

Supplementary information

Organocatalytic Enantioselective Michael Addition of Cyclic Hemiacetals to Nitroolefins: A Facile Access to Chiral Substituted 5- and 6-Membered Cyclic Ethers

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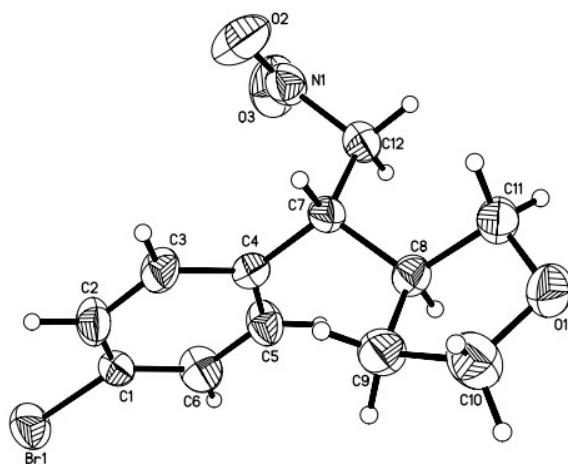
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Zhang, zhangshilei@suda.edu.cn.

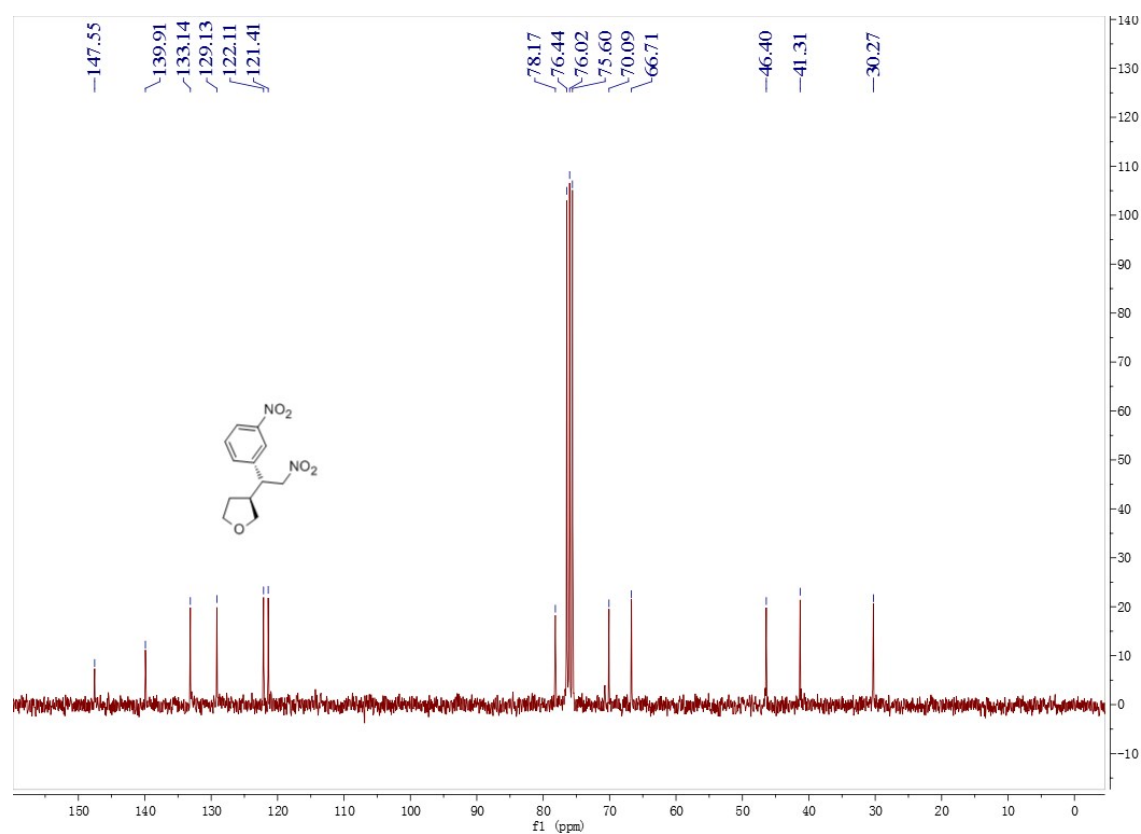
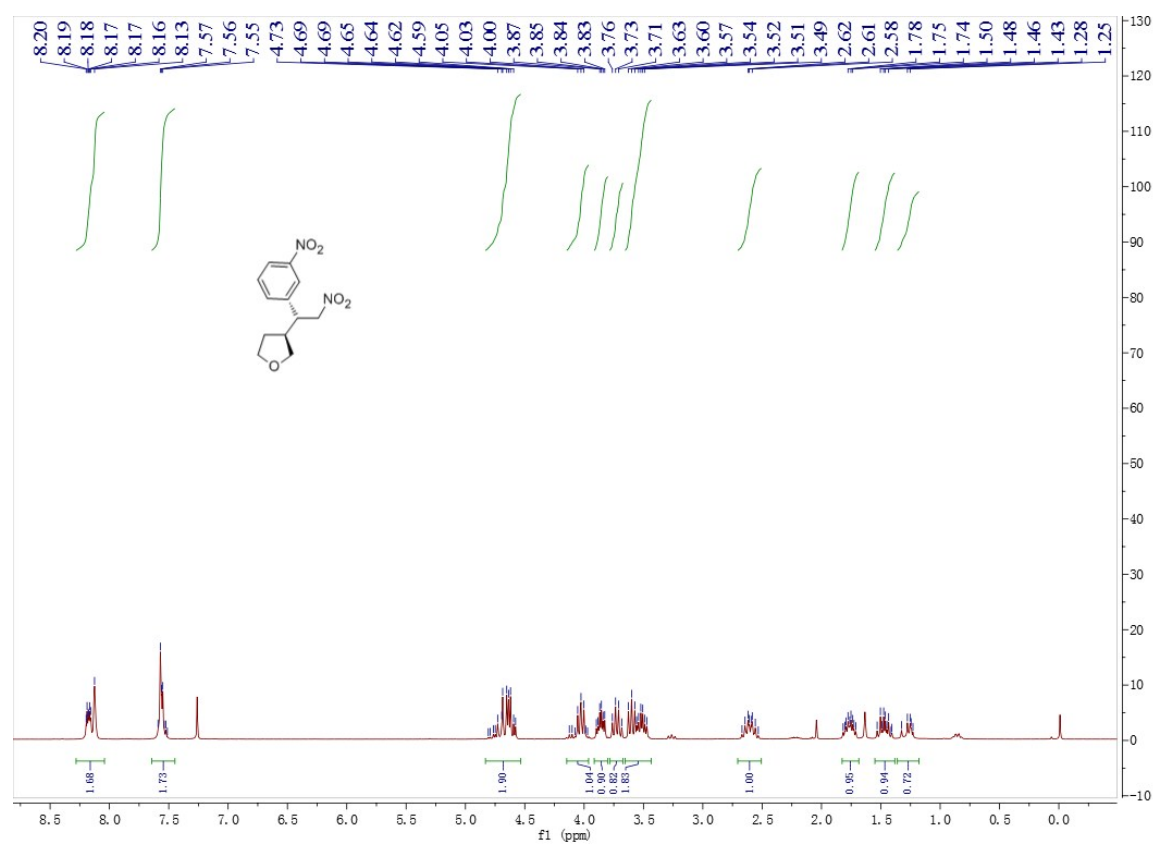
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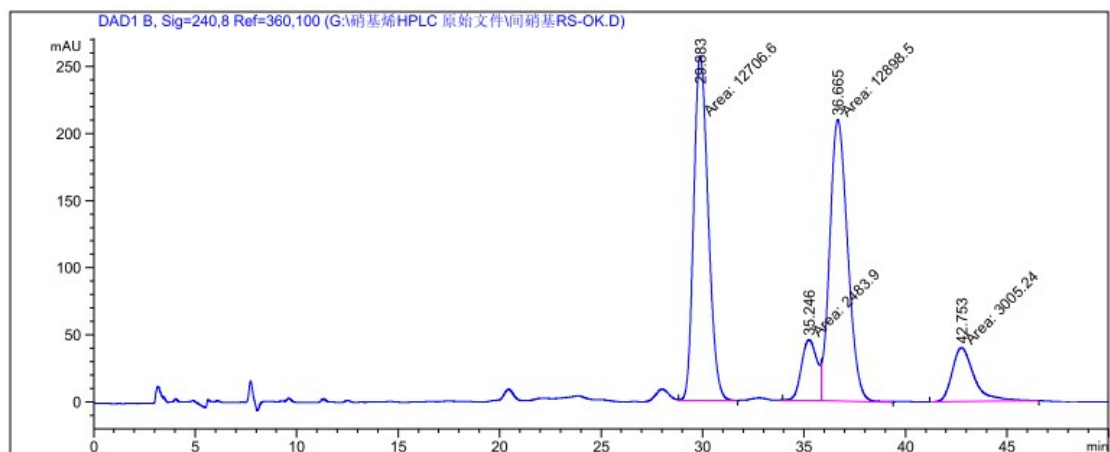
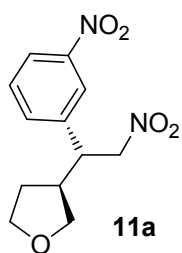
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1. The Single Crystal X-ray Diffraction of Compound 11K

