

N-Aryl Pyrazoles: DFT Calculations of CH Acidity And Deprotonative Metallation Using a Combination of Lithium and Zinc Amides

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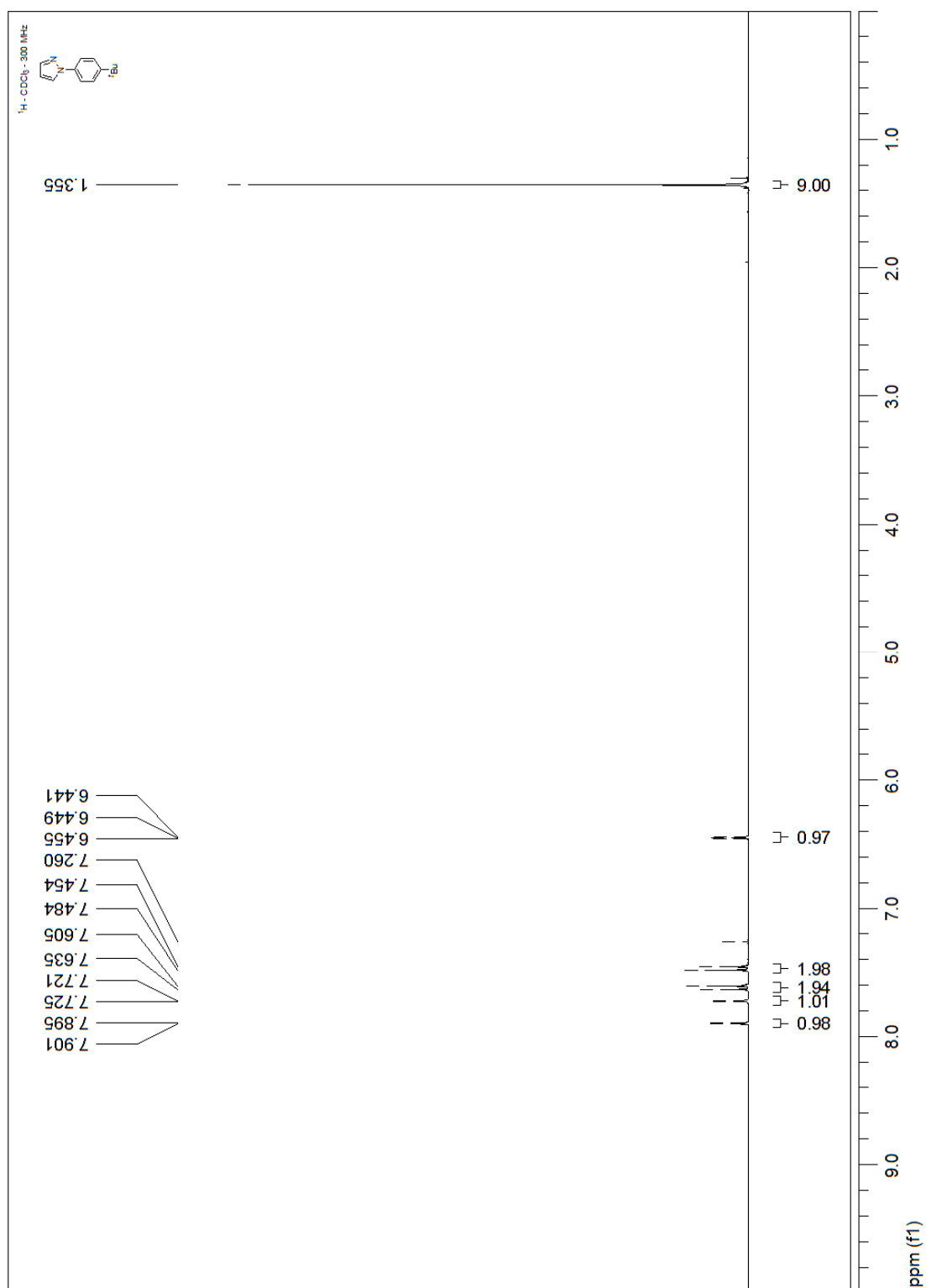
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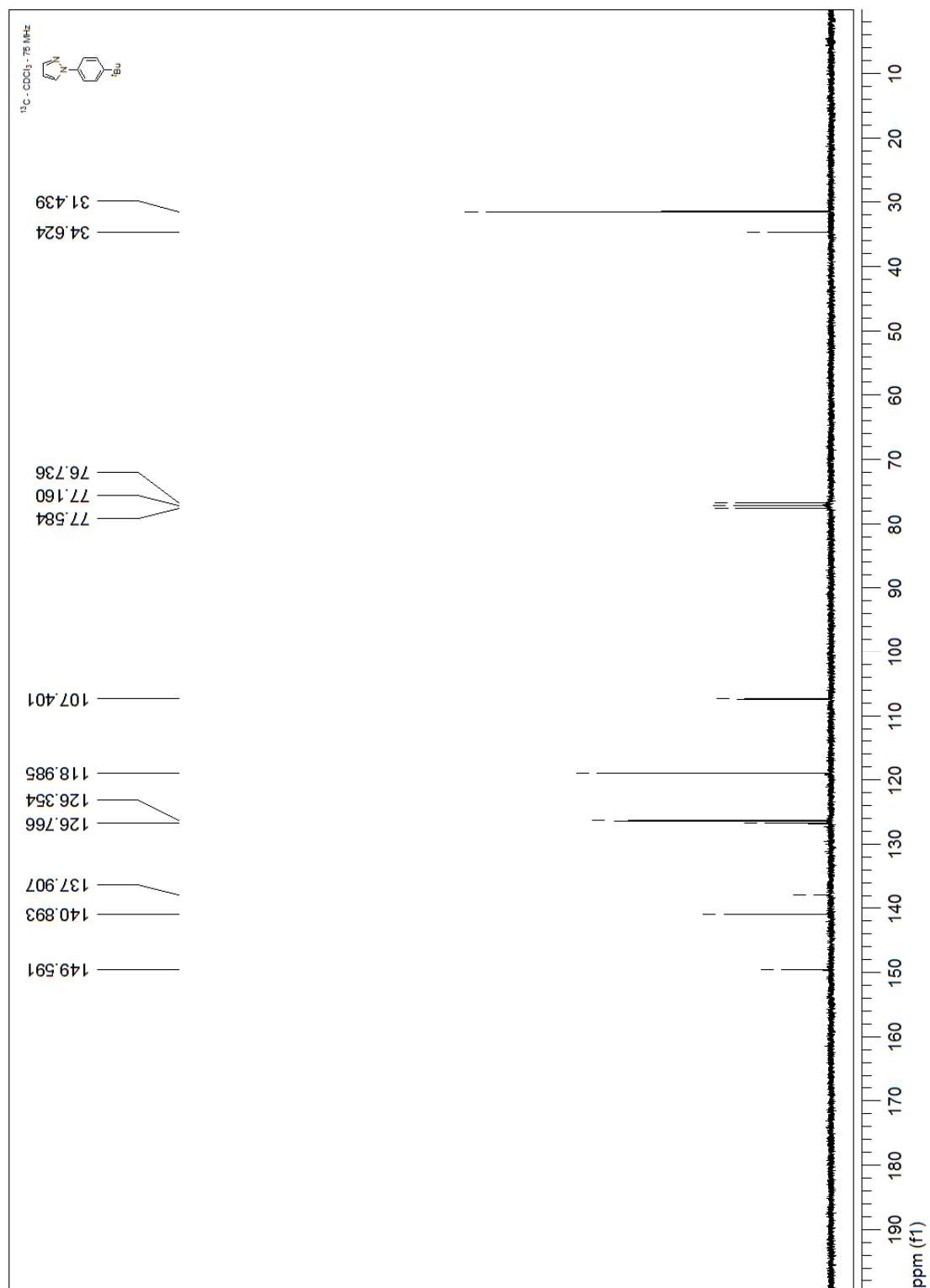
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^1H and ^{13}C NMR spectra

