	1.01708236429491	0.24655892104766
C	0.74053780295896	0.22247891122108	1.27218823302241
C	1.32127958226658	-1.01173003744764	1.56593874743333
C	2.44765578707531	-1.45693252503280	0.86595236859369
C	2.99818320207449	-0.64904049821591	-0.13550462354082
C	2.41253461812786	0.57782134801718	-0.45127487612231
C	-1.83239202339916	0.63676884228074	-0.19991109401960
C	-2.70185520934894	-0.11847694727975	0.61272102139019
C	-2.88386186317900	-1.47980563209622	0.39928750370005
C	-2.22109088199295	-2.12566843430459	-0.65824590687672
O	-2.46319246391939	-3.47596827086488	-0.78725233694429
C	-1.80675745872608	-4.16599599066110	-1.86777610088080
C	-1.38525075971971	-1.38008729138468	-1.50267563826851
C	-1.19310835634353	-0.01629175233813	-1.26750619155611
H	-0.12424275825391	0.56192781997145	1.83132004690019
H	0.88943642182910	-1.62643339011474	2.35347221379327
H	2.89528971212698	-2.42018695692638	1.10221111917547
H	3.87867753424393	-0.97970175454276	-0.68363952333070
H	2.82229846055722	1.19513464439689	-1.24966735846704
H	-3.22092974251235	0.38260423712431	1.42769004275614
H	-3.54526425646207	-2.06040322152498	1.03959267146138
H	-2.12150405878560	-5.21065854170694	-1.78545256618407
H	-2.11835576463539	-3.76785848157708	-2.84458387922255
H	-0.71231033739781	-4.10650716413869	-1.77589403661609
H	-0.87252561124903	-1.84667238718369	-2.33827787457562
H	-0.53265385191692	0.54134926618104	-1.92630085619976
H	1.36438560358130	2.99004283505830	-0.39820596390231
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Coordinates V

N	-1.57044409500916	2.08763987531524	-0.03785555453207
C	-0.40589372120070	2.80189500896397	-0.03757154124232
N	-0.68909854370298	4.09363090508037	0.15948430000699
N	-2.05173667120618	4.16091347517605	0.28871056241060
N	-2.60459066680402	2.99210299766770	0.19093566205573
N	0.8537662727267	2.31423936561023	-0.27406122817346
C	1.39419391581408	1.08578191966481	0.19071992371239
C	0.81532819975718	0.35543863383819	1.23907454272624
C	1.36929492830257	-0.86786538006341	1.62142036711907
C	2.51333132206380	-1.36319225817747	0.98783837544970
C	3.10557027944685	-0.61838933892483	-0.03909345514340
C	2.54592279399588	0.59377111174752	-0.44483467512084
C	-1.84037445424992	0.70890551227215	-0.28759770044552
C	-2.72226800957635	0.02148741414057	0.55729271841104
C	-2.96809146543676	-1.32834372679230	0.34344119311779
C	-2.32530178278258	-2.00888801898096	-0.70780101109697
O	-2.61980866632265	-3.34176721725862	-0.82187579037703
C	-1.98451453404507	-4.08006596826049	-1.88857856833657
C	-1.44763194427868	-1.31274849228787	-1.55445067926181
C	-1.21361792673480	0.04756116674742	-1.34339169178266
H	-0.05772140537826	0.73646471185087	1.75882216372810
H	0.90605491764548	-1.43000960149223	2.43019850988279
H	2.94279222840473	-2.31475089740306	1.29432399371485
H	4.00023726711350	-0.98772054672317	-0.53730526385770
H	2.98922710473639	1.16079943304903	-1.26219289152902
H	-3.20445016736000	0.54889184361361	1.37617591343904
H	-3.64926111749919	-1.87827954286310	0.98887270686965
H	-2.34703544671230	-5.10699816341262	-1.78924224774090
H	-2.27360610228227	-3.68323428576075	-2.87181362437802
H	-0.89043900058114	-4.06560318605351	-1.78523302345353
H	-0.94622143024055	-1.81174363966446	-2.37704878179252
H	-0.53462614697088	0.58326251118015	-2.00018619878840
H	1.52761406832128	3.04421437820091	-0.49077700559129

