

Supplementary Information

Chemoselective Oxidation of Phenoxathiin-Based Thiacalix[4]arene and Stereoselective Alkylation of Products

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Additional synthetic procedures for compounds **3**, **4** and **5** (not mentioned in the Experimental section)

Compound 3. Macrocycle **2b** (165 mg, 0.23 mmol) was dissolved in acetonitrile (200 mL). Concentrated hydrochloric acid (5 mL) was added and the solution was boiled vigorously for 45 min. After the reaction mixture cooled down to room temperature, the solvent was removed under reduced pressure. Subsequently, the residual solid was triturated with chloroform (5 x 30 mL), dissolved in further chloroform (30 mL) and the white adduct of acetonitrile and HCl was filtered off. The filtrate was evaporated to dryness under reduced pressure and the residue was recrystallized from acetonitrile:chloroform 3:1 v/v (2 mL). White microcrystals were filtered off and dried under vacuum to yield compound **3** as a racemic mixture (41 mg, 25 %).

Compound 4. Macrocycle **3** (251 mg, 0.35 mmol) was dissolved in chloroform (4 mL). Trifluoroacetic acid (1 mL) and hydrogen peroxide (30% aq. sol., 3.25 mL) were added and the solution was refluxed (62 °C) for 4 days. Subsequently, the reaction mixture was cooled on an ice bath to 0 °C and Na₂SO₃ was slowly added until no oxidation reaction was observable by potassium iodine starch test. The mixture was extracted with chloroform (3 x 20 mL) and the combined organic layers were dried over MgSO₄. The solvent was subsequently removed under reduced pressure to yield compound **4** as a racemic mixture in sufficient purity (white solid, 255 mg, 86 %).

Compound 4 and 5. Macrocycle **2b** (190 mg, 0.27 mmol) was dissolved in chloroform (3.2 mL). Trifluoroacetic acid (0.8 mL) and hydrogen peroxide (30% aq. sol., 2.6 mL) were added and the solution was refluxed (62 °C) for 4 days. Subsequently, the reaction mixture was cooled on an ice bath to 0 °C and Na₂SO₃ was slowly added until no oxidation reaction was observable by potassium iodine starch test. The mixture was extracted with chloroform (3 x 10 mL) and the combined organic layers were dried over MgSO₄. The solvent was subsequently removed under reduced pressure to yield the mixture of compounds **4** and **5** in sufficient purity (147 mg, ca 66 %). The particular yields of compounds **4** (56 %) and **5** (10 %) were calculated after following alkylation with iodomethane.

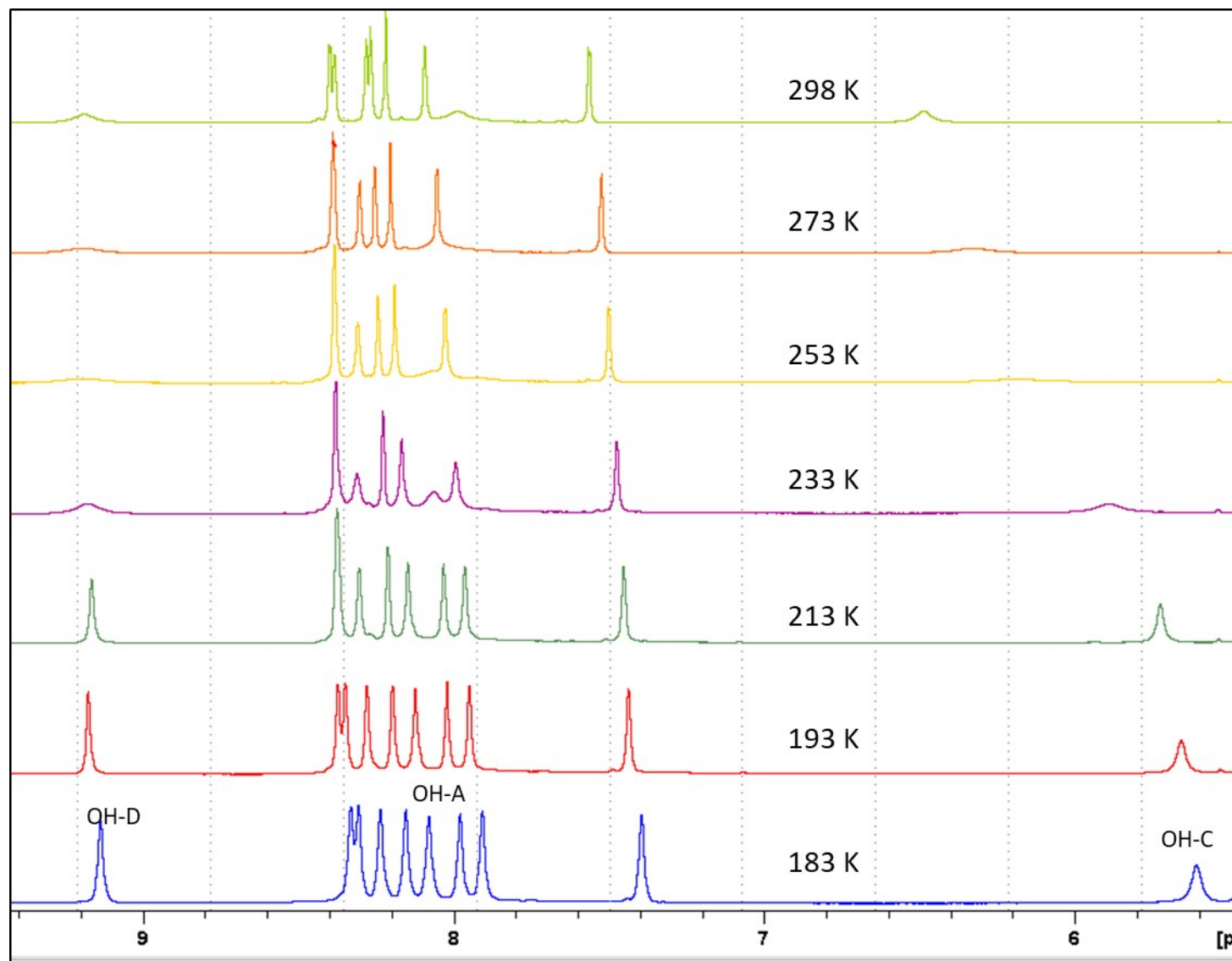


Figure S1. Temperature dependent ^1H NMR spectra (CD_2Cl_2) of compound 4.

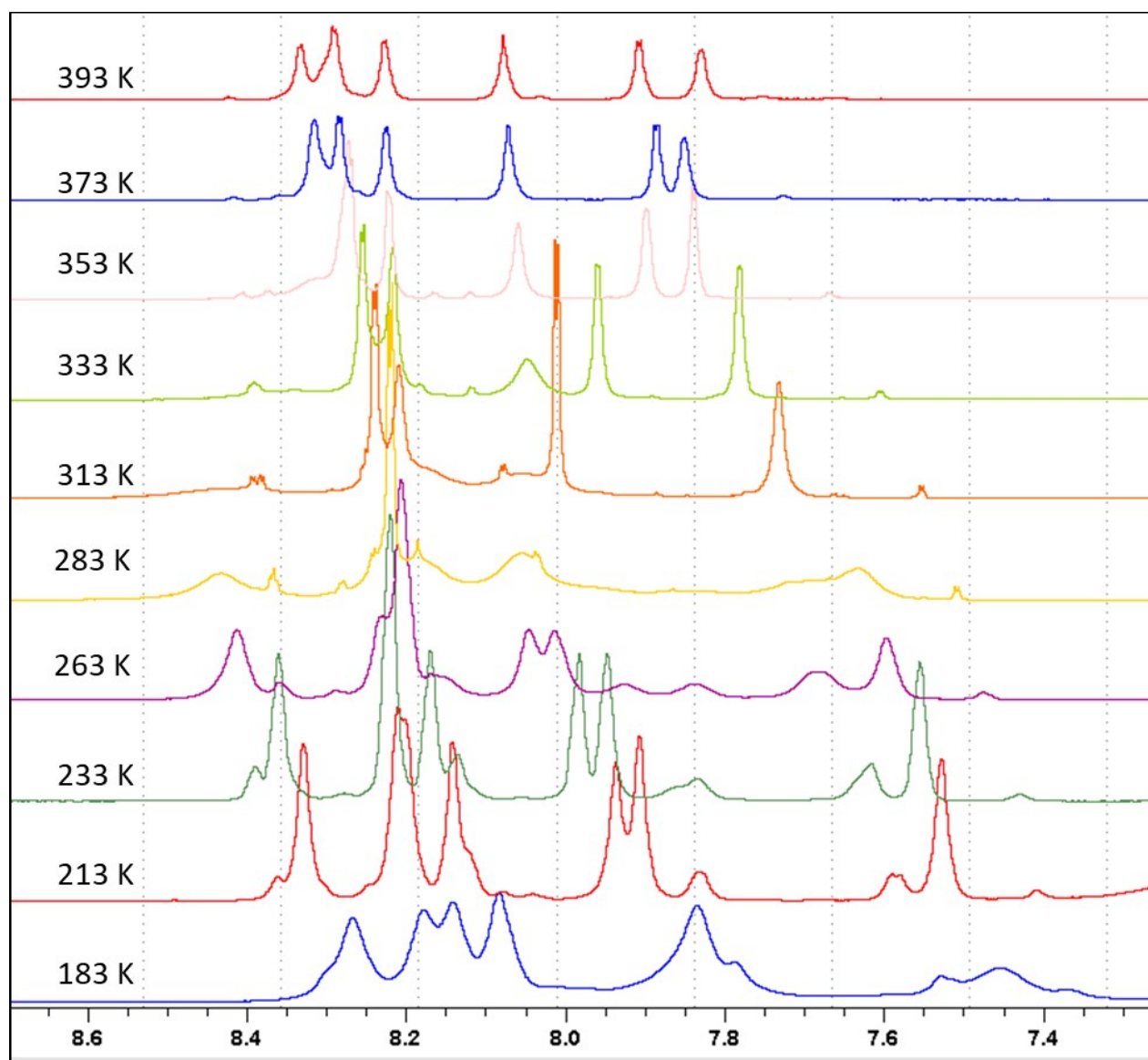
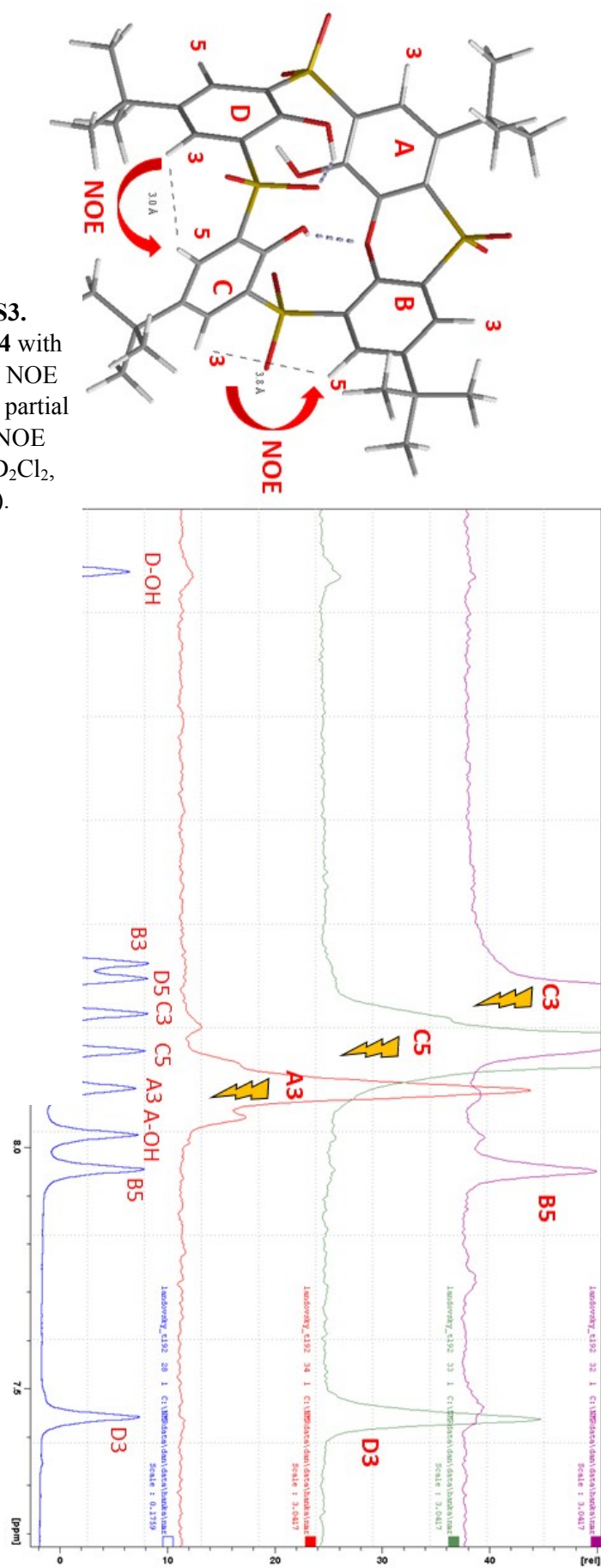


Figure S2. Temperature dependent ^1H NMR spectra (CD_2Cl_2 or $\text{C}_2\text{D}_2\text{Cl}_4$) of compound **5**.

Figure S3.
Compound 4 with
highlighted NOE
contacts and partial
 ^1H NMR NOE
spectra (CD_2Cl_2 ,
183 K).



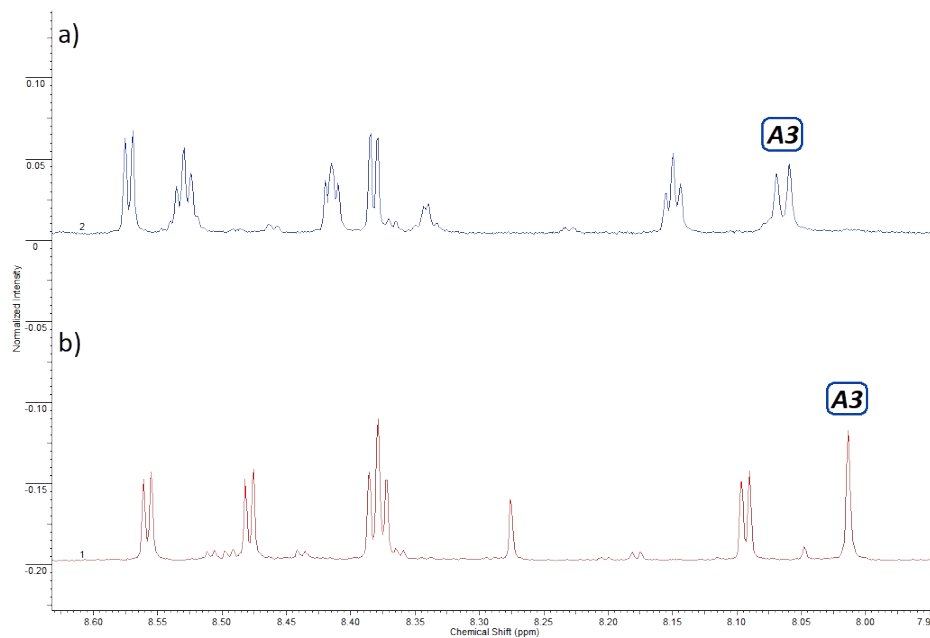


Figure S4. ^1H NMR spectra (400 MHz, 298 K, CDCl_3) of: (a) **6a** with 1 molar eq. of $\text{Eu}(\text{hfc})_3$; (b) free **6a**.

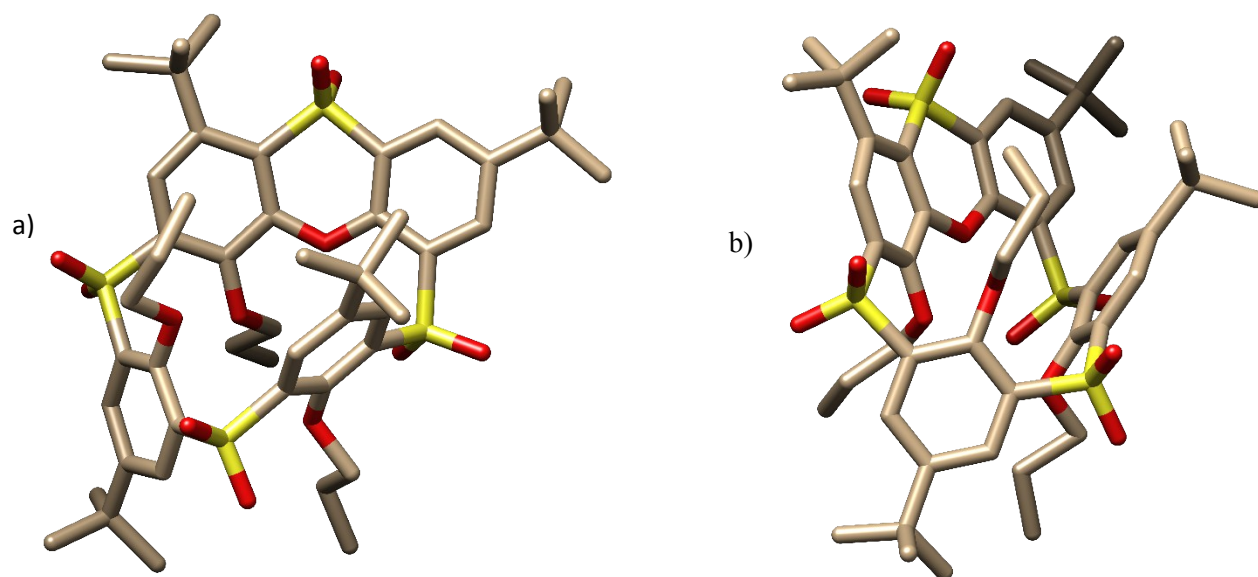


Figure S5. Single crystal X-ray structure of **6c**: (a) front view, (b) side view (hydrogen atoms omitted for better clarity).

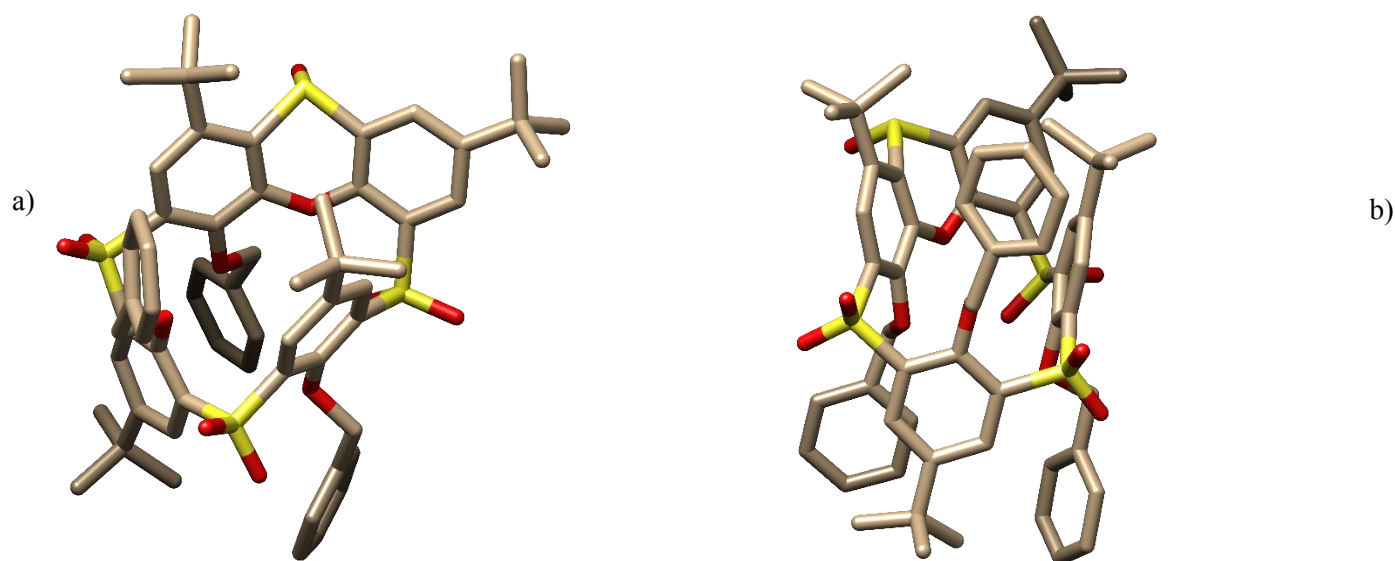
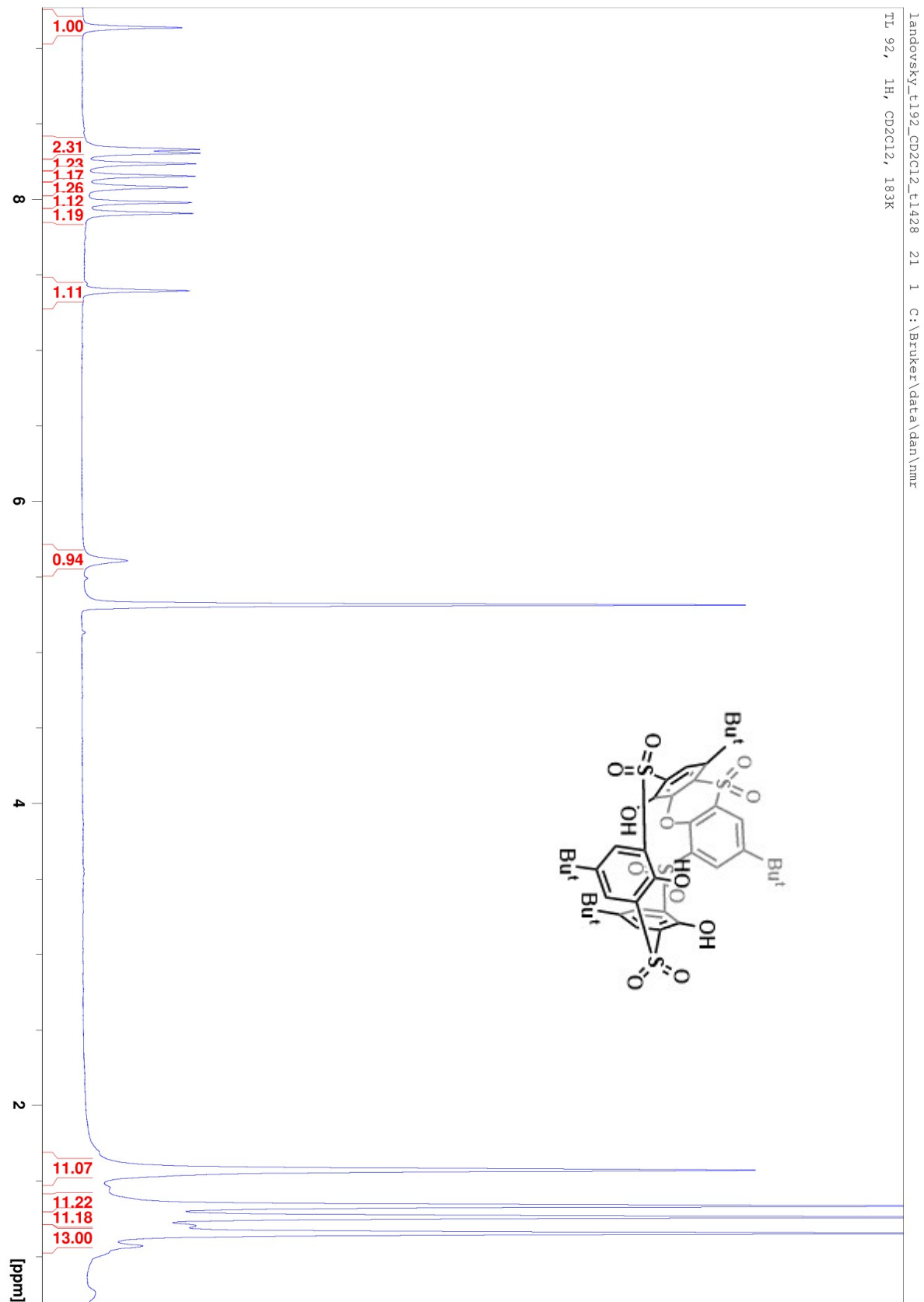
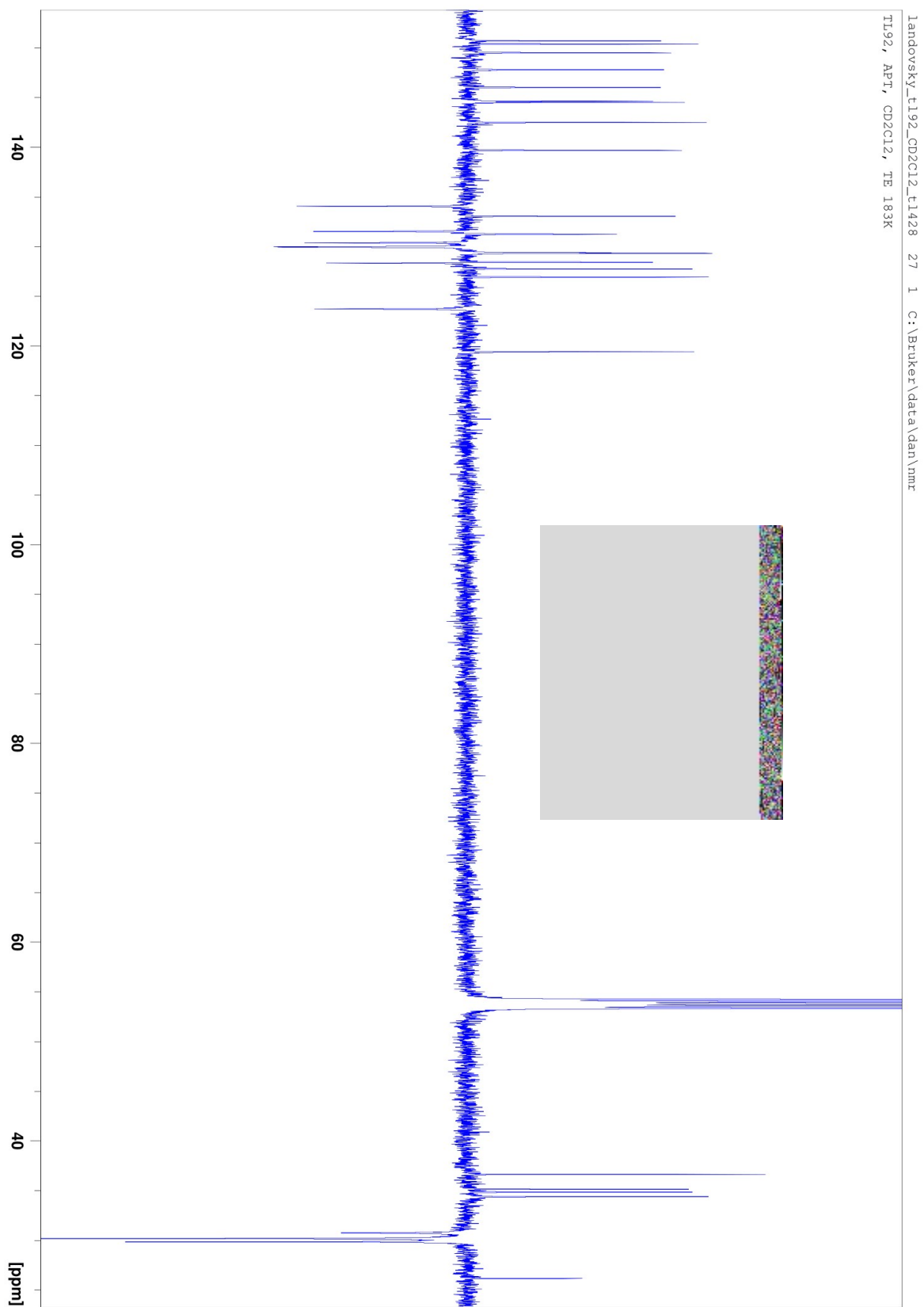


Figure S6. Single crystal X-ray structure of **7d**: (a) front view, (b) side view (hydrogen atoms omitted for better clarity).

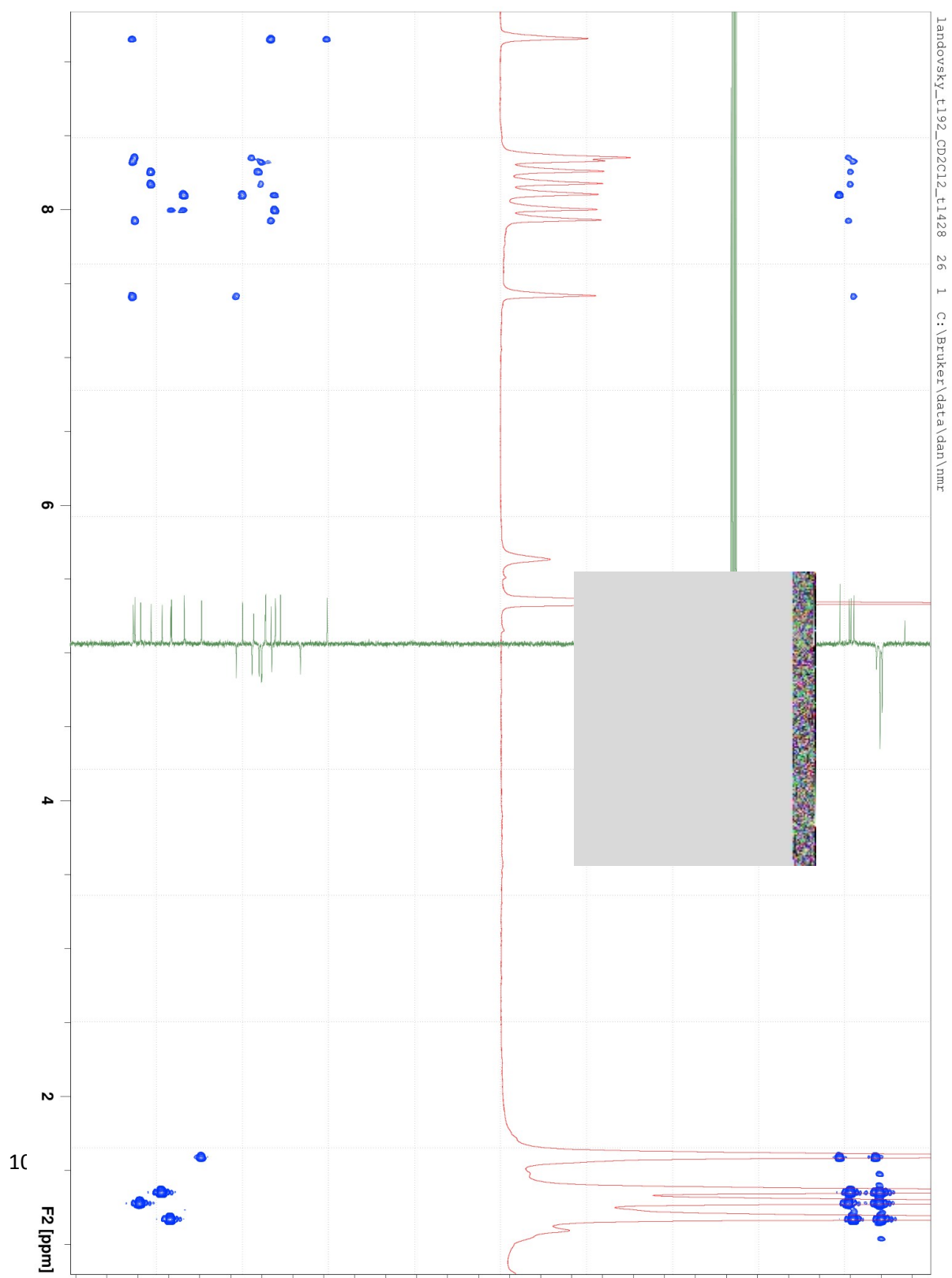
^1H NMR spectrum of compound **4** (CD_2Cl_2 , 183 K)



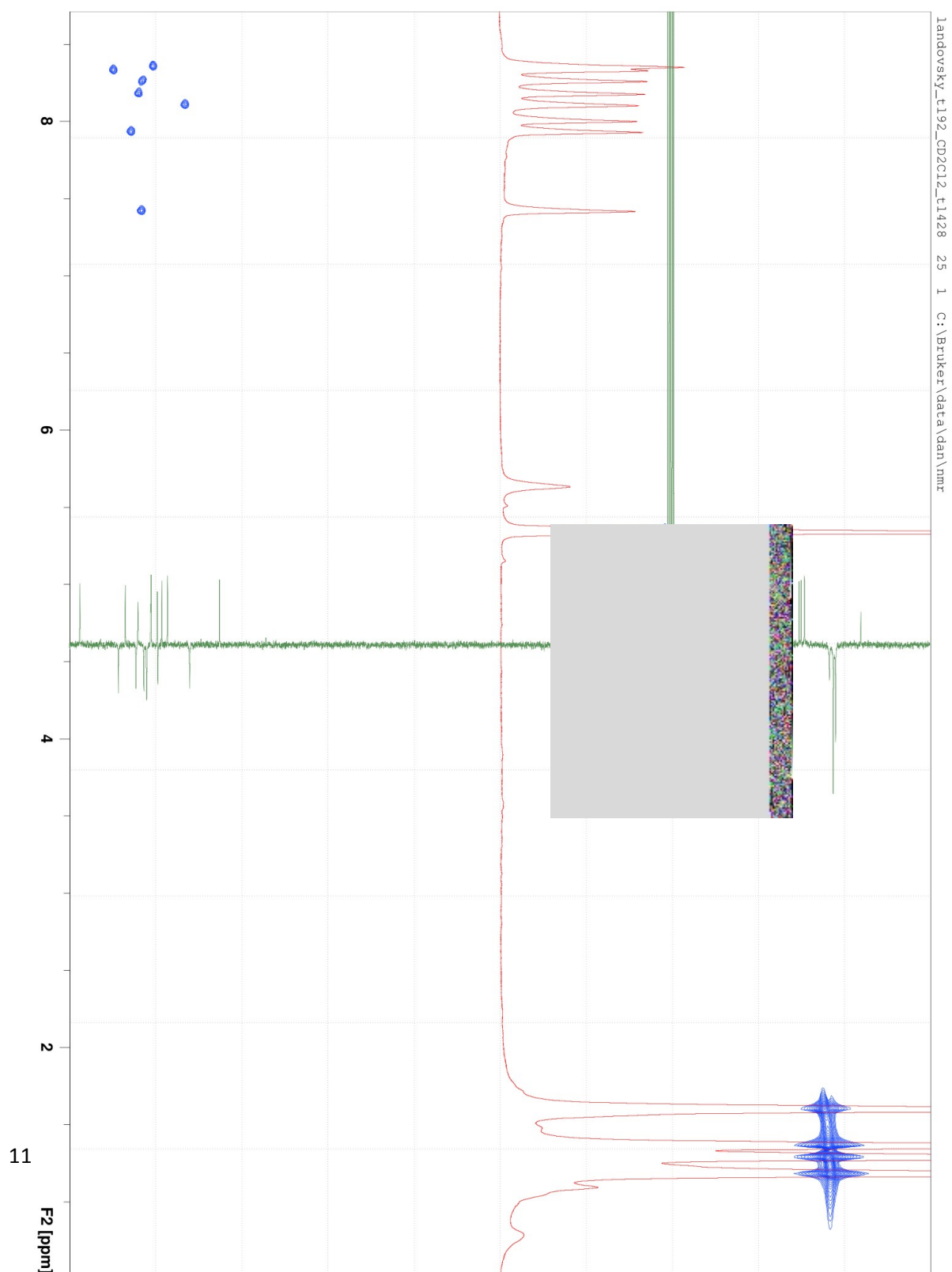
^{13}C APT spectrum of compound **4** (CD_2Cl_2 , 183 K)