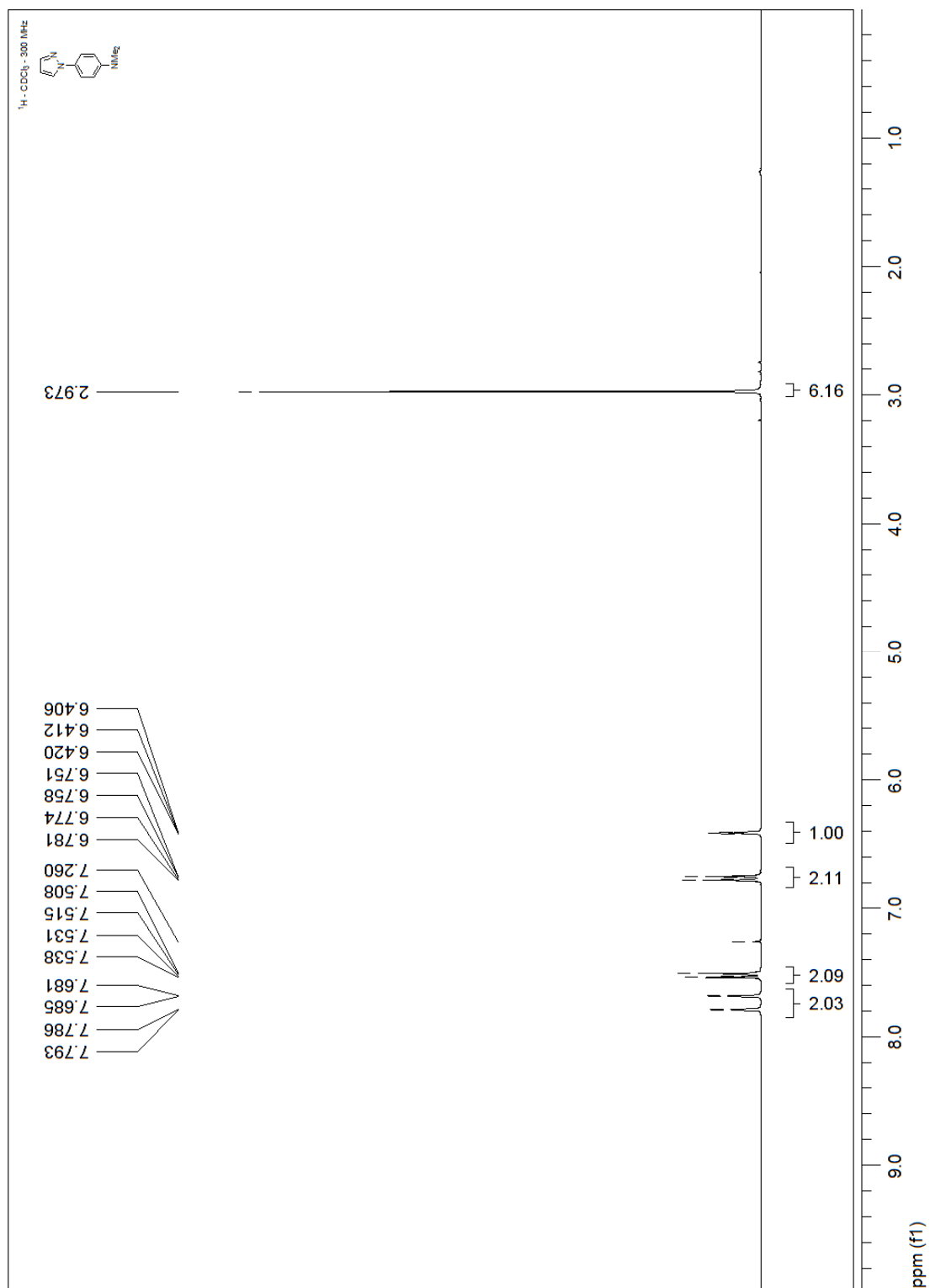
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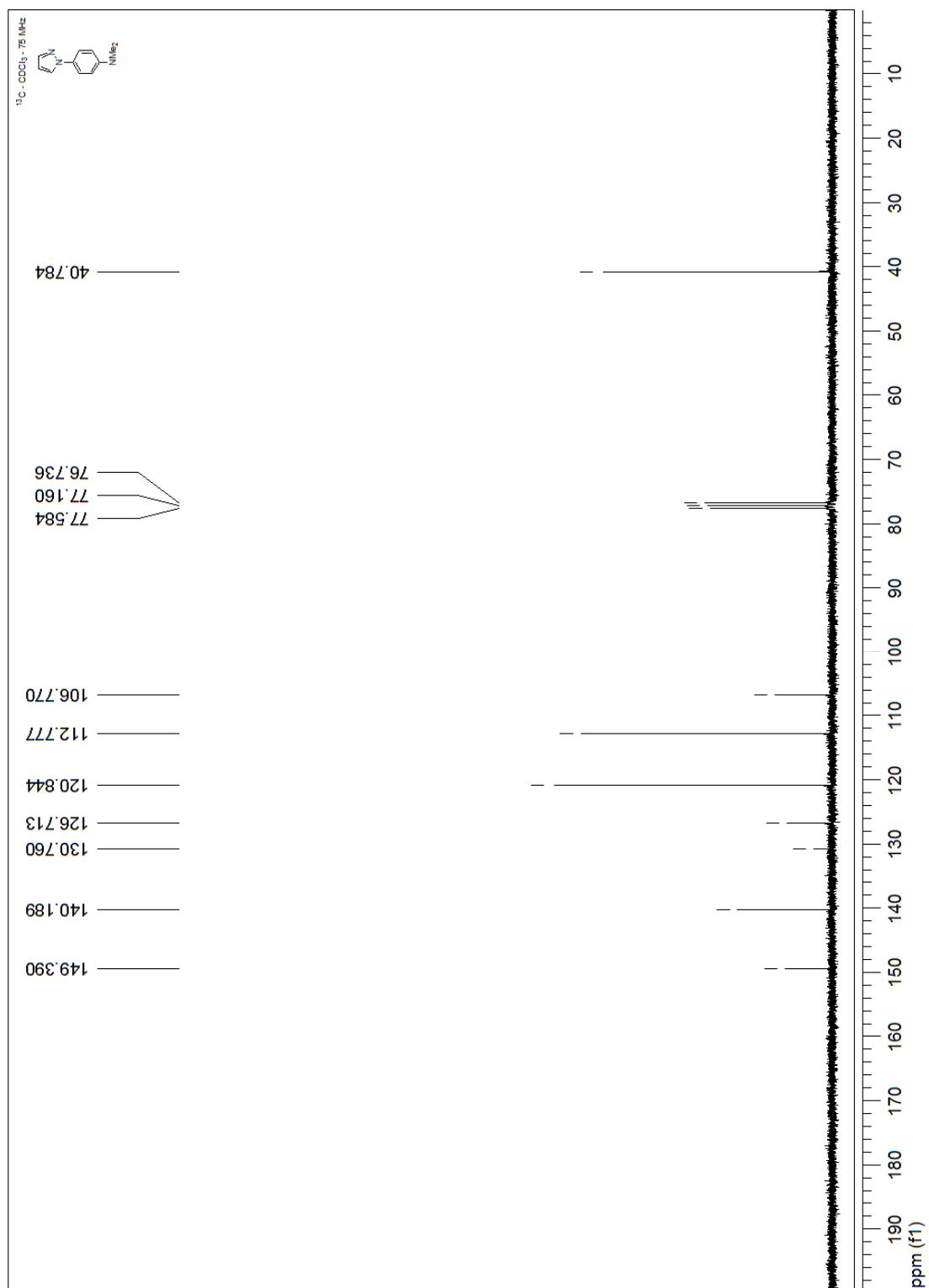
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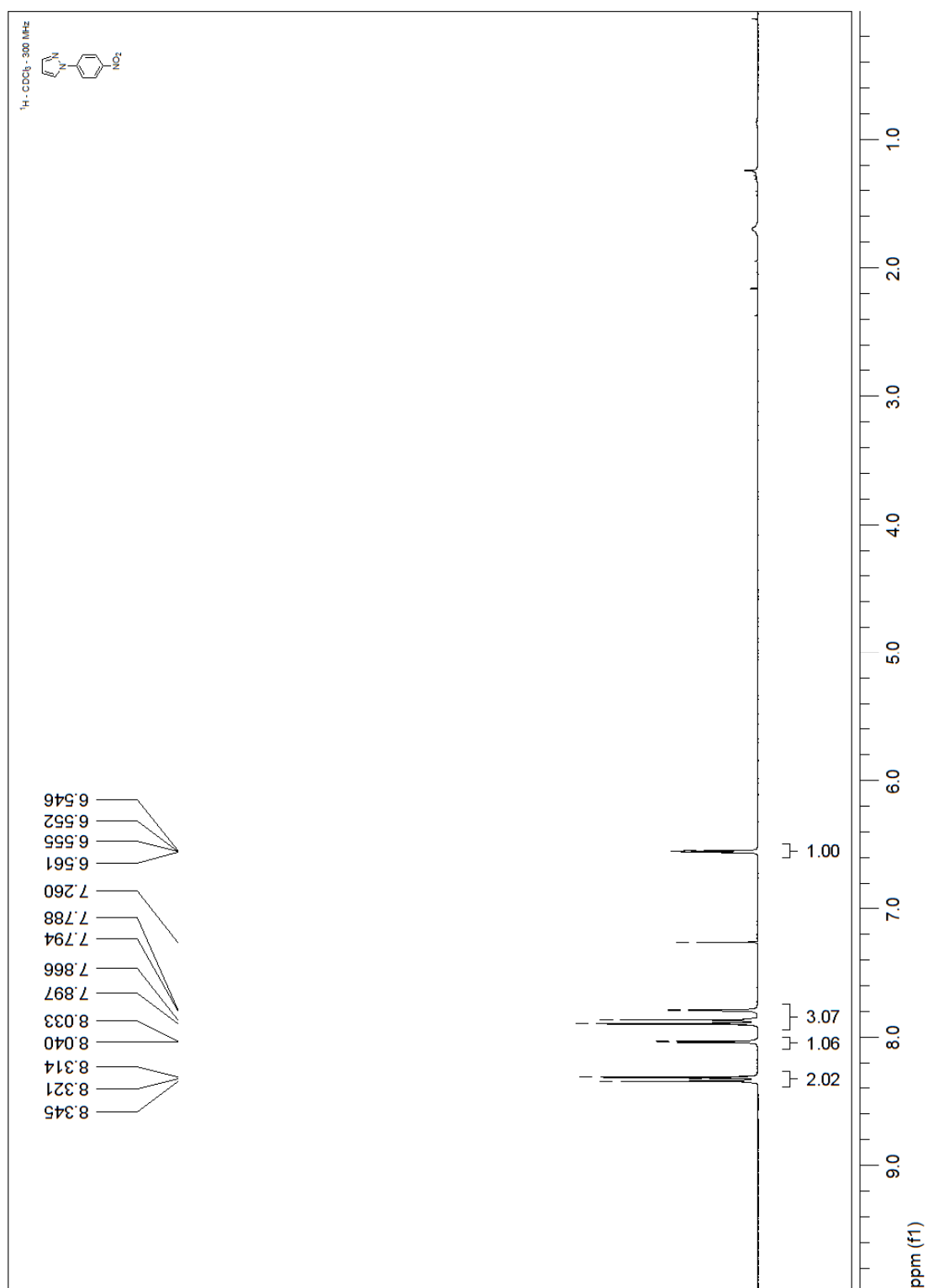
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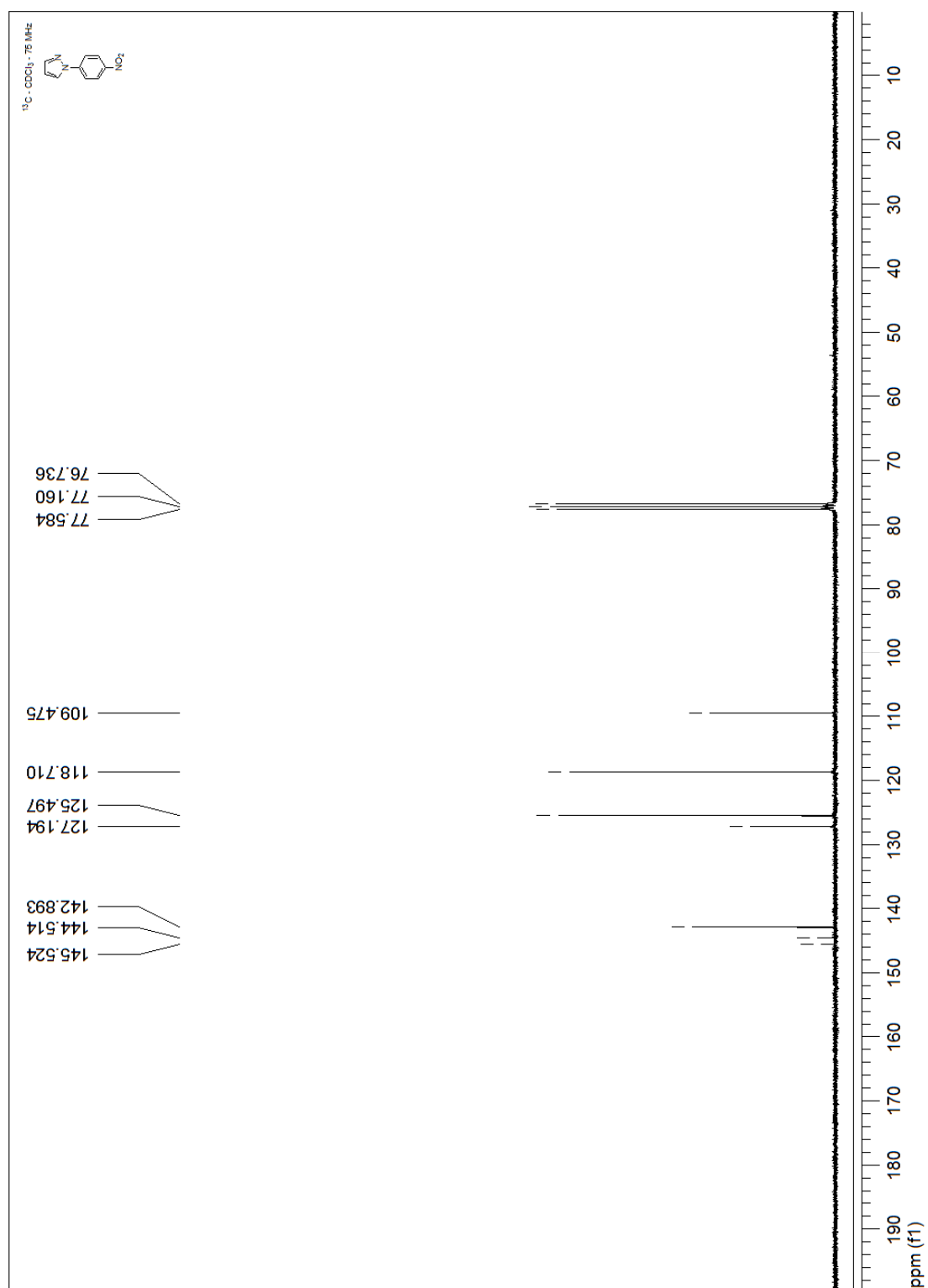
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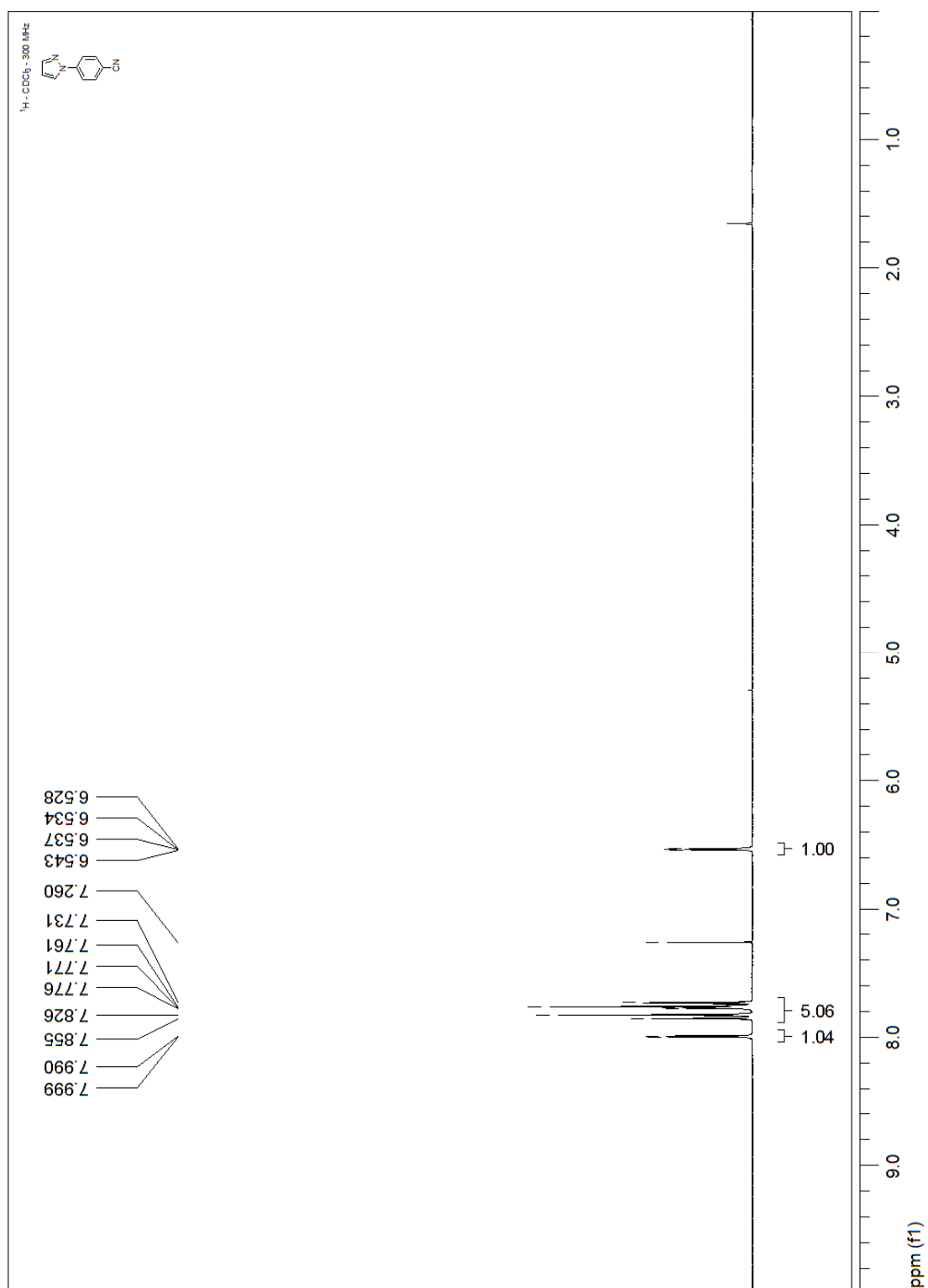
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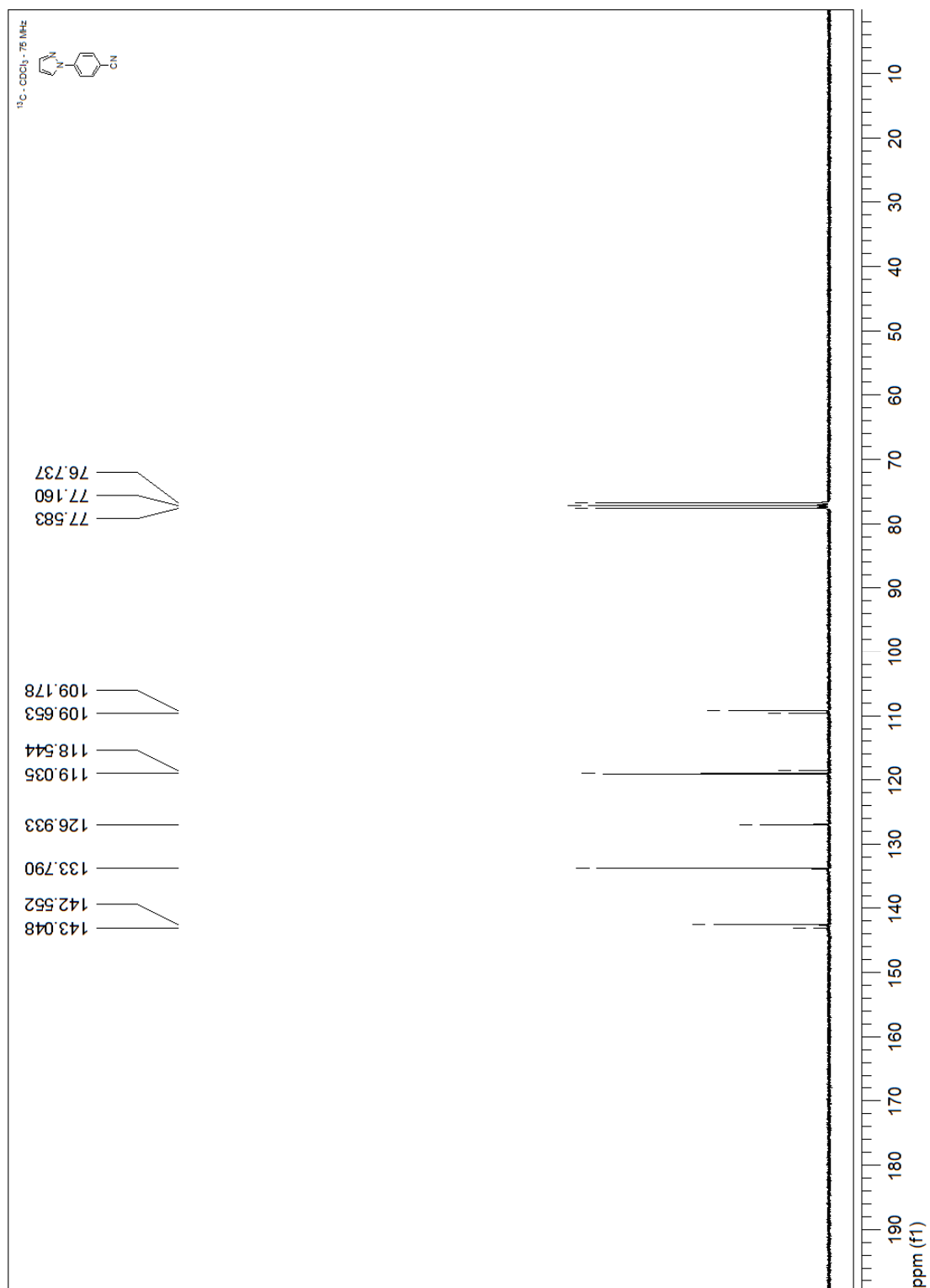
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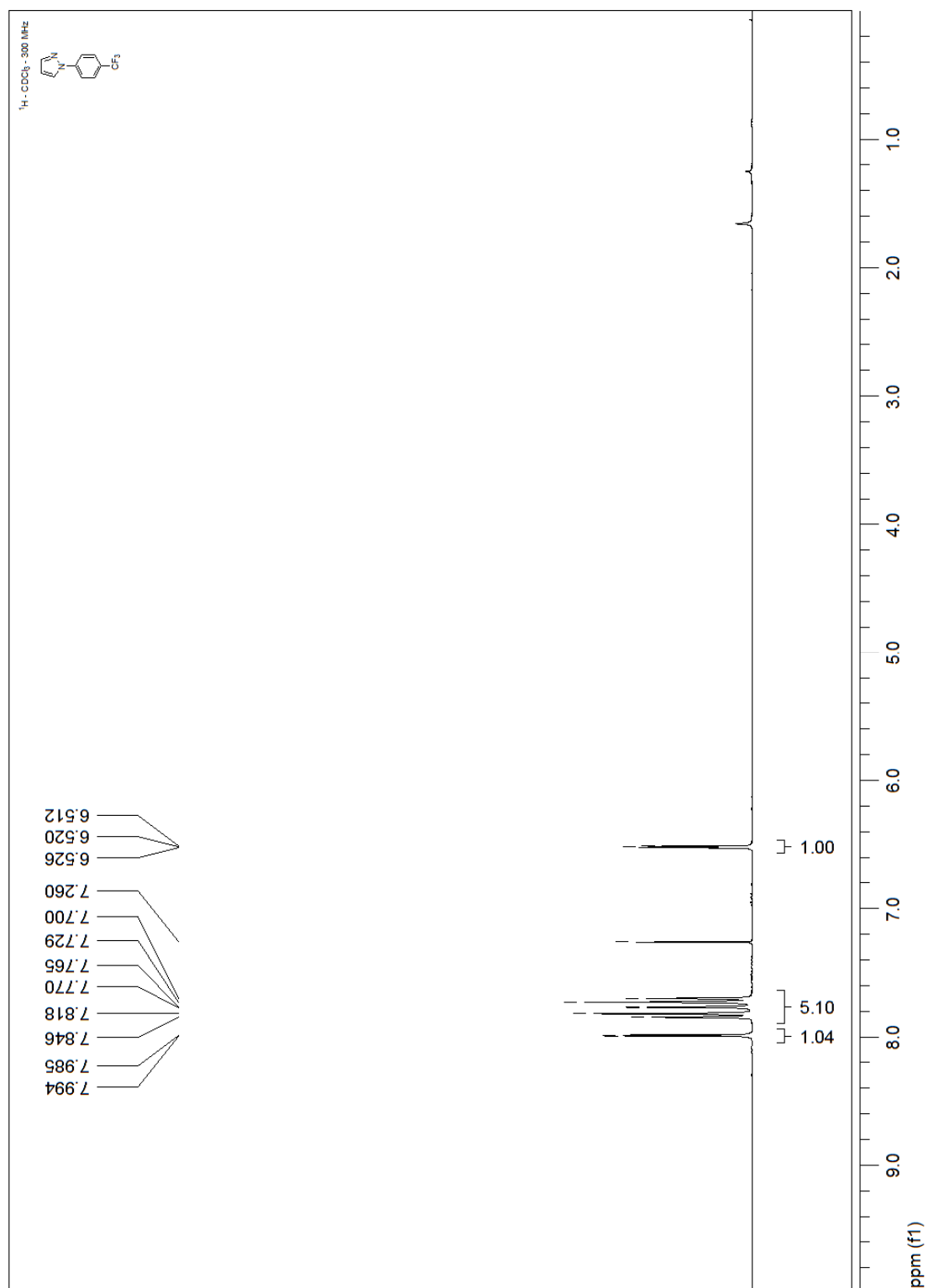
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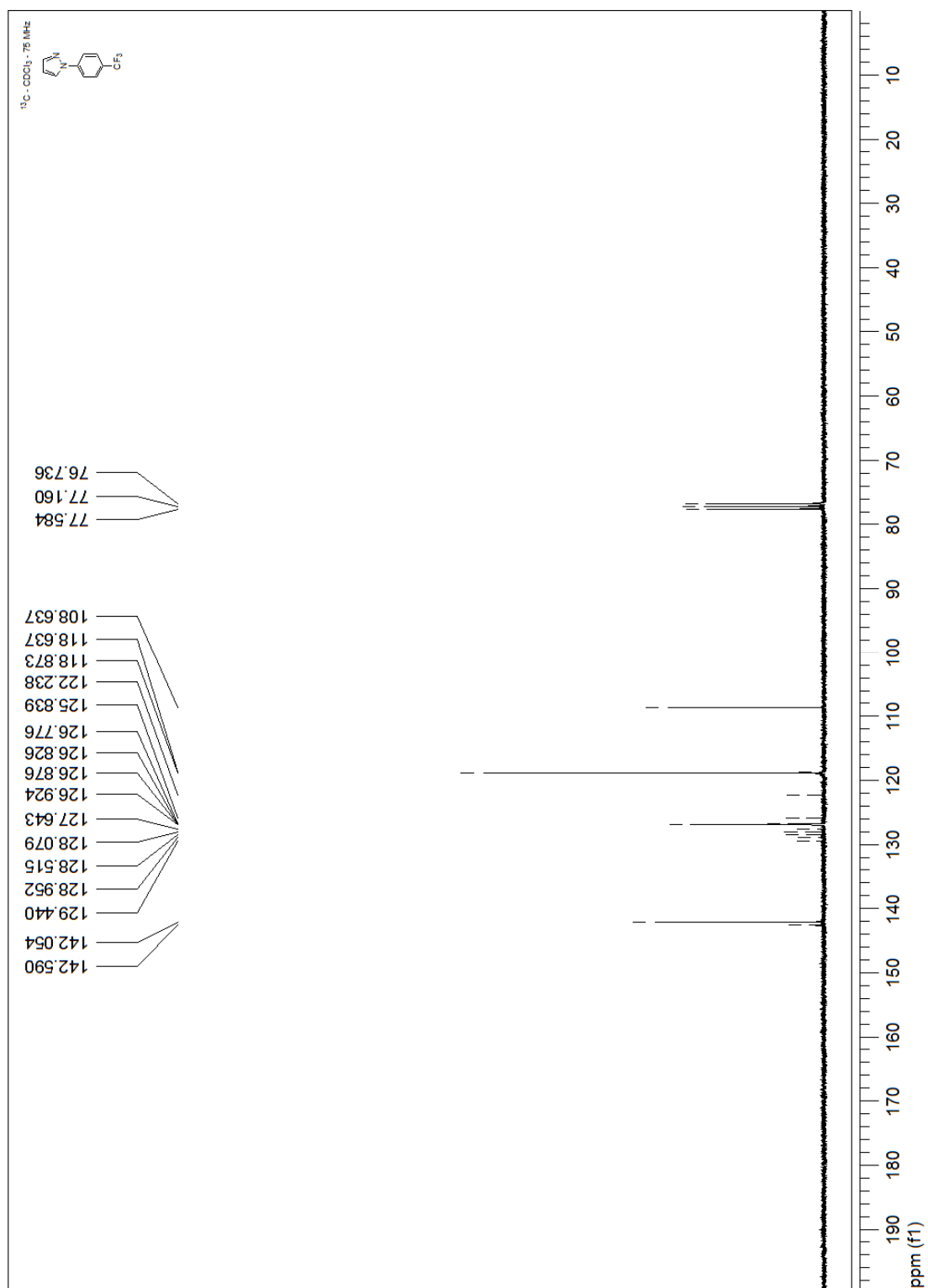
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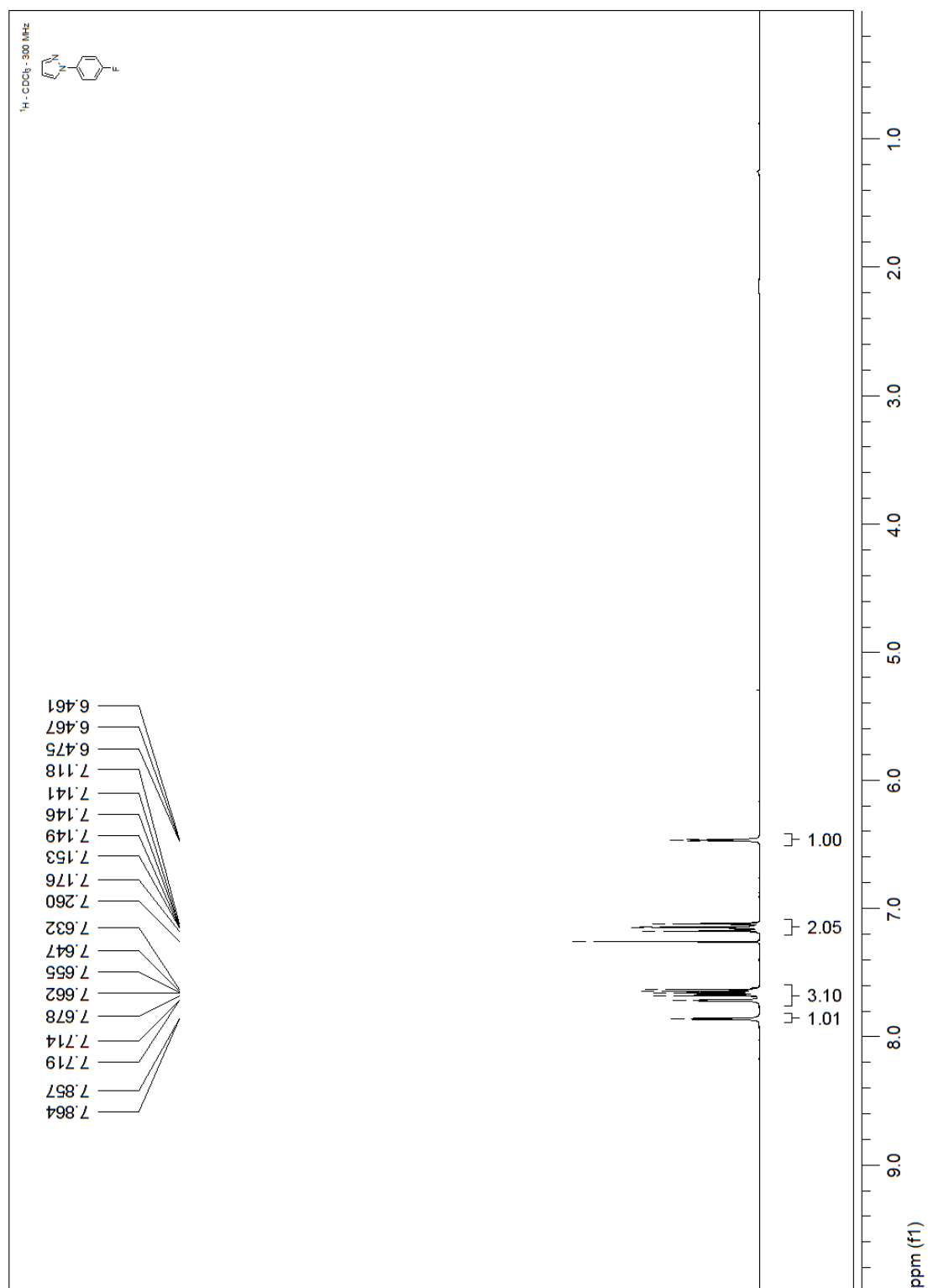
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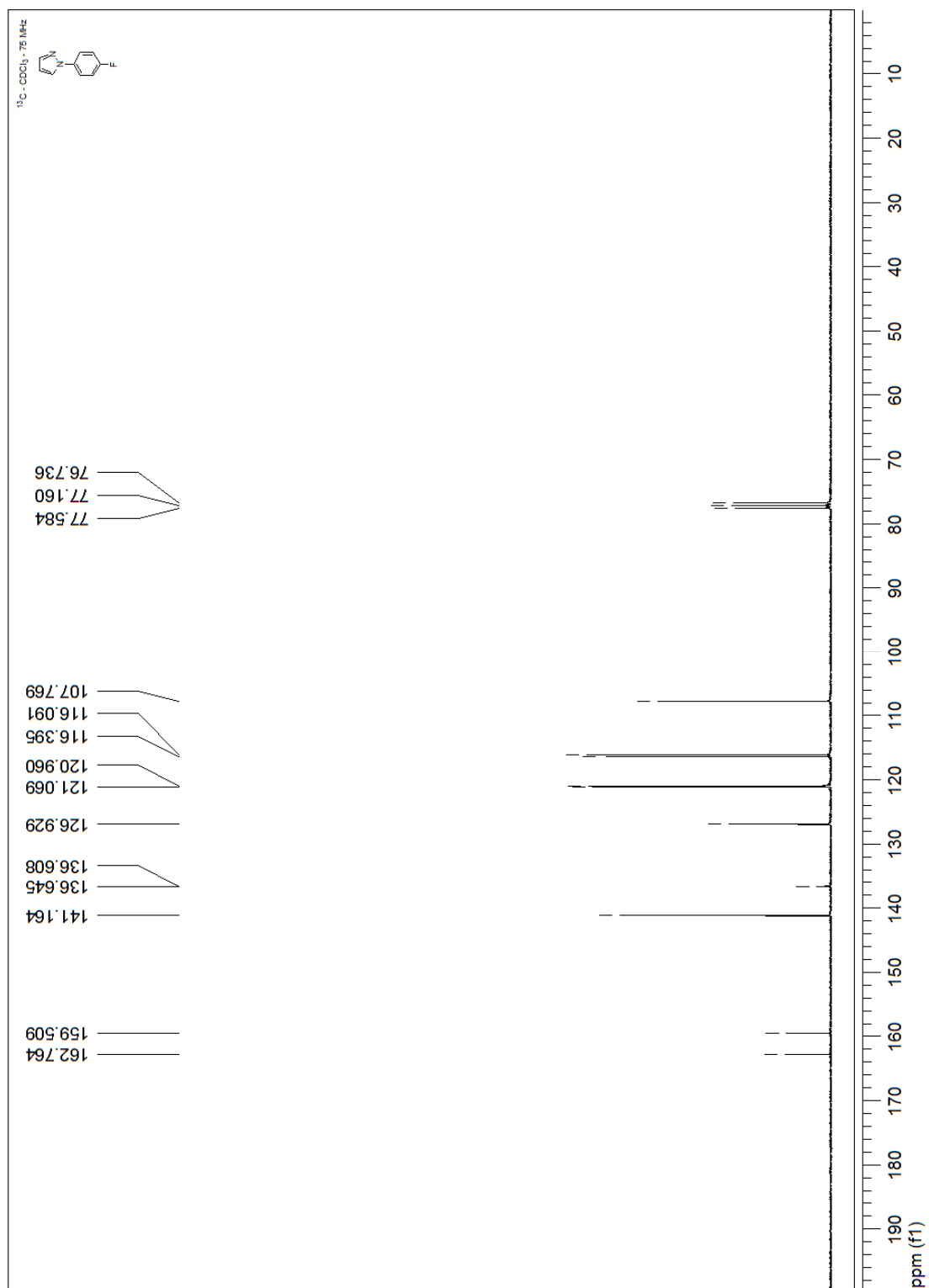
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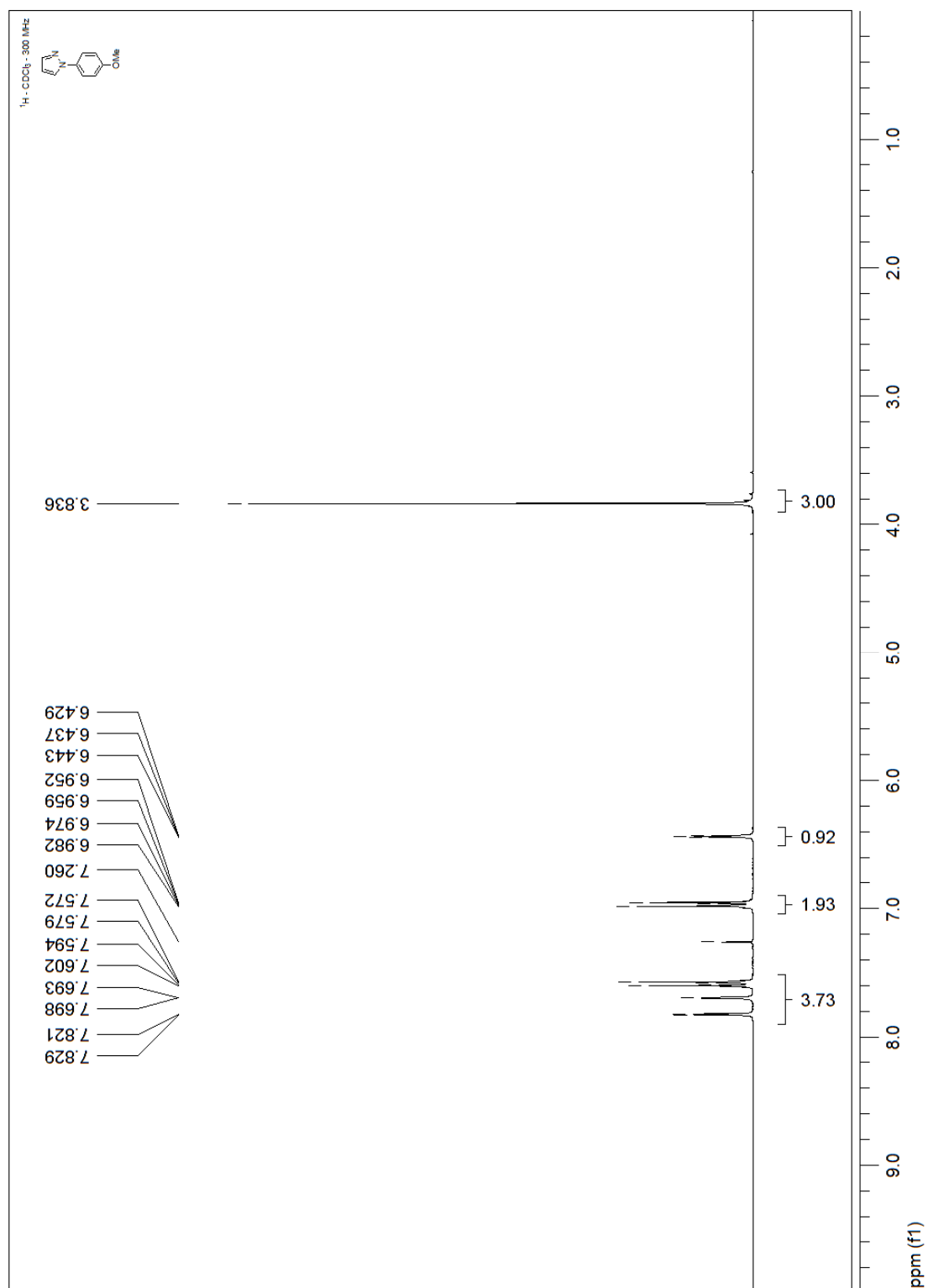
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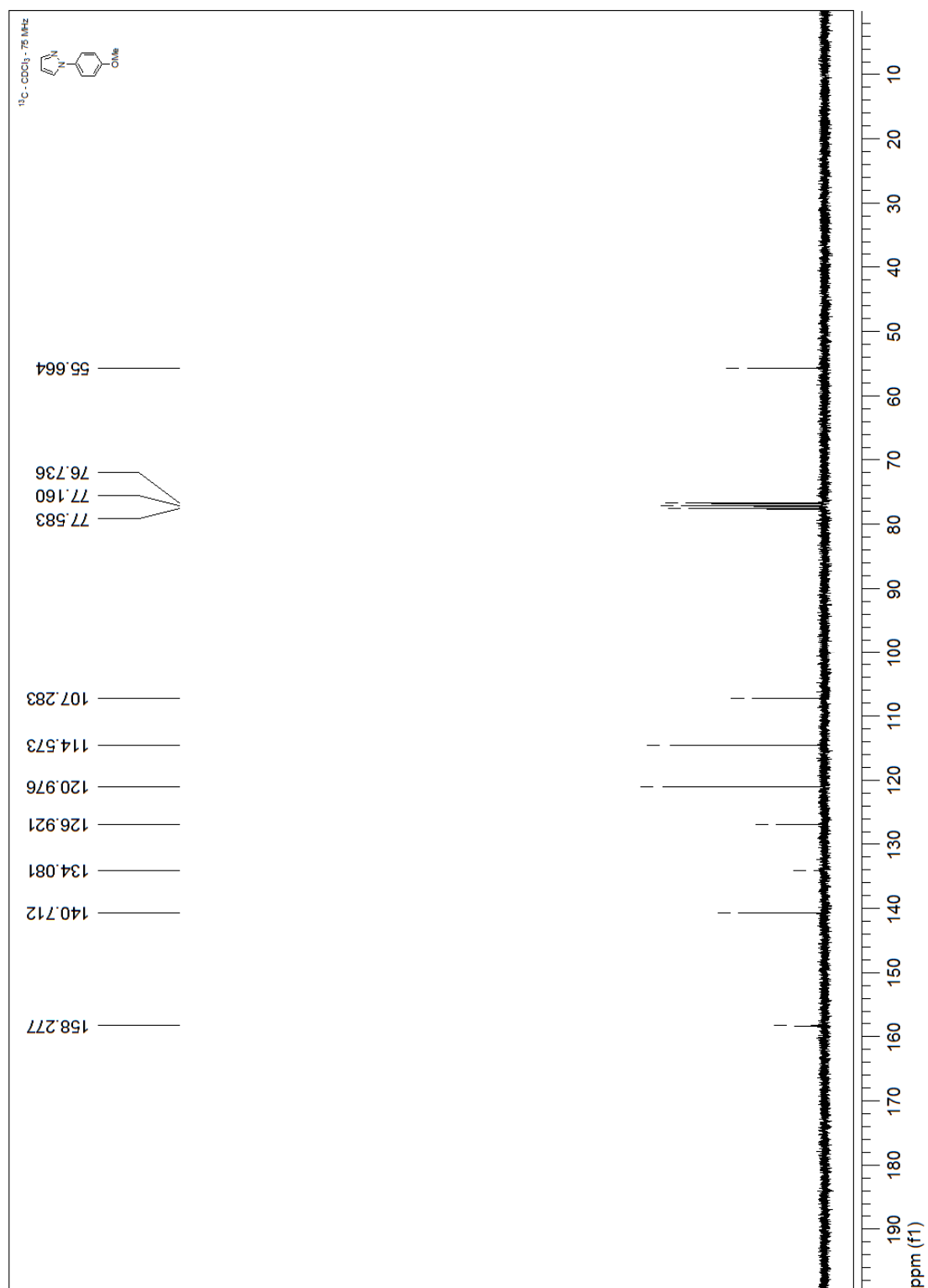
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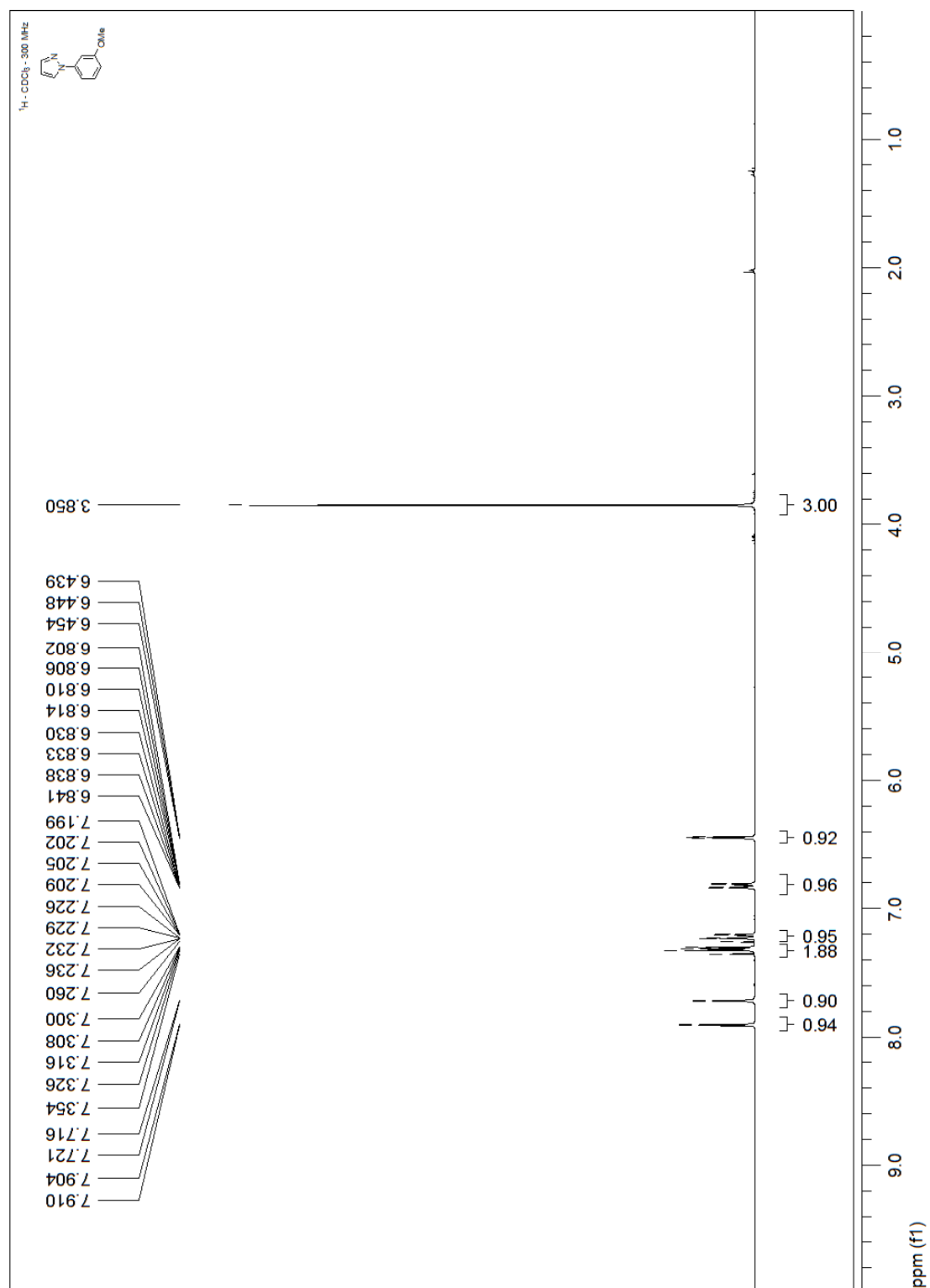
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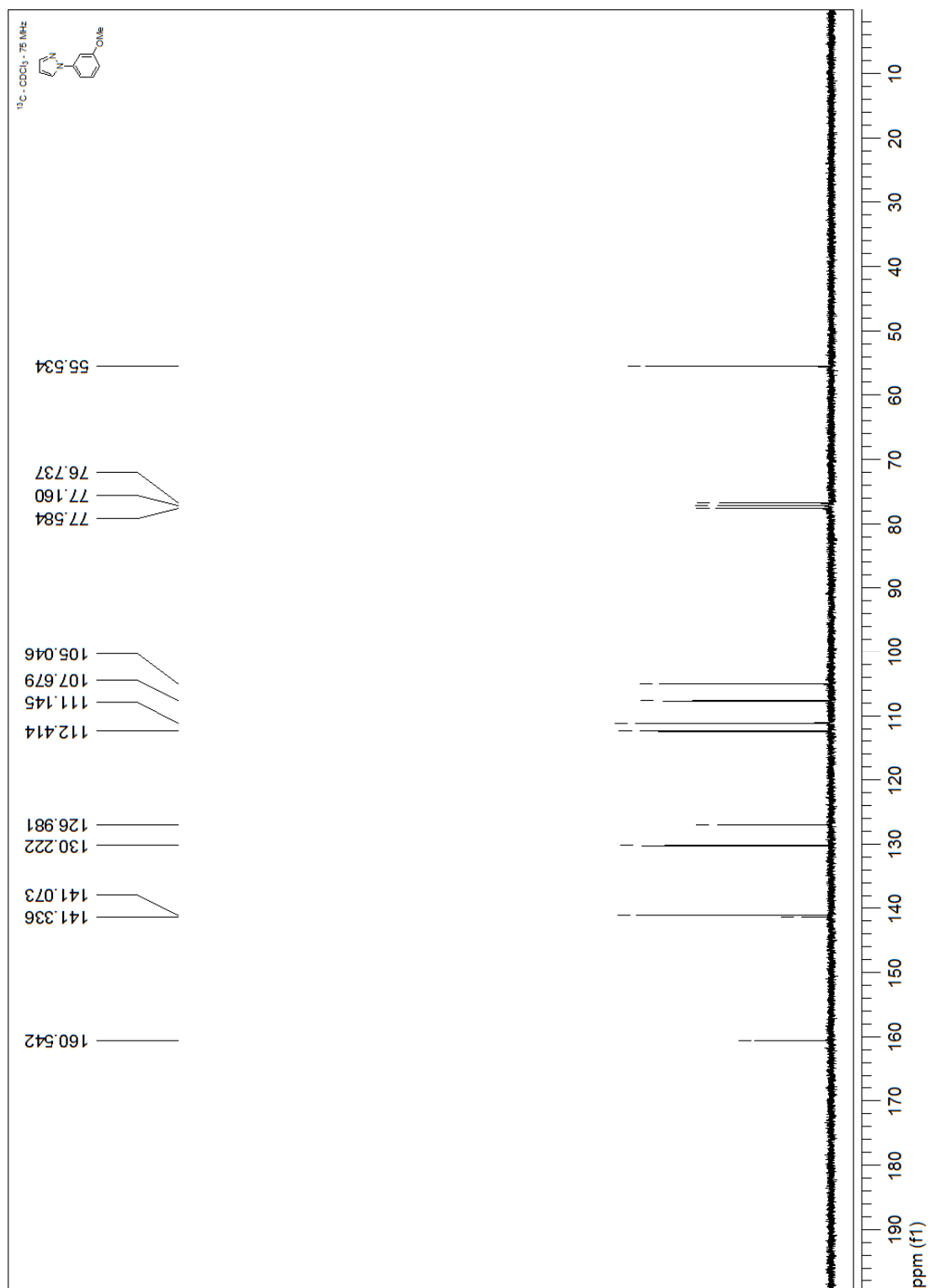