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Coordinates VI

N	-2.09175360392900	1.88319816644885	-0.01875055571783
C	-1.06251894428135	2.65113579464814	-0.03743223785462
N	-1.35970769779683	4.05542432101425	0.00252707489520
N	-0.43894552590680	4.85261107057295	0.24808461614523
N	0.30418568546467	5.69902500270163	0.44892570600177
N	0.29668208888910	2.34712906196638	-0.06844630878257
C	0.91255577124165	1.13245068489084	0.31280955553538
C	0.41377863075827	0.34938764473204	1.36511969514795
C	1.04088966806600	-0.85342671270460	1.68913925379885
C	2.18033152220267	-1.27609224117676	0.99552641689250
C	2.69589441201880	-0.47633111166934	-0.02995742304865
C	2.06228494725695	0.71785543035613	-0.37762989485582
C	-2.05823555293552	0.50597835746237	-0.29669946494559
C	-2.86372874208265	-0.34219691179852	0.49000301923346
C	-2.87620587745485	-1.71595325839342	0.28223541894663
C	-2.10600163914327	-2.28279458742164	-0.74746581523356
O	-2.18177242541447	-3.65218859864596	-0.87310252397104
C	-1.39858267320973	-4.26713169407921	-1.91410178420234
C	-1.33842246103343	-1.44704122169383	-1.57242917033784
C	-1.31439128100005	-0.06984409329683	-1.34106061606530
H	-0.46337698095522	0.67090184637511	1.91653668869354
H	0.63505936931168	-1.46216418715772	2.49488128277344

H	2.66459009763995	-2.21487570550939	1.25651803141575
H	3.58655966972096	-0.78812300158968	-0.57271144387591
H	2.44661632939311	1.32611596136780	-1.19581218702392
H	-3.46385195407993	0.09874635587893	1.28352857775754
H	-3.48574170693447	-2.36836962238387	0.90451114339426
H	-1.59085364666354	-5.34110988932370	-1.83269441312873
H	-1.70831285778650	-3.91613830522015	-2.90931501450386
H	-0.32472609390110	-4.07674772121861	-1.77221657098089
H	-0.75010099385269	-1.85353767843669	-2.38920791011725
H	-0.70531377616109	0.56014284350293	-1.98364707156321
H	0.90271624255866	3.00686399980158	-0.54846607442255

33			
Coordinates TS1			
H	0.22795771477341	2.16421308507452	-1.23649788531897
N	0.52619469075896	1.36974302930717	-1.79582071253120
C	1.90057627173390	1.14386484934665	-1.82937576541036
N	2.74477903714461	1.52703448954335	-2.78185285362085
N	3.98141537600759	1.07815638732657	-2.40279070254880
N	3.92152960120813	0.42653221489300	-1.26922079916002
N	2.61010830298713	0.44898022425202	-0.88238966472225
C	2.18903644304346	-0.08691173331749	0.38271839030192
C	1.38865166987773	-1.23031214582929	0.42852099319963
C	0.98635128534887	-1.72351261137087	1.67212451072441
C	1.38982484478672	-1.08352637033867	2.84900280443434
H	1.07515180129893	-1.47403444452050	3.81483953153985
C	2.20203407298280	0.05469840594498	2.78738421184689
C	2.60460614374385	0.56150927040576	1.54954932690367
C	-0.38558178071081	0.27862985838188	-1.82825000546564
C	-0.16709536703430	-0.81064726216970	-2.67879577808648
C	-1.05967647099258	-1.88910145525492	-2.70345239414614
C	-2.20162669110430	-1.87376334798935	-1.88942740215668
C	-2.43240720774711	-0.76937908498981	-1.05152181096214
C	-1.53033465131979	0.28834846069426	-1.01471413596235
H	1.08682295748579	-1.72126322948961	-0.49100761590051
H	0.36112079888478	-2.61253821159288	1.71907655859279
H	2.52190622777211	0.55018200489525	3.70169877199465
H	3.23486560596724	1.44471778712532	1.47891881372746
H	0.70152759531307	-0.82552592811377	-3.33354171950623
H	-0.85741519746993	-2.72103500362568	-3.37084716023200
O	-3.14731964542692	-2.87457339131965	-1.84083952887172
H	-3.32005149099928	-0.76140940201354	-0.42227430621180
H	-1.70668965167751	1.12499348287016	-0.33986340867157
C	-2.96449253646359	-4.00137533752415	-2.72012584884068
H	-3.82139786159646	-4.65736306484927	-2.54062687229038
H	-2.95850597041983	-3.68898282817260	-3.77453992927518
H	-2.03616591815667	-4.54464869757913	-2.48975761337363

