Supporting Information

Copper Cluster Complex Catalyzed C-S Bond Formation

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Table of Contents

Table S1. Crystallographic Data of Complexes **A**, **B** and **C**.

Complex	**A**	**B**	**C**
Formula	$C_{80}H_{84}Cu_8N_{24}O_{36}$	$C_{64}H_{58}Cu_4N_8O_{14}$	$C_{46}H_{62}Cu_4N_{14}O_{22}$
CCDC no.	2013079	2013080	2013078
Formula weight	2466.03	1417.38	1417.30
Temp (K)	200(2) K	150(2) K	150(2) K
Crystal system	monoclinic	monoclinic	triclinic
Space group	C 2/c	I 2/a	P-1
a (Å)	23.249(4)	24.8301(13)	6.9977(3)
b (Å)	24.663(4)	11.1779(6)	13.6034(8)
c (Å)	19.015(3)	25.5838(10)	16.4938(9)
α (deg)	90	90	111.441(5)
β (deg)	114.638(3)	117.139(3)	91.672(4)
γ (deg)	90	90	104.326(5)
V(Å^3)	9910(3)	6319.0(6)	1403.47(14)
Z	4	4	1
D_{calc}(g/cm^3)	1.653	1.490	1.677
μ (Mo Kα) (mm^{-1})	1.778	1.399	1.587
F(000)	5008.0	2904.0	728.0
N_{ref}, N_{par}	8781, 629	6224, 409	5521, 376
$R1[I > 2\sigma(I)]$	0.0717	0.0530	0.0742
w$R2$ $[I > 2\sigma(I)]$	0.2091	0.2183	0.2996
S	0.987	1.027	1.063

Table S2. Selected angle and bond lengths (Å) for complexes **A**

C1-O1	1.293(10)	C21-C22	1.382(12)	N4-Cu2	1.937(6)
C1-C7	1.372(12)	C22-C23	1.375(12)	N5-N6	1.382(9)
C1-C2	1.453(11)	C23-C24	1.432(12)	N5-Cu3	1.942(6)
C2-O2	1.362(10)	C24-C25	1.412(11)	N6-Cu4	1.982(6)
C2-C4	1.367(12)	C25-N5	1.304(10)	N7-N8	1.408(8)
C3-O2	1.417(9)	C26-O8	1.272(9)	N8-Cu4	1.939(8)
C4-C5	1.393(12)	C26-N6	1.337(11)	N11-O17	1.12(4)
C5-C6	1.330(11)	C26-N7	1.353(10)	N11-O16	1.32(2)
C6-C7	1.420(12)	C27-N8	1.301(10)	N11-O18	1.33(7)
C7-C8	1.435(10)	C27-C28	1.429(11)	N11'-O16'	1.08(5)
C8-N1	1.300(9)	C28-C29	1.401(12)	N11'-O18'	1.26(4)
C9-O3	1.277(8)	C28-C34	1.403(12)	N11'-O17'	1.37(3)
C9-N3	1.330(9)	C29-C30	1.380(12)	N12-O14	1.196(9)
C9-N2	1.360(9)	C30-C31	1.390(13)	N12-O13	1.236(9)
C10-N4	1.302(9)	C31-C32	1.346(13)	N12-O15	1.244(9)
C10-C11	1.447(10)	C32-O9	1.387(11)	O1-Cu1	1.874(5)
C11-C17	1.391(10)	C32-C34	1.441(12)	O3-Cu2	1.937(5)
C11-C12	1.415(10)	C33-O9	1.426(9)	O4-Cu2	1.938(5)
C12-C13	1.342(11)	C34-O10	1.291(10)	O4-Cu3	1.997(4)
C13-C14	1.401(11)	C35-O11	1.253(10)	O5-Cu3	2.270(5)
C14-C15	1.355(10)	C35-N9	1.296(11)	O6-Cu3	1.932(5)
C15-O5	1.370(9)	C36-N9	1.429(11)	O6-Cu2	1.982(5)
C15-C17	1.438(11)	C37-N9	1.449(13)	O7-Cu2	2.230(6)
C16-O5	1.398(10)	C38-N10	1.31(2)	O8-Cu3	1.961(5)
C17-O4	1.354(8)	C38-O12	1.427(19)	O10-Cu4	1.881(6)
C18-O6	1.377(9)	C39-N10	1.366(13)	O11-Cu1	1.969(6)
C18-C19	1.392(11)	C40-N10	1.439(15)	O12-Cu4	2.175(11)
C18-C24	1.396(10)	N1-N2	1.414(8)	O16-Cu4	2.028(14)
C19-O7	1.361(9)	N1-Cu1	1.921(6)	O16'-Cu4	2.20(2)
C19-C21	1.387(12)	N3-N4	1.386(8)	Cu2-O6	1.982(5)
C20-O7	1.420(9)	N3-Cu1	1.980(6)	Cu2-O7	2.230(6)

∠C1-C7-C6	120.5(9)	∠C26-N6-Cu4	119.4(9)	∠N1-C8-C7	126.8(6)
∠C1-C7-C8	114.4(8)	∠C26-N6-N5	120.2(9)	∠N1-Cu1-N3	112.7(5)
∠C1-O1-Cu1	116.3(7)	∠C26-N7-N8	117.0(9)	∠N1-Cu1-O11	119.4(4)
∠C10-N4-Cu2	123.9(7)	∠C27-N8-Cu4	117.8(9)	∠N10-C38-O12	113.9(2)
∠C10-N4-N3	124.1(7)	∠C27-N8-N7	116.9(8)	∠N11-O16-Cu4	111.8(5)
∠C11-C17-C15	121.9(8)	∠C28-C34-C32	119.4(8)	∠N11'-O16'-Cu4	129.8(5)
∠C12-C11-C10	124.2(7)	∠C29-C28-C27	122.8(10)	∠N2-N1-Cu1	127.2(5)
∠C12-C13-C14	119.6(7)	∠C29-C30-C31	113.1(9)	∠N3-N4-Cu2	108.8(6)
∠C13-C12-C11	121.2(8)	∠C29-C28-C34	123.6(9)	∠N3-C9-N2	114.6(6)
∠C14-C15-C17	119.1(8)	∠C30-C29-C28	121.2(8)	∠N4-C10-C11	134.8(6)
∠C14-C15-O5	117.6(7)	∠C31-C32-C34	115.2(9)	∠N4-N3-Cu1	127.8(6)
∠C15-C14-C13	118.3(6)	∠C31-C32-O9	125.9(16)	∠N4-Cu2-O4	114.9(5)
∠C15-O5-C16	118.2(7)	∠C32-C31-C30	125.0(8)	∠N4-Cu2-O6	128.2(6)
∠C15-O5-Cu3	120.6(7)	∠C32-O9-C33	121.9(9)	∠N4-Cu2-O7	118.9(12)
∠C16-O5-Cu3	113.7(6)	∠C34-C28-C27	107.3(15)	∠N5-C25-C24	107(3)
∠C17-C11-C10	120.4(8)	∠C34-O10-Cu4	126.7(13)	∠N5-N6-Cu4	120.7(18)
∠C17-C11-C12	116.6(8)	∠C35-N9-C36	119.4(8)	∠N5-Cu3-O4	90.7(3)
∠C17-O4-Cu2	117.9(7)	∠C35-N9-C37	120.9(8)	∠N5-Cu3-O5	112.6(6)
∠C17-O4-Cu3	120.4(9)	∠C35-O11-Cu1	126.0(8)	∠N5-Cu3-O8	118.2(7)
∠C18-C24-C23	117.2(8)	∠C36-N9-C37	120.0(9)	∠N6-N5-Cu3	116.7(7)
∠C18-C24-C25	116.8(8)	∠C38-N10-C39	123.1(8)	∠N6-C26-N7	116.4(7)
∠C18-O6-Cu2	115.7(6)	∠C38-N10-C40	121.9(8)	∠N6-Cu4-O12	125.1(7)
∠C18-O6-Cu3	123.1(8)	∠C38-O12-Cu4	117.2(8)	∠N6-Cu4-O16	81.1(3)
∠C19-O7-C20	118.9(9)	∠C39-N10-C40	129.0(6)	∠N6-Cu4-O16'	171.0(3)
∠C19-C18-C24	115.8(8)	∠C4-C2-C1	114.6(5)	∠N7-N8-Cu4	99.2(2)
∠C19-O7-Cu2	117.6(7)	∠C5-C6-C7	113.2(5)	∠N8-C27-C28	120.8(6)
∠C2-O2-C3	121.5(8)	∠C6-C5-C4	136.8(5)	∠N8-Cu4-N6	82.4(2)
∠C2-C4-C5	120.5(8)	∠C6-C7-C8	129.4(6)	∠N8-Cu4-O12	109.9(6)
∠C20-O7-Cu2	123.0(8)	∠C7-C1-C2	121.0(6)	∠N8-Cu4-O16	91.4(3)
∠C21-C19-C18	124.2(7)	∠C8-N1-Cu1	126.2(5)	∠N8-Cu4-O16'	110.6(7)
∠C22-C21-C19	126.5(8)	∠C8-N1-N2	112.8(5)	∠O1-C1-C2	125.0(8)
∠C22-C23-C24	117.5(9)	∠C9-N3-Cu1	109.0(5)	∠O1-C1-C7	79.2(3)
∠C23-C22-C21	123.1(8)	∠C9-O3-Cu2	124.8(5)	∠O1-Cu1-N1	168.1(3)
∠C25-C24-C23	123.0(8)	∠C9-N2-N1	117.3(5)	∠O1-Cu1-N3	120.4(7)
∠C25-N5-Cu3	121.3(10)	∠C9-N3-N4	113.7(3)	∠O1-Cu1-O11	116.6(7)
∠C25-N5-N6	125.3(8)	∠Cu2-O4-Cu3	110.3(5)	∠O10-C34-C28	118.4(9)
∠C26-O8-Cu3	117.4(7)	∠Cu3-O6-Cu2	121.1(5)	∠O10-C34-C32	117.2(8)

∠O10-Cu4-N6	91.9(3)	∠O17-N11-O16	130(6)	∠O5-C15-C17	125.6(8)
∠O10-Cu4-N8	112.7(7)	∠O17-N11-O18	96.2(6)	∠O6-C18-C19	109.7(2)
∠O10-Cu4-O12	124.4(9)	∠O18'-N11'-O17'	96.5(8)	∠O6-C18-C24	75.88(19)
∠O10-Cu4-O16	178.9(3)	∠O2-C2-C1	92.6(6)	∠O6-Cu3-N5	101.7(2)
∠O10-Cu4-O16'	89.0(2)	∠O2-C2-C4	99.2(8)	∠O6-Cu3-O4	90.2(2)
∠O11-Cu1-N3	114.7(19)	∠O3-C9-N2	44.4(8)	∠O6-Cu3-O5	173.8(2)
∠O11-C35-N9	99.6(4)	∠O3-C9-N3	116.3(18)	∠O6-Cu2-O7	94.3(2)
∠O12-Cu4-O16'	164.3(4)	∠O3-Cu2-N4	113(3)	∠O6-Cu3-O8	90.2(2)
∠O13-N12-O15	86.8(4)	∠O3-Cu2-O4	106(3)	∠O7-C19-C18	107.7(2)
∠O14-N12-O13	55.2(5)	∠O3-Cu2-O6	124(3)	∠O7-C19-C21	92.4(2)
∠O14-N12-O15	121.5(10)	∠O3-Cu2-O7	129(3)	∠O8-C26-N6	98.0(2)
∠O16-Cu4-O12	119.0(9)	∠O4-C17-C11	92.3(2)	∠O8-C26-N7	77.5(2)
∠O16-Cu4-O16'	119.5(10)	∠O4-C17-C15	169.4(2)	∠O8-Cu3-O4	82.2(3)
∠O16-N11-O18	97.1(4)	∠O4-Cu3-O5	174.1(2)	∠O8-Cu3-O5	167.9(2)
∠O16'-N11'-O17'	140.5(4)	∠O4-Cu2-O6	89.3(2)	∠O9-C32-C34	124.0(9)
∠O16'-N11'-O18'	94.8(4)	∠O4-Cu2-O7	96.1(2)		

Table S3. Selected angle and bond lengths (Å) for complexes **B**

C10-C11	1.395(6)	C25-C29	1.379(5)	Cu2-O3	2.296(2)
C10-C12	1.379(6)	C28-C30	1.376(5)	Cu2-O5	2.004(2)
C12-C13	1.386(6)	C29-C30	1.401(6)	Cu2-O6	1.965(2)
C15-C16	1.450(5)	C2-C4	1.395(6)	N1-C23	1.290(5)
C16-C17	1.411(5)	C3-C5	1.383(6)	N1-N2	1.405(4)
C16-C20	1.412(5)	C41-C42	1.473(10)	N2-C35	1.327(5)
C17-C16	1.411(5)	C4-C6	1.366(7)	N3-C15	1.286(4)
C17-C21	1.413(5)	C5-C6	1.392(7)	N3-N4	1.389(4)
C18-C19	1.395(5)	C8-C13	1.396(5)	N4-C14	1.335(5)
C18-C21	1.377(5)	C8-C14	1.488(5)	O1-C35	1.278(4)
C19-C20	1.378(5)	C8-C9	1.402(5)	O2-C14	1.278(4)
C1-C2	1.365(6)	C9-C11	1.389(6)	O3-C21	1.374(4)
C1-C3	1.412(6)	Cu1-N3	1.918(3)	O3-C22	1.421(4)
C1-C35	1.491(5)	Cu1-O2	1.936(2)	O4-C25	1.370(4)
C21-C18	1.377(5)	Cu1-O4	2.280(2)	O4-C26	1.429(4)
C23-C24	1.441(5)	Cu1-O5	1.955(2)	O5-C17	1.350(4)
C24-C27	1.392(5)	Cu1-O6	1.989(2)	O5-Cu1	1.955(2)
C24-C28	1.412(5)	Cu2-N1	1.917(3)	O6-C27	1.348(4)
C25-C27	1.428(4)	Cu2-O1	1.936(2)	O7-C41	1.430(10)

∠C5-C3-C1	120.0(5)	∠C29-C25-C27	121.1(3)	∠C35-O1-Cu2	110.6(2)
∠N2-C35-C1	116.2(3)	∠O4-C25-C27	115.3(3)	∠Cu1-O5-Cu2	112.84(11)
∠O1-C35-C1	119.3(3)	∠C27-C24-C28	119.8(3)	∠N2-N1-Cu2	114.4(2)
∠C13-C12-C10	120.5(4)	∠C28-C30-C29	120.2(3)	∠C35-N2-N1	108.8(3)
∠C9-C11-C10	120.0(4)	∠O4-C25-C29	123.6(3)	∠C23-N1-N2	116.1(3)
∠C12-C10-C11	120.0(4)	∠C2-C1-C3	119.5(4)	∠O1-C35-N2	124.5(3)
∠C13-C8-C14	121.6(3)	∠C25-C29-C30	119.6(3)	∠C14-N4-N3	108.4(3)
∠C9-C8-C14	119.0(3)	∠C2-C1-C35	119.9(4)	∠C15-N3-N4	117.3(3)
∠C17-C16-C15	124.0(3)	∠C3-C1-C35	120.5(4)	∠O2-C14-N4	124.4(3)
∠C20-C16-C15	116.3(3)	∠C1-C2-C4	119.8(4)	∠N1-Cu2-O1	81.69(11)
∠C19-C20-C16	120.9(3)	∠O7-C41-C42	117.9(7)	∠N3-Cu1-O2	81.26(11)
∠C21-C17-C16	118.1(3)	∠C4-C6-C5	119.5(4)	∠N1-Cu2-O3	110.88(11)
∠N3-C15-C16	125.1(3)	∠C3-C5-C6	119.8(5)	∠O1-Cu2-O3	89.77(9)
∠O5-C17-C16	123.8(3)	∠C11-C9-C8	120.0(4)	∠O5-Cu2-O3	74.60(9)
∠C18-C21-C17	121.3(3)	∠C12-C13-C8	120.1(4)	∠O6-Cu2-O3	95.50(9)
∠O3-C21-C17	114.3(3)	∠N4-C14-C8	117.0(3)	∠N3-Cu1-O4	111.79(10)
∠O3-C21-C18	124.4(3)	∠O2-C14-C8	118.6(3)	∠O2-Cu1-O4	87.71(10)
∠C21-C18-C19	120.5(3)	∠C13-C8-C9	119.4(3)	∠O5-Cu1-O4	96.88(9)
∠C6-C4-C2	121.2(4)	∠C14-O2-Cu1	110.7(2)	∠O6-Cu1-O4	76.07(9)
∠C17-C16-C20	119.6(3)	∠C15-N3-Cu1	127.4(2)	∠N1-Cu2-O5	174.16(12)
∠C18-C19-C20	119.6(3)	∠C17-O5-Cu1	125.3(2)	∠N3-Cu1-O5	93.68(11)
∠O5-C17-C21	118.1(3)	∠C25-O4-Cu1	110.41(19)	∠O1-Cu2-O5	96.57(10)
∠C21-O3-C22	117.8(3)	∠C26-O4-Cu1	125.5(2)	∠O2-Cu1-O5	174.18(10)
∠C27-C24-C23	123.8(3)	∠C27-O6-Cu1	119.7(2)	∠O6-Cu2-O5	90.14(9)
∠C28-C24-C23	116.4(3)	∠Cu2-O6-Cu1	111.79(11)	∠N1-Cu2-O6	91.28(11)
∠C30-C28-C24	120.8(3)	∠N4-N3-Cu1	115.3(2)	∠N3-Cu1-O6	171.72(11)
∠N1-C23-C24	124.2(3)	∠C17-O5-Cu2	120.9(2)	∠O1-Cu2-O6	172.38(10)
∠O6-C27-C24	123.8(3)	∠C21-O3-Cu2	111.89(19)	∠O2-Cu1-O6	96.85(10)
∠C24-C27-C25	118.4(3)	∠C22-O3-Cu2	127.3(2)	∠O5-Cu1-O6	87.76(9)
∠O6-C27-C25	117.7(3)	∠C23-N1-Cu2	129.5(2)		
∠C25-O4-C26	117.8(3)	∠C27-O6-Cu2	126.7(2)		