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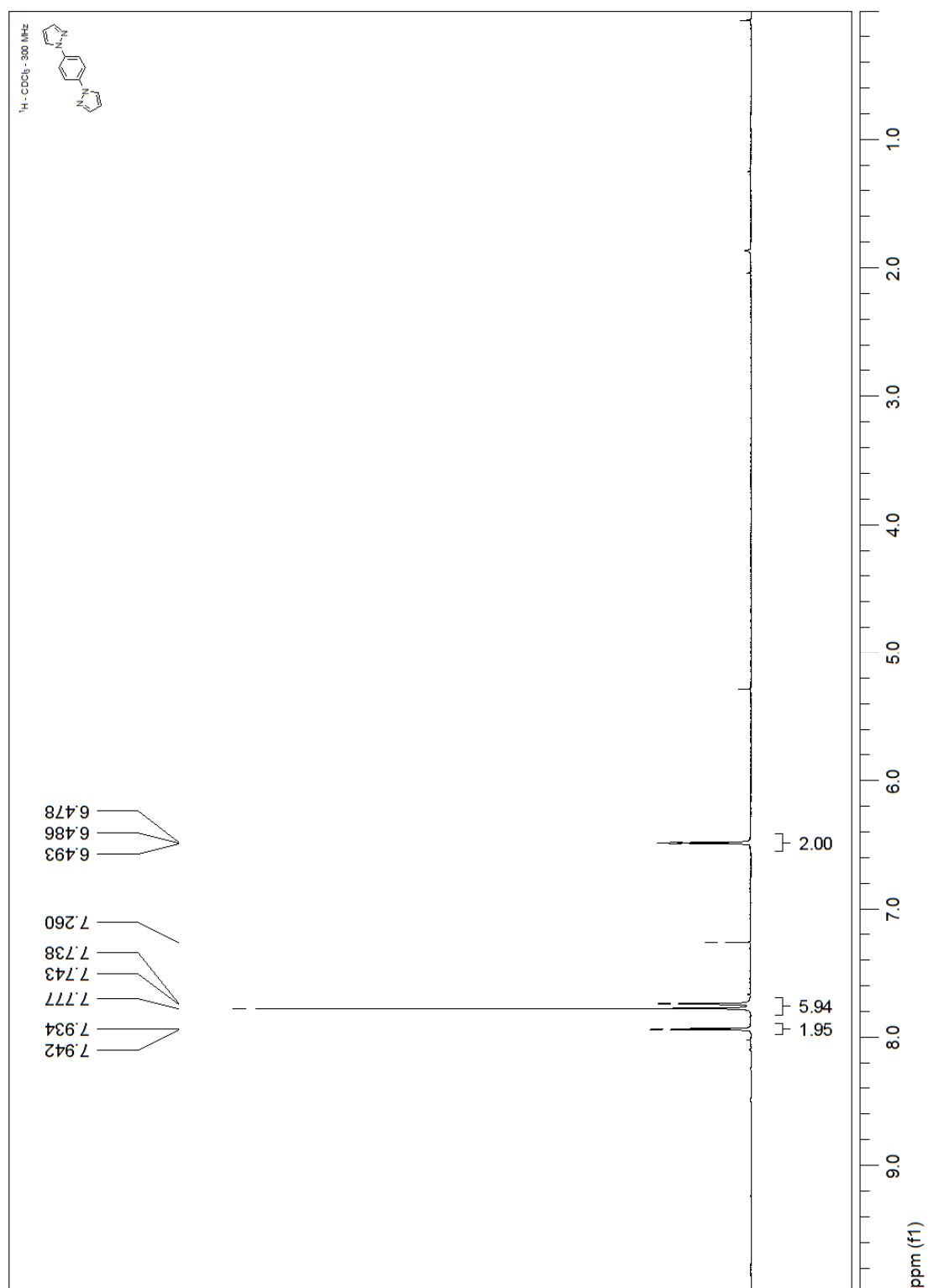
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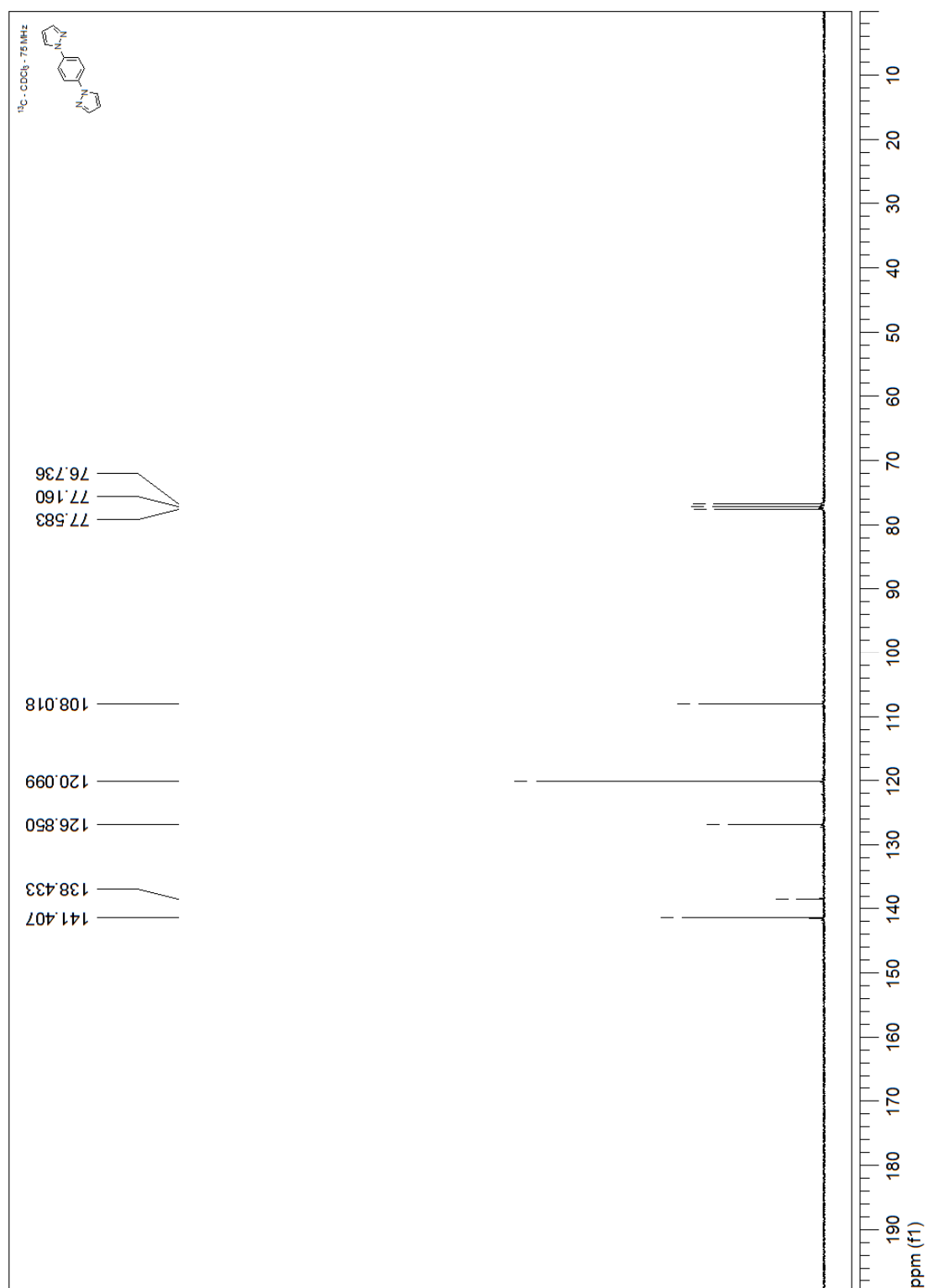
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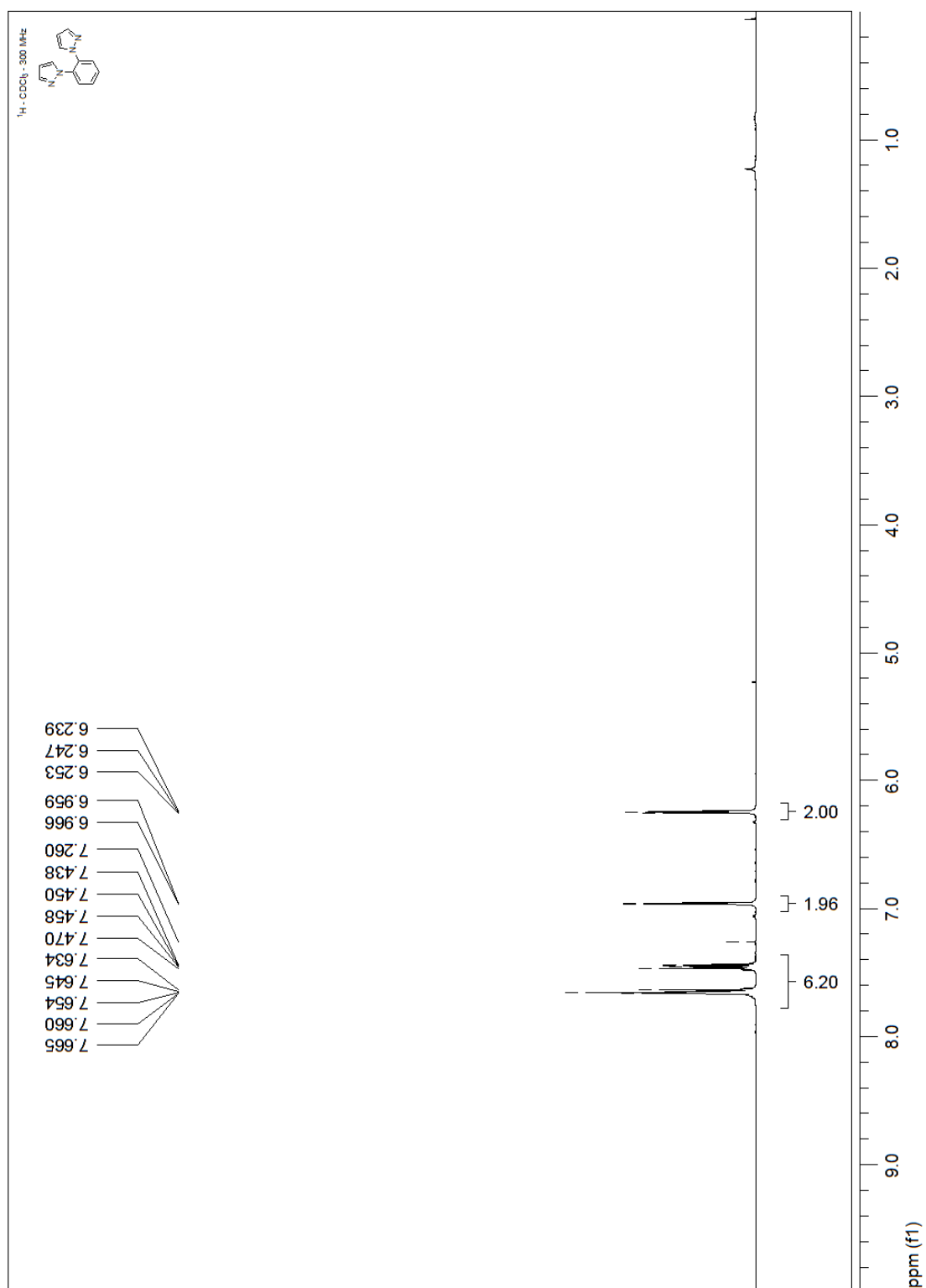
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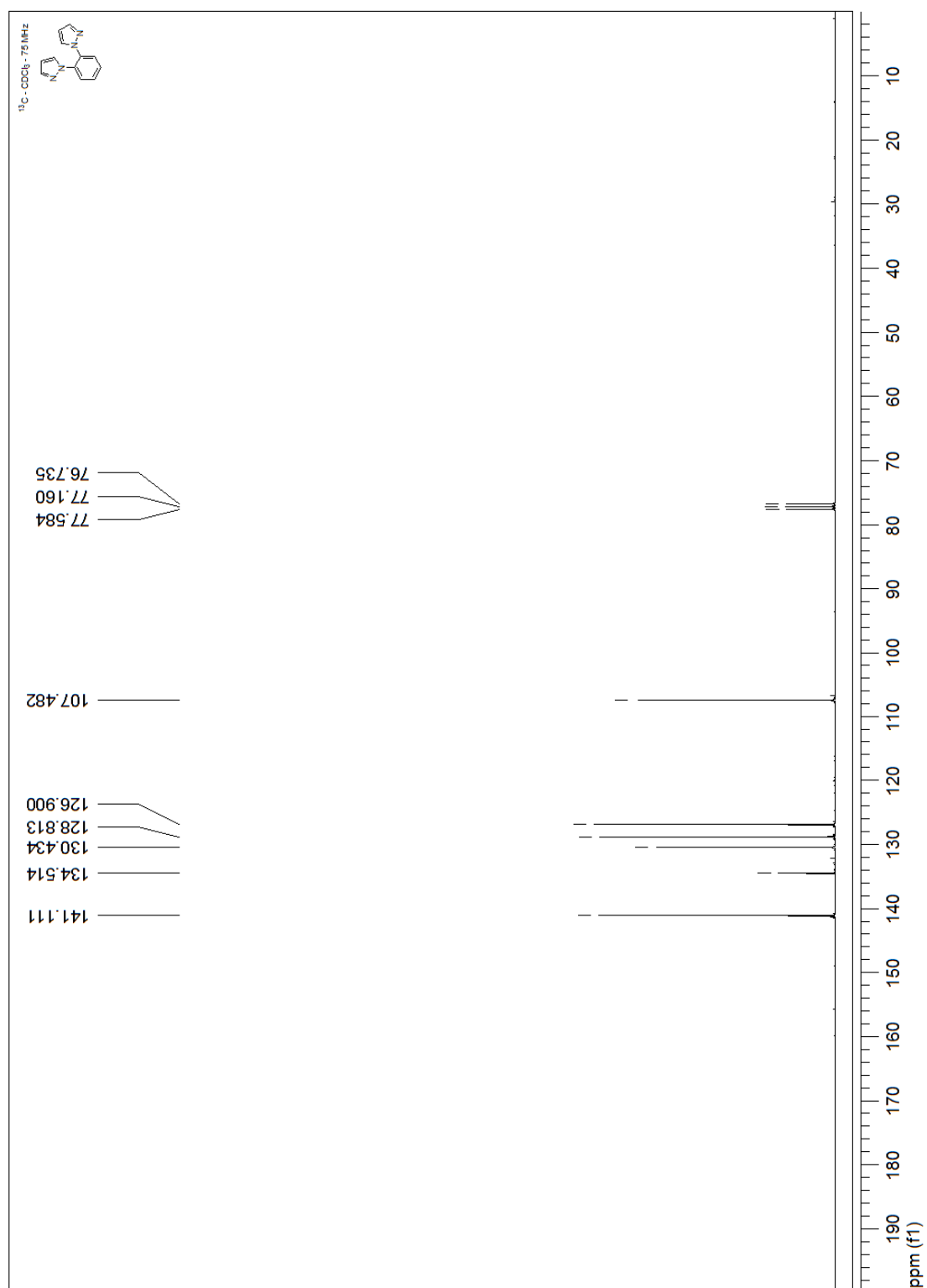
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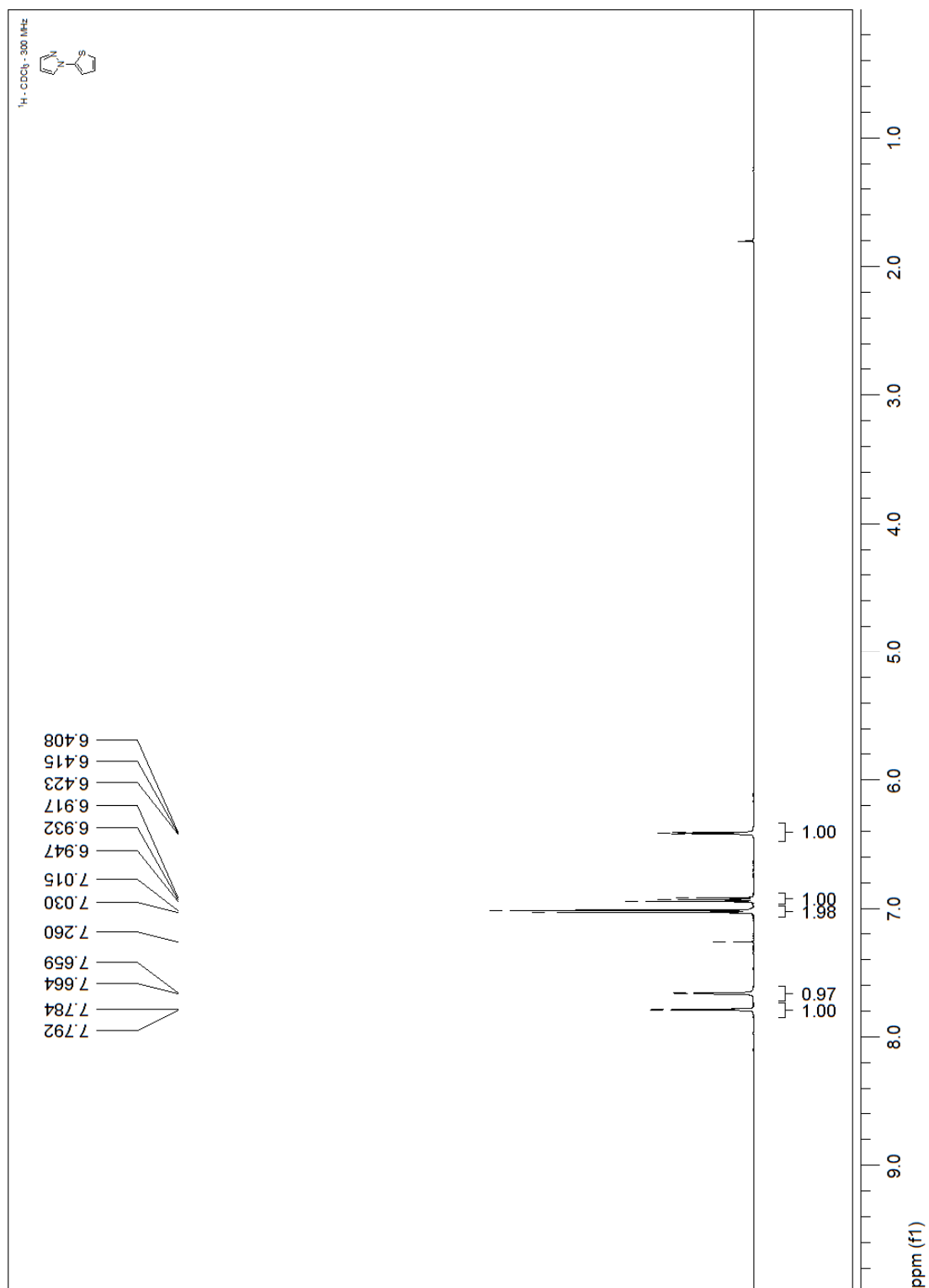
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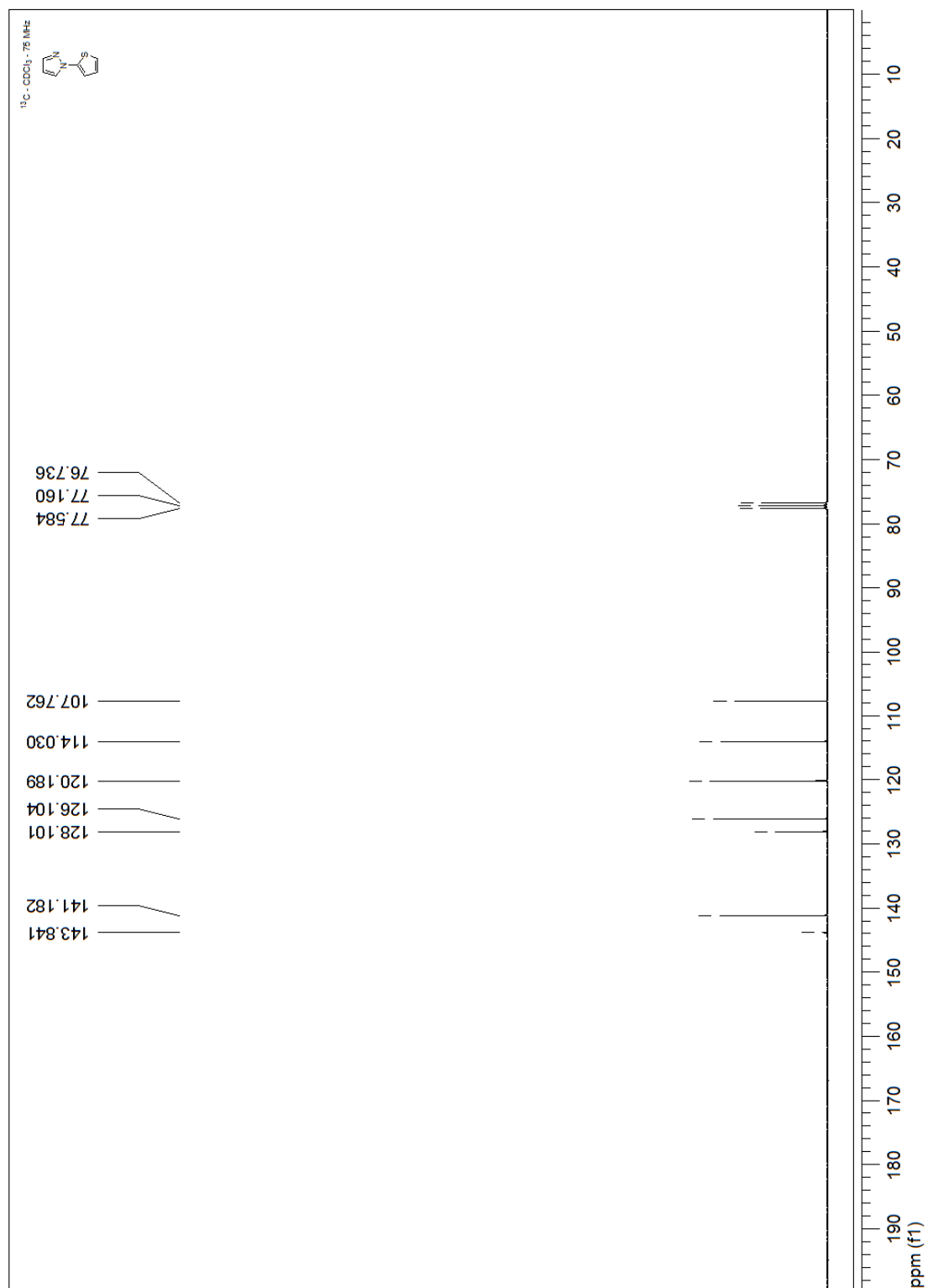
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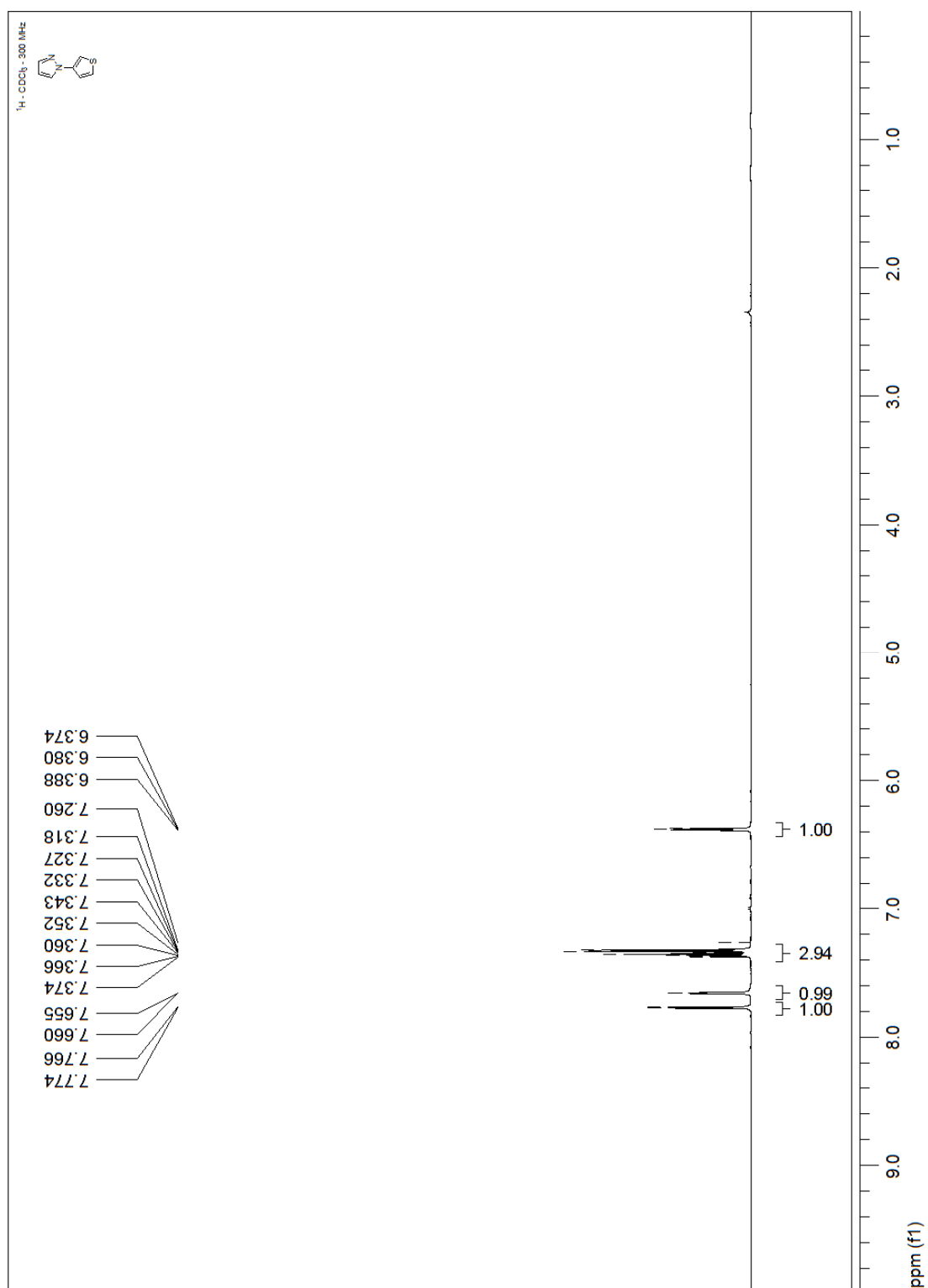
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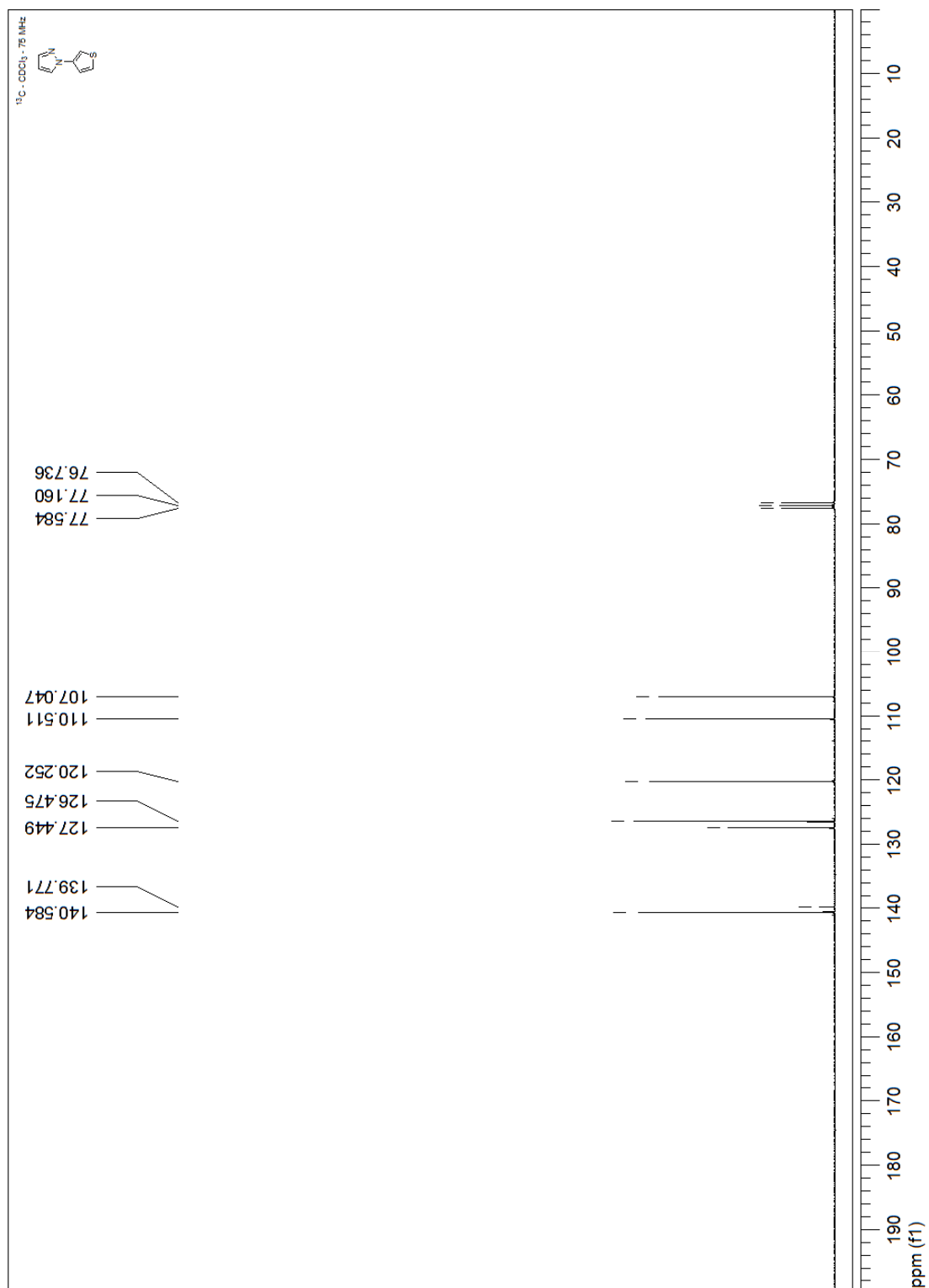
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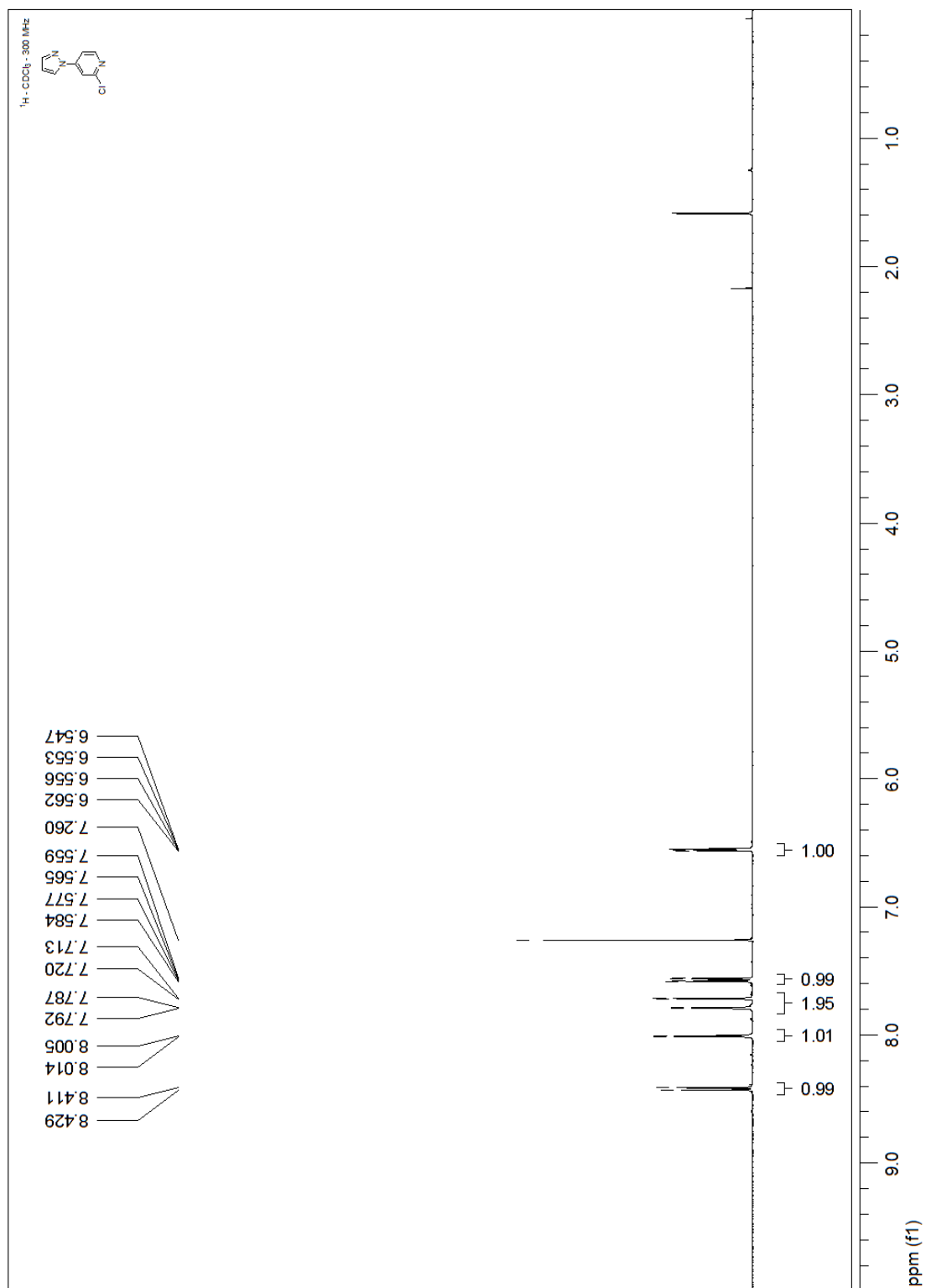
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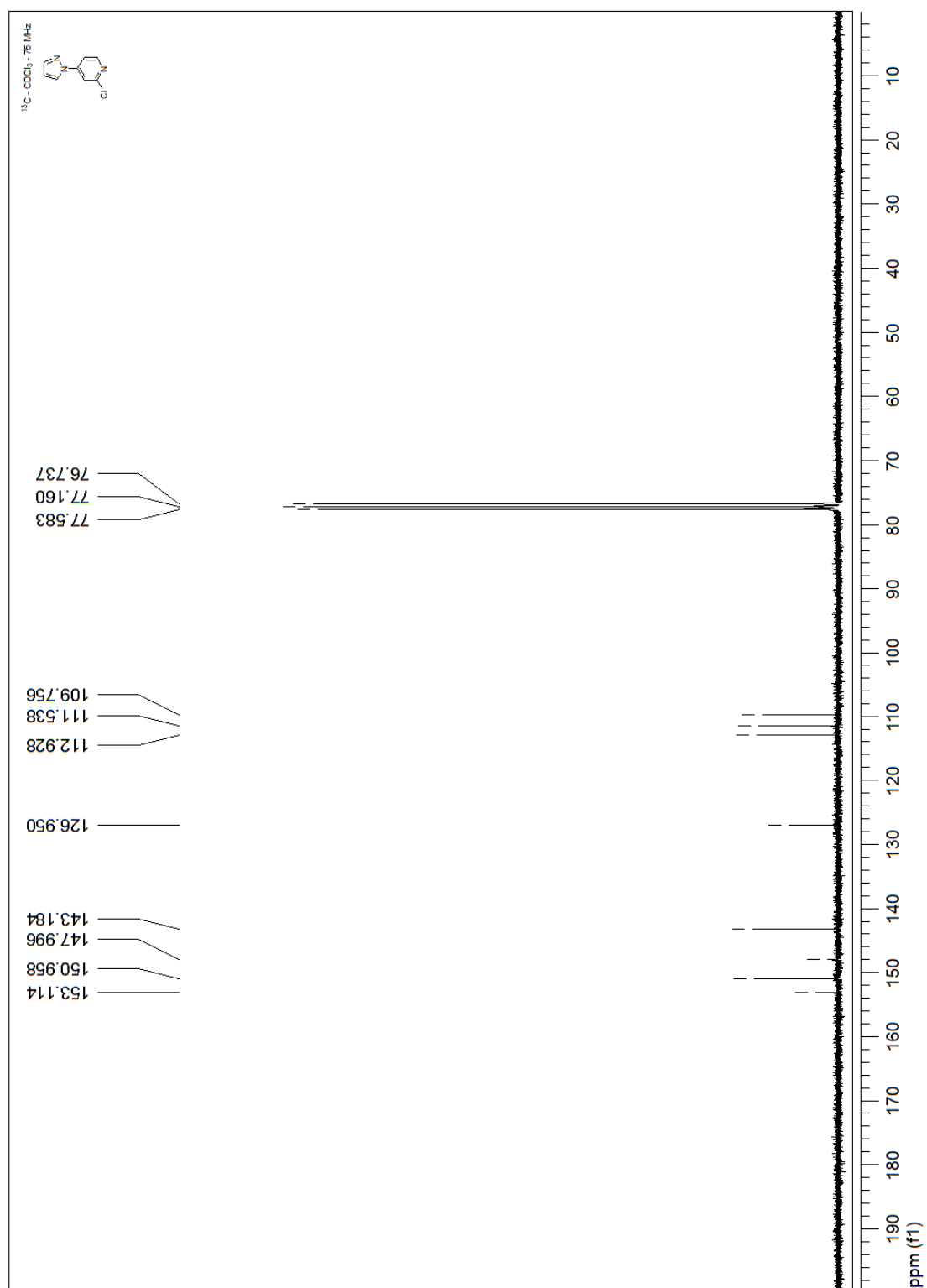
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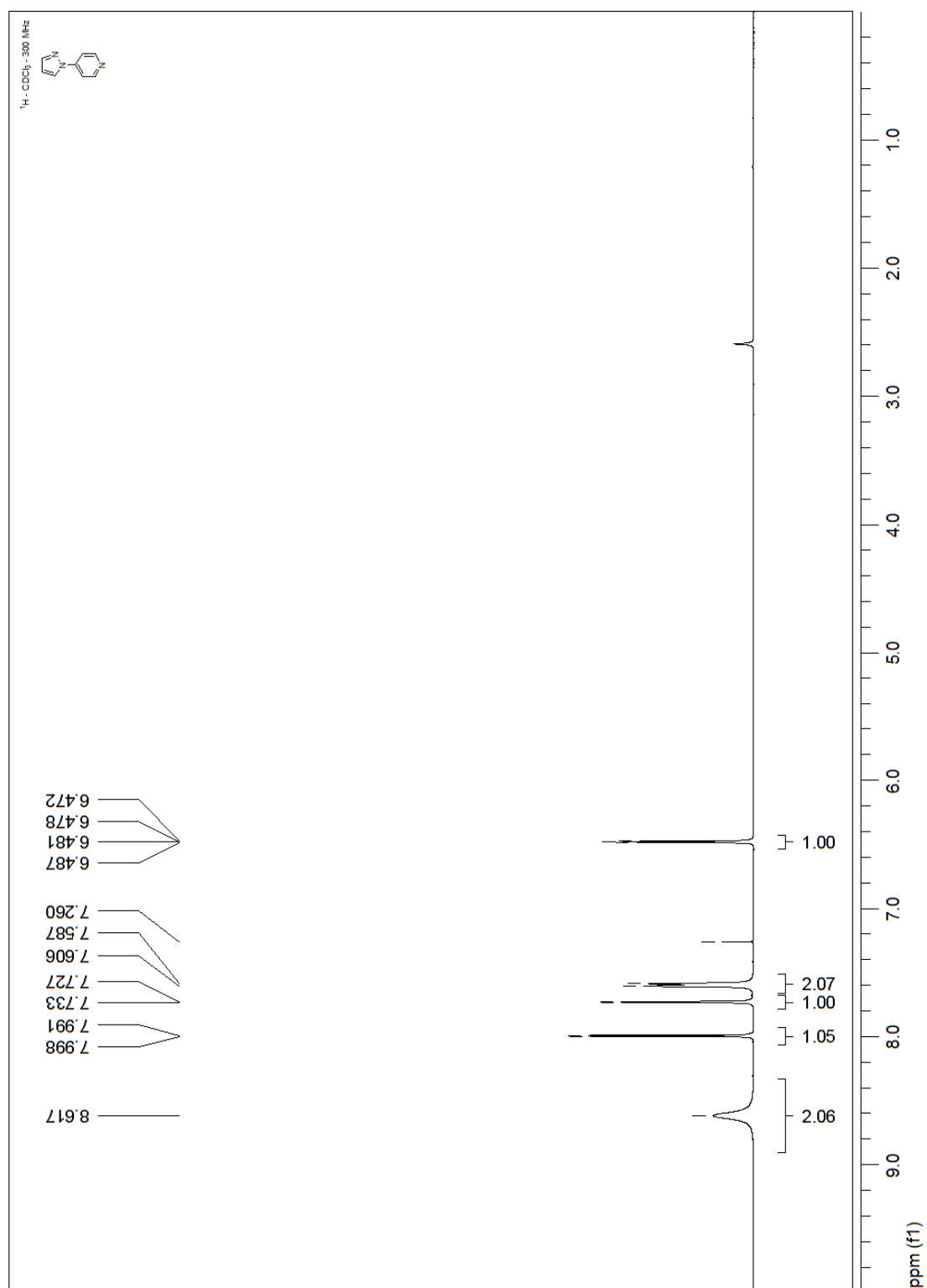
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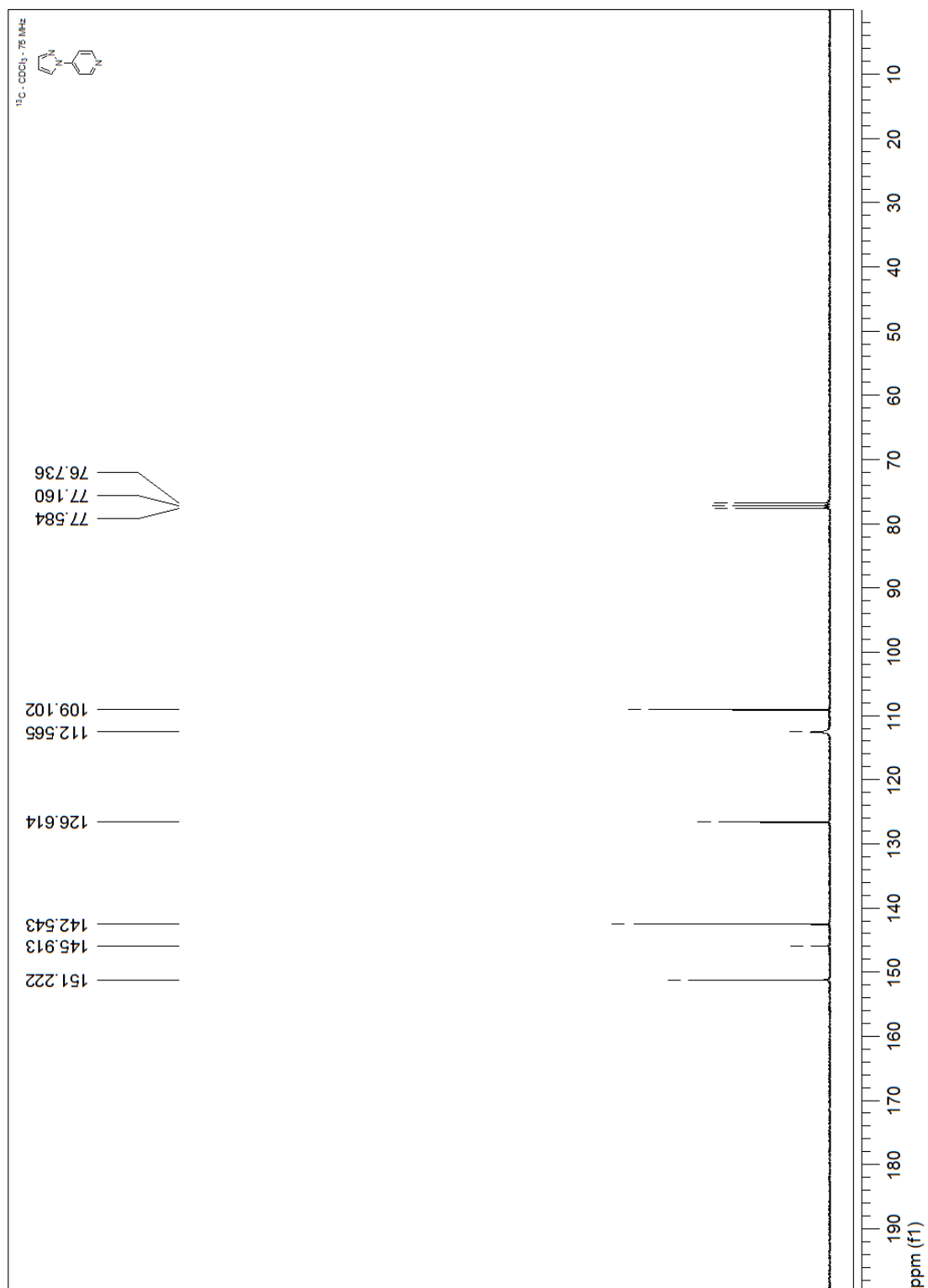
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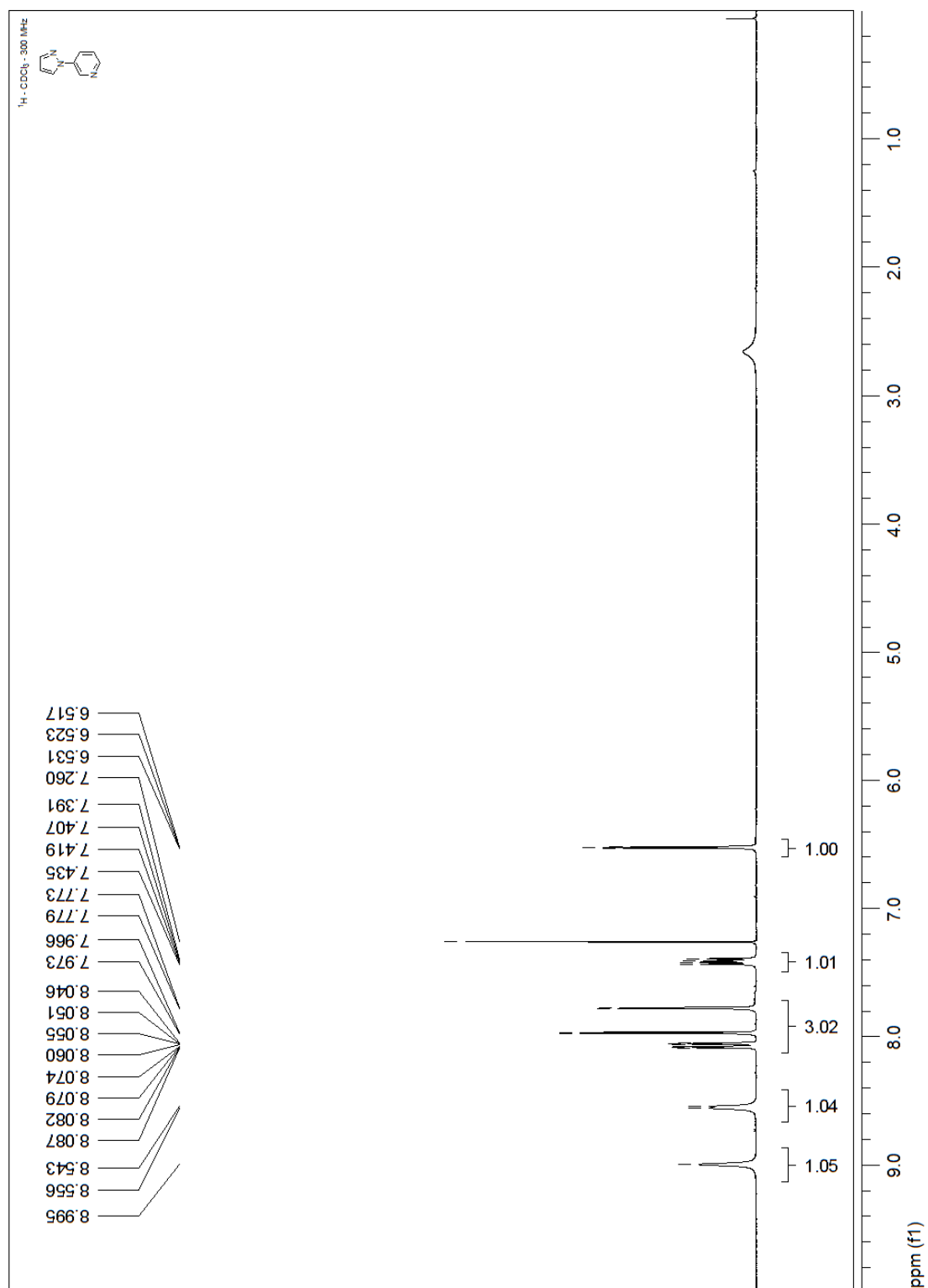
