

Squaramide-catalysed Enantioselective Michael Addition of Pyrazolin-5-ones to Nitroalkenes

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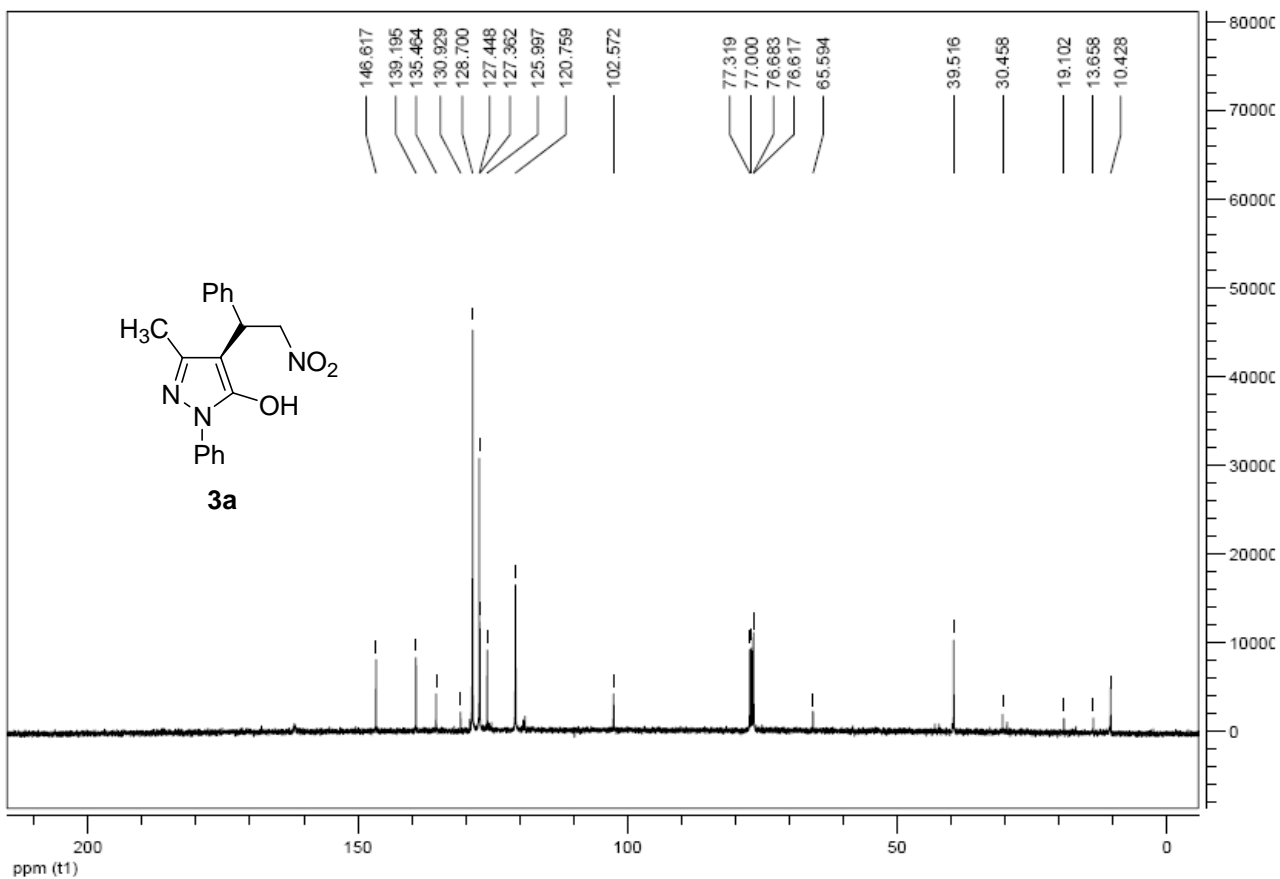
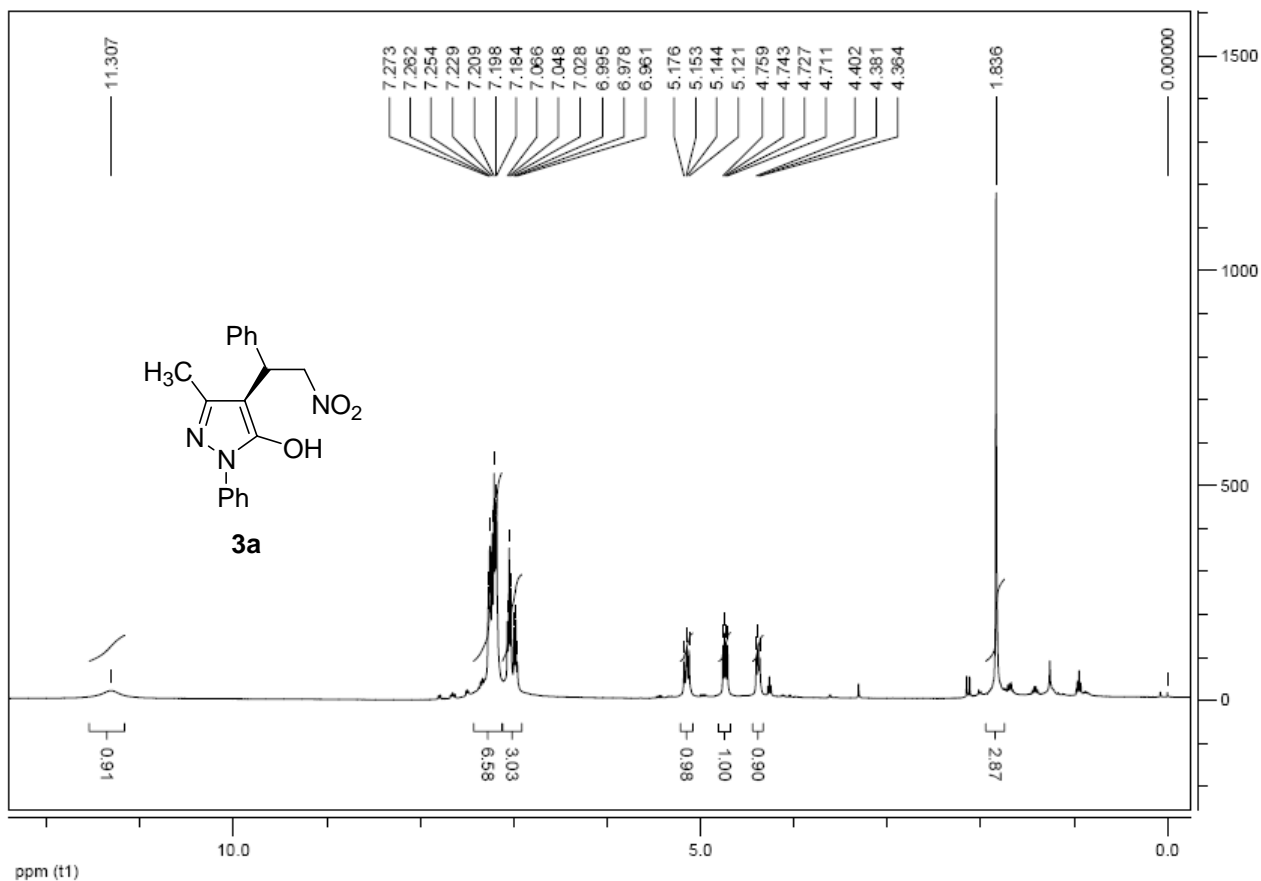
dudm@bit.edu.cn

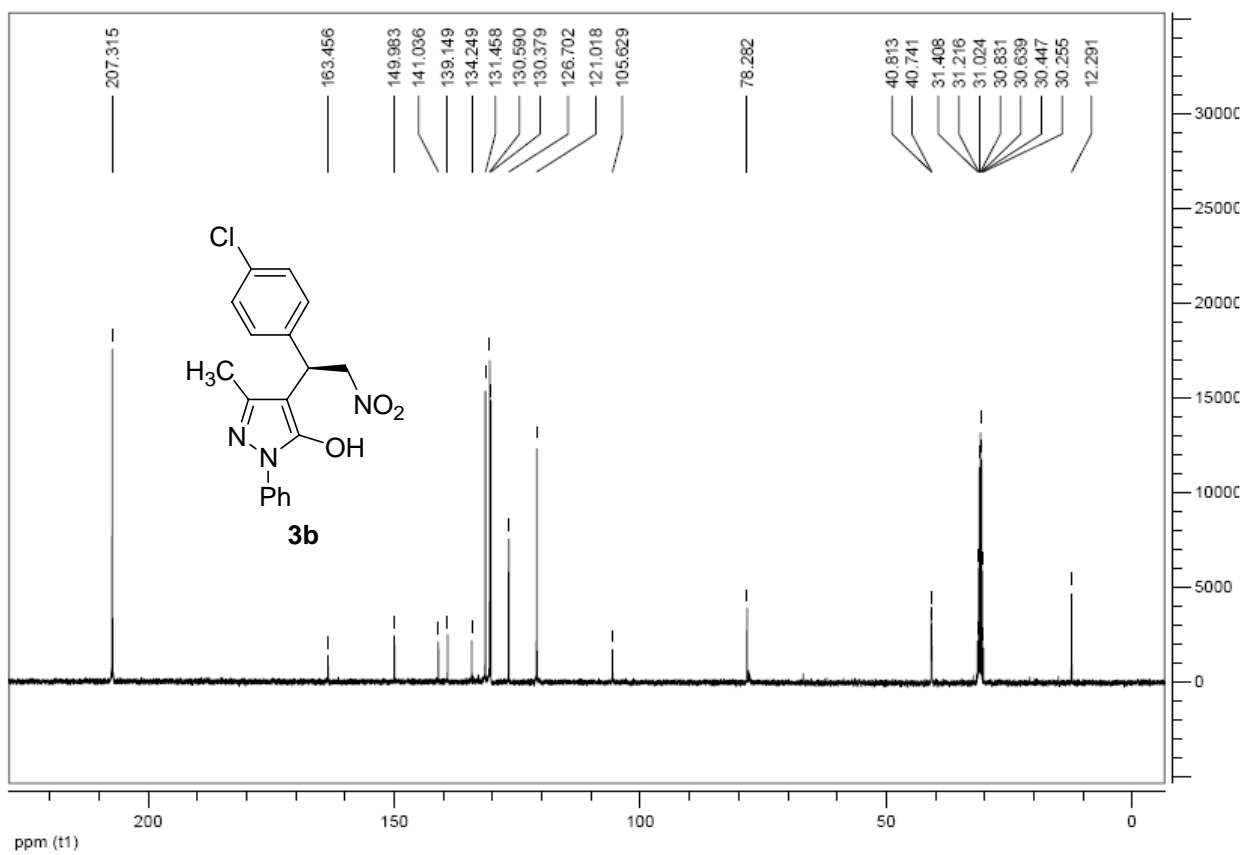
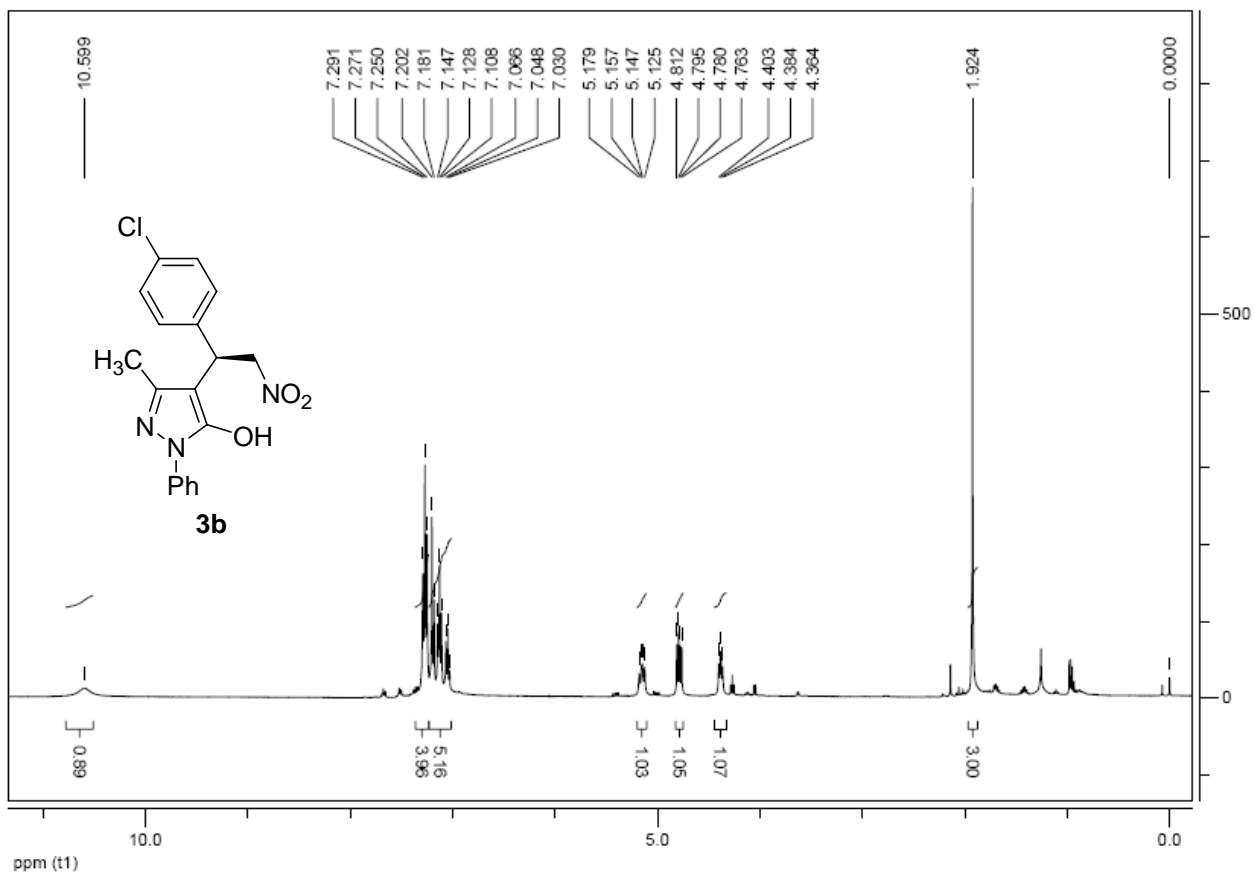
Supporting Information

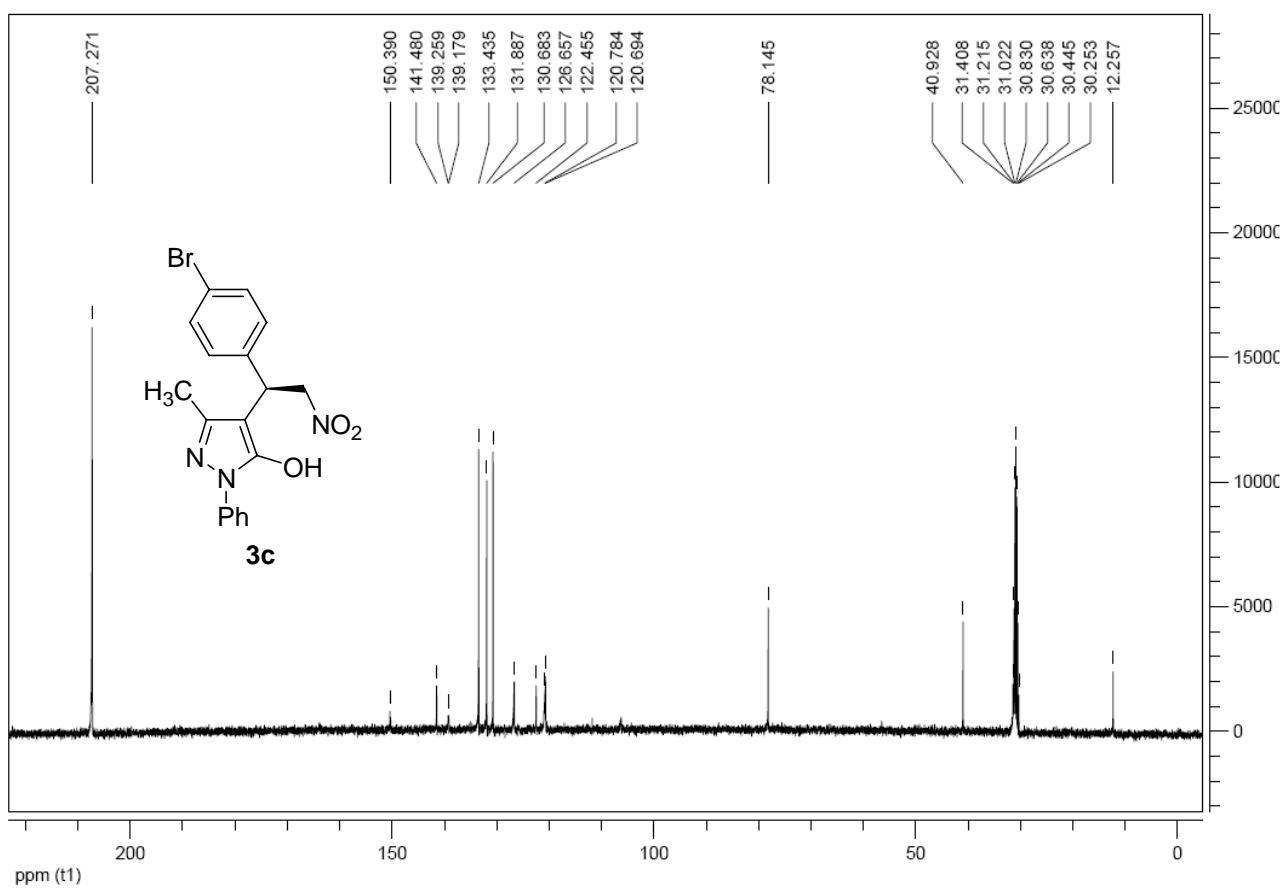
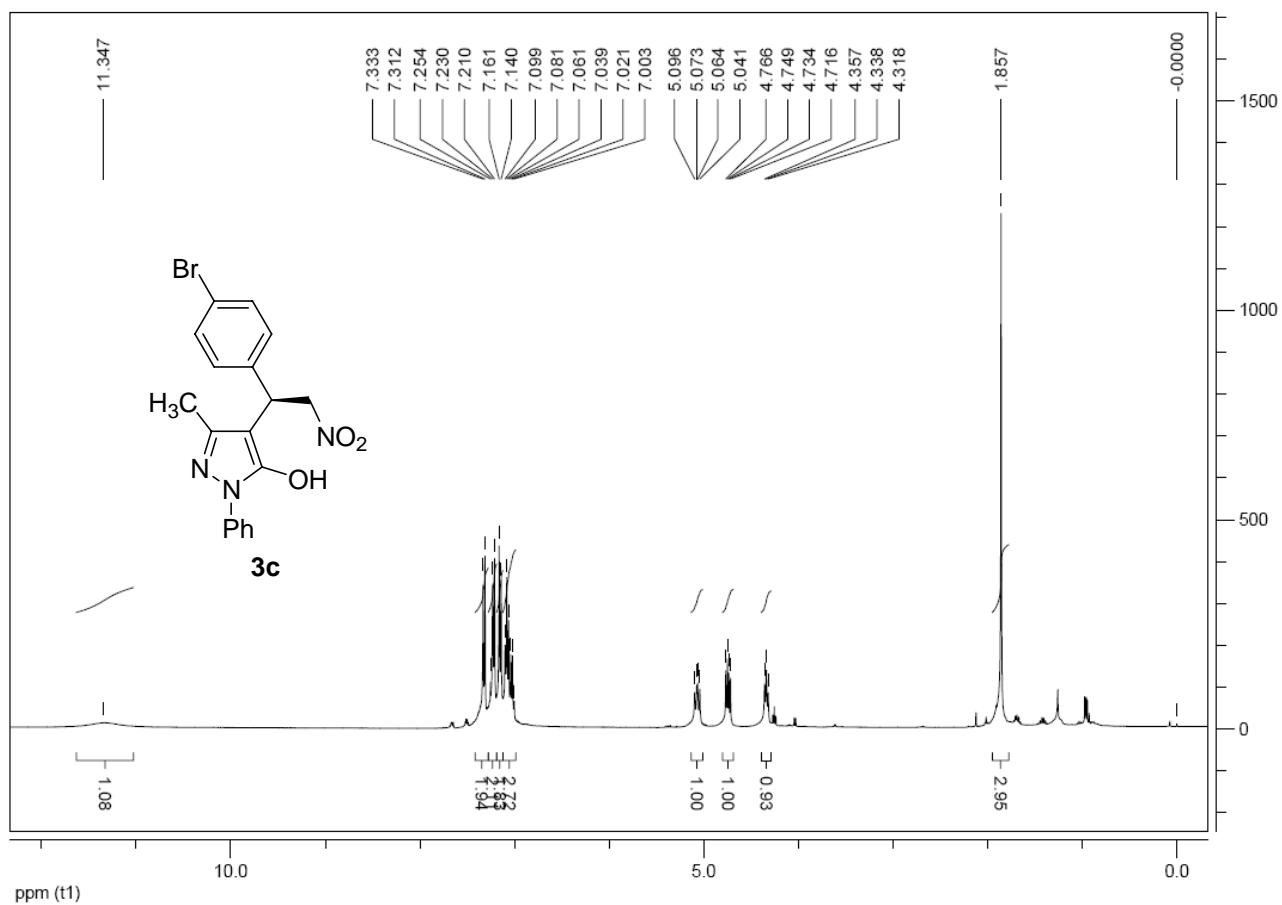
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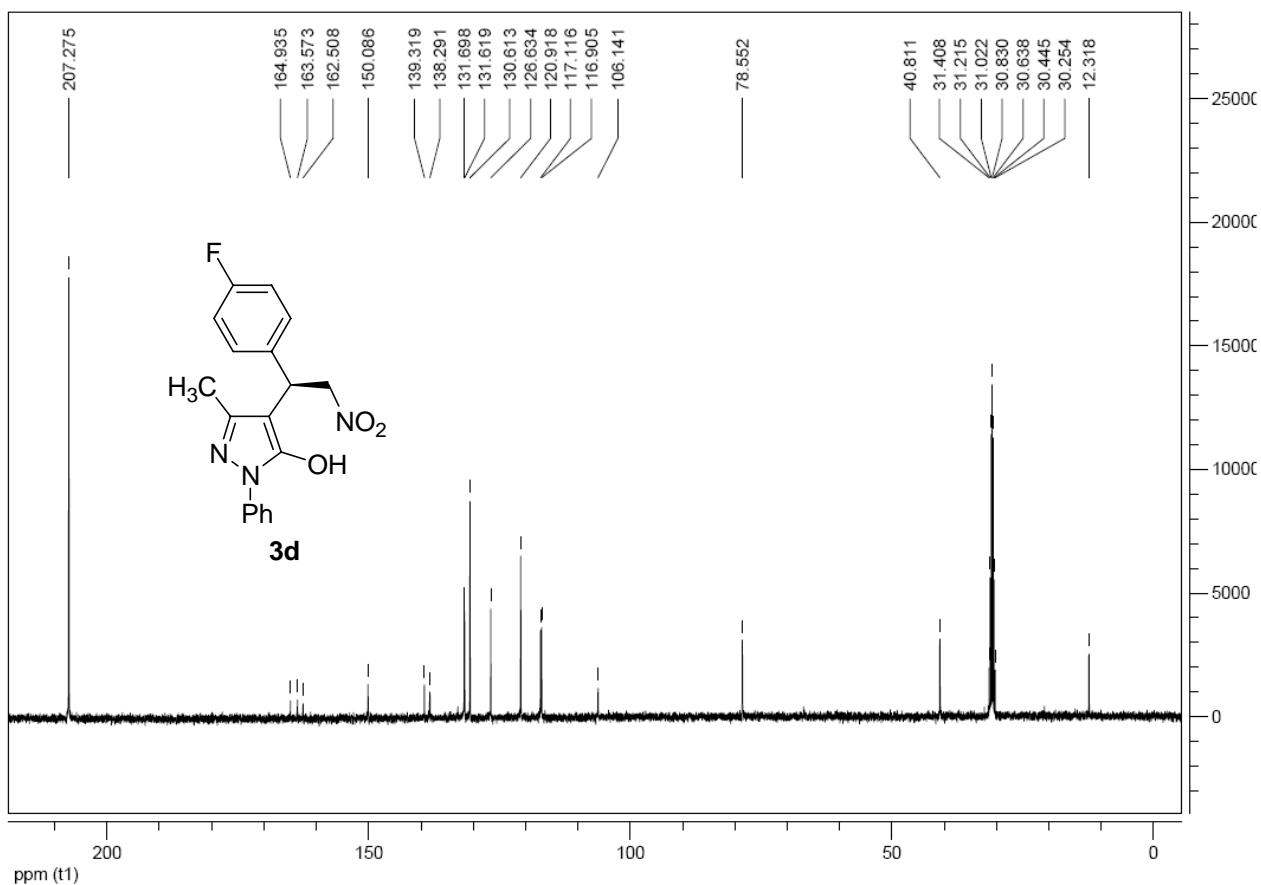
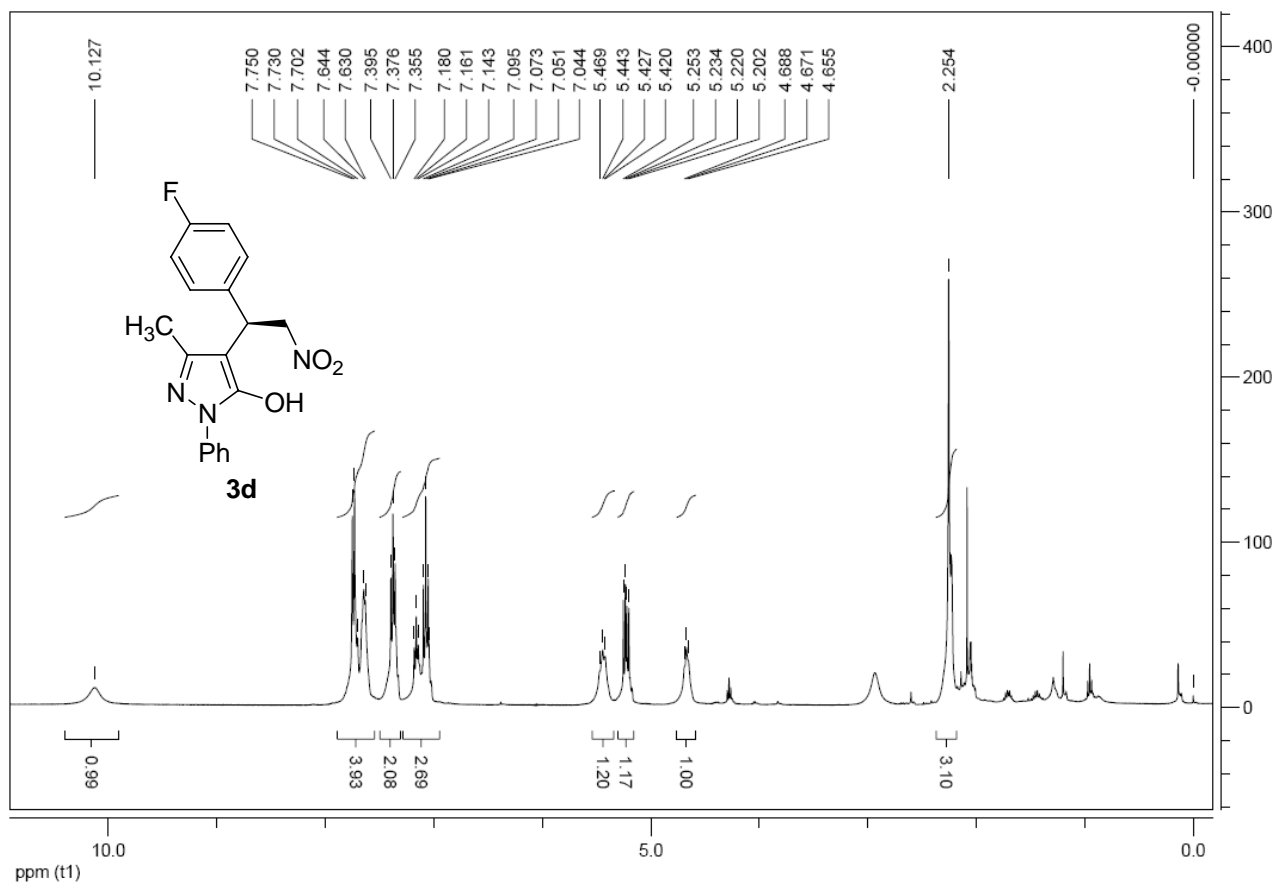
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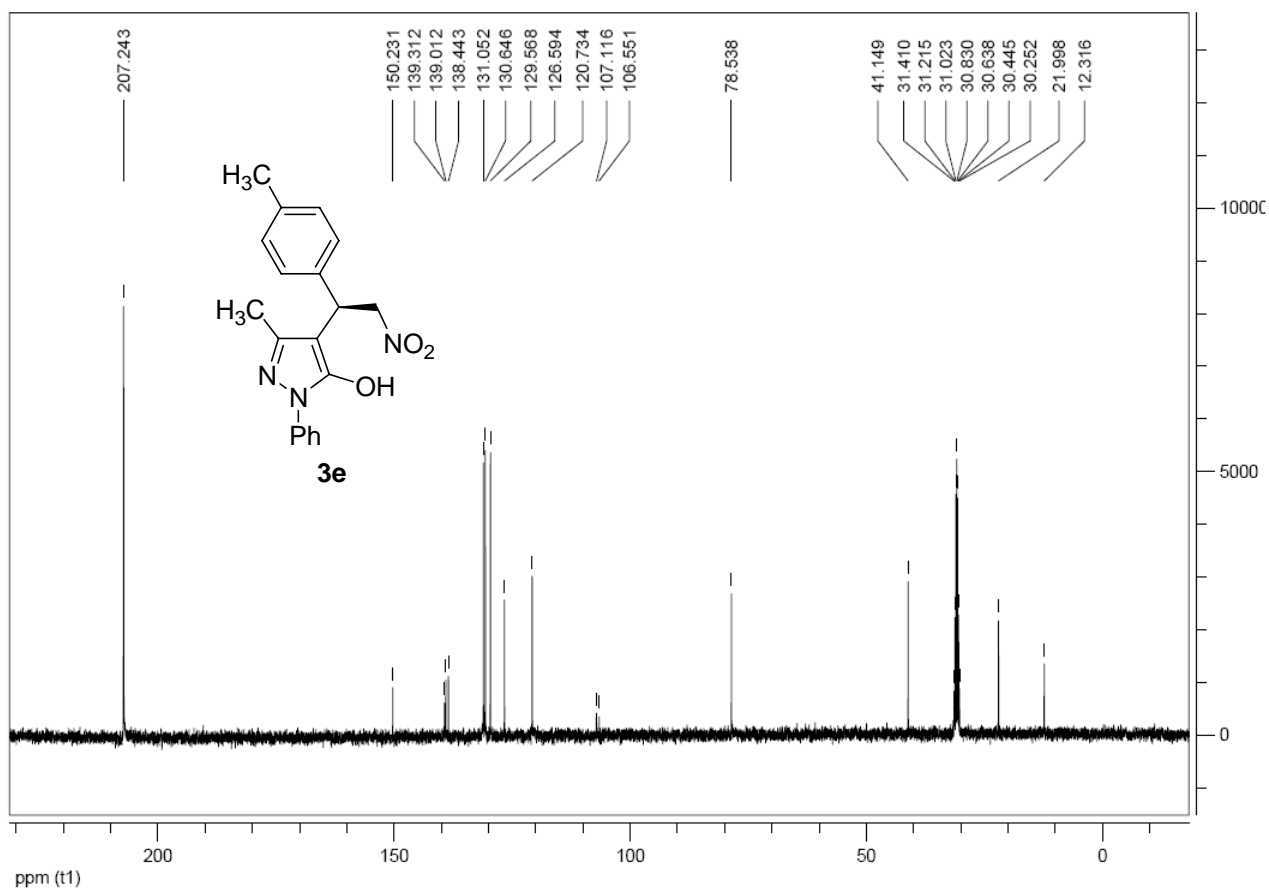
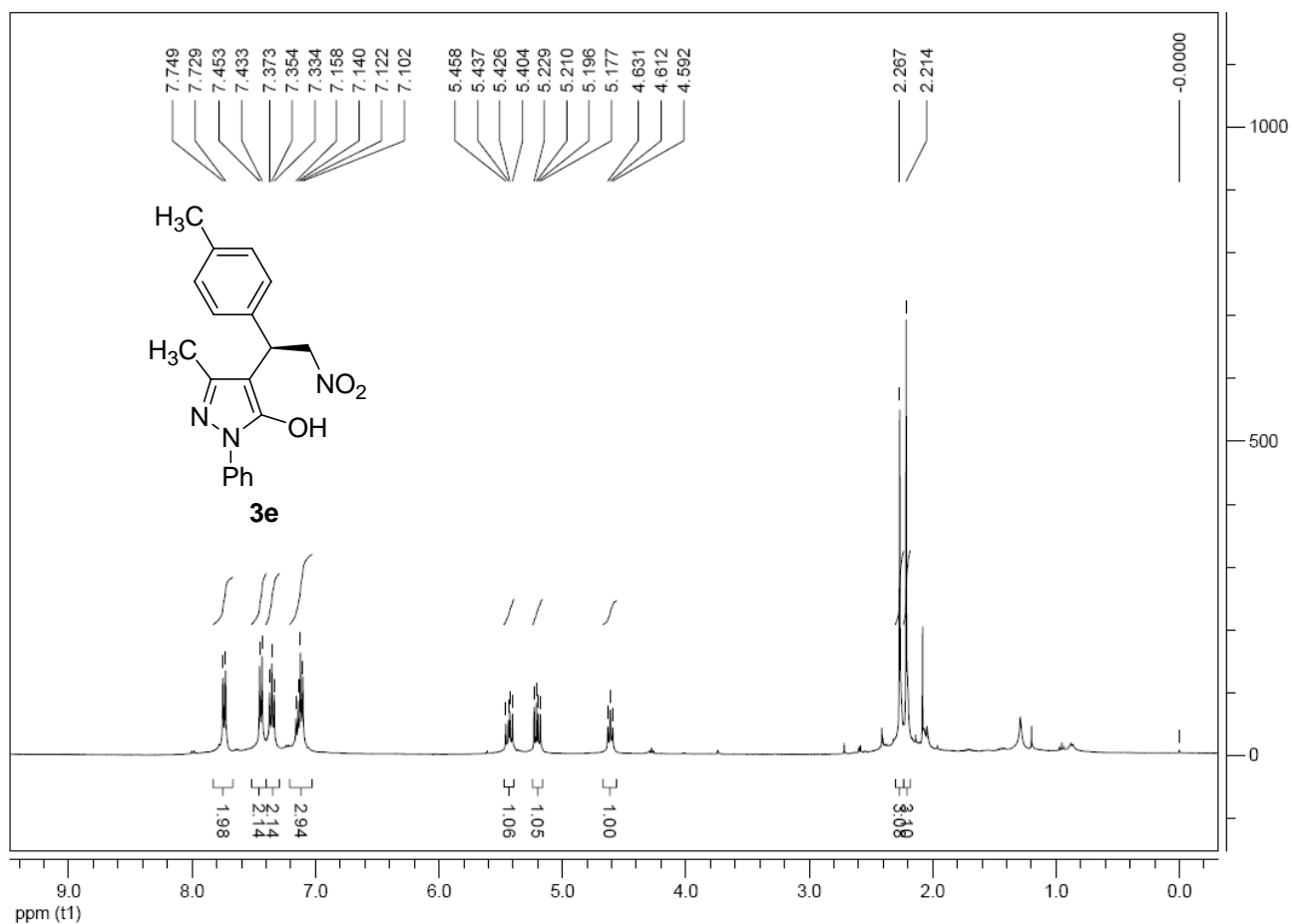
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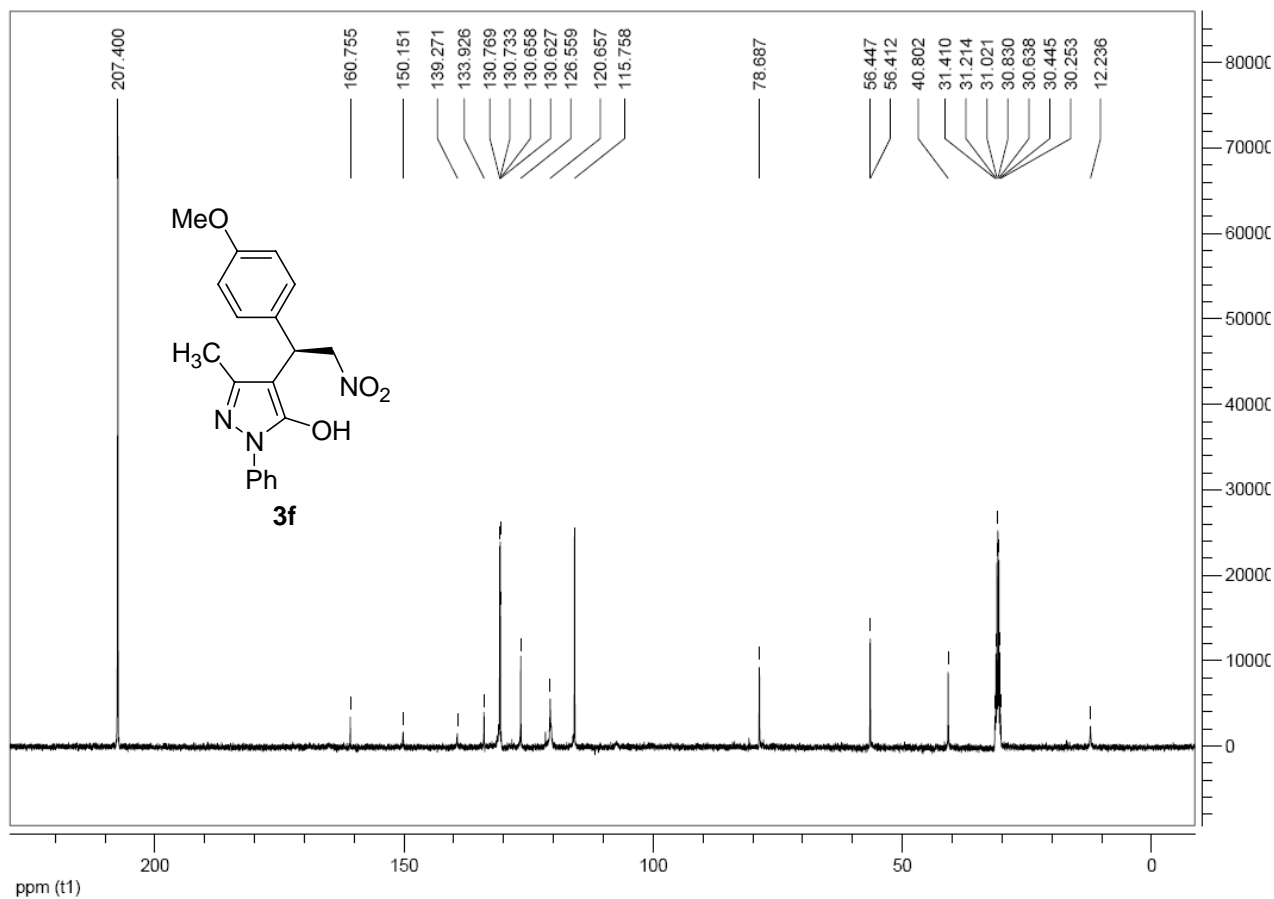
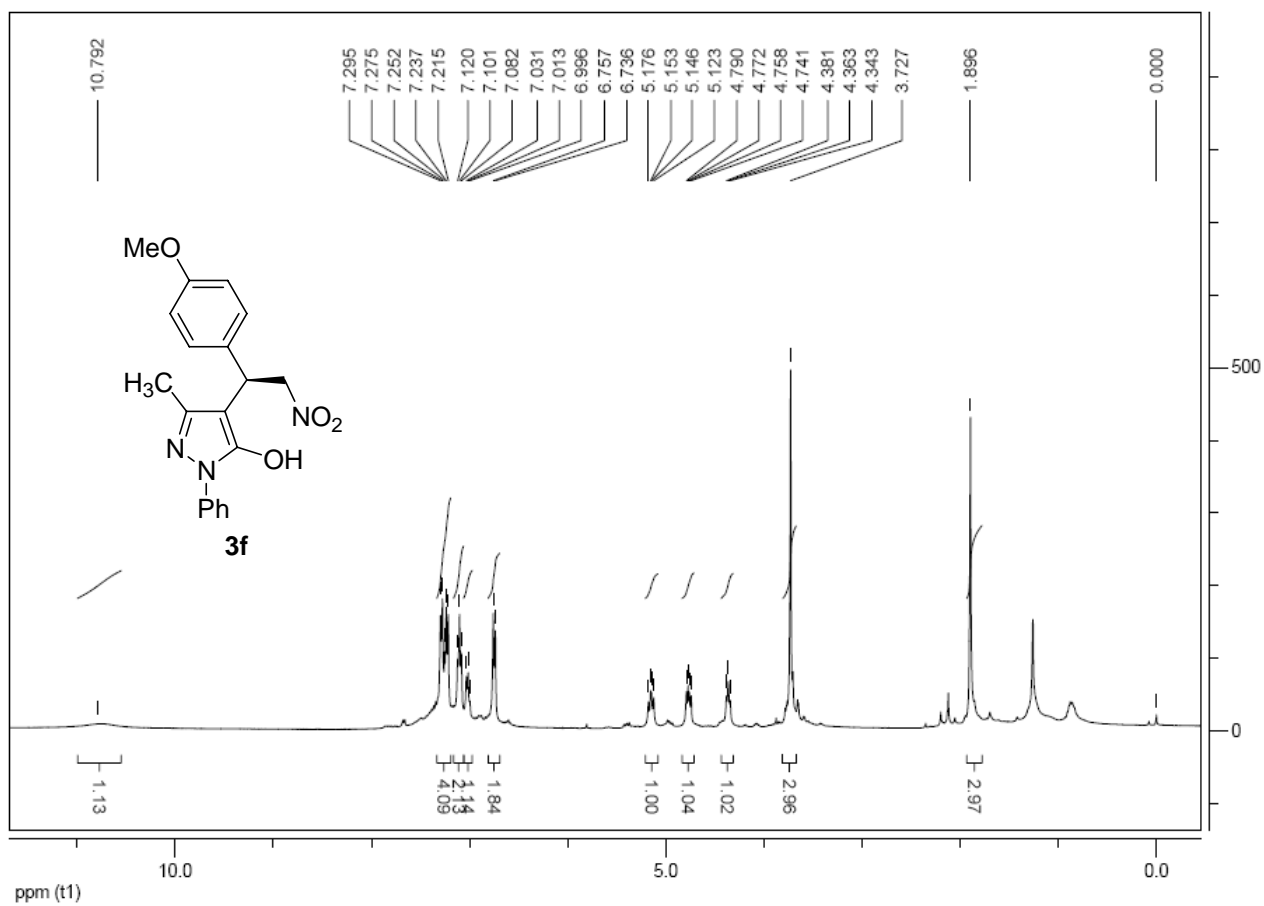


