

Supplementary Material

Phosphorylation of 10-bromoanthracen-9-yl-cyclopenta[*d*]isoxazol-6-ols: chemistry suitable for antivirals

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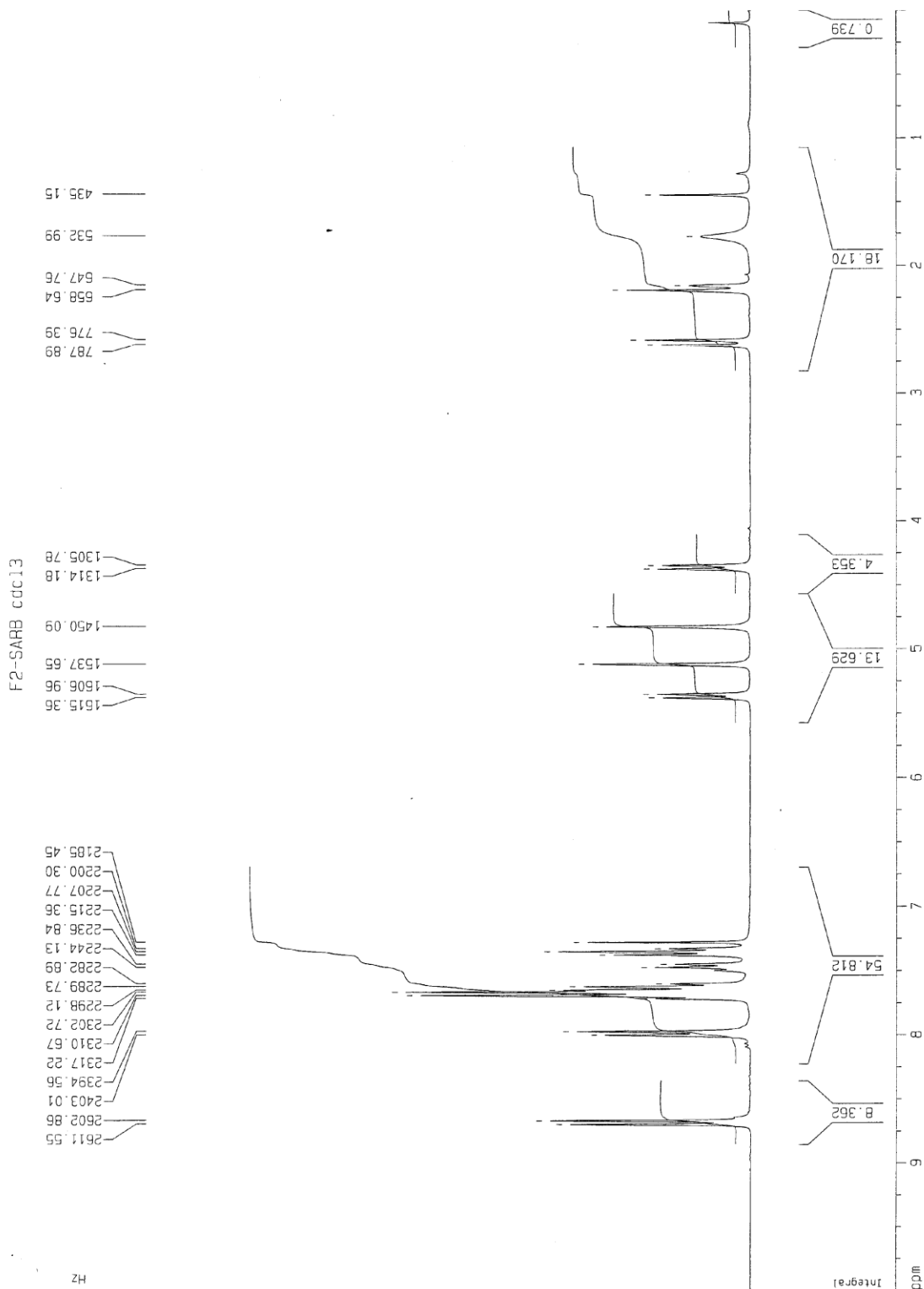
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^d*Centro Grandi Strumenti (CGS), University of Pavia, Via A. Bassi 21, 27100 - Pavia (Italy)*
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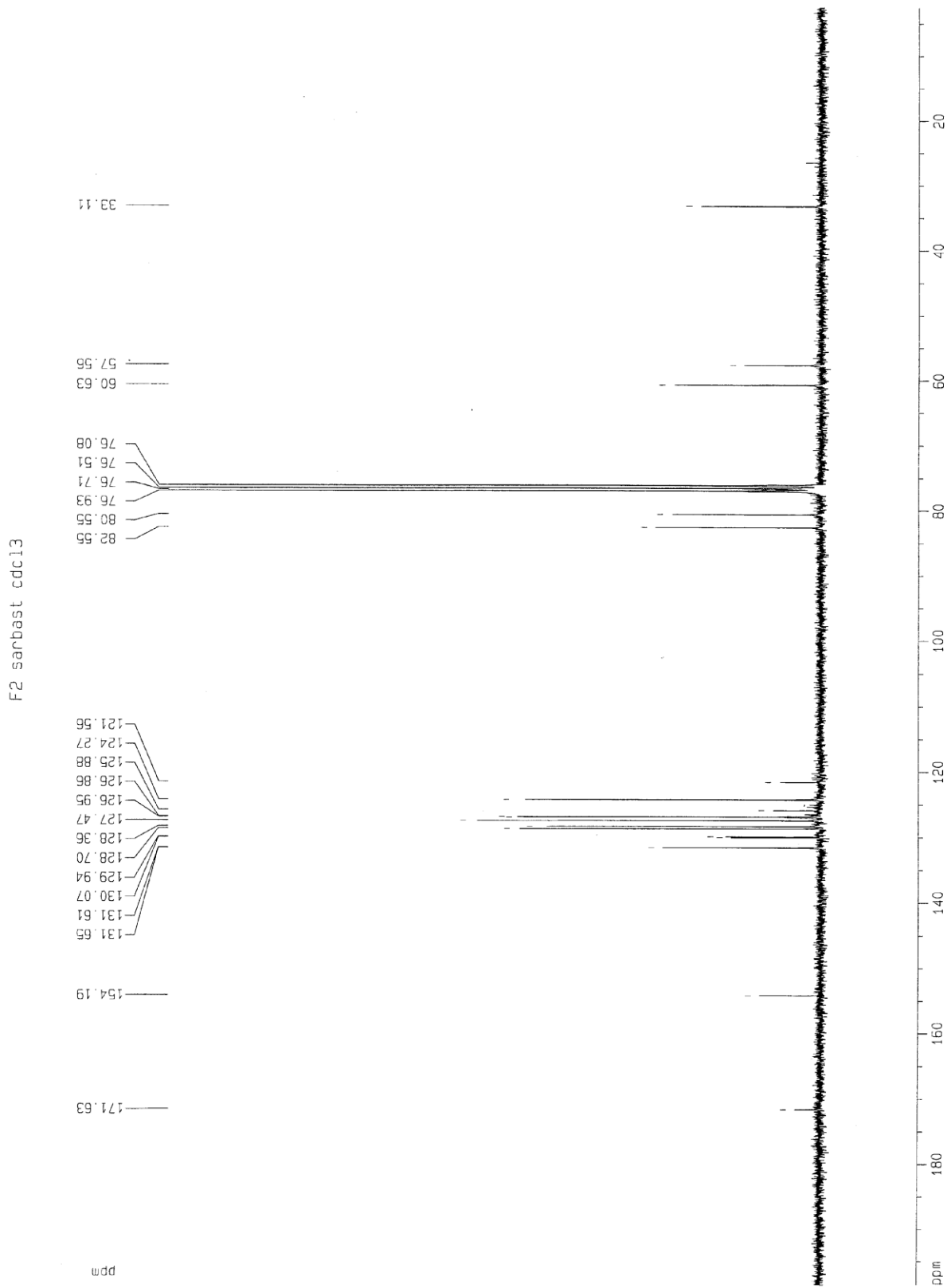
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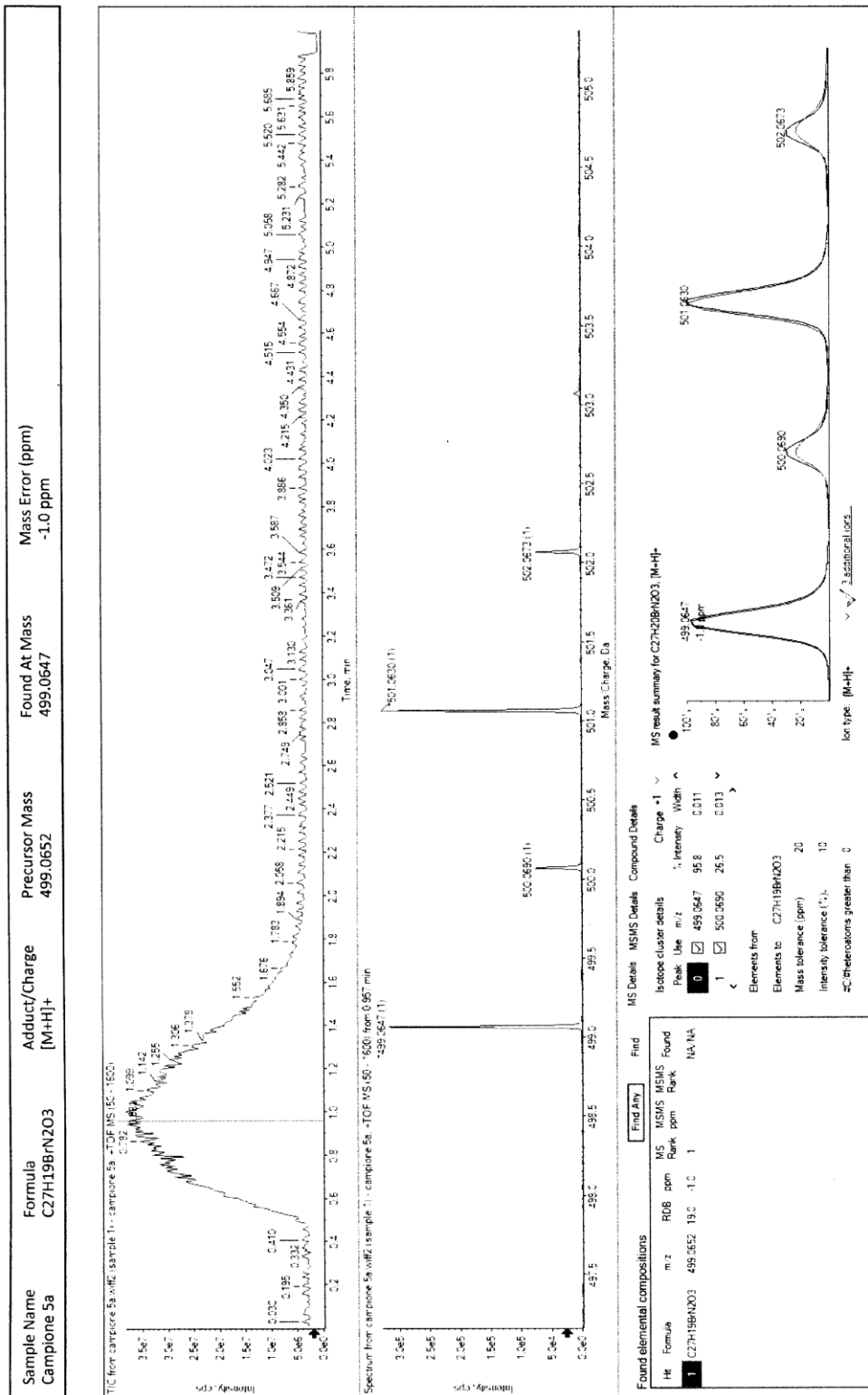
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1. ^1H , ^{13}C and ^{31}P NMR spectra and HRMS spectra of synthesized compounds

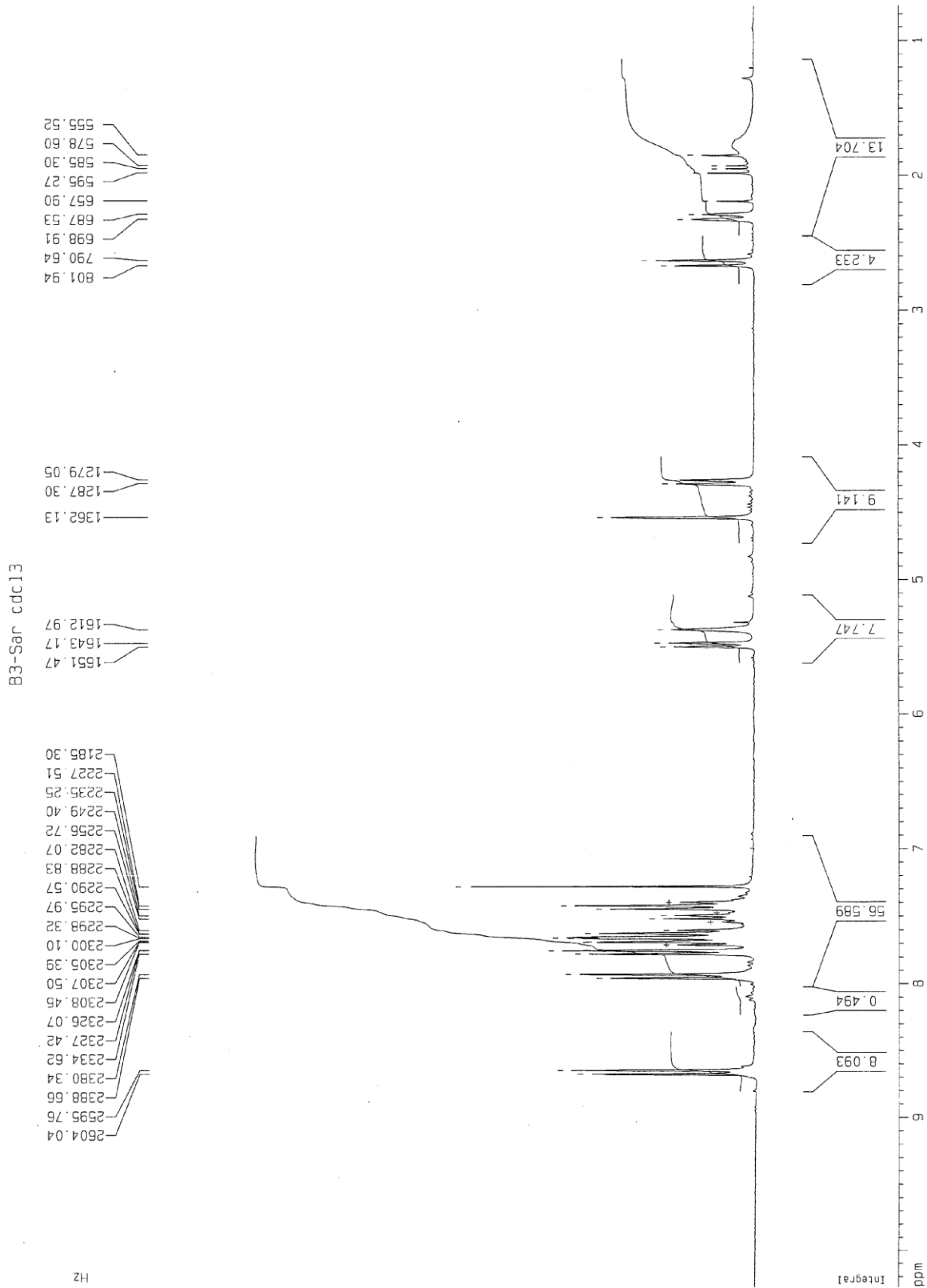
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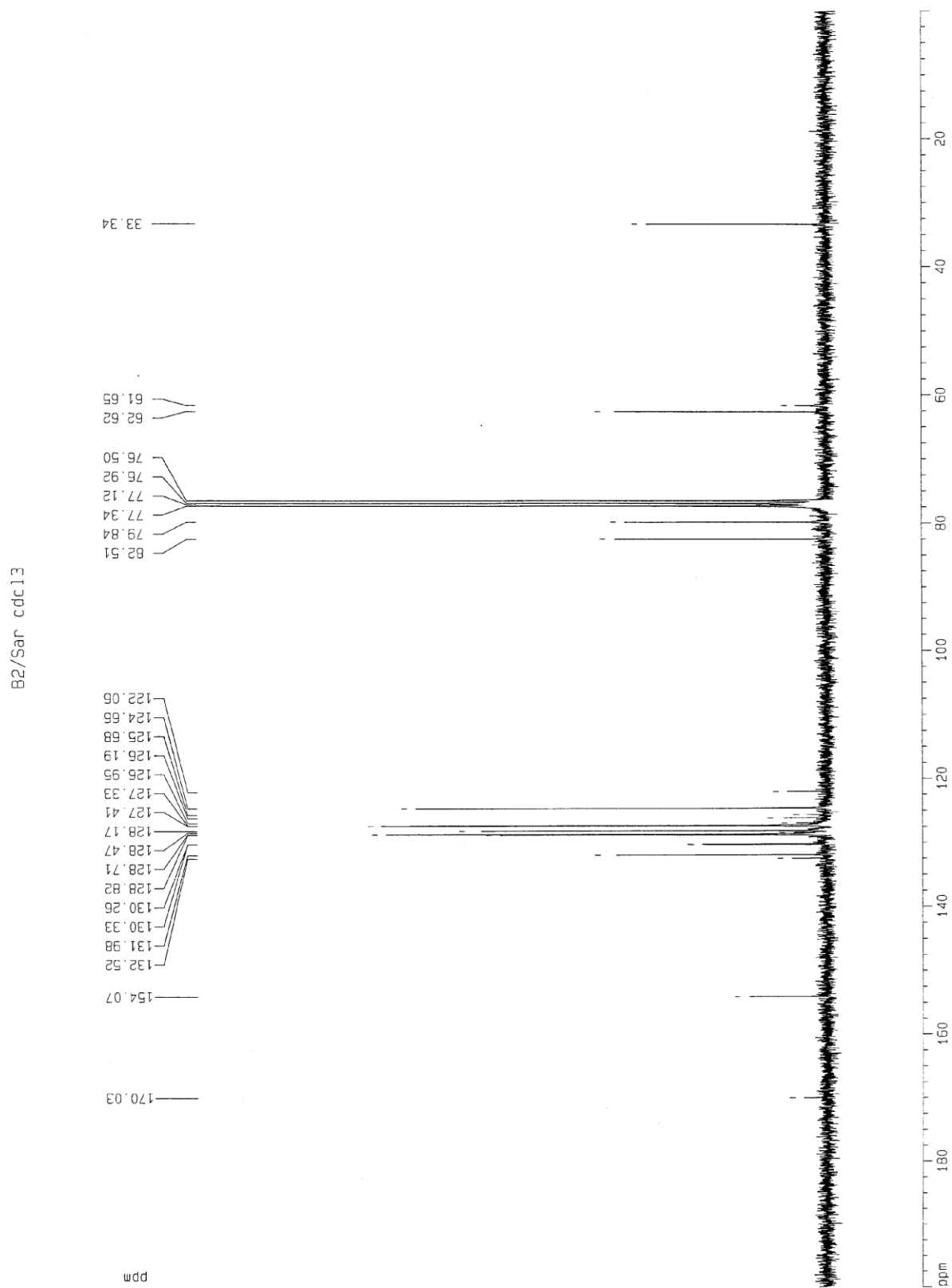


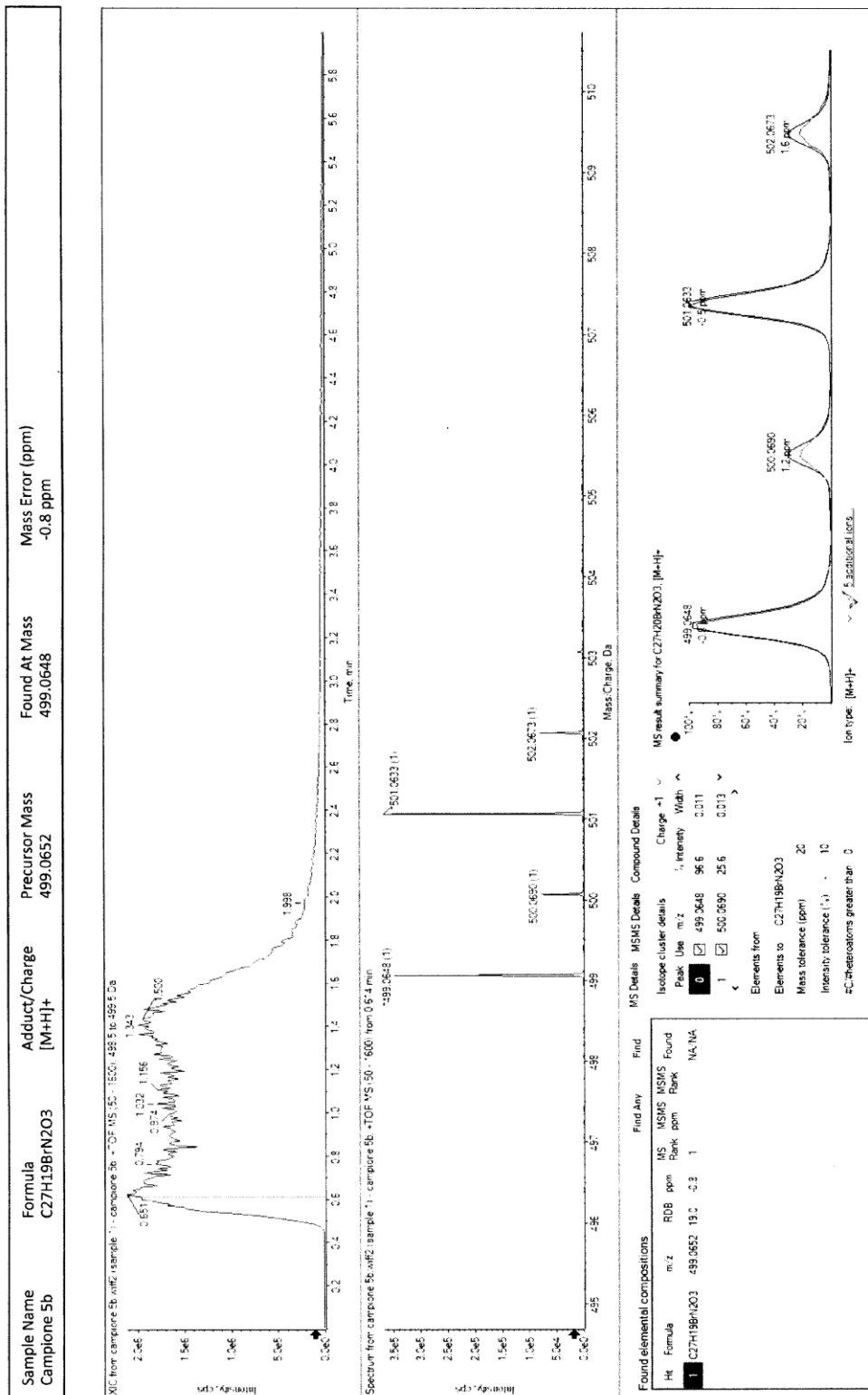




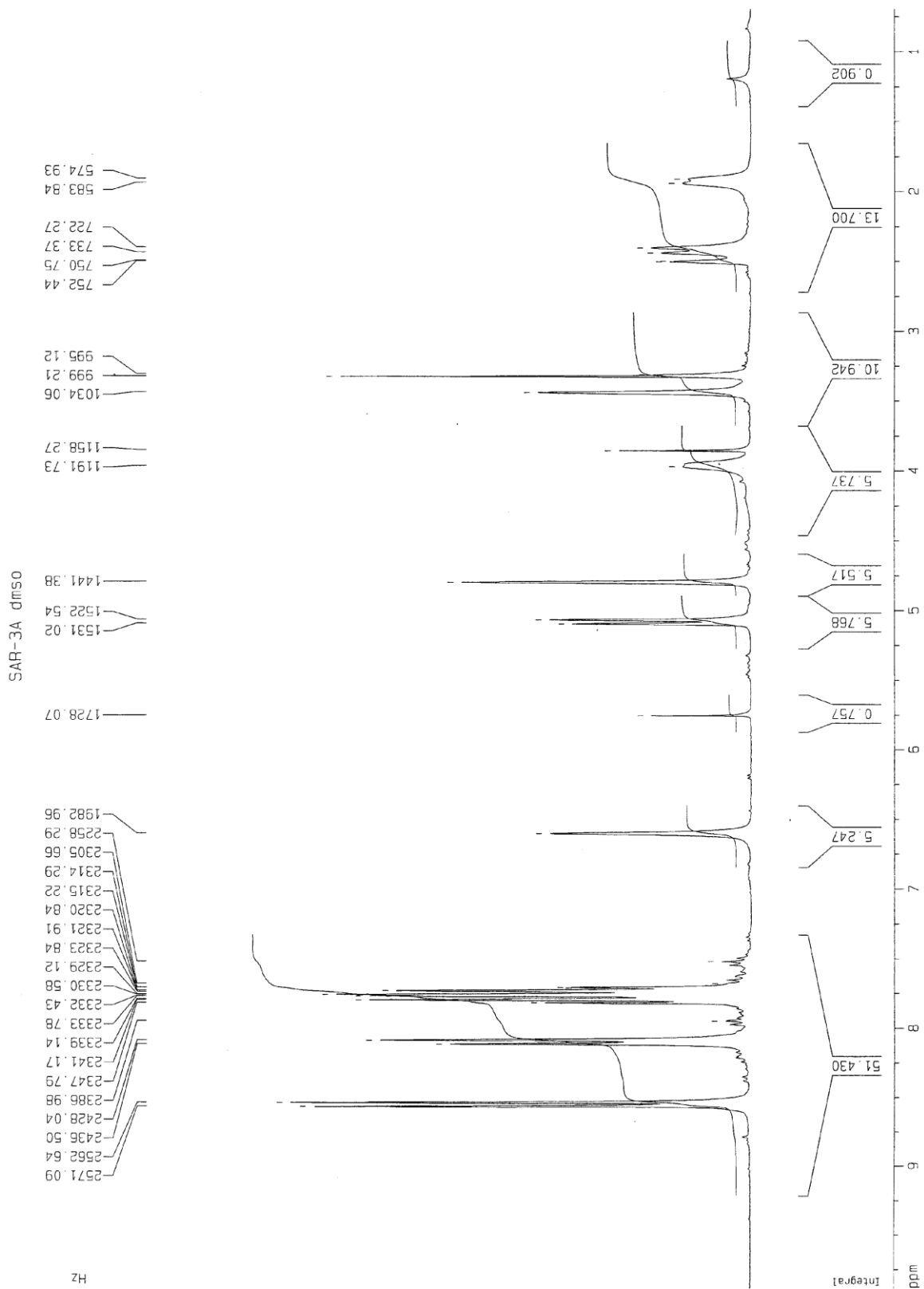
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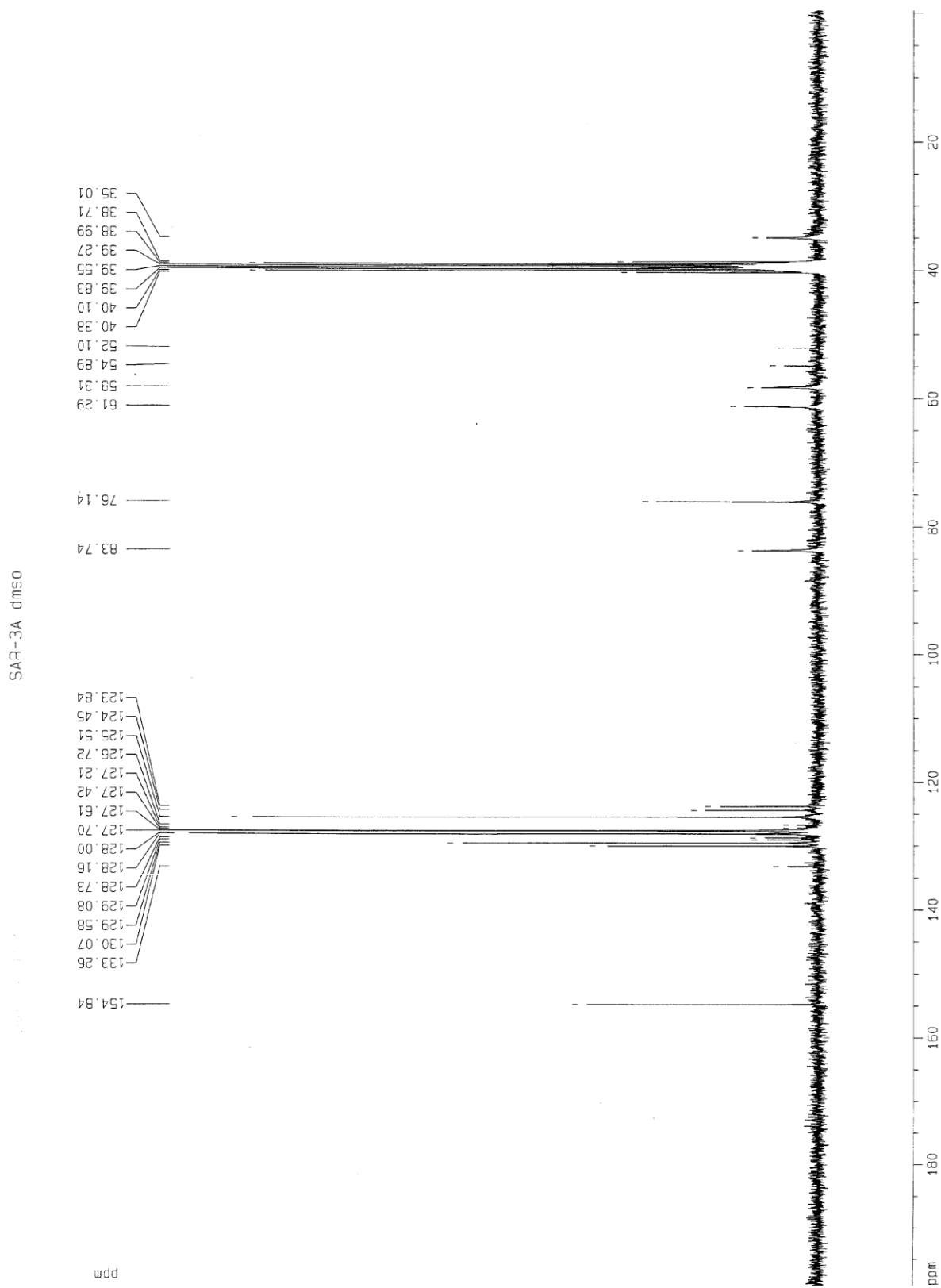


