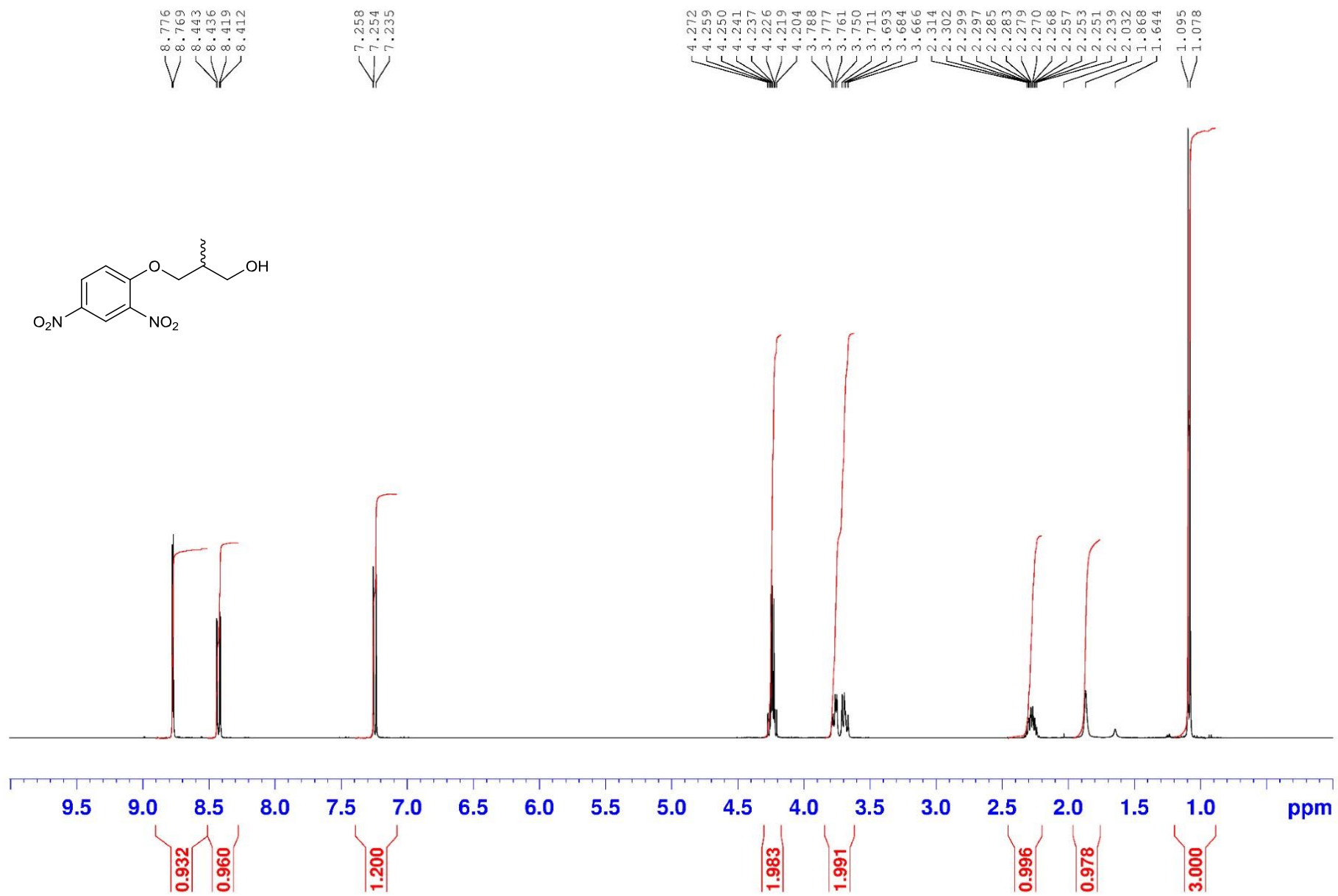
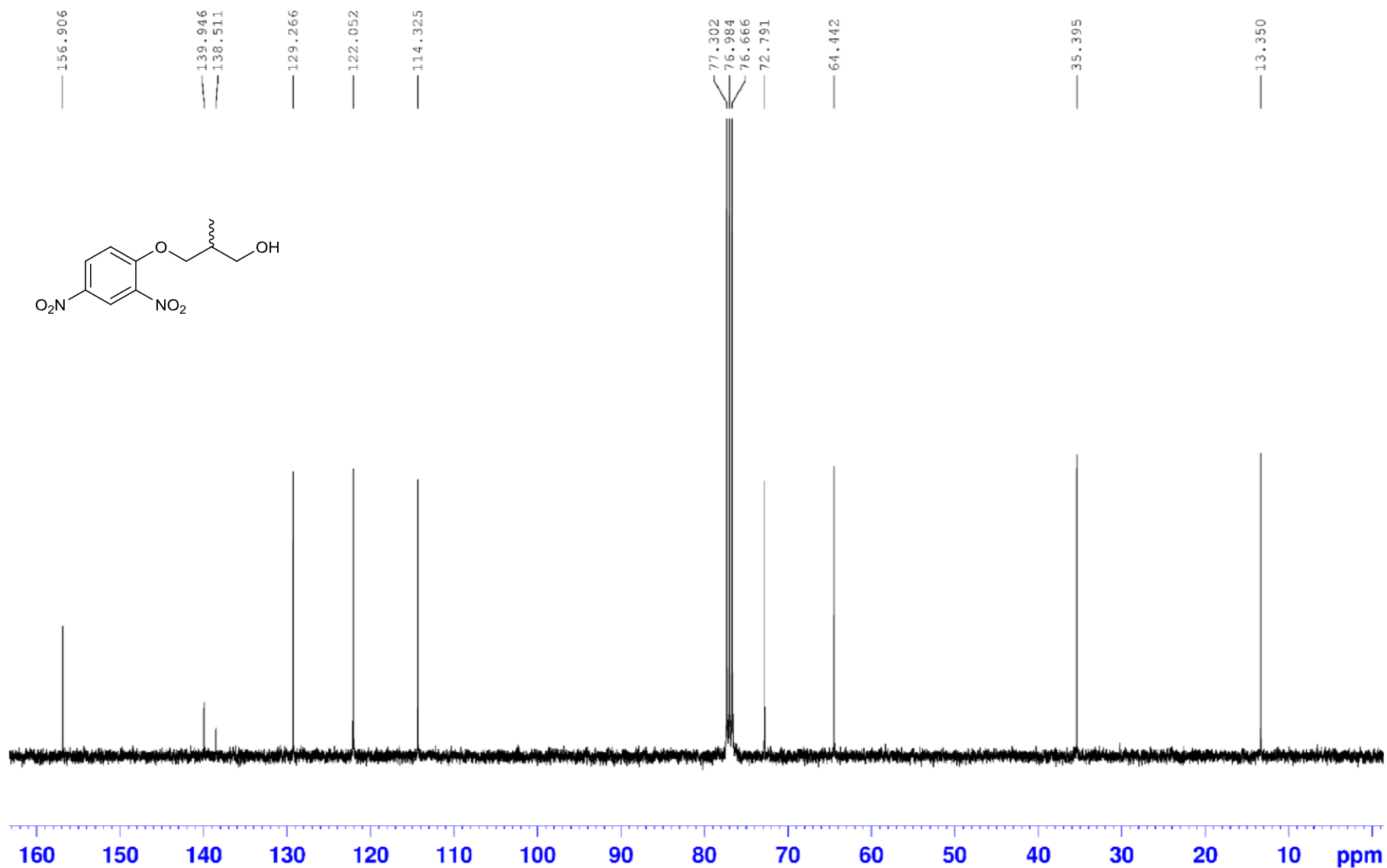