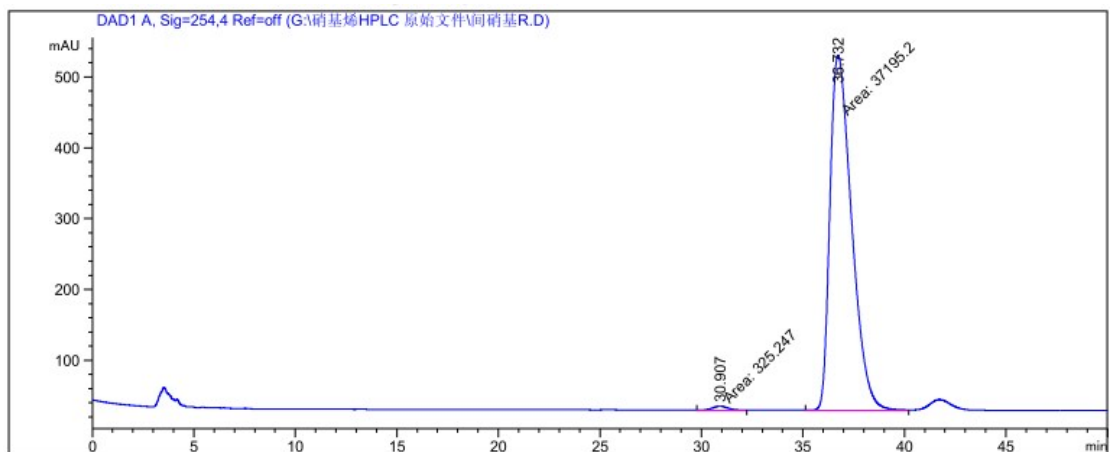


2. NMR and HPLC Spectra for All Compounds

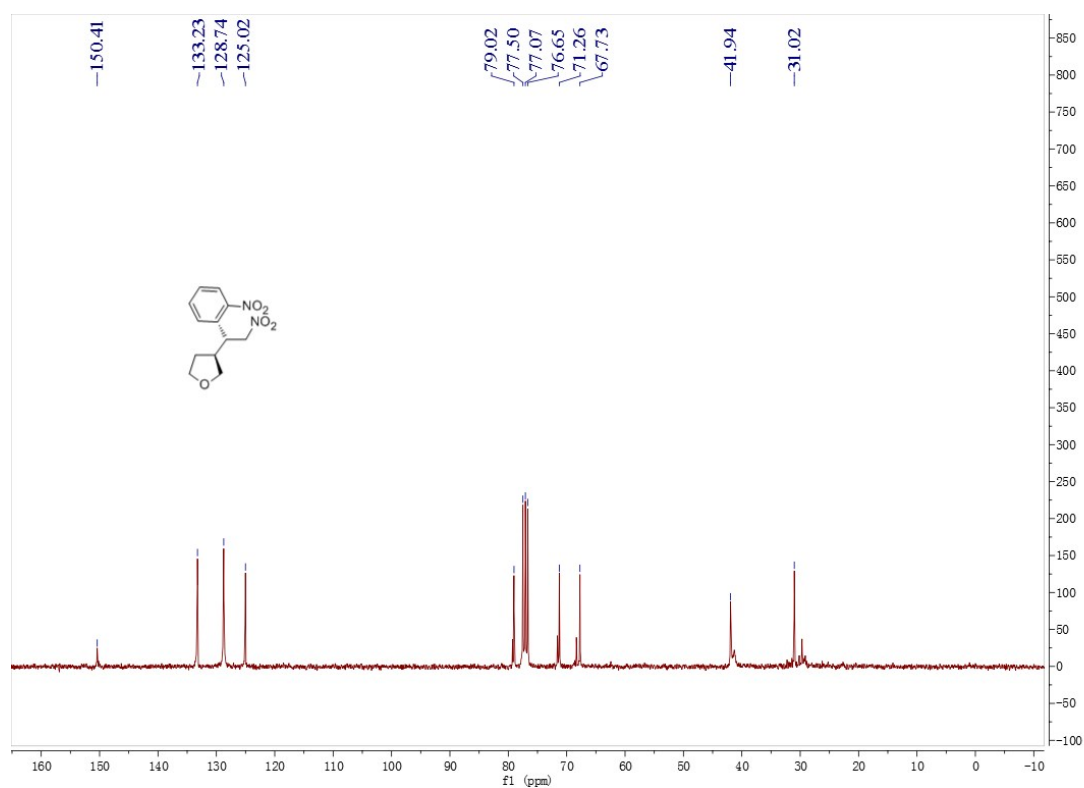
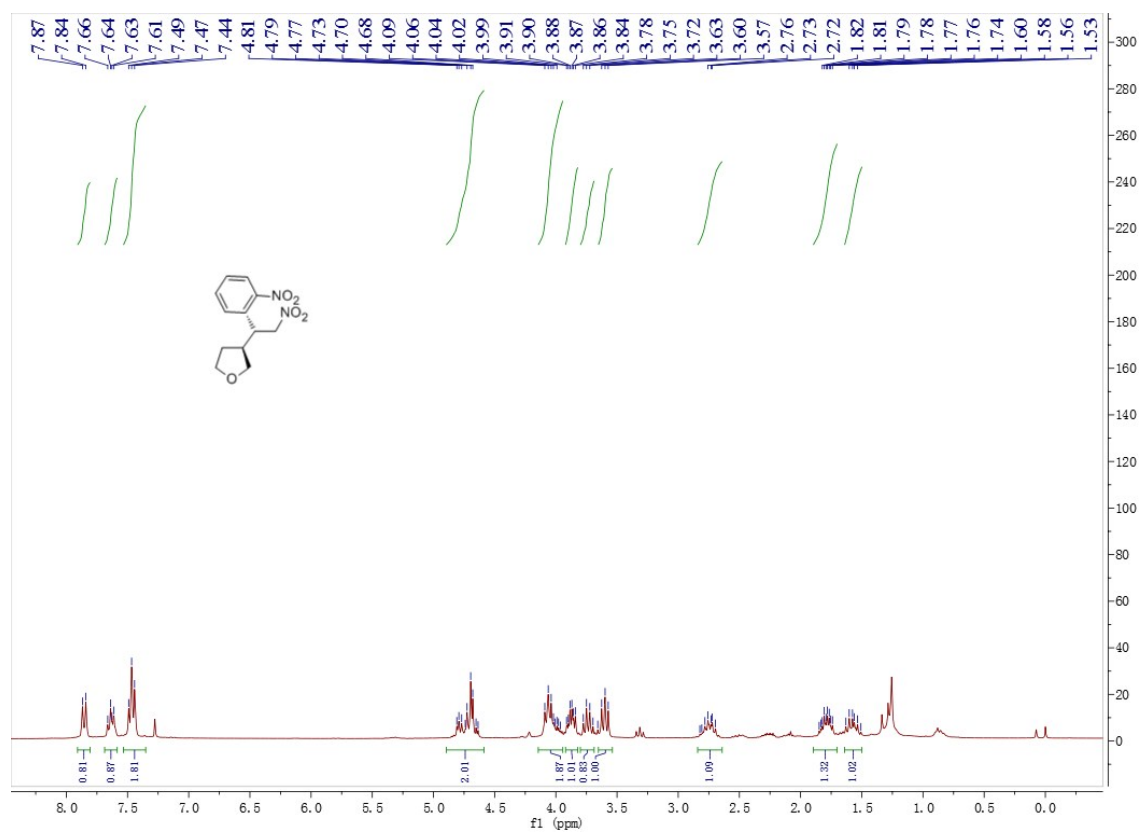


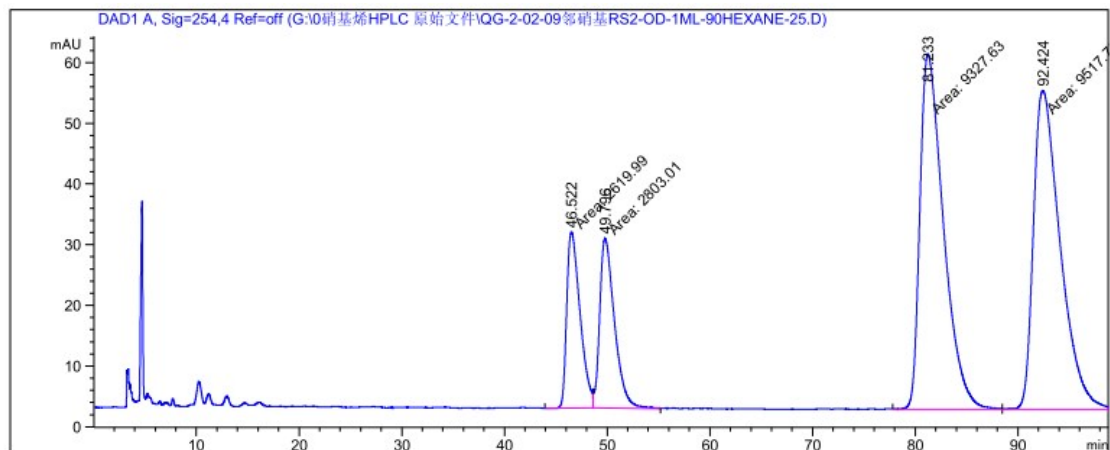
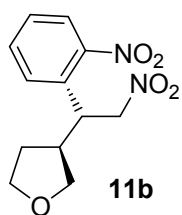


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1	29.883	MM	0.8239	1.27066e4	257.03036	40.8647
2	35.246	MM	0.9142	2483.89795	45.28357	7.9883
3	36.665	MM	1.0256	1.28985e4	209.60298	41.4820
4	42.753	MM	1.2465	3005.24365	40.18242	9.6650

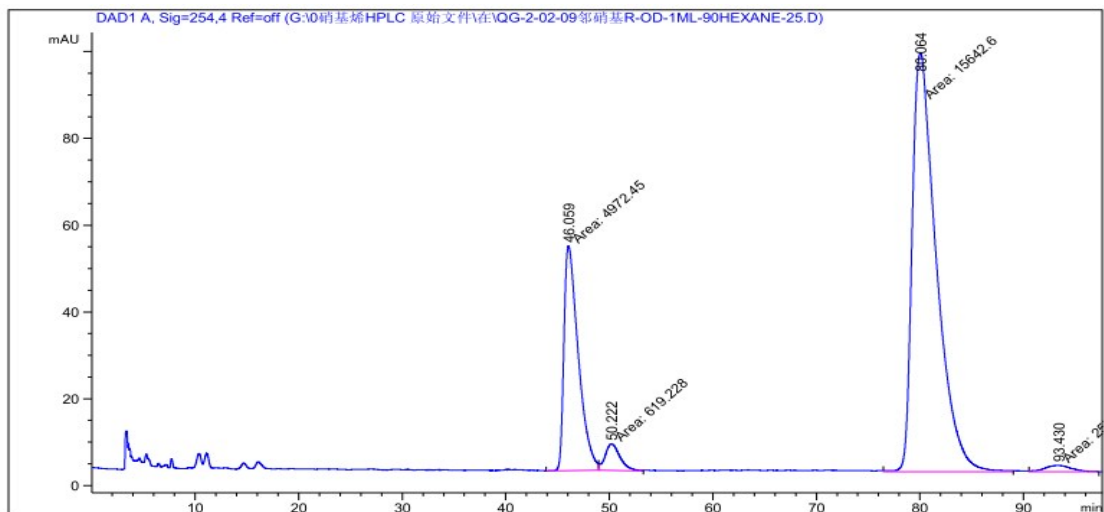


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1	30.907	MM	0.9512	325.24725	5.69897	0.8669
2	36.732	MM	1.2363	3.71952e4	501.43430	99.1331

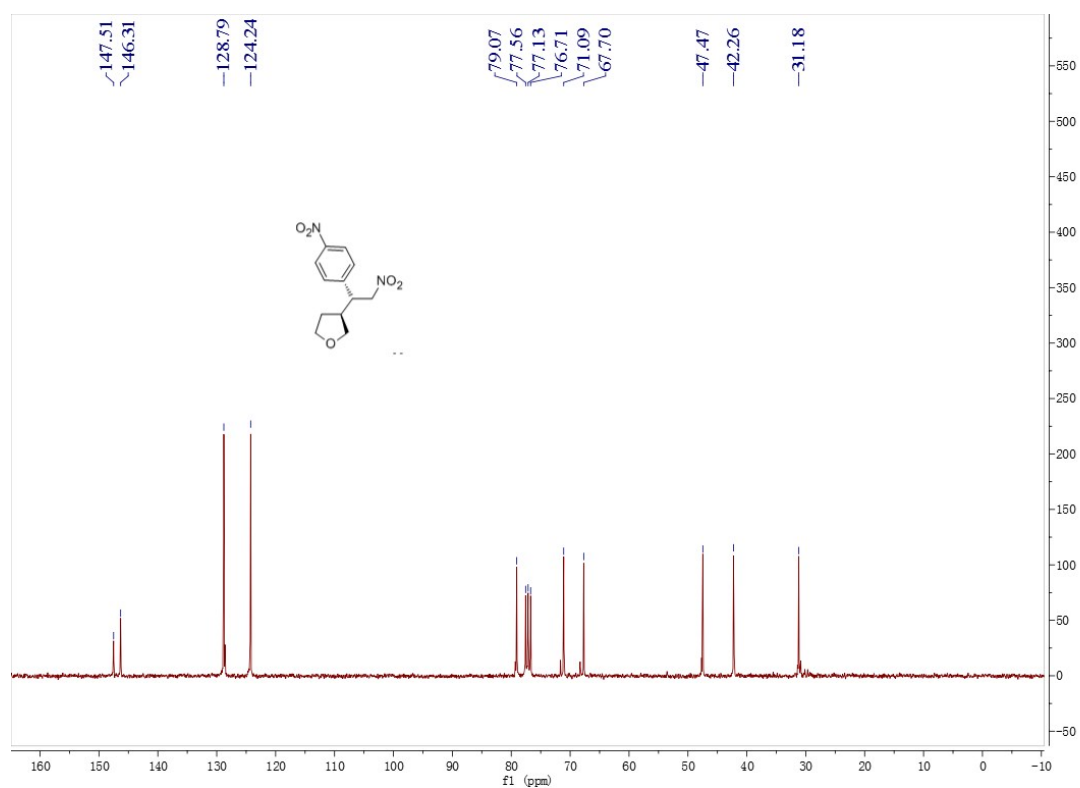
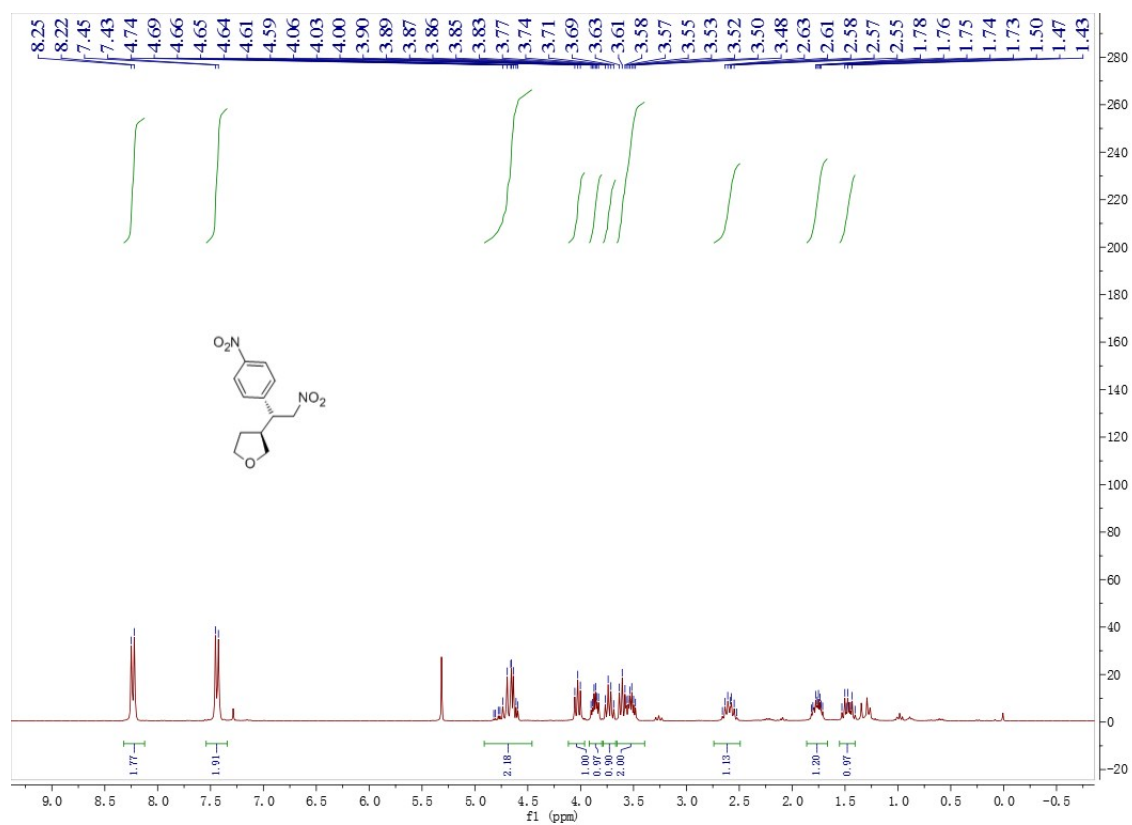


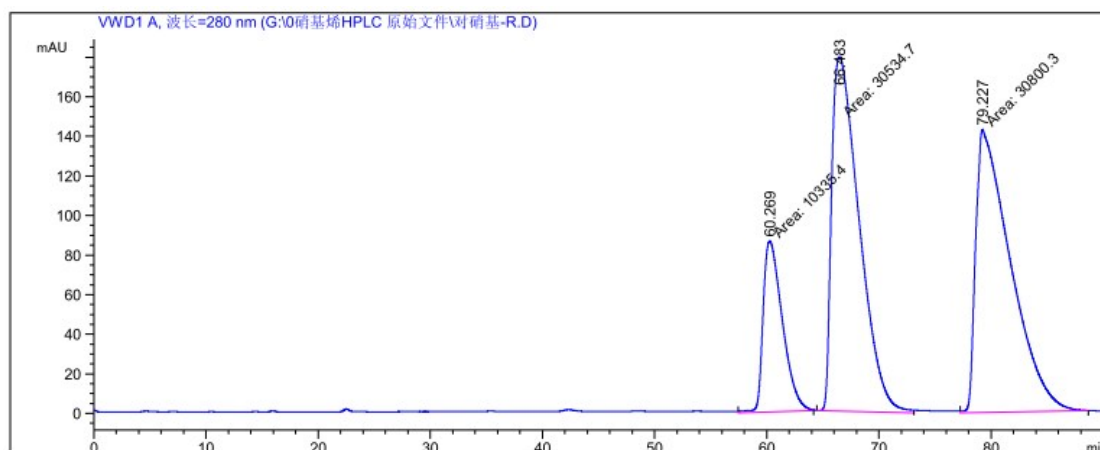
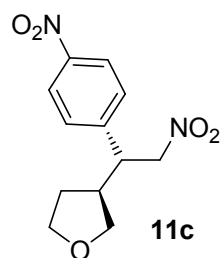


