

VNiVERSiDAD D SALAMANCA

FACULTAD DE CIENCIAS QUÍMICAS

Departamento de Química Orgánica



**VNiVERSiDAD
D SALAMANCA**

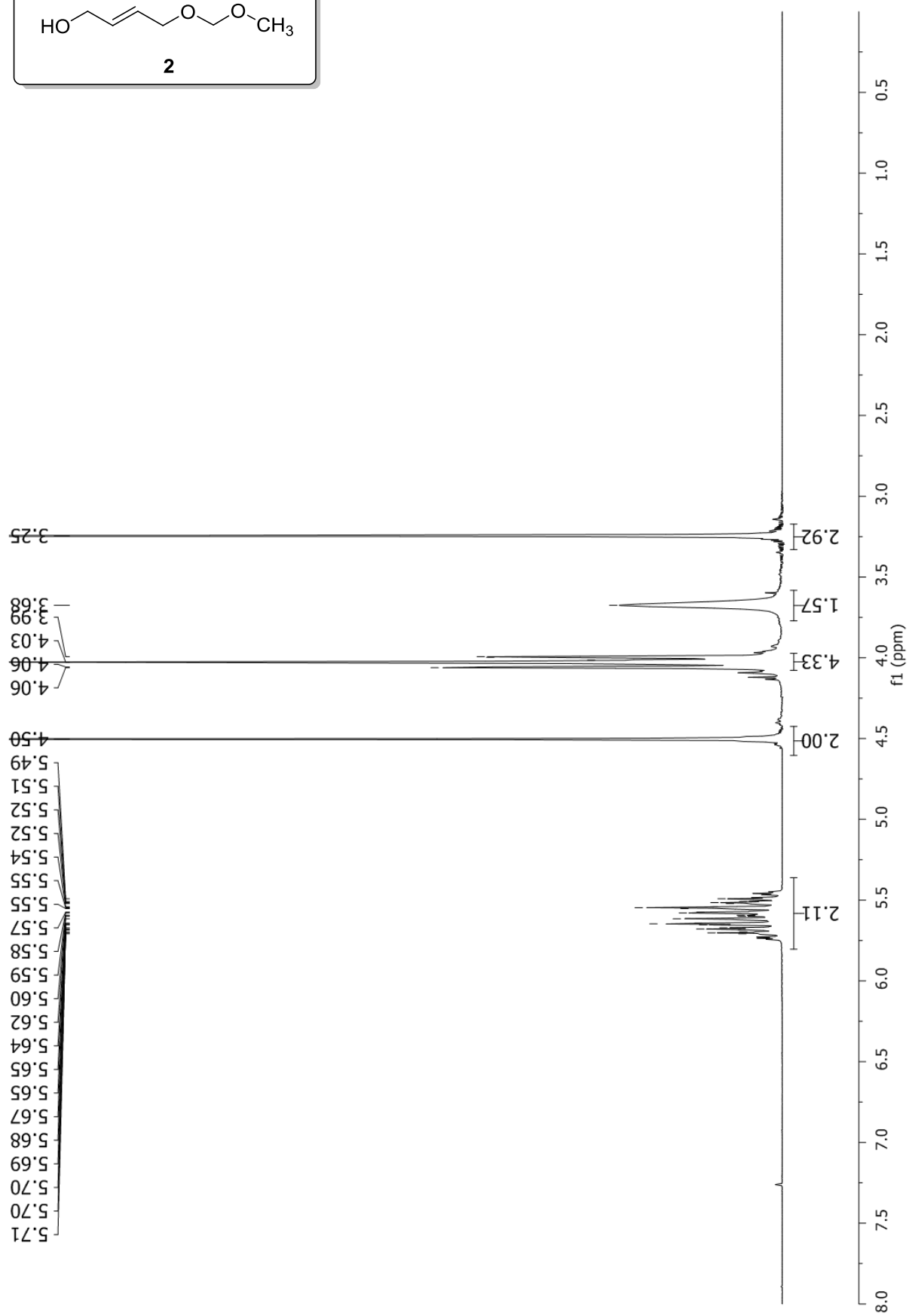
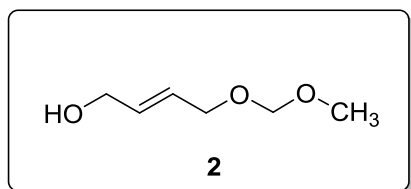
CAMPUS OF INTERNATIONAL EXCELLENCE

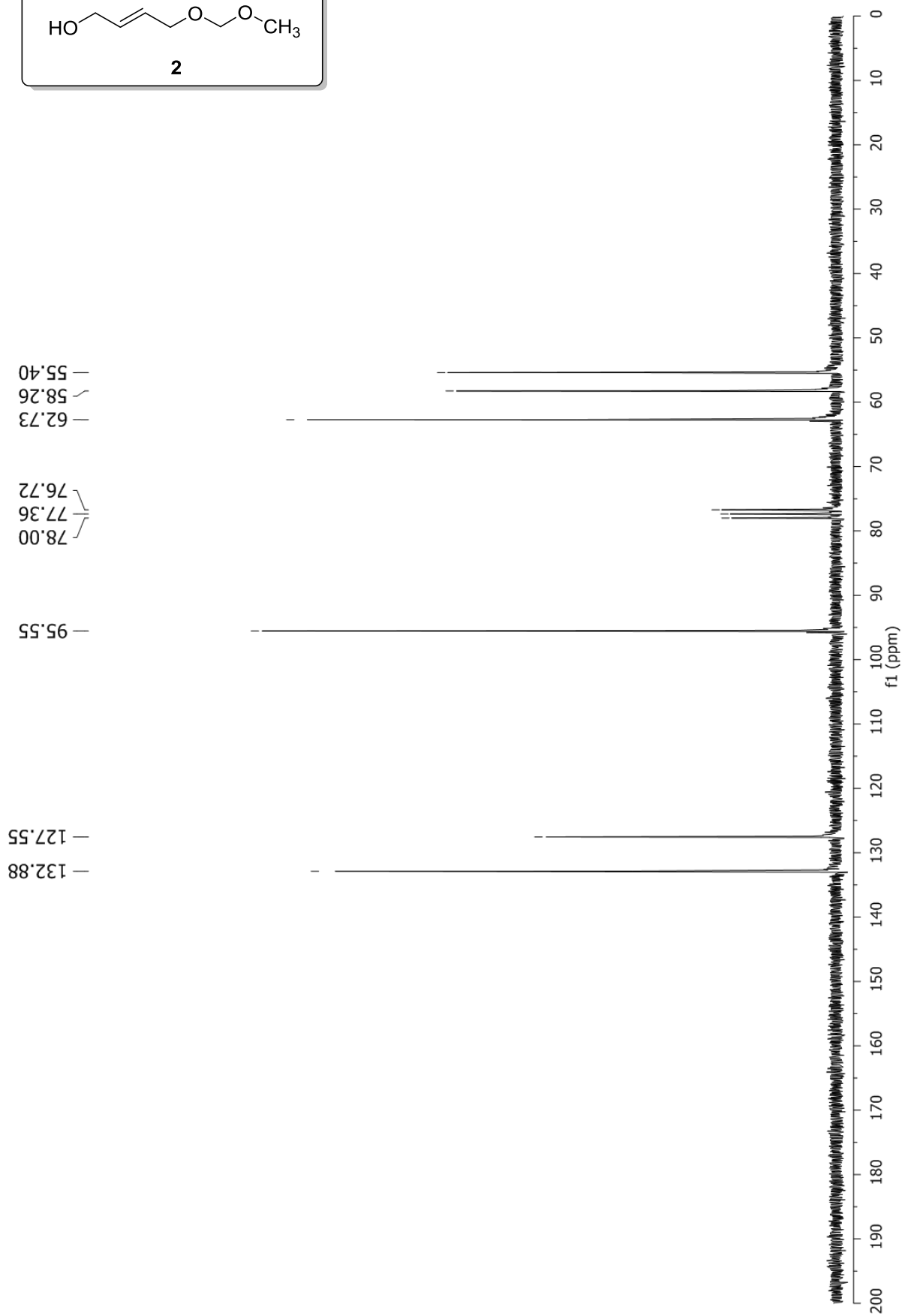
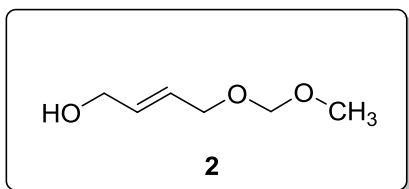
**SYNTHESIS OF SULFONYL NAZAROV
REAGENTS AND APPLICATION IN
ORGANOCATALYSIS**

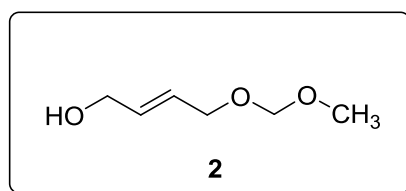
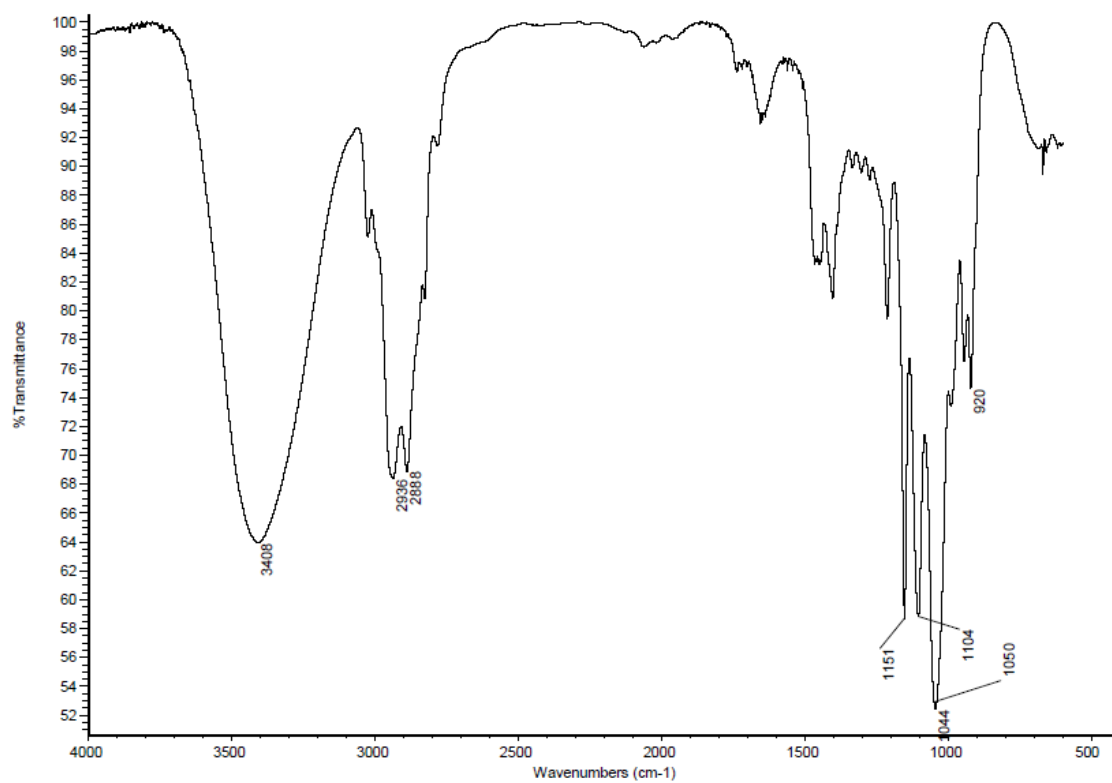
JAVIER PEÑA GONZÁLEZ

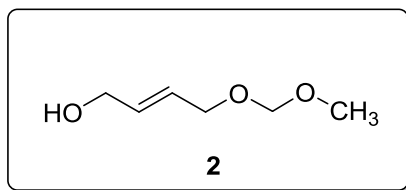
JULY 2014

FULL SPECTROSCOPY

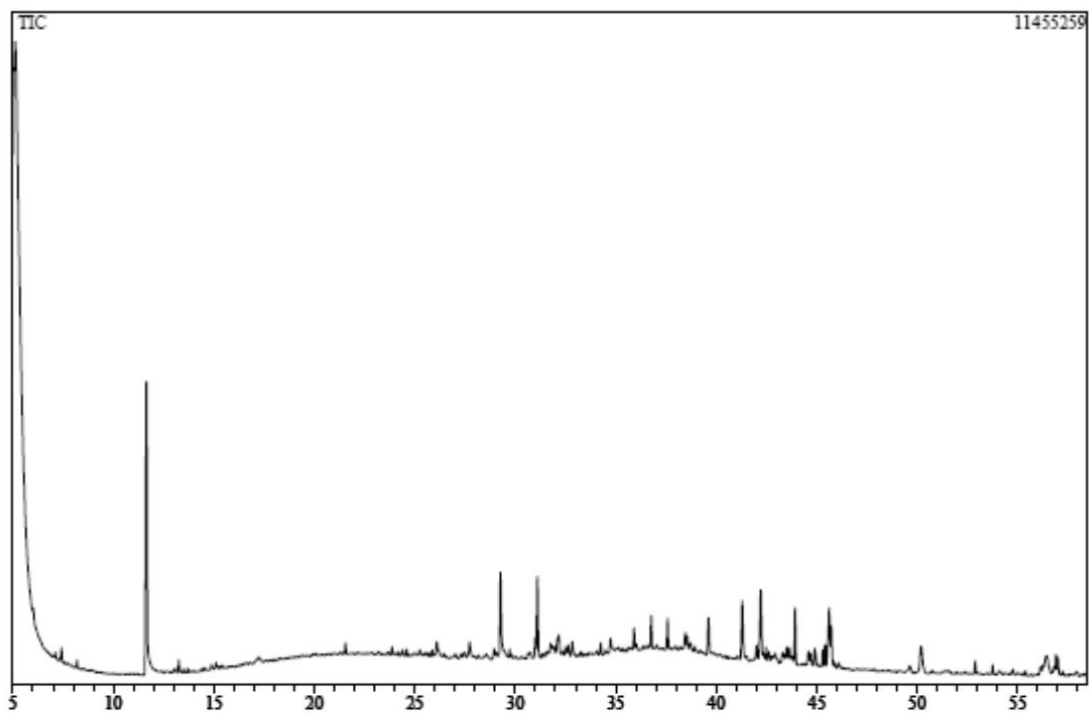




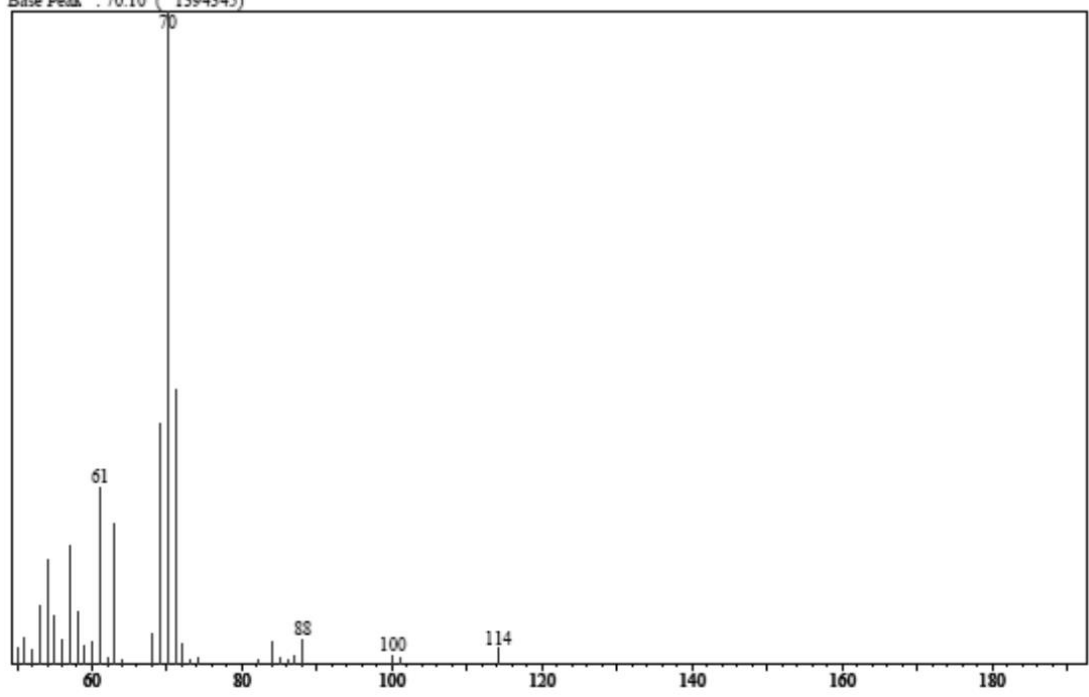


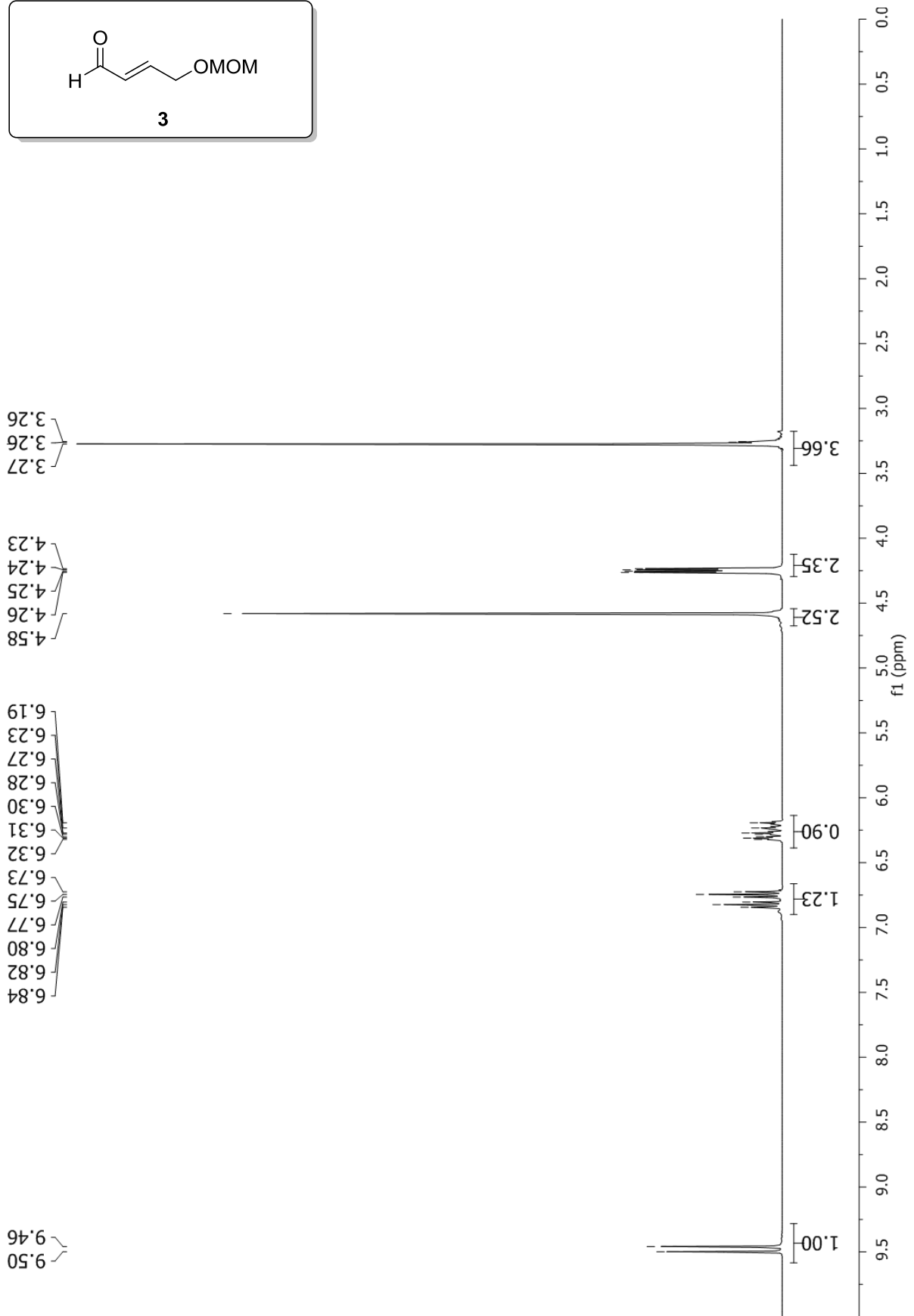
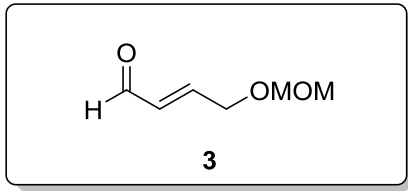


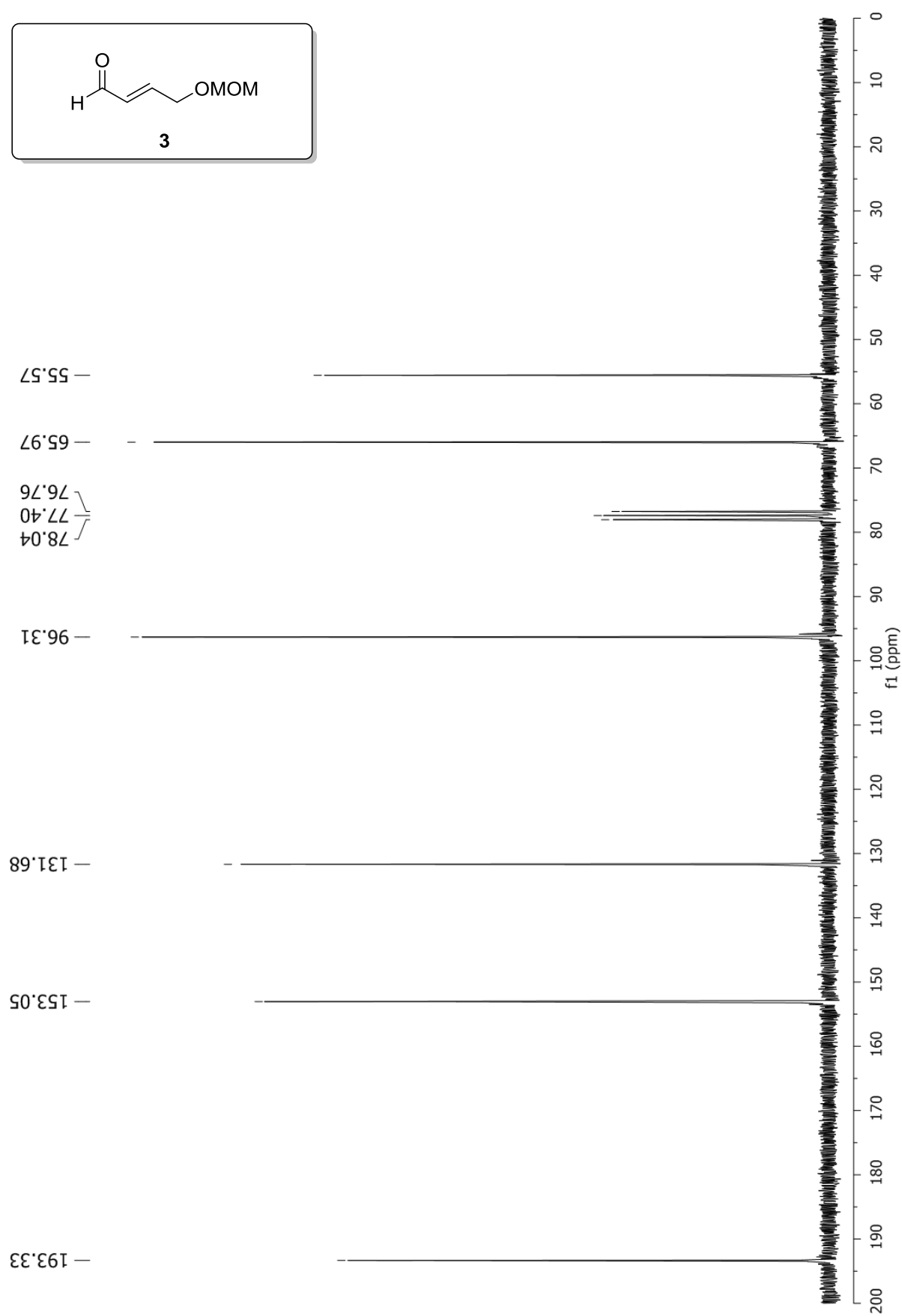
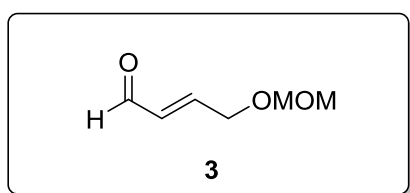
Data : JULIO.D01
 Sample : PR-147-crudo
 Method File Name : NMG3.MET

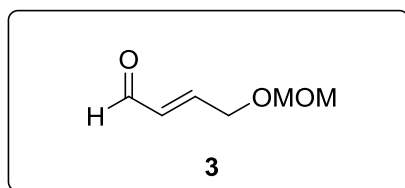
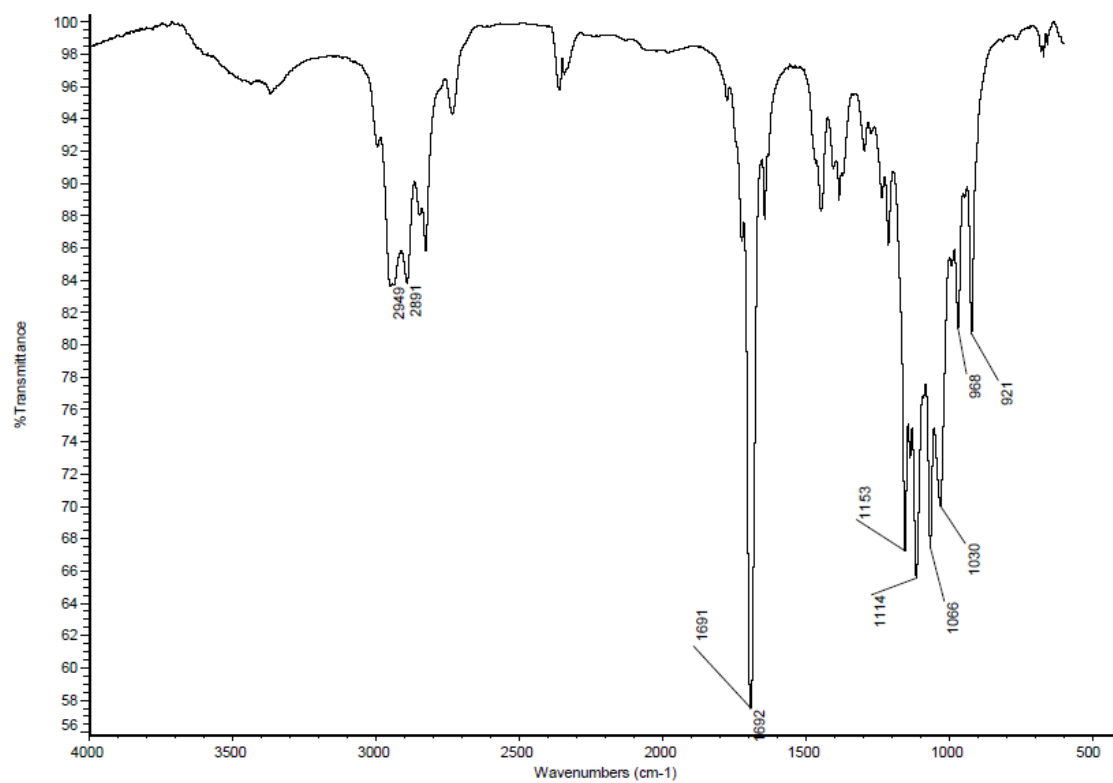


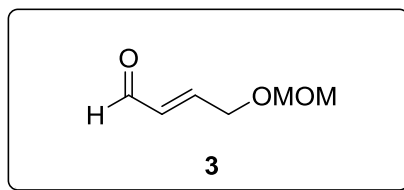
Scan # : (794 - 802) B.G. Scan# : (742 - 769)
 Mass Peak # : 31 Ret. Time : (11.608 - 11.675)
 Base Peak : 70.10 (1394345)



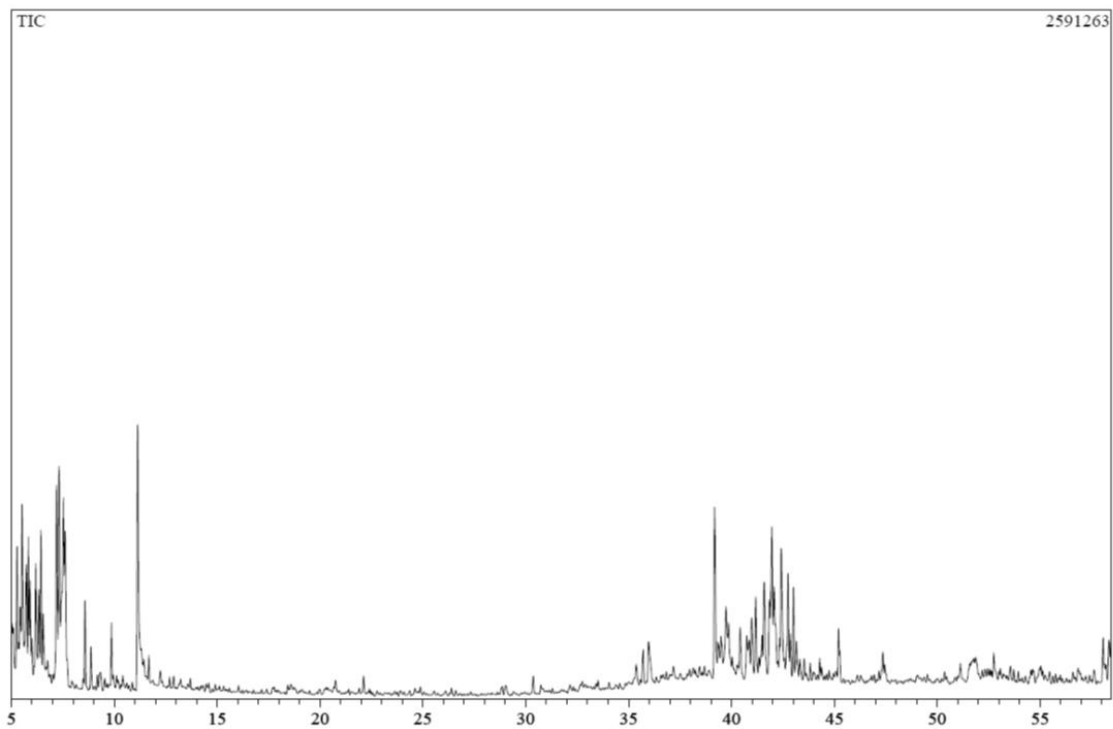




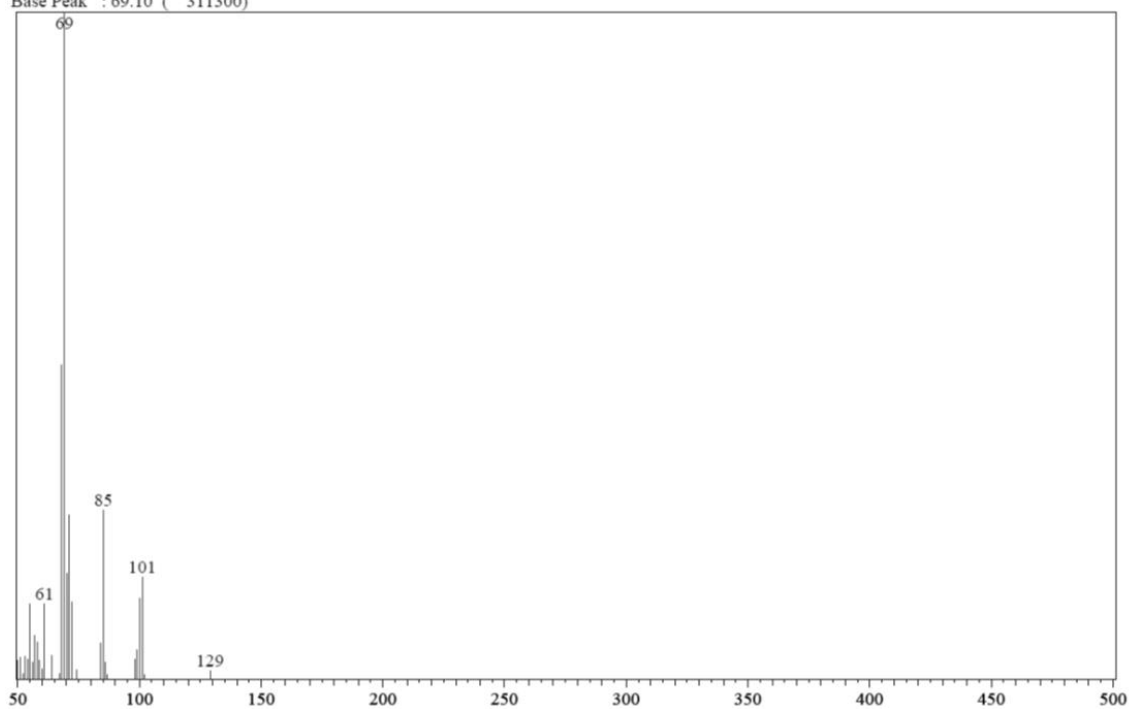


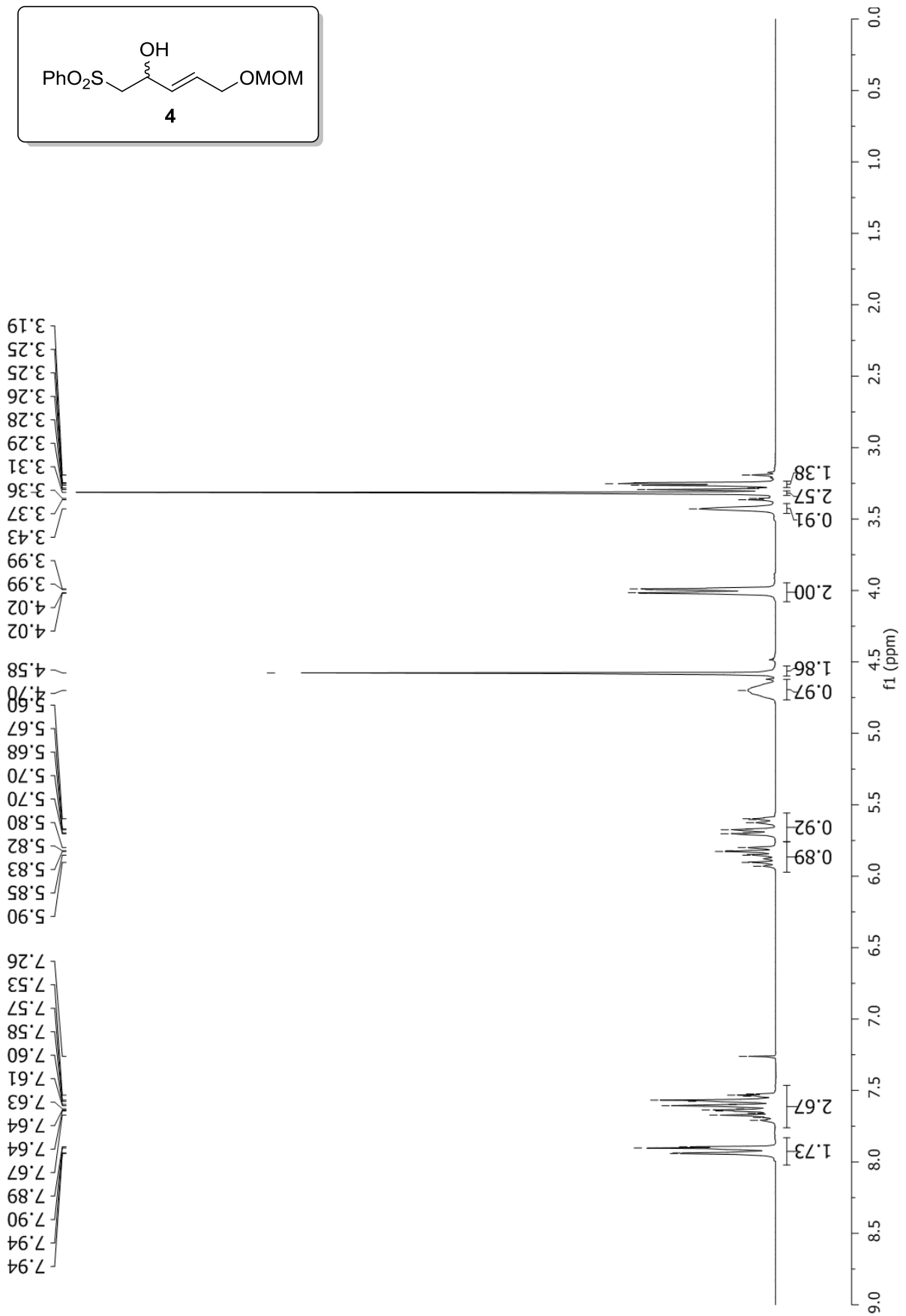
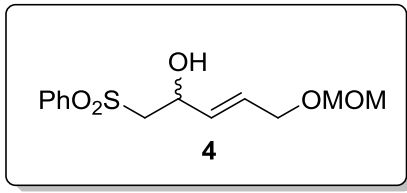


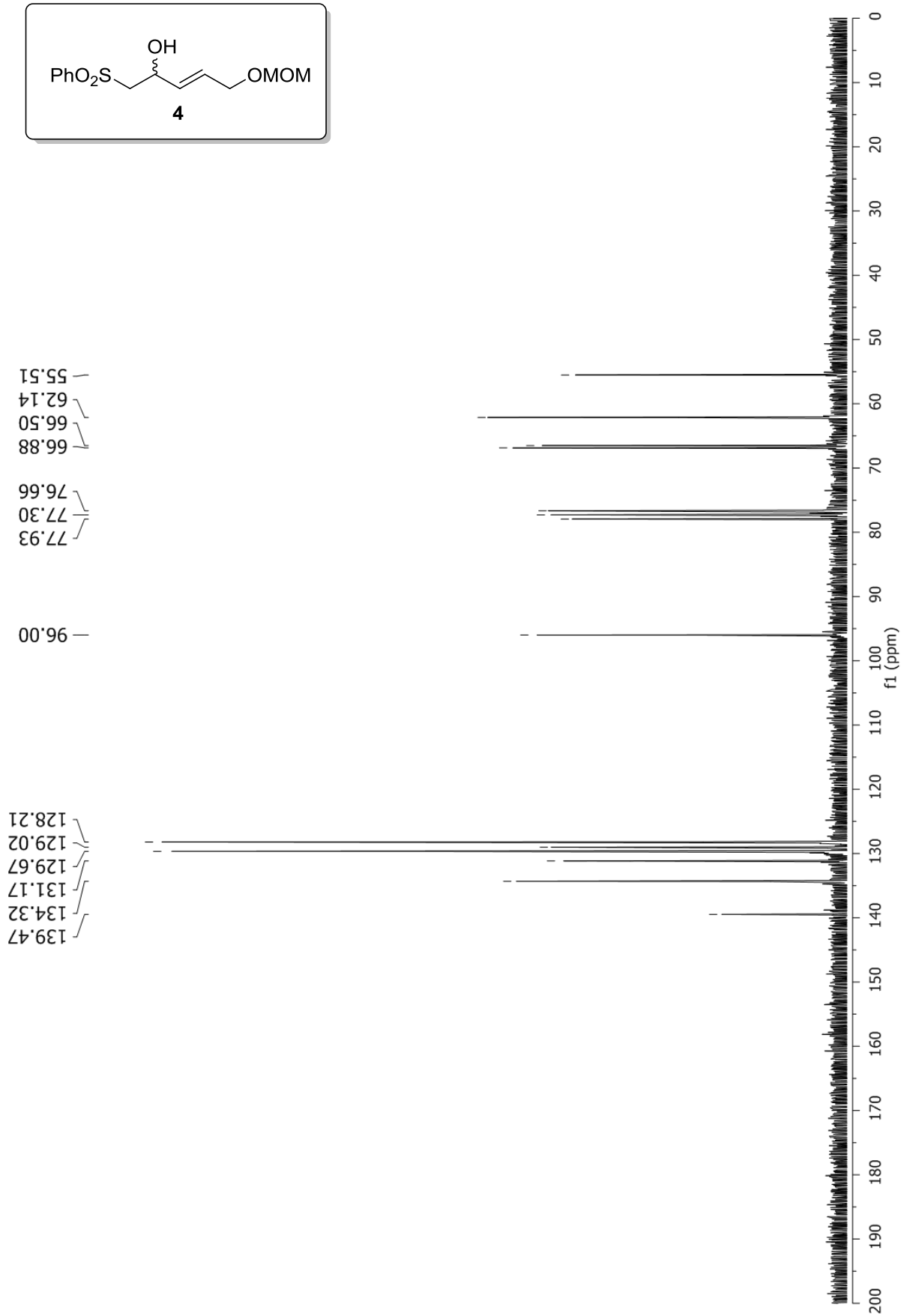
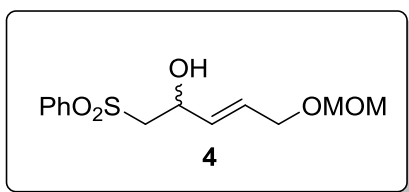
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 Method File Name : NMG3.MET

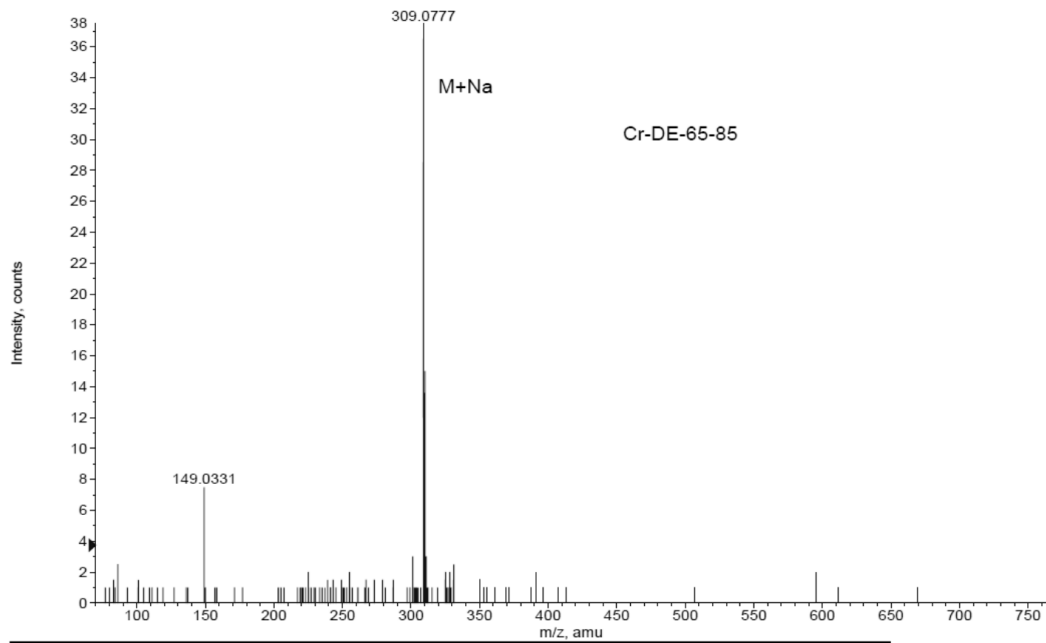
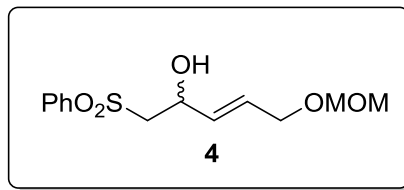
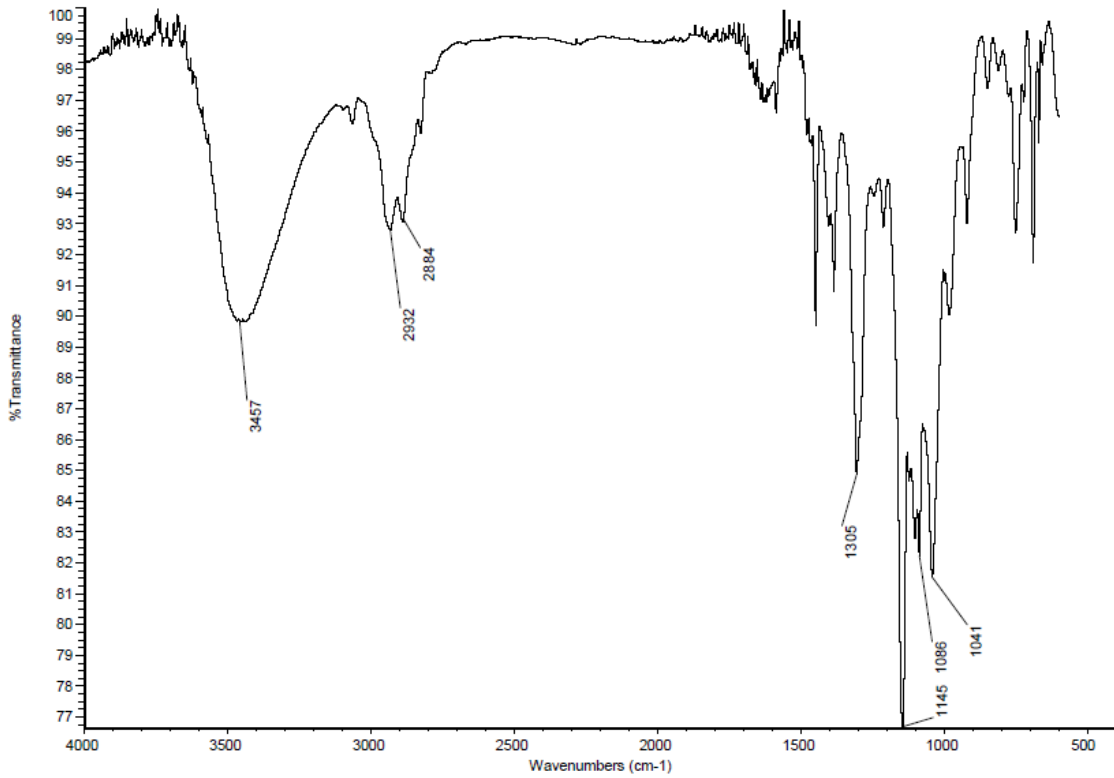


Scan # : (735 - 741)
 Mass Peak # : 30 Ret. Time : (11.115 - 11.163)
 Base Peak : 69.10 (311300)

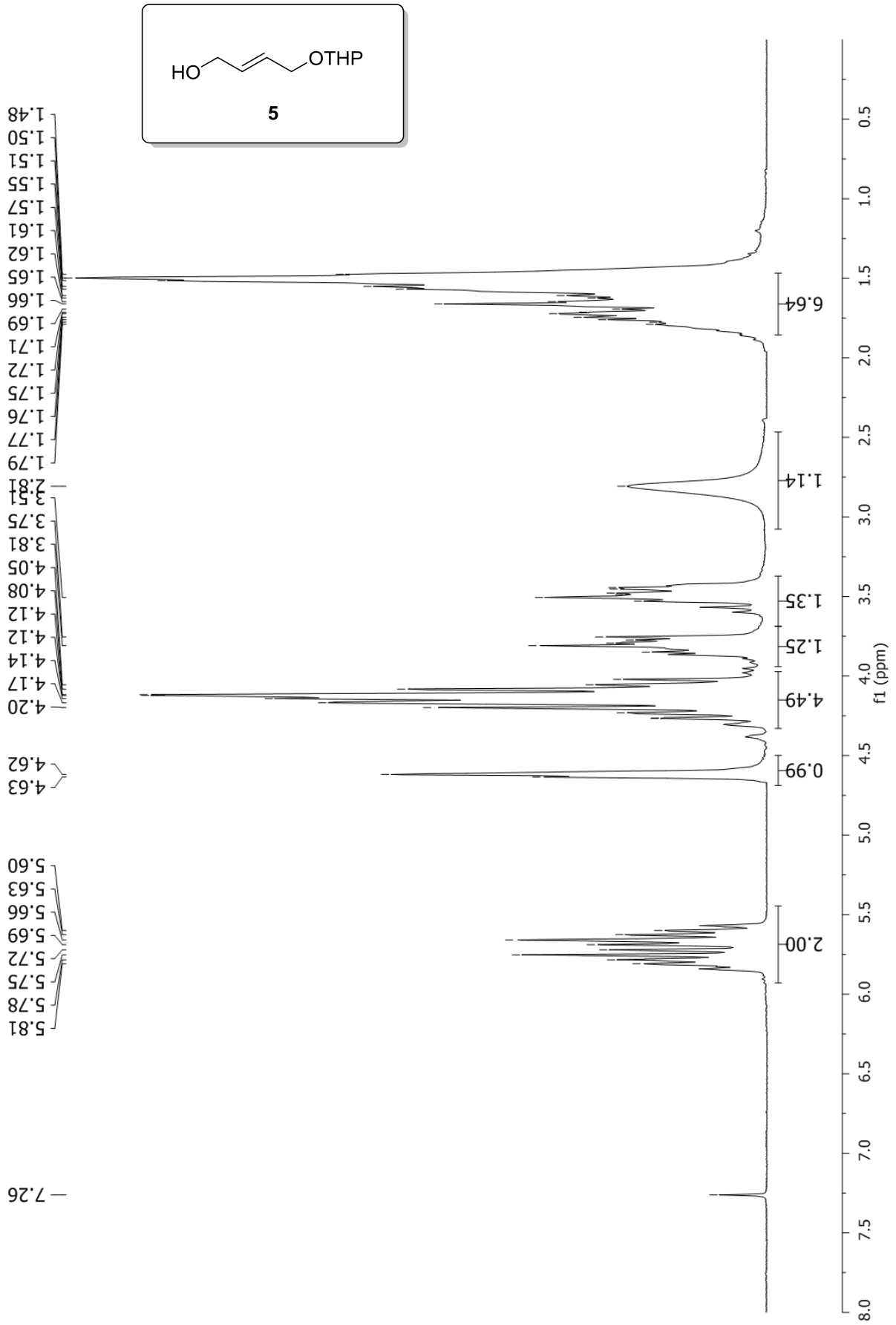


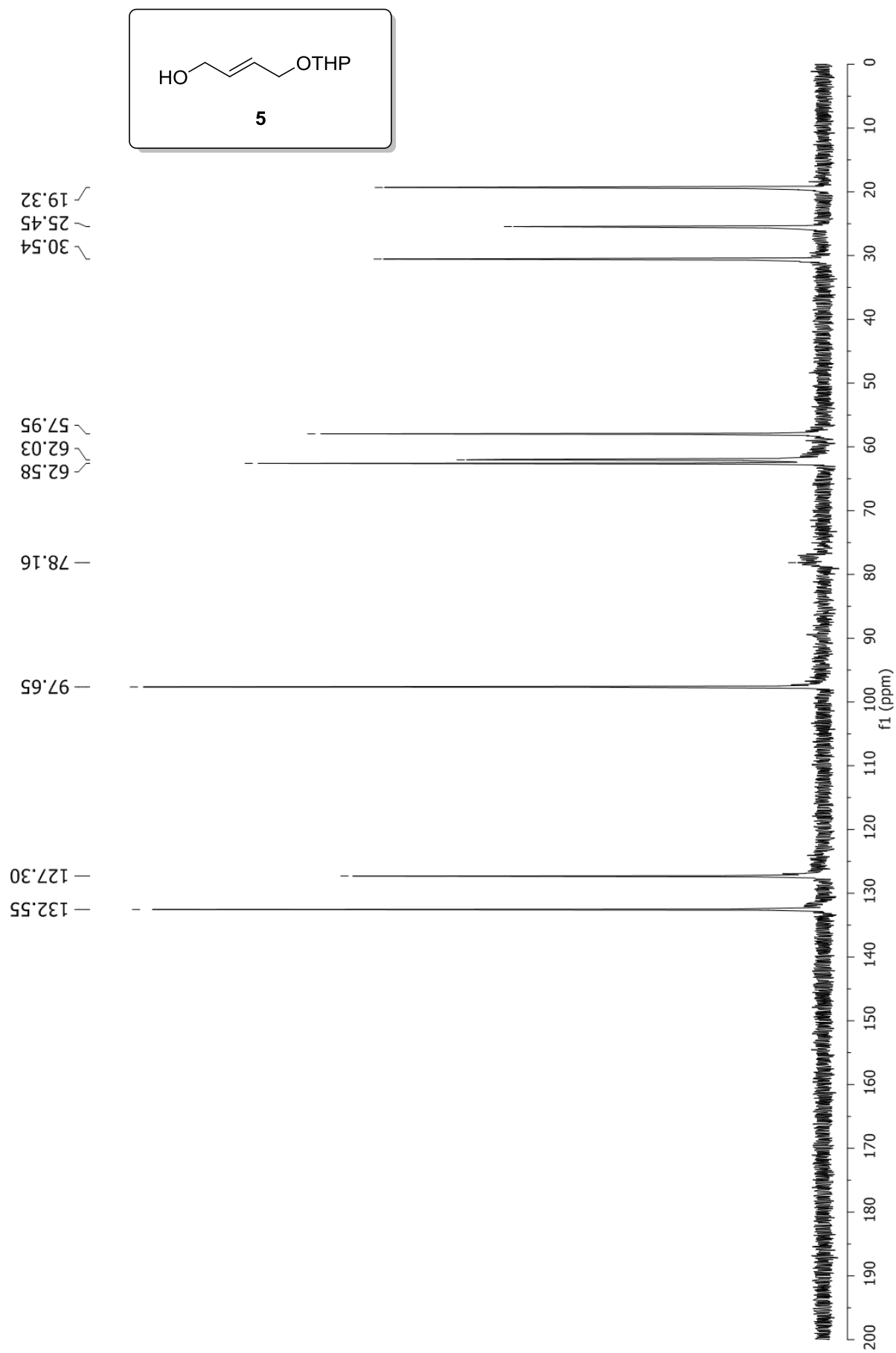


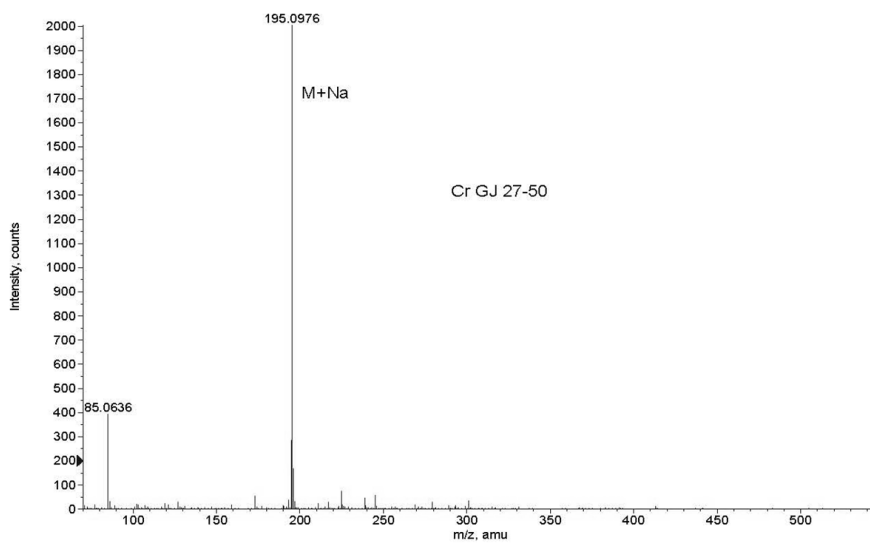
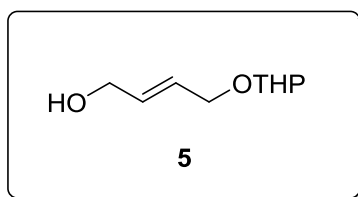
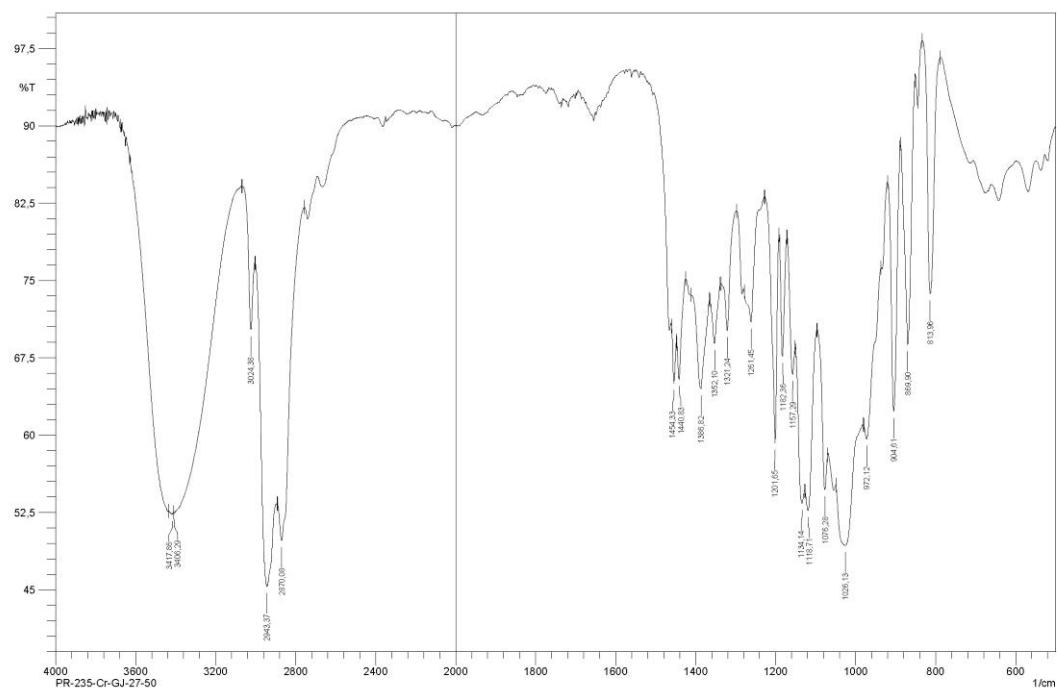




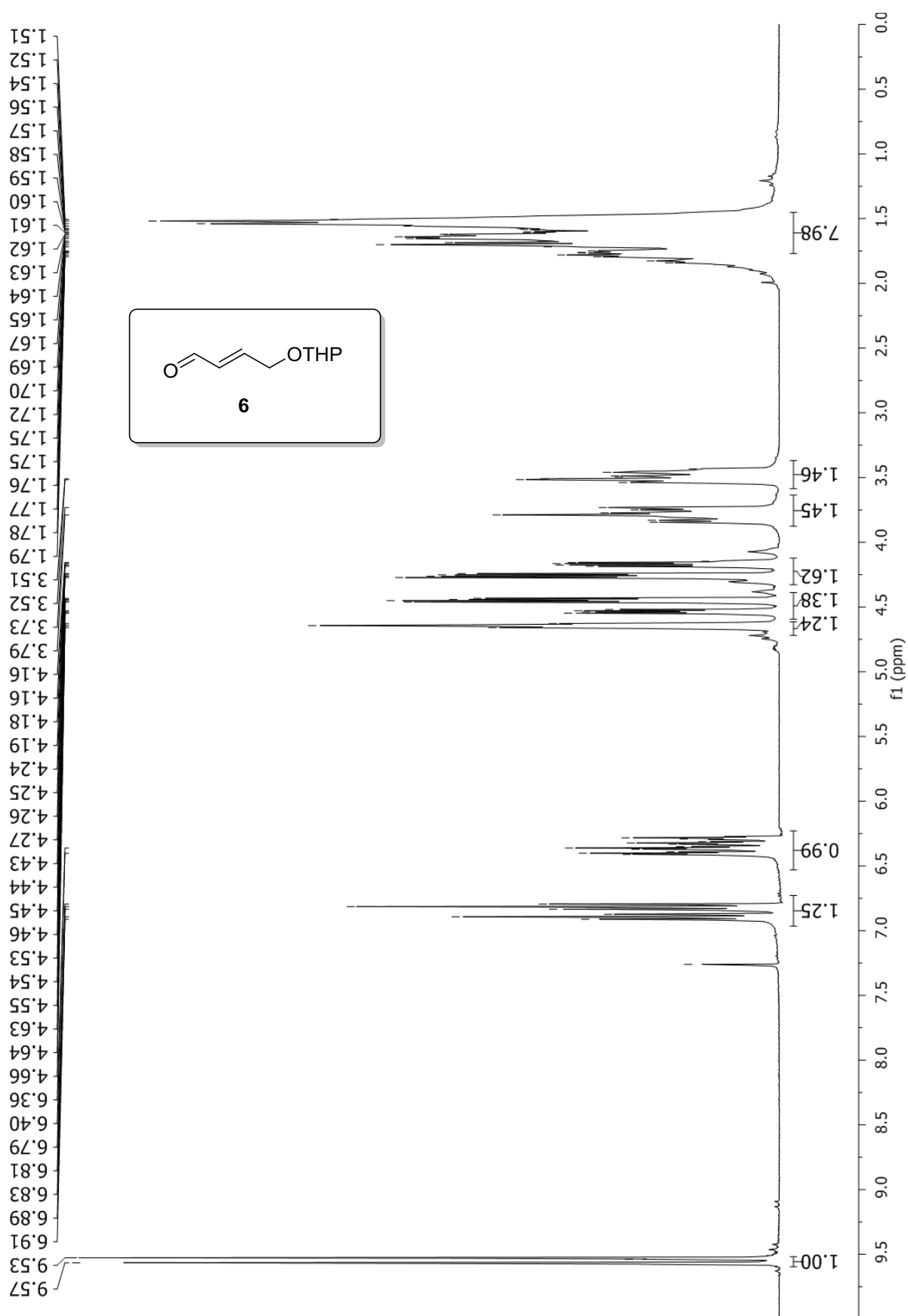
Formula	CalculatedMass	mDaError	ppmError	RDB
C ₁₄ H ₁₄ N ₄ O Na S	309.078054	-0.354152	-1.145833	9.5
C ₁₃ H ₁₈ O ₅ Na S	309.076717	0.98316	3.180942	4.5

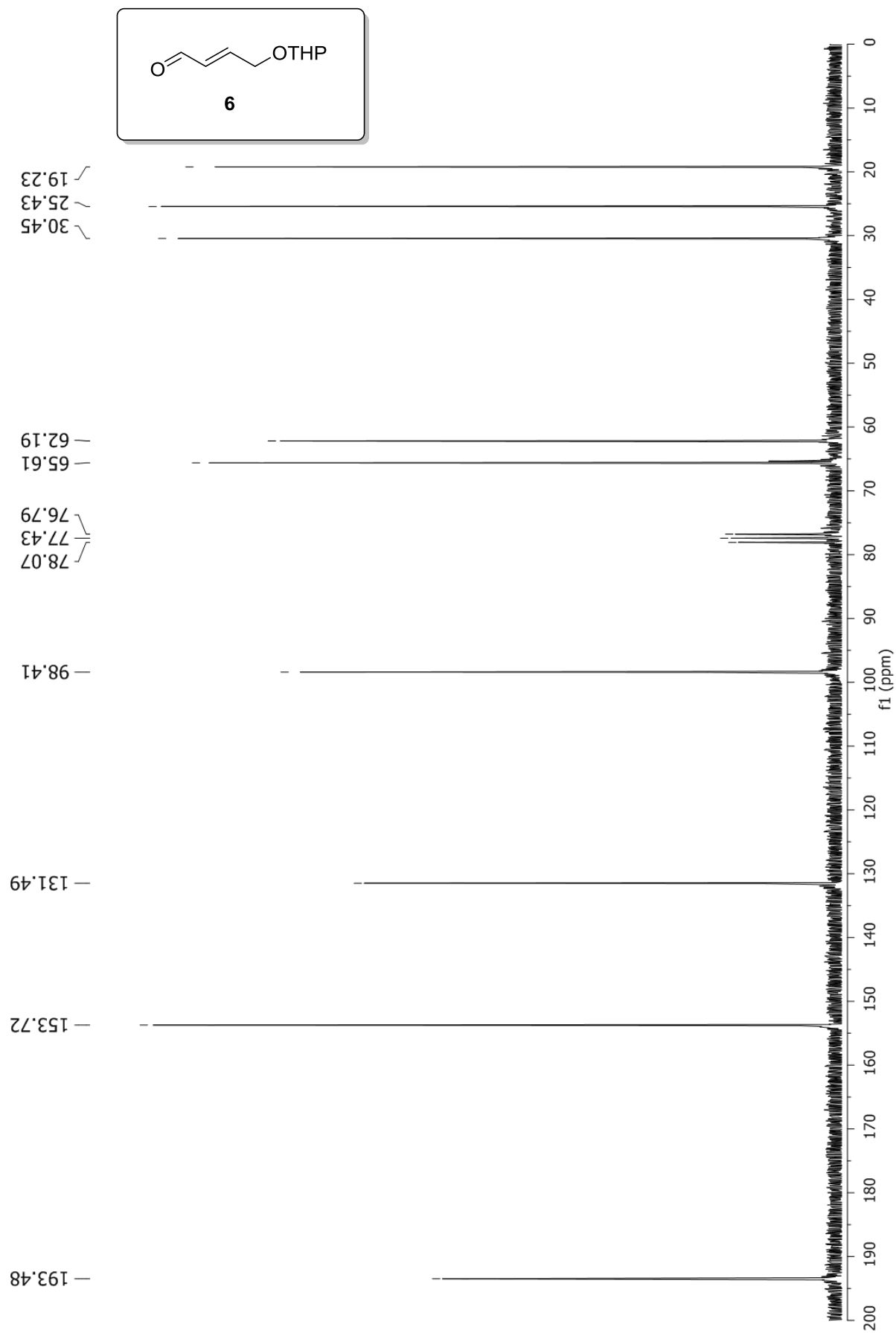


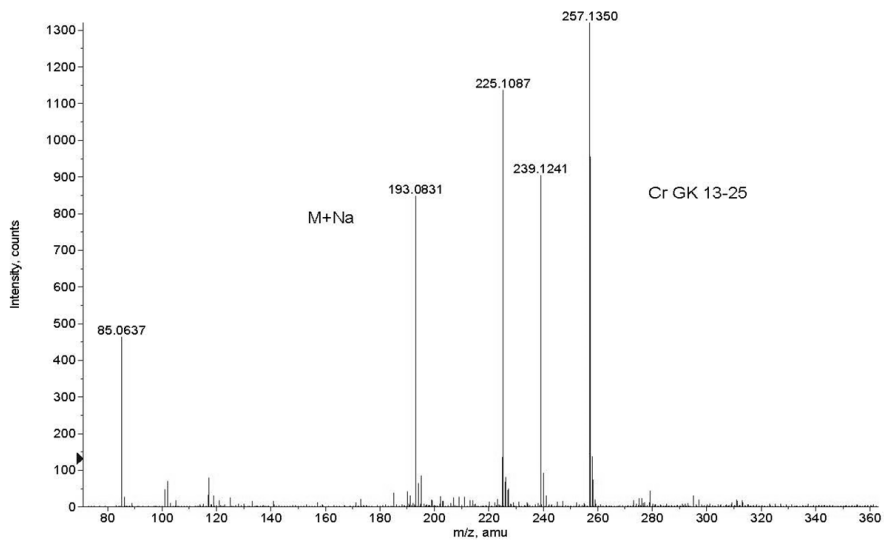
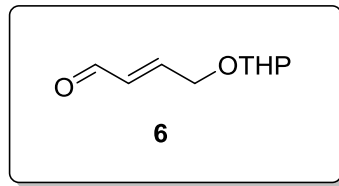
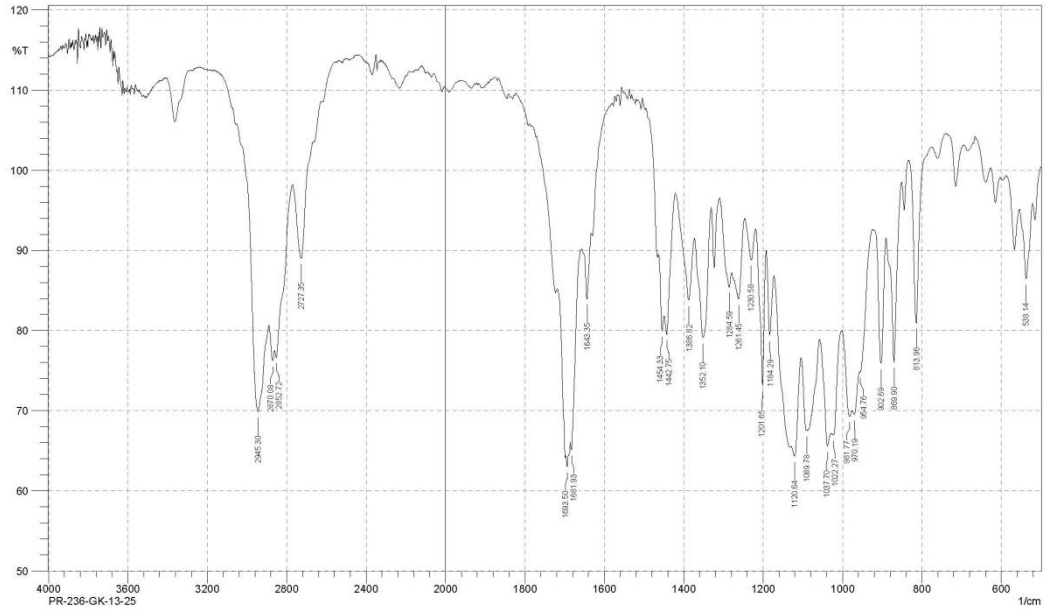




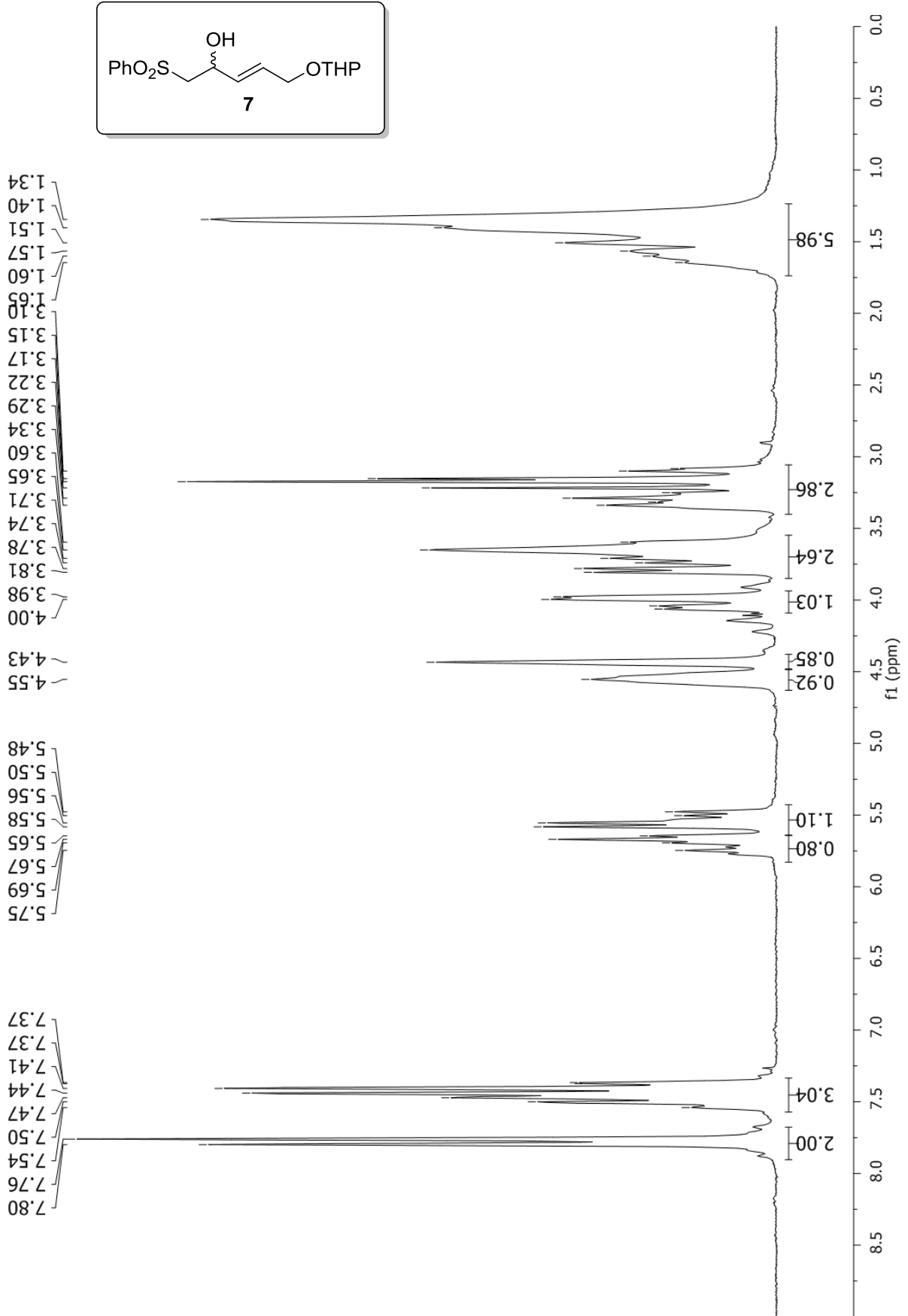
Formula	CalculatedMass	mDaError	ppmError	RDB
C6 H15 N2 O5	195.097548	0.051764	0.265323	0.5
C5 H12 N6 O Na	195.09648	1.119712	5.739224	2.5
C7 H11 N6 O	195.098886	-1.285548	-6.589237	5.5
C9 H16 O3 Na	195.099166	-1.56568	-8.025089	1.5

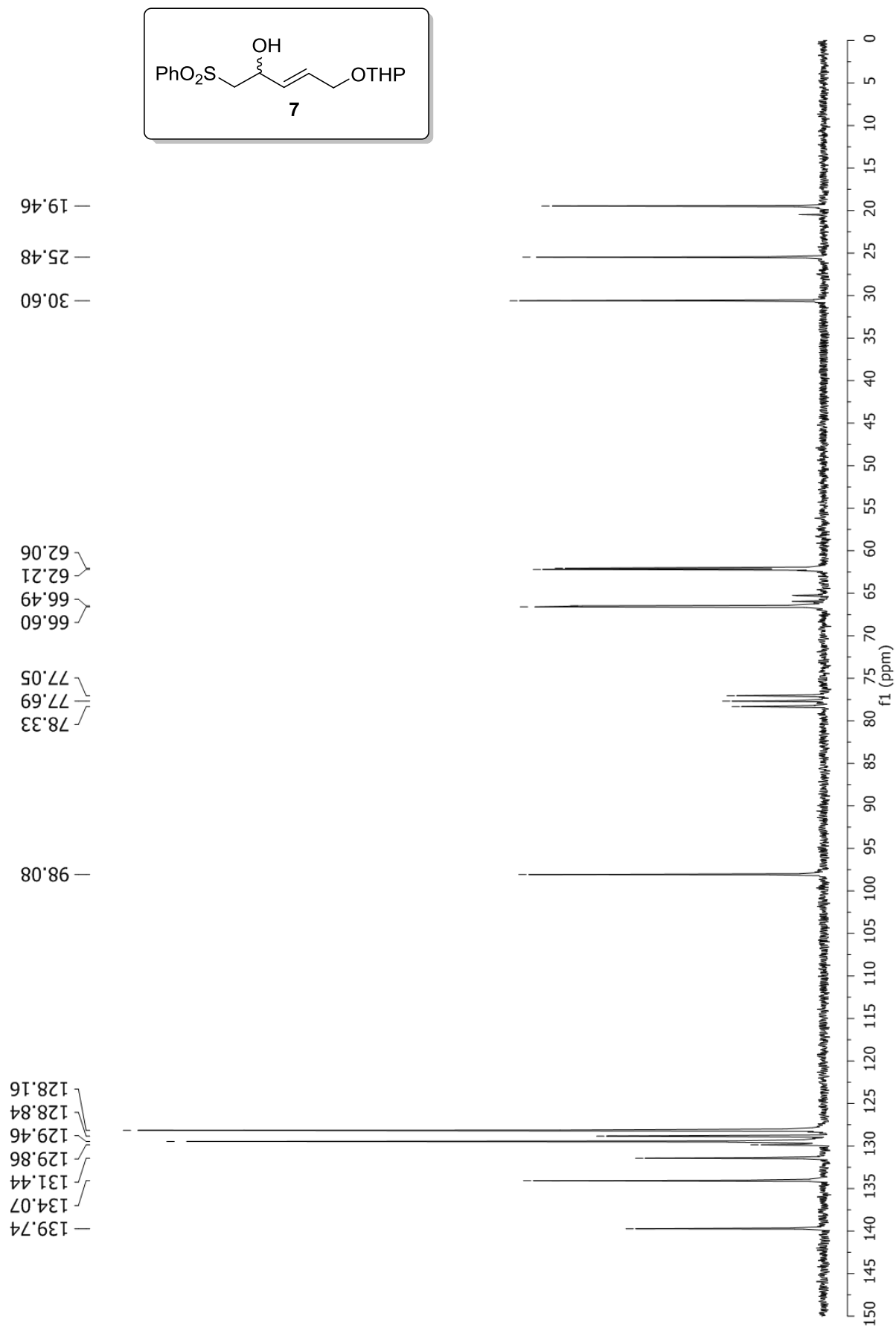




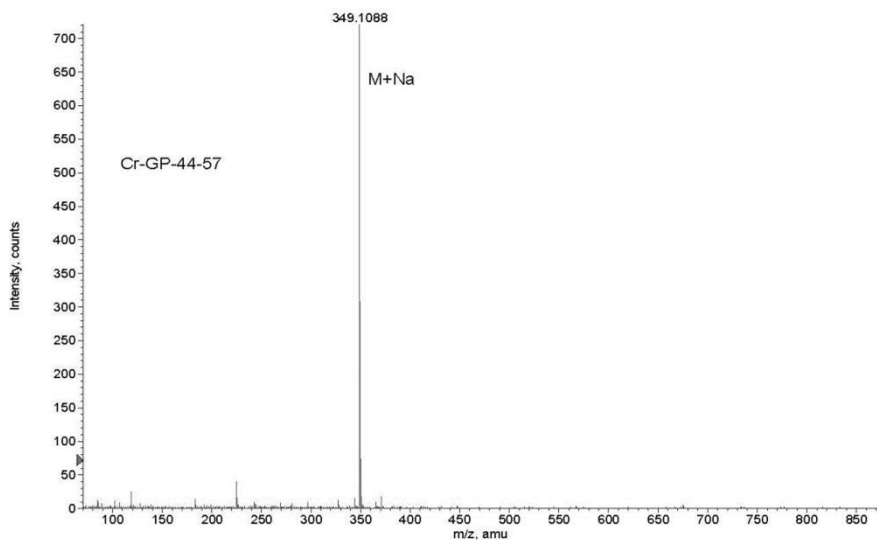
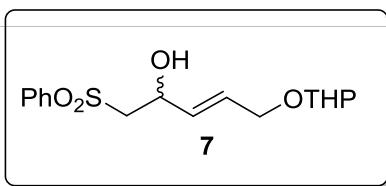
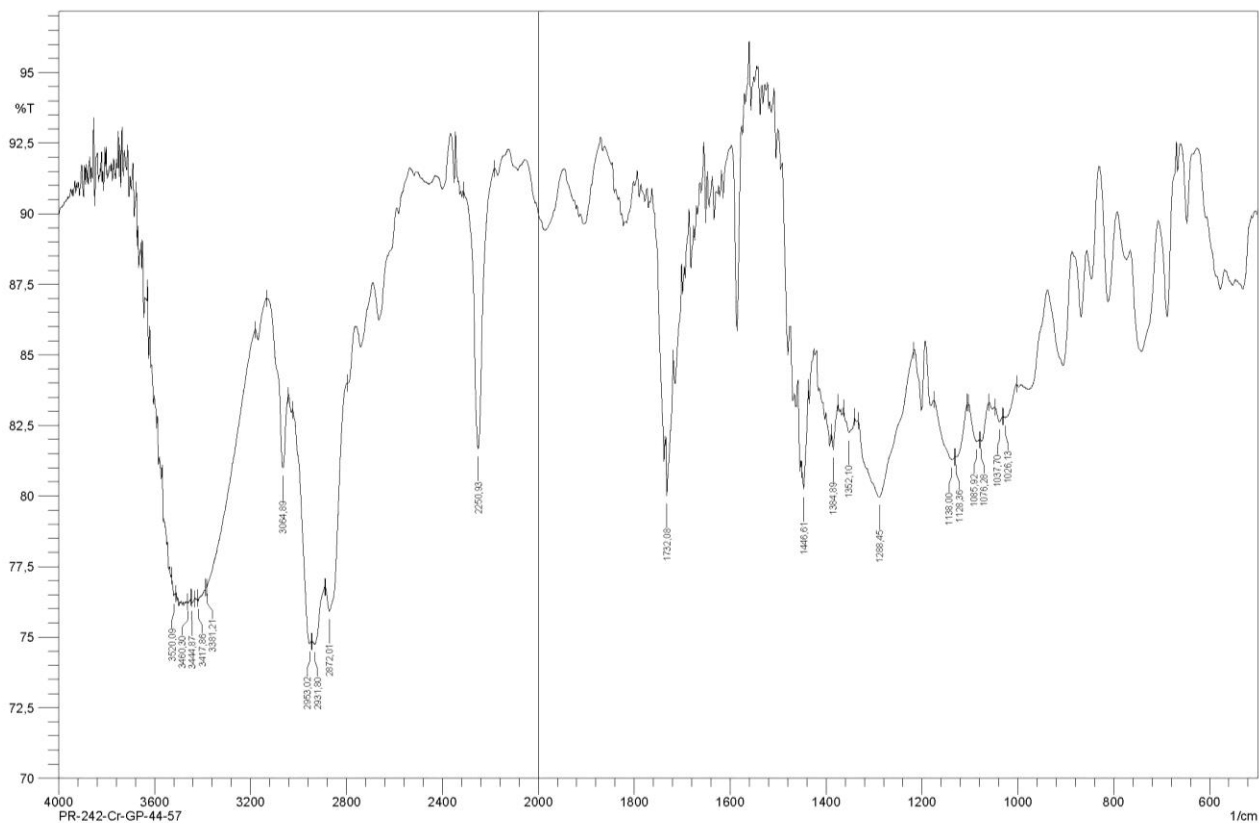


Formula	CalculatedMass	mDaError	ppmError	RDB
C7 H9 N6 O	193.083235	-0.135468	-0.701603	6.5
C9 H14 O3 Na	193.083516	-0.4156	-2.152435	2.5
C6 H13 N2 O5	193.081898	1.201844	6.224473	1.5

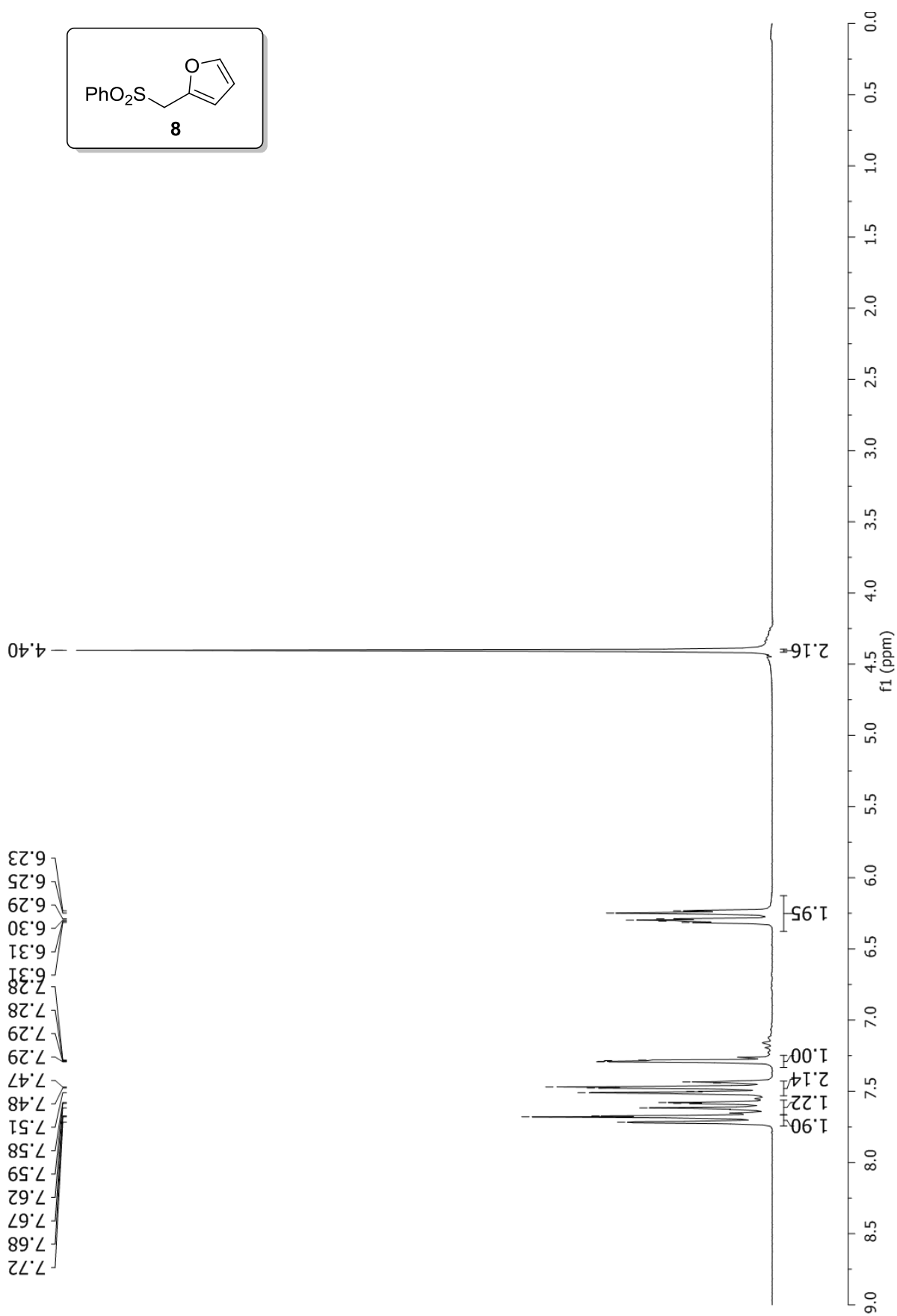


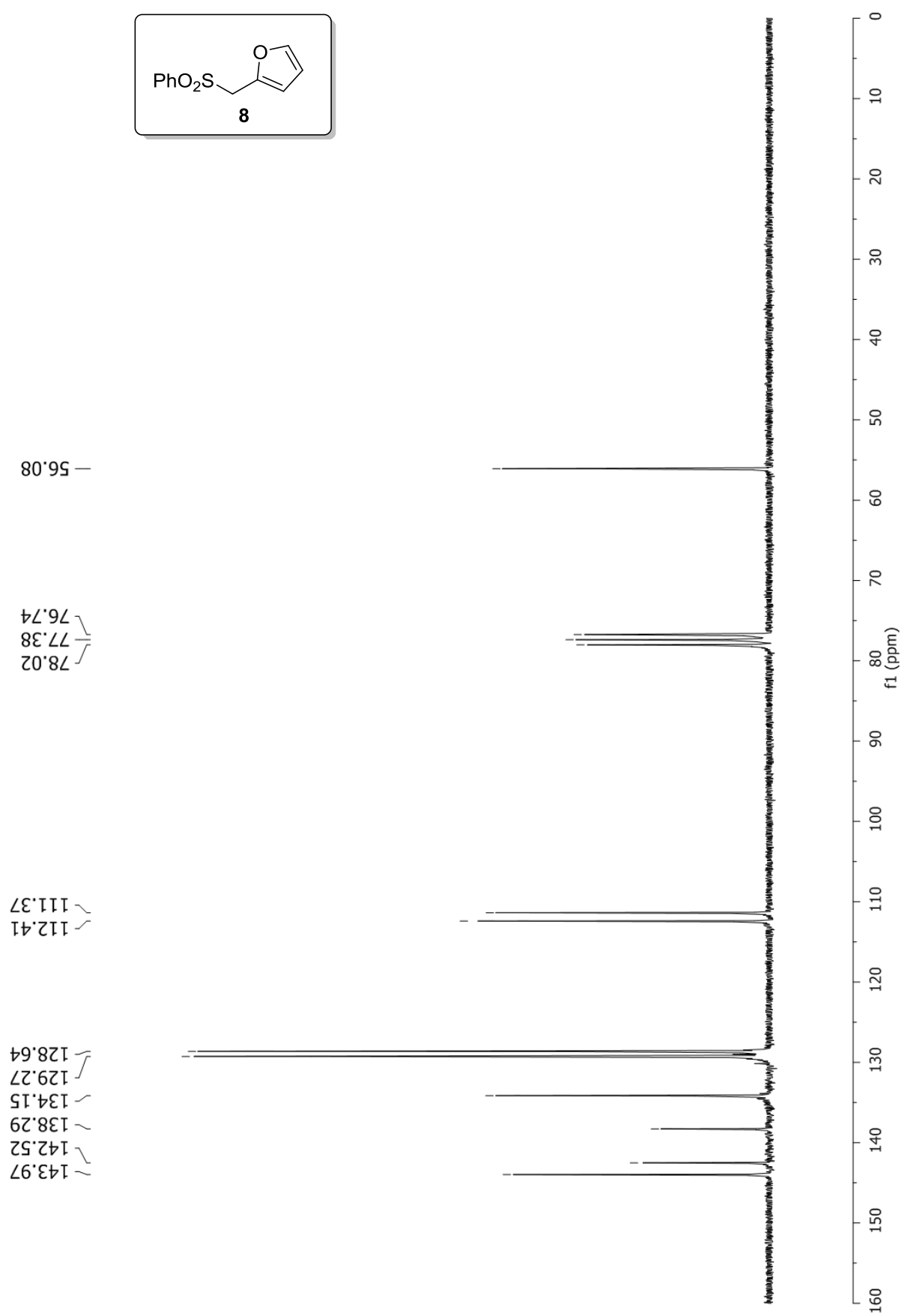
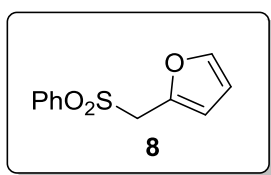


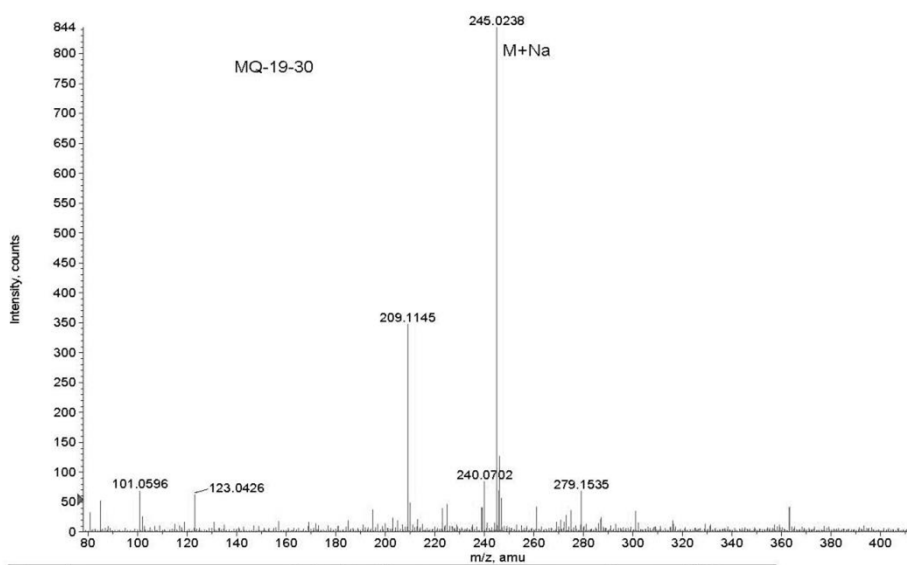
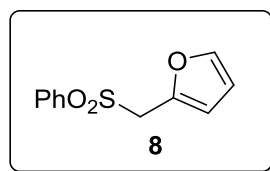
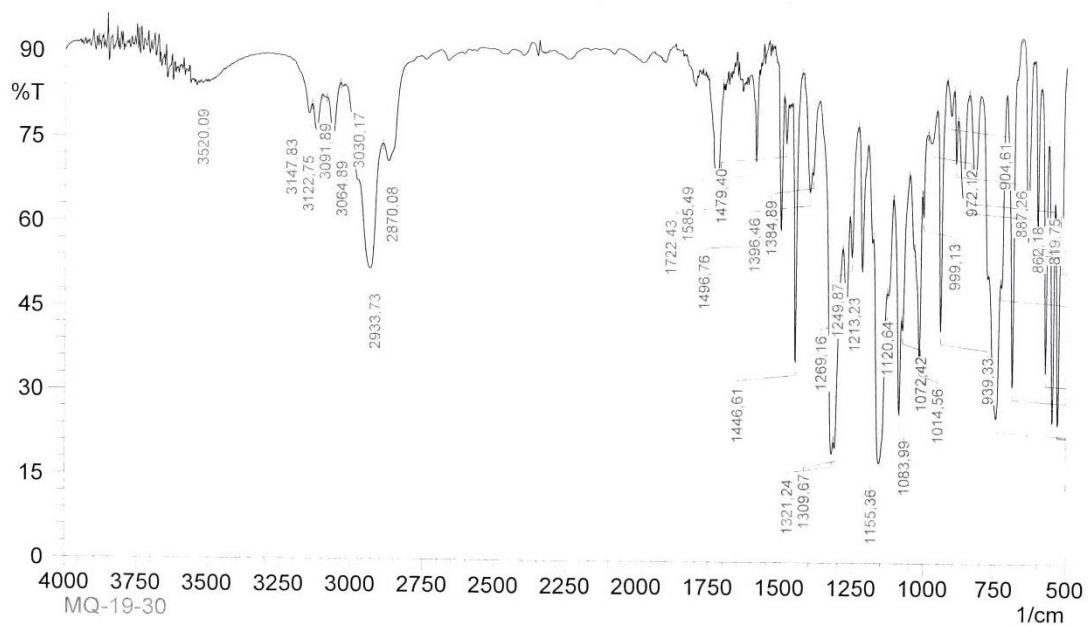
Full Spectroscopy



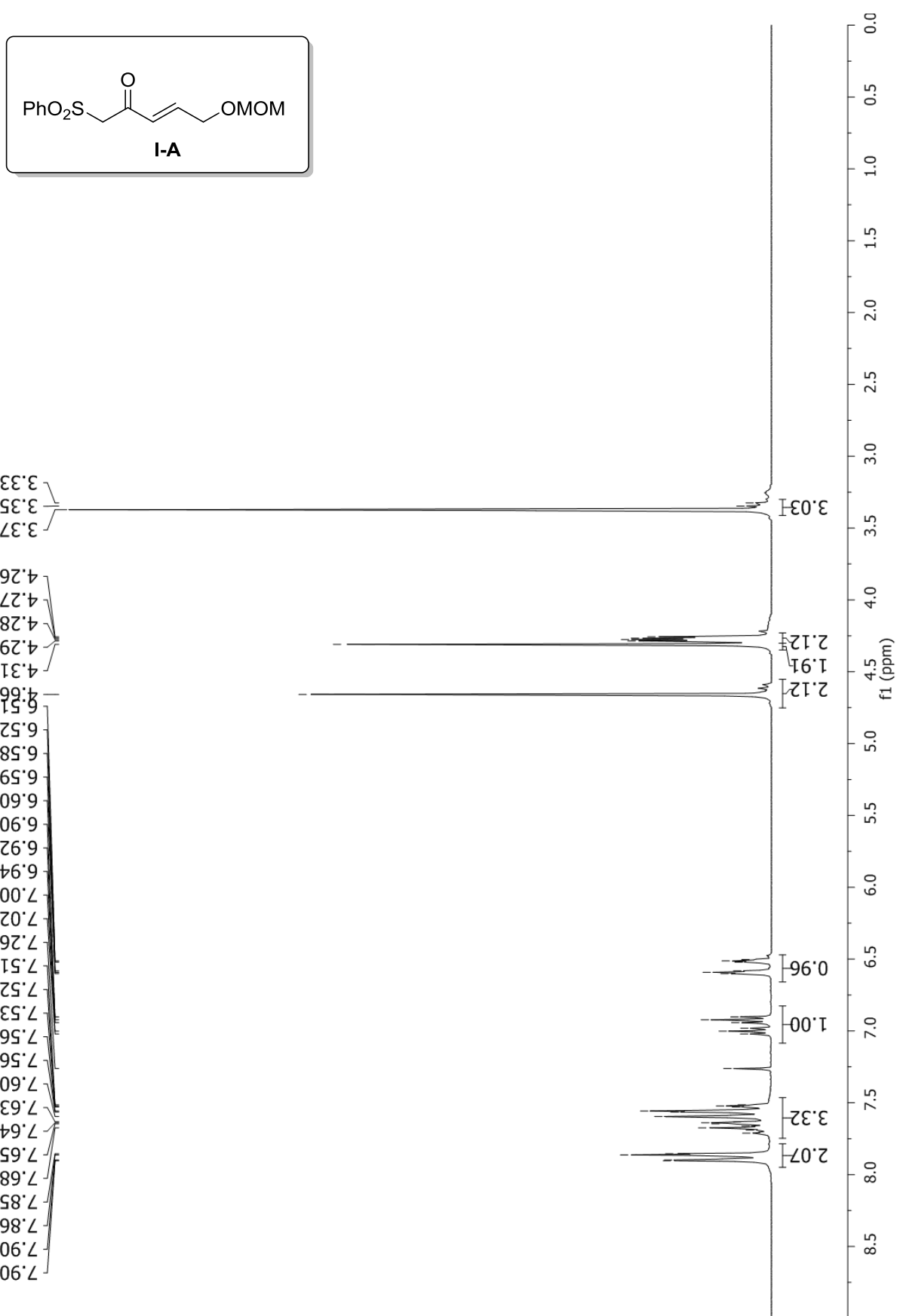
Formula	CalculatedMass	mDaError	ppmError	RDB
C17 H18 N4 O Na S	349.109354	-0.554312	-1.587789	10.5
C16 H22 O5 Na S	349.108017	0.783	2.24285	5.5
C14 H17 N6 O3 S	349.107737	1.063132	3.045269	9.5
C18 H21 O5 S	349.110422	-1.62226	-4.646854	8.5
C3 H17 N12 O6 S	349.110925	-2.124836	-6.086448	1.5
C13 H21 N2 O7 S	349.1064	2.400444	6.875909	4.5
C19 H17 N4 O S	349.11176	-2.959572	-8.477493	13.5
C12 H18 N6 O3 Na S	349.105332	3.468392	9.934973	6.5

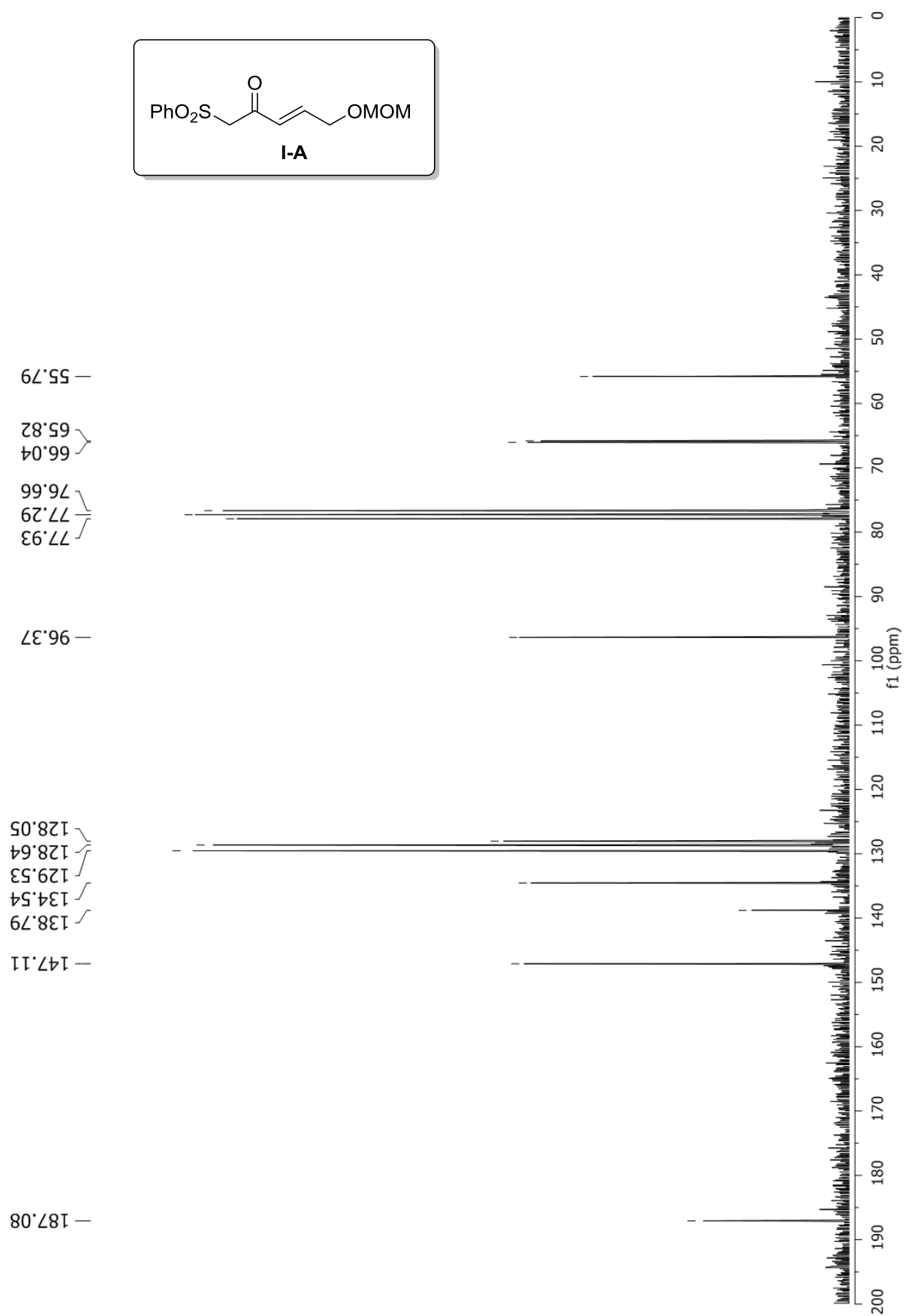




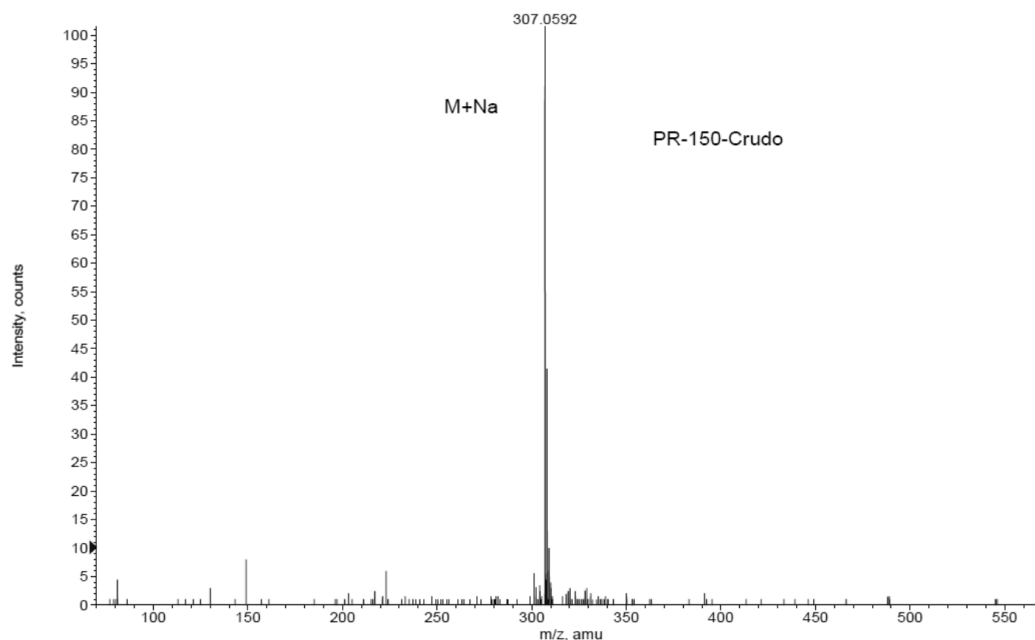
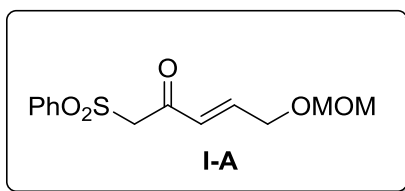
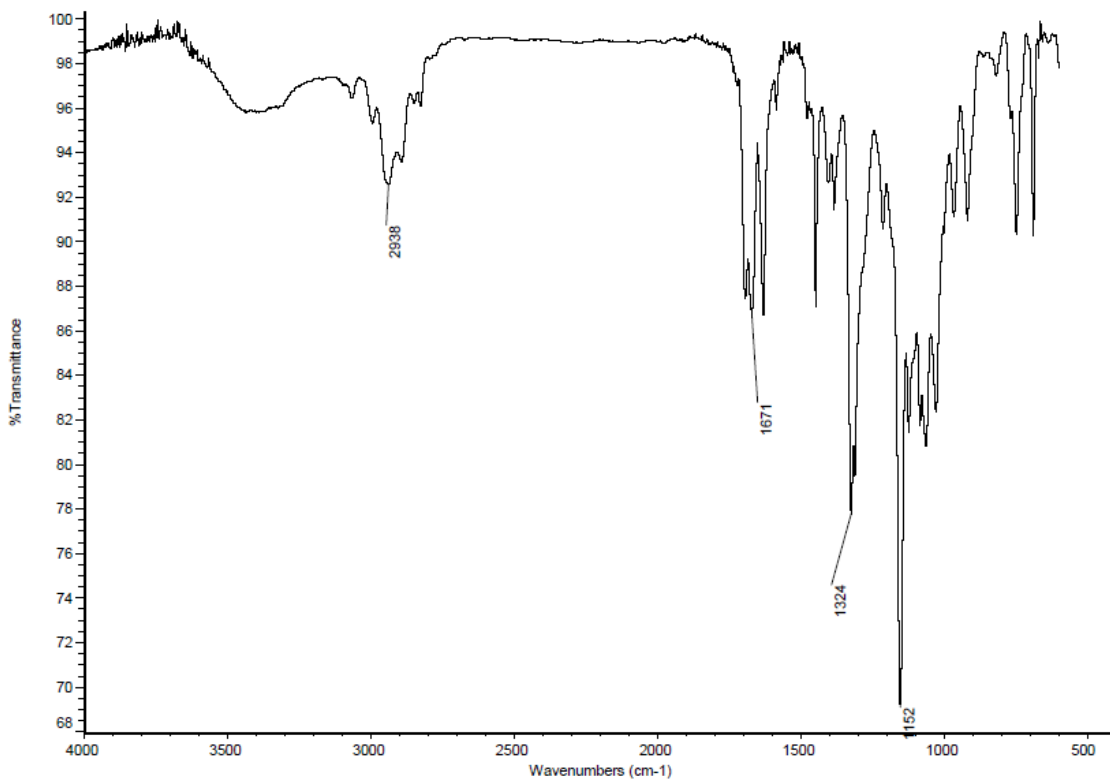


Formula	CalculatedMass	mDaError	ppmError	RDB
C9 H5 N6 O S	245.024007	-0.207108	-0.845255	10.5
C3 H6 N6 O6 Na	245.024103	-0.303248	-1.237624	3.5
C16 H5 O3	245.023321	0.47946	1.956785	14.5
C11 H10 O3 Na S	245.024287	-0.48724	-1.988537	6.5

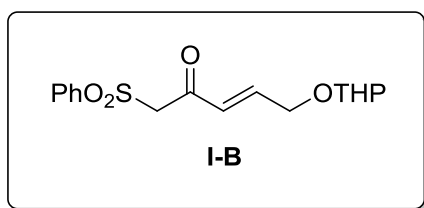


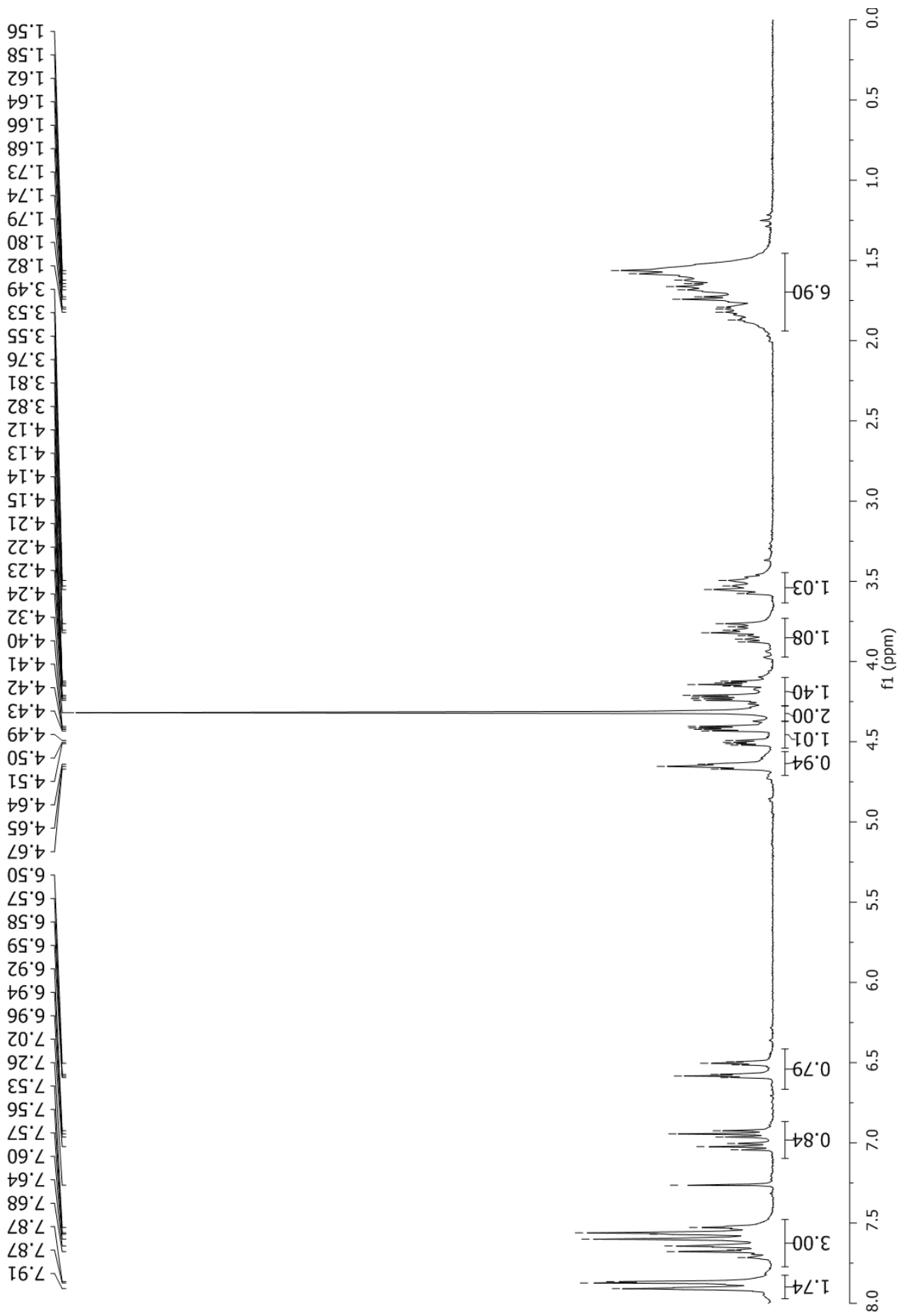


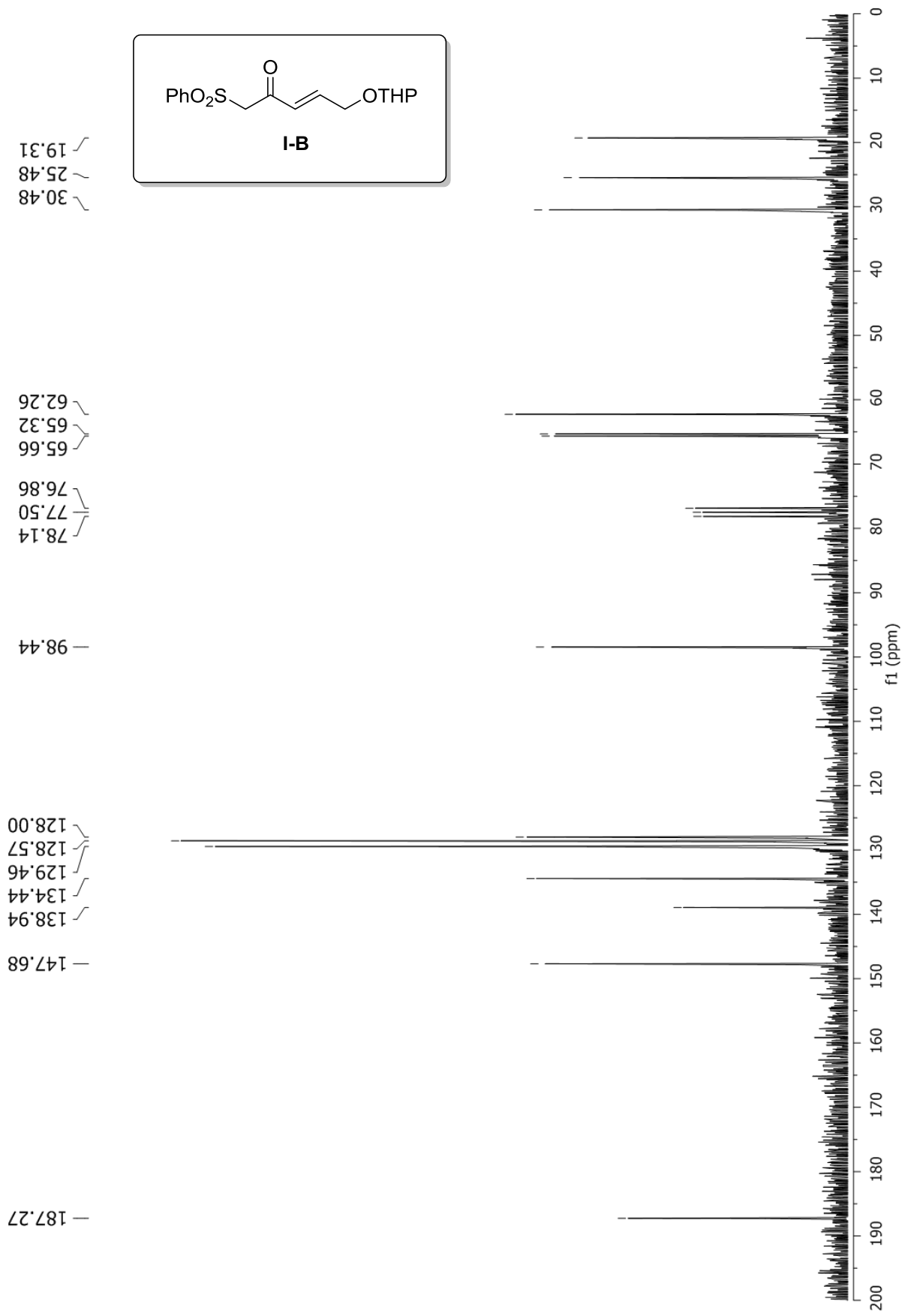
Full Spectroscopy

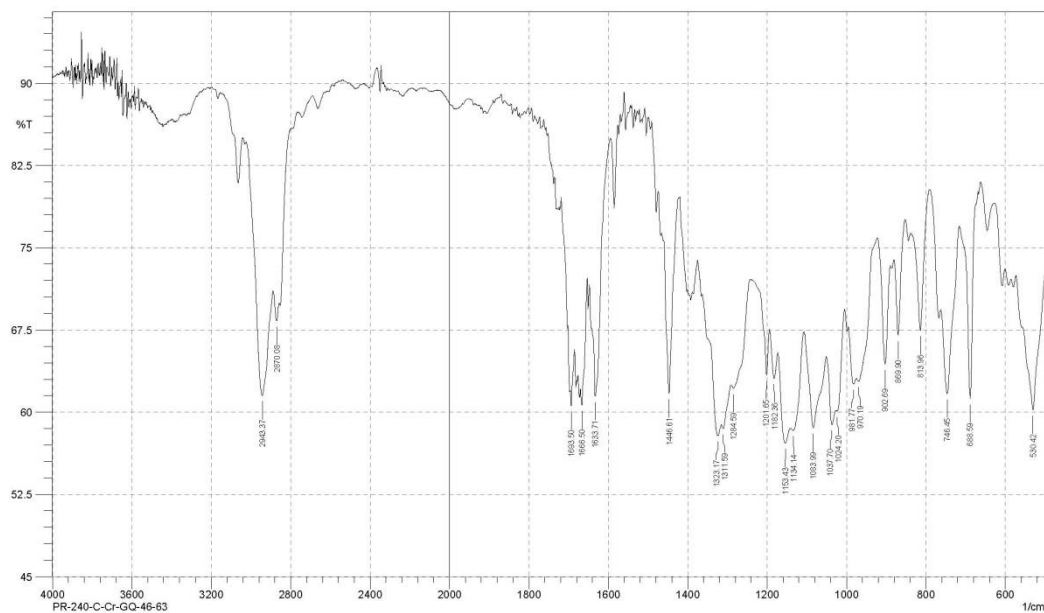


Formula	CalculatedMass	mDaError	ppmError	RDB
C10 H15 N2 O7 S	307.059449	-0.249316	-0.811946	4.5
C9 H12 N6 O3 Na S	307.058381	0.818632	2.666035	6.5
C7 H7 N12 O S	307.058101	1.098764	3.578339	10.5
C11 H11 N6 O3 S	307.060787	-1.586628	-5.167164	9.5
C22 H11 S	307.057599	1.60134	5.215076	17.5
C13 H16 O5 Na S	307.061067	-1.86676	-6.079468	5.5





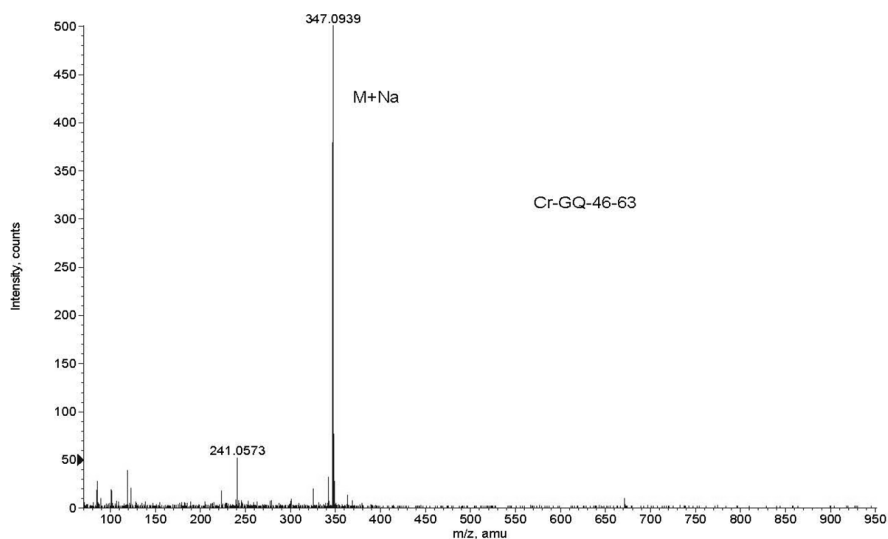
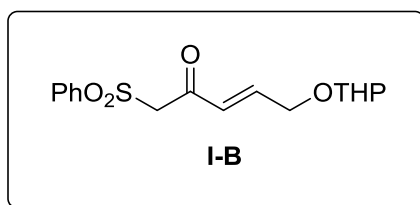




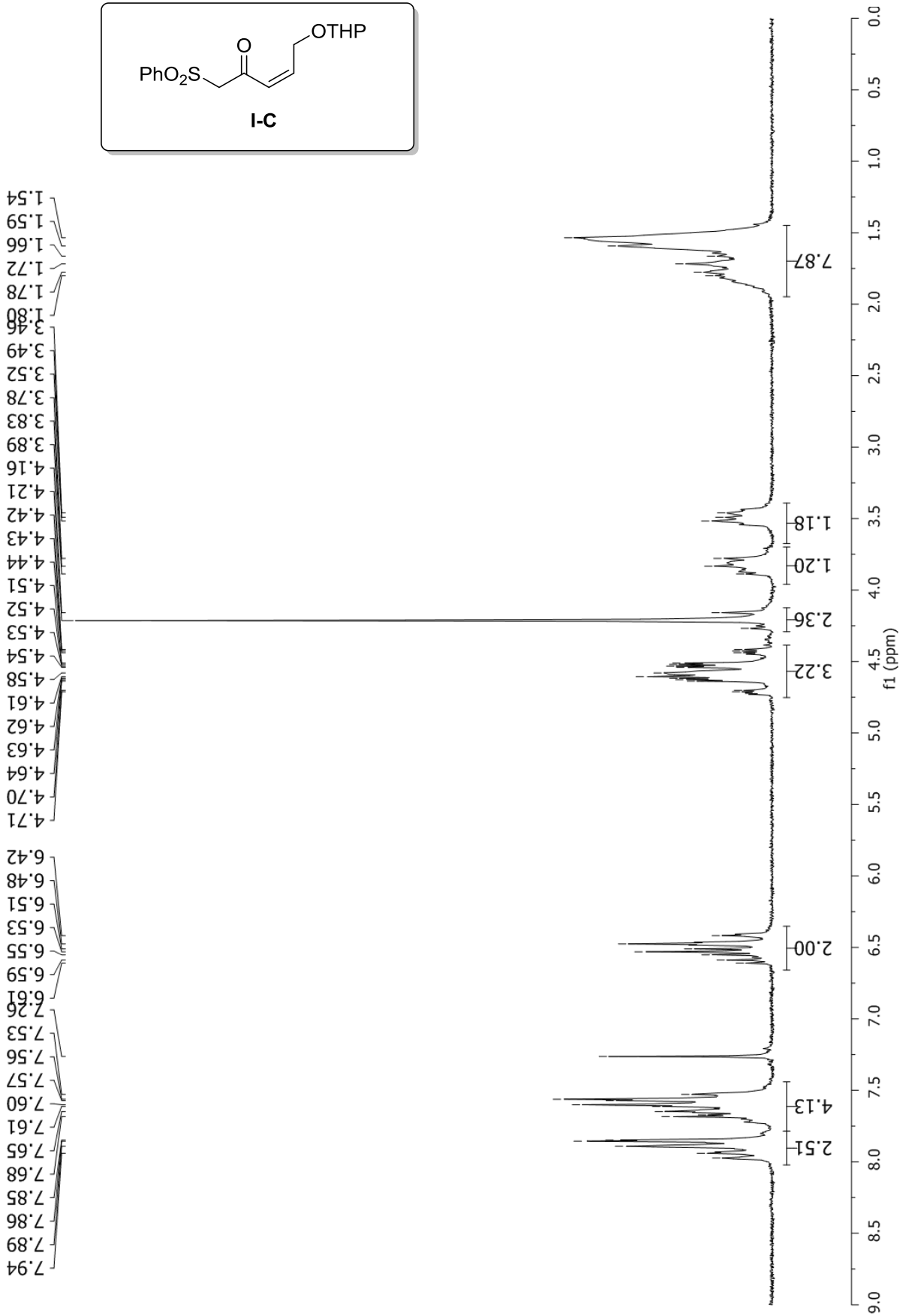
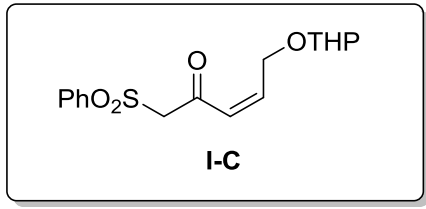
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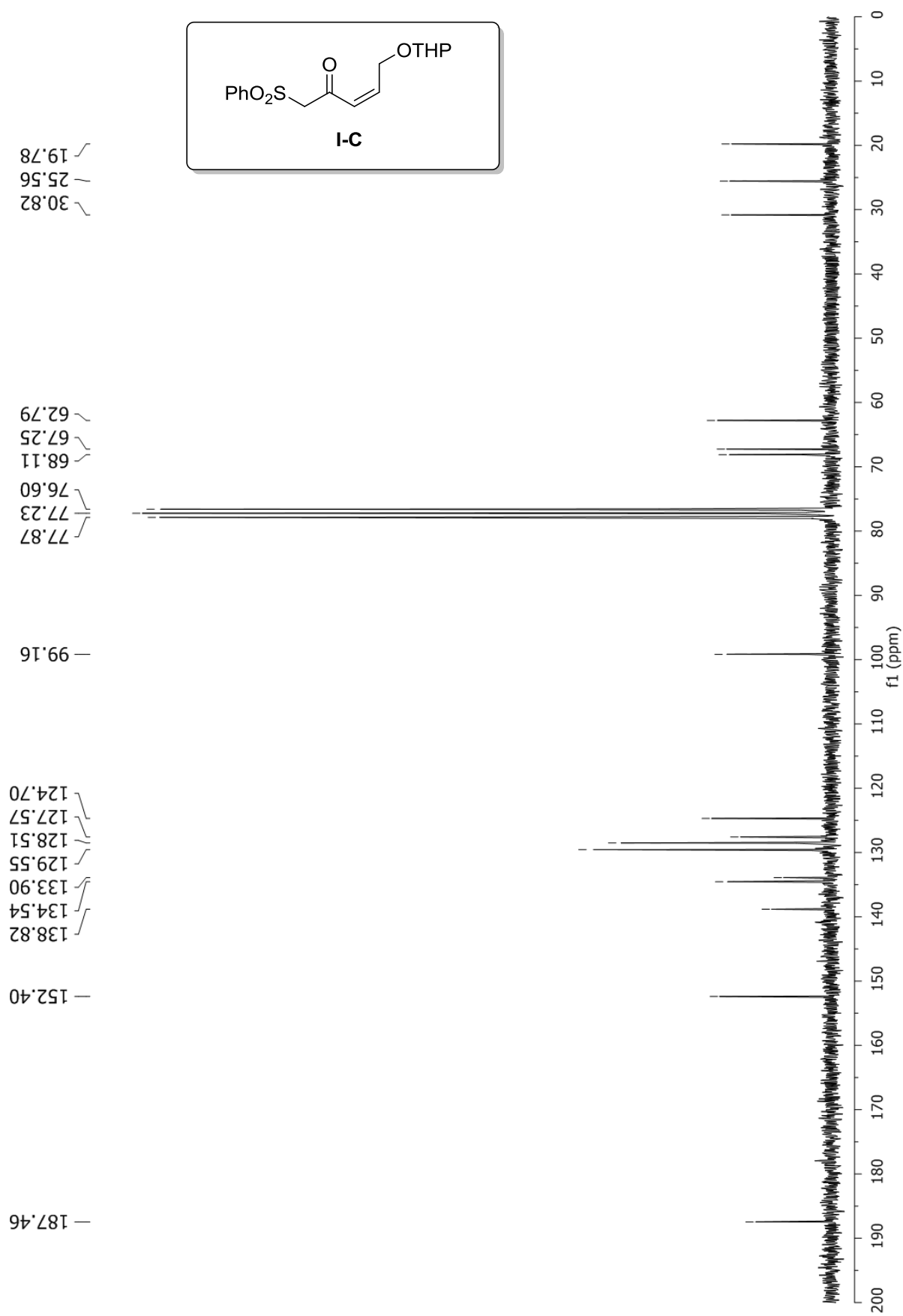
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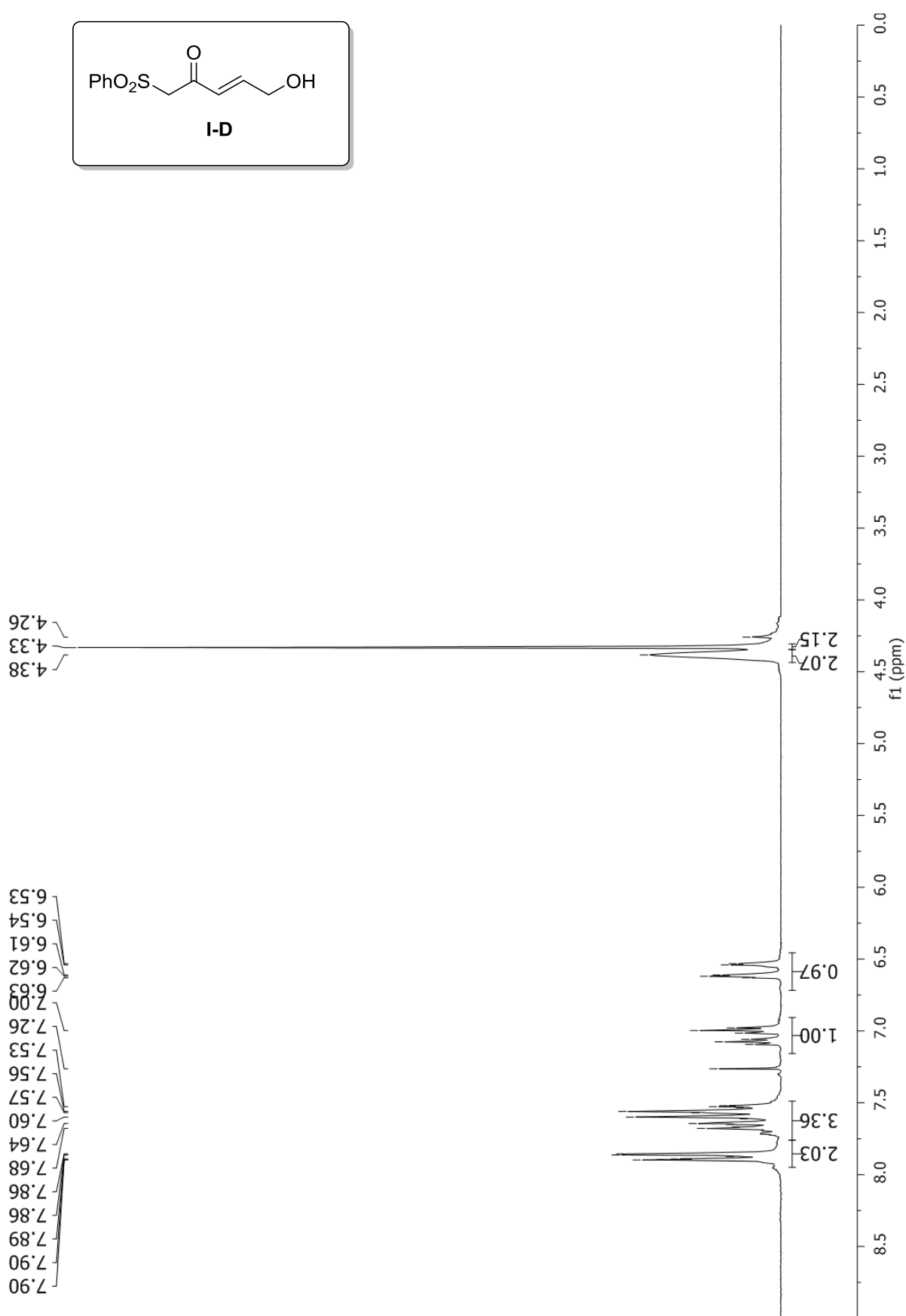
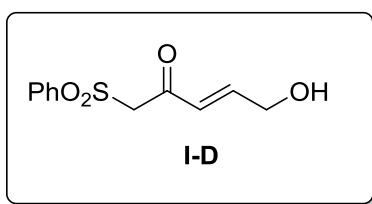
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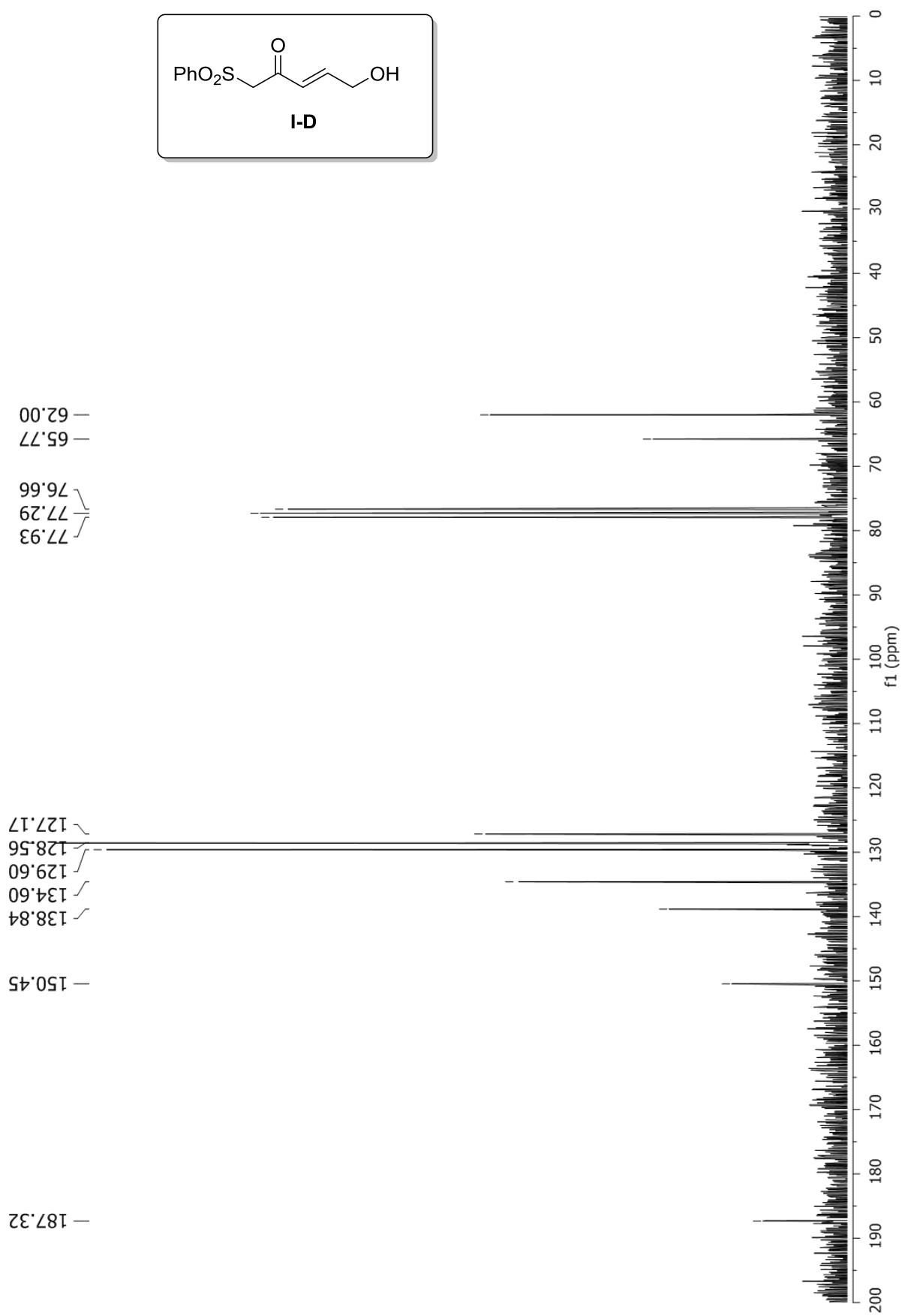


Formula	CalculatedMass	mDaError	ppmError	RDB
C17 H16 N4 O Na S	347.093704	0.195768	0.564019	11.5
C9 H12 N10 O4 Na	347.09352	0.37976	1.094111	8.5
C9 H19 N2 O12	347.093251	0.649124	1.870165	1.5
C10 H15 N6 O8	347.094588	-0.688188	-1.982711	6.5
C18 H19 O5 S	347.094772	-0.87218	-2.512803	9.5
C10 H8 N14 Na	347.094858	-0.957552	-2.758765	13.5
C12 H20 O10 Na	347.094868	-0.96832	-2.789788	2.5
C H16 N12 O6 Na S	347.092869	1.030504	2.968944	-0.5
C22 H11 N4 O	347.092738	1.162468	3.34914	19.5
C3 H15 N12 O6 S	347.095275	-1.374756	-3.960755	2.5
C16 H20 O5 Na S	347.092367	1.53308	4.416896	6.5

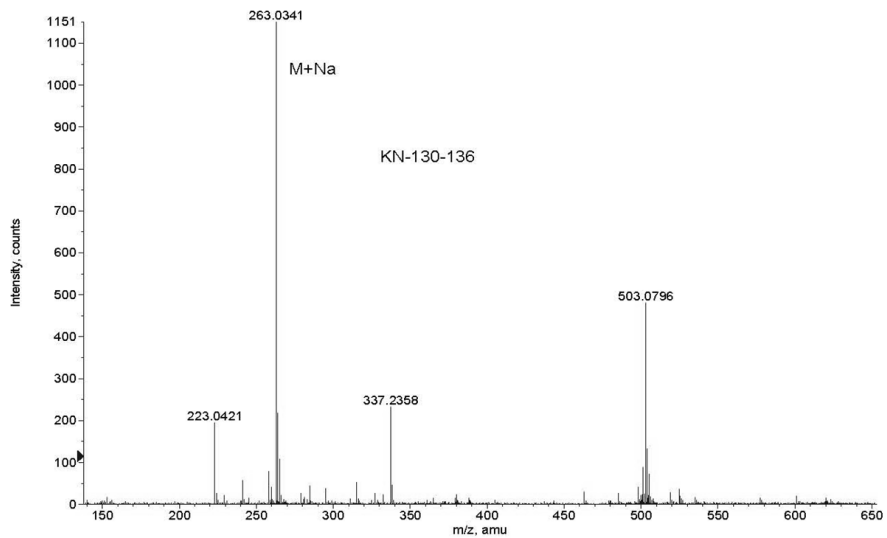
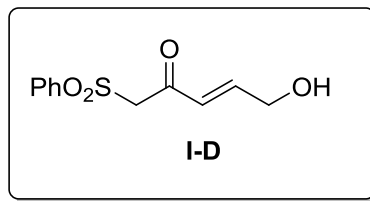
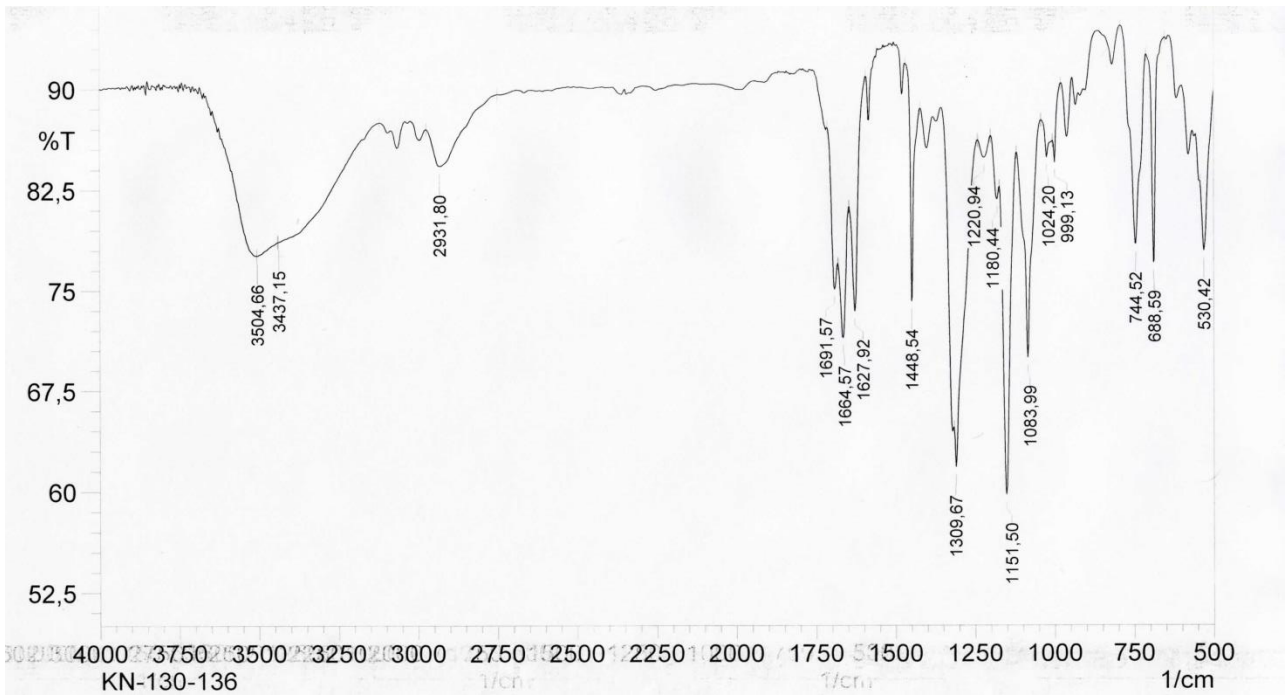




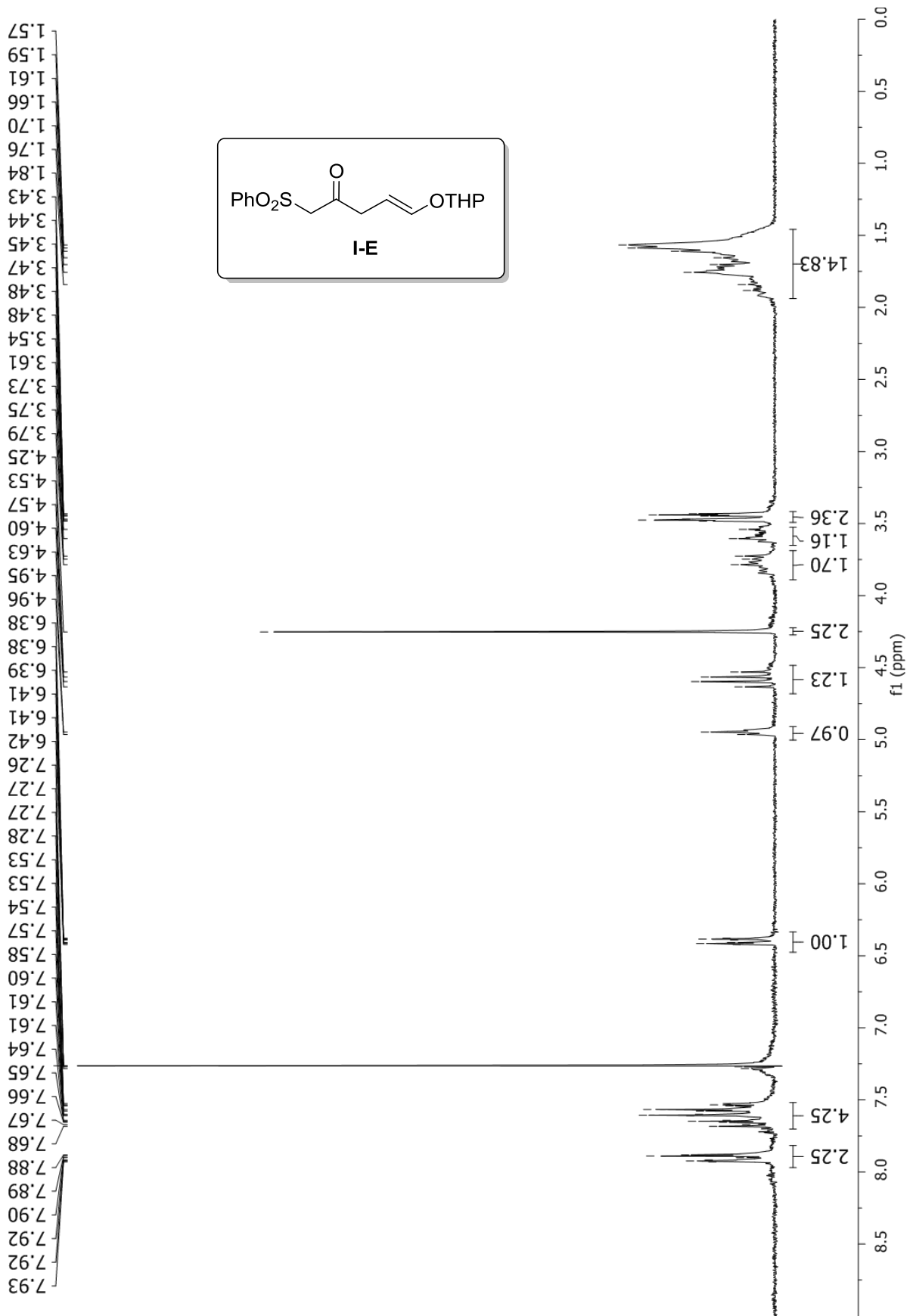


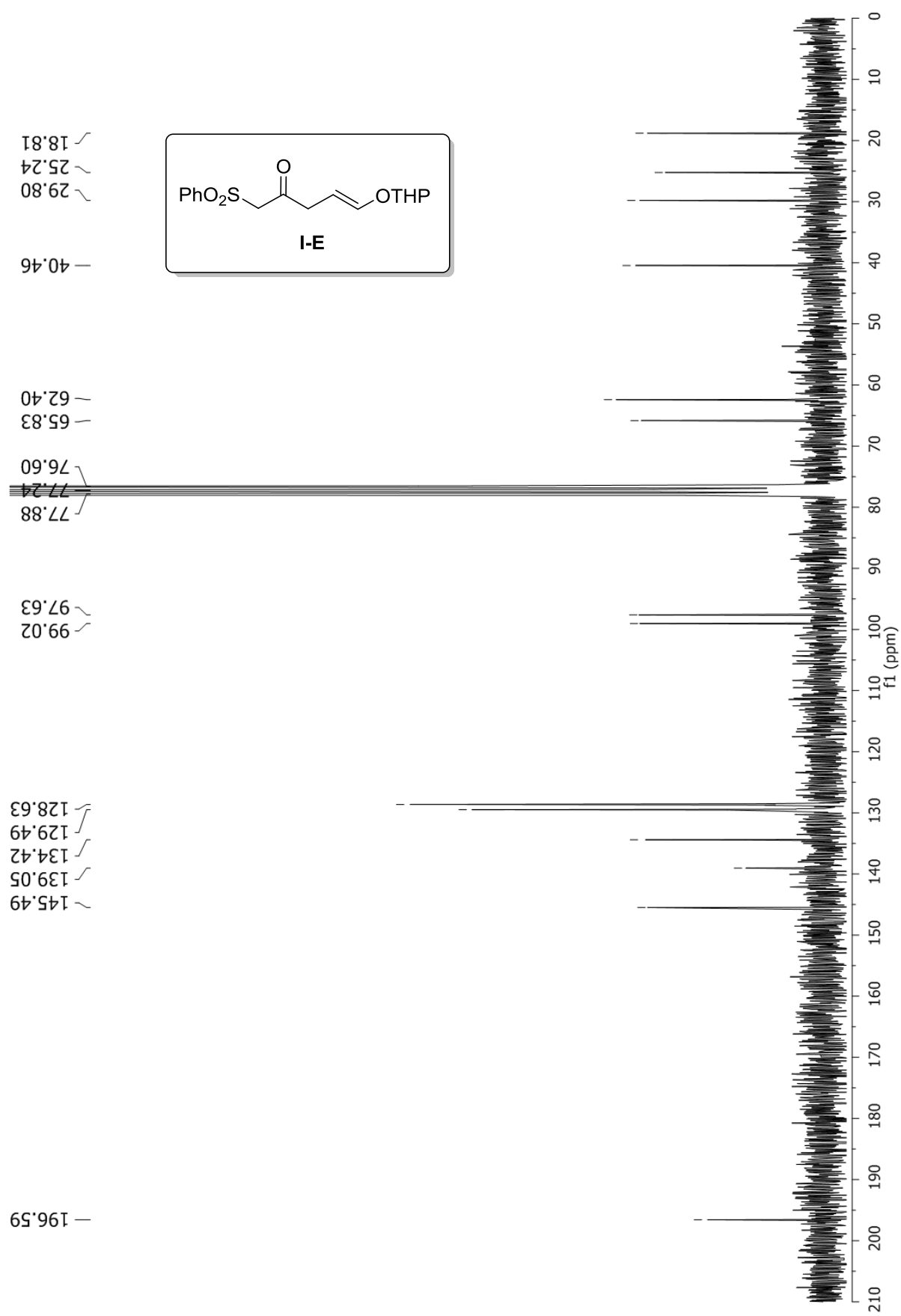


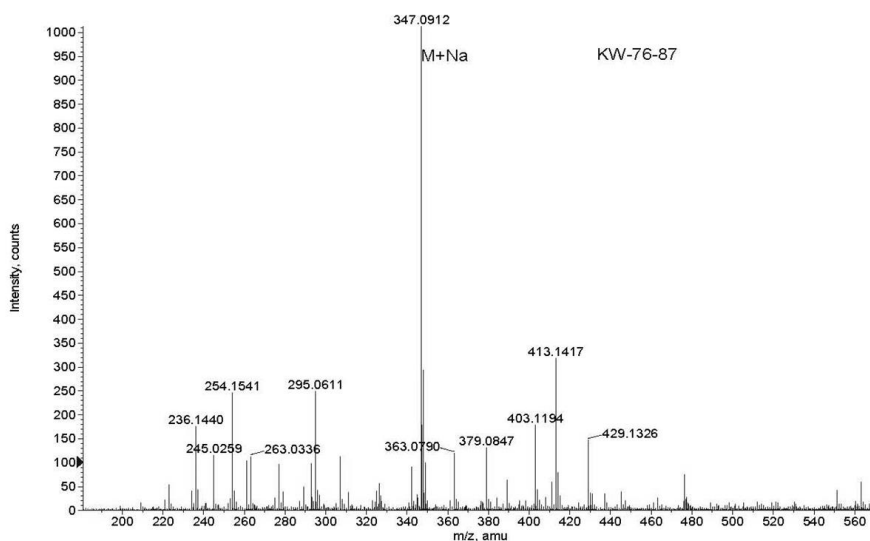
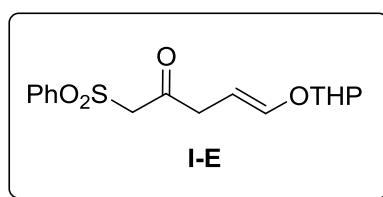
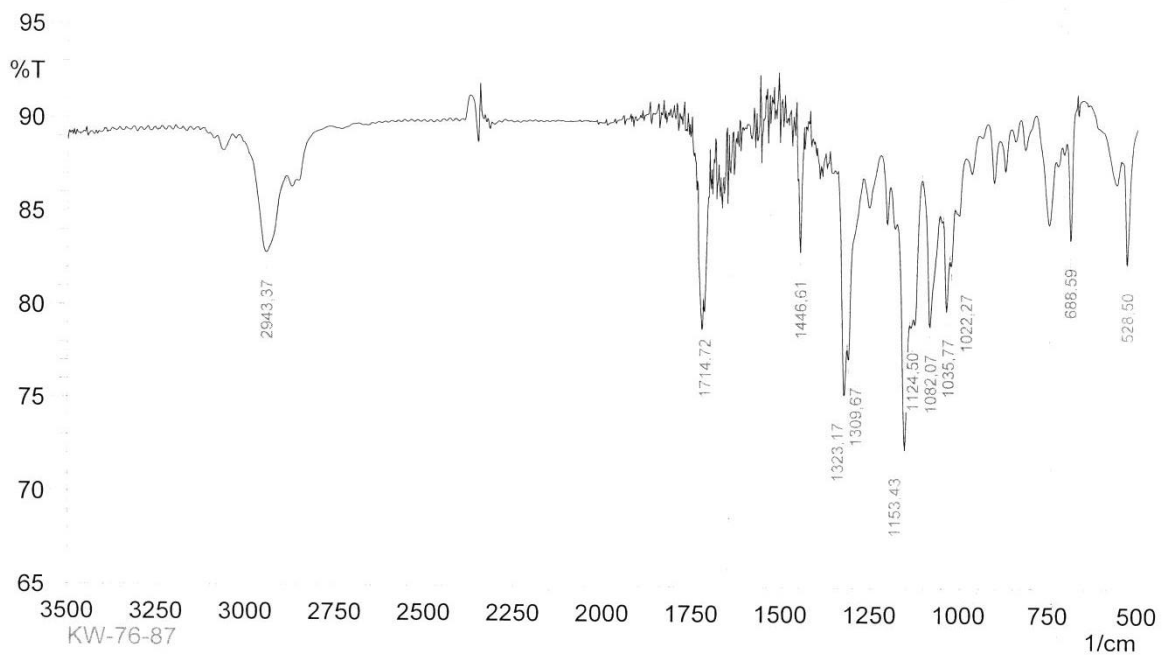
Full Spectroscopy



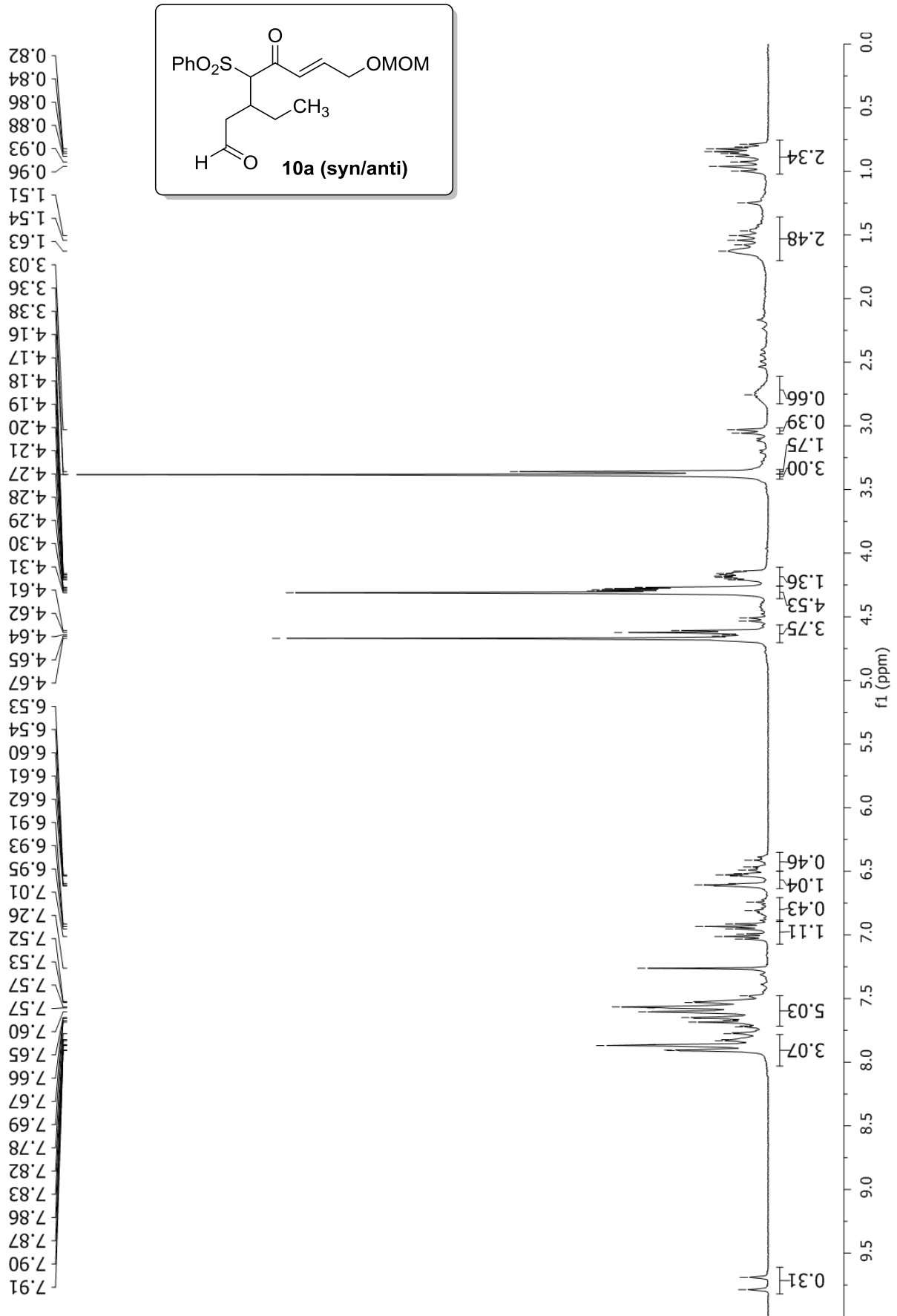
Formula	CalculatedMass	mDaError	ppmError	RDB
C9 H7 N6 O2 S	263.034572	-0.471828	-1.793786	9.5
C11 H12 O4 Na S	263.034852	-0.75196	-2.858787	5.5
C8 H11 N2 O6 S	263.033235	0.865484	3.29038	4.5
C7 H8 N6 O2 Na S	263.032167	1.933432	7.350484	6.5
C12 H8 N4 Na S	263.036189	-2.089272	-7.942954	10.5