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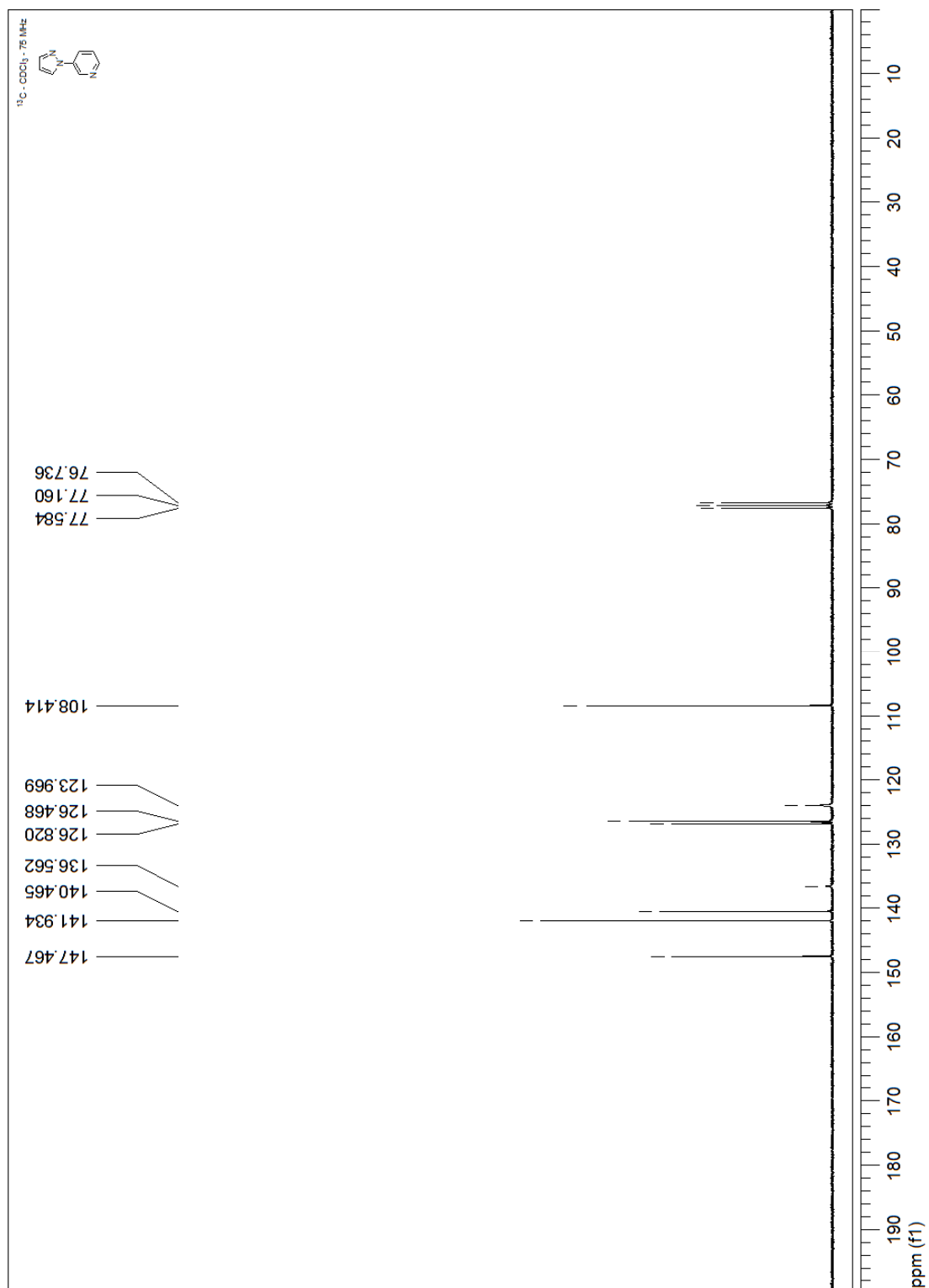
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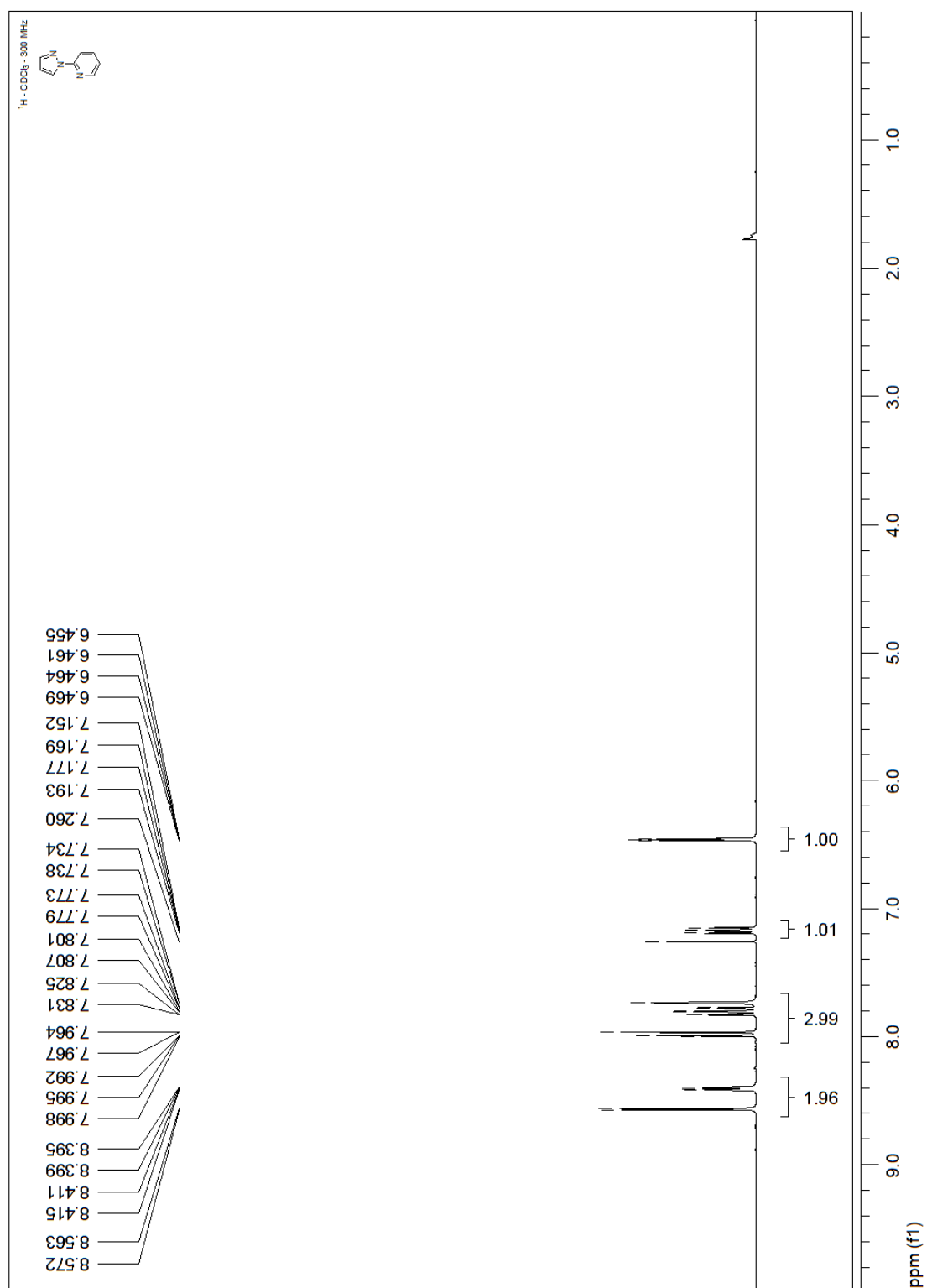
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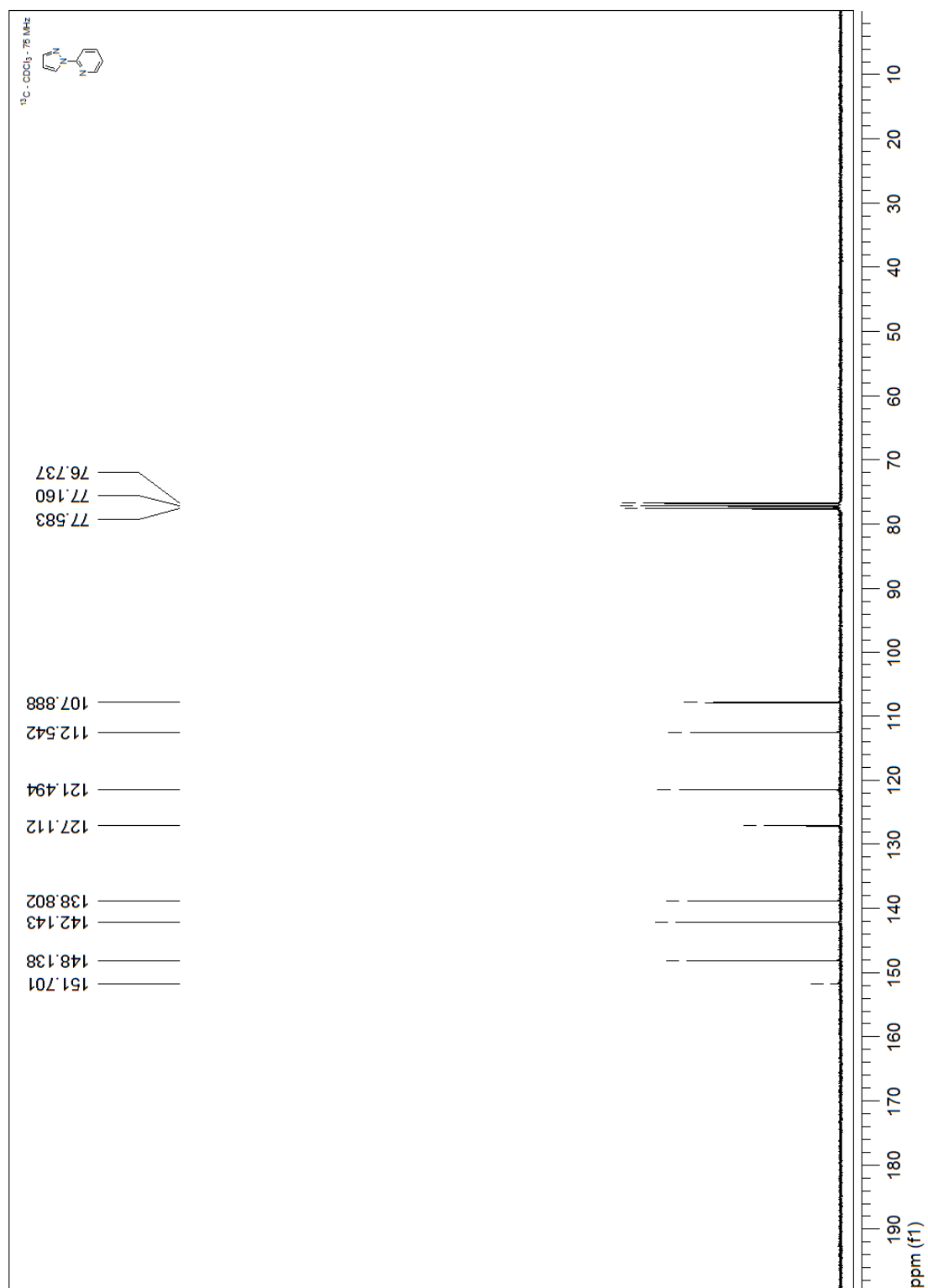
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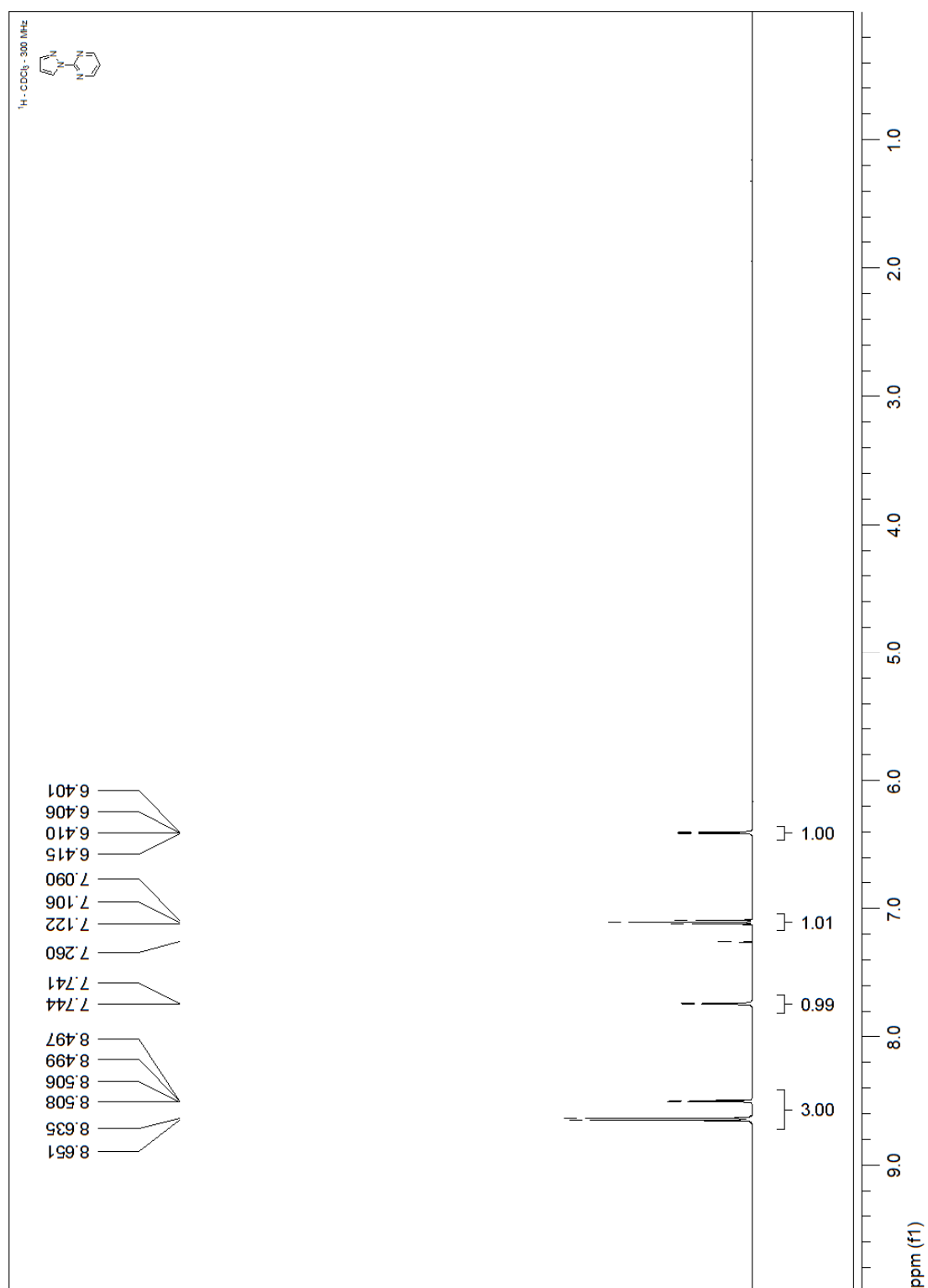
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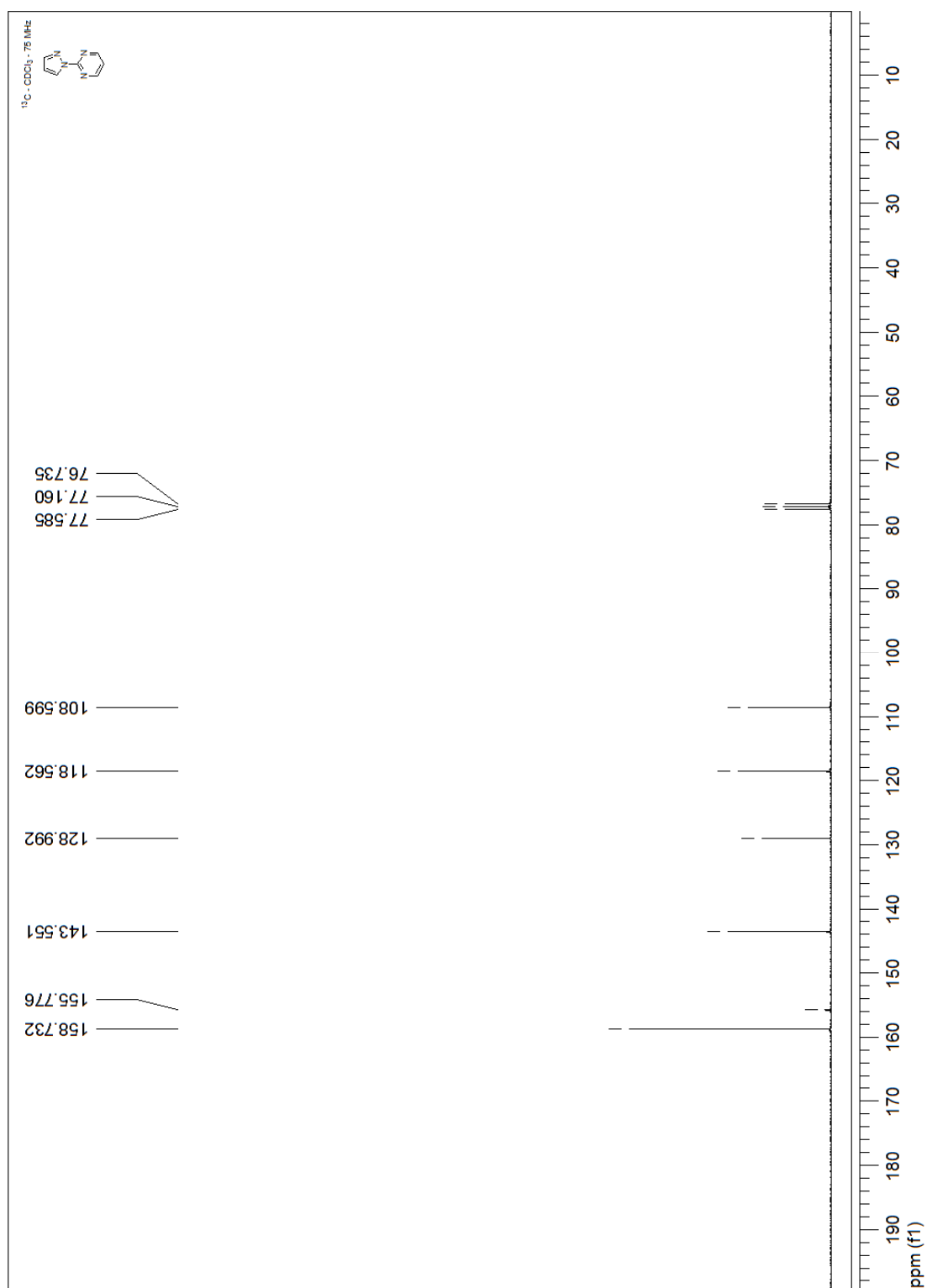
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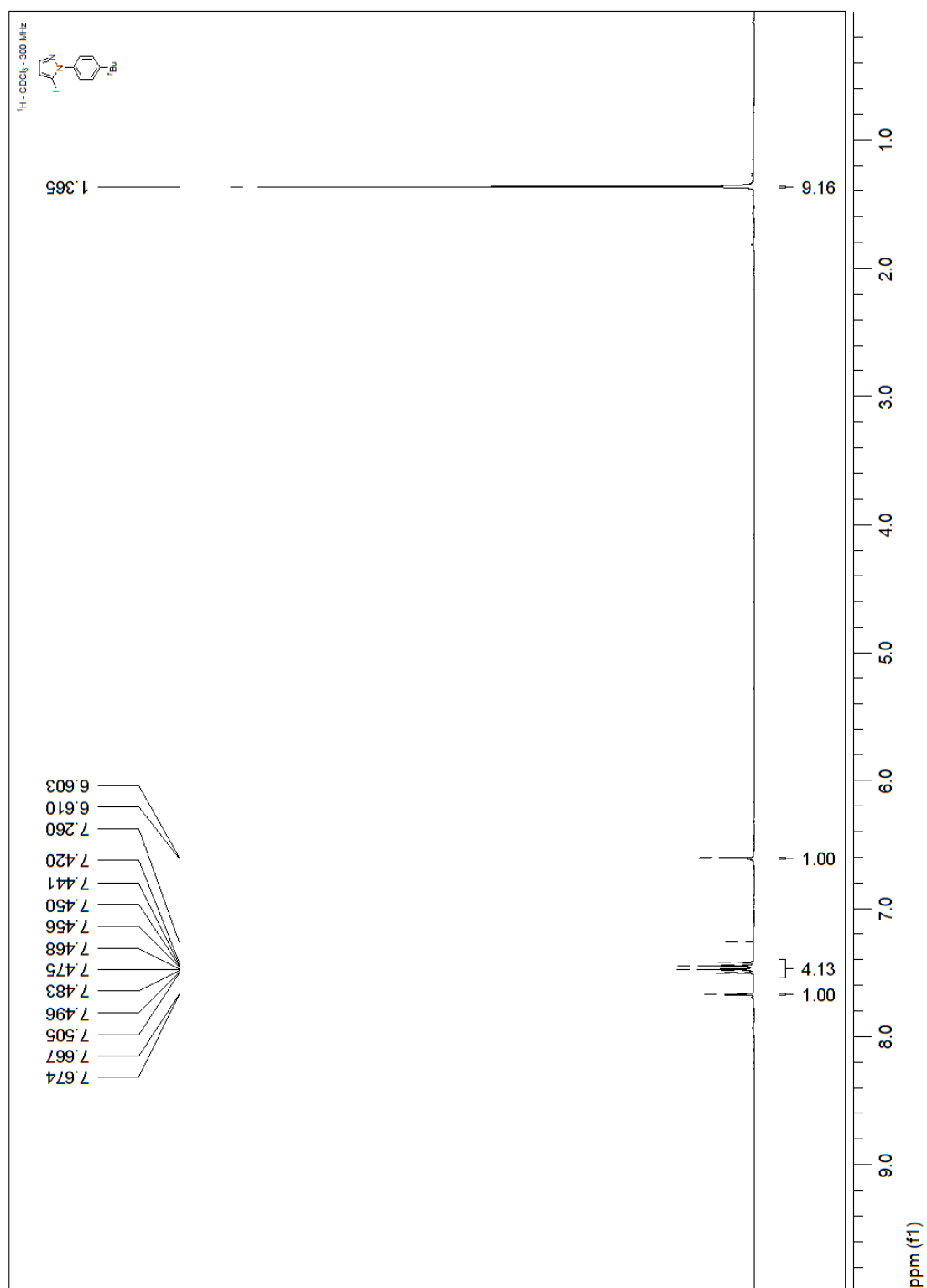
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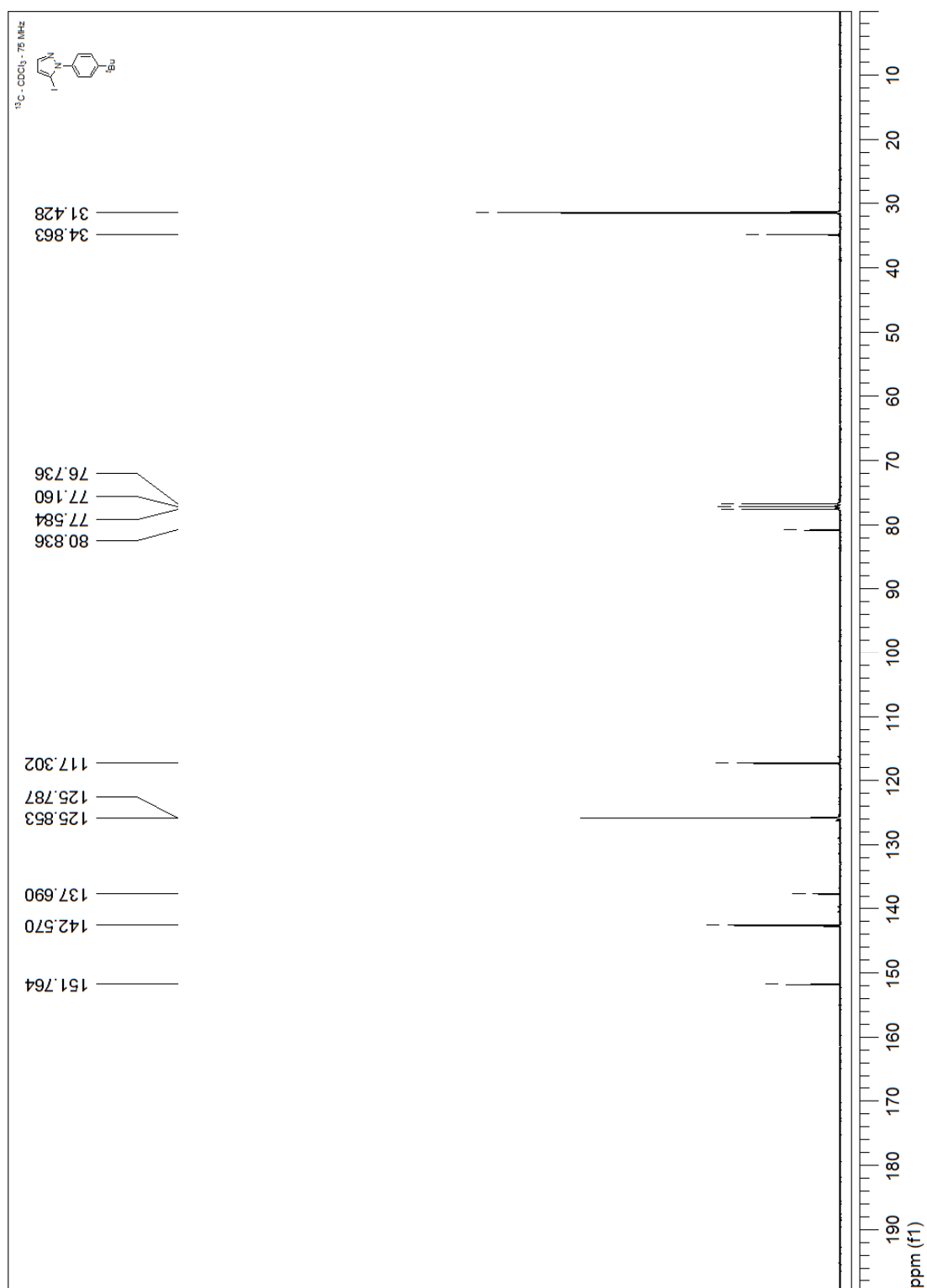
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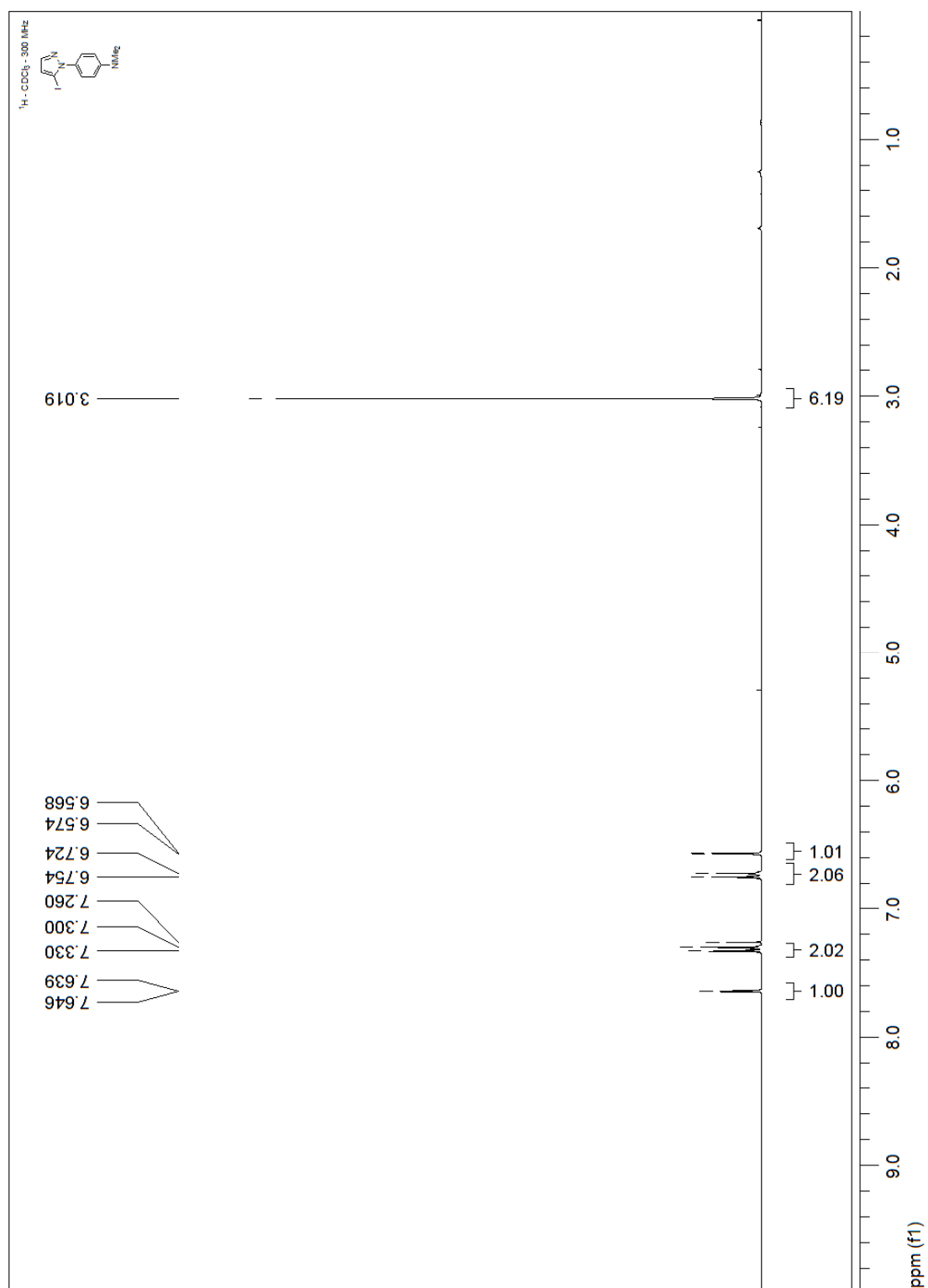
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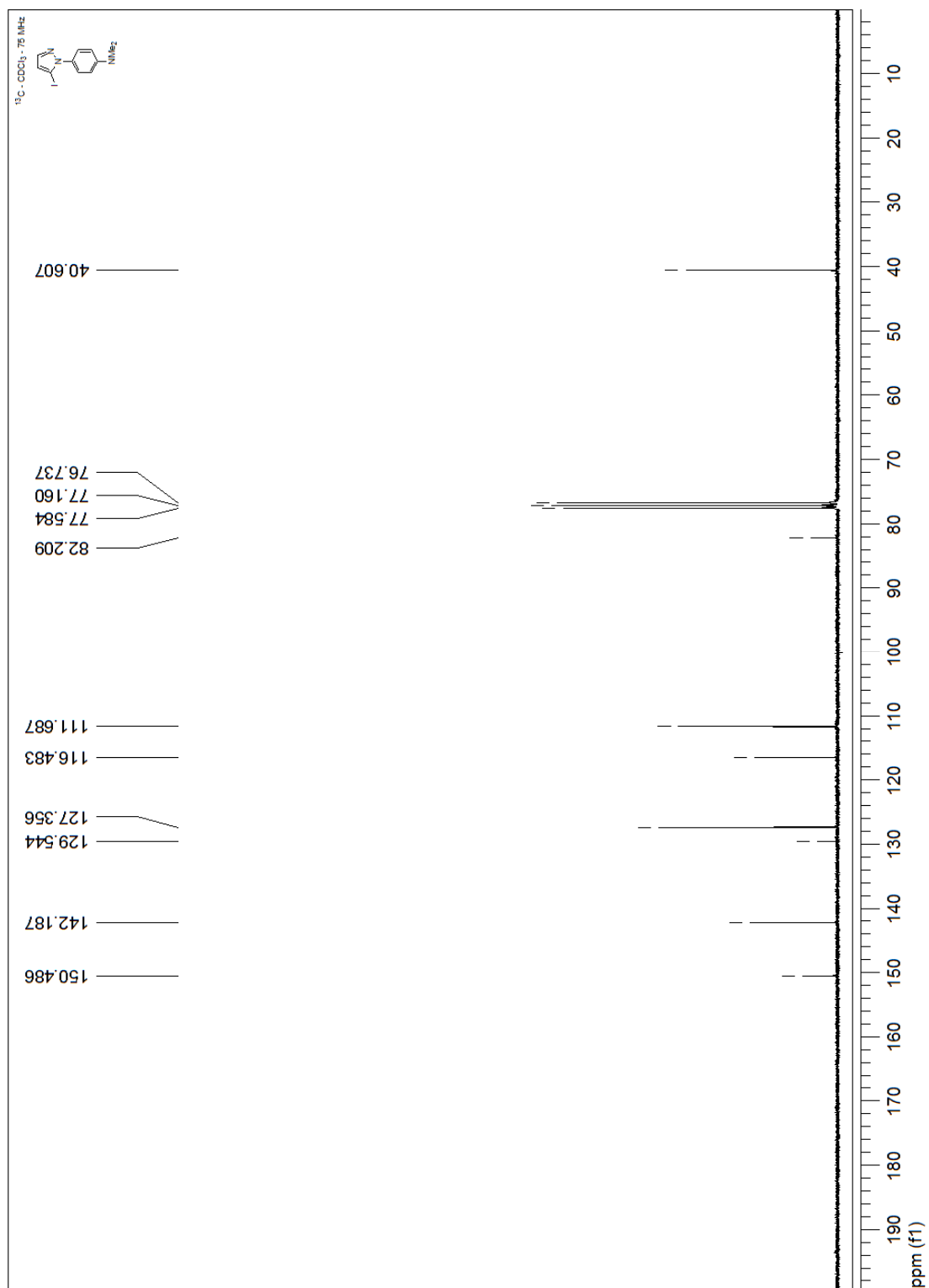
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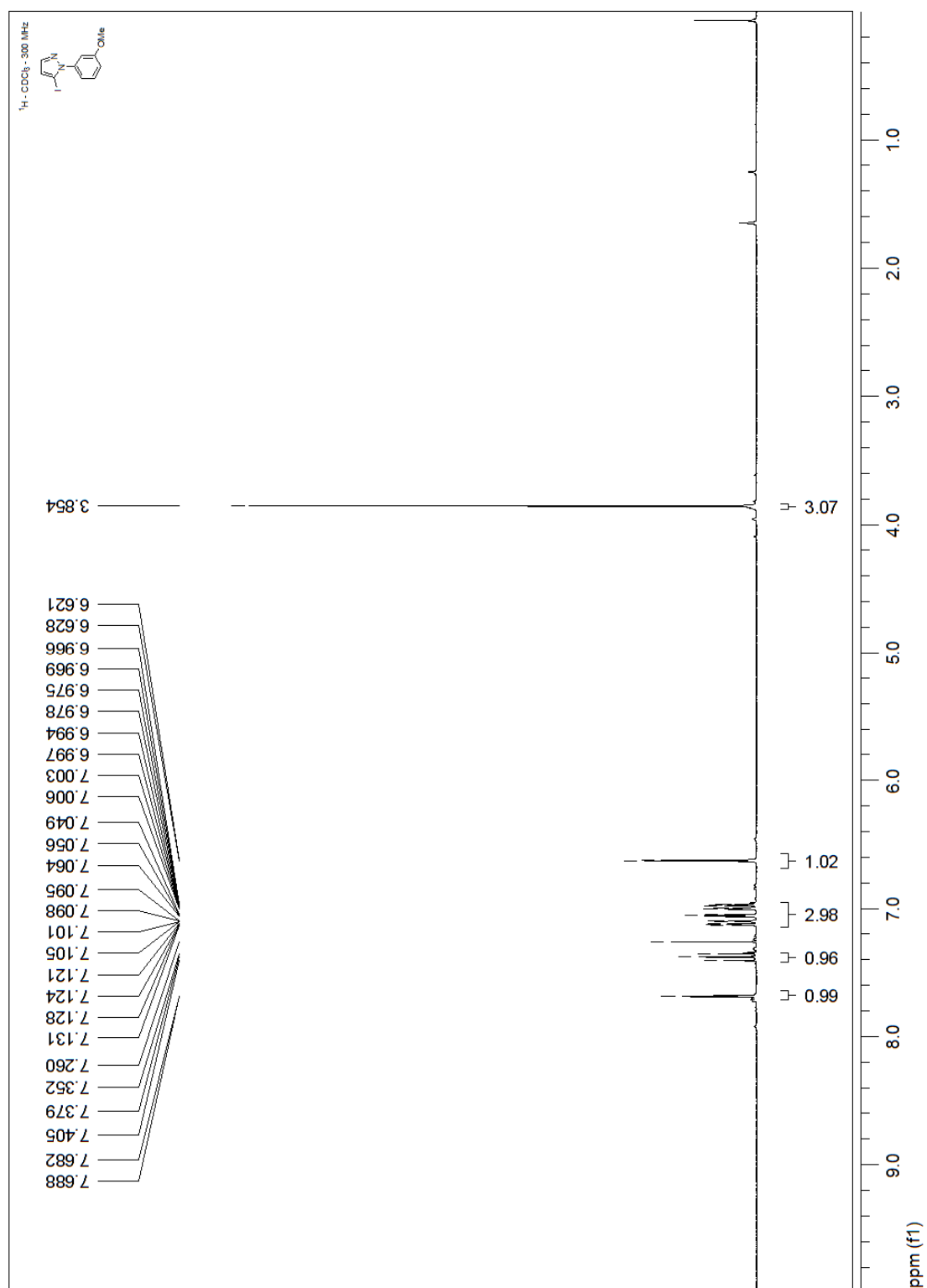
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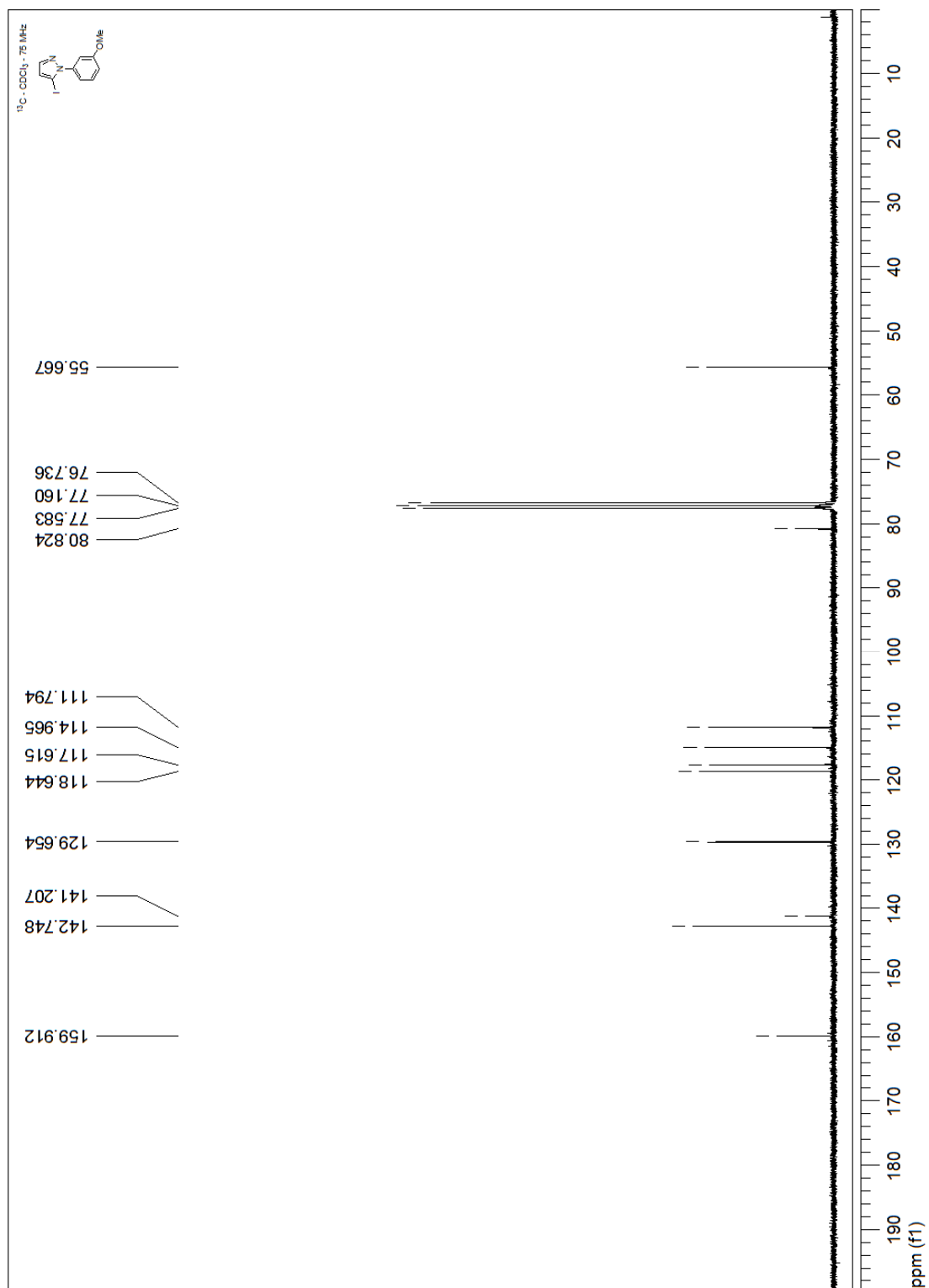
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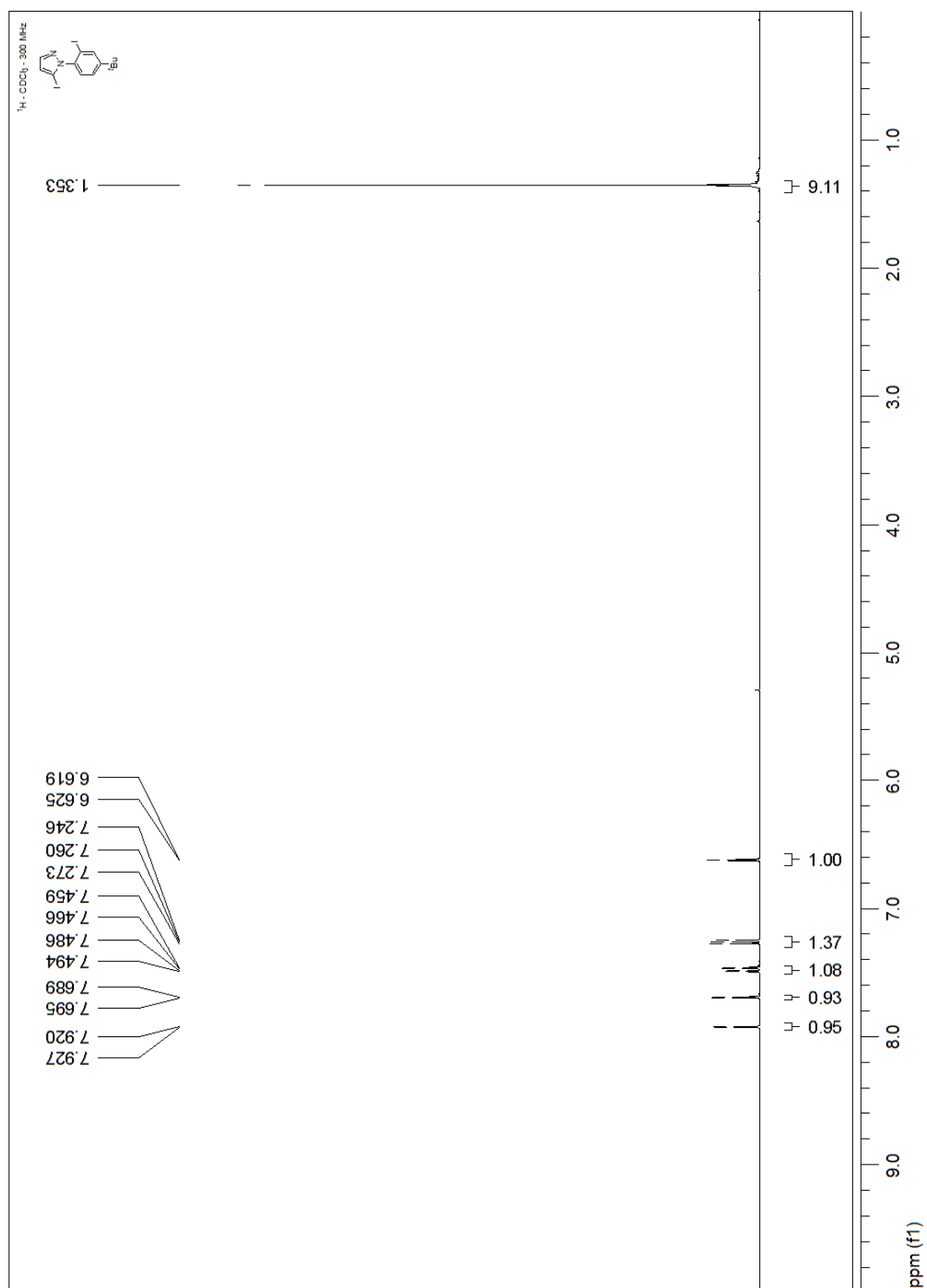
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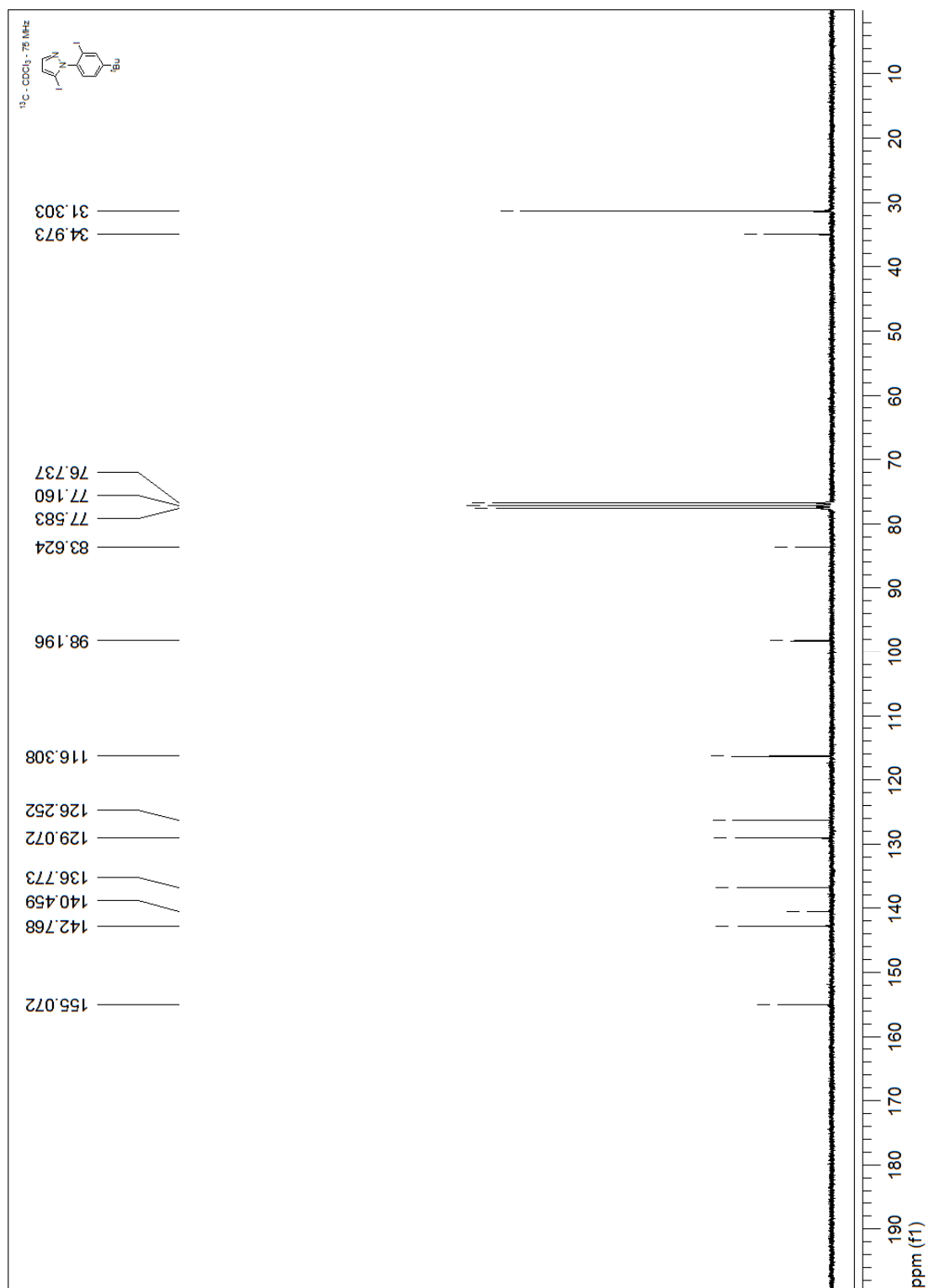