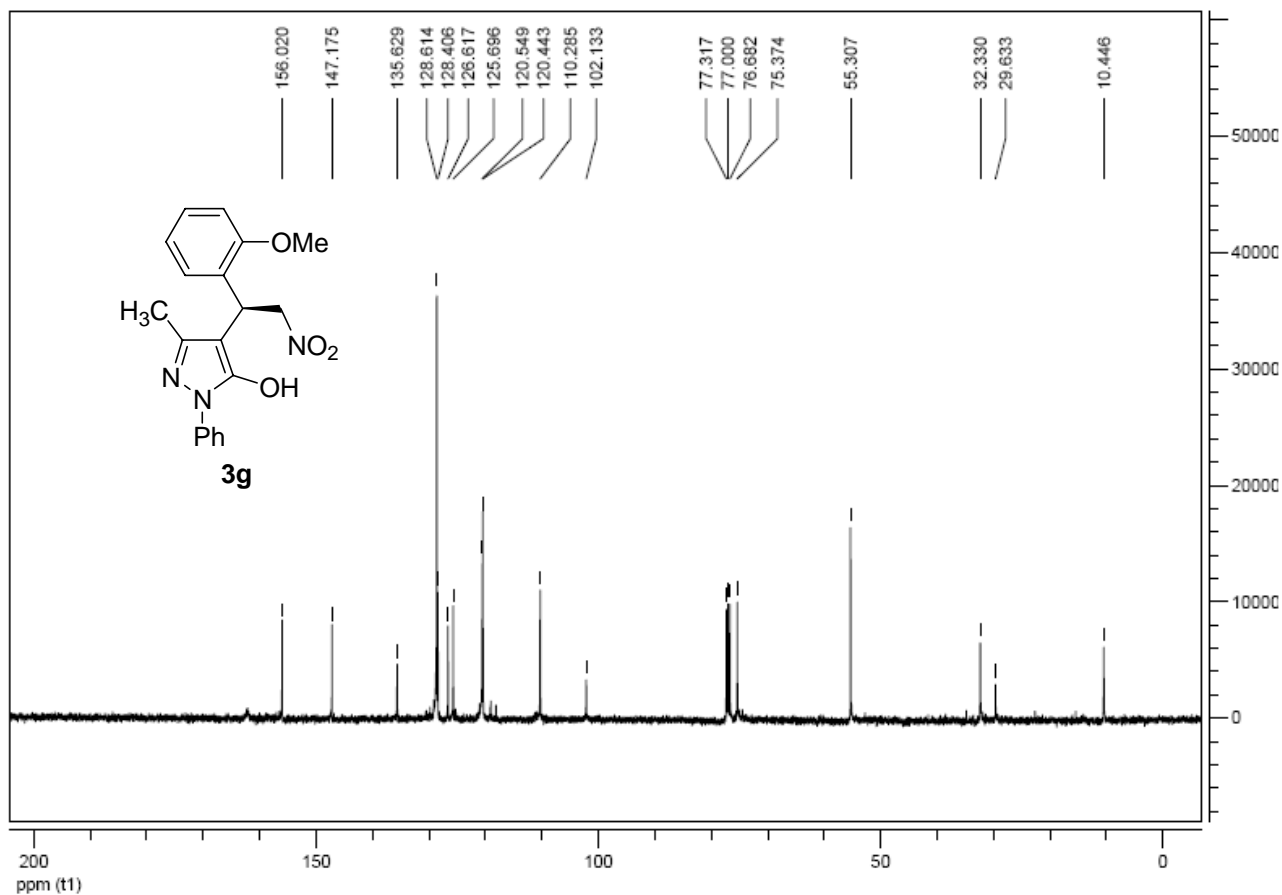
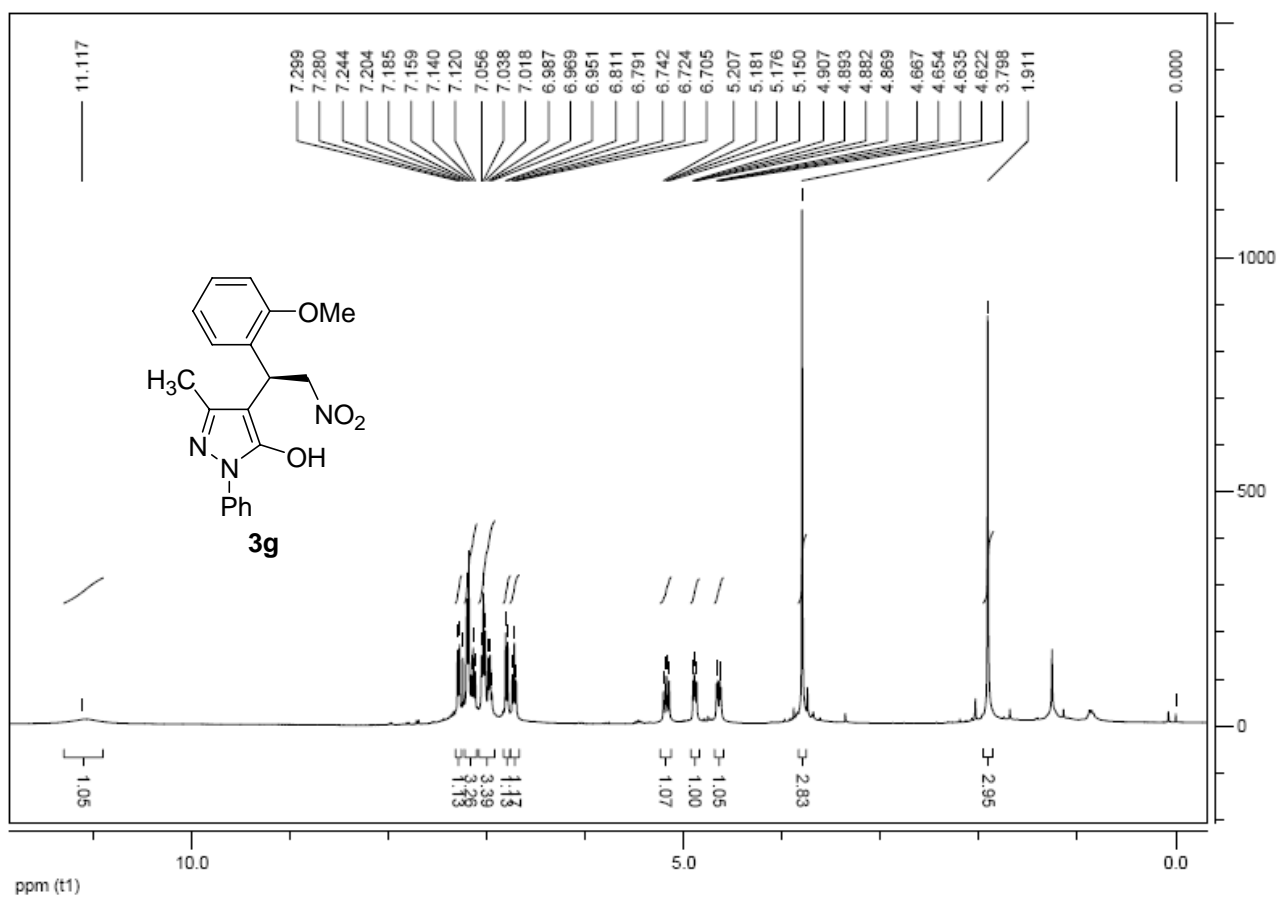


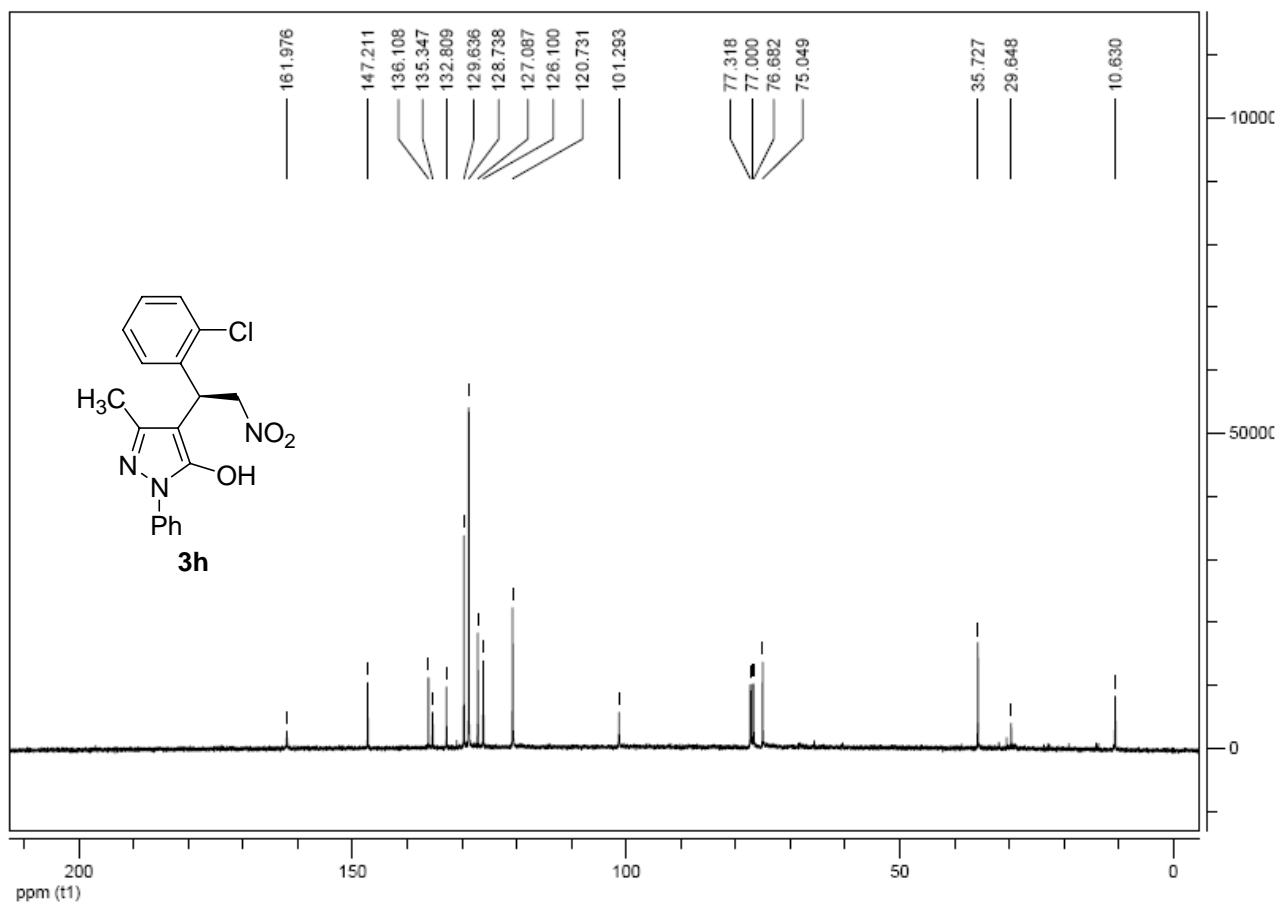
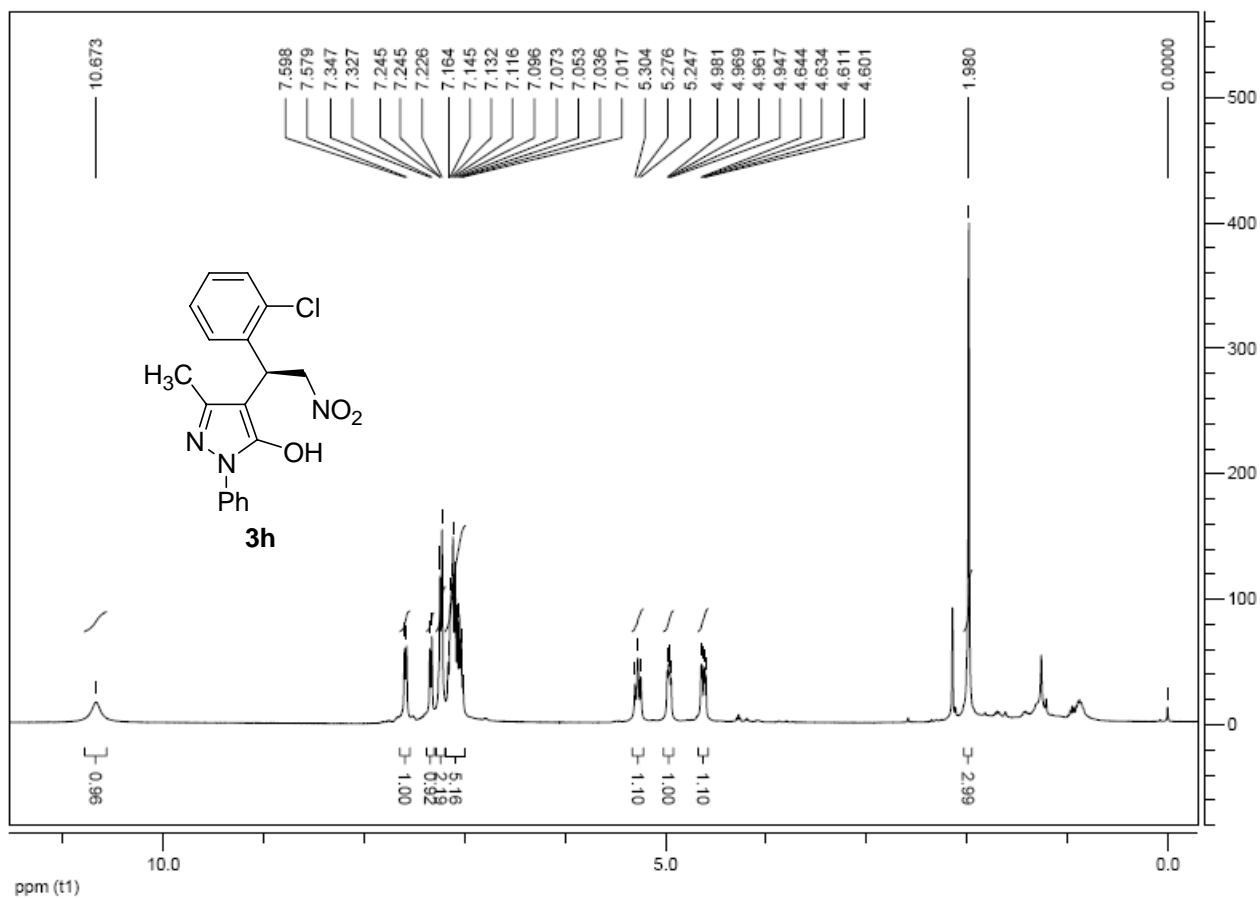


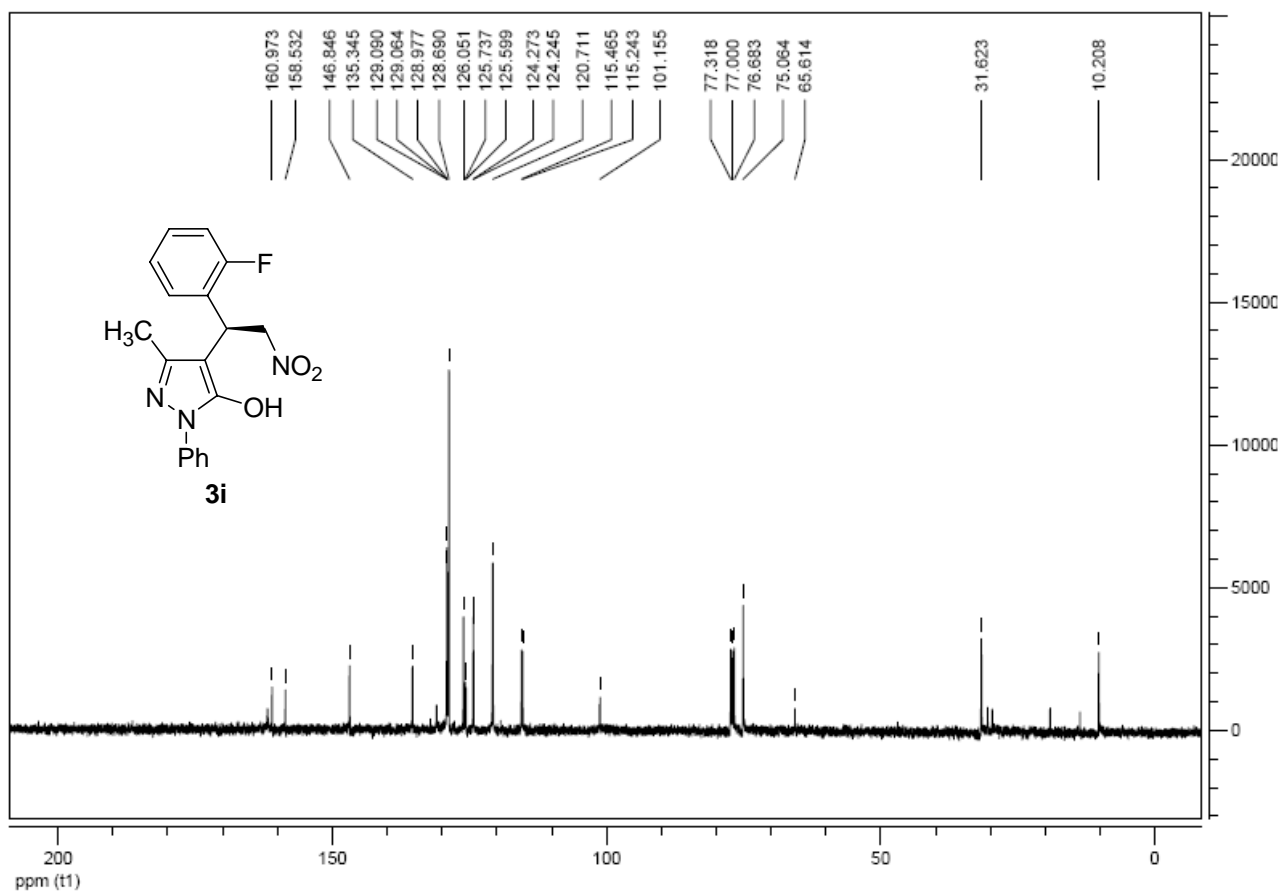
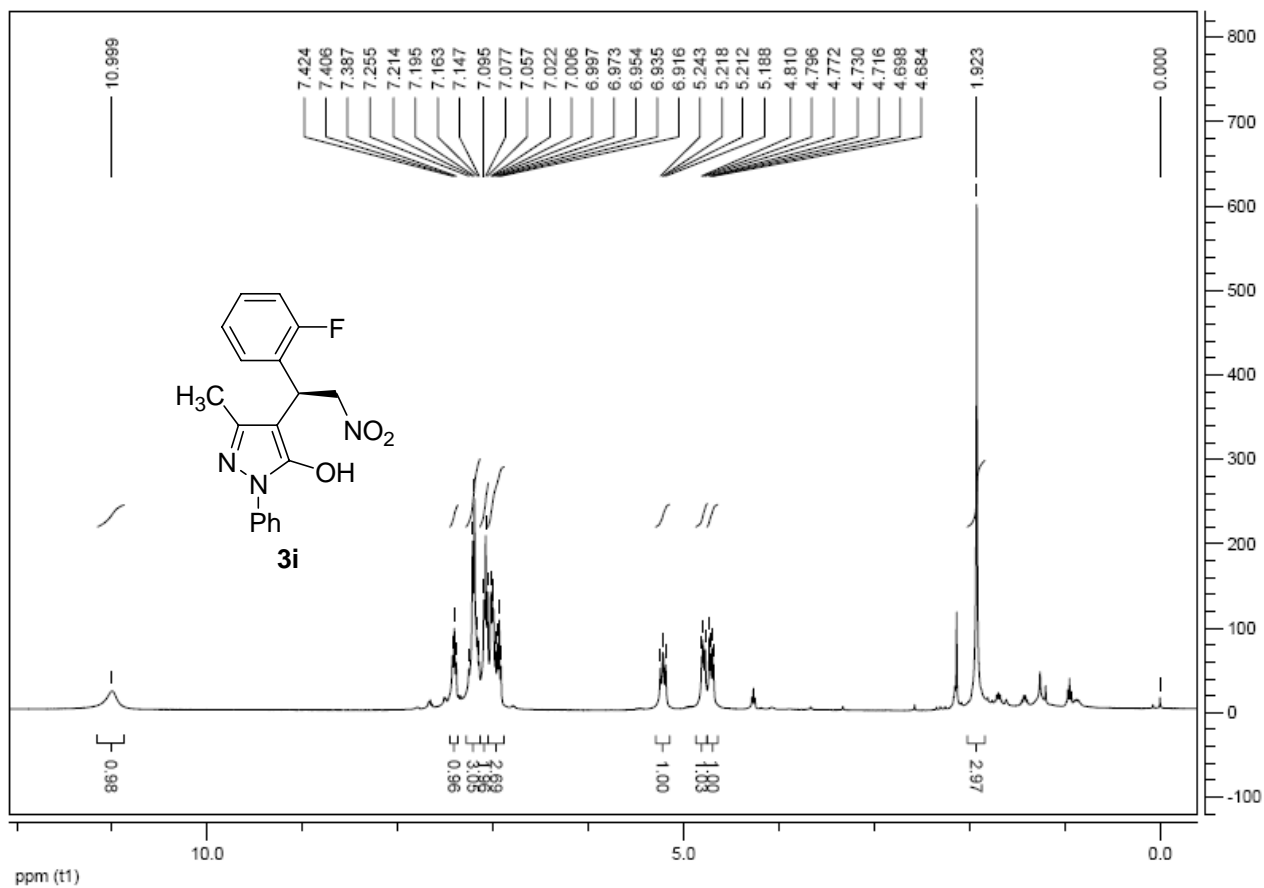


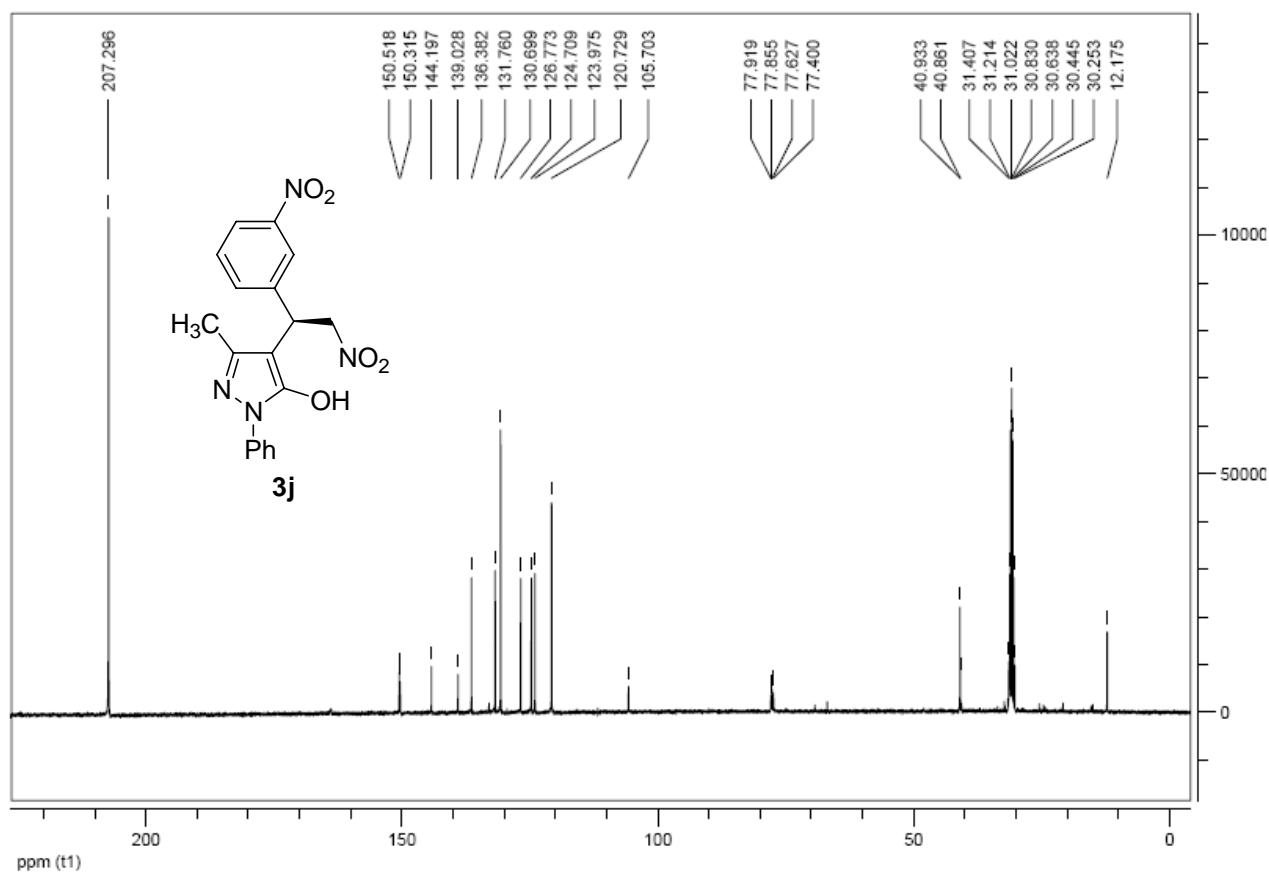
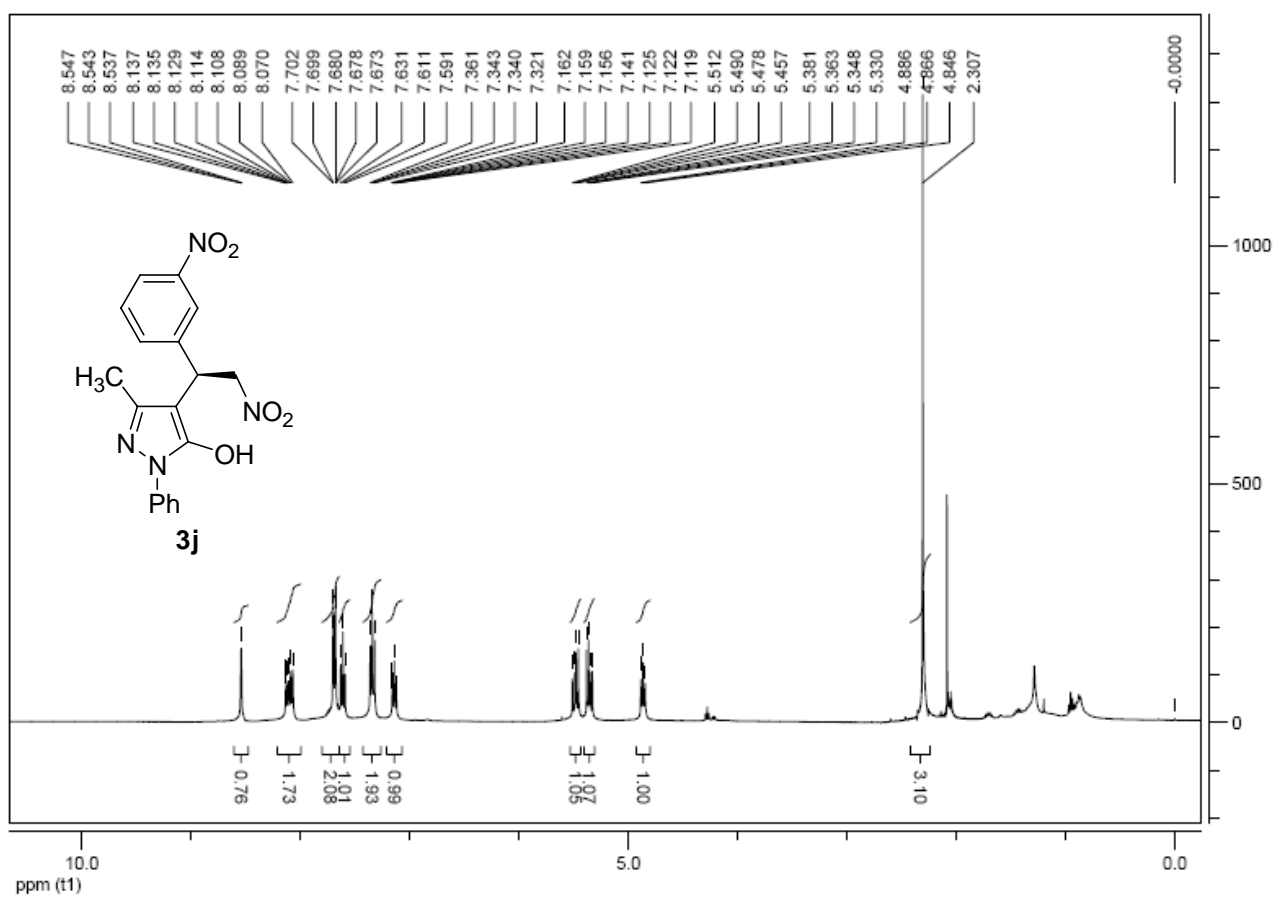