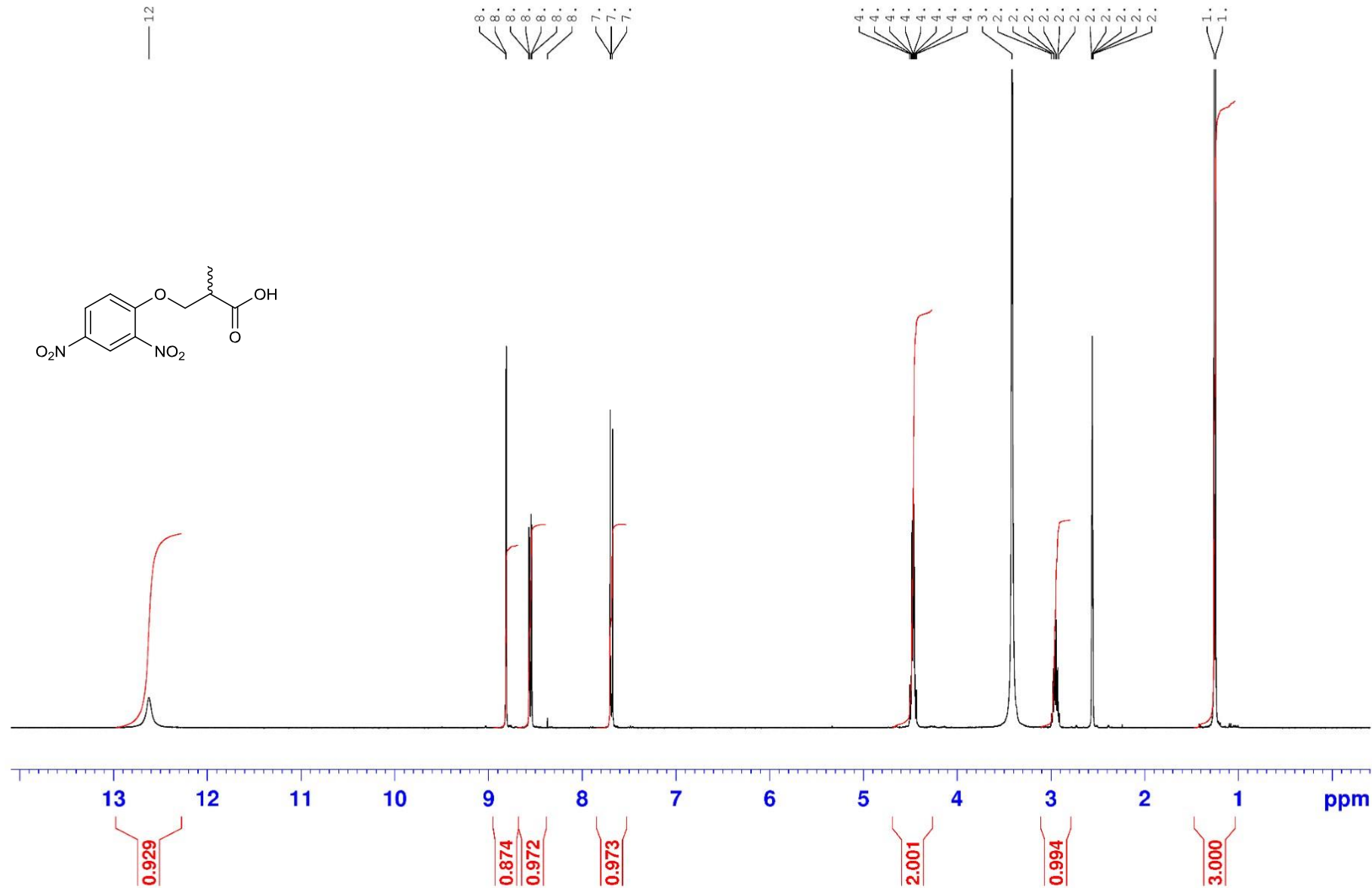