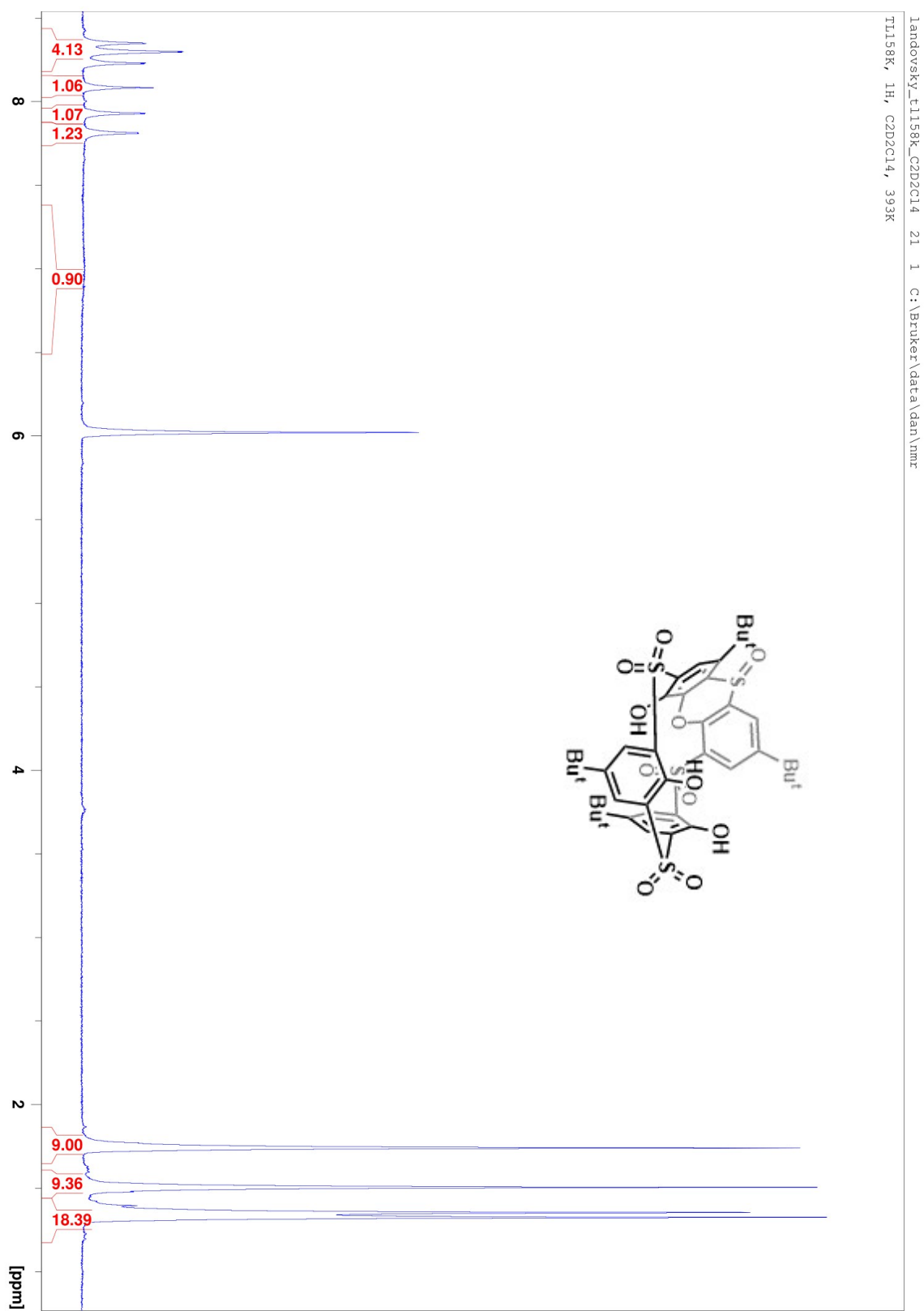
HMBC spectrum of compound **4** (CD₂Cl₂, 183 K)



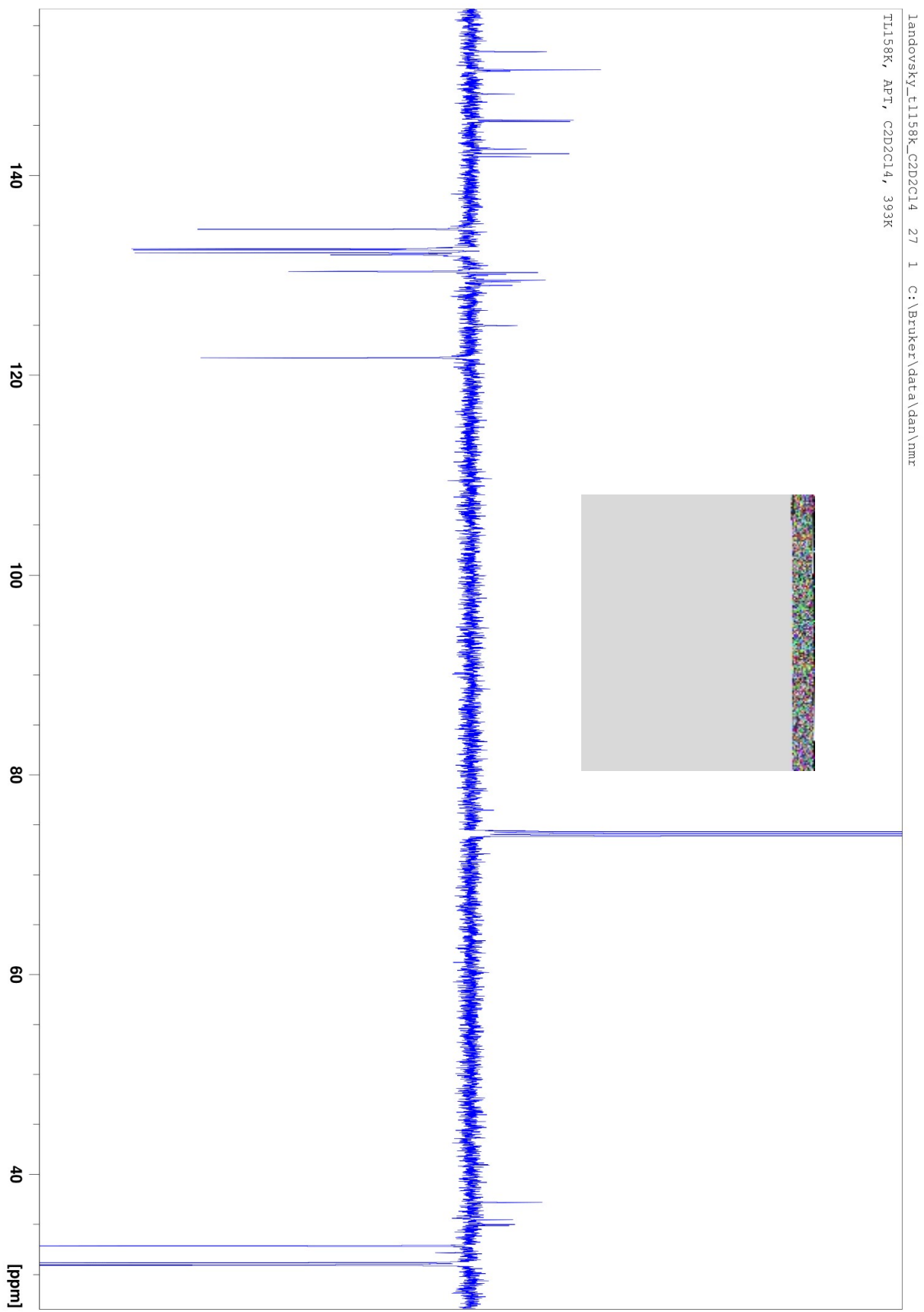
HMQC spectrum of compound **4** (CD₂Cl₂, 183 K)



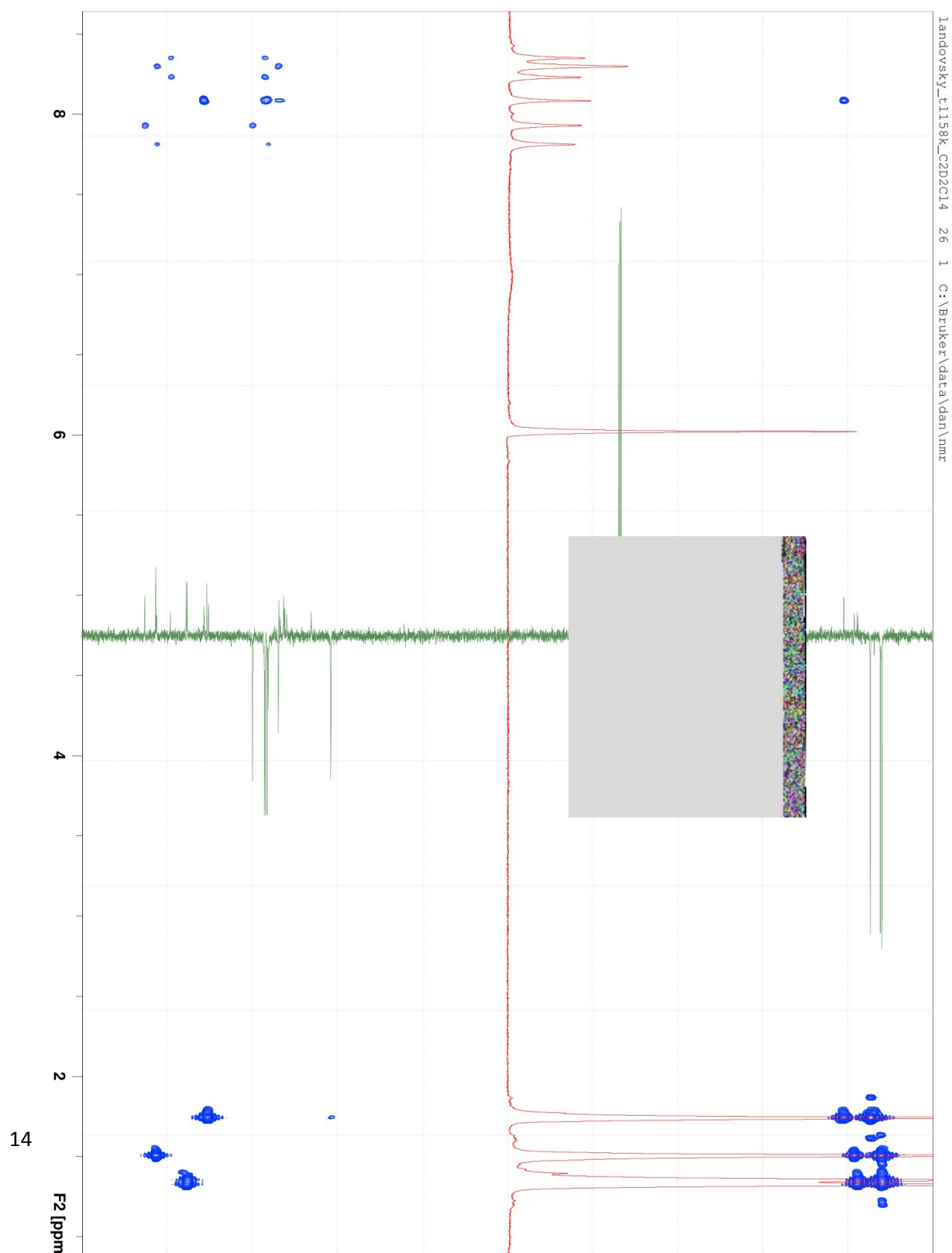
^1H NMR spectrum of compound **5** ($\text{C}_2\text{D}_2\text{Cl}_4$, 393 K)



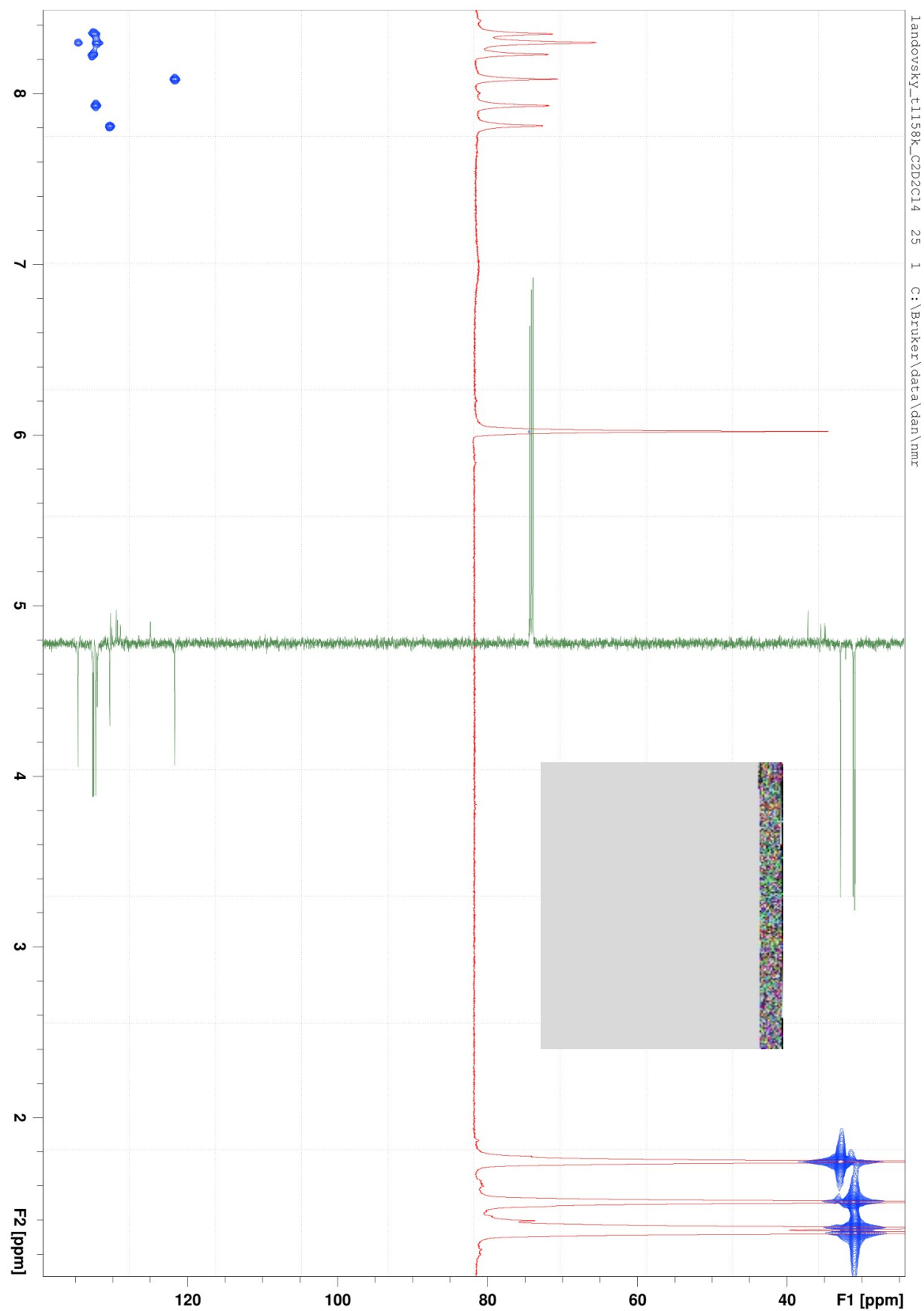
^{13}C APT spectrum of compound **5** ($\text{C}_2\text{D}_2\text{Cl}_4$, 393 K)



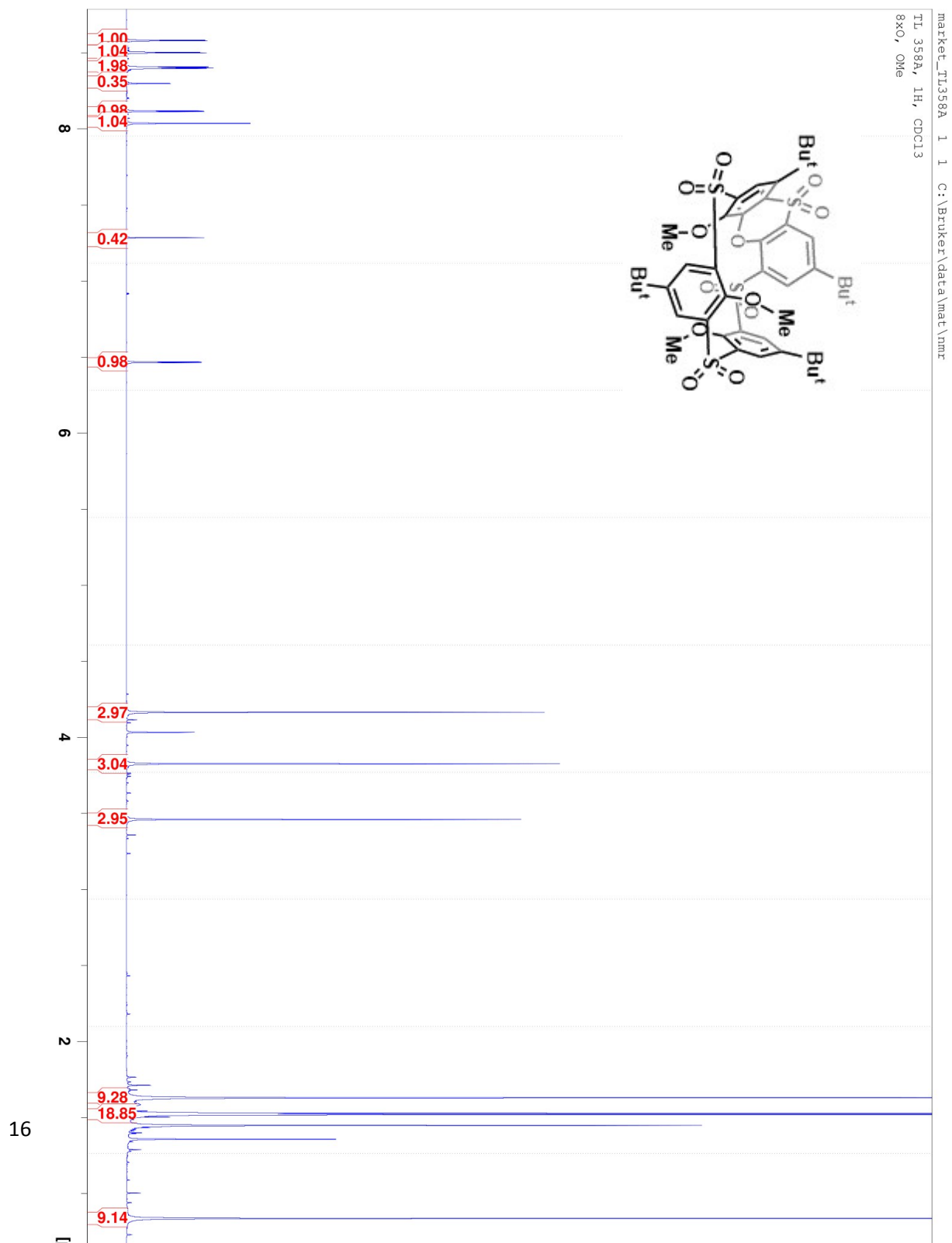
HMBC spectrum of compound **5** ($\text{C}_2\text{D}_2\text{Cl}_4$, 393 K)



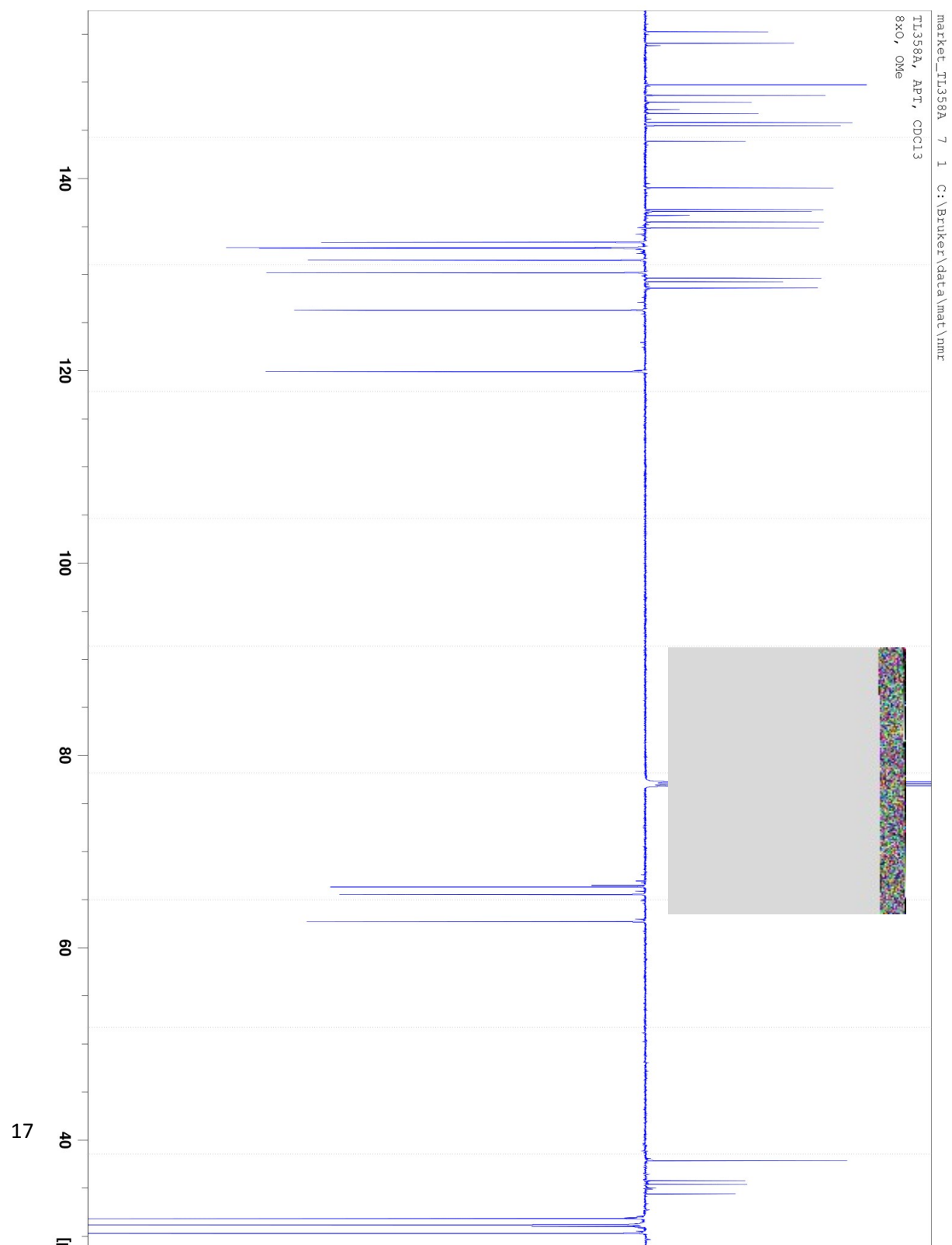
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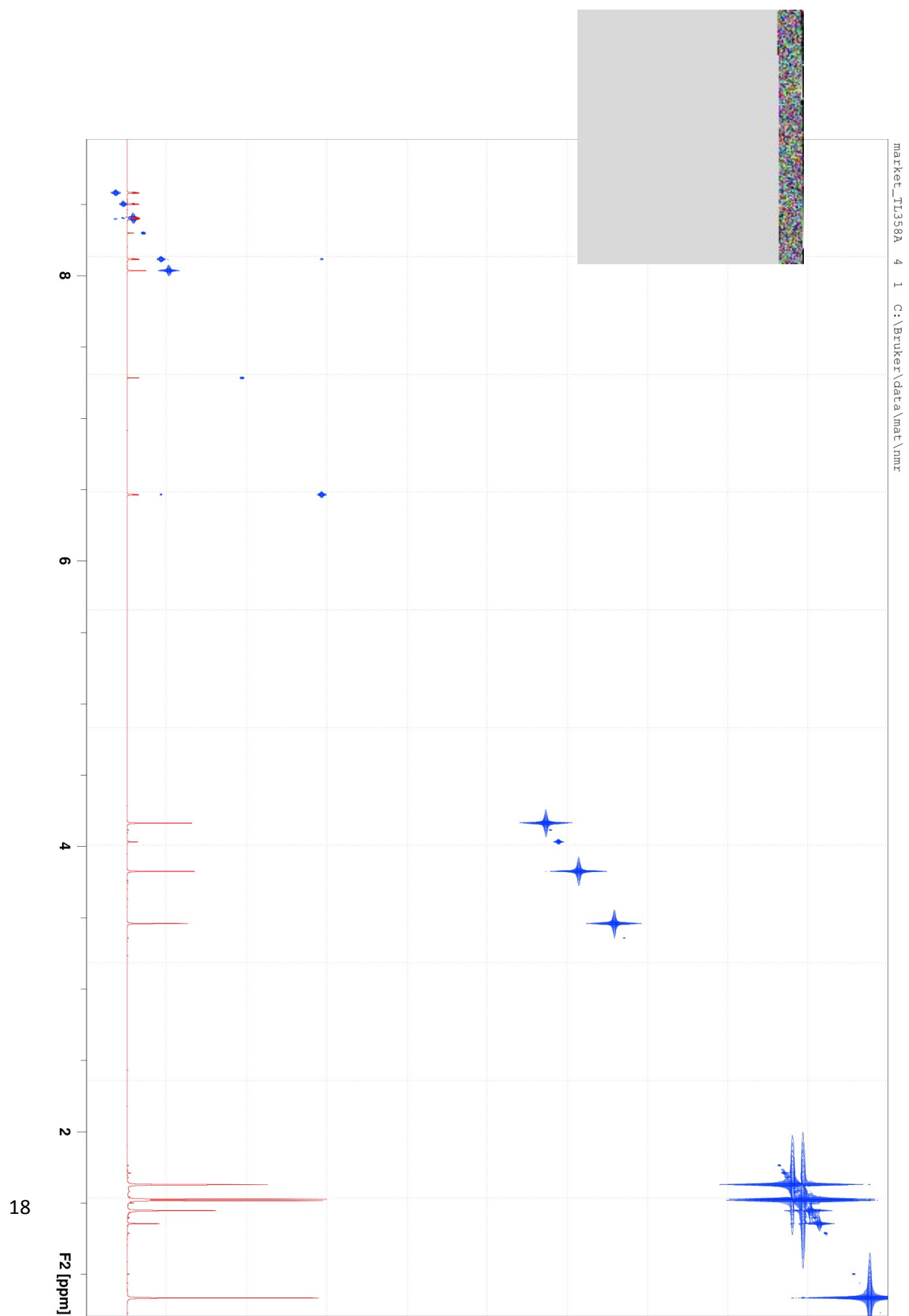
^1H NMR spectrum of compound **6a** (CDCl_3 , 298 K)



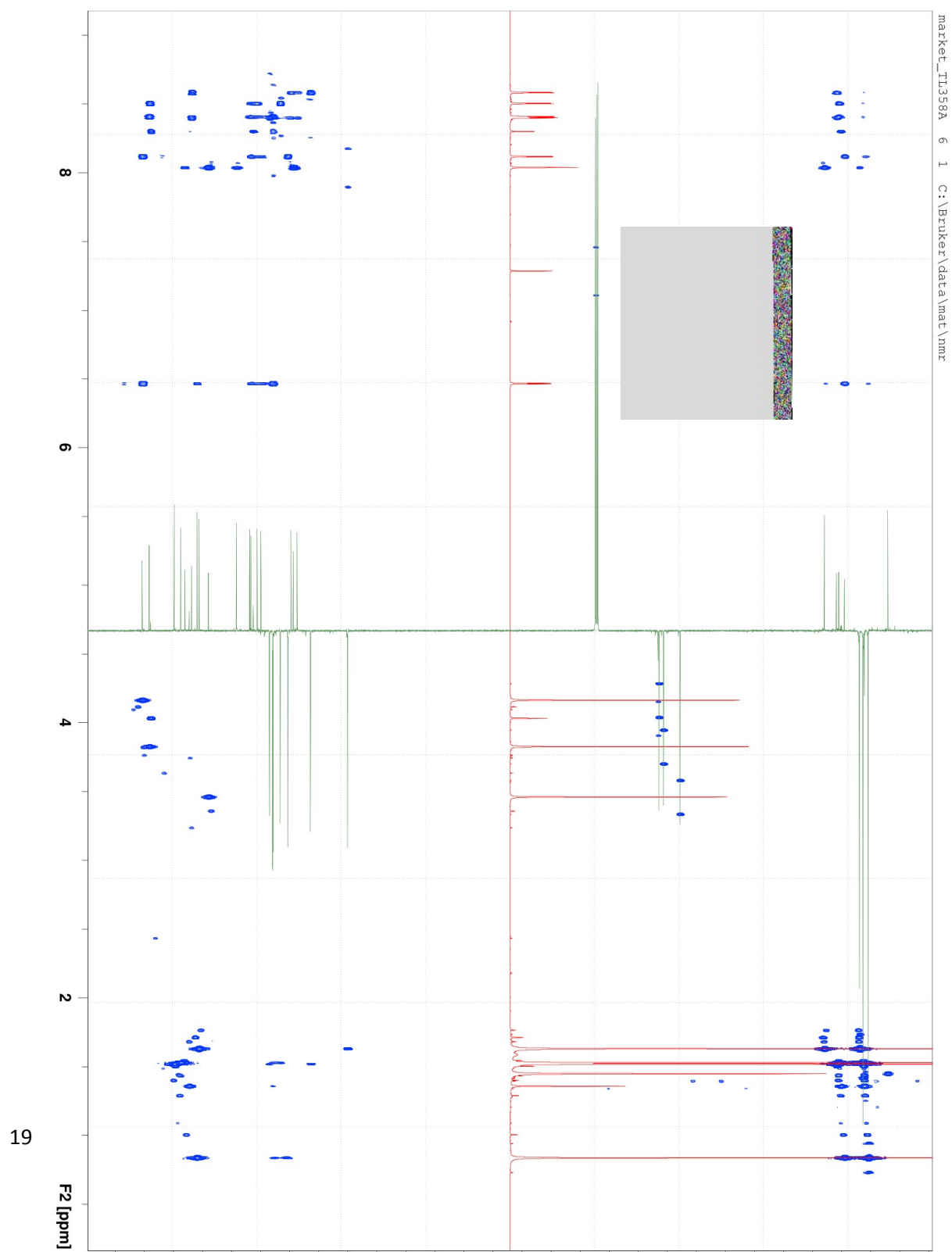
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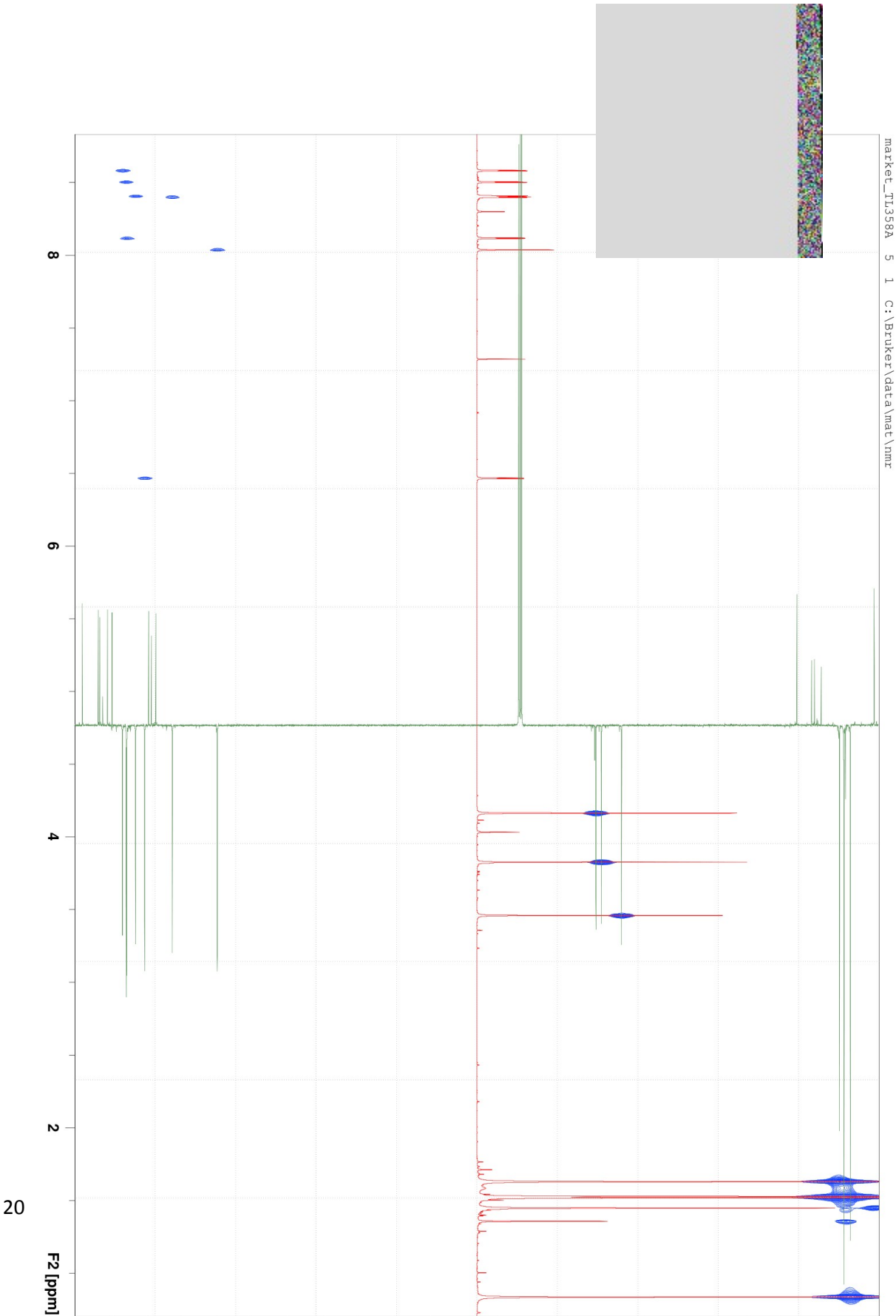
COSY spectrum of compound **6a** (CDCl₃, 298 K)