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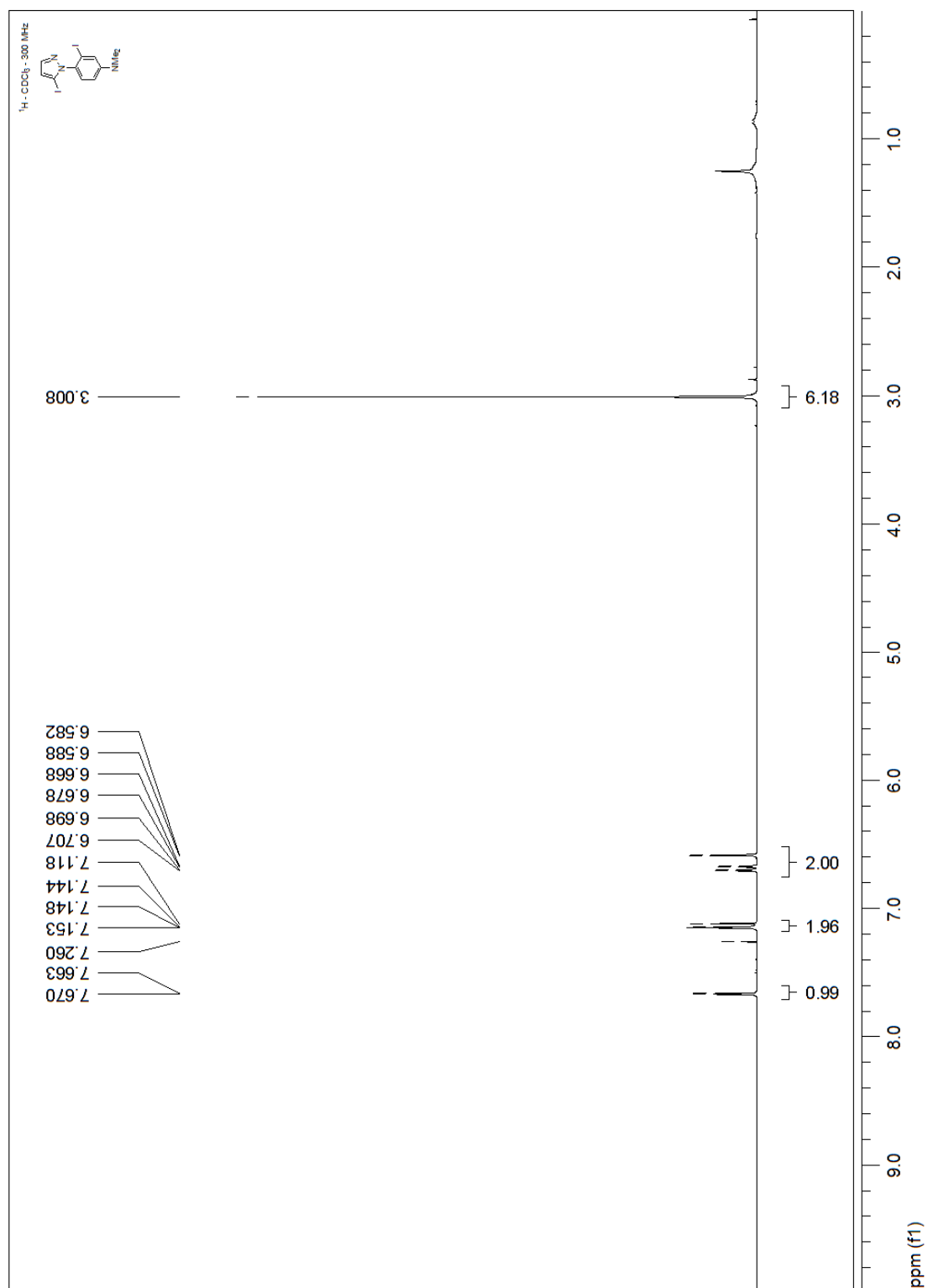
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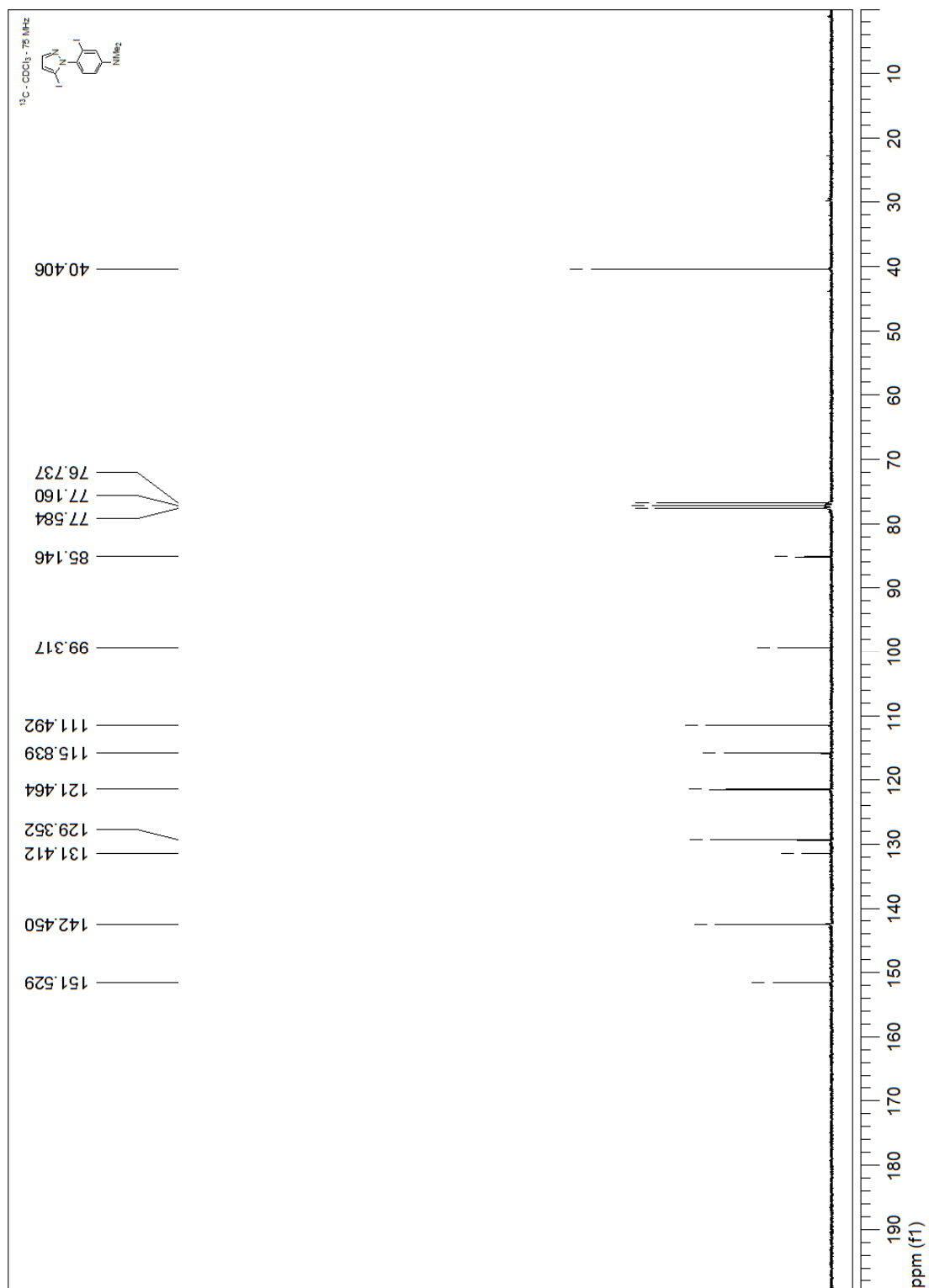
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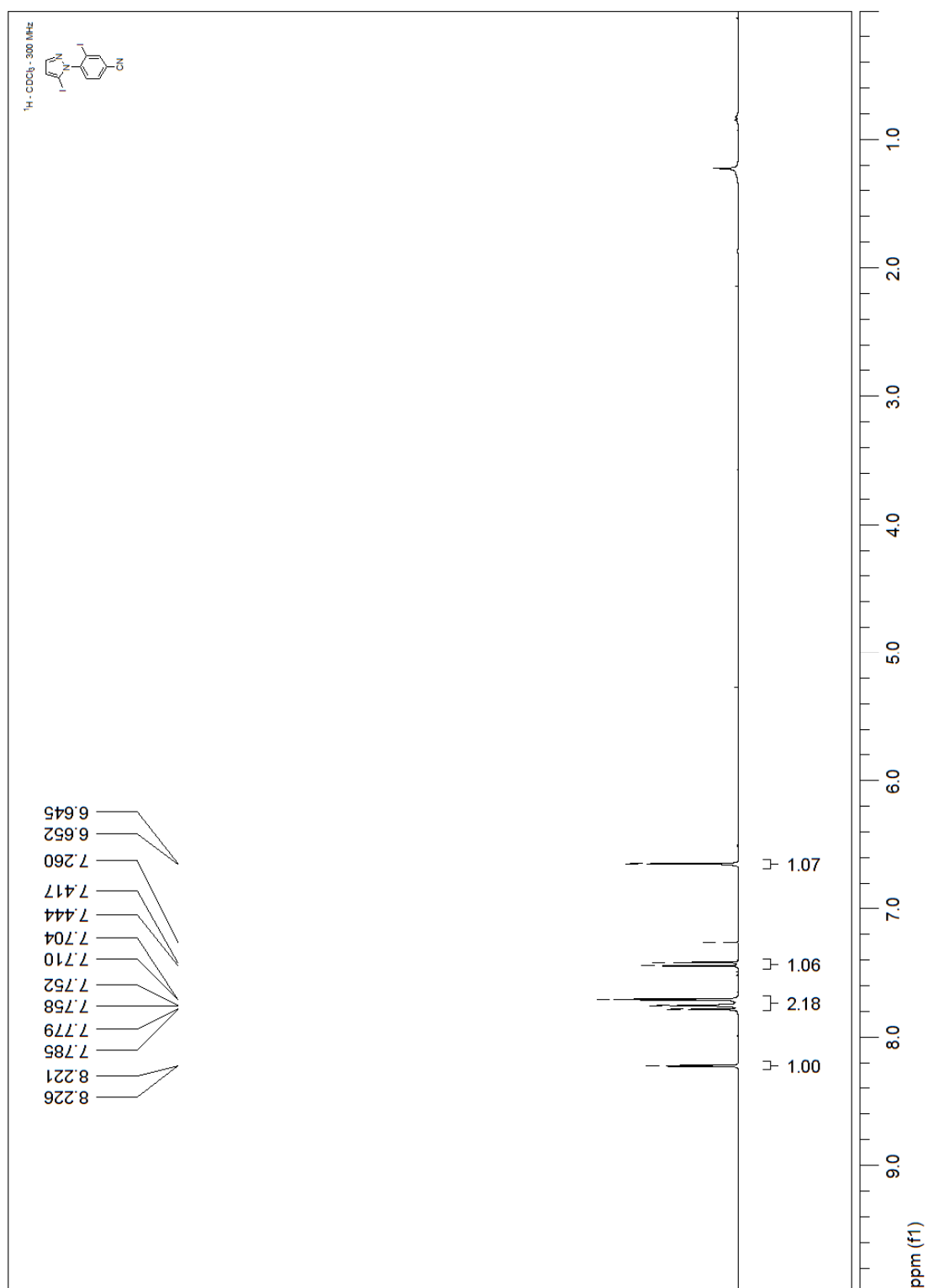
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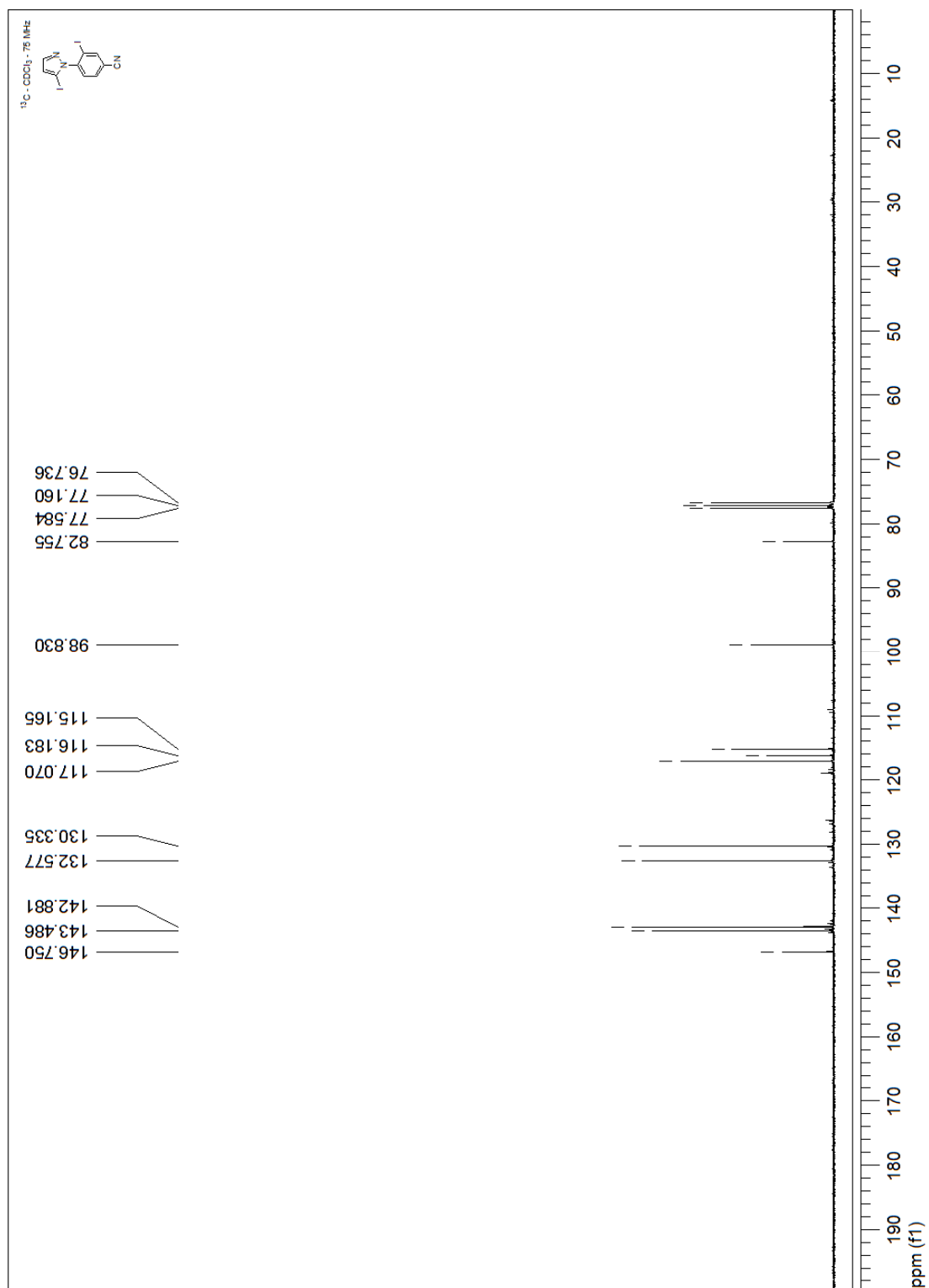
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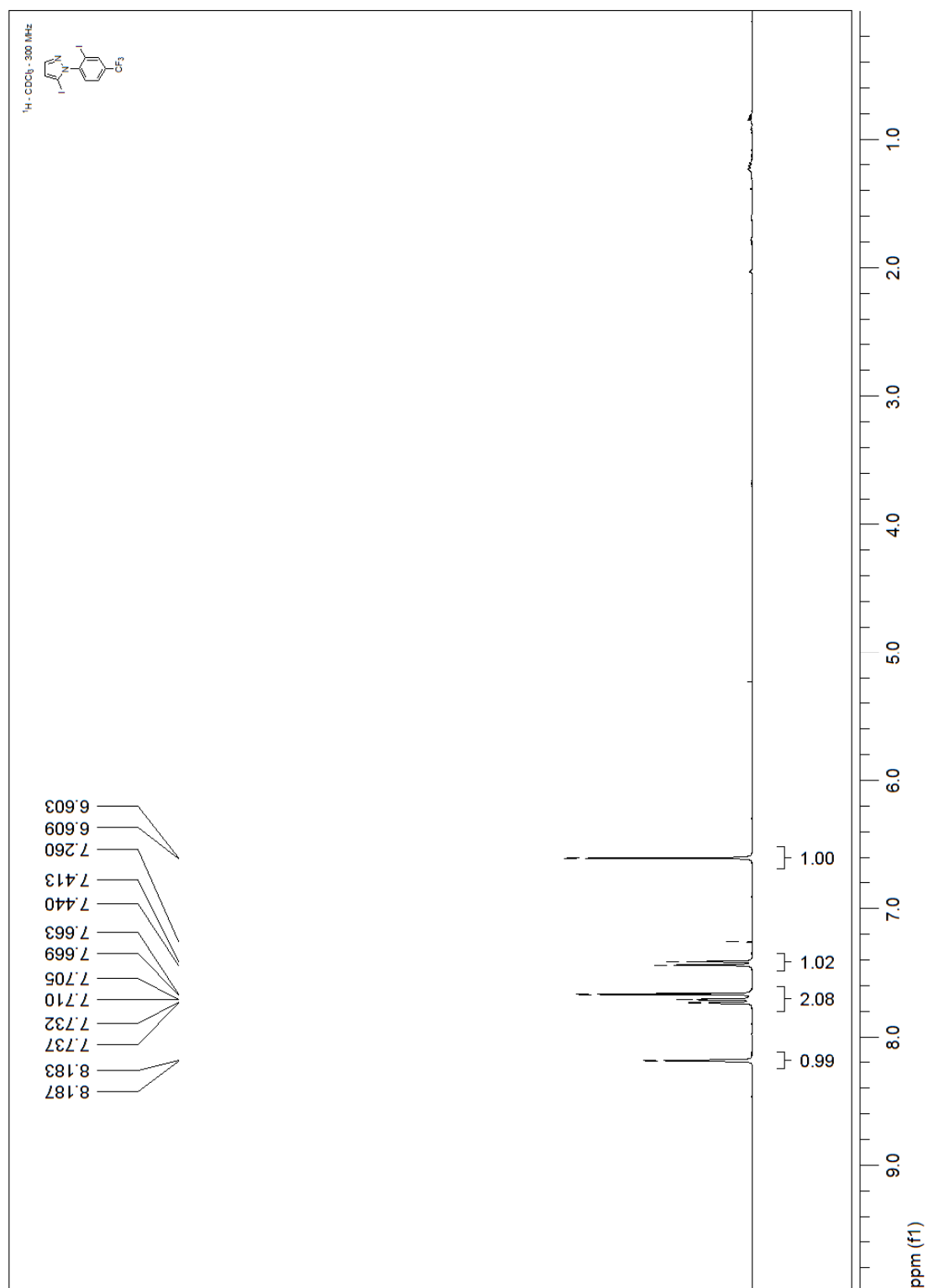
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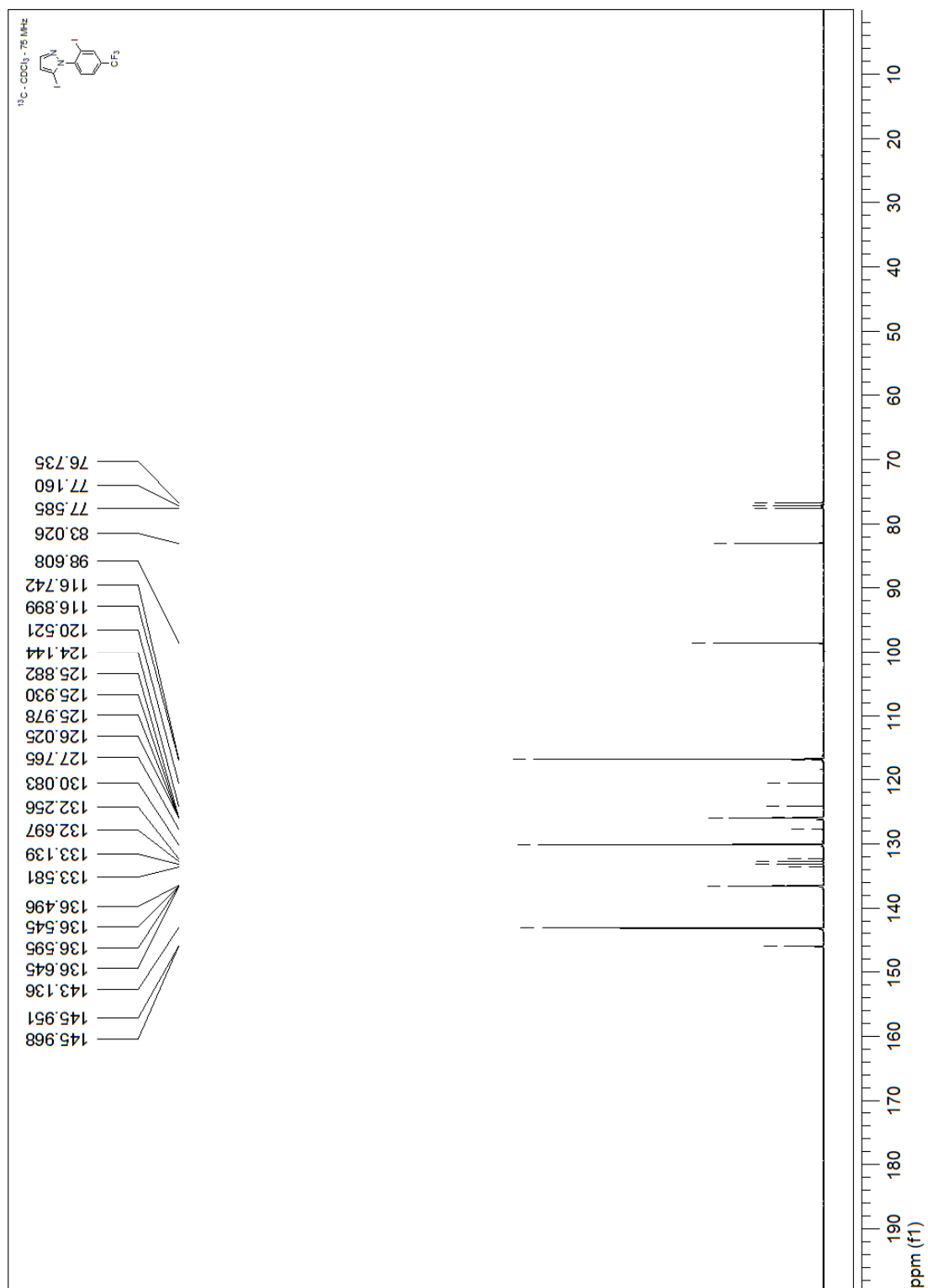
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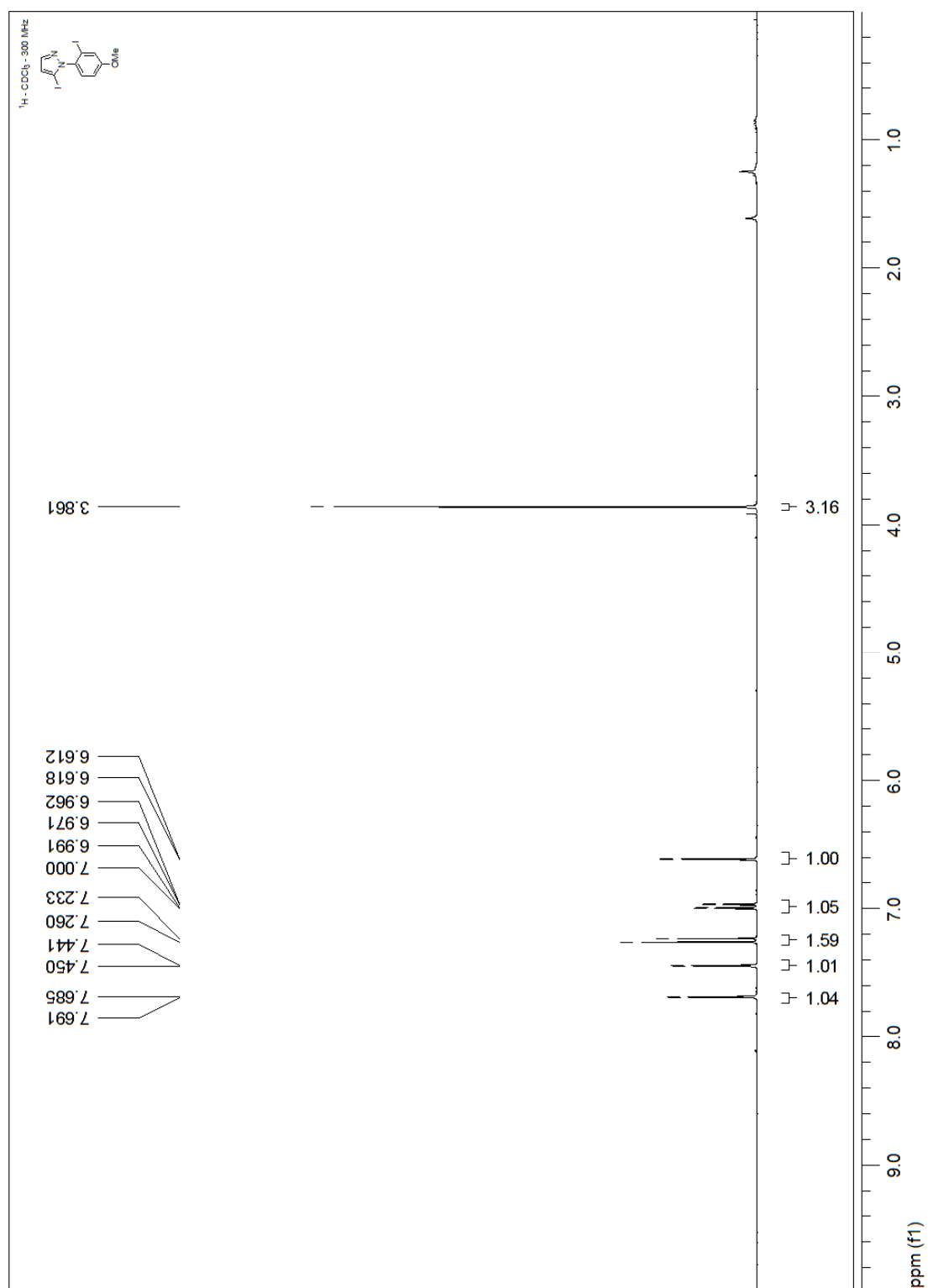
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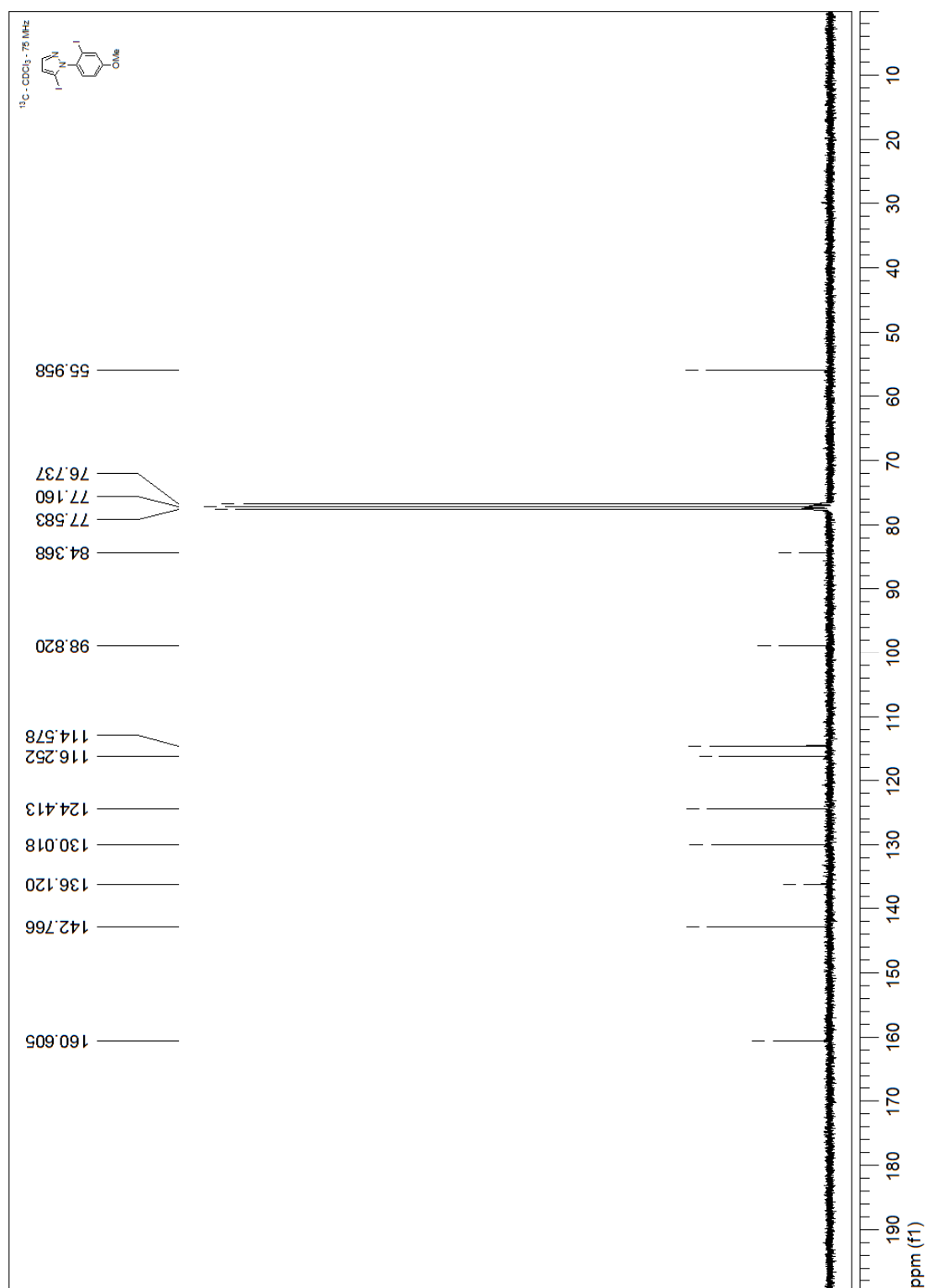
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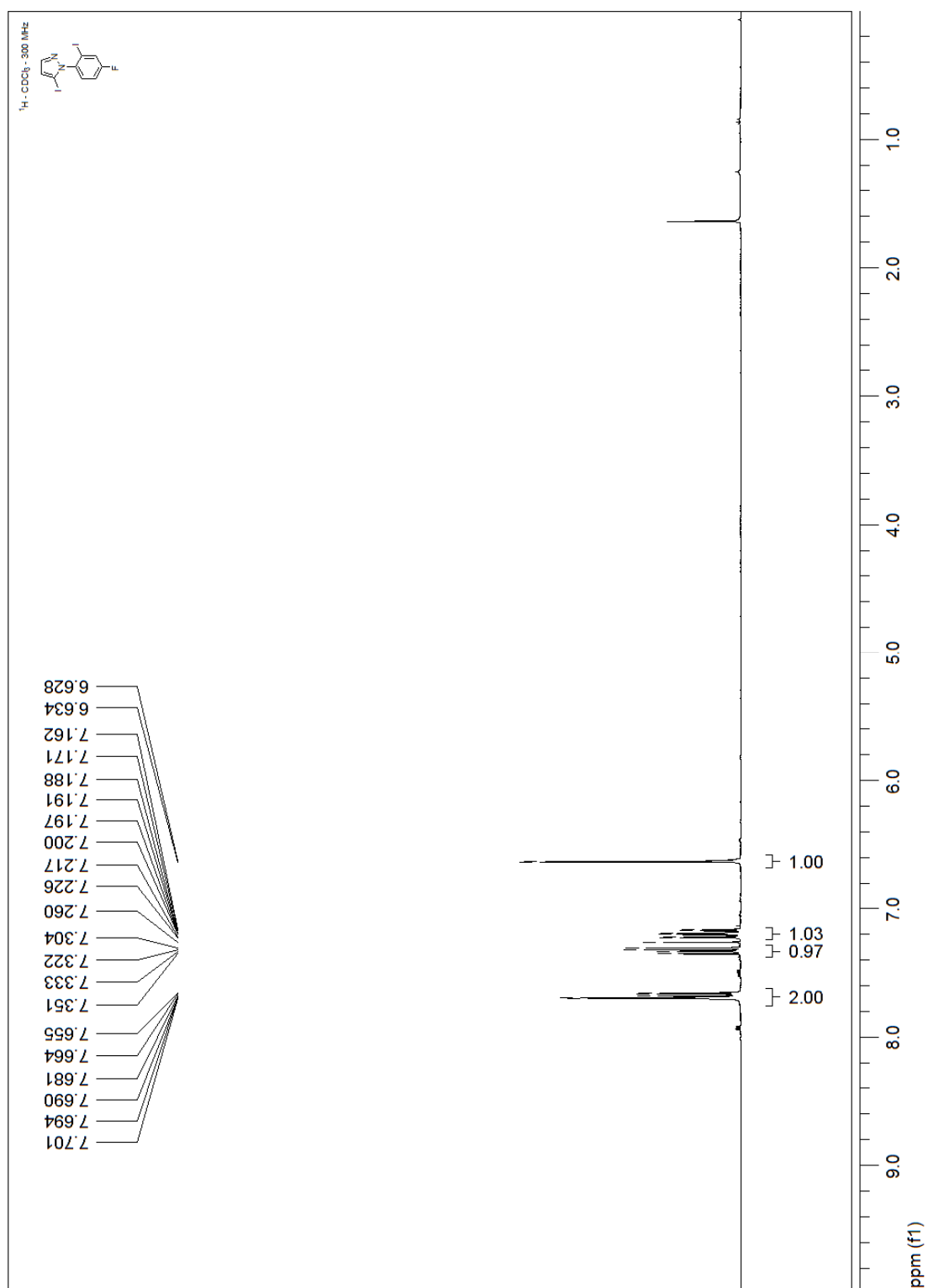
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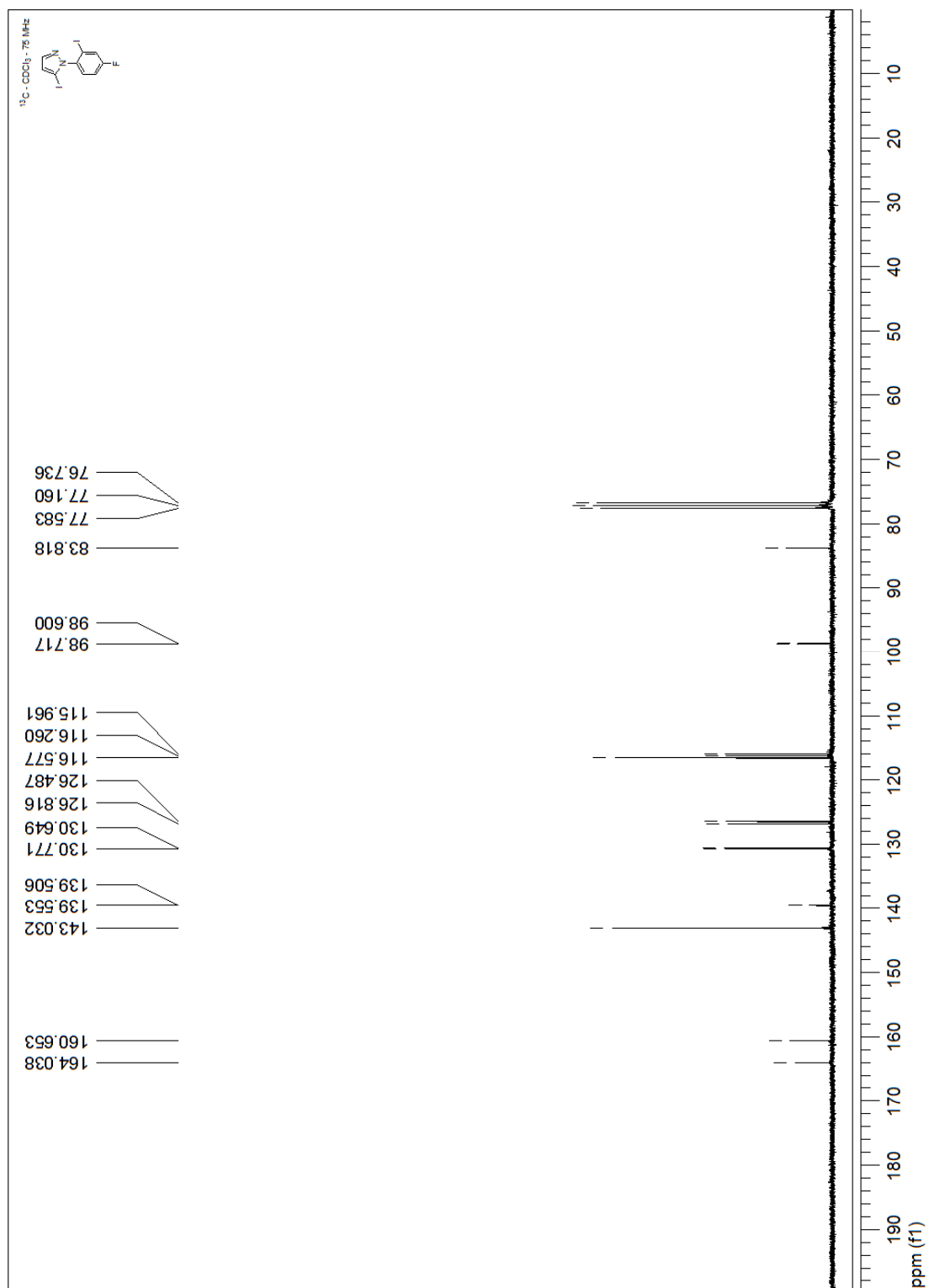
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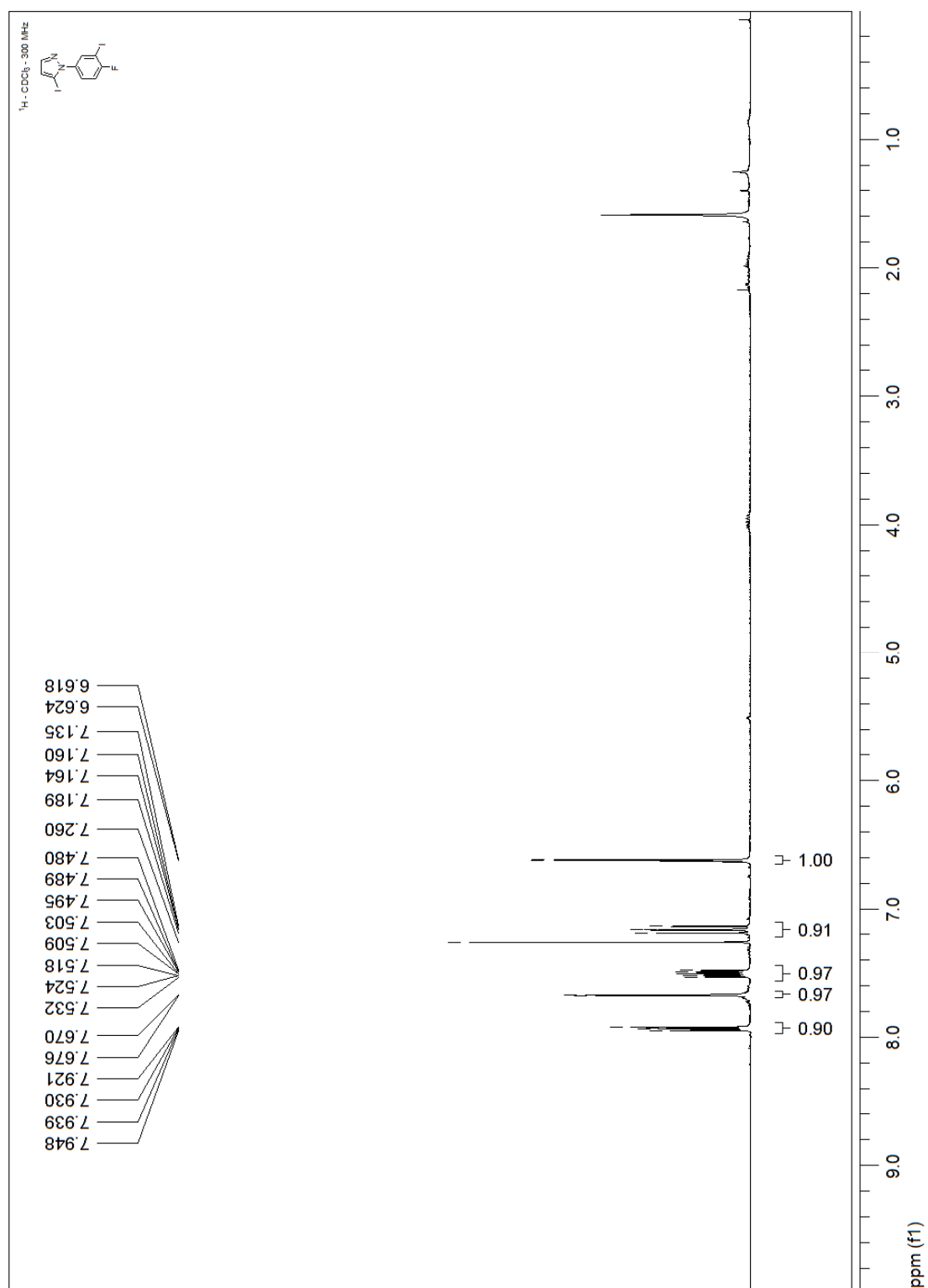
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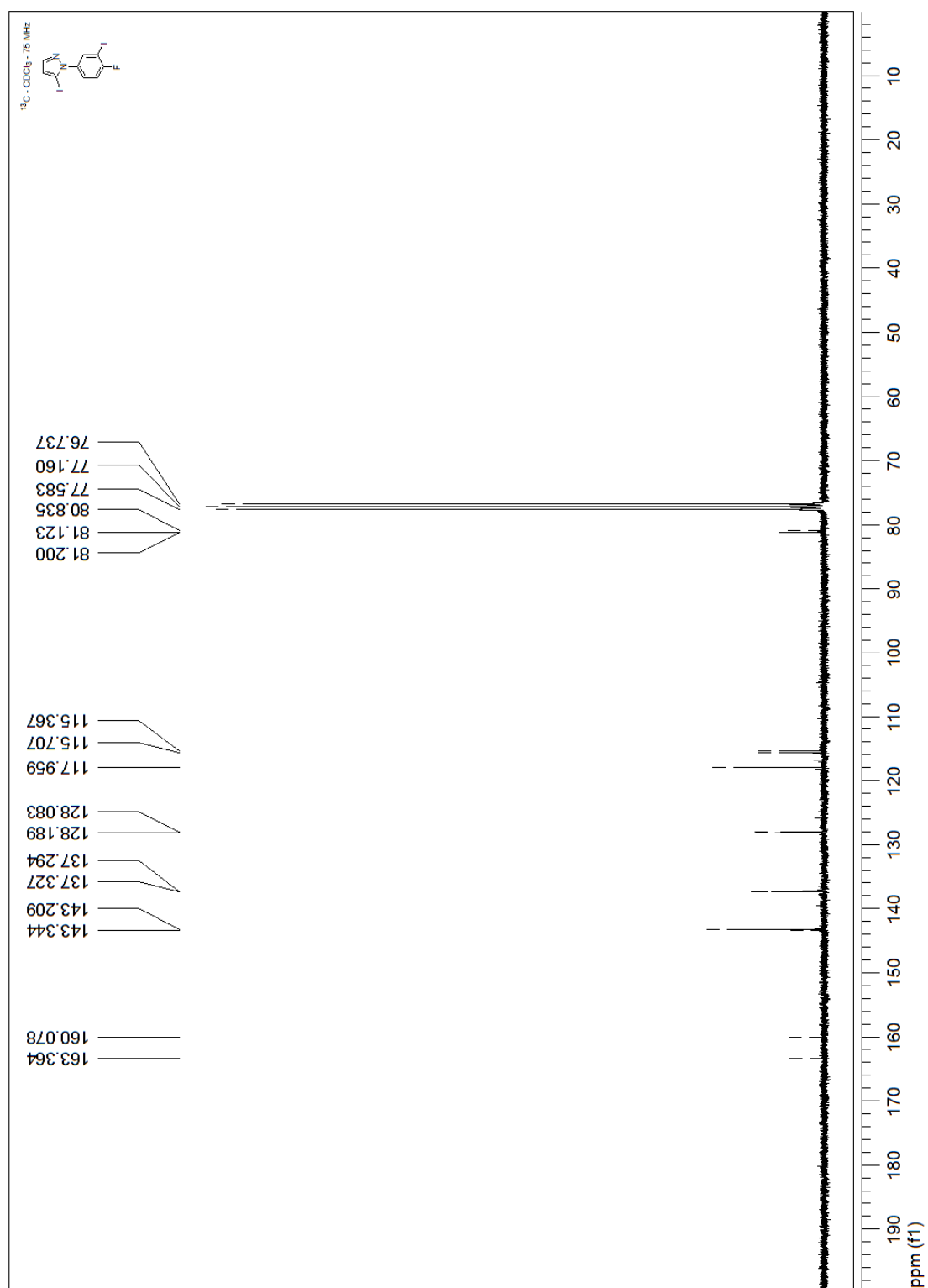
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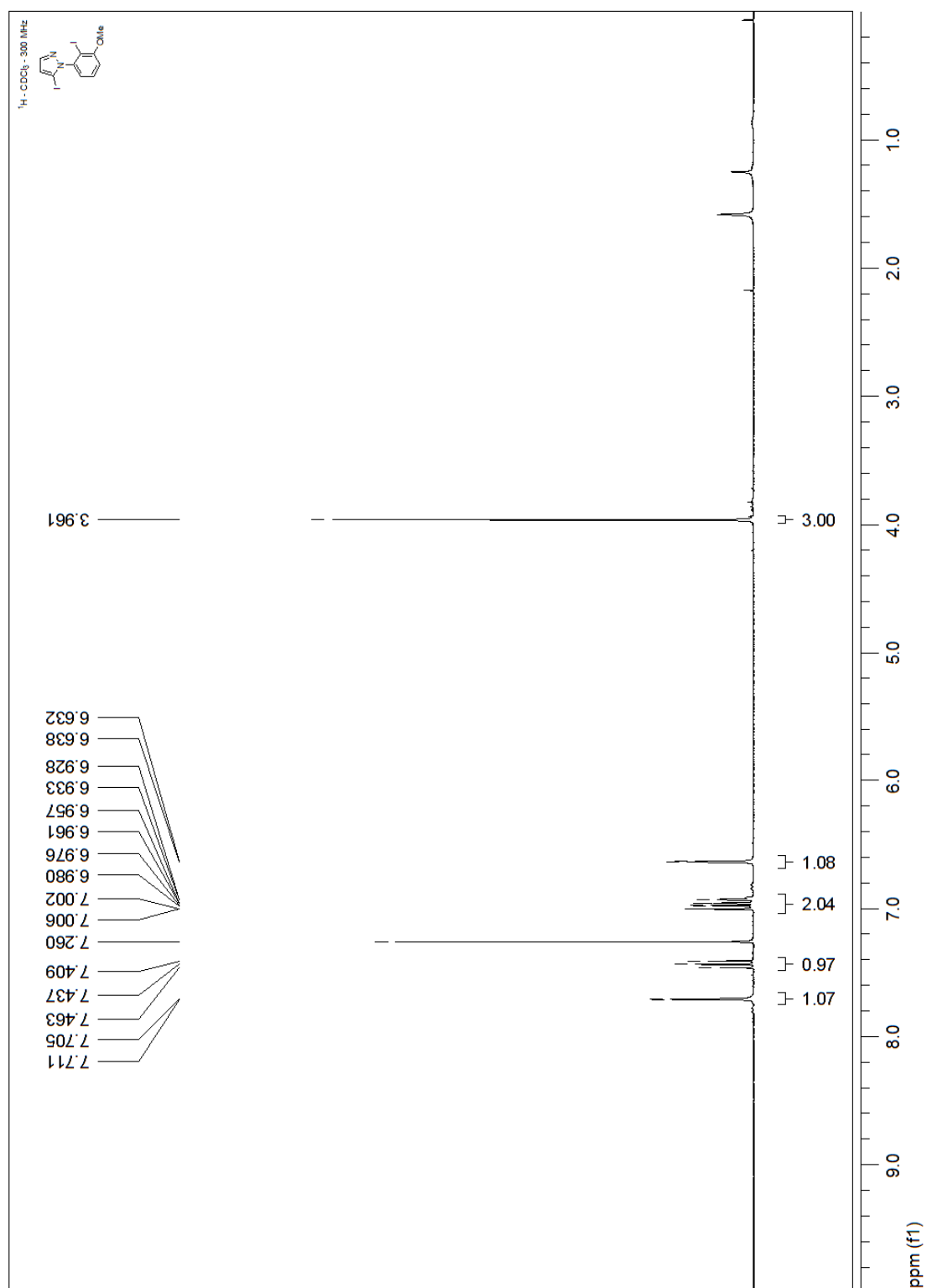