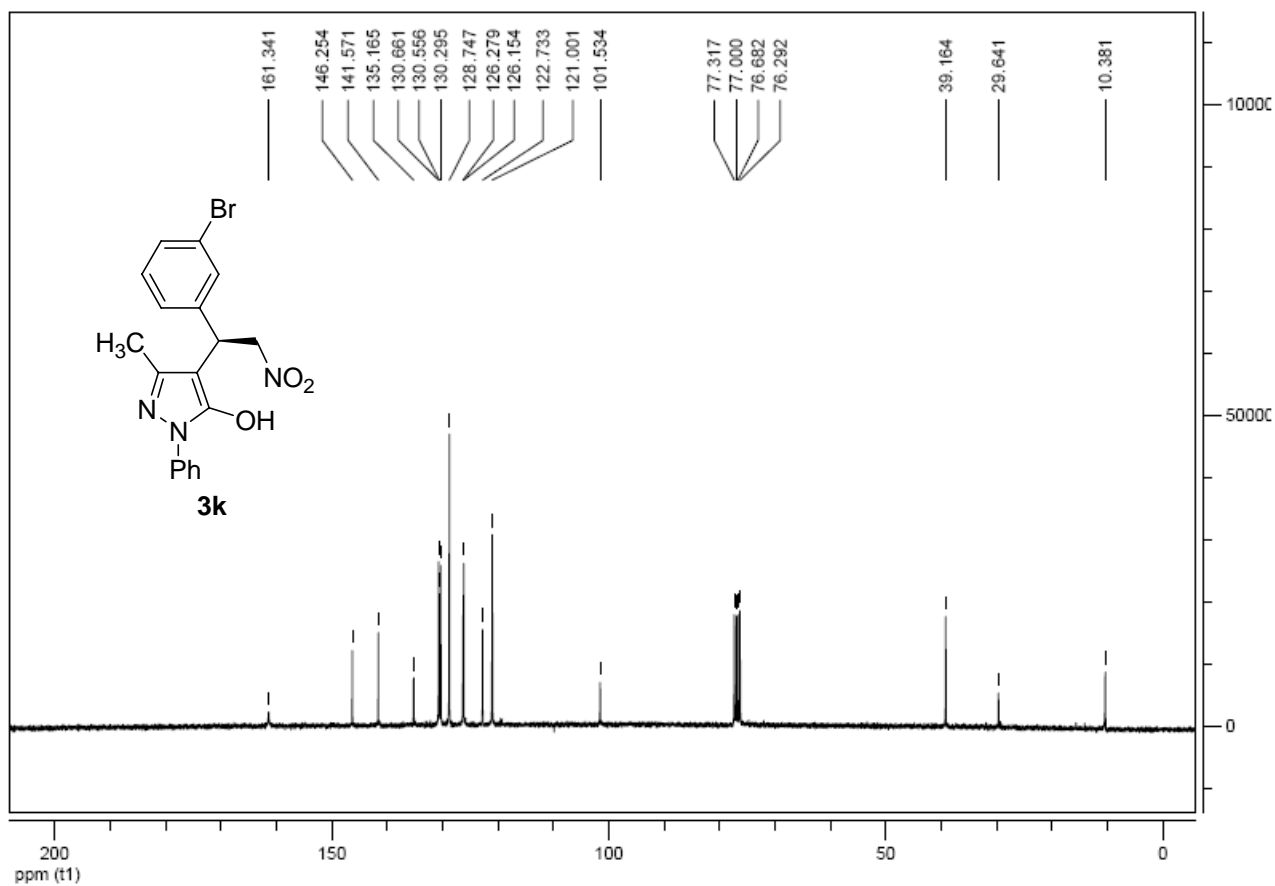
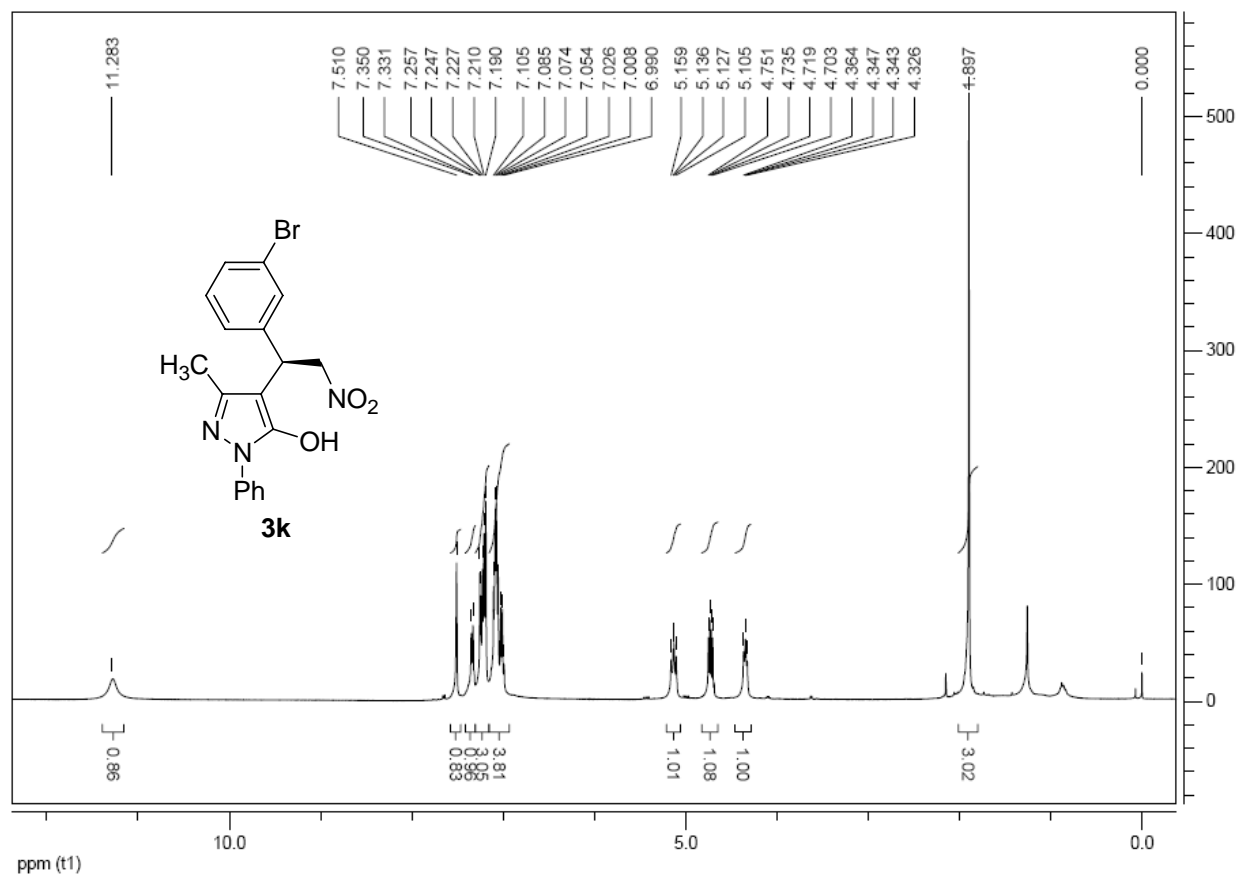


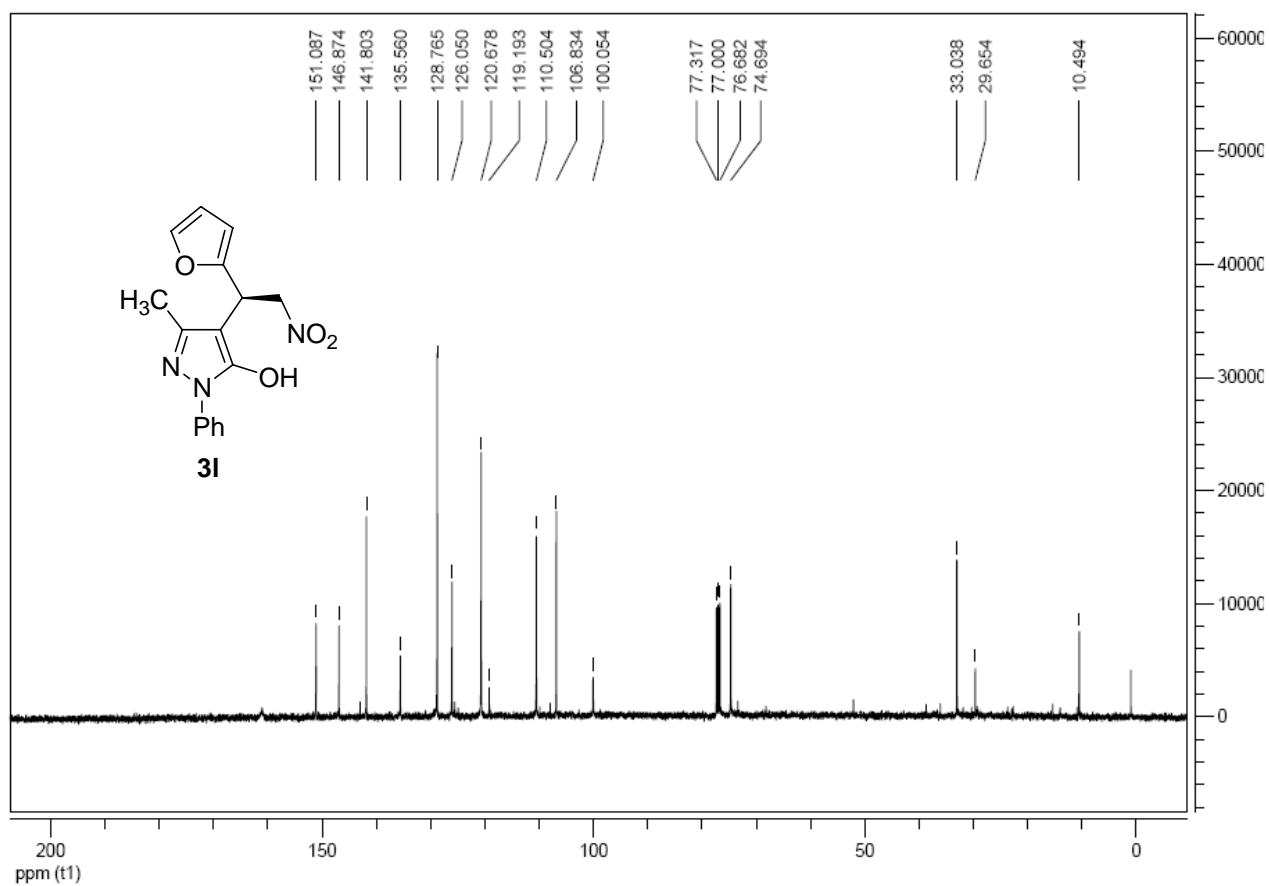
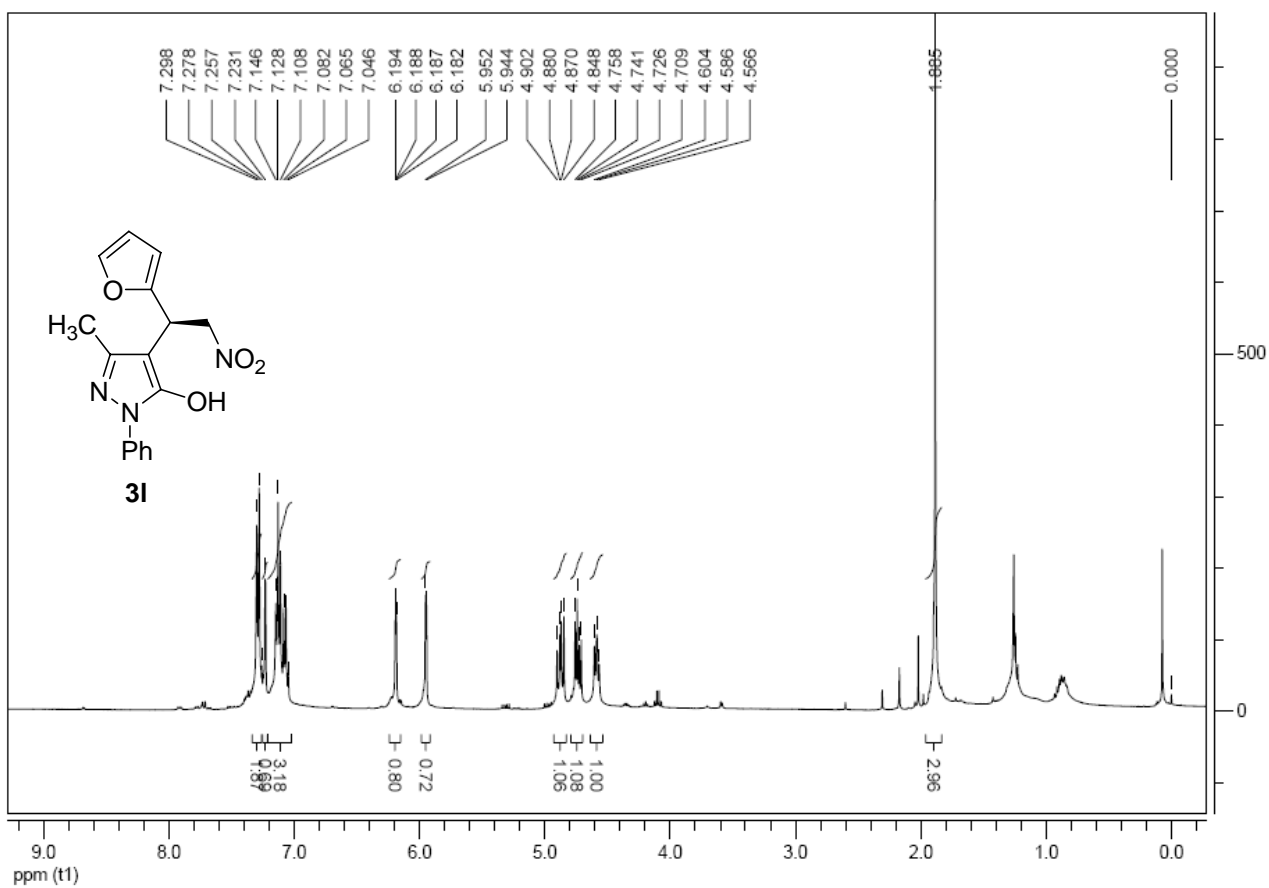


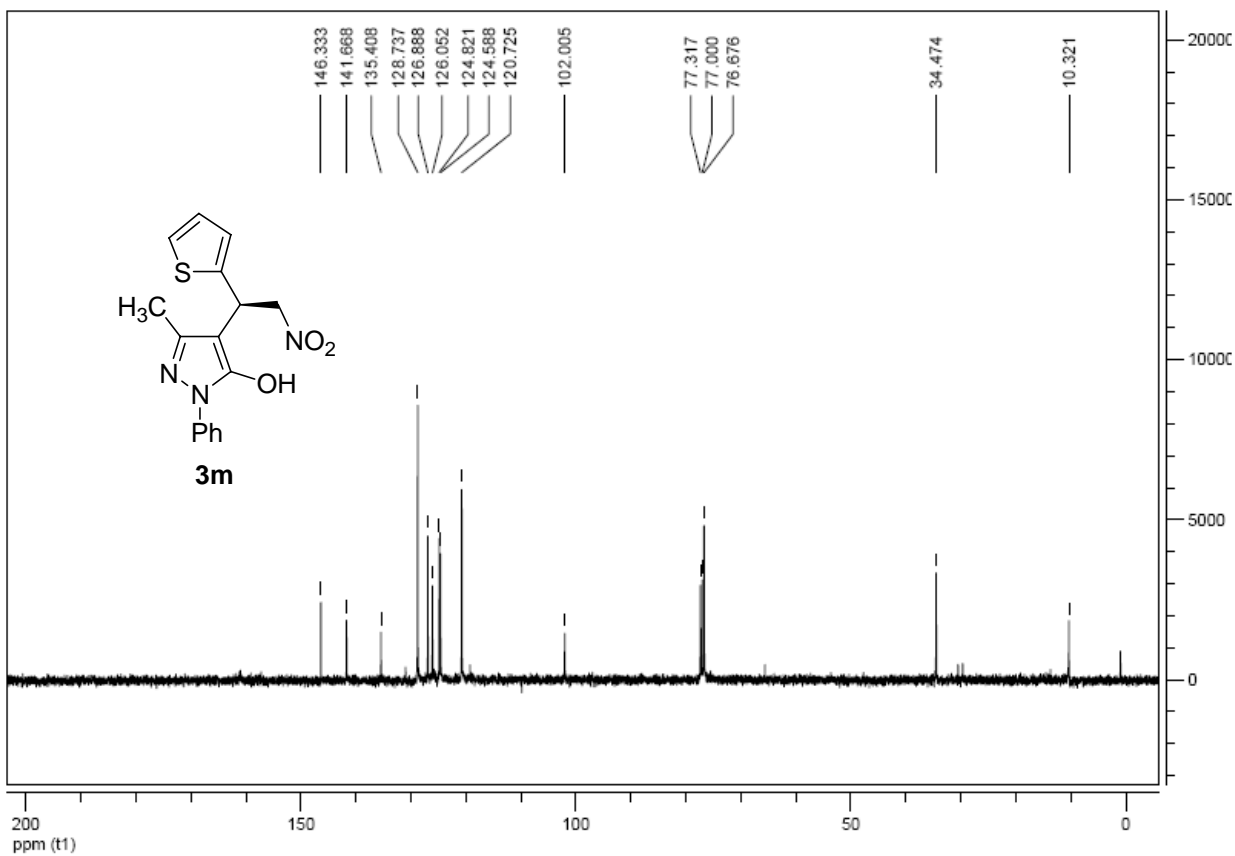
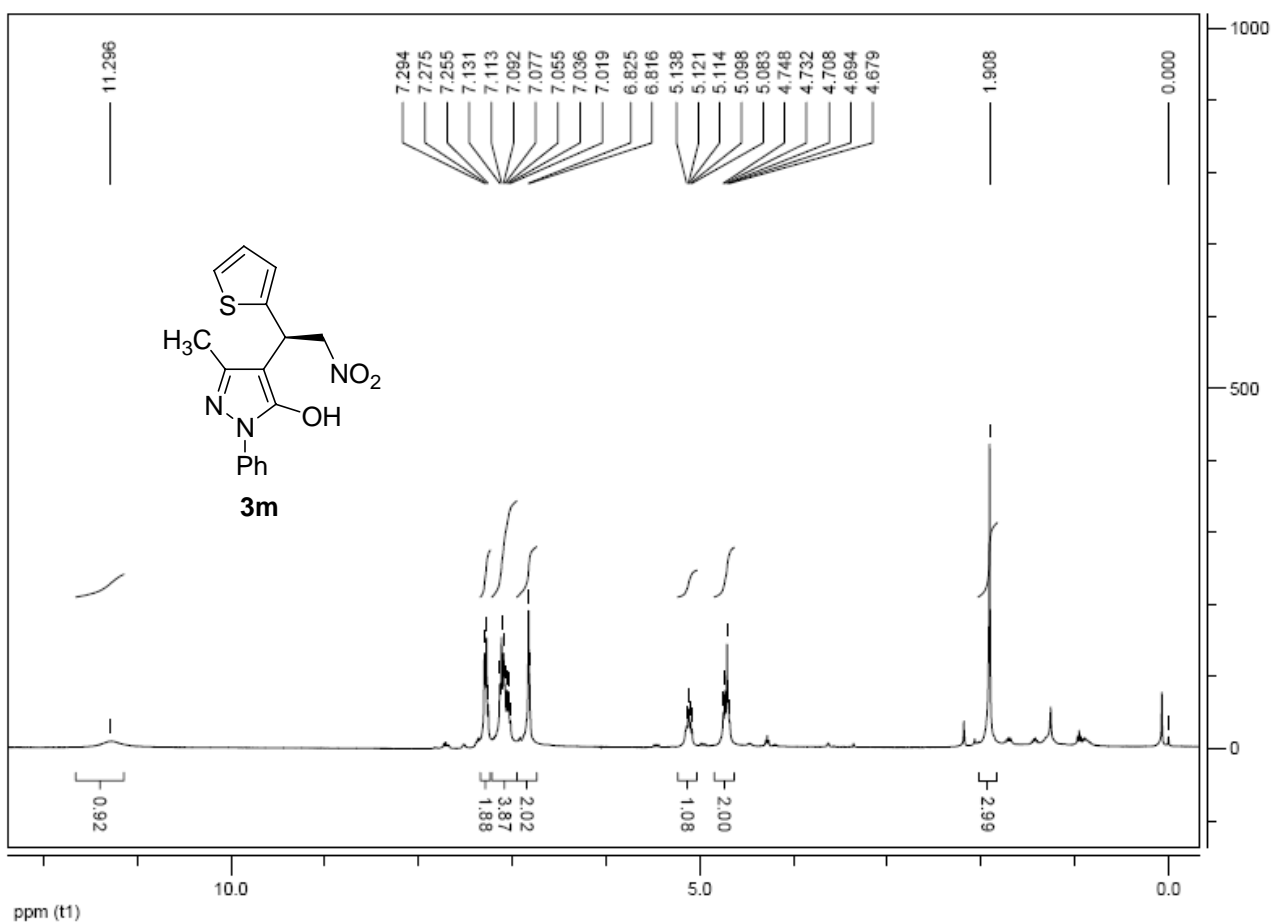


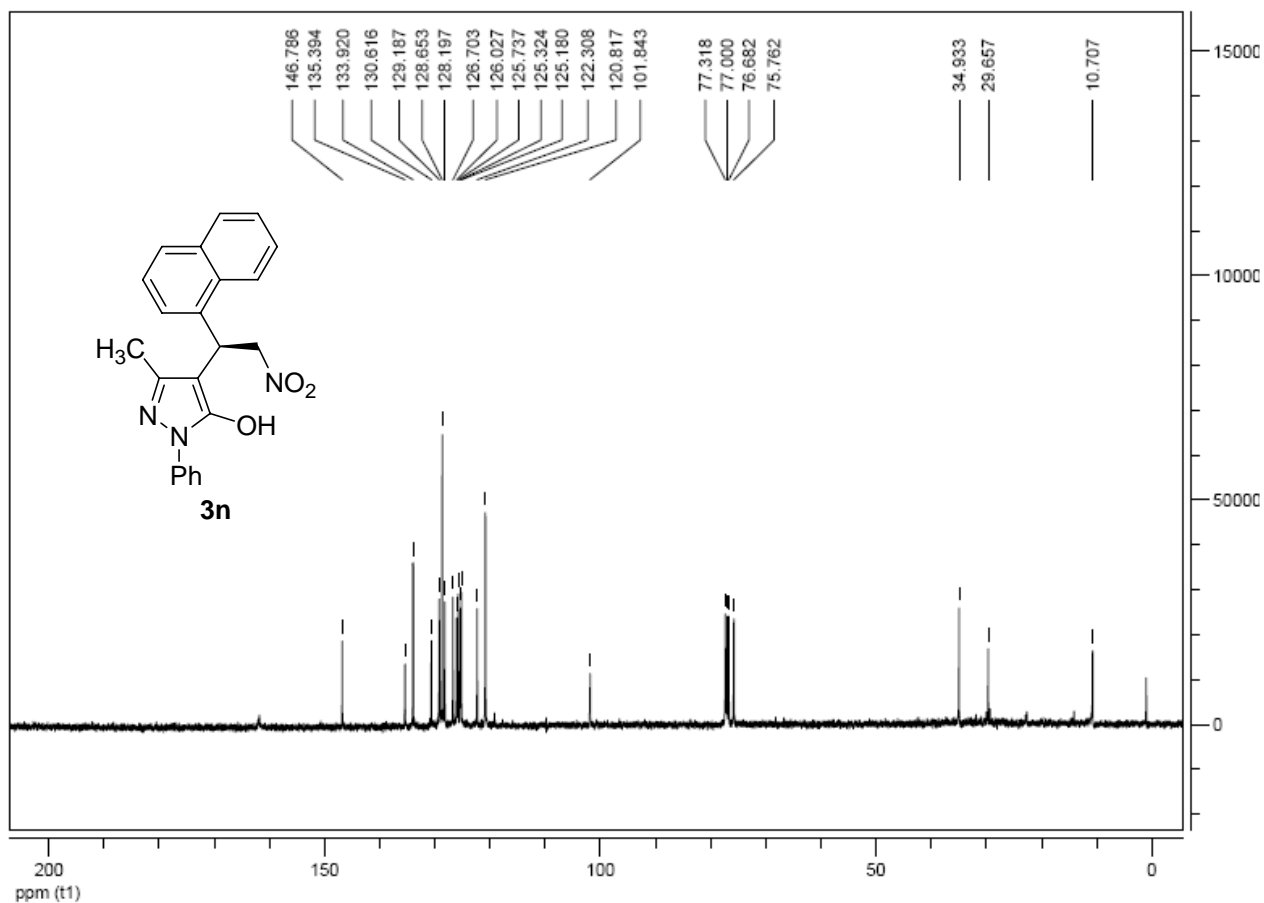
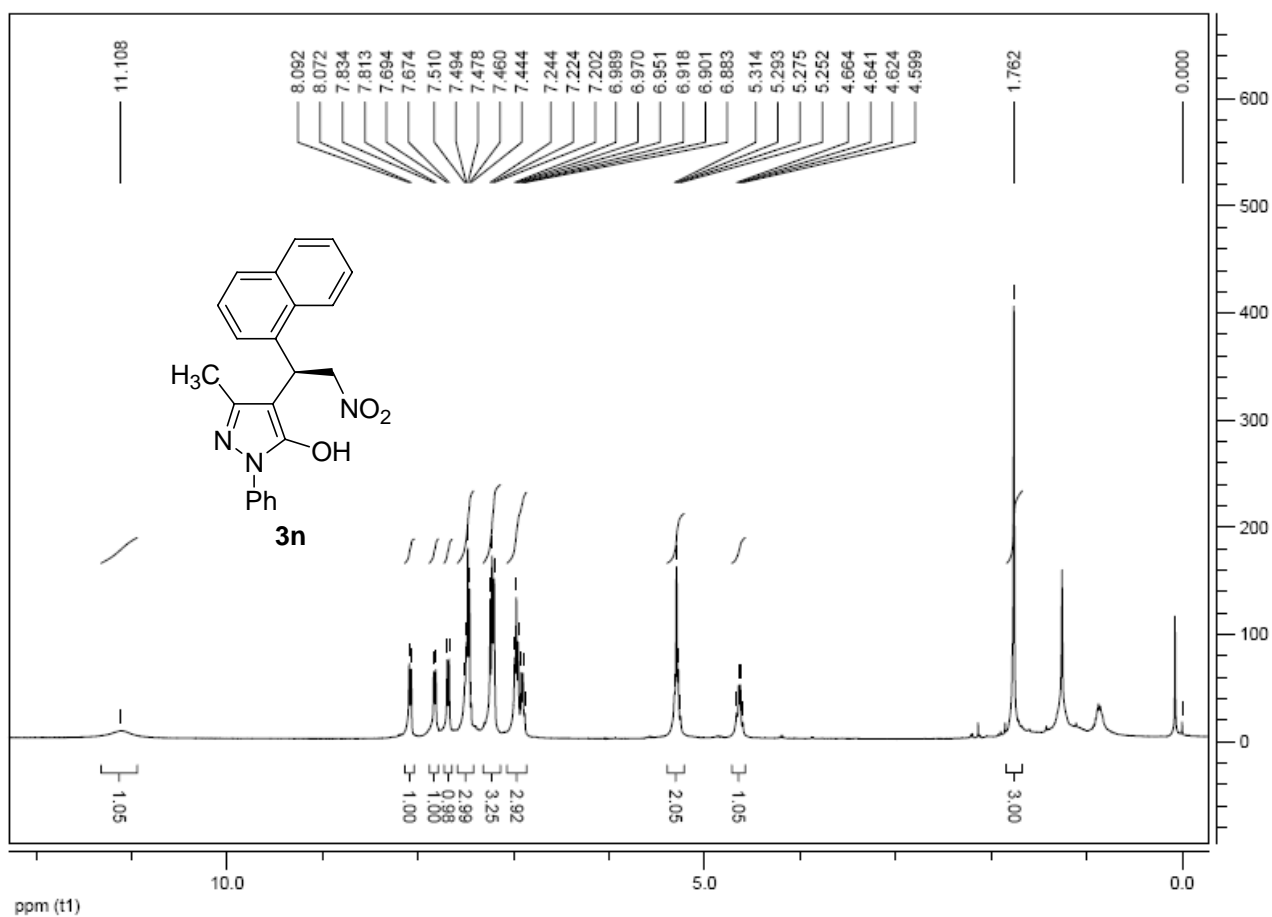


