Electronic Supplementary Information

Stereoselective organocatalytic sulfa-Michael reactions of aryl substituted α,β-unsaturated *N*-acyl pyrazoles

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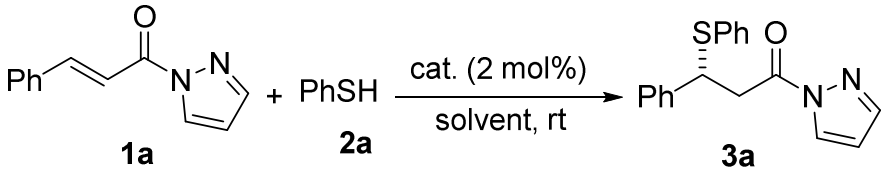
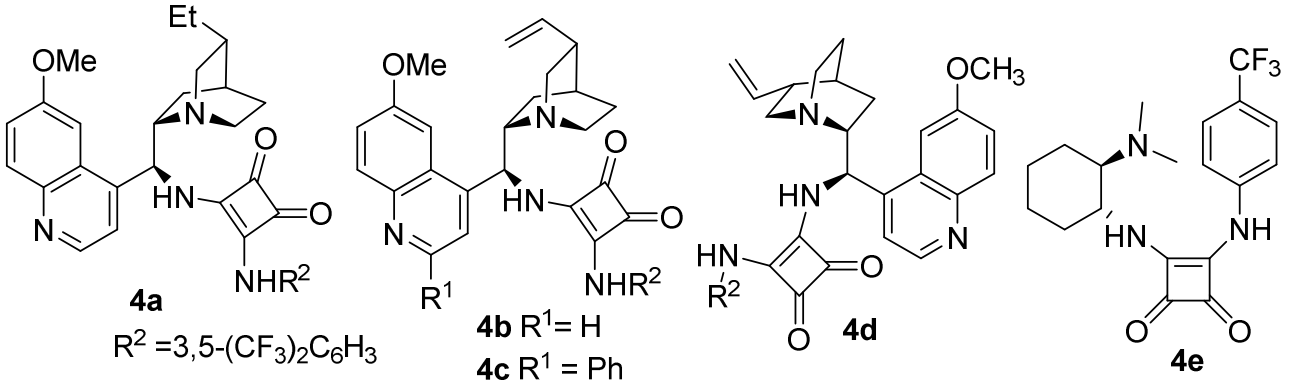
Additional Tables and Compounds Characterization

Table S1. Optimization of the reaction conditions for the asymmetric sulfa-Michael reaction of pyrazolamide **1a** with thiophenol[a]

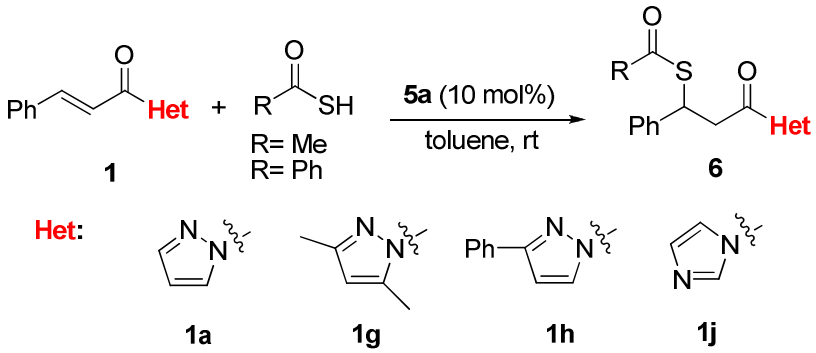




entry	cat.	solvent	time (h)	yield (%)[b]	ee (%)[c]
1	**4a**	toluene	3	98	80 (*R*)
2	**4b**	toluene	2	55	75 (*R*)
3	**4c**	toluene	2	68	49 (*R*)
4	**4d**	toluene	2.5	72	-71 (*S*)
5	**4e**	toluene	3	99	-8 (*S*)
6	**4a**	chlorobenzene	1	98	-79 (*R*)
7	**4a**	mesitylene	1.5	98	-73 (*R*)
8	**4a**	CH_2Cl_2	1.5	98	-75 (*R*)
9	**4a**	AcOEt	1	98	-78 (*R*)
10	**4a**	Et_2O	1	98	-81 (*R*)
11[d]	**4a**	Et_2O	16	85	-78 (*R*)
12[e]	**4a**	Et_2O	15	71	-87 (*R*)

[a]Molar ratios: **1a**/**2a** 1/1.3 at C = 0.1 M. [b]Isolated yield after chromatography. [c]The ee values determined by chiral HPLC analysis. [d] Performed at 0° C. [e] The reaction was carried out at C = 0.05 M.

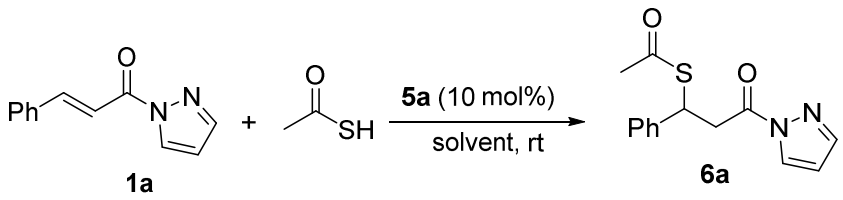
Table S2. Screening of *N*-acyl pyrazolamides **1** in the asymmetric sulfa-Michael reaction with tioacetic and thiobenzoic acid[a]



entry	**1**	R	time (h)	**6**	yield **6**(%)[b]	*ee* **6**(%)[c]
1	**1a**	Me	8	**6a**	98	64
2	**1g**	Me	23	**6g**	88	46
3	**1h**	Me	16	**6h**	71	27
4[d]	**1j**	Me	118	**6j**	no reaction	-
5	**1a**	Ph	28	**6i**	68	13
6[e]	**1a**	Me	23	**6a**	80	66
7[f]	**1a**	Me	21	**6a**	50	69

[a]Molar ratios: **1a**/thioacetic acid 1/2 at C = 0.1 M. [b]Isolated yield after chromatography. [c]The ee values determined by chiral HPLC analysis. [d]The reaction was performed at C = 0.05 M in a mixture toluene/DCM 1/1 to improve the solubility of **1j**. [e]Perfomed at 0 °C. [f]Performed at -20 °C.

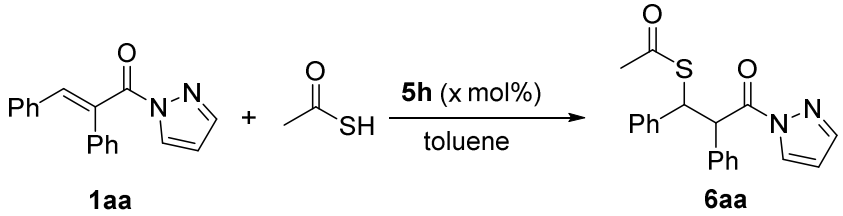
Table S3. Solvent screening in the asymmetric sulfa-Michael reaction of *N*-acyl pyrazolamide **1a** with tioacetic acid[a]



entry	solvent	time (h)	yield (%)[b]	ee (%)[c]
1	toluene	8	98%	64
2	chlorobenzene	3	95%	60
3	mesitylene	4	75%	63
4	$CF_3C_6H_5$	4.5	75%	65
5	$CHCl_3$	6.5	98%	55
6	AcOEt	4	85%	18
7	MeO*t*Bu	4	99%	54

[a]Molar ratios: **1a**/thioacetic acid 1/2 at C = 0.1 M. [b] Determined by ^{1}H NMR analysis using 1,3,5-$(MeO)_3C_6H_3$ as an internal standard. [c]The ee values determined by chiral HPLC analysis.

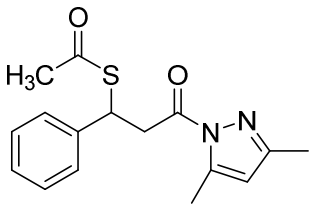
Table S4. Optimization of the reaction conditions for the asymmetric sulfa-Michael reaction of α,β–diphenyl α,β-unsaturated *N*-acyl pyrazole **1aa** with thioacetic acid[a]



entry	**5h** (x mol%)	C (M)	T (°C)	time (h)	yield **6**(%)[b]	dr **6aa**[c]	*ee* **6aa**(%)[d]
1	5	0.1	0	7	87	90/10	90
2	5	0.1	-20	25	93	92/8	84
3	5	0.05	rt	8	93	81/19	96
4	2	0.1	rt	69	75	89/11	95

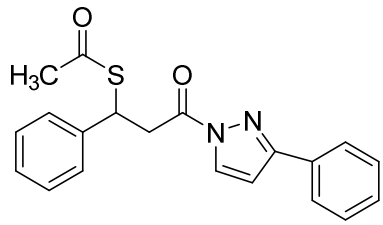
[a]Molar ratios: **1a**/thioacetic acid 1/2. [b]Determined by ^{1}H NMR analysis using 1,3,5-$(MeO)_3C_6H_3$ as an internal standard. [c]Determined by ^{1}H NMR analysis of the crude reaction mixture. [d]The ee values determined by chiral HPLC analysis for the major diastereomer of **6aa**.

S-(3-(3,5-dimethyl-1H-pyrazol-1-yl)-3-oxo-1-phenylpropyl) ethanethioate (6g)



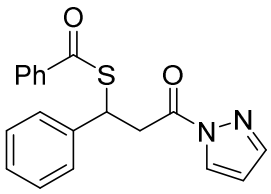
White liquid, 26.5 mg, 88% yield. $[\alpha]_D^{18}$ = +83.1 (c 0.43, $CHCl_3$), 46% ee. **^{1}H NMR** ($CDCl_3$, 250 MHz): δ 7.43- 7.39 (m, 2H), 7.33- 7.21 (m, 3H), 5.91 (s, 1H), 5.22 (dd, 1H, *J*= 8.2, 6.6 Hz), 3.89 (dd, 1H, *J*= 17.6, 8.2 Hz) 3.72 (dd, 1H, *J*= 17.6, 6.6 Hz), 2.44 (s, 3H), 2.28 (s, 3H), 2.22 (s, 3H). **^{13}C NMR** ($CDCl_3$, 62.5 MHz): δ 194.3, 170.3, 152.2, 144.1, 140.6, 128.6, 127.8, 127.5, 111.2, 43.2, 41.3, 30.3, 14.4, 13.8. **HRMS (MALDI-FT ICR)** exact mass calculated $[M+H]^+$ calculated for $C_{16}H_{19}N_2O_2S$: 303.1162, found: 303.1162. HPLC analysis with Chiralpak AD column, 98:2 *n*-hexane:2-propanol, 1 mL/min, 254 nm; minor enantiomer t_R= 10.3 min, major enantiomer t_R= 11.8 min. IR (neat, cm^{-1}): 1728, 1691, 1585, 1491, 1453, 1411, 1382, 1362, 1310, 1251, 1134, 1108, 1026, 962, 808, 770, 700, 631, 588, 514, 424.

S-(3-oxo-1-phenyl-3-(3-phenyl-1H-pyrazol-1-yl)propyl) ethanethioate (6h)



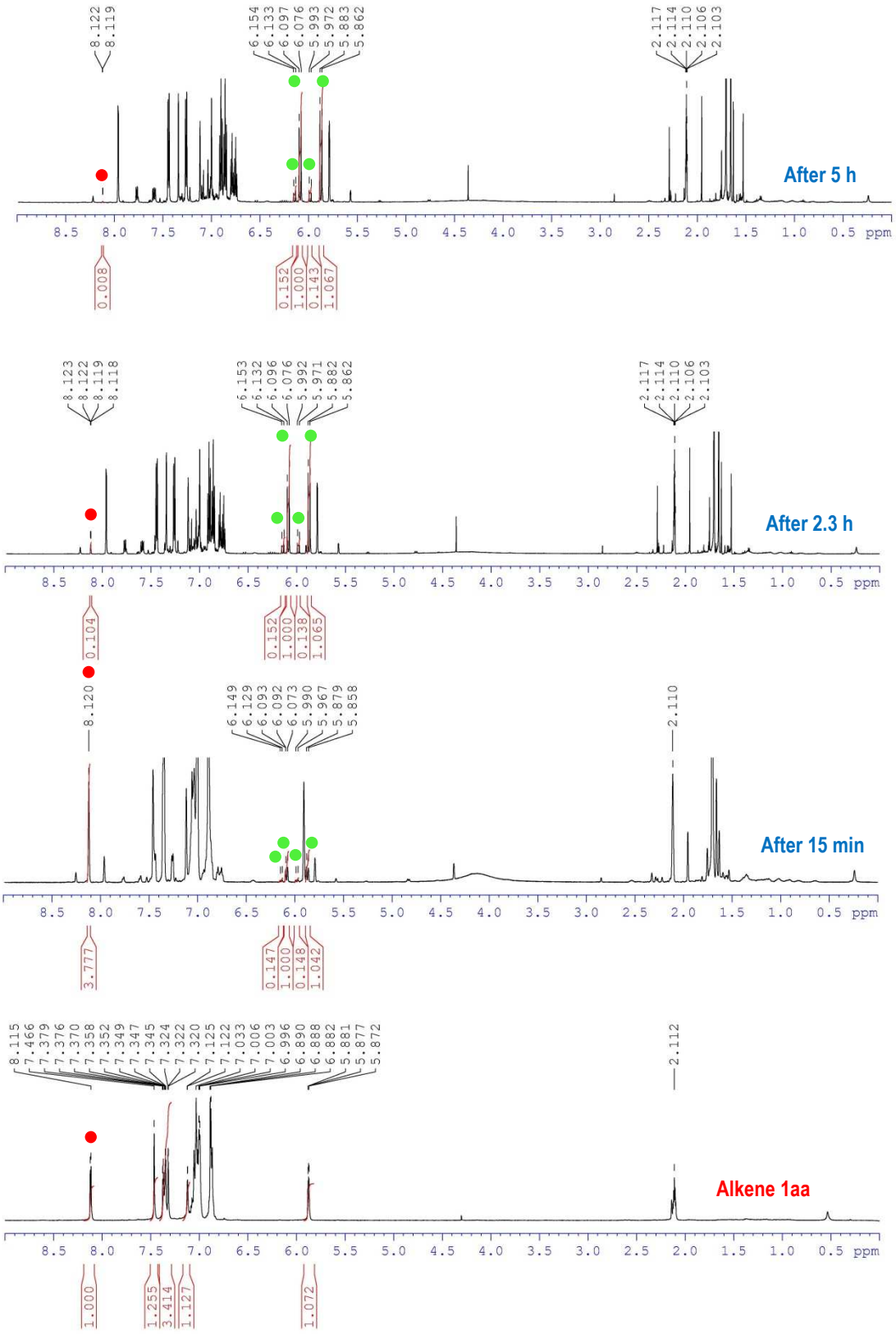
White solid, 24.9 mg, 71% yield. **mp** 105.6-107.4 °C. $[\alpha]_D^{18}$ = +57.6 (c 0.54, $CHCl_3$), 27% ee. **^{1}H NMR** ($CDCl_3$, 250 MHz): δ 8.19 (d, 1H *J*= 2.8 Hz), 7.90-7.87 (m, 2H), 7.48-7.38 (m, 5H), 7.34-7.23 (m, 3H), 6.74 (d, 1H, *J*= 2.8 Hz), 5.32 (dd, 1H, *J*= 7.5, 7.5 Hz), 4.00 (dd, 1H, *J*= 17.3, 8.5 Hz), 3.84 (dd, 1H, *J*= 17.3, 6.7 Hz), 2.31 (s, 3H). **^{13}C NMR** ($CDCl_3$, 62.5 MHz): δ 194.1, 168.8, 155.5, 140.1, 131.6, 129.5, 129.3, 128.8, 128.7, 127.7, 126.3, 107.6, 43.3, 40.2, 30.3. **HRMS (MALDI-FT ICR)** exact mass calculated $[M+Na]^+$ calculated for $C_{20}H_{18}N_2NaO_2S$: 373.0981, found: 373.0978. HPLC analysis with Chiralpak IC column, 95:5 *n*-hexane:2-propanol, 1 mL/min, 254 nm; minor enantiomer t_R= 16.3 min, major enantiomer t_R= 14.3 min. IR (neat, cm^{-1}): 1734, 1691, 1541, 1505, 1494, 1454, 1411, 1363, 1305, 1286, 1237, 1132, 1097, 1076, 1043, 936, 762, 696, 630.

S-(3-oxo-1-phenyl-3-(1H-pyrazol-1-yl)propyl) benzothioate (6i)



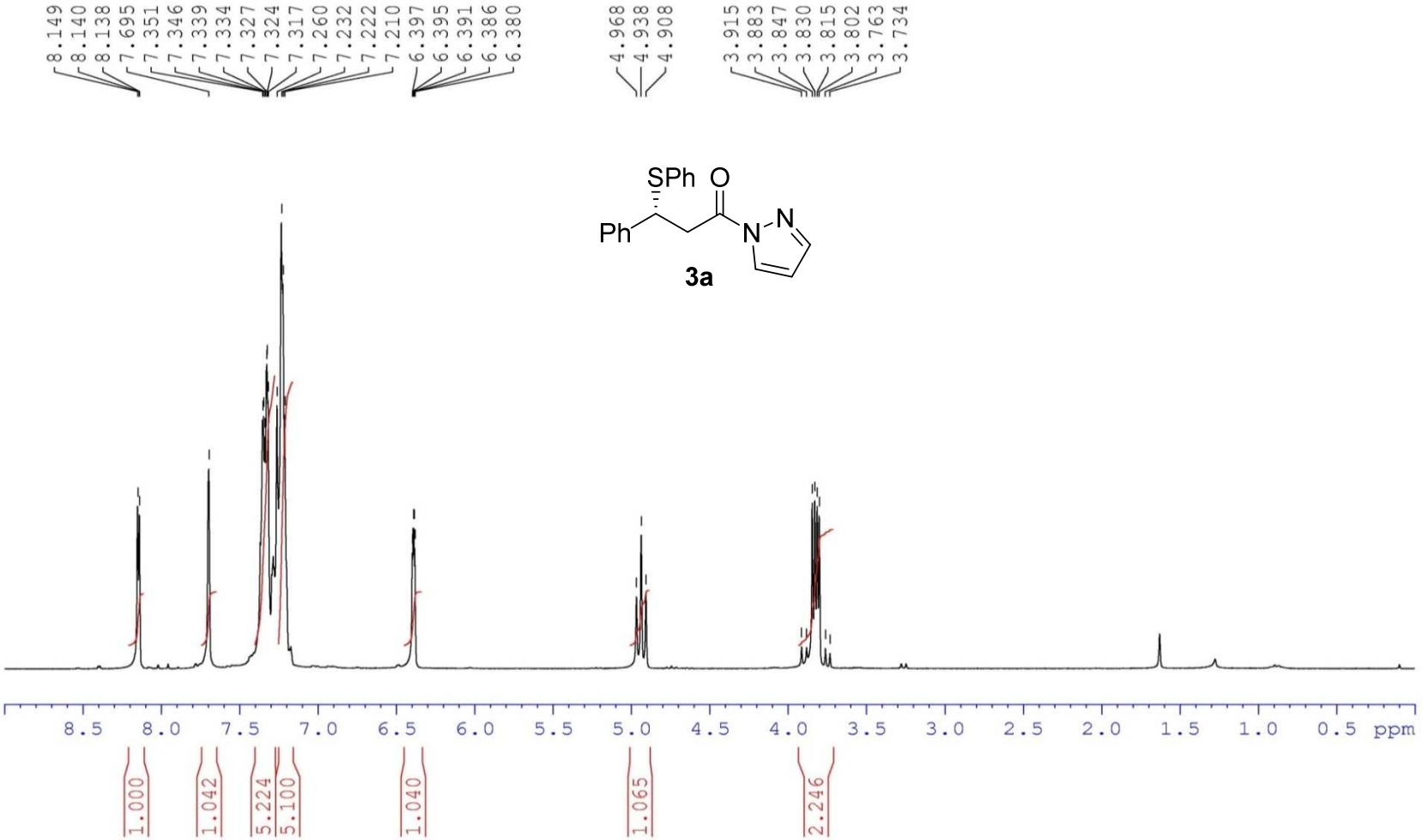
White solid, 22.9 mg, 68% yield. **mp** 91.7-93.5 °C. $[\alpha]_D^{19}$ = +18.8 (c 0.68, $CHCl_3$), 13% ee. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.18 dd, 1H, *J*= 2.9 Hz, 0.4 Hz), 7.93-7.90 (m, 2H), 7.71(s, 1H), 7.55-7.48 (m, 3H), 7.44-7.39 (m, 2H), 7.36-7.31 (m, 2H), 7.28-7.25 (m, 1H), 6.42 (dd 1H, *J*= 3.0, 1.5 Hz) 5.50 (dd, 1H, *J*= 8.5, 6.5 Hz) 4.04 (dd 1H *J*= 17.4, 8.5 Hz) 3.92 (dd, 1H *J*= 17.4, 6.5 Hz). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 190.3, 168.8, 144.1, 140.0. 136.5, 133.5, 128.7, 128.6, 128.4, 127.9, 127.8, 127.3, 109.8, 43.2, 40.4. **HRMS (MALDI-FT ICR)** exact mass calculated $[M+Na]^+$ calculated for $C_{19}H_{16}N_2NaO_2S$: 359.0825, found: 359.0821. HPLC analysis with Chiralpak AD column, 90:10 *n*-hexane:2-propanol, 1 mL/min, 254 nm; minor enantiomer t_R= 26.0 min, major enantiomer t_R= 20.9 min. IR (neat, cm^{-1}): 1734, 1662, 1581, 1533, 1494, 1449, 1417, 1386, 1343, 1315, 1247, 1208, 1176, 1093, 1037, 909, 772, 689, 648.

Figure S1. Monitoring of the reaction in Table 3 (entry 7) by ^{1}H NMR in toluene-d_8 (600 MHz at rt). Red spots refer to alkene **1aa** and green spots to the mixture of diastereomers of **6aa**. The diasteroselectivity does not change over time.

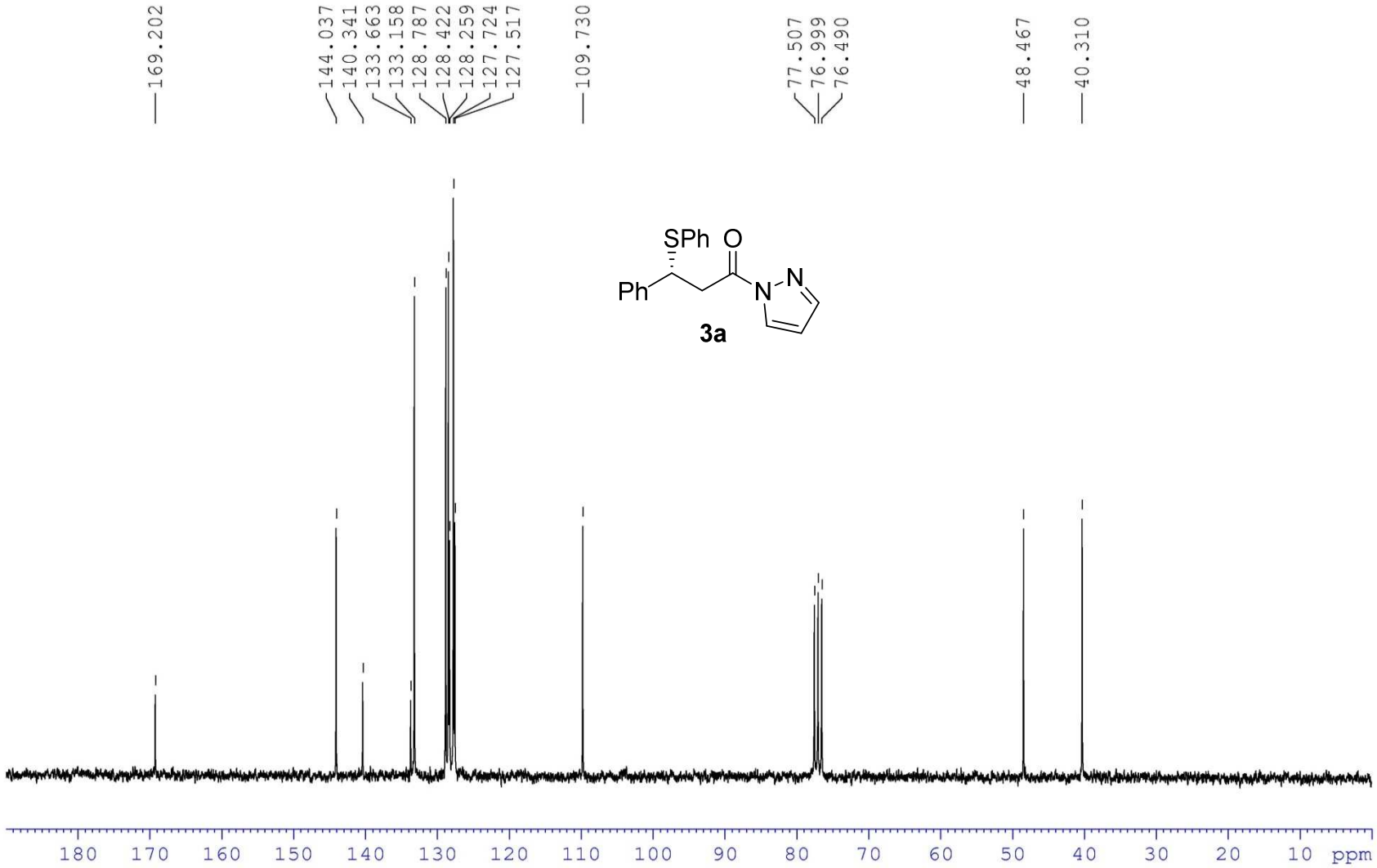


NMR Spectra

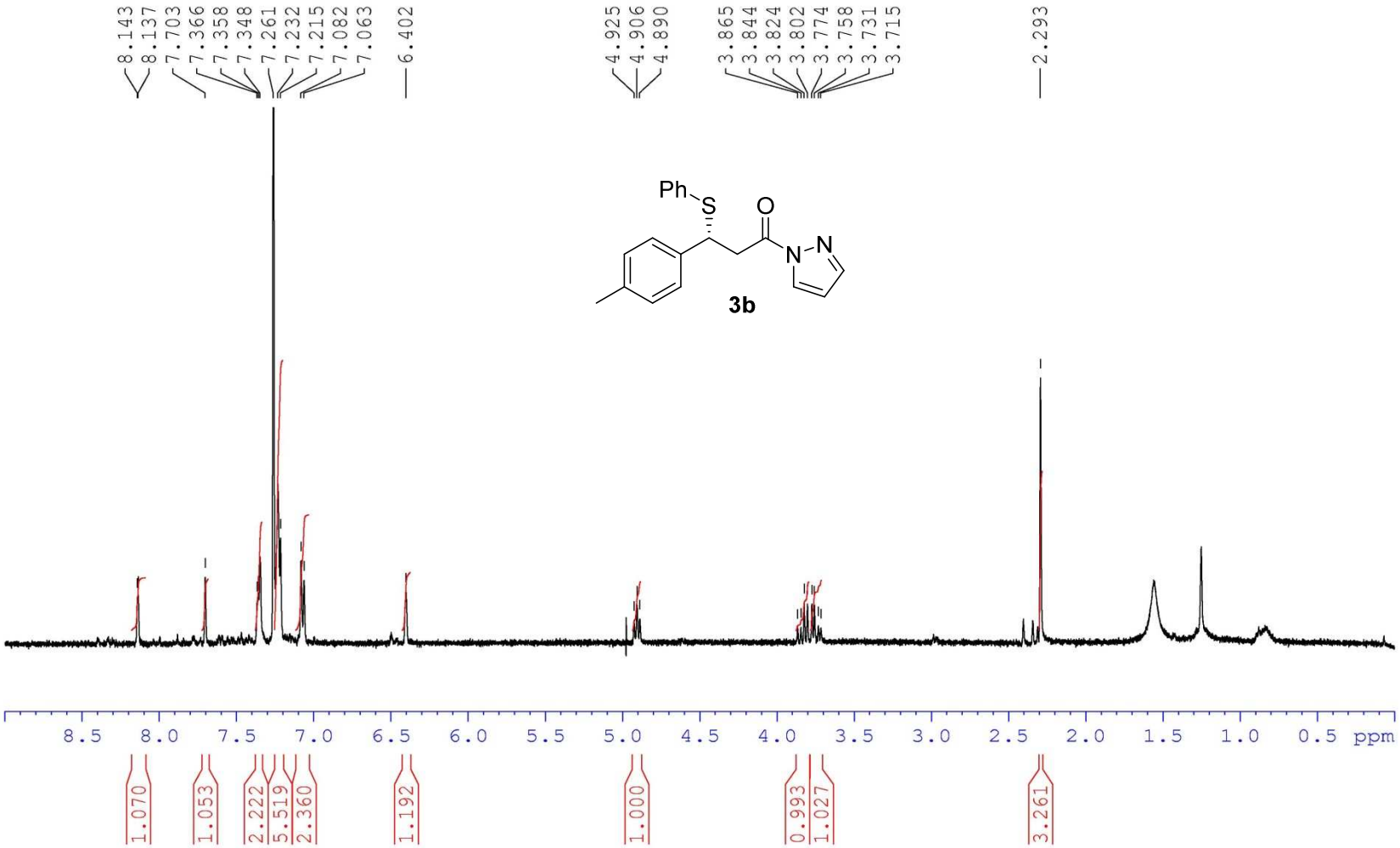
^{1}H NMR in $CDCl_3$ (250 MHz)



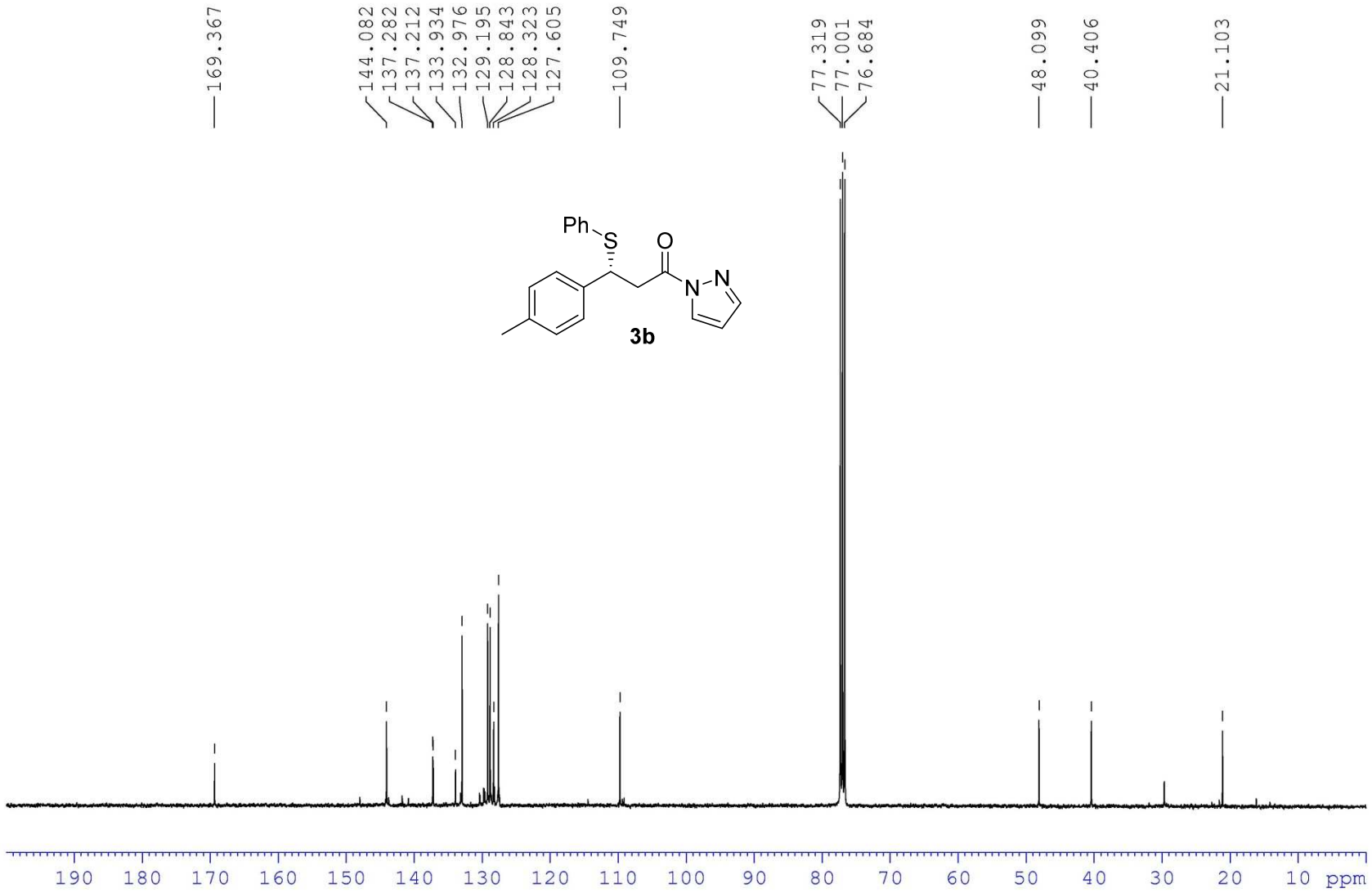
^{13}C NMR in $CDCl_3$ (62.5 MHz)



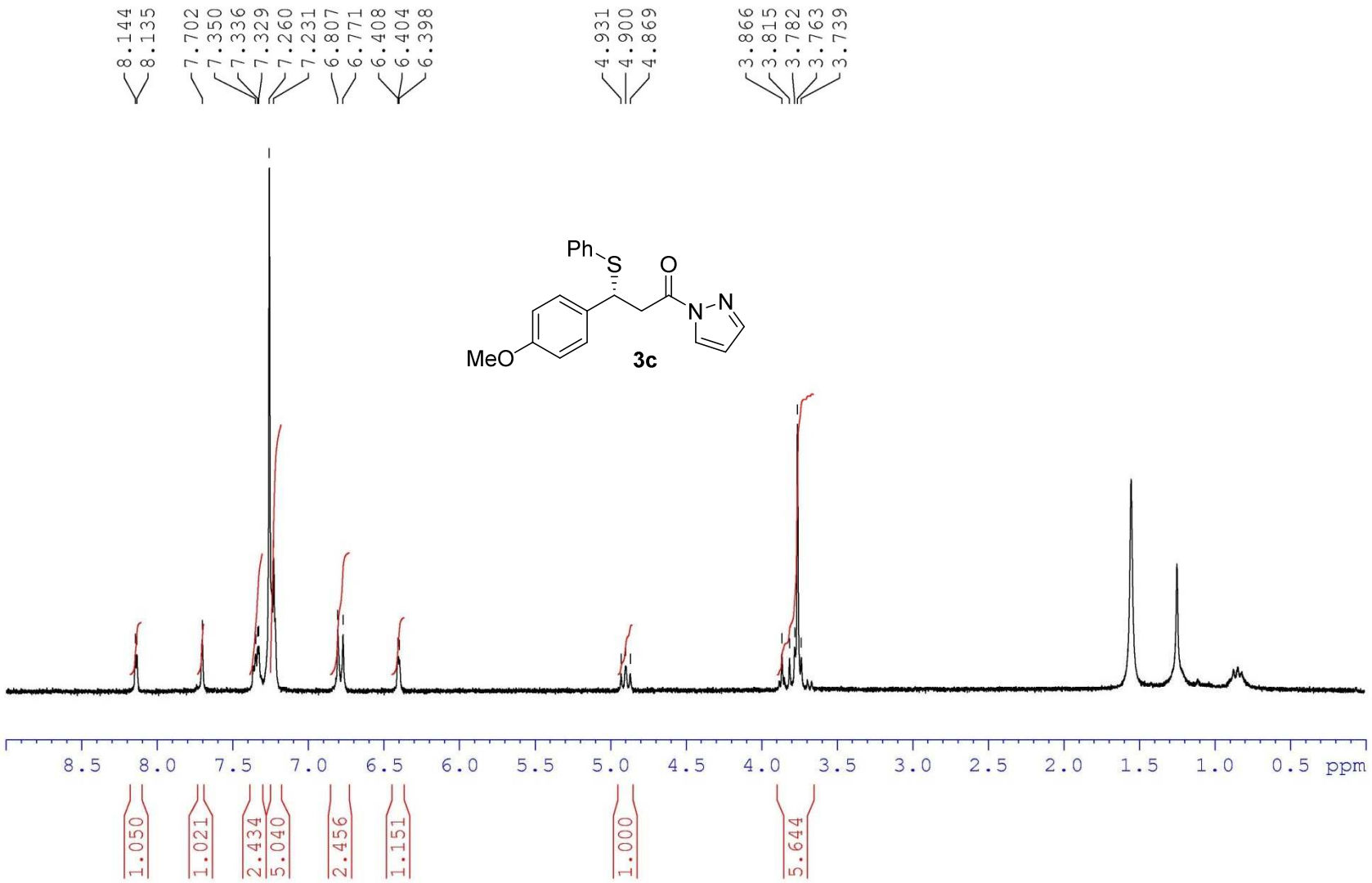
^{1}H NMR in $CDCl_3$ (400 MHz)



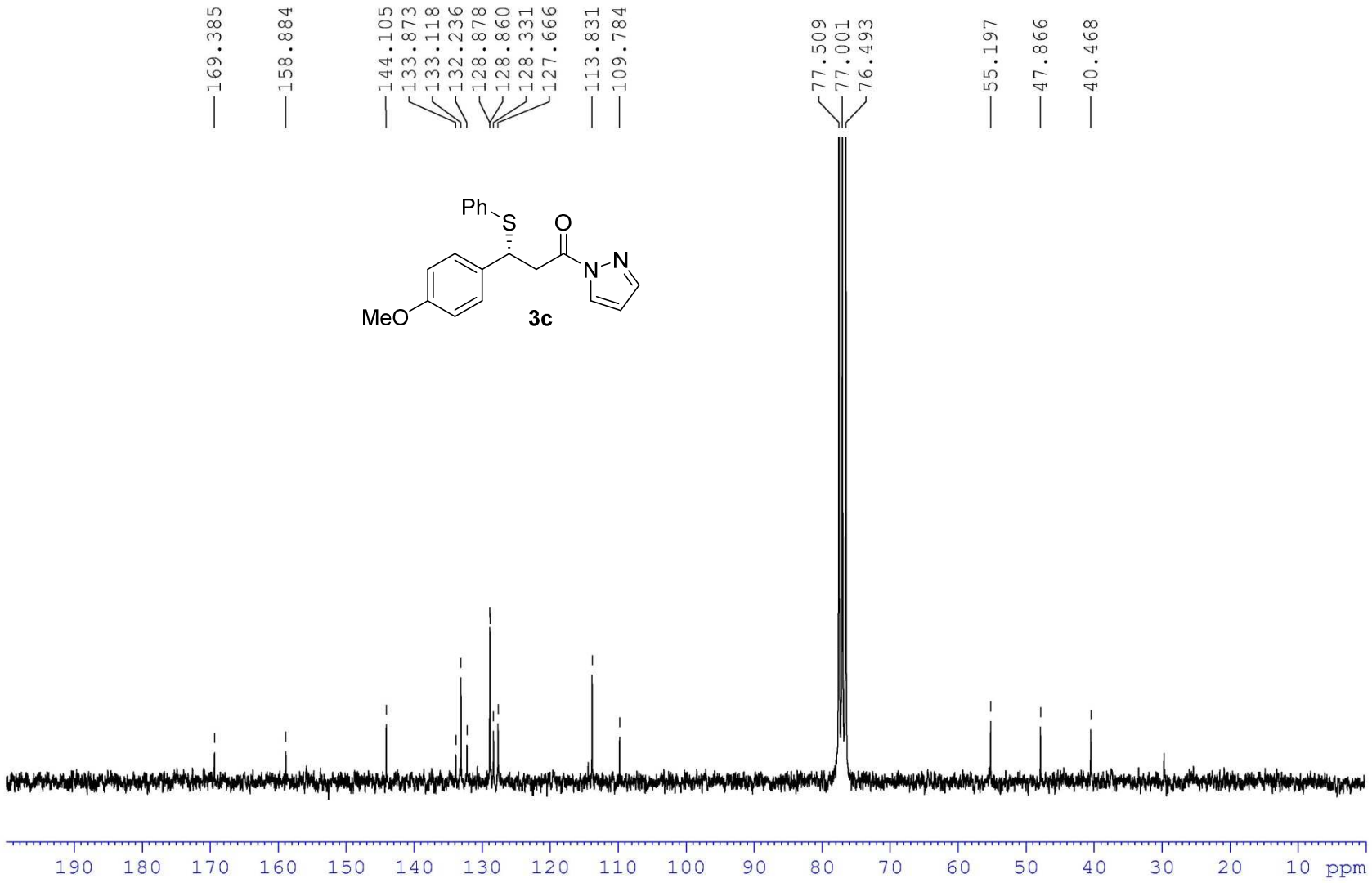
^{13}C NMR in $CDCl_3$ (100 MHz)



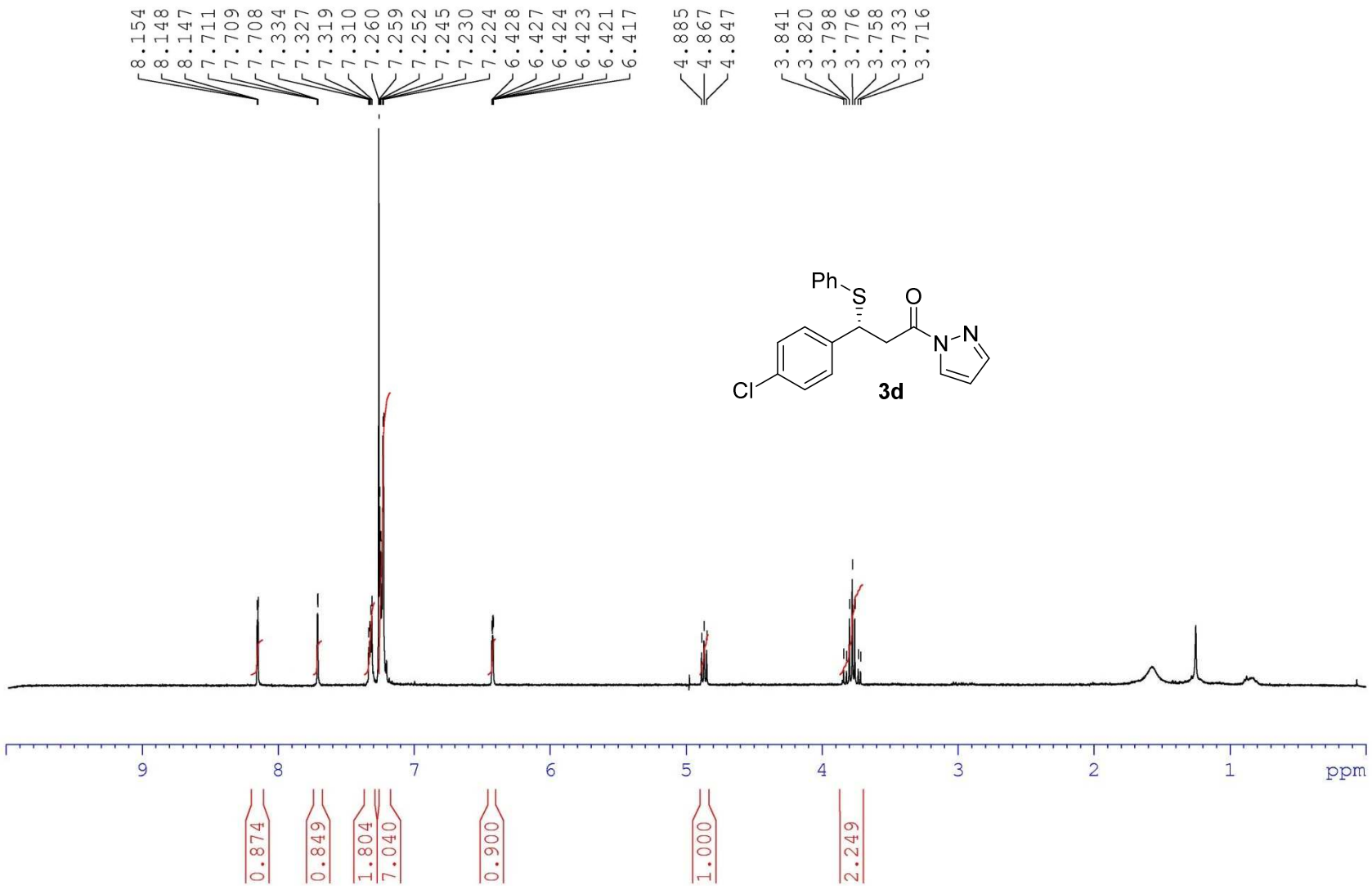
^{1}H NMR in $CDCl_3$ (250 MHz)



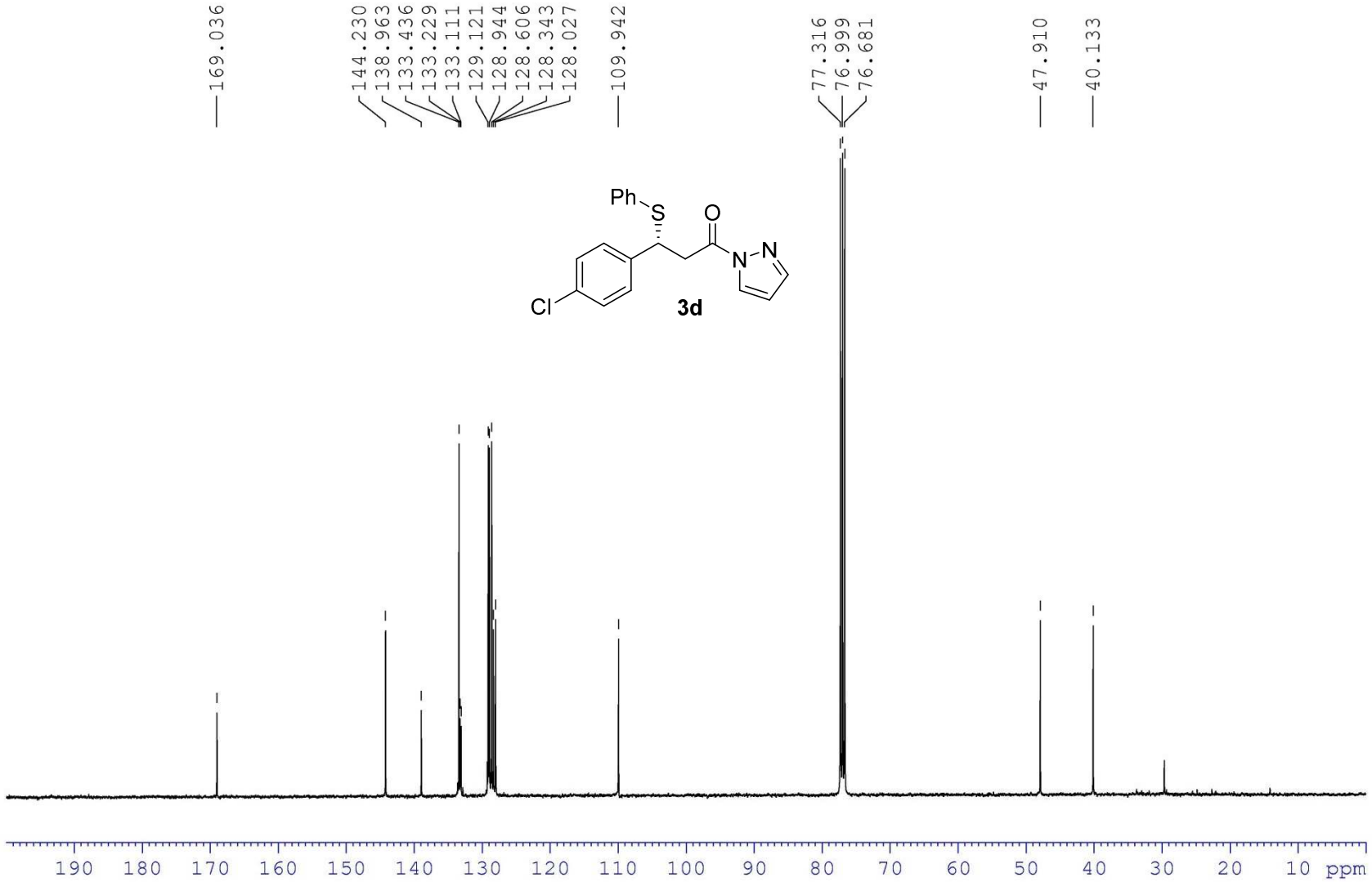
^{13}C NMR in $CDCl_3$ (62.5 MHz)



^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)