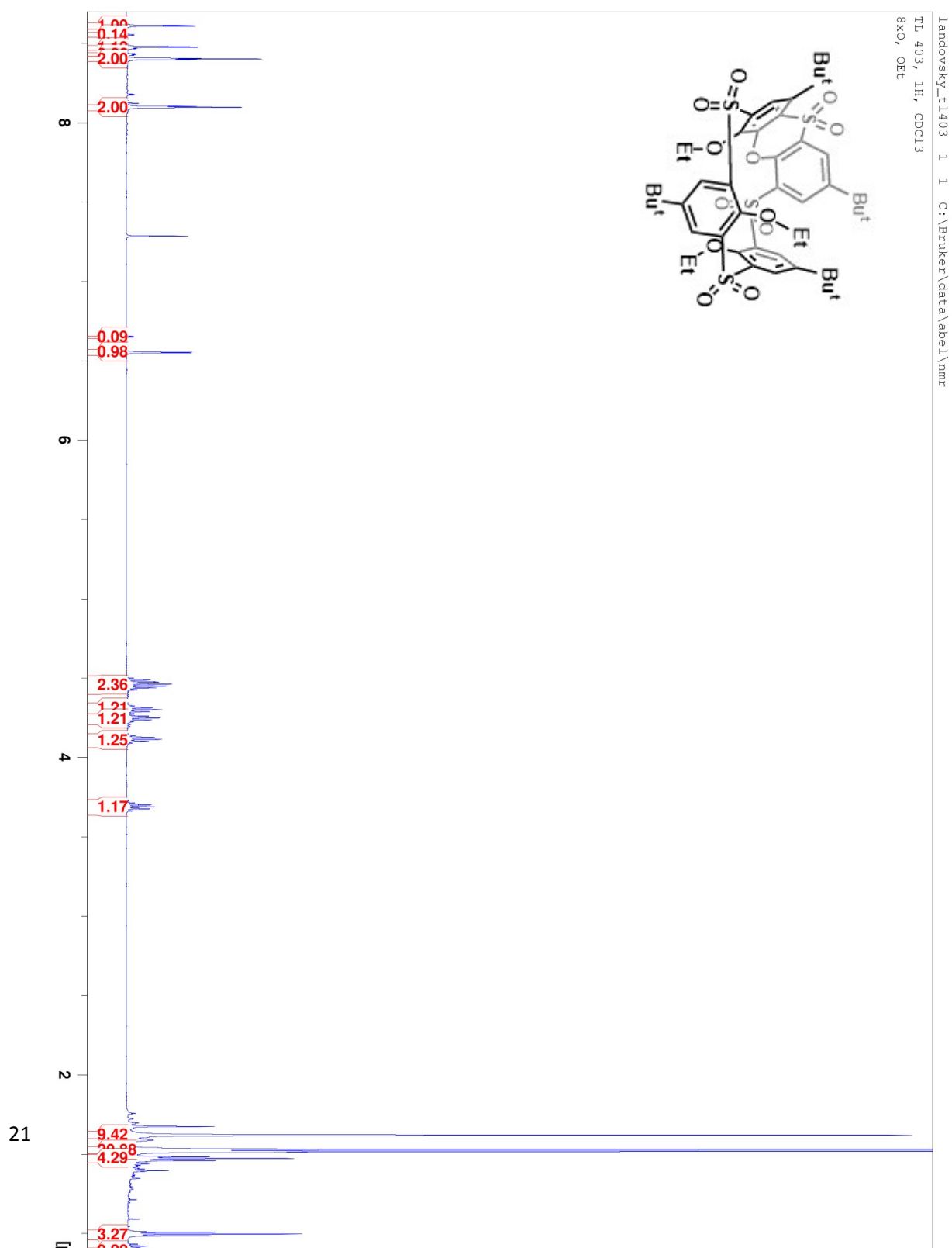
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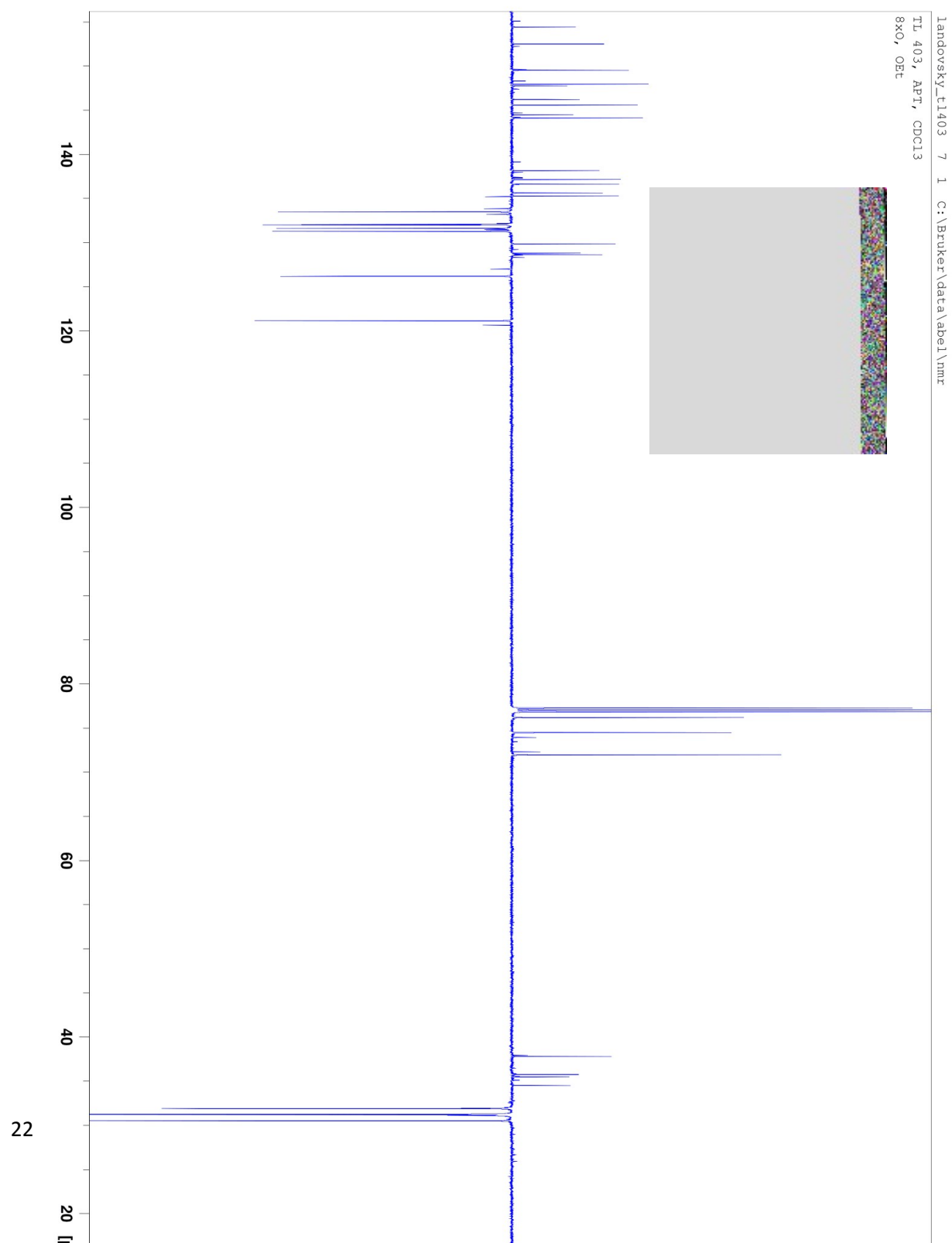
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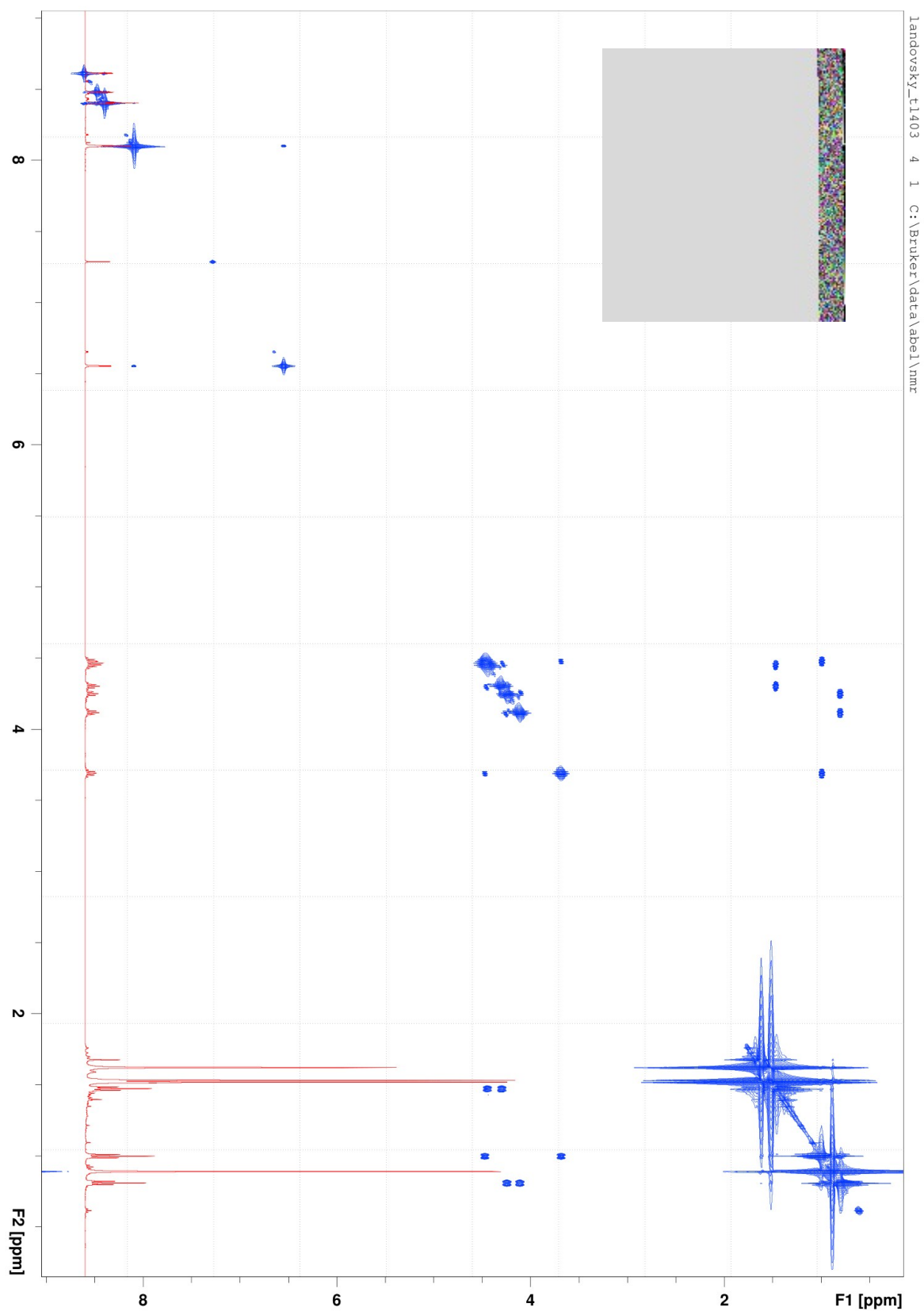
^1H NMR spectrum of compound **6b** (CDCl_3 , 298 K)



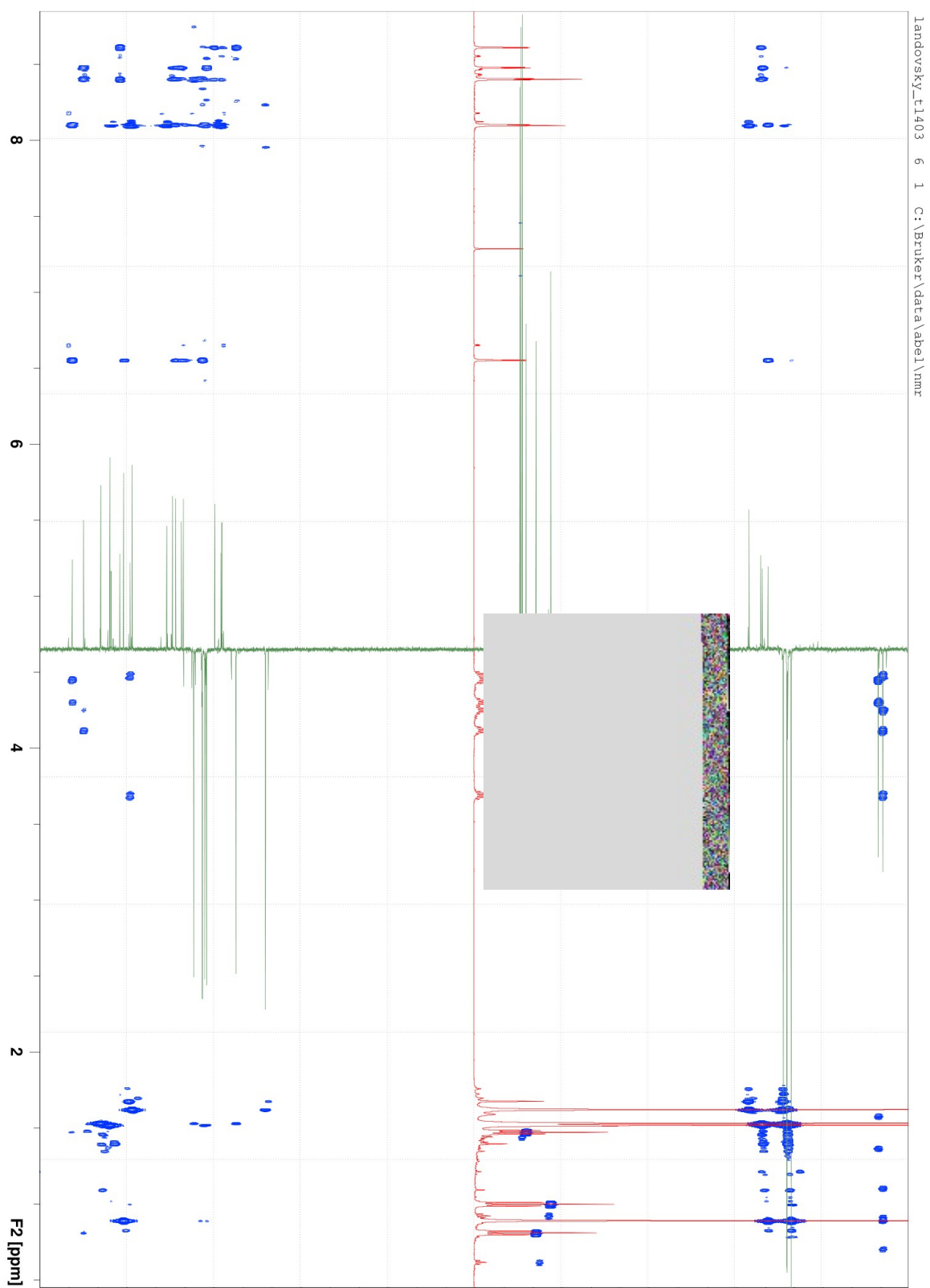
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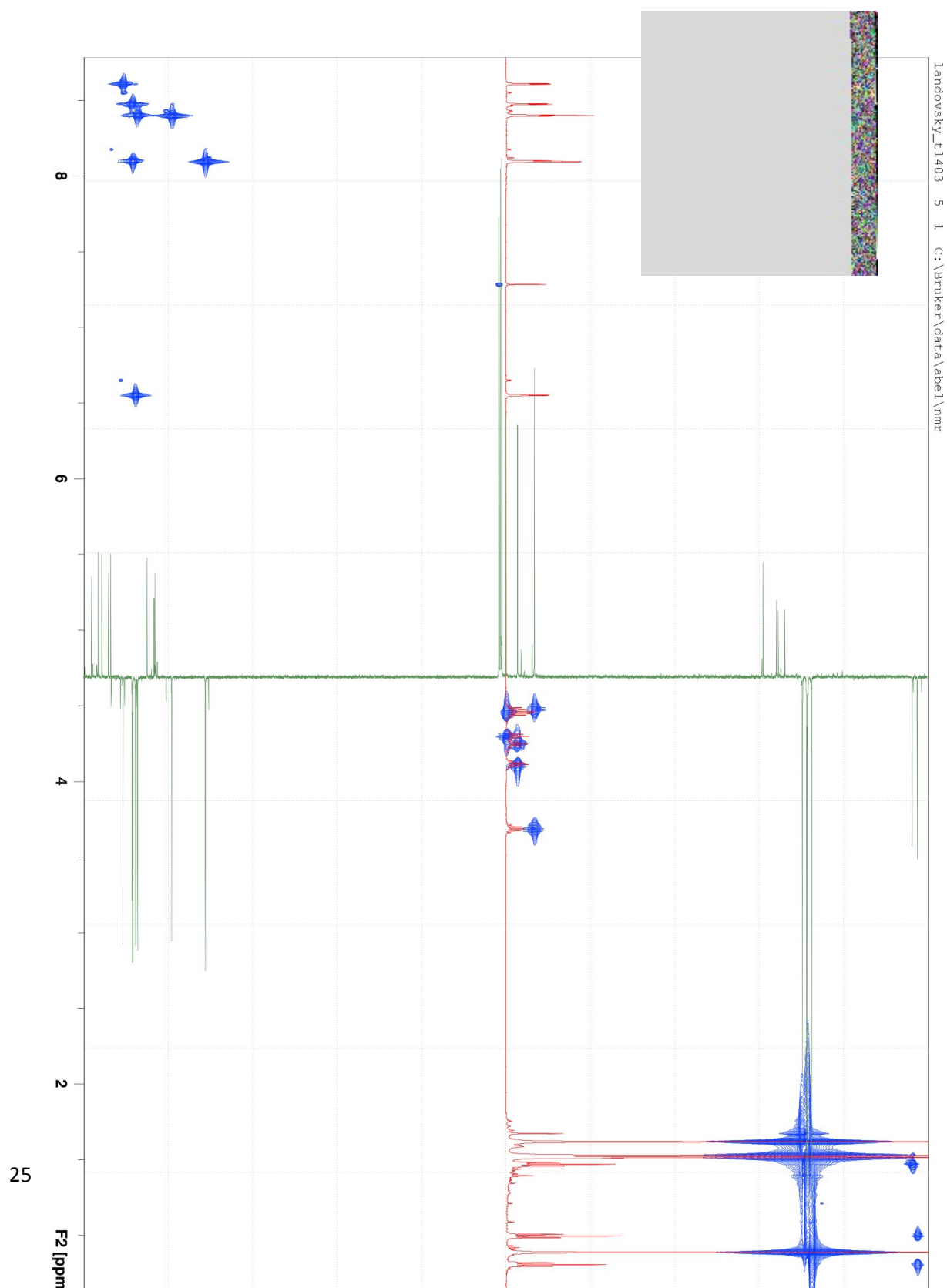
COSY spectrum of compound **6b** (CDCl₃, 298 K)