33			
Coordinates TS2			
H	-3.02929868887828	2.38512647867525	0.00025642369814
N	-2.13719406427731	1.90559997765804	-0.08814502196103
C	-1.04266936632623	2.71066741668965	0.02358006159500
N	-1.42818379954111	4.10329473351522	0.04385982575366
N	-0.33422088759976	4.76551825599860	0.16481336073066
N	0.81508479367171	4.58232179110175	0.26994755068997
N	0.21187067710628	2.41858012999691	0.07251679111020
C	0.85578827594250	1.21603904483120	0.35839820275274
C	0.43190164751346	0.36263021256686	1.39750862133157
C	1.08538159972524	-0.84896269837078	1.61704507410652

C	2.17746228892000	-1.22245692237772	0.82452485293541
C	2.62325815516263	-0.36118180187287	-0.18520743622620
C	1.97400485573712	0.85202858841322	-0.41472282041995
C	-2.14714568975051	0.50551222297297	-0.34621943367158
C	-3.00022315767023	-0.31859161105981	0.40451716305861
C	-3.00977438471058	-1.69376644929739	0.20040512973881
C	-2.14459468178218	-2.27396500259230	-0.74388910980140
O	-2.20145620899838	-3.64287902276310	-0.84699170432583
C	-1.30839070353308	-4.27744809481905	-1.78555089765463
C	-1.29993963898373	-1.45174181368697	-1.50469756195494
C	-1.31670134795001	-0.06844397983838	-1.31258371997287
H	-0.41680562894472	0.64418522766451	2.01468996699228
H	0.73736422577144	-1.50760805495035	2.41104314214103
H	2.68263790139507	-2.17031799354977	0.99998335088712
H	3.48003341766712	-0.63628993132518	-0.79826250228356
H	2.30737476545540	1.52614006066397	-1.20105263386187
H	-3.64376005871119	0.12344577260983	1.16322915333853
H	-3.66671224135570	-2.33823846199481	0.78063225235916
H	-1.49703076517889	-5.35066695078802	-1.69053757122988
H	-1.52096175705350	-3.96017944928874	-2.81658397205520
H	-0.25757351489411	-4.06726847689971	-1.54002868915792
H	-0.62877609991128	-1.86952602442529	-2.24761894138742
H	-0.66374891801713	0.55844282654228	-1.91186290725510