Table S4. Selected angle and bond lengths (Å) for complexes **C**

C10-C11	1.465(8)	Cu1-O2	1.876(6)	N6-C21	1.329(10)
C11-C12	1.39	Cu1-O3	1.926(6)	N6-C22	1.441(12)
C11-C16	1.39	Cu1-O7	2.308(5)	N6-C23	1.449(11)
C12-C13	1.39	Cu1-O8	2.015(5)	O10-N7	1.272(9)
C13-C14	1.39	Cu2-N2	1.967(7)	O11-N7	1.235(10)
C14-C15	1.39	Cu2-N4	1.956(6)	O1-C1	1.424(11)
C15-C16	1.39	Cu2-O4	1.890(5)	O1-C2	1.368(7)
C2-C3	1.39	Cu2-O6	1.979(6)	O2-C7	1.333(7)
C2-C7	1.39	N1-C8	1.297(11)	O3-C9	1.276(9)
C3-C4	1.39	N1-N2	1.393(9)	O4-C16	1.350(6)
C4-C5	1.39	N3-C9	1.366(10)	O5-C15	1.376(7)
C5-C6	1.39	N3-N4	1.385(9)	O5-C17	1.432(10)
C6-C7	1.39	N4-C10	1.296(10)	O6-C18	1.273(10)
C6-C8	1.464(9)	N5-C18	1.305(11)	O7-C21	1.247(10)
C9-N2	1.347(10)	N5-C19	1.469(13)	O9-N7	1.246(11)
Cu1-N1	1.936(6)	N5-C20	1.463(15)		

∠C10-N4-Cu2	129.4(5)	∠C6-C5-C4	120	∠O1-C2-C7	115.4(4)
∠C10-N4-N3	117.8(7)	∠C6-C7-C2	120	∠O2-C7-C2	115.6(4)
∠C12-C11-C10	118.0(4)	∠C7-C6-C5	120	∠O2-C7-C6	124.4(4)
∠C12-C11-C16	120	∠C7-C6-C8	123.5(5)	∠O2-Cu1-N1	93.5(3)
∠C13-C12-C11	120	∠C7-O2-Cu1	127.2(4)	∠O2-Cu1-O3	174.4(2)
∠C13-C14-C15	120	∠C8-N1-Cu1	126.5(5)	∠O2-Cu1-O7	89.1(2)
∠C14-C13-C12	120	∠C8-N1-N2	119.6(6)	∠O2-Cu1-O8	91.6(2)
∠C14-C15-C16	120	∠C9-N2-Cu2	113.4(5)	∠O3-C9-N2	124.9(7)
∠C15-C16-C11	120	∠C9-N2-N1	108.7(6)	∠O3-C9-N3	118.6(7)
∠C15-O5-C17	118.2(6)	∠C9-N3-N4	115.0(7)	∠O3-Cu1-N1	82.2(2)
∠C16-C11-C10	121.8(4)	∠C9-O3-Cu1	110.2(5)	∠O3-Cu1-O7	90.5(2)
∠C16-O4-Cu2	127.3(4)	∠N1-C8-C6	123.3(6)	∠O3-Cu1-O8	93.9(2)
∠C18-N5-C19	121.0(8)	∠N1-Cu1-O7	125.1(2)	∠O4-C16-C11	123.2(4)
∠C18-N5-C20	121.7(9)	∠N1-Cu1-O8	146.5(2)	∠O4-C16-C15	116.5(4)
∠C18-O6-Cu2	120.3(5)	∠N1-N2-Cu2	137.9(5)	∠O4-Cu2-N2	170.2(3)
∠C20-N5-C19	117.3(9)	∠N2-C9-N3	116.5(6)	∠O4-Cu2-N4	89.5(3)
∠C21-N6-C22	120.4(8)	∠N2-Cu2-O6	100.7(2)	∠O4-Cu2-O6	89.0(2)
∠C21-N6-C23	121.9(7)	∠N2-N1-Cu1	113.7(5)	∠O5-C15-C14	124.8(4)
∠C21-O7-Cu1	121.0(5)	∠N3-N4-Cu2	112.8(5)	∠O5-C15-C16	115.2(4)
∠C22-N6-C23	117.4(7)	∠N4-C10-C11	123.0(7)	∠O6-C18-N5	123.2(8)
∠C2-O1-C1	118.9(7)	∠N4-Cu2-N2	81.3(3)	∠O7-C21-N6	125.0(8)
∠C3-C2-C7	120	∠N4-Cu2-O6	171.01(19)	∠O8-Cu1-O7	88.0(2)
∠C3-C4-C5	120	∠O11-N7-O10	119.1(7)	∠O9-N7-O10	119.0(8)
∠C4-C3-C2	120	∠O11-N7-O9	121.9(7)		
∠C5-C6-C8	116.4(5)	∠O1-C2-C3	124.5(4)		

Table S5. Summary of SHAPE[1] analysis for complexes **A**, **B** and **C**.

Vertices	Code	Label	Shape	Symmetry
4	1	SP-4	Square	D_{4h}
	2	T-4	Tetrahedron	T_d
	3	SS-4	Seesaw or sawhorse‡ (cis-divacant octahedron)	C_{2v}
	4	vTBPY-4	Axially vacant trigonal bipyramid	C_{3v}
5	1	PP-5	Pentagon	D_{5h}
	2	vOC-5	Vacant octahedron‡ (Johnson square pyramid, J1)	C_{4v}
	3	TBPY-5	Trigonal bipyramid	D_{3h}
	4	SPY-5	Square pyramid §	C_{4v}
	5	JTBPY-5	Johnson trigonal bipyramid (J12)	D_{3h}
6	1	HP-6	Hexagon	D_{6h}
	2	PPY-6	Pentagonal pyramid	C_{5v}
	3	OC-6	Octahedron	O_h
	4	TPR-6	Trigonal prism	D_{3h}
	5	JPPY-5	Johnson pentagonal pyramid (J2)	C_{5v}

Complex A

[1] a) M. Pinsky and D. Avnir, *Inorg. Chem.*, 1998, **37**, 5575; b) D. Casanova, J. Cirera, M. Llunell, P. Alemany, D. Avnir and S. Alvarez, *J. Am. Chem. Soc.*, 2004, **126**, 1755; c) J. Cirera, E. Ruiz and S. Alvarez, *Chem. Eur. J.*, 2006, **12**, 3162; d) D. Casanova, M. Llunell, P. Alemany and S. Alvarez, *Chem. Eur. J.*, 2005, **11**, 1479; e) A. Ruiz-Martínez, D. Casanova and S. Alvarez, *Chem. Eur. J.*, 2008, **14**, 1291.

	SP-4	T-4	SS-4	vTBPY-4
Cu-1	**0.463**	31.565	17.654	31.996

	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Cu-2	34.321	23.116	**4.579**	11.389	26.204
Cu-3	33.310	22.891	**3.955**	12.160	26.044
Cu-4	32.857	16.425	15.537	**9.922**	20.168

Complex B

	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Cu-1	31.115	21.571	**4.521**	12.364	24.047
Cu-2	33.185	22.163	**4.513**	12.691	24.987

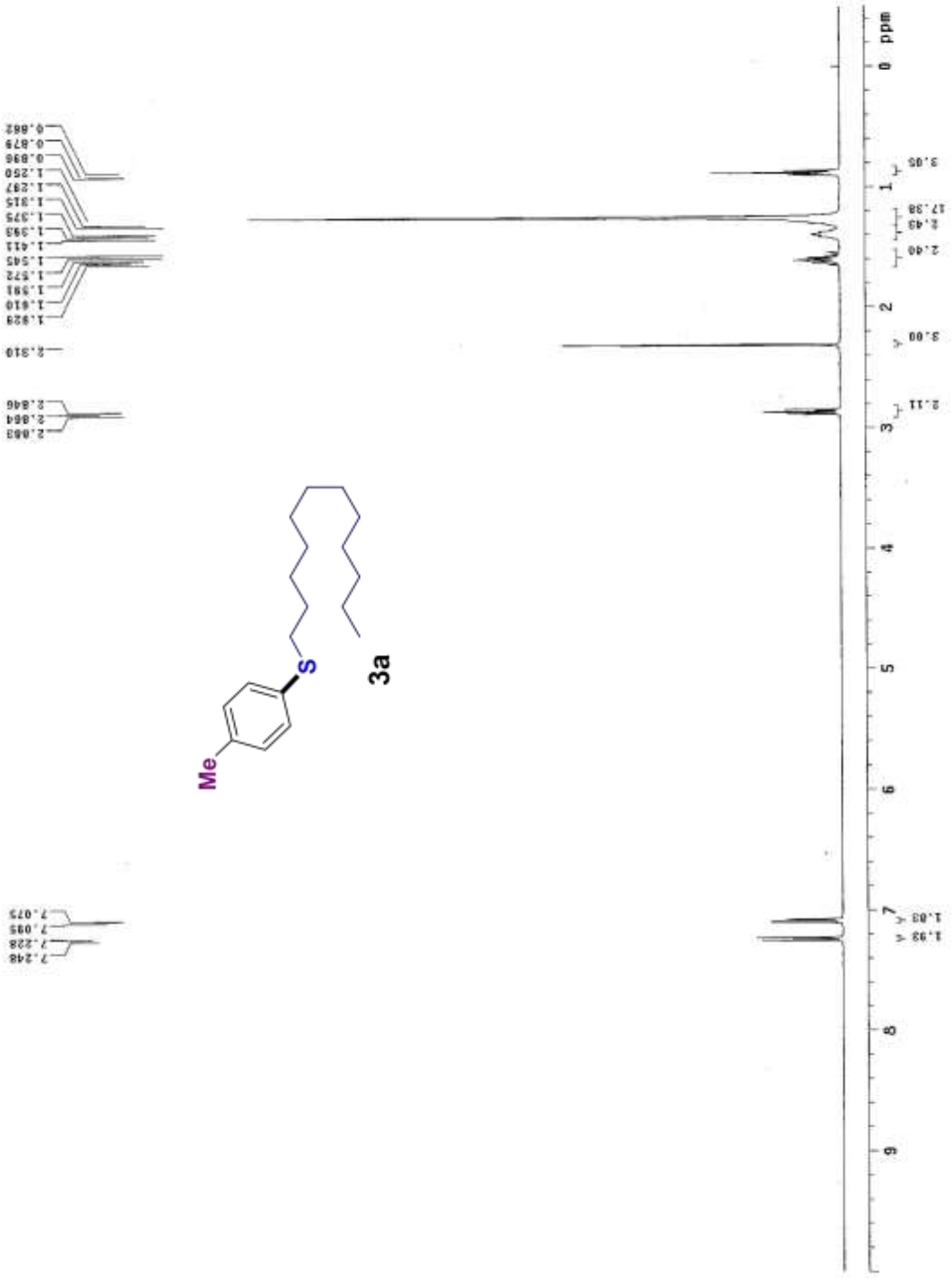
Complex C

	PP-5	vOC-5	TBPY-5	SPY-5	JTBPY-5
Cu-1	28.269	4.757	**3.046**	3.570	6.915
Cu-2	32.465	1.775	4.906	**1.400**	8.450

NMR measurement

^{1}H and ^{13}C NMR spectra were recorded by using d-chloroform and TMS as internal standard. Coupling constant are reported in hertz (Hz) and chemical shifts are in parts per million (ppm).

^{1}H & ^{13}C NMR Spectra

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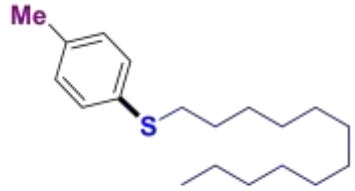
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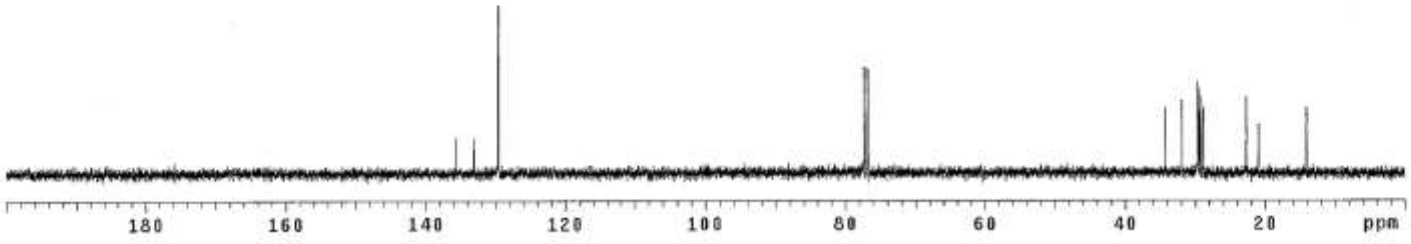
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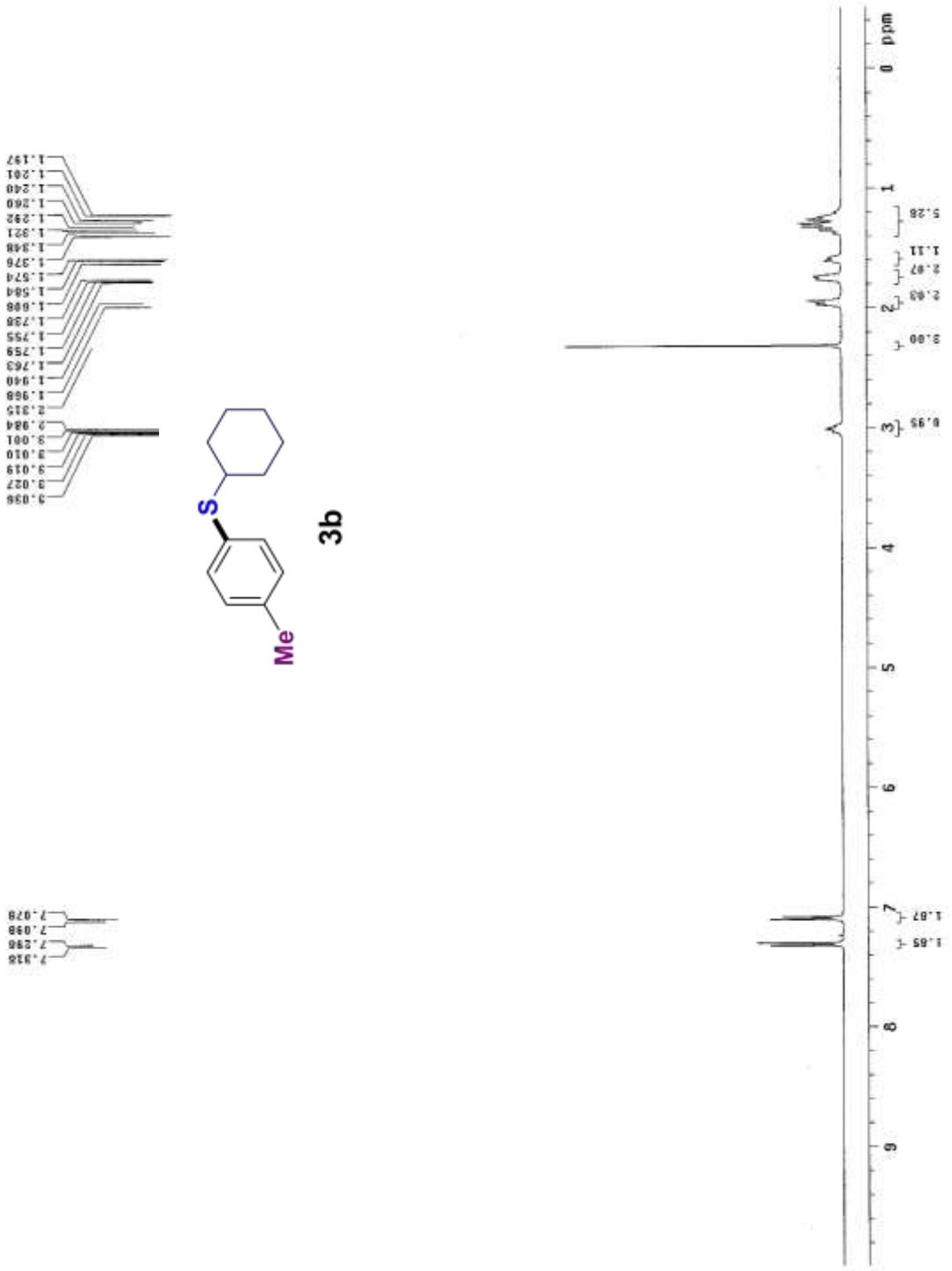
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2.315
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3.010
3.019
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3.038
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7.098
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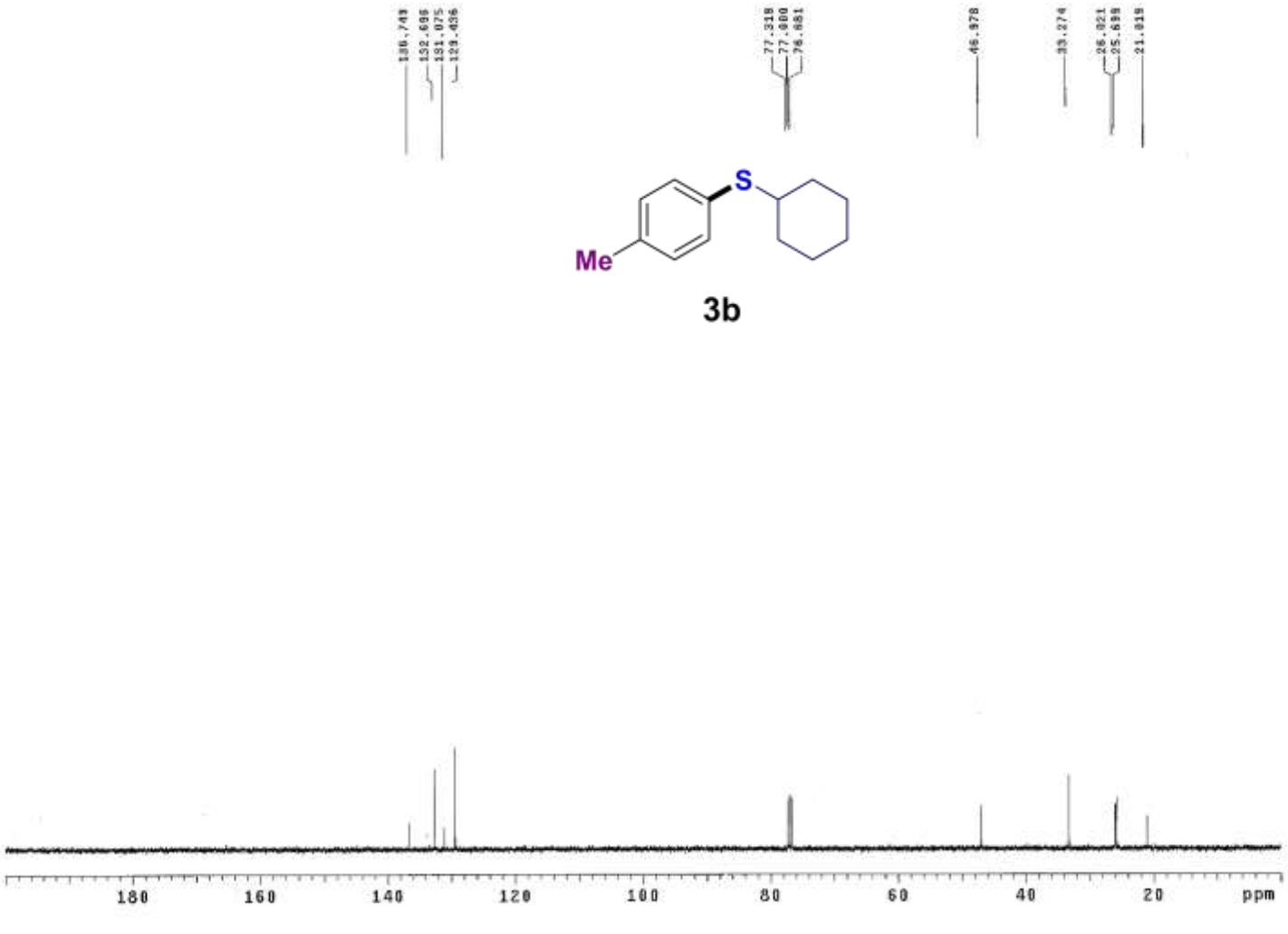
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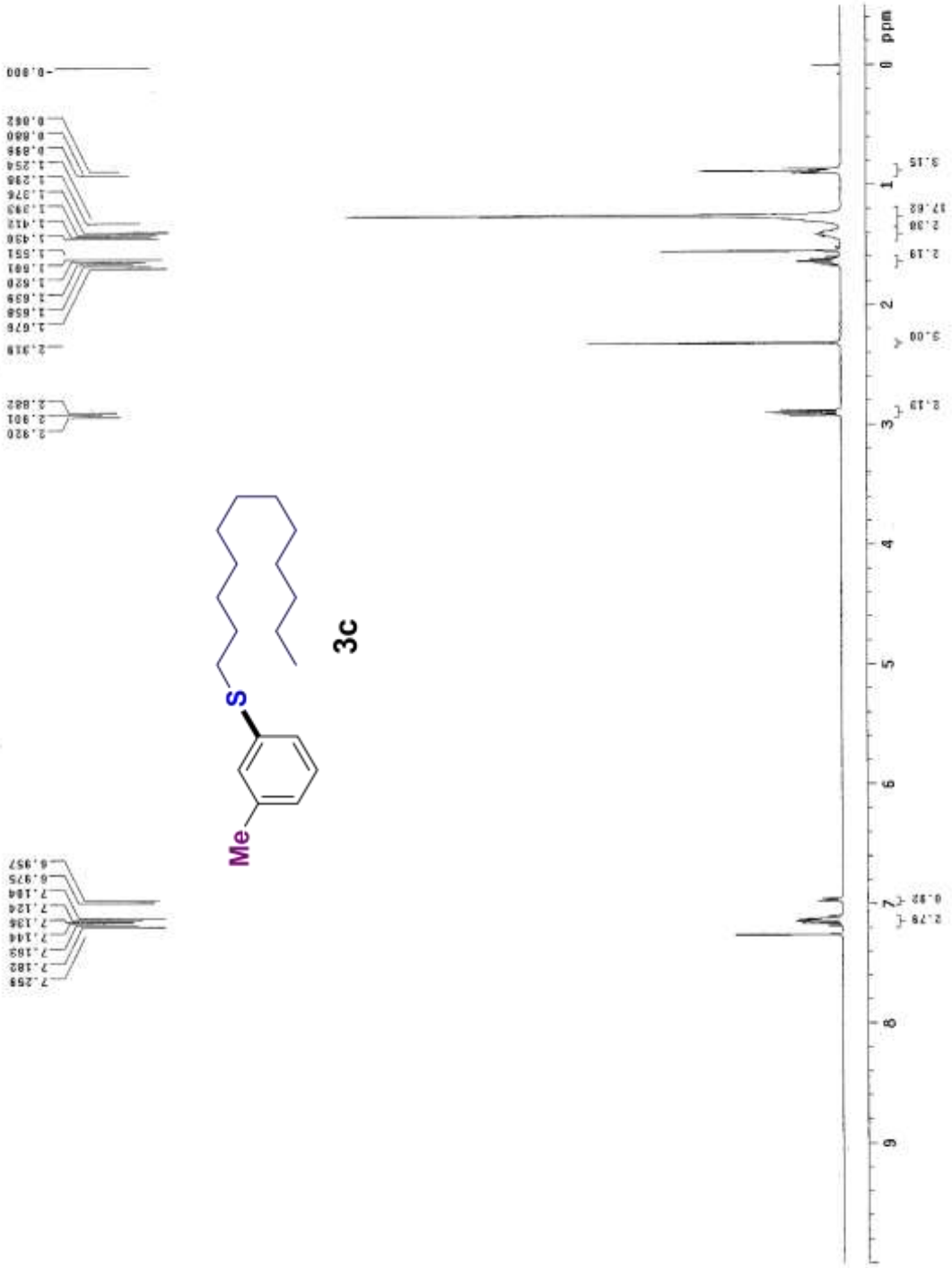
ppm