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1	46.522	MM	1.5068	2619.99121	28.97902	10.7959
2	49.796	MM	1.6699	2803.00830	27.97629	11.5500
3	81.233	MM	2.6551	9327.63477	58.55096	38.4353
4	92.424	MM	3.0198	9517.78418	52.53016	39.2188

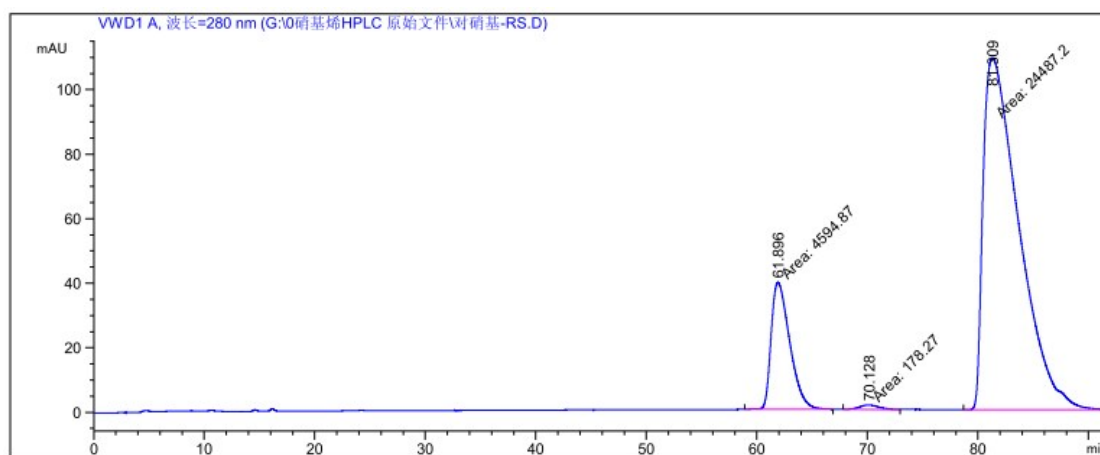


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2	50.222	MM	1.6863	619.22791	6.12015	2.8812
3	80.064	MM	2.7032	15642.6e4	96.44337	72.7842
4	93.430	MM	2.9811	257.46204	1.43943	1.1980

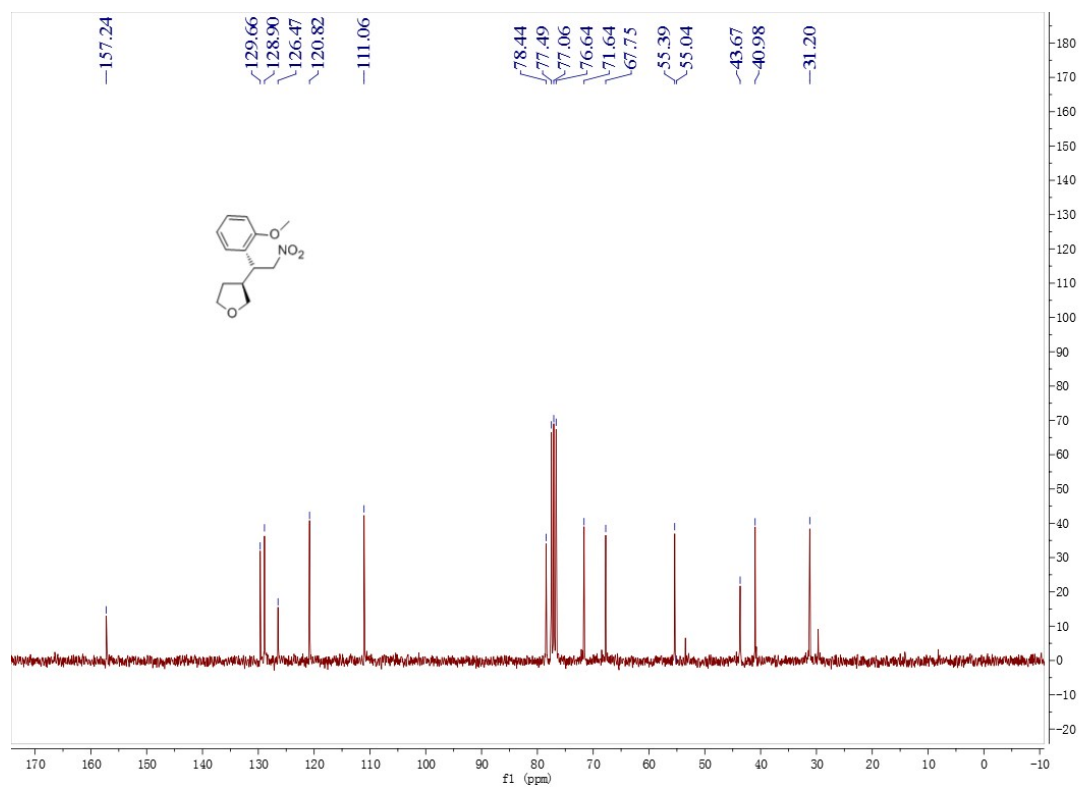
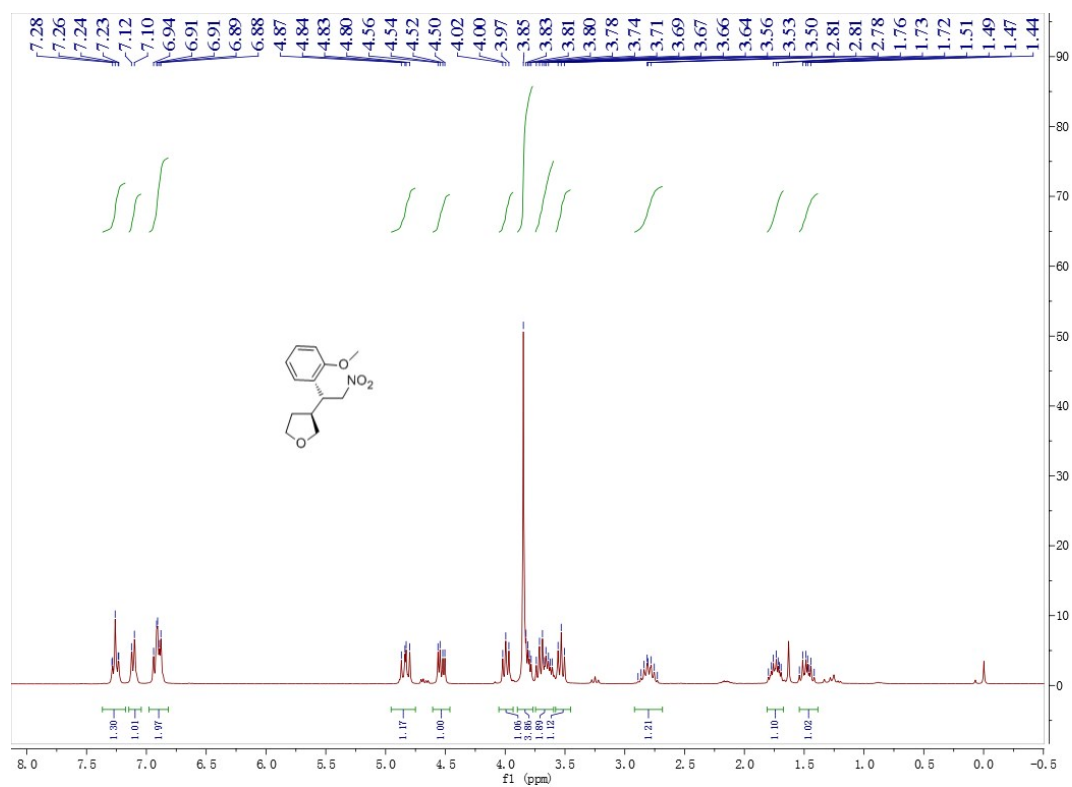


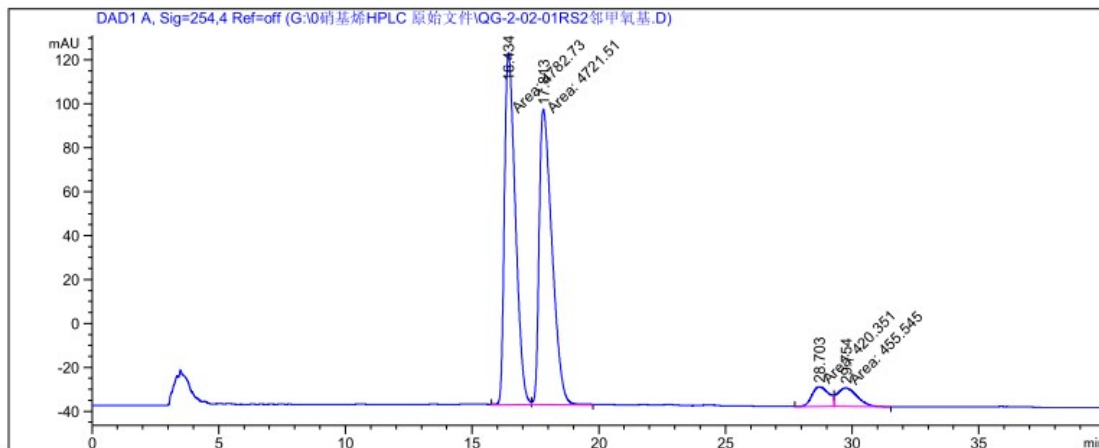
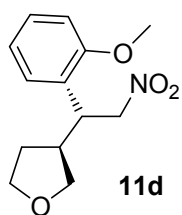


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	60.269	MM	1.9932	1.03354e4	86.42022	14.4207
2	66.483	MM	2.8409	3.05347e4	179.13666	42.6044
3	79.227	MM	3.5931	3.08003e4	142.86621	42.9749

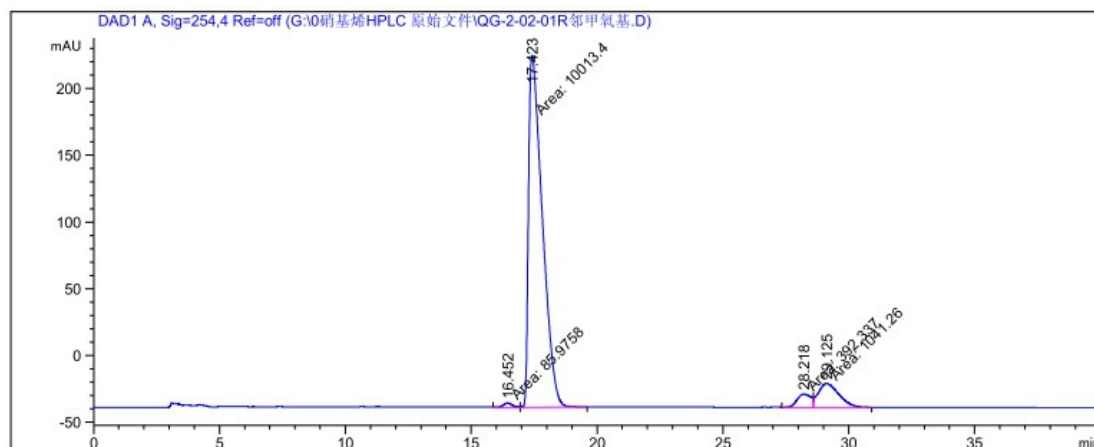


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1	61.896	MM	1.9502	4594.87061	39.26748	15.7034
2	70.128	MM	2.1175	178.26950	1.40317	0.6093
3	81.309	MM	3.7405	2.44872e4	109.10786	83.6873