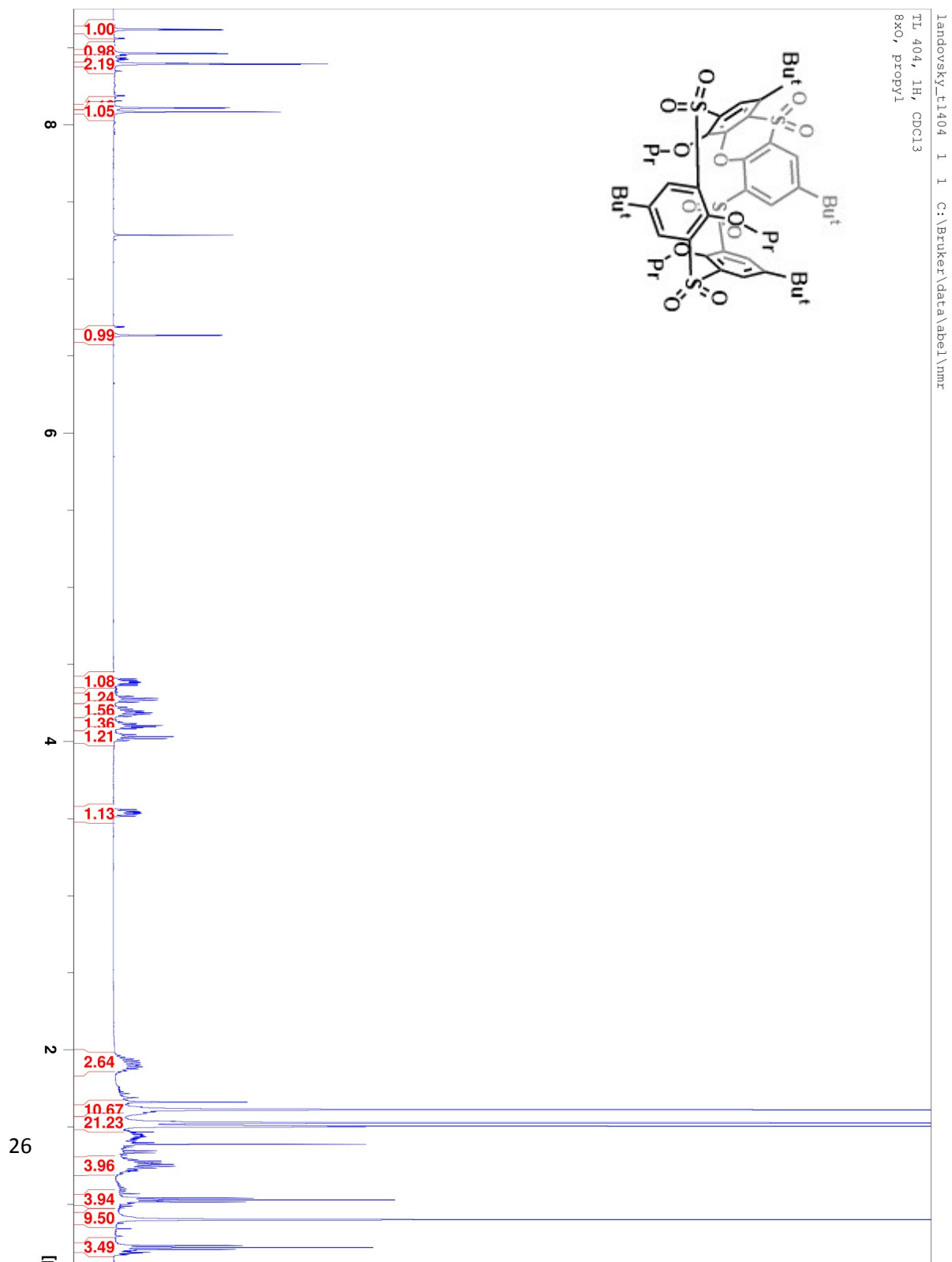
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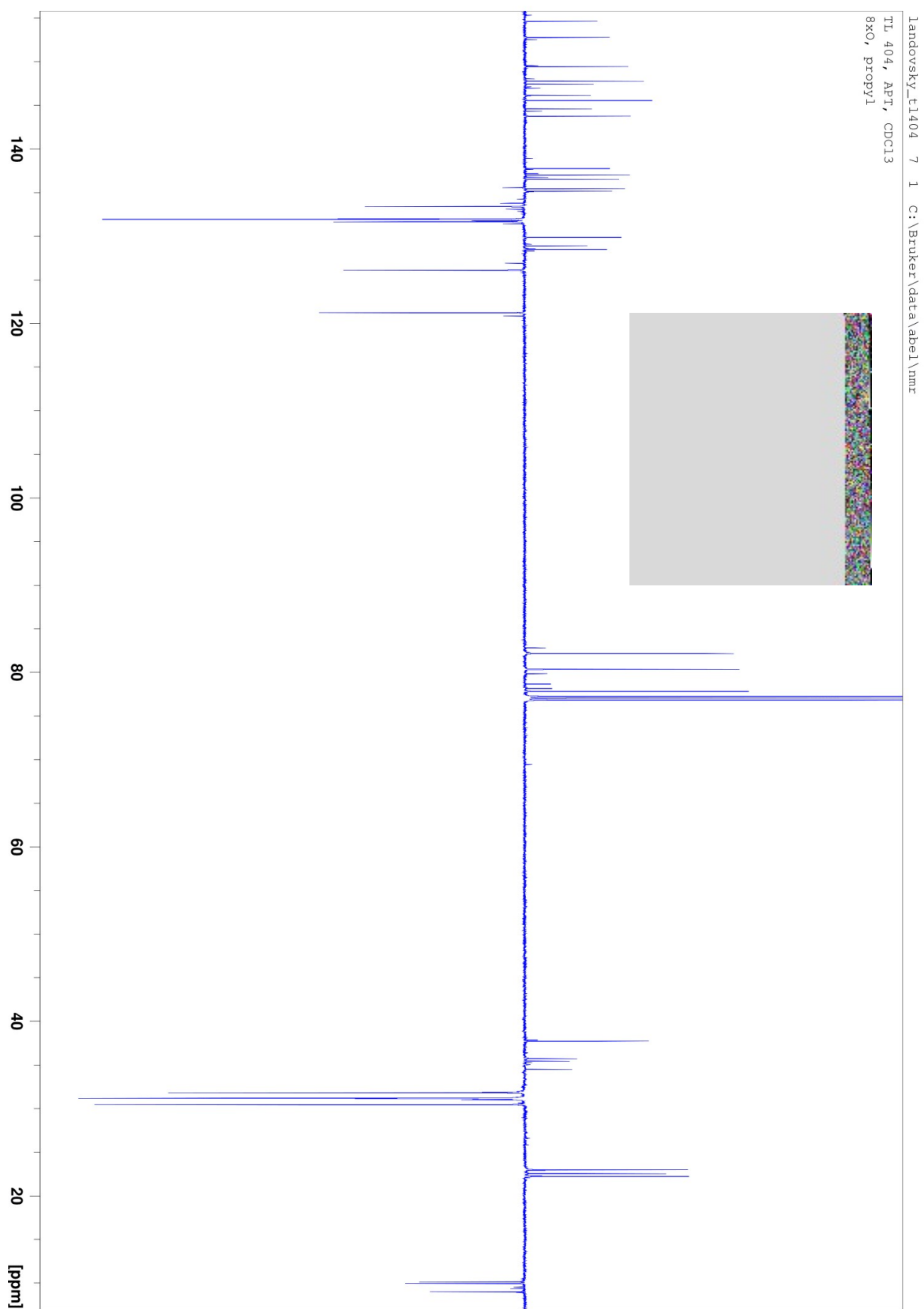
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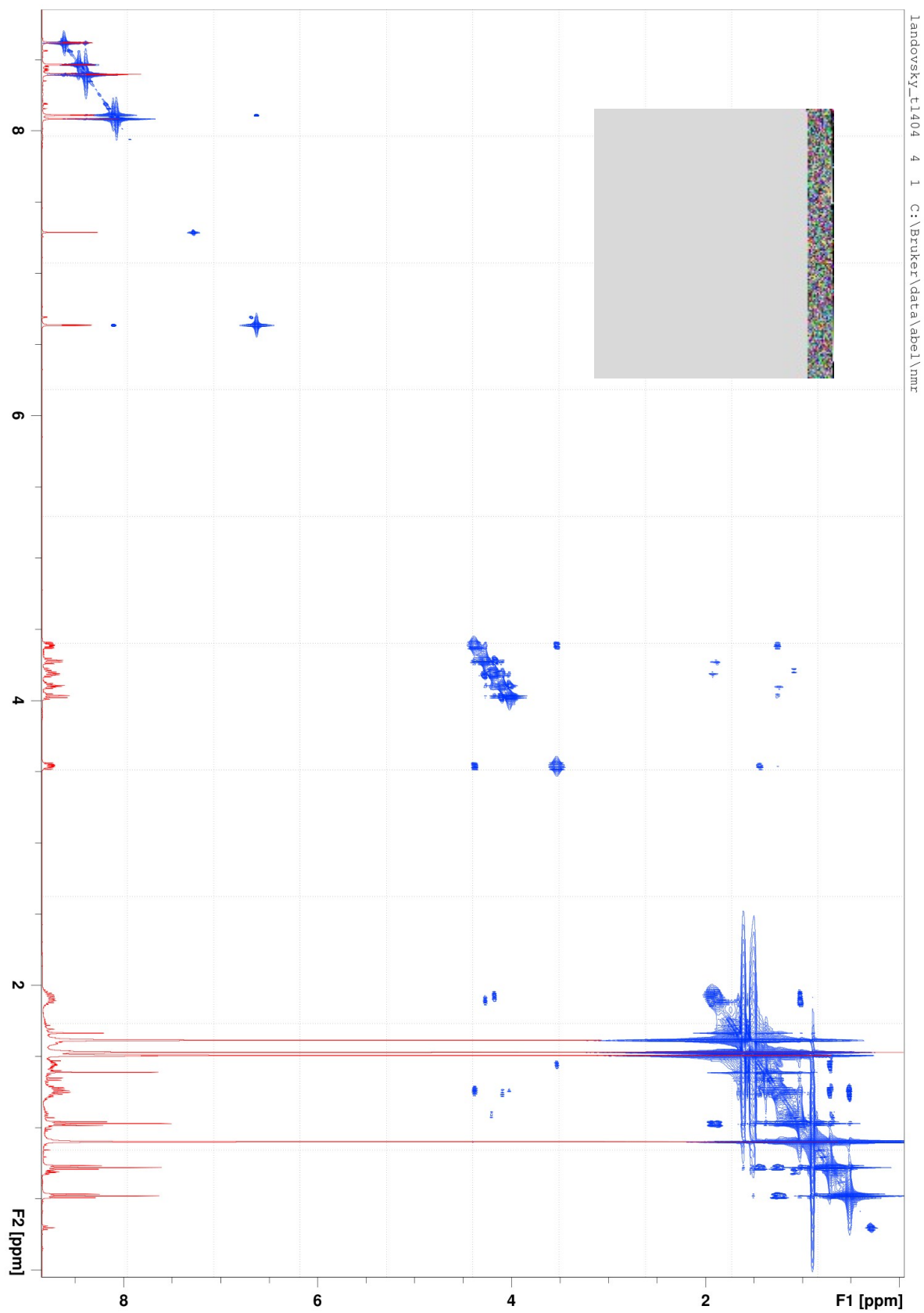
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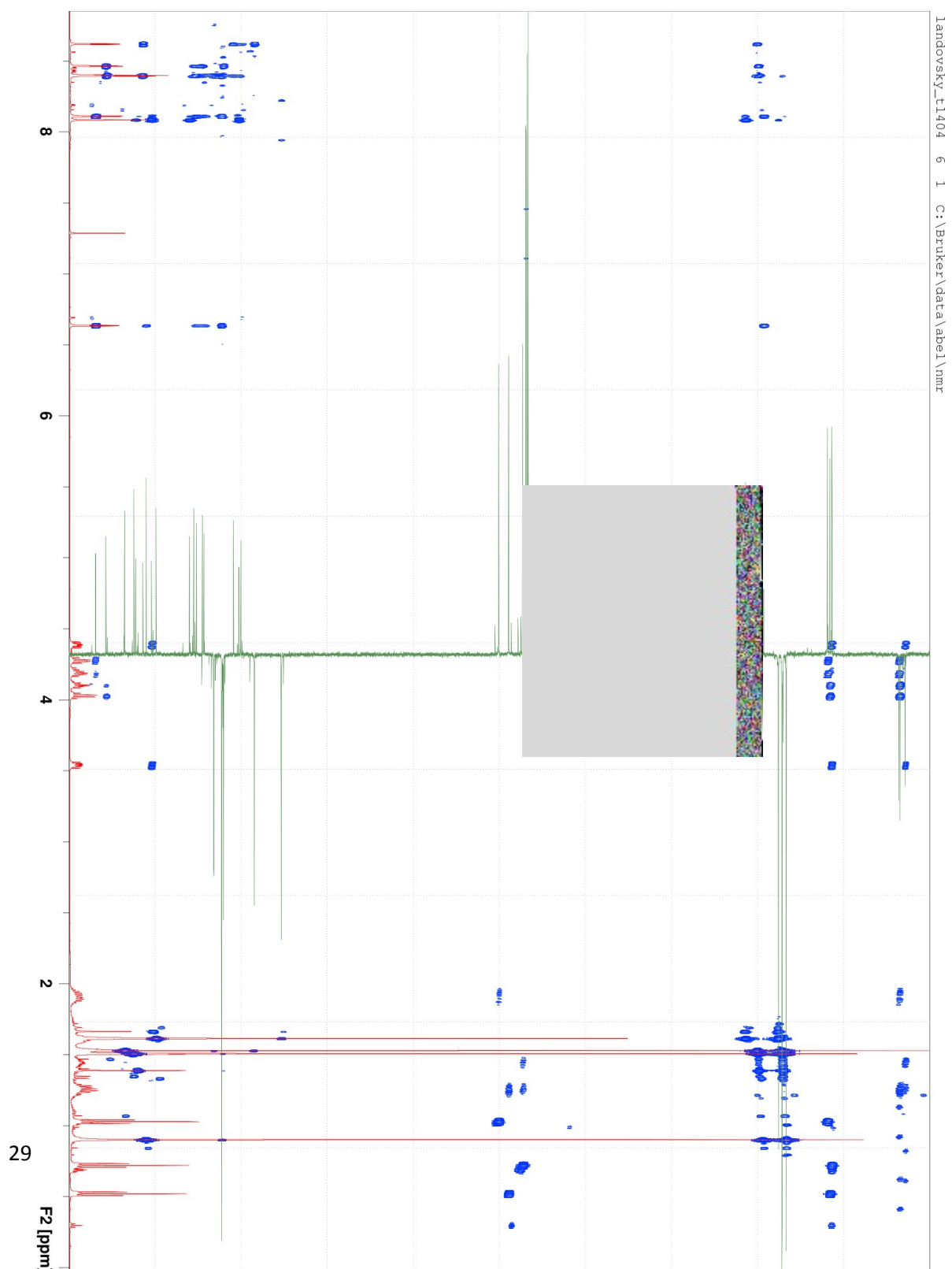
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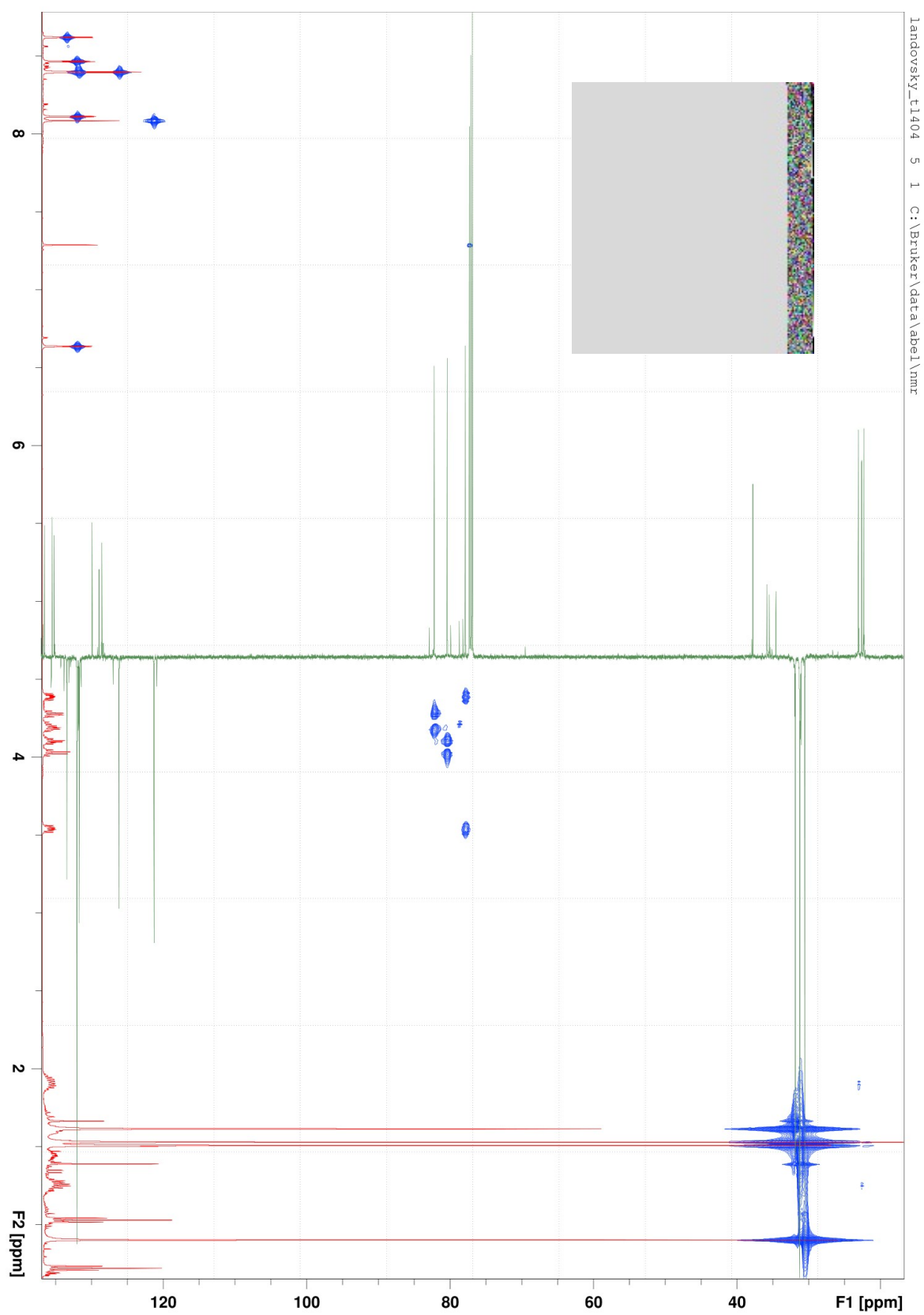
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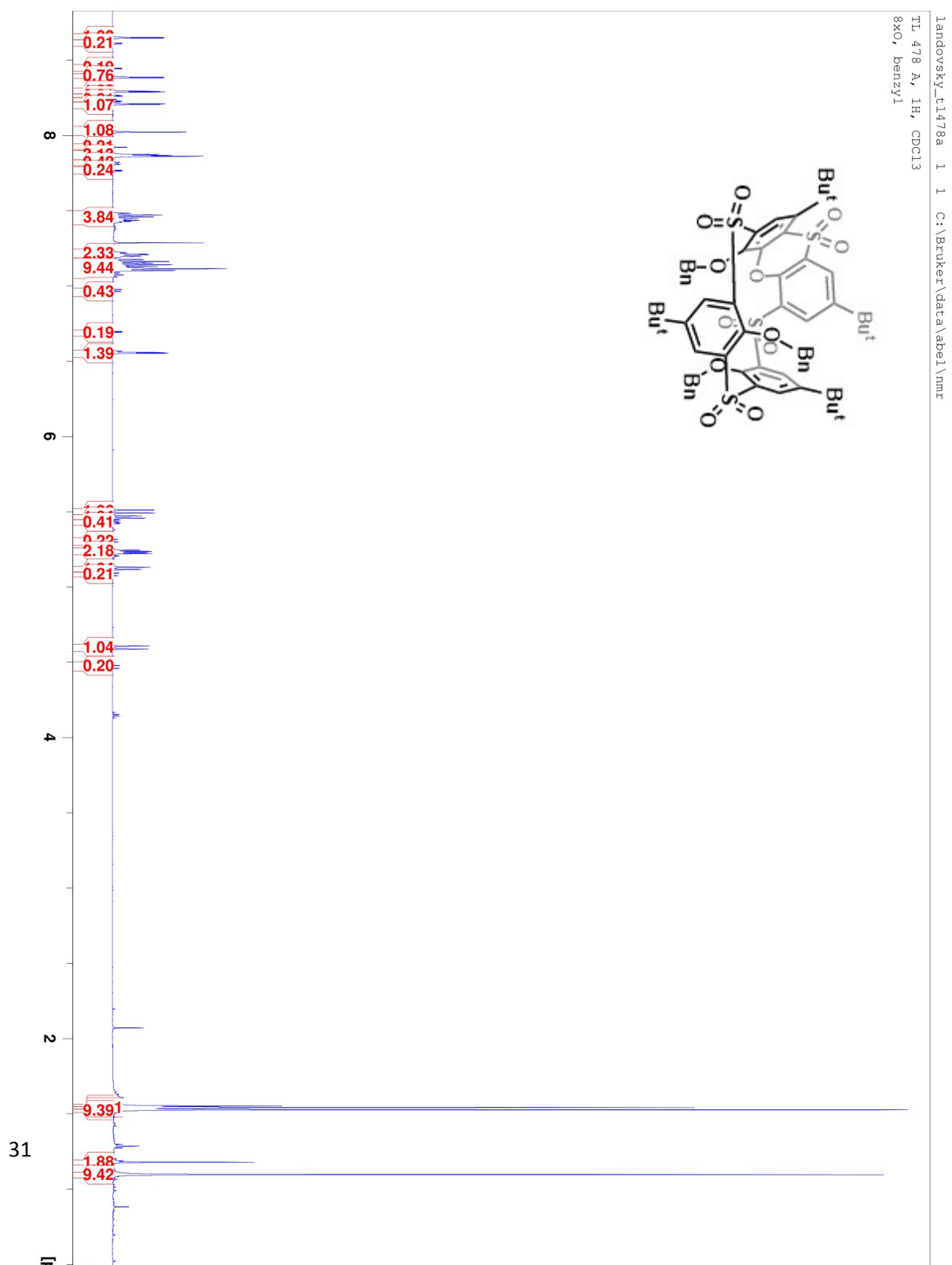
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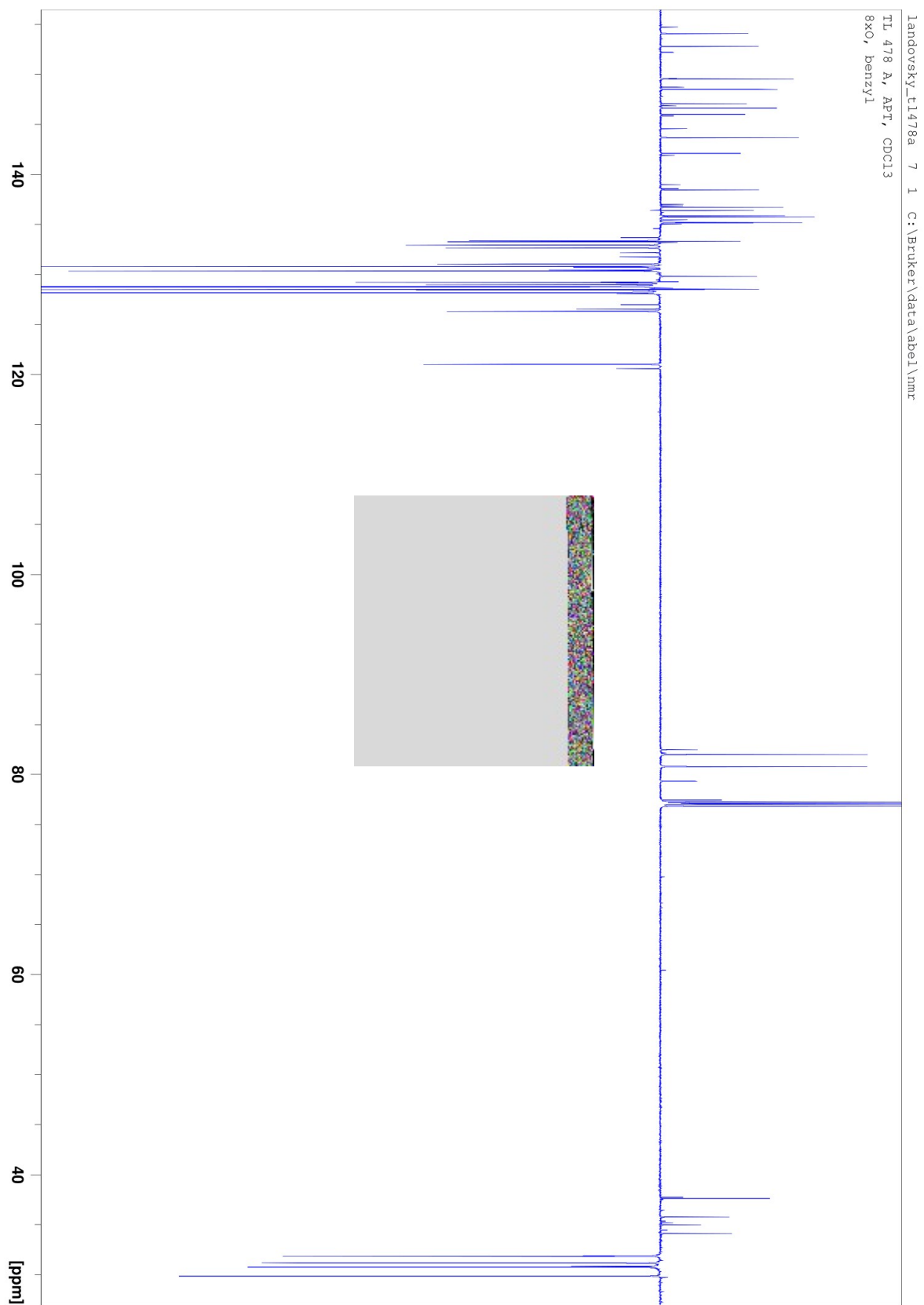
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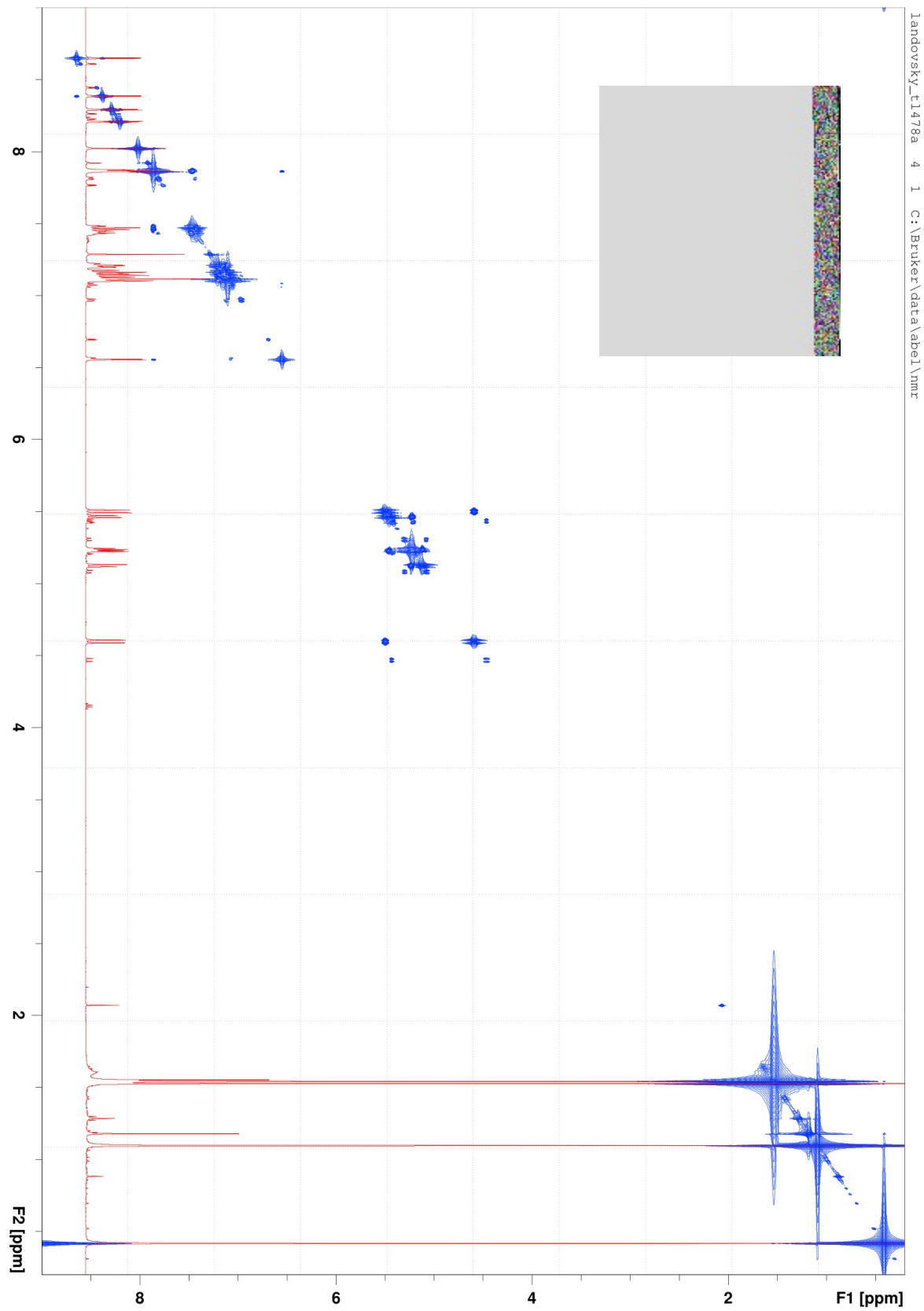
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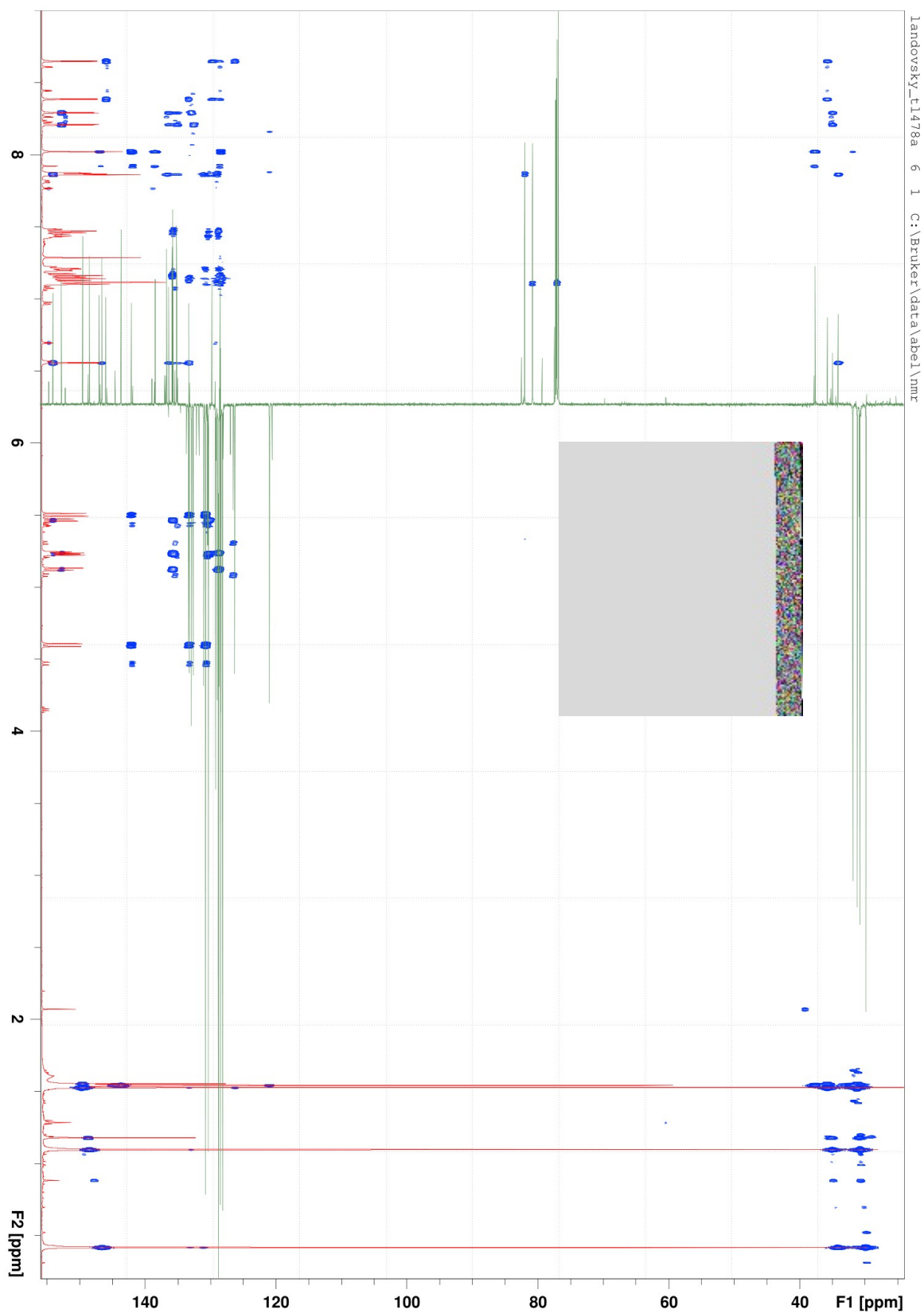
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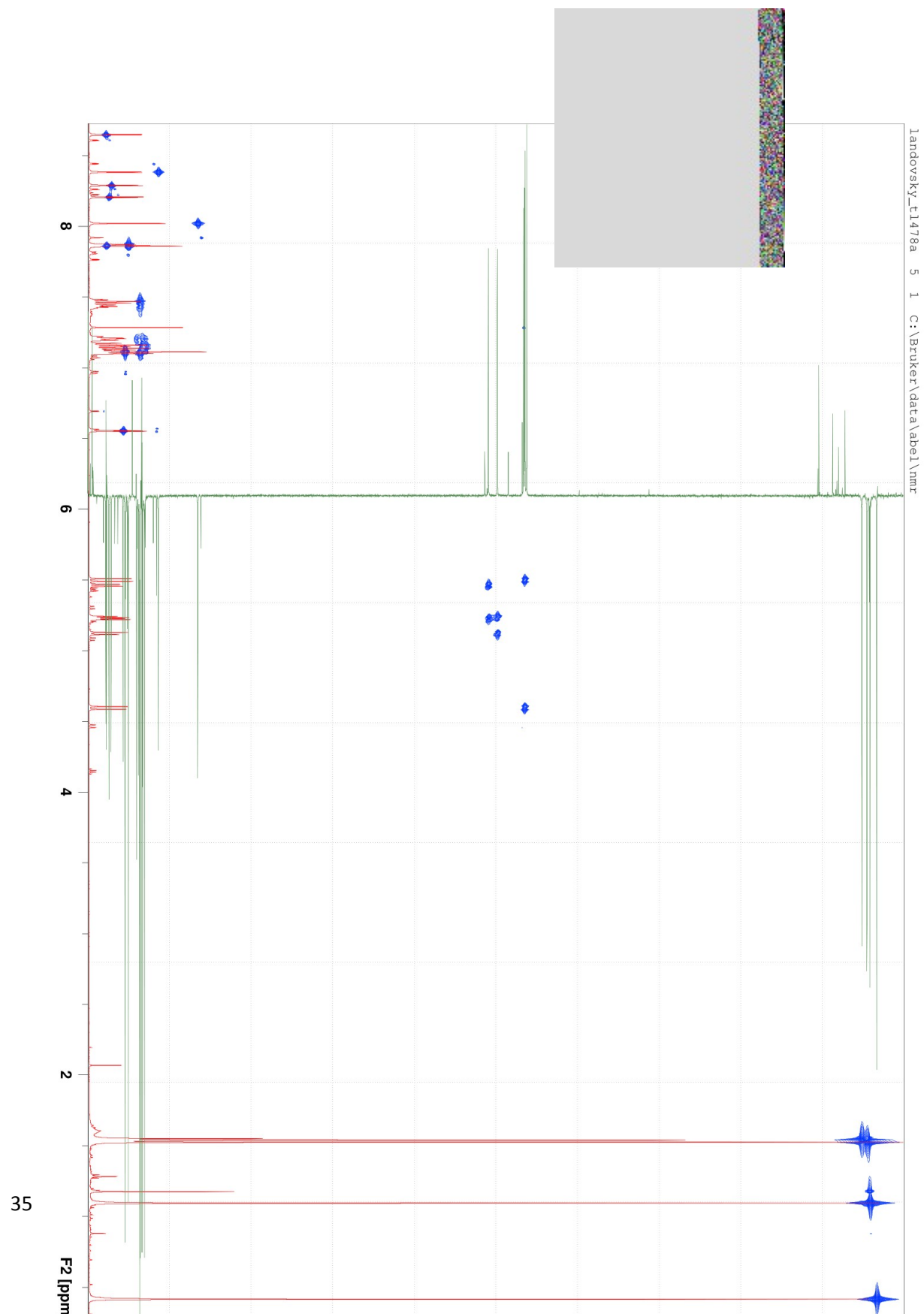
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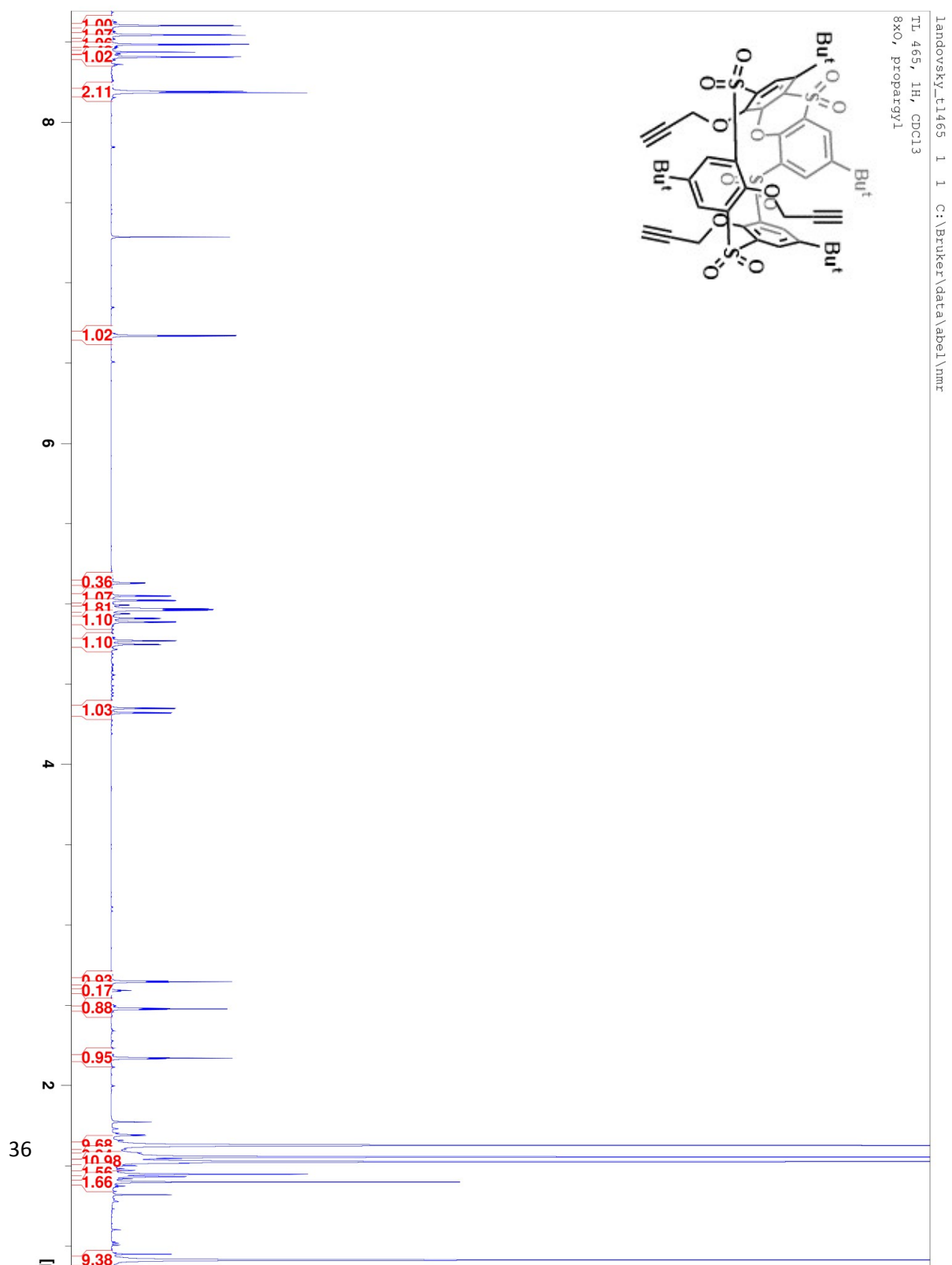
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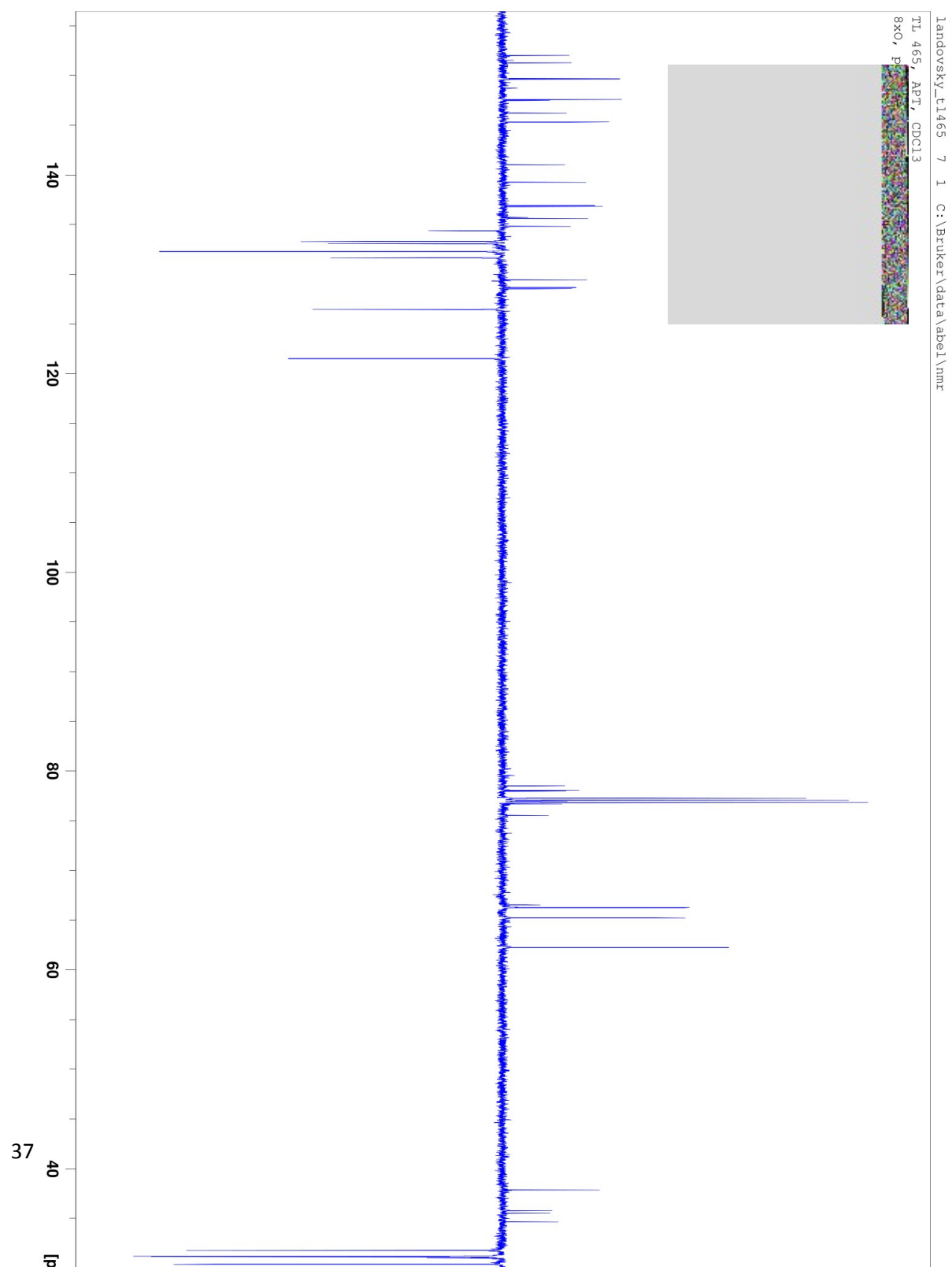
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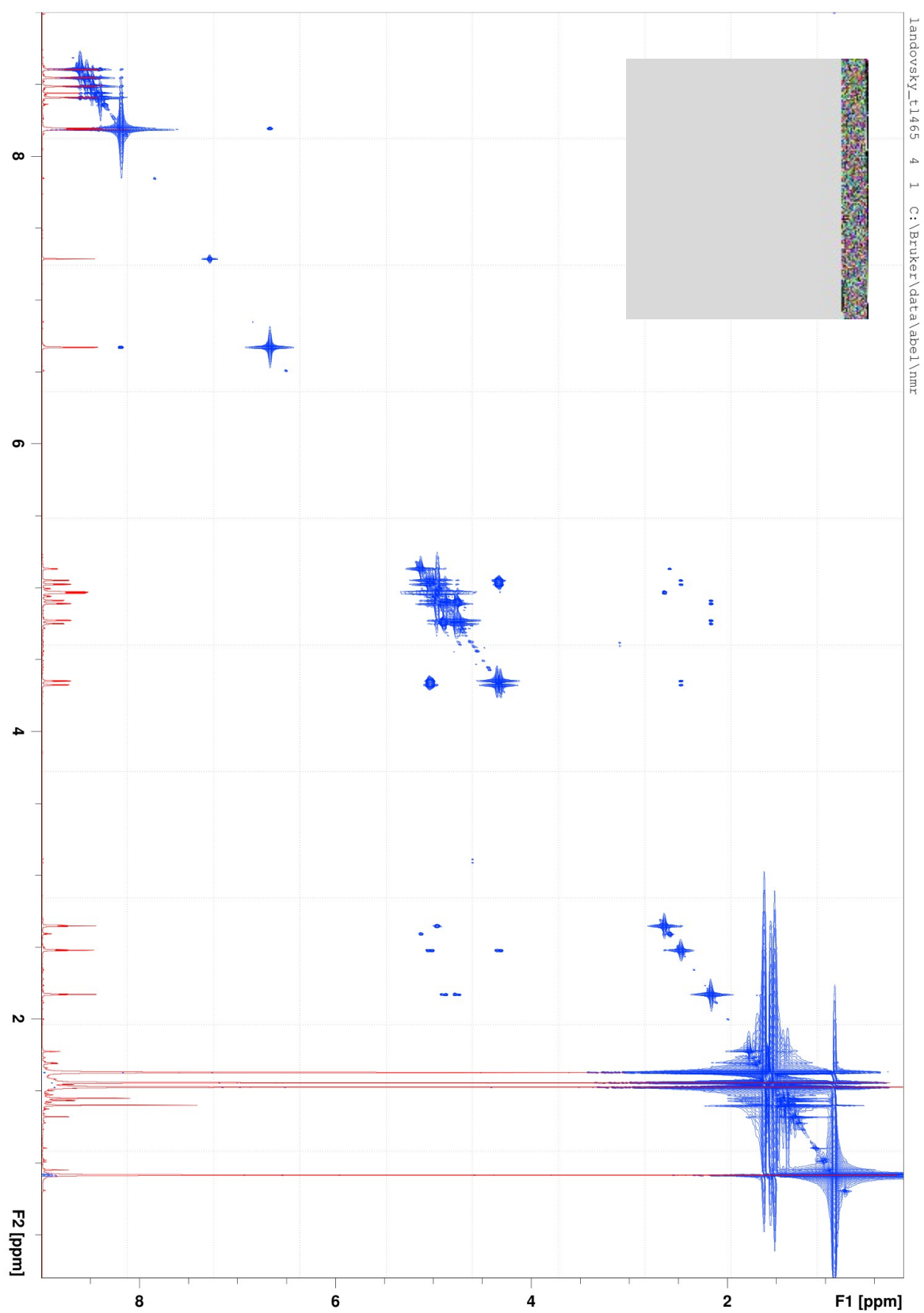
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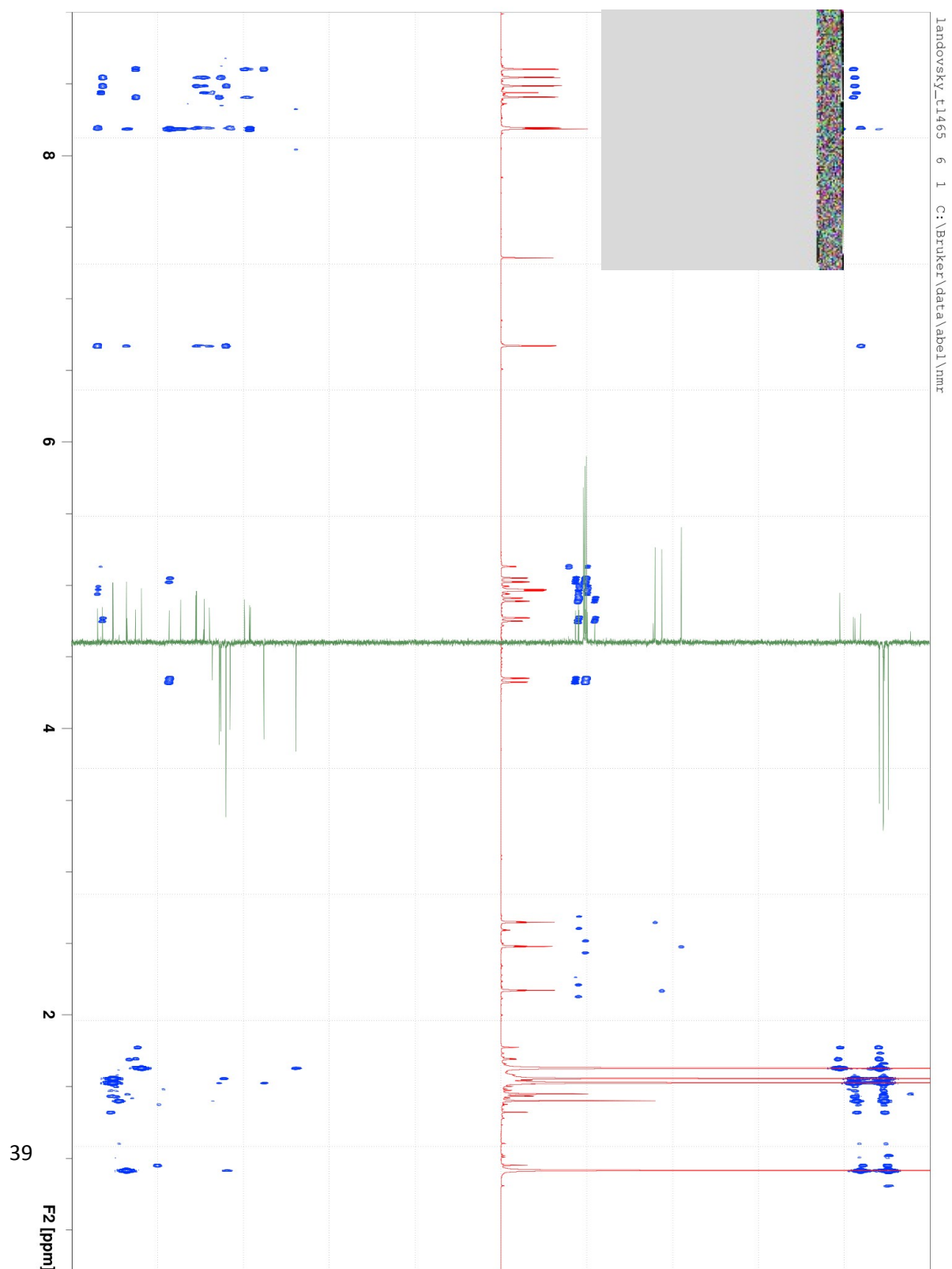
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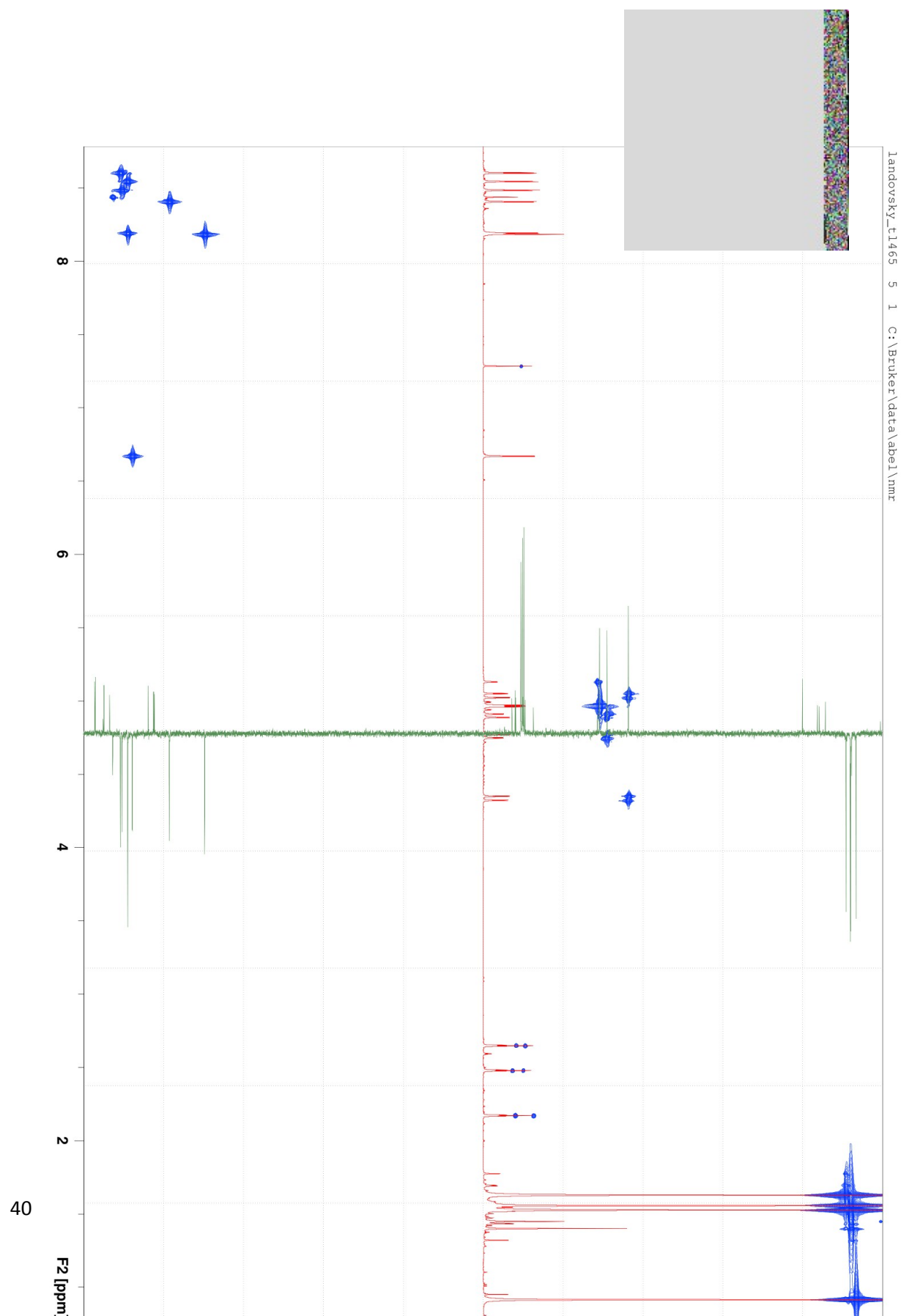
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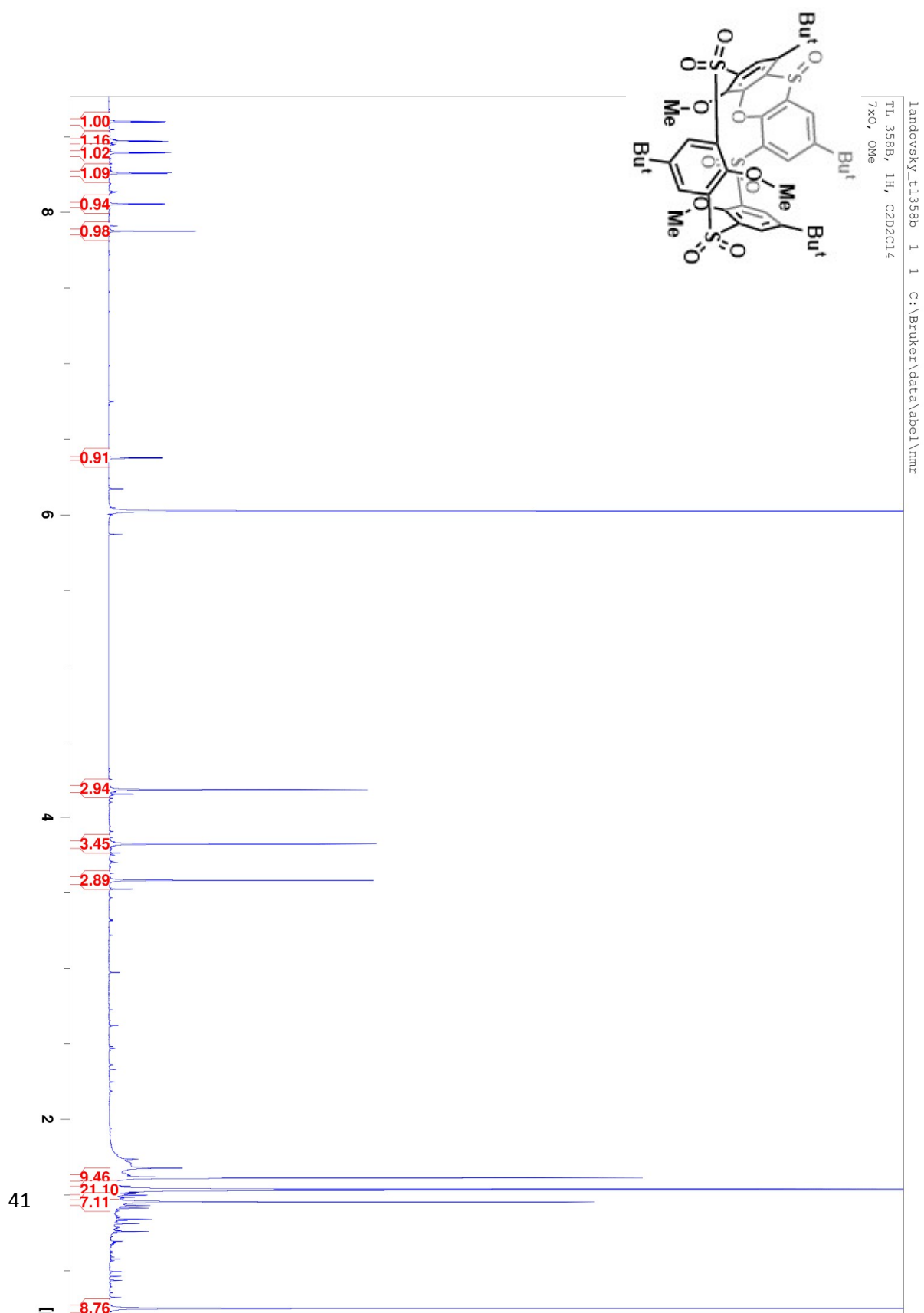
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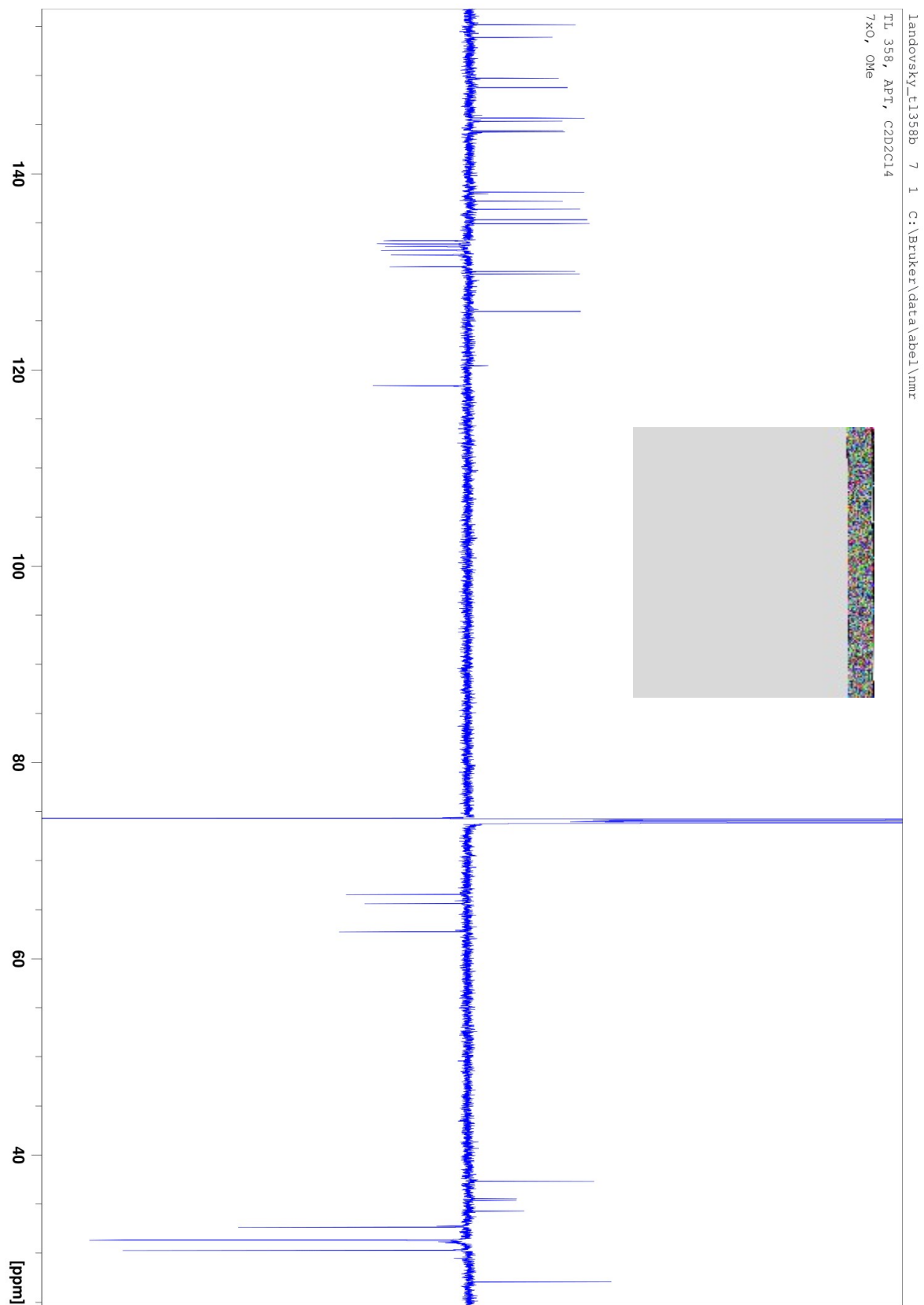
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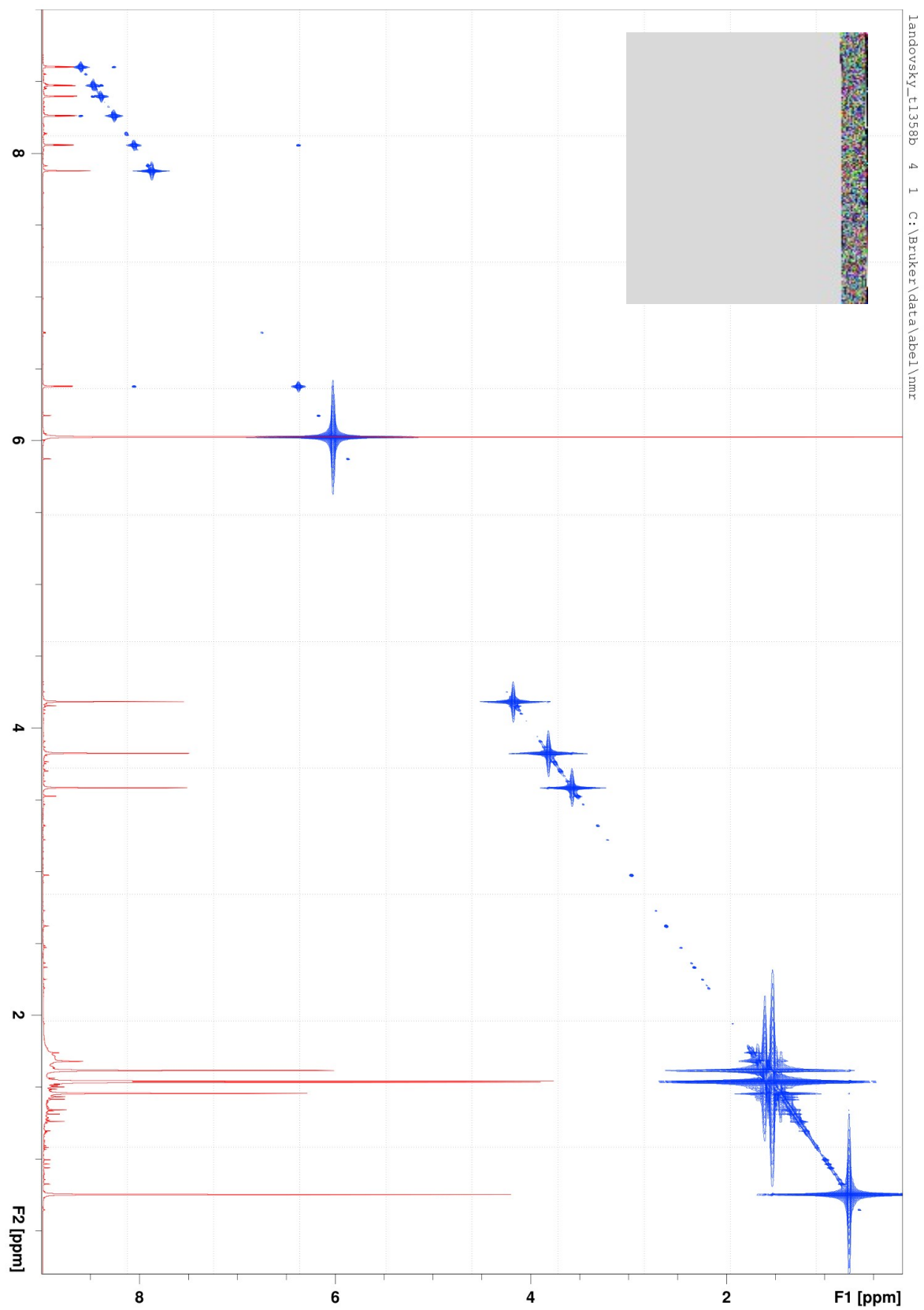
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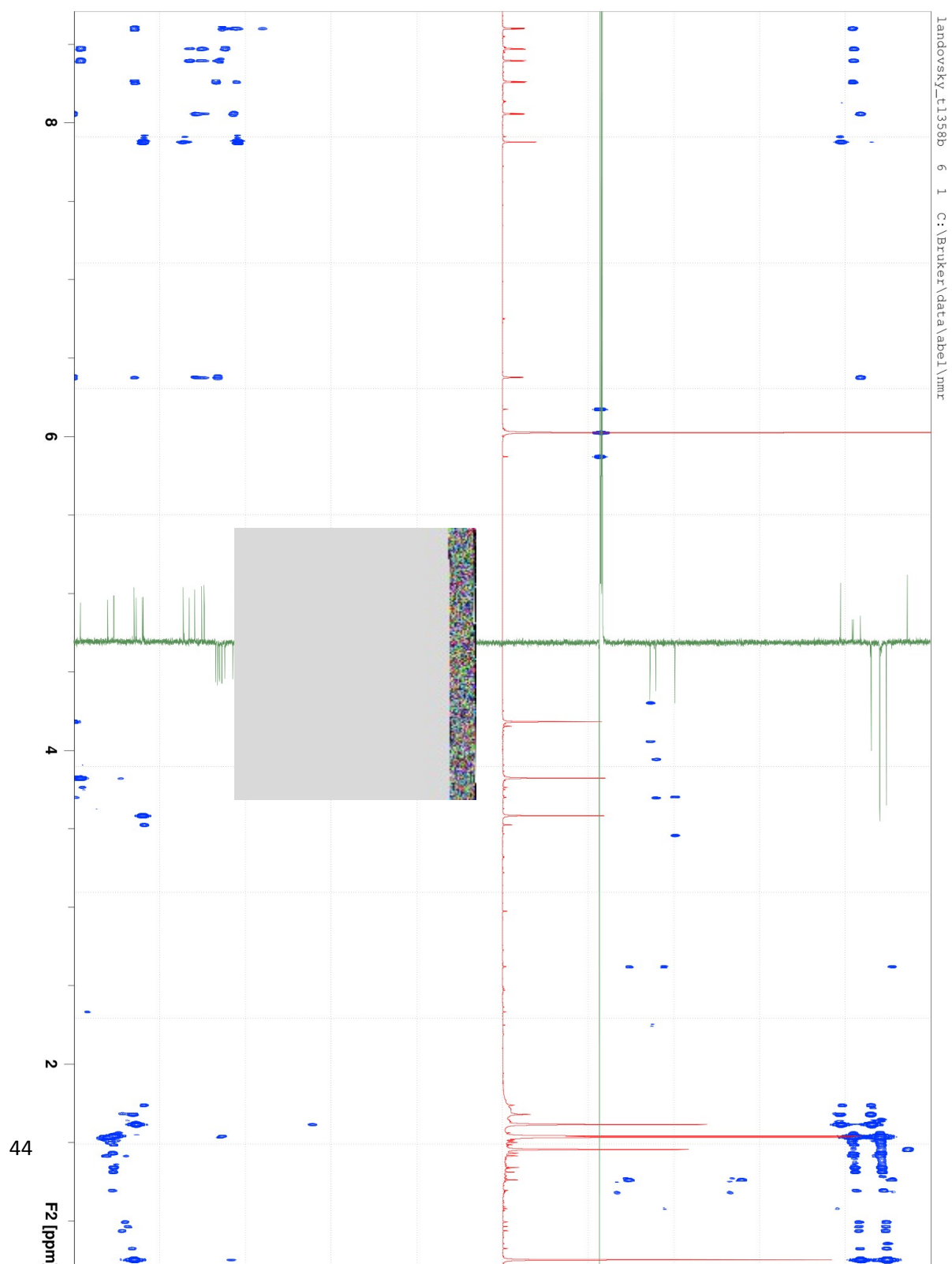
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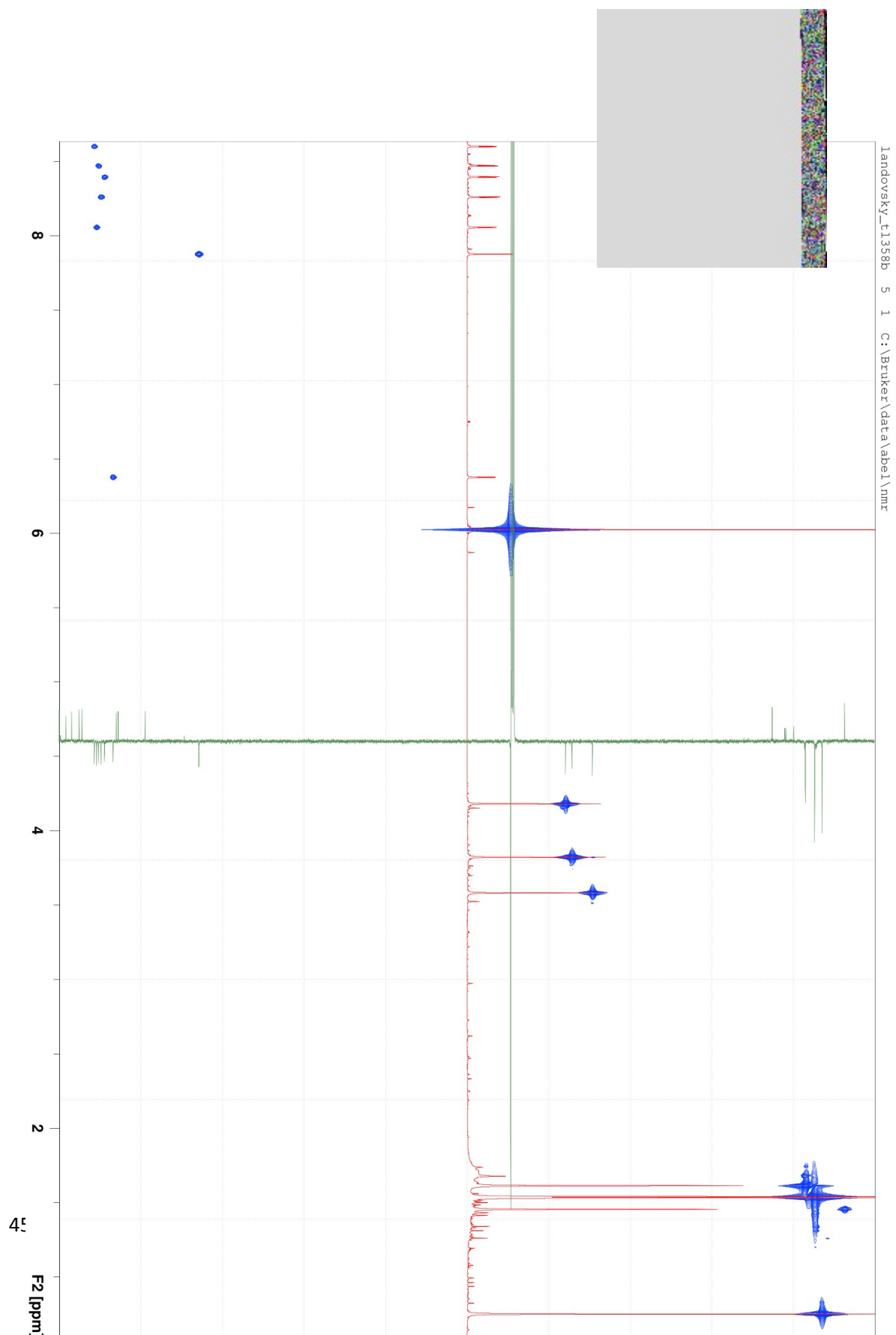
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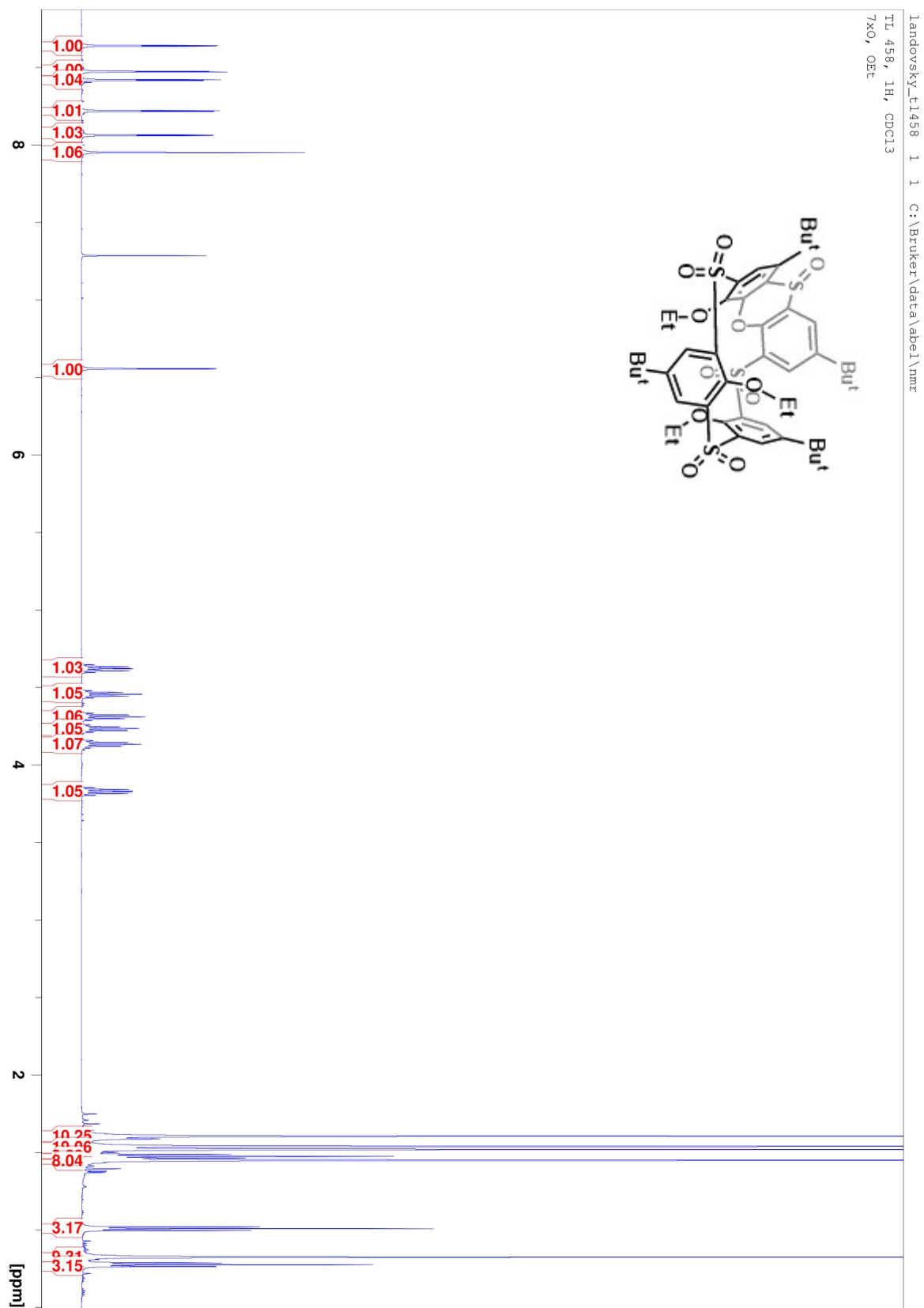
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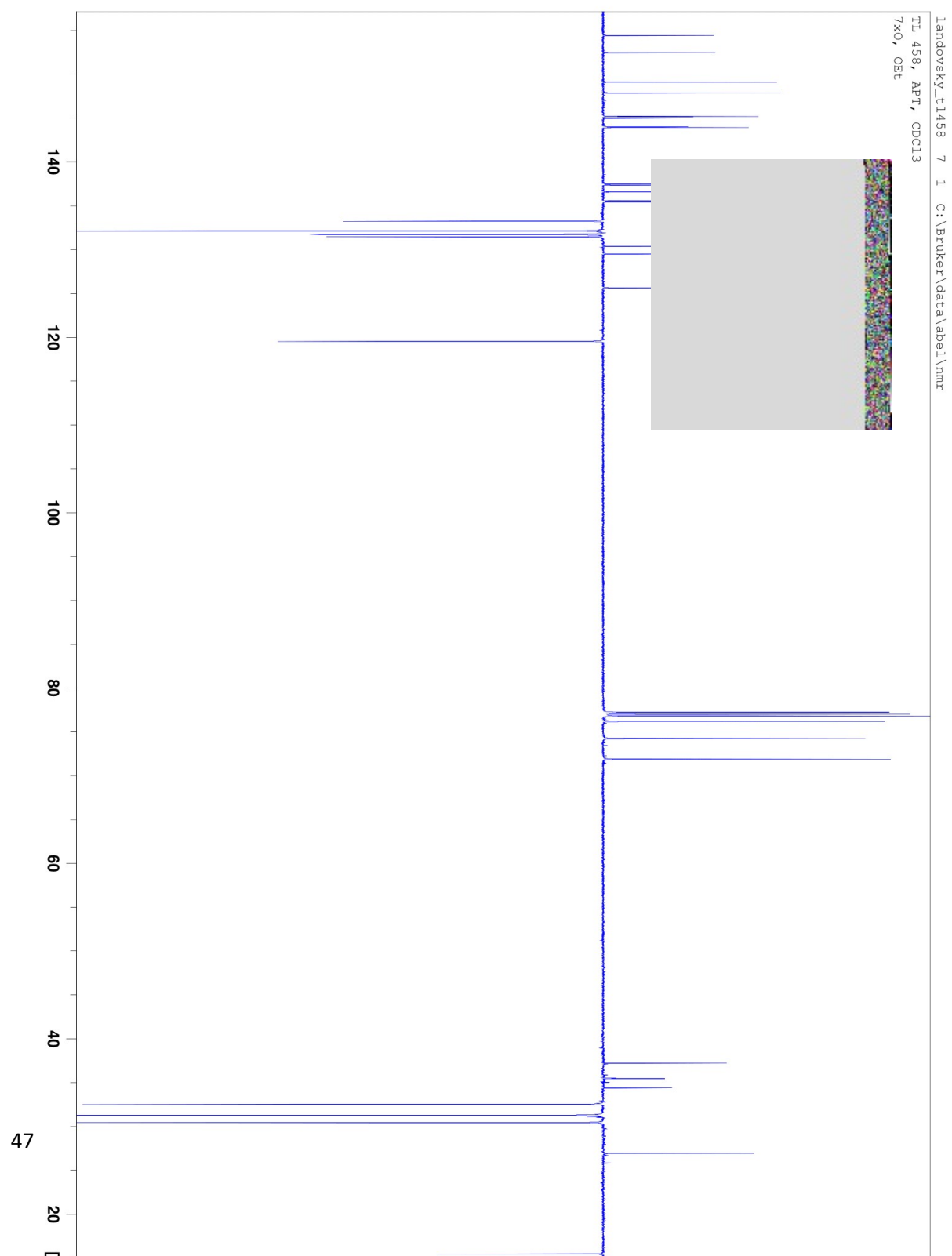
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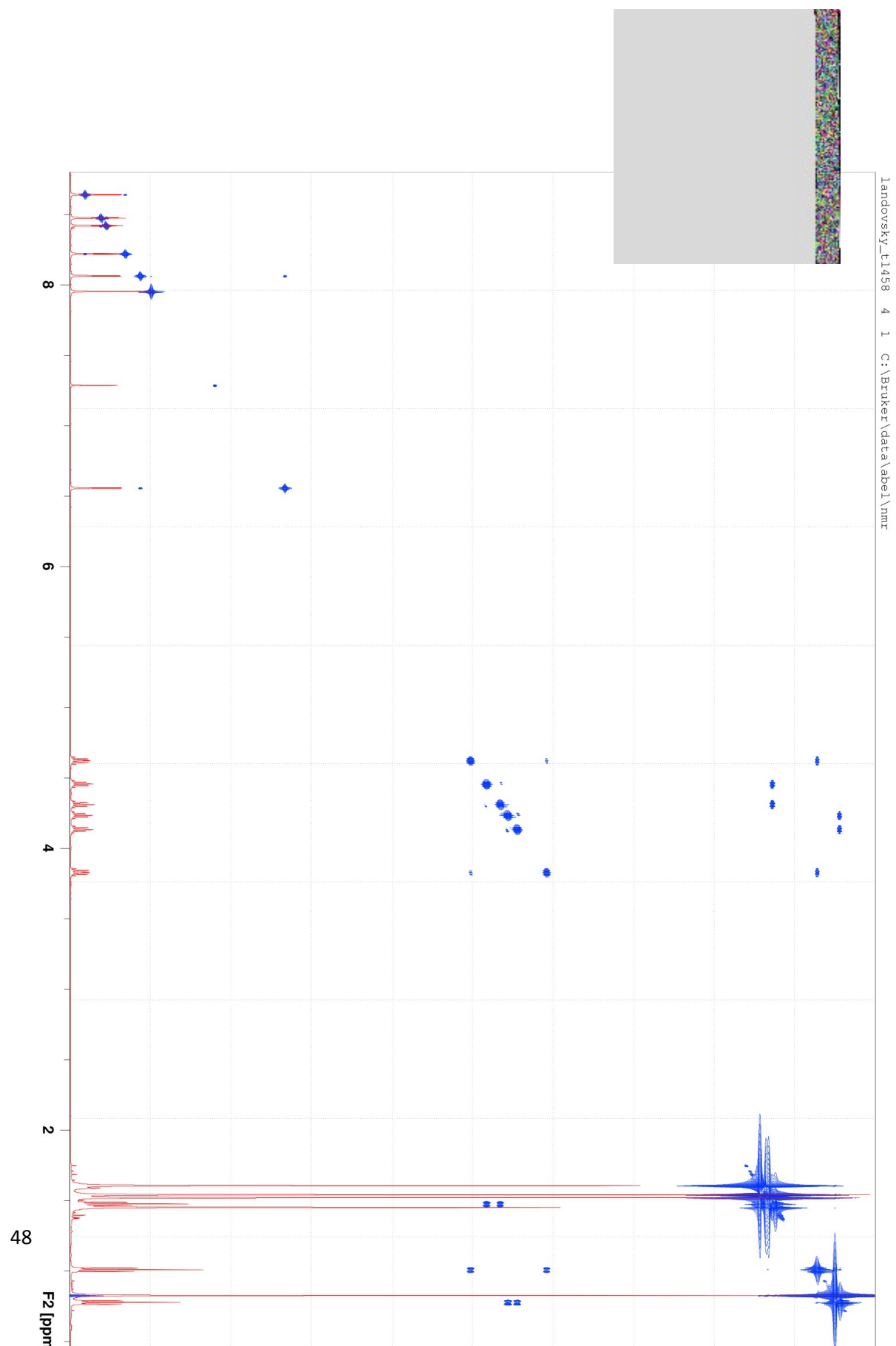
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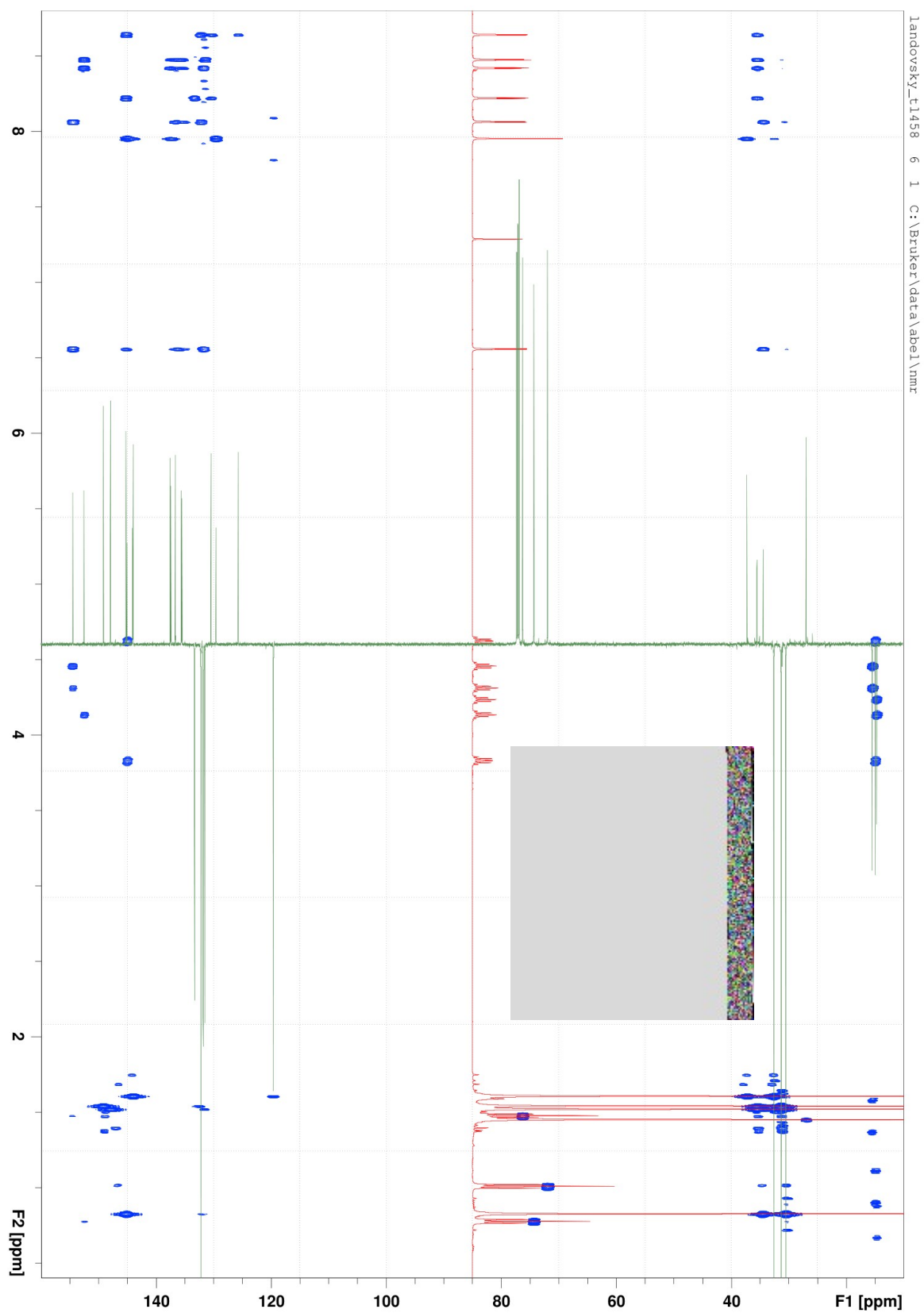
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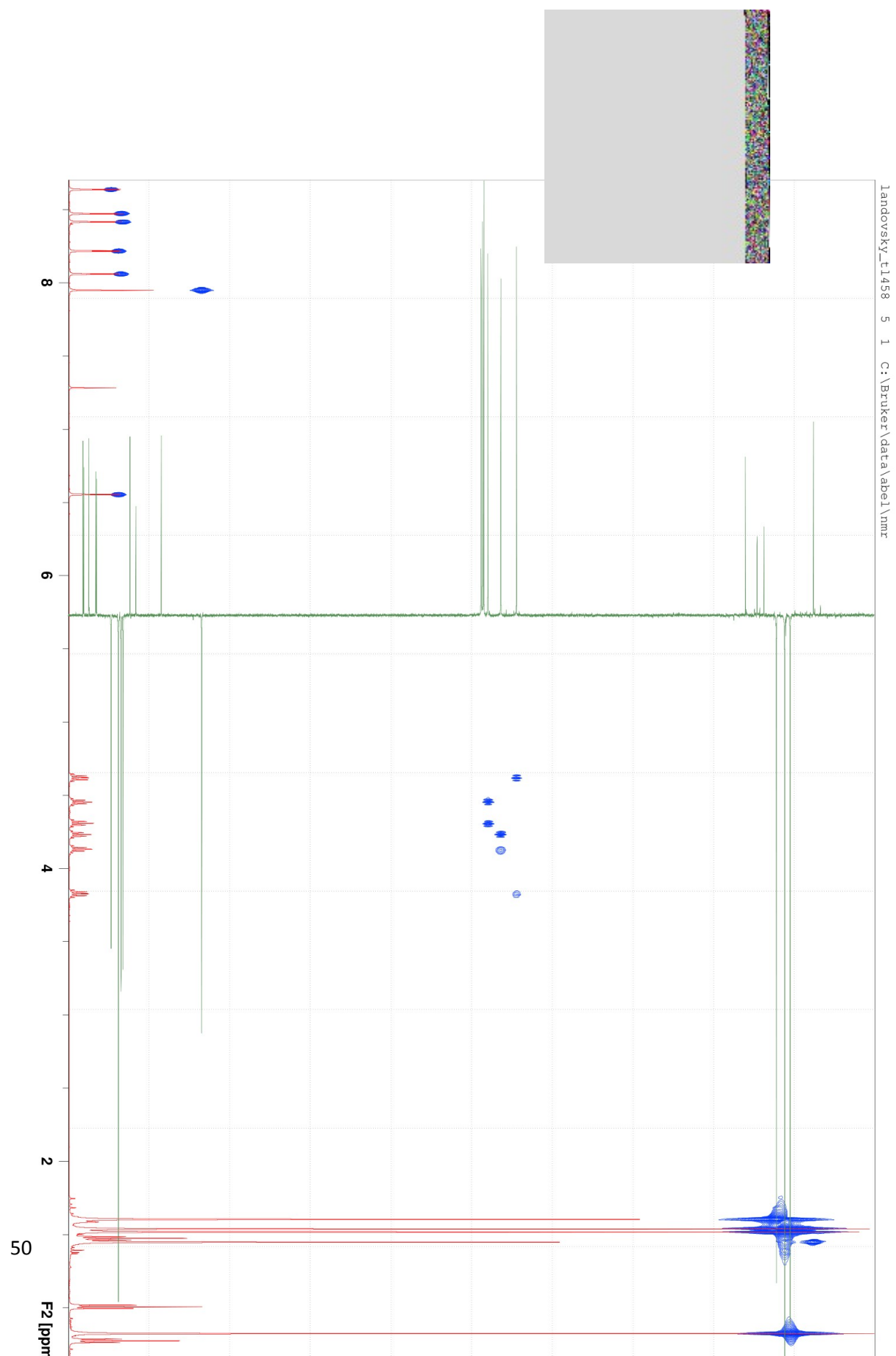
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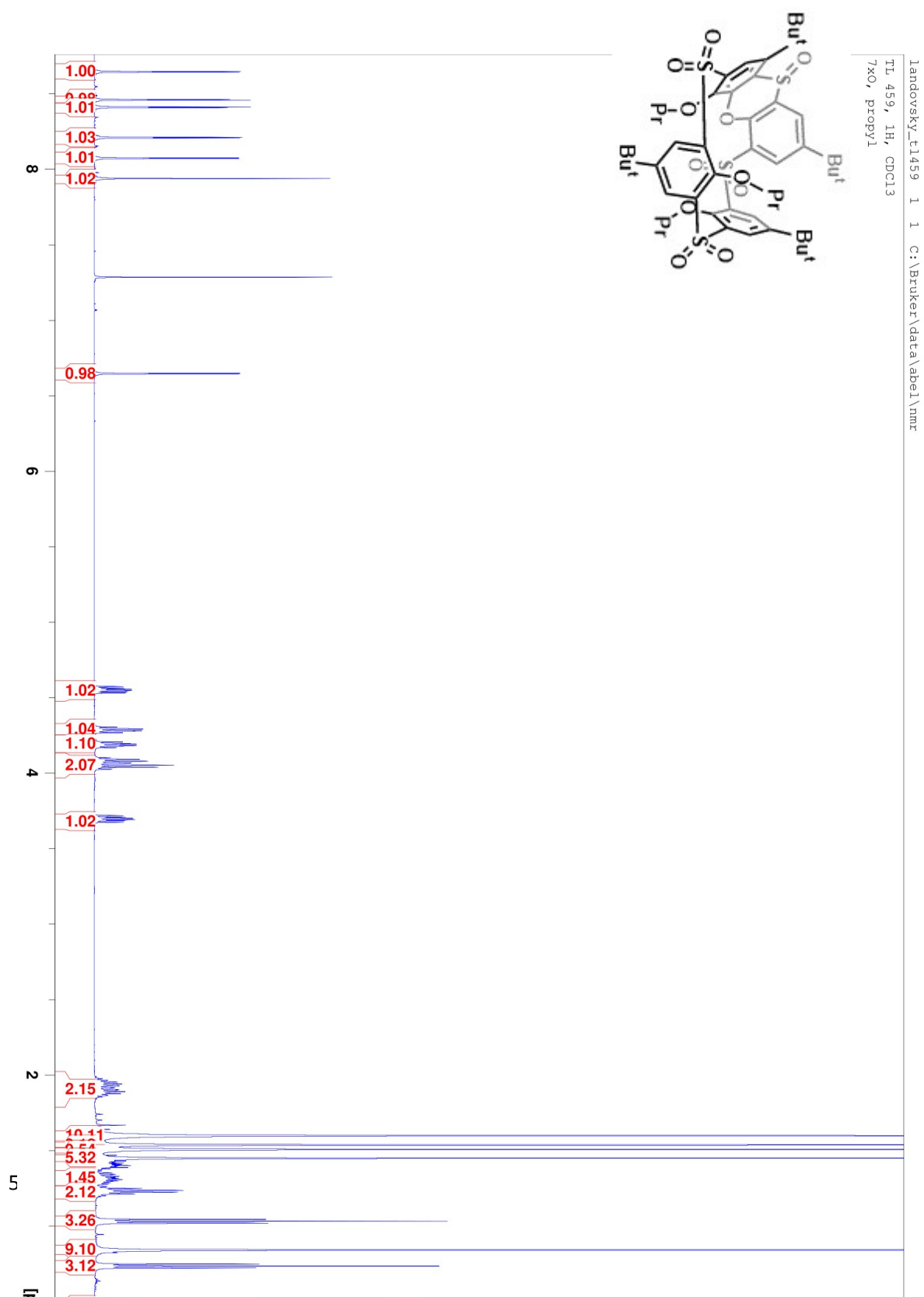
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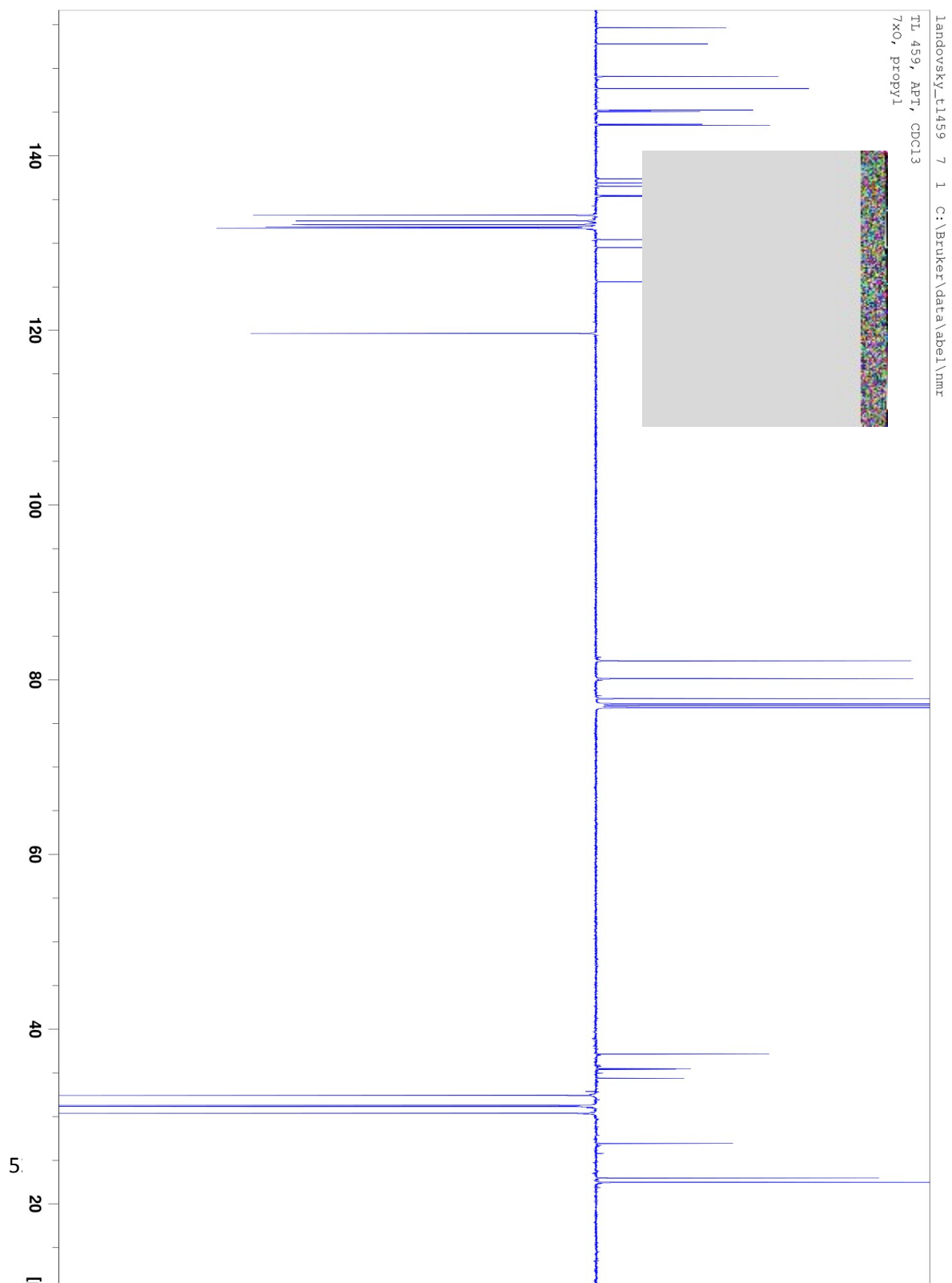
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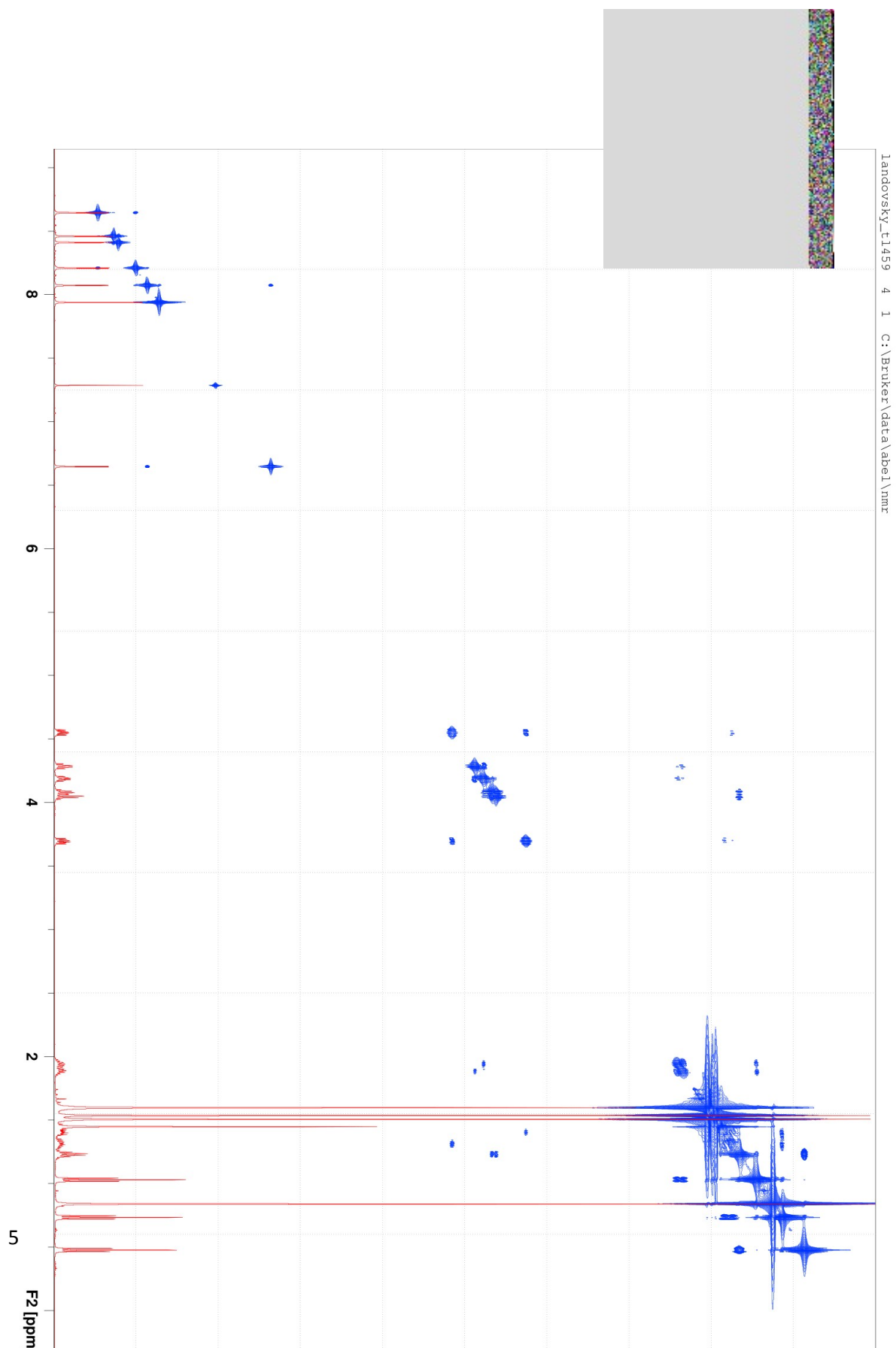
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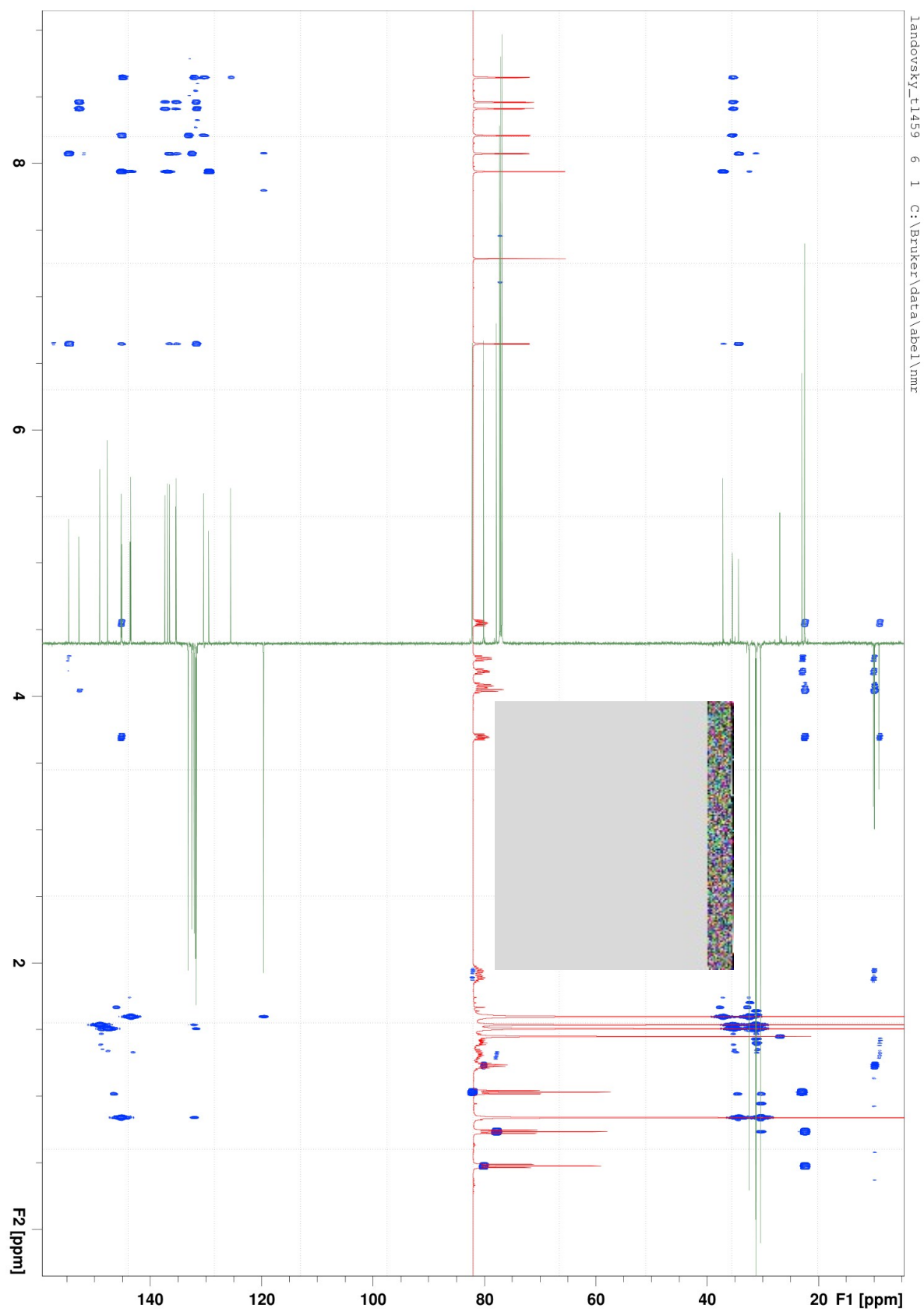
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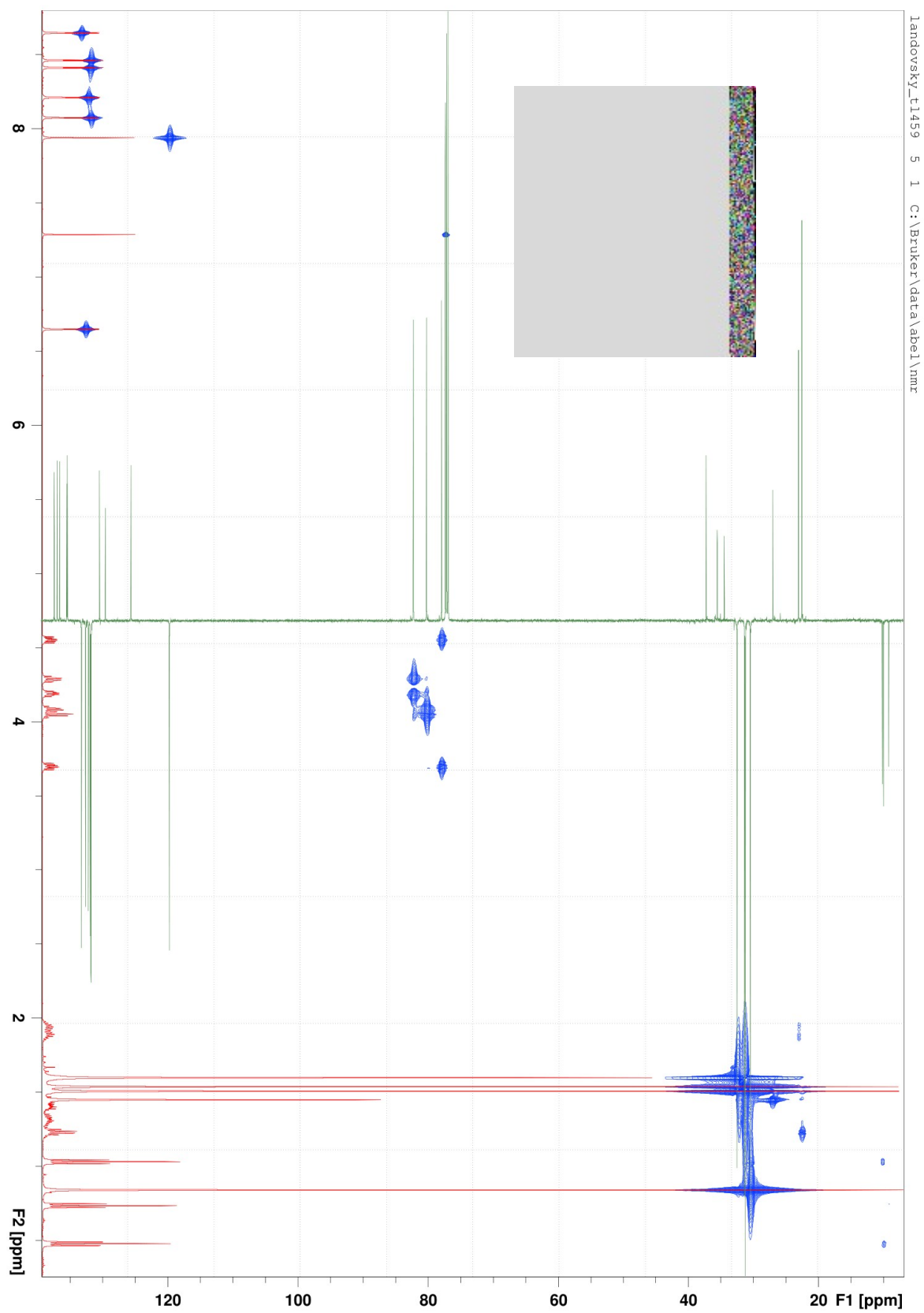
COSY spectrum of compound **7c** (CDCl₃, 298 K)