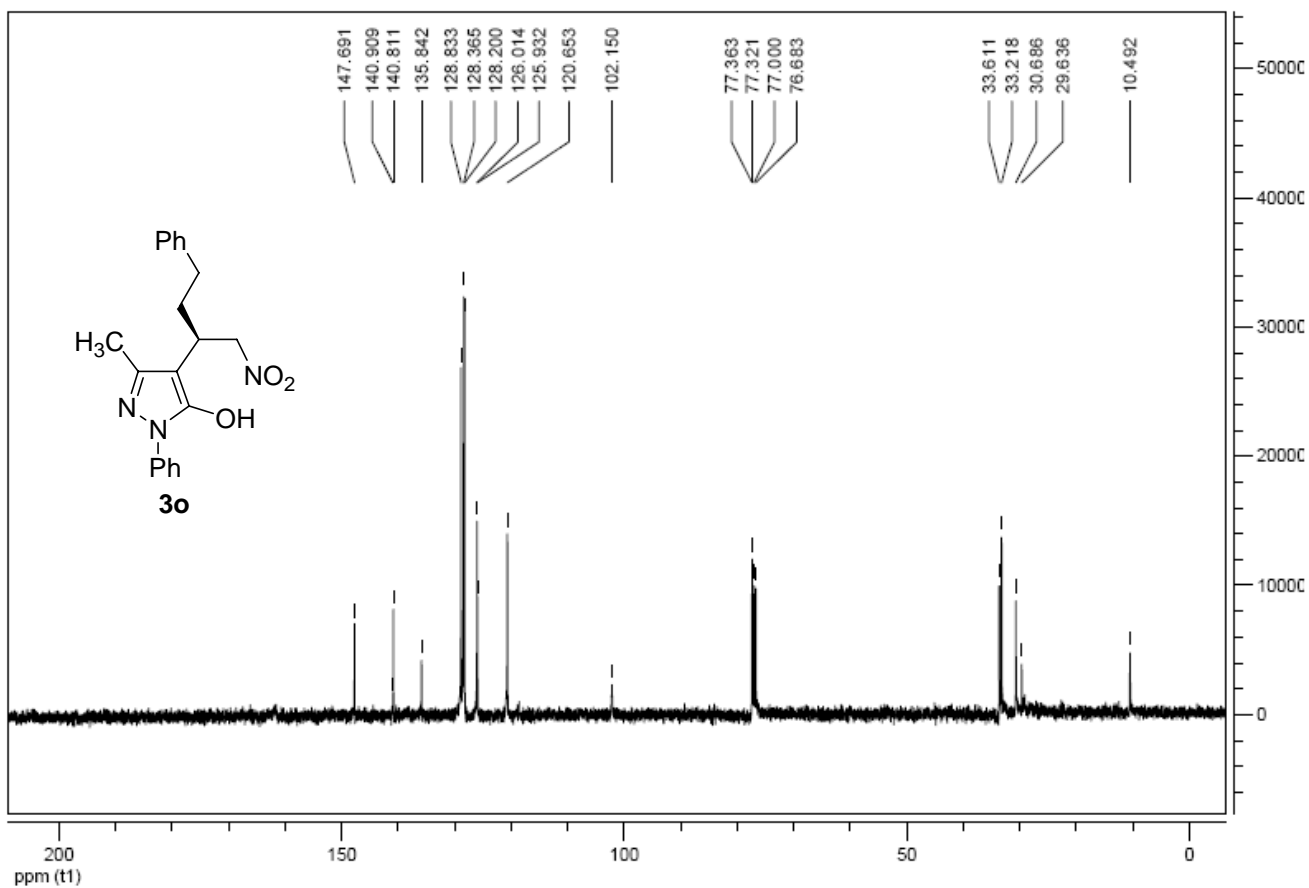
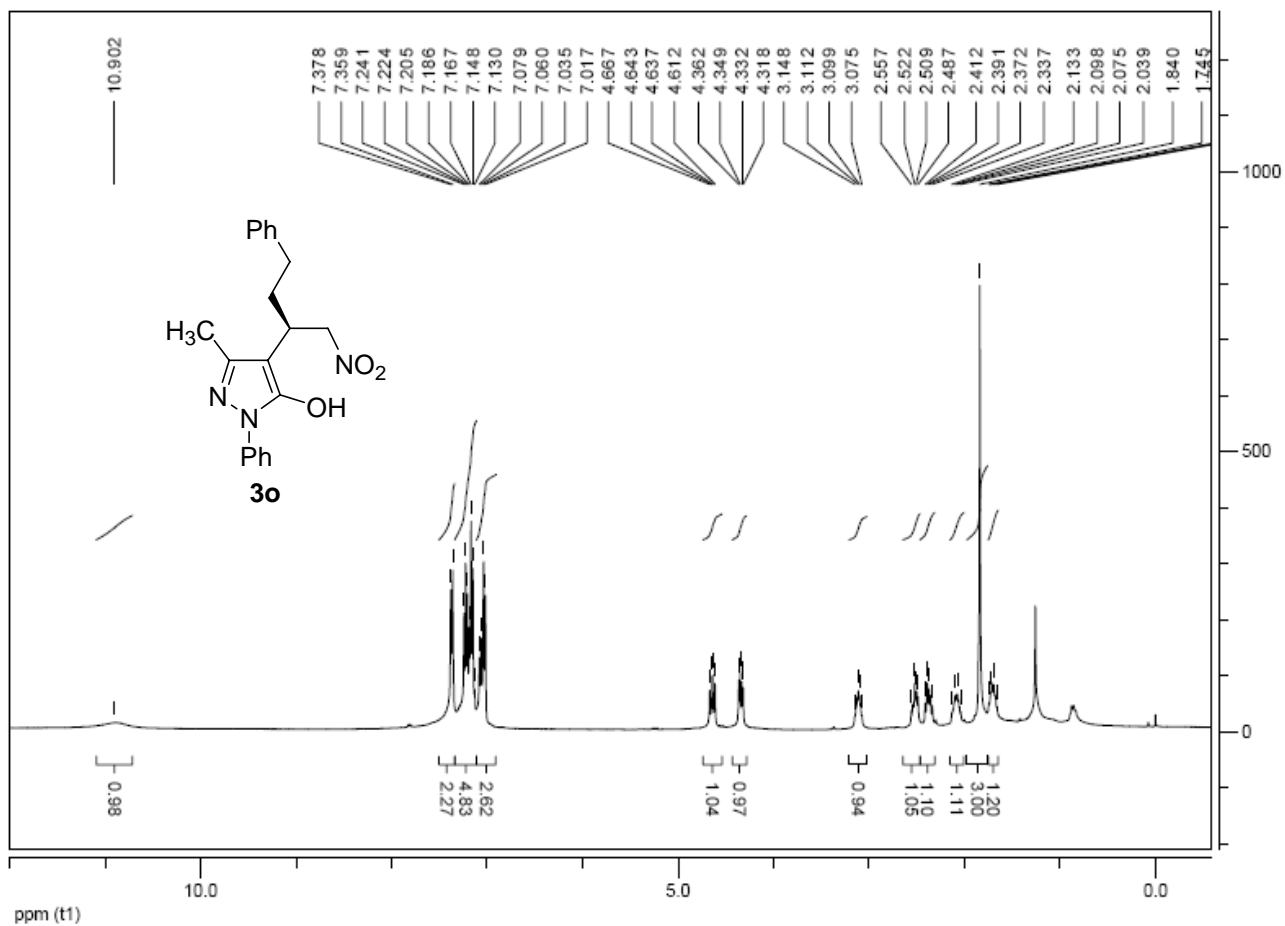


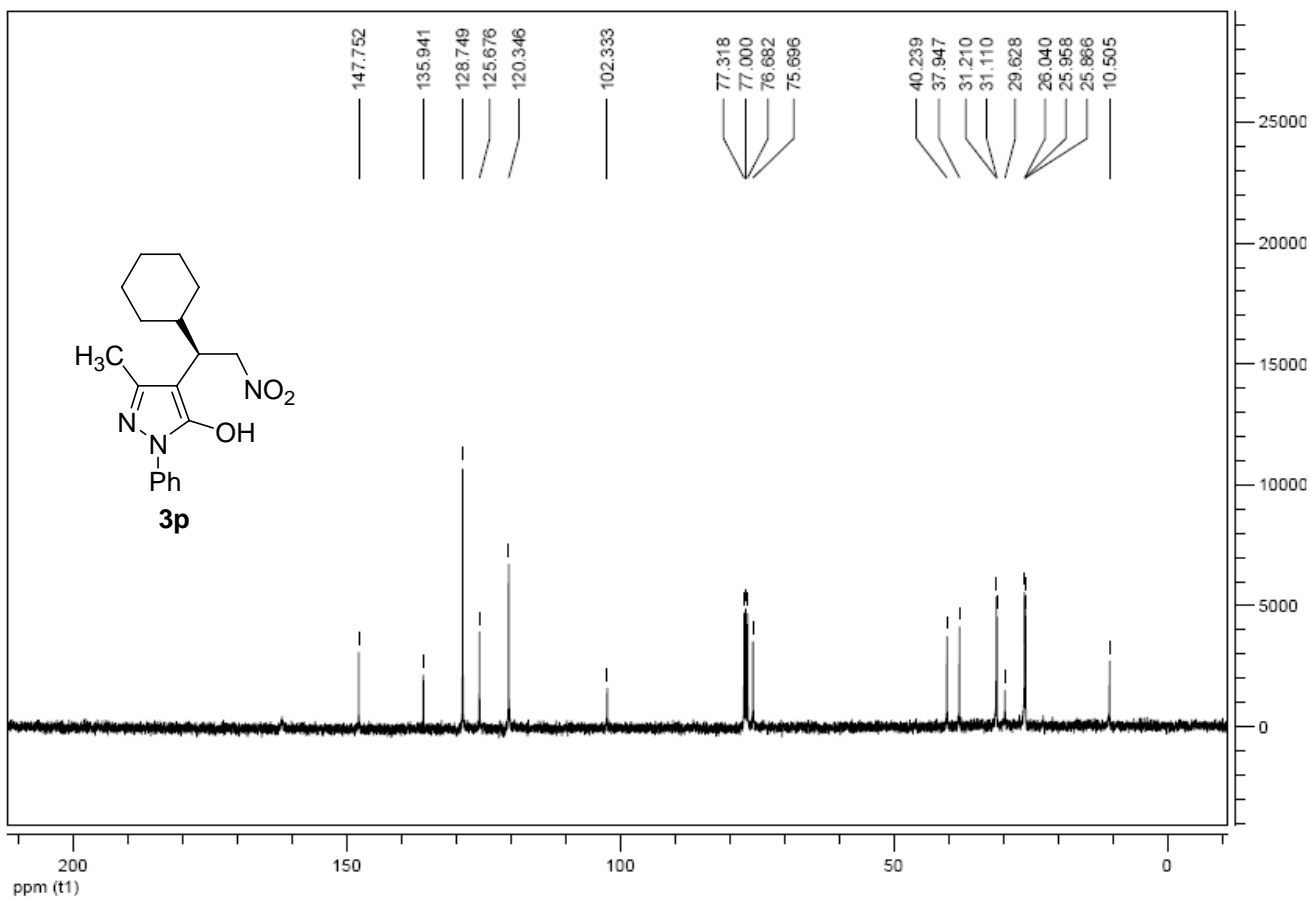
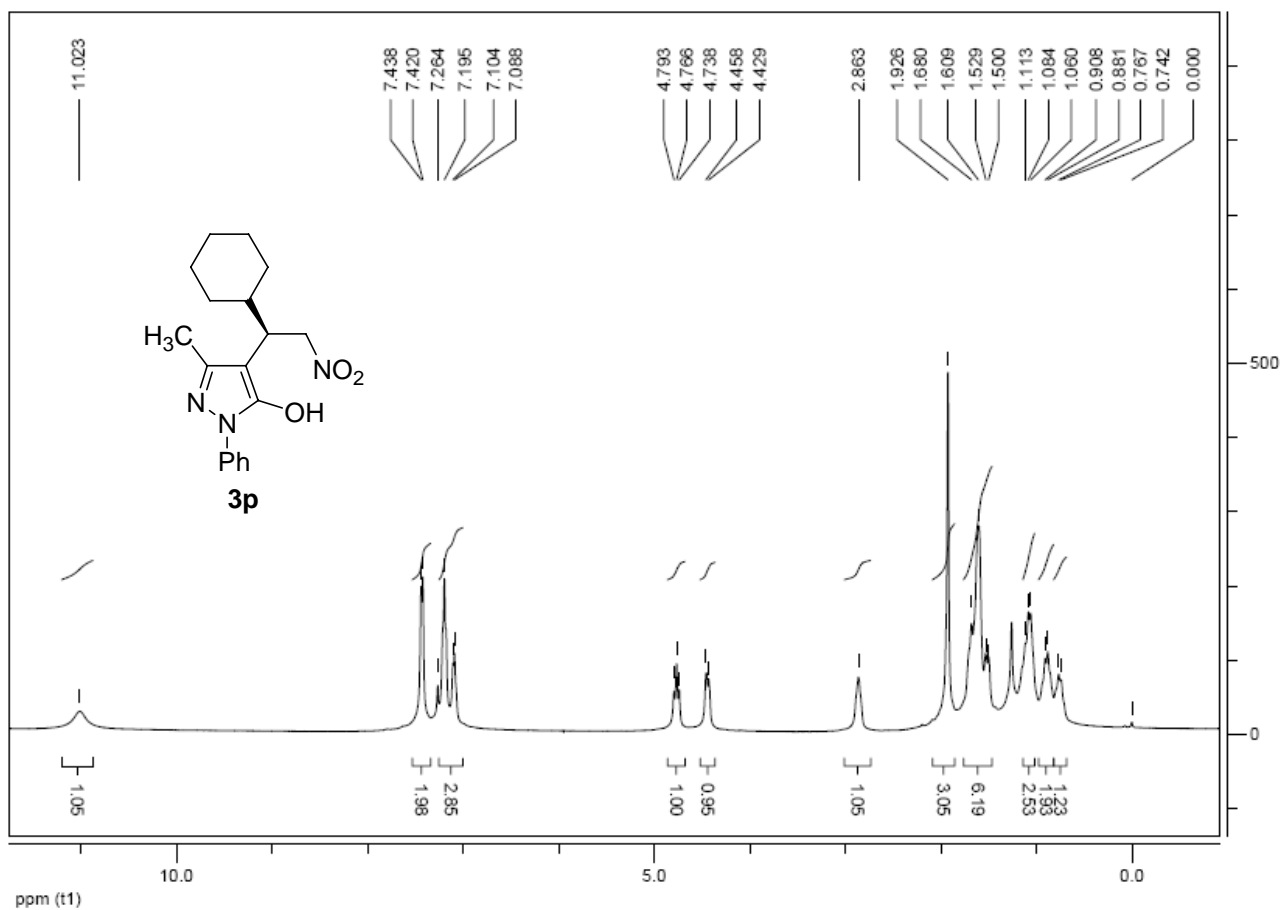


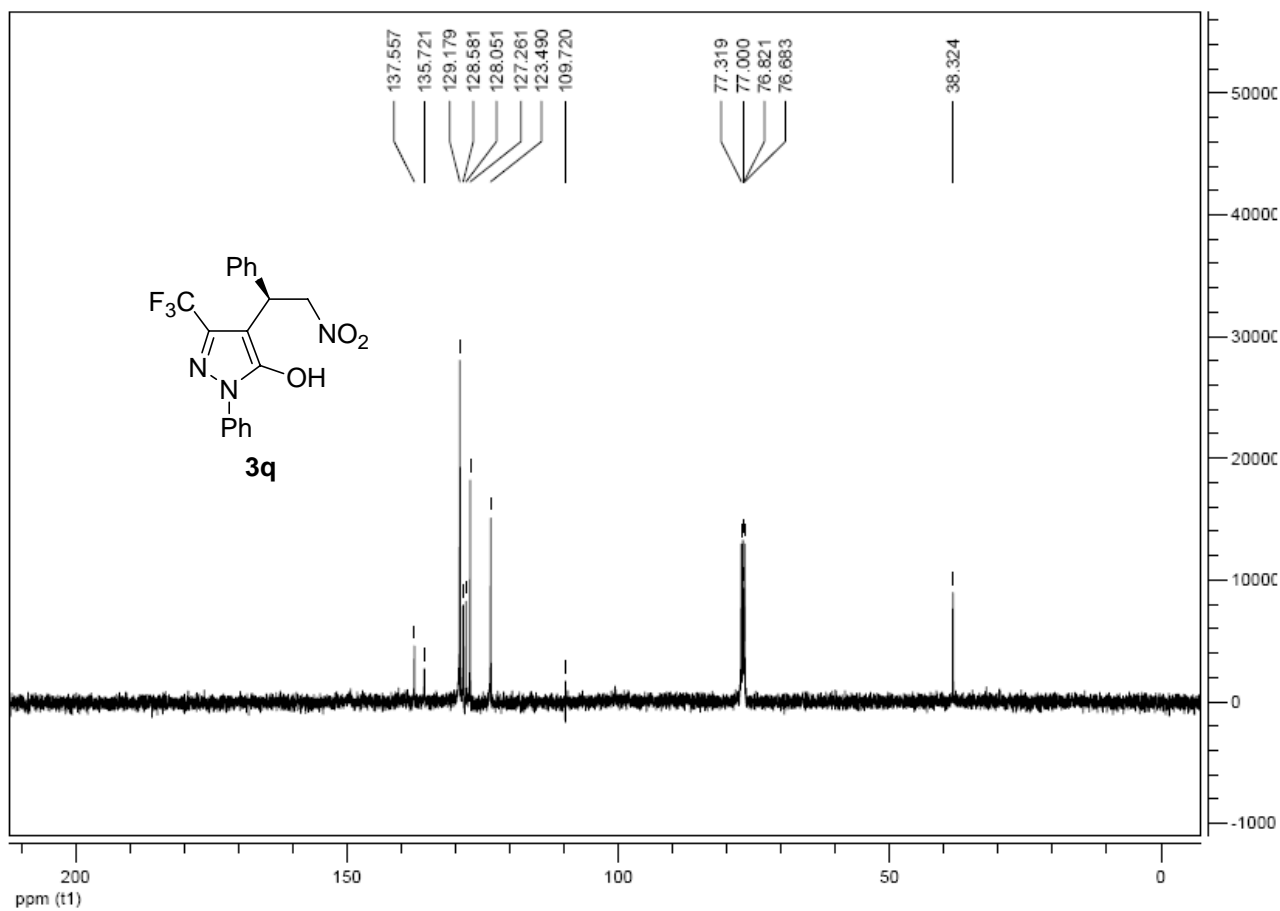
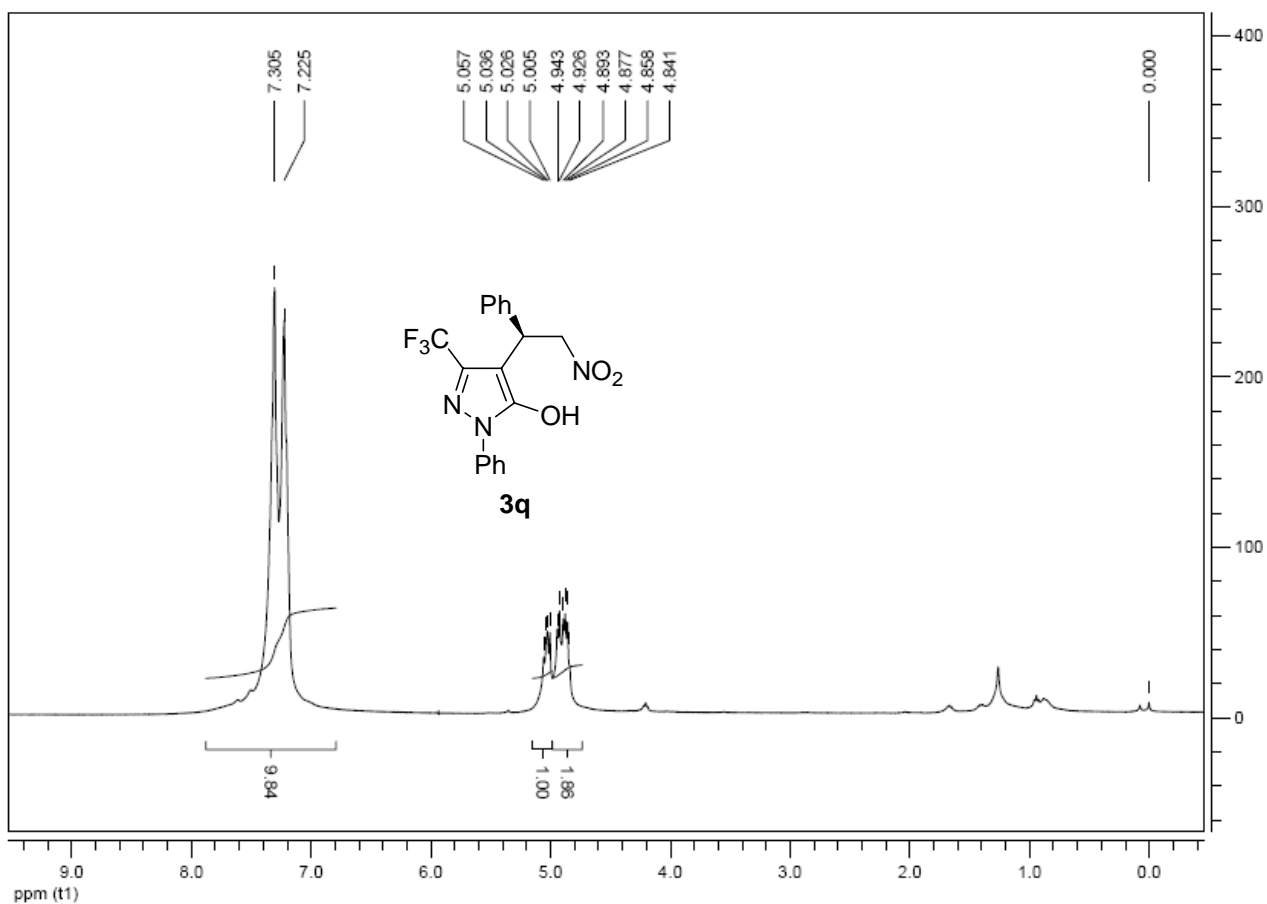


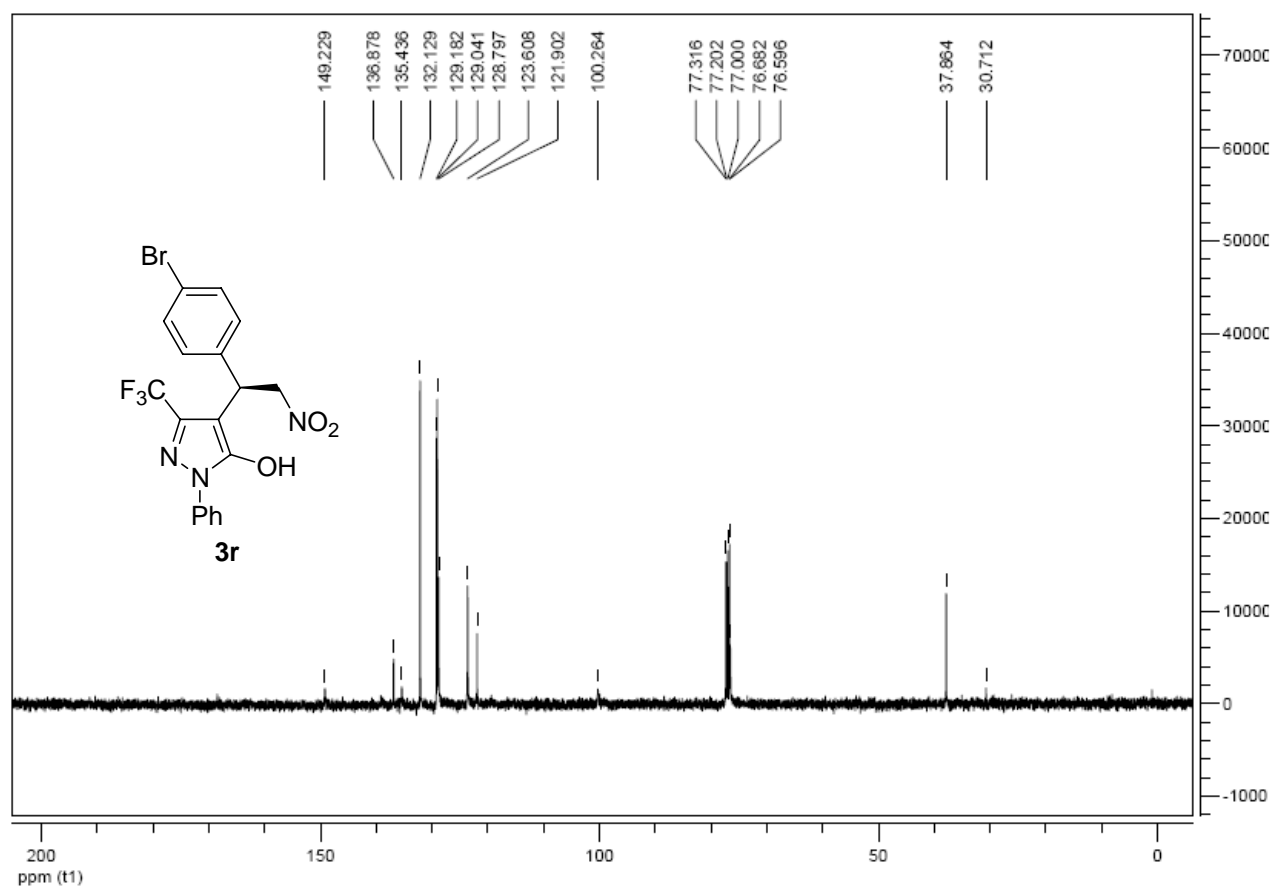
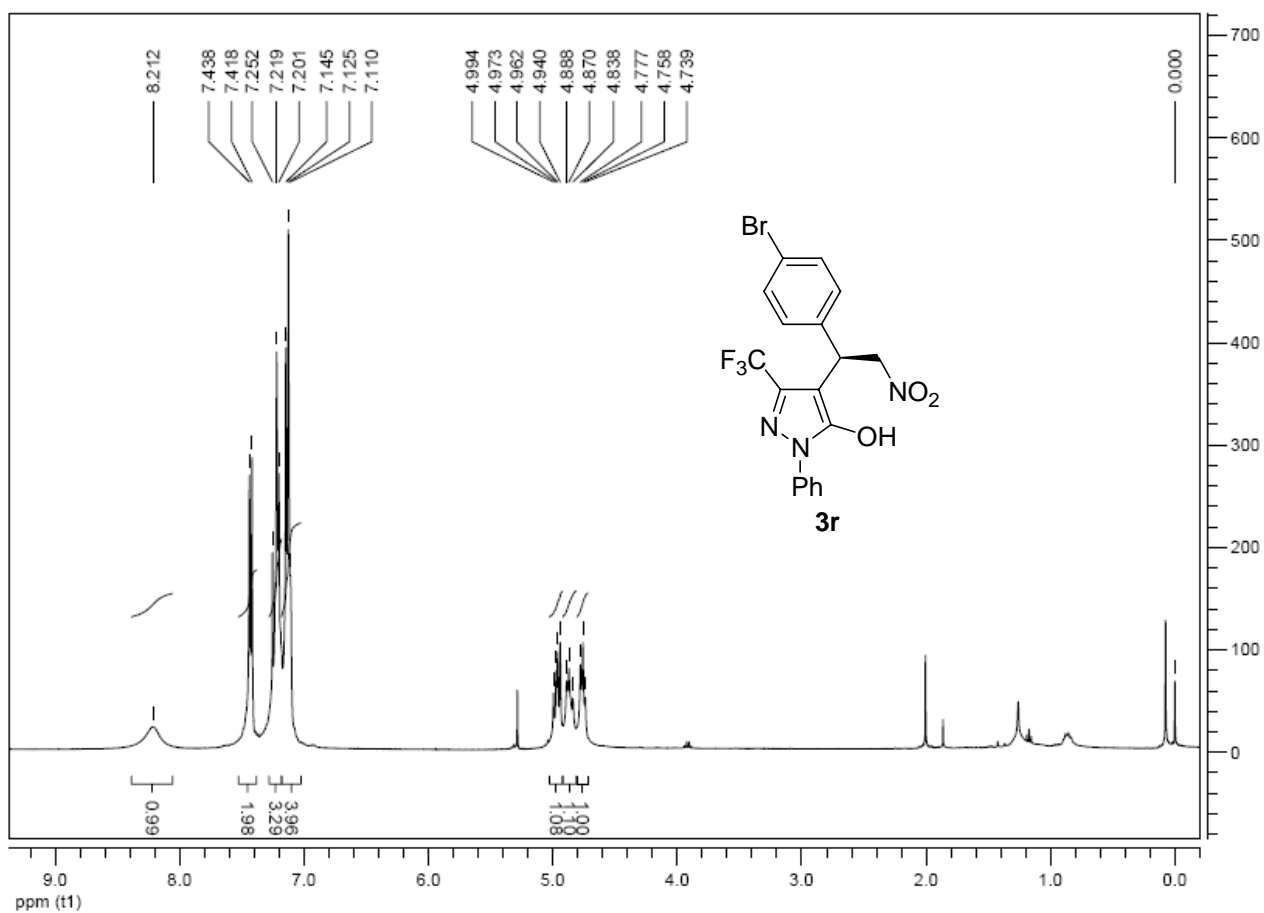


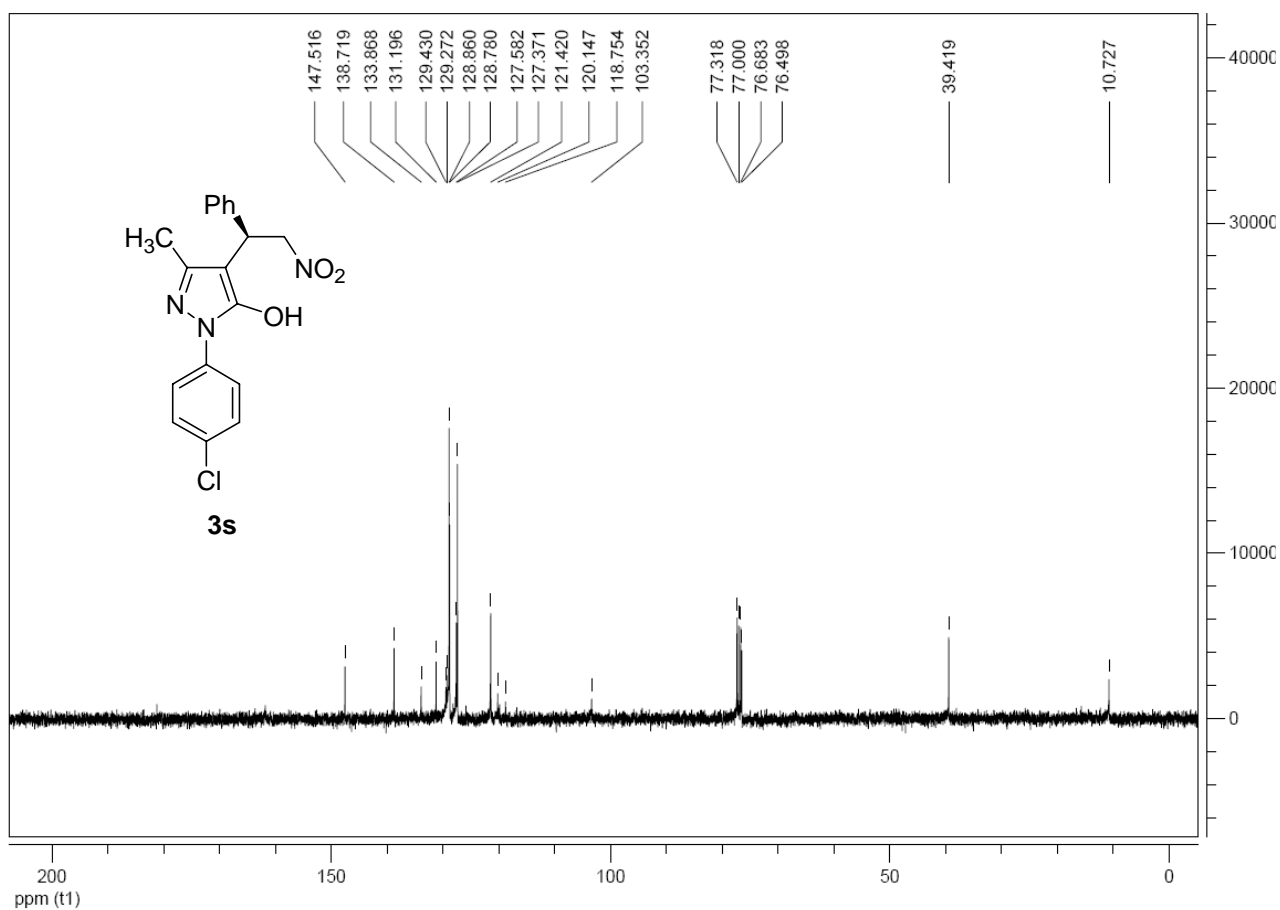
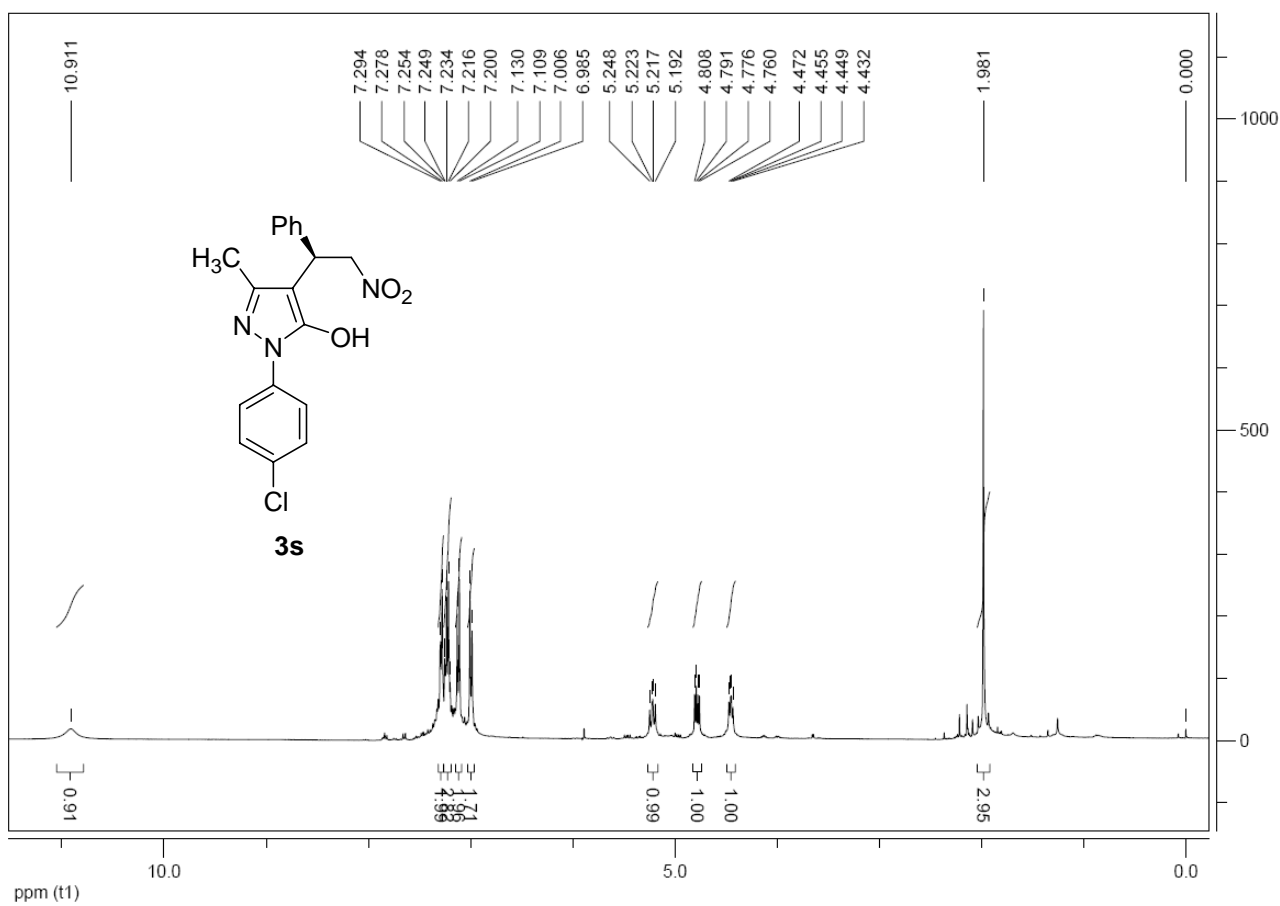