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Coordinates TS3

H	-2.60735382724932	2.61771686060805	-0.38628348510592
N	-1.75979882681946	2.06160451534793	-0.32372442514179
C	-0.59333882704969	2.76551687530145	-0.13877996959999
N	-0.82296695007231	4.20835488275099	-0.27263645173817
N	-1.32375698073892	4.79548880383998	0.69534357981969
N	-1.77211417981002	5.46052270353956	1.51229555747885
N	0.61633827999398	2.39649002297792	0.03923084094226
C	1.04622187426497	1.07441286718952	0.25581580081251
C	0.55302988595970	0.27592392500226	1.30588262888891
C	1.01191777999630	-1.03063017701113	1.47108843352999
C	1.97711064110787	-1.56156632767315	0.60712844722788
C	2.50172982776153	-0.75741109497872	-0.41074712878552
C	2.05292533488295	0.55386975134231	-0.57801727416536
C	-1.89052425876651	0.64586046768164	-0.48249823960401
C	-2.75576545521992	-0.06162270355133	0.36438170224013
C	-2.84626467866529	-1.44630265543647	0.27803759373343
C	-2.05050413808275	-2.14863017231777	-0.64391477001029
O	-2.16996908701699	-3.51626635339524	-0.61827264469224
C	-1.31872708853486	-4.27514980688257	-1.50258235889260
C	-1.20553248860126	-1.44058350130402	-1.51170032272641
C	-1.14407663935122	-0.04792018350521	-1.43714328632423
H	-0.20410463800201	0.67568957868363	1.97536891429397
H	0.60321314870471	-1.64218306516038	2.27393006538344
H	2.32495322639348	-2.58485332334406	0.73522269619954
H	3.26666984222170	-1.15169152320768	-1.07829723355462
H	2.45287909497868	1.18407869354771	-1.37012669184451
H	-3.33515026759866	0.47621319790235	1.11287364882512
H	-3.50679622983973	-2.00410584282697	0.93845922068411
H	-1.54493934587757	-5.32548854034520	-1.29765926464531
H	-1.53860049127895	-4.05367106653858	-2.55668505611538
H	-0.25719904617545	-4.08057093523157	-1.29410588001169
H	-0.58763760693723	-1.95560869612225	-2.23951445242393
H	-0.48486588457773	0.49251082311700	-2.10937419467784

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Coordinates TS4

N	-1.58736486775228	2.00311346566192	0.09945758964287
C	-0.51732360279753	2.70991258596936	-0.00493359838169
N	-0.63065985626371	4.15087859474428	-0.03613645617537
N	-1.88836389297717	4.40710646491459	0.00153105832371
N	-2.92017945530171	3.86152990135484	0.02594391261373
N	0.79721612739601	2.33574447771643	-0.07974747713011
C	1.37778685855089	1.09353583900405	0.27404735009133
C	0.82801791881948	0.26176044028714	1.26118210217806
C	1.43906447430832	-0.95811926143486	1.55640553248581
C	2.60651199179088	-1.35200838849878	0.89439564093964
C	3.16744471754865	-0.50787662927301	-0.07092869830916
C	2.55417322340109	0.70520556572813	-0.38740610750498
C	-1.81806922984213	0.65778844221862	-0.18519530795922
C	-2.72984547135332	-0.05408984837737	0.62047377790702
C	-2.98259713495457	-1.39949081064279	0.38969106435685
C	-2.34007243058156	-2.07079088099366	-0.66669090583829
O	-2.65077822565860	-3.40174593409119	-0.80889907985639
C	-2.01969601983859	-4.12186098056246	-1.88743624571250
C	-1.45172993524194	-1.36609228401395	-1.49437664344257
C	-1.19813850267937	-0.01498518417959	-1.25265795957152
H	-0.06556299389867	0.56307428180590	1.79633762813011
H	0.99916730581501	-1.60026743010854	2.31714193179611
H	3.07769153479584	-2.30356052868007	1.13207970175915
H	4.07951517950262	-0.79841222382342	-0.58923606102794
H	2.97574265883847	1.35269247786172	-1.15501174914013
H	-3.22669695572068	0.46780796838742	1.43562780404906
H	-3.67982977595264	-1.95111778509009	1.01706706334783
H	-2.39547555803845	-5.14667882572876	-1.81587859250758
H	-2.29593943237529	-3.69890996192870	-2.86395841519345
H	-0.92554255145519	-4.12514207193286	-1.77907383500329
H	-0.95009295220181	-1.85567256424270	-2.32327537563066
H	-0.50288356204011	0.51661034371598	-1.89686511621088
H	1.43410841615810	3.09295874423245	-0.31447353302557