2*R*,5*S*-3-(2,4-Dinitrophenoxy)-2-methylpropan-1-ol ¹H NMR

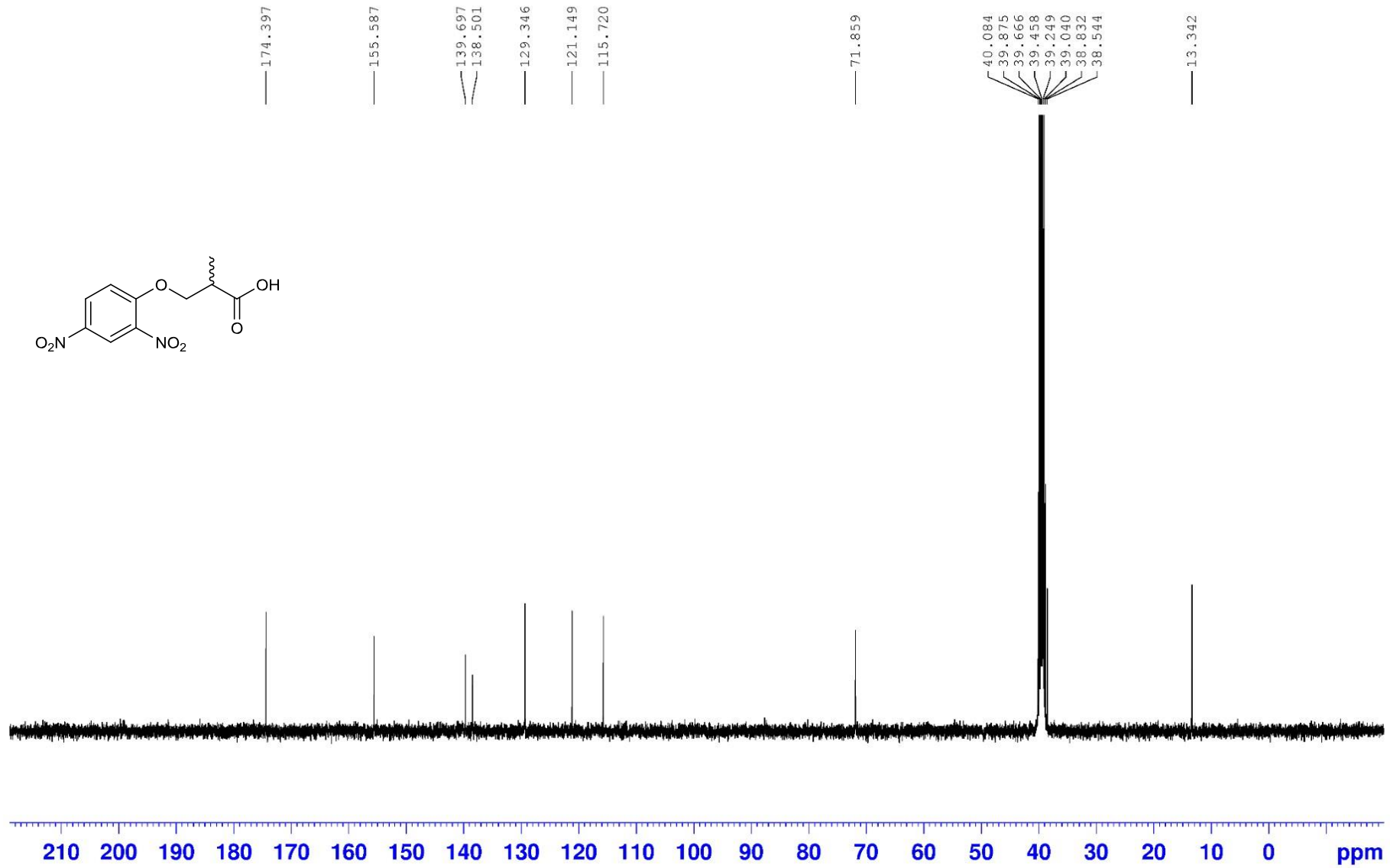
2R,S-3-(2,4-Dinitrophenoxy)-2-methylpropan-1-ol 9 ¹³C NMR