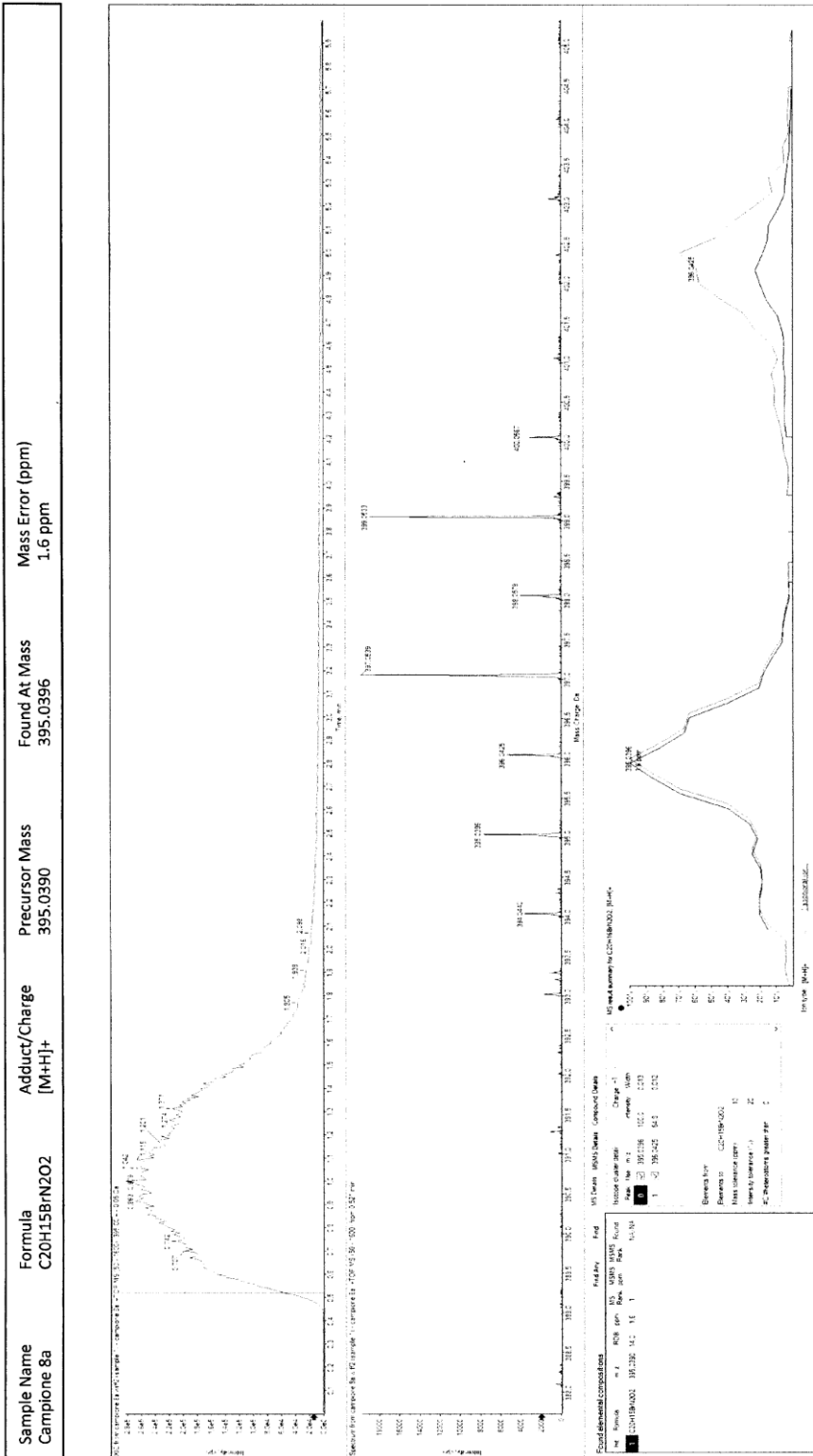




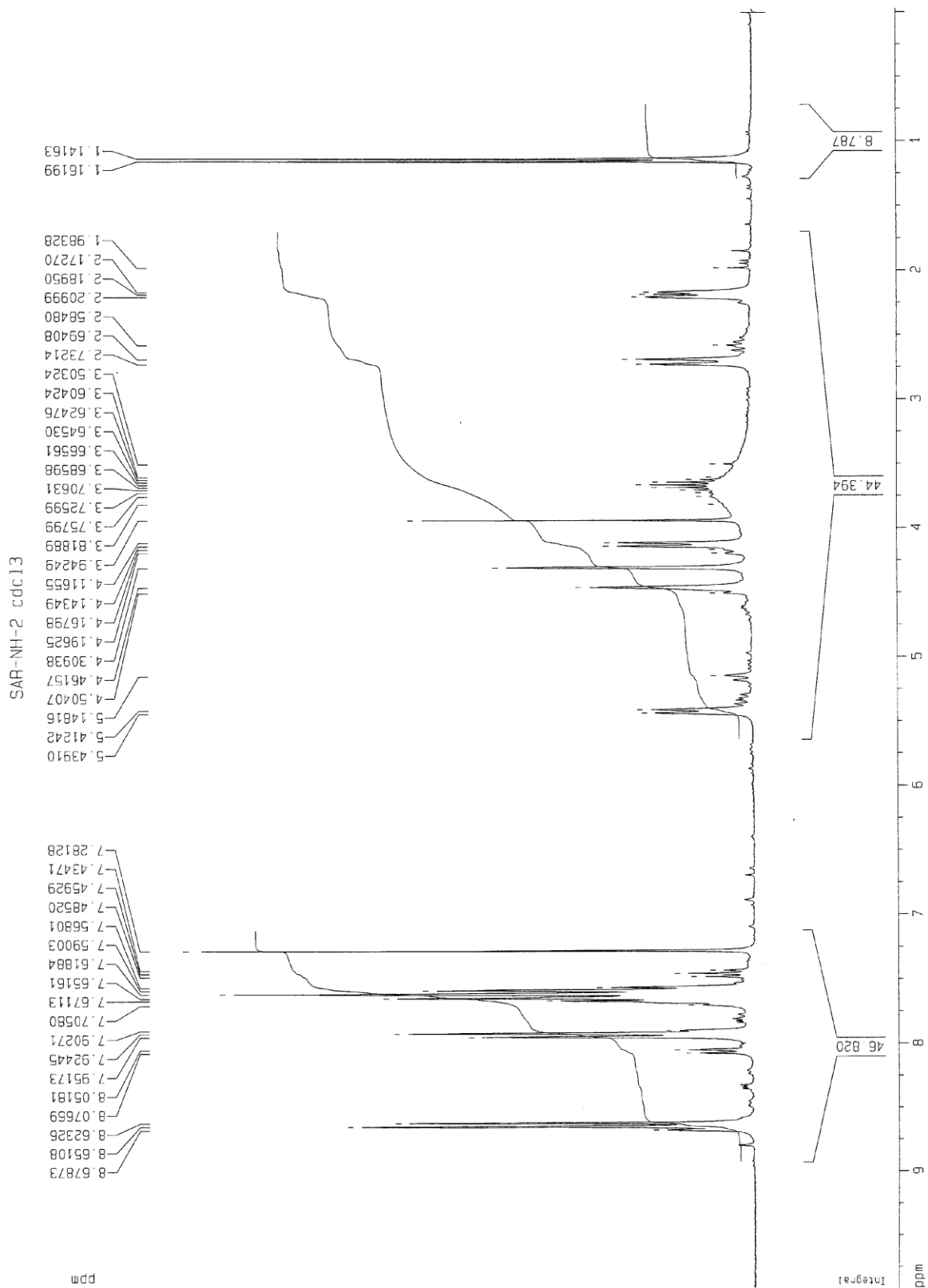
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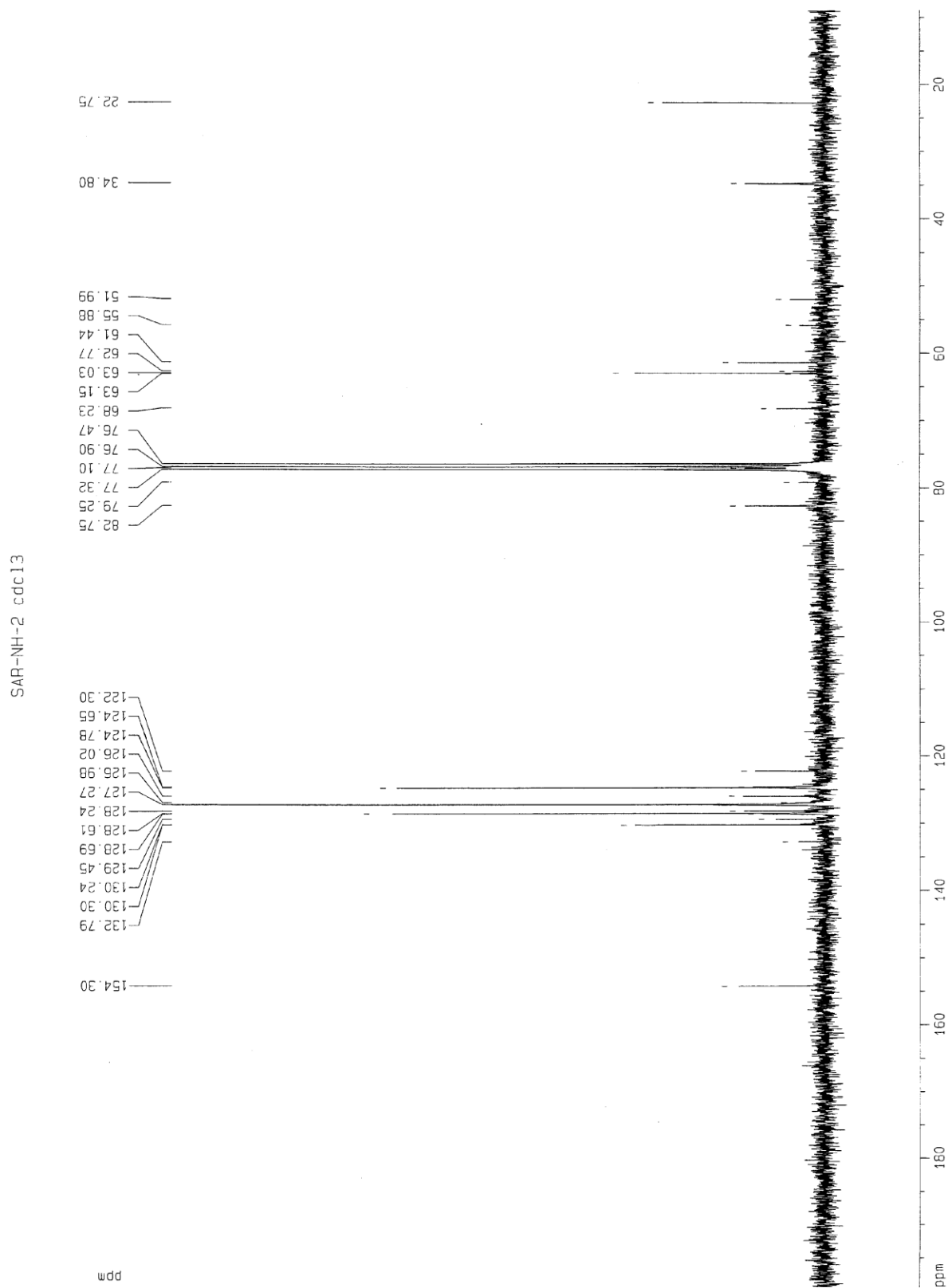


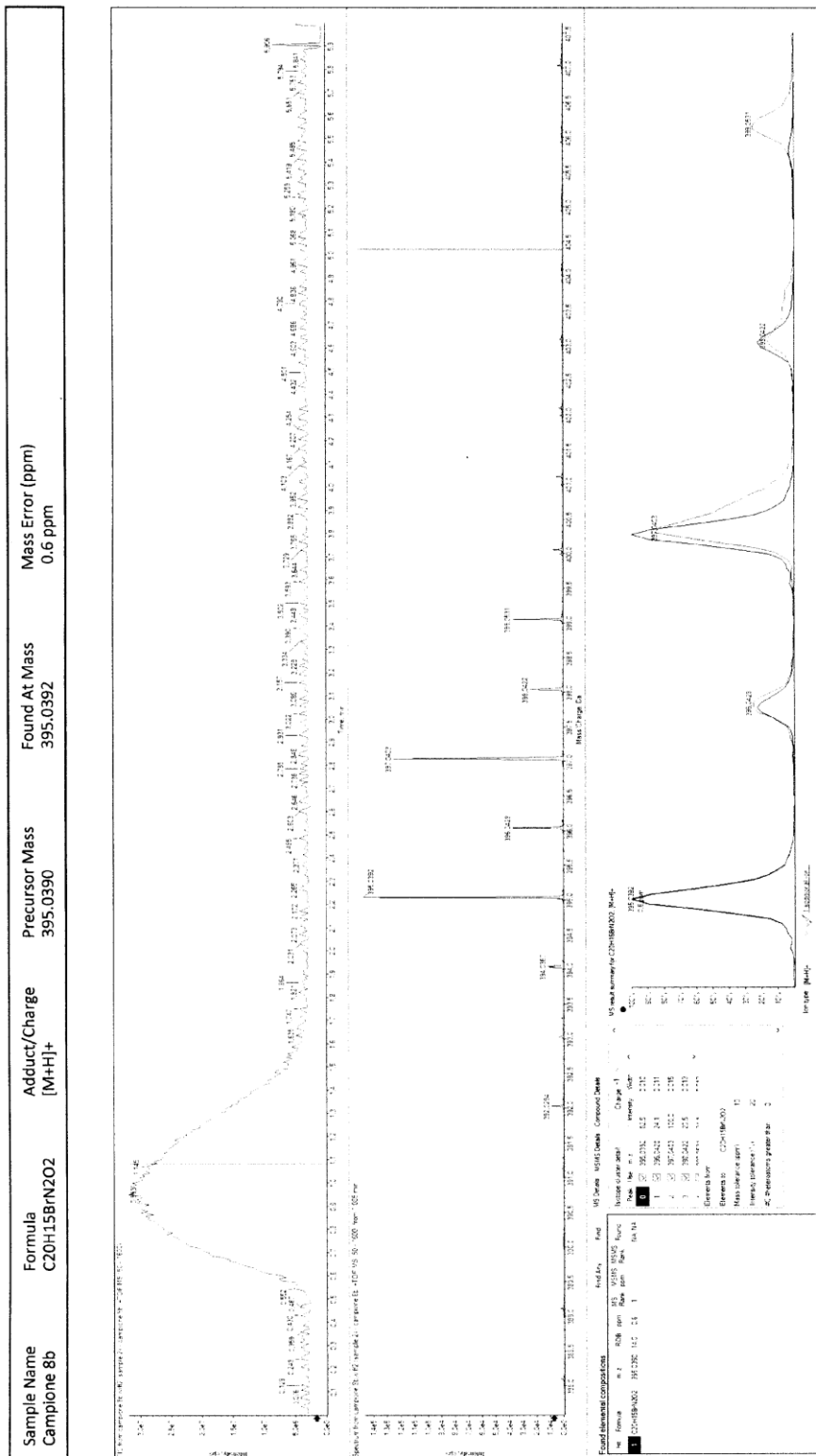




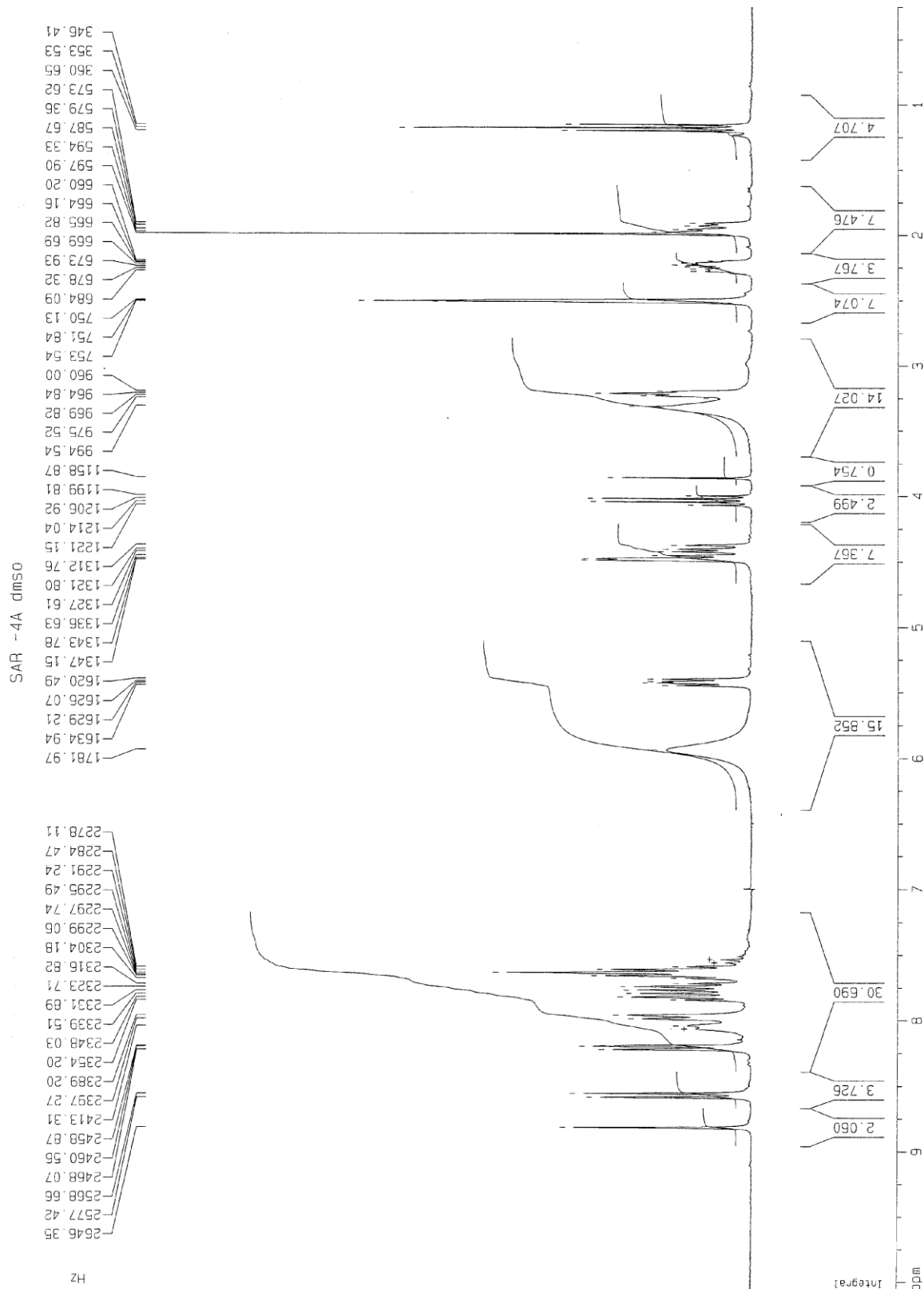
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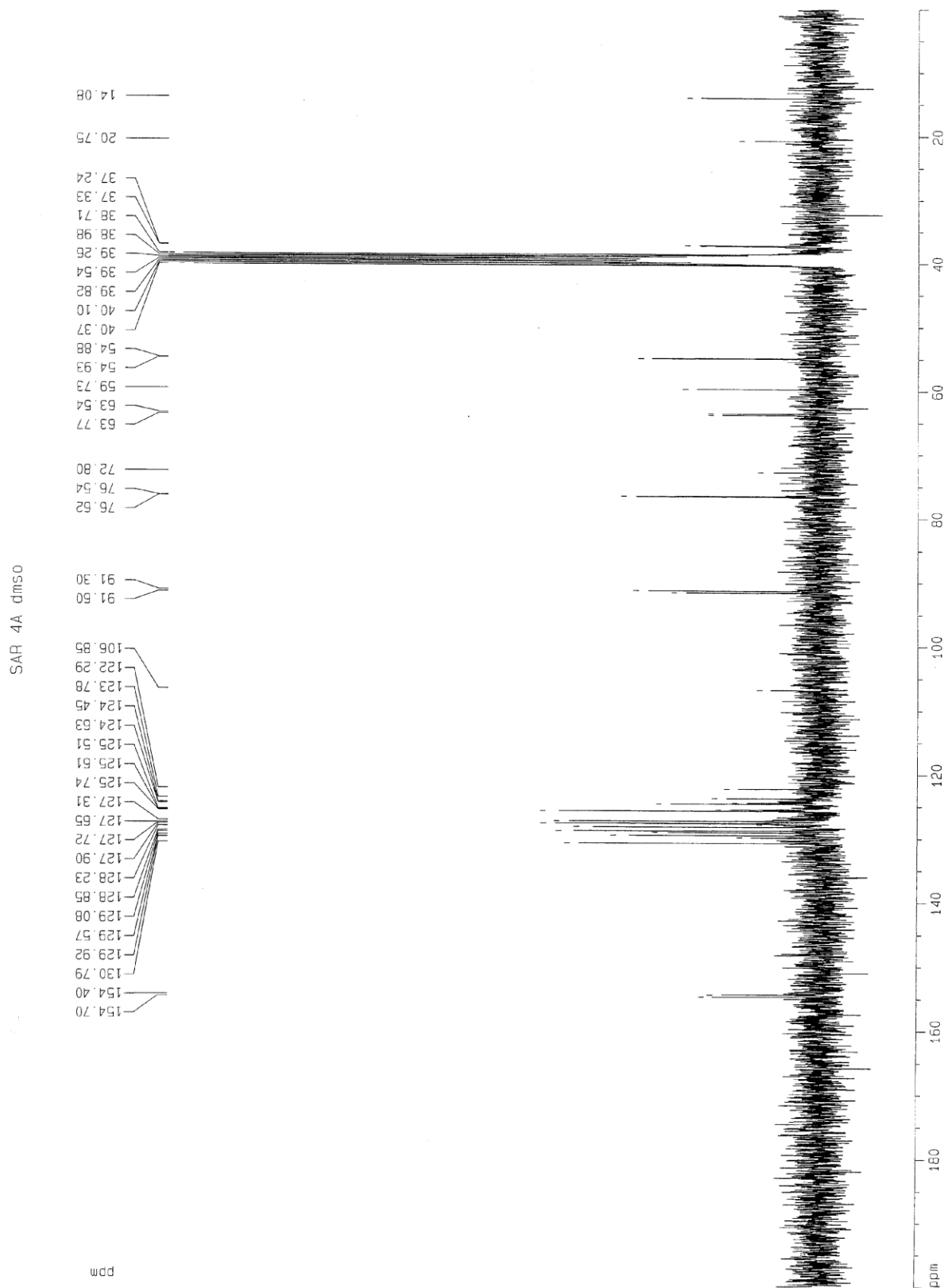


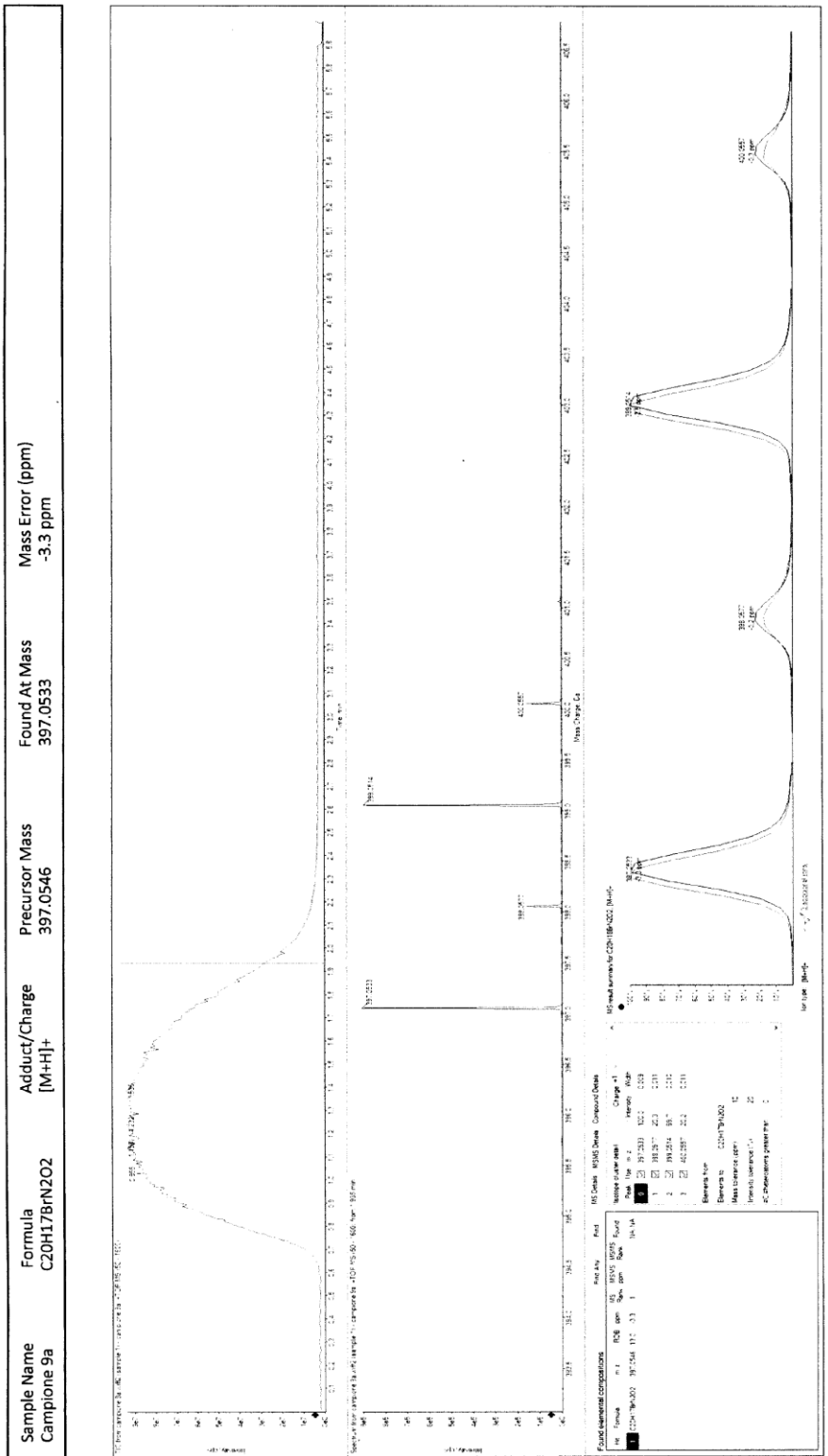




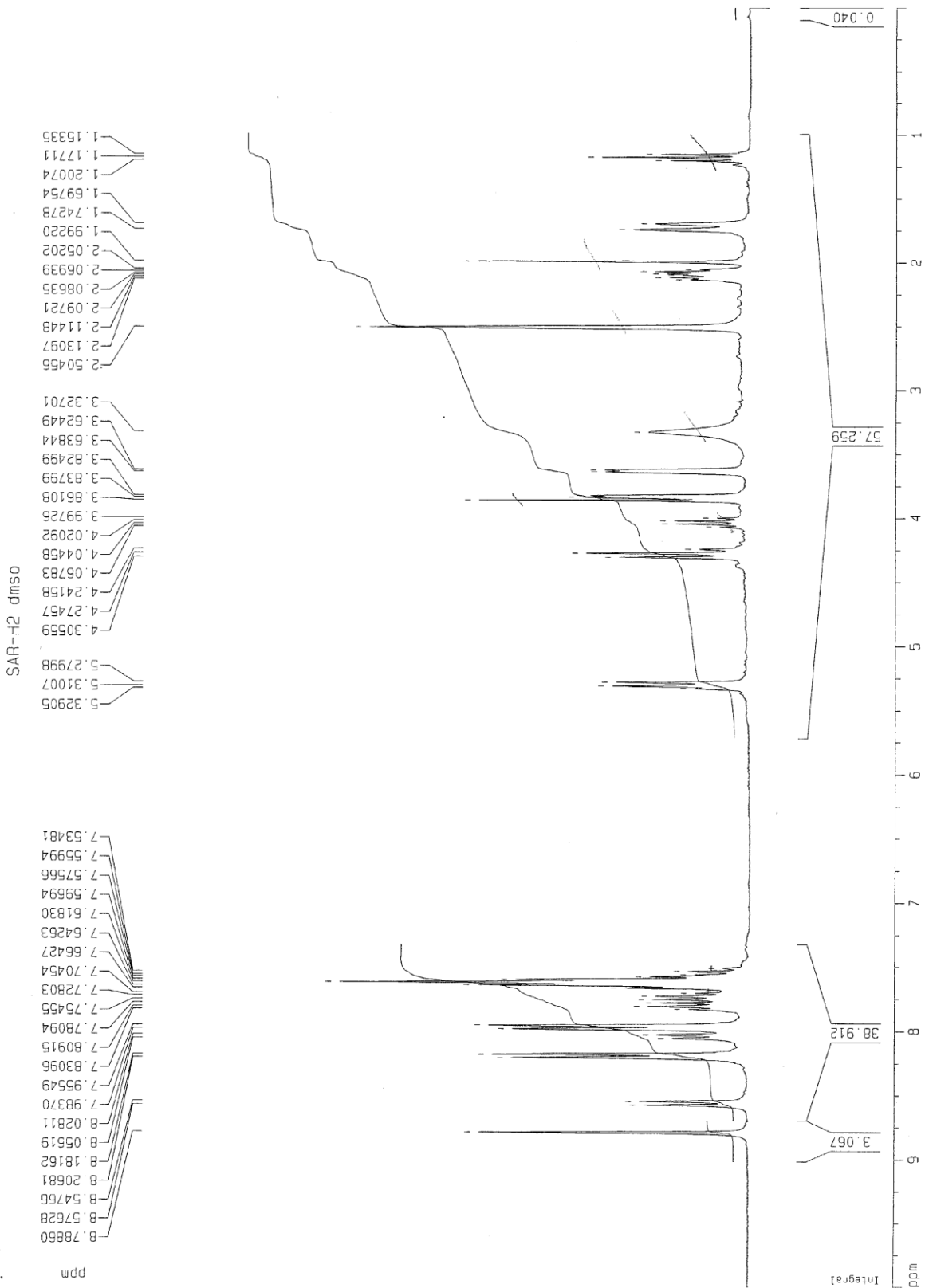
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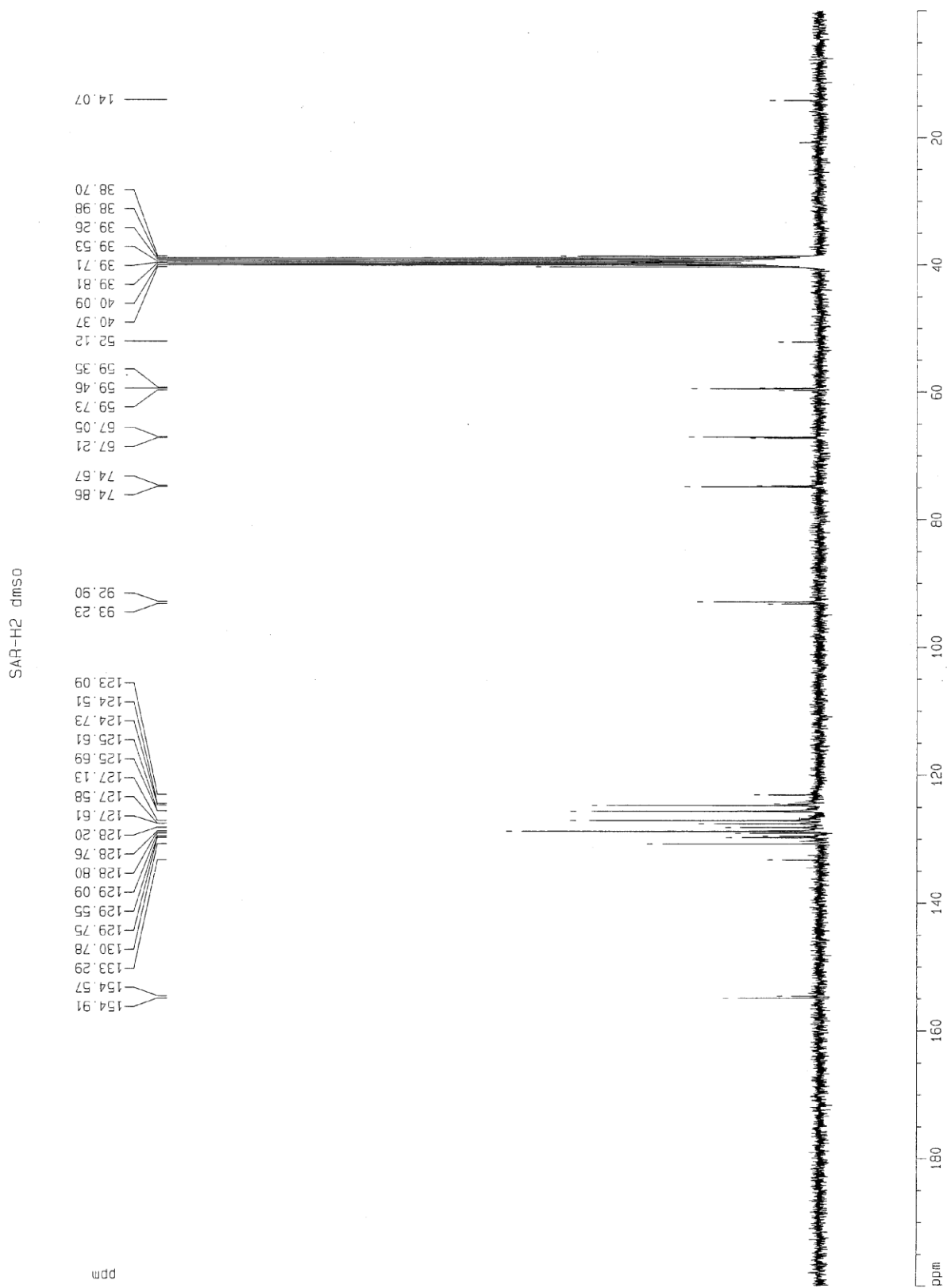


