

Supplemental Information

**Synthetic routes to trifluoromethylphenyl diazirine photolabeling reagents containing an alkyne
substituent (TPDYNE) for chemical biology applications**

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Taylor Family Institute for Innovative Psychiatric Research

Washington University in St. Louis

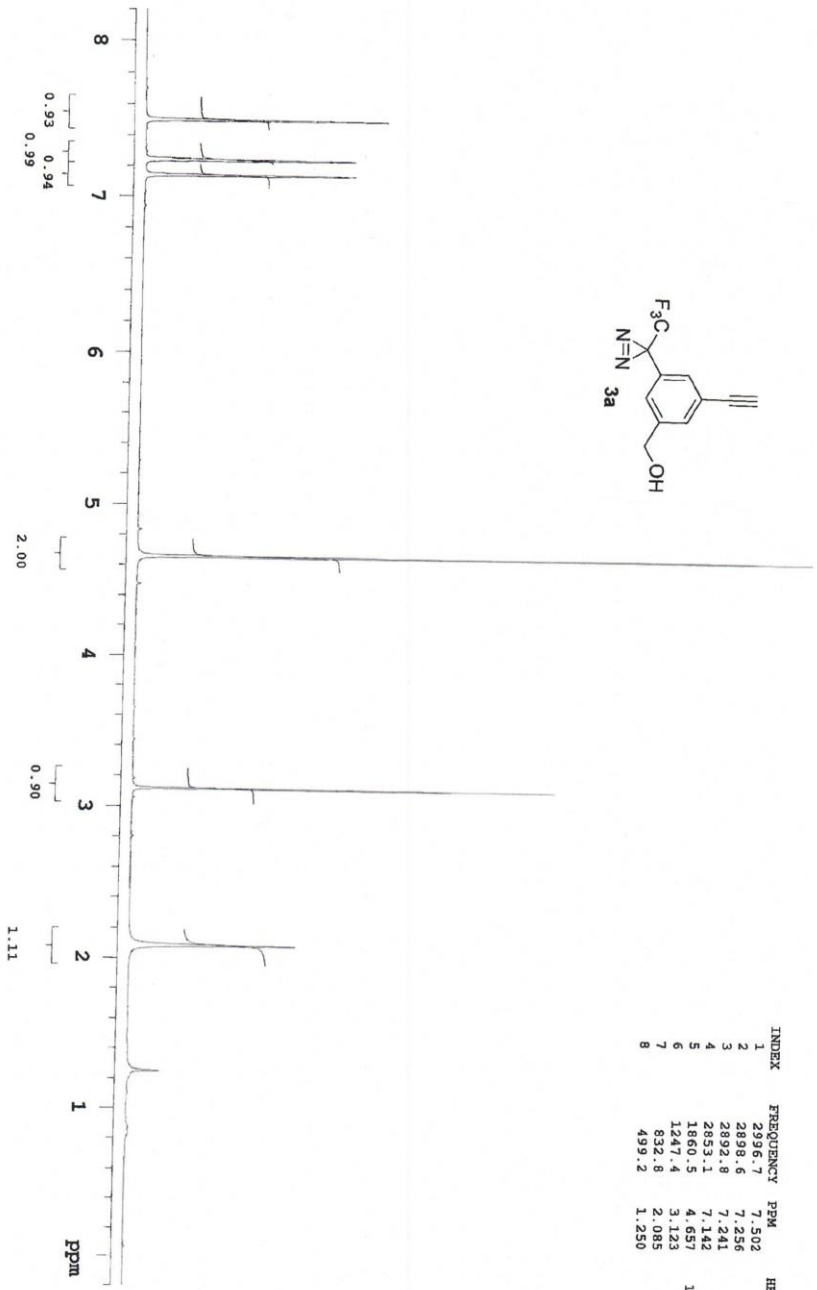
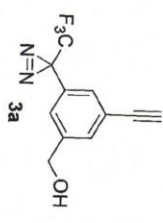
660 S. Euclid Ave.

St. Louis, MO 63110

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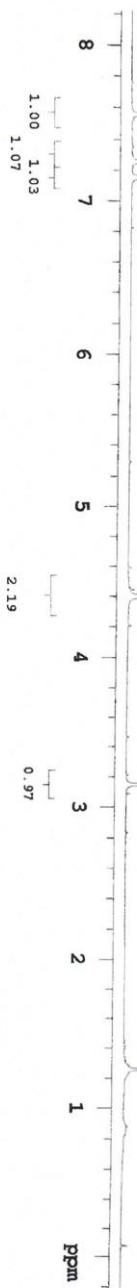
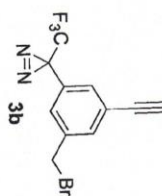
12055



mq12088



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FIDFile: PROTON_01
Pulse Sequence: PROTON (a2pu1)
Solvent: cdcl3
Data collected on: Jan 5 2022



mg12068

Sample Name:

mg12078

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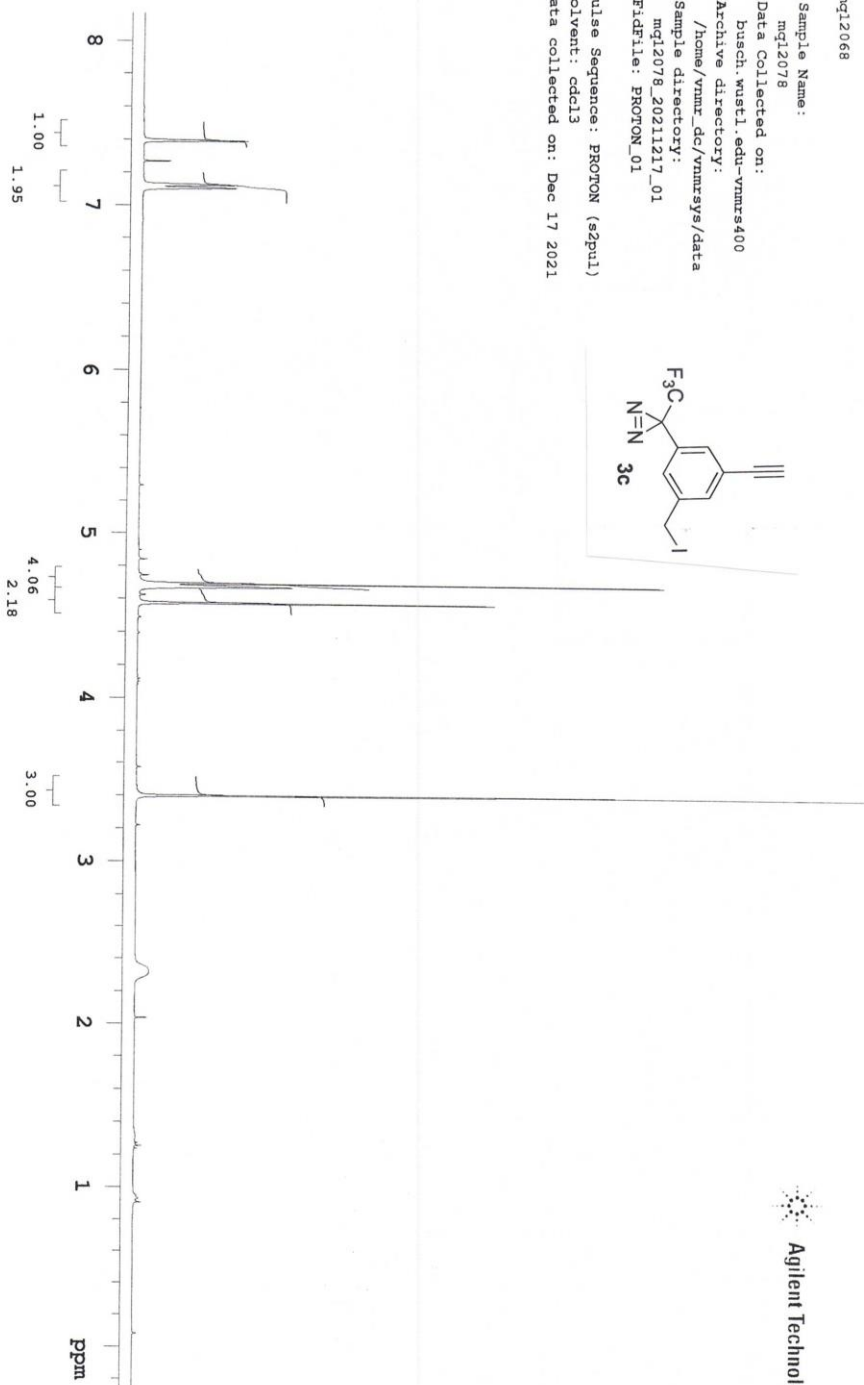
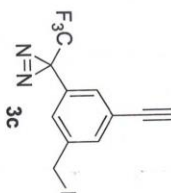
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Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 17 2021

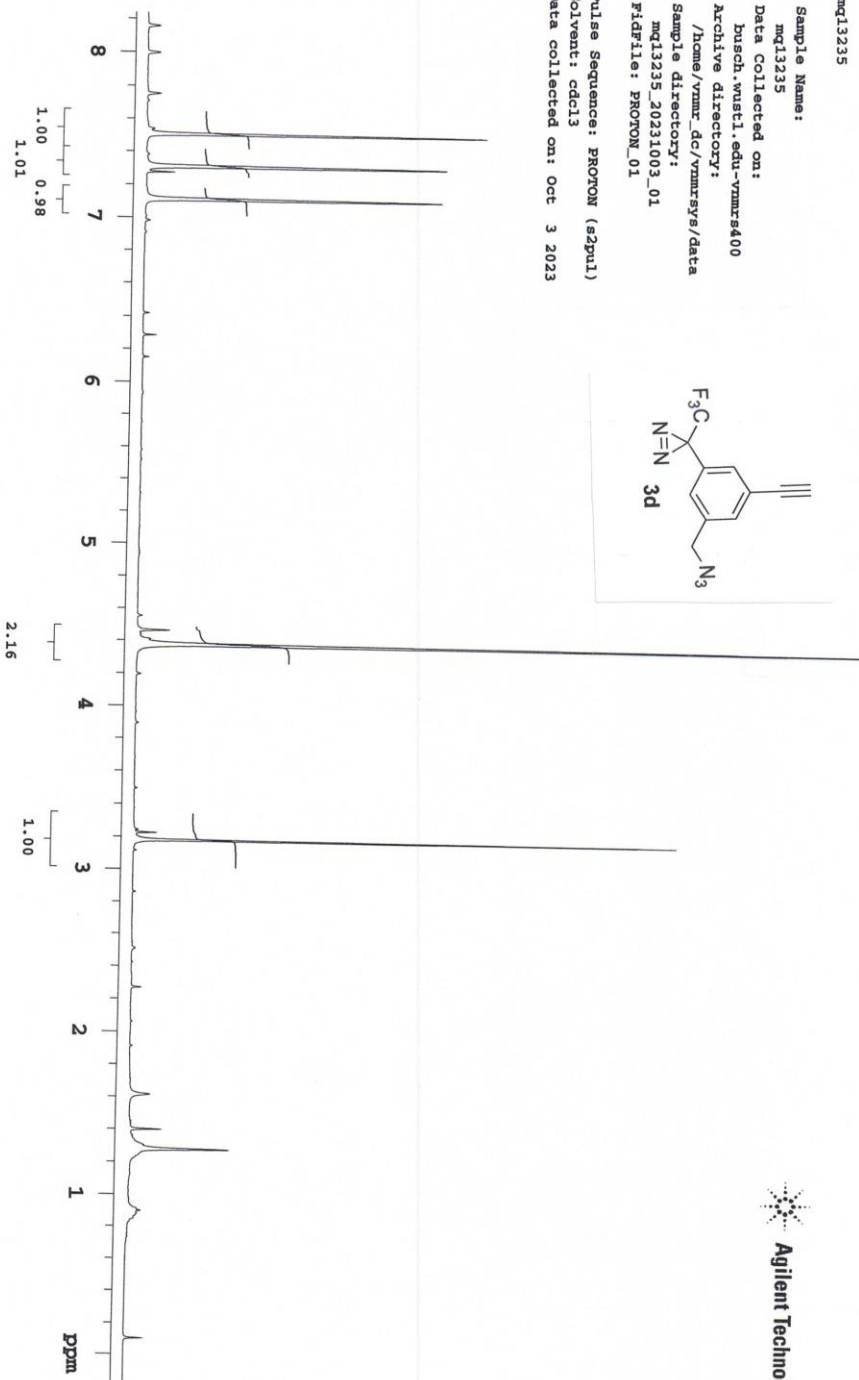
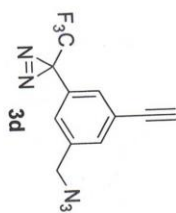


Agilent Technologies

mq13235

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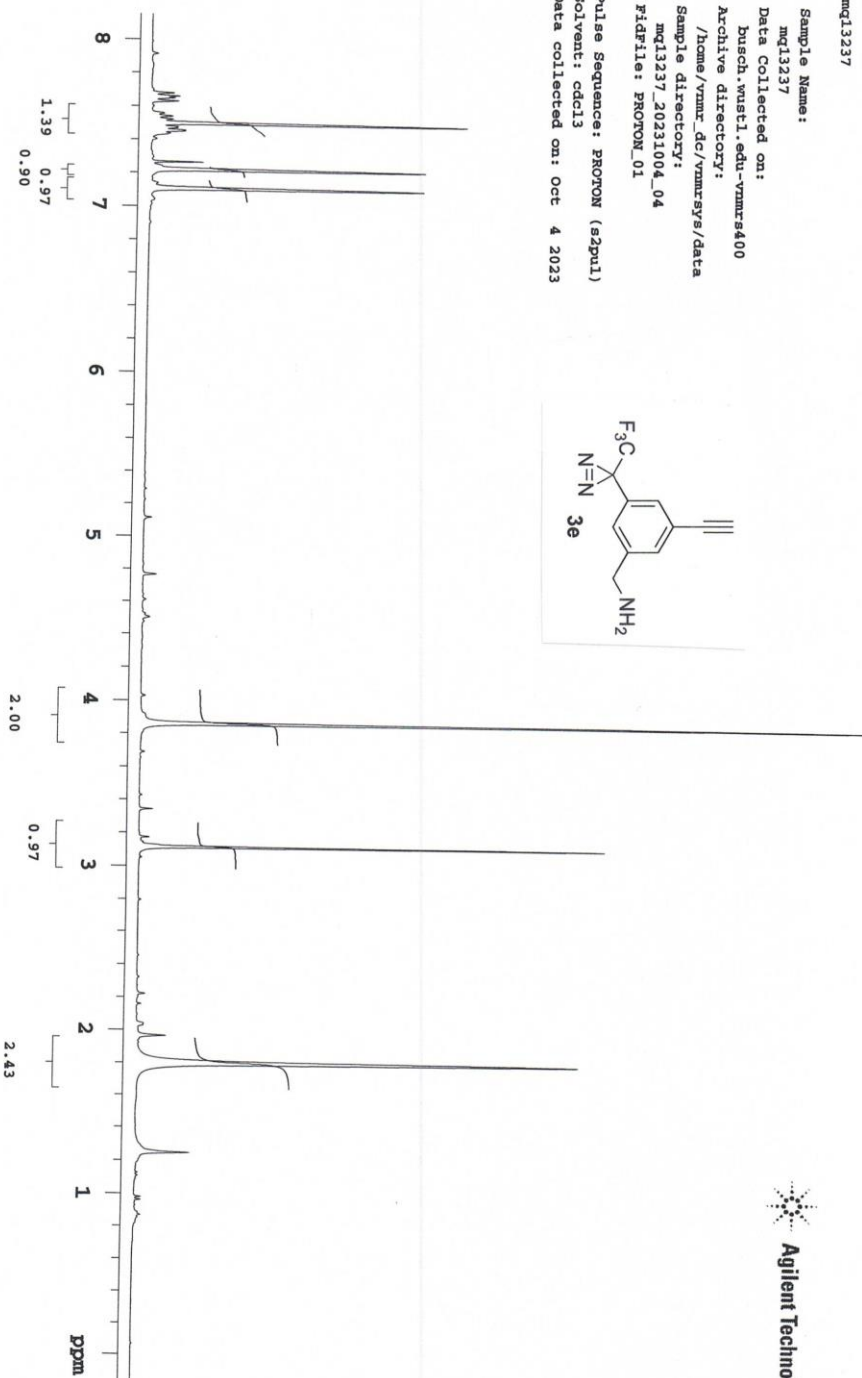
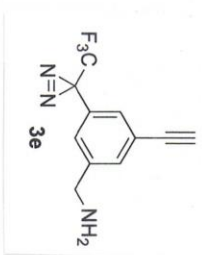
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Solvent: cdcl3
Data collected on: Oct 3 2023



Agilent Technologies

mg13237

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Archive directory:
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mg13237_20231004_04
FIDFile: PROTON_01
Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Oct 4 2023



Agilent Technologies

mq12018

Sample Name:

mq12018

Data Collected on:

busch.wustl.edu-ymrs400

Archive directory:

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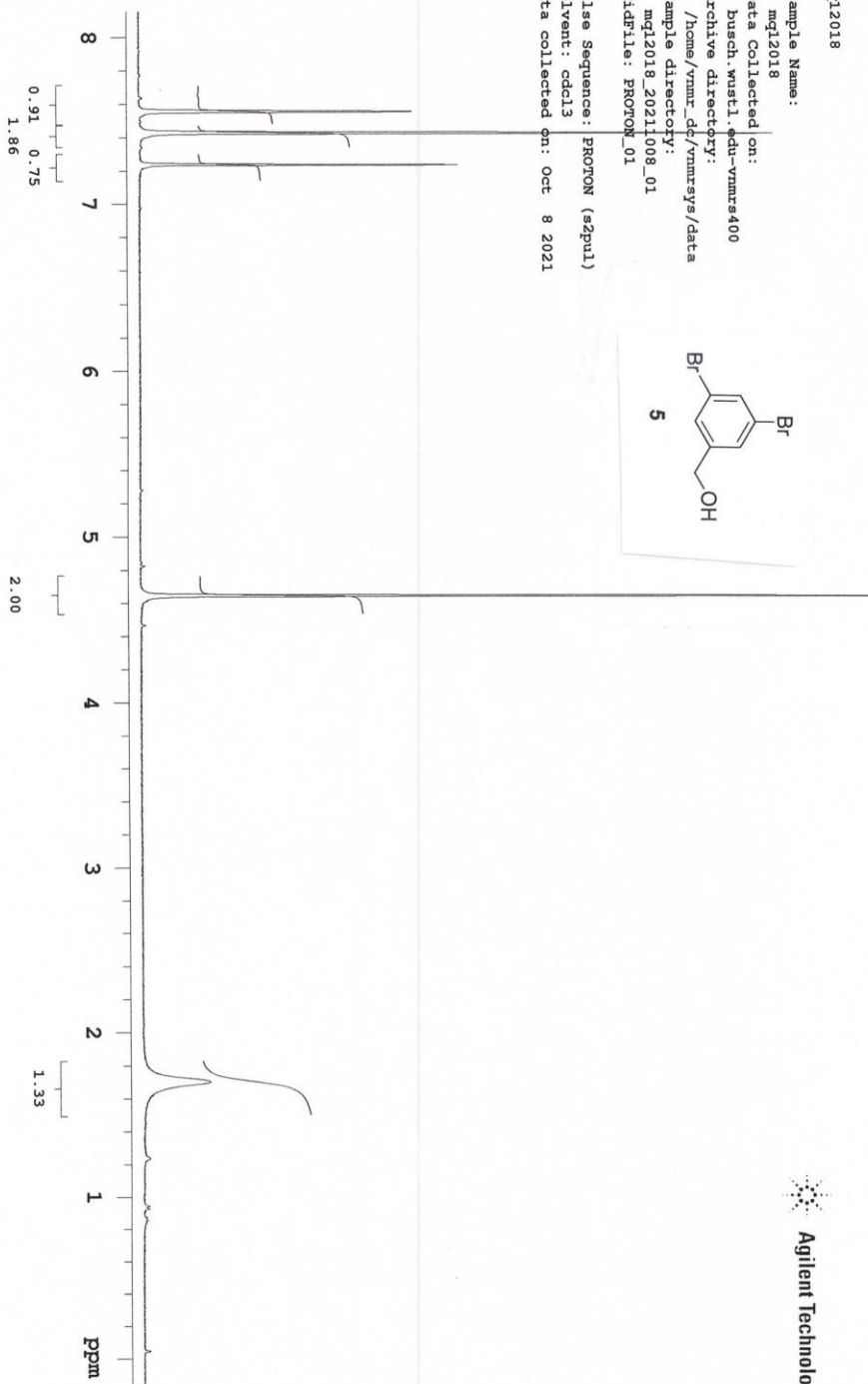
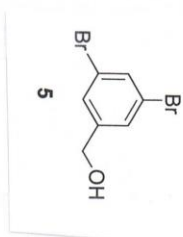
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Solvent: cdcl3

Data collected on: Oct 8 2021



 Agilent Technologies

mq12020

Sample Name:

mq12020

Data Collected on:

busch.wustl.edu-ymms400

Archive directory:

/home/ymr_dc/ymmsys/data

Sample directory:

mq12020_20211011_01

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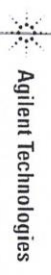
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Solvent: cdcl3

