

Electronic Supplementary Information

Iridium-Catalyzed Asymmetric Allylation of Sodium Triisopropylsilanethiolate: a New Way to Form Chiral Thiols

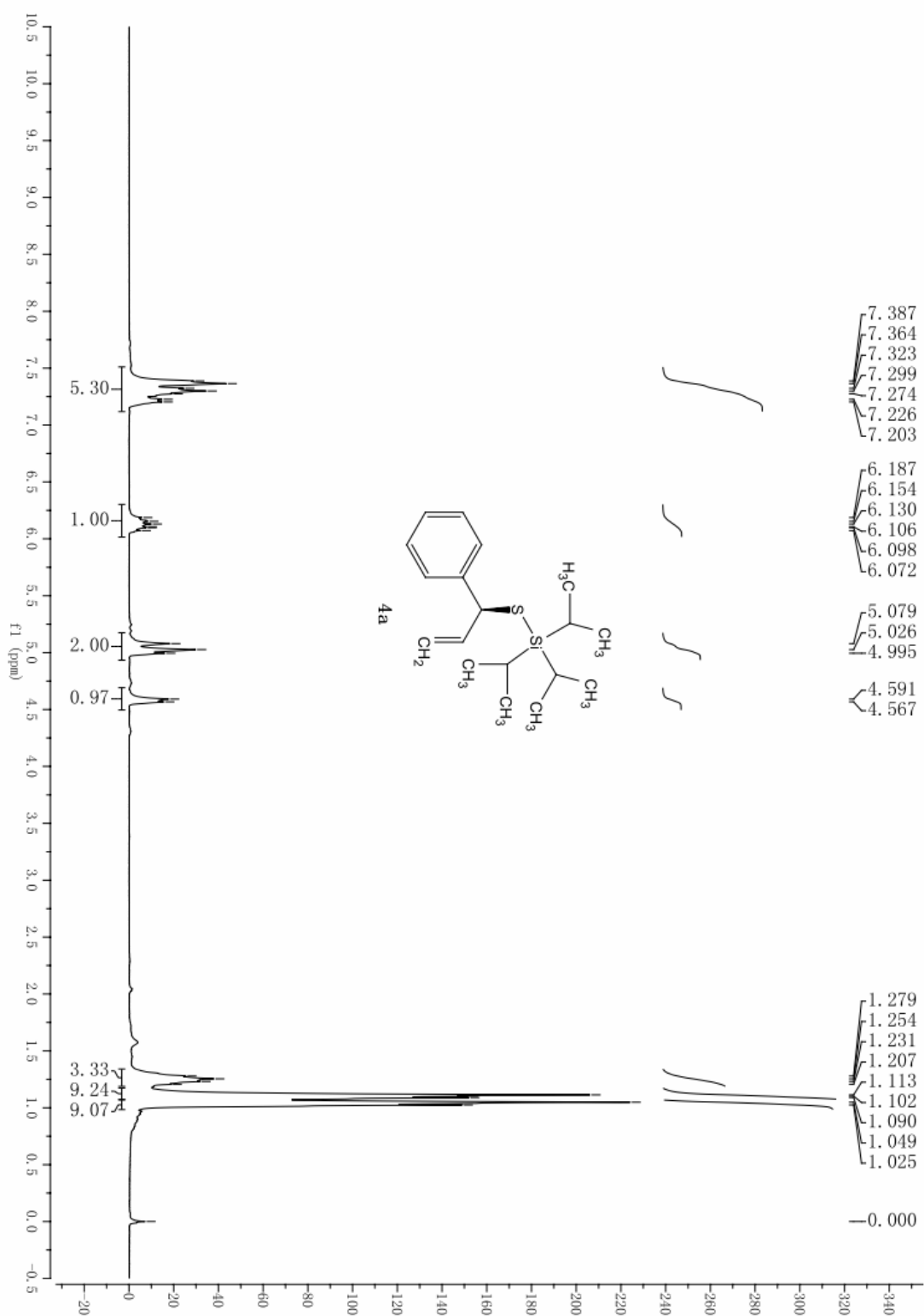
Weiqing Huang^a, Shengcai Zheng^a, Jialiang Tang^a, and Xiaoming Zhao^{a*}

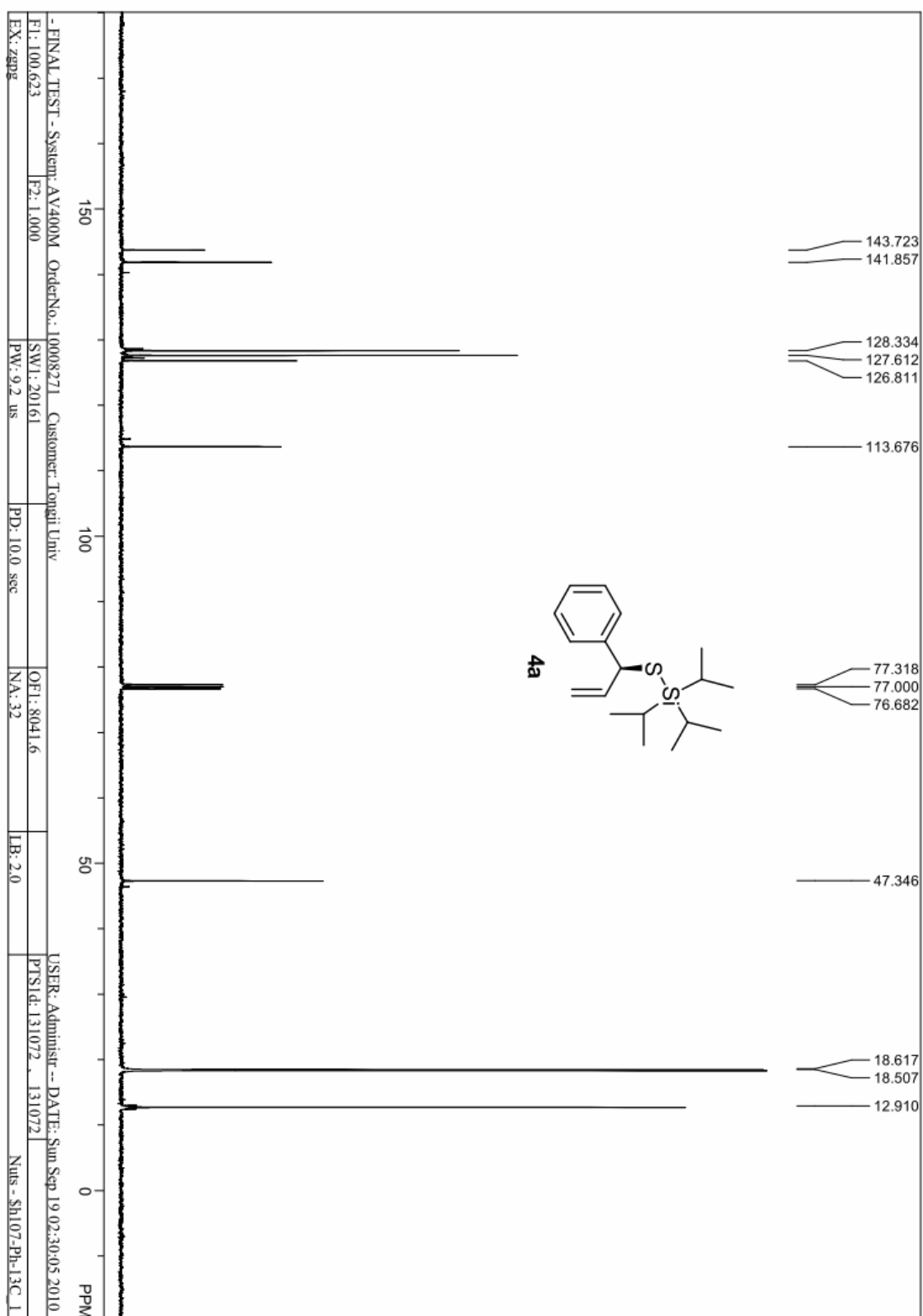
a Department of Chemistry, Tongji University, 1239 Siping Road, Shanghai, 200092 P.R. China

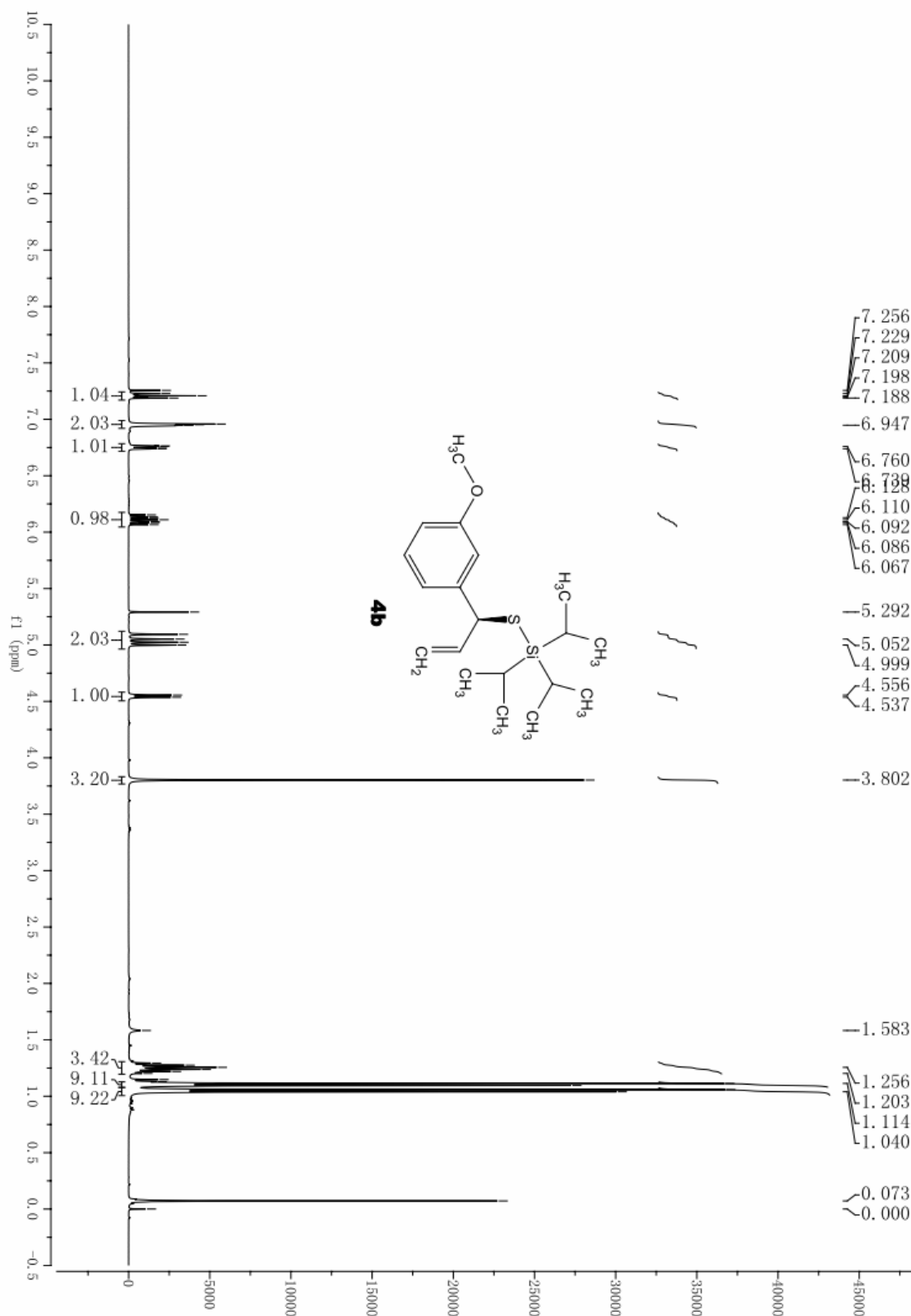
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Dalian, P.R. China, 116012*

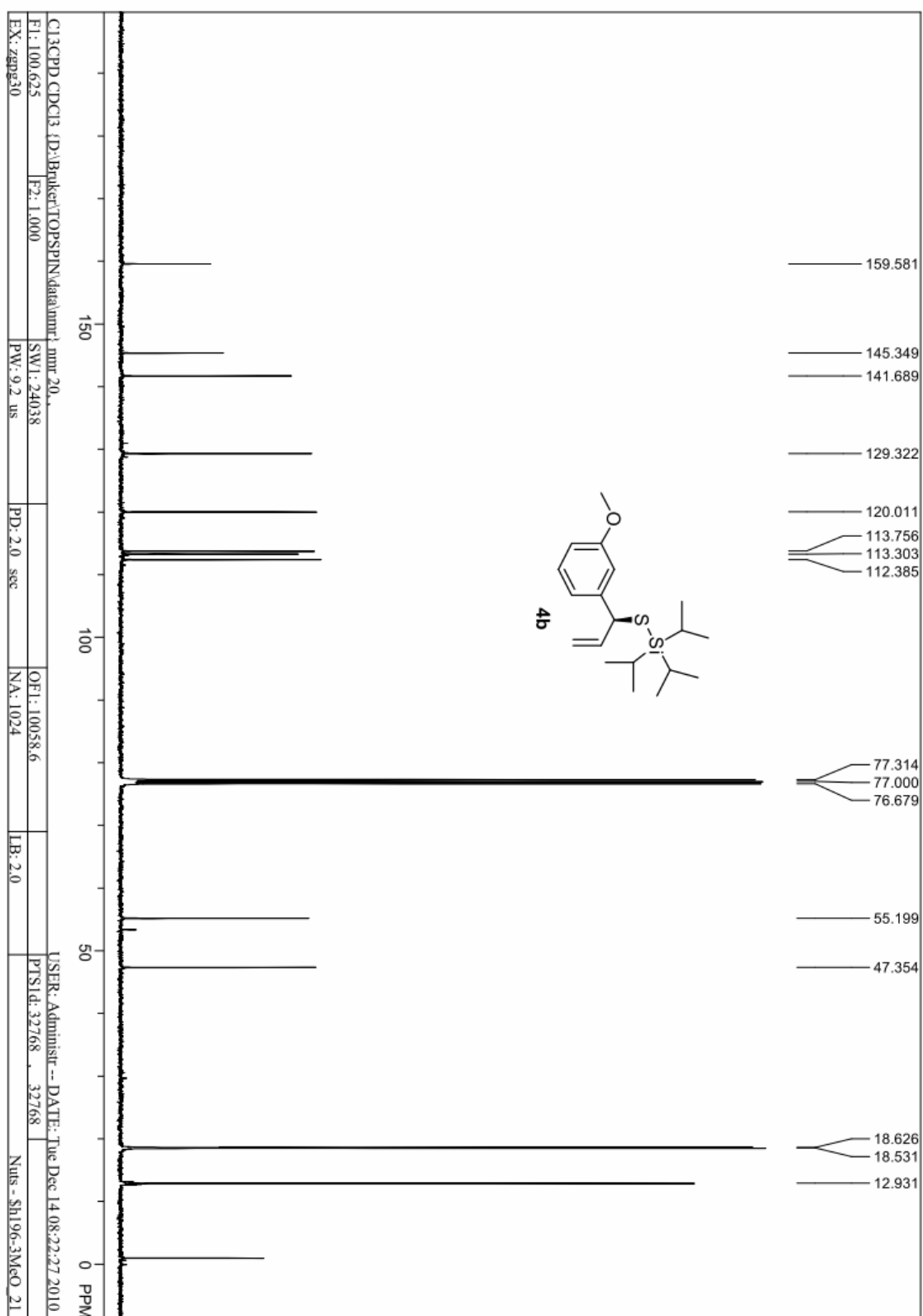
xmzhao08@mail.tongji.edu.cn

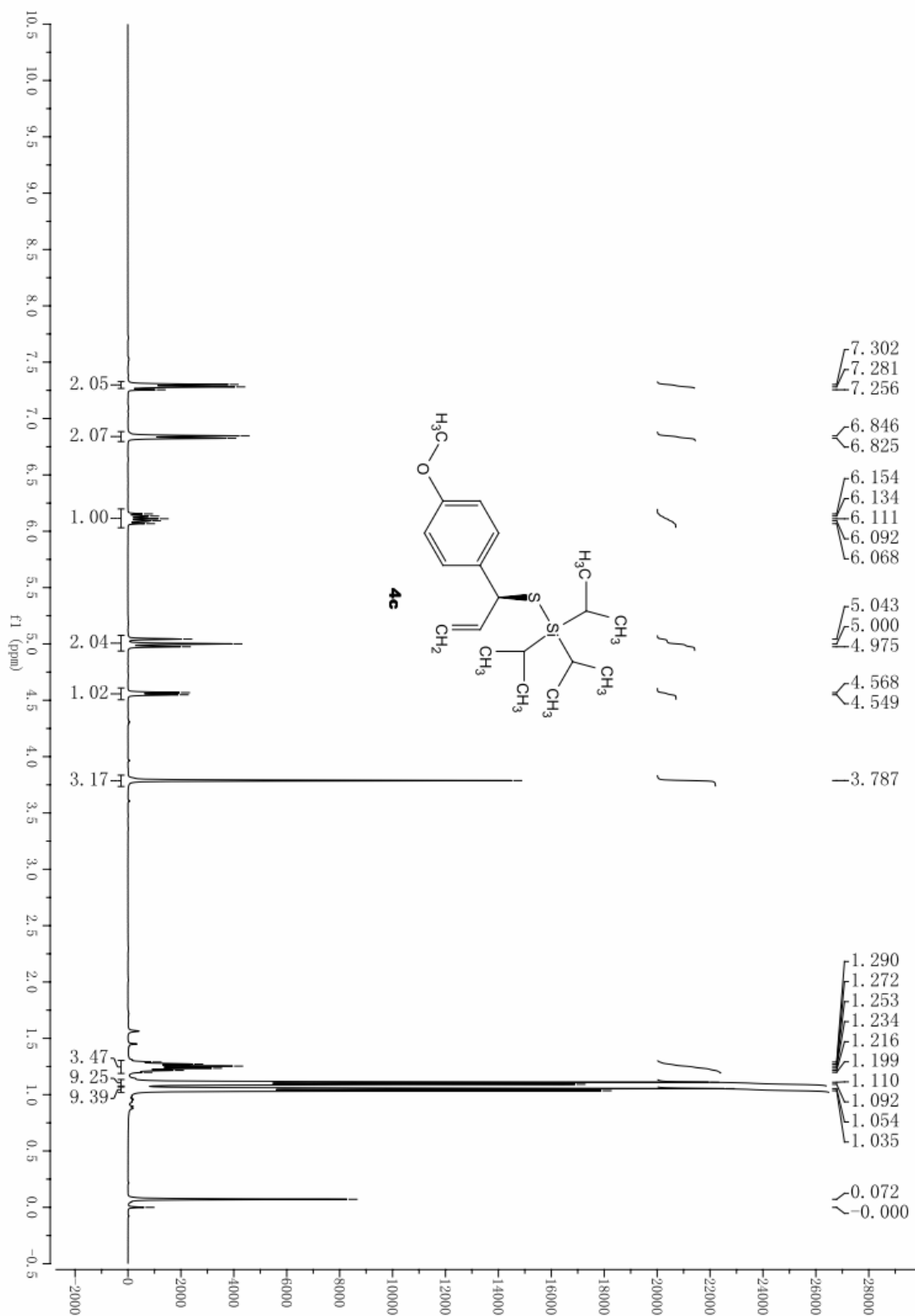
NMR Spectra of the Compounds:

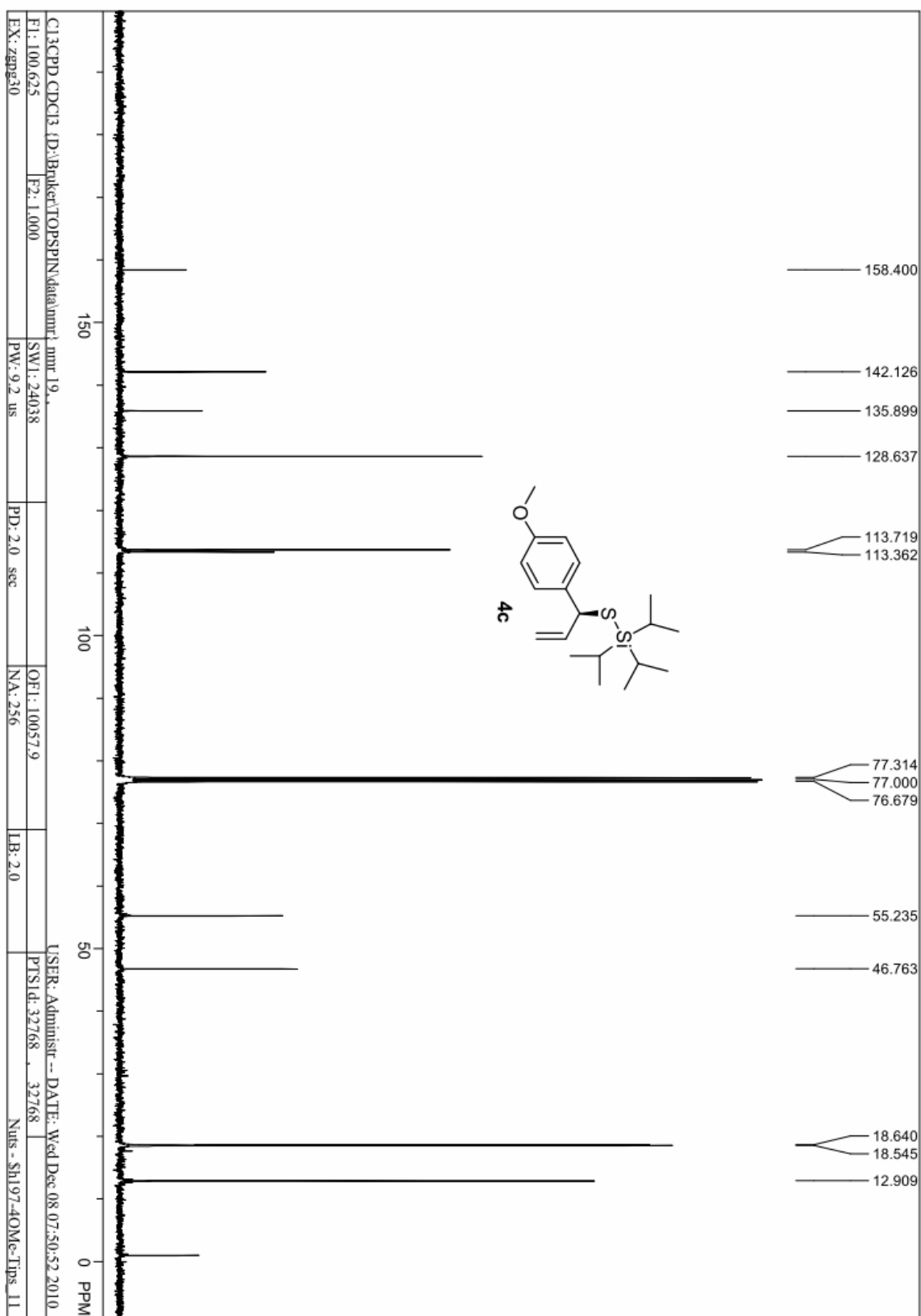


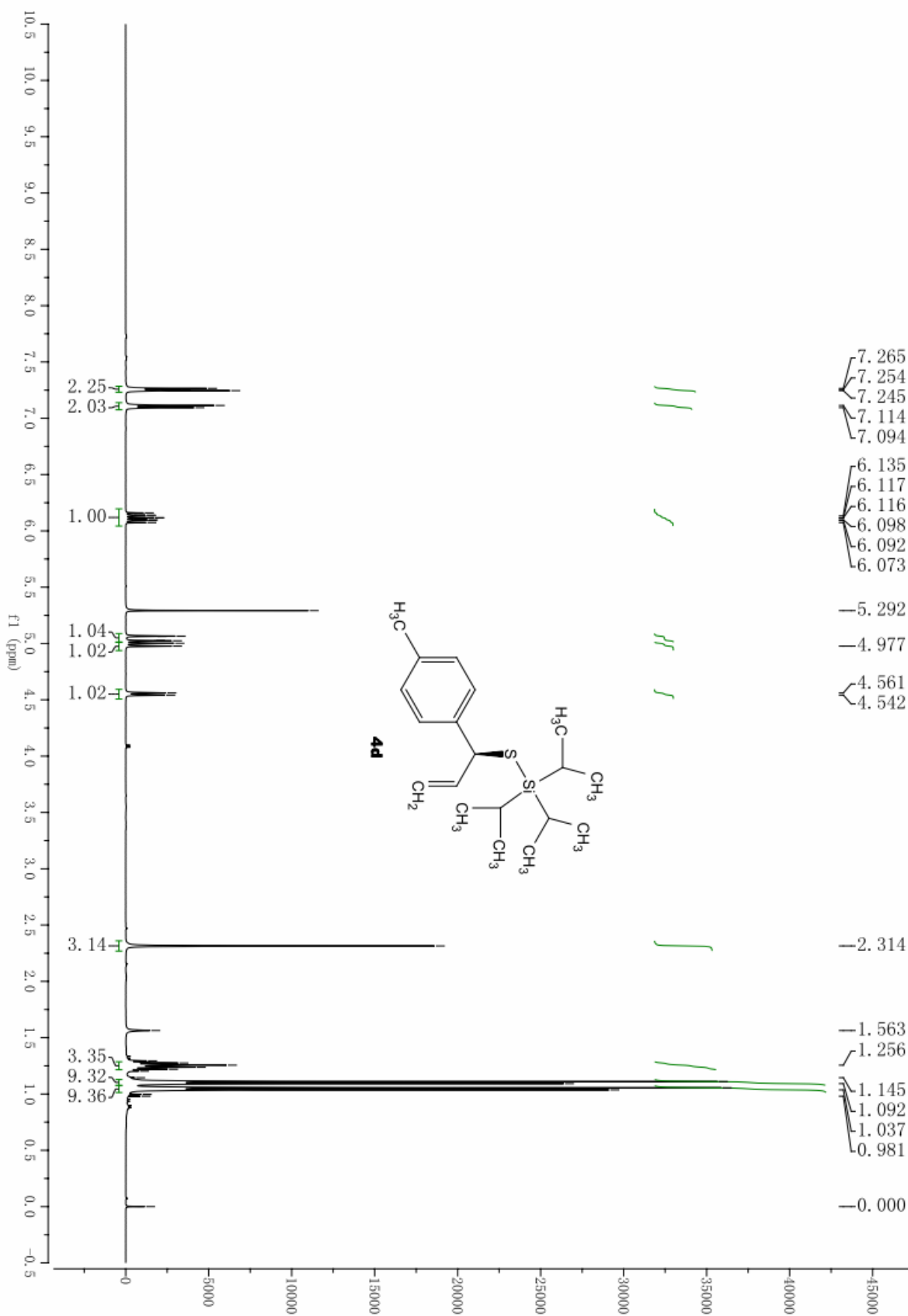


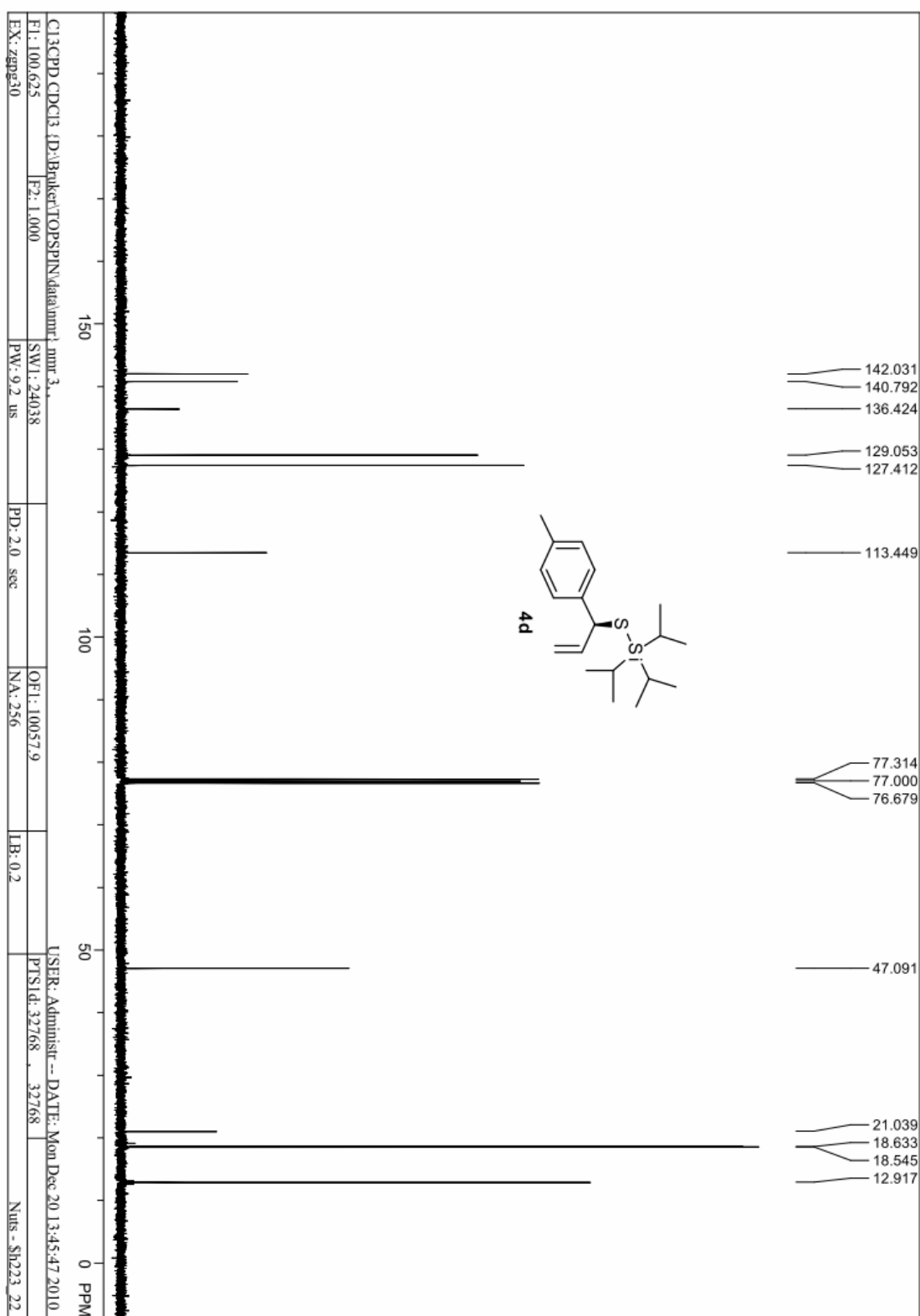


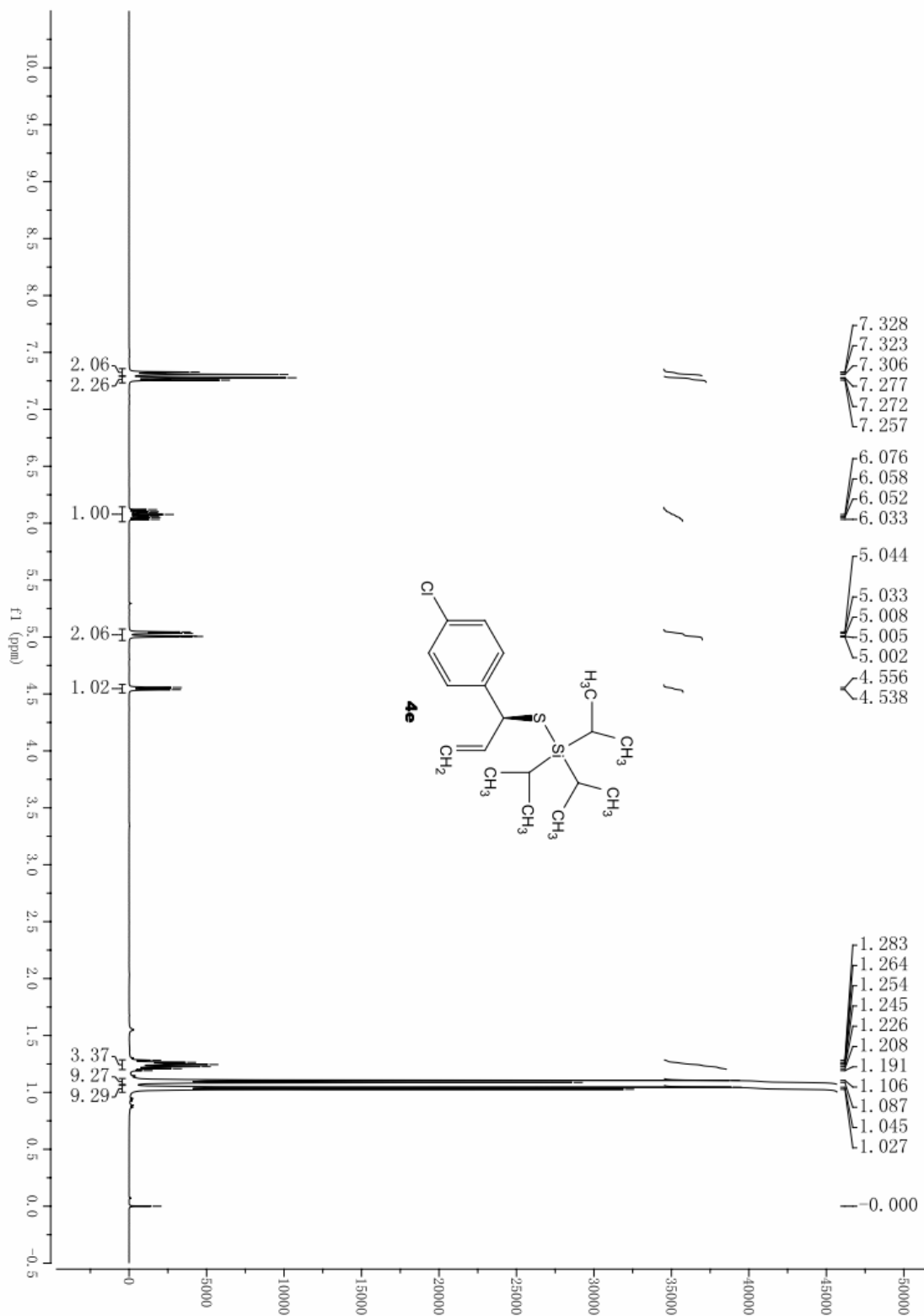


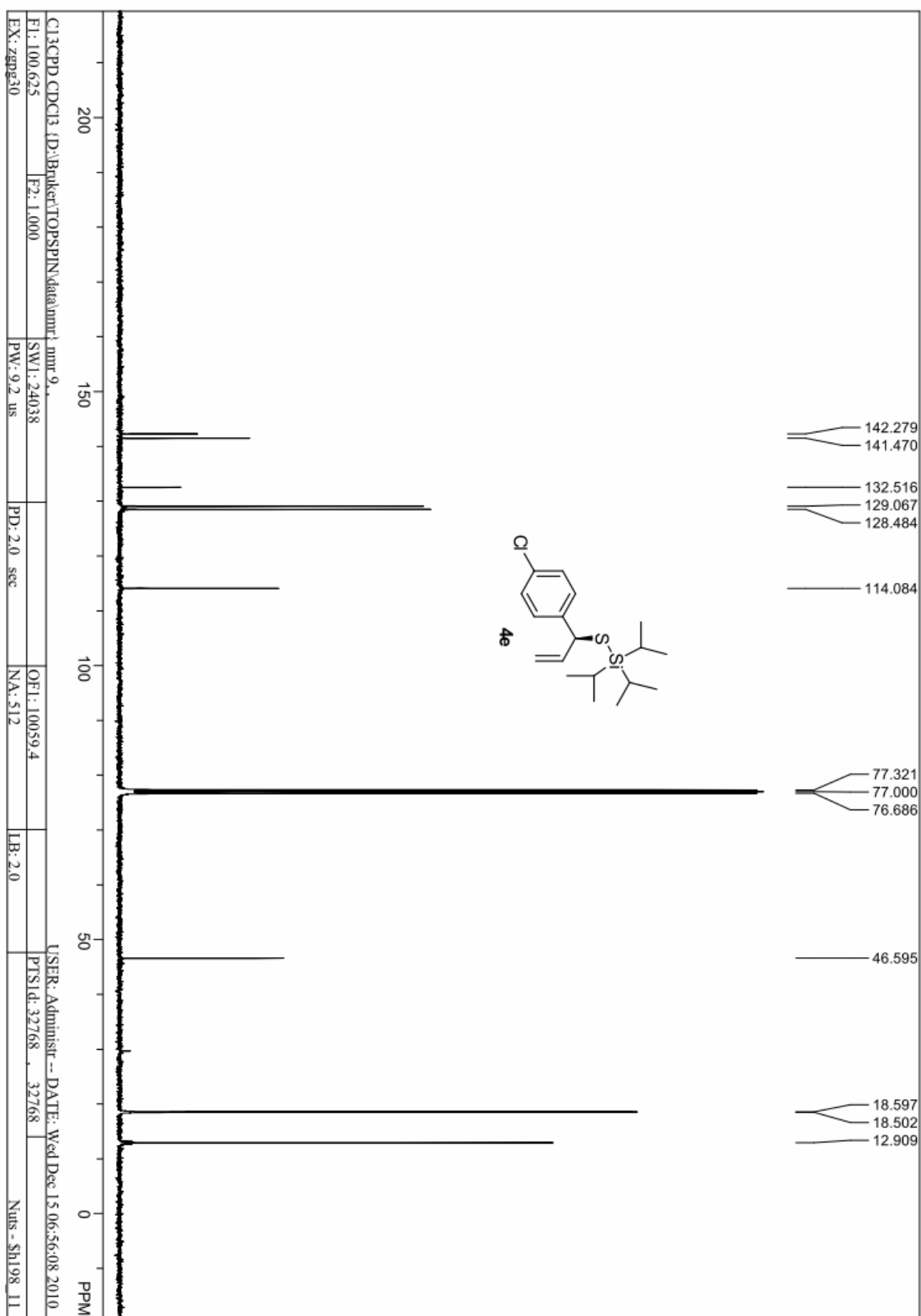


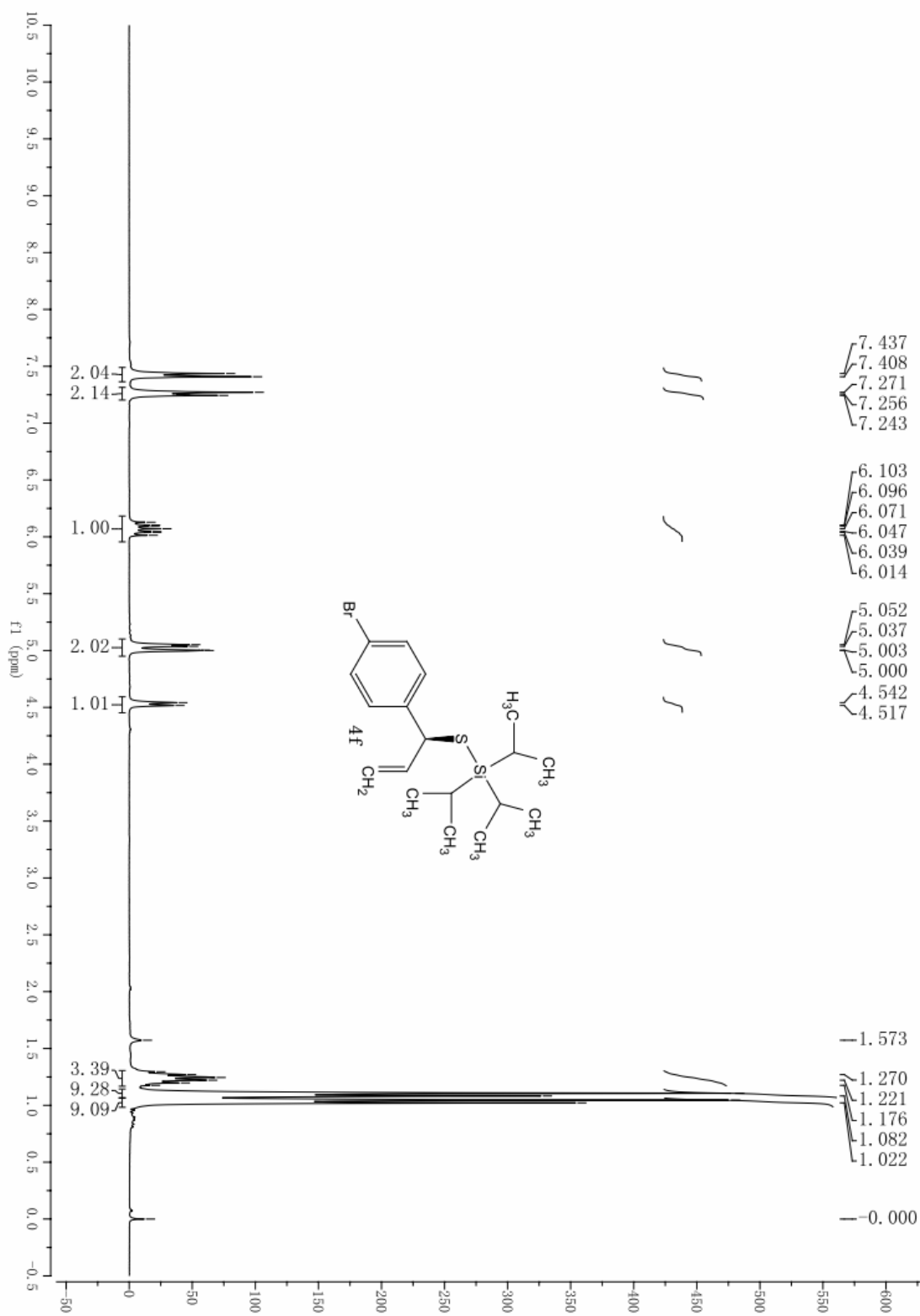


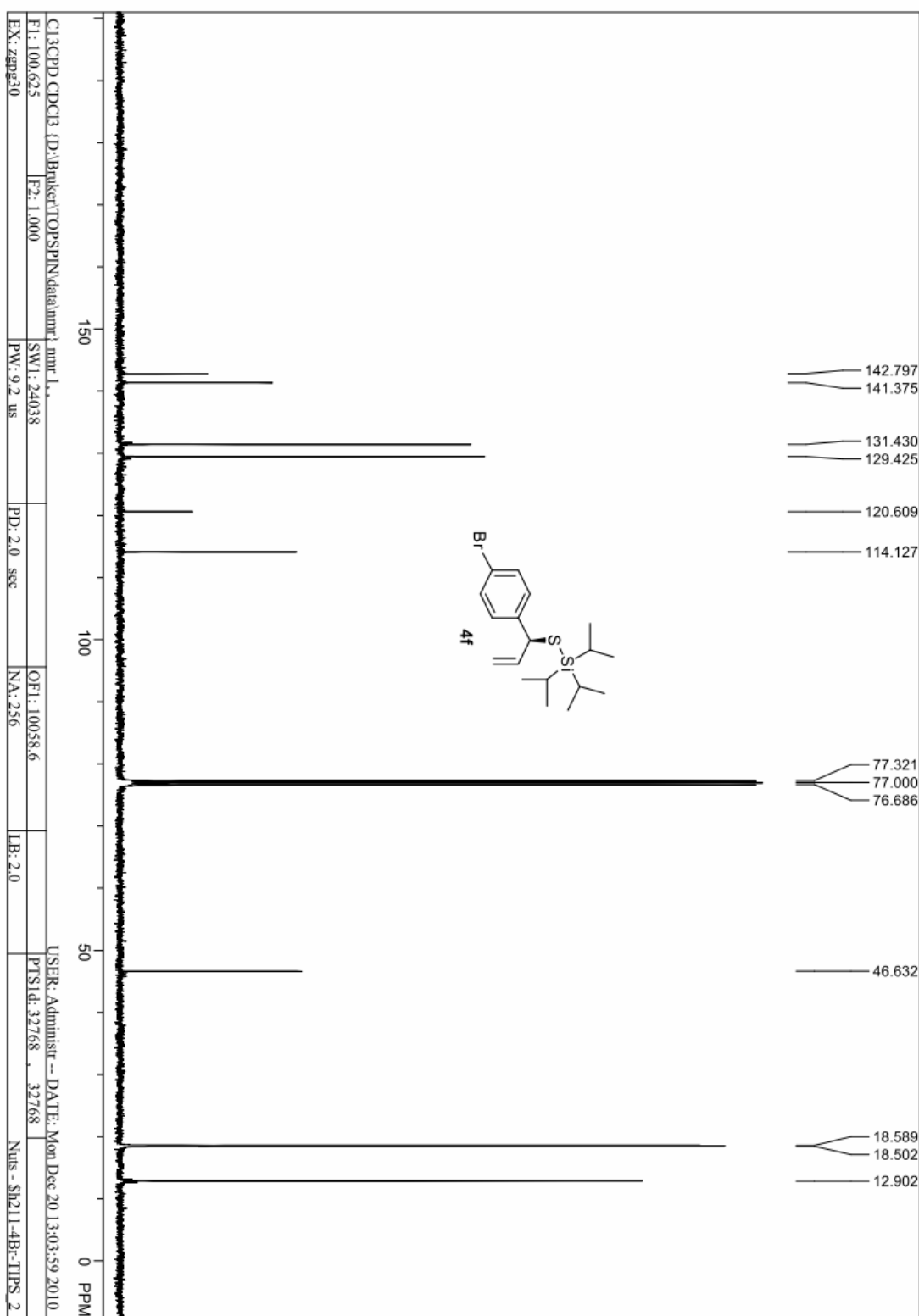


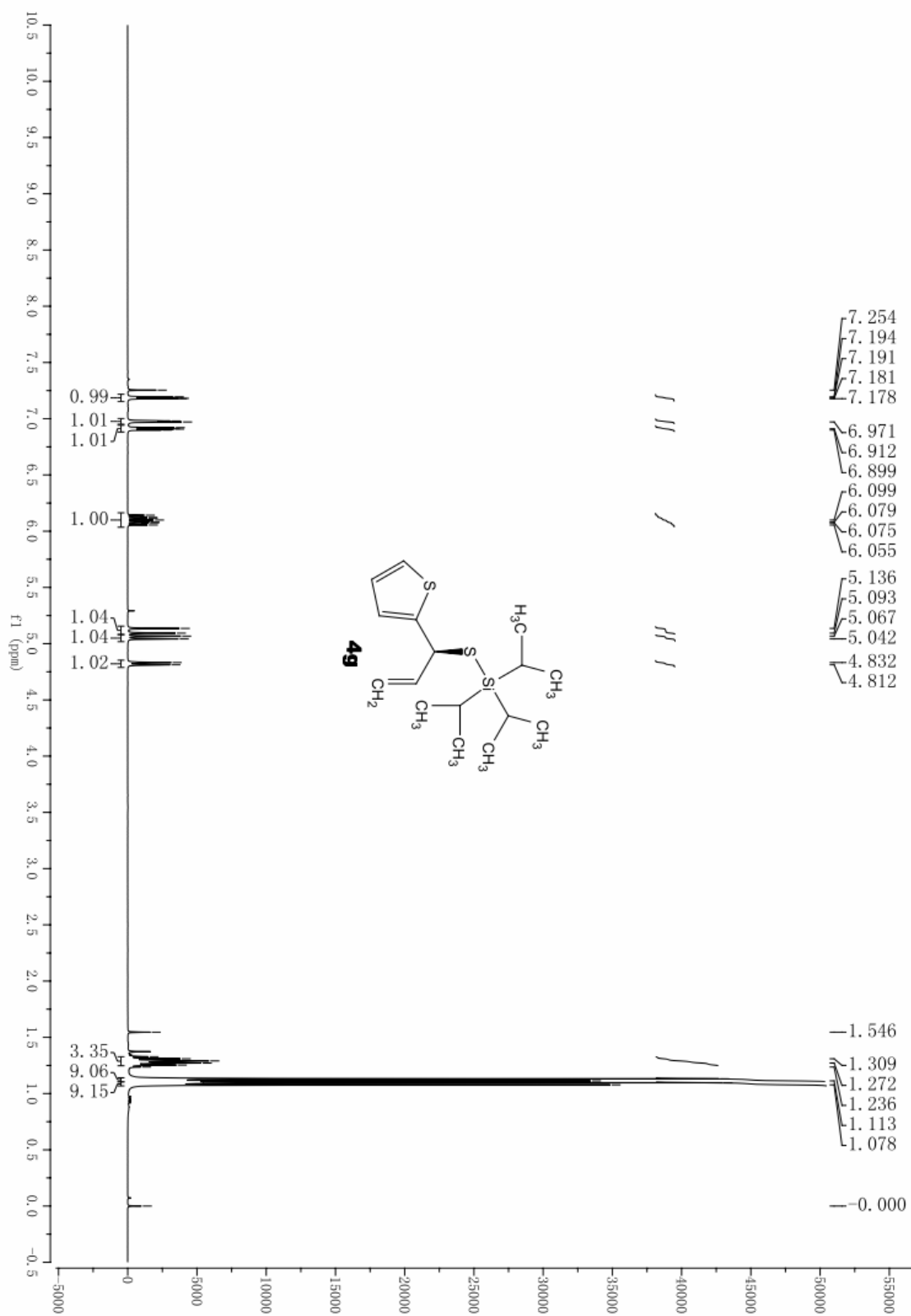


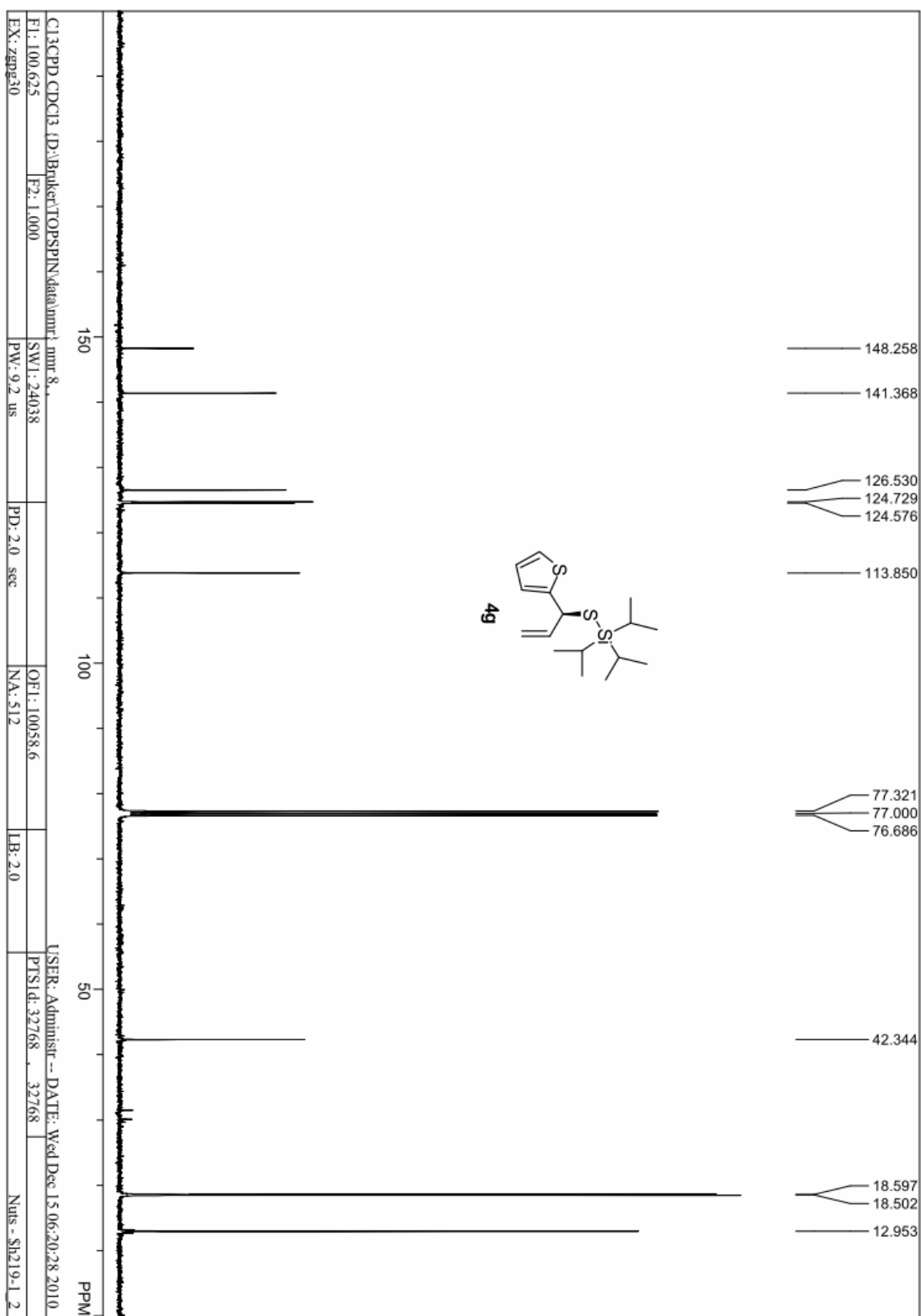


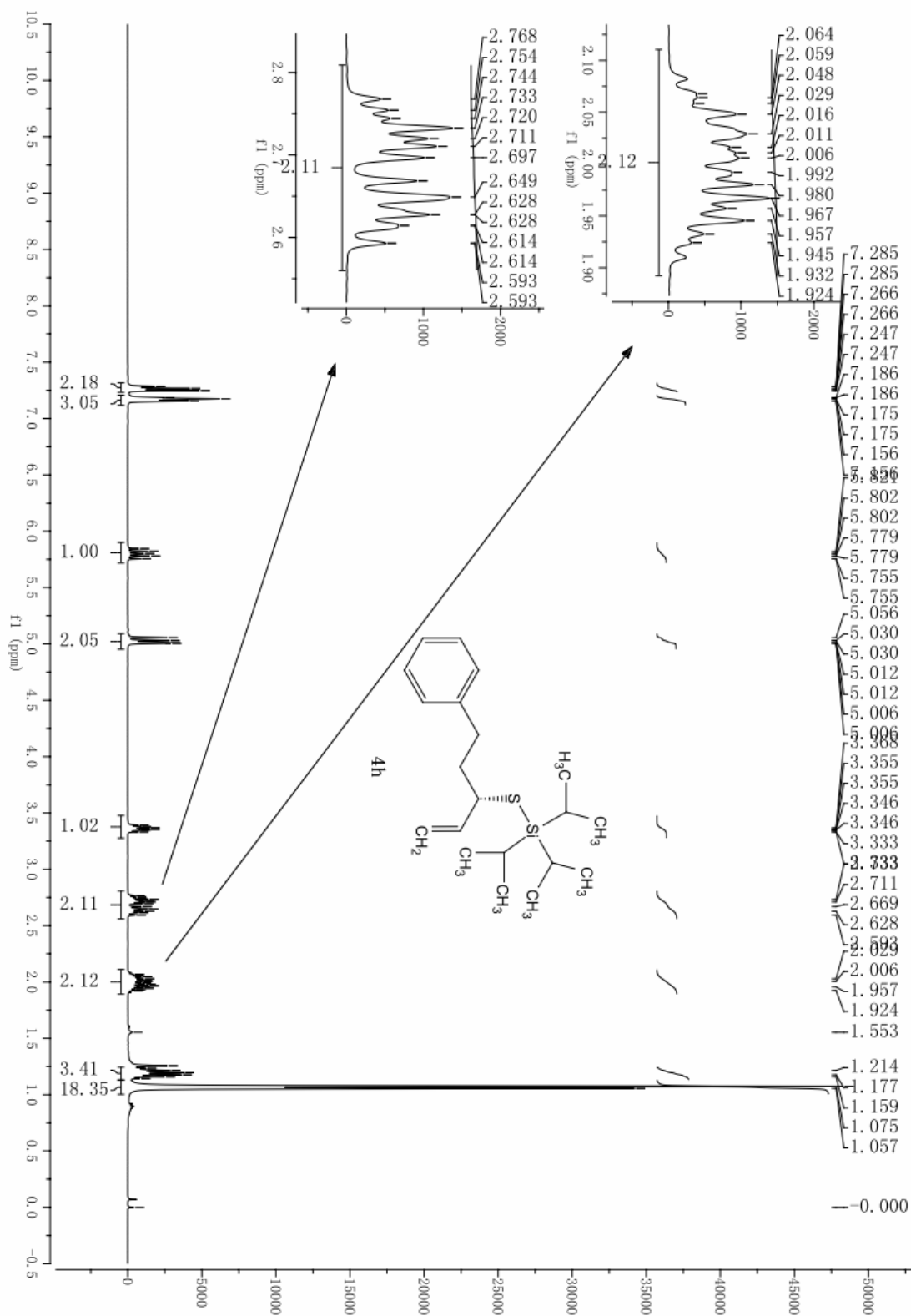


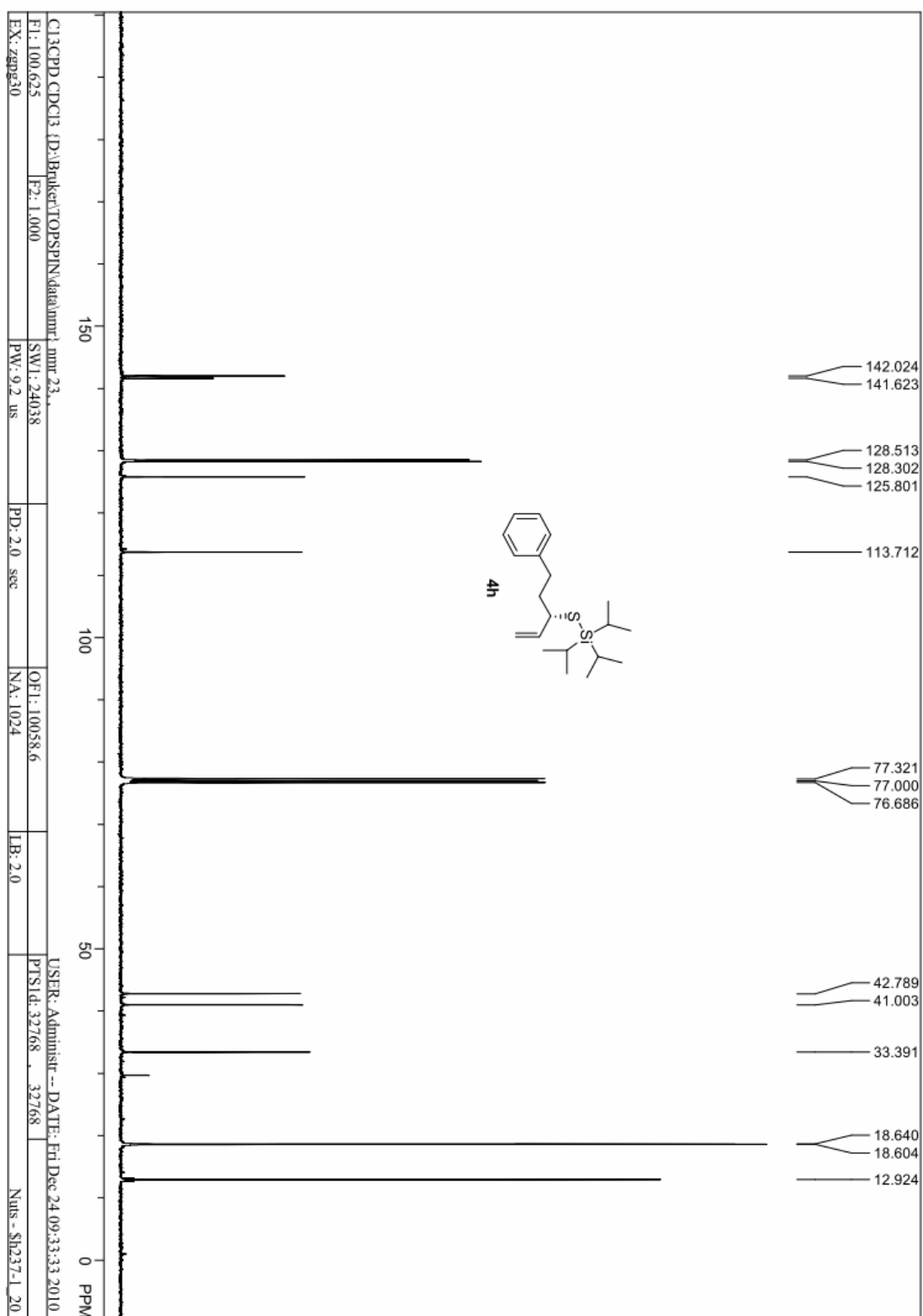


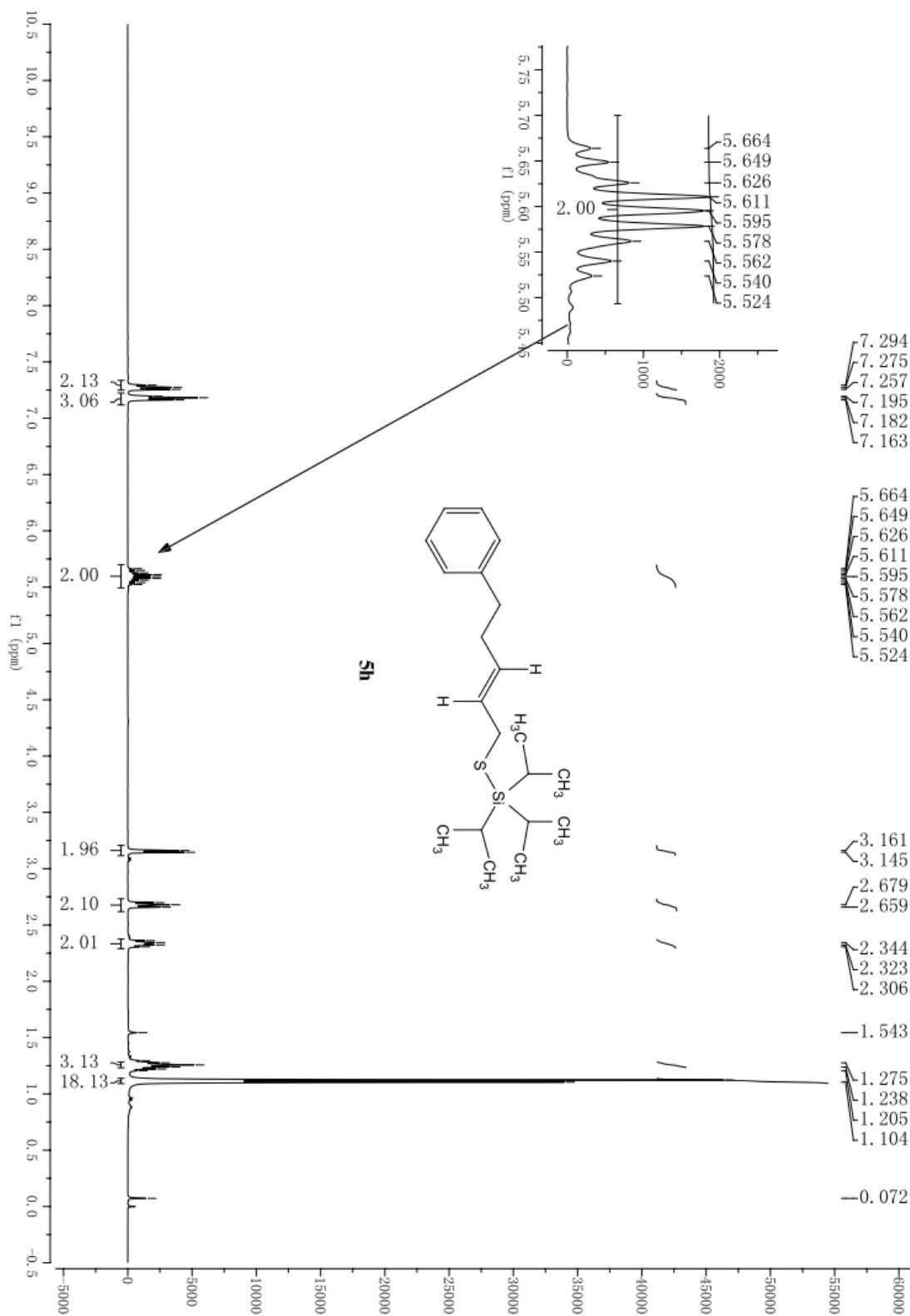