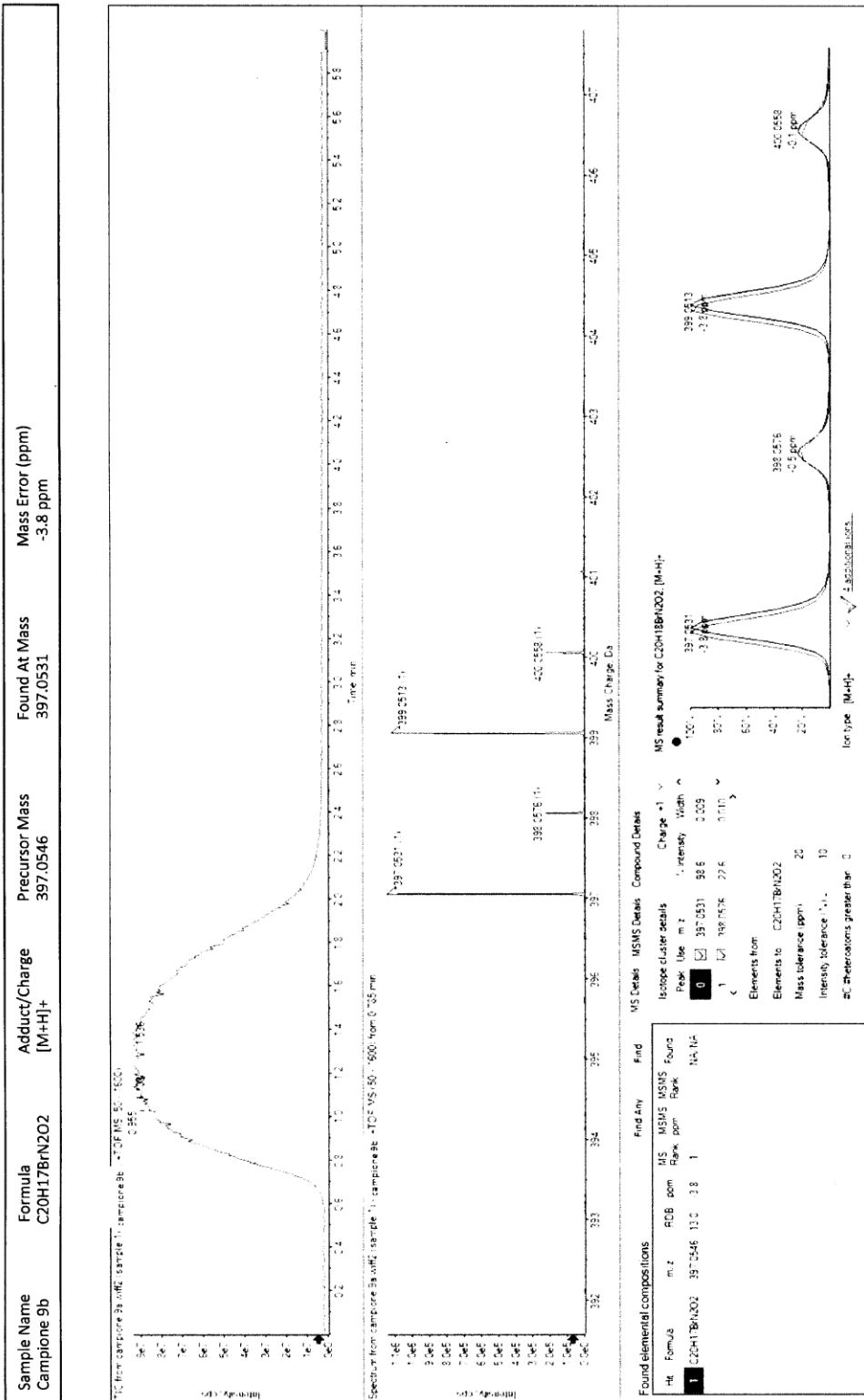




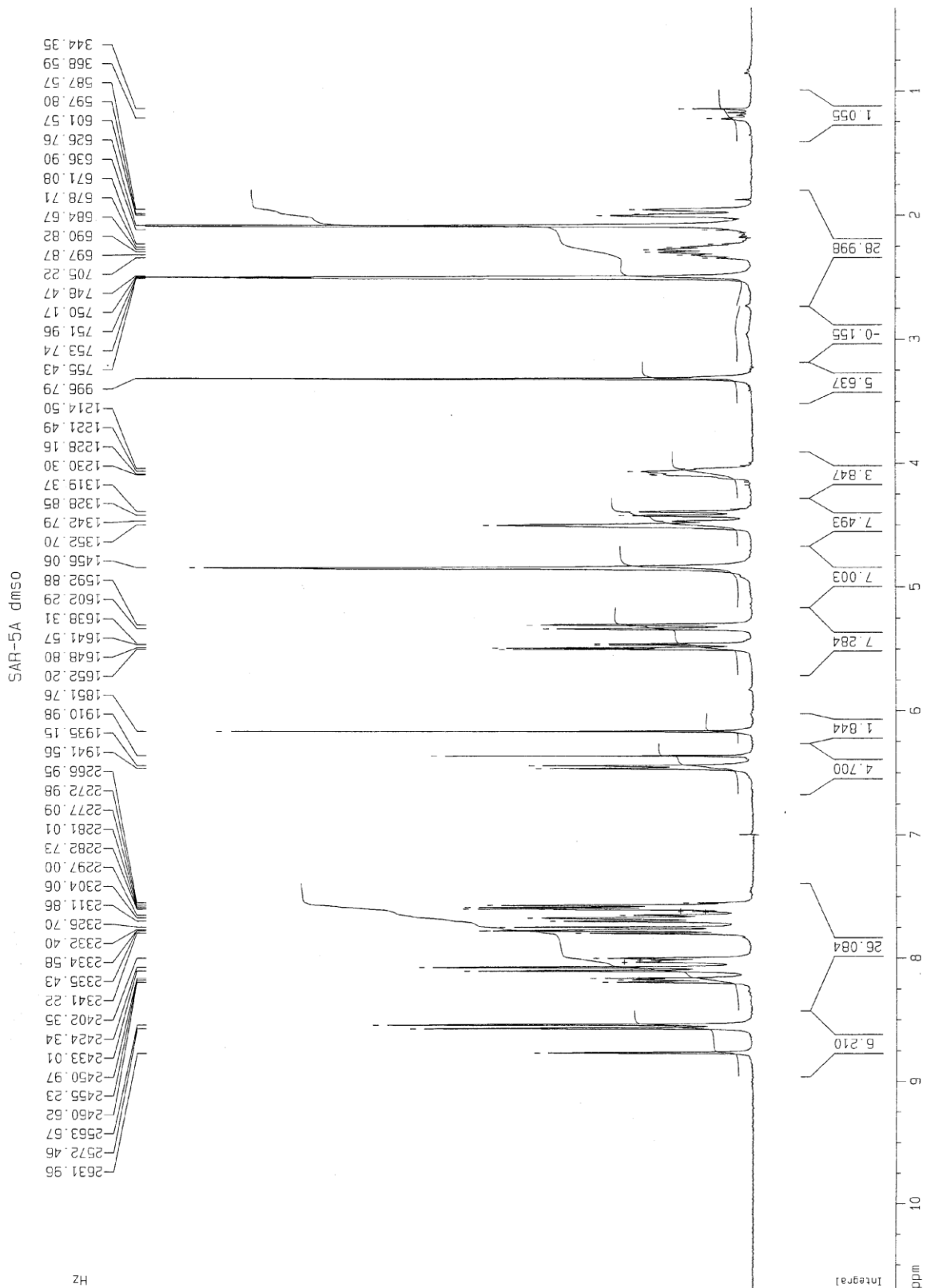
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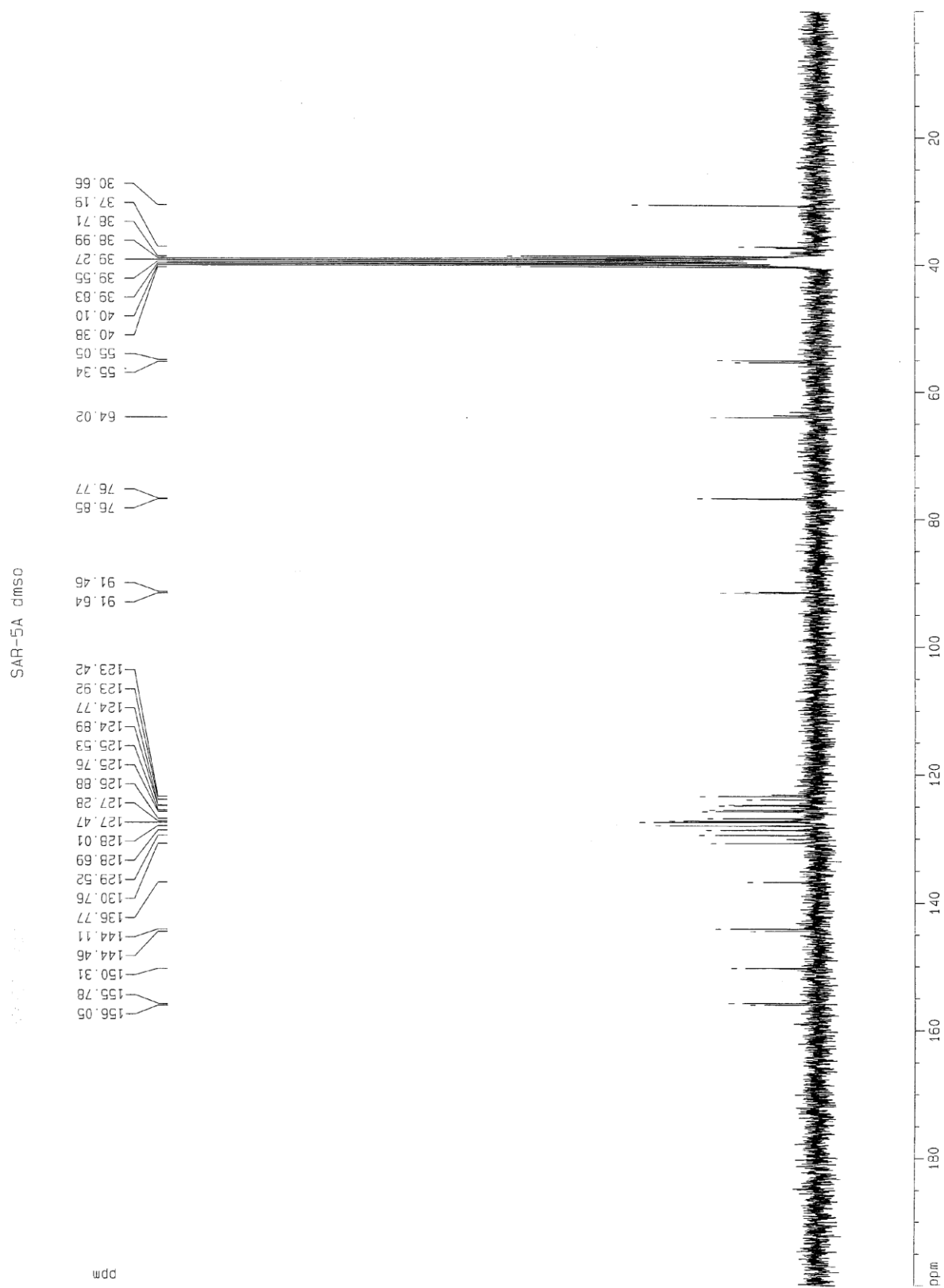


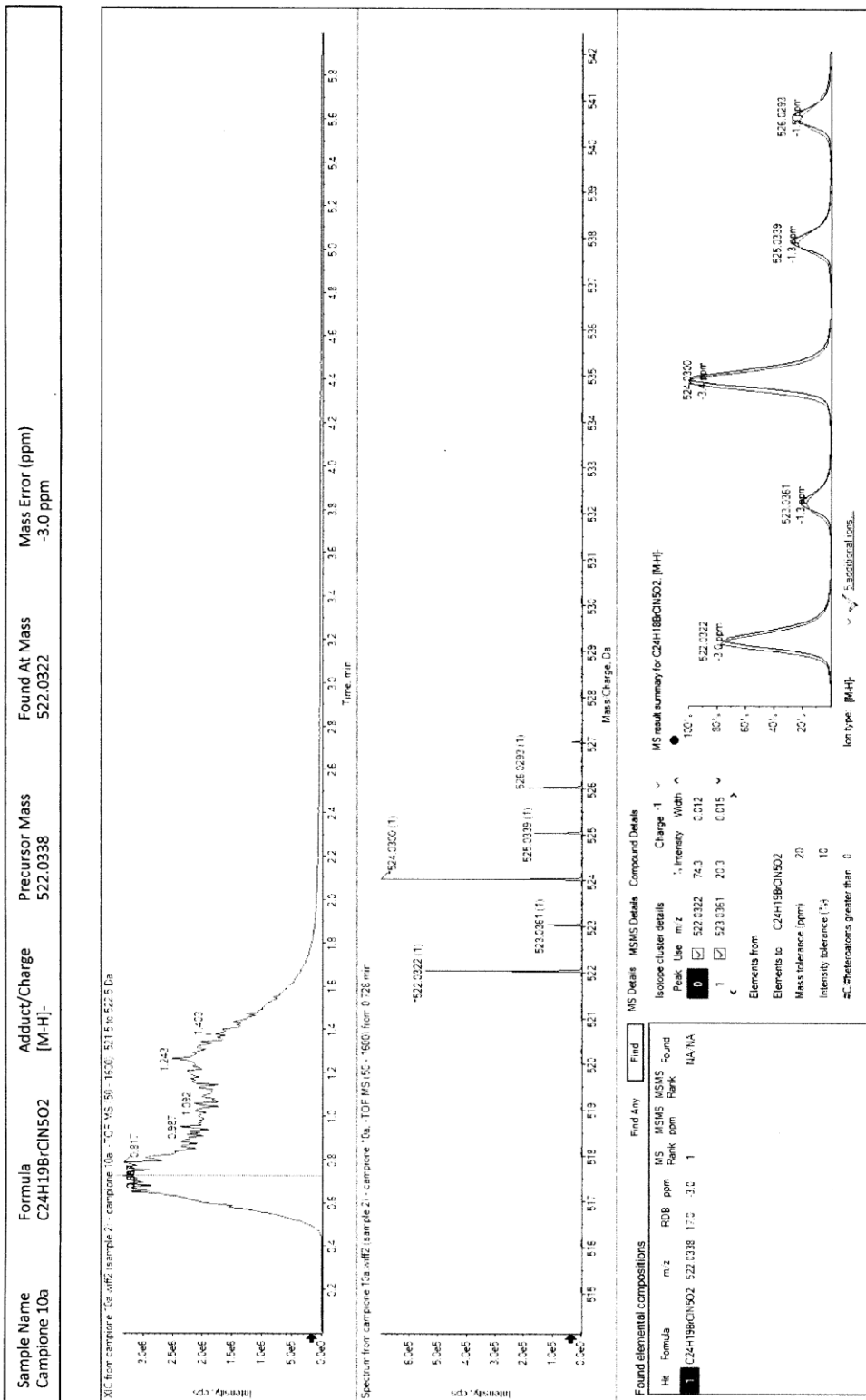




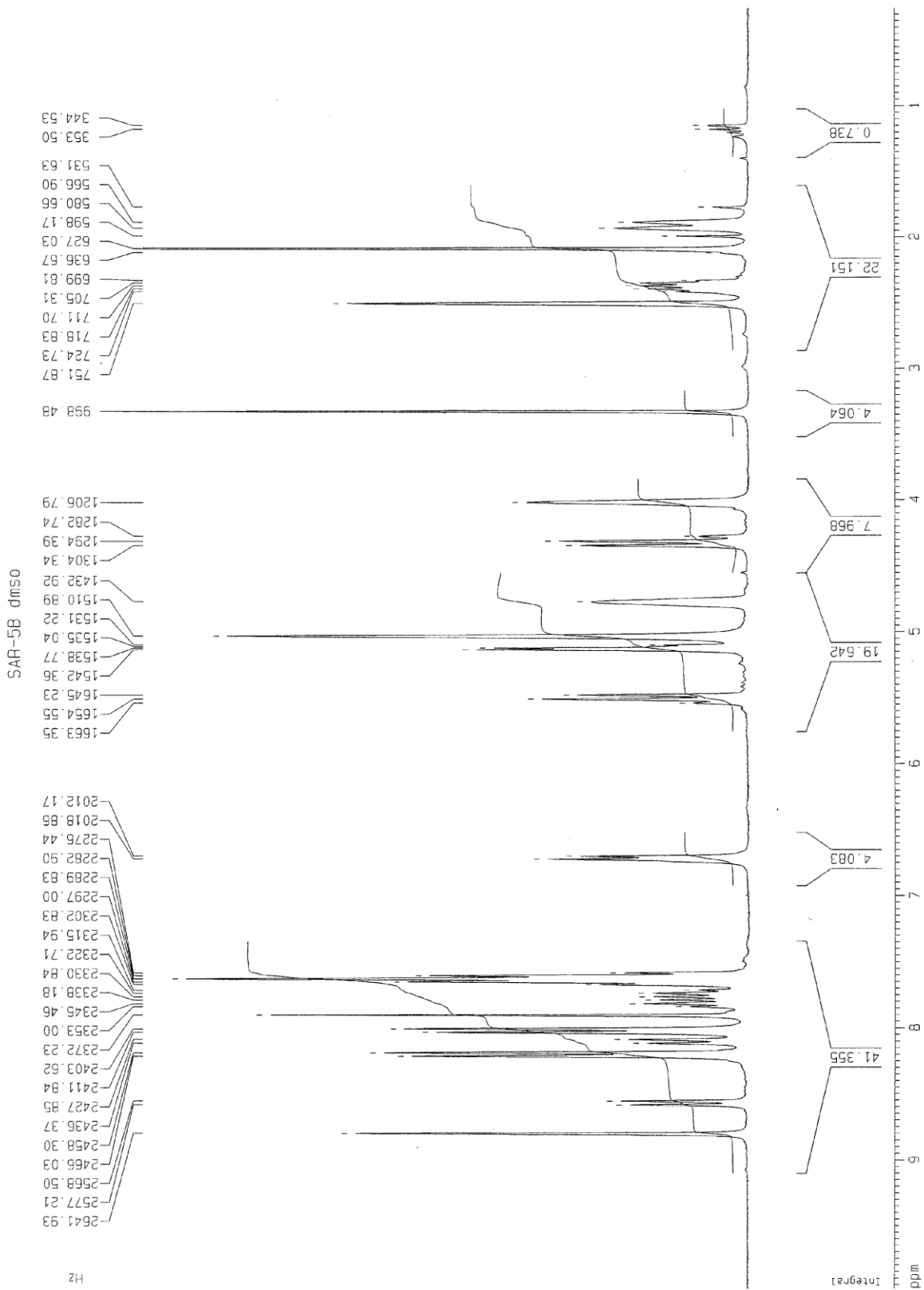
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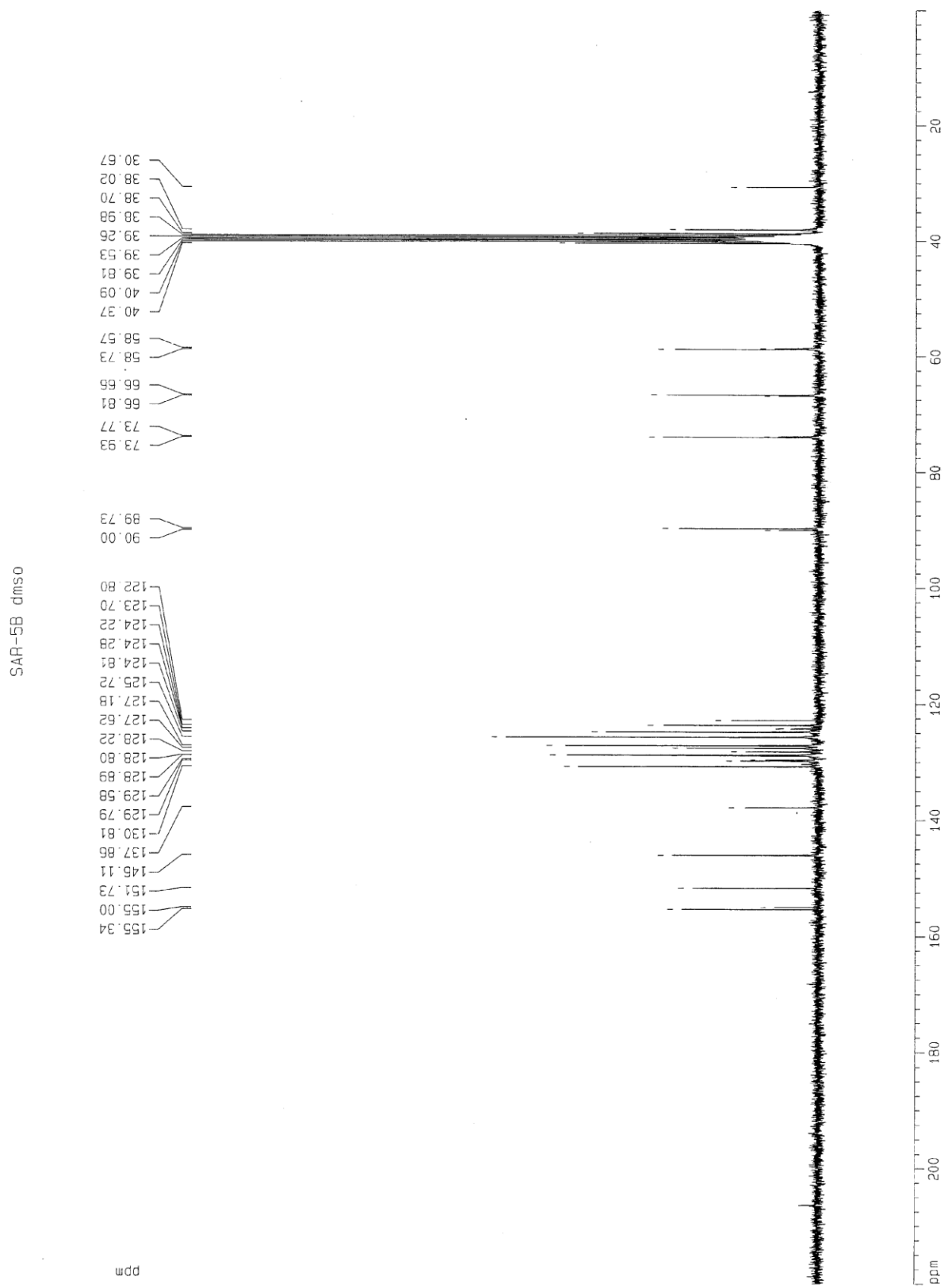




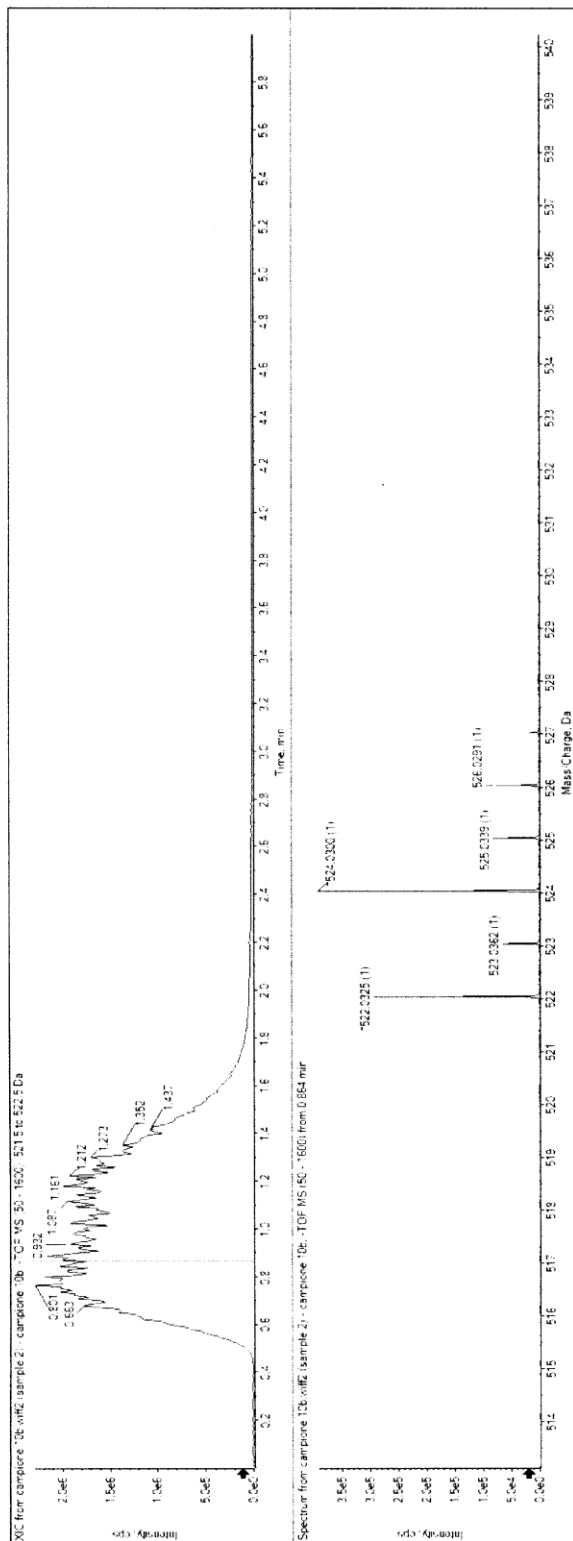


10b





Sample Name: **C24H19BrClNSO2** Adduct/Charge: **[M-H]⁻** Found At Mass: **522.0325** Mass Error (ppm): **-2.5 ppm**
 Campione 10b Precursor Mass: **522.0338**