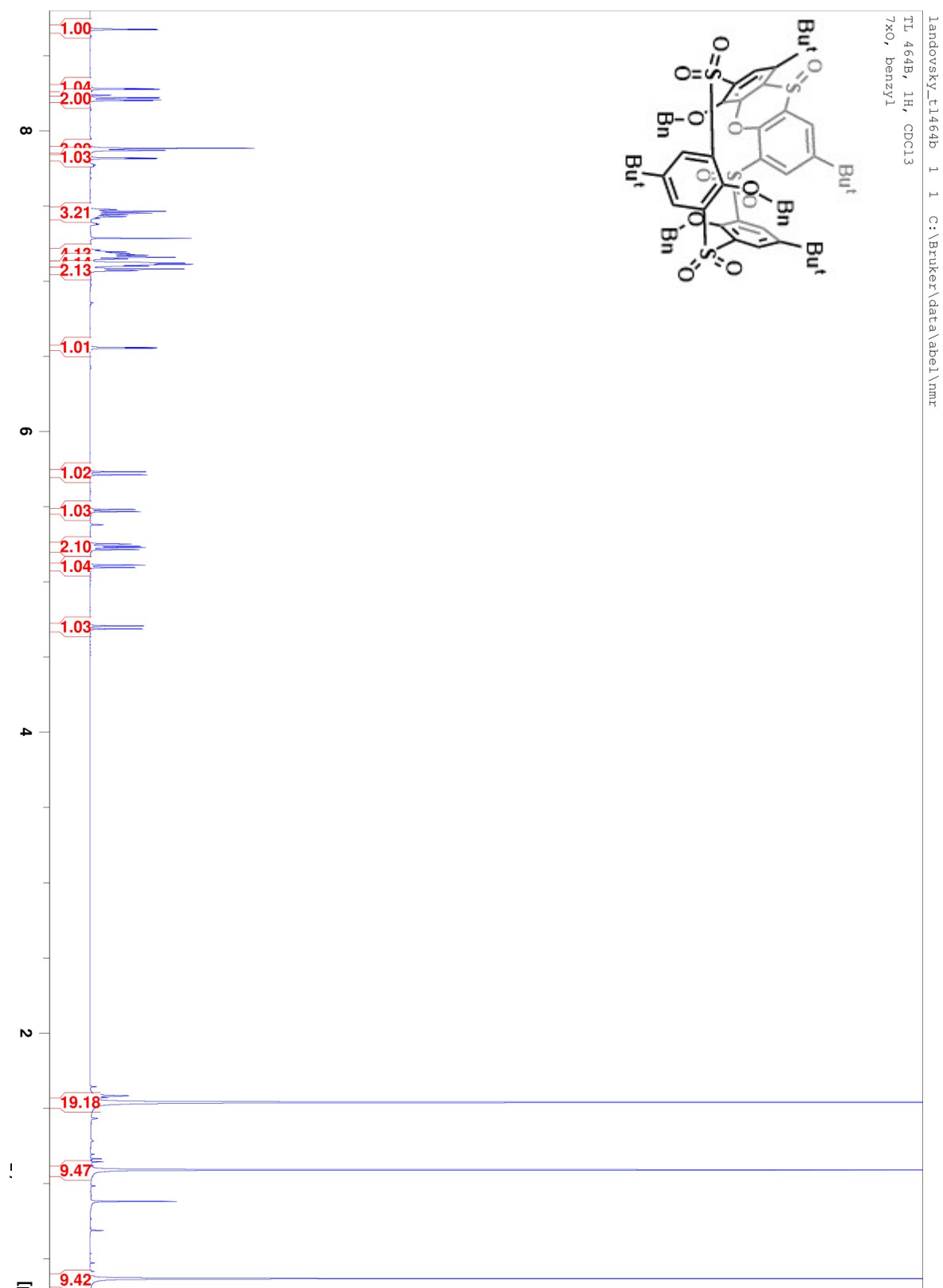
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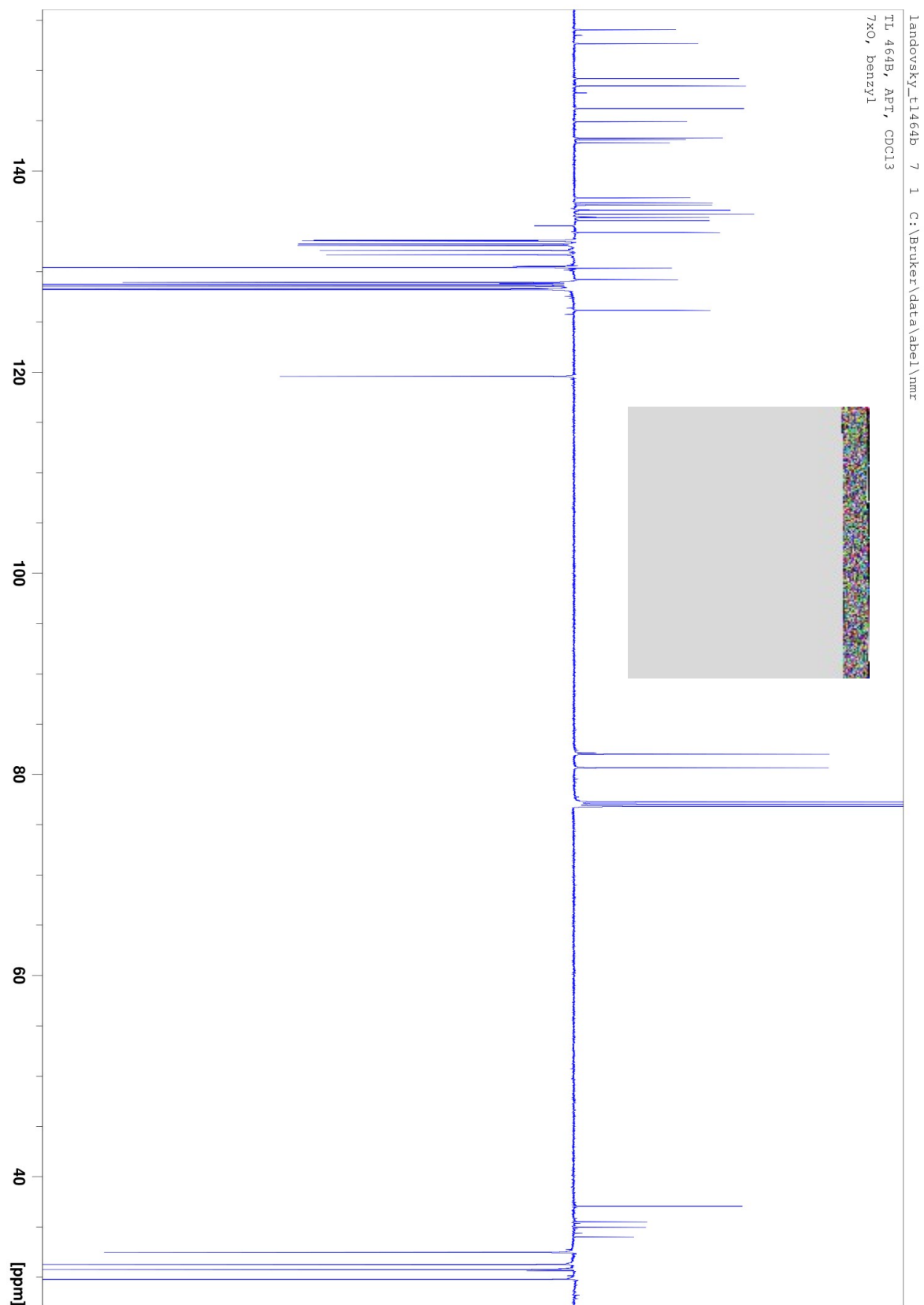
HMQC spectrum of compound **7c** (CDCl₃, 298 K)