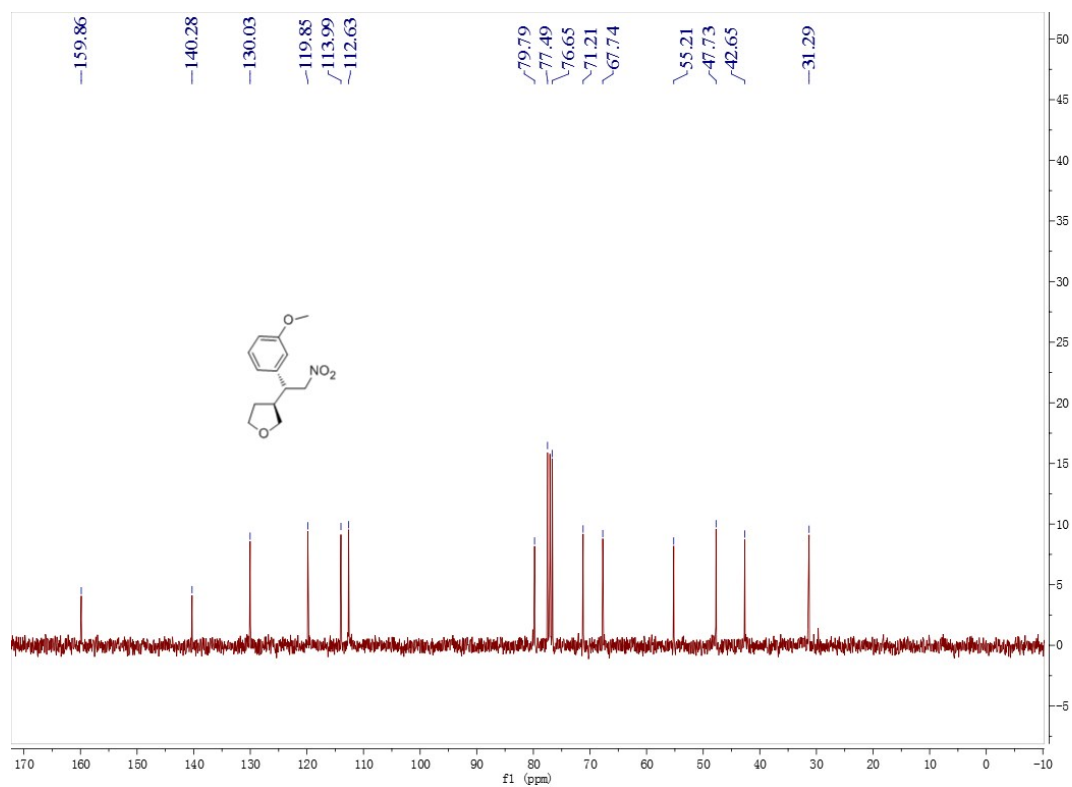
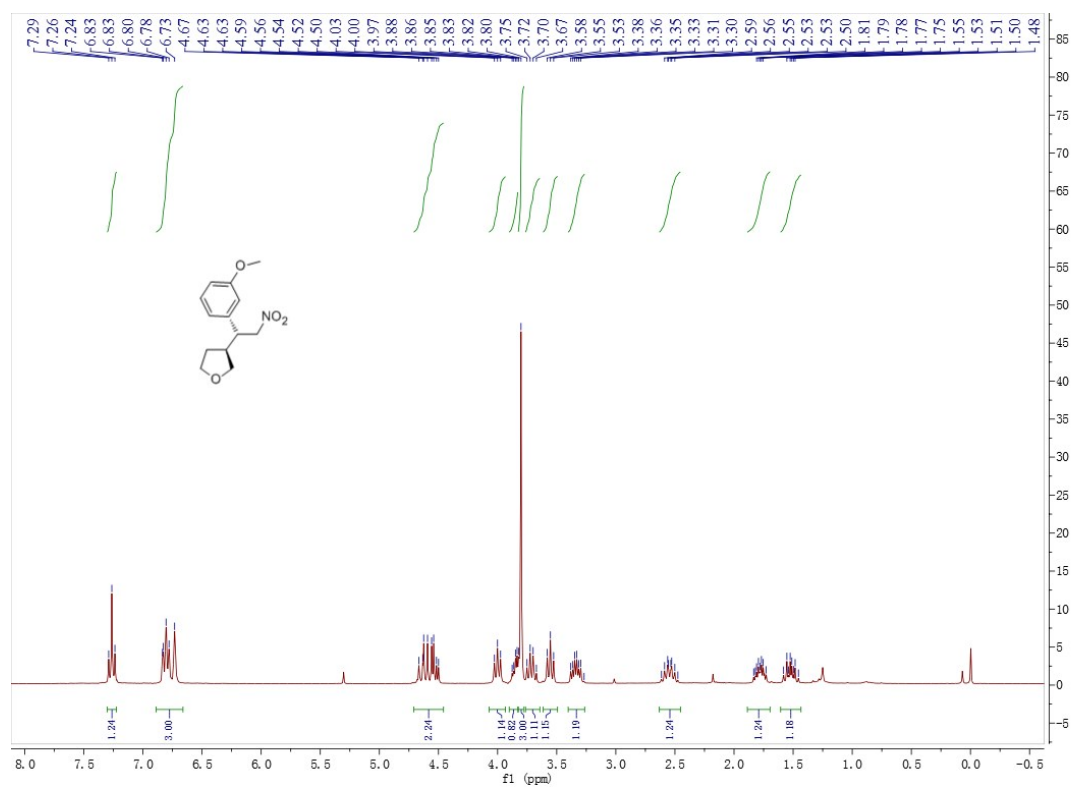


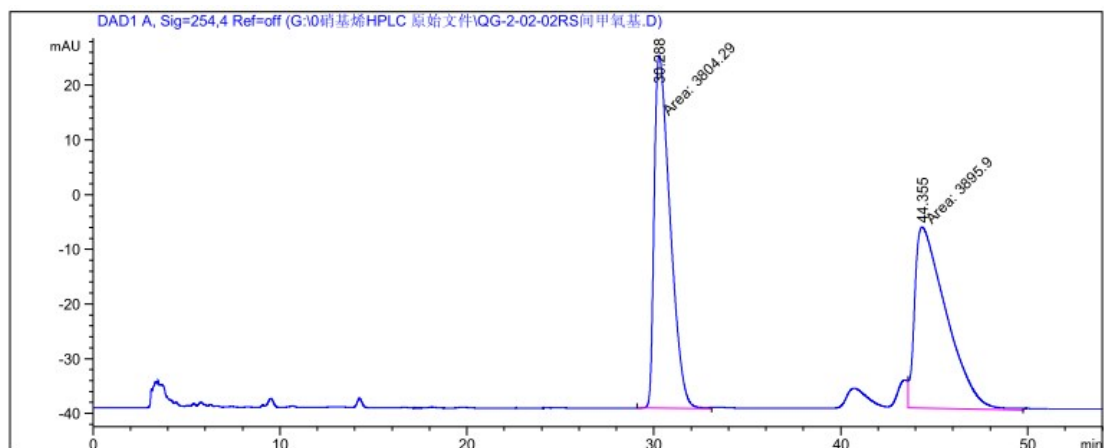
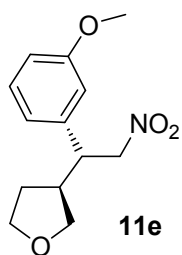


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1	16.434	MM	0.4974	4782.72949	160.24741	46.0758
2	17.813	MM	0.5853	4721.50879	134.45769	45.4860
3	28.703	MM	0.7790	420.35132	8.99302	4.0496
4	29.754	MM	0.9064	455.54541	8.37629	4.3886

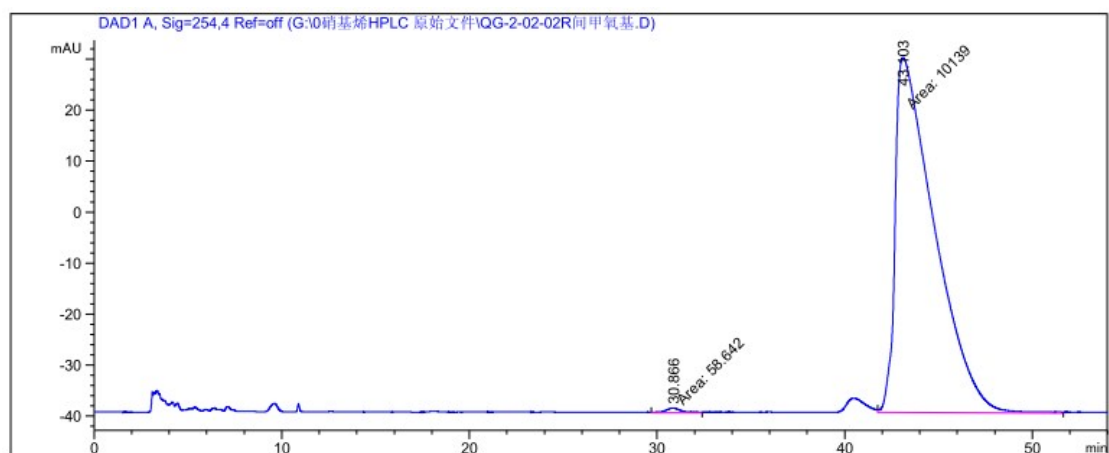


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2	17.423	MM	0.6333	1.00134e4	263.53598	86.8240
3	28.218	MM	0.6498	392.33713	10.06276	3.4019
4	29.125	MM	0.9652	1041.26355	17.97919	9.0286

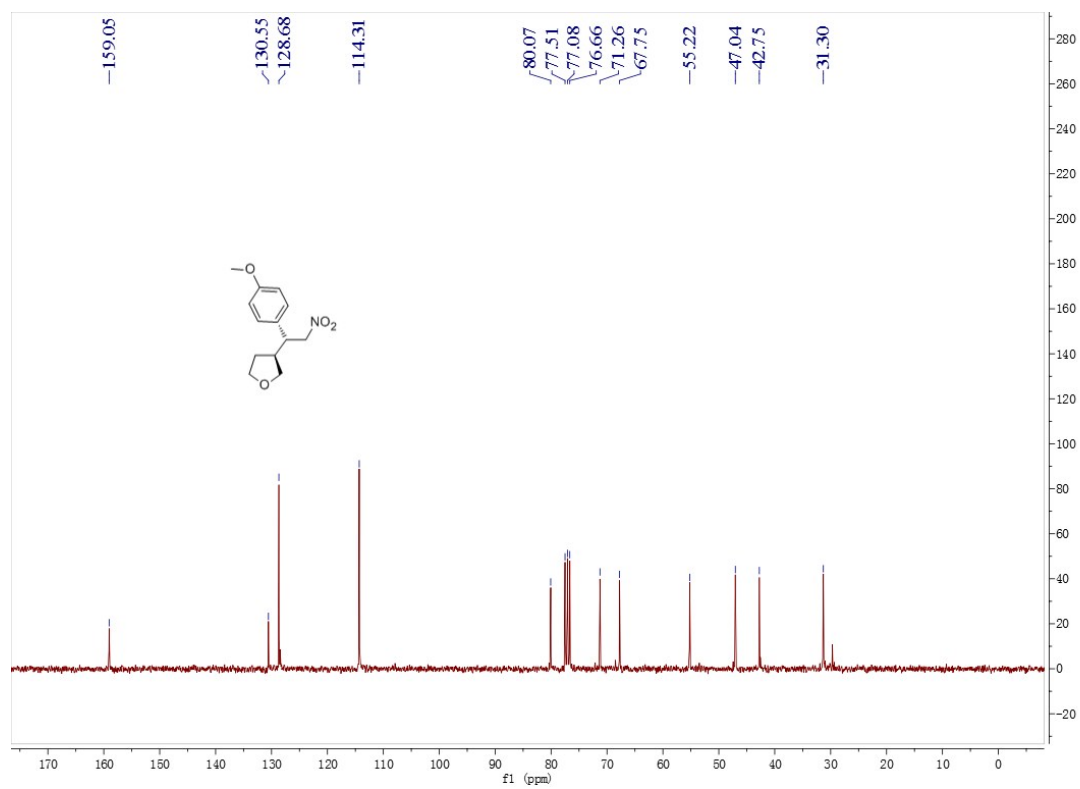
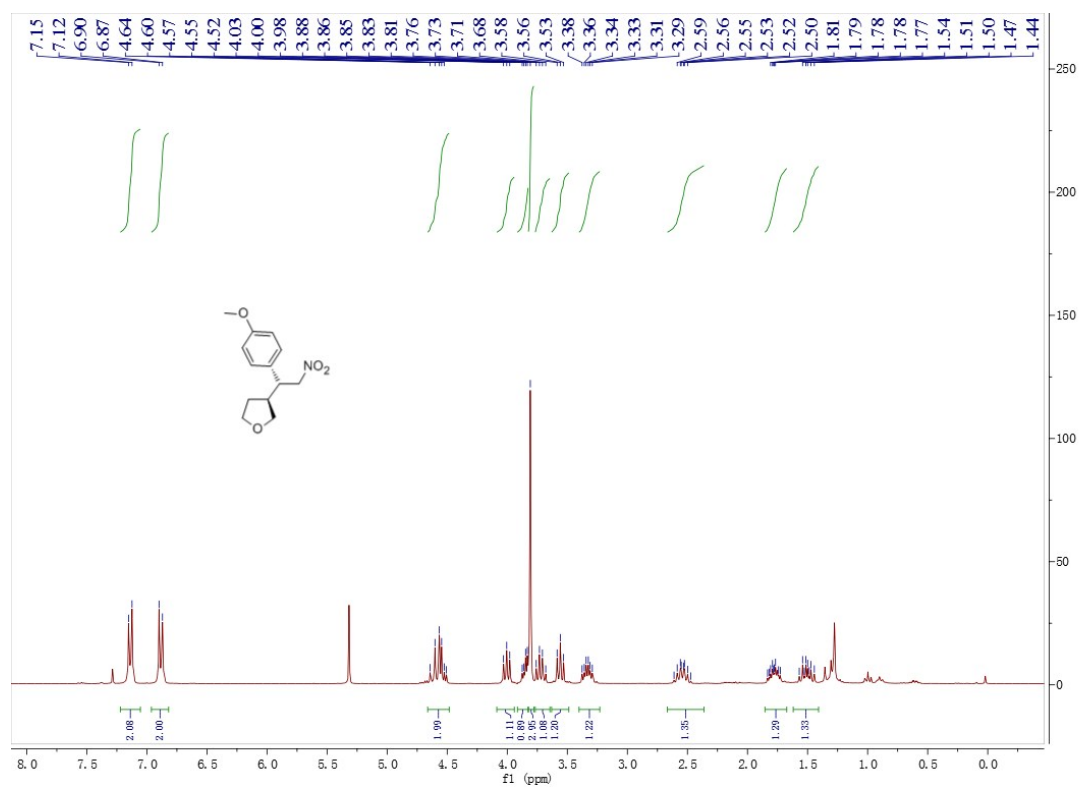