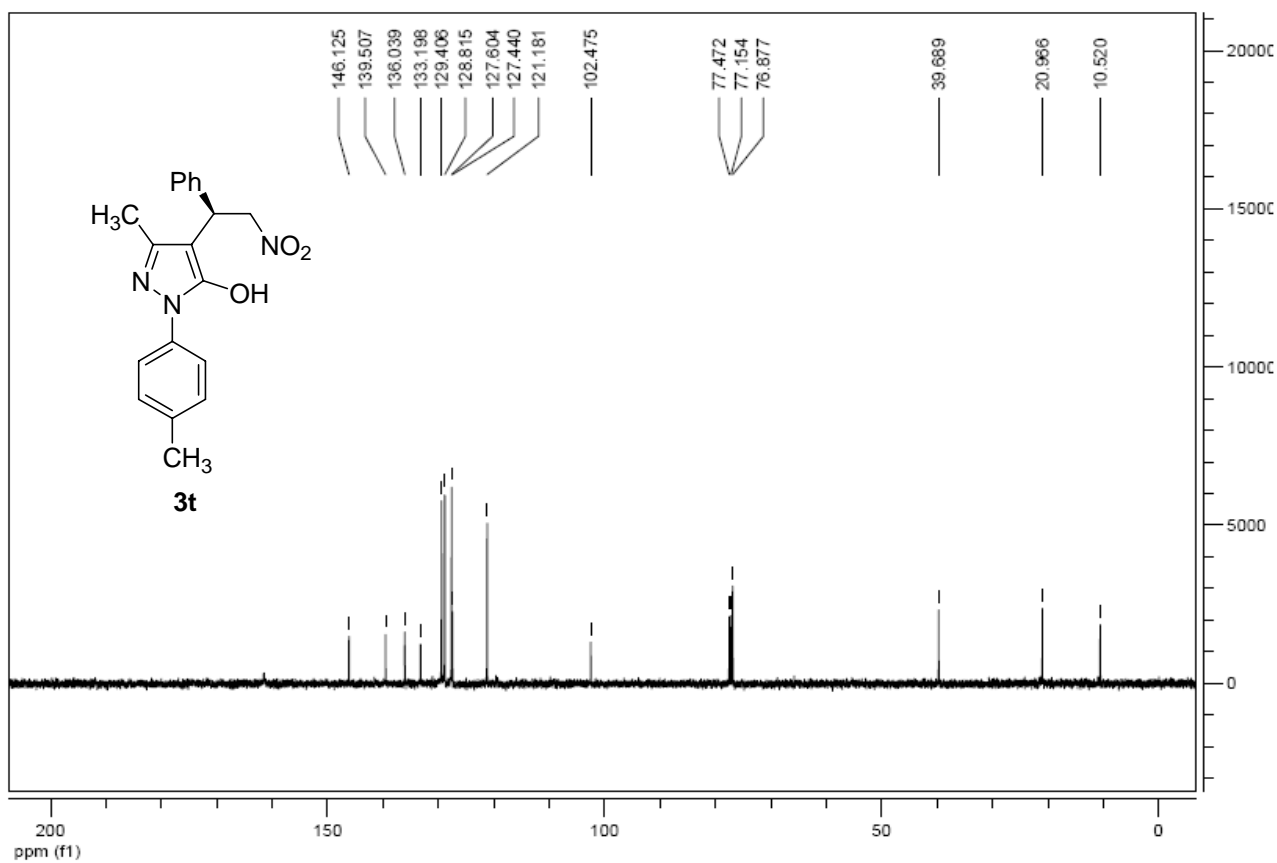
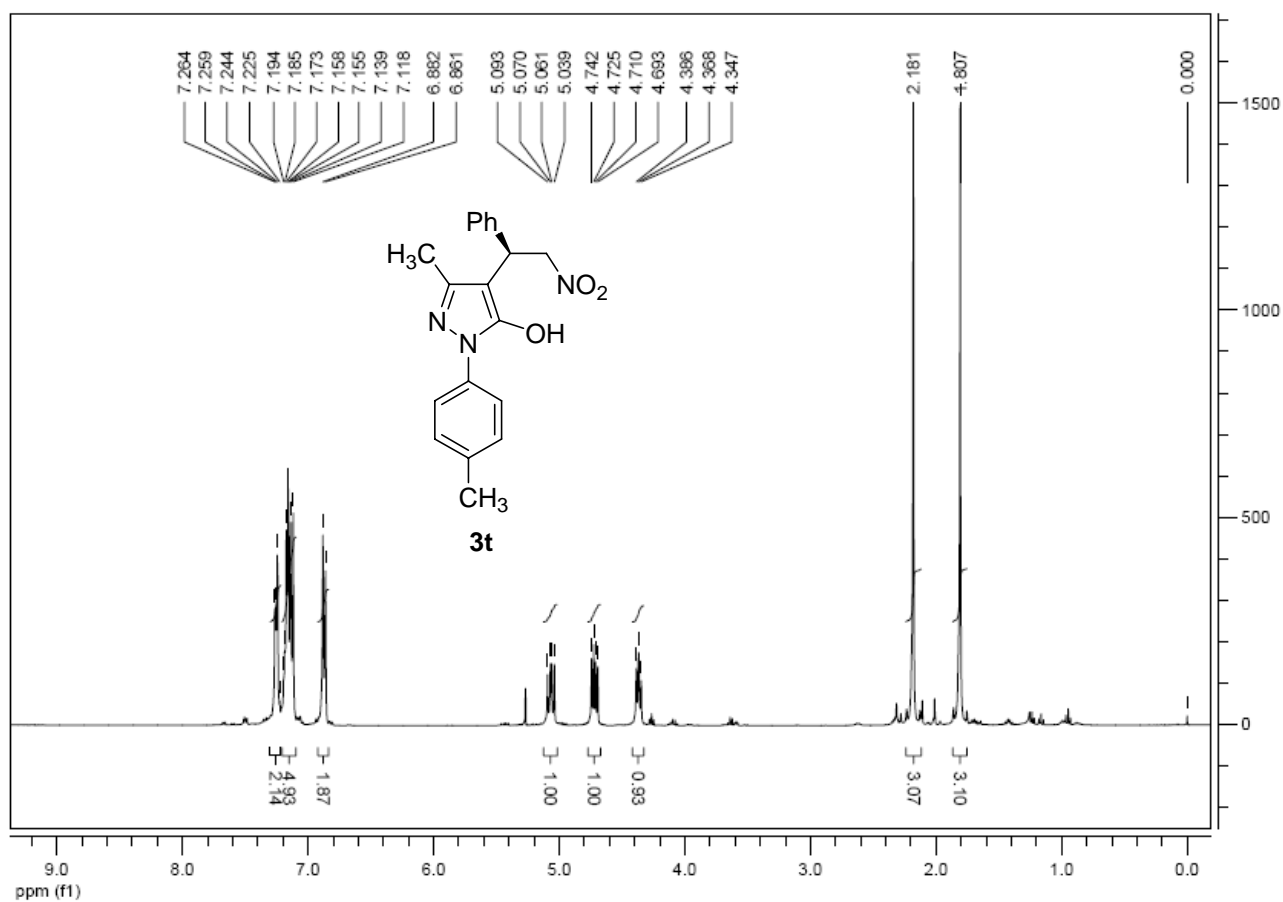


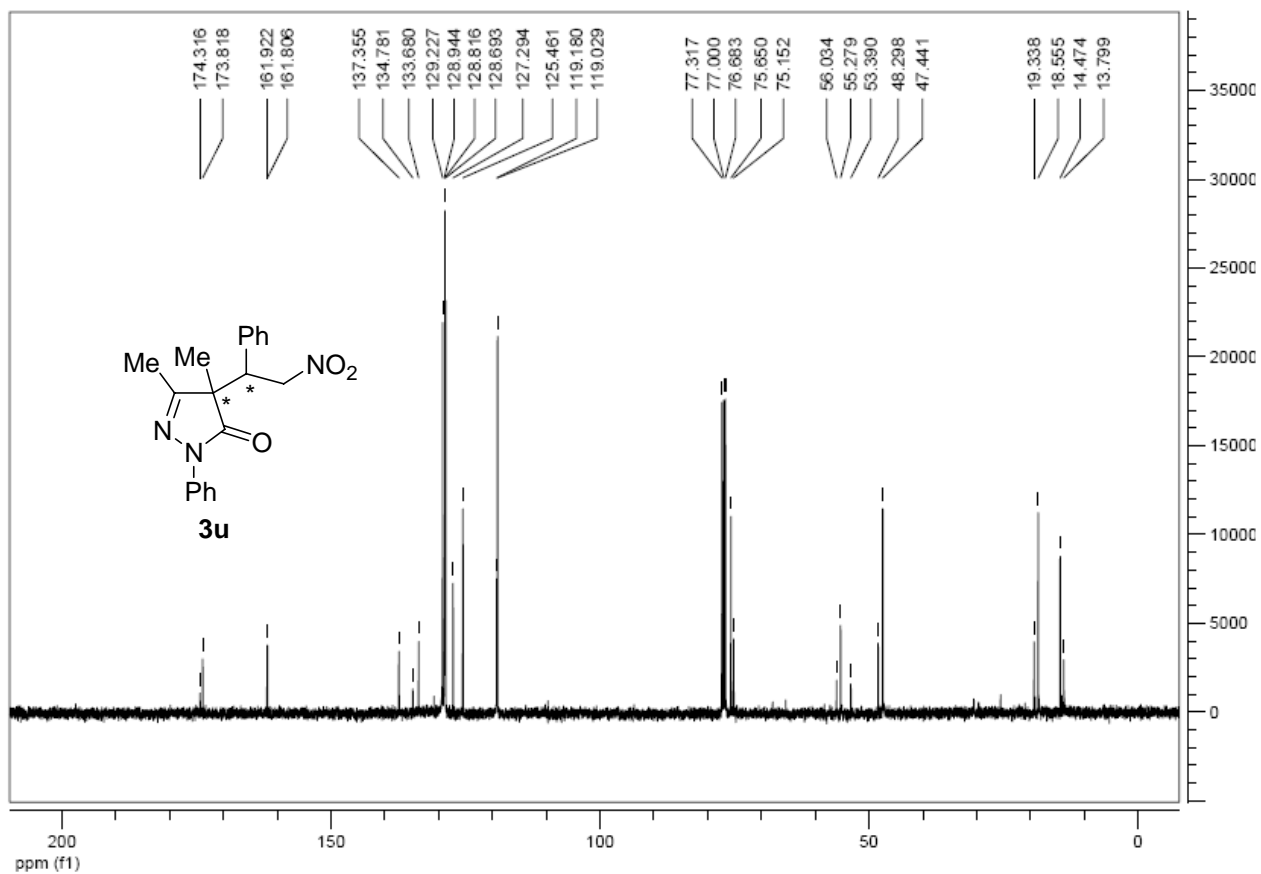
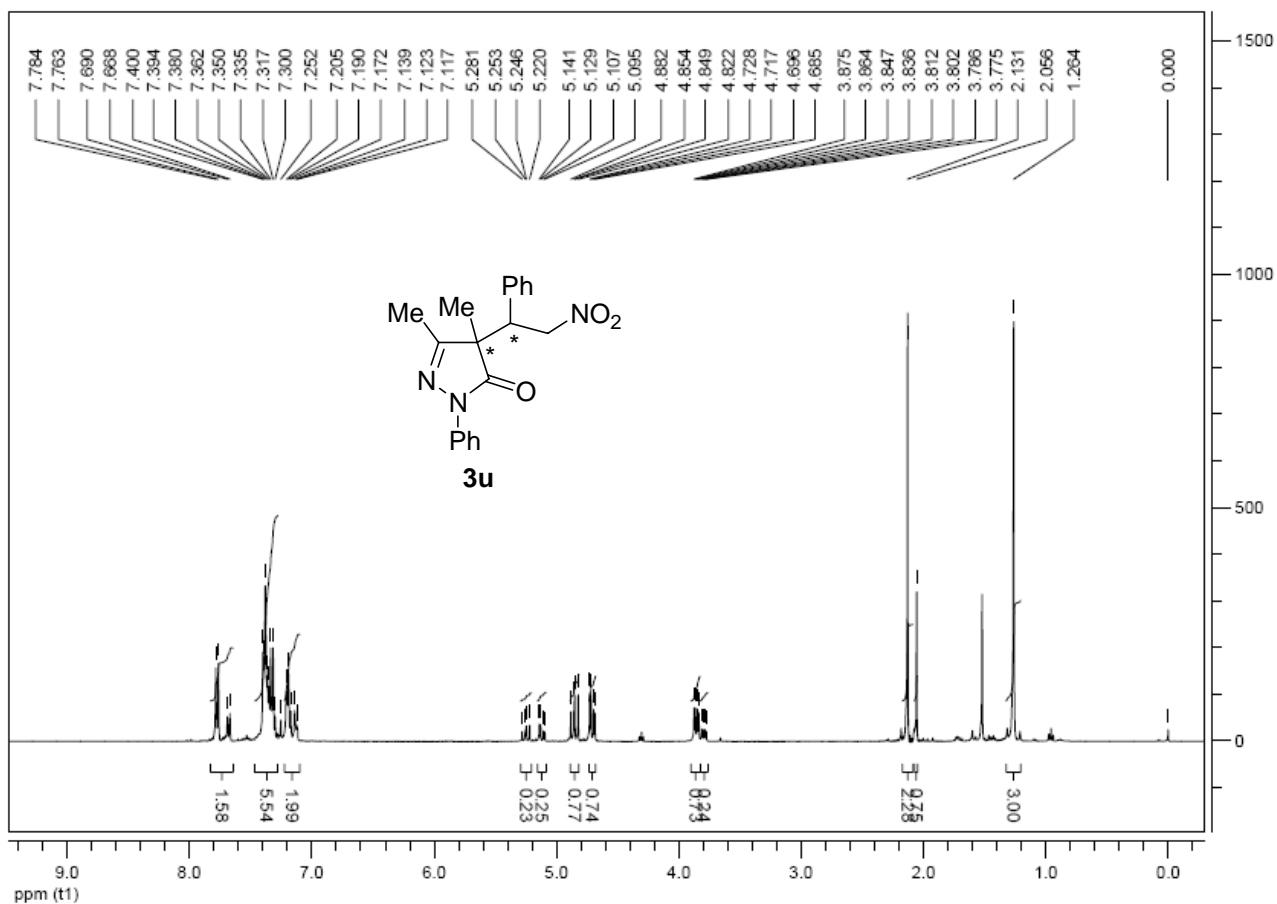


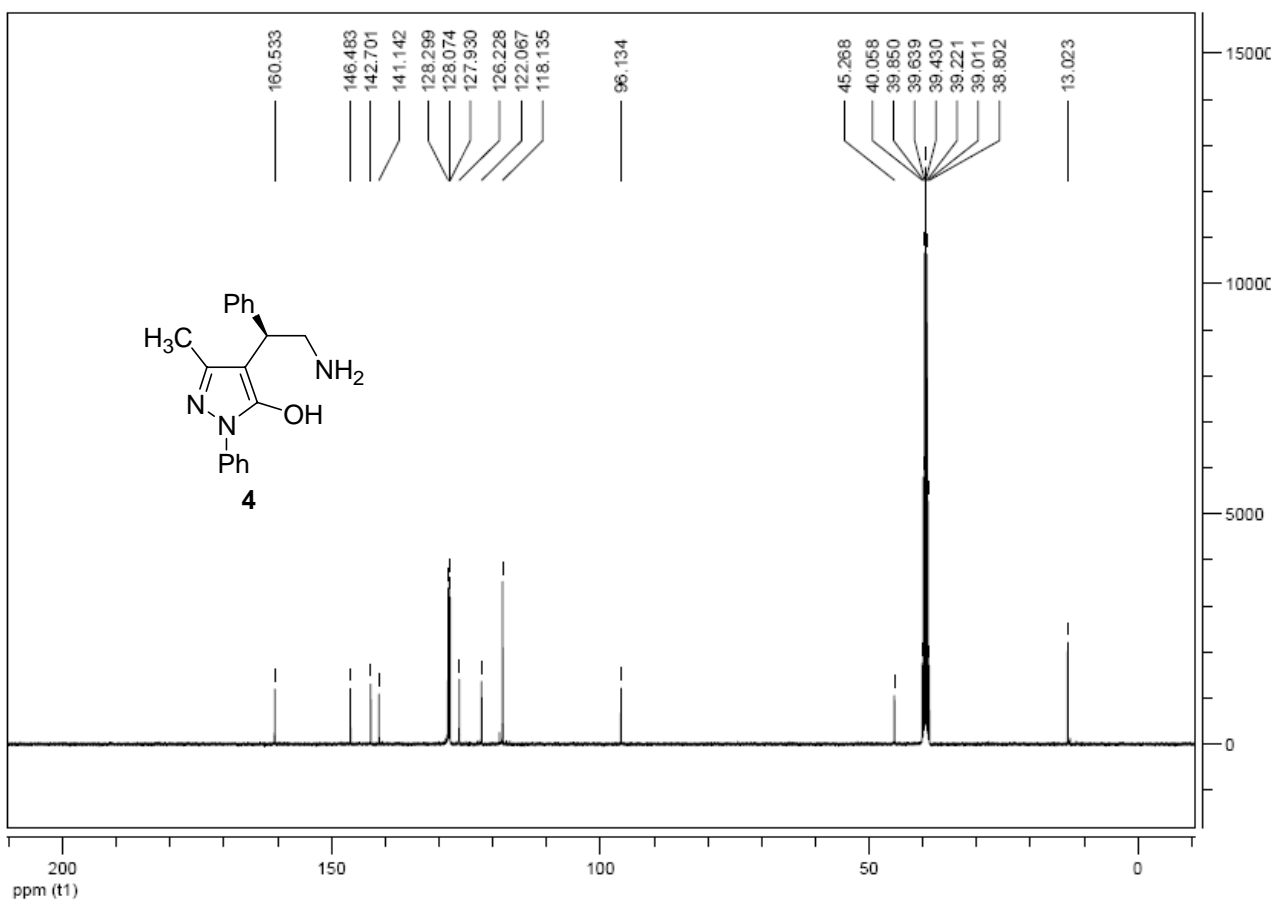
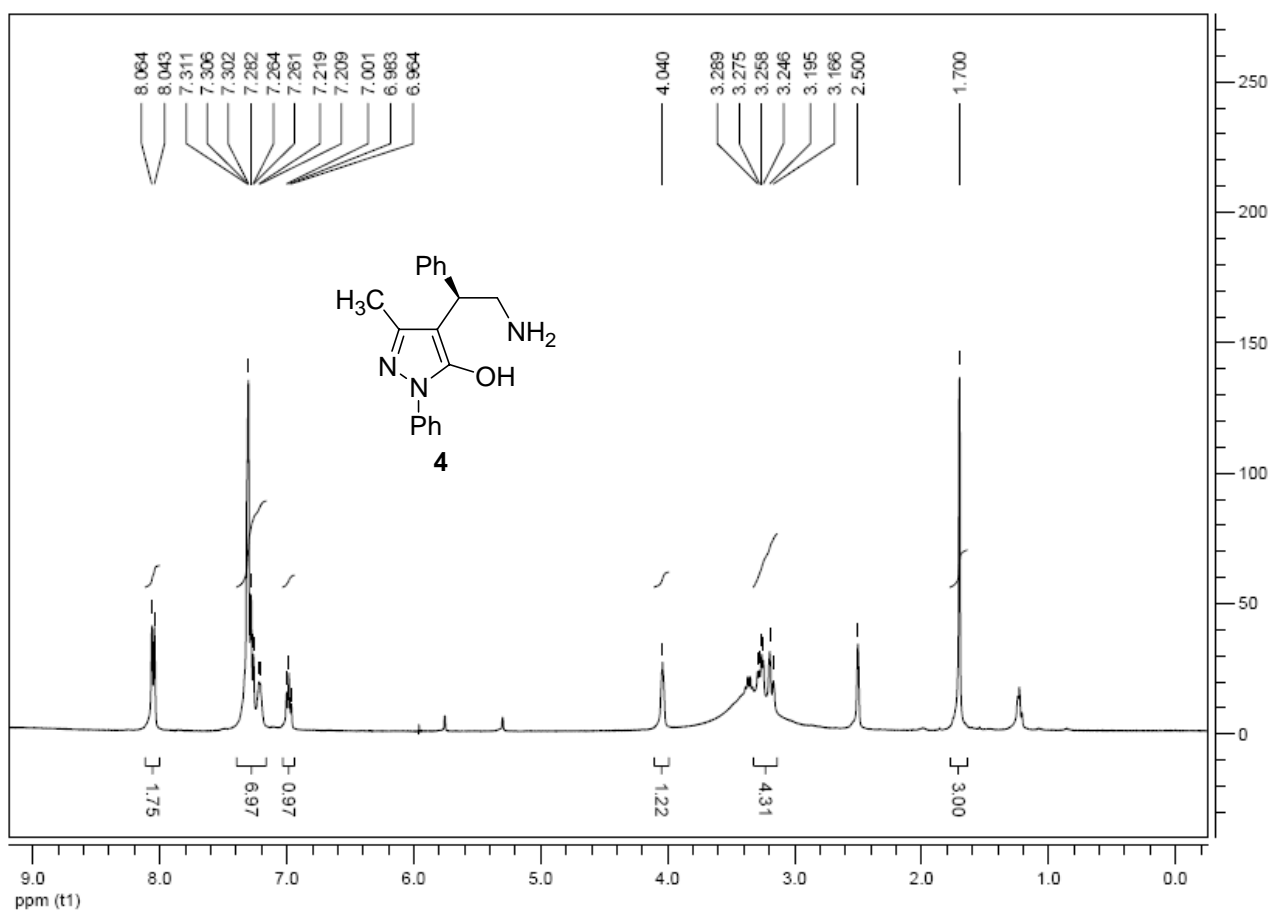


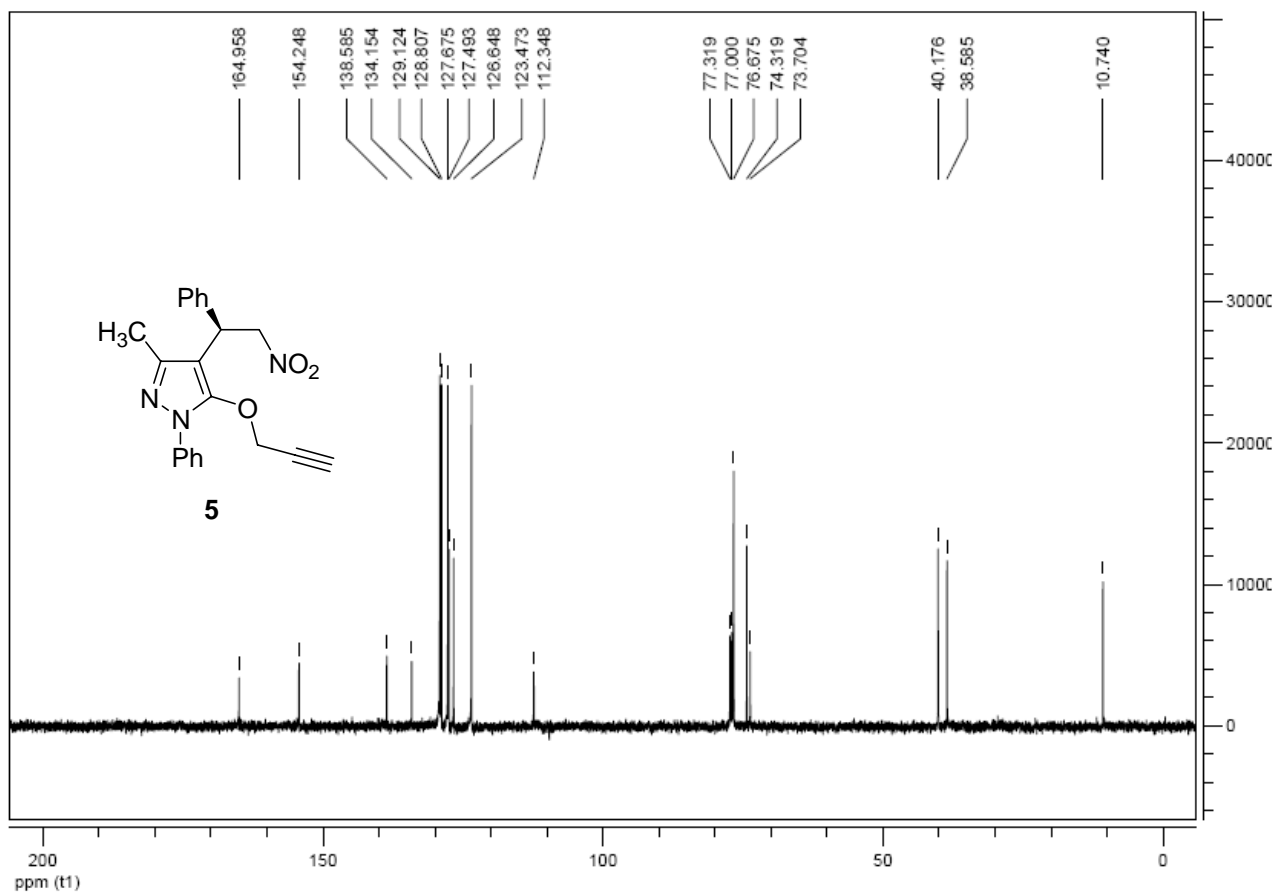
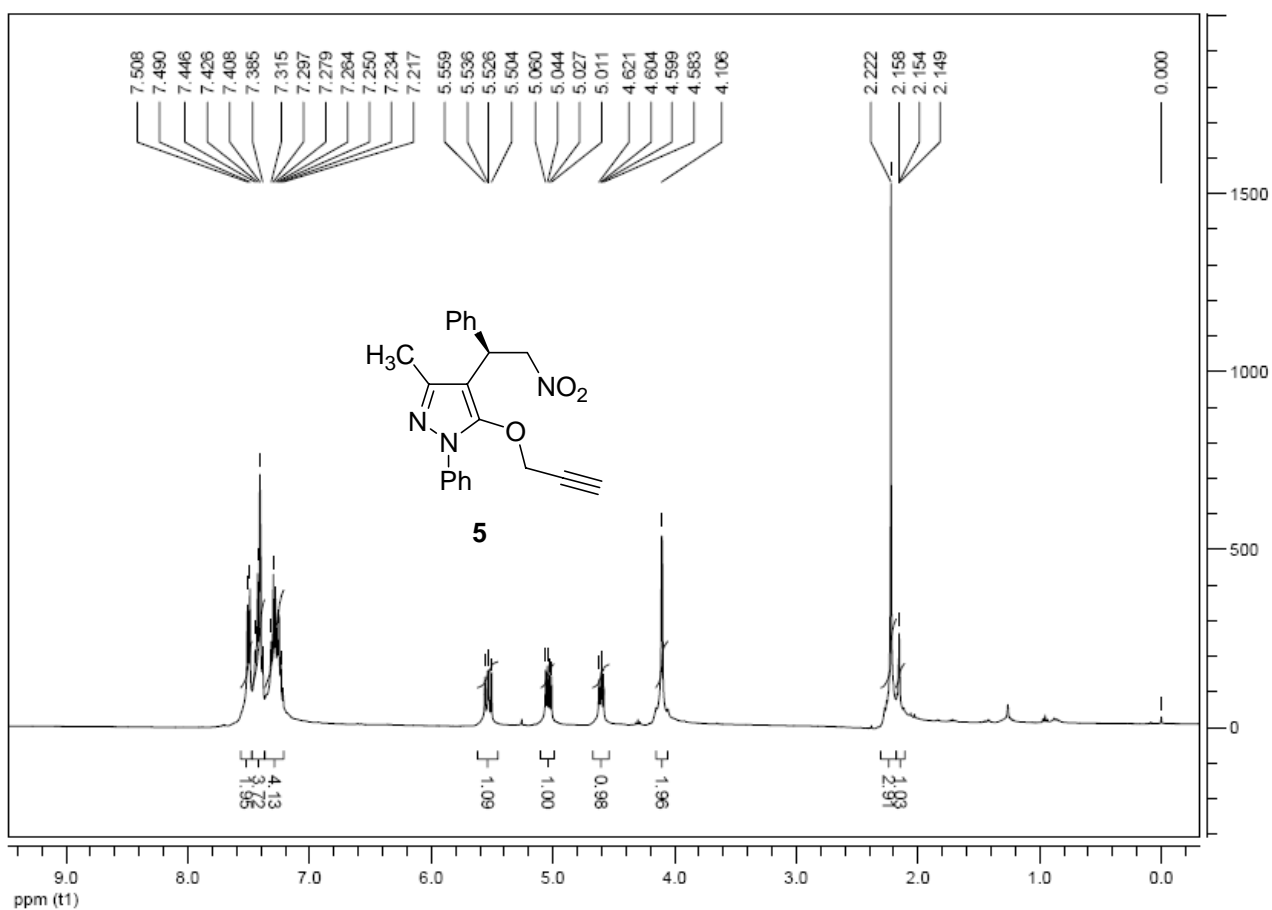




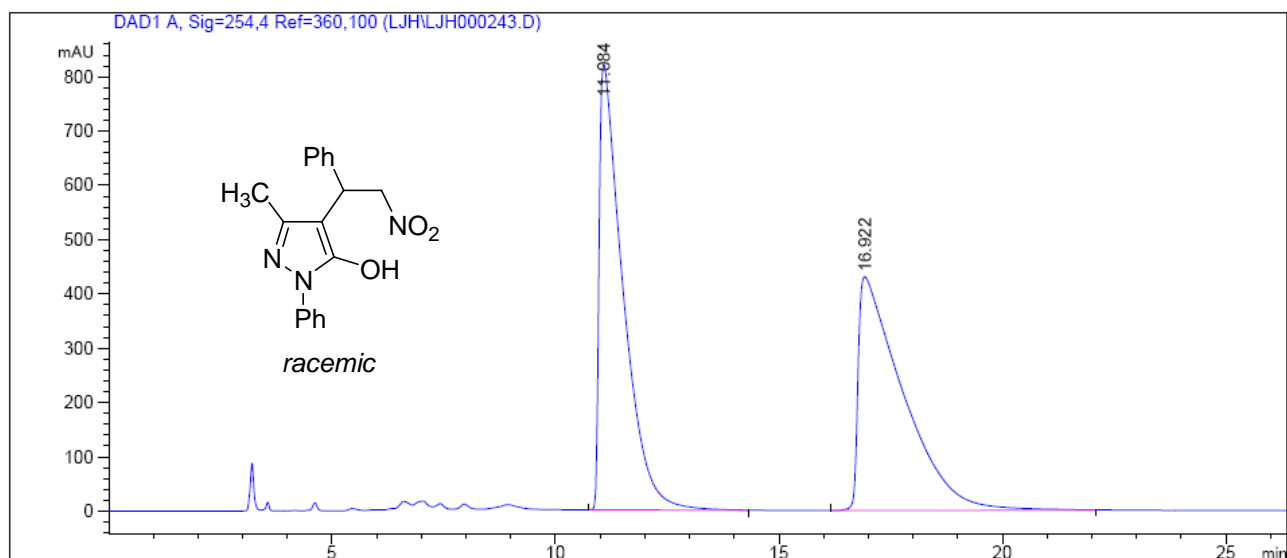






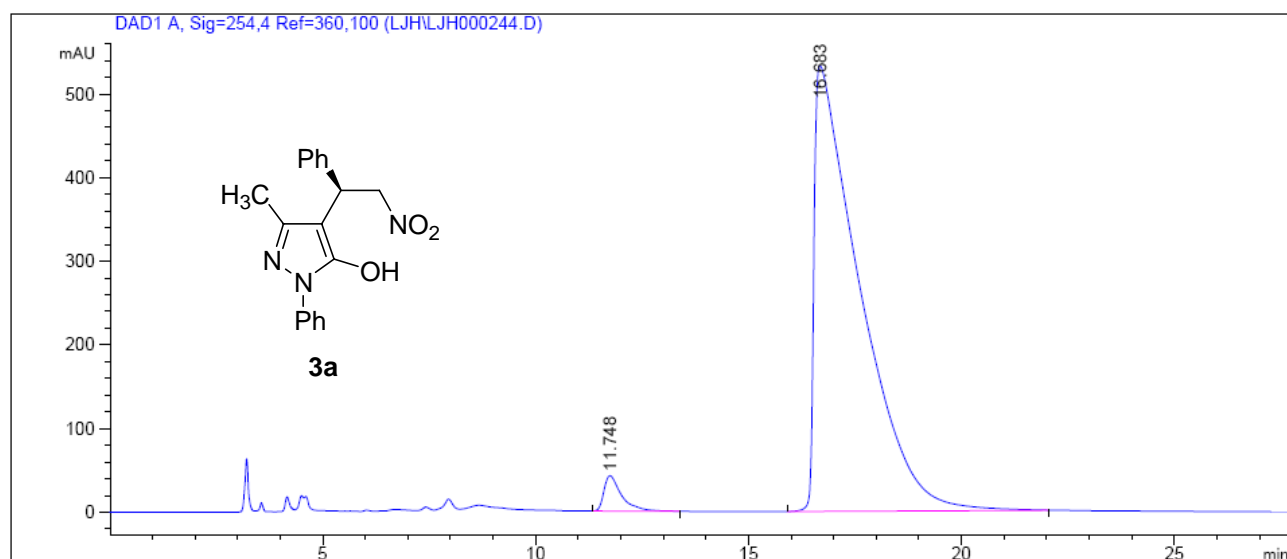


Copies of HPLC chromatographs of products

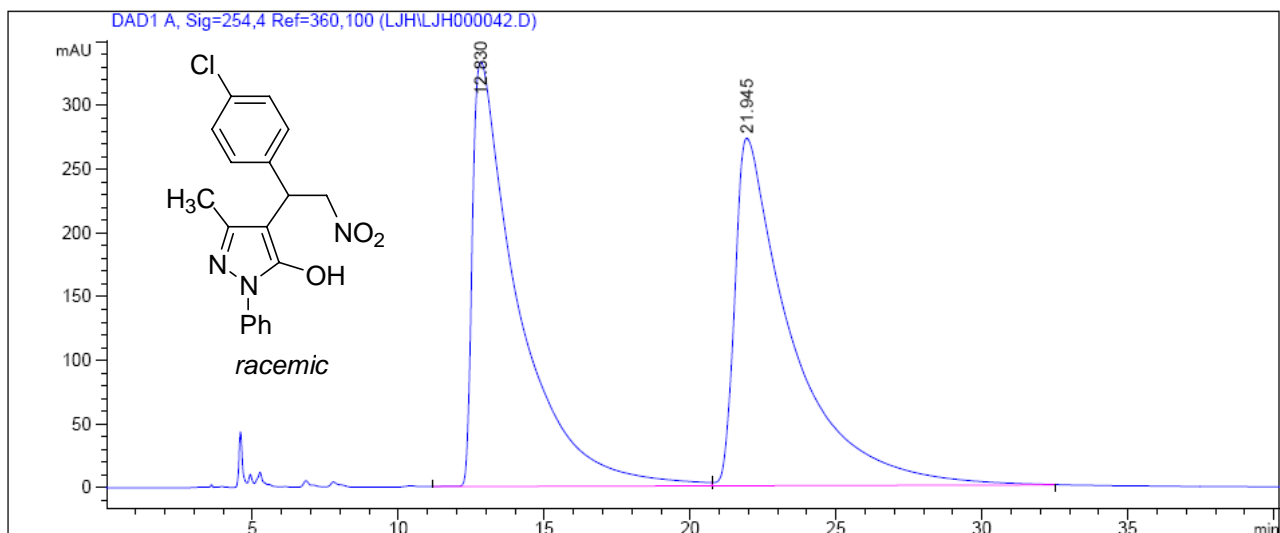


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3a (AD-H column; *n*-hexane–isopropanol 80:20)