3b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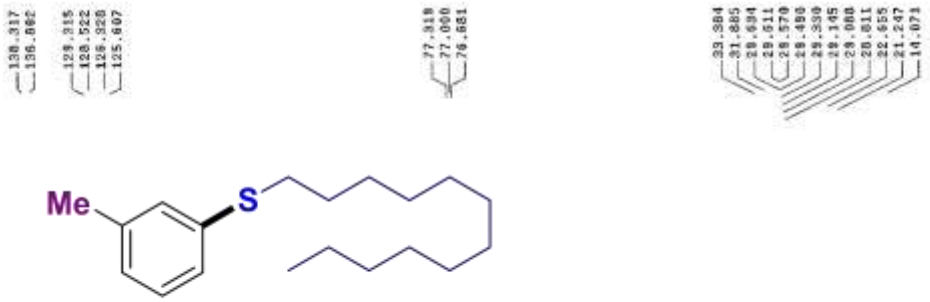
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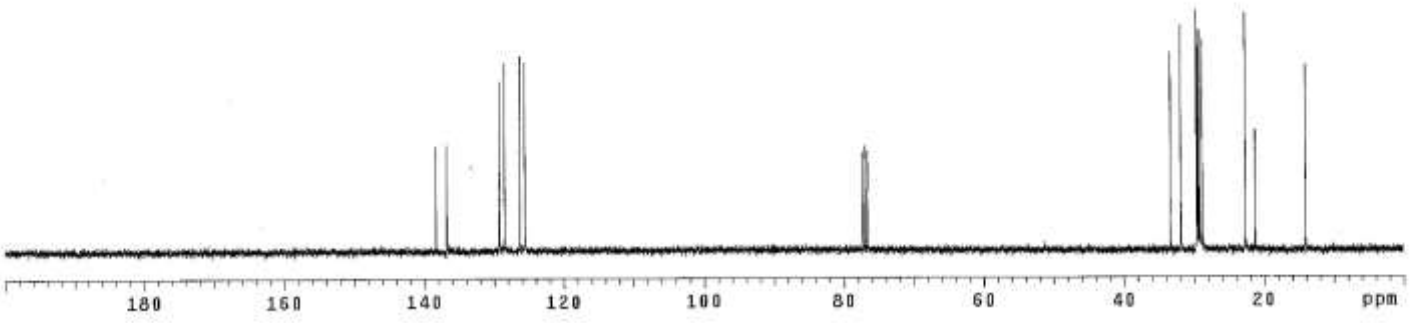
Me
S

3c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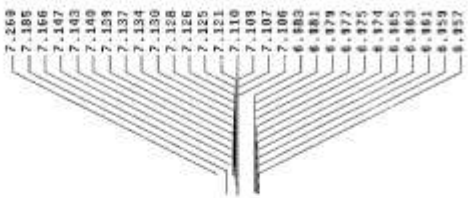
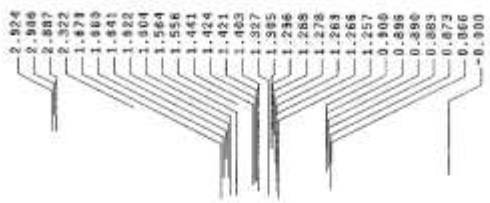
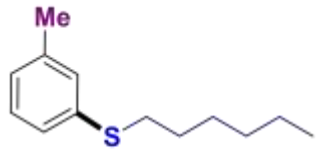
60
40
20
ppm







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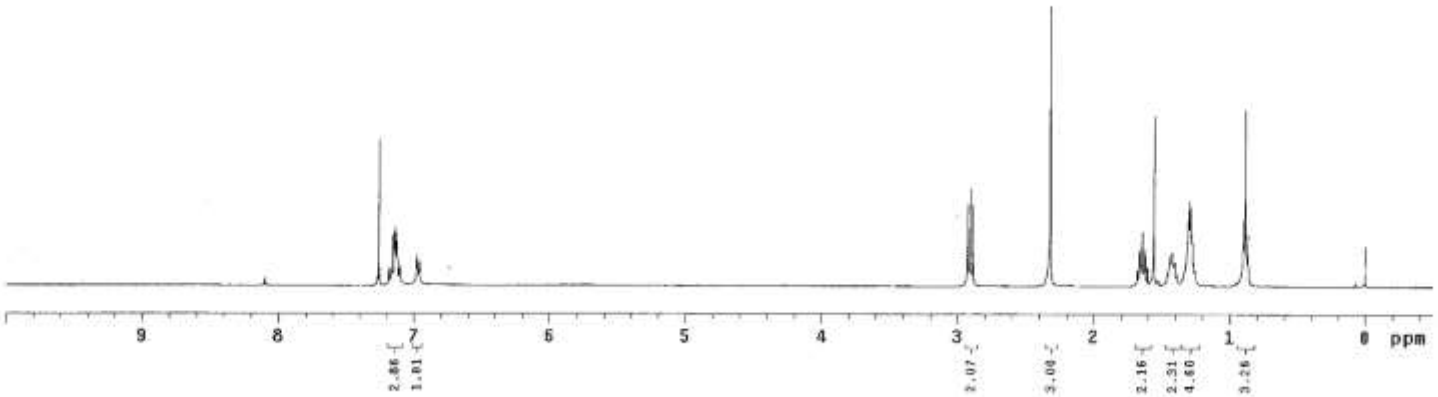

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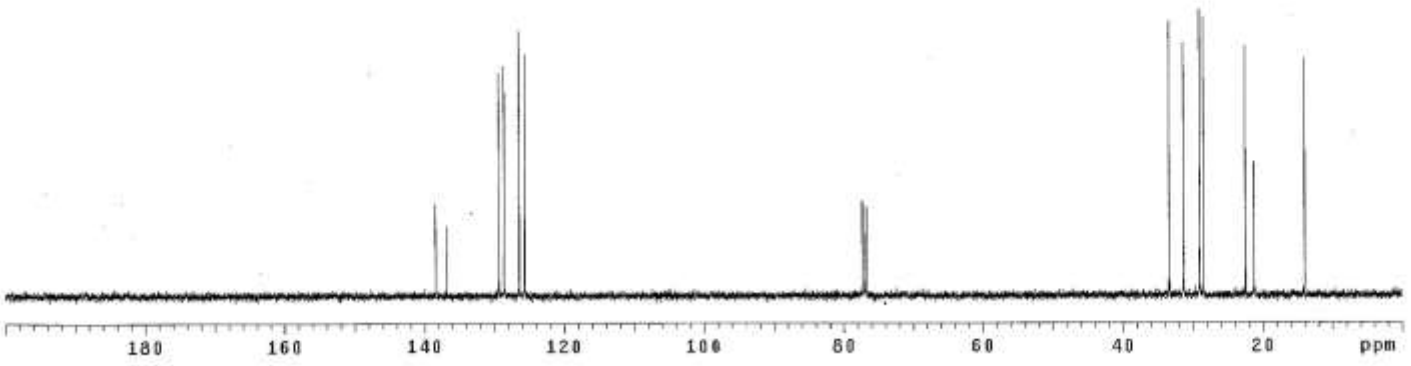

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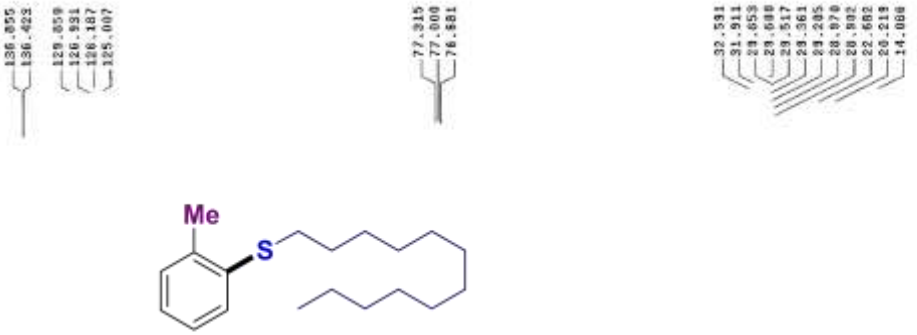
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S