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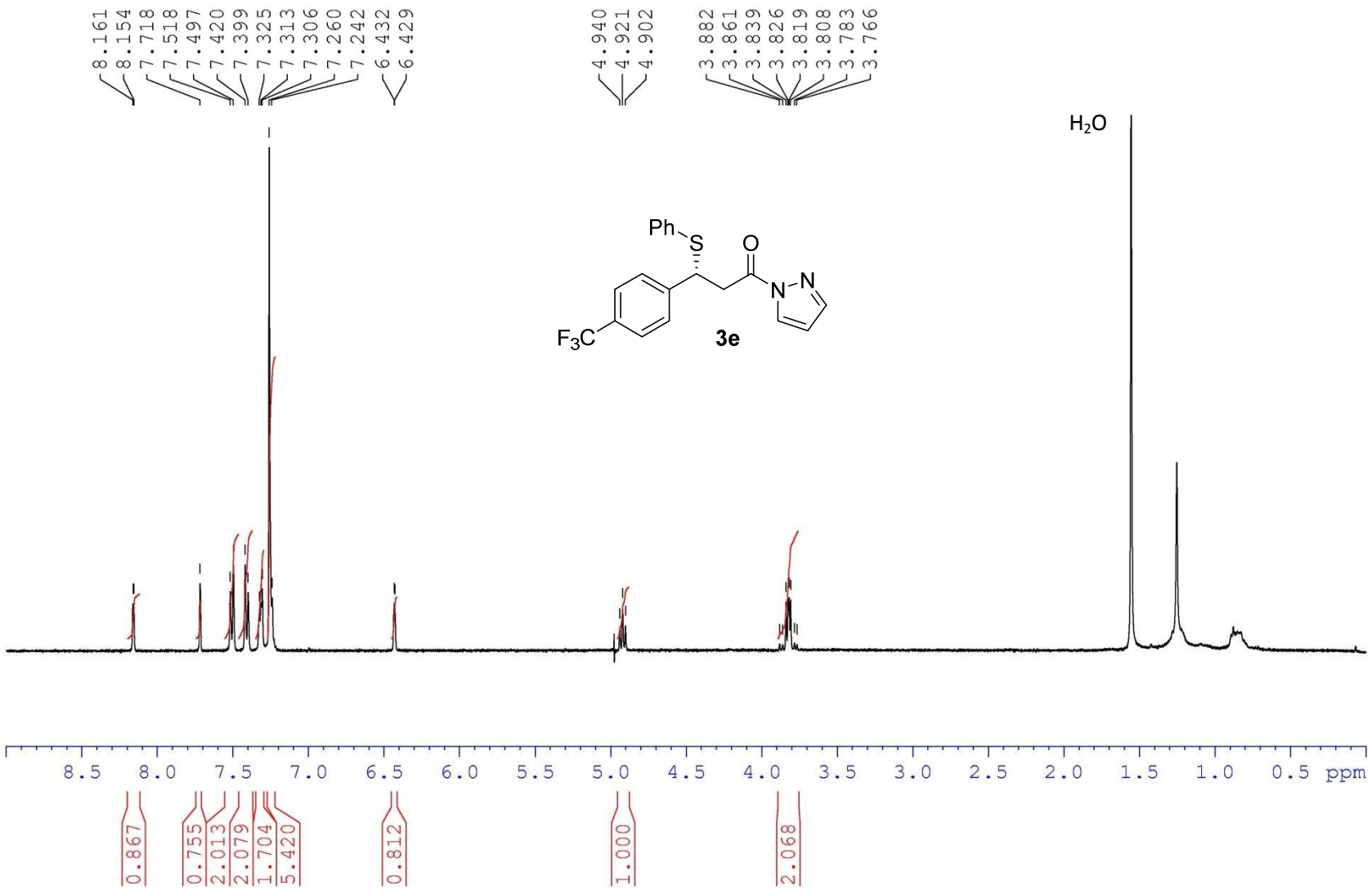
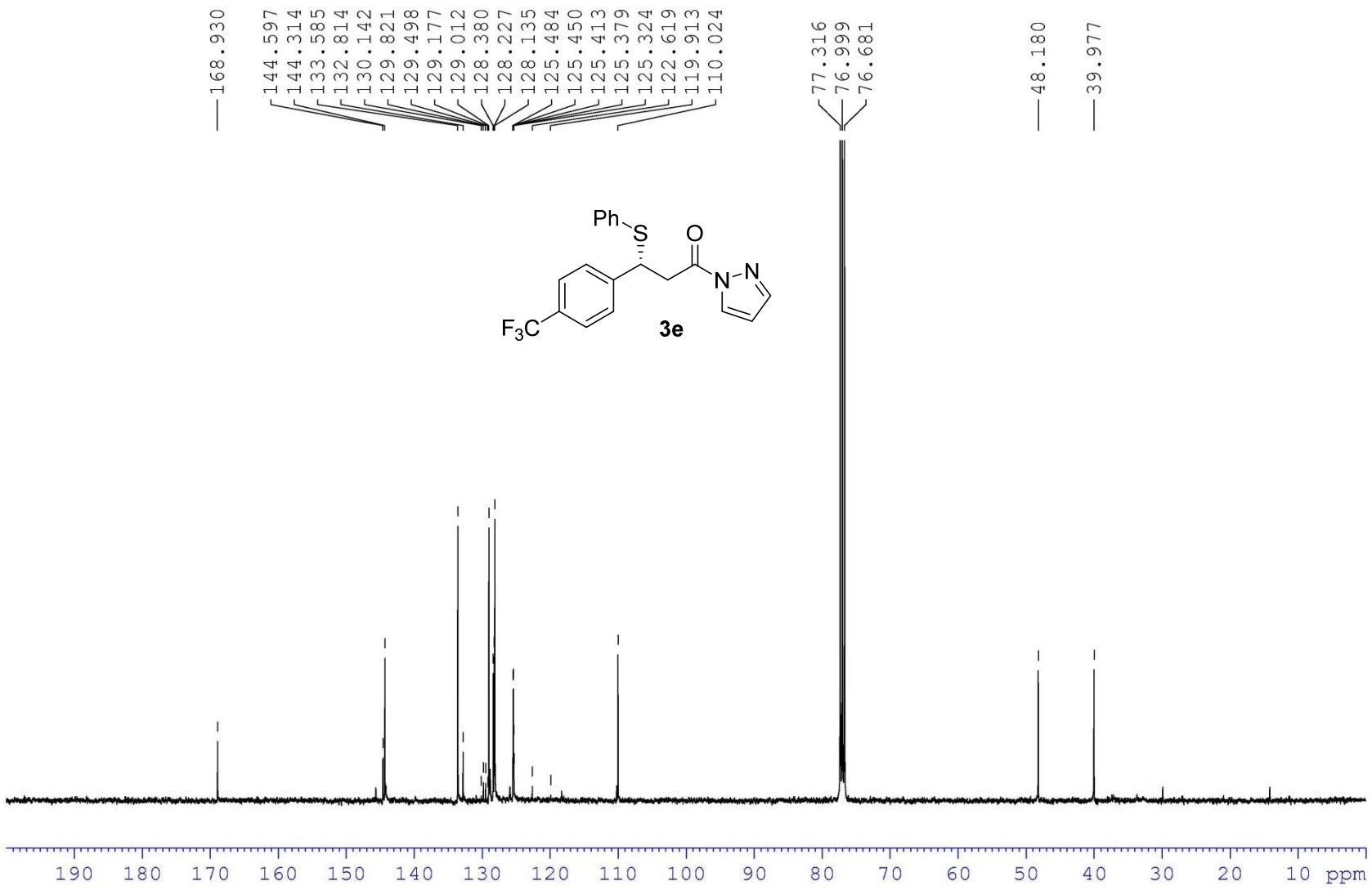
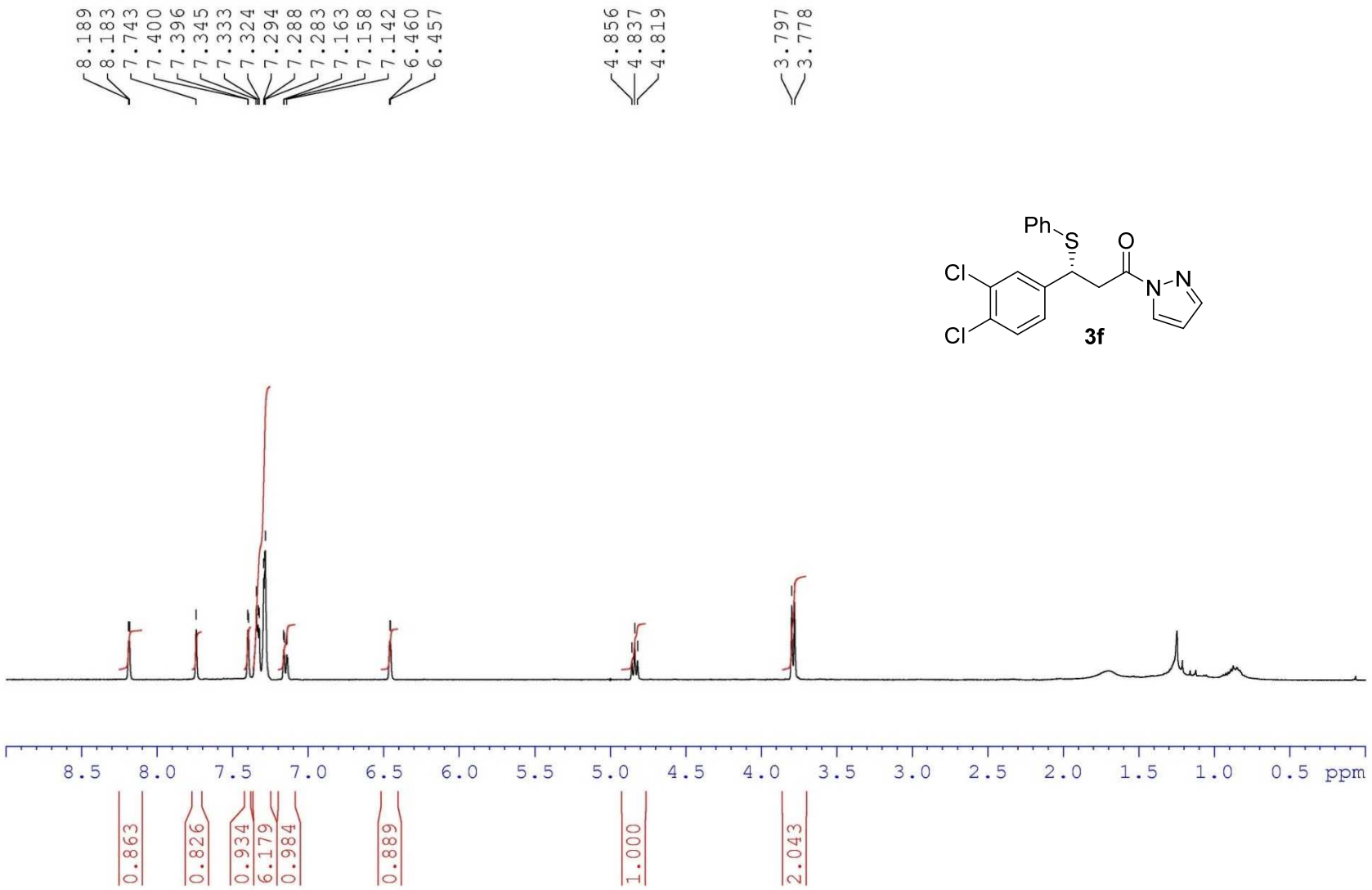


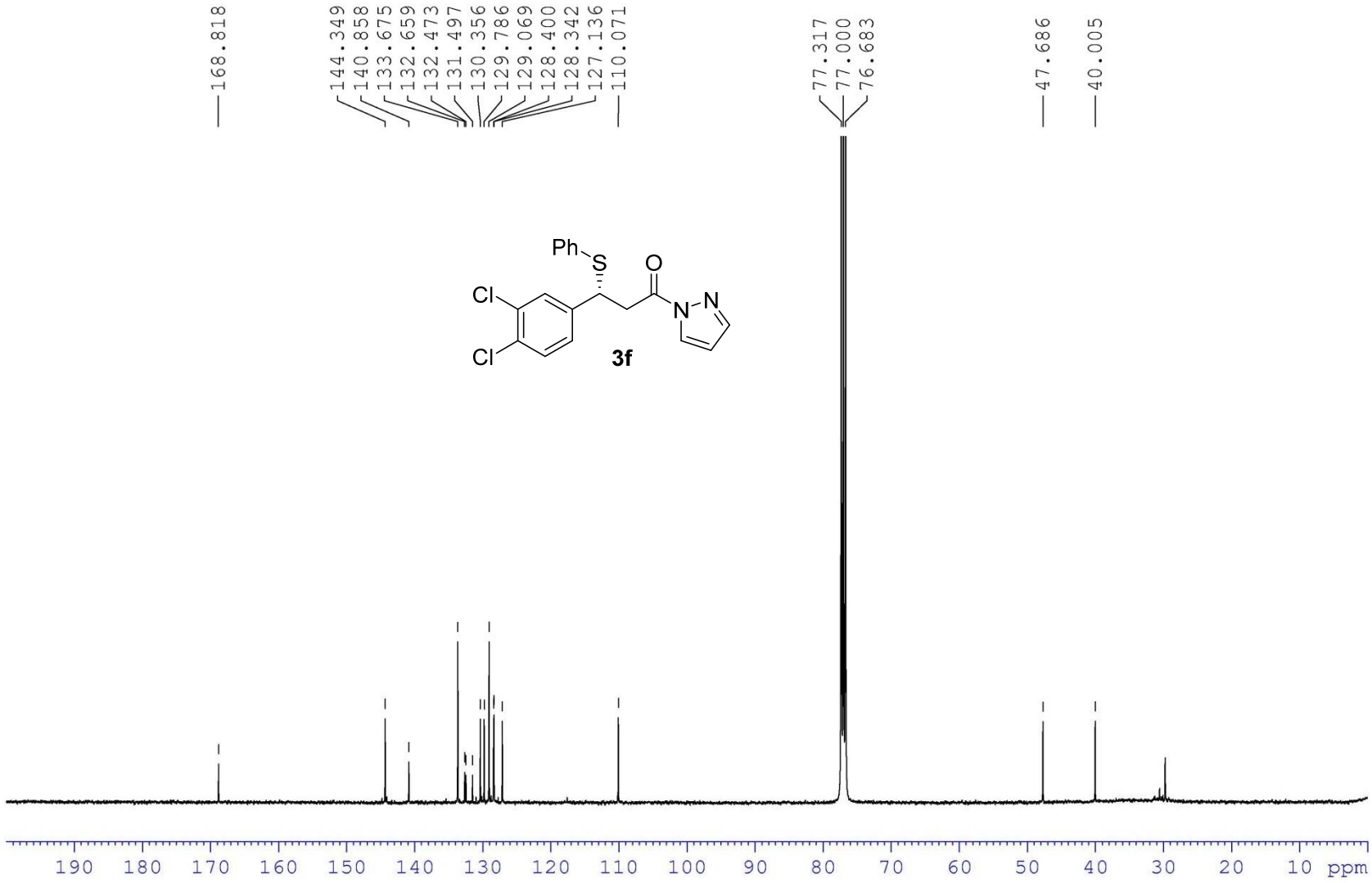
^{13}C NMR in $CDCl_3$ (100 MHz)



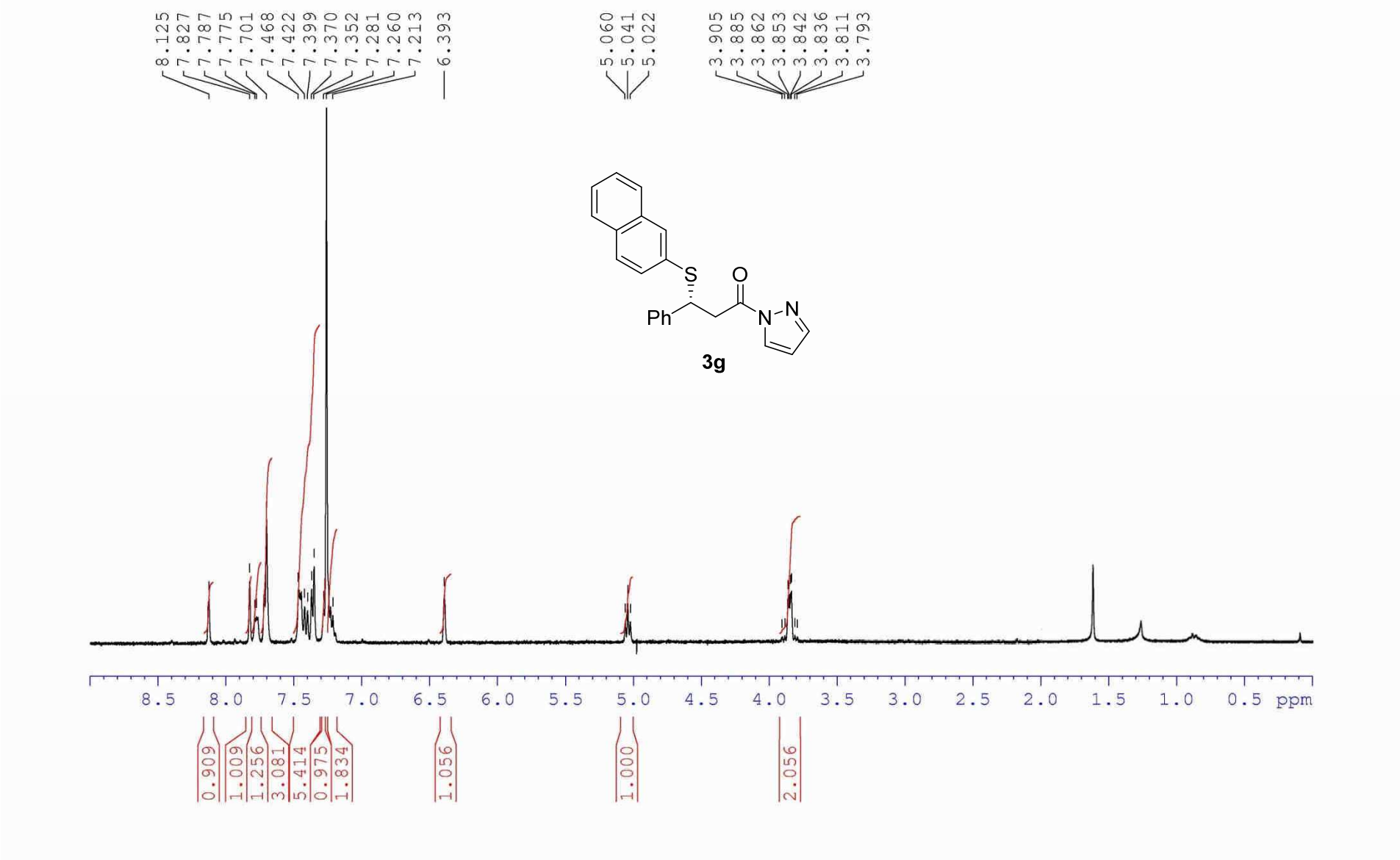
^{1}H NMR in $CDCl_3$ (400 MHz)



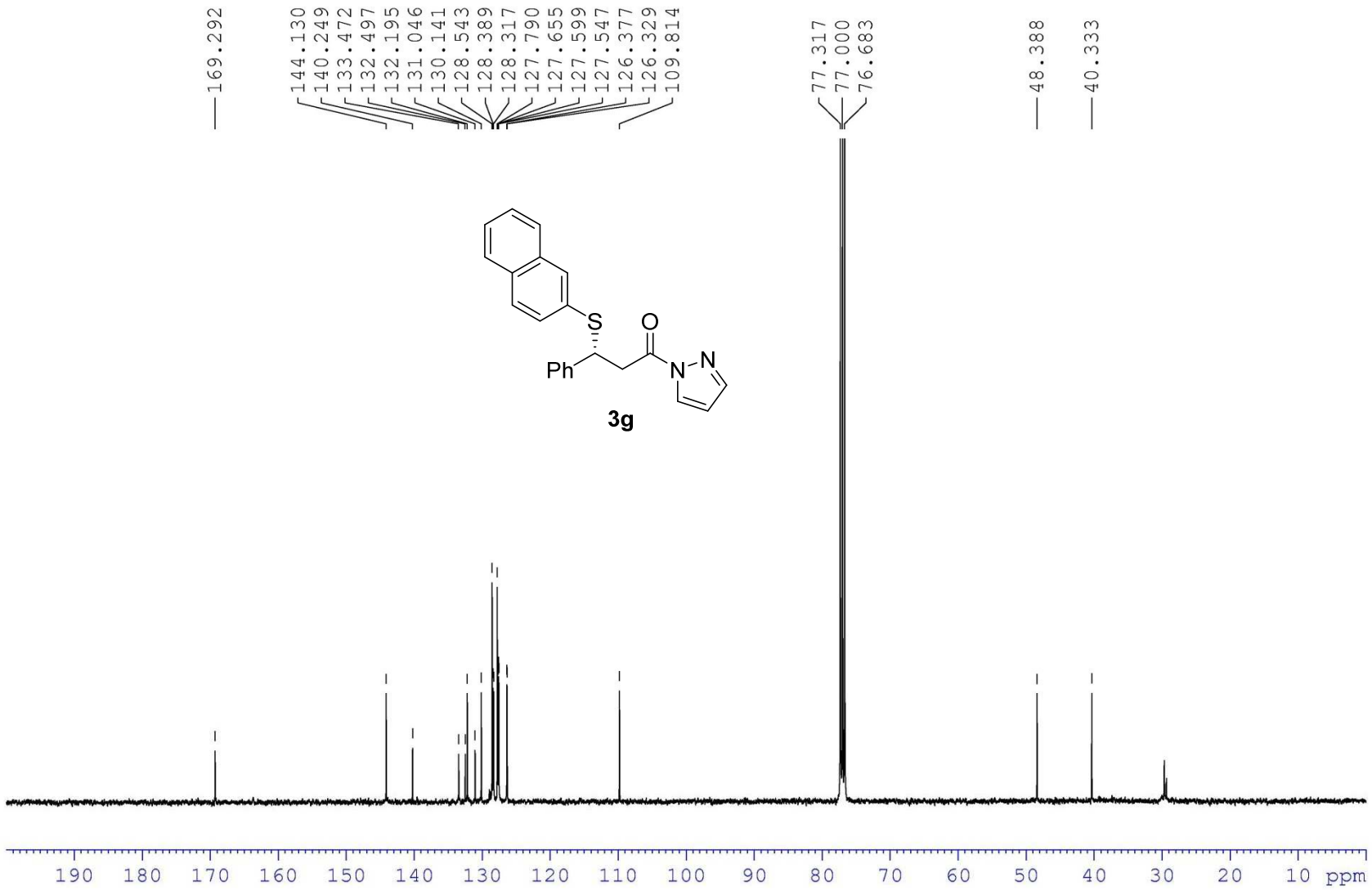
^{13}C NMR in $CDCl_3$ (100 MHz)



^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)



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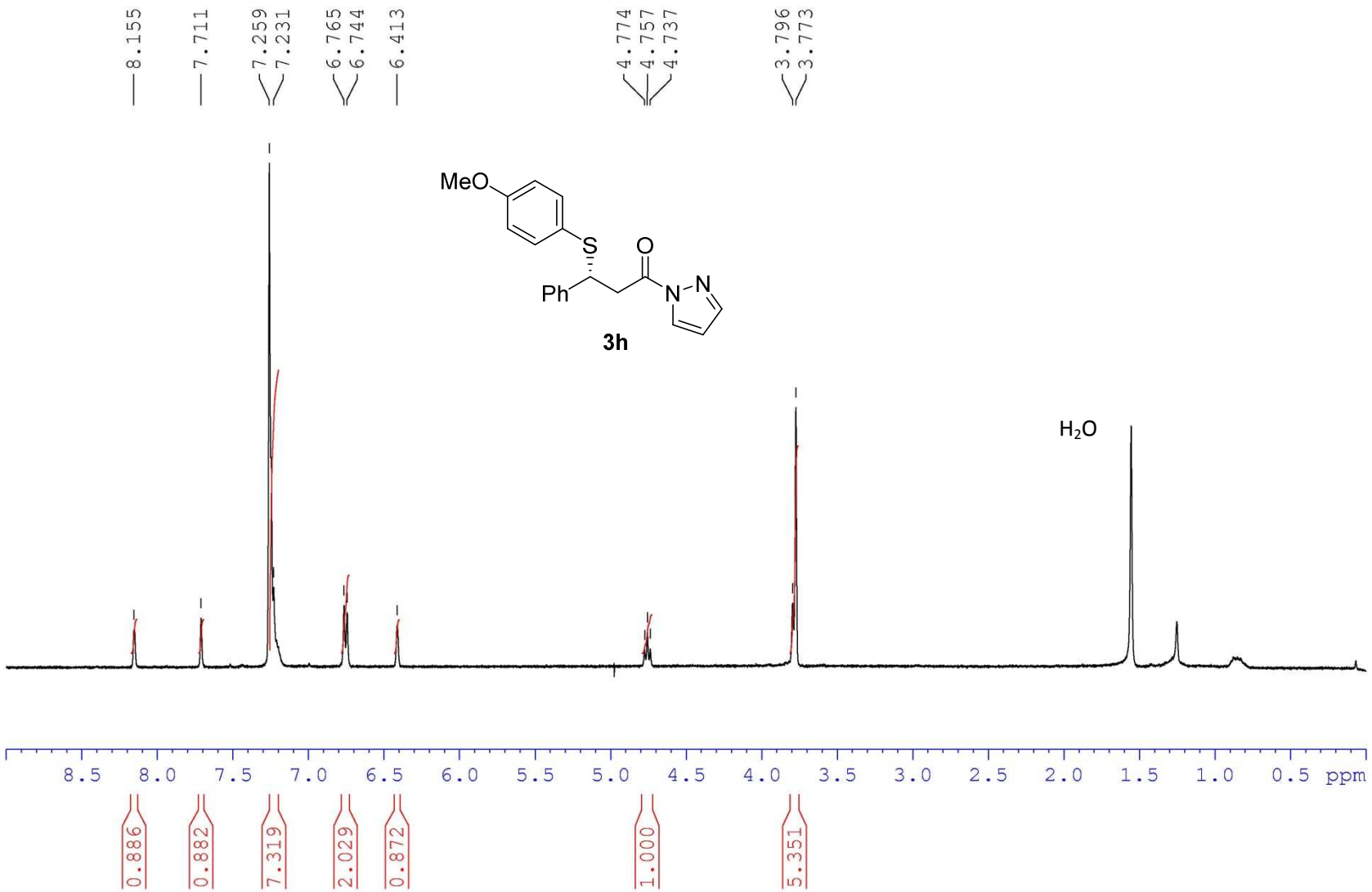
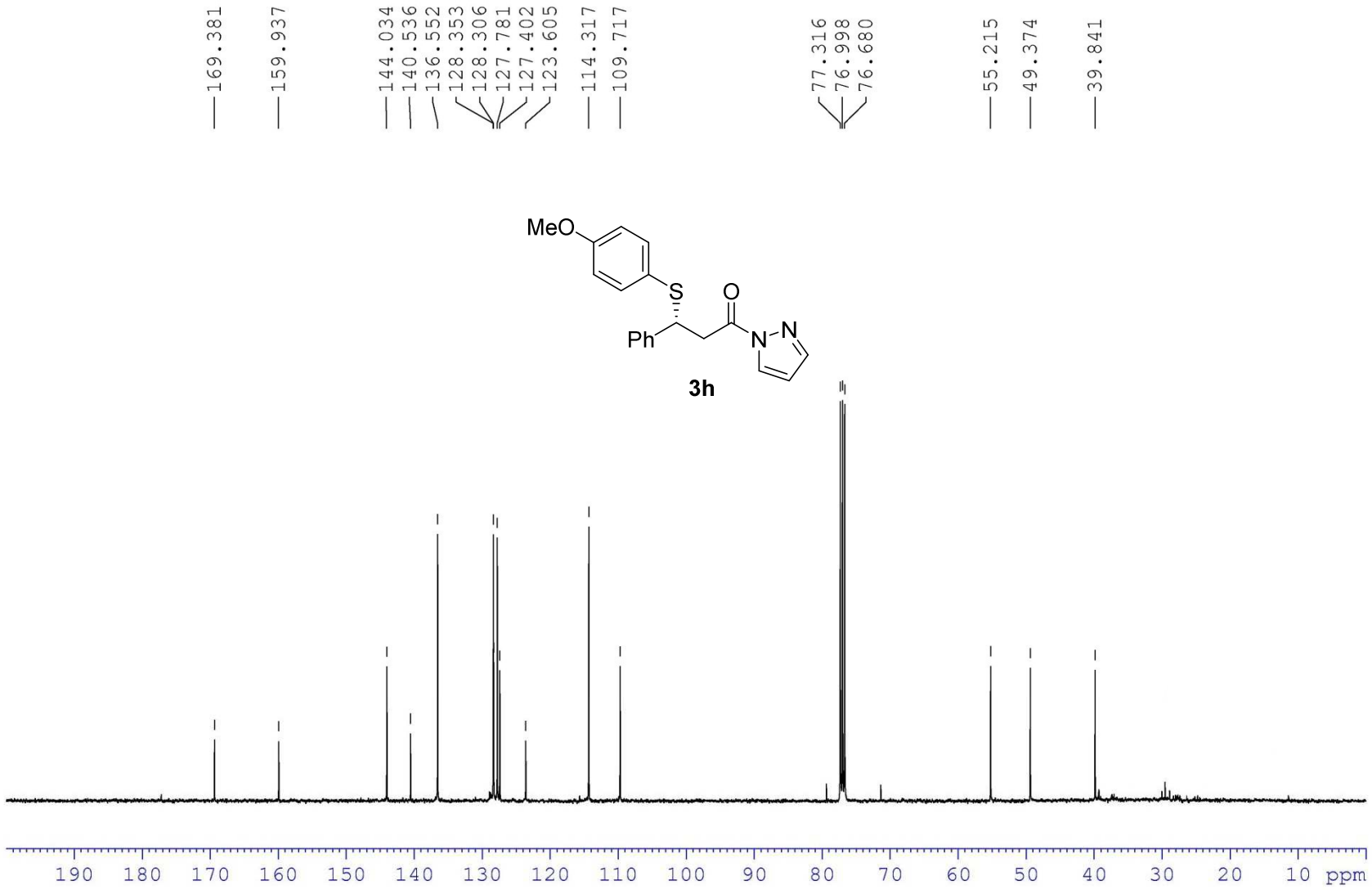
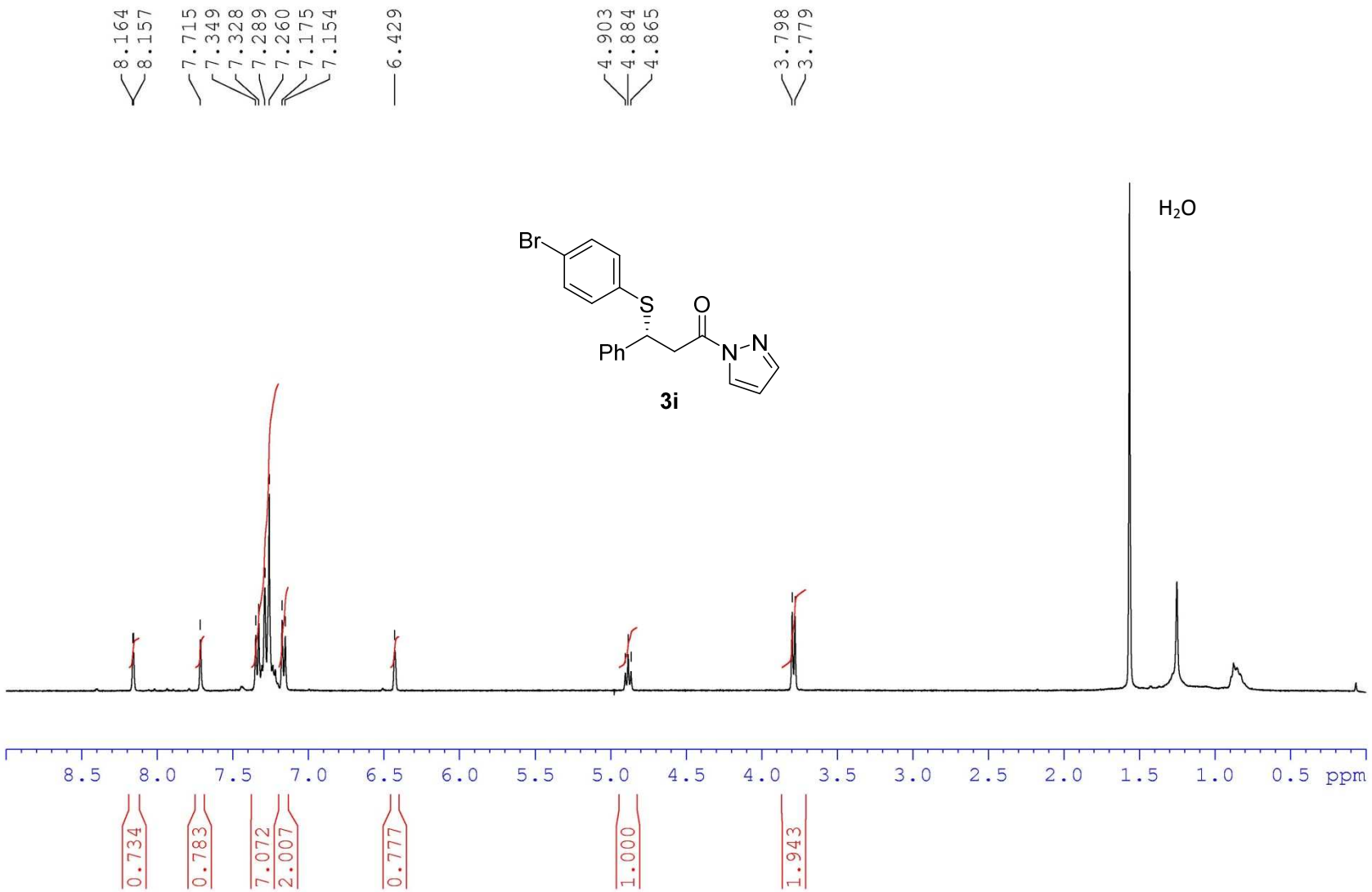


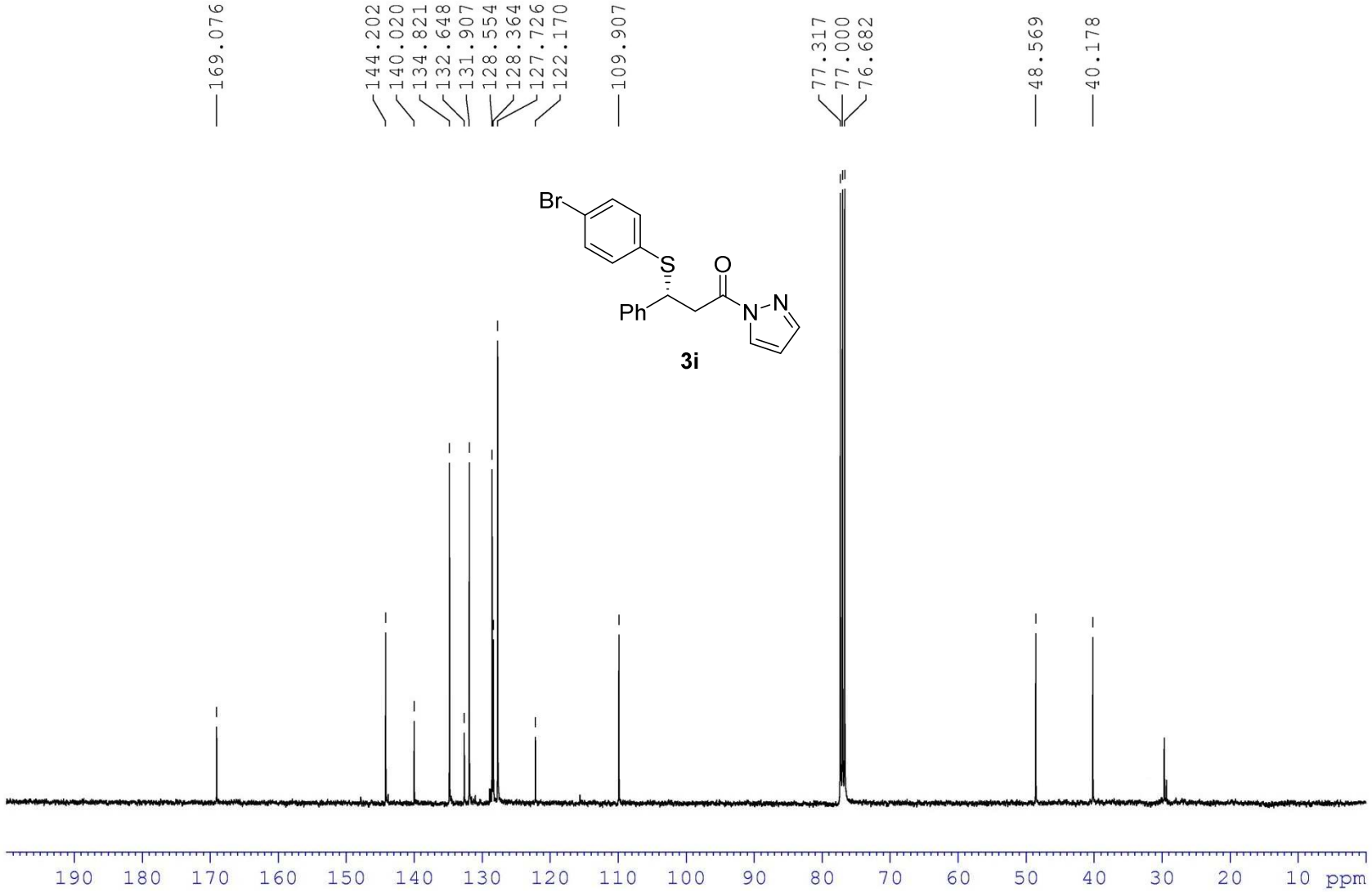
^{13}C NMR in $CDCl_3$ (100 MHz)



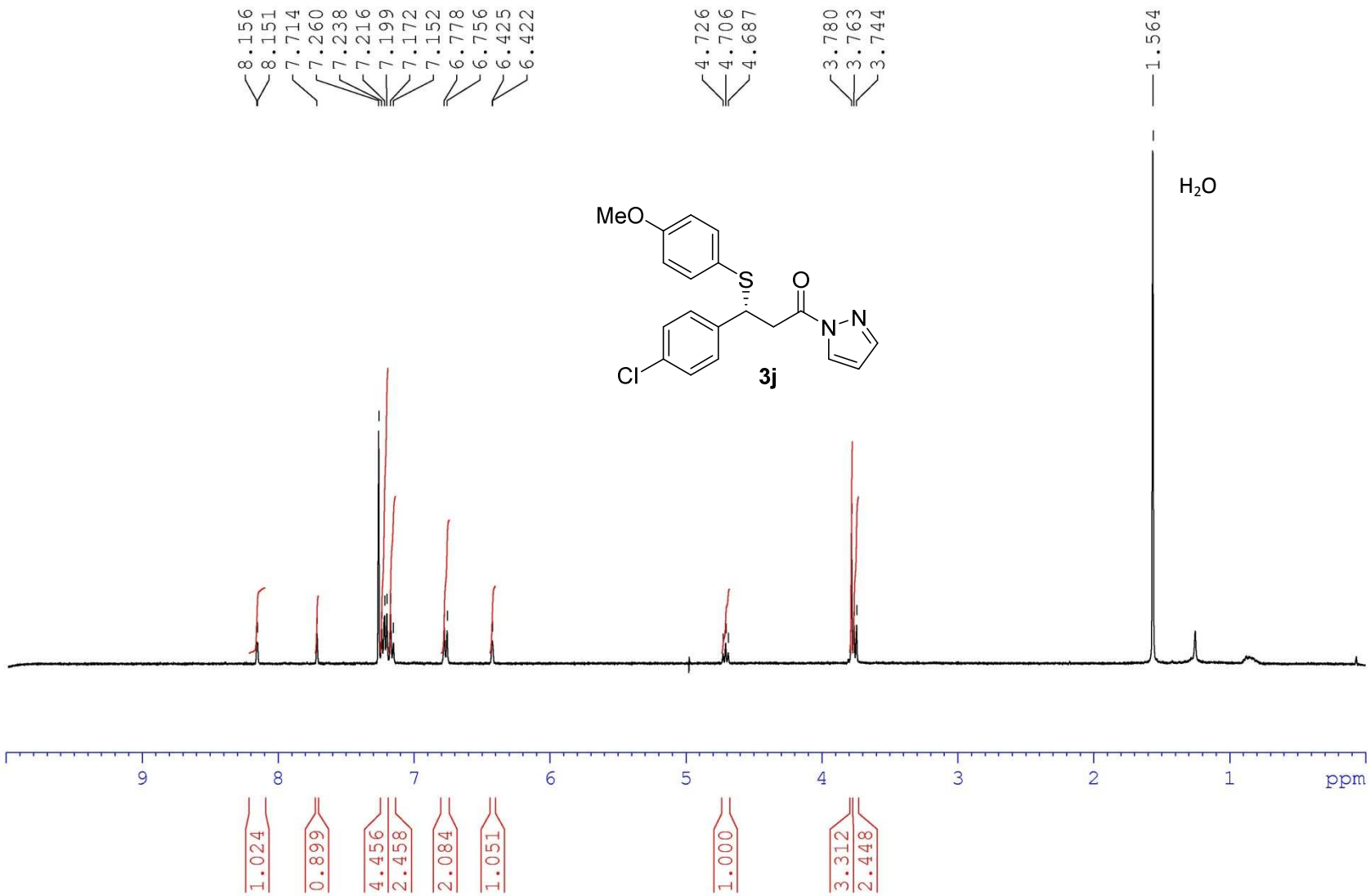
^{1}H NMR in $CDCl_3$ (400 MHz)



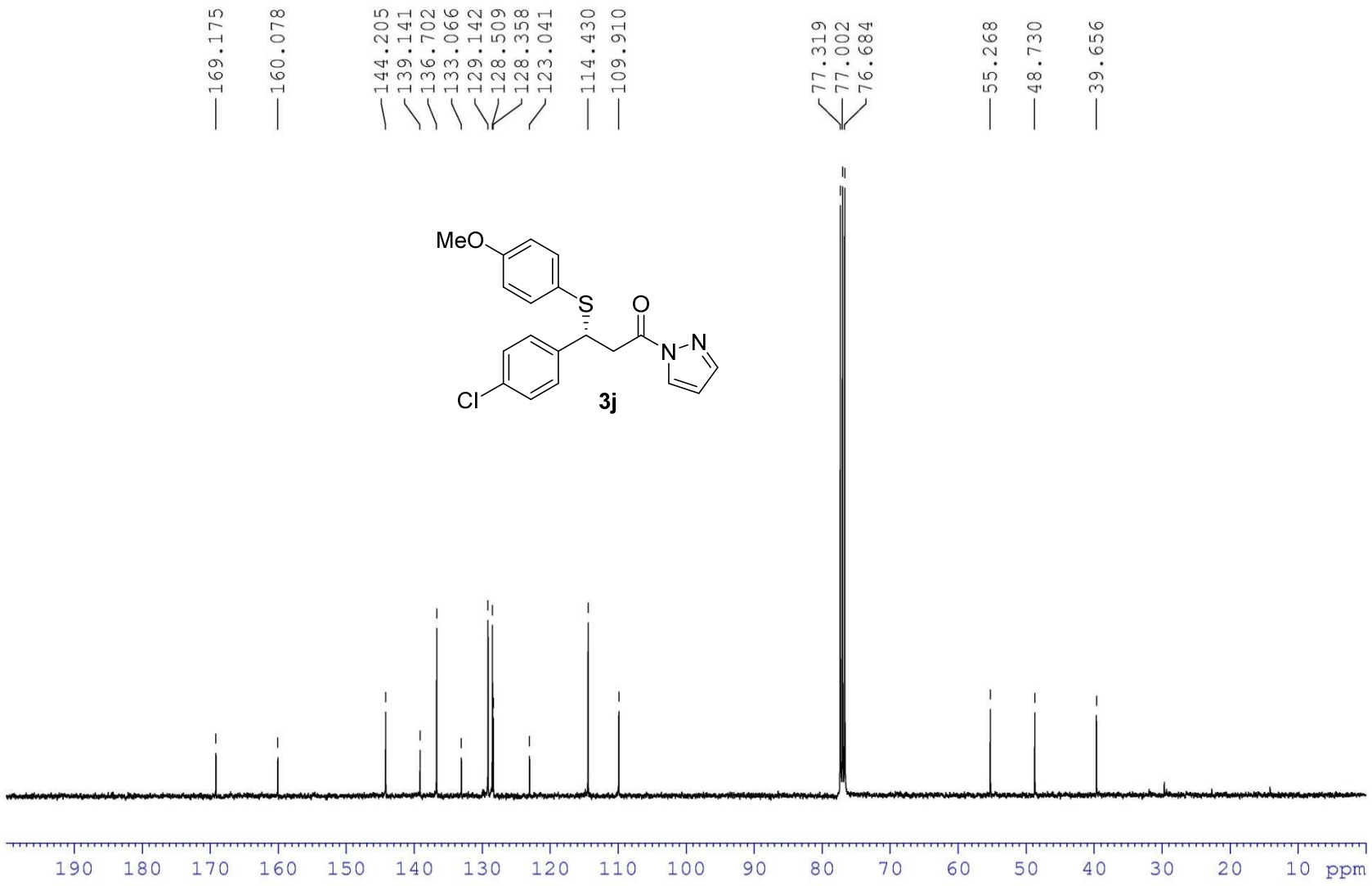
^{13}C NMR in $CDCl_3$ (100 MHz)



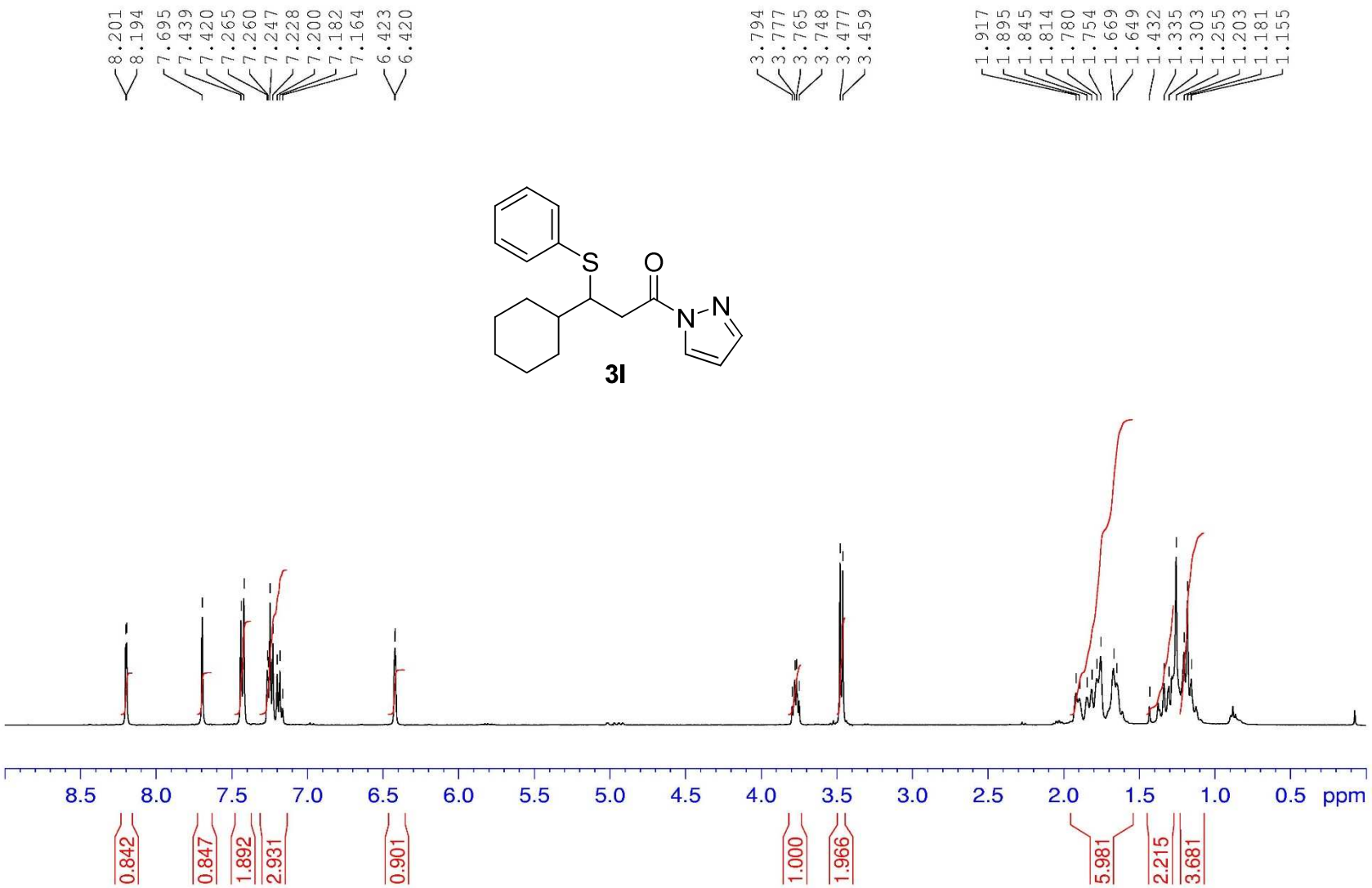
^{1}H NMR in $CDCl_3$ (400 MHz)



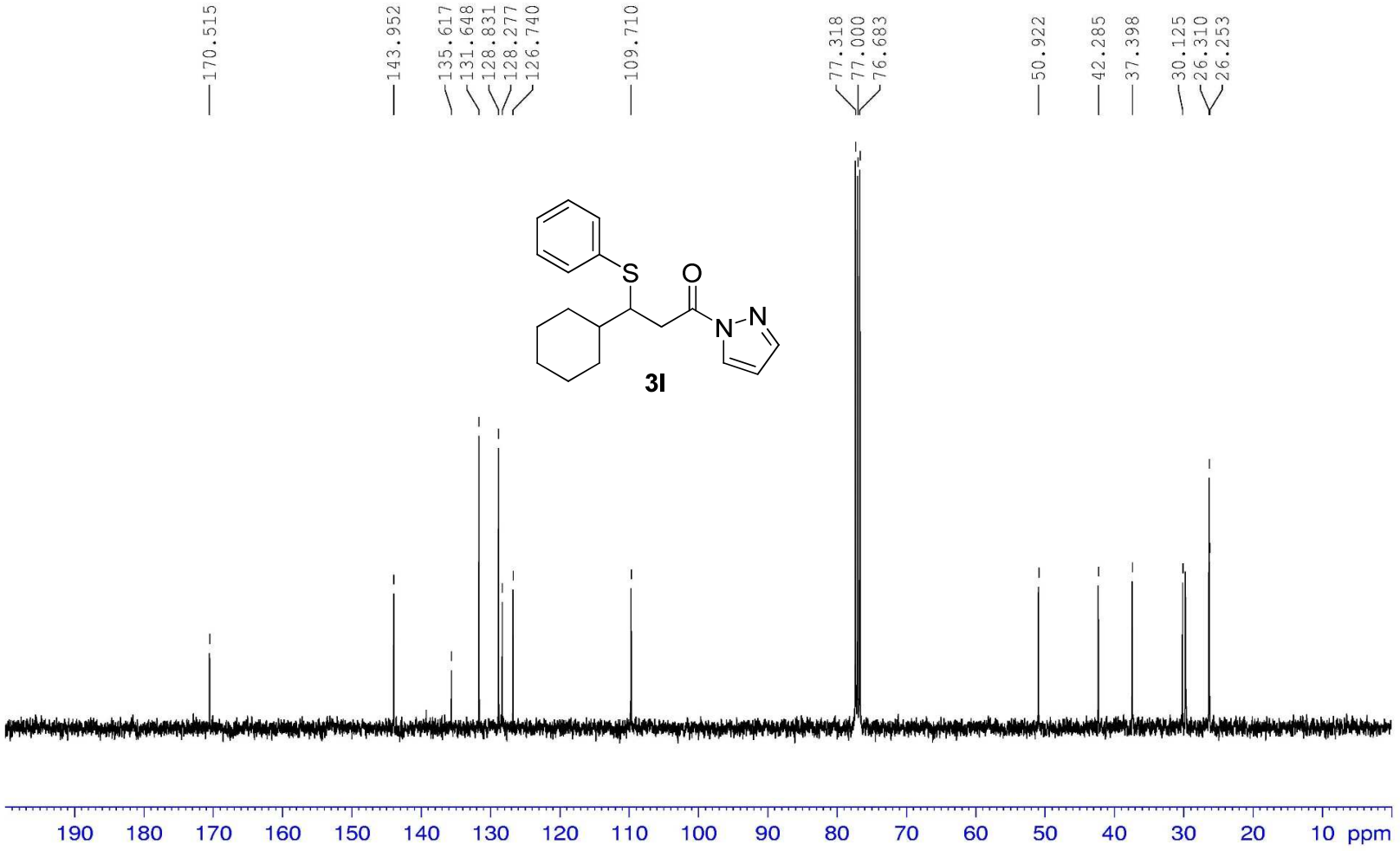
^{13}C NMR in $CDCl_3$ (100 MHz)



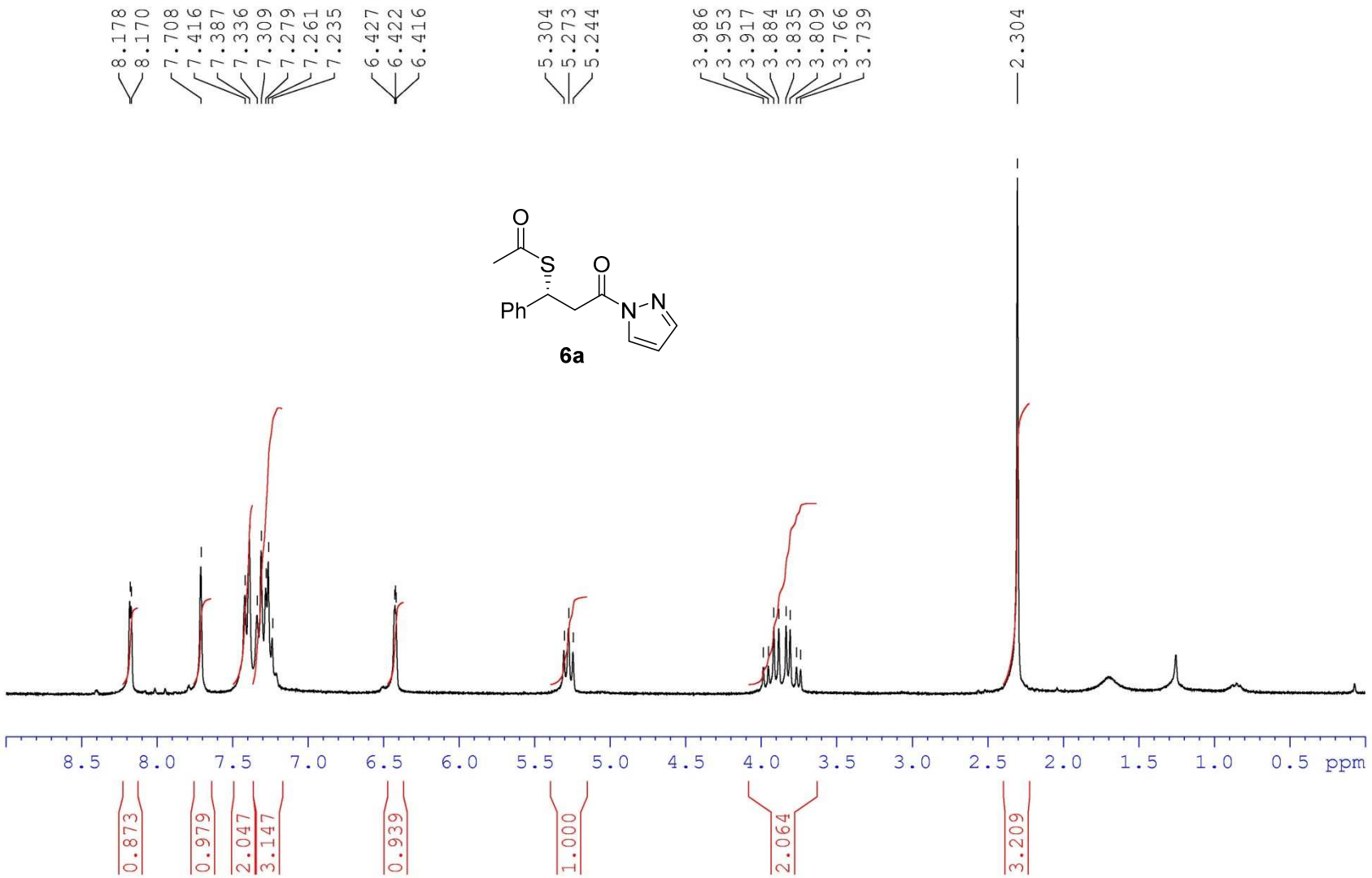
^{1}H NMR in $CDCl_3$ (400 MHz)