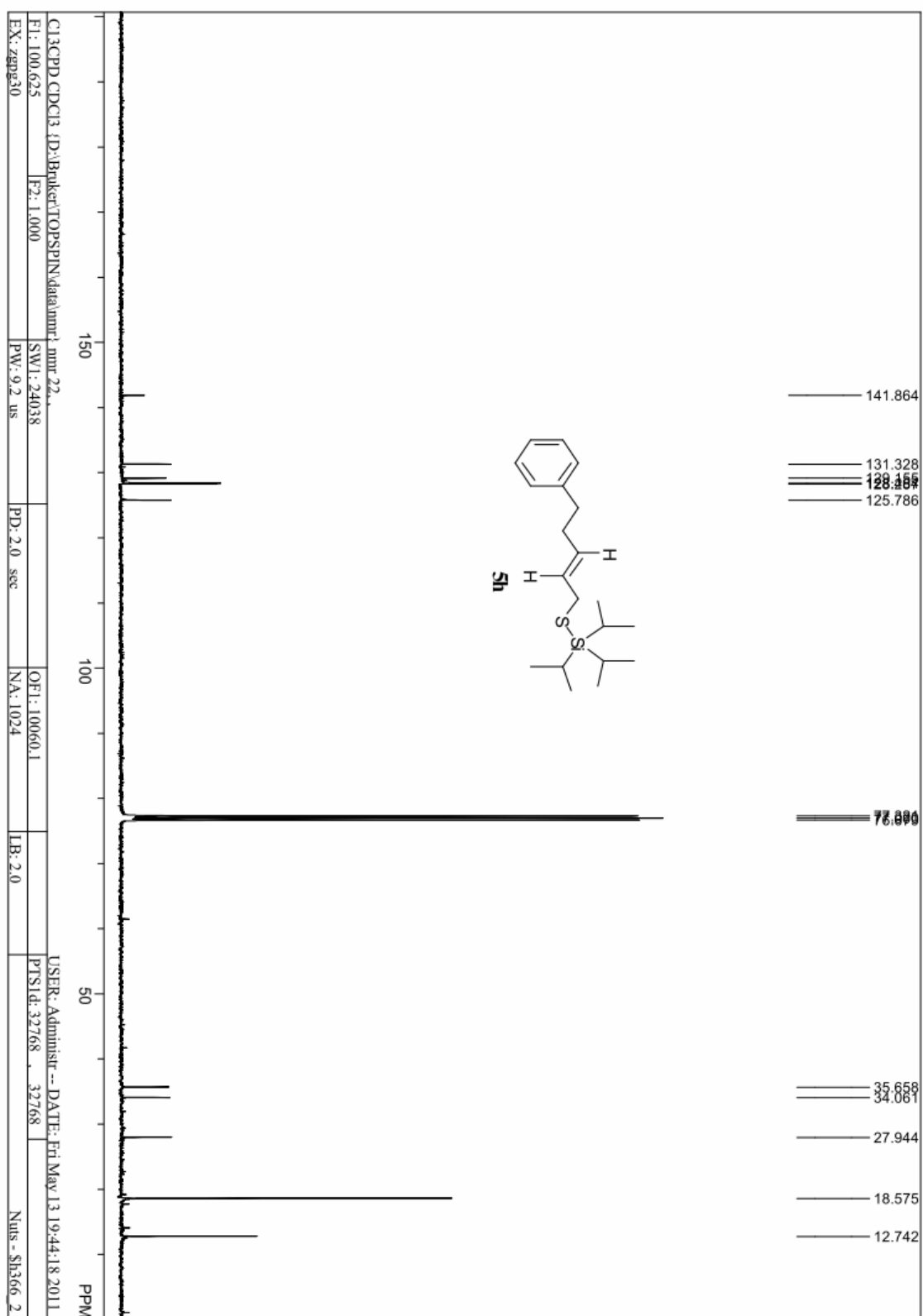


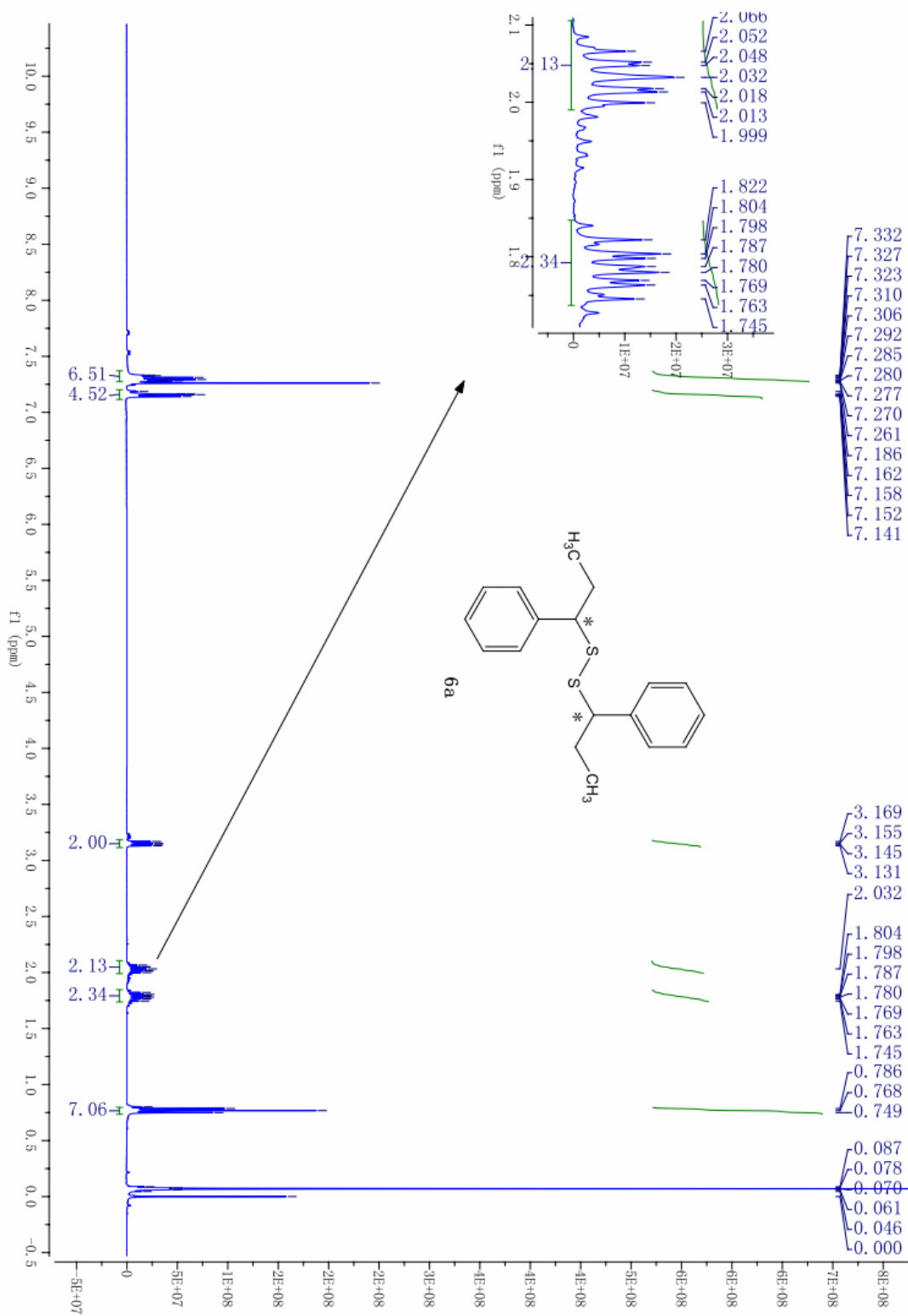


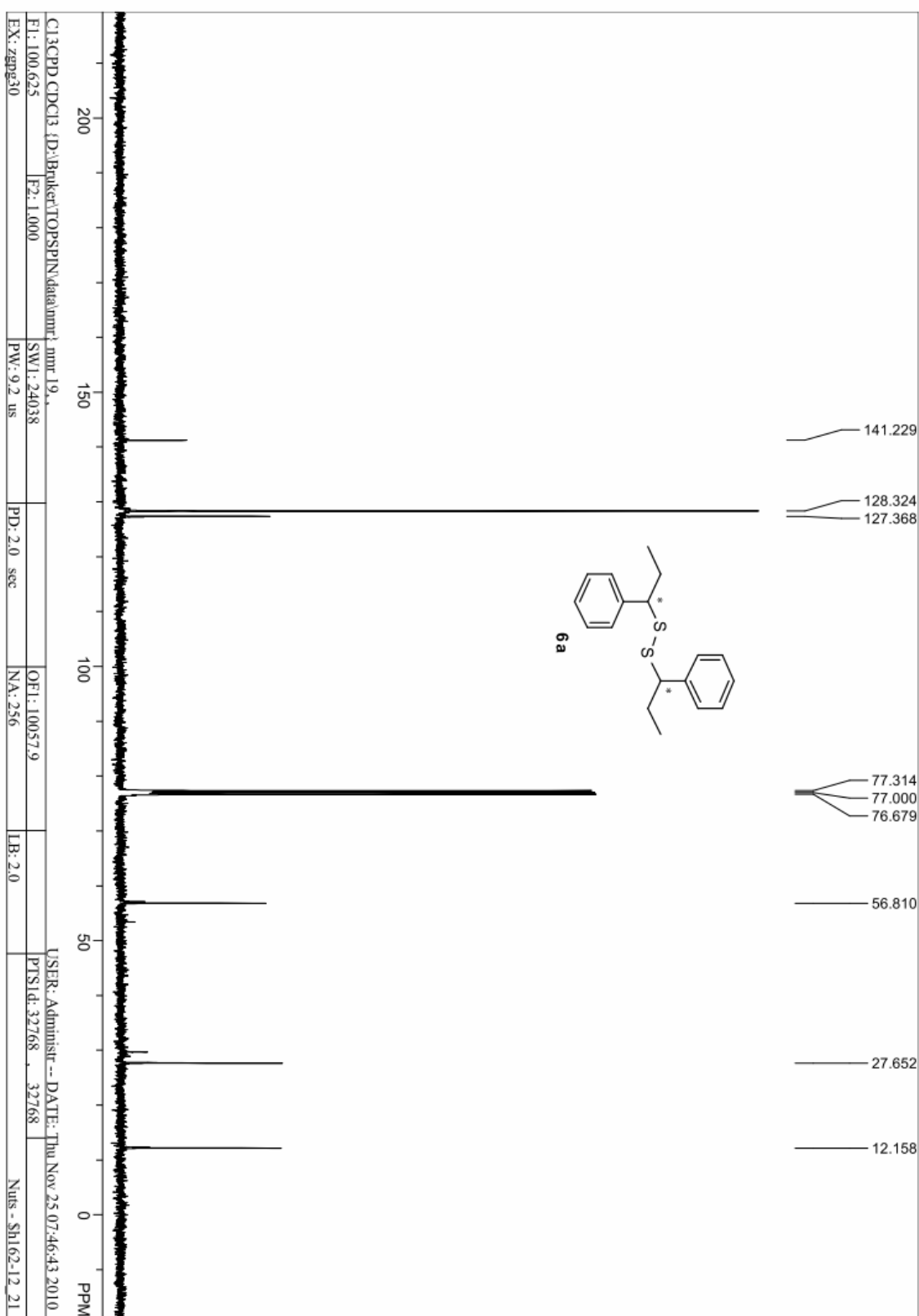


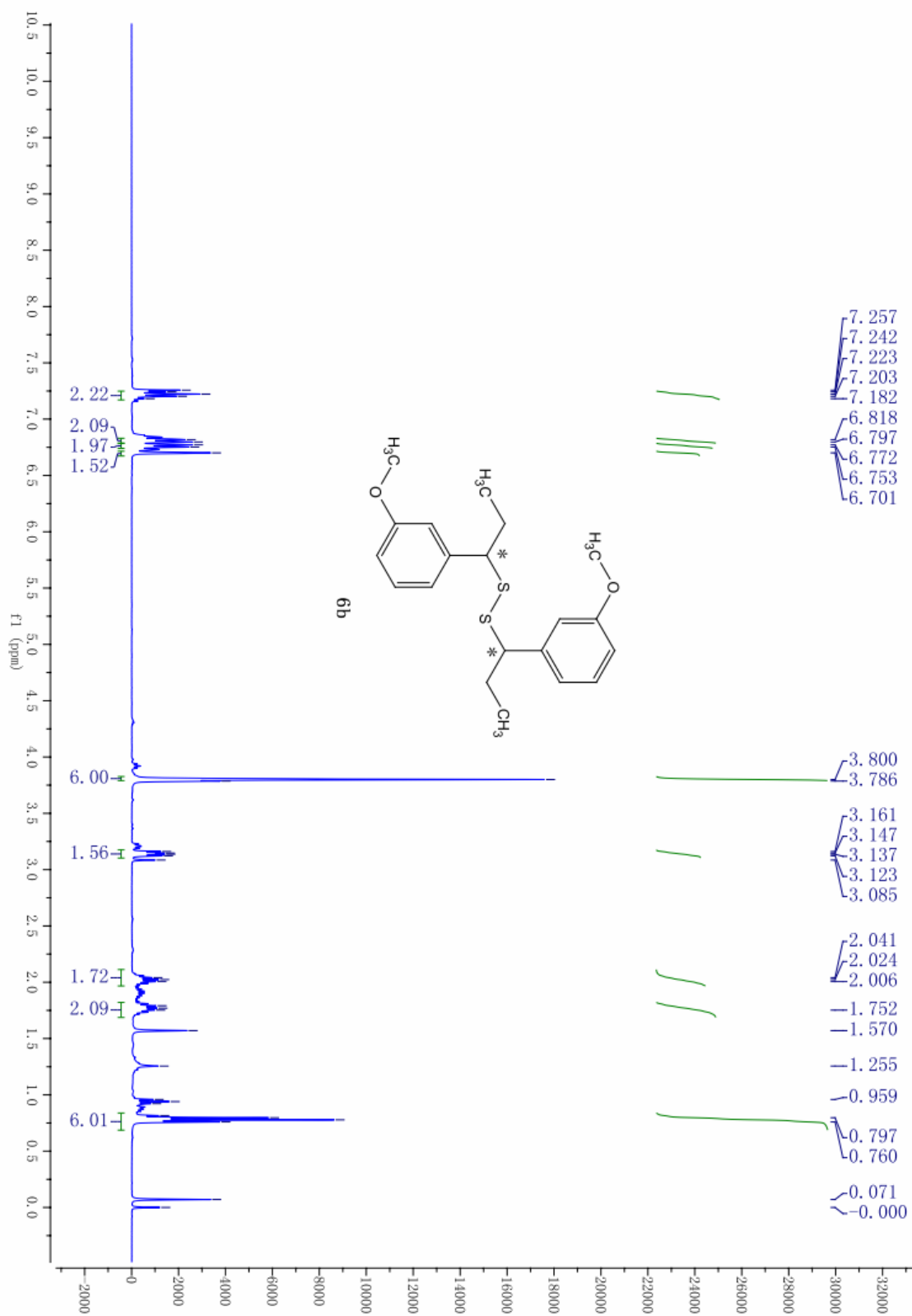


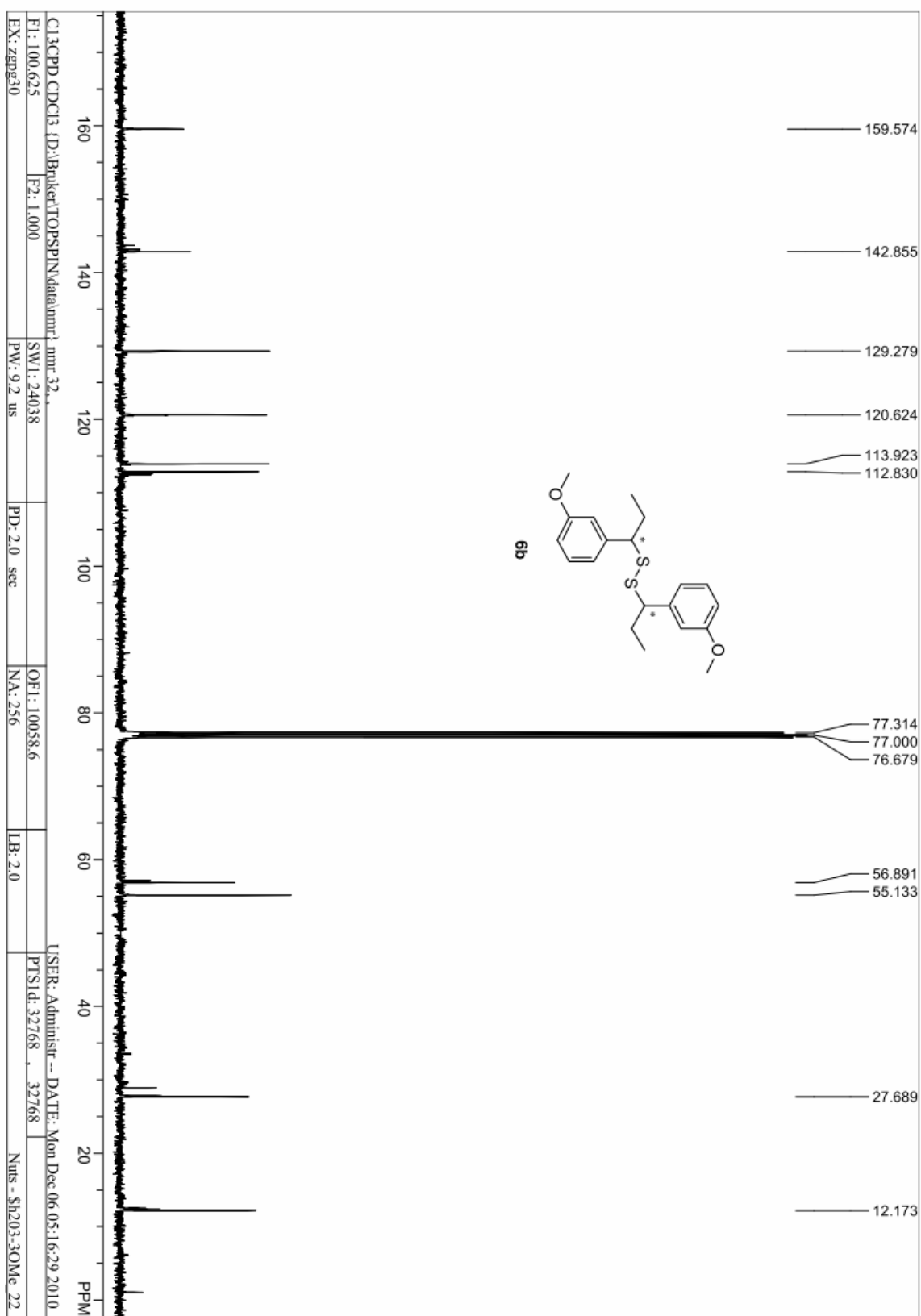


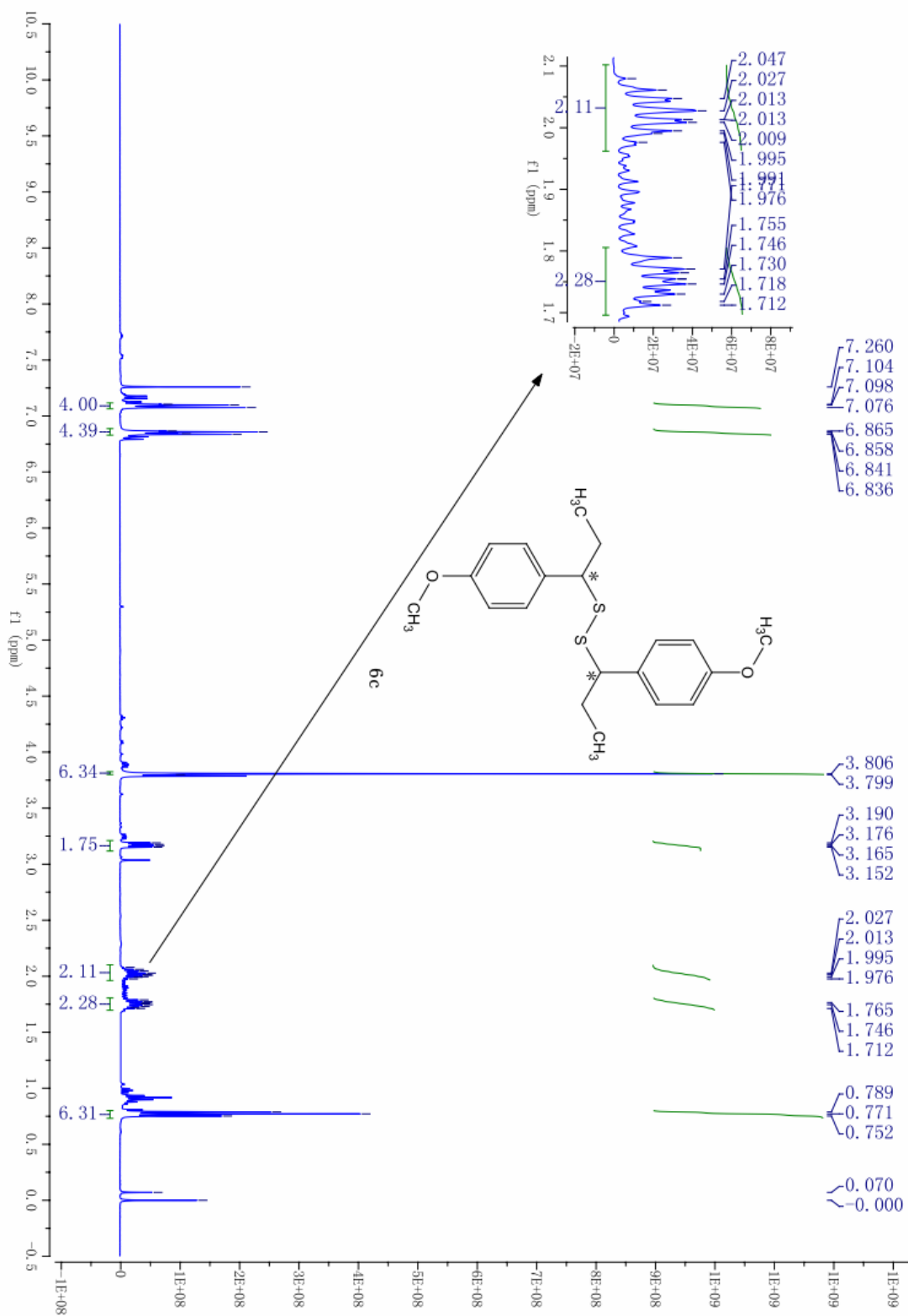


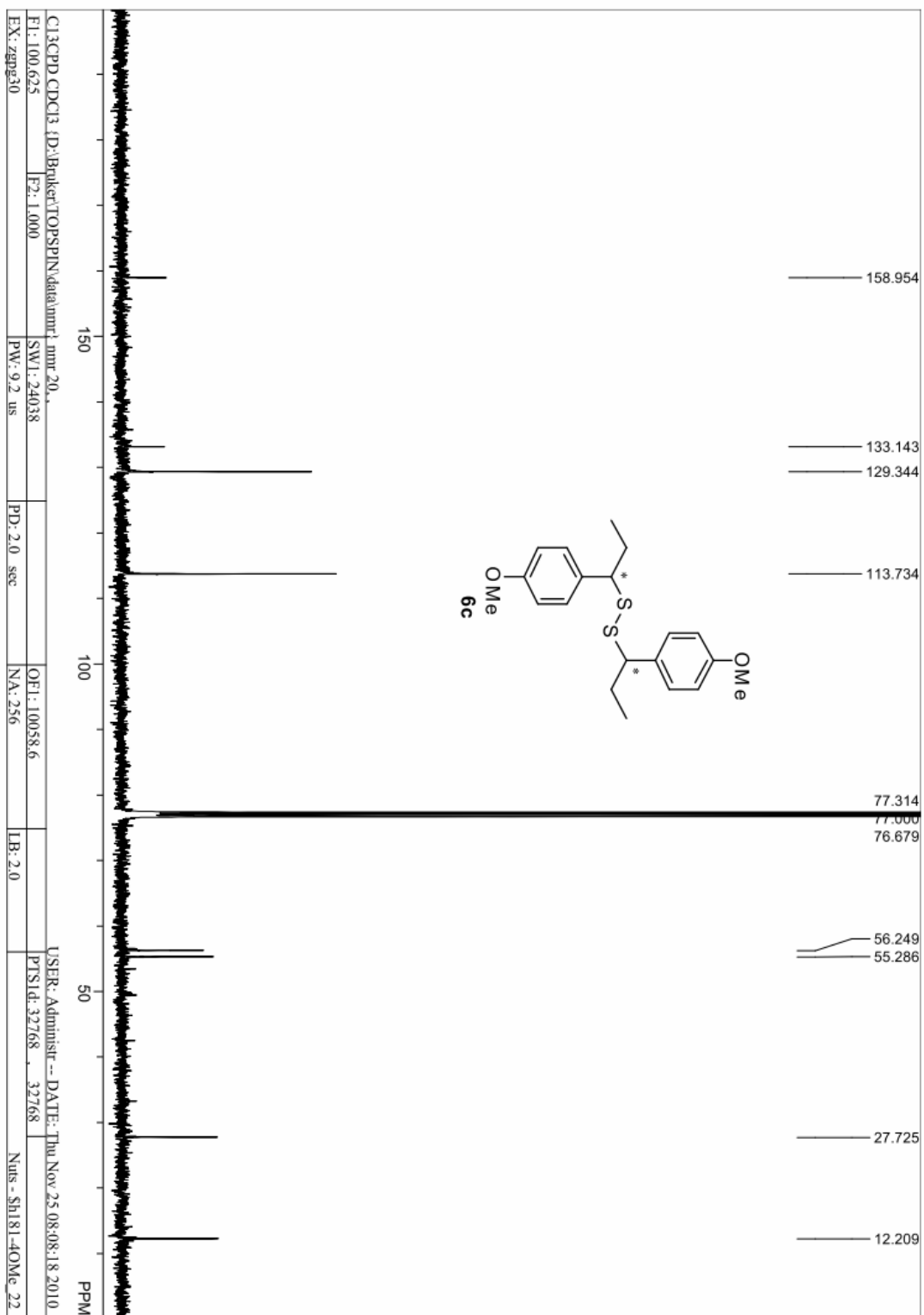


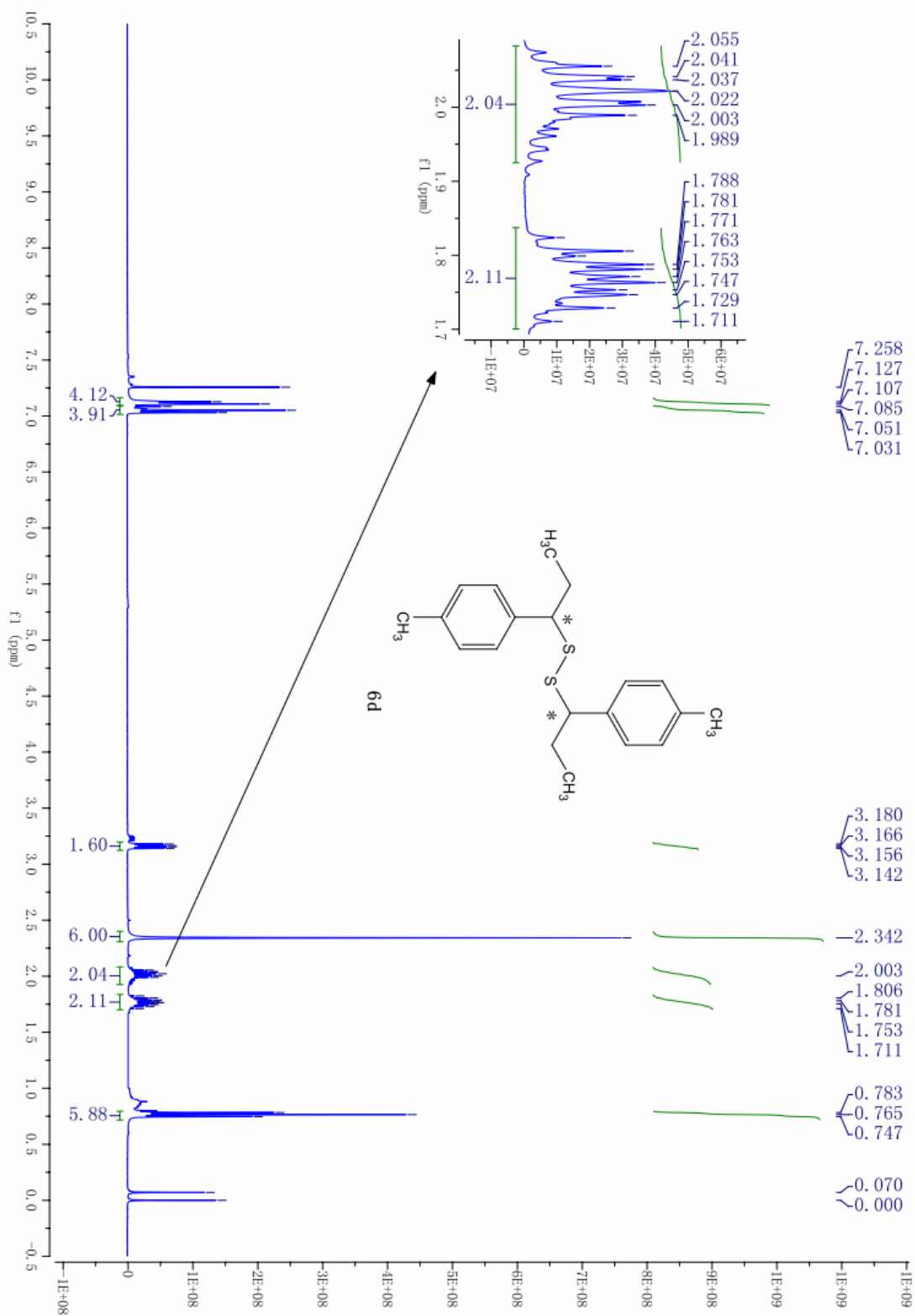


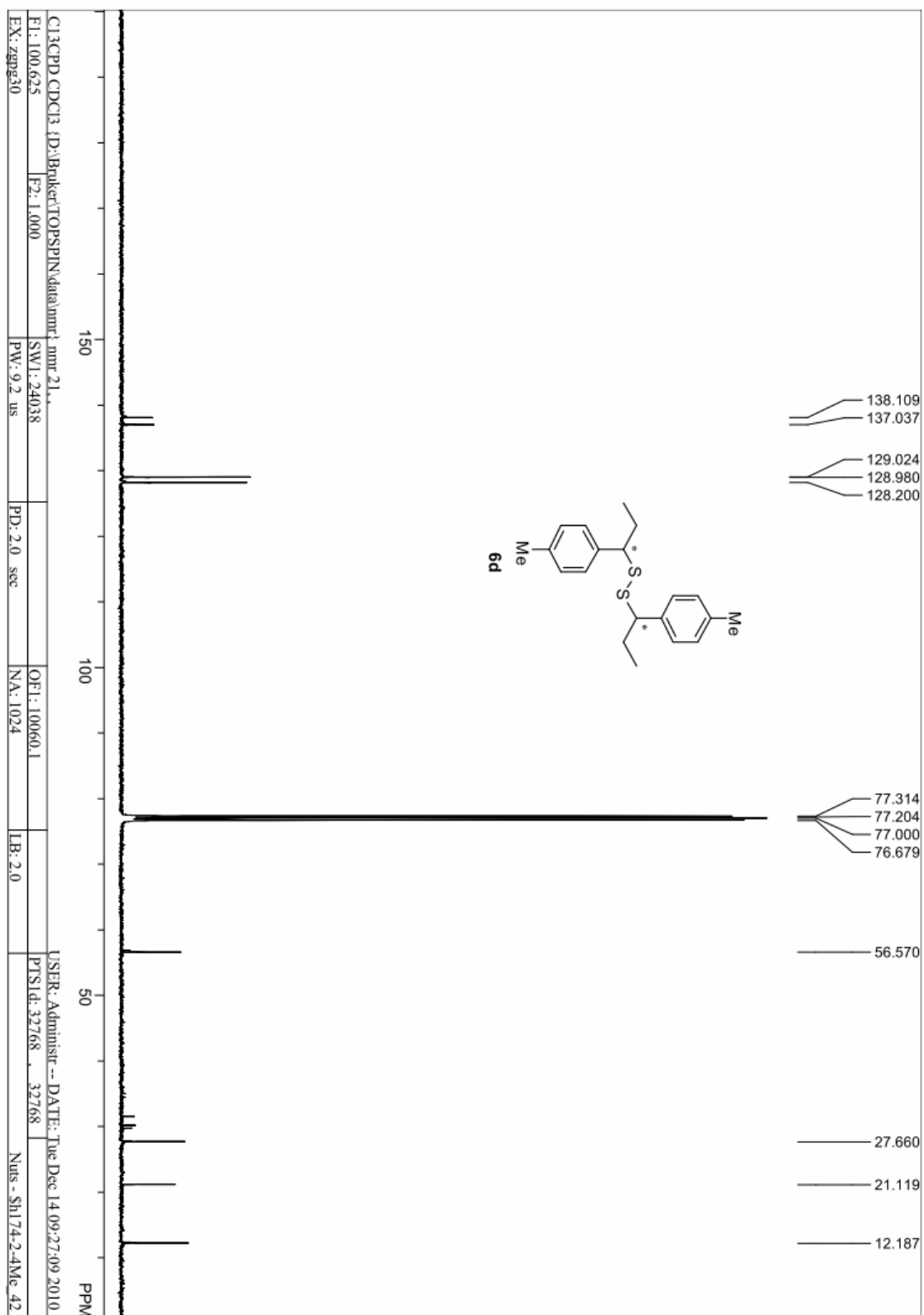


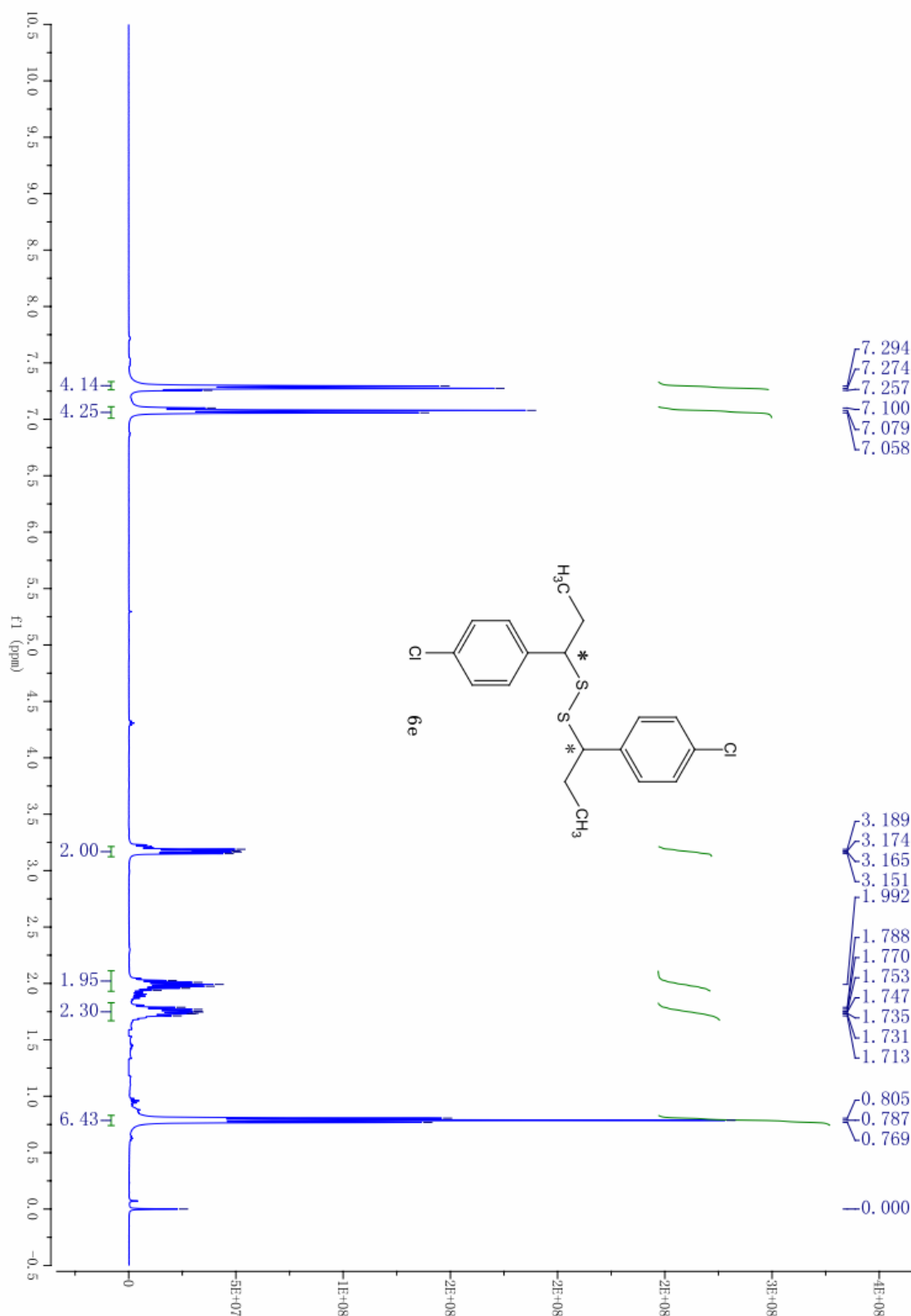


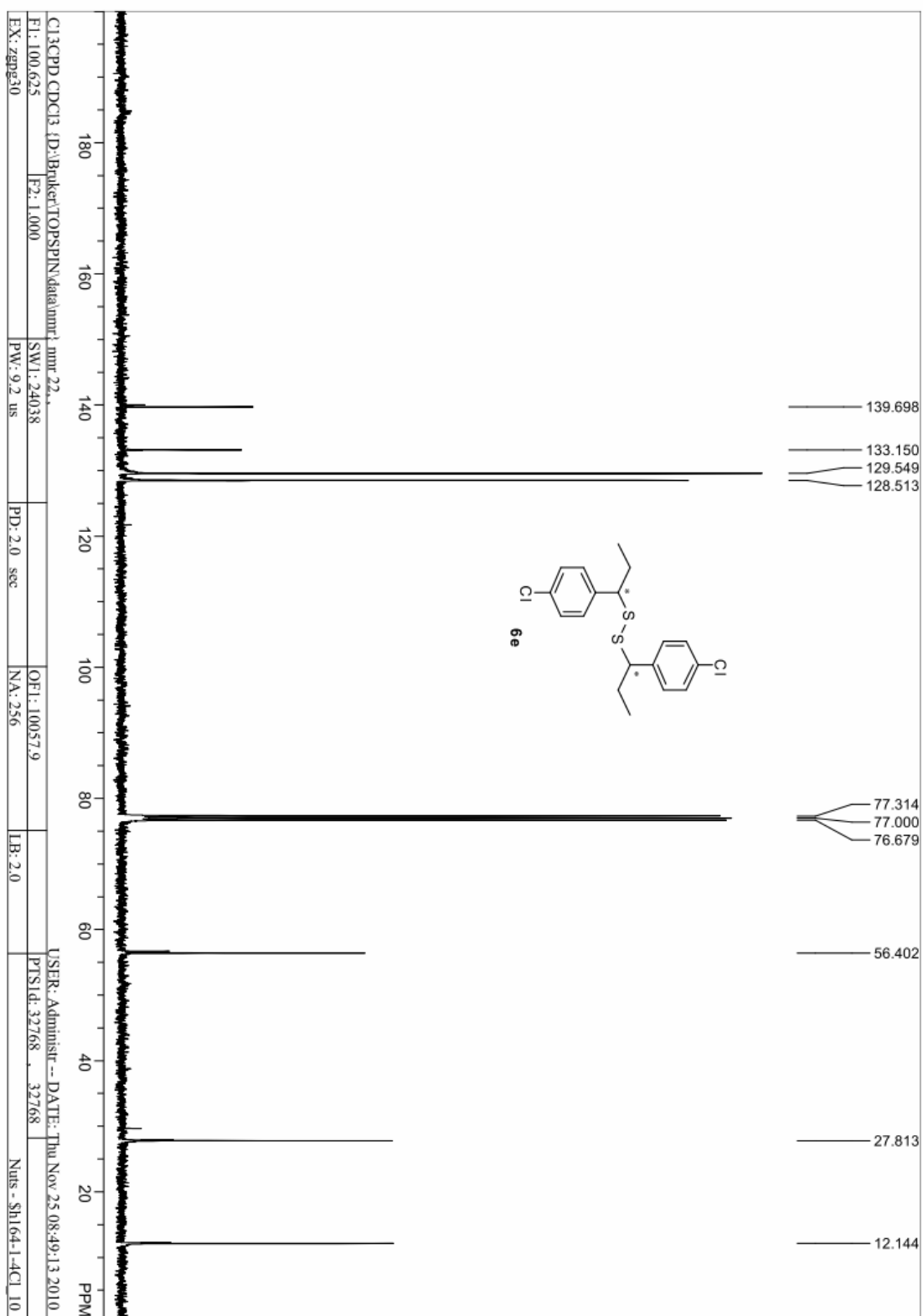