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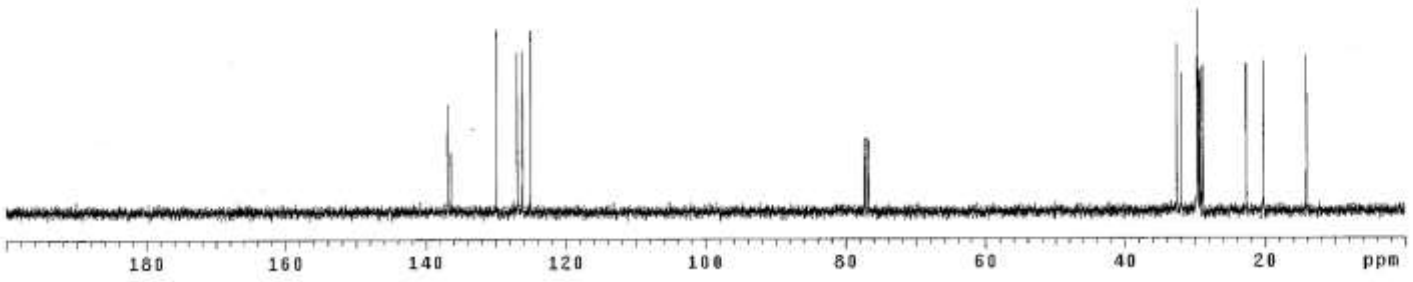
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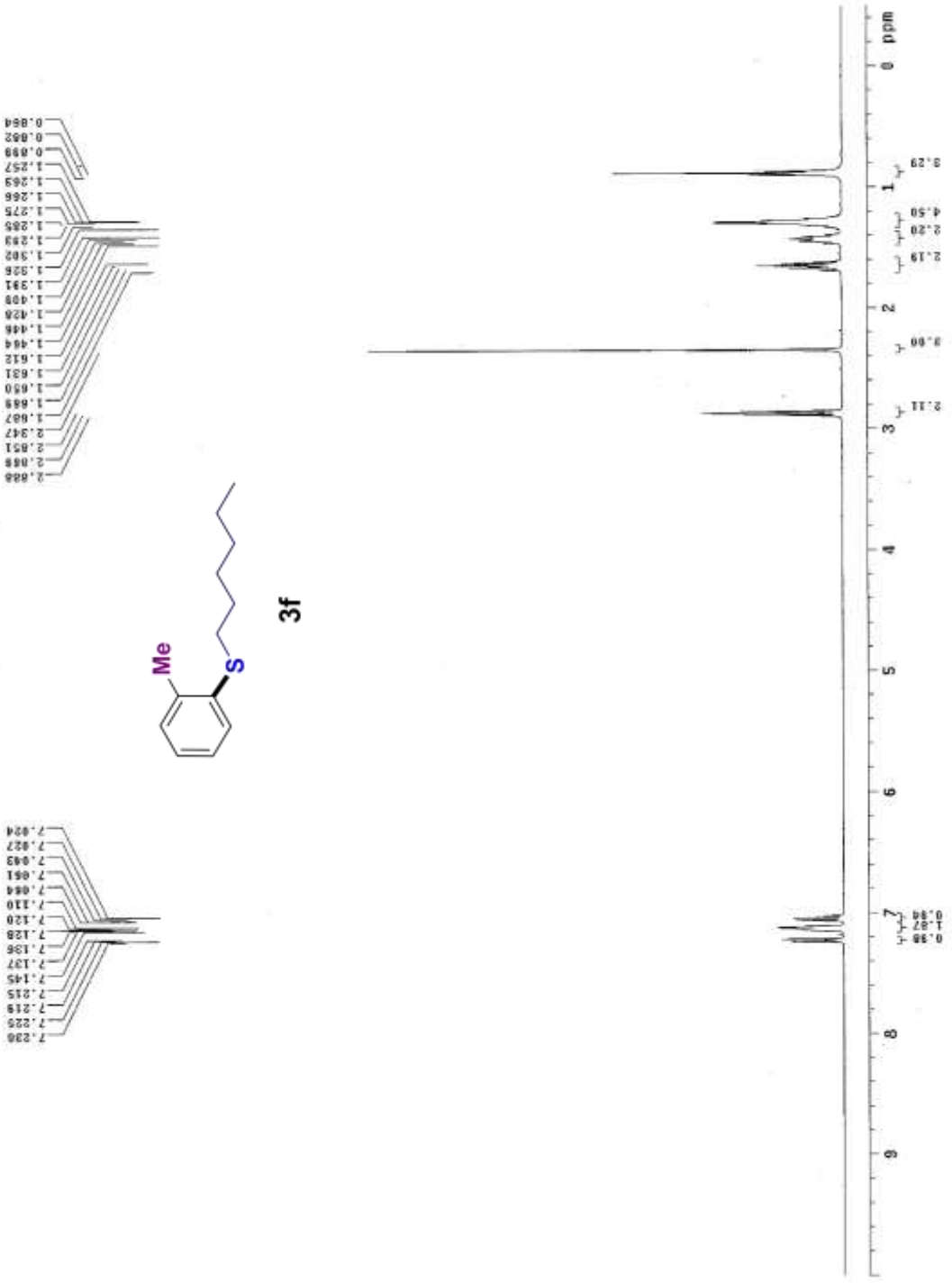
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S
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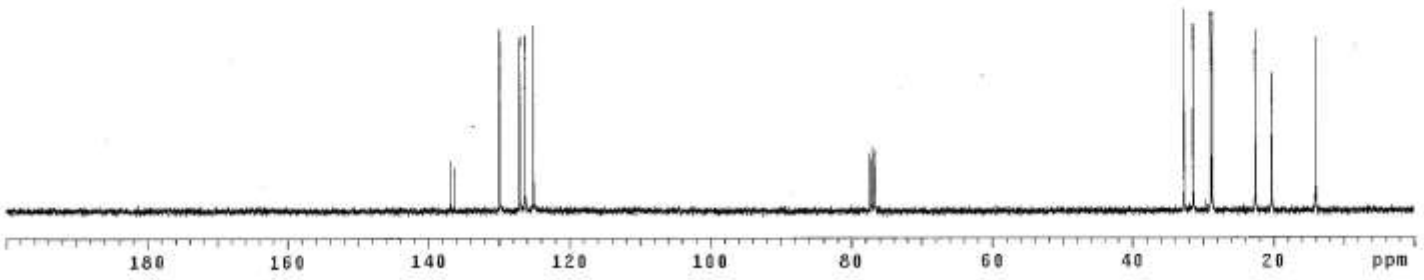
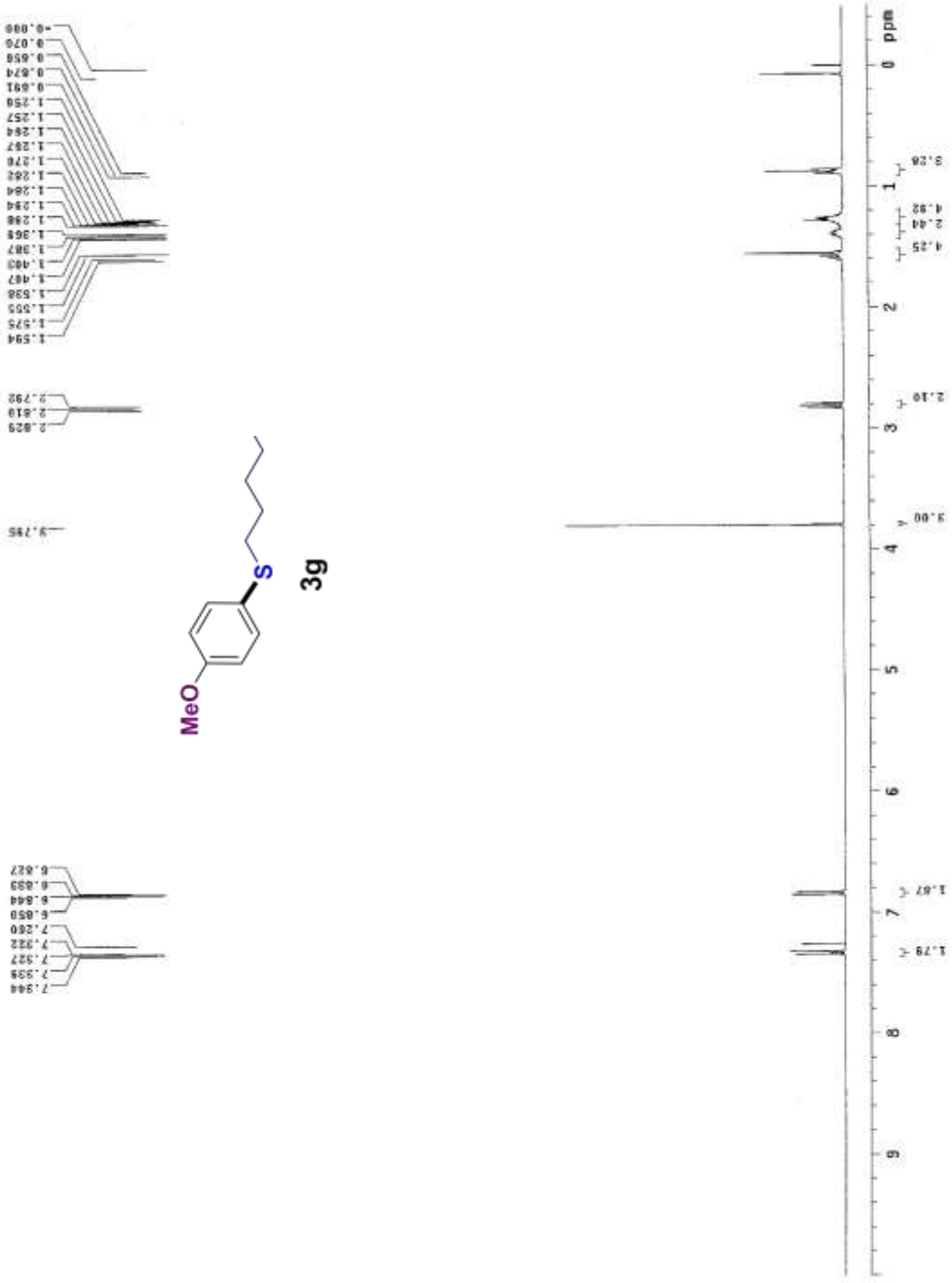
3f

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1.575
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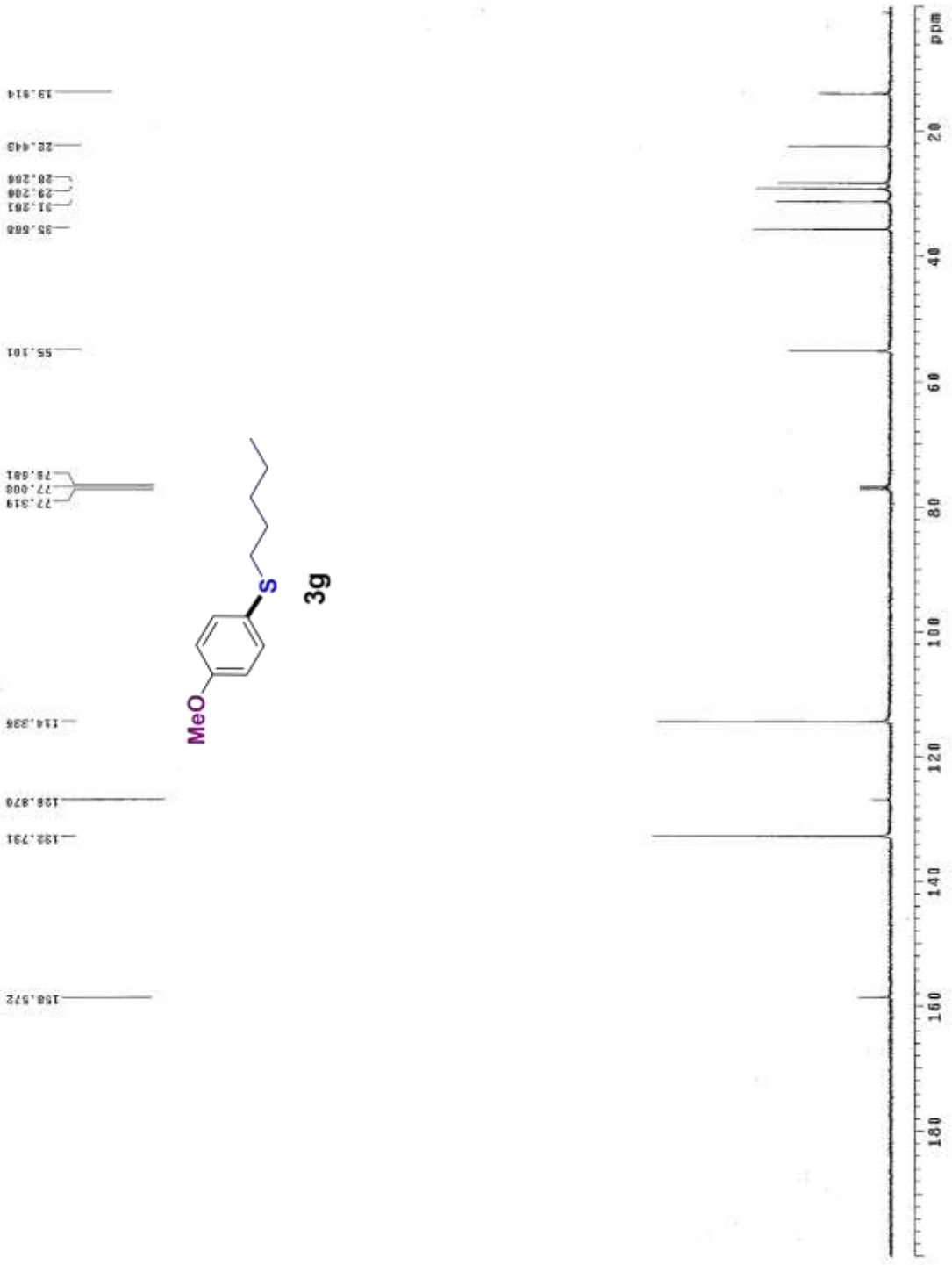
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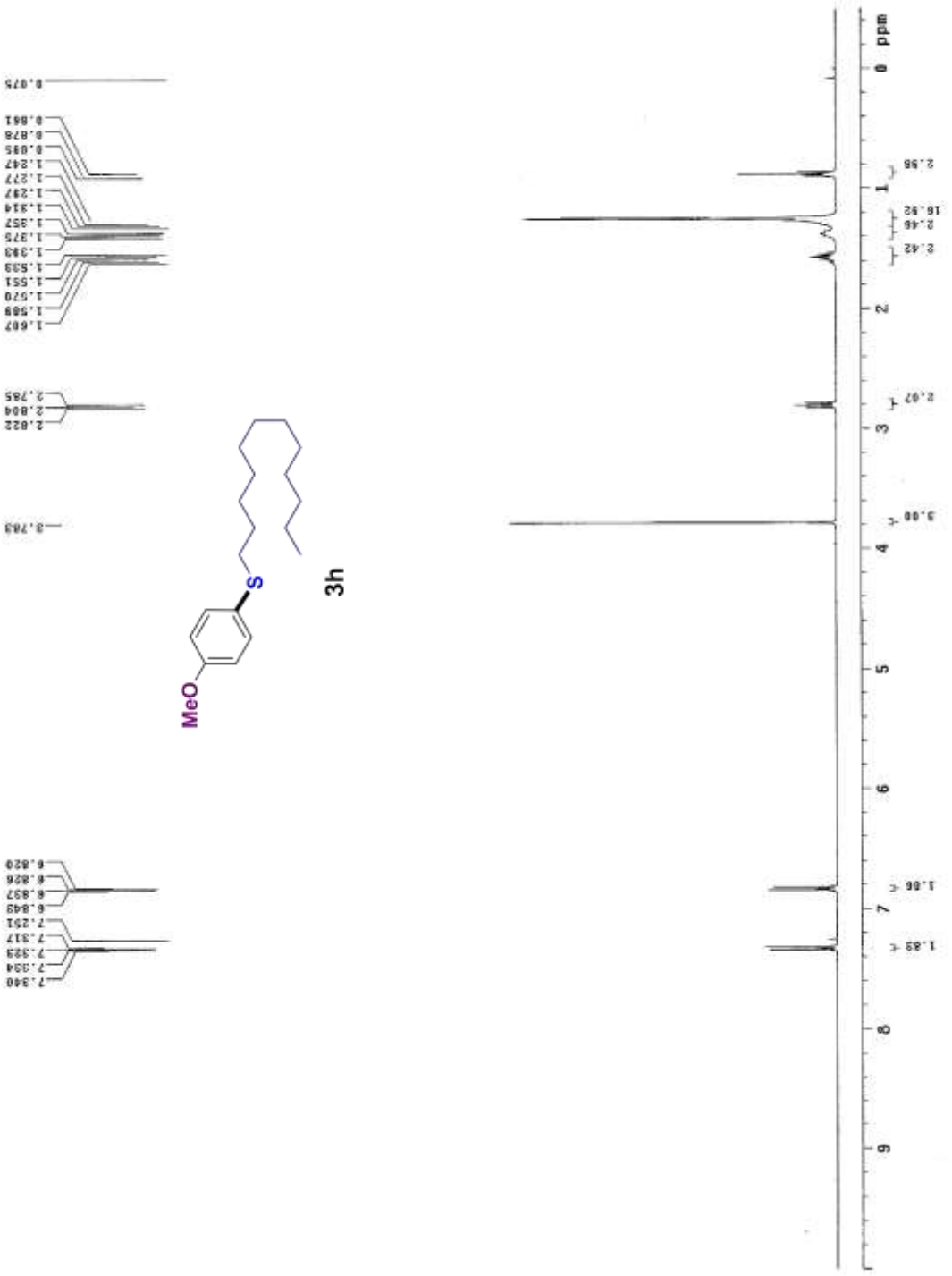
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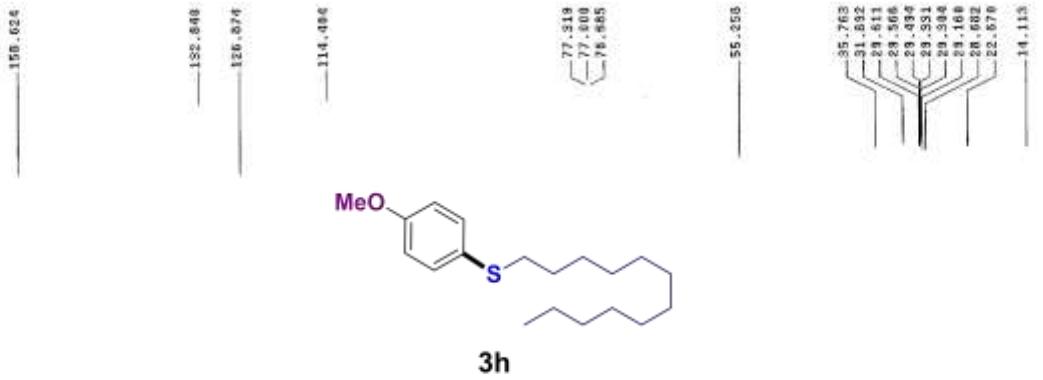
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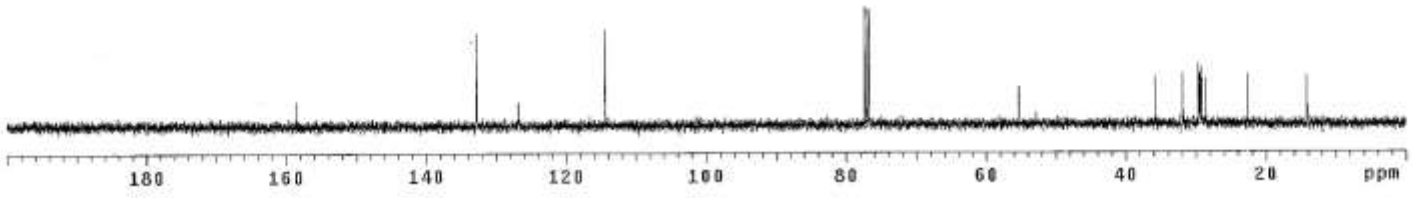
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Me
S
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Me
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ppm
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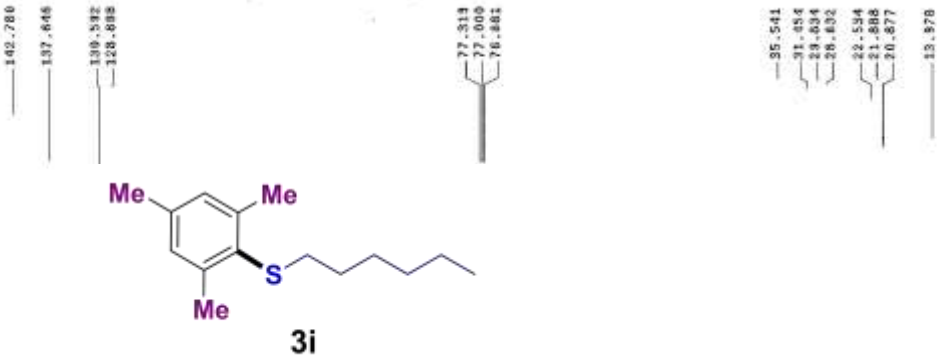
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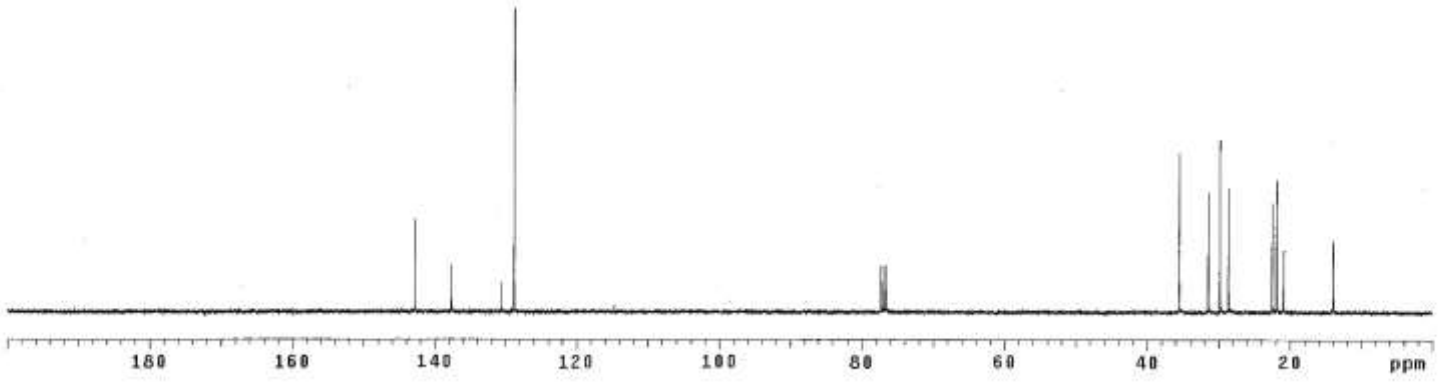
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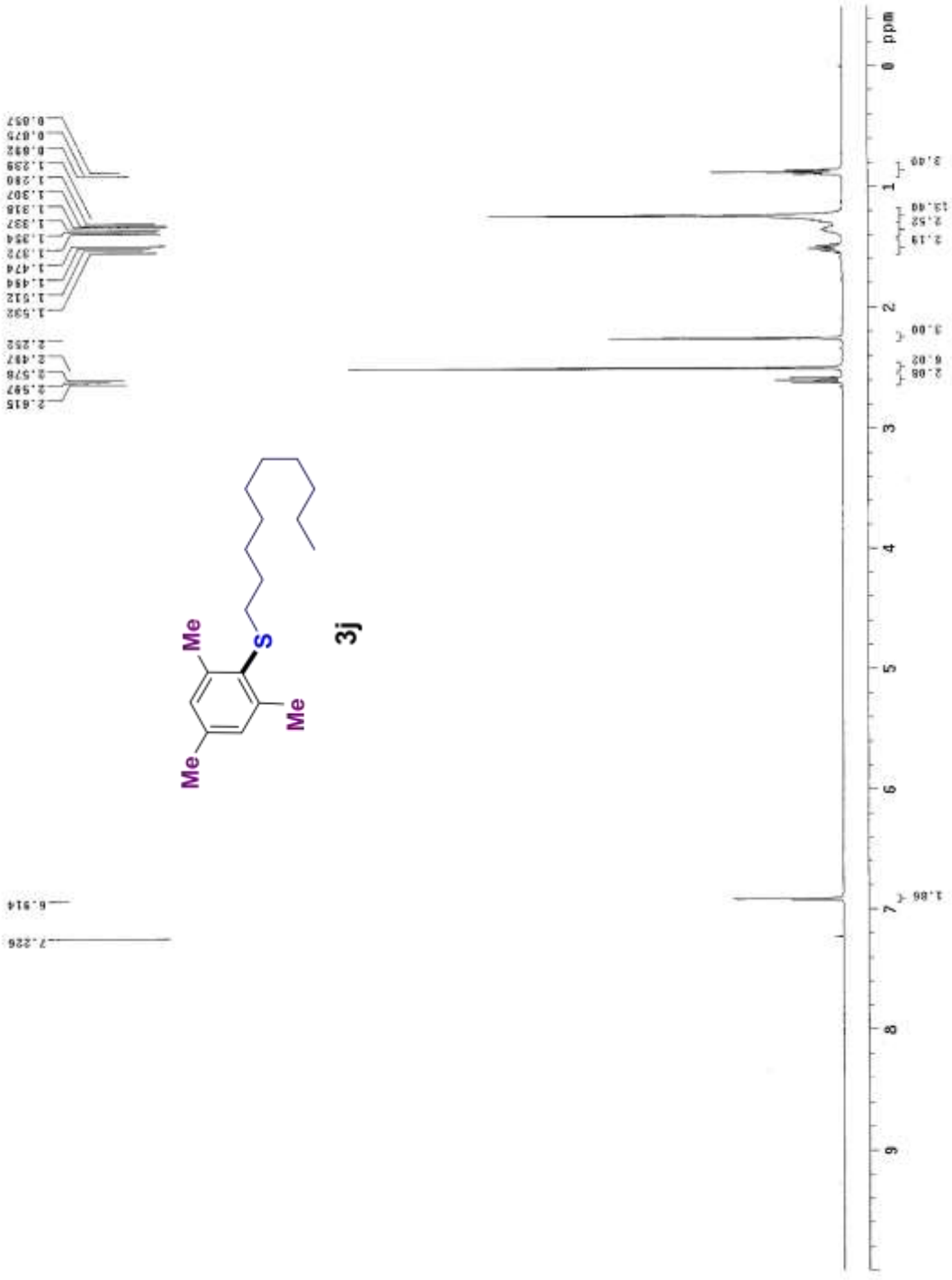
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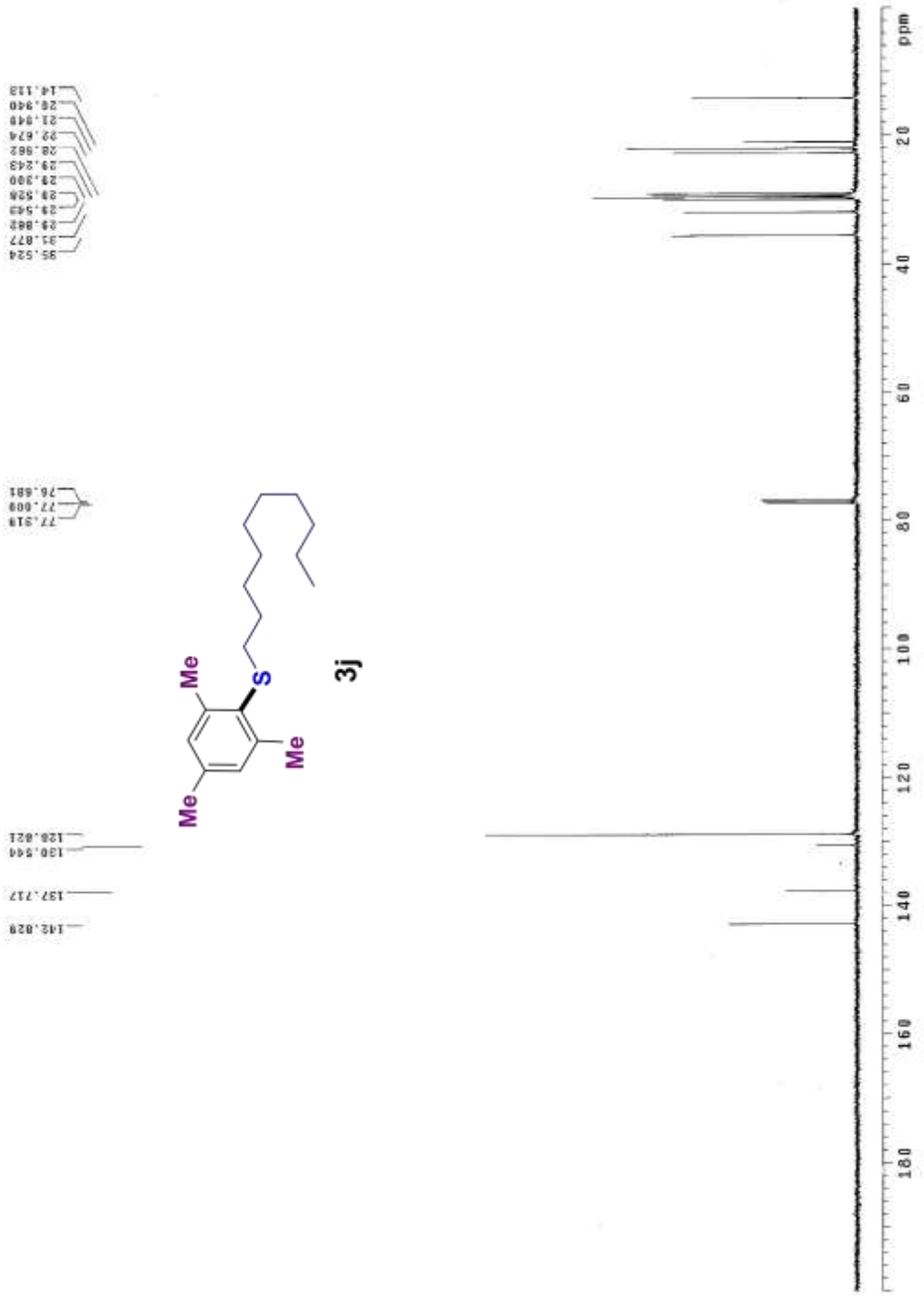
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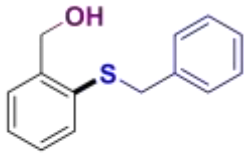
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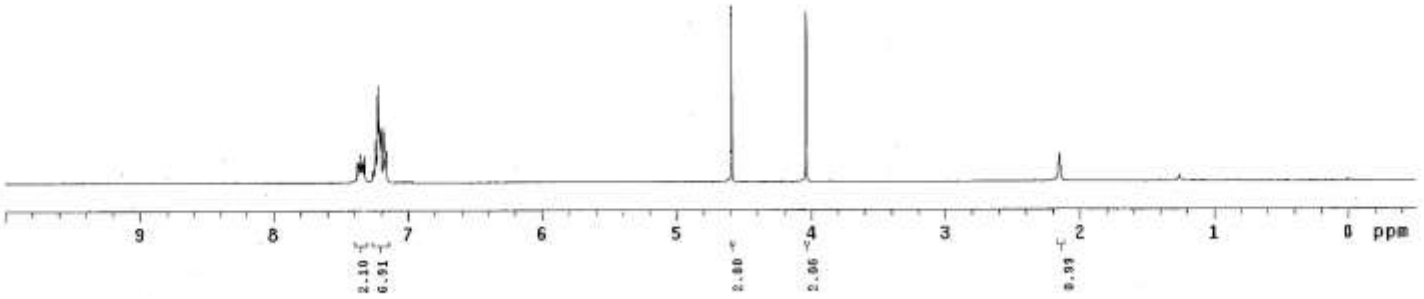
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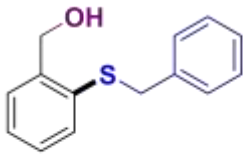
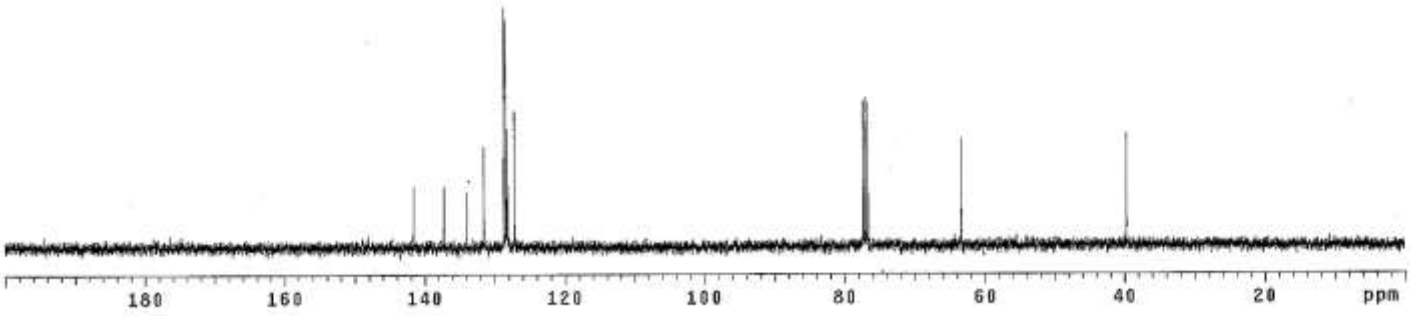
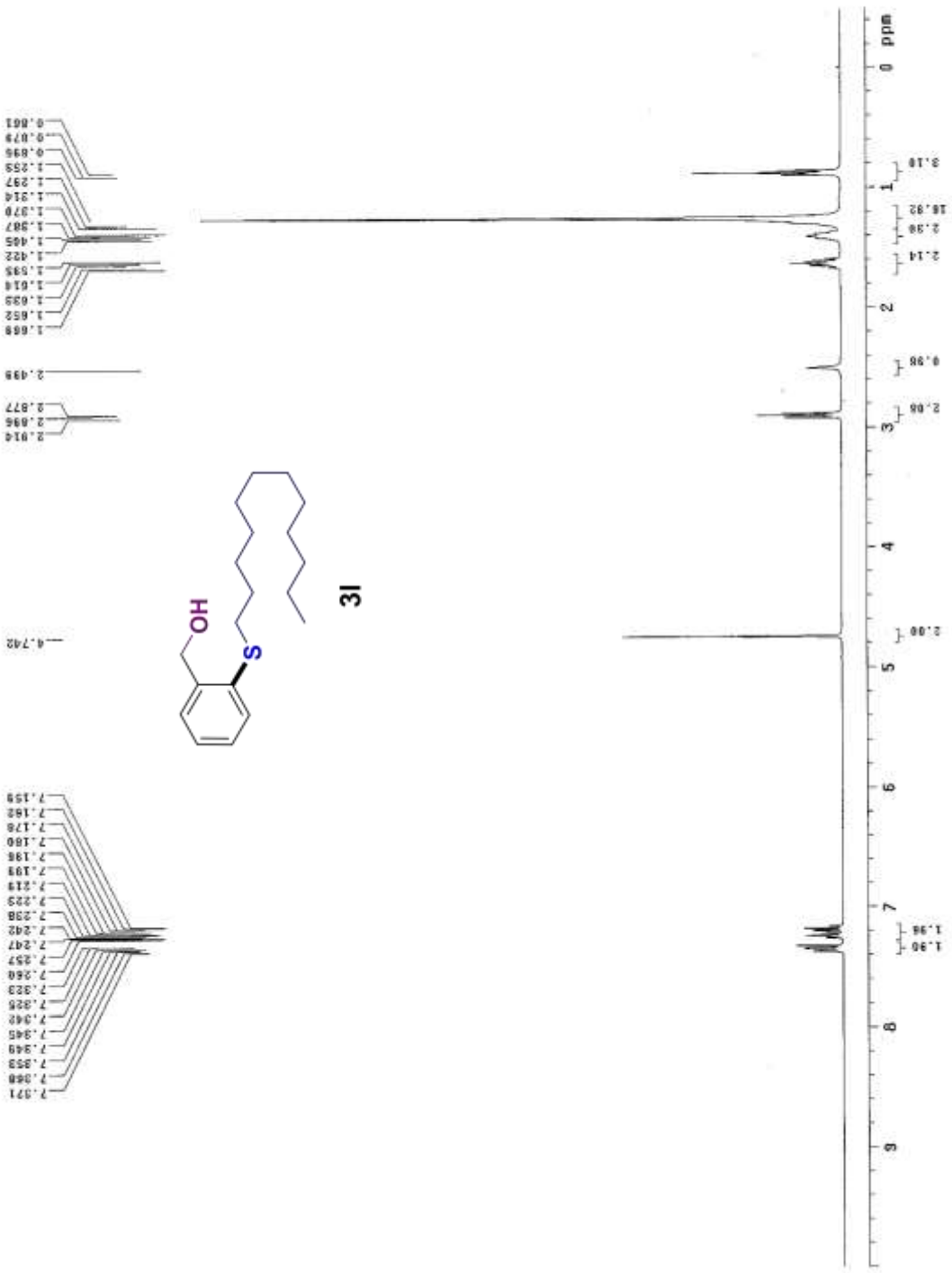
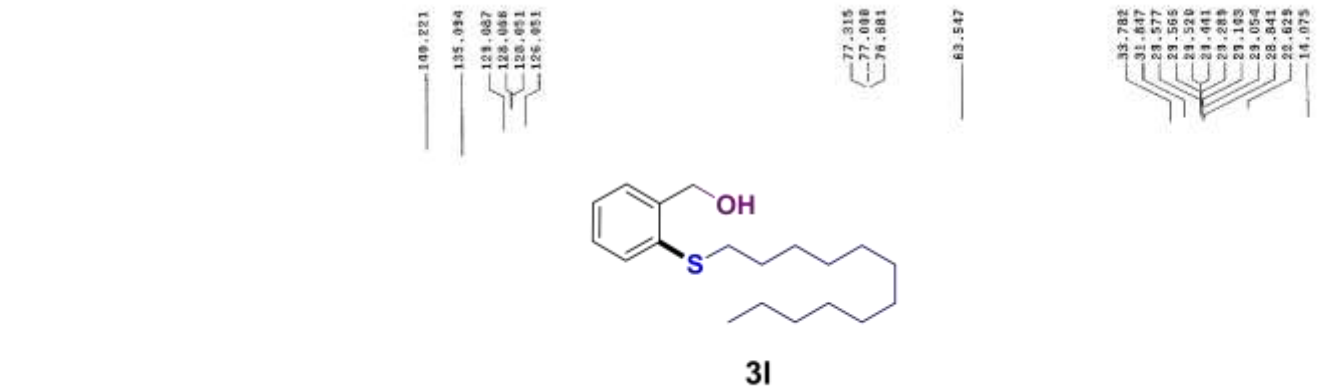
69.361
39.676


OH
S

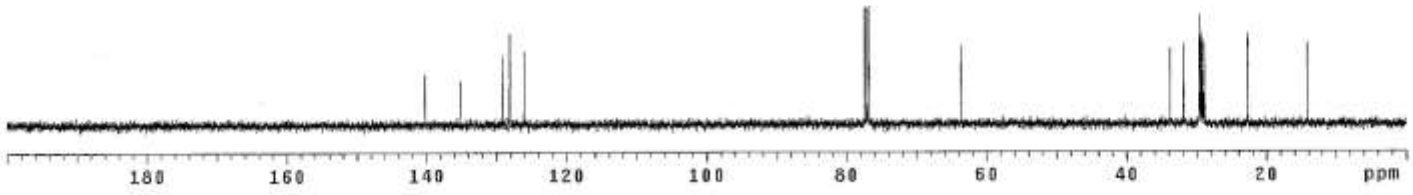
3k

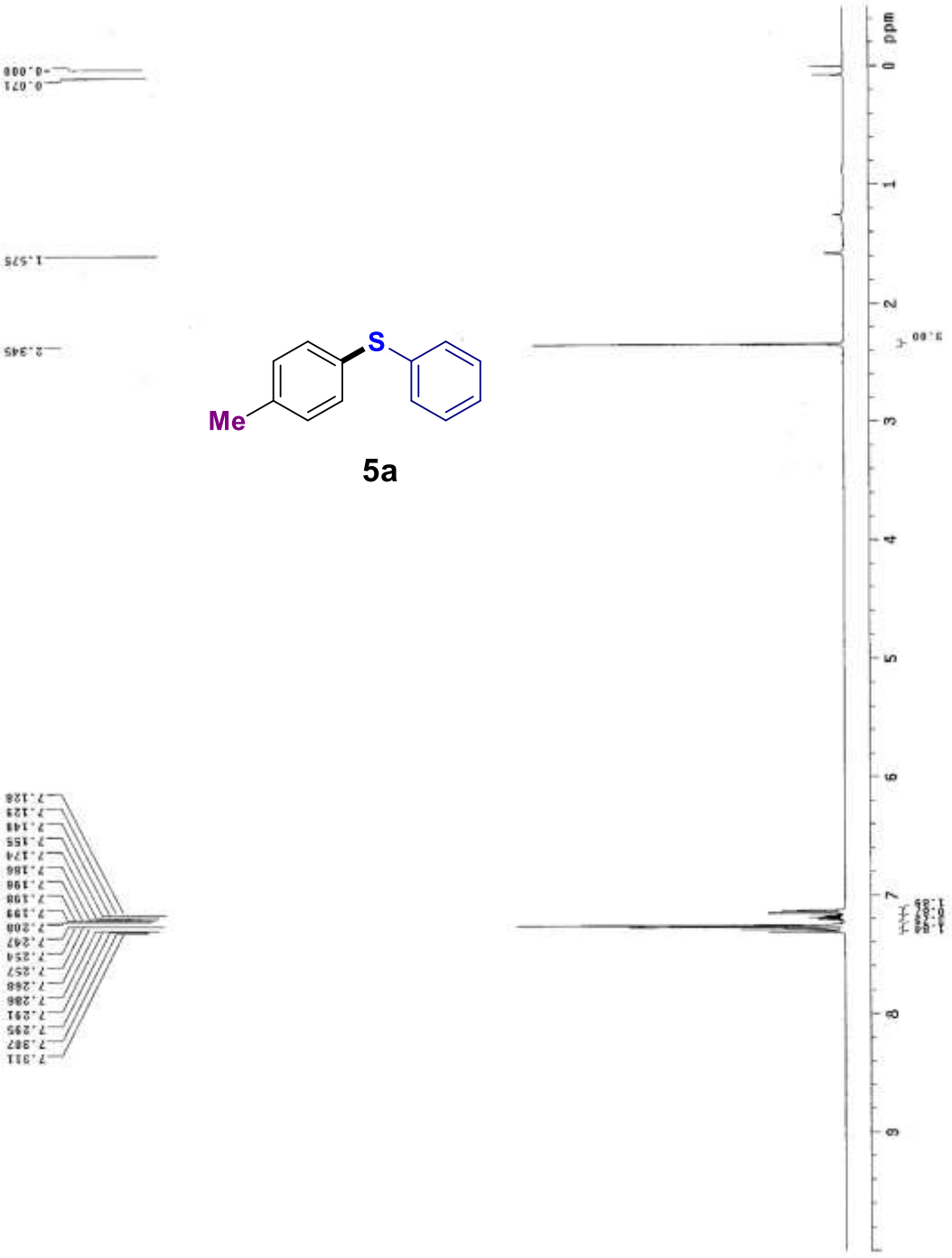

180
160
140
120
100
80
60
40
20
ppm


OH
S
3l

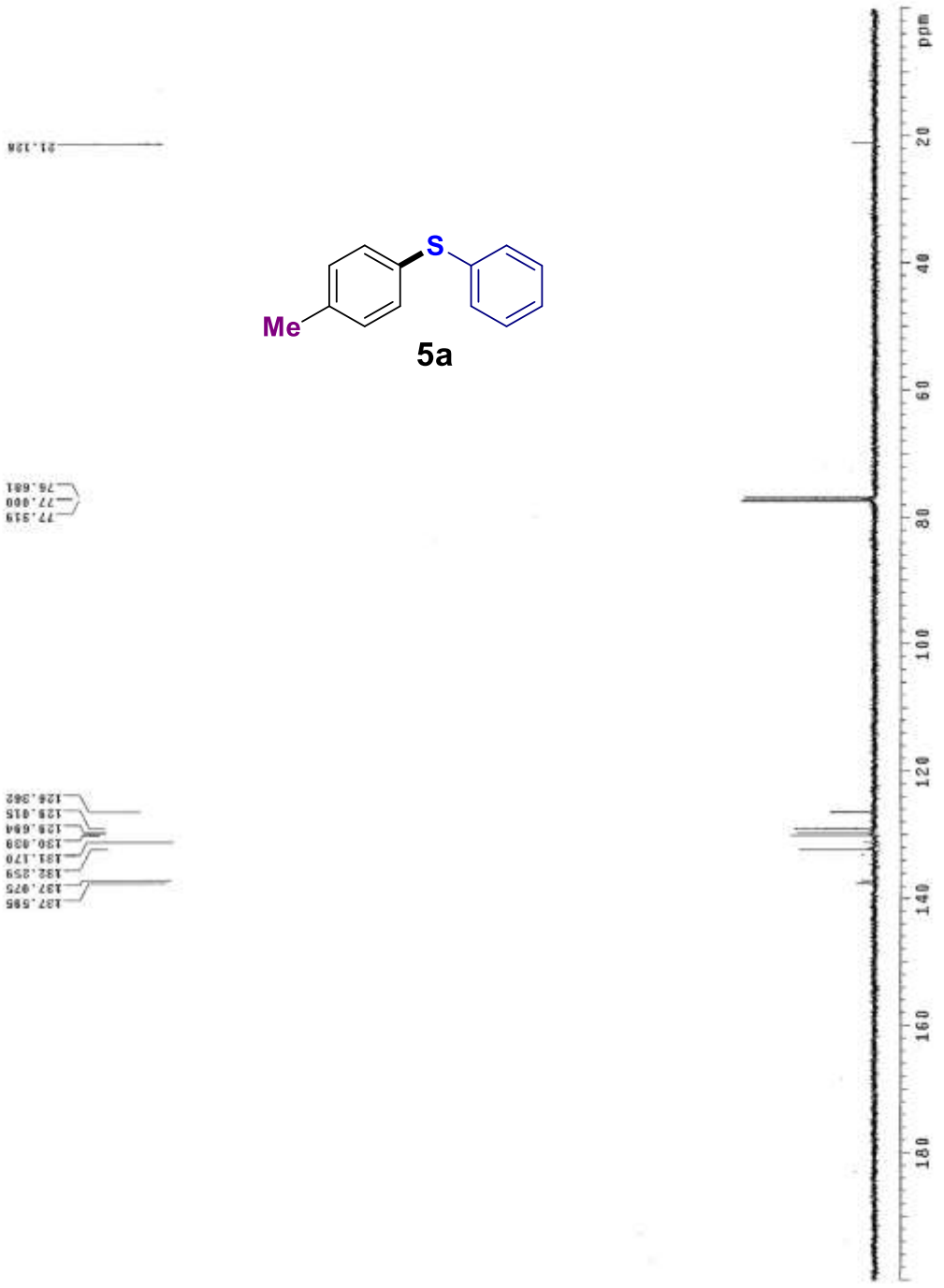

140.221
135.034
129.087
129.046
128.051
126.051
77.315
77.098
76.881
63.547
33.782
31.847
29.577
29.565
29.520
29.441
29.289
29.165
29.054
28.841
22.625
14.075
OH
S

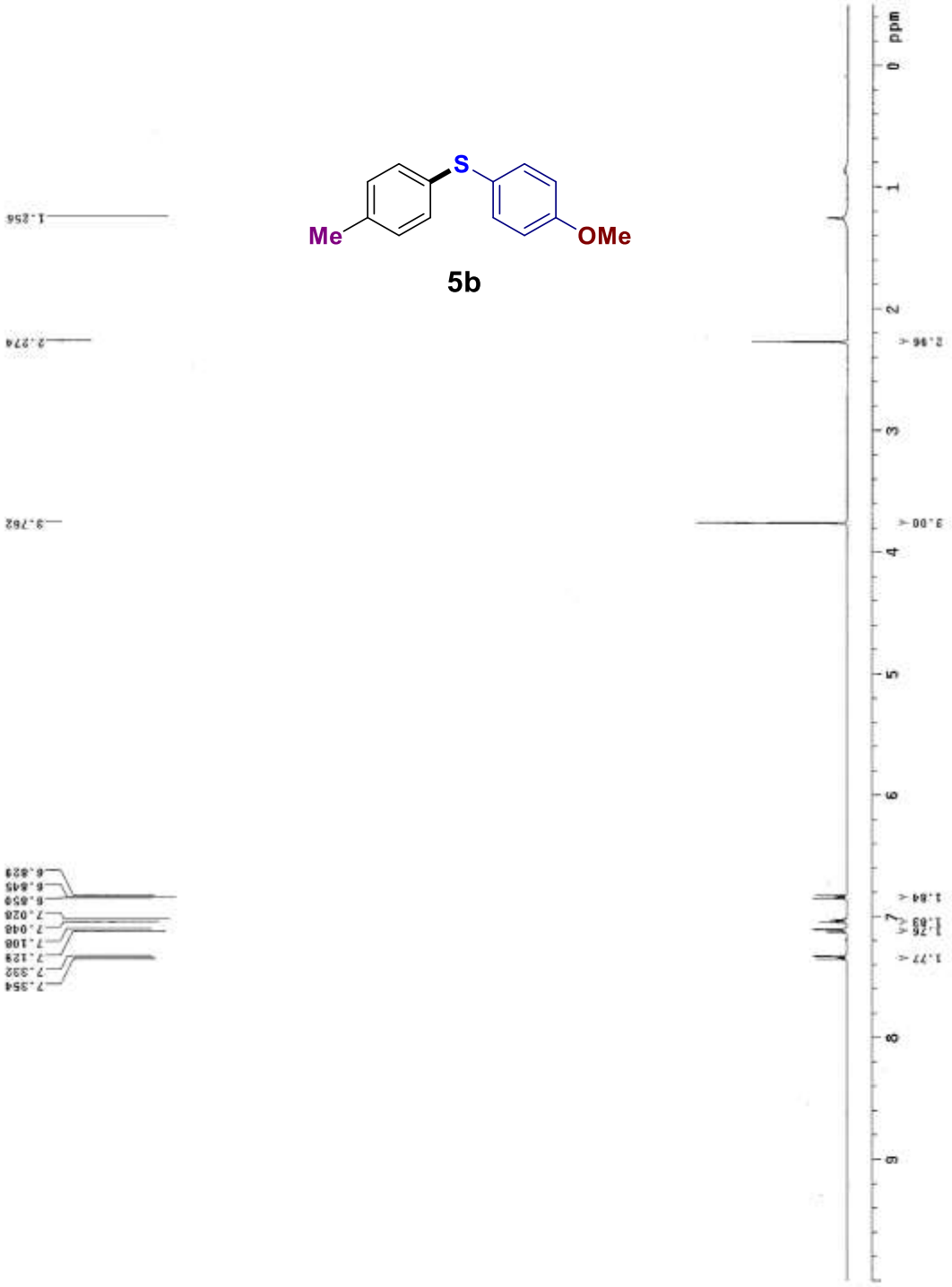
3l


180
160
140
120
100
80
60
40
20
ppm

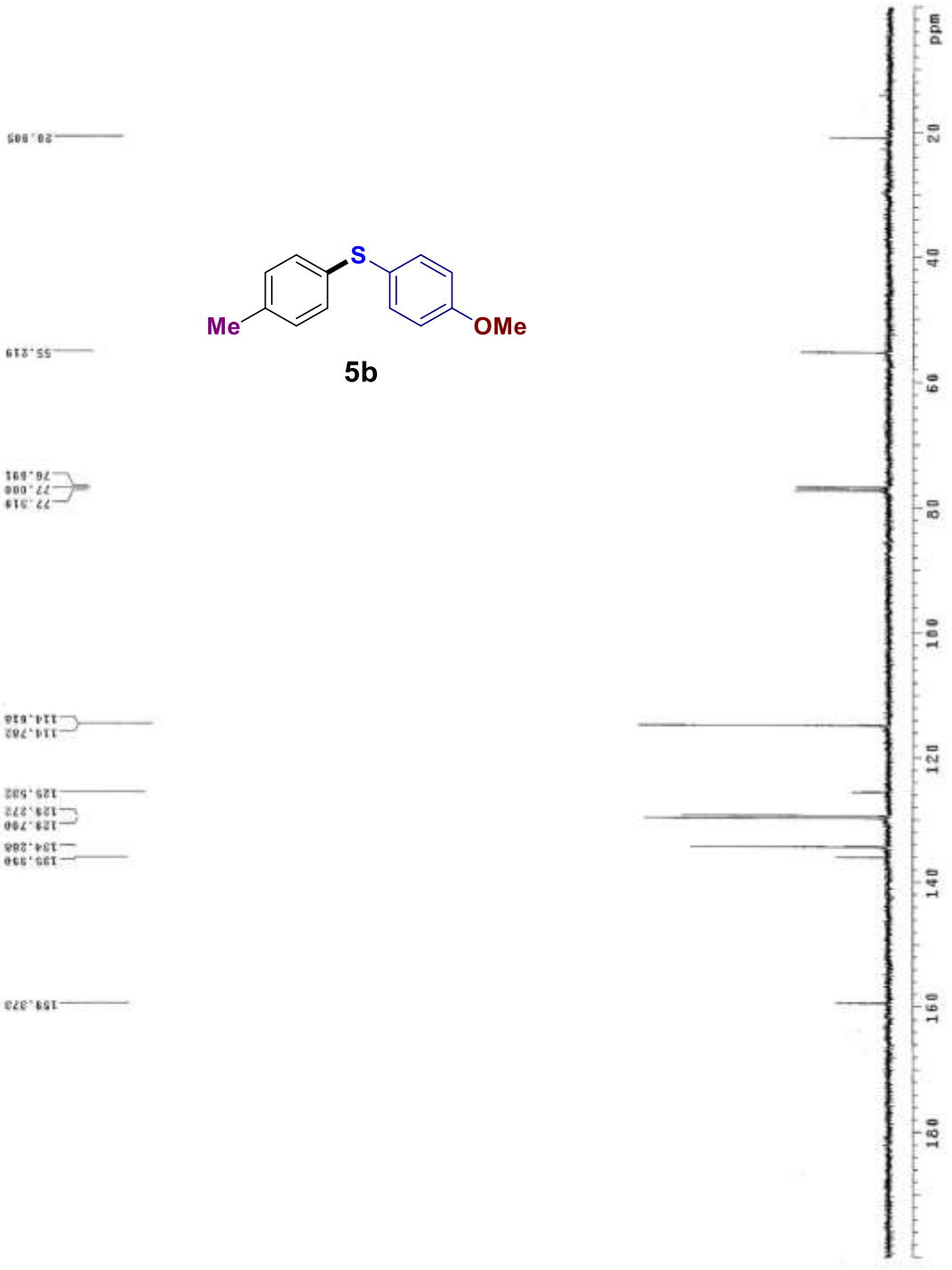


5a

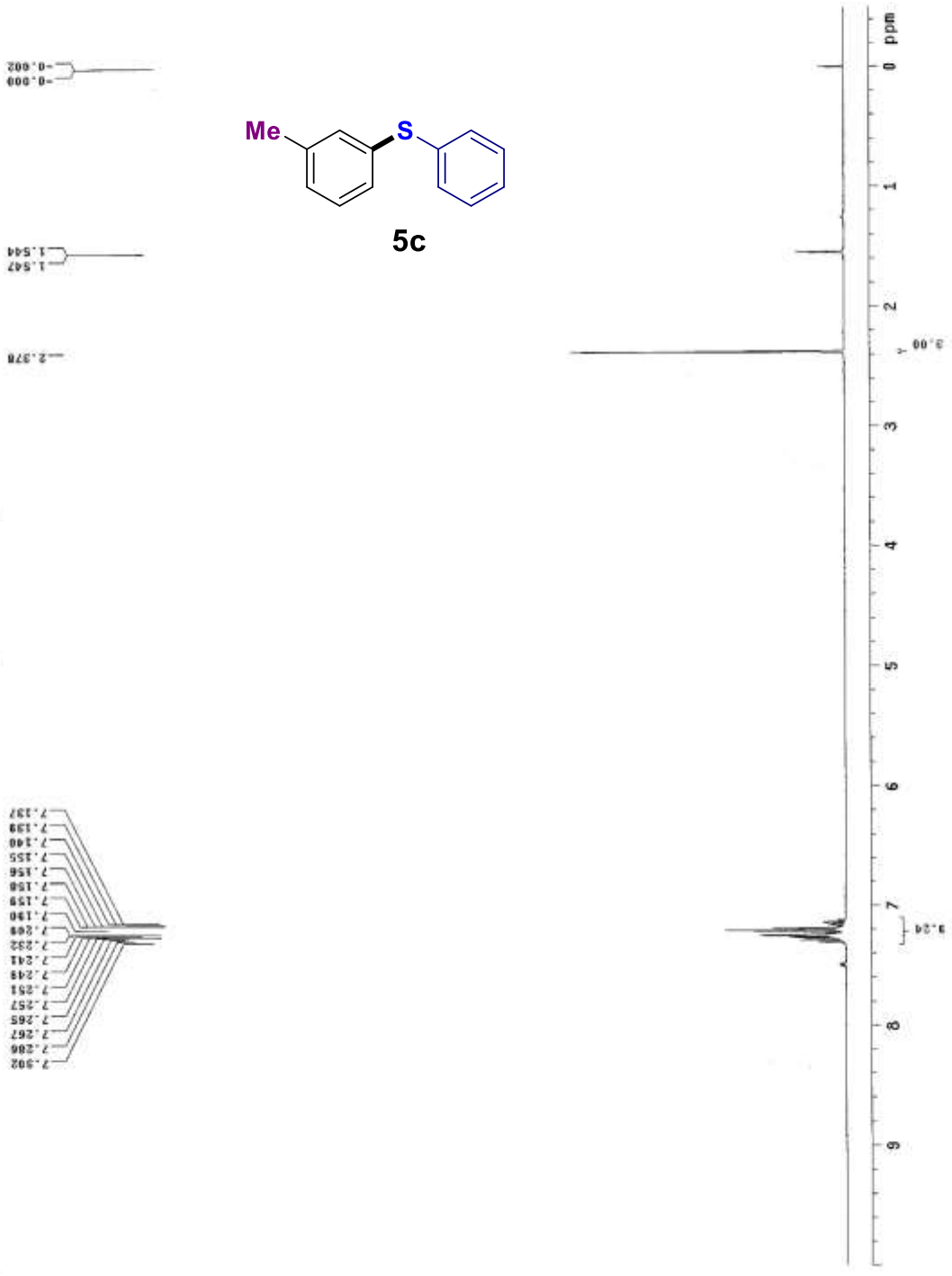

S
Me
5a
ppm
20
40
60
80
100
120
140
160
180


S
Me
OMe
1.256
3.774
3.762
6.829
6.845
6.859
7.028
7.048
7.108
7.129
7.332
7.354
2.96
3.00
1.84
1.76
1.69
1.77
ppm
0
1
2
3
4
5
6
7
8
9

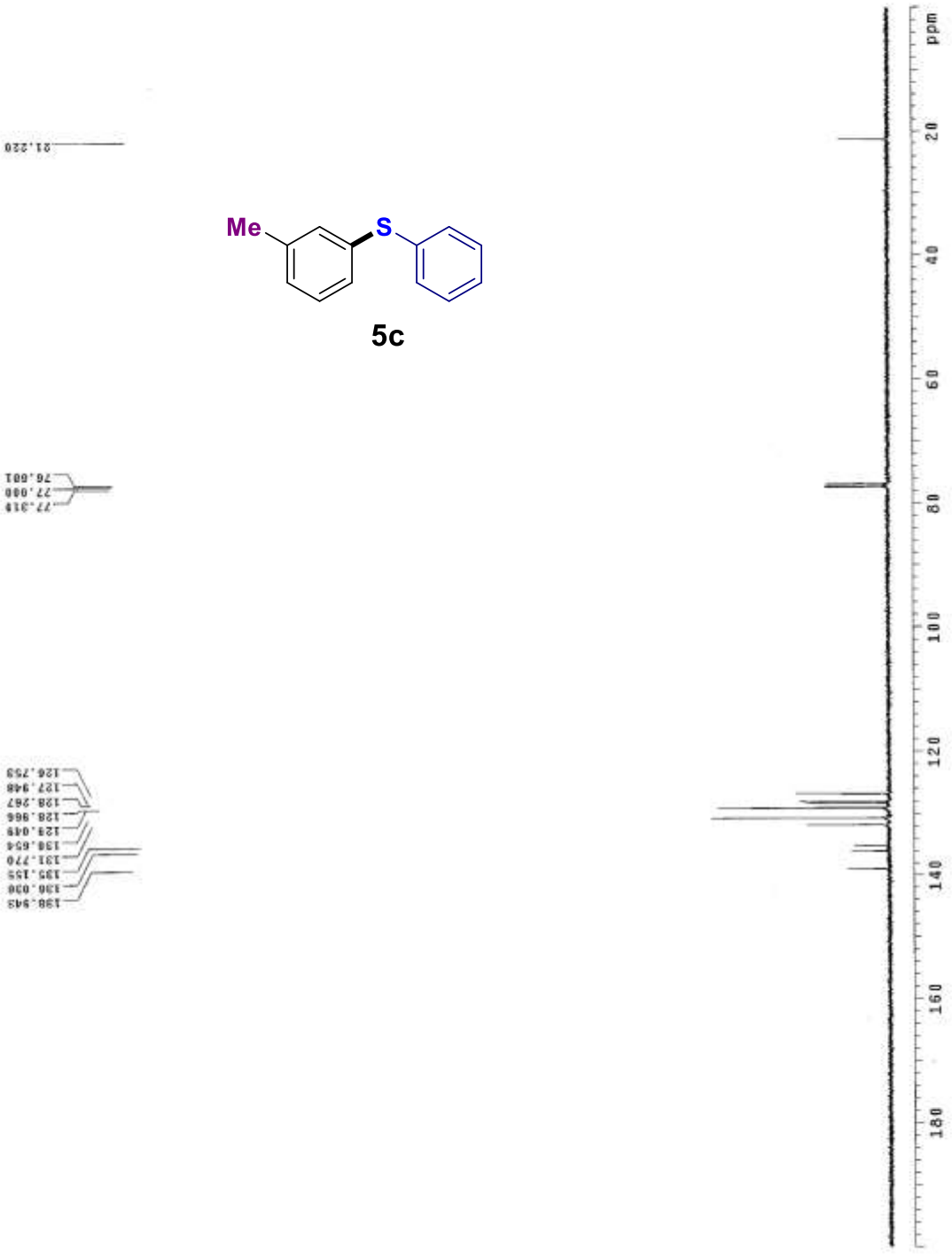
5b

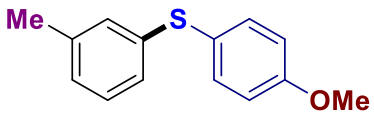

S
Me
OMe
28.805
55.219
77.319
77.000
76.681
114.838
114.782
125.582
129.272
129.790
134.288
135.990
159.373
ppm
20
40
60
80
100
120
140
160
180

5b

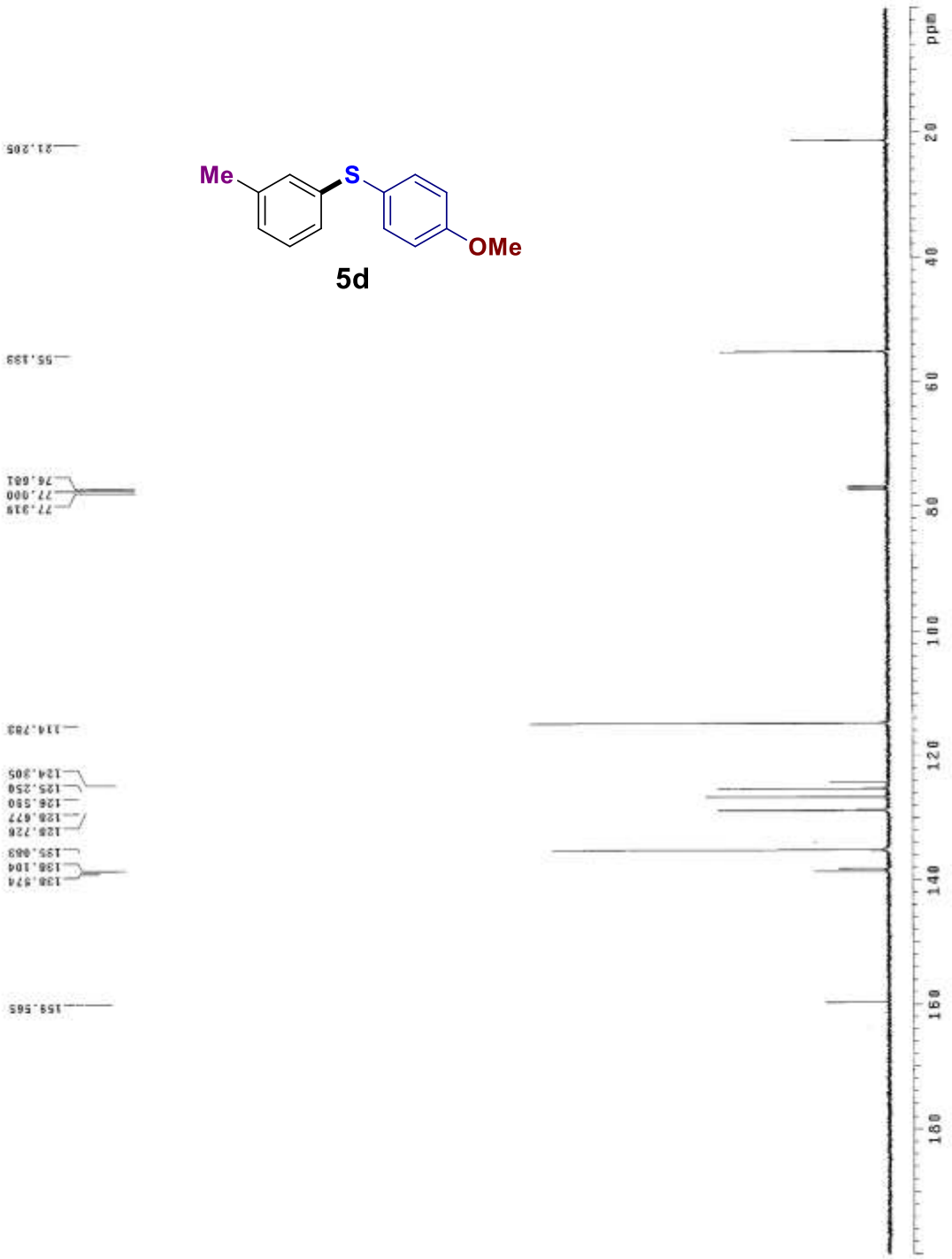


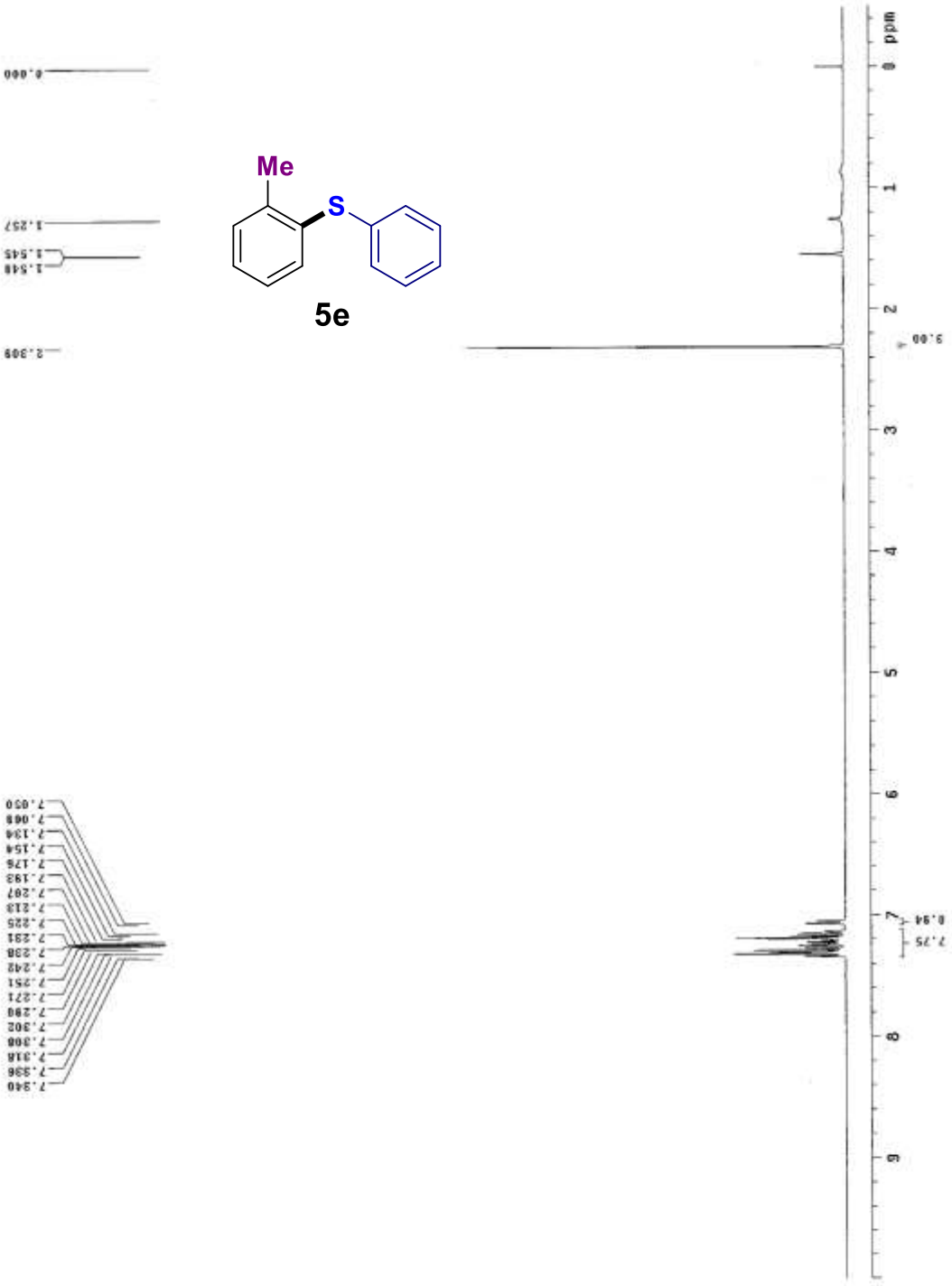
5c

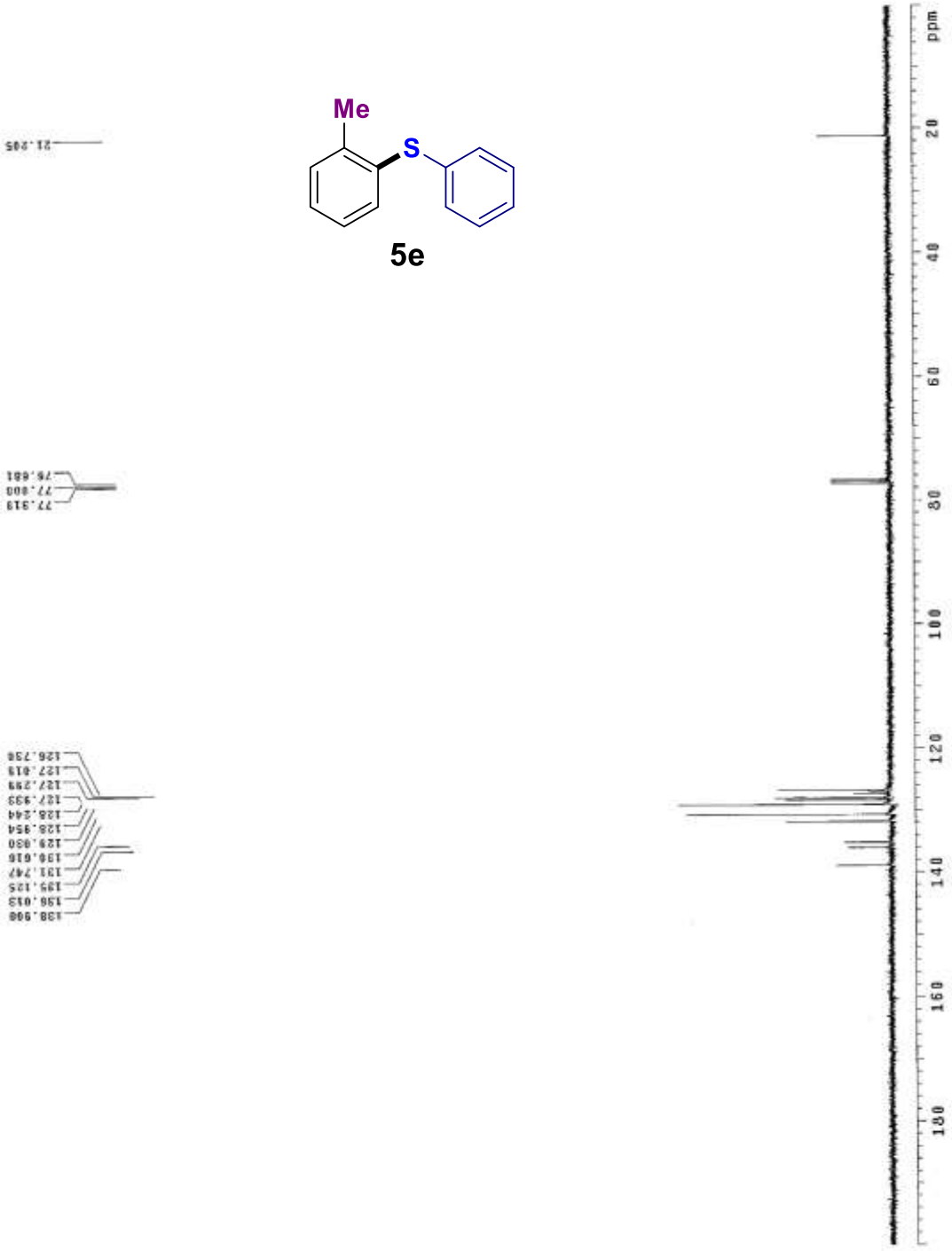

Me
S
5c
ppm
20
40
60
80
100
120
140
160
180



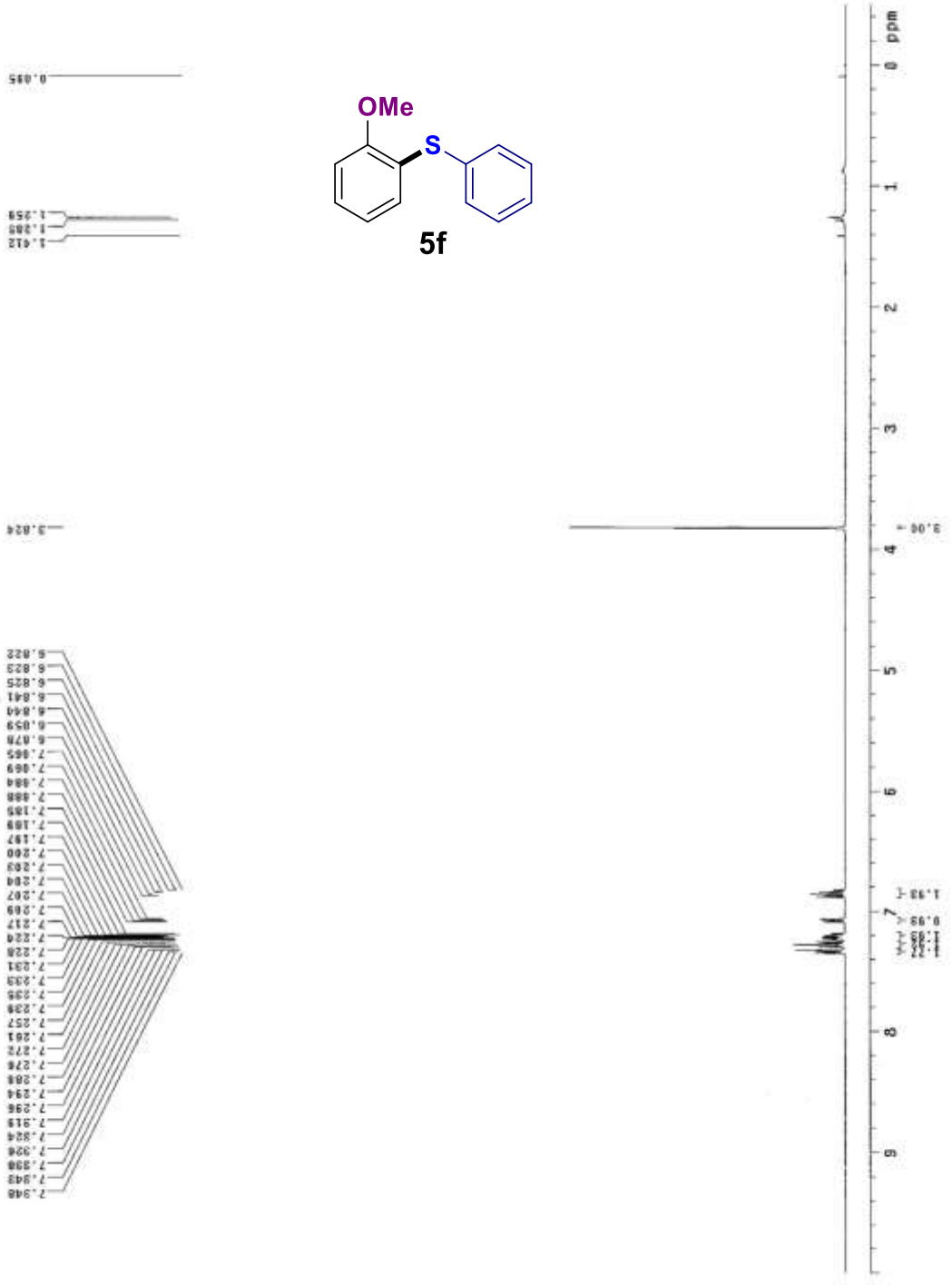
5d

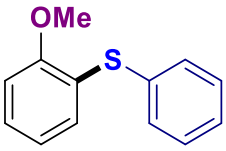

Me
S
OMe
5d
21.205
55.189
76.681
77.000
77.319
114.783
124.305
125.250
126.580
128.677
128.726
135.083
136.104
138.974
159.565
ppm
20
40
60
80
100
120
140
160
180


Me
S
5e


Me
S
21.205
76.681
77.000
77.319
126.758
127.019
127.299
127.993
128.244
128.954
129.080
130.616
131.747
135.125
136.013
138.900
ppm
20
40
60
80
100
120
140
160
180

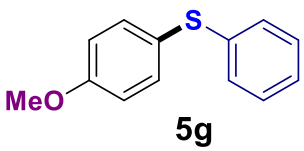
5e


OMe
S
5f

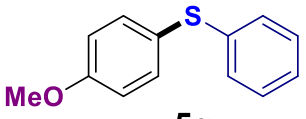

OMe
S

5f

55.729
76.681
77.000
77.319
110.750
121.126
129.920
126.993
128.244
129.027
134.911
134.502
184.615
197.197
ppm
20
40
60
80
100
120
140
160
180

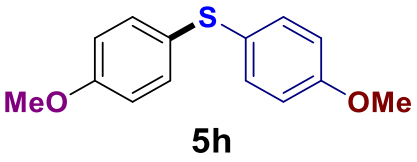


5g

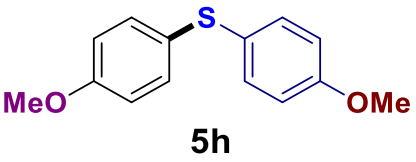

S
MeO

5g

55.152
76.681
77.080
77.915
114.844
124.813
125.592
127.950
128.798
135.276
136.517
159.671
ppm
20
40
60
80
100
120
140
160
180

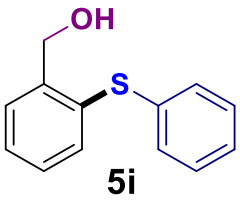


5h

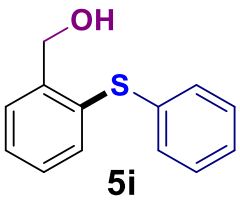

S
MeO
OMe

5h

55.229
76.681
77.000
77.318
114.085
127.227
138.618
158.896
ppm
20
40
60
80
100
120
140
160
180

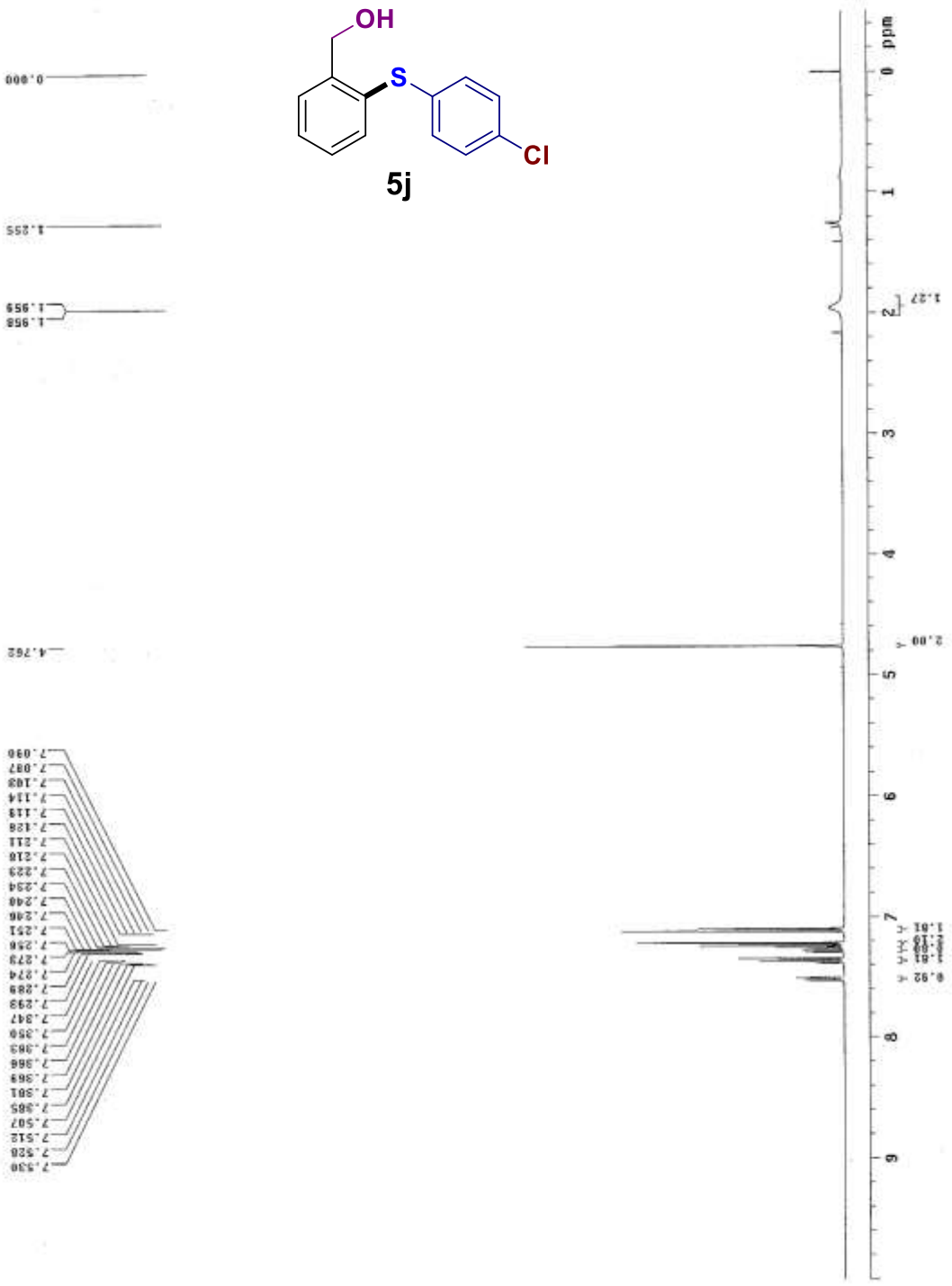


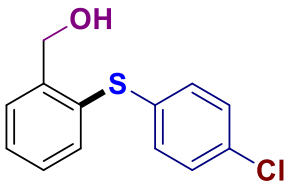
5i


OH
S

5i

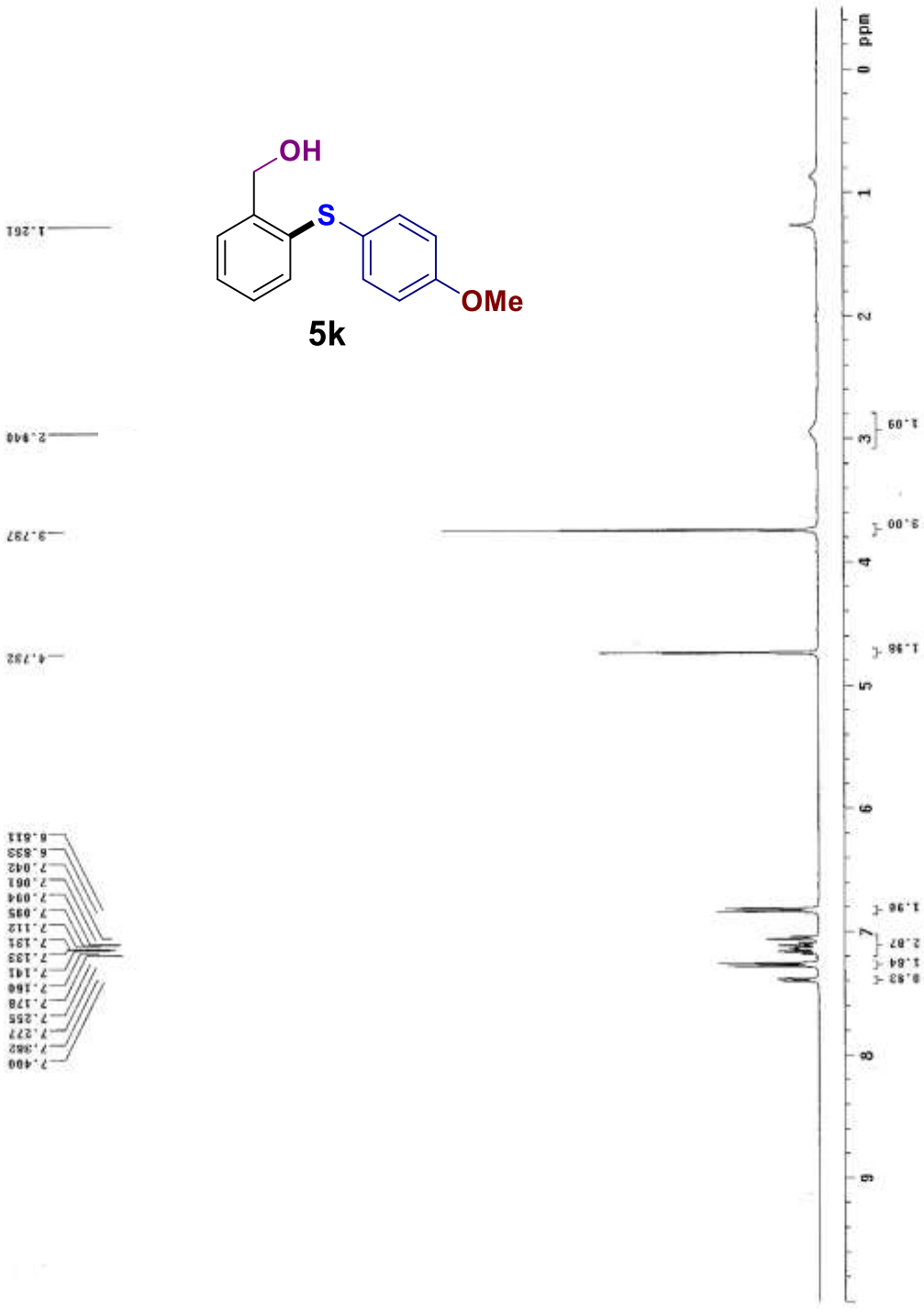
62.966
76.685
77.000
77.319
128.389
128.858
128.156
128.225
129.043
129.293
132.028
139.576
139.000
142.176
ppm
20
40
60
80
100
120
140
160
180

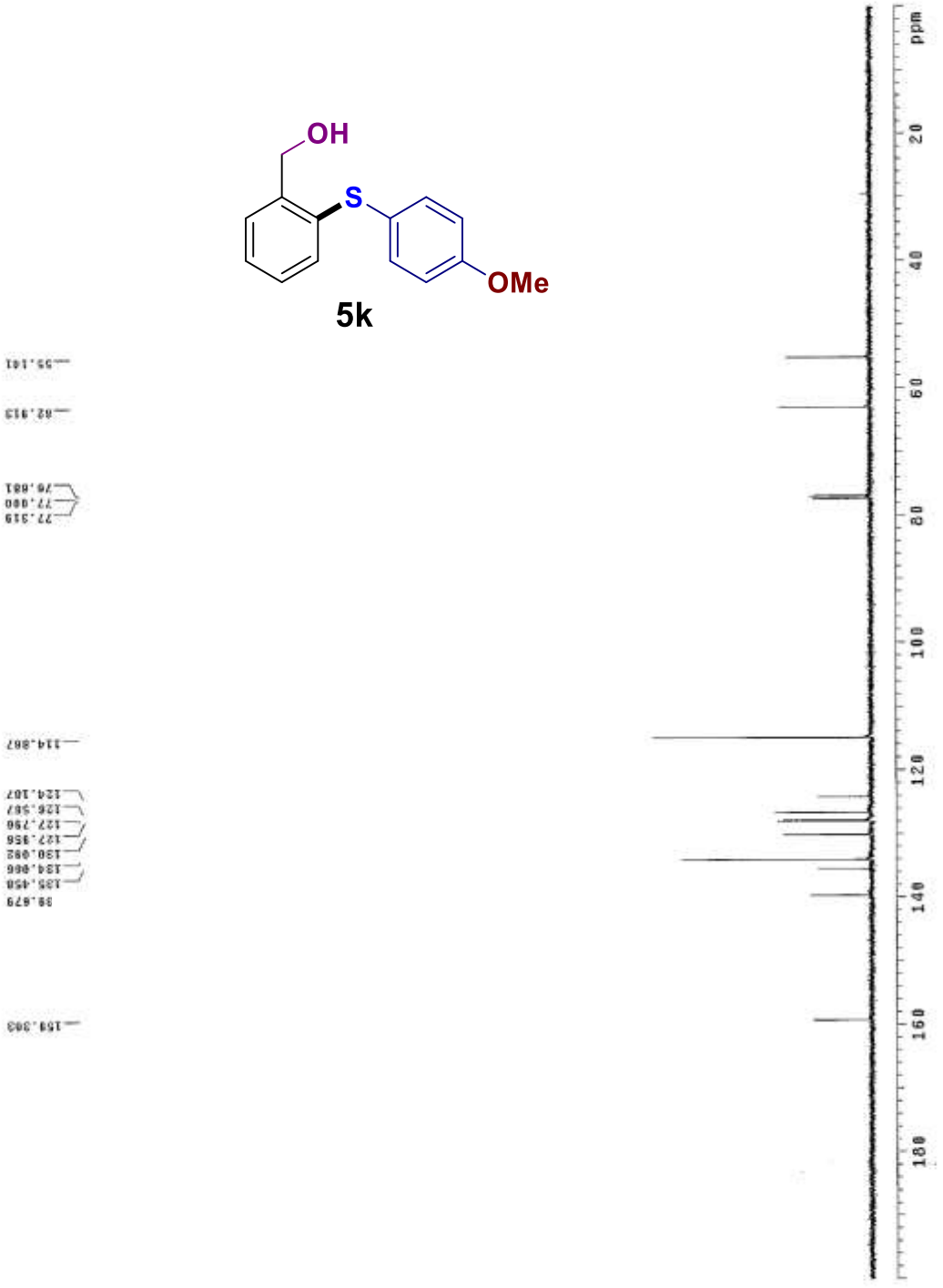

OH
S
Cl
5j


OH
S
Cl

5j

ppm
20
40
60
80
100
120
140
160
180
63.418
76.681
77.000
77.319
120.556
128.586
128.776
129.318
130.514
131.898
132.521
134.047
134.677
142.428


OH
S
OMe
5k


OH
S
OMe
5k
55.161
82.913
76.881
77.080
77.319
114.867
124.107
126.587
127.796
127.956
130.082
134.066
135.458
89.679
159.383
ppm
20
40
60
80
100
120
140
160
180