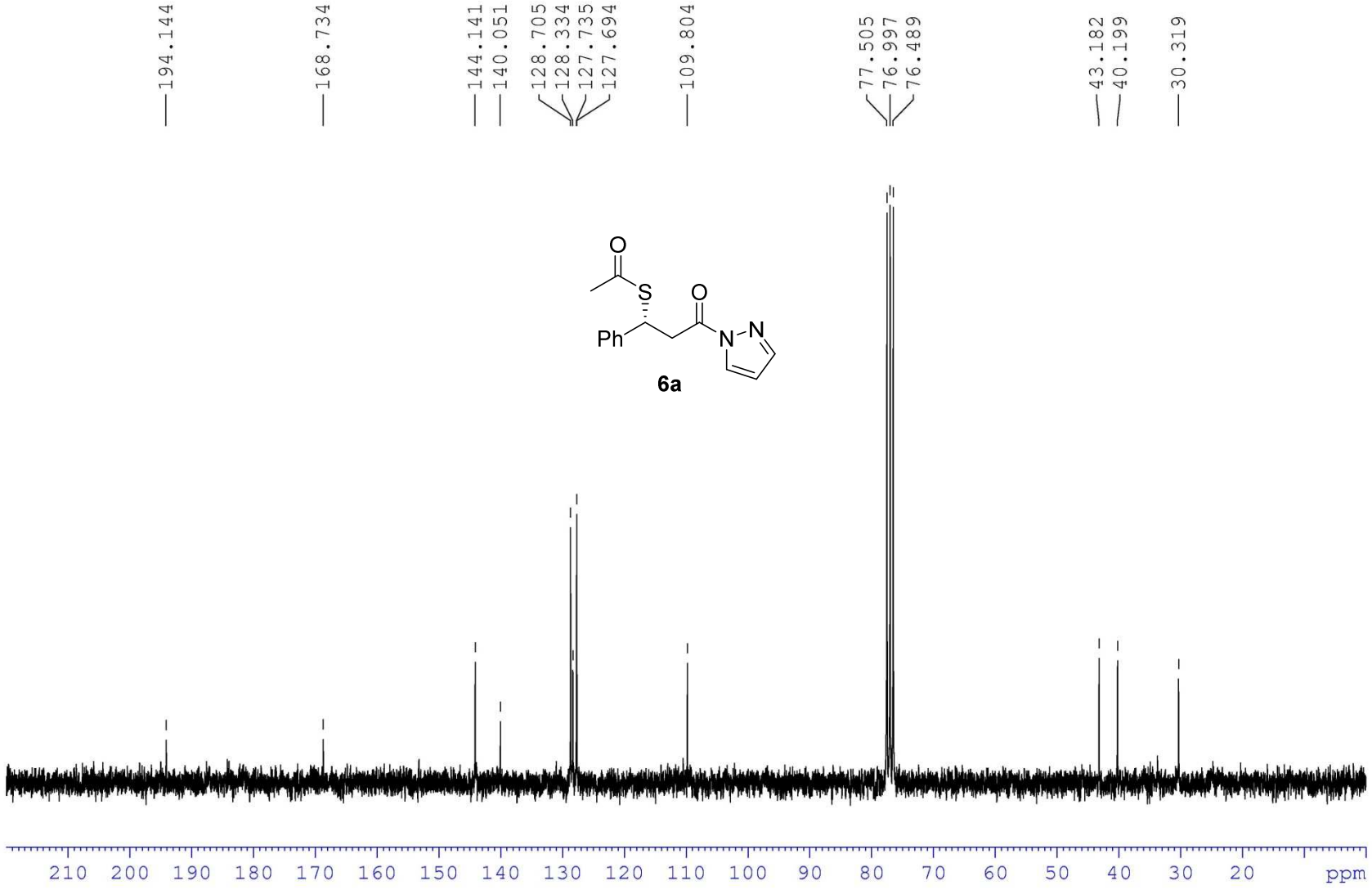
^{13}C NMR in $CDCl_3$ (100 MHz)



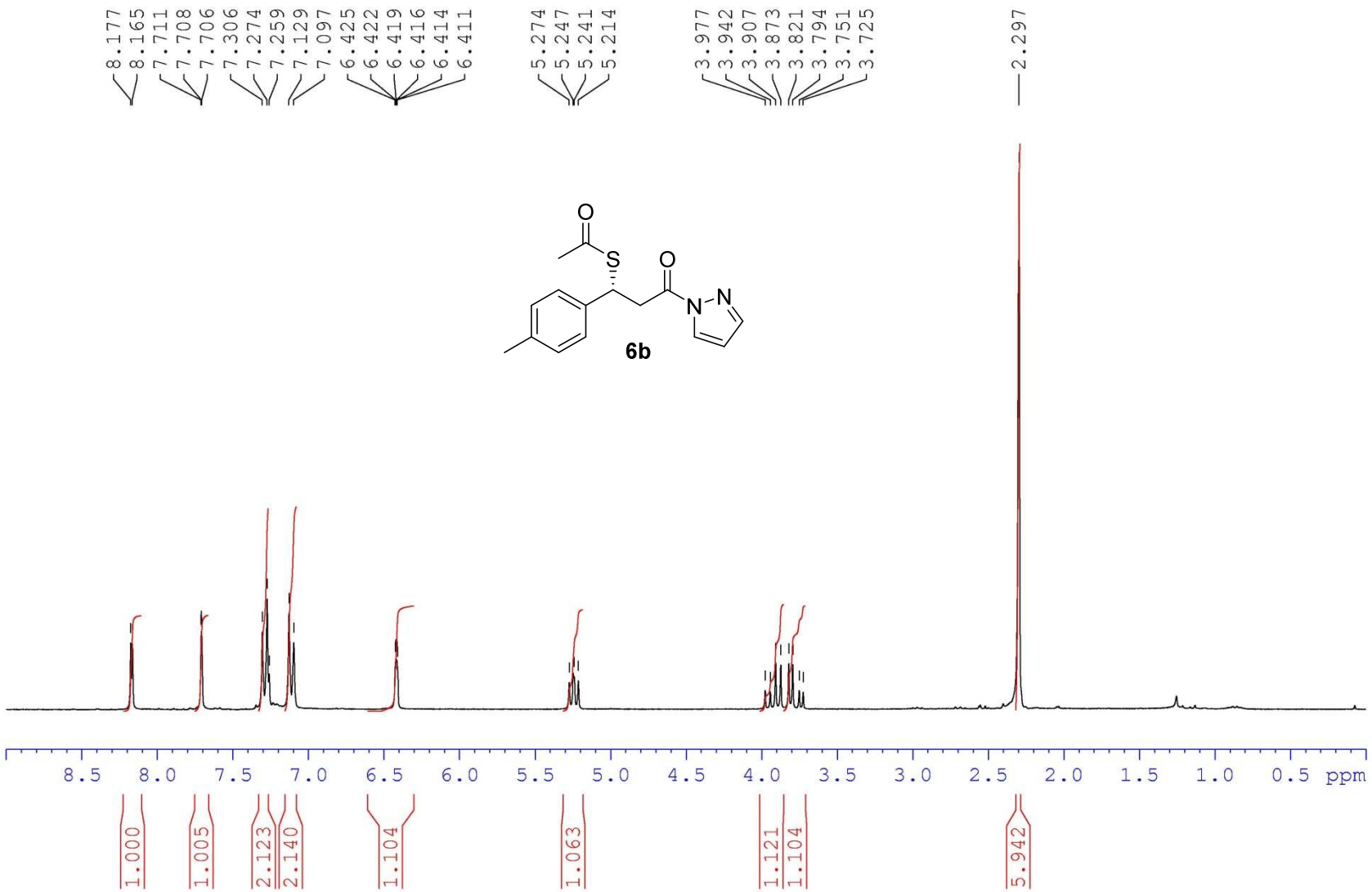
^{1}H NMR in $CDCl_3$ (250 MHz)



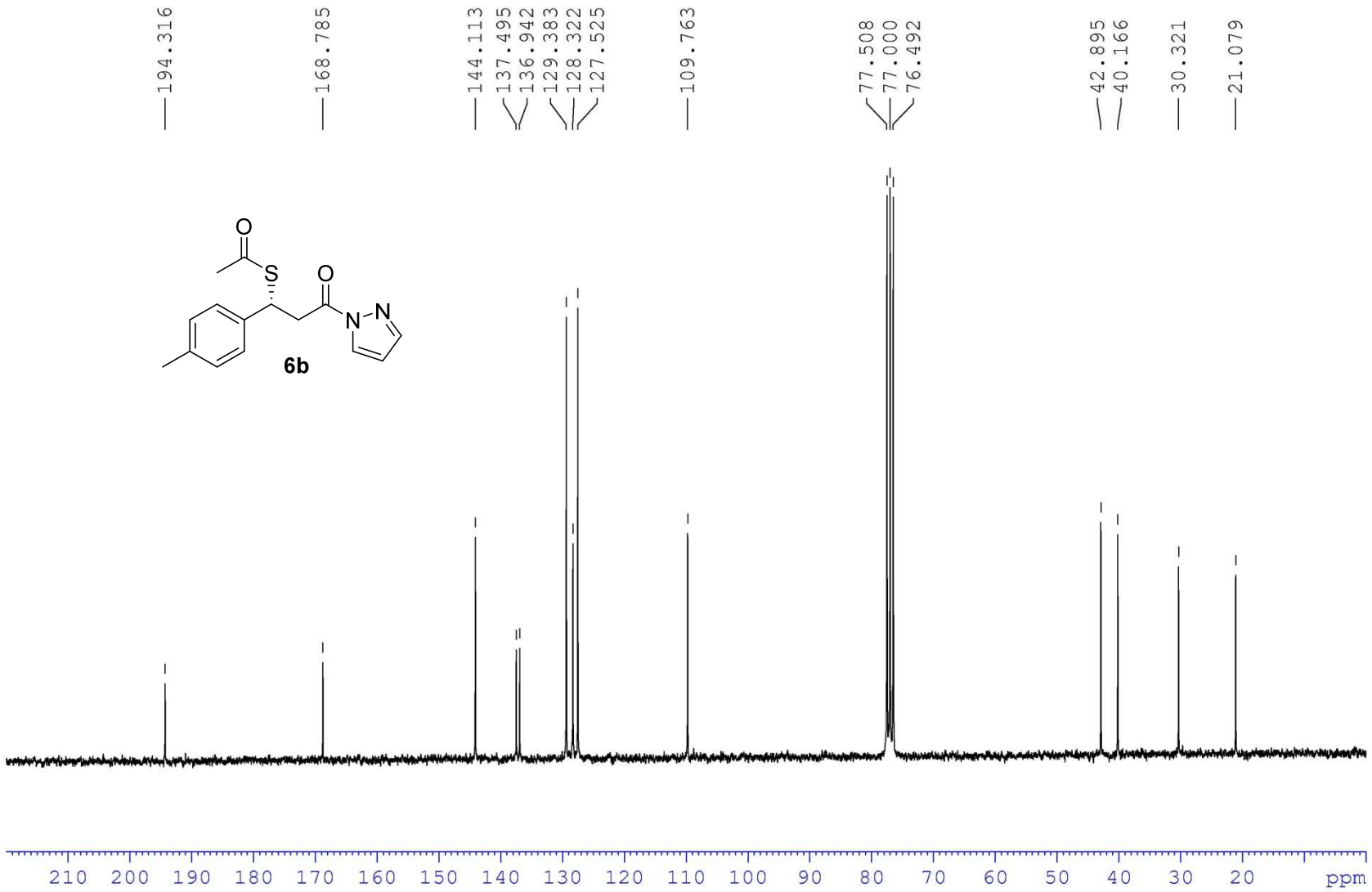
^{13}C NMR in $CDCl_3$ (62.5 MHz)



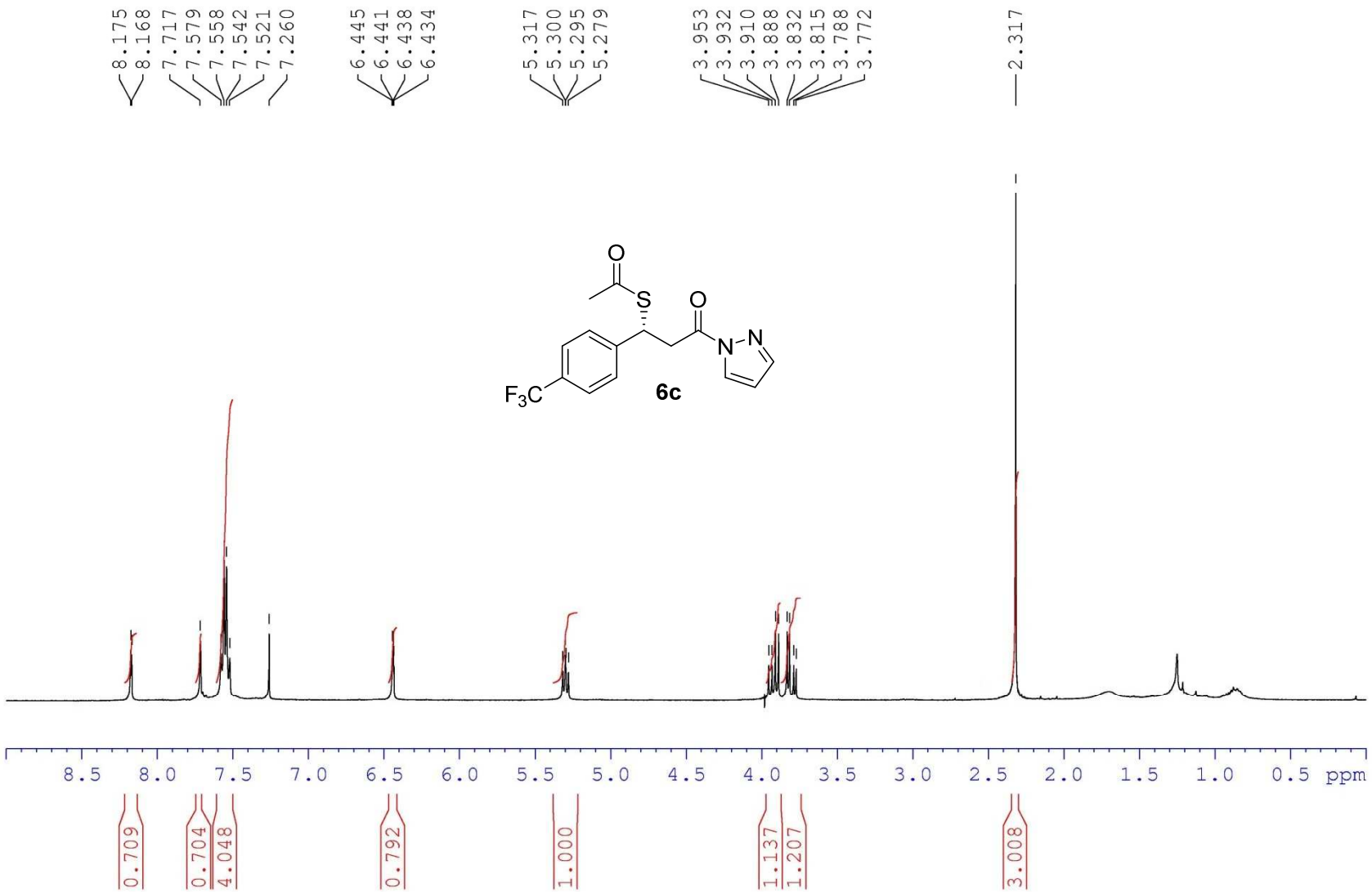
^{1}H NMR in $CDCl_3$ (250 MHz)



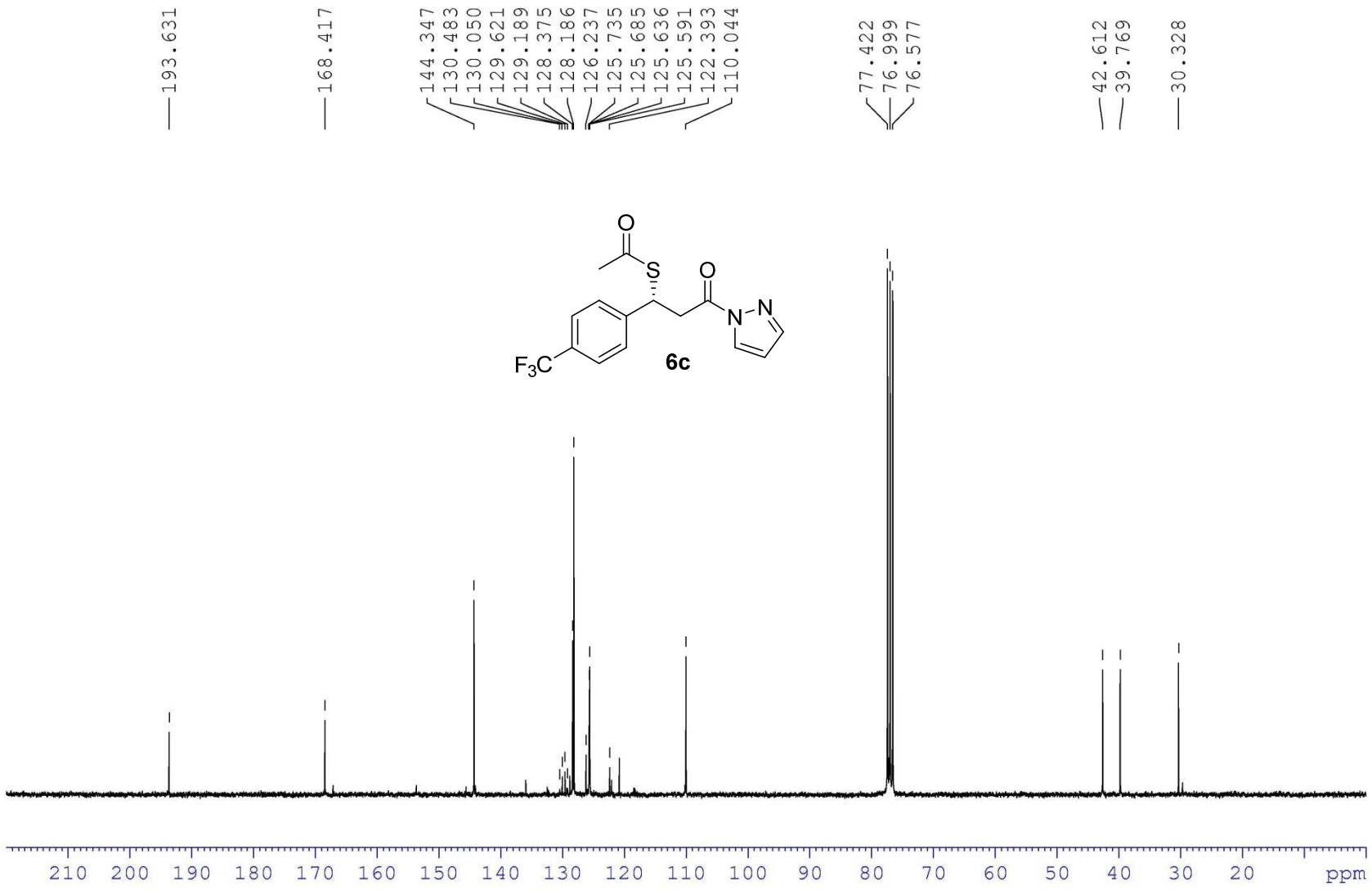
^{13}C NMR in $CDCl_3$ (62.5 MHz)



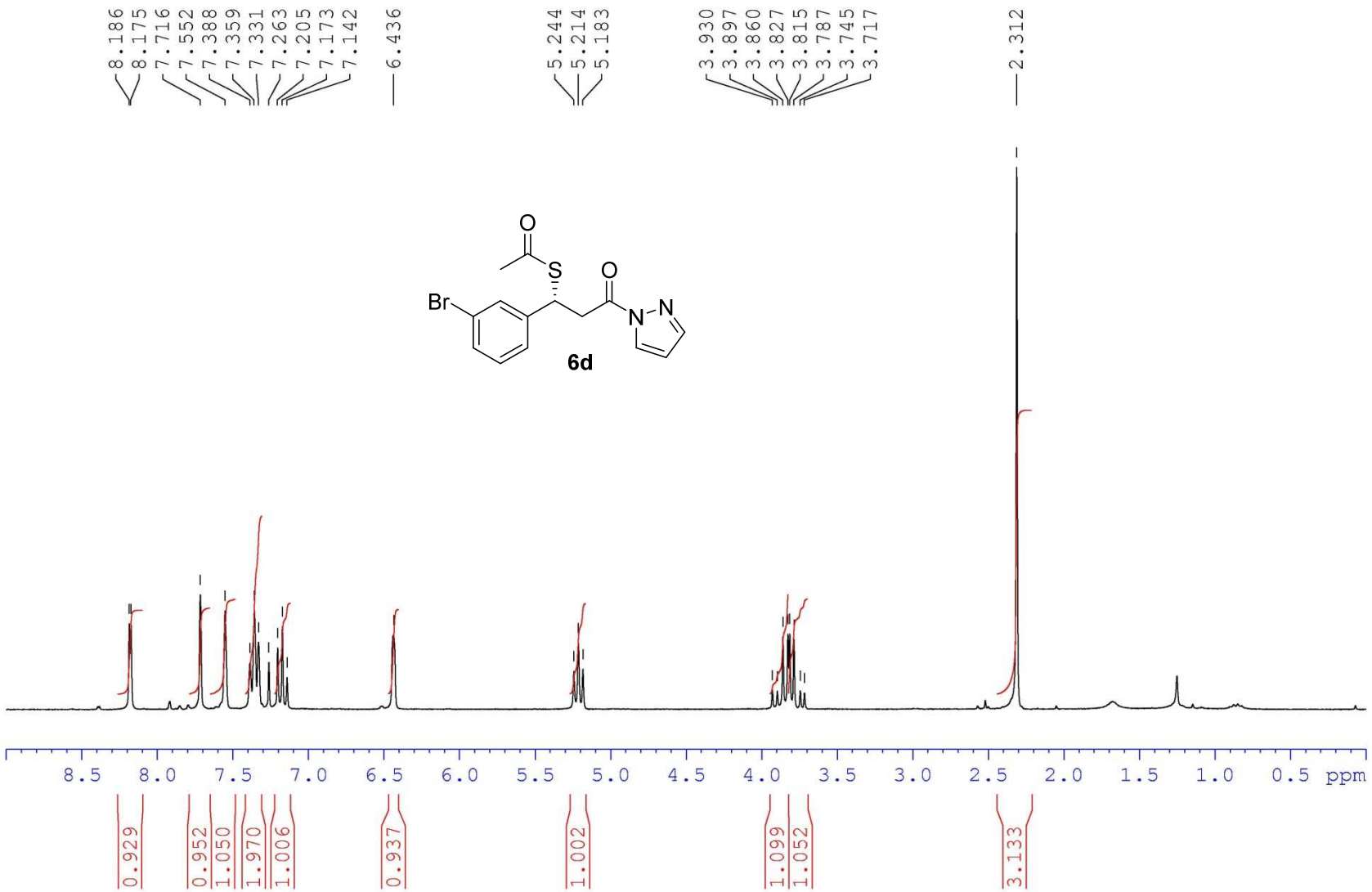
^{1}H NMR in $CDCl_3$ (400 MHz)



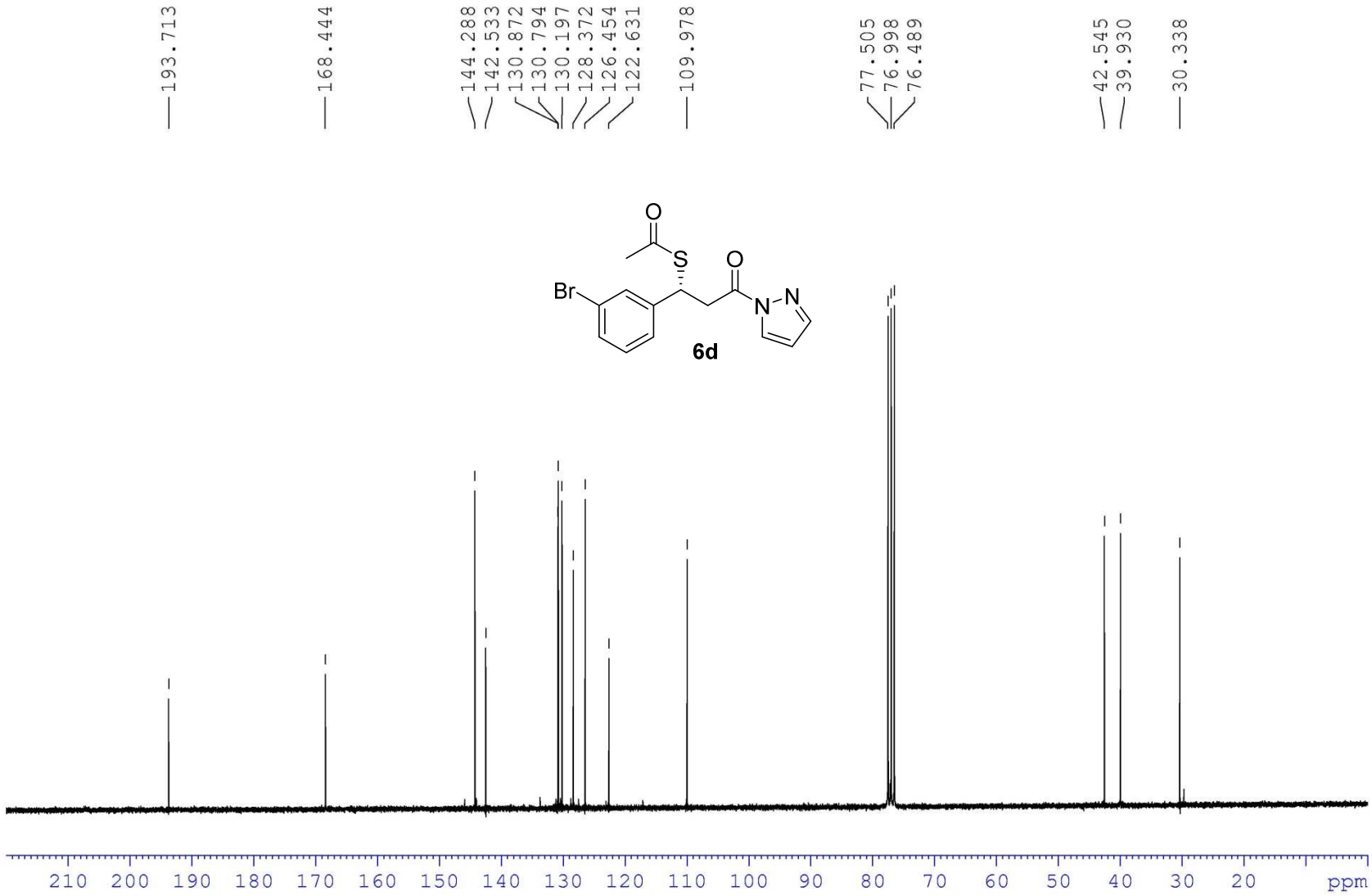
^{13}C NMR in $CDCl_3$ (75 MHz)



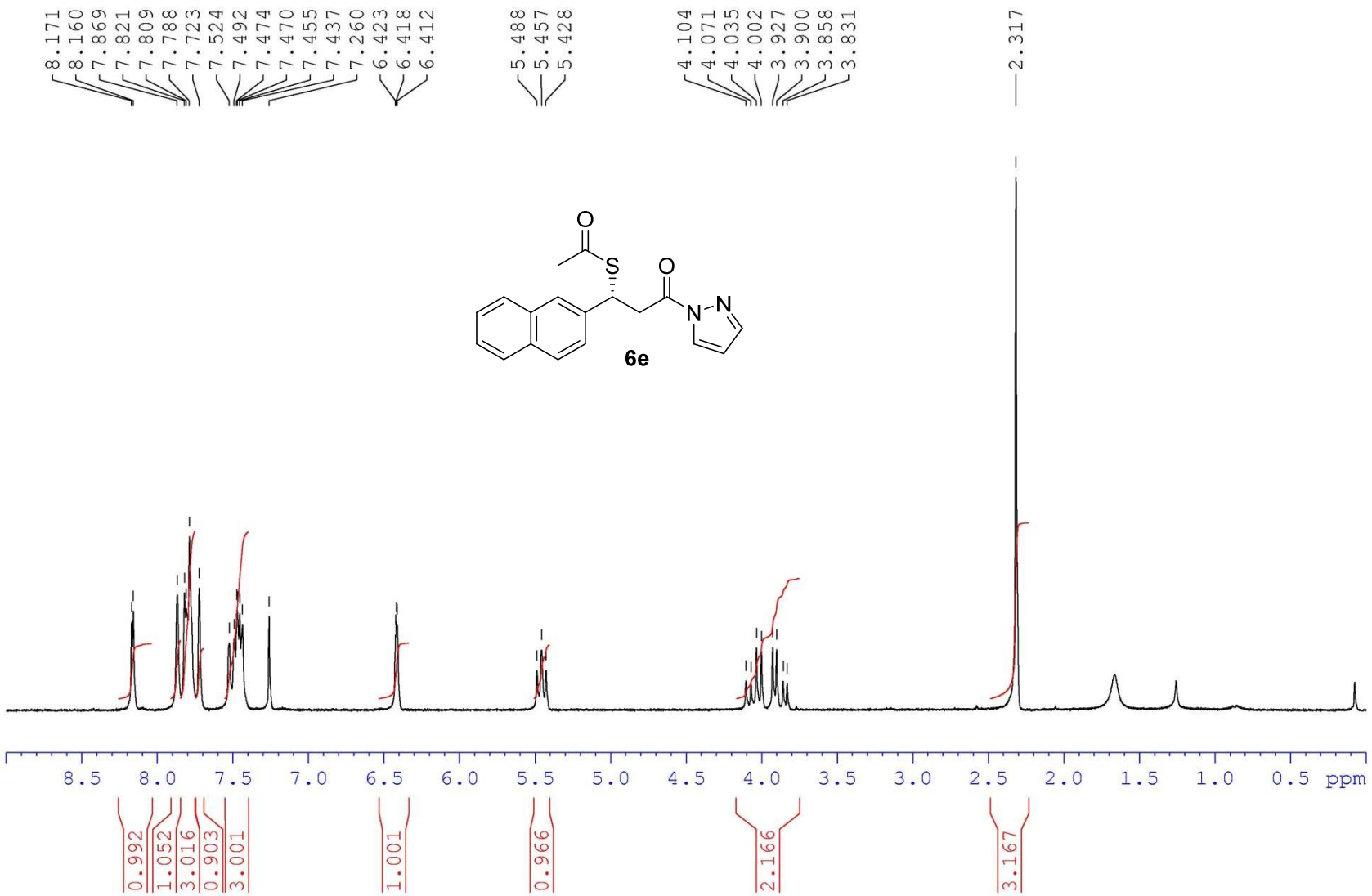
^{1}H NMR in $CDCl_3$ (250 MHz)



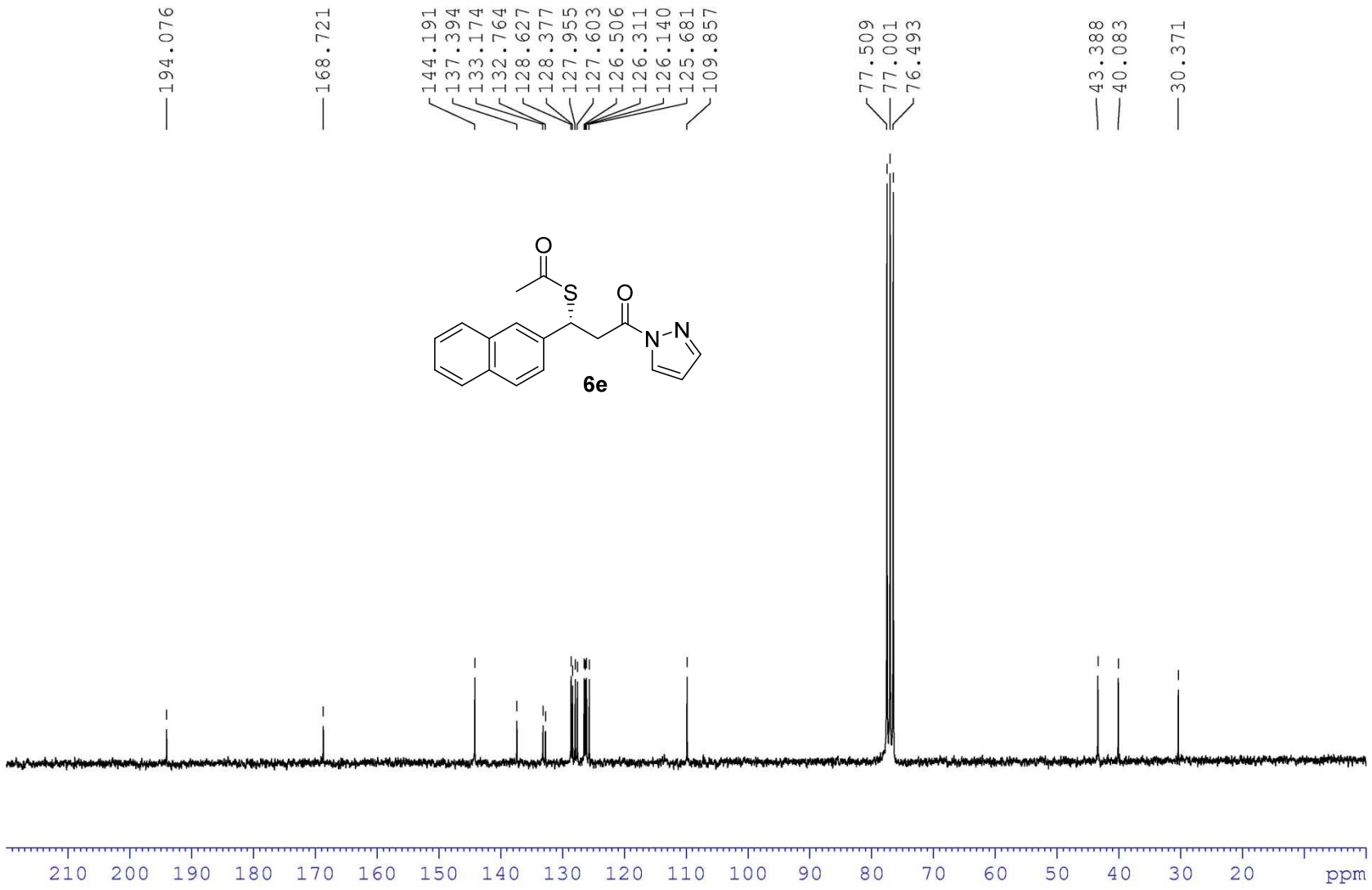
^{13}C NMR in $CDCl_3$ (62.5 MHz)



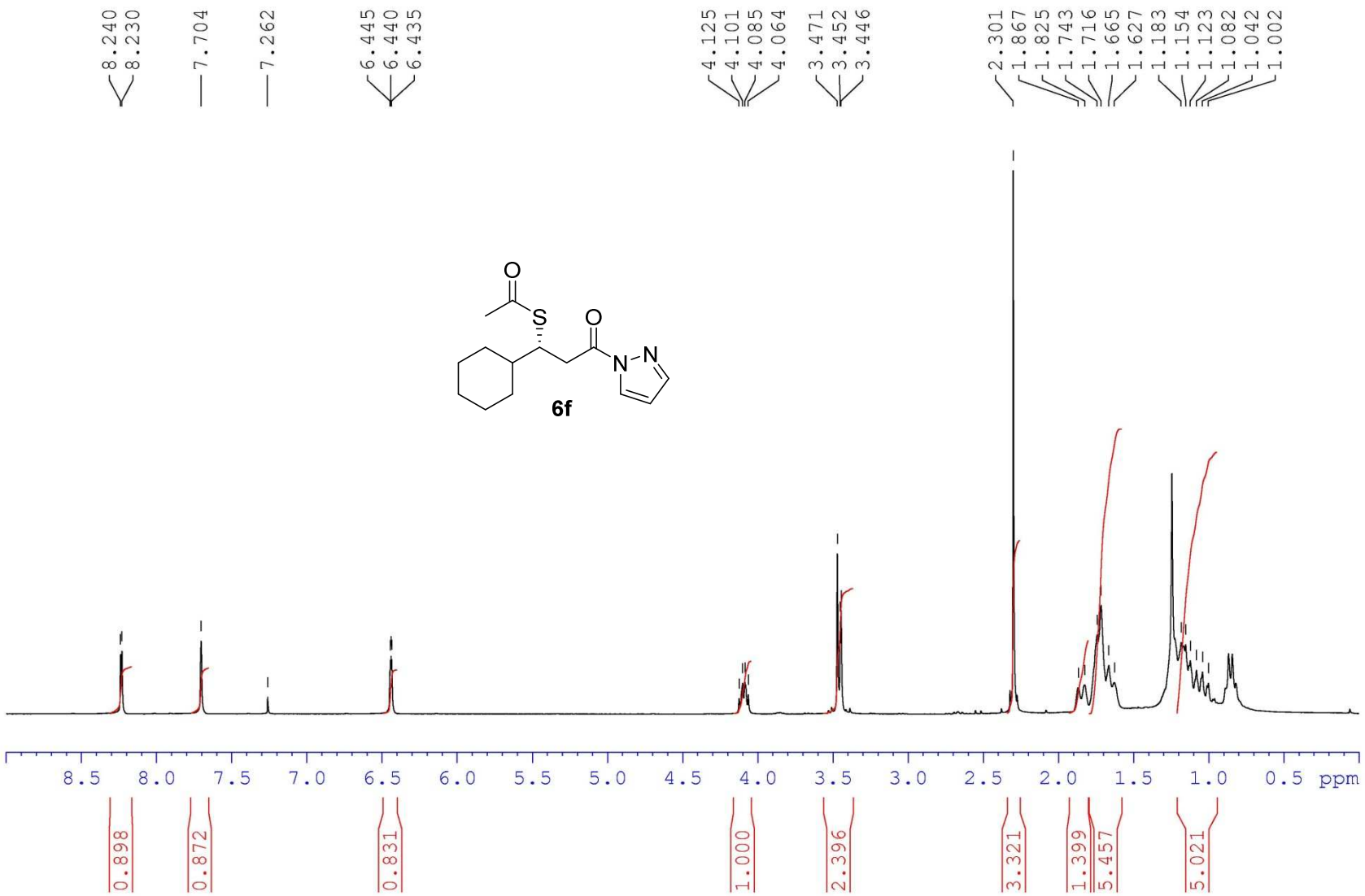
^{1}H NMR in $CDCl_3$ (250 MHz)



^{13}C NMR in $CDCl_3$ (62.5 MHz)

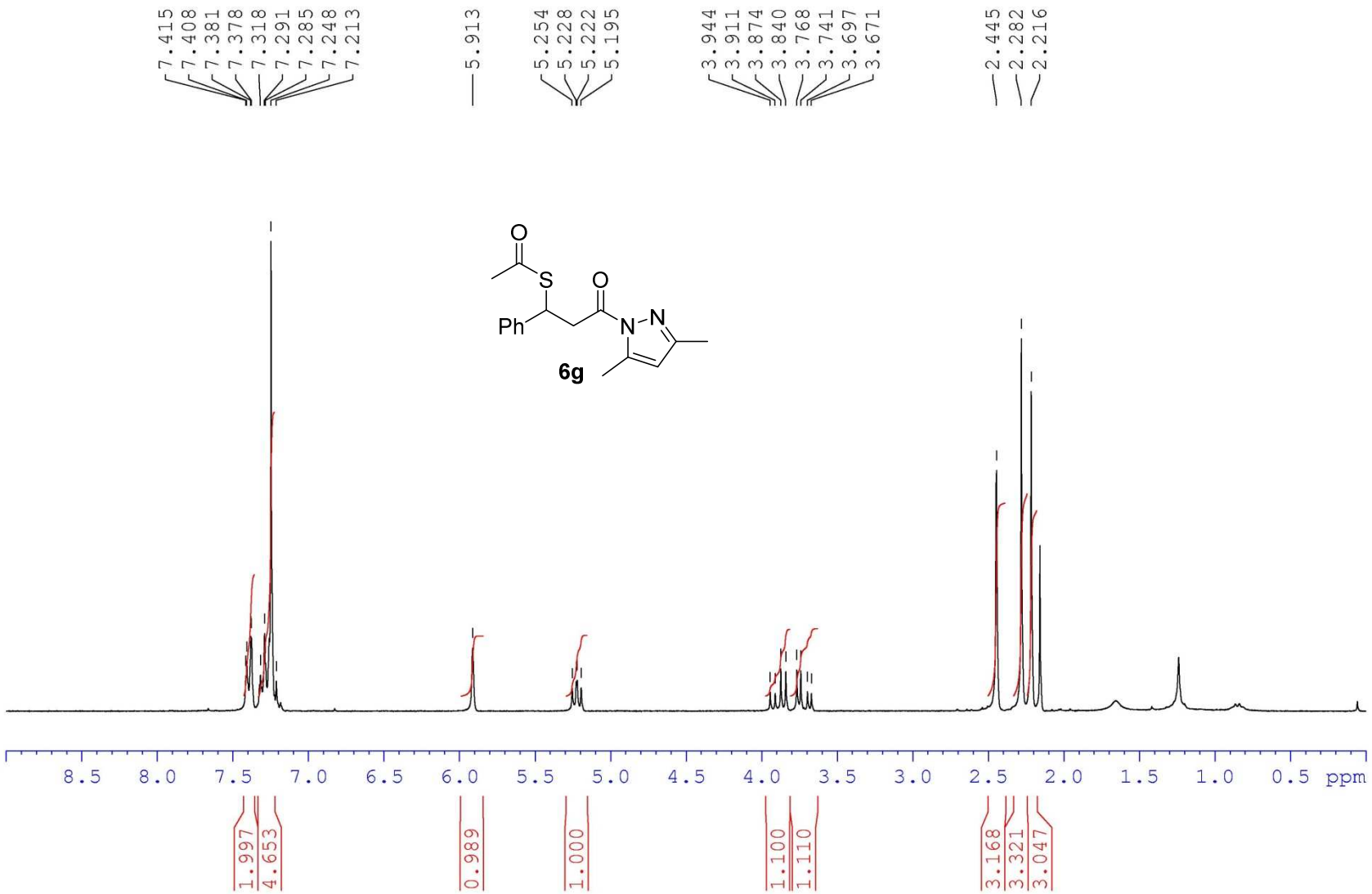


^{1}H NMR in $CDCl_3$ (300 MHz)

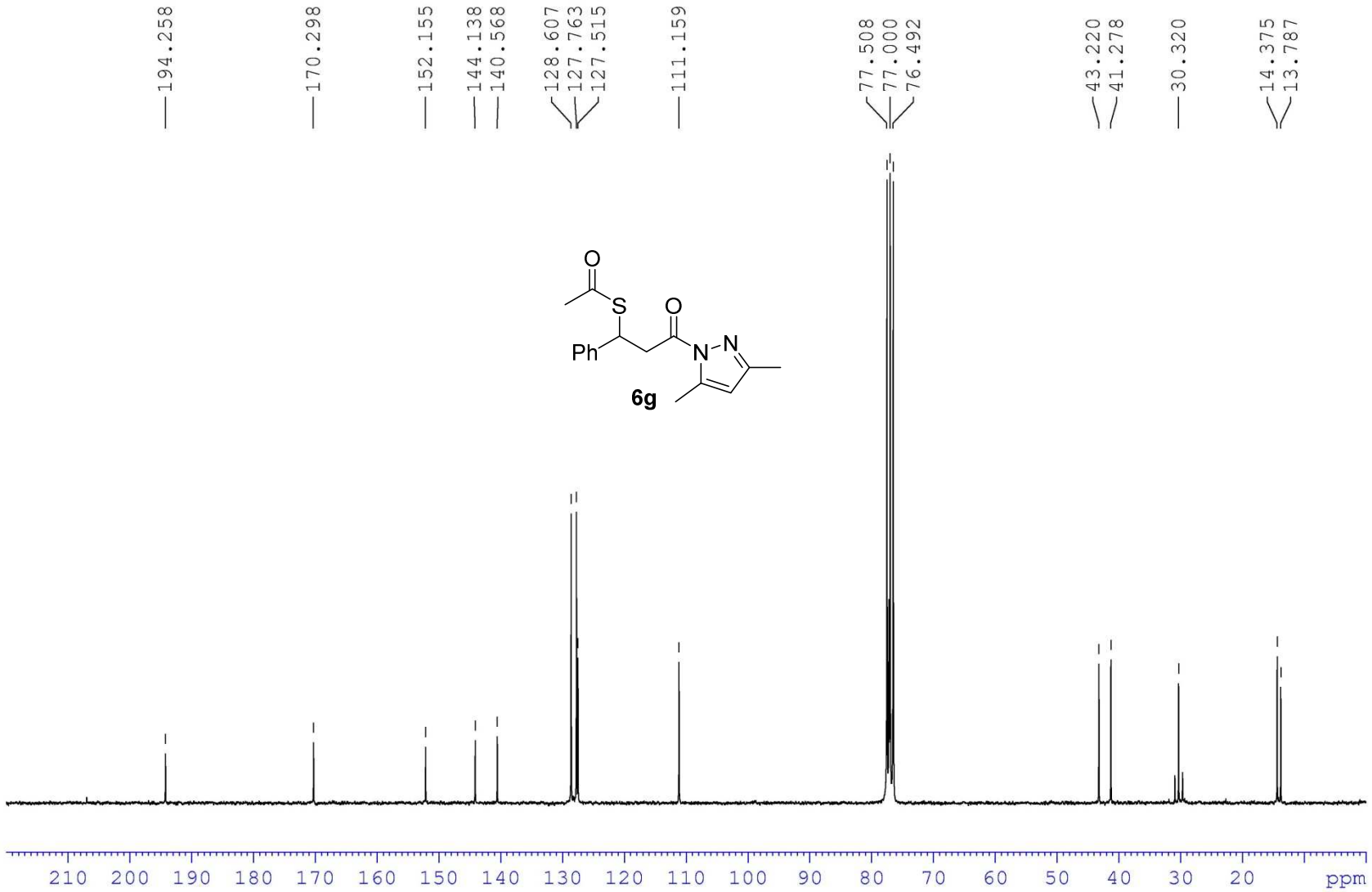


^{13}C NMR in $CDCl_3$ (75 MHz)

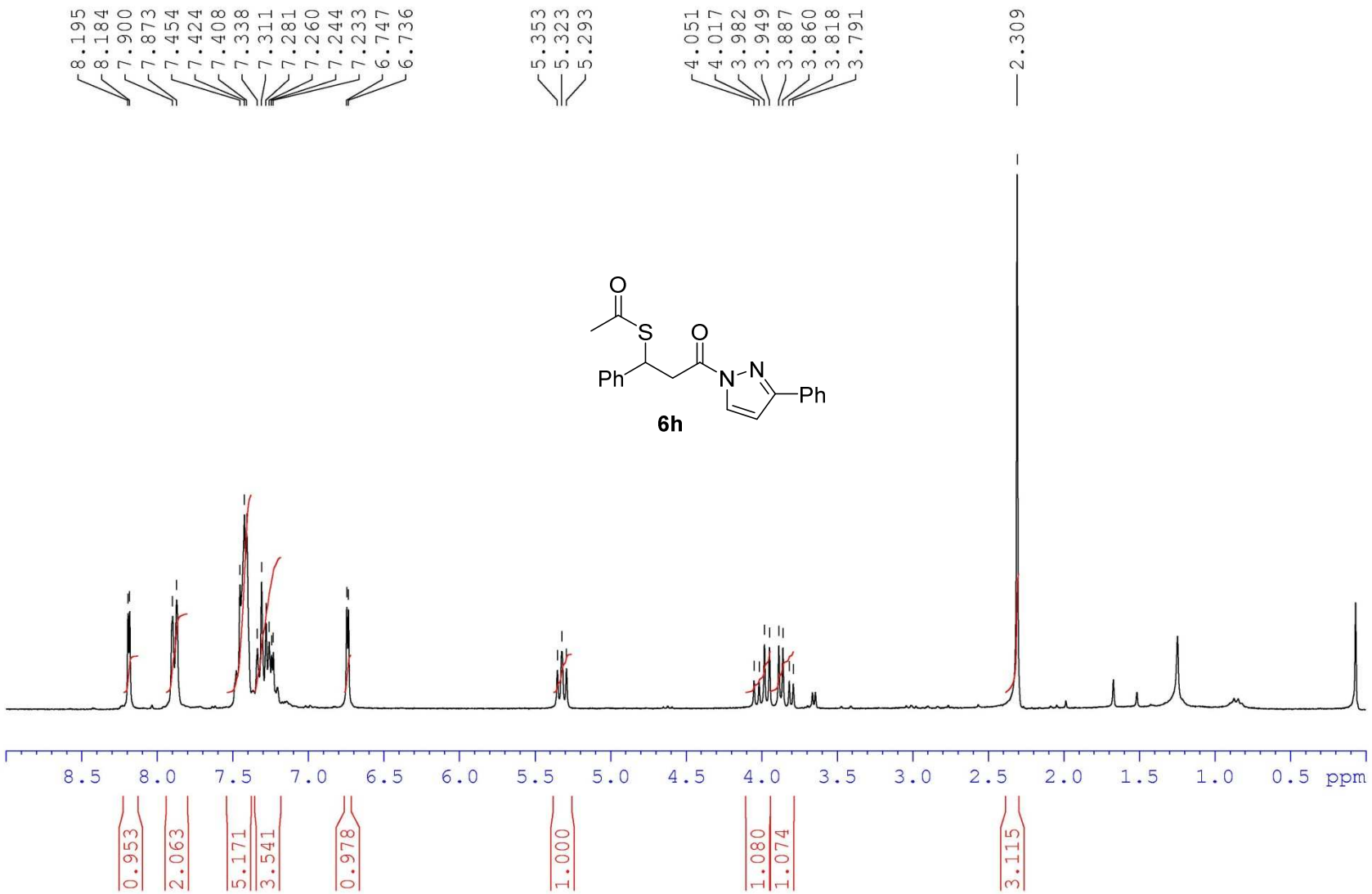
^{1}H NMR in $CDCl_3$ (250 MHz)