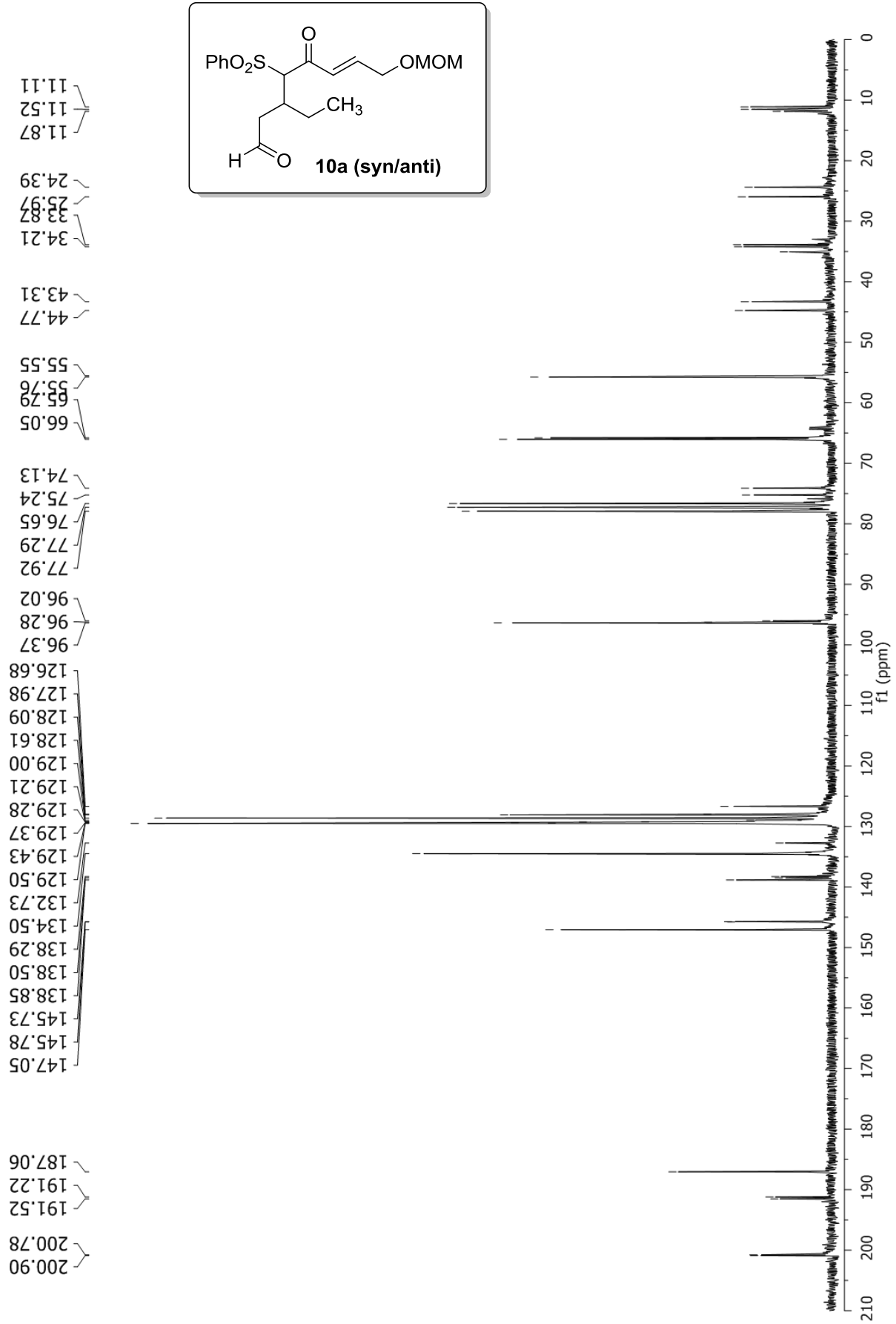




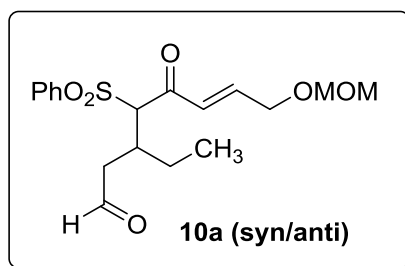
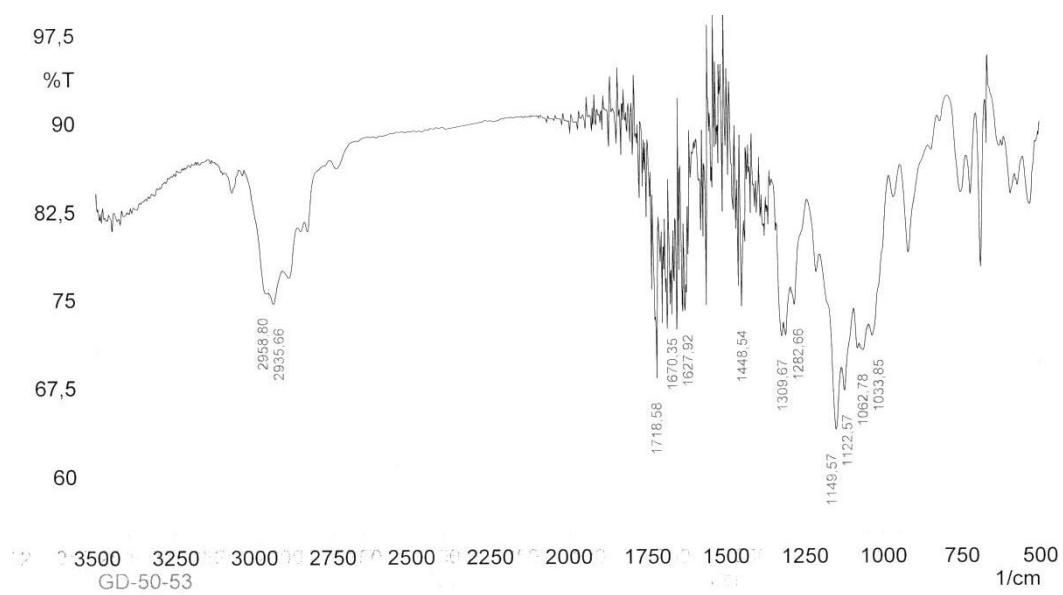


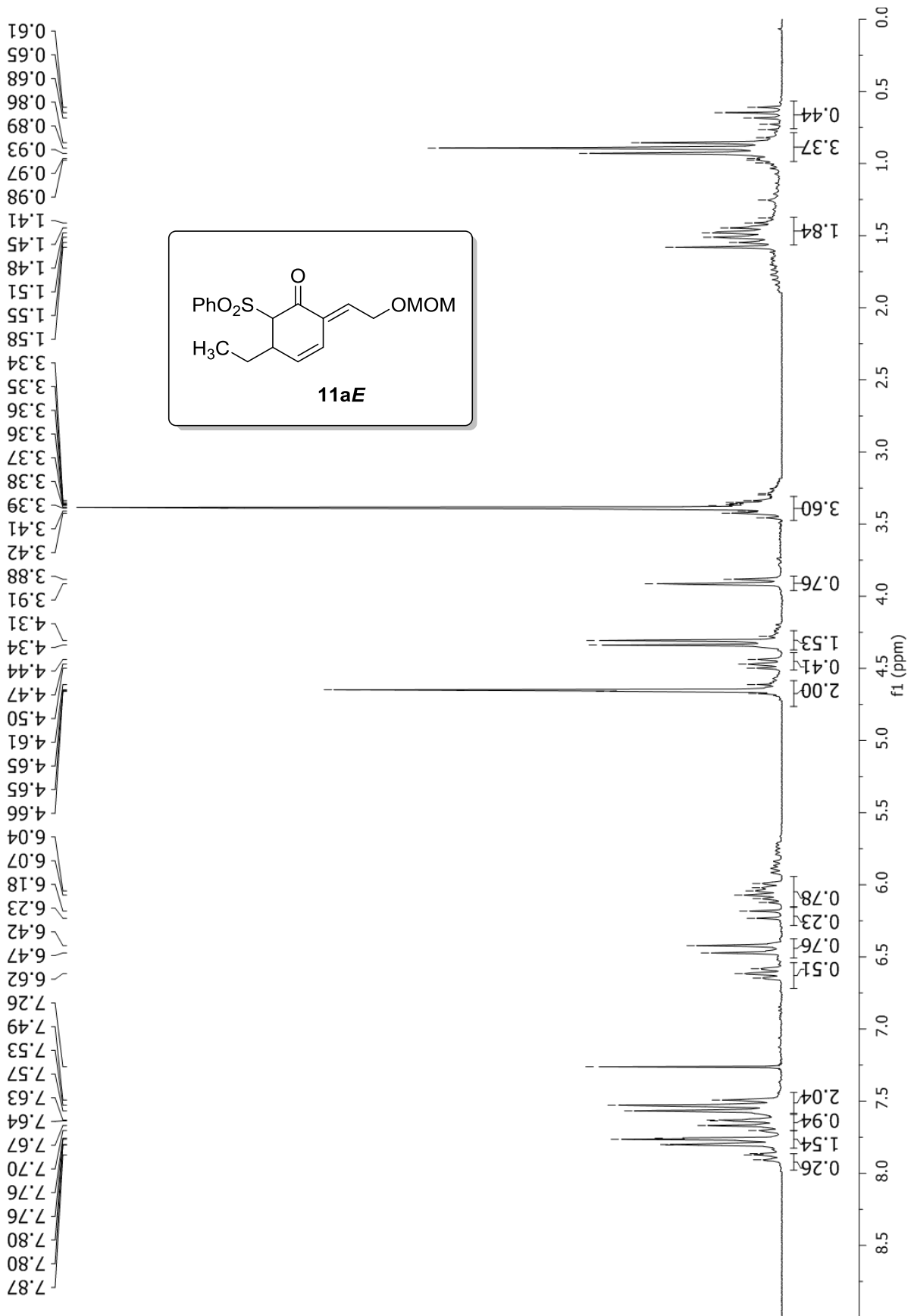
Formula	CalculatedMass	mDaError	ppmError	RDB
C21 H15 O5	347.0914	-0.20022	-0.57685	14.5
C13 H19 N2 O7 S	347.090749	0.450524	1.297997	5.5
C16 H20 O5 Na S	347.092367	-1.16692	-3.361993	6.5
C19 H16 O5 Na	347.088995	2.20504	6.352902	11.5
C25 H15 S	347.088899	2.30118	6.62989	18.5
C11 H20 N2 O7 Na S	347.088344	2.855784	8.22775	2.5

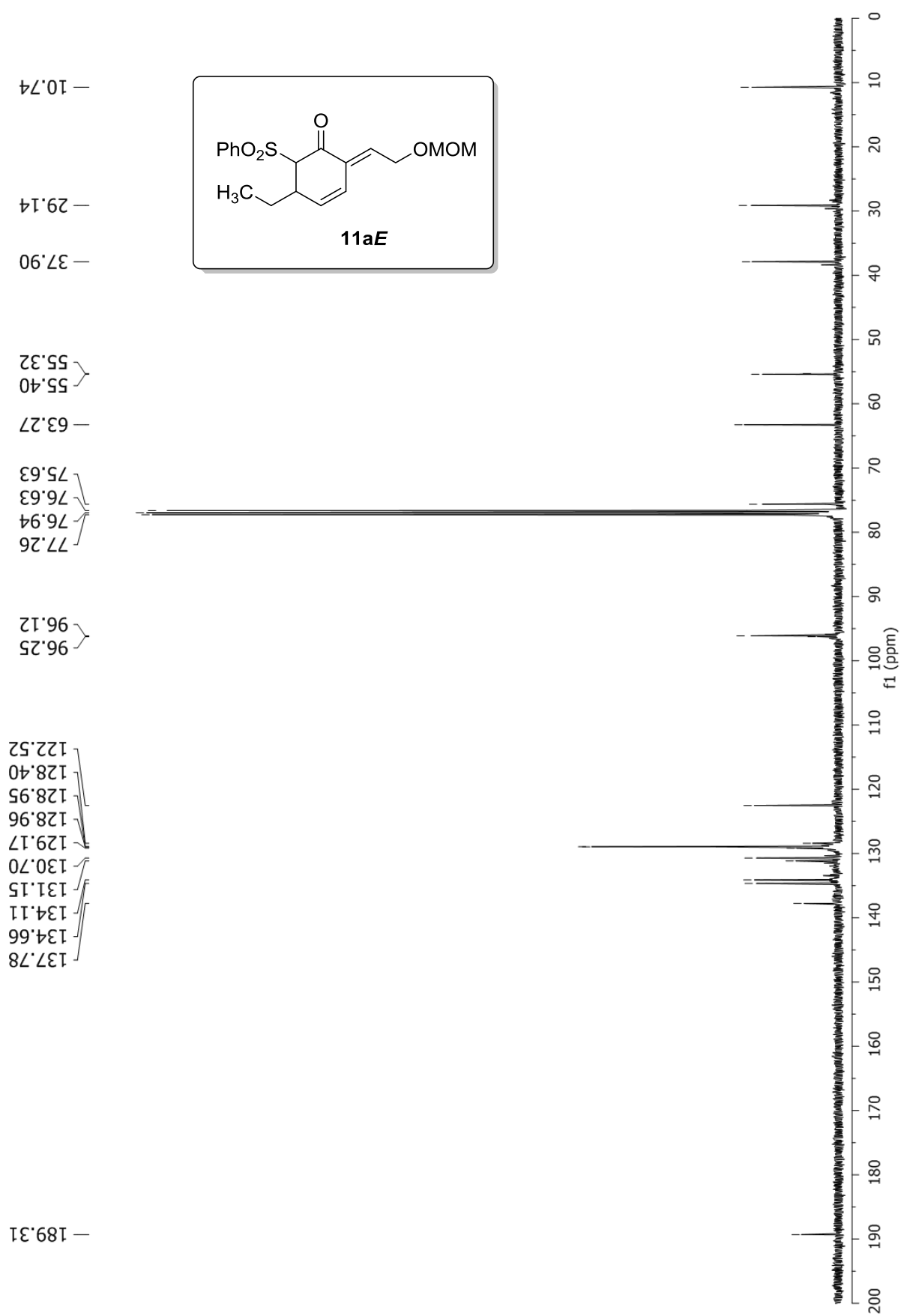


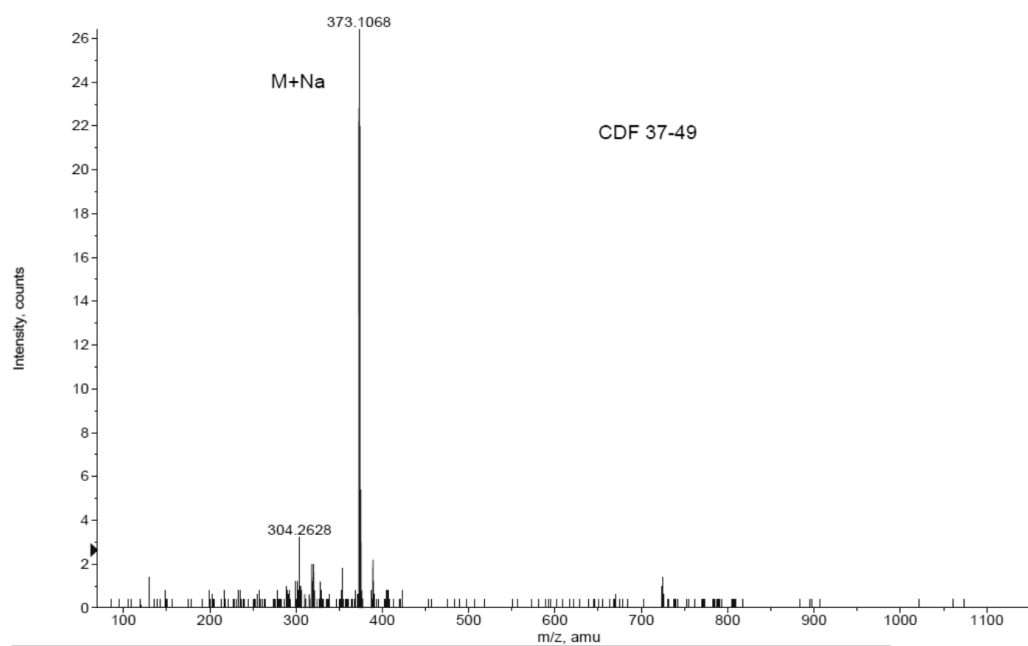
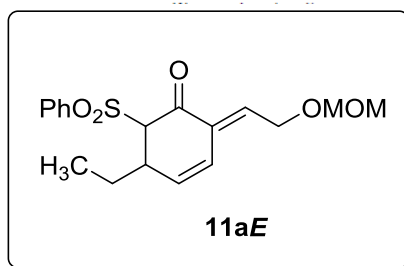
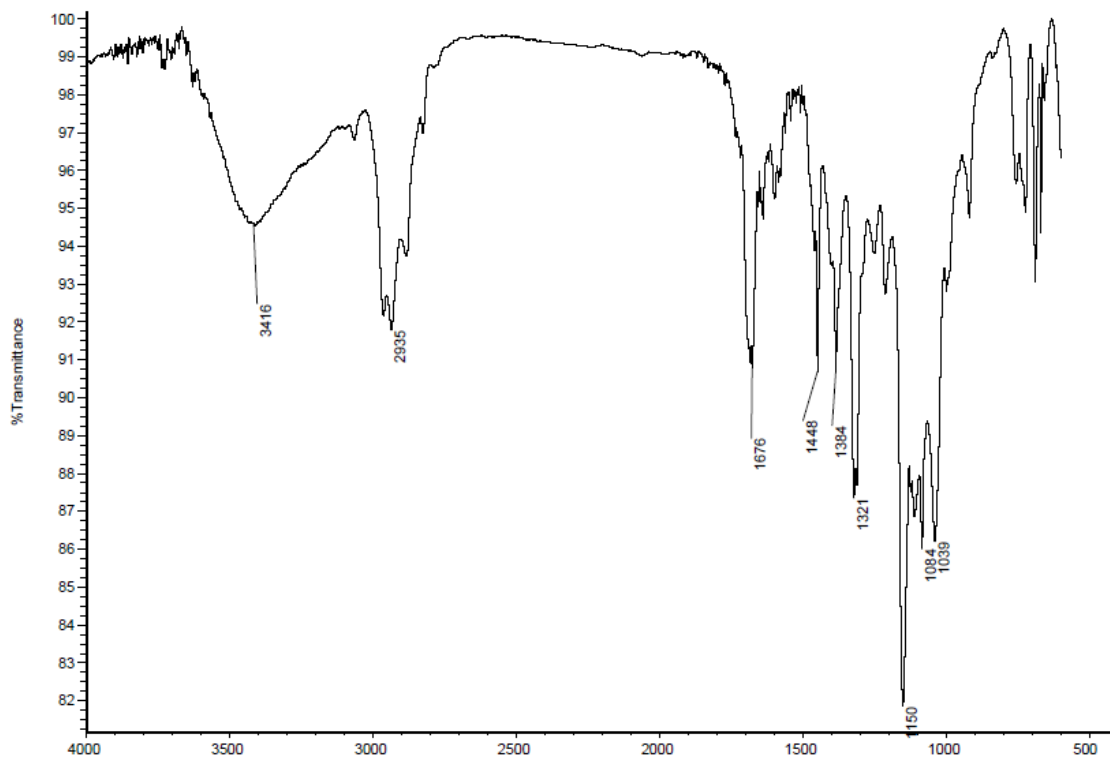


Full Spectroscopy

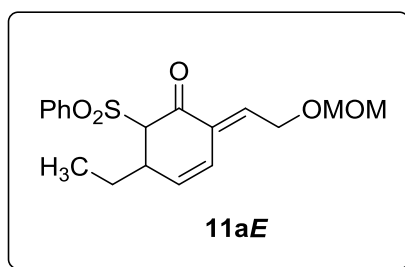
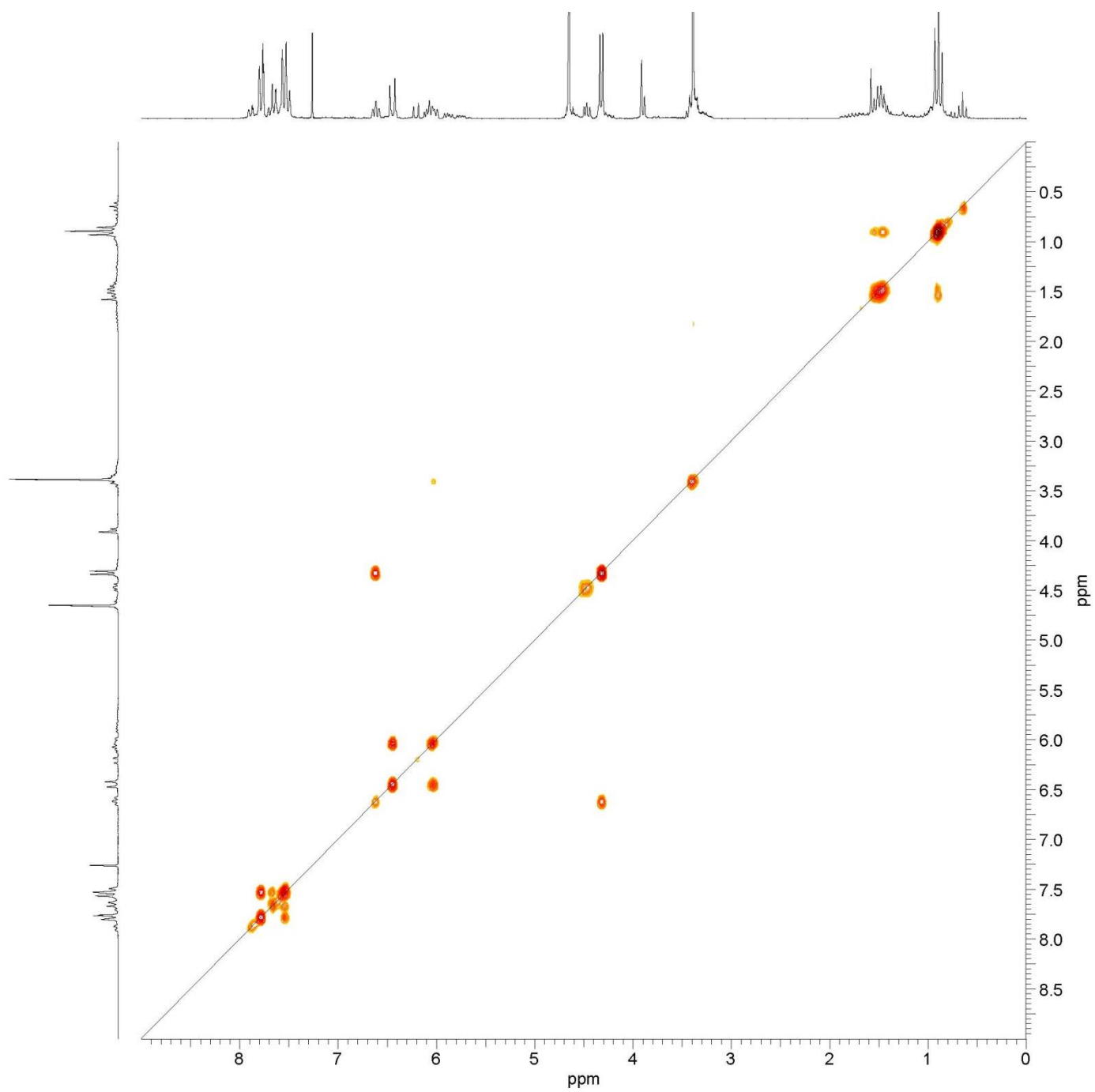


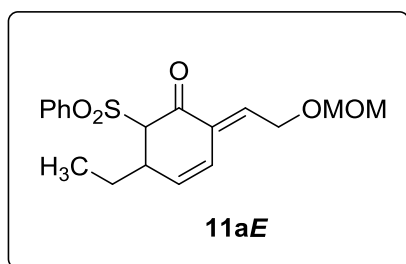
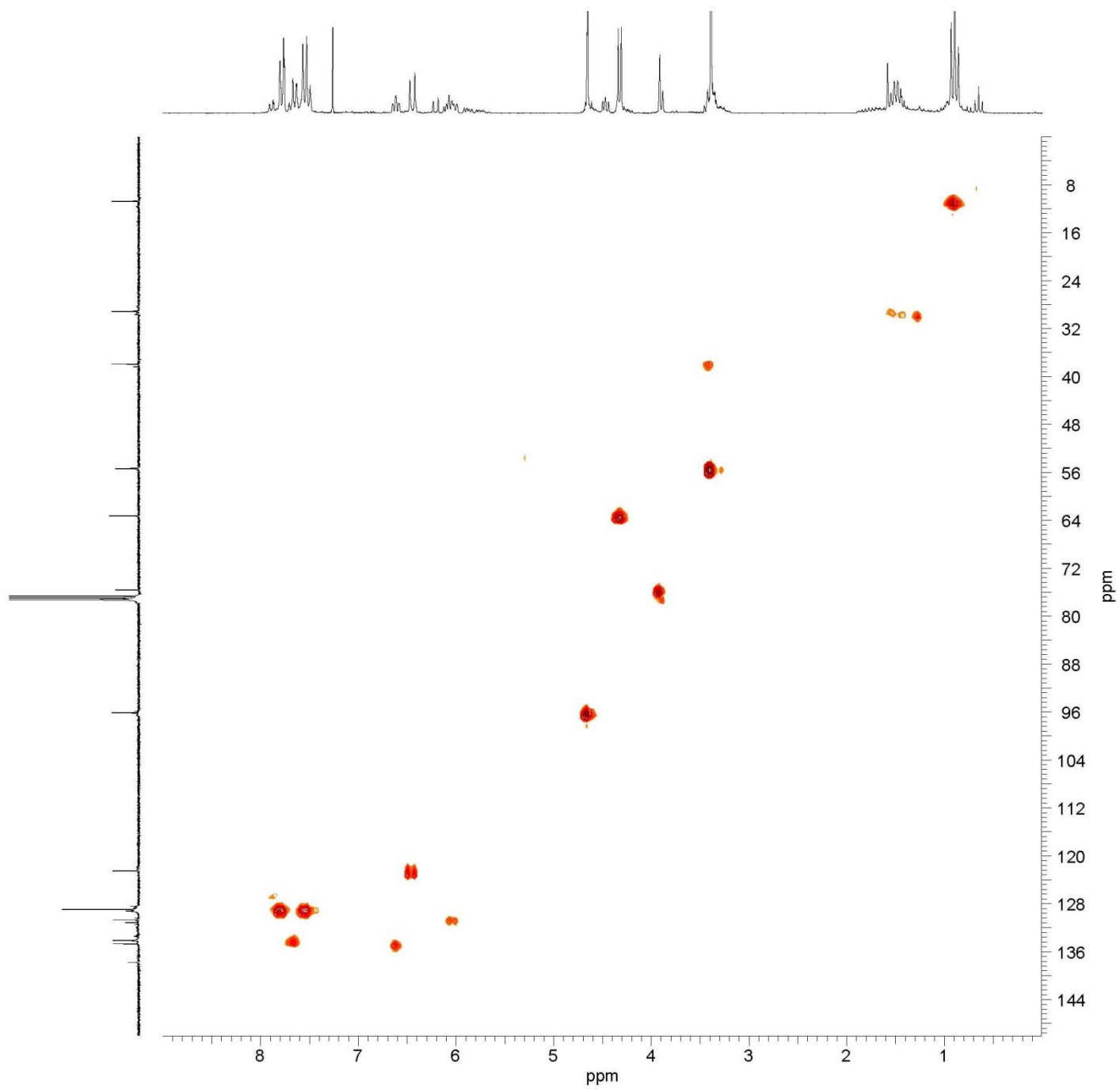


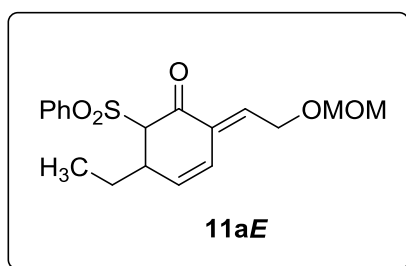
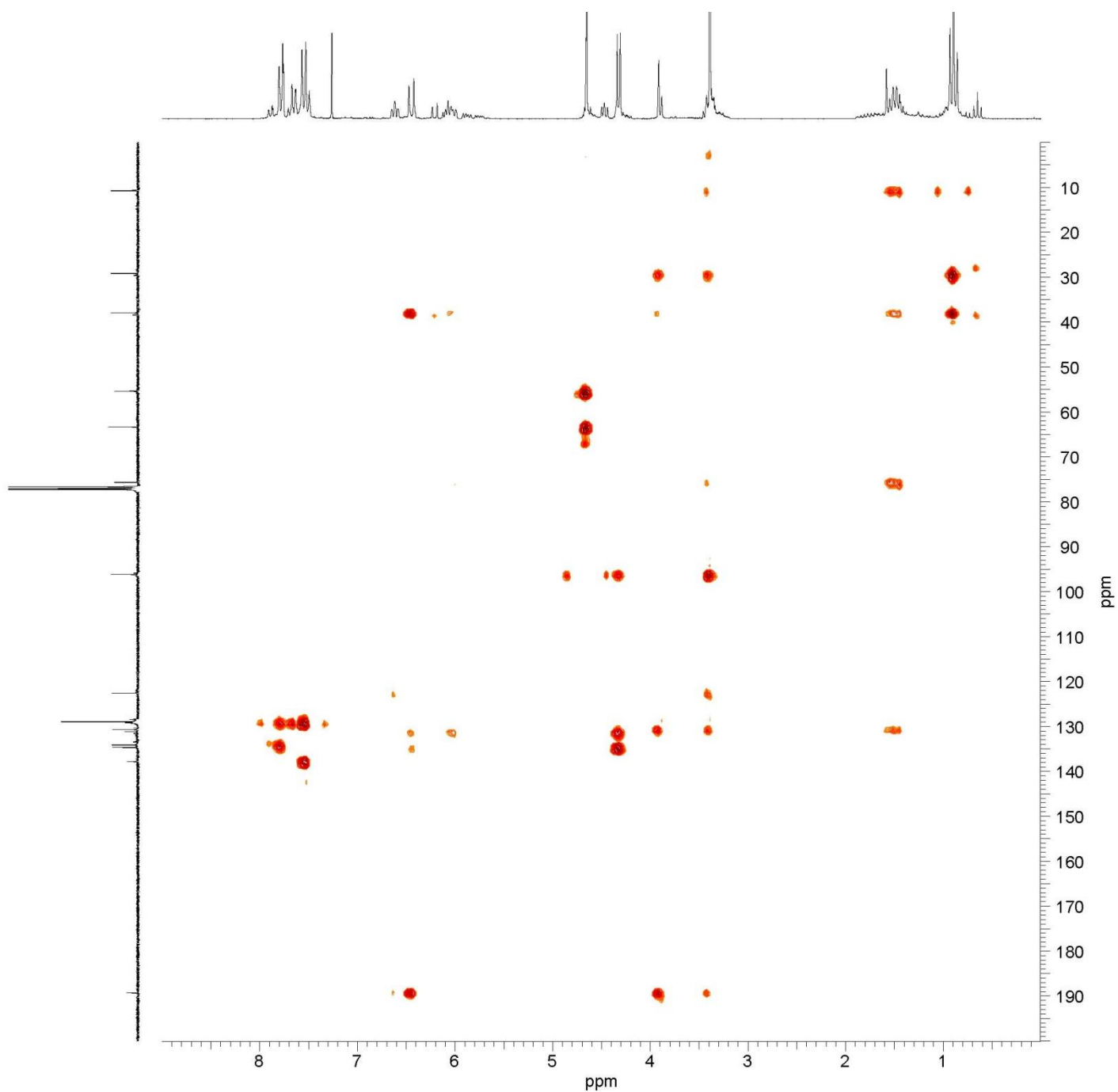


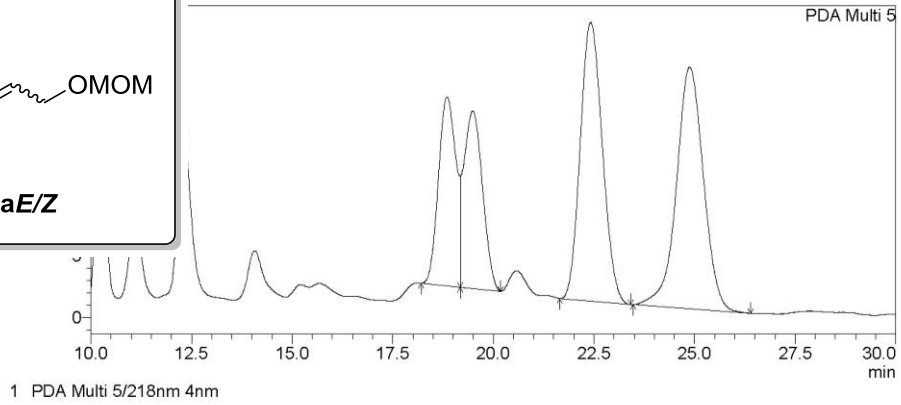
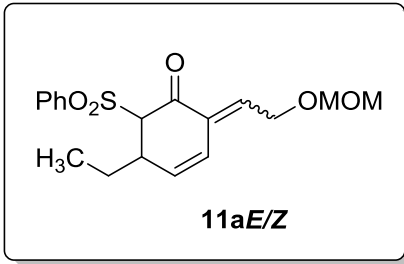


Formula	CalculatedMass	mDaError	ppmError	RDB
H17 N14 O8 S	373.106902	-0.102132	-0.273734	-0.5
C15 H21 N2 O7 S	373.1064	0.400444	1.073268	6.5
C16 H17 N6 O3 S	373.107737	-0.936868	-2.510988	11.5
C18 H22 O5 Na S	373.108017	-1.217	-3.261796	7.5



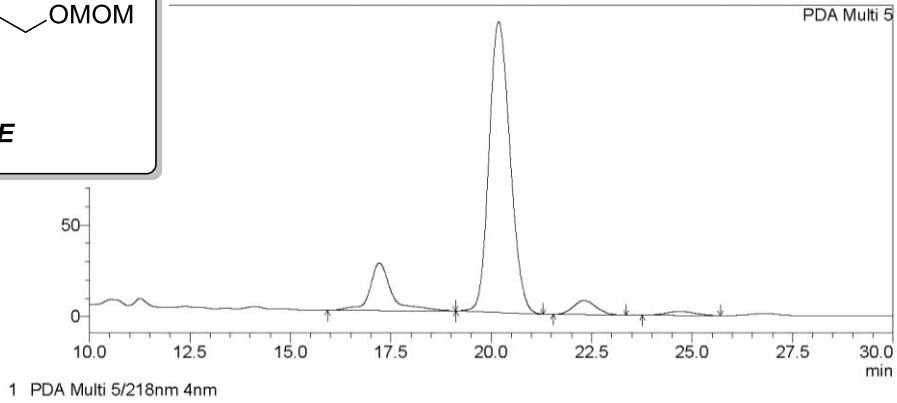
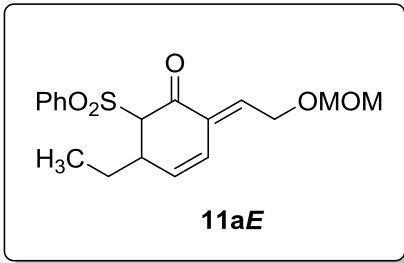






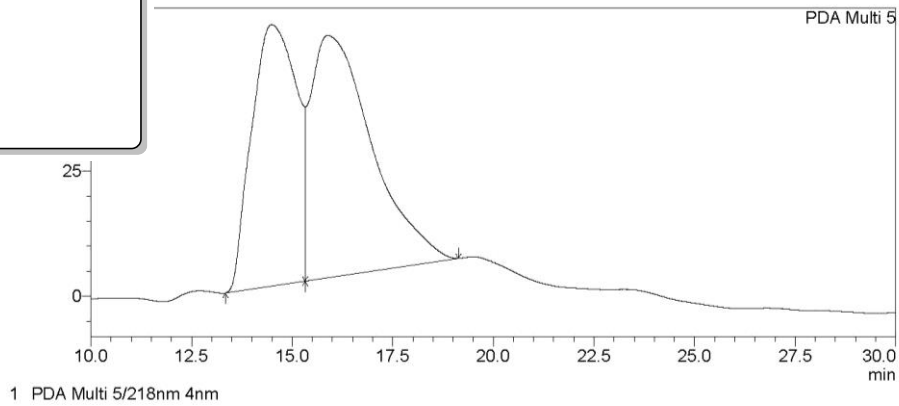
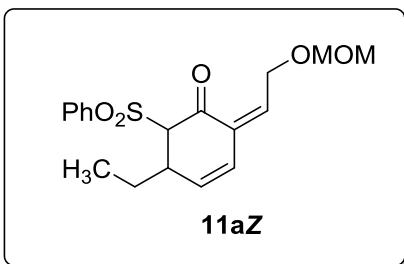
PeakTable
PDA Ch5 218nm 4nm

Peak#	Ret. Time	Area %
1	18.843	17.247
2	19.483	17.154
3	22.411	31.830
4	24.875	33.770
Total		100.000



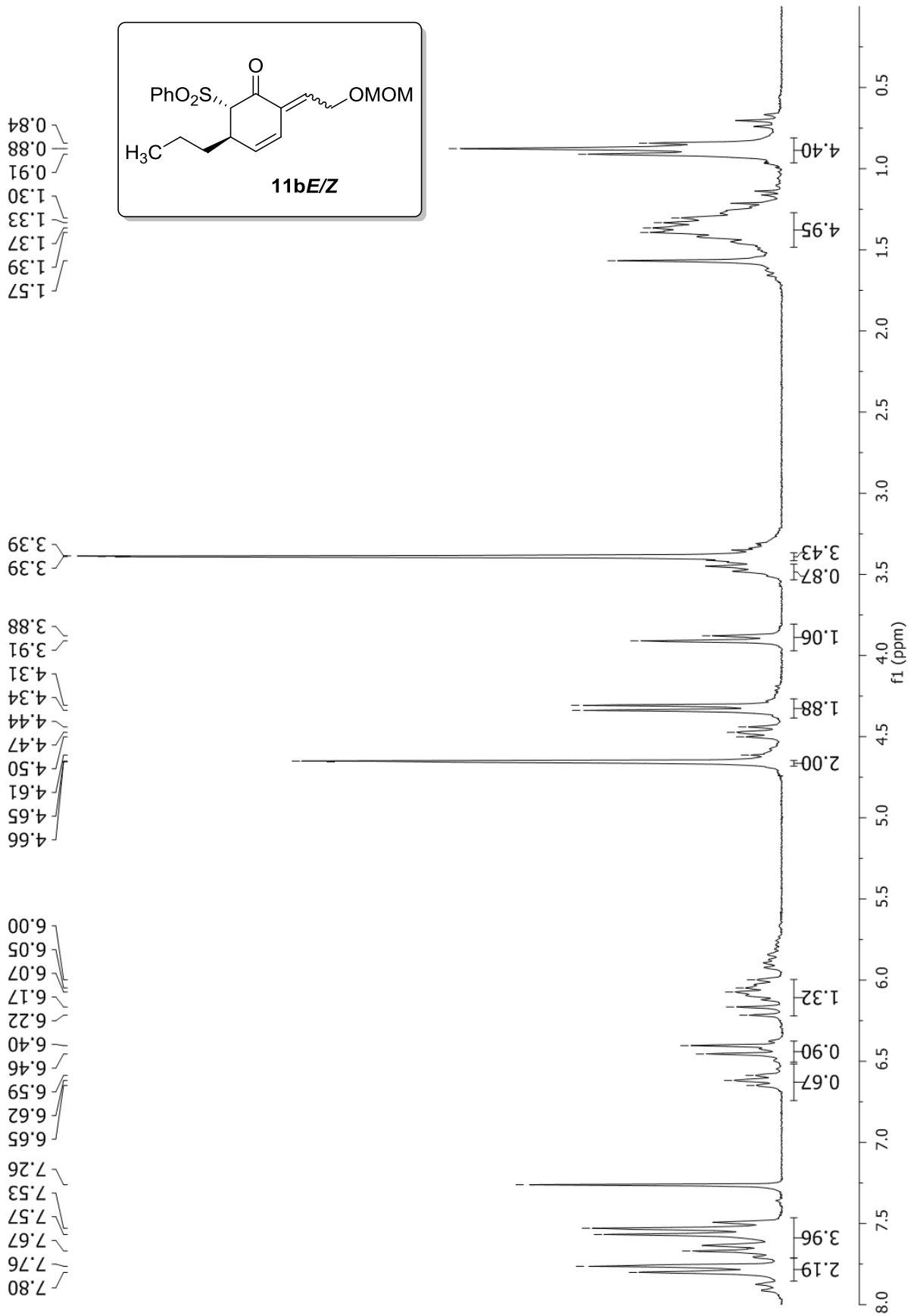
PeakTable
PDA Ch5 218nm 4nm

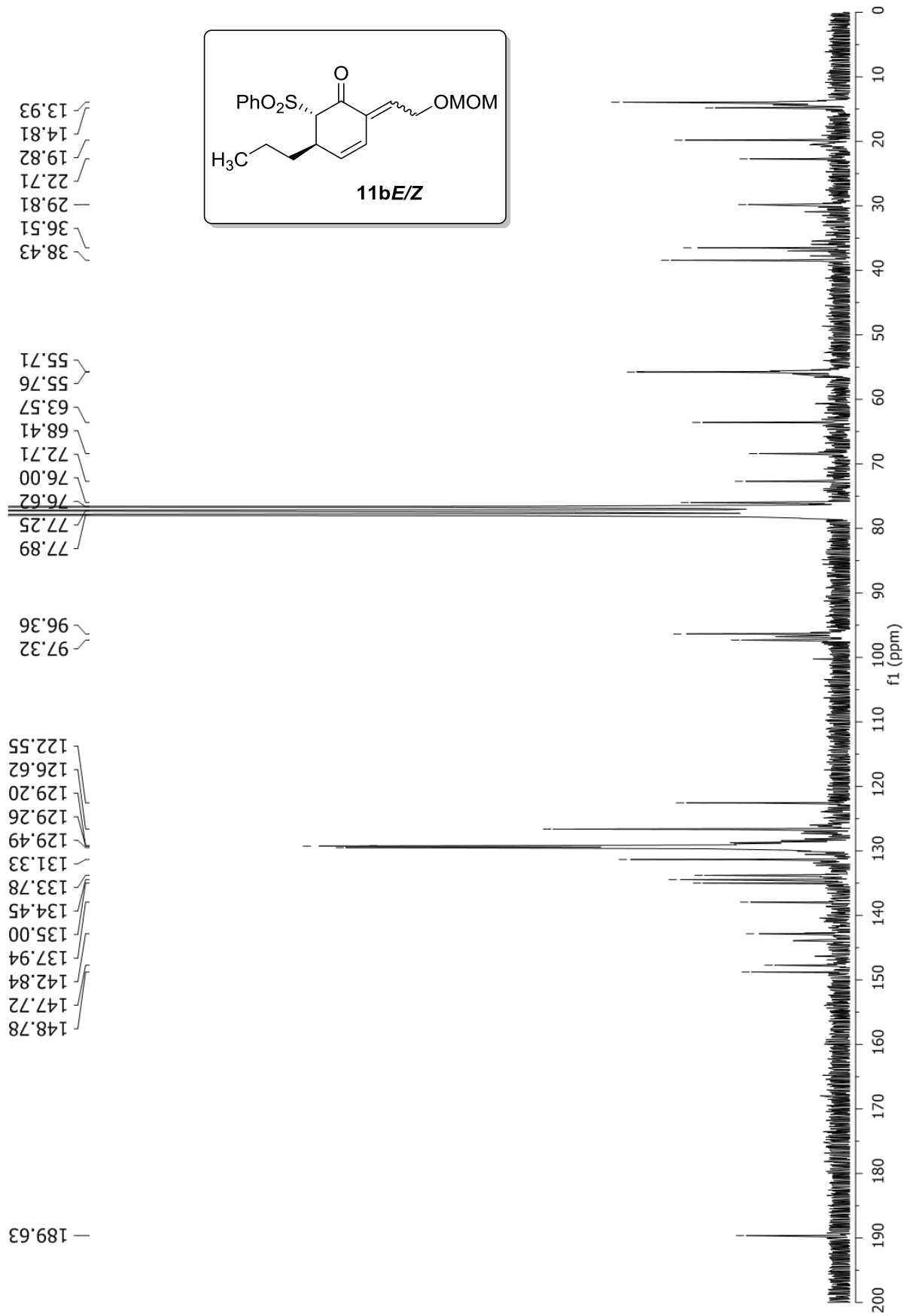
Peak#	Ret. Time	Area %
1	17.210	13.438
2	20.179	80.791
3	22.301	4.248
4	24.675	1.524
Total		100.000



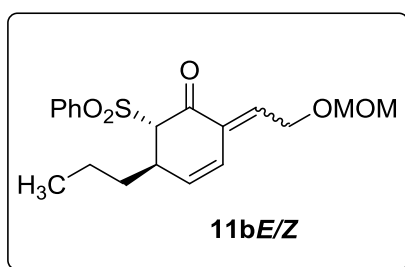
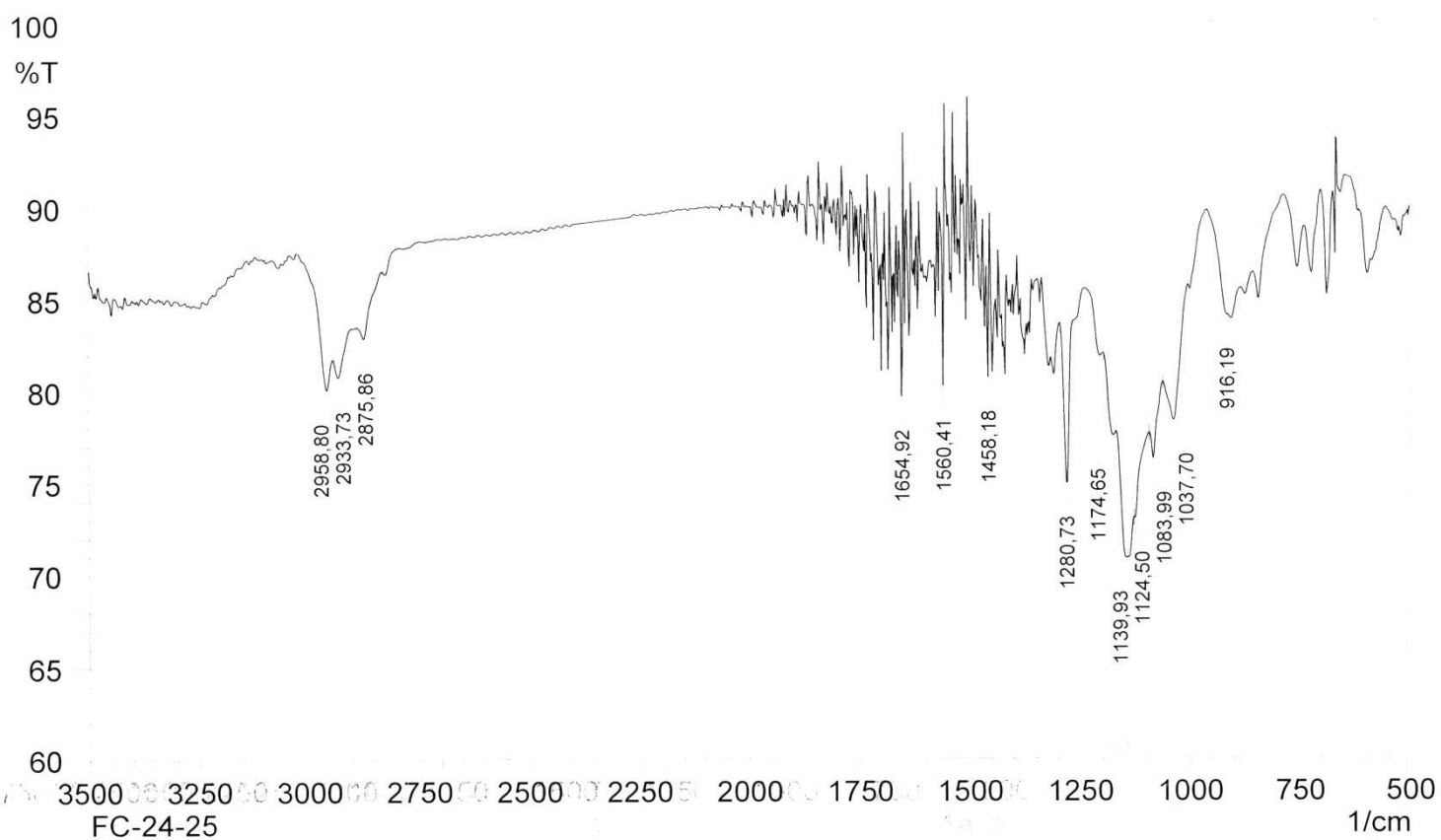
PeakTable
PDA Ch5 218nm 4nm

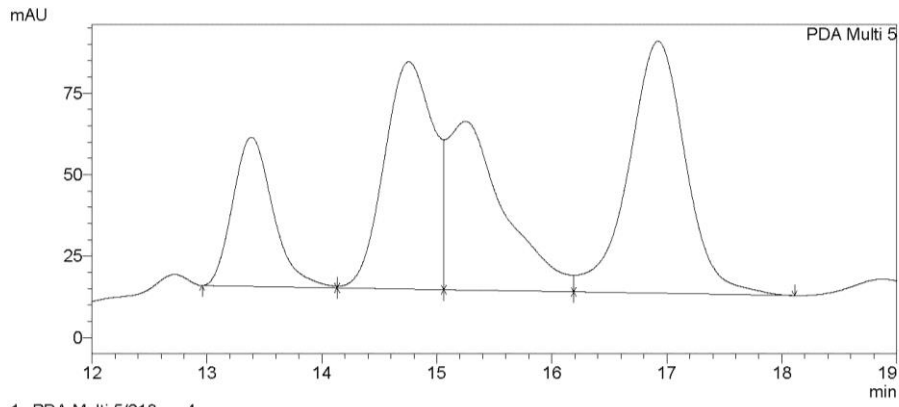
Peak#	Ret. Time	Area %
1	14.487	44.166
2	15.887	55.834
Total		100.000





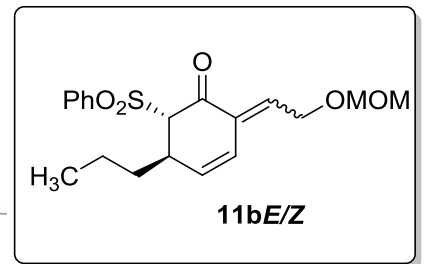
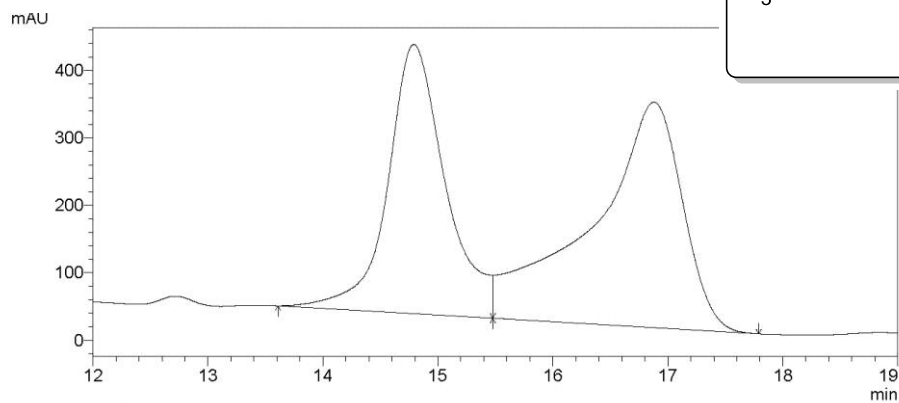
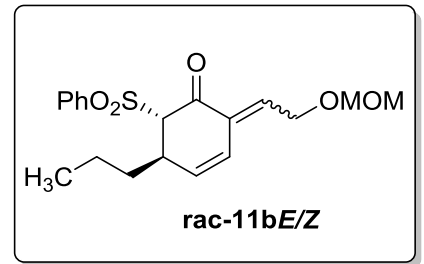
Full Spectroscopy





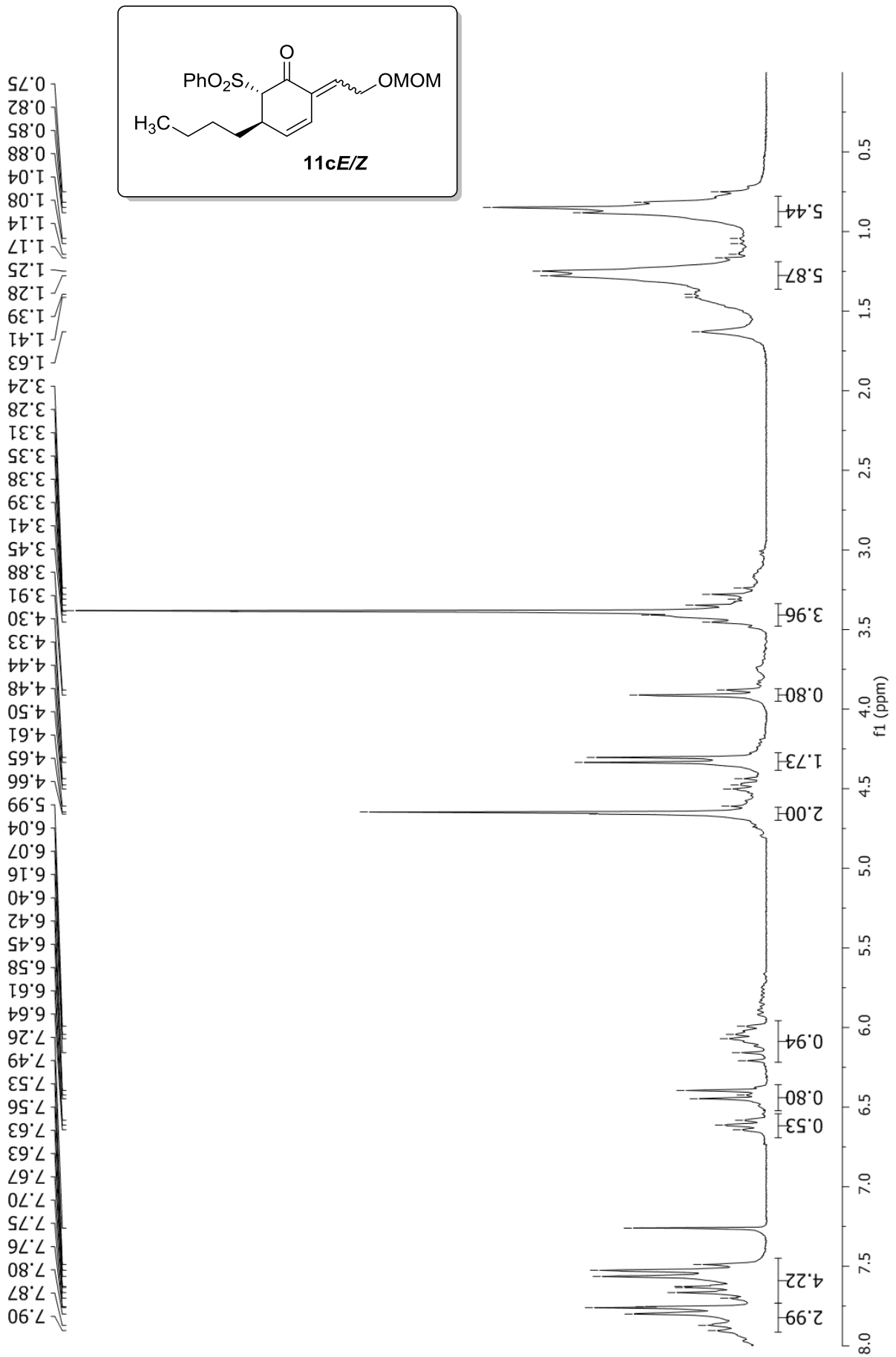
PeakTable
PDA Ch5 218nm 4nm

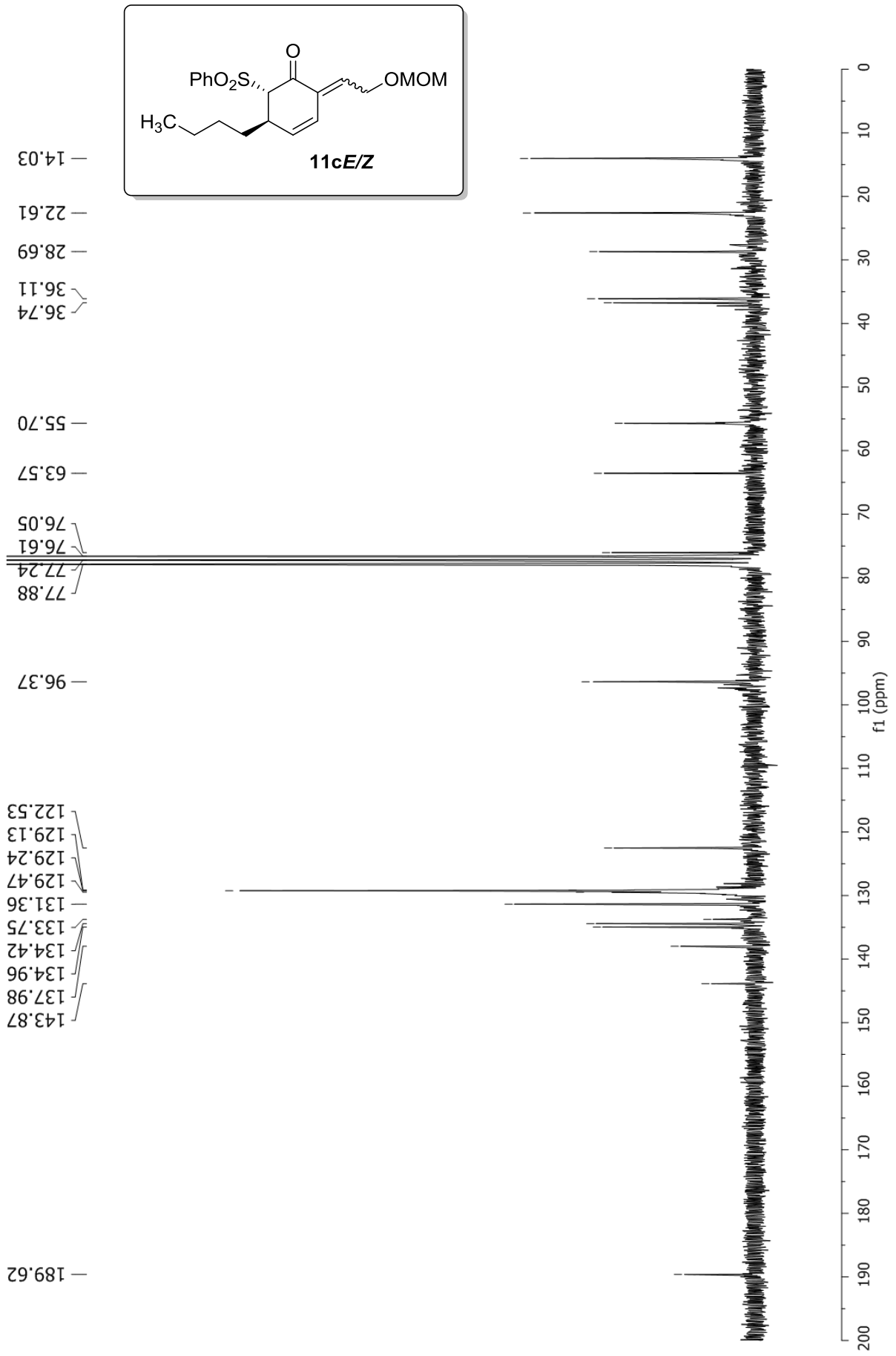
Peak#	Ret. Time	Area %
1	13.381	14.555
2	14.750	27.379
3	15.244	23.243
4	16.918	34.823
Total		100.000



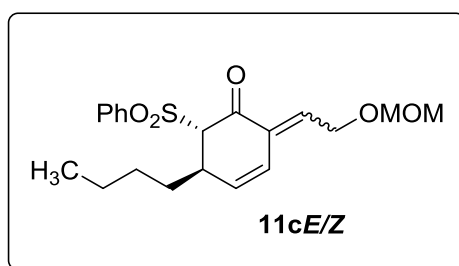
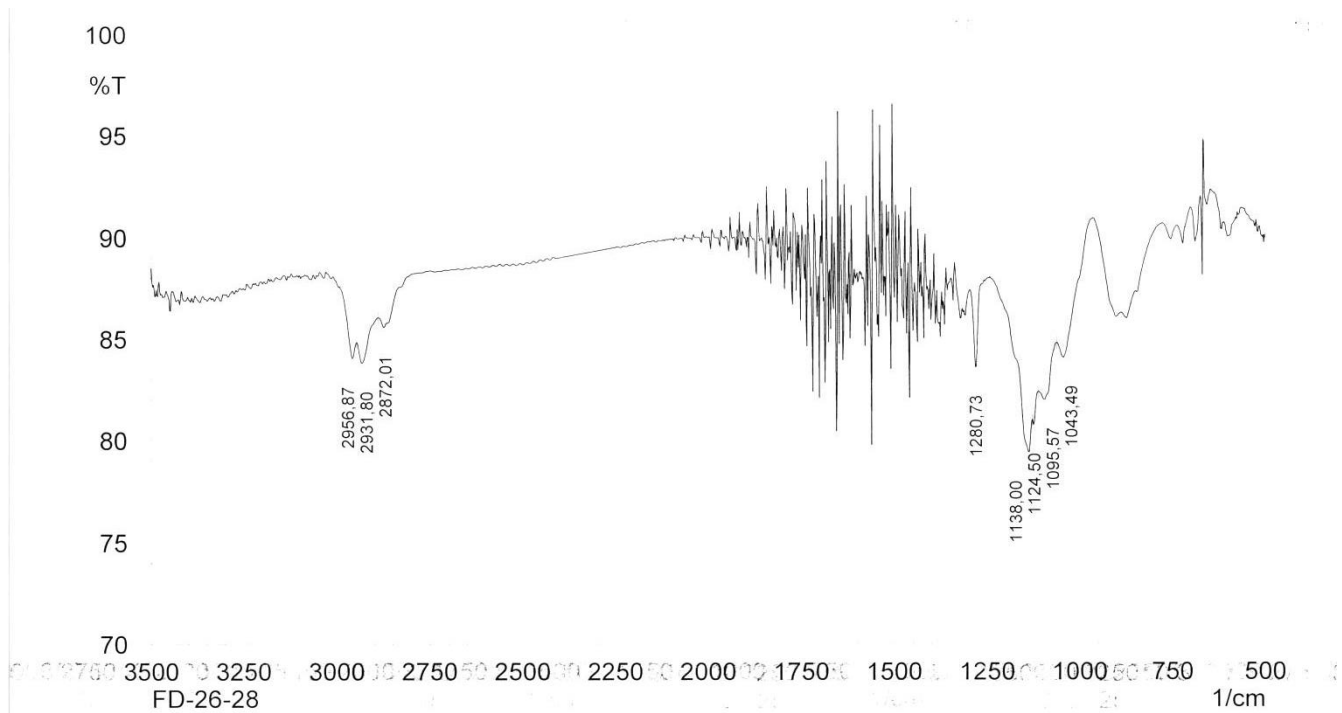
PeakTable
PDA Ch5 218nm 4nm

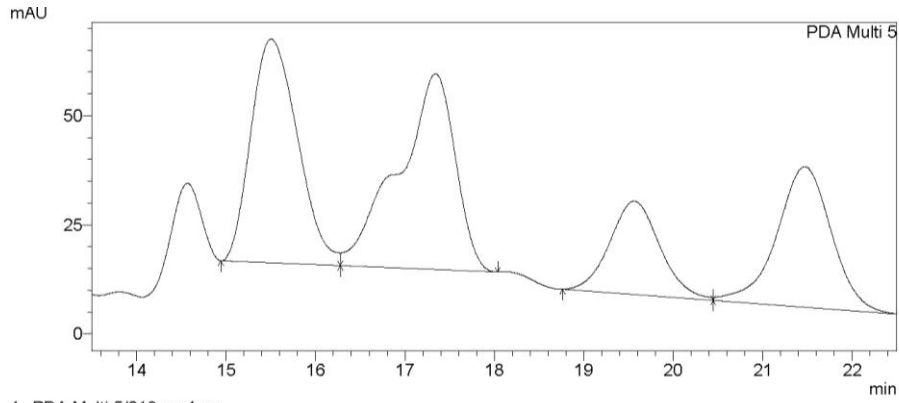
Peak#	Ret. Time	Area %
1	14.785	43.341
2	16.874	56.659
Total		100.000





Full Spectroscopy

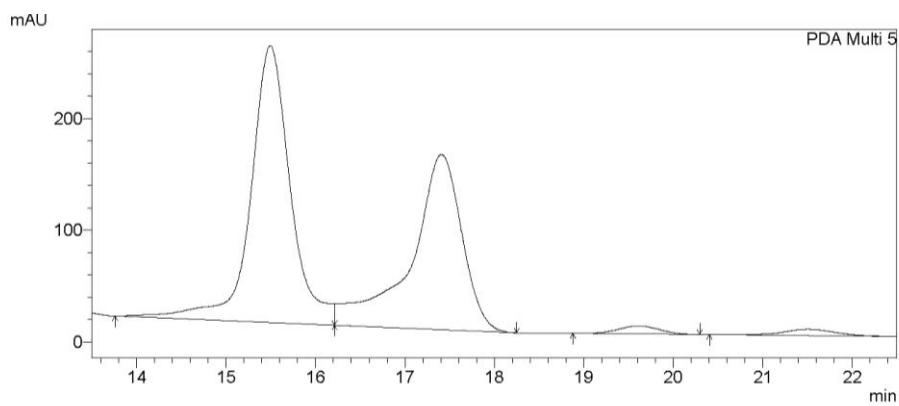
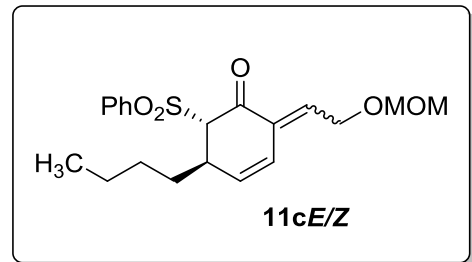
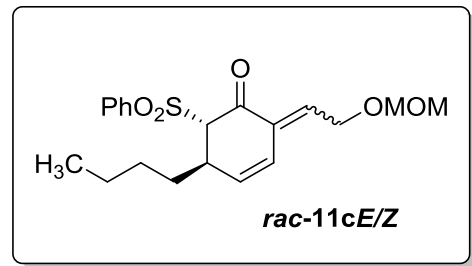




1 PDA Multi 5/218nm 4nm

PeakTable
PDA Ch5 218nm 4nm

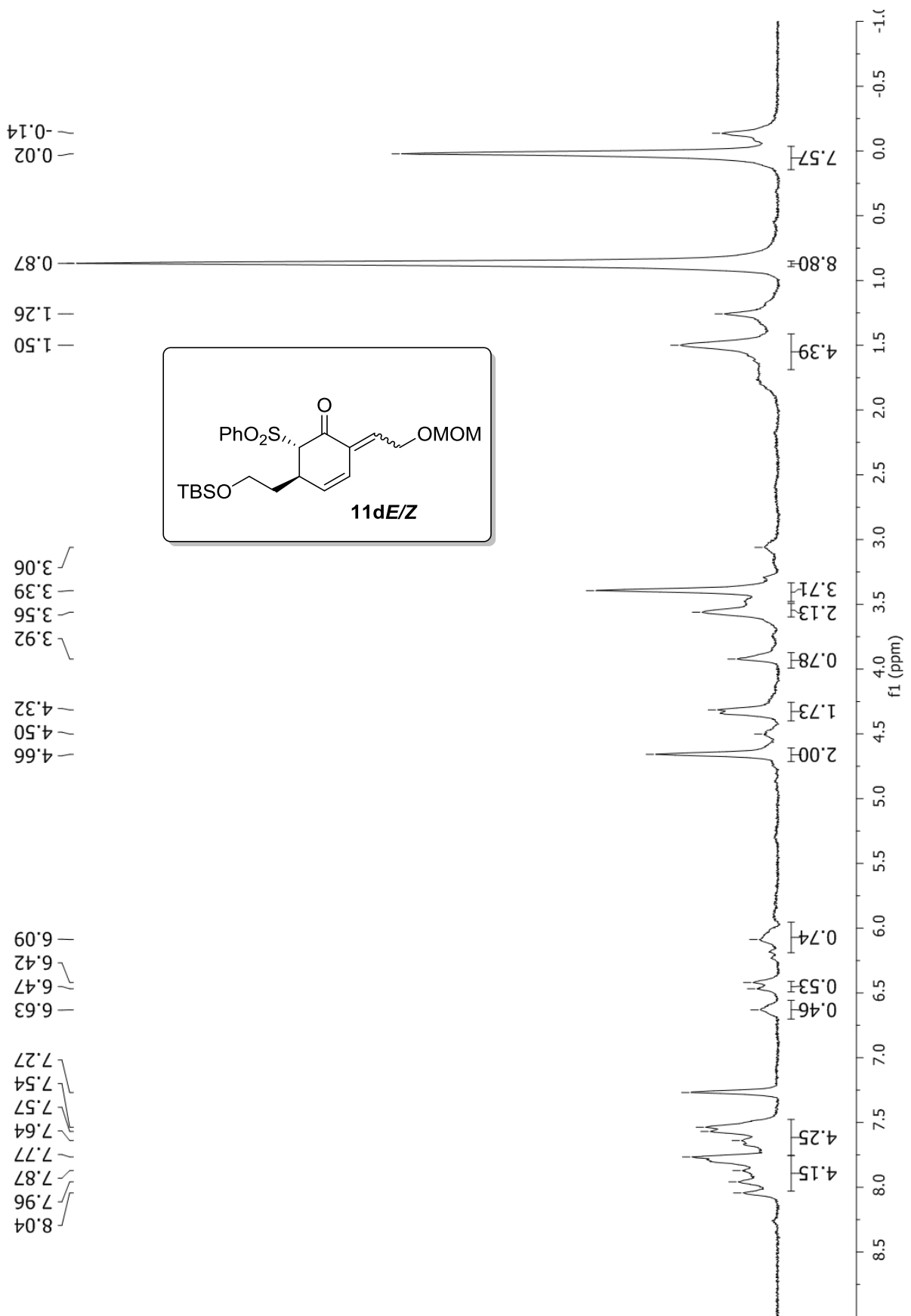
Peak#	Ret. Time	Area %
1	15.498	30.870
2	17.336	32.771
3	19.559	13.790
4	21.465	22.570
Total		100.000

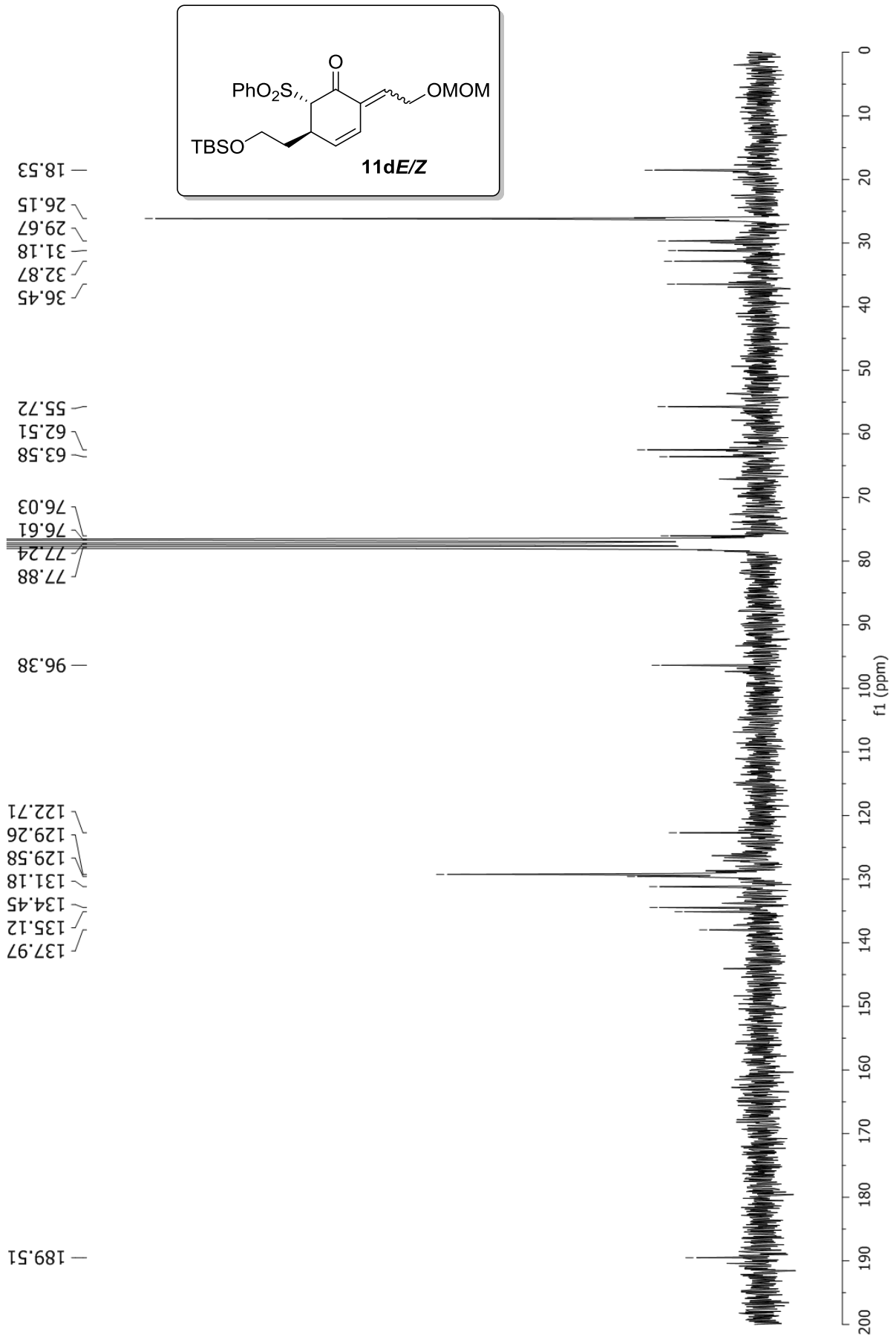


1 PDA Multi 5/218nm 4nm

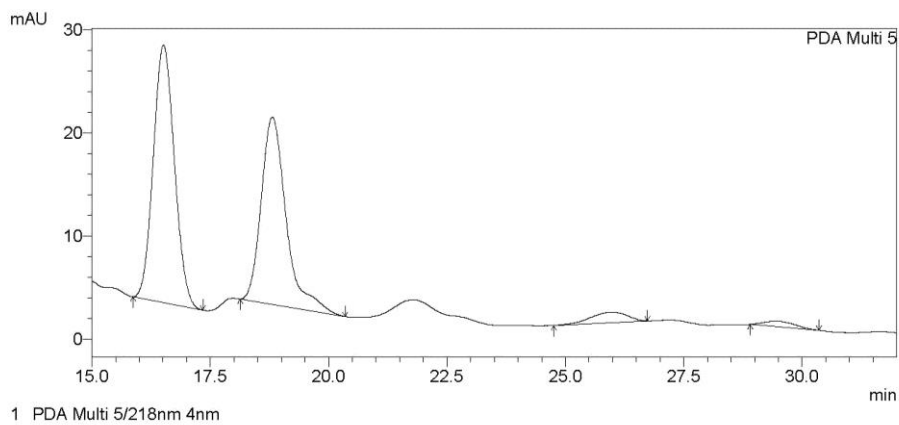
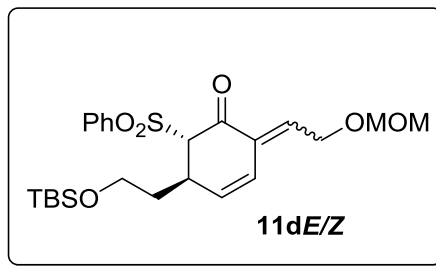
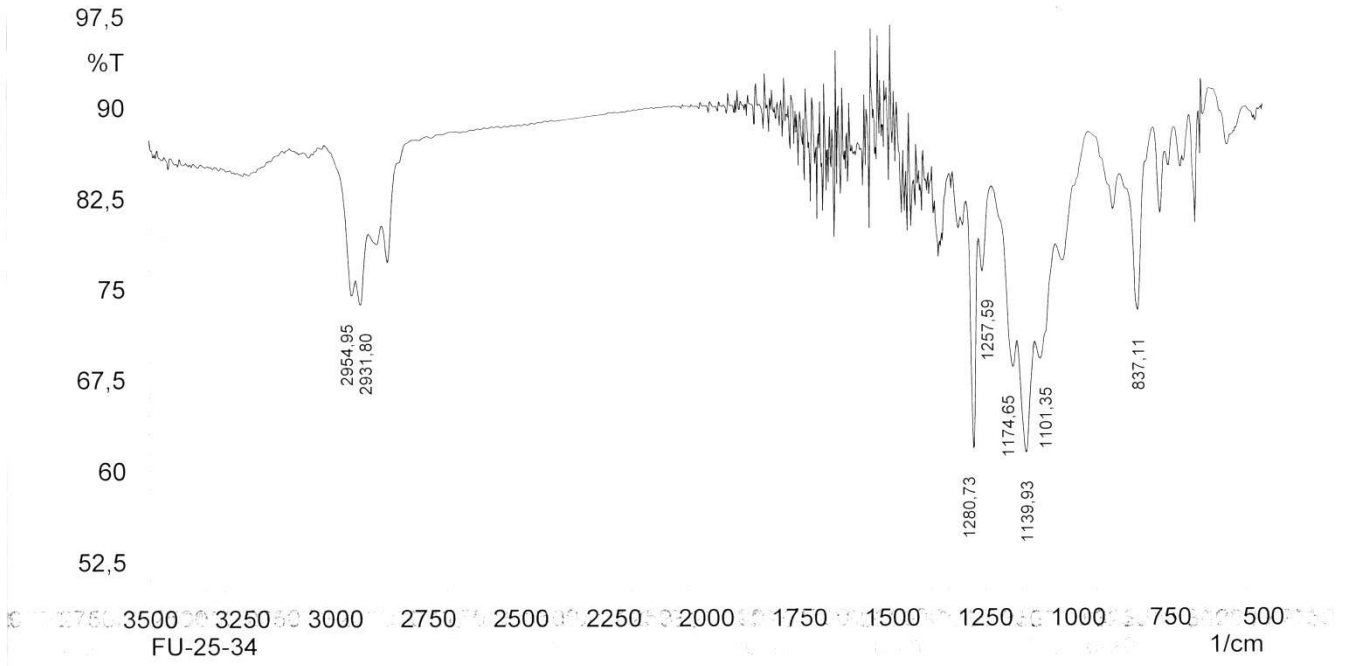
PeakTable
PDA Ch5 218nm 4nm

Peak#	Ret. Time	Area %
1	15.488	53.353
2	17.403	43.416
3	19.601	1.586
4	21.503	1.645
Total		100.000





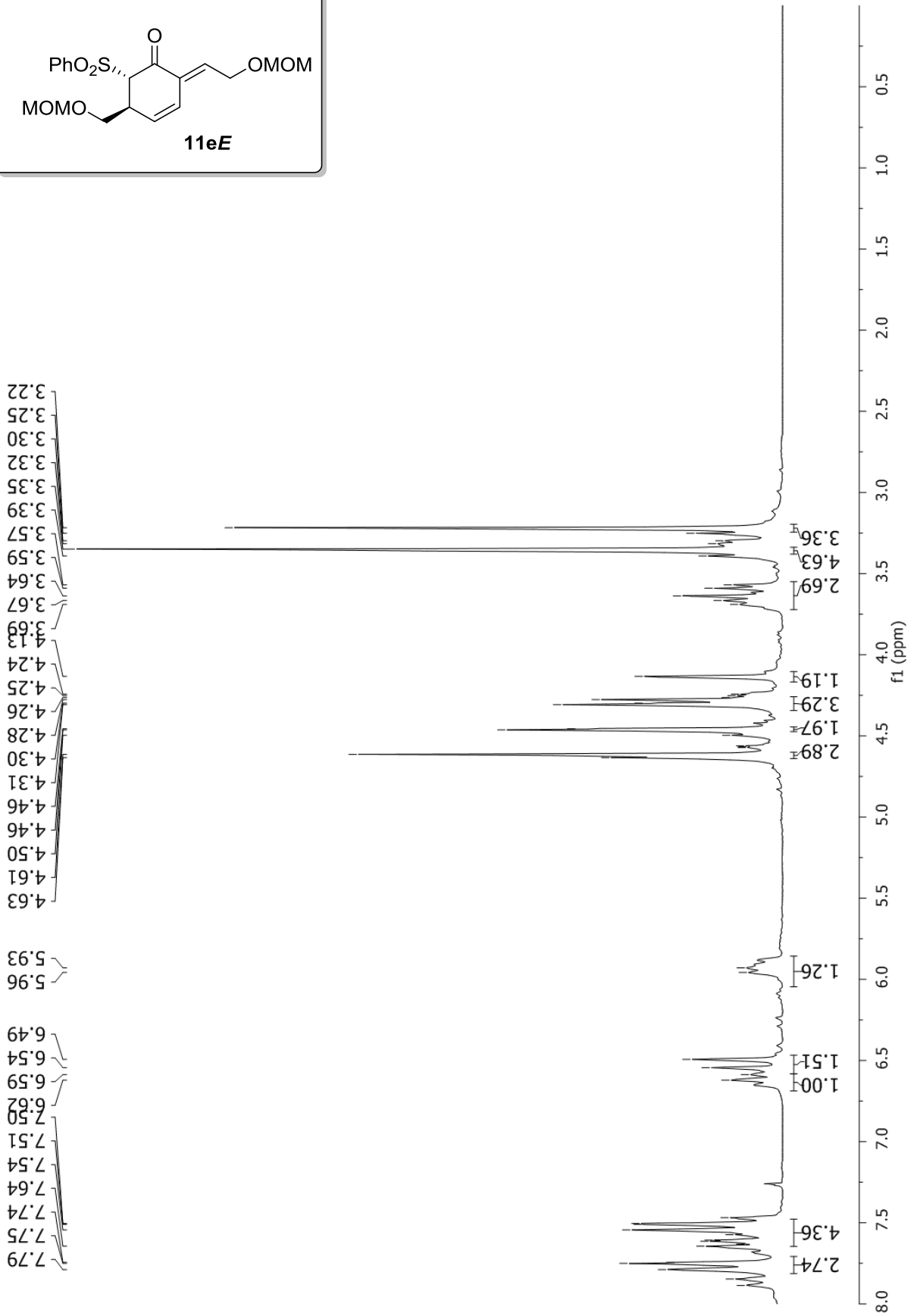
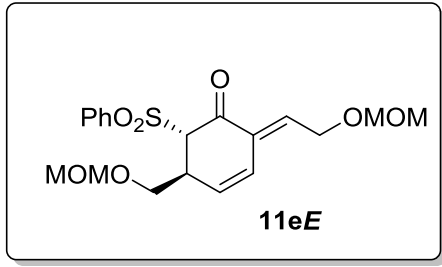
Full Spectroscopy

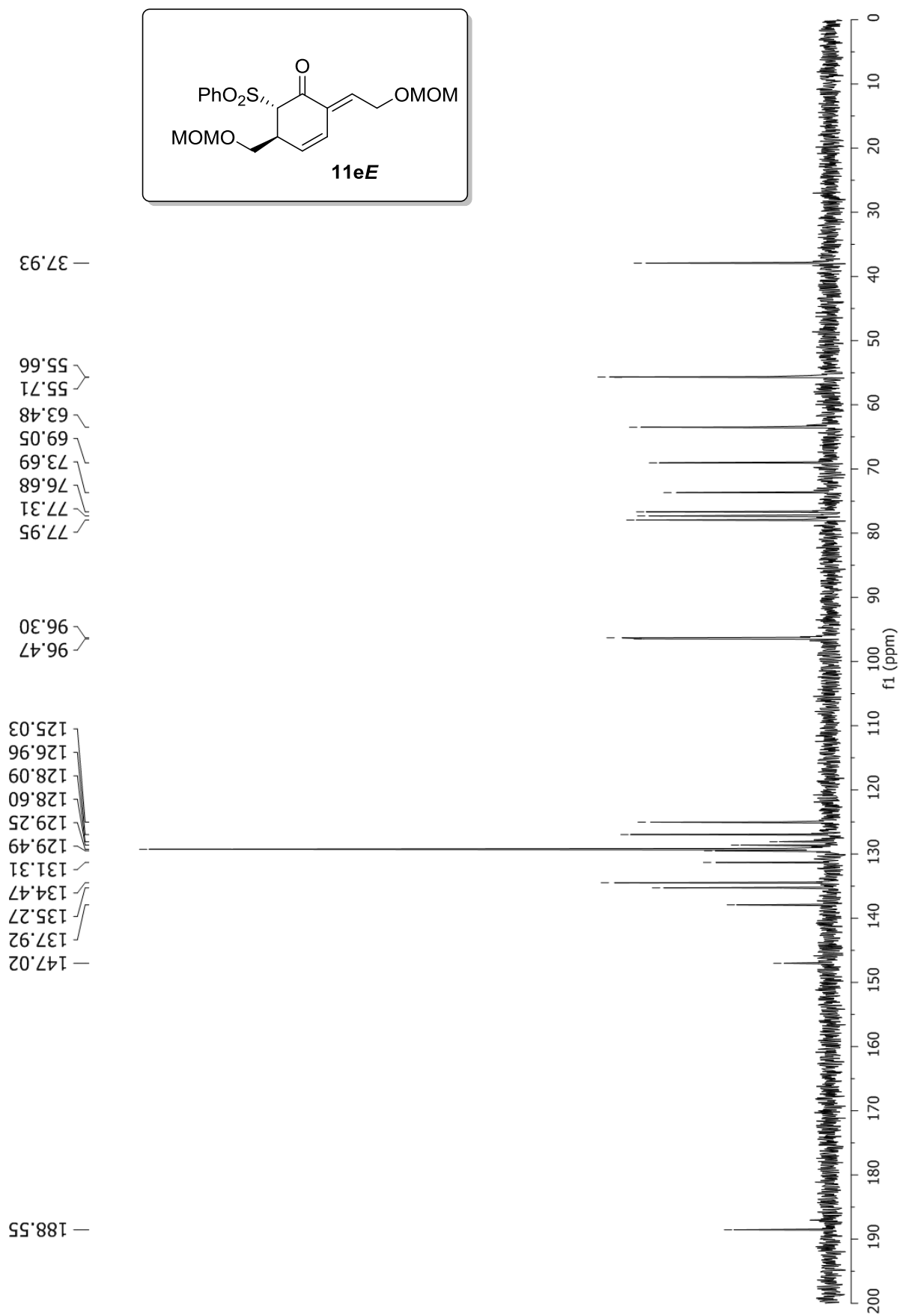
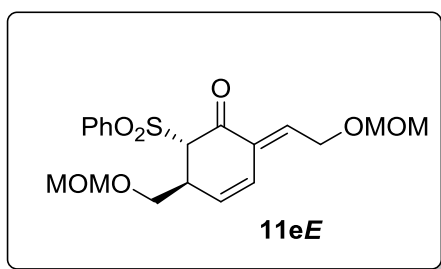


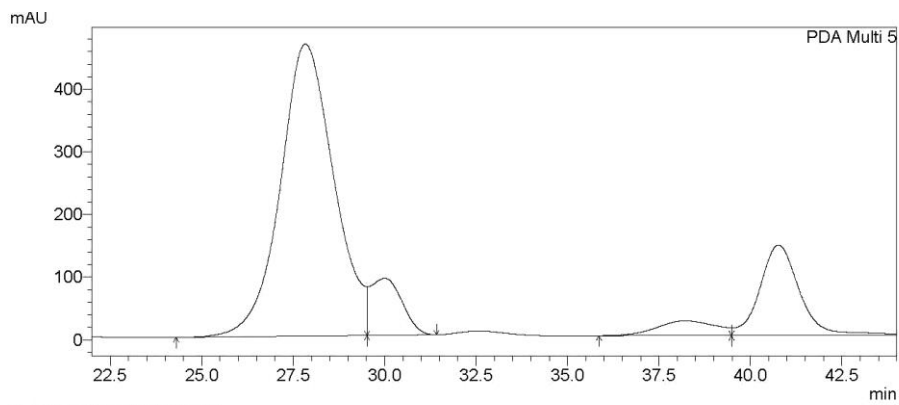
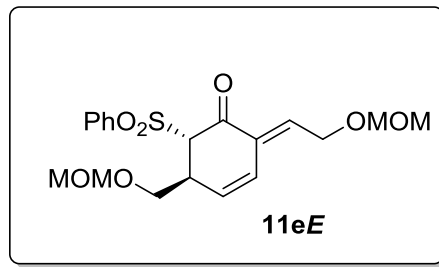
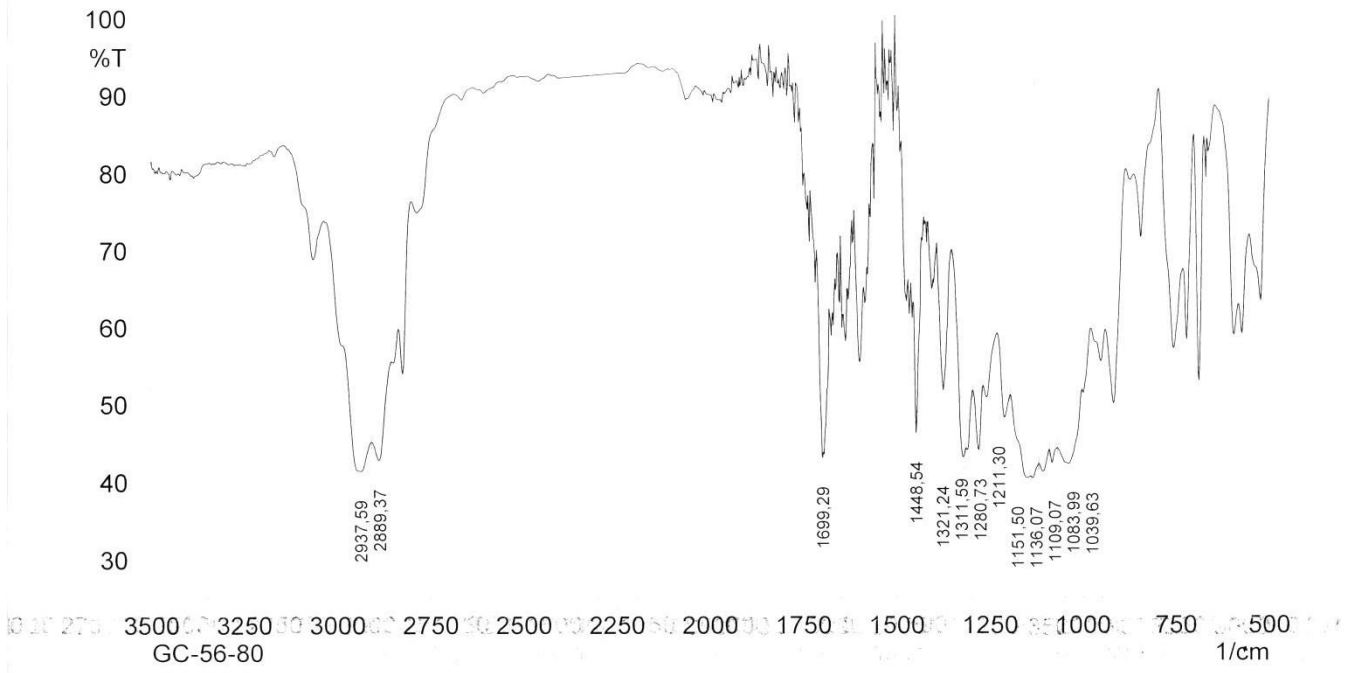
PeakTable

PDA Ch5 218nm 4nm

Peak#	Ret. Time	Area %
1	16.505	51.135
2	18.808	43.654
3	25.979	3.635
4	29.456	1.577
Total		100.000



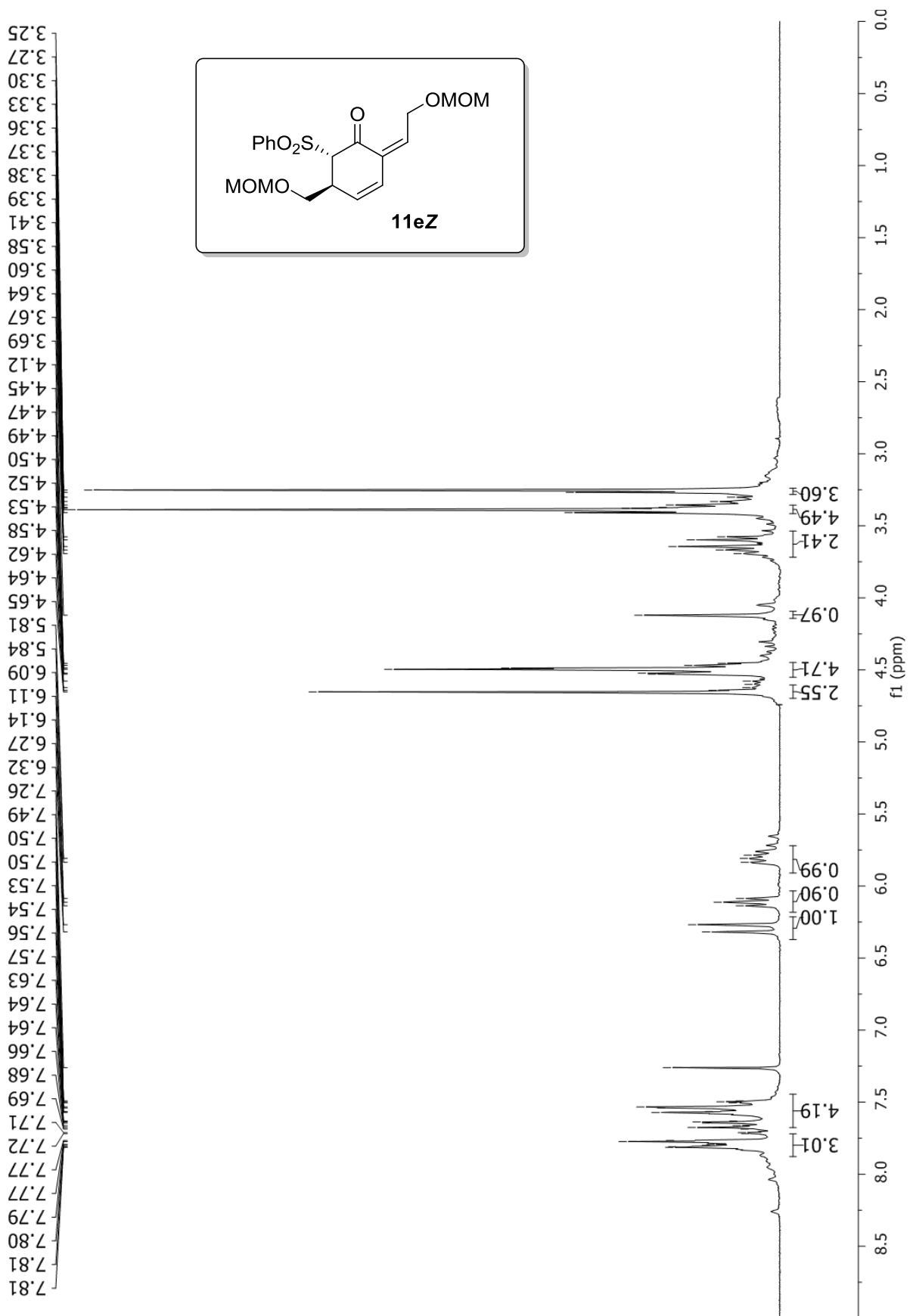


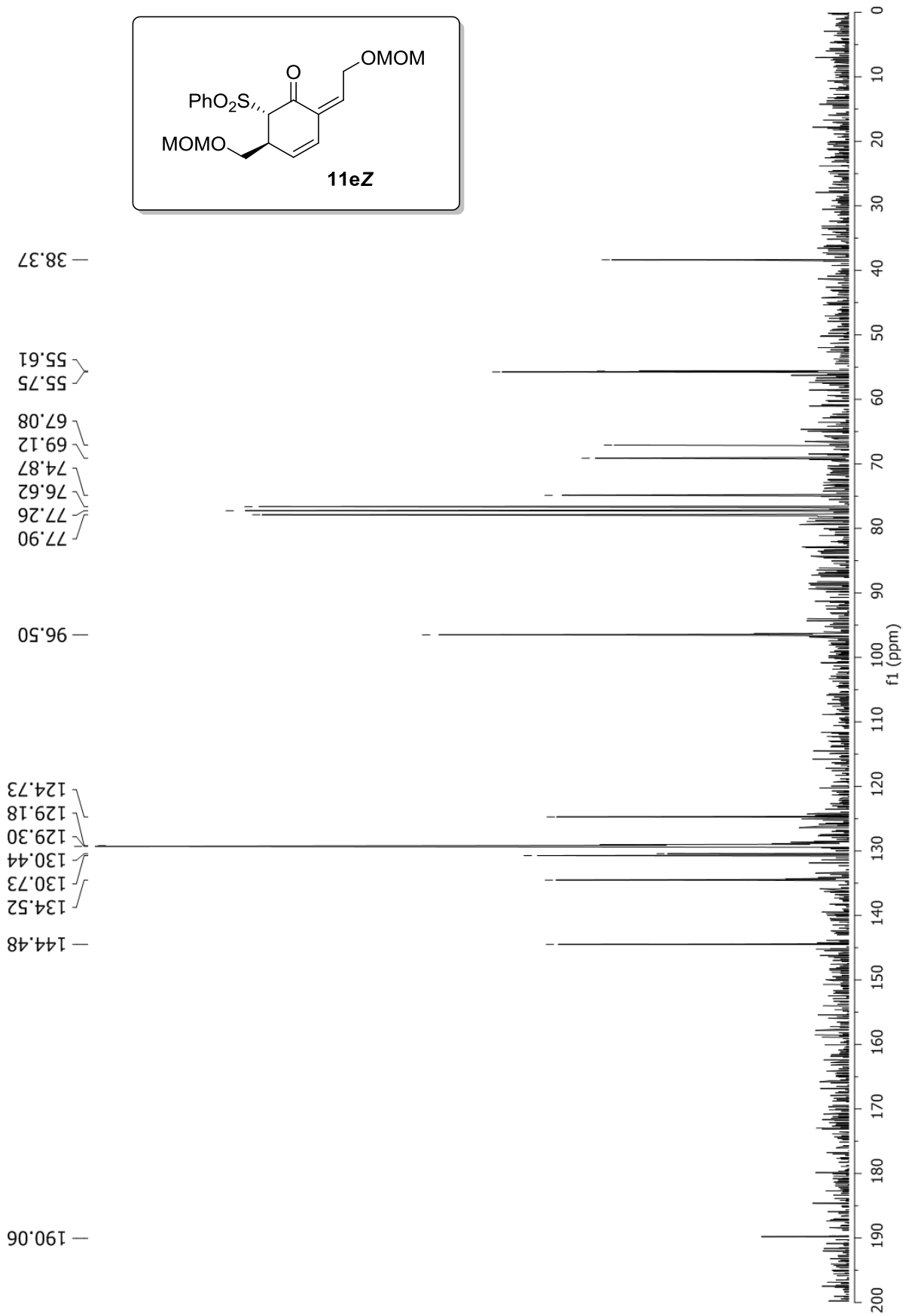
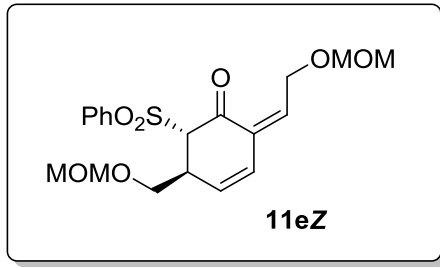


PeakTable

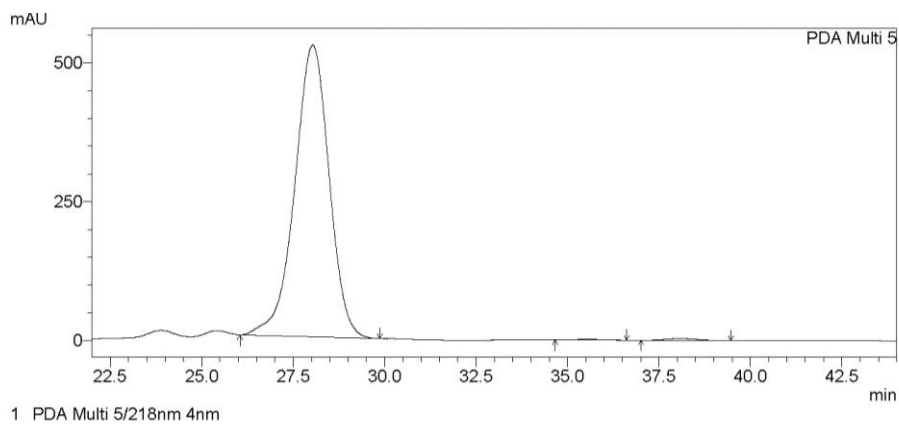
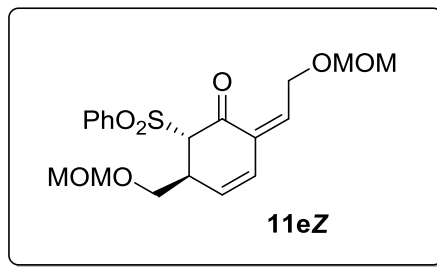
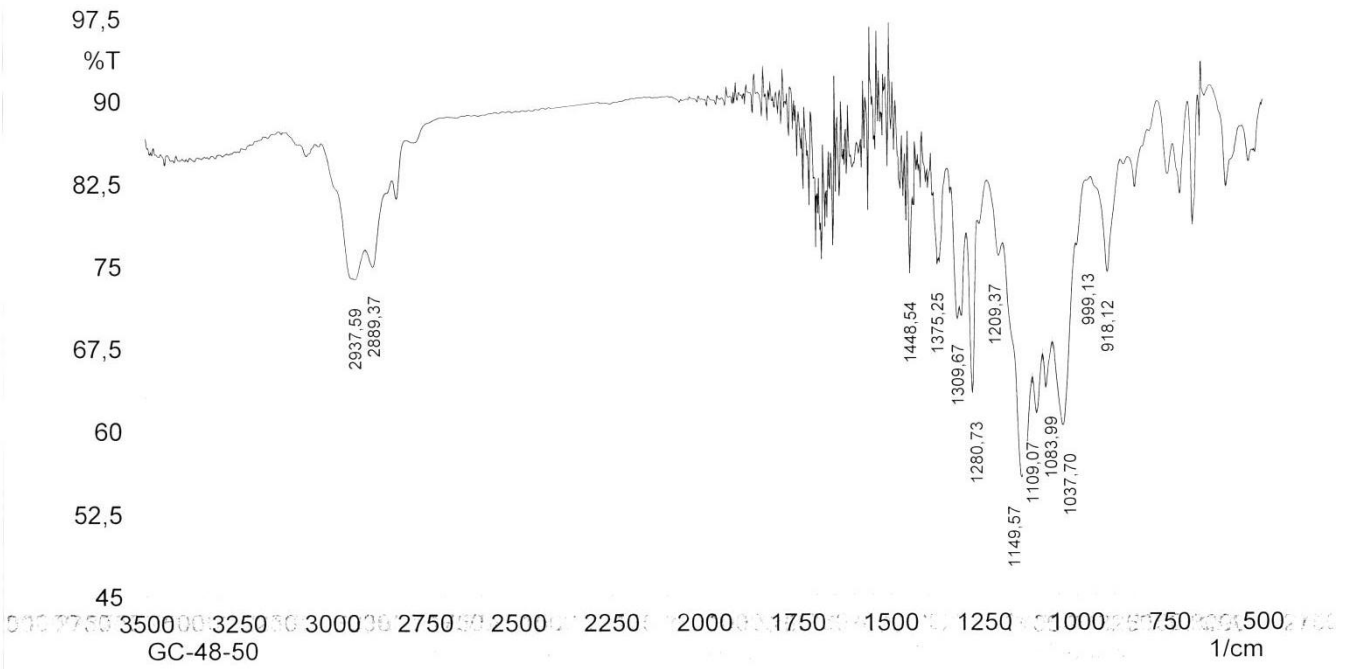
PDA Ch5 218nm 4nm

Peak#	Ret. Time	Area %
1	27.830	71.351
2	29.999	8.180
3	38.222	3.969
4	40.760	16.500
Total		100.000





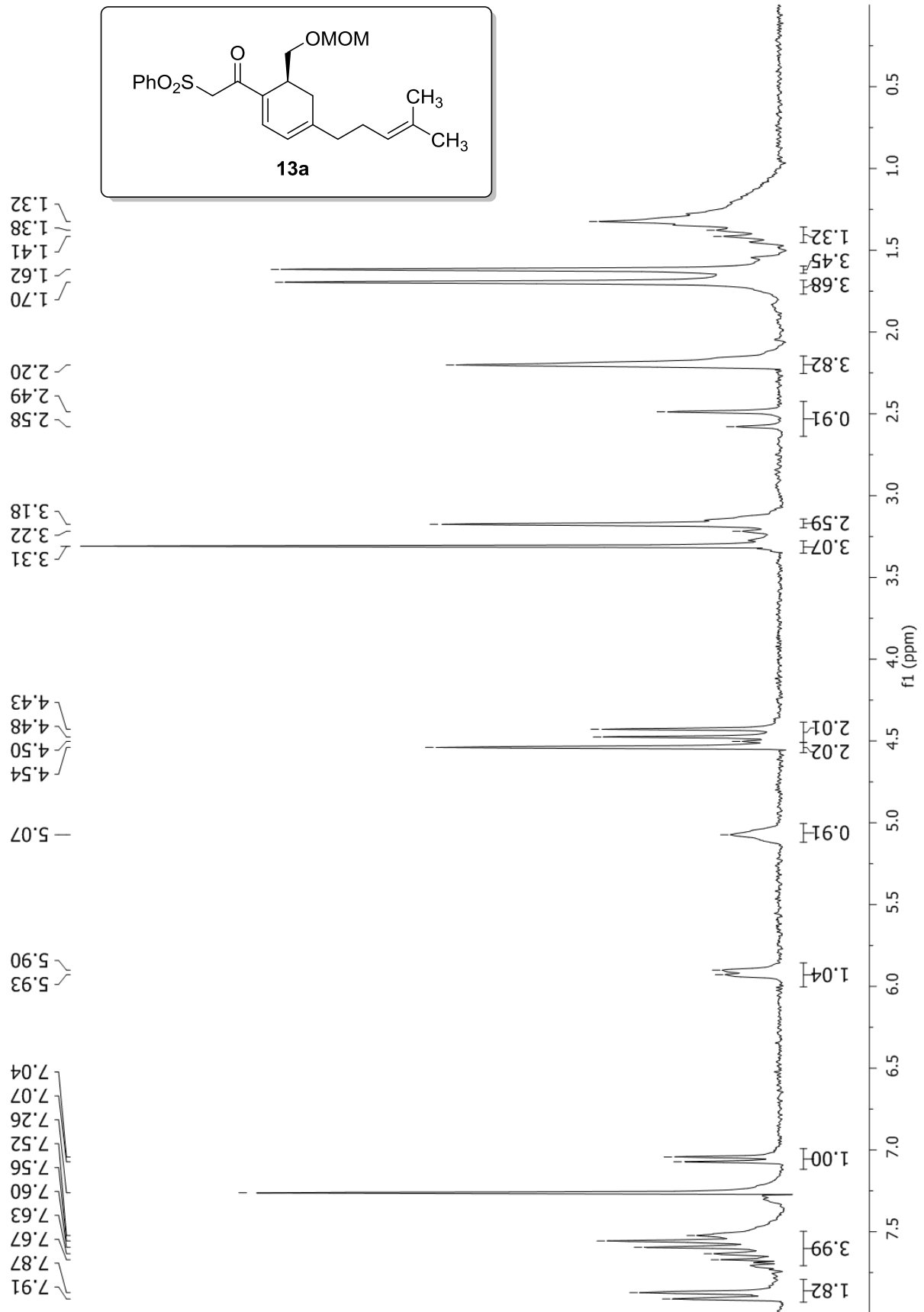
Full Spectroscopy

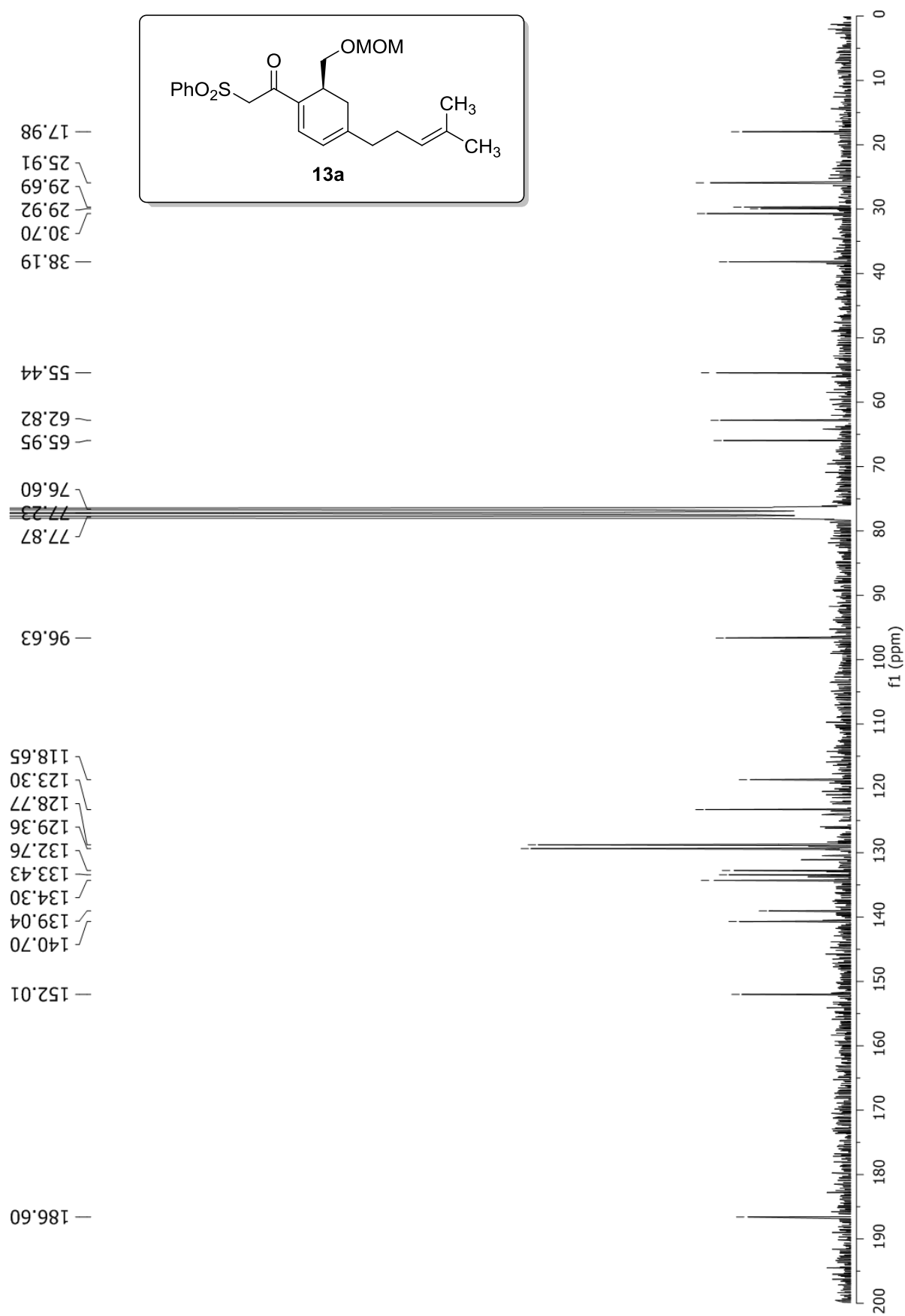


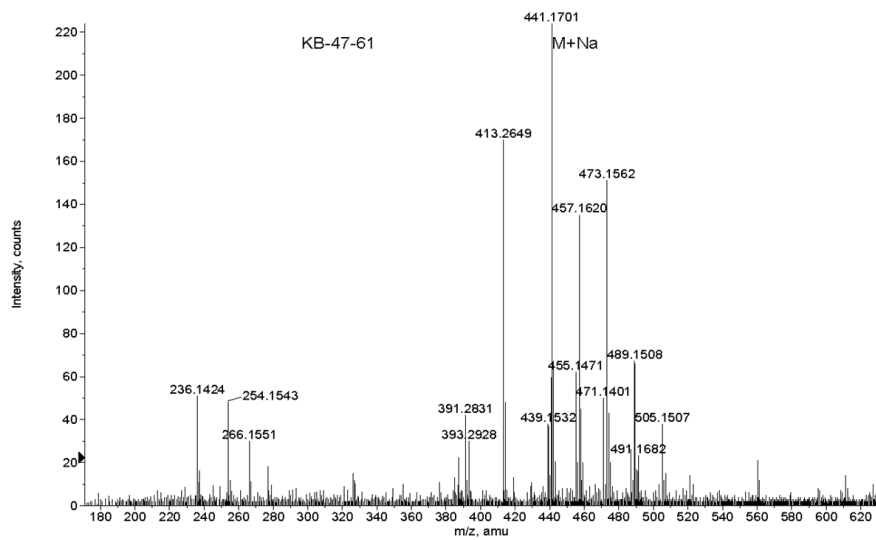
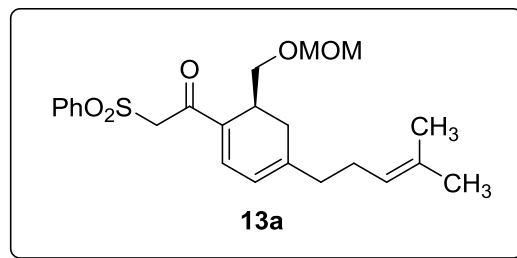
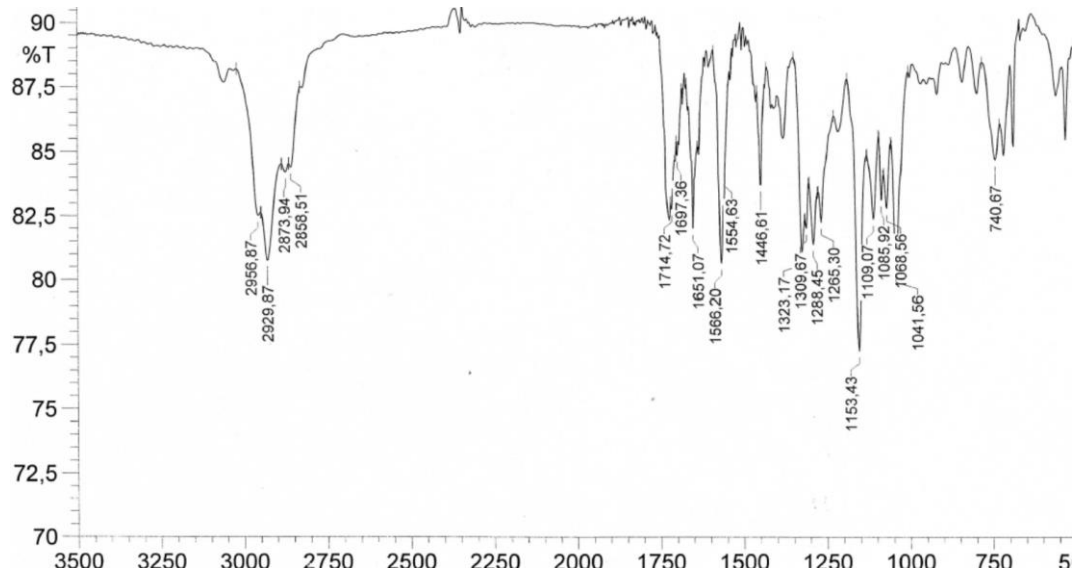
1 PDA Multi 5/218nm 4nm

PeakTable

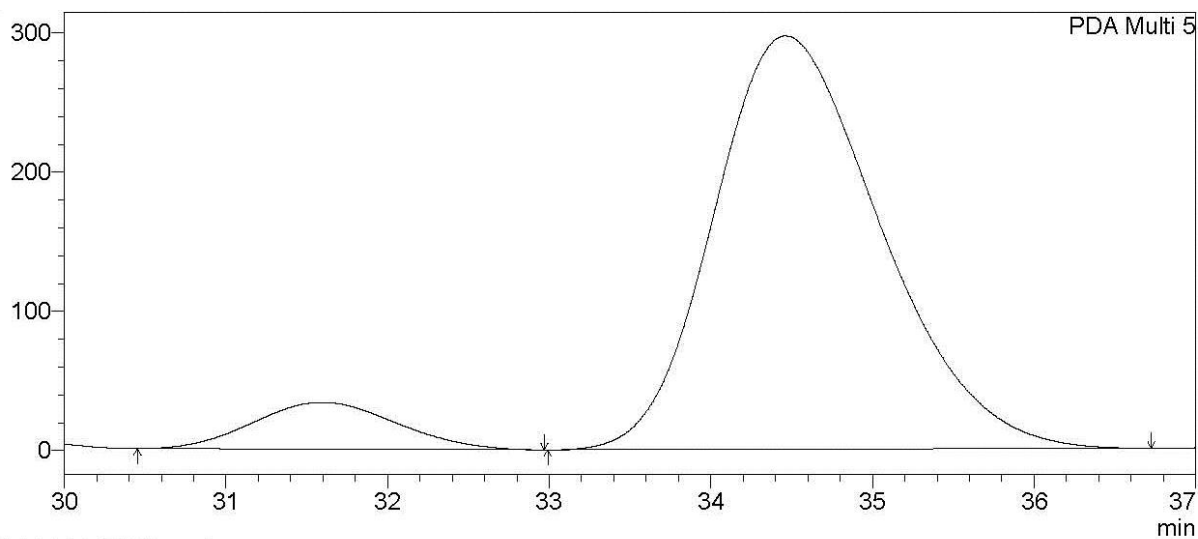
Peak#	Ret. Time	Area %
1	28.030	99.197
2	35.518	0.198
3	38.064	0.605
Total		100.000







Formula	CalculatedMass	mDaError	ppmError	RDB
C ₂₁ H ₂₅ N ₆ O ₃ S	441.170337	-0.237188	-0.537633	12.5
C ₂₃ H ₃₀ O ₅ NaS	441.170617	-0.51732	-1.172607	8.5

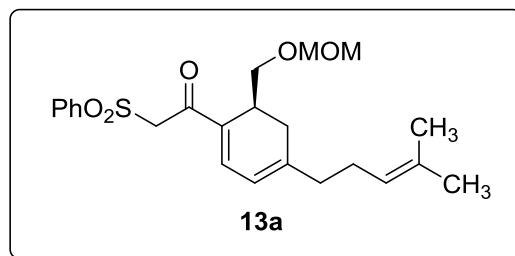


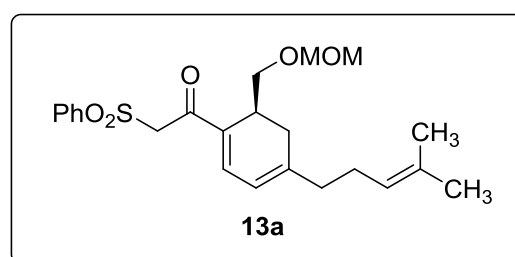
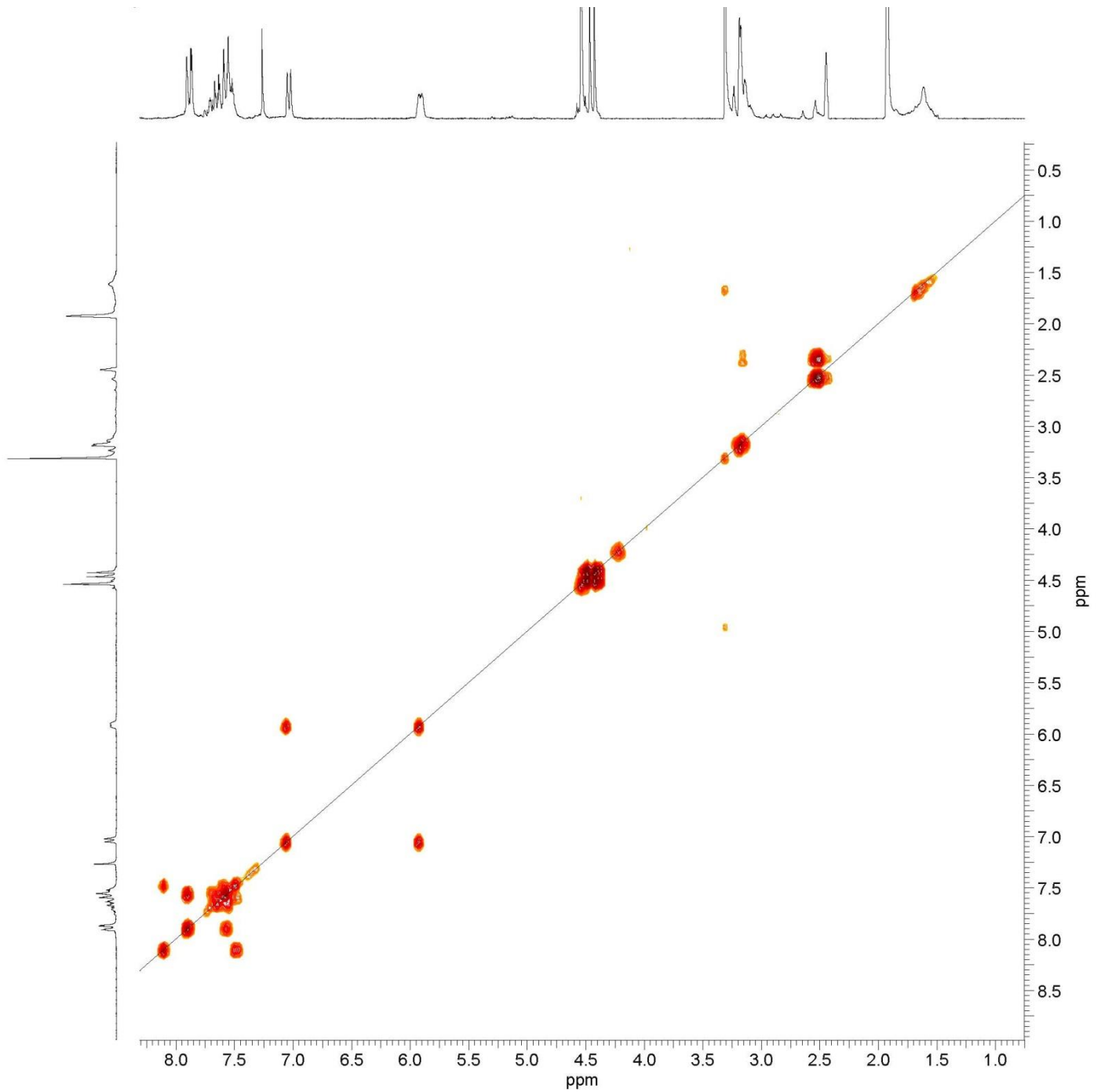
1 PDA Multi 5/325nm 4nm

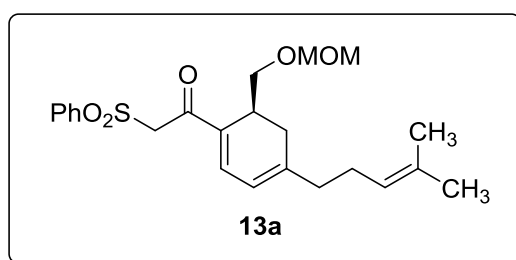
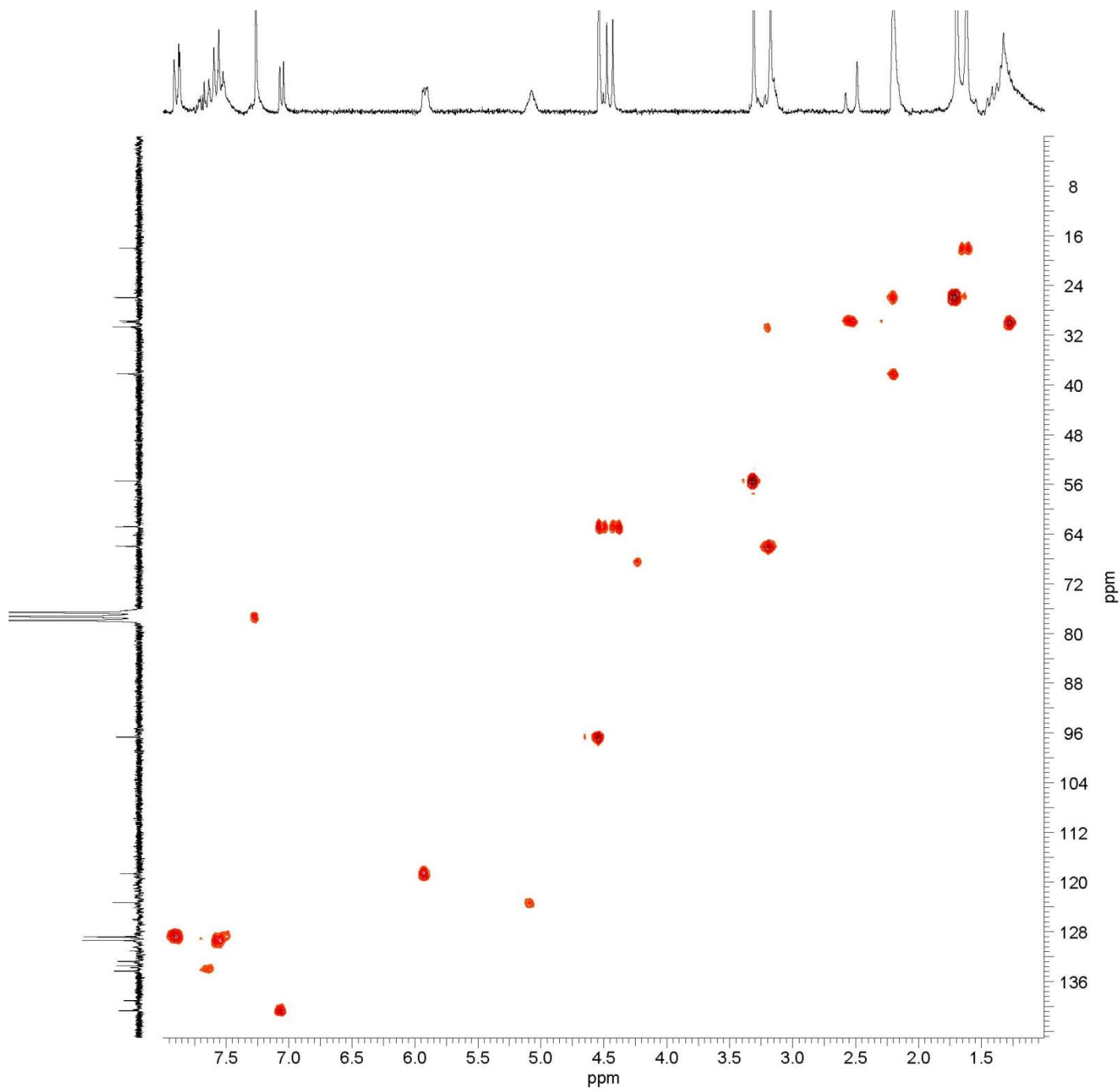
PeakTable

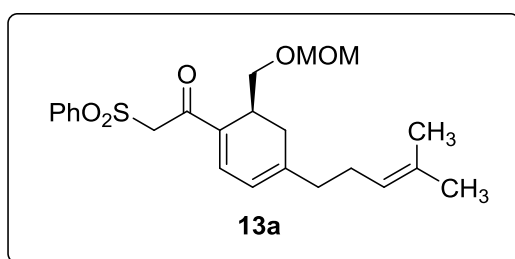
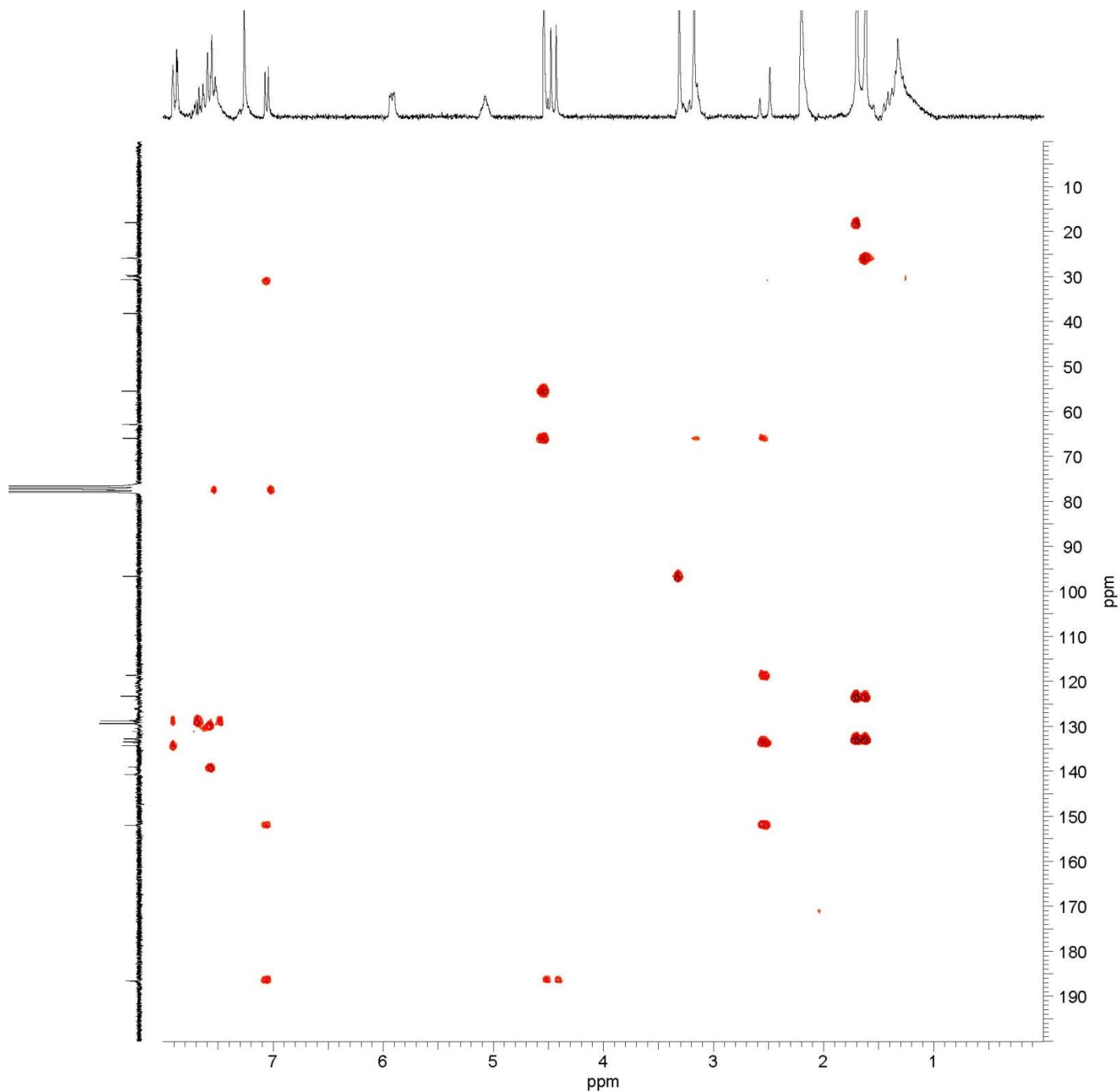
PDA Ch5 325nm 4nm

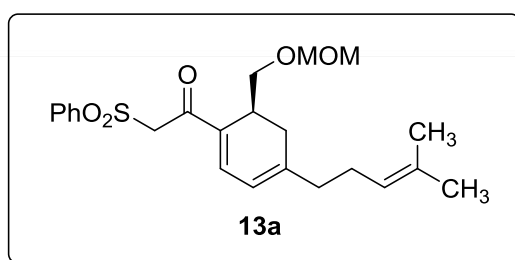
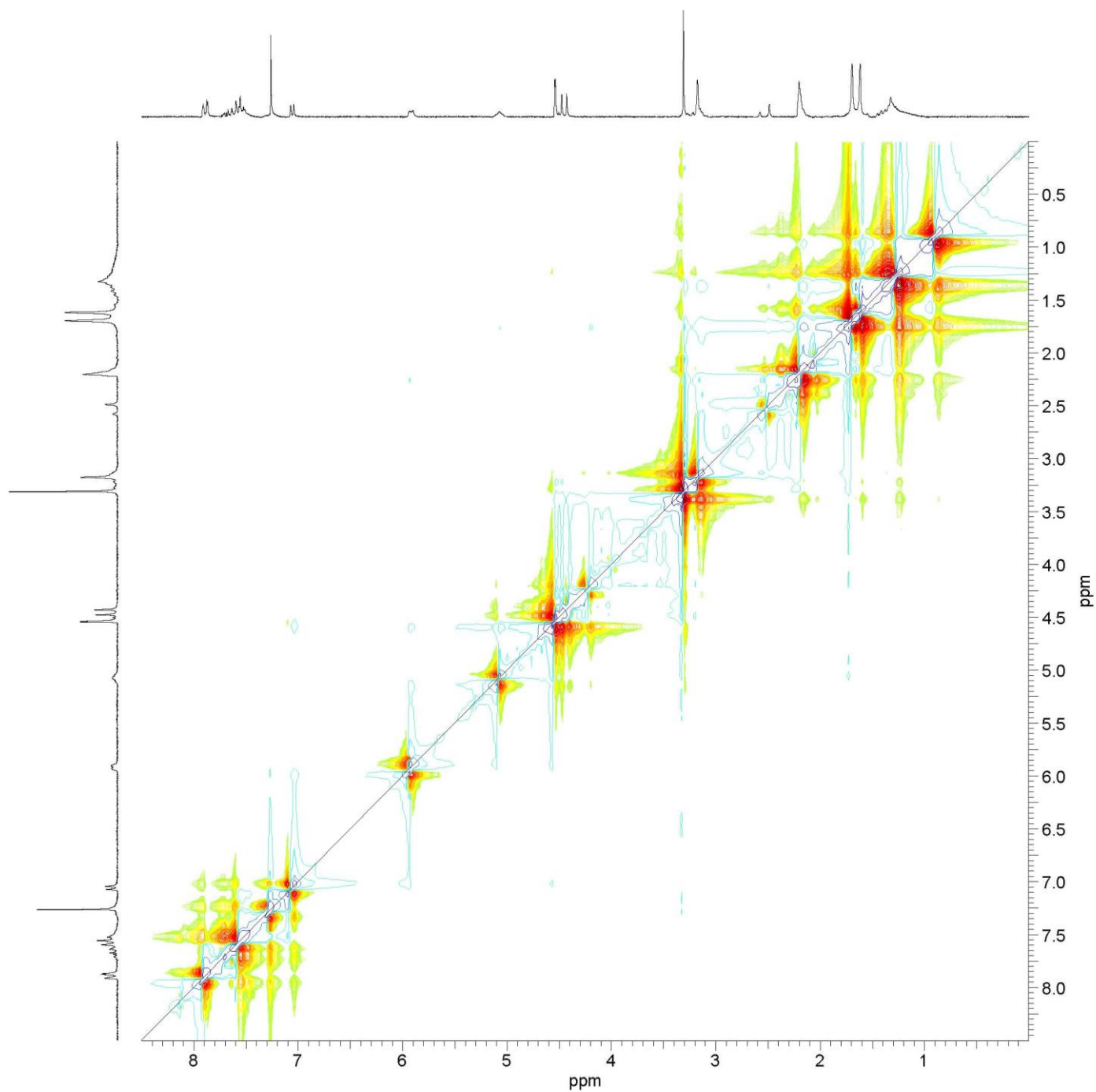
Peak#	Ret. Time	Area %
1	31.586	8.846
2	34.456	91.154
Total		100.000

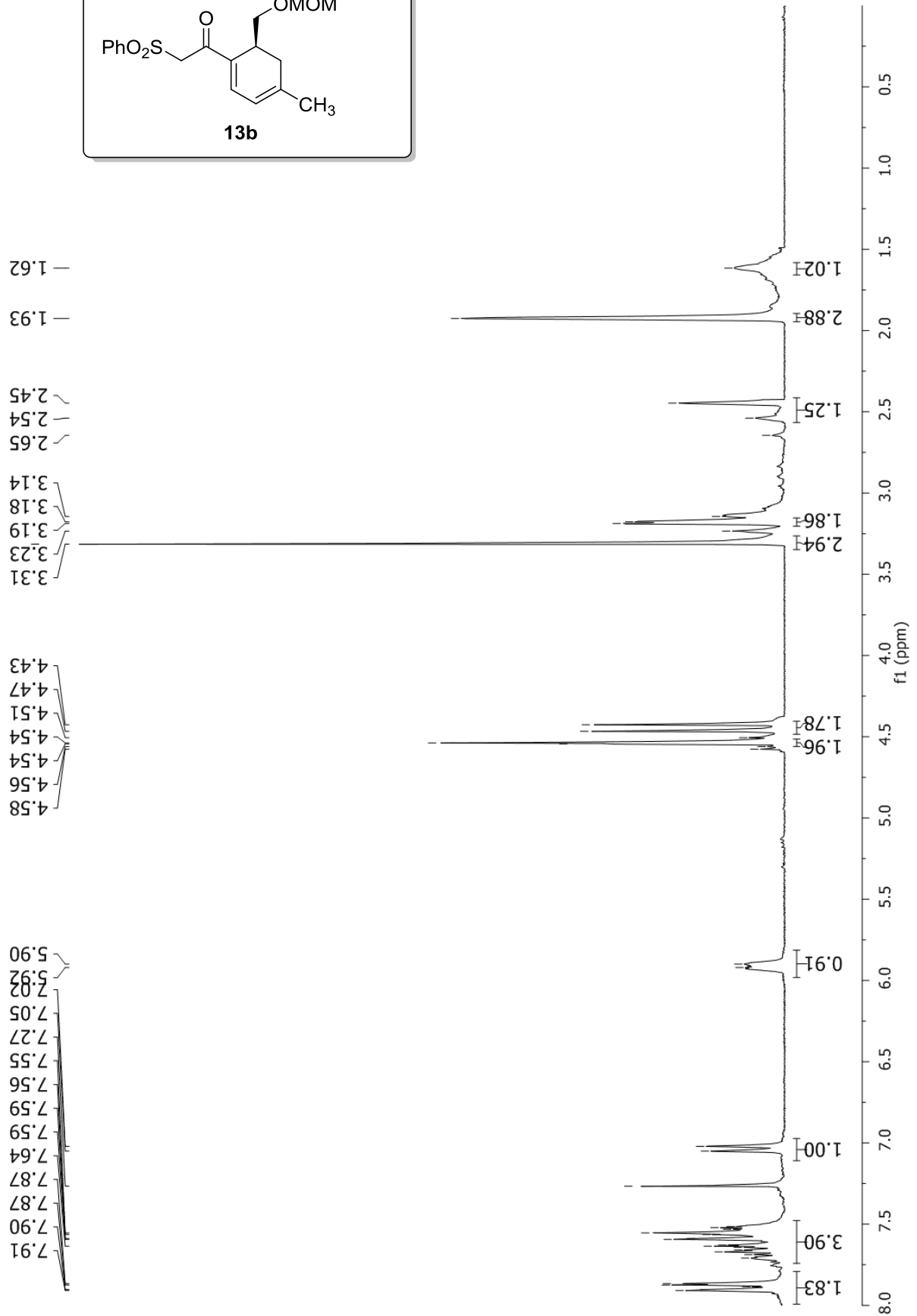
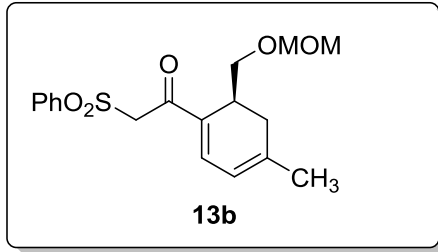


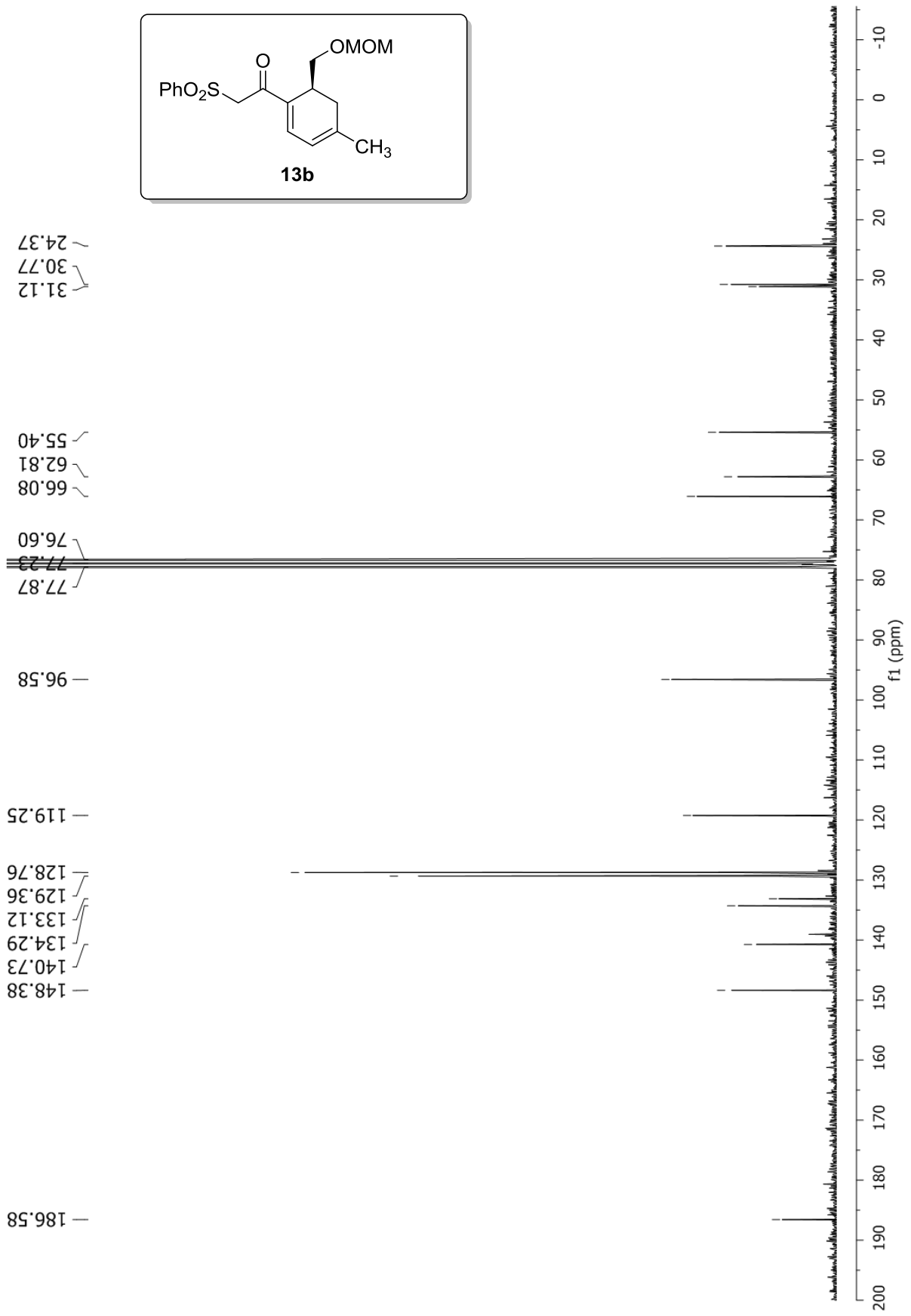
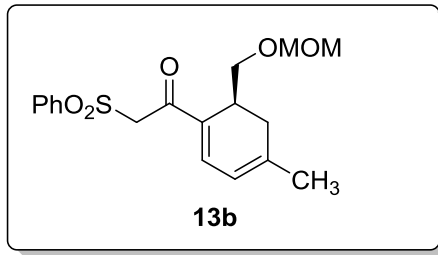


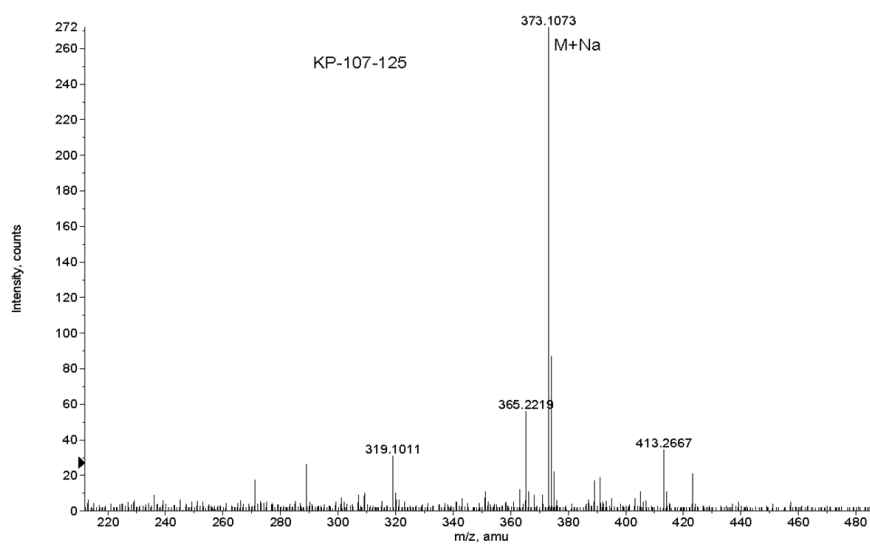
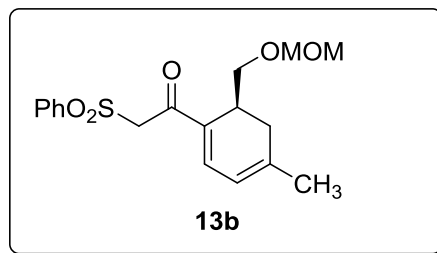
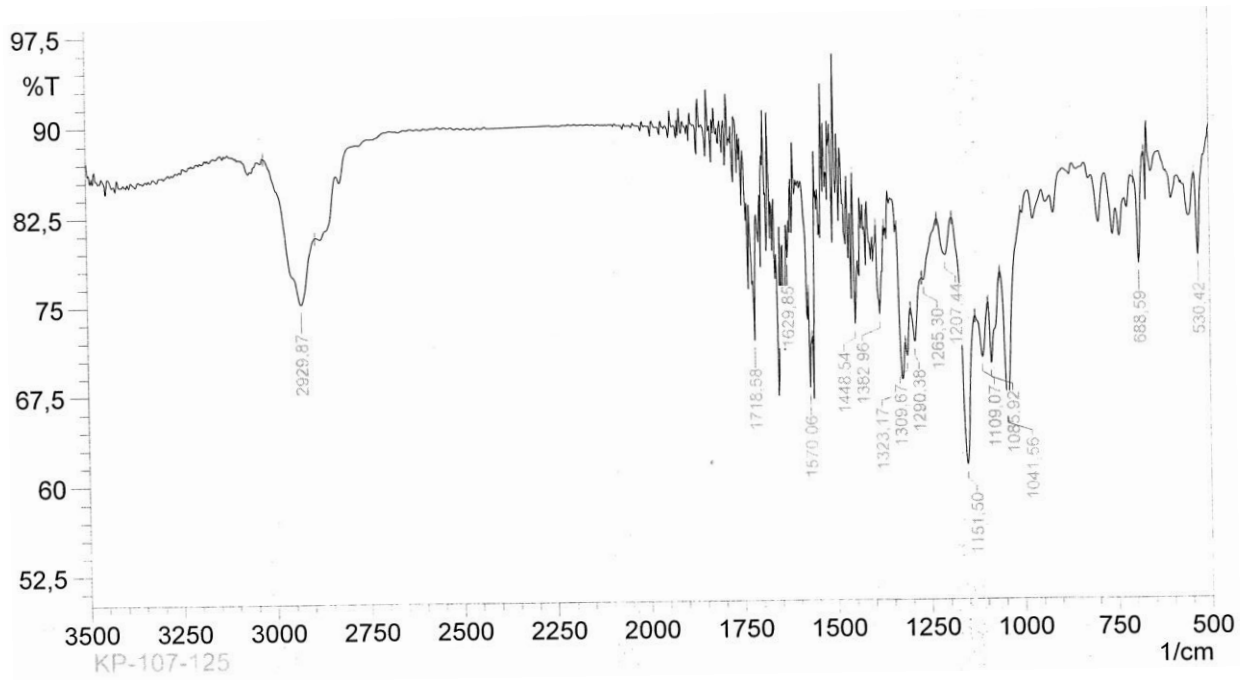




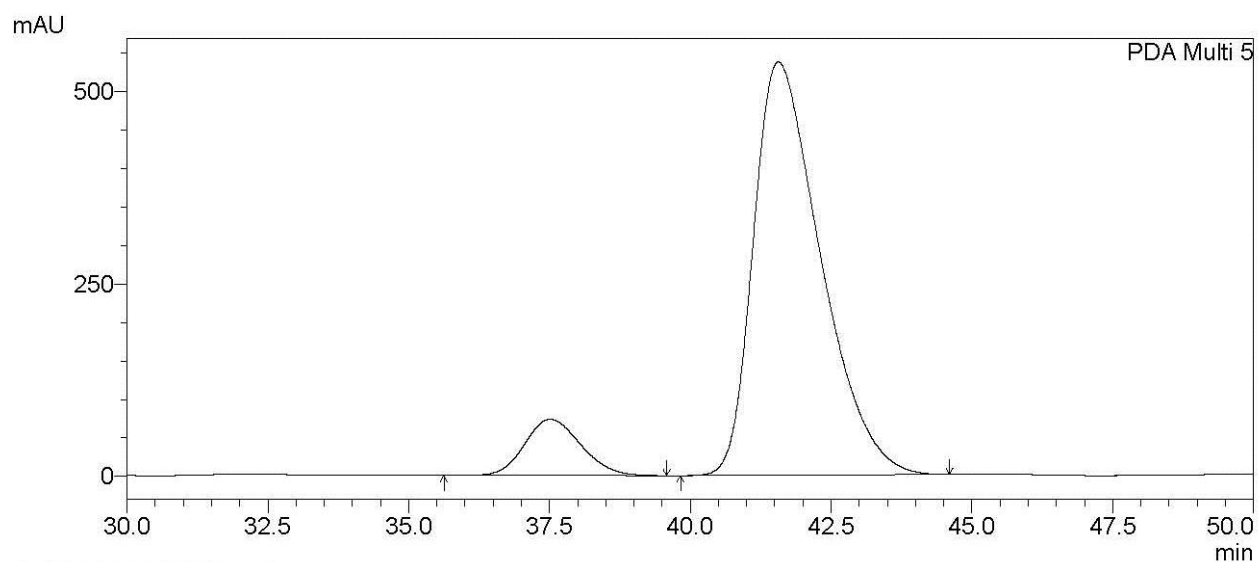








Formula	CalculatedMass	mDaError	ppmError	RDB
C23 H17 O5	373.10705	0.2497	0.669243	15.5
C16 H17 N6 O3 S	373.107737	-0.436868	-1.170889	11.5
C10 H18 N6 O8 Na	373.107833	-0.533008	-1.428563	4.5
C18 H22 O5 Na S	373.108017	-0.717	-1.921696	7.5

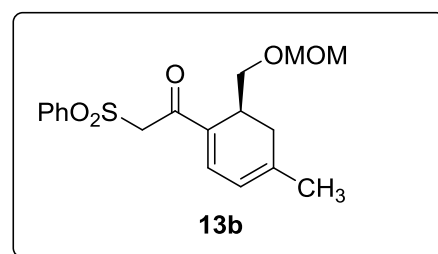


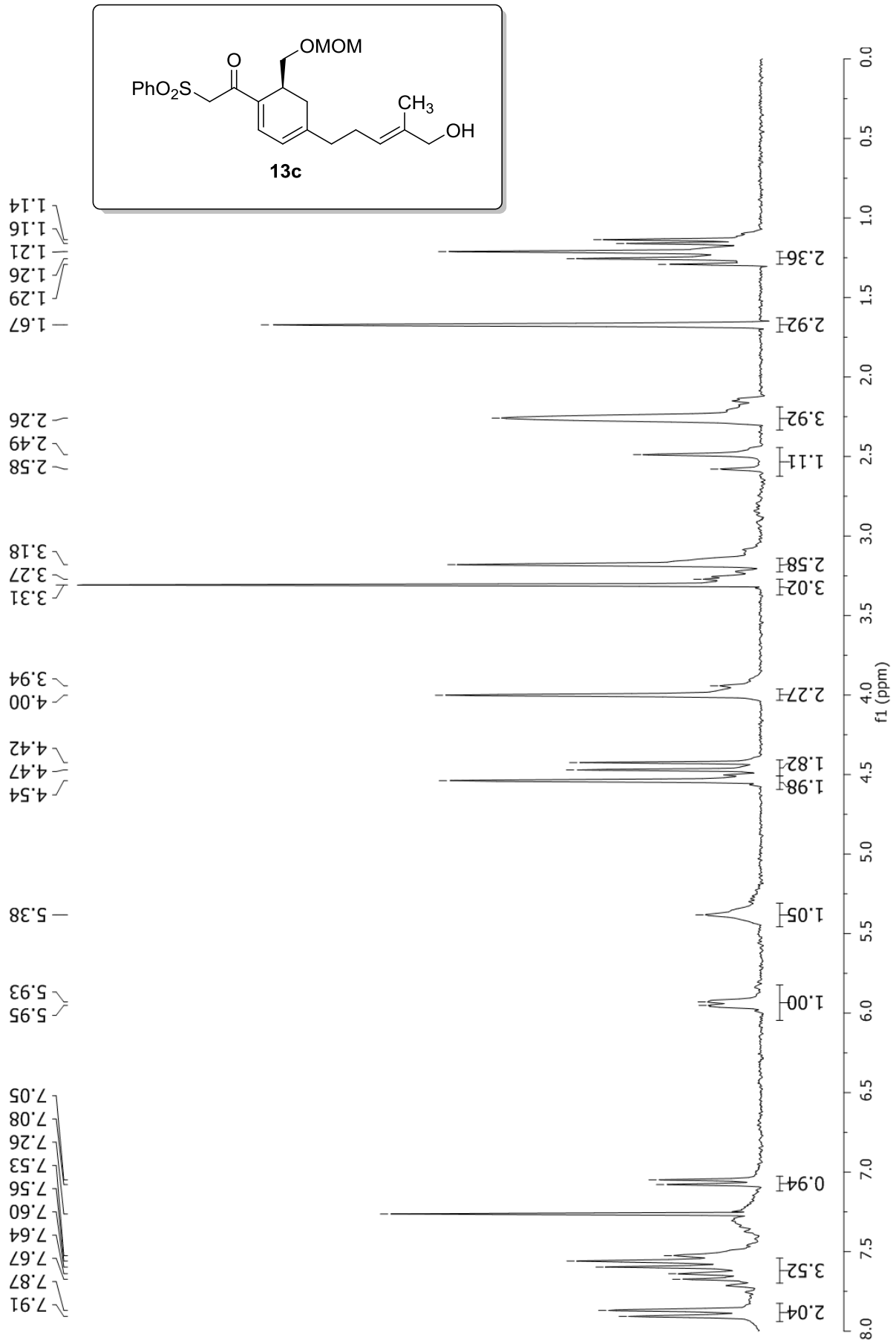
1 PDA Multi 5/325nm 4nm

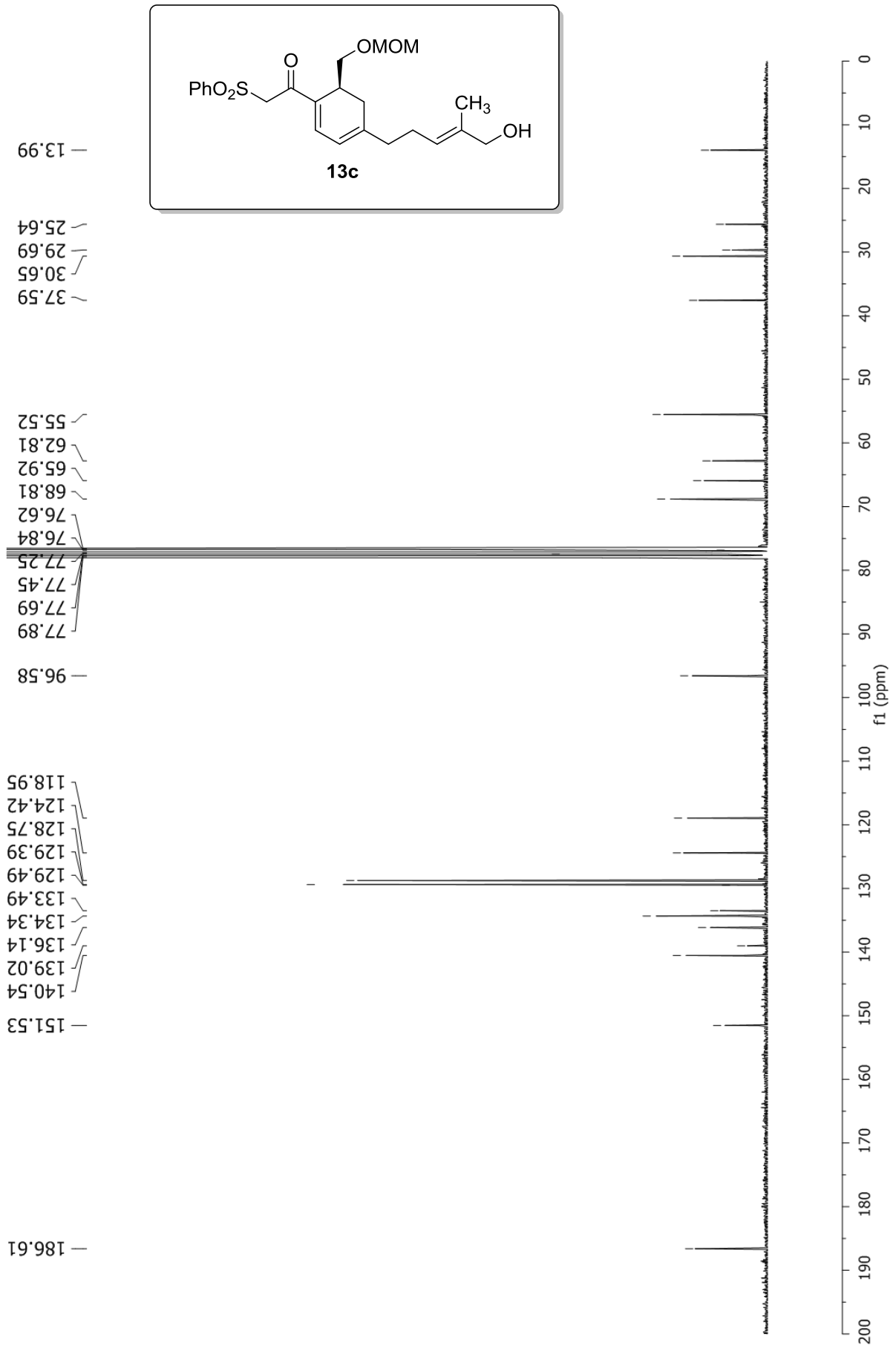
PeakTable

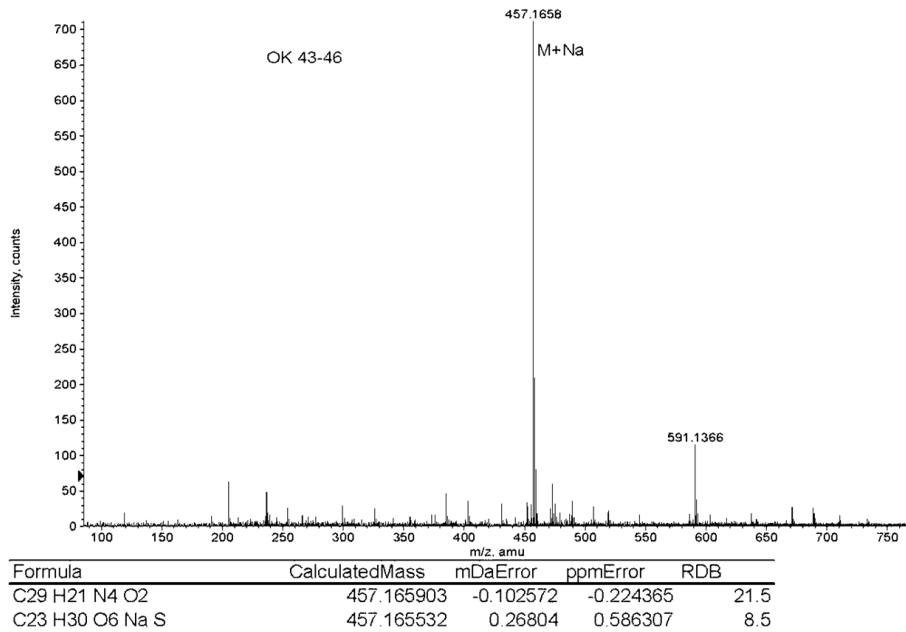
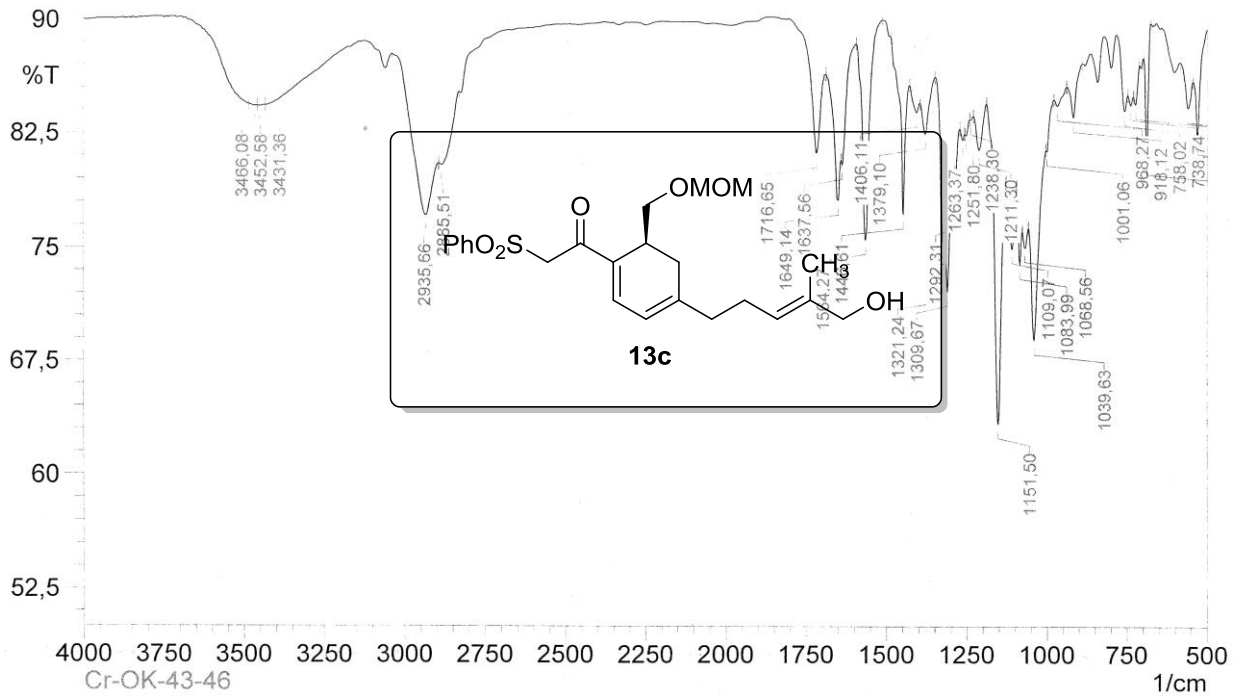
PDA Ch5 325nm 4nm