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Coordinates TS5

N	-1.58323248455995	1.59358397396246	-0.03480191176528
C	-0.31746295336338	2.11393328001315	-0.06466584812934
N	-0.33851943440714	3.30930107743421	0.51839497844158
N	-1.63463076860232	3.52848284141424	0.89149212198250
N	-2.39793482380702	2.51391276196347	0.56672525973540
N	0.78613387910557	1.40856195126255	-0.54689517209292
C	1.80144801106544	0.97050641128893	0.34033161311185
C	1.56173233726749	0.81206444904538	1.71456545544896
C	2.57352681196579	0.32252770708611	2.54429178617385
C	3.82774036960825	-0.01452557558800	2.02477849373469
C	4.06280102341418	0.14550294279239	0.65394102268225
C	3.06070472097359	0.63376535478104	-0.18525260847976
C	-2.07769068246181	0.31809448088041	-0.44604948240695
C	-2.99135622418164	-0.35172360136643	0.38144613361093
C	-3.48270446877662	-1.59222648195086	-0.00071891167169
C	-3.06027513649235	-2.18380362073522	-1.20660995393524
O	-3.59816488043109	-3.41035713743336	-1.48670748507267
C	-3.18862832227575	-4.06177430941334	-2.70992701706260
C	-2.14490178156428	-1.50793434908475	-2.03004604237731
C	-1.66070176272194	-0.25385824152016	-1.64839163034754
H	0.59623579687581	1.07649254893070	2.13831243802610

H	2.37550729395191	0.20829680299448	3.60869673062790
H	4.61142838112676	-0.39234391929071	2.67783862323487
H	5.03452867955284	-0.10688103996847	0.23272348900618
H	3.24854502269529	0.75684111854882	-1.25162800493405
H	-3.30709042155117	0.10445202342050	1.31558792513845
H	-4.19121405227572	-2.12601918296569	0.62842736082084
H	-3.72449280321101	-5.01475379974862	-2.72623110309378
H	-3.47147767292454	-3.46664394613449	-3.58944136454321
H	-2.10595257492716	-4.24971473920073	-2.71569479565962
H	-1.81185558541264	-1.93643040057721	-2.96945731567581
H	-0.96782820546812	0.27189309511704	-2.29703978499363
H	1.13238271181270	1.71817752404209	-1.45159499953498

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Coordinates TS6

N	-1.90866784828826	2.00030393026681	-0.26519489995089
C	-0.83873162435502	2.69660200371924	-0.24488538908035
N	-0.97628113713355	4.15229417125999	-0.37939396196184
N	-1.06818336402214	4.80071155598258	0.67239856115231
N	-1.17997766222505	5.50533299997973	1.56600317810739
N	0.49703698116647	2.35501404069758	-0.15697027139752
C	1.05954248357290	1.10322977139242	0.20359565073411
C	0.50676998881249	0.31851965308294	1.22605657445031
C	1.06531562552000	-0.92493113502218	1.52149027855326
C	2.19221583224672	-1.38224869896232	0.82961320062225
C	2.76591490461852	-0.57902367623258	-0.16197077155632
C	2.19898352497215	0.65628579686581	-0.48161577743168
C	-1.94972525894896	0.60017669284480	-0.43351252185886
C	-2.79801489450279	-0.14782747929426	0.40483681237272
C	-2.86656591035297	-1.53246743253848	0.29983812866160
C	-2.11148879913382	-2.20730399458651	-0.67405605038476
O	-2.24071763369411	-3.57889530387357	-0.69381445826649
C	-1.47708767880064	-4.30155737298958	-1.67827163092271
C	-1.30392178993739	-1.46926321147929	-1.55181172049364
C	-1.22555292810819	-0.08017063145024	-1.42514862387112
H	-0.36004965978105	0.67036033868948	1.77503183912867
H	0.61712249430756	-1.53727450723479	2.30143134490355
H	2.62359037952478	-2.35286135055783	1.06612389046580
H	3.64810505838110	-0.92016822558901	-0.70083250256507
H	2.62191884246960	1.26891302134011	-1.27663508457457
H	-3.38448000291146	0.37475818600708	1.15814619060984
H	-3.50820441145851	-2.10974374812901	0.96278681369889
H	-1.71593850420874	-5.35752840319988	-1.52030644924938
H	-1.76382261160531	-4.01237341369505	-2.69993035693572
H	-0.39690234372393	-4.14730178754862	-1.53961349771623
H	-0.72359860651964	-1.95985010986049	-2.32703295684728
H	-0.58332423156524	0.47509712007342	-2.10378408580076
H	1.14431878568446	3.07608920004168	-0.46337045259552