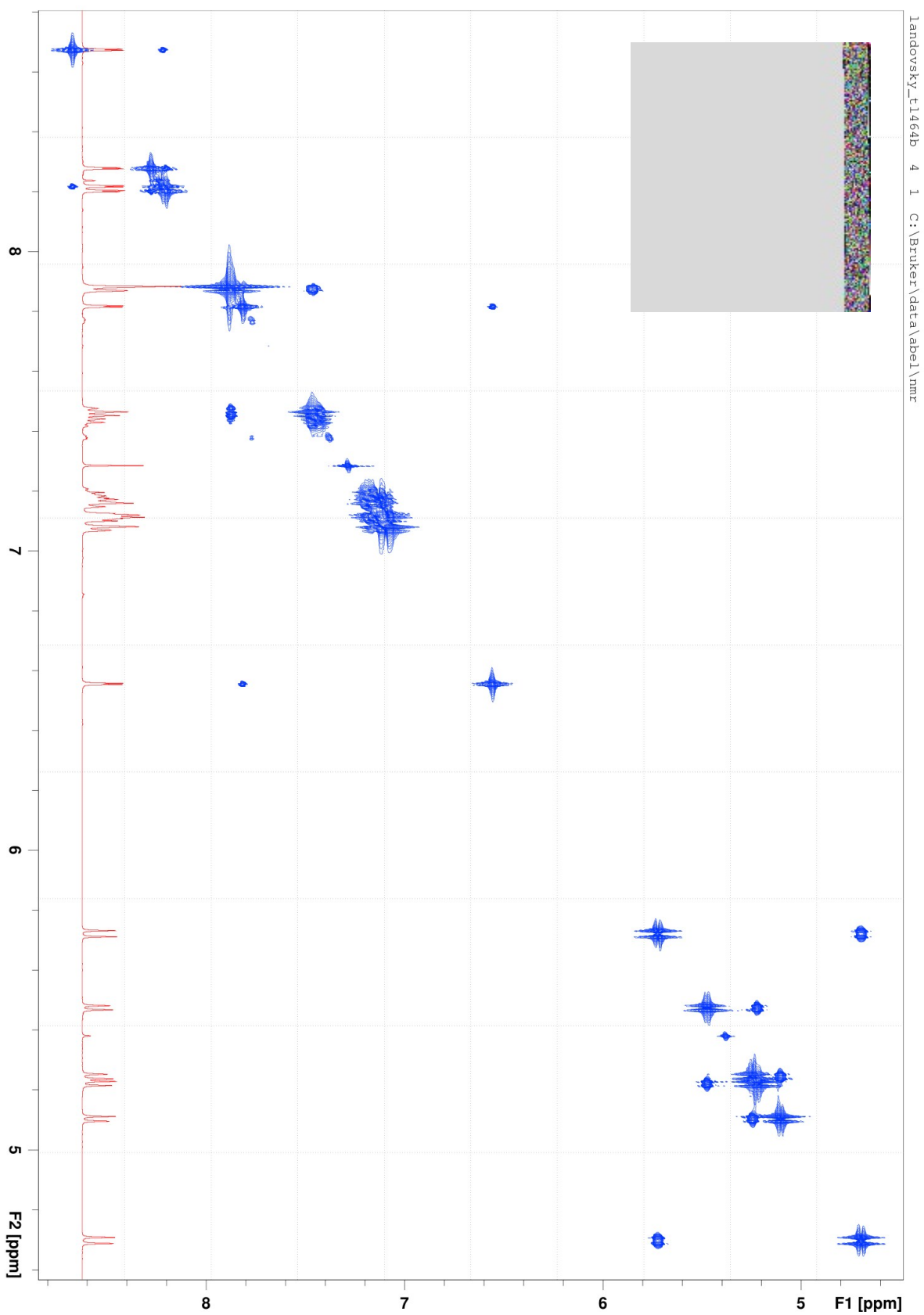
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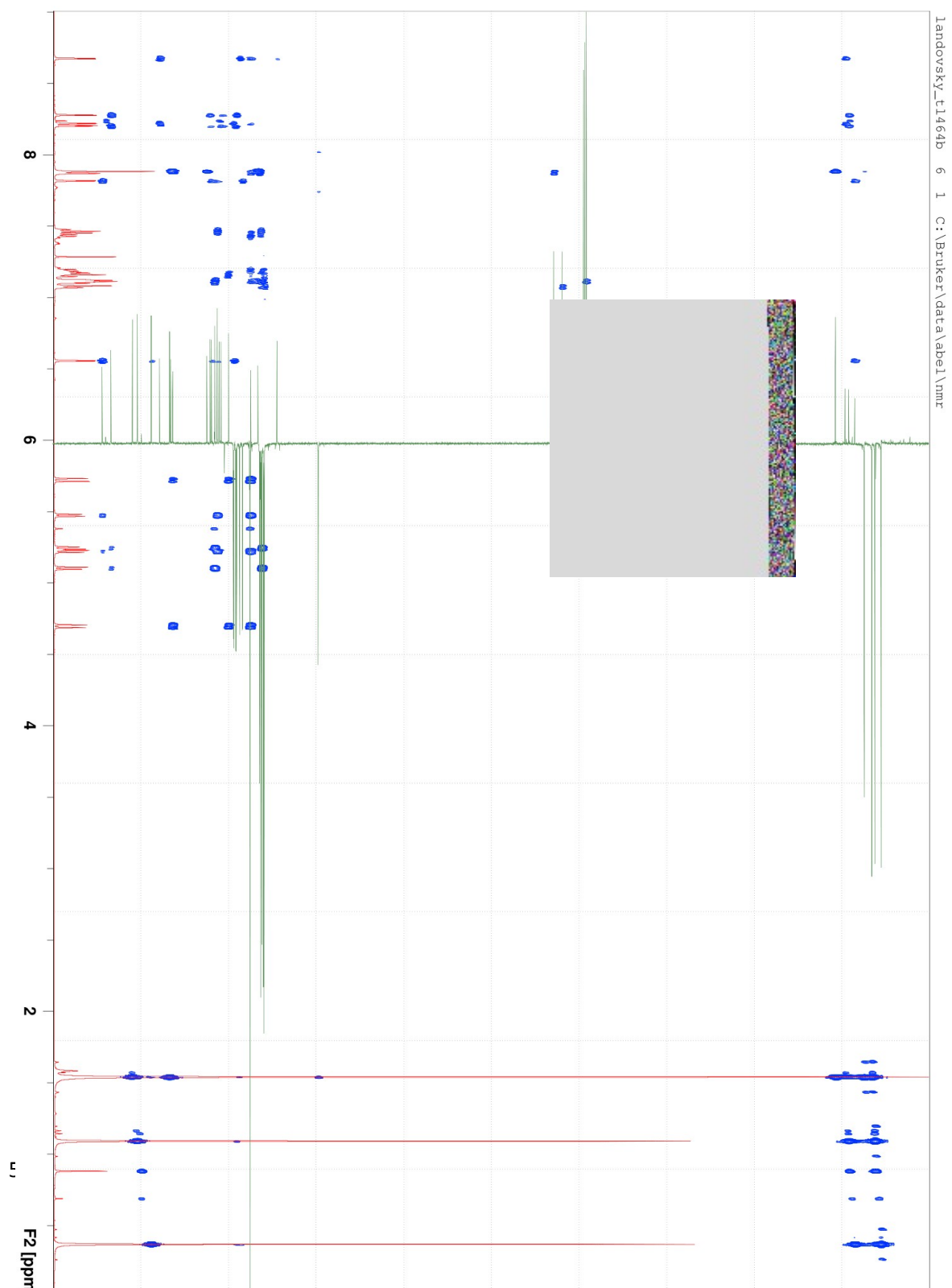
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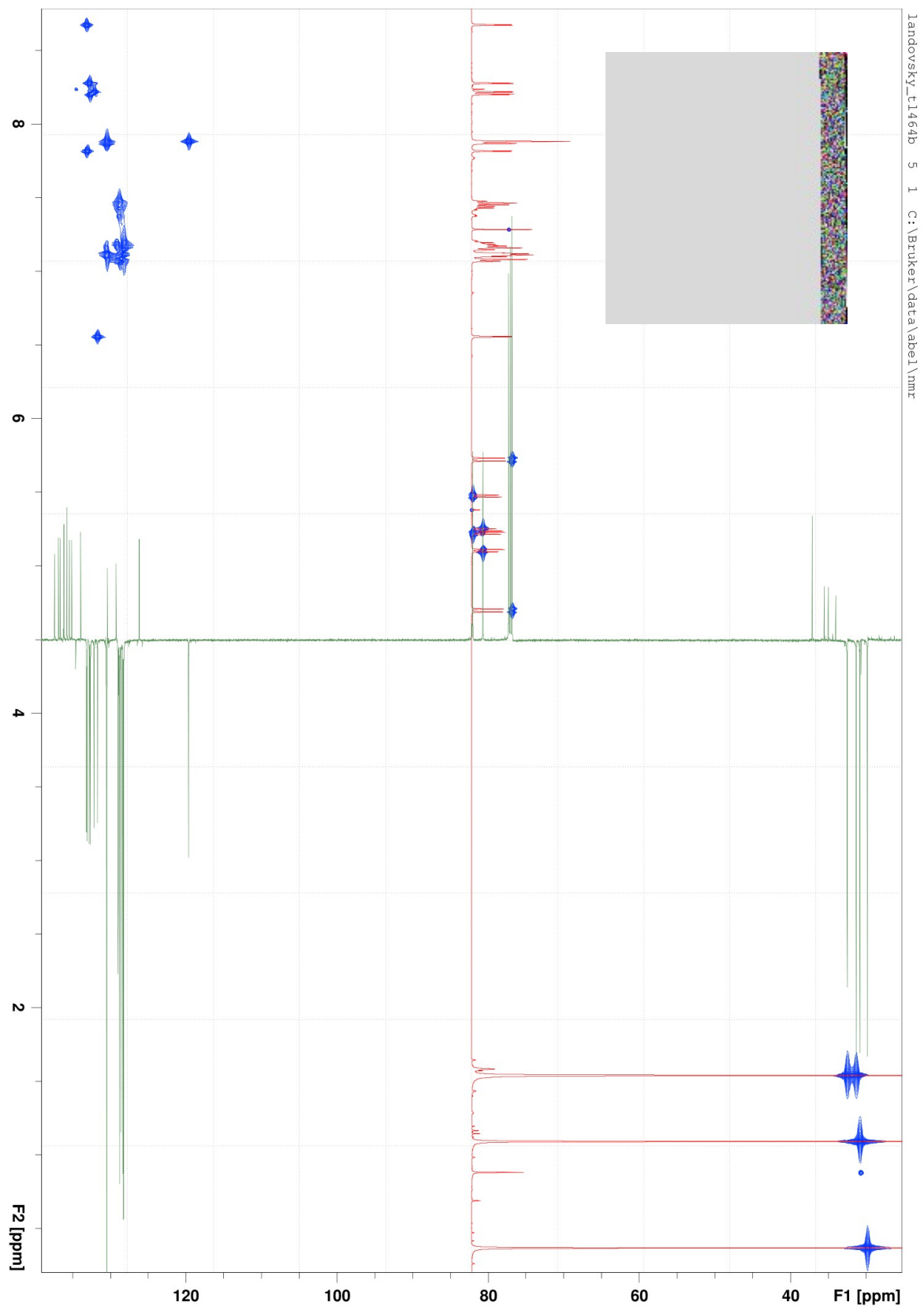
COSY spectrum of compound **7d** (CDCl₃, 298 K)