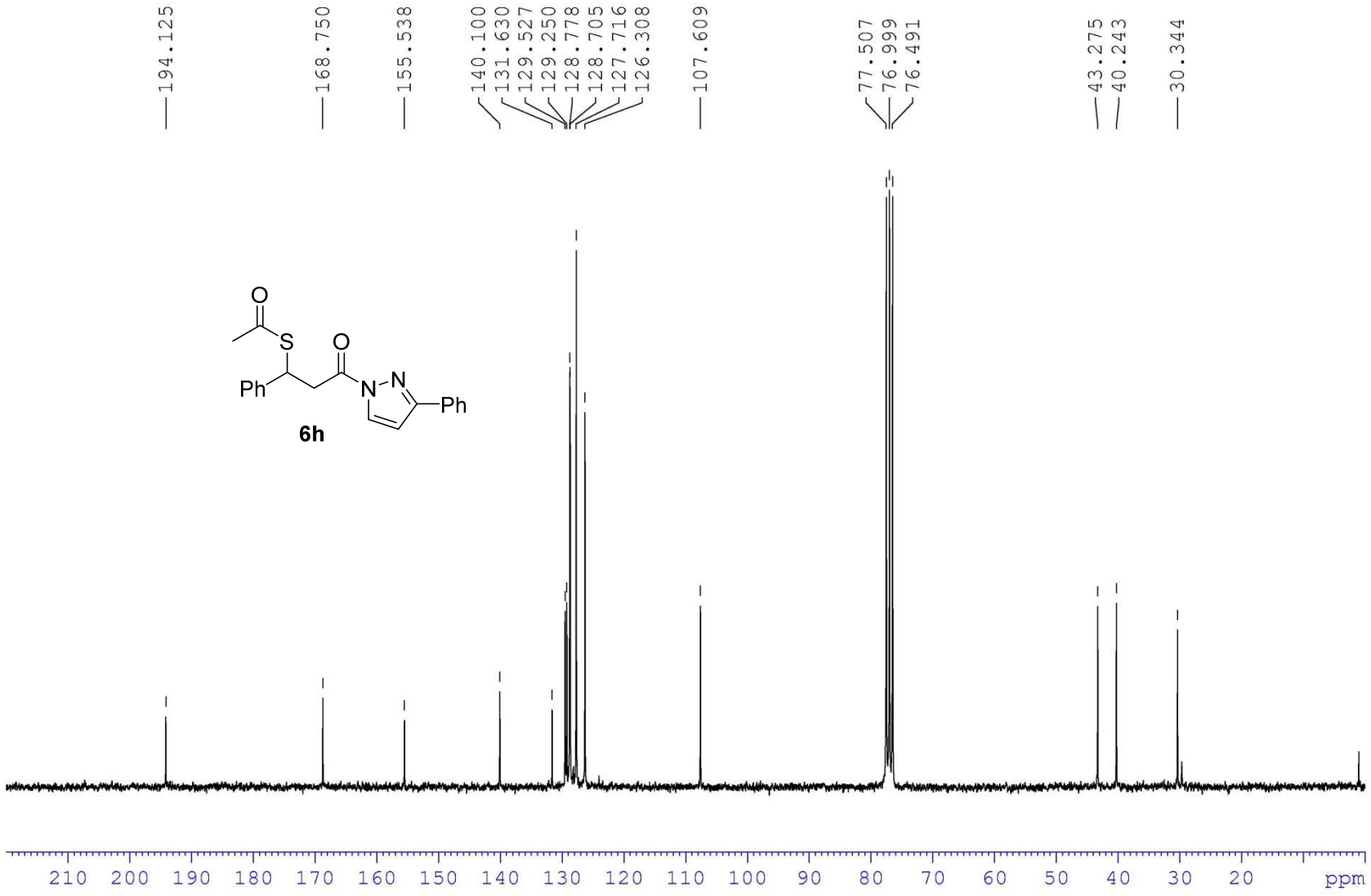
^{13}C NMR in $CDCl_3$ (62.5 MHz)



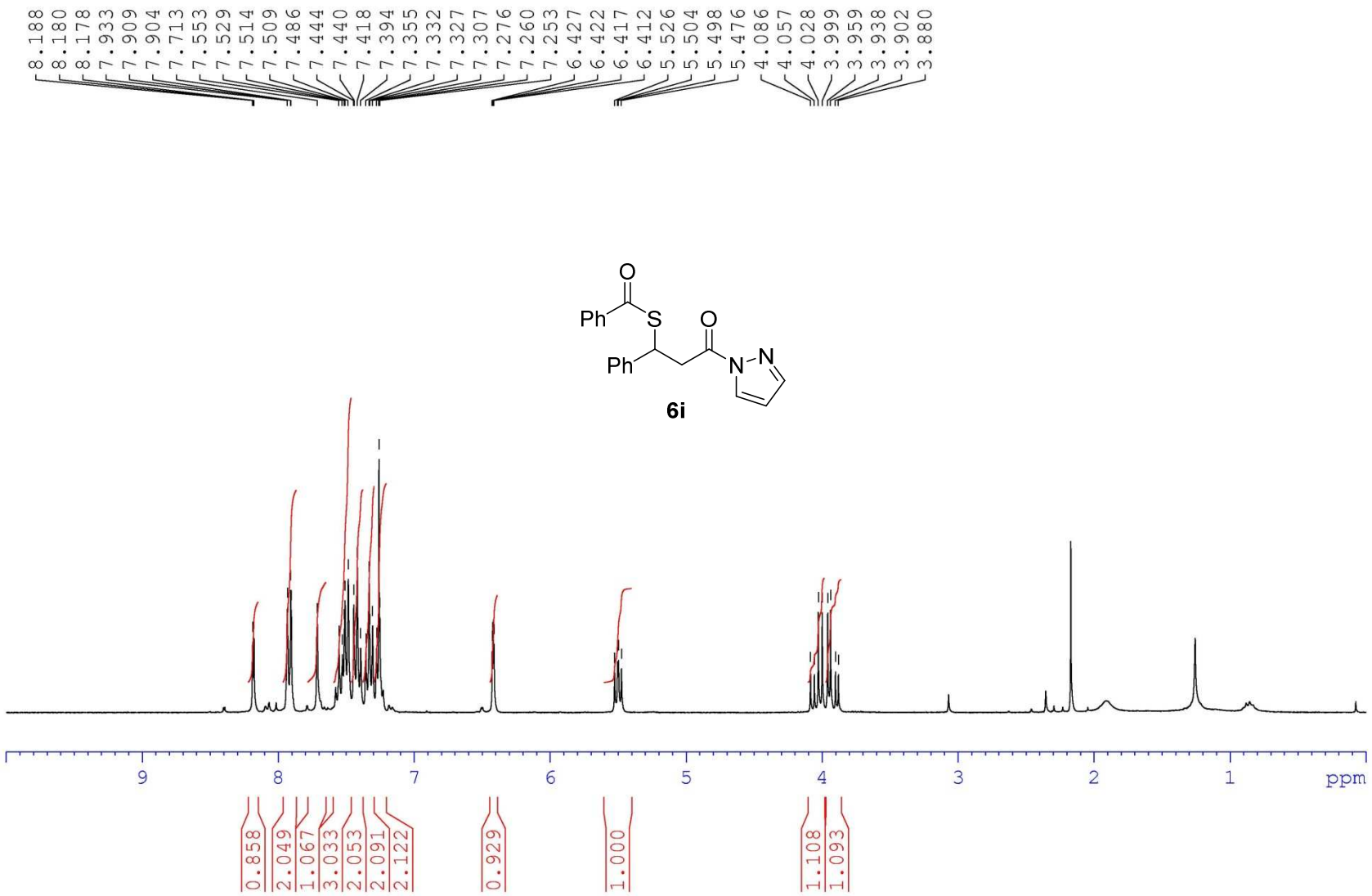
^{1}H NMR in $CDCl_3$ (250 MHz)



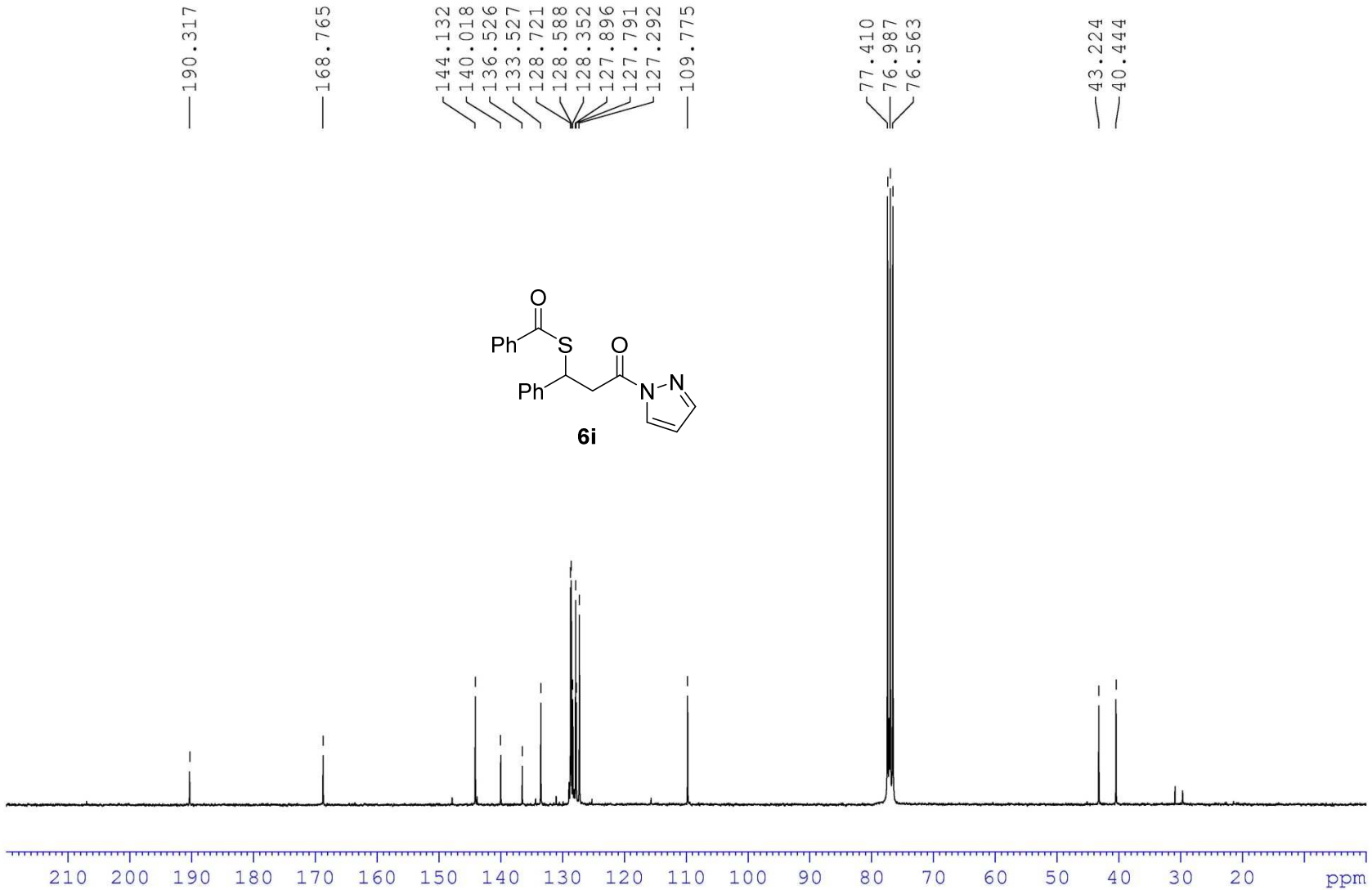
^{13}C NMR in $CDCl_3$ (62.5 MHz)



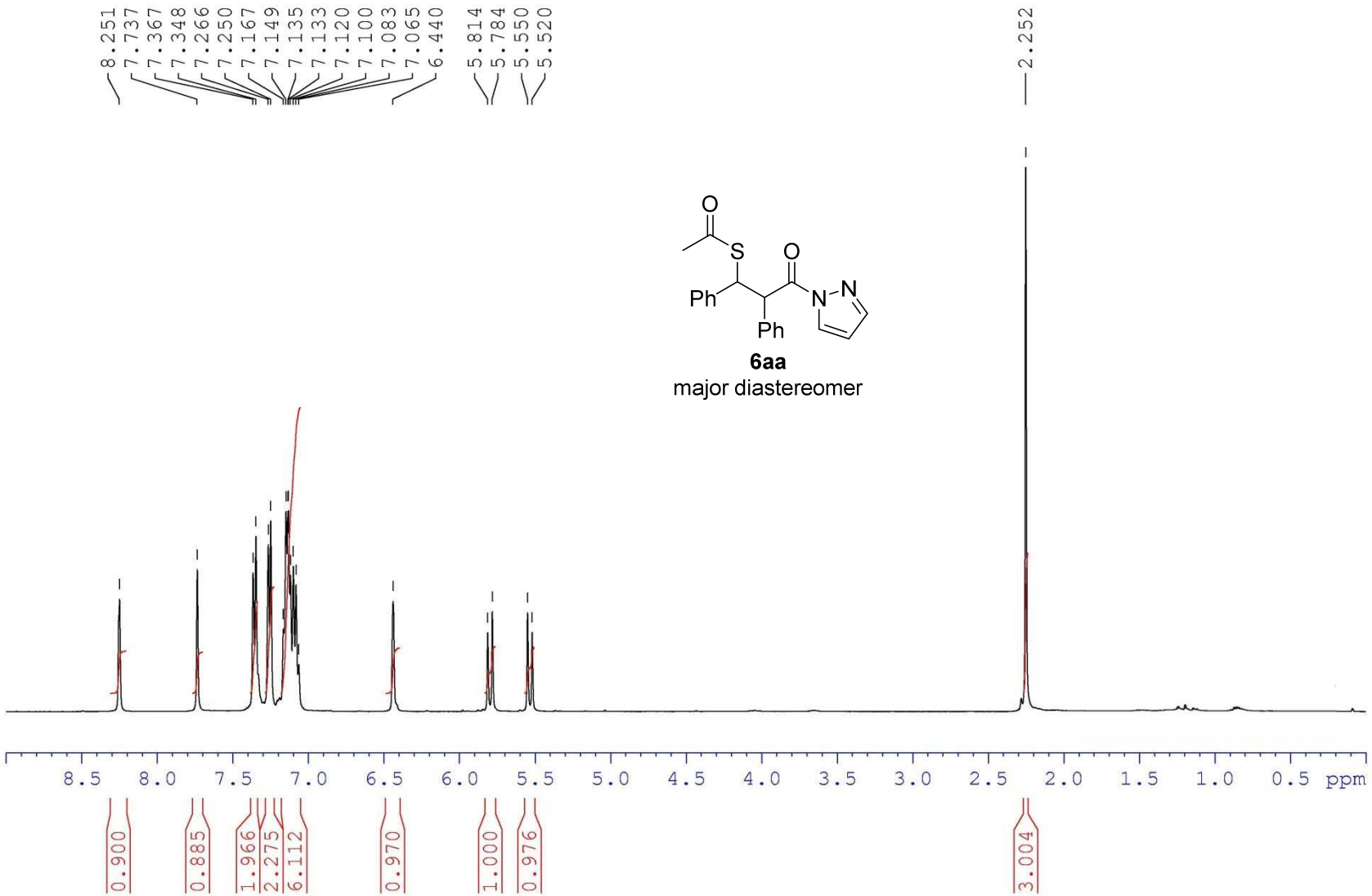
^{1}H NMR in $CDCl_3$ (300 MHz)



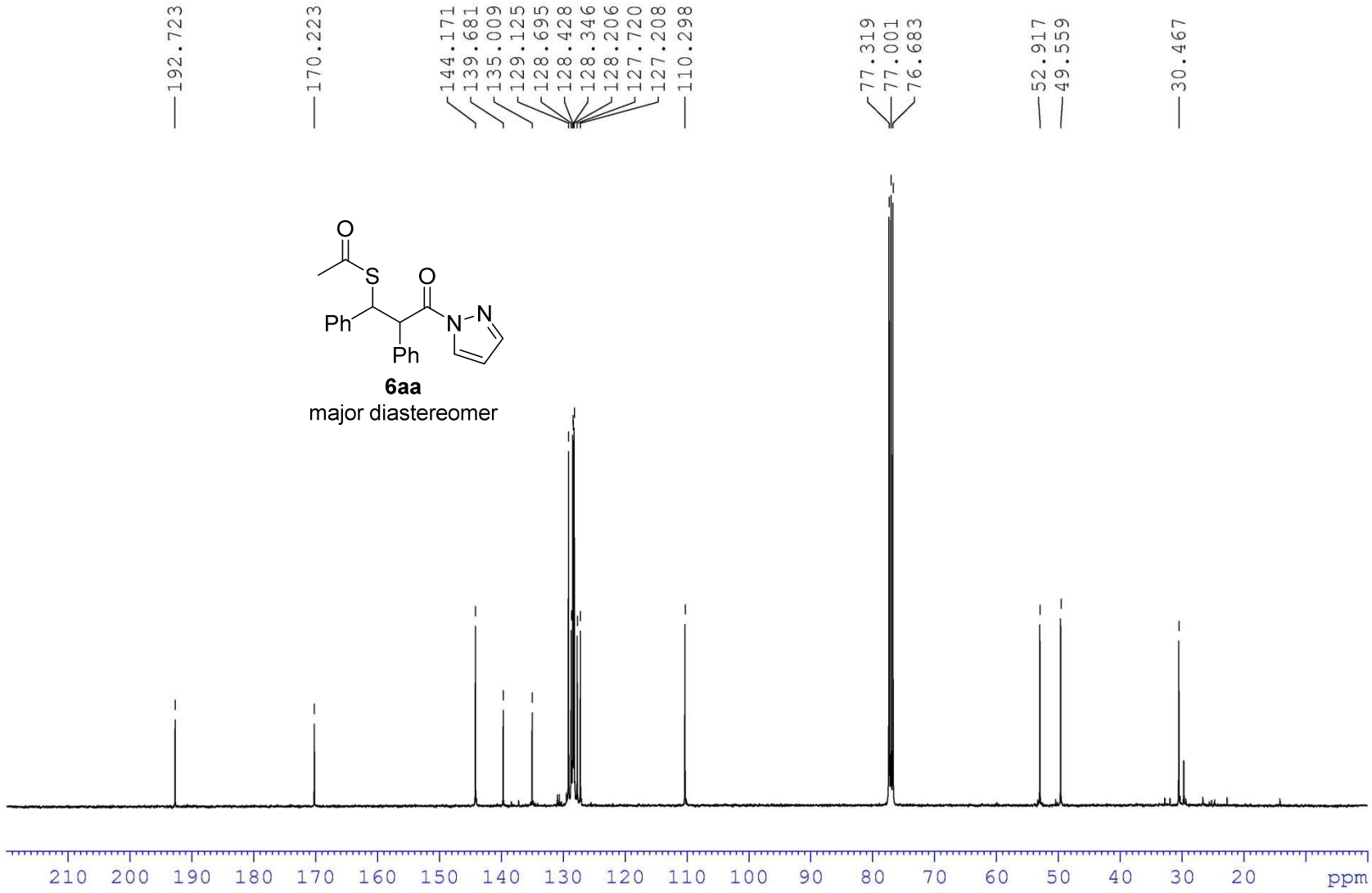
^{13}C NMR in $CDCl_3$ (75 MHz)



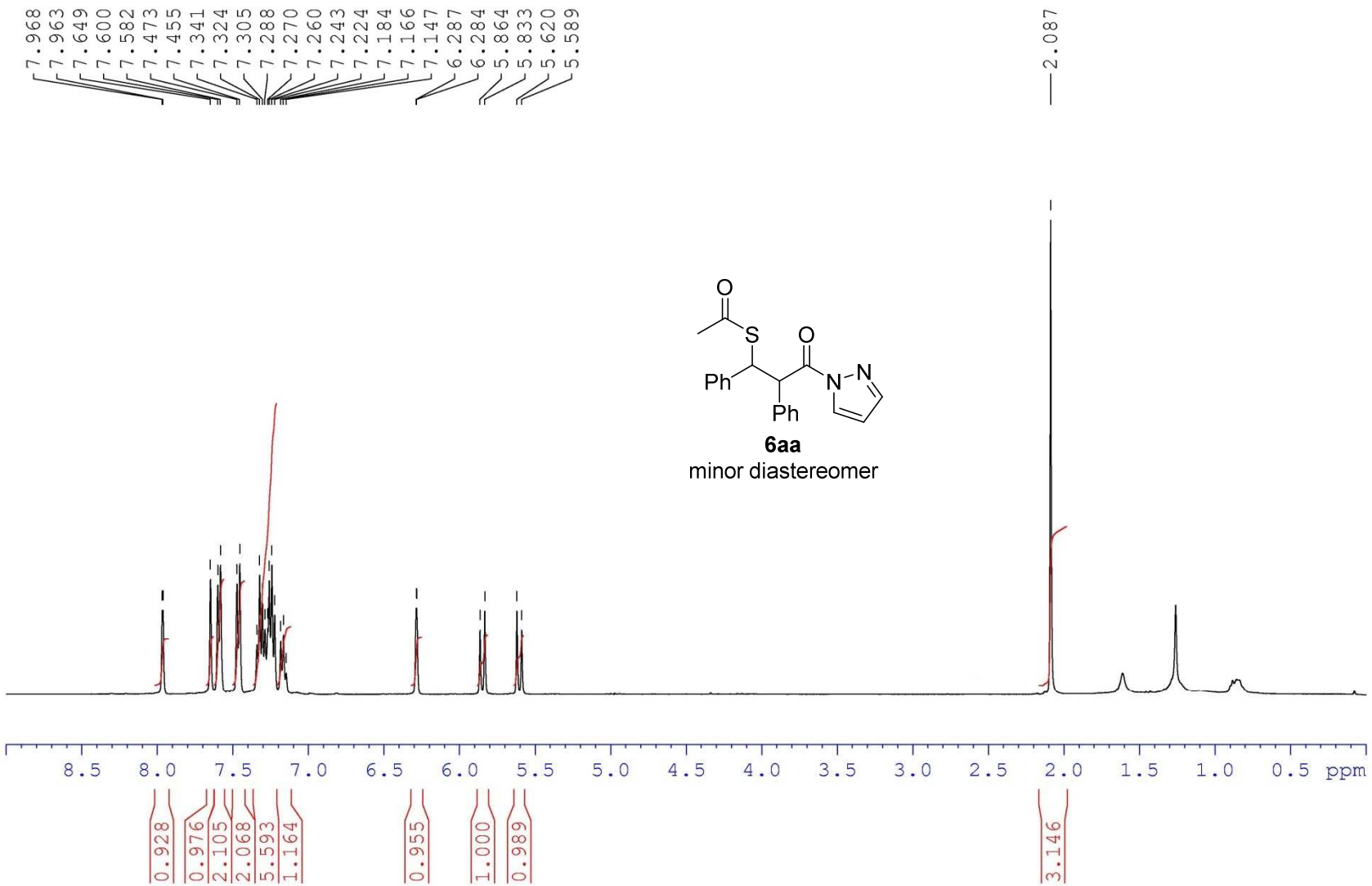
^{1}H NMR in $CDCl_3$ (400 MHz)



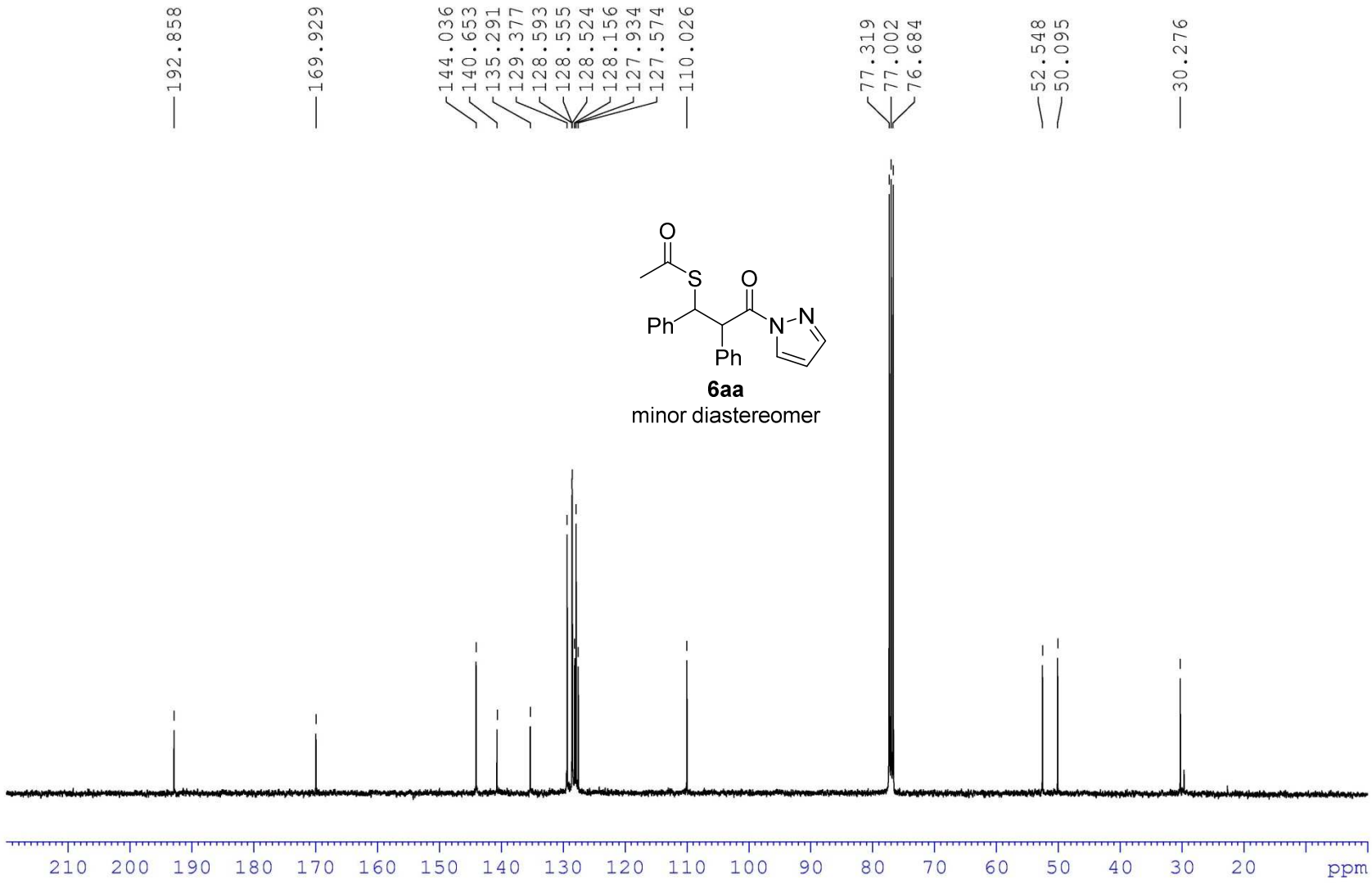
^{13}C NMR in $CDCl_3$ (100 MHz)



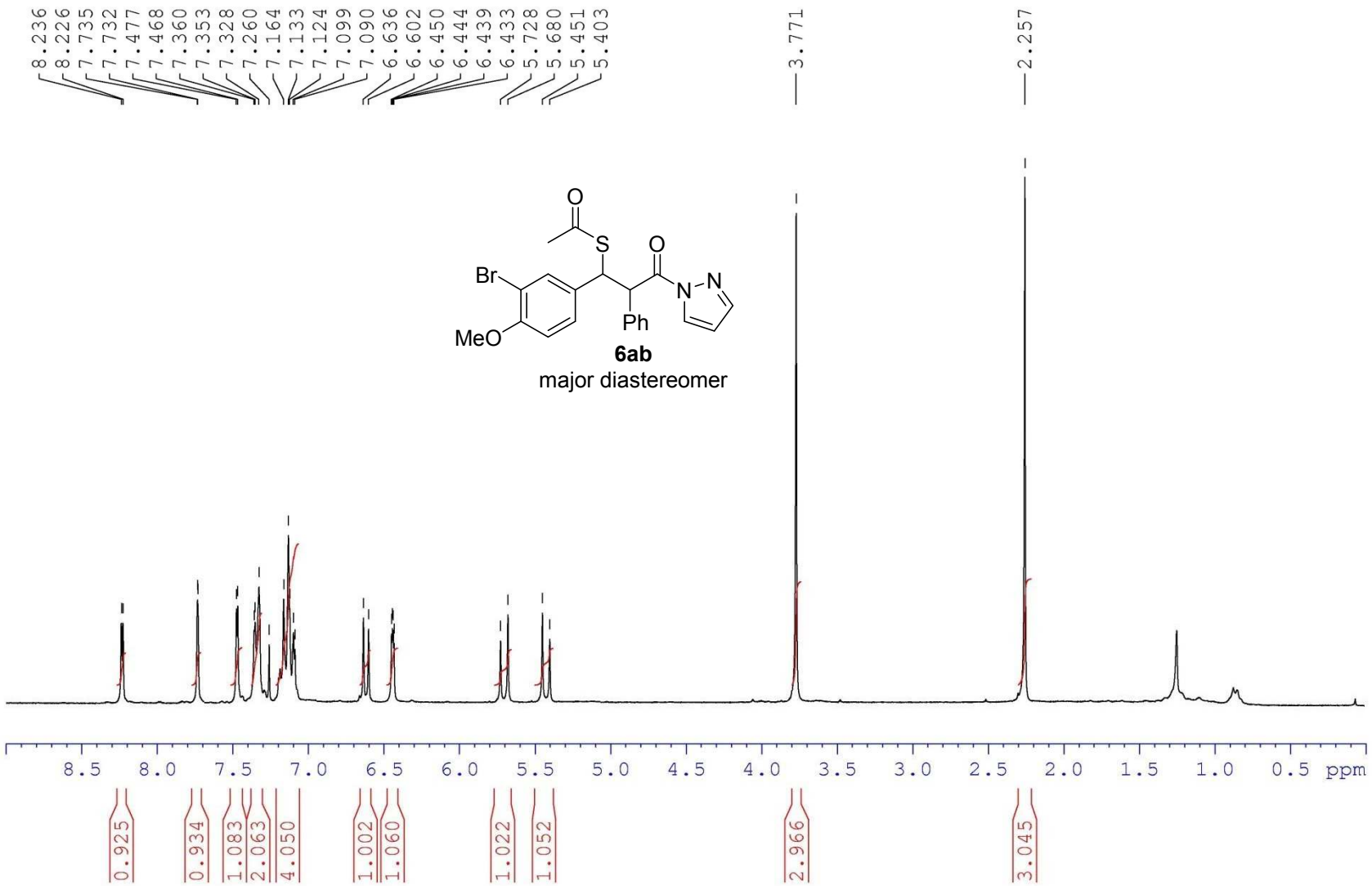
^{1}H NMR in $CDCl_3$ (400 MHz)



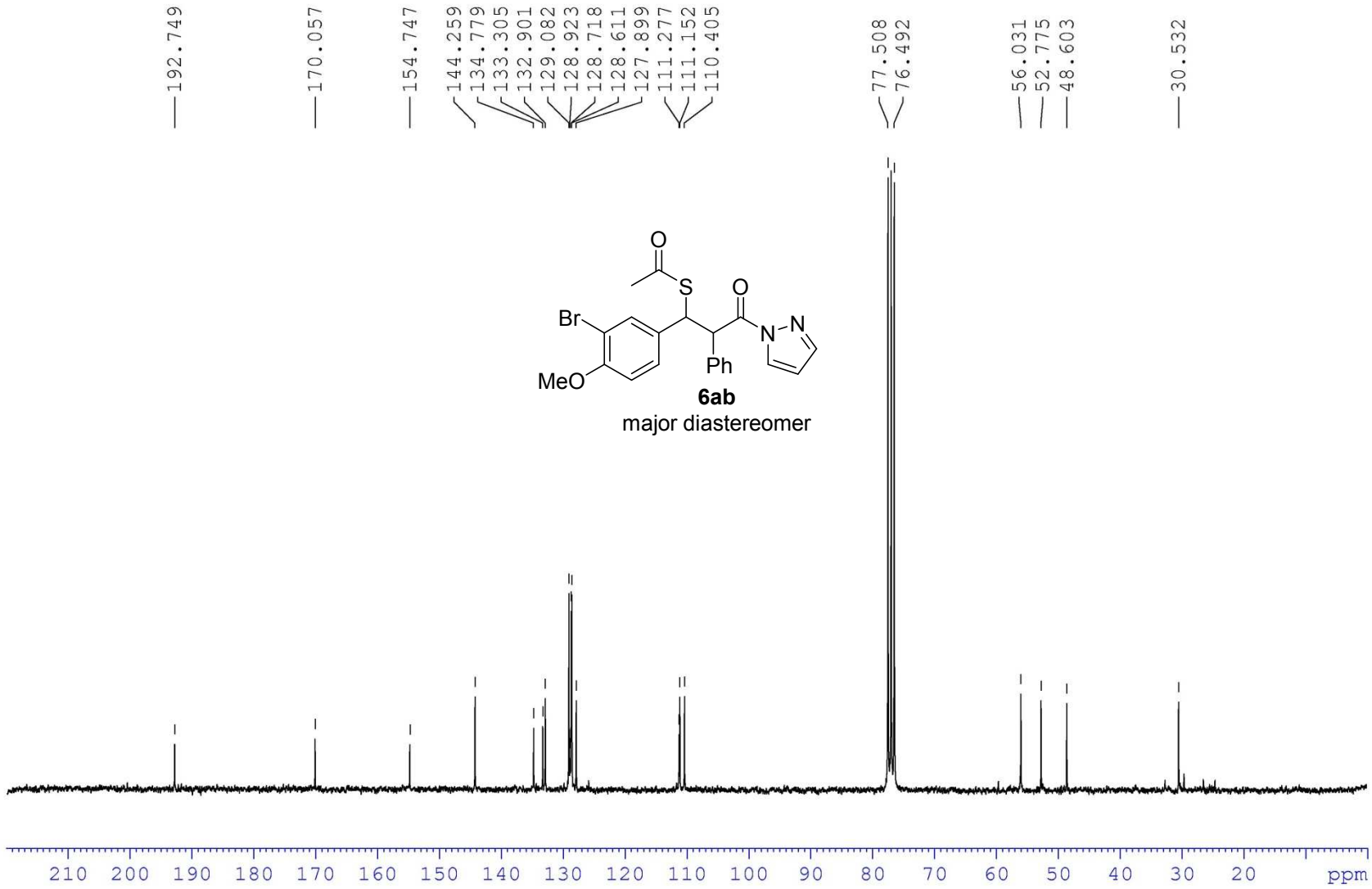
^{13}C NMR in $CDCl_3$ (100 MHz)



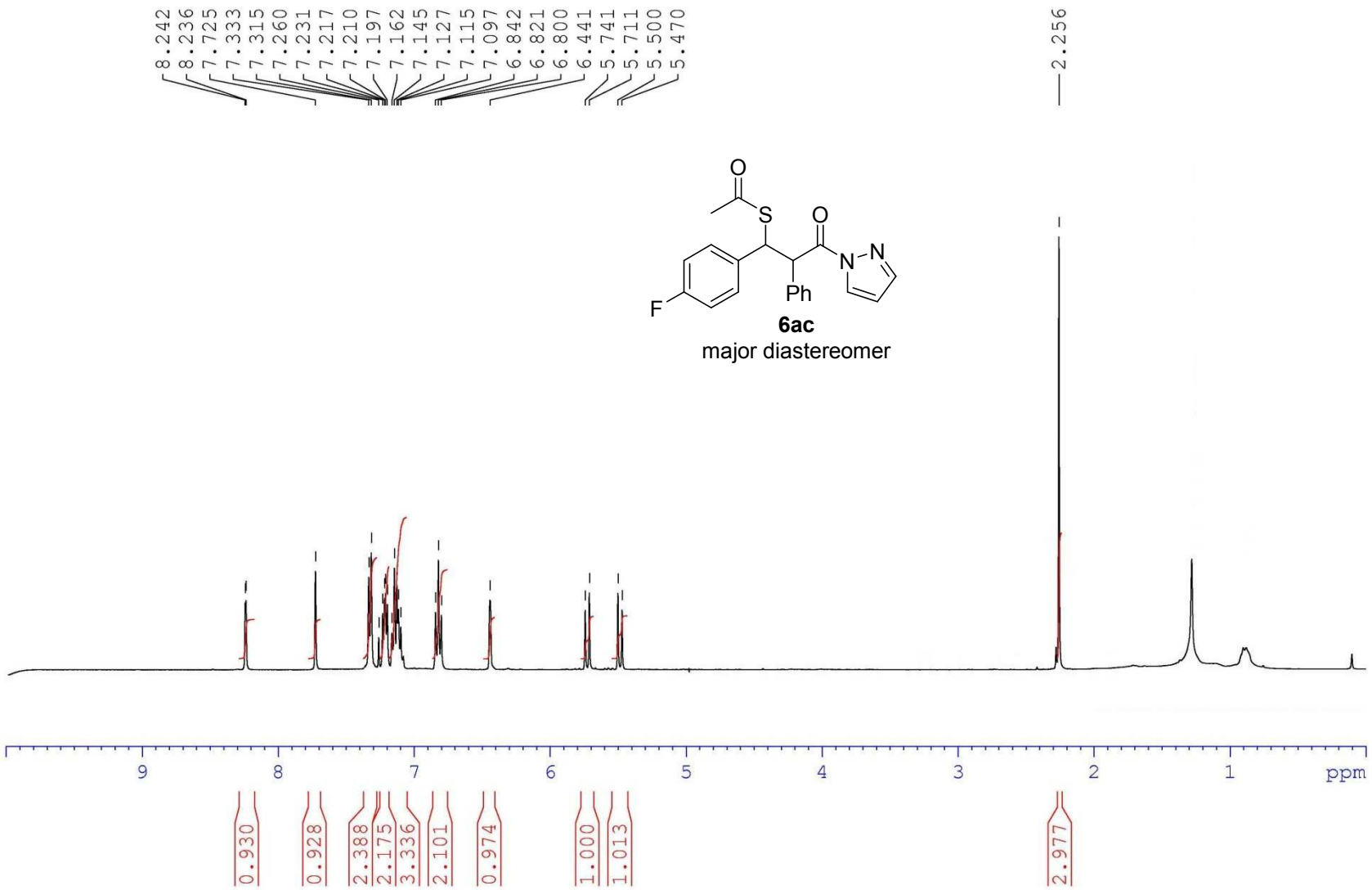
^{1}H NMR in $CDCl_3$ (250 MHz)



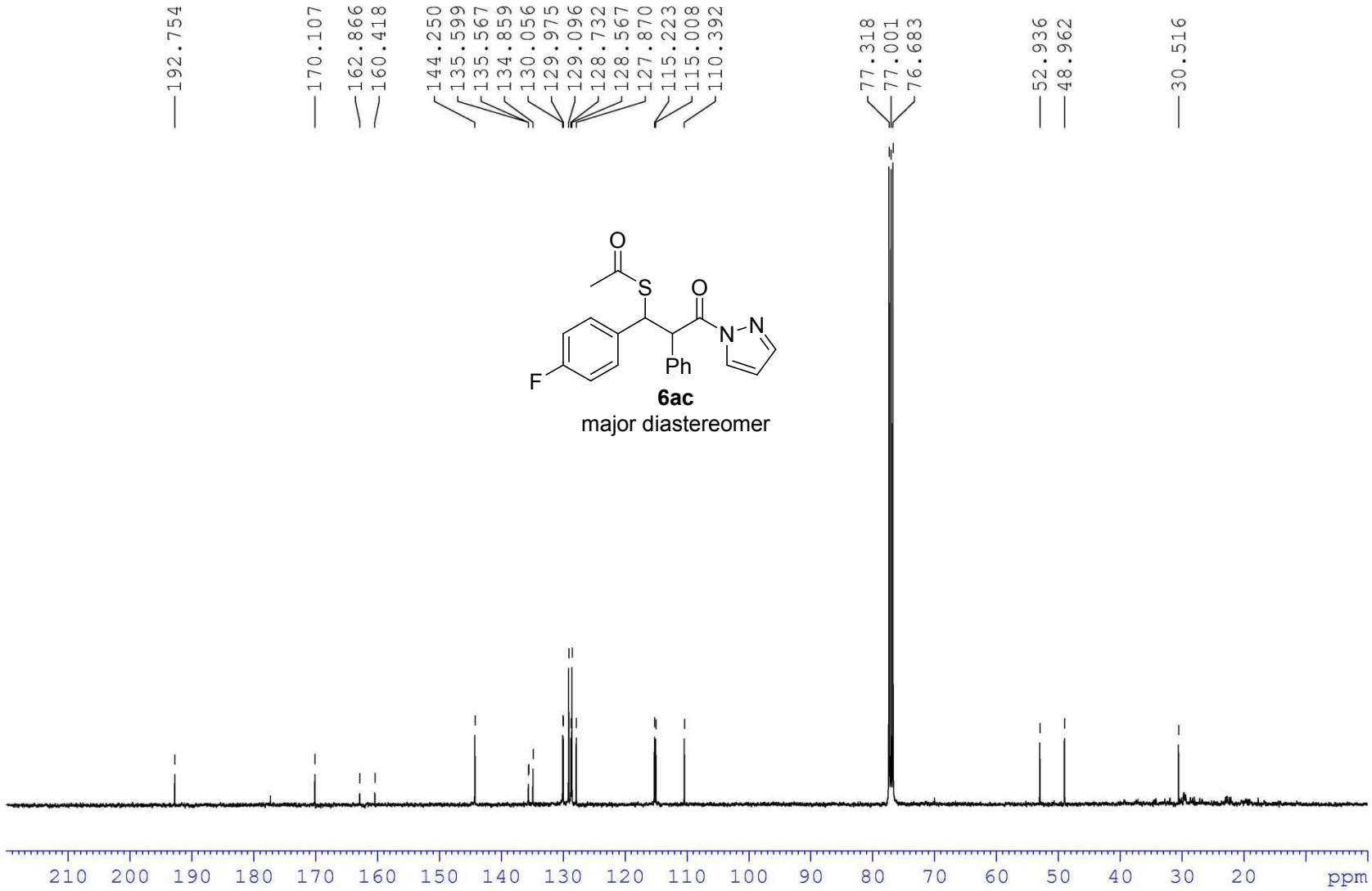
^{13}C NMR in $CDCl_3$ (62.5 MHz)



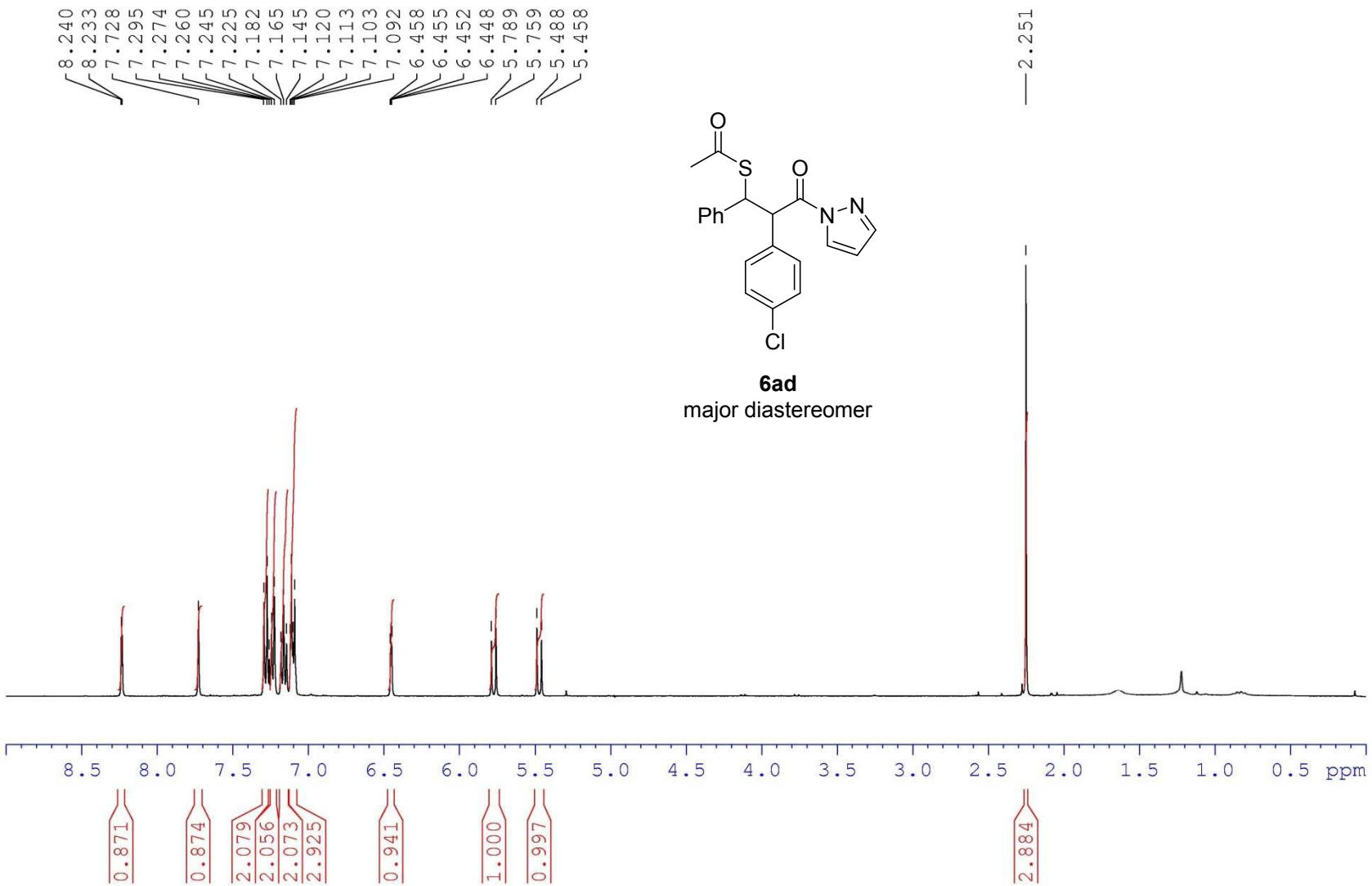
^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)

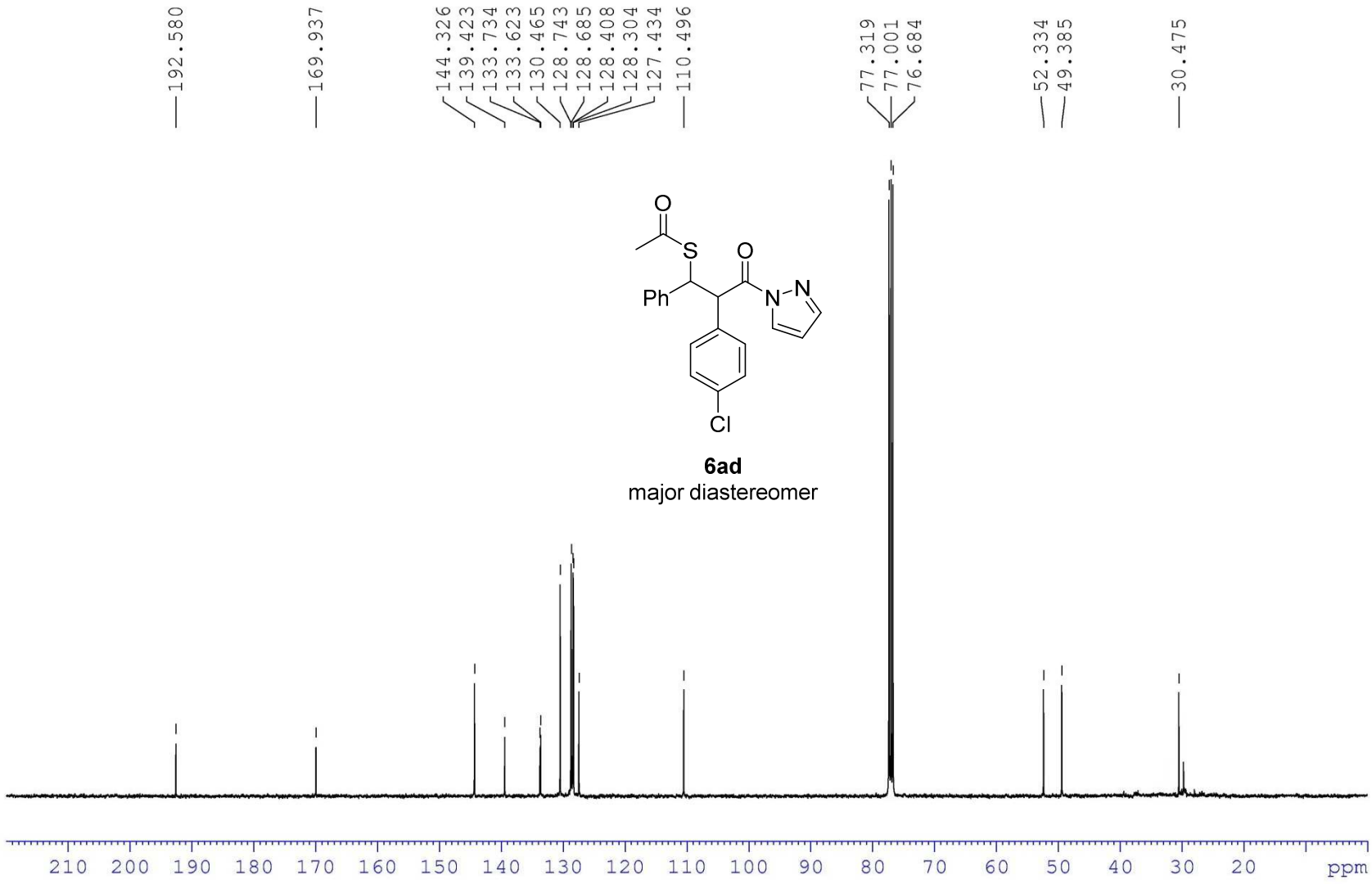


^{1}H NMR in $CDCl_3$ (400 MHz)

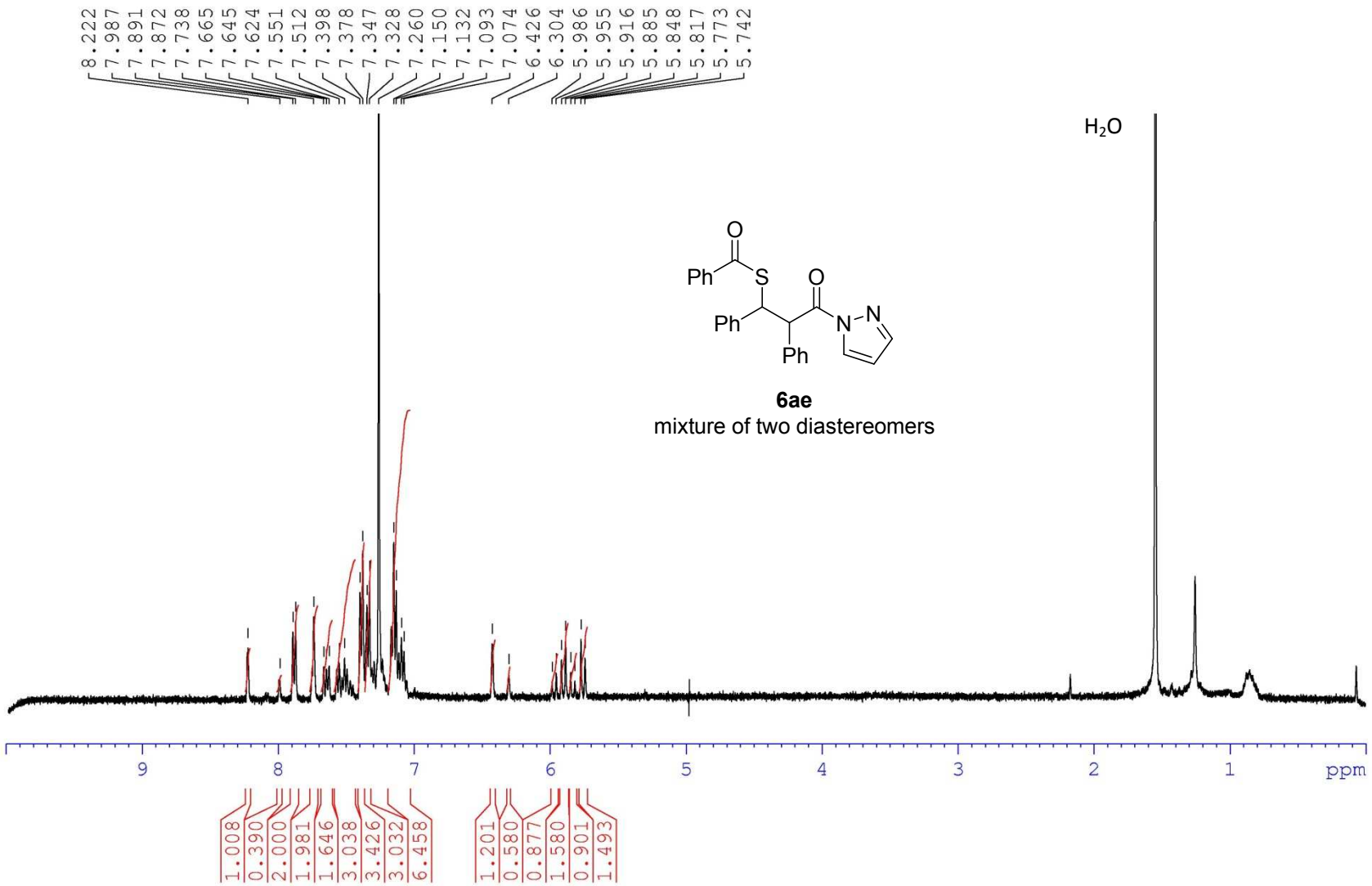


6ad
major diastereomer

^{13}C NMR in $CDCl_3$ (100 MHz)