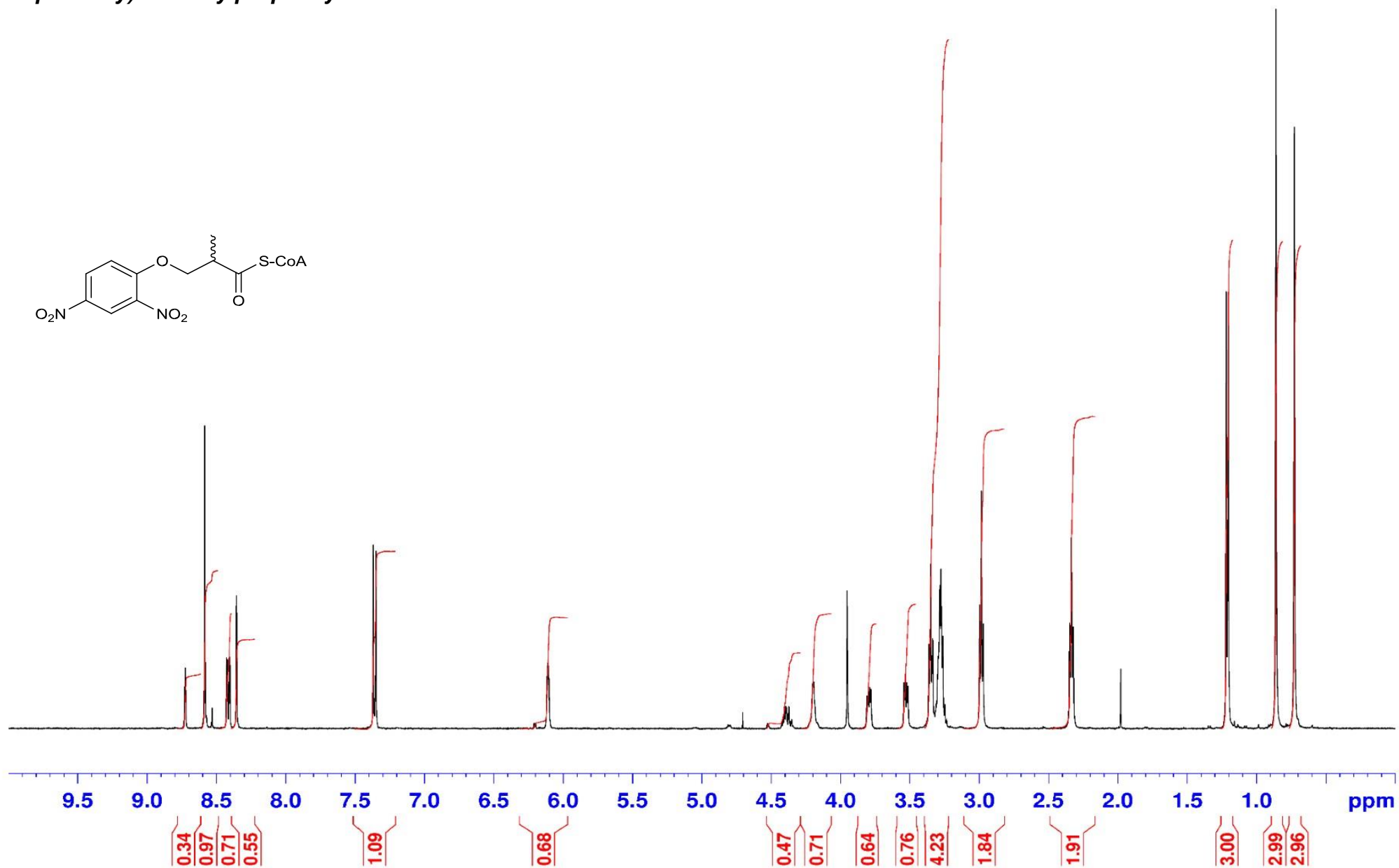
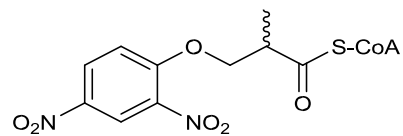
2R,S-3-(2,4-Dinitrophenoxy)-2-methylpropanoic acid 10 ¹H NMR