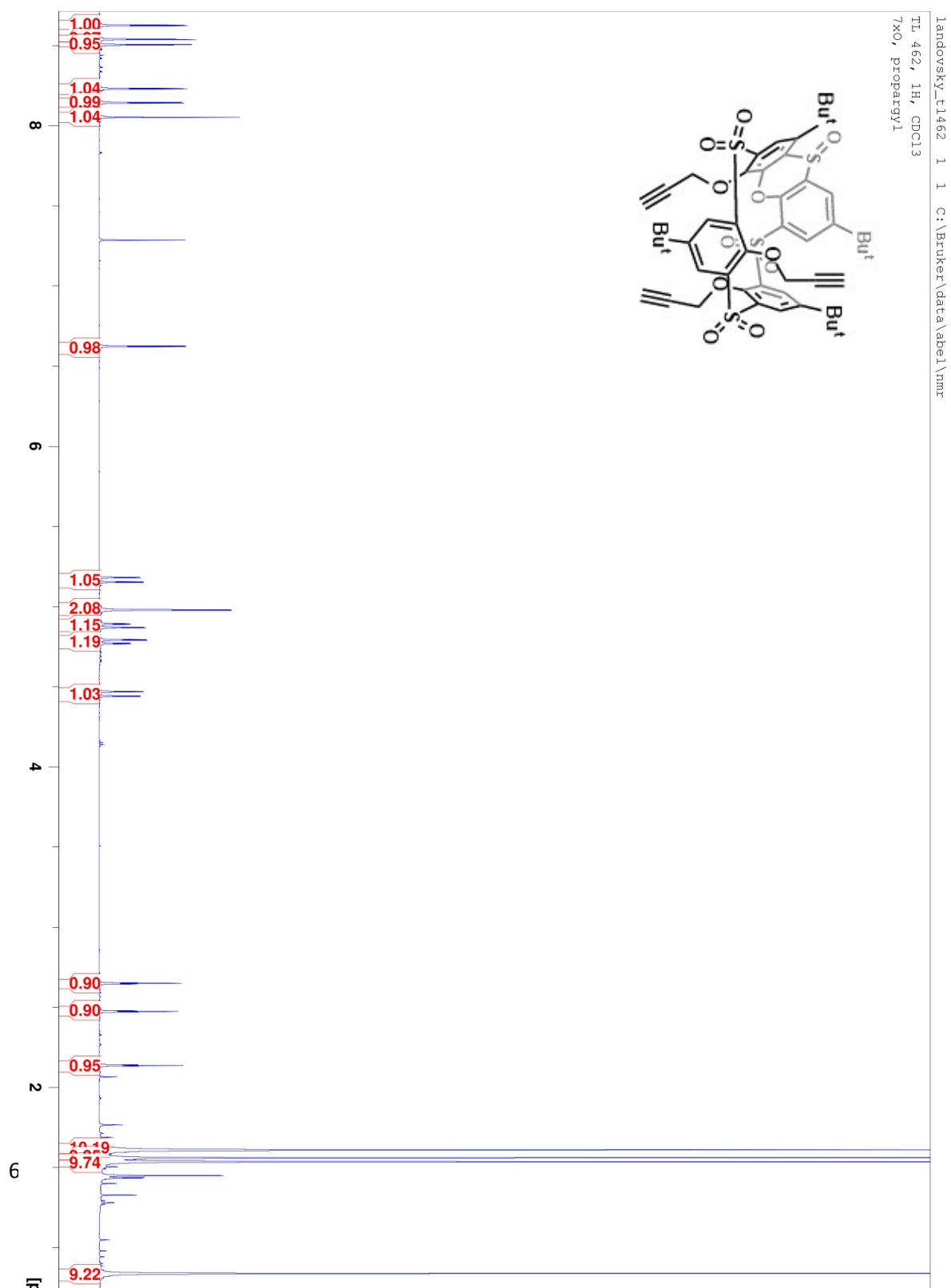
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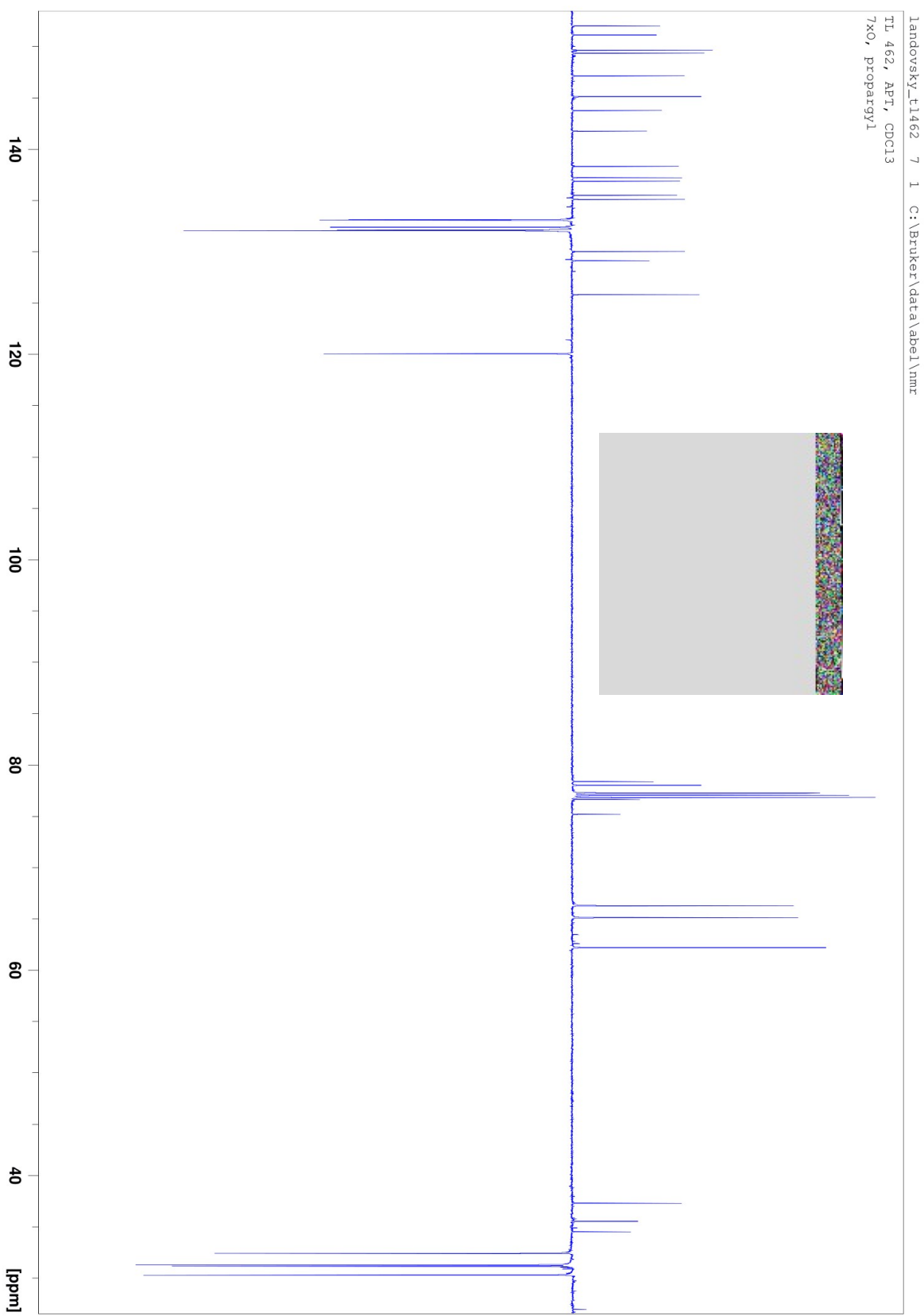
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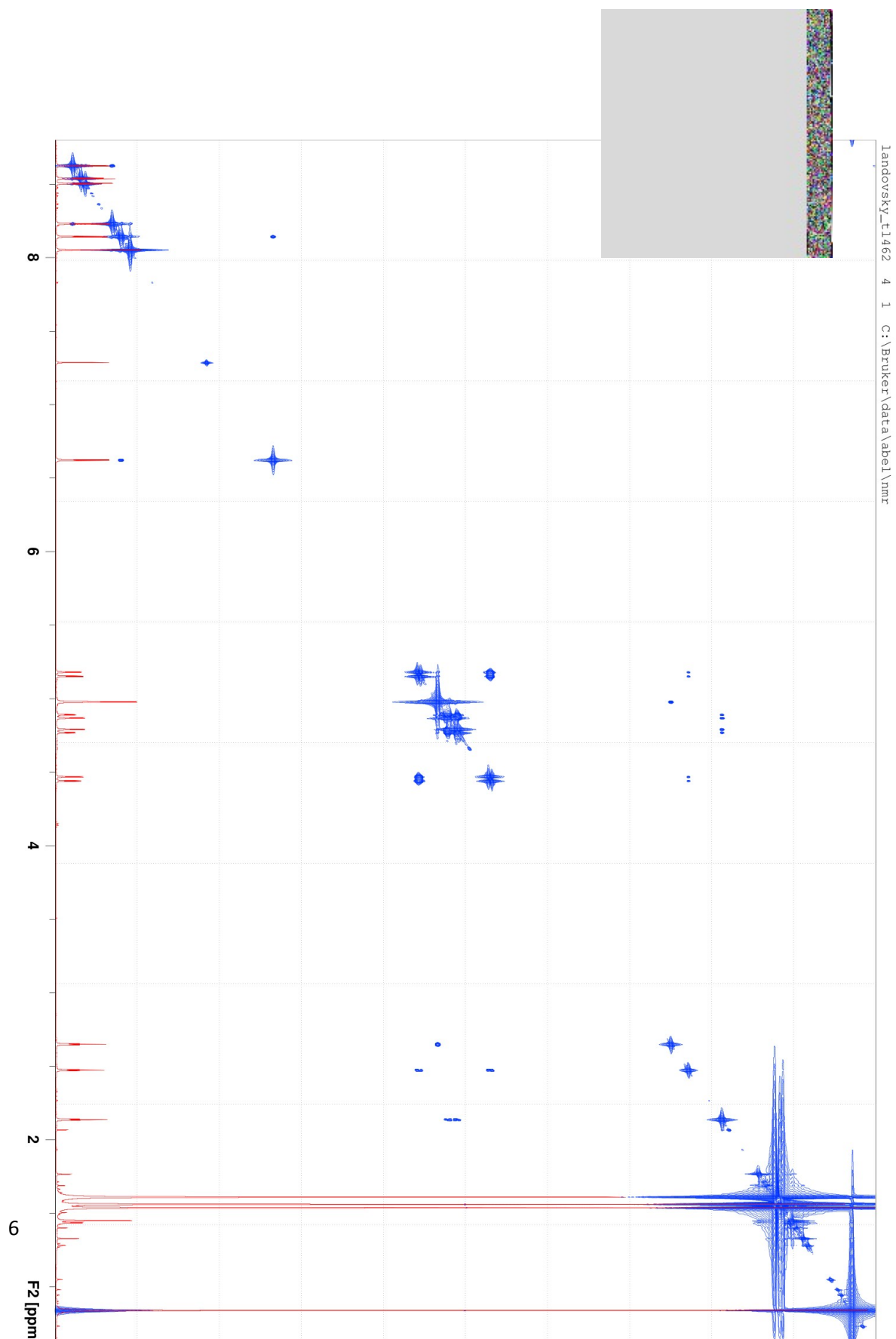
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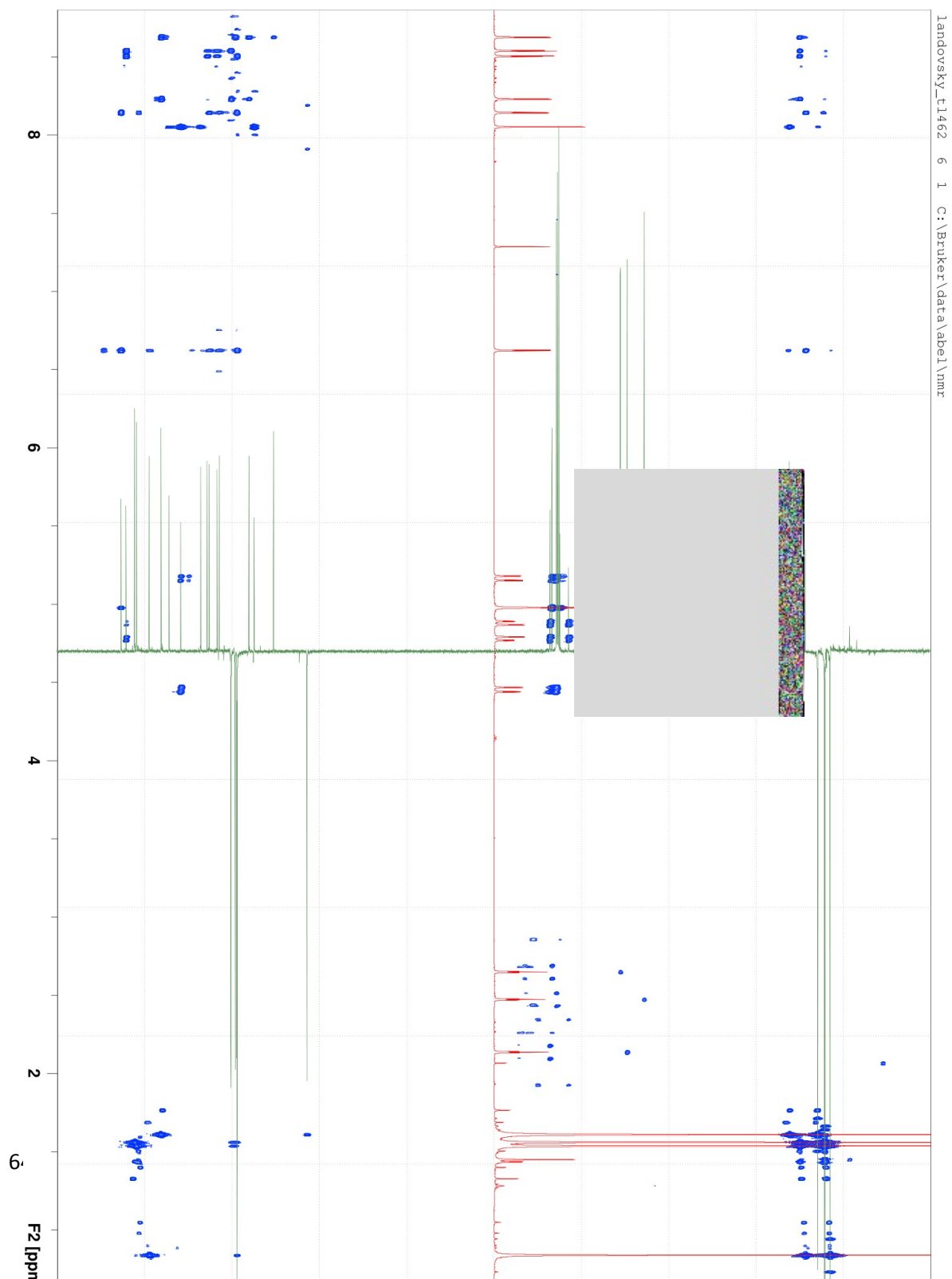
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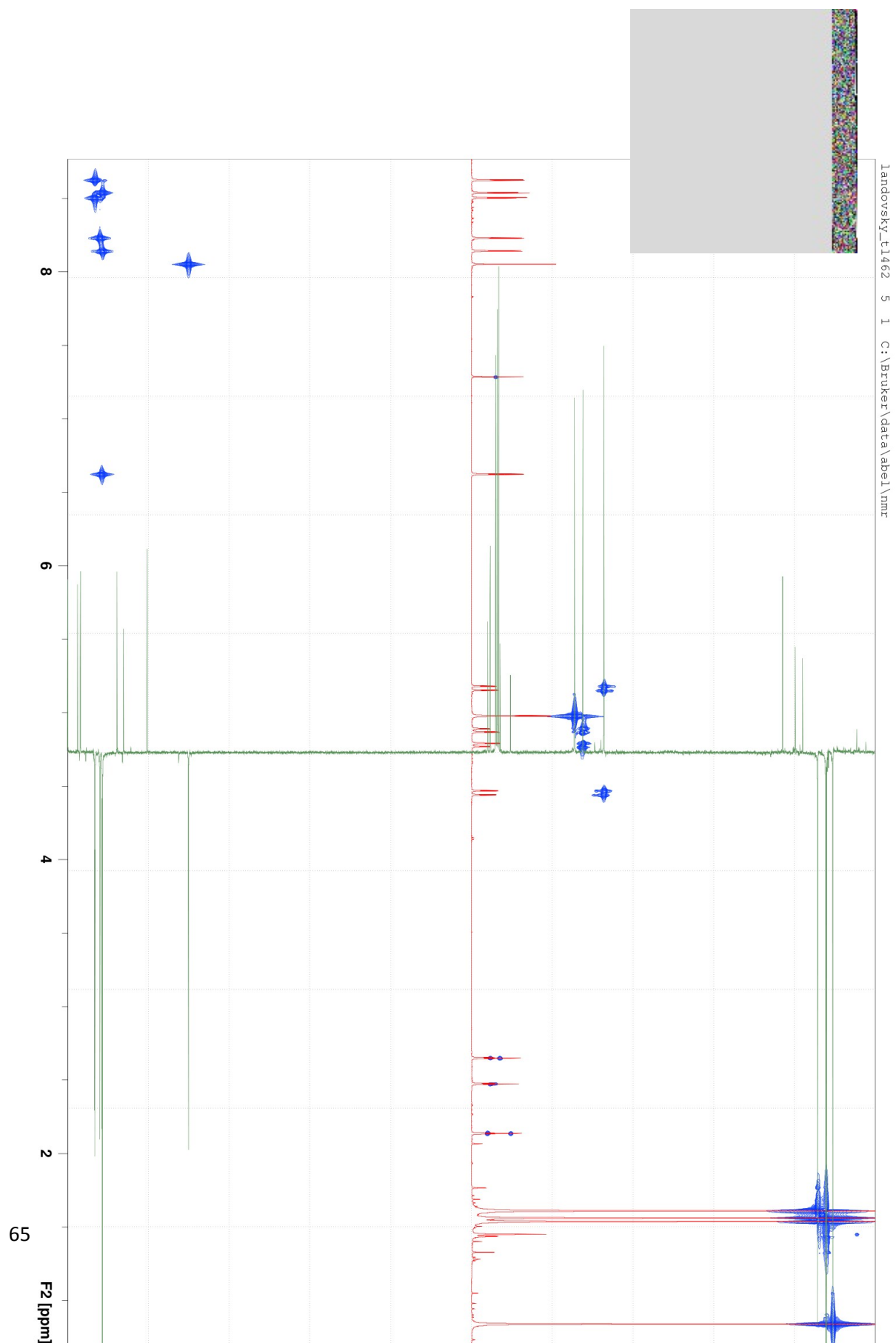
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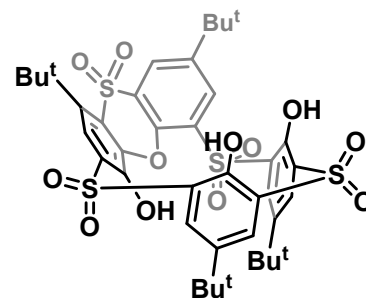
HMBC spectrum of compound **7e** (CDCl₃, 298 K)



HMQC spectrum of compound **7e** (CDCl₃, 298 K)