^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (75 MHz)

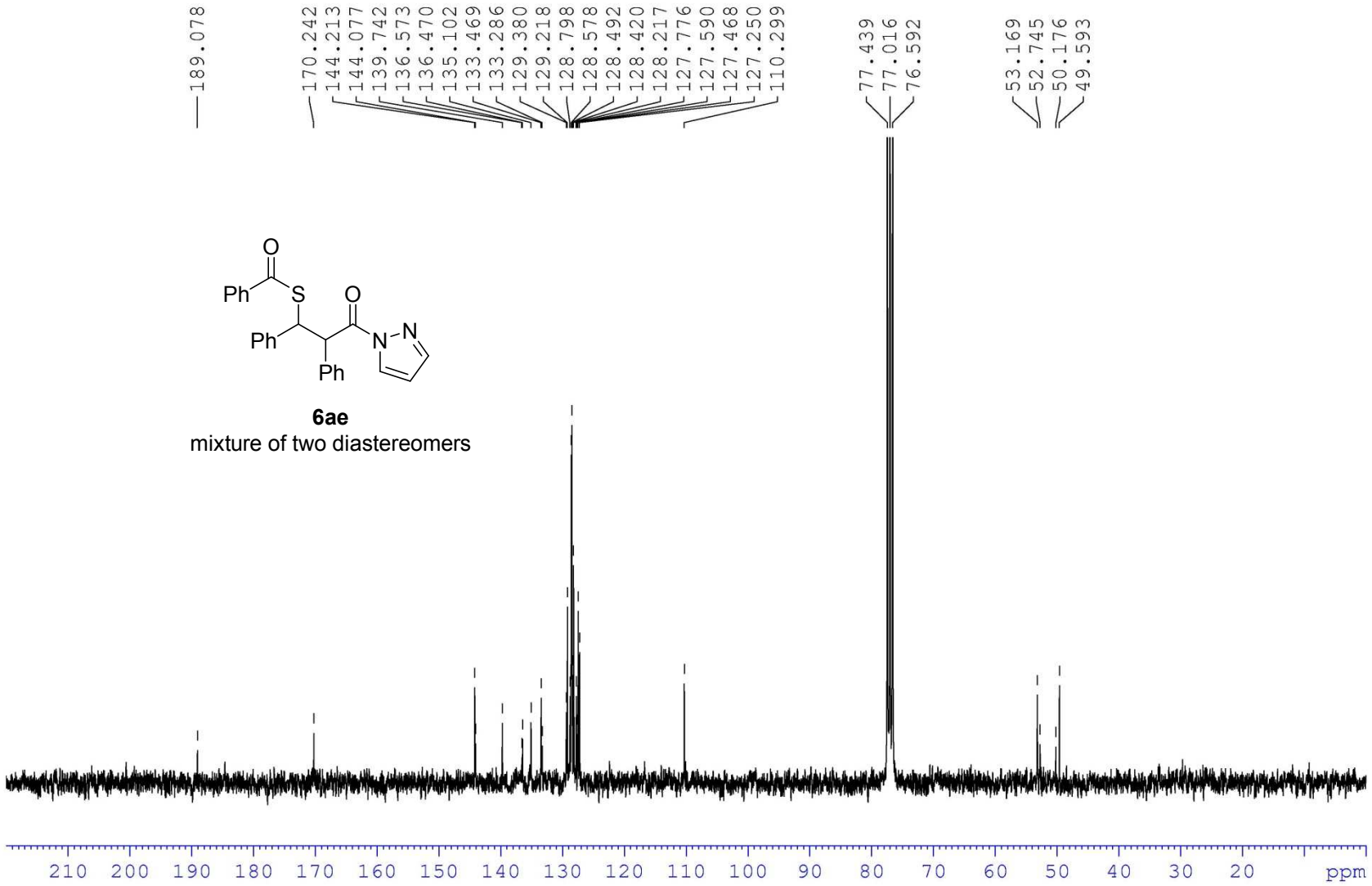
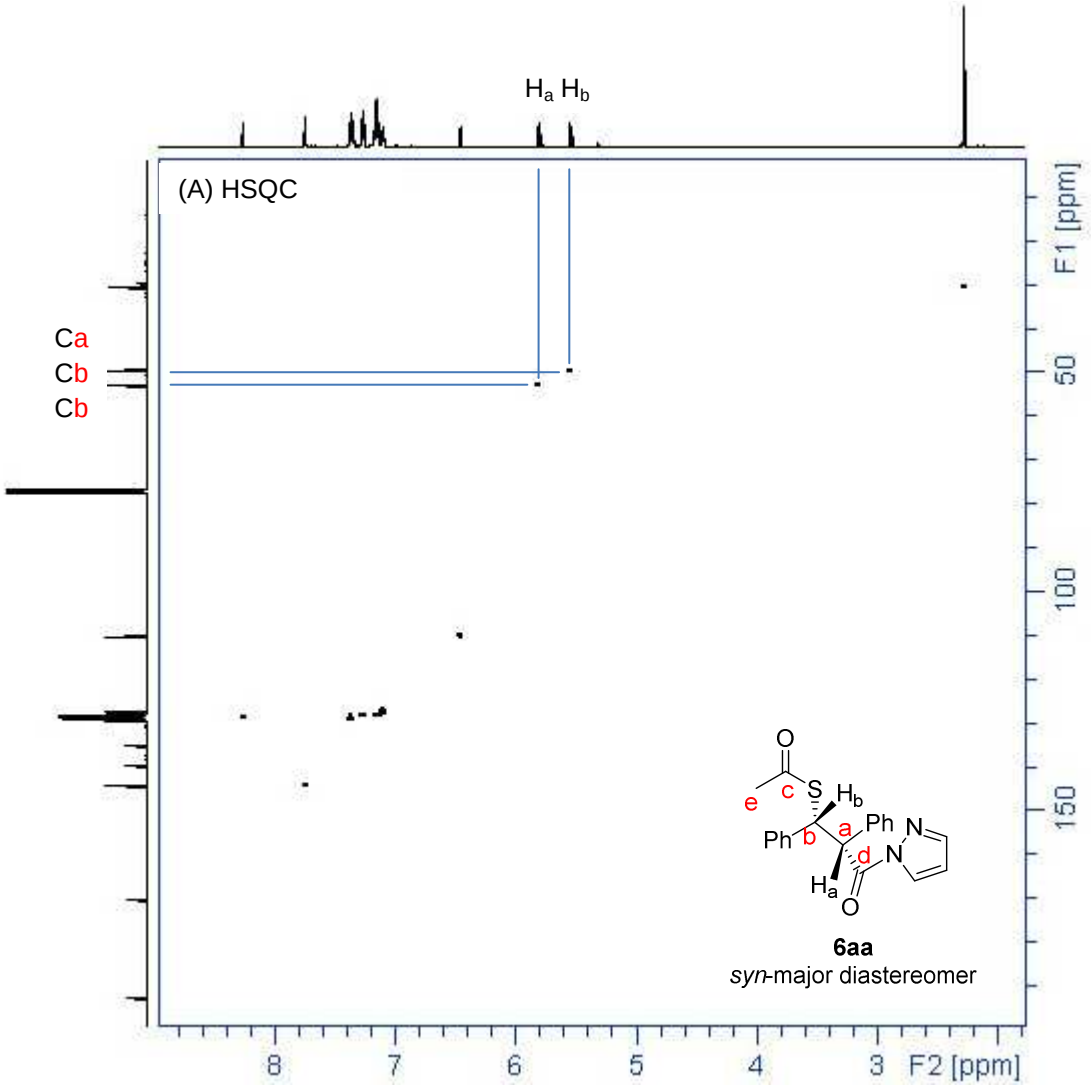


Figure S2. 2D NMR of *syn*-major diastereomer of **6aa** (600 MHz in $CDCl_3$ at rt). (A) HSQC of **6aa**. (B) HMBC of **6aa**.



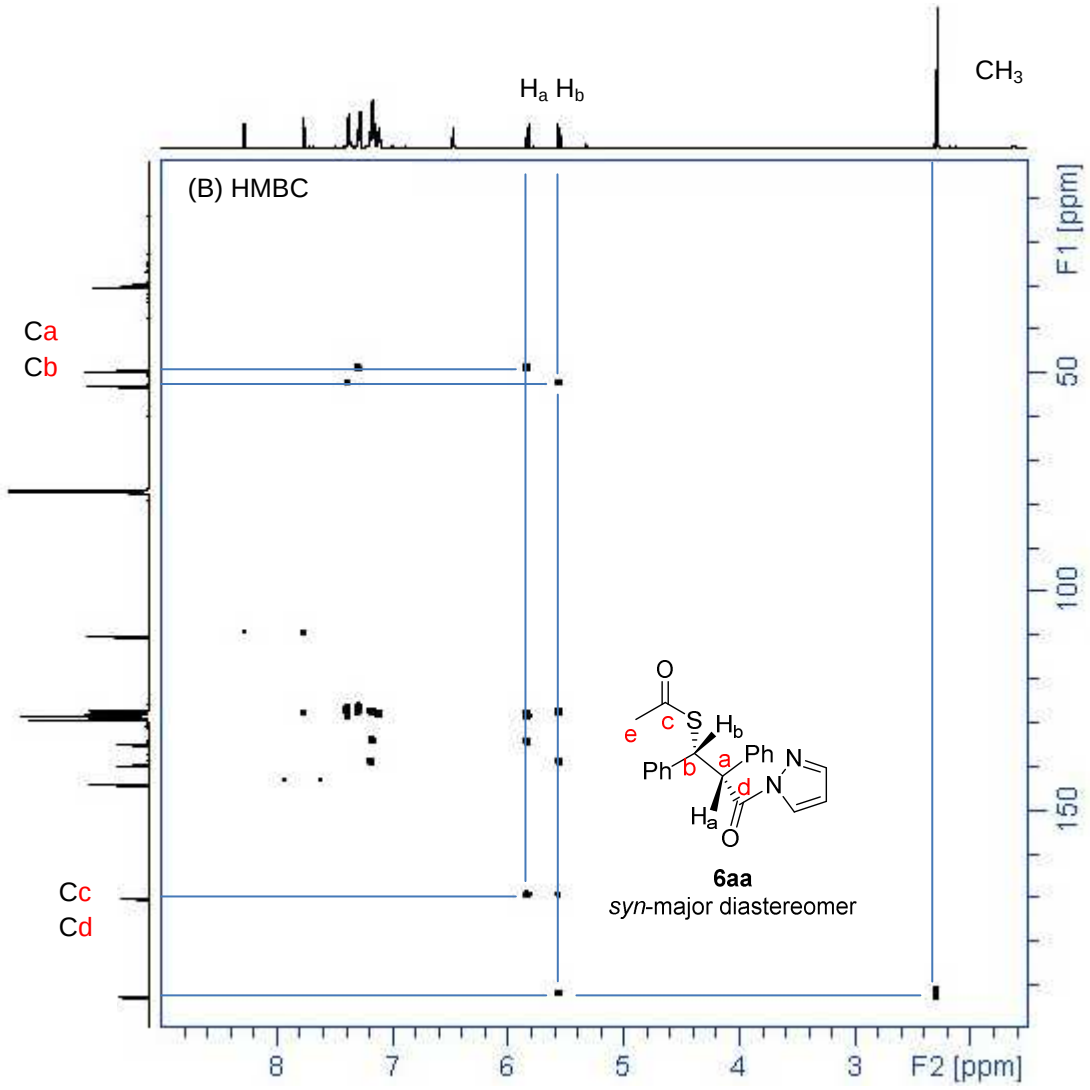
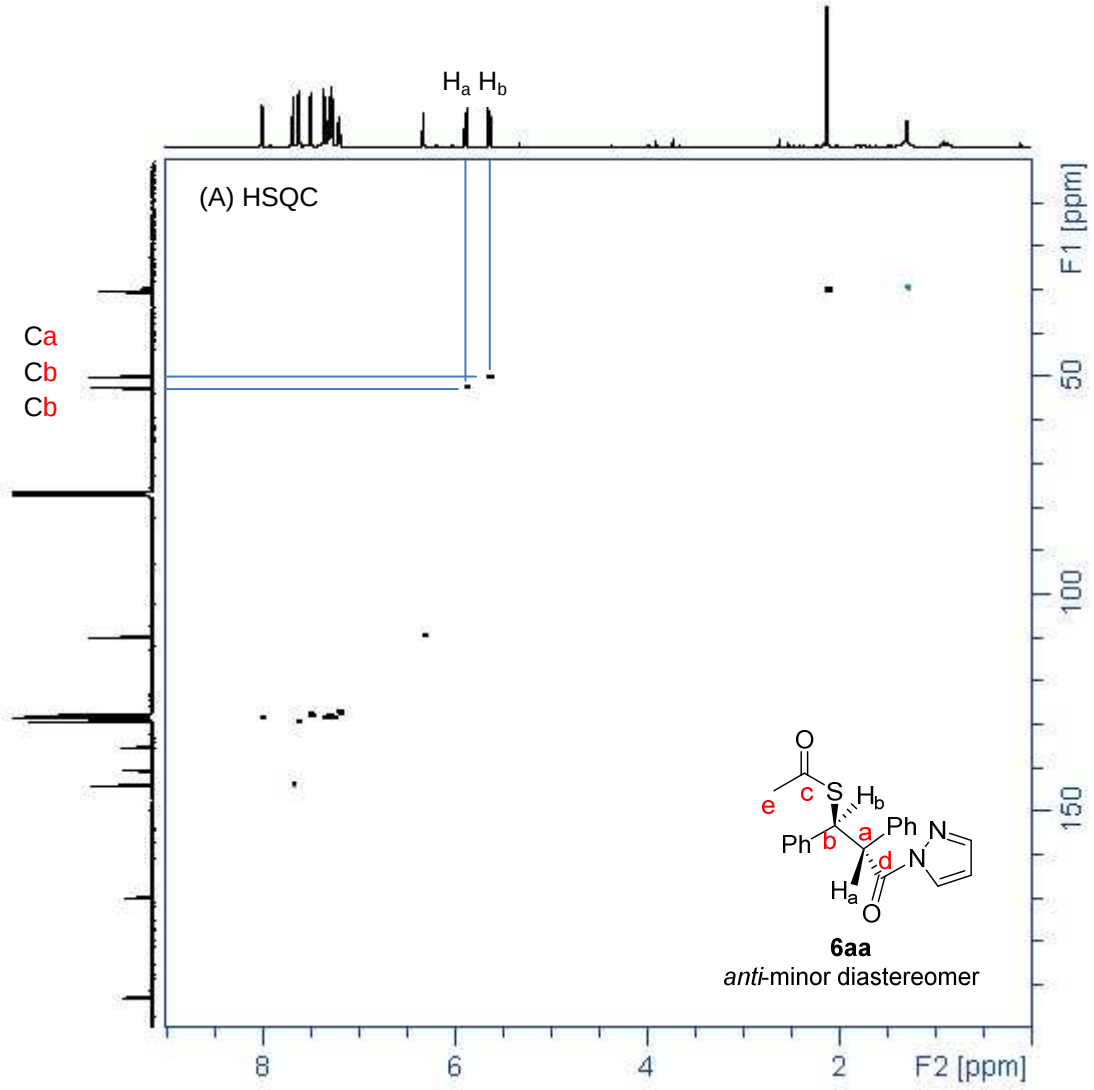
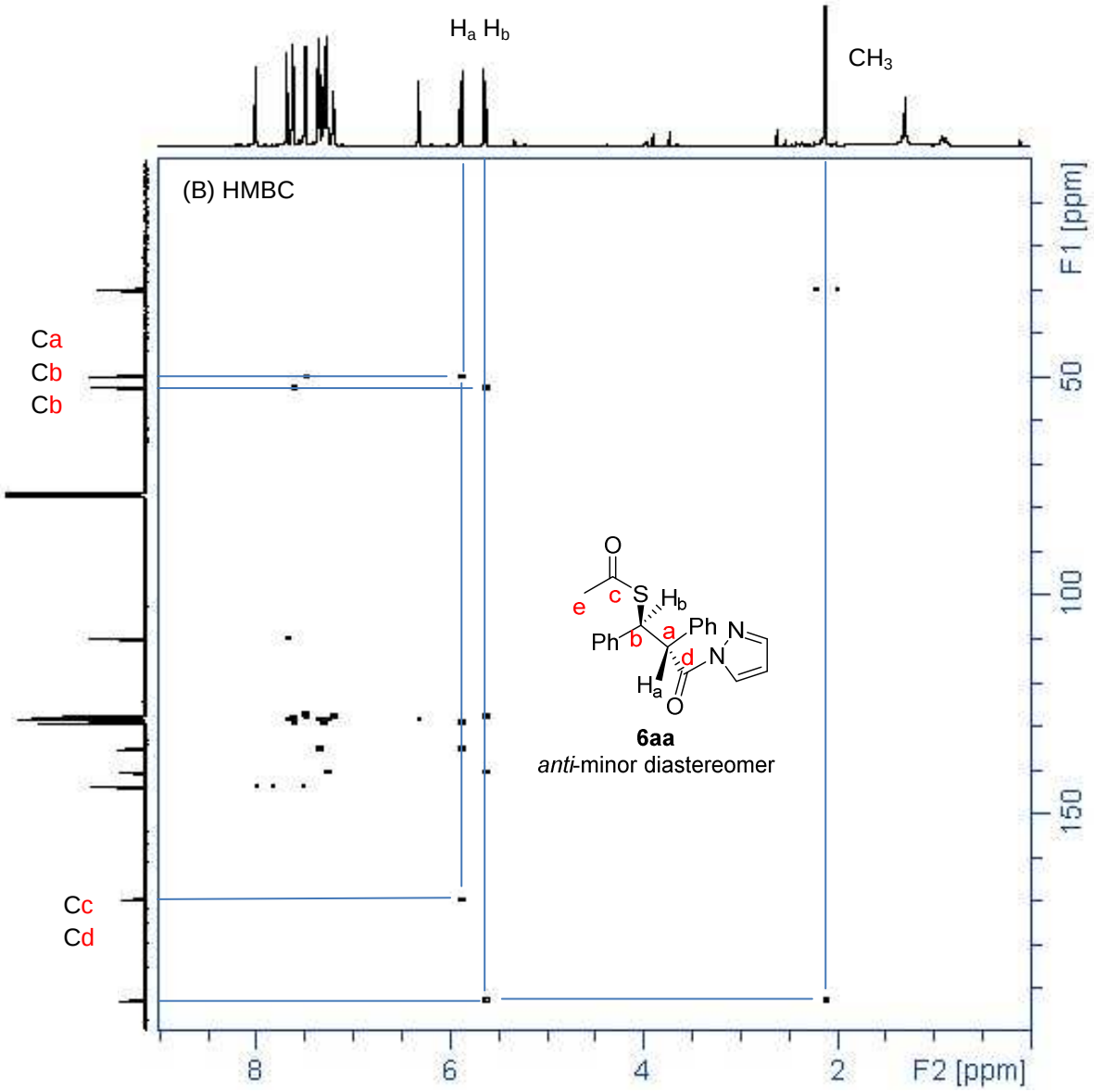

Ha Hb
CH3
(B) HMBC
Ca
Cb
Cc
Cd
F1 [ppm]
50
100
150
8
7
6
5
4
3
F2 [ppm]
O
c
S
Hb
e
Ph
b
a
Ph
N
N
d
Ha
O
6aa
syn-major diastereomer

Figure S3. 2D NMR of *anti*-minor diastereomer of **6aa** (600 MHz in $CDCl_3$ at rt). (A) HSQC of **6aa**. (B) HMBC of **6aa**.

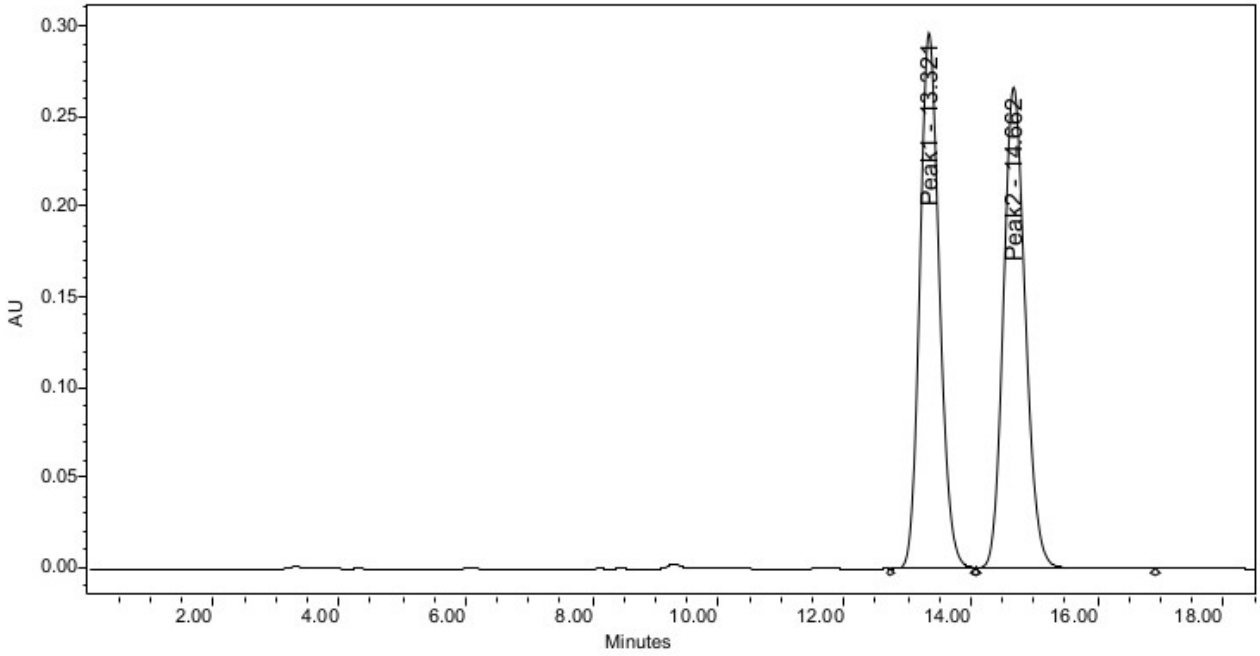




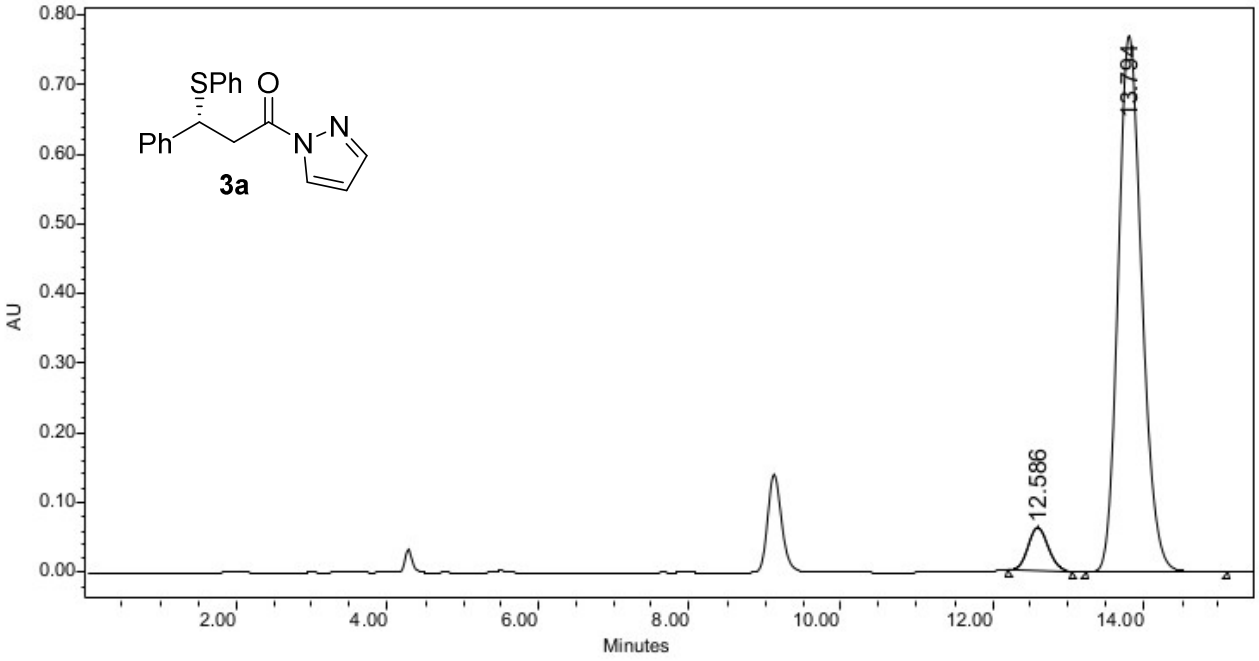
6aa

anti-minor diastereomer

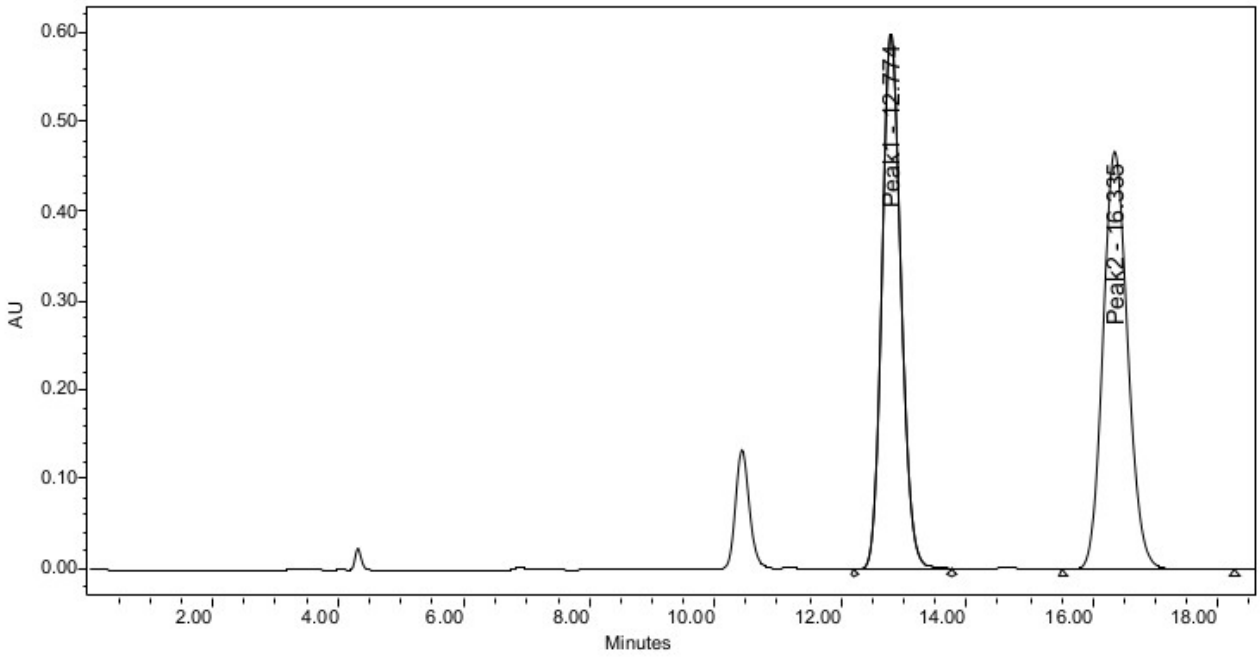
HPLC chromatograms



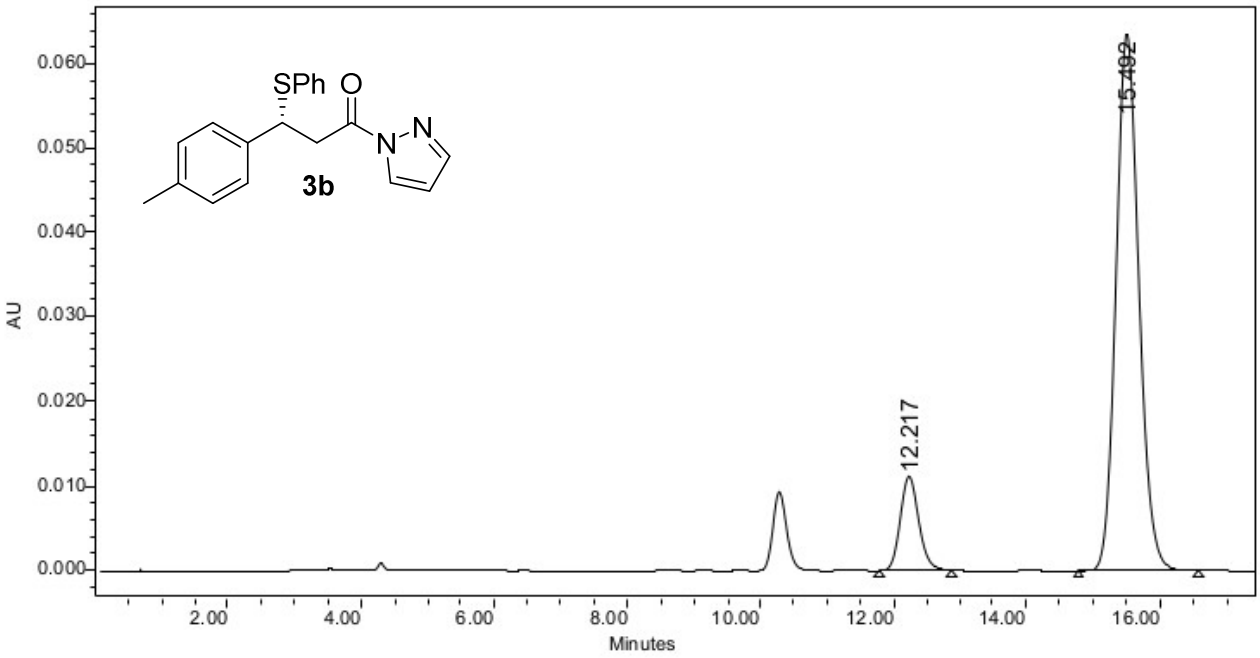
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	13.321	6412362	49.80	297098	52.69
2	Peak2	14.662	6463912	50.20	266799	47.31



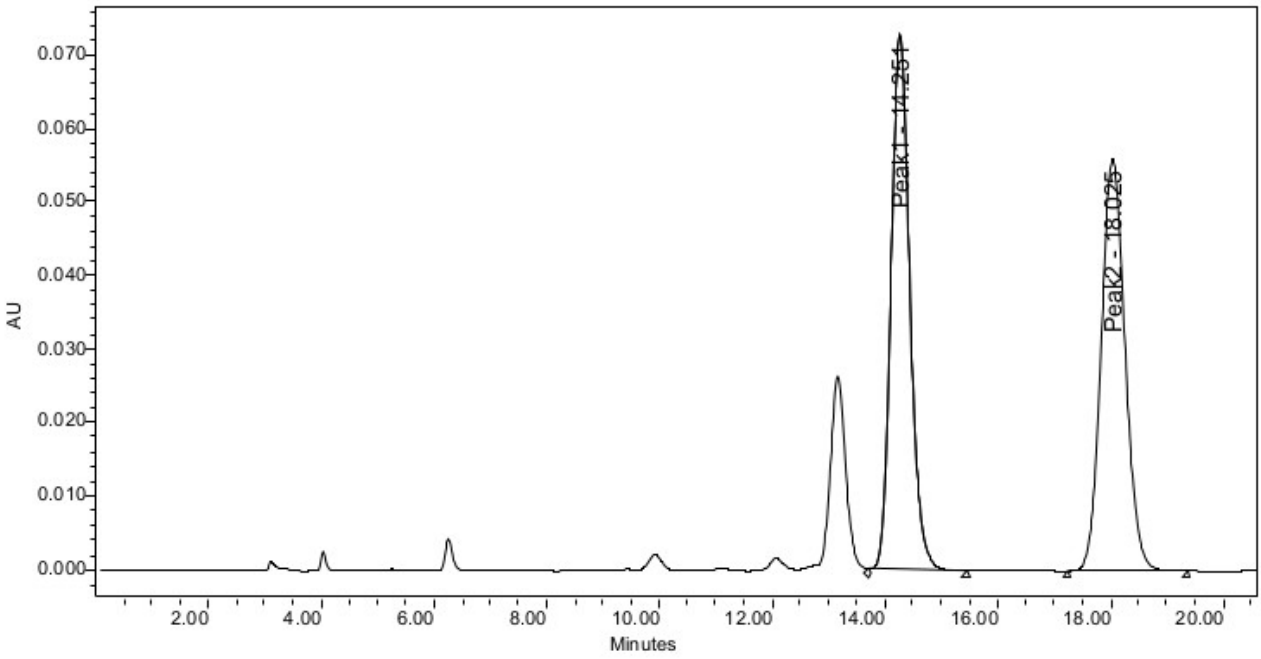
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.586	1168263	6.49	62387	7.48
2	13.794	16837899	93.51	772044	92.52



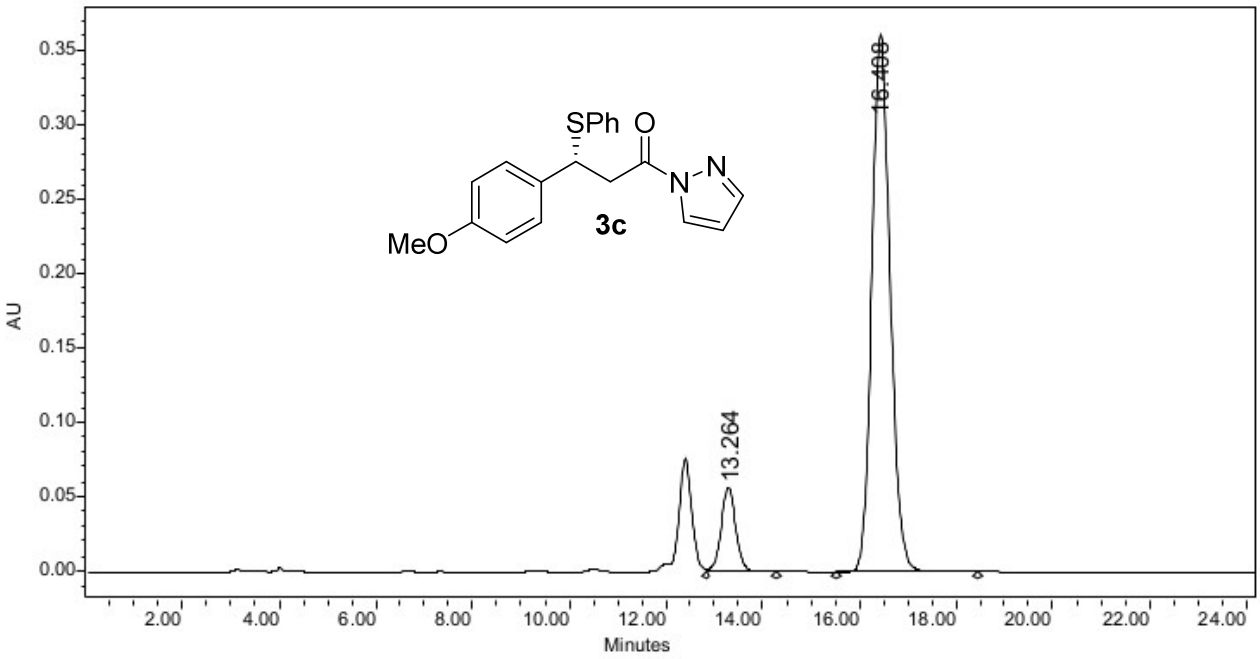
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.774	12746619	49.83	599806	56.16
2	Peak2	16.335	12833698	50.17	468168	43.84



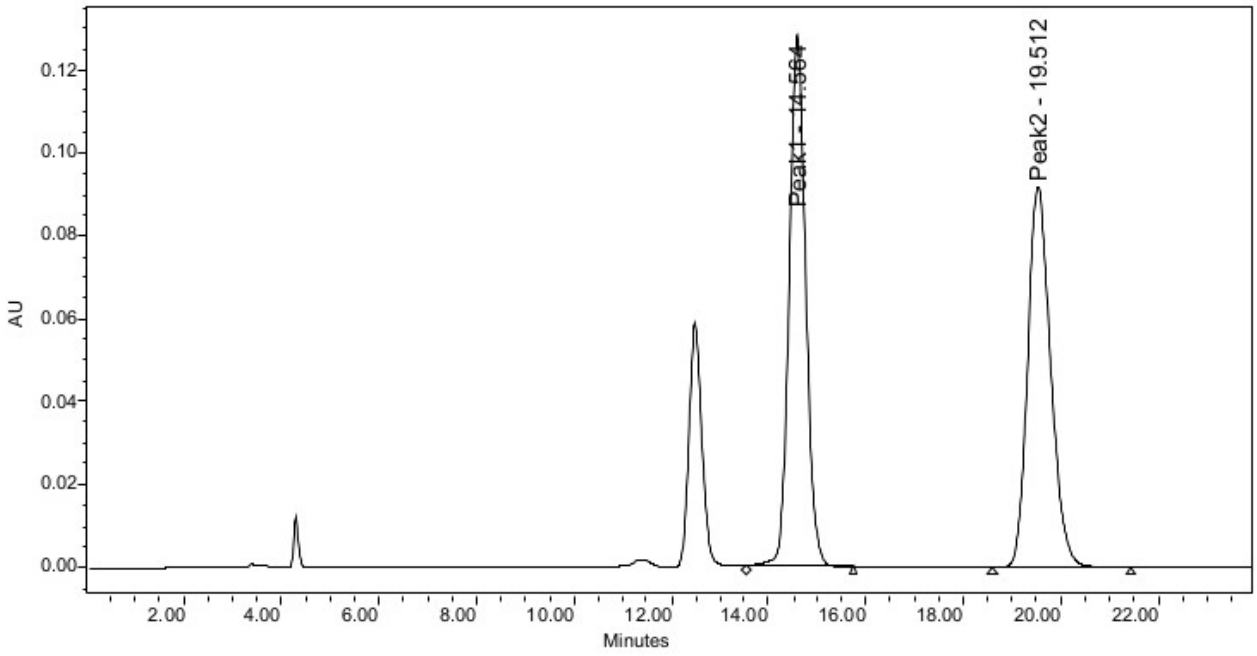
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.217	216939	12.51	11188	14.95
2	15.492	1517577	87.49	63631	85.05



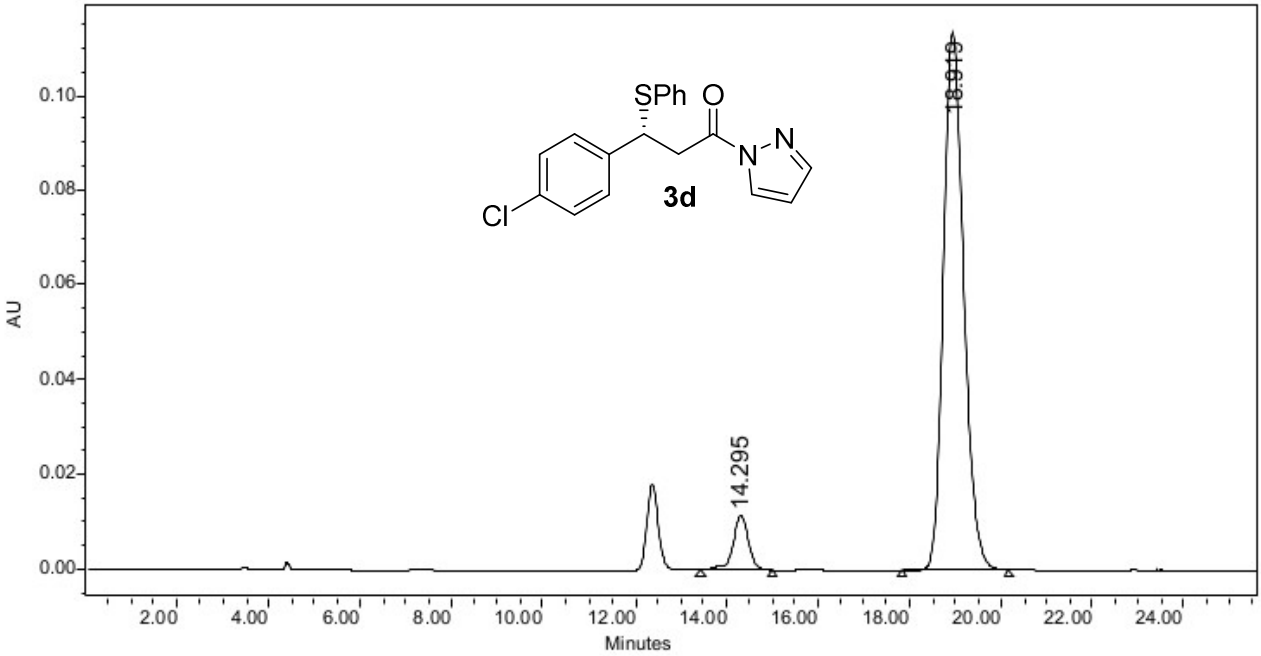
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	14.251	1682607	50.44	72766	56.50
2	Peak2	18.025	1653398	49.56	56025	43.50



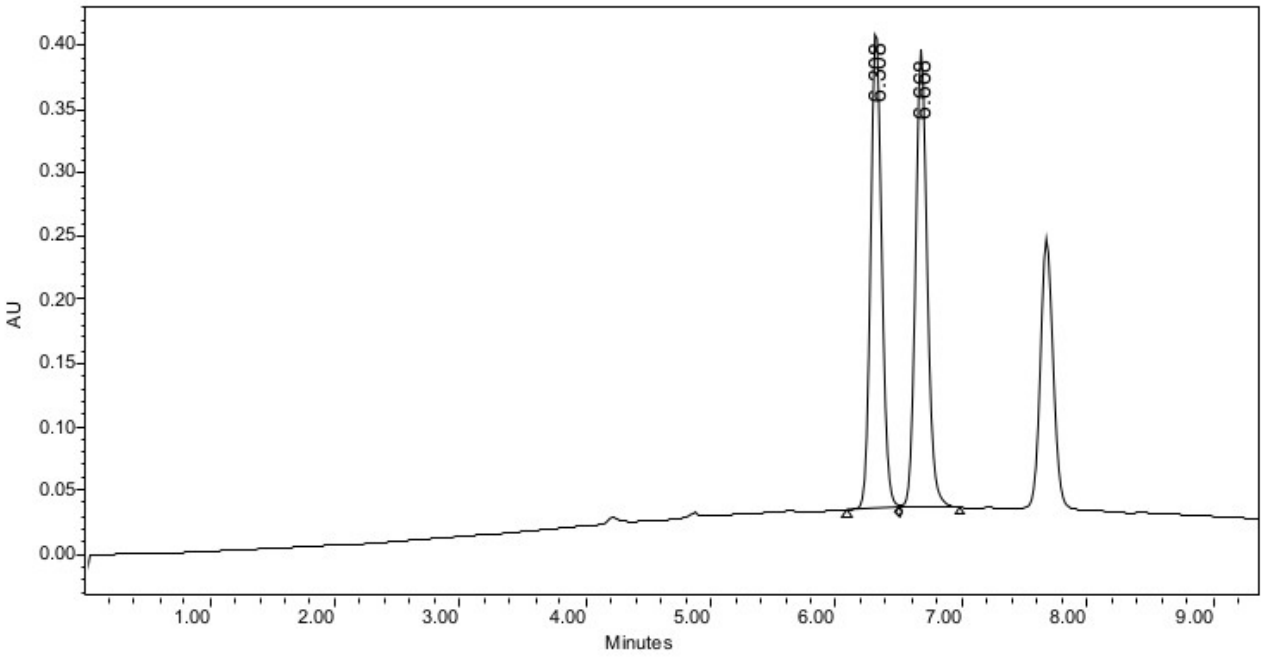
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.264	1208919	11.28	56926	13.61
2	16.408	9511091	88.72	361252	86.39



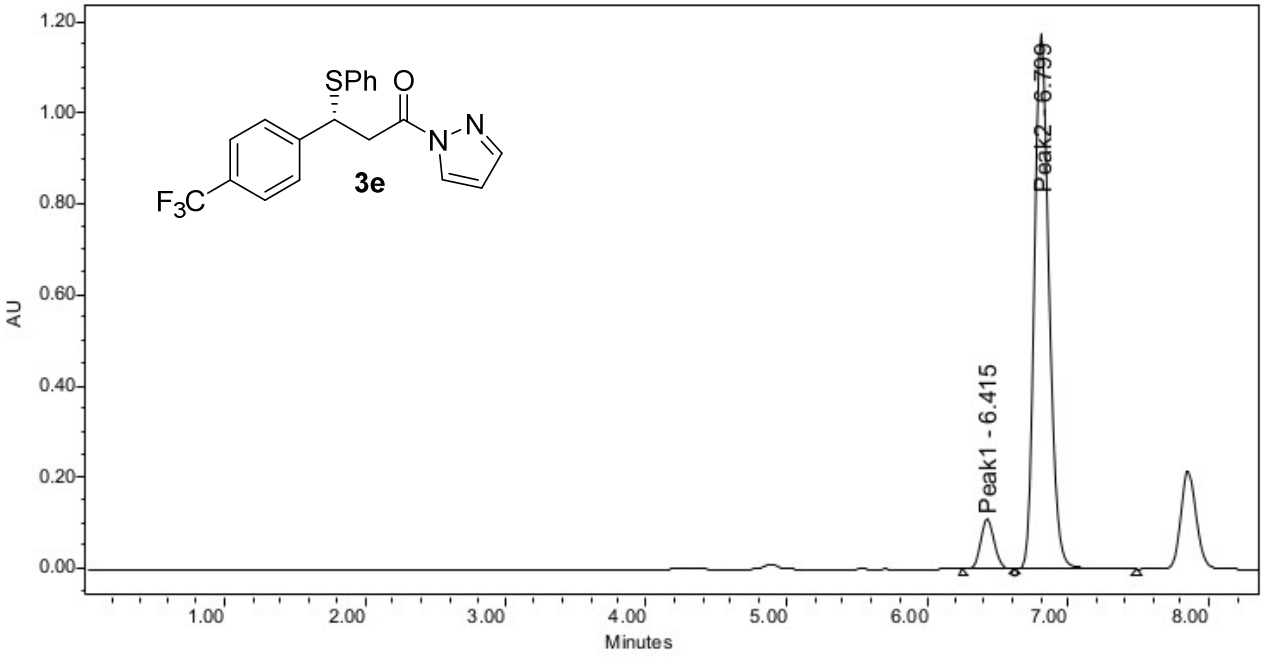
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	14.564	3033957	50.10	128417	58.28
2	Peak2	19.512	3022027	49.90	91921	41.72



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	14.295	269792	7.20	11545	9.24
2	18.919	3479363	92.80	113361	90.76



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	6.308	2334304	49.64	376245	51.15
2	6.668	2367851	50.36	359279	48.85



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	6.415	733040	7.92	109556	8.55
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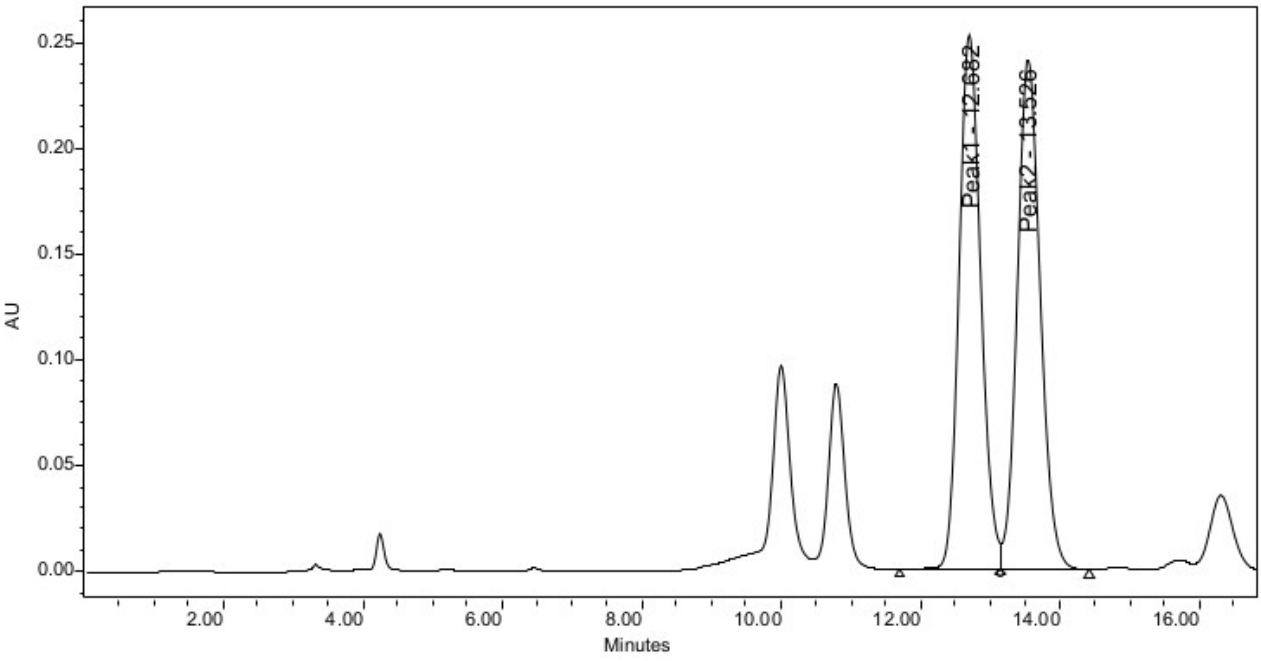
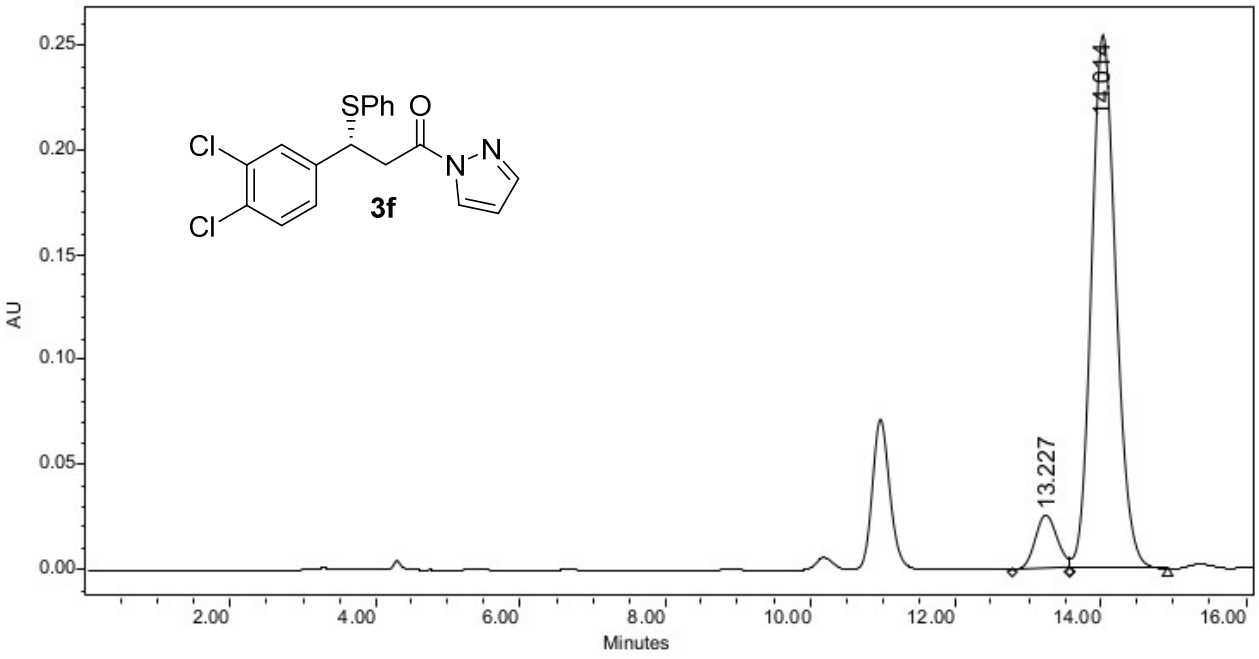
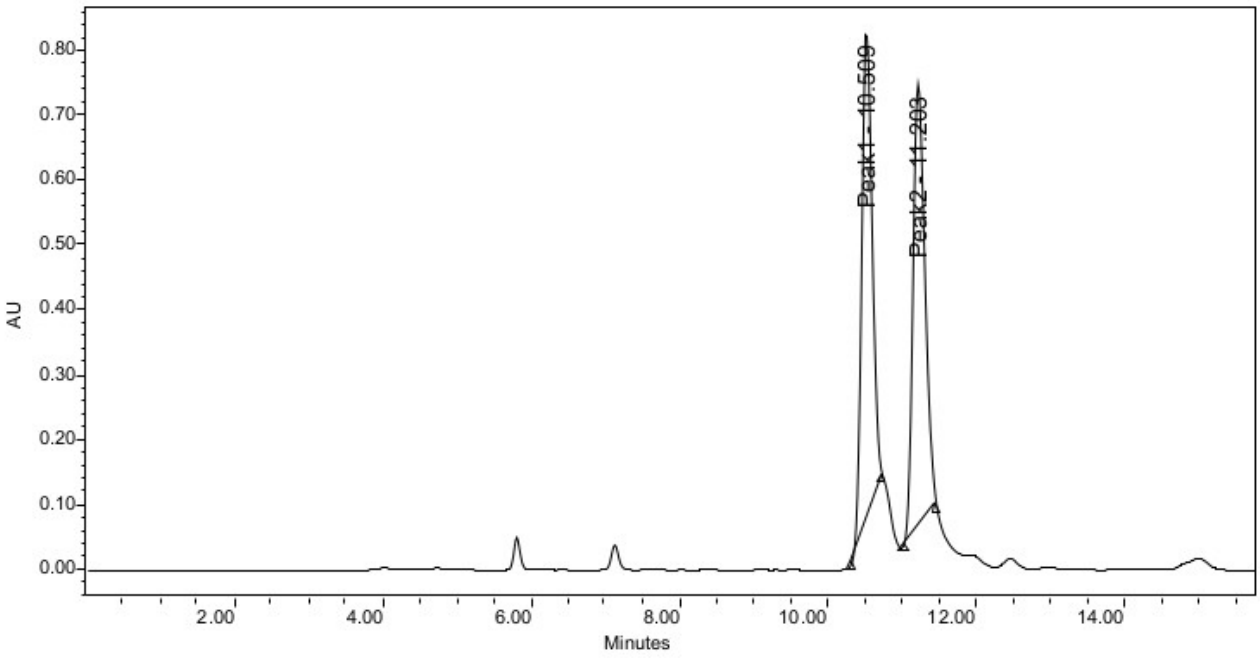