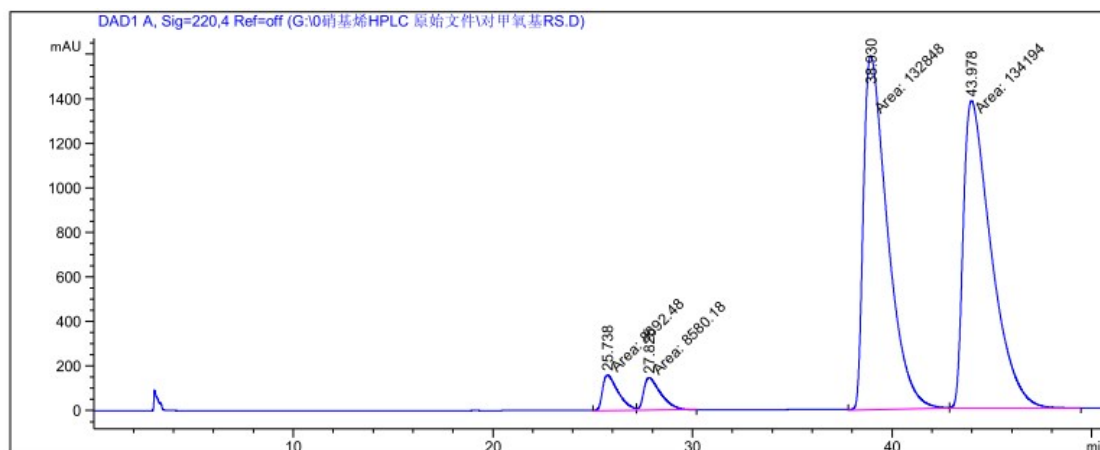
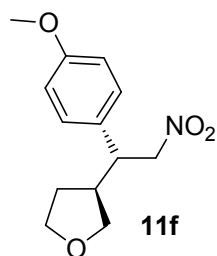


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1	30.288	MM	0.9831	3804.29102	64.49437	49.4052
2	44.355	MM	1.9600	3895.89575	33.12800	50.5948

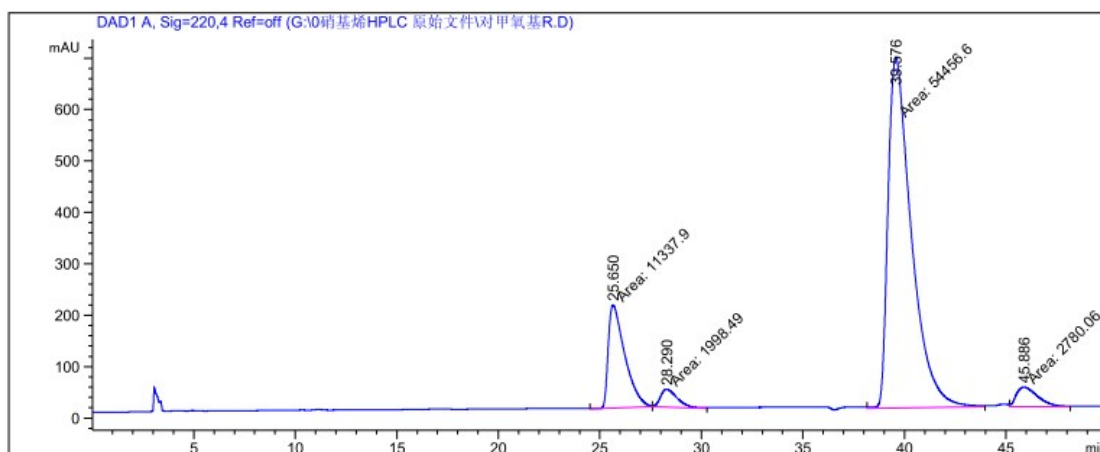


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1	30.866	MM	1.0628	58.64198	9.19594e-1	0.5751
2	43.103	MM	2.4298	1.01390e4	69.54636	99.4249

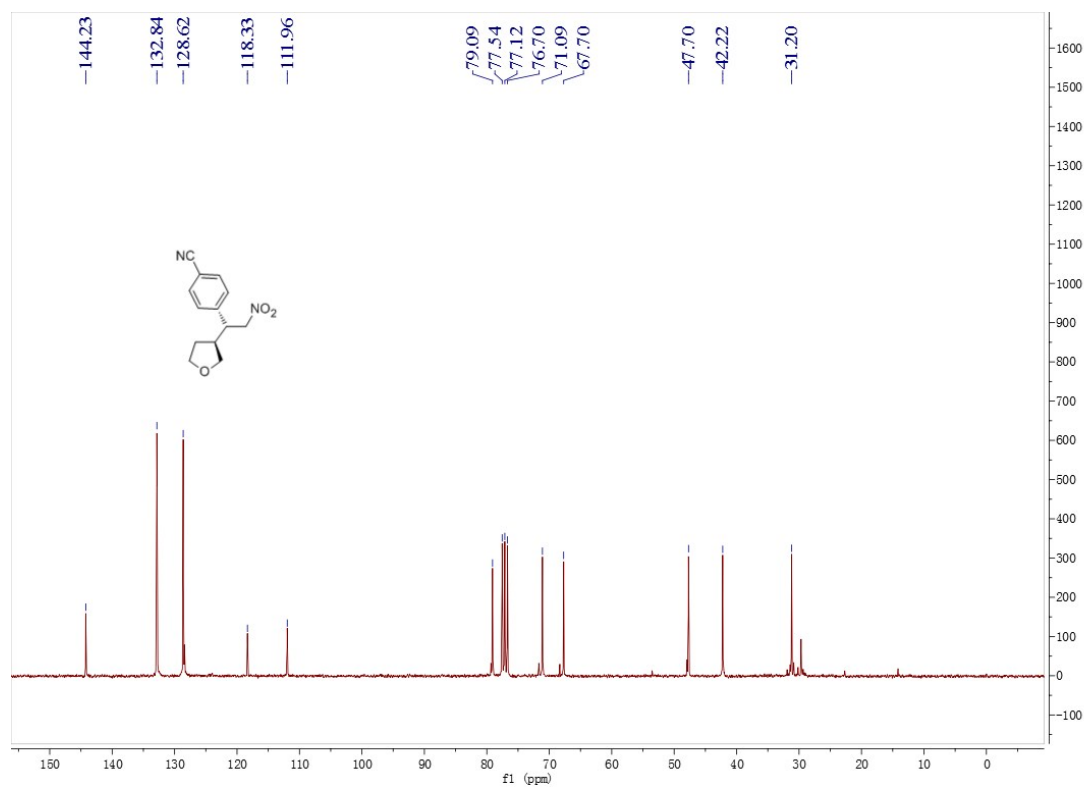
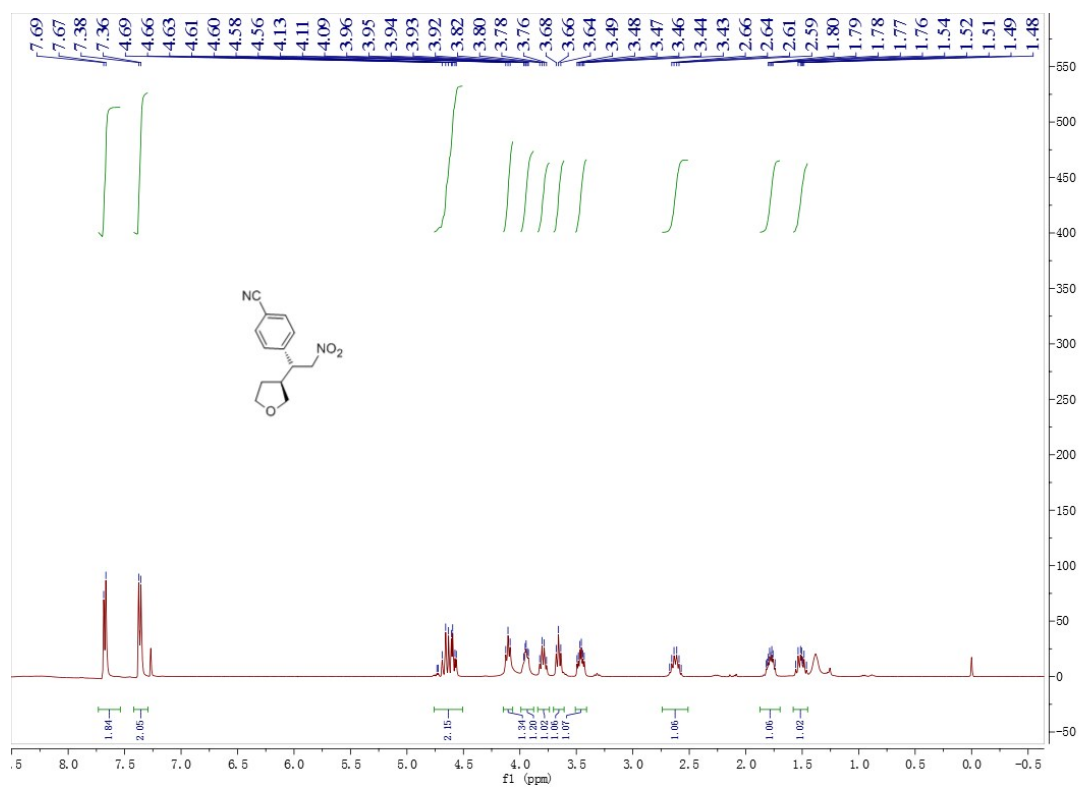


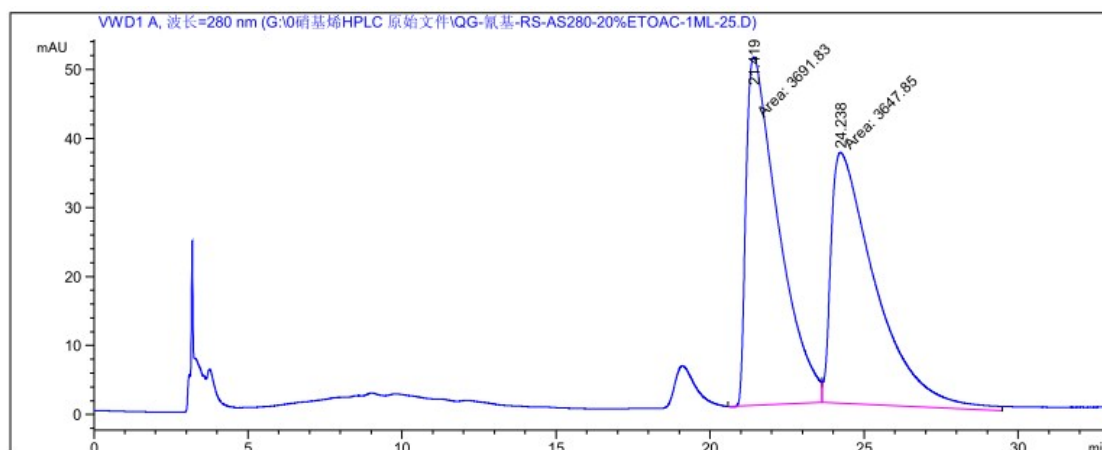
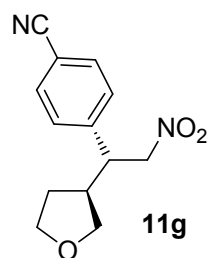


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1	25.738	MM	0.9052	8692.48047	160.04019	3.0574
2	27.825	MM	0.9867	8580.18066	144.92542	3.0179
3	38.930	MM	1.3928	1.32848e5	1589.66406	46.7258
4	43.978	MM	1.6191	1.34193e5	1381.35986	47.1990

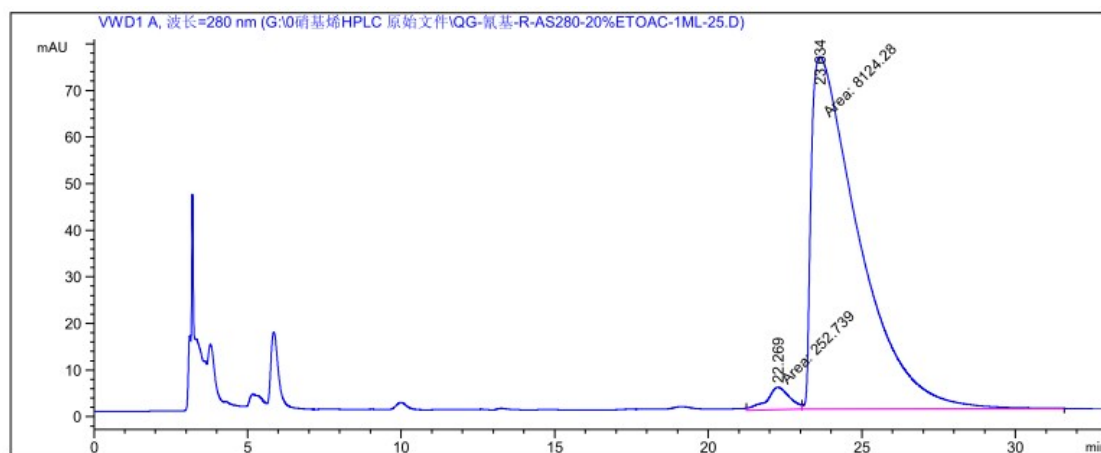


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1	25.650	MM	0.9421	1.13379e4	200.58028	16.0654
2	28.290	MM	0.9589	1998.48950	34.73691	2.8318
3	39.576	MM	1.3290	5.44566e4	682.93280	77.1635
4	45.886	MM	1.2218	2780.06372	37.92447	3.9393