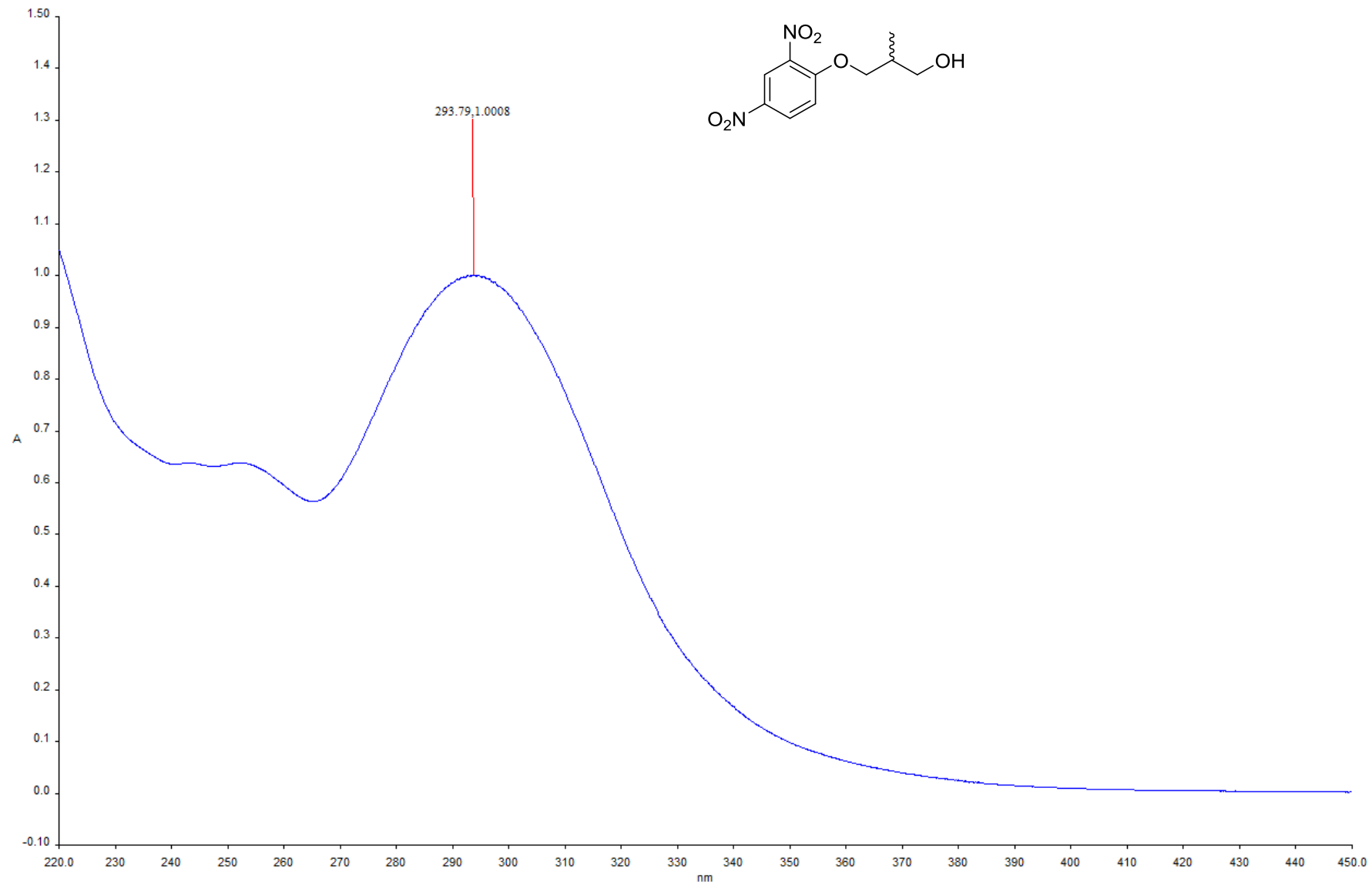
2R,S-3-(2,4-Dinitrophenoxy)-2-methylpropanoic acid 10 ¹³C NMR