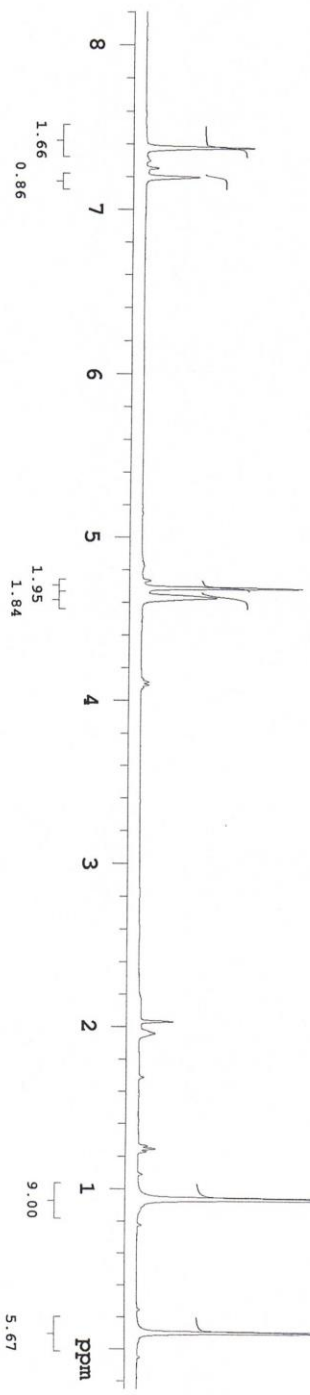
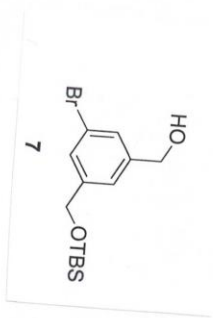
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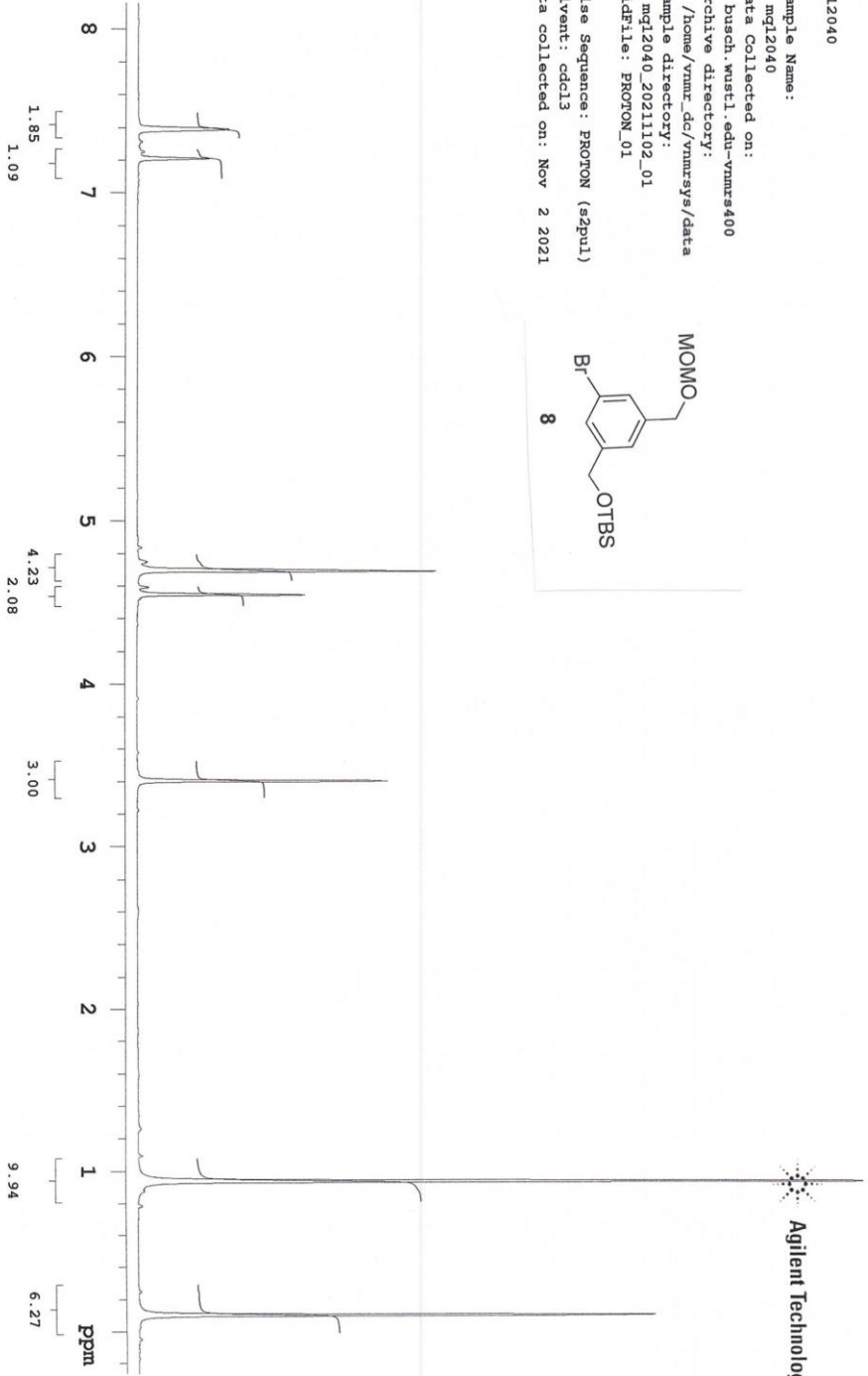
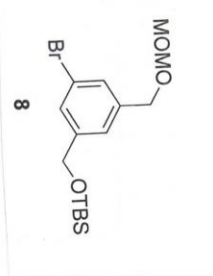


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Solvent: cdcl3
Data collected on: Nov 1 2021



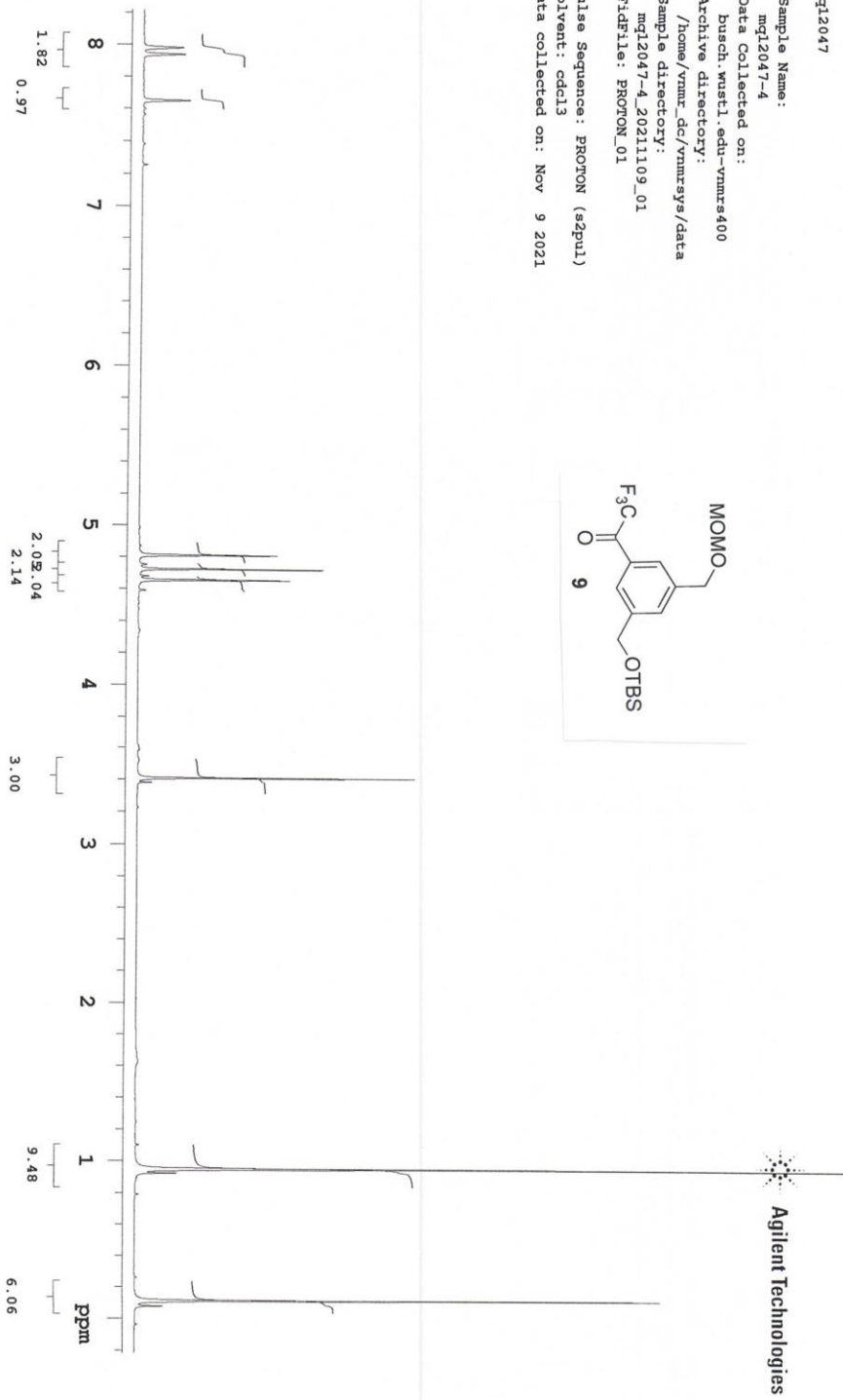
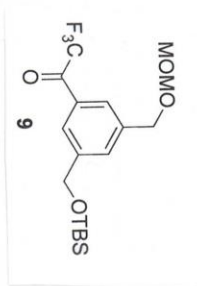
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Solvent: cdcl3
Data collected on: Nov 2 2021



mq12047

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Archive directory:
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Sample directory:
mq12047-4_2021109_01
FidFile: PROTON_01
Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Nov 9 2021



mq12048

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mq12048

Data Collected on:

busch.wustl.edu~vnmr400

Archive directory:

/home/vnmr_dc/vnmrsys/data

Sample directory:

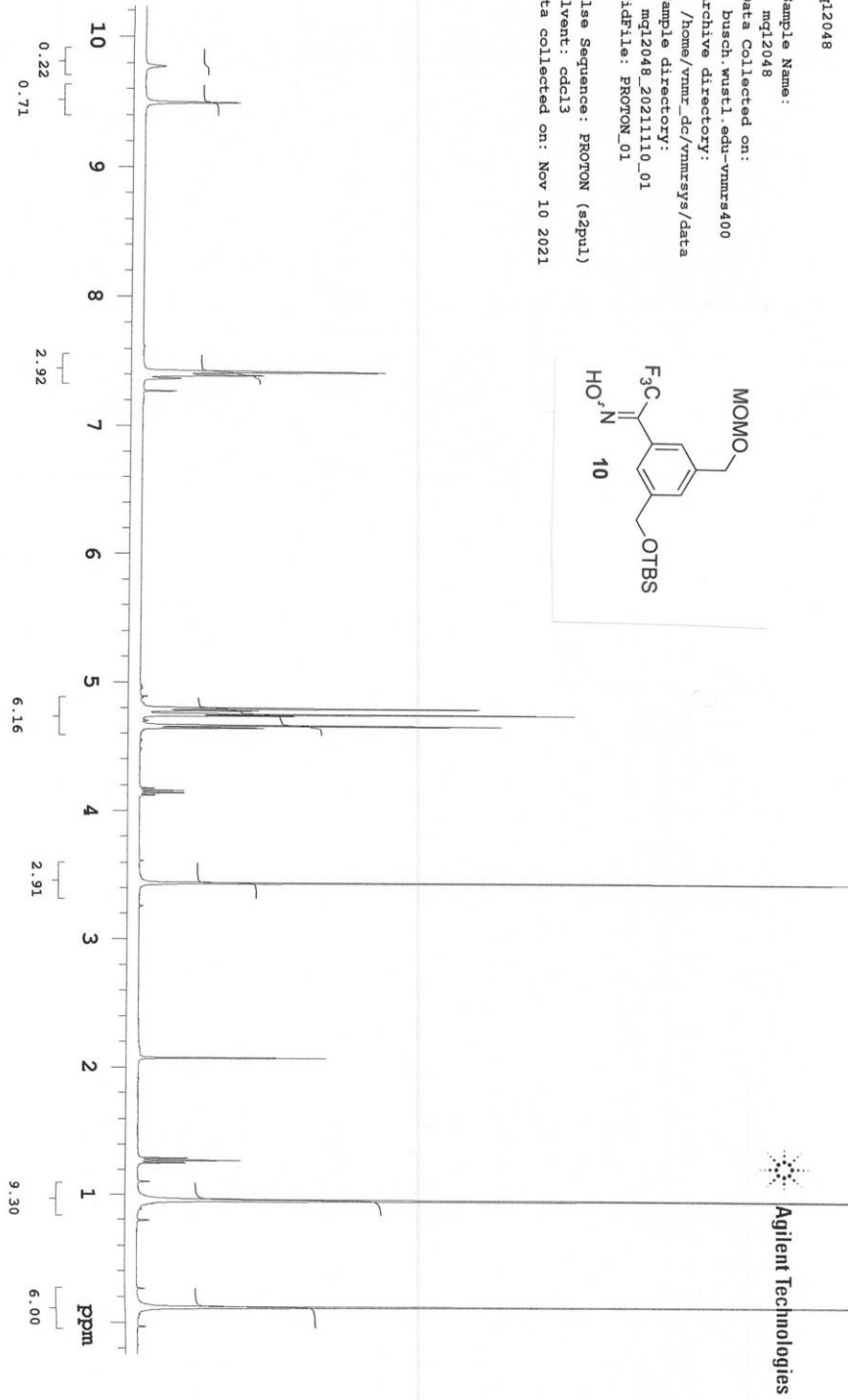
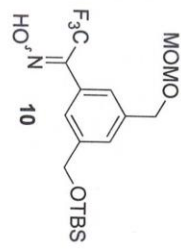
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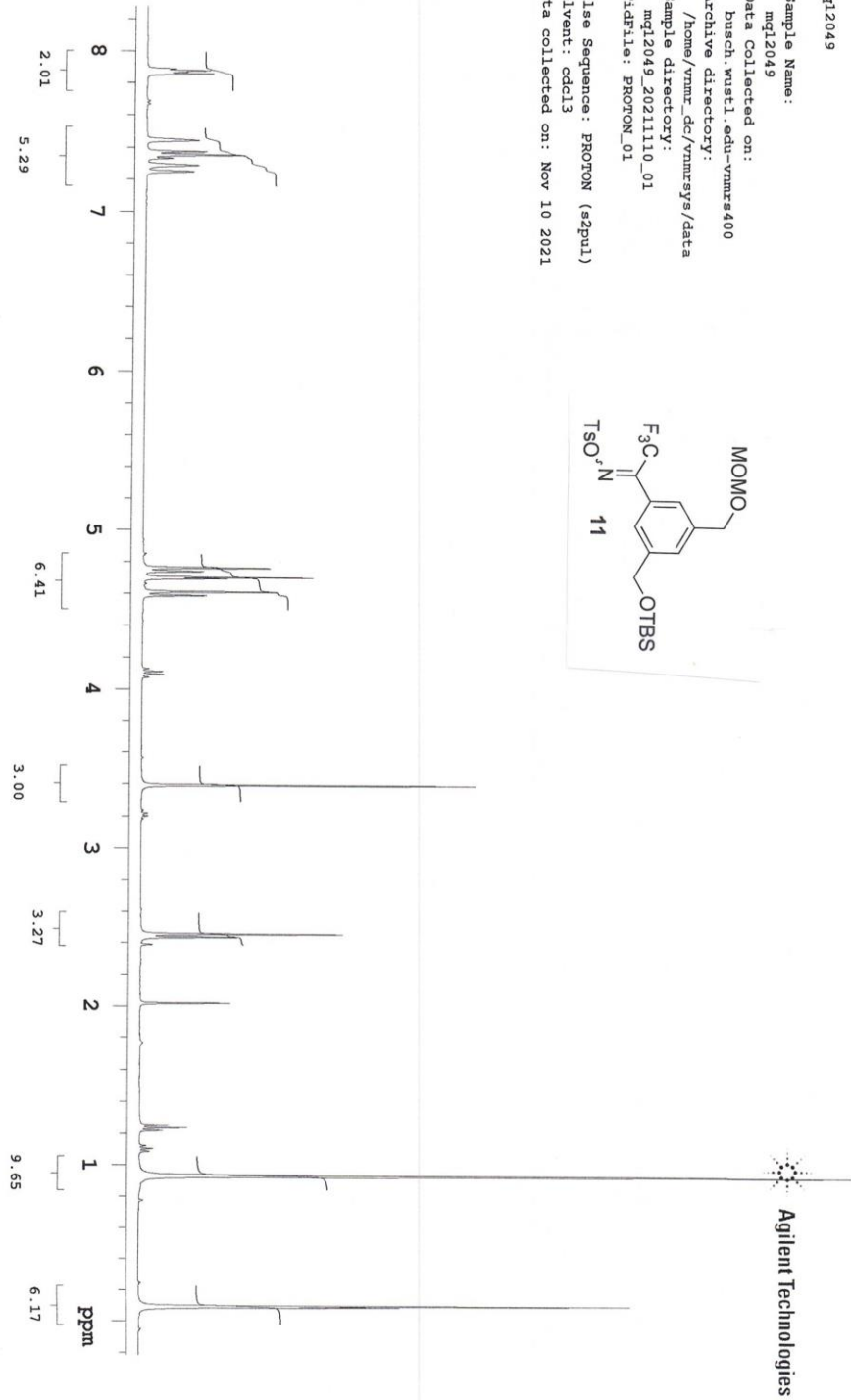
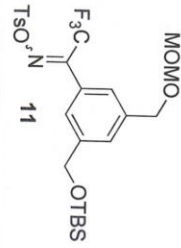
Solvent: cdcl3

Data collected on: Nov 10 2021



mq12049

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mq12049_2021110_01
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Solvent: cdcl3
Data collected on: Nov 10 2021



mq12050

Sample Name:

mq12050

Data Collected on:

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Archive directory:

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Sample directory:

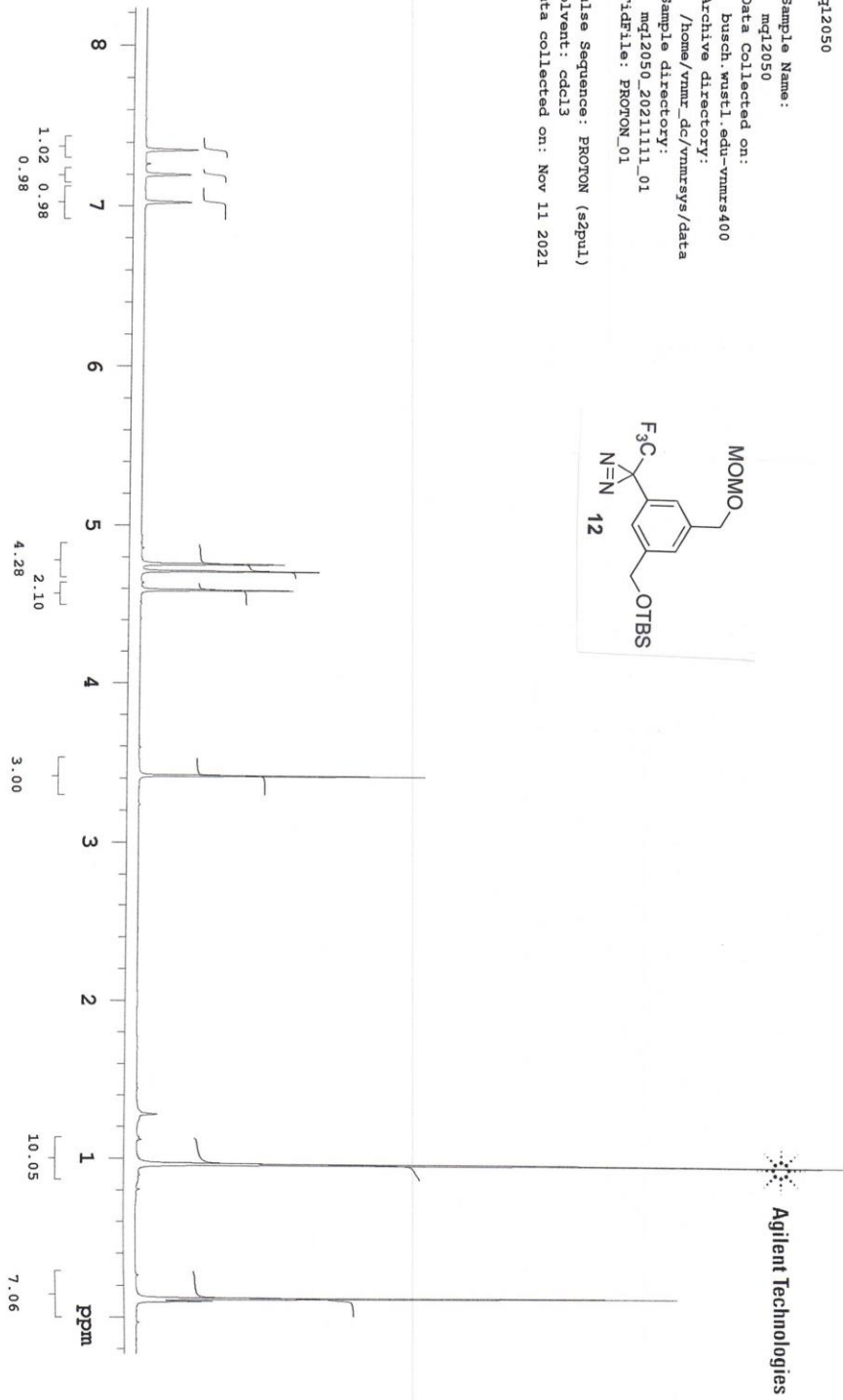
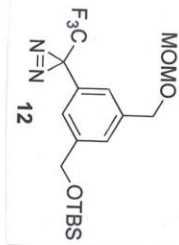
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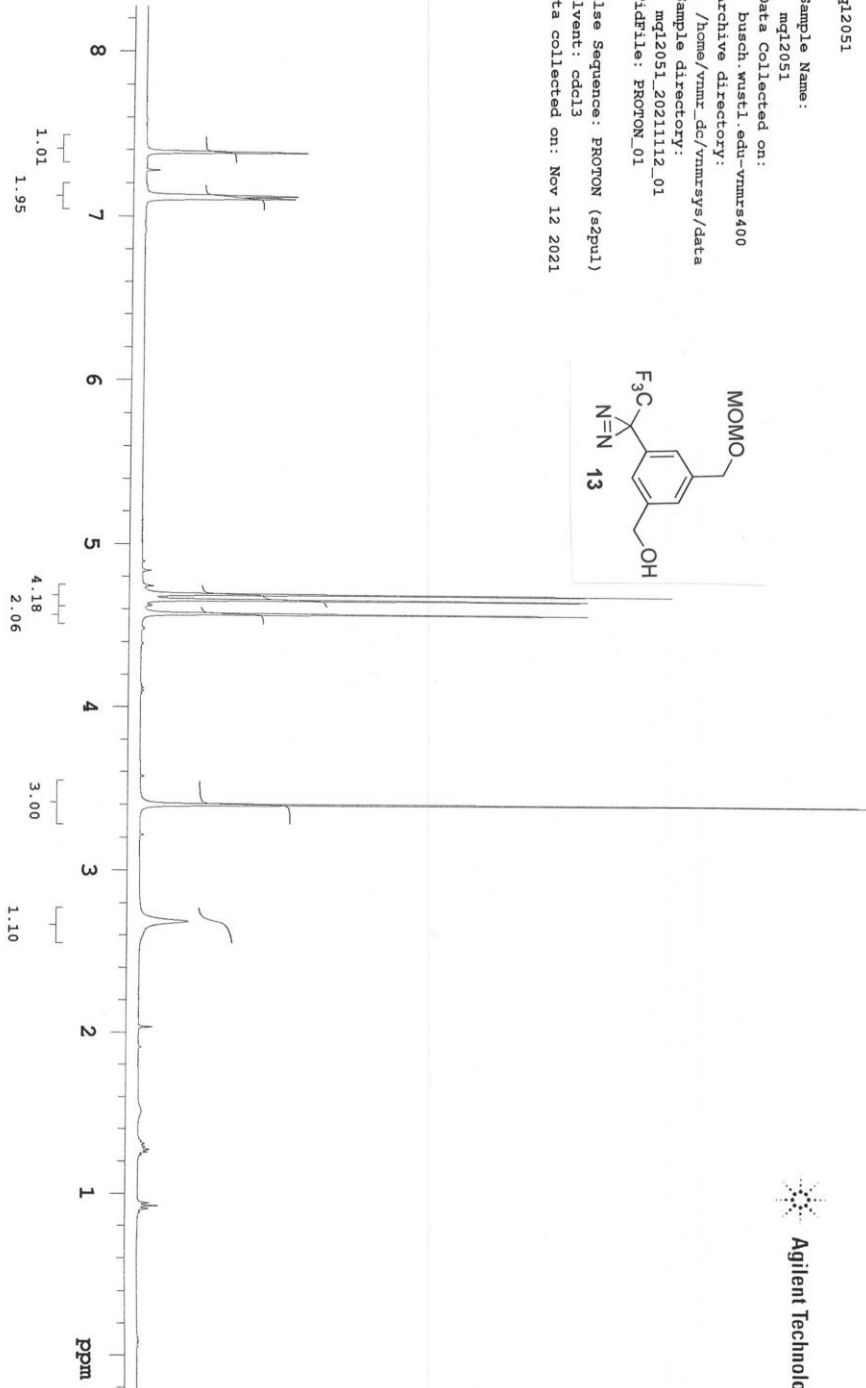
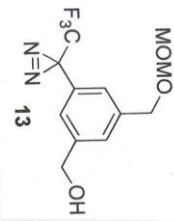
Solvent: cdcl3

Data collected on: Nov 11 2021



mq12051

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Sample directory:
mq12051_2021112_01
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Pulse Sequence: PROTON (szpul)
Solvent: cdcl3
Data collected on: Nov 12 2021



mg12053

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Data Collected on:

busch.wustl.edu~vnmrs400

Archive directory:

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Sample directory:

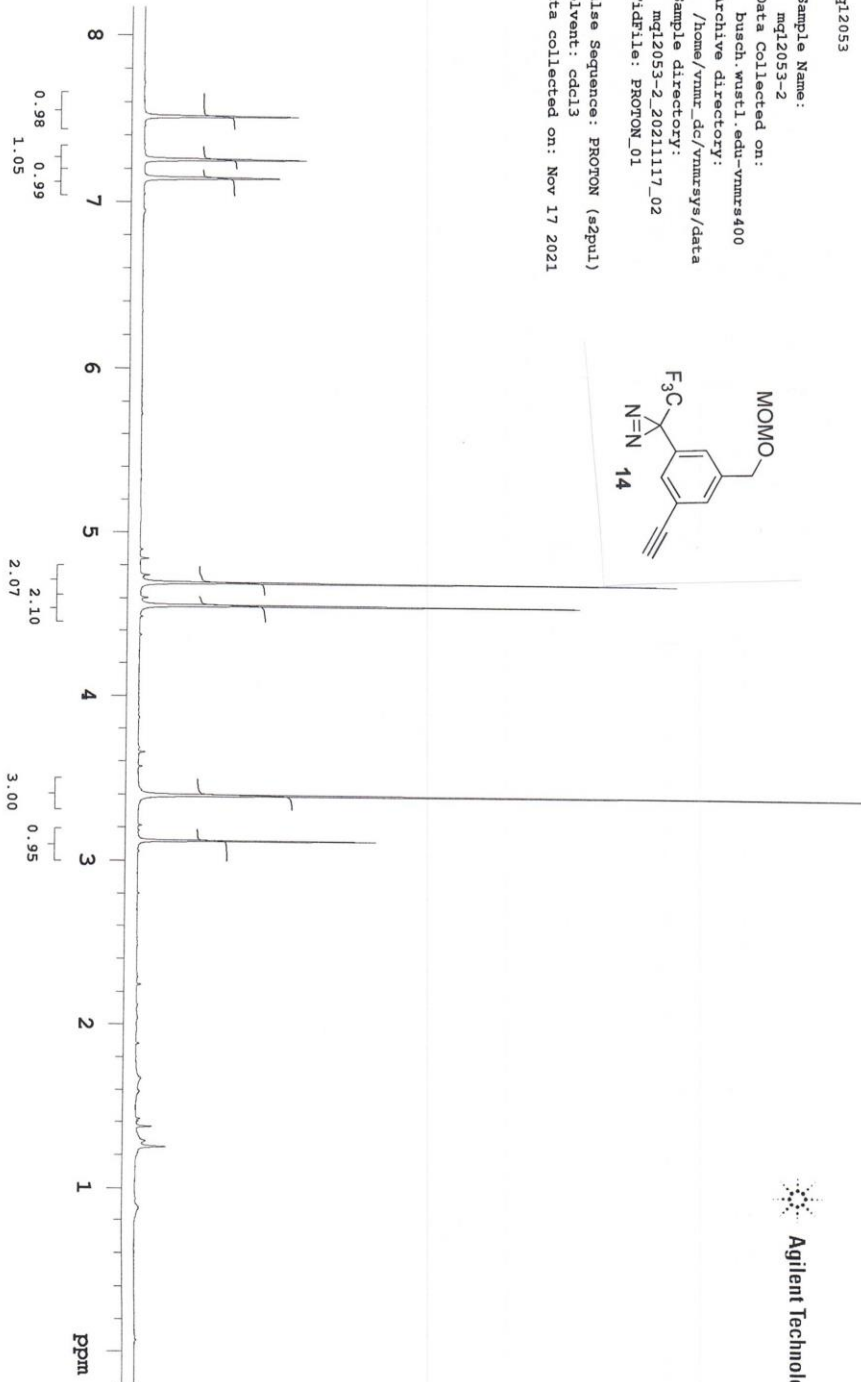
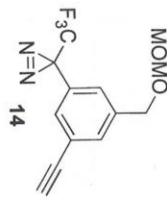
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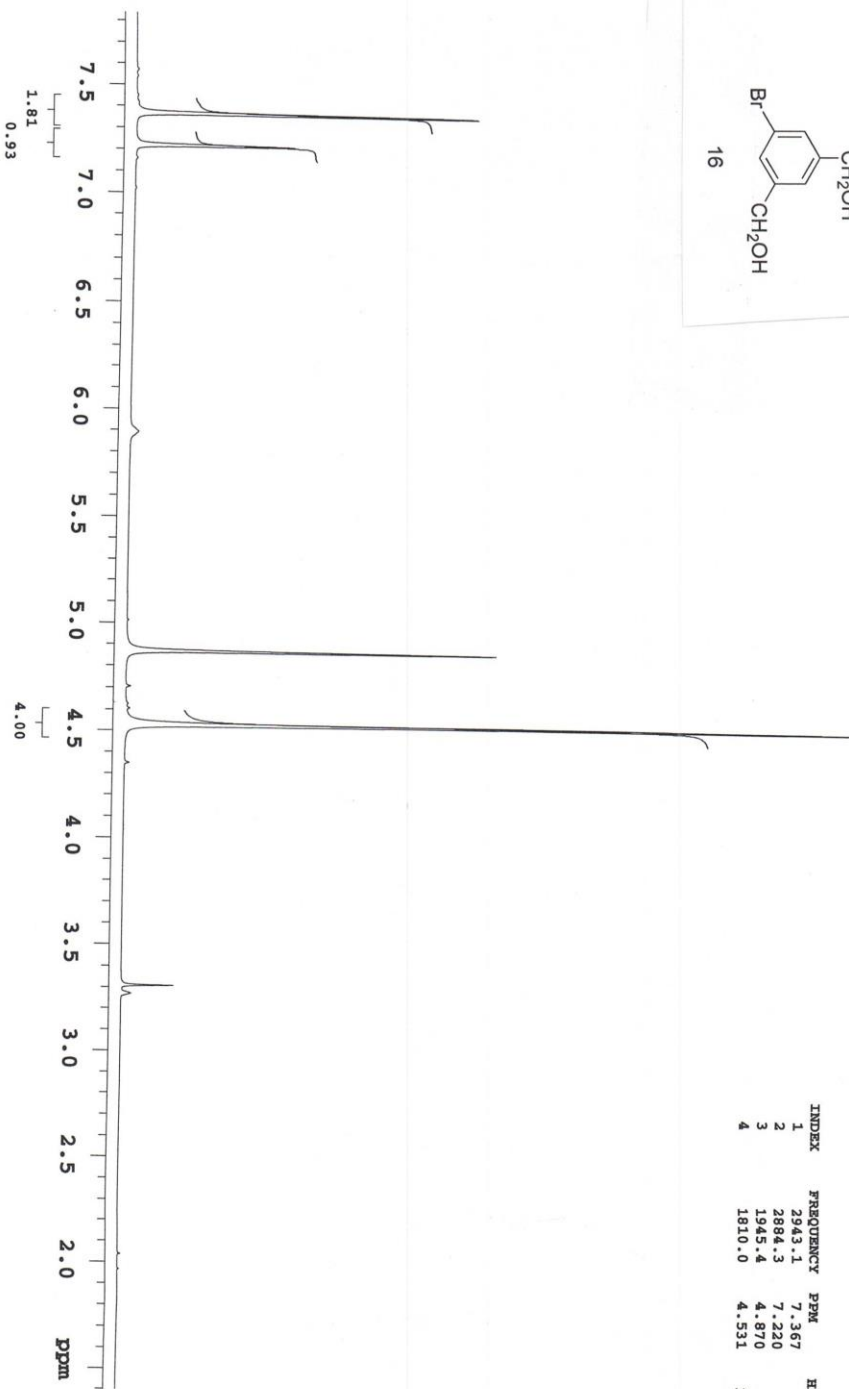
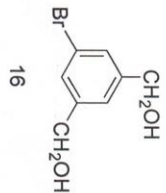
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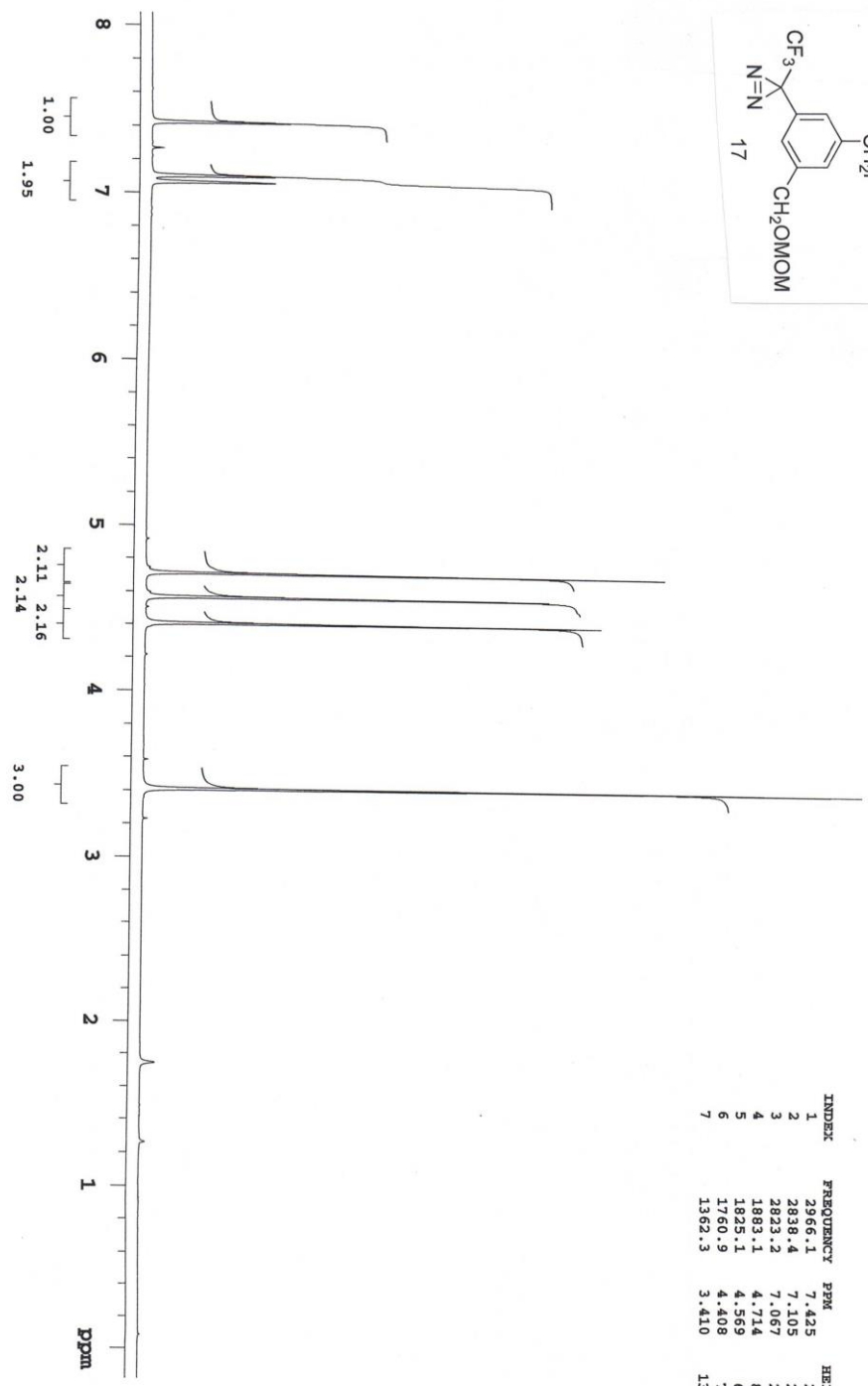
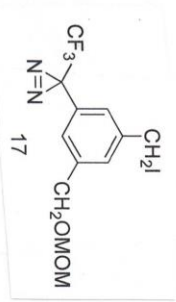
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Solvent: cdcl3

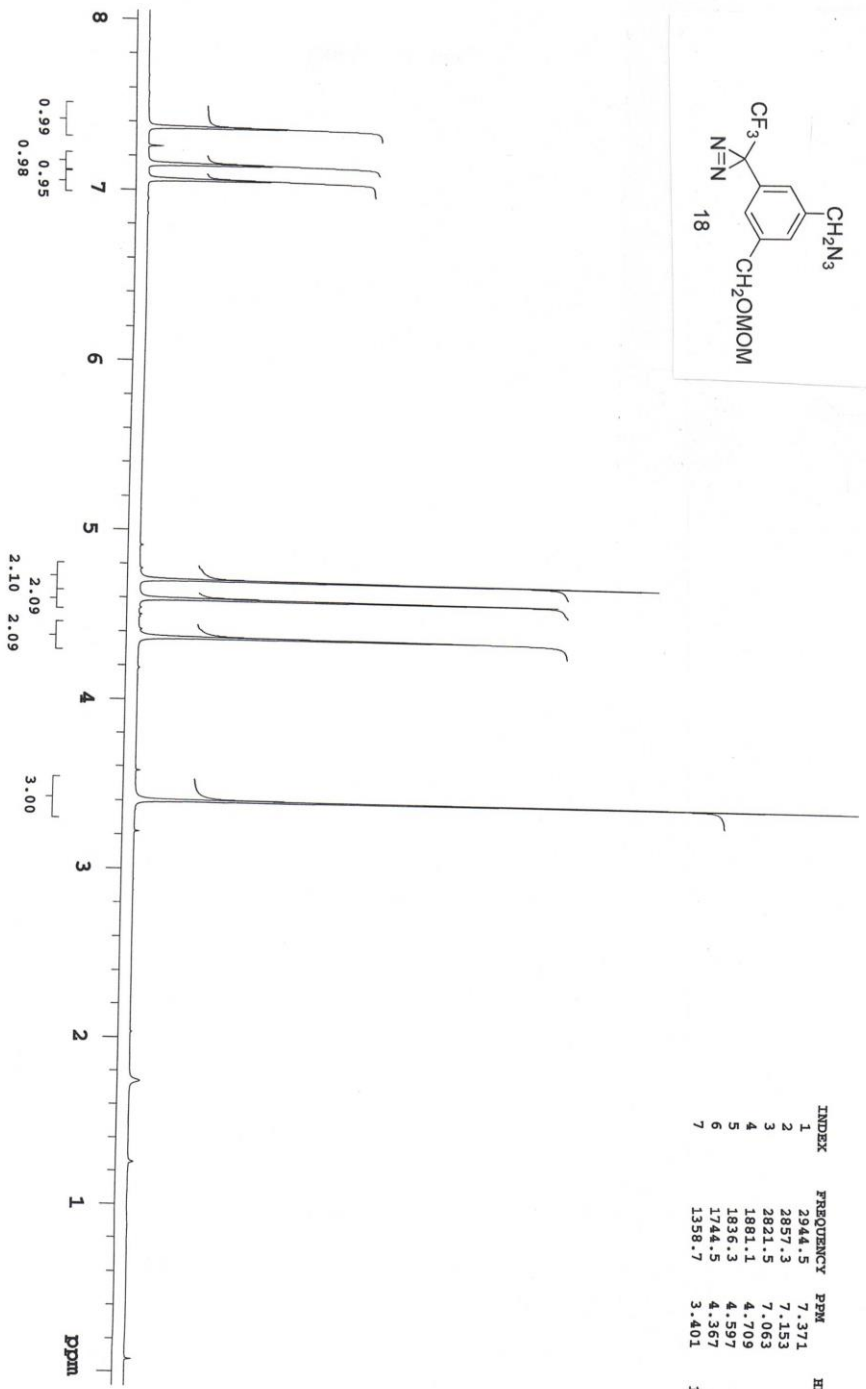
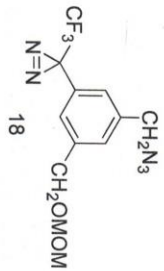
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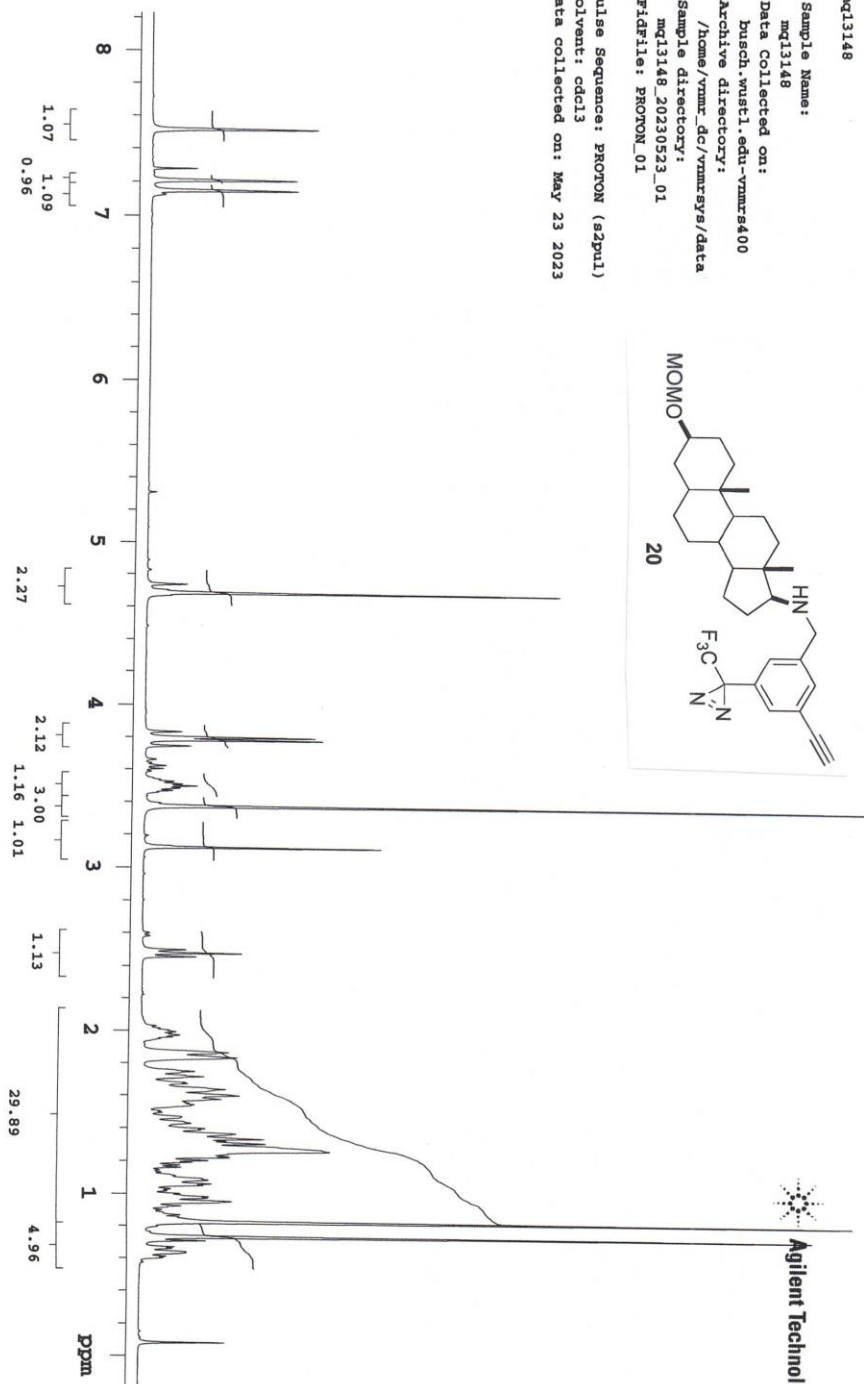
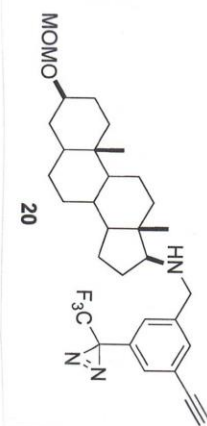
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2	2838.4	7.105	21.2
3	2823.2	7.067	21.2
4	1883.1	4.714	88.8
5	1825.1	4.569	89.0
6	1760.9	4.408	78.0
7	1362.3	3.410	132.3



mq13148

Sample Name:
mq13148
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Sample directory:
mq13148_20230523_01
FIDFile: PROTON_01

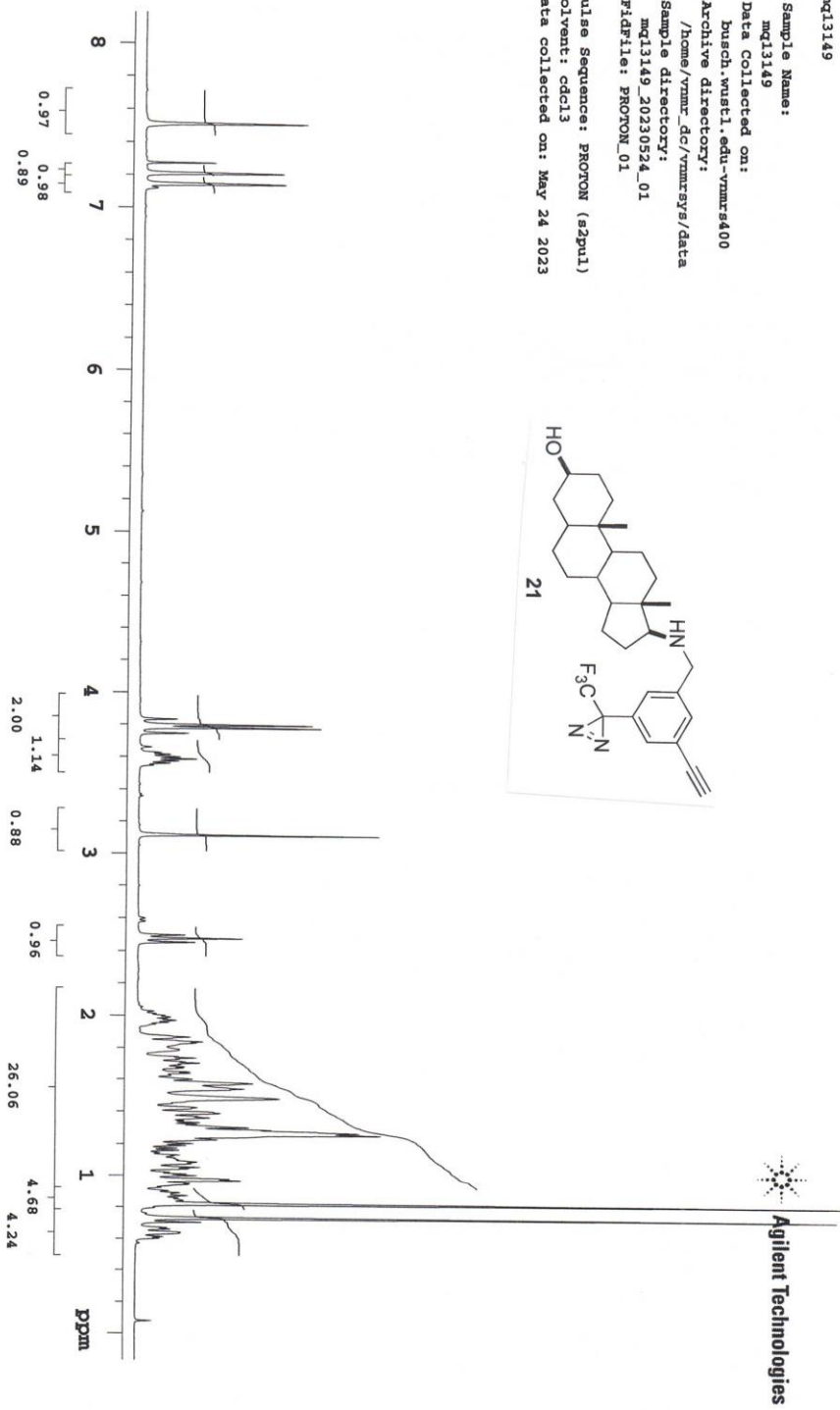
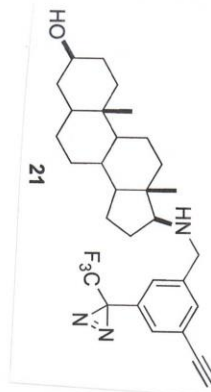
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Solvent: cdcl3
Data collected on: May 23 2023



Agilent Technologies

mq13149

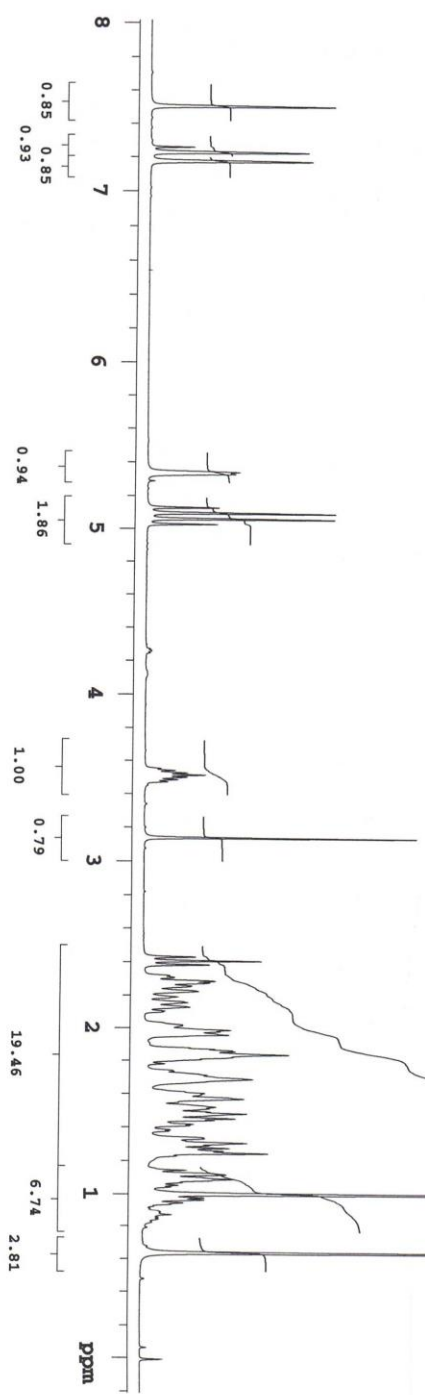
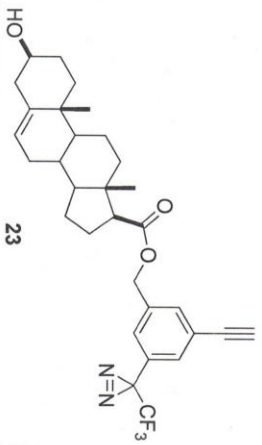
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Solvent: cdcl3
Data collected on: May 24 2023



mq13108

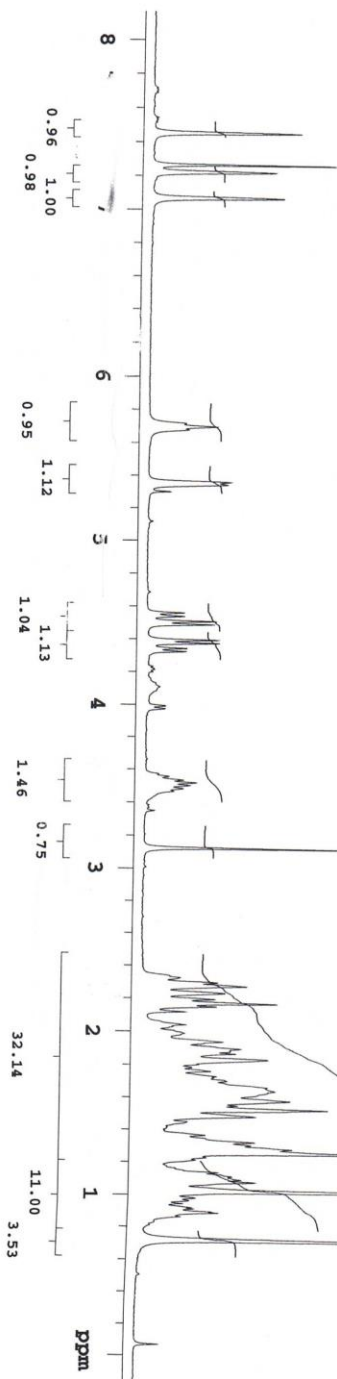
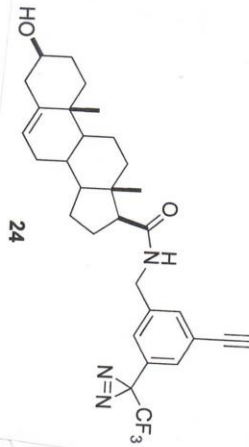
Agilent Technologies

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Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 24 2023

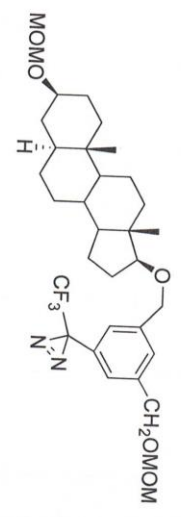


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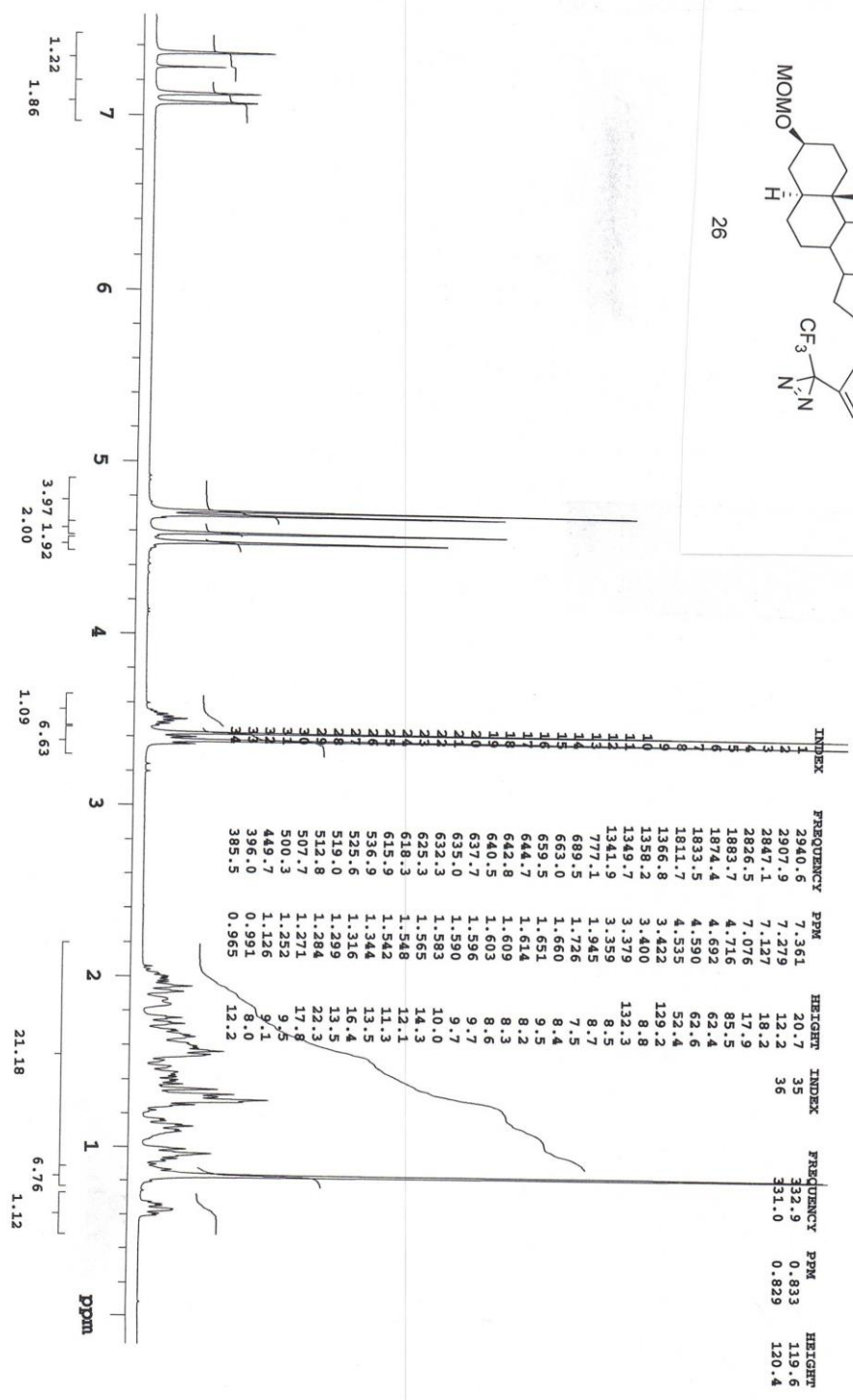
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Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Jun 2 2023

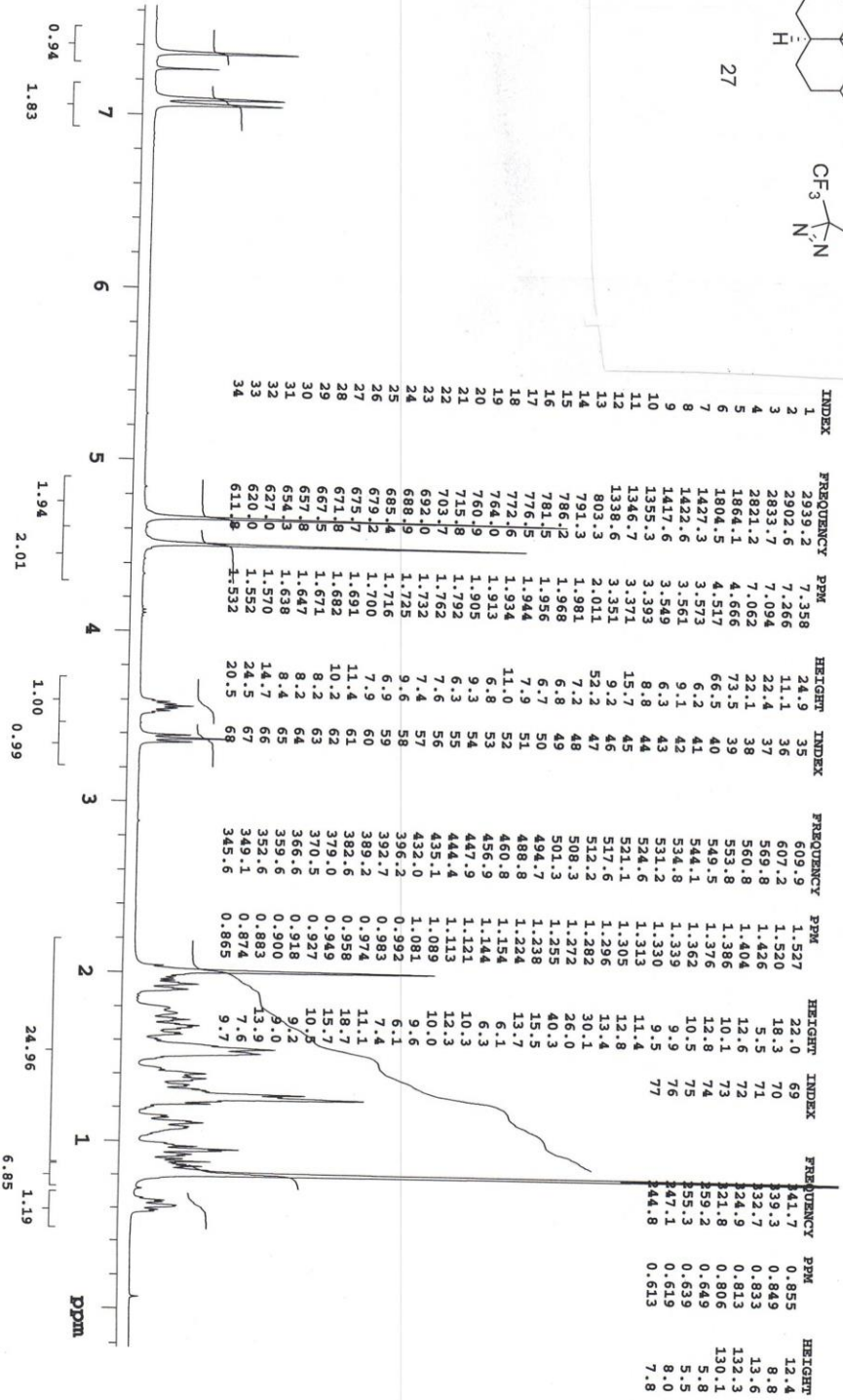
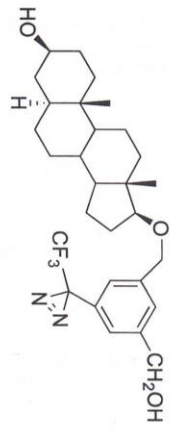


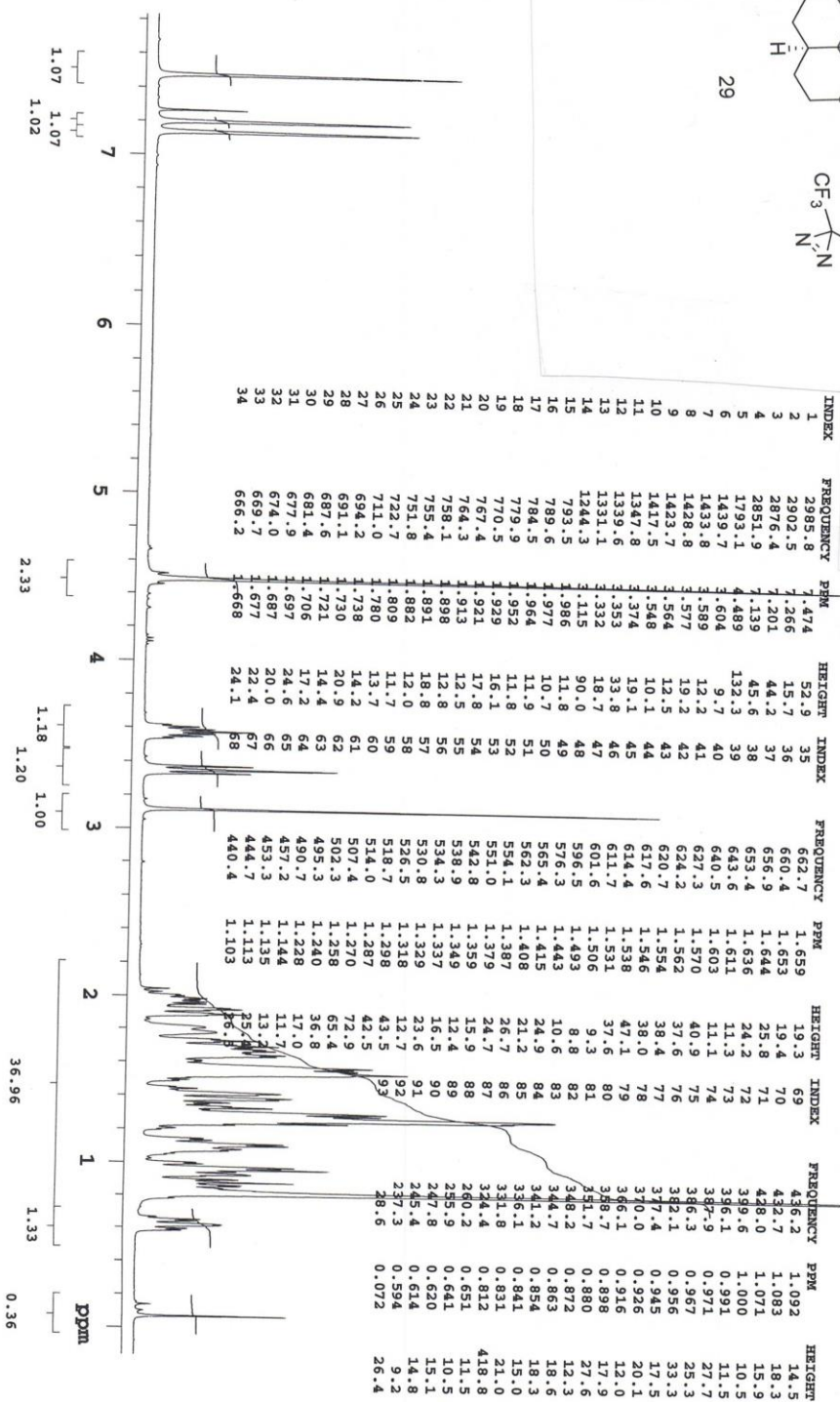
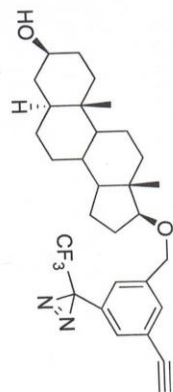
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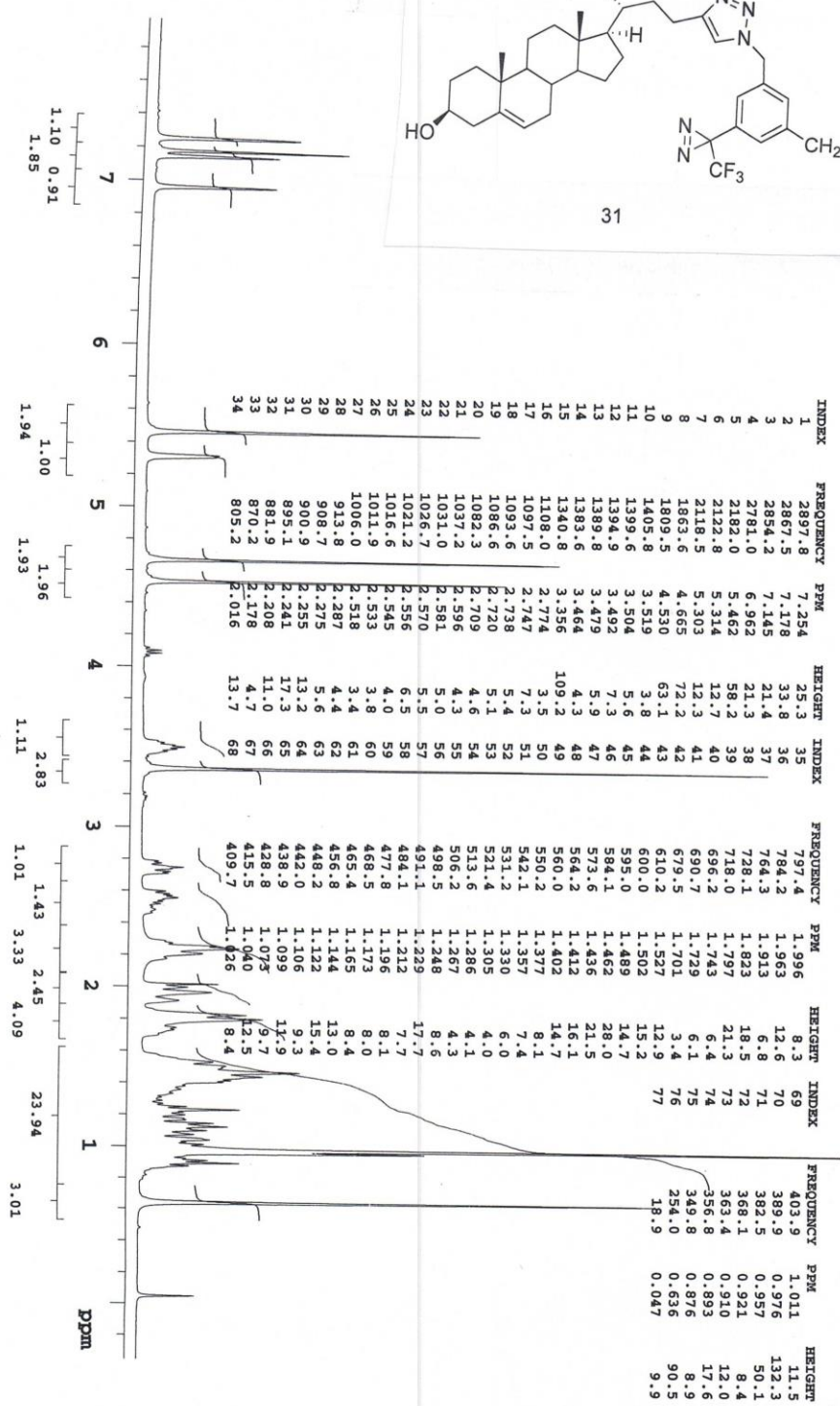
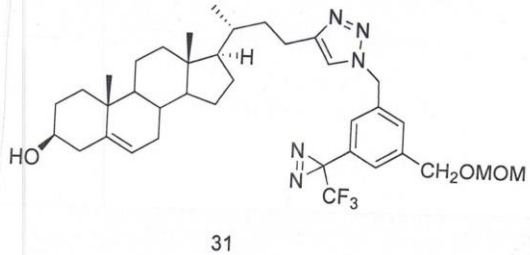


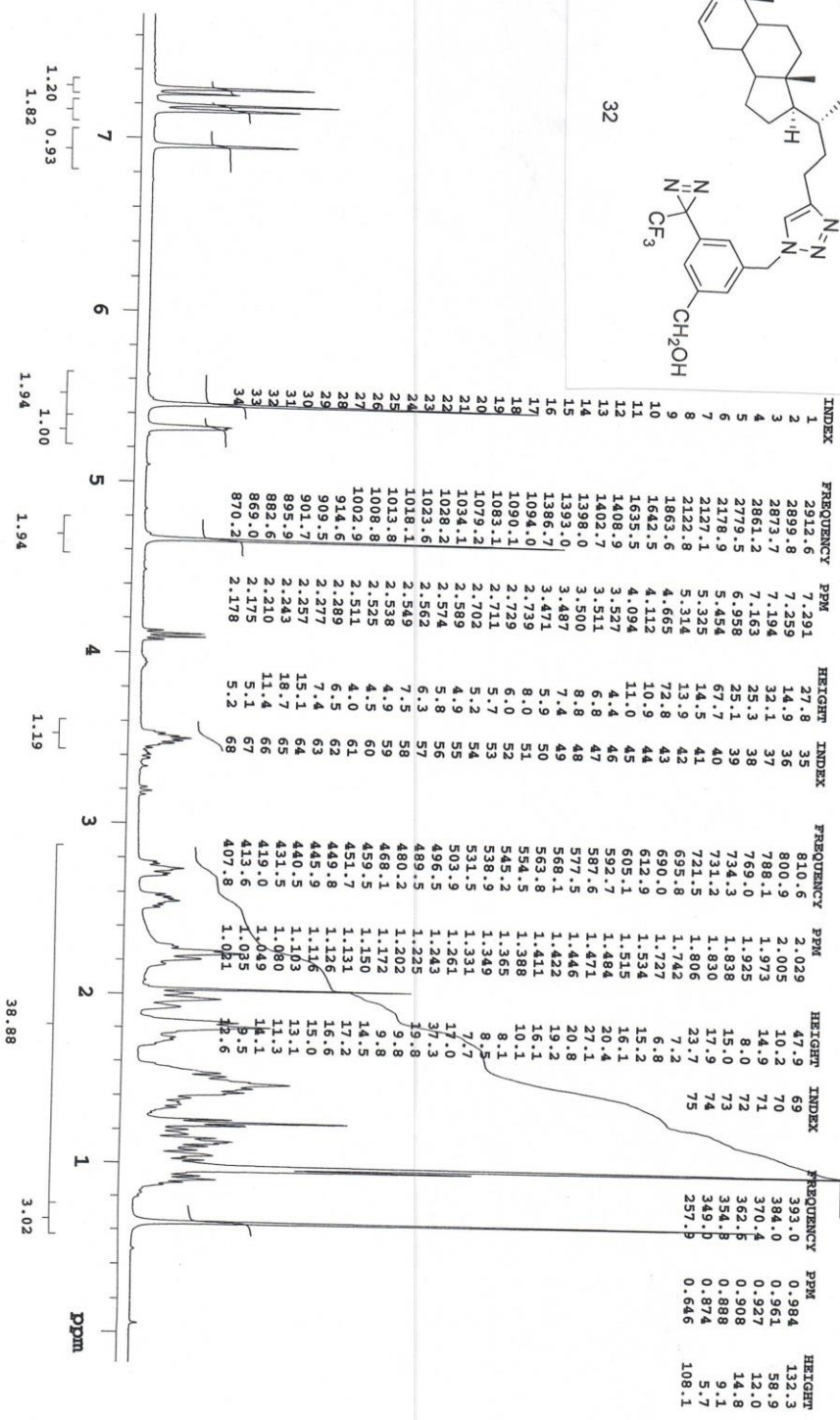
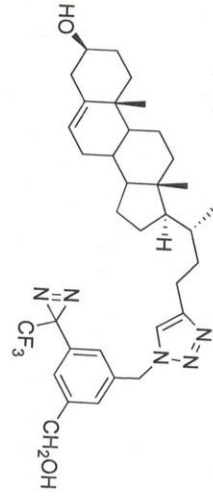
26

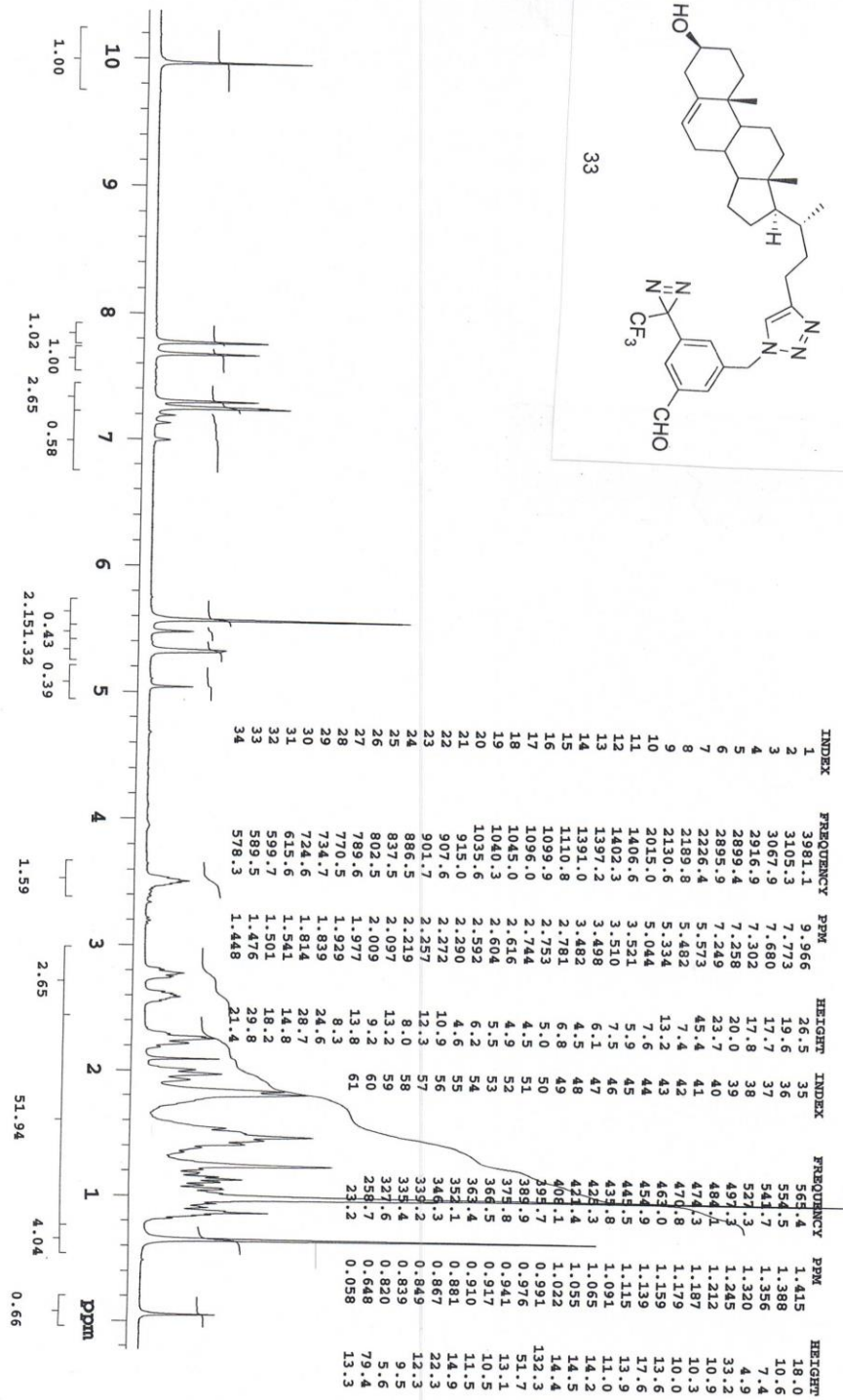
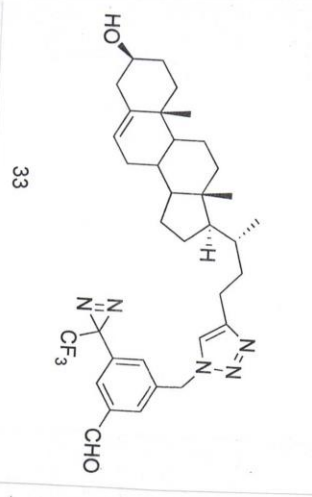


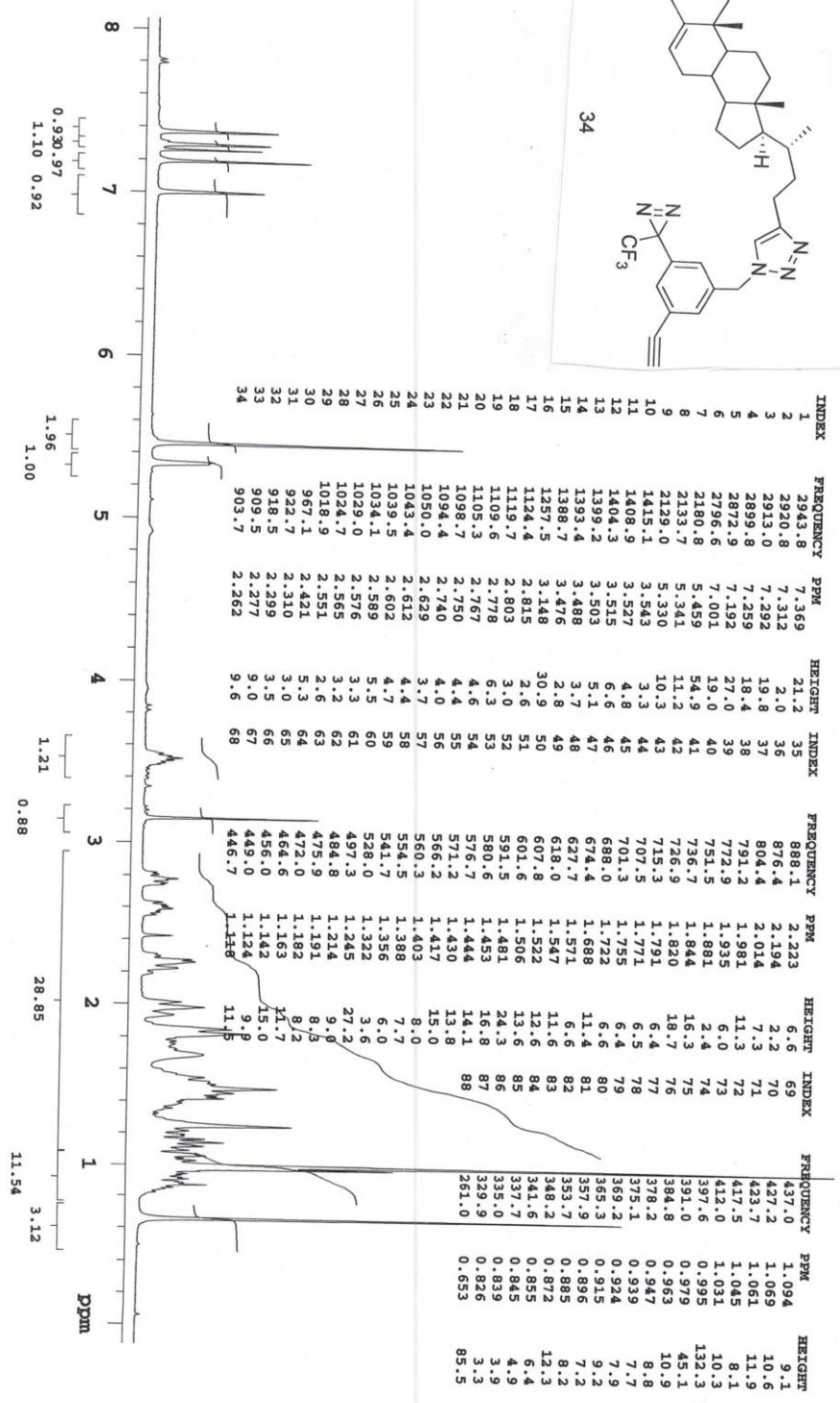
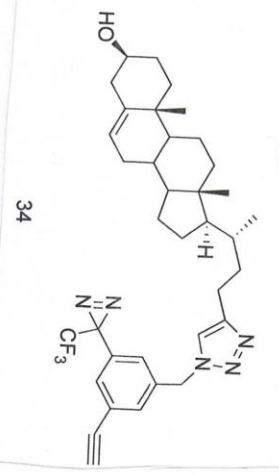


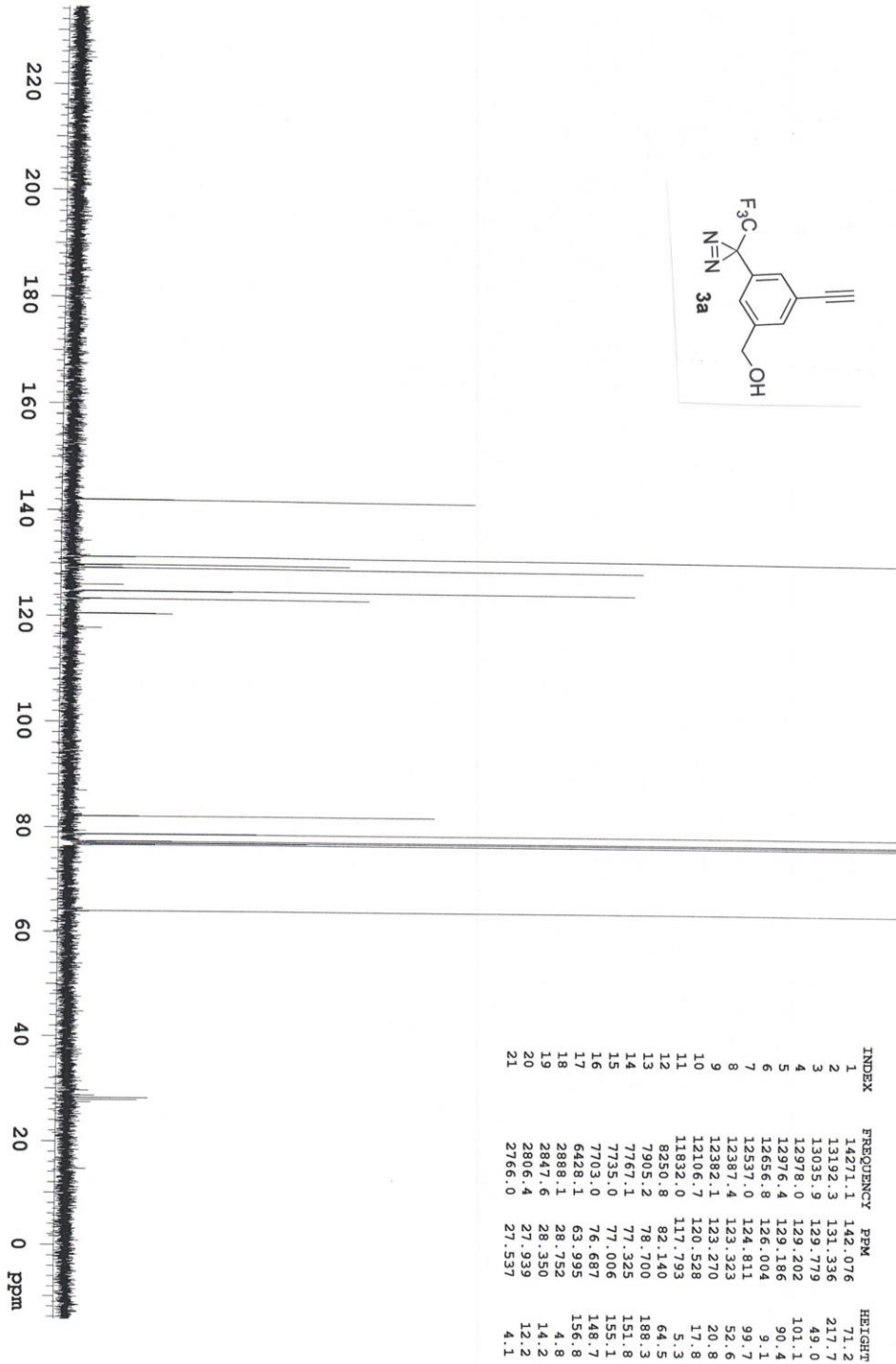
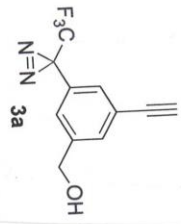


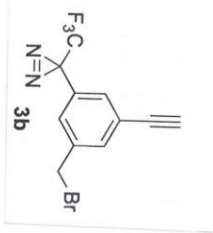




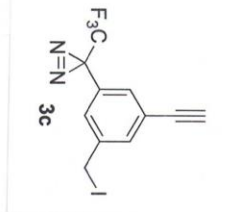




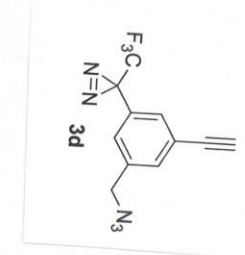




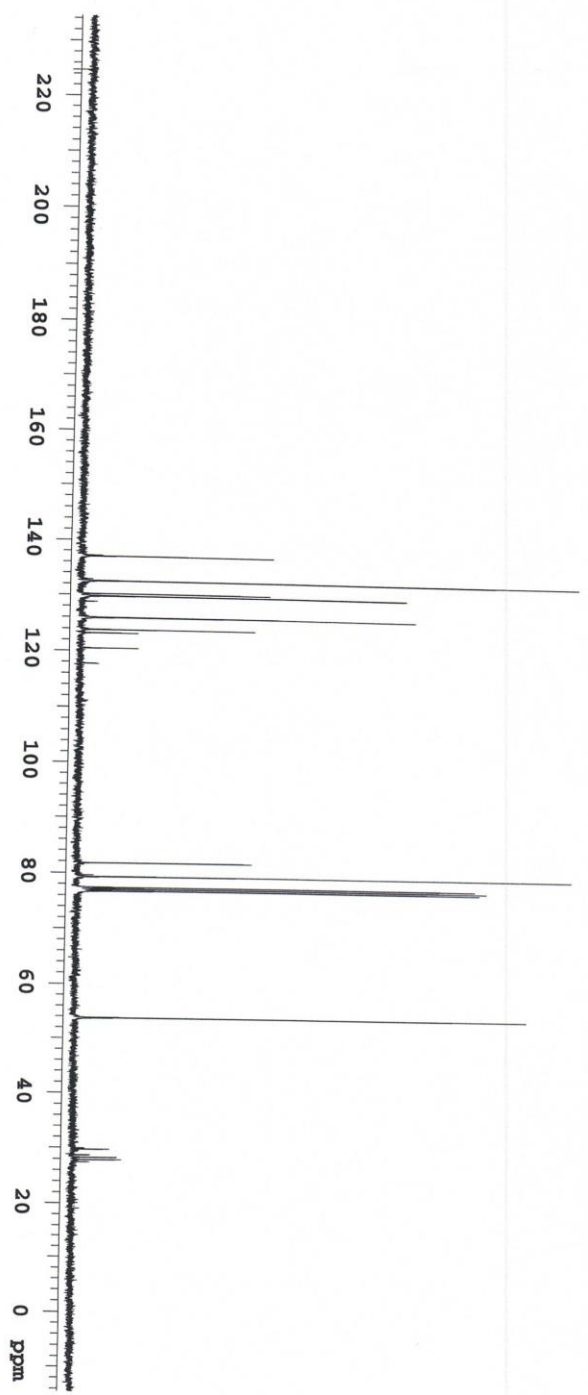
INDEX	FREQUENCY	PPM	HEIGHT
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2	13428.3	133.685	56.9
3	13078.1	130.198	46.7
4	13049.8	129.917	51.3
5	12765.3	127.084	56.7
6	12435.7	123.803	51.1
7	12371.6	123.165	14.4
8	12096.9	120.431	18.5
9	11822.3	117.696	6.2
10	8200.6	81.641	40.4
11	7958.0	79.225	99.9
12	7766.5	77.319	87.3
13	7734.4	77.000	87.0
14	7703.2	76.689	84.2
15	3136.2	31.222	106.4
16	2982.1	29.688	5.5
17	2835.6	28.230	10.7
18	2795.2	27.827	11.9

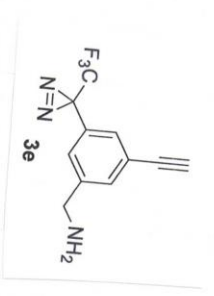


INDEX	FREQUENCY	PPM	HEIGHT
1	14278.8	142.152	48.9
2	13991.9	139.296	55.5
3	13019.9	129.619	56.7
4	12773.5	127.166	106.7
5	12673.5	126.171	7.7
6	12527.8	124.720	83.8
7	12451.5	123.961	85.2
8	12398.9	123.437	26.3
9	12124.2	120.702	21.2
10	11849.6	117.968	8.1
11	9637.0	95.941	27.1
12	9634.8	95.919	84.5
13	7768.6	77.340	83.3
14	7736.6	77.021	84.8
15	7704.5	76.702	84.6
16	6882.8	68.522	108.6
17	6464.7	64.560	58.3
18	5569.0	55.443	46.6
19	5566.8	55.420	40.3
20	2872.1	28.593	11.0
21	2831.6	28.190	11.8



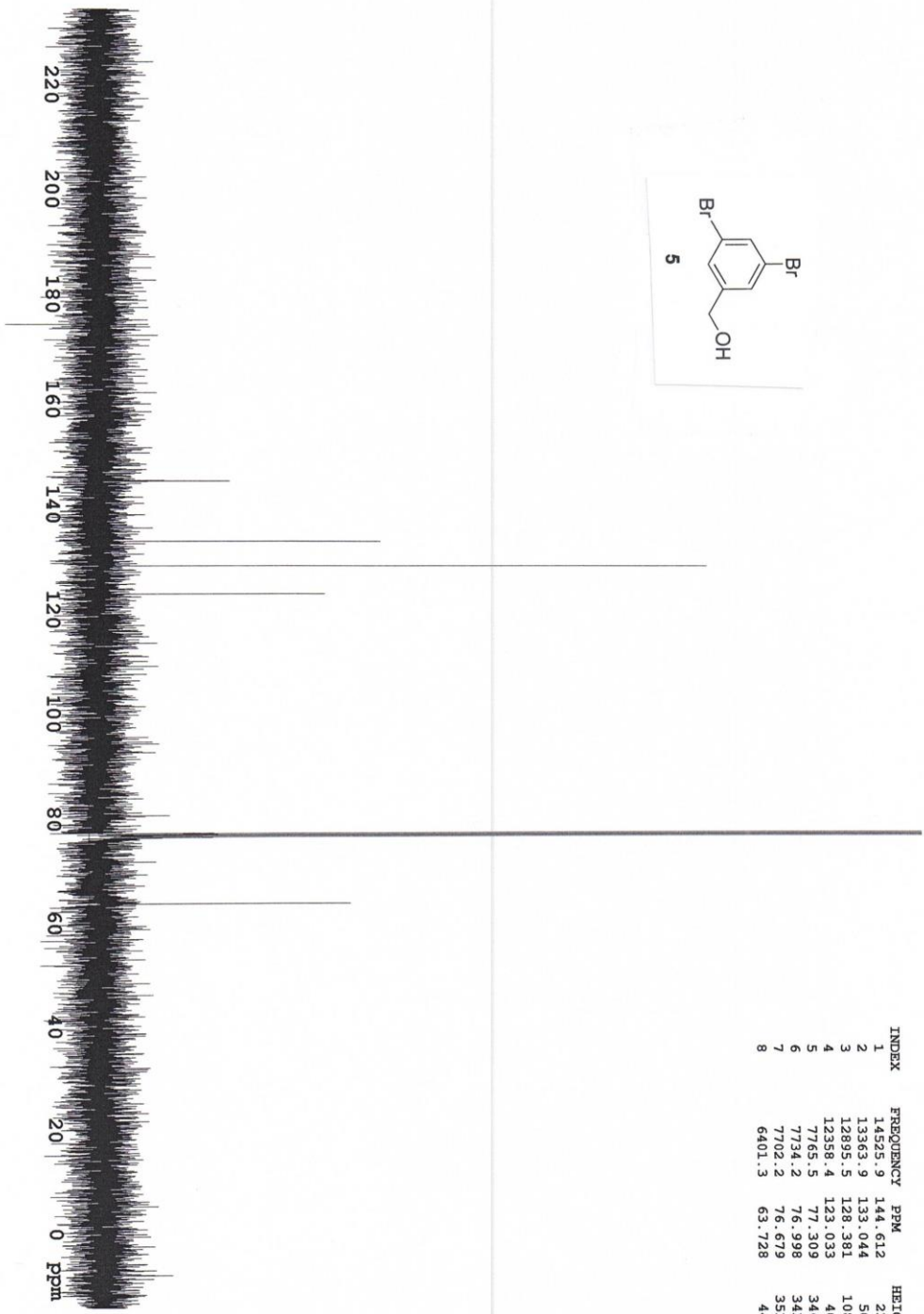
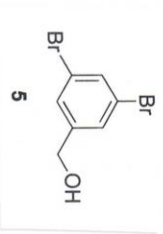
INDEX	FREQUENCY	PPM	HEIGHT
1	13758.6	136.973	32.1
2	13310.0	132.507	83.8
3	13077.3	130.190	31.6
4	13036.8	129.788	54.7
5	12653.1	125.967	56.3
6	12433.3	123.780	29.1
7	12372.3	123.172	9.5
8	12097.7	120.438	9.5
9	8207.4	81.709	39.1
10	7959.5	79.240	83.3
11	7766.4	77.319	67.1
12	7734.4	77.000	69.1
13	7702.4	76.681	67.8
14	5393.7	53.697	76.2
15	2838.6	28.260	7.4
16	2797.4	27.850	8.1

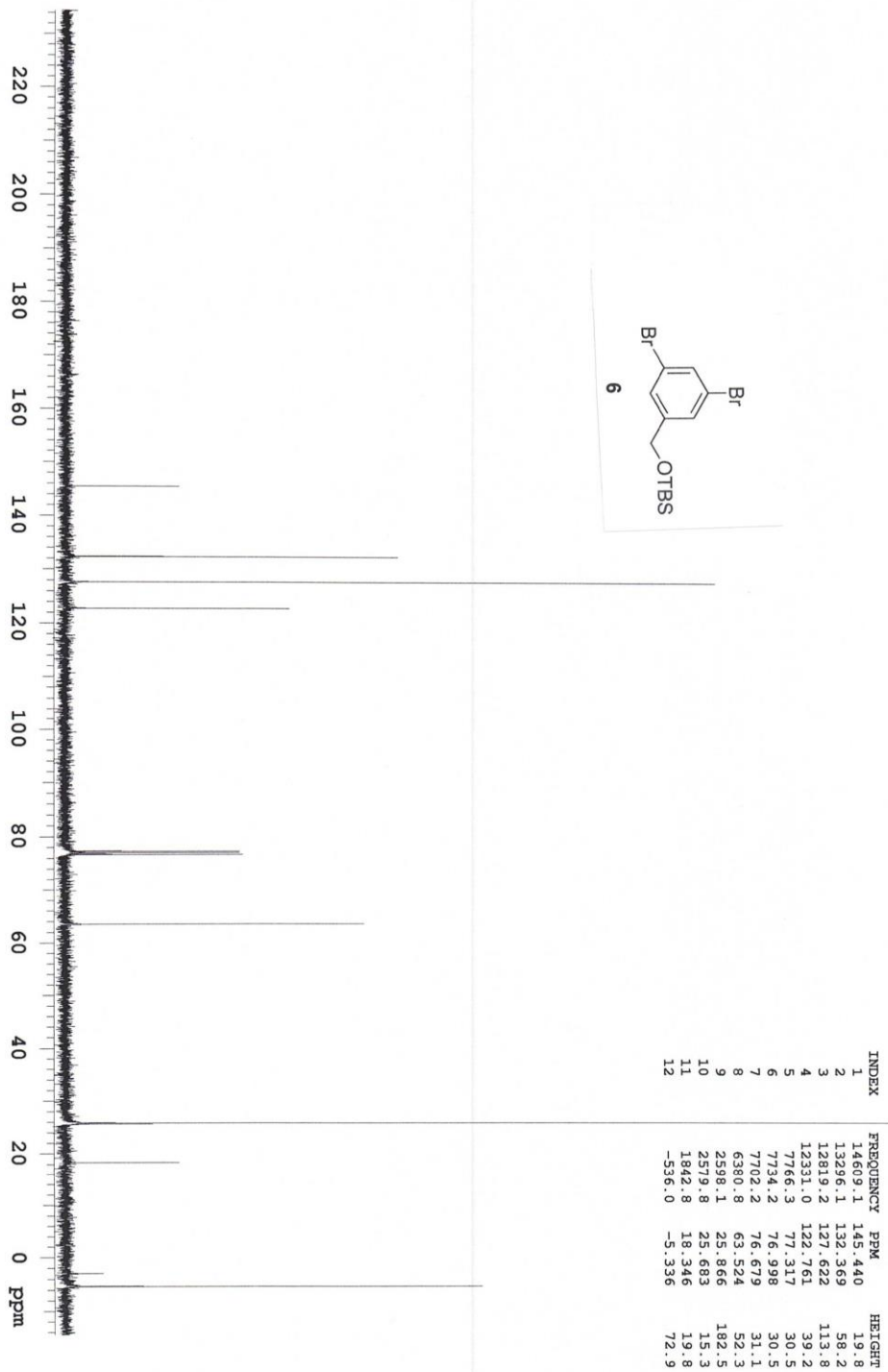
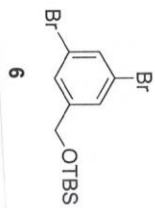


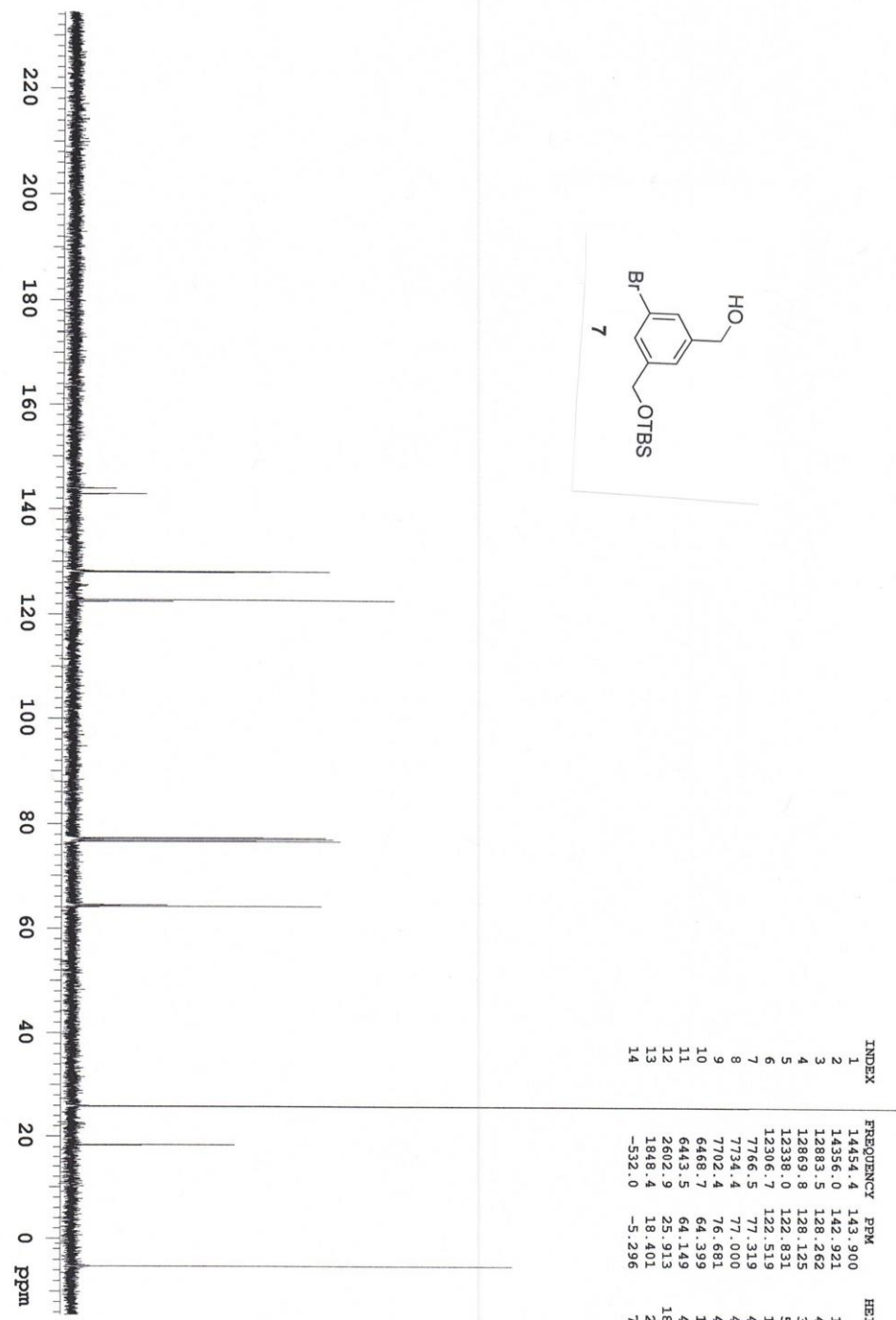
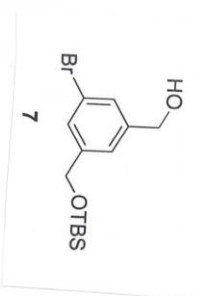


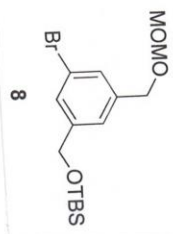
INDEX	FREQUENCY PPM	HEIGHT
1	14484.8	144.203
2	13270.2	132.111
3	13260.2	132.012
4	13254.1	131.951
5	13026.0	129.680
6	12917.7	128.602
7	12901.7	128.442
8	12598.0	125.419
9	12384.4	123.292
10	12379.0	123.239
11	12109.7	120.558
12	8285.3	82.285
13	7884.6	78.495
14	7769.4	77.348
15	7757.9	77.234
16	7737.3	77.029
17	7705.3	76.710
18	4578.0	45.576
19	2849.2	28.365
20	2808.7	27.952



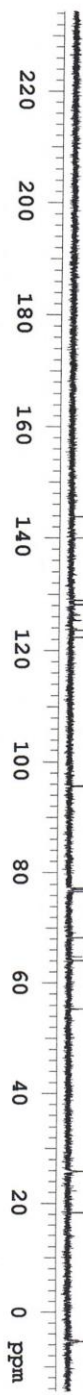


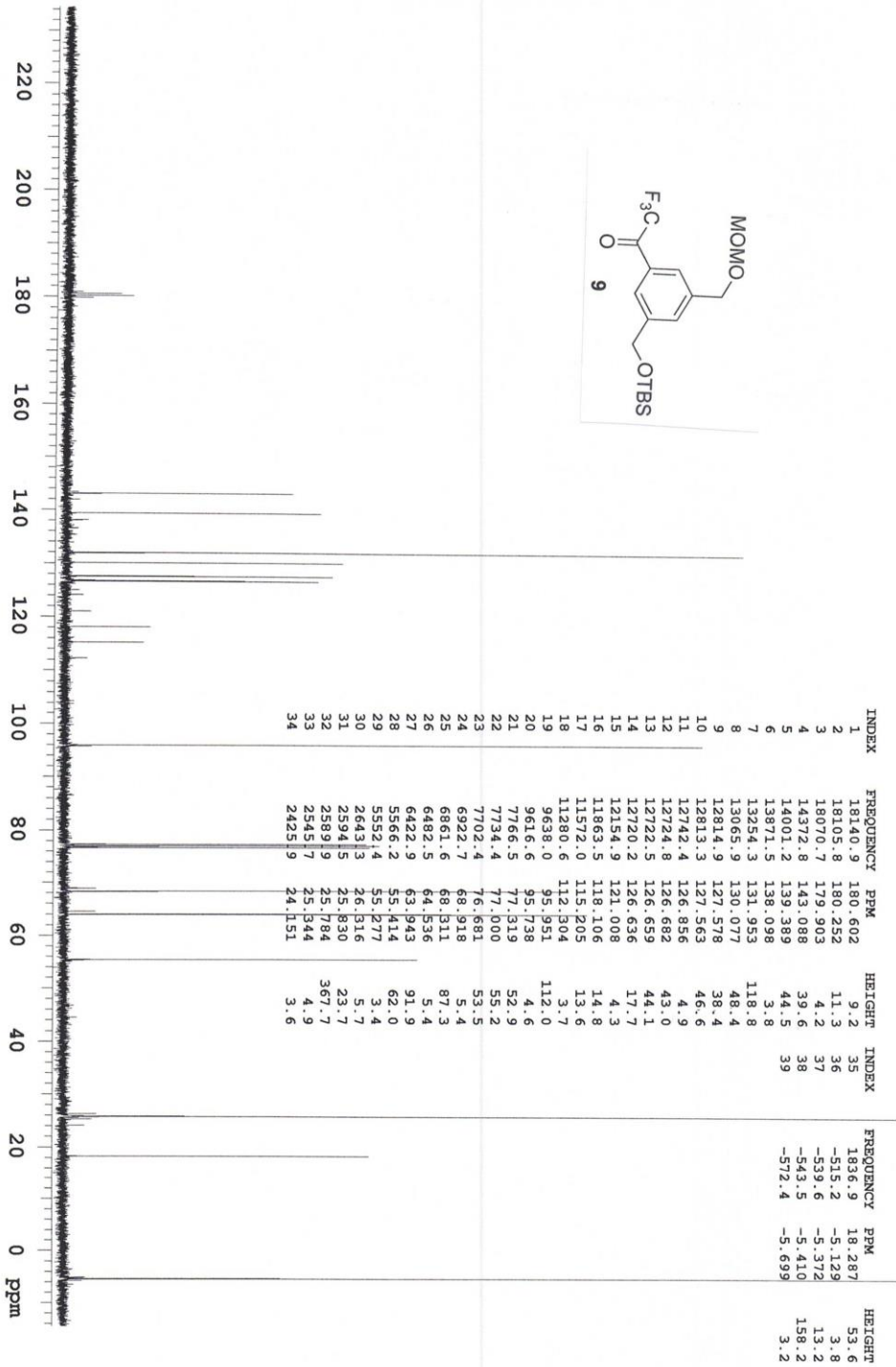
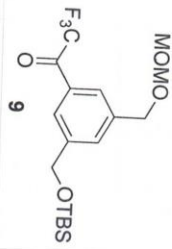


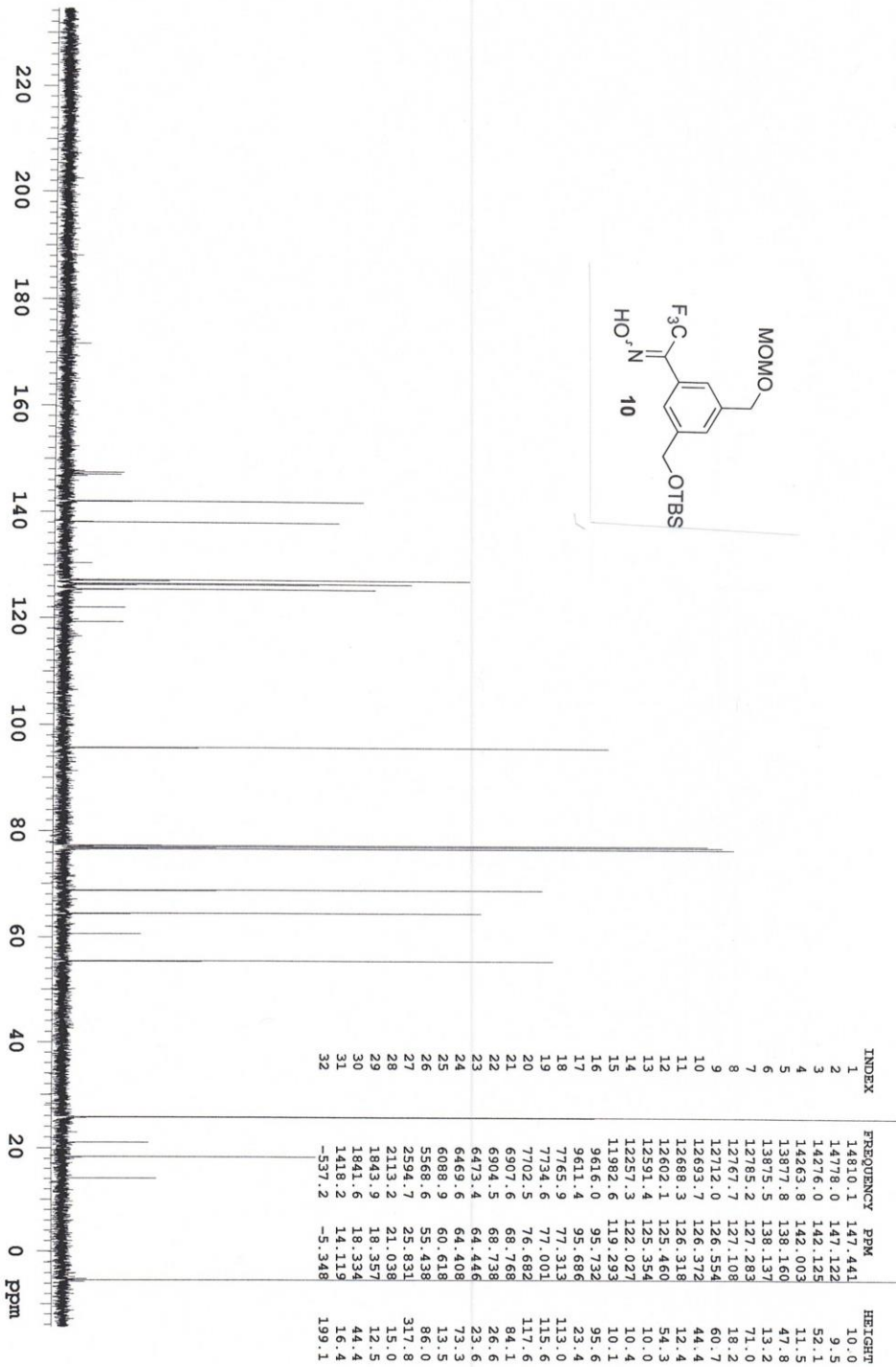


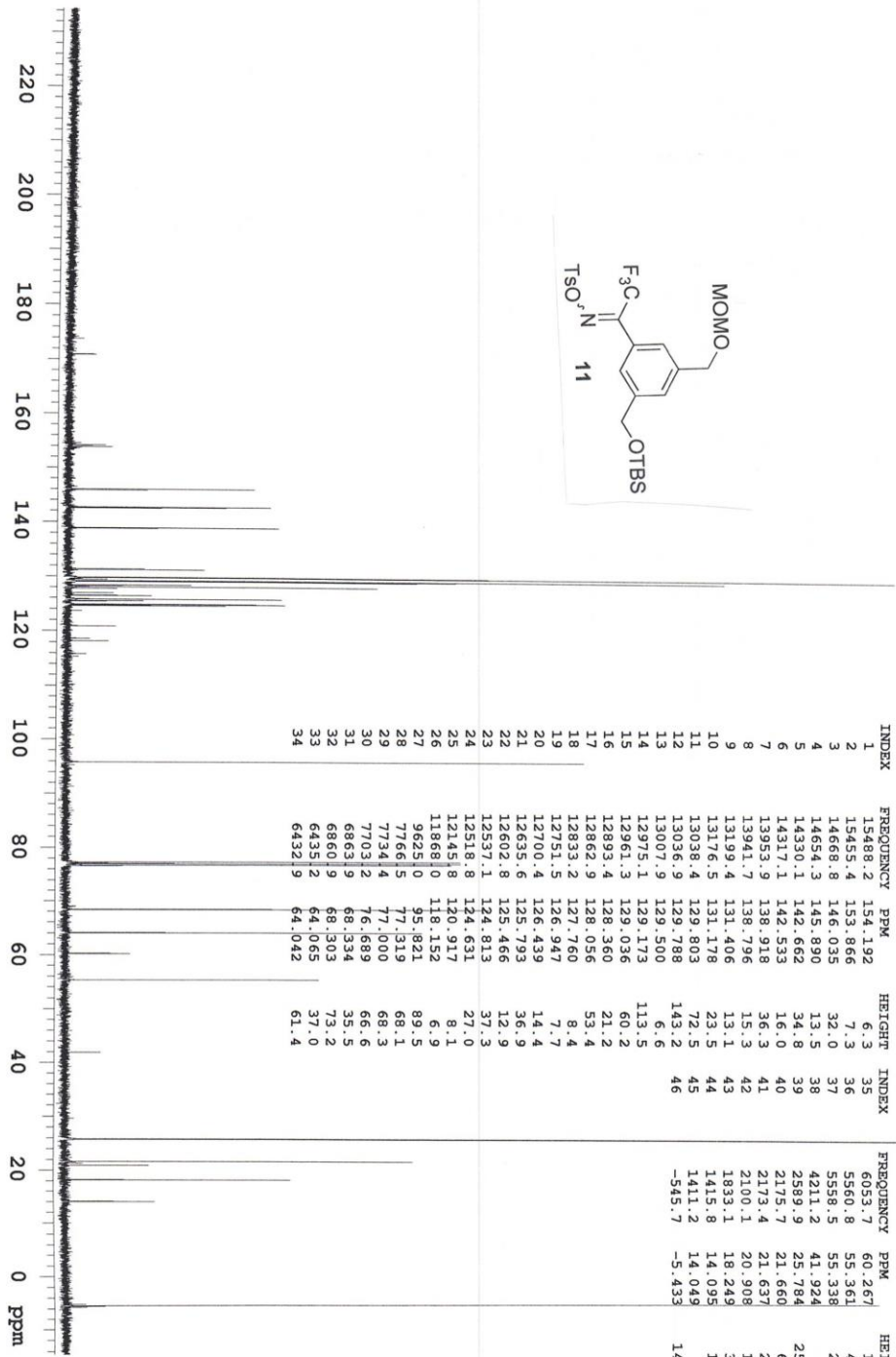
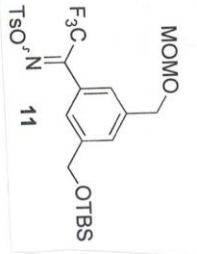


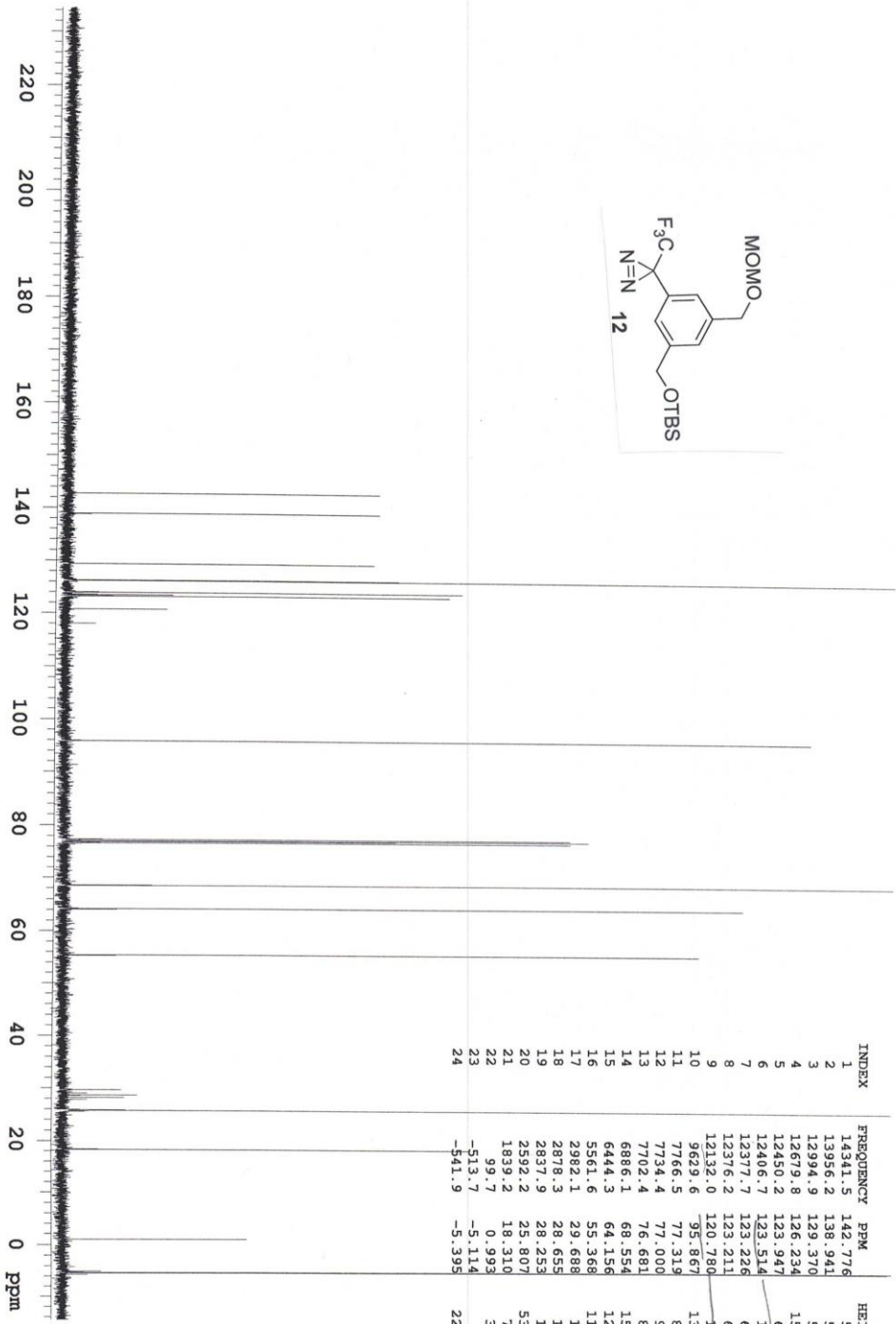
INDEX	FREQUENCY	PPM	HEIGHT
1	1447.5	143.832	20.4
2	14063.0	140.004	12.3
3	12961.3	129.036	46.5
4	12874.4	128.170	43.2
5	12421.2	123.659	46.5
6	12296.1	122.413	22.0
7	9612.8	95.700	41.8
8	7766.5	77.319	15.1
9	7734.4	77.000	15.5
10	7702.4	76.681	15.3
11	6854.8	68.242	37.3
12	6434.4	64.057	51.7
13	5562.4	55.376	20.6
14	2602.9	25.913	12.1
15	2599.1	25.875	185.2
16	1843.0	18.348	20.7
17	-535.1	-5.327	76.6

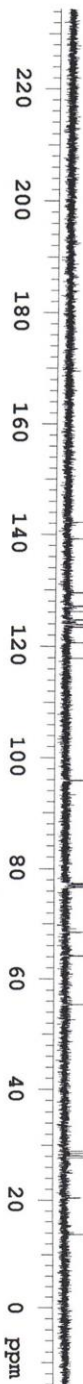
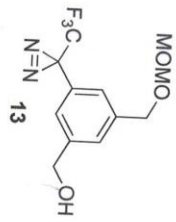




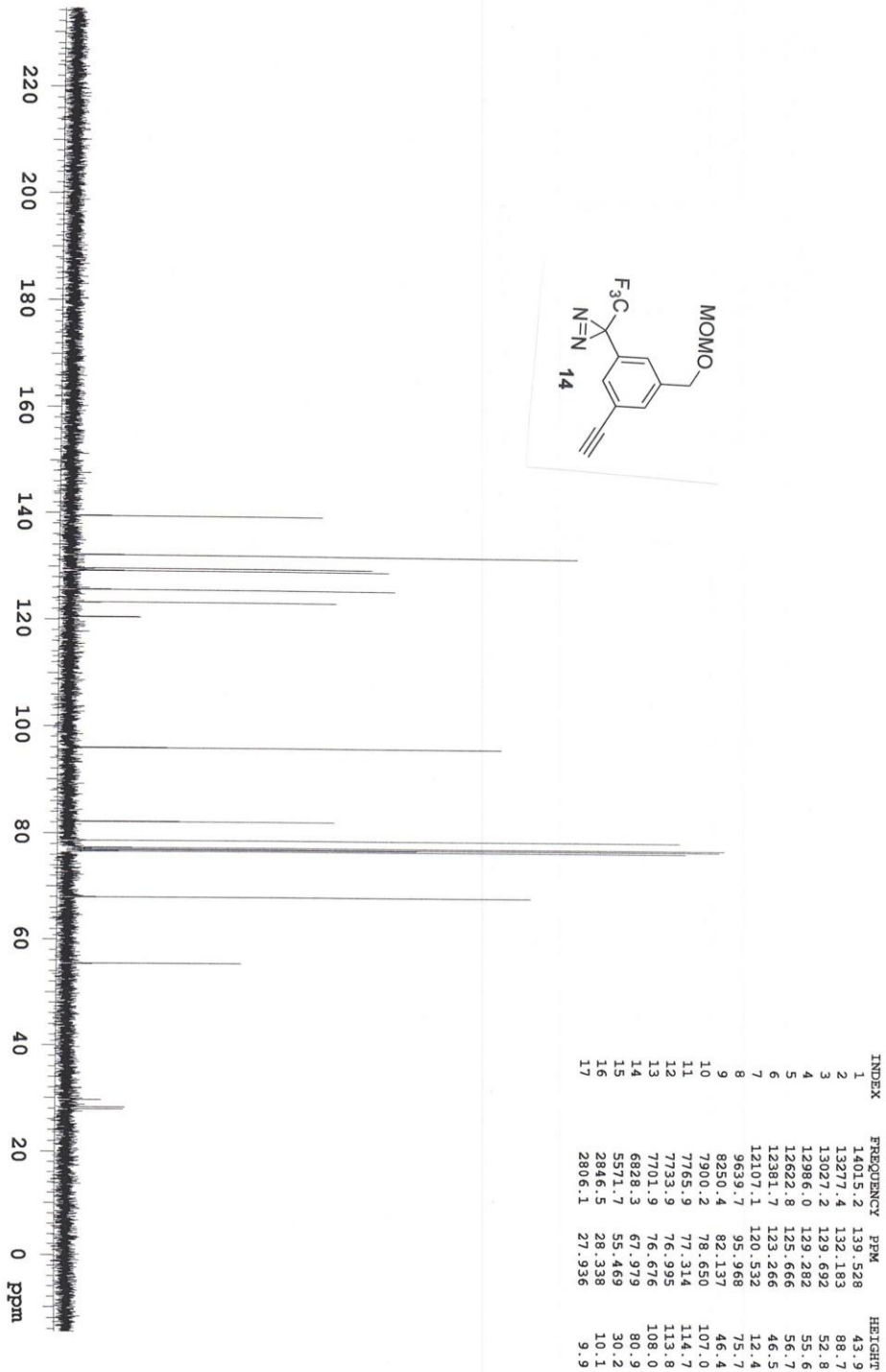
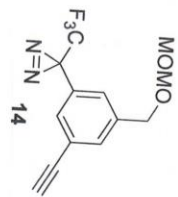


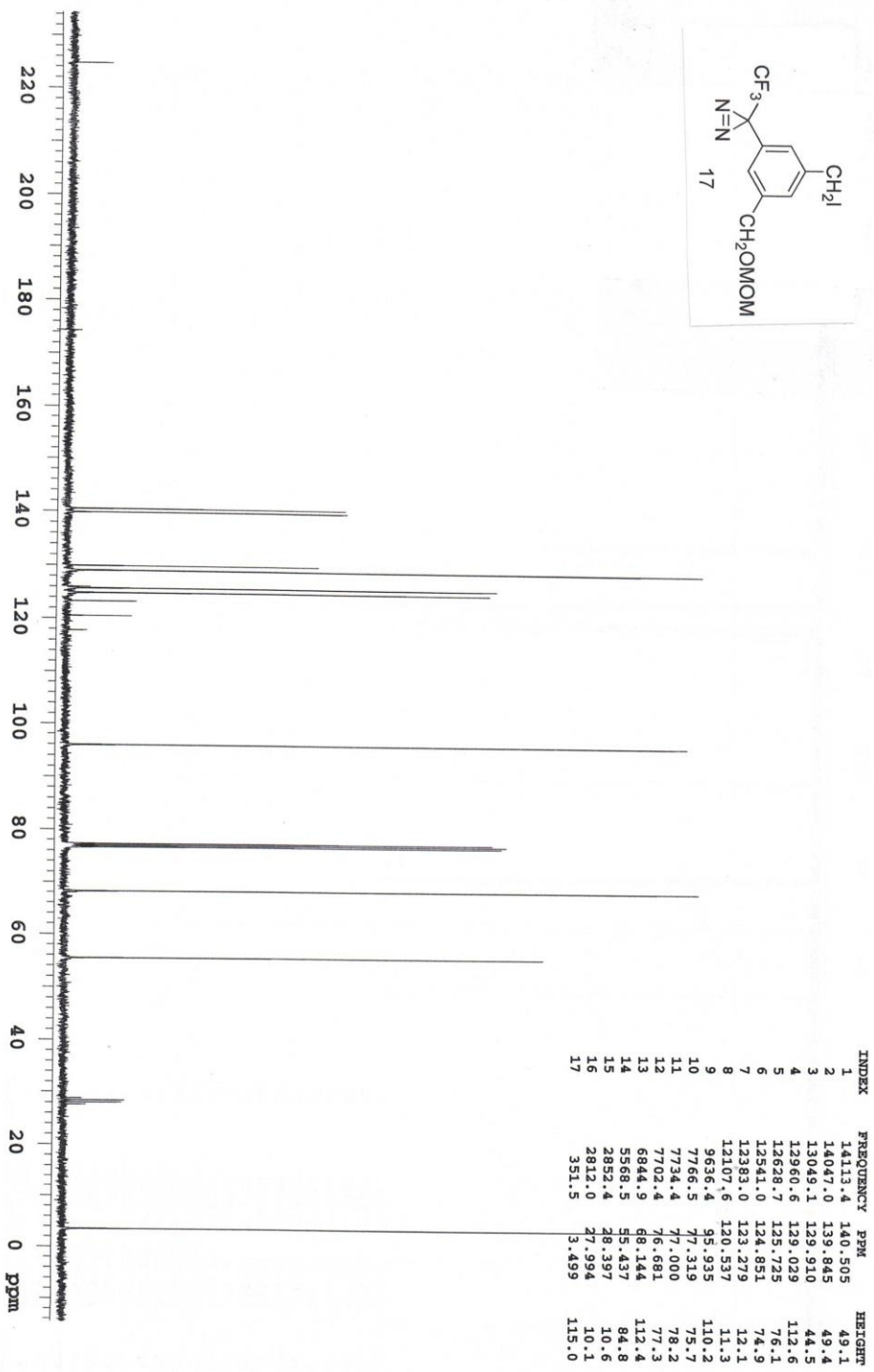
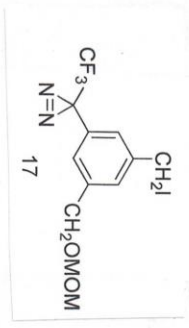


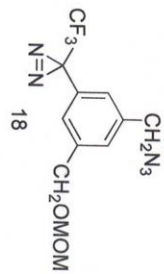




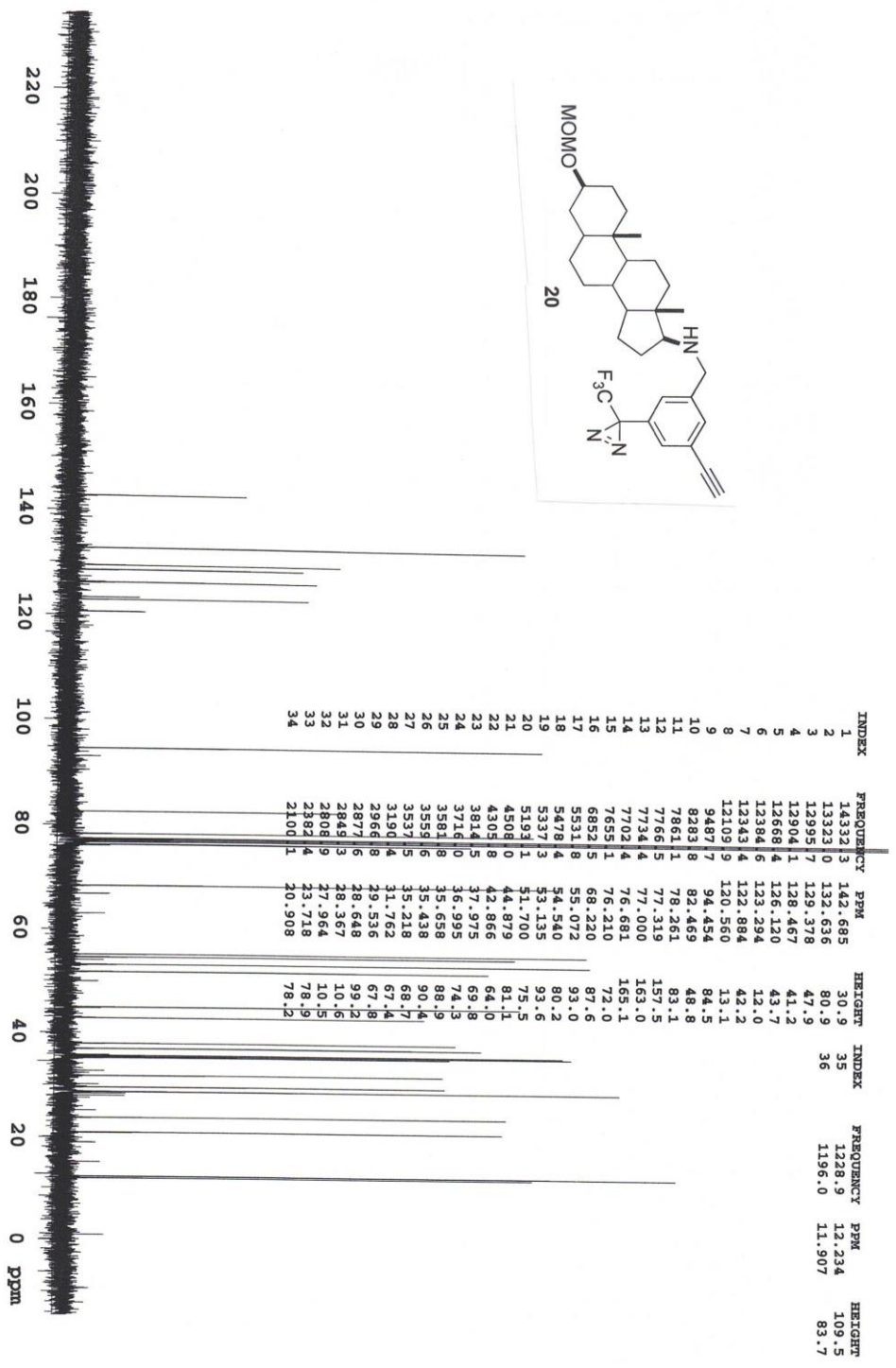
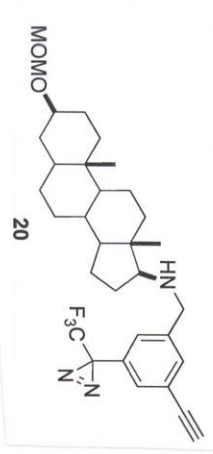
INDEX	FREQUENCY	PPM	HEIGHT
1	14281.4	142.178	55.3
2	13983.1	139.208	42.5
3	13013.4	129.555	40.9
4	12767.7	127.109	116.4
5	12670.1	126.137	5.1
6	12520.5	124.648	58.3
7	12445.0	123.896	58.7
8	12395.4	123.402	15.2
9	12120.8	120.668	14.0
10	11846.1	117.934	4.3
11	9628.2	95.854	120.0
12	7766.7	77.321	67.4
13	7734.6	77.002	70.4
14	7702.6	76.683	70.7
15	6879.4	68.487	130.2
16	6449.8	64.211	126.3
17	5561.0	55.362	72.2
18	2867.8	28.551	8.6
19	2827.4	28.148	9.7
20	2787.0	27.745	3.5
21	1380.1	13.740	3.4

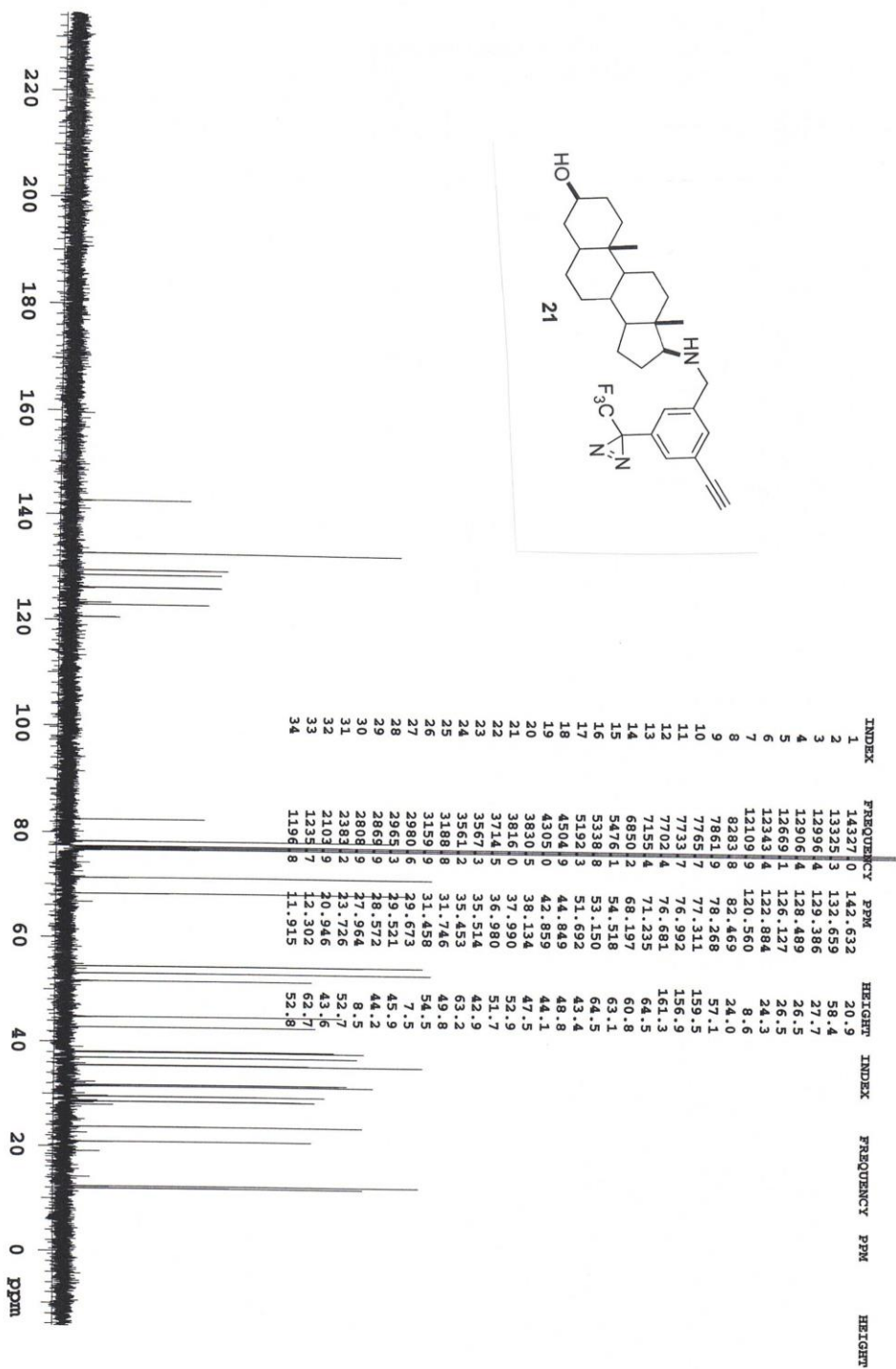
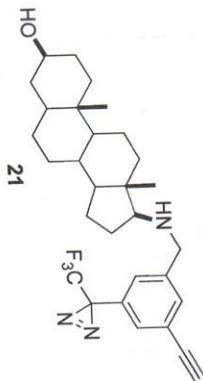


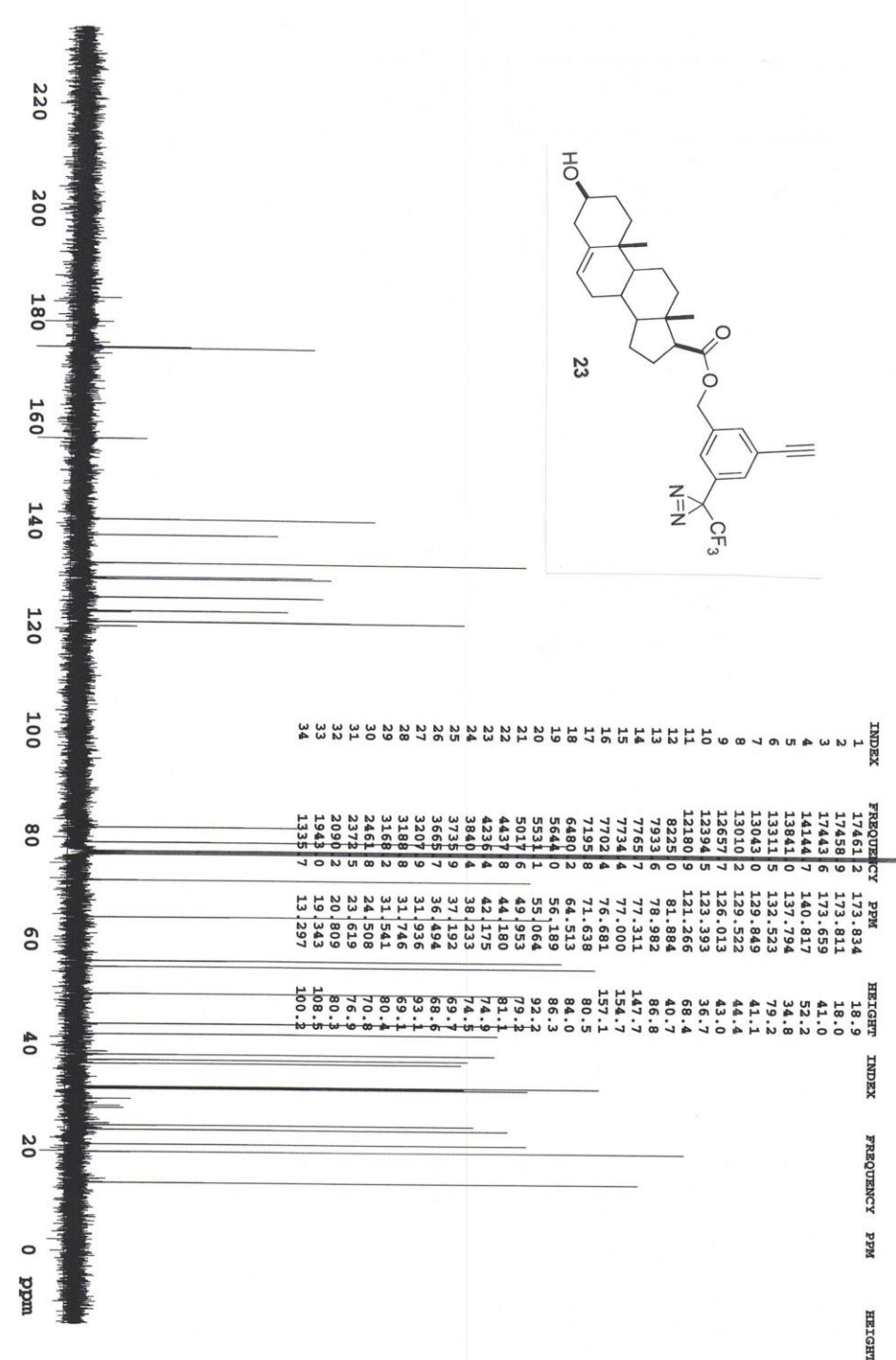
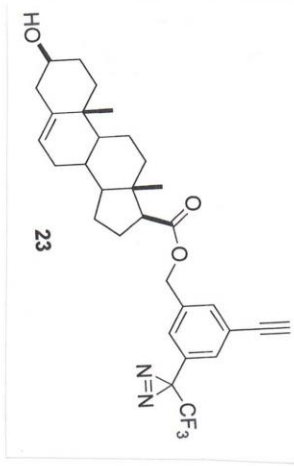


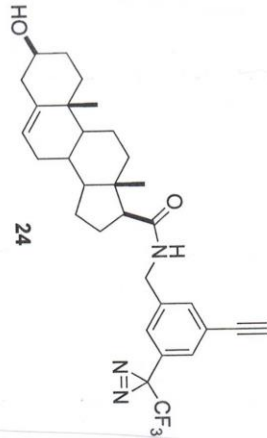


INDEX	FREQUENCY	PPM	HEIGHT
1	22569.0	224.685	8.2
2	14053.1	139.905	37.6
3	13734.2	136.730	32.2
4	13055.2	129.970	39.3
5	12893.5	128.262	81.2
6	12581.4	125.254	44.9
7	12567.7	125.117	43.1
8	12566.1	125.102	45.3
9	12386.8	123.317	9.0
10	12112.2	120.583	10.5
11	9637.2	95.943	88.2
12	7766.5	77.319	58.9
13	7734.4	77.000	61.7
14	7702.4	76.681	61.3
15	6851.7	68.212	108.5
16	5565.4	55.406	93.5
17	5431.1	54.069	94.4
18	2860.8	28.480	7.8
19	2819.6	28.070	7.9

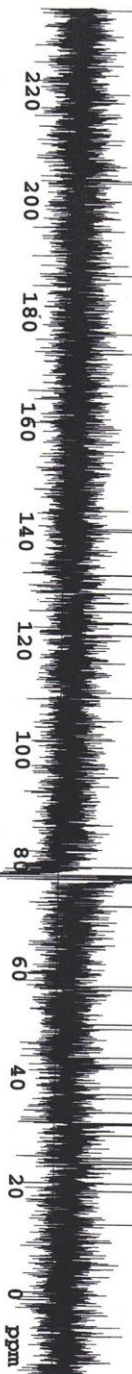


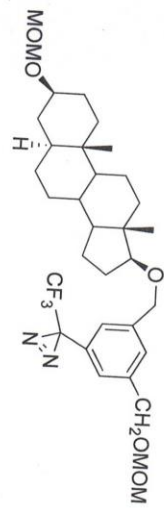




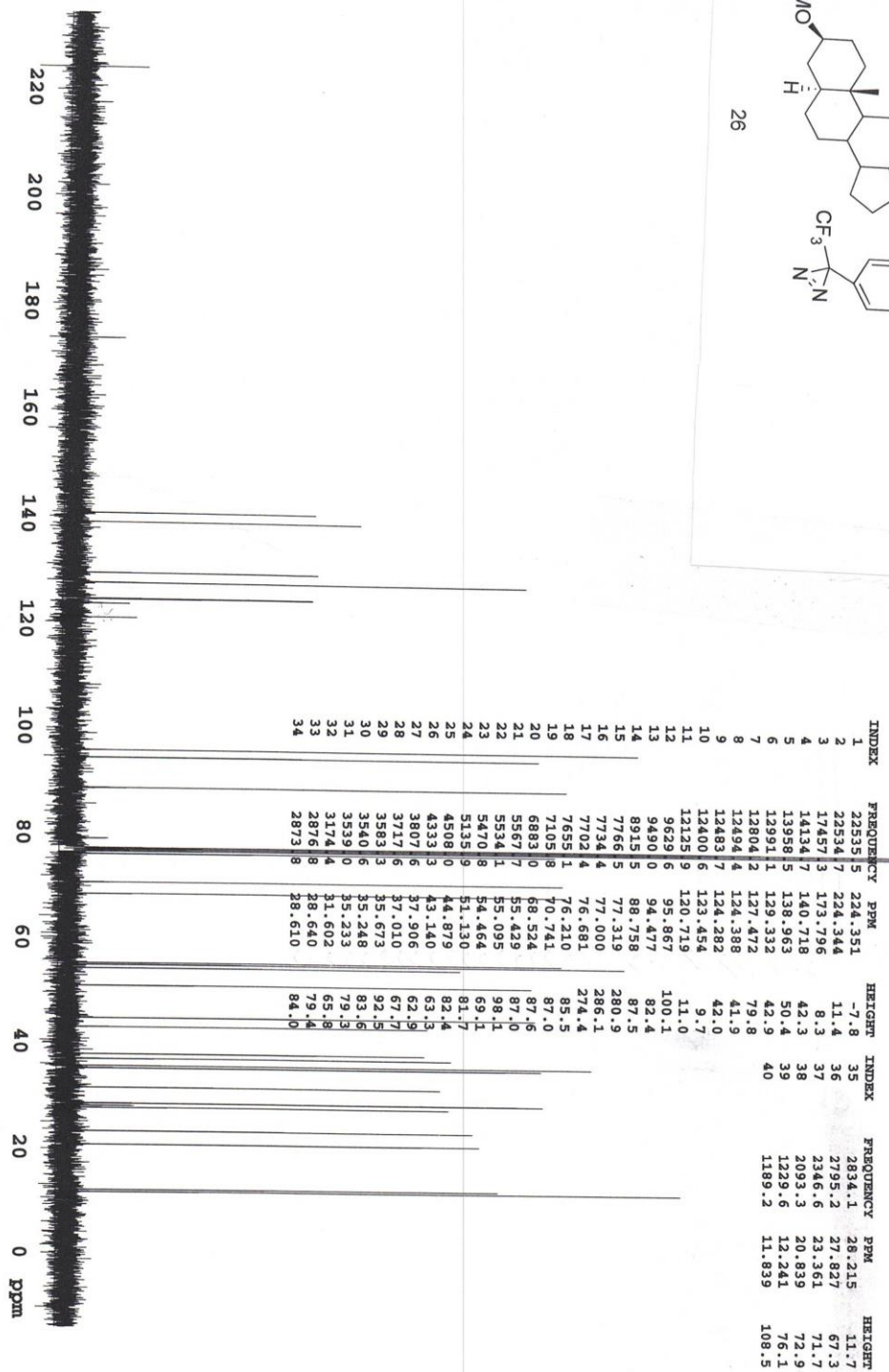


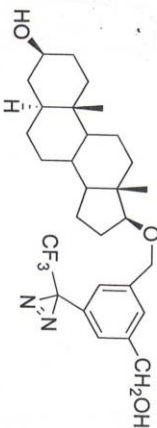
INDEX	FREQUENCY PPM	HEIGHT	INDEX	FREQUENCY PPM	HEIGHT
1	130.35	172.891	16	43.018	57.056
2	106.14	140.785	17	42.570	56.461
3	105.86	140.403	18	37.749	50.067
4	99.85	133.438	19	32.181	42.681
5	97.96	129.935	20	31.112	43.917
6	97.29	129.035	21	31.835	42.224
7	94.79	128.724	22	29.132	38.638
8	93.11	123.496	23	28.073	37.234
9	91.47	121.329	24	27.544	36.532
10	59.44	78.846	25	25.57	33.522
11	58.40	77.458	26	24.04	31.893
12	58.37	77.427	27	23.95	31.771
13	58.05	77.000	28	23.81	31.588
14	57.73	76.573	29	22.37	29.680
15	54.05	71.690	30	19.29	25.591
16	43.01	57.056	31	18.78	24.919
17	42.57	56.461	32	18.46	24.492
18	37.74	50.067	33	17.86	23.699
19	32.18	42.681	34	15.75	20.891
20	31.11	43.917			
21	31.83	42.224			
22	29.13	38.638			
23	28.07	37.234			
24	27.54	36.532			
25	25.57	33.522			
26	24.04	31.893			
27	23.95	31.771			
28	23.81	31.588			
29	22.37	29.680			
30	19.29	25.591			
31	18.78	24.919			
32	18.46	24.492			
33	17.86	23.699			
34	15.75	20.891			





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