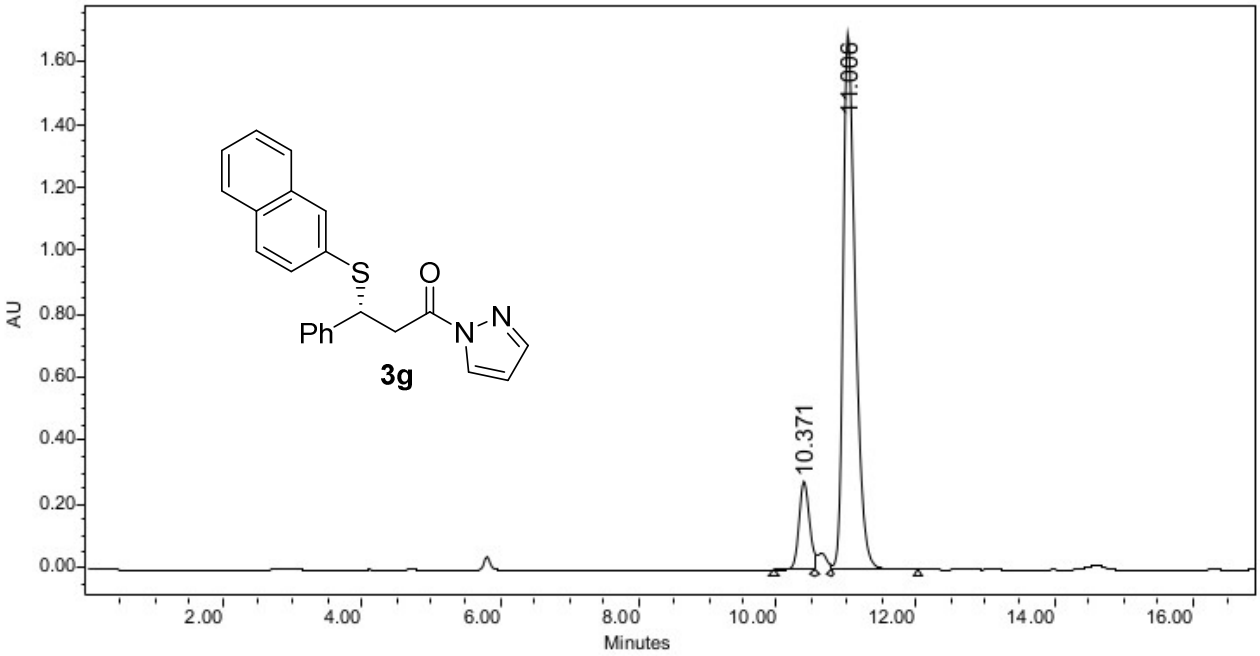
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.682	5485752	49.68	252844	51.17
2	Peak2	13.526	5557126	50.32	241306	48.83



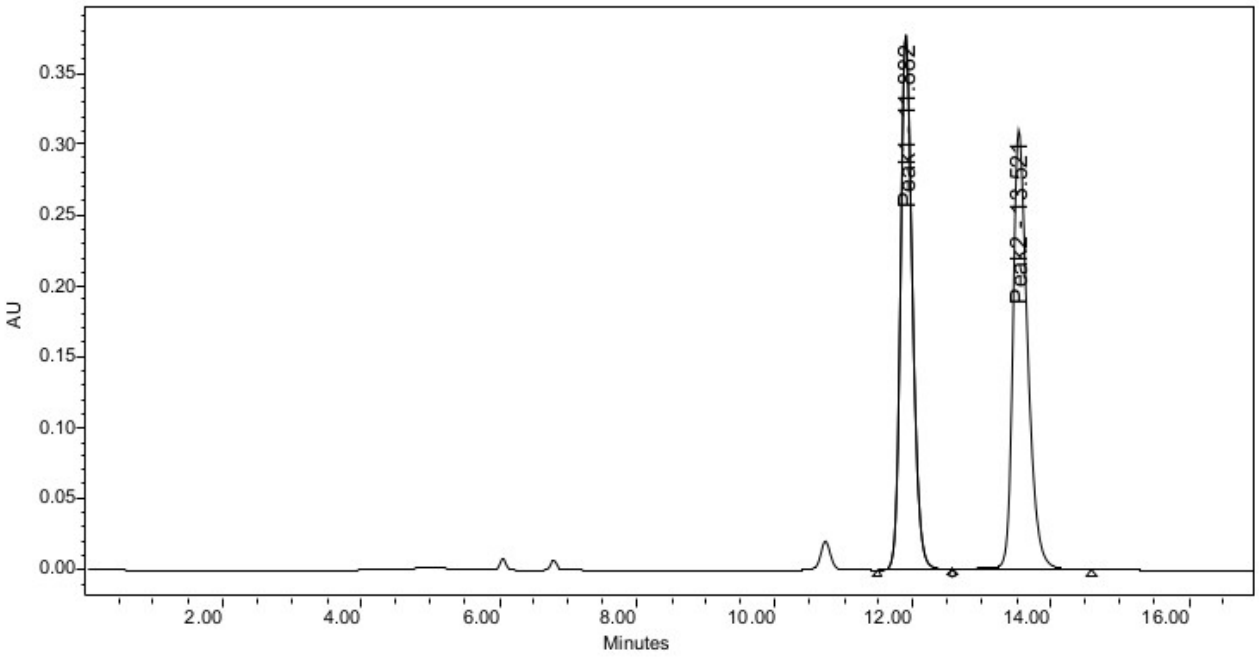
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.227	555194	8.52	25998	9.25
2	14.014	5964628	91.48	254934	90.75



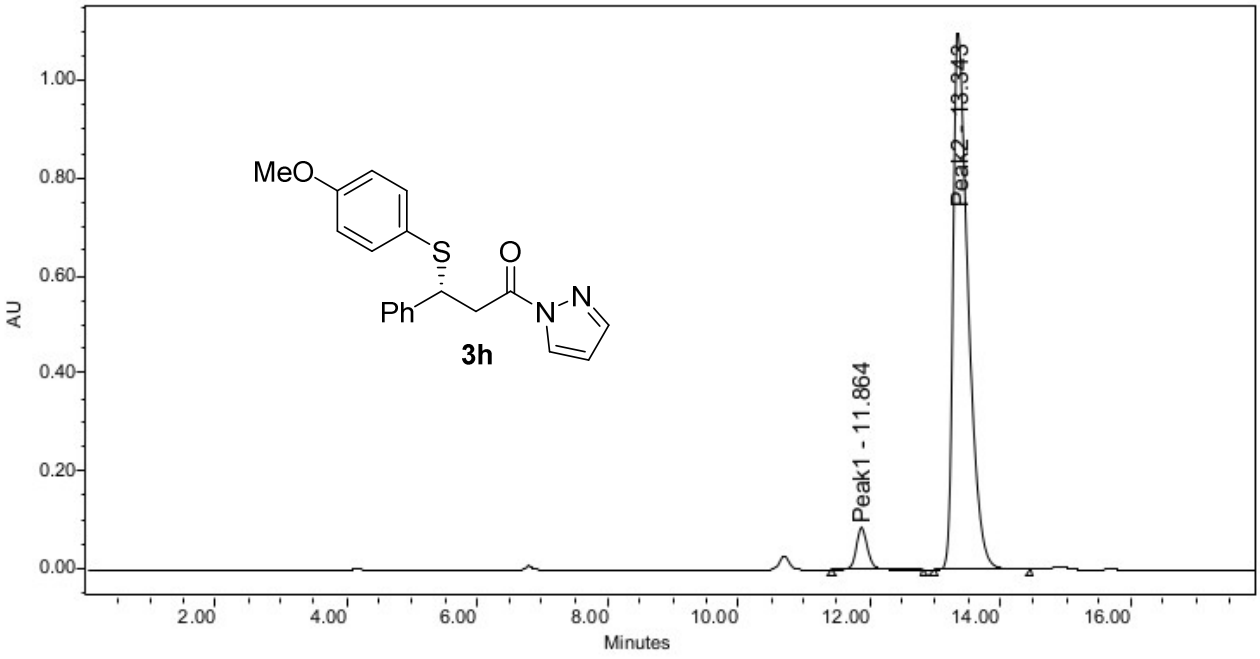
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	10.509	7362880	49.23	751828	52.43
2	Peak2	11.203	7592077	50.77	682015	47.57



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.371	2997831	12.61	279996	14.14
2	11.006	20766486	87.39	1699893	85.86



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	11.882	4547865	49.46	378258	54.87
2	Peak2	13.521	4646316	50.54	311174	45.13



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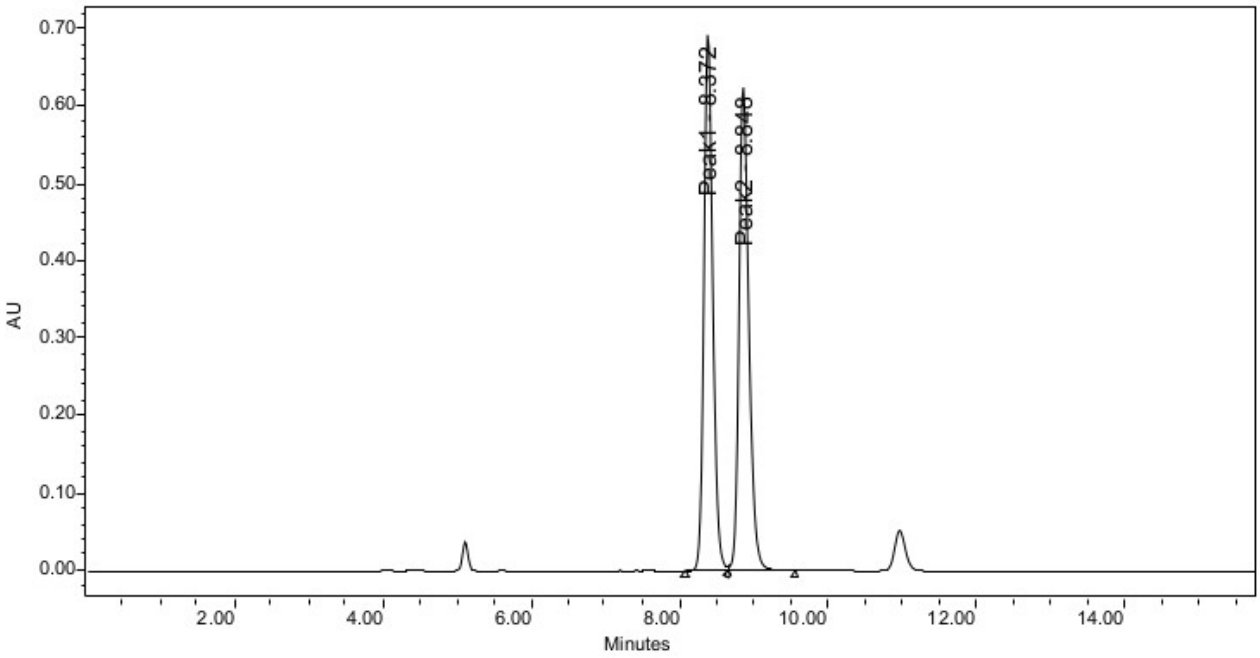
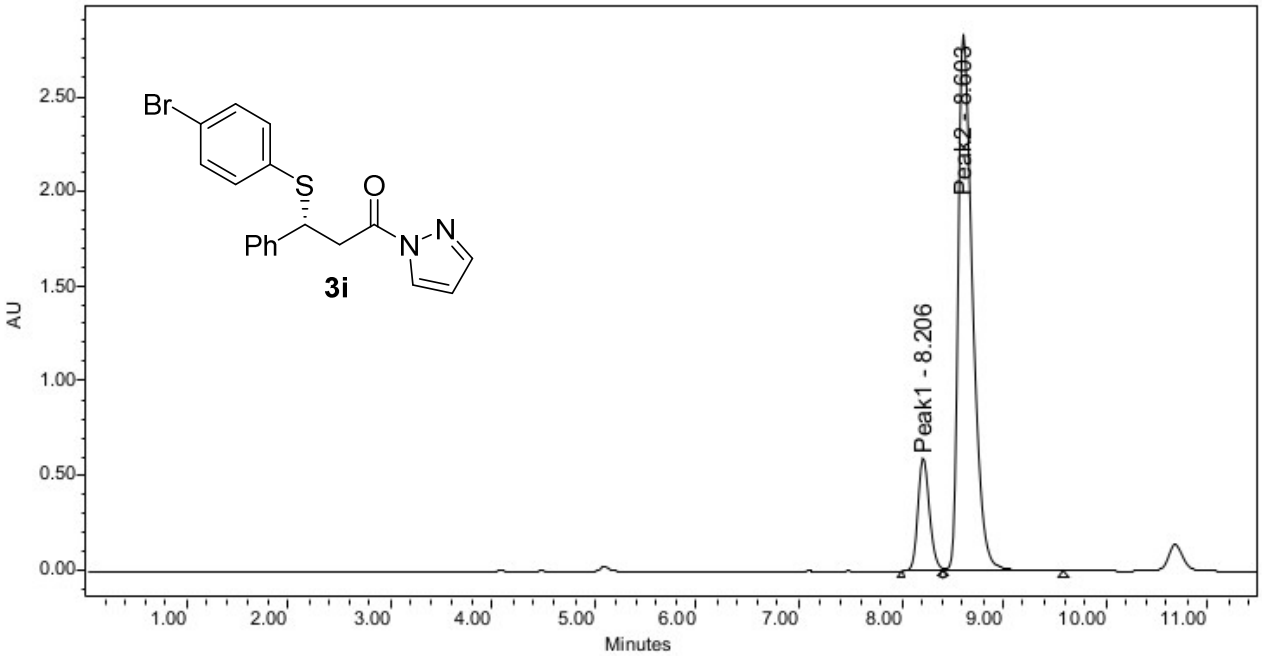
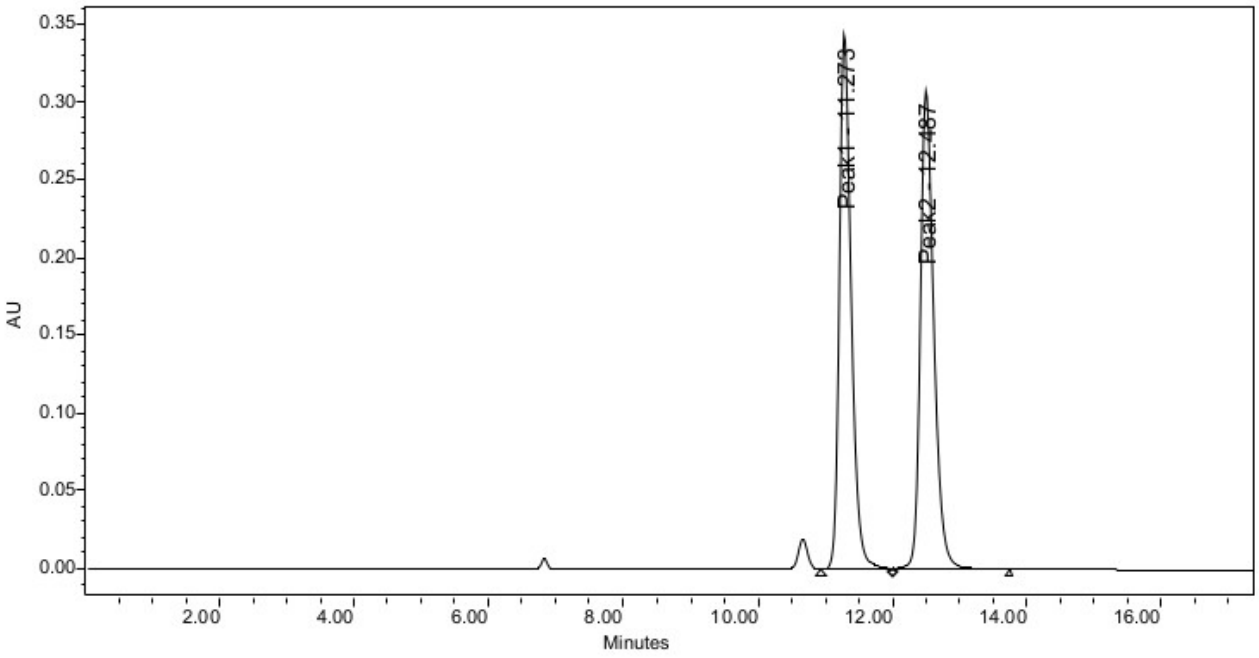
1	Peak1	11.864	1032020	5.54	85648	7.20
2	Peak2	13.343	17586174	94.46	1104169	92.80



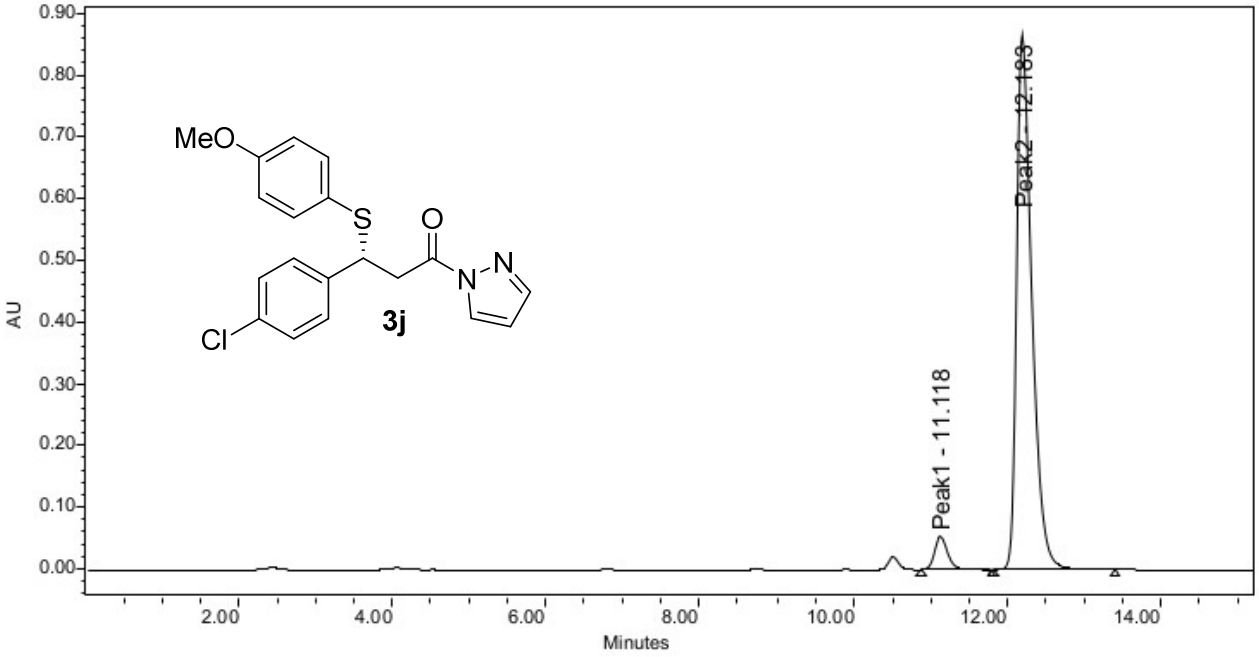
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.372	5751668	49.82	694664	52.66
2	Peak2	8.848	5792315	50.18	624442	47.34



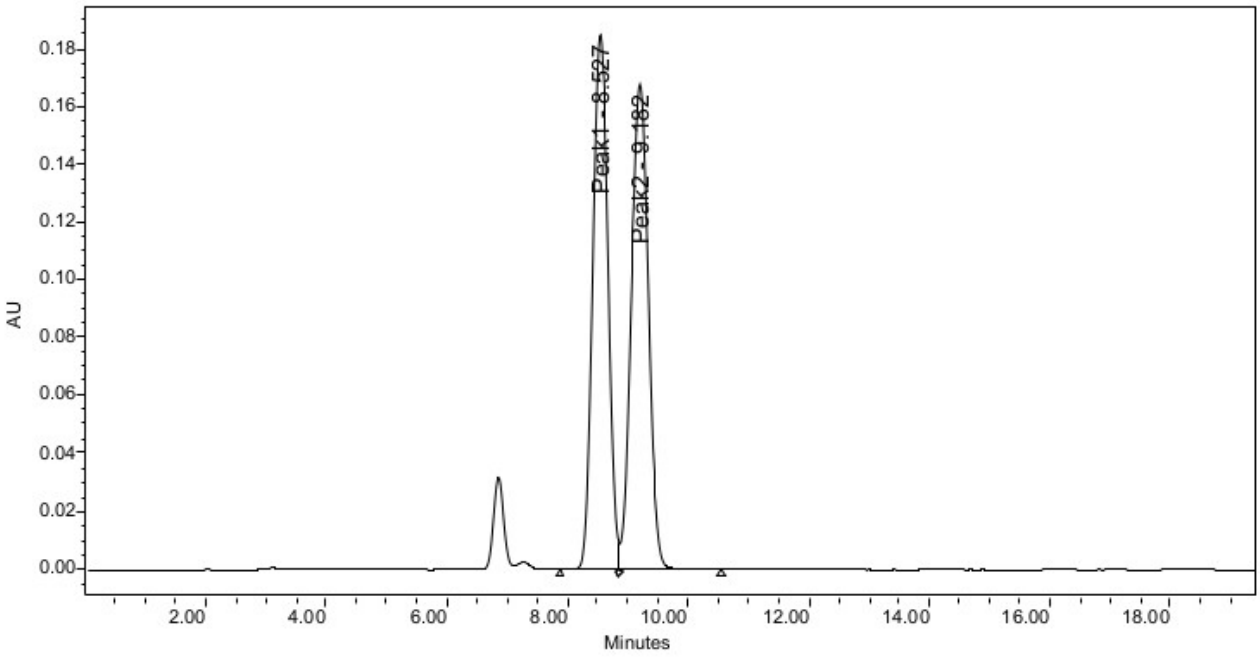
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.206	4731333	14.54	597360	17.39
2	Peak2	8.603	27816886	85.46	2838637	82.61



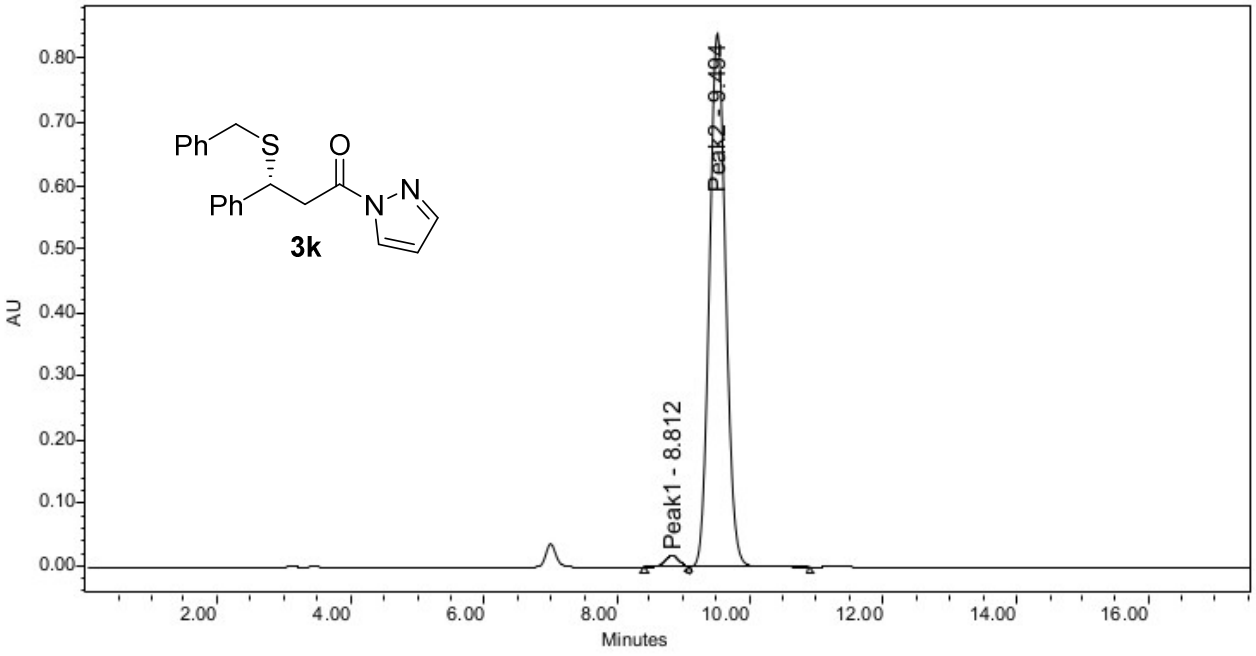
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	11.273	4215792	49.65	344385	52.83
2	Peak2	12.487	4274975	50.35	307493	47.17



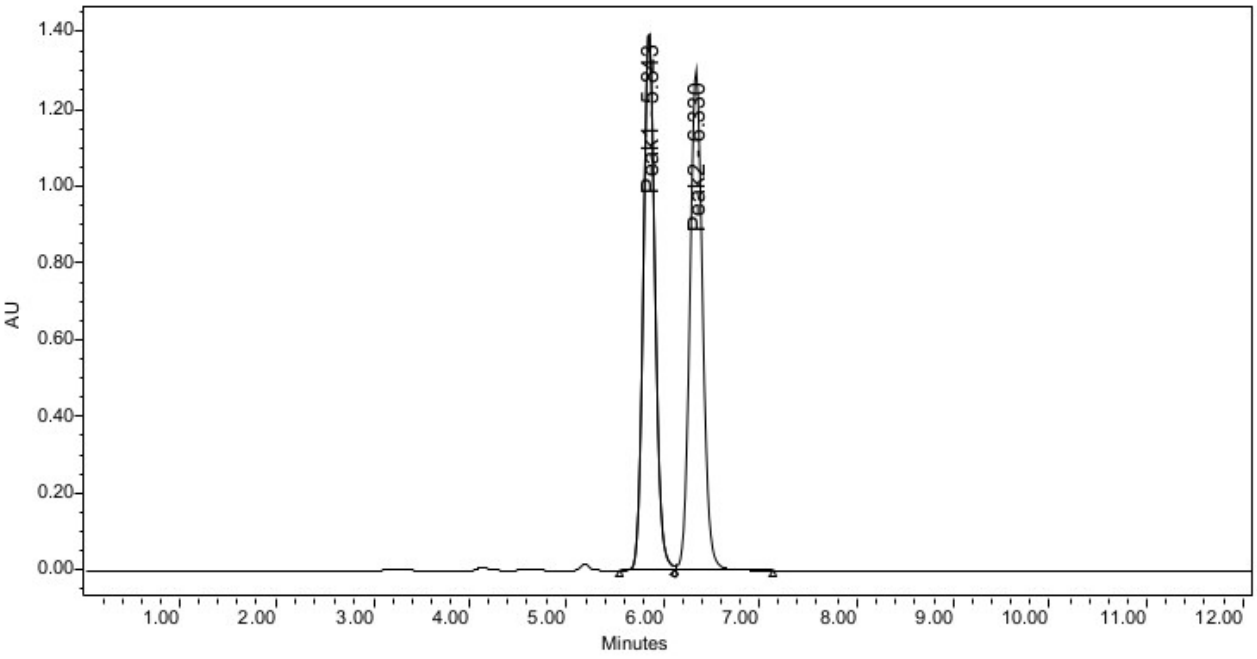
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	11.118	631605	5.05	53485	5.81
2	Peak2	12.183	11884201	94.95	866633	94.19



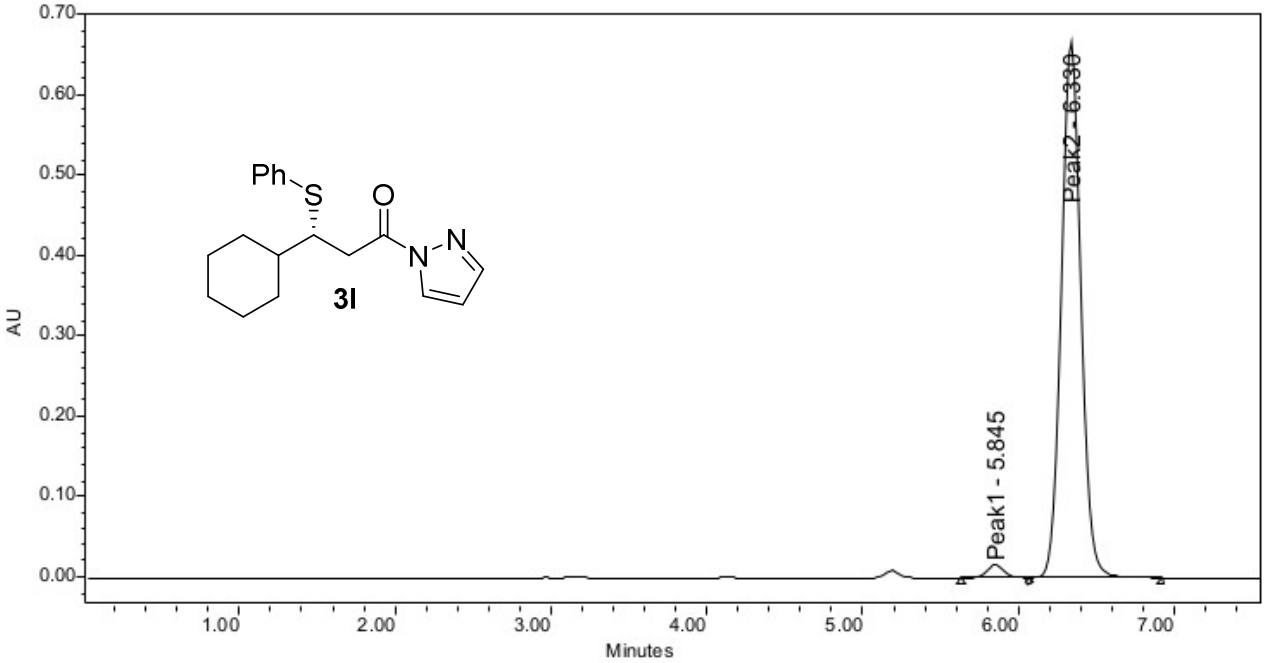
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.527	3260002	49.66	185193	52.46
2	Peak2	9.182	3304664	50.34	167857	47.54



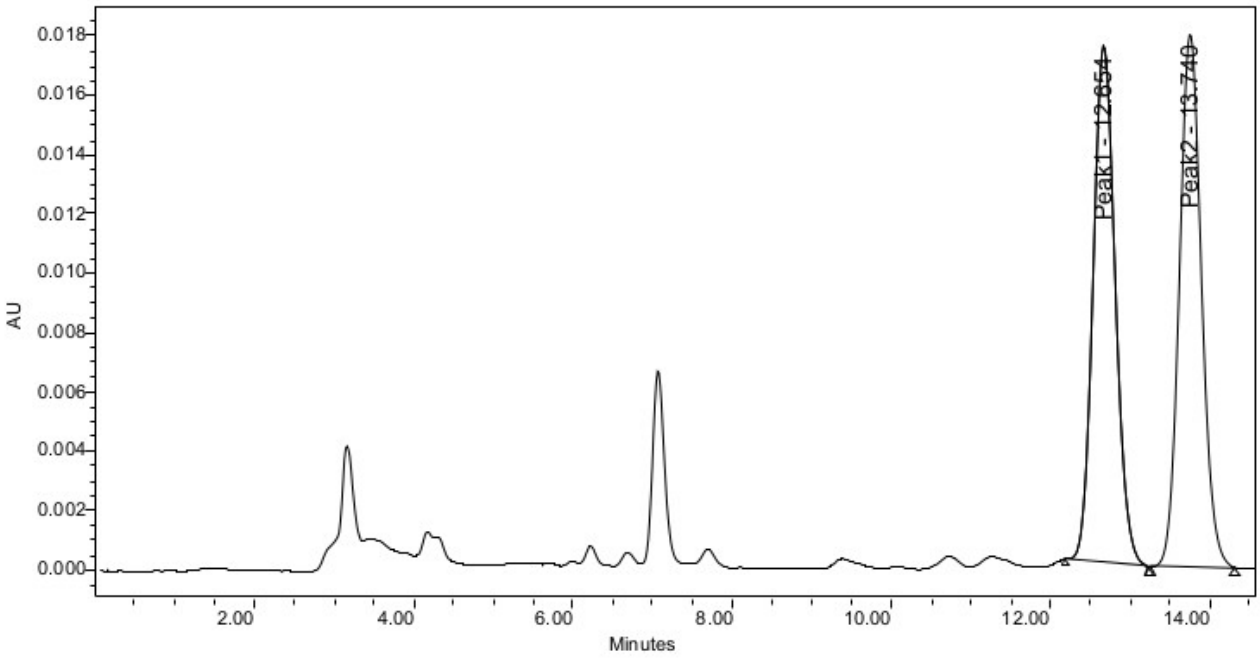
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.812	268984	1.85	18118	2.10
2	Peak2	9.494	14272823	98.15	842710	97.90



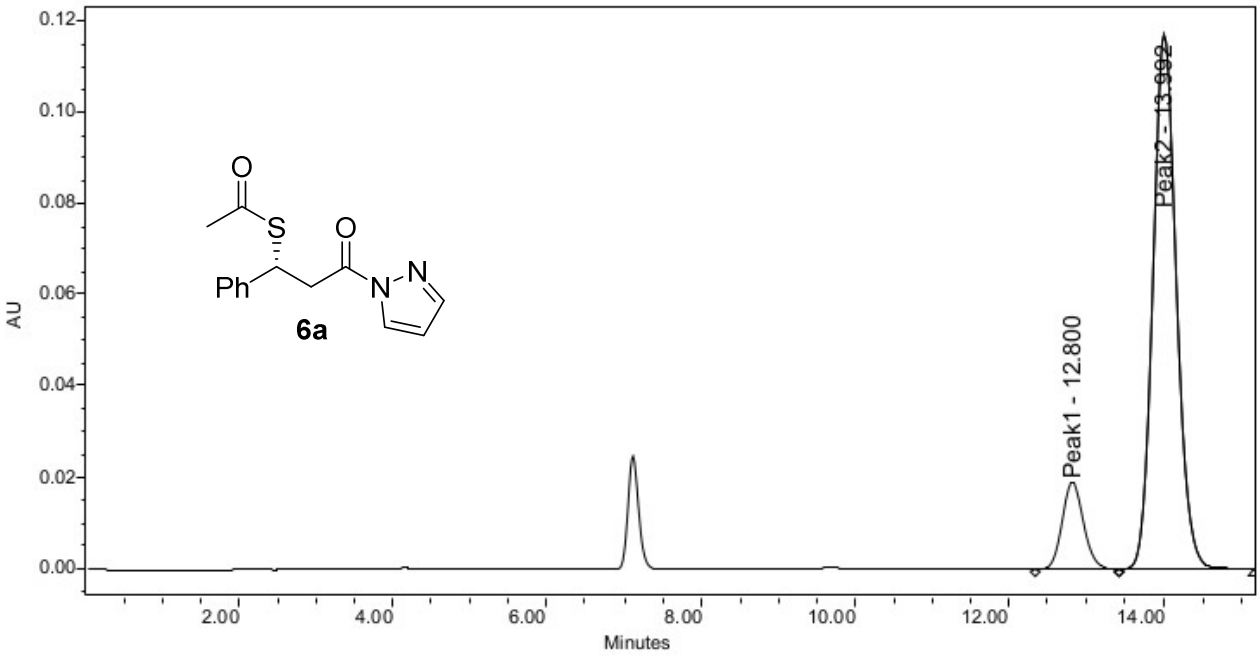
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	5.843	11823688	49.79	1402564	51.86
2	Peak2	6.330	11924428	50.21	1302055	48.14



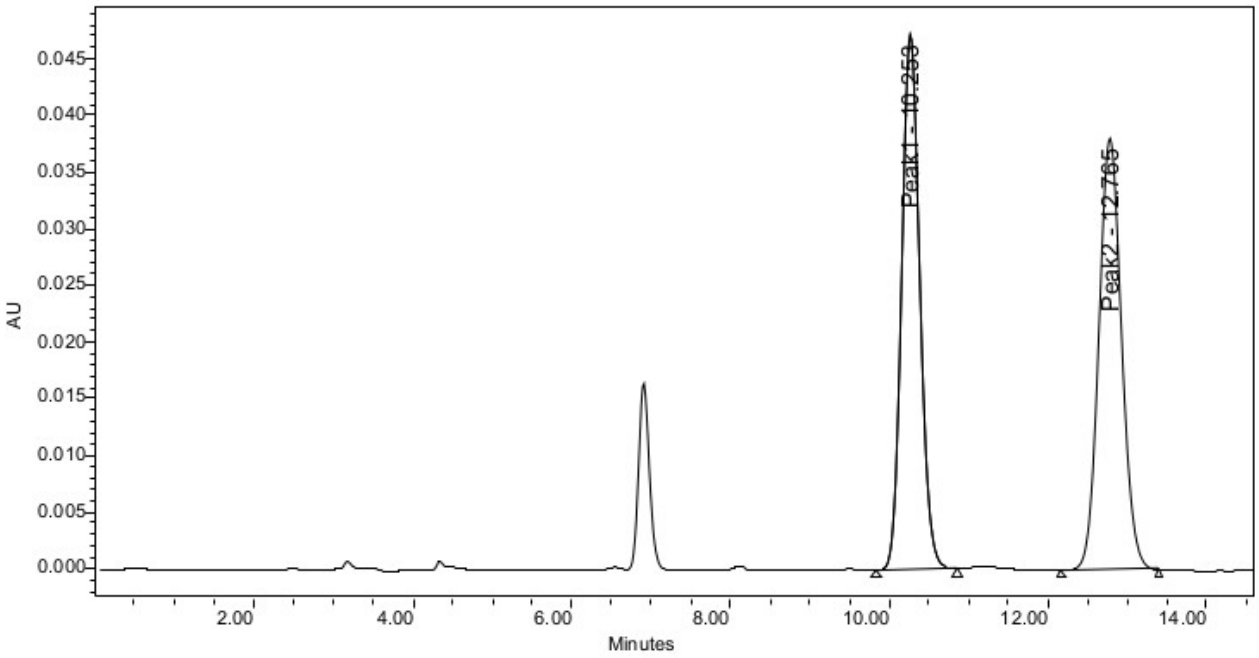
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	5.845	123775	2.09	15844	2.32
2	Peak2	6.330	5811562	97.91	666628	97.68



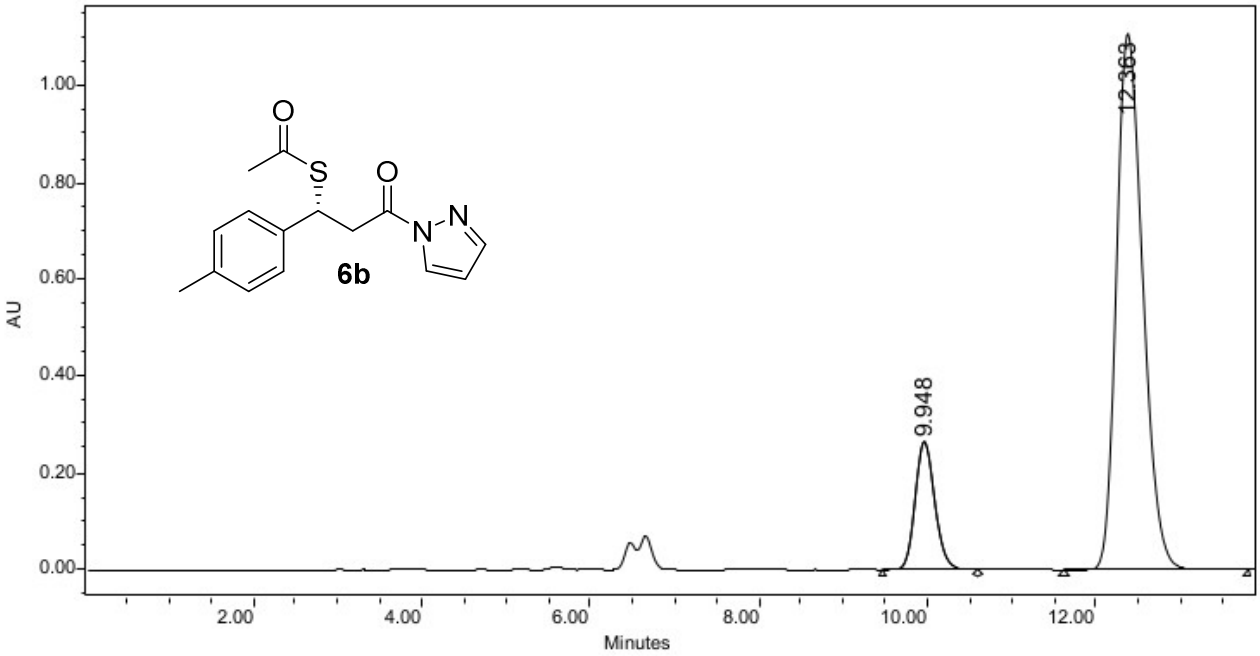
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.654	336011	49.23	17413	49.20
2	Peak2	13.740	346549	50.77	17981	50.80



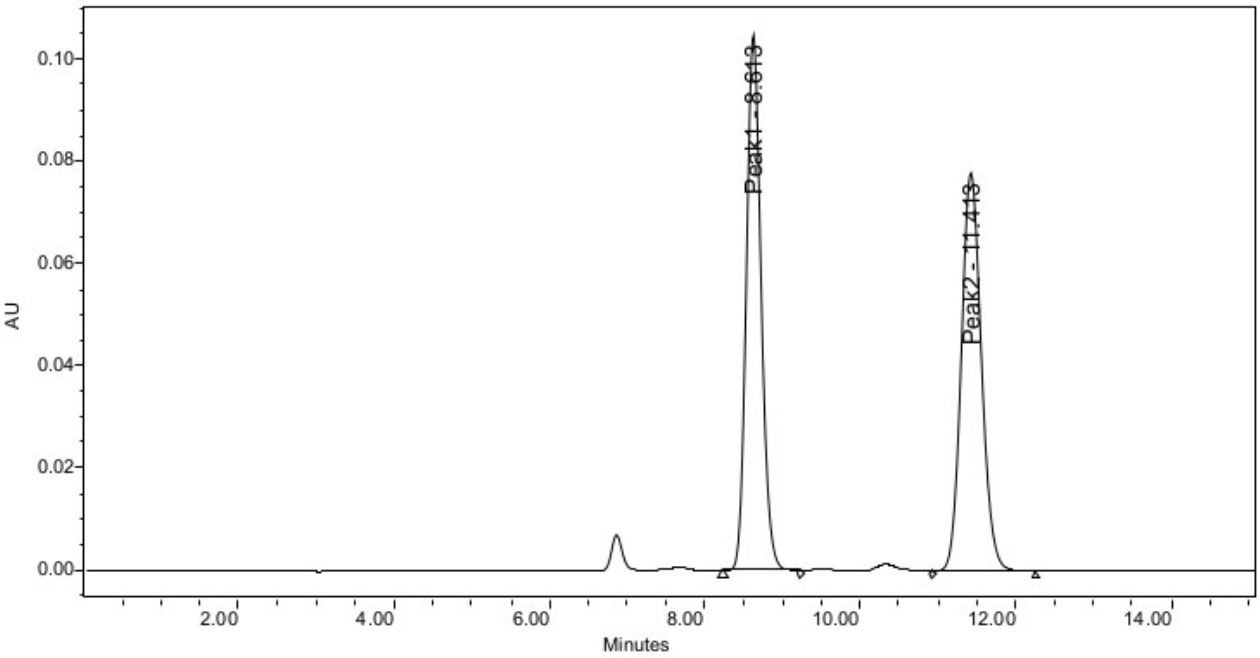
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.800	370531	13.00	19099	13.99
2	Peak2	13.992	2480781	87.00	117413	86.01



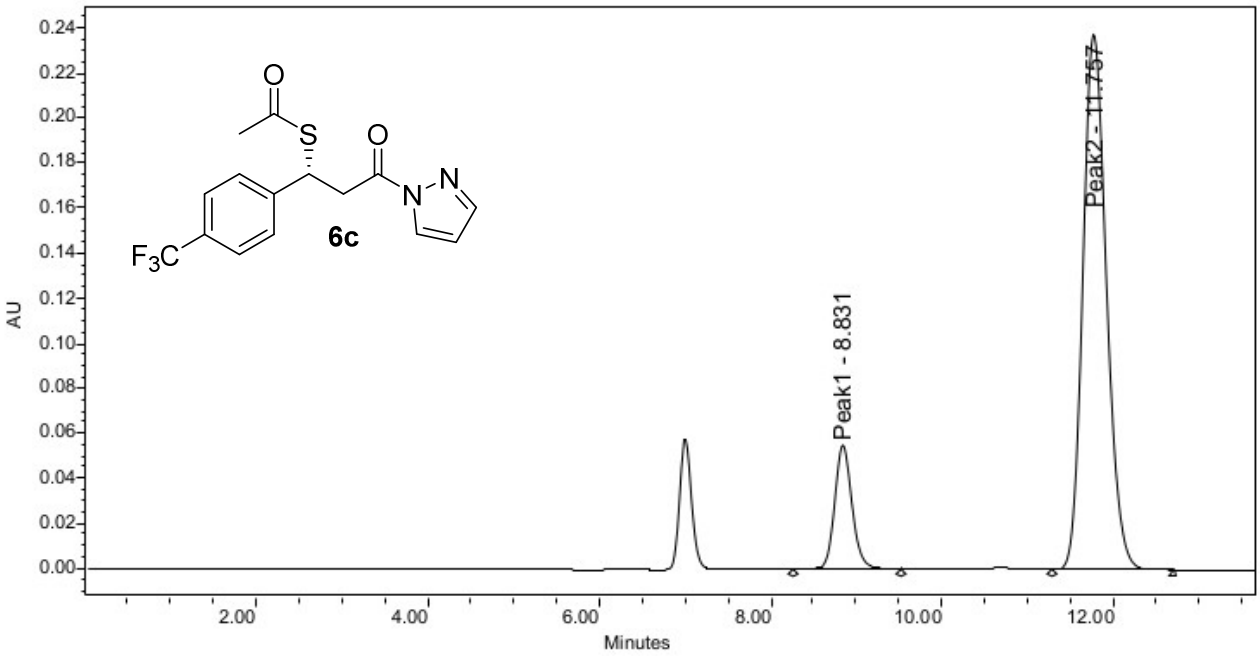
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	10.253	748906	49.72	47183	55.34
2	Peak2	12.765	757380	50.28	38081	44.66



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.948	4300098	15.17	265216	19.30
2	12.363	24044697	84.83	1108814	80.70

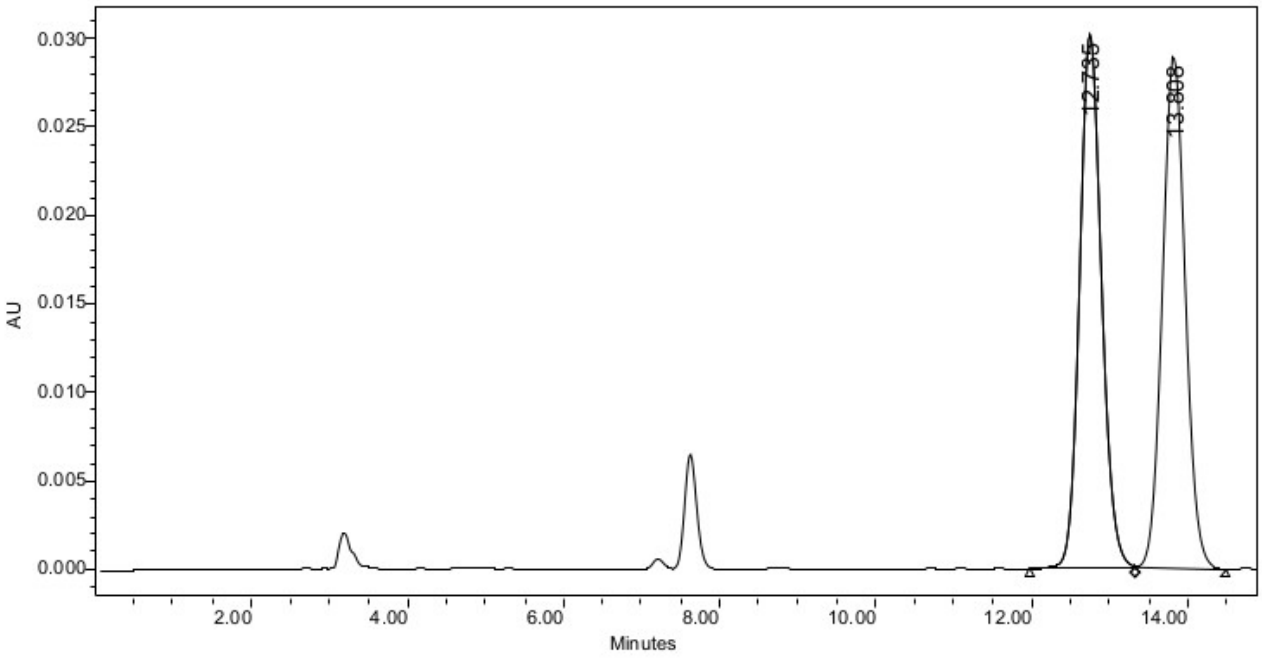


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.613	1385418	49.81	104996	57.39
2	Peak2	11.413	1395755	50.19	77970	42.61