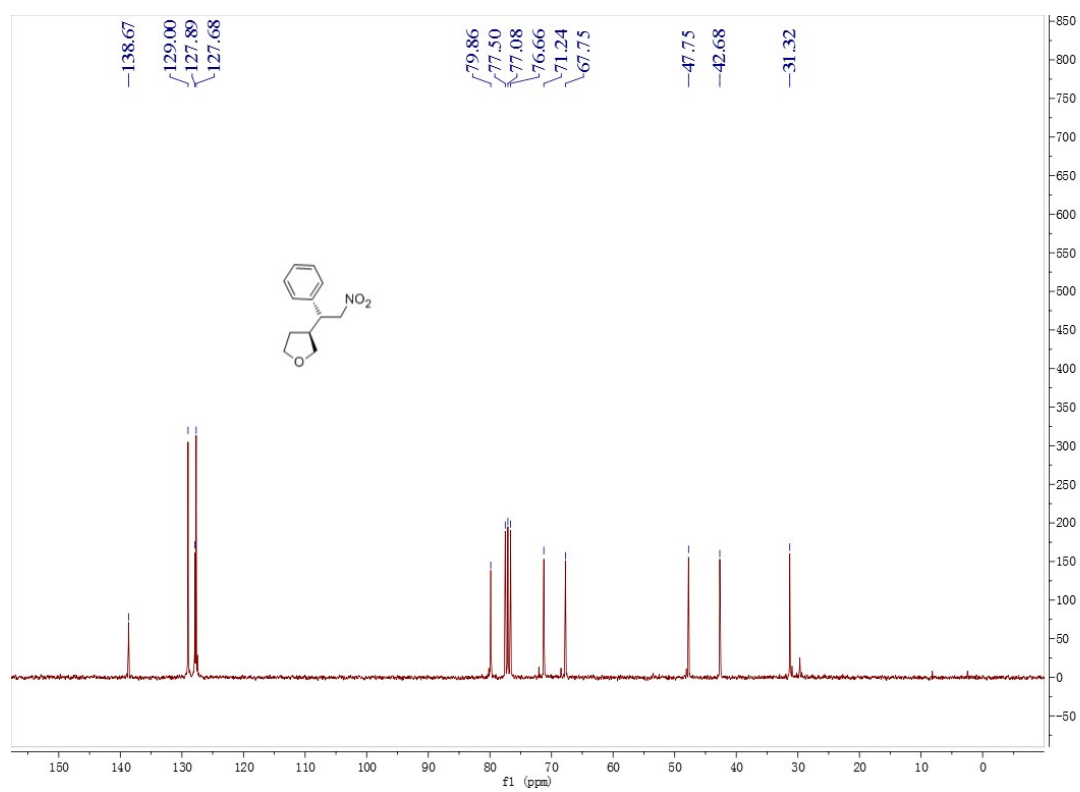
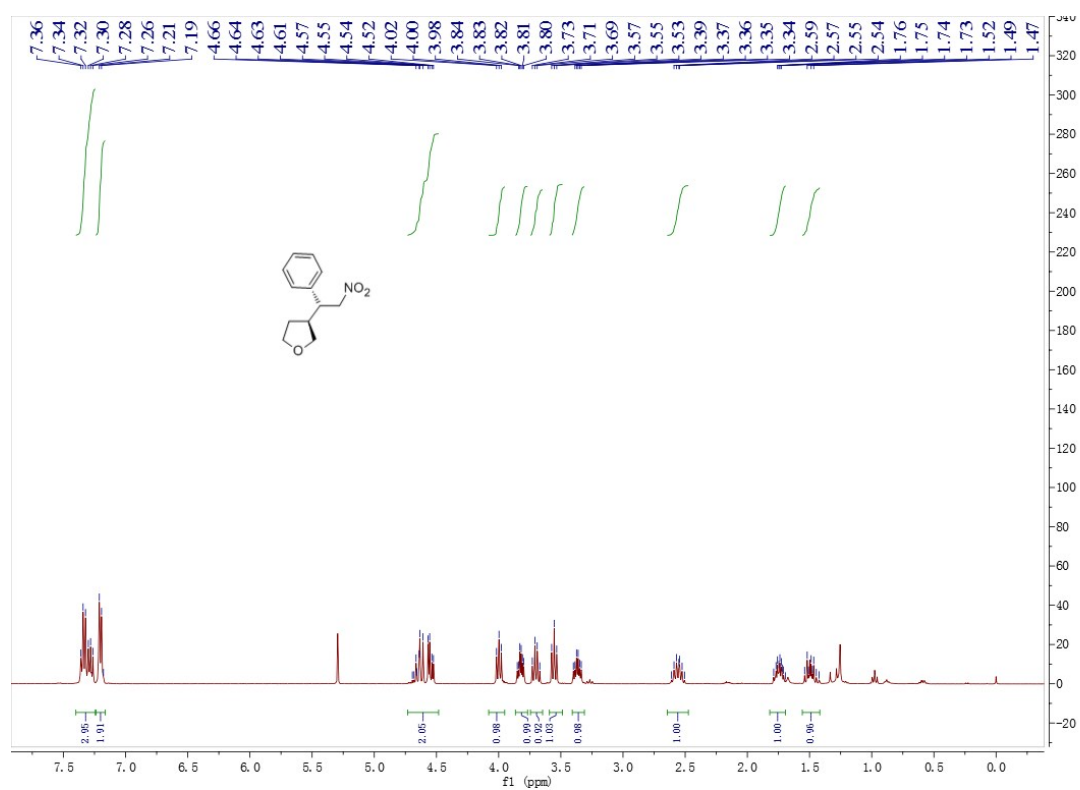


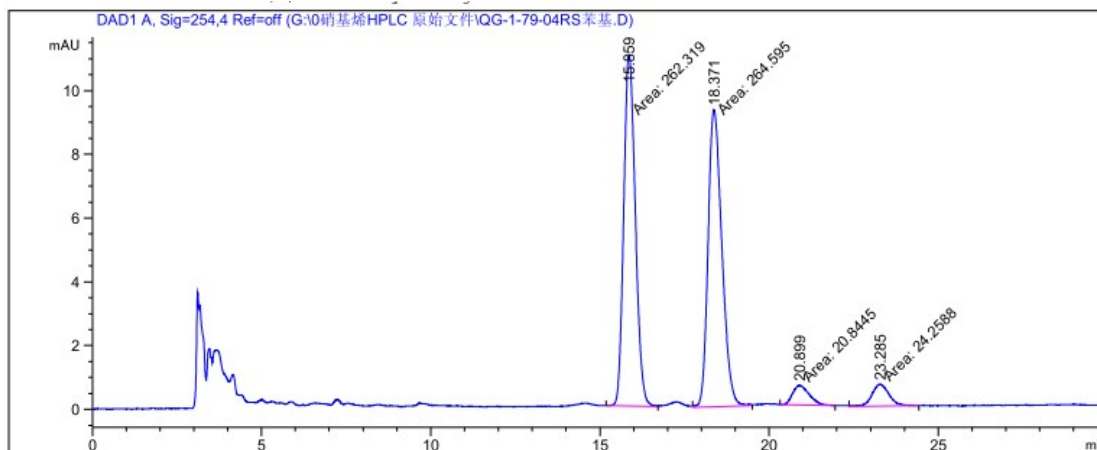
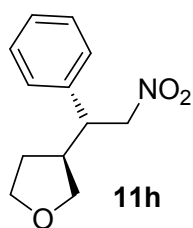


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1	21.419	MM	1.2186	3691.83447		50.49432	50.2997
2	24.238	MM	1.6747	3647.84521		36.30298	49.7003

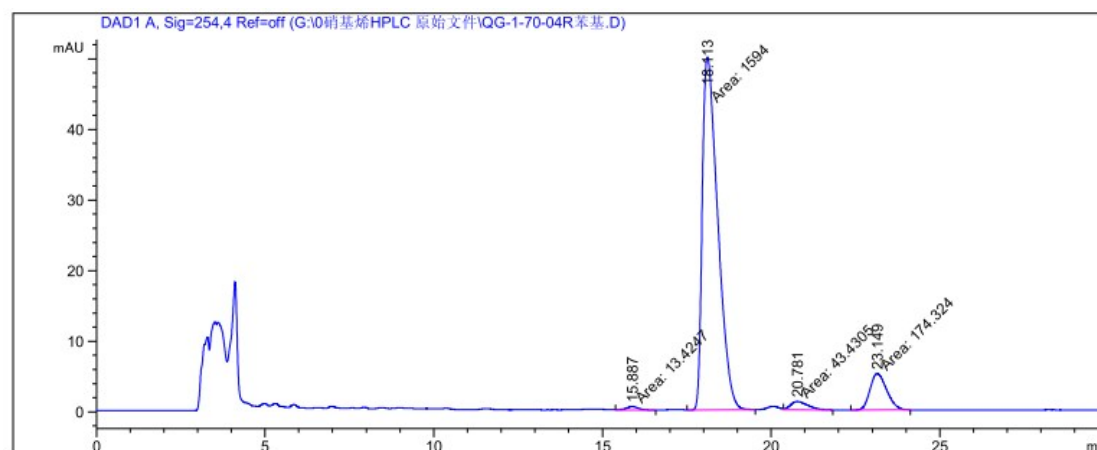


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1	22.269	MM	0.8732	252.73865		4.82393	3.0170
2	23.634	MM	1.7904	8124.28174		75.62841	96.9830

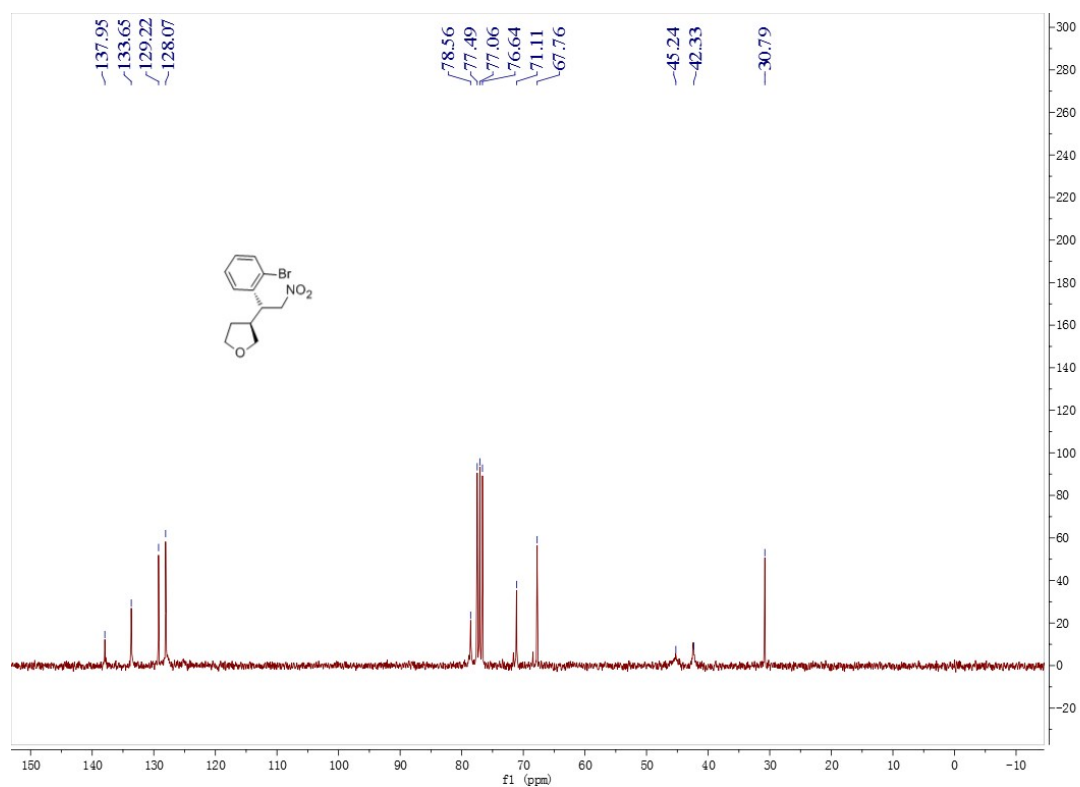
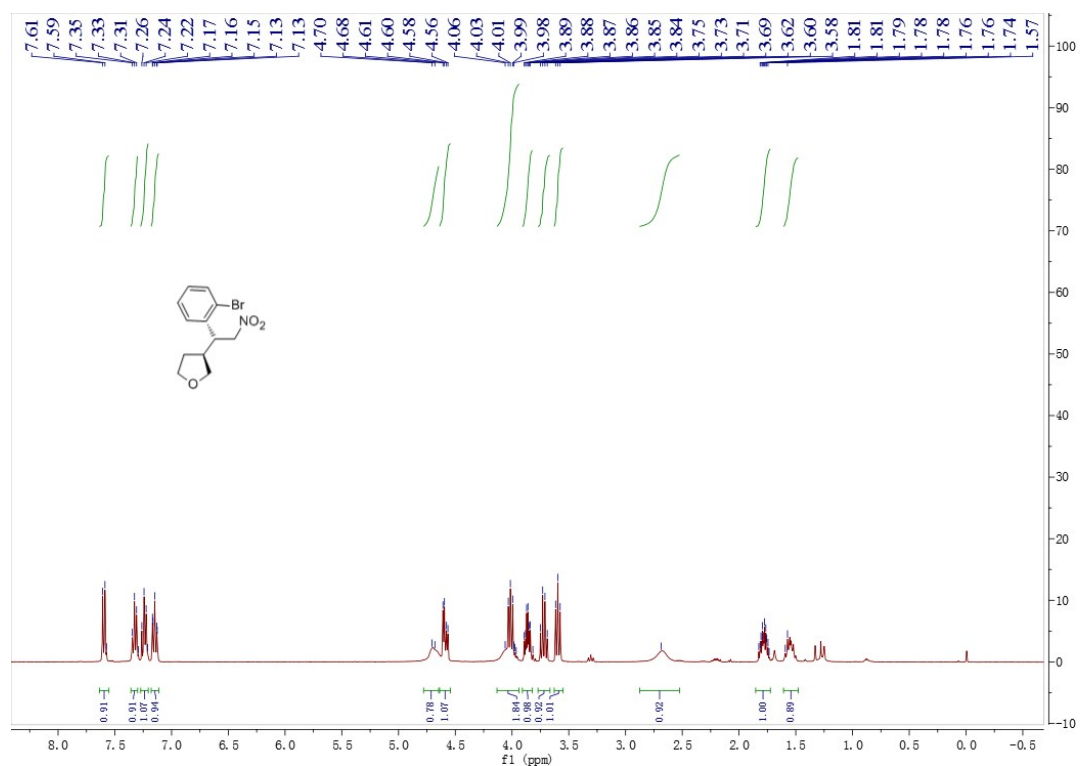


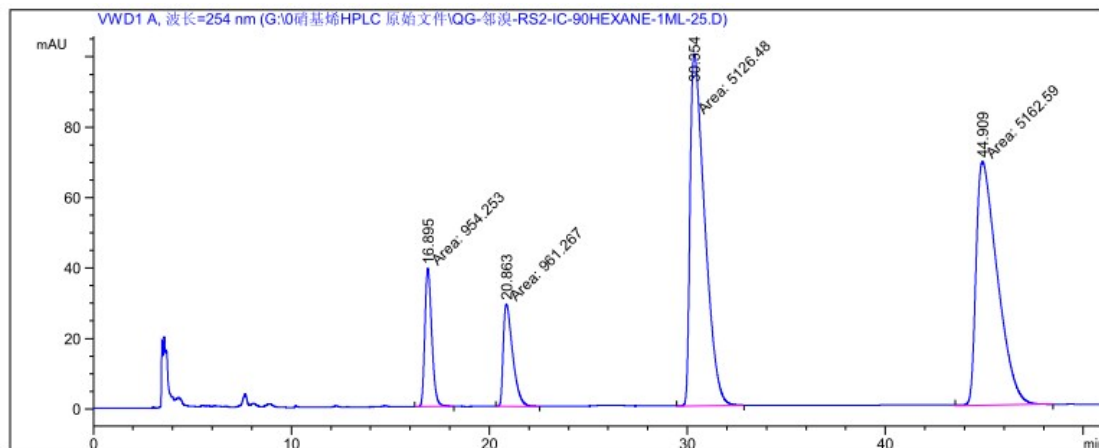
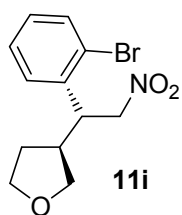


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1	15.859	MM	0.3965	262.31882	11.02641	45.8586
2	18.371	MM	0.4734	264.59488	9.31485	46.2565
3	20.899	MM	0.5651	20.84450	6.14765e-1	3.6440
4	23.285	MM	0.5922	24.25881	6.82708e-1	4.2409

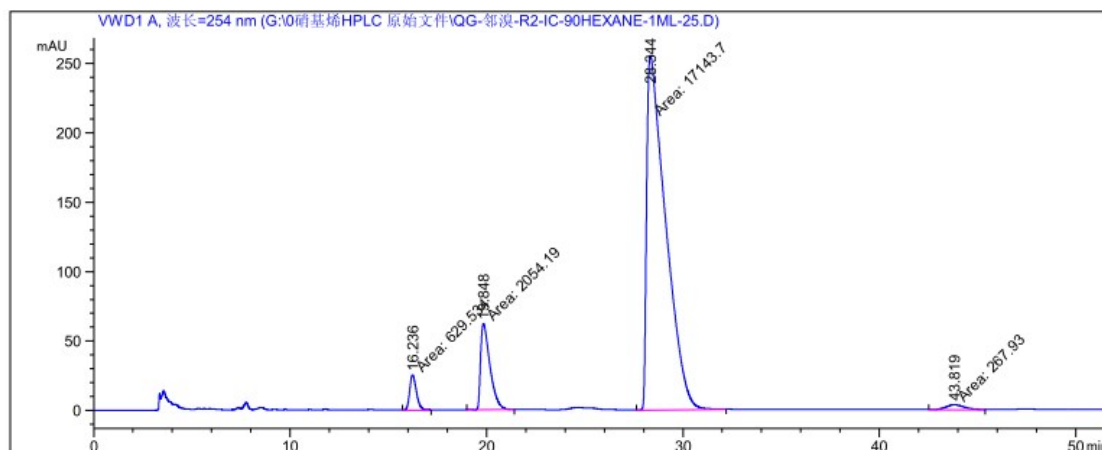


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1	15.887	MM	0.4408	13.42469	5.07613e-1	0.7355
2	18.113	MM	0.5312	1594.00122	50.01206	87.3339
3	20.781	MM	0.6188	43.43047	1.16984	2.3795
4	23.149	MM	0.5682	174.32405	5.11345	9.5511

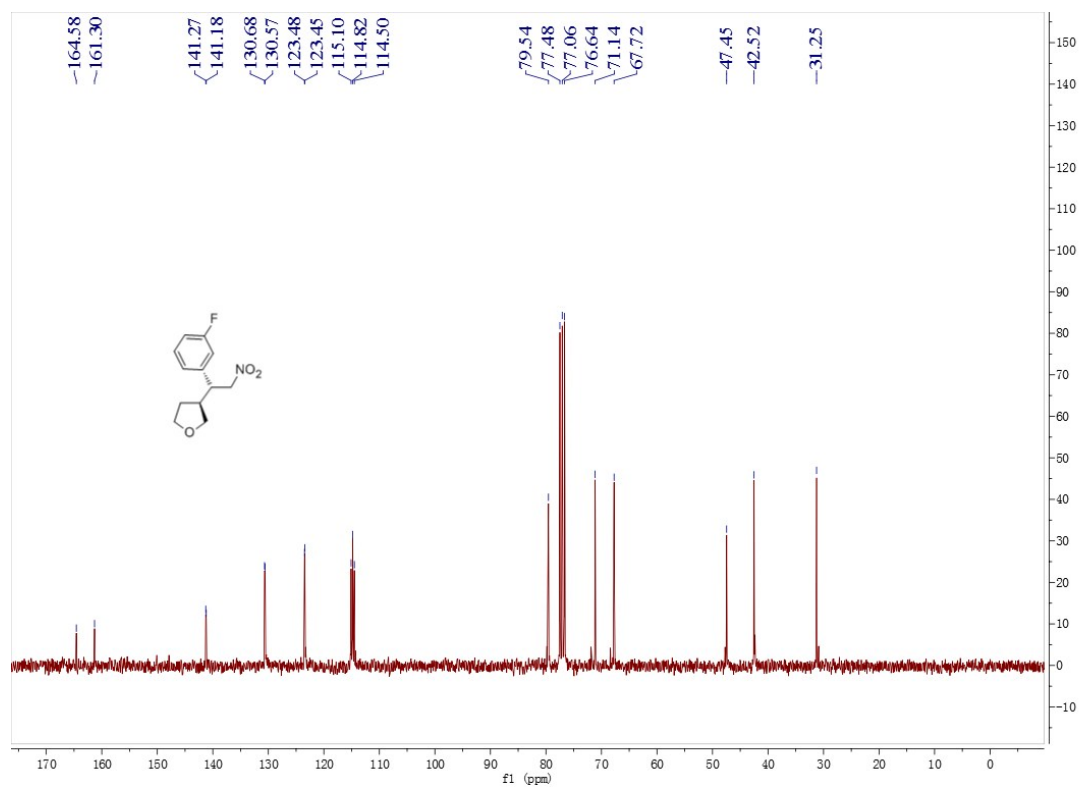
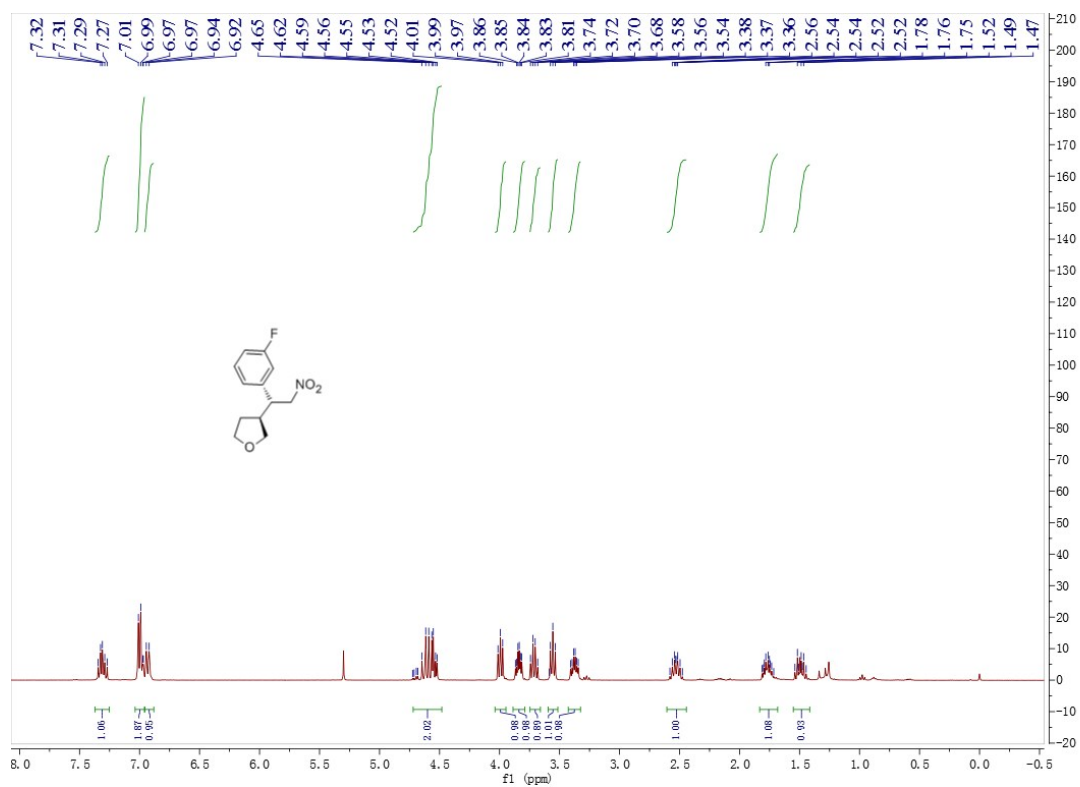


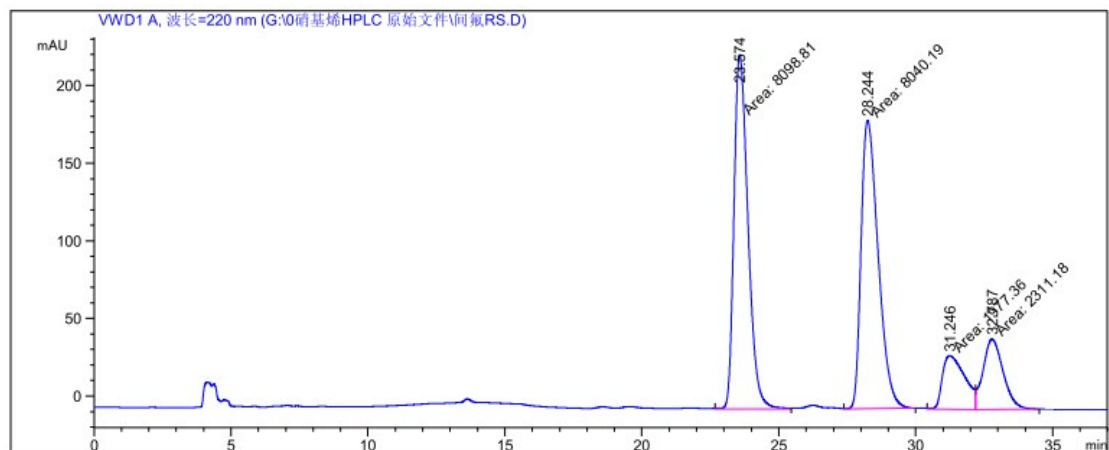
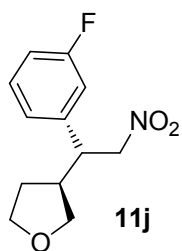


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1	16.895	MM	0.4053	954.25250	39.23817	7.8188
2	20.863	MM	0.5519	961.26697	29.02834	7.8763
3	30.354	MM	0.8539	5126.47852	100.05771	42.0045
4	44.909	MM	1.2431	5162.59326	69.21854	42.3004

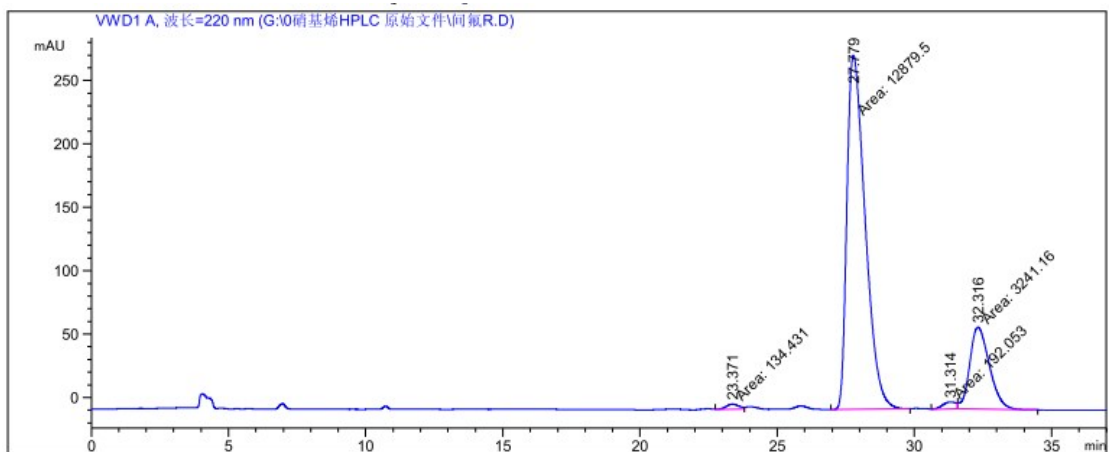


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	16.236	MM	0.4114	629.53357	25.50305	3.1327
2	19.848	MM	0.5530	2054.18872	61.90949	10.2222
3	28.344	MM	1.1172	1.71437e4	255.75224	85.3117
4	43.819	MM	1.2005	267.93042	3.71984	1.3333