MS result summary for C24H19BrClNSO2 [M-H]⁻

MS Details: MSMS Details Compound Details

Isotope cluster details: Charge: -1

Peak Use: 522.0325 73.4 0.012

523.0362 19.5 0.014

Elements from: C24H19BrClNSO2

Elements to: C24H19BrClNSO2

Mass tolerance (ppm): 20

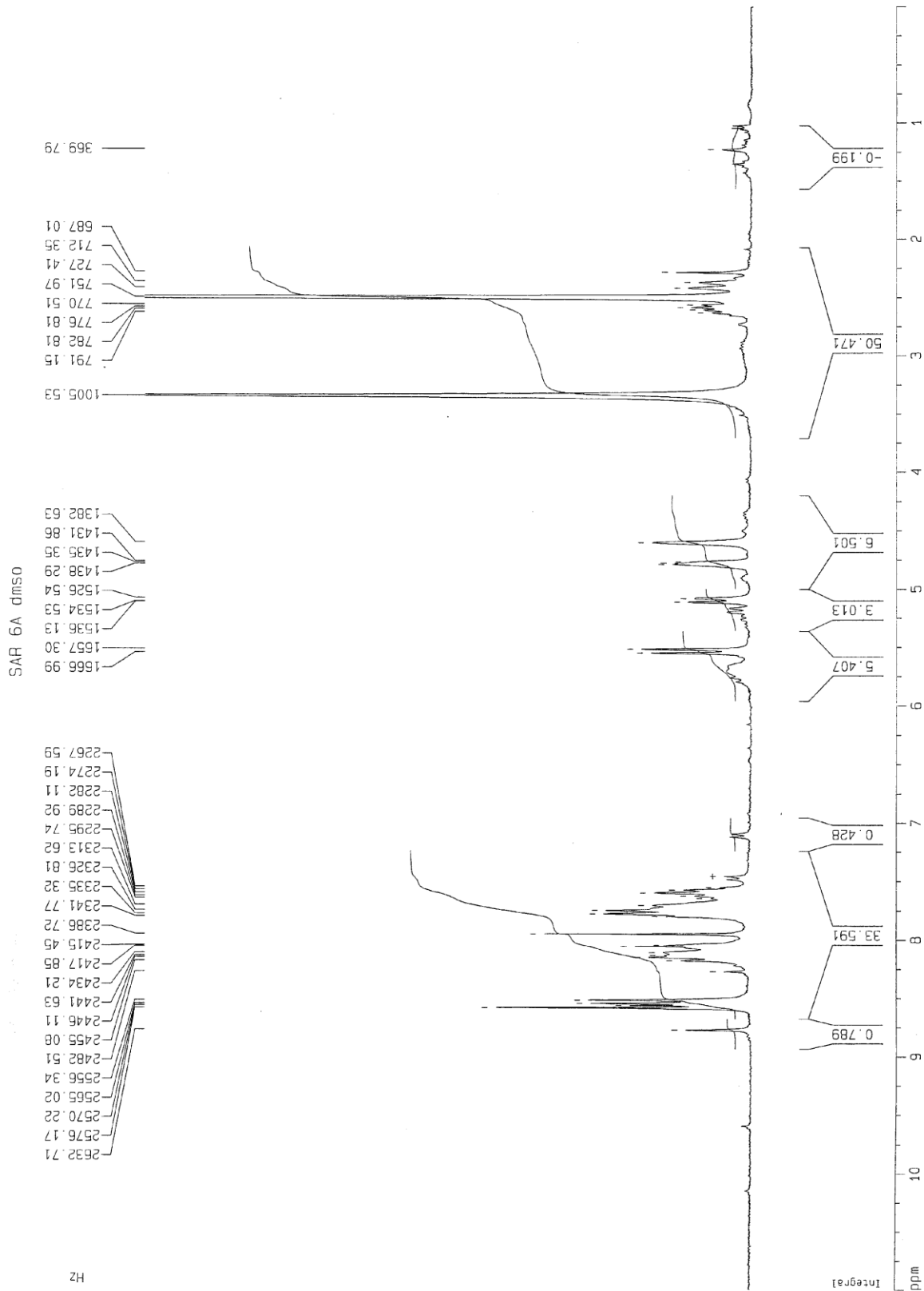
Intensity tolerance (%): 10

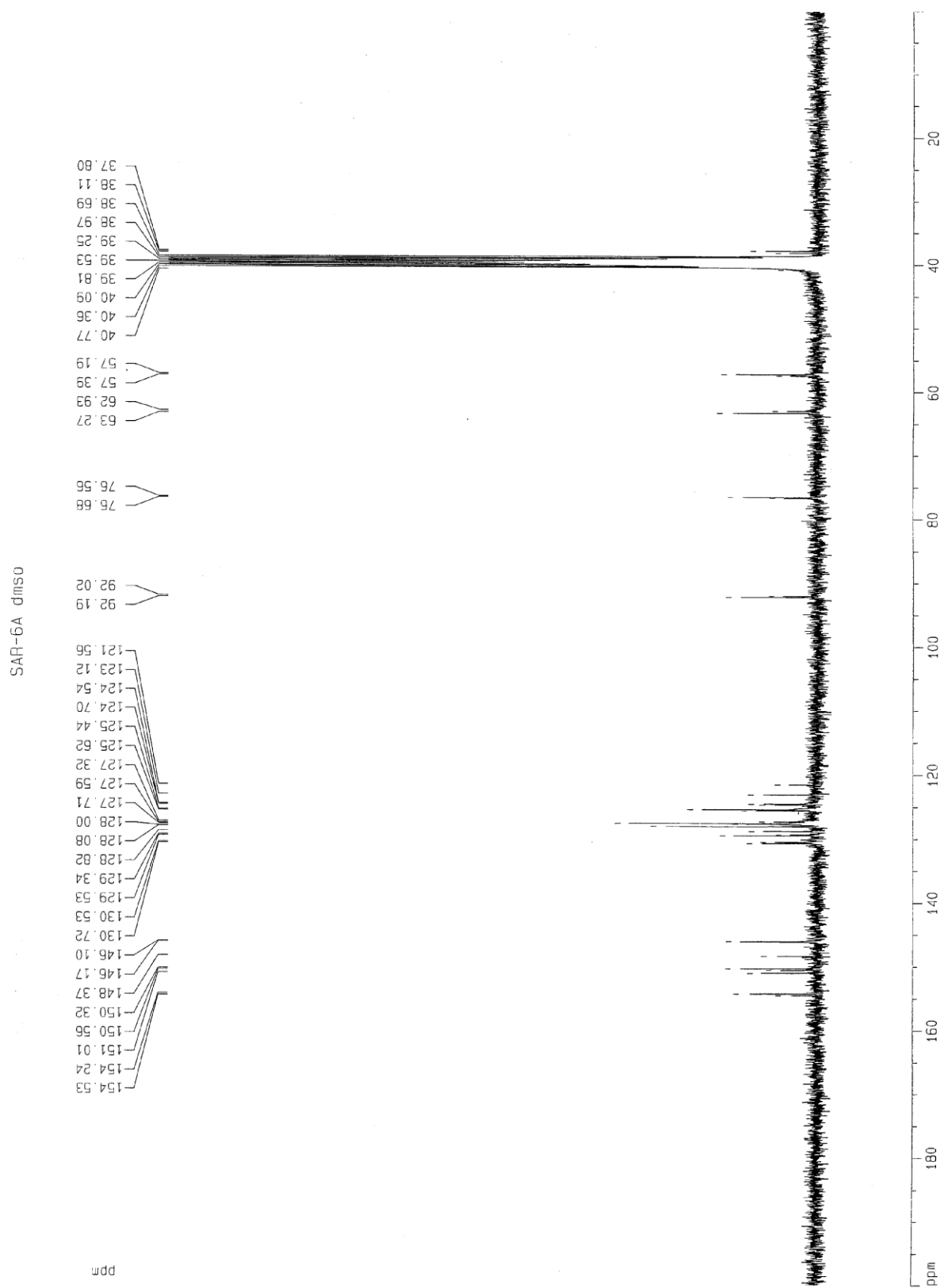
ΔC: Retentions greater than: 0

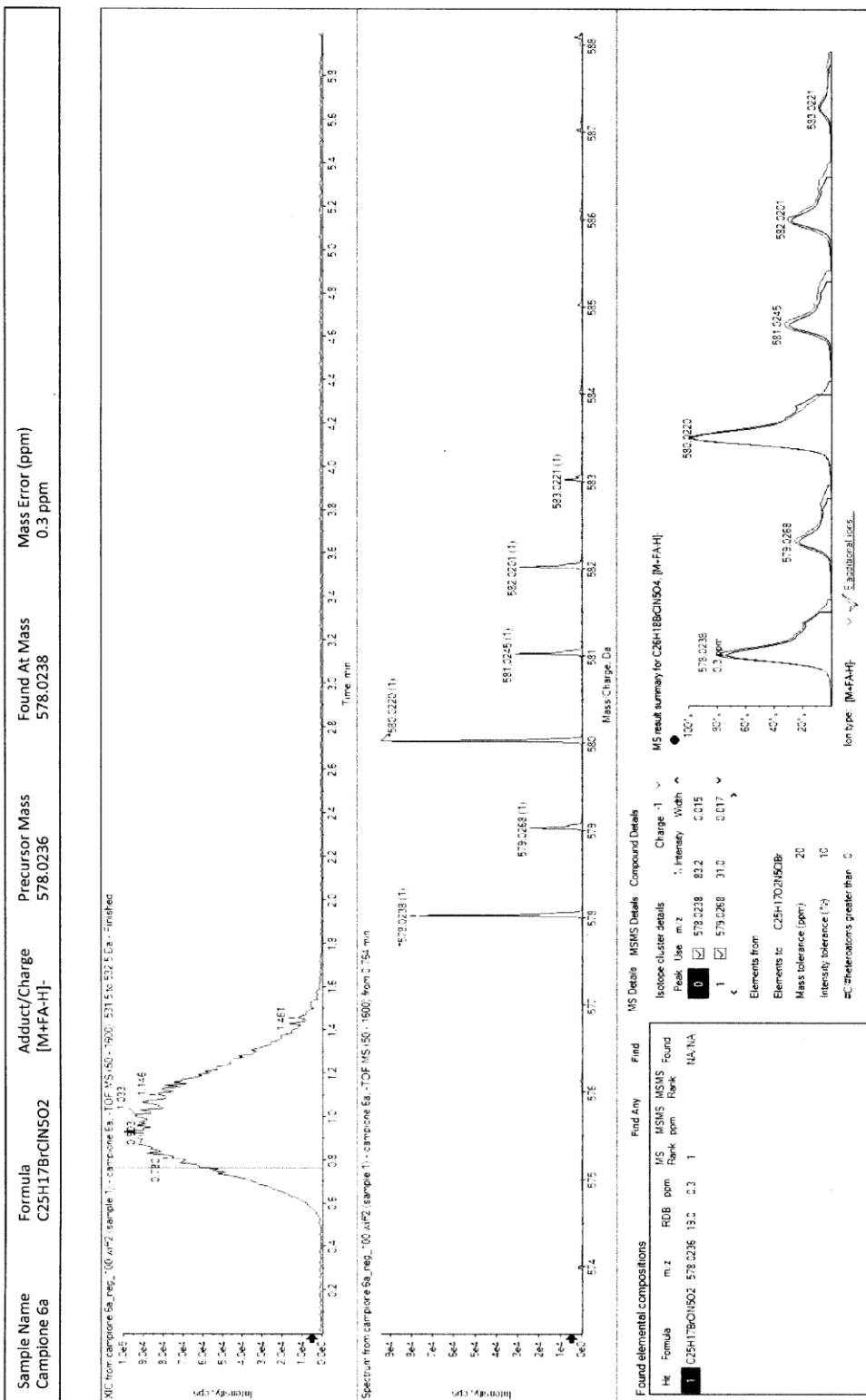
Ion type: [M-H]⁻

Found	Any	Find	MS Rank	MS Rank	MS Rank	MS Rank
1		C24H19BrClNSO2	522.0338	17.0	-2.5	1
		NA	NA	NA	NA	NA

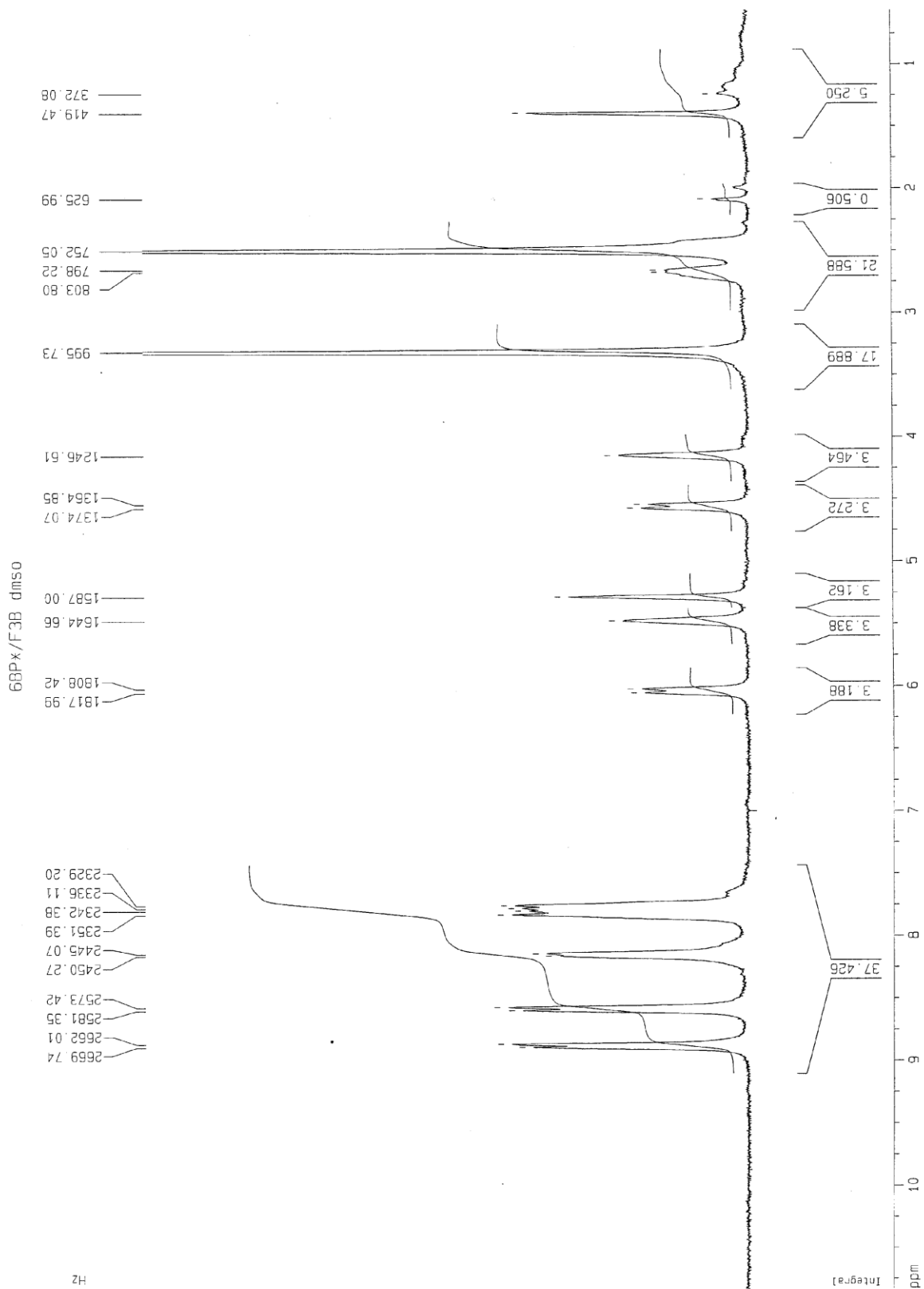
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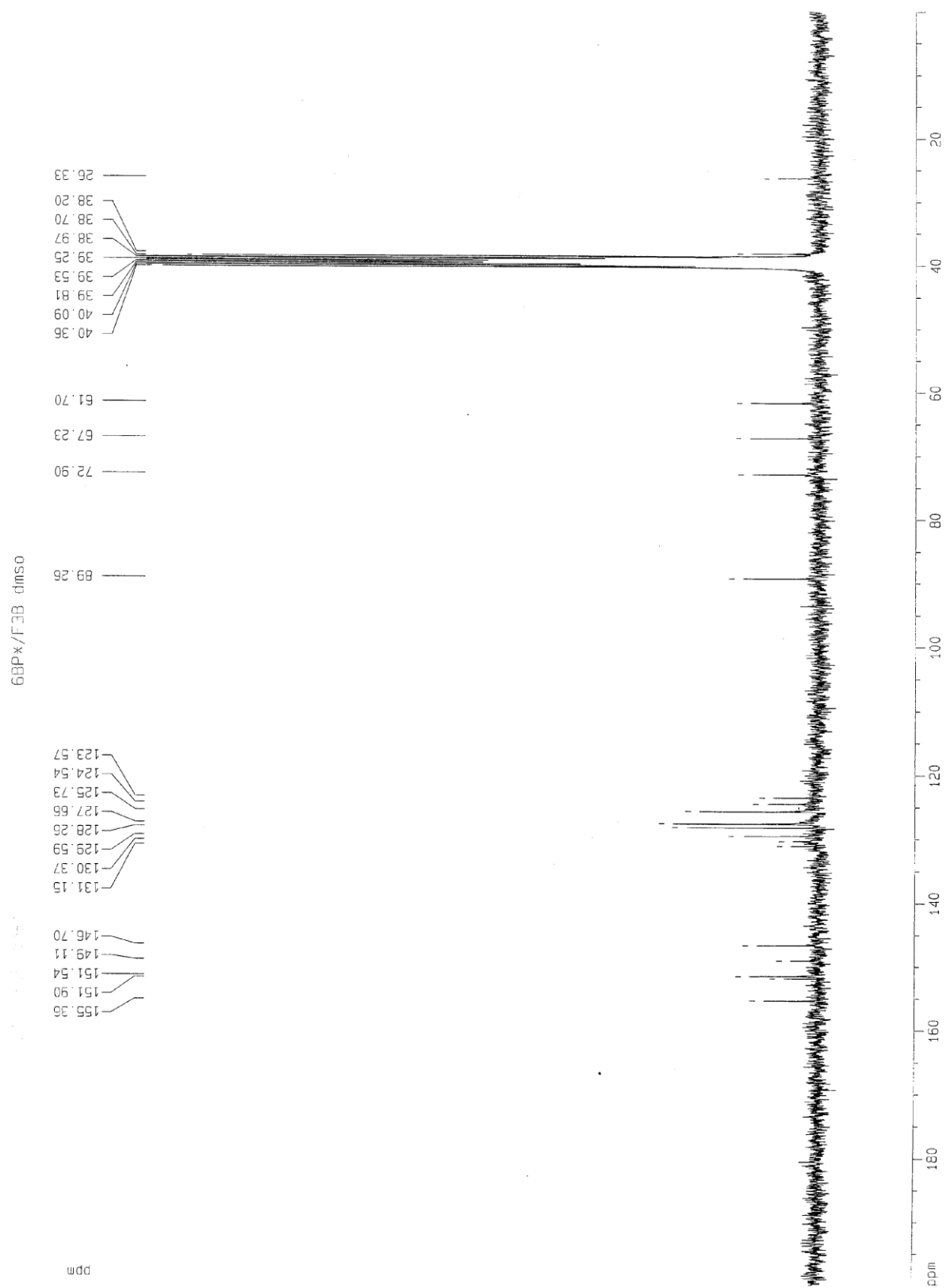


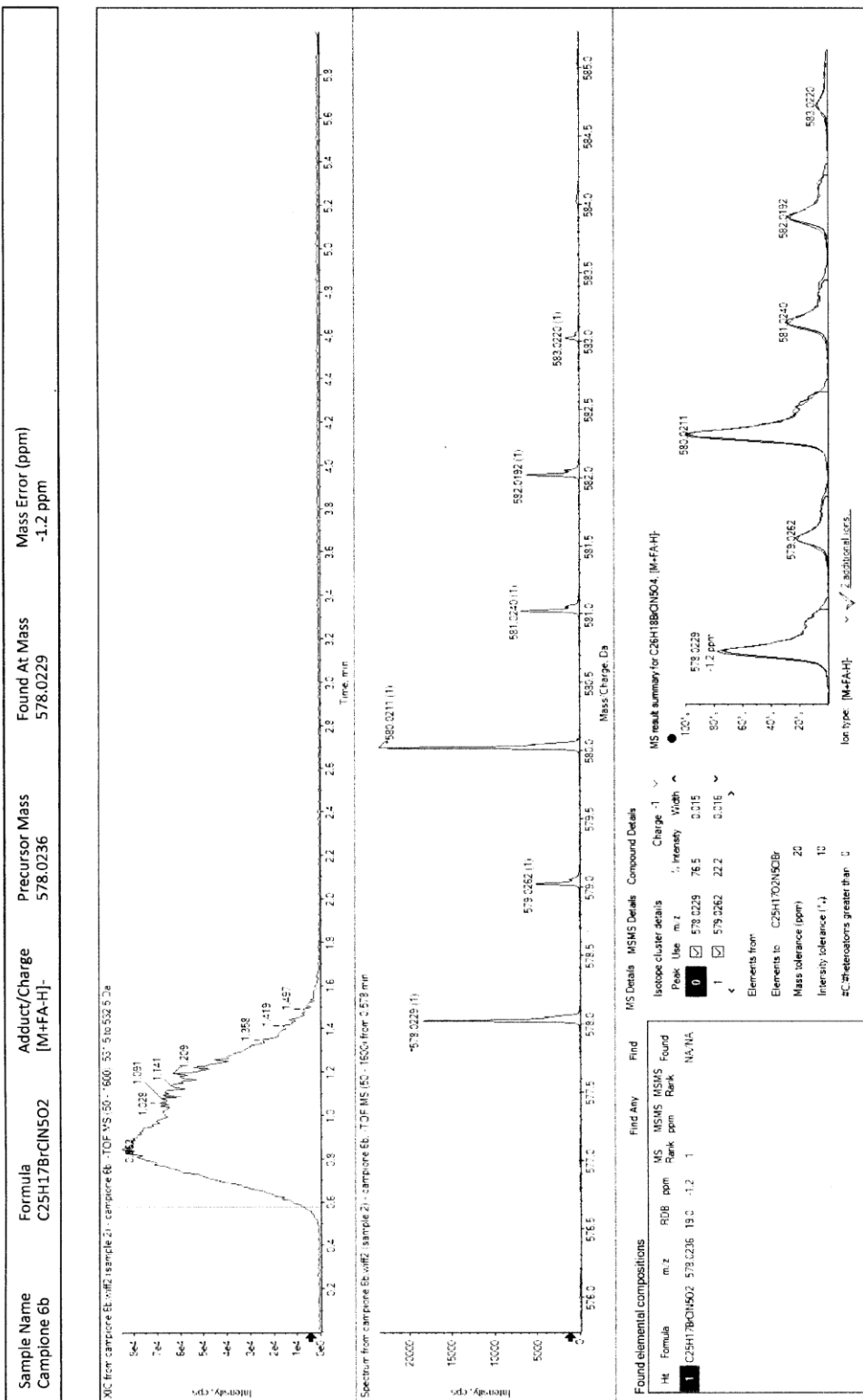




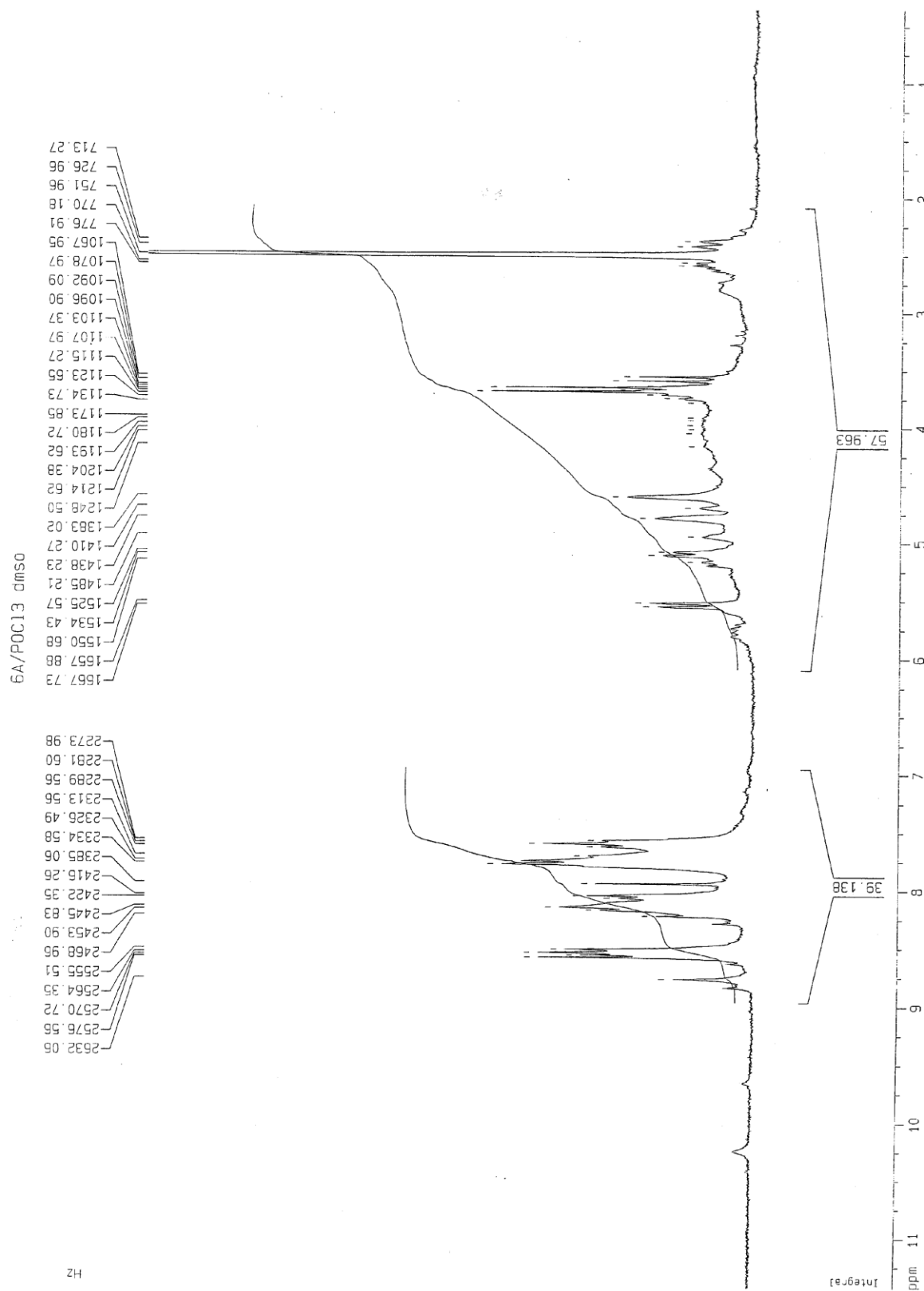
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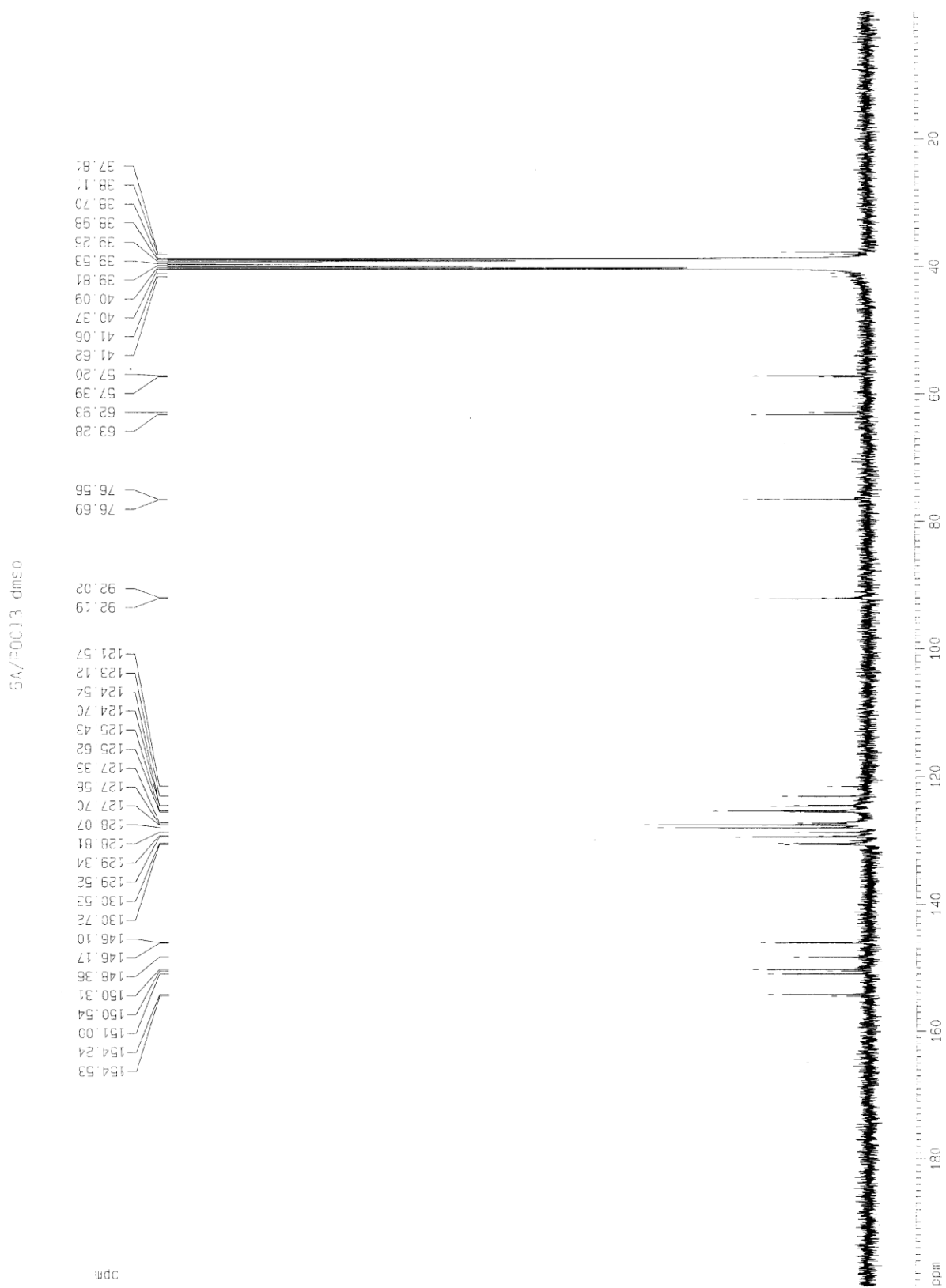






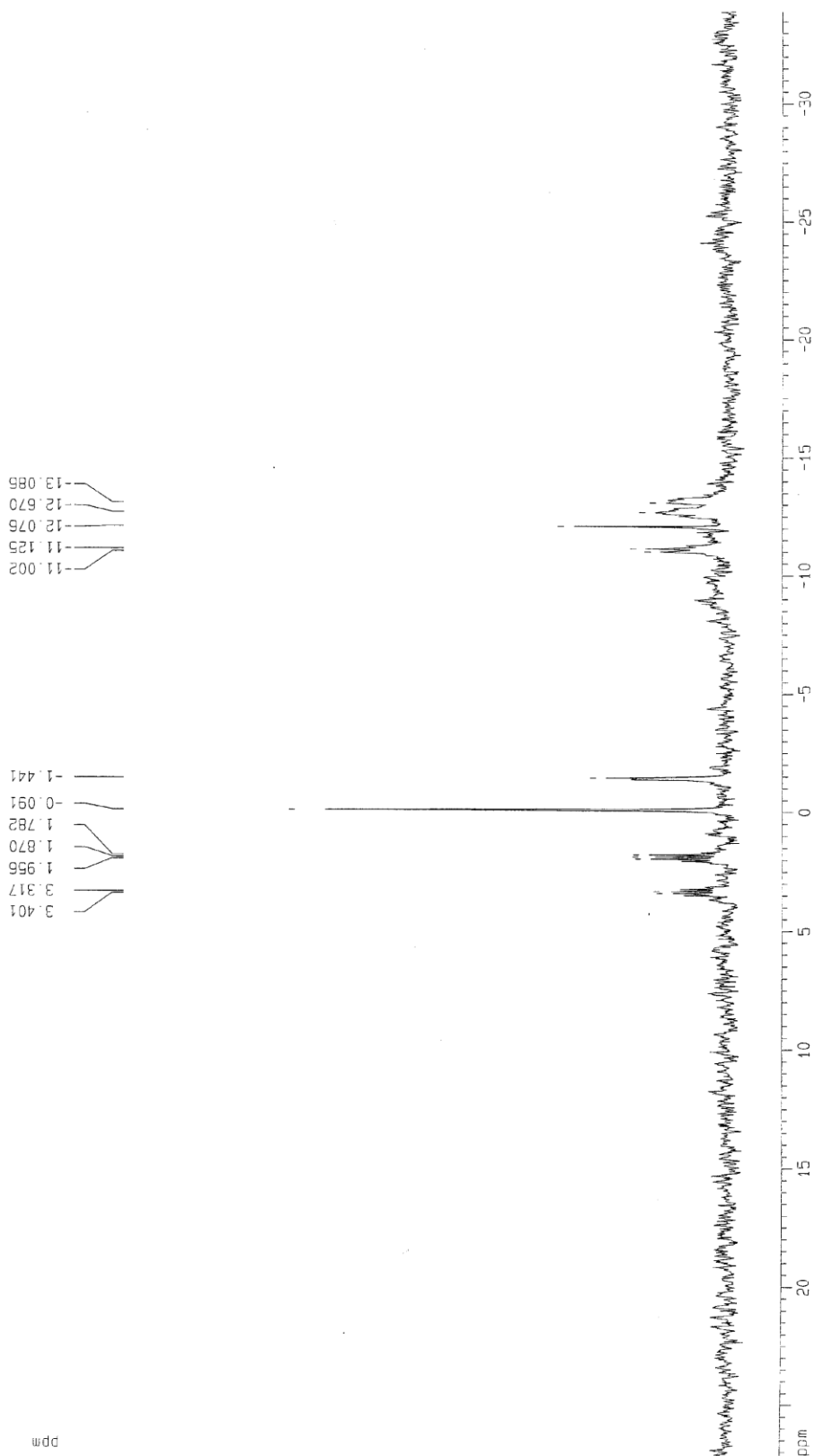
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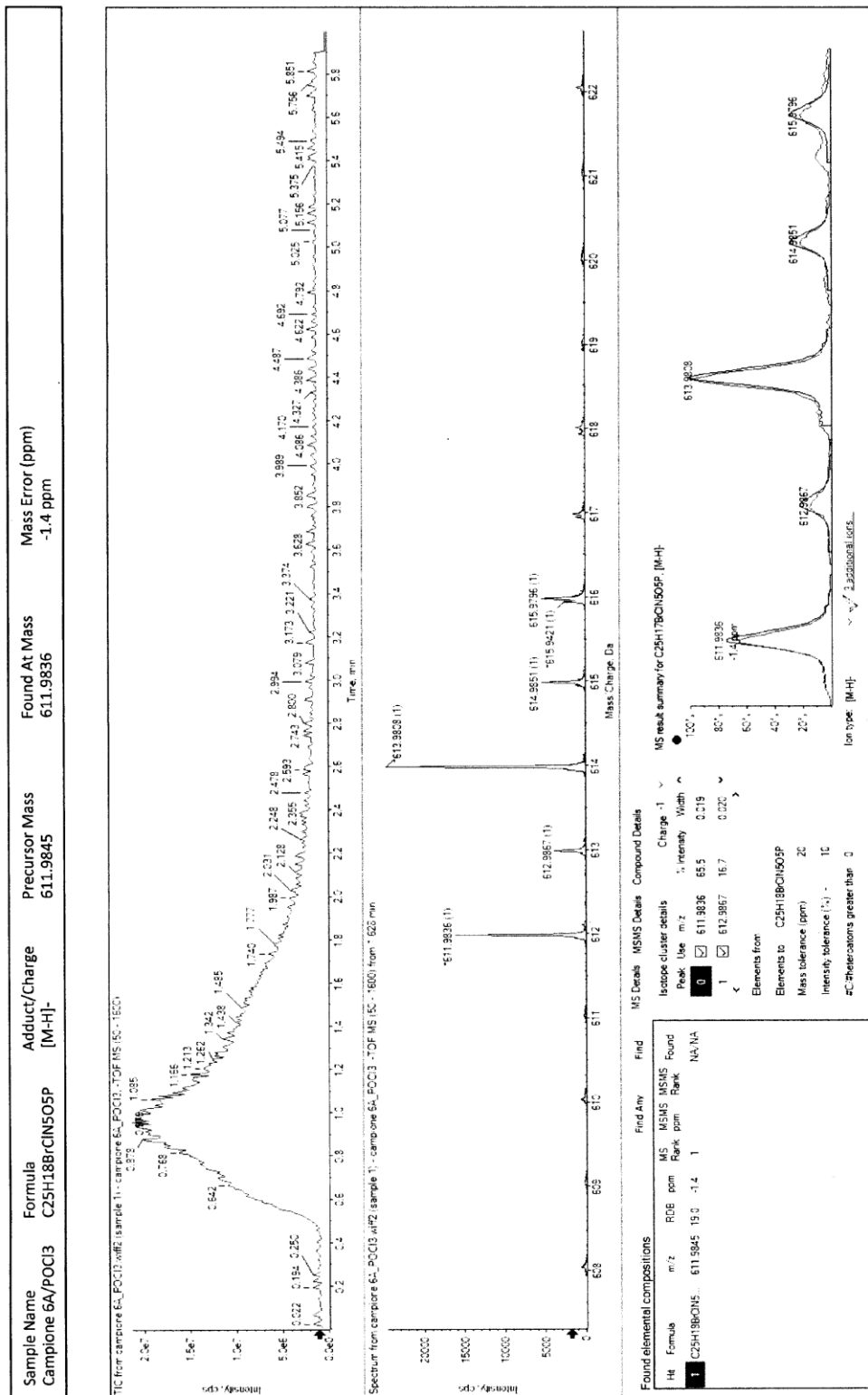




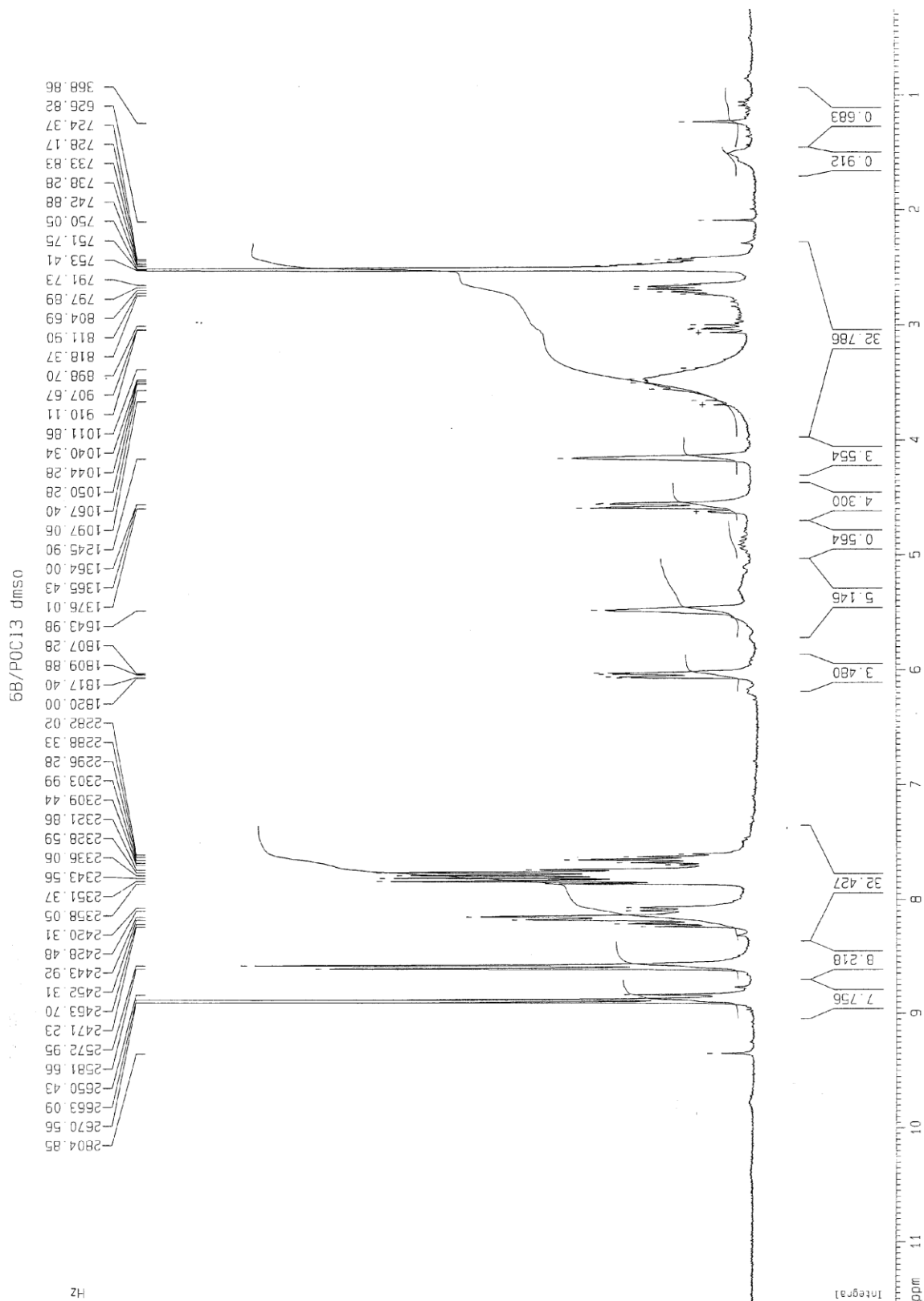
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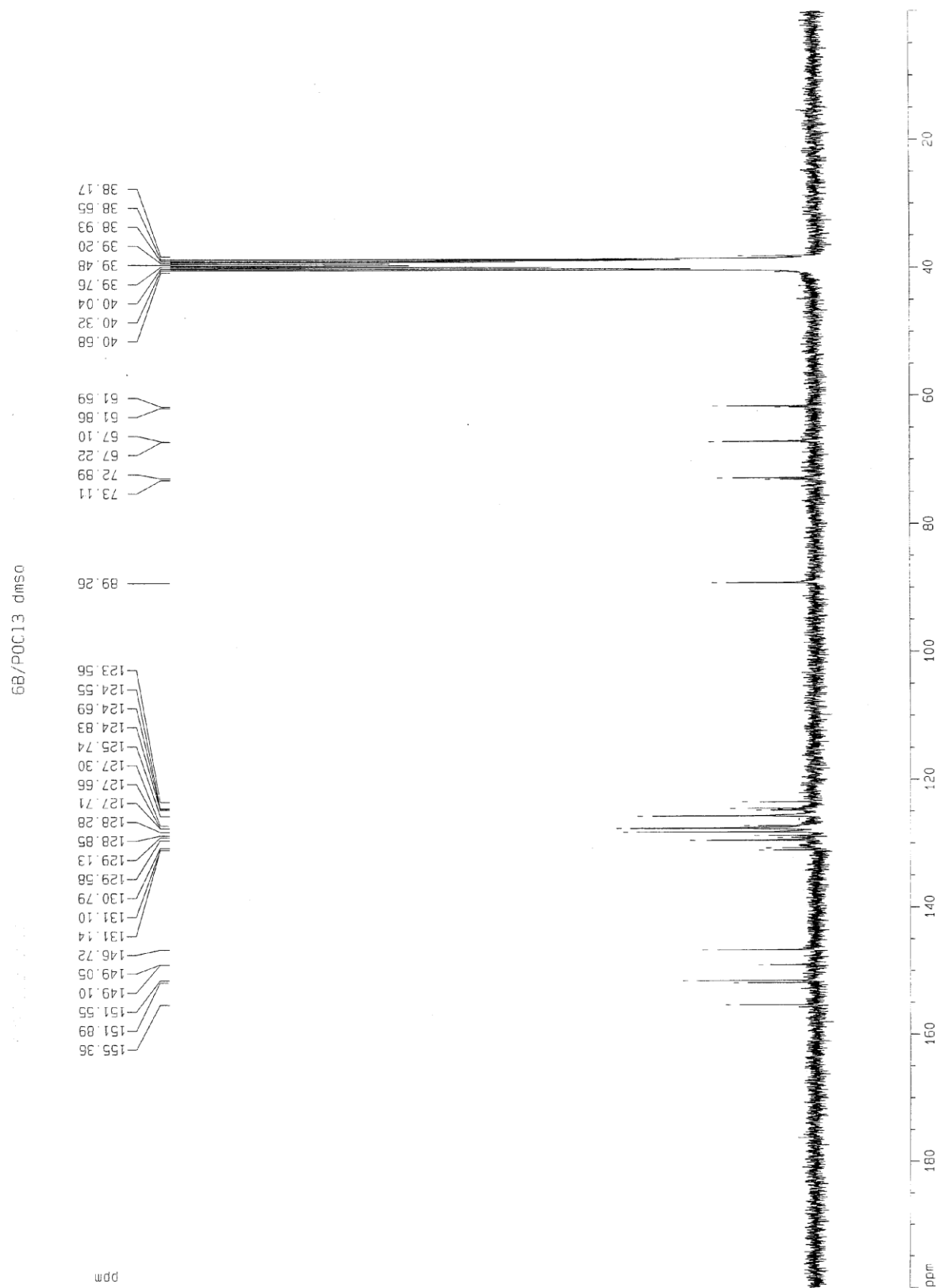
6A/POC13 dms0 non dec



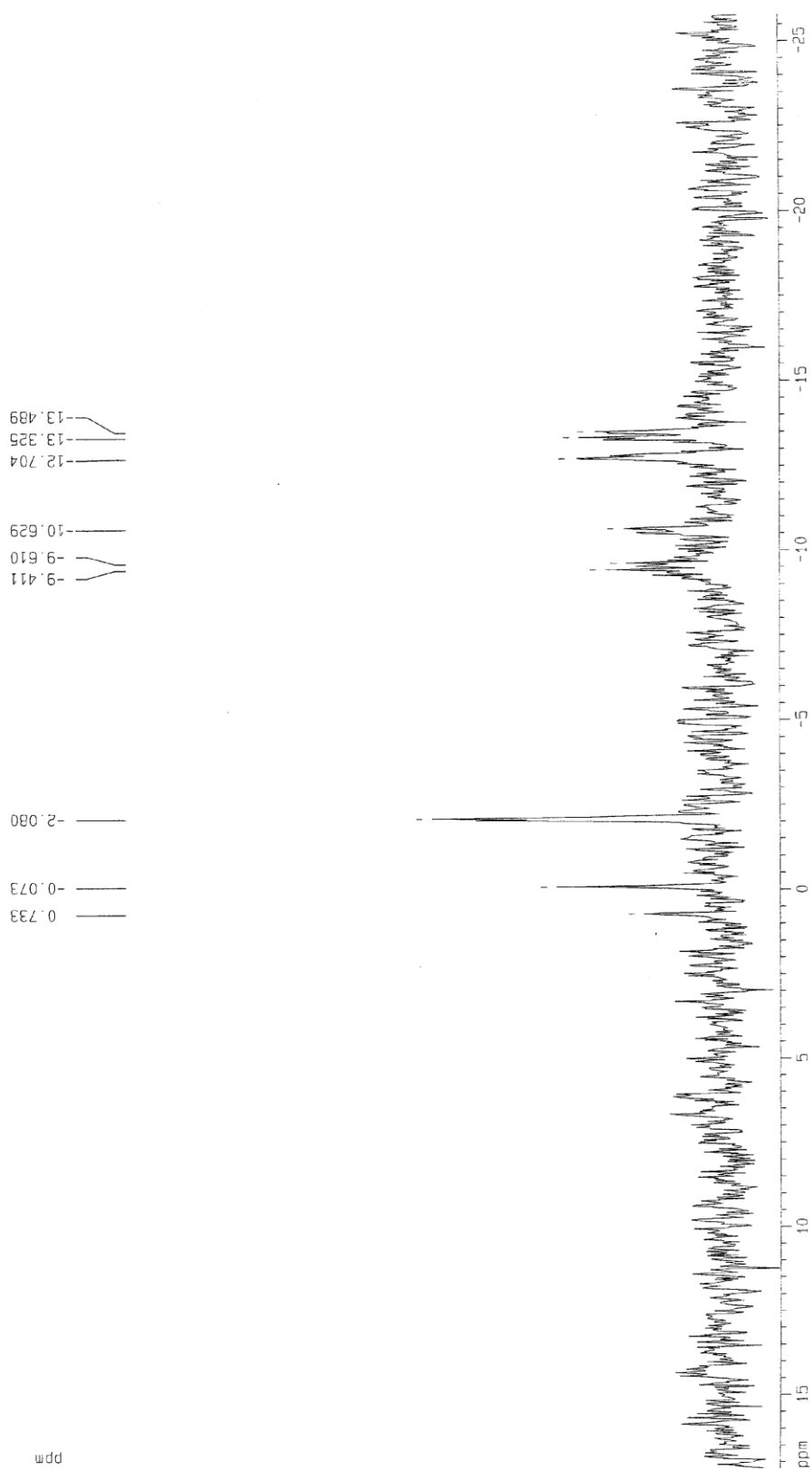


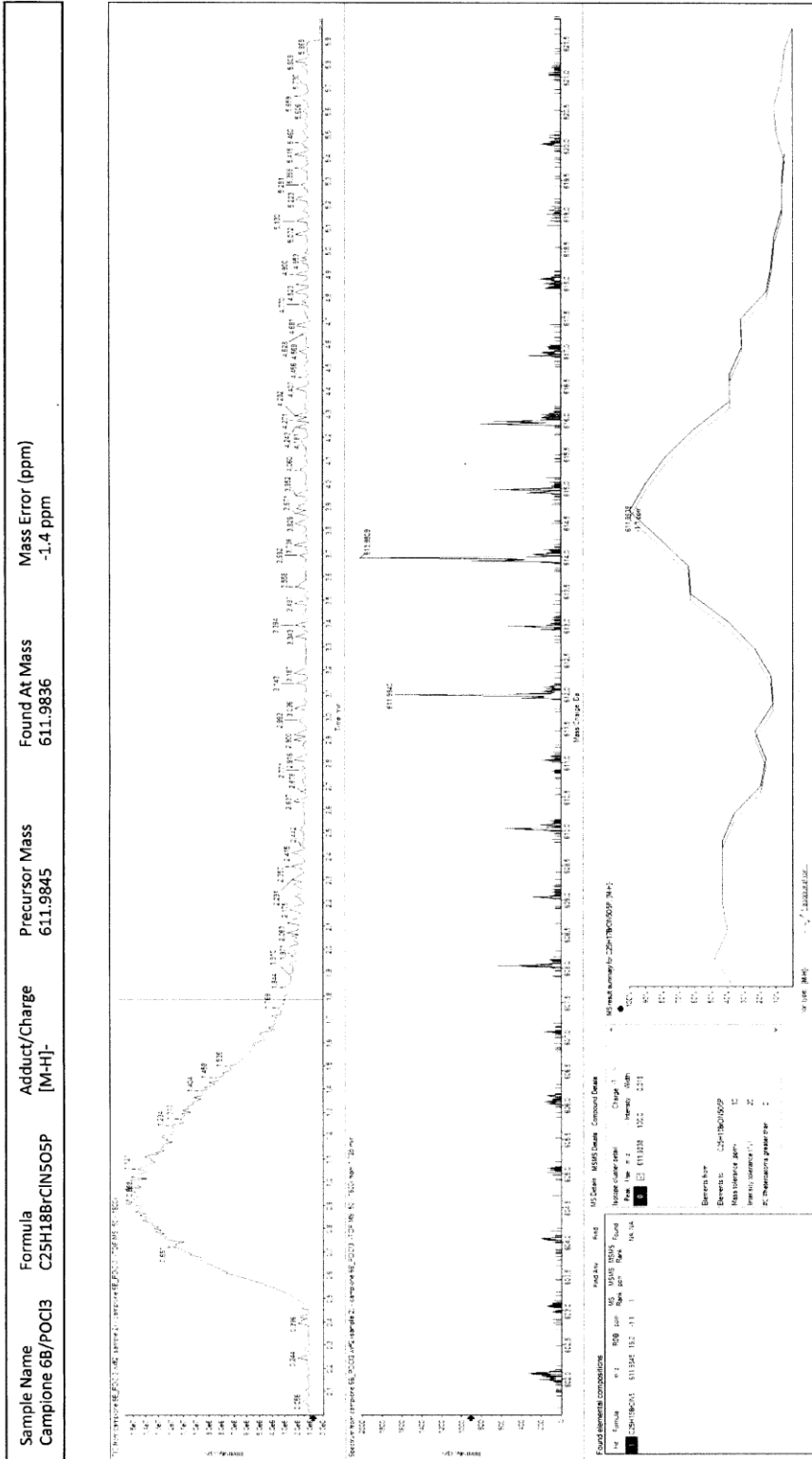
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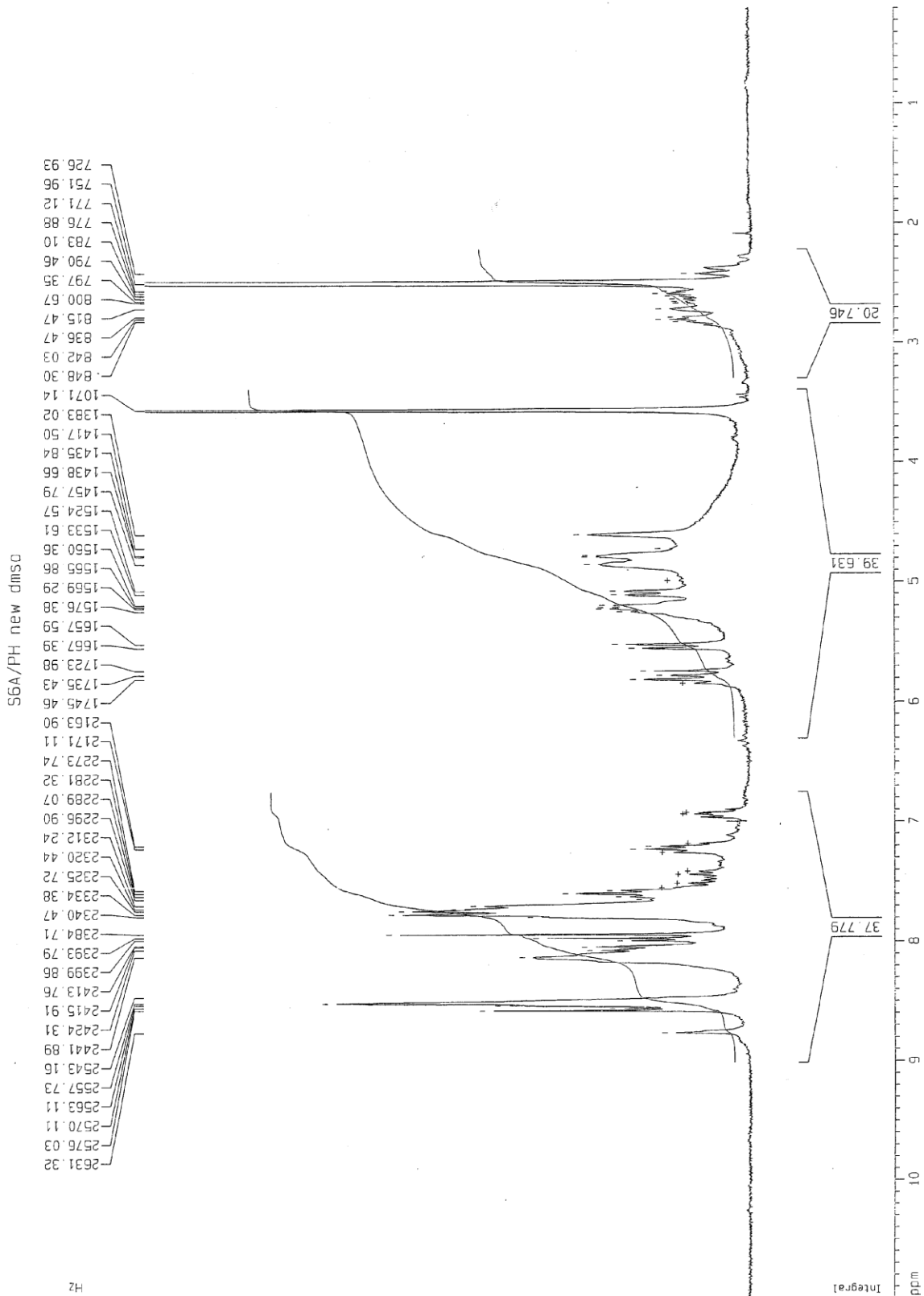