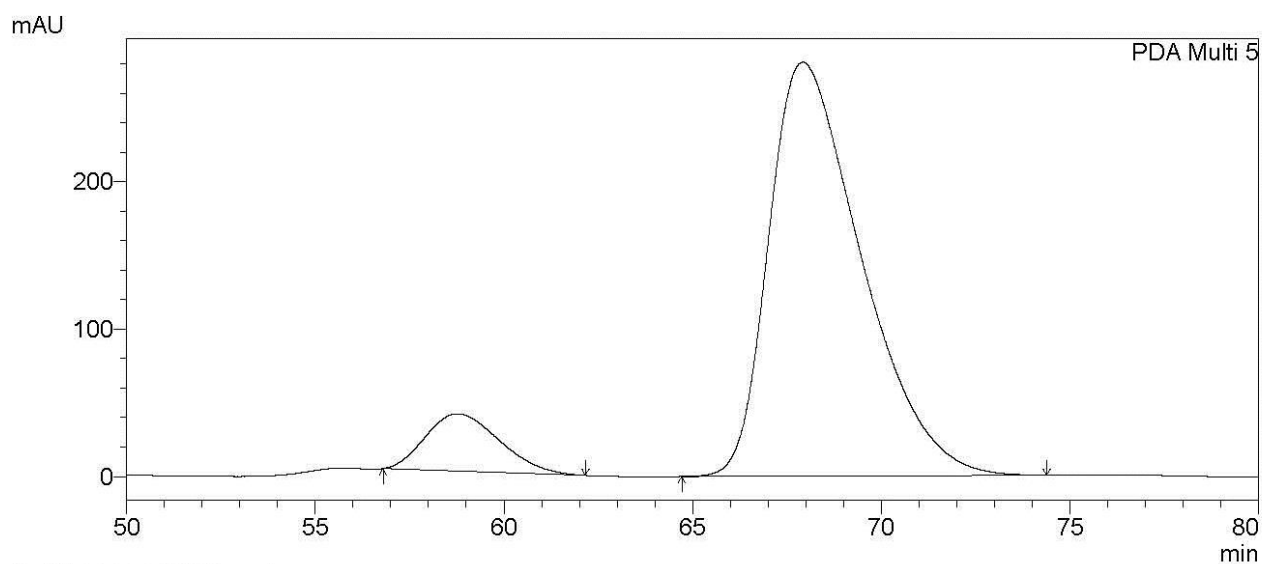
Peak#	Ret. Time	Area %
1	37.508	10.239
2	41.560	89.761
Total		100.000









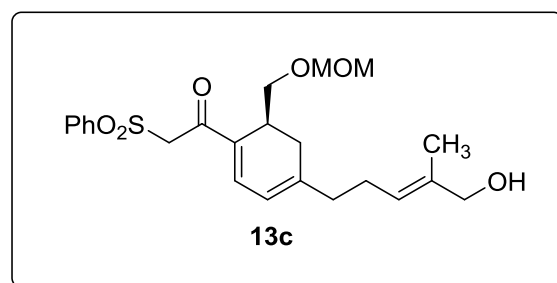


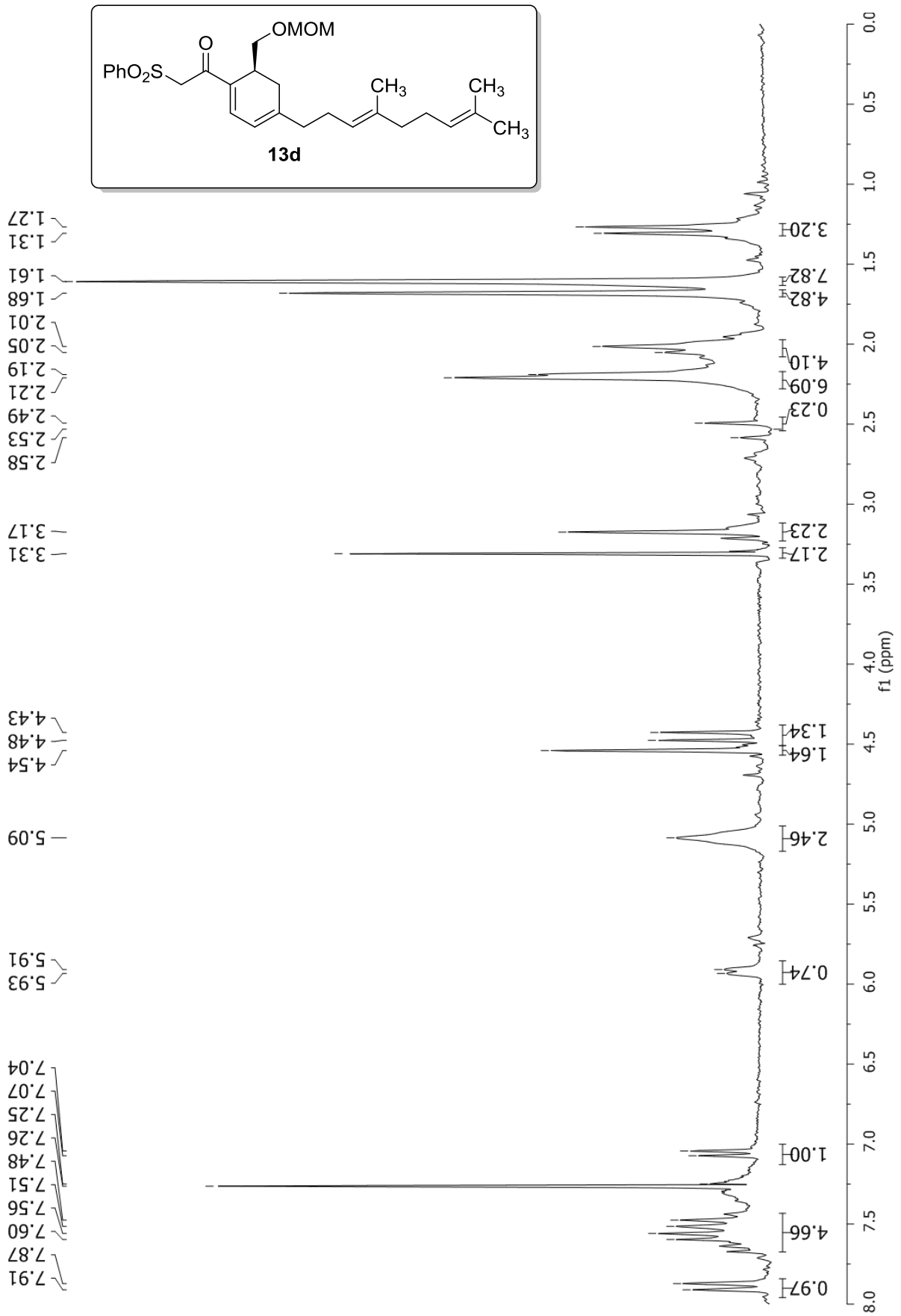
1 PDA Multi 5/325nm 4nm

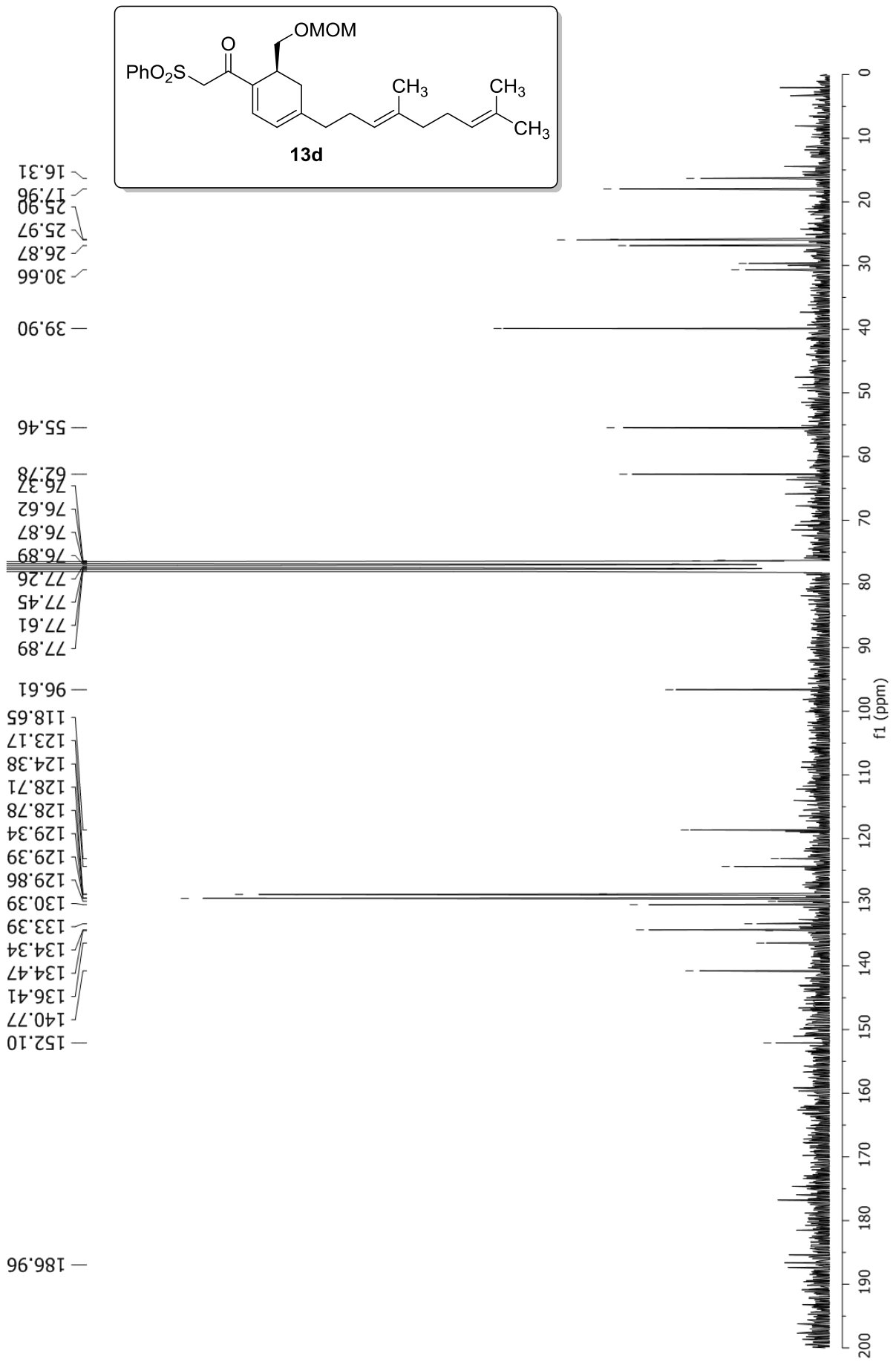
PeakTable

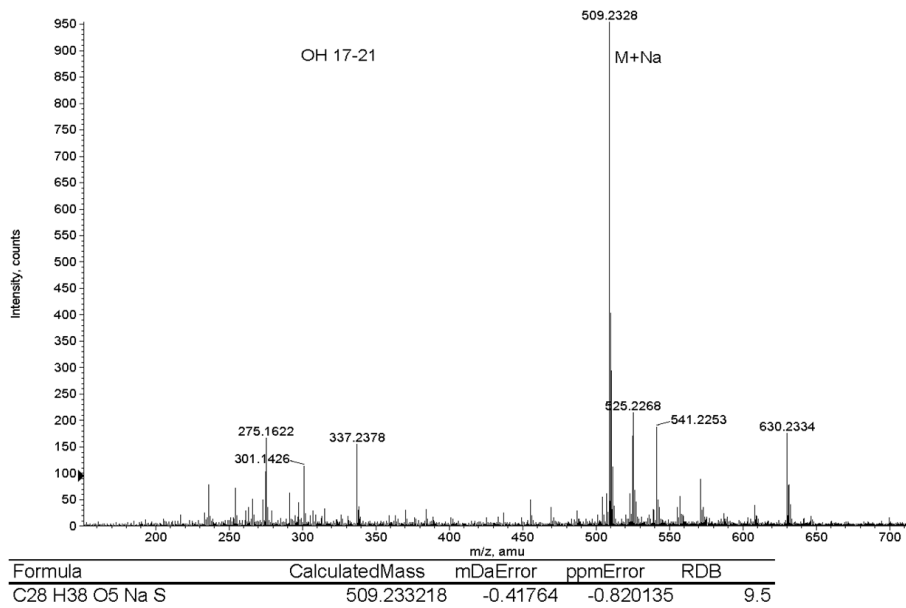
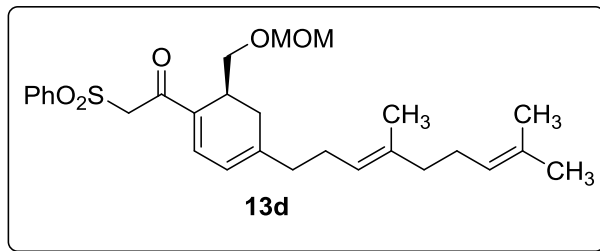
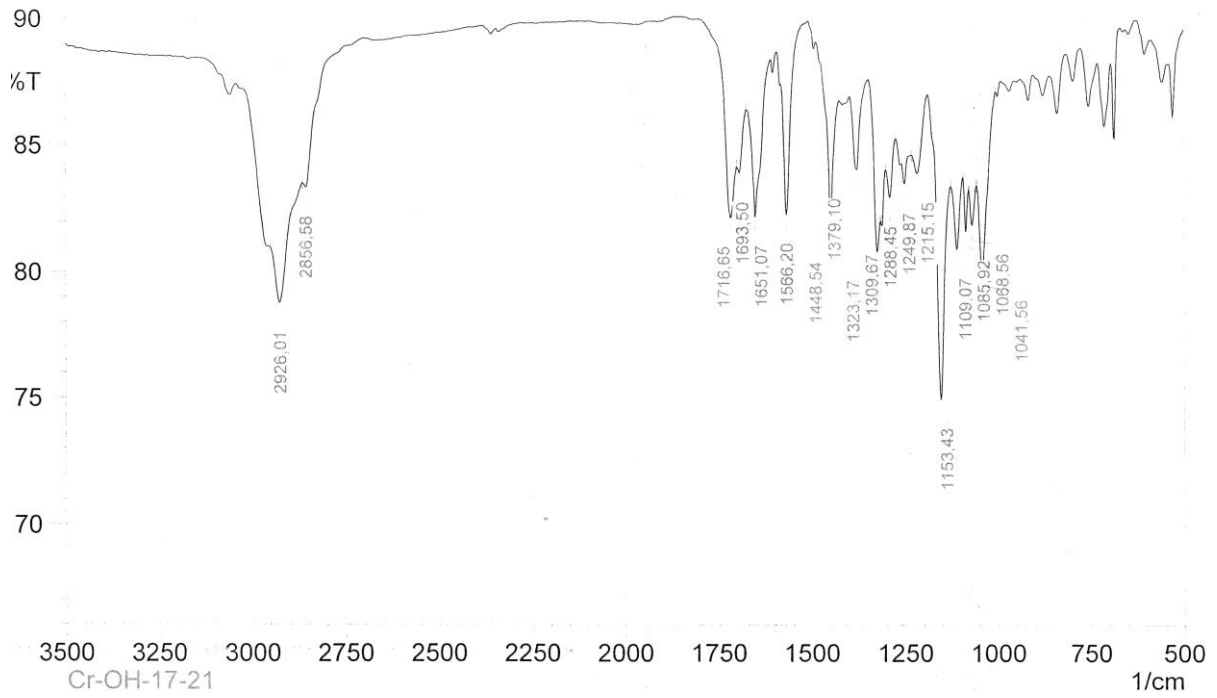
PDA Ch5 325nm 4nm

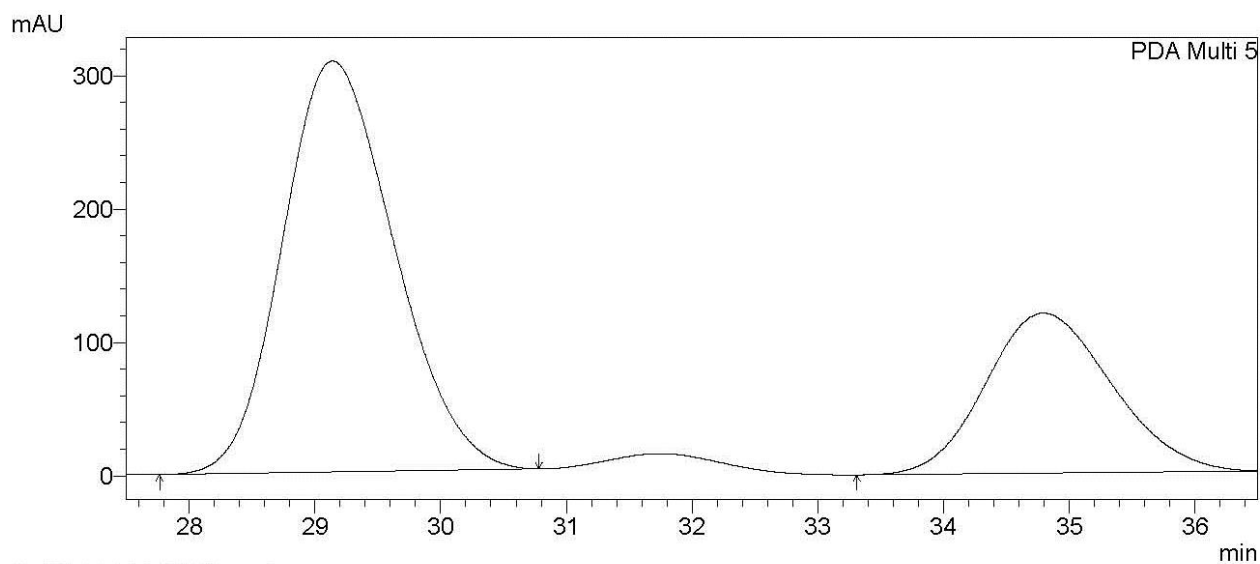
Peak#	Ret. Time	Area %
1	58.775	9.923
2	67.918	90.077
Total		100.000







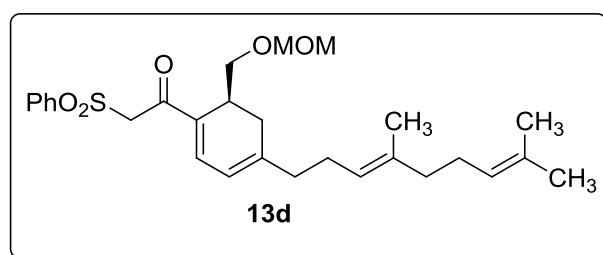


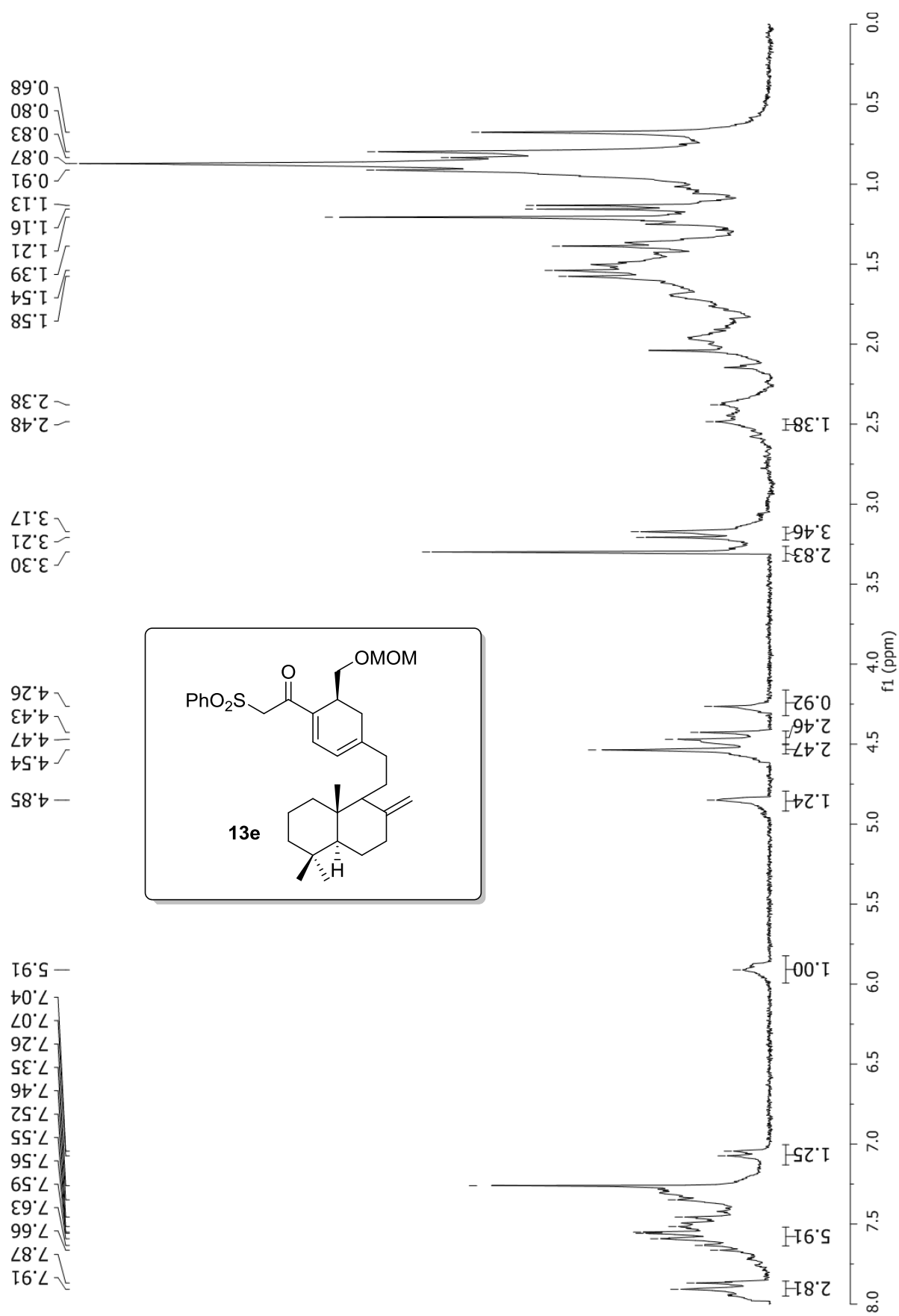


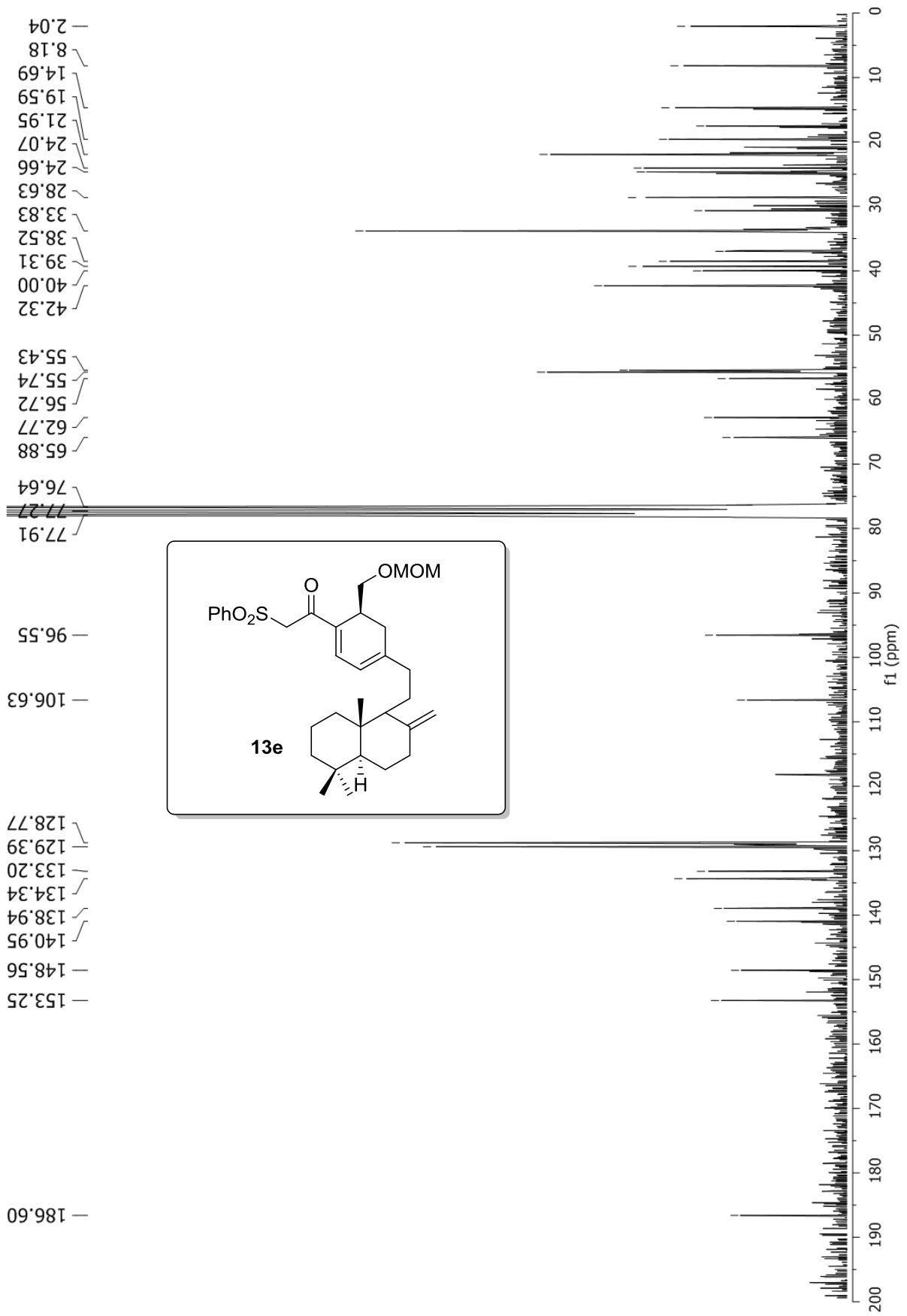
1 PDA Multi 5/325nm 4nm

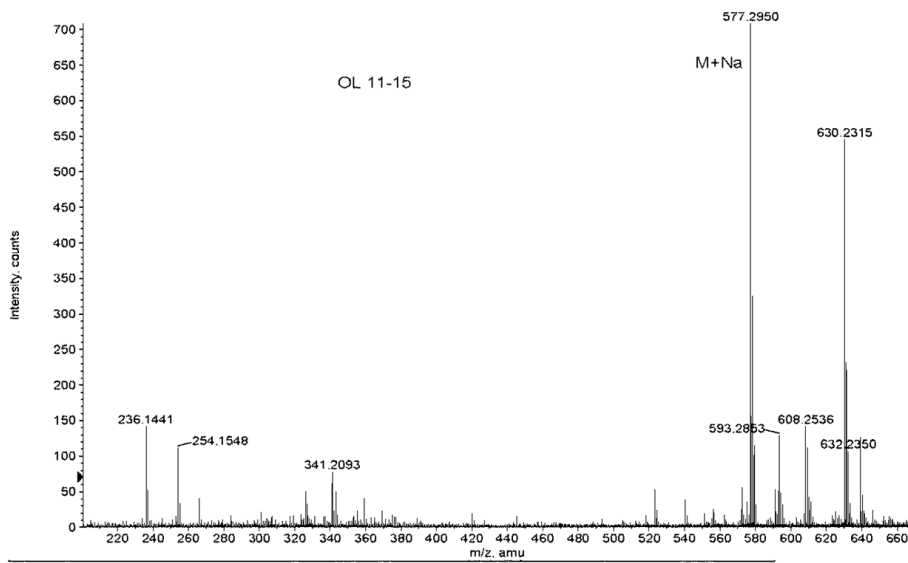
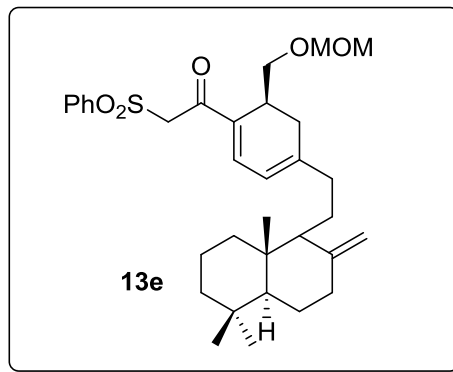
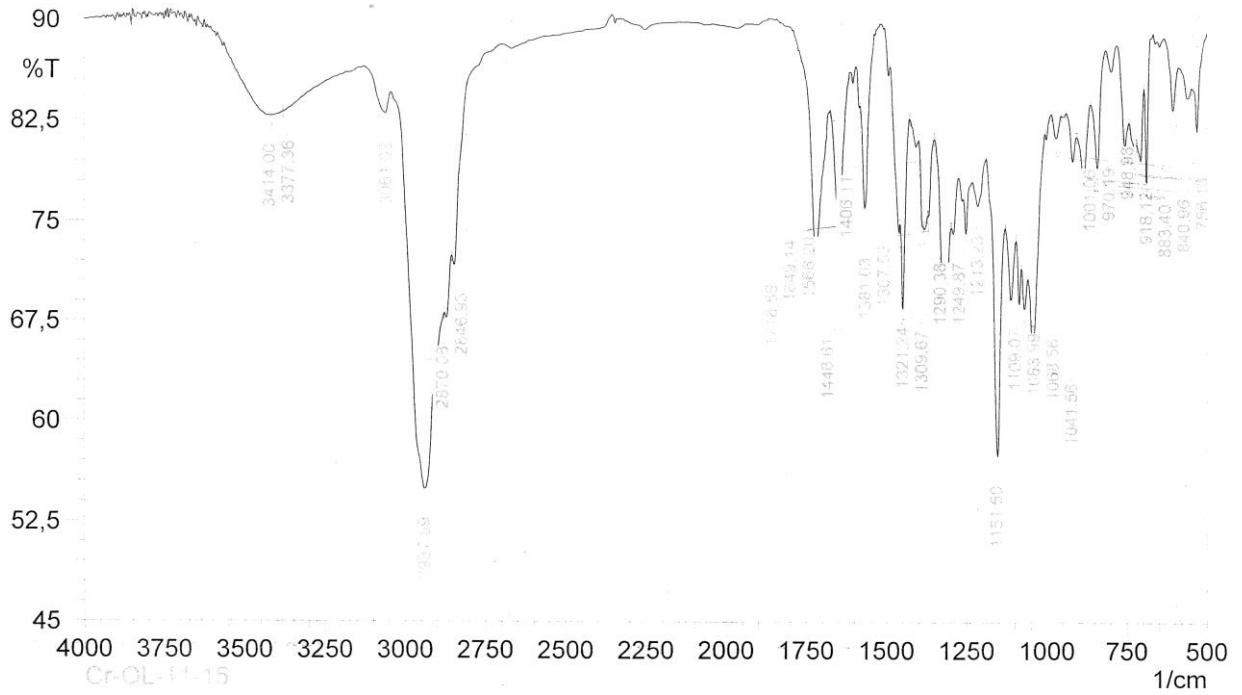
PeakTable
PDA Ch5 325nm 4nm

Peak#	Ret. Time	Area %
1	29.135	69.482
2	34.789	30.518
Total		100.000

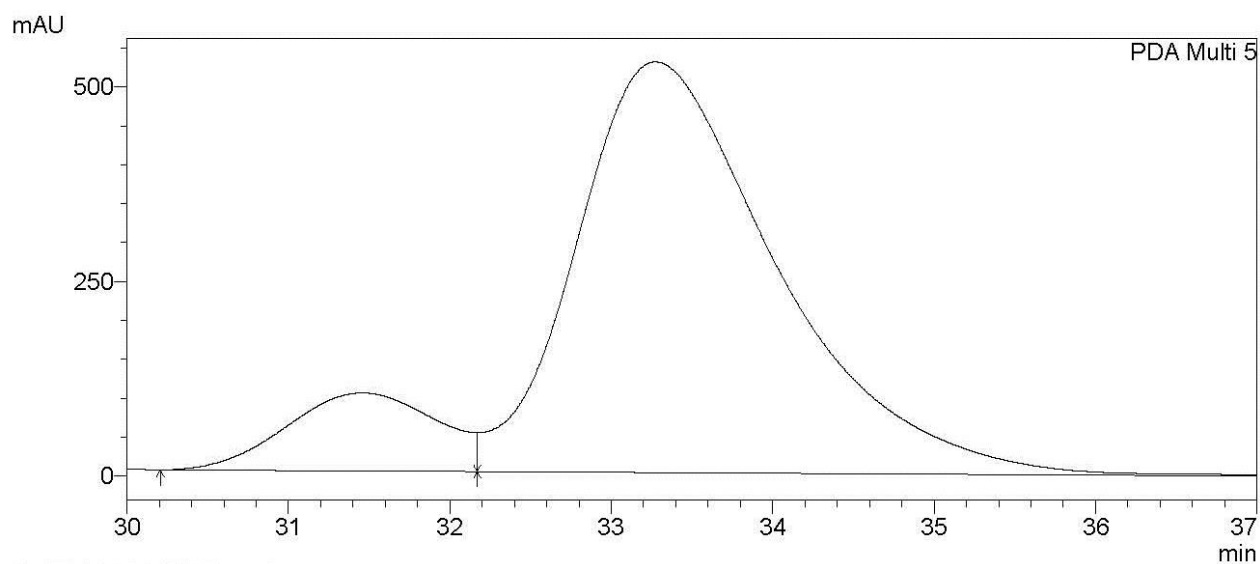








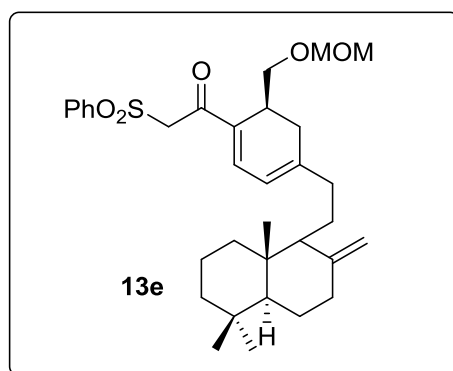
Formula	CalculatedMass	mDaError	ppmError	RDB
C38 H41 O5	577.294851	0.14874	0.25765	18.5
C30 H45 N2 O7 S	577.294201	0.799484	1.384878	9.5
C33 H46 O5 Na S	577.295818	-0.81796	-1.416883	10.5

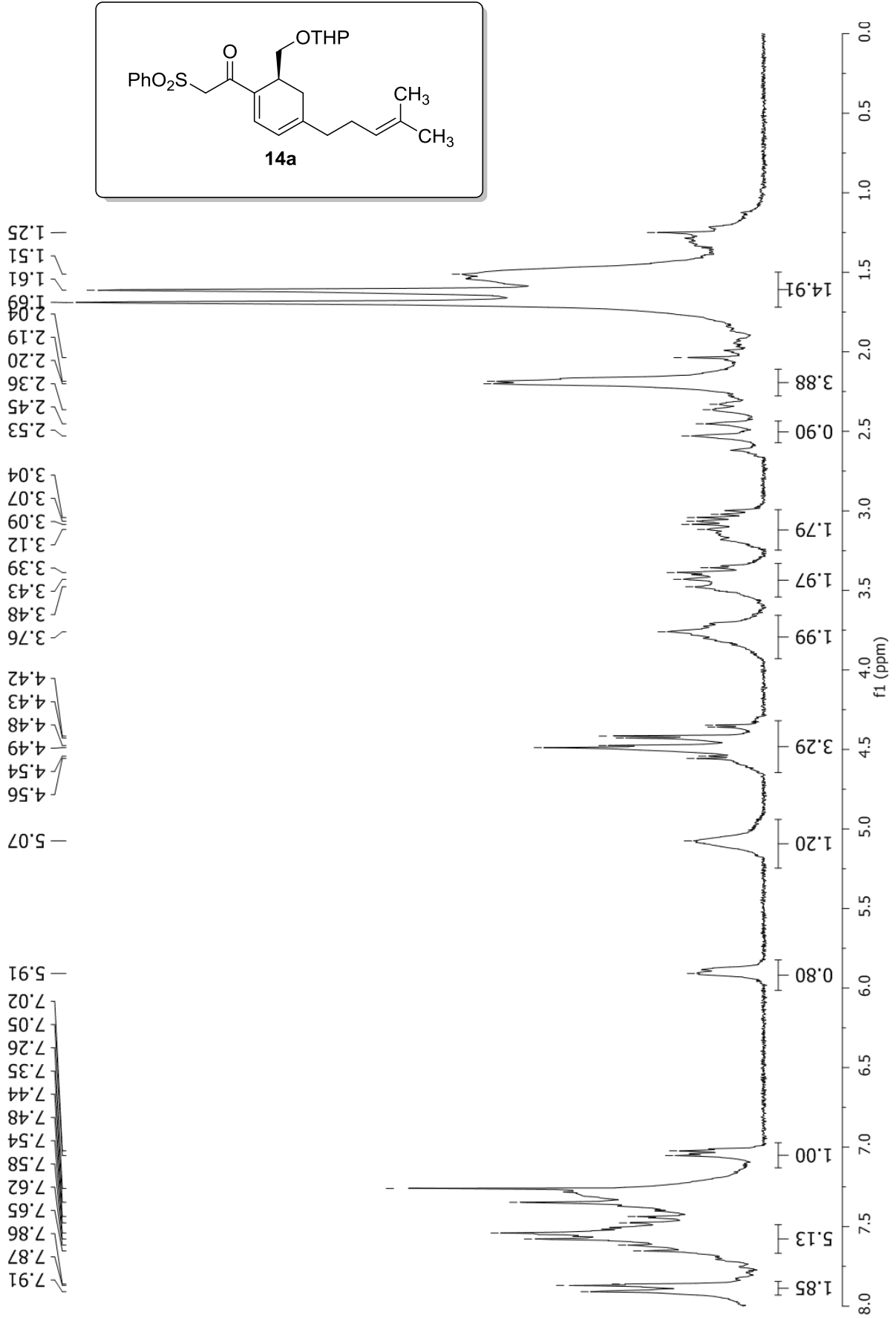


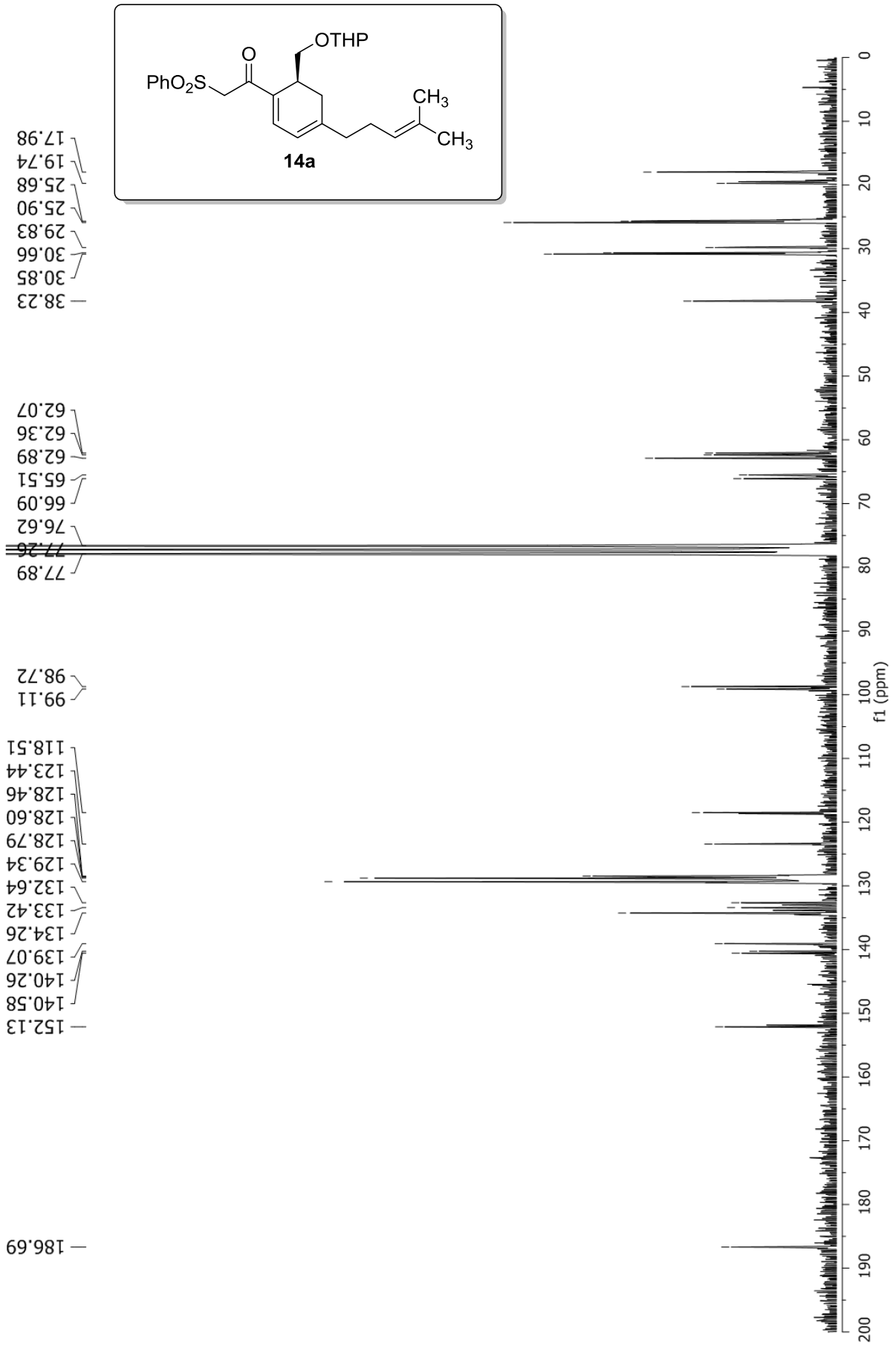
PeakTable

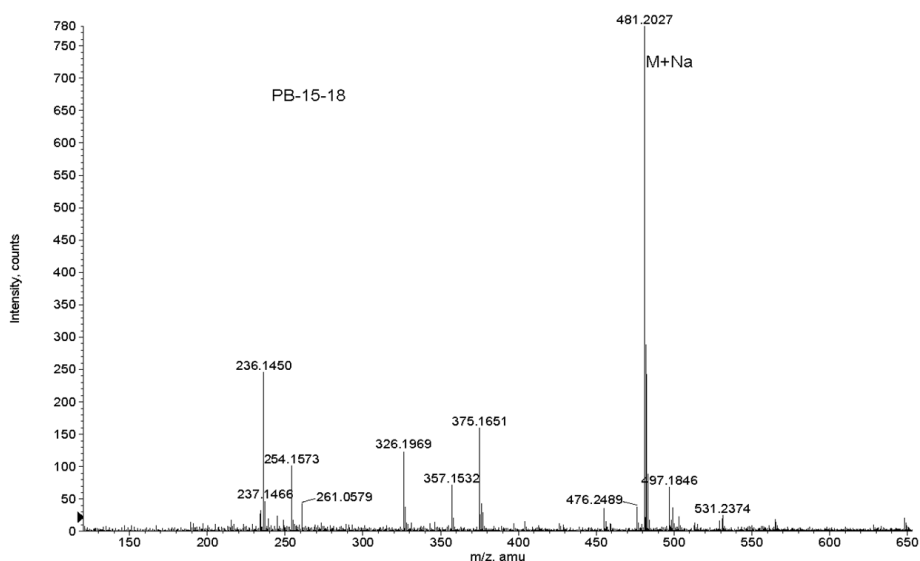
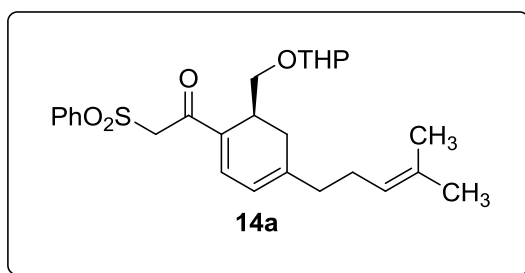
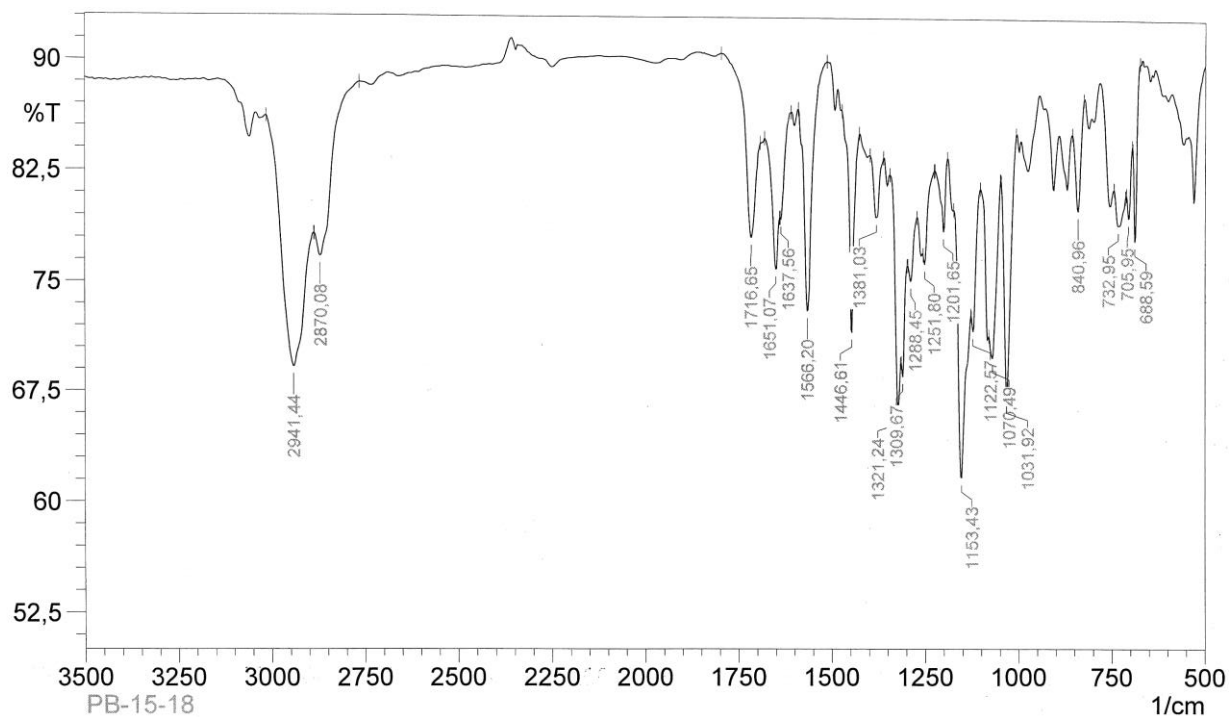
PDA Ch5 325nm 4nm

Peak#	Ret. Time	Area %
1	31.450	12.405
2	33.269	87.595
Total		100.000

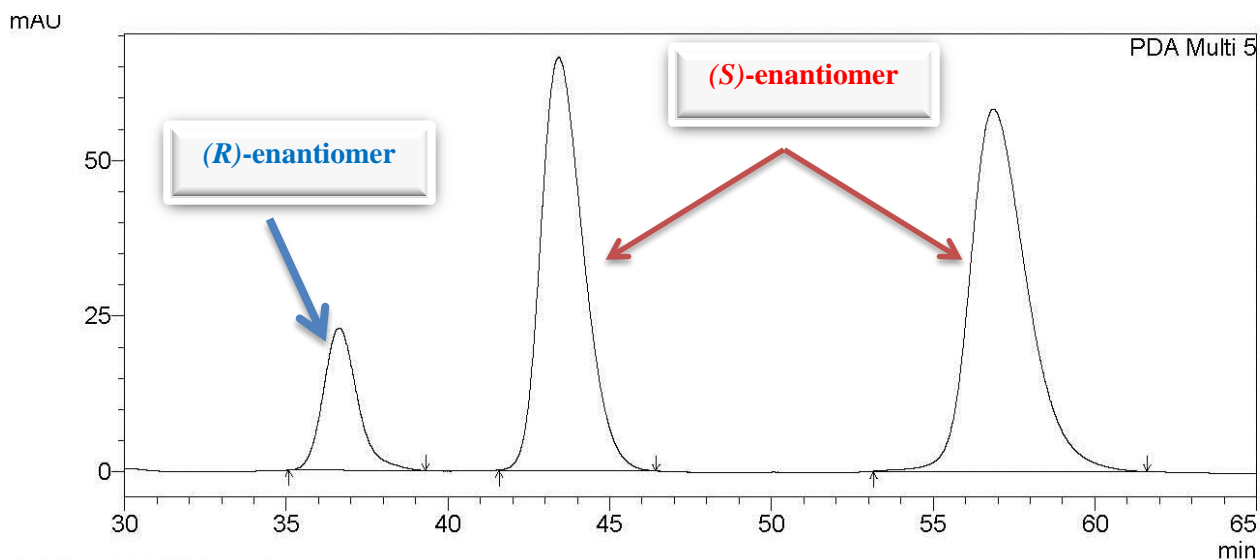






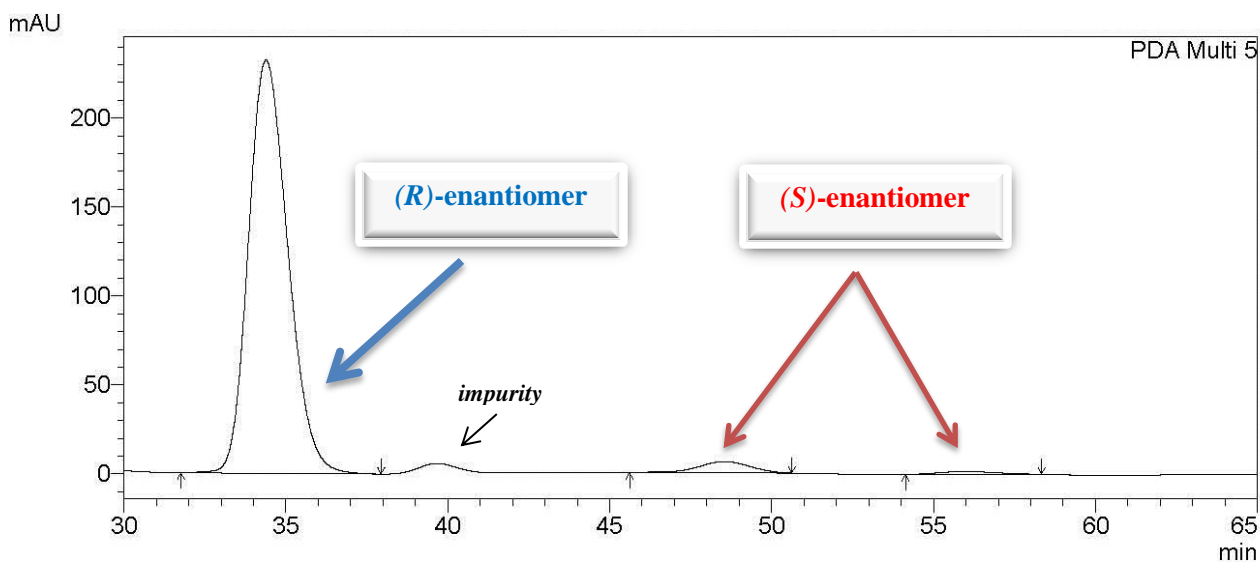
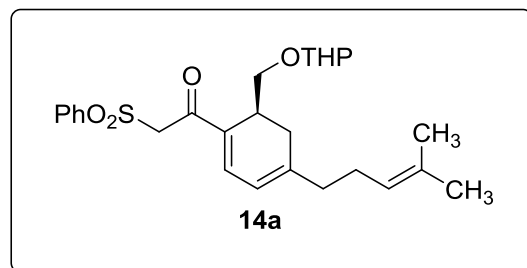


Formula	CalculatedMass	mDaError	ppmError	RDB
C32 H25 N4 O	481.202288	0.411908	0.855996	22.5
C27 H30 N4 O Na S	481.203255	-0.554792	-1.152927	14.5
C26 H34 O5 Na S	481.201917	0.78252	1.626174	9.5



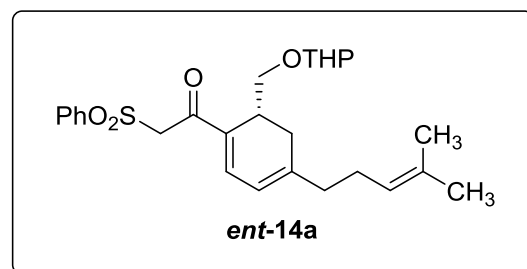
PeakTable
PDA Ch5 325nm 4nm

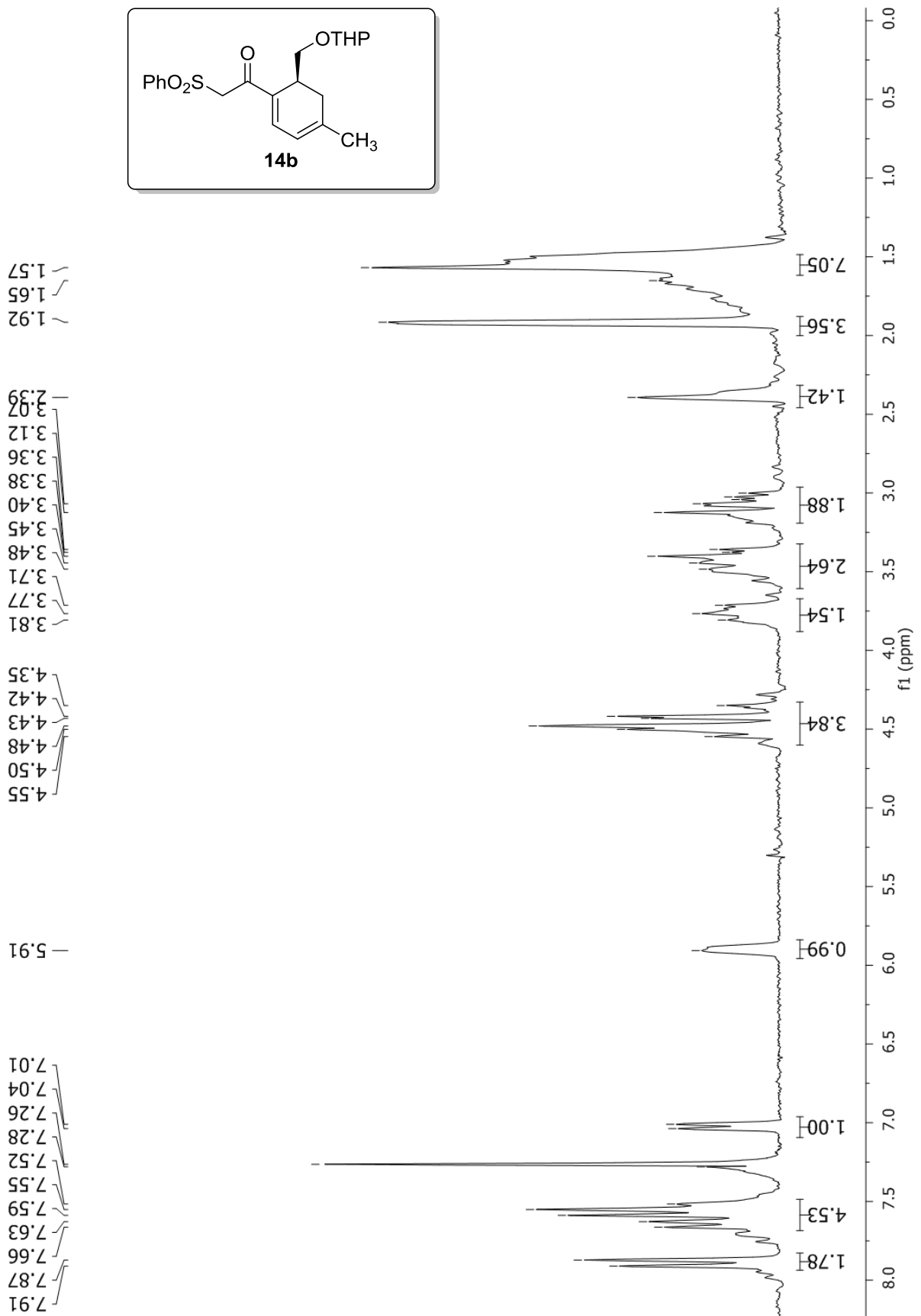
Peak#	Ret. Time	Area %
1	36.632	4.841
2	43.413	43.792
3	56.852	51.366
Total		100.000

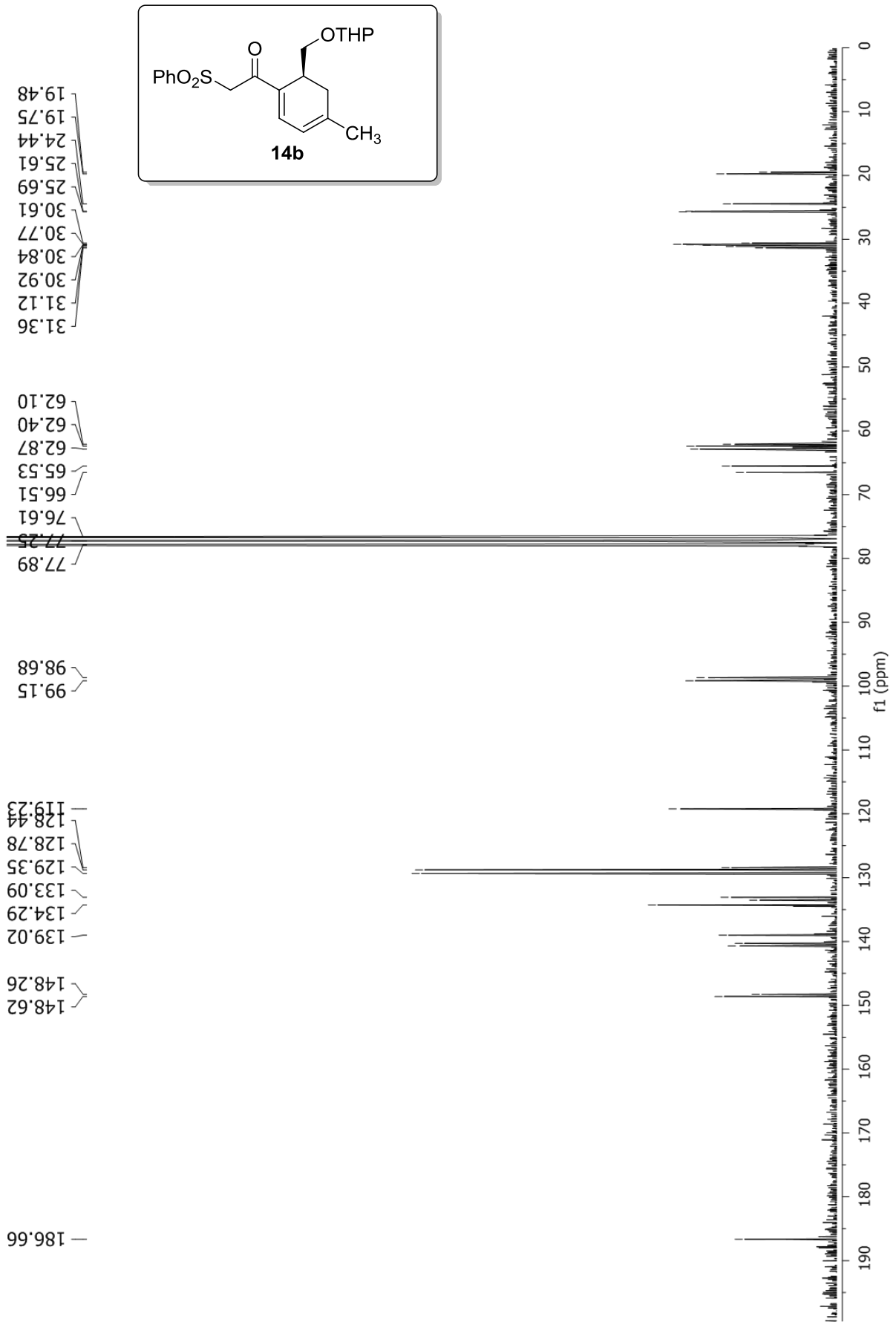


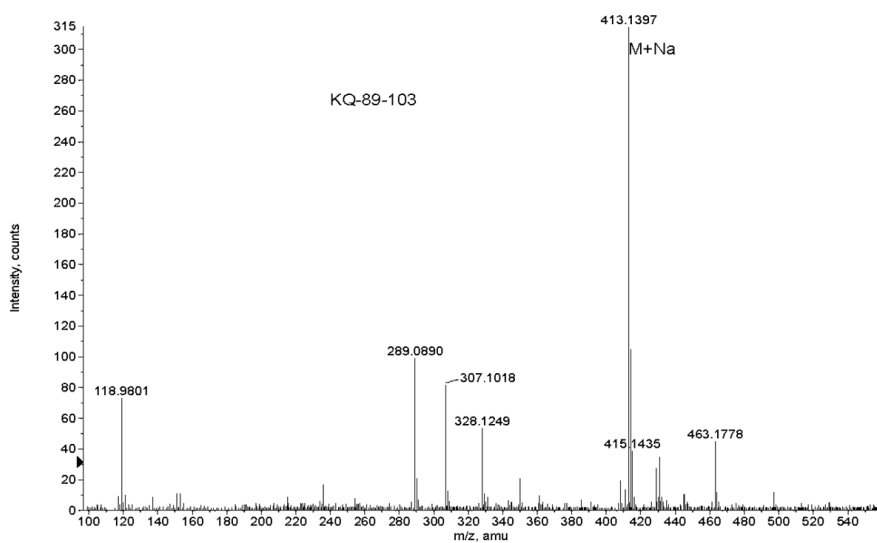
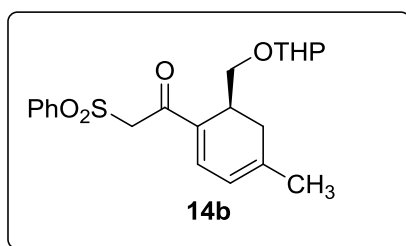
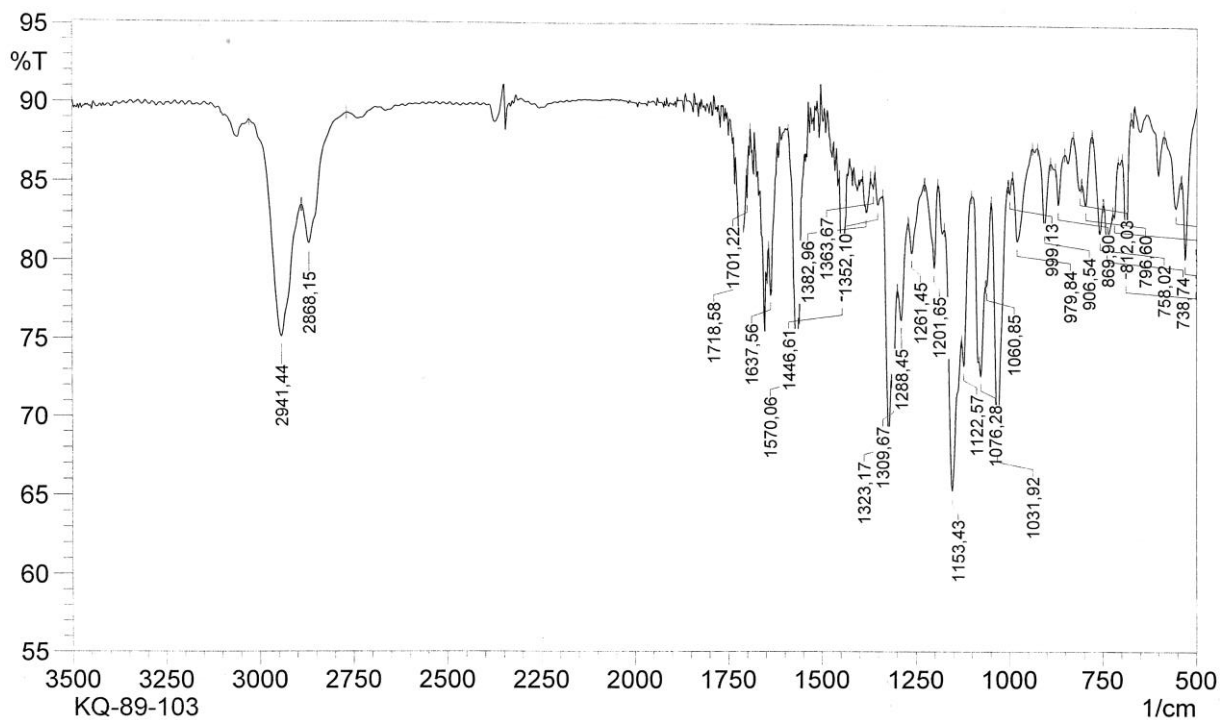
PeakTable
PDA Ch5 325nm 4nm

Peak#	Ret. Time	Area %
1	34.384	95.616
2	48.558	3.427
3	55.995	0.957
Total		100.000

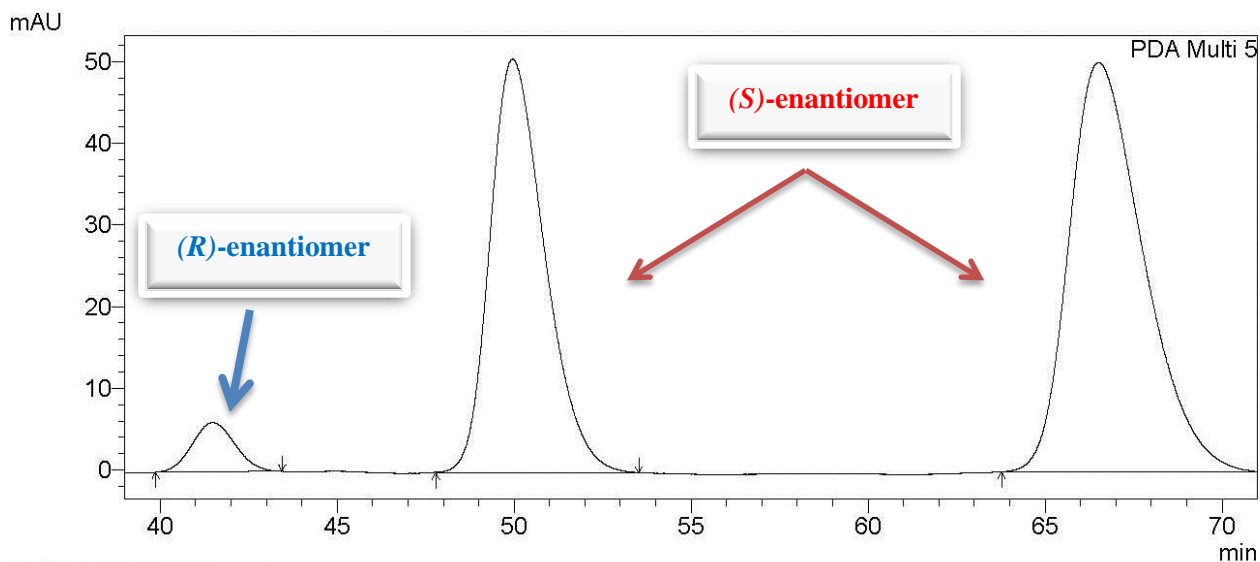








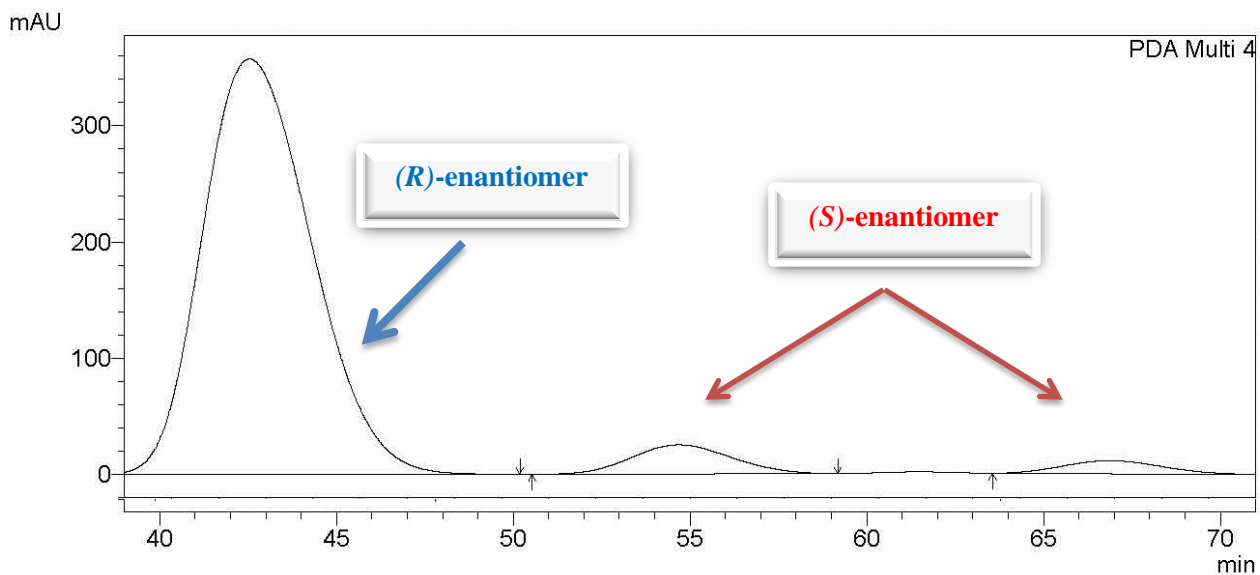
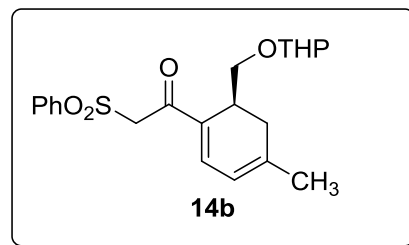
Formula	CalculatedMass	mDaError	ppmError	RDB
C27 H17 N4 O	413.139688	0.012228	0.029598	21.5
C21 H26 O5 Na S	413.139317	0.38284	0.926659	8.5



1 PDA Multi 5/325nm 4nm

PeakTable
PDA Ch5 325nm 4nm

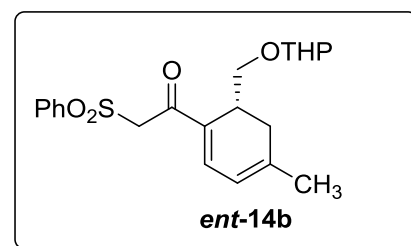
Peak#	Ret. Time	Area %
1	41.480	3.813
2	49.950	41.129
3	66.505	55.058
Total		100.000

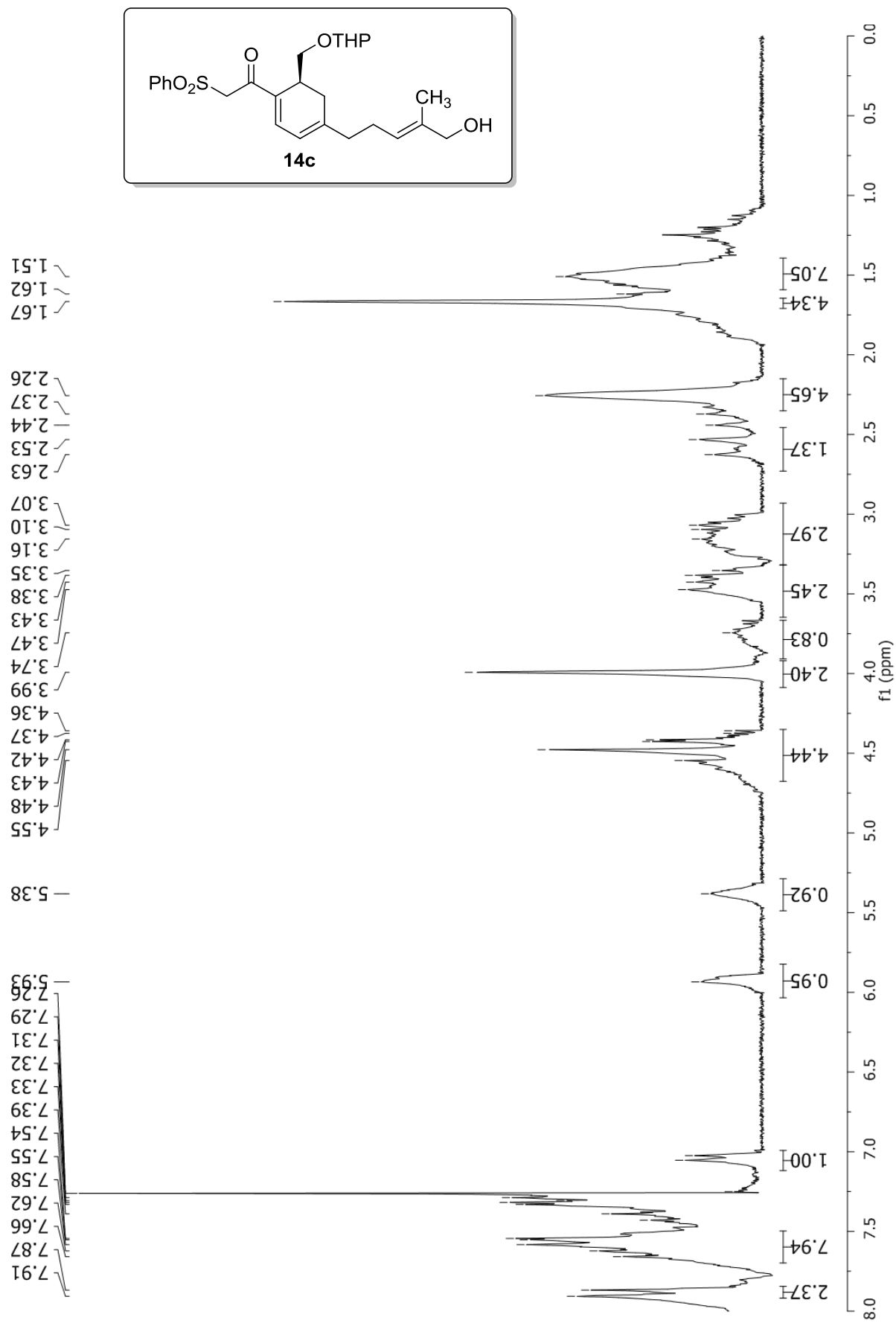


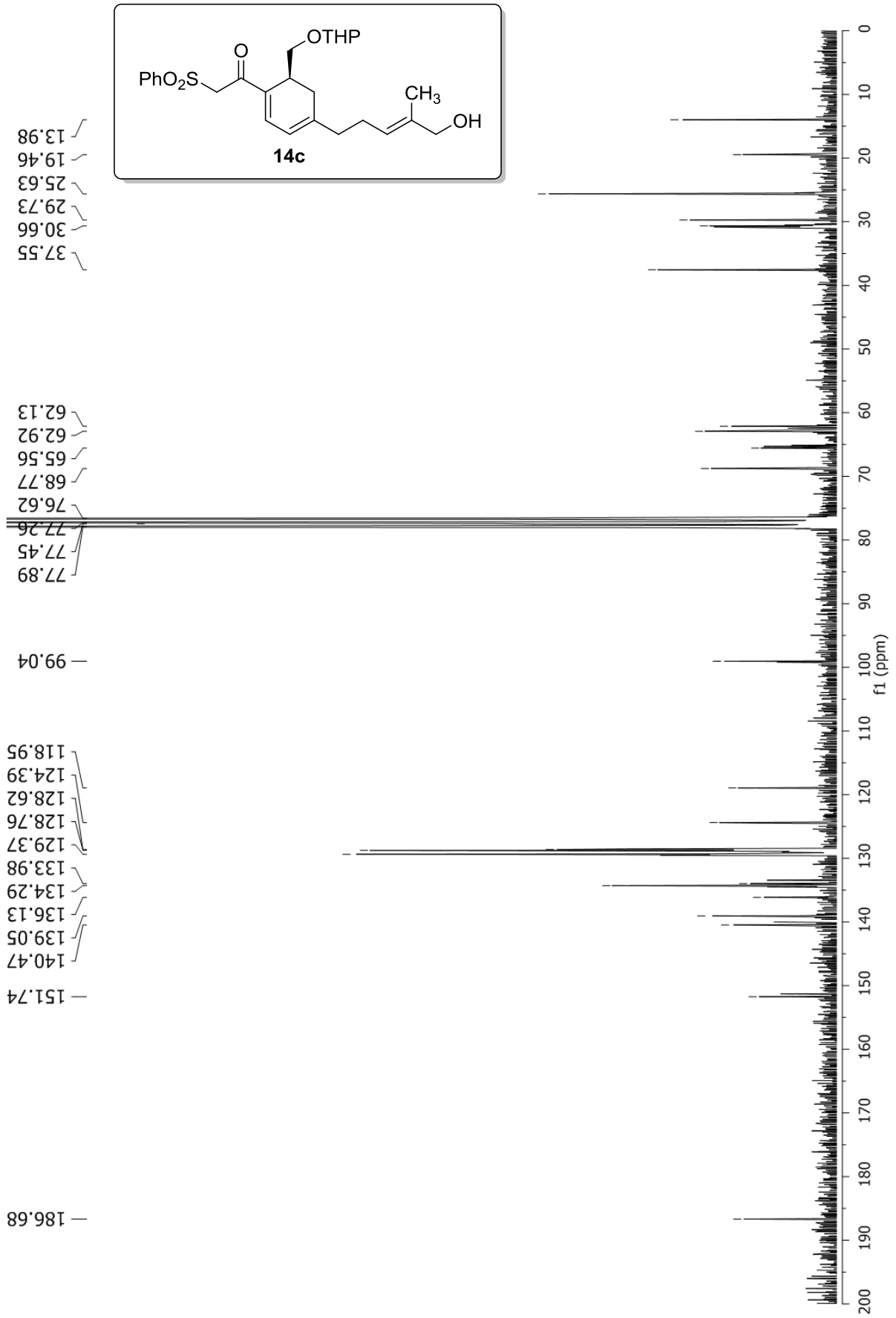
1 PDA Multi 5/325nm 4nm

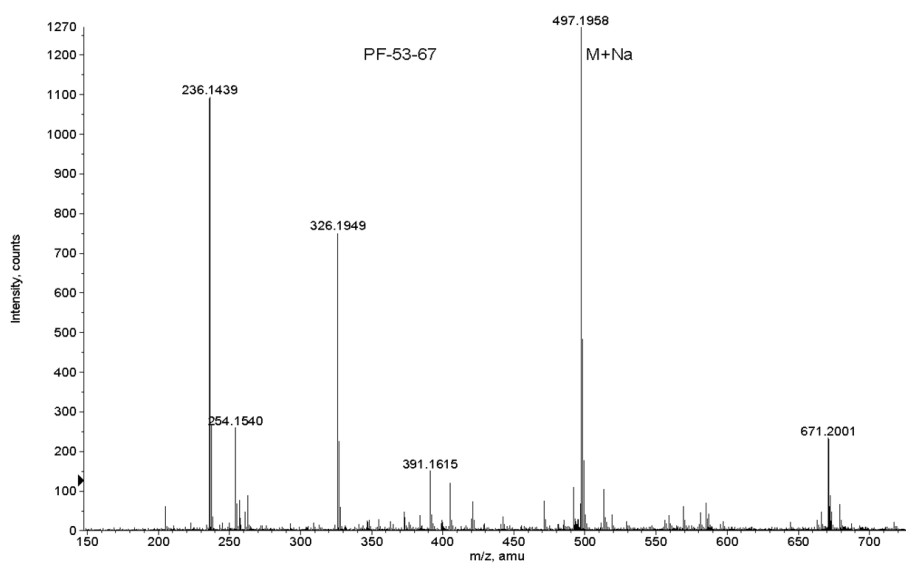
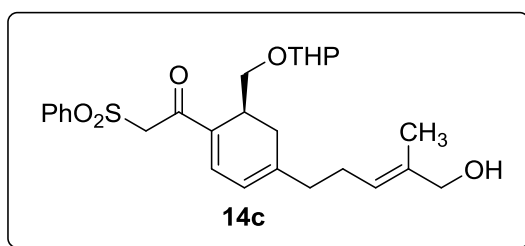
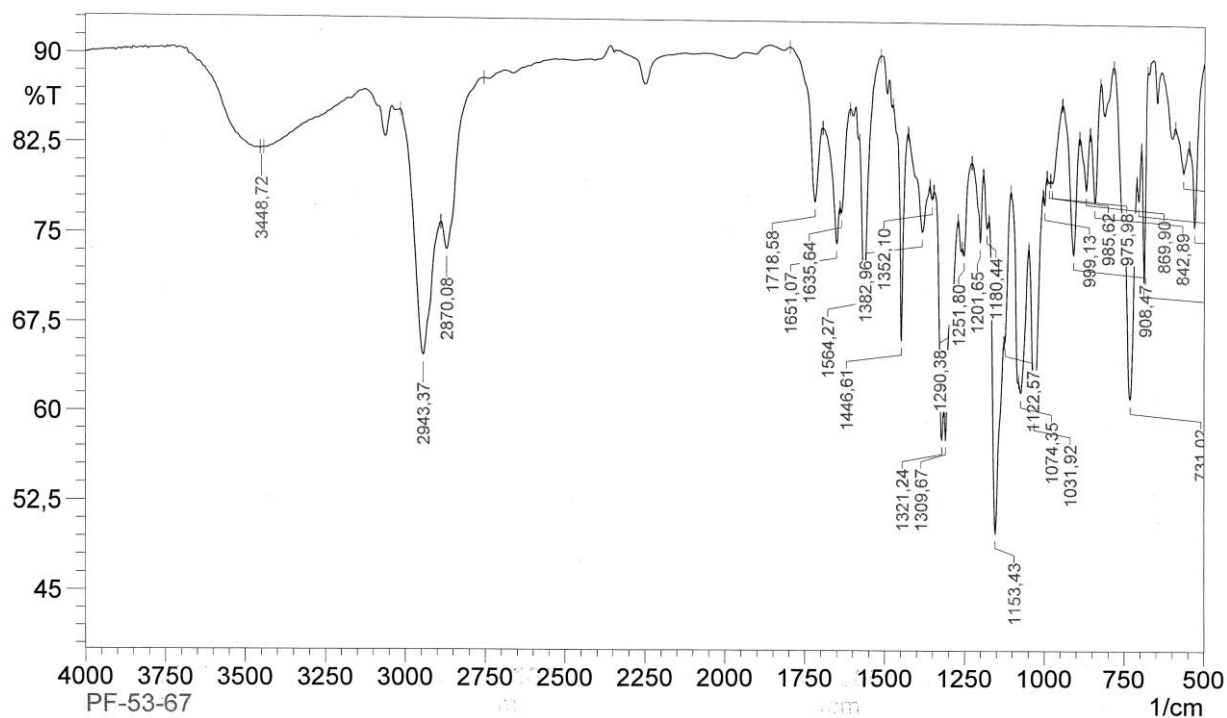
PeakTable
PDA Ch4 325nm 4nm

Peak#	Ret. Time	Area %
1	41.664	95.981
2	54.227	3.235
3	66.505	0.784
Total		100.000

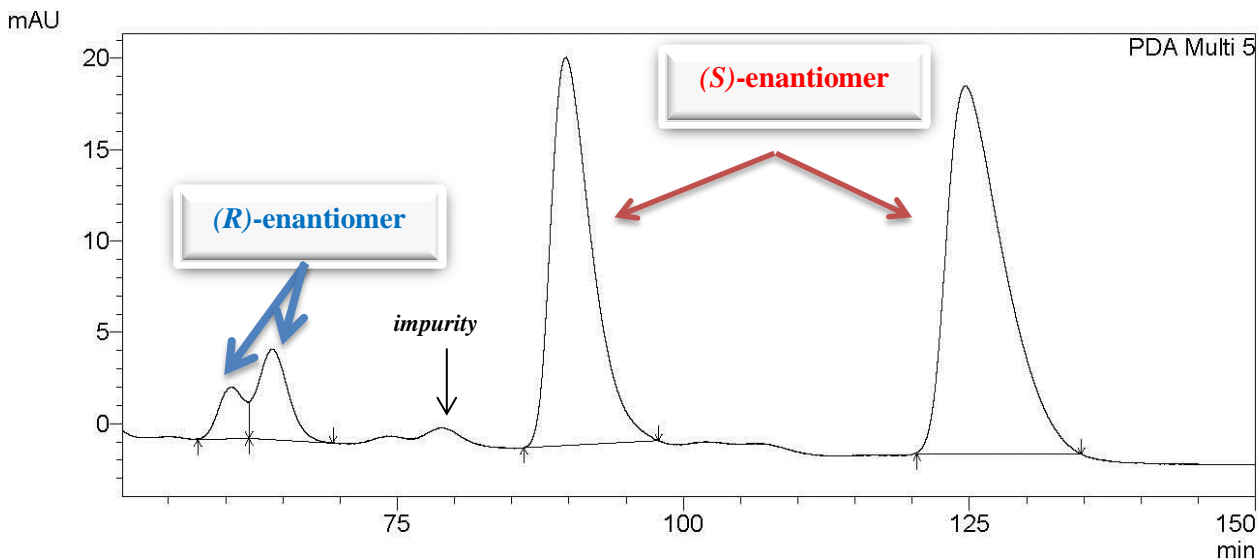








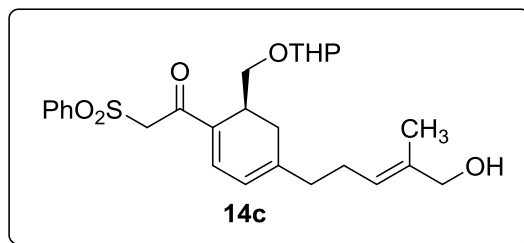
Formula	CalculatedMass	mDaError	ppmError	RDB
C31 H29 O6	497.195865	-0.06542	-0.131578	17.5
C23 H33 N2 O8 S	497.195215	0.585324	1.177249	8.5
C30 H26 N4 O2 Na	497.194797	1.002528	2.016362	19.5
C26 H34 O6 Na S	497.196832	-1.03212	-2.07588	9.5

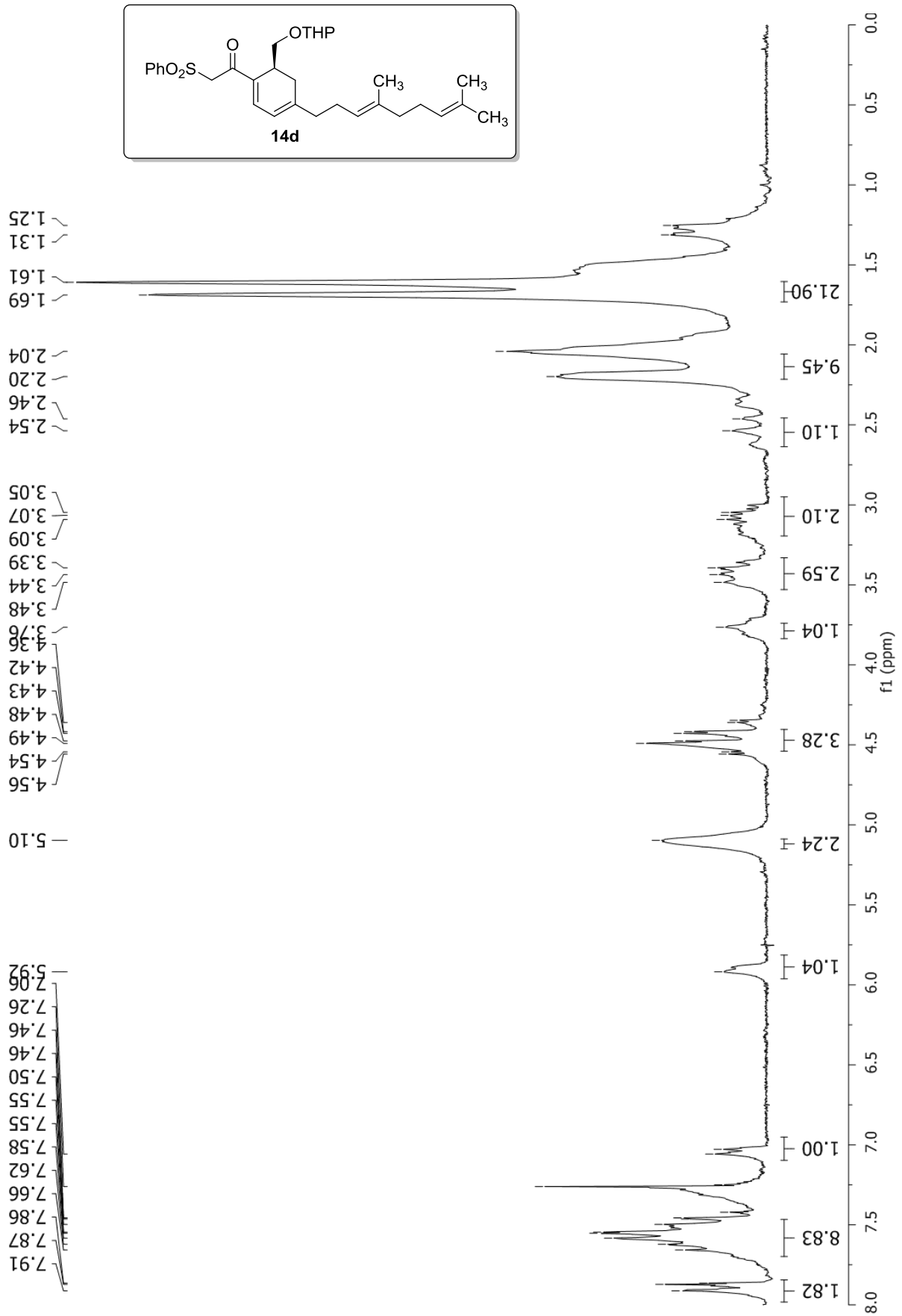


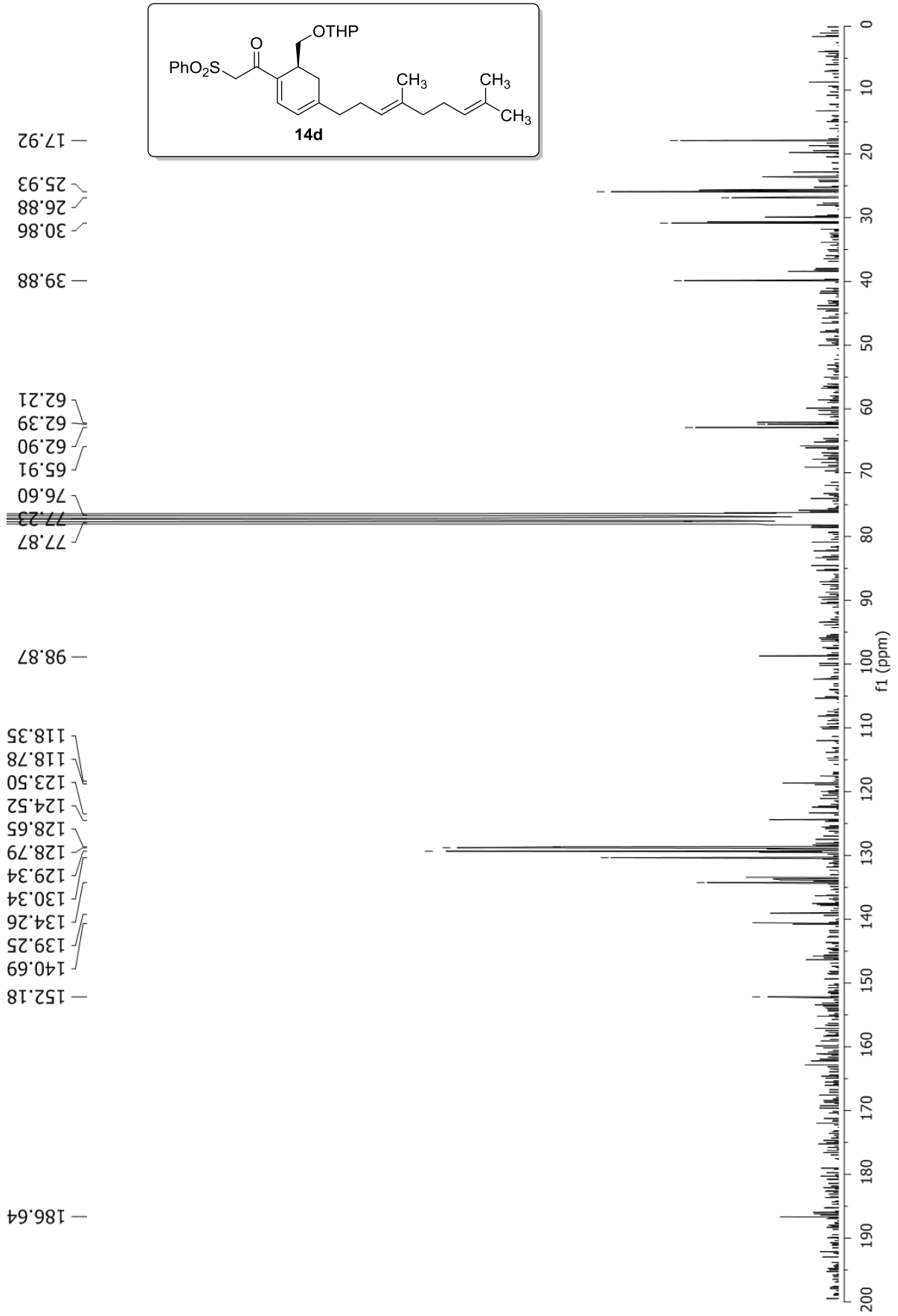
1 PDA Multi 5/360nm 4nm

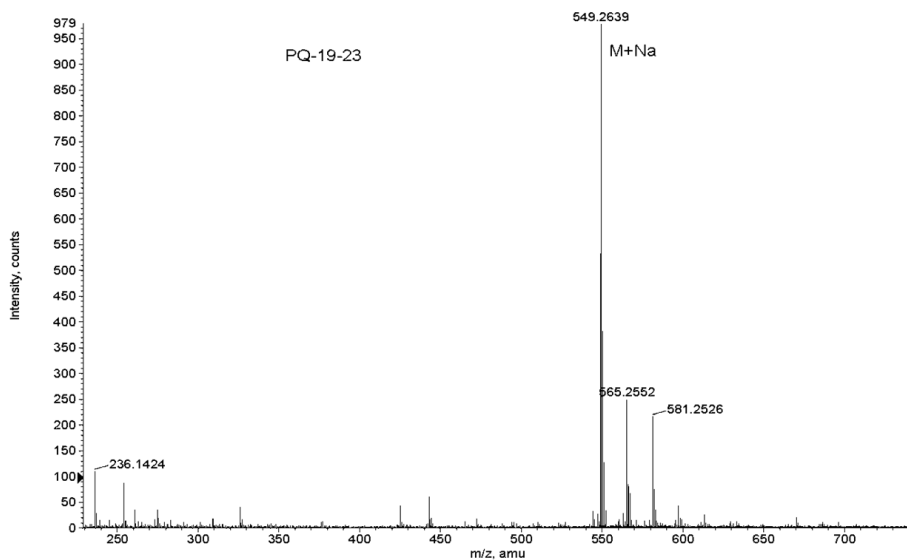
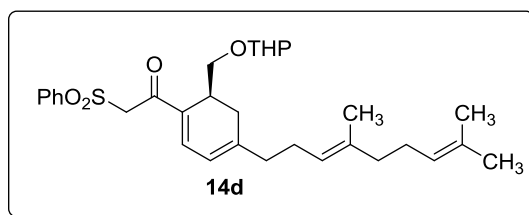
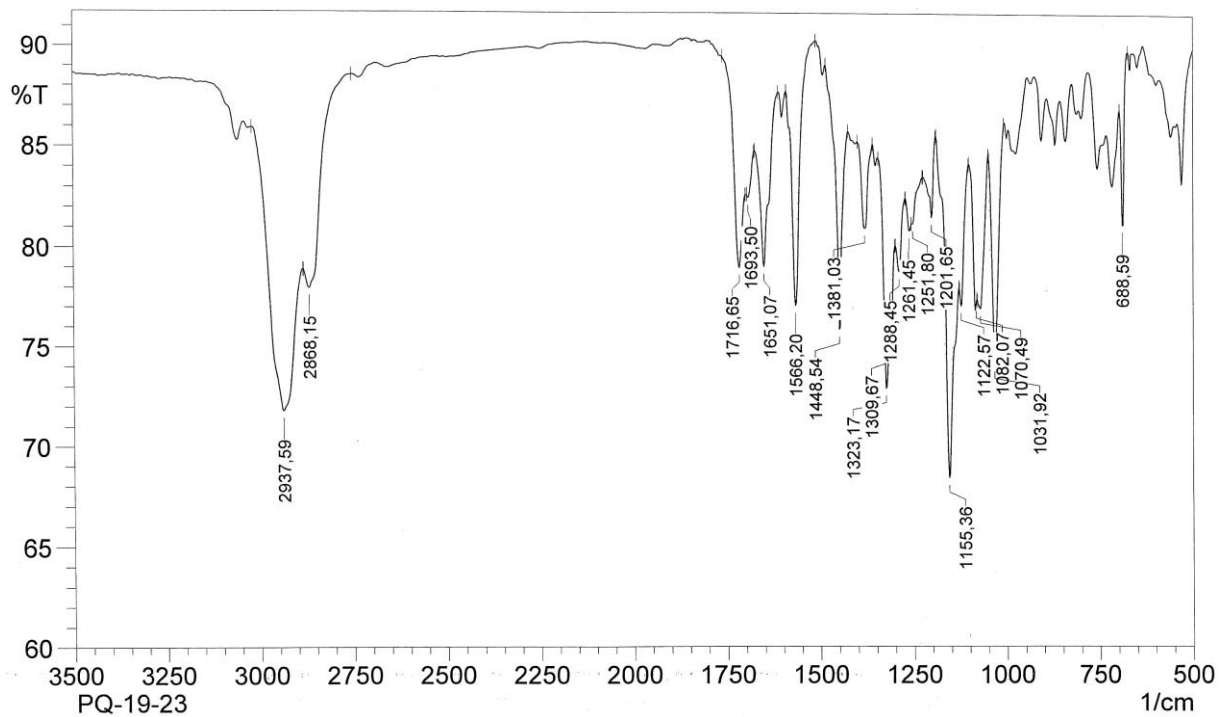
PeakTable
PDA Ch5 360nm 4nm

Peak#	Ret. Time	Area %
1	60.398	3.276
2	64.045	6.704
3	89.756	38.586
4	124.625	51.435
Total		100.000

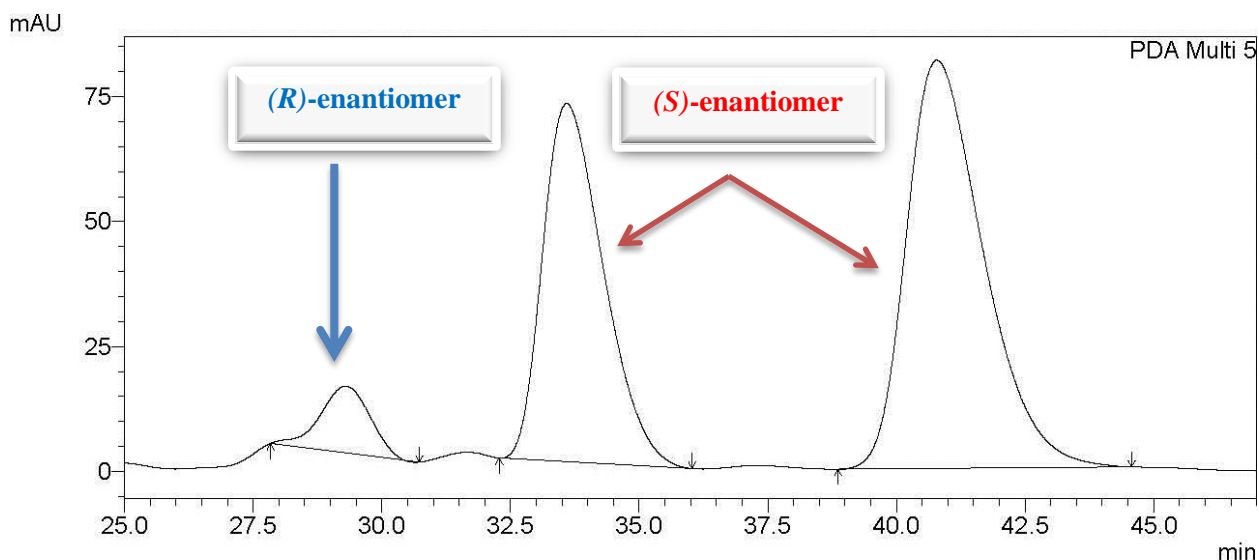








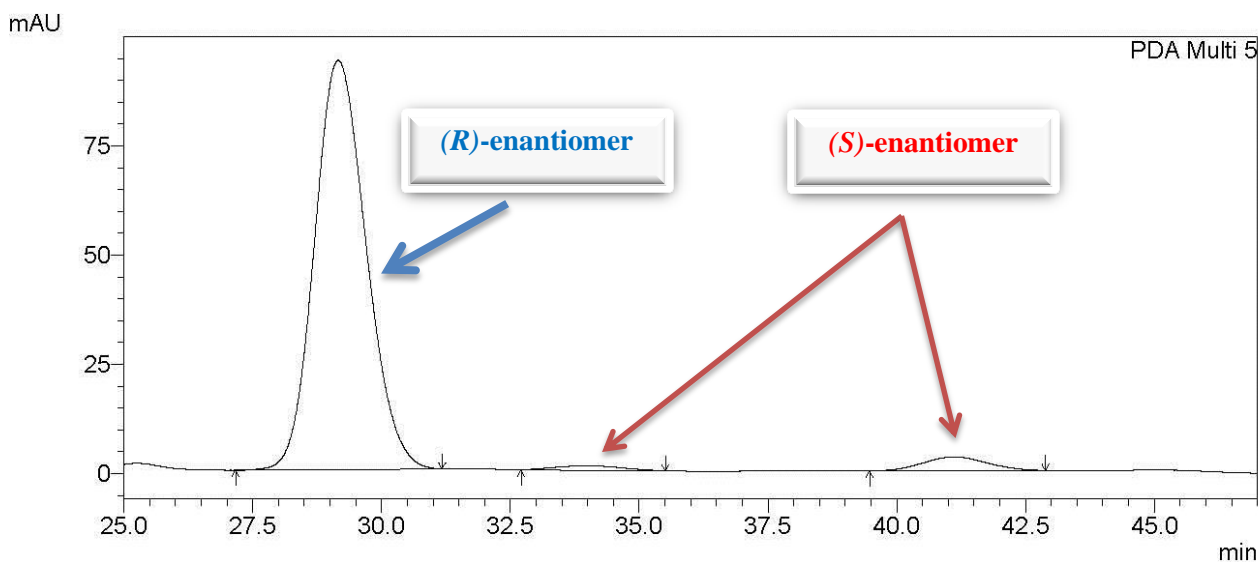
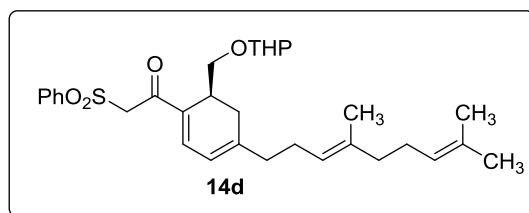
Formula	CalculatedMass	mDaError	ppmError	RDB
$\text{C}_{36}\text{H}_{37}\text{O}_5$	549.263551	0.3489	0.635213	18.5
$\text{C}_{31}\text{H}_{42}\text{O}_5\text{Na S}$	549.264518	-0.6178	-1.124777	10.5



1 PDA Multi 5/360nm 4nm

PeakTable
PDA Ch5 360nm 4nm

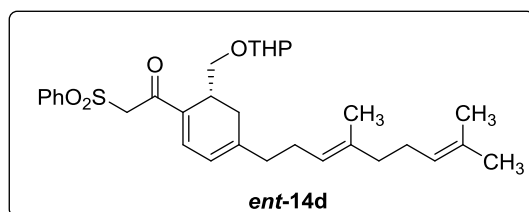
Peak#	Ret. Time	Area %
1	29.284	5.159
2	33.589	38.762
3	40.781	56.079
Total		100.000

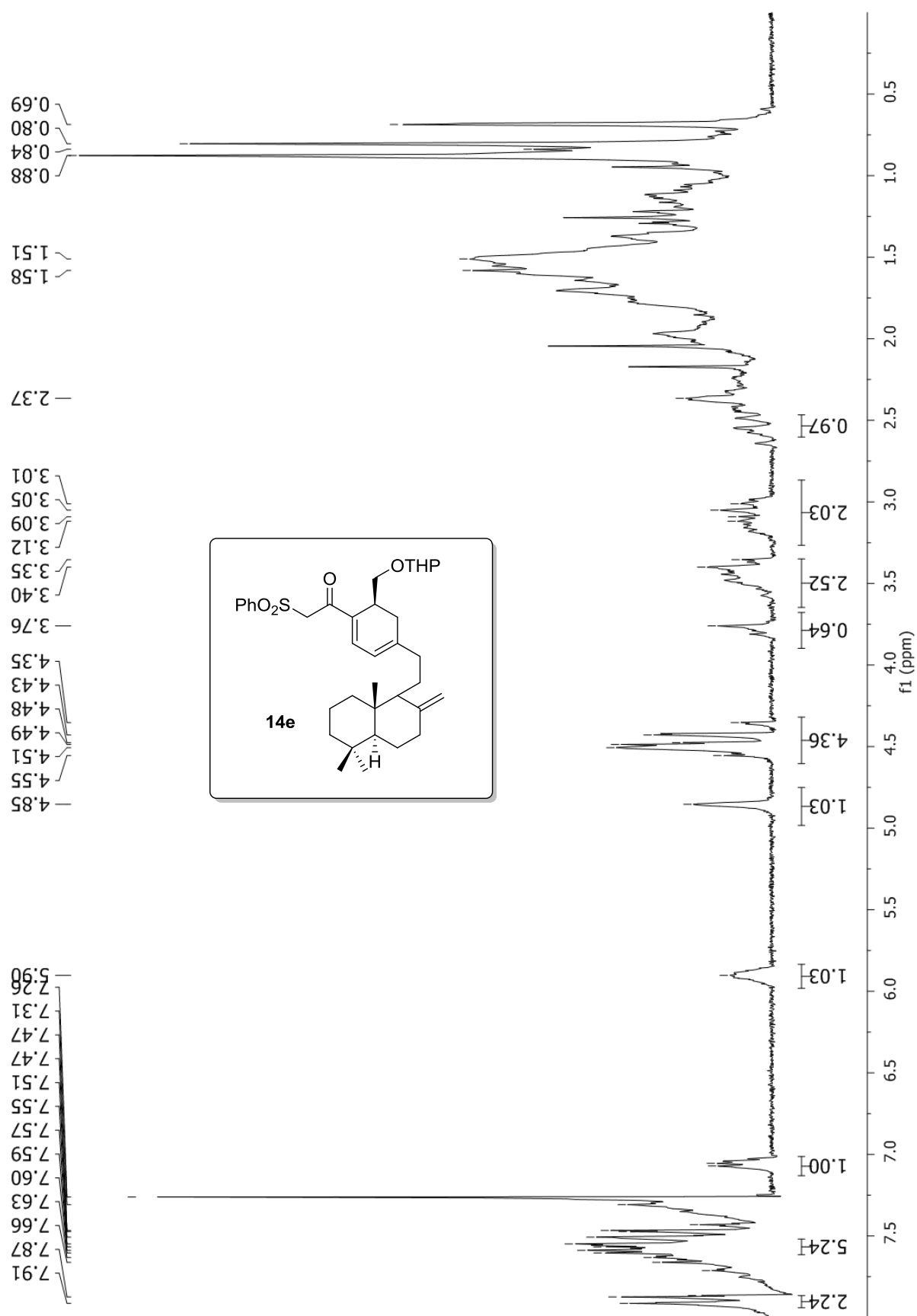


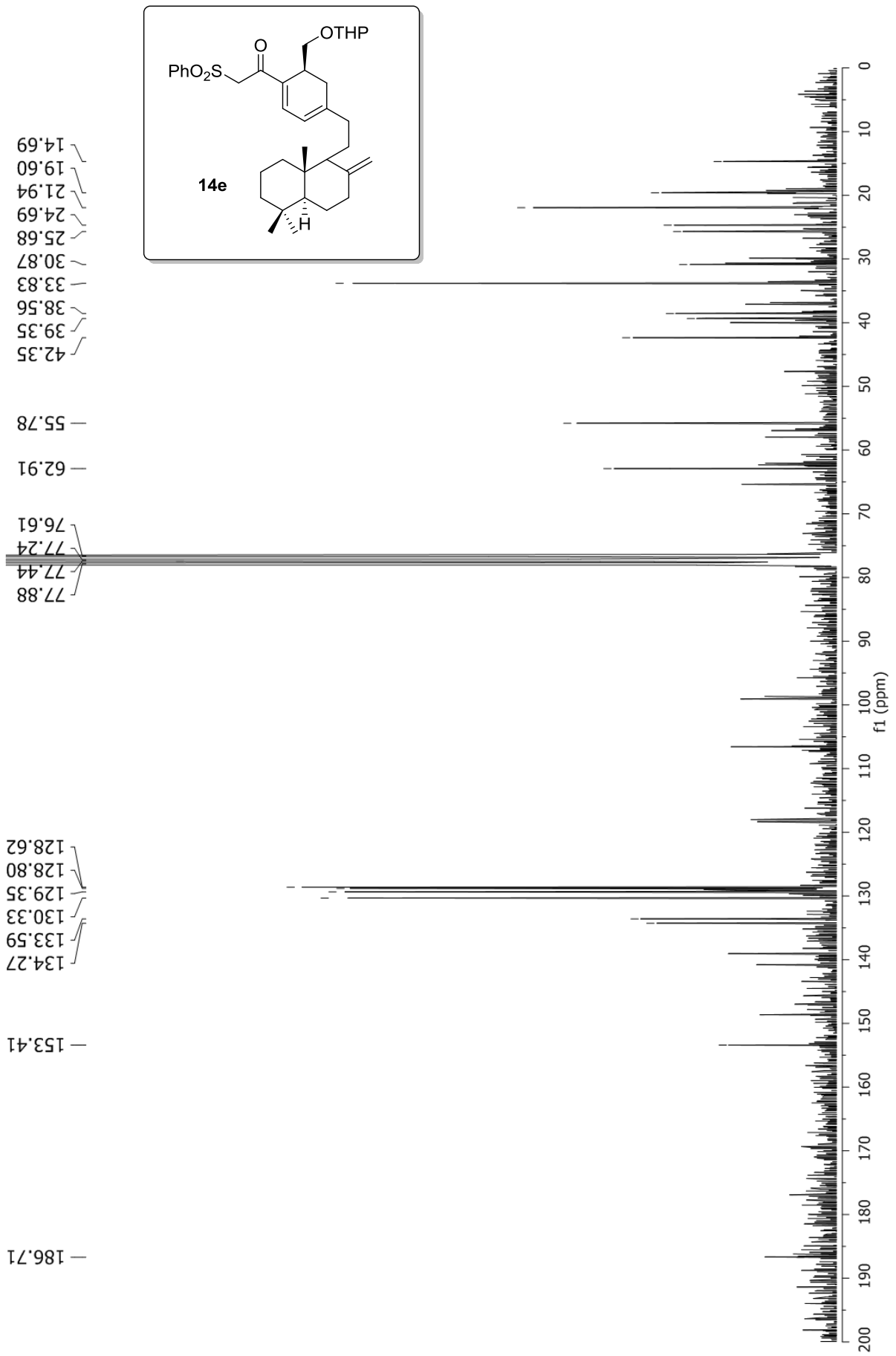
1 PDA Multi 5/360nm 4nm

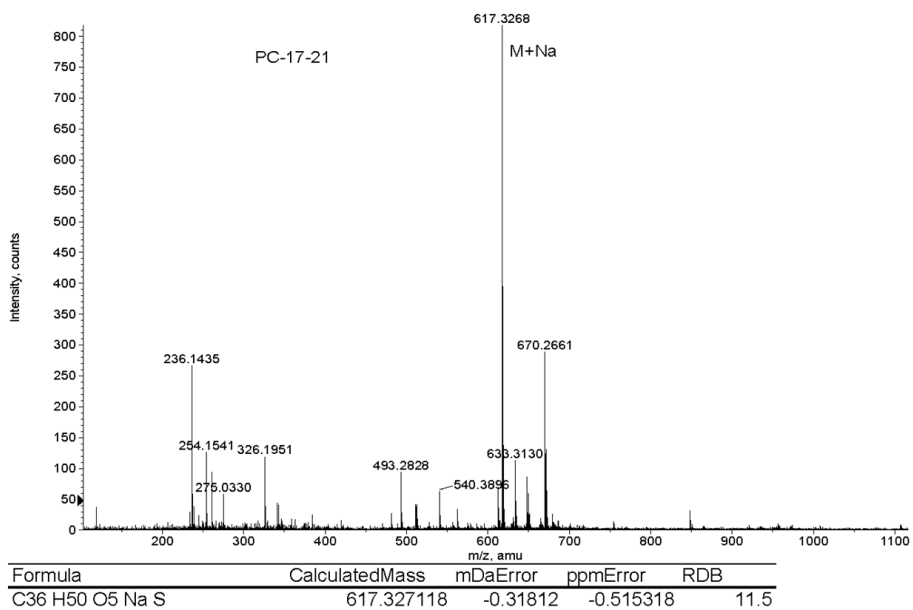
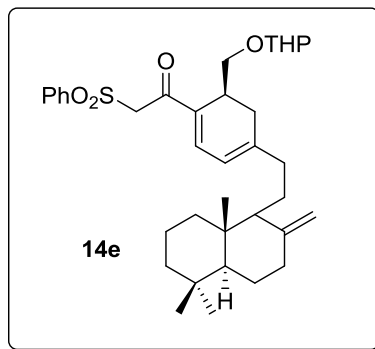
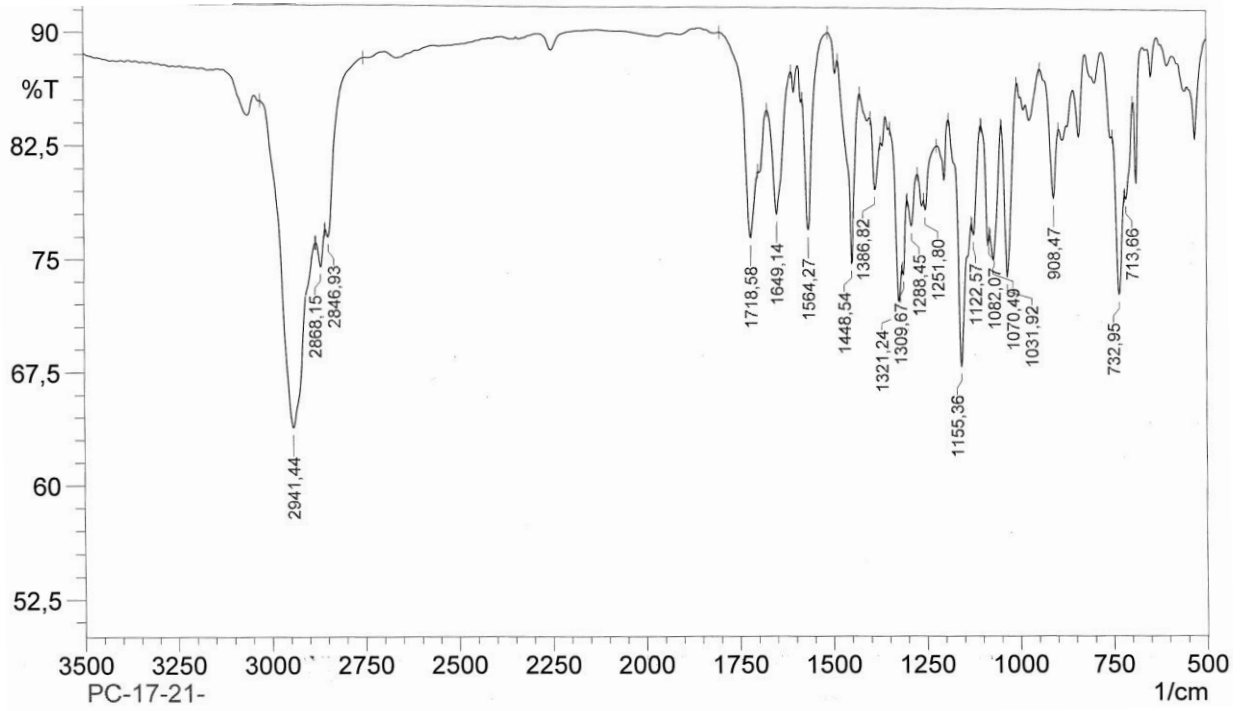
PeakTable
PDA Ch5 360nm 4nm

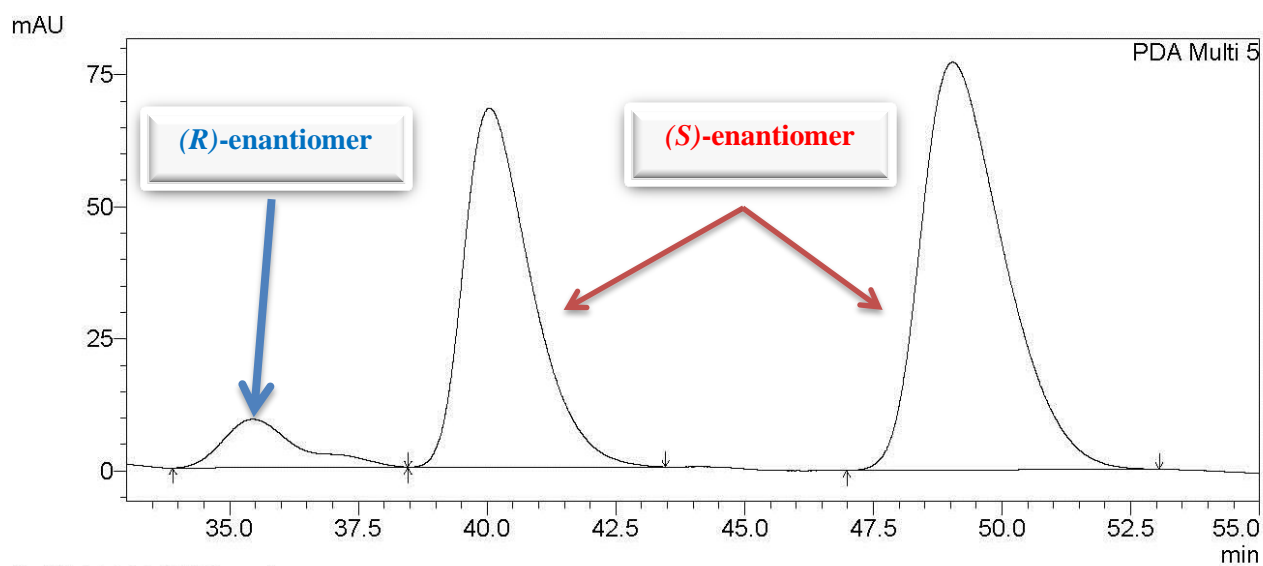
Peak#	Ret. Time	Area %
1	29.155	94.550
2	33.973	1.407
3	41.092	4.043
Total		100.000









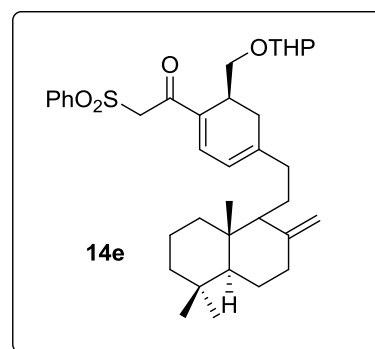


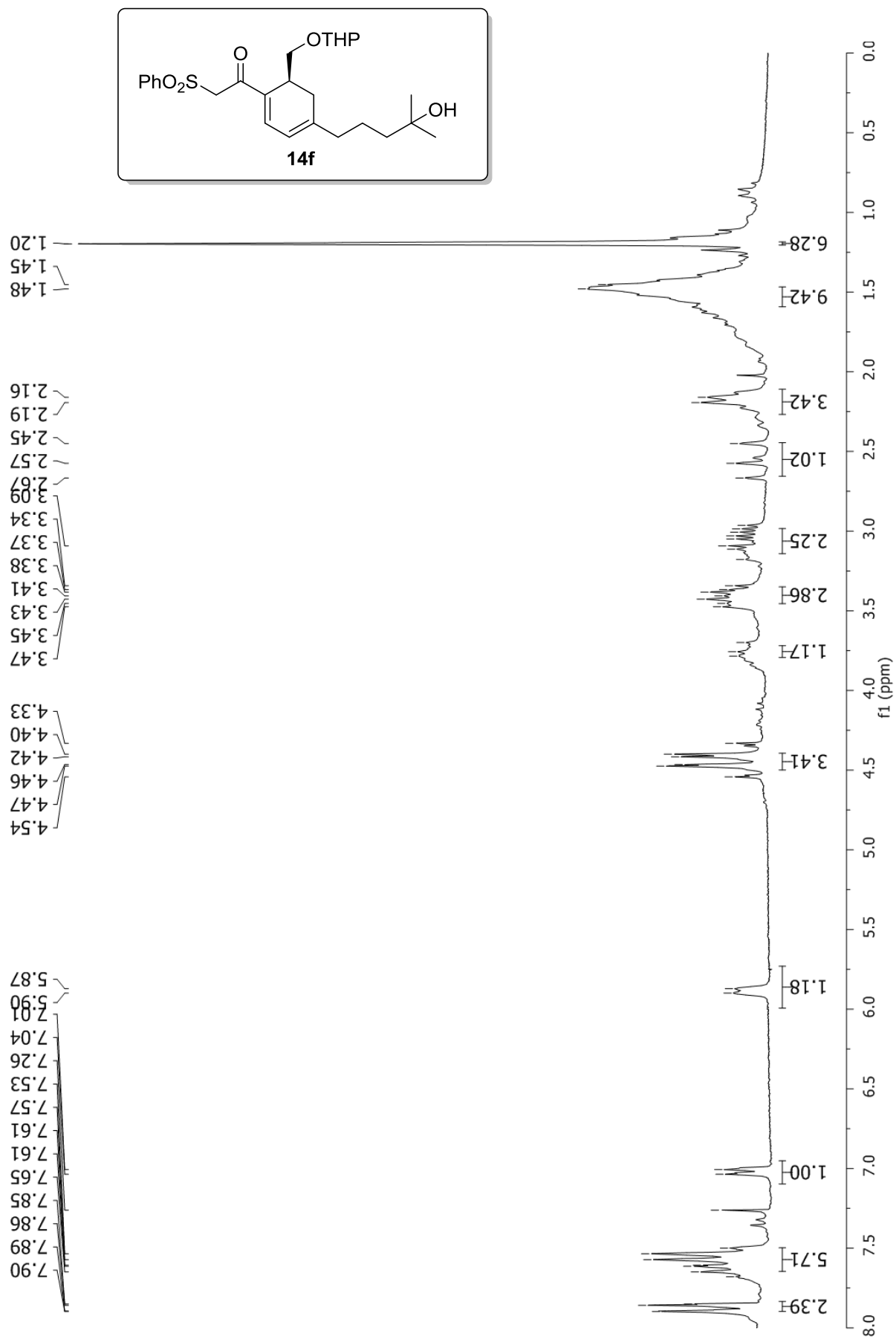
1 PDA Multi 5/360nm 4nm

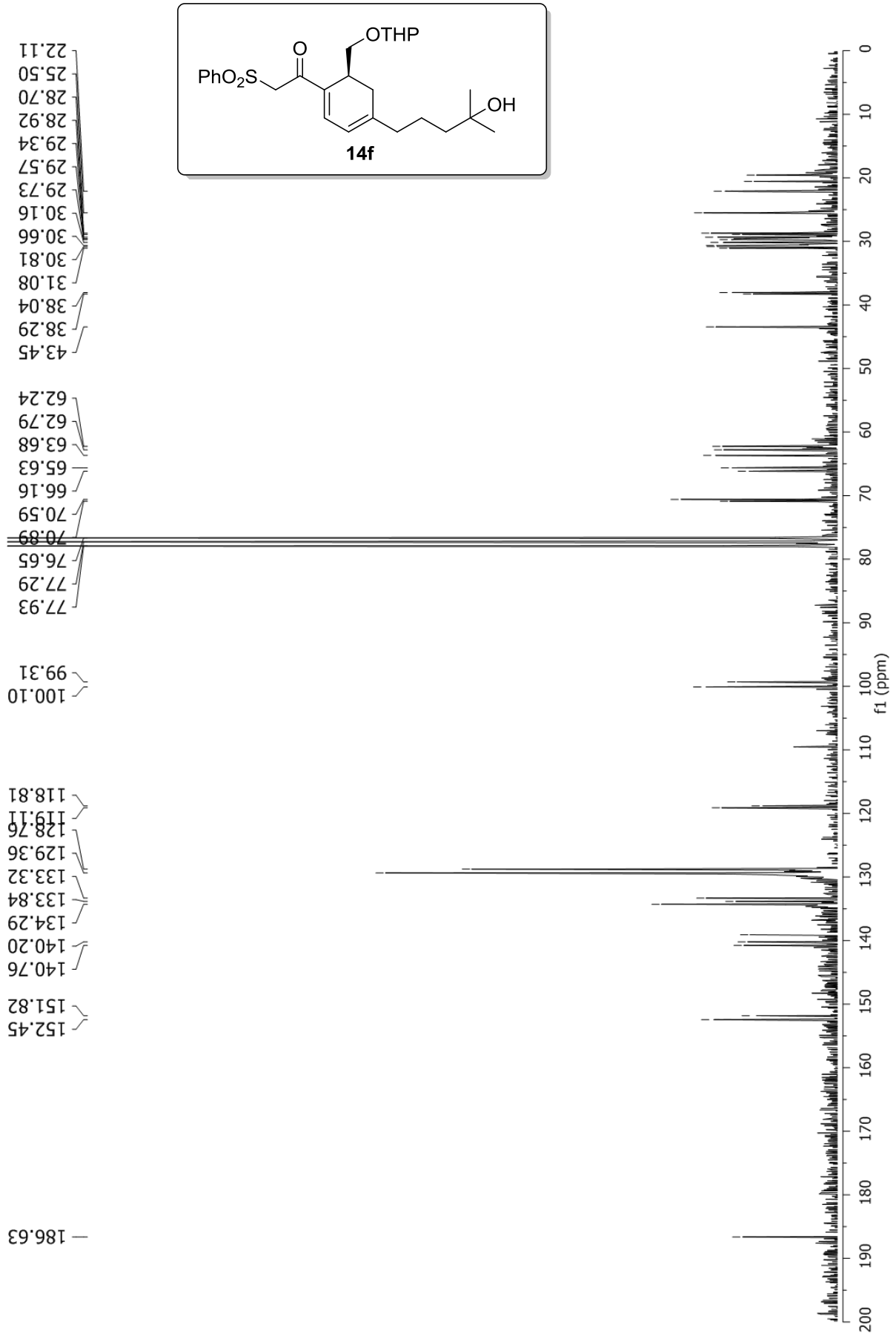
PeakTable

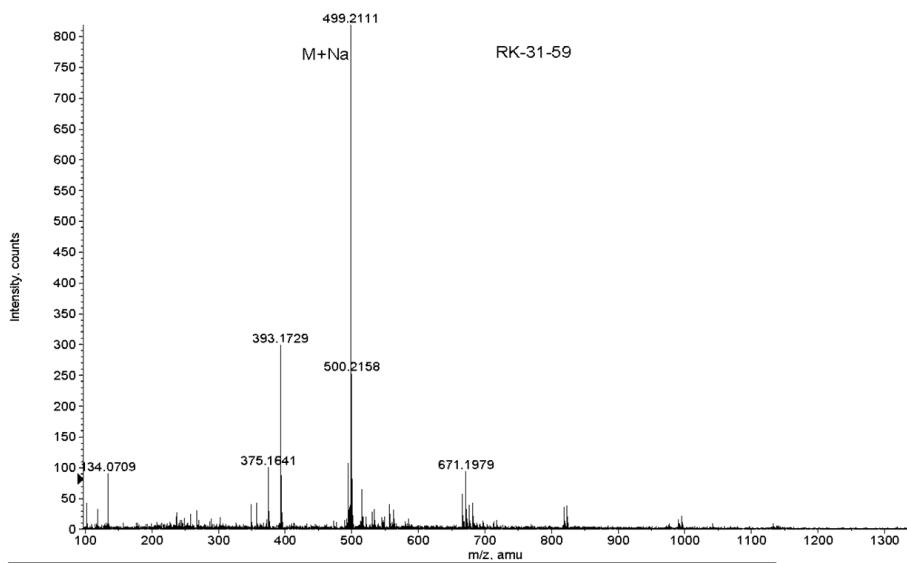
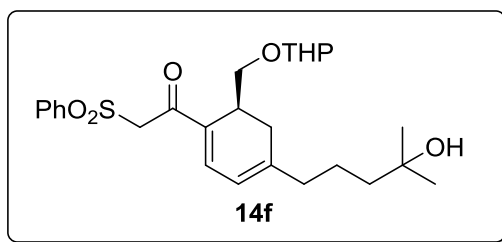
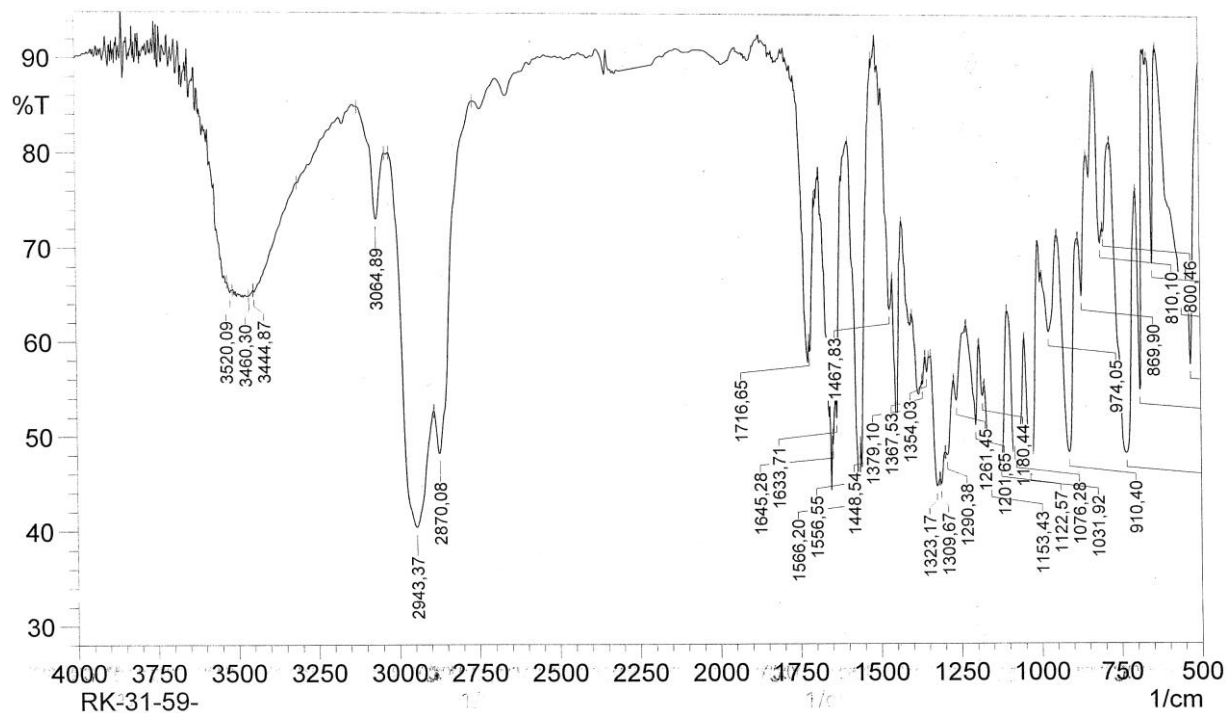
PDA Ch5 360nm 4nm

Peak#	Ret. Time	Area %
1	35.451	6.060
2	40.042	39.201
3	49.039	54.739
Total		100.000

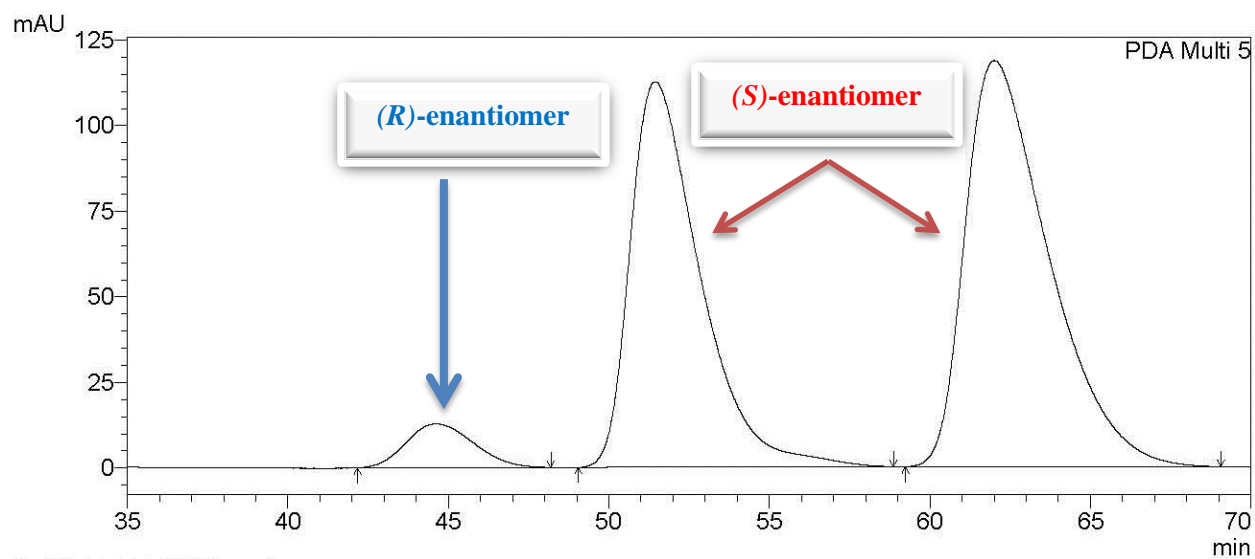








Formula	CalculatedMass	mDaError	ppmError	RDB
C23 H28 N10 Na S	499.211134	-0.03412	-0.068348	14.5
C23 H35 N2 O8 S	499.210865	0.235244	0.471231	7.5
C24 H31 N6 O4 S	499.212202	-1.102068	-2.207617	12.5
C22 H32 N6 O4 Na S	499.209797	1.303192	2.6105	9.5
C26 H36 O6 Na S	499.212482	-1.3822	-2.768766	8.5

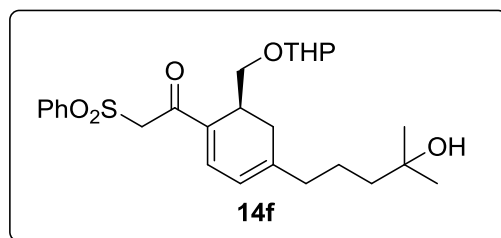


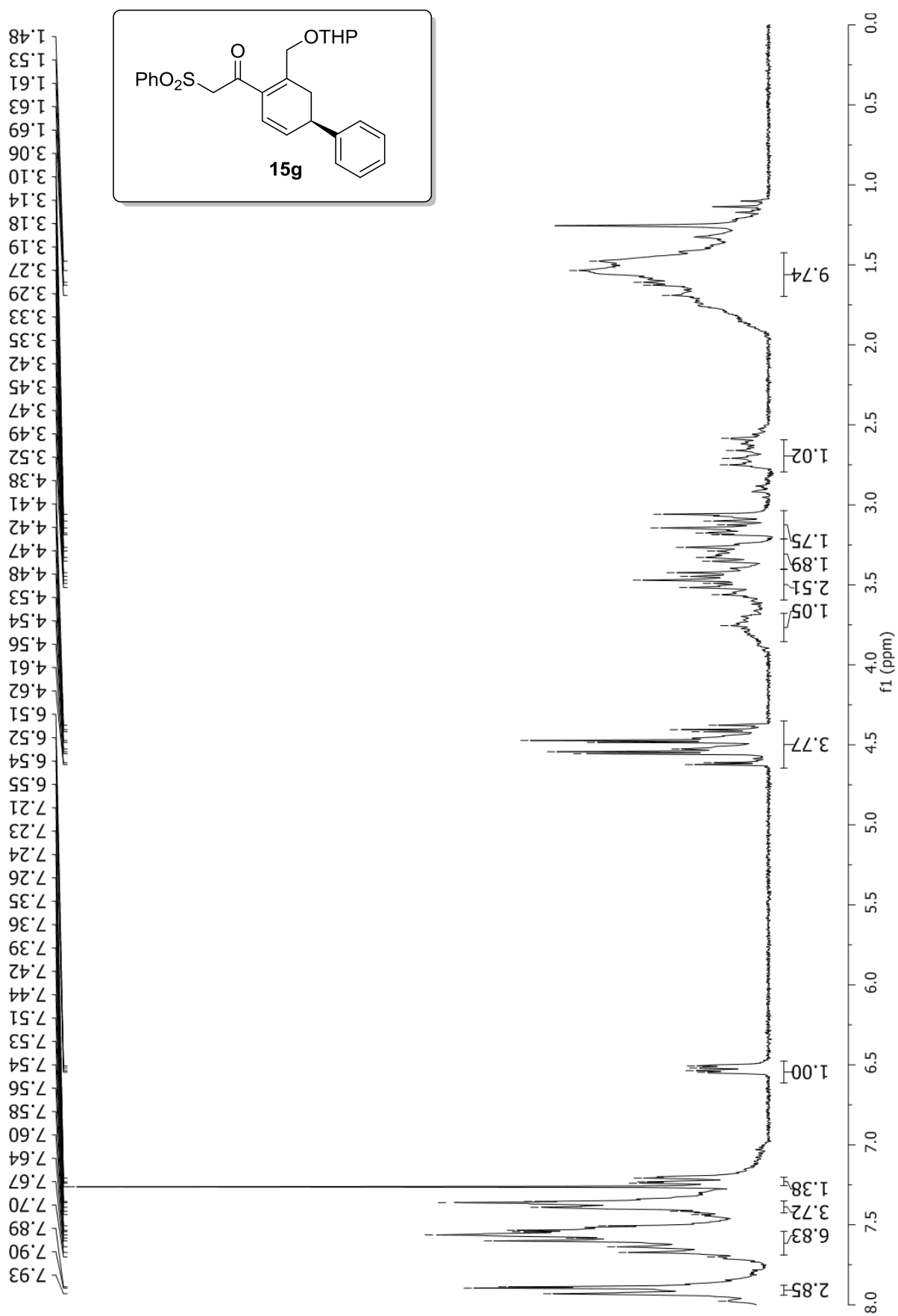
1 PDA Multi 5/350nm 4nm

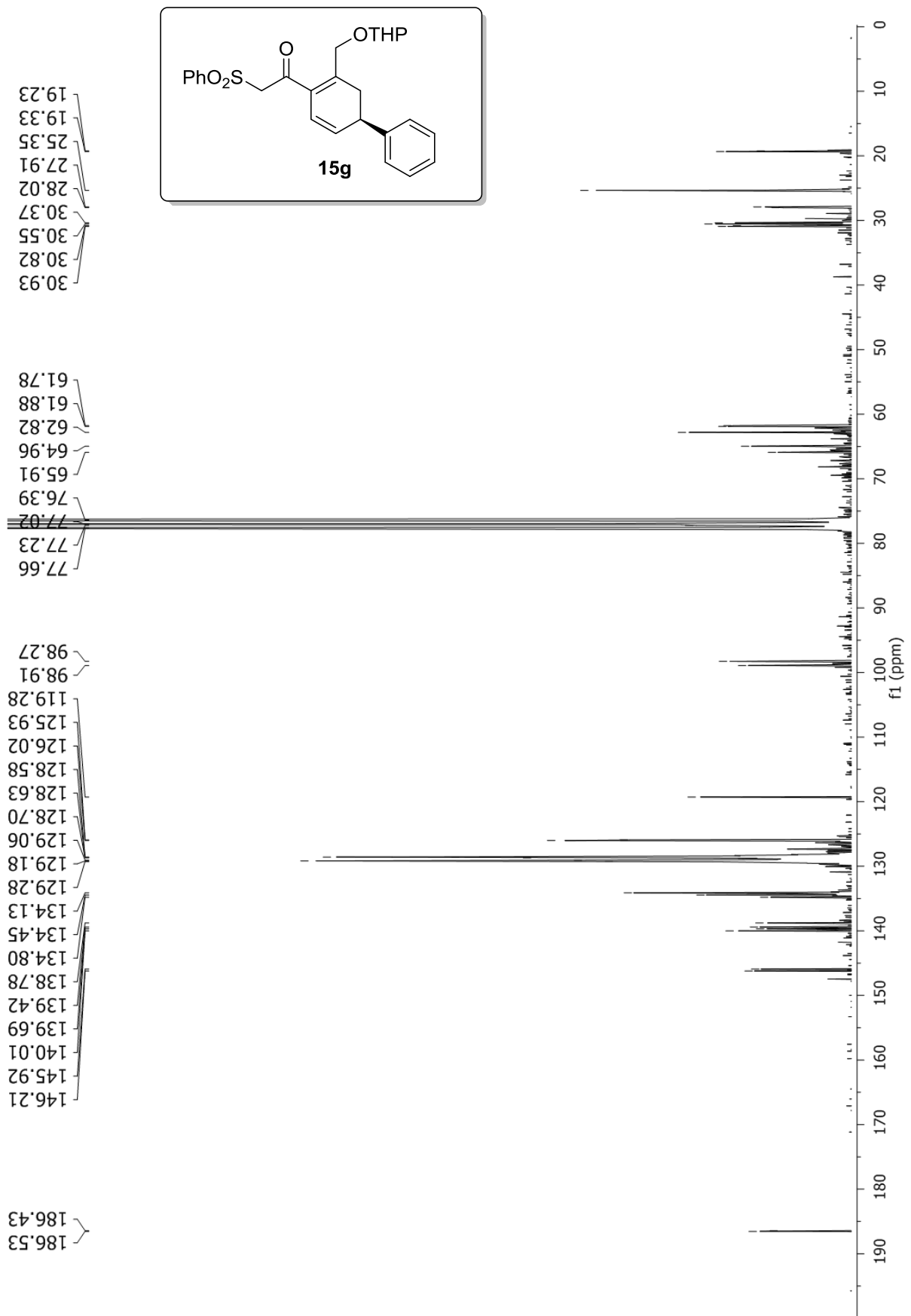
PeakTable

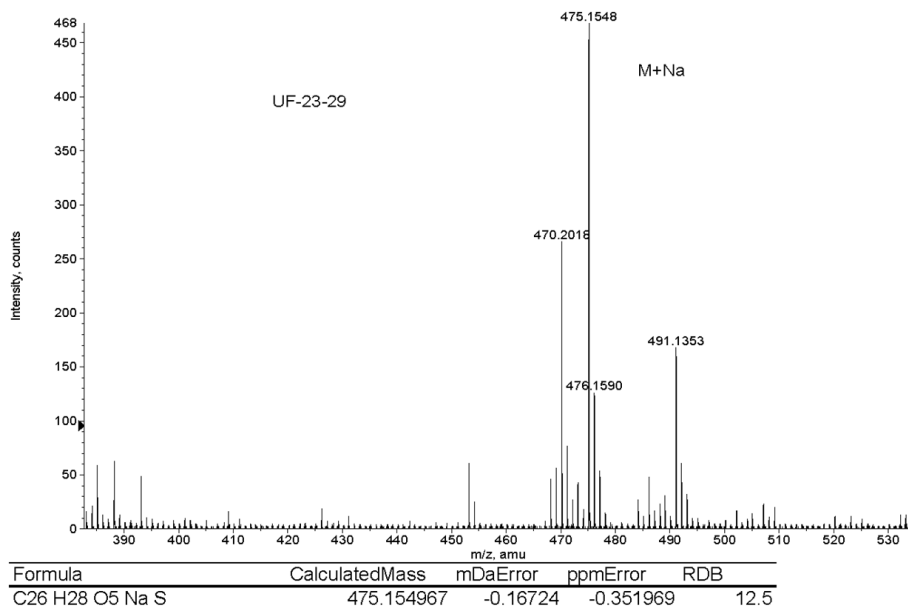
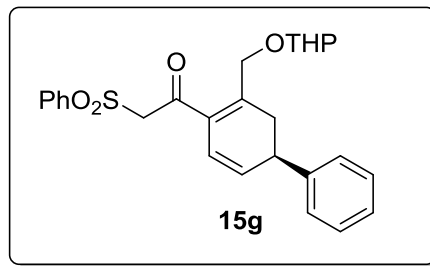
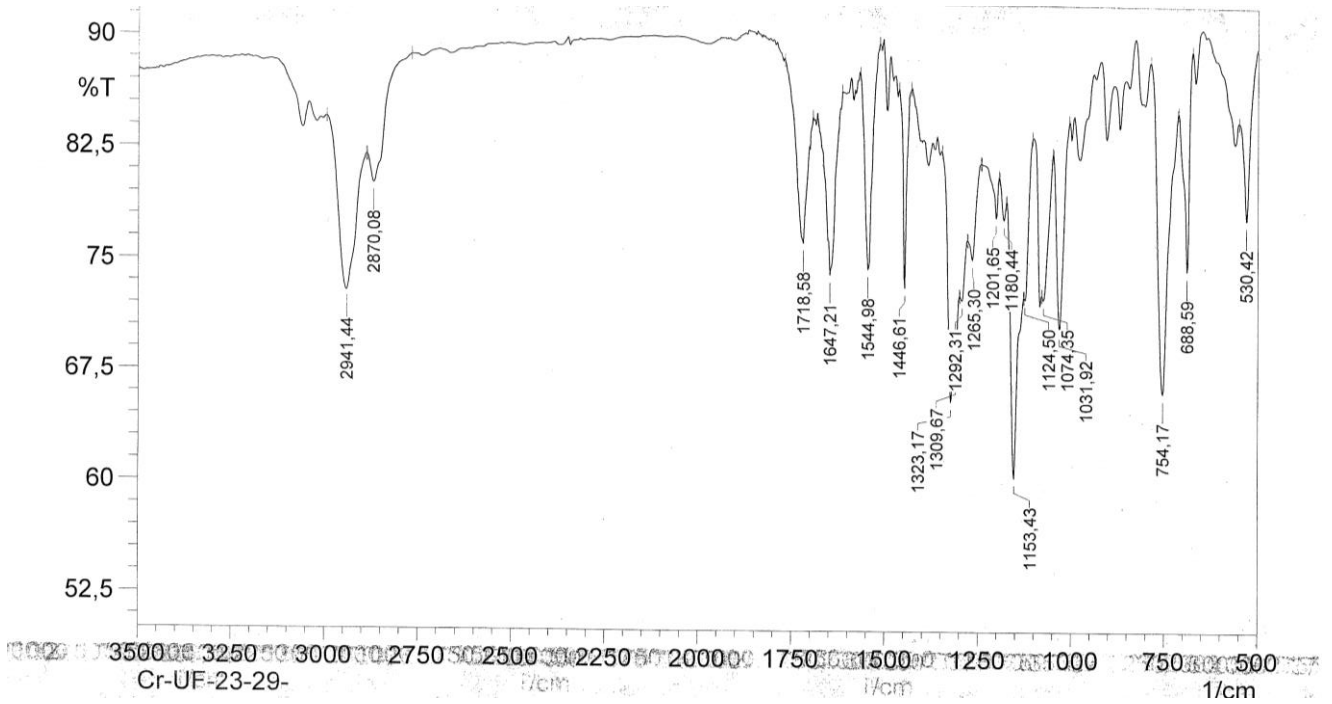
PDA Ch5 350nm 4nm

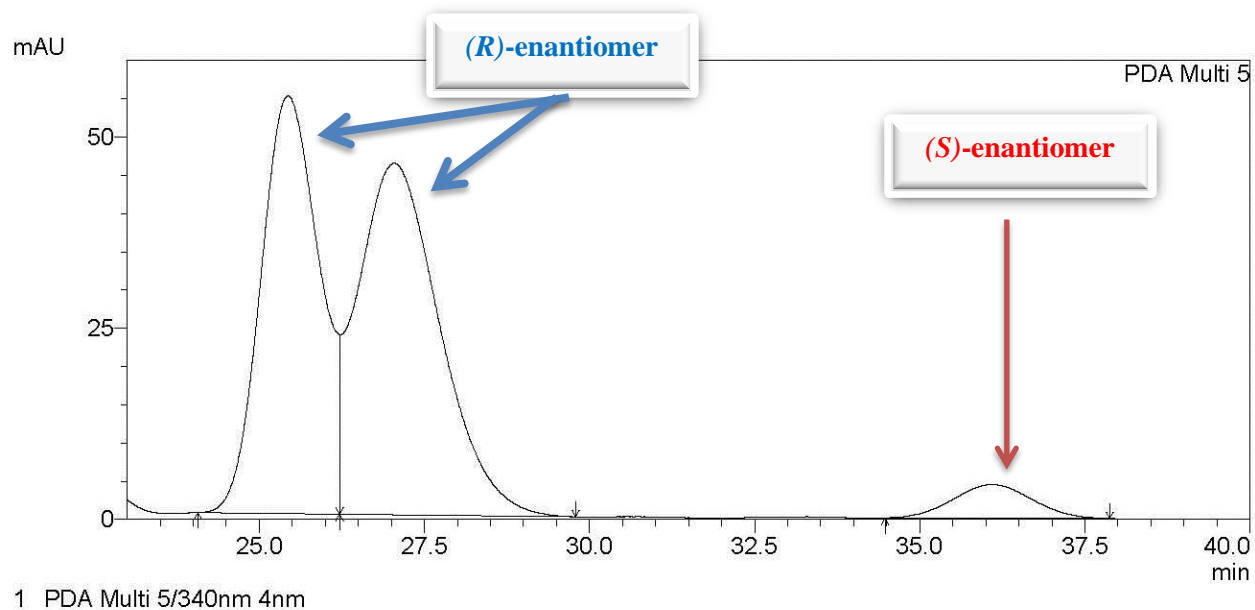
Peak#	Ret. Time	Area %
1	44.627	4.663
2	51.433	42.145
3	61.993	53.192
Total		100.000







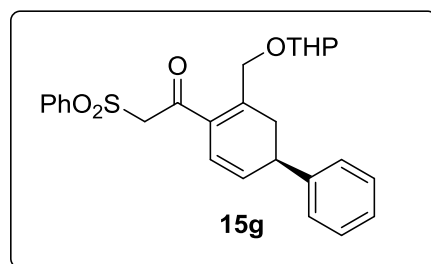


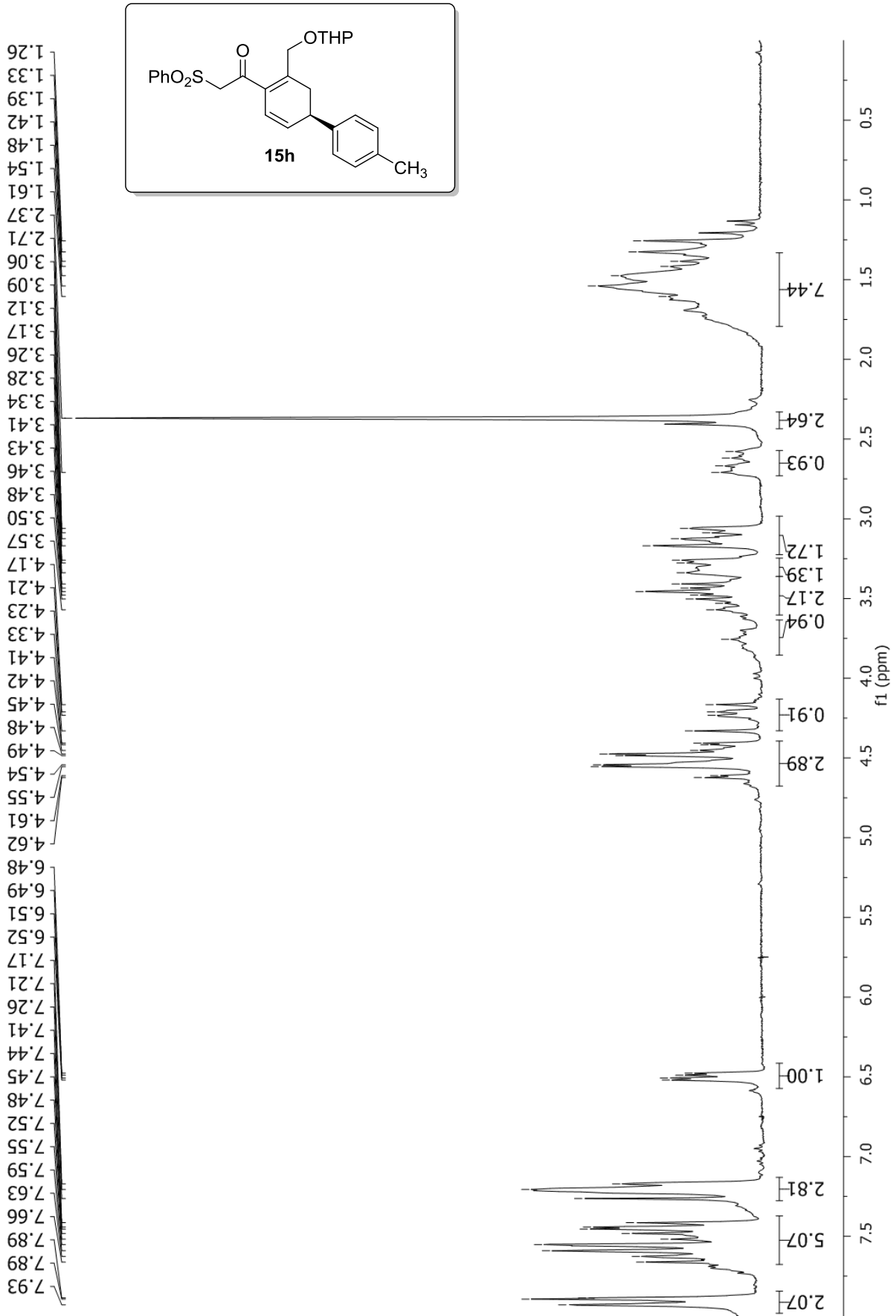


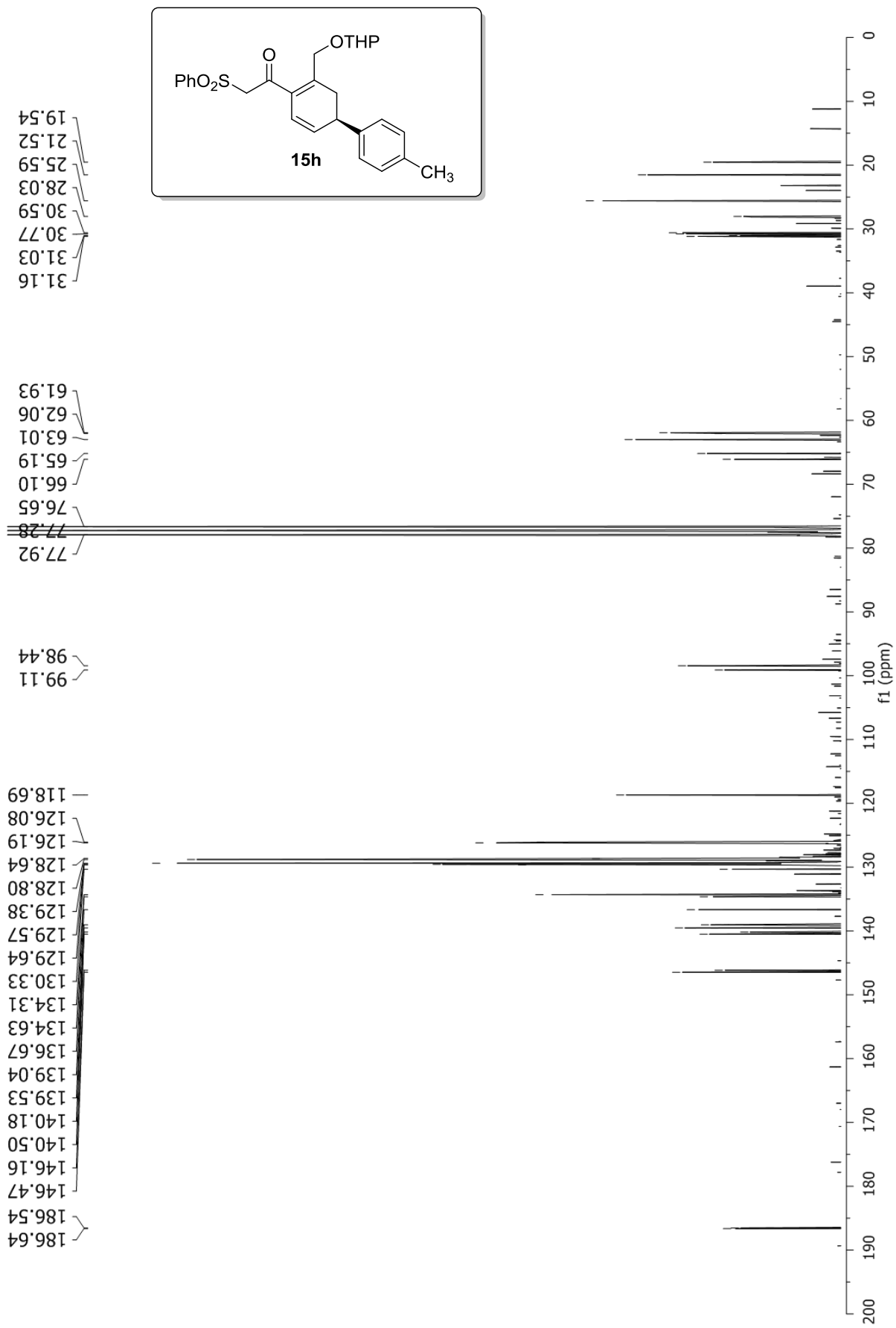
PeakTable

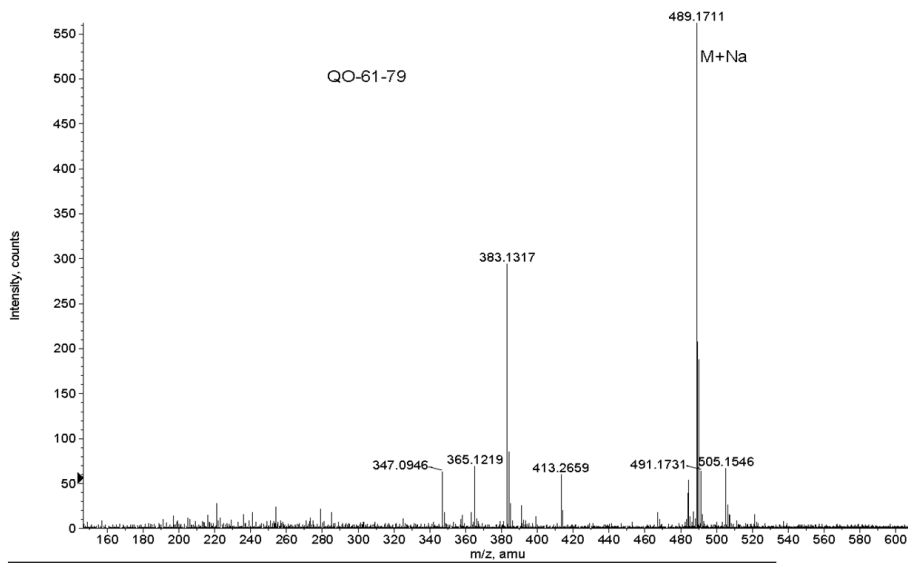
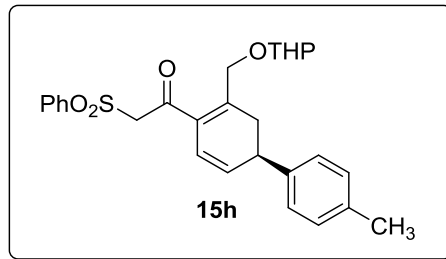
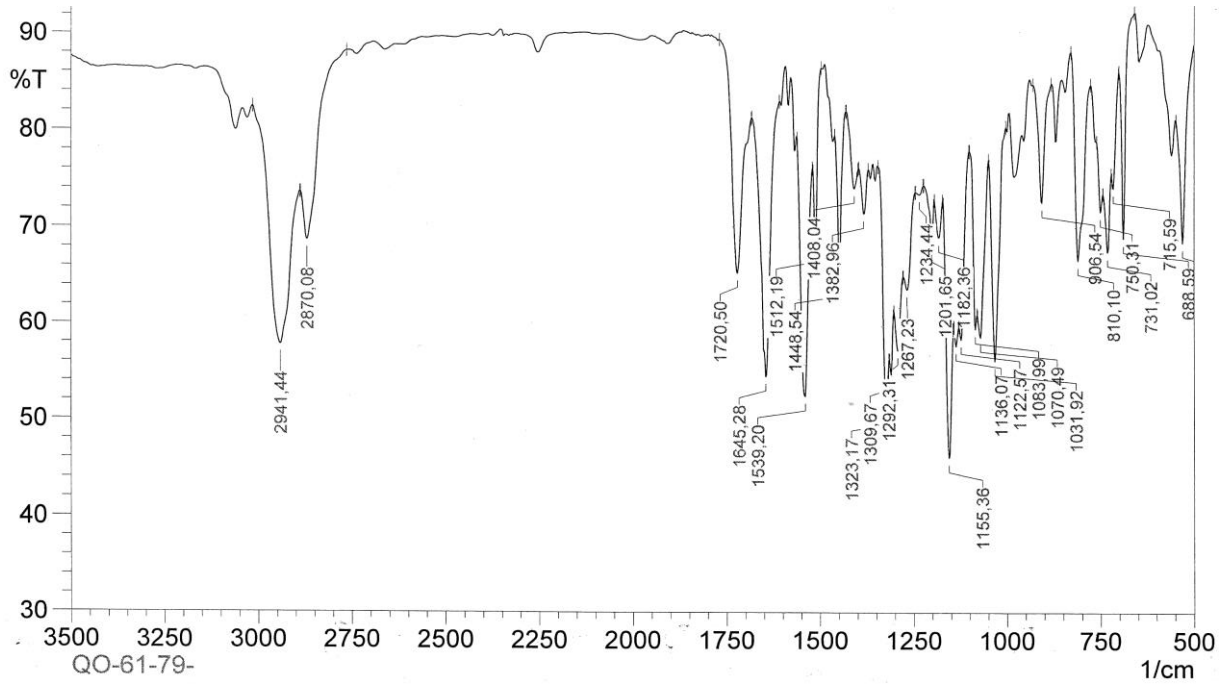
PDA Ch5 340nm 4nm

Peak#	Ret. Time	Area %
1	25.431	43.750
2	27.042	51.512
3	36.072	4.739
Total		100.000

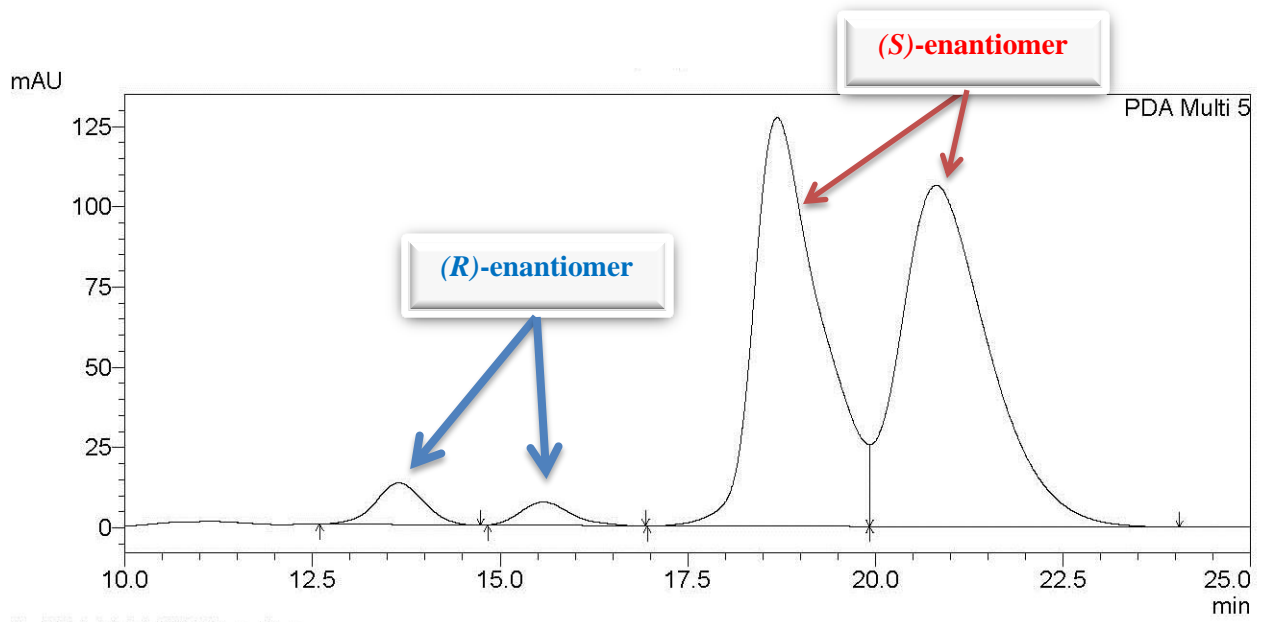








Formula	CalculatedMass	mDaError	ppmError	RDB
C33 H21 N4 O	489.170988	0.112068	0.229097	25.5
C27 H30 O5 Na S	489.170617	0.48268	0.986729	12.5

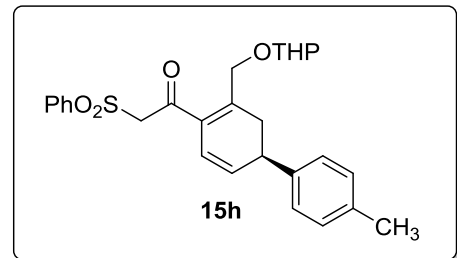


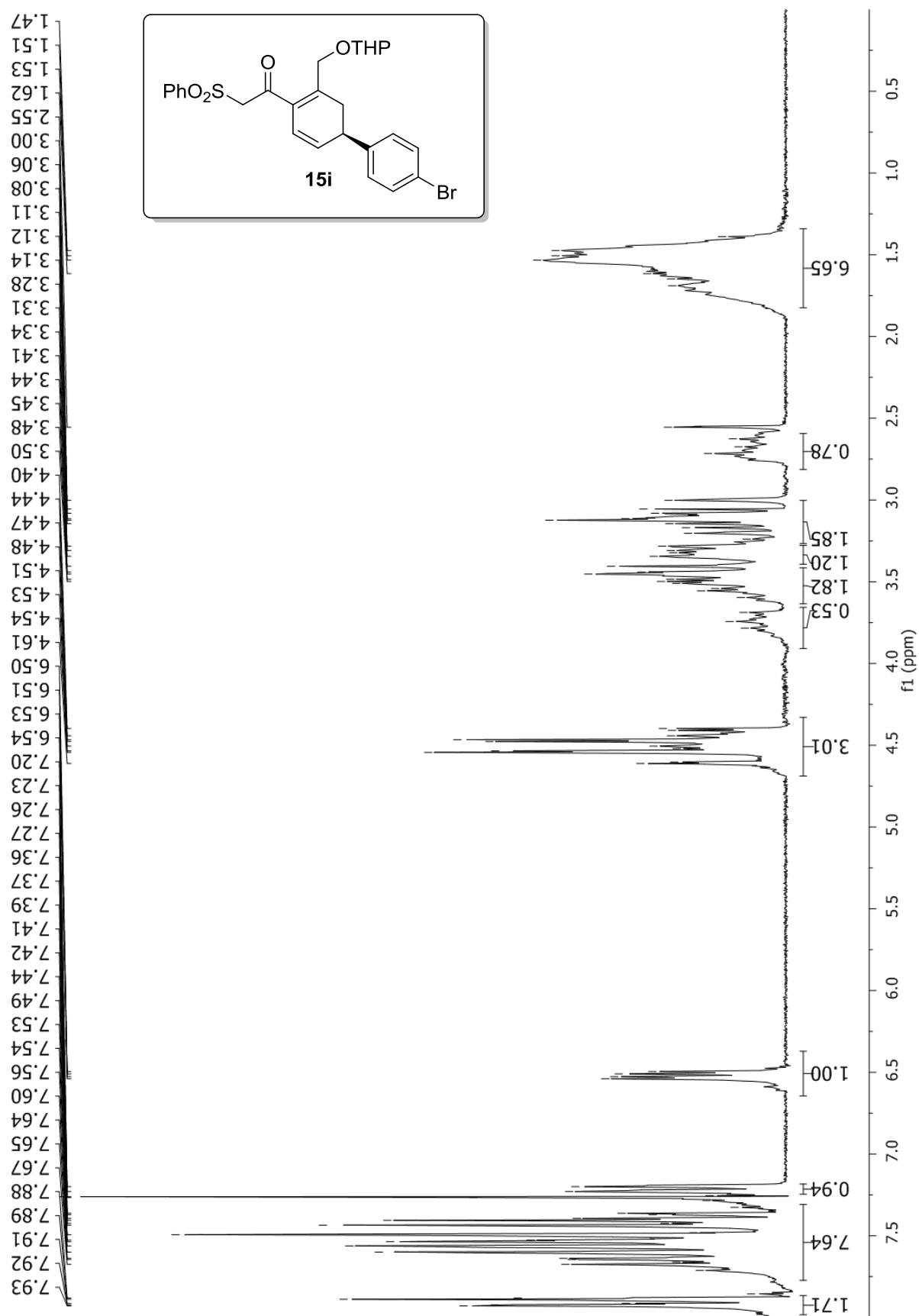
1 PDA Multi 5/420nm 4nm

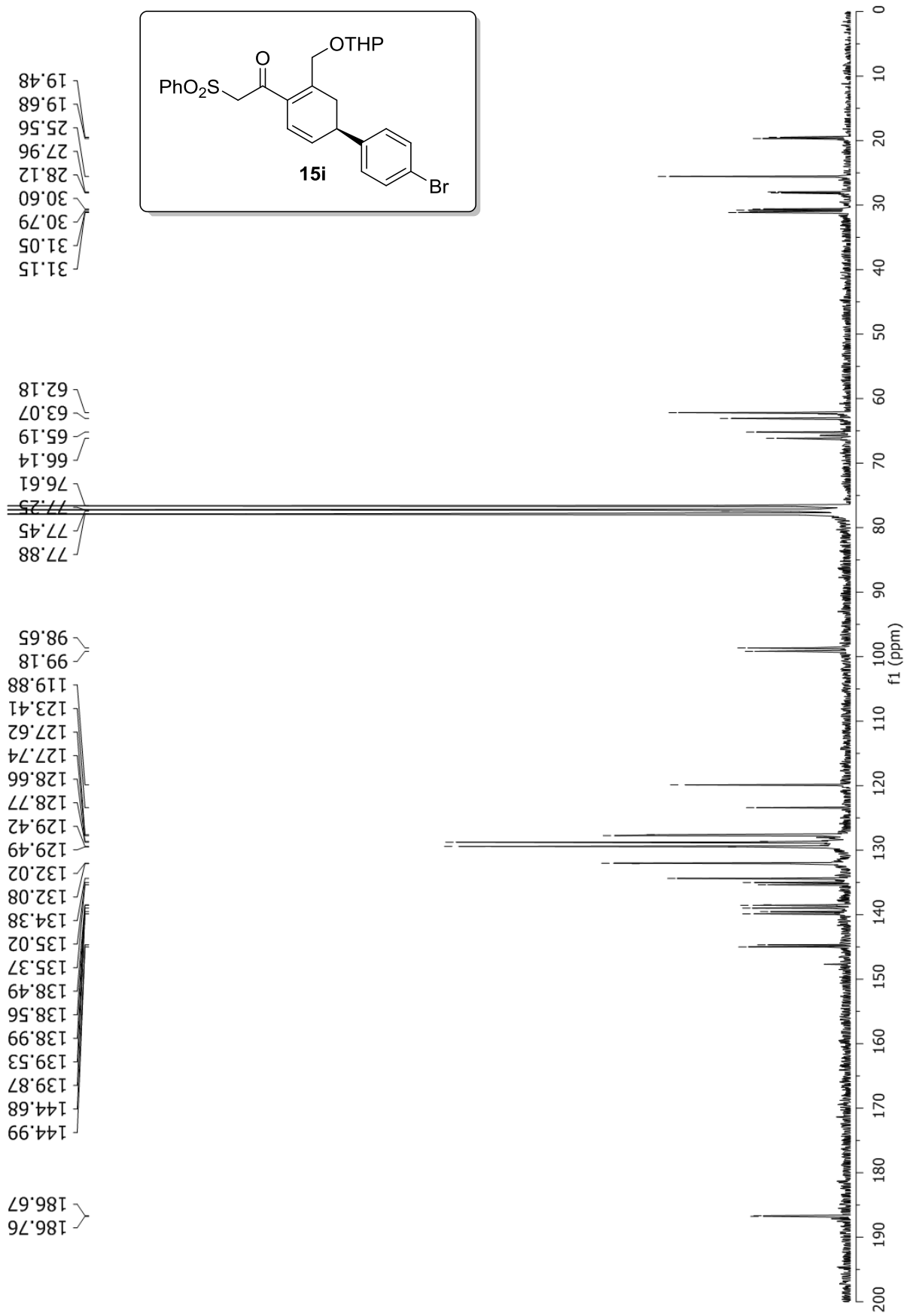
PeakTable

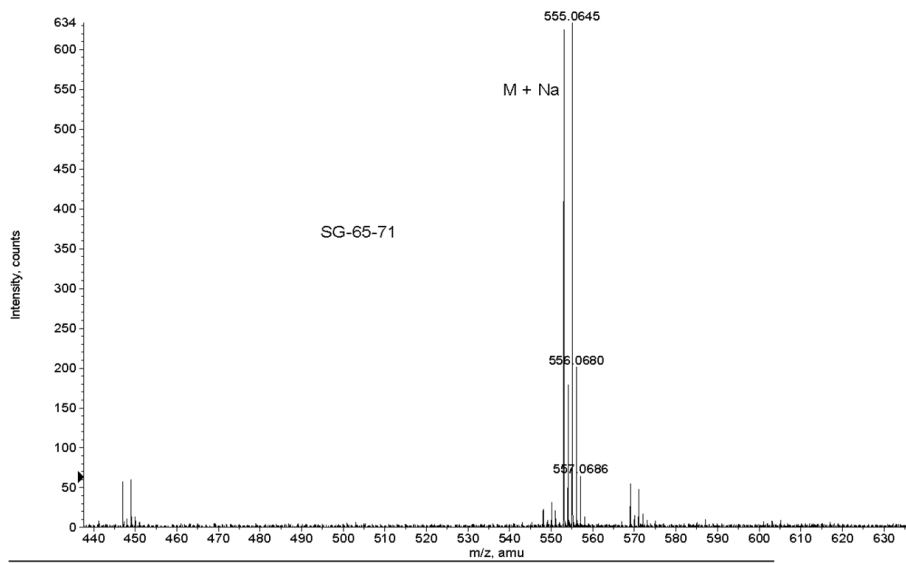
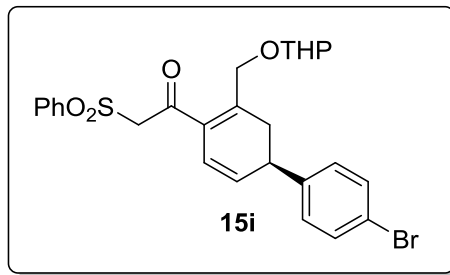
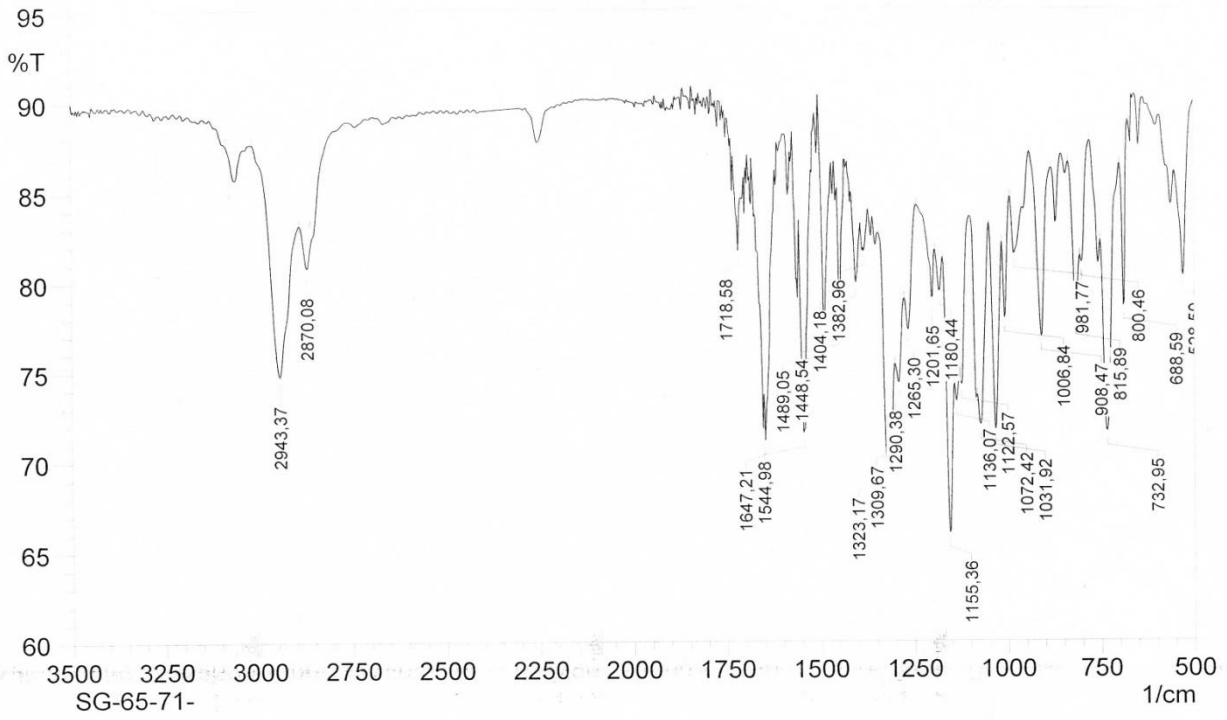
PDA Ch5 420nm 4nm

Peak#	Ret. Time	Area %
1	13.642	3.330
2	15.573	1.928
3	18.687	44.894
4	20.807	49.848
Total		100.000

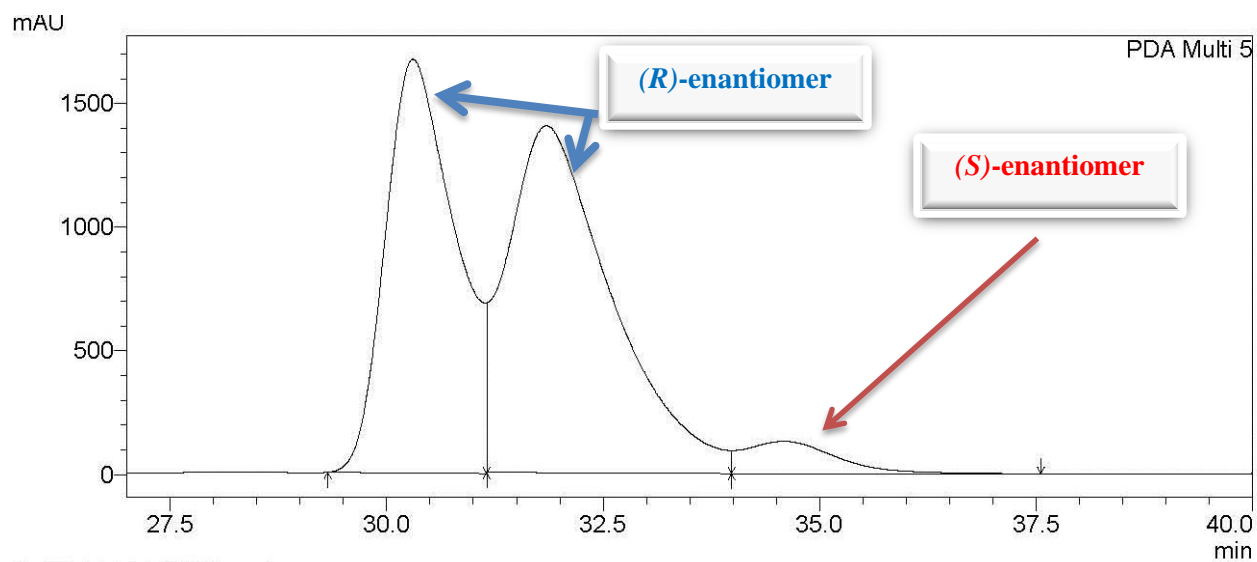








Formula	CalculatedMass	mDaError	ppmError	RDB
C39 H14 O Na S	553.065758	0.04188	0.075723	32.5
C26 H27 O5 Na S Br	553.065478	0.3217	0.581666	12.5

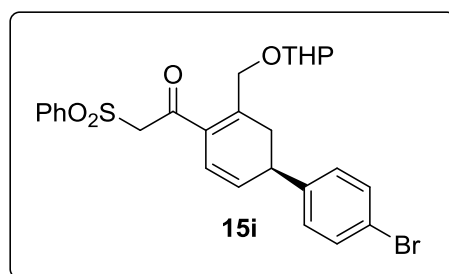


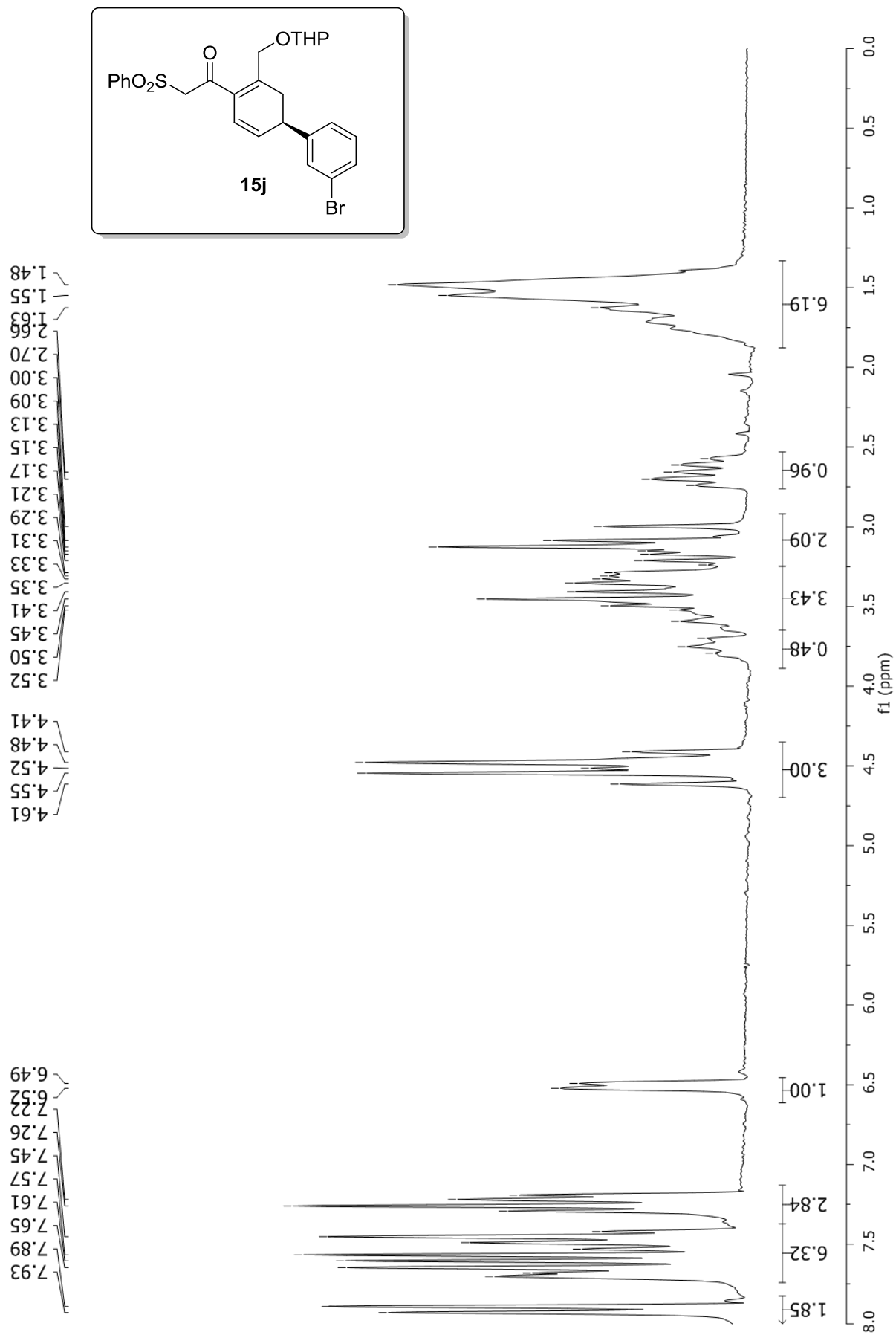
1 PDA Multi 5/350nm 4nm

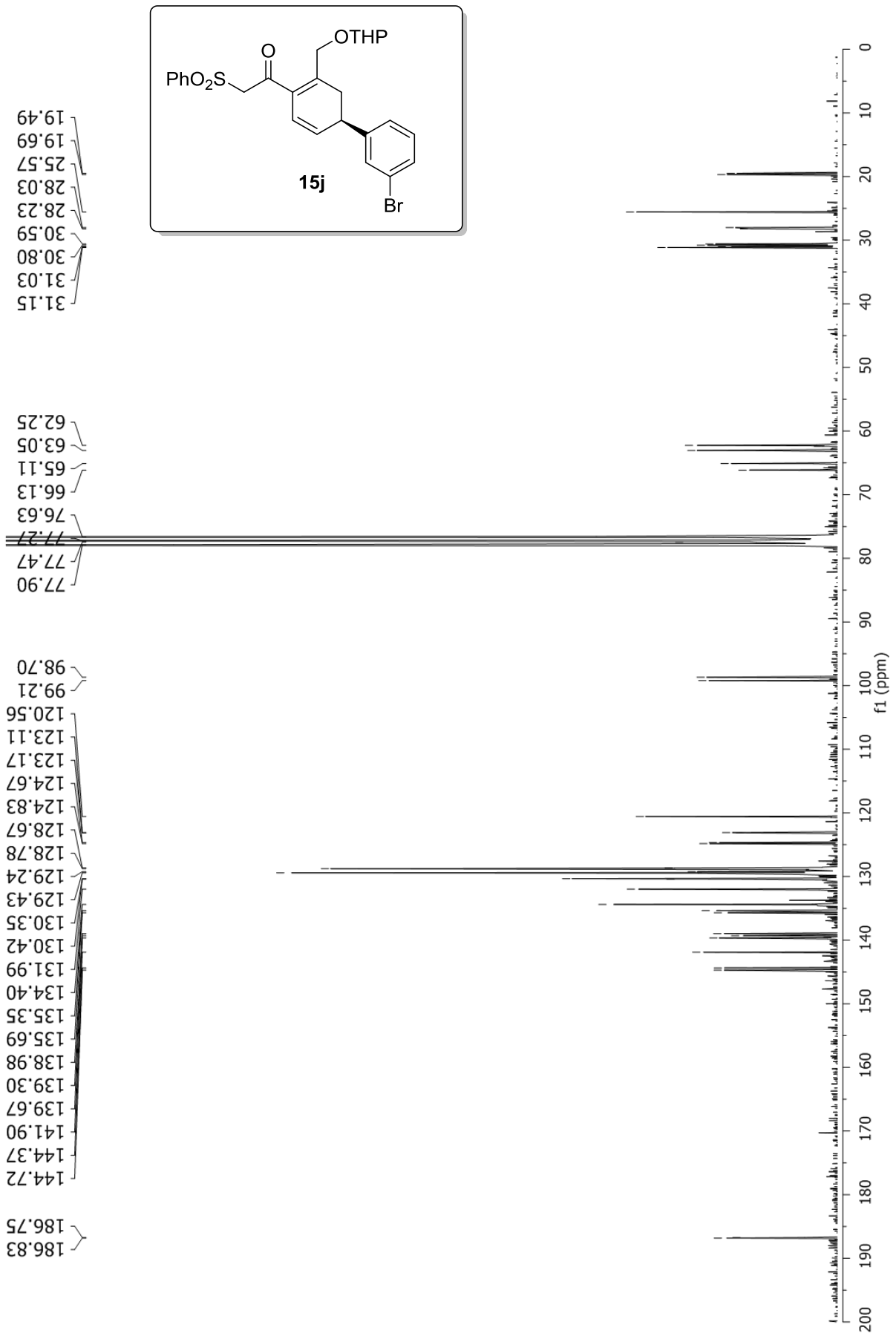
PeakTable

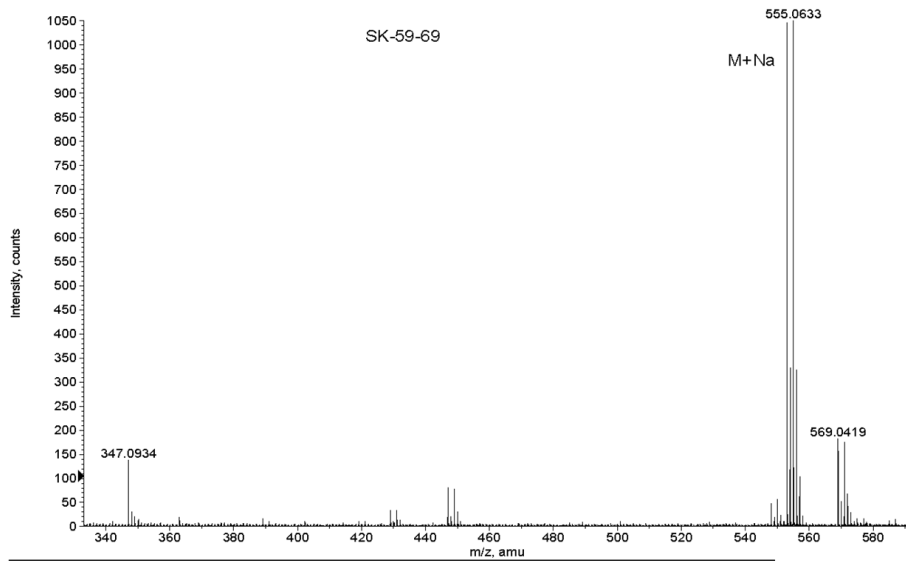
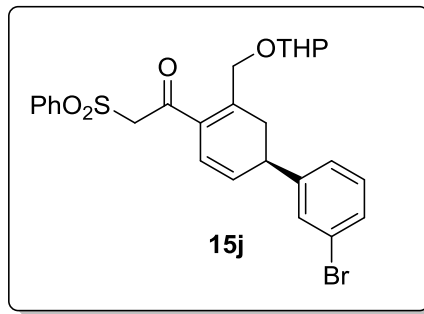
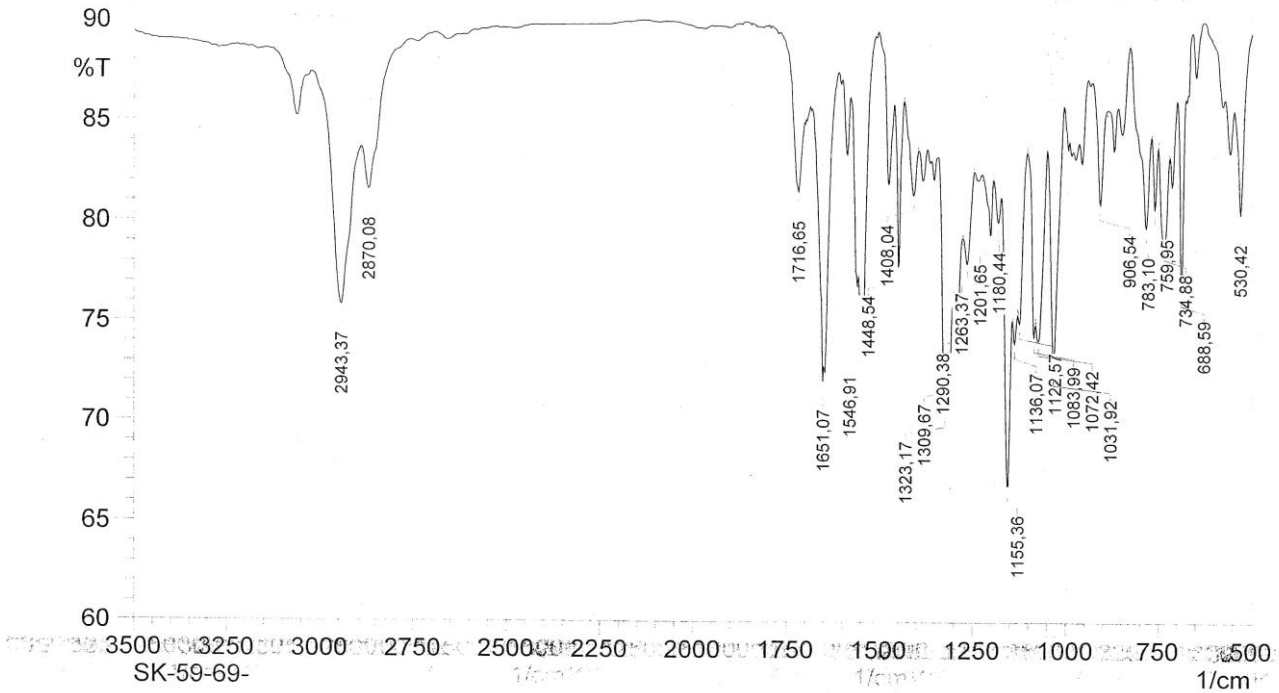
PDA Ch5 350nm 4nm

Peak#	Ret. Time	Area %
1	30.299	42.671
2	31.840	53.024
3	34.581	4.305
Total		100.000

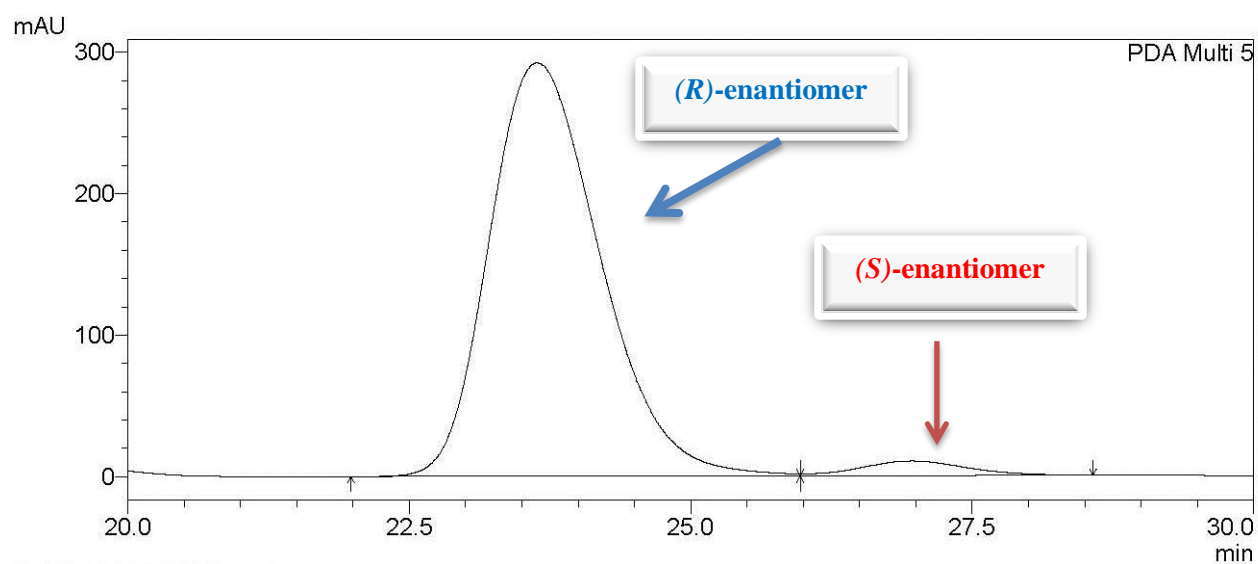








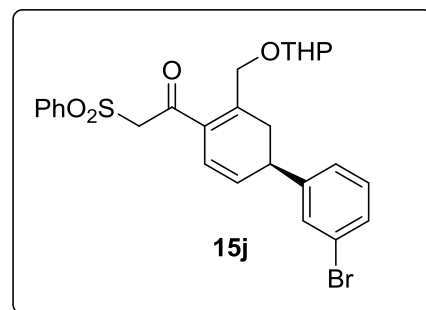
Formula	CalculatedMass	mDaError	ppmError	RDB
C39 H14 O Na S	553.065758	0.04188	0.075723	32.5
C26 H27 O5 Na S Br	553.065478	0.3217	0.581666	12.5

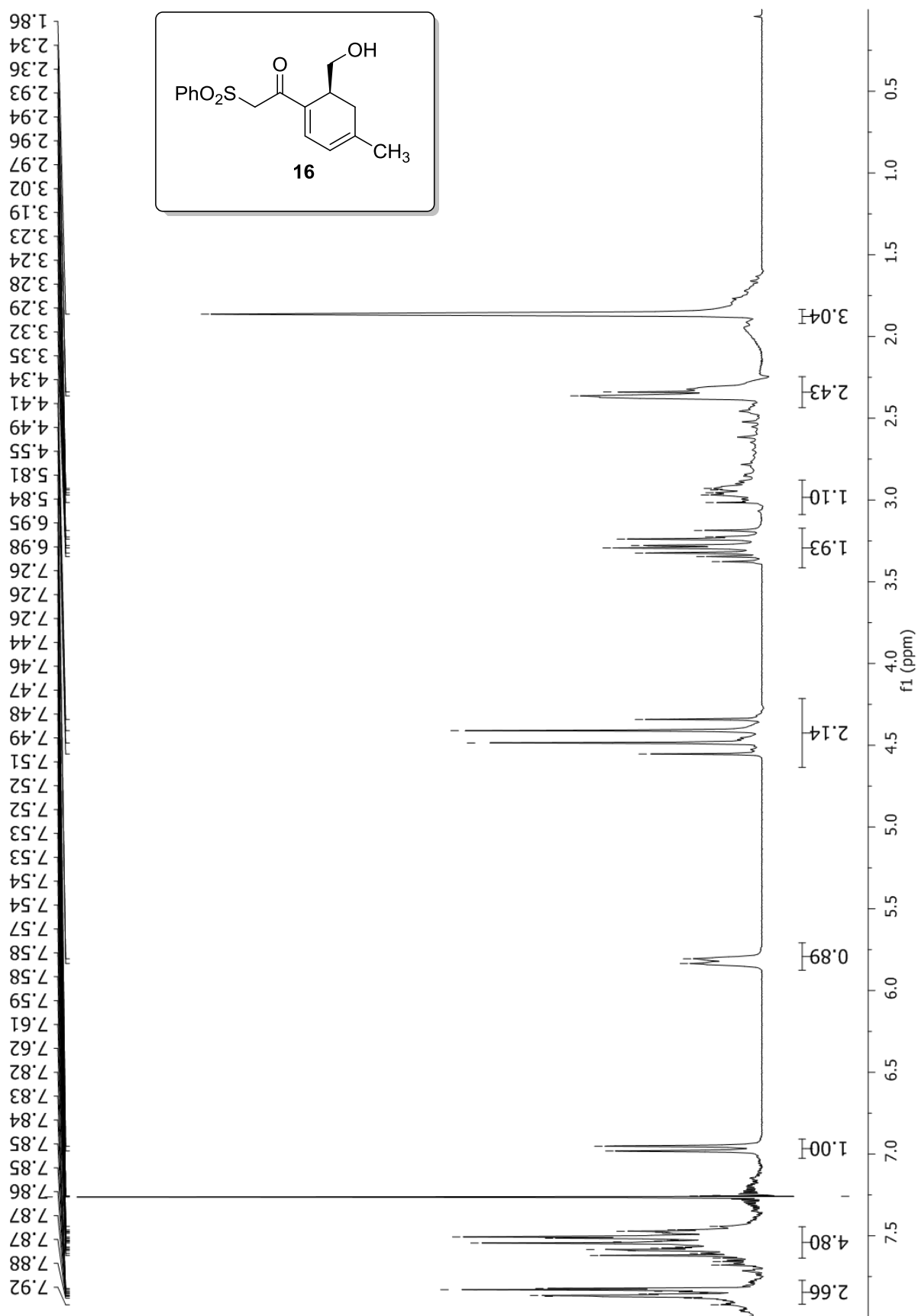


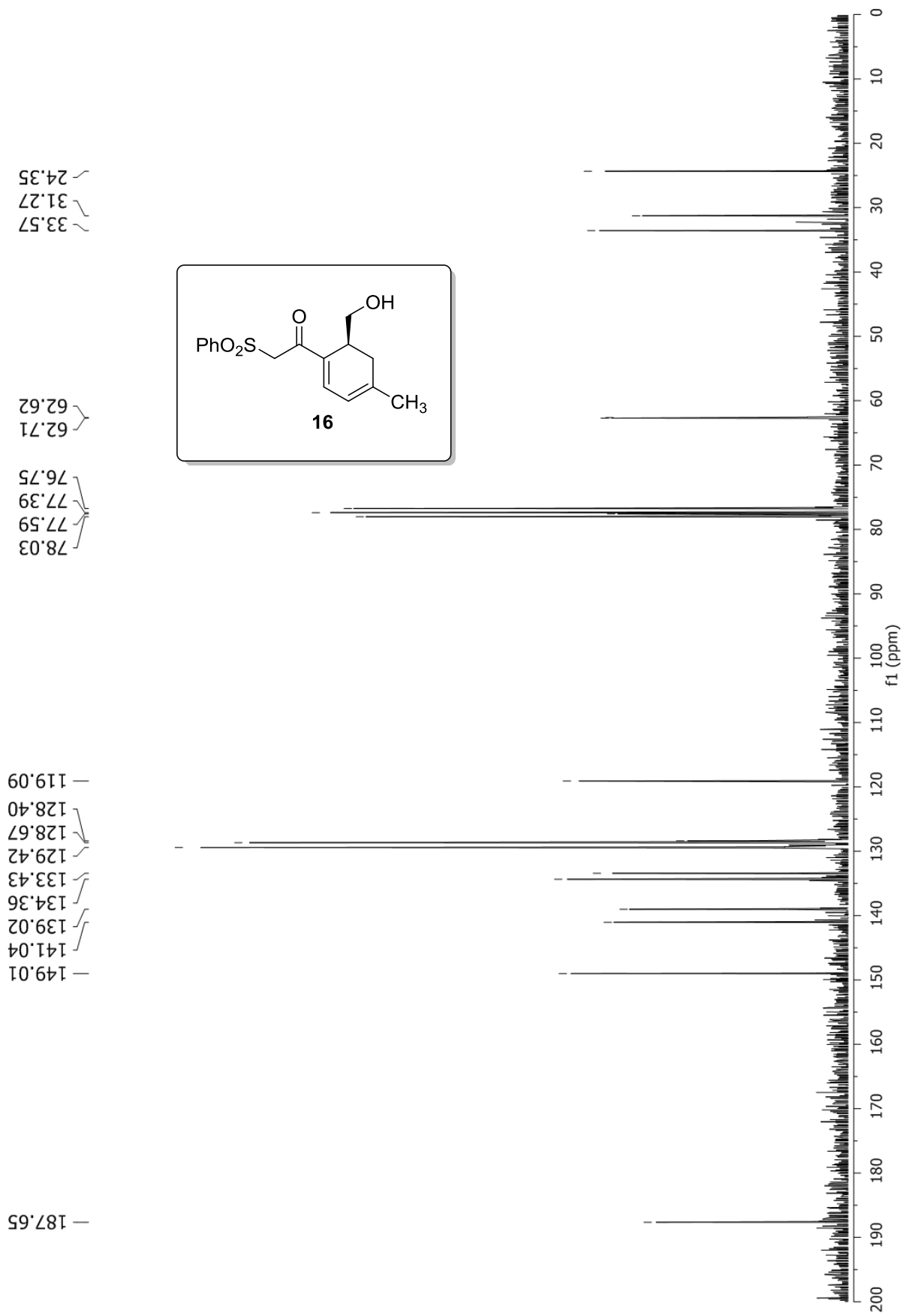
1 PDA Multi 5/350nm 4nm

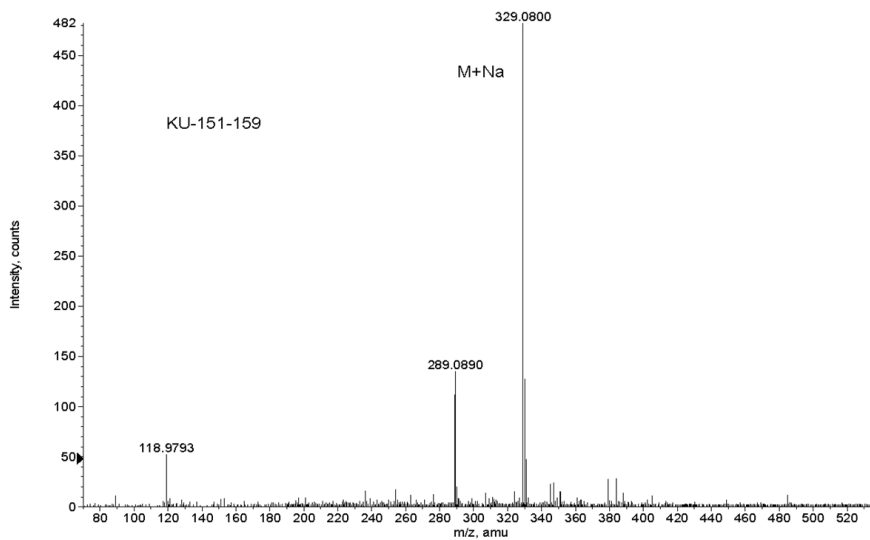
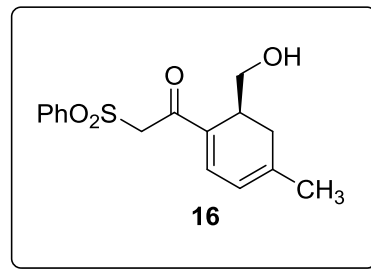
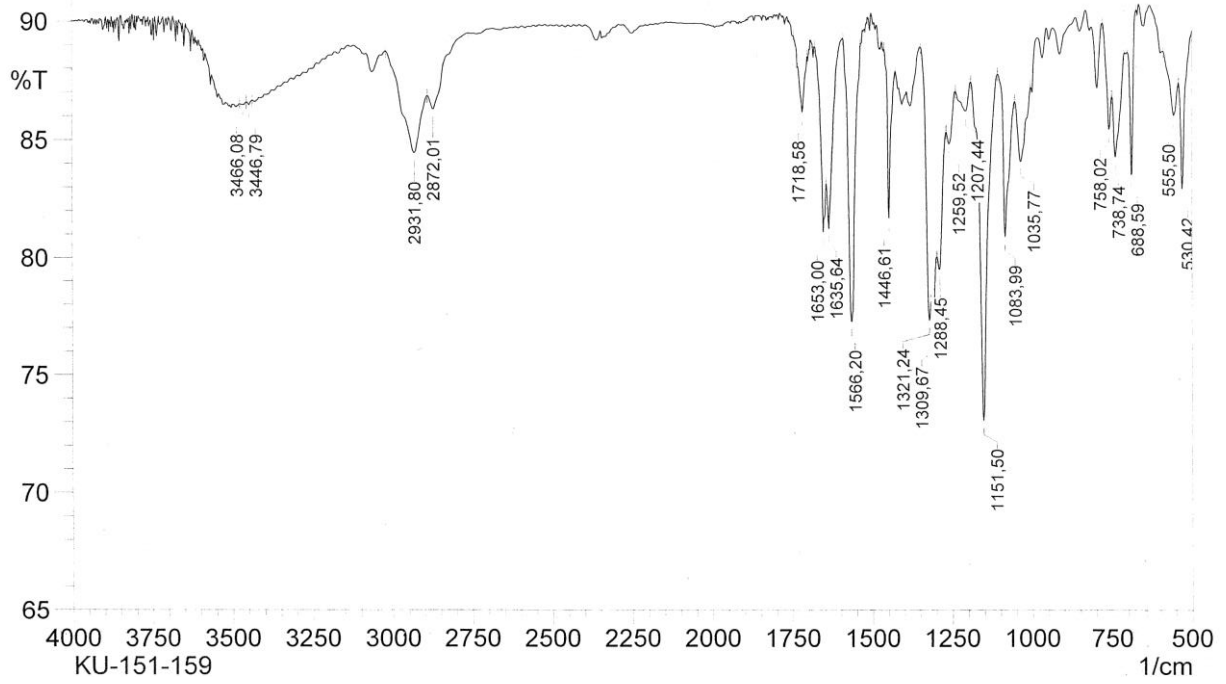
PeakTable
PDA Ch5 350nm 4nm

Peak#	Ret. Time	Area %
1	23.630	96.748
2	26.951	3.252
Total		100.000

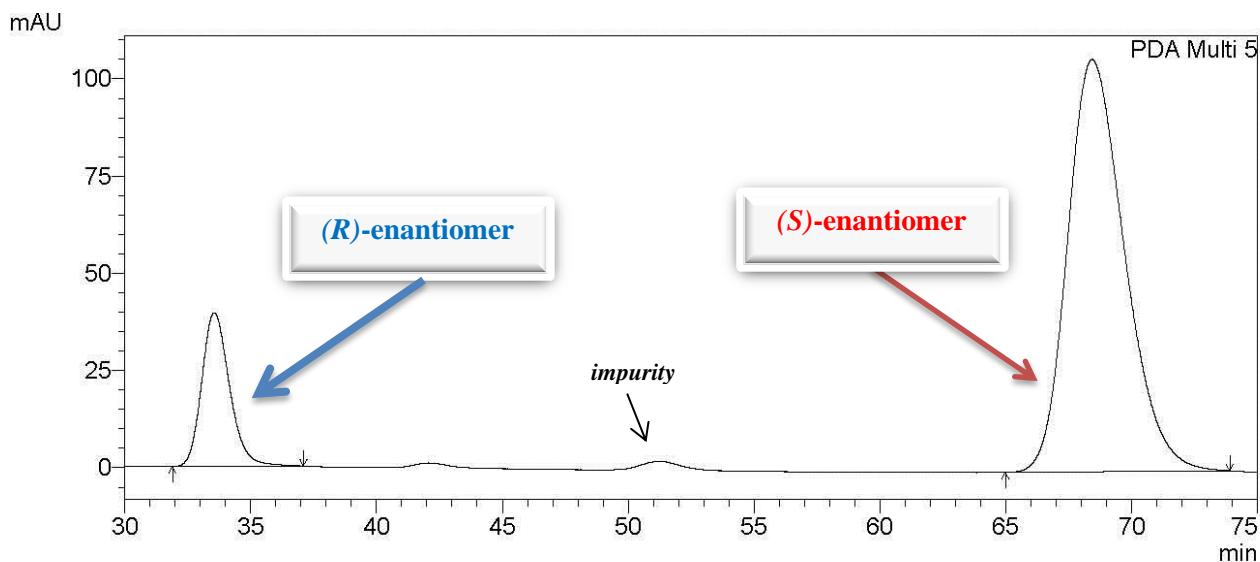








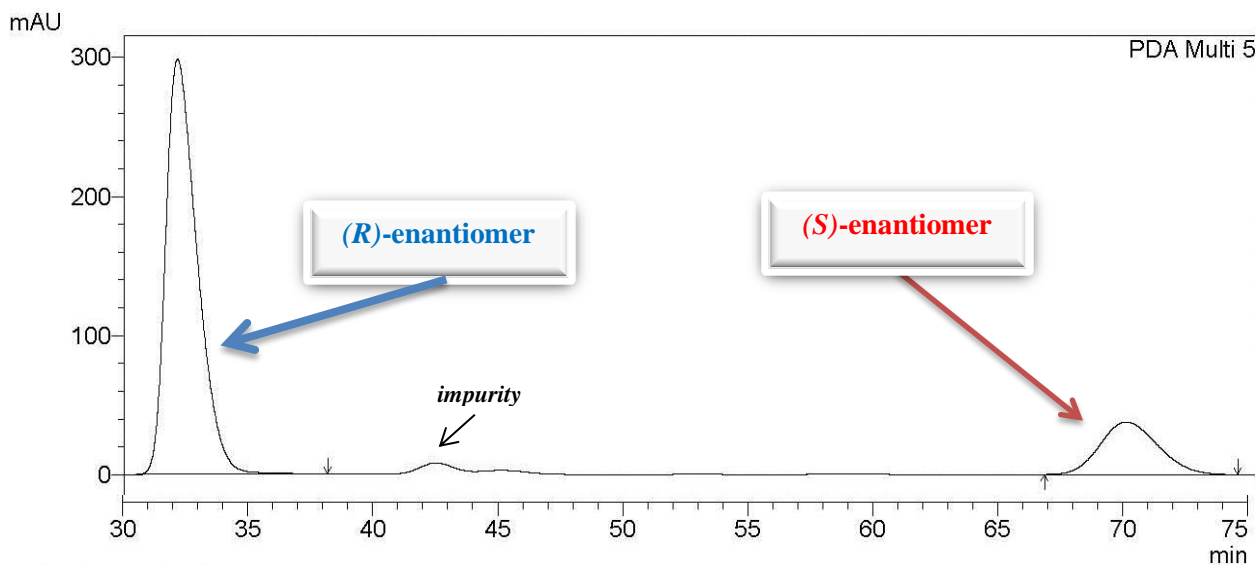
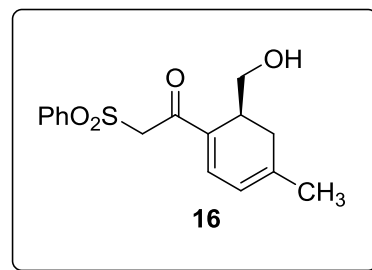
Formula	CalculatedMass	mDaError	ppmError	RDB
C21 H13 O4	329.080836	-0.8355	-2.538892	15.5
C19 H14 O4 Na	329.07843	1.56976	4.770139	12.5
C16 H18 O4 Na S	329.081802	-1.8022	-5.476471	7.5



1 PDA Multi 5/325nm 4nm

PeakTable
PDA Ch5 325nm 4nm

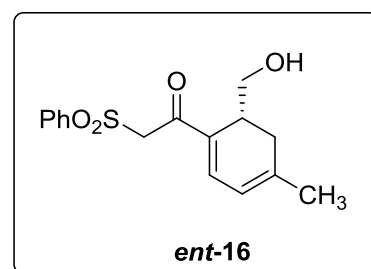
Peak#	Ret. Time	Area %
1	33.553	15.411
2	68.425	84.589
Total		100.000

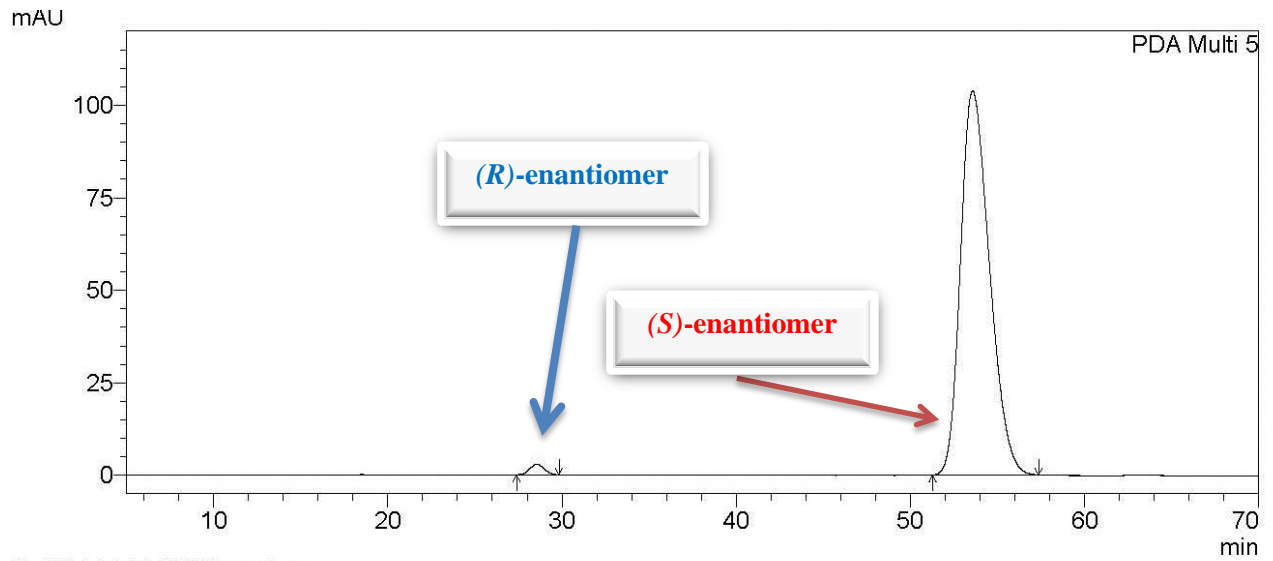


1 PDA Multi 5/325nm 4nm

PeakTable
PDA Ch5 325nm 4nm

Peak#	Ret. Time	Area %
1	31.819	81.094
2	69.774	18.906
Total		100.000



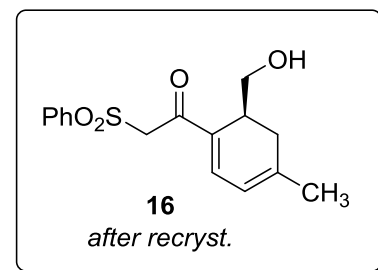


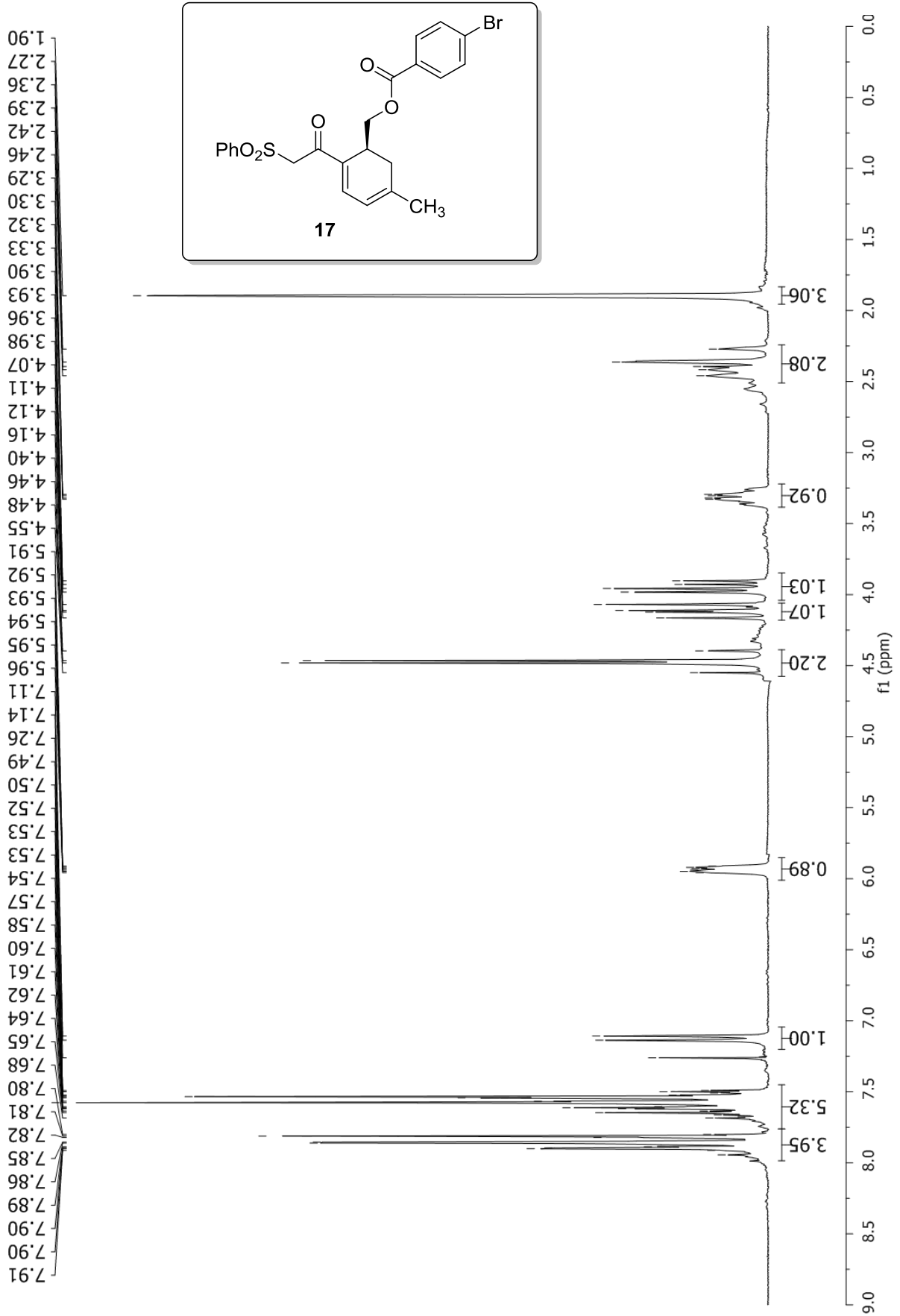
1 PDA Multi 5/360nm 4nm

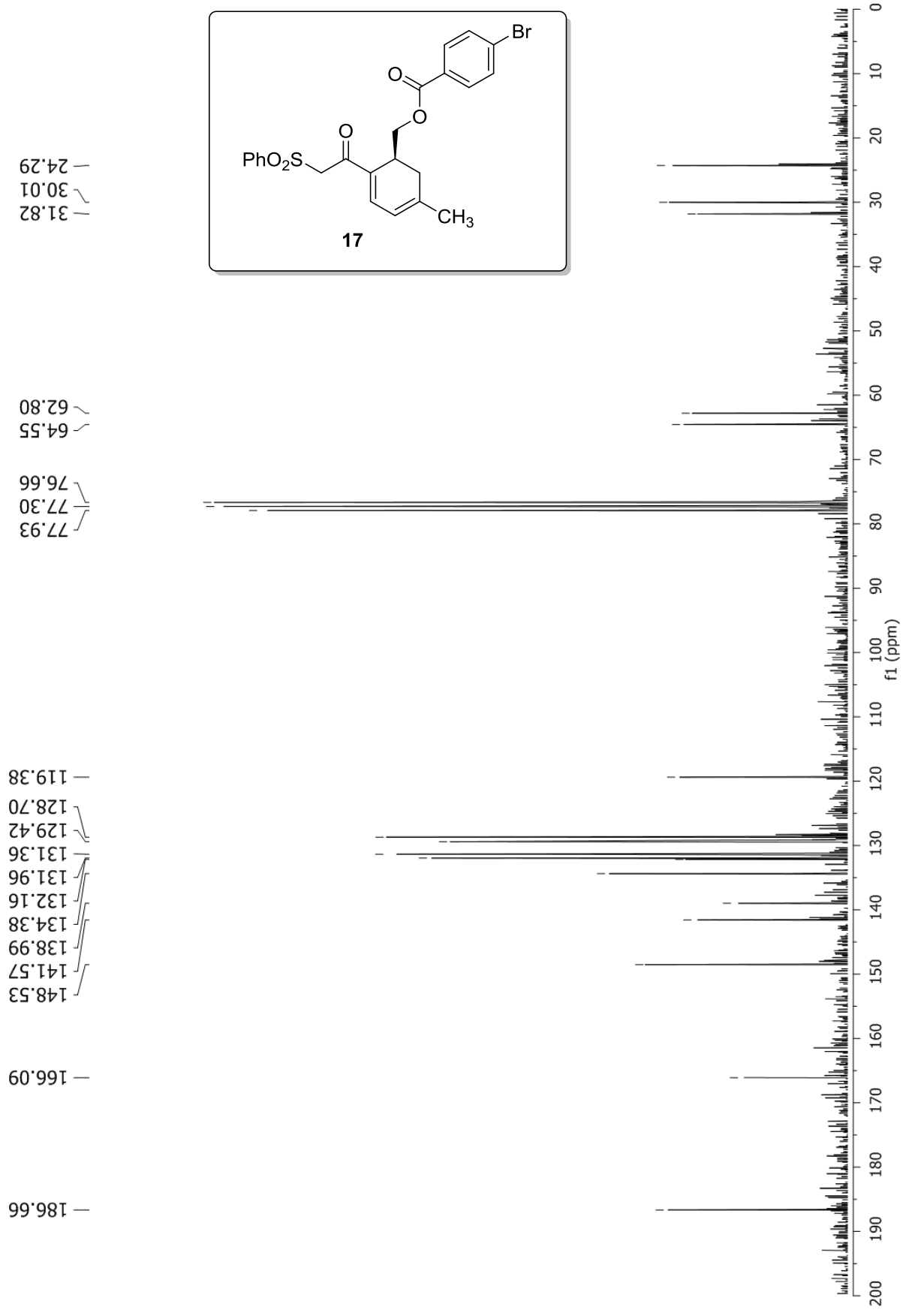
PeakTable

PDA Ch5 360nm 4nm

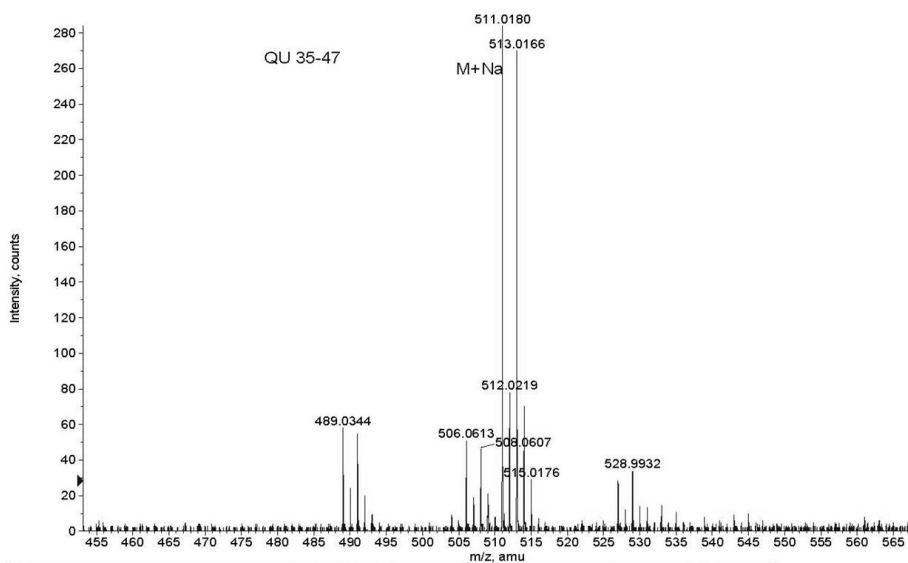
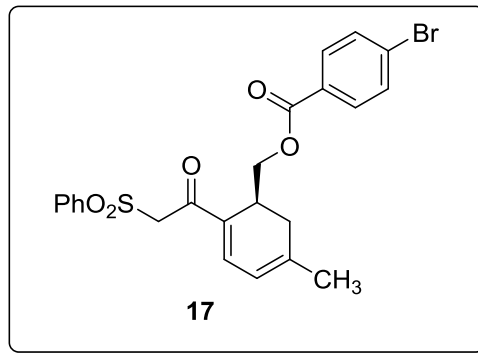
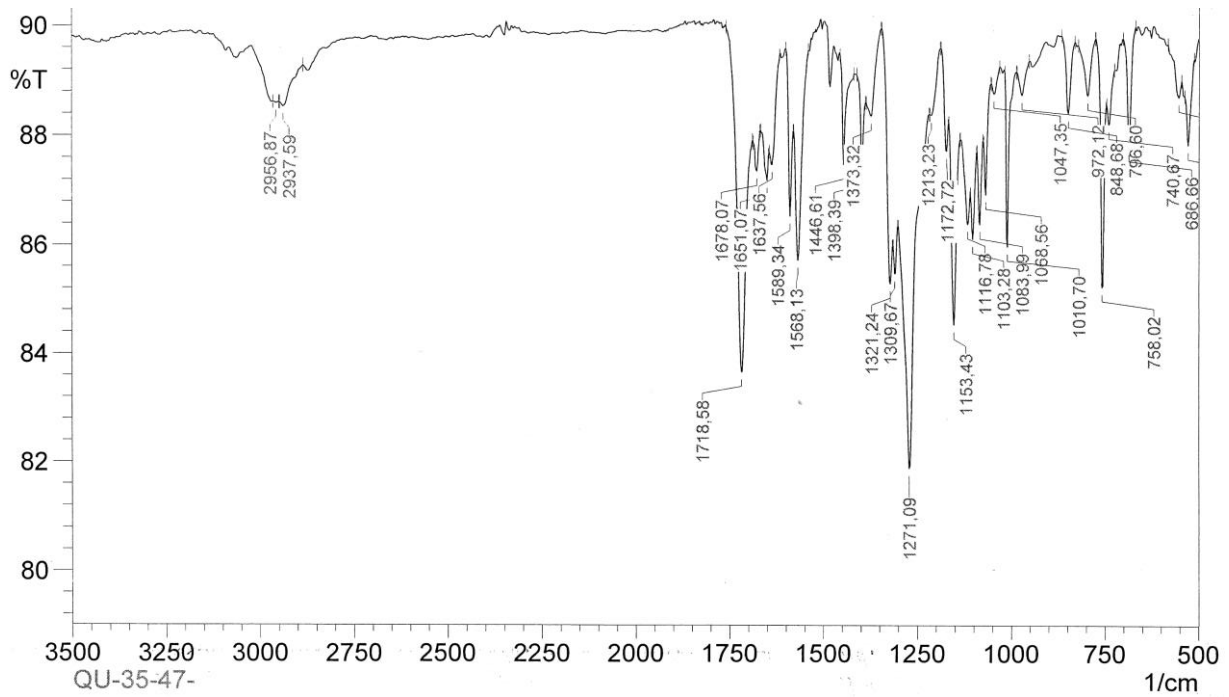
Peak#	Ret. Time	Area %
1	28.539	1.367
2	53.573	98.633
Total		100.000



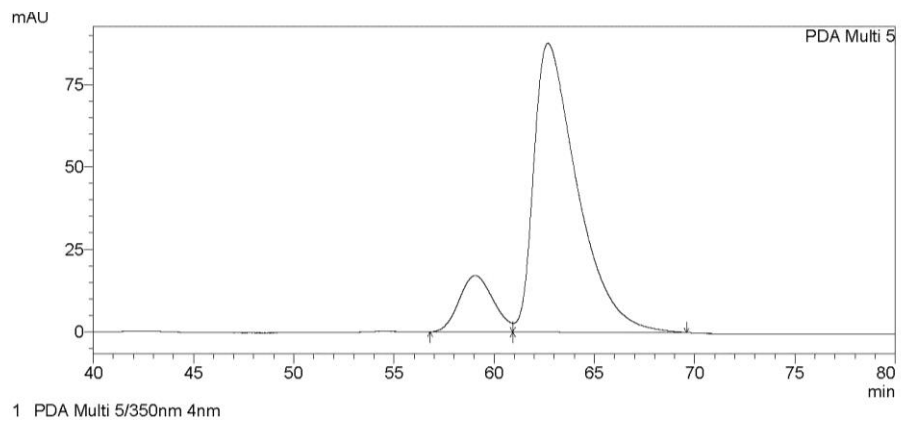




Full Spectroscopy



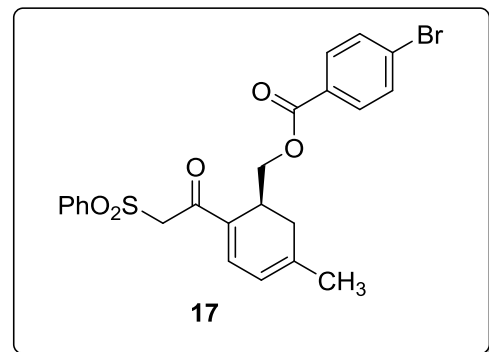
Formula	CalculatedMass	mDaError	ppmError	RDB
C41 H3 O	511.017841	0.15882	0.310791	40.5
C28 H16 O5 Br	511.017561	0.43864	0.858364	20.5
C23 H21 O5 Na S Br	511.018528	-0.52806	-1.033348	12.5

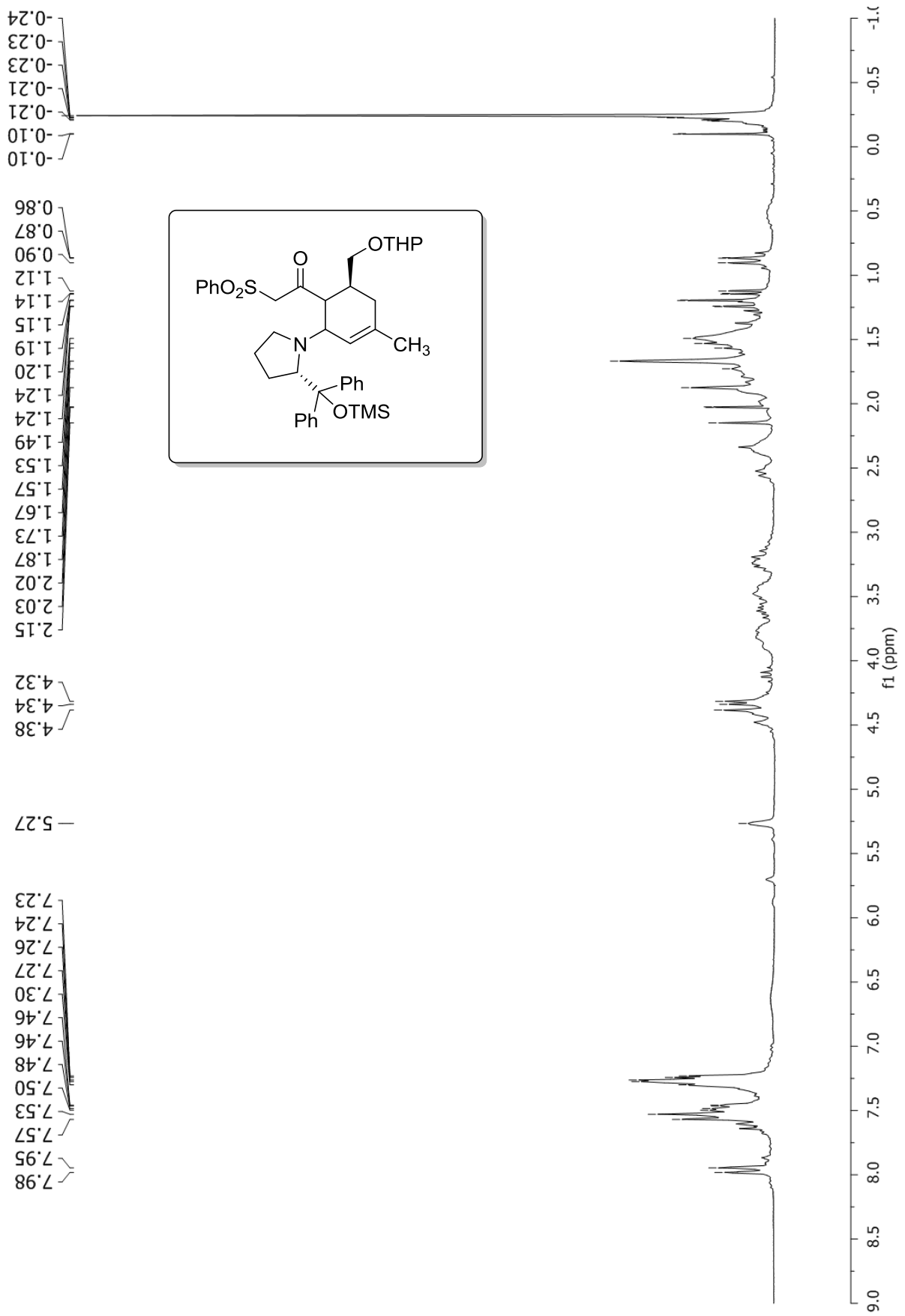


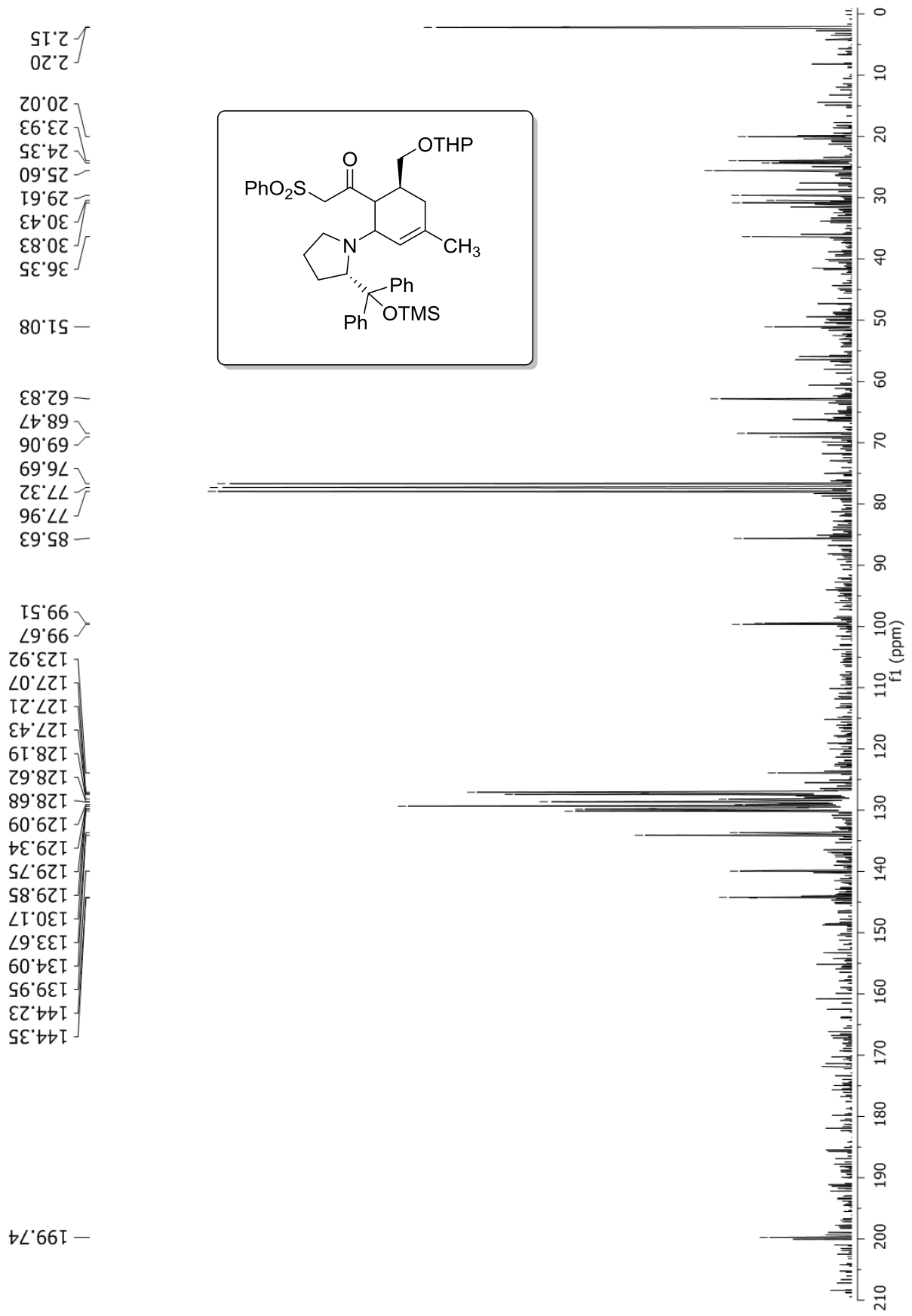
PeakTable

PDA Ch5 350nm 4nm

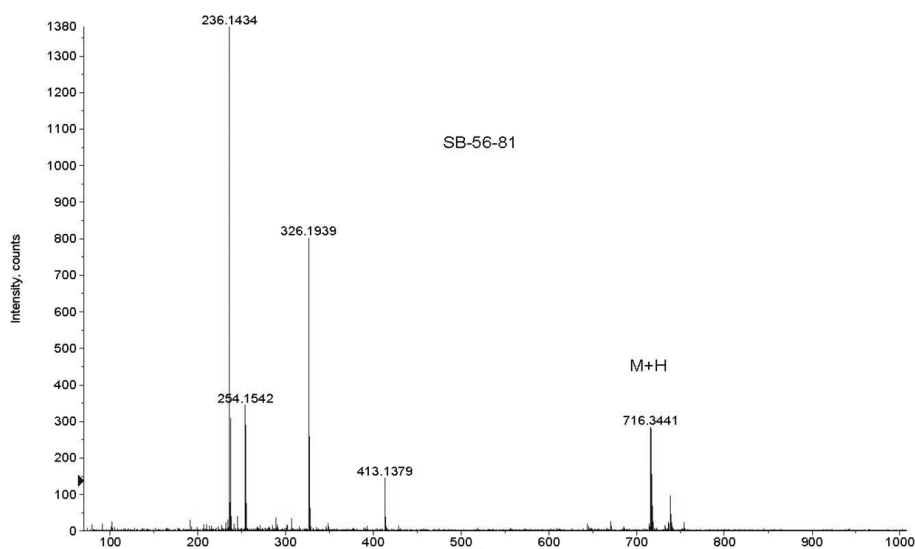
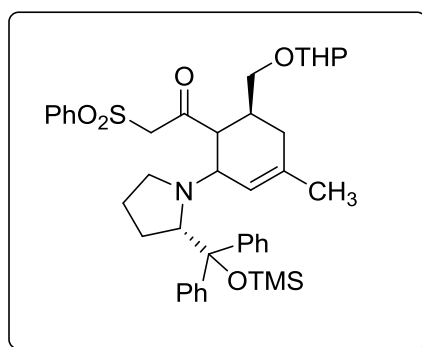
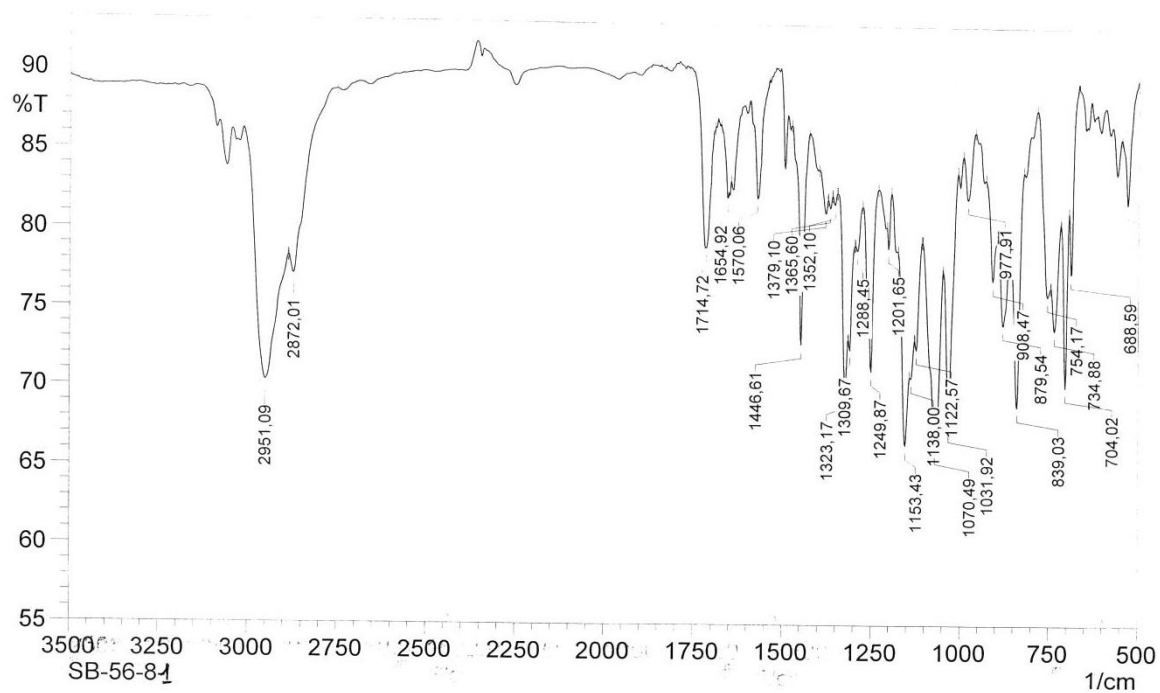
Peak#	Ret. Time	Area %
1	59.039	13.222
2	62.682	86.778
Total		100.000



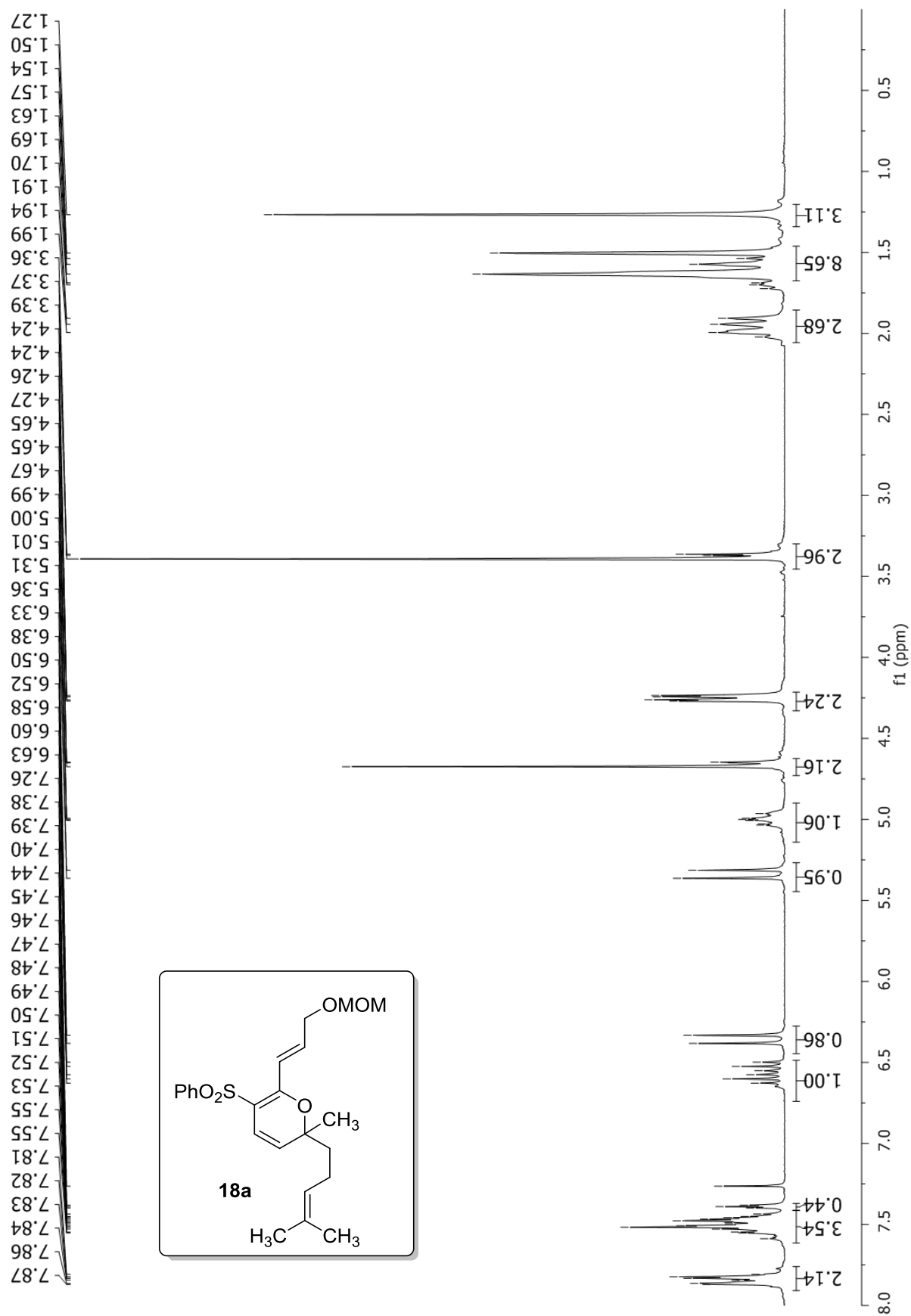


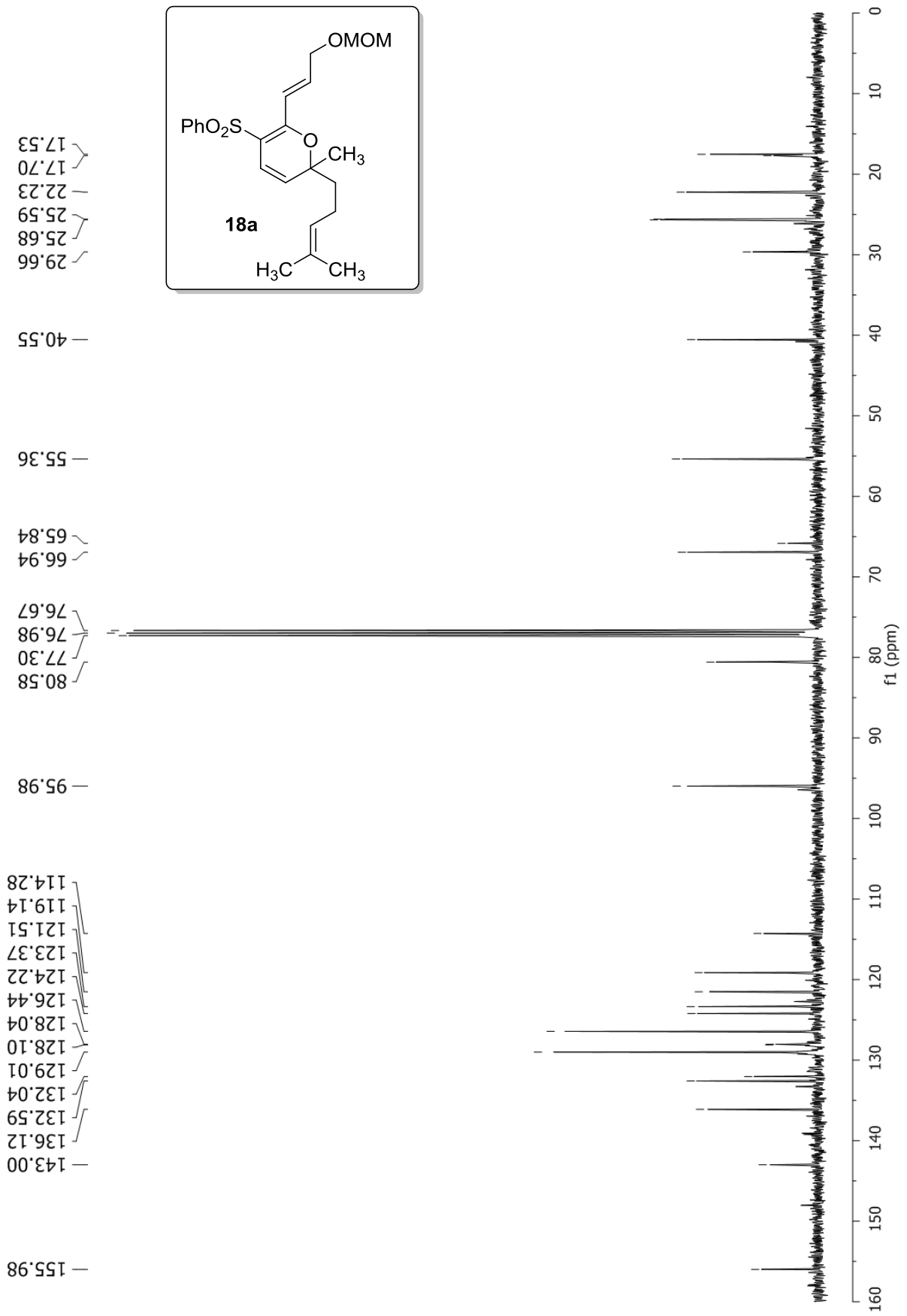


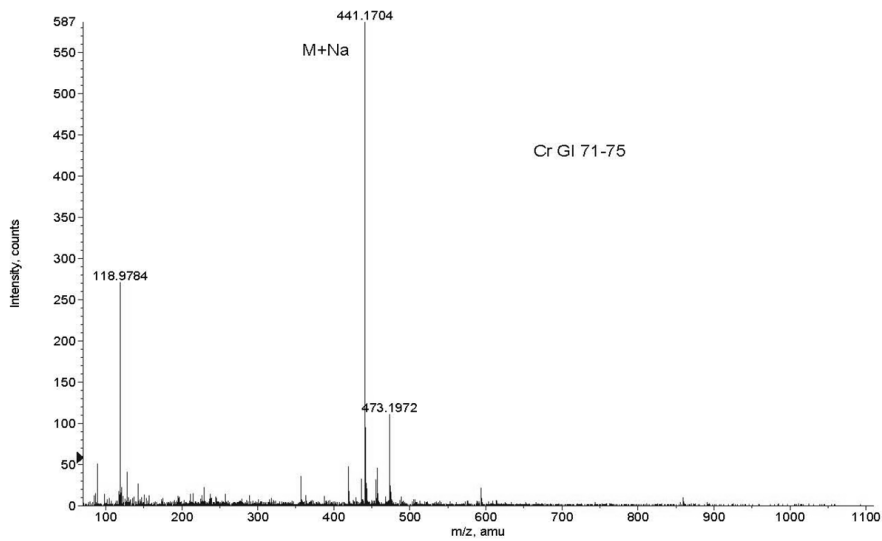
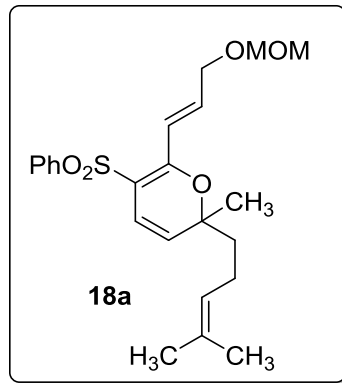
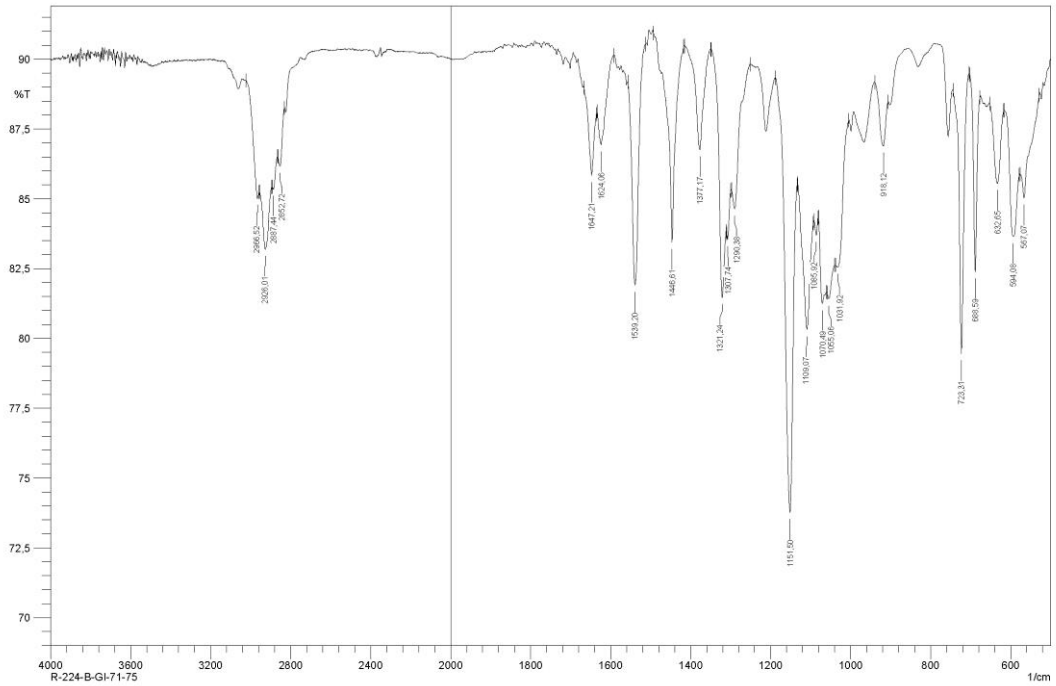
Full Spectroscopy



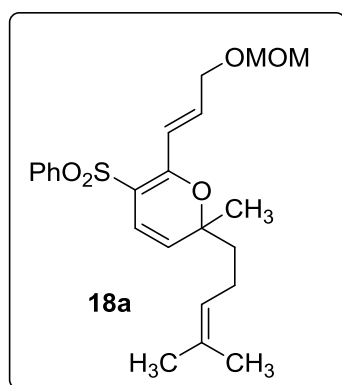
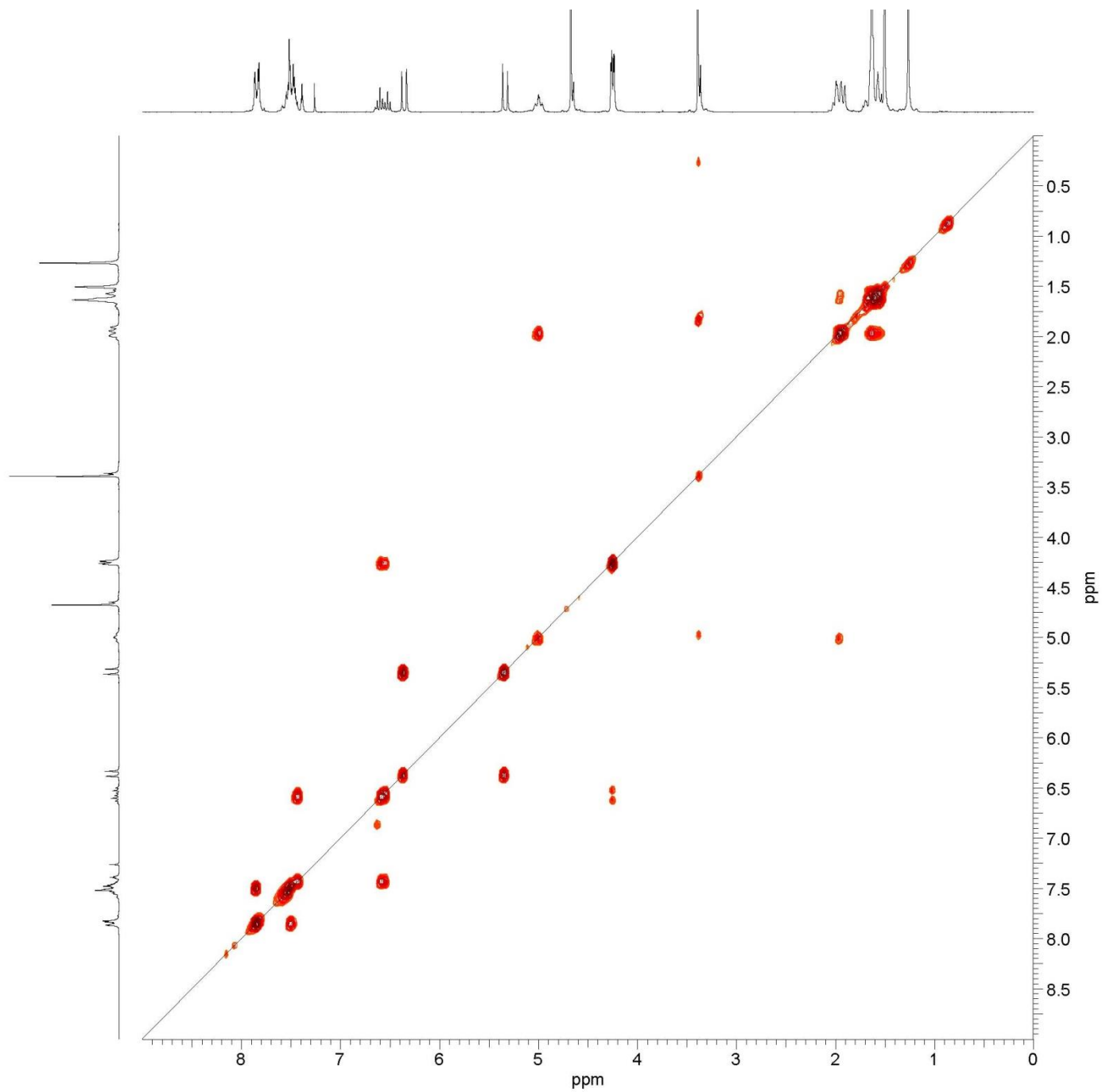
Formula	CalculatedMass	m/z, amu	ppmError	RDB
C41 H54 N O6 Si S	716.343566	0.534372	0.745971	16.5
C42 H50 N5 O2 Si S	716.344903	-0.80294	-1.120885	21.5
C40 H51 N5 O2 Na Si S	716.342498	1.60232	2.2368	18.5
C45 H51 N3 Na Si S	716.34652	-2.420384	-3.378798	22.5

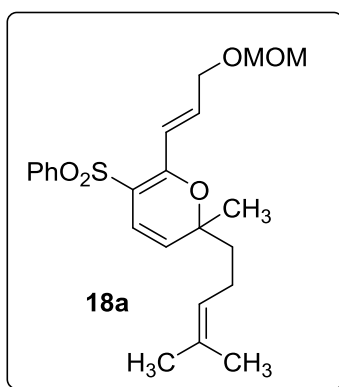
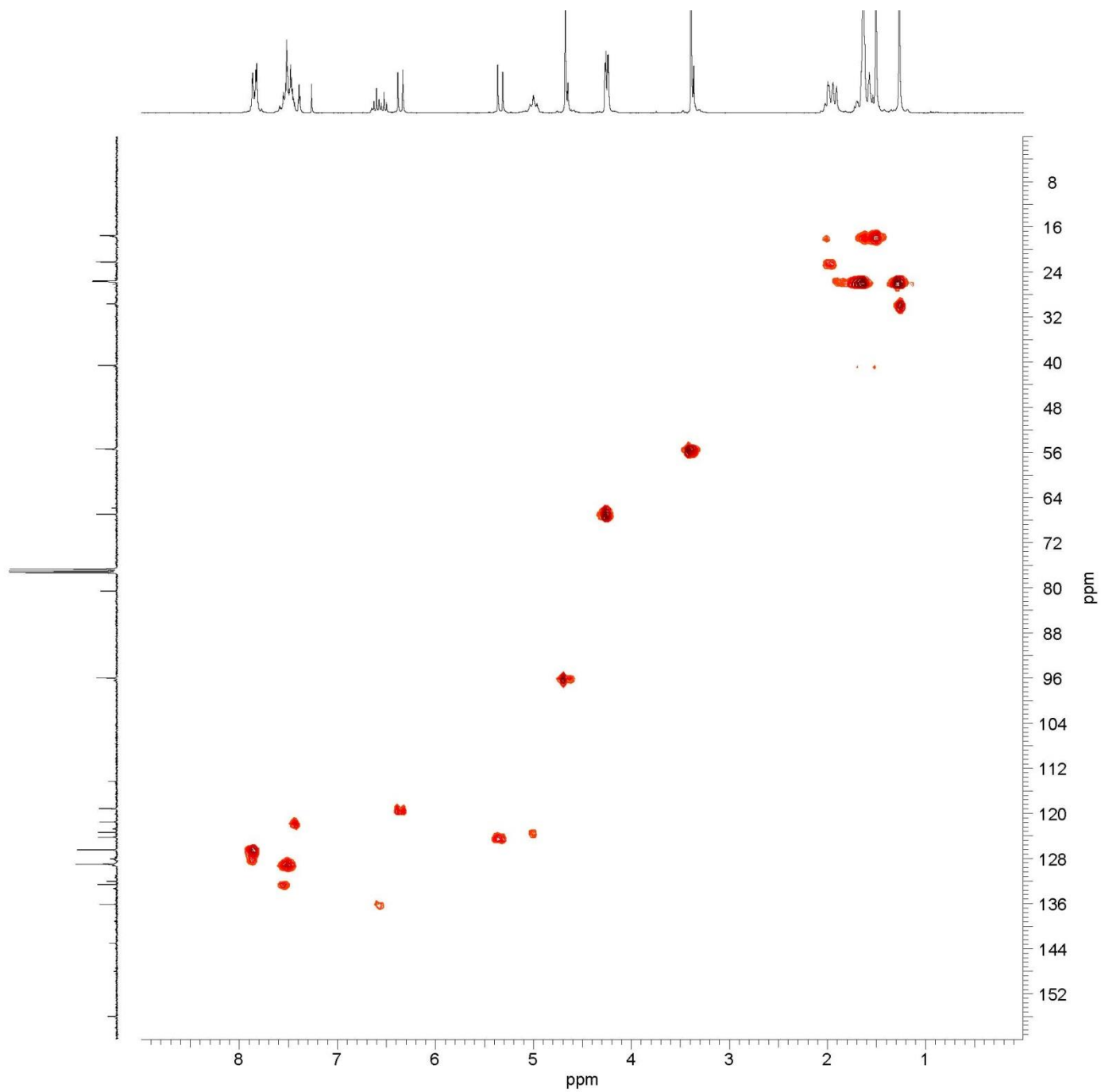


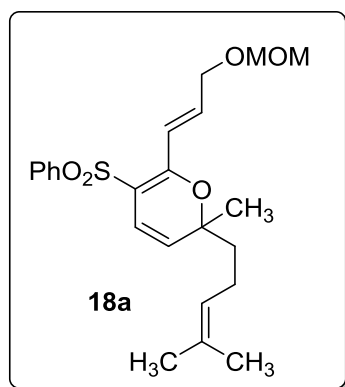
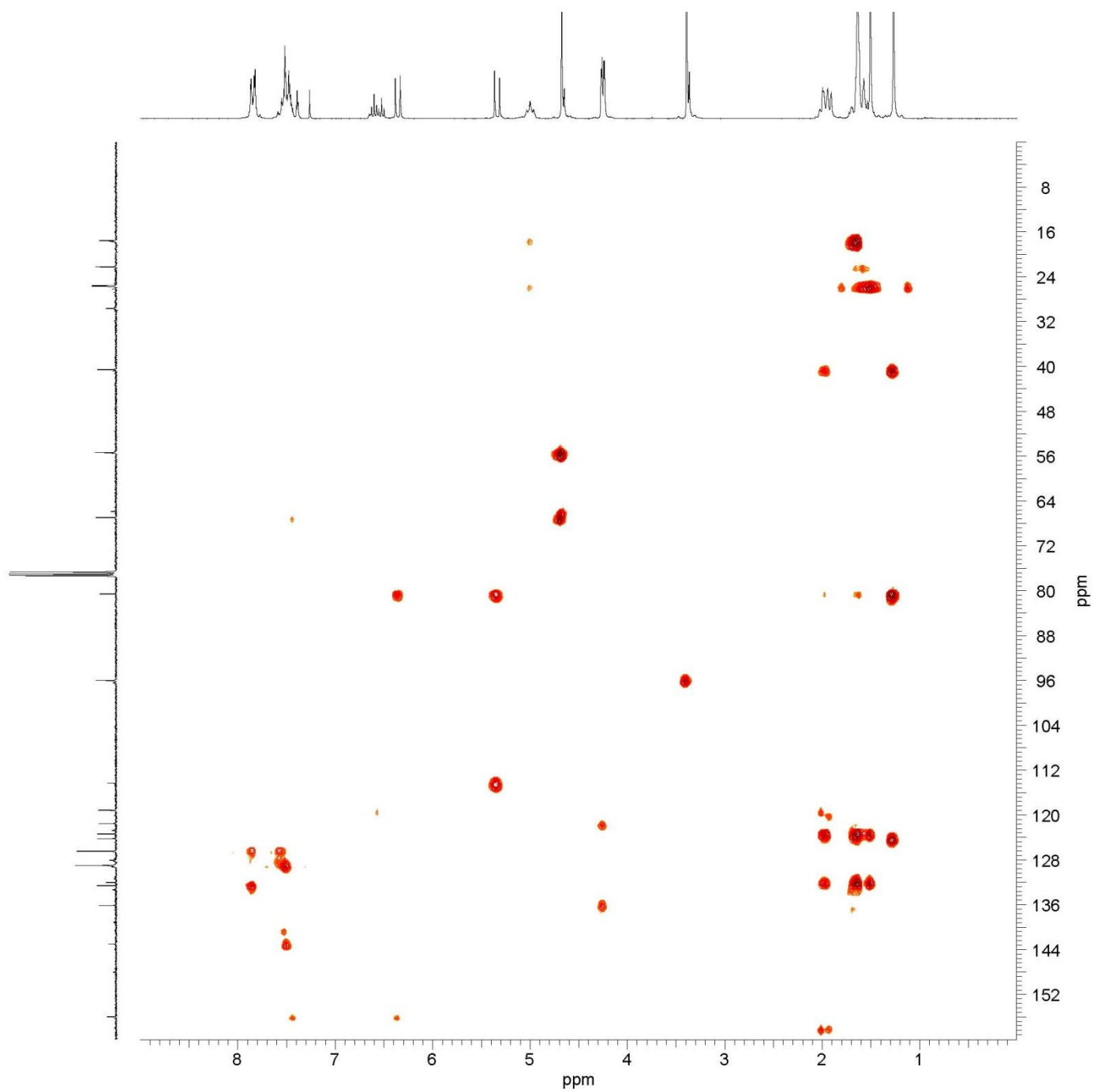


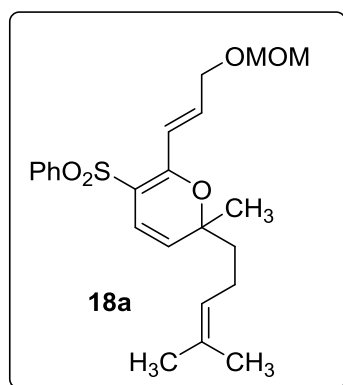
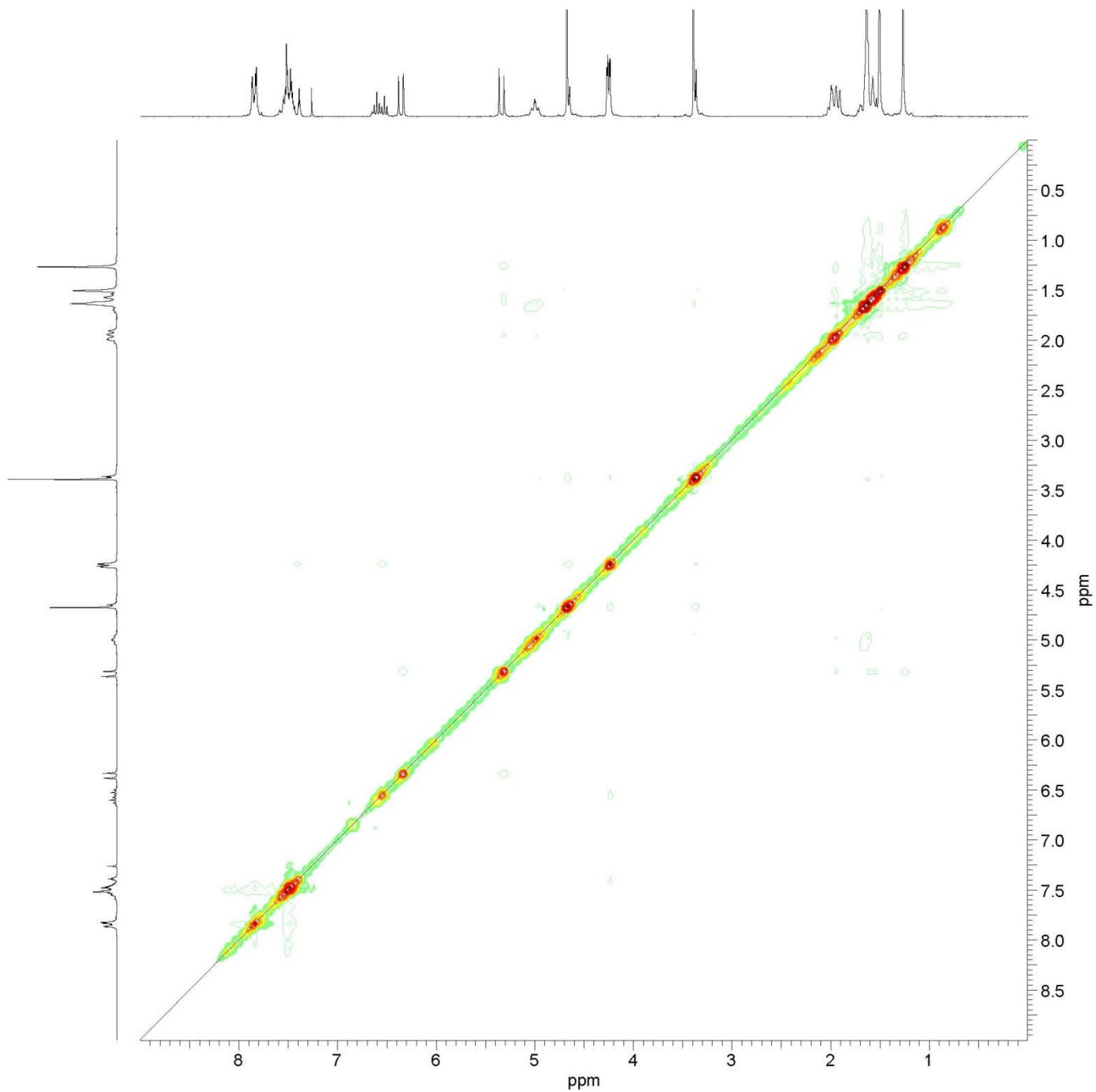


Formula	CalculatedMass	mDaError	ppmError	RDB
C ₂₁ H ₂₅ N ₆ O ₃ S	441.170337	0.062812	0.142376	12.5
C ₂₃ H ₃₀ O ₅ Na S	441.170617	-0.21732	-0.492598	8.5

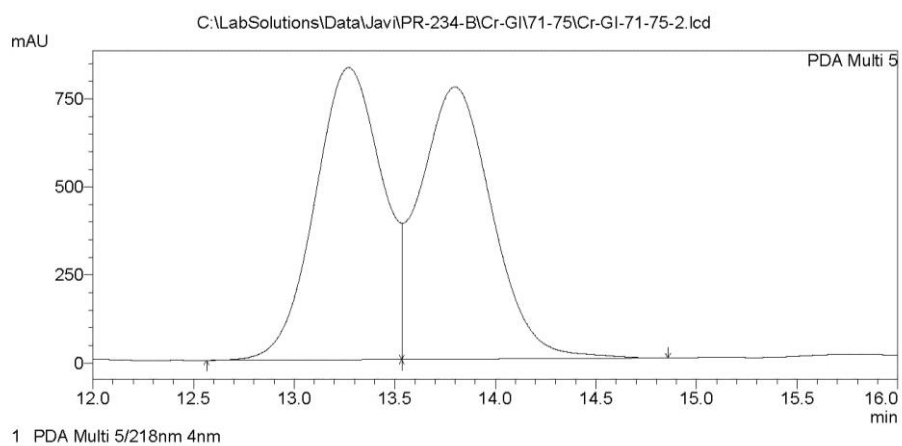








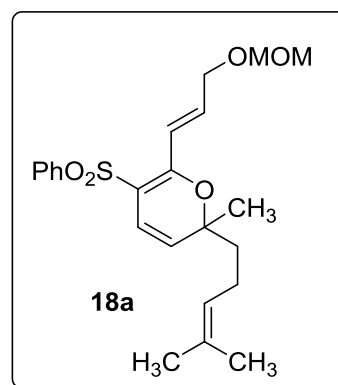
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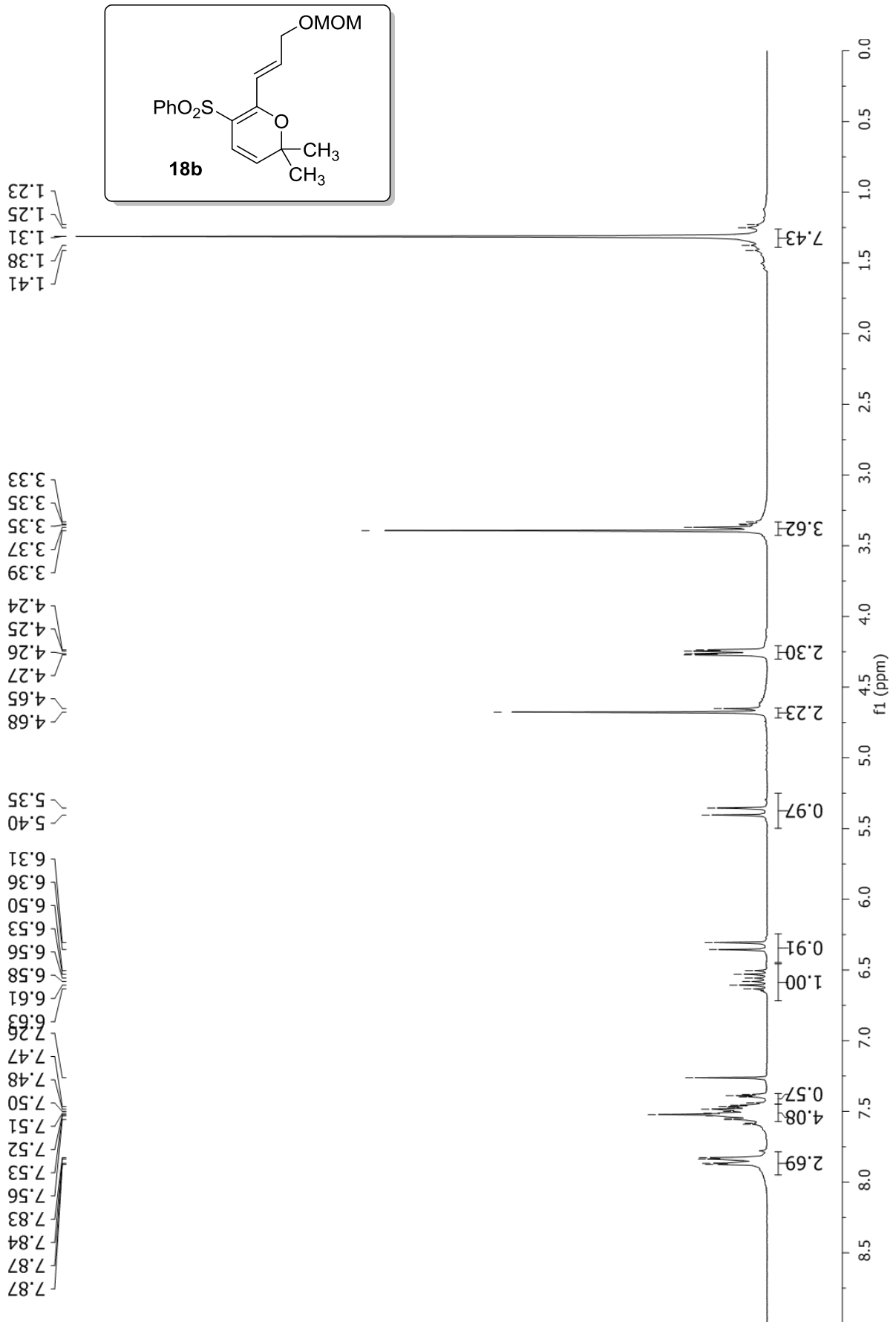


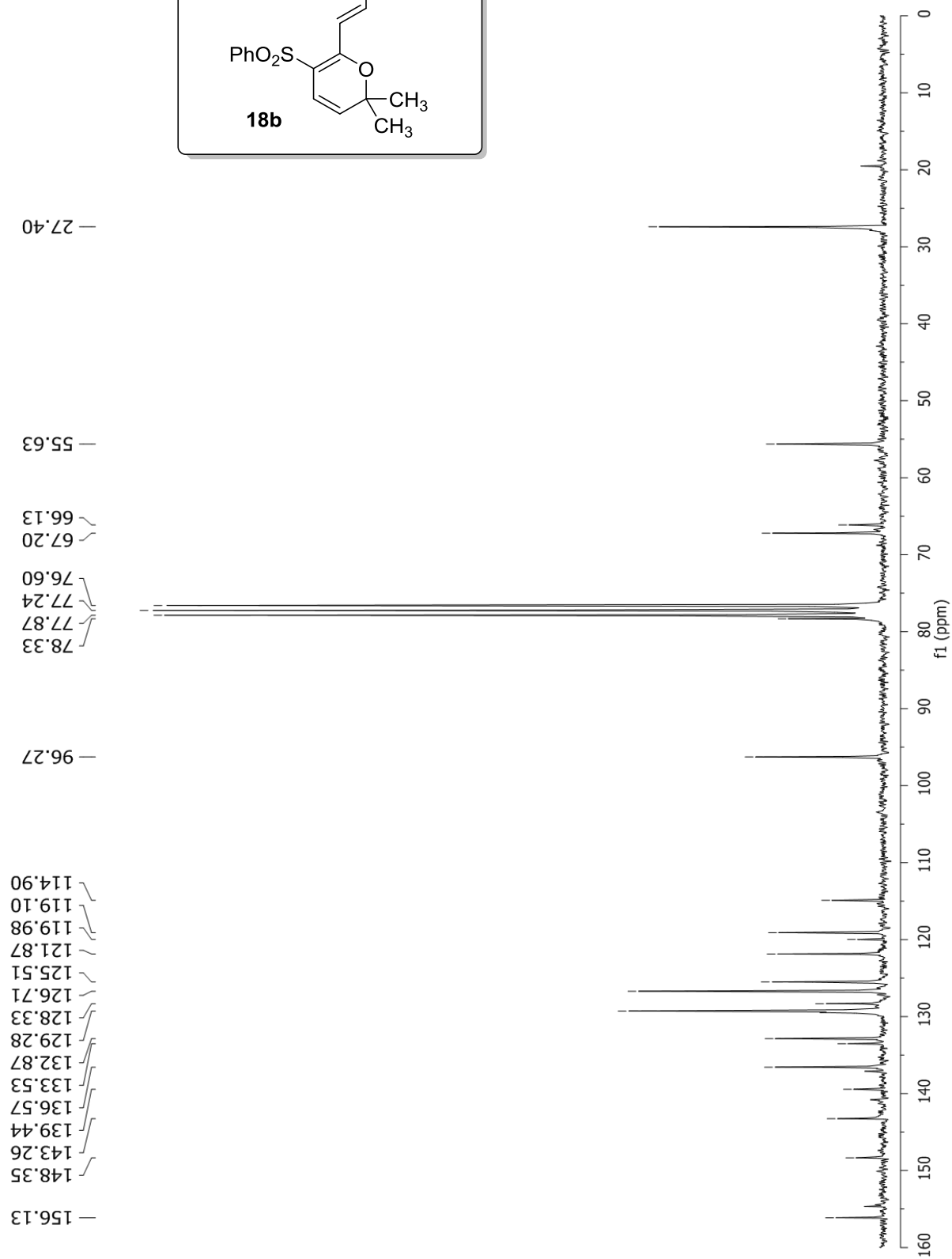
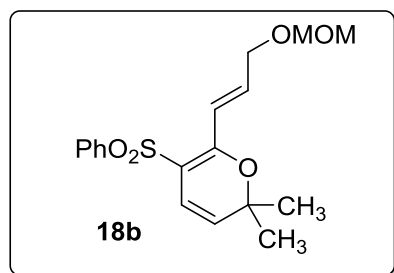
PeakTable

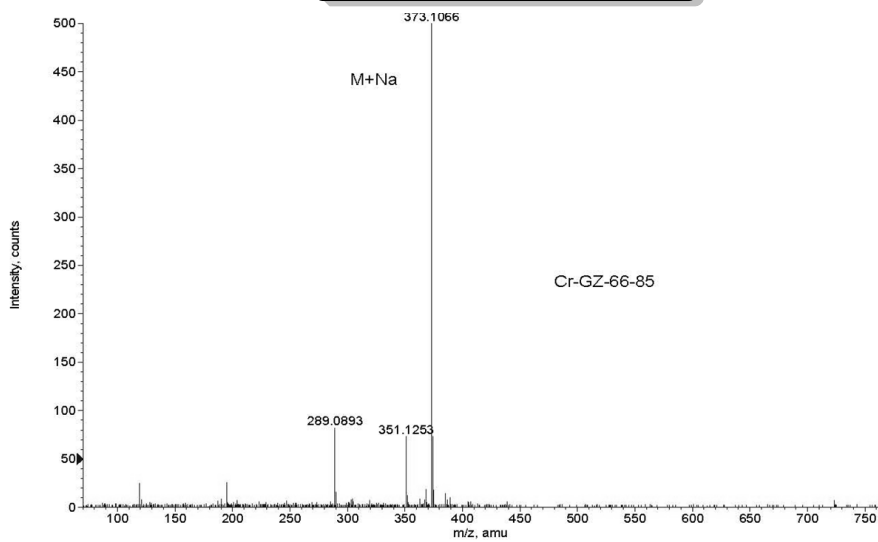
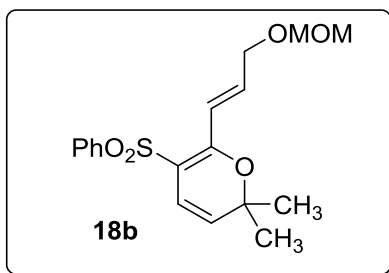
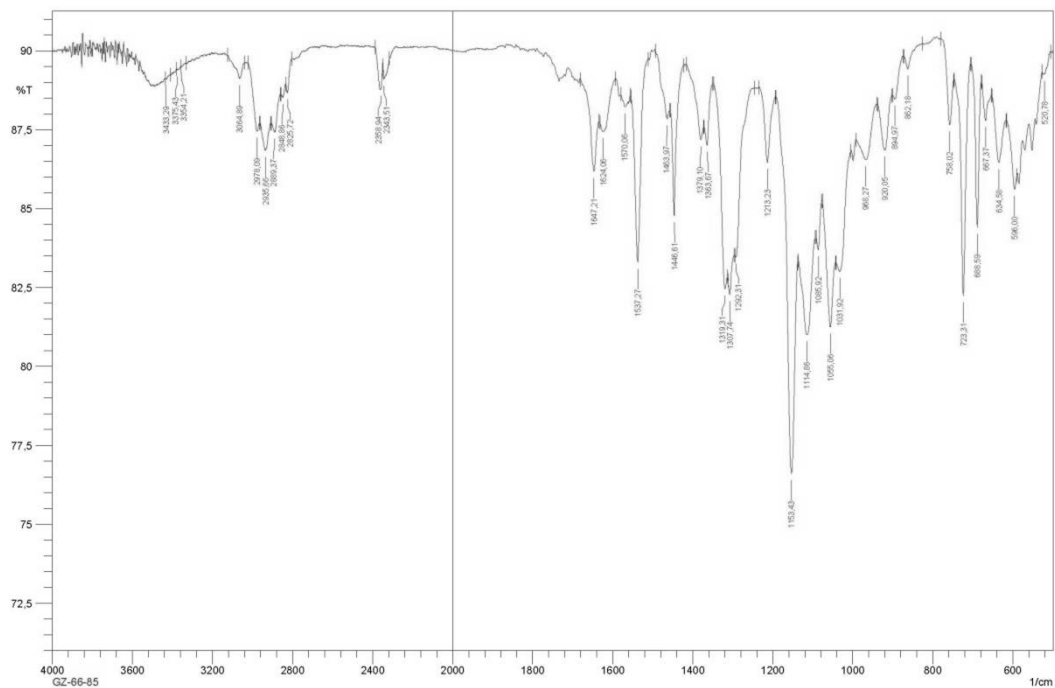
PDA Ch5 218nm 4nm

Peak#	Ret. Time	Area %
1	13.265	50.162
2	13.794	49.838
Total		100.000

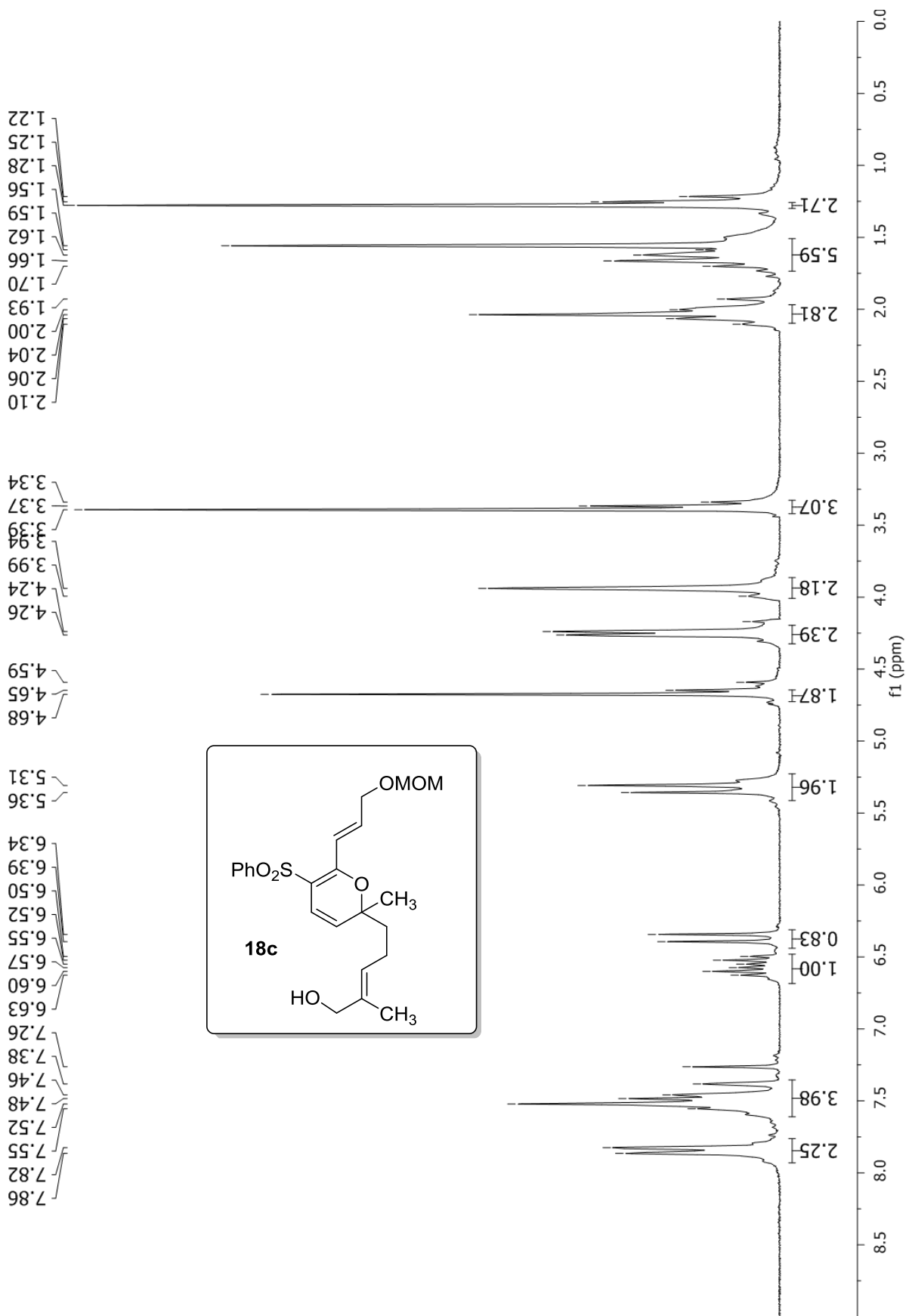


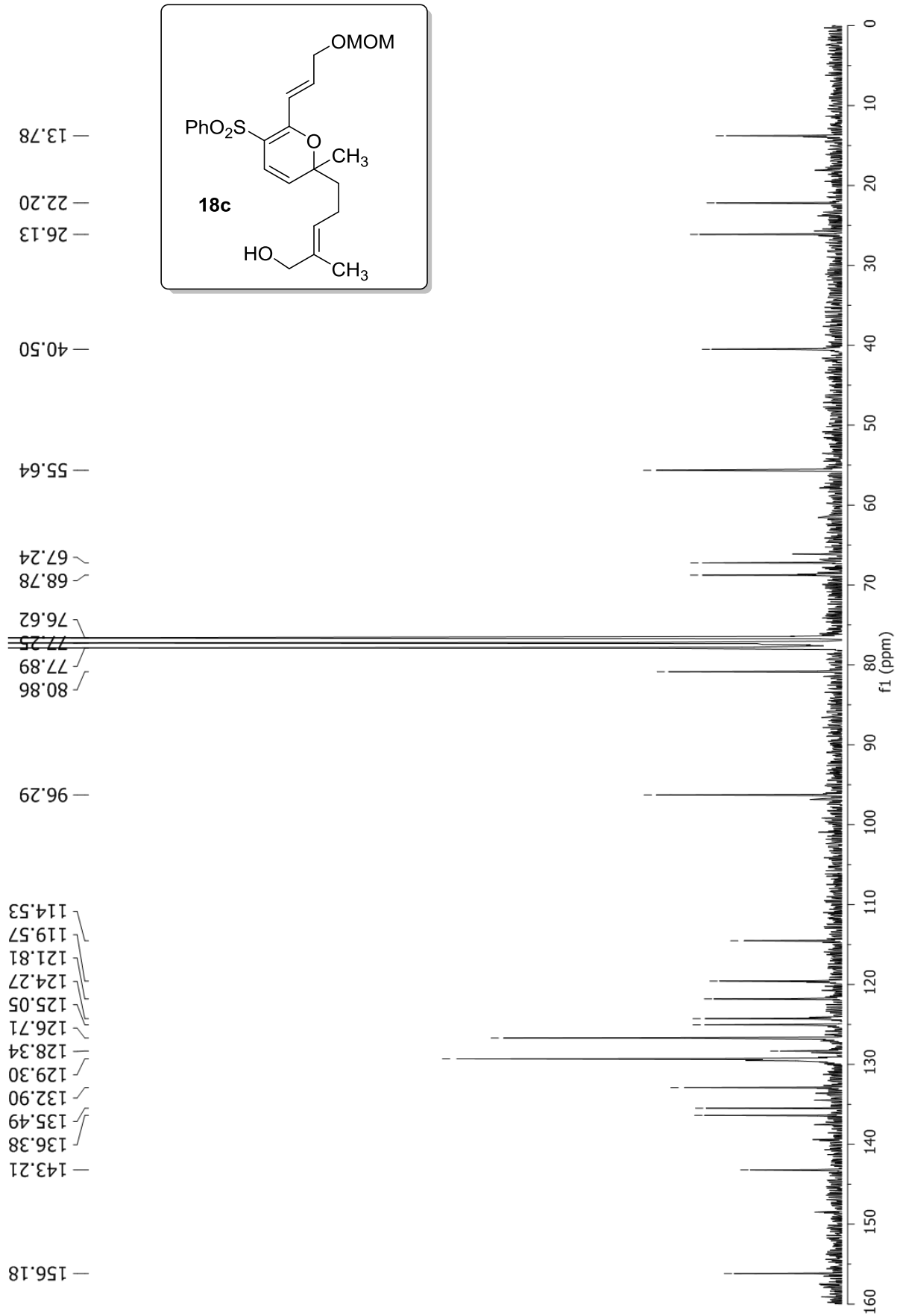


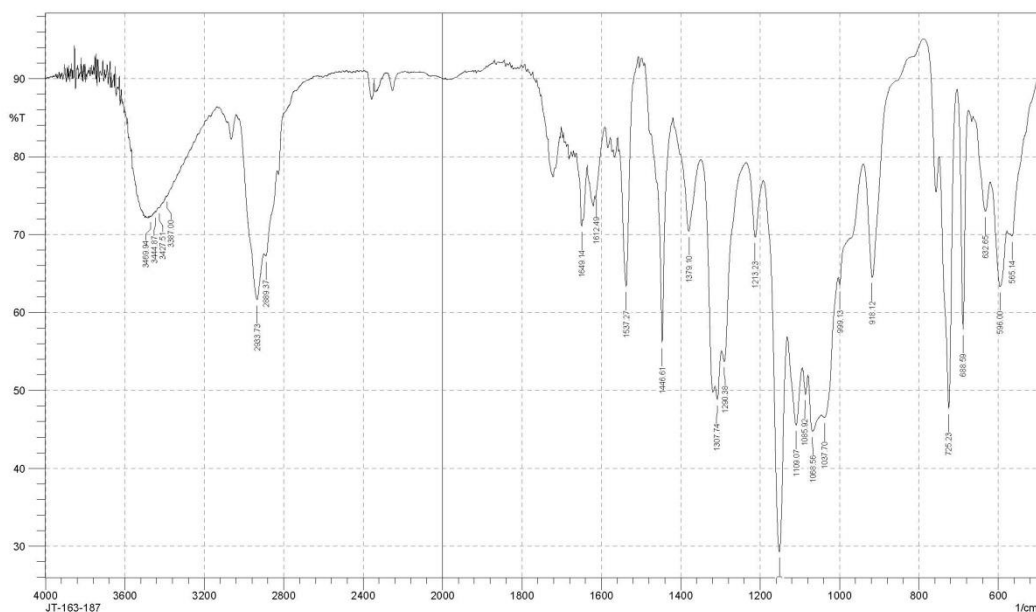




Formula	CalculatedMass	mDaError	ppmError	RDB
C15 H21 N2 O7 S	373.1064	0.200444	0.537229	6.5
H17 N14 O8 S	373.106902	-0.302132	-0.809773	-0.5
C16 H17 N6 O3 S	373.107737	-1.136868	-3.047028	11.5
C14 H18 N6 O3 Na S	373.105332	1.268392	3.399538	8.5
C18 H22 O5 Na S	373.108017	-1.417	-3.797837	7.5
C12 H13 N12 O S	373.105051	1.548524	4.150347	12.5
C3 H18 N12 O6 Na S	373.10852	-1.919576	-5.144838	0.5
C27 H17 S	373.104549	2.0511	5.497348	19.5
C13 H22 N2 O7 Na S	373.103994	2.605704	6.983795	3.5
C19 H18 N4 O Na S	373.109354	-2.754312	-7.382094	12.5
C11 H17 N8 O5 S	373.103714	2.885836	7.734604	7.5



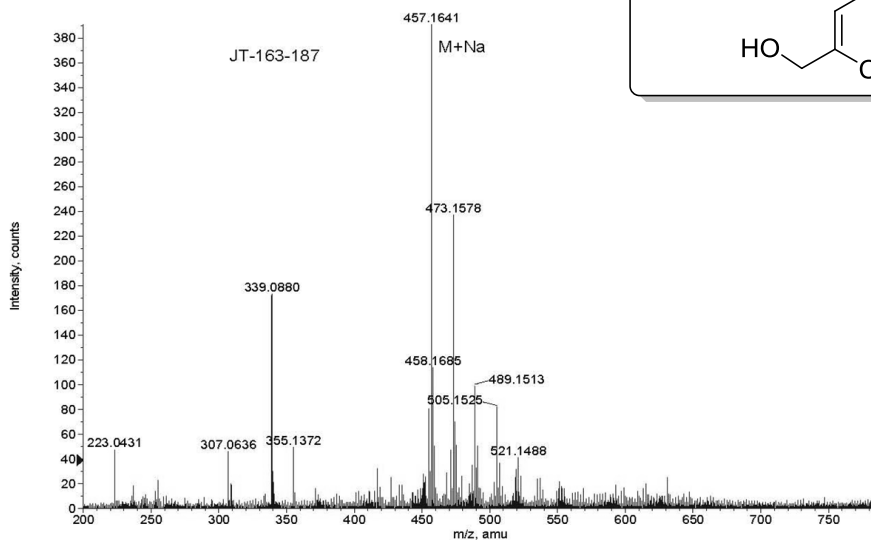
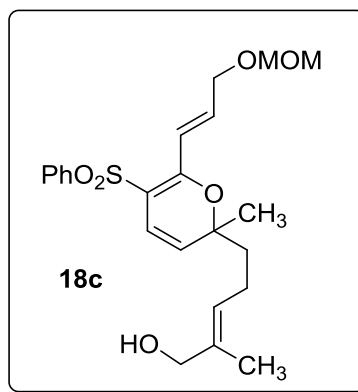




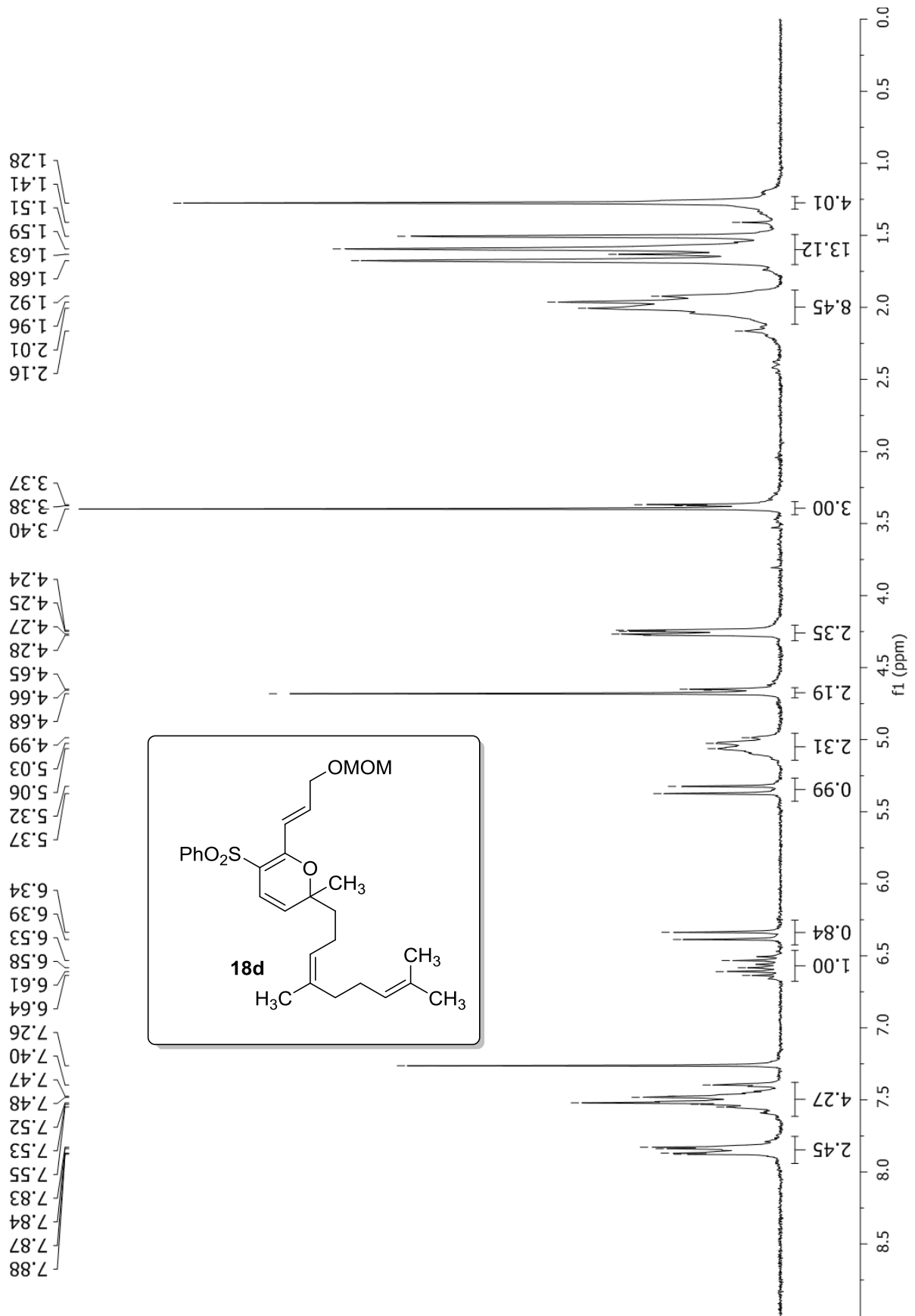
Comment:
JT-163-187

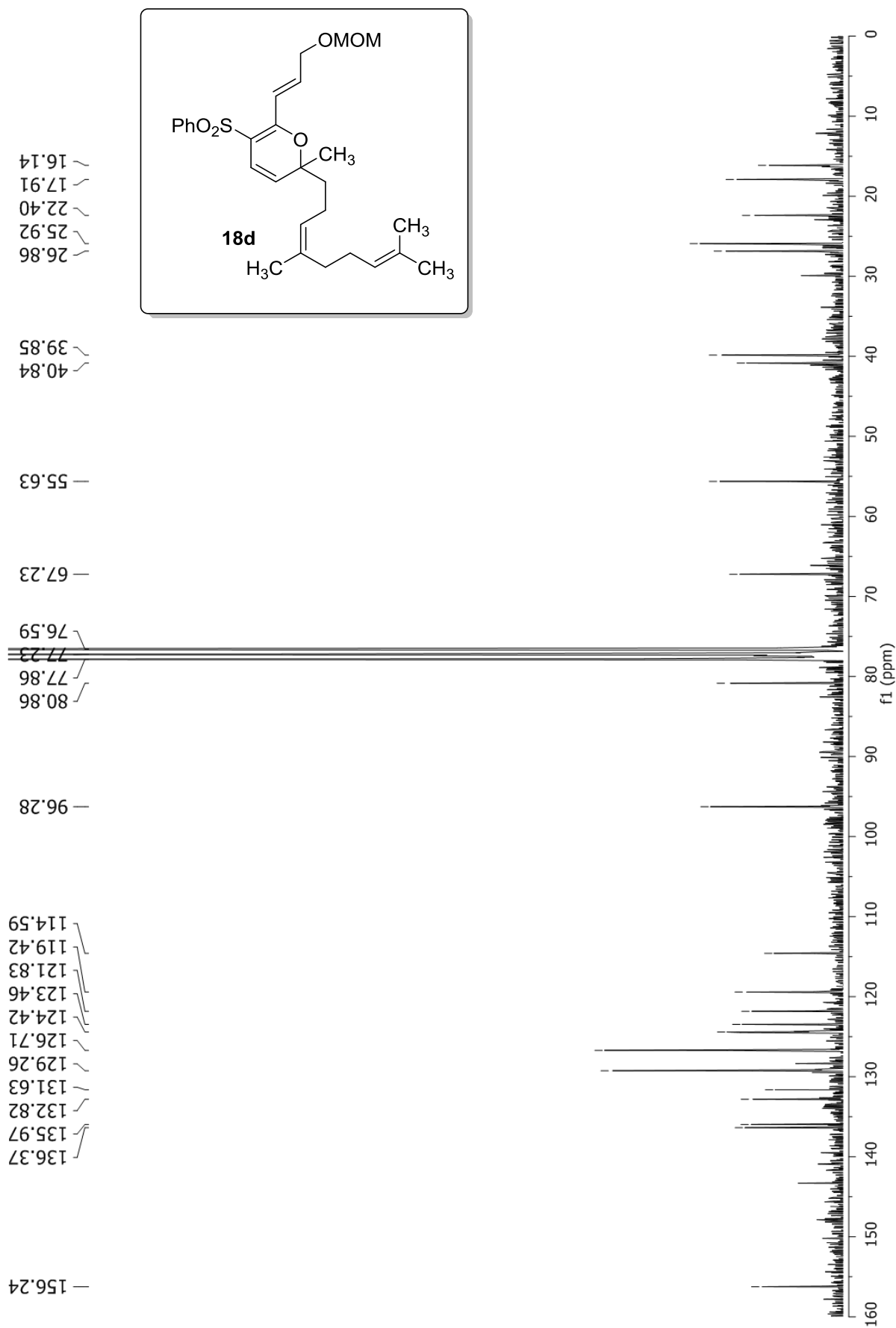
No. of Scans;
Resolution;
Apodization;

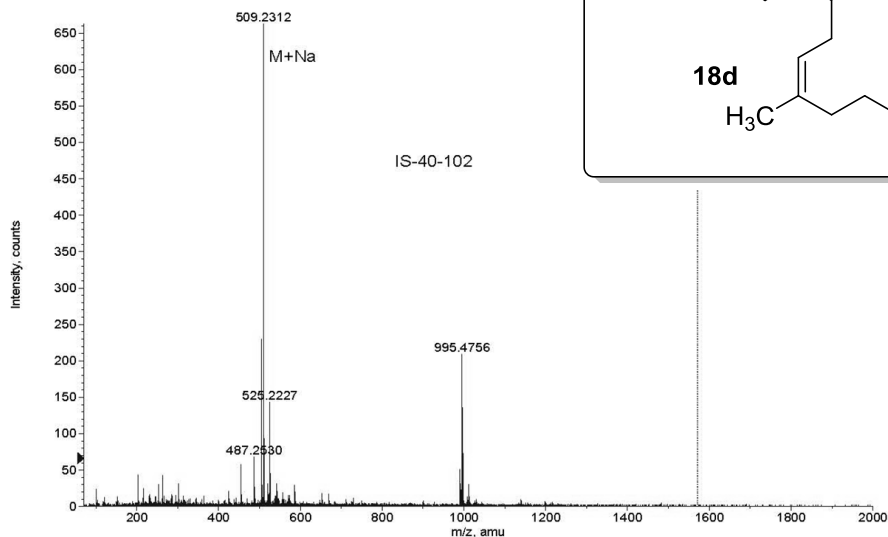
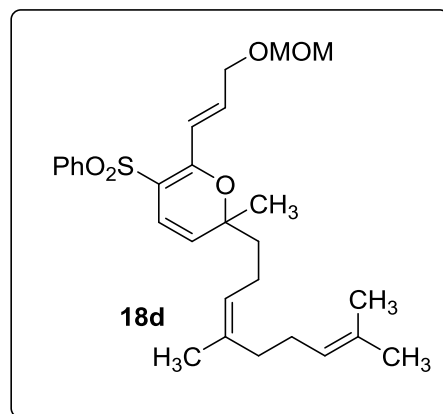
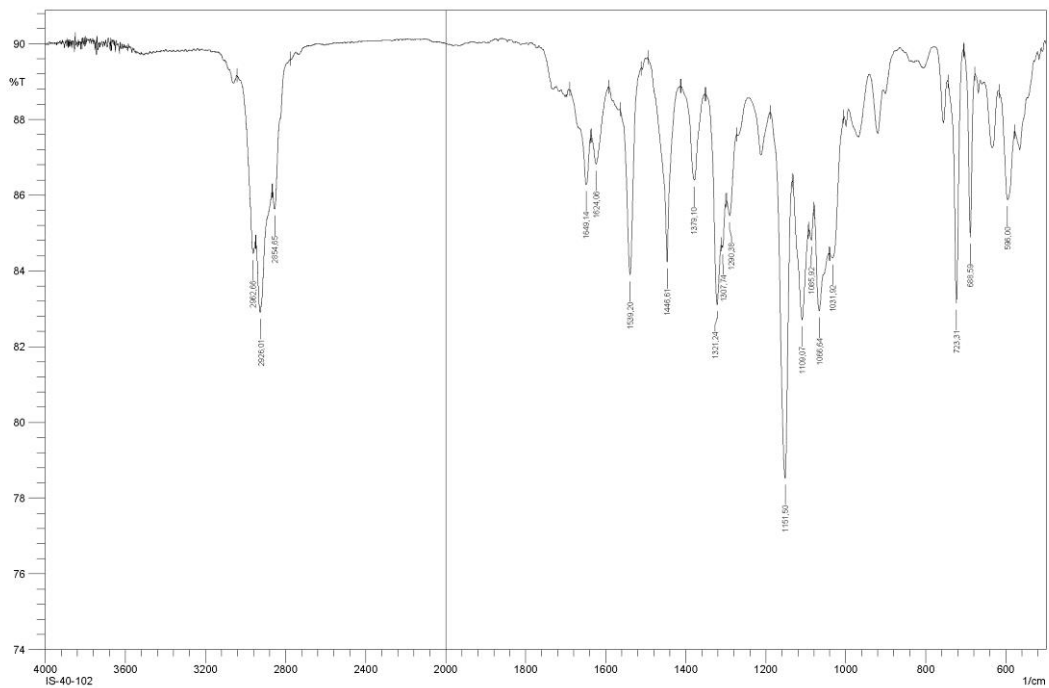
Date/Time: 26/03/2012 10:06:59
User: Usuario



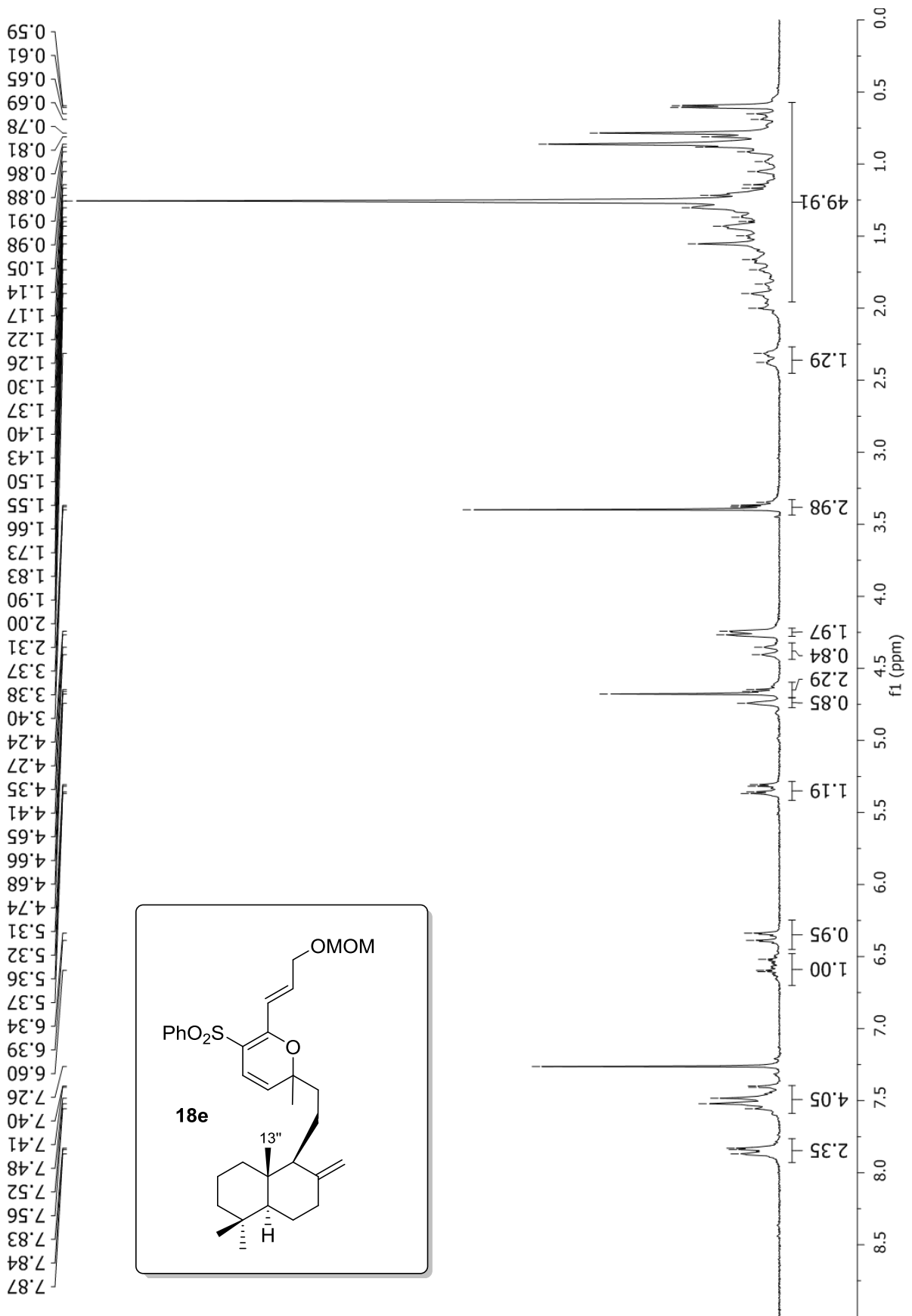
Formula	CalculatedMass	mDaError	ppmError	RDB
C ₂₀ H ₂₂ N ₁₀ Na S	457.164184	-0.08388	-0.183479	14.5
C ₂₀ H ₂₉ N ₂ O ₈ S	457.163915	0.185484	0.405727	7.5
C ₅ H ₂₅ N ₁₄ O ₉ S	457.164417	-0.317092	-0.693606	0.5
C ₂₁ H ₂₅ N ₆ O ₄ S	457.165252	-1.151828	-2.519504	12.5
C ₁₉ H ₂₆ N ₆ O ₄ Na S	457.162847	1.253432	2.741752	9.5
C ₂₃ H ₃₀ O ₆ Na S	457.165532	-1.43196	-3.132263	8.5
C ₁₇ H ₂₁ N ₁₂ O ₂ S	457.162566	1.533564	3.354511	13.5
C ₈ H ₂₆ N ₁₂ O ₇ Na S	457.166035	-1.934536	-4.231596	1.5
C ₃₂ H ₂₅ O S	457.162064	2.03614	4.453844	20.5
C ₂₂ H ₂₁ N ₁₀ S	457.166580	2.48014	5.444724	17.5

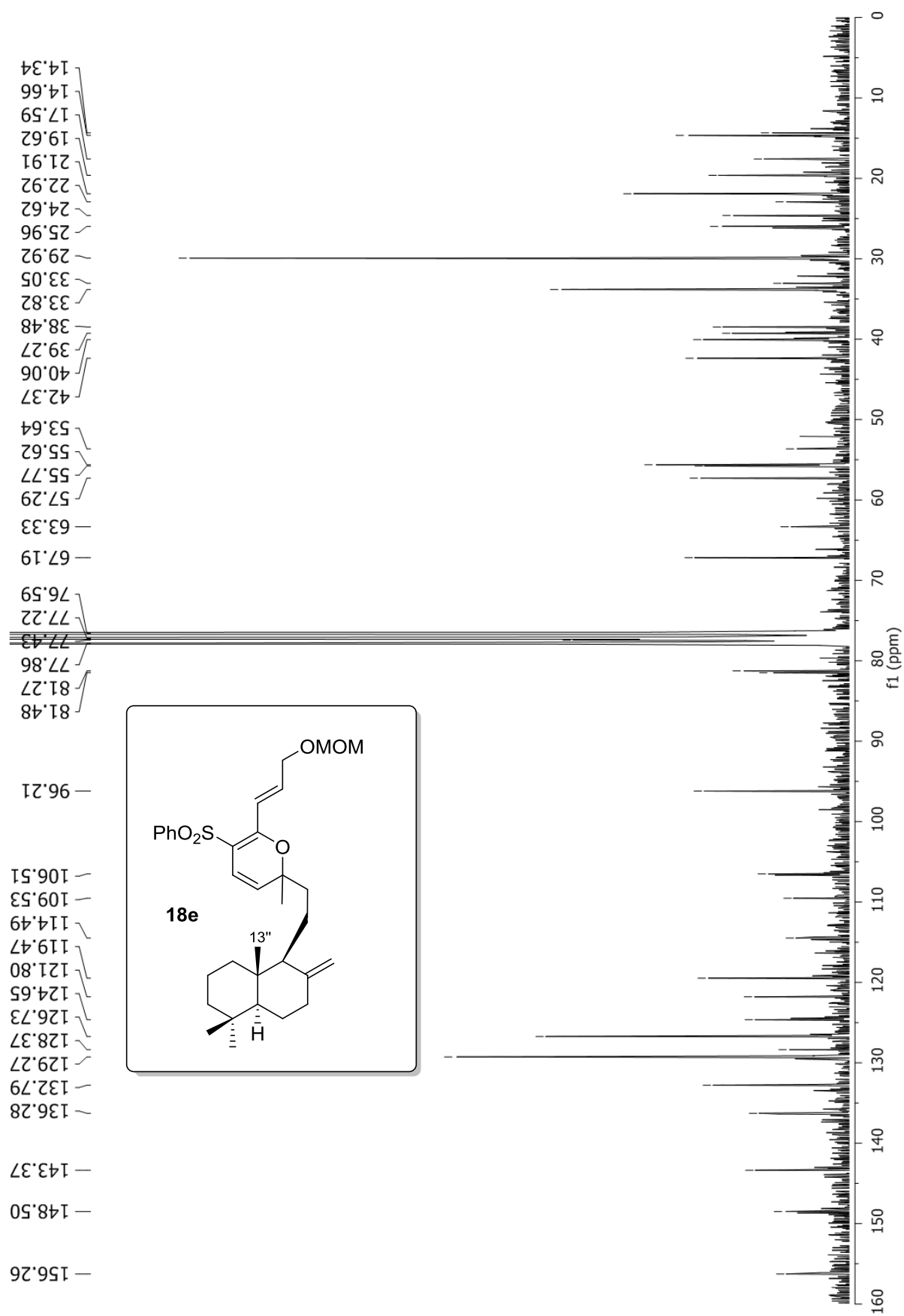


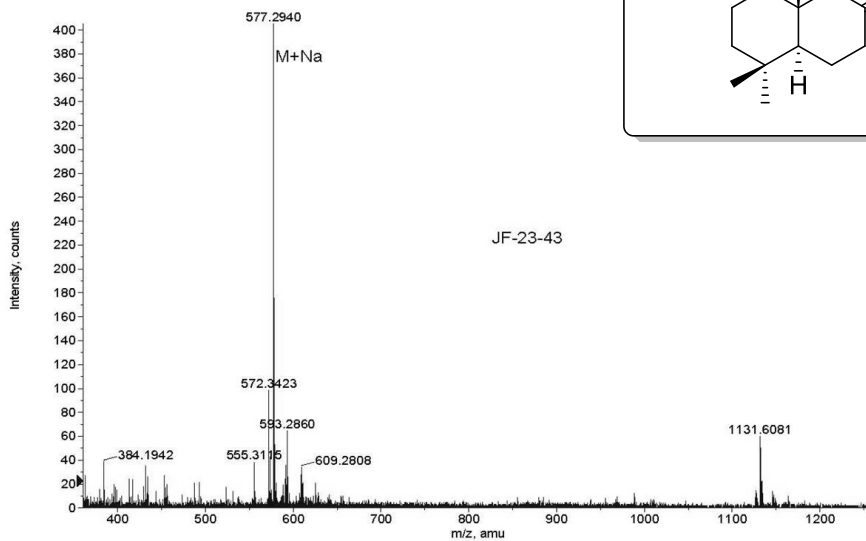
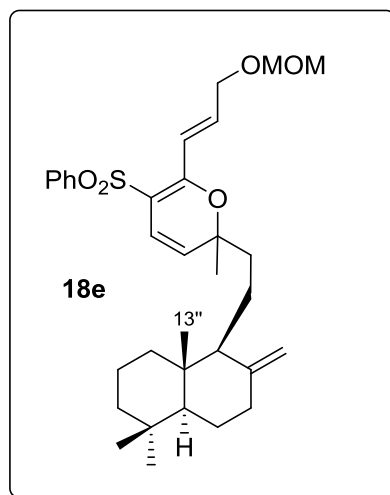
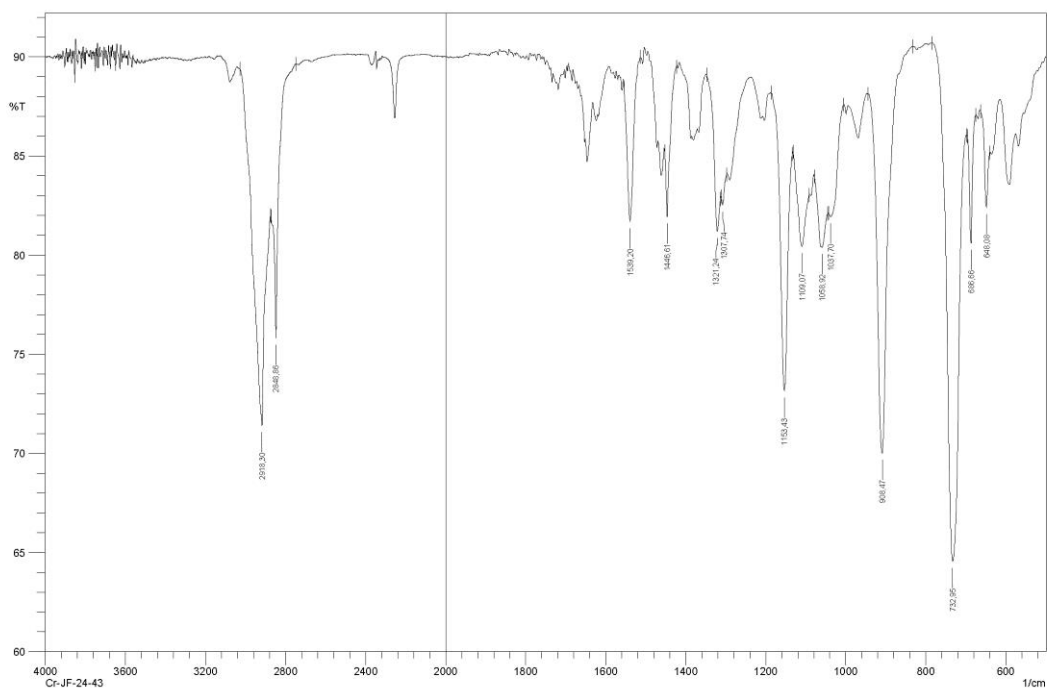




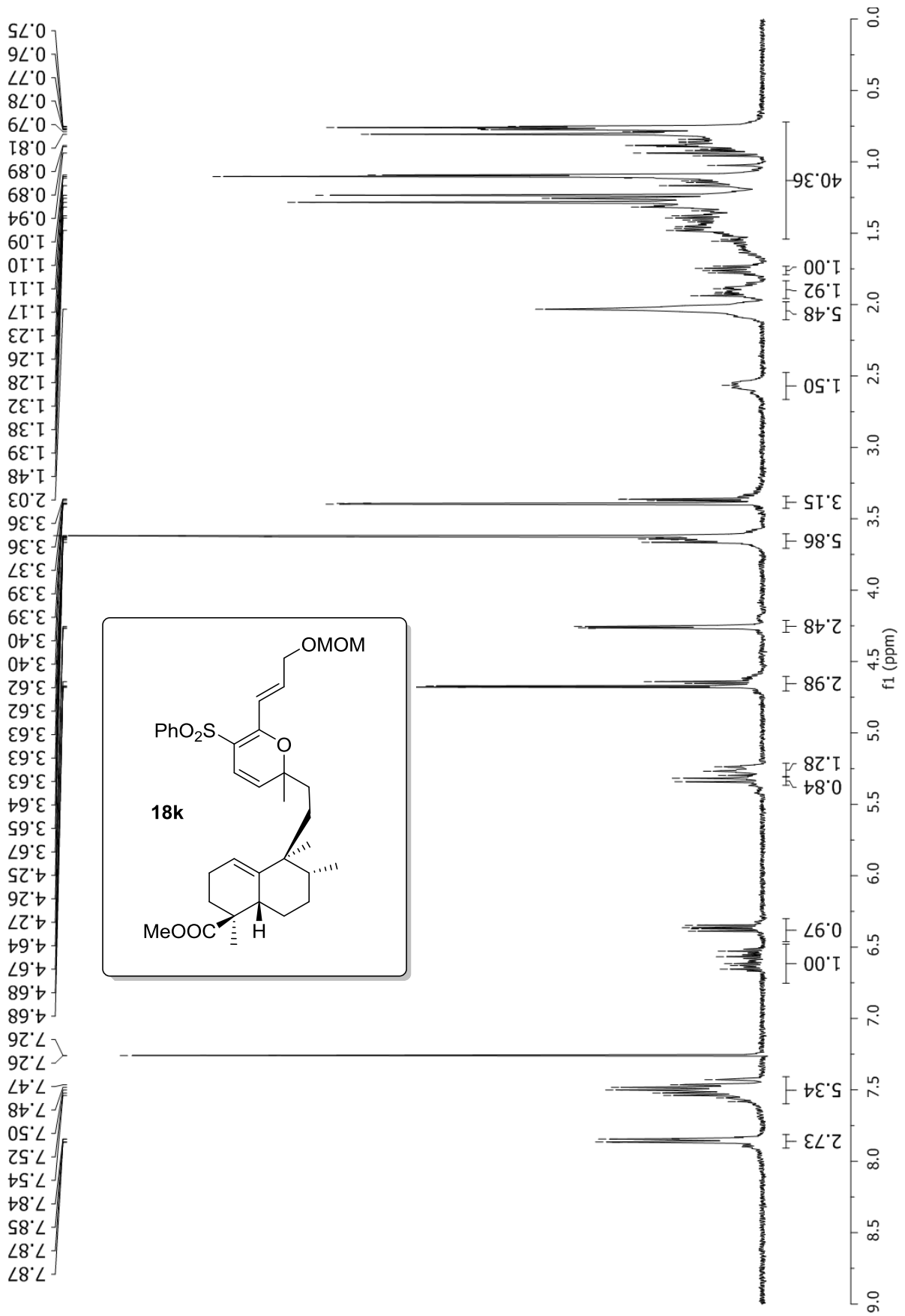
Formula	CalculatedMass	mDaError	ppmError	RDB
C ₂₅ H ₃₇ N ₂ O ₇ S	509.2316	-0.400196	-0.785882	8.5
C ₂₄ H ₃₄ N ₆ O ₃ NaS	509.230532	0.667752	1.311293	10.5
C ₁₀ H ₃₃ N ₁₄ O ₈ S	509.232103	-0.902772	-1.772812	1.5
C ₂₂ H ₂₉ N ₁₂ O ₅ S	509.230252	0.947884	1.8614	14.5
C ₃₇ H ₃₃ S	509.22975	1.45046	2.84833	21.5
C ₂₆ H ₃₃ N ₆ O ₃ S	509.232938	-1.737508	-3.412018	13.5
C ₂₃ H ₃₈ N ₂ O ₇ NaS	509.229195	2.005064	3.937429	5.5
C ₂₈ H ₃₈ O ₅ Na ₂ S	509.233218	-0.01764	-3.962125	9.5

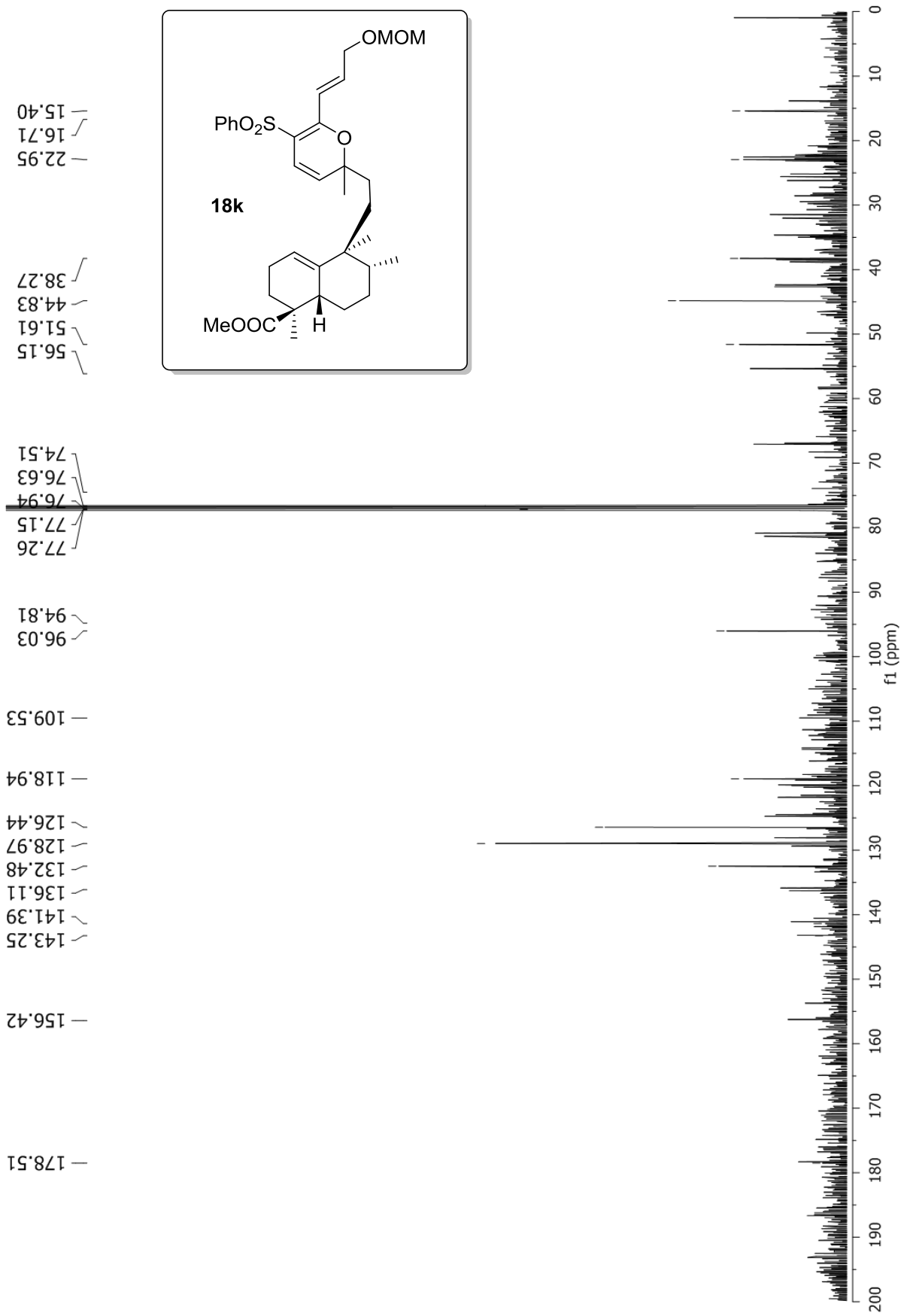


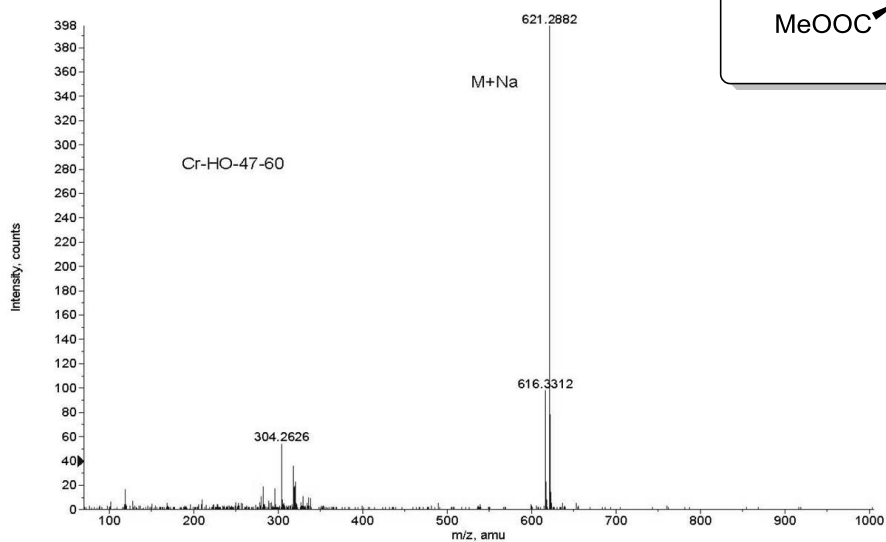
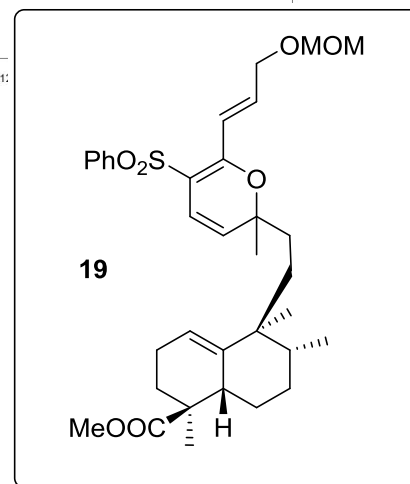
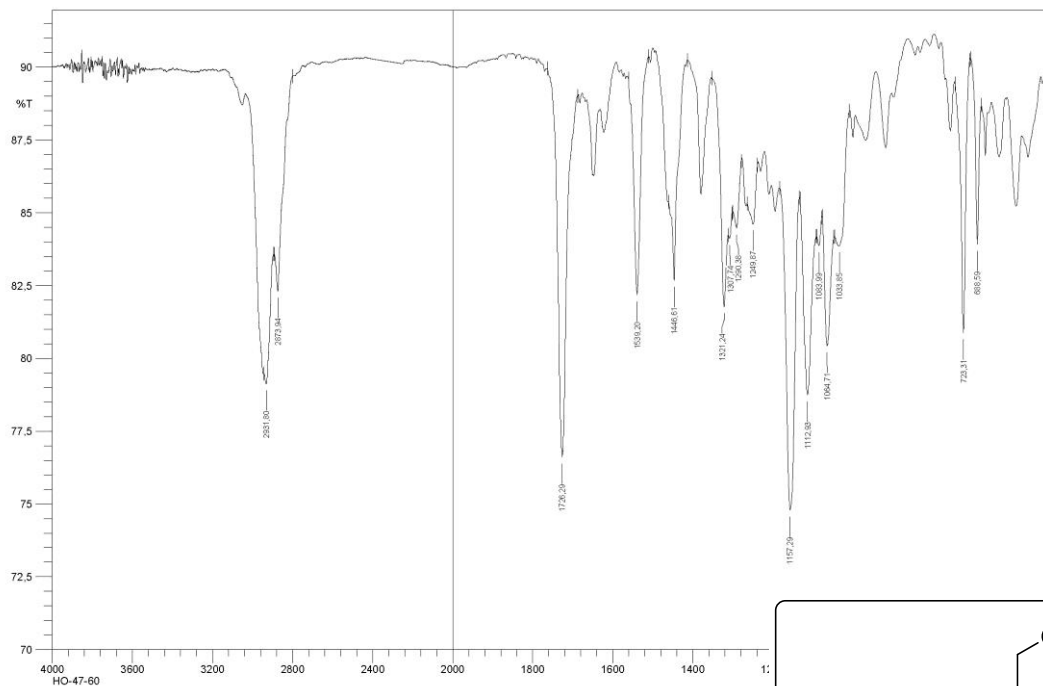




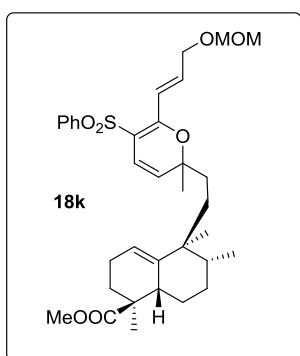
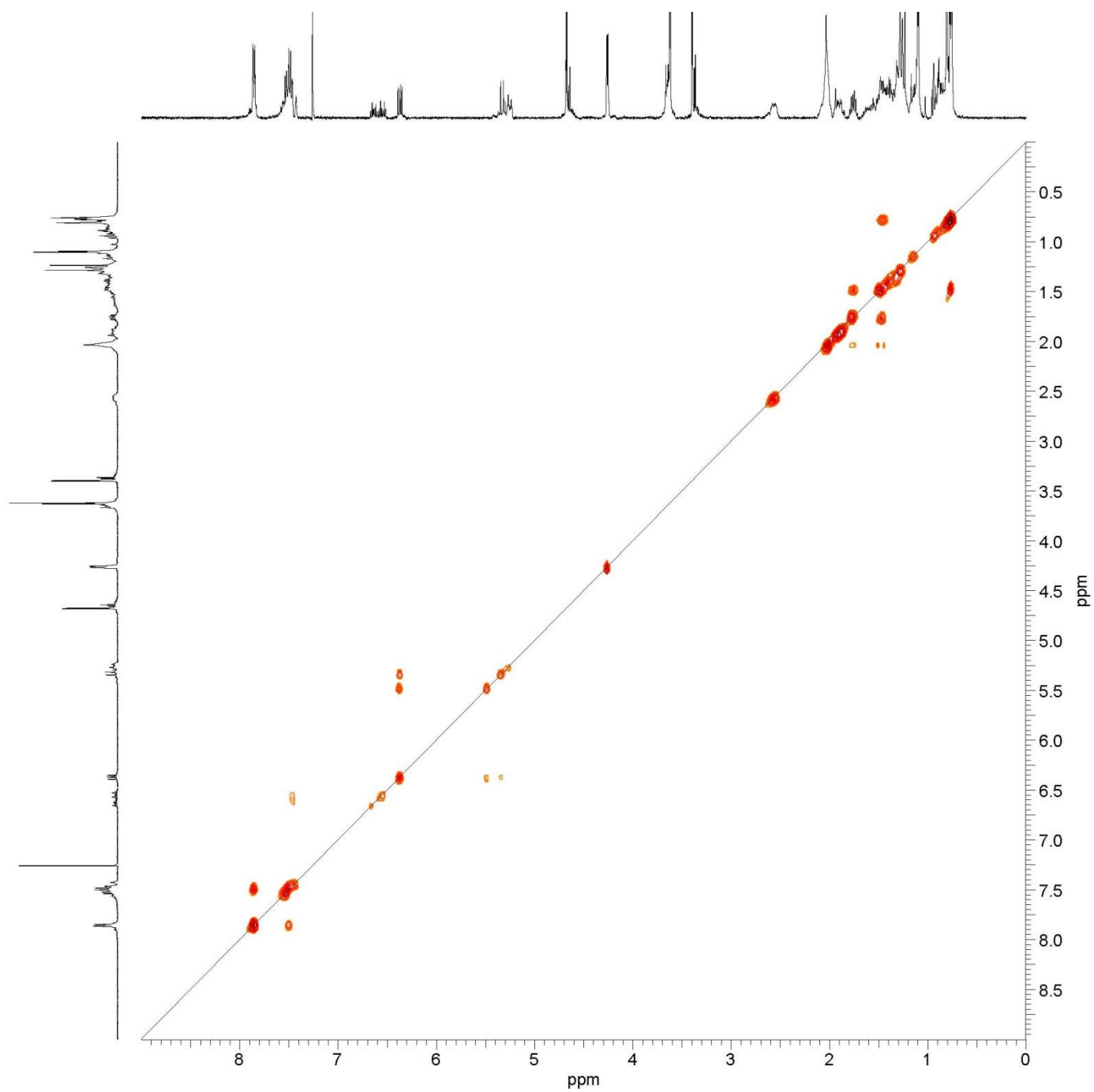
Formula	CalculatedMass	mDaError	ppmError	RDB
C42 H41 S	577.29235	1.65014	2.858402	22.5
C33 H46 O5 Na S	577.295818	-1.81796	-3.149103	10.5
C40 H42 Na S	577.289945	4.0554	7.024837	19.5
C35 H45 O5 S	577.298223	-4.22322	-7.315538	13.5
C24 H49 O13 S	577.28884	5.1595	8.937379	0.5

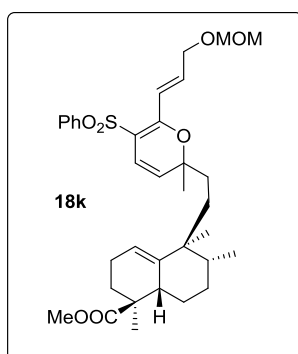
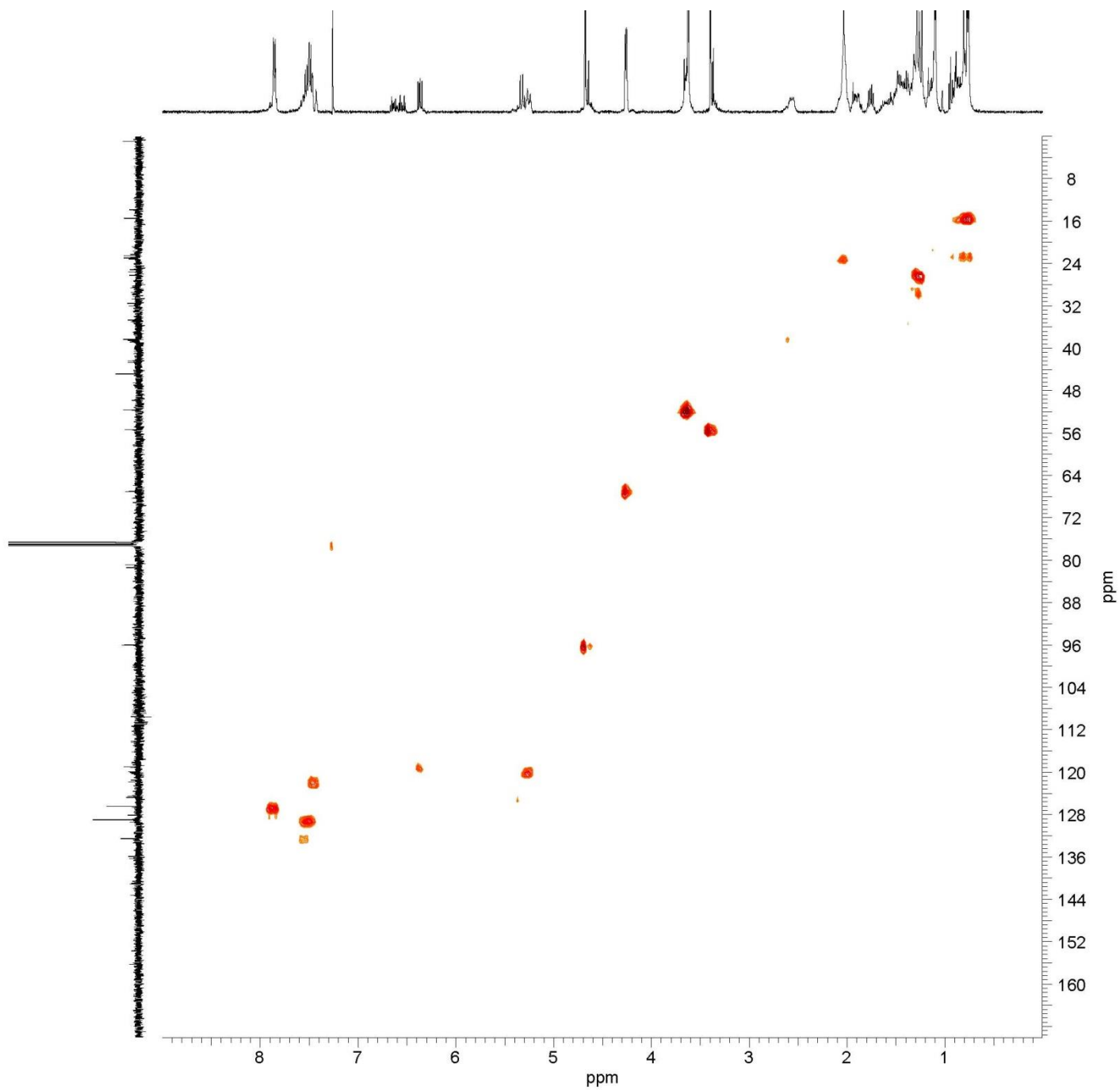


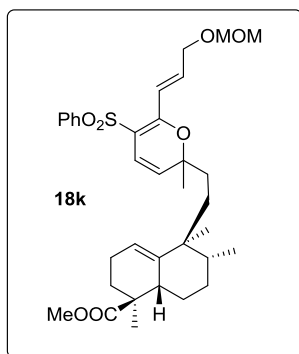
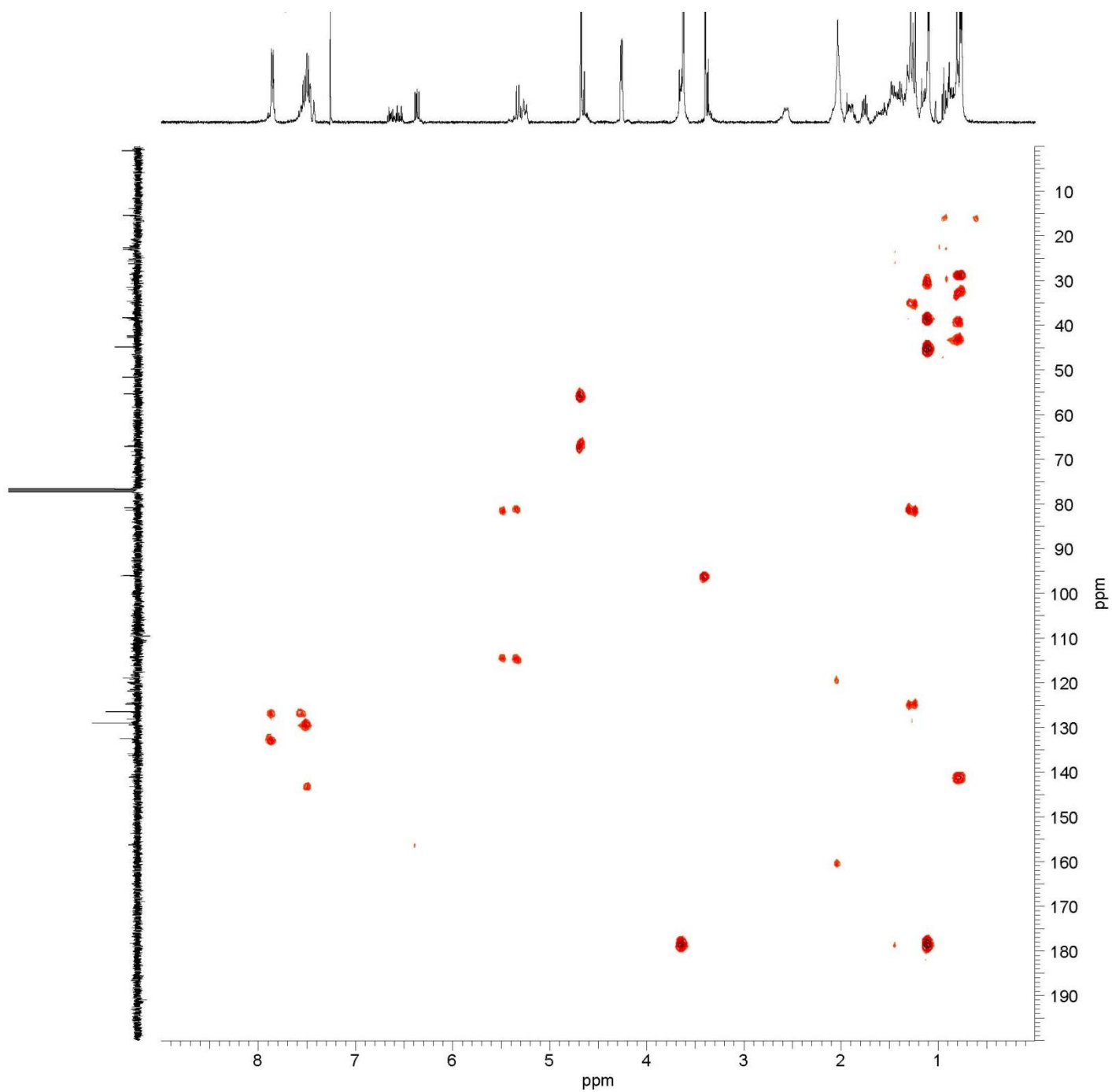


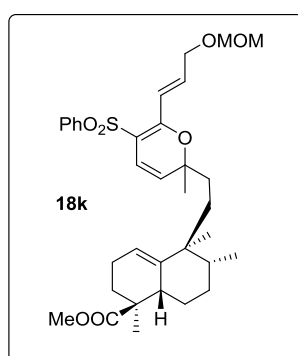
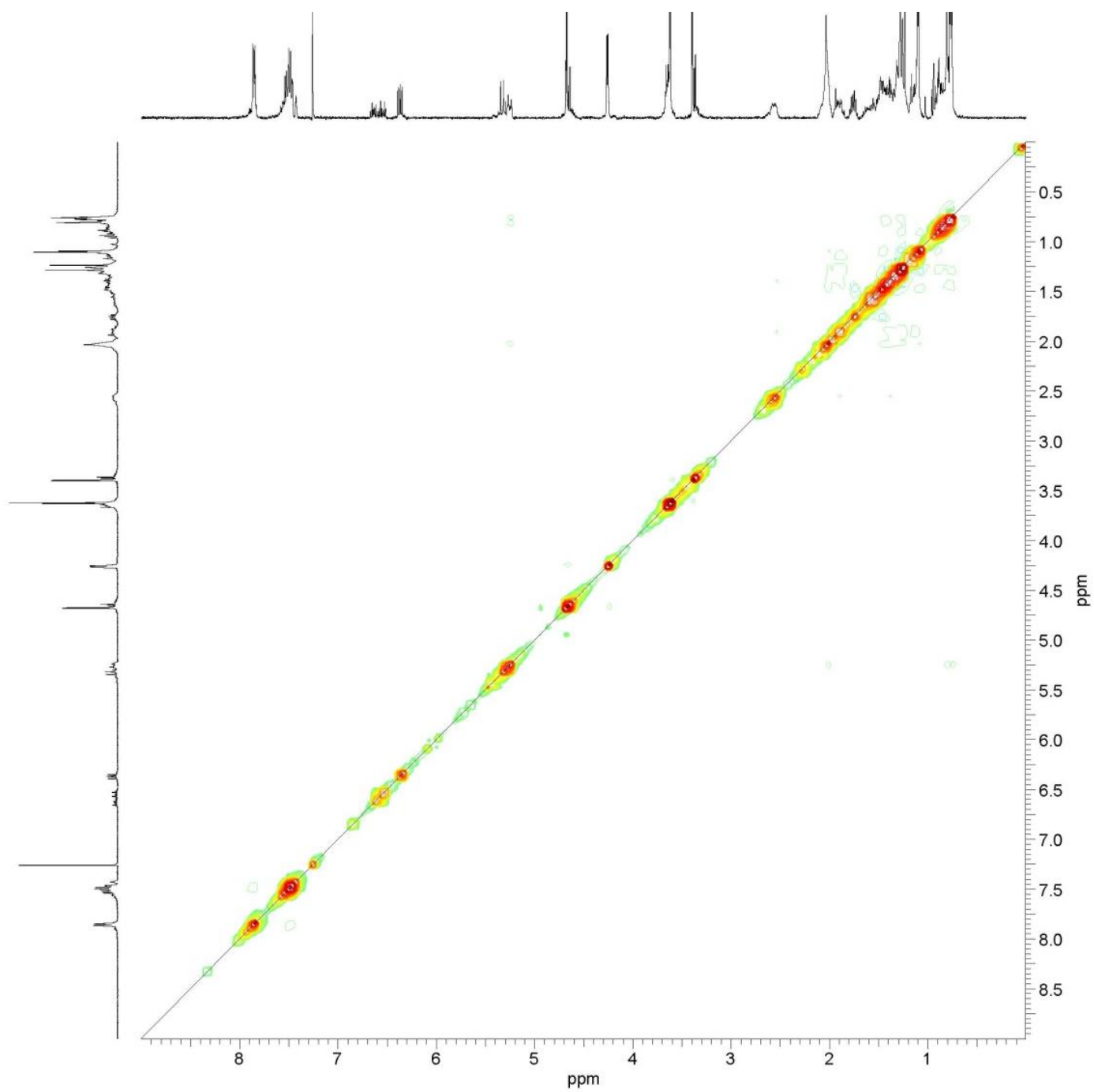


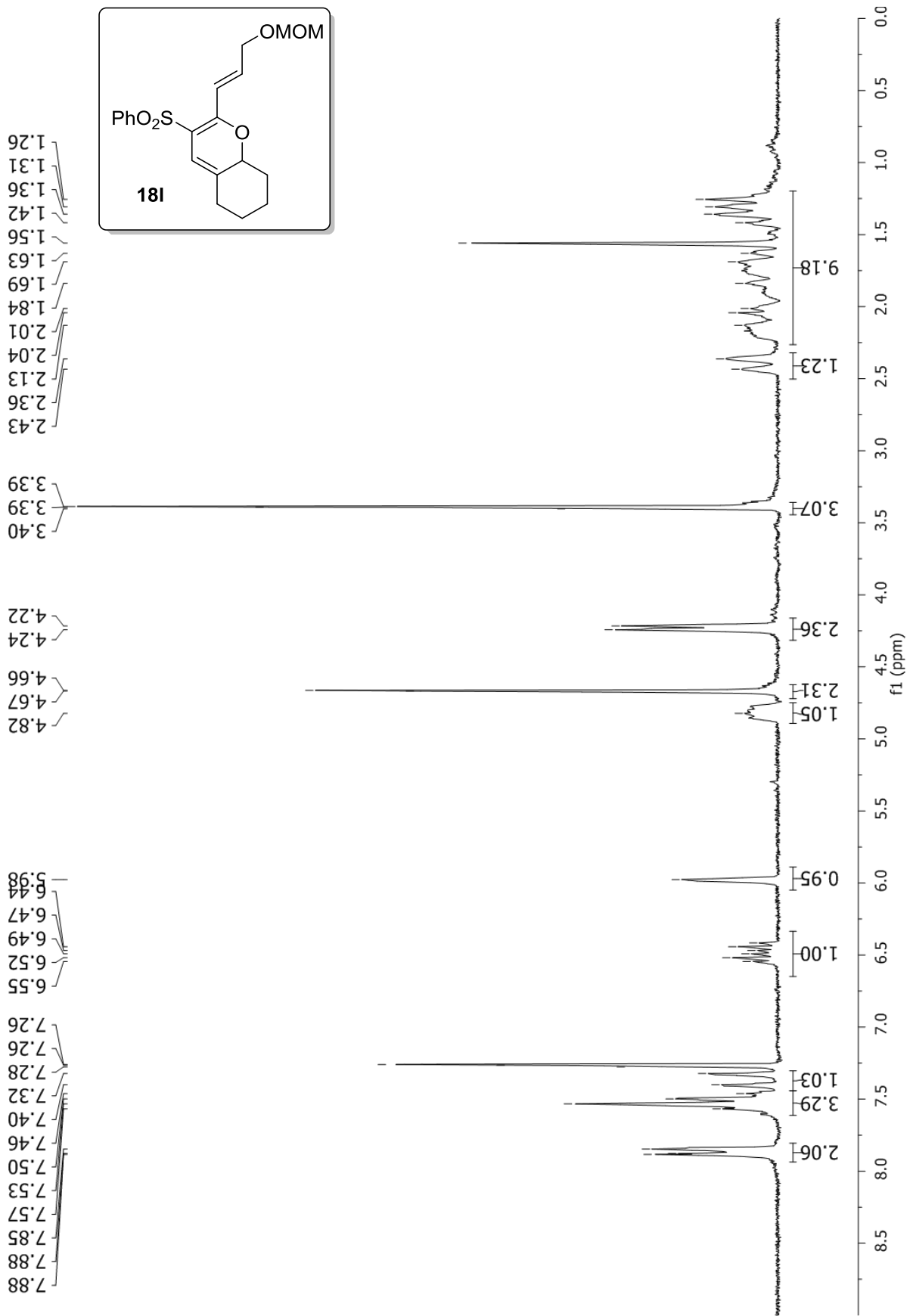
Formula	CalculatedMass	mDaError	ppmError	RDB
C36 H45 O7 S	621.288052	0.1475	0.23741	14.5
C21 H41 N12 O8 S	621.288555	-0.355076	-0.571515	7.5
C23 H46 N6 O10 Na S	621.288835	-0.635208	-1.022404	3.5
C20 H45 N8 O12 S	621.287218	0.982236	1.580965	2.5
C37 H41 N4 O3 S	621.28939	-1.189812	-1.915071	19.5
C35 H42 N4 O3 Na S	621.286985	1.215448	1.956334	16.5
C33 H37 N10 O S	621.286704	1.49558	2.407222	20.5
C24 H49 N2 O14 S	621.289903	-1.703156	-2.741328	1.5
C24 H49 N10 O6 Na S	621.289172	1.07252	2.174894	8.5

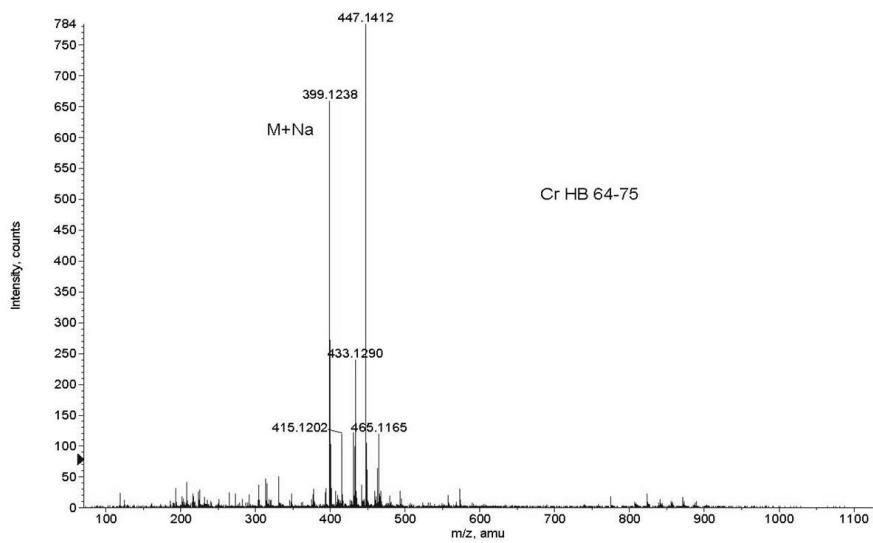
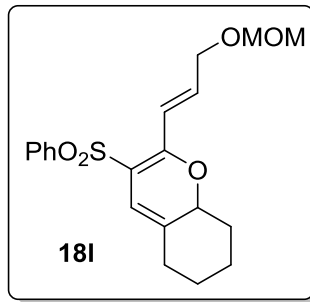
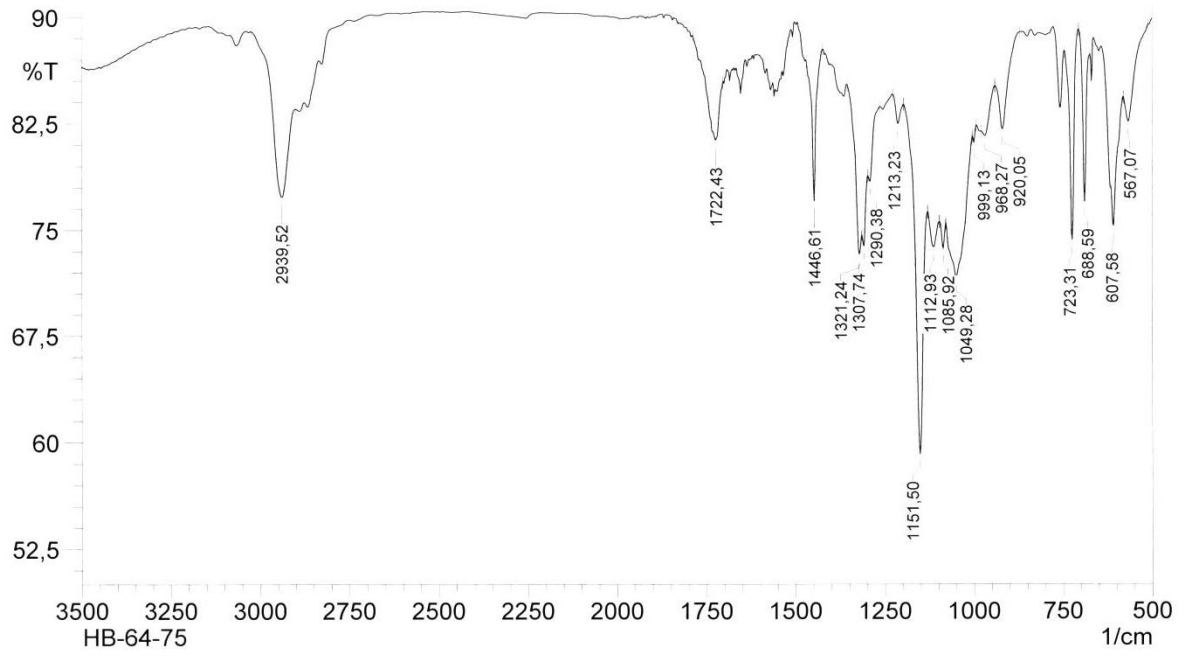




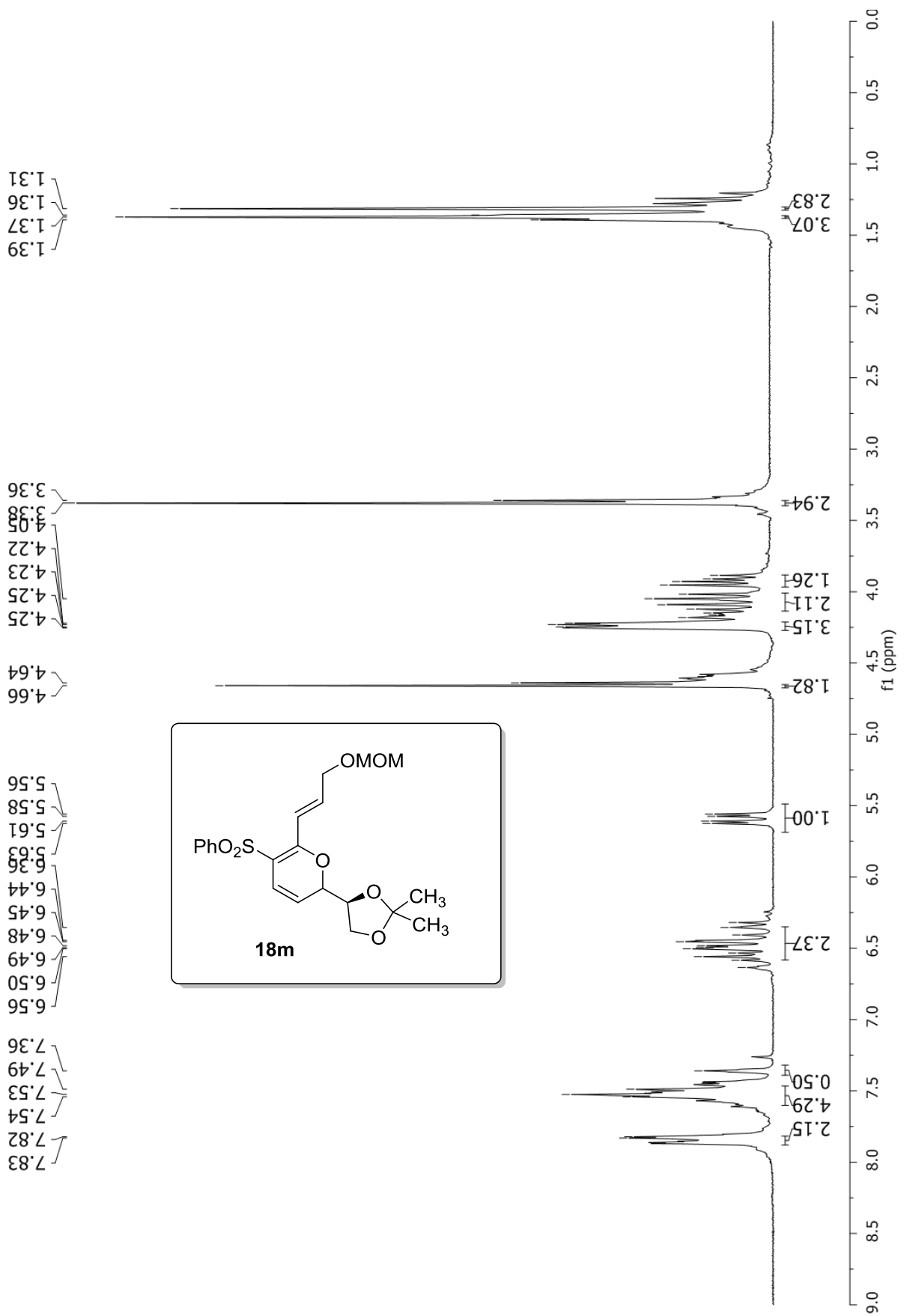


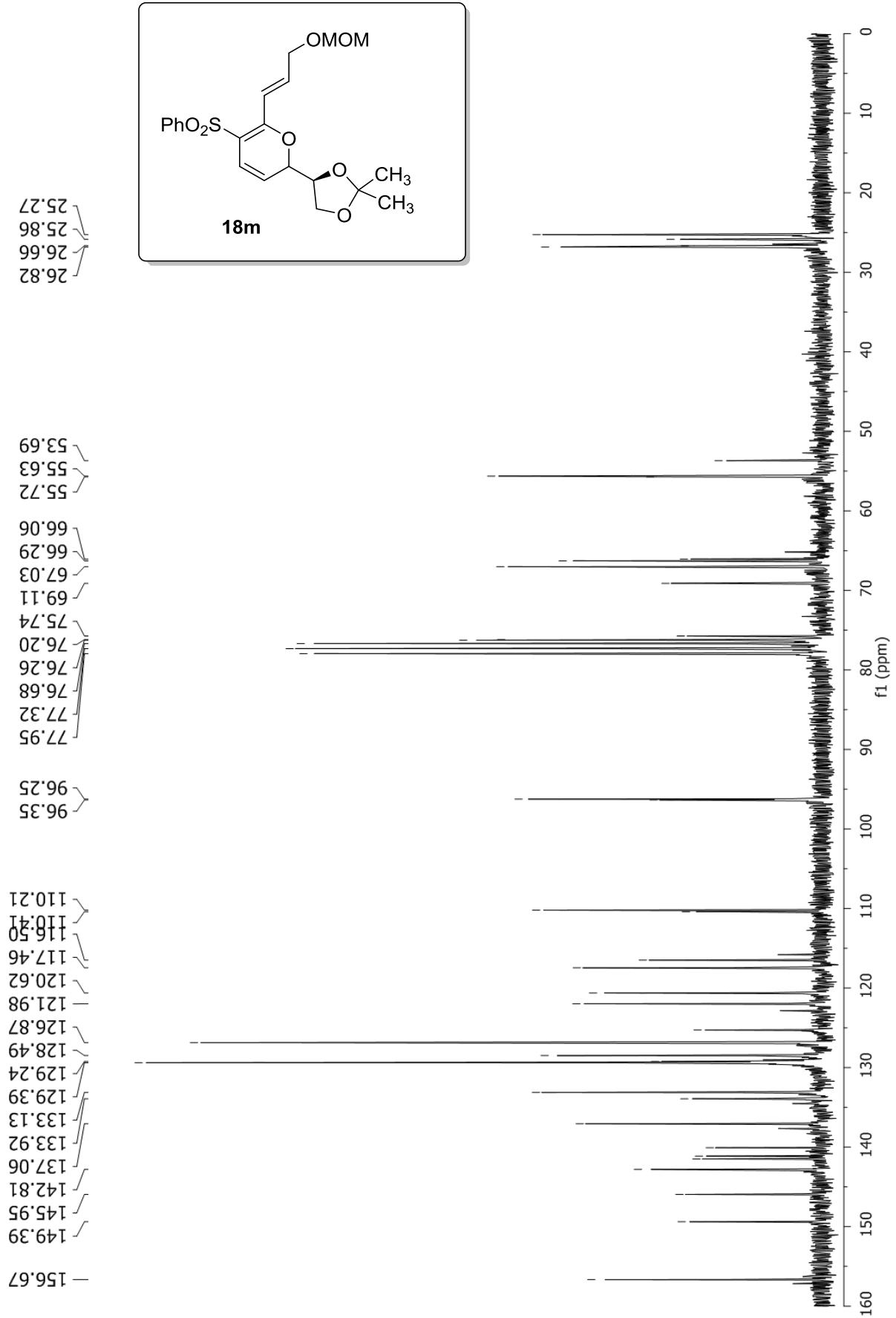




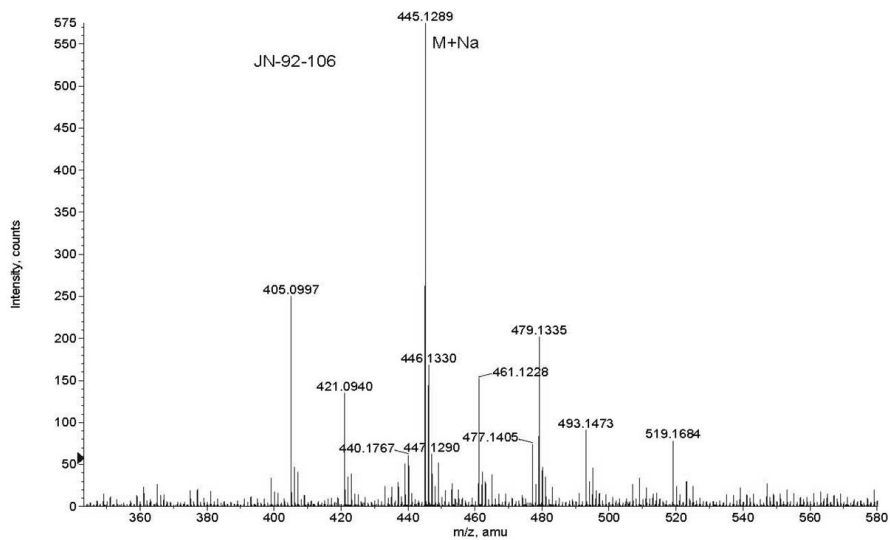
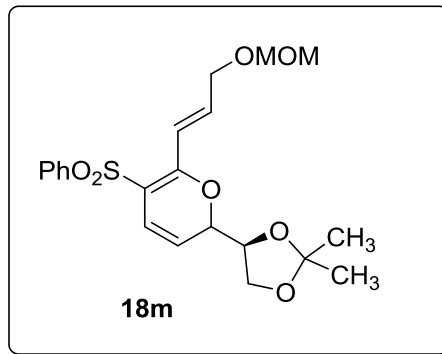
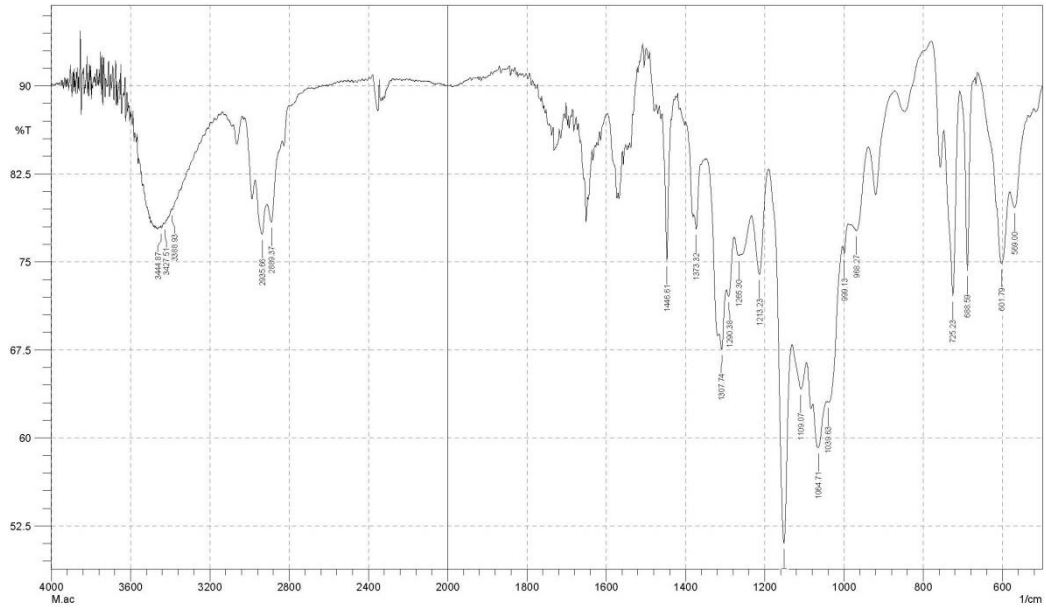


Formula	CalculatedMass	mDaError	ppmError	RDB
C ₂₀ H ₂₄ O ₅ NaS	399.123667	0.13292	0.333029	8.5

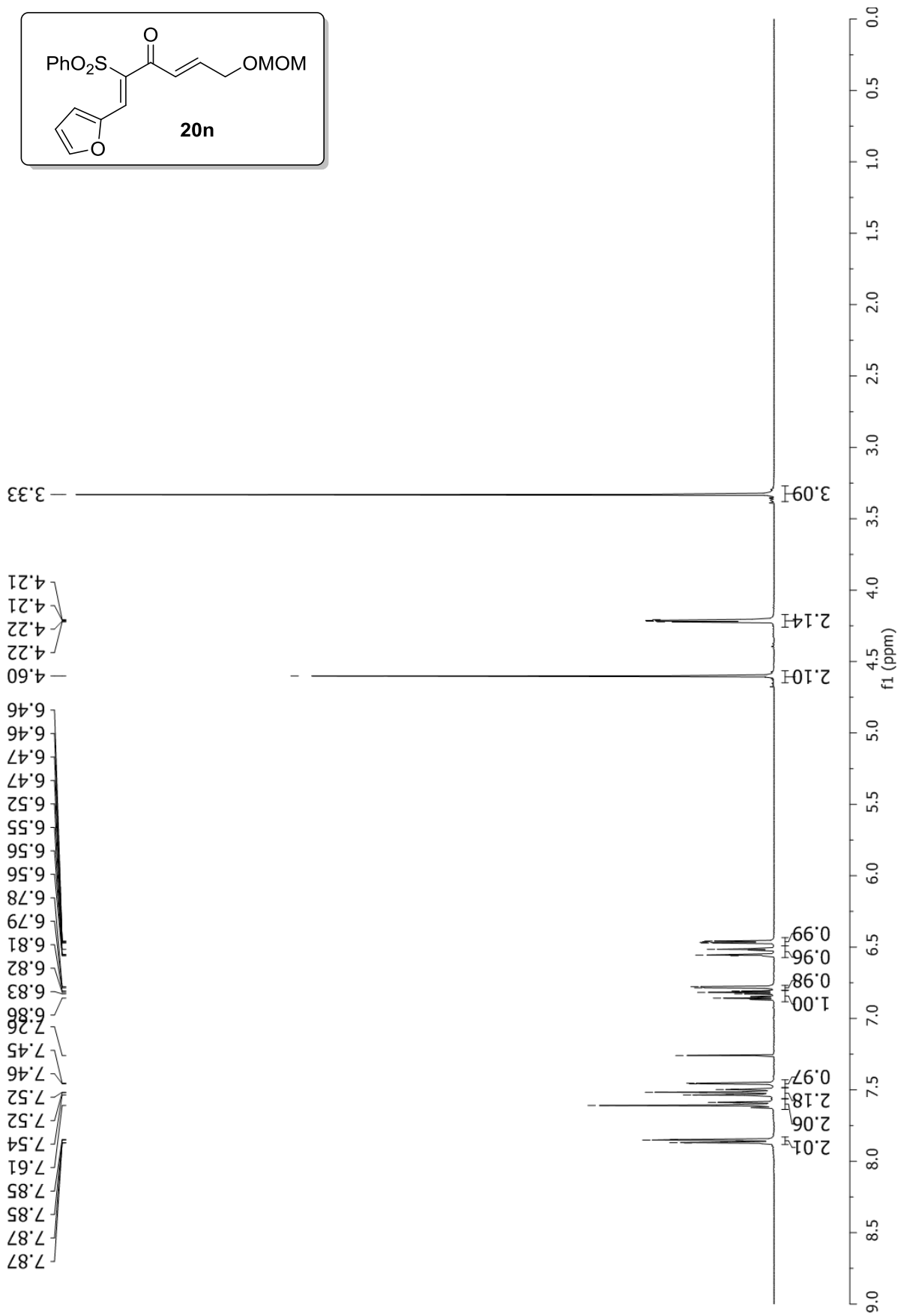
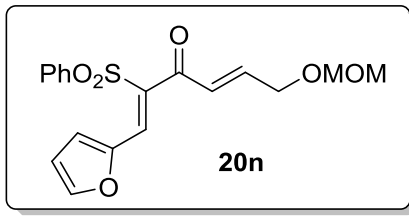


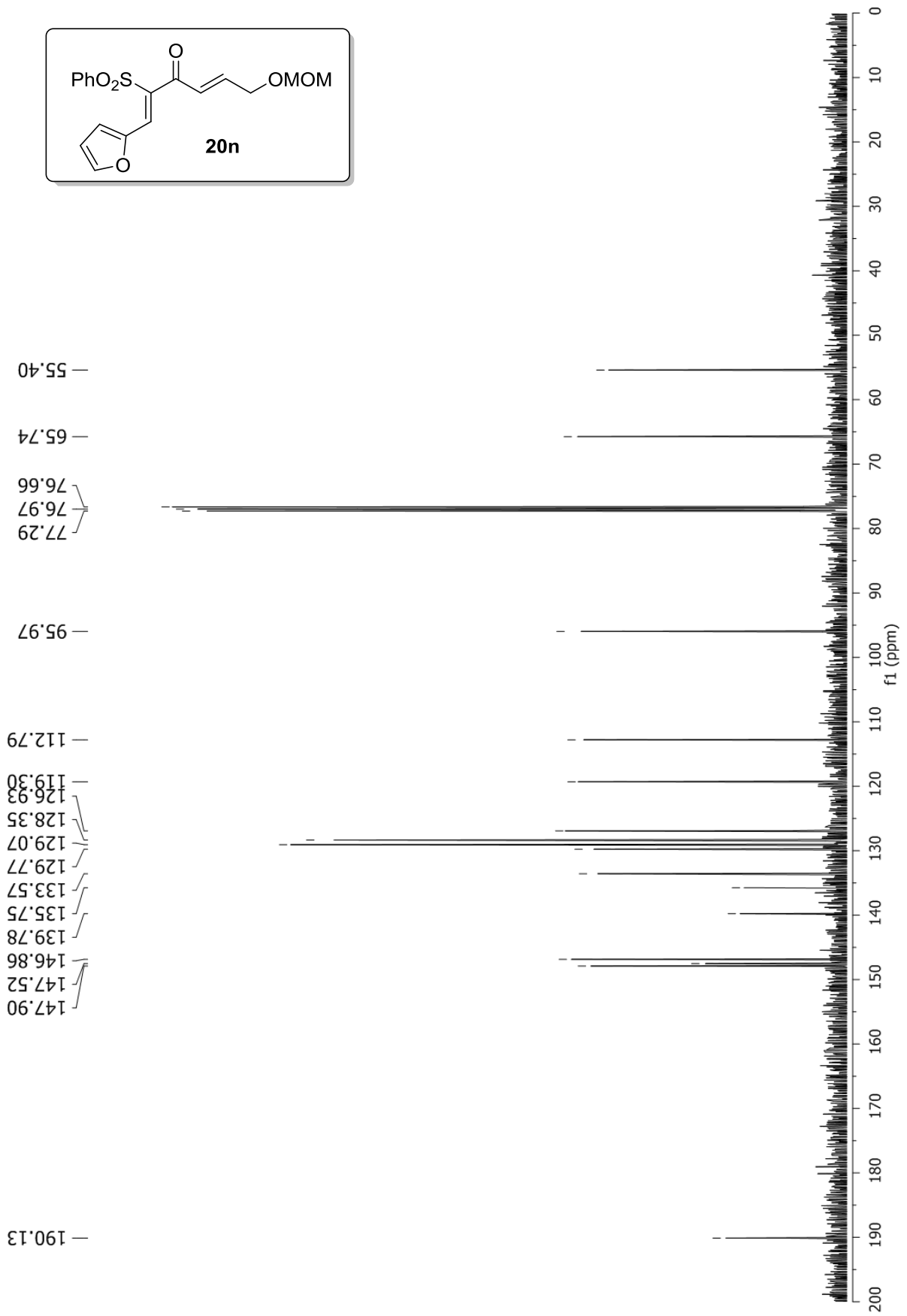
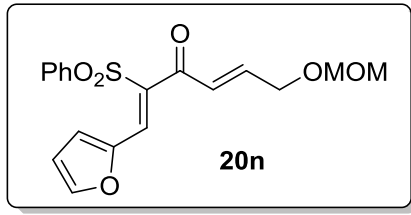


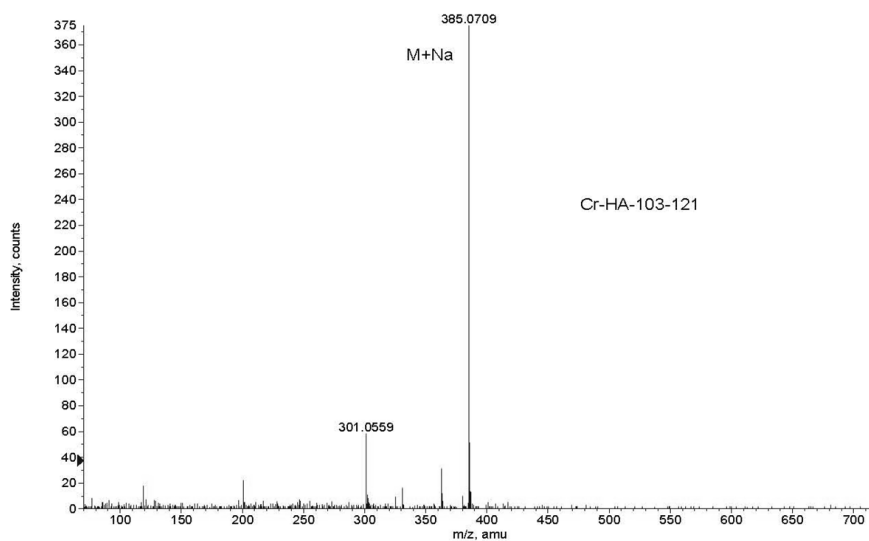
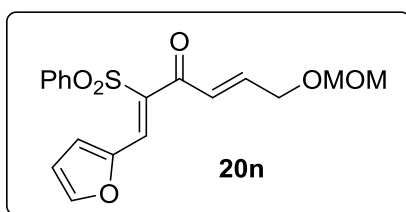
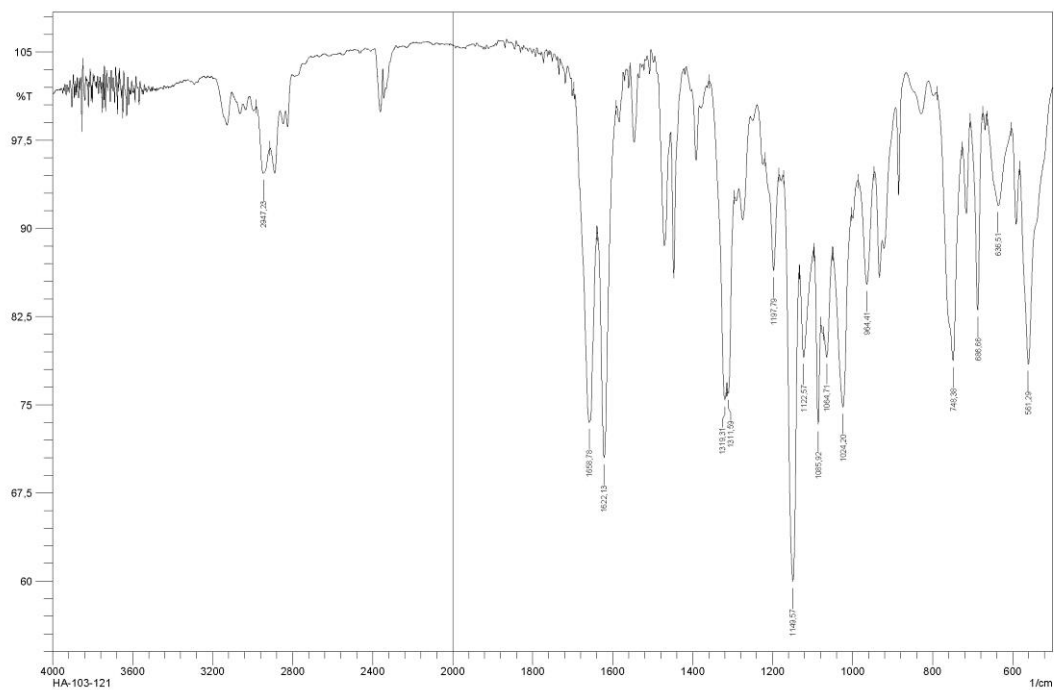
Full Spectroscopy



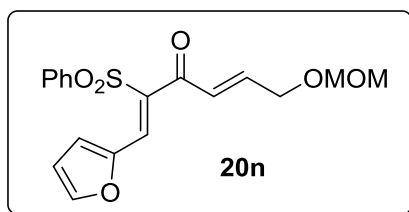
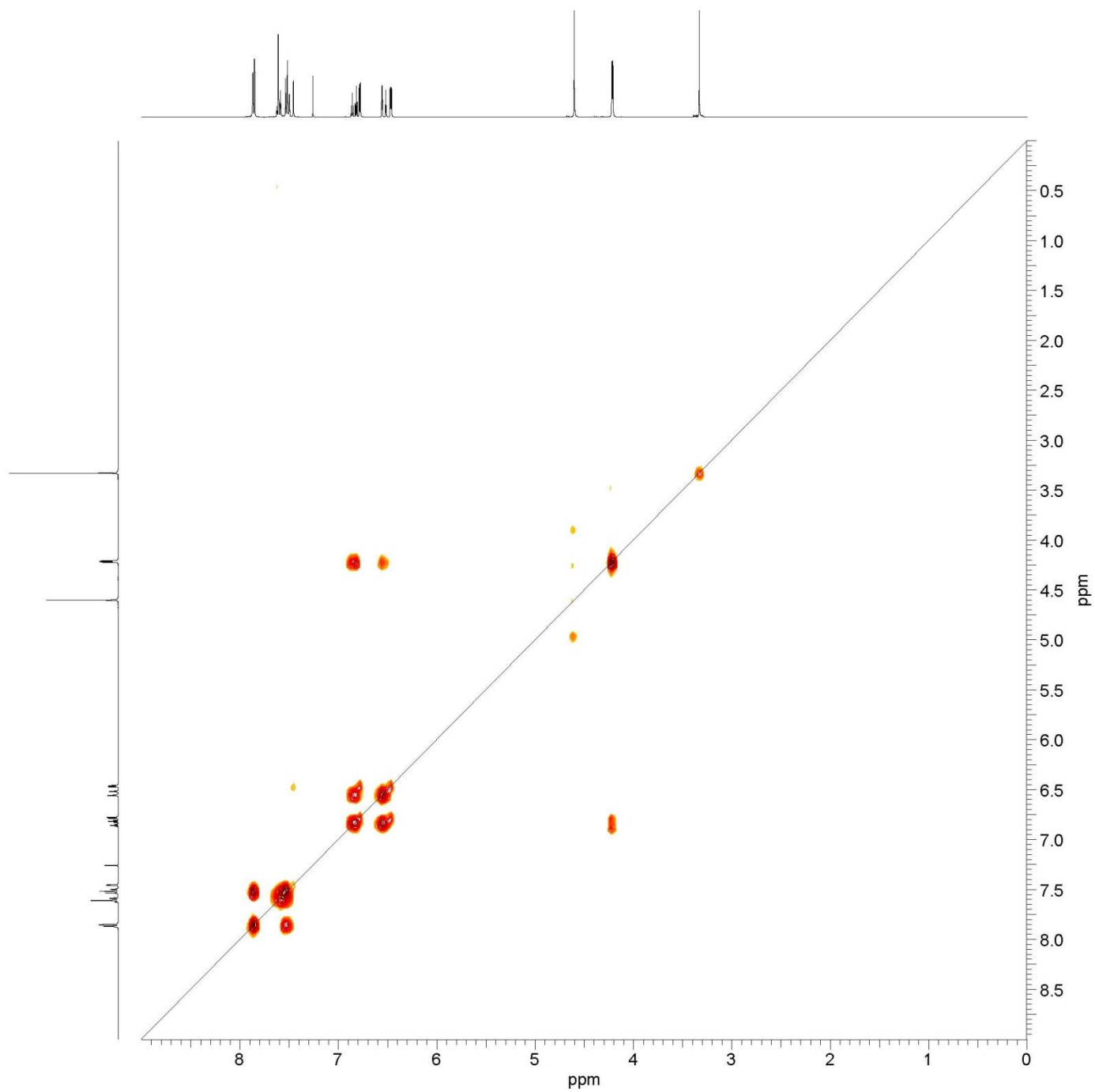
Formula	CalculatedMass	mDaError	ppmError	RDB
C19 H21 N6 O5 S	445.128866	0.033692	0.07569	12.5
C21 H26 O7 Na S	445.129146	-0.24644	-0.553637	8.5

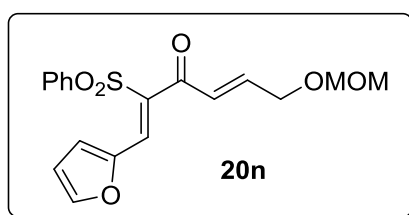
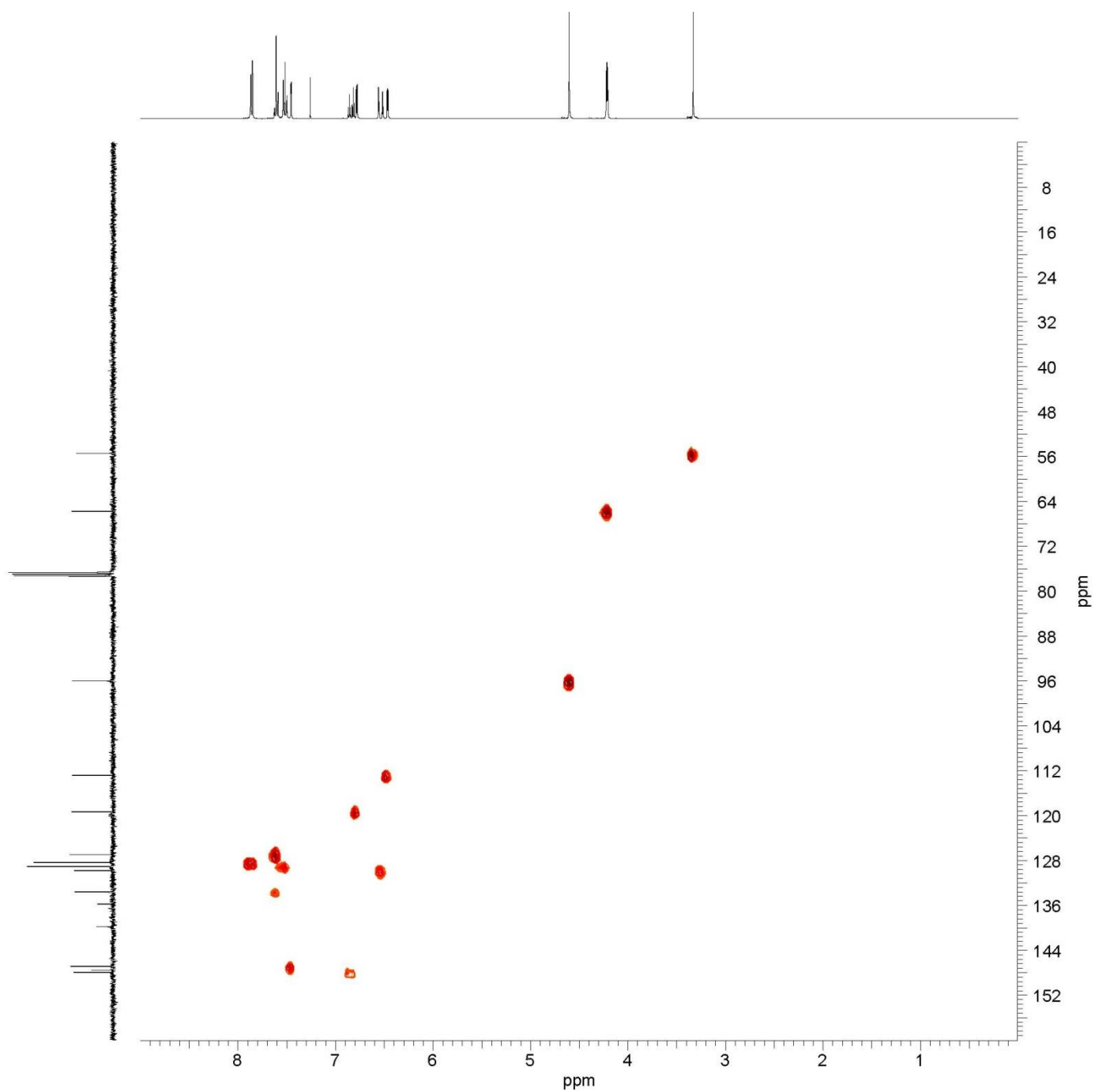


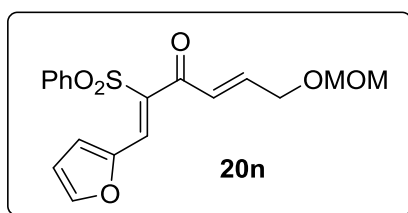
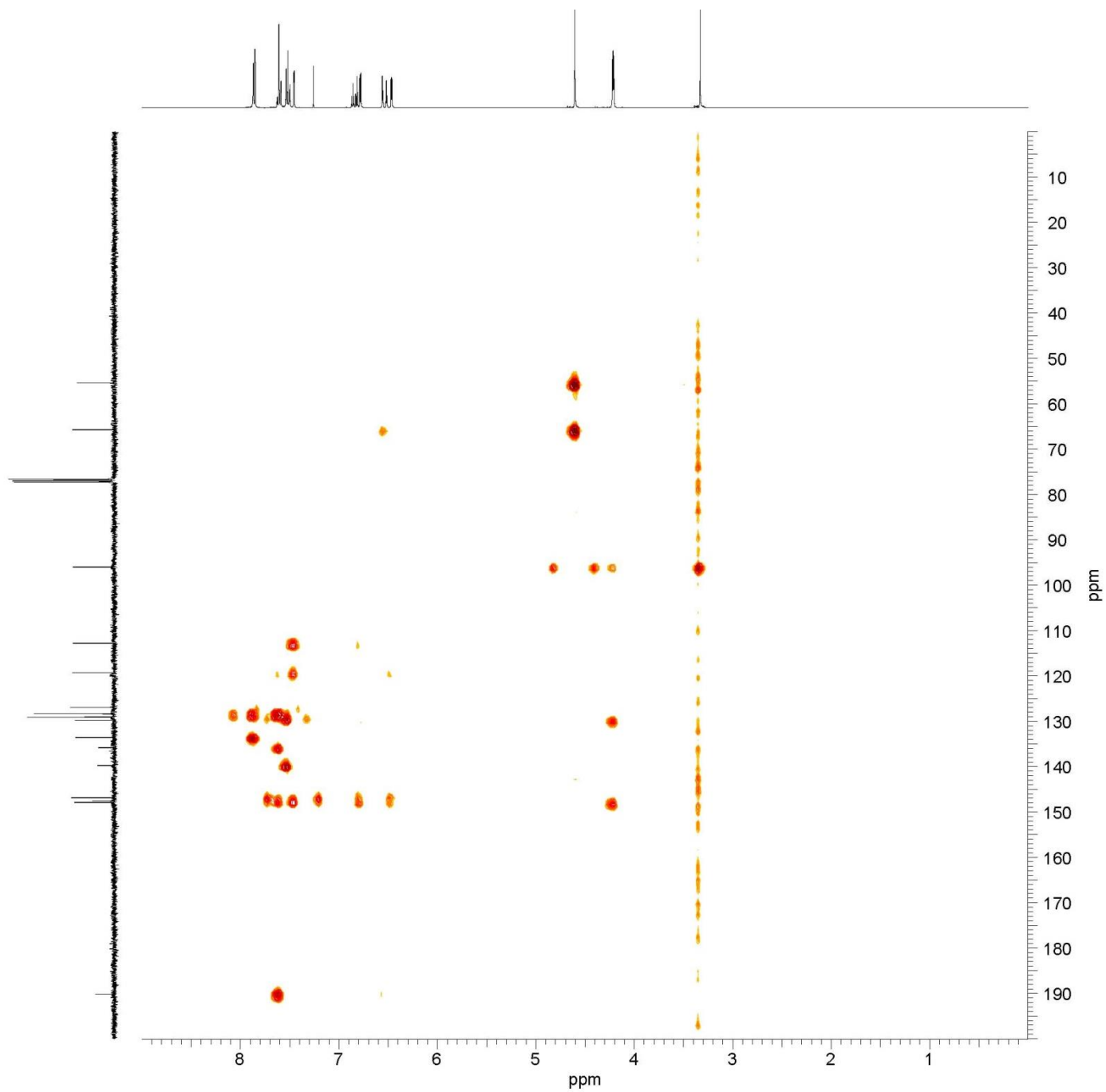


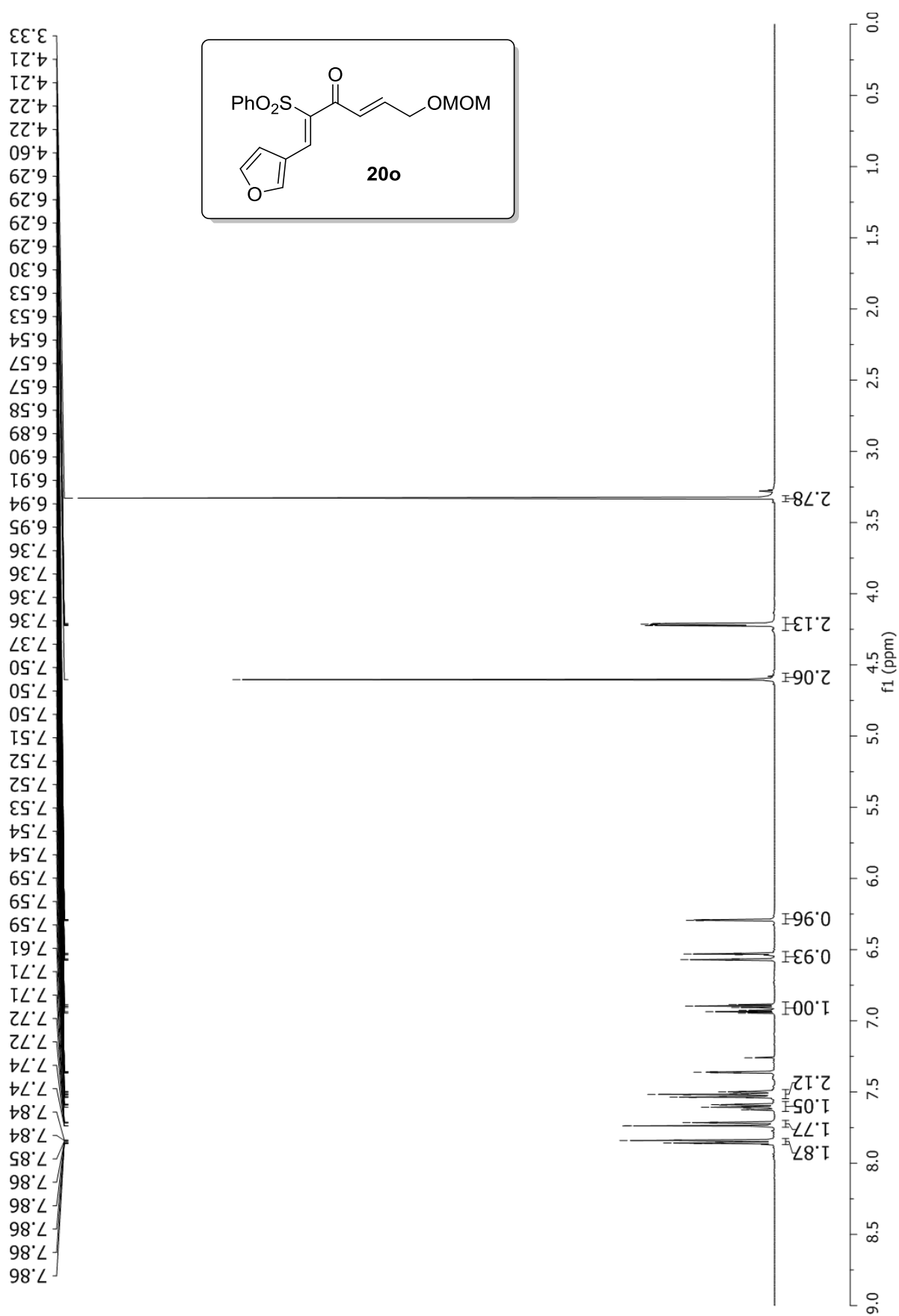


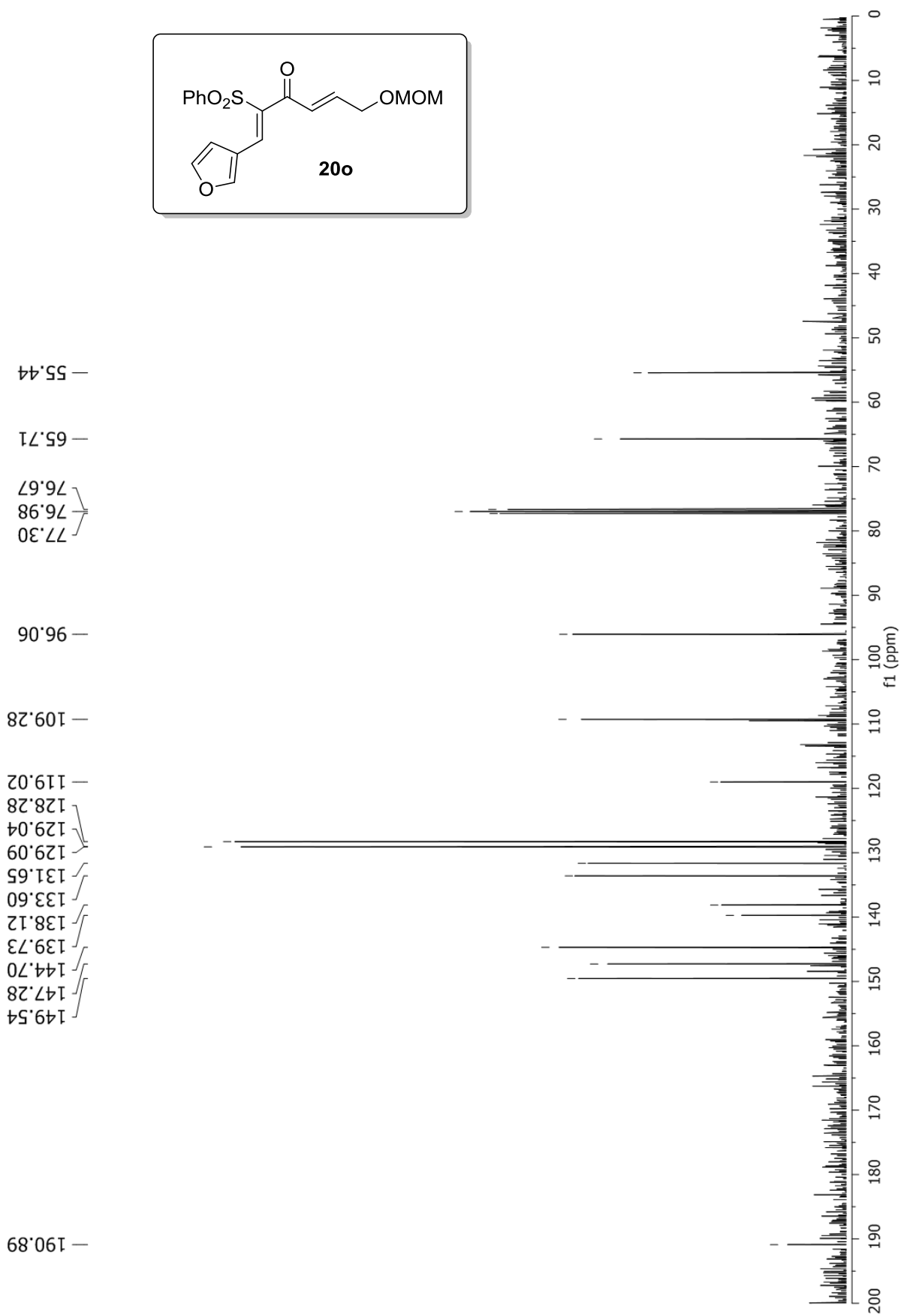
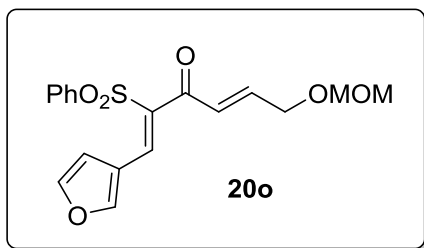
Formula	CalculatedMass	mDaError	ppmError	RDB
H13 N14 O9 S	385.070517	0.383388	0.995628	1.5
C16 H13 N6 O4 S	385.071351	-0.451348	-1.172115	13.5
C15 H10 N10 Na S	385.070283	0.6166	1.601261	15.5
C18 H18 O6 Na S	385.071631	-0.73148	-1.899596	9.5
C15 H17 N2 O8 S	385.070014	0.885964	2.300778	8.5
C3 H14 N12 O7 Na S	385.072134	-1.234056	-3.204746	2.5

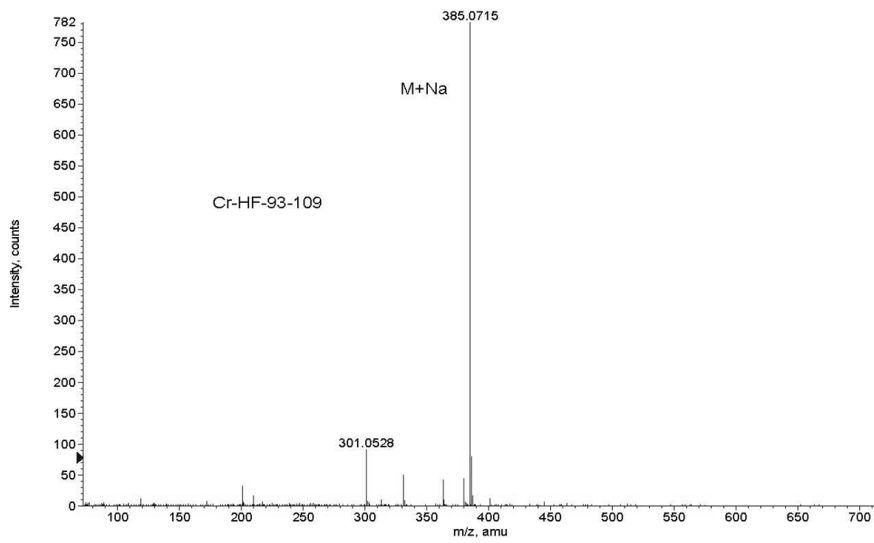
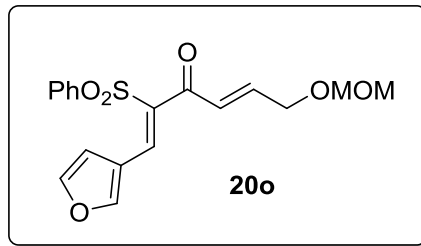
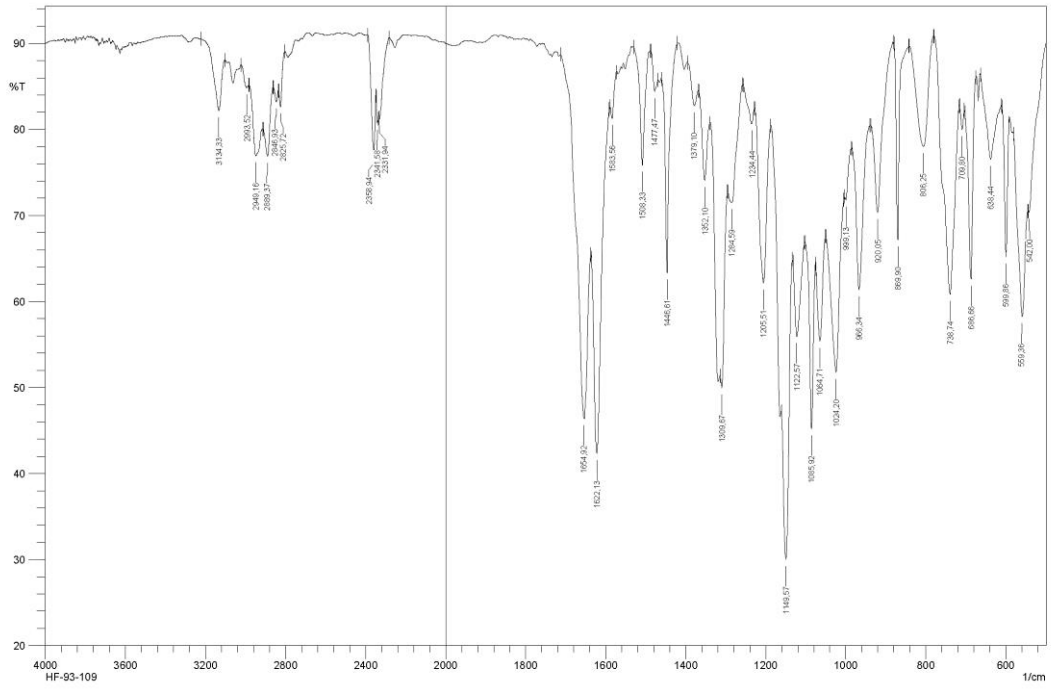




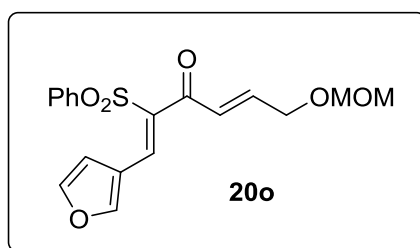
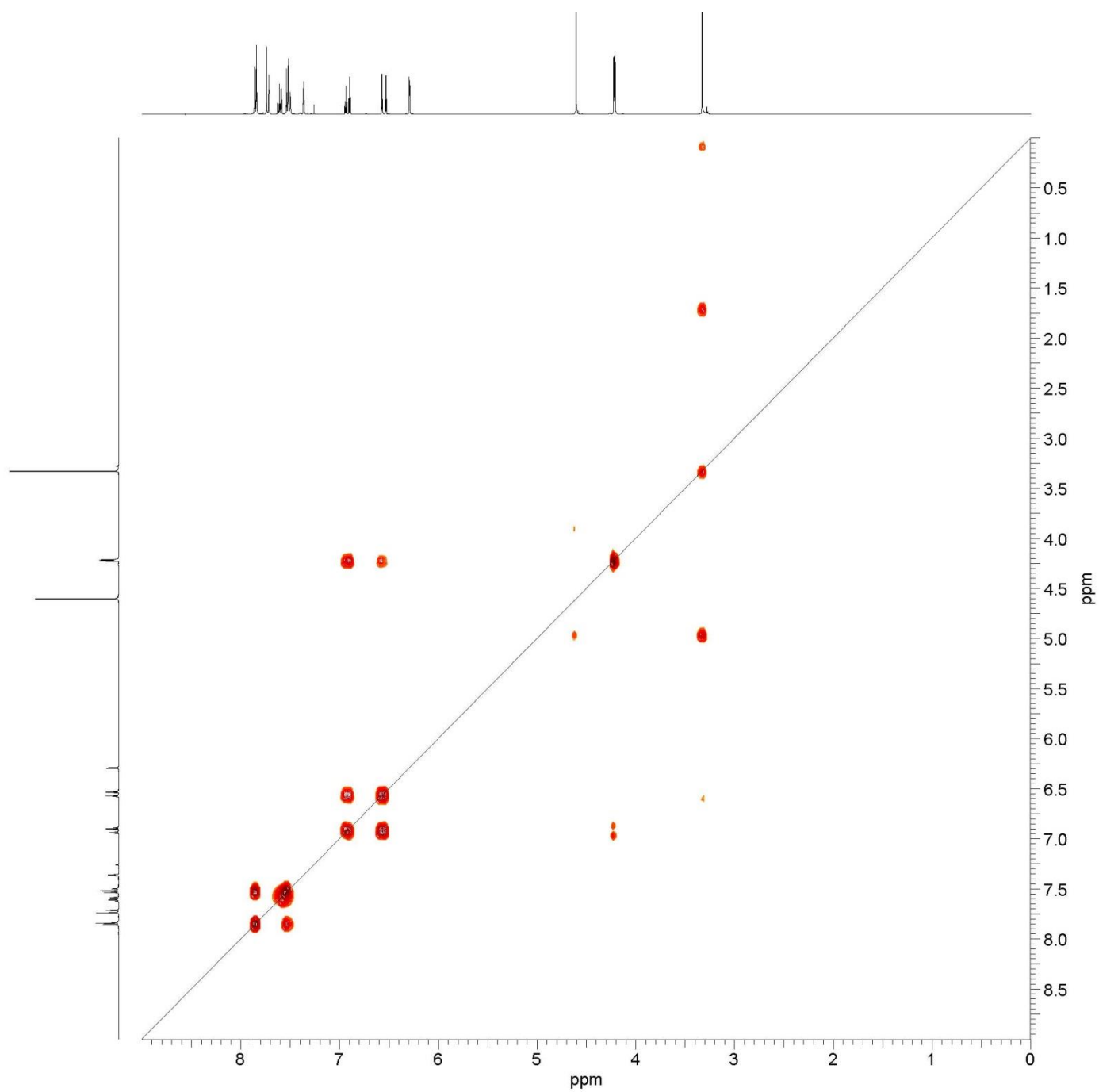


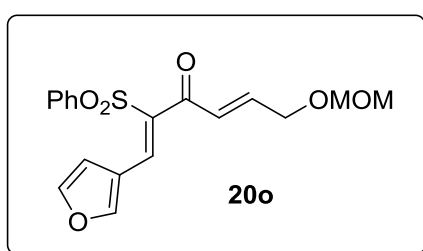
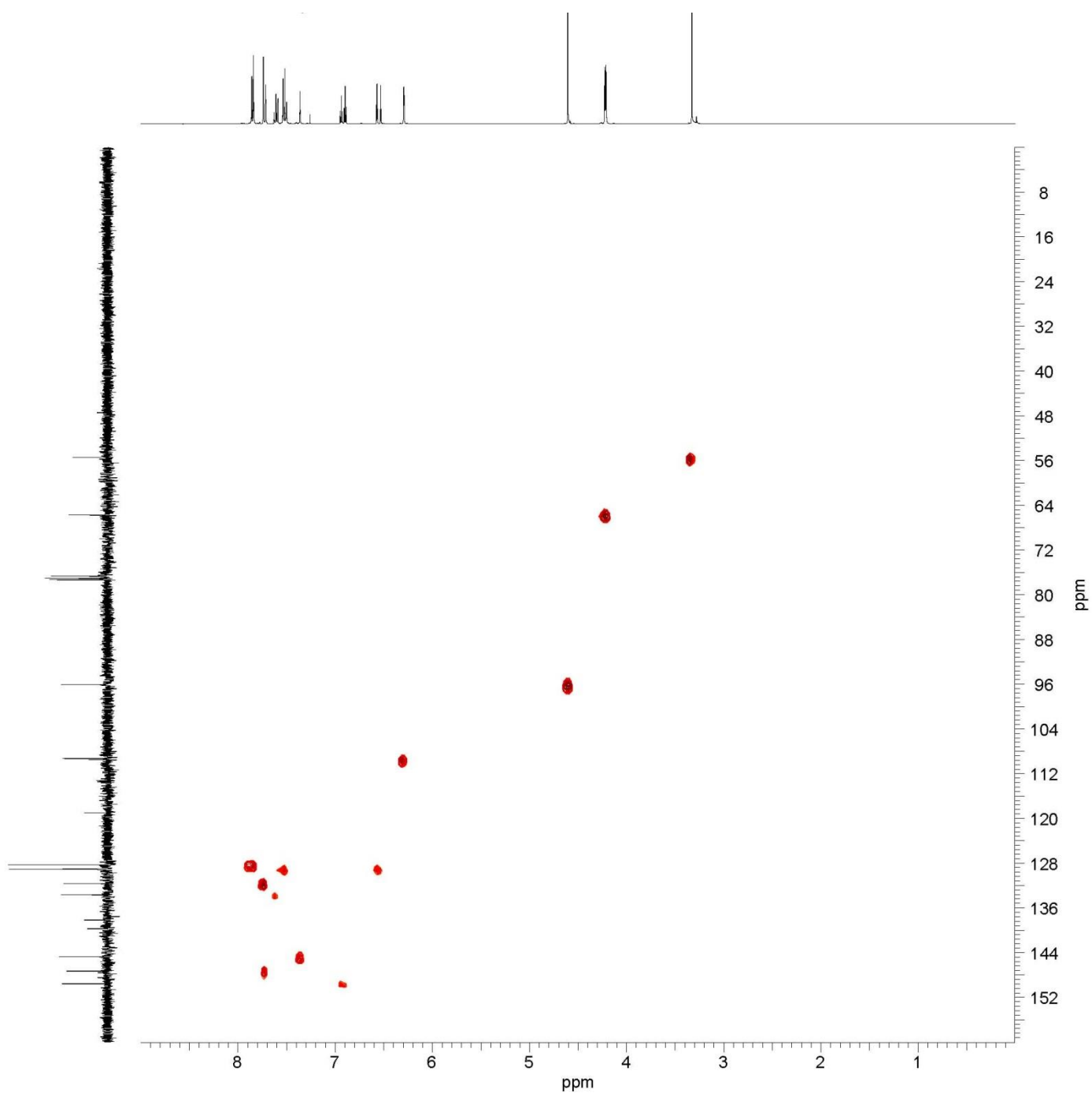


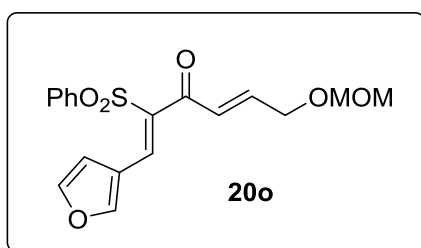
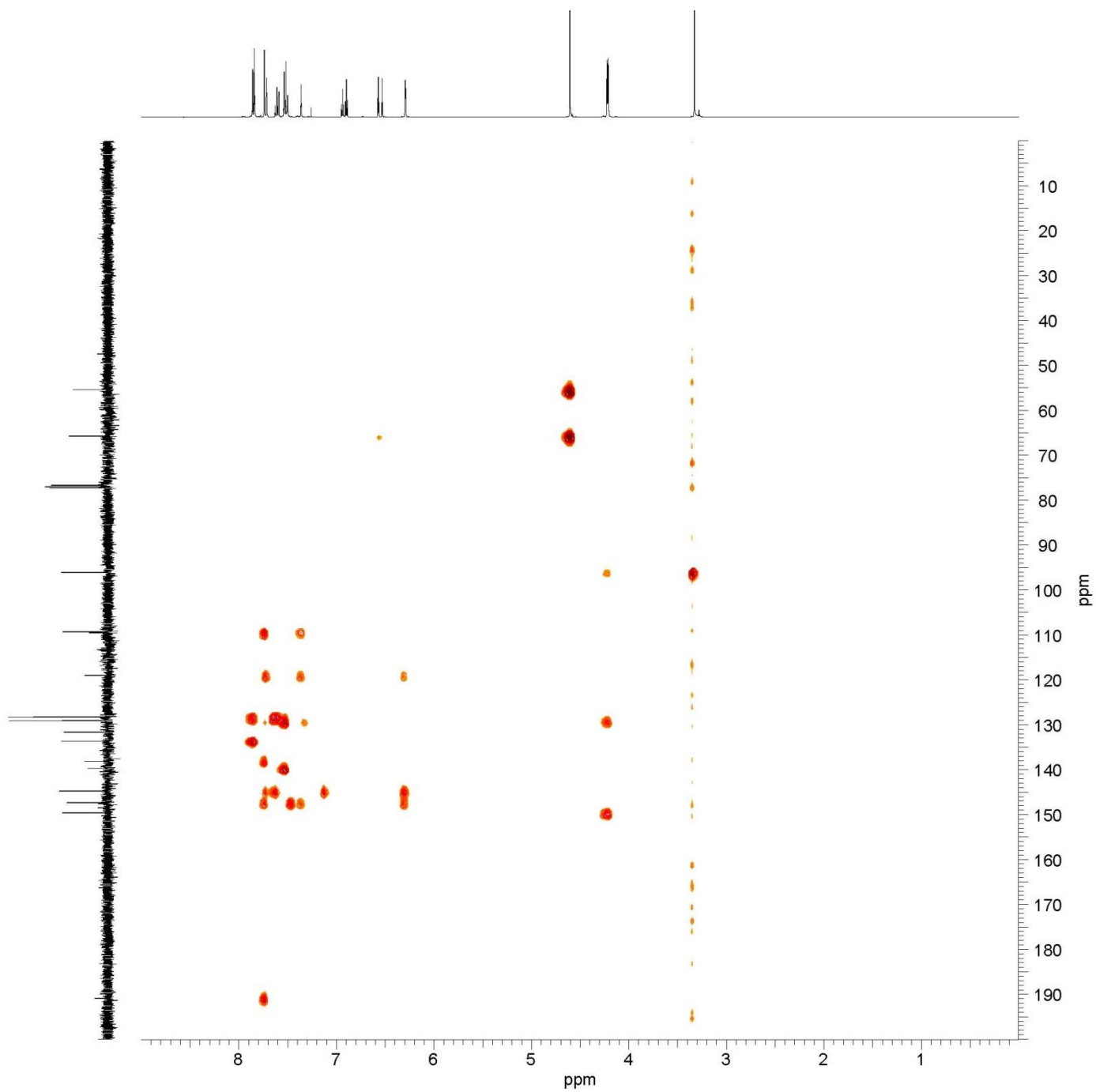


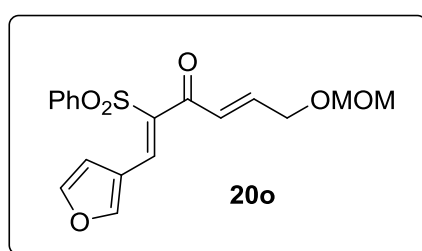
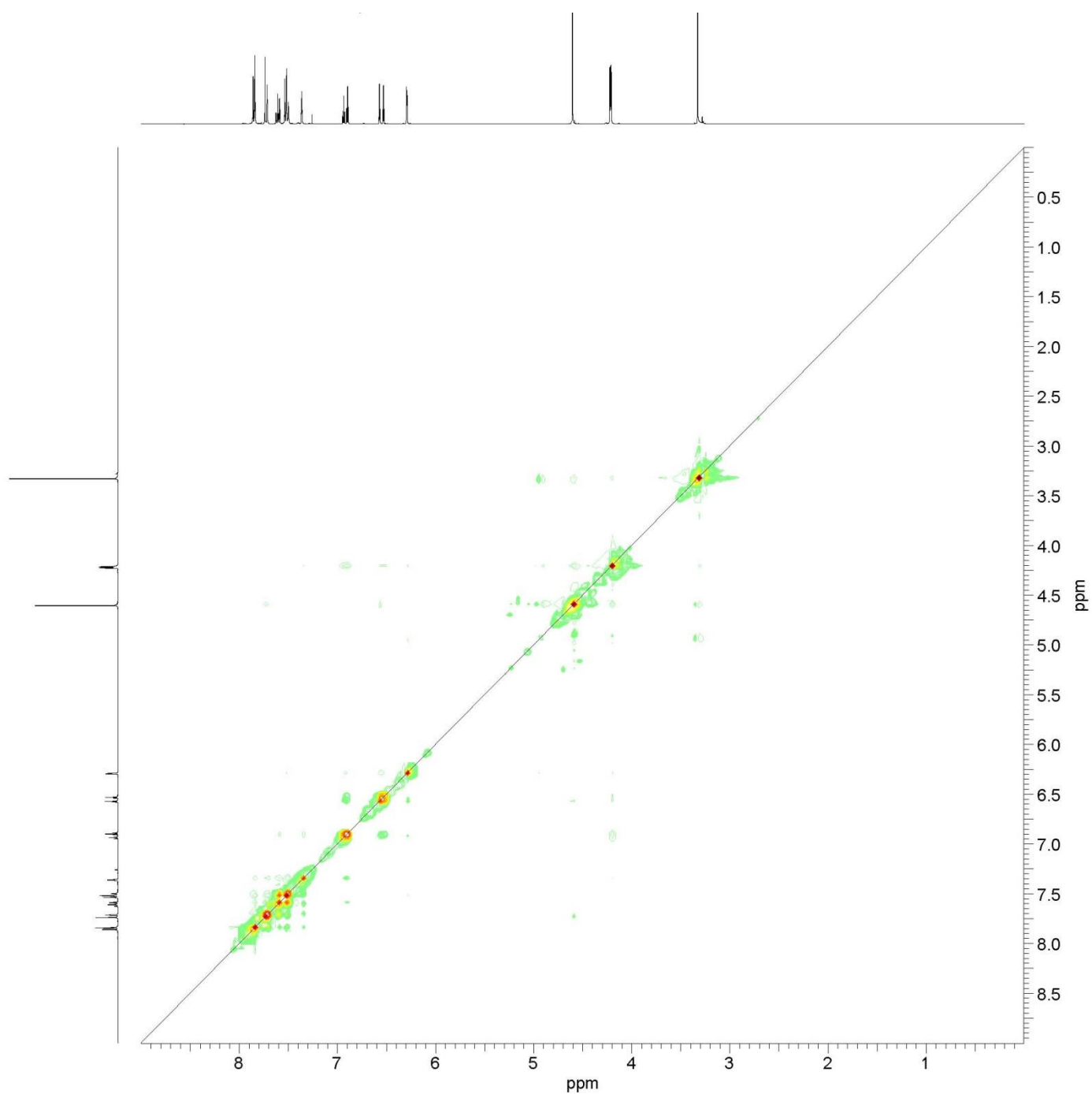


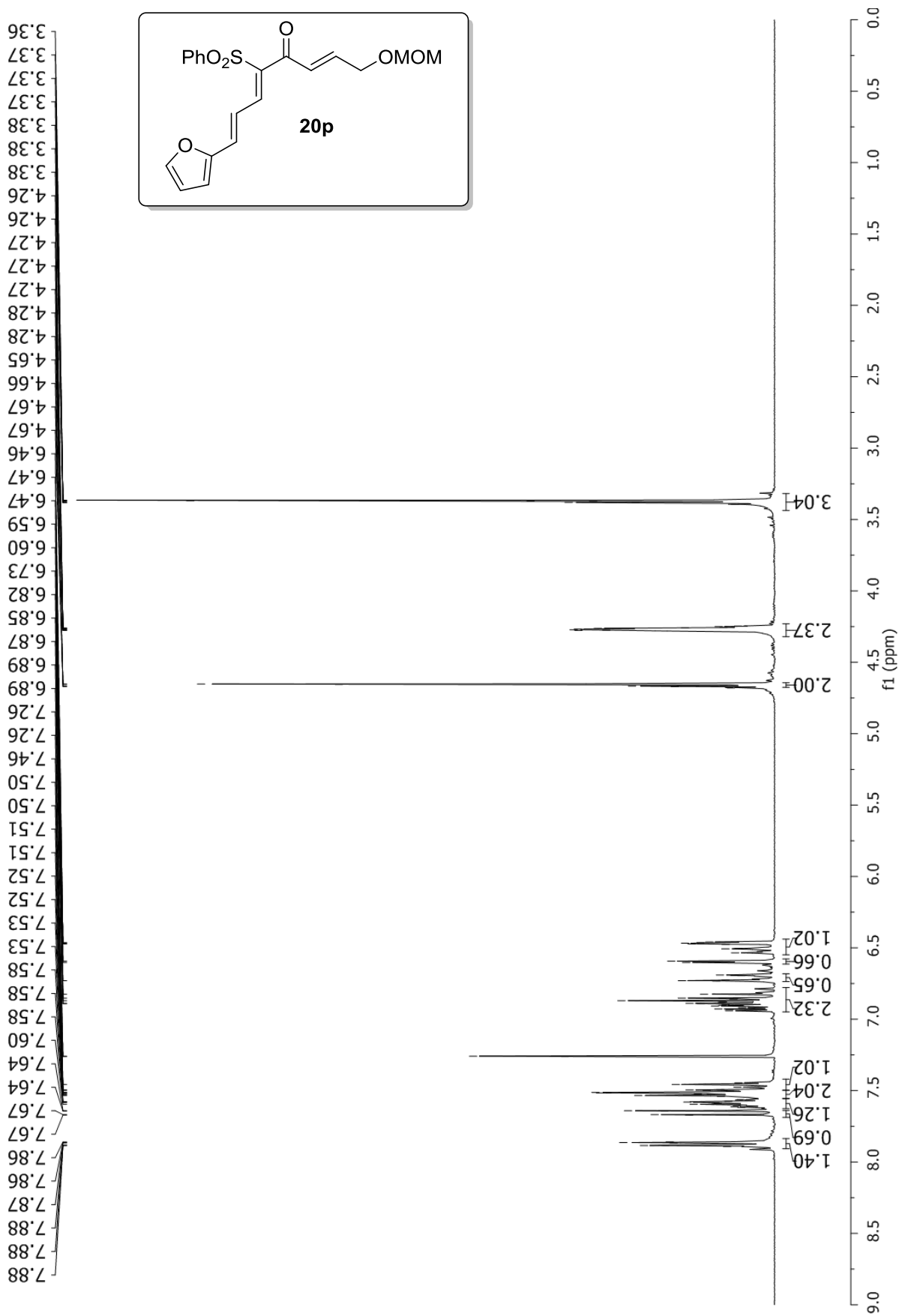
Formula	CalculatedMass	mDaError	ppmError	RDB
C18 H18 O6 Na S	385.071631	-0.13148	-0.341443	9.5
C16 H13 N6 O4 S	385.071351	0.148652	0.386037	13.5
C3 H14 N12 O7 Na S	385.072134	-0.634056	-1.646591	2.5
H13 N14 O9 S	385.070517	0.983388	2.553777	1.5
C17 H9 N10 S	385.072689	-1.18866	-3.086851	18.5
C15 H10 N10 Na S	385.070992	1.2166	3.150400	15.5

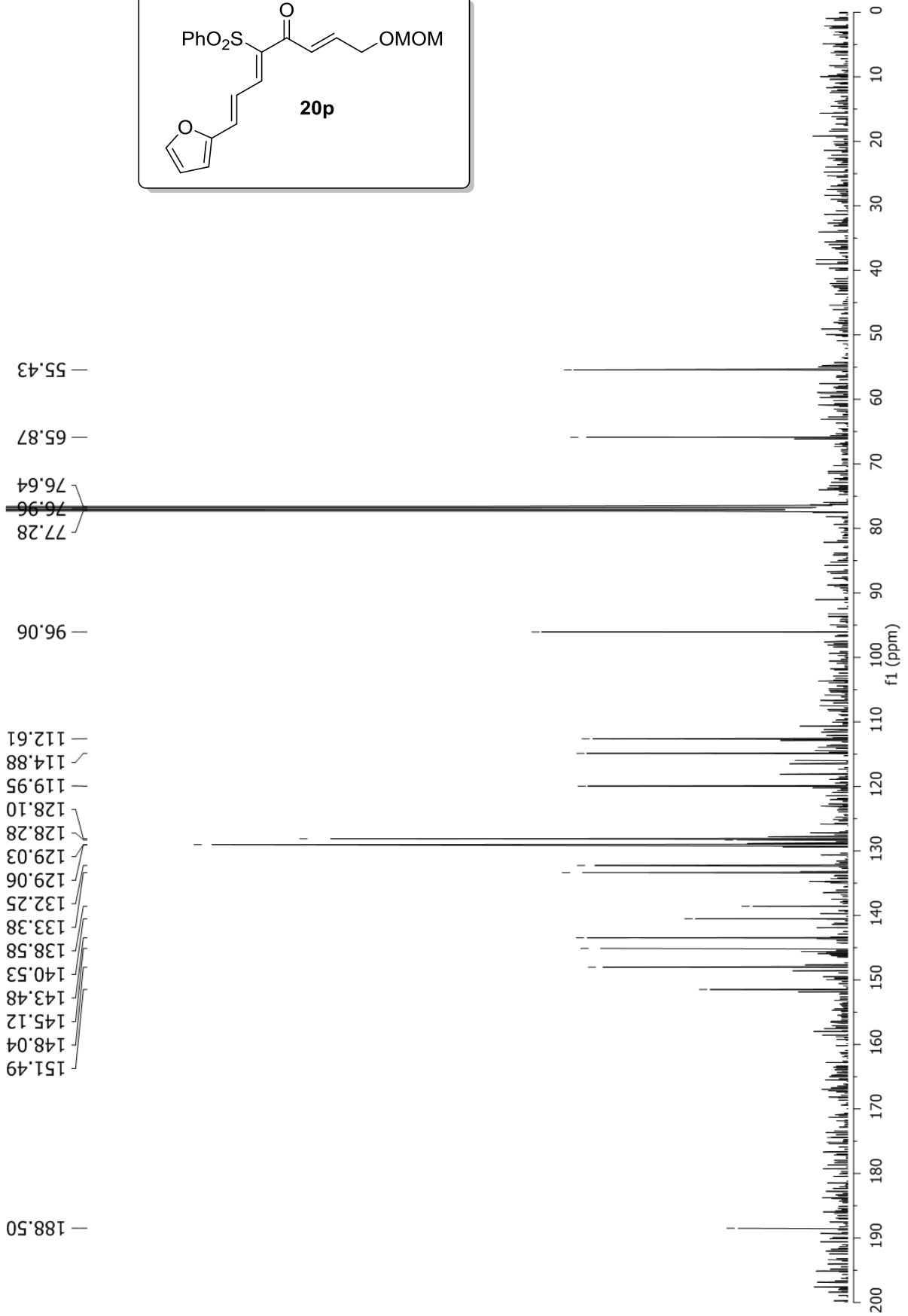
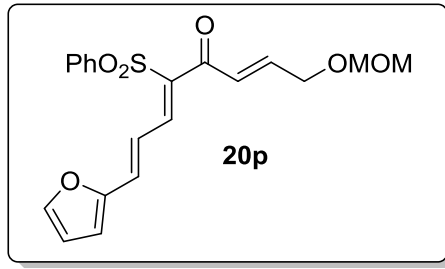


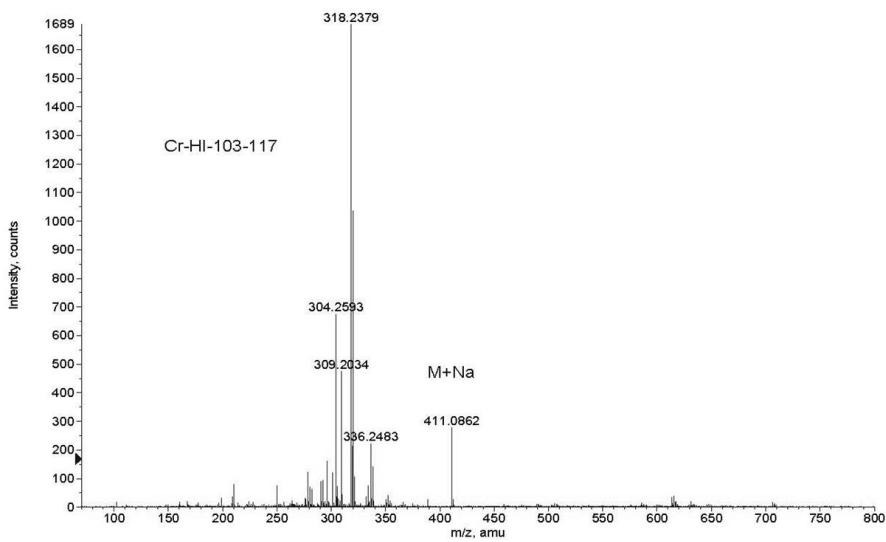
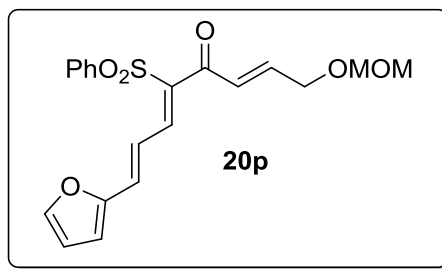
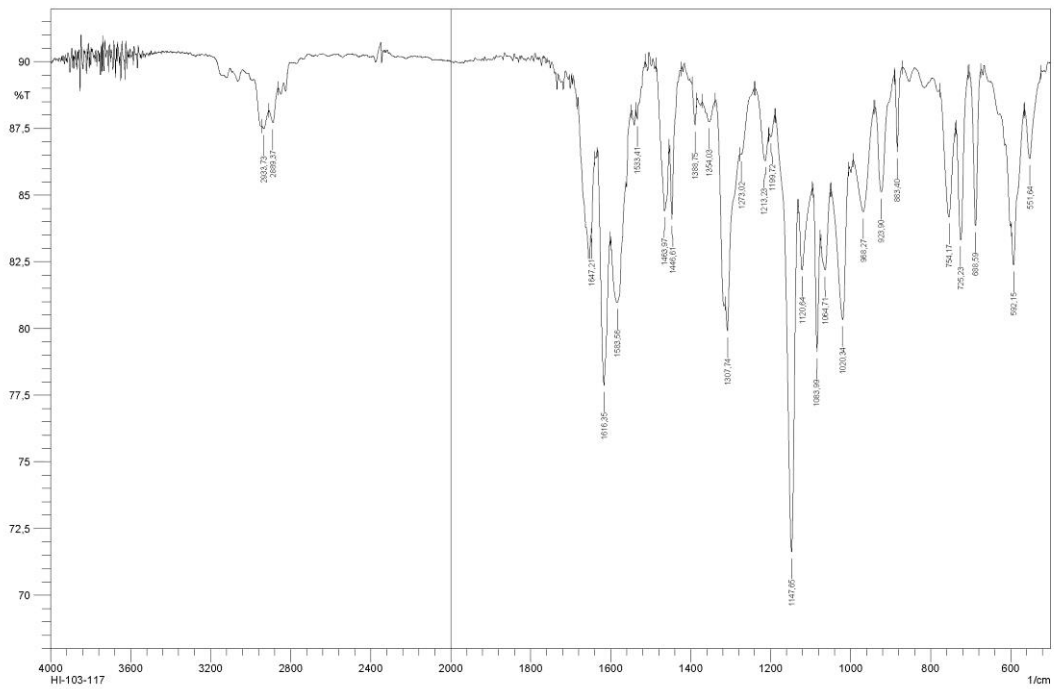




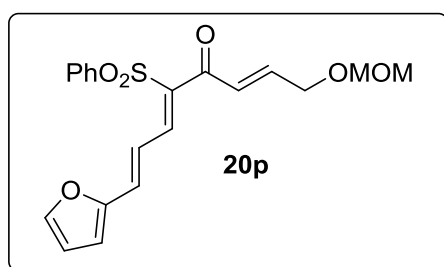
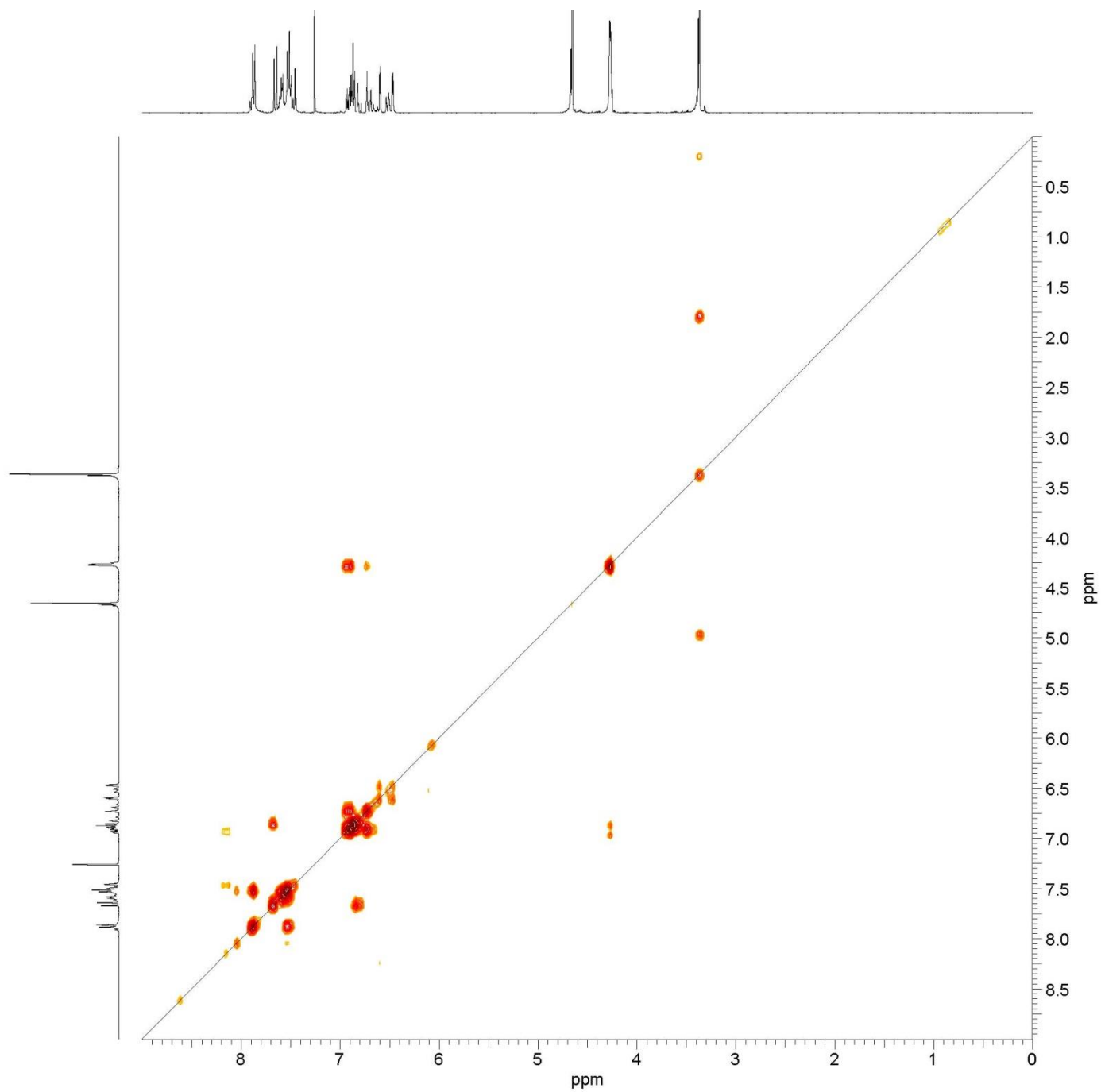


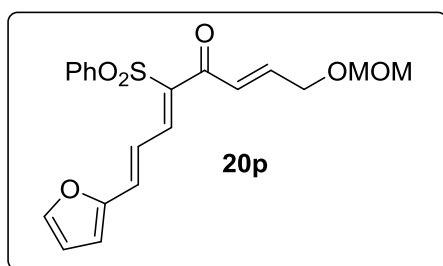
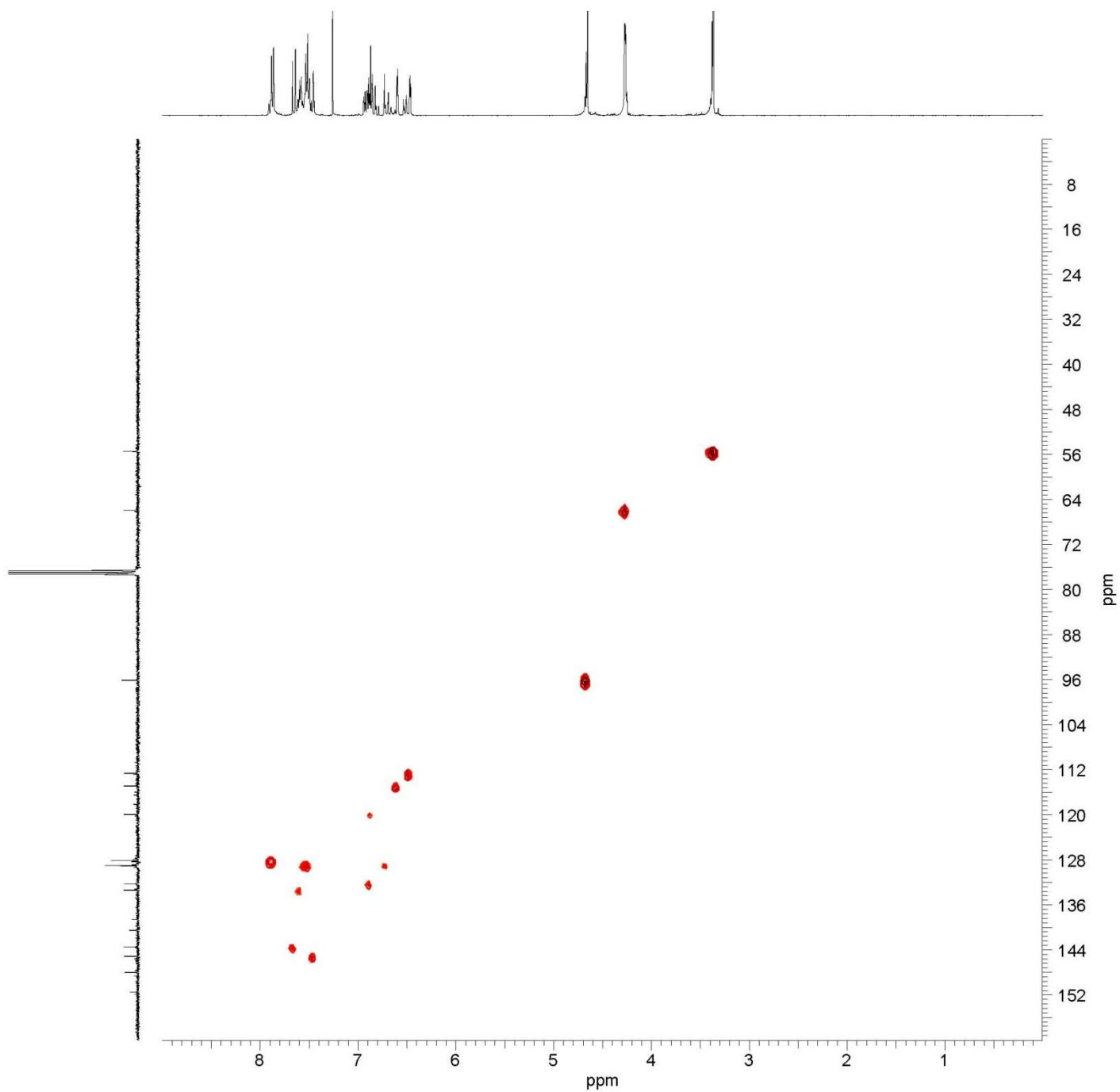


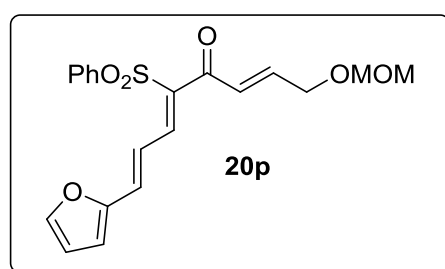
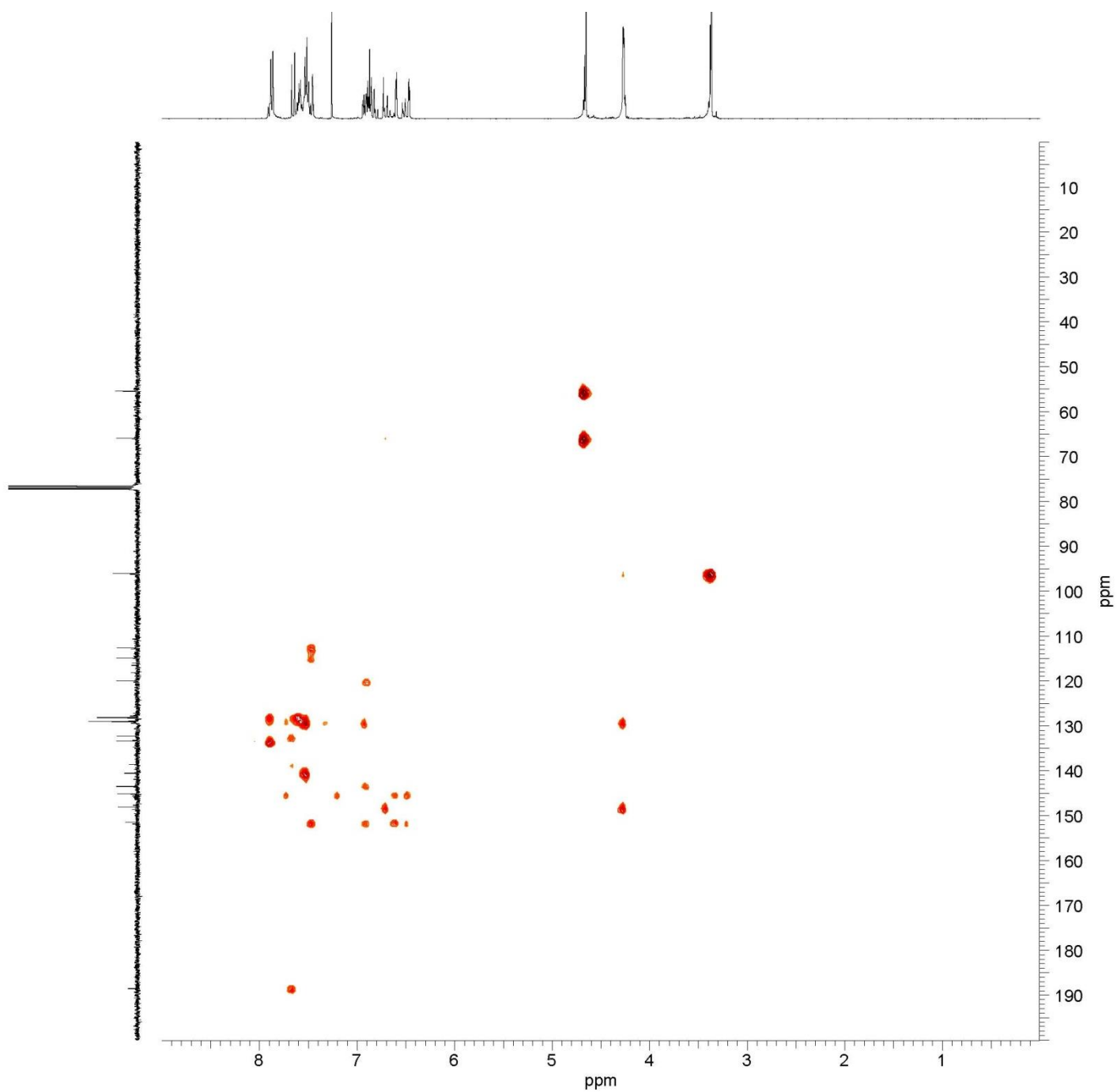


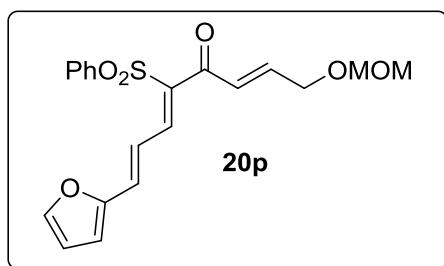
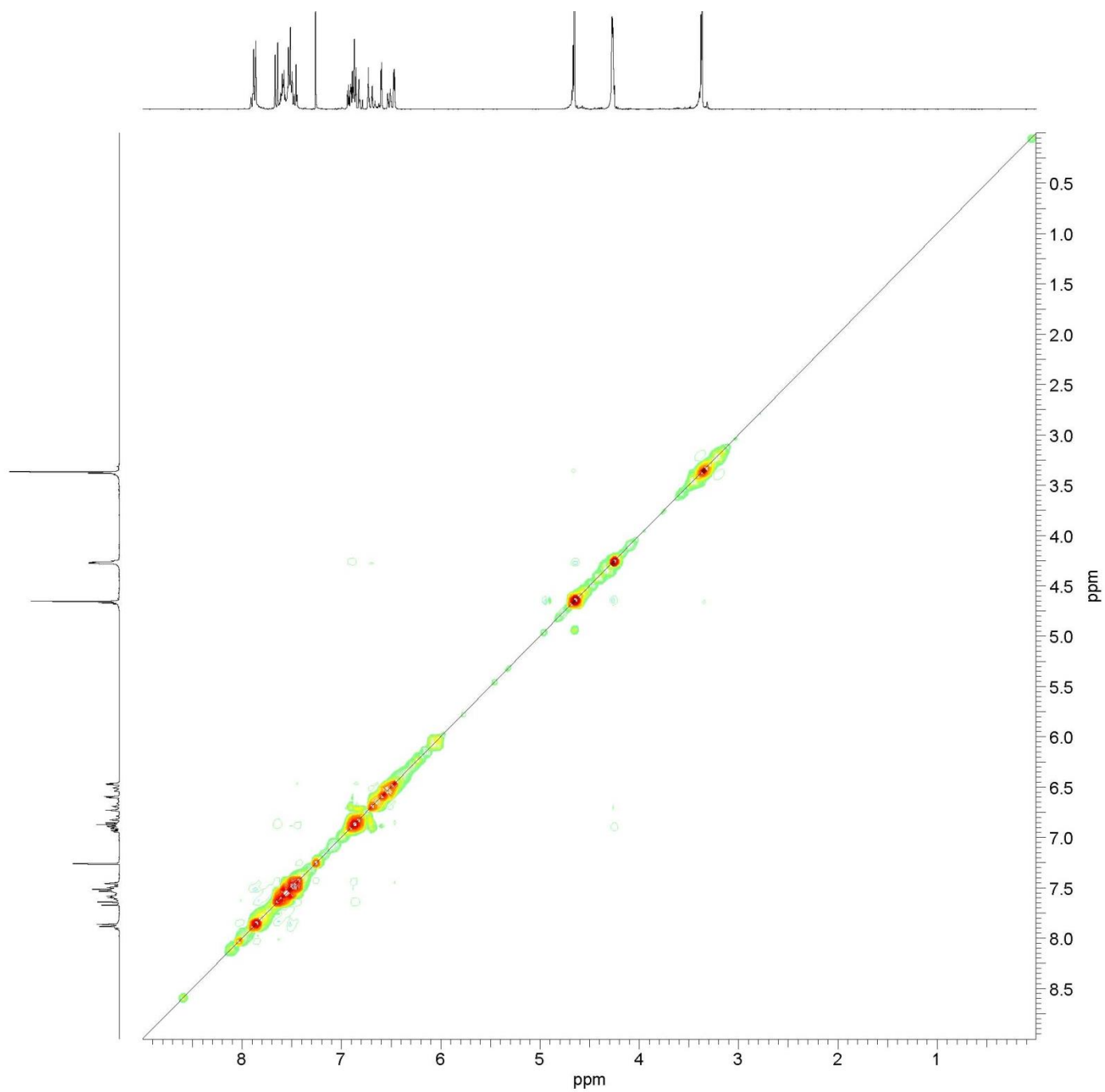


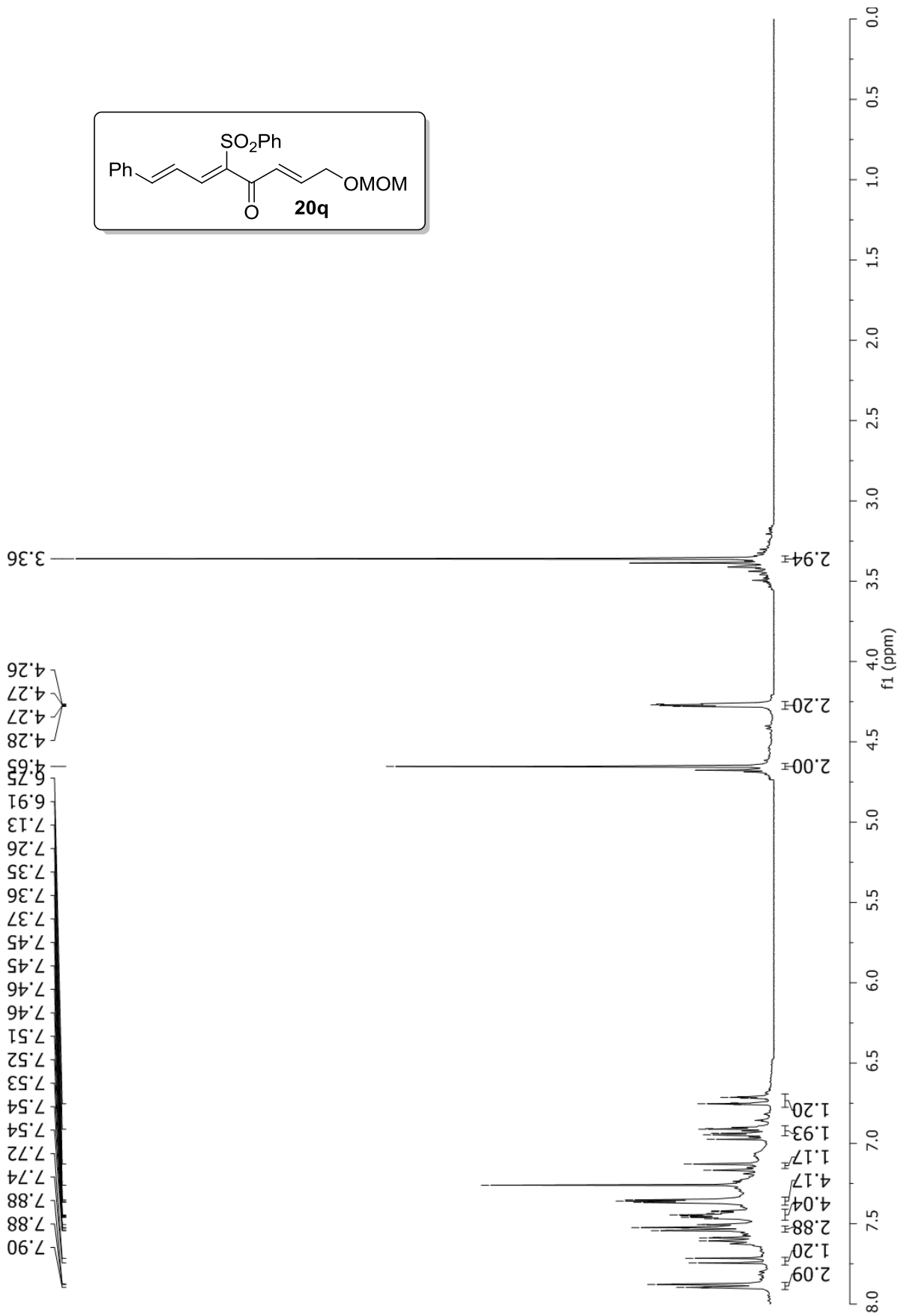
Formula	CalculatedMass	mDaError	ppmError	RDB
C2 H15 N14 O9 S	411.086167	0.033308	0.081024	2.5
C17 H12 N10 Na S	411.085933	0.26652	0.64833	16.5
C17 H19 N2 O8 S	411.085664	0.535884	1.303579	9.5
C18 H15 N6 O4 S	411.087001	-0.801428	-1.949535	14.5
C20 H20 O6 Na S	411.087282	-1.08156	-2.630978	10.5
C5 H16 N12 O7 Na S	411.087784	-1.584136	-3.853532	3.5

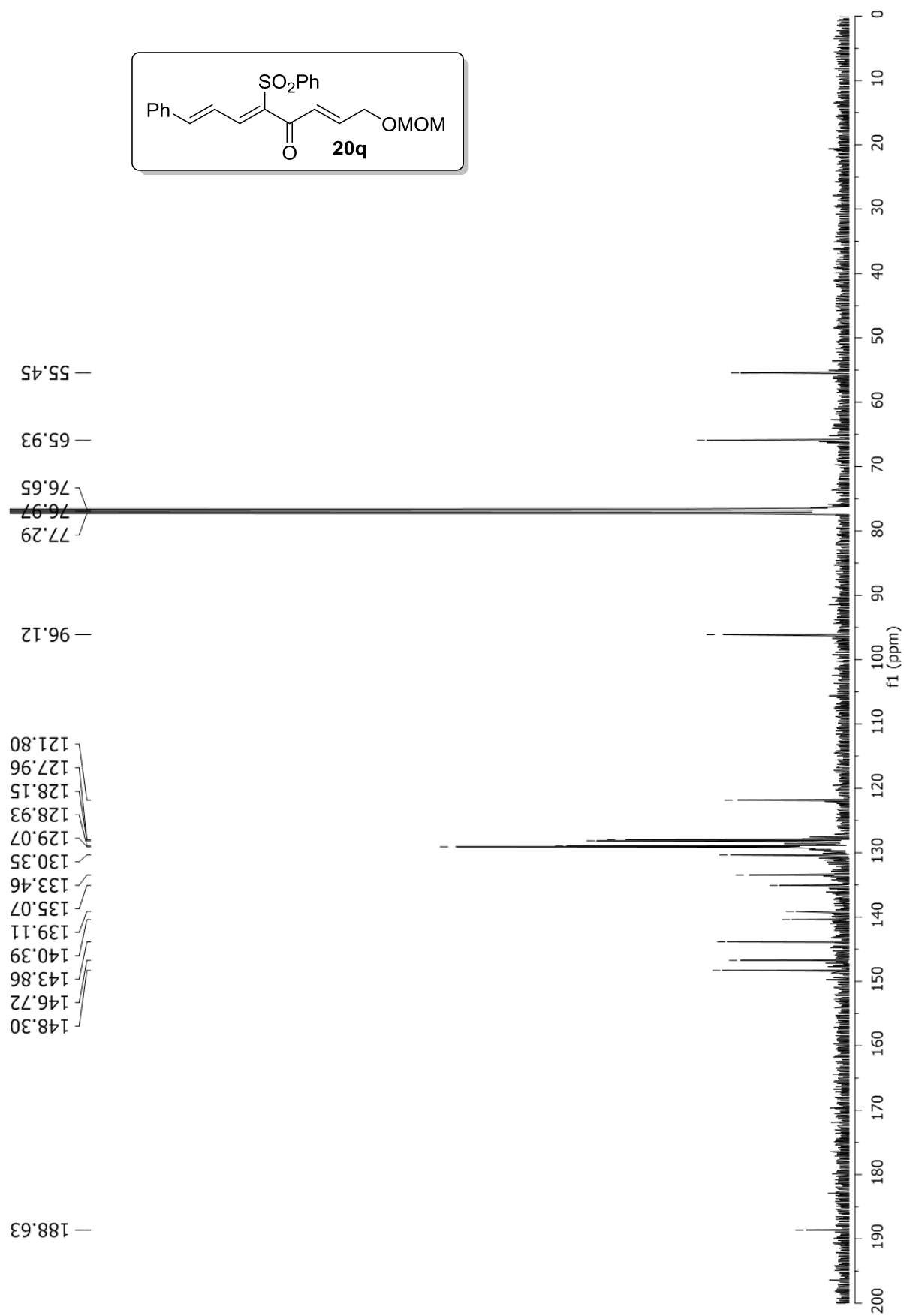
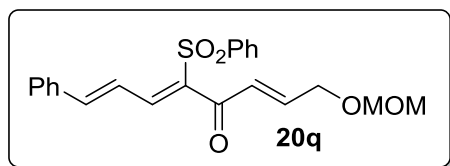