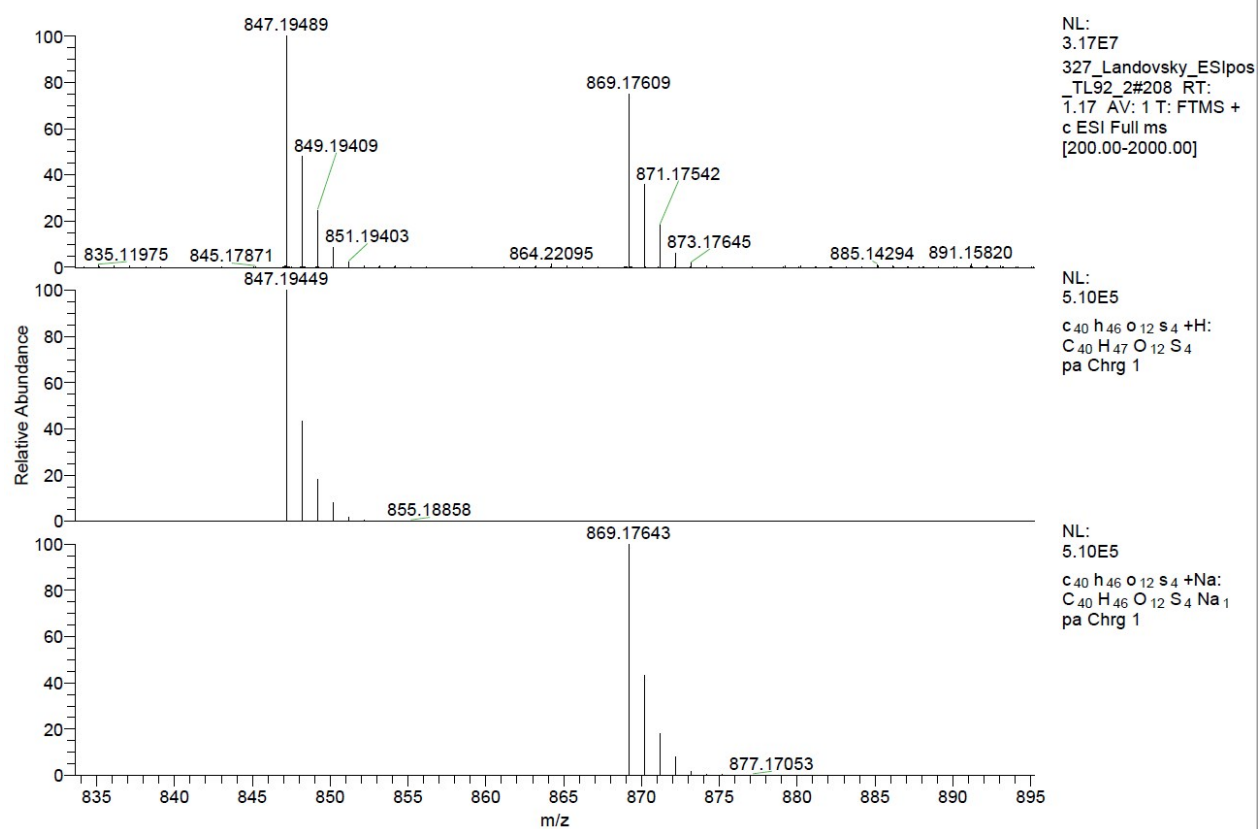


HRMS ESI+ spectrum of compound 4

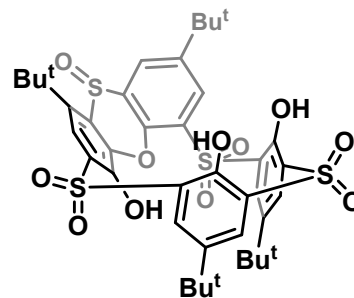


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10/9/2015 9:46:58 AM

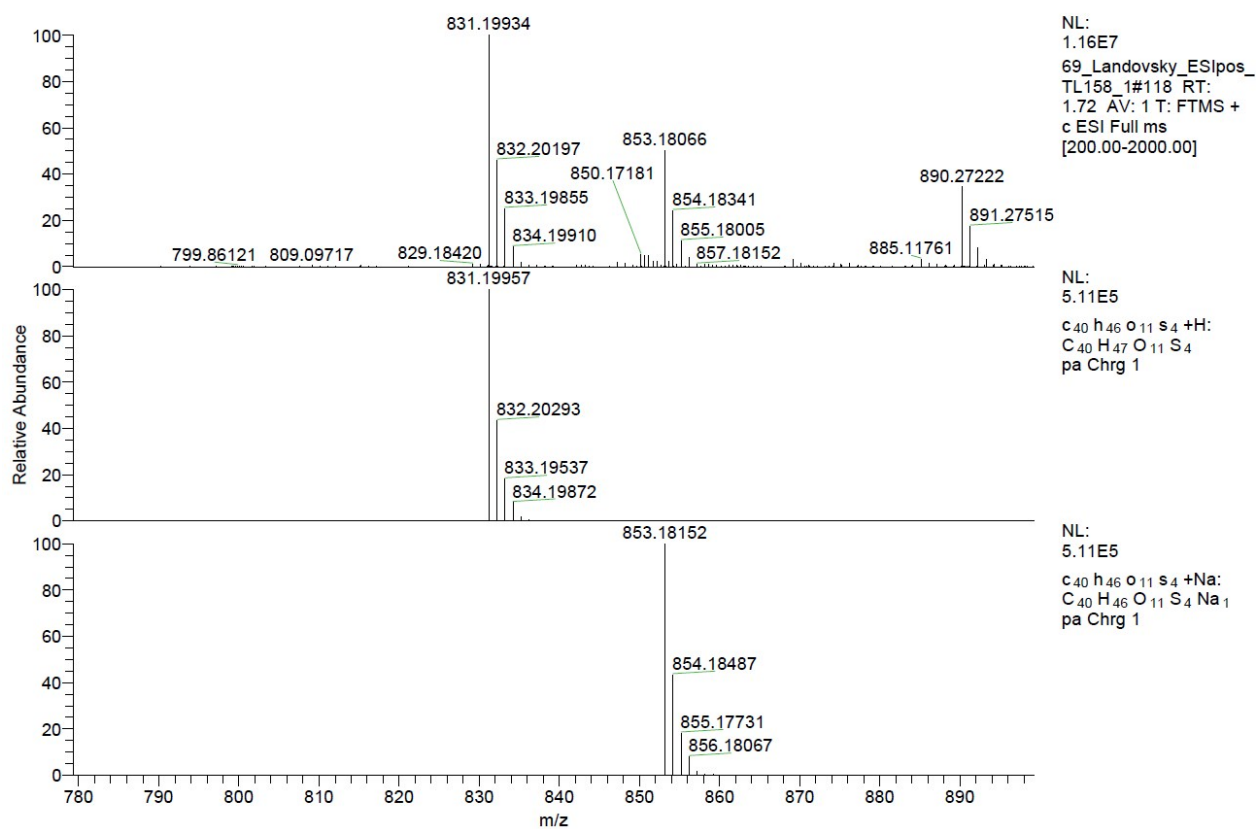


HRMS ESI+ spectrum of compound **5**

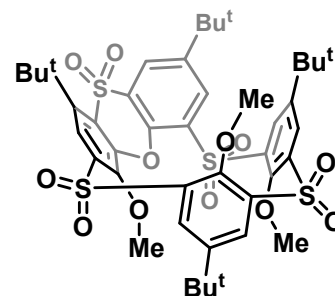


69_Landovsky_ESIpos_TL158_1
MeOH

3/23/2016 9:26:58 AM

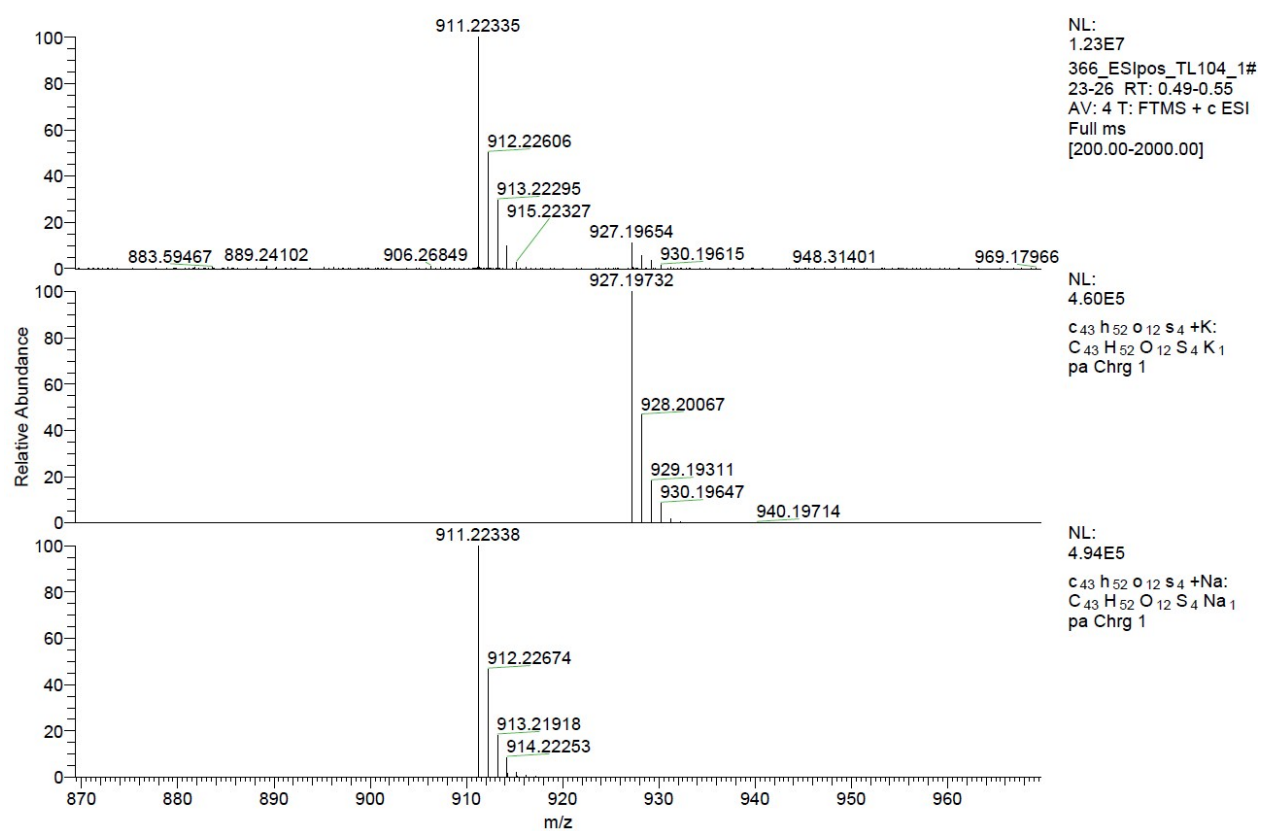


HRMS ESI+ spectrum of compound **6a**

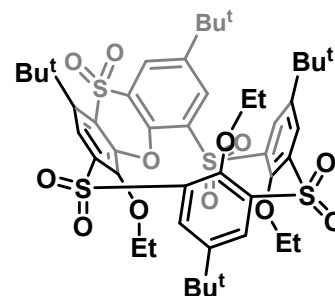


E:\ORBITRAP_2015\366\366_ESIpos_TL104_1

11/6/2015 8:43:10 AM

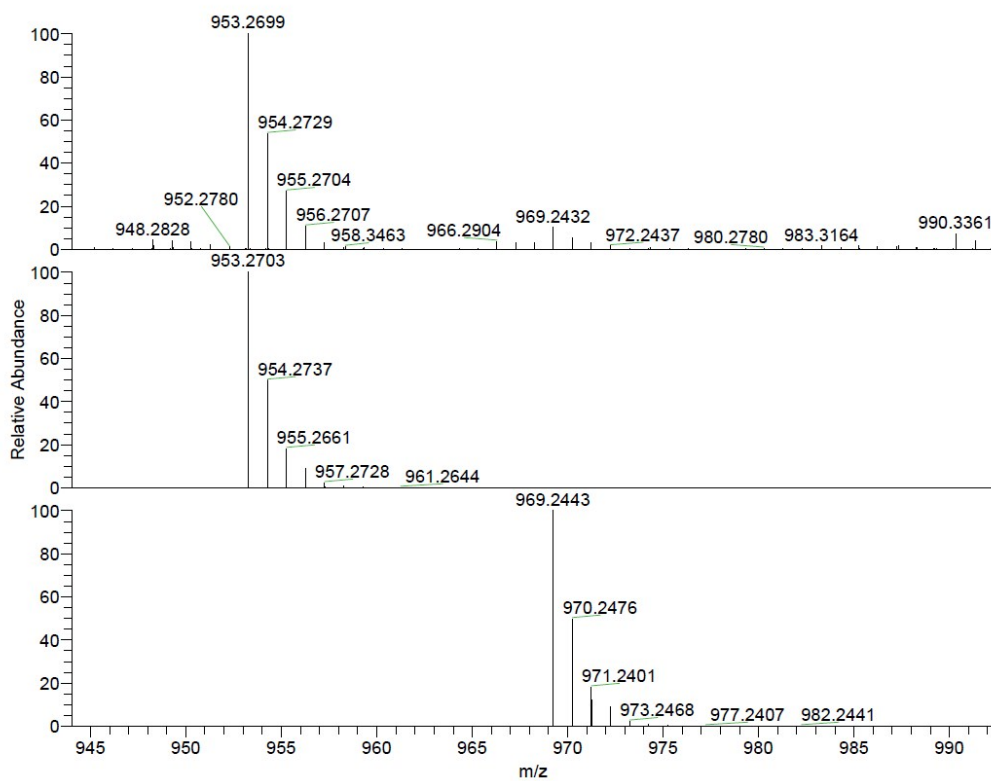


HRMS ESI+ spectrum of compound **6b**

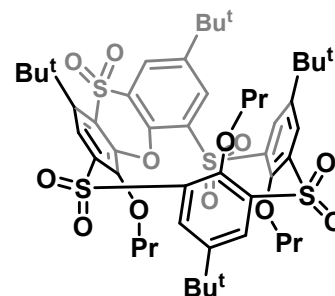


E:\ORBITRAP_2017\249\249_ESIpos_TL359A_1
MeOH

8/18/2017 2:04:41 PM

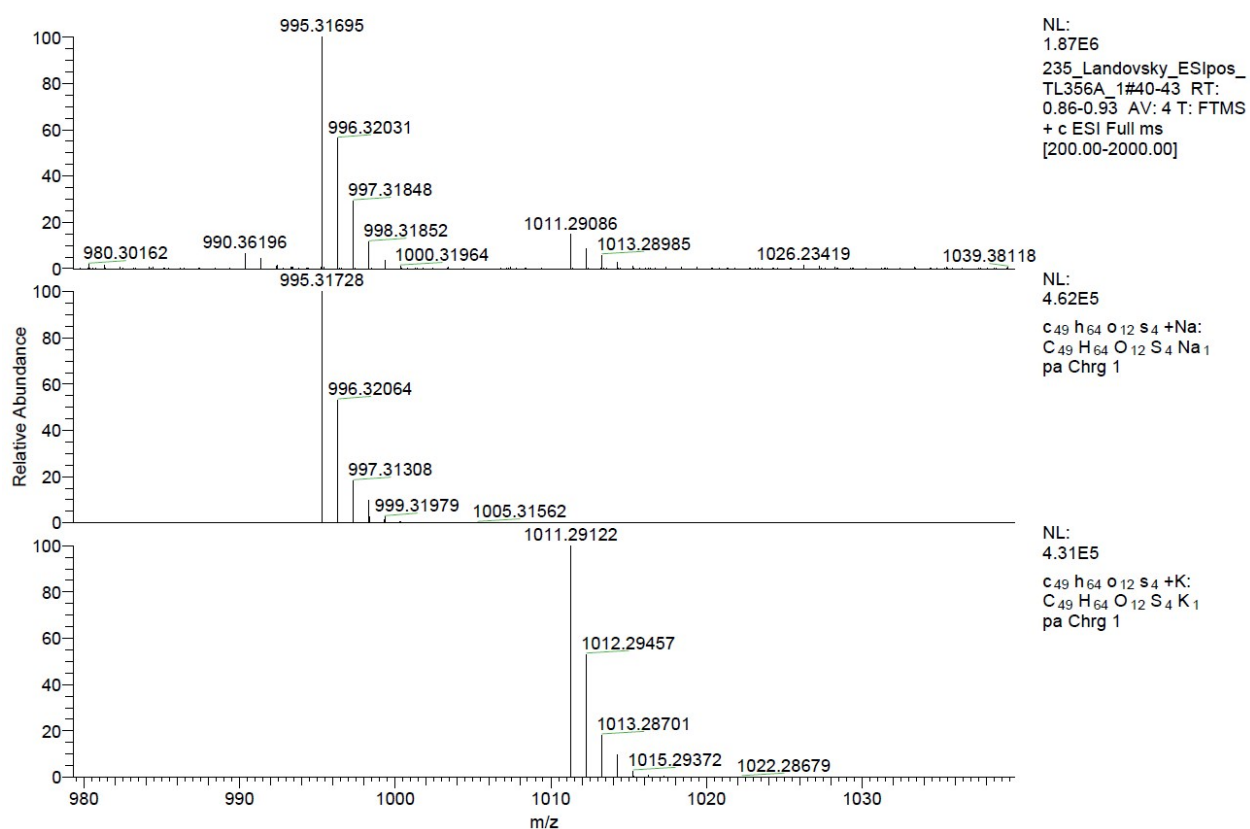


HRMS ESI+ spectrum of compound **6c**

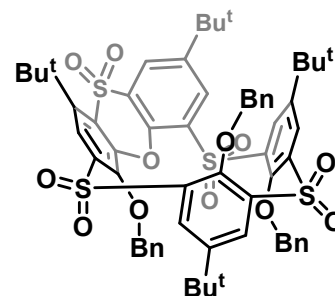


235_Landovsky_ESIpos_TL356A_1
MeOH

8/3/2017 7:37:15 AM

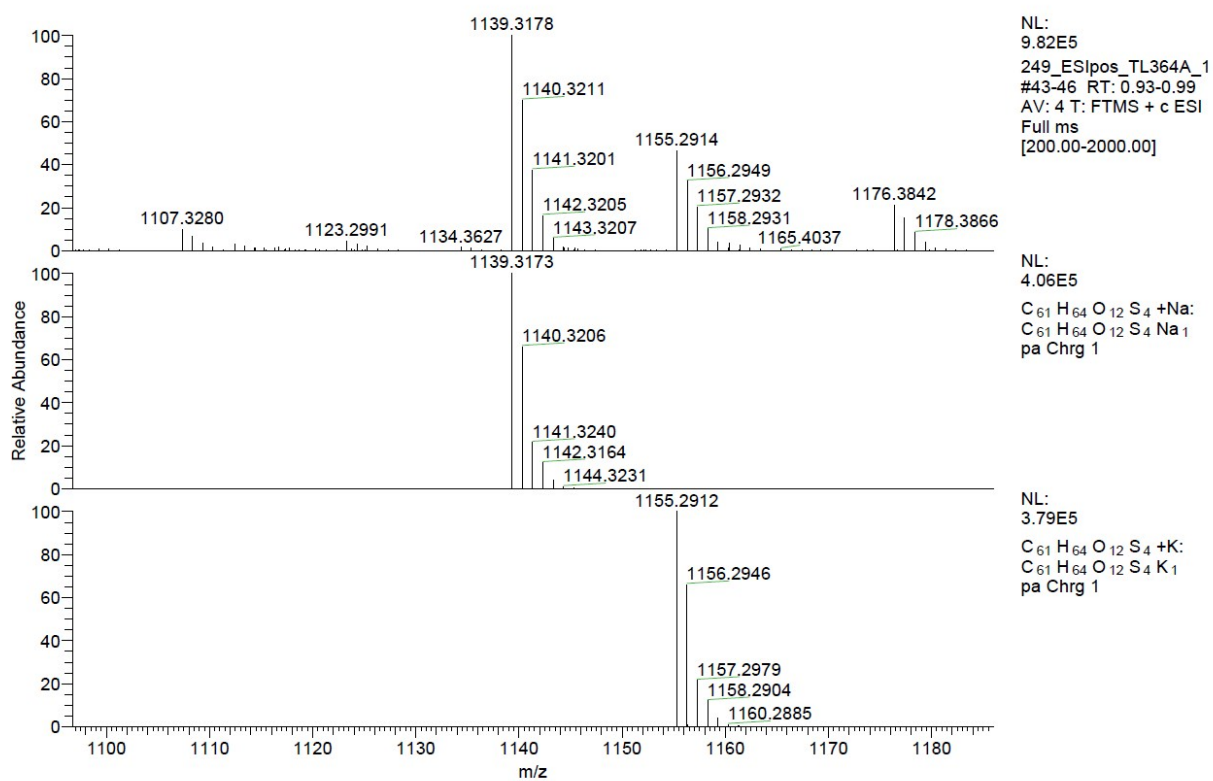


HRMS ESI+ spectrum of compound **6d**

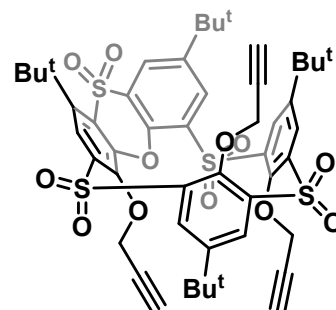


E:\ORBITRAP_2017\249\249_ESIpos_TL364A_1
MeOH

8/18/2017 5:58:02 PM

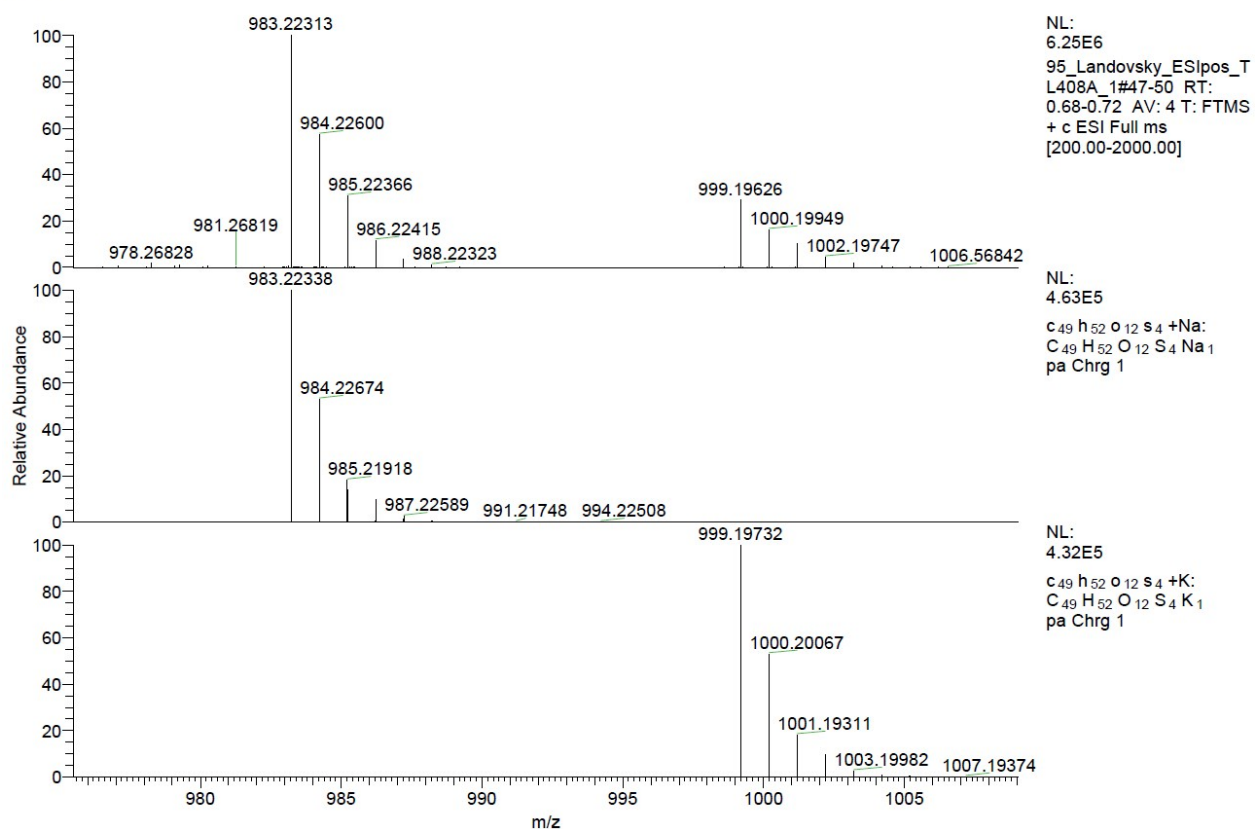


HRMS ESI+ spectrum of compound **6e**

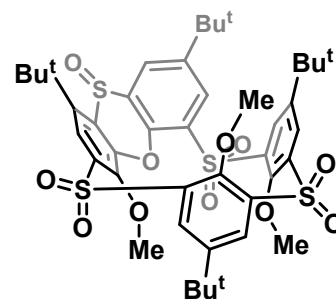


95_Landovsky_ESIpos_TL408A_1
MeOH

3/27/2018 8:17:32 AM

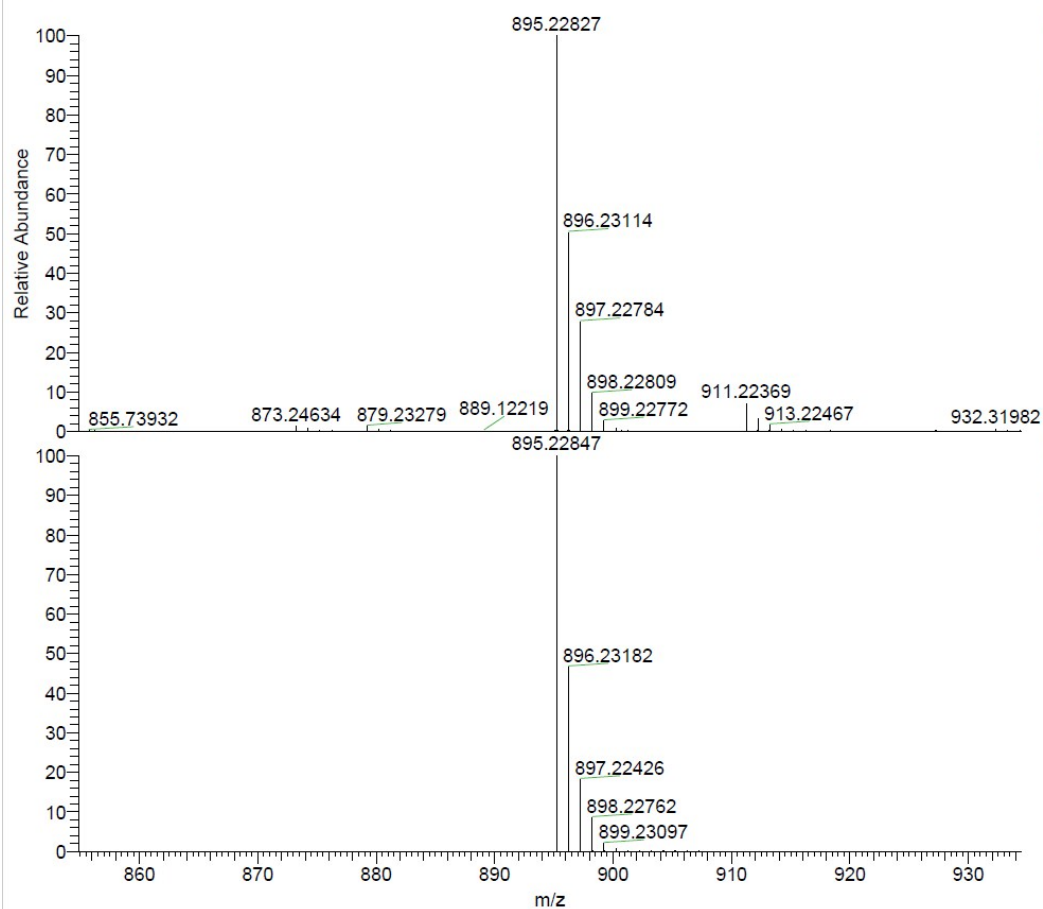


HRMS ESI+ spectrum of compound **7a**



318_Landovsky_ESIpos_TL88_1
MeOH

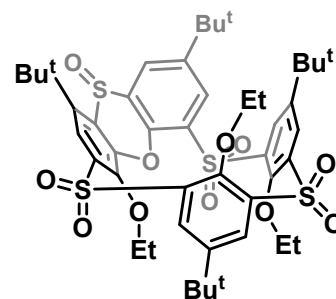
9/25/2015 8:08:36 AM



NL:
1.11E7
318_Landovsky_ESIpos_TL88_1#41 RT:
0.72 AV: 1 T: FTMS +
c ESI Full ms
[200.00-2000.00]

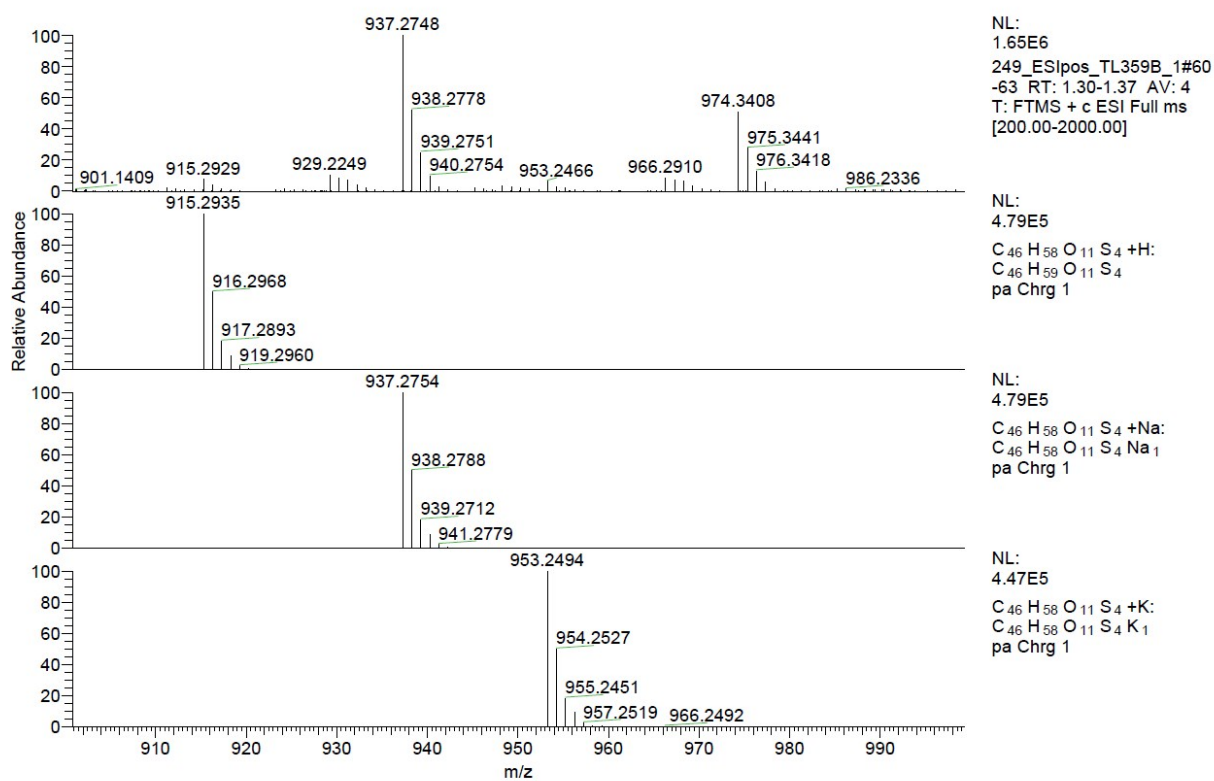
NL:
4.95E5
c₄₃ h₅₂ O₁₁ S₄ +Na:
C₄₃ H₅₂ O₁₁ S₄ Na₁
pa Chrg 1

HRMS ESI+ spectrum of compound **7b**

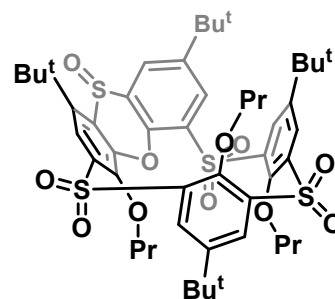


E:\ORBITRAP_2017\249\249_ESIpos_TL359B_1
MeOH

8/18/2017 2:26:13 PM

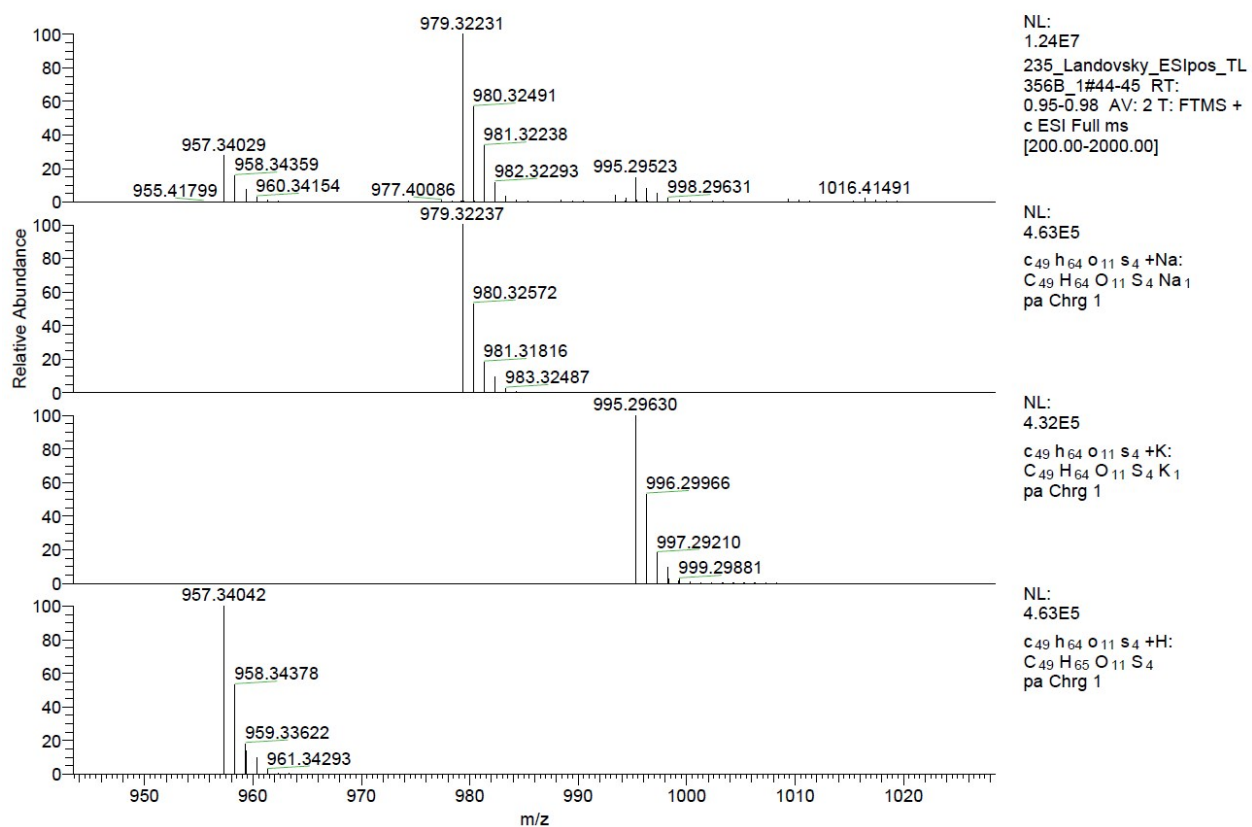


HRMS ESI+ spectrum of compound **7c**

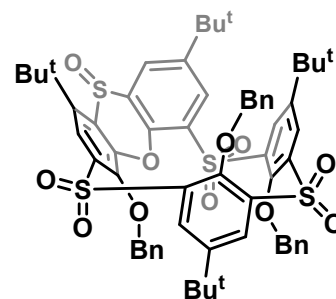


235_Landovsky_ESIpos_TL356B_1
MeOH

8/3/2017 7:38:59 AM

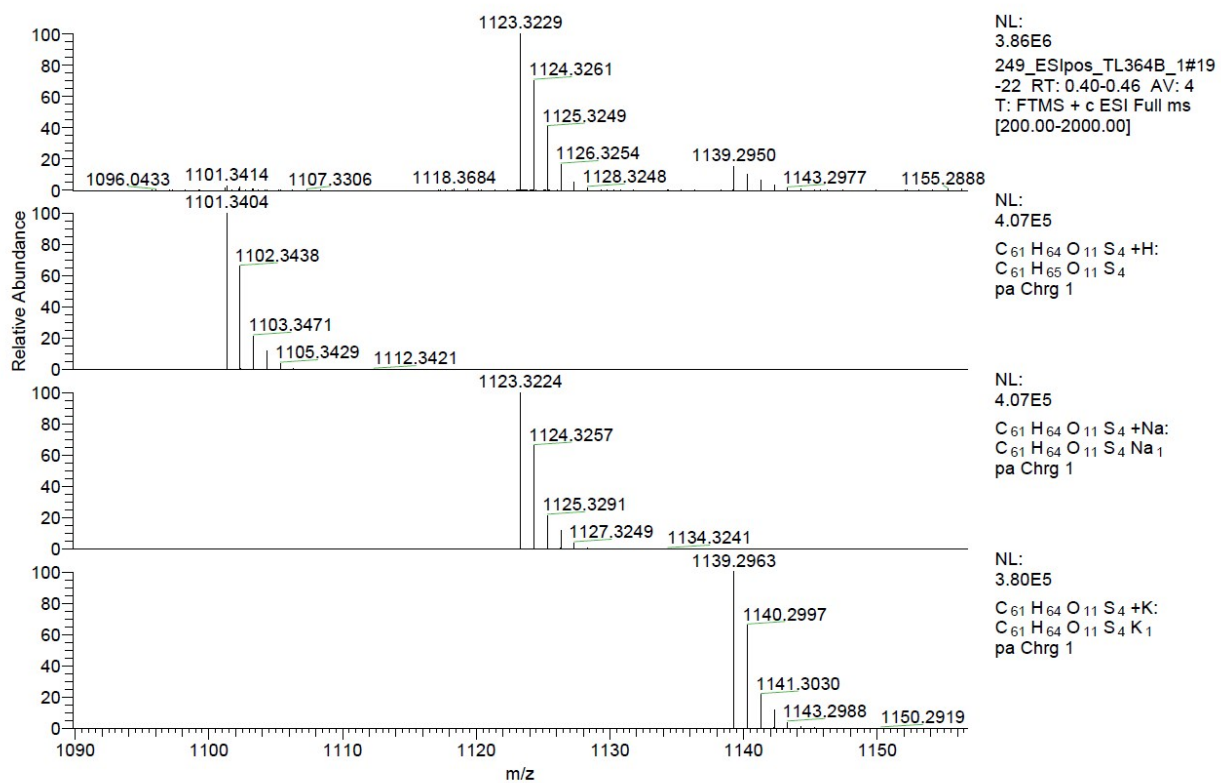


HRMS ESI+ spectrum of compound **7d**

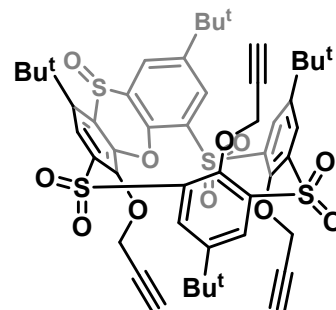


E:\ORBITRAP_2017\249\249_ESIpos_TL364B_1
MeOH

8/18/2017 6:20:03 PM

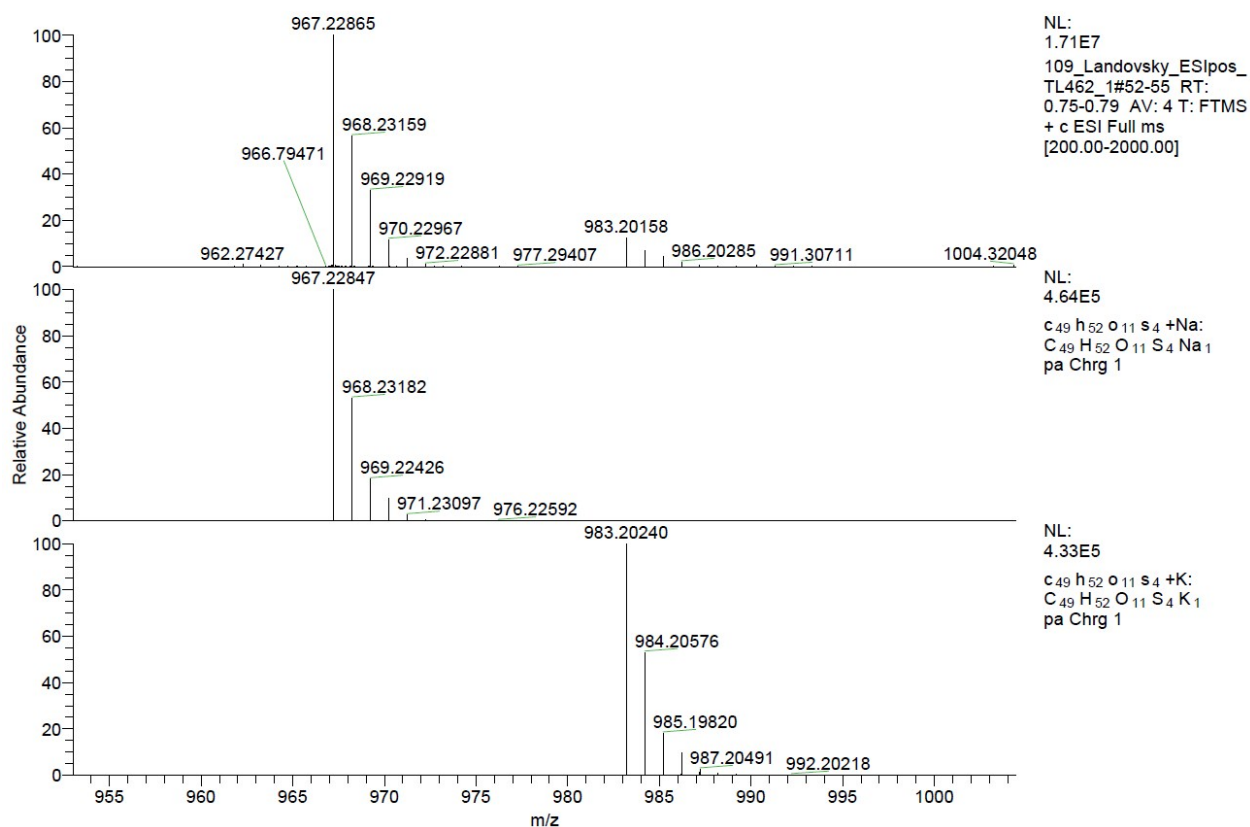


HRMS ESI+ spectrum of compound 7e



109_Landovsky_ESIpos_TL462_1
MeOH

4/9/2018 7:16:24 AM



DFT Calculations

Coordinates of molecules **7a** and **6a** of main articles in conformations **A** to **D**, obtained at B3LYP/def2-TZVPP level of theory.

7a-A

110

C	-0.33089871019039	-2.33426375358056	-1.86636088040910
C	0.99554364227228	-2.21904294281588	-1.40622609131895
C	1.39816428377469	-2.84445829031253	-0.22956843370701
C	0.53842624317164	-3.63292496107234	0.53473704389380
C	-0.73599837859275	-3.83826663448514	0.01448642645296
C	-1.15707273469811	-3.23220664197098	-1.17037769537147
S	2.33778078548552	-1.47369855551877	-2.35474984443819
O	3.36650986504725	-1.12751645638098	-1.40010526049690
C	1.04689654920071	-4.32632145537269	1.80884631773486
C	-0.08122521204548	-5.03879151608455	2.56955290420240
S	-2.66133605380669	-3.91969444821591	-1.90038355884041
O	-3.36175686874687	-4.58239863490765	-0.82397500853570
O	-0.78259705477629	-1.66327299505848	-2.94495180431142
C	-1.49292293584214	-0.44348157939091	-2.66950330876671
C	-1.94098936063841	-5.24495240556189	-2.90533426292965
C	-1.72322679010908	-5.17875823210421	-4.29308057130326
C	-1.10510185975916	-6.30036810010701	-4.88504946153061
C	-0.73948403341885	-7.40638723865117	-4.12653053532492
C	-0.94204303198918	-7.46463998002847	-2.74904614574353
C	-1.55961867712784	-6.36475914865252	-2.16954630477046
O	-2.03168683022716	-4.08203818937494	-5.01194020402576
C	-3.31541850034889	-4.04716911263732	-5.65676947137963
S	-0.80022057532852	-6.46342431077016	-6.65972540188828
O	-0.81330282544565	-5.19566137995563	-7.33363118355608
C	-0.52366515837795	-8.69750873292870	-1.93742952565404
C	0.92794036883514	-9.09183471345083	-2.28232566589972
O	-1.68116525380827	-7.51617906465982	-7.11393596058087
C	0.86686821417143	-7.14562379265887	-6.73697046011873
C	1.01033979422643	-8.40963982519640	-7.29332525618606
C	2.24962271517267	-9.05654913385361	-7.38347670917296
C	3.33773429403037	-8.38588556754569	-6.83361310812972
C	3.21605944572475	-7.11102412733875	-6.28142823588239
C	1.99313601906489	-6.45872872462503	-6.26333989249123
O	1.83860816957745	-5.19609110411698	-5.80266713437309
C	2.71889366417313	-4.62480859091902	-4.92121944996273

C	3.98531422926684	-5.12444823089172	-4.61934487048248
S	4.72858395655500	-6.29018433819507	-5.80241723243334
C	4.73106272235448	-4.57434640316506	-3.54202507753966
C	4.17911667786298	-3.47053408935955	-2.89532302856663
C	2.95778862013575	-2.91211251065280	-3.27120265444604
C	2.19898770022525	-3.48554476585537	-4.28195708352023
C	2.40926216258218	-10.39921384500511	-8.11367034188607
C	1.15222871693097	-11.27705961600052	-7.96944626141571
O	5.16948735767254	-5.48068358884019	-6.96951215814913
O	0.95544390504697	-3.05360377920994	-4.56089699742023
C	0.78827381430571	-2.30342322972491	-5.78286312679834
C	6.05870883614344	-5.17722474605700	-3.02490263712990
C	7.18714426410998	-5.07832316982680	-4.07661477068651
O	-3.36574511709009	-2.97304789348636	-2.71849453087449
C	-0.58759957549591	-8.43223004049820	-0.42589908768046
C	-1.47779262926562	-9.86169270284947	-2.26984389313161
C	2.64843421729845	-10.10270554762817	-9.61138050078552
C	3.60940992645403	-11.19969506625906	-7.57574469985996
C	6.55796056505834	-4.44454610629806	-1.76491871230838
C	5.83163006596245	-6.65220887003898	-2.61889927087228
O	1.85669431342303	-0.47525370285257	-3.27017885303135
C	1.68927106559290	-3.30057945327964	2.76325294406893
C	2.10403986209499	-5.37677453020232	1.40251050632974
H	0.11074097400902	-8.88505945761345	-7.65317475560180
H	4.32276840448349	-8.83110051700544	-6.84669695511626
H	4.69764383858002	-2.99974484662826	-2.07771530170865
H	2.42367208398040	-2.70160889858039	0.07729366471289
H	-1.43451787313526	-4.49453320126638	0.50931697744210
H	-1.77163216395263	-6.35887906361962	-1.11347428266841
H	-0.27693807685655	-8.24308011750733	-4.63035233887263
H	3.63673444413672	-12.17746027880934	-8.05719433656037
H	3.53780395228366	-11.36113547576528	-6.49858181203258
H	4.56161055634990	-10.71453408561994	-7.79054626810830
H	1.31387395846206	-12.22627361593450	-8.48181954750010
H	0.93008573781903	-11.49428014782861	-6.92300166765034
H	0.27021262164458	-10.81951485684842	-8.41597920515223
H	2.82110999311754	-11.03164210031243	-10.15895277350893
H	3.51881757467500	-9.46050175037332	-9.75282297093984
H	1.78901284478624	-9.59731628971591	-10.05537506802680
H	6.75017110269344	-7.06351711078834	-2.19590181194341
H	5.54763451945660	-7.27590596479764	-3.46403411908459
H	5.05054511494968	-6.73189822848917	-1.86037352940063

H	8.12167747454624	-5.42936494112450	-3.63471830834535
H	7.00570918130216	-5.68034802295959	-4.96329822177076
H	7.33098148040881	-4.04761639010258	-4.40214618483236
H	7.46761828386763	-4.93322603019408	-1.41546333857262
H	5.83078298196997	-4.48449449007390	-0.95251994978318
H	6.80249292309422	-3.40021973467992	-1.96163242783926
H	2.48925467305890	-5.89206627537651	2.28513792511714
H	1.67104431377511	-6.12433984805389	0.73611388284094
H	2.94933535111407	-4.92014263414784	0.88648408866827
H	0.32734840880545	-5.50930343692847	3.46481530046877
H	-0.55195497730260	-5.82393144623853	1.97598053760292
H	-0.85597708888289	-4.33840086475884	2.88454223372770
H	2.09280664172933	-3.81105420731699	3.63990255798051
H	0.95422618721439	-2.57119420573571	3.10641395066792
H	2.50800652127169	-2.75475526139459	2.29463616244419
H	-1.22797421463878	-10.74012778557689	-1.67121738083879
H	-1.41708311618662	-10.14113438352881	-3.32298300620166
H	-2.51190939816559	-9.58867049734539	-2.05401381101003
H	1.23973535314551	-9.94115809237170	-1.67228039534489
H	1.04531752397727	-9.38255097061721	-3.32675744372587
H	1.61162880502856	-8.26474145571909	-2.08450249735177
H	-0.22353199268221	-9.30816362782823	0.11190500089813
H	0.04065890434078	-7.58757215280863	-0.14107421955651
H	-1.60328716486672	-8.23578603634824	-0.08143561108187
H	-1.85821395693289	-0.08823557132459	-3.62869724375414
H	-2.34020277742455	-0.62763182640929	-2.00901414870501
H	-0.81622516557195	0.29349698658614	-2.23391579008788
H	-0.26030447666293	-2.02987849351177	-5.81204070307351
H	1.41145080382162	-1.41021761254666	-5.74769077328159
H	1.03226898491455	-2.92236068286100	-6.64462365514331
H	-3.27794691607952	-3.21362363880686	-6.35187561488282
H	-3.49670174371867	-4.96794143357447	-6.21299784159443
H	-4.09642528162868	-3.87777436233619	-4.91634449848275

7a-B

110

C	1.46814509774148	1.28826143614146	0.58931588913839
C	1.27053874125489	2.31068498495248	-0.35286541283708
C	2.04845254881227	3.45593559707940	-0.36684601554498
C	3.07094563528012	3.65638680652592	0.56289459821540
C	3.23539854335625	2.67105141763345	1.52904213411878

C	2.45192691205641	1.51288839951724	1.56282091798289
S	-0.07578073271631	2.24486383489527	-1.54208193054764
O	0.03960488910637	1.03243133190635	-2.31987420424613
C	3.94451895468654	4.91720717591239	0.49550689864883
C	4.84636436300547	5.06250241316478	1.72921573868936
S	2.74392160267413	0.44938686379042	2.98862729480879
O	2.21394175242444	-0.87277951268839	2.77556147941487
O	0.66196983457870	0.19918434646368	0.58140310547684
C	1.16201810787694	-0.97831182419800	-0.08613716565773
C	1.83707689633756	1.31650837272379	4.30892132138390
C	0.42812047640178	1.40166470358540	4.39182168641292
C	-0.09849470611529	2.23527629762039	5.38147270466456
C	0.73504424950192	2.91005125747099	6.27617288197859
C	2.11632467866908	2.80689073769255	6.22042124282610
C	2.64472629478867	1.99934379405836	5.20957981670376
O	-0.38865658211220	0.75792768630508	3.51641511676906
C	-0.66500352644335	-0.62724520727898	3.80550177656856
S	-1.82074744780549	2.77138777294379	5.62099967806970
O	-1.95268838801218	4.04129105576379	4.95099427178349
C	3.03692554710544	3.55201880038778	7.19530545794362
C	4.02506372027040	4.43330554931048	6.40790442994158
O	-2.03203041284424	2.70413920391255	7.04980817725918
C	-3.03018596315730	1.65500599757985	4.89839620601034
C	-3.62571329527902	0.73295187357611	5.75301260705822
C	-4.71273421869046	-0.06381679762210	5.37056882843301
C	-5.22593117333077	0.15476497135587	4.09674075684184
C	-4.65310964608753	1.08127849971449	3.23105508422067
C	-3.52558302379581	1.80697872011790	3.59262879721605
O	-2.91494364265890	2.62958537588008	2.70863401900962
C	-2.92981653889828	2.31162457023485	1.37005105184244
C	-3.98070129574320	1.64242998721013	0.74251870051447
S	-5.50357211663703	1.51137450572586	1.71450312717819
C	-3.86837493207448	1.20012605143999	-0.59848660992637
C	-2.62607502298302	1.39434613126513	-1.19450982420691
C	-1.59592285677842	2.10466106222179	-0.58161612770992
C	-1.76079740127097	2.66855987673895	0.67788428133460
C	-5.32338817838594	-1.07578469031841	6.35112404276071
C	-4.22867507294892	-2.03339703675573	6.86416089752744
O	-6.03491596090616	2.88958190814522	1.88595301768133
O	-0.79033325216743	3.41575170587432	1.25124775197816
C	-1.15084020593044	4.75052474666485	1.67066242797135
C	-5.01524925289130	0.53688451816713	-1.40036472933236

C	-6.24771368578746	1.46972753054212	-1.45025718207445
O	4.14267300638190	0.58554457899449	3.32388685957358
C	2.25351912461090	4.47707964916181	8.13533243552578
C	3.80916029366340	2.53187245919417	8.05230635021221
C	-5.94871784553676	-0.32009366861292	7.54198418144566
C	-6.42635205116754	-1.91569249187582	5.69074022230041
C	-4.60826295193997	0.28808632408505	-2.86595530888553
C	-5.38787881812679	-0.84138333893538	-0.80797416910420
O	-0.09539052810828	3.51366110720441	-2.23165686029906
C	3.06638022810172	6.18124700215697	0.41421635282299
C	4.82840103711310	4.84040223123708	-0.76607687310914
H	-3.23180642841042	0.66633548536617	6.75696936419227
H	-6.10476593459292	-0.37368253423362	3.75644052685410
H	-2.42983593031404	1.00452220258318	-2.17924441160588
H	1.82114513169167	4.20126239110858	-1.11445020858477
H	3.99084559420947	2.77993690139675	2.29027211923313
H	3.71326653535567	1.89044823456203	5.09600849467907
H	0.26552604518481	3.52792580281954	7.02436164071441
H	-6.82086285047607	-2.63142962383057	6.41341106882121
H	-6.05064614188557	-2.48220097489049	4.83668894952178
H	-7.26214745325589	-1.30007001152924	5.35503008658696
H	-4.65861933932640	-2.75138099359146	7.56537352037457
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