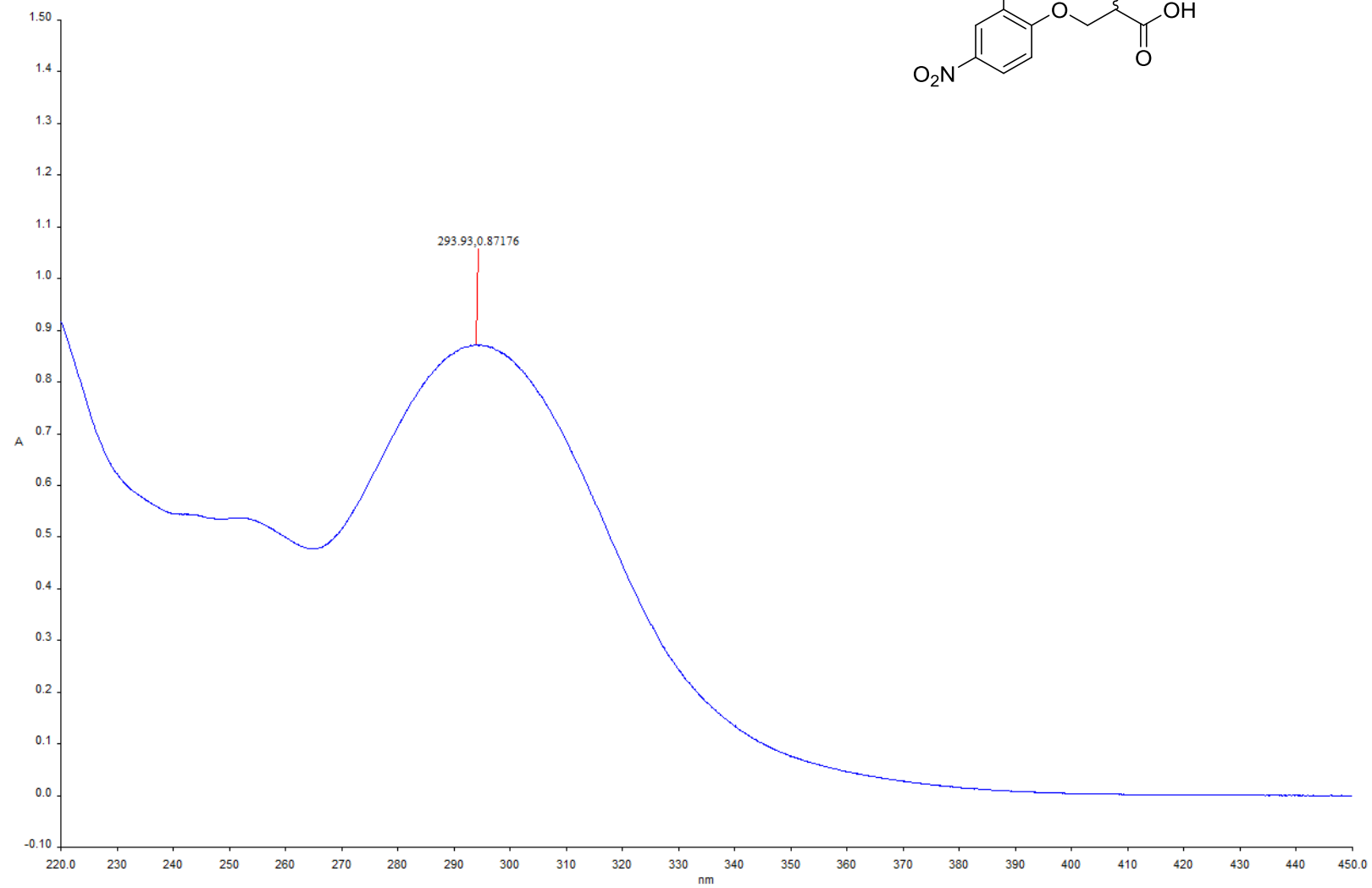
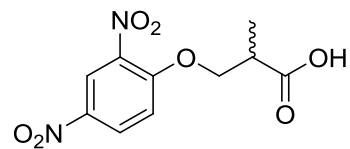
2R,S-3-(2,4-Dinitrophenoxy)-2-methylpropanoyl-CoA ^1H NMR



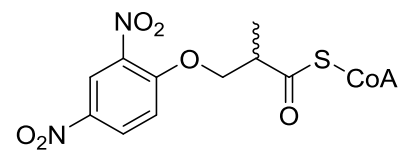
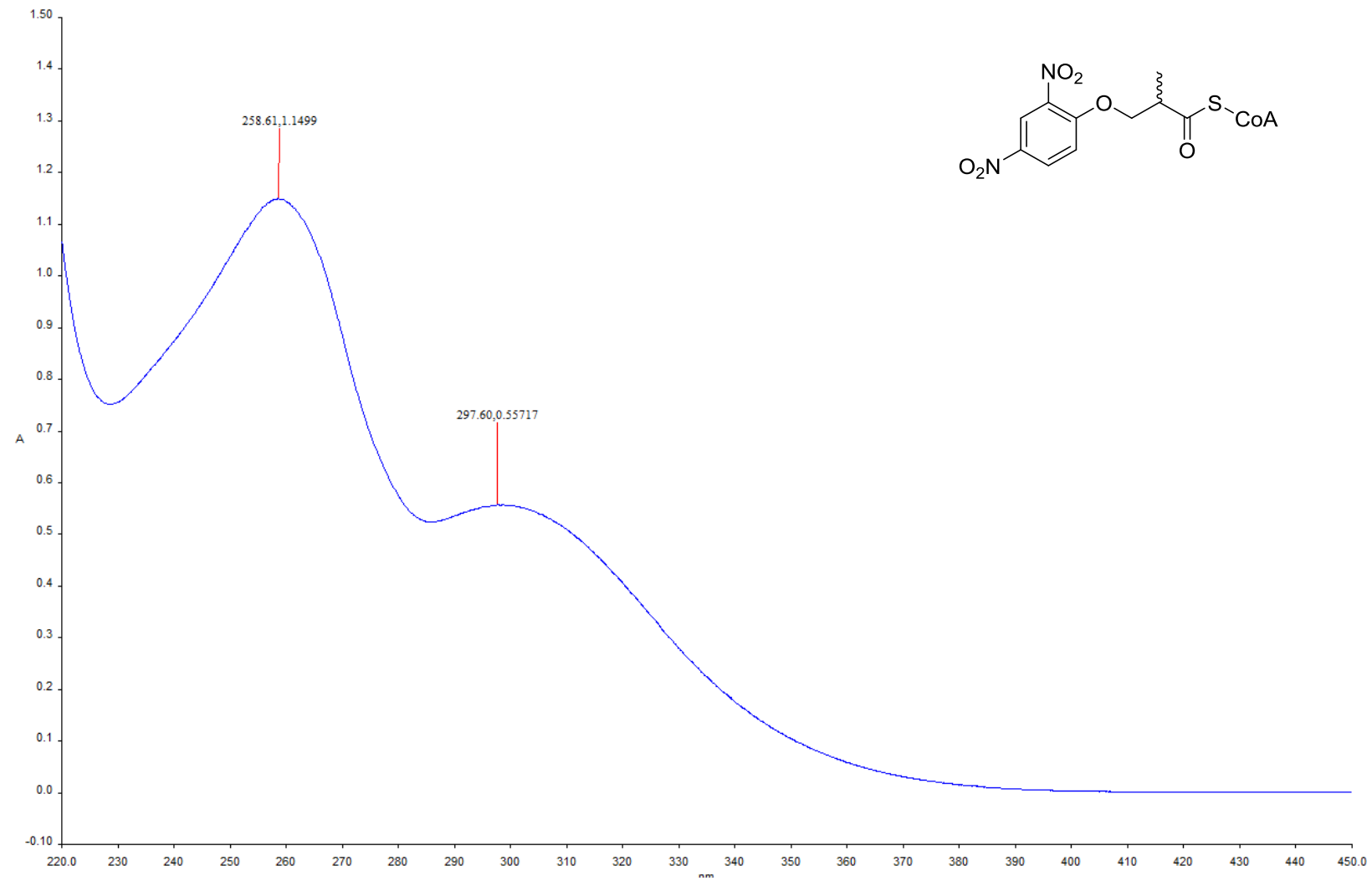
2R,S-3-(2,4-dinitrophenoxy)-2-methylpropan-1-ol 9 (72 μ M in EtOH)