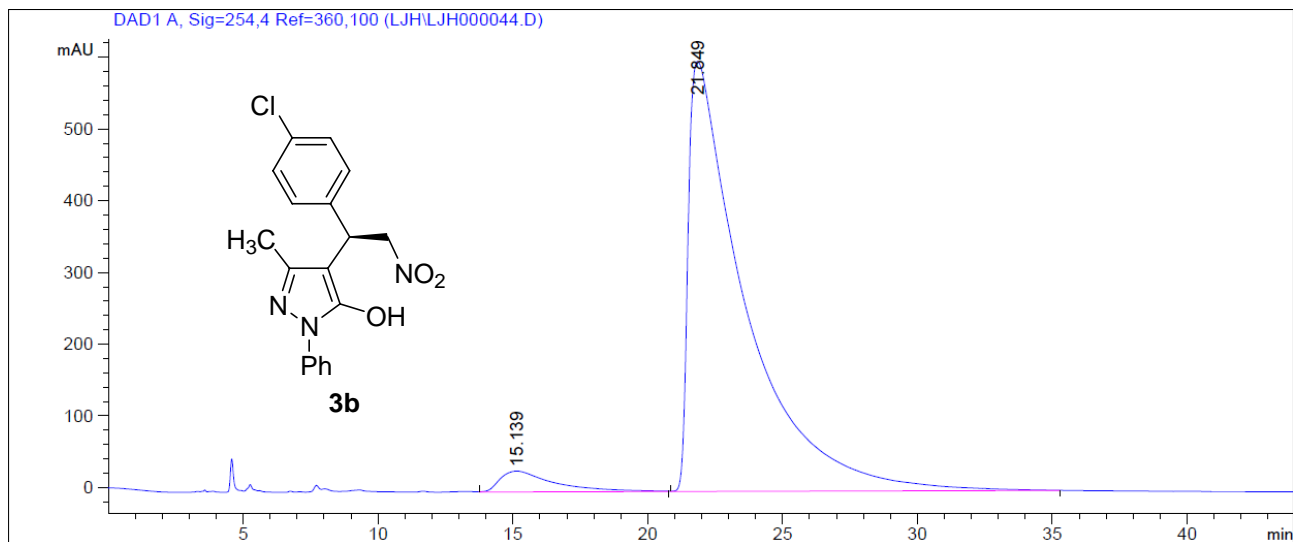


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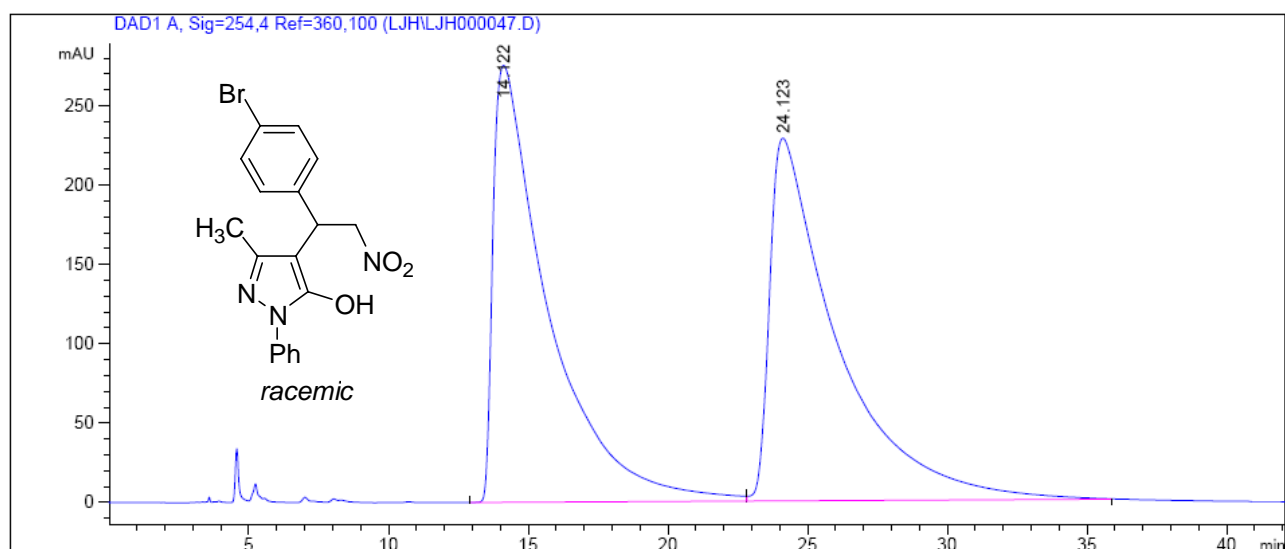


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3b

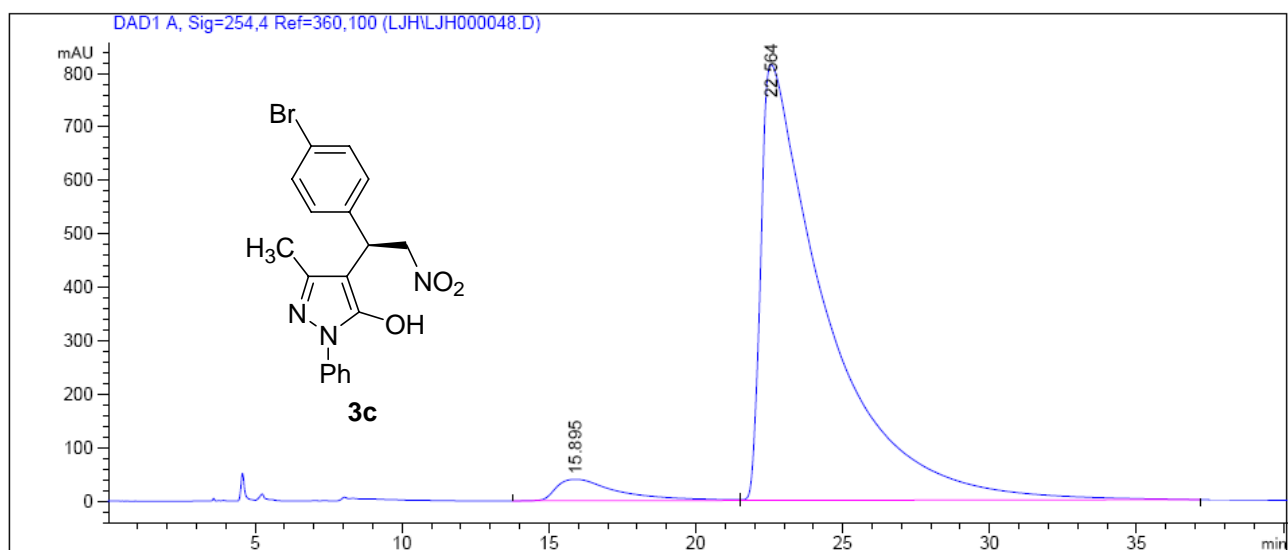


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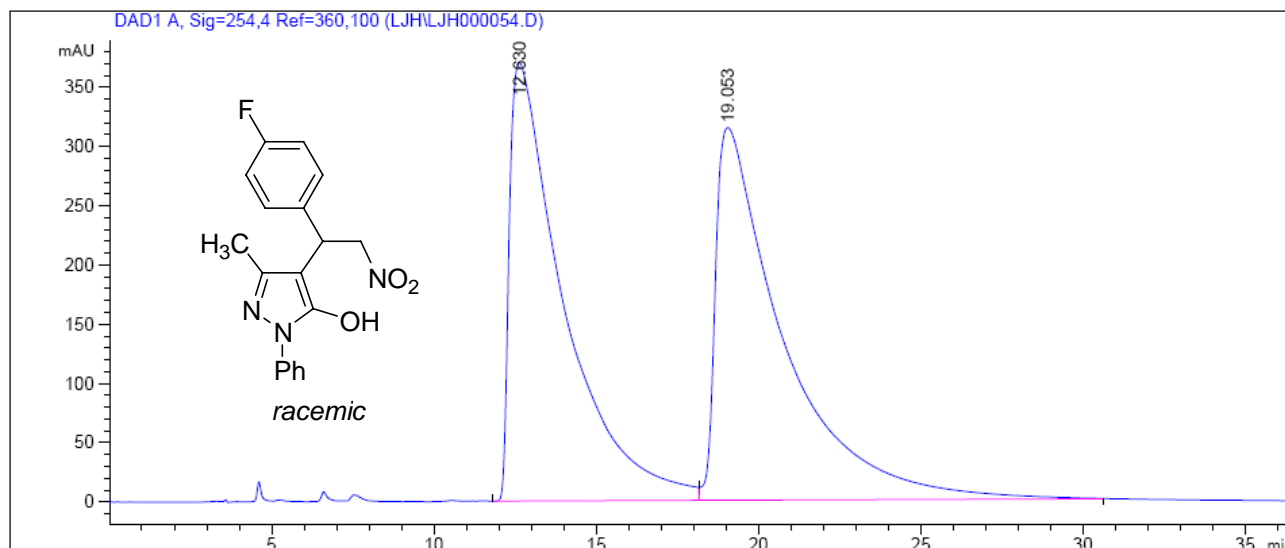


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2	24.123	VB	2.2611	3.84111e4	228.50797	50.3625

3c

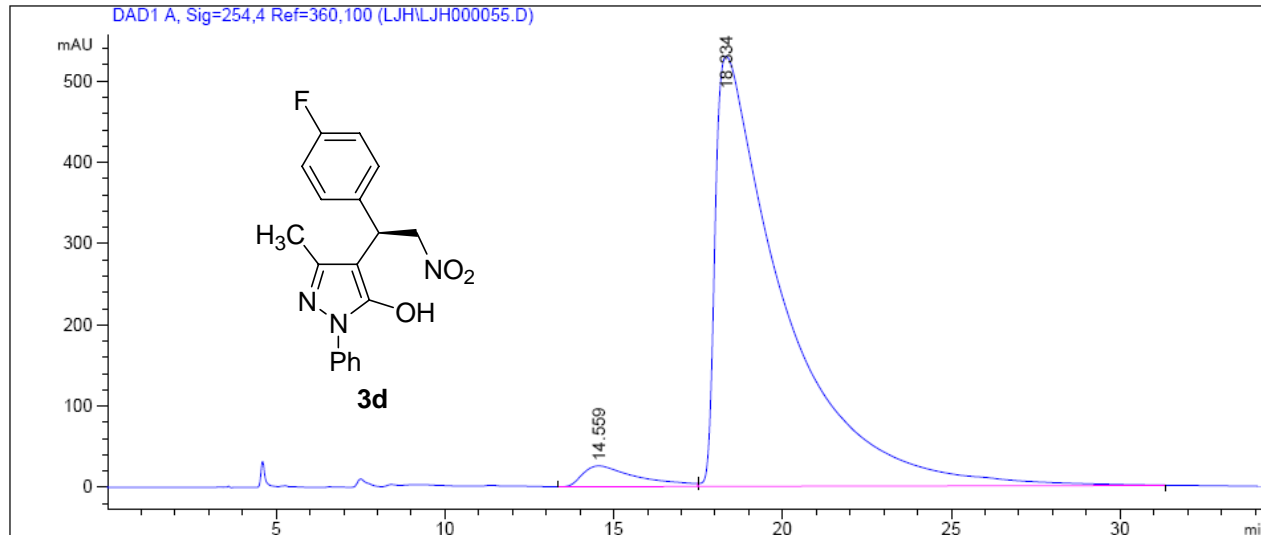


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1	15.895	BV	2.1305	5866.79541	39.92146	4.4472
2	22.564	VB	2.0599	1.26054e5	815.23413	95.5528

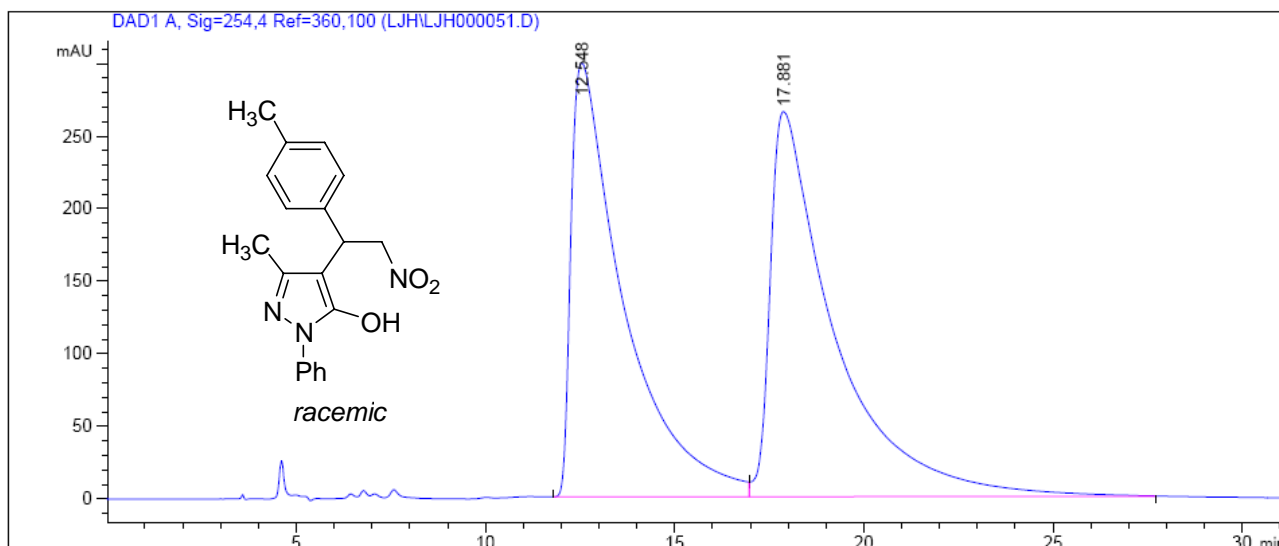


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3d

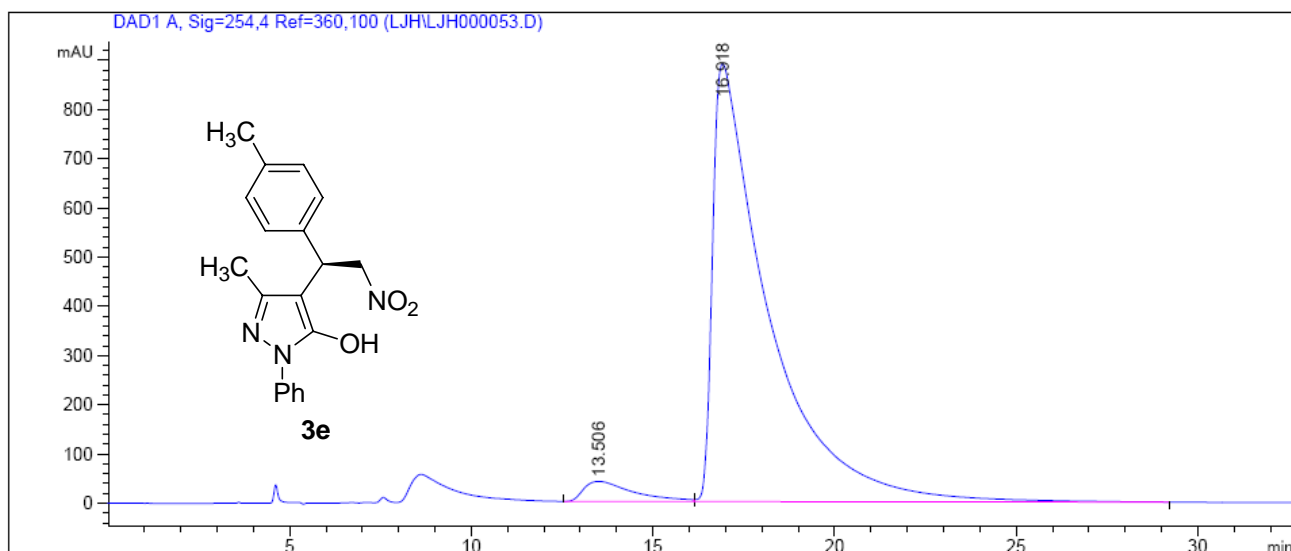


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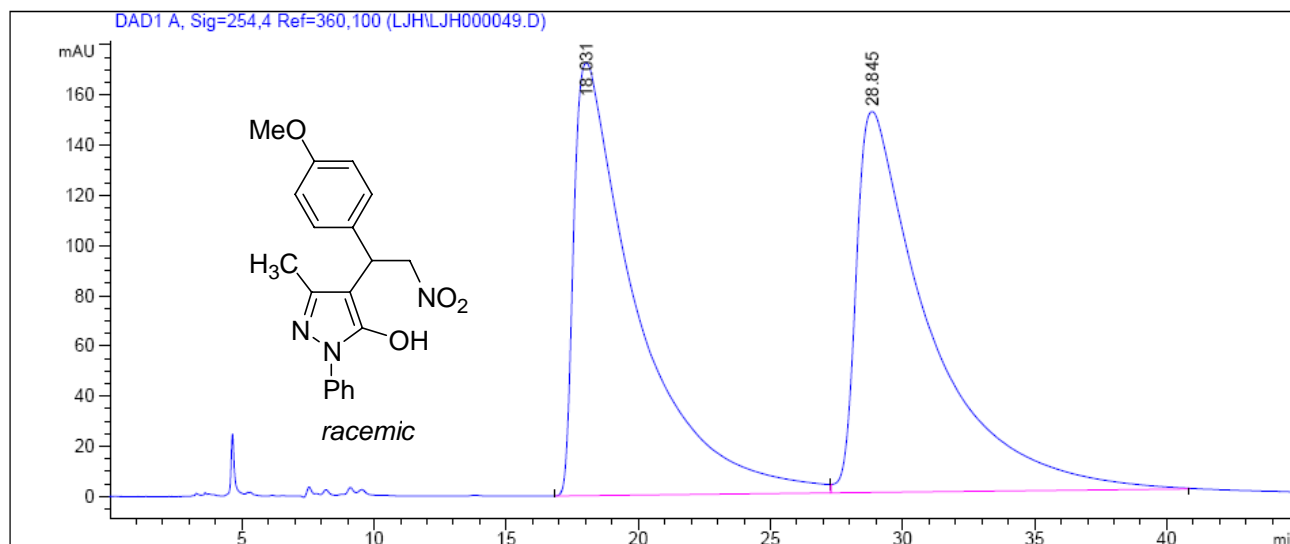


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3e

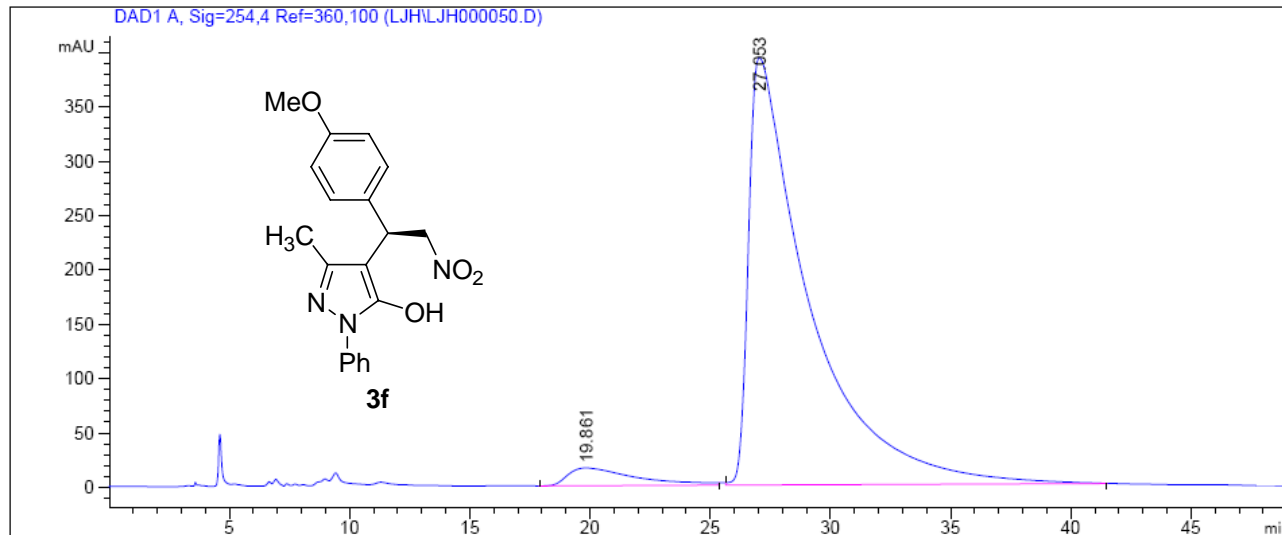


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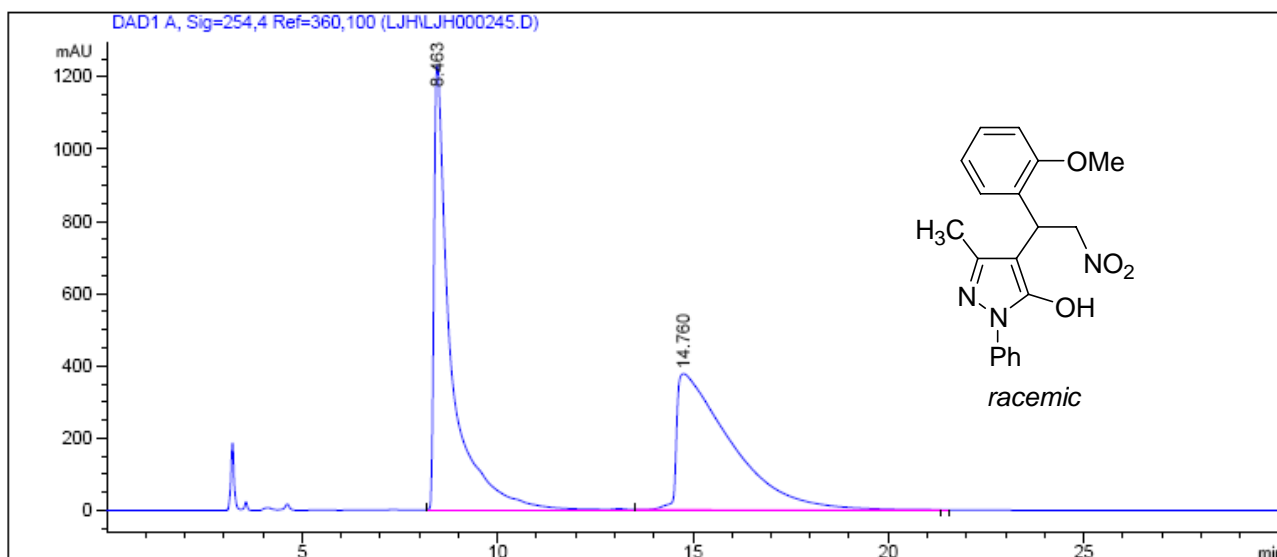


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3f

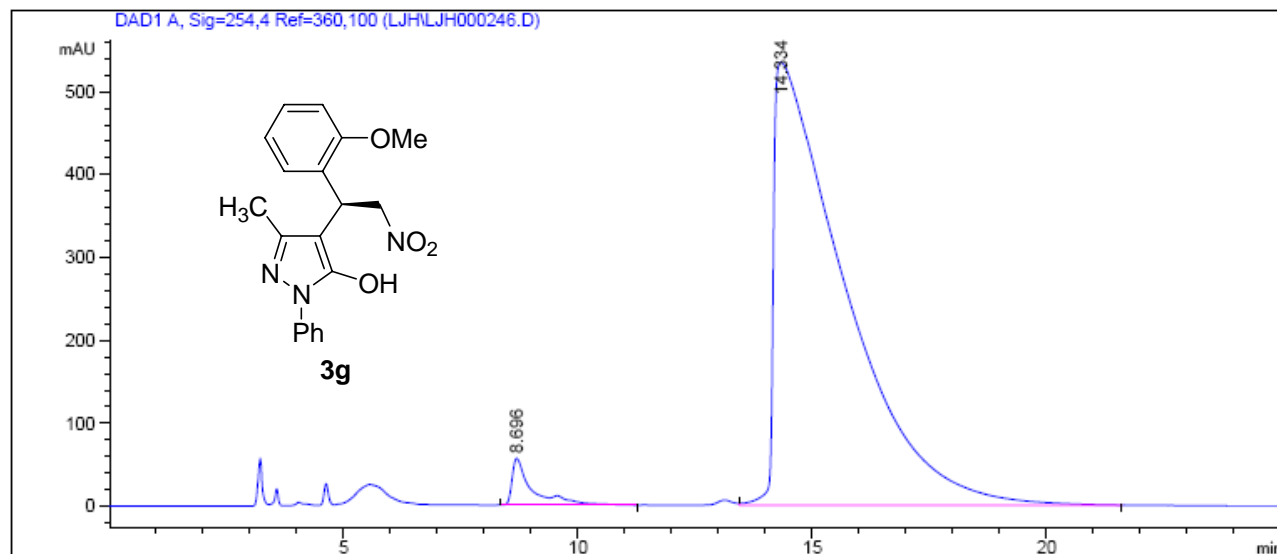


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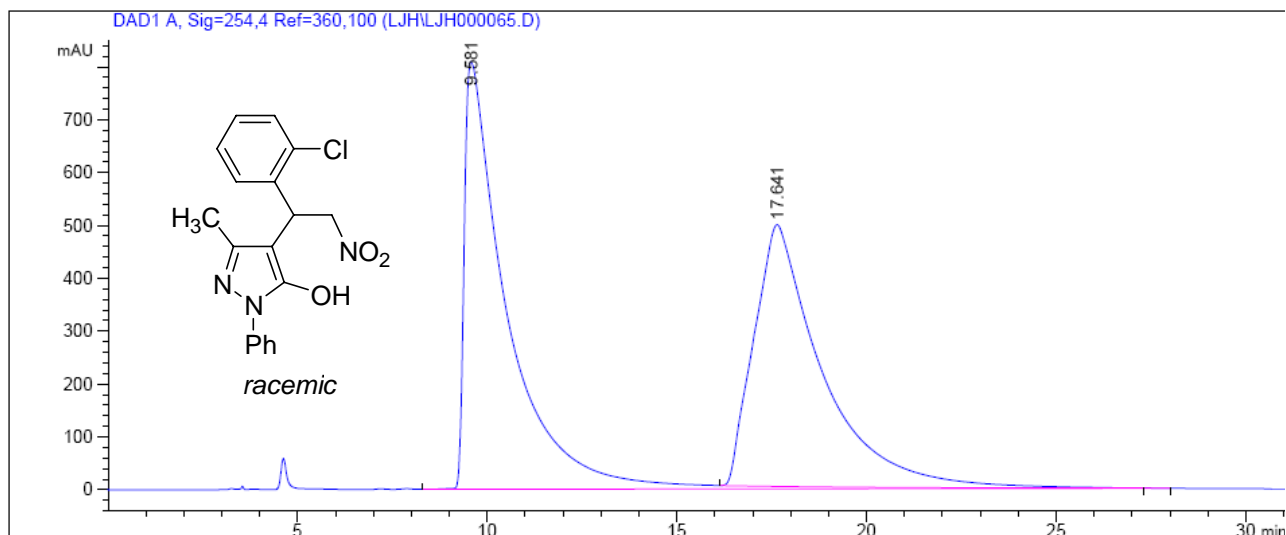


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2	14.760	VB X	1.2442	3.63688e4	376.10168	49.4201

3g

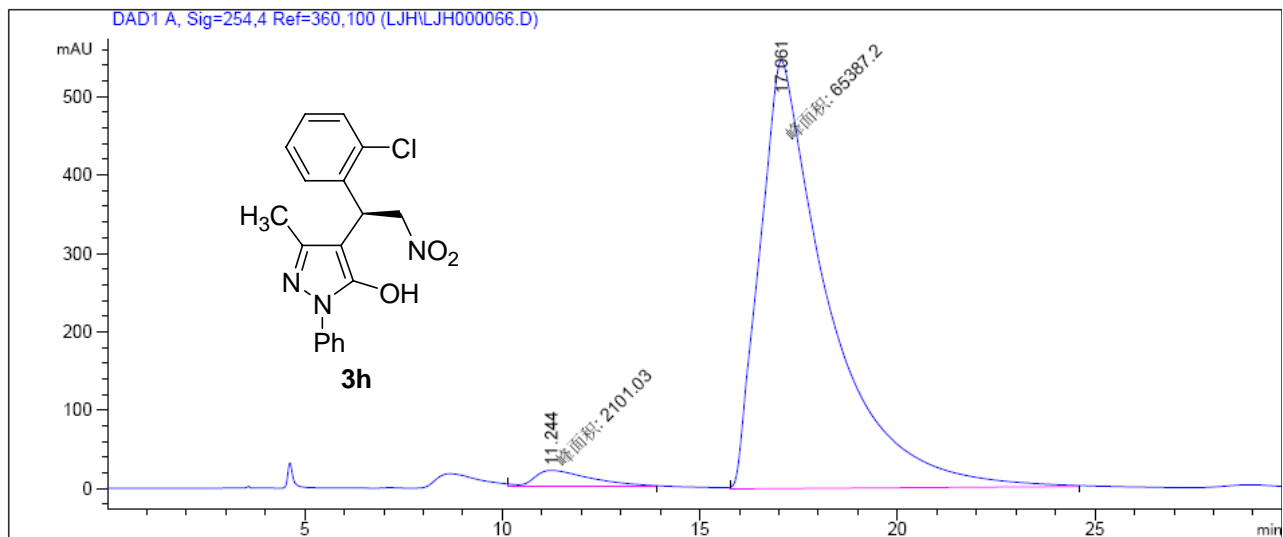


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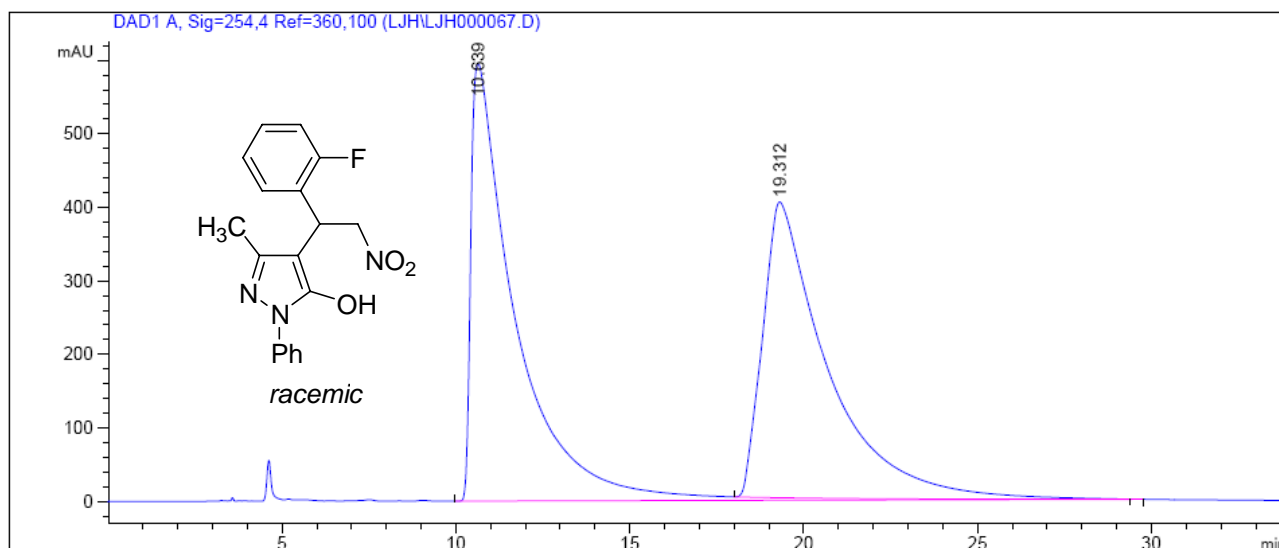


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2	17.641	BB X	1.6567	6.18447e4	495.31610	49.1786