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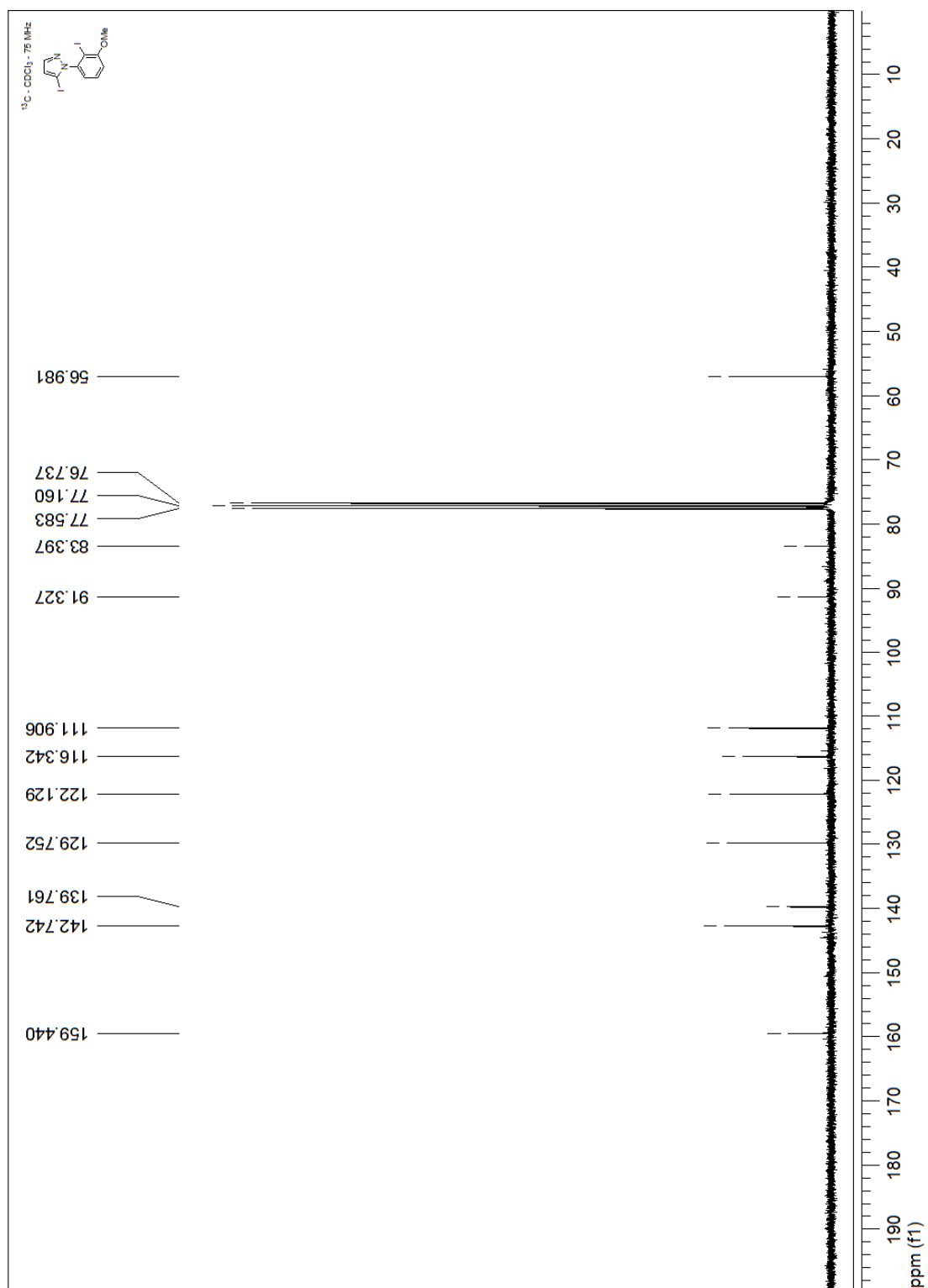
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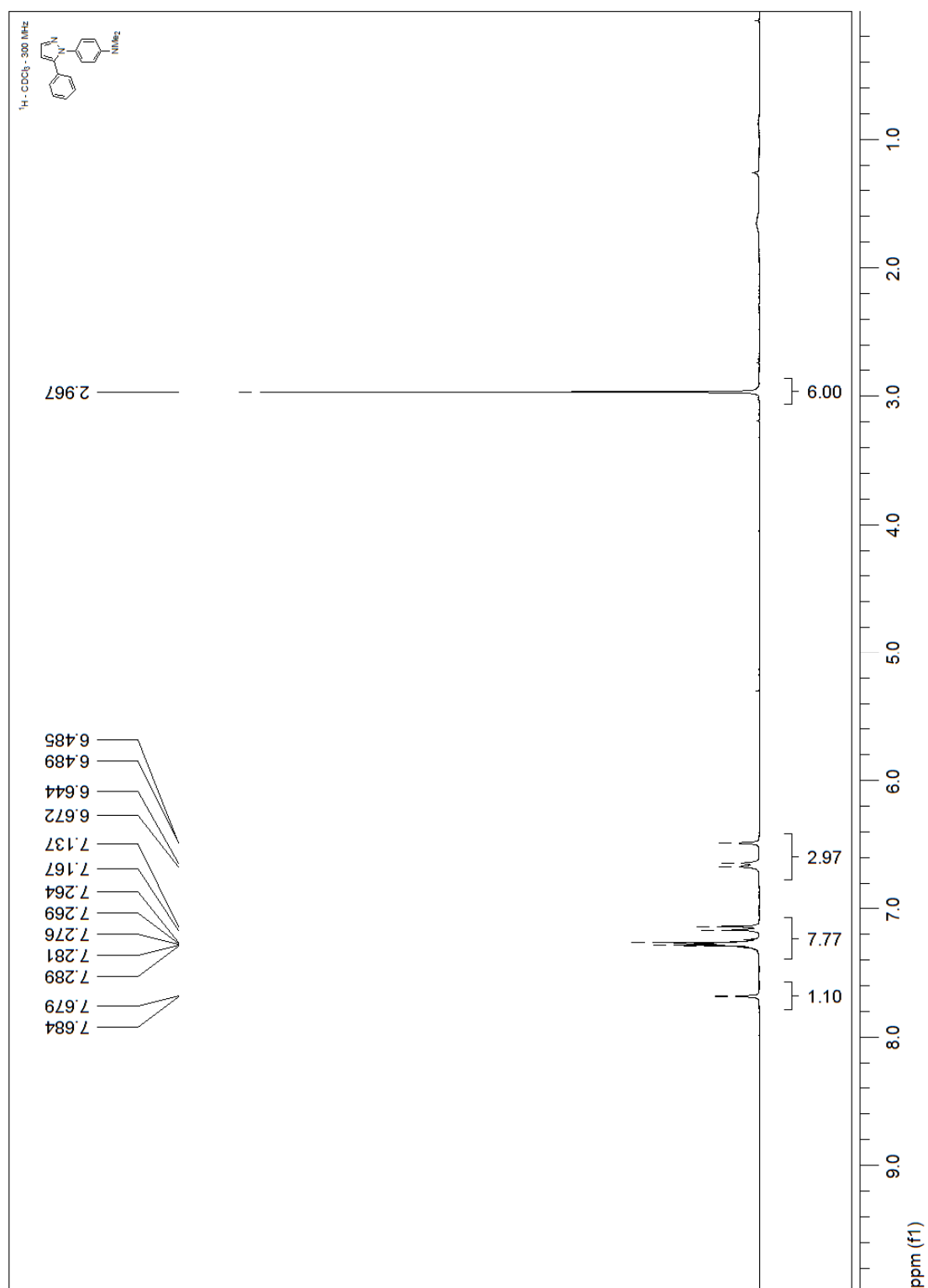
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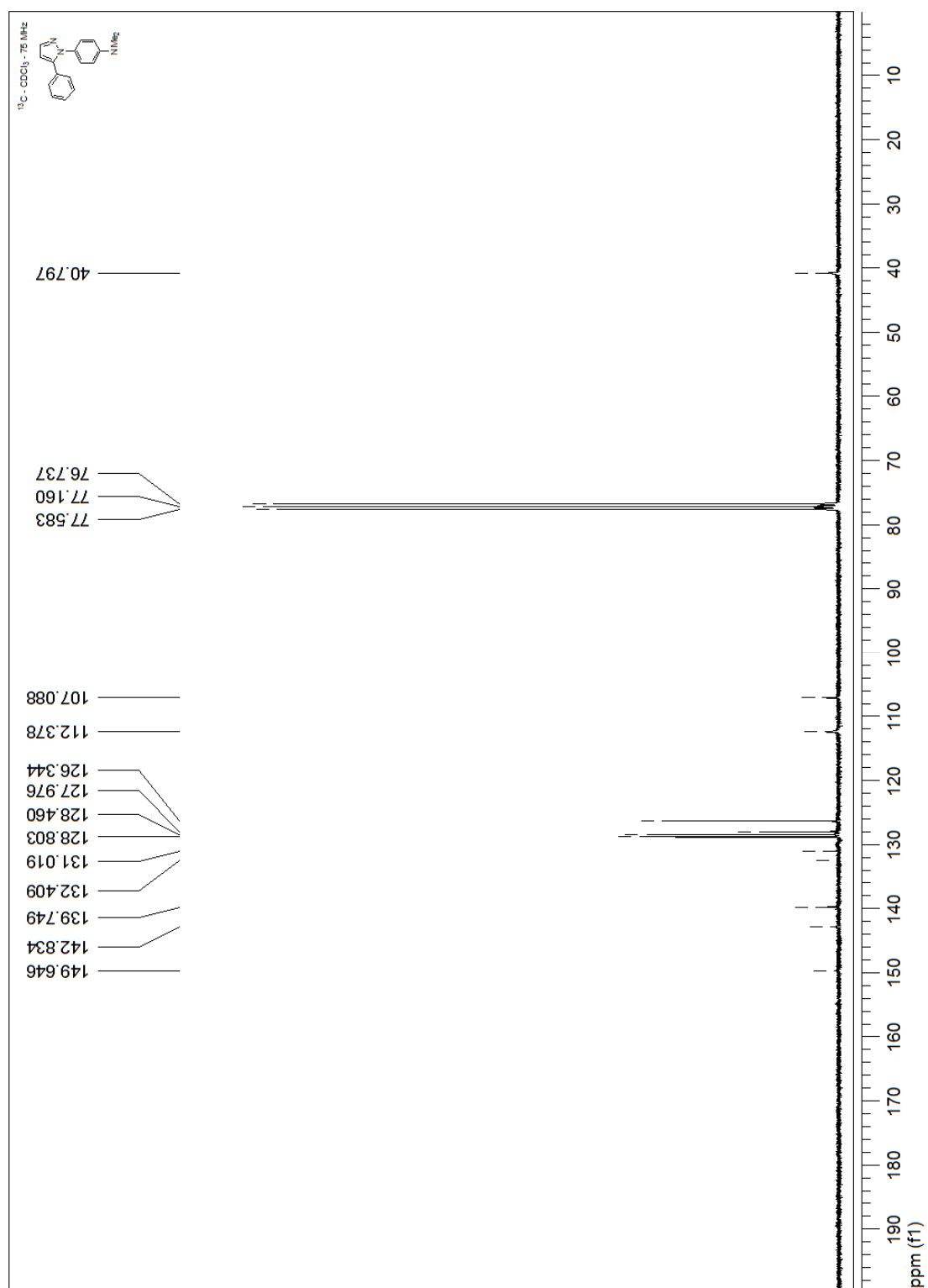
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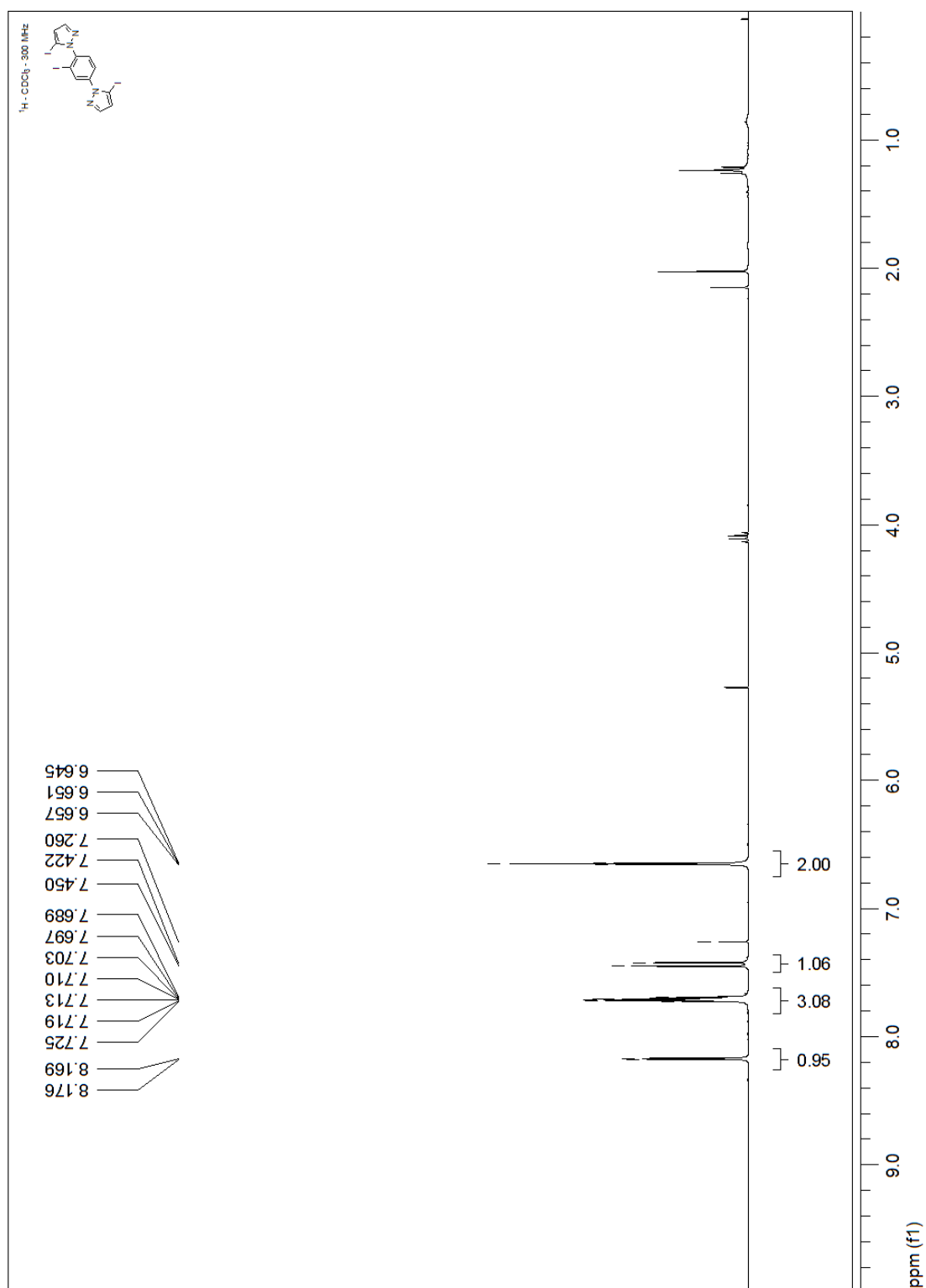
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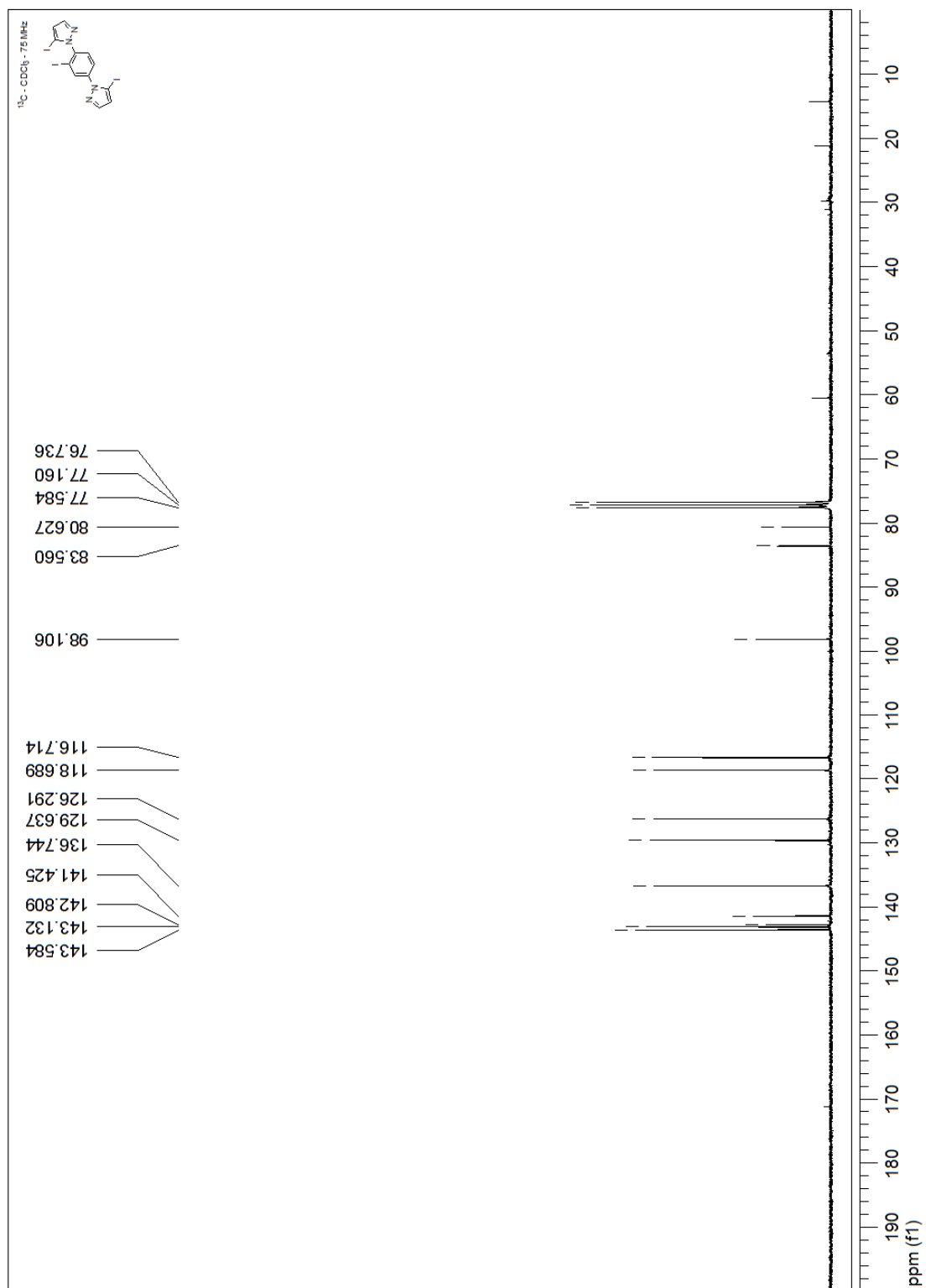
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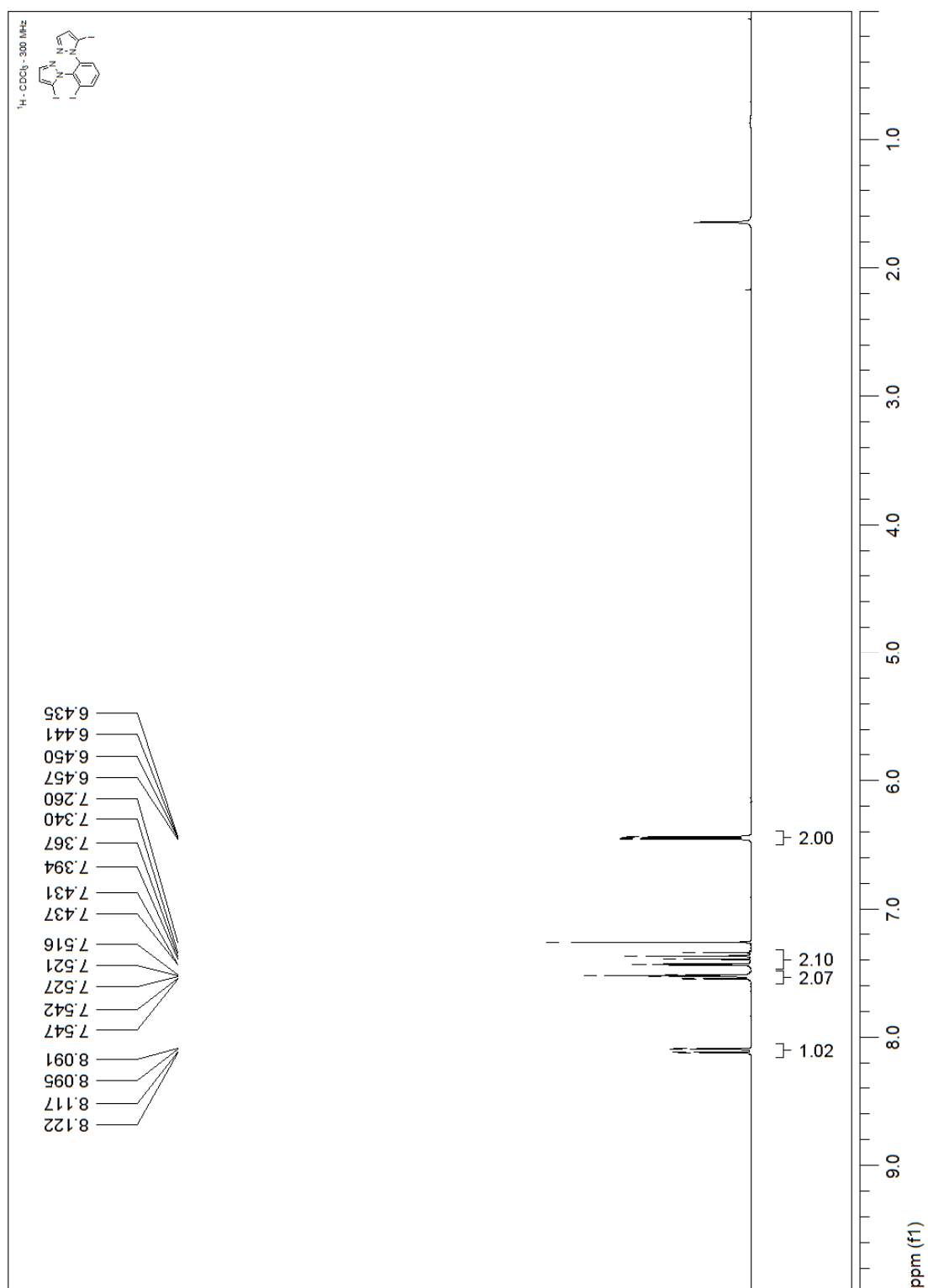
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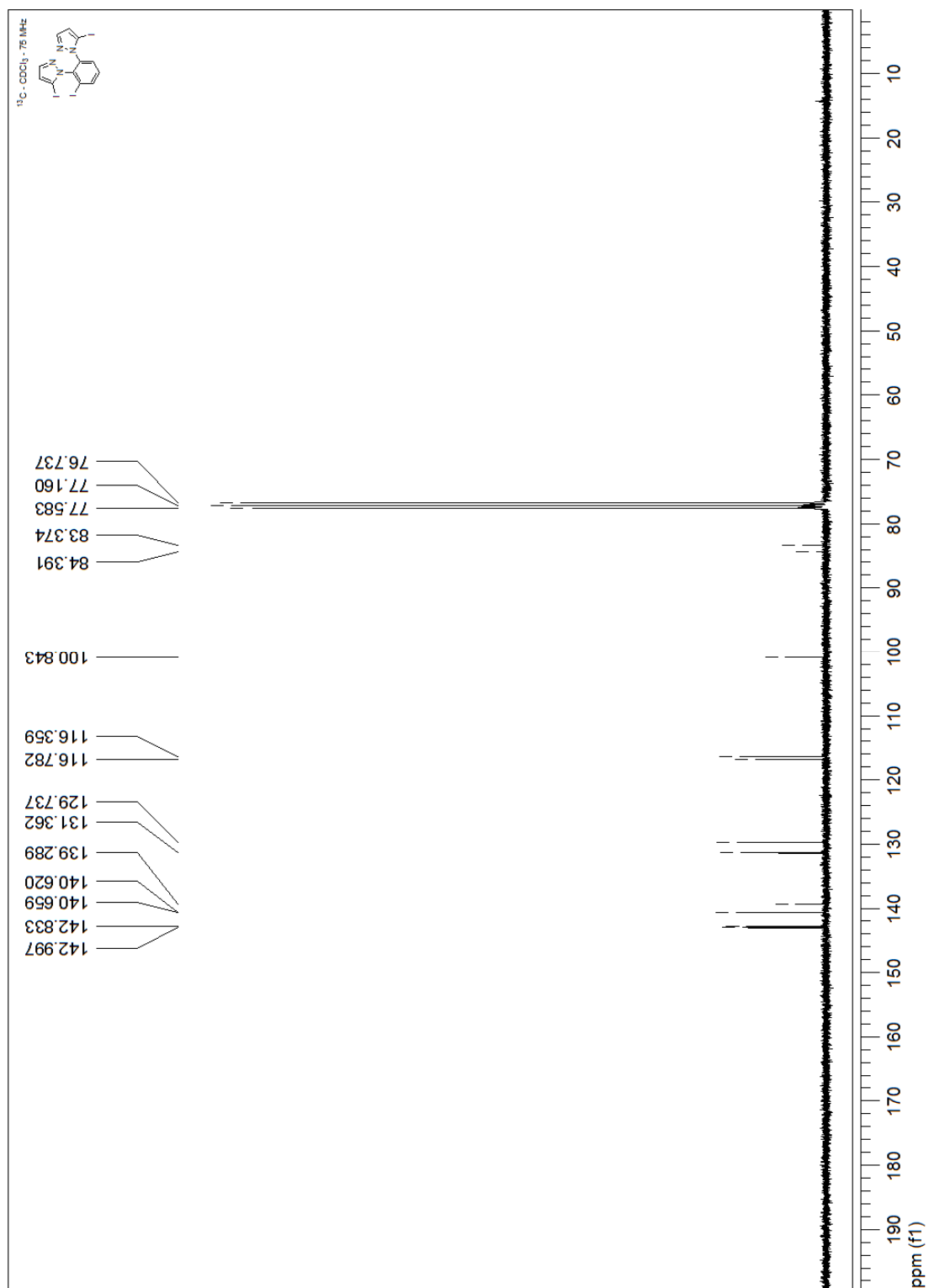
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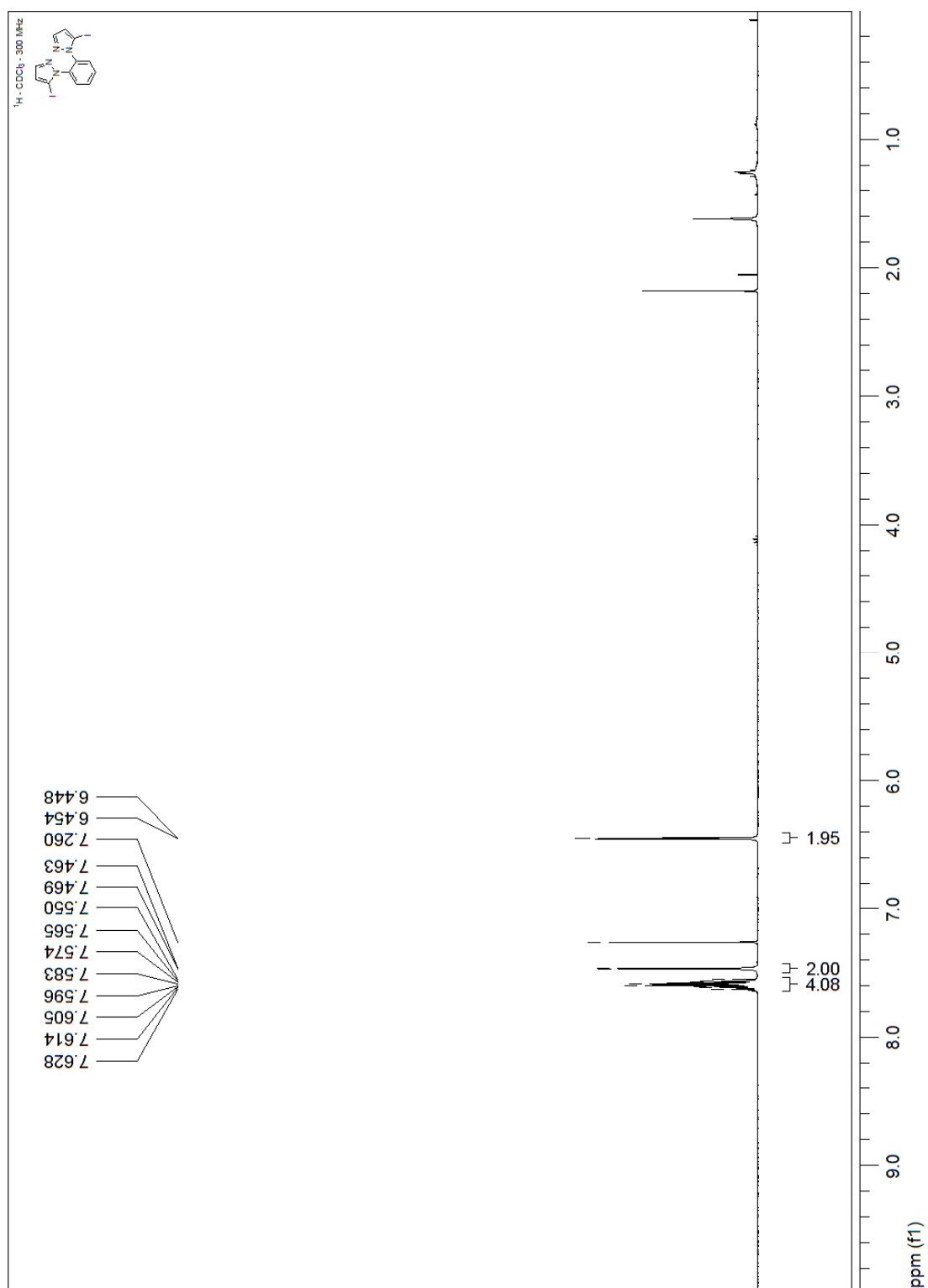
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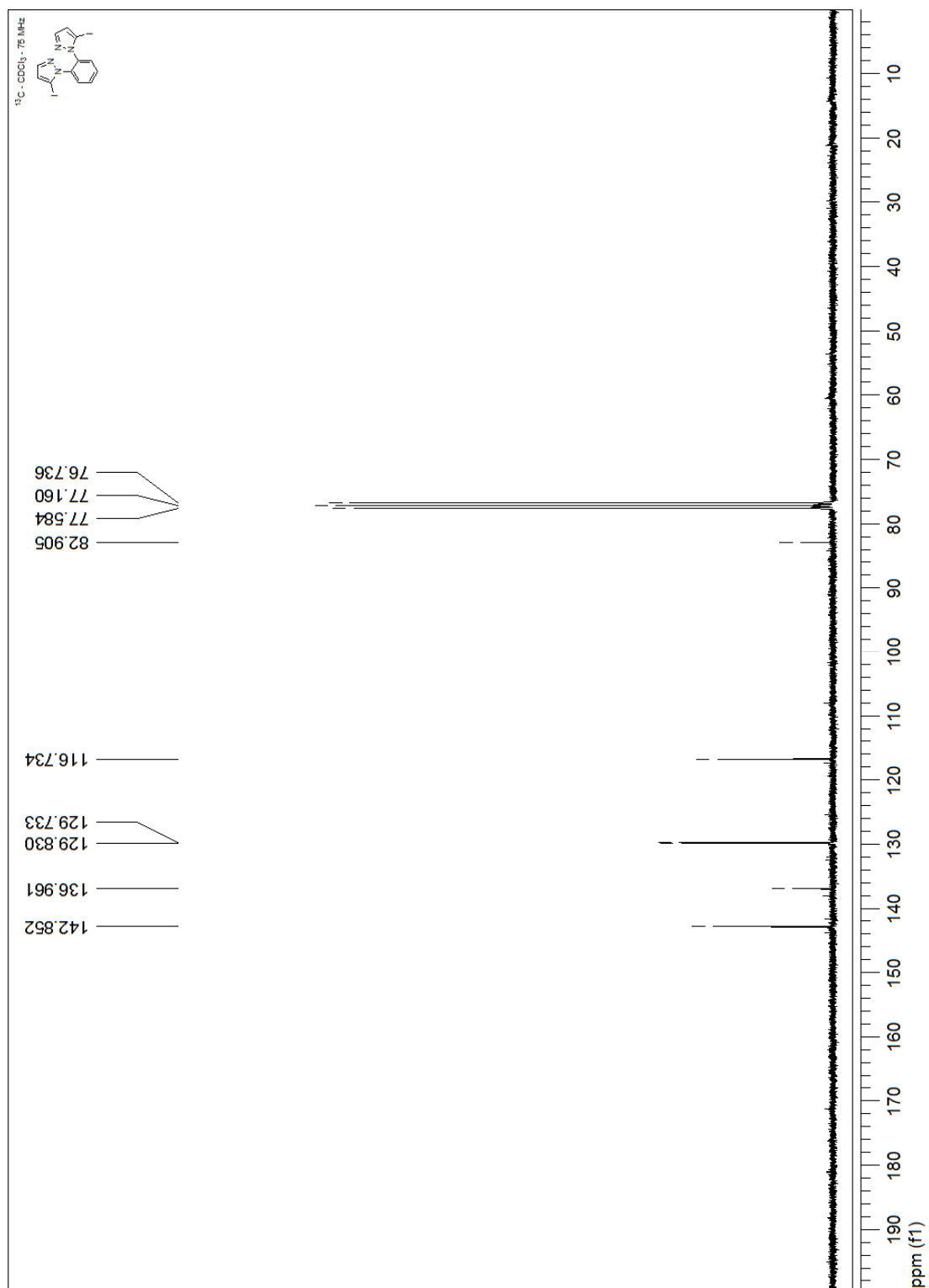
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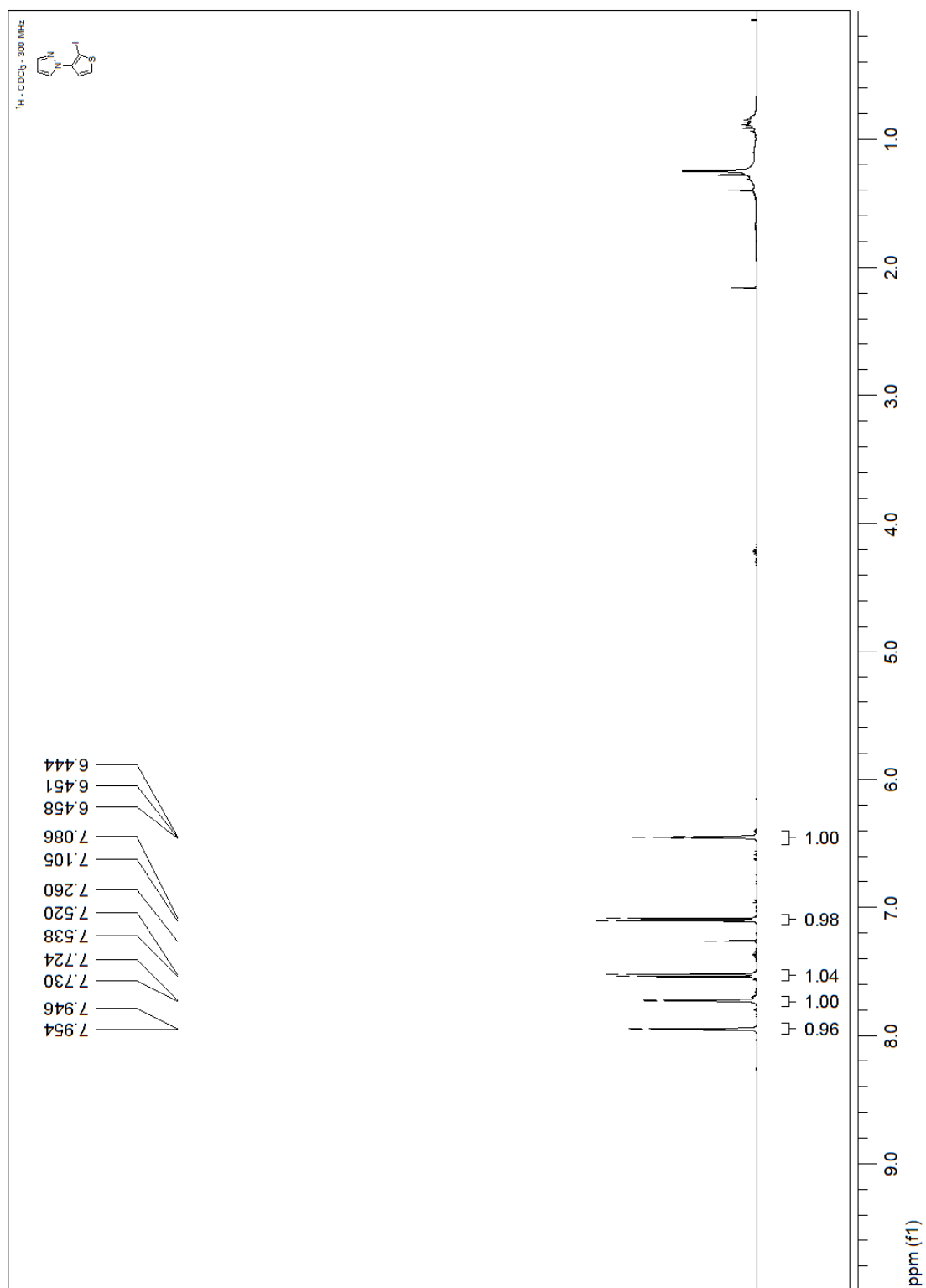
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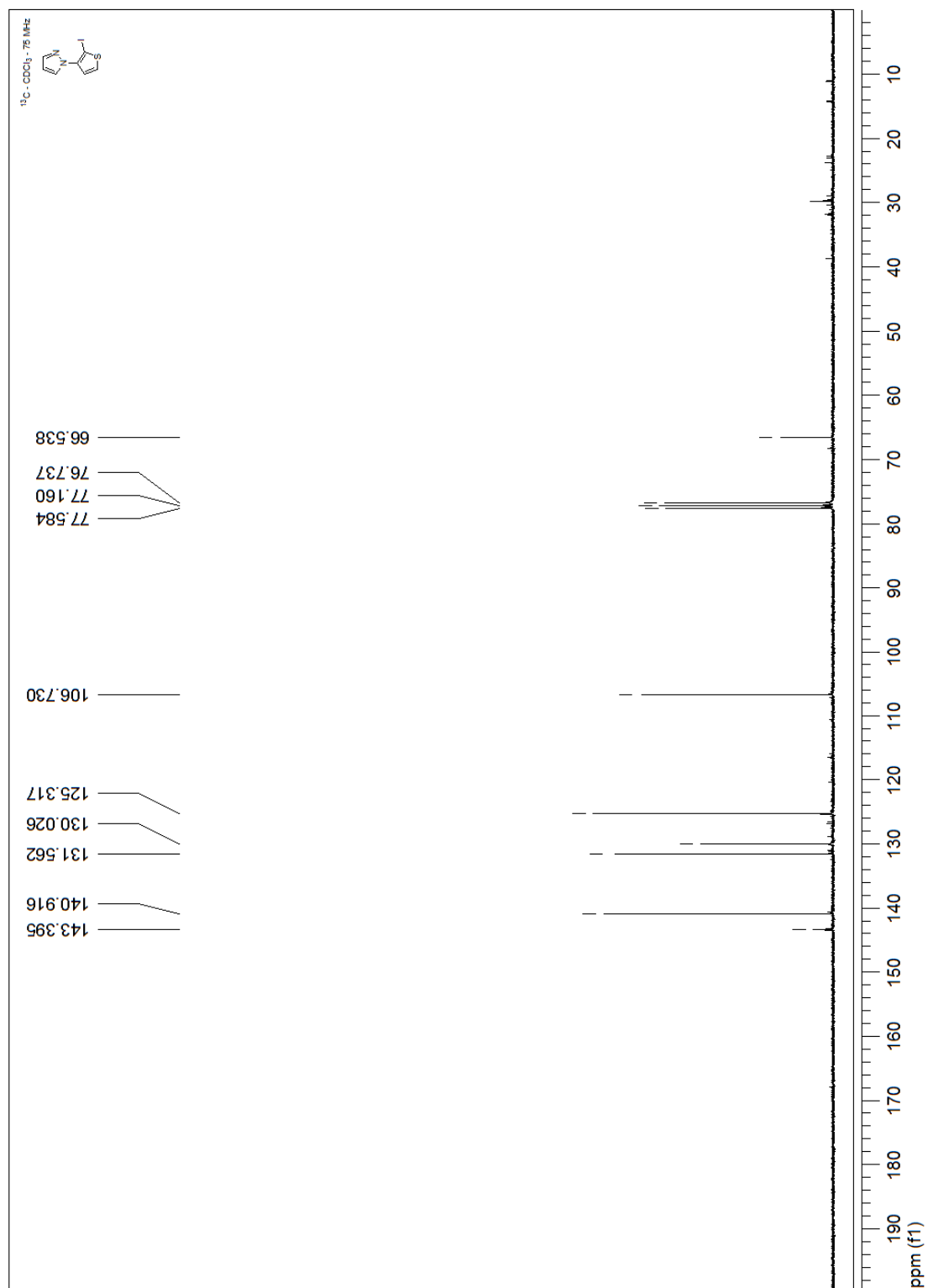
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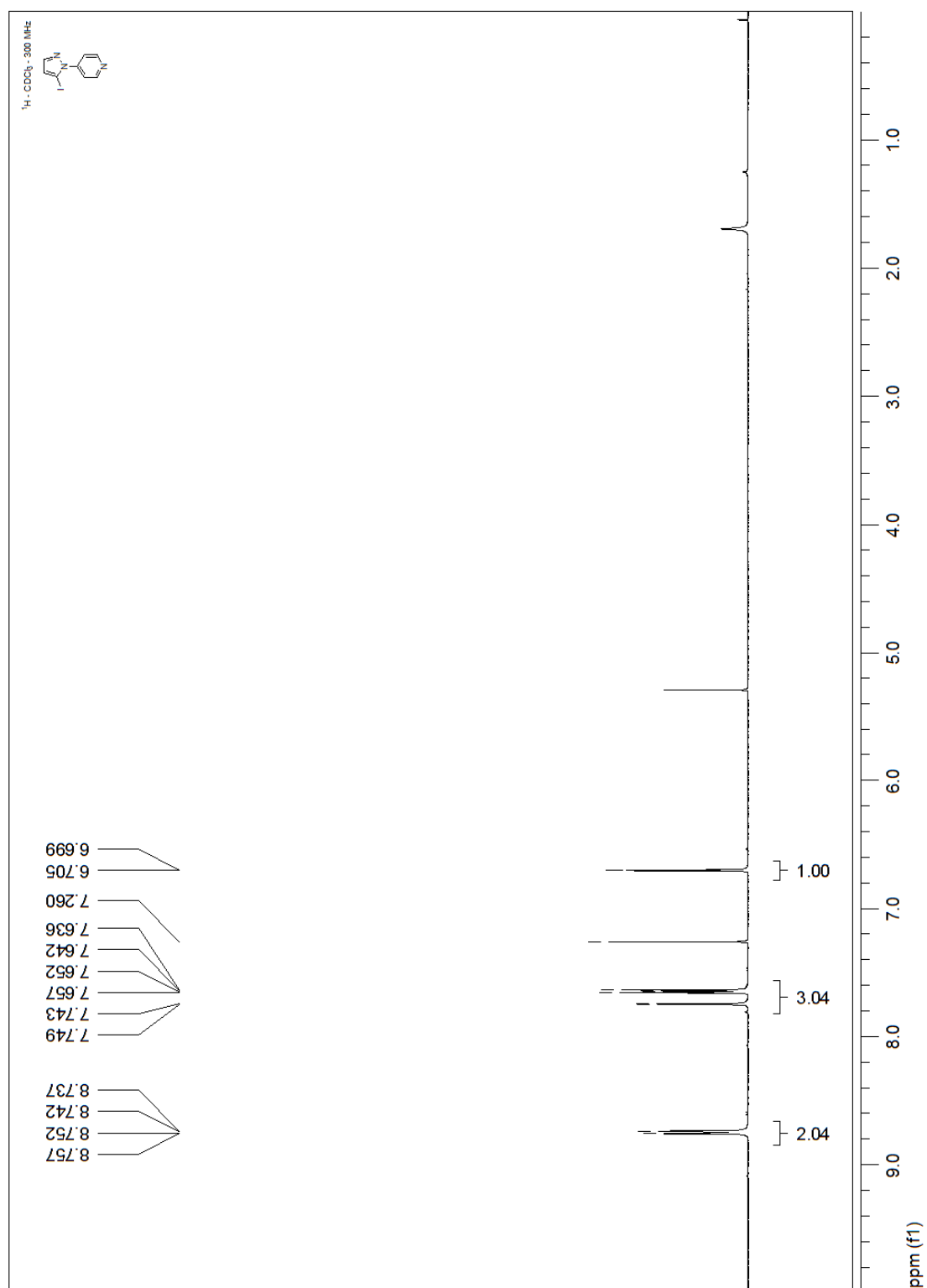
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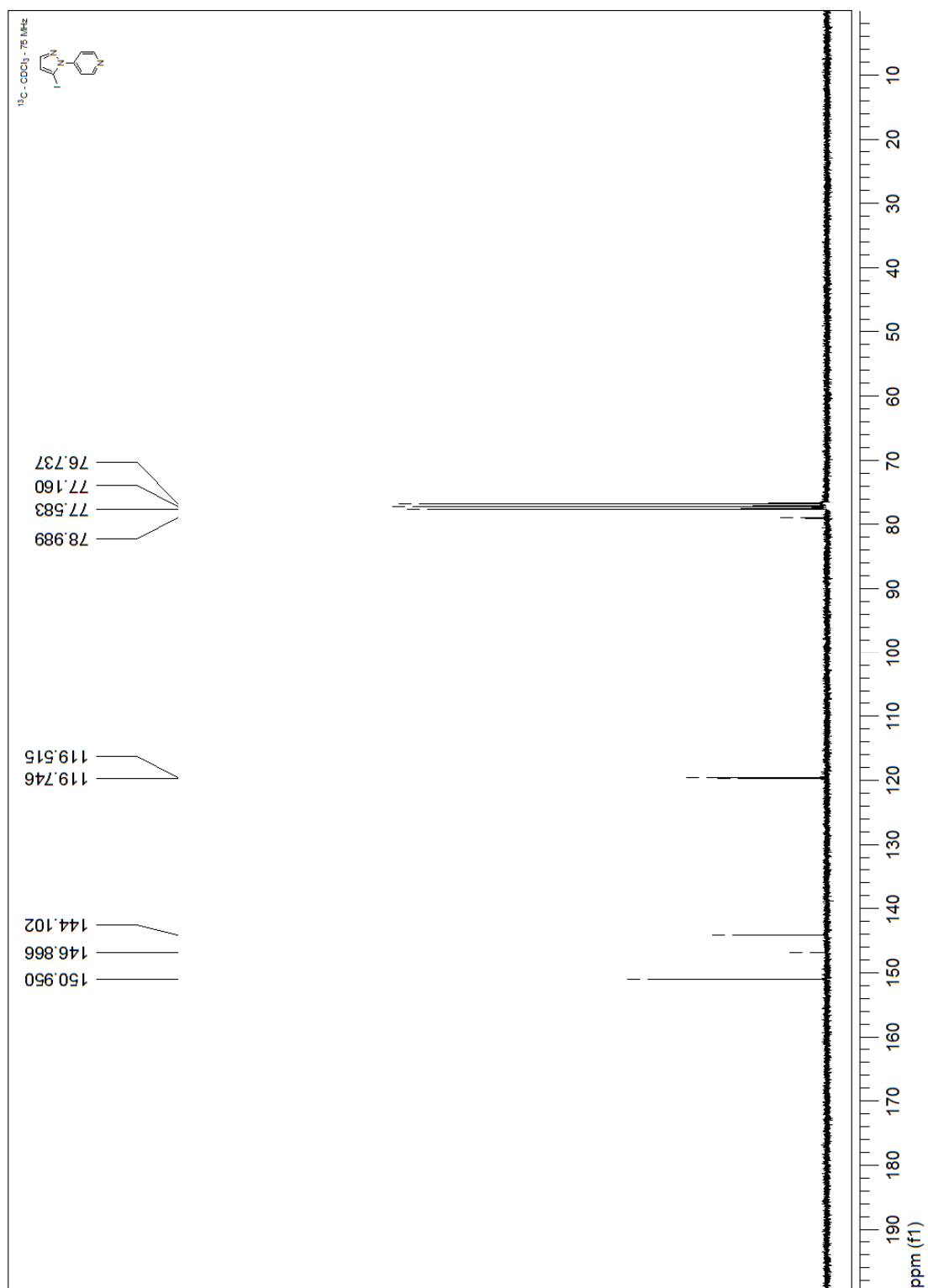
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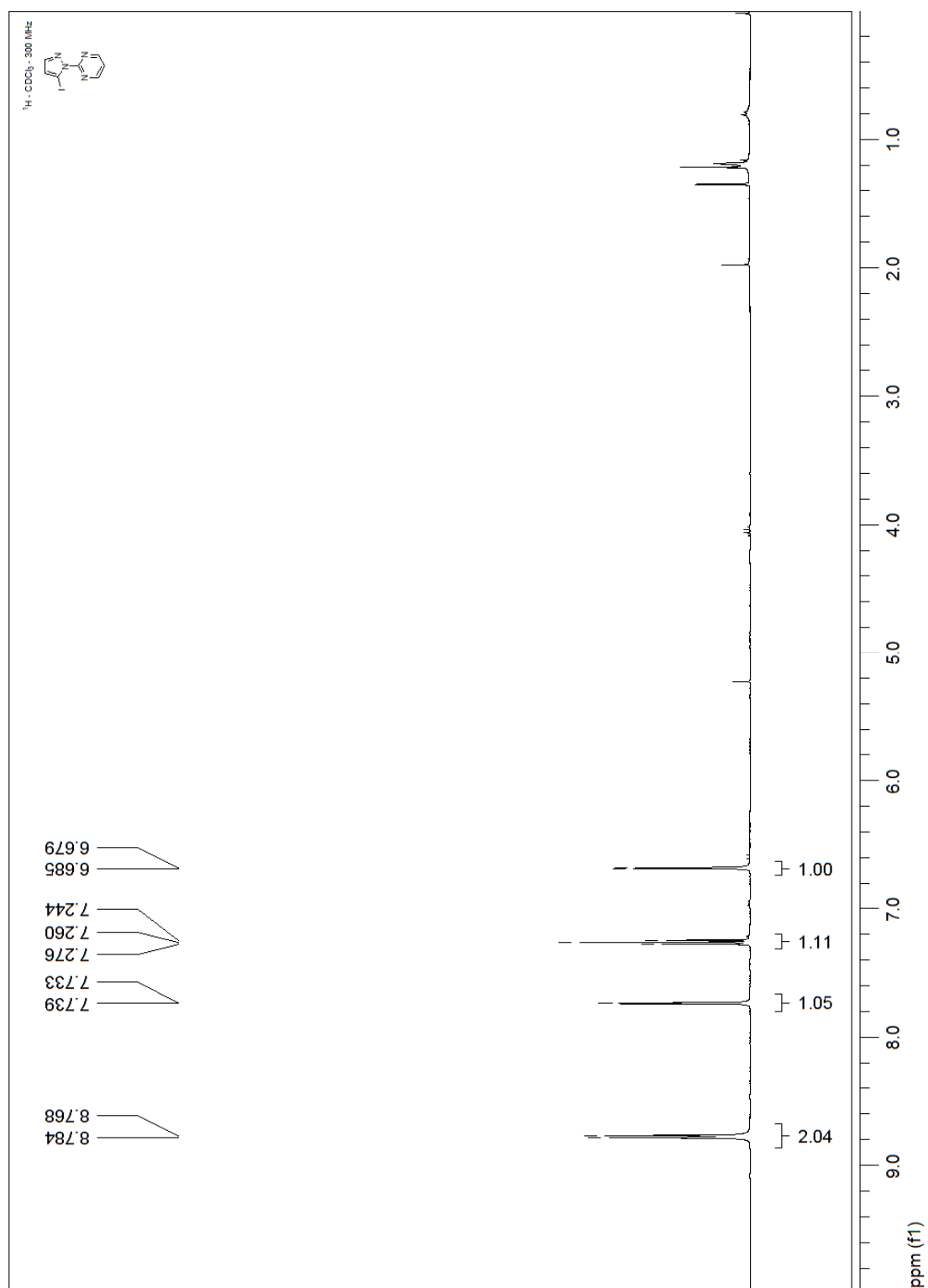
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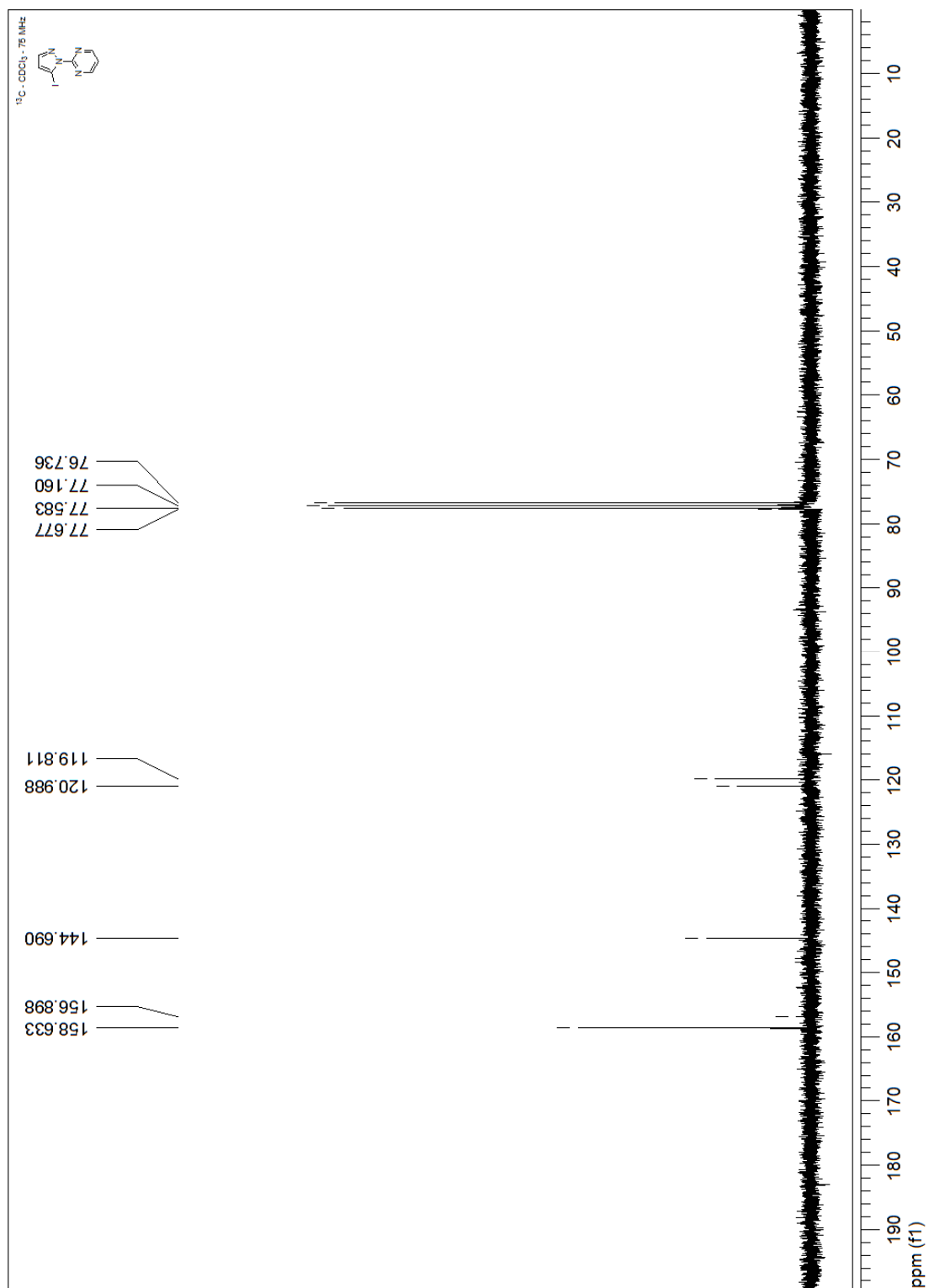
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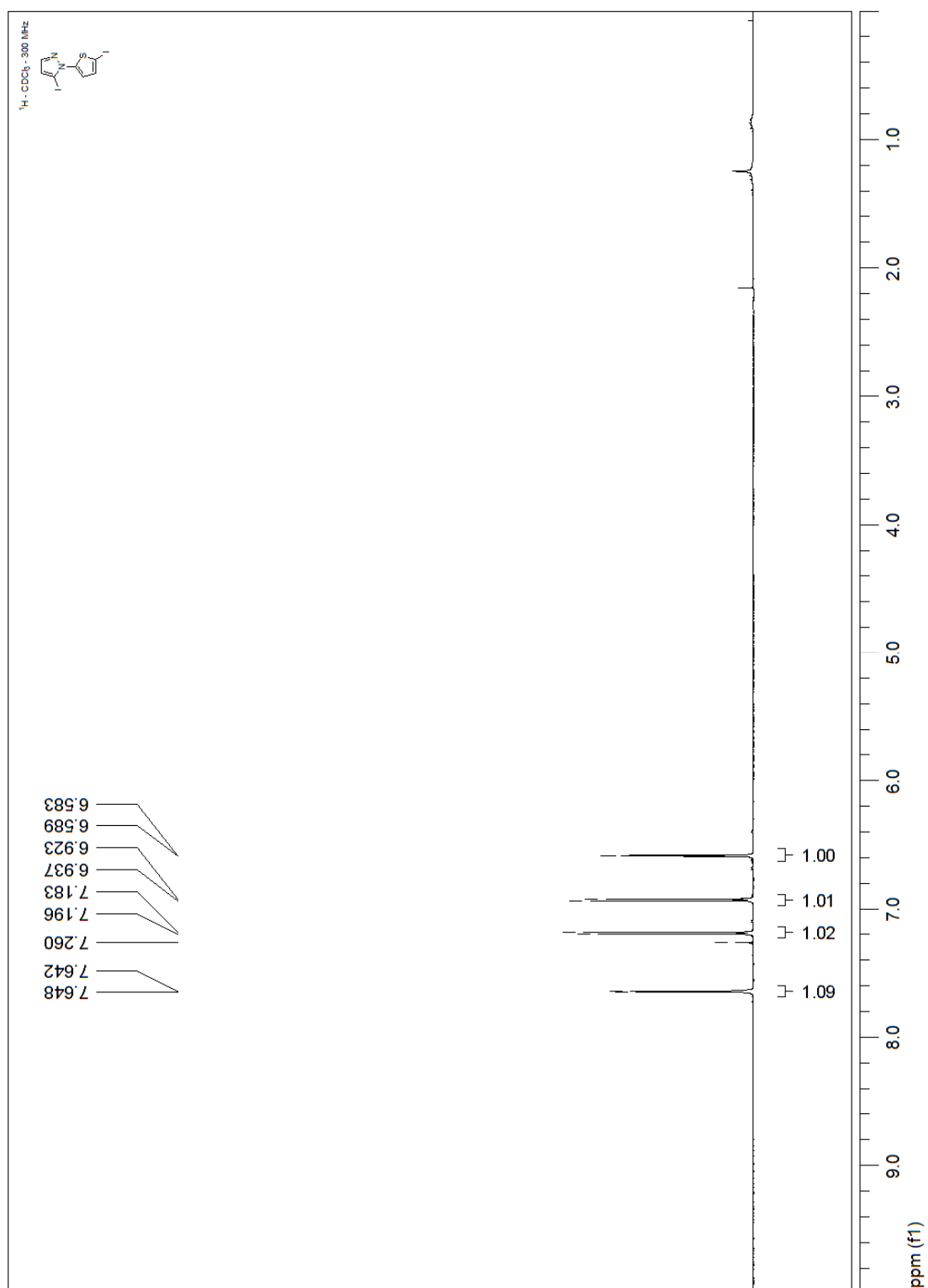
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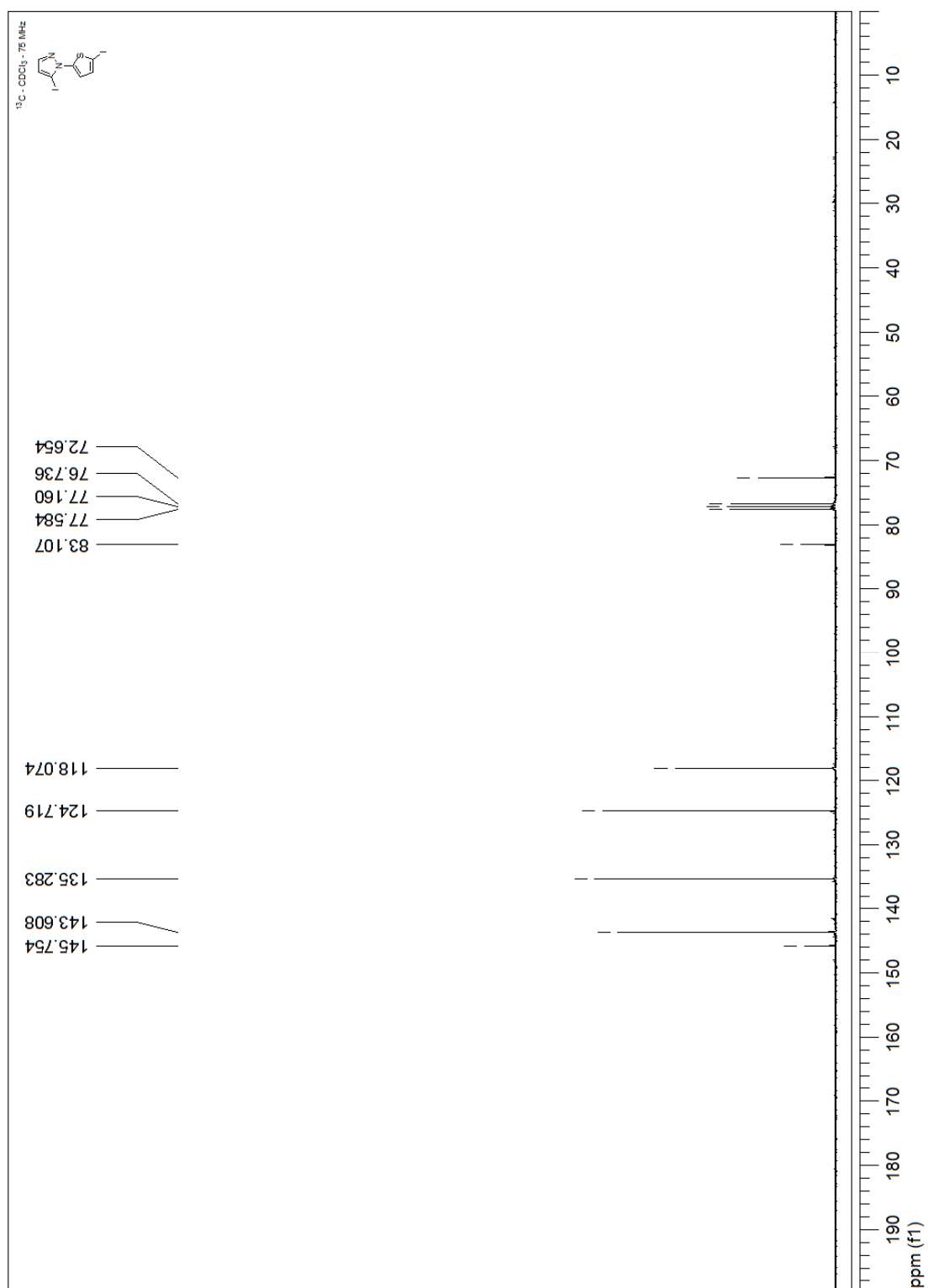
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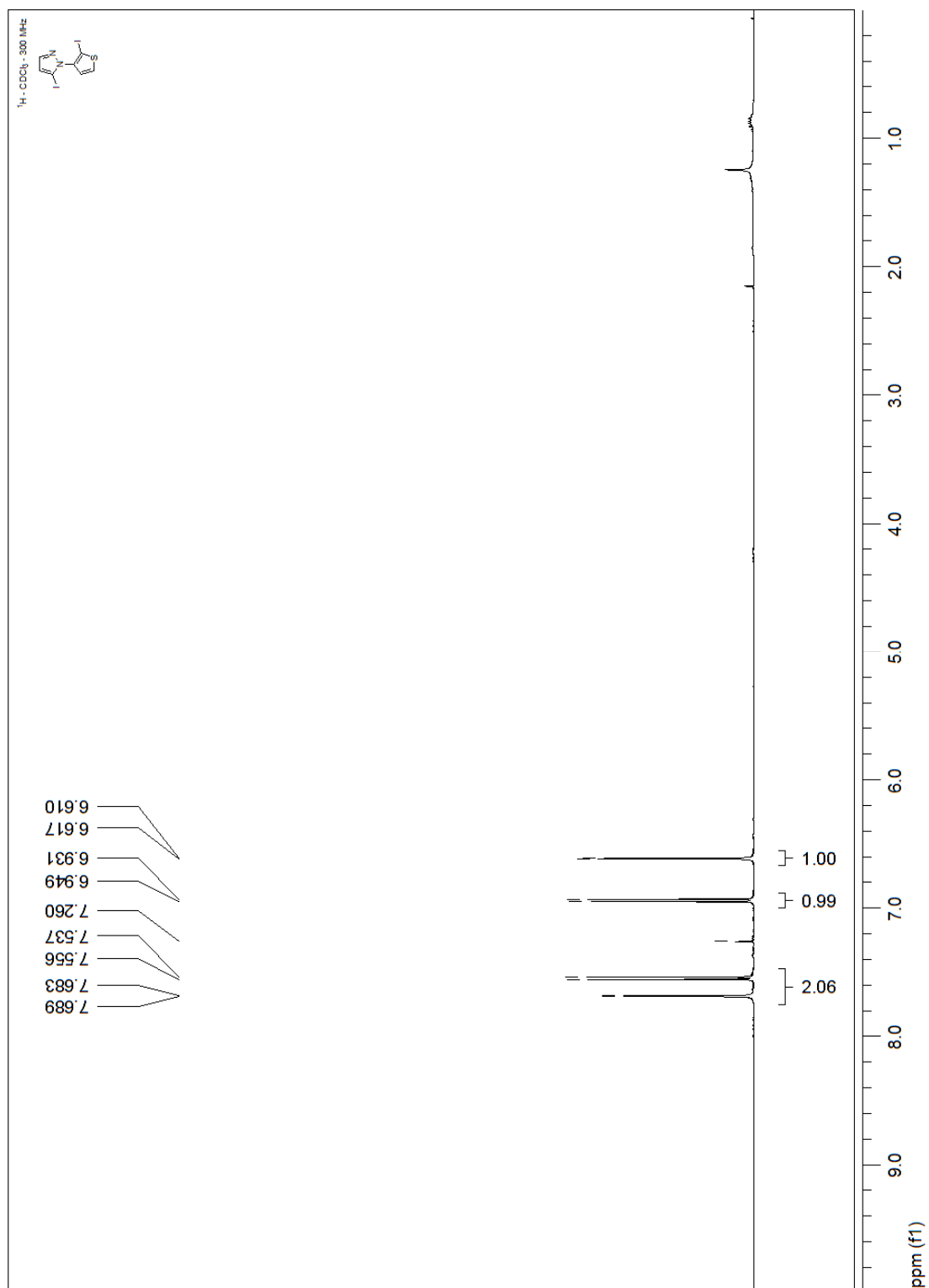
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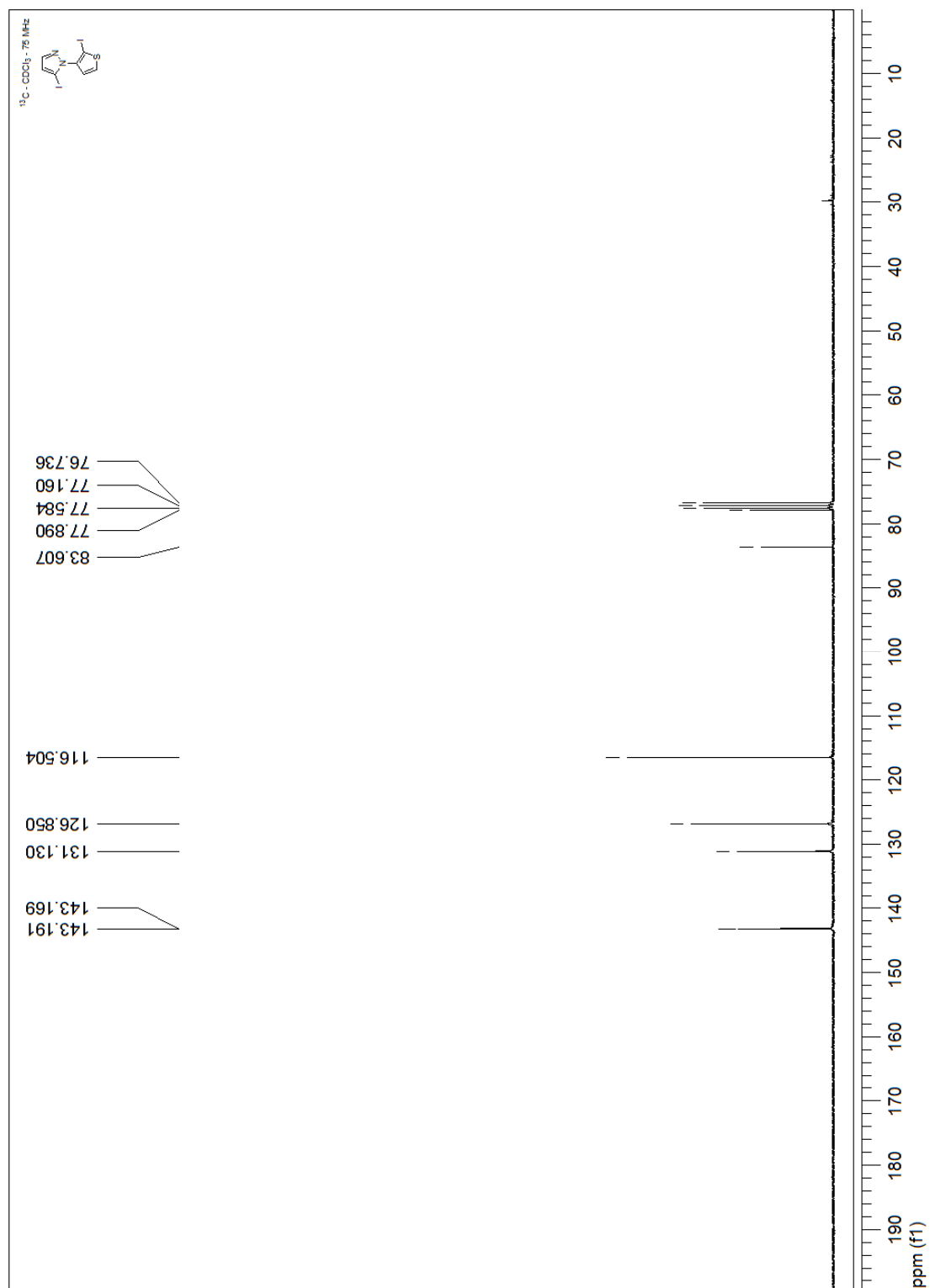
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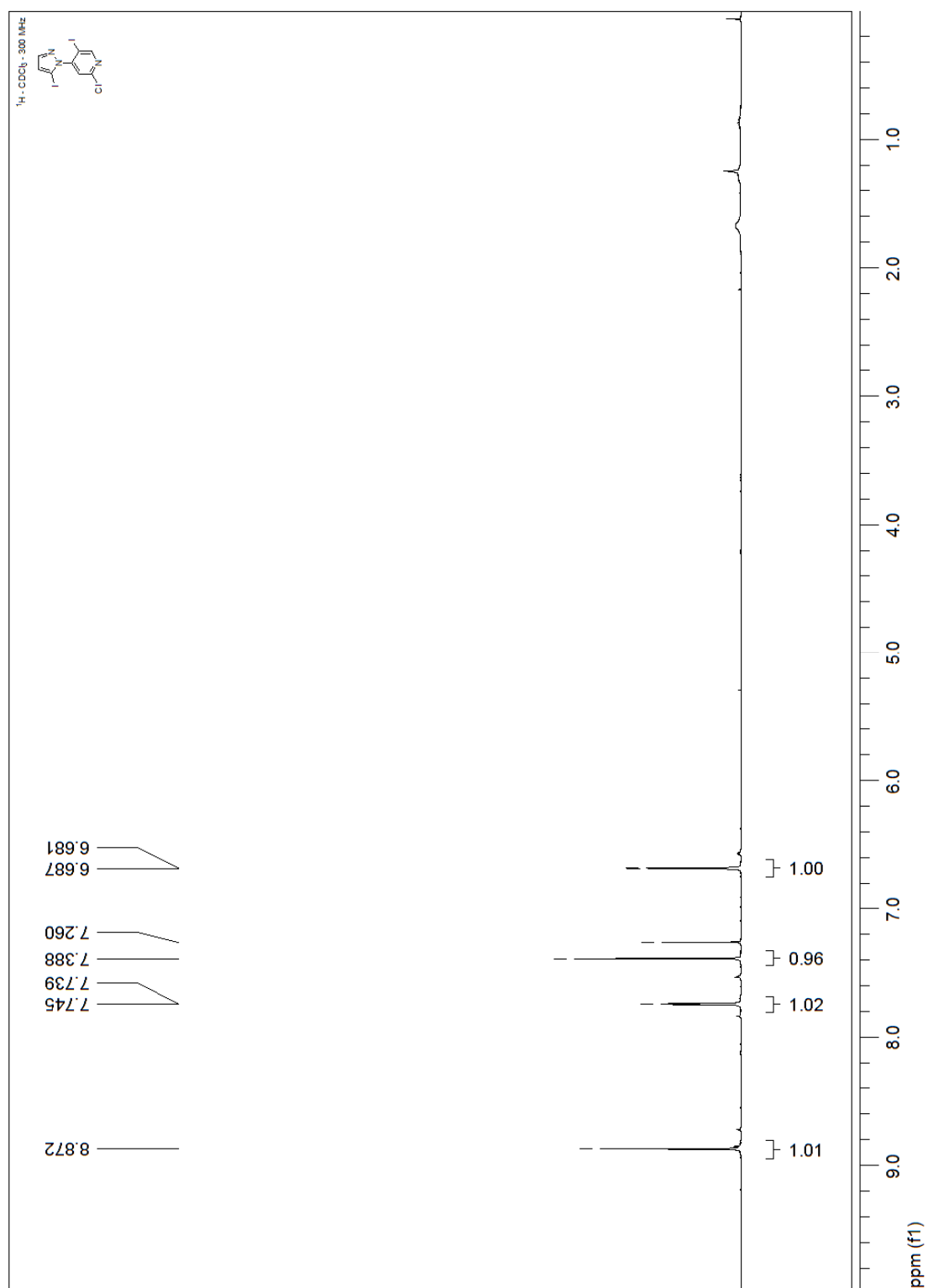
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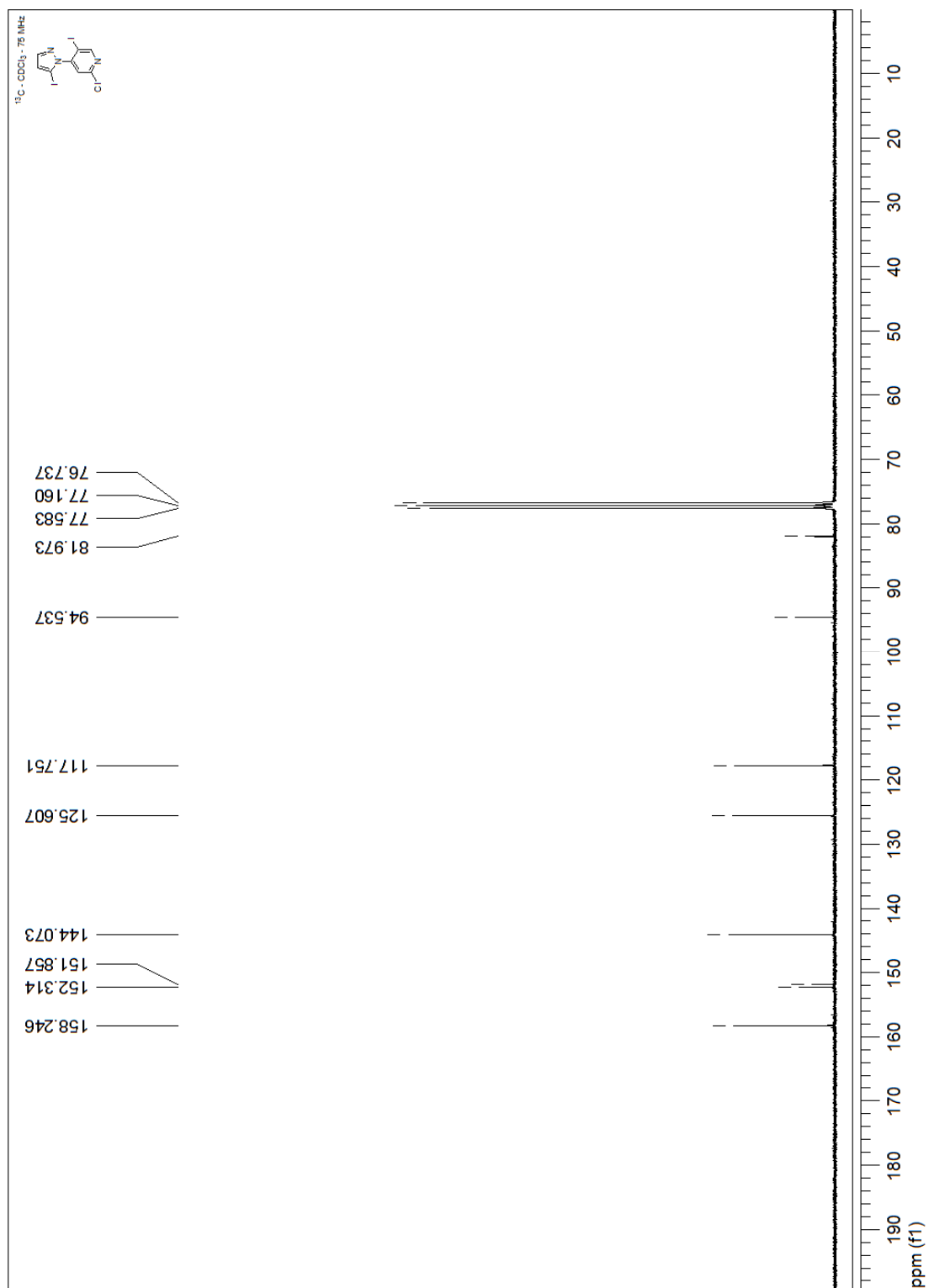
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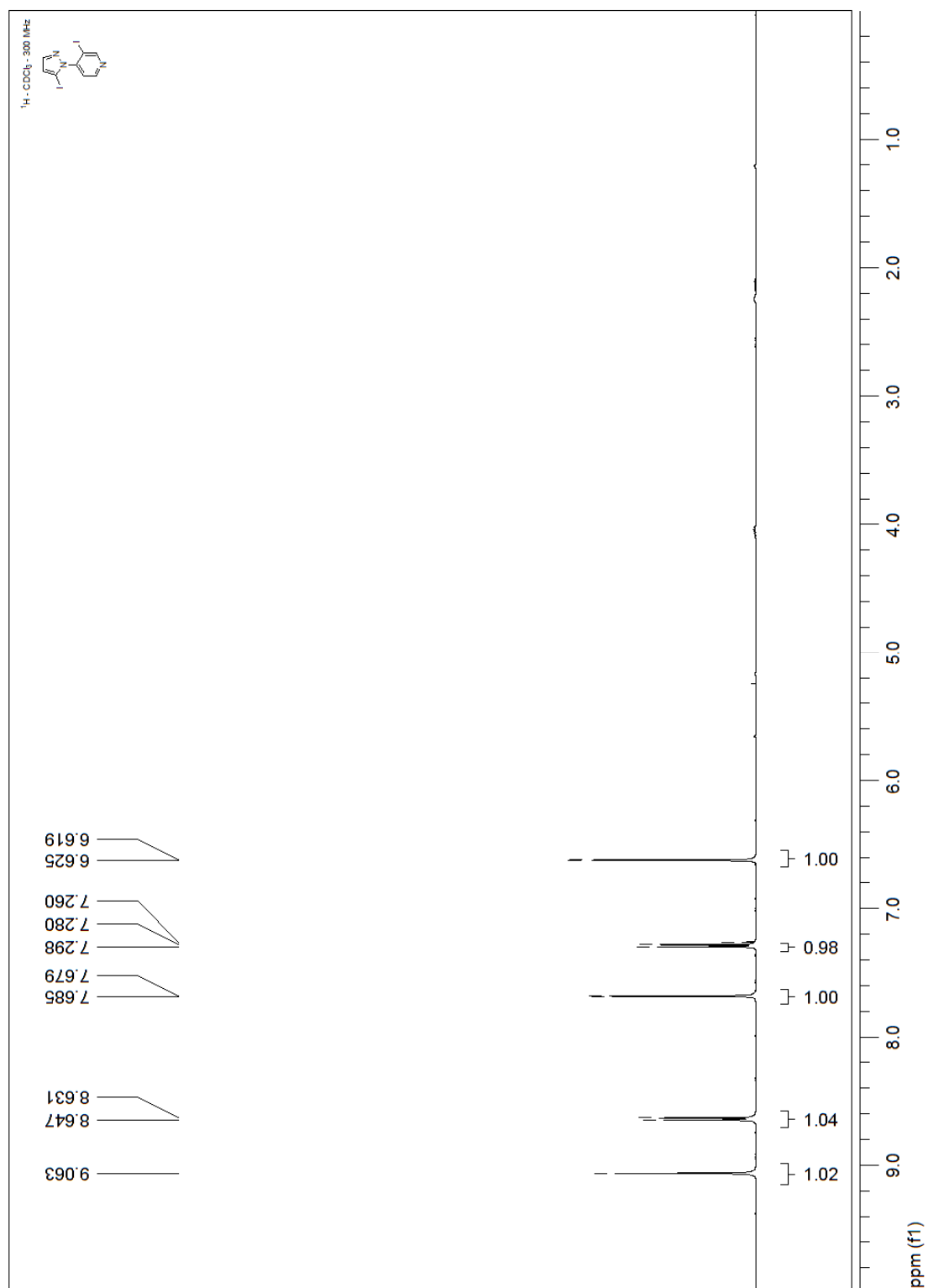
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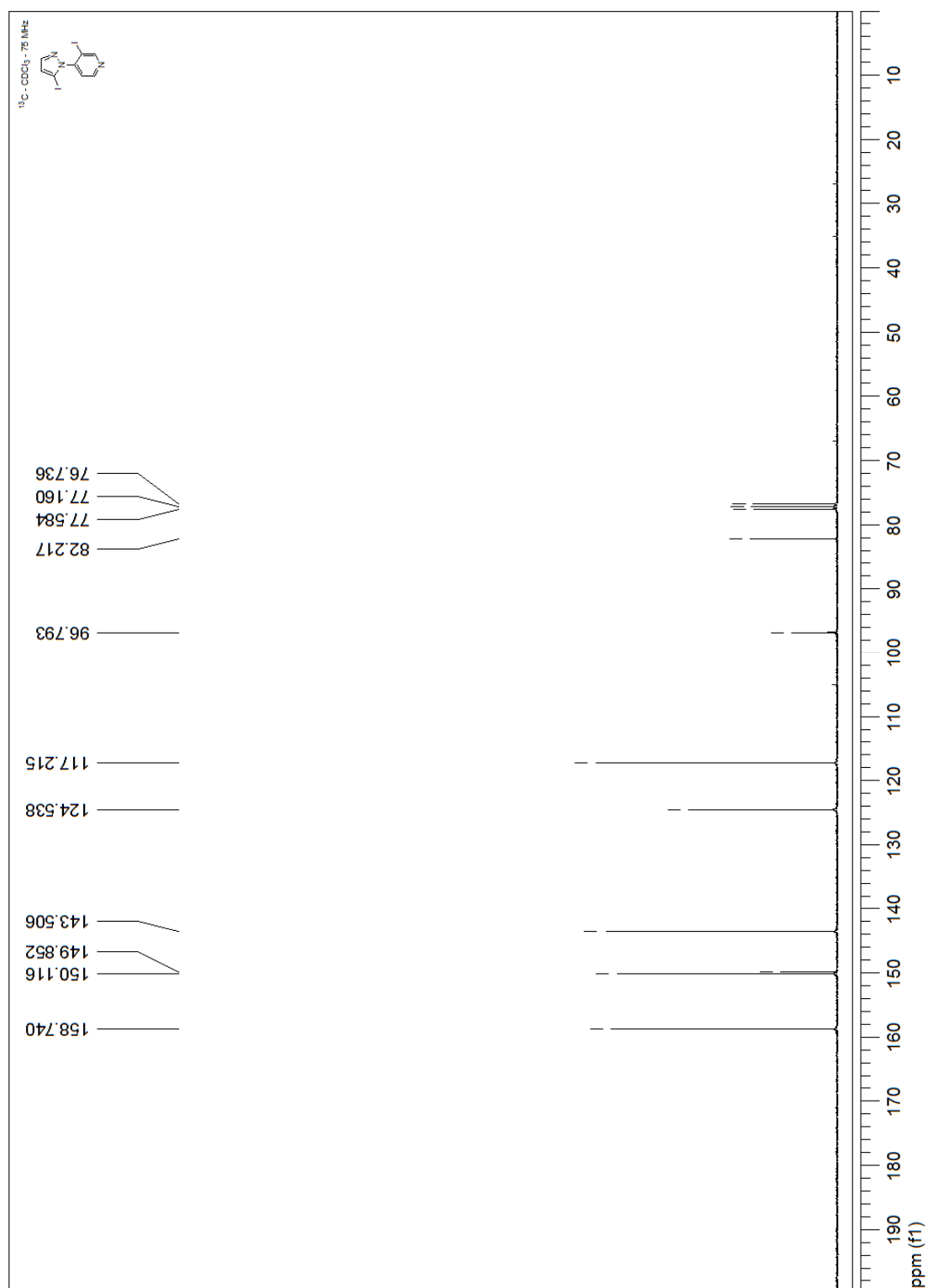
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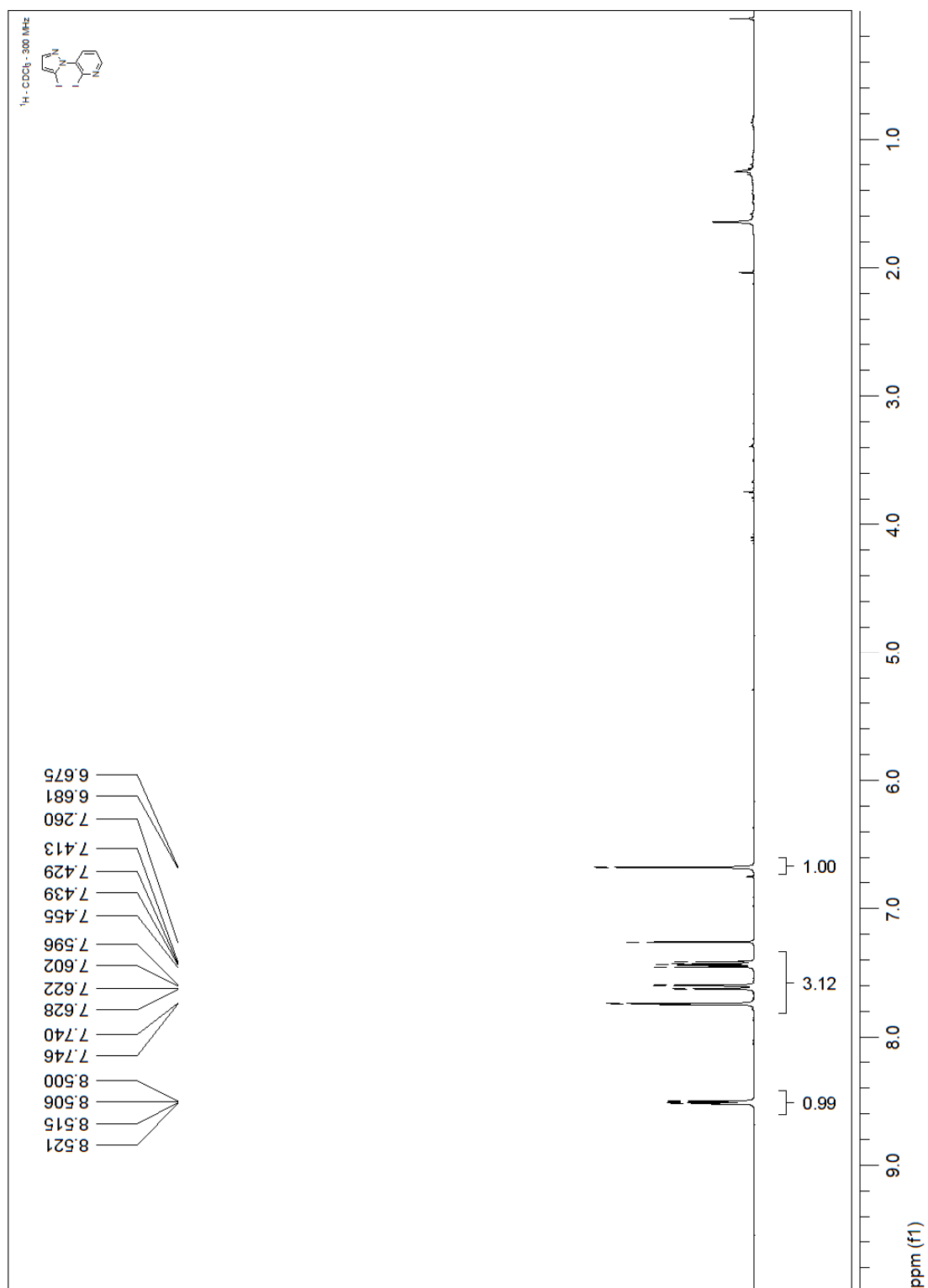
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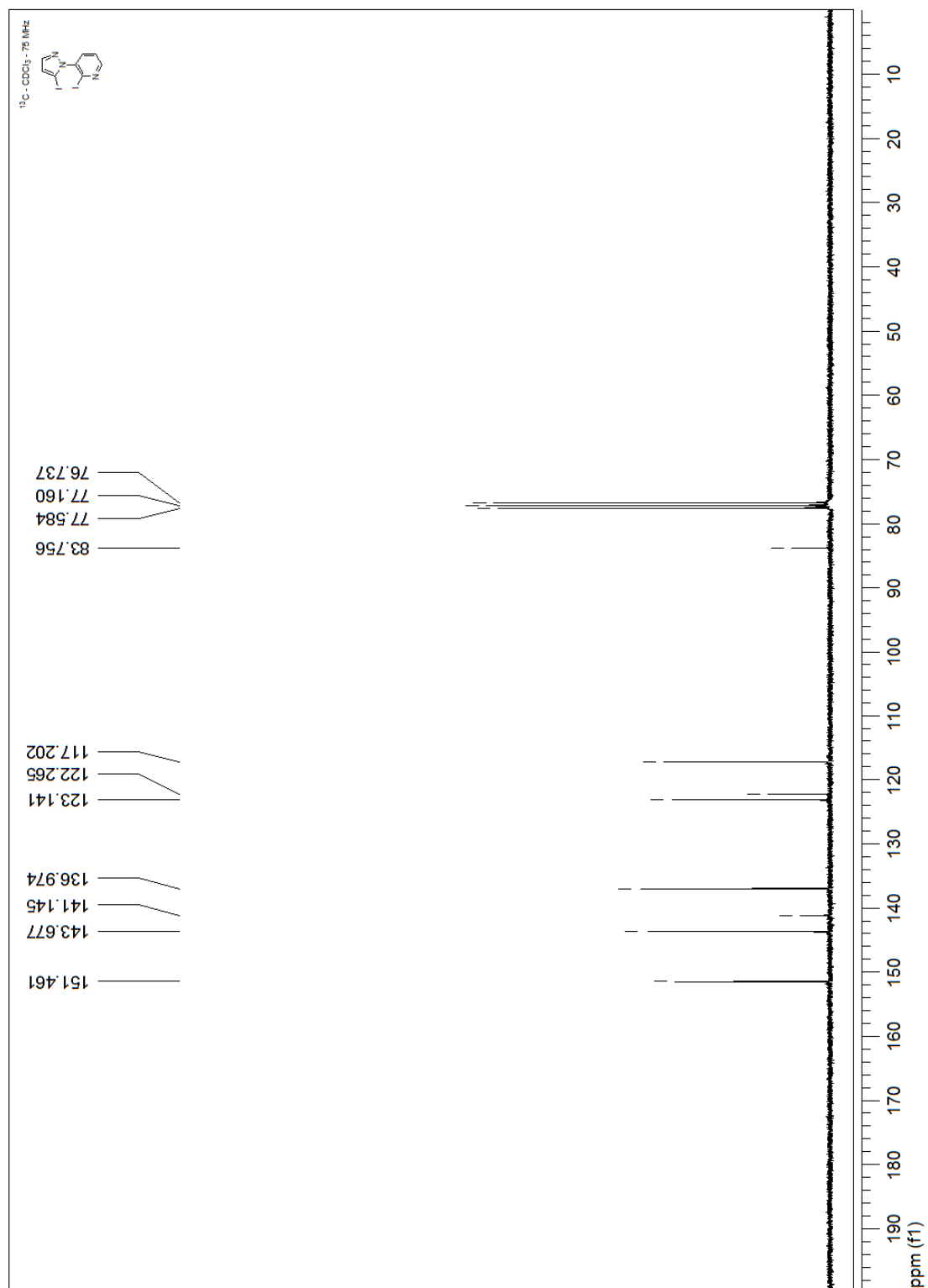
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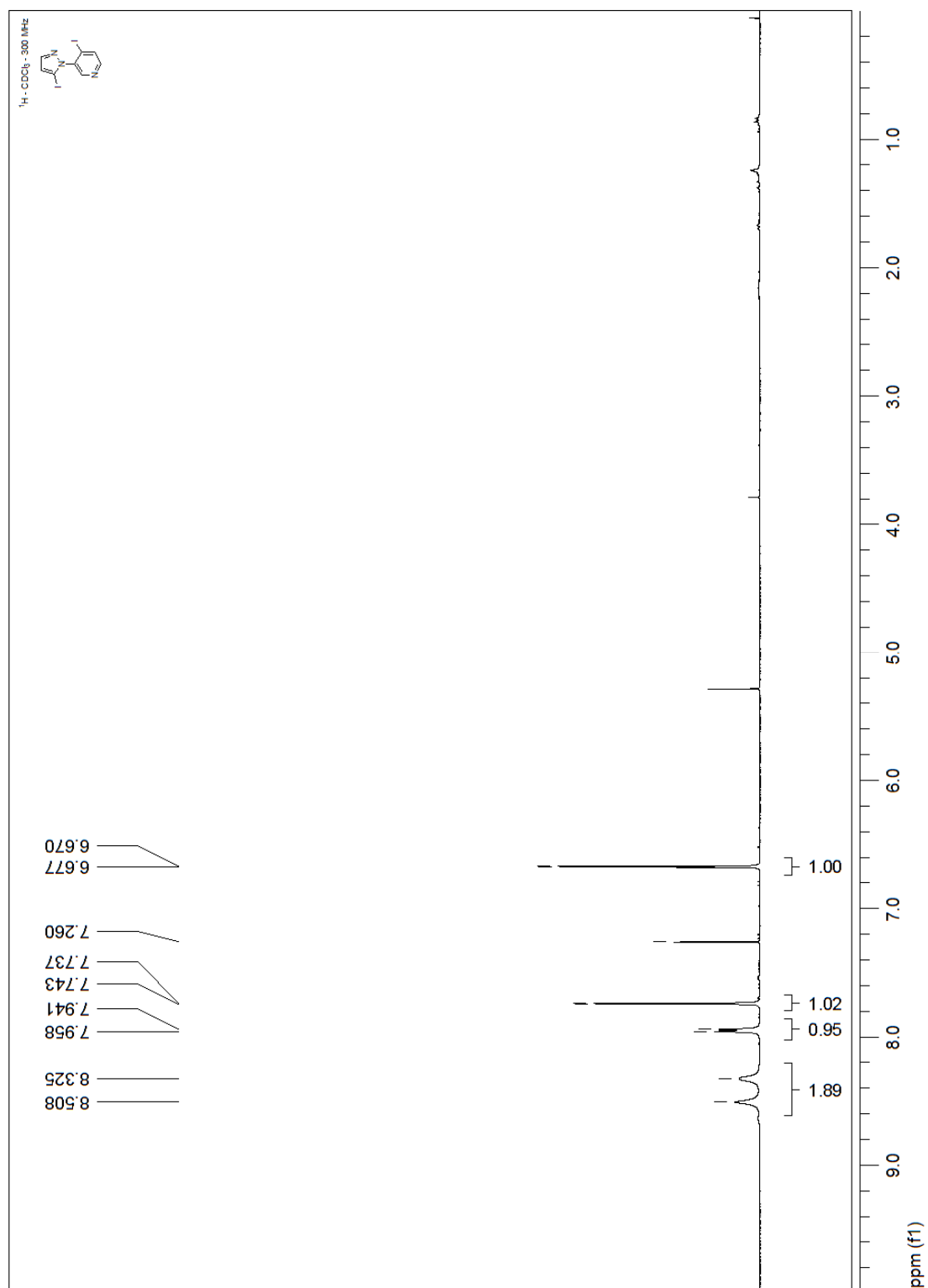
Compound 8o, ^1H -NMR



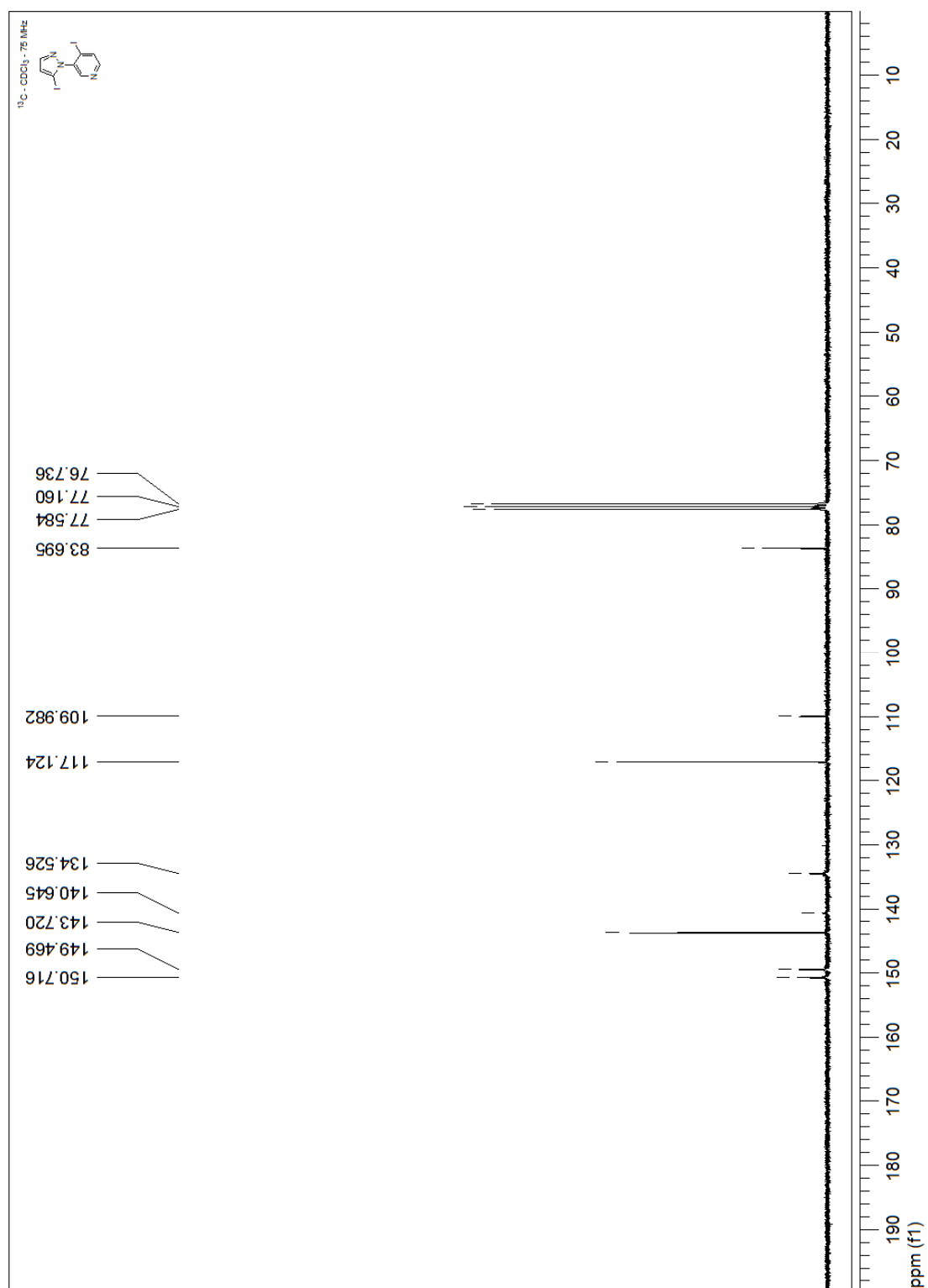
Compound 8o, ^{13}C -NMR



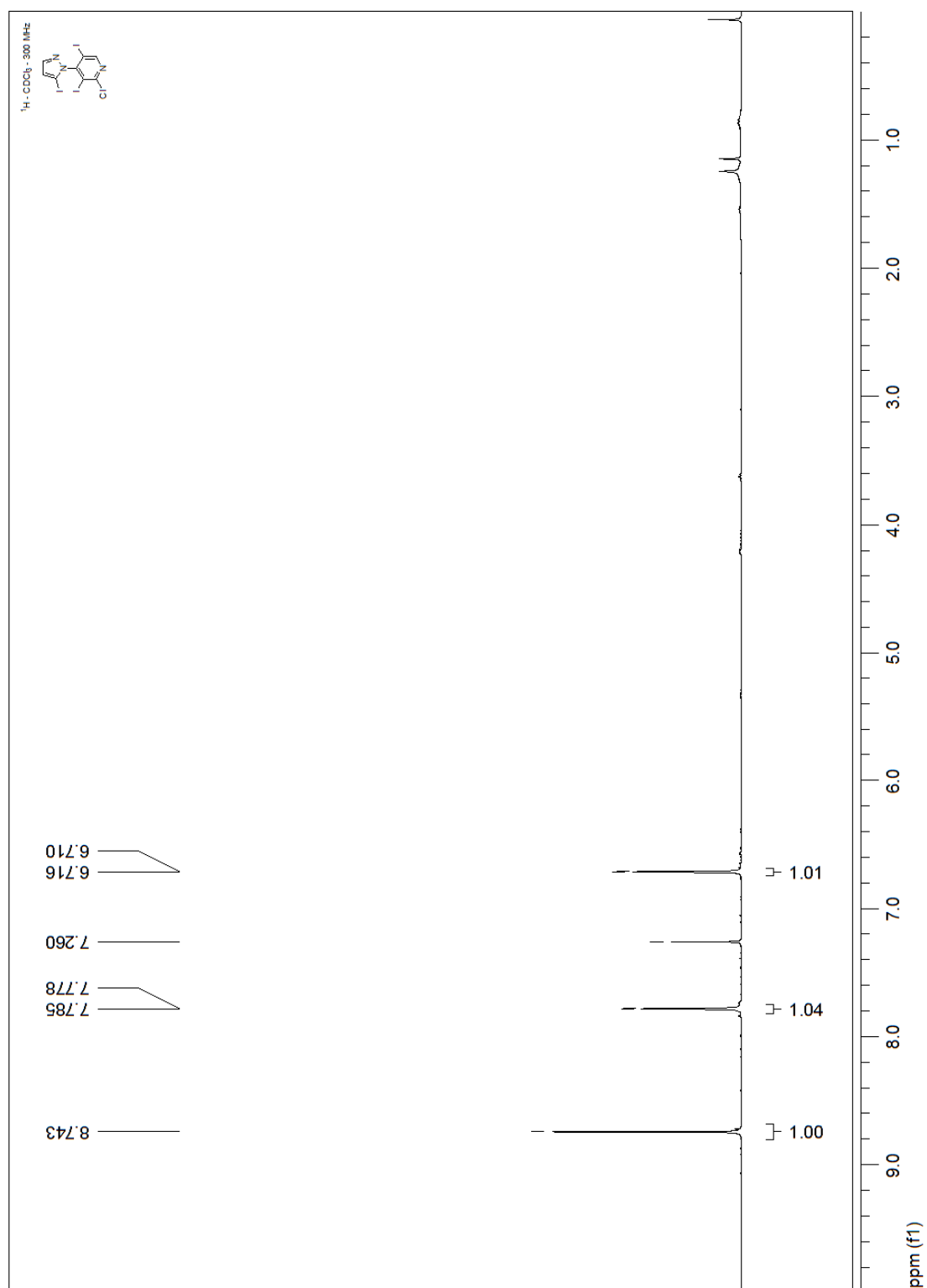
Compound 8'o, ^1H -NMR



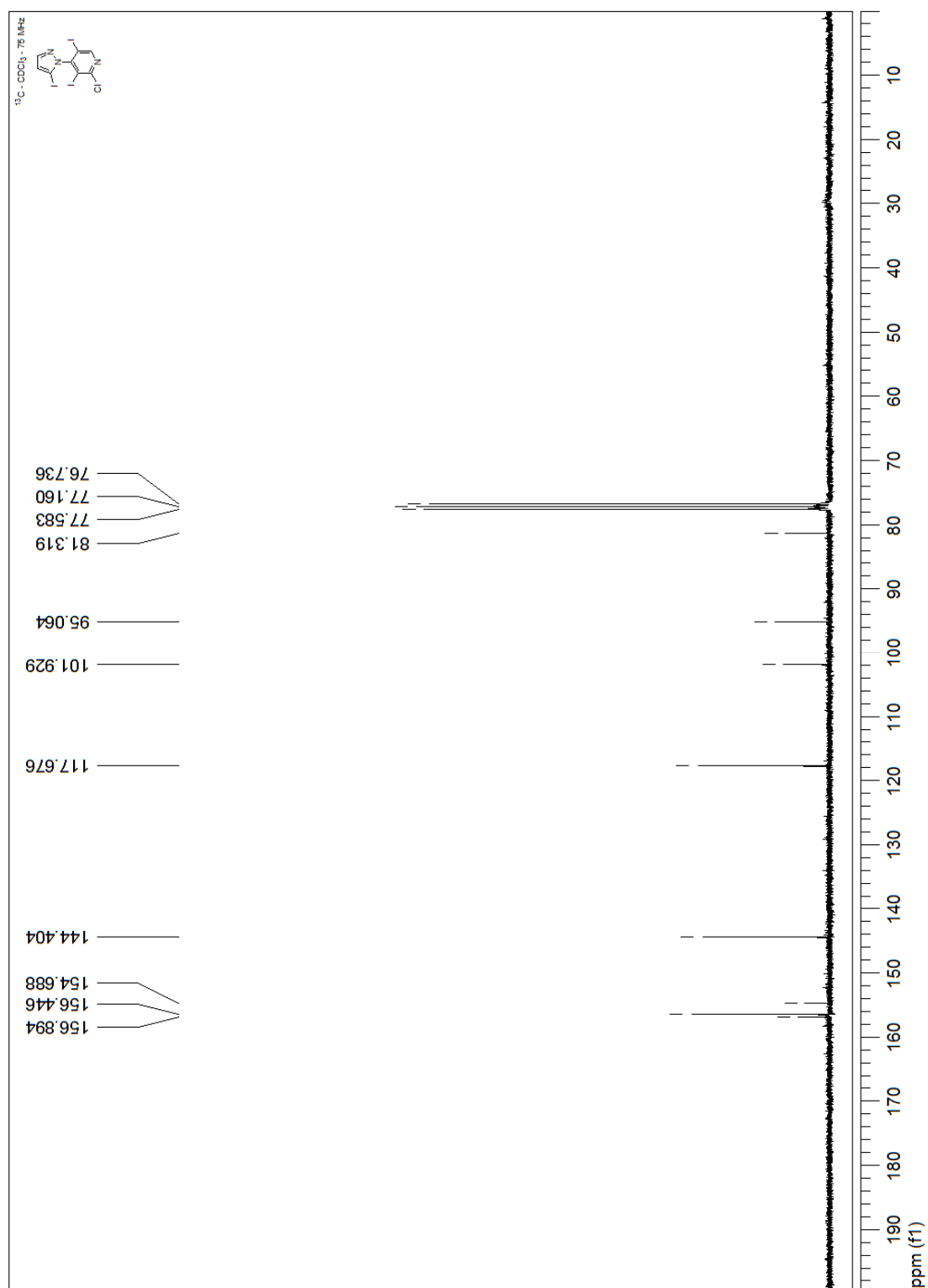
Compound 8'o, ^{13}C -NMR



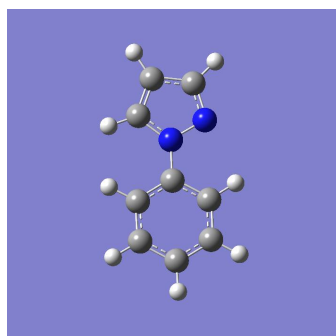
Compound 9m, ^1H -NMR



Compound 9m, ^{13}C -NMR

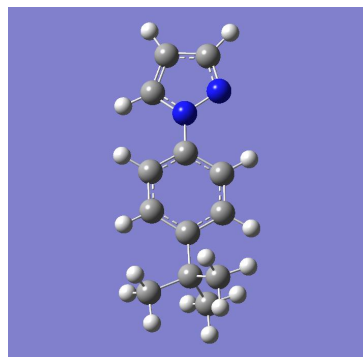


**Cartesian coordinates of molecular geometries for most stable rotamer forms
of investigated pyrazoles (neutral molecule, gas phase)
optimized at B3LYP/6-31G(d) level of theory**



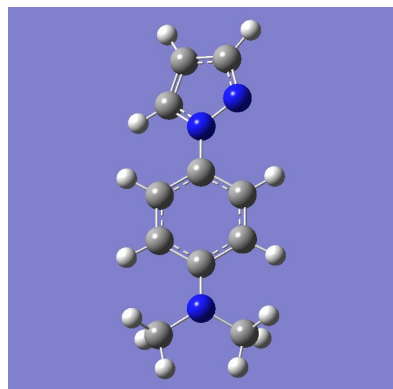
phenylpyrazole

C	1.36617582	-0.82540800	-0.00021998
N	0.08171234	-1.15994395	-0.00027983
N	-0.58972604	0.02324385	-0.00003068
C	1.54866700	0.57709806	0.00005246
C	0.27008351	1.08806744	0.00027824
H	2.47457797	1.13369254	0.00013508
H	-0.07943094	2.10836801	0.00055902
H	2.11819071	-1.60389786	-0.00041210
C	-2.01093012	0.03023049	-0.00003745
C	-2.70211811	-1.18767969	-0.00023933
C	-2.72259516	1.23612160	0.00016939
C	-4.09495661	-1.18980263	-0.00024488
H	-2.13655558	-2.11084510	-0.00039702
C	-4.11670673	1.21777308	0.00017714
H	-2.20464534	2.18899696	0.00032417
C	-4.81182374	0.00826179	-0.00003366
H	-4.62196389	-2.14018594	-0.00041165
H	-4.65819854	2.15985517	0.00033657
H	-5.89796105	-0.00027289	-0.00003430



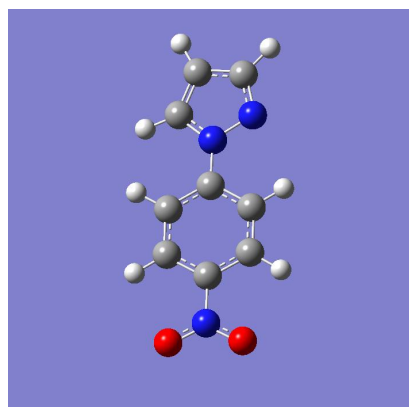
1a

C	1.25994867	0.78385832	-1.23285019
N	0.03837220	1.14093704	-0.84997825
N	-0.66837736	-0.01984859	-0.81660637
C	1.36200460	-0.60941555	-1.45022718
C	0.10259615	-1.09267185	-1.16934946
C	-2.03454110	-0.01115363	-0.43175490
C	-2.88521733	-1.06014286	-0.78251600
C	-2.53986874	1.06262246	0.30930516
C	-4.22079082	-1.04247936	-0.37687059
C	-3.87581986	1.06694339	0.69223595
C	-4.75330925	0.01674050	0.36836792
H	2.02481703	1.54185789	-1.34231468
H	2.22715508	-1.17900798	-1.75707462
H	-0.28892365	-2.09839383	-1.16649580
H	-1.87850519	1.87991529	0.57057570
H	-2.52423127	-1.88446574	-1.38932195
H	-4.23850857	1.91491786	1.26638432
H	-4.84942266	-1.87581473	-0.66961814
C	-6.22315983	0.07071264	0.82082967
C	-6.28541136	0.16172926	2.36442974
C	-6.90404770	1.31762961	0.20746935
C	-7.01653645	-1.17448685	0.38190439
H	-5.81544289	-0.71281172	2.82867872
H	-5.77536158	1.05415513	2.74177371
H	-7.32824135	0.20687937	2.70166010
H	-6.88743005	1.27412825	-0.88748937
H	-7.95071433	1.37875166	0.53003447
H	-6.40692180	2.24462122	0.51200276
H	-8.05269797	-1.09287822	0.72881765
H	-7.04147652	-1.27886439	-0.70879895
H	-6.59844060	-2.09496623	0.80531756



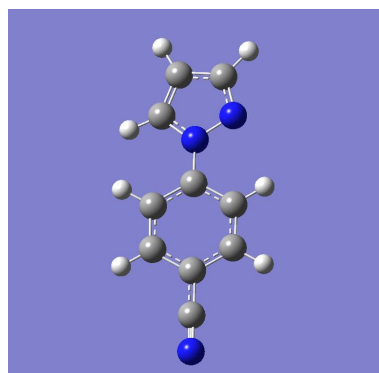
1b

C	1.24449795	0.83550465	-1.24123388
N	0.01359156	1.13809546	-0.83474065
N	-0.64457925	-0.04951446	-0.80925151
C	1.39752925	-0.54722697	-1.48367851
C	0.16099876	-1.08447175	-1.18984856
C	-2.00478595	-0.10472433	-0.40169221
C	-2.84618073	-1.13032001	-0.83719959
C	-2.51909367	0.87338016	0.45316839
C	-4.16957090	-1.19223274	-0.41248936
C	-3.84390849	0.82390982	0.86739020
C	-4.71214519	-0.20920652	0.44465264
H	1.97692471	1.62523526	-1.34870642
H	2.27907044	-1.07759157	-1.81360185
H	-0.19305314	-2.10432401	-1.19350060
H	-1.86877543	1.67294474	0.78842606
H	-2.47937986	-1.88476968	-1.52659290
H	-4.78431509	-2.00852839	-0.77140587
H	-4.19887557	1.59877961	1.53582406
N	-6.04503305	-0.24717636	0.84167000
C	-6.82788753	-1.44165913	0.57678741
H	-6.41229428	-2.34345562	1.05585919
H	-7.84305309	-1.29327943	0.95026084
H	-6.89942667	-1.63402916	-0.50056166
C	-6.49680633	0.64776577	1.89320664
H	-6.35903109	1.69580330	1.60220086
H	-7.56477545	0.49227803	2.05905270
H	-5.97182213	0.48839064	2.84932223



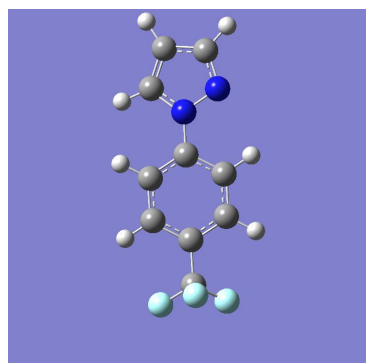
1c

C	1.09211885	0.73431806	-1.63732416
N	-0.16742739	1.06823082	-1.39763287
N	-0.71291175	-0.03028304	-0.80192552
C	1.38724338	-0.58121355	-1.20038659
C	0.20640688	-1.04044688	-0.66913419
C	-2.06617214	-0.01174081	-0.40321036
C	-2.70375455	-1.18681899	0.02423438
C	-2.77535189	1.19931368	-0.43956574
C	-4.03336752	-1.15042599	0.42433427
C	-4.10556656	1.23457333	-0.04534638
C	-4.72200447	0.06033664	0.38672199
H	1.74886114	1.44797869	-2.11752317
H	2.32608661	-1.11188973	-1.26061203
H	-0.03782389	-1.98108273	-0.20114088
H	-2.17682447	-2.13380761	0.03420716
H	-4.54444415	-2.04541096	0.75645629
H	-4.67101972	2.15801870	-0.06328593
H	-2.26866435	2.09356715	-0.77831449
N	-6.12538871	0.09751829	0.80736512
O	-6.70837072	1.18135363	0.76145002
O	-6.63901205	-0.95769421	1.18262858



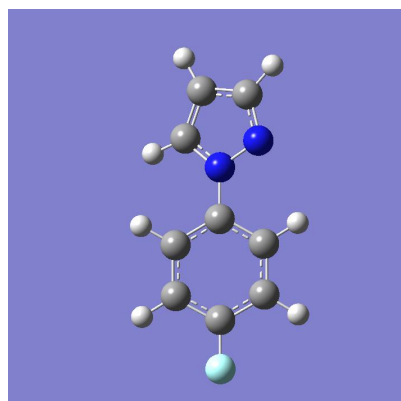
1d

C	1.06230614	0.69312802	-1.72591866
N	-0.20834658	1.01103768	-1.52074435
N	-0.71750842	-0.03056842	-0.80497115
C	1.39938502	-0.55444308	-1.14601378
C	0.23291324	-0.98887696	-0.56252620
C	-2.07193700	-0.01155607	-0.40413205
C	-2.68529573	-1.16504073	0.10420734
C	-2.80576926	1.17767948	-0.52103008
C	-4.01424697	-1.12557636	0.50681638
C	-4.13528863	1.21176479	-0.12512045
C	-4.75408904	0.06280800	0.39762079
H	1.69550097	1.36943640	-2.28530571
H	2.35500535	-1.05793416	-1.14873588
H	0.01845513	-1.87636343	0.01210611
H	-2.31872349	2.05668219	-0.92331652
H	-2.13997331	-2.09940504	0.17324519
H	-4.48760977	-2.01946981	0.89933343
H	-4.70251831	2.13251146	-0.21393379
C	-6.12481297	0.10065250	0.81102538
N	-7.23826576	0.13051556	1.14793521



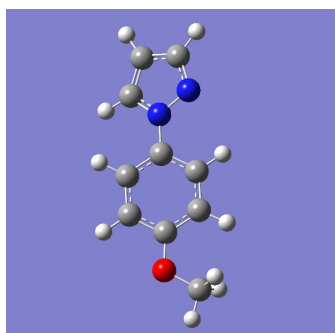
1e

C	1.07484983	0.70006004	-1.71507427
N	-0.19209879	1.02640808	-1.49443693
N	-0.71081031	-0.03185758	-0.81277348
C	1.39822051	-0.56952300	-1.17889127
C	0.22733307	-1.00842409	-0.60539914
C	-2.06548626	-0.01155350	-0.40360935
C	-2.70375783	-1.18591616	0.01385069
C	-2.76904818	1.19983172	-0.41721811
C	-4.03134083	-1.14348755	0.42868959
C	-4.09741081	1.23010687	-0.00981927
C	-4.73495675	0.06235154	0.41999249
H	1.71397701	1.38712036	-2.25432778
H	2.34756630	-1.08436288	-1.20103498
H	0.00230143	-1.91020064	-0.05744247
H	-2.26199588	2.09783435	-0.74655204
H	-2.18043887	-2.13551862	0.00306277
H	-4.52108370	-2.05403329	0.75699645
H	-4.63822179	2.17074718	-0.01319747
C	-6.18644632	0.09377447	0.80750948
F	-6.49322022	-0.88268503	1.69155222
F	-6.99746059	-0.08022826	-0.26334614
F	-6.53146078	1.27440305	1.36874539



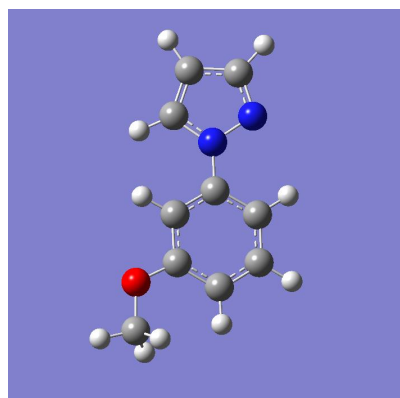
1f

C	1.05406188	0.63073201	-1.82092273
N	-0.22941057	0.93214904	-1.65261225
N	-0.70657164	-0.03380638	-0.82367250
C	1.42515272	-0.52992348	-1.10403311
C	0.26716423	-0.92727099	-0.47189178
C	-2.06594281	-0.01203241	-0.41672994
C	-2.69443218	-1.18075378	0.02726774
C	-2.77845980	1.19223556	-0.46478179
C	-4.02370305	-1.14392295	0.44561290
C	-4.11051452	1.22863889	-0.06227184
C	-4.71278273	0.06122150	0.39414190
H	1.66768373	1.25732266	-2.45515885
H	2.39509976	-1.00217637	-1.04812039
H	0.07205113	-1.74155908	0.20924644
H	-2.27893850	2.08400543	-0.82283400
H	-2.16160183	-2.12568693	0.02969396
H	-4.52934078	-2.03874145	0.79249753
H	-4.68132025	2.15079292	-0.09137020
F	-6.00178848	0.09786489	0.79195920



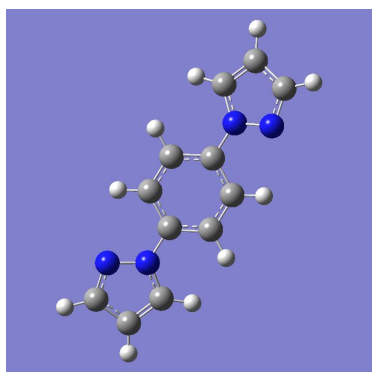
1g

C	1.24484201	0.74312082	-1.36989105
N	0.04223470	1.12588865	-0.94952747
N	-0.66631197	-0.02714463	-0.83043917
C	1.33039789	-0.65827183	-1.52737369
C	0.08203734	-1.11984834	-1.16679625
C	-2.01329249	0.00599649	-0.38040566
C	-2.90180249	-1.02680118	-0.70794341
C	-2.45936517	1.07734082	0.39374850
C	-4.21000277	-0.99439353	-0.24433491
C	-3.77794579	1.12025404	0.84746479
C	-4.66076860	0.07879711	0.53734740
H	2.00719990	1.49041632	-1.54855591
H	2.17767396	-1.24730361	-1.84716231
H	-0.31441787	-2.12145185	-1.09697037
H	-1.76816093	1.87708475	0.63160735
H	-2.58096338	-1.84731667	-1.34177453
H	-4.90862076	-1.78714038	-0.49177826
H	-4.09865280	1.96529987	1.44559968
O	-5.96475115	0.01616487	0.93658275
C	-6.47645681	1.08074539	1.72239567
H	-7.51929882	0.82938428	1.92407022
H	-5.93637955	1.17653689	2.67375445
H	-6.43166051	2.03742207	1.18510829



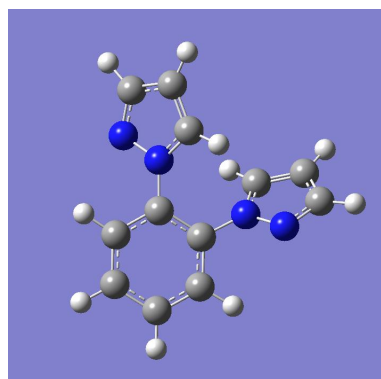
1h

C	1.30075819	0.67174191	-1.11473097
N	0.09708417	1.09602763	-0.74625280
N	-0.69379925	-0.00865661	-0.80538478
C	1.30800591	-0.71041212	-1.41442595
C	0.00837888	-1.11364895	-1.20125483
C	-2.06826841	0.08148177	-0.46208671
C	-2.96130858	-0.89556875	-0.89697710
C	-2.51305289	1.15983730	0.31570255
C	-4.31321934	-0.81482236	-0.53727016
C	-3.85941465	1.23055167	0.65122530
C	-4.77189070	0.25330230	0.24088185
H	2.12238000	1.37526112	-1.15450777
H	2.13914533	-1.32425247	-1.72981527
H	-0.45532235	-2.08542354	-1.27268948
H	-1.80416384	1.91274844	0.63482304
H	-2.65025424	-1.71684108	-1.53216178
H	-4.21313363	2.06240830	1.25419561
H	-5.81444523	0.33586900	0.52401017
O	-5.09856664	-1.82574467	-1.01181100
C	-6.48455185	-1.79642161	-0.70919847
H	-6.91330394	-2.67883652	-1.18761779
H	-6.66287542	-1.84843257	0.37295870
H	-6.96638745	-0.89550261	-1.11119864



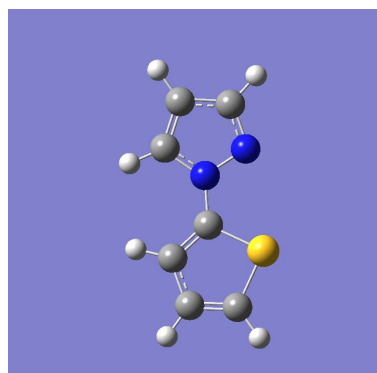
1i

C	1.04891073	0.65051478	-1.72222370
N	-0.22260914	0.98627376	-1.53354640
N	-0.74641601	-0.03344706	-0.80198042
C	1.36695375	-0.58666977	-1.11574407
C	0.18840123	-0.99499982	-0.53135903
C	-2.10646925	0.00564438	-0.40362607
C	-2.77190578	-1.15907554	-0.00439684
C	-2.79498419	1.22300637	-0.41642823
C	-4.09819741	-1.10429843	0.40959643
C	-4.12852711	1.27352431	-0.02588092
C	-4.78396347	0.11467236	0.40570281
H	1.69304168	1.30867097	-2.29086339
H	2.31657968	-1.10134792	-1.09959564
H	-0.04426008	-1.86331505	0.06569122
H	-2.28005673	2.11529382	-0.75008092
H	-2.26605474	-2.11851055	-0.02513626
N	-6.13540968	0.15884225	0.83189253
C	-6.85858037	1.24428378	1.24476512
C	-8.06264819	-0.60237365	1.32638625
C	-8.11695143	0.78925639	1.57140991
N	-6.87010876	-0.98446120	0.88258658
H	-8.84389810	-1.34076933	1.45232663
H	-8.94761734	1.37363515	1.93940803
H	-6.42430739	2.23072481	1.29879538
H	-4.61981079	-2.00052653	0.72159324
H	-4.65538182	2.22064876	-0.07292832



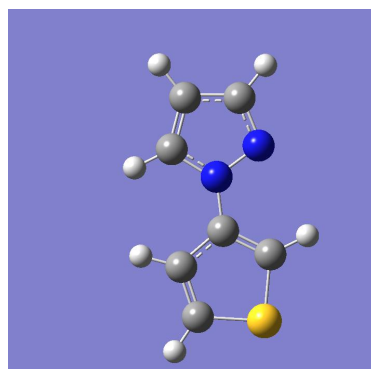
1j

C	1.07730985	0.64560620	-1.91118587
N	-0.24701488	0.75439820	-1.88506686
N	-0.63258878	-0.02550203	-0.83568758
C	1.56485533	-0.19169028	-0.88011670
C	0.43694443	-0.60158607	-0.20497692
C	-1.99925160	-0.06349409	-0.45111721
C	-2.62506023	-1.25312332	-0.03781853
C	-2.73222033	1.12844077	-0.46802878
C	-3.94301781	-1.21618565	0.42771037
C	-4.05381881	1.14907295	-0.03396879
C	-4.65468514	-0.02069509	0.43773098
H	-4.39223009	-2.14388657	0.76445132
H	-5.67953914	-0.00643542	0.79646879
N	-1.96004822	-2.50957757	-0.09266174
C	-1.34956307	-3.08616250	-1.17080611
C	-1.32493397	-4.42405004	0.58528952
C	-0.91985928	-4.33133580	-0.76654324
H	-1.27676816	-2.56799656	-2.11565822
H	-1.17998429	-5.24333337	1.27776164
H	-0.39571188	-5.06583654	-1.36050590
N	-1.95771285	-3.32825955	0.99650111
H	2.58897640	-0.45506512	-0.65920812
H	0.30356647	-1.23751866	0.65749059
H	-2.23668176	2.02833669	-0.81344877
H	-4.60746383	2.08333773	-0.04686413
H	1.63710063	1.17052166	-2.67460885



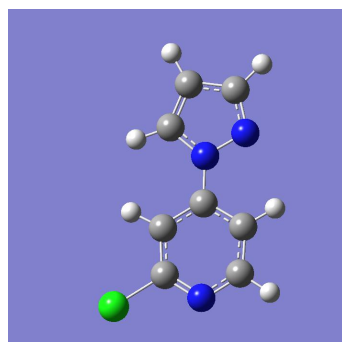
1k

C	2.90969988	0.63297196	-0.42980341
N	1.61753769	0.86904901	-0.63020888
N	0.97656889	-0.11154386	0.05905947
C	3.11961423	-0.50024404	0.39077140
C	1.85286715	-0.95612900	0.68376693
H	3.64514087	1.28516815	-0.88204856
H	4.05739445	-0.92558728	0.71707399
H	1.50973090	-1.79903632	1.26430040
C	-0.42269845	-0.15912932	0.05423258
C	-1.24860378	-0.96188108	0.79689146
S	-1.30865413	0.89307066	-1.01852575
C	-2.62669537	-0.73312497	0.49851965
H	-0.89913177	-1.67880798	1.53069565
C	-2.81471616	0.23063382	-0.45024349
H	-3.43784892	-1.26563148	0.98290421
H	-3.74640172	0.60715017	-0.85013341



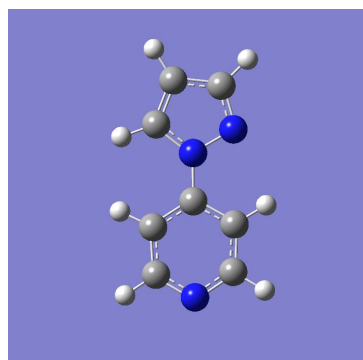
11

C	2.91659675	0.70556713	0.36215899
N	1.62473695	0.94487216	0.56428829
N	0.98391853	-0.09147557	-0.03669877
C	3.12835048	-0.48516701	-0.37000071
C	1.86093239	-0.97043203	-0.60885984
H	3.65166008	1.39852490	0.75053513
H	4.06524540	-0.92535772	-0.67863314
H	1.52408566	-1.85345318	-1.13007158
C	-0.42497735	-0.15293977	-0.01170881
C	-1.20402082	0.79411801	0.59916003
C	-1.18666359	-1.20433071	-0.61784879
S	-2.88516256	0.41421176	0.44234088
H	-0.86579772	1.67589410	1.12092586
C	-2.53033933	-1.02778915	-0.45096287
H	-0.75979996	-2.04634108	-1.14931717
H	-3.33041345	-1.66435337	-0.80298830



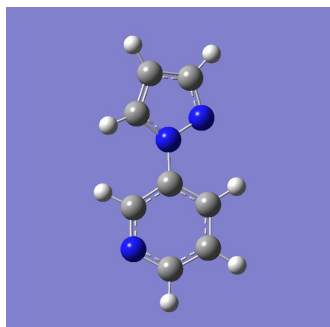
1m

C	2.97713210	-0.70911831	-0.25059523
N	1.71710477	-1.06901865	-0.44241771
N	0.97972344	-0.04171708	0.06831248
C	3.08045360	0.55364841	0.38577851
C	1.77975794	0.95164547	0.57509184
H	3.77296939	-1.36690885	-0.57491226
H	3.97467480	1.09175430	0.66413938
H	1.37269512	1.84544707	1.02125547
C	-0.42671965	-0.10441137	0.02484048
C	-1.06245551	-1.21742487	-0.54325324
C	-1.21389015	0.92880556	0.54079244
C	-2.45038106	-1.23428043	-0.56336288
H	-0.47587191	-2.03032508	-0.94938232
C	-2.59807339	0.77868289	0.45322370
H	-0.79290310	1.81655059	0.99344129
H	-2.97787776	-2.08118469	-0.99603583
N	-3.22732178	-0.25362348	-0.07409322
Cl	-3.60514575	2.07469867	1.10015538



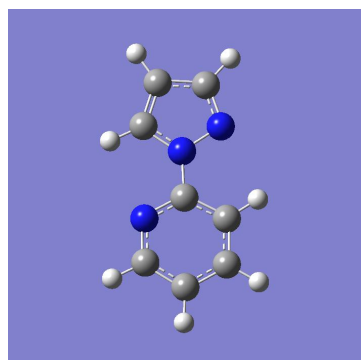
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C	1.37763301	-0.82624509	0.01659572
N	0.09583102	-1.16335321	0.01173951
N	-0.57664011	0.02157214	0.00747881
C	1.55887155	0.57886378	0.01717757
C	0.28287711	1.08971685	0.01164324
H	2.48493214	1.13490120	0.02320985
H	-0.07019001	2.10894581	0.01814600
H	2.13154344	-1.60276312	0.01917005
C	-1.98854447	0.02773967	0.00504377
C	-2.69494460	-1.17596045	0.09921019
C	-2.71605807	1.21882750	-0.09065331
C	-4.08594797	-1.12317707	0.09538518
H	-2.16158089	-2.11478792	0.17191730
C	-4.10768431	1.14393591	-0.08170631
H	-2.23148338	2.18473632	-0.17698545
H	-4.65690253	-2.04716295	0.16789300
H	-4.69265574	2.05929237	-0.15480025
N	-4.80384336	0.00529120	0.00898821



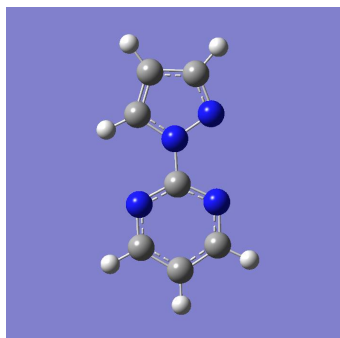
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C	2.97275581	-0.76239343	-0.10445271
N	1.70055488	-1.13126840	-0.19779666
N	0.99165840	-0.00050080	0.06863757
C	3.10655444	0.60708707	0.22508464
C	1.81210792	1.06353046	0.33117708
C	-0.42213328	-0.03872331	0.06185097
C	-1.09430707	-1.26017480	0.16367878
C	-1.17941932	1.13432692	-0.05287449
C	-2.48480113	-1.24639448	0.16076975
C	-3.15048860	-0.02275671	0.06541200
H	3.75177343	-1.49303234	-0.27956690
H	4.01336513	1.17536957	0.37185759
H	1.41964034	2.03475741	0.59090350
H	-0.69220706	2.09986073	-0.17112348
H	-4.23779821	0.02018588	0.06949012
H	-3.04587222	-2.17286750	0.23813019
N	-2.51410599	1.14926281	-0.04173234
H	-0.52444938	-2.17863064	0.23808607



1p

C	2.98330338	0.23154783	-0.64688004
N	1.73476818	0.30929084	-1.08919685
N	0.97008476	0.04659062	0.00581239
C	3.04142744	-0.08108388	0.73471327
C	1.72609702	-0.19286790	1.12140036
C	-0.44014136	0.04163081	-0.08449693
C	-1.06932534	0.30820444	-1.30745668
C	-2.42563151	-0.24222785	1.00355938
C	-2.45868524	0.28744520	-1.32785847
C	-3.16123240	0.00732863	-0.15251661
H	3.80196678	0.40253766	-1.33419997
H	3.91731997	-0.20569809	1.35463424
H	1.25388574	-0.41604614	2.06449743
H	-0.47376754	0.51874350	-2.18622799
H	-2.98900411	0.48844703	-2.25463768
H	-4.24598433	-0.01705457	-0.13199867
H	-2.92677881	-0.46522424	1.94363766
N	-1.08795772	-0.22796450	1.04881310



1q

C	2.92016231	-0.64637631	-0.31897198
N	1.68129759	-1.04918245	-0.55052458
N	0.90390821	-0.09164094	0.03212245
C	2.96758171	0.57172733	0.41322053
C	1.65278597	0.89994878	0.62216854
H	3.74677315	-1.24230265	-0.68475024
H	3.83823448	1.12296455	0.73780085
H	1.17366724	1.72573948	1.12231091
C	-0.50117182	-0.16258564	0.00204375
C	-2.38688793	-1.23107226	-0.62325570
C	-2.46690651	0.79300136	0.59363271
H	-2.84508959	-2.07951883	-1.12890604
H	-2.98679445	1.61081180	1.08960093
N	-1.13324353	0.84727986	0.61434380
N	-1.05203634	-1.20602632	-0.61987934
C	-3.16573478	-0.24278672	-0.02261995
H	-4.24927997	-0.27770329	-0.03419596