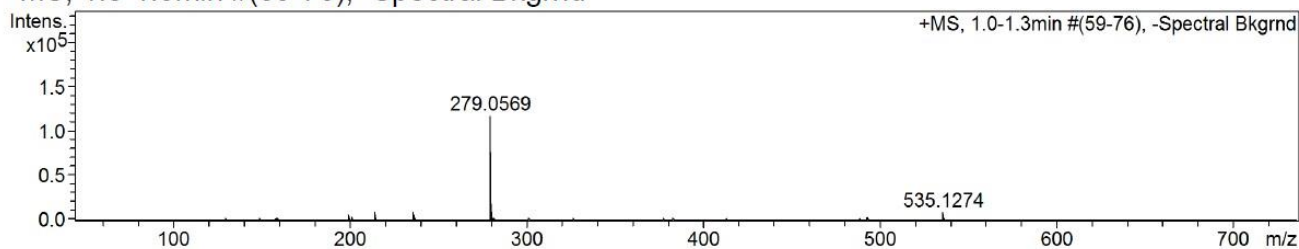
2R,S-3-(2,4-dinitrophenoxy)-2-methylpropanoic acid 10 (72 μ M in EtOH)



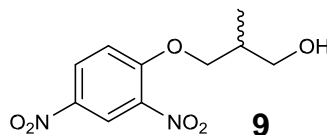
2R,S-3-(2,4-dinitrophenoxy)-2-methylpropanoyl-CoA 6 (72 μM in H_2O)



+MS, 1.0-1.3min #(59-76), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	199.0043	5990	5.1	281	1855.4
2	201.0008	2746	2.3	123	822.5
3	214.0950	8150	7.0	169	2261.7
4	236.0792	8757	7.5	234	2435.8
5	279.0569	117254	100.0	5662	14325.3
6	280.0592	14630	12.5	832	1751.1
7	281.0613	2344	2.0	131	275.0
8	413.2699	1931	1.6	153	321.4
9	492.1403	2878	2.5	335	425.0
10	535.1274	8848	7.5	1080	1173.1



Generate Molecular Formula Parameters

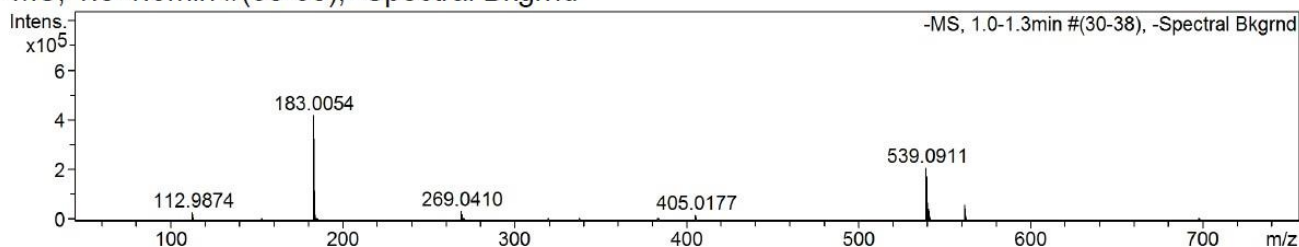
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C₁₀H₁₂N₂O₆ Adduct(s): H, Na