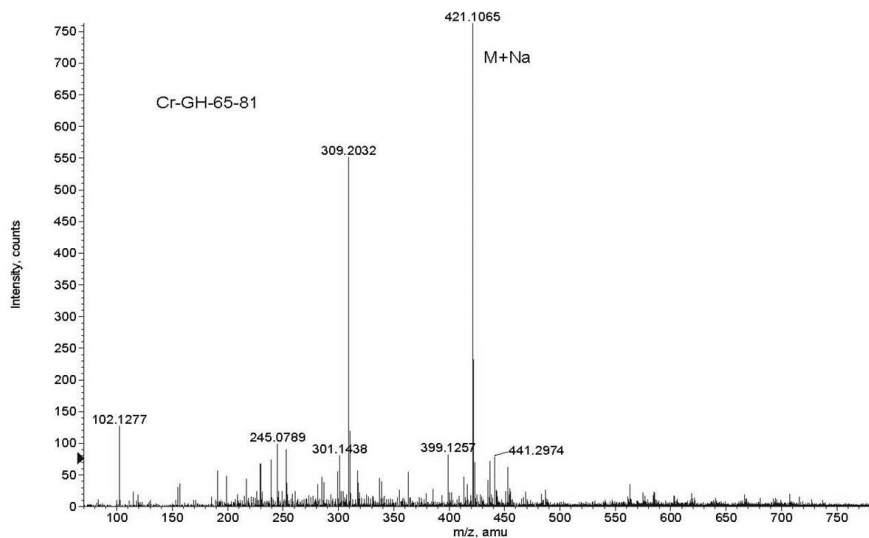
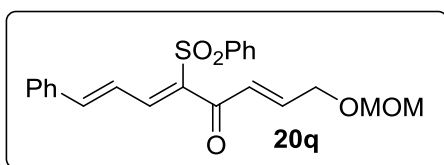
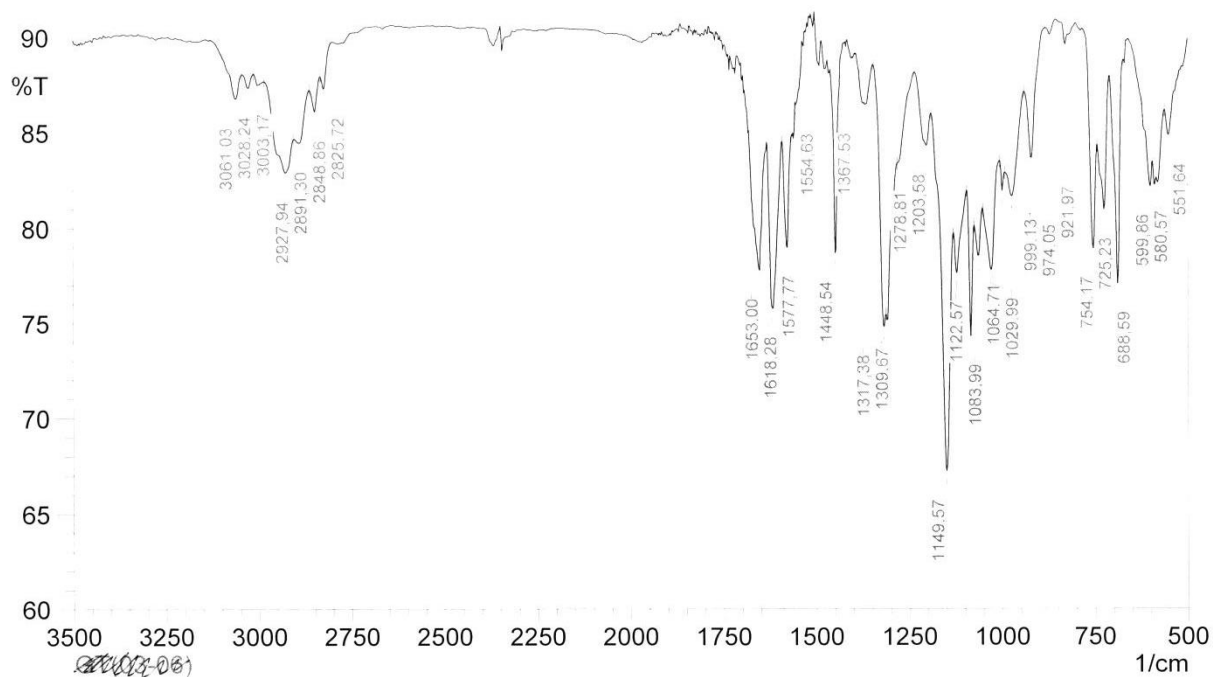




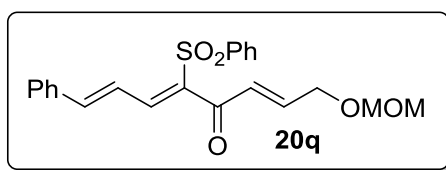
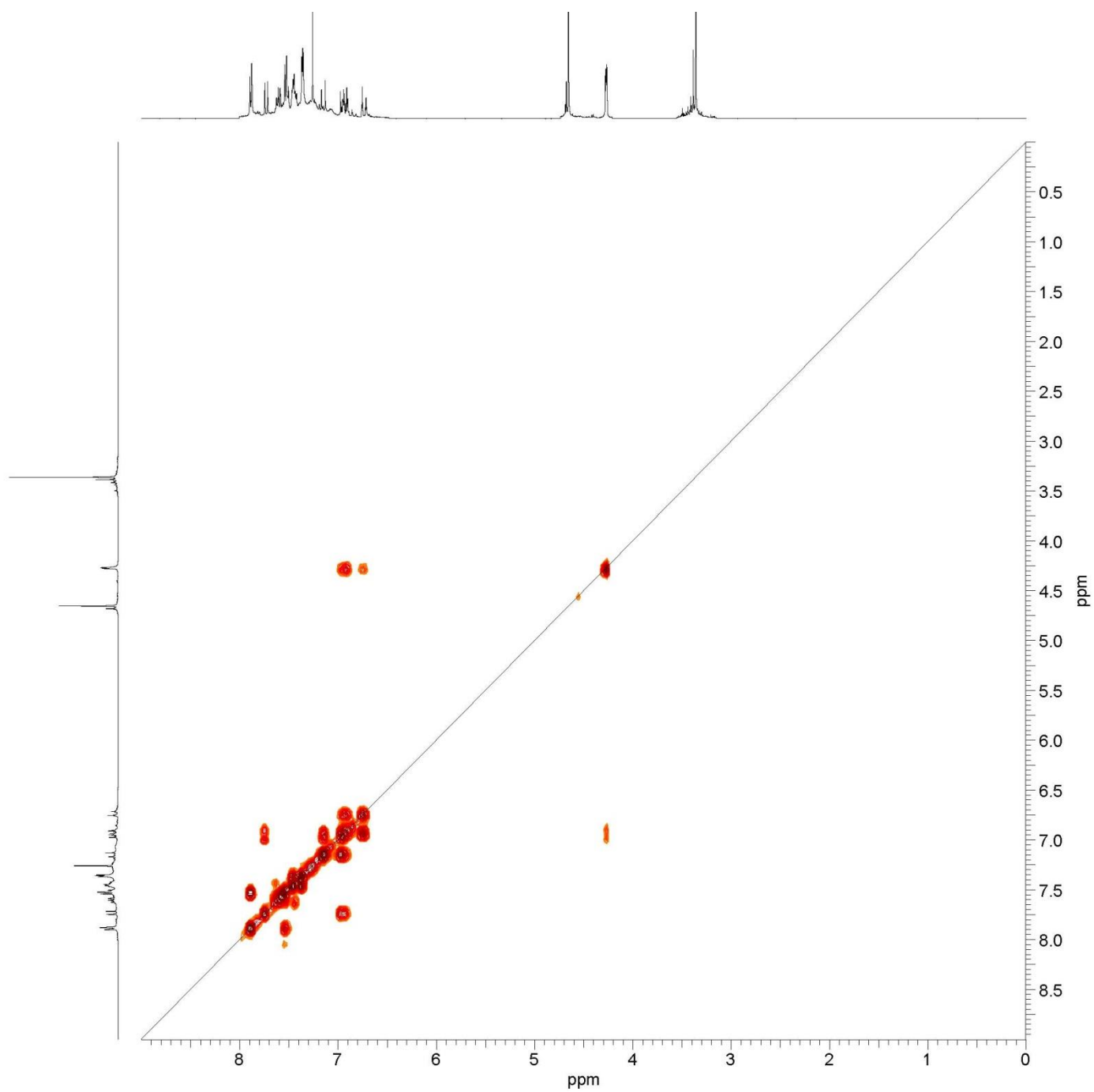


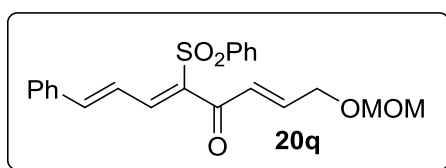
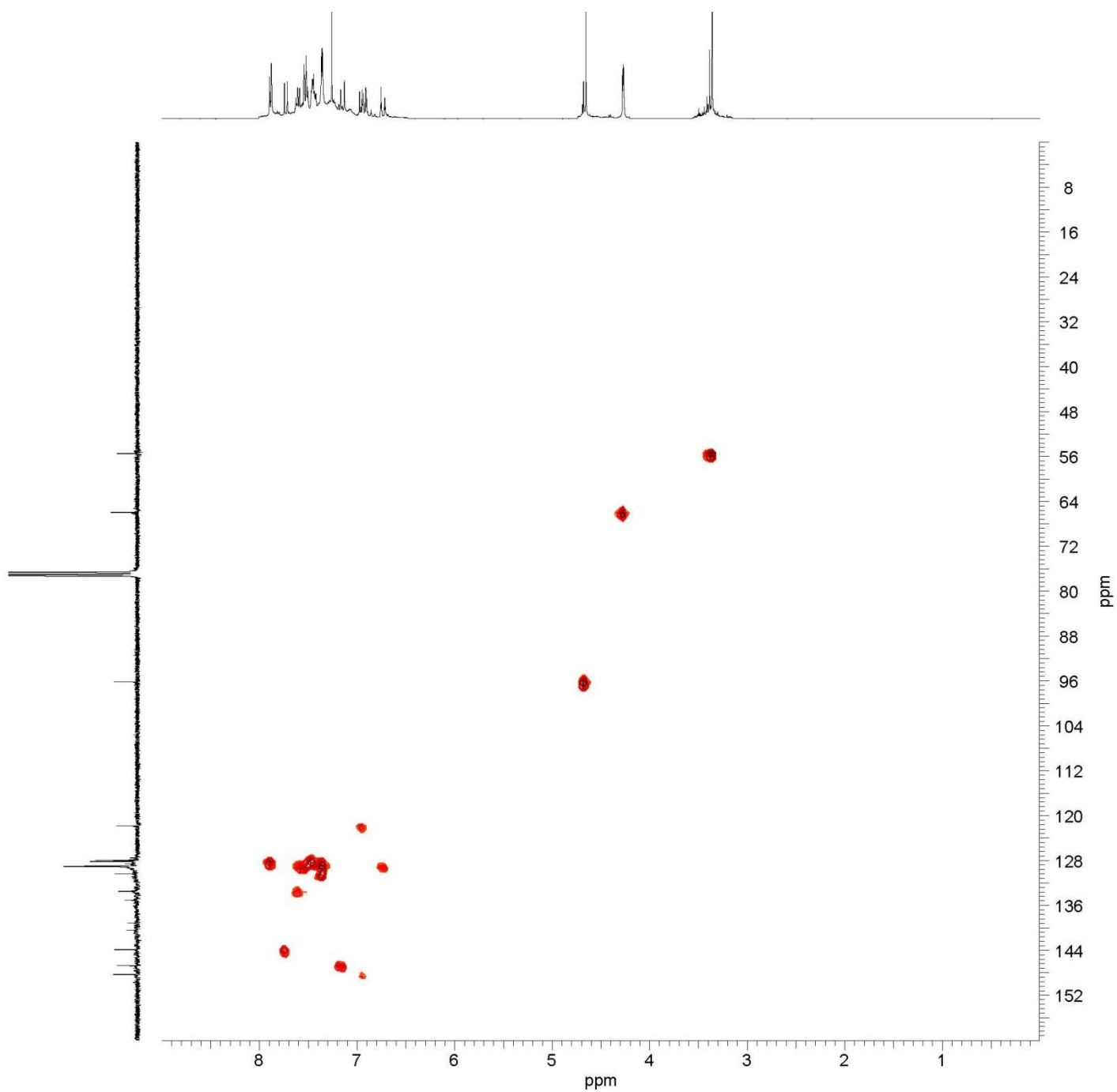


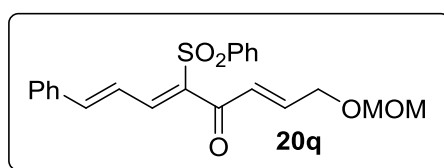
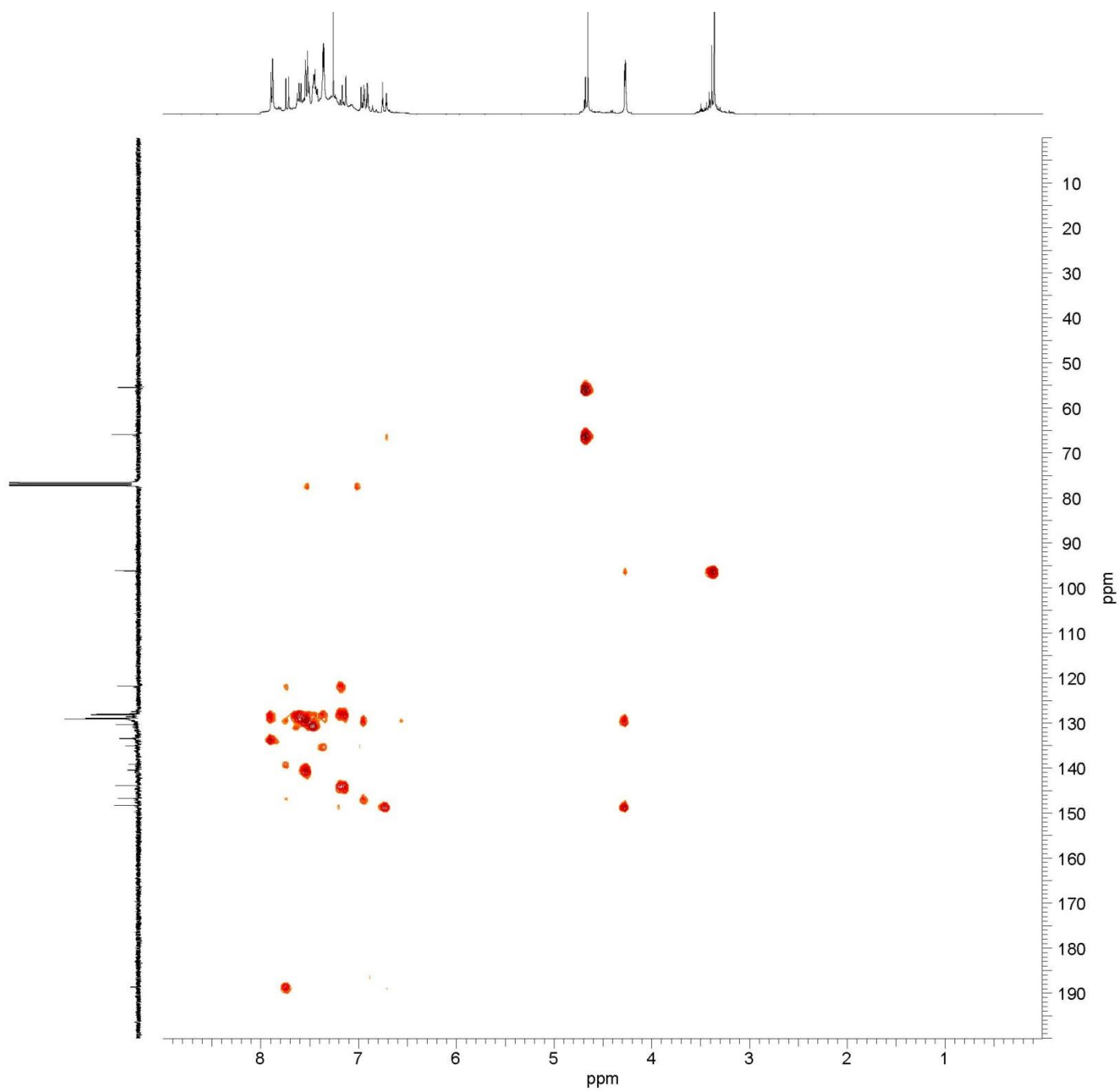


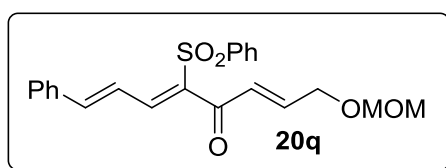
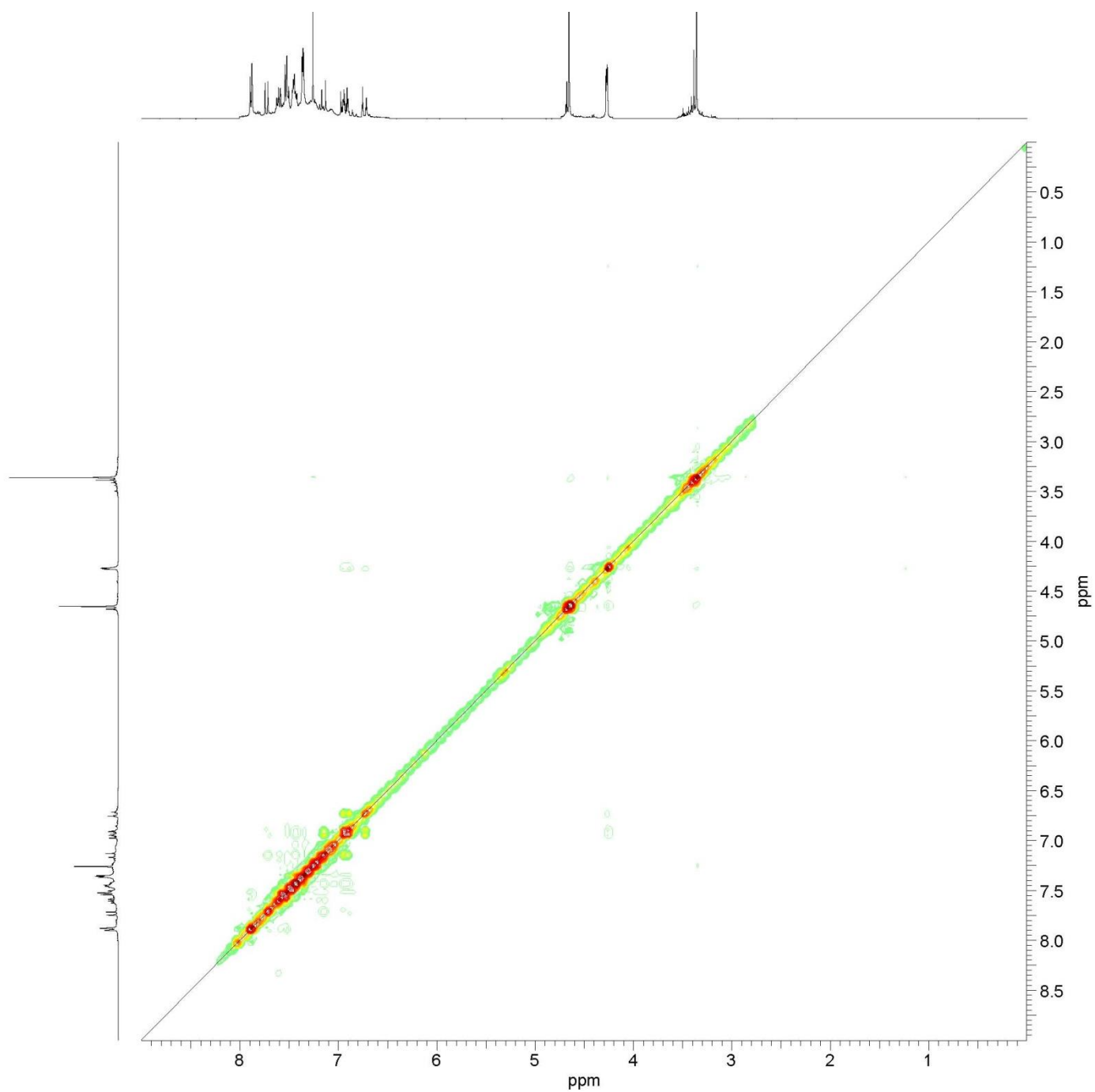


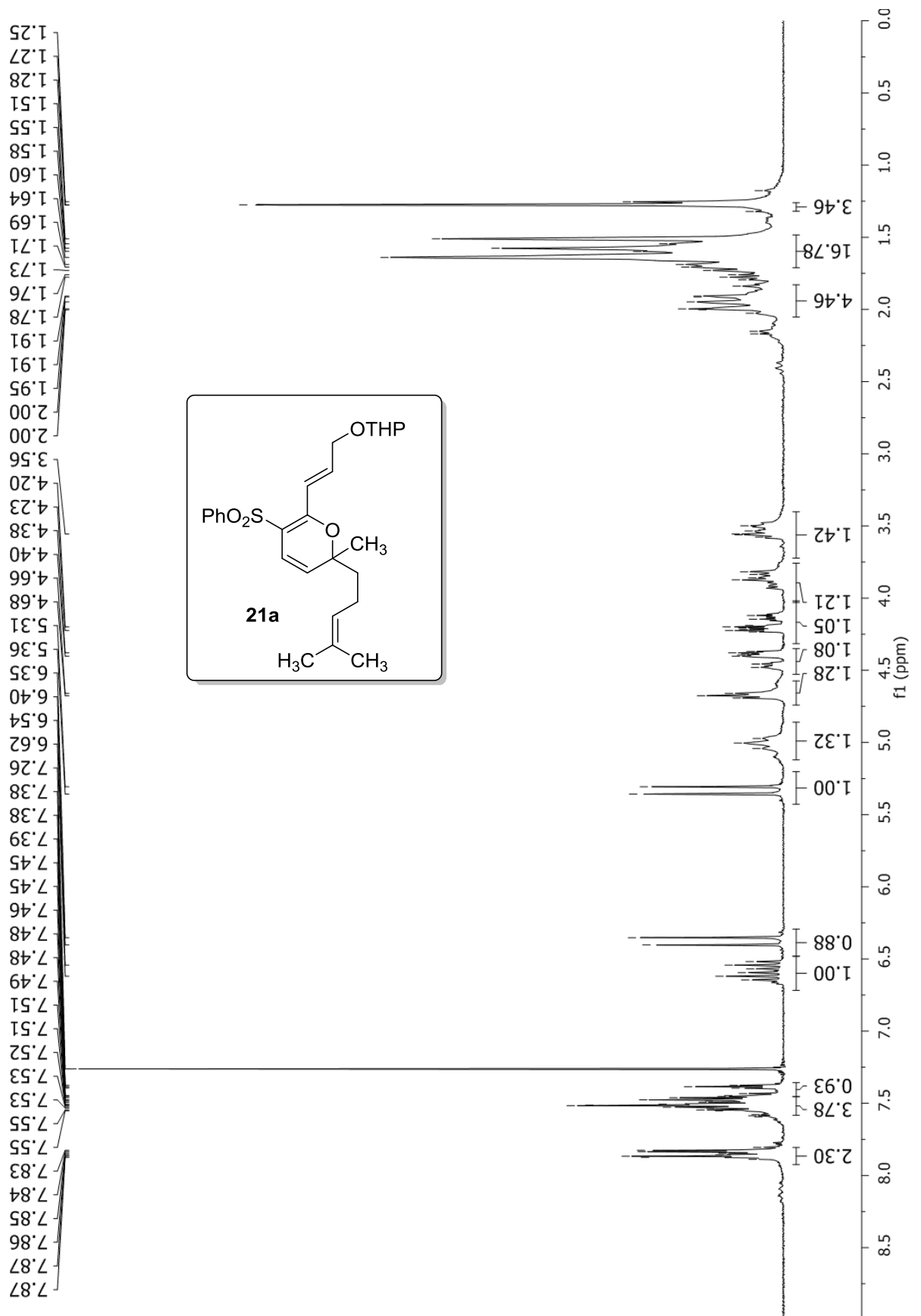
Formula	CalculatedMass	mDaError	ppmError	RDB
C13 H22 N2 O12 Na	421.106496	0.004304	0.010221	3.5
C19 H21 N2 O7 S	421.1064	0.100444	0.238524	10.5
C11 H17 N8 O10	421.106216	0.284436	0.675448	7.5
C4 H17 N14 O8 S	421.106902	-0.402132	-0.95494	3.5
C26 H14 N4 O Na	421.105982	0.517648	1.229255	21.5
C27 H17 O5	421.10705	-0.5503	-1.306794	19.5
C6 H22 N8 O10 Na S	421.107182	-0.682264	-1.620168	-0.5
C12 H13 N12 O6	421.107553	-1.052876	-2.500257	12.5
C18 H18 N6 O3 Na S	421.105332	1.168392	2.774572	12.5
C20 H17 N6 O3 S	421.107737	-1.236868	-2.937182	15.5
C14 H18 N6 O8 Na	421.107833	-1.333008	-3.165485	8.5
C10 H14 N12 O6 Na	421.105148	1.352384	3.211497	9.5
C16 H13 N12 O S	421.105051	1.448524	3.4398	16.5
C22 H22 O5 Na S	421.108017	-1.517	-3.602409	11.5

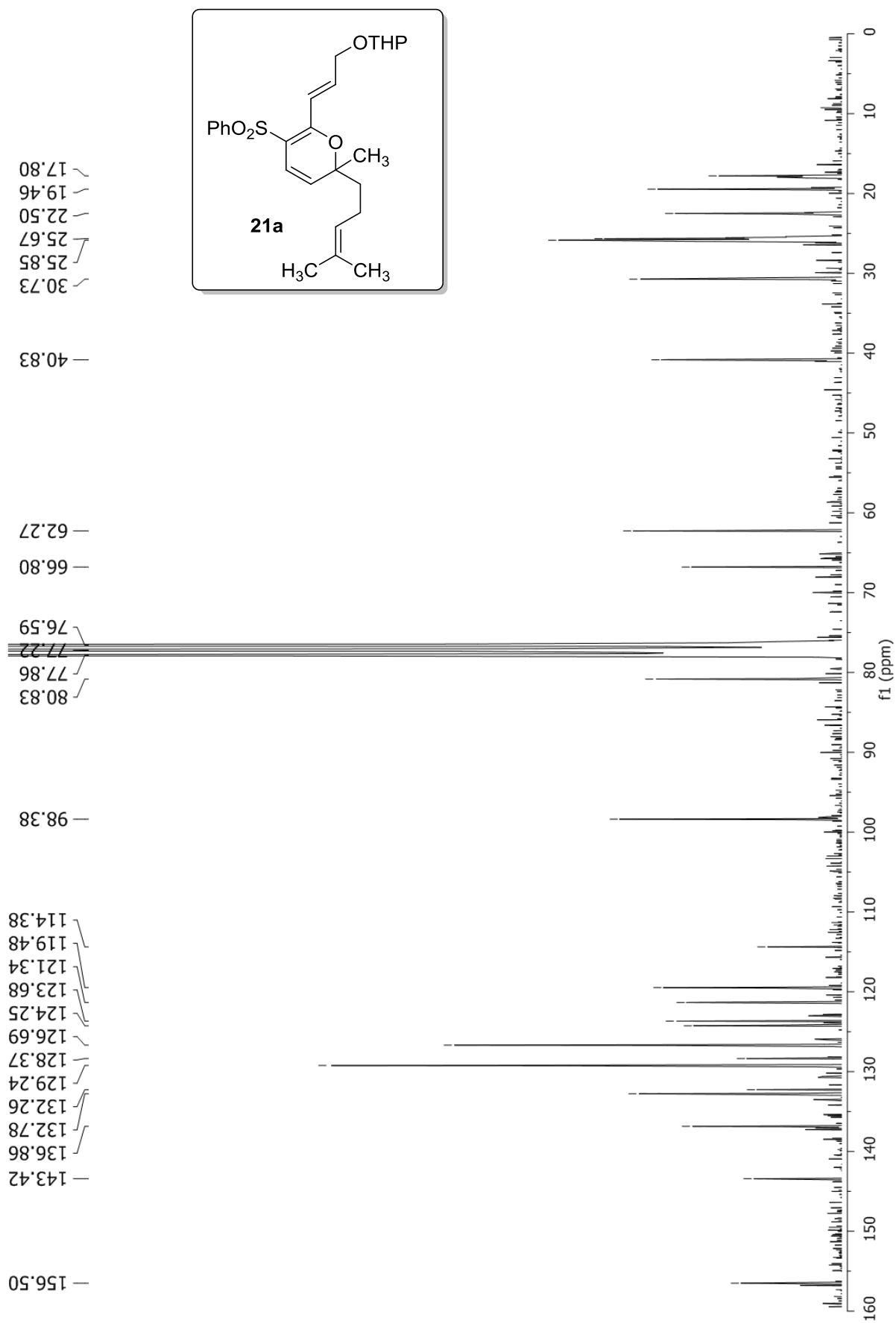


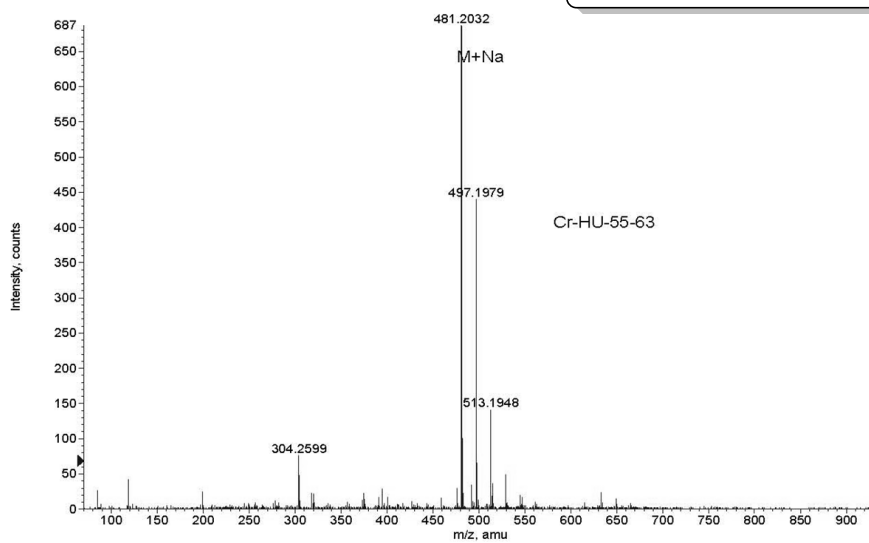
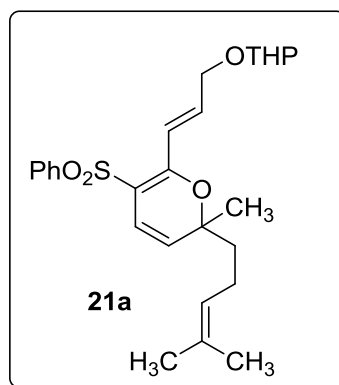
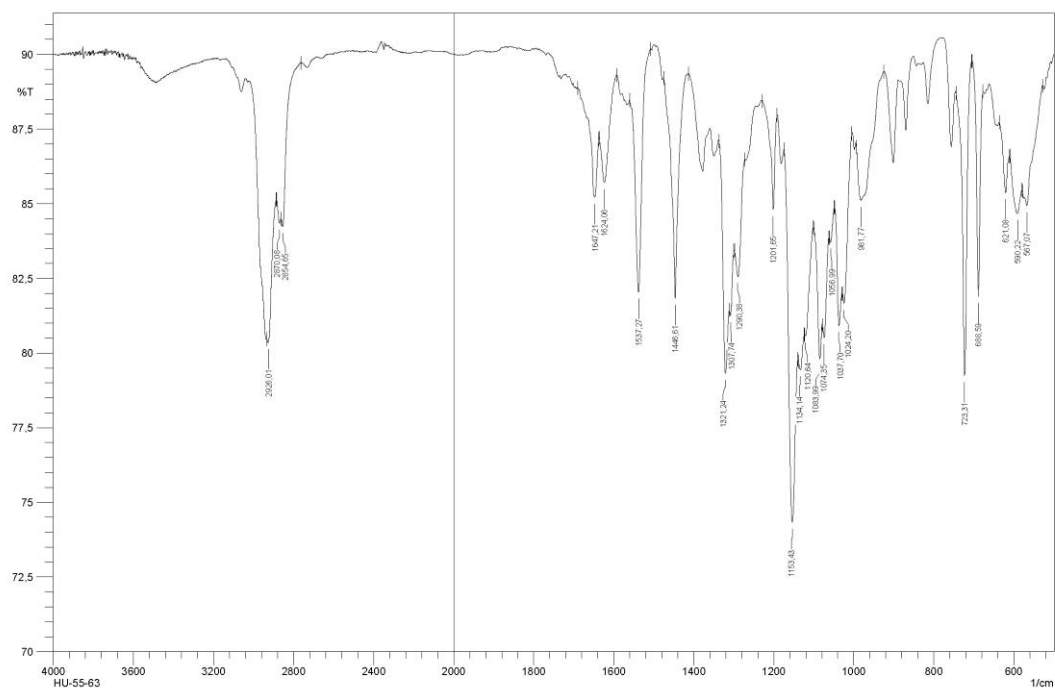




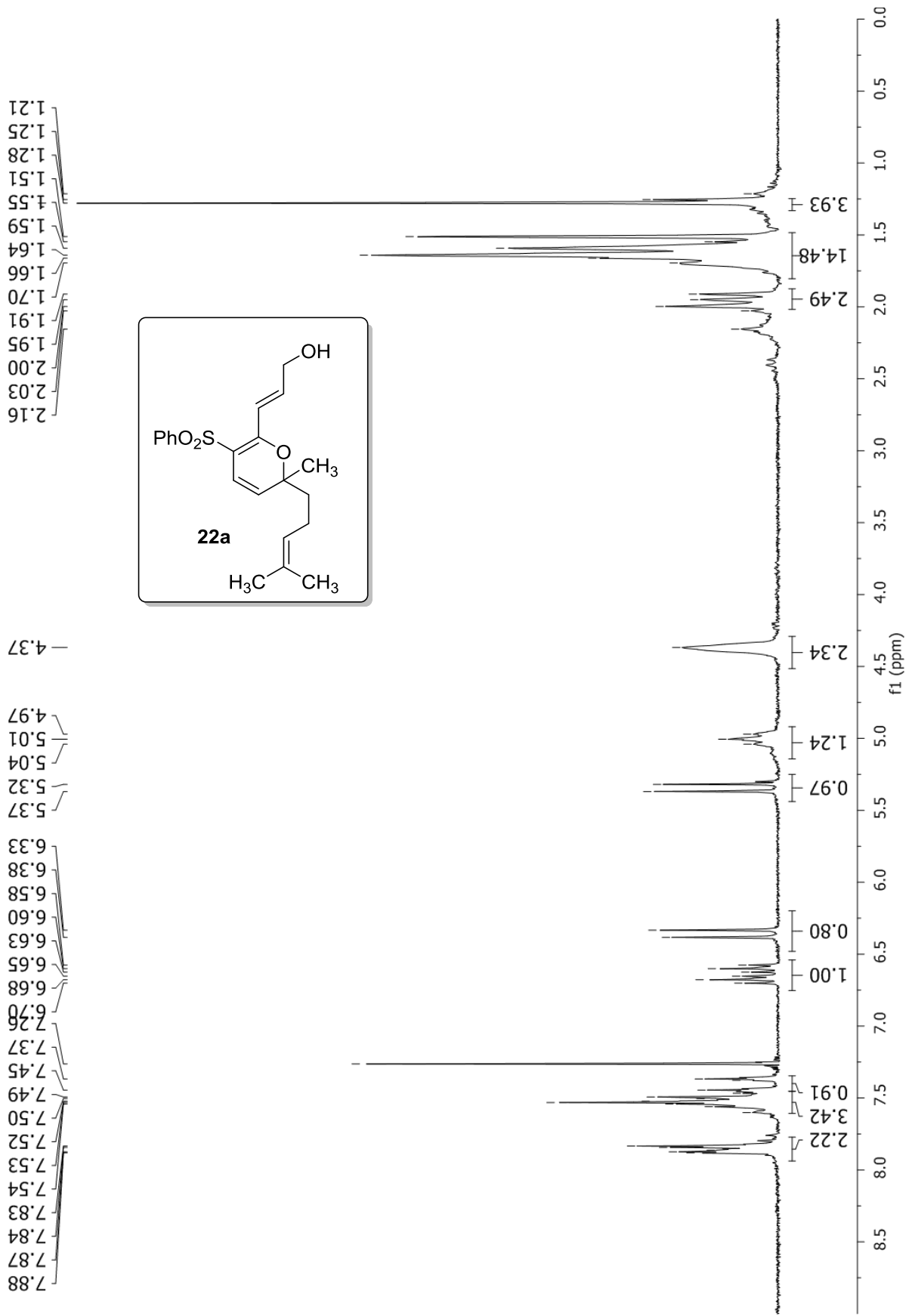


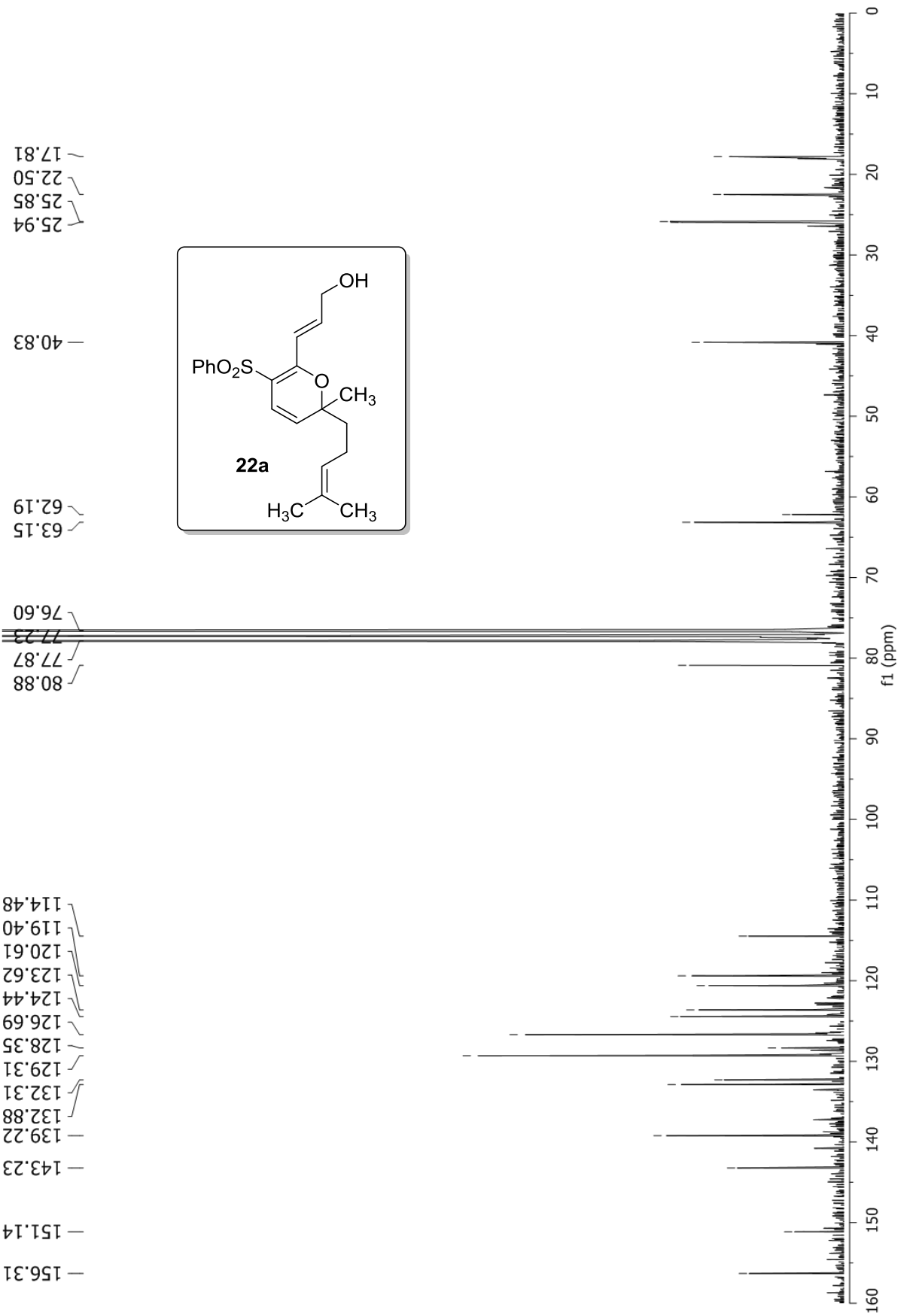


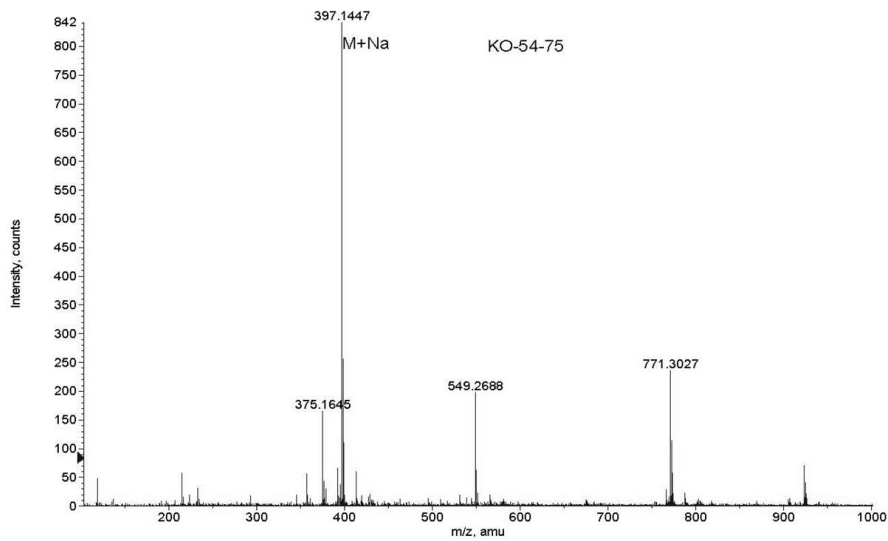
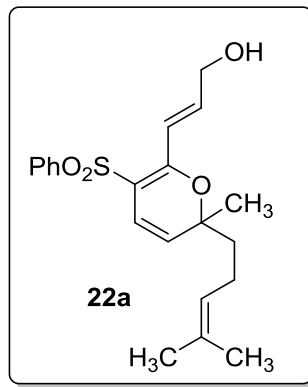
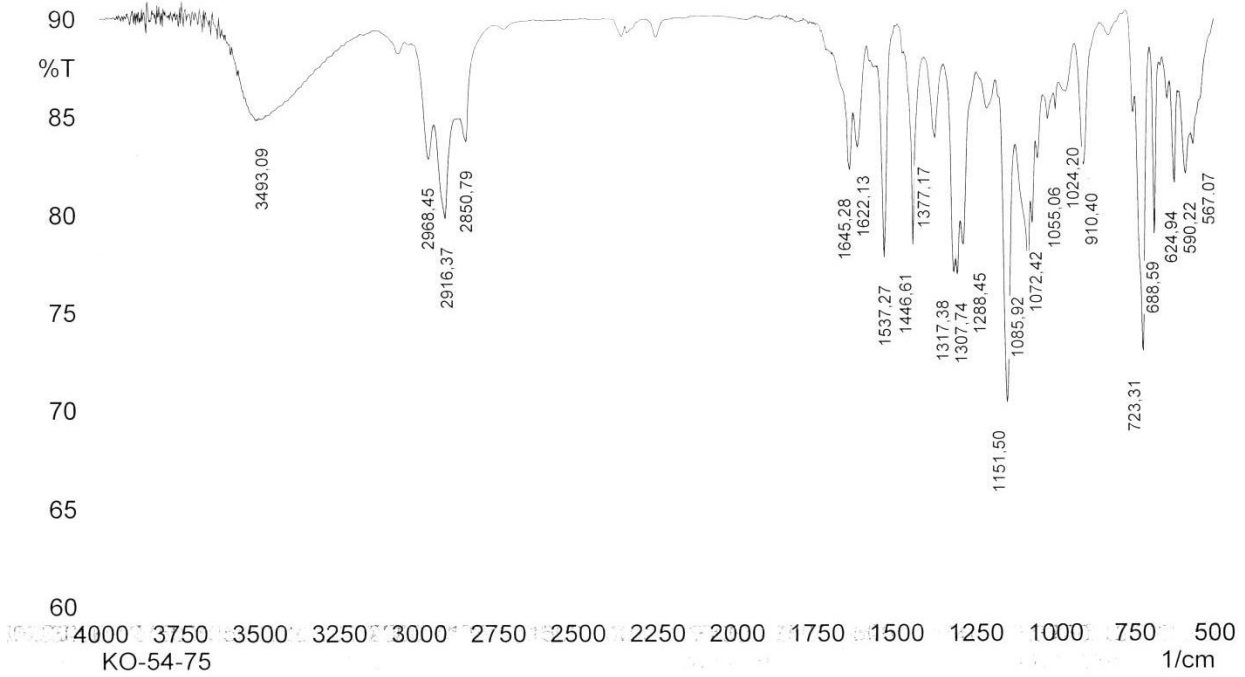




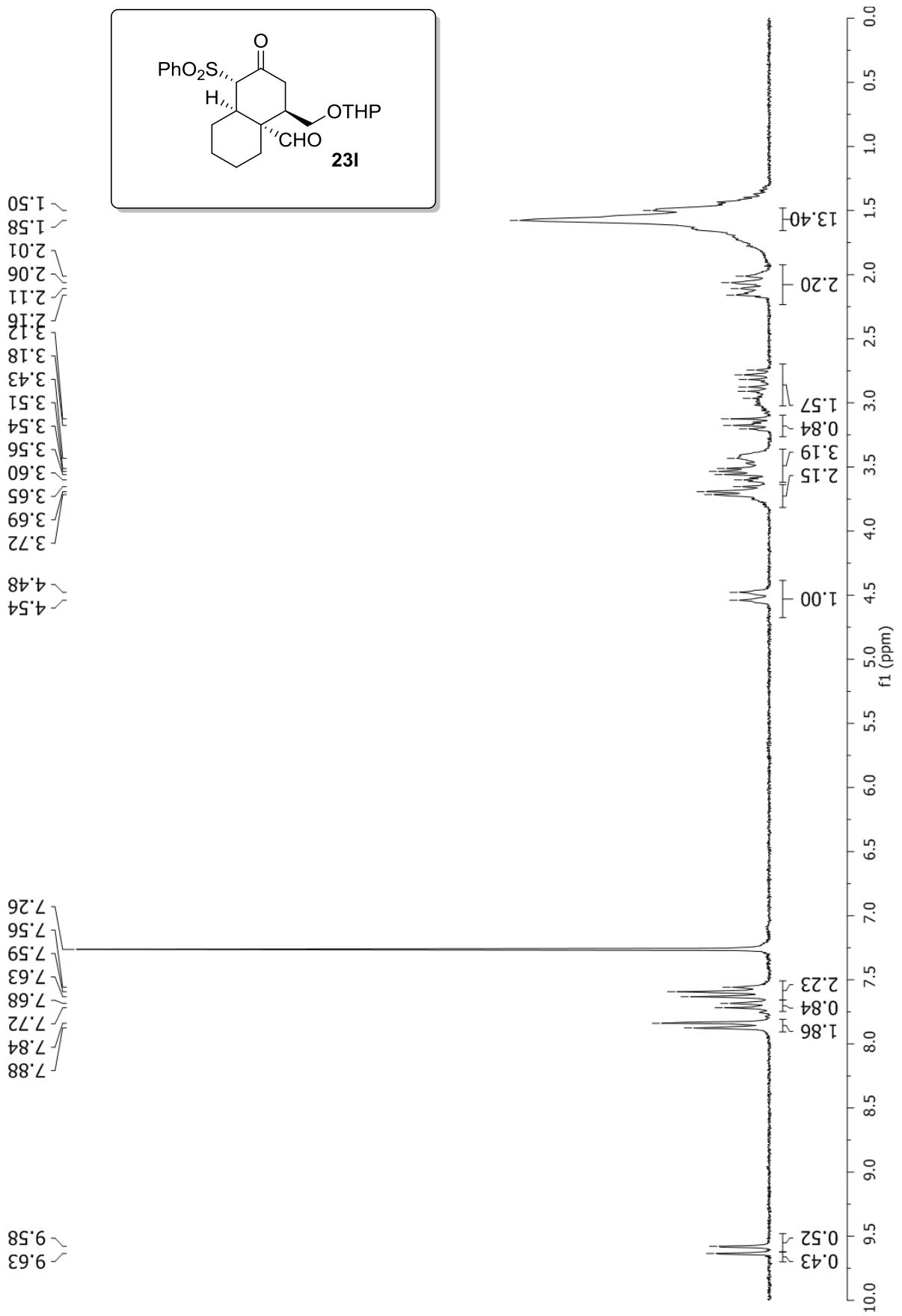
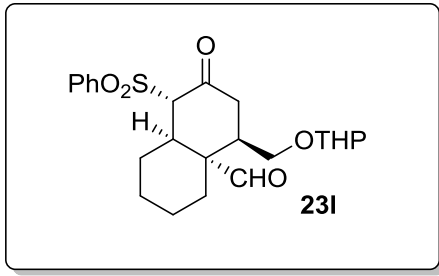
Formula	CalculatedMass	mDaError	ppmError	RDB
C27 H30 N4 O Na S	481.203255	-0.054792	-0.113864	14.5
C12 H33 N8 O10 S	481.203488	-0.288004	-0.598507	0.5
C11 H30 N12 O6 Na S	481.20242	0.779944	1.620819	2.5
C28 H33 O5 S	481.204323	-1.12274	-2.33319	12.5
C26 H34 O5 Na S	481.201917	1.28252	2.665233	9.5

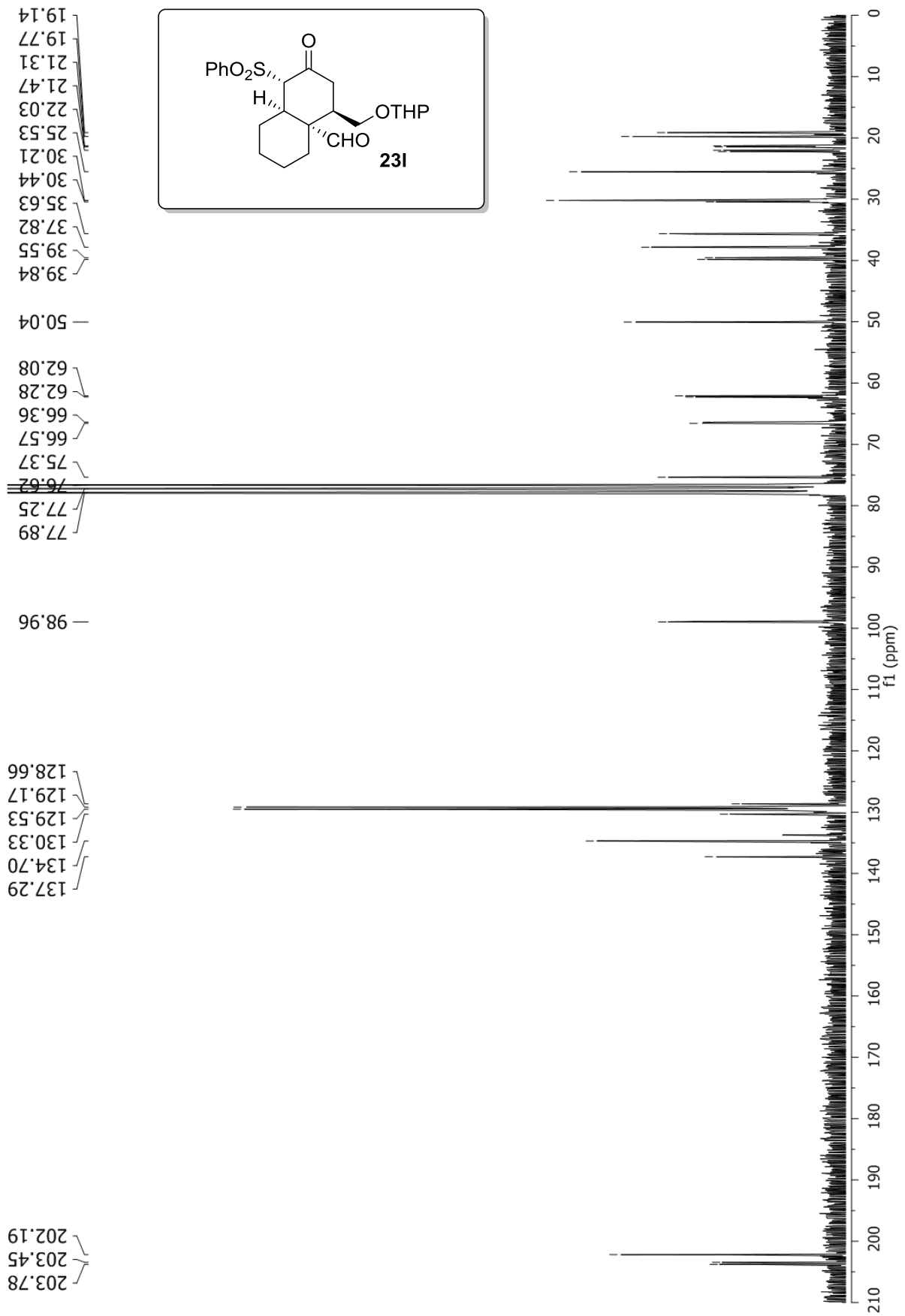




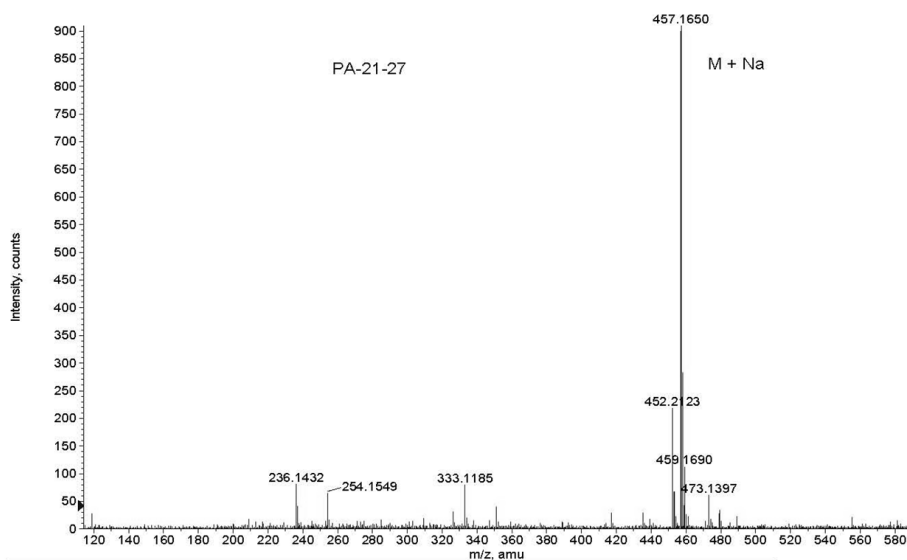
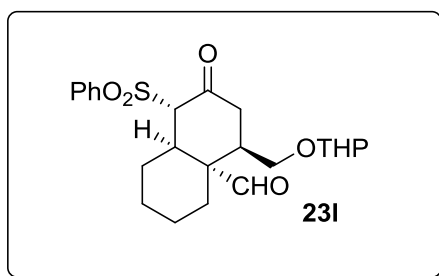
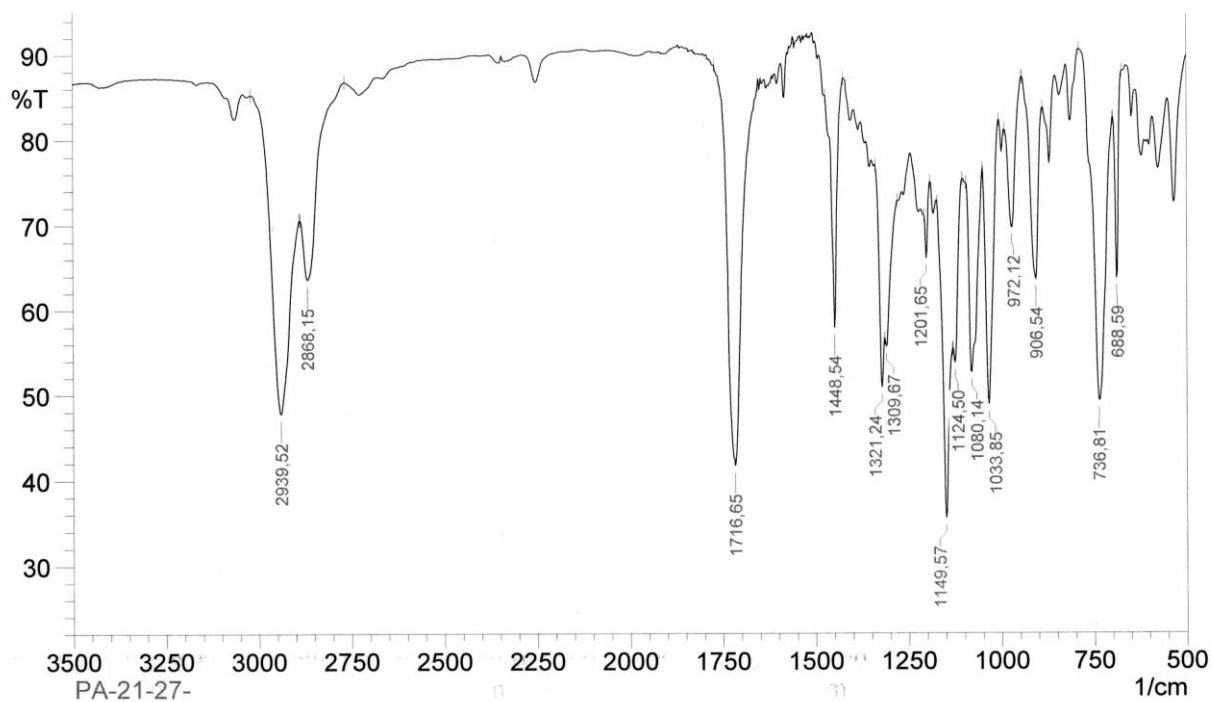


Formula	CalculatedMass	mDaError	ppmError	RDB
C27 H17 N4	397.144773	-0.073132	-0.184144	21.5
C21 H26 O4 Na S	397.144403	0.29748	0.749046	8.5

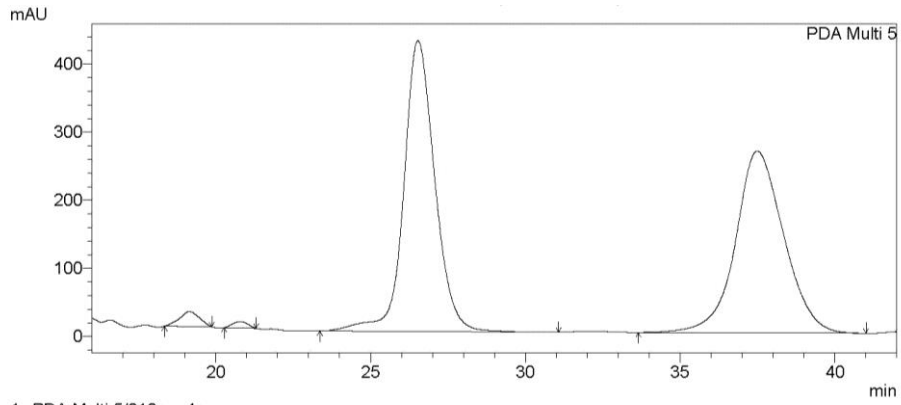




Full Spectroscopy



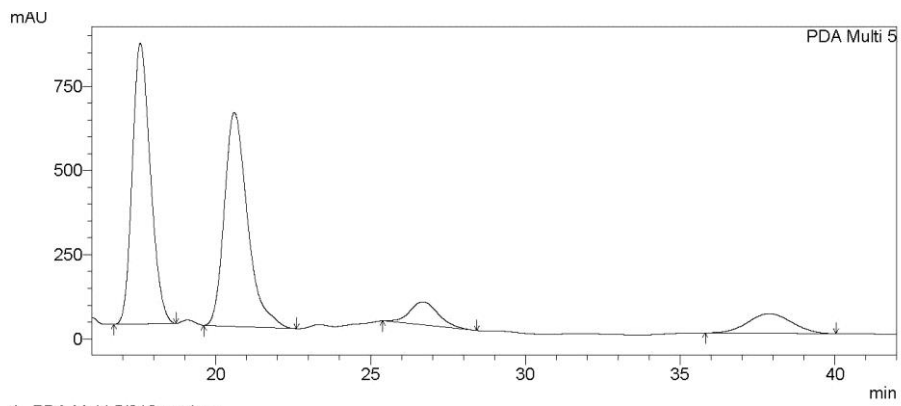
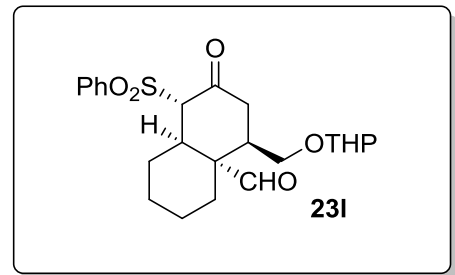
Formula	CalculatedMass	mDaError	ppmError	RDB
C21 H25 N6 O4 S	457.165252	-0.251828	-0.550846	12.5
C15 H26 N6 O9 Na	457.165348	-0.347968	-0.761142	5.5
C28 H25 O6	457.164565	0.43474	0.950947	16.5
C23 H30 O6 Na S	457.165532	-0.53196	-1.163605	8.5



1 PDA Multi 5/210nm 4nm

PeakTable

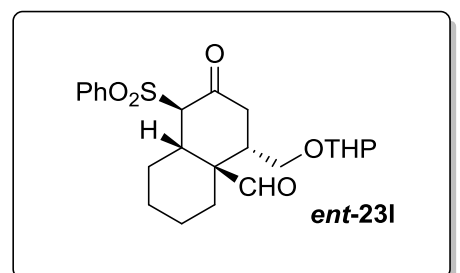
Peak#	Ret. Time	Area %
1	19.141	1.612
2	20.775	0.527
3	26.527	49.707
4	37.486	48.154
Total		100.000

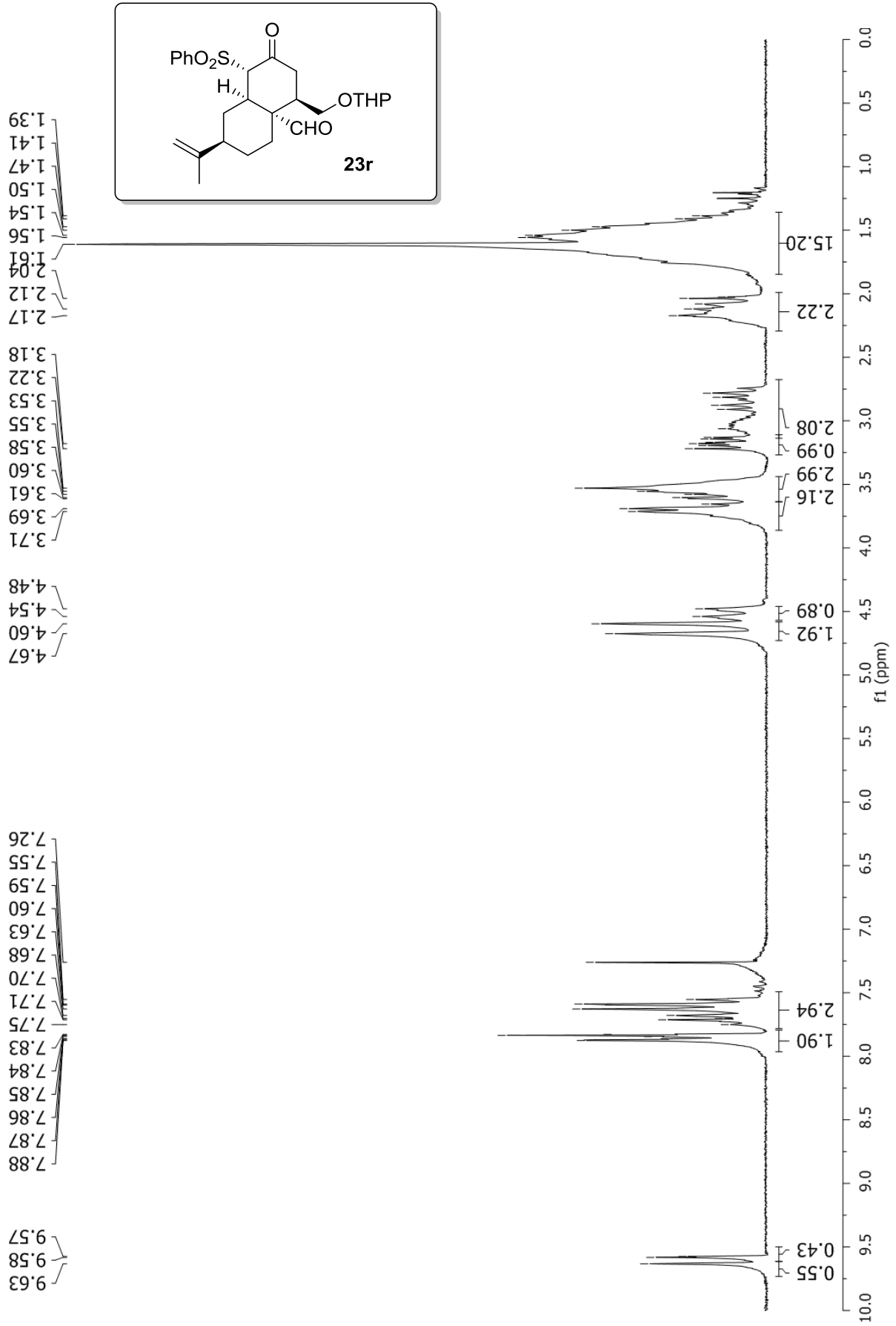


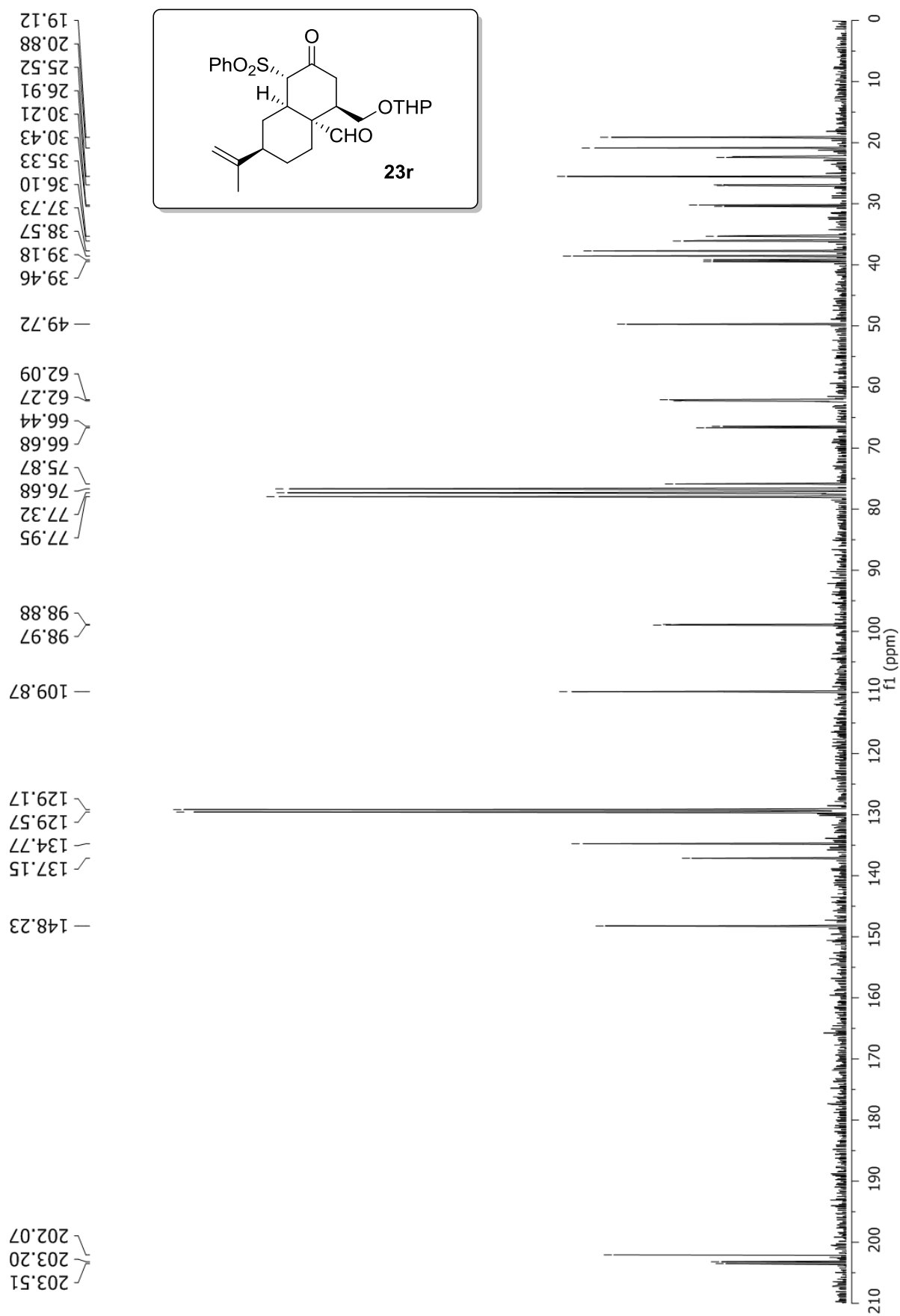
1 PDA Multi 5/210nm 4nm

PeakTable

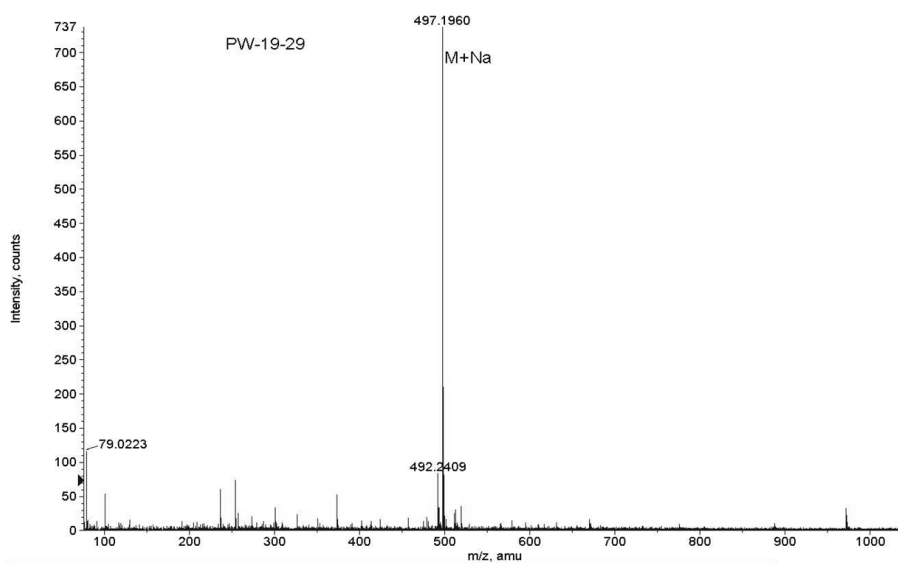
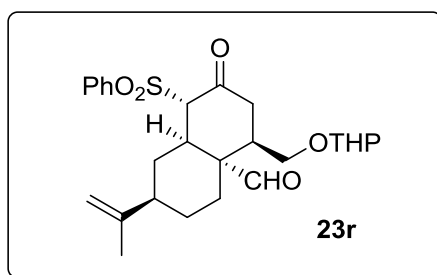
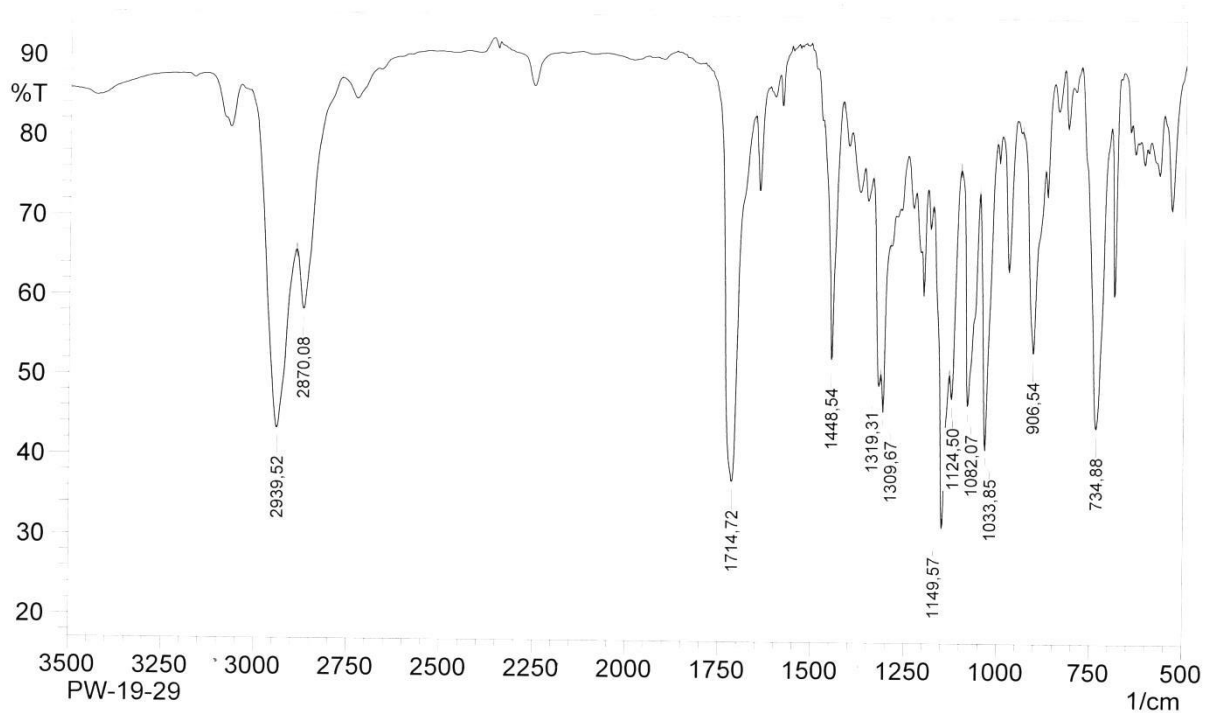
Peak#	Ret. Time	Area %
1	17.557	43.999
2	20.595	42.994
3	26.682	5.655
4	37.883	7.351
Total		100.000



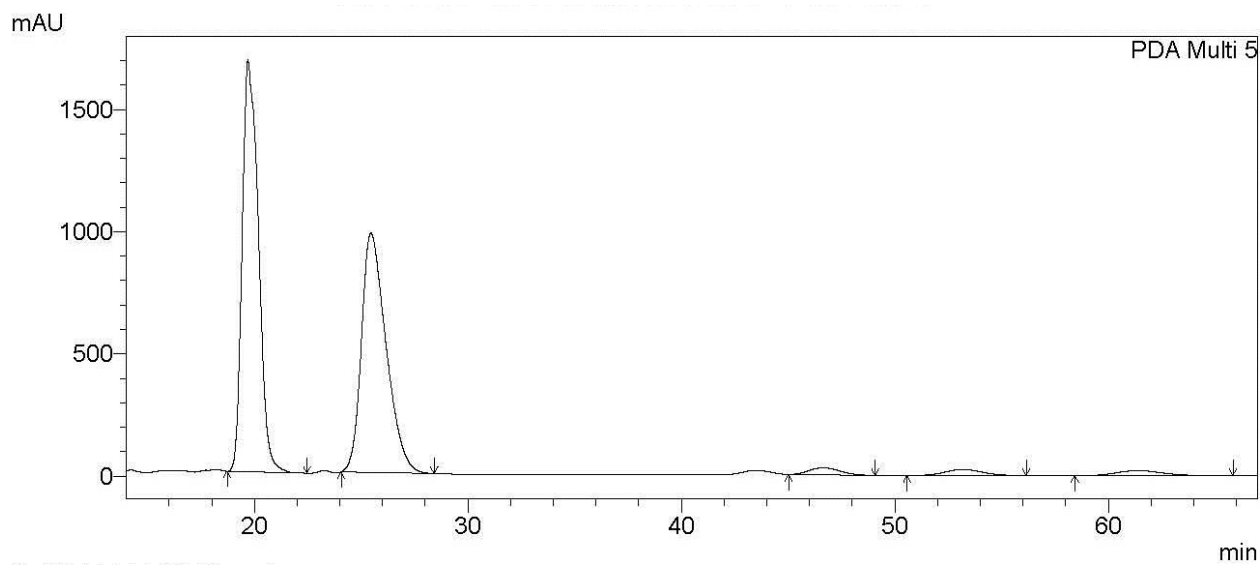




Full Spectroscopy



Formula	CalculatedMass	mDaError	ppmError	RDB
C31 H29 O6	497.195865	0.13458	0.270678	17.5
C23 H33 N2 O8 S	497.195215	0.785324	1.579504	8.5
C26 H34 O6 Na S	497.196832	-0.83212	-1.673624	9.5

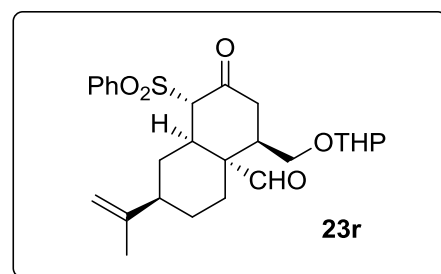


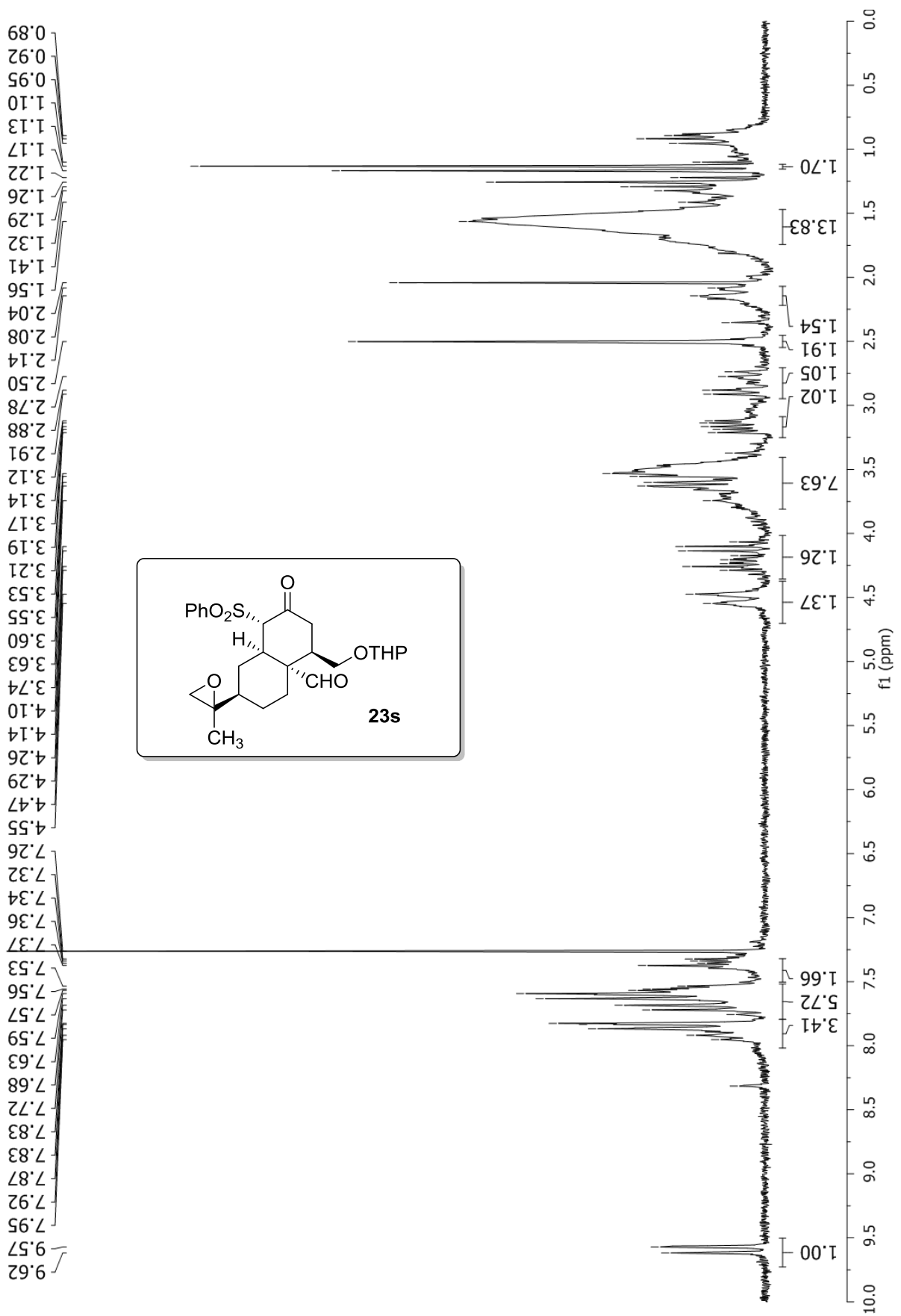
1 PDA Multi 5/210nm 4nm

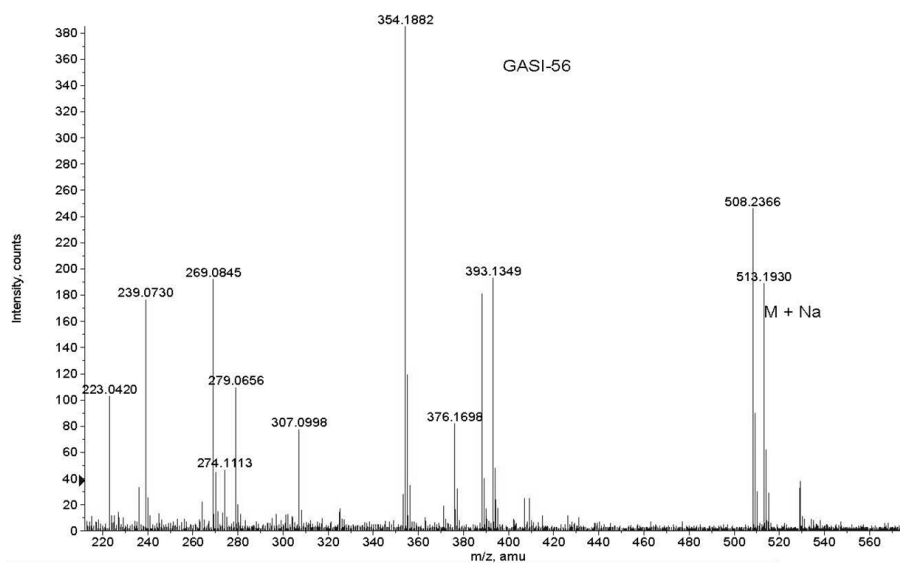
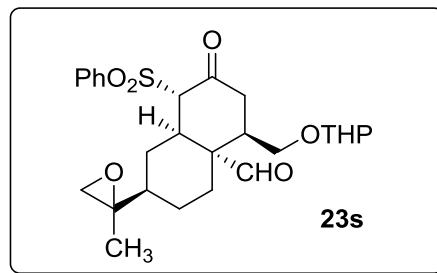
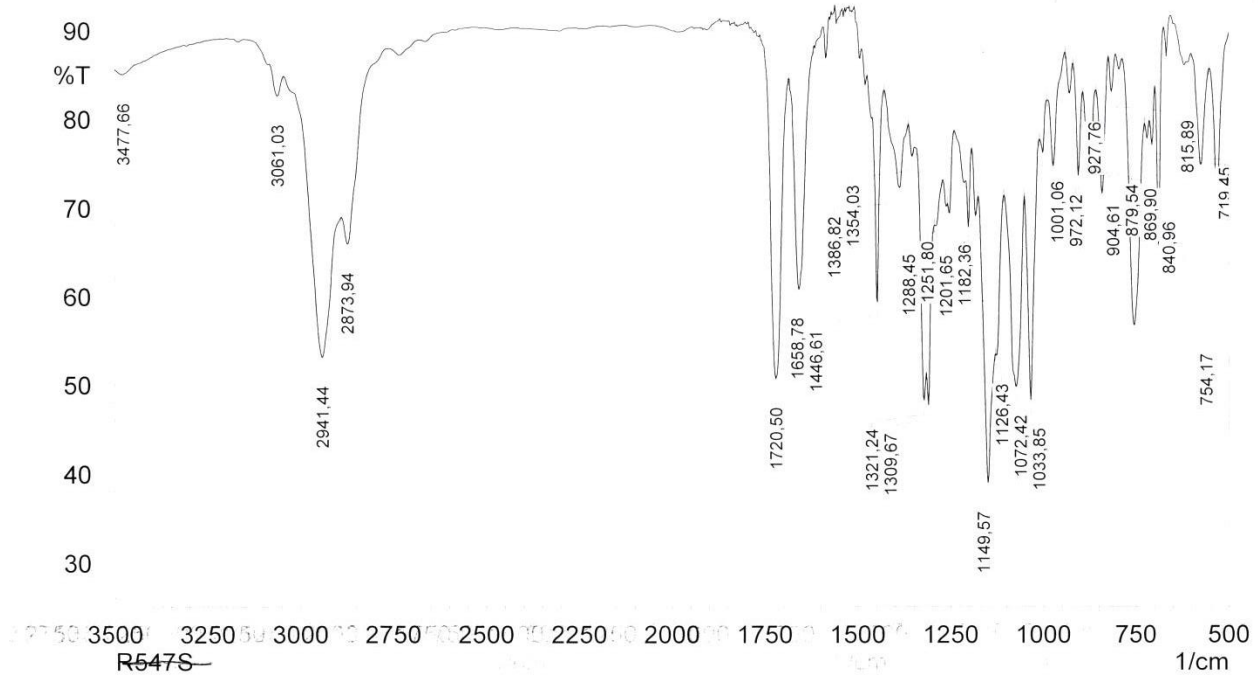
PeakTable

PDA Ch5 210nm 4nm

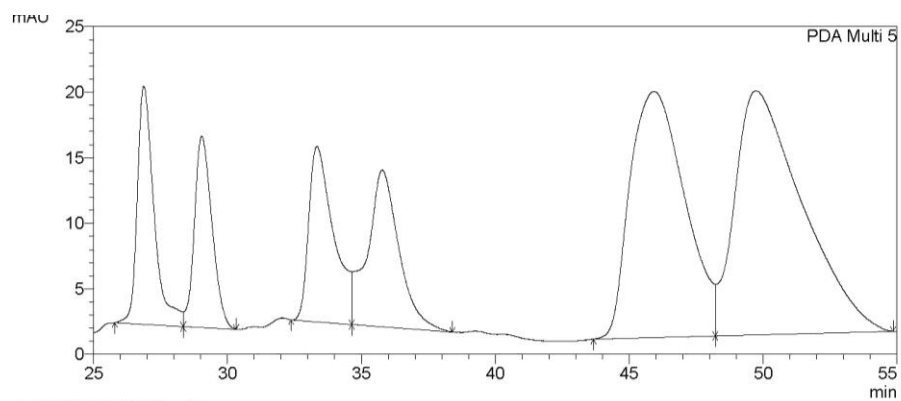
Peak#	Ret. Time	Area %
1	19.688	50.436
2	25.454	44.540
3	46.618	1.631
4	53.177	1.672
5	61.389	1.720
Total		100.000







Formula	CalculatedMass	mDaError	ppmError	RDB
C27 H30 N4 O3 Na S	513.193084	-0.084072	-0.163821	14.5
C35 H26 N2 O Na	513.193735	-0.734816	-1.43185	23.5
C32 H25 N4 O3	513.192117	0.882628	1.719874	22.5
C28 H33 O7 S	513.194152	-1.15202	-2.244806	12.5
C26 H34 O7 Na S	513.191747	1.25324	2.442042	9.5

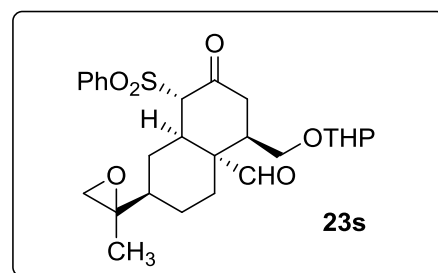


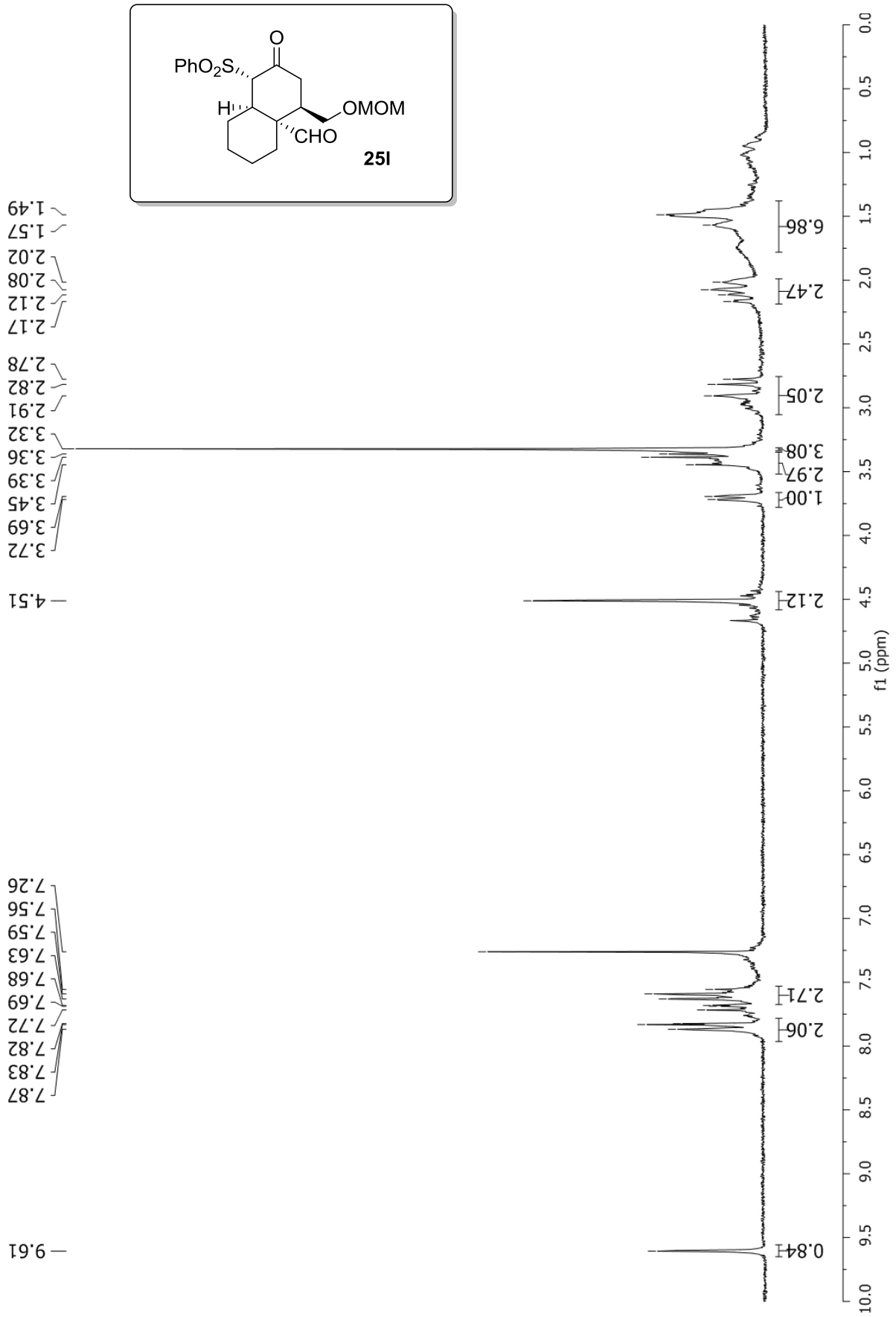
1 PDA Multi 5/290nm 4nm

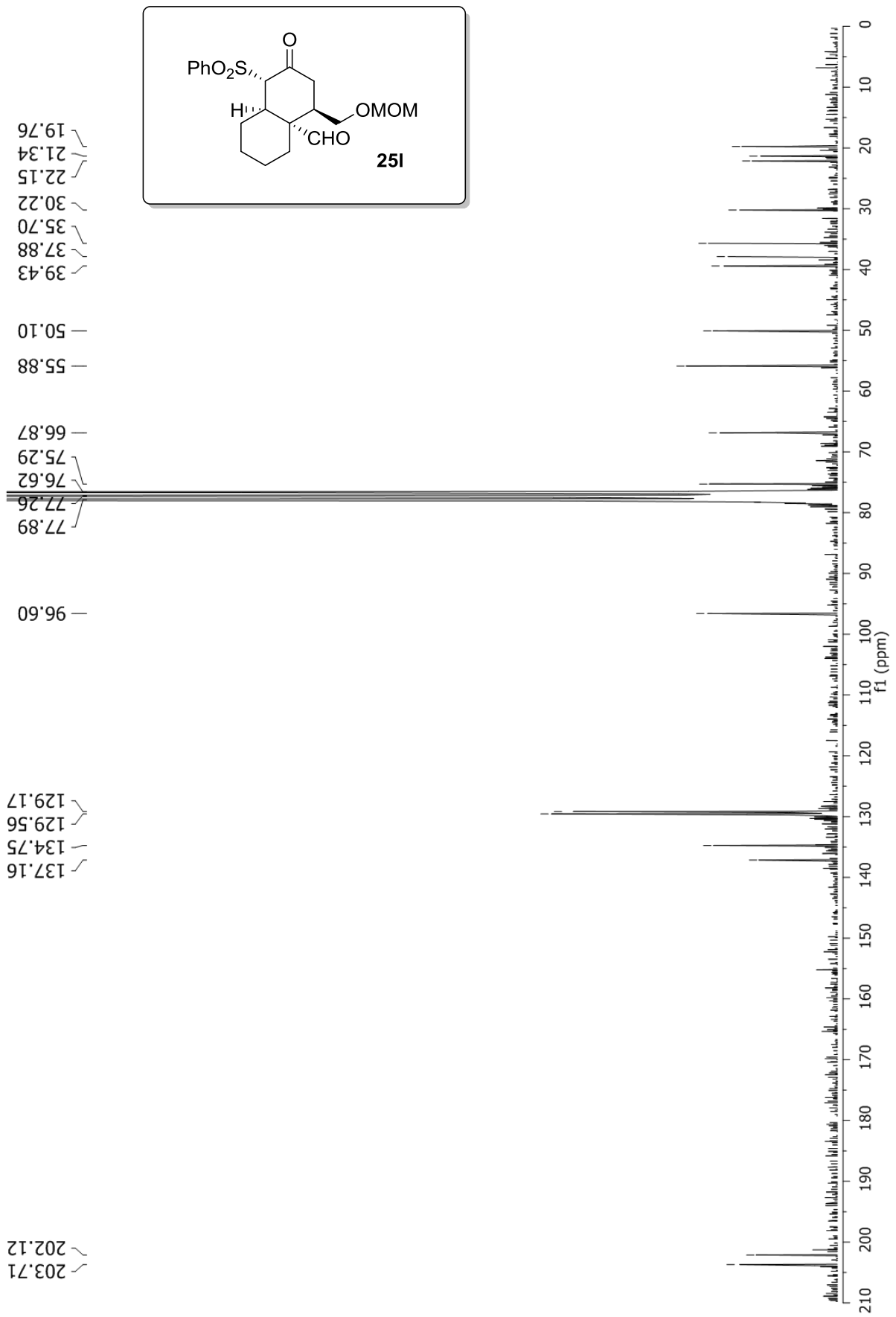
PeakTable

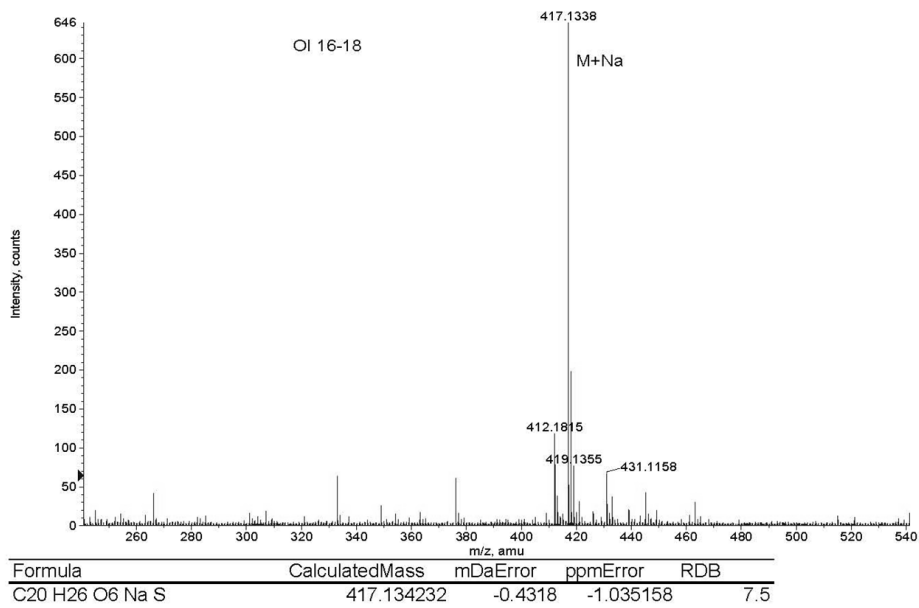
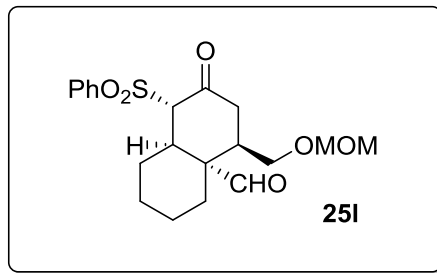
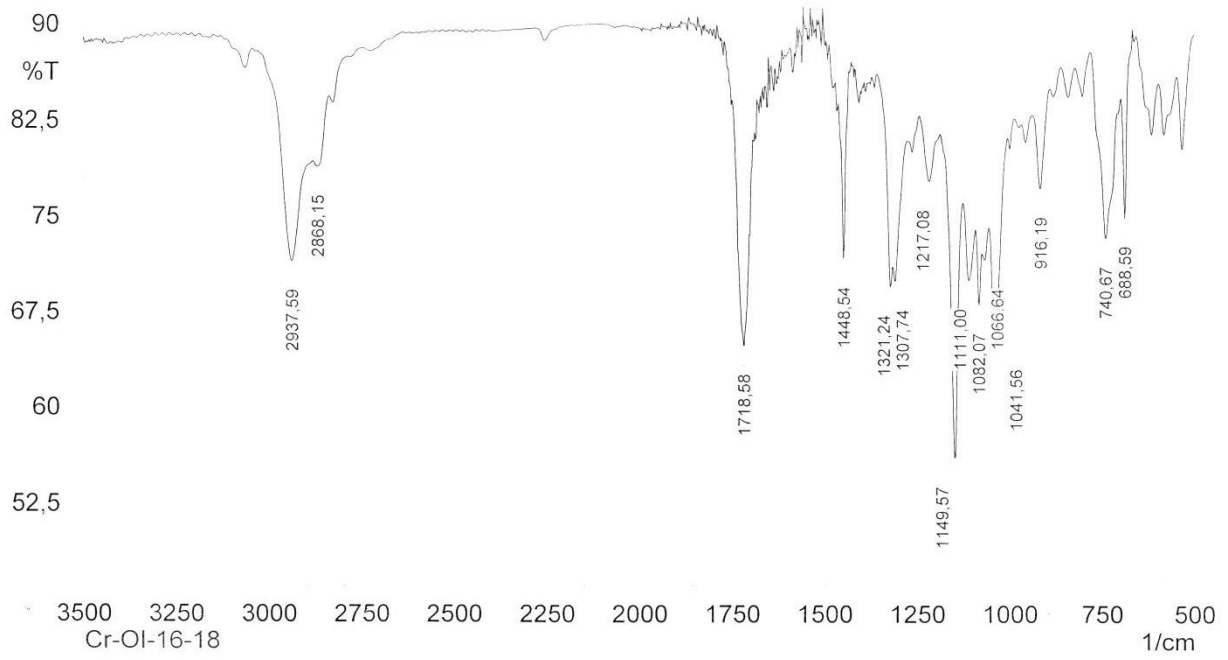
PDA Ch5 290nm 4nm

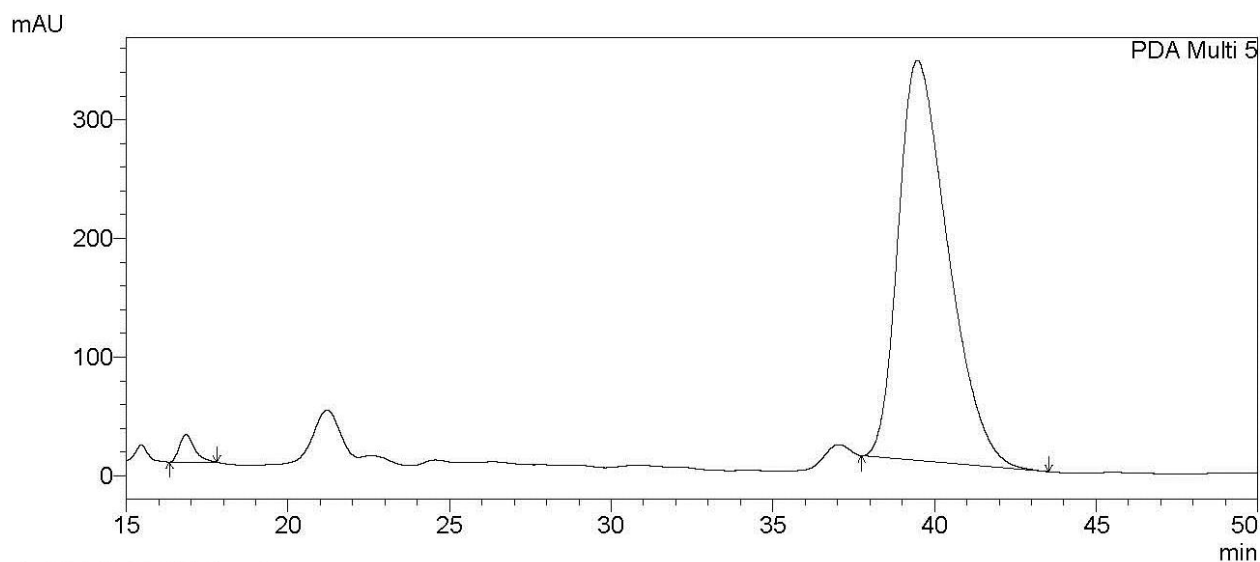
Peak#	Ret. Time	Area %
1	26.868	8.619
2	29.039	7.220
3	33.330	9.398
4	35.781	10.560
5	45.924	28.911
6	49.734	35.290
Total		100.000









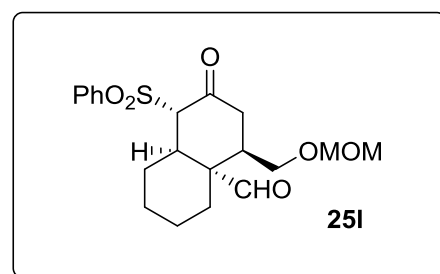


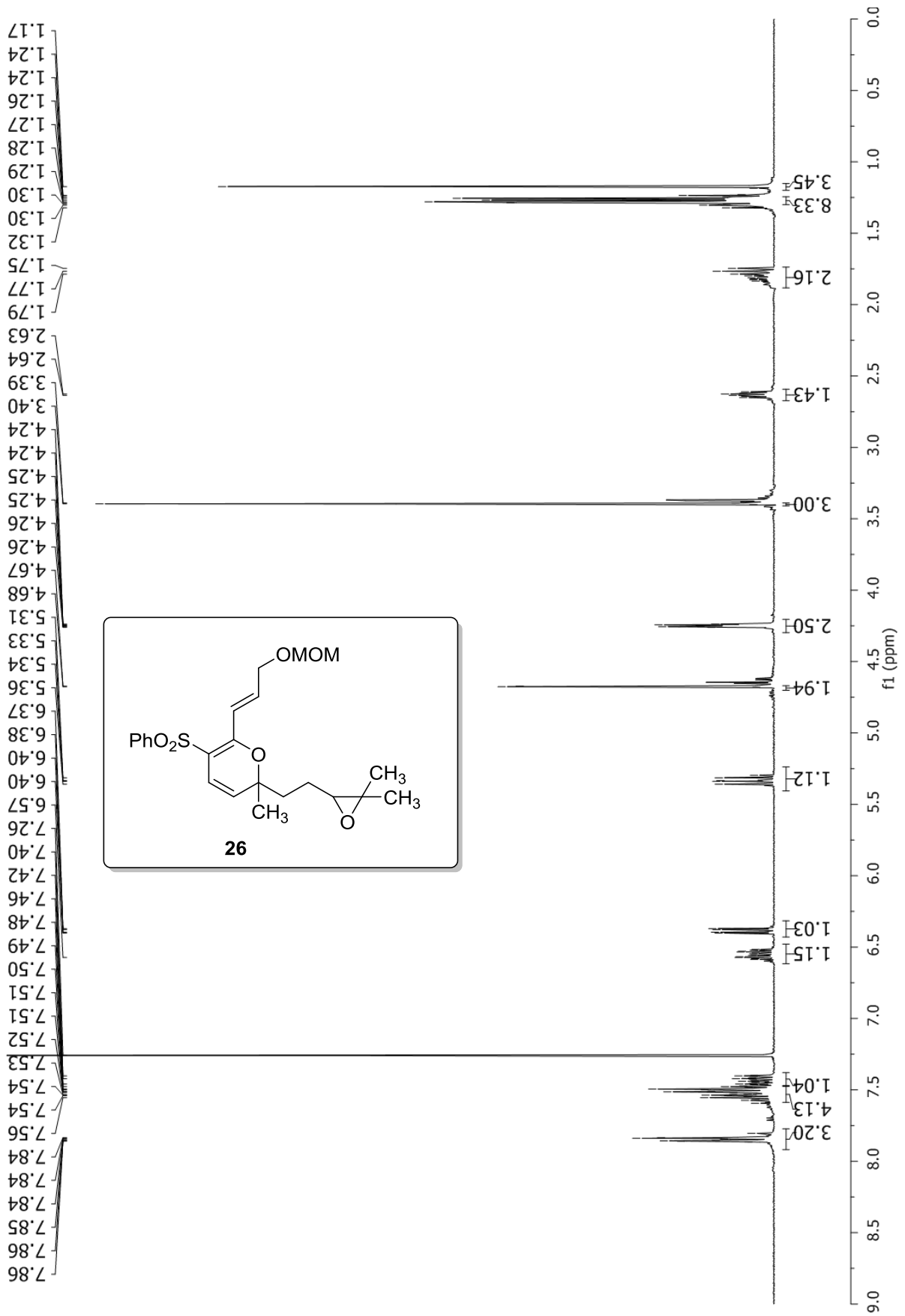
1 PDA Multi 5/210nm 4nm

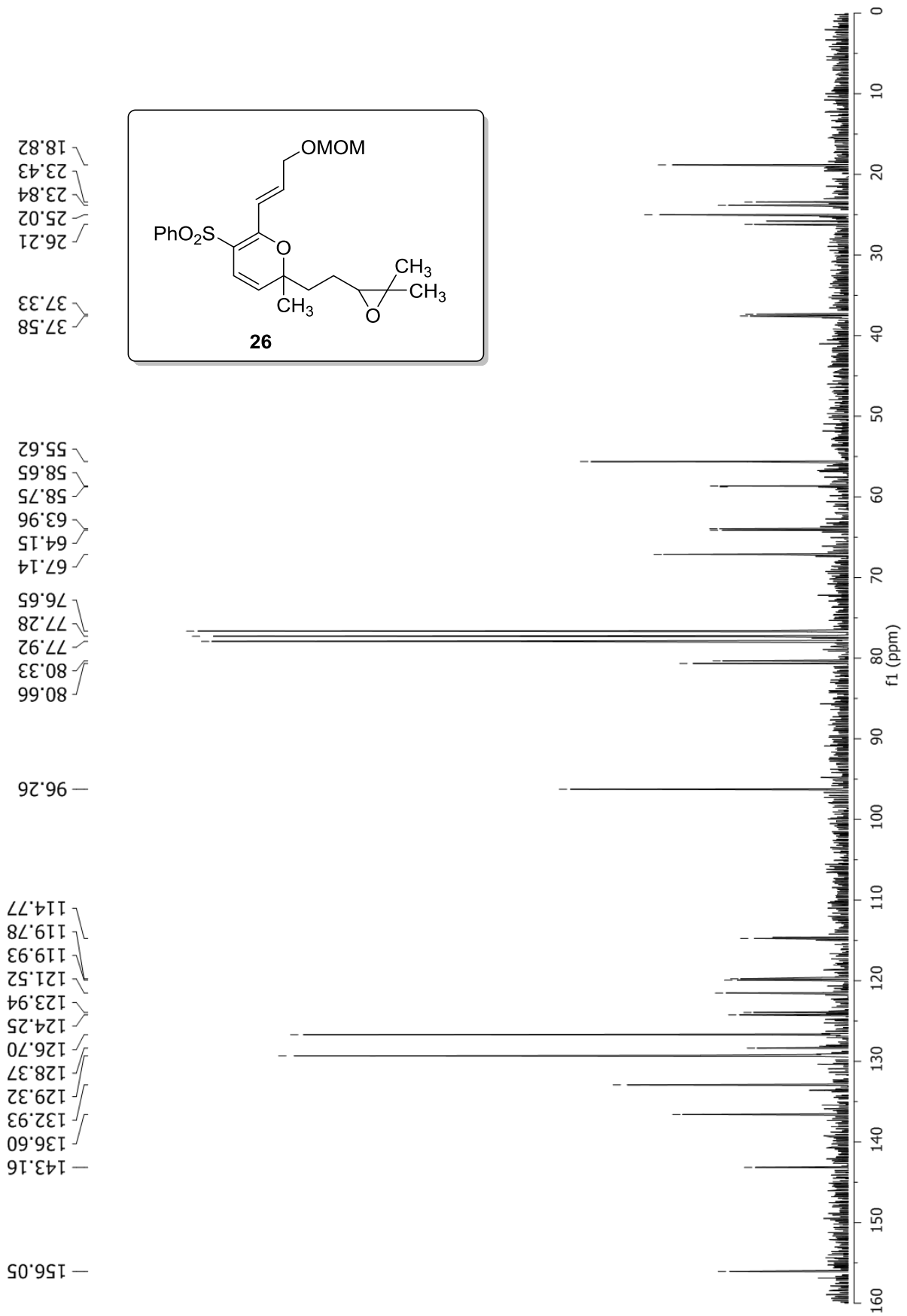
PeakTable

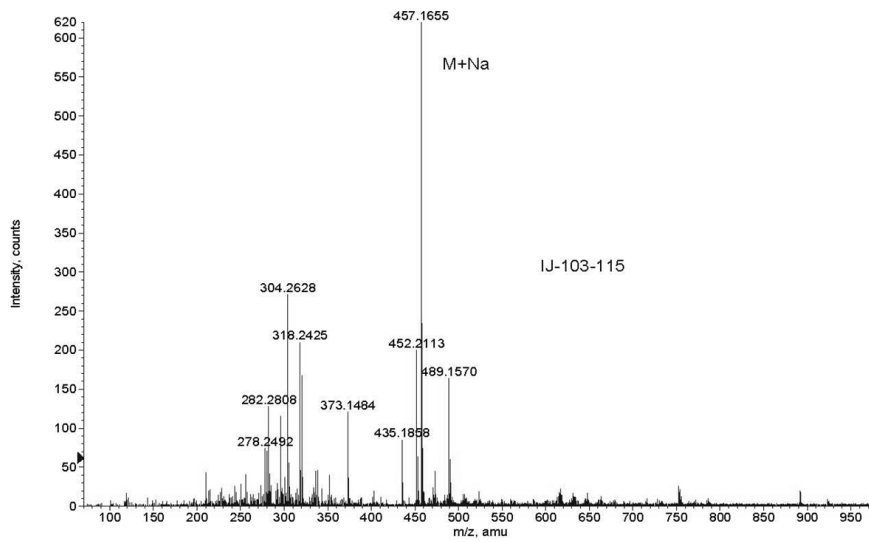
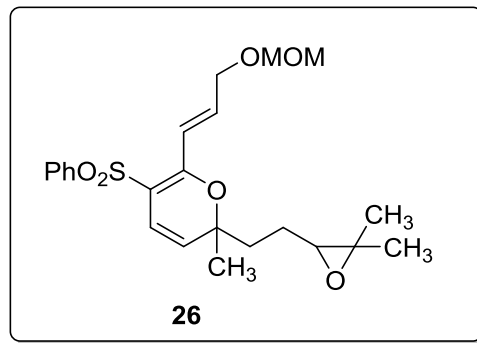
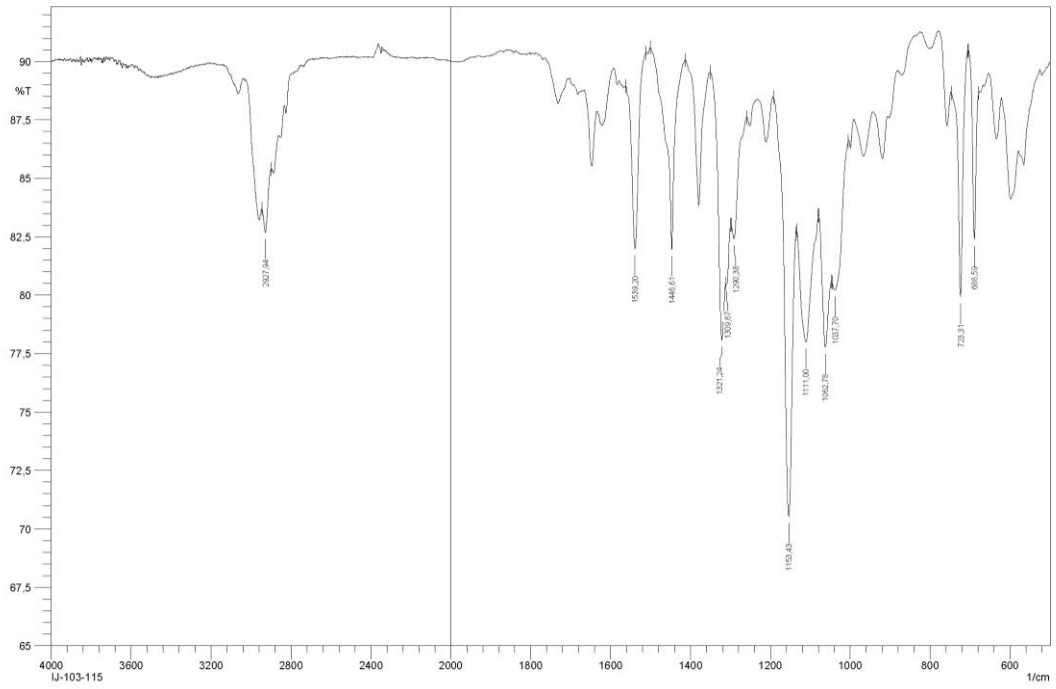
PDA Ch5 210nm 4nm

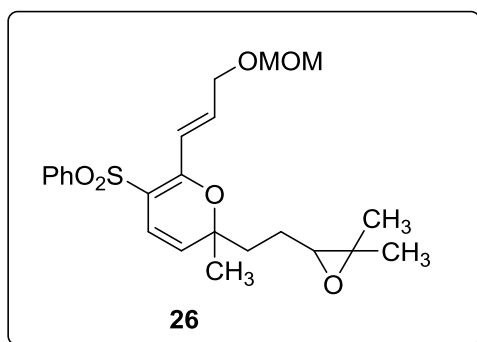
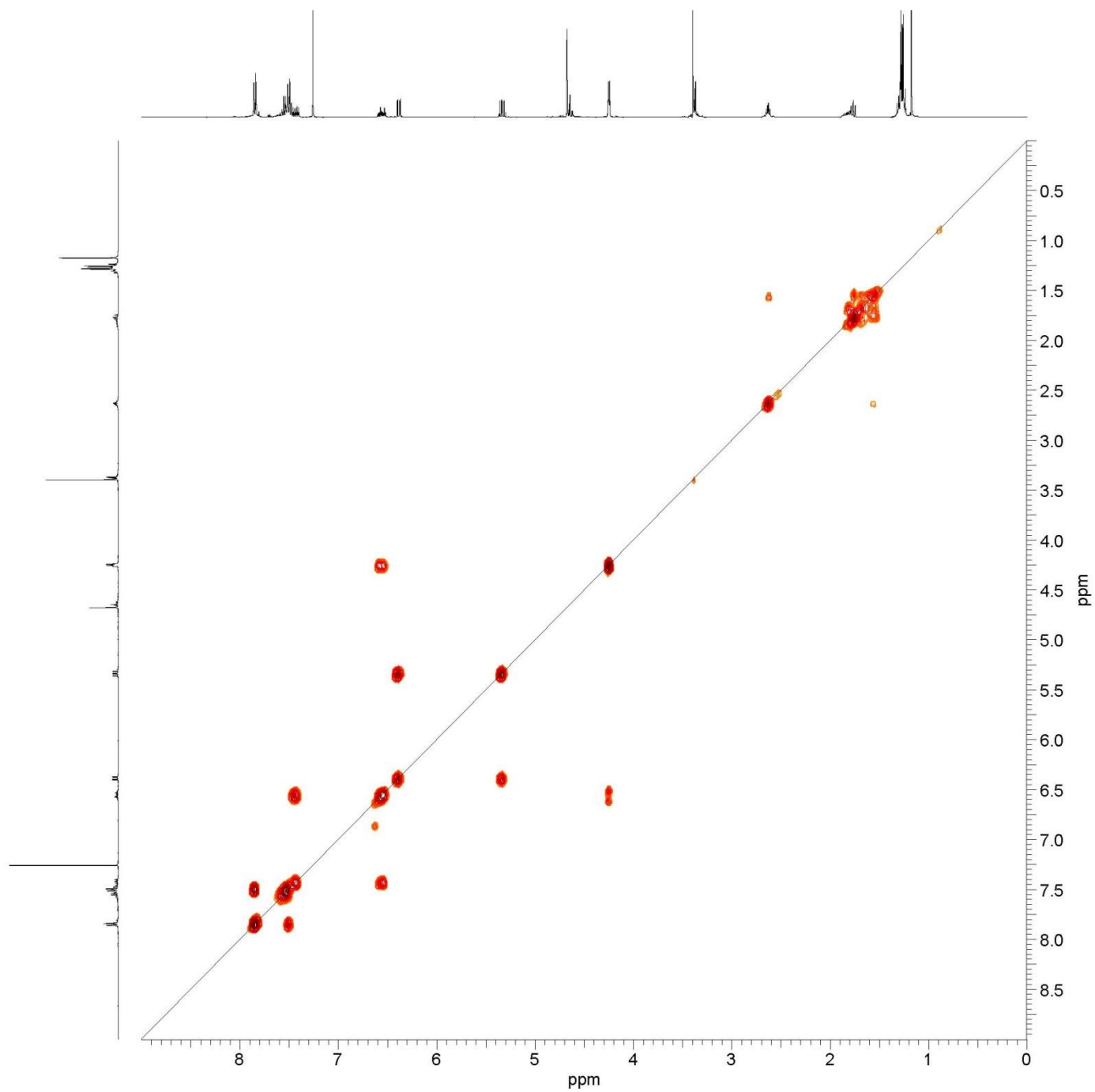
Peak#	Ret. Time	Area %
1	16.837	2.056
2	39.465	97.944
Total		100.000

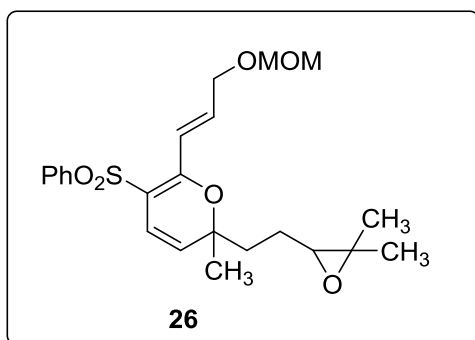
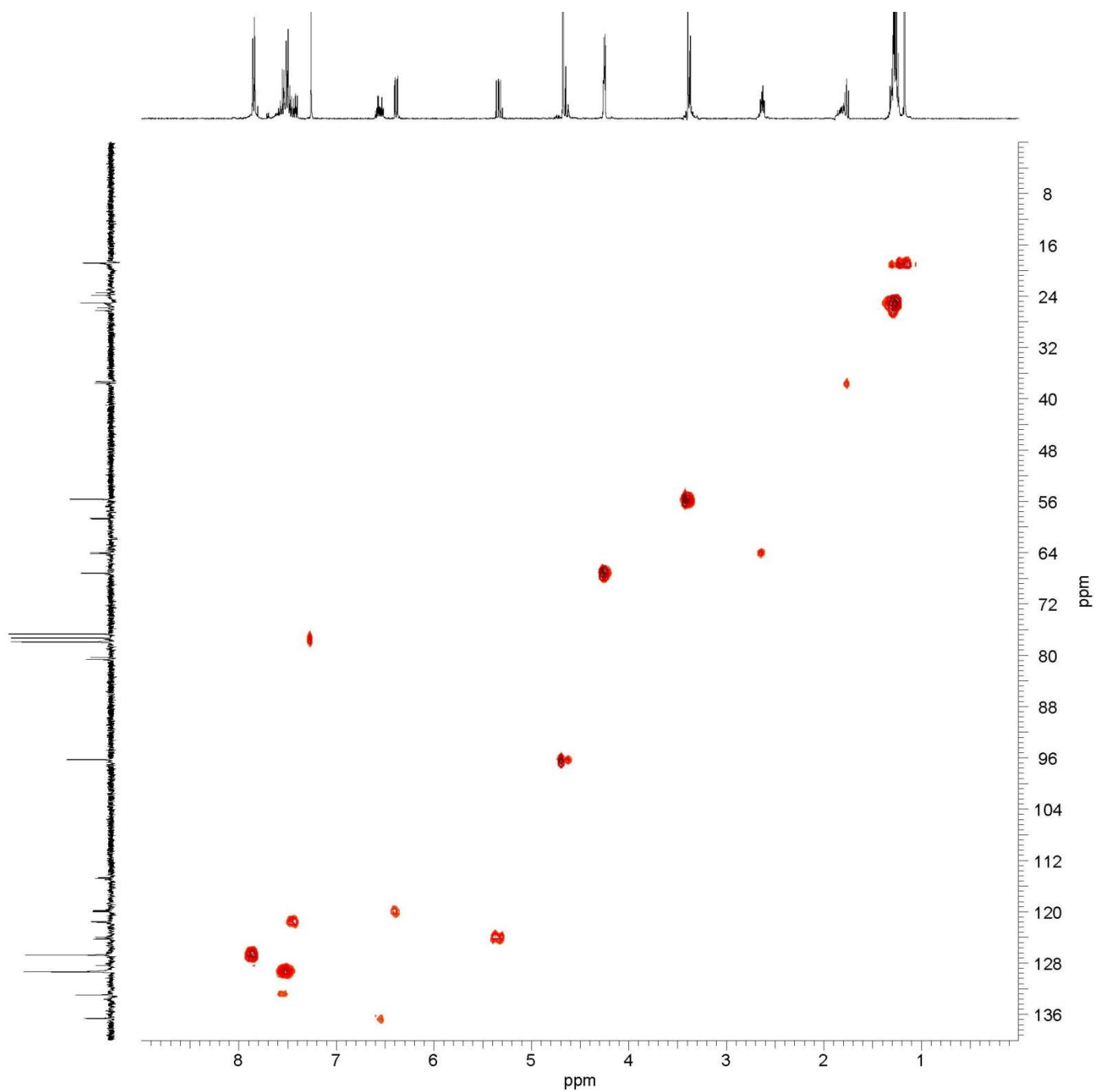


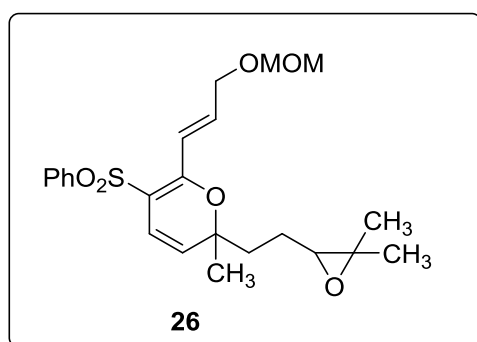
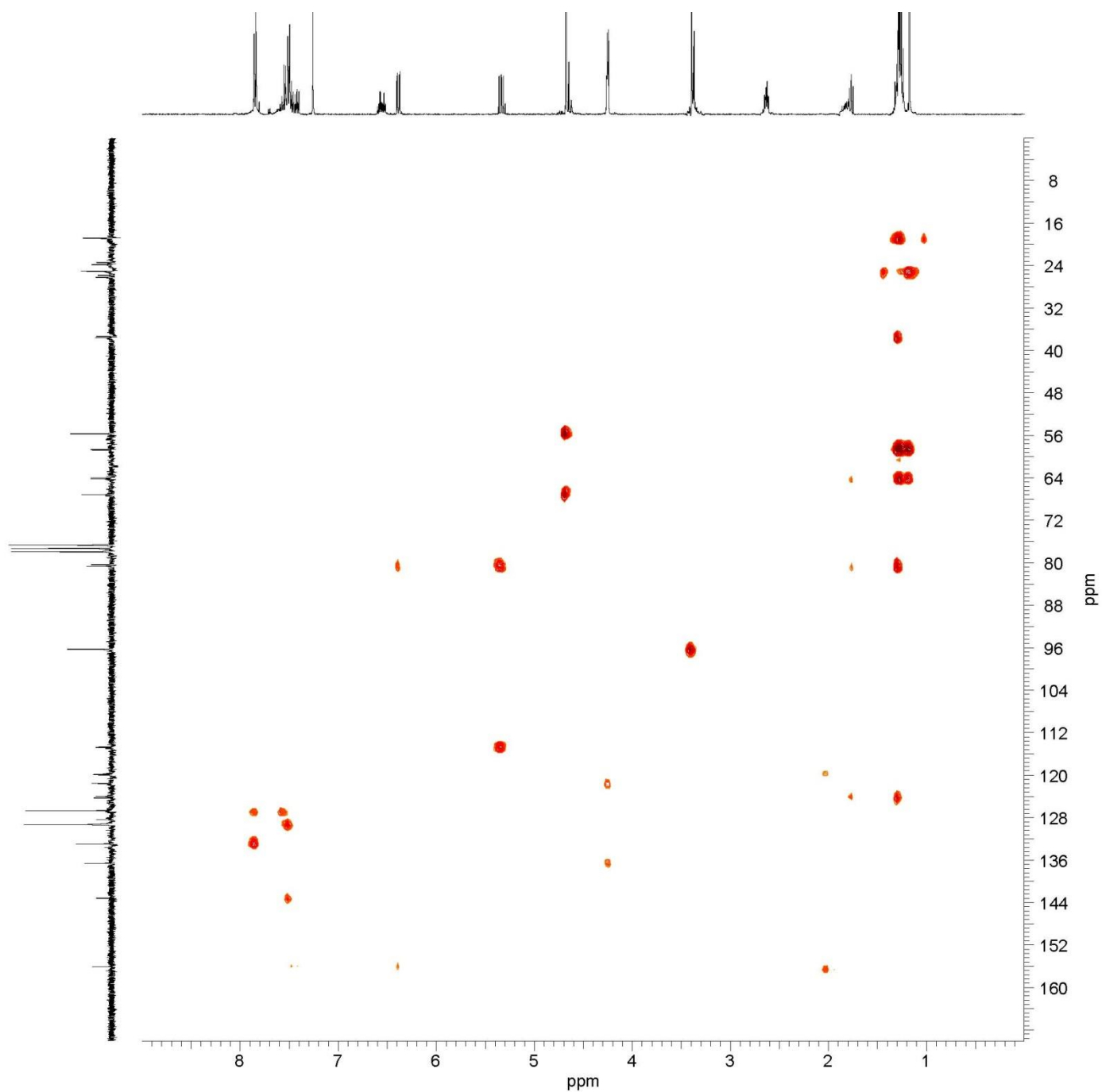


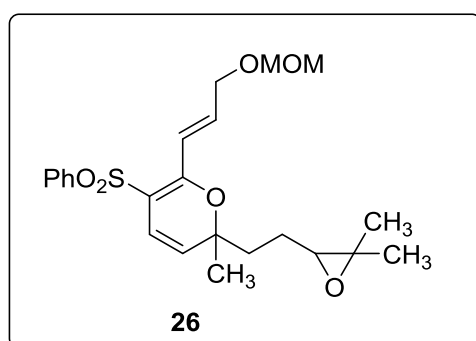
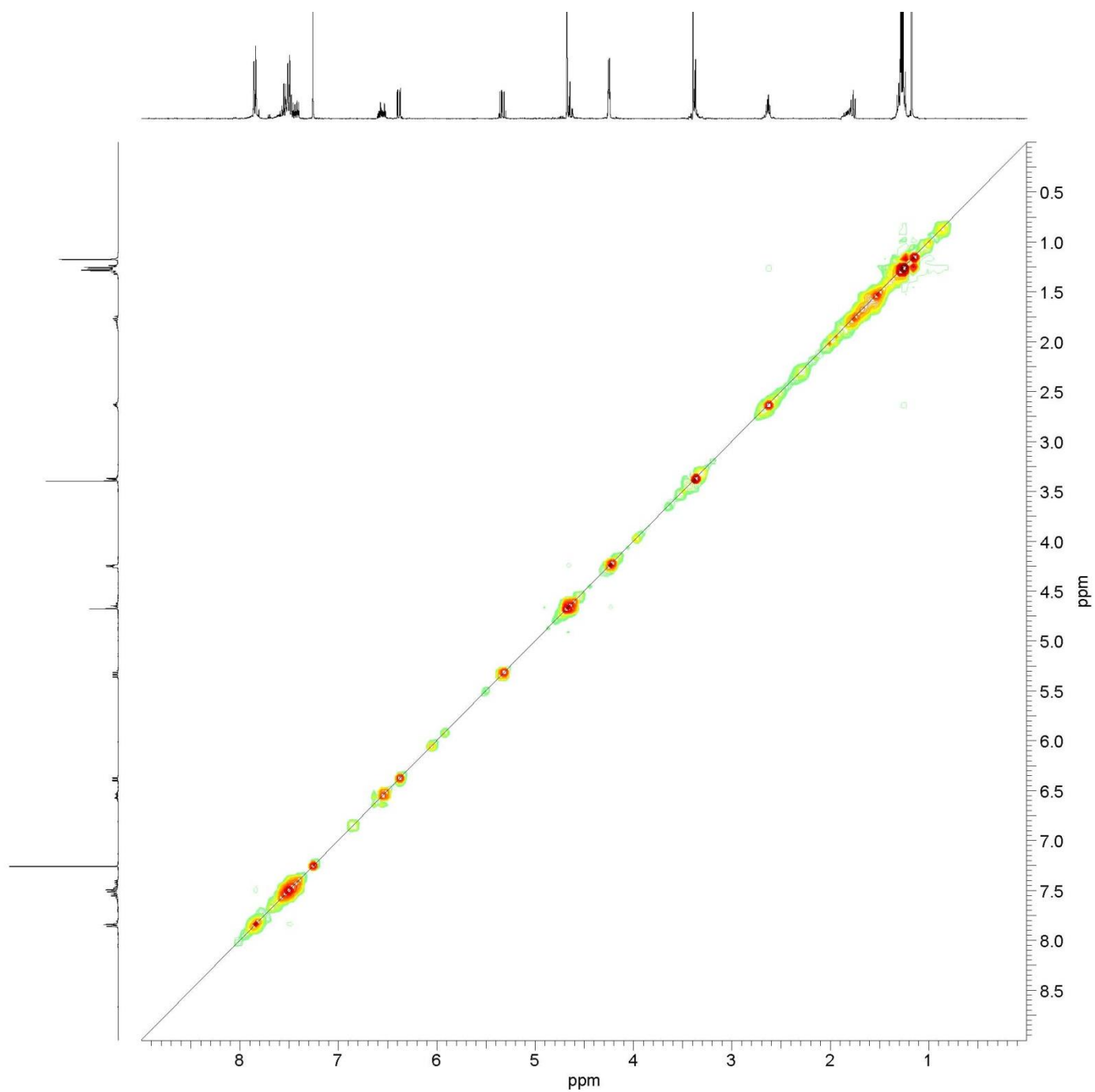


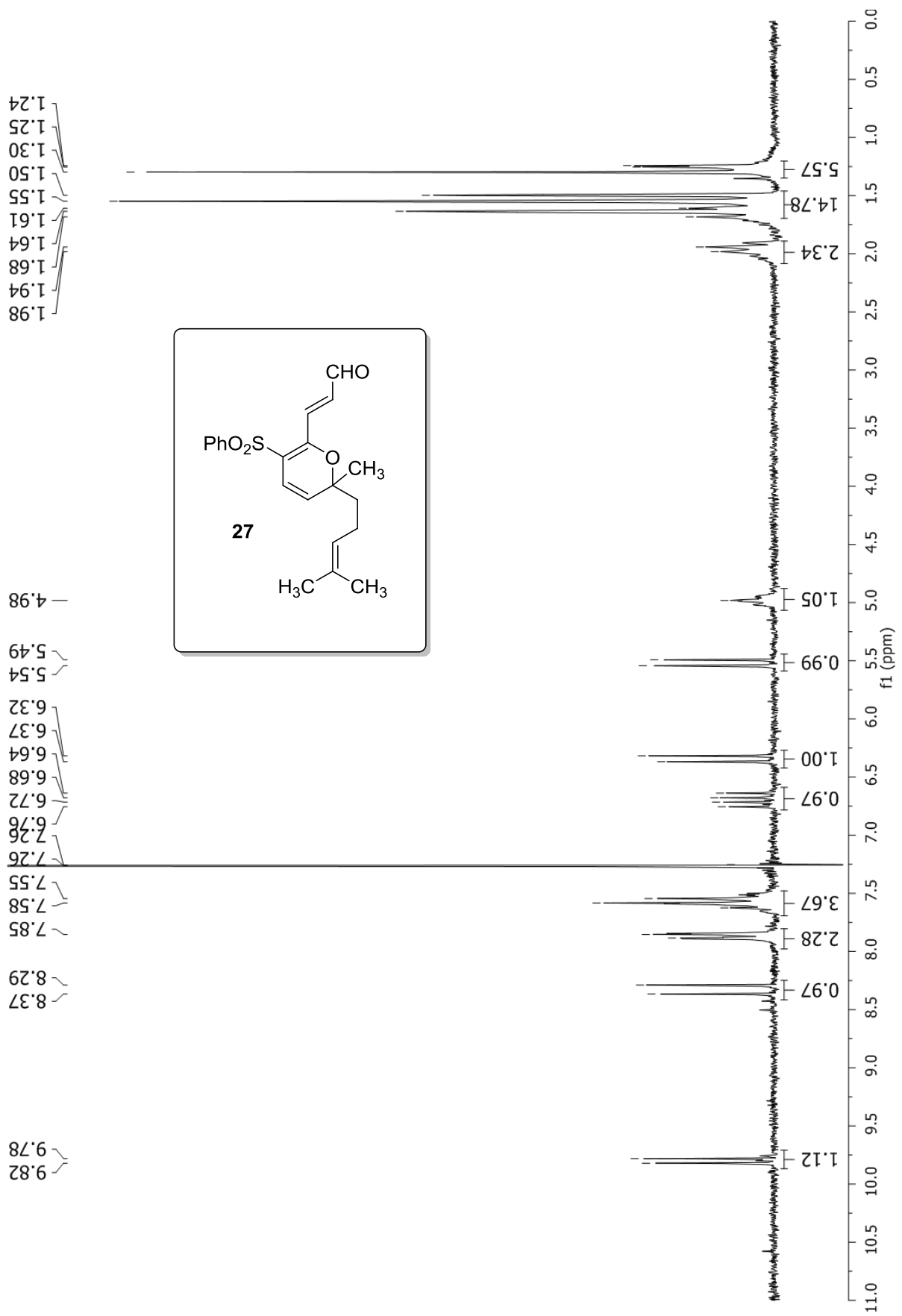


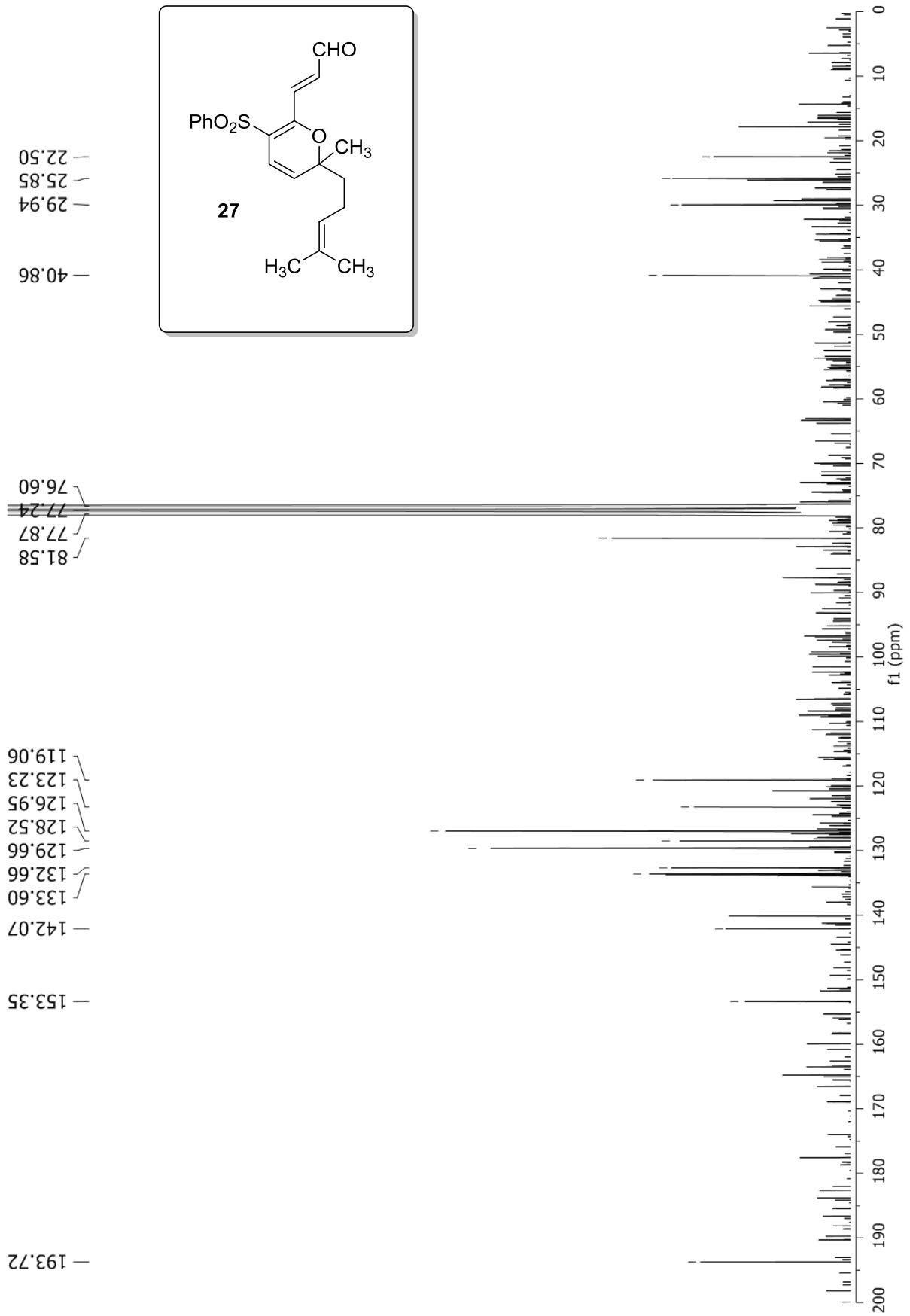




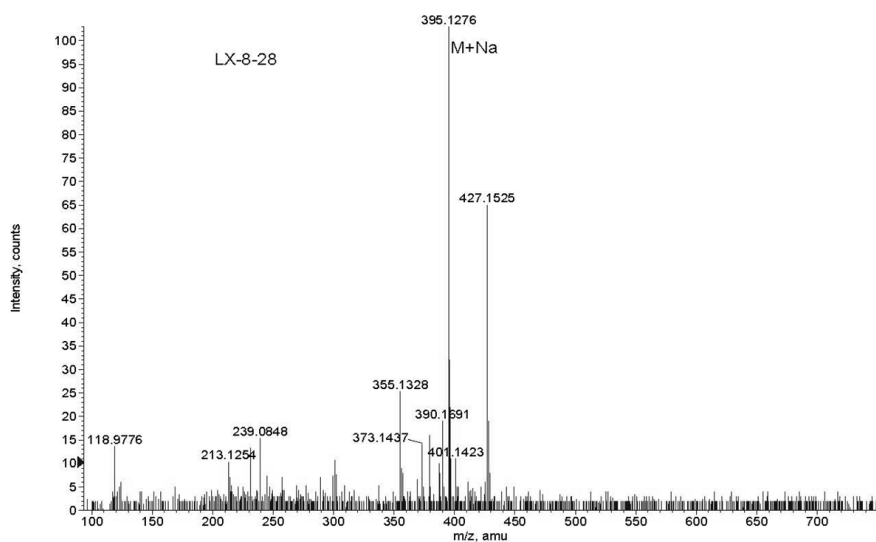
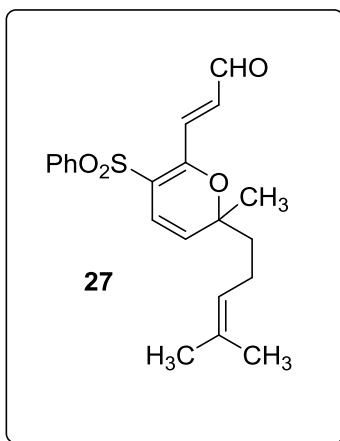
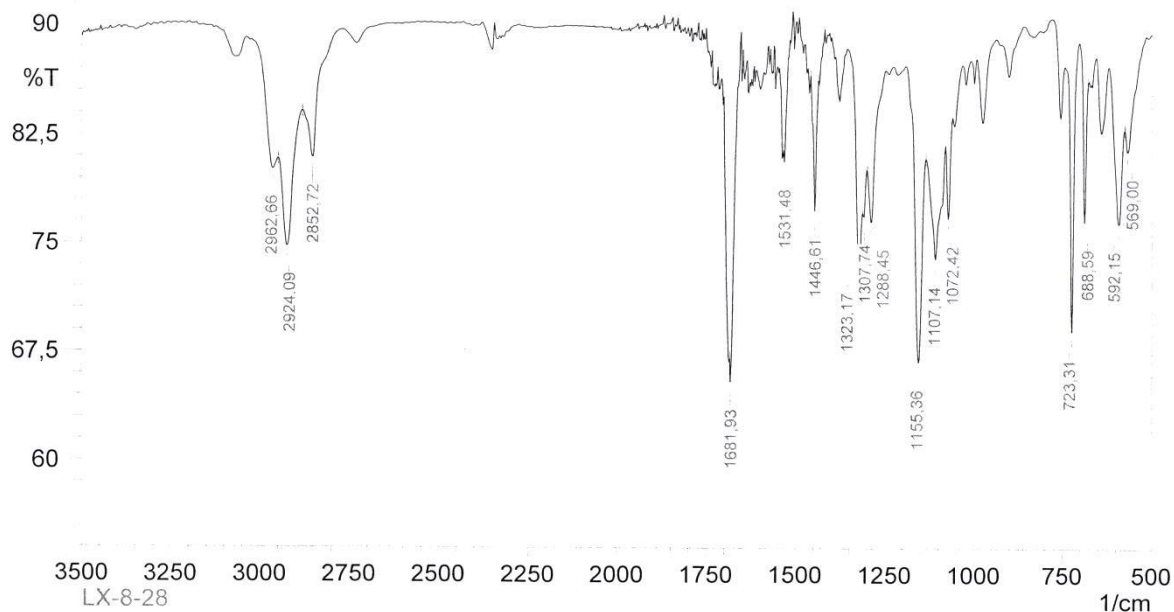




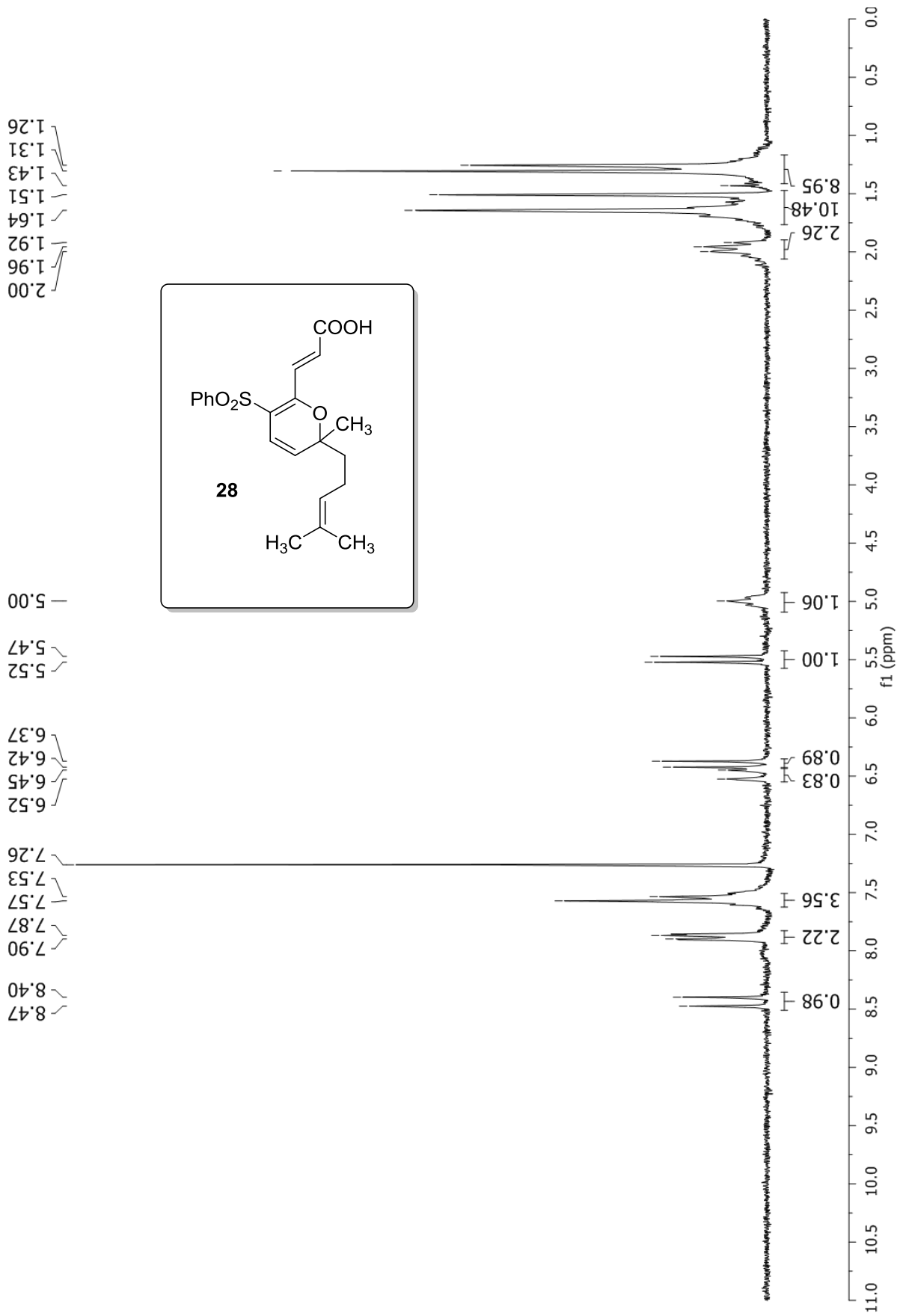


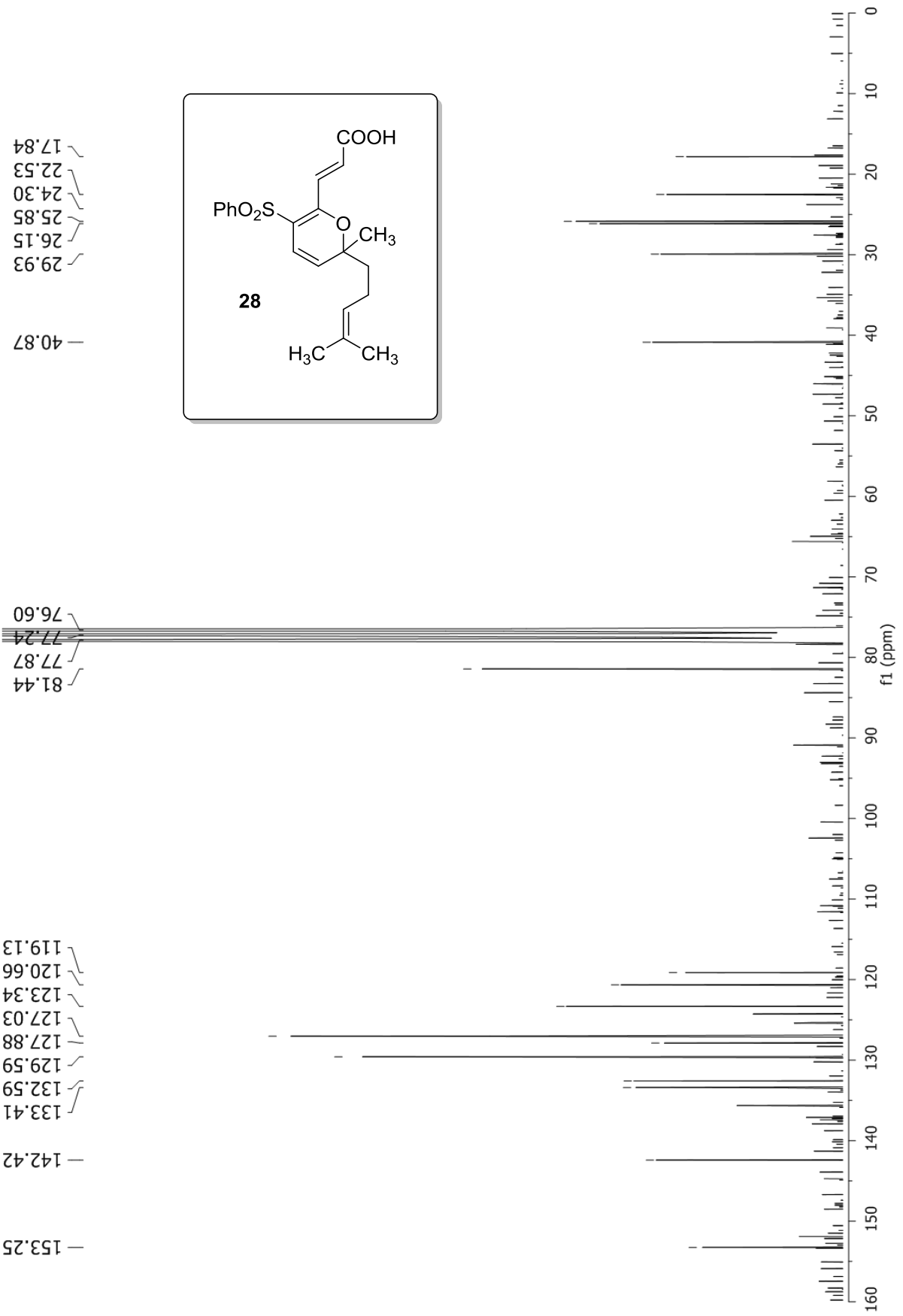


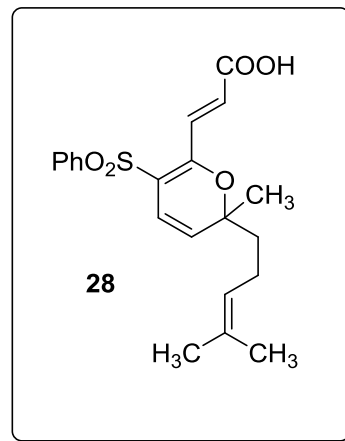
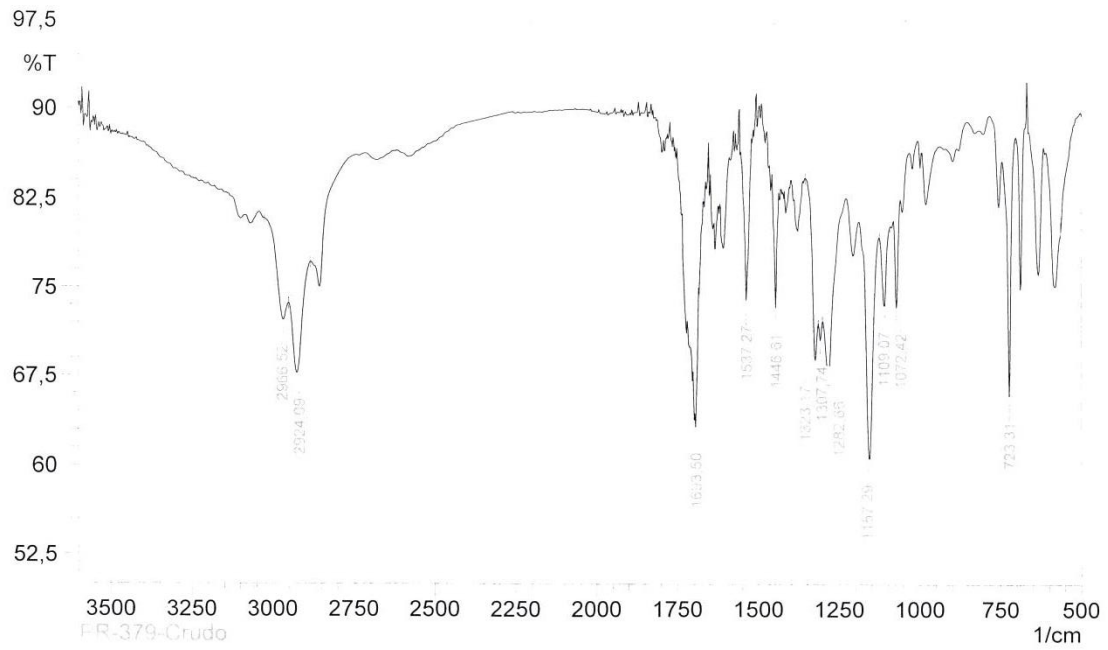
Full Spectroscopy