3h

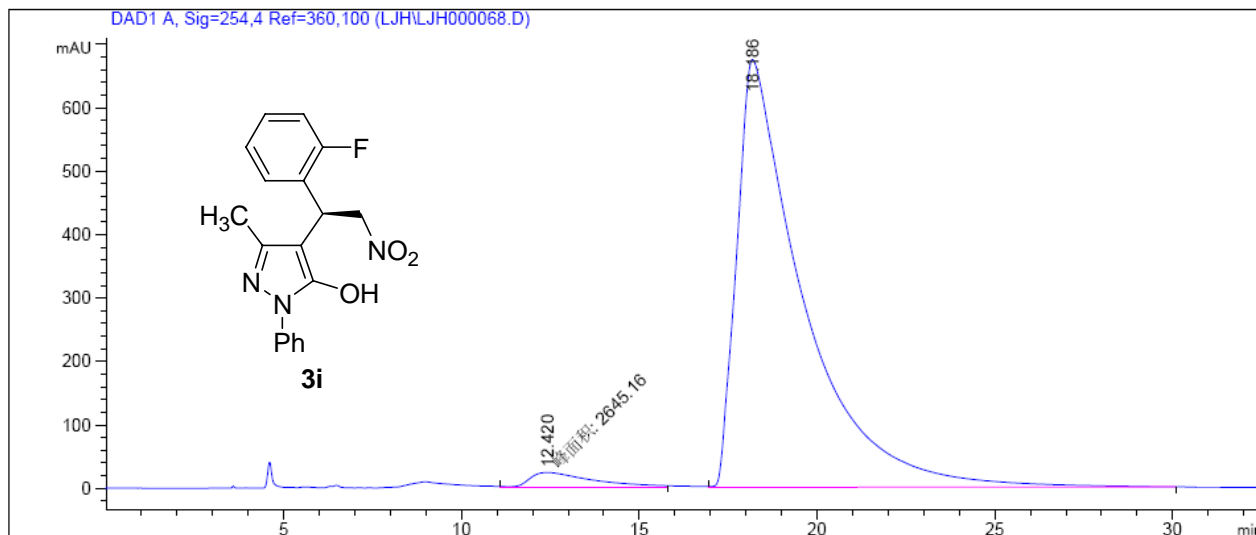


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1	11.244	MM T	1.6075	2101.03223	20.73529	3.1132
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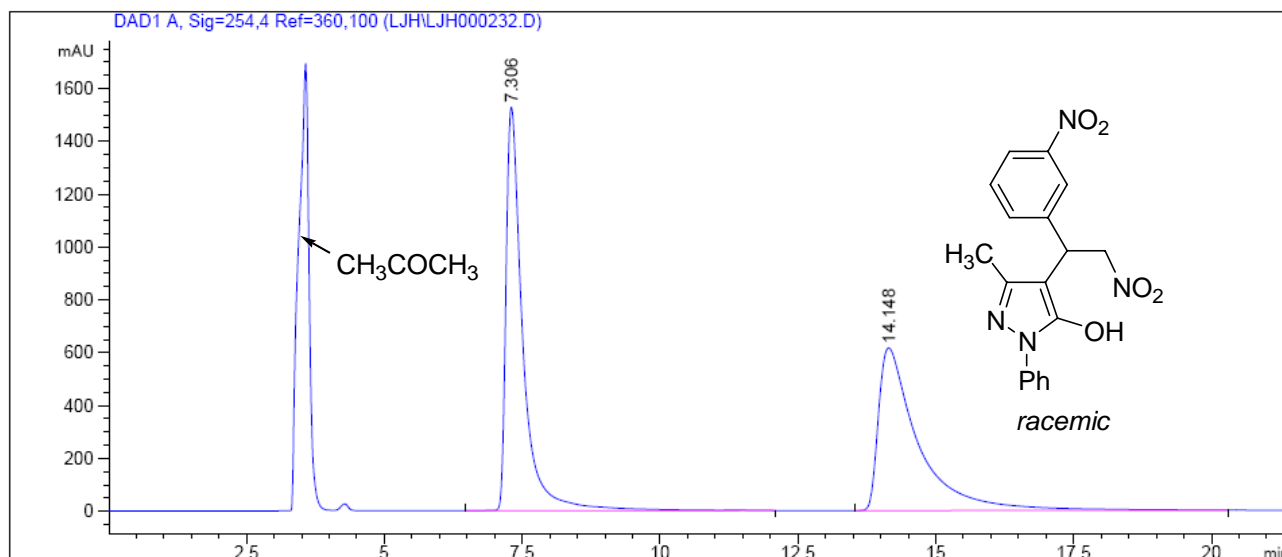


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1	10.639	VB S	1.2010	5.35136e4	595.17010	50.6277
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3i

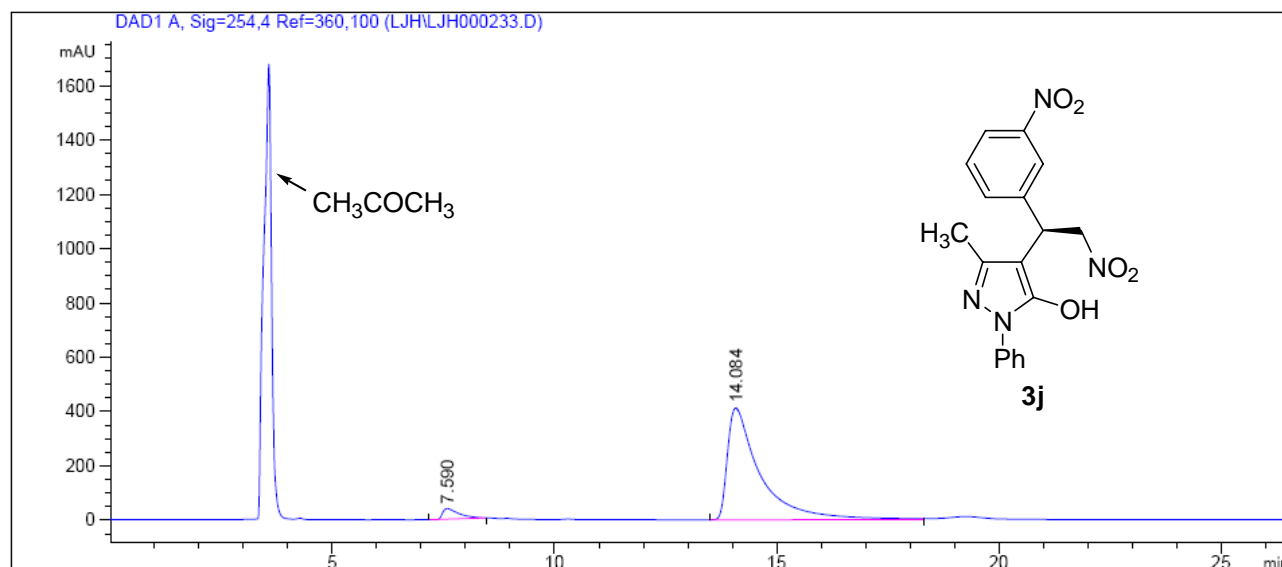


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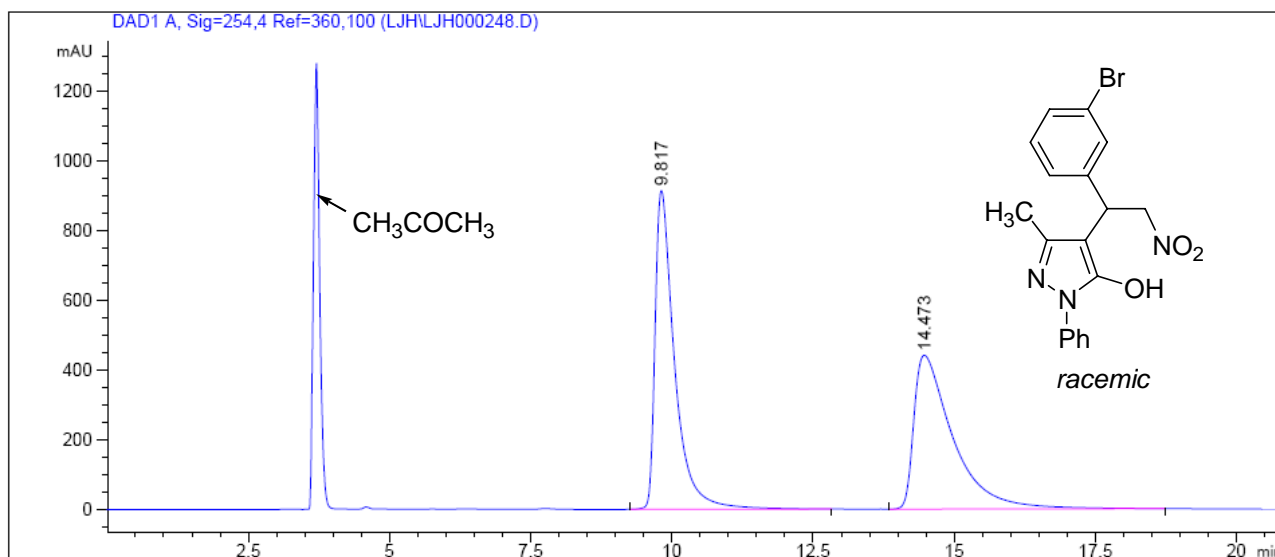


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3j

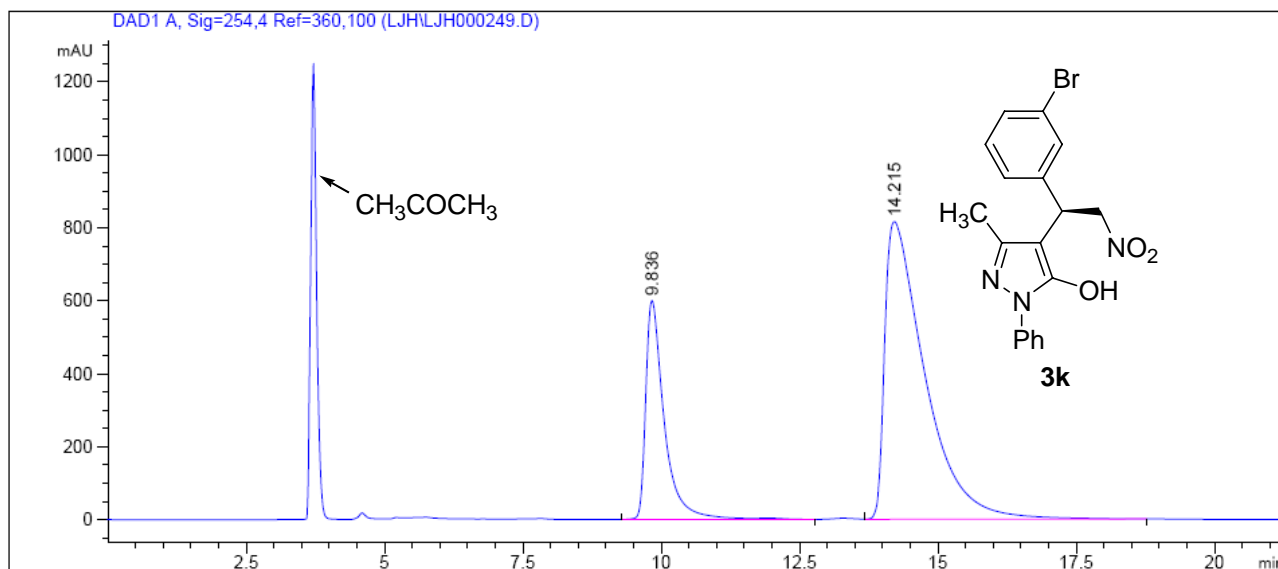


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1	7.590	BB S	0.3674	991.44727	39.15594	4.4724
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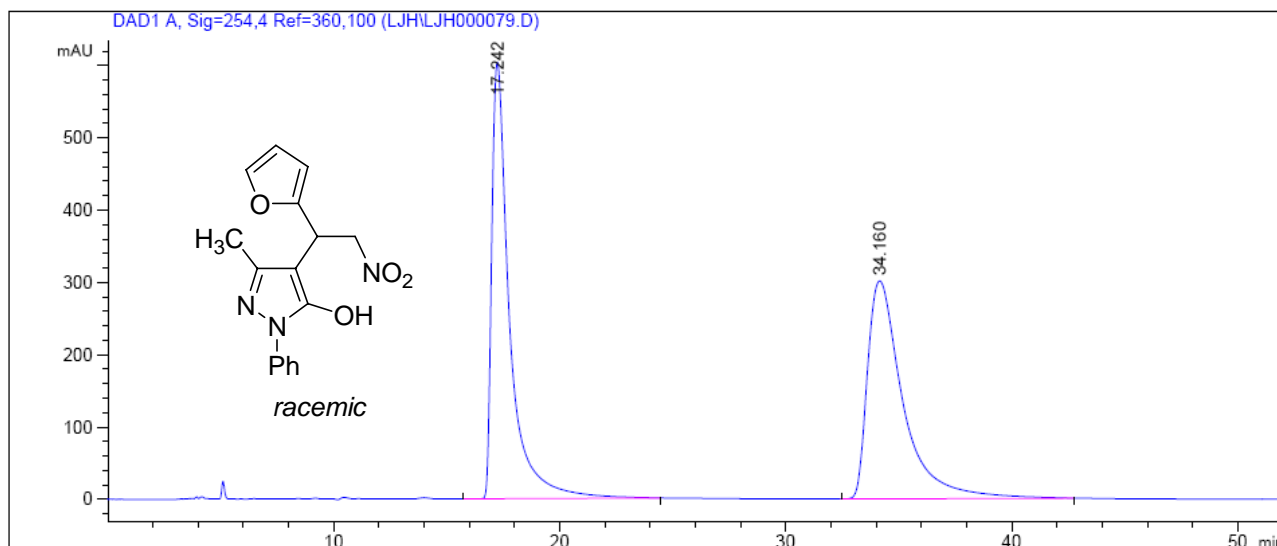


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1	9.817	BB S	0.3524	2.19941e4	915.25928	50.7388
2	14.473	BB	0.7115	2.13536e4	442.13046	49.2612

3k

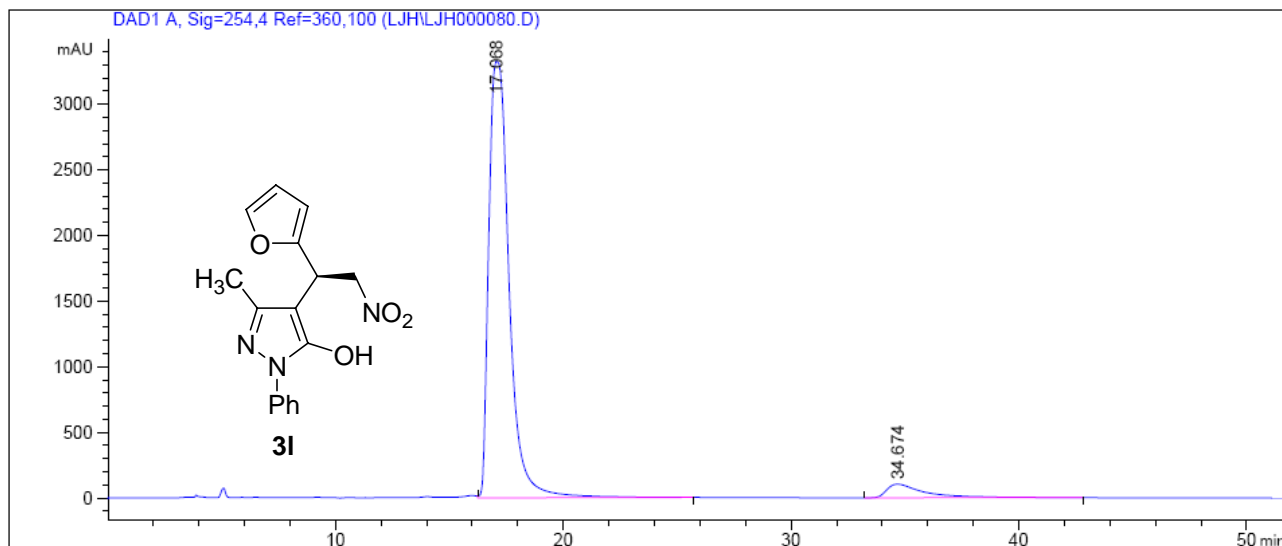


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.836	BB S	0.3440	1.40600e4	600.09302	25.4354
2	14.215	VB	0.7413	4.12171e4	816.05420	74.5646

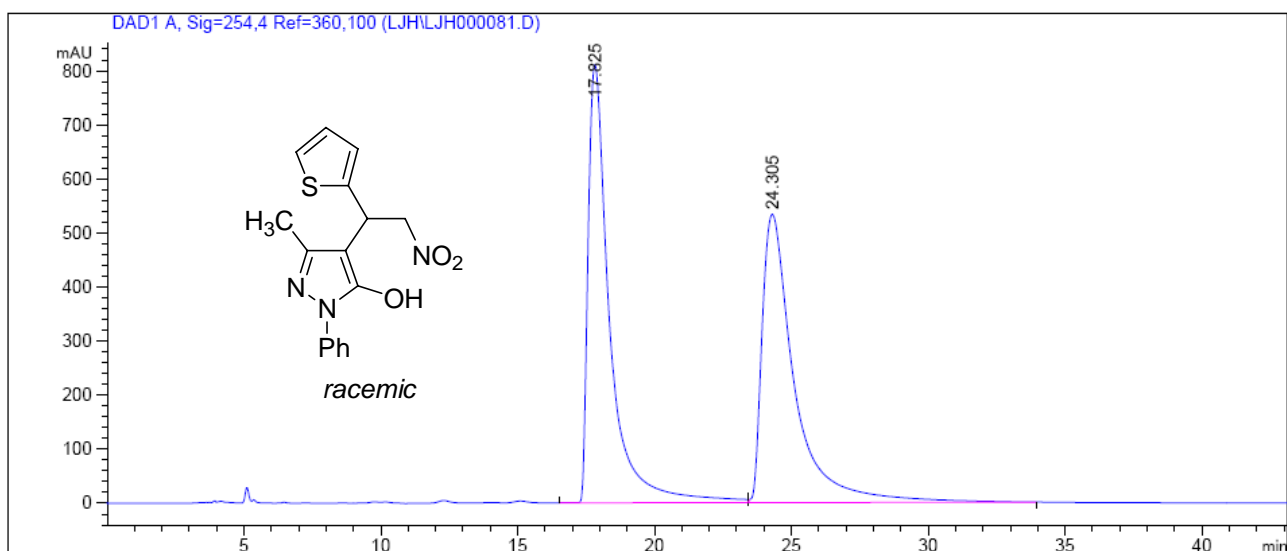


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.242	BB	0.8159	3.32998e4	603.31097	50.2256
2	34.160	BB	1.6297	3.30007e4	301.33463	49.7744

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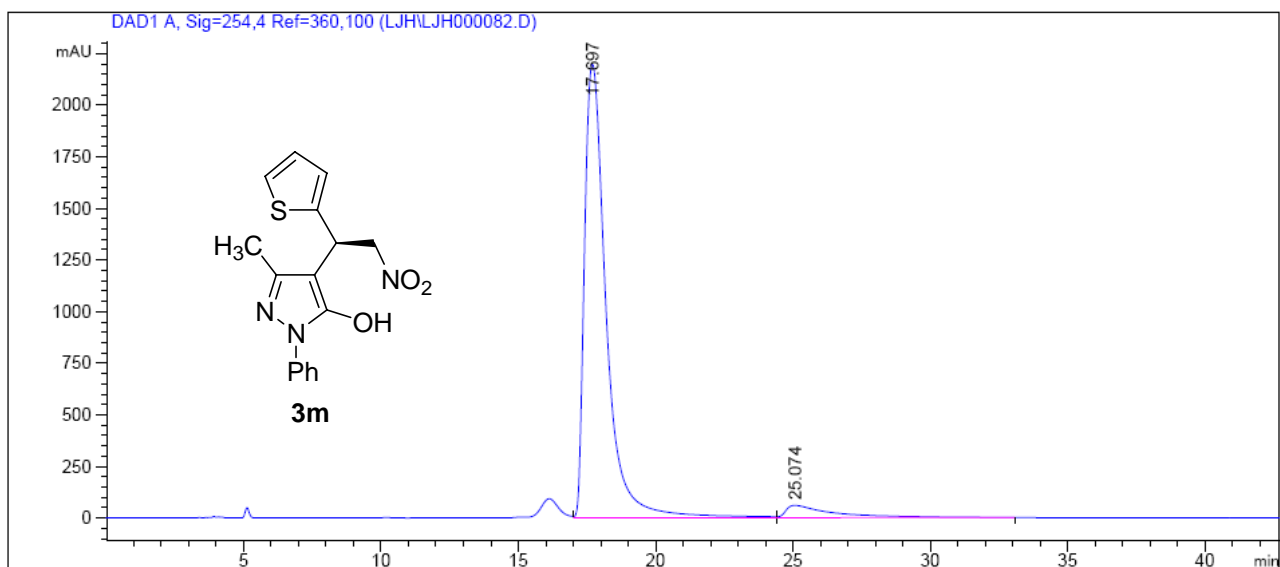


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.068	VB S	0.8591	2.06270e5	3327.84619	94.4360
2	34.674	BB	1.6857	1.21530e4	103.51668	5.5640

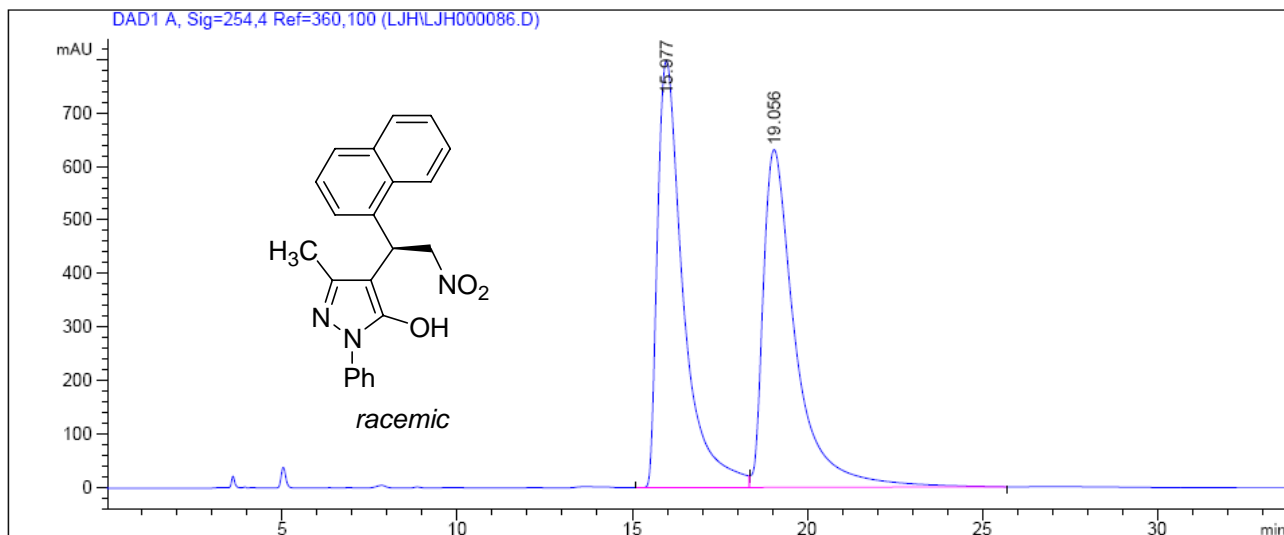


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.825	BV	0.8148	4.46478e4	810.28503	50.4421
2	24.305	VB	1.2279	4.38652e4	533.12964	49.5579

3m

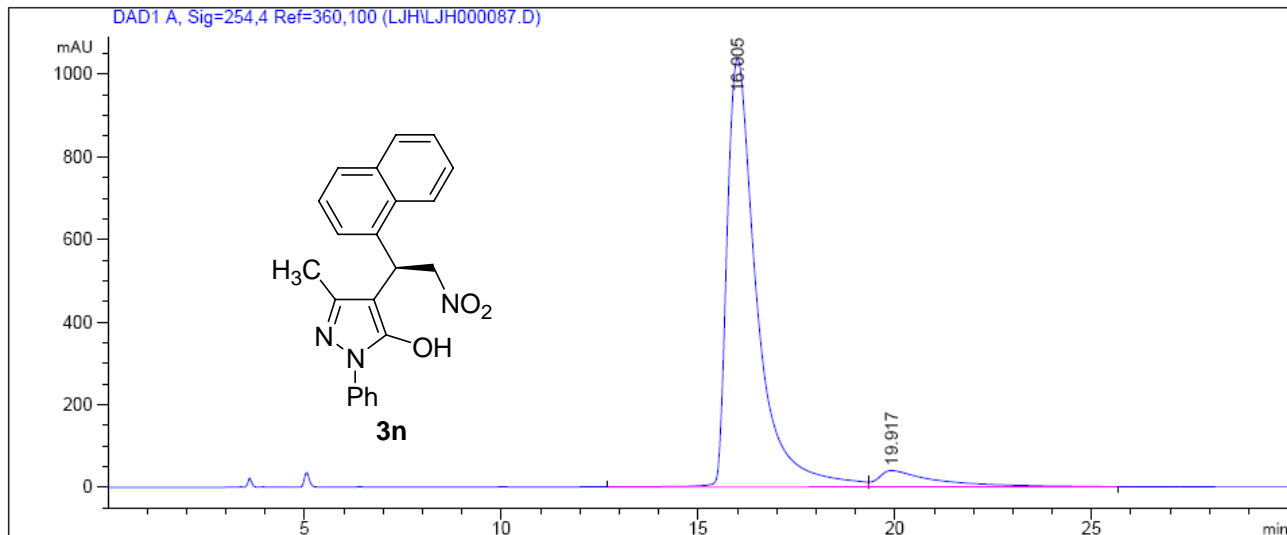


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.697	VV T	0.8396	1.20533e5	2198.68555	94.3267
2	25.074	VB T	1.6278	7249.53760	59.90956	5.6733

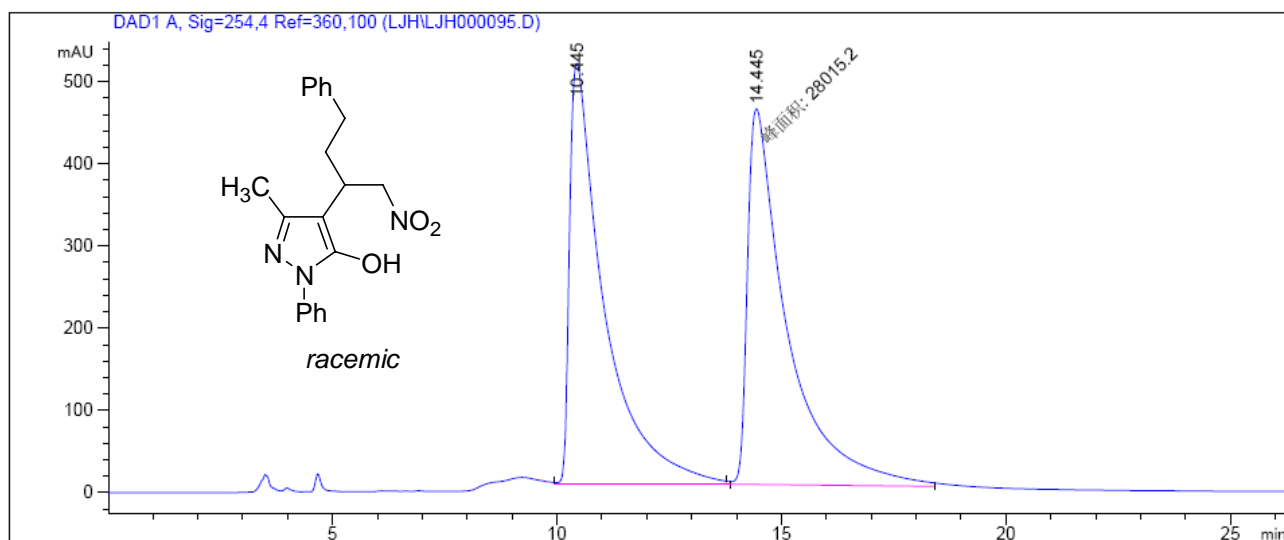


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.977	BV	0.7716	4.09990e4	797.79510	50.3221
2	19.056	VB	0.9644	4.04743e4	630.97375	49.6779

3n

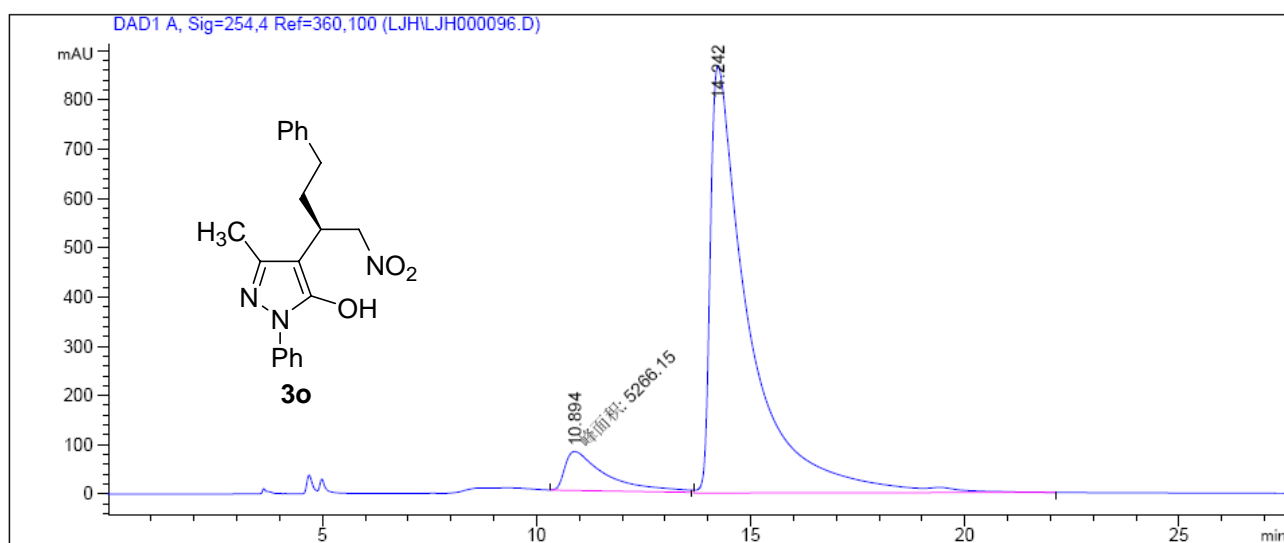


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.005	VV	0.7801	5.44174e4	1037.15747	93.1134
2	19.917	VB	1.3870	4024.69189	39.42617	6.8866

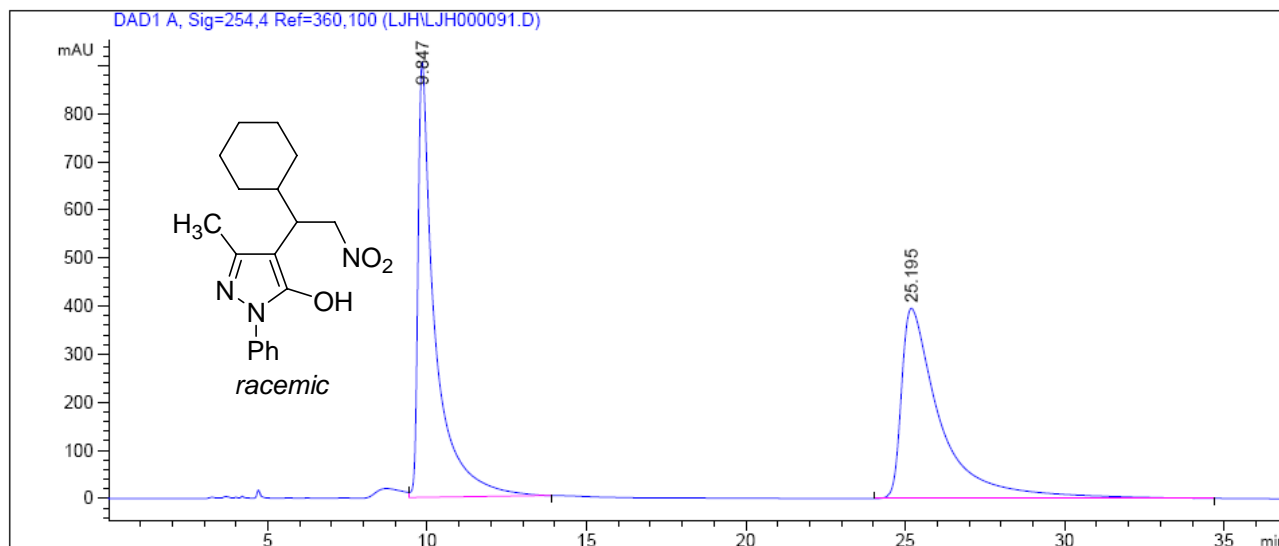


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.445	MM R	0.8368	2.73709e4	511.64197	49.4184
2	14.445	MM T	0.9855	2.80152e4	457.03885	50.5816

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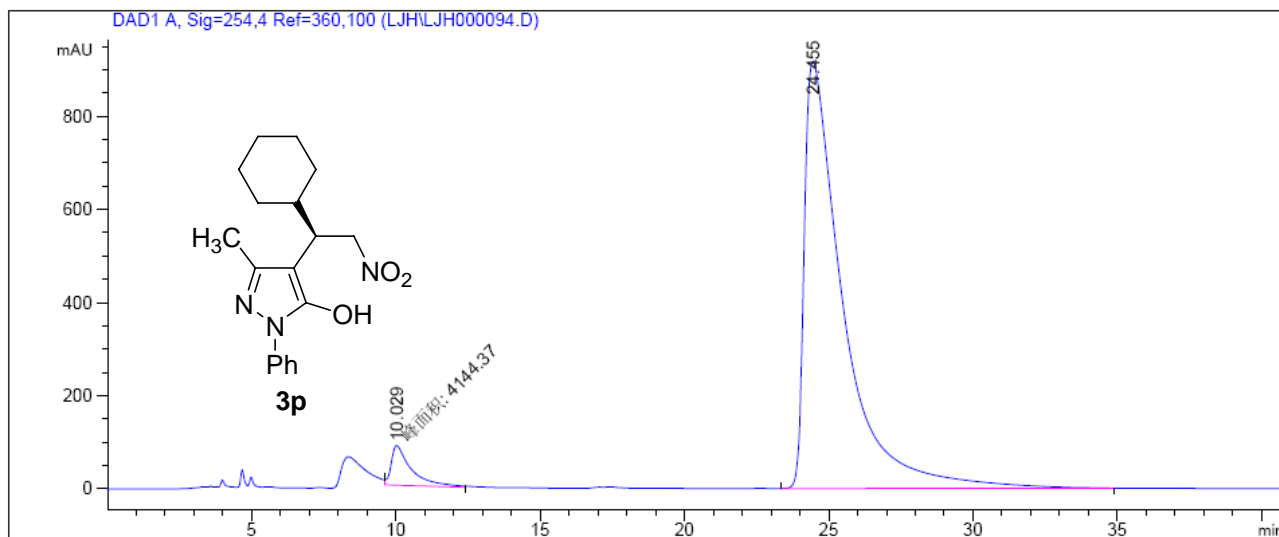


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.894	MM	1.1049	5266.15430	79.43681	8.8590
2	14.242	VB S	0.8581	5.41782e4	868.11761	91.1410

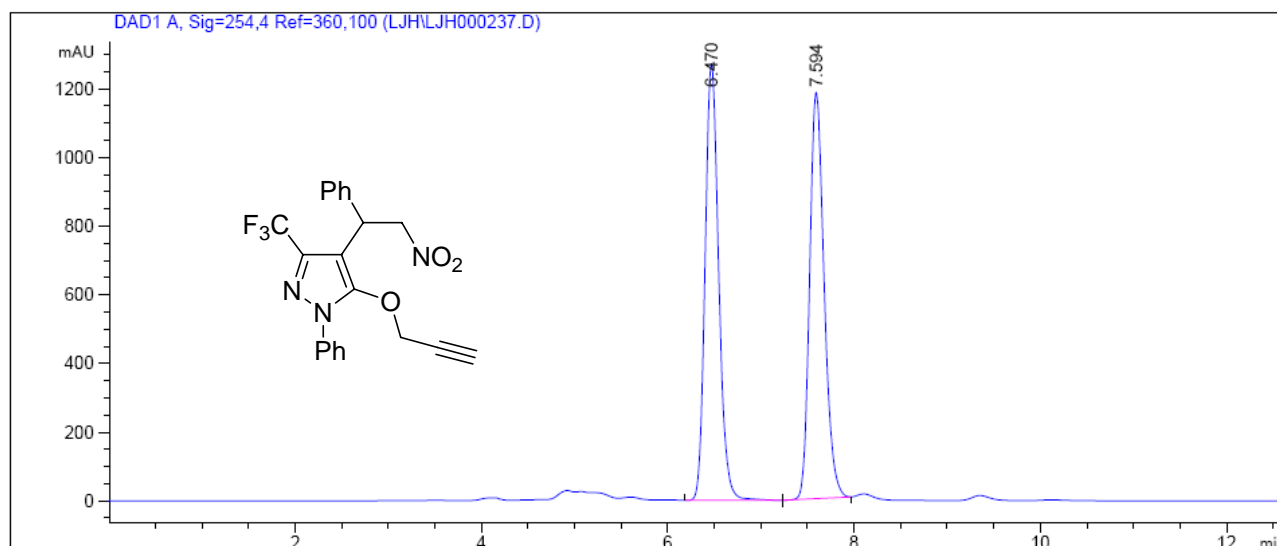


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.847	VB S	0.5070	3.34619e4	905.70752	49.7625
2	25.195	BB	1.2004	3.37812e4	395.52261	50.2375

3p

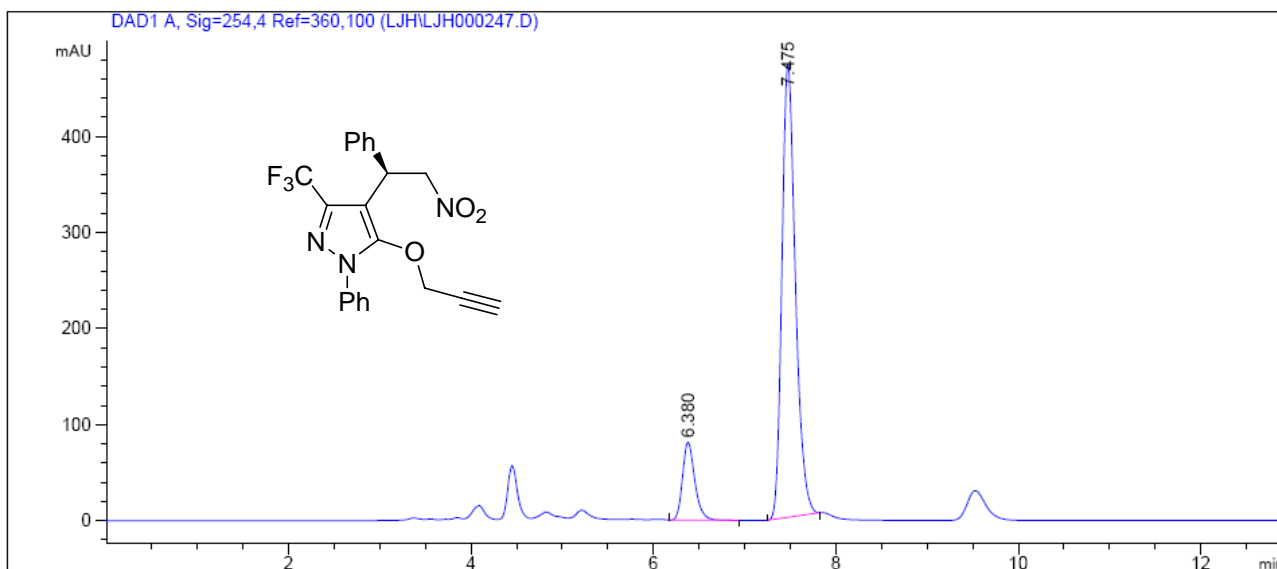


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.029	MM T	0.8091	4144.37158	85.37071	4.6402
2	24.455	BB	1.3317	8.51696e4	916.88892	95.3598

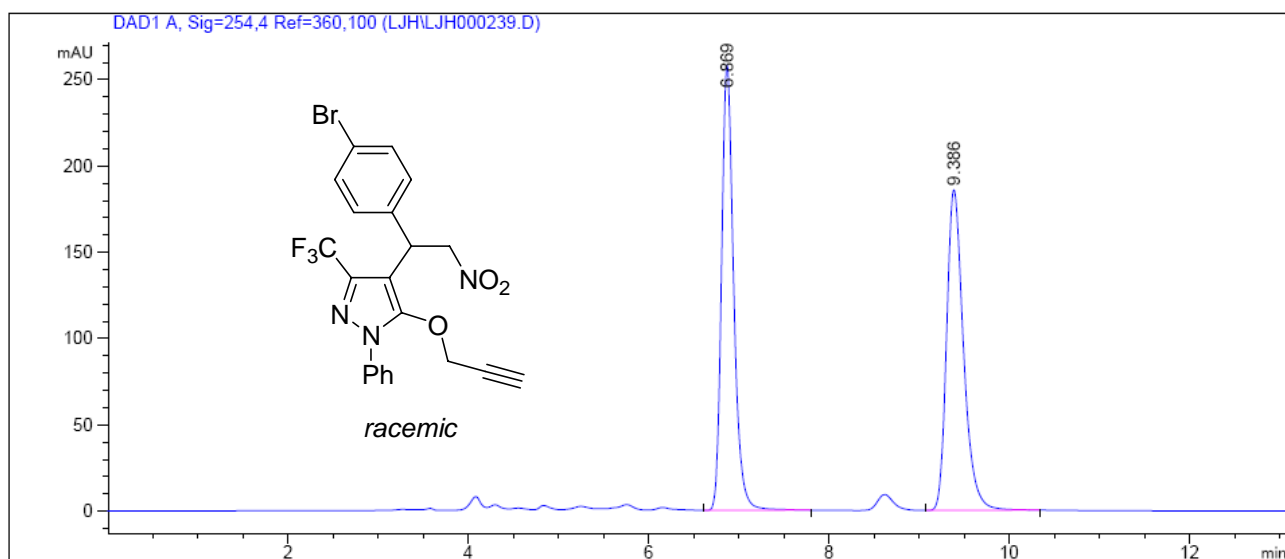


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.470	BB	0.1581	1.28592e4	1270.05566	50.1919
2	7.594	BB S	0.1659	1.27609e4	1182.16187	49.8081

3q was determined by its propargyloxy derivative

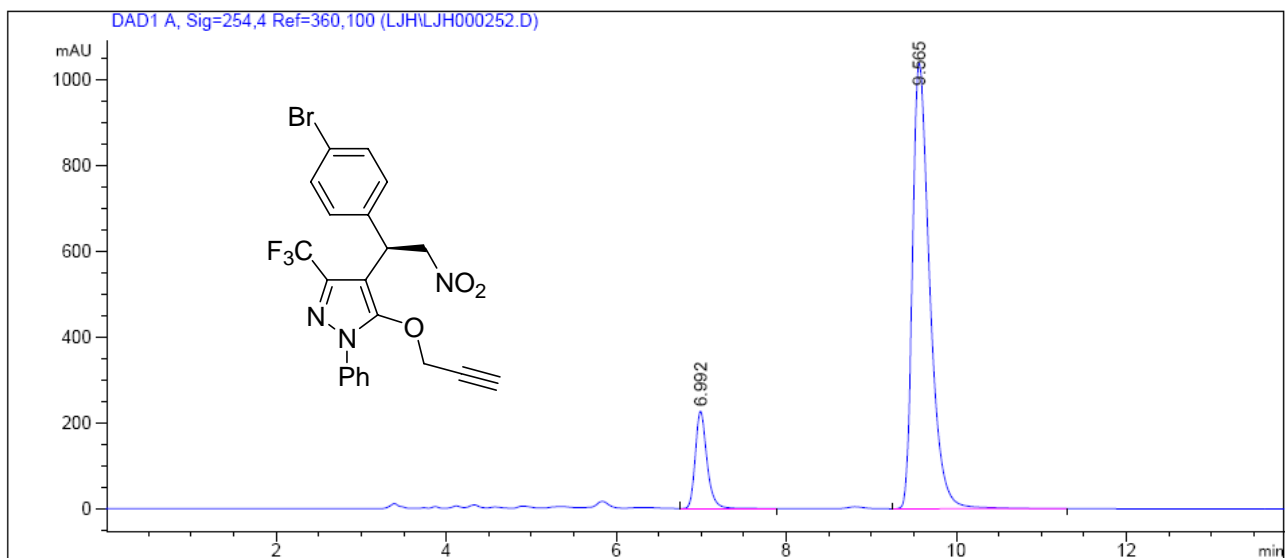


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.380	BB	0.1452	758.12915	80.97334	13.5595
2	7.475	BB S	0.1596	4832.99805	471.59232	86.4405

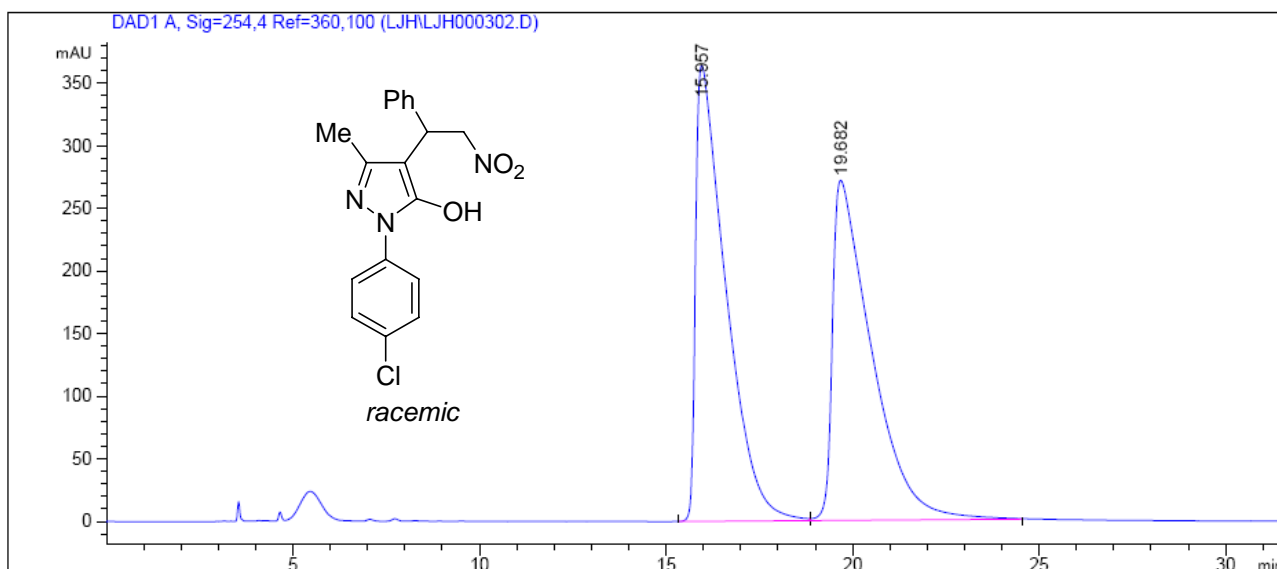


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.869	BB S	0.1454	2415.68262	257.63870	50.0040
2	9.386	VB S	0.1999	2415.29932	185.51678	49.9960

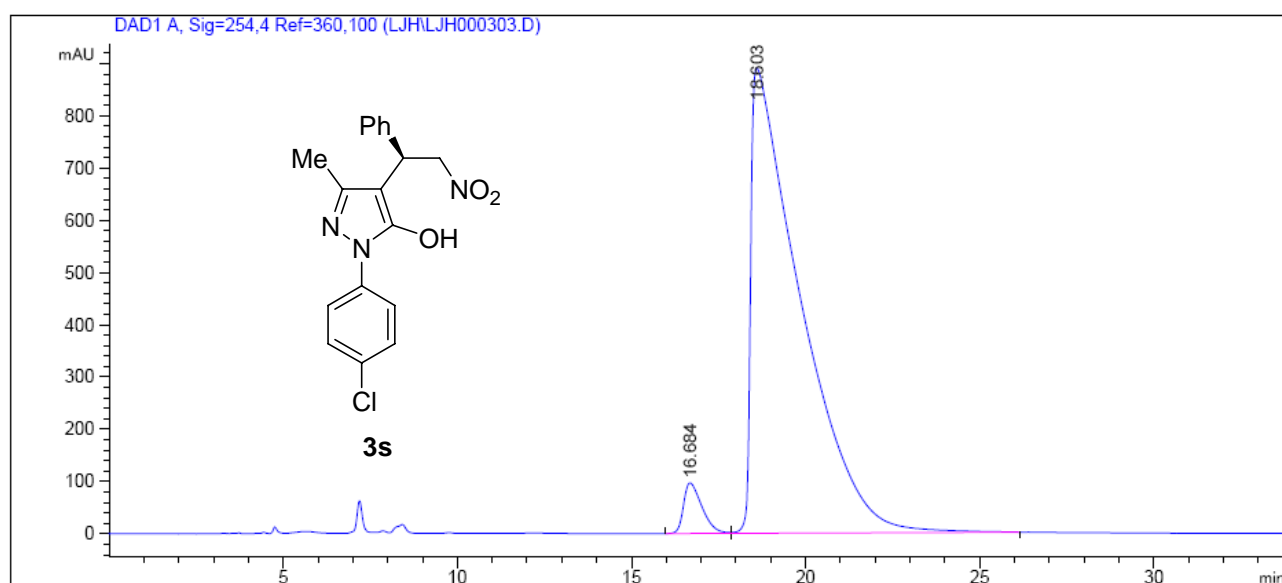
Compound **3r** was determined by its propargyloxy derivative



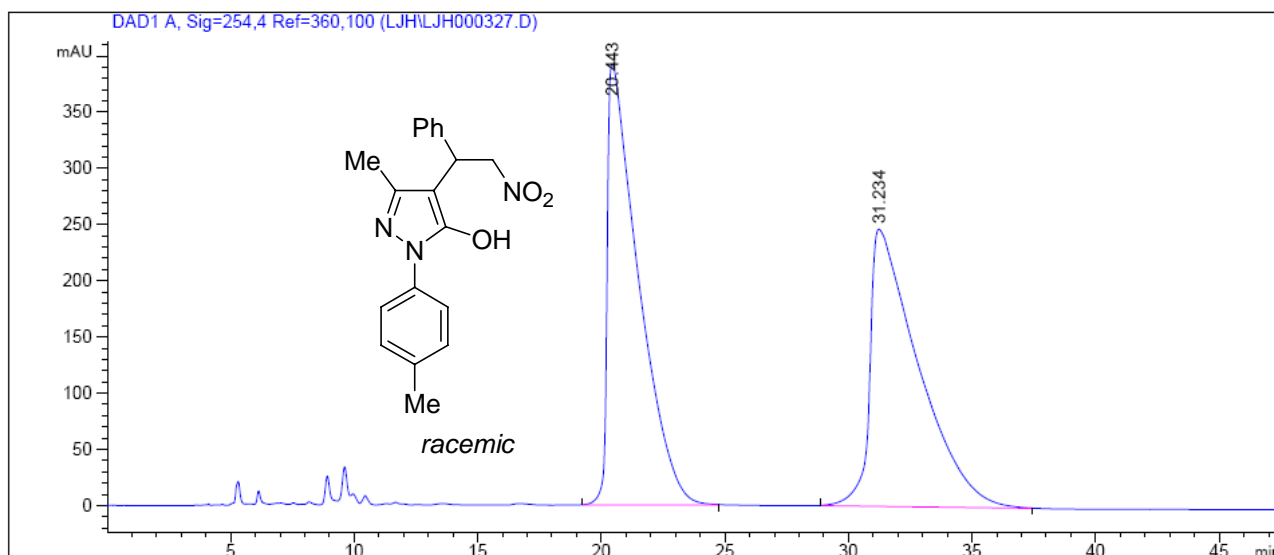
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.992	BB S	0.1477	2163.94043	225.93787	12.8928
2	9.565	VB S	0.2165	1.46201e4	1036.99011	87.1072



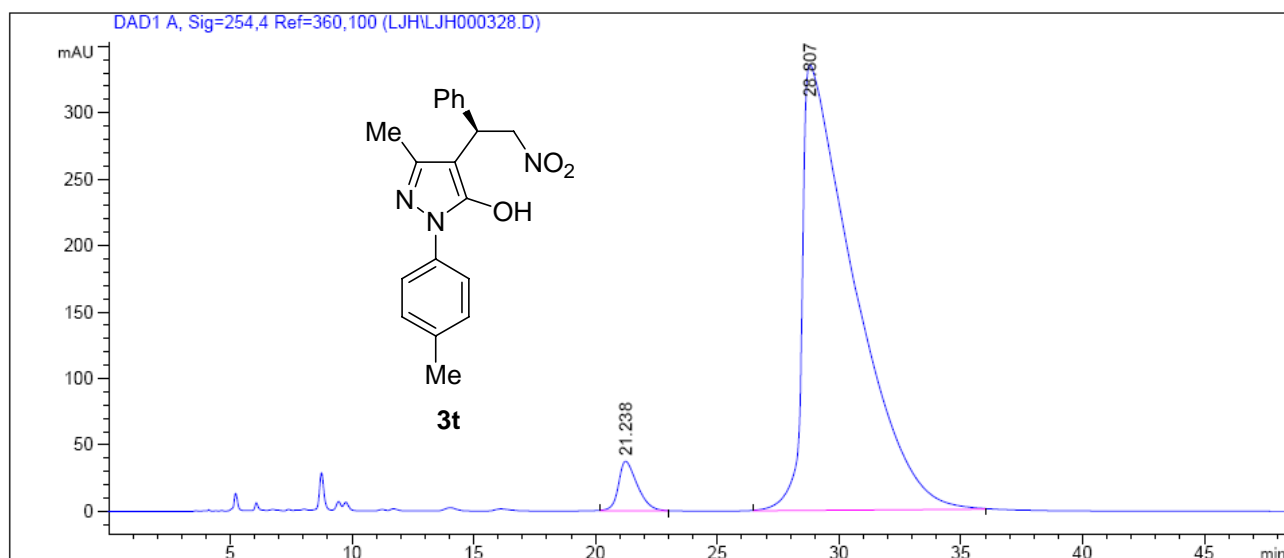
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.957	BV	0.8166	2.04805e4	363.92163	50.9157
2	19.682	VB	1.0004	1.97438e4	271.50012	49.0843



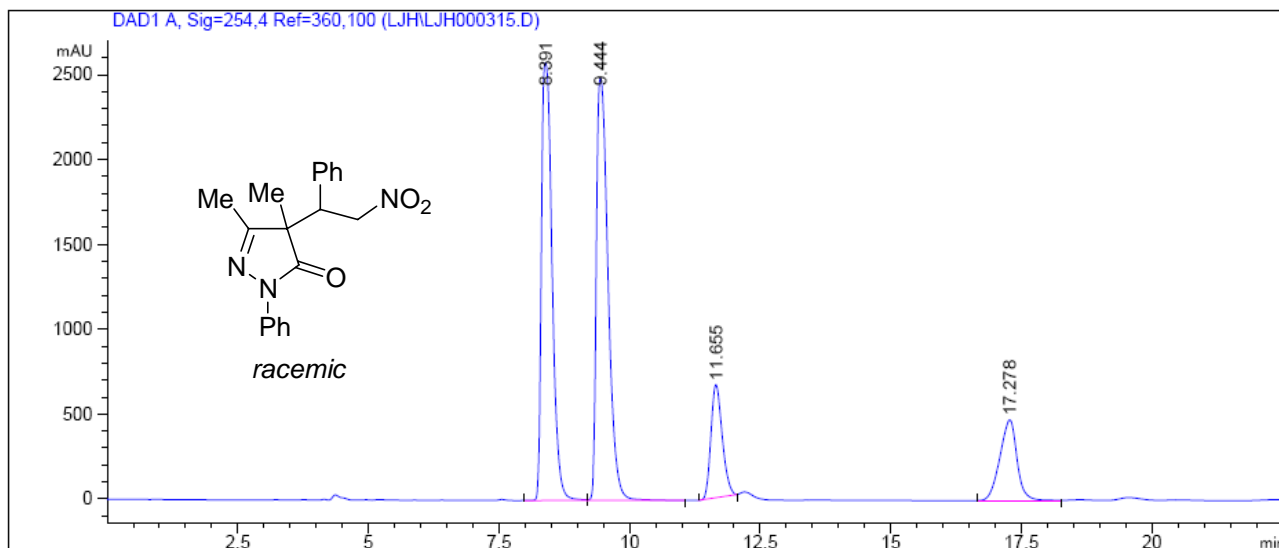
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.684	BV	0.5613	3562.41260	96.80896	3.8914
2	18.603	VB	1.3653	8.79823e4	890.03815	96.1086



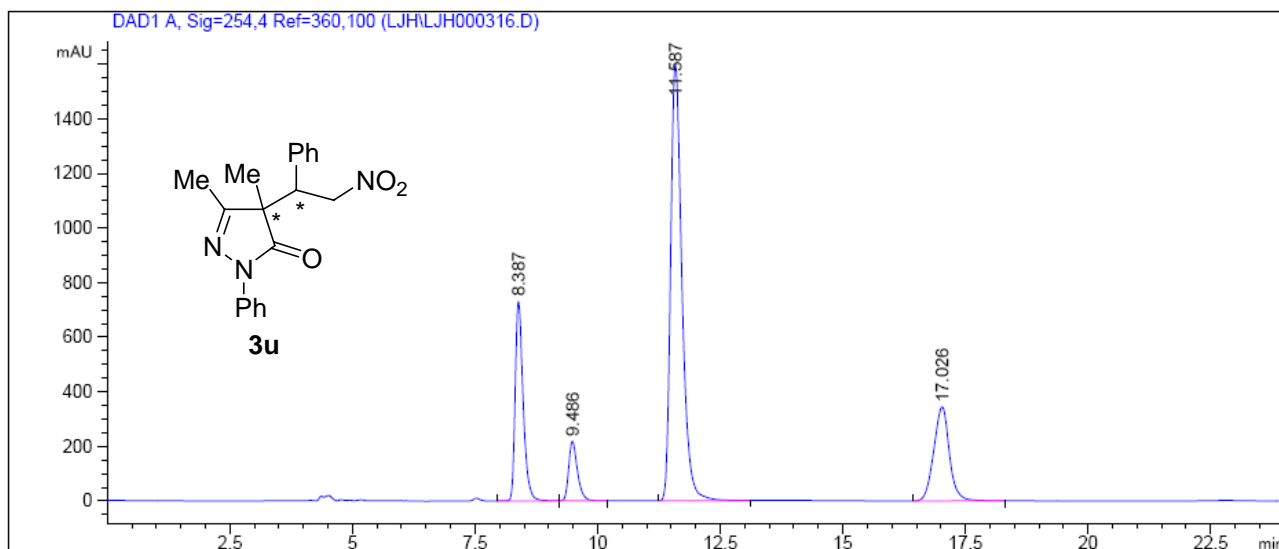
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.443	BB	1.1865	3.43361e4	392.54123	50.5021
2	31.234	BB	1.7950	3.36533e4	246.77774	49.4979



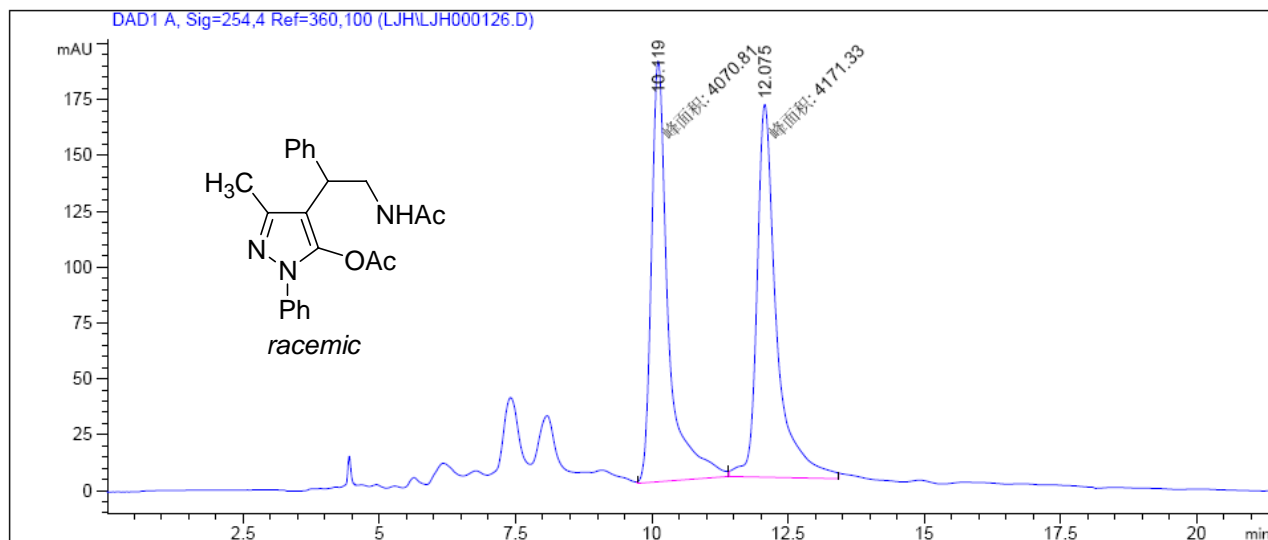
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.238	BB	0.8216	2008.24744	37.21607	3.8791
2	28.807	BB	1.8826	4.97624e4	335.46152	96.1209



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.391	BV	0.2228	3.64304e4	2579.44482	38.0220
2	9.444	VB S	0.2406	3.85249e4	2488.85913	40.2081
3	11.655	BB	0.2312	9992.22559	665.48059	10.4288
4	17.278	BV	0.3507	1.08663e4	475.34451	11.3411

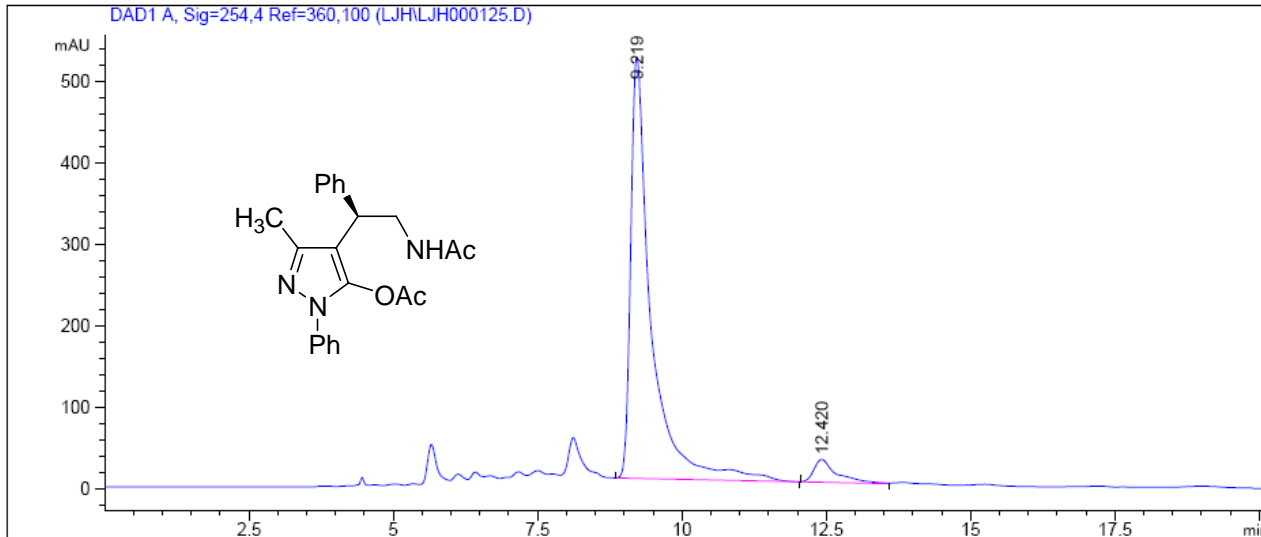


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.387	BV	0.1712	8222.27246	731.02222	18.6108
2	9.486	VB S	0.1890	2706.95142	217.76132	6.1271
3	11.587	BB	0.2449	2.56494e4	1601.27661	58.0564
4	17.026	BB	0.3374	7601.47656	344.50128	17.2057

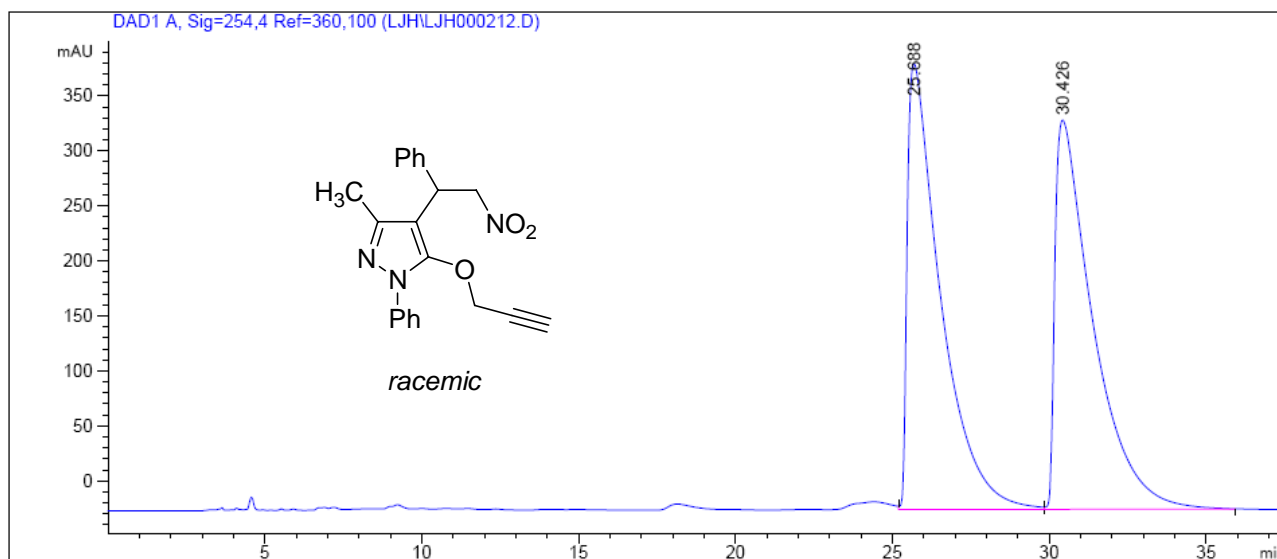


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.119	MM T	0.3602	4070.81152	188.36588	49.3902
2	12.075	MM T	0.4166	4171.32764	166.86177	50.6098

Compound **4** was determined by its acetyl derivative

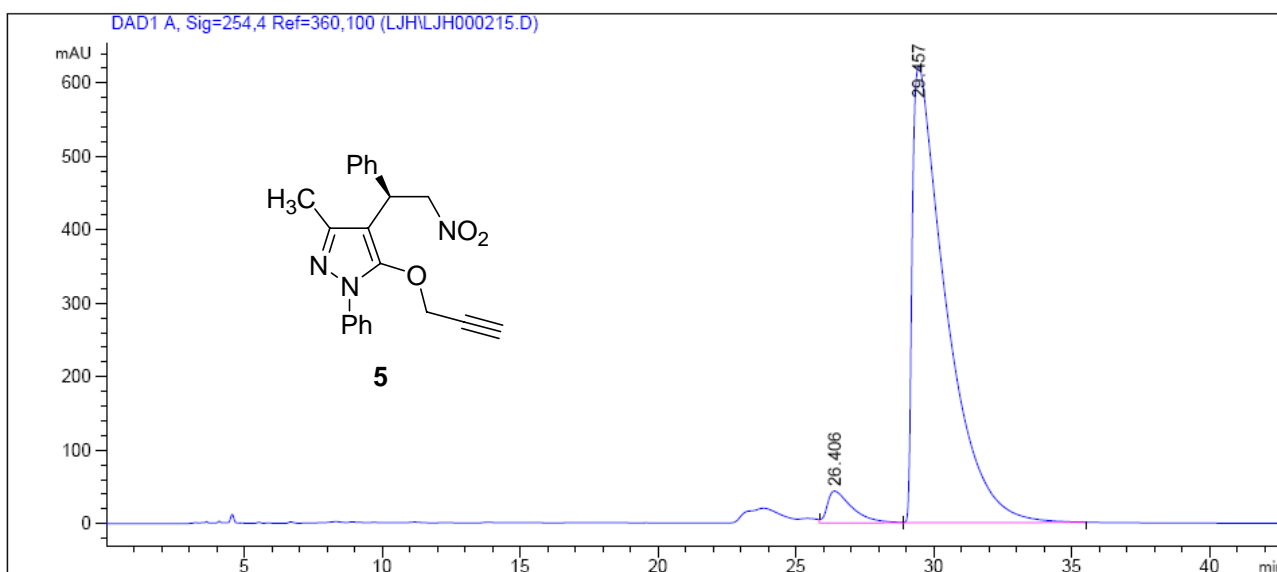


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.219	BB S	0.3450	1.26902e4	517.01080	94.3021
2	12.420	BV	0.3917	766.77008	27.97937	5.6979



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.688	VV	1.0673	2.98607e4	405.40359	50.1459
2	30.426	VB	1.2107	2.96869e4	353.88205	49.8541

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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.406	VV	0.9159	2682.06909	43.22739	4.8511
2	29.457	VB	1.2027	5.26054e4	622.00244	95.1489