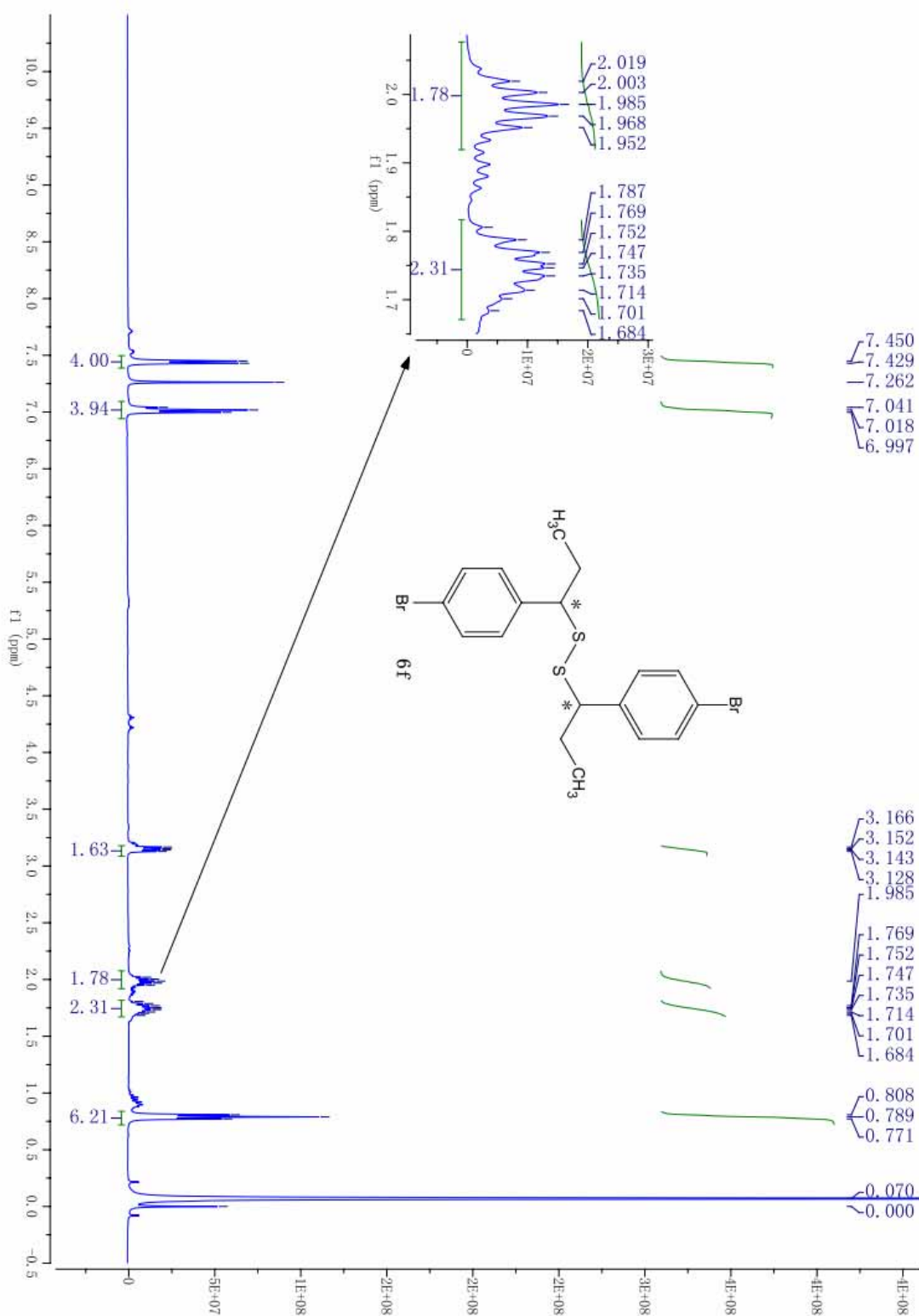


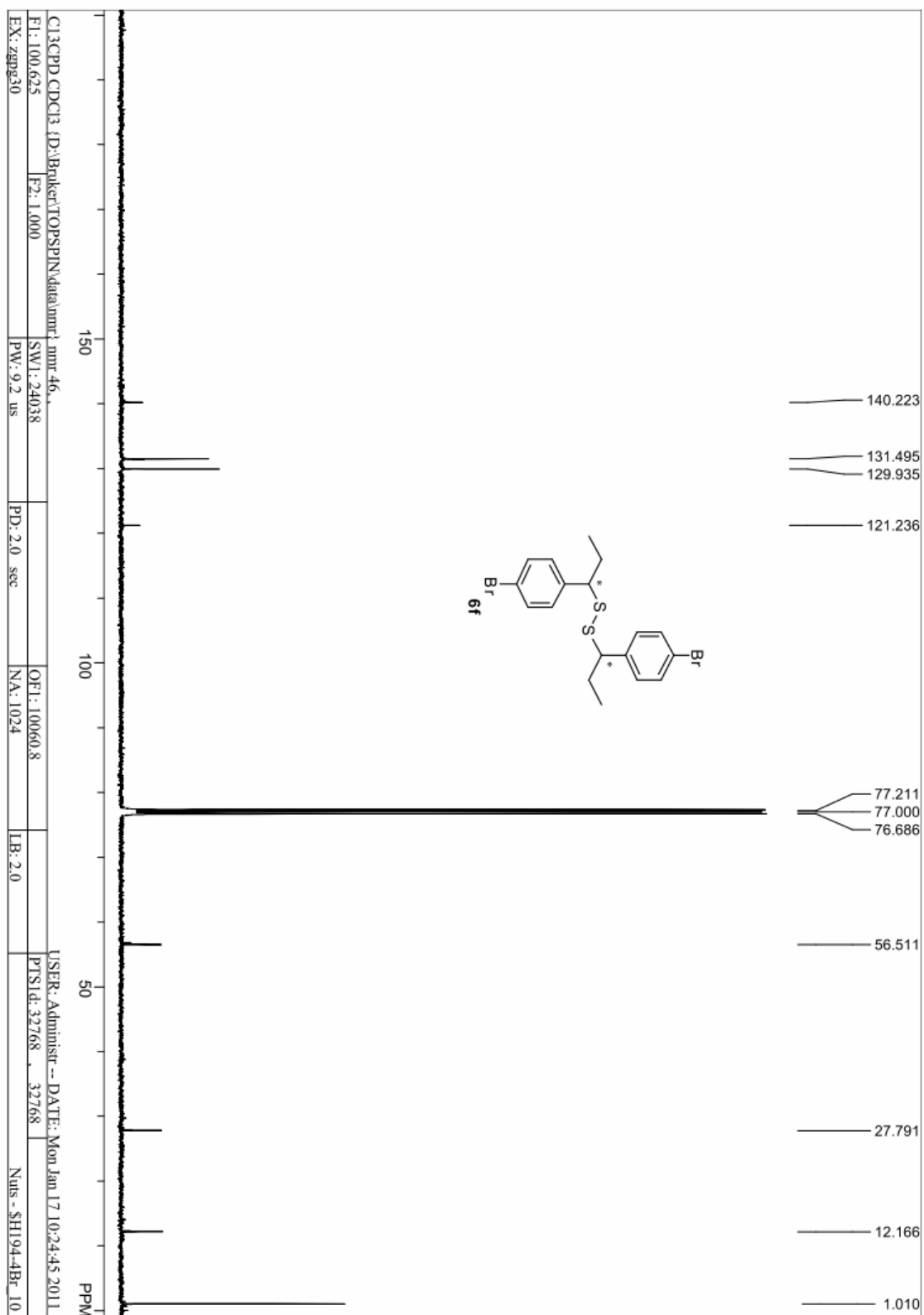


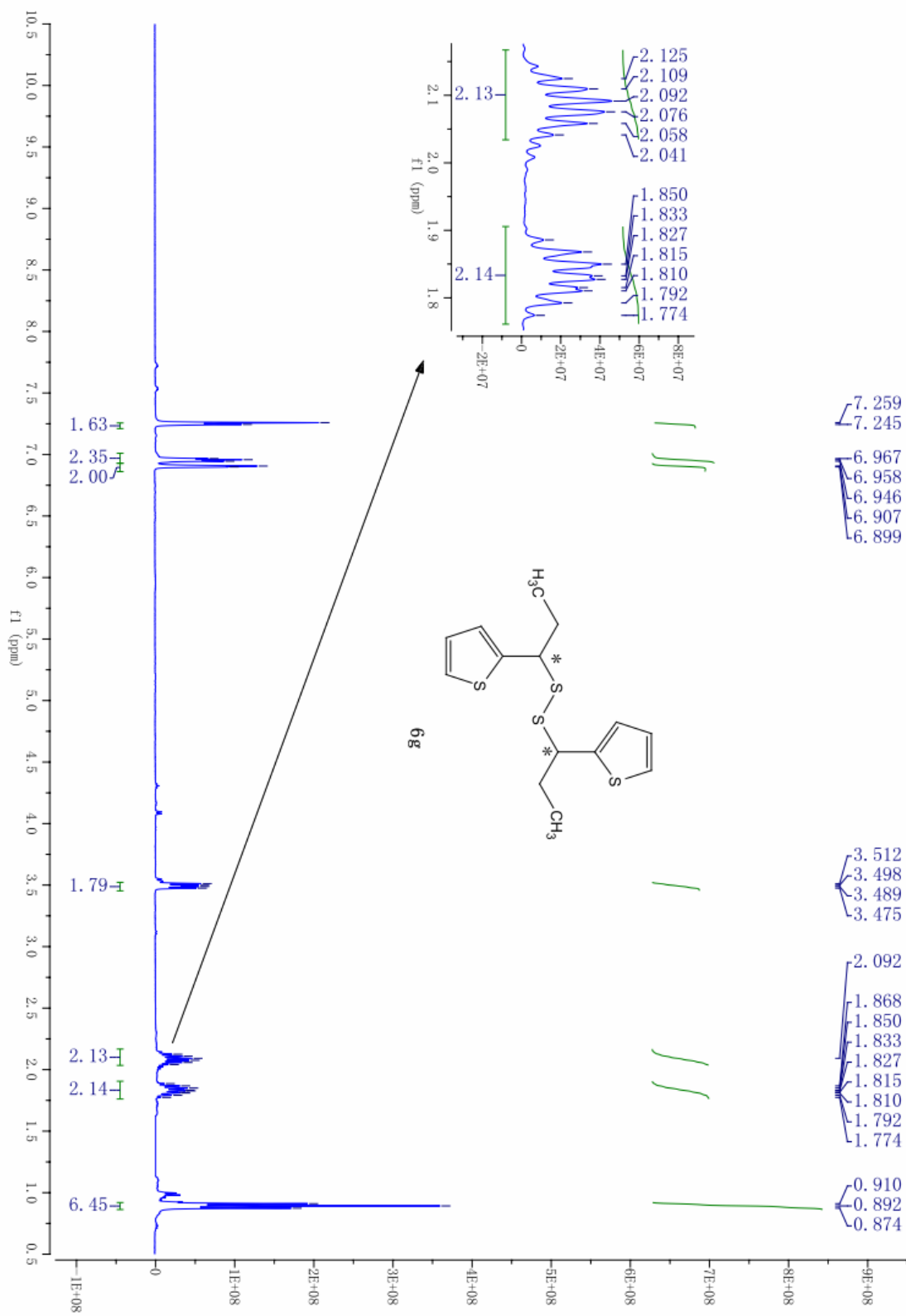


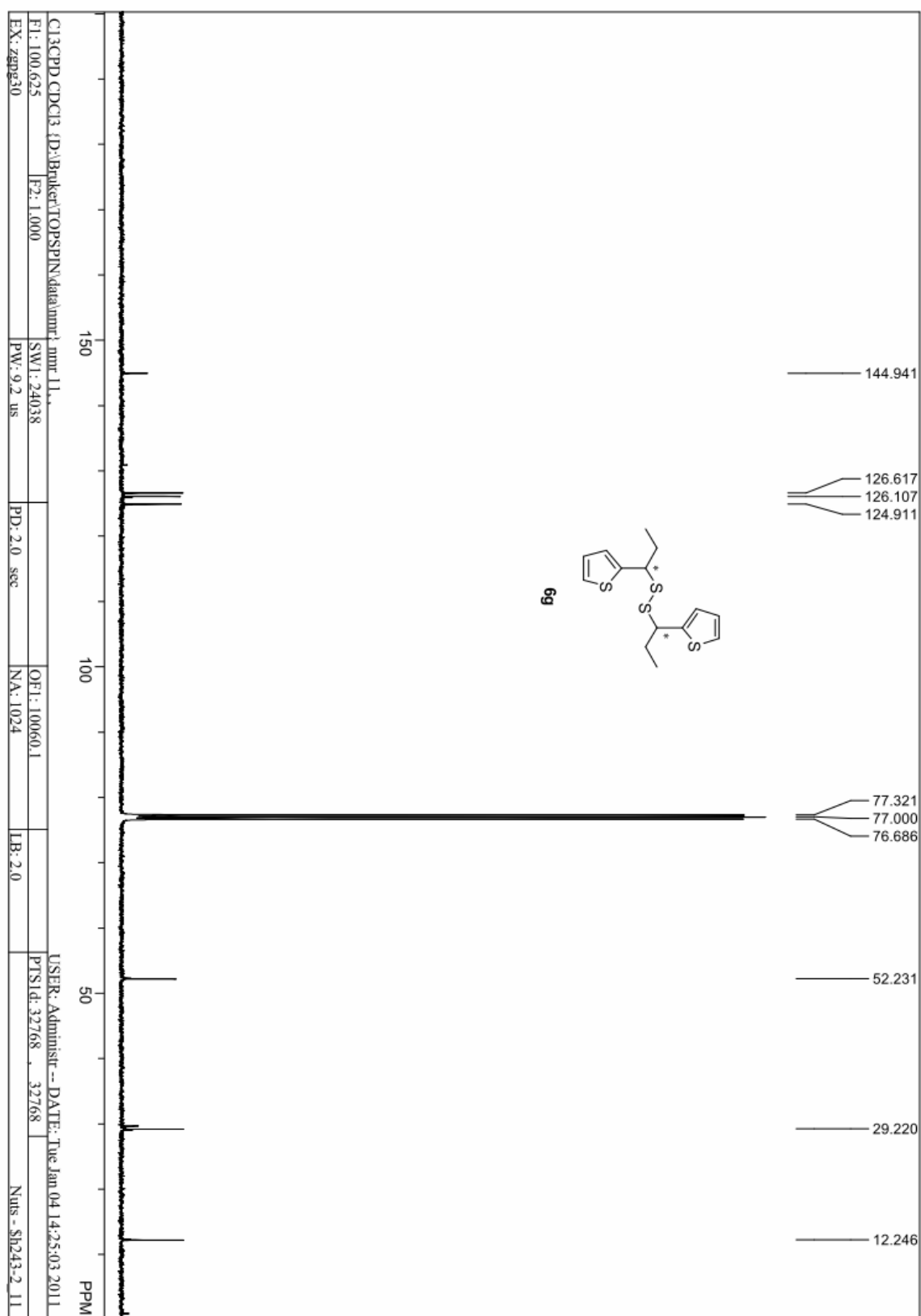


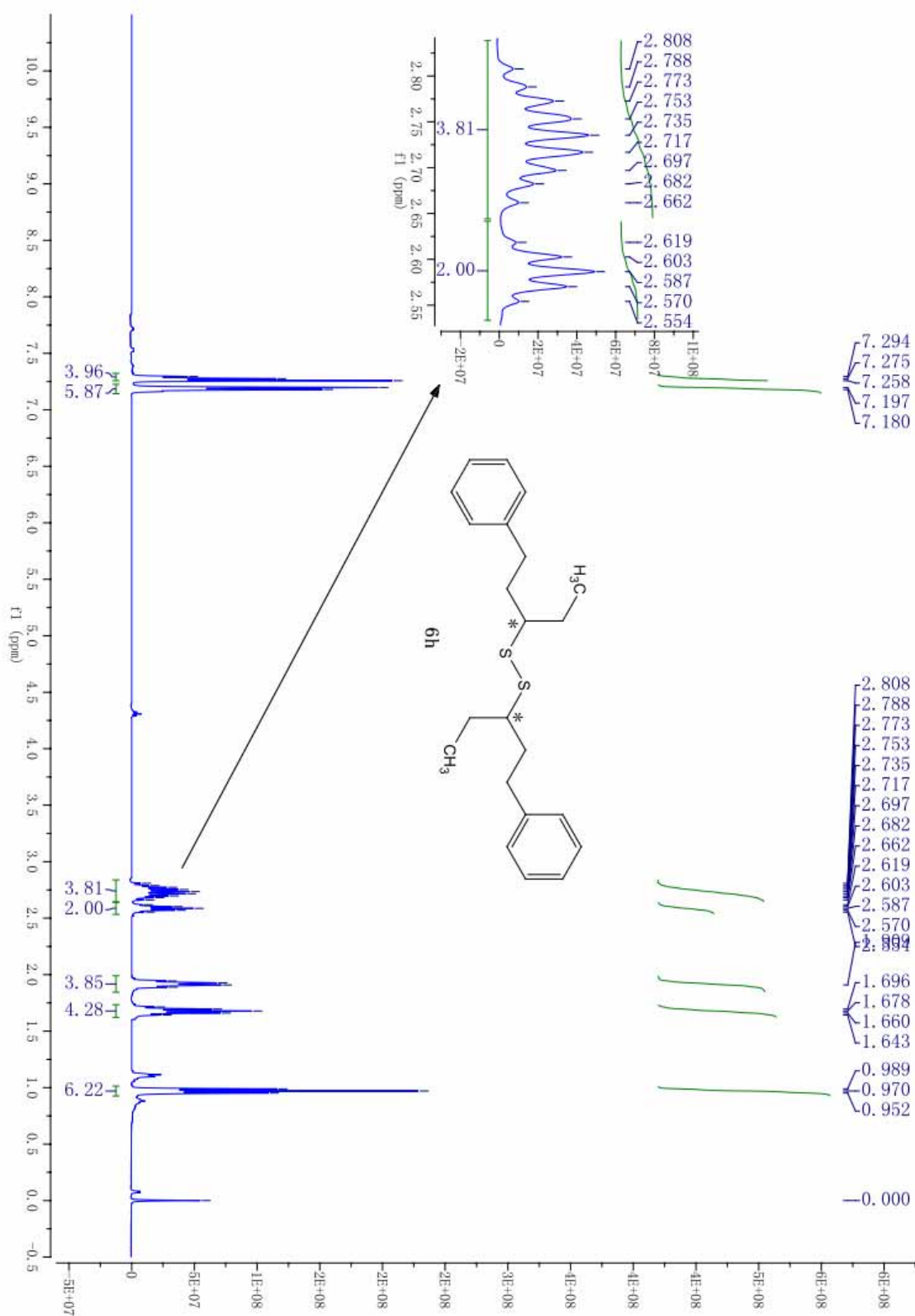


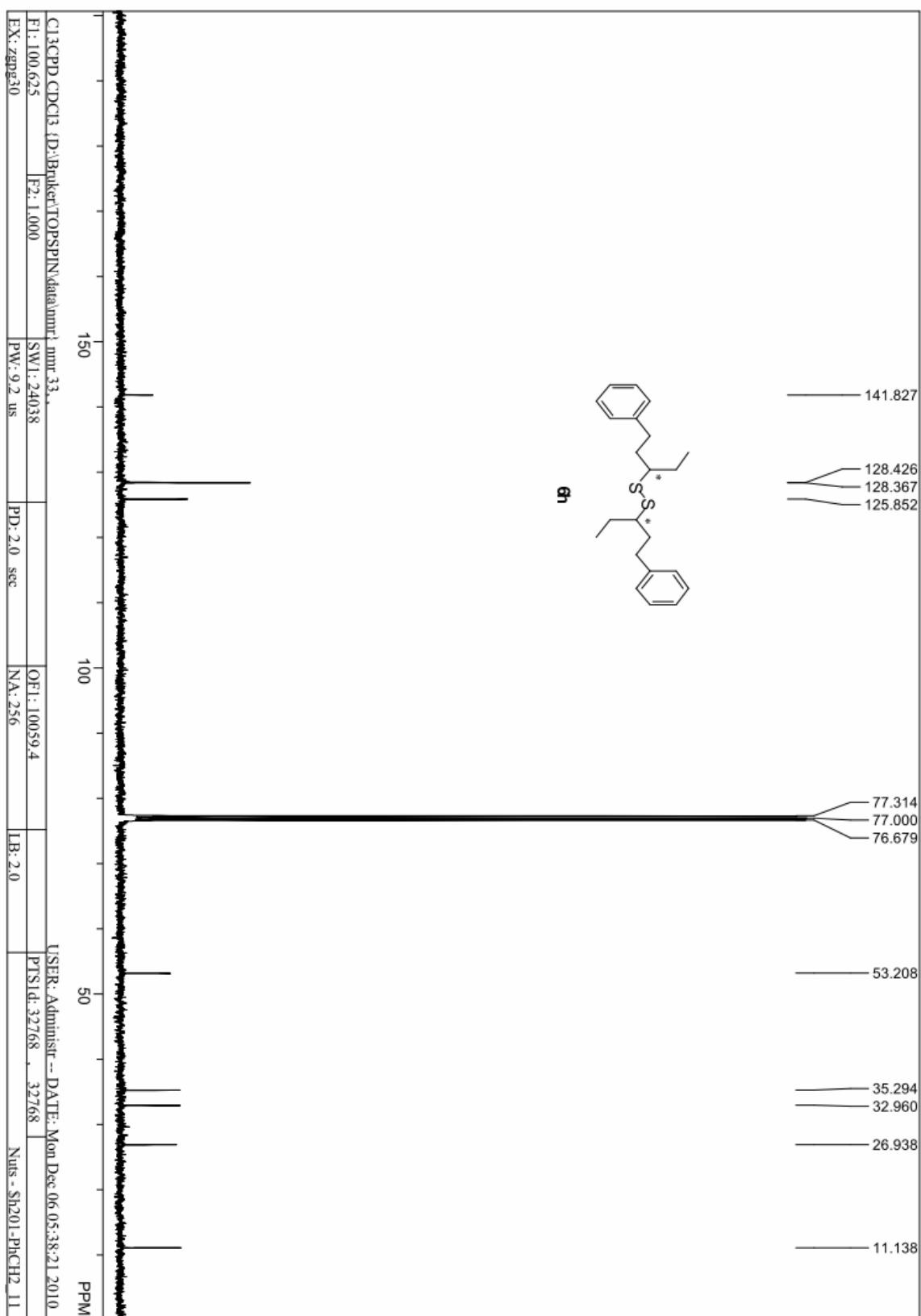


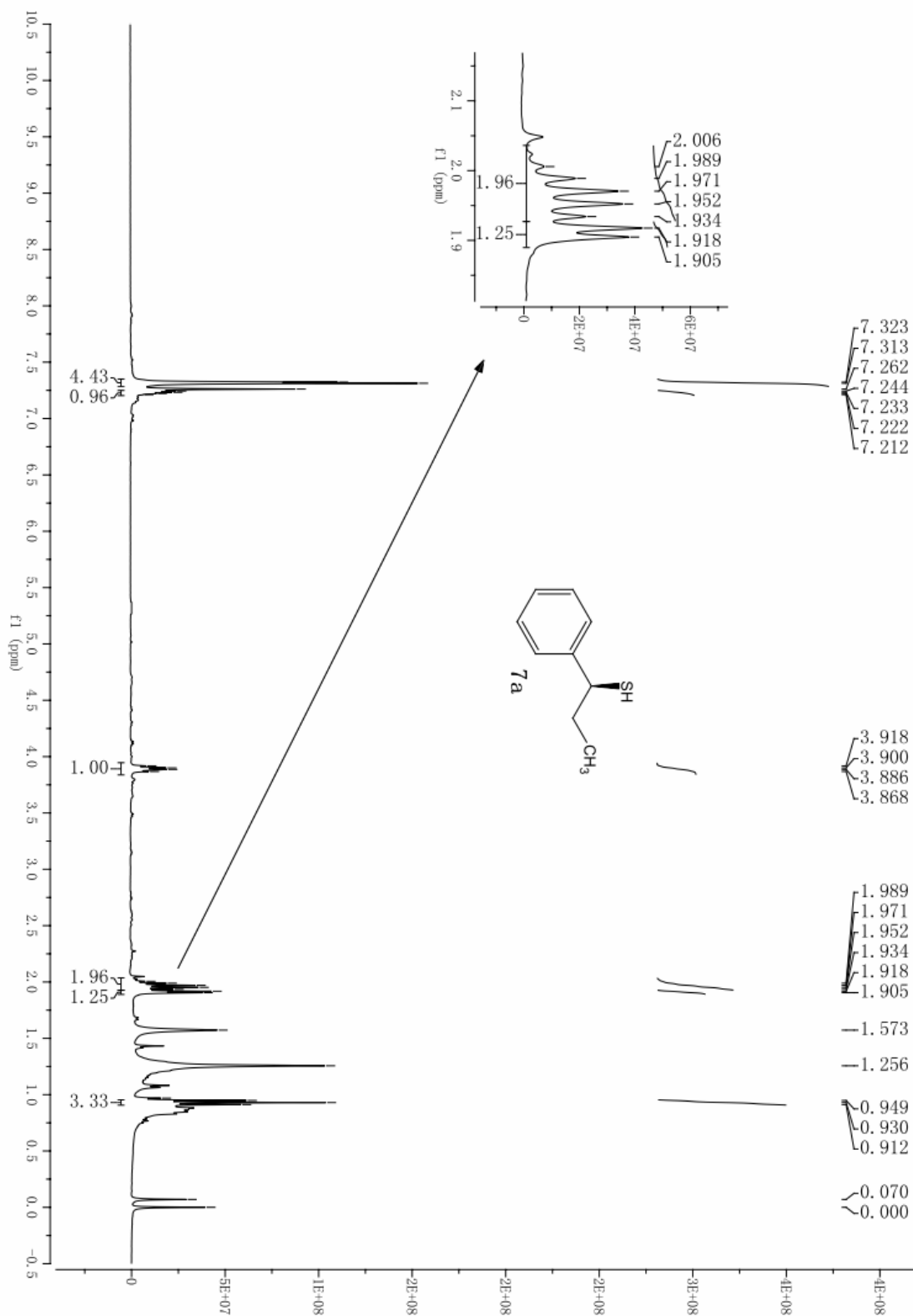


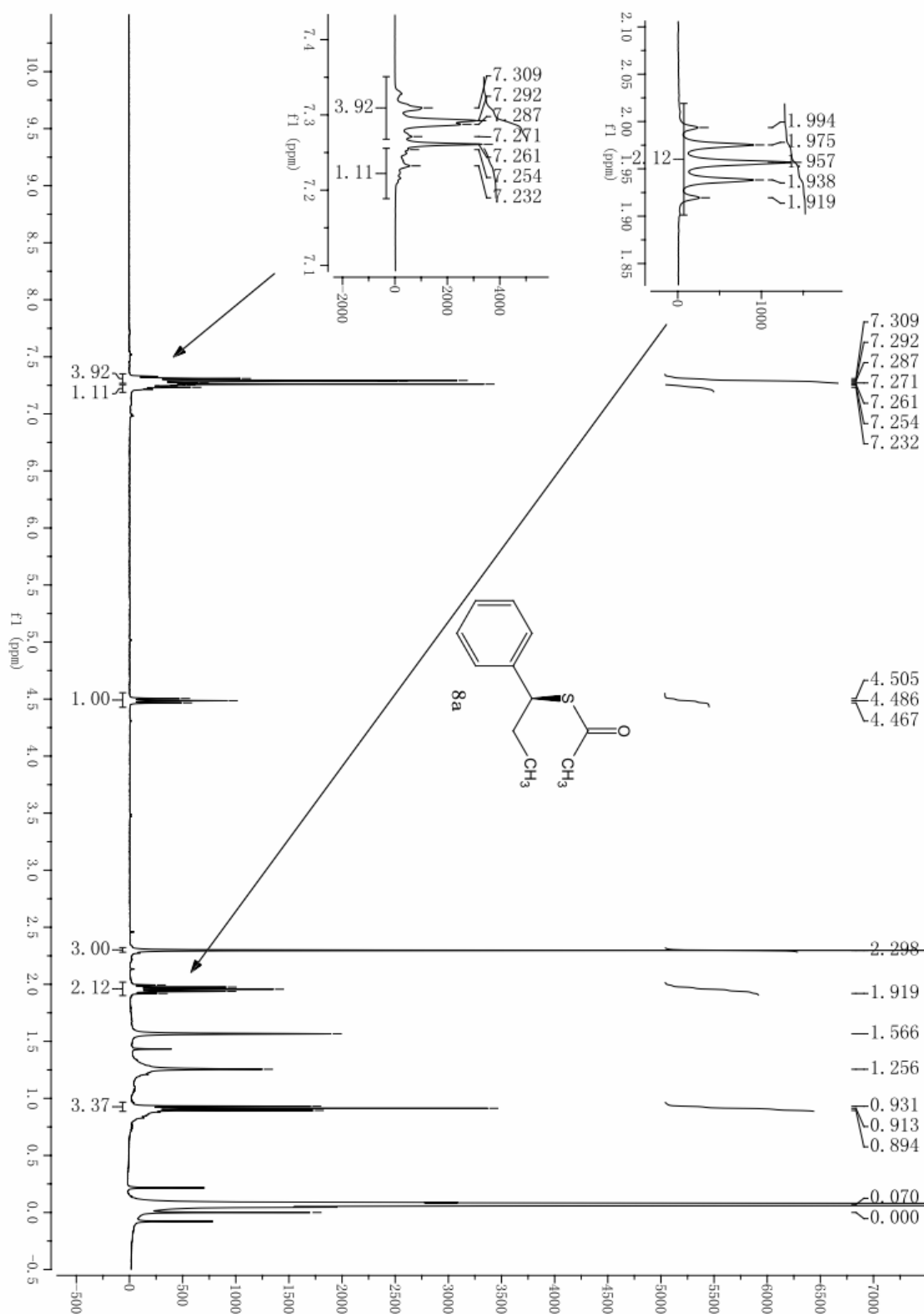




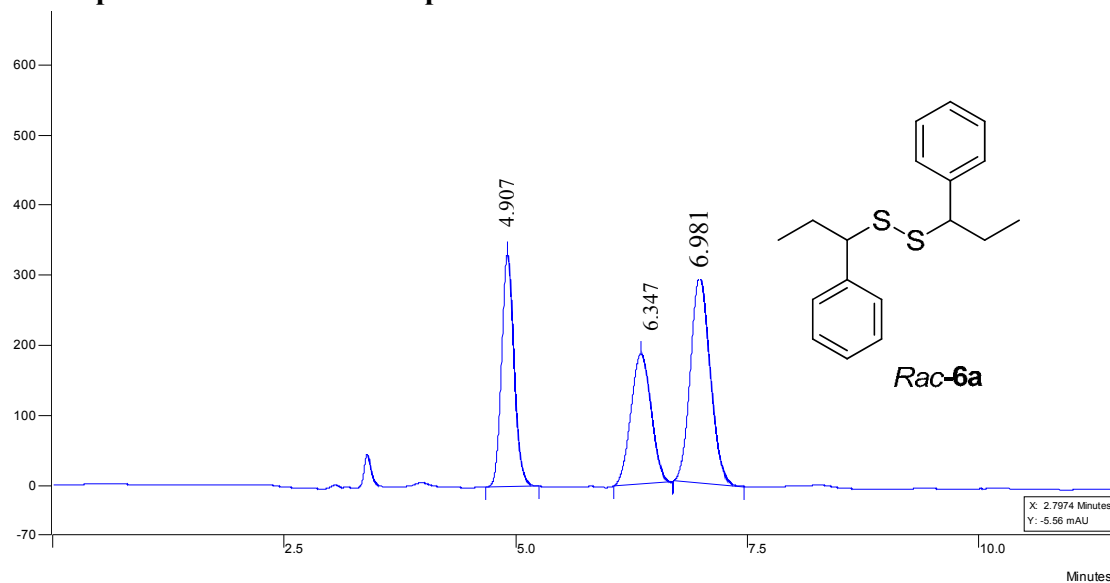




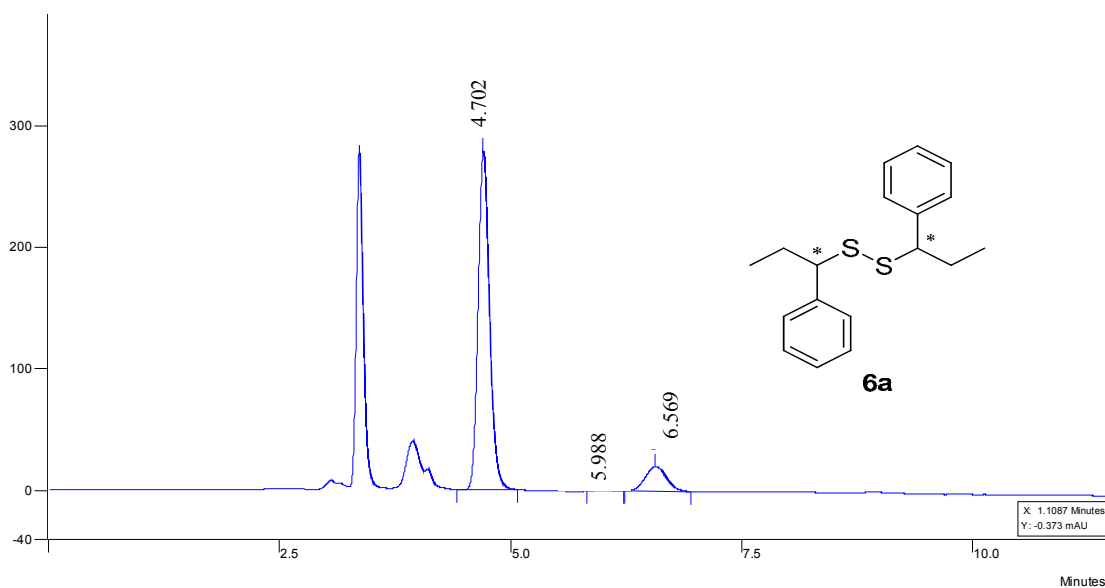




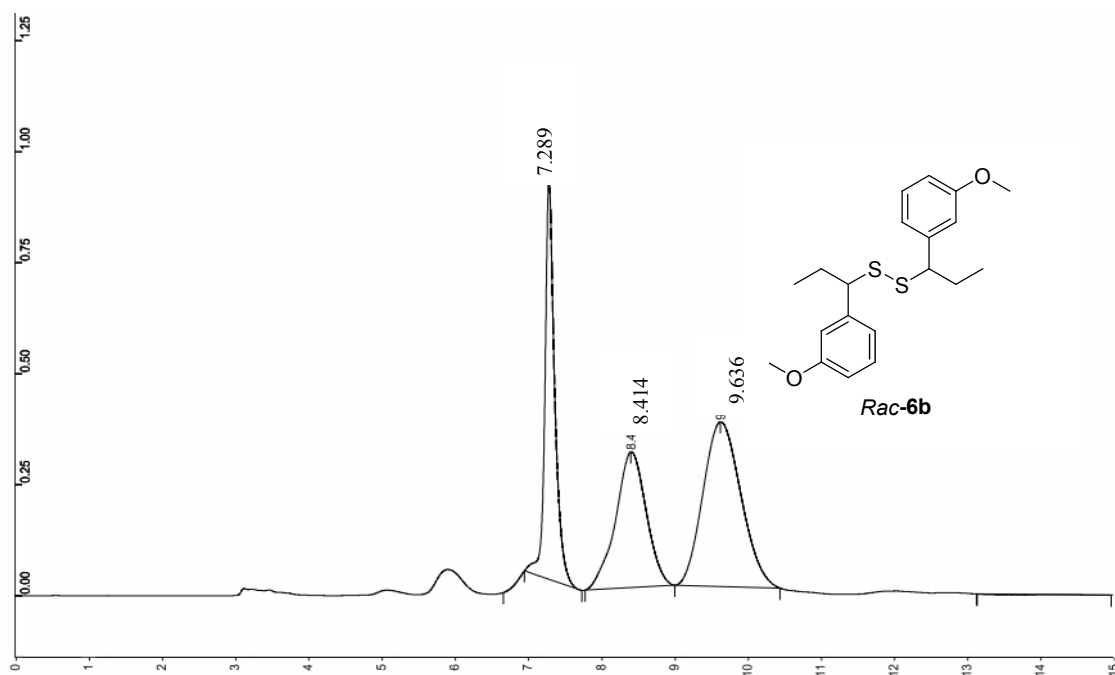