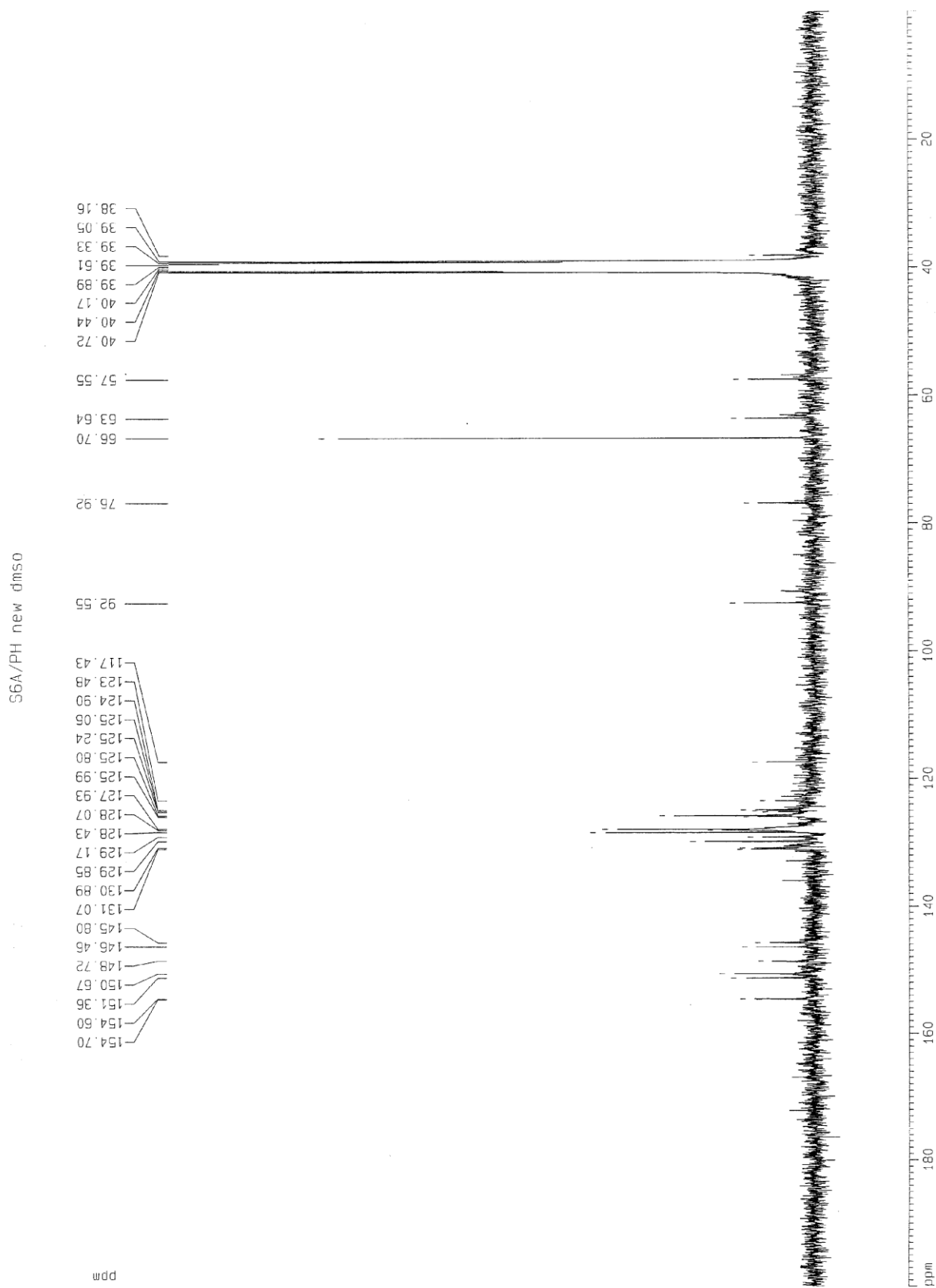
6B/POC13 dmso P non Dec



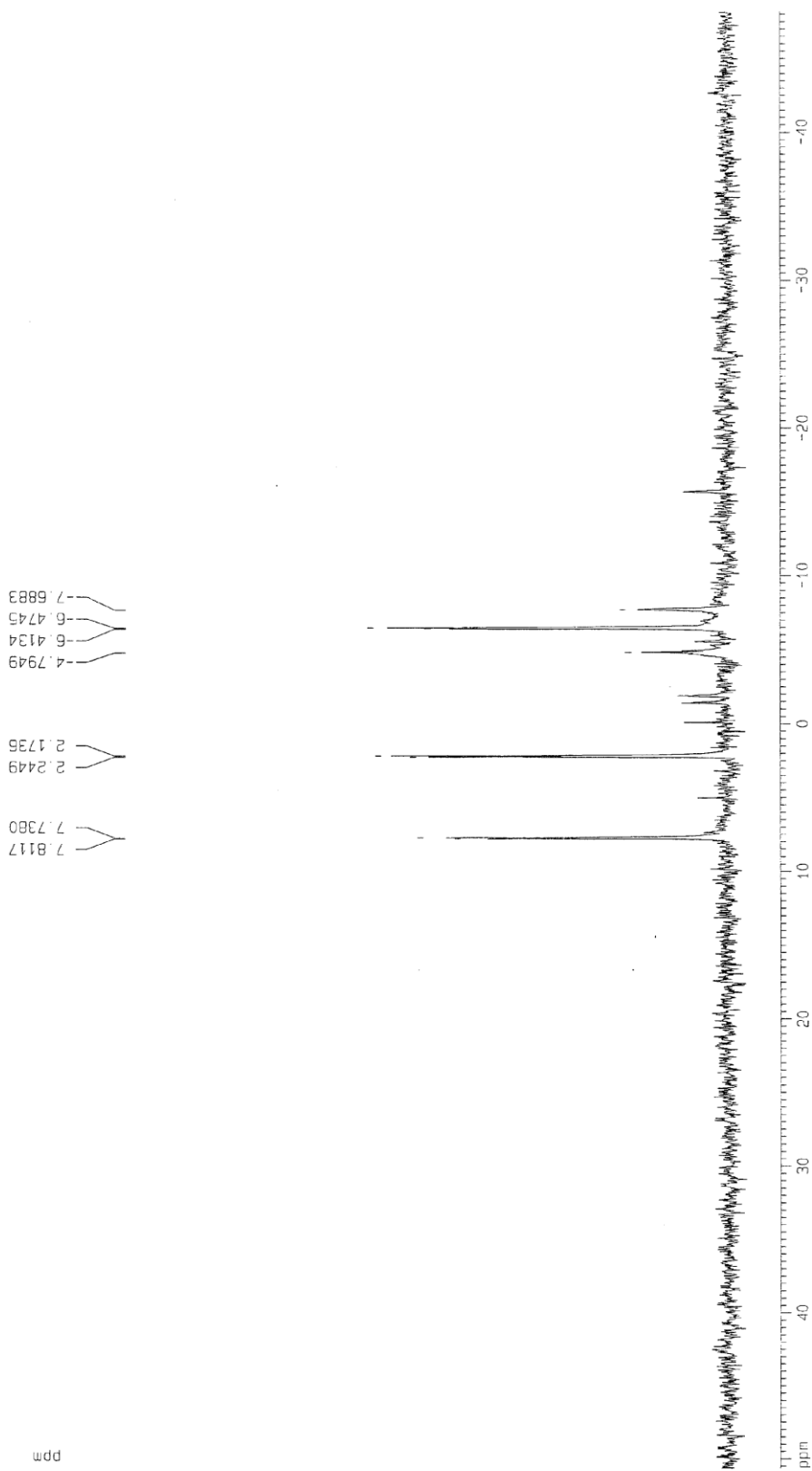


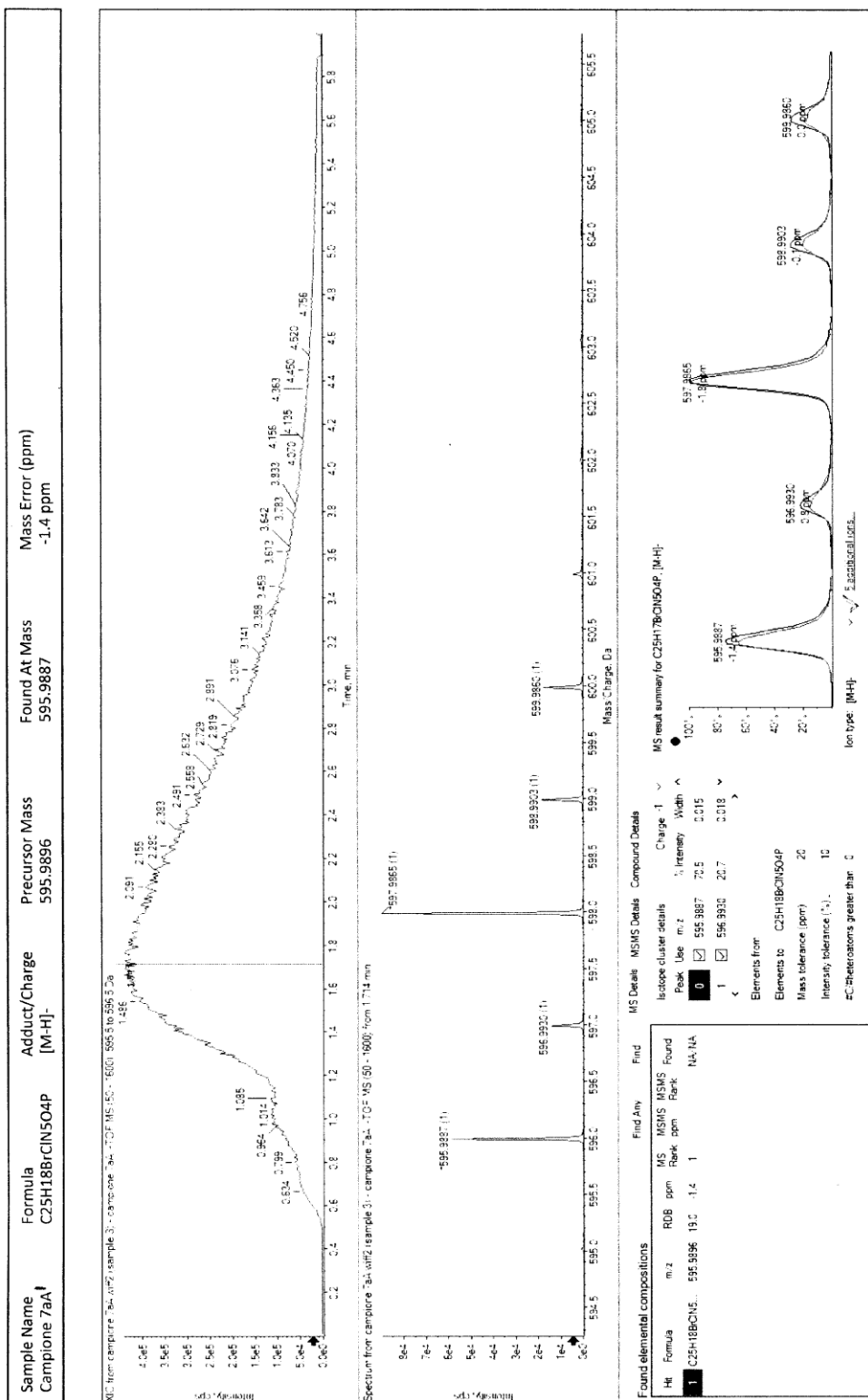
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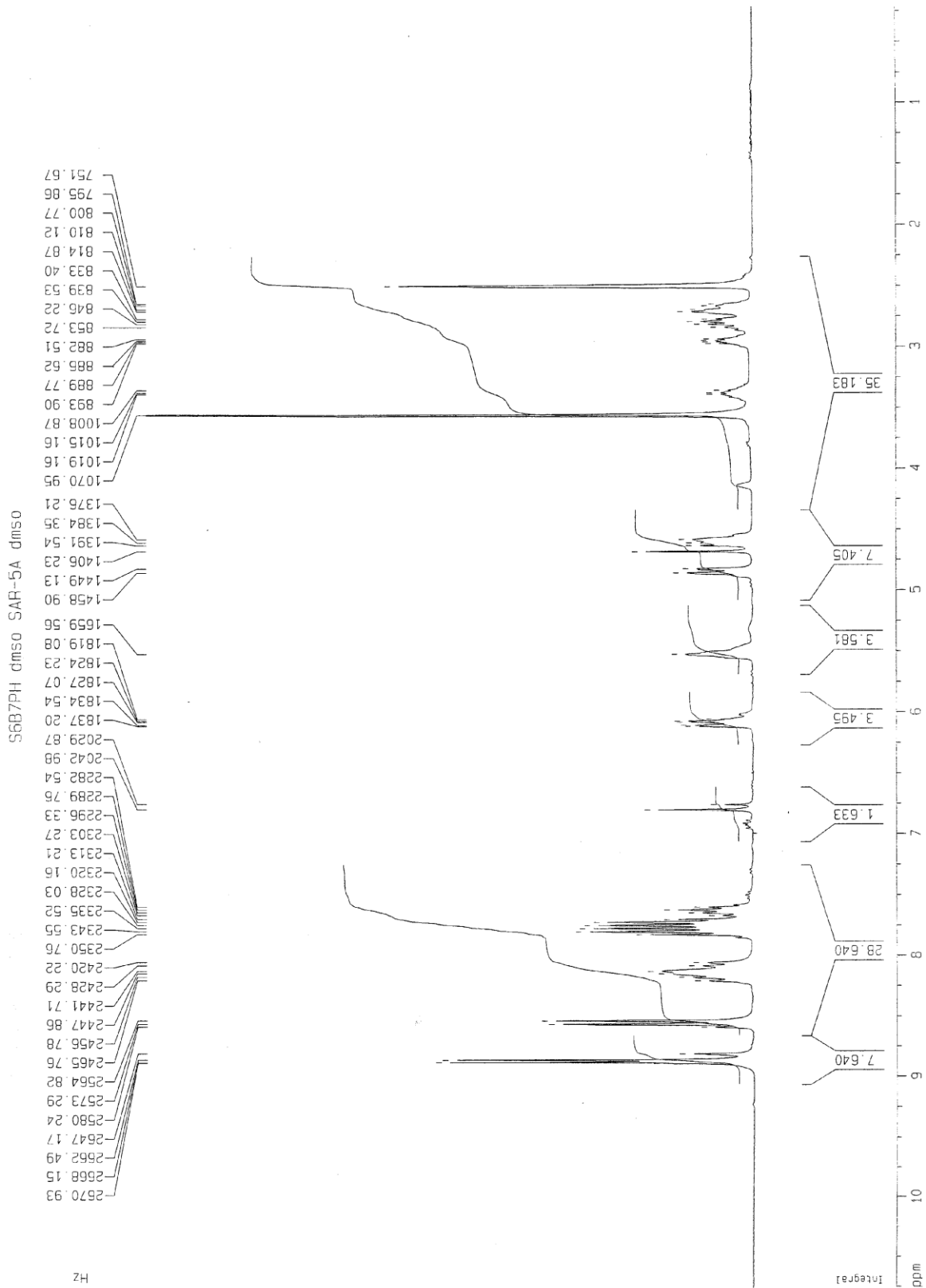


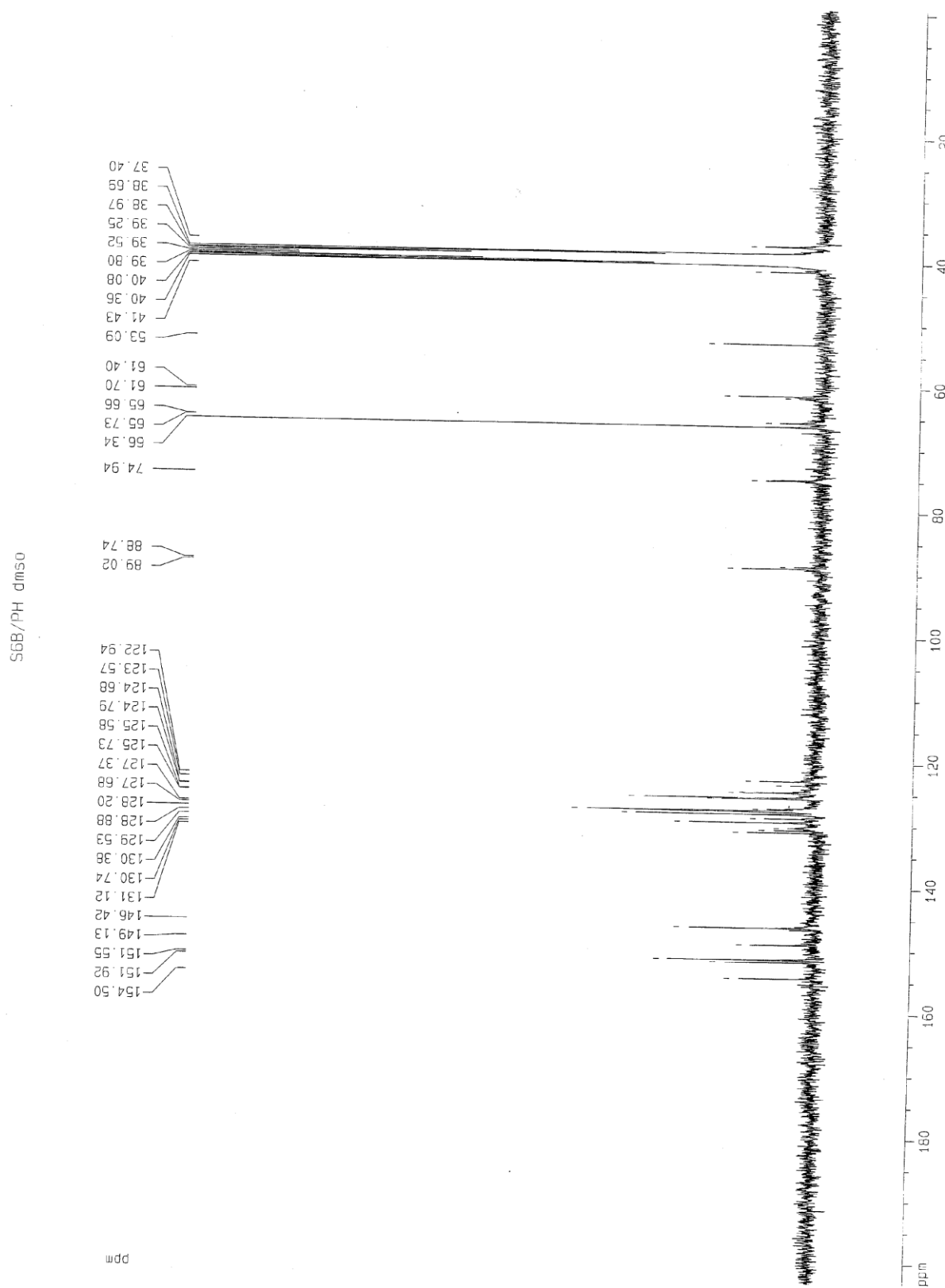
S6A/PH dmsO



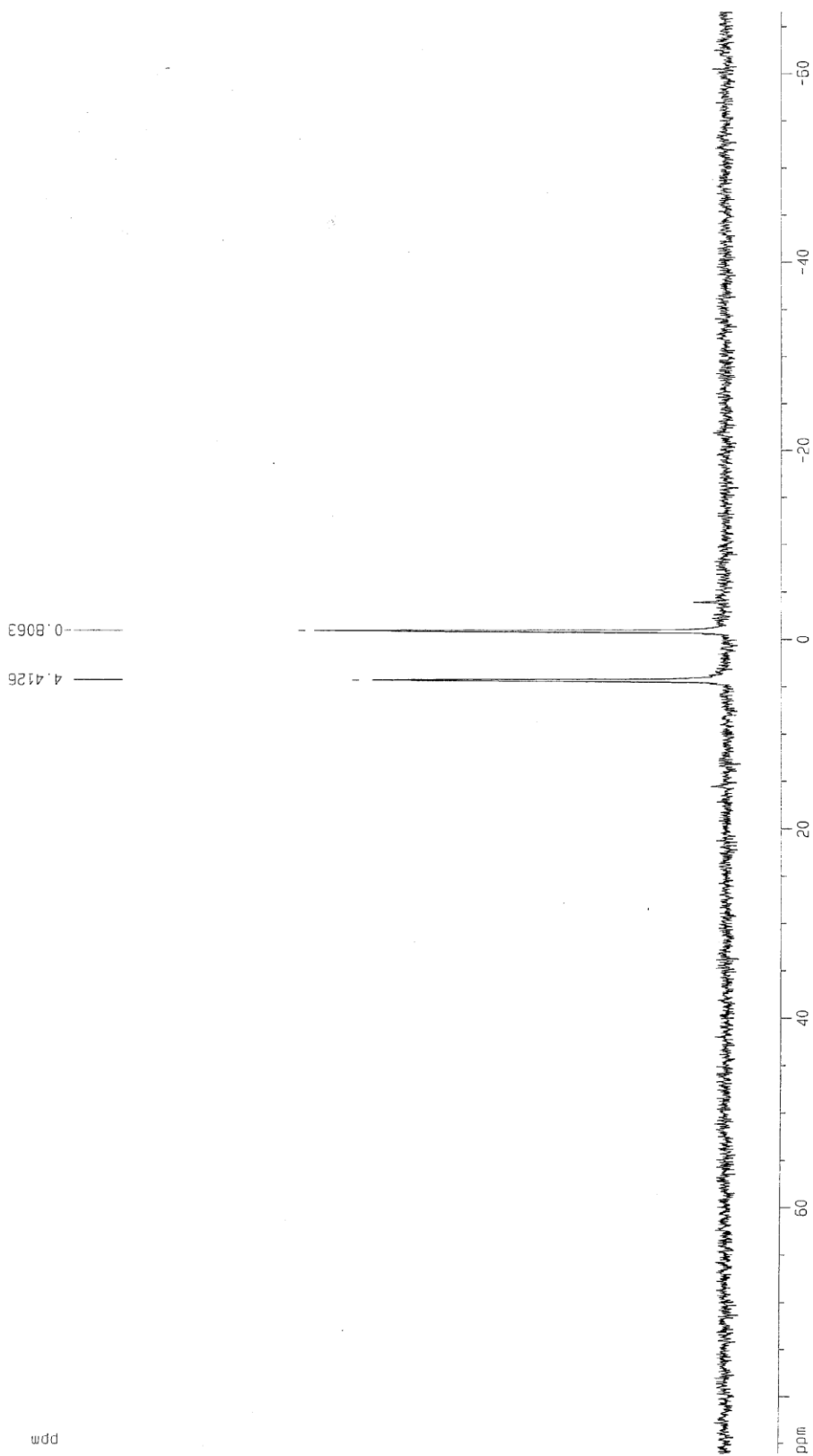


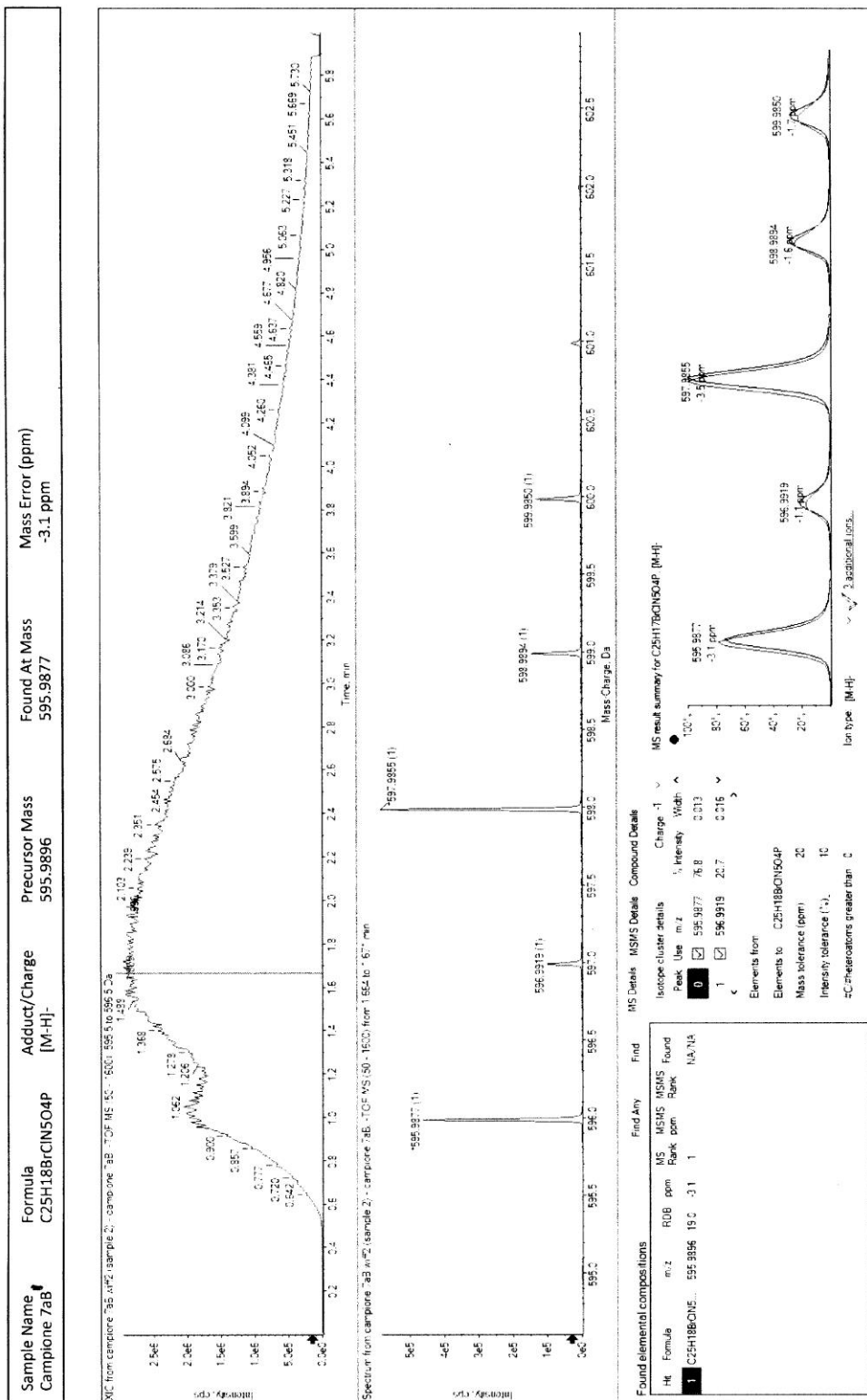
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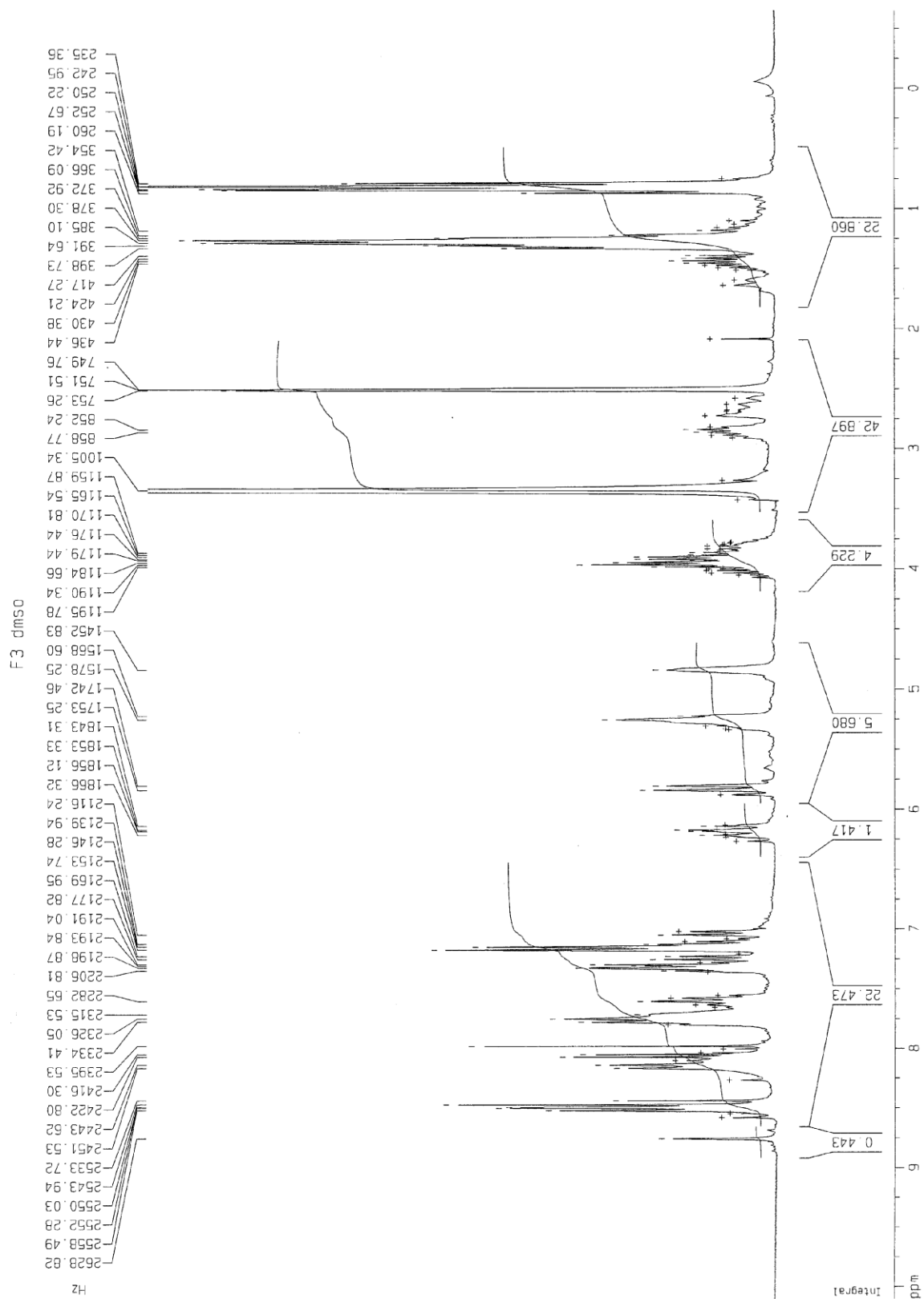


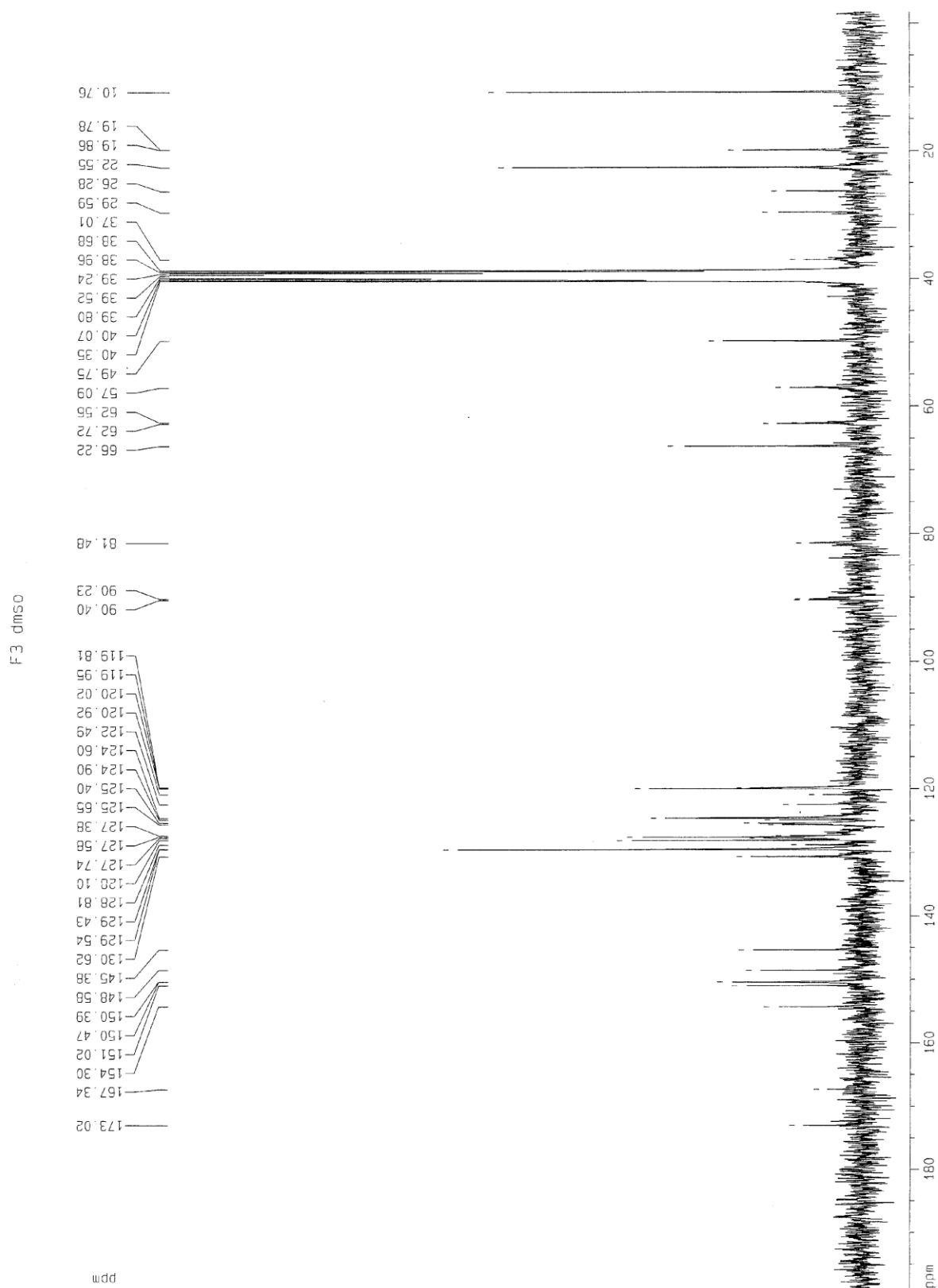
S6B7PH P





7cA

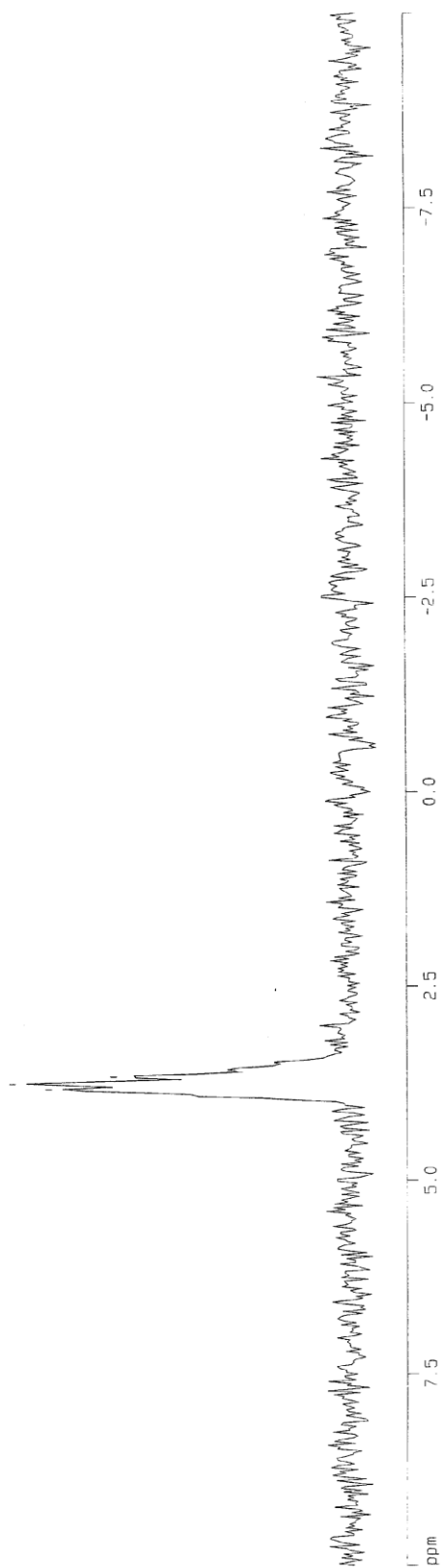


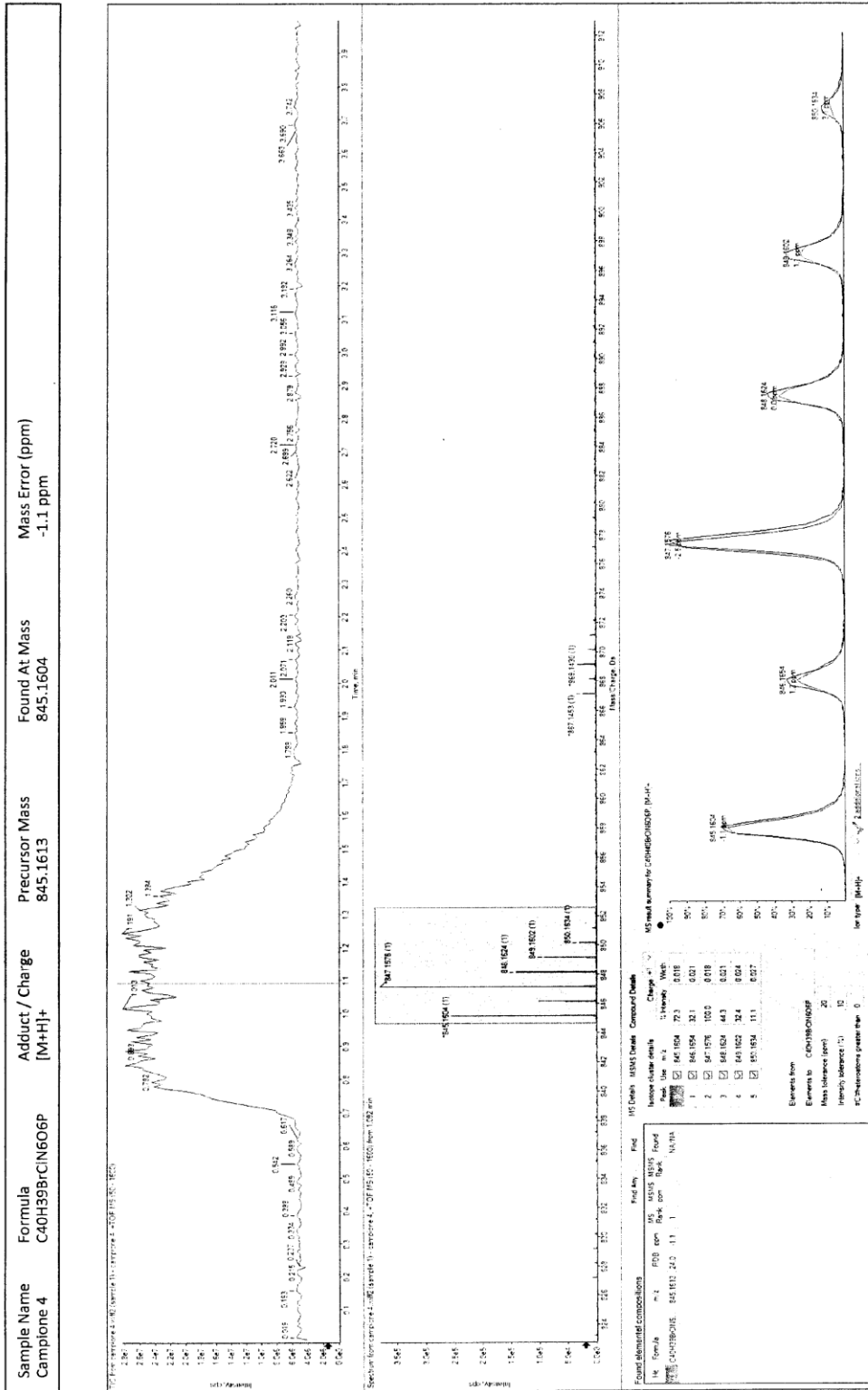


F3 prnon dec dimso

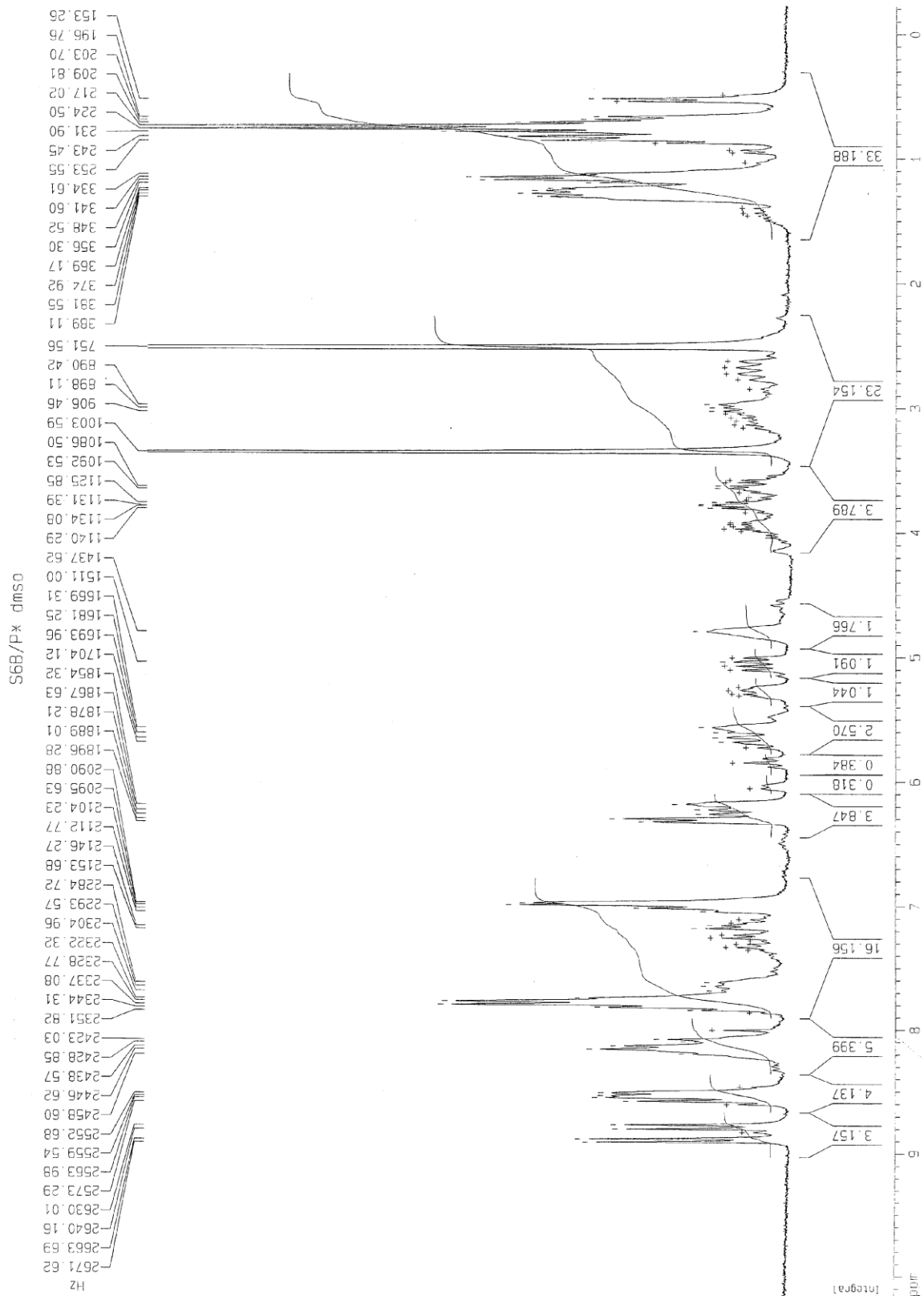
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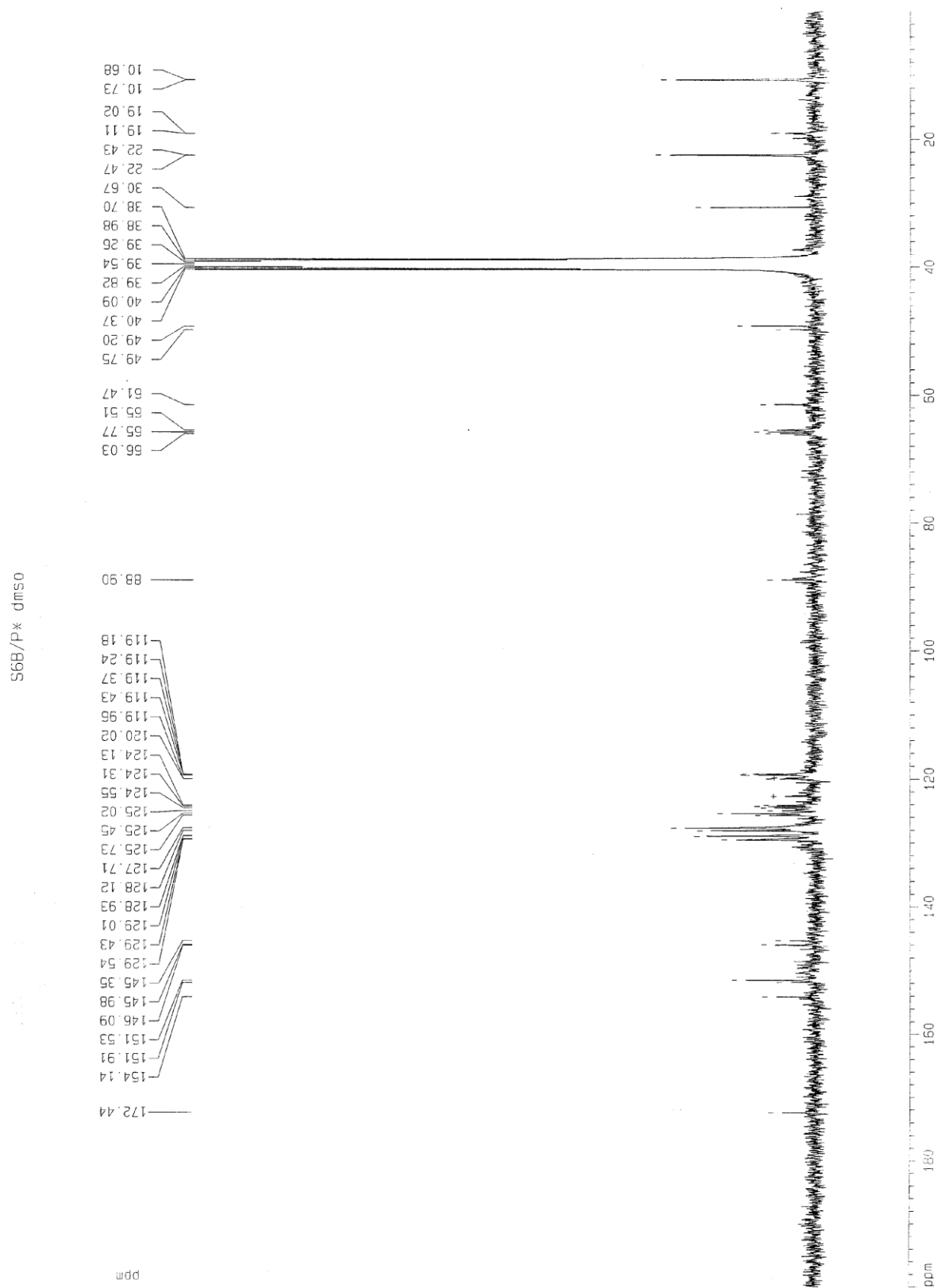
HZ



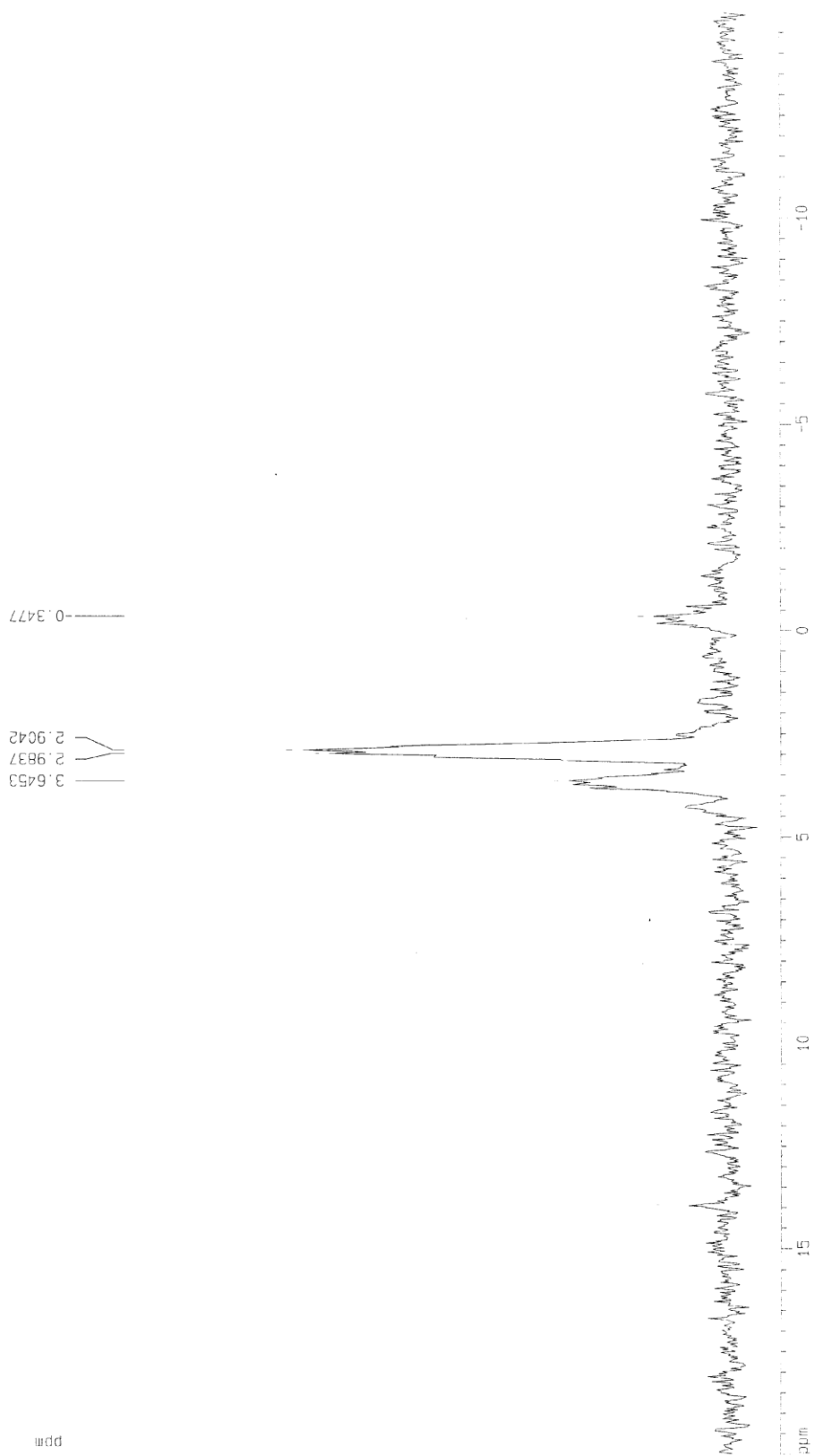


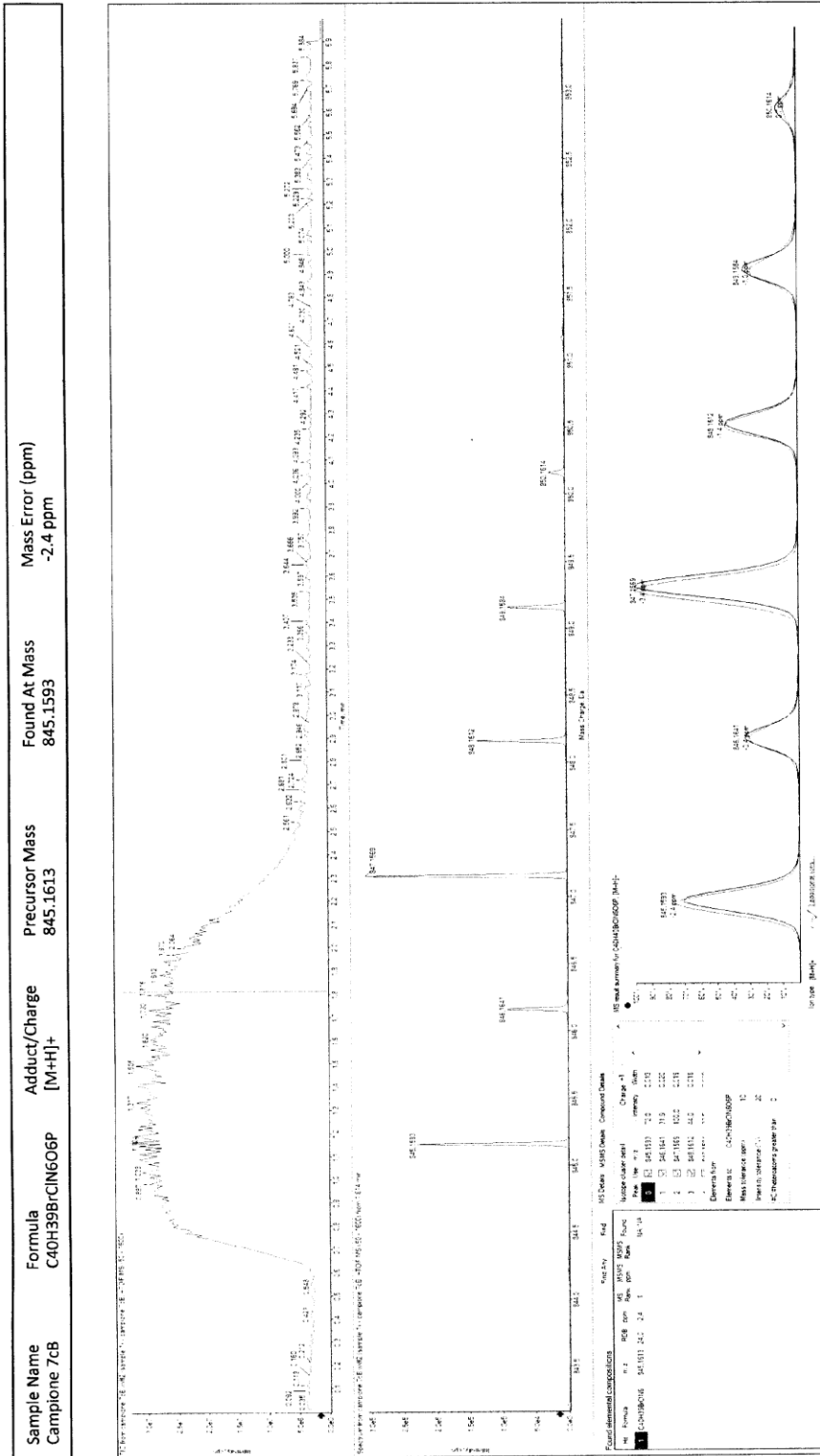
7cB





S6B7x dms0 P non dec





2. Cartesian Coordinates of optimized structures

6°

Stoichiometry C25H17BrClN5O2
 Framework group C1[X(C25H17BrClN5O2)]
 Deg. of freedom 147
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.966031	3.431296	0.783909
2	6	0	1.299597	2.045108	0.682774
3	6	0	1.911174	1.325831	-0.567257
4	6	0	2.678111	2.446481	-1.314623
5	6	0	3.096210	3.477983	-0.252709
6	1	0	2.334866	3.696508	1.778852
7	1	0	1.416221	1.421295	1.571539
8	1	0	1.123766	0.911952	-1.200813
9	1	0	3.521520	2.059878	-1.896029
10	1	0	1.988178	2.925998	-2.018608
11	1	0	3.194331	4.488352	-0.668841
12	6	0	-0.152189	2.458646	0.468003
13	8	0	0.925958	4.377859	0.418590
14	7	0	-0.303268	3.723733	0.307615
15	8	0	4.284928	3.108159	0.449857
16	1	0	5.023016	3.111410	-0.179778
17	6	0	-1.282138	1.500730	0.352225
18	6	0	-1.666539	0.756796	1.489447
19	6	0	-1.912034	1.284518	-0.894798
20	6	0	-1.118409	1.025066	2.784505
21	6	0	-2.657888	-0.290079	1.373832
22	6	0	-2.916904	0.247824	-1.023360
23	6	0	-1.586441	2.052627	-2.059490
24	6	0	-1.479415	0.292074	3.883015
25	1	0	-0.430812	1.856626	2.897349
26	6	0	-2.997500	-1.037112	2.545618
27	6	0	-3.239814	-0.512767	0.113663
28	6	0	-3.525705	0.044577	-2.302120
29	1	0	-0.865032	2.855135	-1.965893
30	6	0	-2.196518	1.823028	-3.262944
31	6	0	-2.423273	-0.762580	3.757599
32	1	0	-1.054003	0.523602	4.855348
33	1	0	-3.730406	-1.829678	2.458452
34	6	0	-3.178372	0.803574	-3.386218
35	1	0	-4.277246	-0.729086	-2.397953
36	1	0	-1.935431	2.427780	-4.126861
37	1	0	-2.700902	-1.344308	4.631788
38	1	0	-3.658169	0.629004	-4.344979
39	35	0	-4.541090	-1.915510	-0.058688
40	6	0	2.484526	-1.122558	-0.669980
41	6	0	3.815322	0.046680	0.633350
42	6	0	3.468017	-1.929836	-0.056379
43	1	0	4.222879	0.924392	1.116078
44	6	0	3.394664	-3.283233	-0.396091

45	6	0	1.589288	-2.845440	-1.735009
46	1	0	0.842513	-3.255070	-2.409520
47	17	0	4.532665	-4.431233	0.266811
48	7	0	4.286923	-1.171676	0.753463
49	7	0	2.724284	0.157931	-0.215646
50	7	0	1.534363	-1.530747	-1.508310
51	7	0	2.466508	-3.731173	-1.224435

6a_up

Stoichiometry C₂₅H₁₇BrClN₅O₂
 Framework group C1[X(C₂₅H₁₇BrClN₅O₂)]
 Deg. of freedom 147
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.850097	2.994776	1.148476
2	6	0	1.138643	1.704523	0.714210
3	6	0	1.546584	1.431094	-0.777665
4	6	0	2.445946	2.630943	-1.189486
5	6	0	2.937535	3.327939	0.103495
6	1	0	2.272958	2.968707	2.157295
7	1	0	1.366242	0.836112	1.335284
8	1	0	0.651293	1.409576	-1.403151
9	1	0	3.284640	2.330216	-1.823106
10	1	0	1.831116	3.329580	-1.767085
11	1	0	2.987776	4.411718	-0.033351
12	6	0	-0.316399	2.138821	0.829279
13	8	0	0.799918	4.007743	1.131097
14	7	0	-0.449246	3.402611	1.020438
15	8	0	4.221014	2.932883	0.527054
16	1	0	4.233831	1.956034	0.623115
17	6	0	-1.471462	1.231609	0.606048
18	6	0	-1.719895	0.199582	1.537994
19	6	0	-2.257034	1.344353	-0.564586
20	6	0	-1.003817	0.118463	2.774906
21	6	0	-2.733876	-0.796858	1.271085
22	6	0	-3.281500	0.356906	-0.843488
23	6	0	-2.070035	2.405319	-1.510290
24	6	0	-1.234233	-0.889258	3.672486
25	1	0	-0.290911	0.900135	3.015291
26	6	0	-2.934428	-1.836988	2.232428
27	6	0	-3.471640	-0.686428	0.079334
28	6	0	-4.042290	0.487908	-2.048587
29	1	0	-1.339478	3.173434	-1.287011
30	6	0	-2.823726	2.490281	-2.650050
31	6	0	-2.205781	-1.887204	3.390290
32	1	0	-0.683378	-0.921034	4.608161
33	1	0	-3.686043	-2.589718	2.029216
34	6	0	-3.821364	1.516177	-2.924105
35	1	0	-4.807670	-0.249045	-2.257912
36	1	0	-2.666937	3.312084	-3.343078
37	1	0	-2.380368	-2.686679	4.104461
38	1	0	-4.415813	1.592305	-3.830027
39	35	0	-4.803348	-2.017965	-0.299471

40	6	0	3.248968	-0.468054	-0.397191
41	6	0	1.621664	-0.885128	-1.803301
42	6	0	3.321466	-1.779596	-0.923803
43	1	0	0.726647	-0.696653	-2.383469
44	6	0	4.390136	-2.543591	-0.448287
45	6	0	5.072249	-0.783861	0.847277
46	1	0	5.800411	-0.408464	1.560324
47	17	0	4.626105	-4.180019	-0.993036
48	7	0	2.288394	-2.011092	-1.804887
49	7	0	2.139699	0.101780	-0.979406
50	7	0	4.101206	0.062101	0.483505
51	7	0	5.249489	-2.046056	0.428083

6b

Stoichiometry C25H17BrClN5O2
 Framework group C1[X(C25H17BrClN5O2)]
 Deg. of freedom 147
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.653988	-0.327969	0.337904
2	6	0	1.676712	0.773202	0.644080
3	6	0	2.861151	0.152016	1.398468
4	6	0	2.193117	-0.988723	2.187823
5	6	0	0.996274	-1.484767	1.340733
6	1	0	0.707809	-0.709007	-0.683848
7	1	0	1.976292	1.383319	-0.216388
8	1	0	3.305785	0.901157	2.057224
9	1	0	2.886052	-1.798386	2.437917
10	1	0	1.817469	-0.568407	3.125466
11	1	0	0.141893	-1.719654	1.985739
12	7	0	-0.405685	1.453199	1.400671
13	8	0	1.321274	-2.629056	0.540811
14	1	0	1.466423	-3.383213	1.134665
15	6	0	-0.642548	0.439496	0.629705
16	8	0	0.970130	1.612018	1.592755
17	6	0	-2.035659	0.244903	0.149586
18	6	0	-2.819769	1.407703	-0.134555
19	6	0	-2.632353	-1.041963	0.016637
20	6	0	-2.255563	2.718008	-0.285558
21	6	0	-4.250340	1.288328	-0.343456
22	6	0	-4.065299	-1.163380	-0.176892
23	6	0	-1.885468	-2.261481	0.058245
24	6	0	-3.023522	3.817232	-0.560301
25	1	0	-1.187719	2.843096	-0.190488
26	6	0	-5.020381	2.469844	-0.589213
27	6	0	-4.826813	0.009413	-0.301661
28	6	0	-4.651118	-2.467827	-0.232358
29	1	0	-0.809549	-2.239238	0.092729
30	6	0	-2.483167	-3.491818	-0.030415
31	6	0	-4.430807	3.698624	-0.689328
32	1	0	-2.547601	4.785649	-0.685457
33	1	0	-6.090536	2.368010	-0.715254
34	6	0	-3.890264	-3.601400	-0.154188

35	1	0	-5.724018	-2.542690	-0.355781
36	1	0	-1.866981	-4.386827	-0.021248
37	1	0	-5.036223	4.578291	-0.888480
38	1	0	-4.360494	-4.578912	-0.209846
39	35	0	-6.737166	-0.144727	-0.457677
40	6	0	5.142410	0.425026	0.378894
41	6	0	4.035384	-1.316338	-0.385882
42	6	0	5.877872	-0.283968	-0.596294
43	1	0	3.222565	-2.025446	-0.475007
44	6	0	7.138554	0.254172	-0.869173
45	6	0	6.758859	1.910390	0.666561
46	1	0	7.151906	2.796557	1.157144
47	17	0	8.188890	-0.490495	-2.048997
48	7	0	3.950305	-0.257877	0.508030
49	7	0	5.161395	-1.368287	-1.056547
50	7	0	7.568833	1.337167	-0.244321
51	7	0	5.536277	1.516301	1.031863

6b_up

Stoichiometry C25H17BrClN5O2
 Framework group C1[X(C25H17BrClN5O2)]
 Deg. of freedom 147
 Full point group C1 NOP 1
 Largest Abelian subgroup C1 NOP 1
 Largest concise Abelian subgroup C1 NOP 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.853380	0.162422	0.808187
2	6	0	1.683877	1.424940	1.025277
3	6	0	2.963147	1.066458	1.795582
4	6	0	2.557470	-0.159633	2.634936
5	6	0	1.335453	-0.837547	1.943728
6	1	0	0.989116	-0.300388	-0.170888
7	1	0	1.872362	2.023696	0.123748
8	1	0	3.234756	1.912228	2.432208
9	1	0	3.370957	-0.878193	2.761964
10	1	0	2.270898	0.191202	3.630230
11	1	0	0.540291	-0.977738	2.680071
12	7	0	-0.487307	1.841677	1.711532
13	8	0	1.623286	-2.124630	1.448718
14	1	0	2.335482	-2.008552	0.782701
15	6	0	-0.544878	0.762360	1.000058
16	8	0	0.859542	2.190457	1.938325
17	6	0	-1.863222	0.377719	0.424540
18	6	0	-2.677363	1.409207	-0.137411
19	6	0	-2.340825	-0.961739	0.435876
20	6	0	-2.208041	2.746009	-0.366047
21	6	0	-4.034137	1.115177	-0.560384
22	6	0	-3.700364	-1.256671	0.025402
23	6	0	-1.534769	-2.068961	0.846134
24	6	0	-3.002020	3.715836	-0.915571
25	1	0	-1.193538	2.997480	-0.096685
26	6	0	-4.839312	2.168468	-1.100948
27	6	0	-4.505780	-0.199838	-0.426859
28	6	0	-4.170445	-2.605939	0.101158
29	1	0	-0.495194	-1.927428	1.088299

30	6	0	-2.017444	-3.350793	0.883321
31	6	0	-4.345388	3.431087	-1.271097
32	1	0	-2.596807	4.710000	-1.082158
33	1	0	-5.857043	1.939339	-1.389522
34	6	0	-3.360273	-3.624458	0.521727
35	1	0	-5.191600	-2.810535	-0.194181
36	1	0	-1.356854	-4.158442	1.185537
37	1	0	-4.974937	4.209915	-1.692064
38	1	0	-3.741509	-4.640784	0.564593
39	35	0	-6.330640	-0.576187	-0.907689
40	6	0	4.434955	-0.124038	0.019034
41	6	0	5.167066	1.789303	0.801050
42	6	0	5.658117	0.268175	-0.577315
43	1	0	5.173038	2.686668	1.407766
44	6	0	6.160776	-0.616427	-1.535141
45	6	0	4.366041	-1.993183	-1.201219
46	1	0	3.867367	-2.918878	-1.473886
47	17	0	7.654819	-0.277716	-2.359671
48	7	0	4.129231	0.877354	0.916704
49	7	0	6.092567	1.470222	-0.065894
50	7	0	5.515707	-1.731453	-1.840397
51	7	0	3.766225	-1.245814	-0.266894

6b'

Stoichiometry C₂₅H₁₇BrClN₅O₂
 Framework group C1[X(C₂₅H₁₇BrClN₅O₂)]
 Deg. of freedom 147
 Full point group C1 NOP 1
 Largest Abelian subgroup C1 NOP 1
 Largest concise Abelian subgroup C1 NOP 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.432510	0.475719	-0.193405
2	6	0	-1.672896	0.208372	-1.071771
3	6	0	-2.599912	-0.767116	-0.299906
4	6	0	-1.688042	-1.377533	0.789596
5	6	0	-0.621299	-0.315354	1.123687
6	1	0	-0.268036	1.527065	0.057249
7	1	0	-2.205926	1.100648	-1.411132
8	1	0	-2.961337	-1.529780	-0.992565
9	1	0	-2.245629	-1.711338	1.670642
10	1	0	-1.191681	-2.258208	0.365827
11	1	0	0.317387	-0.776434	1.455887
12	7	0	0.232381	-0.572595	-2.190181
13	8	0	-1.061145	0.634970	2.097984
14	1	0	-1.164701	0.174831	2.946206
15	6	0	0.668176	-0.060897	-1.097142
16	8	0	-1.159000	-0.468962	-2.252899
17	6	0	2.113641	-0.039402	-0.747527
18	6	0	2.792697	1.198149	-0.728061
19	6	0	2.776302	-1.228259	-0.369608
20	6	0	2.175115	2.401539	-1.197005
21	6	0	4.156344	1.272808	-0.250465
22	6	0	4.143866	-1.171536	0.106999
23	6	0	2.137313	-2.508946	-0.433588
24	6	0	2.831182	3.602538	-1.168305

25	1	0	1.177306	2.344618	-1.618684
26	6	0	4.799732	2.550372	-0.229737
27	6	0	4.778068	0.081661	0.163240
28	6	0	4.776911	-2.392791	0.501273
29	1	0	1.132086	-2.564167	-0.833750
30	6	0	2.784287	-3.652252	-0.049325
31	6	0	4.158777	3.678177	-0.666983
32	1	0	2.342266	4.498483	-1.540023
33	1	0	5.817559	2.610254	0.135349
34	6	0	4.121168	-3.591794	0.429130
35	1	0	5.798354	-2.352349	0.858728
36	1	0	2.279168	-4.611509	-0.119351
37	1	0	4.672148	4.635079	-0.643799
38	1	0	4.627530	-4.503851	0.731908
39	35	0	6.579091	0.171298	0.827026
40	6	0	-5.094458	-0.476790	-0.184549
41	6	0	-3.980275	0.931591	1.085935
42	6	0	-5.952976	0.409006	0.503540
43	1	0	-3.119219	1.384463	1.558778
44	6	0	-7.311556	0.210774	0.242987
45	6	0	-6.785087	-1.510320	-1.172940
46	1	0	-7.161742	-2.276352	-1.845119
47	17	0	-8.520948	1.213437	1.007216
48	7	0	-3.817715	-0.127926	0.205365
49	7	0	-5.228771	1.279077	1.290539
50	7	0	-7.718015	-0.736819	-0.584728
51	7	0	-5.459856	-1.443119	-1.024112

6b'_up

Stoichiometry C₂₅H₁₇BrClN₅O₂
 Framework group C1[X(C₂₅H₁₇BrClN₅O₂)]
 Deg. of freedom 147
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.585898	-0.427057	0.480583
2	6	0	-1.753820	0.071701	1.348551
3	6	0	-2.448202	1.232197	0.566161
4	6	0	-1.646679	1.413409	-0.751215
5	6	0	-0.770849	0.150444	-0.955443
6	1	0	-0.509049	-1.515577	0.398700
7	1	0	-2.470790	-0.694263	1.651321
8	1	0	-2.376370	2.124926	1.191184
9	1	0	-2.290322	1.582831	-1.618427
10	1	0	-1.003563	2.293750	-0.646458
11	1	0	0.197480	0.419452	-1.386437
12	7	0	0.241725	0.674882	2.393484
13	8	0	-1.322179	-0.793020	-1.842787
14	1	0	-2.229414	-1.010493	-1.537762
15	6	0	0.583077	0.130697	1.282016
16	8	0	-1.150956	0.592035	2.558514
17	6	0	2.002203	0.076108	0.837540
18	6	0	2.669264	-1.167517	0.823090
19	6	0	2.645266	1.241494	0.365170

20	6	0	2.077377	-2.343834	1.384486
21	6	0	3.995515	-1.275263	0.254762
22	6	0	3.975884	1.152126	-0.202115
23	6	0	2.022656	2.530503	0.421706
24	6	0	2.721064	-3.551483	1.359962
25	1	0	1.111363	-2.259019	1.870329
26	6	0	4.625867	-2.559371	0.241263
27	6	0	4.595583	-0.108488	-0.250106
28	6	0	4.588673	2.350079	-0.689059
29	1	0	1.048085	2.611629	0.887548
30	6	0	2.649204	3.650945	-0.052782
31	6	0	4.008964	-3.661376	0.769377
32	1	0	2.252933	-4.426650	1.801455
33	1	0	5.614088	-2.645212	-0.193394
34	6	0	3.948680	3.557723	-0.620572
35	1	0	5.582015	2.284495	-1.115299
36	1	0	2.157352	4.617443	0.012856
37	1	0	4.511742	-4.623989	0.748580
38	1	0	4.439014	4.451562	-0.995475
39	35	0	6.345739	-0.243454	-1.032201
40	6	0	-4.552447	0.002395	-0.253245
41	6	0	-4.891568	1.832373	0.901716
42	6	0	-5.929925	0.276397	-0.081190
43	1	0	-4.638640	2.720734	1.467390
44	6	0	-6.789477	-0.659418	-0.662546
45	6	0	-4.984414	-1.853580	-1.409928
46	1	0	-4.634027	-2.723644	-1.957448
47	17	0	-8.516338	-0.475022	-0.545277
48	7	0	-3.890675	1.023280	0.389120
49	7	0	-6.111263	1.432096	0.645958
50	7	0	-6.315247	-1.709297	-1.315714
51	7	0	-4.043964	-1.045398	-0.906677

7cA

Stoichiometry C₄₀H₃₉BrClN₆O₆P
 Framework group C1[X(C₄₀H₃₉BrClN₆O₆P)]
 Deg. of freedom 276
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.015775	-1.697915	0.506217
2	6	0	1.277892	-0.860449	0.538222
3	6	0	1.200245	0.161331	-0.647895
4	6	0	-0.001404	-0.324003	-1.498000
5	6	0	-0.942628	-1.073623	-0.548800
6	1	0	-0.521879	-1.809162	1.469043
7	1	0	1.452995	-0.334818	1.479212
8	1	0	2.119114	0.133892	-1.237502
9	1	0	-0.506286	0.483009	-2.032552
10	1	0	0.373010	-1.036356	-2.242237
11	1	0	-1.535797	-1.843813	-1.045879
12	6	0	2.312752	-1.954436	0.297379
13	8	0	0.398018	-3.015289	0.056015
14	7	0	1.793595	-3.094622	0.016310

15	8	0	-1.807729	-0.155139	0.154799
16	6	0	3.780658	-1.723946	0.278796
17	6	0	4.435332	-1.383855	1.482977
18	6	0	4.496265	-1.774779	-0.939401
19	6	0	3.759471	-1.423704	2.744372
20	6	0	5.832466	-1.009890	1.471136
21	6	0	5.899410	-1.412483	-0.965392
22	6	0	3.880601	-2.165492	-2.172608
23	6	0	4.391745	-1.080091	3.909056
24	1	0	2.733037	-1.773794	2.774897
25	6	0	6.450042	-0.649298	2.710097
26	6	0	6.511125	-1.027515	0.240093
27	6	0	6.591298	-1.457700	-2.216944
28	1	0	2.843115	-2.476108	-2.158193
29	6	0	4.583486	-2.195905	-3.346499
30	6	0	5.753451	-0.675065	3.888246
31	1	0	3.856789	-1.128190	4.853260
32	1	0	7.493016	-0.357852	2.701715
33	6	0	5.957281	-1.834645	-3.369281
34	1	0	7.639467	-1.186603	-2.236554
35	1	0	4.091801	-2.505183	-4.264553
36	1	0	6.247659	-0.398174	4.814932
37	1	0	6.507489	-1.862046	-4.305439
38	35	0	8.360819	-0.509149	0.207880
39	6	0	2.059326	2.517133	-0.518358
40	6	0	0.198375	2.199010	0.612071
41	6	0	1.630125	3.692470	0.136129
42	1	0	-0.665653	1.674873	0.996467
43	6	0	2.460711	4.798238	-0.064151
44	6	0	3.838358	3.521204	-1.373547
45	1	0	4.741689	3.491182	-1.976511
46	17	0	2.084980	6.339478	0.667395
47	7	0	0.464448	3.464008	0.835123
48	7	0	1.120051	1.556088	-0.203780
49	7	0	3.145369	2.383989	-1.276673
50	7	0	3.549439	4.709746	-0.809515
51	15	0	-3.368534	0.104101	-0.220357
52	8	0	-4.007873	-1.389126	-0.241547
53	6	0	-4.722204	-2.010529	0.789461
54	6	0	-4.558946	-1.674486	2.132950
55	6	0	-5.594431	-3.023231	0.390629
56	6	0	-5.295695	-2.375529	3.090822
57	1	0	-3.893964	-0.870442	2.425403
58	6	0	-6.317264	-3.714763	1.362221
59	1	0	-5.705119	-3.245227	-0.665712
60	6	0	-6.171223	-3.394806	2.714058
61	1	0	-5.178355	-2.116955	4.139436
62	1	0	-6.997852	-4.504564	1.056977
63	1	0	-6.736262	-3.935368	3.467713
64	8	0	-3.911358	1.108661	0.716966
65	7	0	-3.423455	0.466293	-1.863320
66	1	0	-3.504130	1.474563	-1.958041
67	6	0	-4.225107	-0.252720	-2.879081
68	6	0	-5.678197	-0.548250	-2.457343
69	8	0	-6.312567	-1.503552	-2.851600
70	8	0	-6.151342	0.407122	-1.646159
71	6	0	-7.492714	0.238272	-1.113581
72	1	0	-8.205238	0.554448	-1.885654
73	1	0	-7.650388	-0.825214	-0.918167

74	6	0	-7.621695	1.072210	0.160694
75	1	0	-6.829360	0.729898	0.840299
76	6	0	-9.001007	0.783223	0.816515
77	1	0	-9.469827	-0.085667	0.332726
78	1	0	-9.679414	1.625715	0.627189
79	6	0	-7.380090	2.567977	-0.124303
80	1	0	-6.427975	2.668182	-0.656705
81	1	0	-8.164143	2.929934	-0.807345
82	6	0	-8.925285	0.508405	2.323774
83	1	0	-8.490207	1.354864	2.865719
84	1	0	-9.921089	0.318504	2.741309
85	1	0	-8.301692	-0.369860	2.529381
86	6	0	-7.336154	3.452817	1.125538
87	1	0	-8.286343	3.443591	1.672009
88	1	0	-6.546223	3.120289	1.808856
89	1	0	-7.124535	4.493717	0.855475
90	1	0	-4.307394	0.451923	-3.717059
91	6	0	-3.535662	-1.515202	-3.397517
92	1	0	-2.549012	-1.261014	-3.795413
93	1	0	-3.422578	-2.255847	-2.601918
94	1	0	-4.136706	-1.966566	-4.190062

7cA_up

Stoichiometry C40H39BrClN6O6P
 Framework group C1[X(C40H39BrClN6O6P)]
 Deg. of freedom 276
 Full point group C1 NOP 1
 Largest Abelian subgroup C1 NOP 1
 Largest concise Abelian subgroup C1 NOP 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.697482	-2.342126	0.337824
2	6	0	1.681731	-1.159798	0.397142
3	6	0	1.256766	-0.146820	-0.726007
4	6	0	0.242514	-0.940357	-1.574285
5	6	0	-0.426319	-1.939404	-0.624482
6	1	0	0.305933	-2.665025	1.305896
7	1	0	1.713435	-0.667624	1.370255
8	1	0	2.123841	0.122610	-1.336727
9	1	0	-0.465144	-0.317644	-2.117181
10	1	0	0.818021	-1.516469	-2.307940
11	1	0	-0.845174	-2.804179	-1.143115
12	6	0	2.985616	-1.874936	0.065421
13	8	0	1.463686	-3.437284	-0.233863
14	7	0	2.816358	-3.096209	-0.295618
15	8	0	-1.433578	-1.304011	0.188662
16	6	0	4.315350	-1.212035	0.045984
17	6	0	4.863625	-0.744120	1.261819
18	6	0	4.985587	-0.983541	-1.178689
19	6	0	4.260000	-1.045356	2.525413
20	6	0	6.080565	0.038858	1.259346
21	6	0	6.213010	-0.212004	-1.194901
22	6	0	4.487312	-1.479458	-2.427334
23	6	0	4.781301	-0.574370	3.700742
24	1	0	3.393074	-1.697105	2.547664
25	6	0	6.584617	0.516467	2.510166

26	6	0	6.706708	0.284090	0.024466
27	6	0	6.857512	0.015783	-2.451971
28	1	0	3.593675	-2.091096	-2.421992
29	6	0	5.139408	-1.236878	-3.606164
30	6	0	5.953255	0.228878	3.690290
31	1	0	4.306818	-0.825631	4.644928
32	1	0	7.488751	1.112548	2.508704
33	6	0	6.339986	-0.477255	-3.618713
34	1	0	7.774589	0.591345	-2.464222
35	1	0	4.742895	-1.634588	-4.536056
36	1	0	6.357999	0.603809	4.625722
37	1	0	6.851468	-0.291072	-4.558639
38	35	0	8.310259	1.339782	0.005598
39	6	0	-0.367947	1.888409	-0.370829
40	6	0	1.557087	1.896154	0.689820
41	6	0	-0.165636	3.071460	0.386184
42	1	0	2.529661	1.539969	1.006210
43	6	0	-1.193259	4.013767	0.317454
44	6	0	-2.347692	2.637264	-1.089237
45	1	0	-3.256671	2.484236	-1.662709
46	17	0	-1.079882	5.515080	1.193497
47	7	0	1.045680	3.047251	1.037383
48	7	0	0.764476	1.124527	-0.148385
49	7	0	-1.448371	1.648480	-1.123030
50	7	0	-2.273100	3.795825	-0.414276
51	15	0	-3.022472	-1.500767	-0.078406
52	8	0	-3.226624	-3.094935	-0.348186
53	6	0	-3.719532	-3.972609	0.629055
54	6	0	-2.868358	-4.971305	1.095759
55	6	0	-5.046678	-3.887233	1.046071
56	6	0	-3.357832	-5.905382	2.010529
57	1	0	-1.845056	-5.017303	0.735509
58	6	0	-5.519225	-4.825728	1.964092
59	1	0	-5.686376	-3.101840	0.658365
60	6	0	-4.681370	-5.833341	2.447939
61	1	0	-2.701414	-6.689369	2.378033
62	1	0	-6.551204	-4.767749	2.298707
63	1	0	-5.059629	-6.561063	3.160338
64	8	0	-3.823090	-0.936388	1.029461
65	7	0	-3.169425	-0.906368	-1.639978
66	1	0	-2.675686	-0.012664	-1.685477
67	6	0	-4.453275	-0.901353	-2.384480
68	6	0	-5.620059	-0.464884	-1.480632
69	8	0	-6.511291	-1.198662	-1.108874
70	8	0	-5.501397	0.826733	-1.131596
71	6	0	-6.405241	1.284758	-0.088207
72	1	0	-7.435299	1.105962	-0.416070
73	1	0	-6.210479	0.672913	0.797082
74	6	0	-6.144978	2.764295	0.185836
75	1	0	-5.083600	2.860285	0.454728
76	6	0	-7.000529	3.203812	1.407778
77	1	0	-7.419214	2.316935	1.903690
78	1	0	-7.866378	3.780949	1.056599
79	6	0	-6.402219	3.621248	-1.070255
80	1	0	-5.861638	3.177437	-1.915846
81	1	0	-7.470775	3.556899	-1.326083
82	6	0	-6.226958	4.015907	2.454220
83	1	0	-5.800144	4.929108	2.025842
84	1	0	-6.878078	4.307709	3.286617

85	1	0	-5.398829	3.428716	2.868310
86	6	0	-5.990116	5.091155	-0.934037
87	1	0	-6.561412	5.604710	-0.152433
88	1	0	-4.925367	5.178251	-0.687983
89	1	0	-6.163683	5.631033	-1.872325
90	1	0	-4.335230	-0.127709	-3.151065
91	6	0	-4.739498	-2.239532	-3.060704
92	1	0	-3.893929	-2.516501	-3.696604
93	1	0	-4.900690	-3.028131	-2.324325
94	1	0	-5.640281	-2.162952	-3.677736

7cB

Stoichiometry C40H39BrClN6O6P

Framework group C1[X(C40H39BrClN6O6P)]

Deg. of freedom 276

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.289188	-2.339505	-0.506420
2	6	0	-1.461024	-3.341159	-0.411071
3	6	0	-2.495785	-2.770670	0.592517
4	6	0	-1.722754	-1.679641	1.366949
5	6	0	-0.635066	-1.144052	0.421382
6	1	0	-0.092812	-1.960242	-1.512852
7	1	0	-1.918046	-3.614955	-1.365738
8	1	0	-2.813677	-3.576515	1.257115
9	1	0	-2.361362	-0.881838	1.750168
10	1	0	-1.232221	-2.155987	2.223838
11	1	0	0.242098	-0.771558	0.955763
12	7	0	0.494381	-4.390049	0.340324
13	8	0	-1.147079	-0.097610	-0.433158
14	6	0	-4.972760	-2.876295	0.218675
15	6	0	-3.969057	-1.350733	-1.009551
16	6	0	-5.879350	-2.190736	-0.618968
17	1	0	-3.162492	-0.738704	-1.389382
18	6	0	-7.206173	-2.612420	-0.496697
19	6	0	-6.570016	-4.143109	1.083333
20	1	0	-6.889274	-4.930354	1.760738
21	17	0	-8.467395	-1.876303	-1.455006
22	7	0	-5.224190	-1.243473	-1.375697
23	7	0	-3.736966	-2.320371	-0.042699
24	7	0	-5.267451	-3.849384	1.078129
25	7	0	-7.542787	-3.575967	0.344190
26	15	0	-1.130320	1.495646	-0.102451
27	8	0	0.427505	1.823814	0.211170
28	6	0	1.453665	1.917877	-0.742240
29	6	0	1.248146	2.477425	-2.003498
30	6	0	2.710282	1.476519	-0.334845
31	6	0	2.339060	2.579683	-2.869817
32	1	0	0.260576	2.814926	-2.295684
33	6	0	3.789199	1.589678	-1.211518
34	1	0	2.834432	1.054922	0.657202
35	6	0	3.605597	2.140202	-2.481539
36	1	0	2.190131	3.009700	-3.856512

37	1	0	4.761528	1.217953	-0.903151
38	1	0	4.445496	2.223890	-3.165117
39	8	0	-1.815140	2.199749	-1.207429
40	7	0	-1.796423	1.732085	1.425351
41	1	0	-2.696405	2.182308	1.281972
42	6	0	-1.101079	2.286530	2.608338
43	6	0	-0.397513	3.634715	2.358135
44	8	0	0.571484	4.018559	2.974507
45	8	0	-1.038730	4.347618	1.418891
46	6	0	-0.457065	5.624323	1.052295
47	1	0	-0.464871	6.279293	1.931649
48	1	0	0.585883	5.451841	0.769847
49	6	0	-1.266561	6.205188	-0.106510
50	1	0	-1.272187	5.441308	-0.897535
51	6	0	-0.550660	7.476197	-0.641503
52	1	0	0.475898	7.515935	-0.250684
53	1	0	-1.050927	8.369778	-0.244617
54	6	0	-2.726761	6.461367	0.319443
55	1	0	-3.127086	5.538205	0.754673
56	1	0	-2.730195	7.210740	1.125685
57	6	0	-0.480677	7.558522	-2.171612
58	1	0	-1.476766	7.543620	-2.626068
59	1	0	0.021080	8.478319	-2.493796
60	1	0	0.081084	6.710927	-2.582191
61	6	0	-3.657369	6.921169	-0.807618
62	1	0	-3.353767	7.889154	-1.221683
63	1	0	-3.674185	6.194194	-1.628308
64	1	0	-4.684184	7.030469	-0.440516
65	1	0	-1.908501	2.513491	3.317546
66	6	0	-0.160397	1.291357	3.286659
67	1	0	-0.710805	0.387804	3.563757
68	1	0	0.672248	1.021262	2.633370
69	1	0	0.260305	1.743680	4.187425
70	8	0	-0.879012	-4.549387	0.156603
71	6	0	0.858070	-3.212491	-0.015334
72	6	0	2.277910	-2.769925	0.038844
73	6	0	2.852270	-2.354477	1.258825
74	6	0	3.015584	-2.706663	-1.162605
75	6	0	2.158236	-2.477629	2.505779
76	6	0	4.180387	-1.775236	1.271153
77	6	0	4.348503	-2.144833	-1.166928
78	6	0	2.486026	-3.199776	-2.397547
79	6	0	2.711759	-2.041280	3.679476
80	1	0	1.189405	-2.963921	2.510782
81	6	0	4.712943	-1.322511	2.519976
82	6	0	4.871052	-1.678716	0.051234
83	6	0	5.059012	-2.088388	-2.406759
84	1	0	1.507516	-3.668074	-2.394223
85	6	0	3.202933	-3.130894	-3.561606
86	6	0	4.003316	-1.447167	3.683947
87	1	0	2.168562	-2.157559	4.612957
88	1	0	5.700887	-0.878681	2.529119
89	6	0	4.505182	-2.561517	-3.565629
90	1	0	6.056011	-1.665646	-2.410744
91	1	0	2.781795	-3.521336	-4.483547
92	1	0	4.433033	-1.098510	4.618498
93	1	0	5.067773	-2.511106	-4.493371
94	35	0	6.600203	-0.838962	0.039164

7cB_up

Stoichiometry C40H39BrClN6O6P

Framework group C1[X(C40H39BrClN6O6P)]

Deg. of freedom 276

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.010849	-2.344846	-0.214053
2	6	0	0.280625	-3.681151	0.018152
3	6	0	-0.868415	-3.433787	1.032644
4	6	0	-0.454492	-2.125498	1.730920
5	6	0	0.336173	-1.292242	0.707268
6	1	0	0.970818	-1.982585	-1.243487
7	1	0	-0.055081	-4.170867	-0.899754
8	1	0	-0.880448	-4.260709	1.748680
9	1	0	-1.276317	-1.575159	2.183328
10	1	0	0.235110	-2.409584	2.534413
11	1	0	1.062424	-0.635846	1.192373
12	7	0	2.517035	-3.926561	0.662113
13	8	0	-0.526496	-0.501535	-0.134720
14	6	0	-3.287250	-2.605214	0.417303
15	6	0	-2.617510	-4.542681	-0.372750
16	6	0	-4.296000	-3.269887	-0.326363
17	1	0	-1.956507	-5.383233	-0.541494
18	6	0	-5.520516	-2.604668	-0.410858
19	6	0	-4.674357	-0.909132	0.860393
20	1	0	-4.854001	0.060148	1.314247
21	17	0	-6.849873	-3.302221	-1.293556
22	7	0	-3.847730	-4.478744	-0.806347
23	7	0	-2.187566	-3.444016	0.360390
24	7	0	-3.452724	-1.427131	1.027549
25	7	0	-5.704729	-1.435205	0.178487
26	15	0	-0.858304	1.067581	0.123188
27	8	0	0.545135	1.745394	0.588482
28	6	0	1.337661	2.604511	-0.186195
29	6	0	0.810860	3.744263	-0.792403
30	6	0	2.699134	2.318042	-0.232050
31	6	0	1.683280	4.595790	-1.473342
32	1	0	-0.249916	3.956343	-0.731258
33	6	0	3.560072	3.183594	-0.906996
34	1	0	3.072492	1.432787	0.270538
35	6	0	3.051826	4.322747	-1.533673
36	1	0	1.284356	5.485430	-1.952917
37	1	0	4.621723	2.955860	-0.930160
38	1	0	3.719556	4.997832	-2.061625
39	8	0	-1.502772	1.670659	-1.063886
40	7	0	-1.662074	1.007303	1.593788
41	1	0	-2.345520	0.247471	1.558481
42	6	0	-2.174477	2.219090	2.279401
43	6	0	-2.905904	3.152508	1.297576
44	8	0	-2.504406	4.244502	0.958317
45	8	0	-4.037863	2.582640	0.846932
46	6	0	-4.701879	3.266400	-0.250760
47	1	0	-4.862720	4.311575	0.034796

48	1	0	-4.018769	3.241240	-1.104898
49	6	0	-6.017731	2.553151	-0.559890
50	1	0	-5.773548	1.504498	-0.781969
51	6	0	-6.642833	3.187534	-1.832984
52	1	0	-5.879793	3.775599	-2.361710
53	1	0	-7.418057	3.907406	-1.536779
54	6	0	-6.959407	2.581806	0.661672
55	1	0	-6.398696	2.244829	1.542578
56	1	0	-7.239176	3.626972	0.862999
57	6	0	-7.228591	2.171542	-2.822314
58	1	0	-8.014593	1.562077	-2.364880
59	1	0	-7.660463	2.677287	-3.693837
60	1	0	-6.451355	1.488340	-3.184523
61	6	0	-8.223470	1.725636	0.524526
62	1	0	-8.874586	2.082326	-0.281194
63	1	0	-7.968072	0.679986	0.315770
64	1	0	-8.808960	1.749747	1.451098
65	1	0	-2.924865	1.848509	2.986613
66	6	0	-1.086174	2.963867	3.048285
67	1	0	-0.578979	2.272911	3.727338
68	1	0	-0.349608	3.400102	2.372131
69	1	0	-1.530574	3.776678	3.631220
70	8	0	1.261242	-4.547110	0.648946
71	6	0	2.426498	-2.737421	0.188310
72	6	0	3.611400	-1.847119	0.062184
73	6	0	4.191899	-1.255531	1.205589
74	6	0	4.107213	-1.559696	-1.228563
75	6	0	3.756235	-1.572365	2.532814
76	6	0	5.255969	-0.283123	1.051468
77	6	0	5.166806	-0.590177	-1.399873
78	6	0	3.603139	-2.219047	-2.394871
79	6	0	4.312778	-0.973646	3.630493
80	1	0	2.991234	-2.329333	2.658629
81	6	0	5.799189	0.323962	2.227725
82	6	0	5.688784	0.025912	-0.249690
83	6	0	5.625146	-0.308332	-2.725049
84	1	0	2.853276	-2.993407	-2.273843
85	6	0	4.076990	-1.926017	-3.645217
86	6	0	5.344564	-0.008502	3.474839
87	1	0	3.969488	-1.239749	4.626159
88	1	0	6.585520	1.059380	2.111252
89	6	0	5.095381	-0.949144	-3.812159
90	1	0	6.411100	0.425443	-2.853470
91	1	0	3.681782	-2.447257	-4.512323
92	1	0	5.776551	0.465238	4.351543
93	1	0	5.462717	-0.718417	-4.807826
94	35	0	7.041139	1.371471	-0.473346

7cB'

Stoichiometry C40H39BrClN6O6P
 Framework group C1[X(C40H39BrClN6O6P)]
 Deg. of freedom 276
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	0.598124	-2.280471	0.391770
2	6	0	1.935903	-3.045523	0.361891
3	6	0	2.820450	-2.421422	-0.749043
4	6	0	1.832635	-1.628106	-1.634045
5	6	0	0.630155	-1.236032	-0.755541
6	1	0	0.392622	-1.767490	1.333349
7	1	0	2.460527	-3.099339	1.320013
8	1	0	3.301148	-3.229837	-1.303626
9	1	0	2.283086	-0.758171	-2.117858
10	1	0	1.475247	-2.296436	-2.425014
11	1	0	-0.294134	-1.224343	-1.335970
12	7	0	0.195180	-4.545061	-0.090308
13	8	0	0.826375	0.082641	-0.179891
14	6	0	5.243081	-2.062810	-0.181107
15	6	0	3.937220	-0.398967	0.420507
16	6	0	5.960246	-1.035468	0.471393
17	1	0	3.026586	0.174705	0.519425
18	6	0	7.330358	-1.280469	0.593391
19	6	0	7.064173	-3.287202	-0.476847
20	1	0	7.548794	-4.186049	-0.847860
21	17	0	8.377555	-0.117962	1.372875
22	7	0	5.118108	-0.007328	0.836659
23	7	0	3.931843	-1.633801	-0.209029
24	7	0	5.745805	-3.195352	-0.667502
25	7	0	7.871278	-2.392240	0.125388
26	15	0	-0.181971	1.294312	-0.596086
27	8	0	0.770473	2.558460	-0.244990
28	6	0	2.020954	2.794191	-0.830513
29	6	0	2.214519	2.682222	-2.207594
30	6	0	3.043749	3.199080	0.023934
31	6	0	3.480192	2.964218	-2.727071
32	1	0	1.389806	2.389735	-2.848894
33	6	0	4.300828	3.478522	-0.513107
34	1	0	2.842804	3.292287	1.086556
35	6	0	4.522936	3.358998	-1.886706
36	1	0	3.645155	2.879521	-3.797766
37	1	0	5.107674	3.780249	0.147727
38	1	0	5.504211	3.573495	-2.299697
39	8	0	-0.736214	1.176099	-1.964530
40	7	0	-1.368766	1.395103	0.569317
41	1	0	-2.239641	1.687290	0.137427
42	6	0	-1.197296	1.923932	1.935606
43	6	0	-0.849841	3.425069	1.959887
44	8	0	-0.046806	3.934480	2.709551
45	8	0	-1.599799	4.102849	1.072267
46	6	0	-1.343023	5.525561	0.970900
47	1	0	-1.508185	5.982931	1.953418
48	1	0	-0.288867	5.660731	0.710030
49	6	0	-2.263954	6.119505	-0.094460
50	1	0	-2.063450	5.575452	-1.029449
51	6	0	-1.890834	7.612787	-0.304398
52	1	0	-0.901604	7.809685	0.131901
53	1	0	-2.591594	8.244354	0.258210
54	6	0	-3.744917	5.905432	0.280101
55	1	0	-3.899368	4.839555	0.485583
56	1	0	-3.945580	6.432302	1.225251
57	6	0	-1.857605	8.054662	-1.772977
58	1	0	-2.824145	7.908158	-2.266143

59	1	0	-1.596656	9.115851	-1.857648
60	1	0	-1.110308	7.482454	-2.335725
61	6	0	-4.756626	6.358977	-0.777766
62	1	0	-4.713526	7.439720	-0.951923
63	1	0	-4.580921	5.858037	-1.737624
64	1	0	-5.778447	6.119807	-0.461888
65	1	0	-2.189169	1.840170	2.398765
66	6	0	-0.211688	1.112739	2.772980
67	1	0	-0.539166	0.070212	2.818142
68	1	0	0.798128	1.156206	2.357634
69	1	0	-0.169424	1.520447	3.785464
70	8	0	1.582056	-4.404385	-0.020148
71	6	0	-0.379457	-3.421989	0.146296
72	6	0	-1.855564	-3.253657	0.104341
73	6	0	-2.548857	-3.325487	-1.125122
74	6	0	-2.542043	-2.943583	1.298596
75	6	0	-1.896394	-3.685555	-2.348529
76	6	0	-3.964347	-3.016498	-1.173332
77	6	0	-3.951918	-2.622518	1.265564
78	6	0	-1.884548	-2.961828	2.570578
79	6	0	-2.577252	-3.737037	-3.534545
80	1	0	-0.847345	-3.953309	-2.316783
81	6	0	-4.632436	-3.082958	-2.436732
82	6	0	-4.609108	-2.659043	0.023352
83	6	0	-4.602453	-2.291442	2.496148
84	1	0	-0.847017	-3.275610	2.615781
85	6	0	-2.547775	-2.646548	3.726675
86	6	0	-3.963672	-3.429541	-3.579013
87	1	0	-2.058227	-4.020792	-4.445596
88	1	0	-5.689982	-2.853155	-2.474171
89	6	0	-3.924170	-2.294756	3.685334
90	1	0	-5.656516	-2.043655	2.472362
91	1	0	-2.027213	-2.681719	4.679511
92	1	0	-4.495891	-3.473427	-4.524835
93	1	0	-4.444311	-2.044395	4.605482
94	35	0	-6.475007	-2.202493	-0.038162