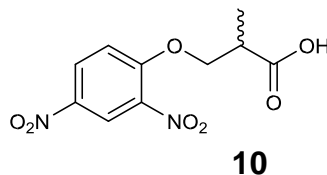
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	279.0569	279.059306	6.70	0.0054	C ₁₀ H ₁₂ N ₂ NaO ₆

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

-MS, 1.0-1.3min #(30-38), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	112.9874	32761	7.8	583	1660.0
2	183.0054	417725	100.0	16034	22540.2
3	184.0079	31339	7.5	1076	1734.5
4	269.0410	37224	8.9	1817	4206.3
5	405.0177	21745	5.2	1492	1227.6
6	539.0911	209548	50.2	19276	4107.9
7	540.0941	46197	11.1	4140	891.2
8	541.0860	11033	2.6	861	209.4
9	561.0730	58567	14.0	5363	1721.6
10	562.0761	13142	3.1	1256	398.0



Generate Molecular Formula Parameters

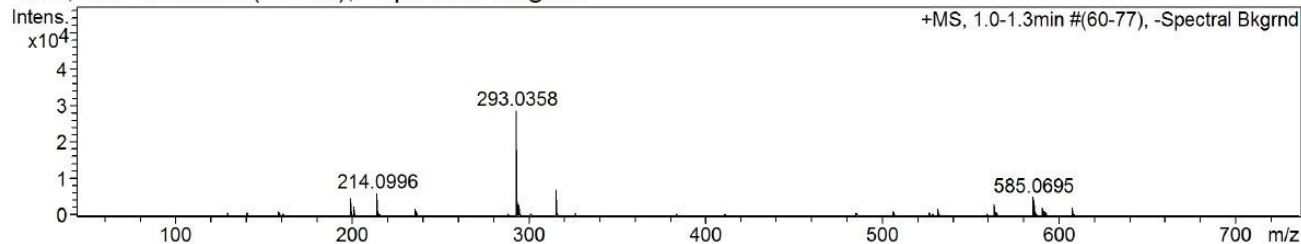
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
negative	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C₁₀H₁₀N₂O₇ Adduct(s): H, Na

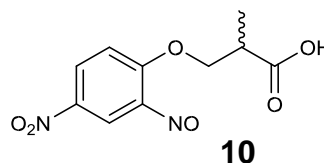
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	269.0410	269.040976	1.90	0.0003	C ₁₀ H ₉ N ₂ O ₇

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	199.0042	4723	16.6	223	3332.8
2	201.0011	2286	8.0	101	1557.0
3	214.0996	6174	21.7	67	4387.1
4	293.0358	28453	100.0	1679	6752.6
5	294.0395	3177	11.2	204	738.4
6	315.0174	6987	24.6	431	2200.0
7	563.0867	2968	10.4	398	534.1
8	585.0695	4950	17.4	662	875.5
9	590.5049	2006	7.0	140	387.3
10	607.0504	2215	7.8	243	592.9



Generate Molecular Formula Parameters

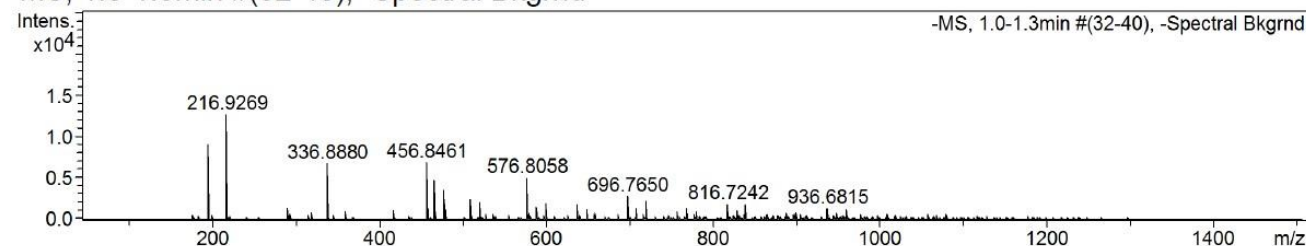
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C₁₀H₁₀N₂O₇ Adduct(s): H, Na

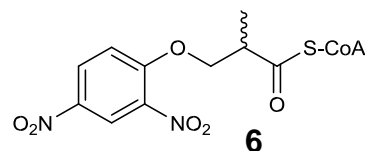
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	293.0358	293.038570	7.70	0.0022	C ₁₀ H ₁₀ N ₂ Na ₁ O ₇

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

-MS, 1.0-1.3min #(32-40), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	194.9457	9063	72.0	381	3074.4
2	216.9269	12596	100.0	565	4353.8
3	336.8880	6695	53.2	433	2443.7
4	456.8461	6838	54.3	511	1411.1
5	465.6174	4667	37.1	346	914.7
6	476.6094	3592	28.5	276	662.1
7	508.5703	2413	19.2	194	464.9
8	576.8058	5039	40.0	454	1241.6
9	696.7650	2804	22.3	293	567.5
10	718.7473	2205	17.5	224	423.0



Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
negative	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C₃₁H₄₄N₉O₂₂P₃S Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication