

Supporting Information

Acridine-based copper(I) PNP pincer complexes: catalysts for alkyne hydroboration and borylation of aryl halides

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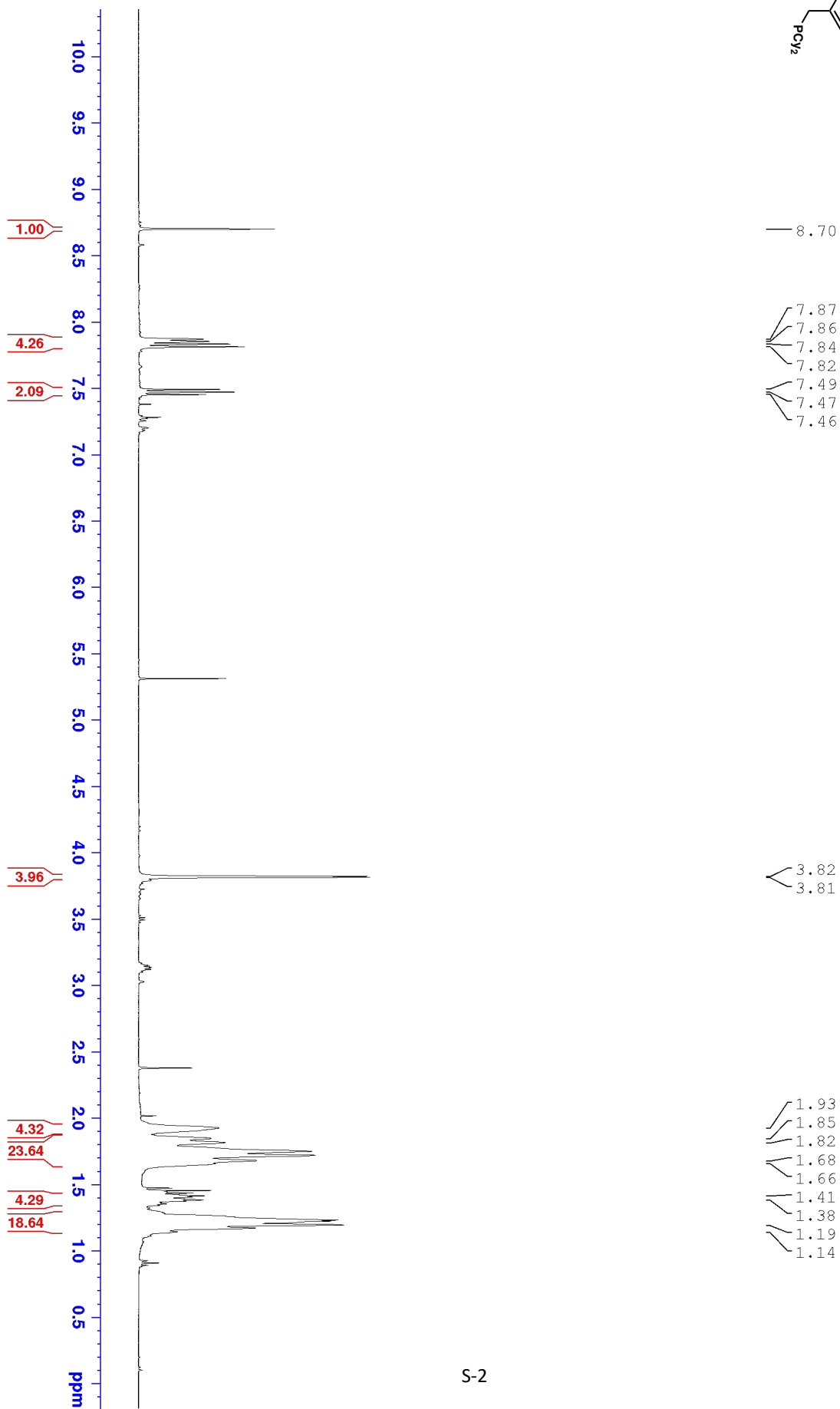
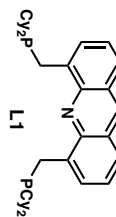
Correspondence to: curtis.ho@utas.edu.au; alex.bissember@utas.edu.au

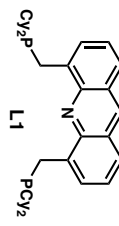
Supporting Information

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I. NMR, IR & Mass Spectra

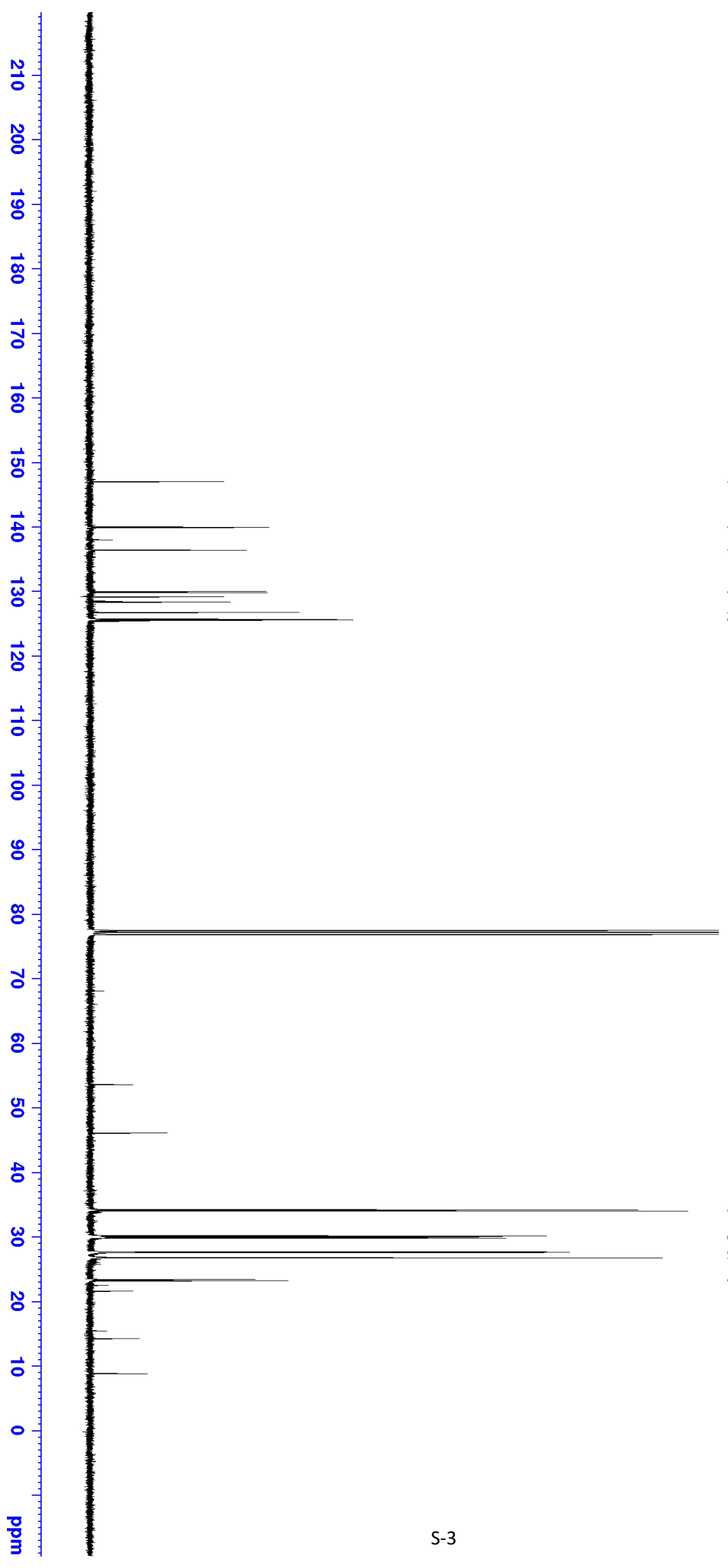


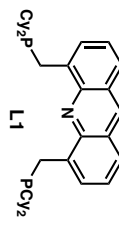


- 147.03
- 147.00
- 139.97
- 139.89
- 136.39
- 129.95
- 129.82
- 126.72
- 125.70
- 125.67
- 125.56
- 125.54

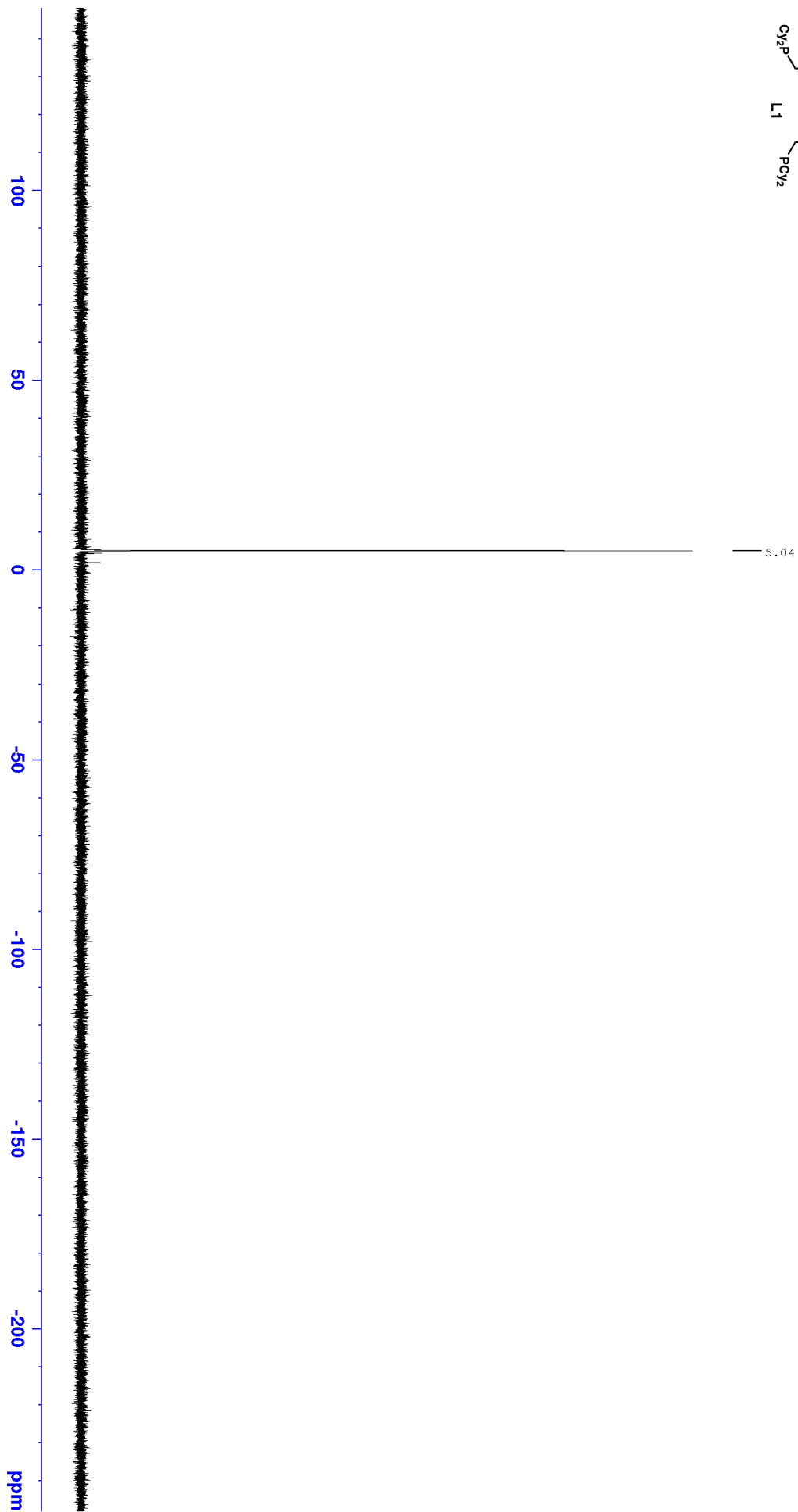
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- 34.01
- 30.12
- 30.00
- 29.88
- 29.78
- 27.65
- 27.59
- 27.55
- 27.51
- 26.71
- 23.36
- 23.19

¹³C NMR experiment performed at 25 °C in CDCl₃

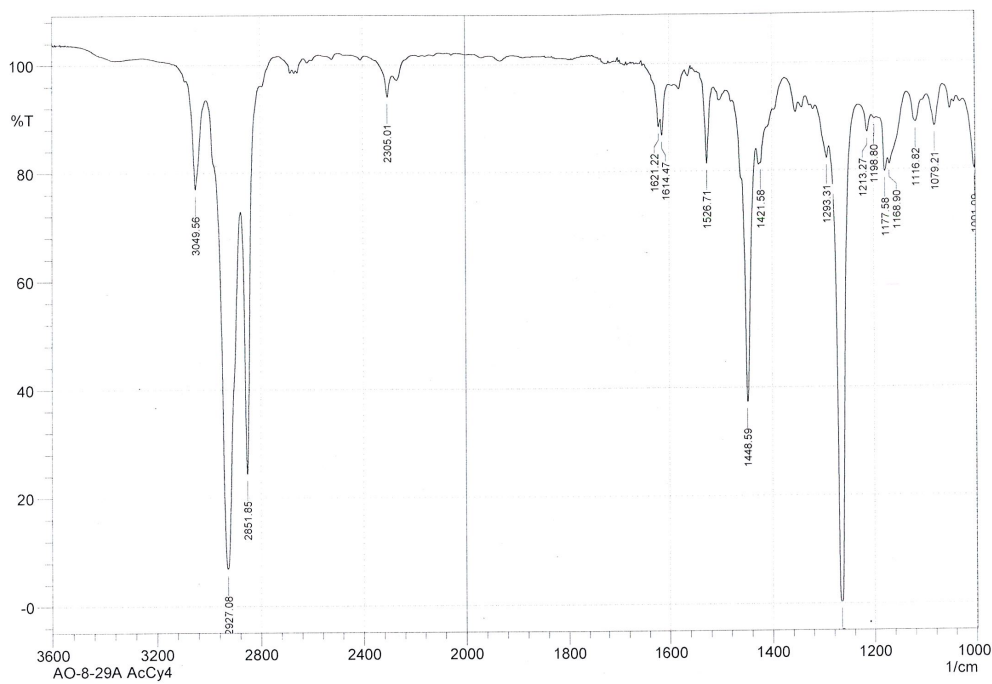
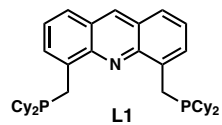




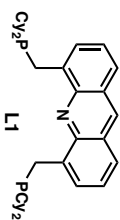
³¹P NMR experiment performed at 25 °C in CDCl₃



IR spectrum



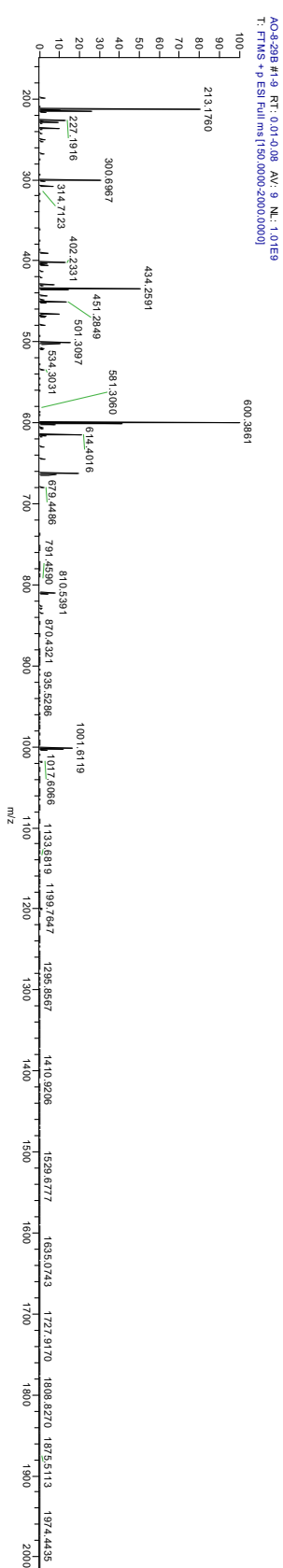
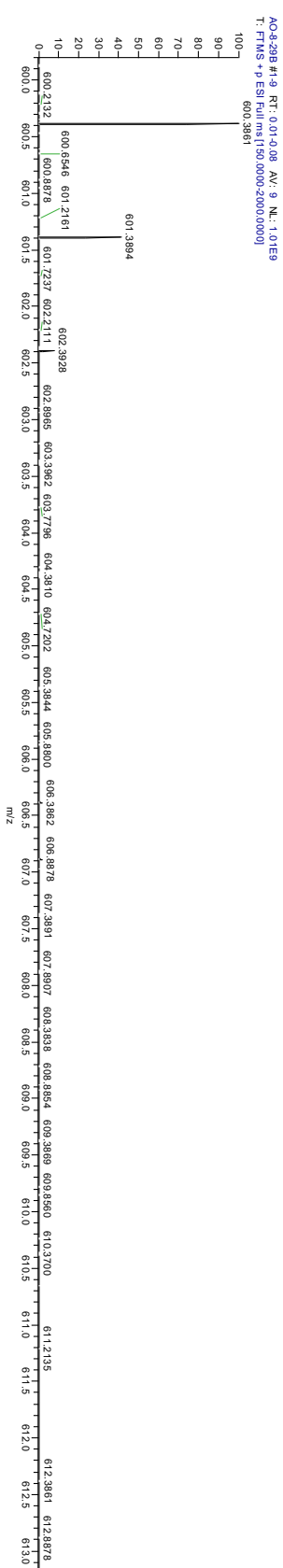
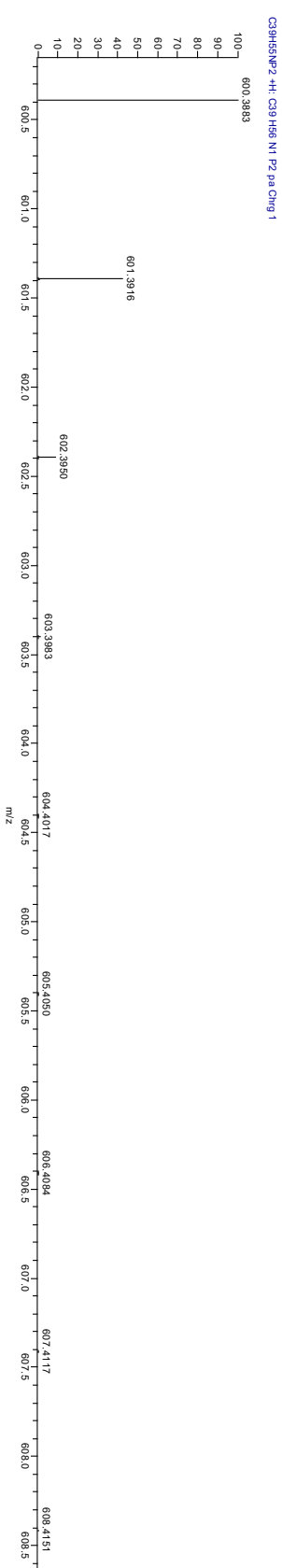
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1	1001.09	80.13	2.67	1023.27	999.16	1.42	0.07
2	1079.21	88	6.65	1093.67	1063.78	1.1	0.4
3	1116.82	88.74	4.63	1133.22	1105.25	1.09	0.27
4	1168.9	80.99	1.95	1171.79	1134.18	2.24	0.2
5	1177.58	79.64	3.95	1193.98	1172.76	1.44	0.1
6	1198.8	89.49	0.33	1203.62	1194.94	0.41	0.01
7	1213.27	86.99	3.77	1229.66	1204.59	1.16	0.13
8	1265.35	0.29	87.12	1288.49	1230.63	24.52	21.37
9	1293.31	82.17	3.3	1314.53	1289.46	1.55	0.16
10	1421.58	81.34	0.87	1423.51	1399.4	1.45	0.01
11	1448.59	37.33	50.04	1476.56	1431.23	6.97	4.51
12	1526.71	81.39	15.34	1542.14	1514.17	0.99	0.6
13	1614.47	86.64	4.12	1617.37	1600.97	0.57	0.09
14	1621.22	88.22	2.32	1648.23	1618.33	0.6	0.04
15	2305.01	94	4.87	2348.41	2284.76	0.58	0.41
16	2851.85	24.39	55.87	2876.92	2798.8	14.7	9.02
17	2927.08	6.91	73.65	3008.09	2877.89	47.16	36.22
18	3049.56	76.97	18.42	3085.24	3009.05	4.22	2.6

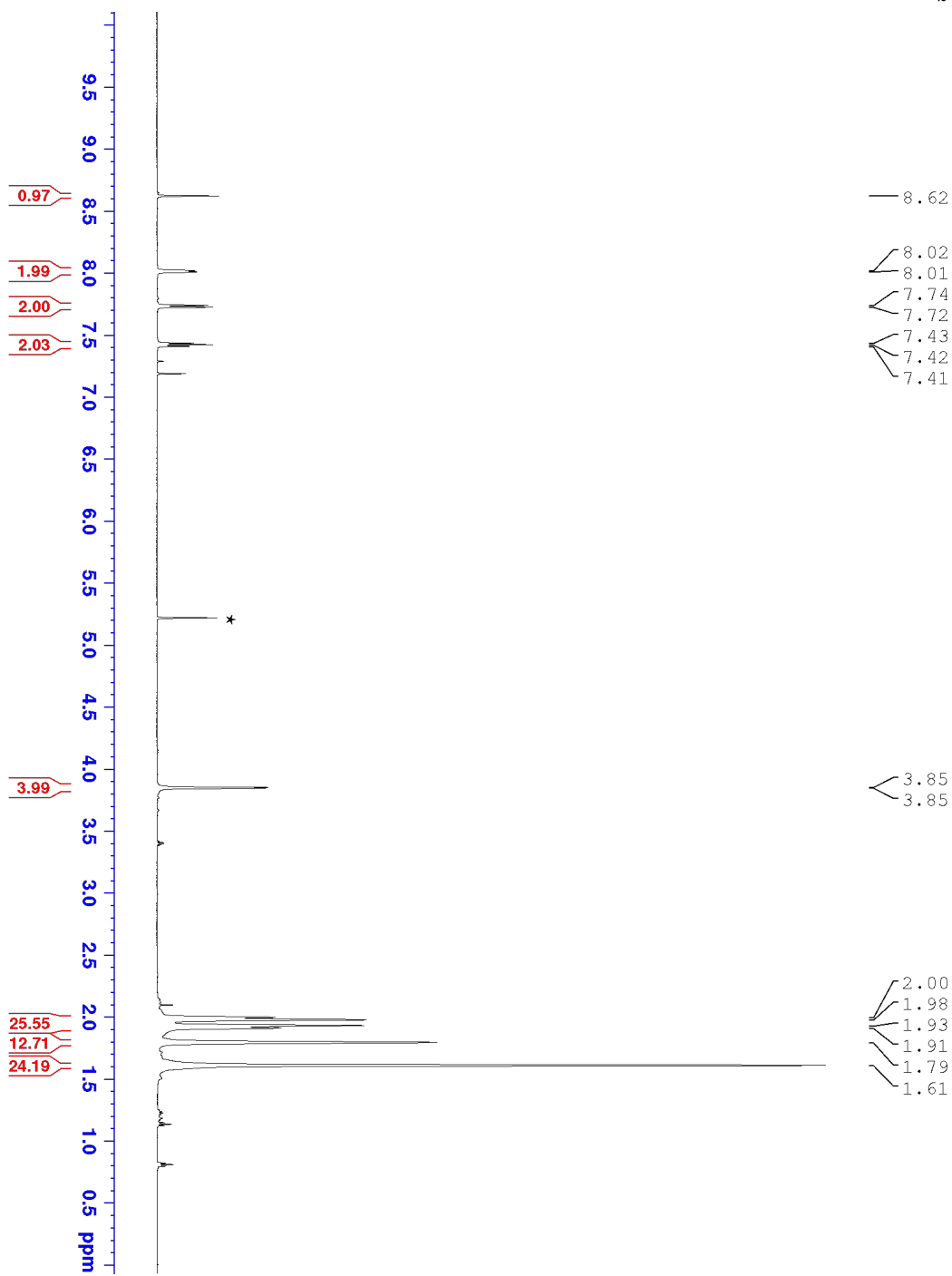
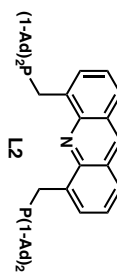


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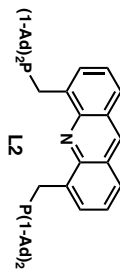
HRESIMS experiment





¹H NMR experiment performed at 25 °C in CDCl₃

* = CH₂Cl₂

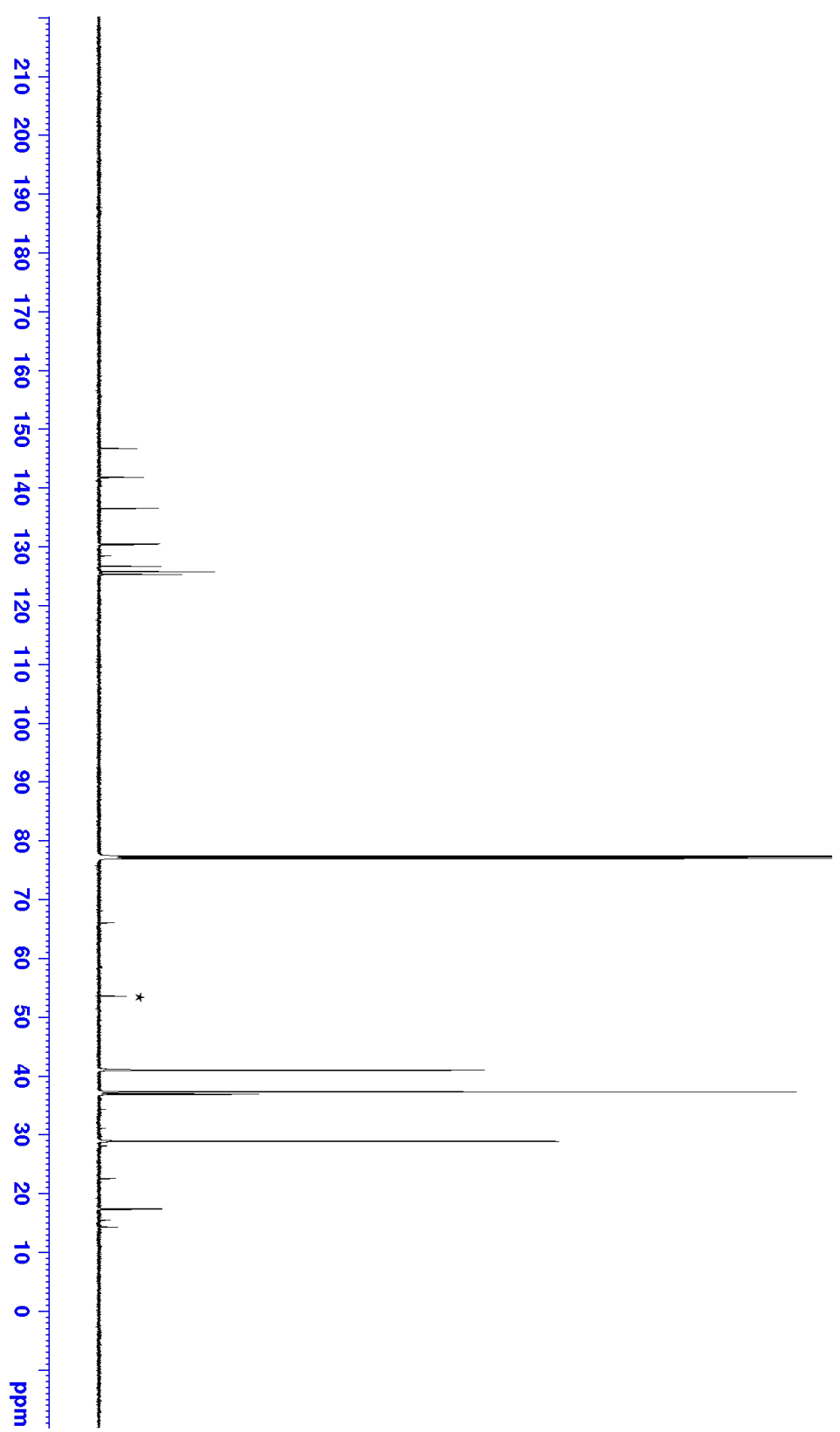


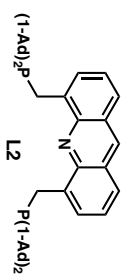
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- 141.82
- 141.73
- 136.49
- 130.46
- 130.34
- 126.63
- 125.72
- 125.26

- 40.99
- 40.92
- 37.23
- 36.93
- 36.78
- 28.89
- 28.84
- 17.39
- 17.27

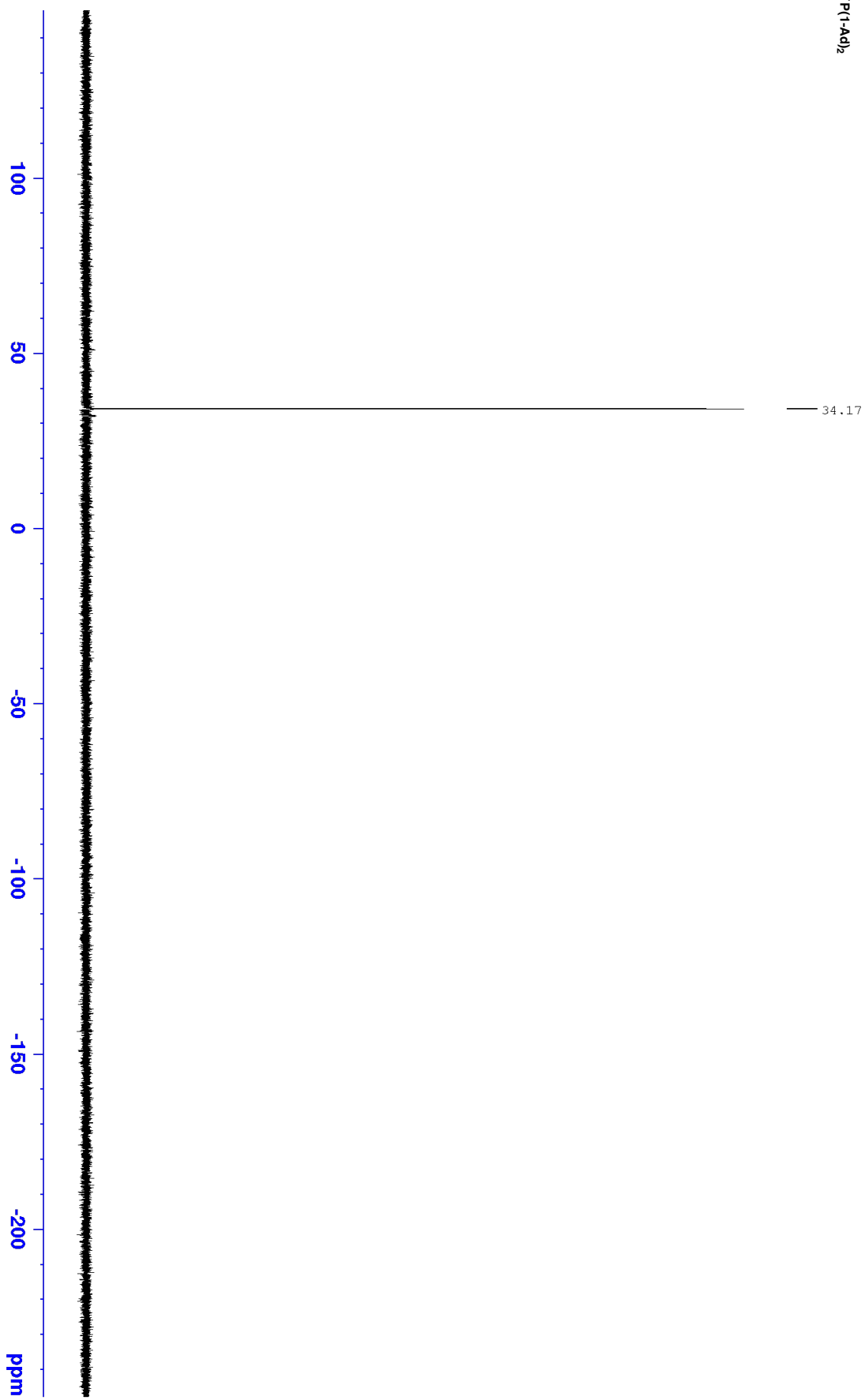
* = CH₂Cl₂

¹³C NMR experiment performed at 25 °C in CDCl₃

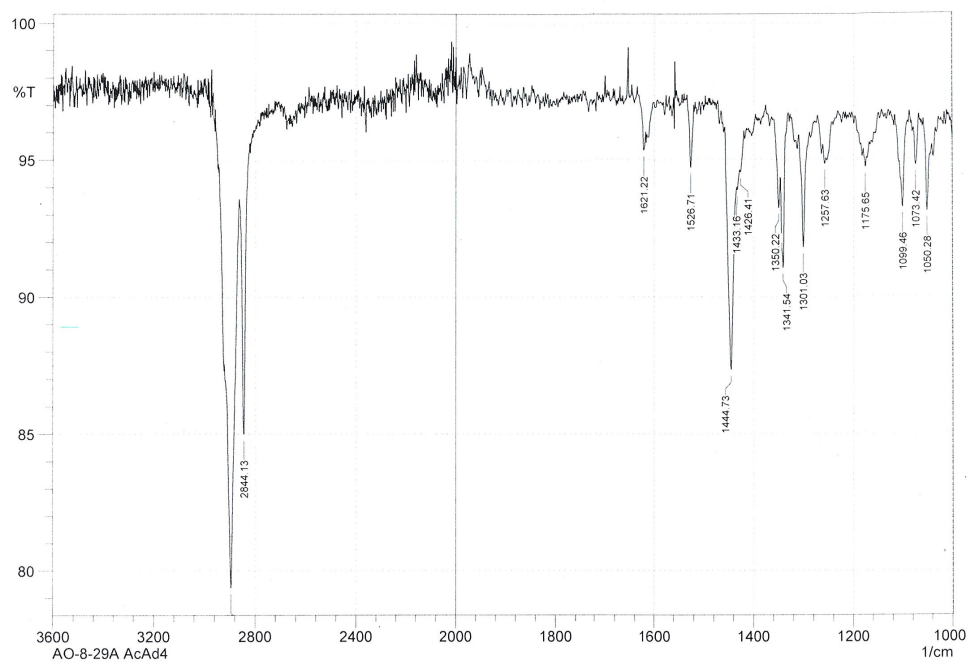
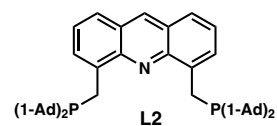




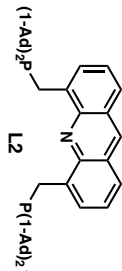
³¹P NMR experiment performed at 25 °C in CDCl₃



IR spectrum



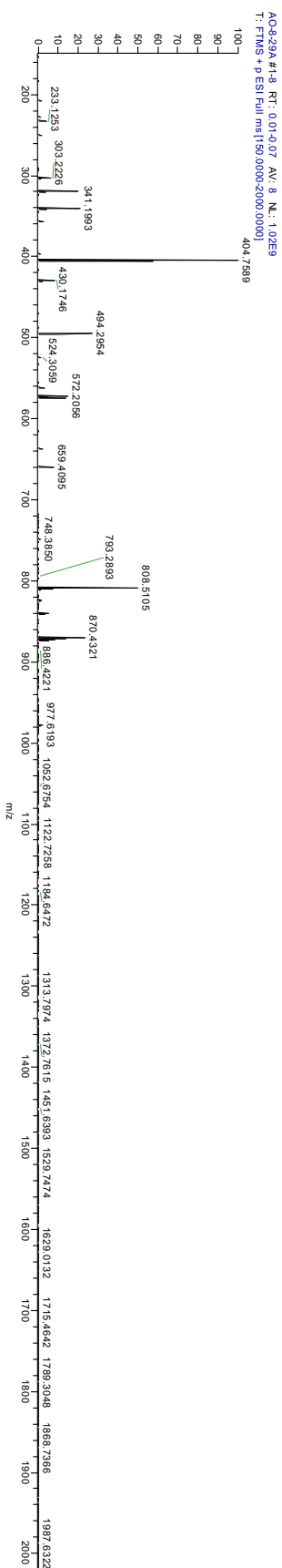
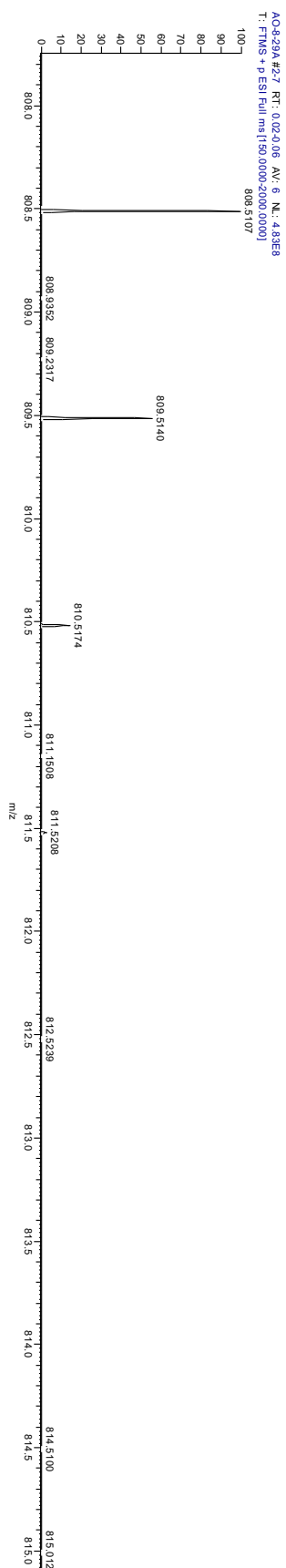
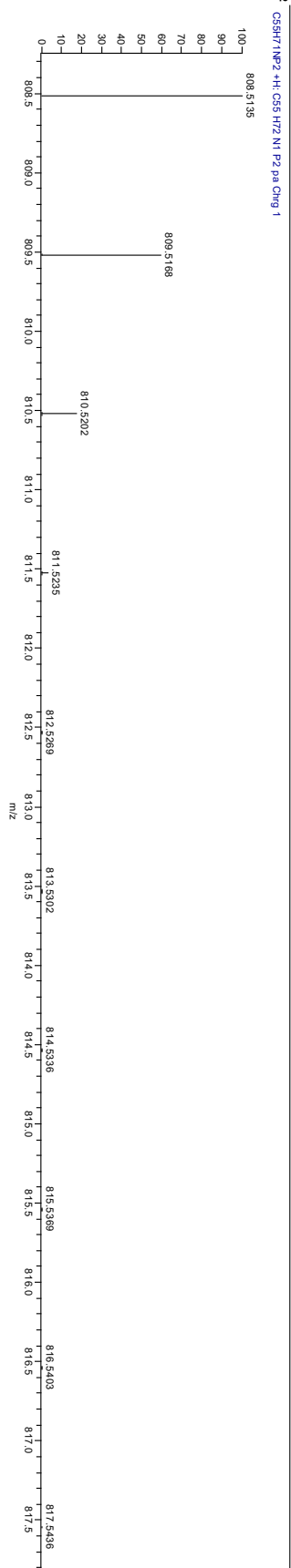
No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	1050.28	93.14	2.853	1057.99	1041.6	0.377	0.081
2	1073.42	94.816	1.484	1077.28	1067.64	0.192	0.037
3	1099.46	93.272	3.204	1114.89	1089.82	0.546	0.158
4	1175.65	94.751	0.471	1179.51	1172.76	0.15	0.007
5	1257.63	94.863	0.361	1261.49	1255.7	0.128	0.006
6	1301.03	91.814	4.136	1309.71	1288.49	0.527	0.147
7	1341.54	91.064	4.011	1346.36	1331.89	0.387	0.101
8	1350.22	93.254	1.553	1360.82	1347.32	0.313	0.034
9	1426.41	94.558	0.387	1428.34	1420.62	0.17	0.009
10	1433.16	93.906	0.198	1434.12	1428.34	0.149	0.003
11	1444.73	87.354	7.499	1458.23	1435.09	0.932	0.415
12	1526.71	94.733	2.431	1534.42	1520.92	0.24	0.072
13	1621.22	95.355	1.014	1635.69	1617.37	0.28	0.025
14	2844.13	85	9.535	2863.42	2822.92	1.612	0.636
15	2895.25	79.37	10.305	2917.43	2864.39	3.641	1.267

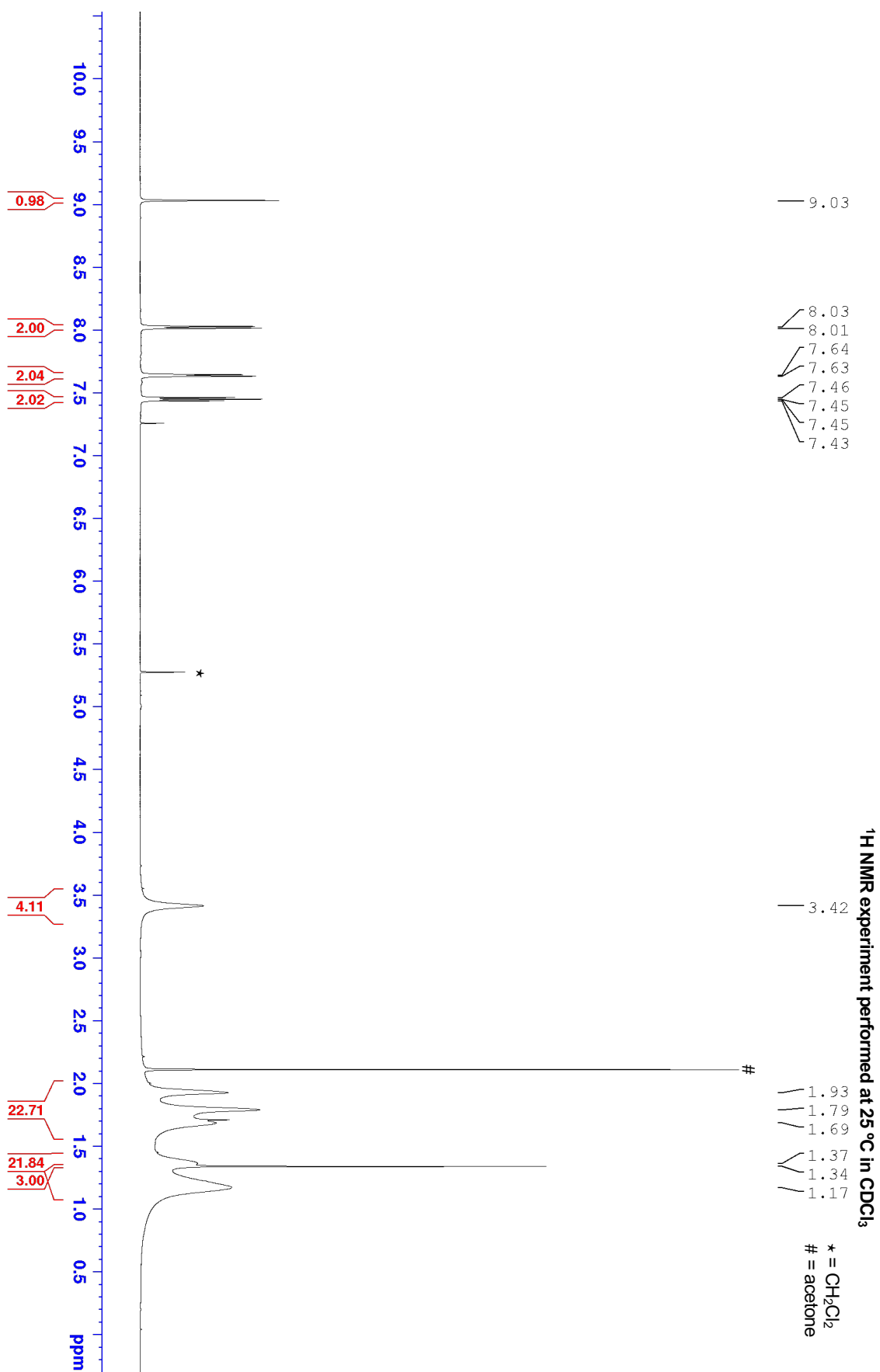
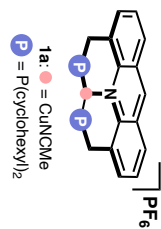


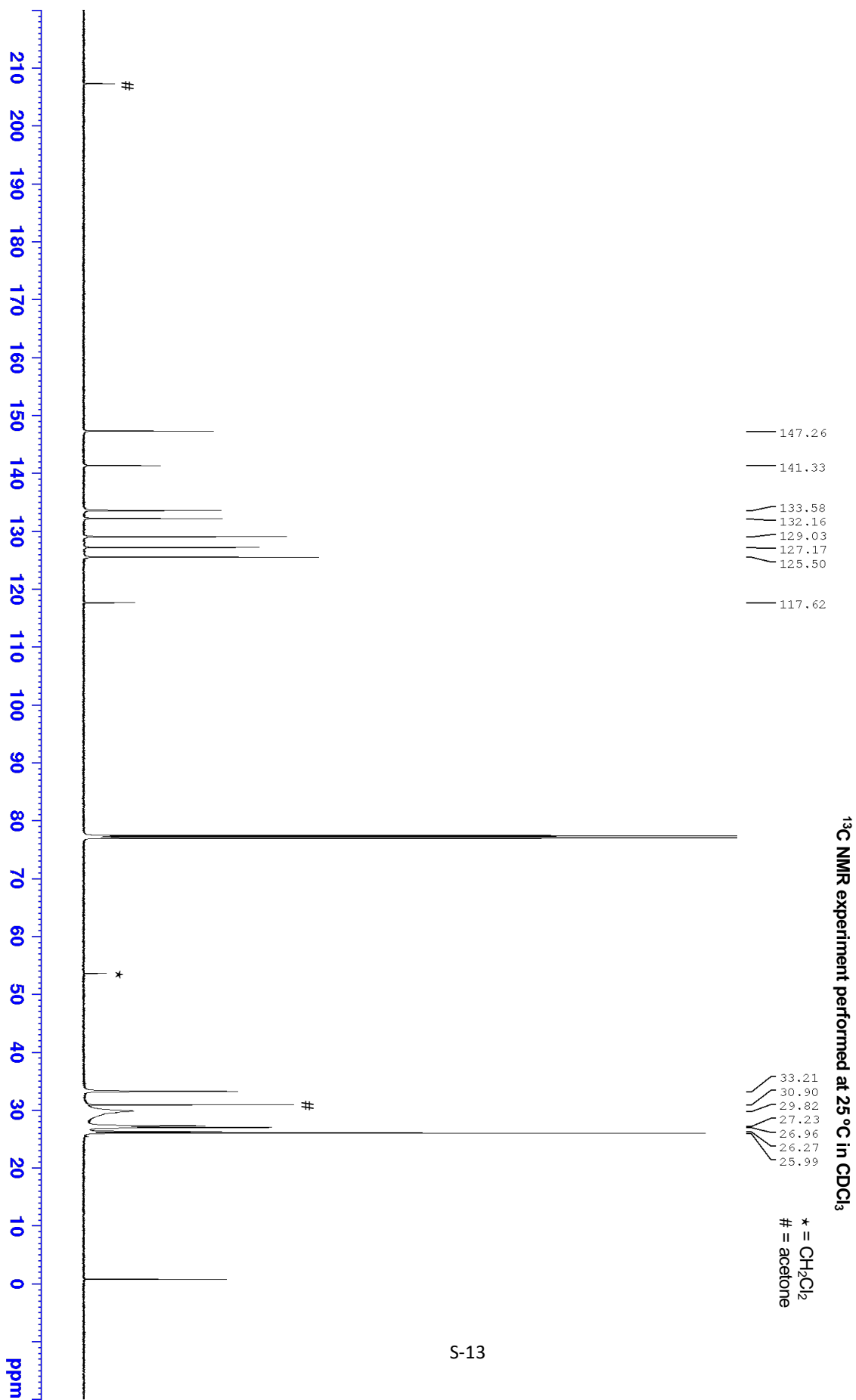
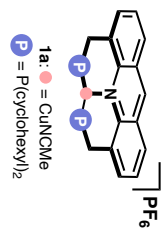
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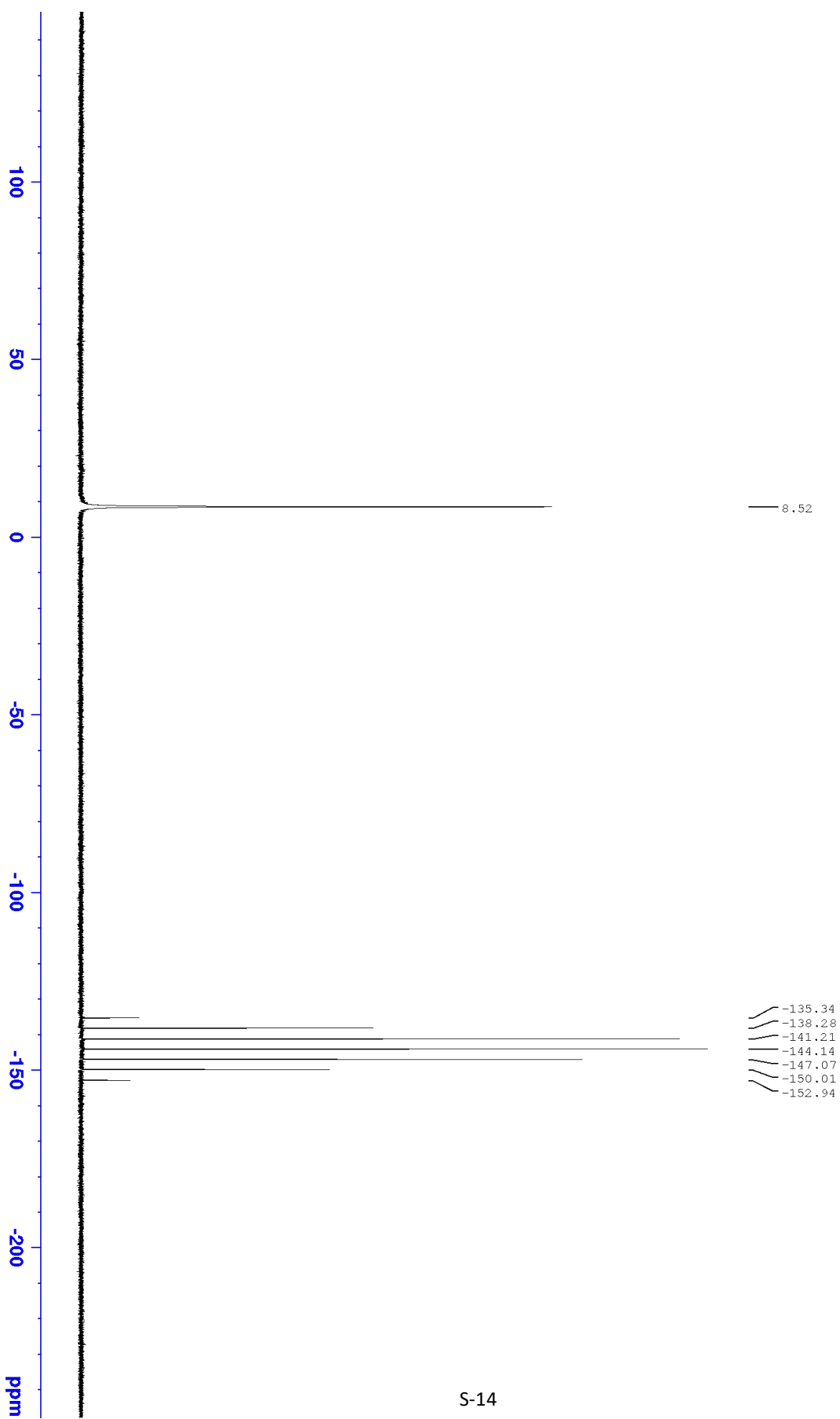
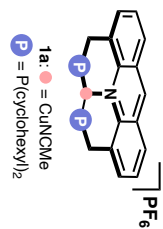
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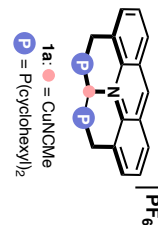
HRESIMS experiment



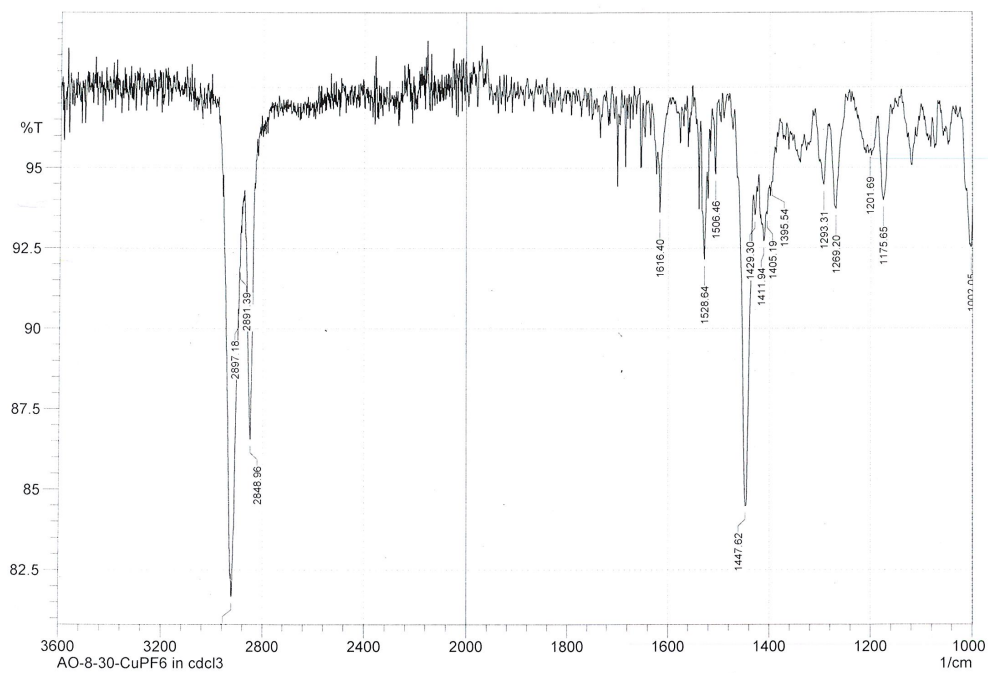




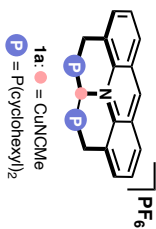




IR spectrum



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	1002.05	92.529	1.371	1009.77	999.16	0.332	0.047
2	1175.65	93.975	2.744	1185.3	1162.15	0.496	0.164
3	1201.69	95.531	0.038	1202.66	1200.73	0.038	0
4	1269.2	93.711	2.987	1281.74	1250.88	0.633	0.197
5	1293.31	94.467	1.254	1300.07	1285.6	0.311	0.041
6	1395.54	94.535	0.181	1396.51	1389.76	0.147	0.003
7	1405.19	93.54	0.23	1406.15	1401.33	0.129	0.002
8	1411.94	92.708	0.612	1413.87	1407.12	0.211	0.011
9	1429.3	93.519	0.675	1431.23	1425.44	0.159	0.011
10	1447.62	84.472	9.945	1462.09	1432.19	1.424	0.676
11	1506.46	94.796	1.978	1510.31	1503.56	0.123	0.027
12	1528.64	92.146	1.874	1531.53	1523.82	0.233	0.035
13	1616.4	93.605	2.167	1620.26	1603.86	0.333	0.052
14	2848.96	86.56	7.887	2874.03	2833.52	1.769	0.759
15	2891.39	91.896	0.294	2892.36	2888.5	0.129	0.001
16	2897.18	90.453	0.406	2898.14	2893.32	0.196	0.007
17	2923.22	81.674	1.548	2926.11	2902	1.722	0.137

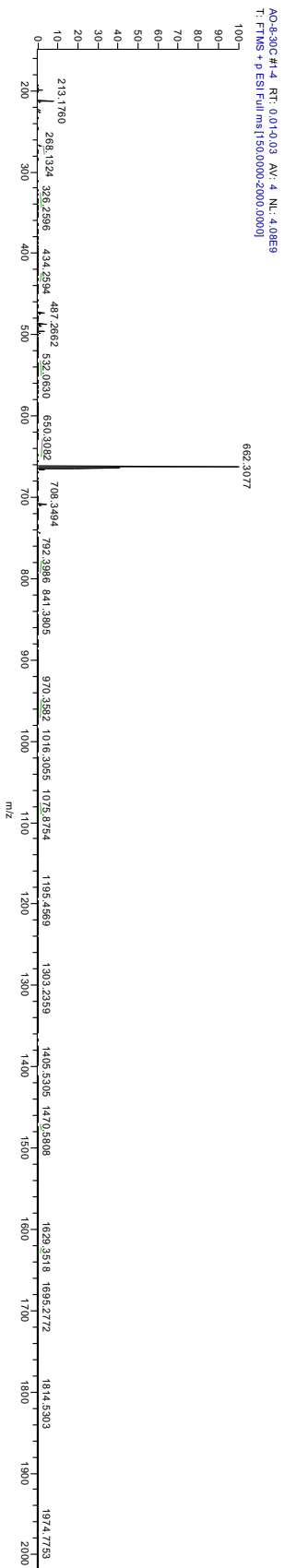
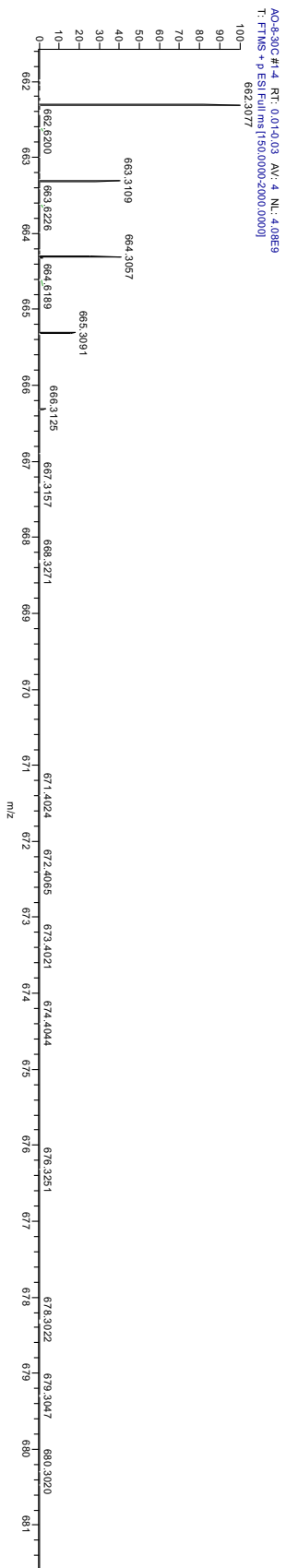
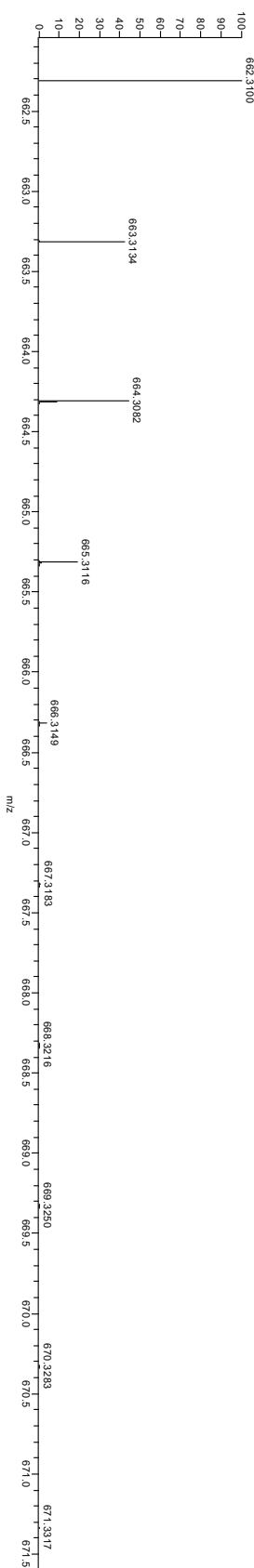


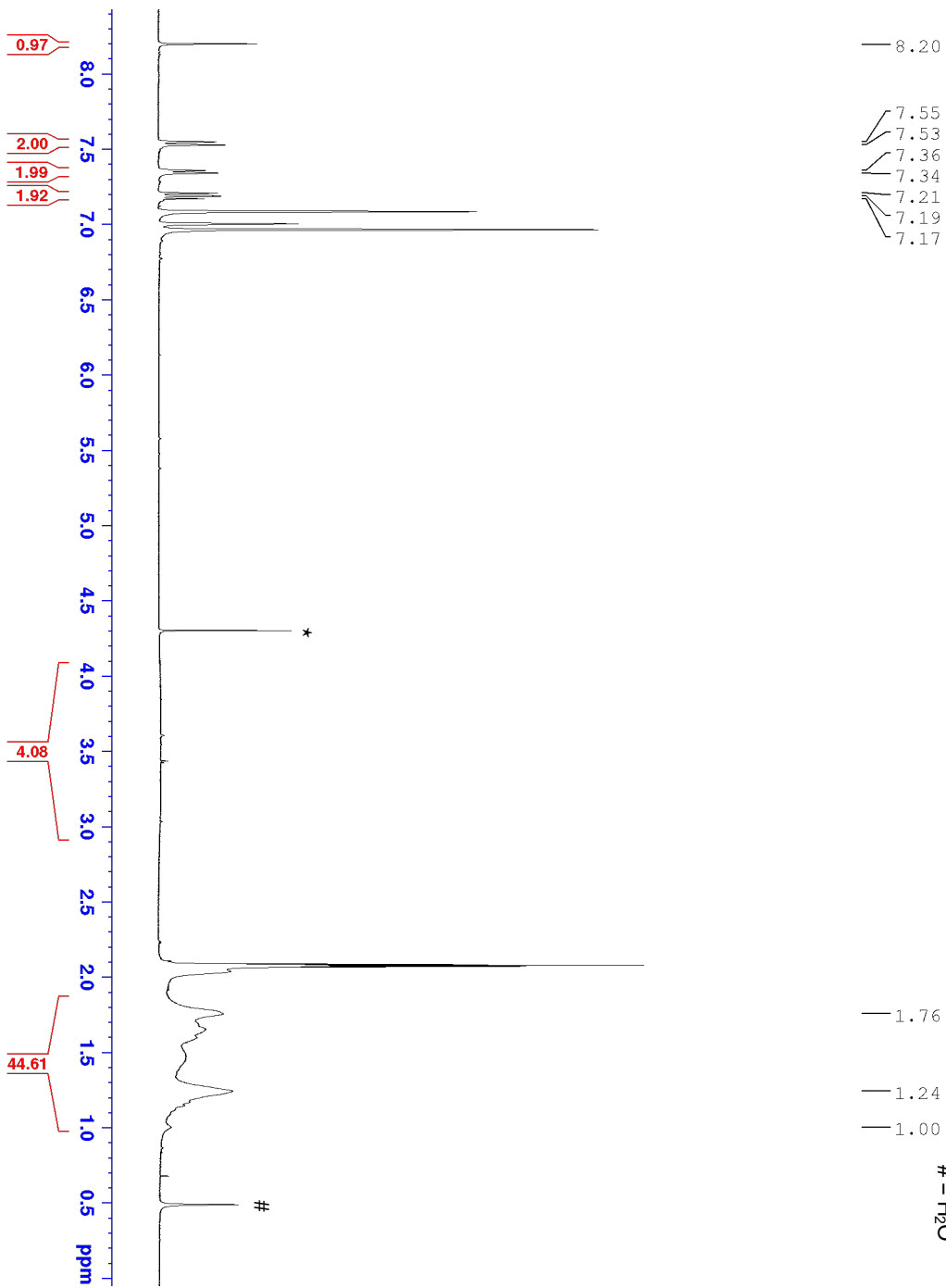
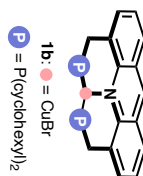
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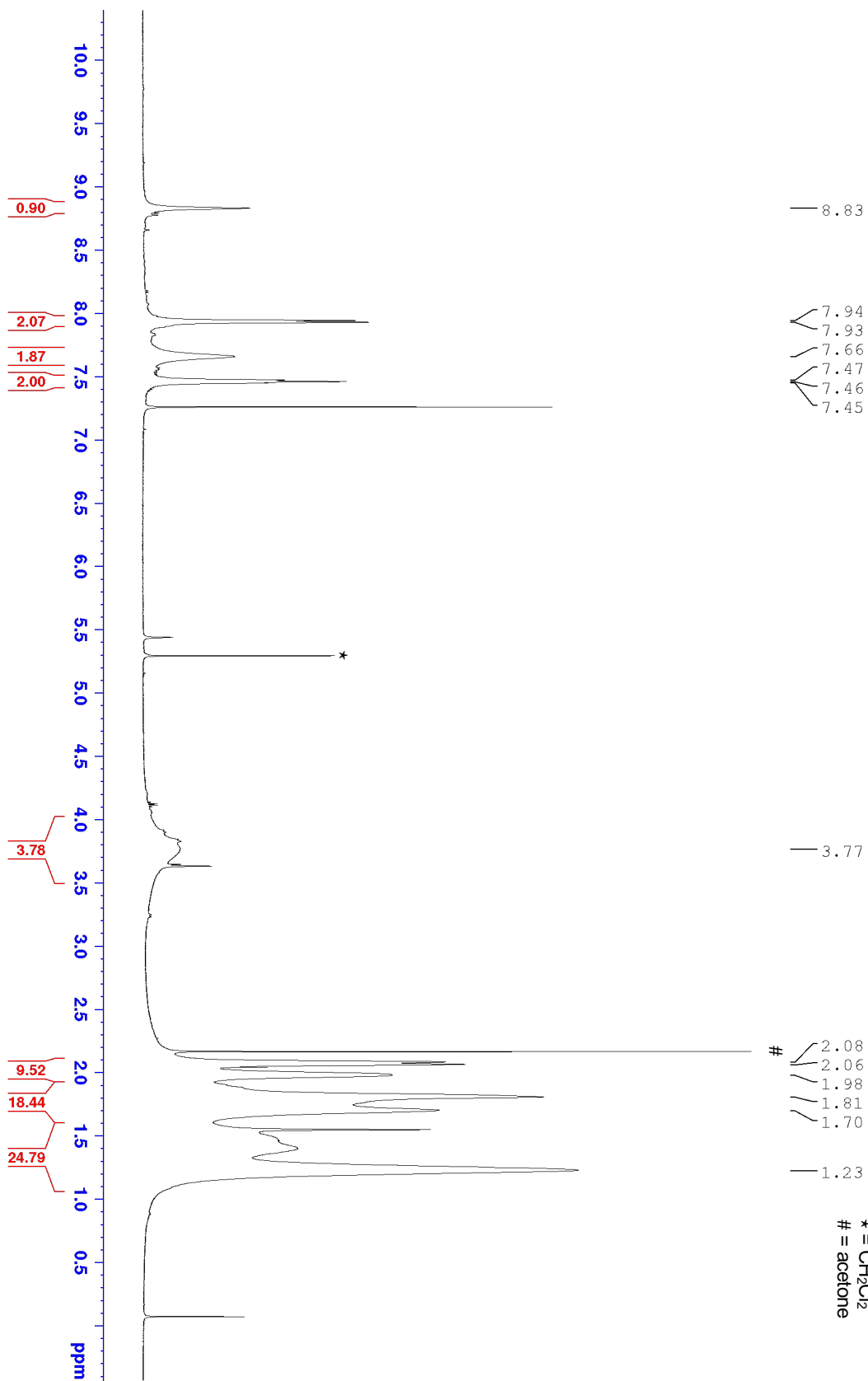
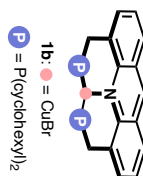
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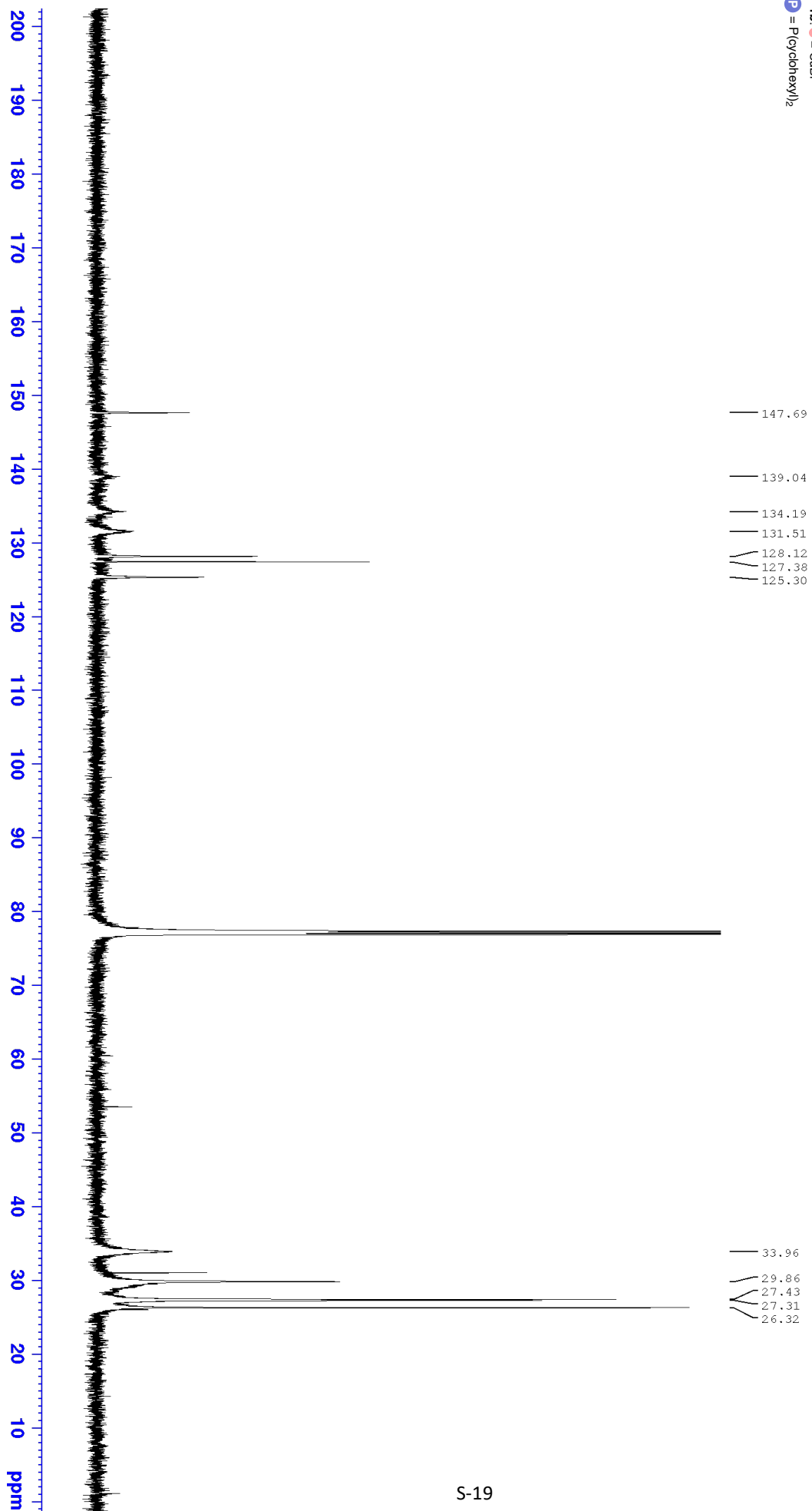
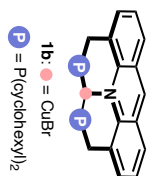
HRESIMS experiment

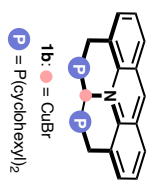
C39H55OINP2: C9 H95 Cu1 Ni1 P2 pa.Chng 1



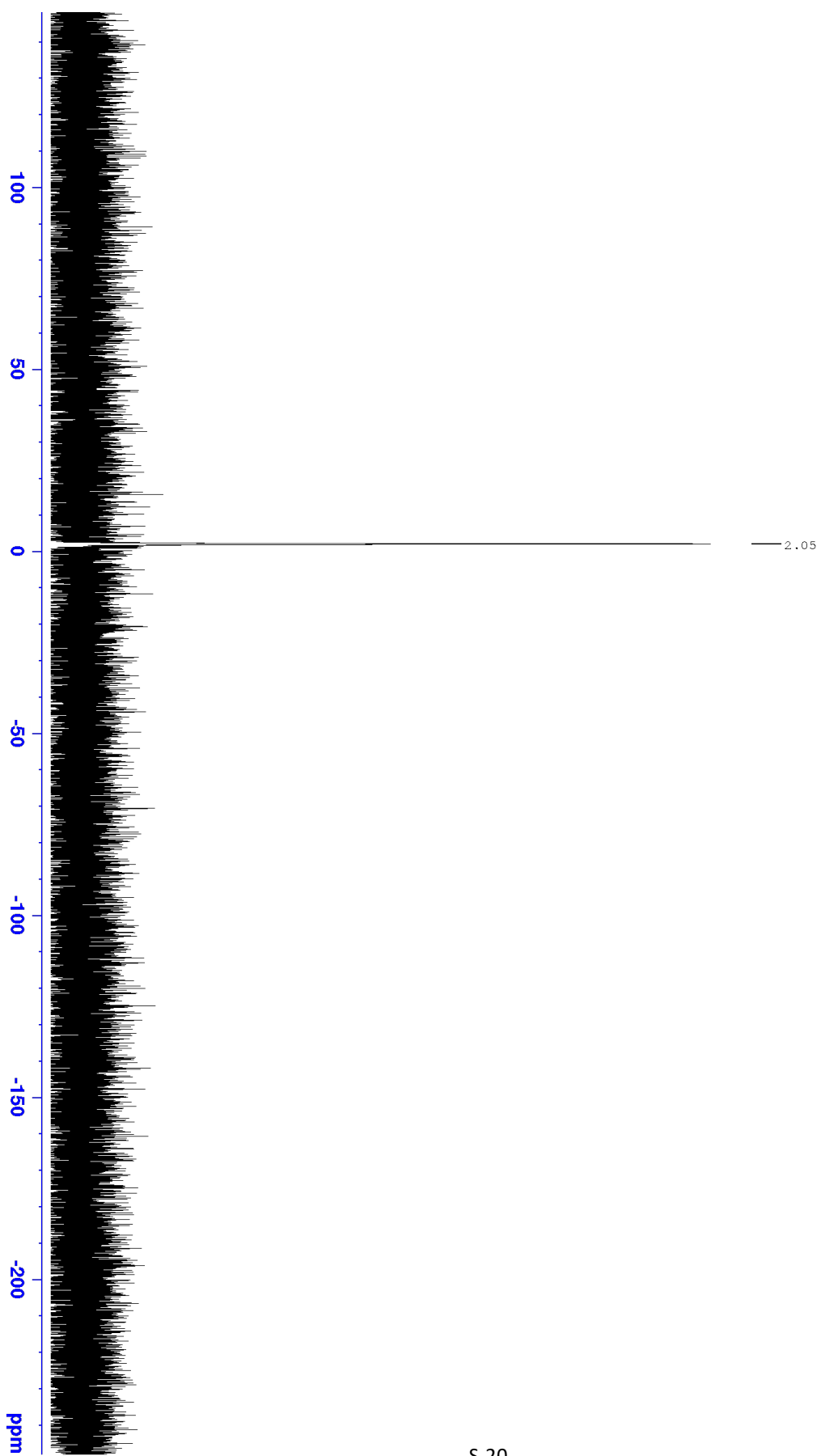




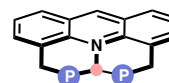




³¹P NMR experiment performed at 25 °C in CDCl₃

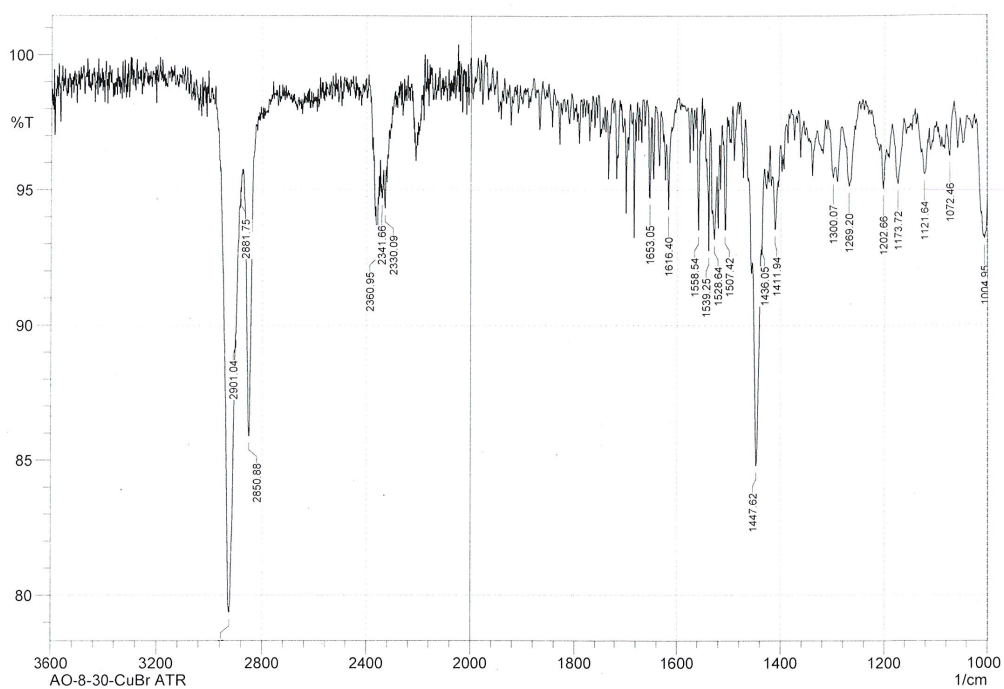


IR spectrum

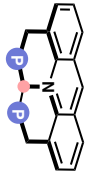


1b: ● = CuBr

● = P(cyclohexyl)₂



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	1004.95	93.196	0.31	1005.91	999.16	0.19	0.011
2	1072.46	96.242	1.522	1079.21	1063.78	0.189	0.041
3	1121.64	95.566	1.075	1126.47	1114.89	0.204	0.034
4	1173.72	95.207	2.316	1185.3	1162.15	0.376	0.124
5	1202.66	95.035	1.556	1208.44	1196.87	0.209	0.035
6	1269.2	95.128	1.763	1274.99	1258.59	0.295	0.078
7	1300.07	95.45	0.929	1310.67	1295.24	0.247	0.023
8	1411.94	93.527	1.827	1415.8	1407.12	0.218	0.037
9	1436.05	92.606	0.631	1437.02	1432.19	0.113	0
10	1447.62	84.787	7.583	1454.38	1438.94	0.834	0.304
11	1507.42	93.511	3.608	1510.31	1503.56	0.14	0.059
12	1528.64	93.176	1.549	1531.53	1523.82	0.204	0.03
13	1539.25	92.753	4.058	1543.1	1536.35	0.141	0.046
14	1558.54	93.506	4.06	1562.39	1555.64	0.131	0.058
15	1616.4	94.263	2.622	1620.26	1611.58	0.157	0.04
16	1653.05	94.702	3.214	1658.84	1650.16	0.125	0.048
17	2330.09	94.316	1.219	2334.91	2328.16	0.154	0.02
18	2341.66	94.688	0.588	2342.62	2335.87	0.145	0.01
19	2360.95	92.964	1.569	2364.81	2356.13	0.253	0.042
20	2850.88	85.884	10.659	2874.03	2825.81	1.709	0.983
21	2881.75	94.916	0.303	2882.71	2877.89	0.098	0.002
22	2901.04	89.667	0.316	2902	2887.53	0.507	0.004
23	2924.18	79.363	12.601	2957.94	2902.96	3.625	1.776



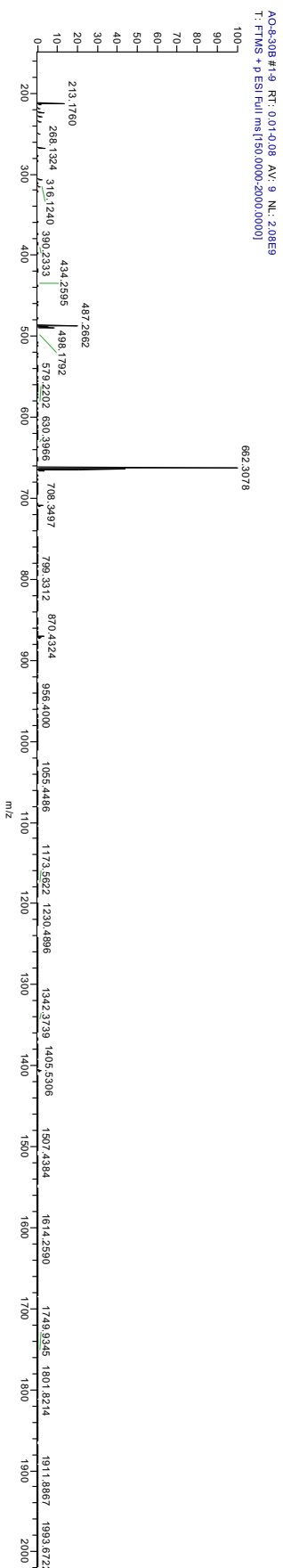
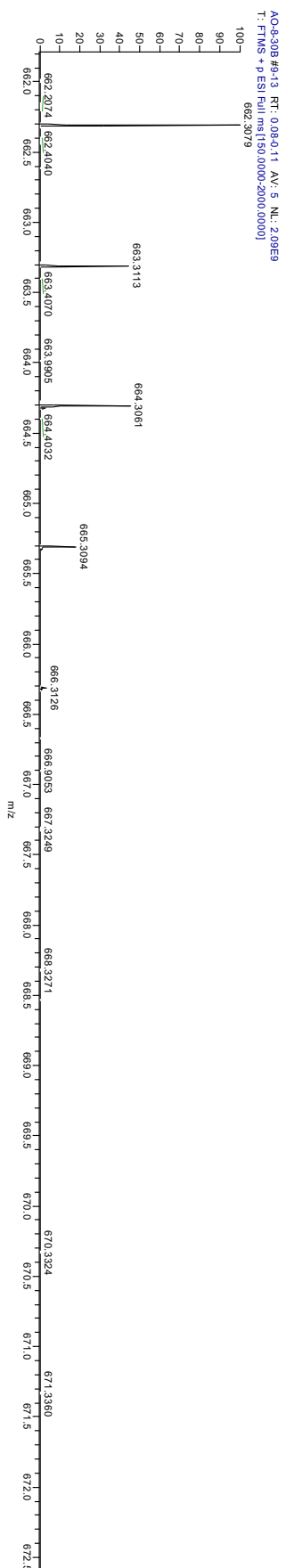
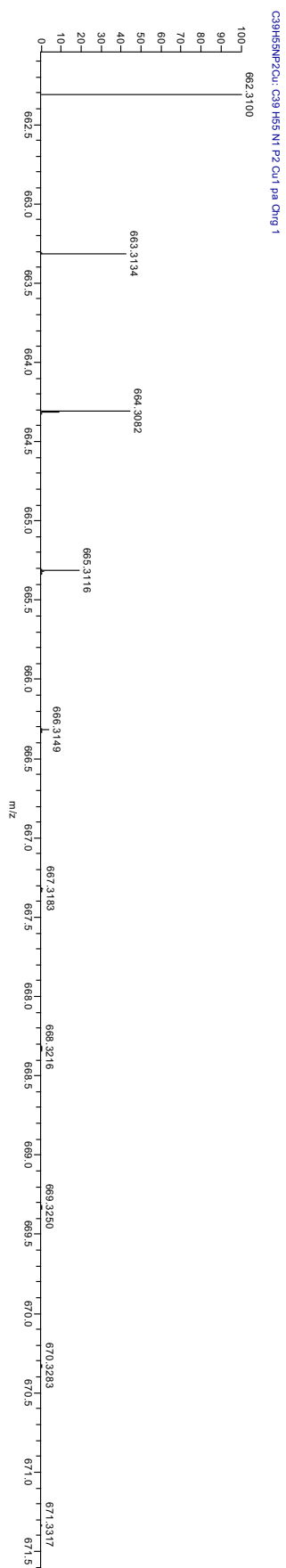
1b: ● = OMe

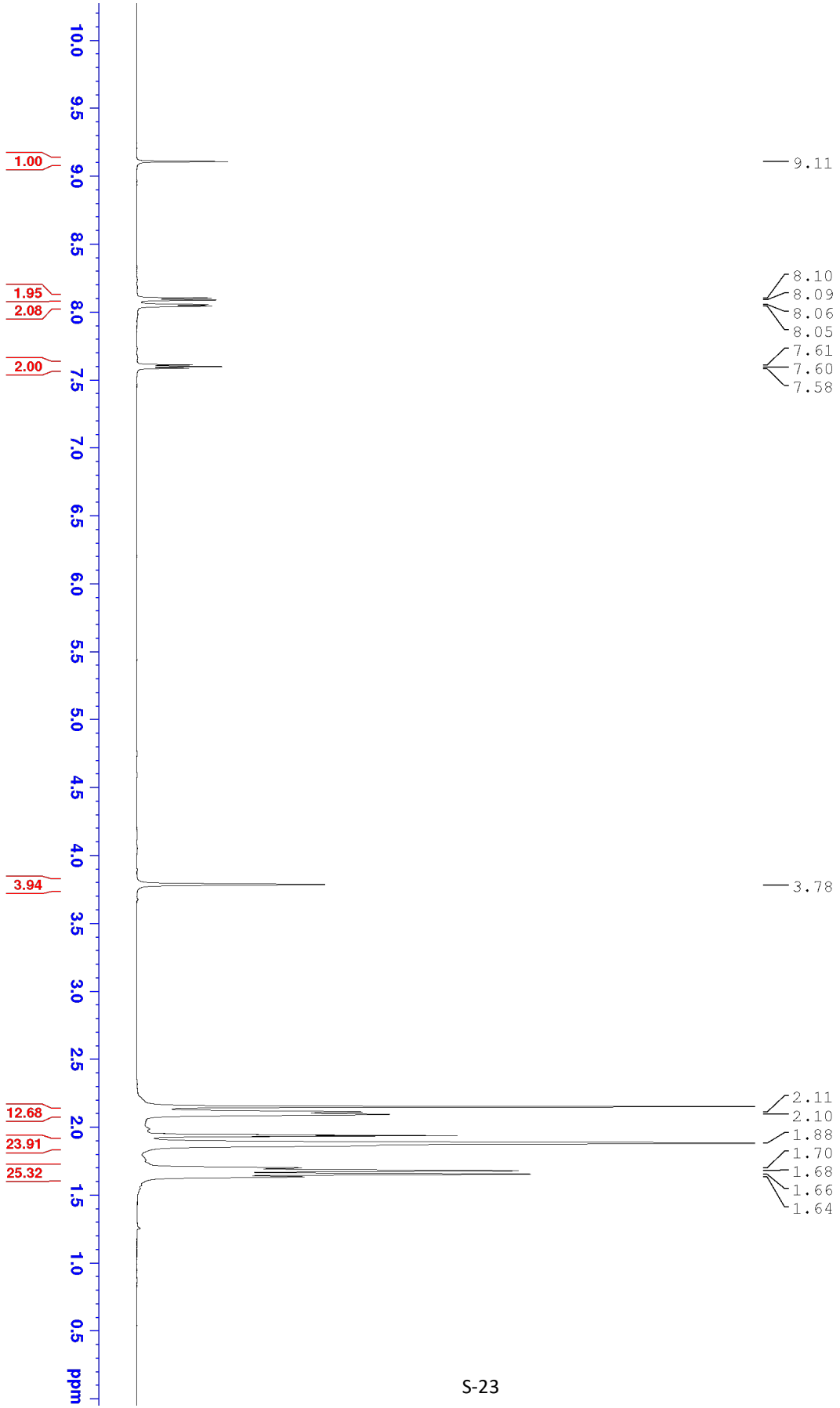
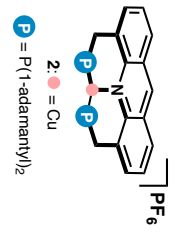
● = P(cyclohexyl)₂

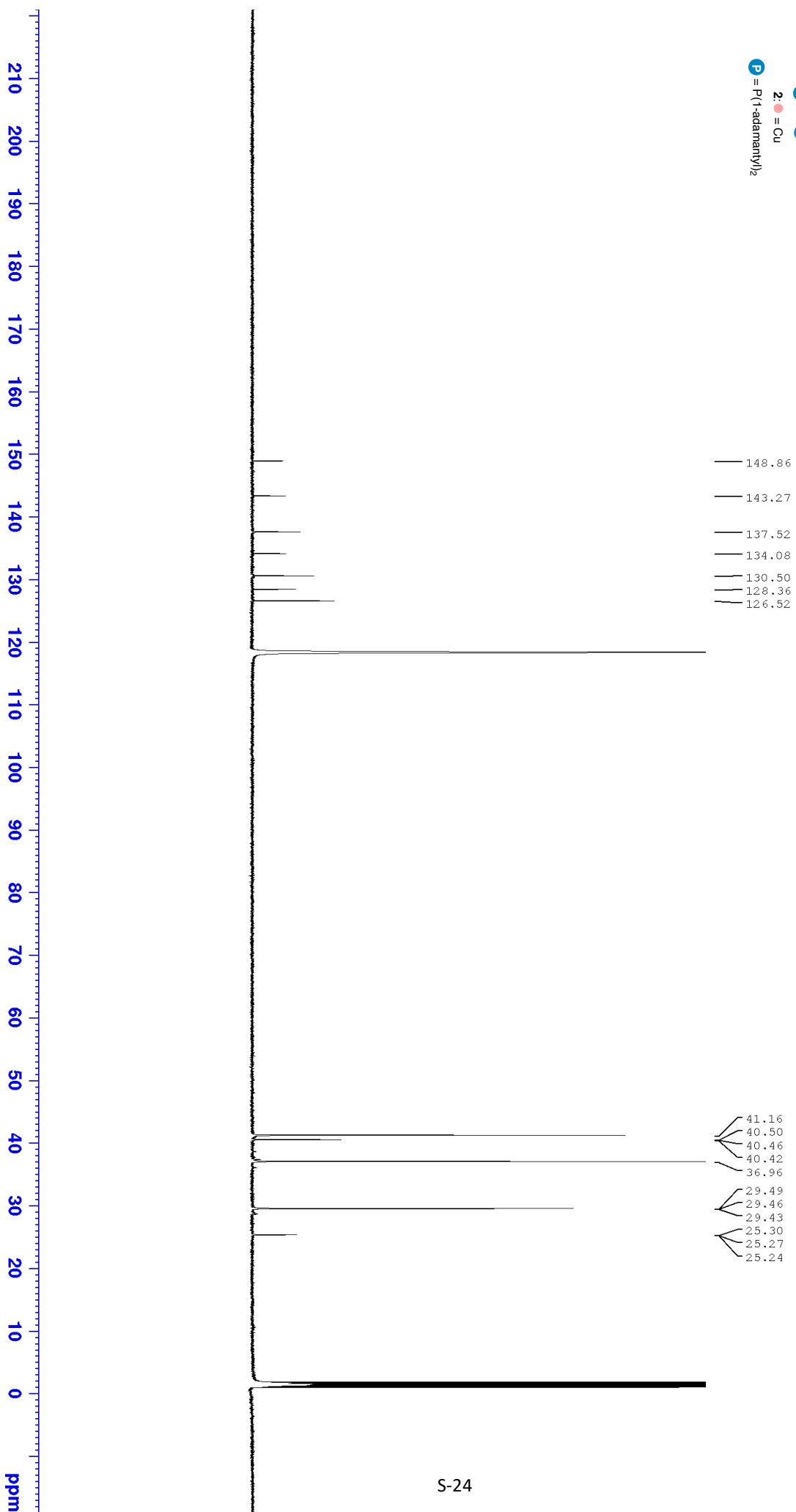
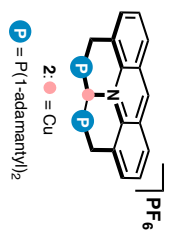
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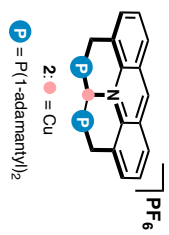
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HRESIMS experiment

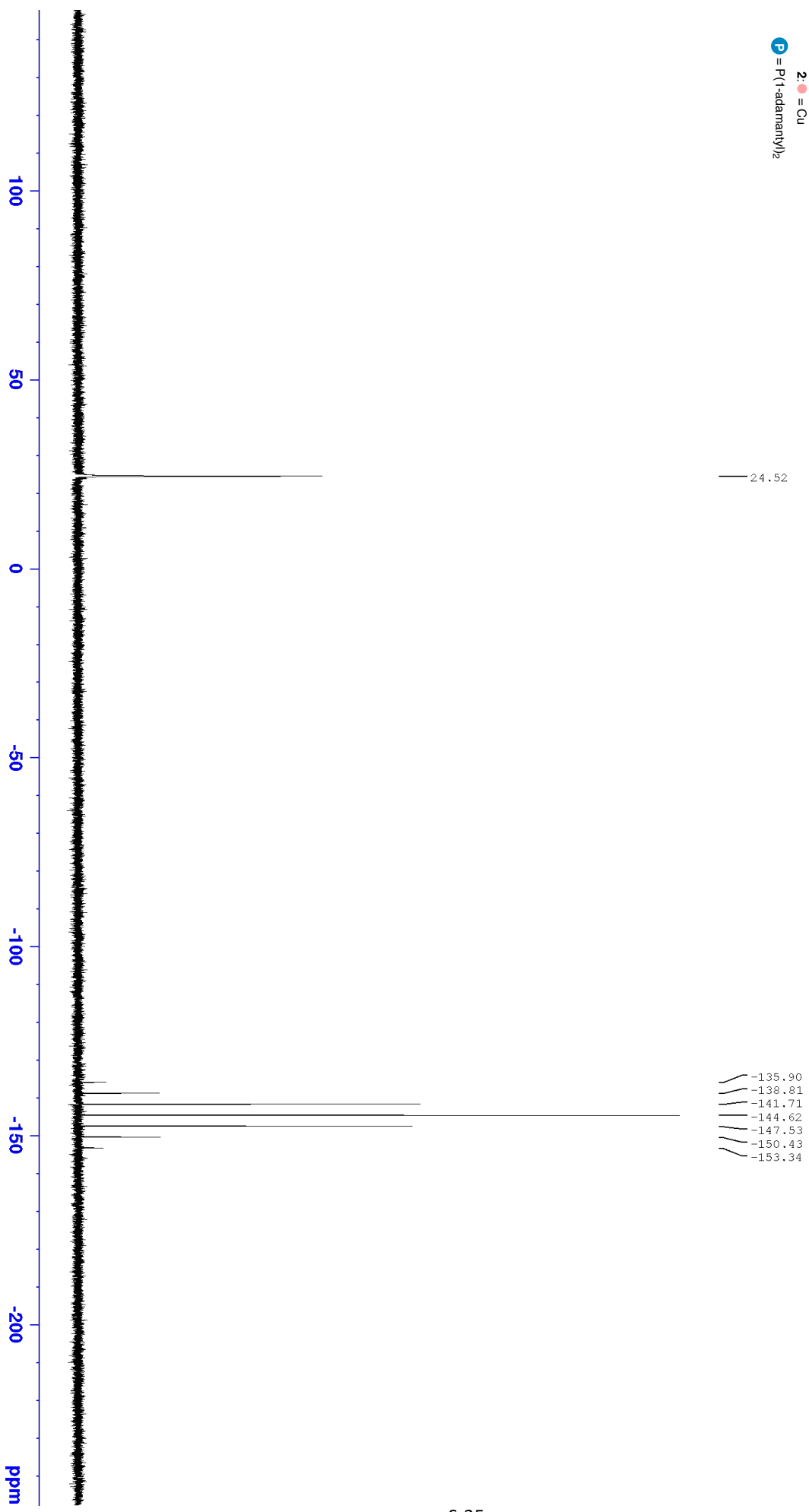




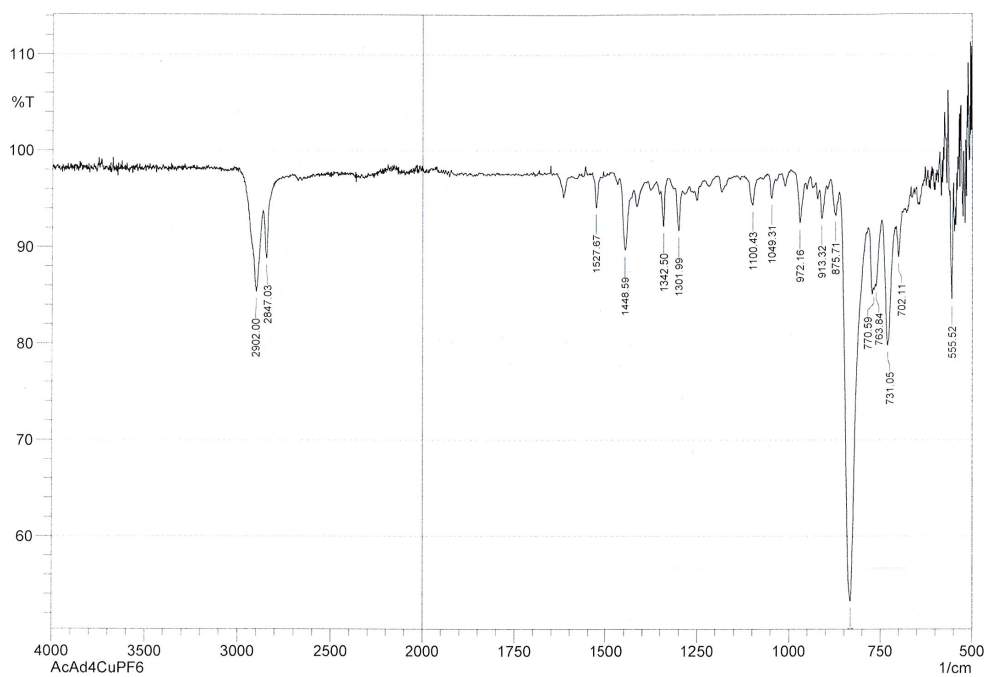
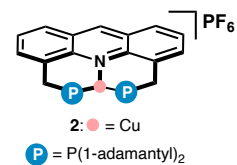




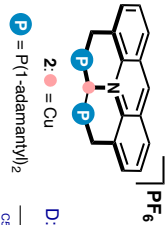
^{31}P NMR experiment performed at 25 °C in CDCl_3



IR spectrum



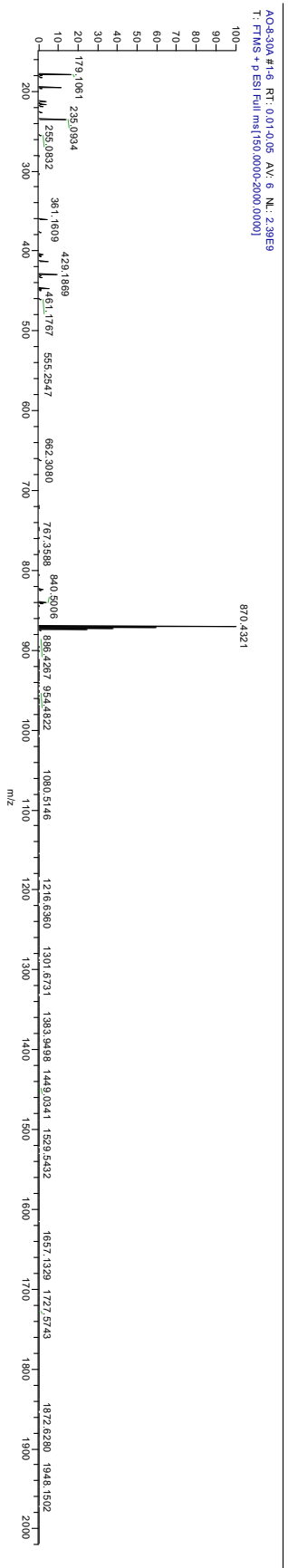
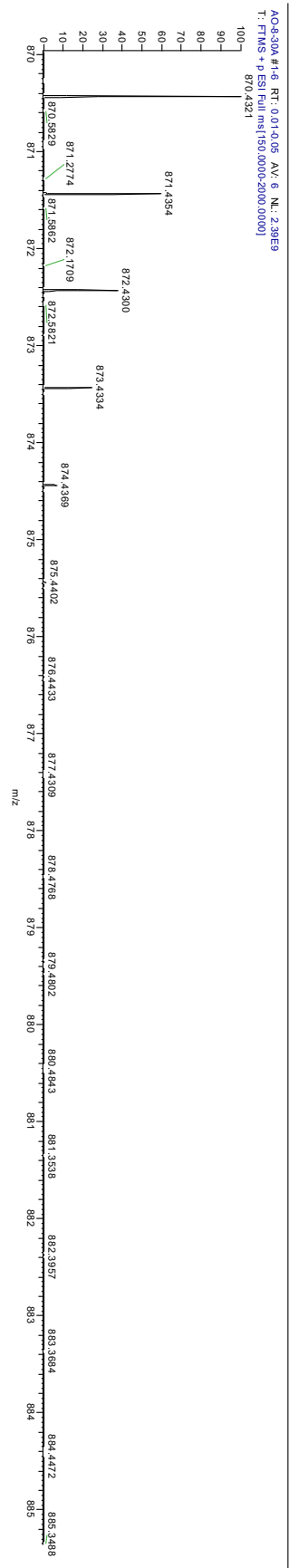
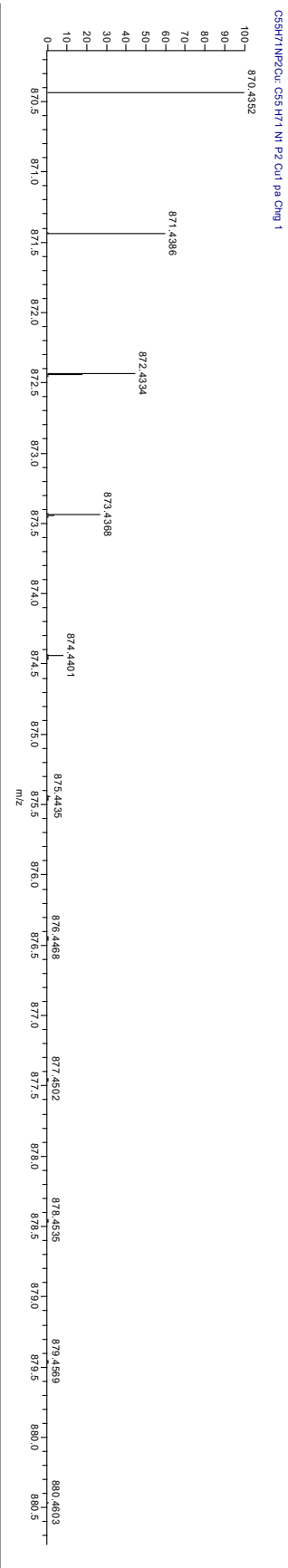
No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	555.52	84.572	11.354	560.34	551.66	0.419	0.262
2	702.11	88.959	3.734	707.9	692.47	0.626	0.135
3	731.05	79.788	12.572	747.44	711.76	2.279	1.04
4	763.84	85.943	0.941	765.77	748.41	0.823	0.016
5	770.59	85.546	0.359	772.52	766.73	0.385	0.006
6	833.28	53.285	40.572	865.1	791.81	9.229	7.102
7	875.71	93.299	1.978	890.18	870.89	0.436	0.082
8	913.32	92.941	3.134	920.08	900.79	0.458	0.128
9	972.16	92.508	4.662	984.69	956.72	0.594	0.239
10	1049.31	95.071	2.236	1059.92	1040.63	0.306	0.08
11	1100.43	94.387	2.632	1113.93	1088.85	0.461	0.132
12	1301.99	91.669	4.327	1312.6	1292.35	0.531	0.172
13	1342.5	92.165	4.232	1350.22	1331.89	0.403	0.119
14	1448.59	89.711	6.473	1464.98	1431.23	1.016	0.436
15	1527.67	94.128	3.445	1539.25	1516.1	0.394	0.147
16	2847.03	88.84	5.539	2862.46	2809.41	1.609	0.431
17	2902	85.348	0.894	2903.93	2867.28	1.786	0.09

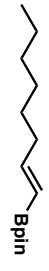


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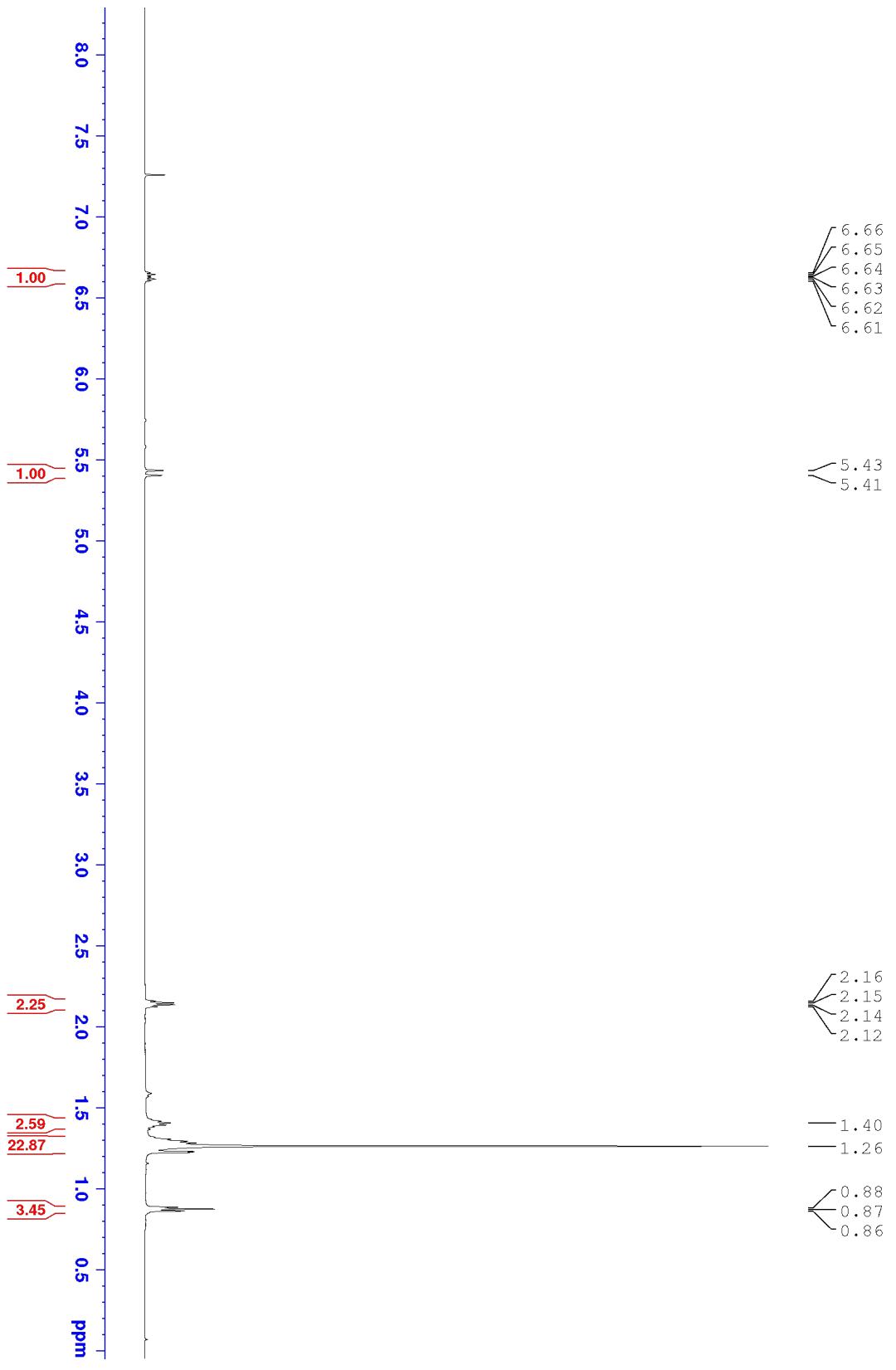
03/02/23 09:32:52

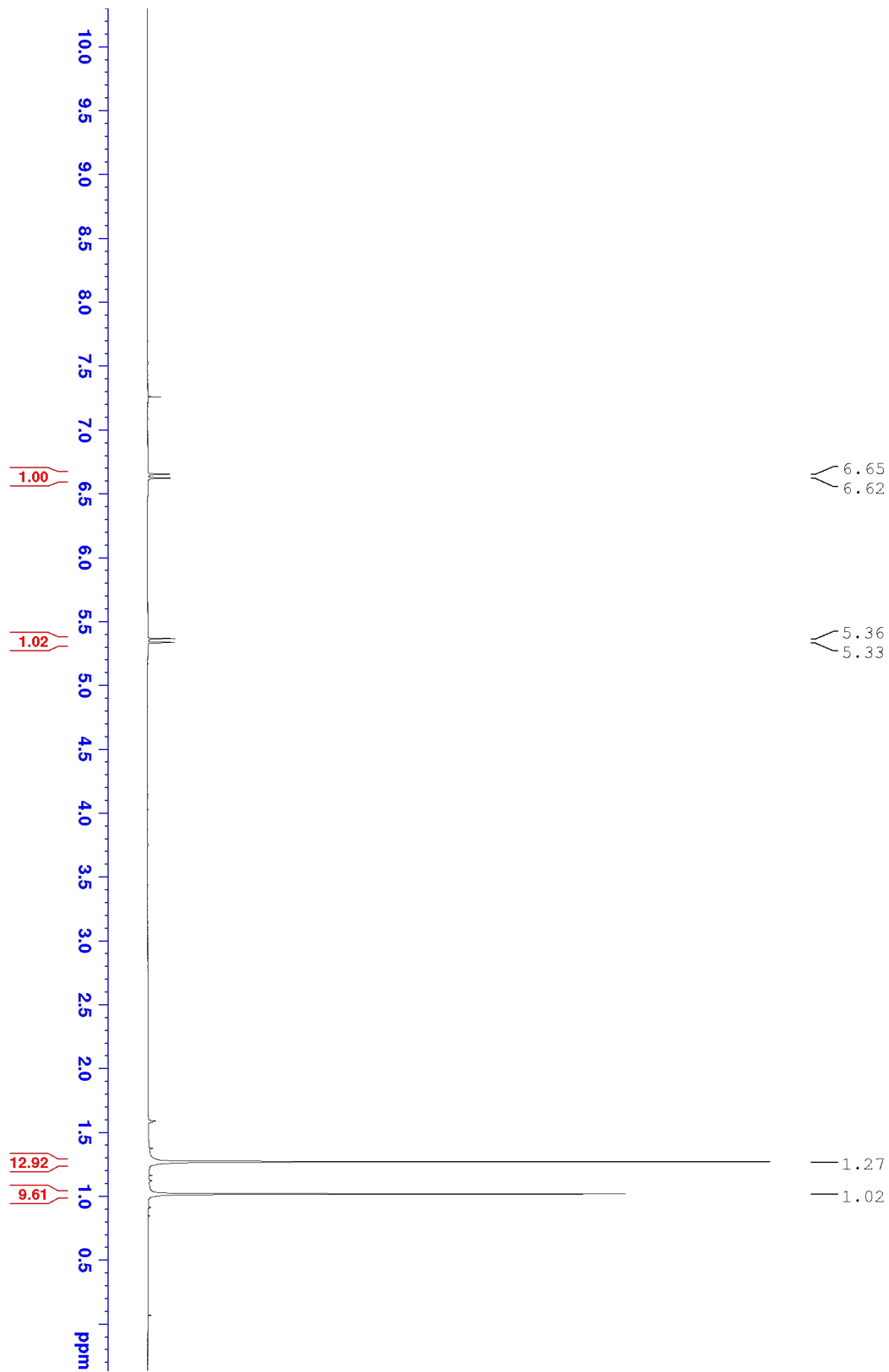
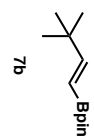
HRESIMS experiment

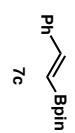




¹H NMR experiment performed at 25 °C in CDCl₃







¹H NMR experiment performed at 25 °C in CDCl₃