HPLC Spectra of the Chiral Compounds:



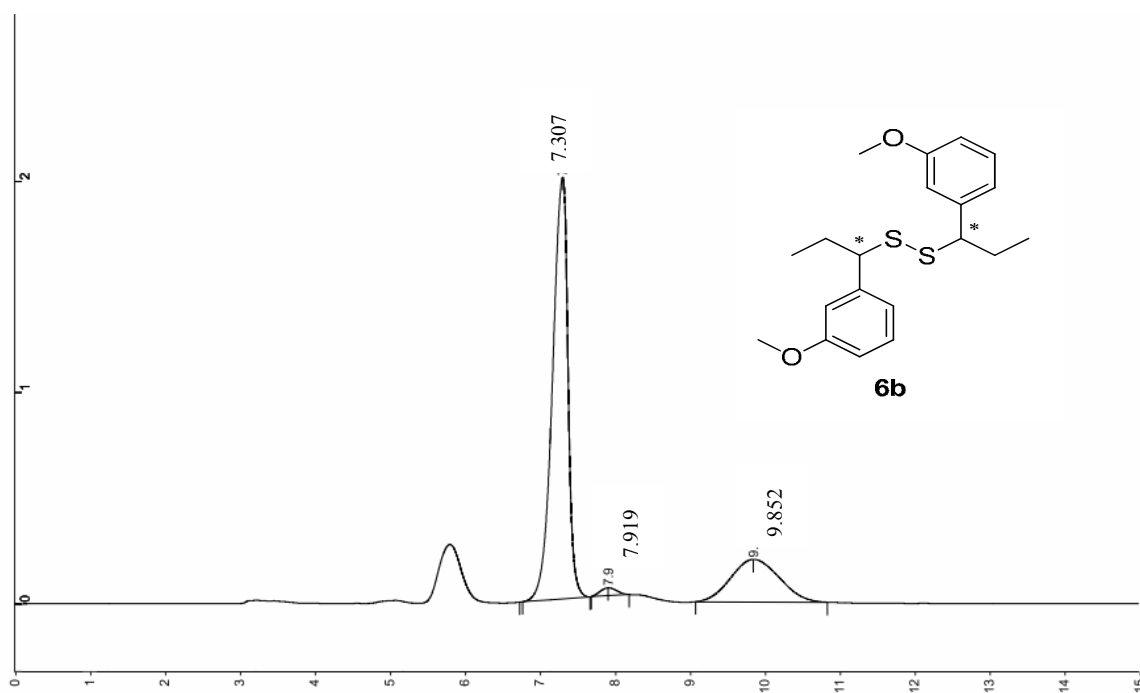
Peak No.	Peak Name	tR (min)	Result	Sep. Code	W 1/2 (sec)	Efficiency Plates	Efficiency Plates/m	k'	R	Tailing (5.0%)
1		4.907	30.232	BB	8.55	6571	43805	3.91		1.13
2		6.347	27.399	BB	14.54	3803	25352	5.35	4.4	1.02
3		6.981	42.369	BB	13.69	5187	34581	5.98	1.6	1.11



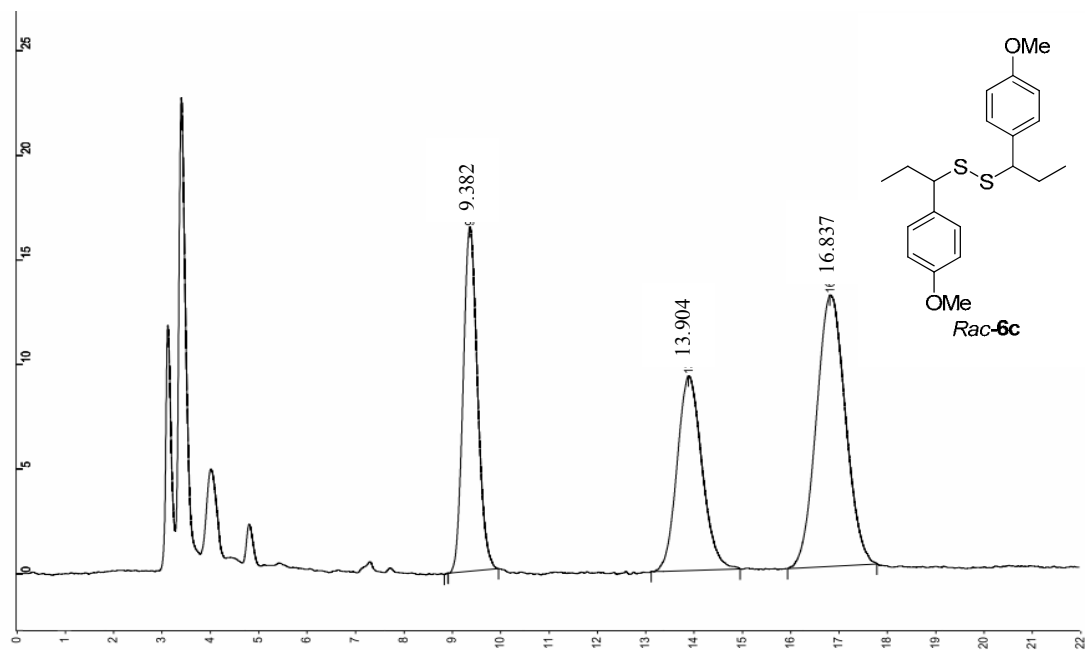
Peak No.	Peak Name	tR (min)	Result	Sep. Code	W 1/2 (sec)	Efficiency Plates	Efficiency Plates/m	k'	R	Tailing (5.0%)