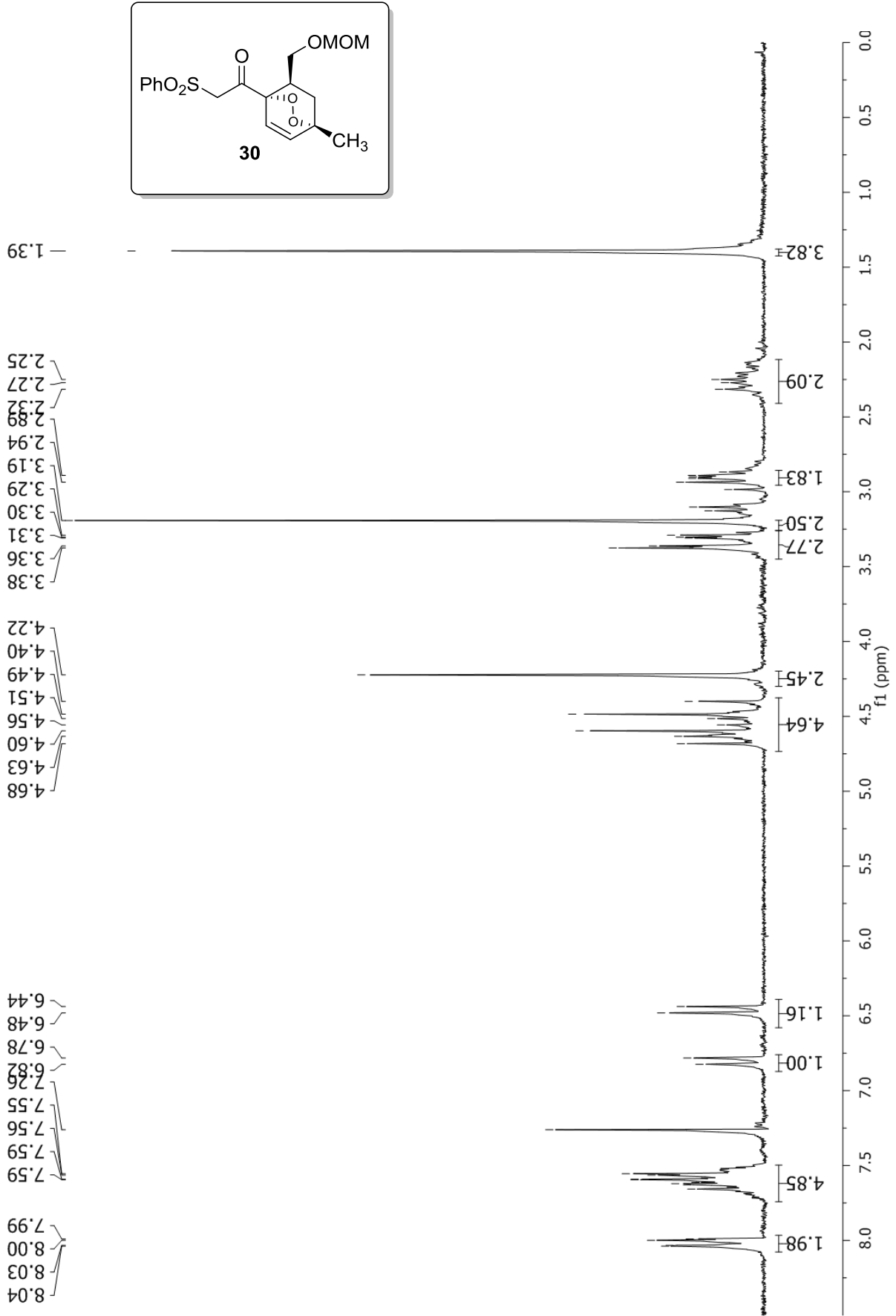


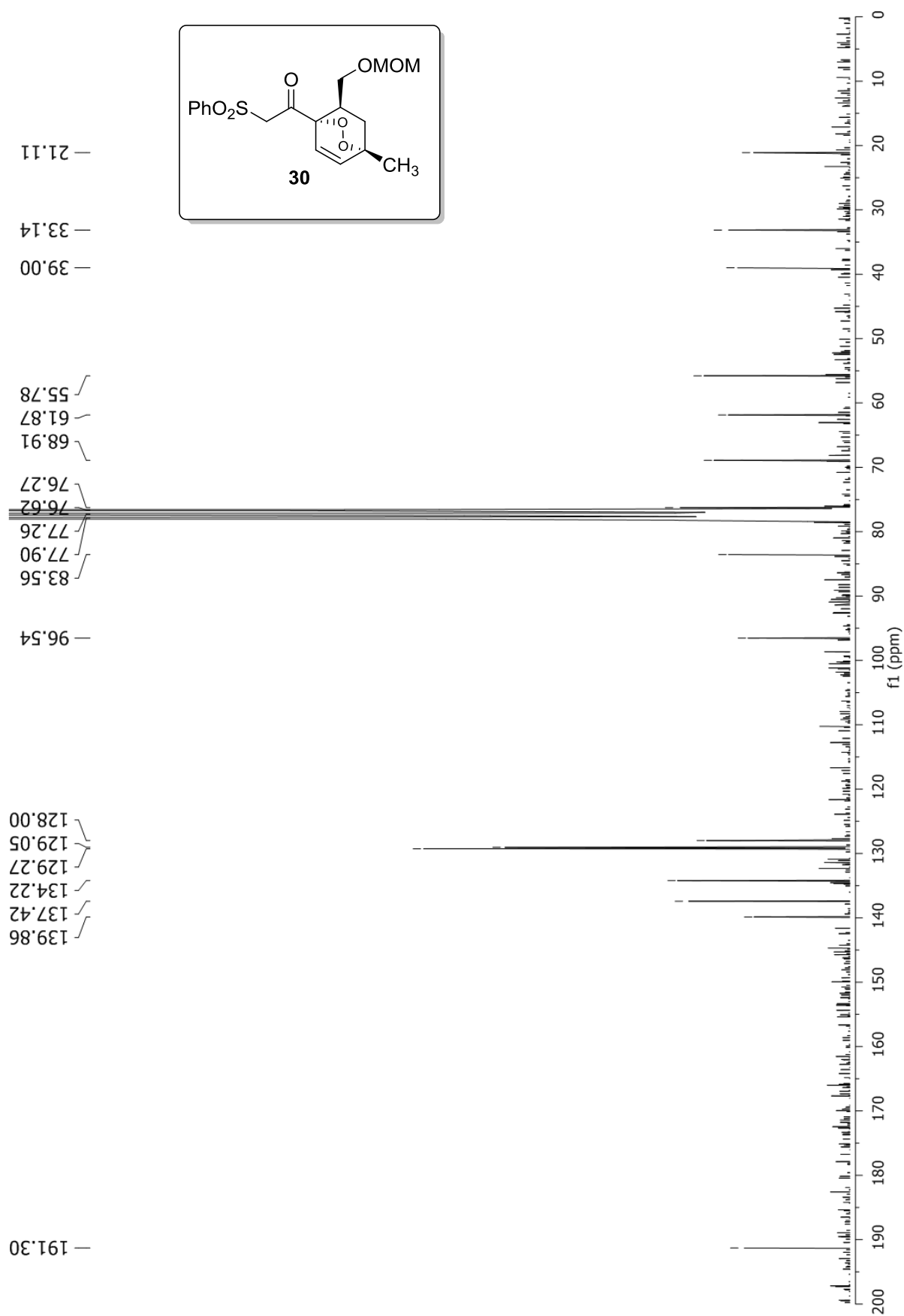
Formula	CalculatedMass	mDaError	ppmError	RDB
C26 H19 O4	395.127786	-0.18574	-0.470075	17.5
C21 H24 O4 Na S	395.128752	-1.15244	-2.916623	9.5
C24 H20 O4 Na	395.12538	2.21952	5.617216	14.5
C23 H23 O4 S	395.131158	-3.5577	-9.003914	12.5
C17 H24 O9 Na	395.131254	-3.65384	-9.247228	5.5



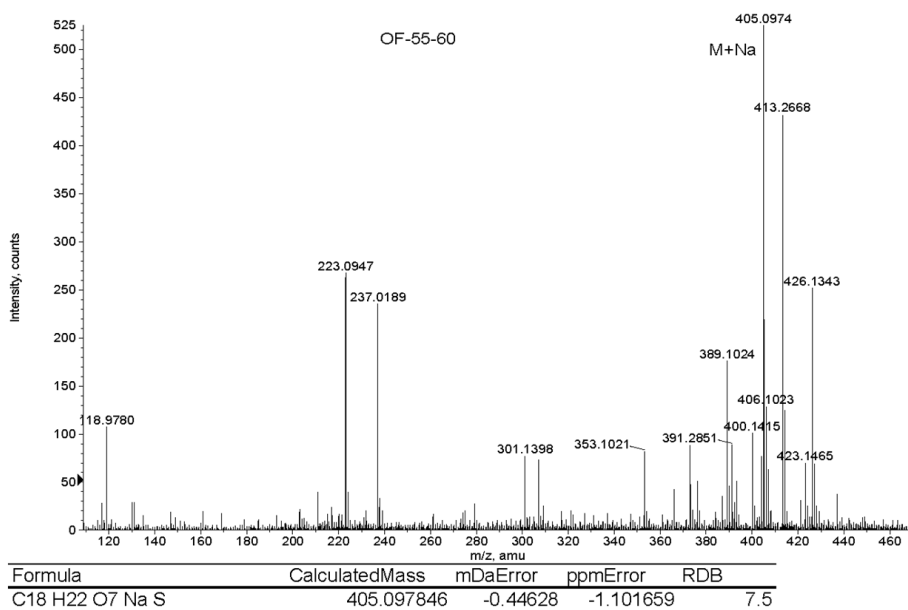
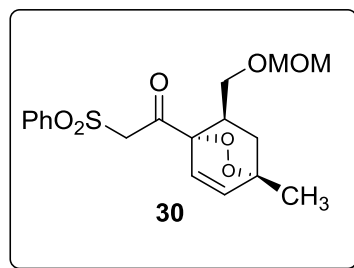
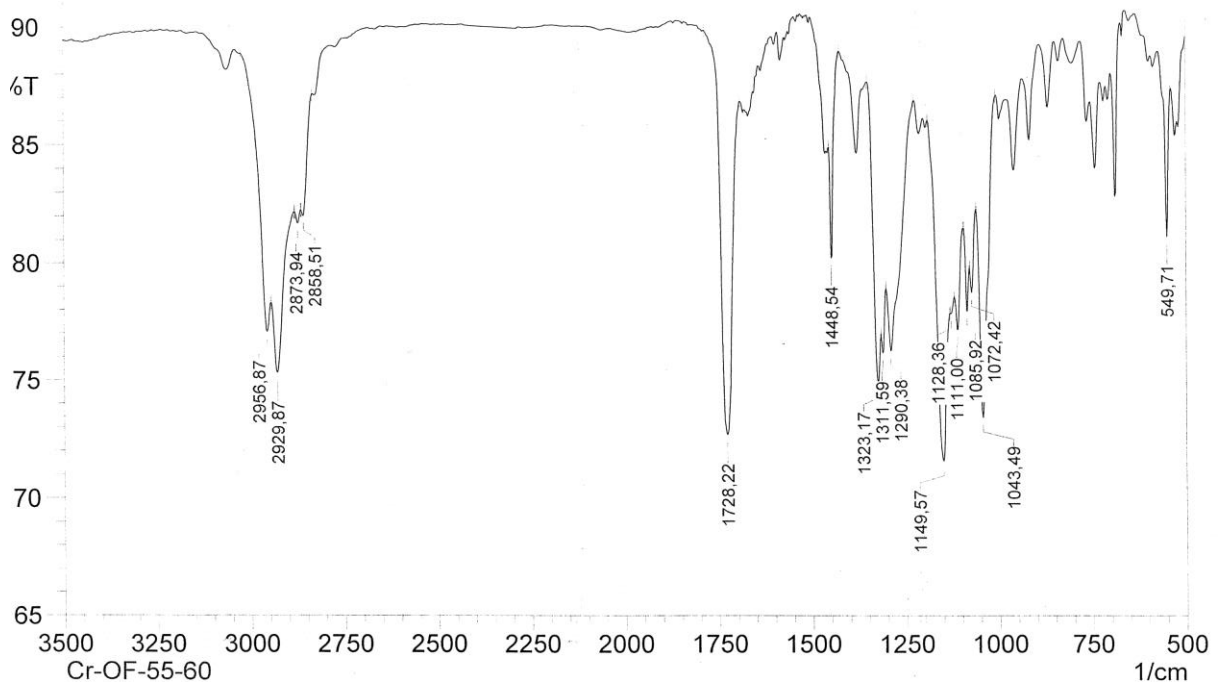


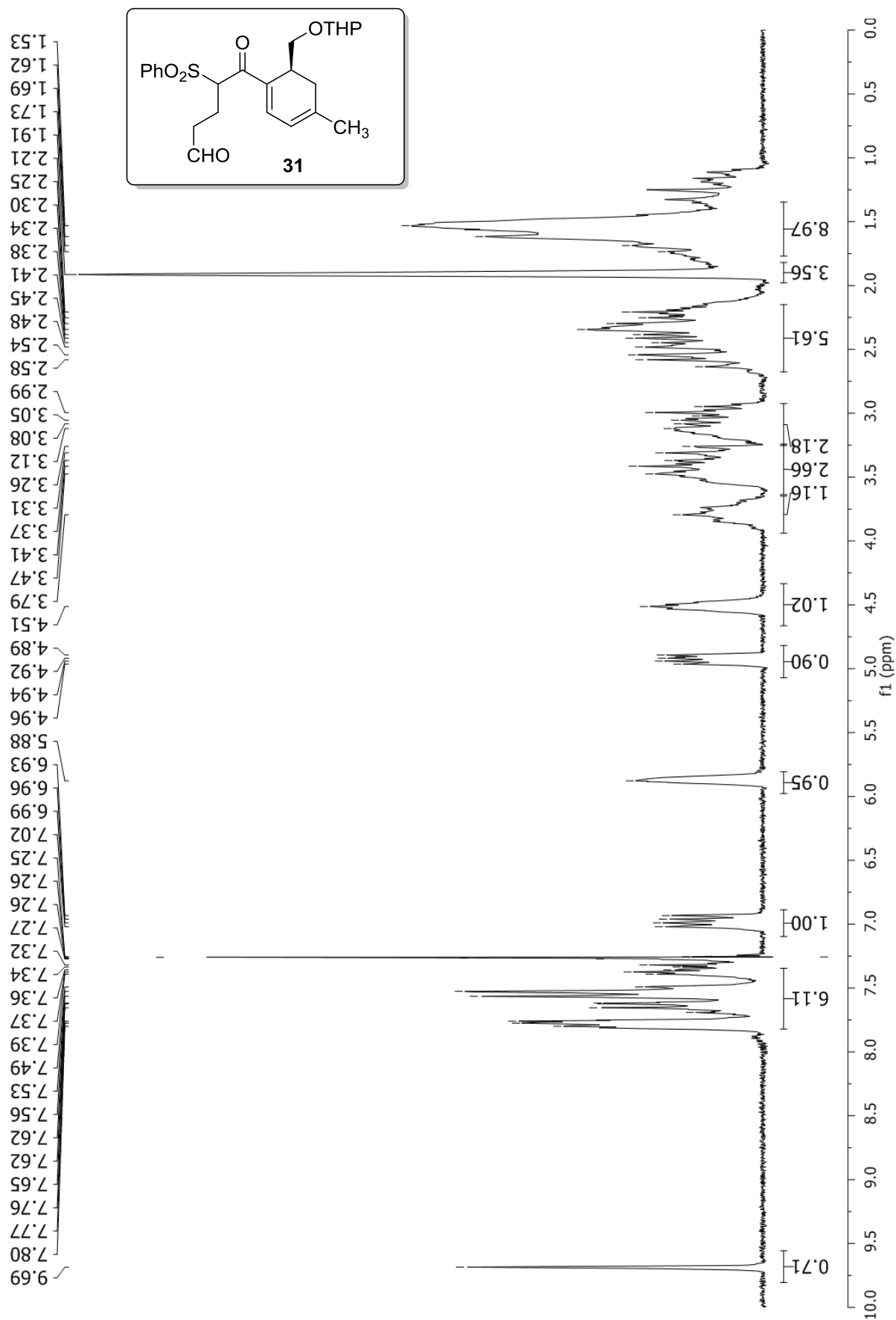


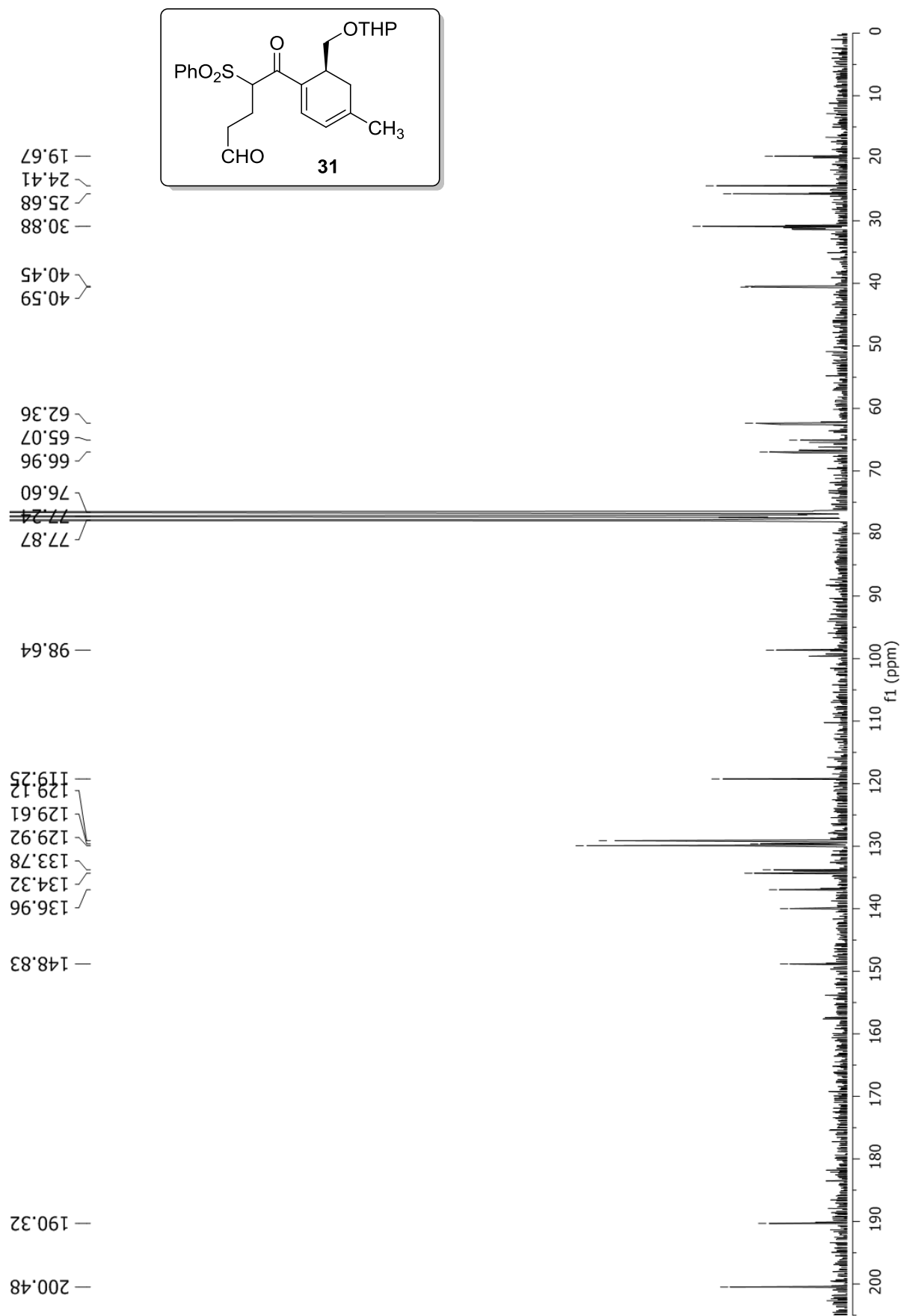


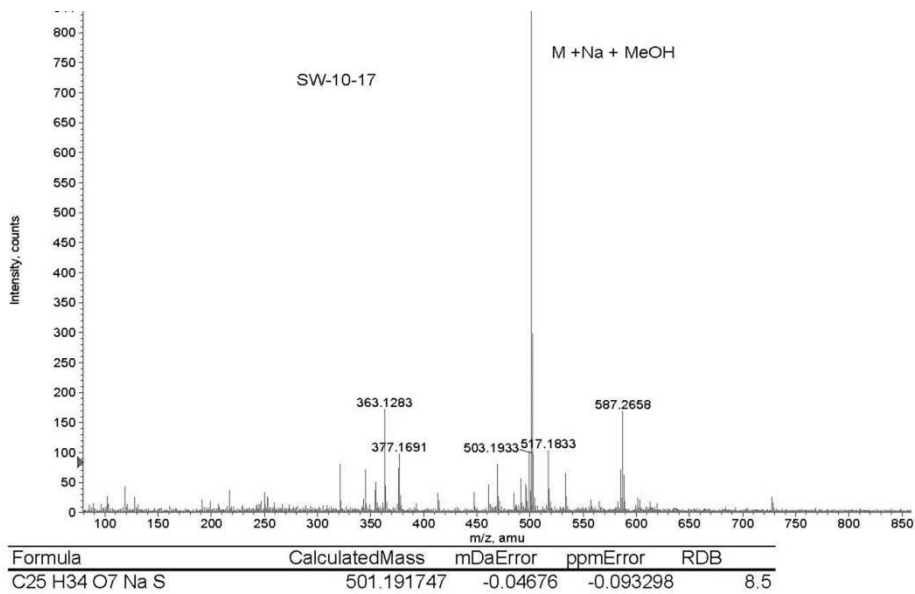
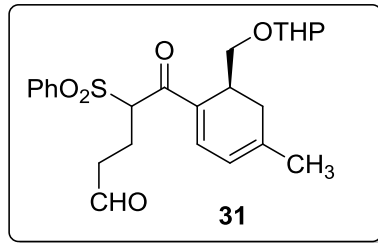
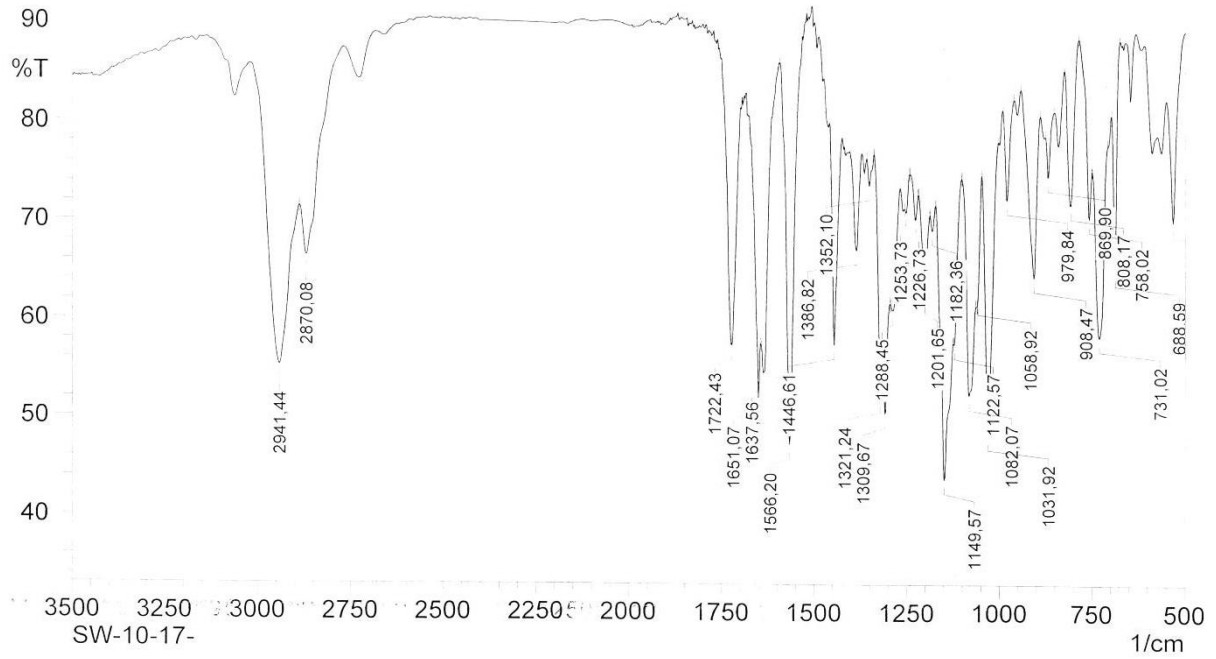


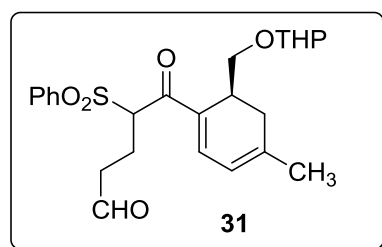
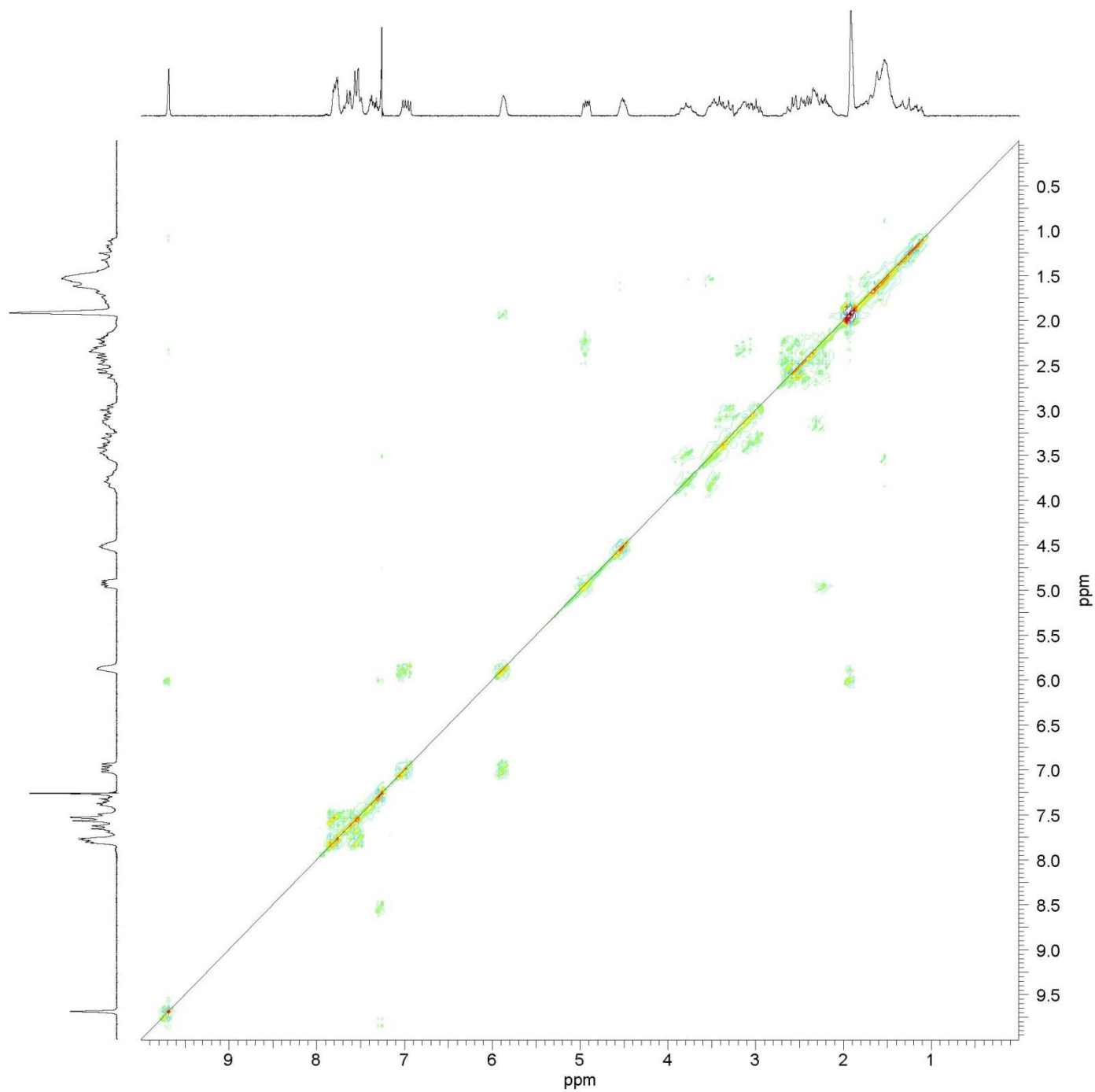
Full Spectroscopy

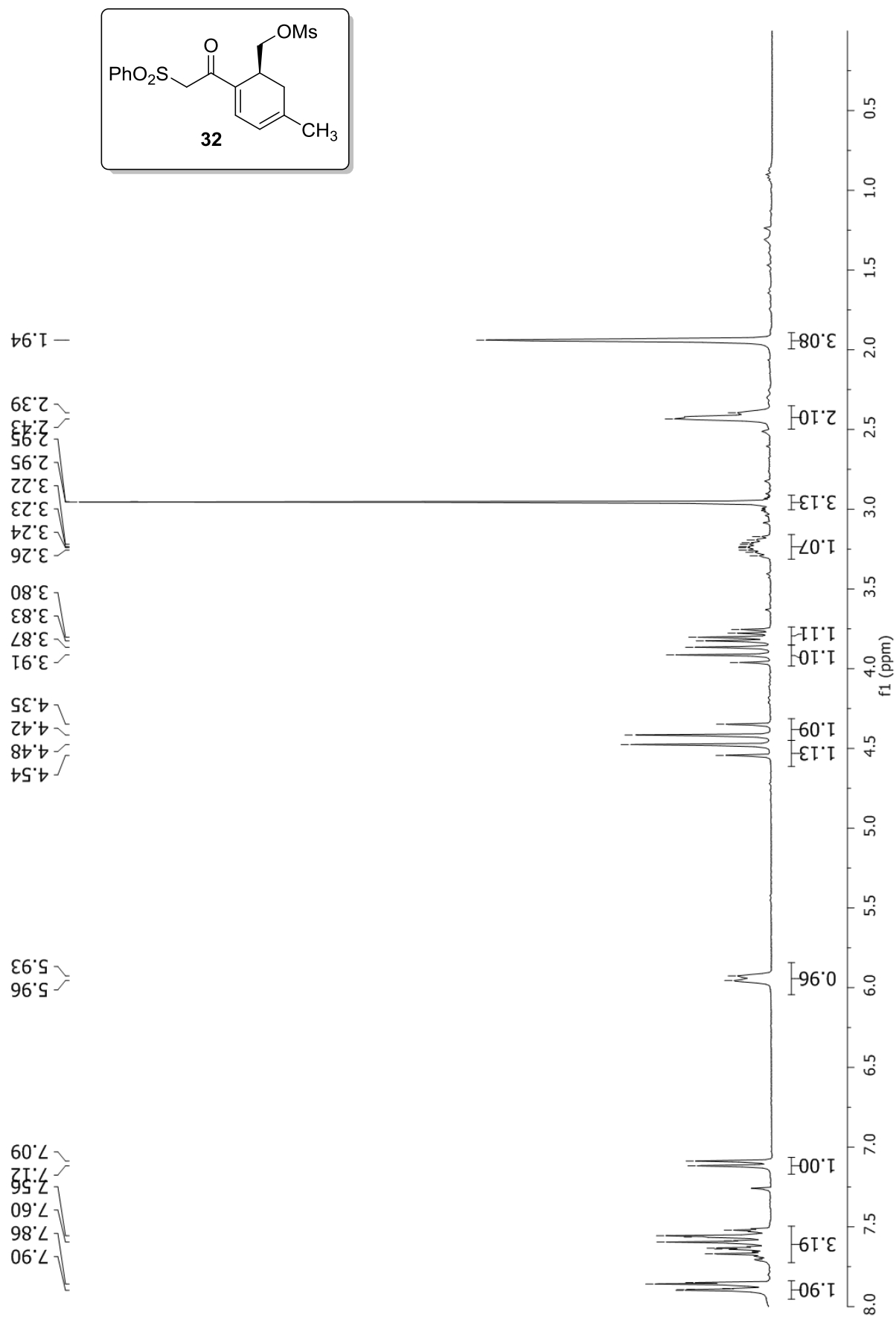


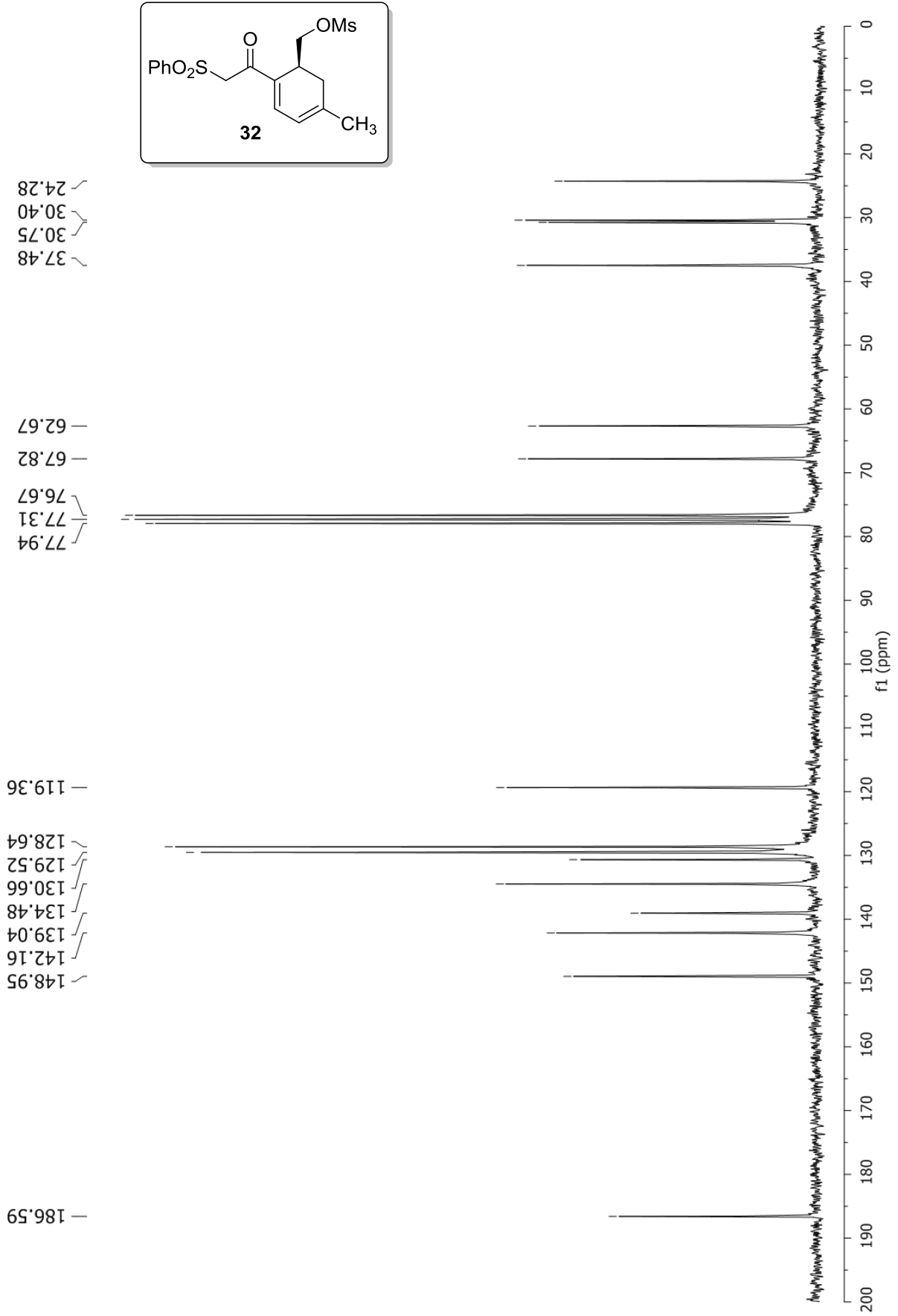


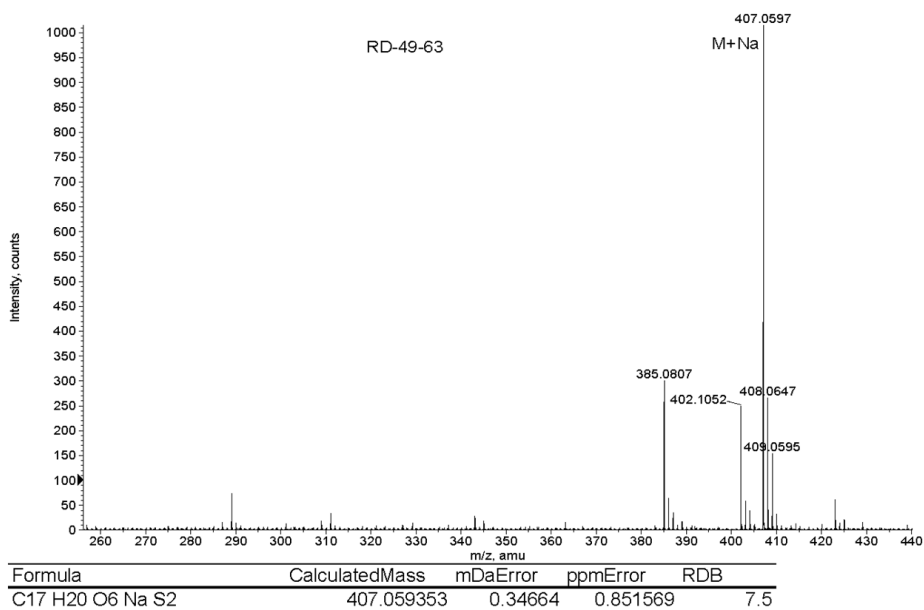
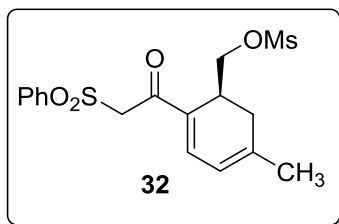
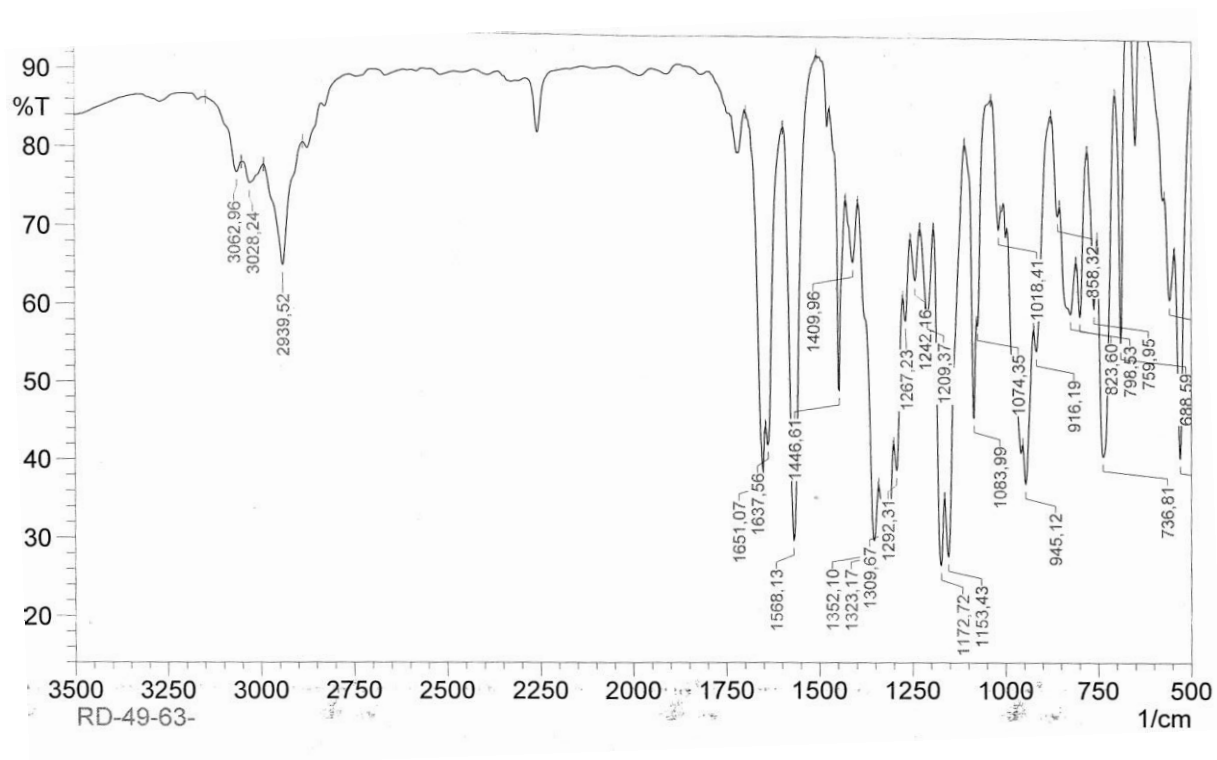


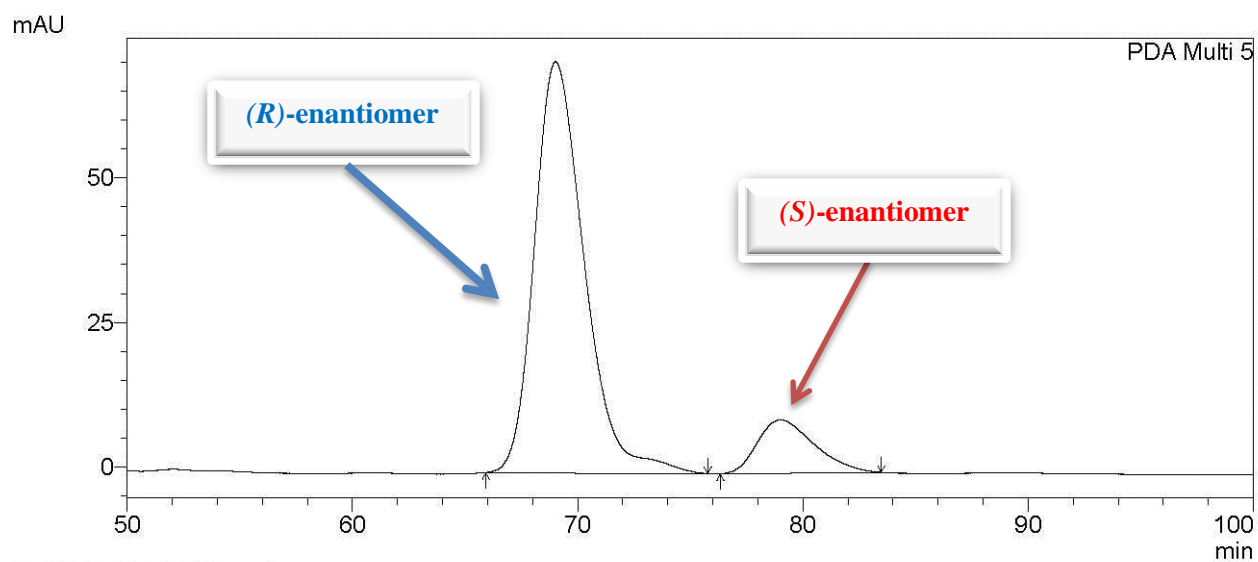








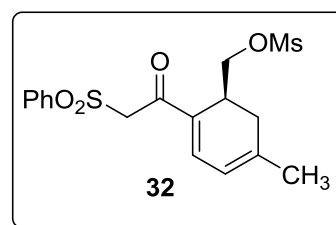


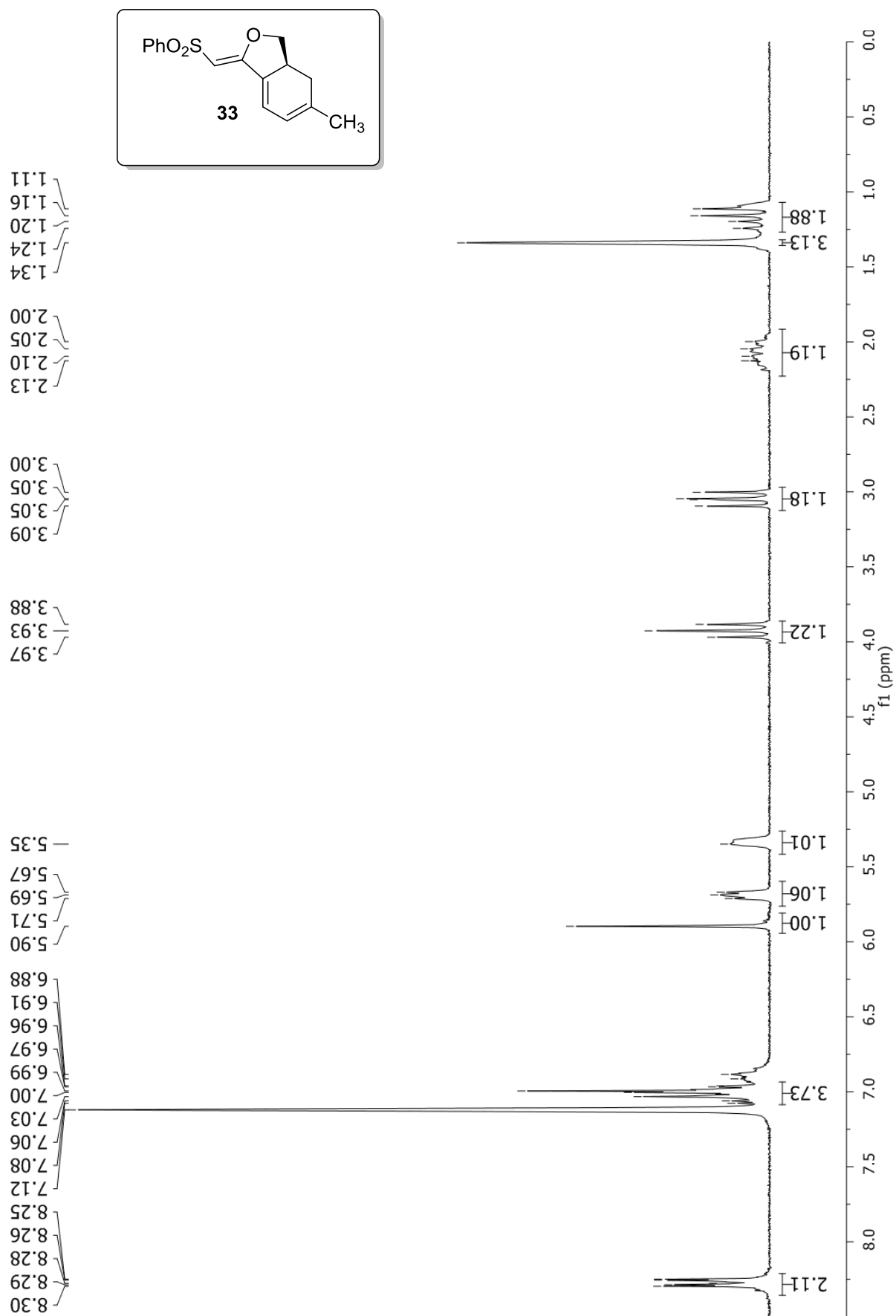


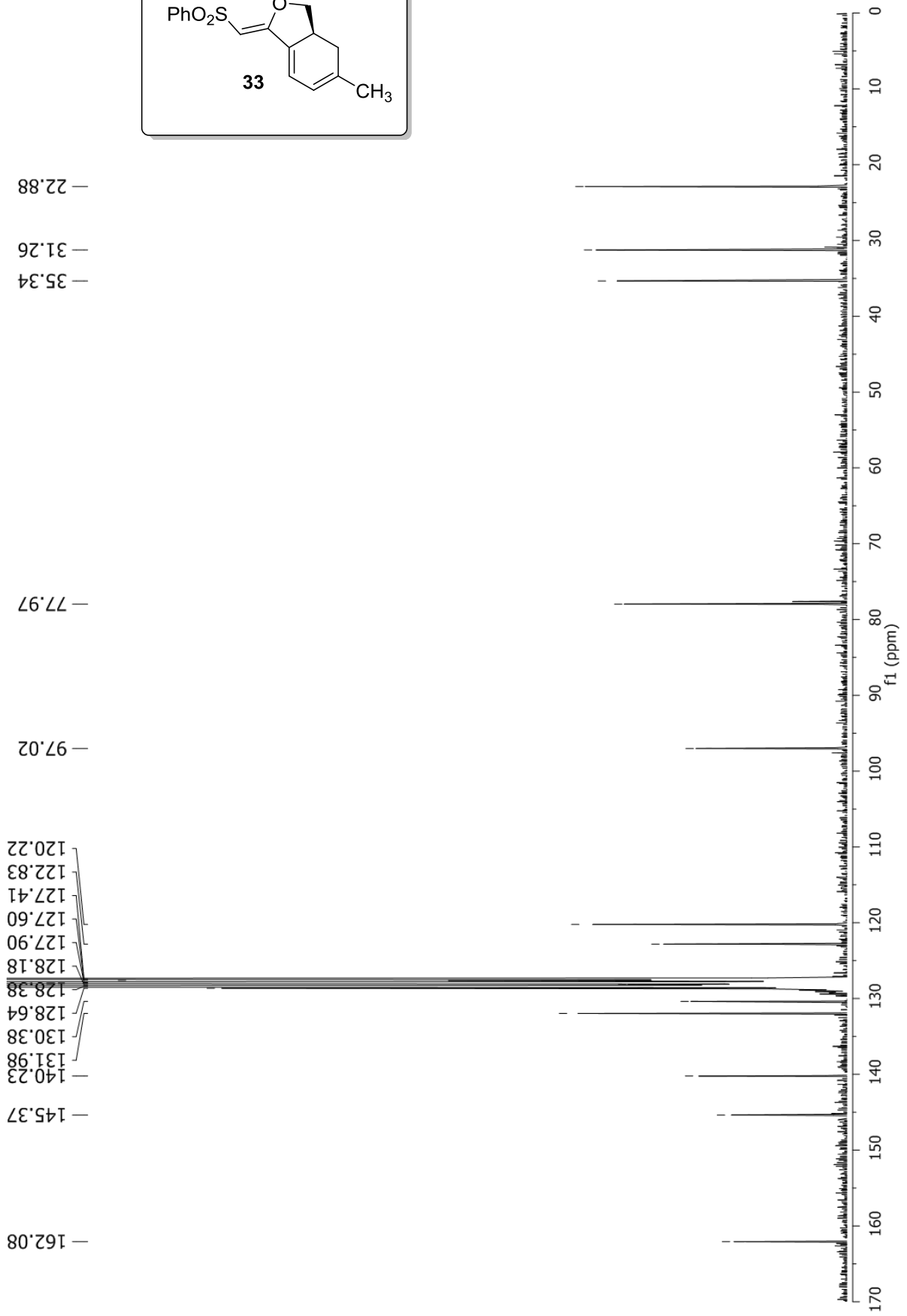
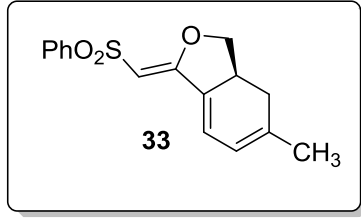
PeakTable

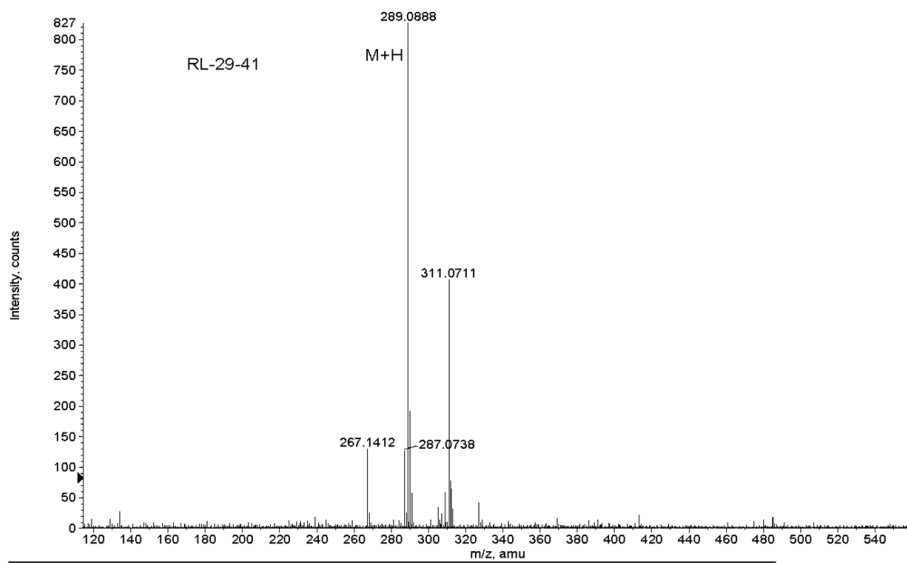
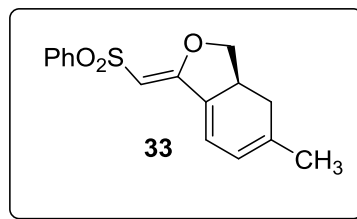
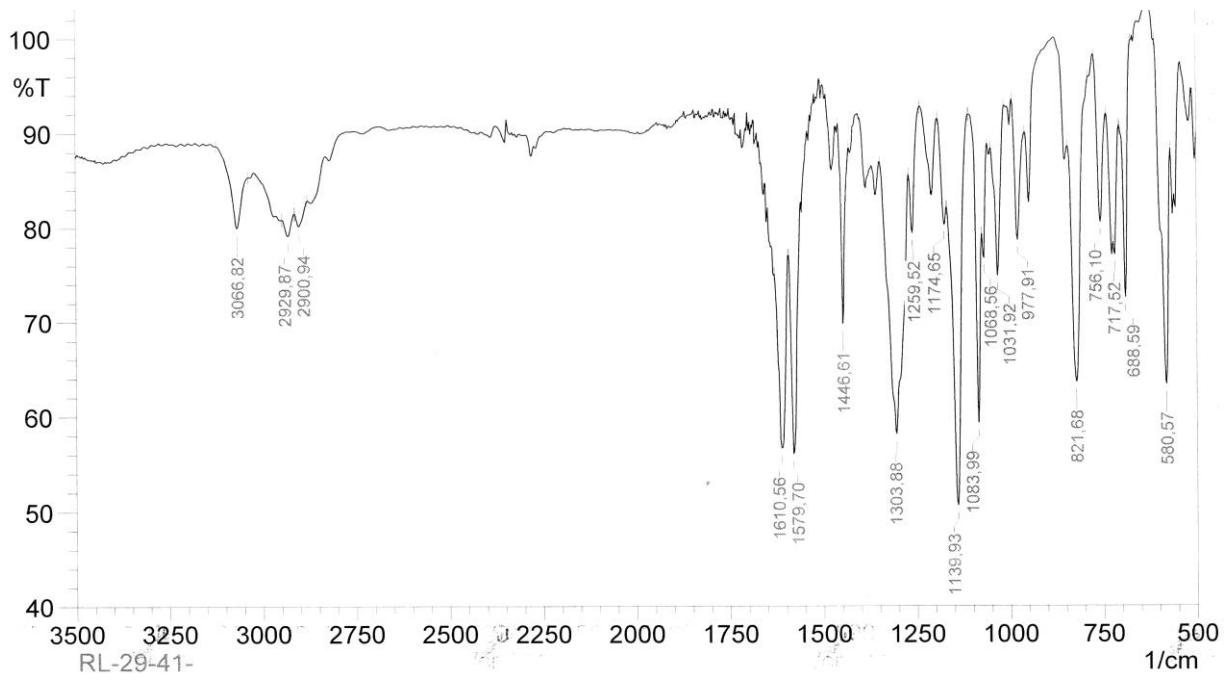
PDA Ch5 350nm 4nm

Peak#	Ret. Time	Area %
1	69.012	87.077
2	79.015	12.923
Total		100.000

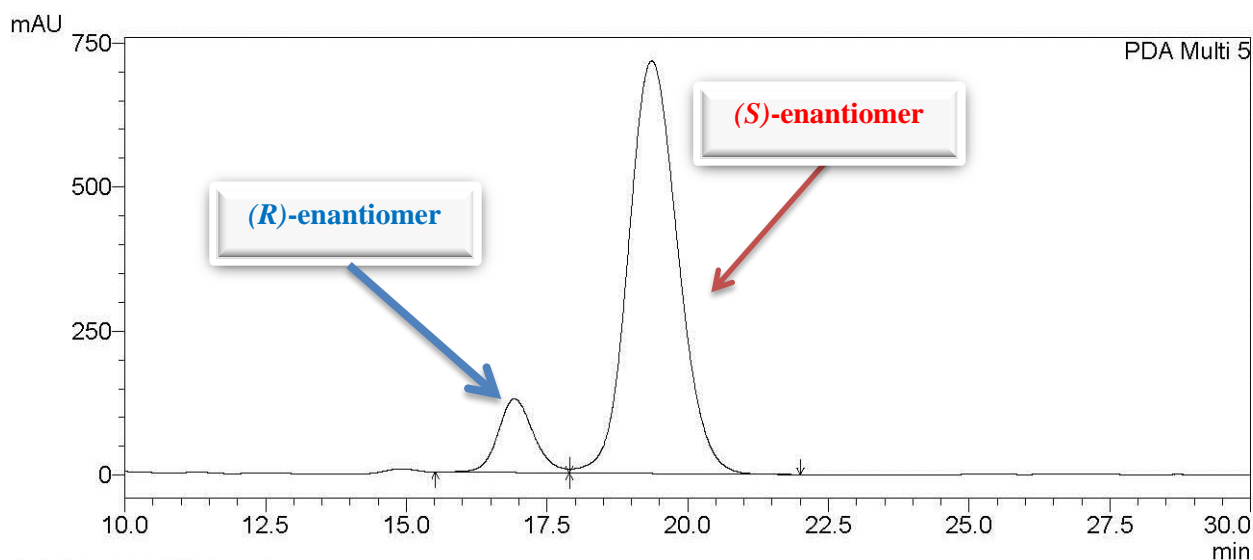




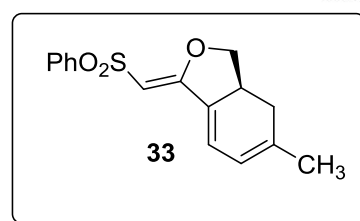




Formula	CalculatedMass	mDaError	ppmError	RDB
C8 H13 N6 O6	289.089109	-0.308828	-1.068279	5.5
C16 H17 O3 S	289.089293	-0.49282	-1.704732	8.5

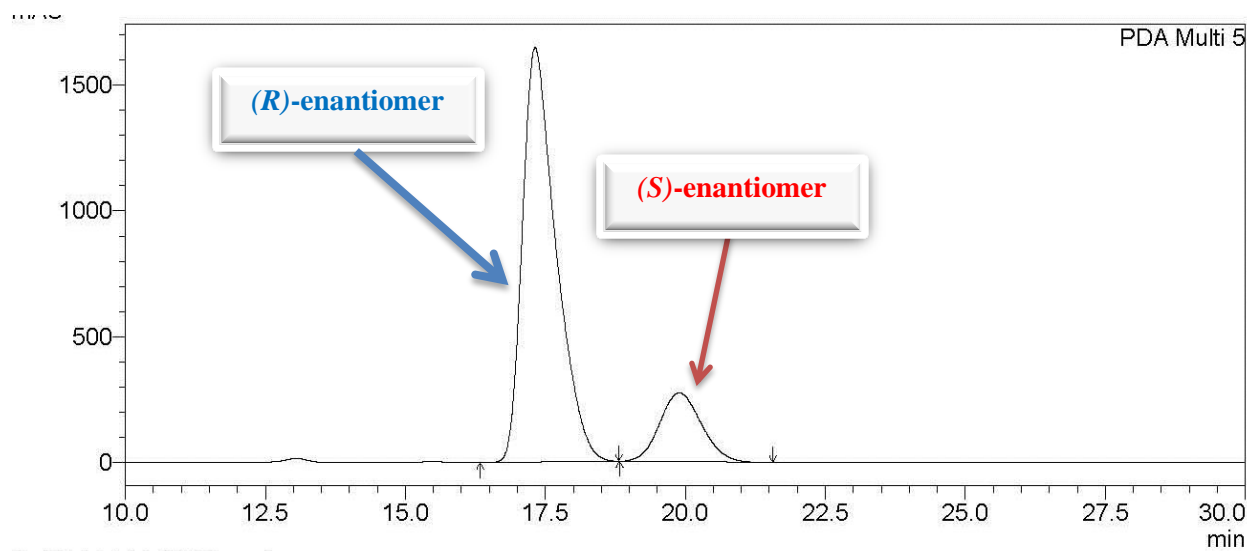


1 PDA Multi 5/350nm 4nm

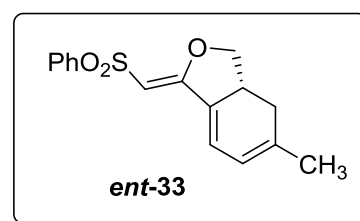


PeakTable
PDA Ch5 350nm 4nm

Peak#	Ret. Time	Area %
1	16.917	11.406
2	19.354	88.594
Total		100.000

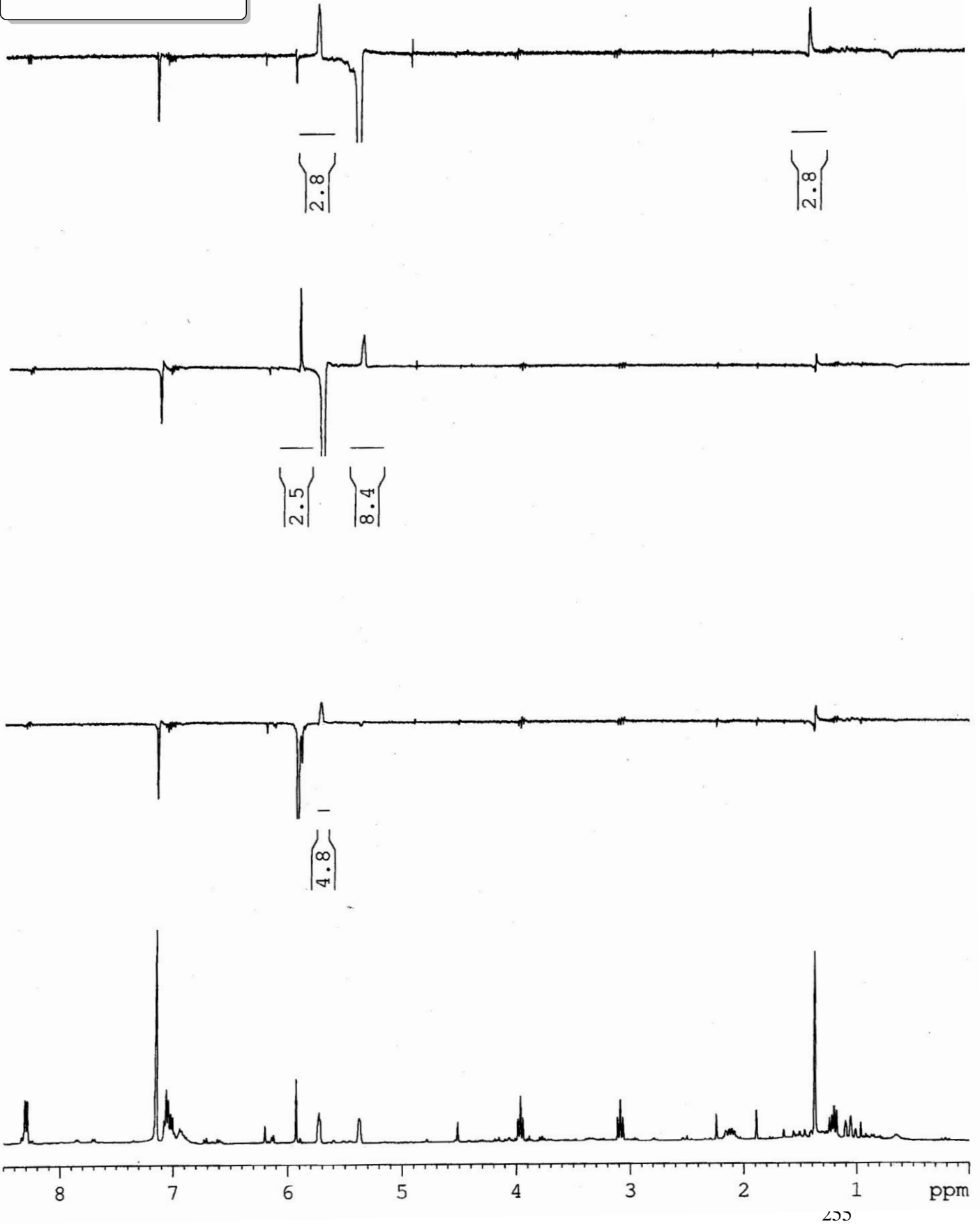
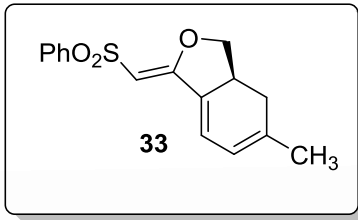


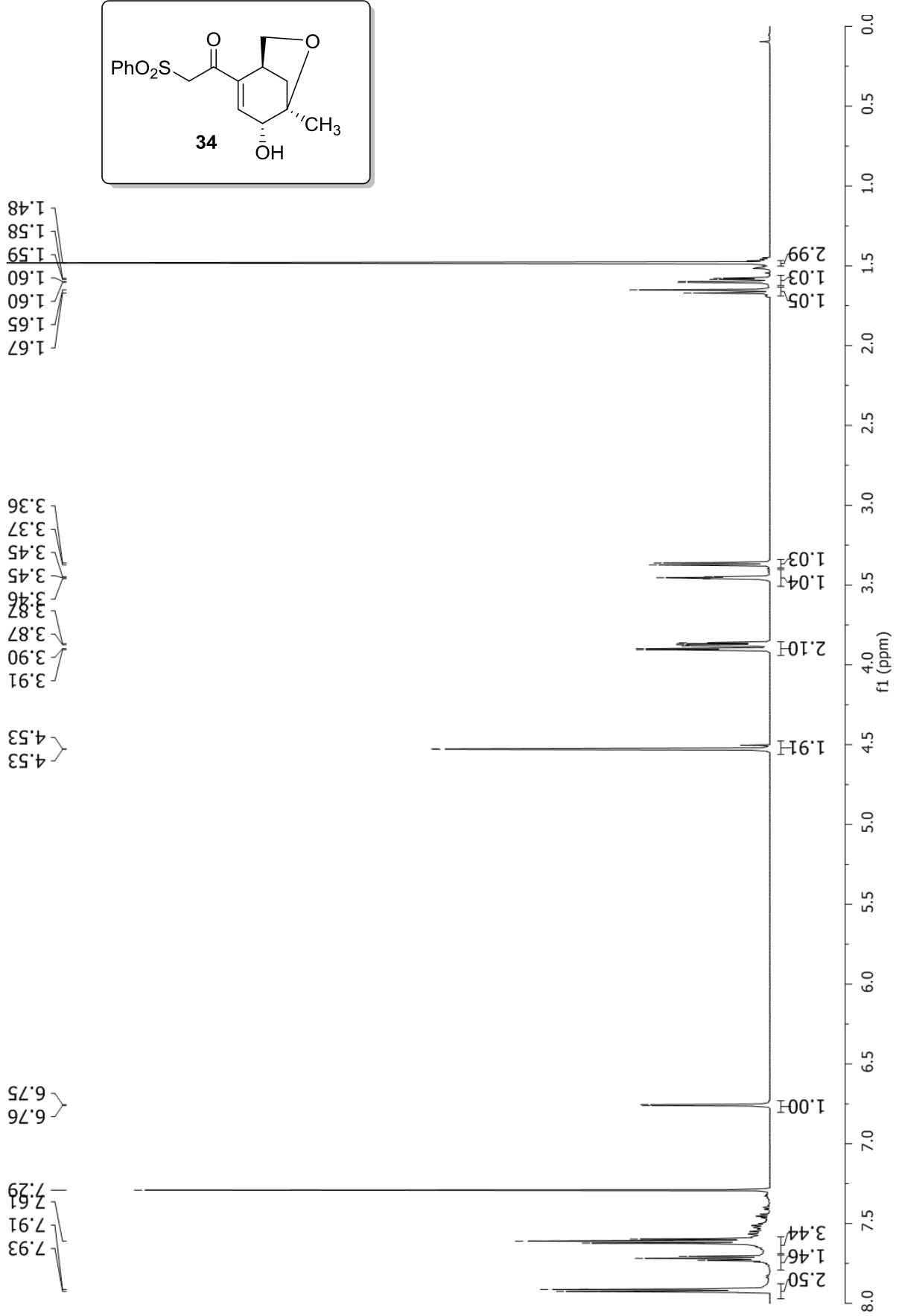
1 PDA Multi 5/350nm 4nm

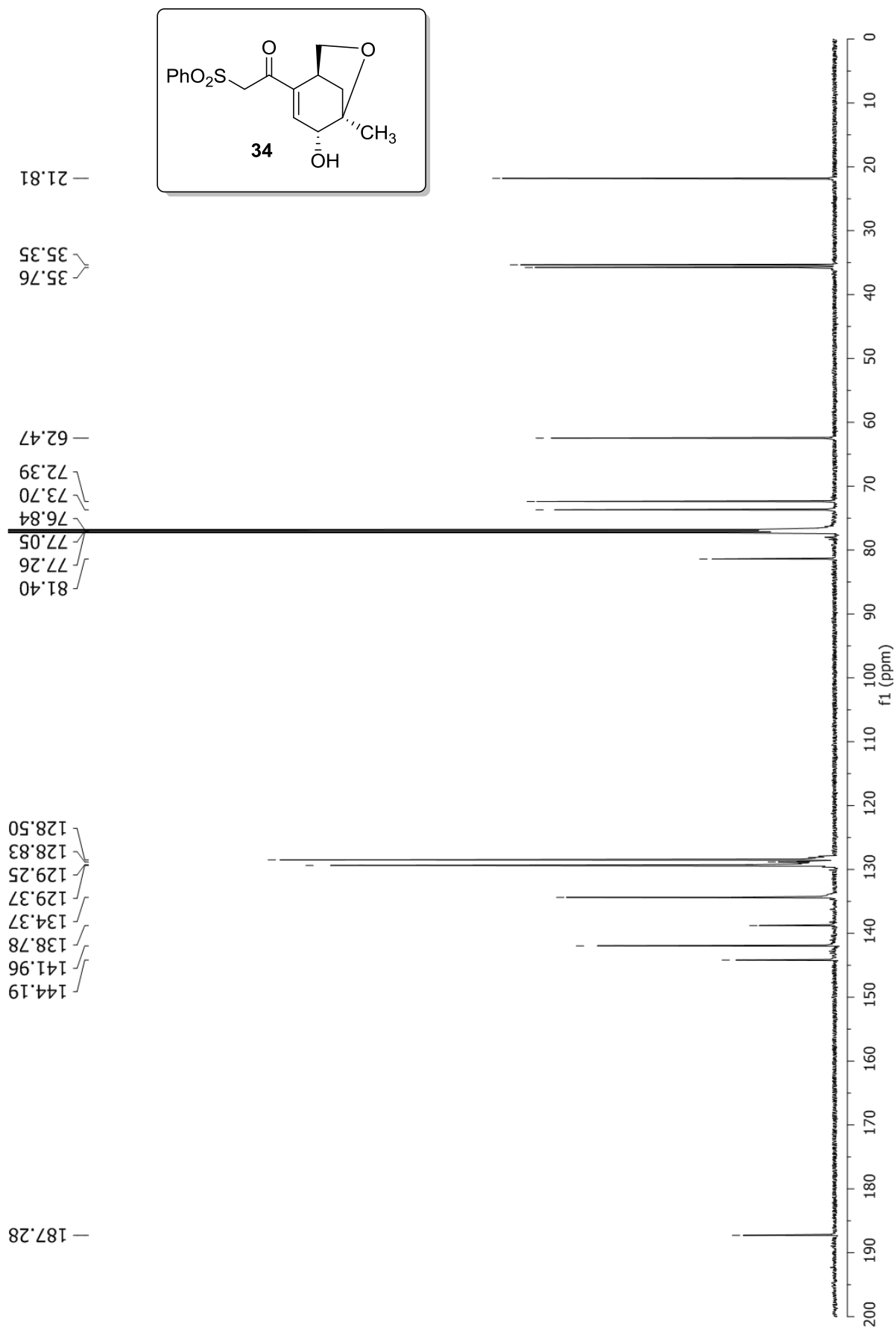


PeakTable
PDA Ch5 350nm 4nm

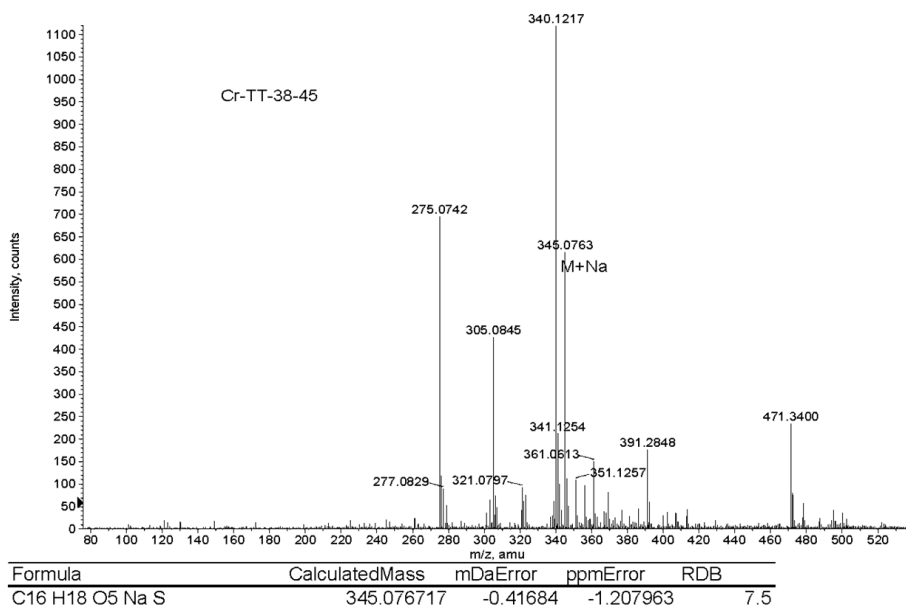
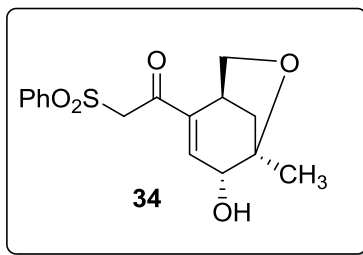
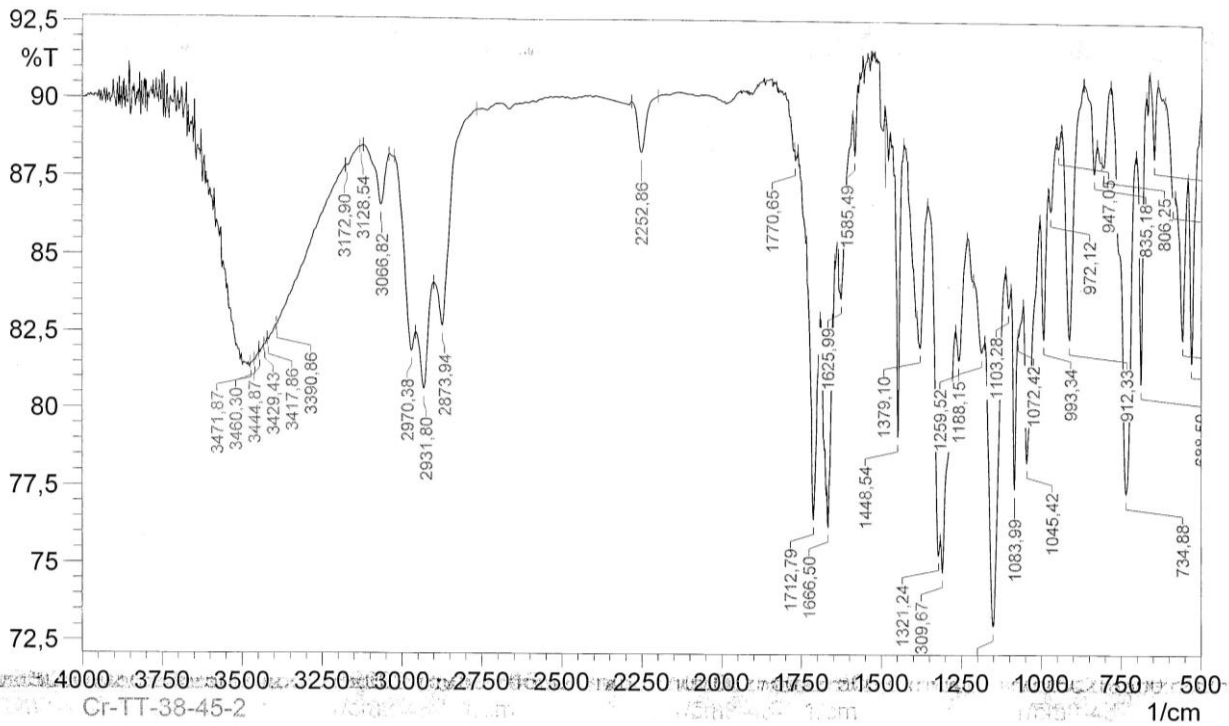
Peak#	Ret. Time	Area %
1	17.313	82.913
2	19.885	17.087
Total		100.000

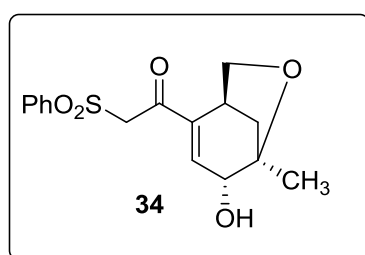
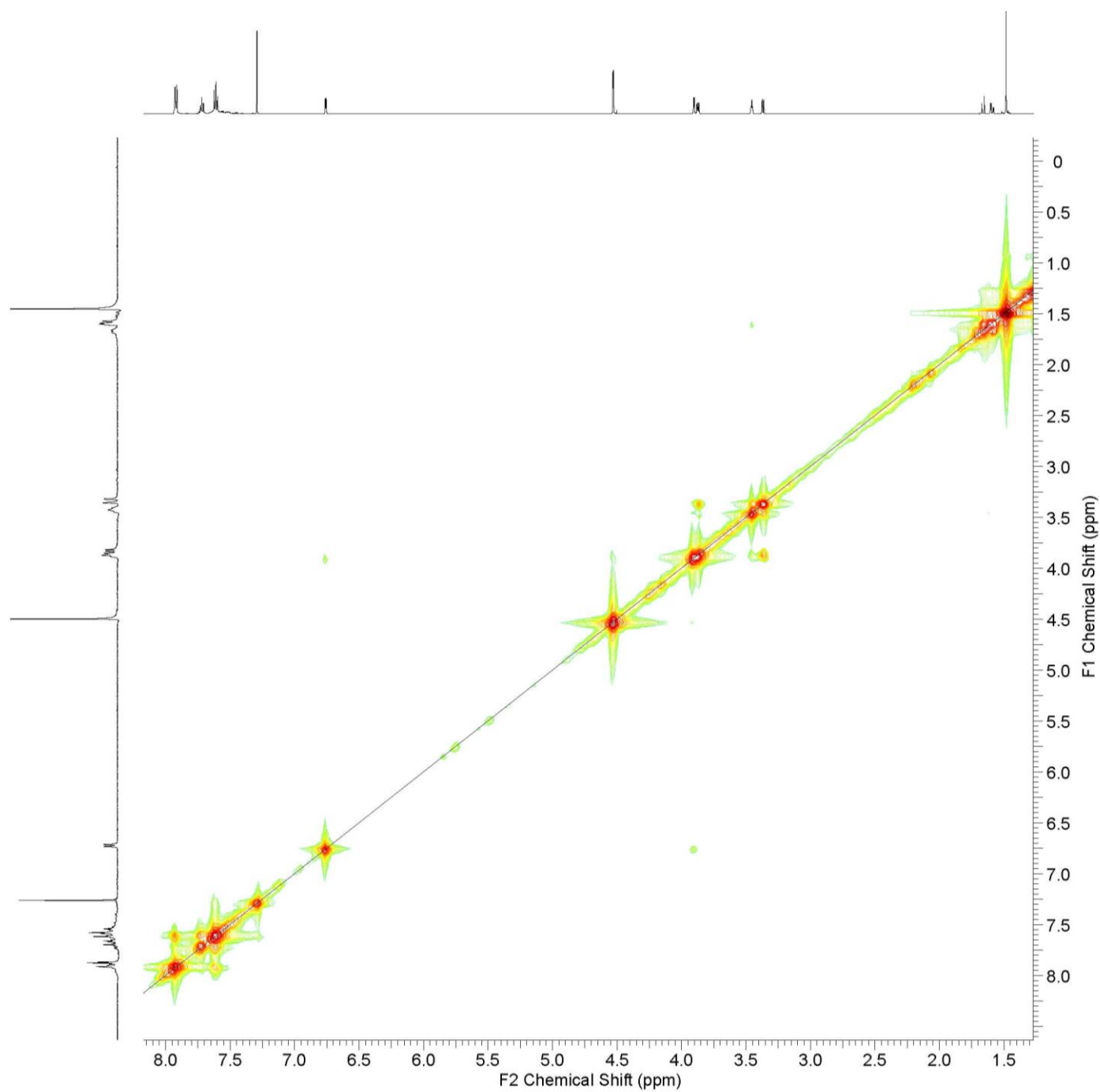


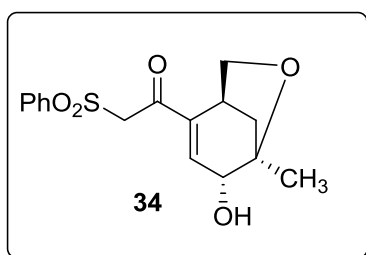
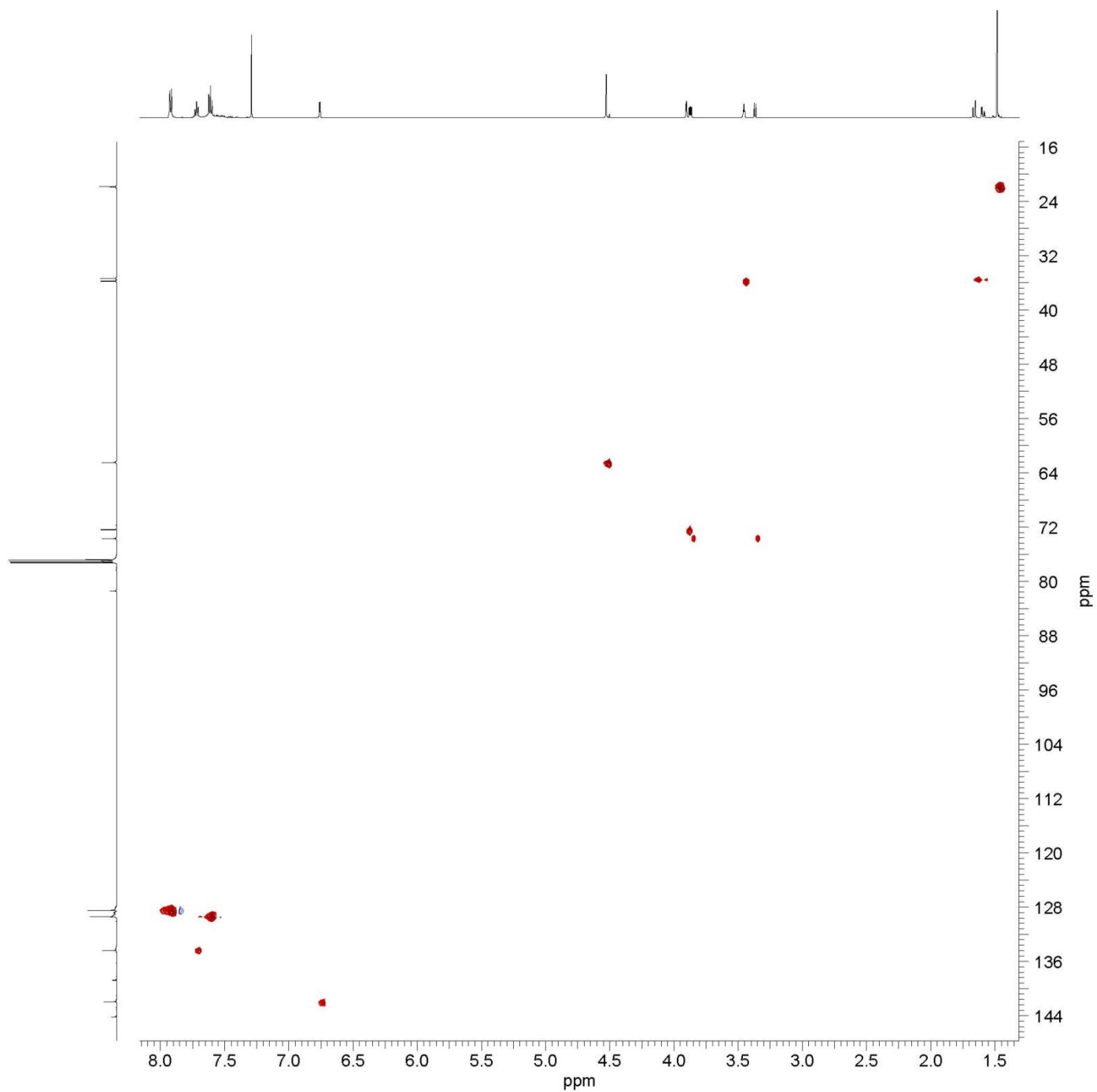


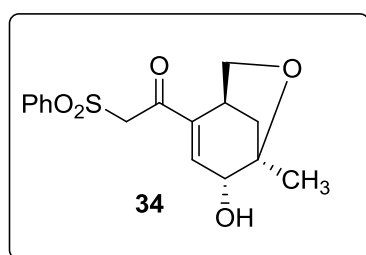
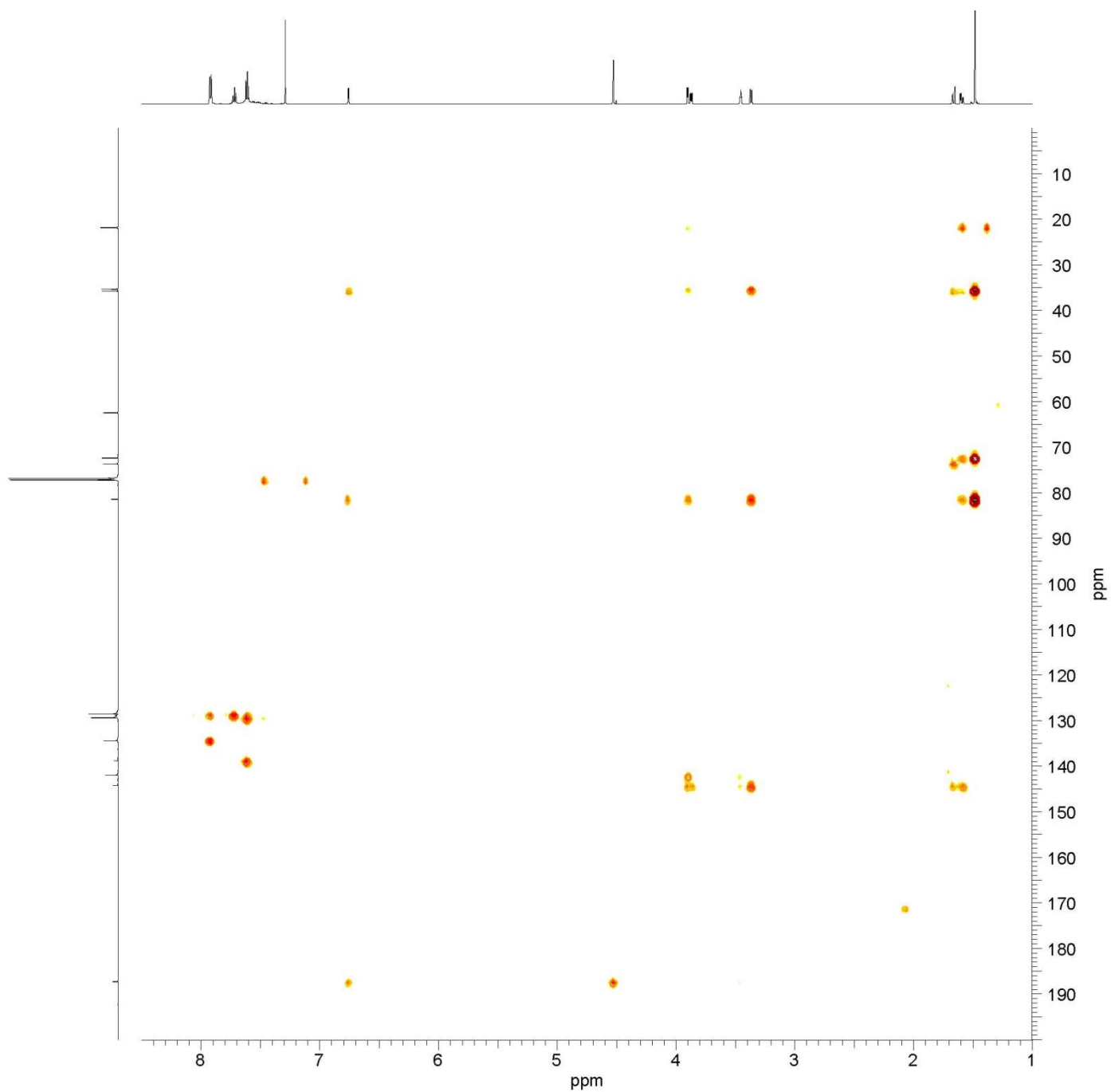


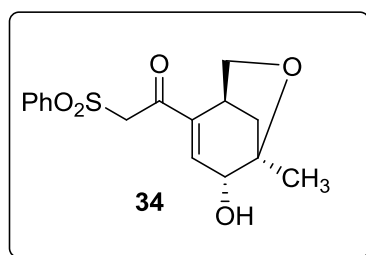
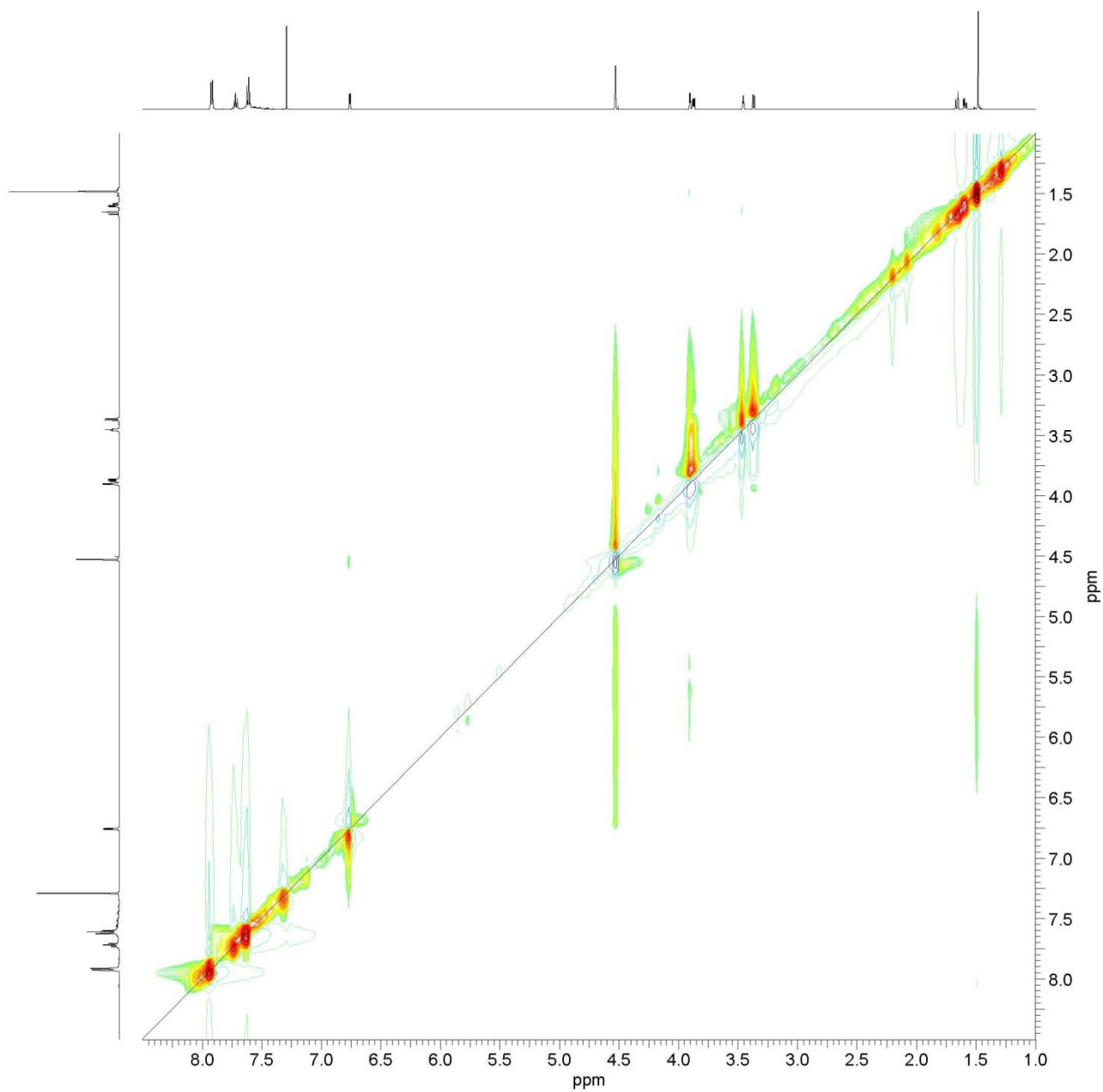
Full Spectroscopy

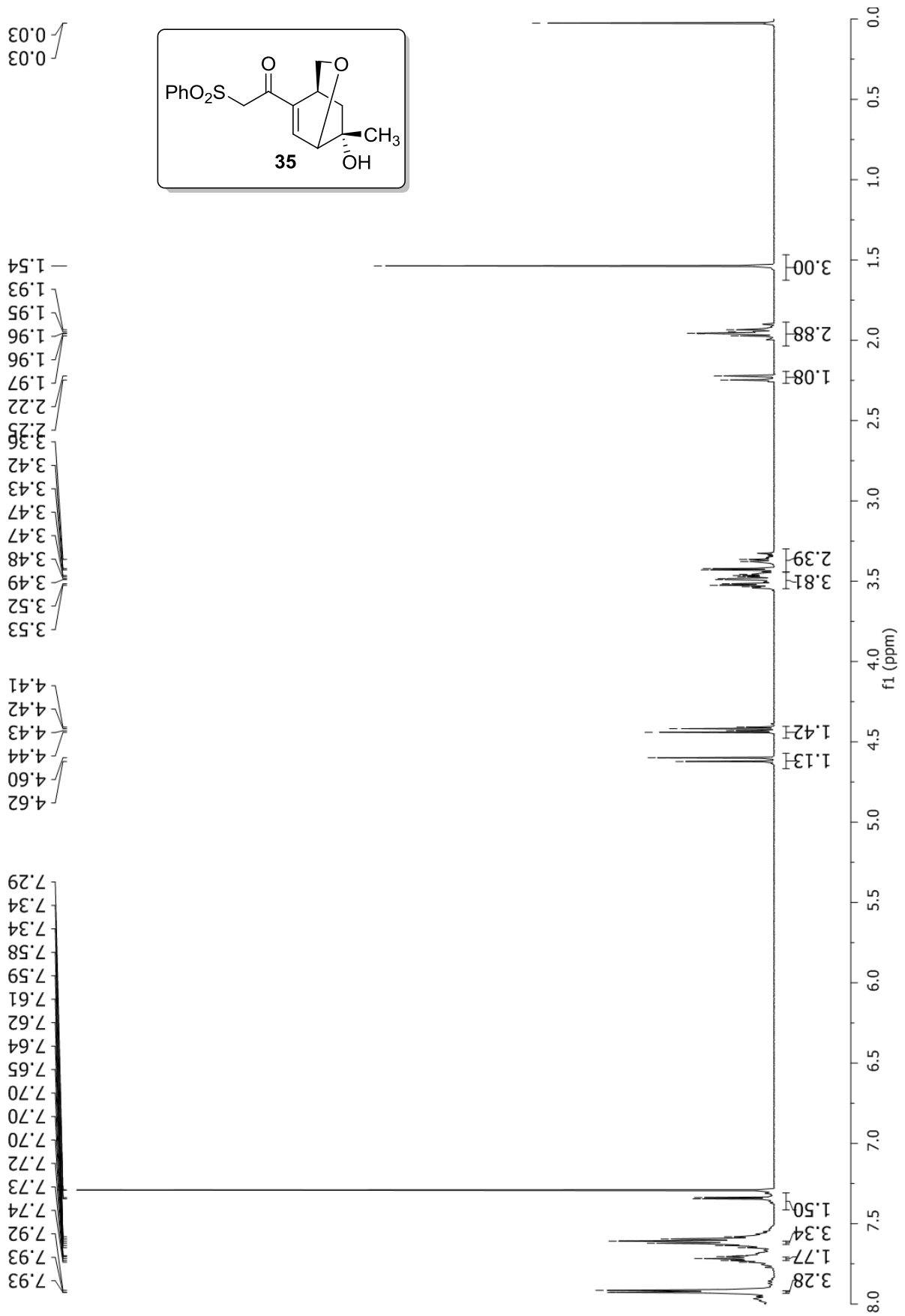


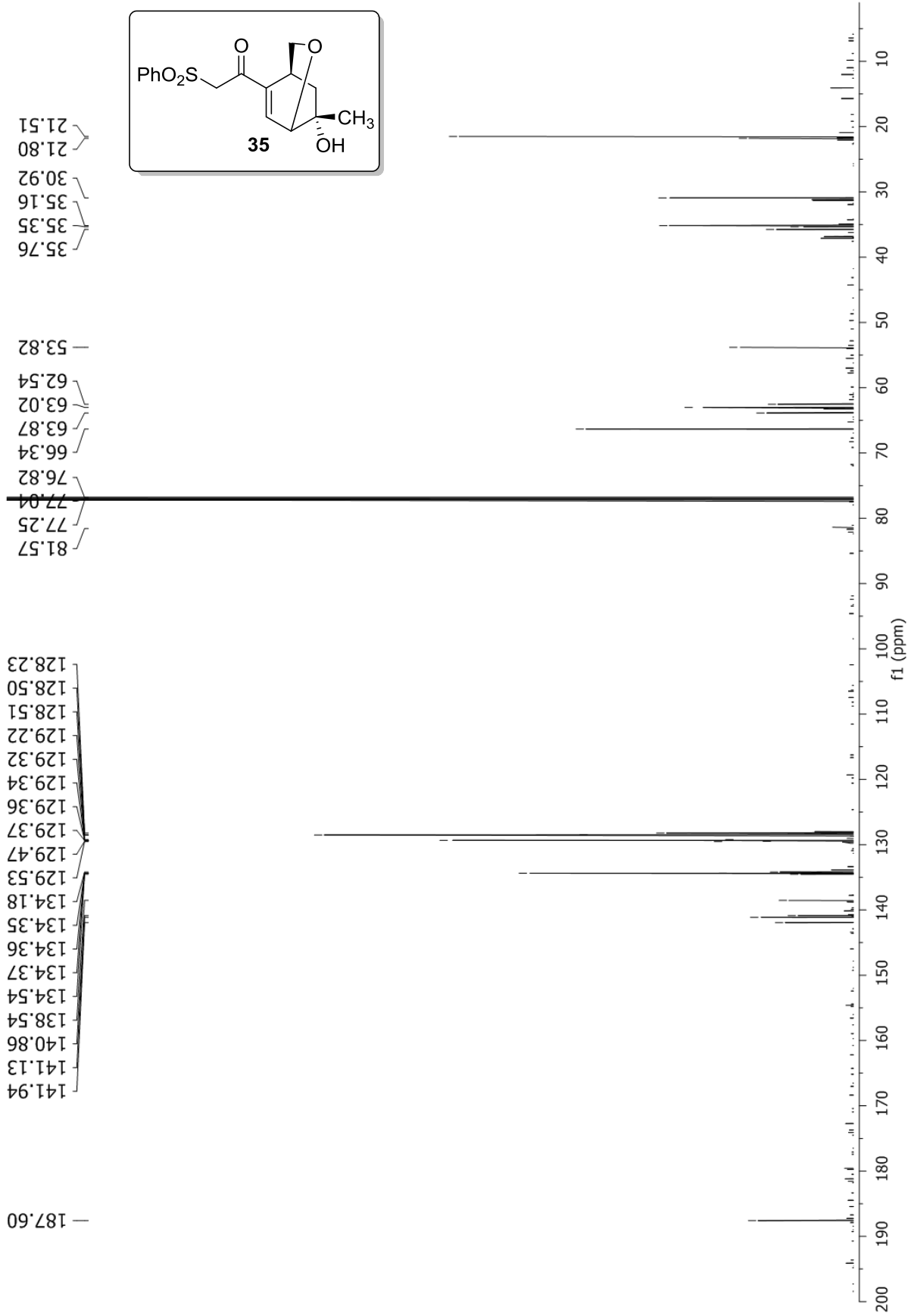


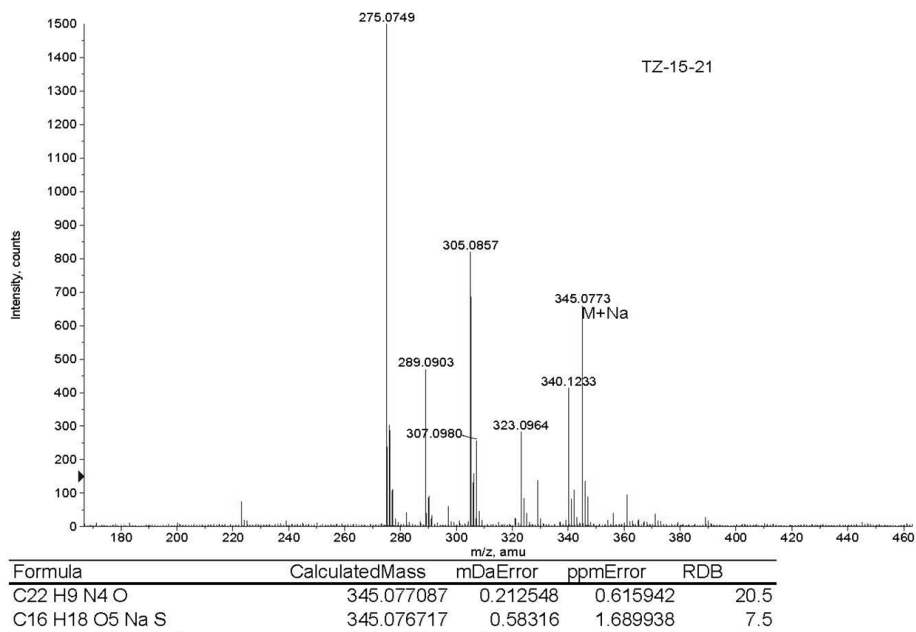
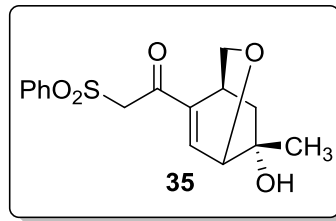
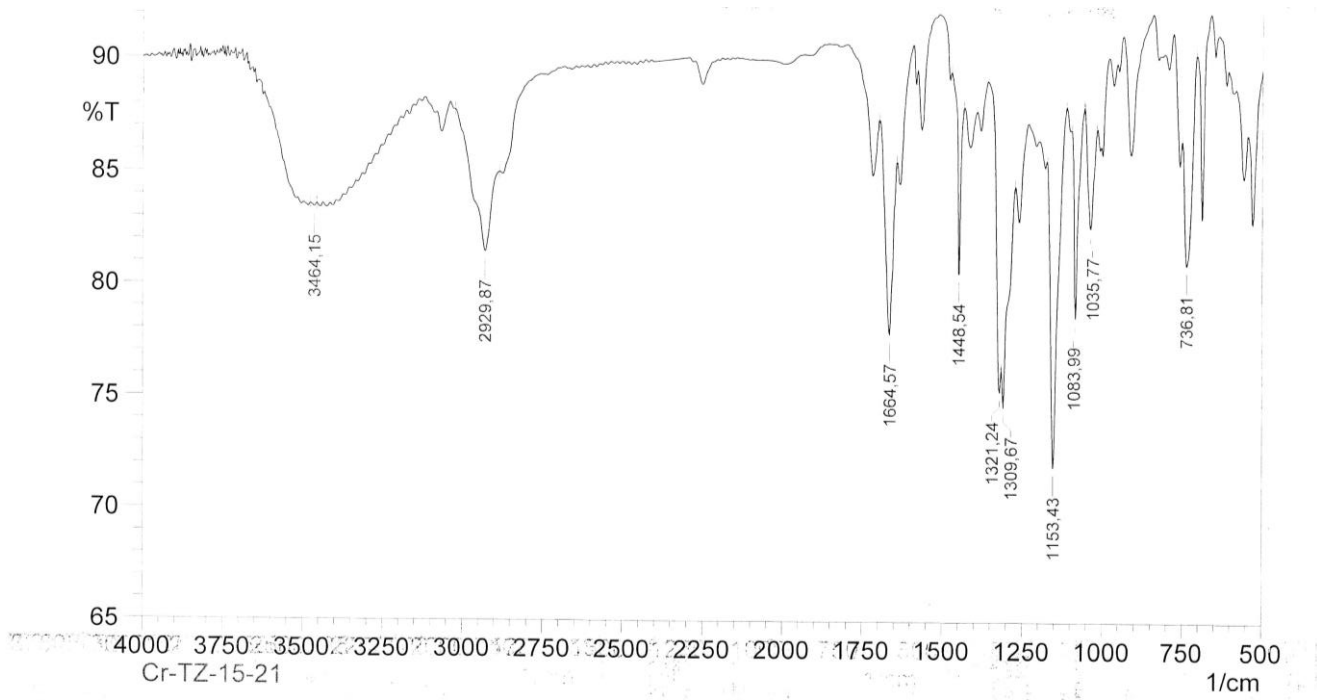


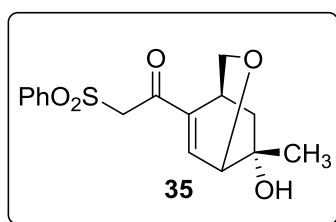
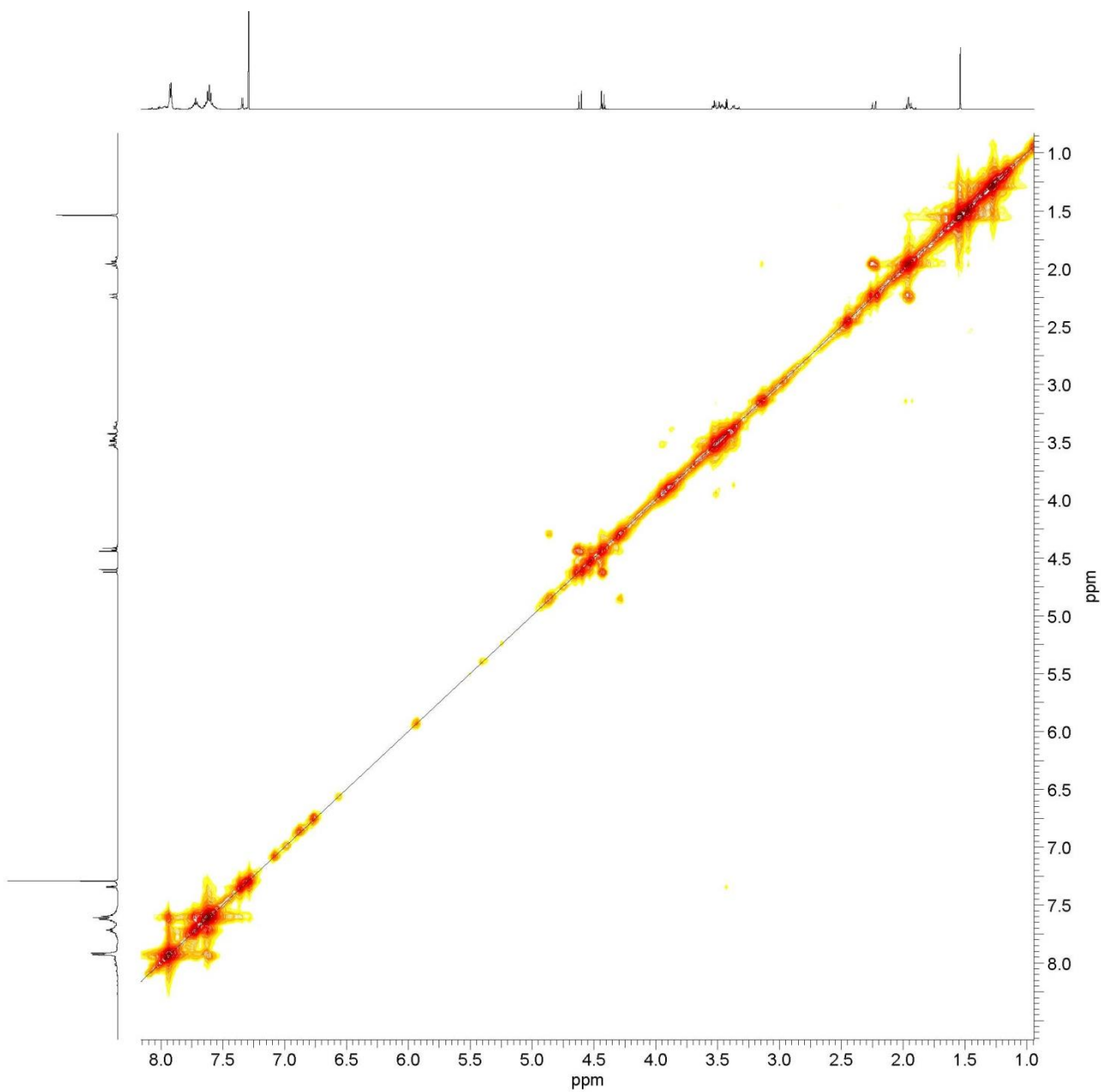


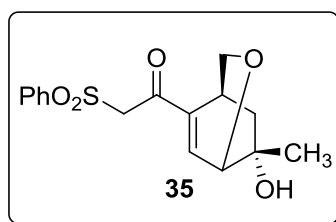
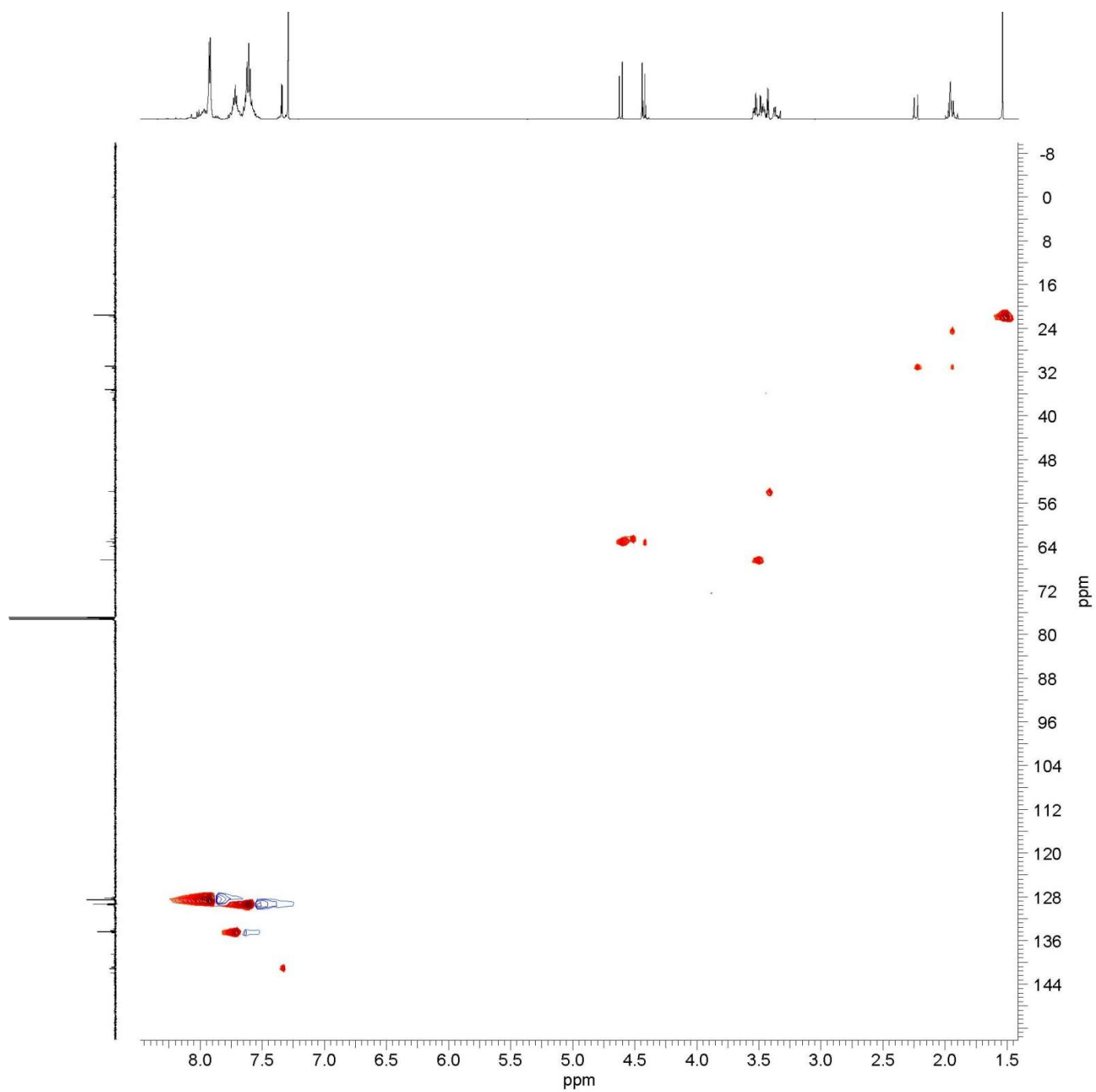


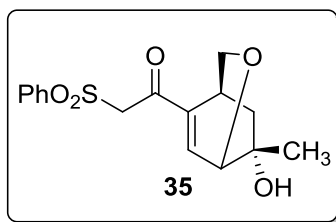
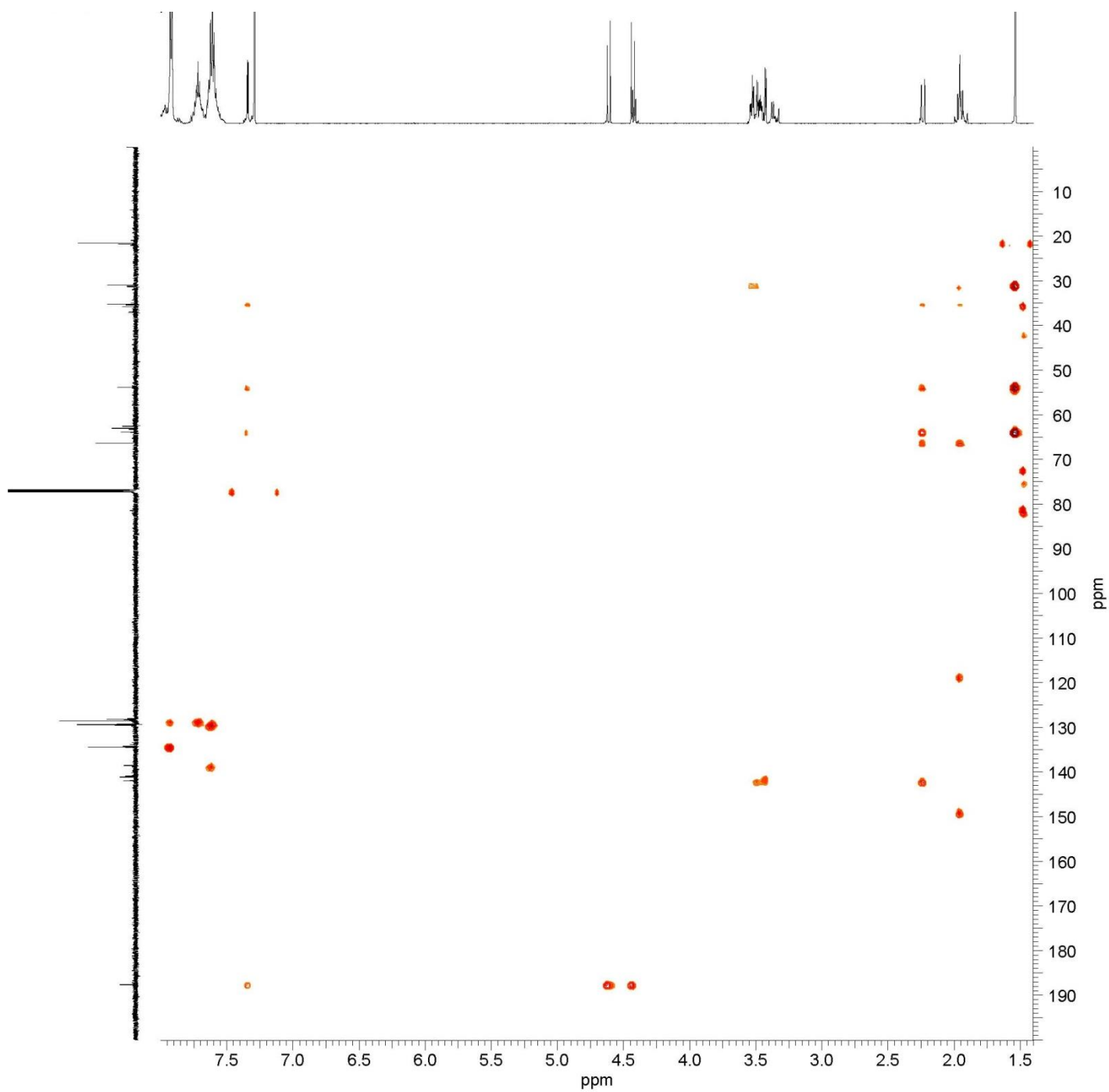


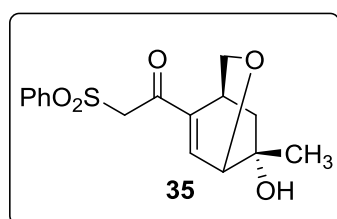
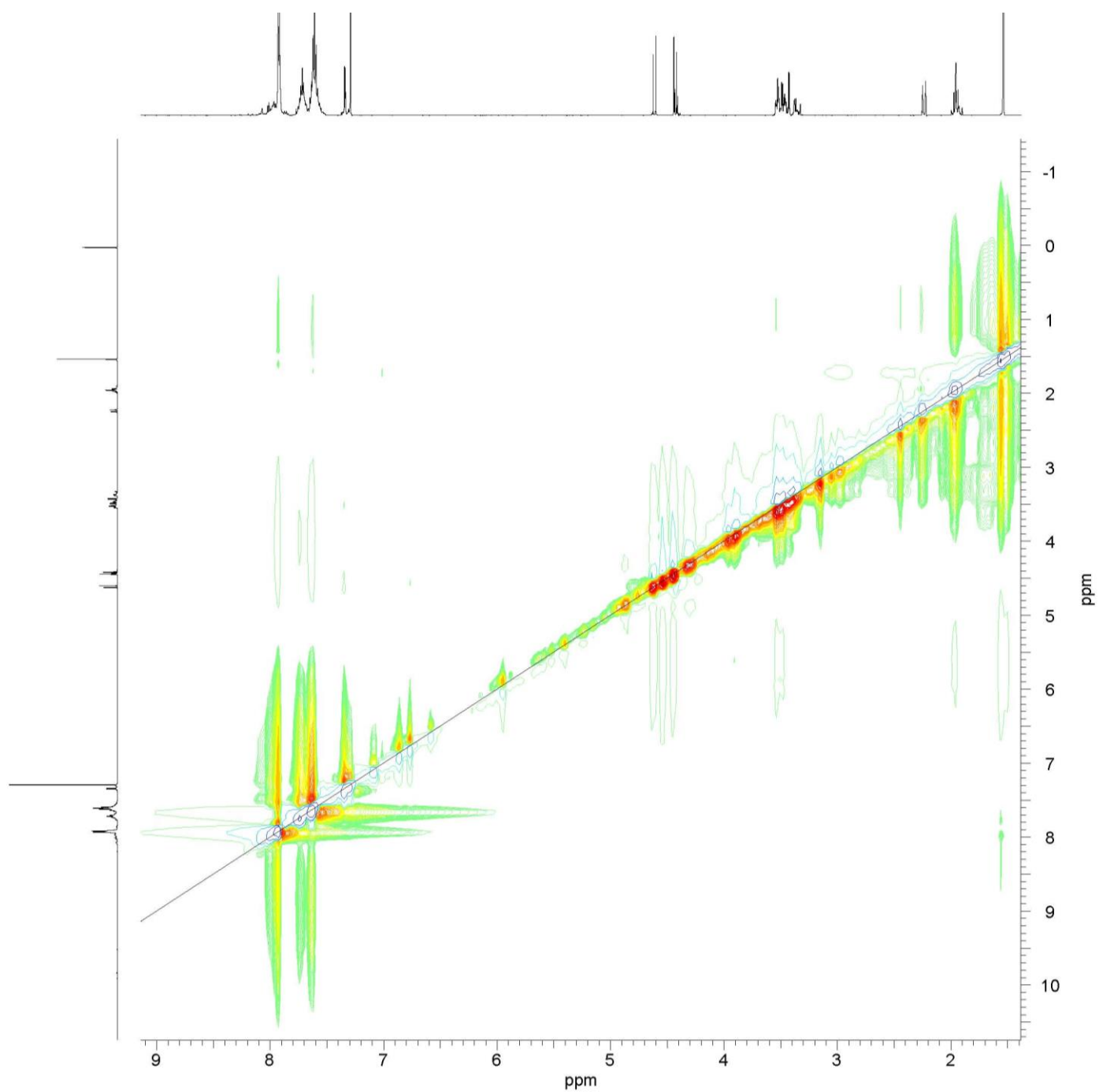


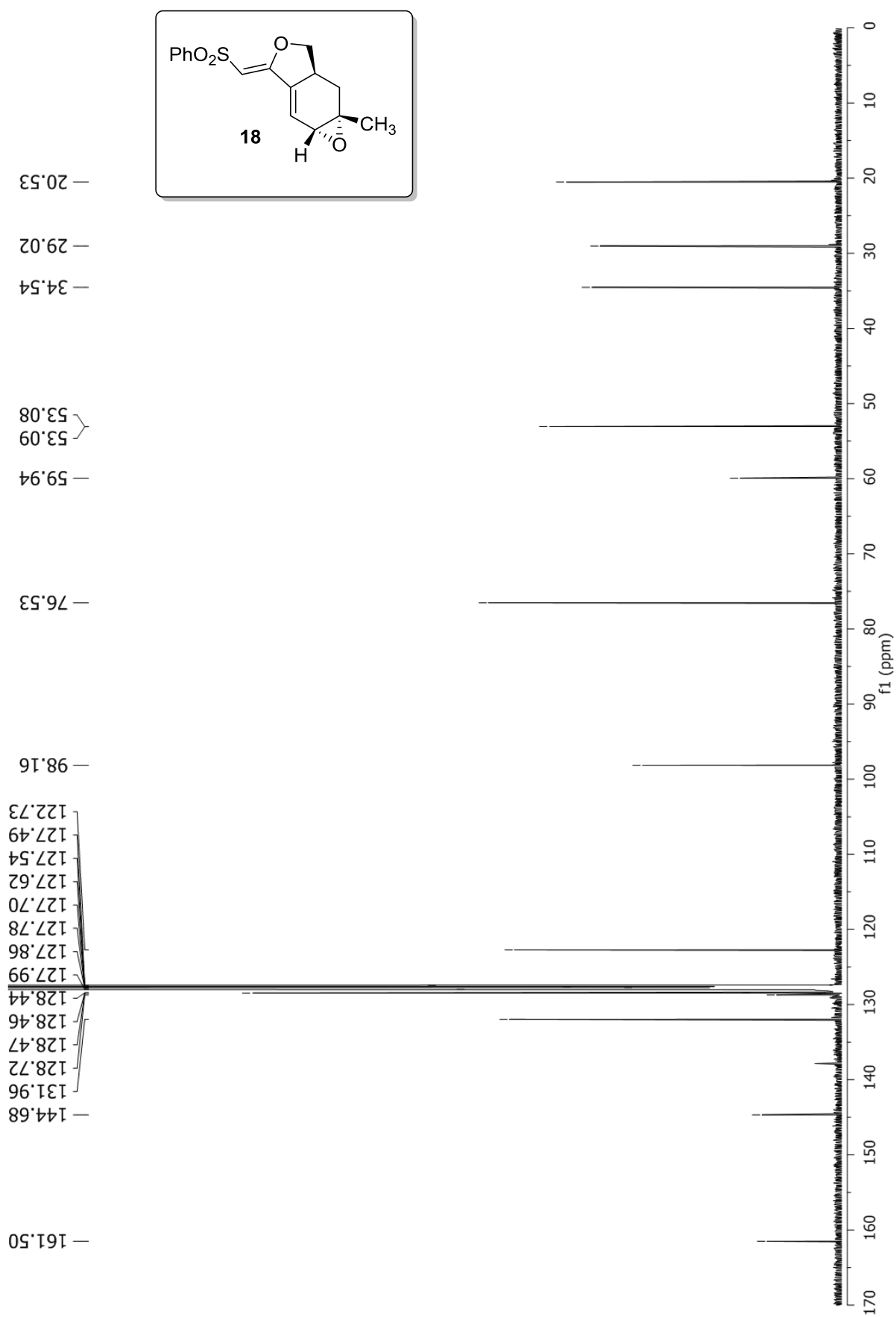




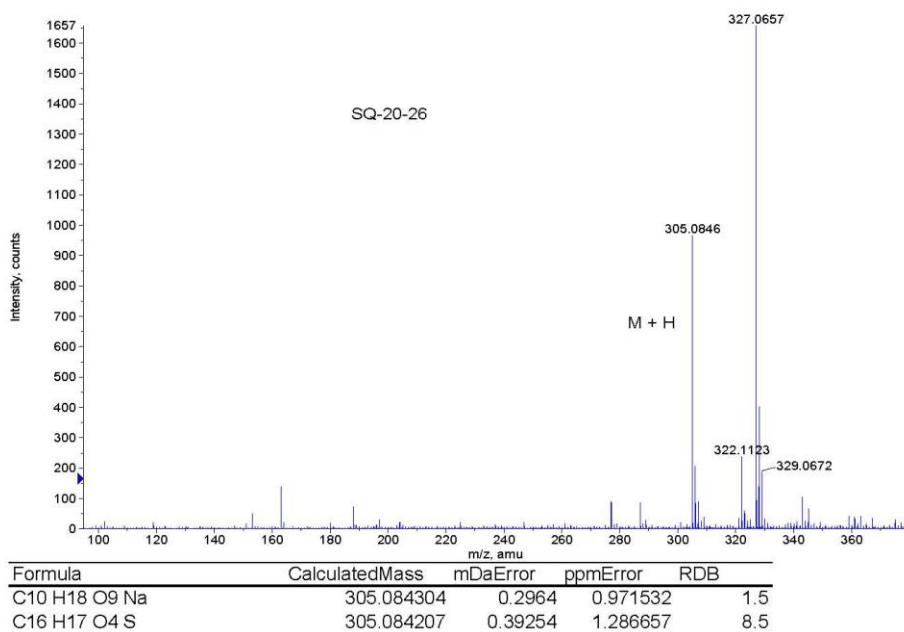
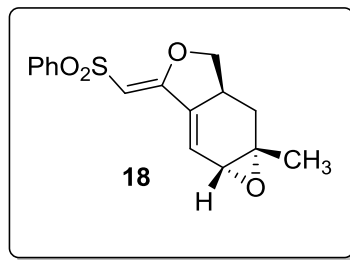
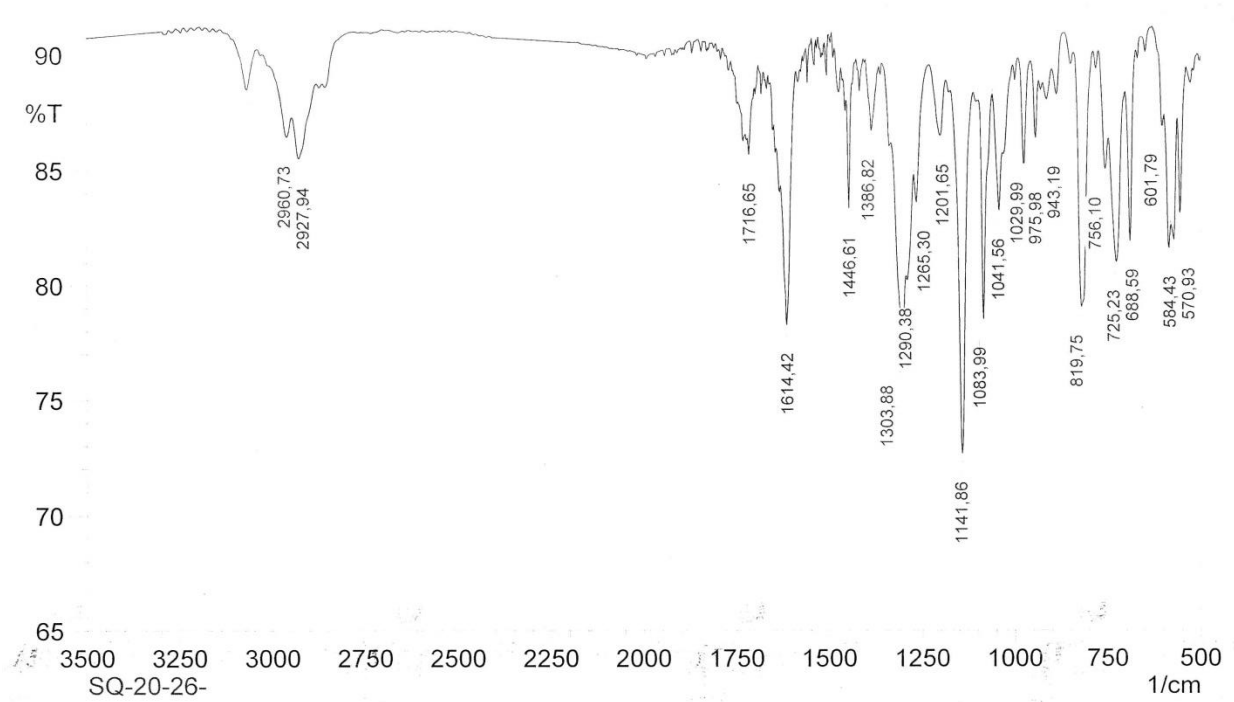


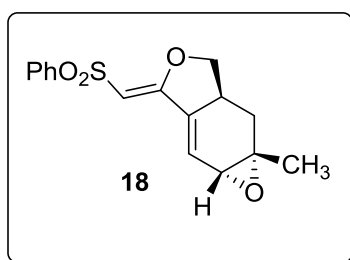
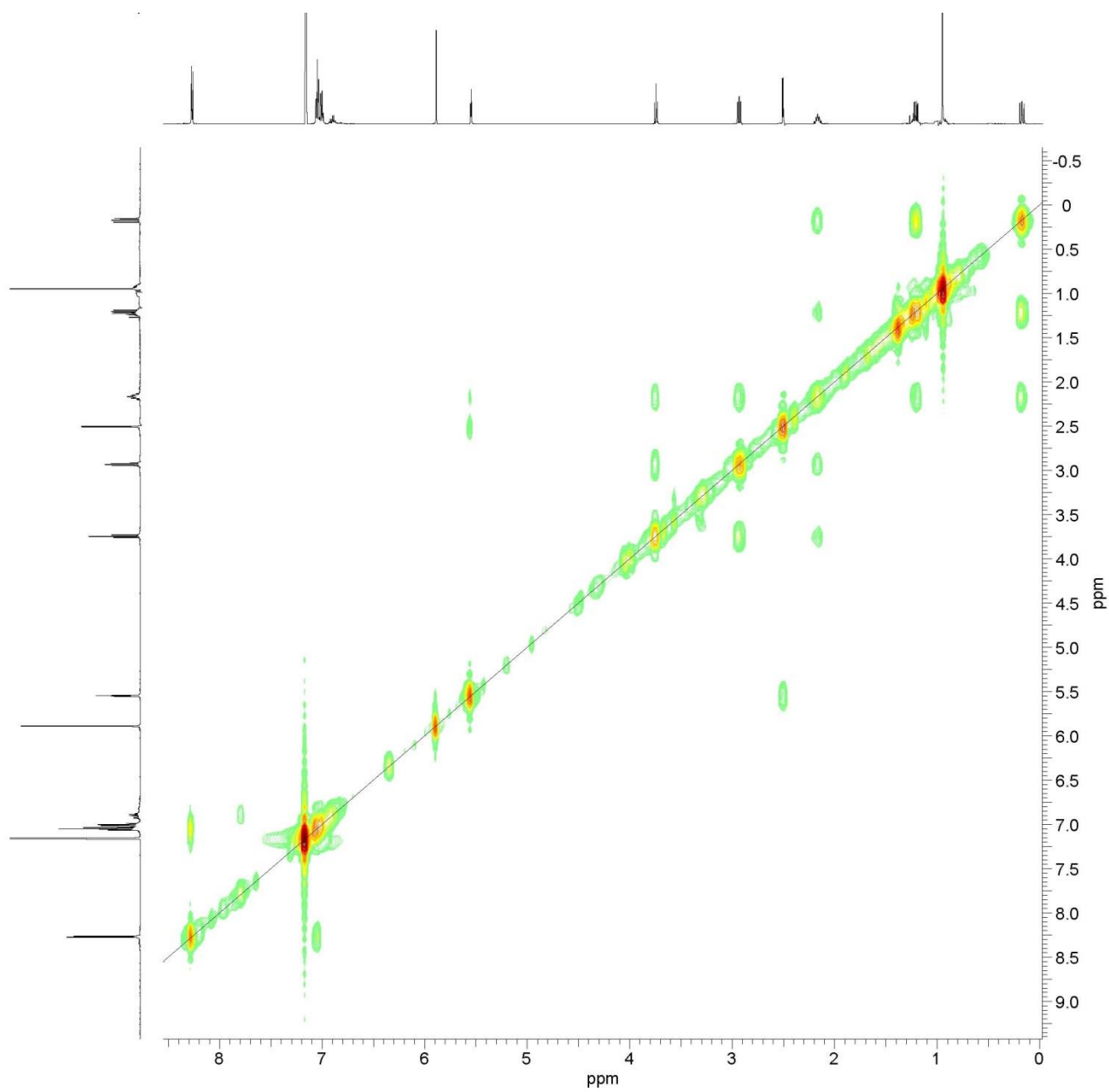


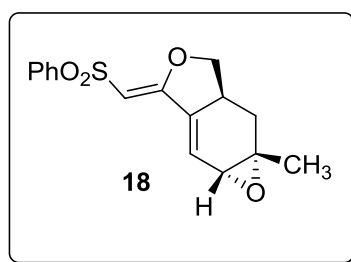
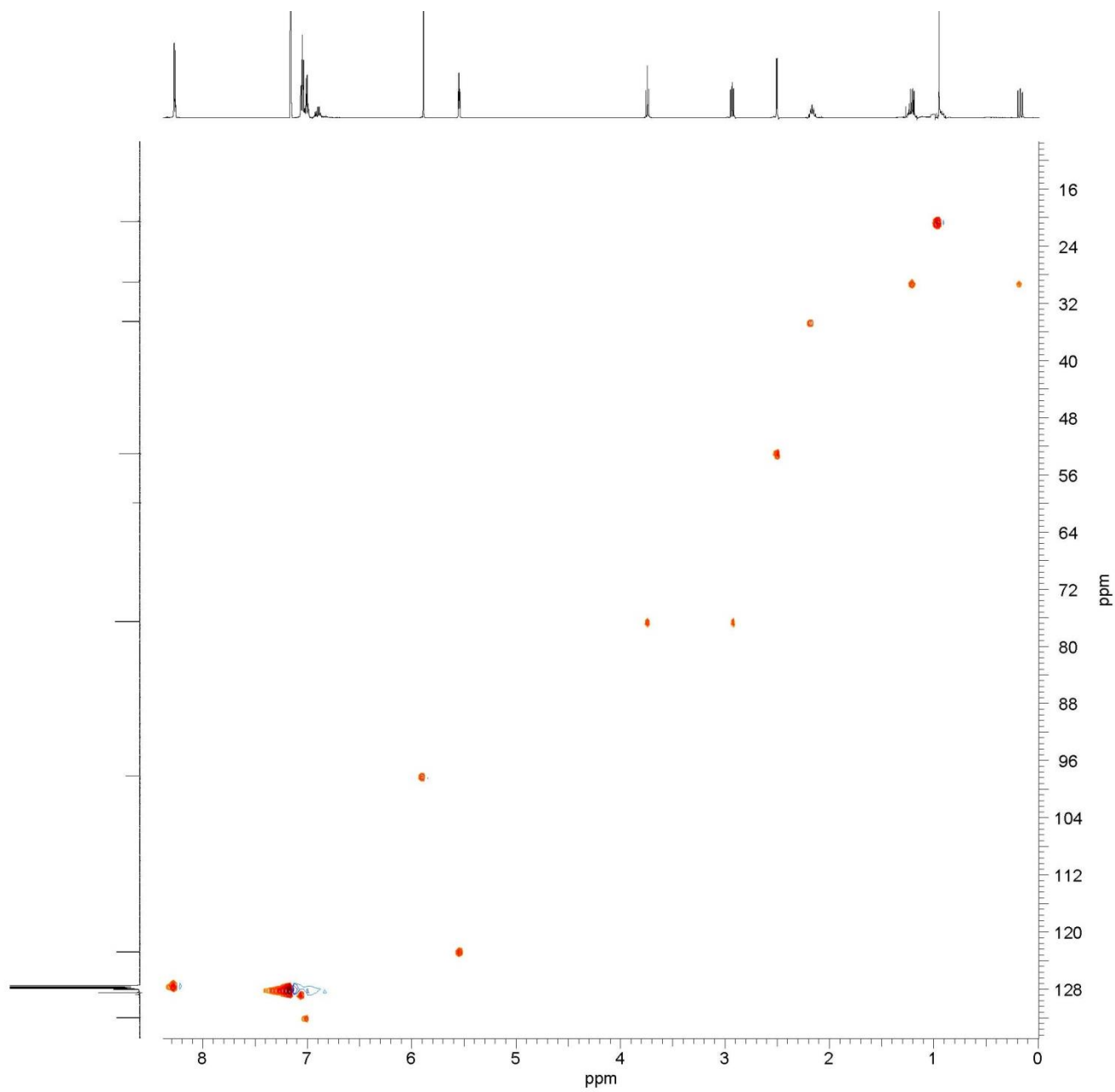


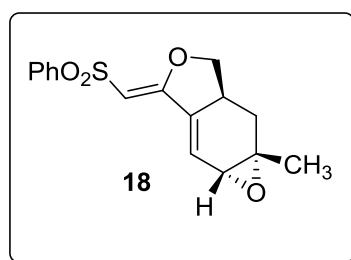
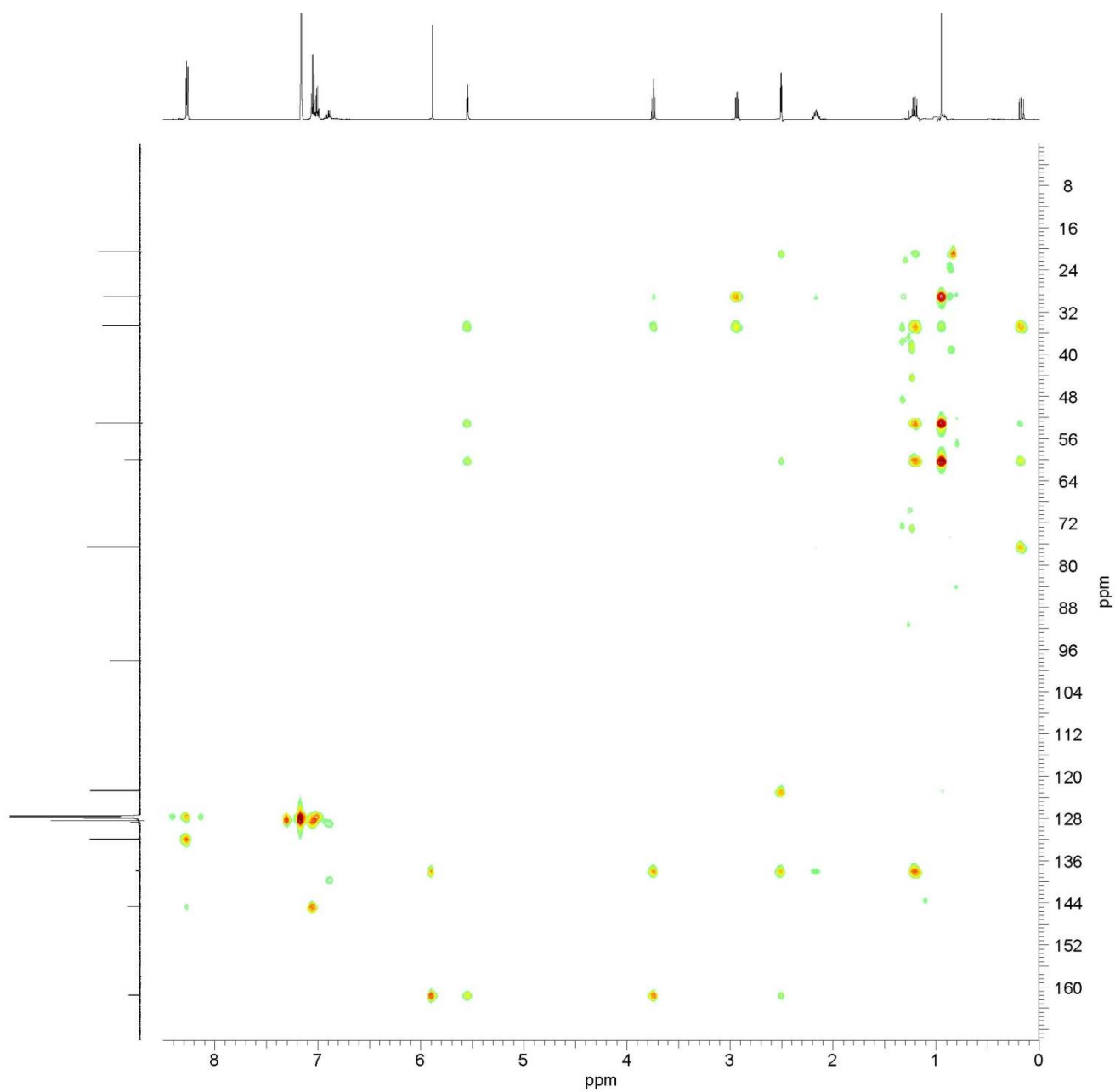


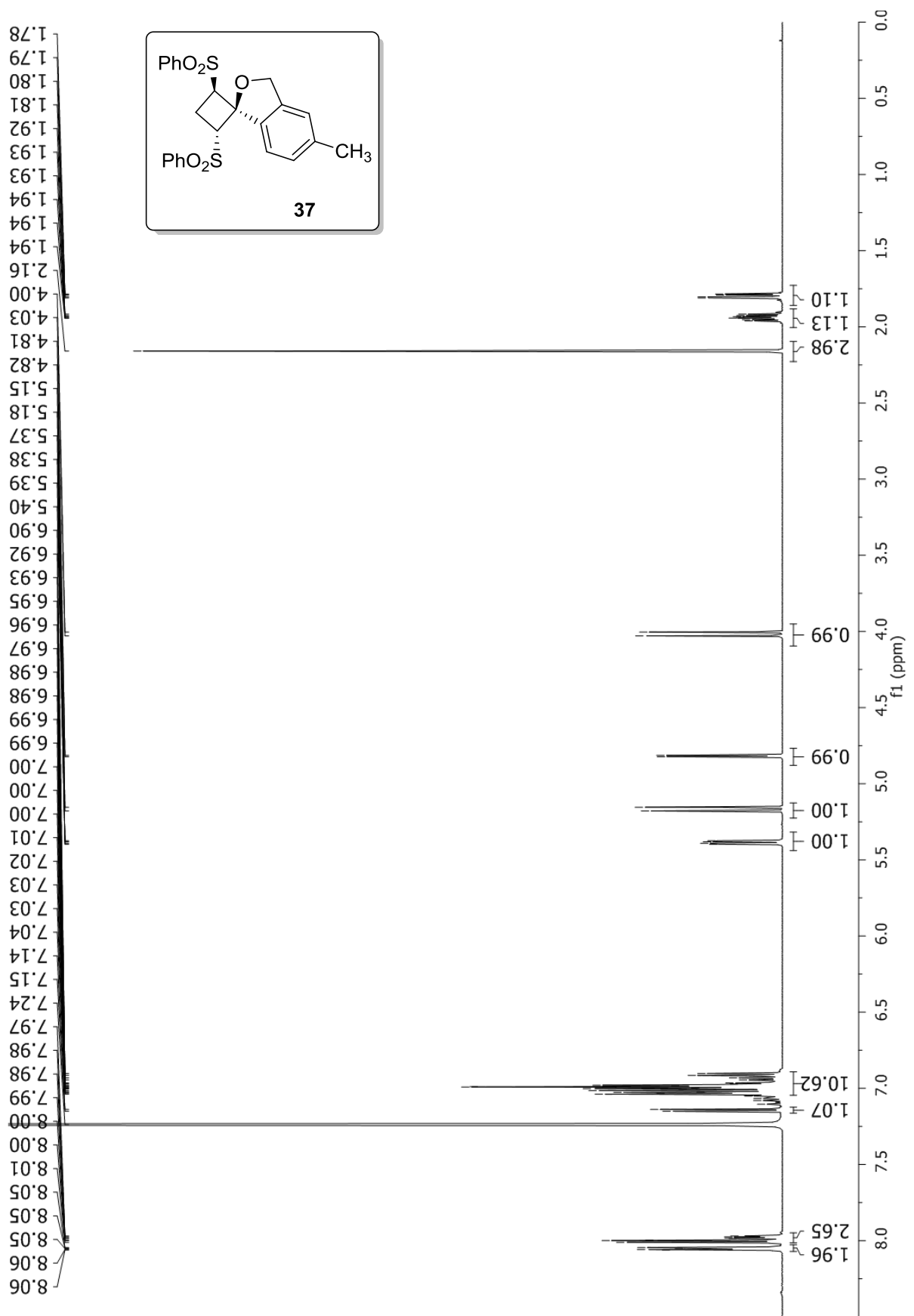
Full Spectroscopy

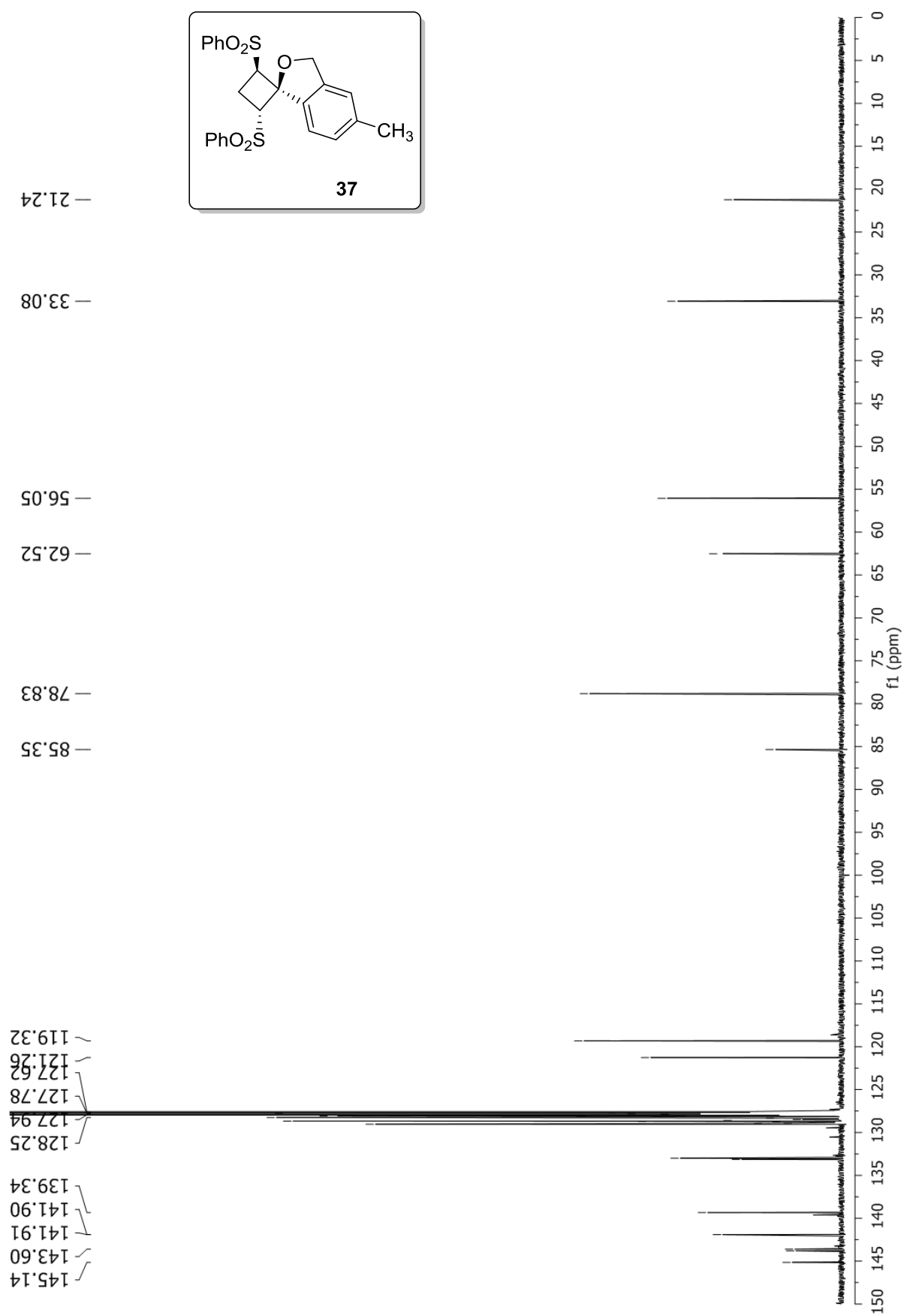




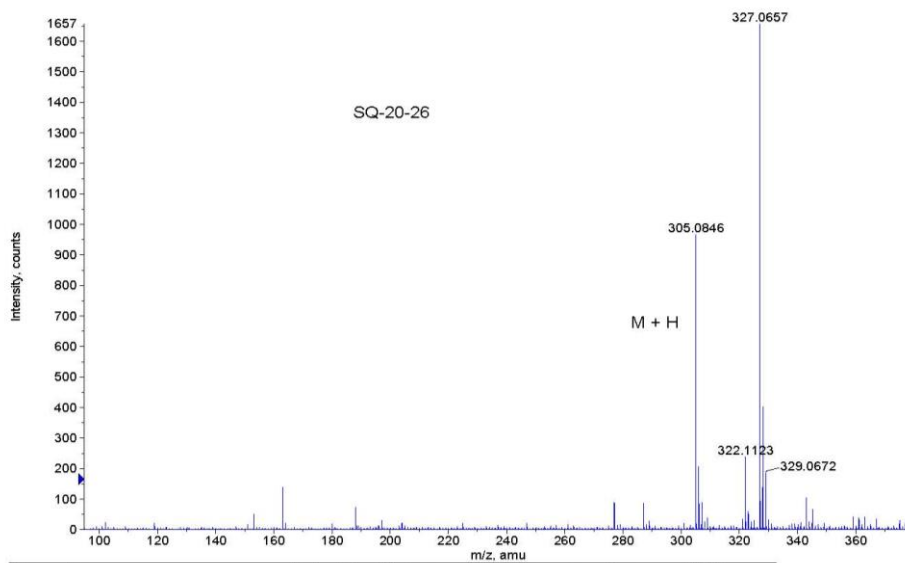
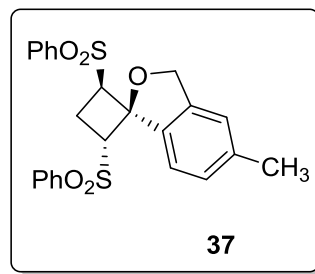
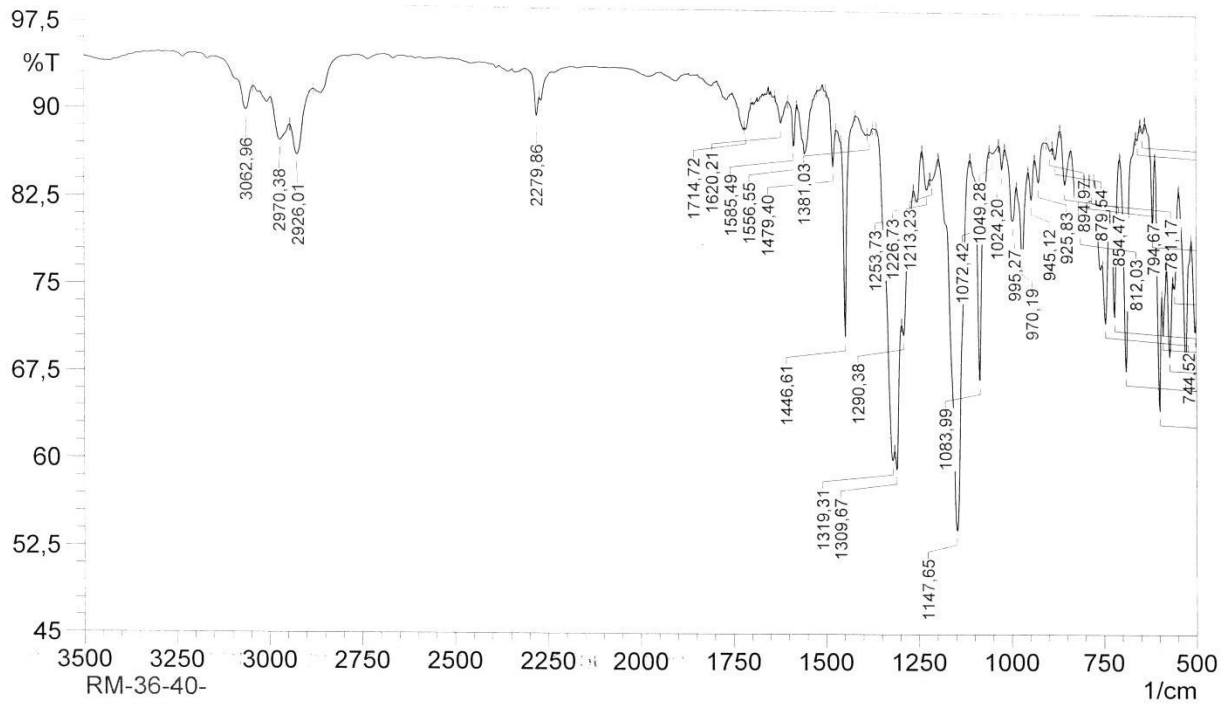




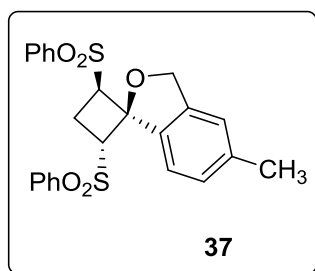
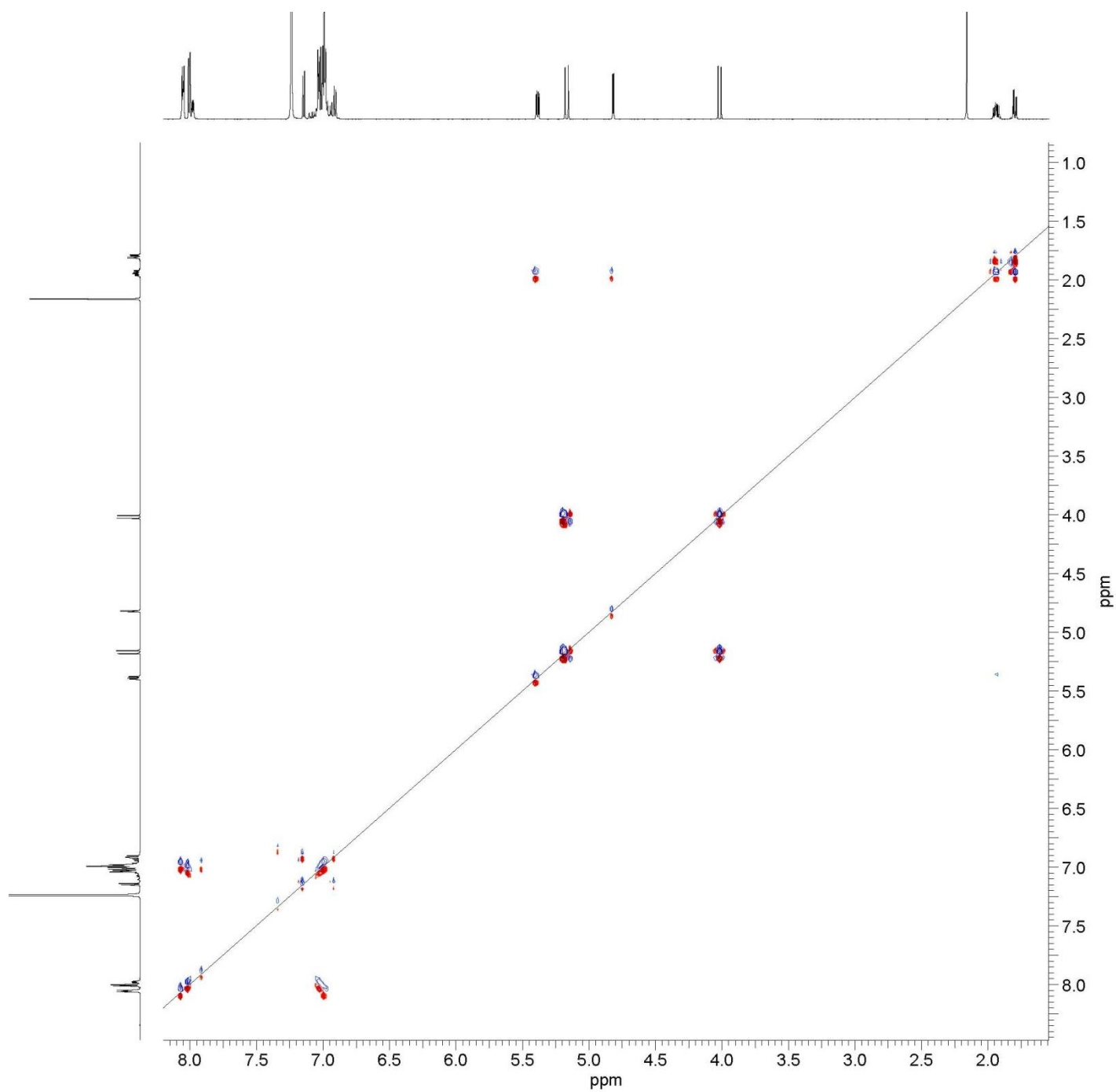


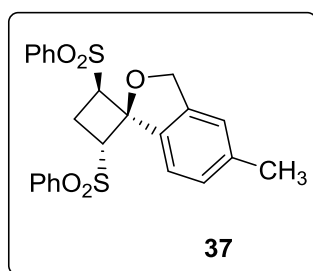
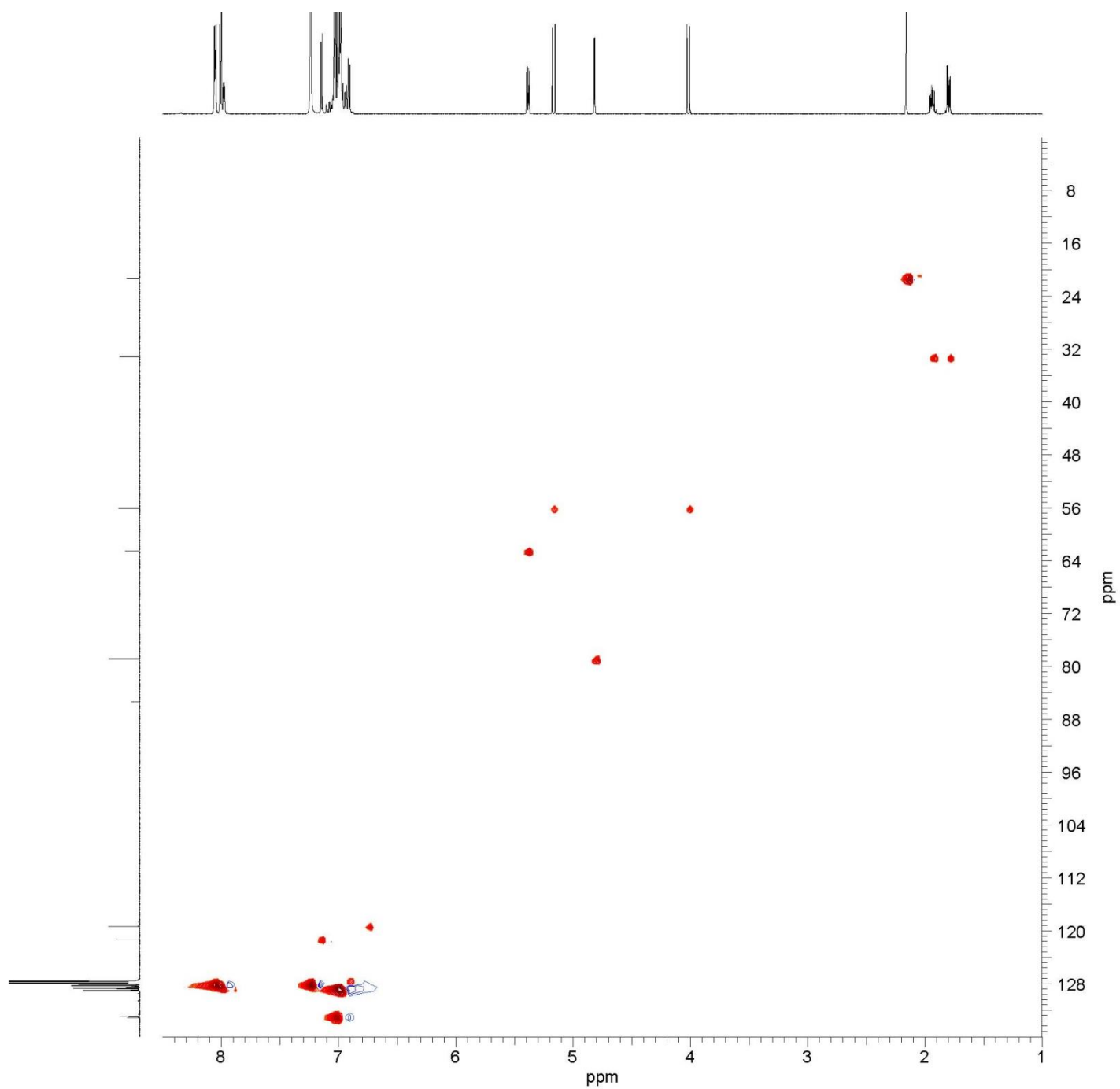


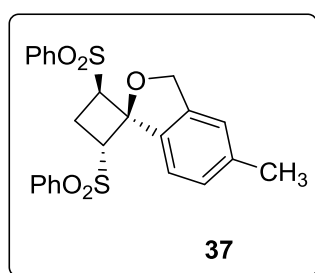
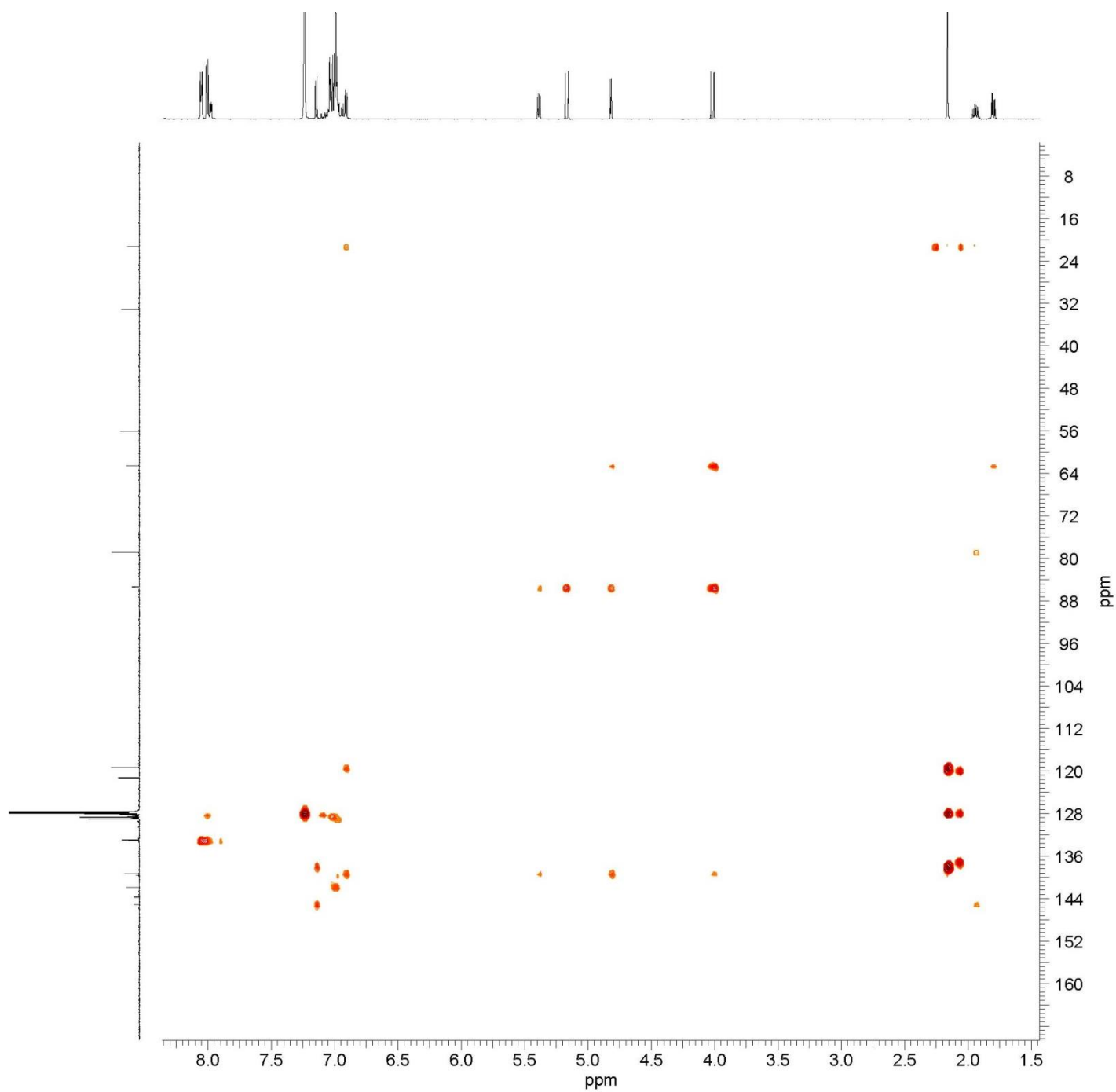
Full Spectroscopy

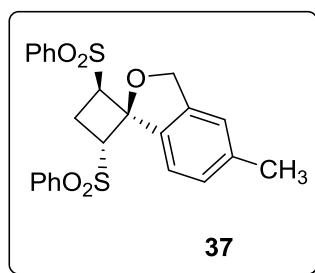
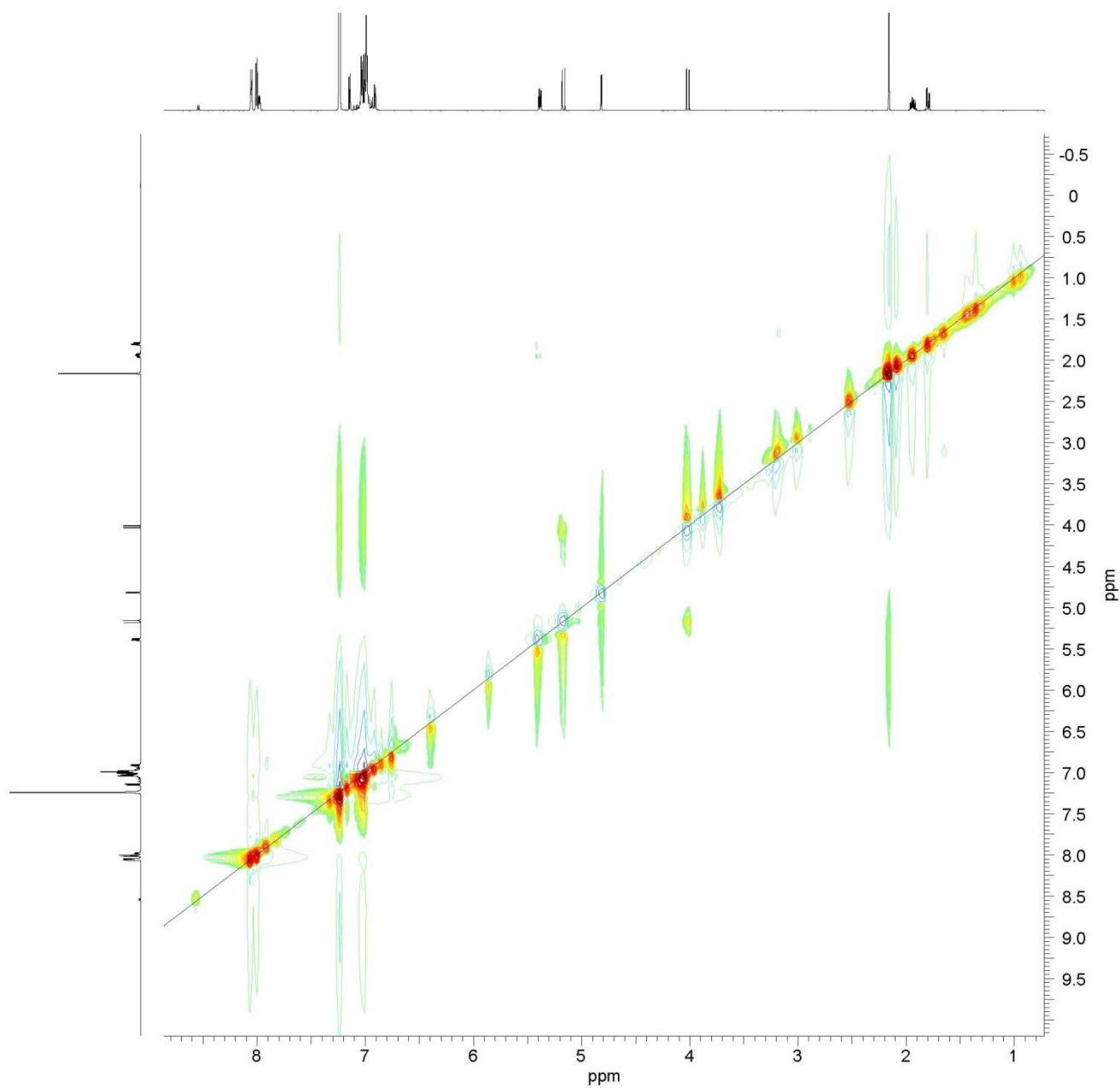


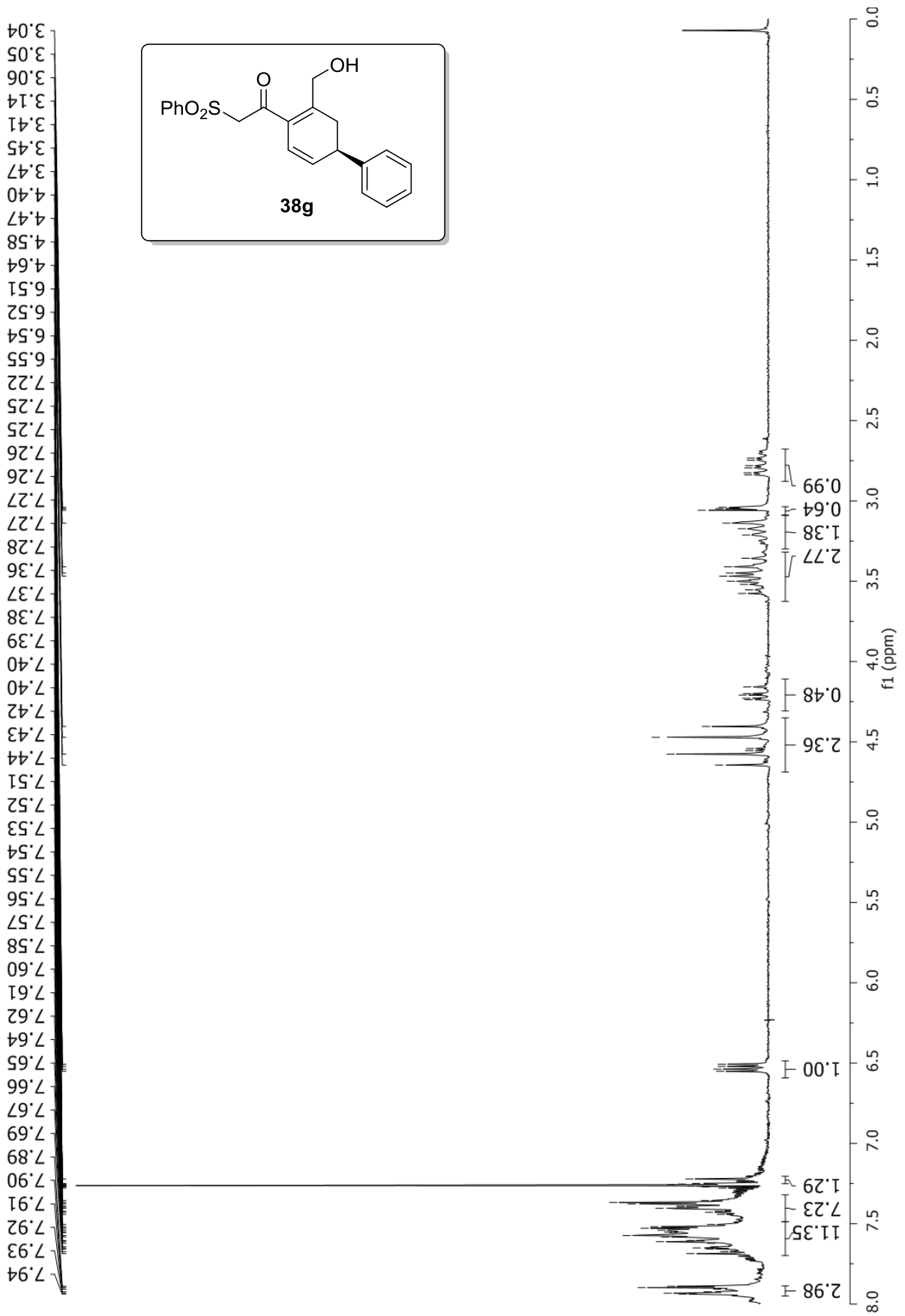
Formula	CalculatedMass	mDaError	ppmError	RDB
C10 H18 O9 Na	305.084304	0.2964	0.971532	1.5
C16 H17 O4 S	305.084207	0.39254	1.286657	8.5
C17 H13 N4 S	305.085545	-0.944772	-3.096749	13.5

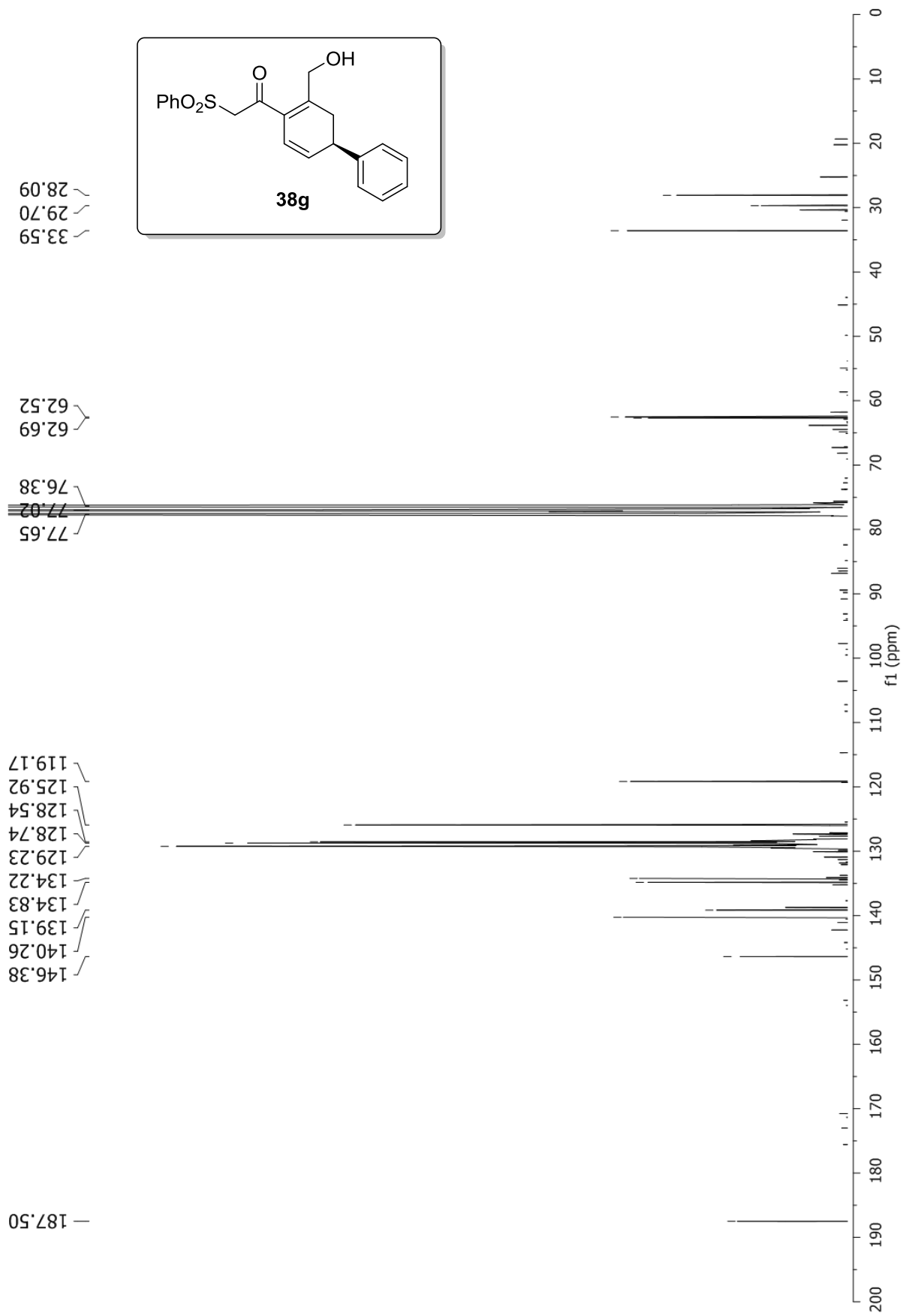


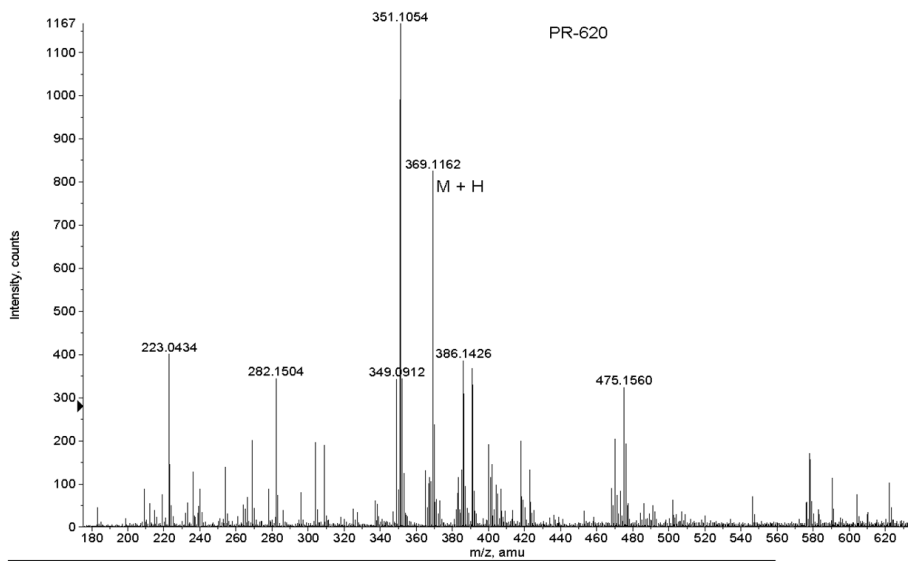
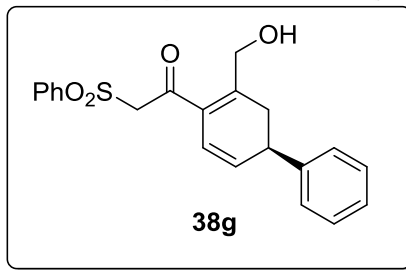
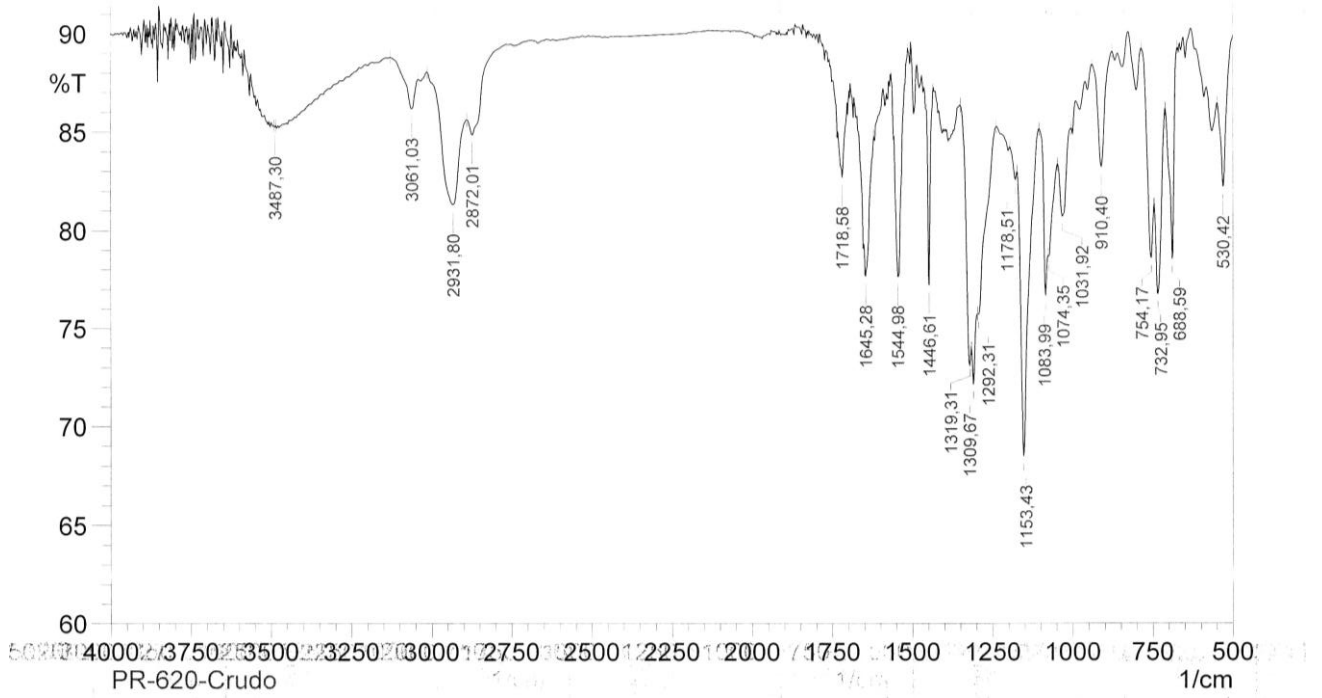




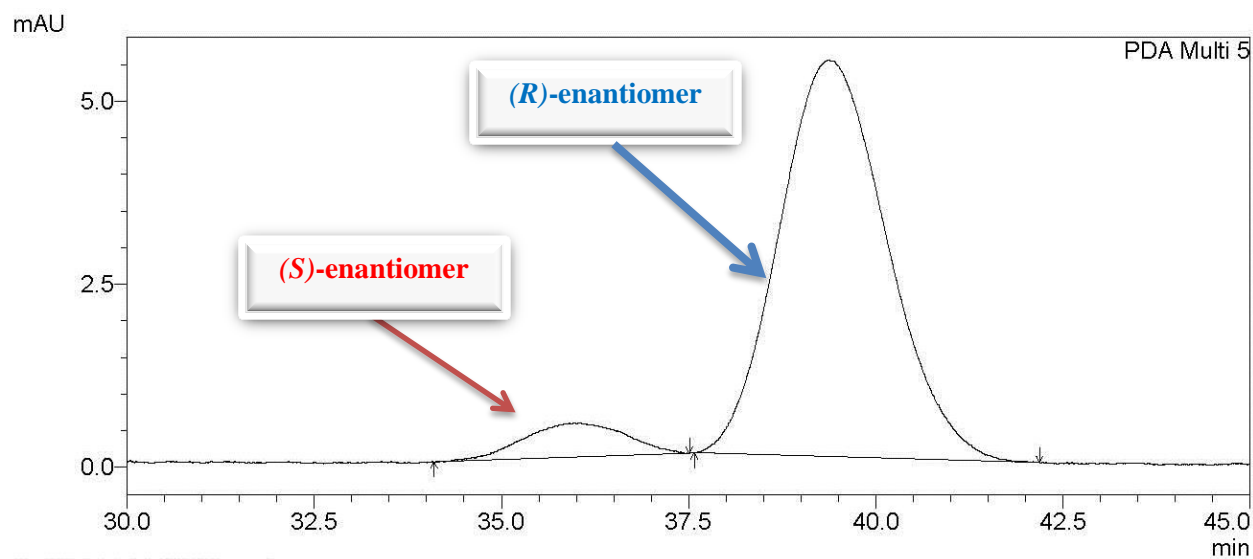








Formula	CalculatedMass	mDaError	ppmError	RDB
C22 H17 N4 S	369.116845	-0.644932	-1.74723	16.5
C21 H21 O4 S	369.115508	0.69238	1.875775	11.5

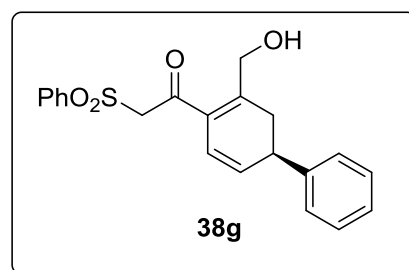


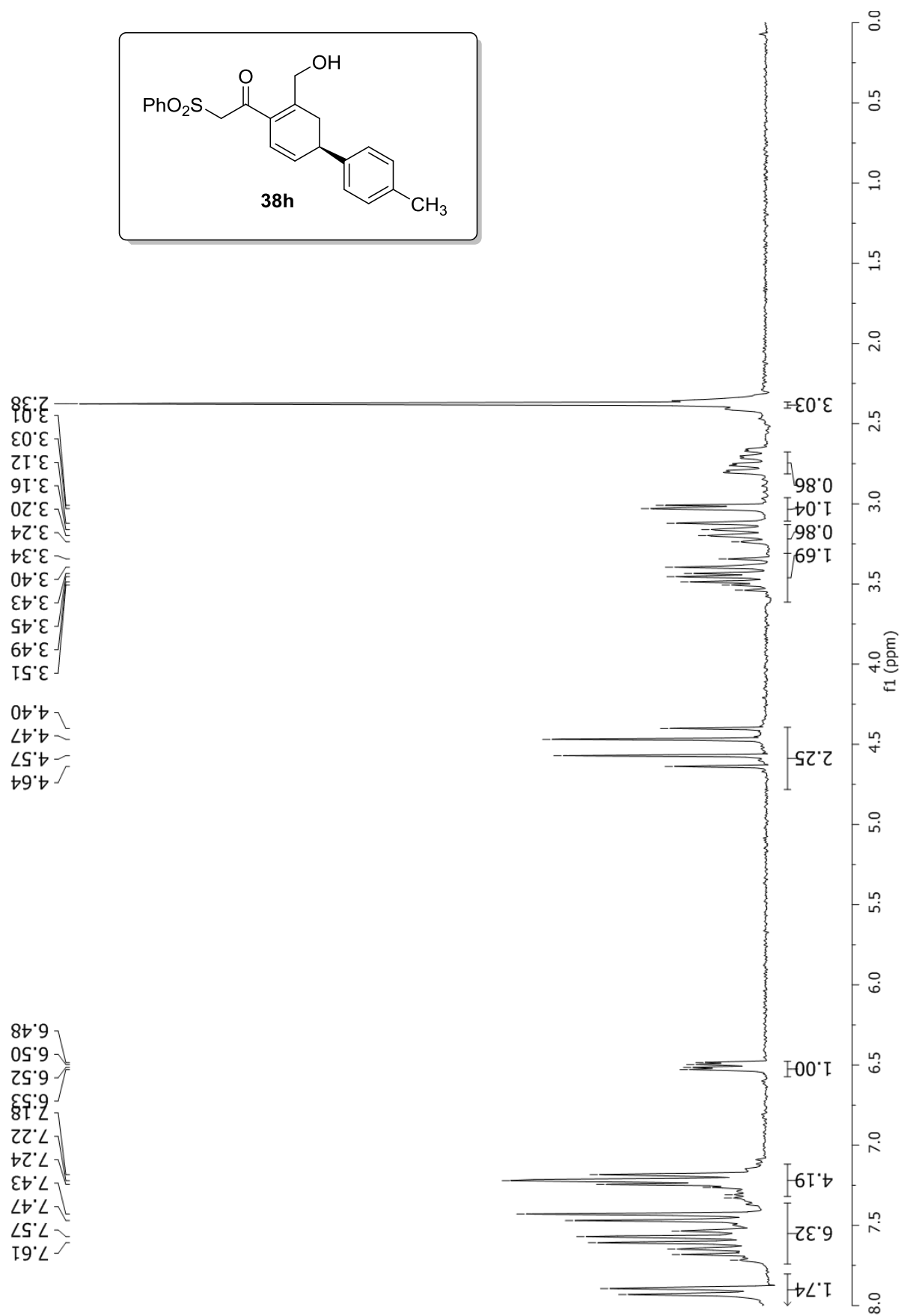
1 PDA Multi 5/430nm 4nm

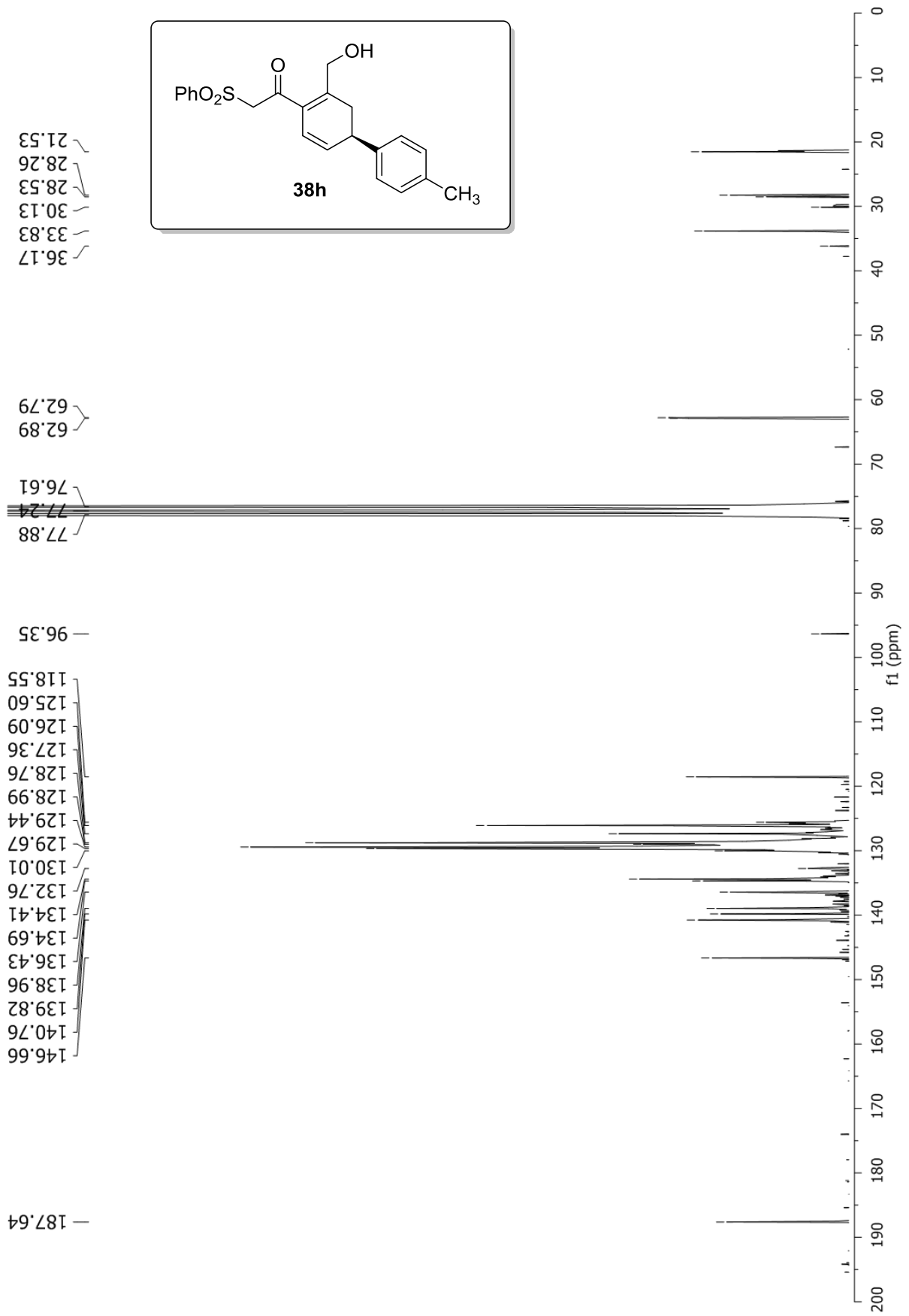
PeakTable

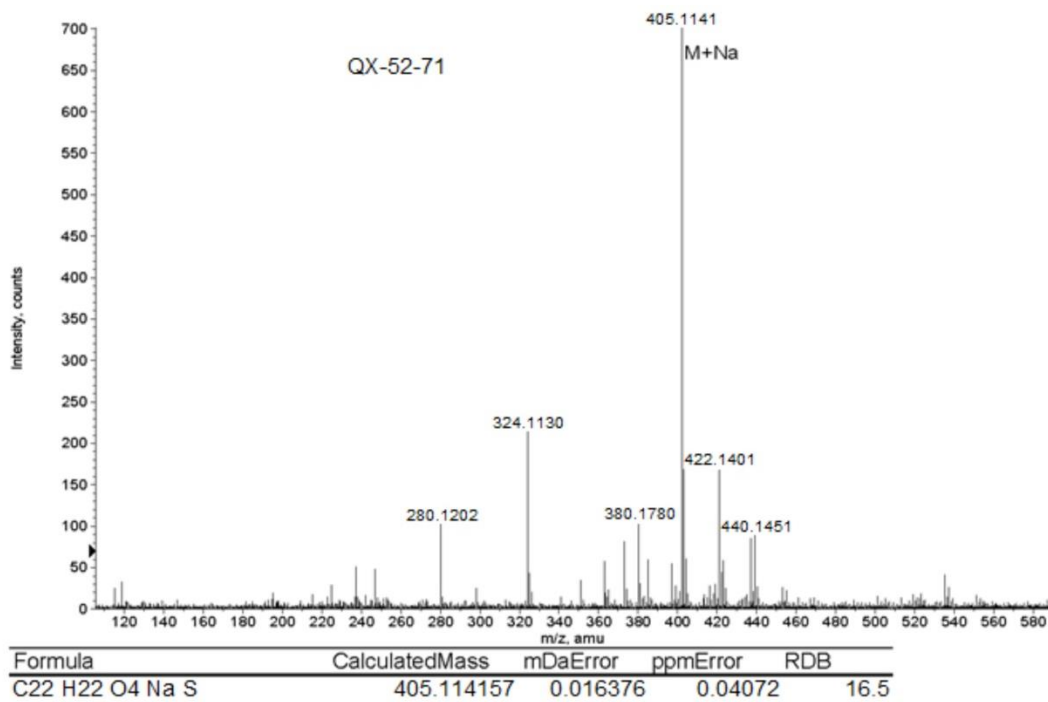
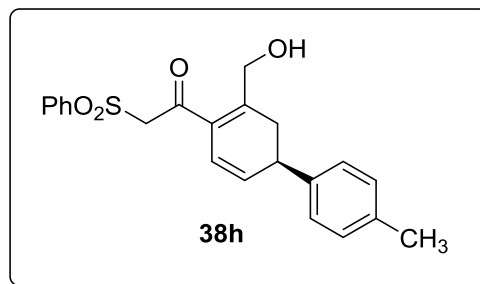
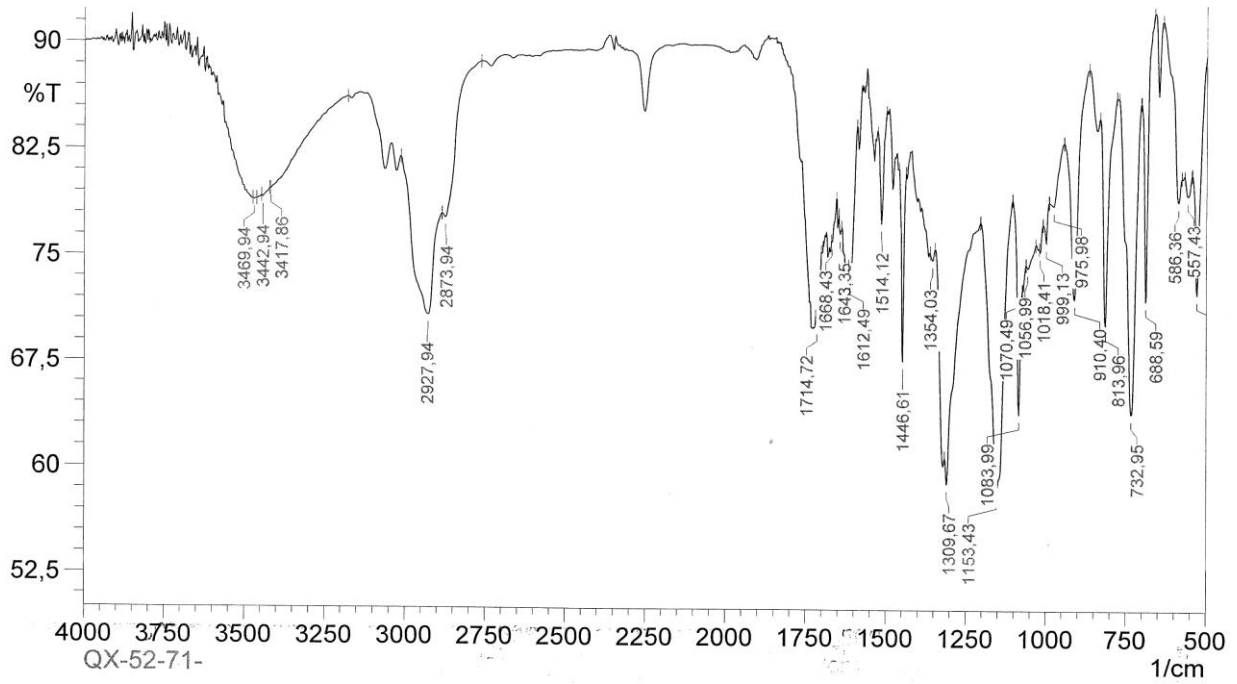
PDA Ch5 430nm 4nm

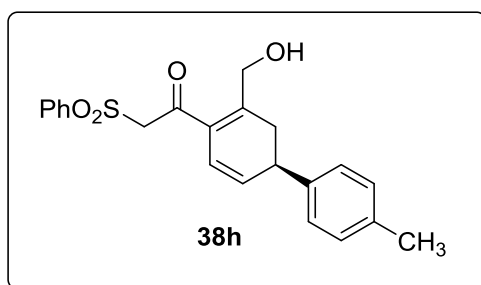
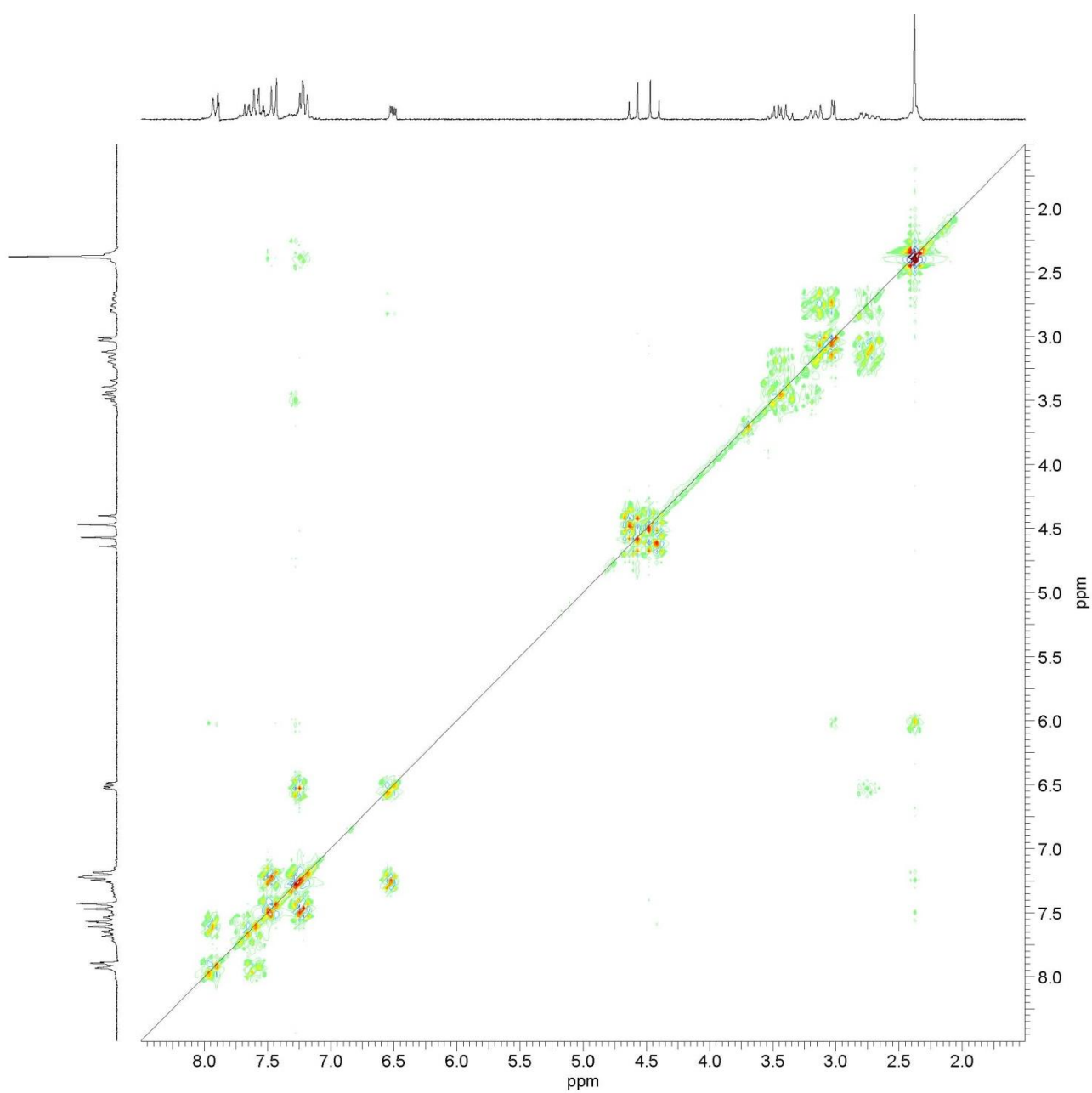
Peak#	Ret. Time	Area %
1	35.961	7.521
2	39.348	92.479
Total		100.000

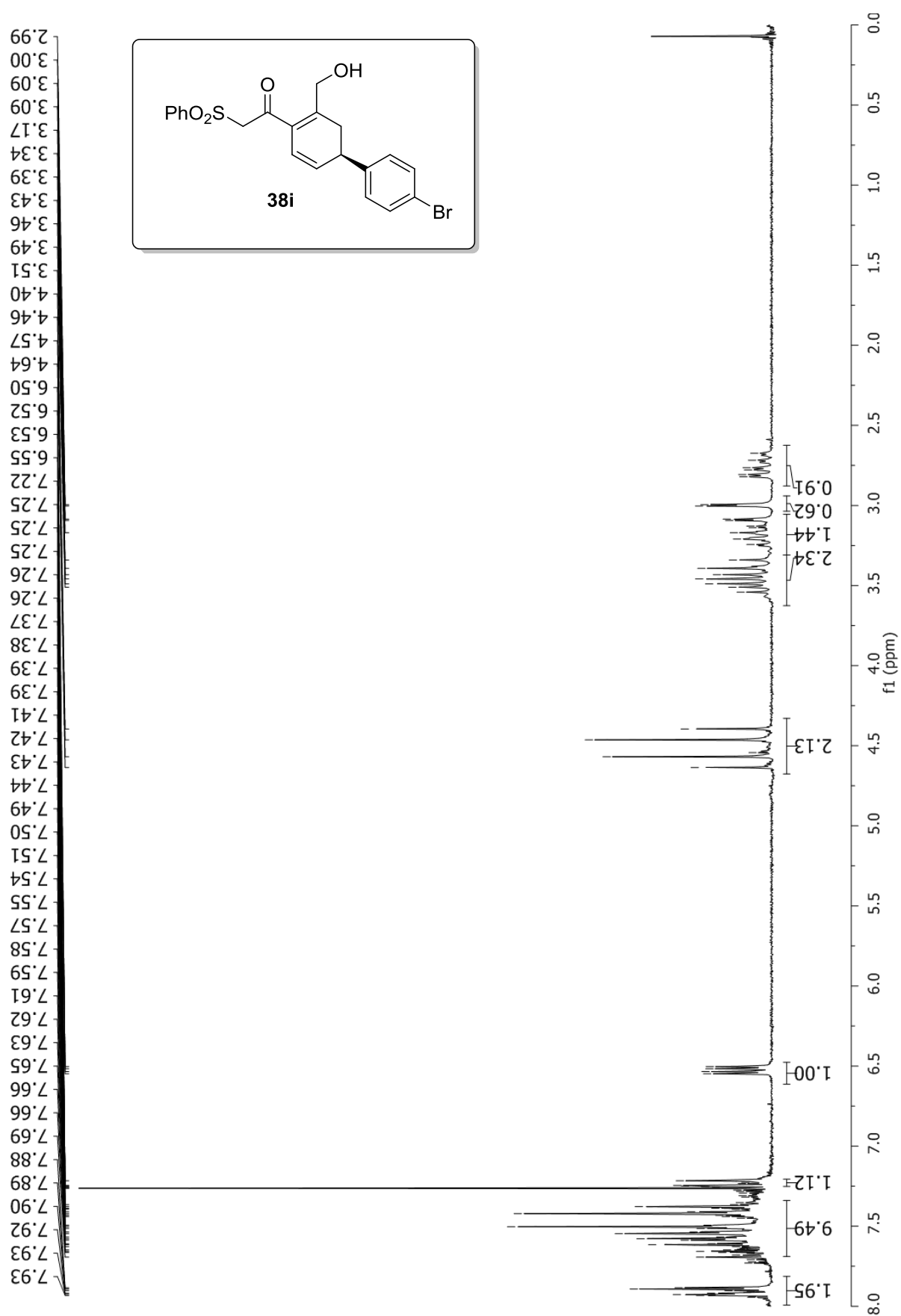


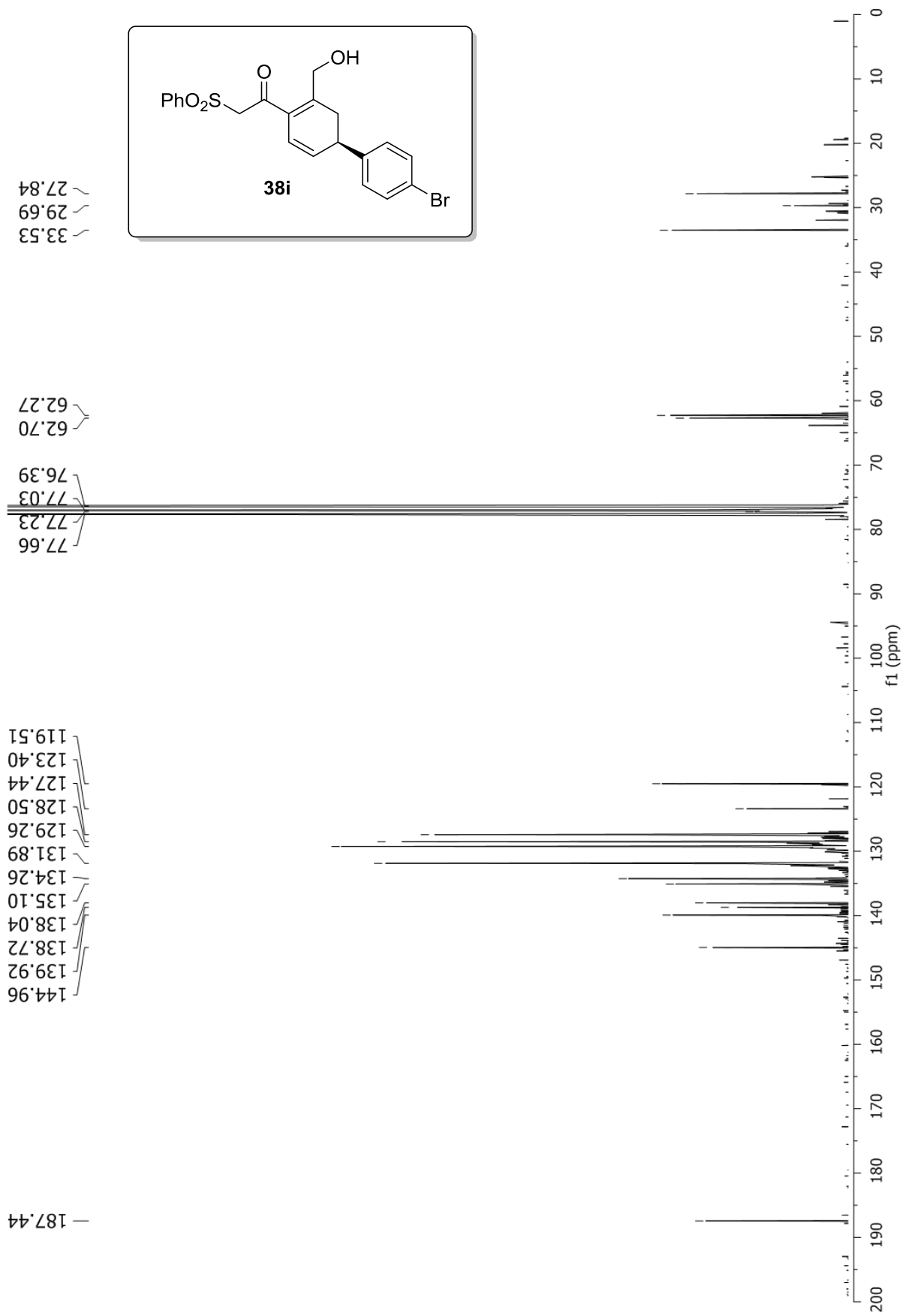


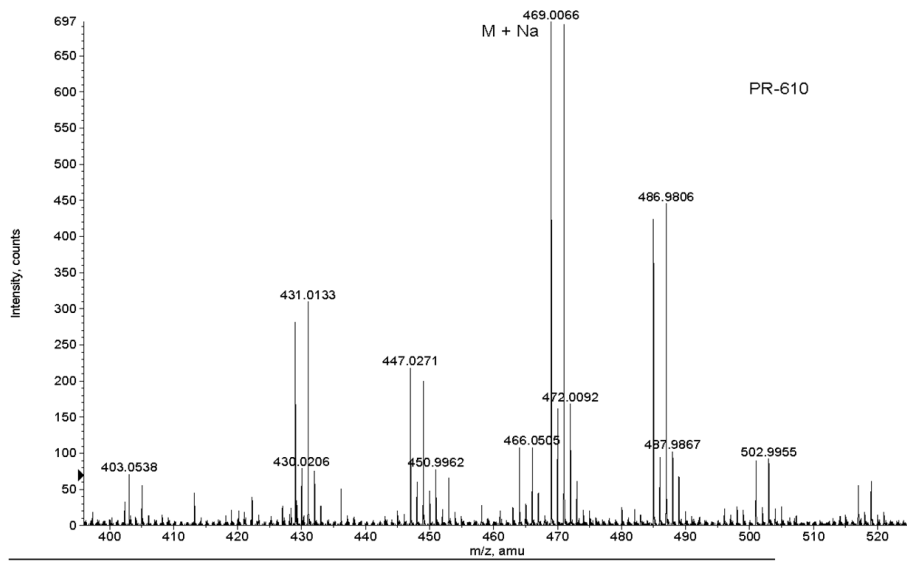
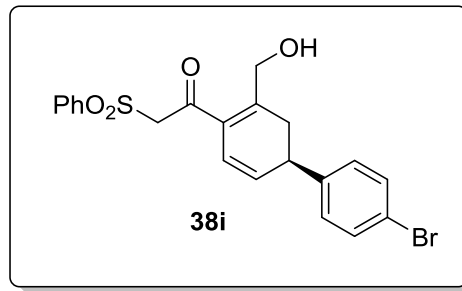
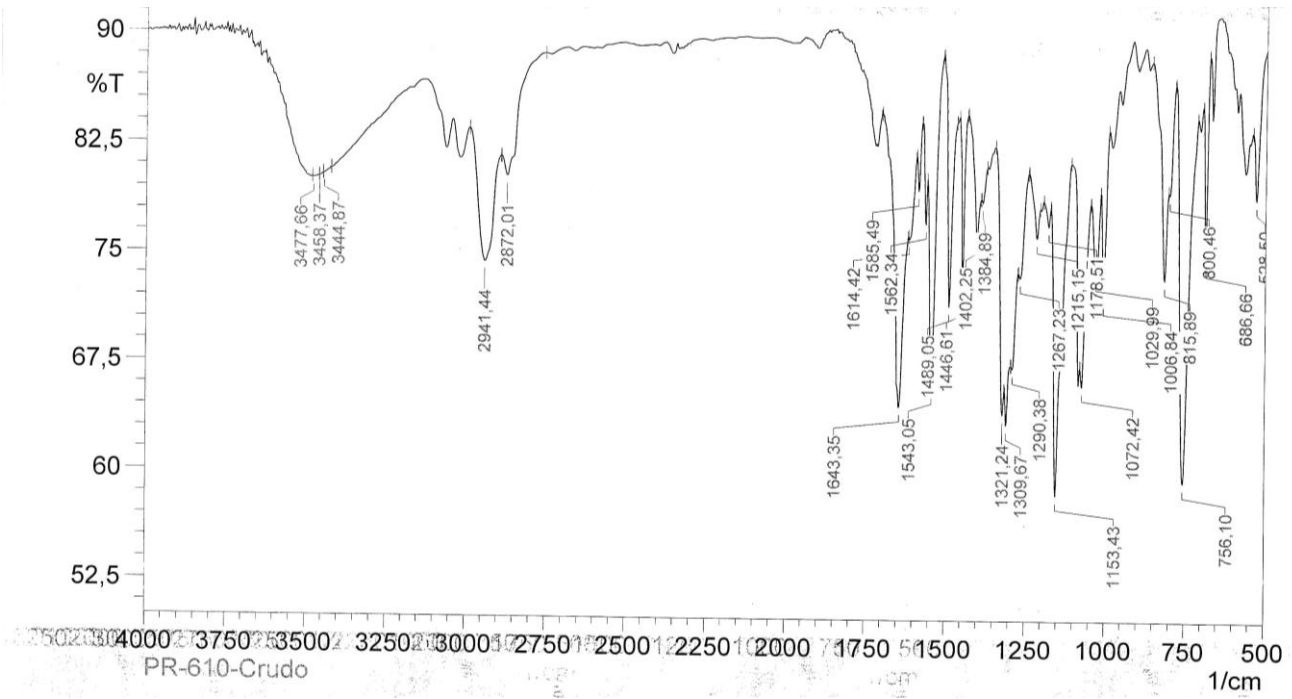




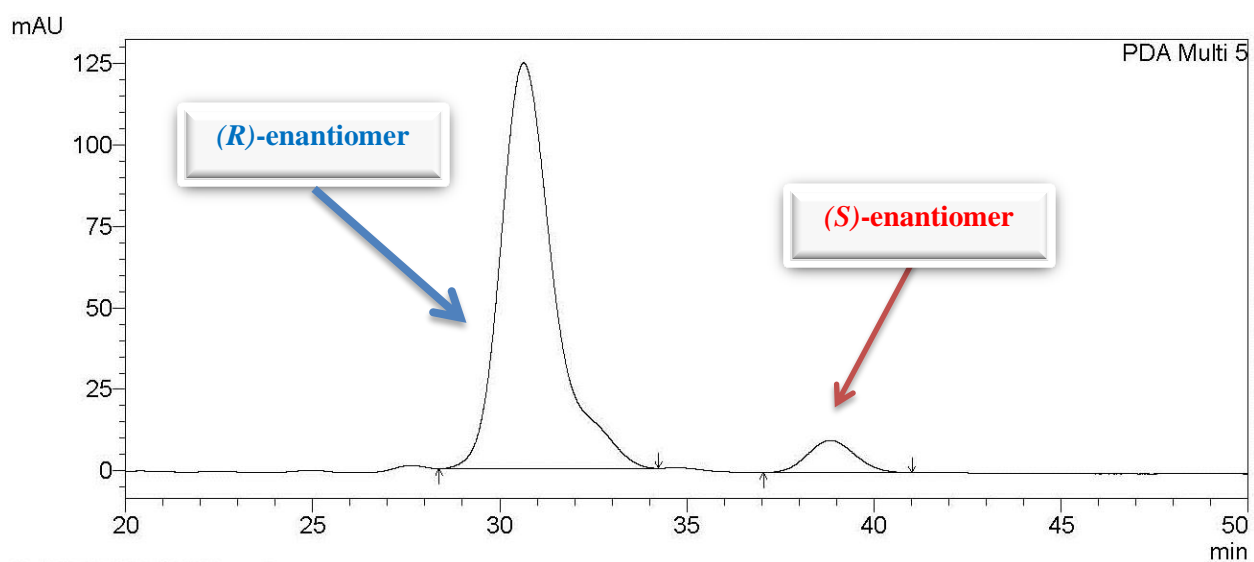








Formula	CalculatedMass	mDaError	ppmError	RDB
C18 H18 N2 O6 S Br	469.006346	0.254104	0.541791	10.5
C21 H19 O4 Na S Br	469.007963	-1.36334	-2.906864	11.5

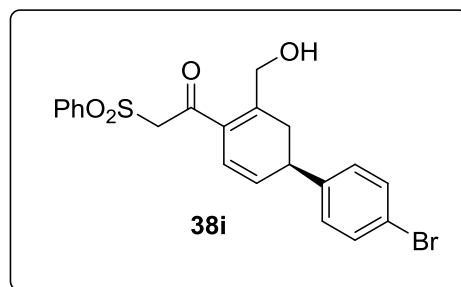


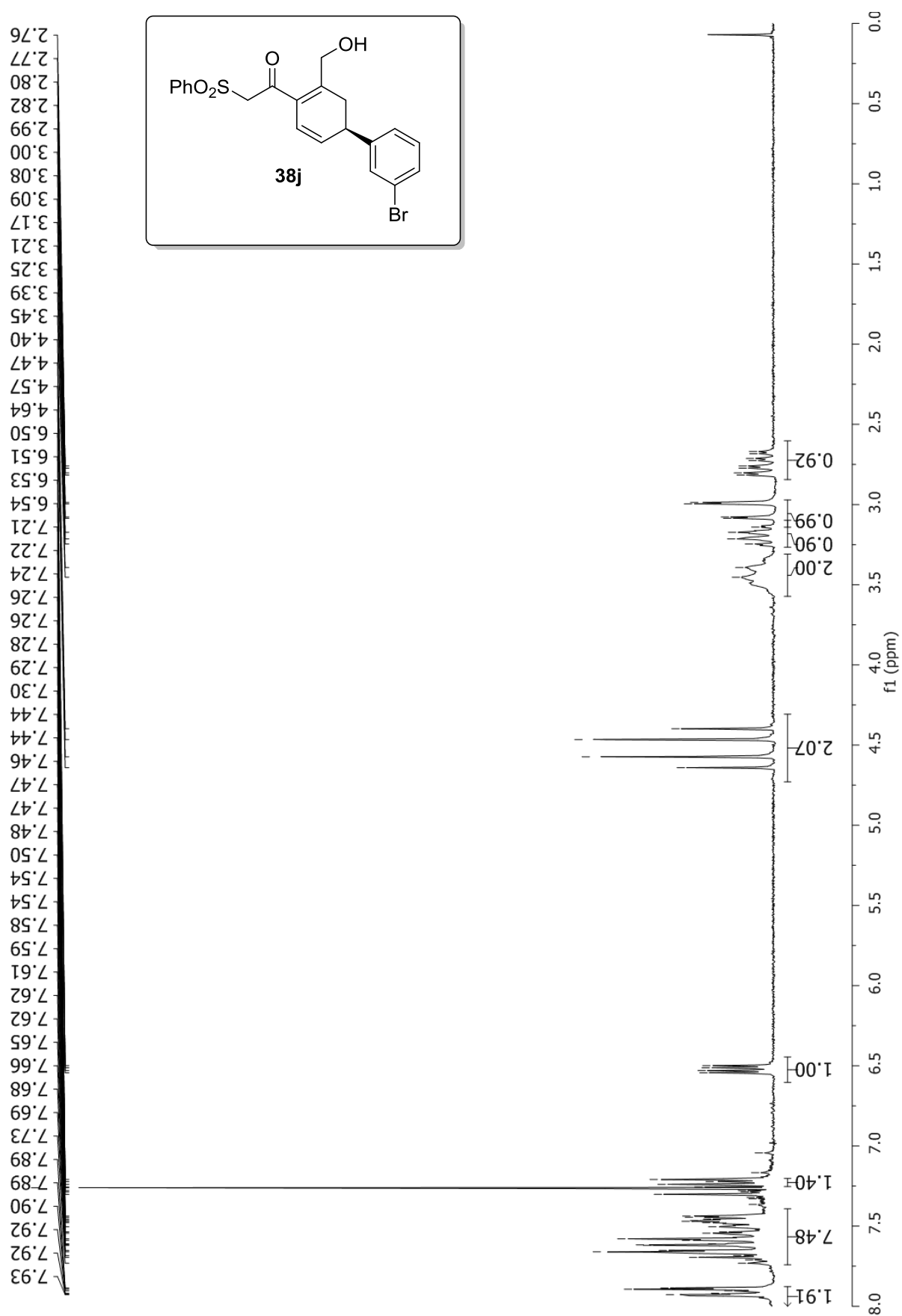
1 PDA Multi 5/350nm 4nm

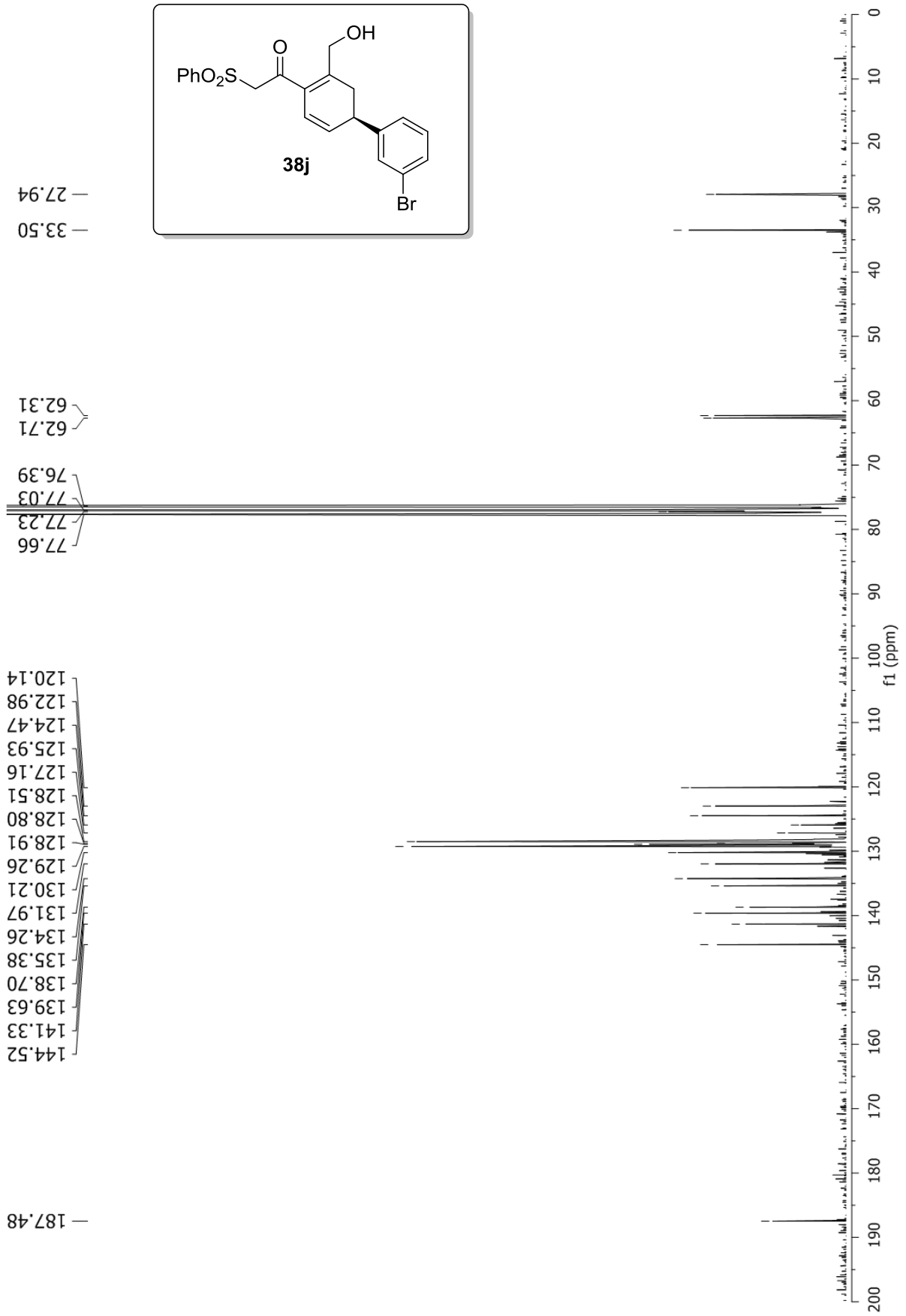
PeakTable

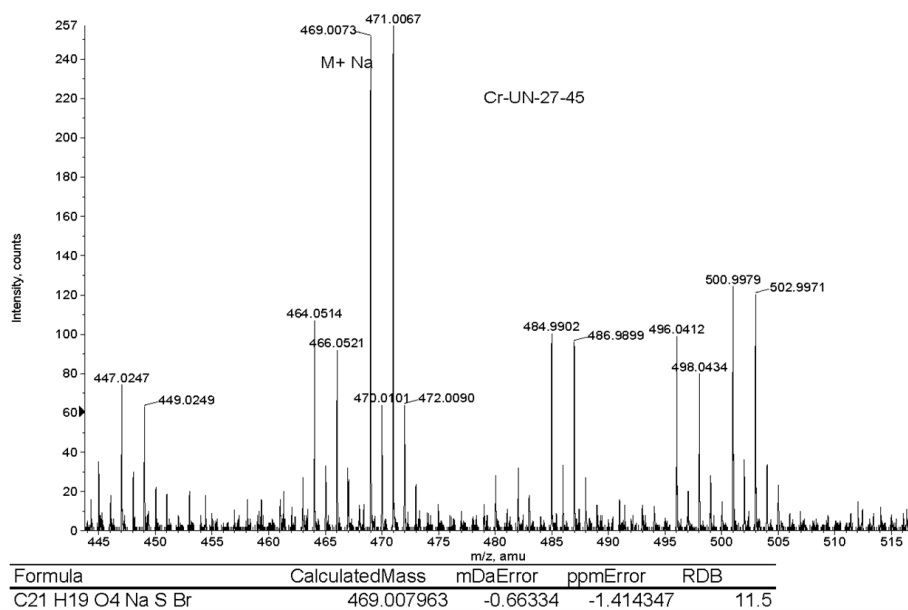
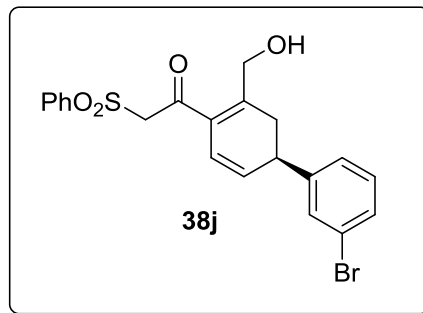
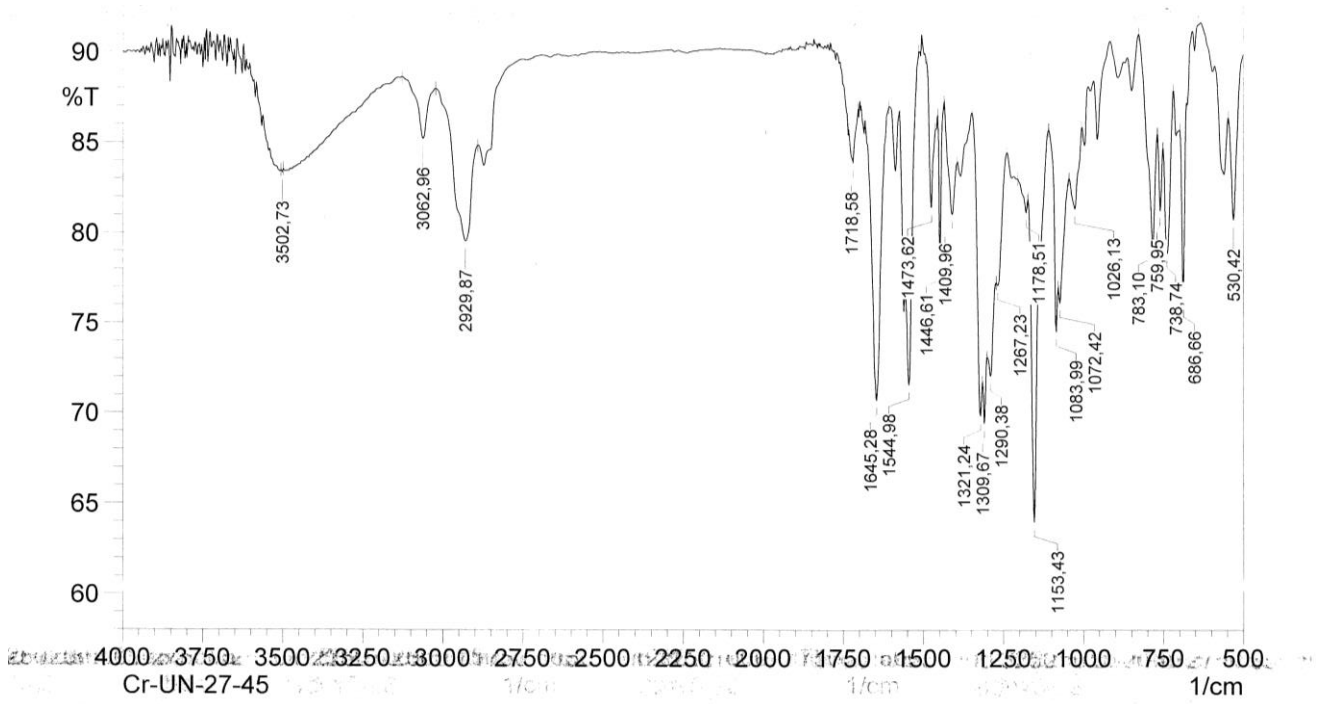
PDA Ch5 350nm 4nm

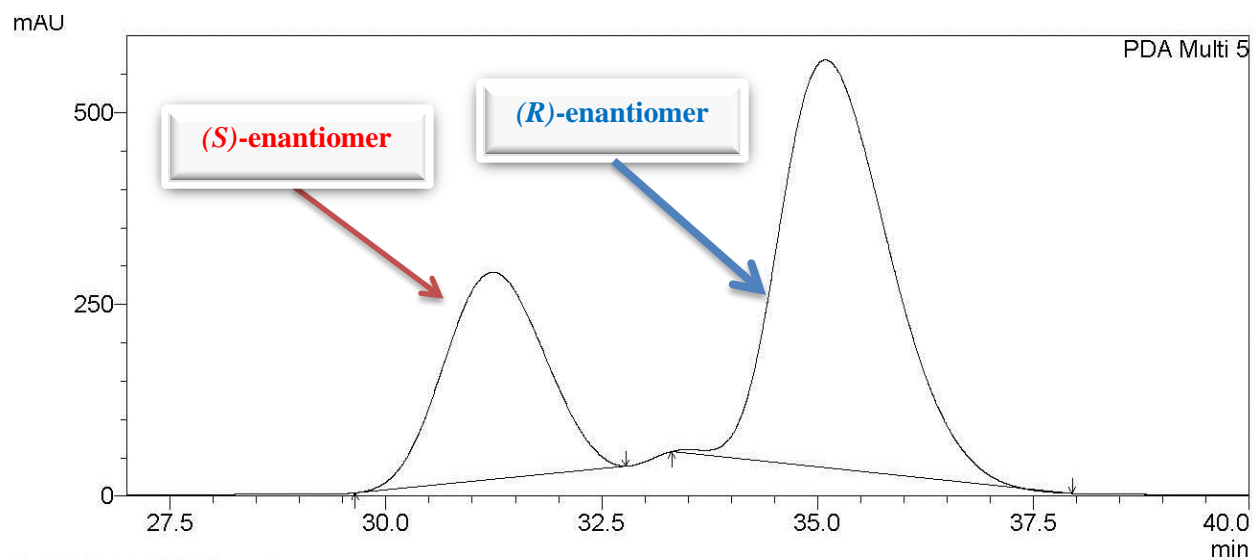
Peak#	Ret. Time	Area %
1	30.637	93.376
2	38.849	6.624
Total		100.000









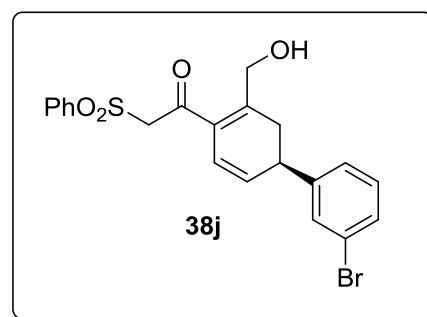


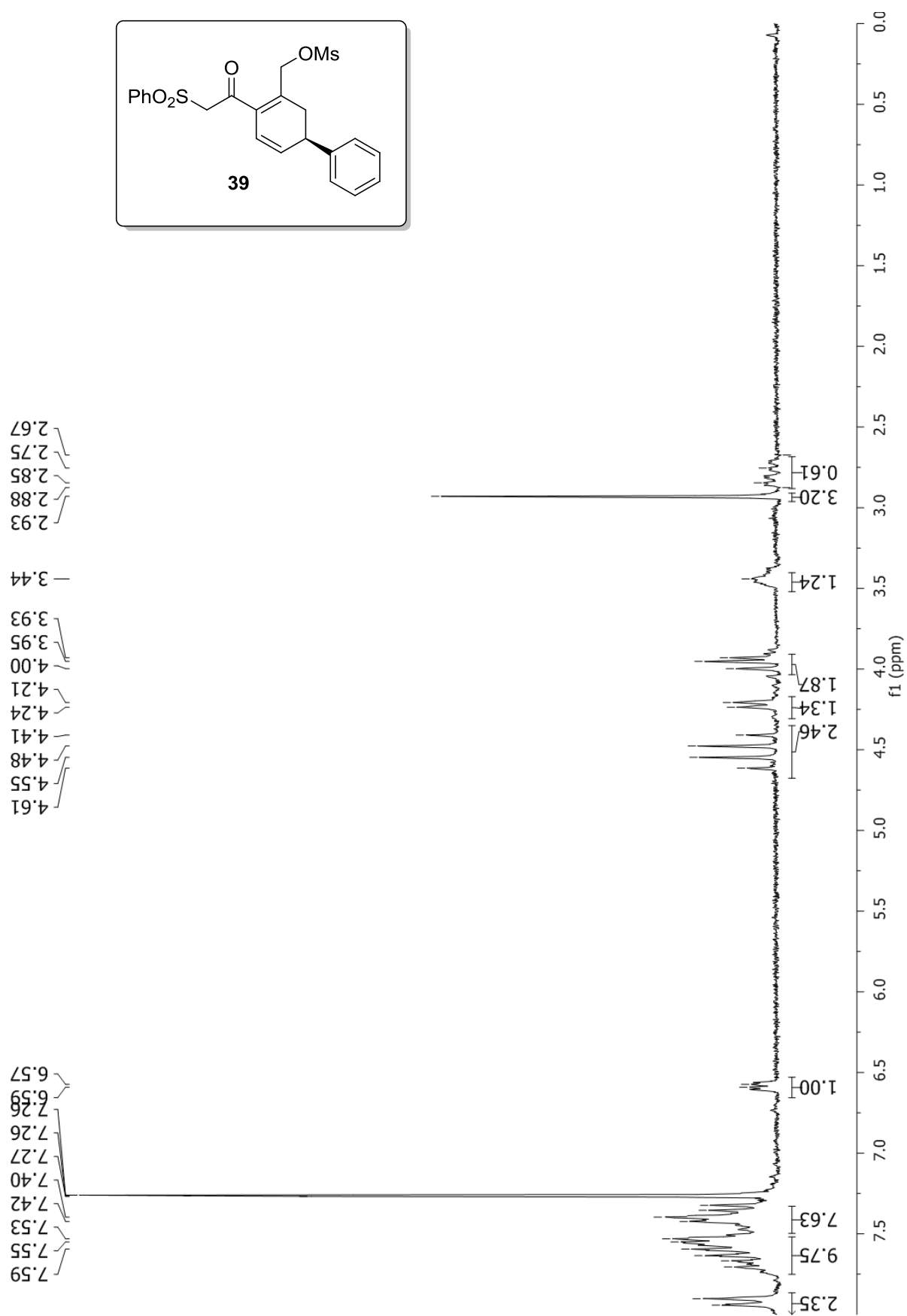
1 PDA Multi 5/360nm 4nm

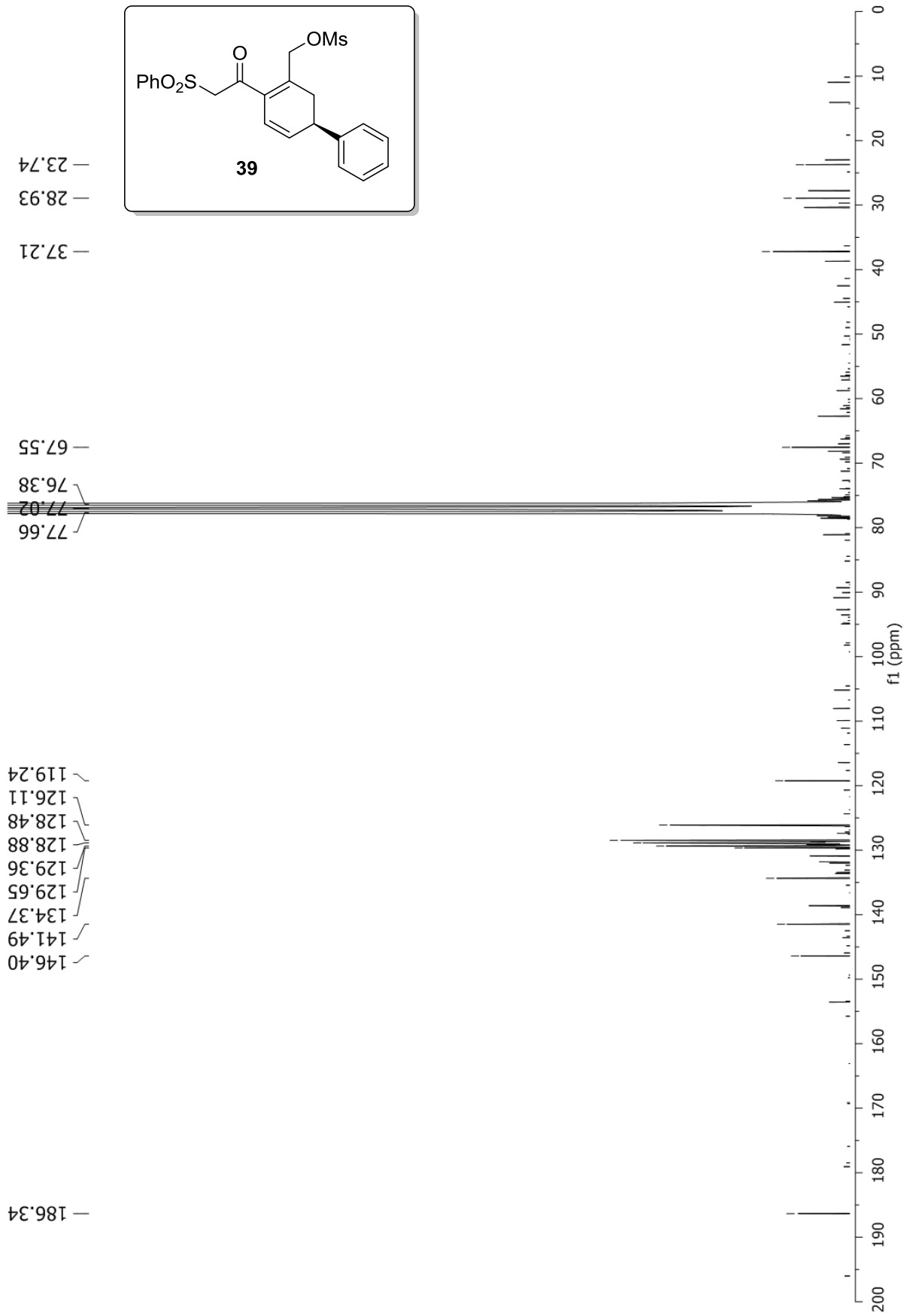
PeakTable

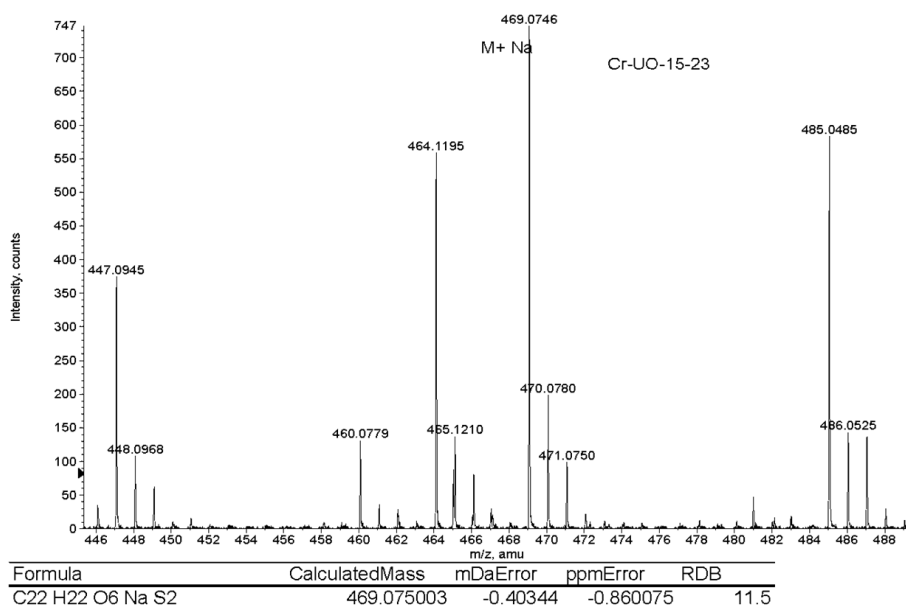
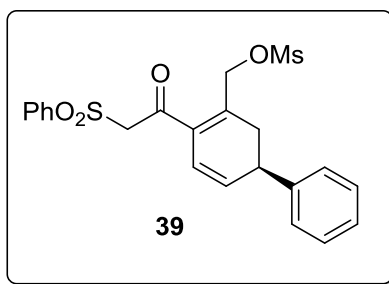
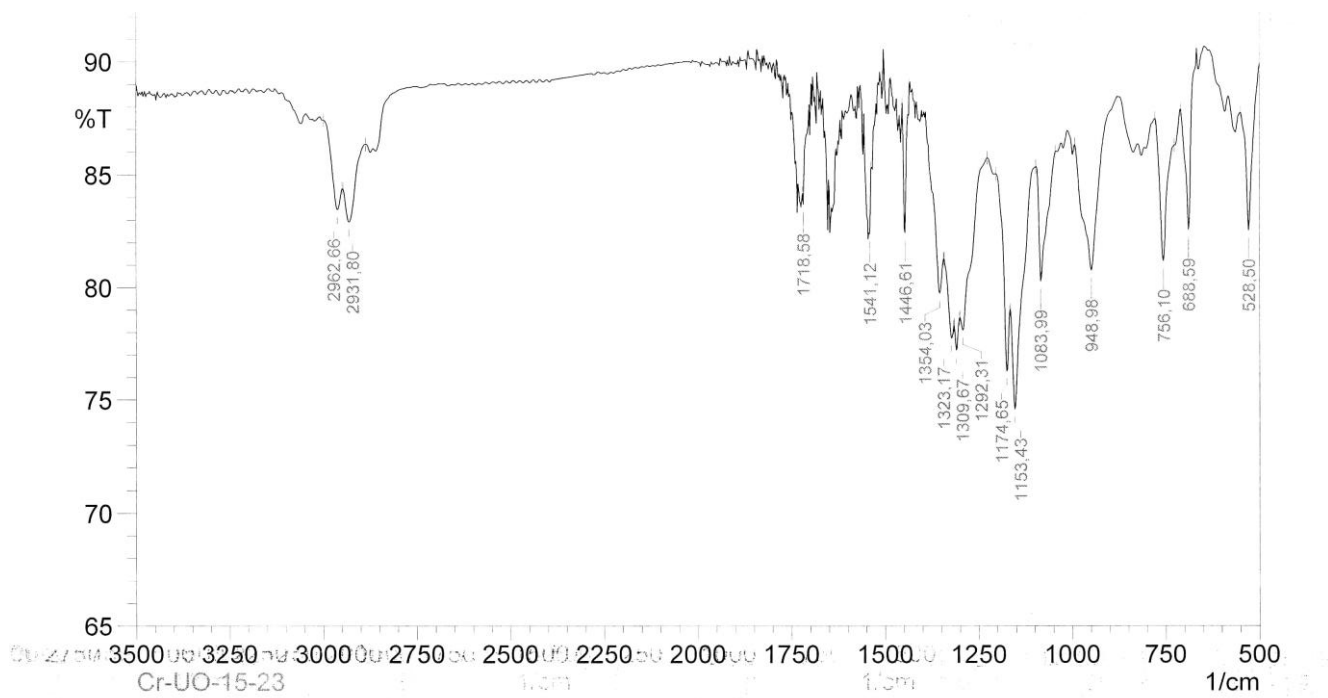
PDA Ch5 360nm 4nm

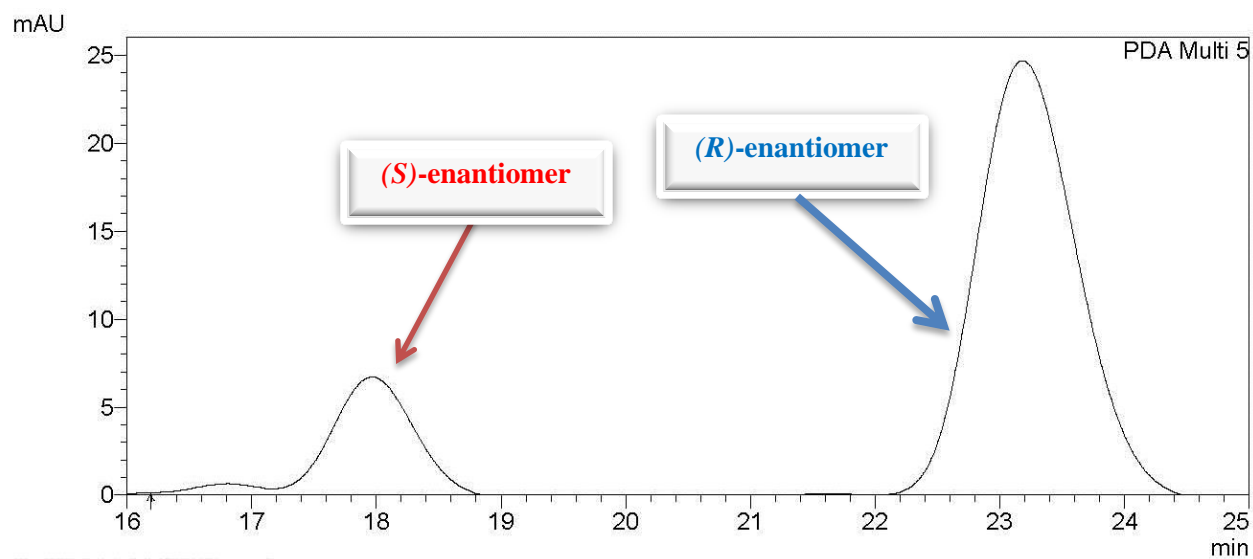
Peak#	Ret. Time	Area %
1	31.235	31.871
2	35.088	68.129
Total		100.000









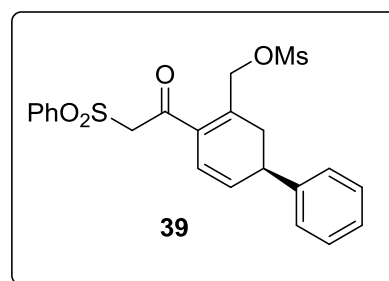


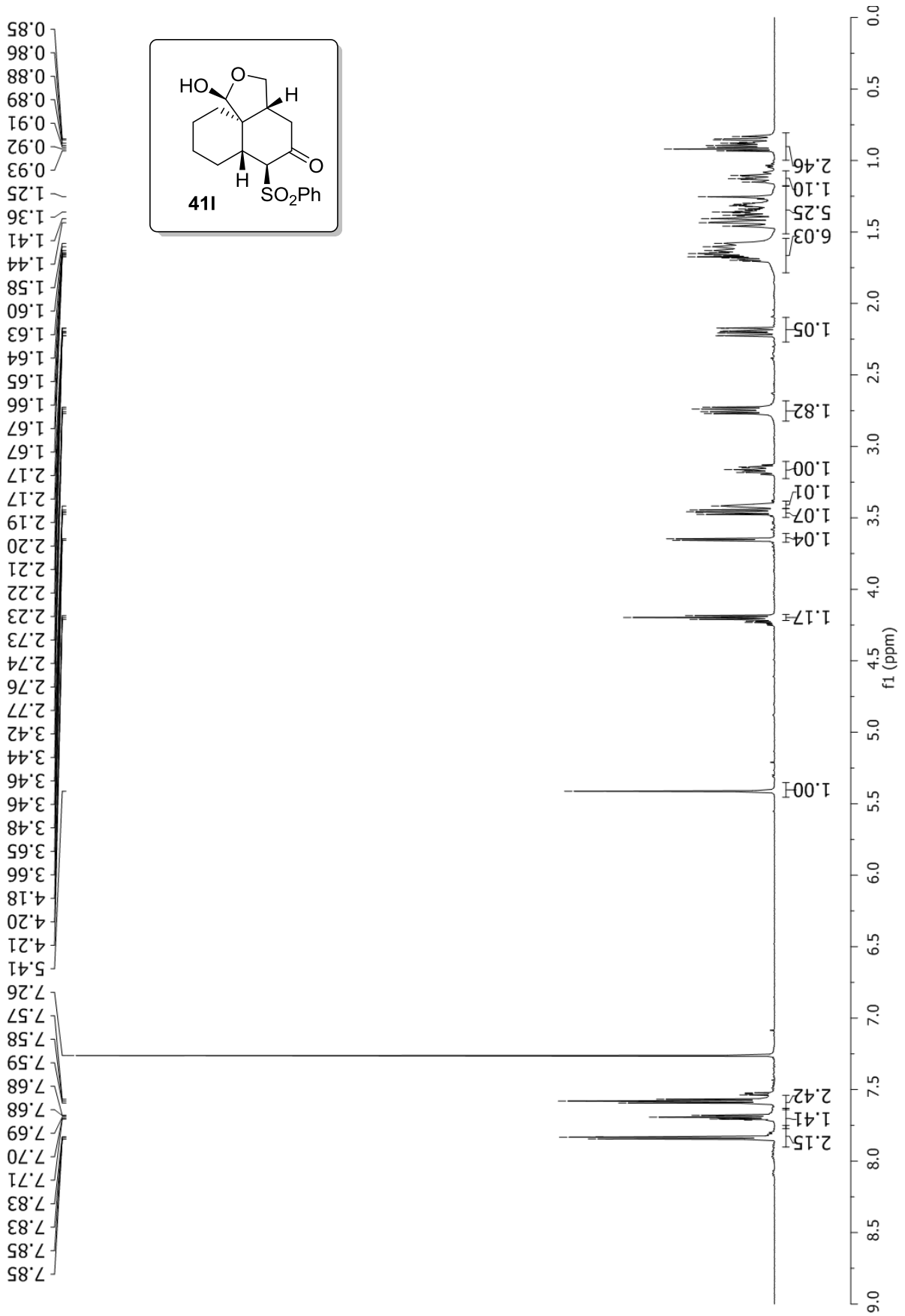
1 PDA Multi 5/325nm 4nm

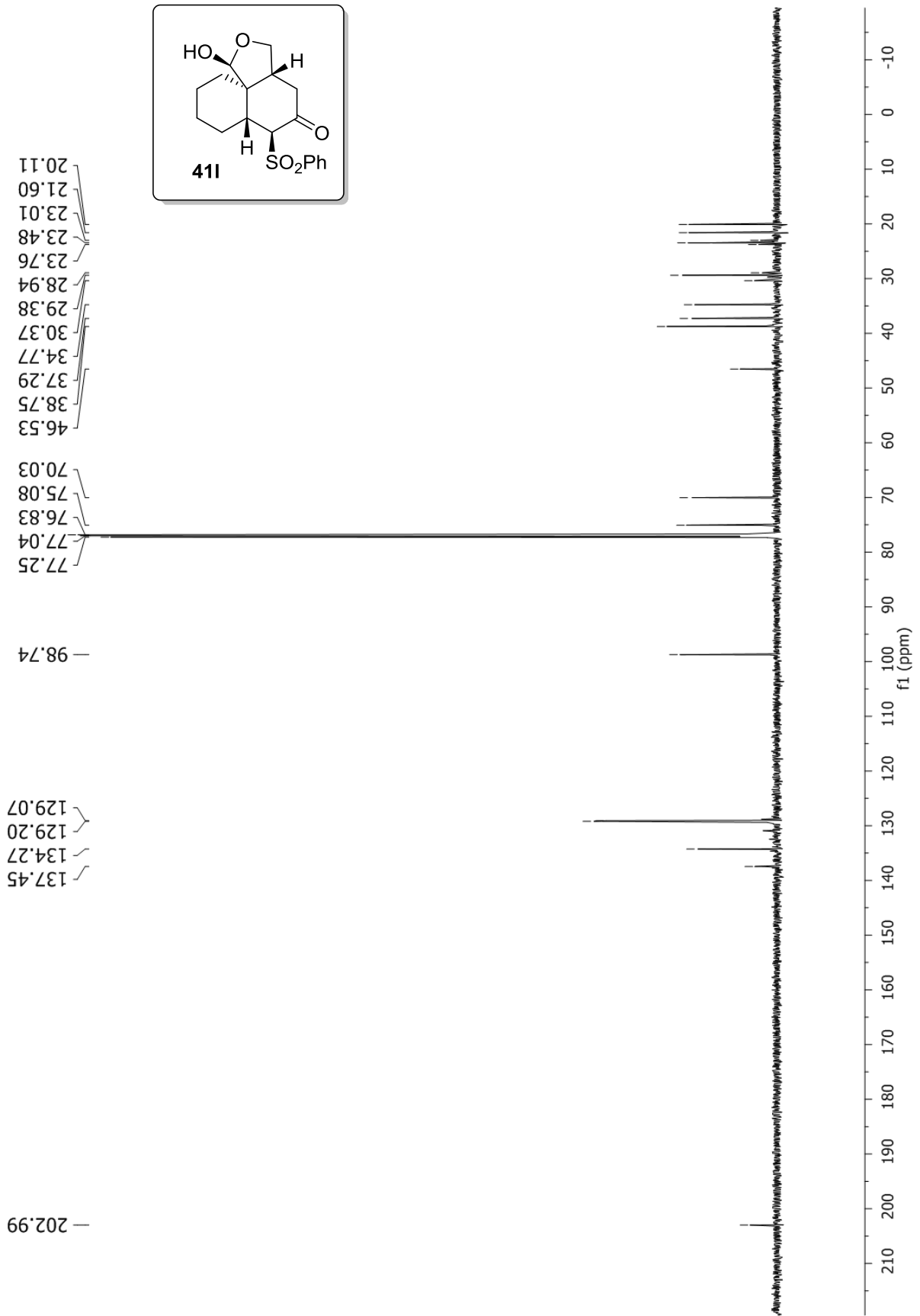
PeakTable

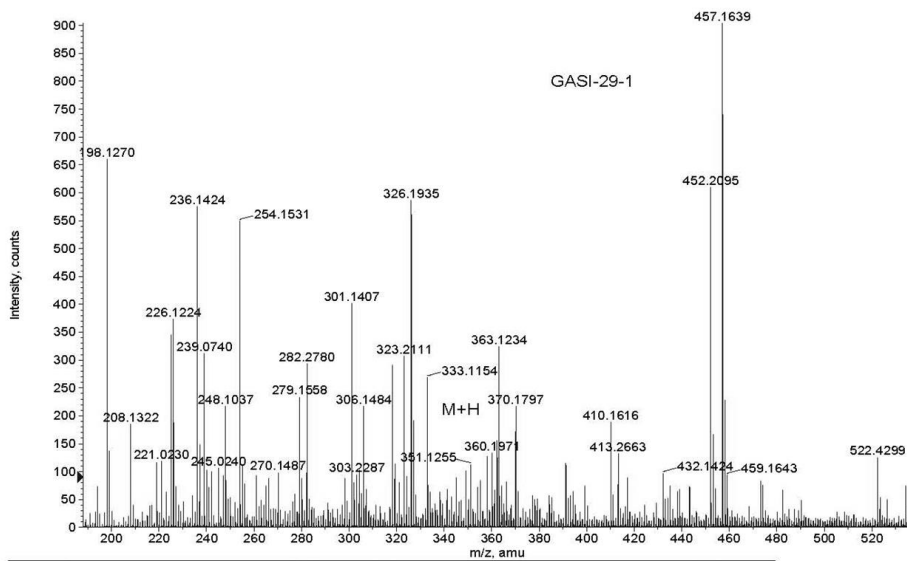
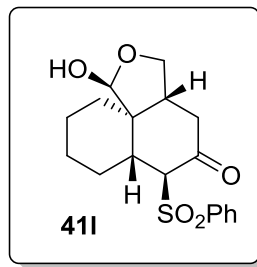
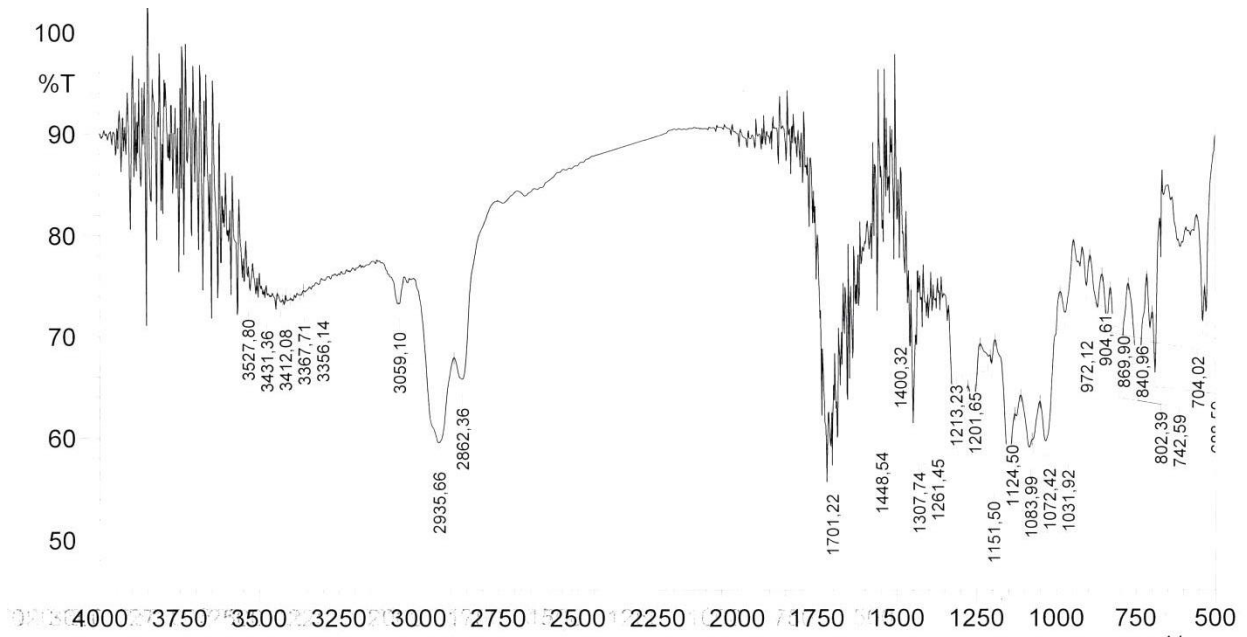
PDA Ch5 325nm 4nm

Peak#	Ret. Time	Area %
1	17.968	18.963
2	23.177	81.037
Total		100.000

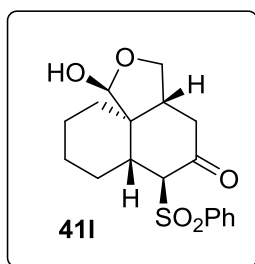
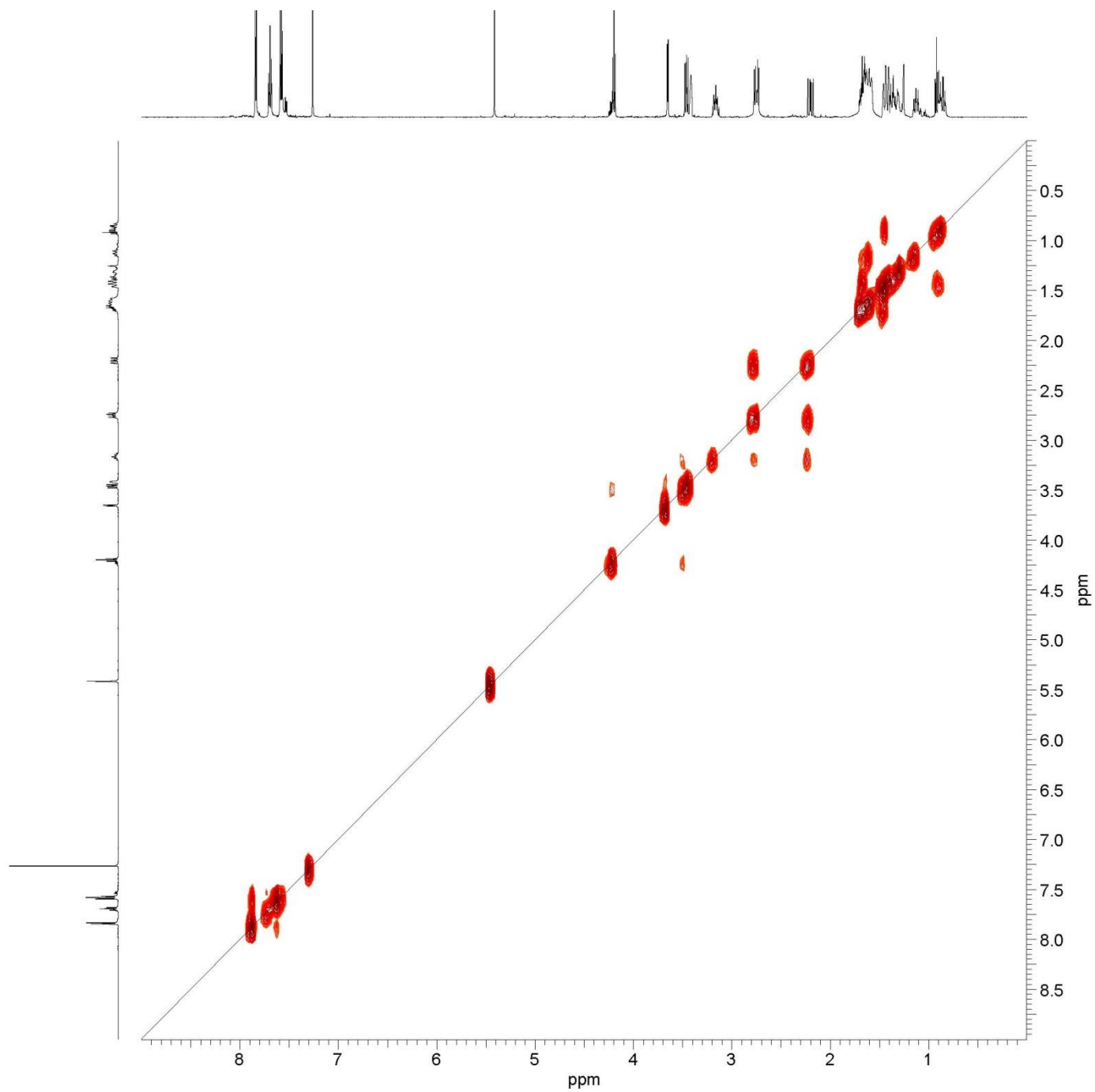


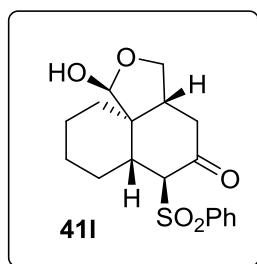
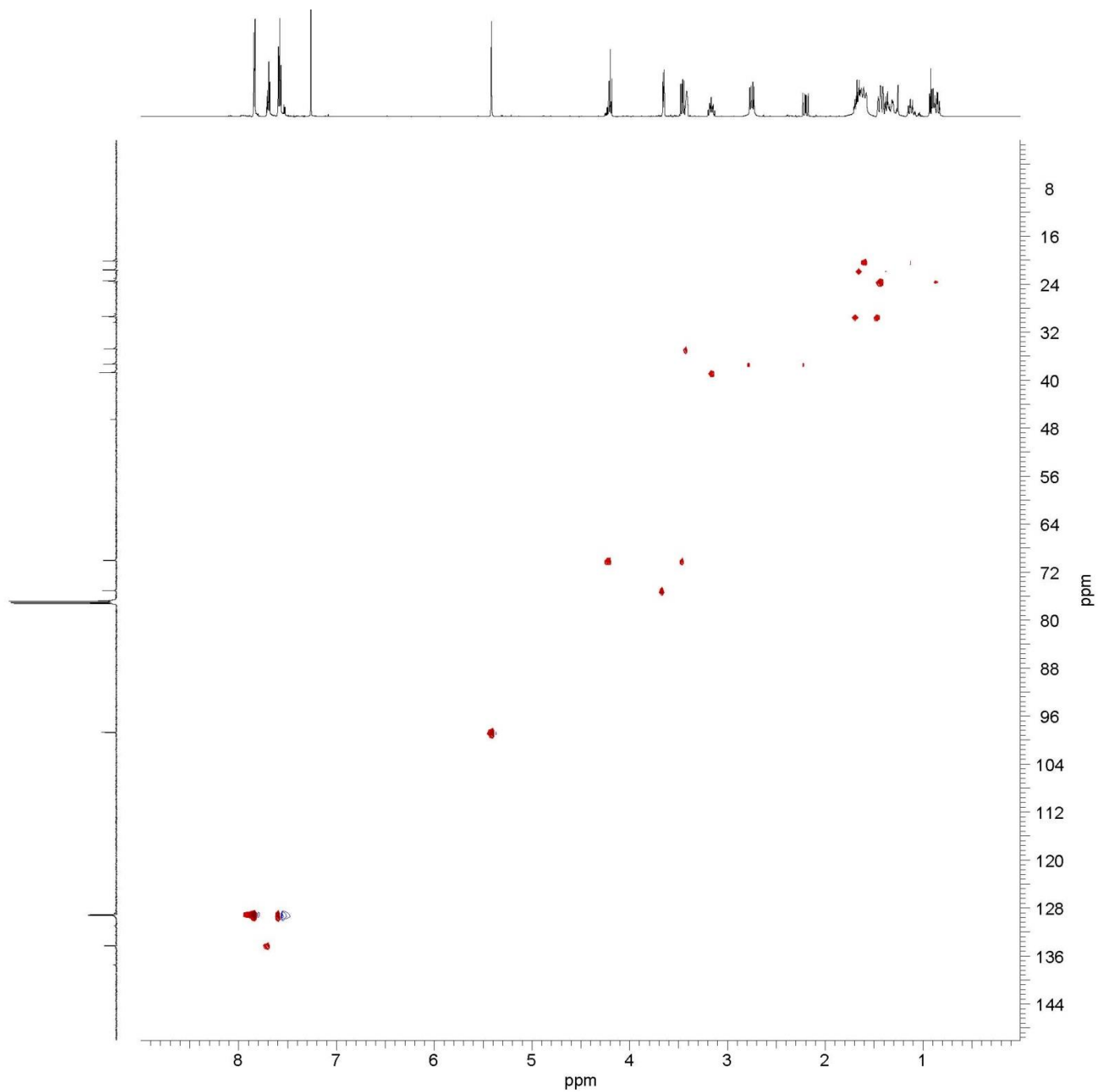


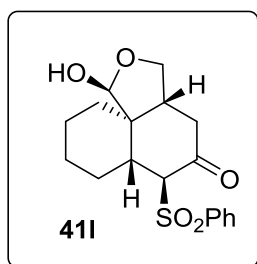
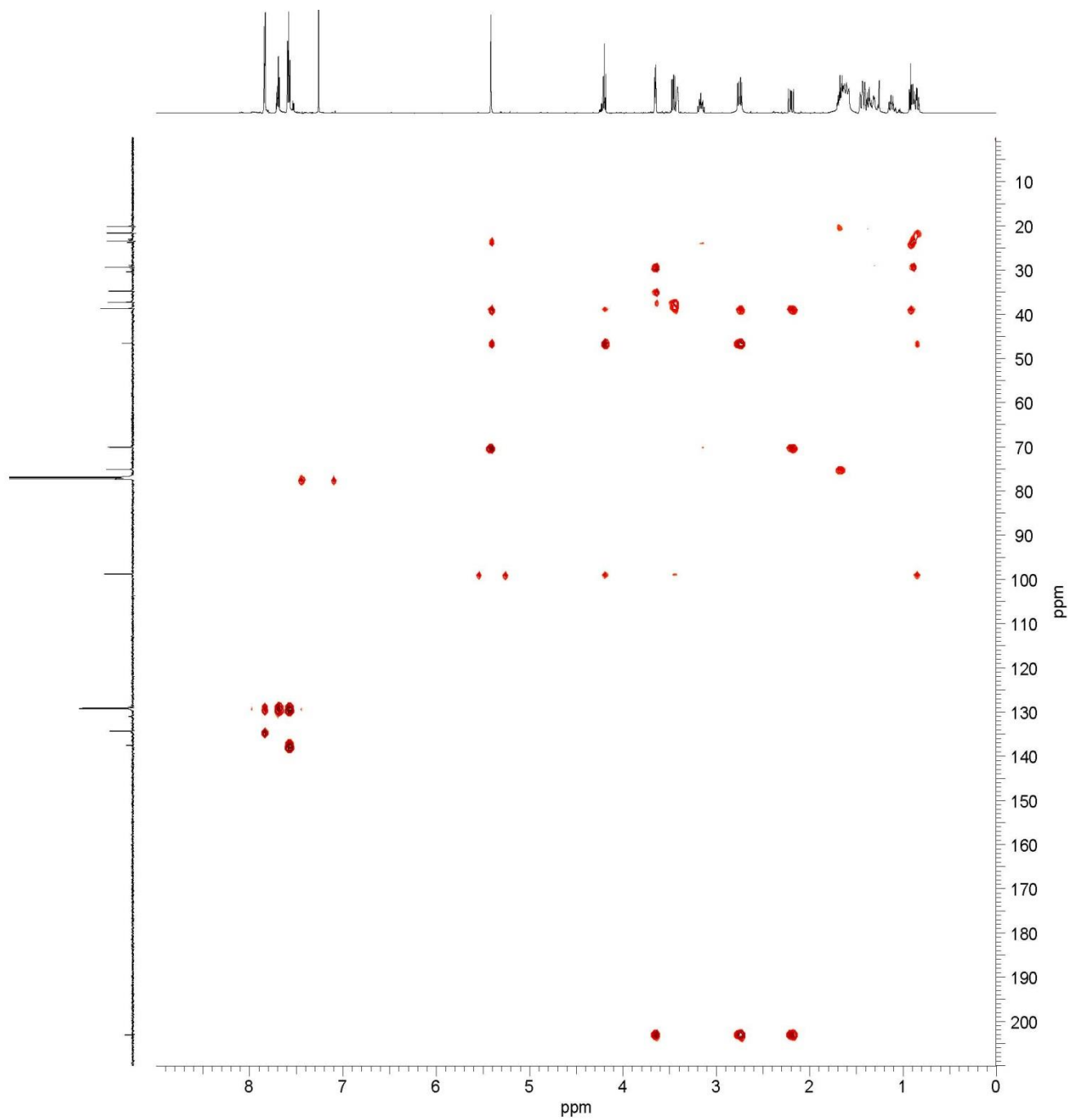


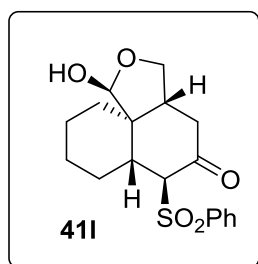
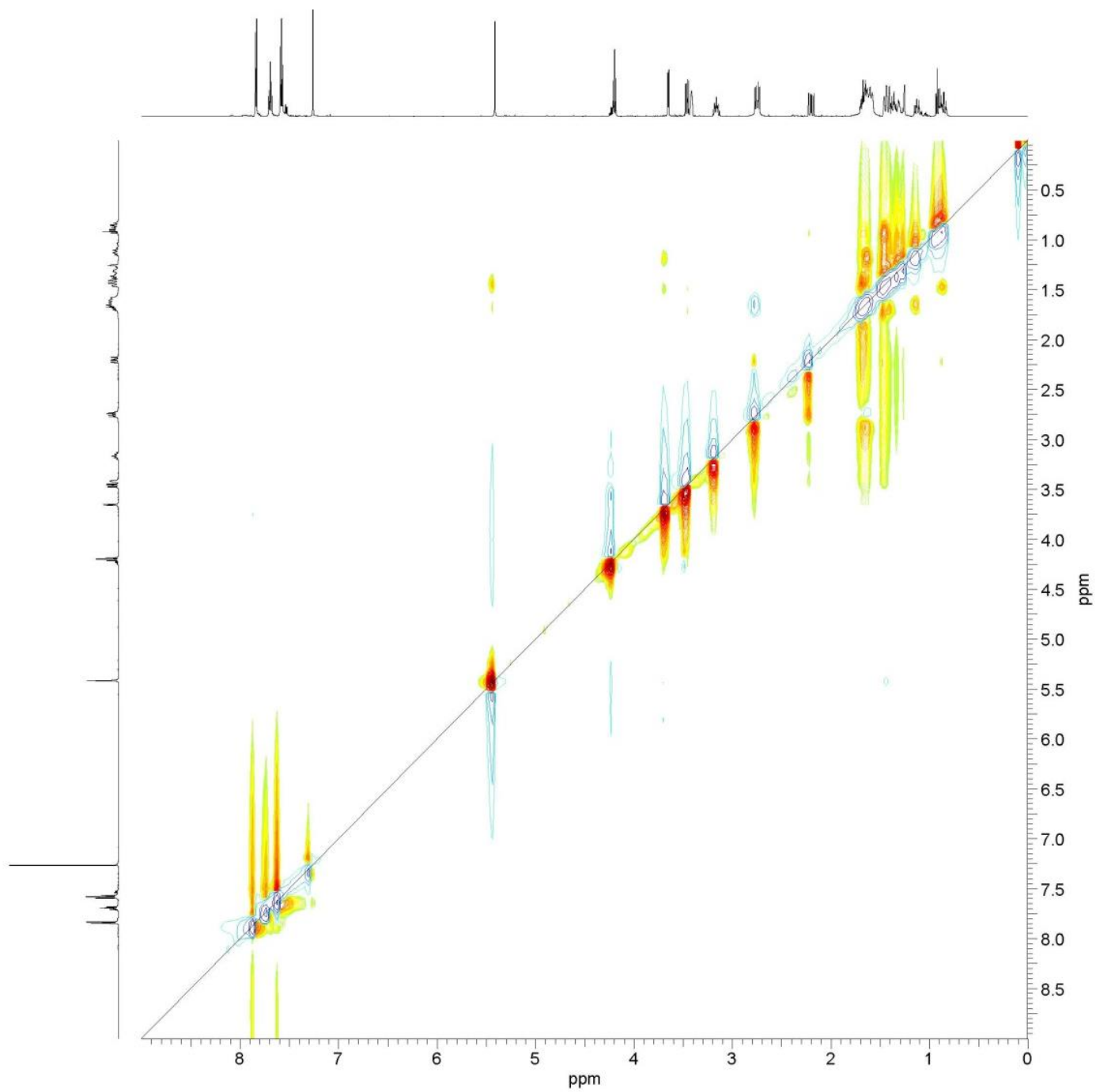


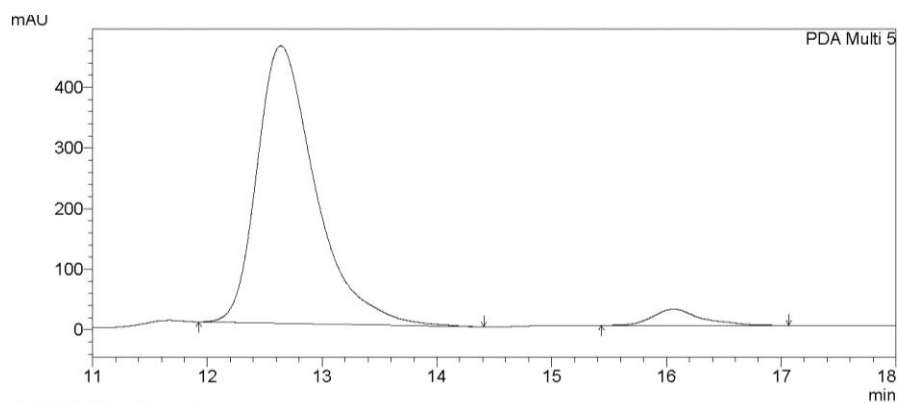
Formula	CalculatedMass	mDaError	ppmError	RDB
C17 H20 N4 O Na S	351.125004	0.495608	1.411482	9.5
C18 H23 O5 S	351.126072	-0.57234	-1.630013	7.5
C16 H24 O5 Na S	351.123667	1.83292	5.22012	4.5
C19 H19 N4 O S	351.12741	-1.909652	-5.438651	12.5
C13 H23 N2 O7 S	351.12205	3.450364	9.826568	3.5







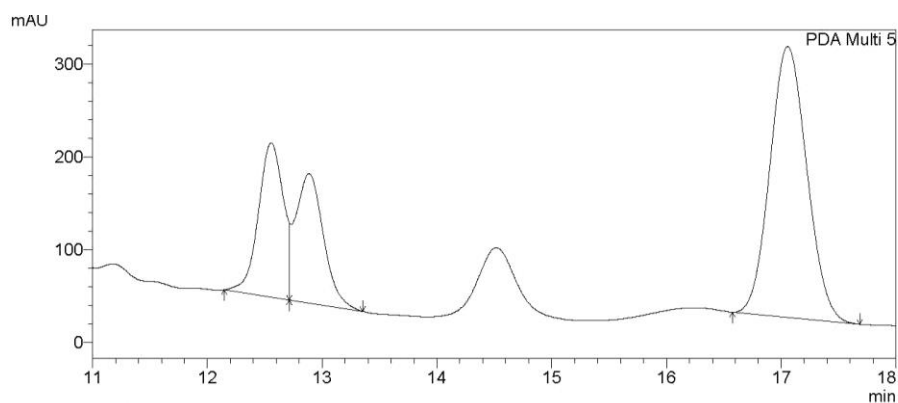
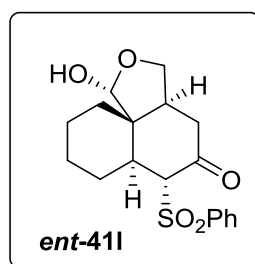
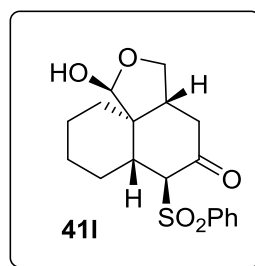




1 PDA Multi 5/210nm 4nm

PeakTable

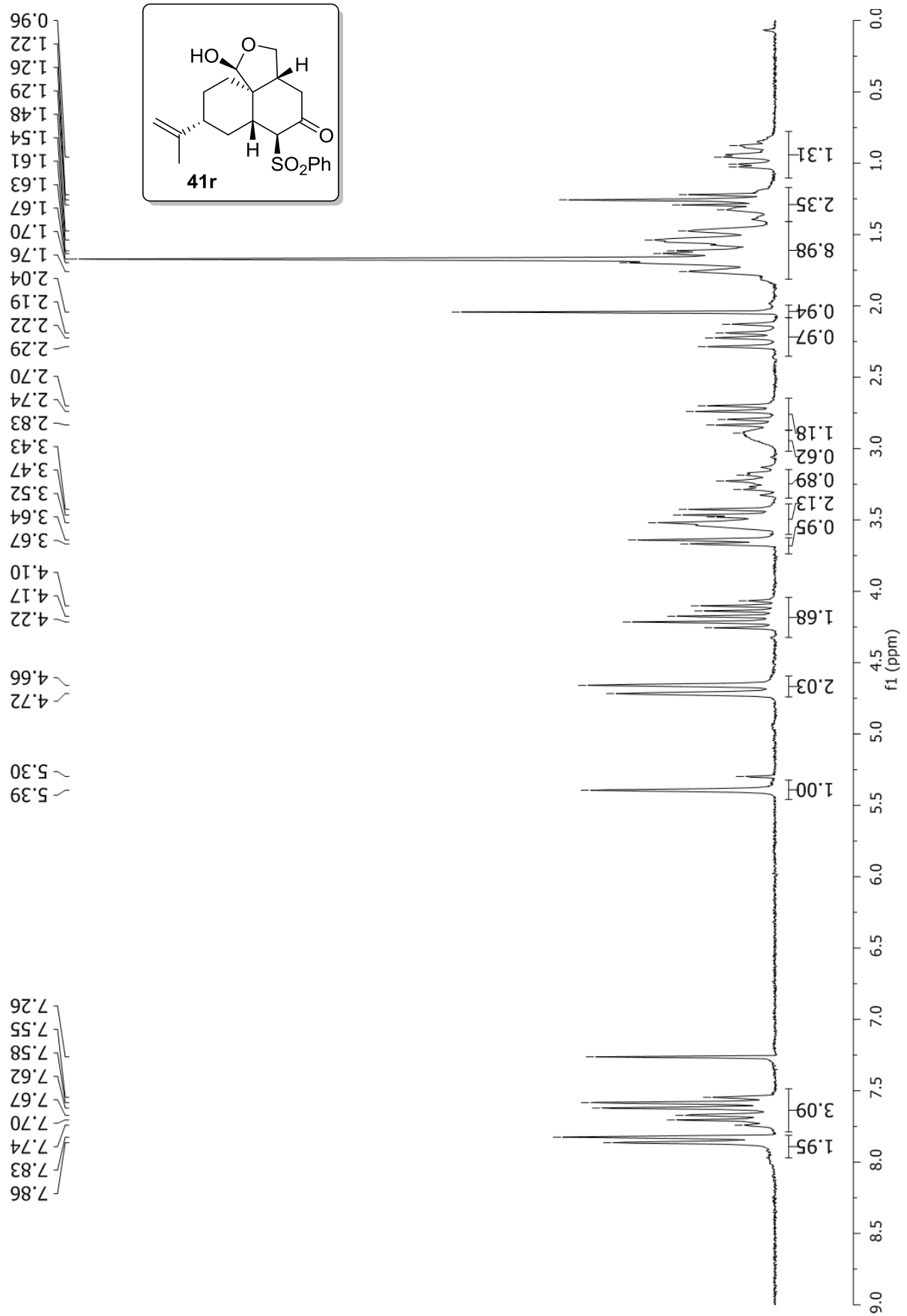
Peak#	Ret. Time	Area %
1	12.634	95.502
2	16.055	4.498
Total		100.000

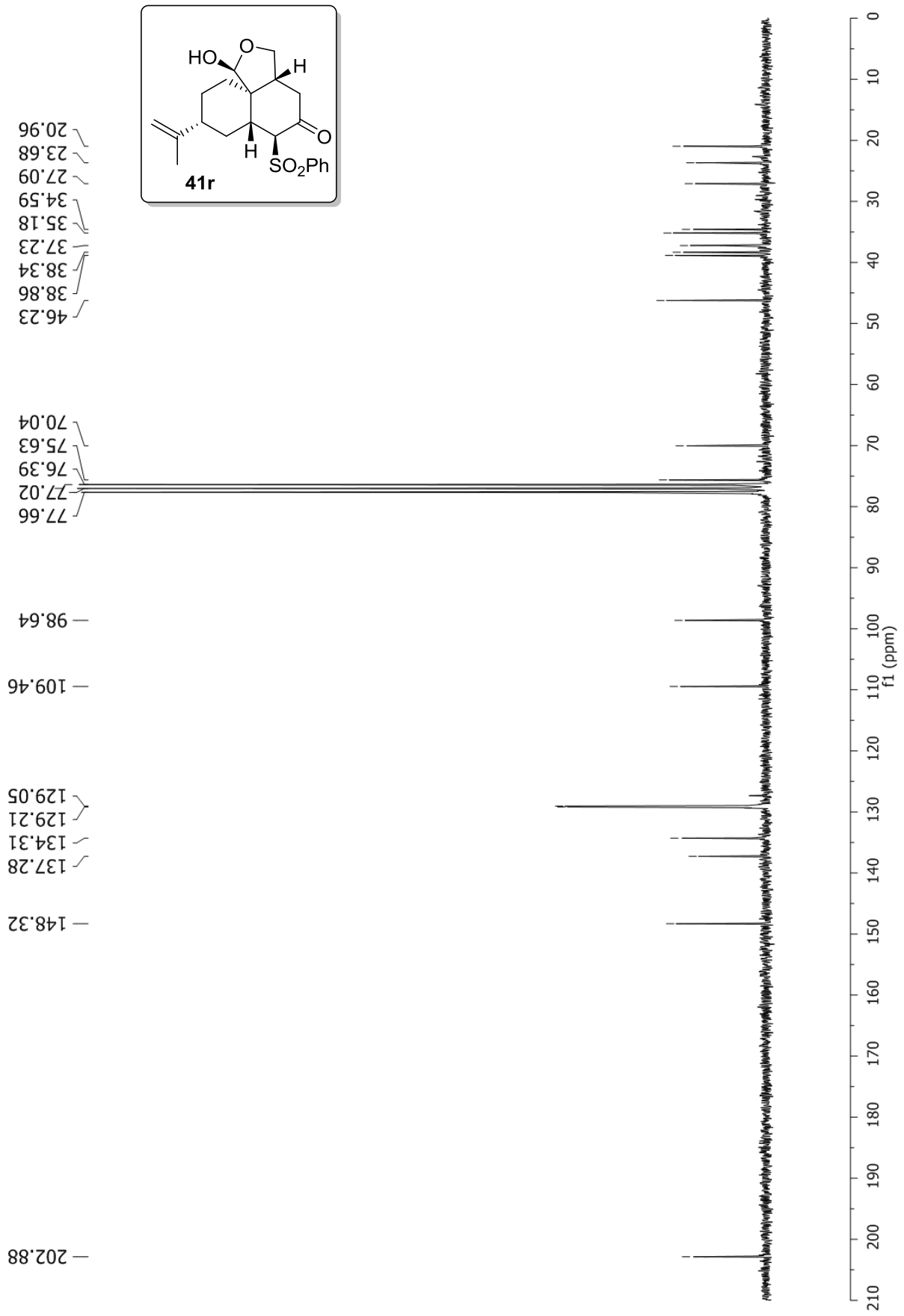


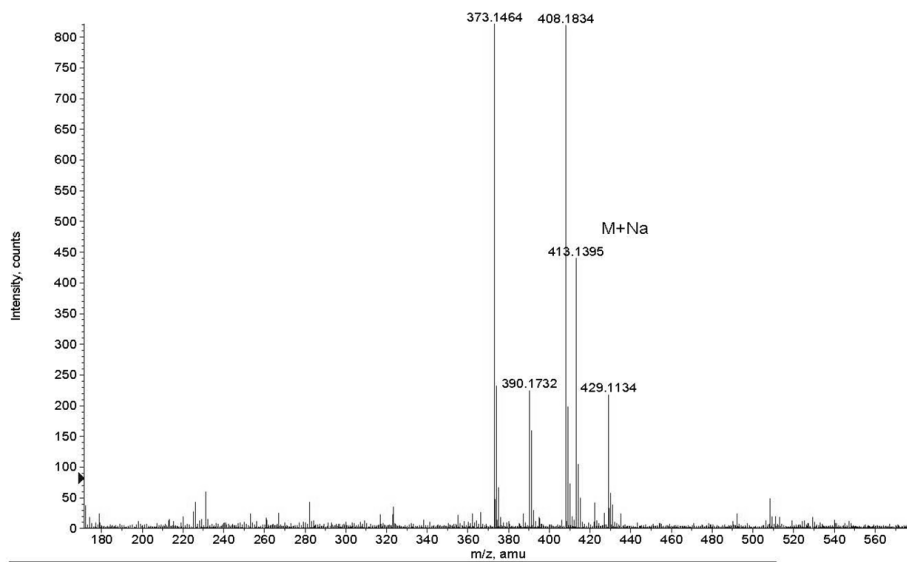
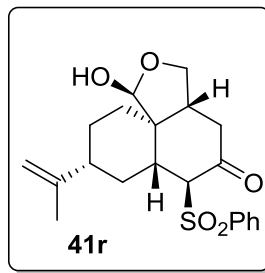
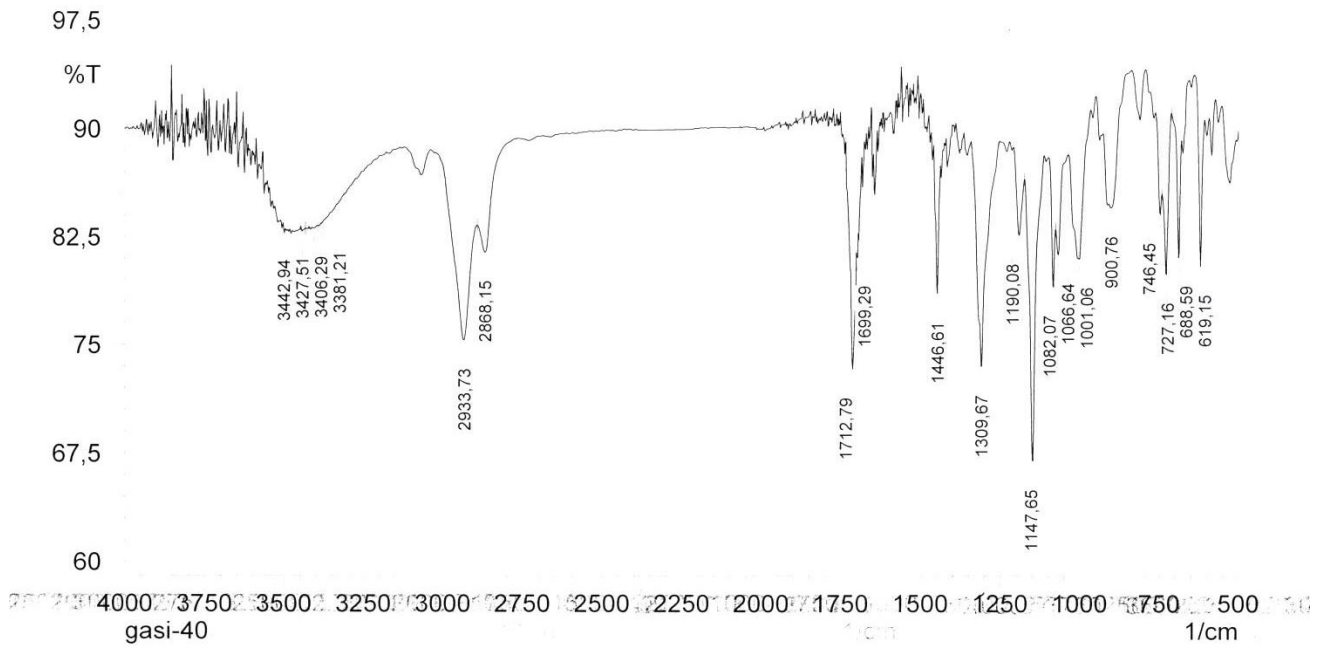
1 PDA Multi 5/210nm 4nm

PeakTable

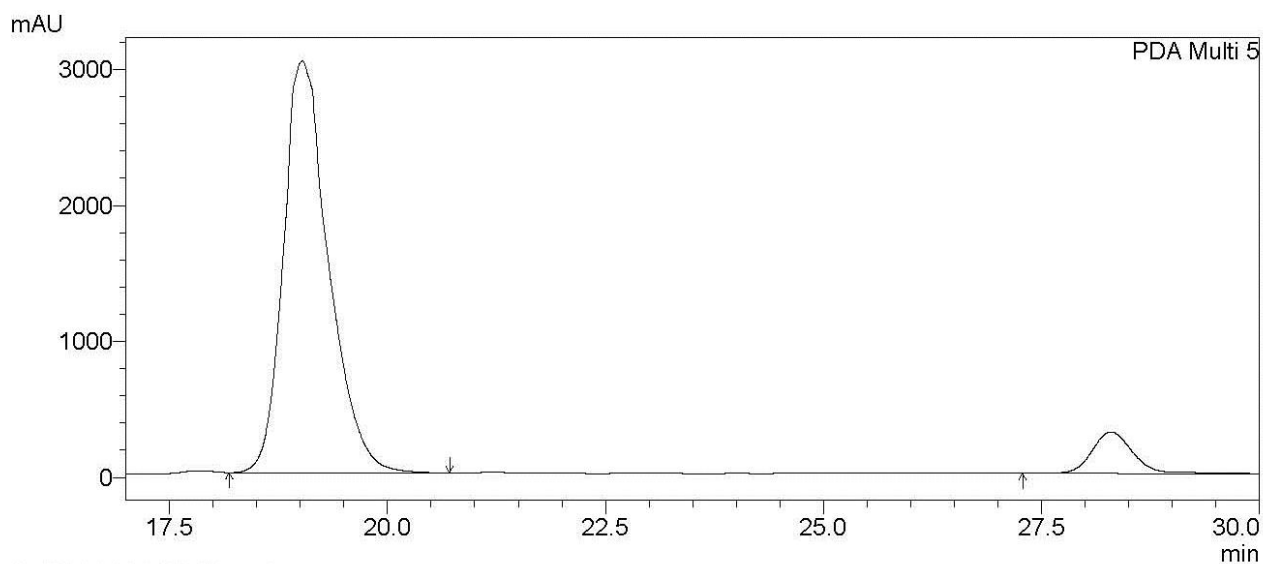
Peak#	Ret. Time	Area %
1	12.551	22.217
2	12.880	20.520
3	17.050	57.263
Total		100.000







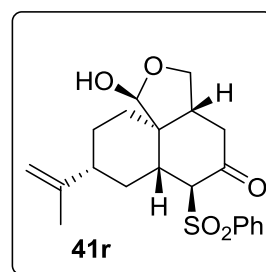
Formula	CalculatedMass	mDaError	ppmError	RDB
C21 H26 O5 Na S	413.139317	0.18284	0.442562	8.5
C27 H17 N4 O	413.139688	-0.187772	-0.4545	21.5
C26 H21 O5	413.13835	1.14954	2.782446	16.5
C22 H22 N4 O Na S	413.140654	-1.154472	-2.794384	13.5
C18 H25 N2 O7 S	413.1377	1.800284	4.357564	7.5
C25 H18 N4 O Na	413.137283	2.217488	5.3674	18.5
C23 H25 O5 S	413.141722	-2.22242	-5.379338	11.5
C17 H26 O10 Na	413.141819	-2.31856	-5.612044	4.5
C24 H22 O5 Na	413.135945	3.5548	8.604346	13.5
C24 H21 N4 O S	413.14306	-3.559732	-8.616284	16.5
C30 H21 S	413.135849	3.65094	8.837052	20.5
C18 H22 N4 O6 Na	413.143156	-3.655872	-8.84899	9.5

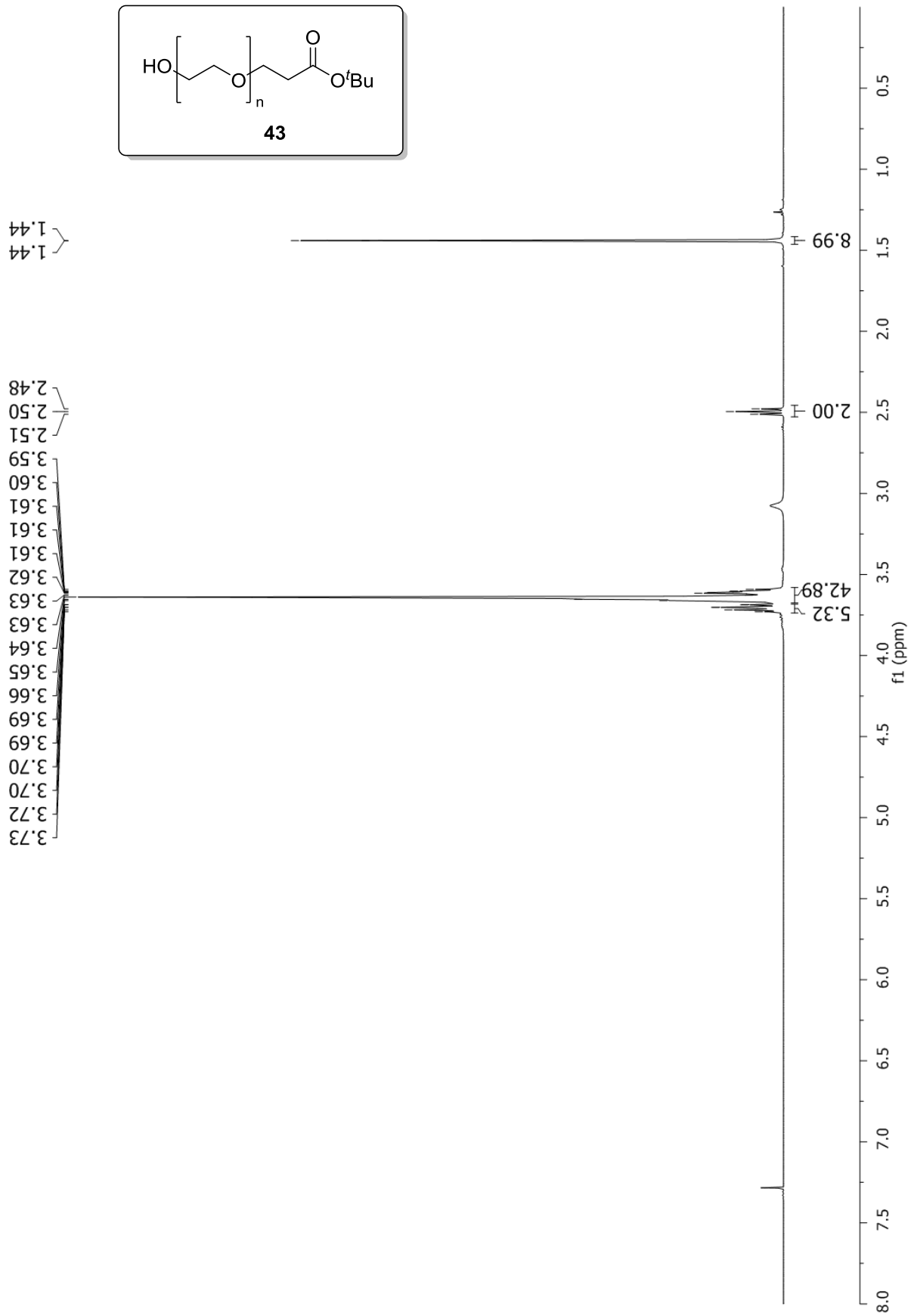


PeakTable

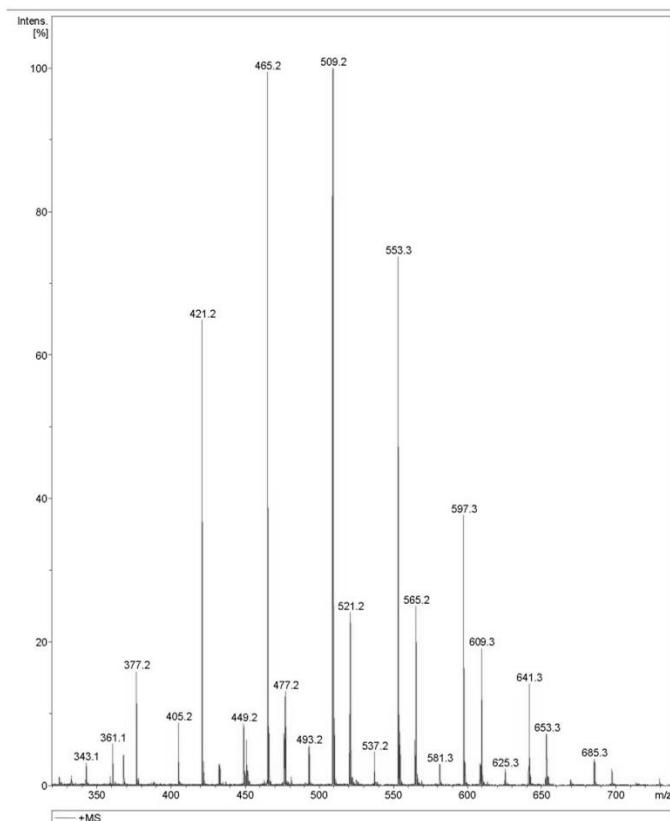
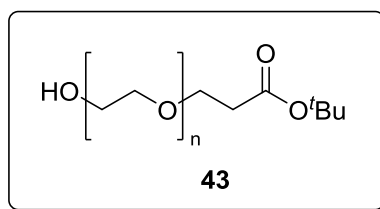
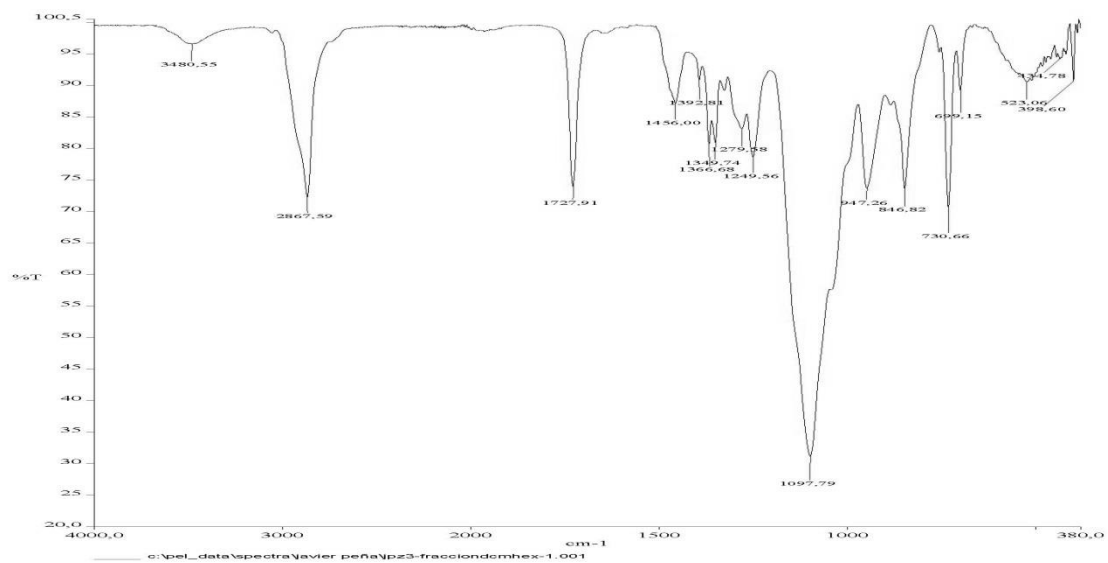
PDA Ch5 215nm 4nm

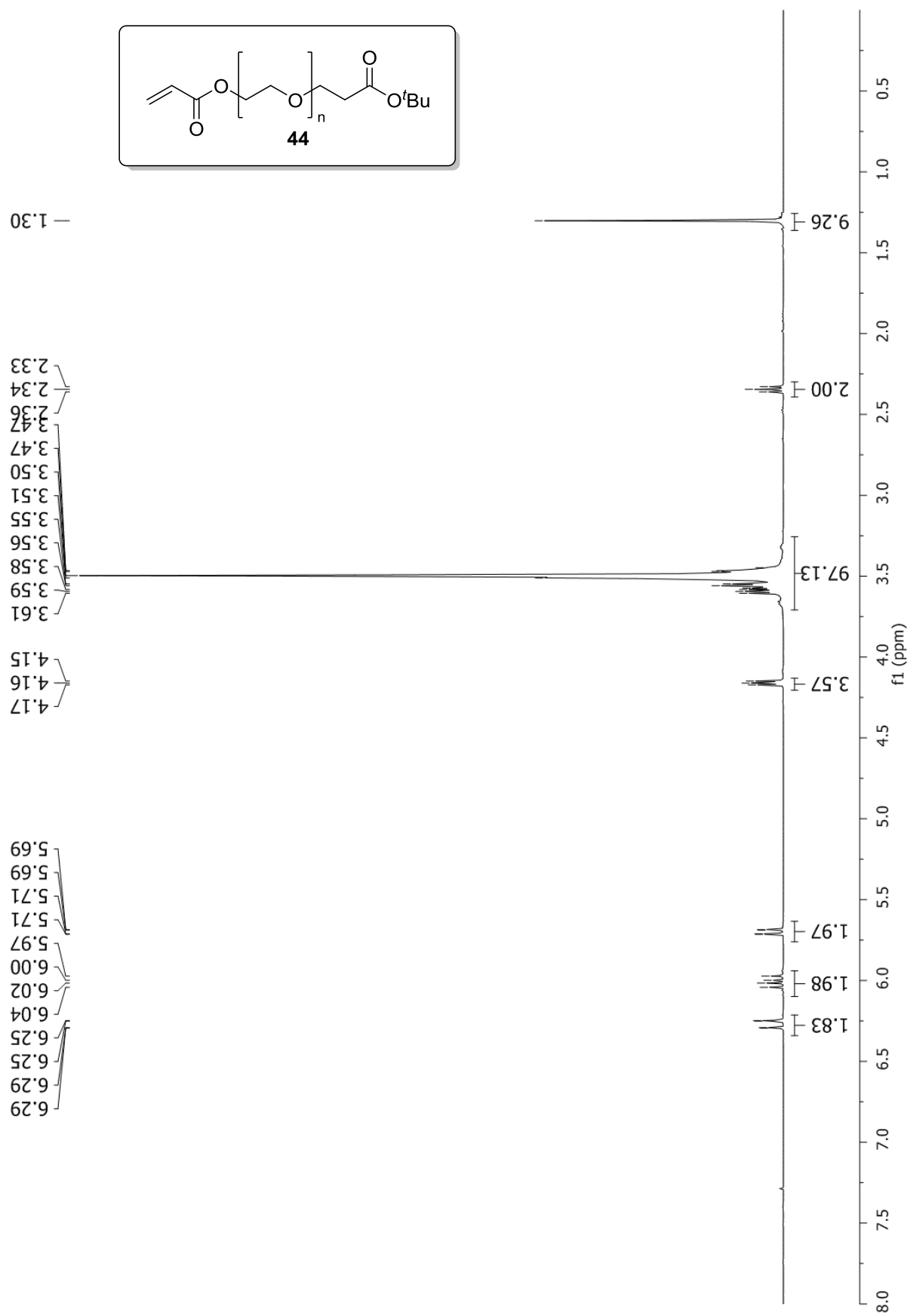
Peak#	Ret. Time	Area %
1	19.020	91.554
2	28.289	8.446
Total		100.000

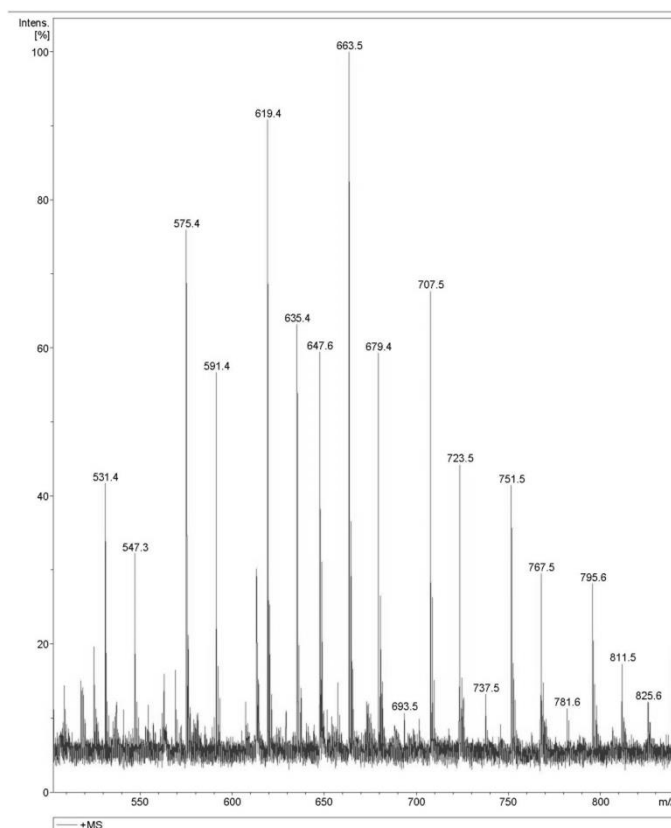
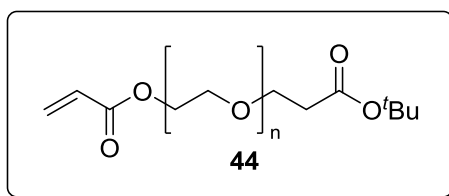
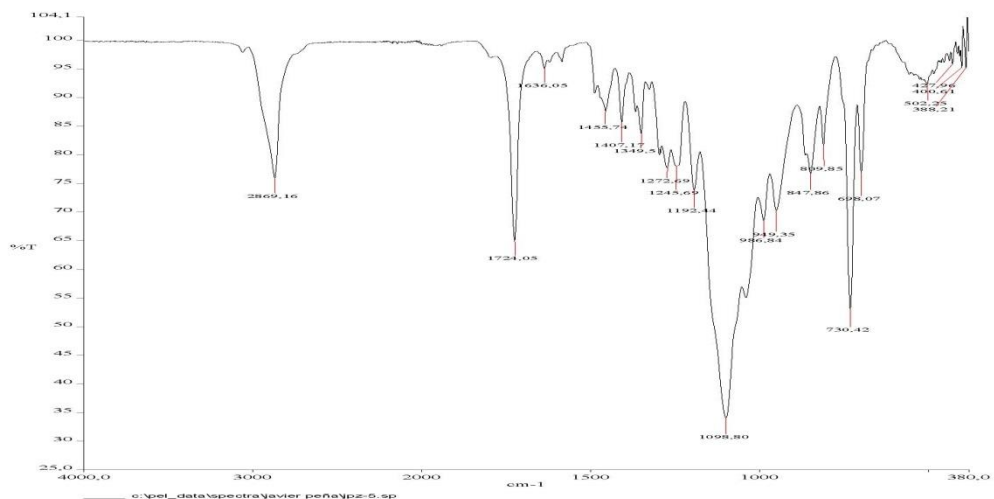


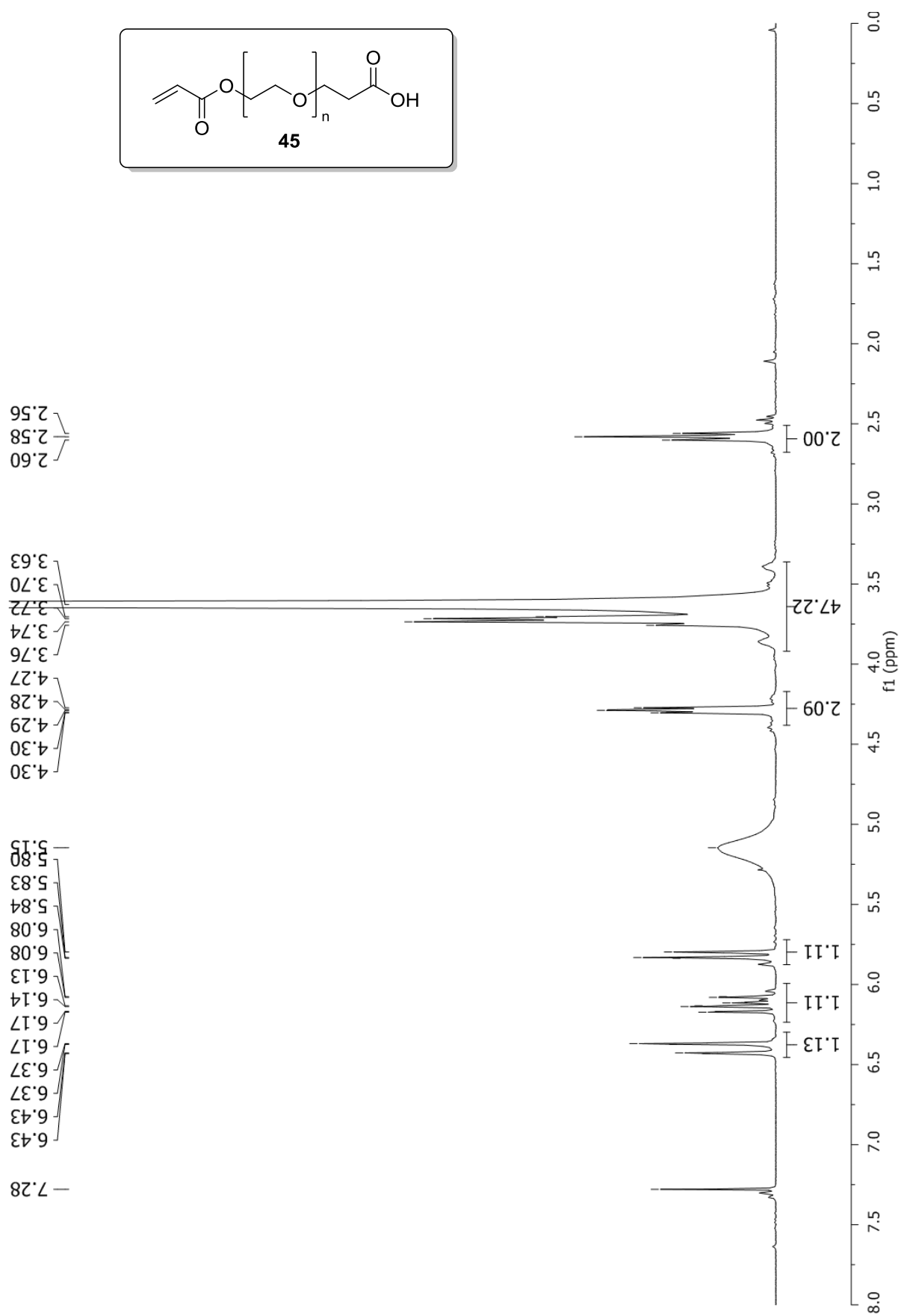


Full Spectroscopy









Full Spectroscopy