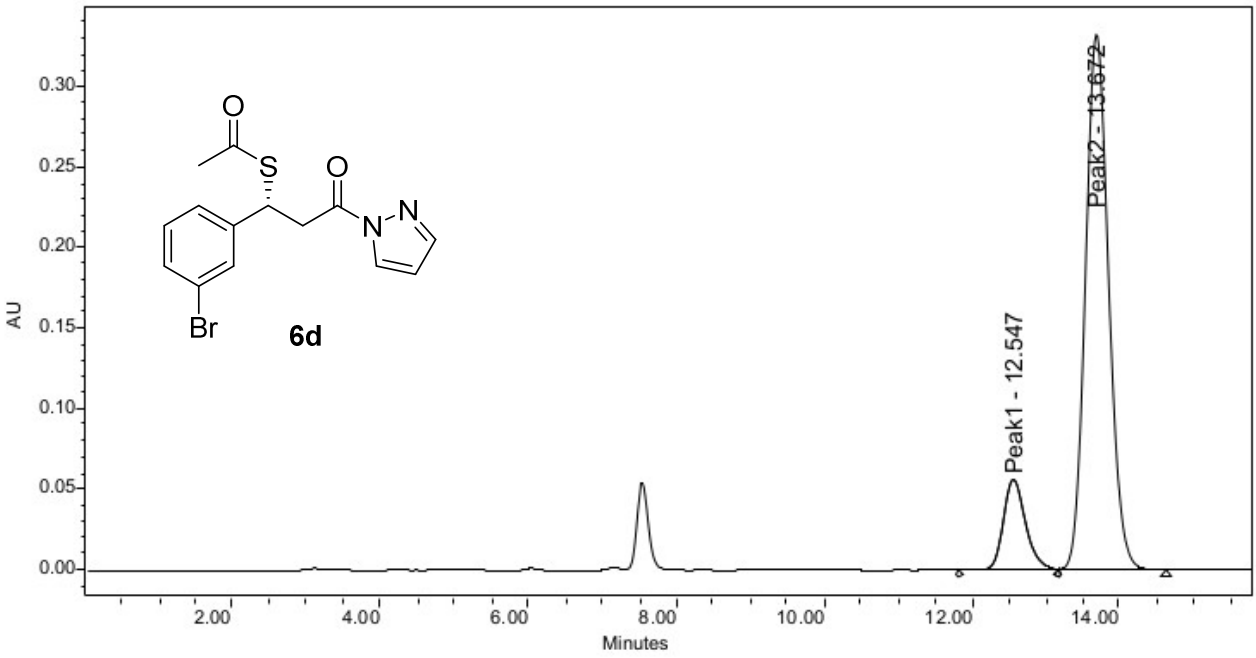


6c

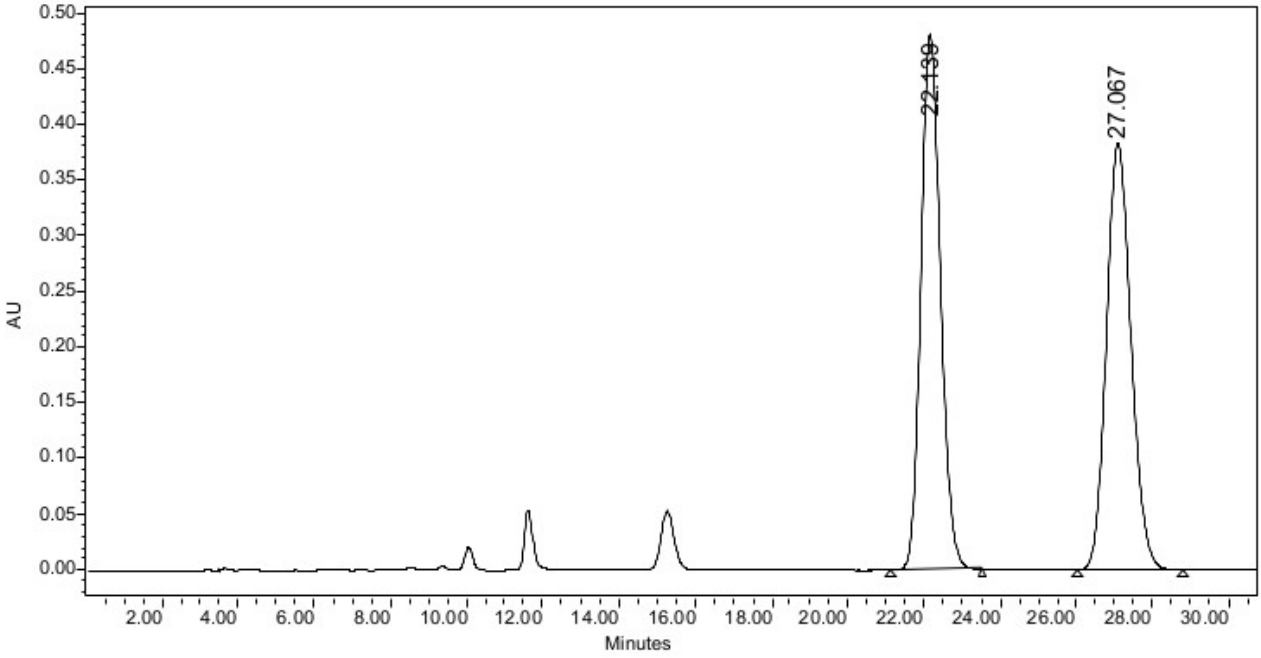
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.831	794681	14.92	55260	18.85
2	Peak2	11.757	4533013	85.08	237956	81.15



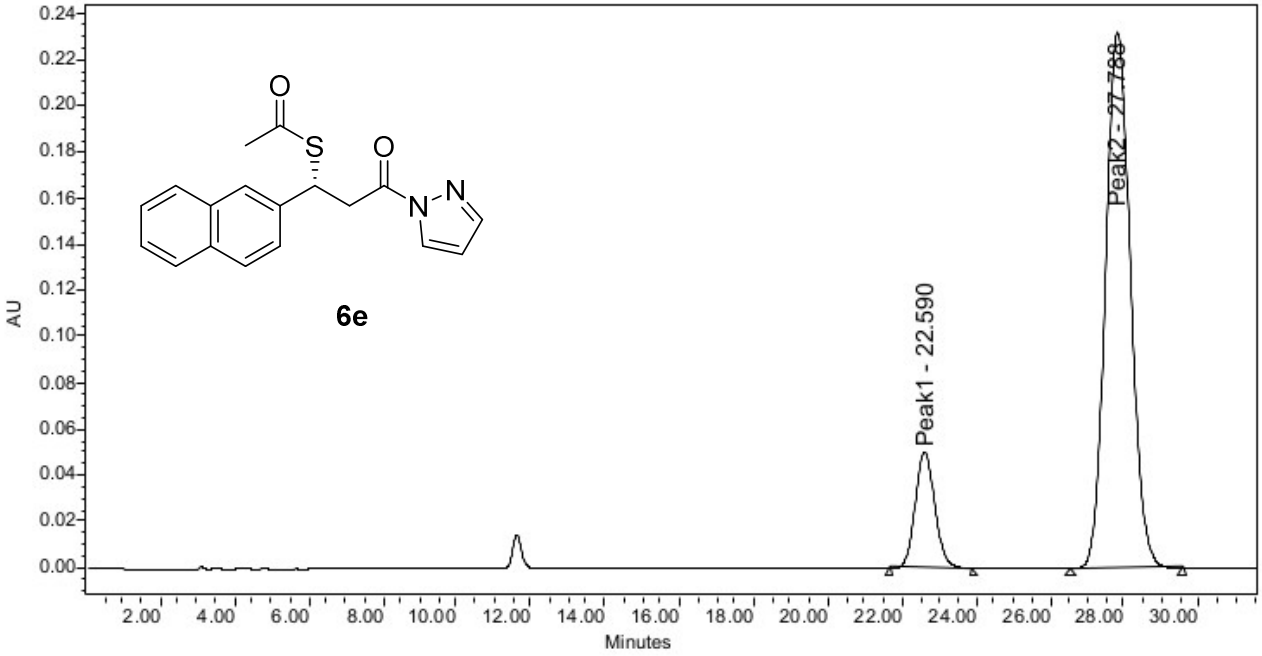
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.735	596327	50.07	30237	51.05
2	13.808	594731	49.93	28993	48.95



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.547	1185512	14.07	56512	14.52
2	Peak2	13.672	7240583	85.93	332702	85.48

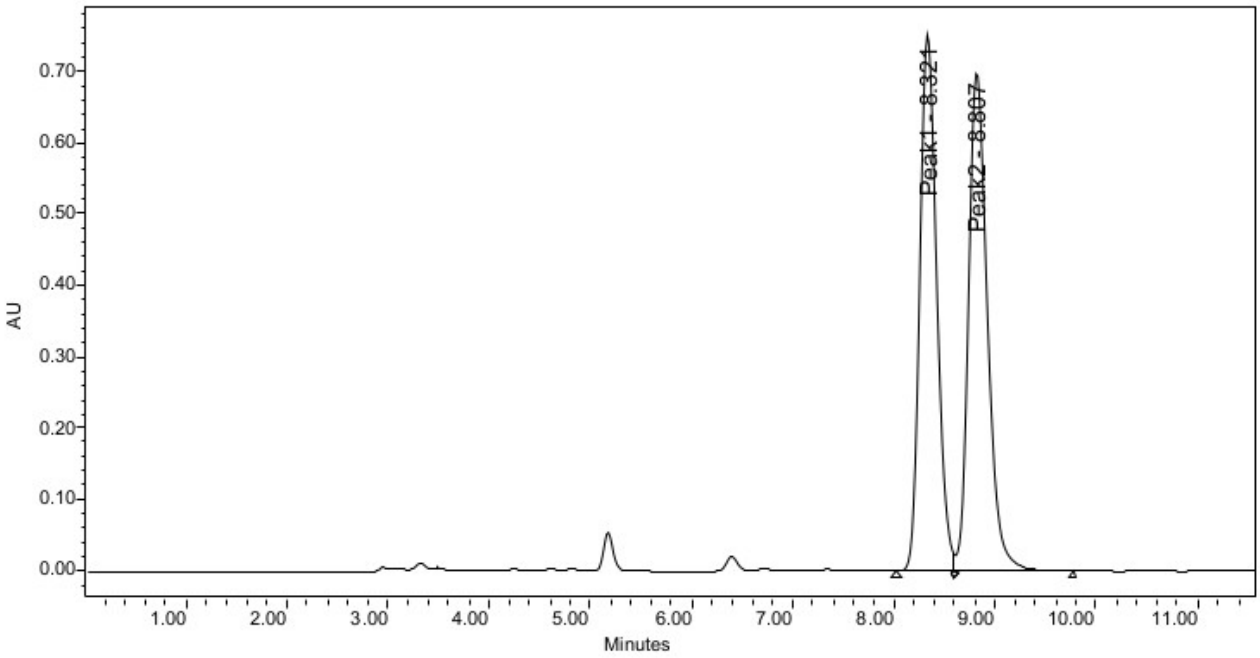


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	22.139	17177056	49.98	480343	55.63
2	27.067	17192806	50.02	383055	44.37

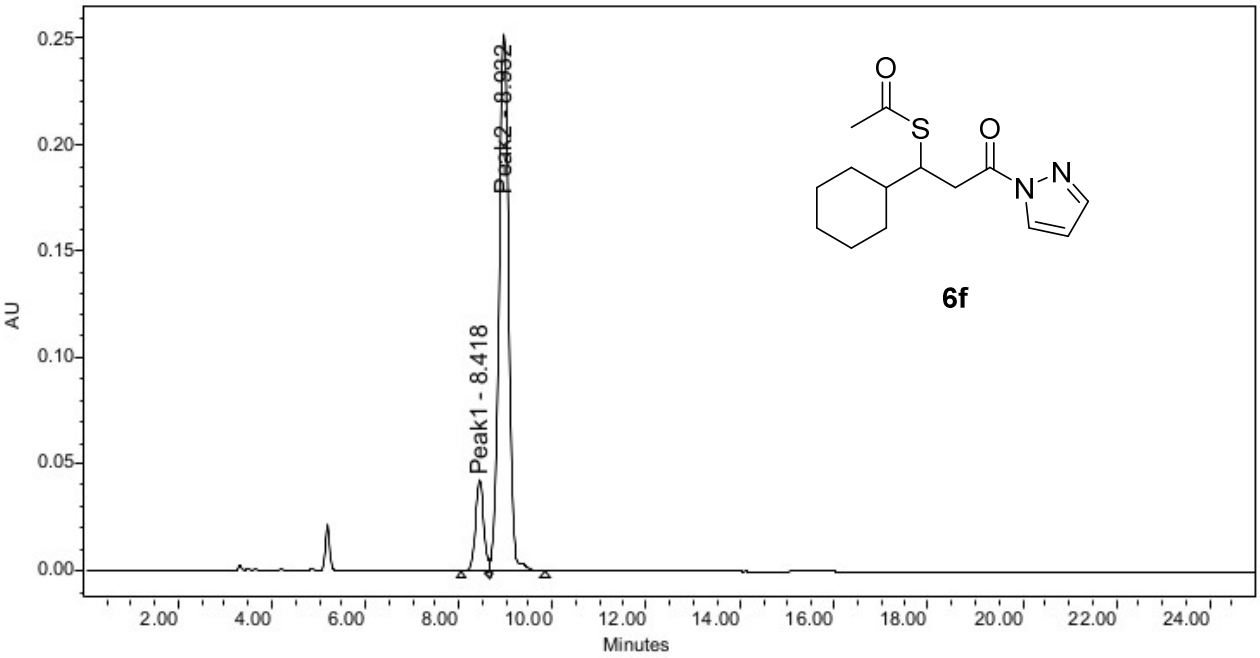


6e

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	22.590	1860394	14.66	50409	17.85
2	Peak2	27.788	10826678	85.34	232001	82.15

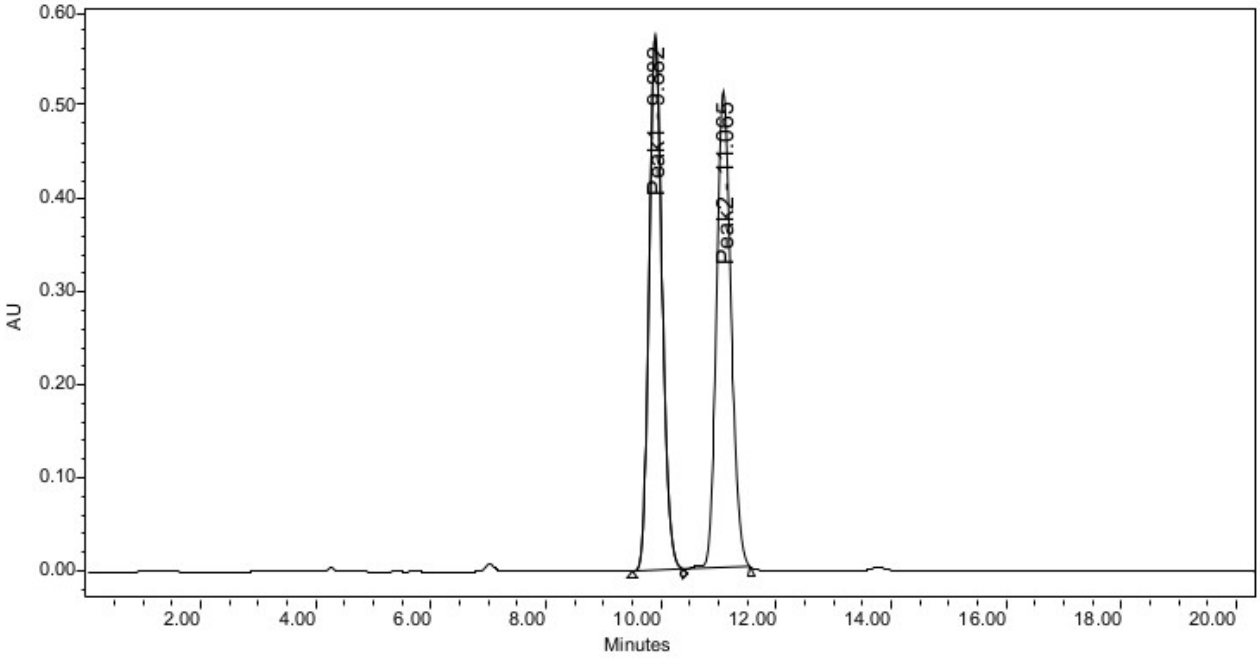


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.321	8742928	49.17	752514	51.82
2	Peak2	8.807	9039098	50.83	699623	48.18

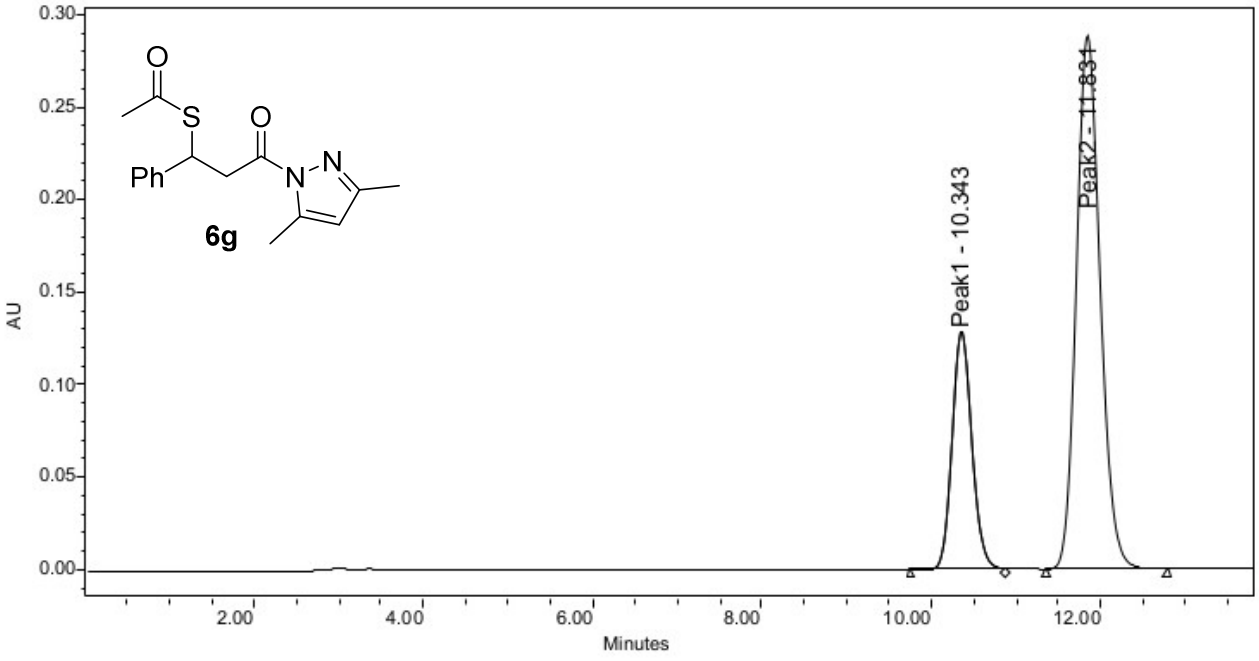


6f

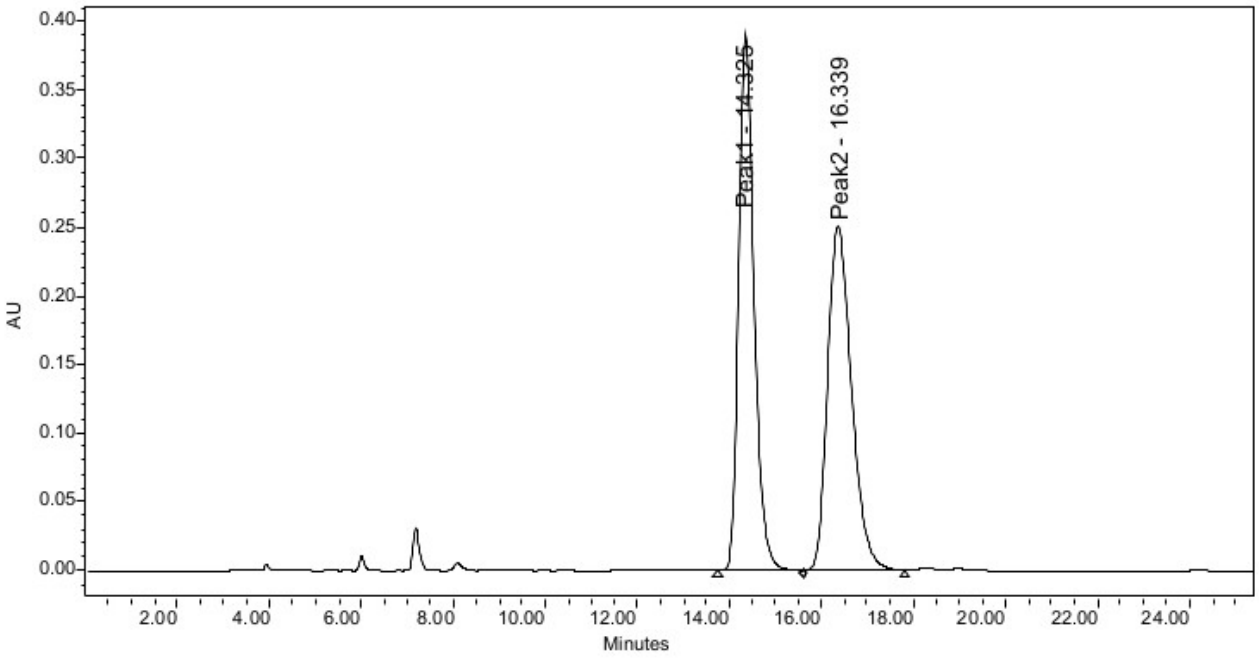
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.418	528449	12.74	42657	14.46
2	Peak2	8.932	3618157	87.26	252352	85.54



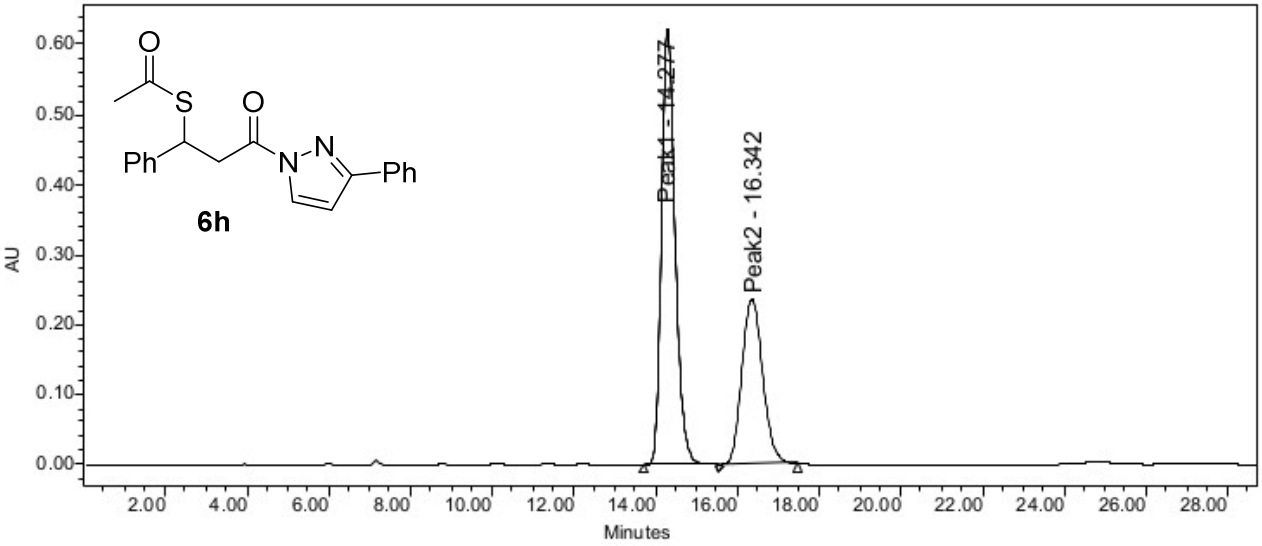
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.882	9111116	49.94	573654	52.79
2	Peak2	11.065	9131443	50.06	513114	47.21



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	10.343	2091248	27.10	128327	30.81
2	Peak2	11.831	5624242	72.90	288221	69.19

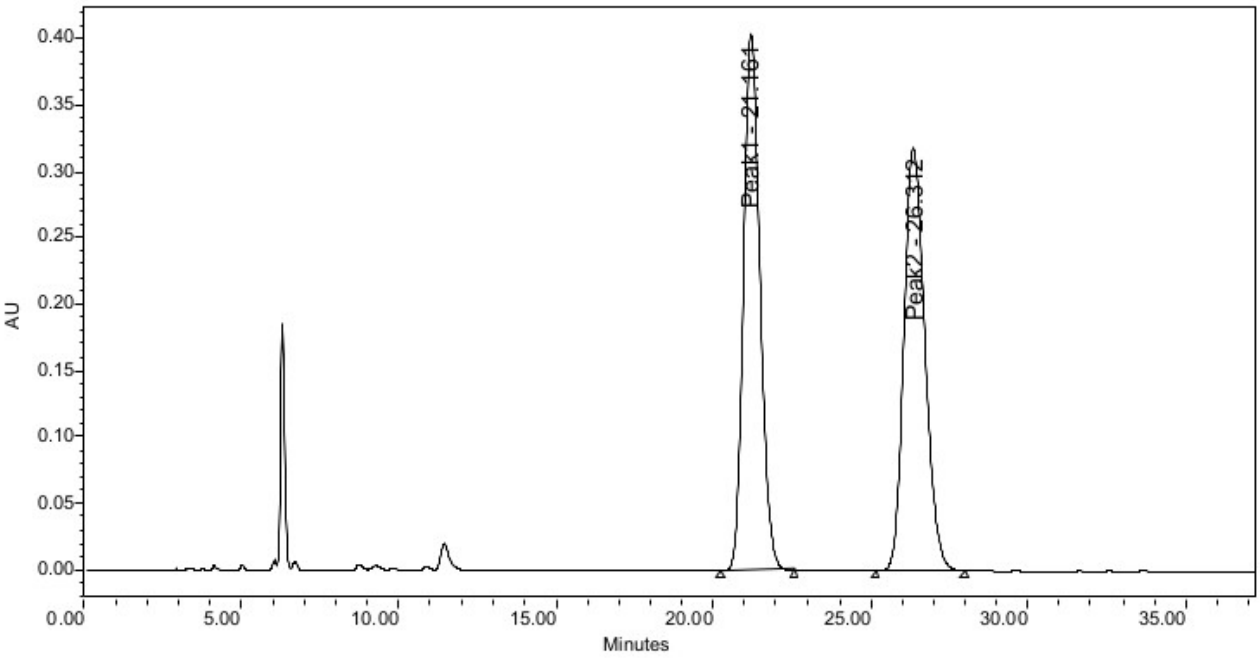


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	14.325	9037152	49.94	391579	60.93
2	Peak2	16.339	9060209	50.06	251049	39.07

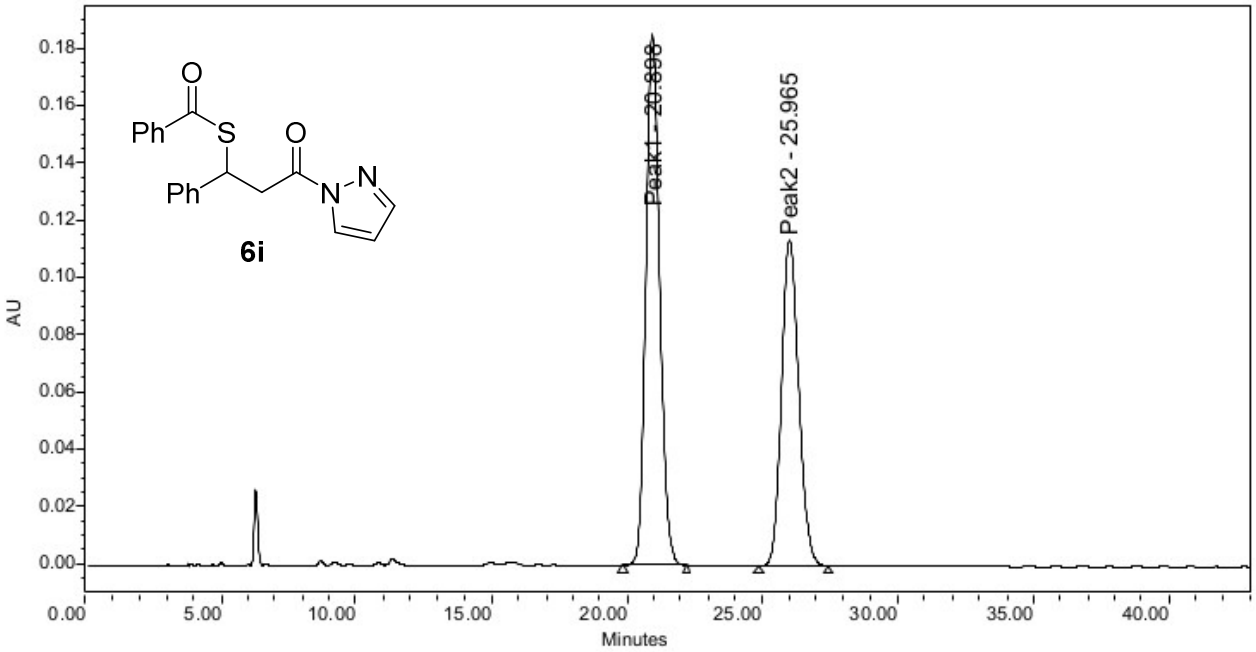


6h

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)
1	Peak1	14.277	14457477	63.27	624154
2	Peak2	16.342	8394335	36.73	236224

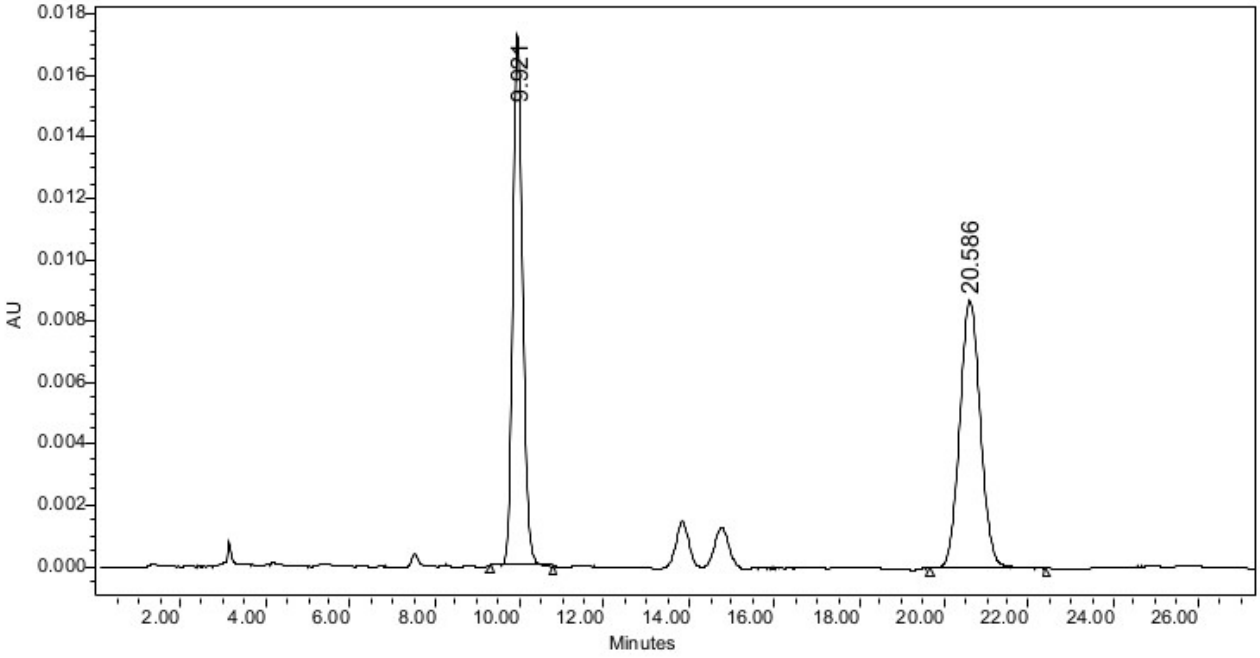


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	21.161	14738486	49.95	403774	55.87
2	Peak2	26.312	14768838	50.05	318906	44.13

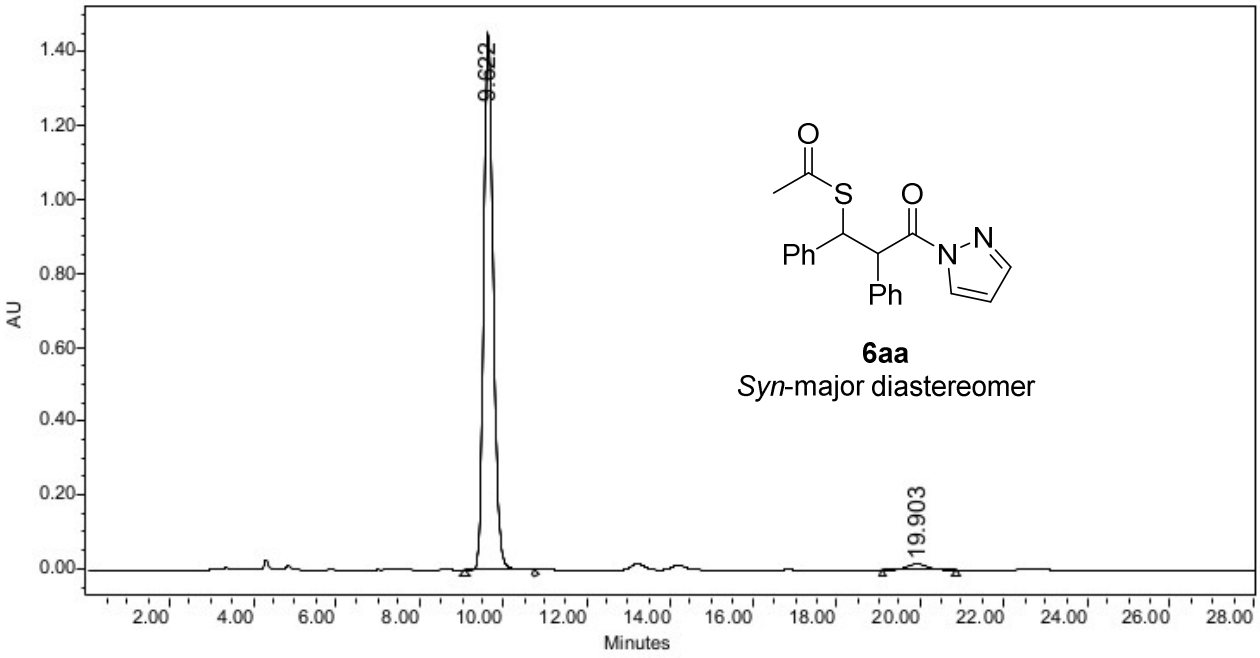


6i

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	20.898	6587314	56.68	185346	62.03
2	Peak2	25.965	5033885	43.32	113462	37.97

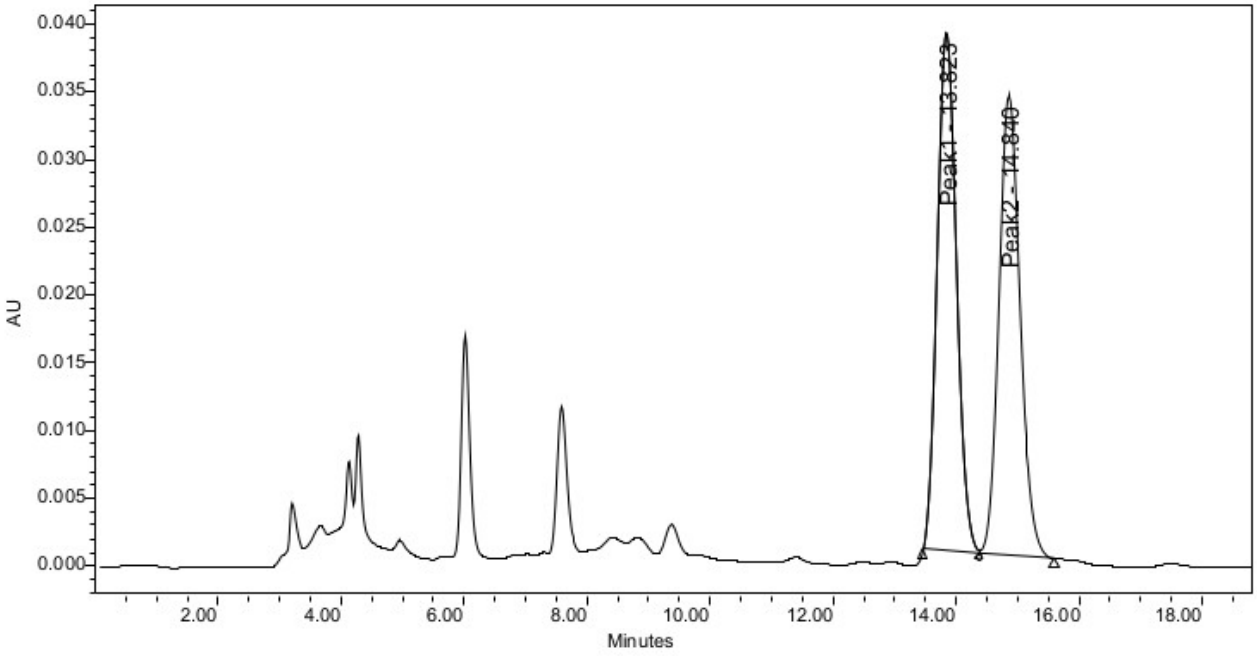


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.921	281769	48.73	17345	66.49
2	20.586	296413	51.27	8741	33.51

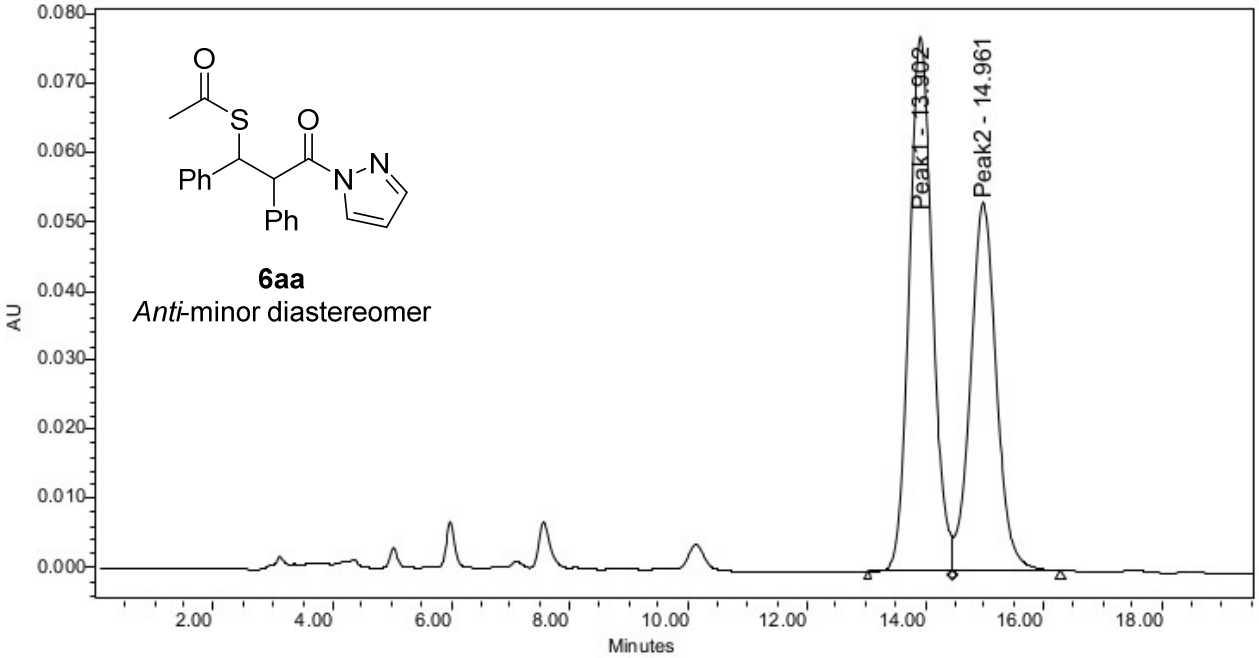


6aa
Syn-major diastereomer

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.622	23385749	97.71	1454059	98.88
2	19.903	547645	2.29	16451	1.12

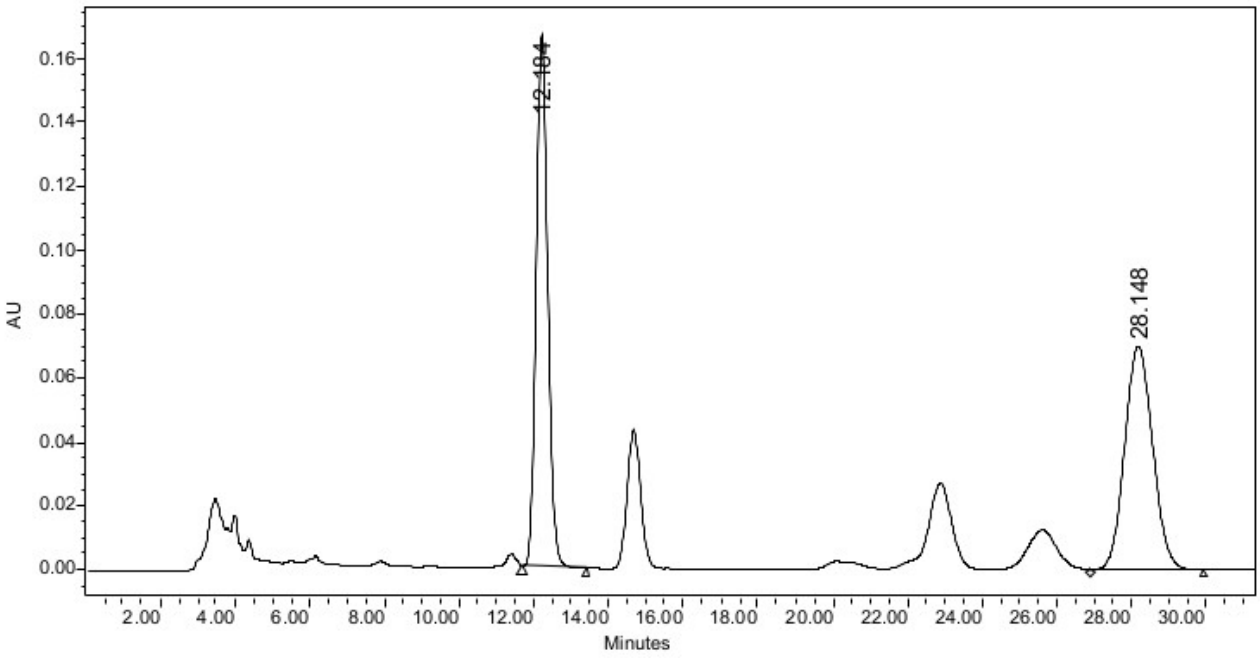


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	13.823	832439	50.60	38271	52.94
2	Peak2	14.840	812753	49.40	34014	47.06

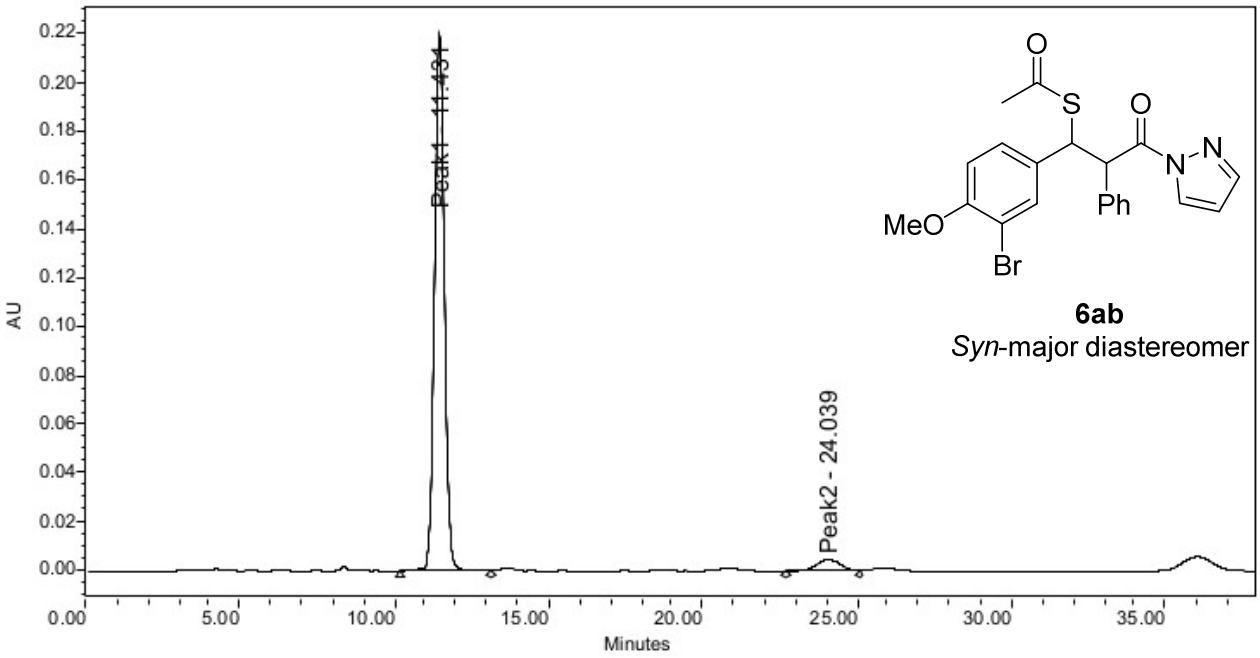


6aa
Anti-minor diastereomer

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	13.902	2098508	56.48	77253	59.17
2	Peak2	14.961	1616843	43.52	53305	40.83

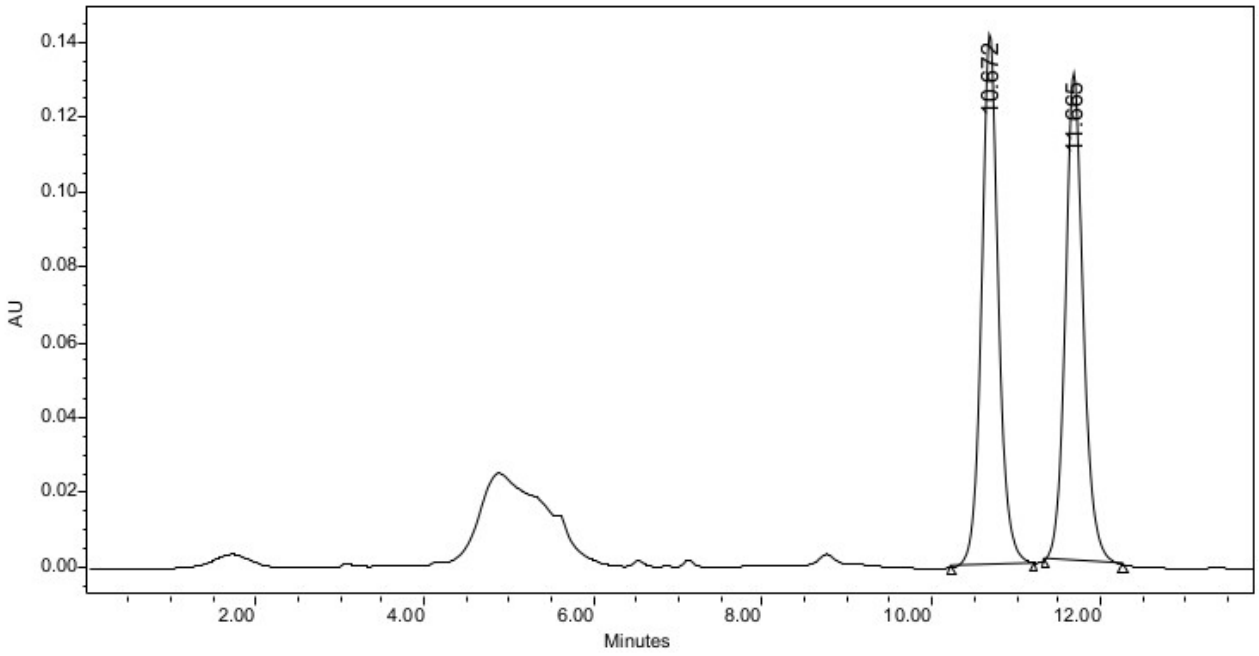


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.184	3612182	49.67	166761	70.41
2	28.148	3659629	50.33	70086	29.59

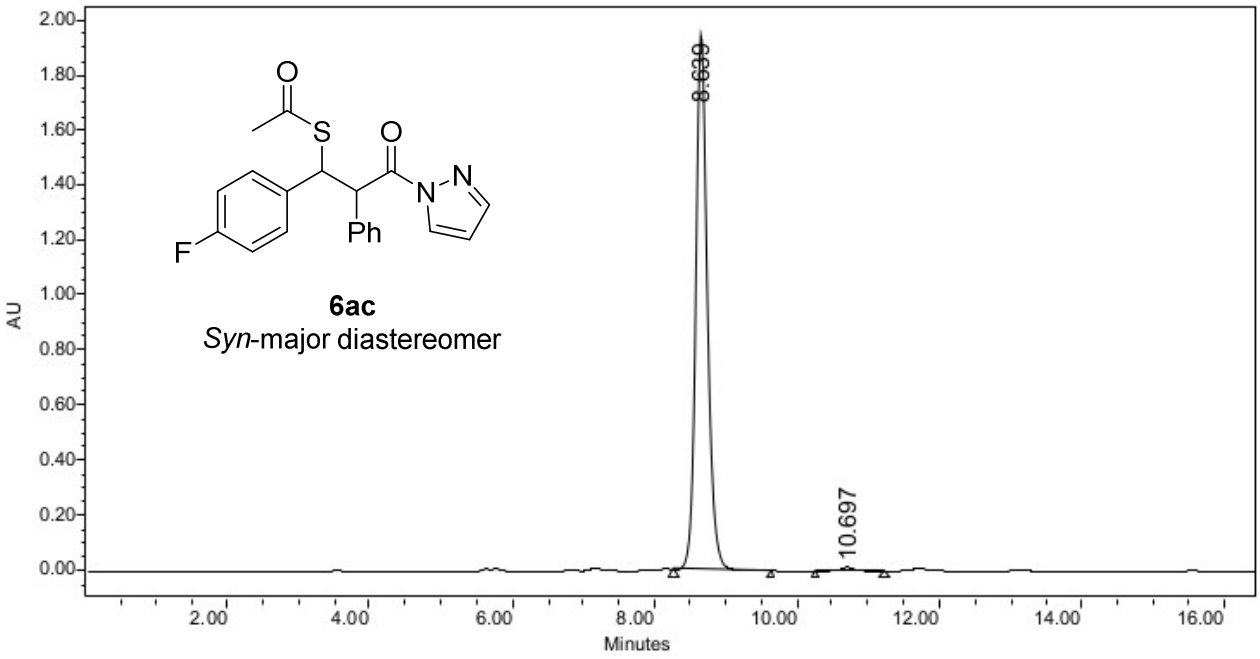


6ab
Syn-major diastereomer

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	11.431	4903233	94.93	219965	97.86
2	Peak2	24.039	261669	5.07	4811	2.14

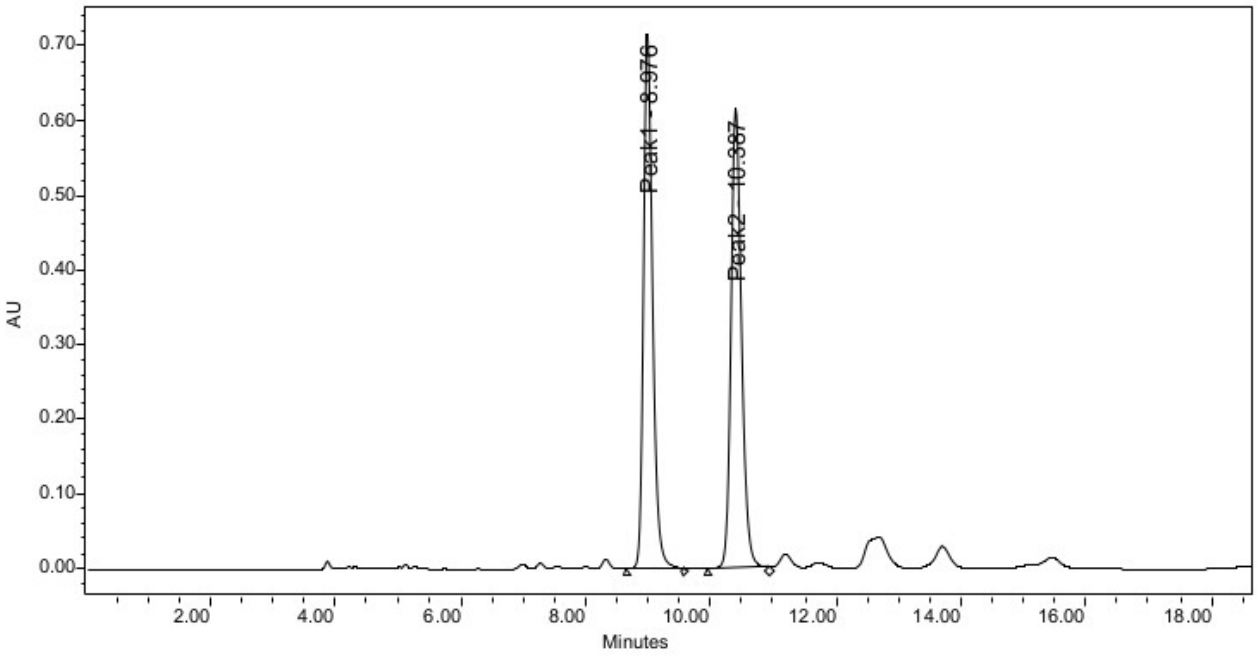


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.672	1965852	50.60	141658	52.14
2	11.665	1919581	49.40	130006	47.86

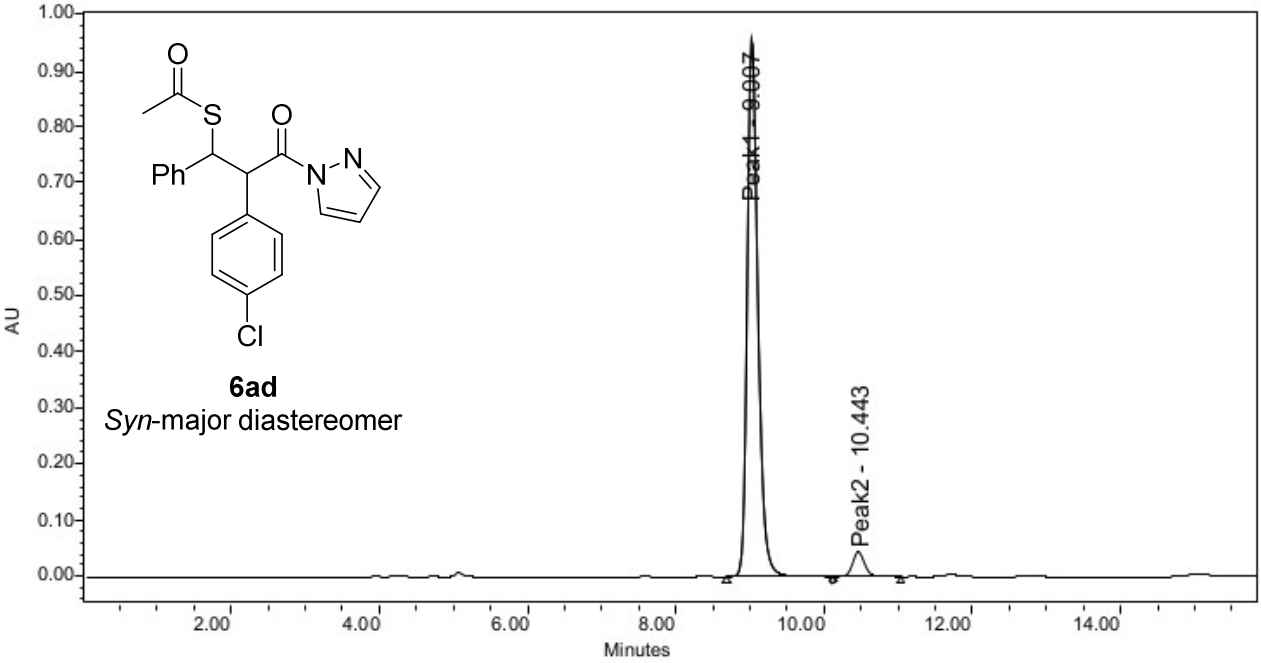


6ac
Syn-major diastereomer

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.639	22085293	99.20	1951228	99.31
2	10.697	178473	0.80	13464	0.69

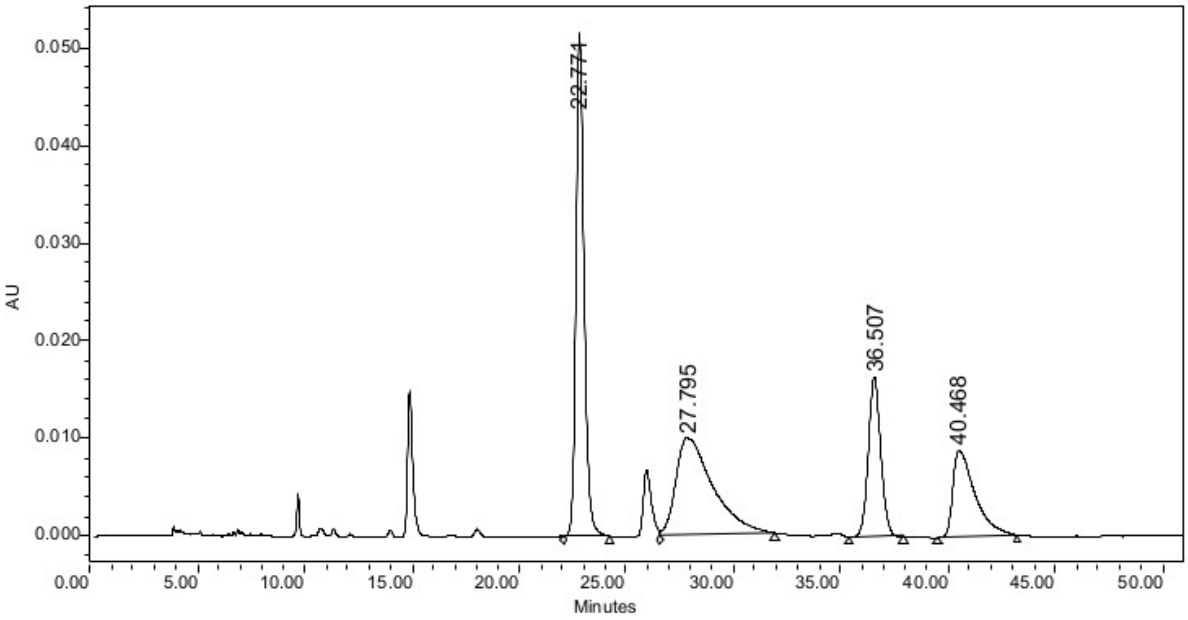


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	8.976	7215683	49.92	721915	53.89
2	Peak2	10.387	7237663	50.08	617654	46.11

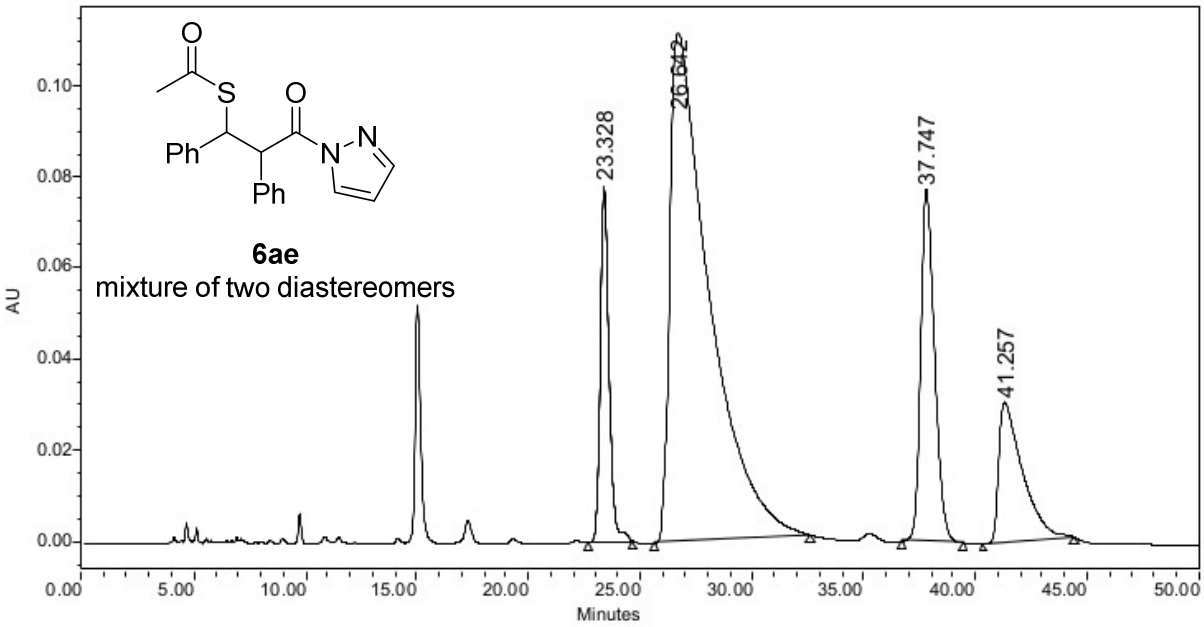


6ad
Syn-major diastereomer

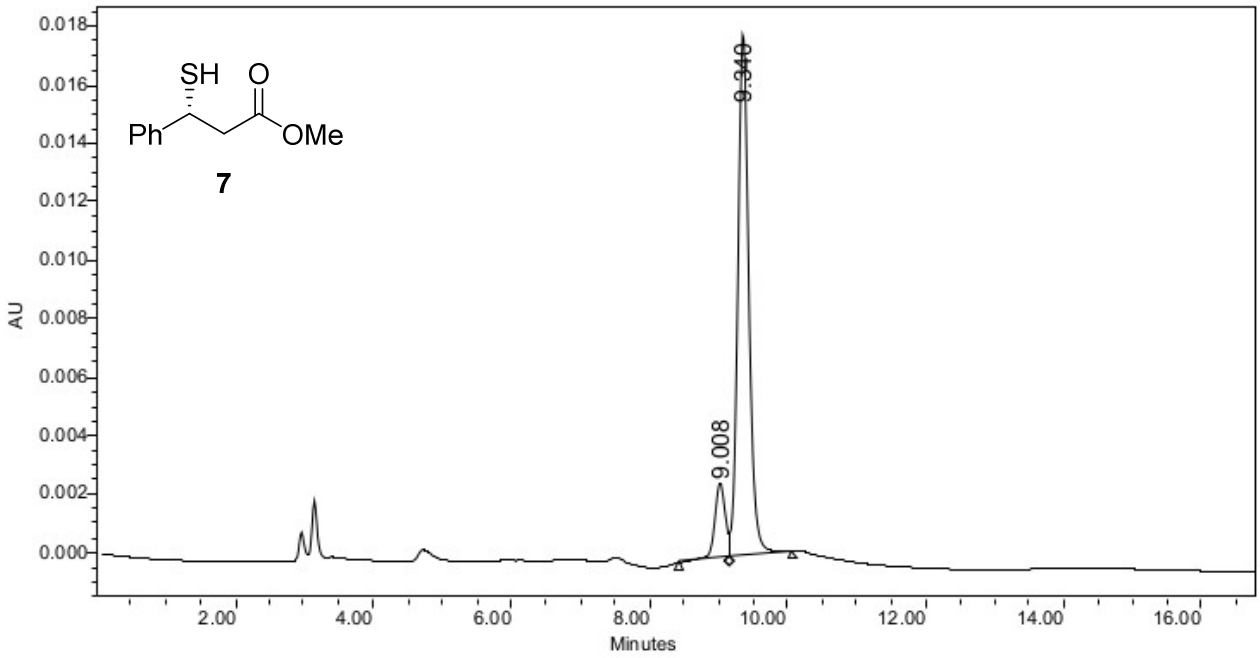
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.007	9670203	95.02	961741	95.61
2	Peak2	10.443	506726	4.98	44170	4.39



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	22.771	1364366	35.22	51737	59.38
2	27.795	1205788	31.13	10019	11.50
3	36.507	665331	17.18	16425	18.85
4	40.468	638275	16.48	8942	10.26



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	23.328	2123981	9.92	77897	26.23
2	26.642	13704498	64.00	111359	37.50
3	37.747	3317975	15.49	77040	25.94
4	41.257	2268449	10.59	30650	10.32



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.008	28333	12.50	2576	12.59
2	9.340	198255	87.50	17891	87.41

Table S5. Relative energy (kcal/mol) of the most populated conformations of *syn* and *anti* diastereoisomers of 6aa. Energy is referred to the most stable conformer of each diastereoisomer.

Conformer	*syn*	*anti*
1	0.00	0.00
2	1.43	0.17
3	1.51	0.59
4	1.77	0.78
5	1.99	1.31
6	2.02	1.74
7	2.28	1.79
8	2.36	2.11
9	2.44	2.23
10	2.47	2.52

Cartesian Coordinates (Å, PCM/M06-2X/6-31+G)**

6aa-syn_conf_1 Energy = -1430.70946256 Hartree

S	-0.898362	-2.309369	0.484416
C	-2.160901	-2.964799	-0.601844
O	-2.629439	-2.319573	-1.509611
C	-0.783007	-0.609299	-0.195796
C	0.603521	-0.036005	0.166288
H	0.758187	-0.070882	1.247217
C	-2.597461	-4.364385	-0.251514
H	-1.818264	-4.914693	0.277944
H	-2.879144	-4.886054	-1.167233
H	-3.476420	-4.291614	0.396271
C	0.725717	1.415236	-0.283491
C	0.827076	4.091695	-1.091531
C	0.781018	2.435985	0.666819
C	0.728433	1.741006	-1.642789
C	0.778896	3.074497	-2.044722
C	0.829134	3.769875	0.265286
H	0.781322	2.183071	1.723596

H	0.688525	0.950766	-2.388842
H	0.779546	3.318133	-3.102458
H	0.867350	4.556295	1.012411
H	0.863918	5.130156	-1.405038
C	1.700509	-0.833180	-0.516366
O	1.581270	-1.376141	-1.590834
C	5.061083	-1.215389	0.597533
H	6.094083	-1.524057	0.558578
C	4.091813	-1.435087	-0.340402
H	4.093704	-1.932319	-1.298036
C	4.402333	-0.491235	1.633657
H	4.816311	-0.123353	2.562507
N	3.132382	-0.281591	1.357564
N	2.943394	-0.862843	0.145458
C	-1.899374	0.281503	0.299457
C	-3.882625	2.052301	1.182550
C	-2.117483	0.475692	1.667199
C	-2.687122	0.975640	-0.619926
C	-3.674907	1.857962	-0.181611
C	-3.101942	1.356529	2.107415
H	-1.518321	-0.069944	2.392835
H	-2.525058	0.822108	-1.683451
H	-4.281455	2.390814	-0.907176
H	-3.261106	1.499570	3.171687
H	-4.650828	2.738407	1.525074
H	-0.851903	-0.720979	-1.281401

6aa-syn_conf_2

S	0.552506	-2.371085	1.051491
C	0.542083	-2.969196	-0.631549
O	0.552570	-2.243207	-1.598817
C	0.770719	-0.546188	0.867604
C	-0.429775	0.097929	0.153600
H	-0.557253	-0.331903	-0.838946
C	0.541978	-4.475494	-0.721117
H	1.581219	-4.808527	-0.802492
H	0.004379	-4.774024	-1.622069
H	0.096972	-4.938996	0.160860
C	-0.291707	1.611328	0.015466
C	-0.040537	4.385104	-0.264829
C	-0.471127	2.213599	-1.231484
C	-0.000637	2.409153	1.125720
C	0.128781	3.789554	0.985189
C	-0.343622	3.594461	-1.372705
H	-0.713787	1.595016	-2.091411
H	0.122283	1.954268	2.105537
H	0.359964	4.399527	1.852715
H	-0.480630	4.051277	-2.347794
H	0.061400	5.460187	-0.373898
C	-1.686877	-0.151819	0.970099
O	-1.714237	-0.210093	2.178837
C	-5.017992	-0.413896	-0.259084
H	-6.092190	-0.502774	-0.212941
C	-4.142270	-0.363526	0.788629

H	-4.273248	-0.393608	1.859256
C	-4.195850	-0.324009	-1.420407
H	-4.498252	-0.330410	-2.458670
N	-2.919498	-0.226019	-1.114123
N	-2.888269	-0.250965	0.242806
C	2.133749	-0.185759	0.316779
C	4.704496	0.475675	-0.595199
C	2.355697	0.093757	-1.034888
C	3.213847	-0.125307	1.204493
C	4.491366	0.199595	0.755262
C	3.633194	0.423716	-1.485635
H	1.533903	0.048149	-1.740634
H	3.049899	-0.334765	2.259173
H	5.316195	0.243546	1.459524
H	3.789040	0.640891	-2.537738
H	5.697346	0.733947	-0.949826
H	0.737280	-0.241204	1.918883

6aa-syn_conf_3

S	1.545858	2.150864	0.667712
C	0.446352	3.513060	0.313560
O	-0.419133	3.444333	-0.530542
C	0.890225	0.923870	-0.528458
C	-0.477571	0.371871	-0.031062
H	-1.039229	1.200709	0.409053
C	0.678092	4.729755	1.172880
H	1.664745	4.724697	1.637837

C	-0.365516	-0.726148	1.010571
C	-0.035360	-2.712191	2.958041
C	-0.397316	-0.397504	2.367602
C	-0.177472	-2.059820	0.636498
C	-0.018053	-3.049116	1.604752
C	-0.226172	-1.383714	3.337842
H	-0.558851	0.635635	2.663000
H	-0.134009	-2.327633	-0.417470
H	-0.249593	-1.115104	4.389335
H	0.093002	-3.481655	3.712811
C	-1.291777	-0.101590	-1.220459
O	-0.848356	-0.326155	-2.323241
C	-4.777056	-0.841159	-1.229379
H	-5.719439	-1.193088	-1.619245
C	-3.567139	-0.828292	-1.864896
H	-3.249061	-1.140192	-2.847688
C	-4.513440	-0.287368	0.057479
H	-5.207268	-0.116778	0.869241
N	-3.245973	0.036808	0.204049
N	-2.667325	-0.296160	-0.976429
C	1.963796	-0.109096	-0.804782
C	3.938333	-2.020955	-1.372136
C	2.262285	-0.451886	-2.126215
C	2.672207	-0.730940	0.230937
C	3.652691	-1.679284	-0.050145
C	3.241349	-1.403738	-2.409509
H	2.449731	-0.483011	1.266543

H	4.190766	-2.152907	0.764980
H	3.459426	-1.659718	-3.441628
H	4.701844	-2.760759	-1.591494
H	0.698305	1.490271	-1.442986
H	1.712013	0.020130	-2.934176
H	0.552243	5.622631	0.558126
H	0.128085	-4.080816	1.300808
H	-0.084181	4.739287	1.957762

6aa-syn_conf_4

S	-0.023322	-2.009033	-1.179211
C	-1.274951	-3.028949	-0.404298
O	-1.489329	-3.038596	0.785447
C	0.567627	-1.071231	0.274259
C	-0.049724	0.345231	0.392379
H	0.348332	0.782437	1.313909
C	-2.067074	-3.839016	-1.399277
H	-2.948323	-3.252792	-1.679160
H	-2.396256	-4.763906	-0.924056
H	-1.491927	-4.054274	-2.301327
C	-1.564610	0.311093	0.520192
C	-4.341540	0.107144	0.821663
C	-2.397355	0.300689	-0.602010
C	-2.134842	0.231489	1.793150
C	-3.514548	0.125625	1.945425
C	-3.780746	0.199530	-0.450918
H	-1.967630	0.363007	-1.598574

H	-1.490983	0.247722	2.669060
H	-3.944013	0.059723	2.940037
H	-4.418105	0.193464	-1.329699
H	-5.417616	0.026183	0.938408
C	0.365786	1.252889	-0.748092
O	0.726069	0.878903	-1.840765
C	0.265727	4.814047	-0.745349
H	0.338412	5.812779	-1.146799
C	0.479301	3.635625	-1.403701
H	0.754099	3.400231	-2.420251
C	-0.072682	4.427423	0.584444
H	-0.313315	5.061600	1.426691
N	-0.069533	3.119449	0.732953
N	0.270301	2.635396	-0.488120
C	2.080910	-1.041671	0.384357
C	4.863758	-0.912836	0.727278
C	2.929381	-0.973650	-0.724533
C	2.643688	-1.044381	1.665773
C	4.024790	-0.978838	1.839001
C	4.311729	-0.912462	-0.553077
H	2.509412	-0.966064	-1.725650
H	1.993518	-1.105246	2.535782
H	4.443448	-0.986970	2.840461
H	4.957545	-0.864243	-1.424255
H	5.940292	-0.866377	0.857698
H	0.169229	-1.635630	1.123831

6aa-syn_conf_5

S	1.072452	-2.004682	0.112801
C	2.370962	-1.650628	-1.063601
O	2.214442	-0.905735	-2.003669
C	-0.226163	-0.810110	-0.403604
C	-0.025947	0.603275	0.230093
H	0.140322	0.472878	1.301298
C	3.673663	-2.333831	-0.740090
H	4.242800	-1.658323	-0.090799
C	-1.249025	1.475855	0.018151
C	-3.557309	3.033063	-0.304915
C	-1.741945	1.753041	-1.261580
C	-1.923893	1.983737	1.129838
C	-3.072228	2.759793	0.972180
C	-2.888729	2.527210	-1.420693
H	-1.225223	1.368617	-2.135343
H	-1.551722	1.765138	2.127699
H	-3.261868	2.735241	-2.418671
H	-4.451979	3.634473	-0.431862
C	1.207270	1.265908	-0.370518
O	1.223717	1.847185	-1.427572
C	4.540045	1.212208	0.894171
H	5.611687	1.336579	0.874587
C	3.655057	1.463408	-0.117805
H	3.774183	1.816737	-1.130483
C	3.731311	0.748084	1.972305
H	4.041506	0.447573	2.963799

N	2.455142	0.709627	1.648836
N	2.410668	1.149695	0.365853
C	-1.559481	-1.409123	-0.011006
C	-4.038009	-2.503651	0.699038
C	-2.486779	-1.754868	-0.994956
C	-1.882461	-1.616876	1.334241
C	-3.114019	-2.162077	1.687645
C	-3.721843	-2.298913	-0.642571
H	-1.169381	-1.351764	2.112029
H	-3.353123	-2.318833	2.734715
H	-4.435924	-2.559779	-1.417258
H	-4.998961	-2.926202	0.974574
H	-0.154477	-0.732625	-1.493080
H	-2.244099	-1.590558	-2.041555
H	3.521014	-3.275362	-0.209781
H	-3.586139	3.146289	1.846680
H	4.233353	-2.495069	-1.662194

6aa-syn_conf_6

S	-1.458291	1.243515	-1.215692
C	-2.670833	2.329037	-0.476241
O	-2.955021	2.307636	0.700258
C	-1.018603	0.262808	0.264689
C	0.493873	-0.048491	0.363716
H	0.620033	-0.643250	1.273538
C	-3.334159	3.250065	-1.469876
H	-2.741285	3.373430	-2.377233

H	-3.506717	4.216284	-0.993142
H	-4.302280	2.816069	-1.737517
C	1.353661	1.198709	0.512729
C	2.868040	3.528973	0.864305
C	1.613623	1.688062	1.795807
C	1.862613	1.883841	-0.593863
C	2.618619	3.042439	-0.417821
C	2.362548	2.849141	1.972601
H	1.230927	1.151592	2.660693
H	1.665634	1.518763	-1.598596
H	3.010359	3.564617	-1.284960
H	2.556775	3.217953	2.974782
H	3.456184	4.431027	1.000019
C	0.994500	-0.883496	-0.796446
O	0.514536	-0.875718	-1.908147
C	3.866256	-2.986914	-0.806603
H	4.620654	-3.640995	-1.215205
C	2.818739	-2.411033	-1.468047
H	2.487333	-2.446962	-2.494283
C	3.737821	-2.531238	0.538578
H	4.368716	-2.759014	1.386825
N	2.697906	-1.739860	0.693580
N	2.133840	-1.667954	-0.539075
C	-1.867257	-0.983439	0.437820
C	-3.356950	-3.317220	0.891110
C	-2.198623	-1.829666	-0.625329
C	-2.297058	-1.315646	1.726722

C	-3.036968	-2.474830	1.954724
C	-2.937000	-2.989916	-0.398134
H	-1.882570	-1.574769	-1.632198
H	-2.056894	-0.655343	2.556921
H	-3.368273	-2.713887	2.960398
H	-3.187830	-3.637451	-1.232607
H	-3.935844	-4.218989	1.063953
H	-1.237649	0.936935	1.098606

6aa-syn_conf_7

S	1.450654	-0.061670	1.923041
C	2.079192	-1.727516	1.846382
O	1.494496	-2.620143	1.273852
C	-0.051823	-0.225691	0.892495
C	0.271184	-0.554206	-0.618547
H	0.449743	-1.633033	-0.631793
C	3.417129	-1.899701	2.518861
H	4.193800	-1.722302	1.767549
H	3.503765	-2.924643	2.881513
H	3.558486	-1.189832	3.335501
C	1.490790	0.137722	-1.185150
C	3.863579	1.330427	-2.099870
C	2.658293	-0.617261	-1.340234
C	1.521667	1.498985	-1.509096
C	2.701496	2.089008	-1.960193
C	3.838380	-0.028713	-1.792200
H	2.641657	-1.677785	-1.098703

H	0.621202	2.095791	-1.423061
H	2.709638	3.145696	-2.209425
H	4.733624	-0.632219	-1.905701
H	4.779322	1.794354	-2.452771
C	-0.981529	-0.304411	-1.444260
O	-1.137962	0.582243	-2.248669
C	-4.074117	-2.054207	-1.145916
H	-5.122863	-2.253202	-1.302488
C	-3.332014	-1.035821	-1.678079
H	-3.572950	-0.216260	-2.337329
C	-3.154254	-2.788843	-0.343826
H	-3.336490	-3.675979	0.247146
N	-1.945799	-2.264197	-0.377432
N	-2.057221	-1.192030	-1.199384
C	-0.919409	1.000867	1.094592
C	-2.618585	3.217540	1.371878
C	-0.397351	2.299078	1.111342
C	-2.301543	0.827083	1.236621
C	-3.146668	1.927272	1.368878
C	-1.241585	3.399522	1.249331
H	0.674414	2.454461	1.020593
H	-2.717199	-0.178706	1.245714
H	-4.215884	1.773962	1.476177
H	-0.820879	4.400015	1.262554
H	-3.274662	4.075587	1.477749
H	-0.583324	-1.099209	1.276324

6aa-syn_conf_8

S	1.165223	-1.558527	-1.323573
C	0.318702	-3.136479	-1.393085
O	-0.794704	-3.298314	-0.952399
C	-0.098898	-0.614092	-0.400156
C	0.076755	0.900222	-0.762453
H	-0.168342	0.969265	-1.827078
C	1.142657	-4.233783	-2.017653
H	1.870992	-3.841963	-2.729471
C	1.475047	1.443365	-0.553824
C	4.117815	2.356118	-0.290570
C	2.014230	1.700346	0.712910
C	2.275073	1.656986	-1.681897
C	3.587793	2.108301	-1.555302
C	3.326629	2.152622	0.839926
H	1.407236	1.557299	1.598850
H	1.865815	1.463846	-2.670477
H	3.730061	2.350201	1.828254
H	5.138687	2.709999	-0.185882
C	-0.983957	1.701864	-0.020193
O	-0.788664	2.446428	0.909211
C	-4.503768	1.544844	-0.571997
H	-5.549583	1.726422	-0.379260
C	-3.434664	1.989458	0.155018
H	-3.350237	2.589645	1.047797
C	-3.928295	0.790927	-1.635298
H	-4.431277	0.269937	-2.438384

N	-2.613046	0.770414	-1.567491
N	-2.311978	1.507720	-0.468659
C	-0.124744	-0.913093	1.084641
C	-0.298252	-1.364823	3.848531
C	-1.367069	-0.921319	1.729989
C	1.028152	-1.153952	1.837038
C	0.941912	-1.375625	3.210745
C	-1.455202	-1.140815	3.103256
H	1.996787	-1.170816	1.345997
H	1.846268	-1.560092	3.782261
H	-2.426947	-1.147412	3.586796
H	-0.363356	-1.541000	4.917568
H	-1.052841	-0.931689	-0.827284
H	-2.274604	-0.768697	1.148317
H	1.681407	-4.749288	-1.216628
H	4.191342	2.267618	-2.443270
H	0.474368	-4.944442	-2.505505

6aa-syn_conf_9

S	0.690070	-2.373357	-0.489283
C	1.917521	-3.311776	0.422319
O	2.083641	-4.461619	0.086985
C	0.746734	-0.674341	0.217883
C	-0.599830	-0.008079	-0.156542
H	-0.752718	-0.062689	-1.237241
C	2.664943	-2.656653	1.552733
H	3.176221	-1.754564	1.205976

C	-0.624261	1.458760	0.254453
C	-0.531344	4.156470	0.990848
C	-0.653952	1.822228	1.603847
C	-0.556941	2.453712	-0.722520
C	-0.507935	3.797627	-0.356521
C	-0.607222	3.166233	1.970083
H	-0.710859	1.053578	2.371025
H	-0.535864	2.172602	-1.771980
H	-0.630351	3.438963	3.020448
H	-0.493117	5.202868	1.276480
C	-1.743971	-0.717578	0.546824
O	-1.655606	-1.226920	1.641265
C	-5.112259	-0.959634	-0.575484
H	-6.159410	-1.216147	-0.536093
C	-4.160757	-1.202932	0.374126
H	-4.192396	-1.675839	1.343467
C	-4.412451	-0.296401	-1.625986
H	-4.802800	0.066977	-2.566750
N	-3.135250	-0.143752	-1.347744
N	-2.982116	-0.701699	-0.119188
C	1.915862	0.150179	-0.275185
C	3.982958	1.822713	-1.161531
C	2.641259	0.924410	0.634100
C	2.237177	0.218748	-1.634044
C	3.263316	1.051333	-2.074960
C	3.671088	1.756036	0.195214
H	1.687354	-0.386802	-2.350056

H	3.502890	1.095682	-3.132711
H	4.226462	2.350758	0.913511
H	4.783969	2.468999	-1.505942
H	0.778294	-0.761655	1.307397
H	2.391049	0.883799	1.691913
H	1.969310	-2.372493	2.348005
H	-0.450923	4.562938	-1.124039
H	3.389427	-3.373107	1.939689

6aa-syn_conf_10

S	-1.227820	1.552491	-1.272544
C	-0.375085	3.122136	-1.415459
O	0.764334	3.280439	-1.045688
C	0.083027	0.609878	-0.414745
C	-0.125964	-0.907627	-0.744534
H	0.053196	-0.993053	-1.821042
C	-1.227200	4.217887	-2.003926
H	-2.000574	3.822718	-2.664542
C	-1.513033	-1.436046	-0.443596
C	-4.141715	-2.322747	-0.007209
C	-1.975884	-1.671394	0.857077
C	-2.381994	-1.658027	-1.517773
C	-3.687957	-2.096457	-1.305200
C	-3.281507	-2.110782	1.070065
H	-1.314900	-1.521598	1.702332
H	-2.032342	-1.481672	-2.532035
H	-3.625393	-2.291630	2.083783

H	-5.156974	-2.666525	0.164371
C	0.971898	-1.708178	-0.057142
O	0.827983	-2.438497	0.892716
C	4.452587	-1.588426	-0.824390
H	5.506795	-1.776254	-0.693181
C	3.426460	-2.014149	-0.027496
H	3.392070	-2.601542	0.877044
C	3.819098	-0.844024	-1.861079
H	4.276117	-0.338160	-2.700485
N	2.510630	-0.811455	-1.713600
N	2.271532	-1.531342	-0.588305
C	0.201686	0.928585	1.061411
C	0.546925	1.415948	3.803042
C	1.481093	0.934958	1.629735
C	-0.901290	1.189300	1.879186
C	-0.729718	1.428684	3.241869
C	1.654511	1.172143	2.991894
H	-1.897918	1.207769	1.447852
H	-1.596089	1.628476	3.864768
H	2.653966	1.177005	3.415225
H	0.678467	1.605924	4.863571
H	1.011535	0.913607	-0.903553
H	2.350261	0.766844	0.996063
H	-1.712127	4.748662	-1.178844
H	-4.345750	-2.262579	-2.152460
H	-0.584507	4.916233	-2.541424

6aa-anti_conf_1 Energy = -1430.70942404 Hartree

S	1.312674	-1.878424	-1.047297
C	2.669080	-2.201825	0.080814
O	2.597351	-2.019027	1.272667
C	0.094610	-1.100813	0.081353
H	0.505543	-1.248225	1.084224
C	-0.003337	0.408279	-0.217560
H	-0.366429	0.567952	-1.233548
C	3.908241	-2.700590	-0.617208
H	3.670858	-3.226764	-1.543251
H	4.463004	-3.349210	0.061771
H	4.525672	-1.829970	-0.860337
C	-1.237358	-1.811892	-0.020838
C	-3.688865	-3.165771	-0.170046
C	-1.609314	-2.719060	0.975239
C	-2.106455	-1.589324	-1.094047
C	-3.325354	-2.262628	-1.167878
C	-2.826596	-3.392940	0.902696
H	-0.940830	-2.890856	1.814971
H	-1.838132	-0.892921	-1.884506
H	-3.989956	-2.079970	-2.006428
H	-3.103372	-4.091200	1.686335
H	-4.638727	-3.687784	-0.226784
C	1.320885	1.145782	-0.074955
C	3.771038	2.479380	0.152818
C	1.840167	1.858517	-1.158314
C	2.030436	1.115709	1.129082

C	3.252310	1.776692	1.240503
C	3.061523	2.521065	-1.047099
H	1.283665	1.891520	-2.090959
H	1.633257	0.567563	1.979256
H	3.798601	1.741083	2.177729
H	3.457346	3.068430	-1.896775
H	4.722936	2.993639	0.240909
C	-0.992638	1.026077	0.755897
O	-1.121315	0.674816	1.906276
C	-3.139341	3.804108	0.156117
H	-3.860988	4.572453	0.385850
C	-2.631867	2.859888	1.003980
H	-2.797569	2.643098	2.047933
C	-2.504628	3.544641	-1.093271
H	-2.631752	4.067031	-2.031600
N	-1.674417	2.525220	-1.021751
N	-1.754071	2.106328	0.266998

6aa-anti_conf_2

S	1.752375	1.439291	-0.961373
C	3.201264	1.804011	0.018618
O	3.369771	1.346571	1.125250
C	0.954997	0.205565	0.137870
H	1.096482	0.576063	1.156559
C	-0.549344	0.171813	-0.197160
H	-0.698543	-0.162494	-1.225425
C	4.189936	2.707270	-0.673978

H	4.950555	2.076538	-1.144096
H	4.672501	3.340238	0.072041
H	3.717069	3.317787	-1.444671
C	1.603789	-1.156032	0.011074
C	2.773479	-3.696085	-0.176655
C	2.306436	-1.692911	1.091962
C	1.494272	-1.902355	-1.167898
C	2.073518	-3.165626	-1.261165
C	2.889759	-2.956195	0.998956
H	2.395219	-1.113623	2.006219
H	0.963320	-1.493938	-2.024694
H	1.979945	-3.734426	-2.180950
H	3.433489	-3.361486	1.846546
H	3.225822	-4.680118	-0.249190
C	-1.248288	1.514124	-0.027902
C	-2.510162	3.995086	0.256721
C	-1.915053	2.093585	-1.108715
C	-1.228307	2.177856	1.202548
C	-1.853912	3.414673	1.342790
C	-2.541354	3.331437	-0.968811
H	-1.942580	1.571598	-2.061312
H	-0.726827	1.725589	2.054713
H	-1.830656	3.923815	2.301064
H	-3.053069	3.775330	-1.816890
H	-2.997013	4.958882	0.366945
C	-1.223915	-0.820506	0.735738
O	-0.899643	-0.996567	1.887418

C	-4.086078	-2.817378	0.030089
H	-4.889618	-3.509987	0.226343
C	-3.132114	-2.381002	0.905914
H	-2.937873	-2.589793	1.946585
C	-3.780147	-2.155939	-1.194851
H	-4.294520	-2.229090	-2.143309
N	-2.725086	-1.376390	-1.083754
N	-2.328542	-1.516169	0.207080

6aa-anti_conf_3

S	0.099102	-0.065581	2.135165
C	1.871889	0.037818	2.363128
O	2.604003	0.571550	1.562055
C	-0.053393	0.700374	0.480234
H	0.791572	1.391369	0.404751
C	0.079430	-0.317362	-0.705359
H	0.013098	0.312625	-1.596539
C	2.352767	-0.632278	3.623433
H	1.592706	-0.621353	4.406233
H	3.262936	-0.137361	3.964186
H	2.585523	-1.673595	3.378925
C	-1.343653	1.481445	0.365374
C	-3.702737	2.952097	0.008911
C	-1.317702	2.716430	-0.288715
C	-2.564451	0.985951	0.835027
C	-3.736208	1.719489	0.661298
C	-2.490535	3.448985	-0.467842

H	-0.372002	3.103373	-0.660664
H	-2.604820	0.018350	1.330409
H	-4.676660	1.324471	1.032346
H	-2.454650	4.408291	-0.974444
H	-4.616552	3.522234	-0.125347
C	-1.031528	-1.343462	-0.766430
C	-3.232759	-3.085486	-0.886578
C	-2.066591	-1.129874	-1.684159
C	-1.109477	-2.448838	0.089884
C	-2.203762	-3.311725	0.026572
C	-3.160257	-1.990690	-1.746641
H	-2.021658	-0.268989	-2.347081
H	-0.314732	-2.638267	0.800118
H	-2.249270	-4.165527	0.695626
H	-3.953625	-1.803482	-2.463409
H	-4.082746	-3.759381	-0.930109
C	1.474837	-0.913342	-0.692862
O	1.784777	-1.971848	-0.196810
C	4.441319	0.668520	-1.866340
H	5.498248	0.793693	-2.042665
C	3.813714	-0.404835	-1.298194
H	4.175328	-1.336411	-0.891574
C	3.389845	1.581270	-2.166301
H	3.459059	2.558506	-2.624359
N	2.211986	1.107007	-1.815715
N	2.474856	-0.116121	-1.291095

6aa-anti_conf_4

S	0.490868	-2.565837	-0.377956
C	0.699514	-2.592180	1.392183
O	0.783419	-1.590328	2.066295
C	0.632104	-0.779510	-0.791651
H	0.436627	-0.795400	-1.869923
C	-0.460299	0.081936	-0.130491
H	-0.290165	0.144817	0.941501
C	0.784828	-3.987168	1.961190
H	0.278328	-4.719676	1.330709
H	0.355374	-3.984774	2.963961
H	1.842570	-4.258878	2.031488
C	2.041891	-0.257853	-0.585957
C	4.671213	0.687187	-0.312323
C	3.009852	-0.545664	-1.555350
C	2.405992	0.513393	0.521697
C	3.713530	0.983859	0.654249
C	4.314737	-0.081458	-1.421652
H	2.733525	-1.138617	-2.424092
H	1.680550	0.743421	1.295627
H	3.980006	1.581939	1.520032
H	5.050577	-0.312871	-2.185363
H	5.687054	1.054474	-0.206074
C	-1.867718	-0.451685	-0.348806
C	-4.433953	-1.506075	-0.713121
C	-2.617289	-0.877402	0.749661
C	-2.414688	-0.546900	-1.631777

C	-3.692074	-1.073722	-1.812841
C	-3.895079	-1.405154	0.568884
H	-2.193223	-0.796235	1.747271
H	-1.843138	-0.203703	-2.490865
H	-4.108717	-1.144449	-2.812658
H	-4.468486	-1.736083	1.429105
H	-5.428821	-1.916121	-0.855372
C	-0.377452	1.474022	-0.732733
O	-0.118898	1.697948	-1.894017
C	-1.045143	4.564852	0.904048
H	-1.175062	5.631272	1.003127
C	-0.729283	3.867503	-0.227905
H	-0.540365	4.165923	-1.247434
C	-1.160786	3.570667	1.919147
H	-1.397012	3.704689	2.965896
N	-0.935410	2.360805	1.451803
N	-0.671597	2.545026	0.132969

6aa-anti_conf_5

S	1.270853	-1.802255	0.829829
C	2.210930	-0.947667	2.096761
O	1.742403	-0.047208	2.752552
C	-0.219926	-0.734912	0.800502
H	-0.451875	-0.527763	1.849248
C	0.104560	0.663118	0.175939
H	0.876381	1.094489	0.813001
C	3.622057	-1.451924	2.236897

H	4.232074	-0.931852	1.491264
H	3.687063	-2.525099	2.047357
H	3.991239	-1.214042	3.234890
C	-1.379925	-1.478483	0.178690
C	-3.609191	-2.759191	-0.942851
C	-2.634576	-1.391039	0.790589
C	-1.252341	-2.224114	-0.997848
C	-2.359973	-2.860429	-1.554665
C	-3.744097	-2.024019	0.234103
H	-2.743780	-0.810215	1.703238
H	-0.287576	-2.304881	-1.490774
H	-2.245542	-3.434756	-2.468514
H	-4.711165	-1.942445	0.720133
H	-4.471090	-3.254577	-1.378716
C	-1.110198	1.572317	0.232440
C	-3.356726	3.225702	0.528862
C	-1.190075	2.484112	1.290477
C	-2.172247	1.491333	-0.675845
C	-3.284363	2.318764	-0.528536
C	-2.306452	3.305213	1.442024
H	-0.370588	2.546795	2.002606
H	-2.130310	0.777163	-1.491390
H	-4.100826	2.247987	-1.240589
H	-2.351511	4.007187	2.268763
H	-4.226736	3.865269	0.640605
C	0.683376	0.526062	-1.217608
O	0.057718	0.229966	-2.209722

C	4.093749	0.889970	-2.196439
H	4.939832	0.892657	-2.865884
C	2.787149	0.634382	-2.507554
H	2.288075	0.382896	-3.430408
C	4.083519	1.154521	-0.796889
H	4.916774	1.406501	-0.154553
N	2.871522	1.067673	-0.288288
N	2.076112	0.751815	-1.340923

6aa-anti_conf_6

S	-0.607893	2.396394	-0.613510
C	-1.236165	2.929599	0.975533
O	-1.035718	2.327316	2.004763
C	0.228099	0.830325	-0.149090
H	0.008000	0.696097	0.909217
C	-0.379060	-0.322830	-0.976732
H	-0.322371	-0.050071	-2.036009
C	-2.067816	4.184052	0.892200
H	-1.810802	4.789043	0.021608
H	-1.934804	4.758285	1.810091
H	-3.117501	3.884559	0.813343
C	1.727650	0.933686	-0.321631
C	4.513035	1.073784	-0.594600
C	2.553097	0.881334	0.804796
C	2.310635	1.055263	-1.588030
C	3.694789	1.126234	-1.724078
C	3.939583	0.951424	0.669859

H	2.102902	0.776725	1.788577
H	1.683103	1.098977	-2.475388
H	4.134865	1.221092	-2.711683
H	4.569669	0.908417	1.552721
H	5.591813	1.127297	-0.701436
C	-1.837255	-0.653979	-0.679133
C	-4.530489	-1.310713	-0.254537
C	-2.606317	-1.209549	-1.707021
C	-2.429321	-0.432324	0.567272
C	-3.770487	-0.753381	0.773229
C	-3.943421	-1.541285	-1.497875
H	-2.152826	-1.380206	-2.680599
H	-1.850157	-0.014315	1.383742
H	-4.219769	-0.569920	1.744311
H	-4.525369	-1.971481	-2.306816
H	-5.573442	-1.561264	-0.088126
C	0.467901	-1.593920	-0.938079
O	0.836823	-2.156488	-1.944078
C	1.715895	-3.407968	1.858290
H	2.272088	-4.169689	2.382006
C	1.621218	-3.229191	0.506891
H	2.041262	-3.755103	-0.336302
C	0.919521	-2.365778	2.416457
H	0.726994	-2.151858	3.458983
N	0.381488	-1.606895	1.485438
N	0.810975	-2.137994	0.314581

6aa-anti_conf_7

S	-0.537235	2.407089	-0.635988
C	-1.070364	3.010090	0.961124
O	-0.912034	2.394704	1.990345
C	0.243173	0.815971	-0.161056
H	0.018611	0.696792	0.898097
C	-0.405554	-0.320882	-0.979468
H	-0.338885	-0.059777	-2.041230
C	-1.712814	4.372916	0.900812
H	-1.001578	5.099192	1.304664
H	-2.599535	4.367505	1.537448
H	-1.979619	4.661260	-0.116459
C	1.745425	0.862419	-0.335163
C	4.533664	0.892276	-0.612162
C	2.569658	0.767946	0.789337
C	2.330876	0.970431	-1.601728
C	3.716432	0.986487	-1.739804
C	3.957802	0.783245	0.652297
H	2.117130	0.673664	1.773115
H	1.703872	1.046913	-2.487286
H	4.158514	1.071239	-2.727433
H	4.586957	0.708113	1.533658
H	5.613563	0.903173	-0.720635
C	-1.873700	-0.601483	-0.678406
C	-4.584367	-1.175058	-0.245829
C	-2.652414	-1.170889	-1.691332
C	-2.465082	-0.322828	0.556638

C	-3.814714	-0.602994	0.766501
C	-3.998417	-1.461403	-1.478032
H	-2.199367	-1.385563	-2.656420
H	-1.879406	0.108540	1.361601
H	-4.263329	-0.375608	1.728528
H	-4.587798	-1.903399	-2.275139
H	-5.633969	-1.393652	-0.076190
C	0.398034	-1.619235	-0.927541
O	0.756830	-2.199834	-1.926873
C	1.560945	-3.455206	1.891160
H	2.087450	-4.231155	2.424590
C	1.484253	-3.282154	0.537861
H	1.894602	-3.826703	-0.298250
C	0.793582	-2.384386	2.435587
H	0.598566	-2.157815	3.474973
N	0.288852	-1.614371	1.495044
N	0.711592	-2.166583	0.331472

6aa-anti_conf_8

S	0.337160	0.770913	1.790428
C	1.109126	2.390128	1.804937
O	1.398833	2.982267	0.792919
C	0.160802	0.567723	-0.020278
H	1.057980	1.025572	-0.443268
C	0.173471	-0.941862	-0.424817
H	0.206342	-0.918313	-1.519198
C	1.320366	2.940439	3.192126

H	0.444238	3.541598	3.453986
H	2.200088	3.585245	3.186689
H	1.431124	2.146692	3.932517
C	-1.045476	1.277698	-0.596487
C	-3.243923	2.513944	-1.817384
C	-0.901075	1.929488	-1.824300
C	-2.300996	1.252973	0.017749
C	-3.393662	1.867842	-0.589723
C	-1.994051	2.544366	-2.434166
H	0.076121	1.956554	-2.300868
H	-2.424991	0.747147	0.971862
H	-4.364082	1.839932	-0.103964
H	-1.866094	3.051959	-3.385122
H	-4.096127	2.994543	-2.287623
C	-1.063683	-1.702455	0.001051
C	-3.478938	-2.946860	0.708358
C	-2.046795	-1.954190	-0.960601
C	-1.301363	-2.088808	1.325453
C	-2.502046	-2.705790	1.674169
C	-3.247196	-2.571486	-0.613661
H	-1.877438	-1.646812	-1.989763
H	-0.546986	-1.919736	2.085723
H	-2.671896	-3.000520	2.705039
H	-3.999558	-2.753598	-1.374520
H	-4.412732	-3.426487	0.984655
C	1.473128	-1.586792	0.032009
O	1.591852	-2.389986	0.925732

C	4.724508	-0.899780	-1.264596
H	5.800813	-0.941951	-1.324394
C	3.918593	-1.504996	-0.341288
H	4.121059	-2.138225	0.508604
C	3.827275	-0.203259	-2.124648
H	4.060328	0.402702	-2.989505
N	2.571996	-0.364273	-1.760616
N	2.629912	-1.162740	-0.663715

6aa-anti_conf_9

S	1.702960	-2.070906	-0.026409
C	3.103331	-2.110152	-1.141786
O	3.360542	-1.213124	-1.910949
C	1.046138	-0.409933	-0.428427
H	1.377942	-0.237504	-1.456826
C	-0.504313	-0.455004	-0.507151
H	-0.769197	-1.097686	-1.352872
C	3.947812	-3.350828	-0.996298
H	4.778673	-3.115433	-0.324214
H	4.354066	-3.618350	-1.972815
H	3.383467	-4.184203	-0.575261
C	1.639736	0.697628	0.422775
C	2.662298	2.857588	1.895369
C	1.992514	1.892817	-0.212986
C	1.823629	0.588977	1.804265
C	2.328884	1.663475	2.534851
C	2.496890	2.968339	0.515630

H	1.860588	1.984431	-1.288577
H	1.563531	-0.335852	2.307133
H	2.463796	1.565293	3.607684
H	2.762066	3.888565	0.004488
H	3.055666	3.692126	2.467475
C	-1.072149	0.929765	-0.777895
C	-1.978085	3.521170	-1.323649
C	-1.261105	1.347818	-2.096186
C	-1.342495	1.817244	0.266910
C	-1.797633	3.106086	-0.004518
C	-1.707898	2.639303	-2.370007
H	-1.058600	0.657626	-2.911505
H	-1.178402	1.510665	1.298091
H	-2.003170	3.787495	0.814959
H	-1.850008	2.953781	-3.399162
H	-2.328974	4.526278	-1.535130
C	-1.156407	-1.062220	0.719376
O	-0.609967	-1.249434	1.782533
C	-4.564360	-2.055364	1.011747
H	-5.463257	-2.398911	1.499440
C	-3.339817	-1.843072	1.579681
H	-2.967239	-1.951173	2.586552
C	-4.386779	-1.721153	-0.362941
H	-5.115300	-1.756639	-1.161350
N	-3.156129	-1.331640	-0.620321
N	-2.515121	-1.406998	0.573065

6aa-anti_conf_10

S	1.326323	-1.294690	1.236407
C	2.567133	-2.470838	0.719781
O	2.873074	-2.639067	-0.438475
C	0.917537	-0.587372	-0.402218
H	0.993862	-1.430319	-1.094621
C	-0.539581	-0.060928	-0.456613
H	-0.632921	0.491582	-1.398892
C	3.214047	-3.208410	1.865714
H	4.189228	-2.749839	2.054569
H	3.370902	-4.247100	1.570005
H	2.617614	-3.159402	2.777686
C	1.899607	0.482758	-0.836476
C	3.615763	2.498182	-1.764566
C	2.292115	0.521403	-2.177934
C	2.382906	1.460123	0.038512
C	3.233360	2.463217	-0.423681
C	3.144590	1.522124	-2.641763
H	1.933756	-0.244626	-2.861472
H	2.094945	1.435468	1.085759
H	3.599539	3.216685	0.266775
H	3.445880	1.533040	-3.684532
H	4.282637	3.276676	-2.121547
C	-0.909811	0.893146	0.667968
C	-1.506796	2.672801	2.747673
C	-0.766075	2.270908	0.483573
C	-1.368503	0.414976	1.898986

C	-1.666092	1.300728	2.934317
C	-1.057498	3.156389	1.518351
H	-0.424372	2.648546	-0.476607
H	-1.495406	-0.654223	2.055506
H	-2.023706	0.916485	3.884307
H	-0.939623	4.224133	1.362542
H	-1.738153	3.362667	3.553030
C	-1.521918	-1.217613	-0.542242
O	-1.256608	-2.376027	-0.323000
C	-4.988157	-0.977609	-1.333249
H	-6.007024	-1.310418	-1.455895
C	-3.917560	-1.715633	-0.912170
H	-3.806914	-2.746422	-0.612809
C	-4.457166	0.323765	-1.571032
H	-4.975157	1.206033	-1.921333
N	-3.167501	0.384068	-1.313152
N	-2.838984	-0.867763	-0.908385