1		4.702	87.597	BB	7.86	7155	47697	3.70		1.17
2		5.988	0.553	BB	11.64	5285	35232	4.99	4.7	1.08
3		6.569	11.851	BB	14.96	3848	25650	5.57	1.5	1.04



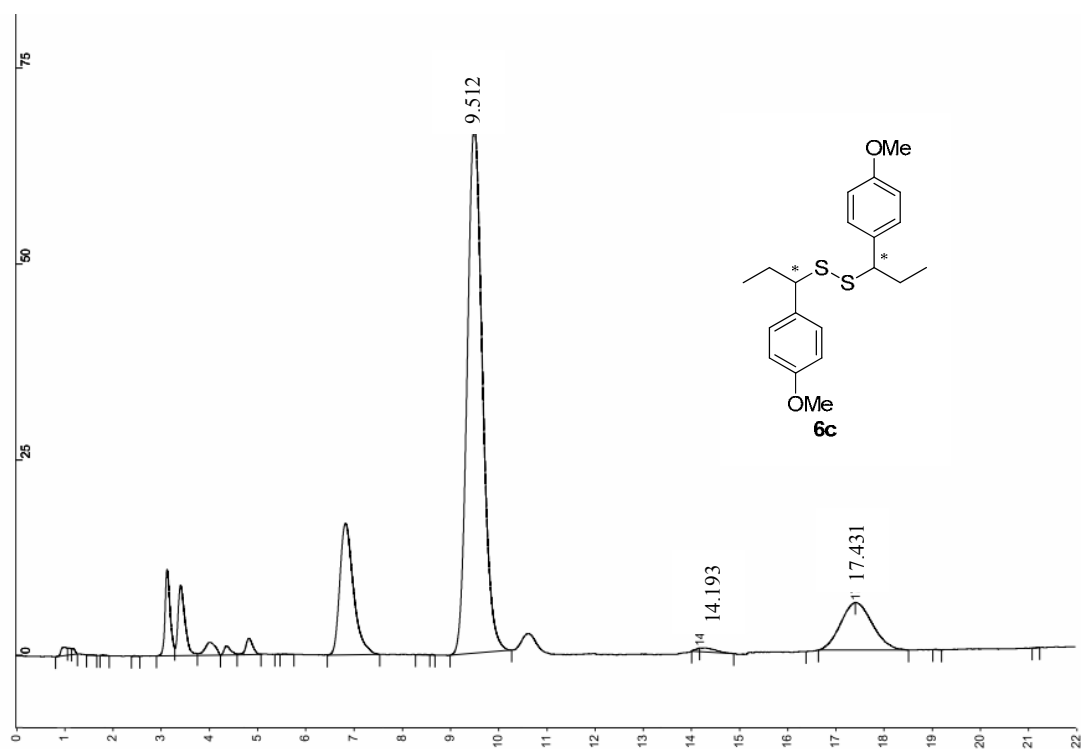
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		27.2086	7.289	0.000	83036672	BB	7.5	
2		29.0169	8.414	0.000	88555512	BB	26.6	
3		43.7745	9.636	0.000	133593648	BB	34.0	
Totals:		100.0000		0.000	305185832			



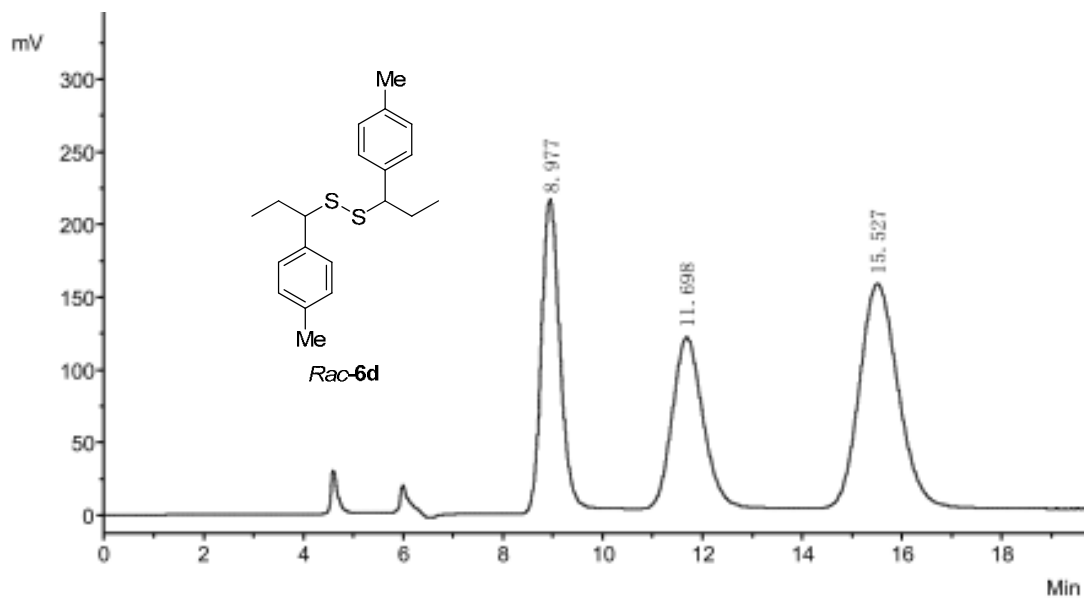
Peak No.	Peak Name	Result (°)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		74.8669	7.307	0.000	285544800	BB	13.0	
2		1.4791	7.919	0.000	5641179	BB	16.5	
3		23.6540	9.852	0.000	90217280	BB	42.8	
Totals:		100.0000		0.000	381403259			



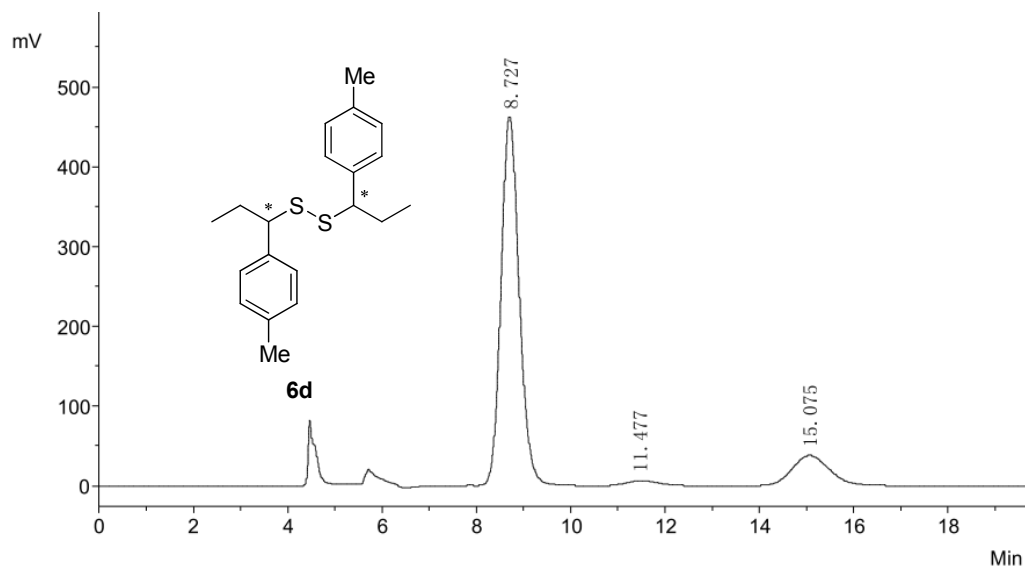
Peak No.	Peak Name	tR (min)	Result	Sep. Code	W 1/2 (sec)	Efficiency Plates	Efficiency Plates/m	k'	R	Tailing (5.0%)
1		9.382	27.912	BB	19.12	4805	32036	8.38		1.15
2		13.904	27.123	BB	33.02	3540	23603	12.90	6.1	1.16
3		16.837	44.965	BB	39.36	3653	24351	15.84	2.9	1.08



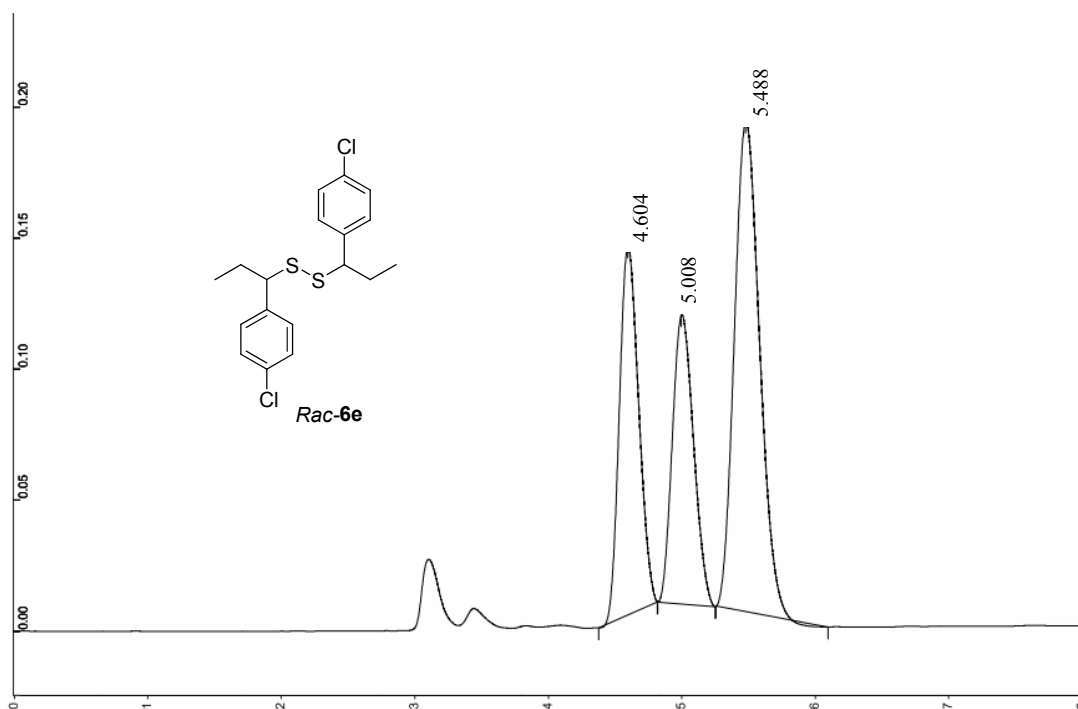
Peak No.	Peak Name	Result (°)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		83.6971	9.512	0.000	14758128	BB	20.2	
2		0.7373	14.193	0.000	130011	BB	21.9	
3		15.5656	17.431	0.000	2744641	BB	42.9	
Totals:		100.0000		0.000	17632780			



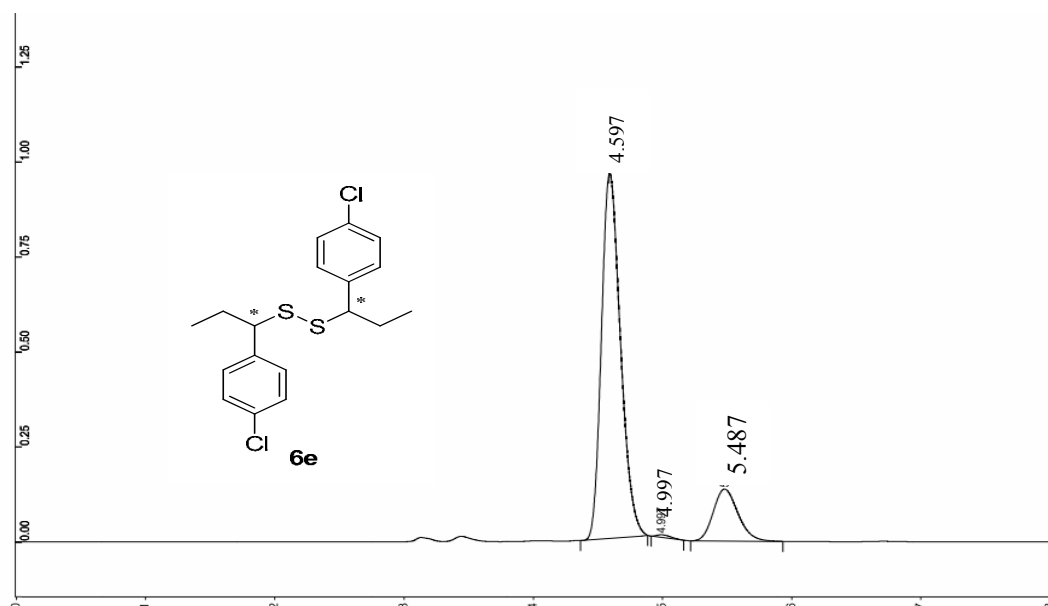
No.	PeakNo	R. Time	PeakHeight	PeakArea	PerCent
1	1	8.977	213458.6	5551725.4	29.2447
2	2	11.698	117612.9	5065982.4	26.6860
3	3	15.527	154762.0	8365995.9	44.0694
Total			485833.6	18983703.7	100.0000



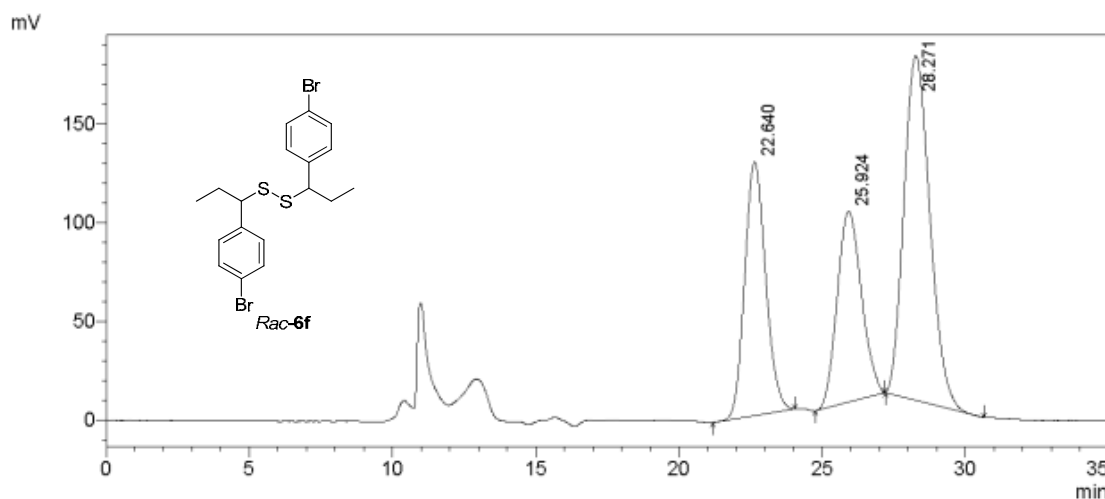
No.	PeakNo	R. Time	PeakHeight	PeakArea	PerCent
1	1	8.727	460584.6	12395019.1	83.8146
2	2	11.477	6692.9	303144.4	2.0498
3	3	15.075	37860.8	2090452.5	14.1356
Total			505138.4	14788615.9	100.0000



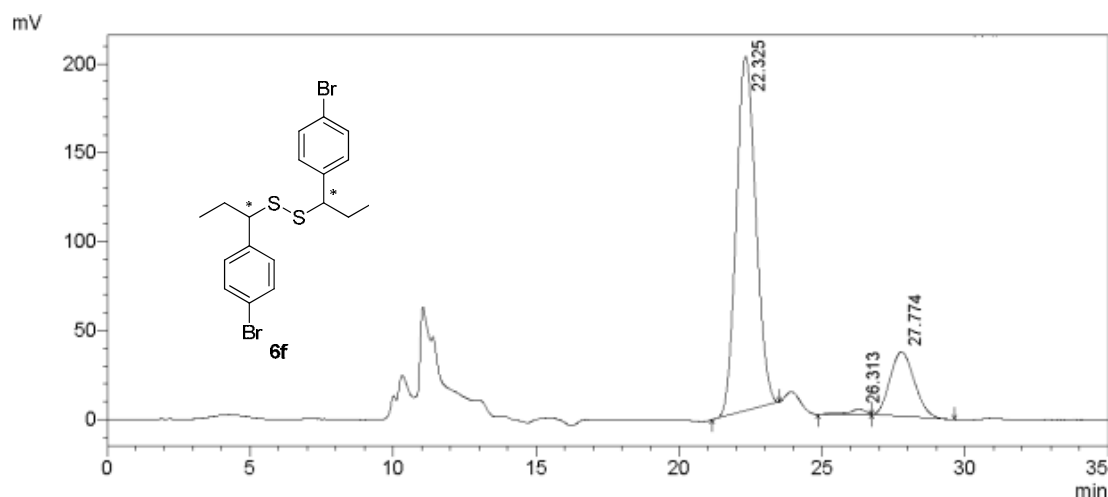
Peak No.	Peak Name	Result (°)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		27.8794	4.604	0.000	14130920	BB	9.9	
2		23.9260	5.008	0.000	12127087	BB	10.5	
3		48.1946	5.488	0.000	24427854	BB	12.2	
Totals:		100.0000		0.000	50685861			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		84.0209	4.597	0.000	98273008	BB	9.5	
2		0.4391	4.997	0.000	513526	BB	4.5	
3		15.5401	5.487	0.000	18176062	BB	12.3	
Totals:		100.0001		0.000	116962596			

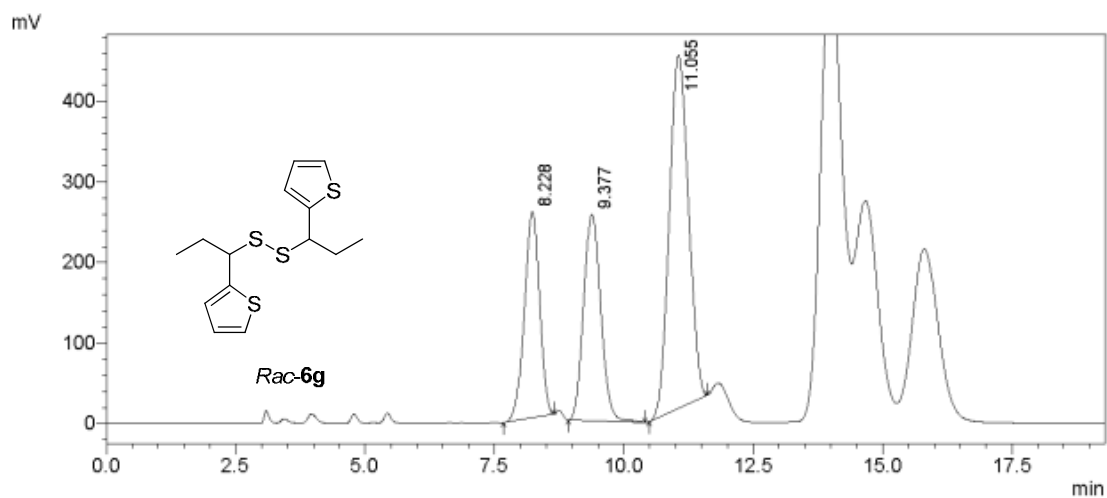


Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	22.640	6542924	128512	28.050	32.131
2	25.924	5737532	96878	24.598	24.222
3	28.271	11045082	175467	47.352	43.646
Total		23325538	399956	100.00	100.00

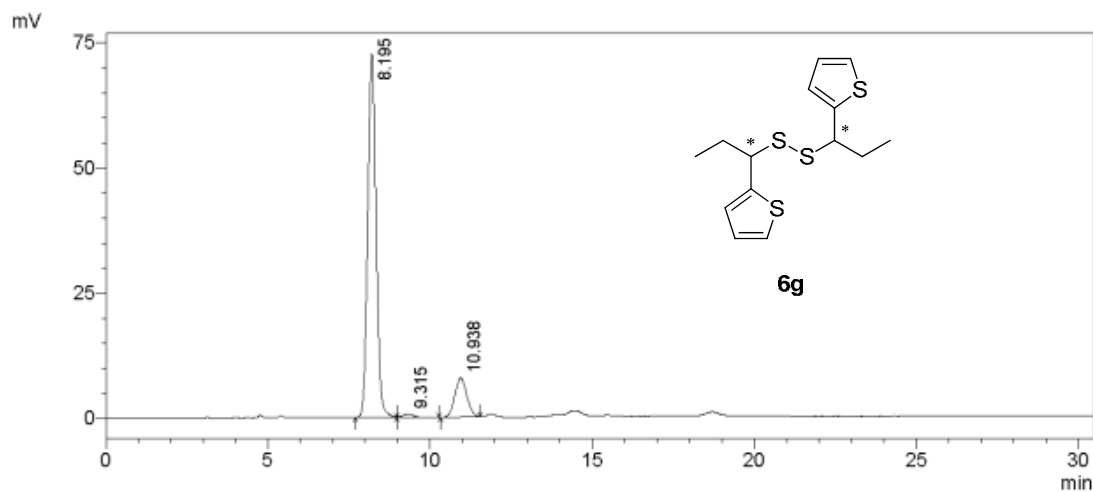


Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	22.325	9519307	199643	80.855	83.730
2	26.313	123104	2704	1.046	1.134

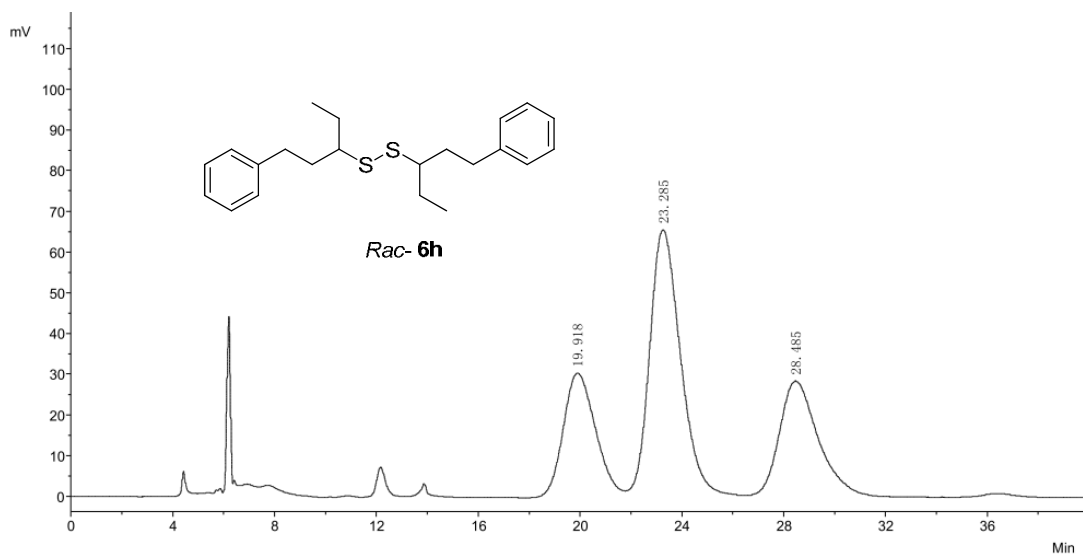
3	27.774	2130890	36090	18.099	15.136
Total		11773301	238436	100.00	100.00



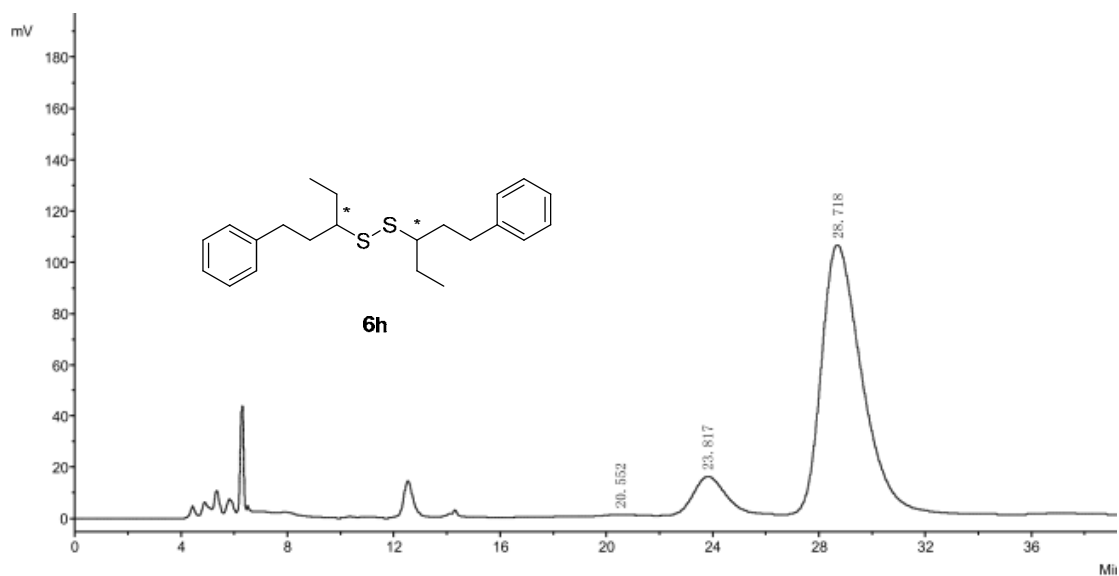
Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	8.228	5263386	255507	23.348	26.909
2	9.377	5912544	256025	26.227	26.964
3	11.055	11367672	437981	50.425	46.127
Total		22543602	949513	100.00	100.00



Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	8.195	1295289	72506	85.682	89.563
2	9.315	16403	688	1.085	0.849
3	10.938	200049	7761	13.233	9.587
Total		1511741	80955	100.00	100.00

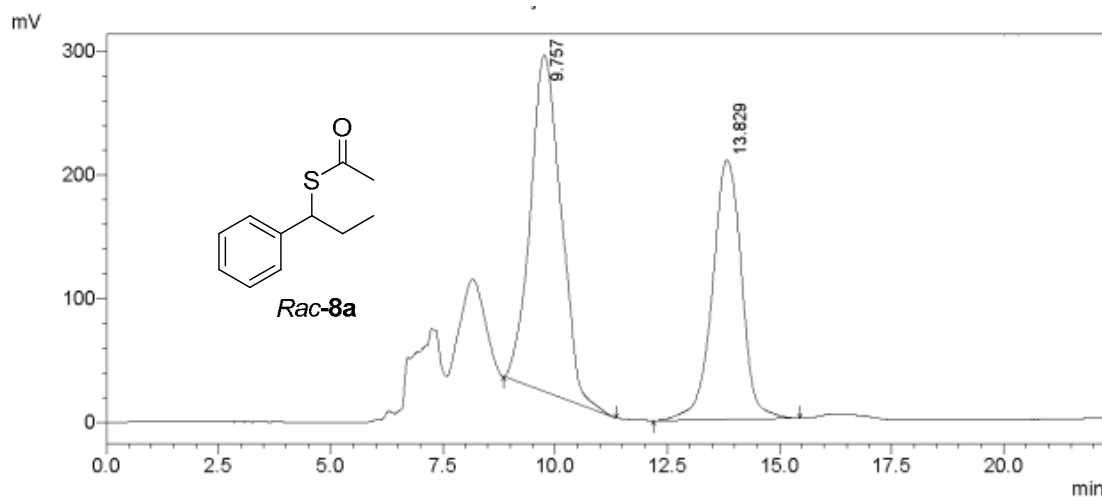


No.	PeakNo	ID. Name	R. Time	PeakHeight	PeakArea	PerCent
1	1		19.918	30512.3	2685604.5	24.0918
2	2		23.285	65460.6	5498902.9	49.3291
3	3		28.485	28183.7	2962882.9	26.5792
Total				124156.6	11147390.4	100.0000

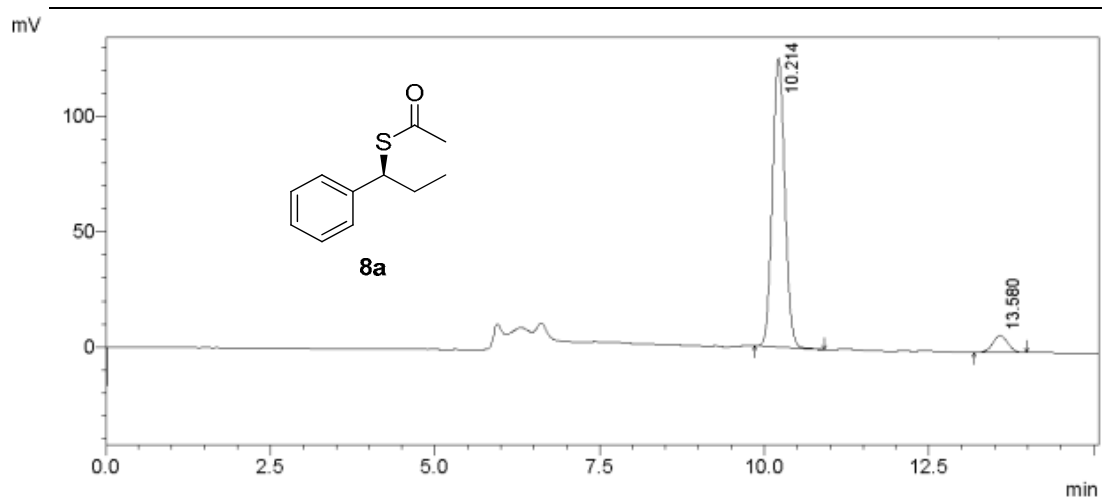


No.	PeakNo	ID. Name	R. Time	PeakHeight	PeakArea	PerCent
1	1		20.552	661.8	50011.3	0.4038
2	2		23.817	14975.6	1274107.8	10.2886
3	3		28.718	105135.6	11059570.4	89.3076
Total				120772.9	12383689.5	100.0000

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Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	9.757	12919675	271984	57.624	56.441
2	13.829	9501091	209905	42.376	43.559
Total		22420767	481889	100.00	100.00



Peak No.	Ret. Time (min)	Area	Height	Area %	Height %
1	10.214	1626951	125332	93.294	94.515
2	13.580	116950	7273	6.706	5.485
Total		1743901	132604	100.00	100.00