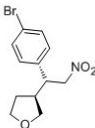
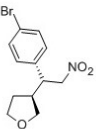


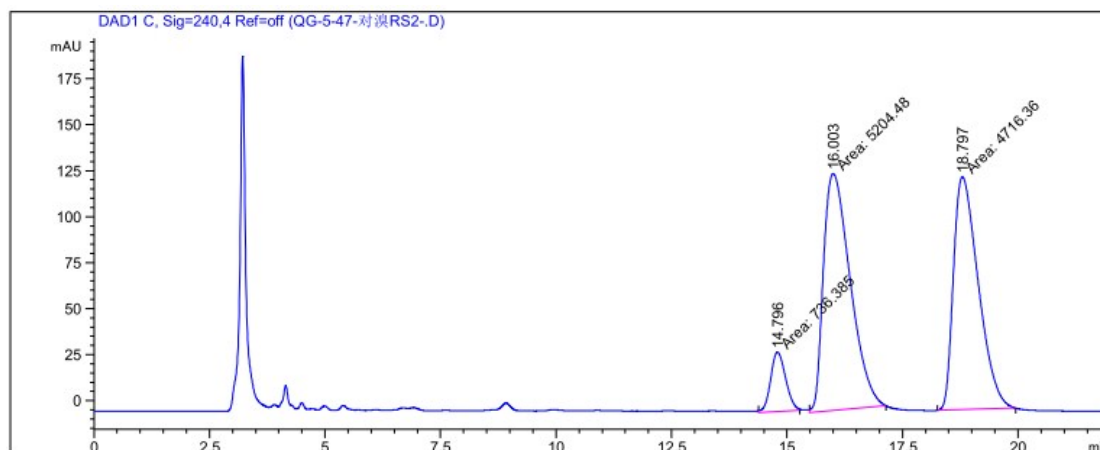
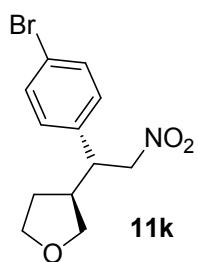


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1	23.574	MM	0.5916	8098.80908	39.6465	228.16852
2	28.244	MM	0.7215	8040.18896	39.3595	185.71689
3	31.246	MM	0.9567	1977.36475	9.6799	34.44757
4	32.787	MM	0.8505	2311.18164	11.3140	45.29087

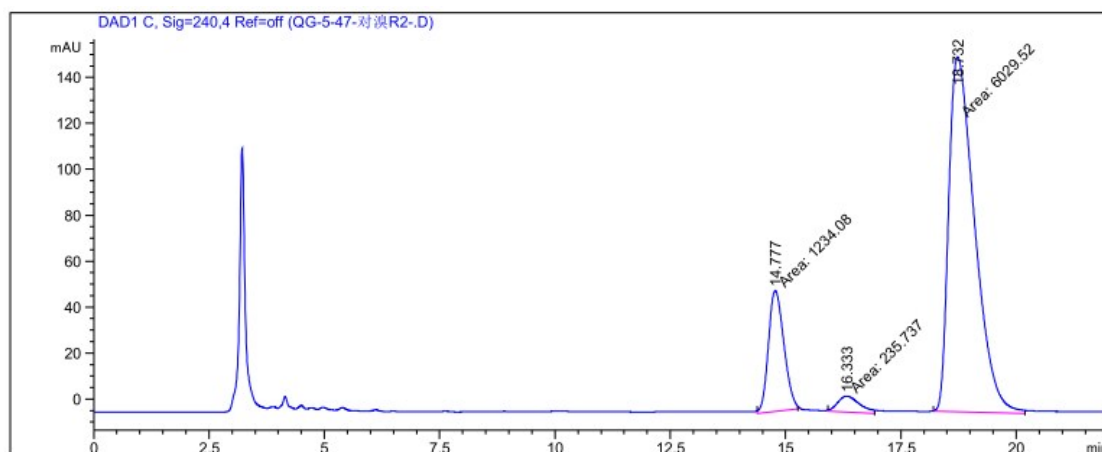


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1	23.371	MM	0.5572	134.43095	0.8174	4.02106
2	27.779	MM	0.7686	1.28795e4	78.3084	279.28769
3	31.314	MM	0.5812	192.05310	1.1677	5.50780
4	32.316	MM	0.8356	3241.15991	19.7066	64.64964

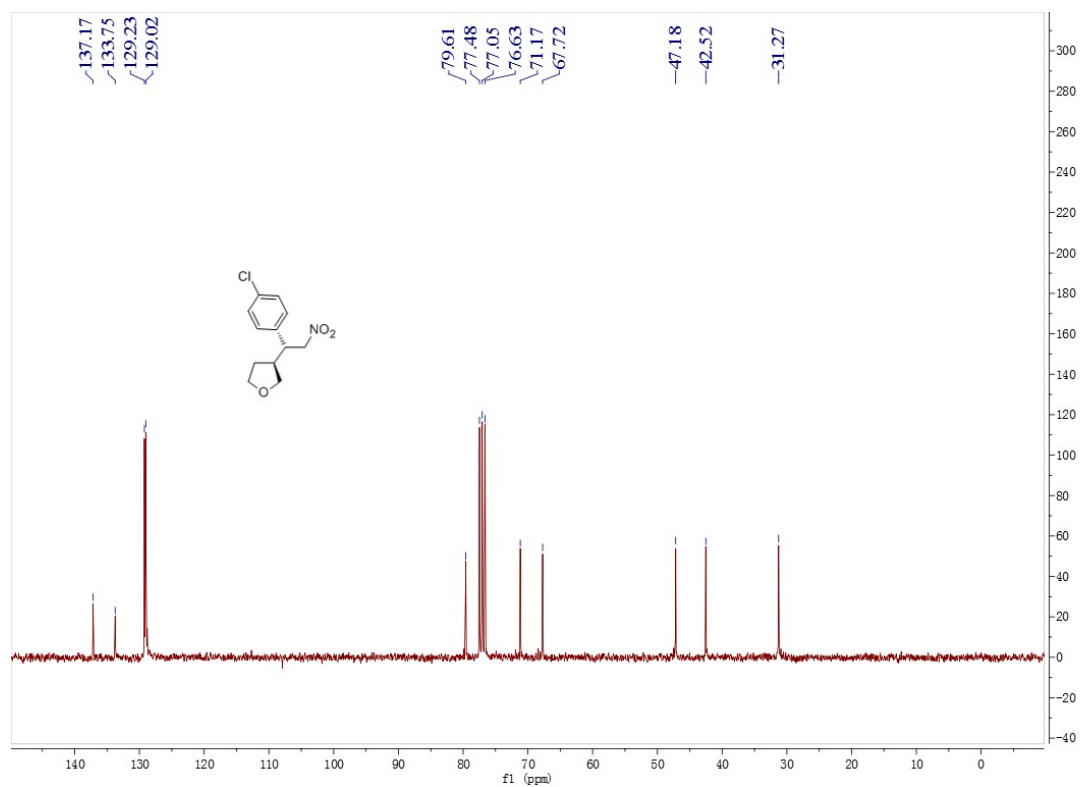
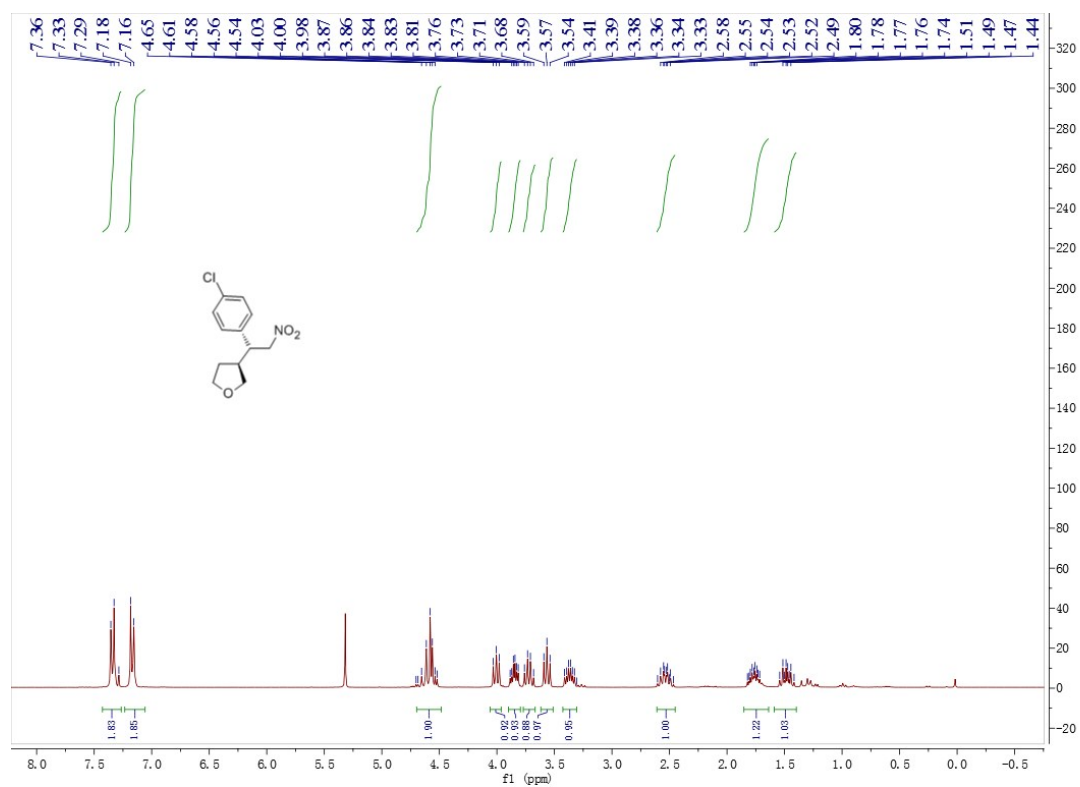


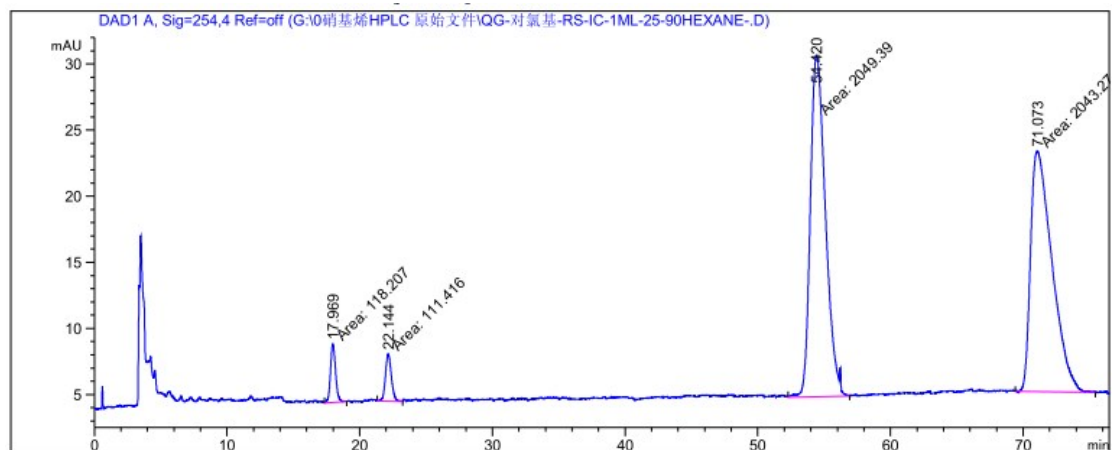
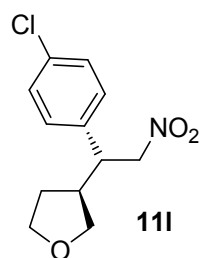


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.796	MM	0.3791	736.38550	32.37293	6.9097
2	16.003	MM	0.6731	5204.48389	128.87700	48.8352
3	18.797	MM	0.6209	4716.36182	126.59889	44.2550

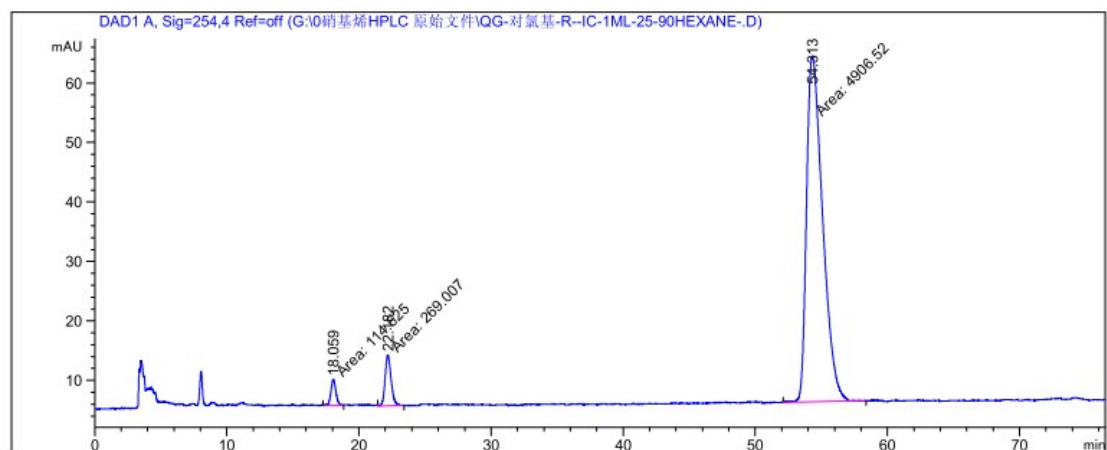


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.777	MM	0.3905	1234.07947	52.66866	16.4559
2	16.333	MM	0.5585	235.73672	7.03493	3.1434
3	18.732	MM	0.6499	6029.51904	154.62196	80.4007

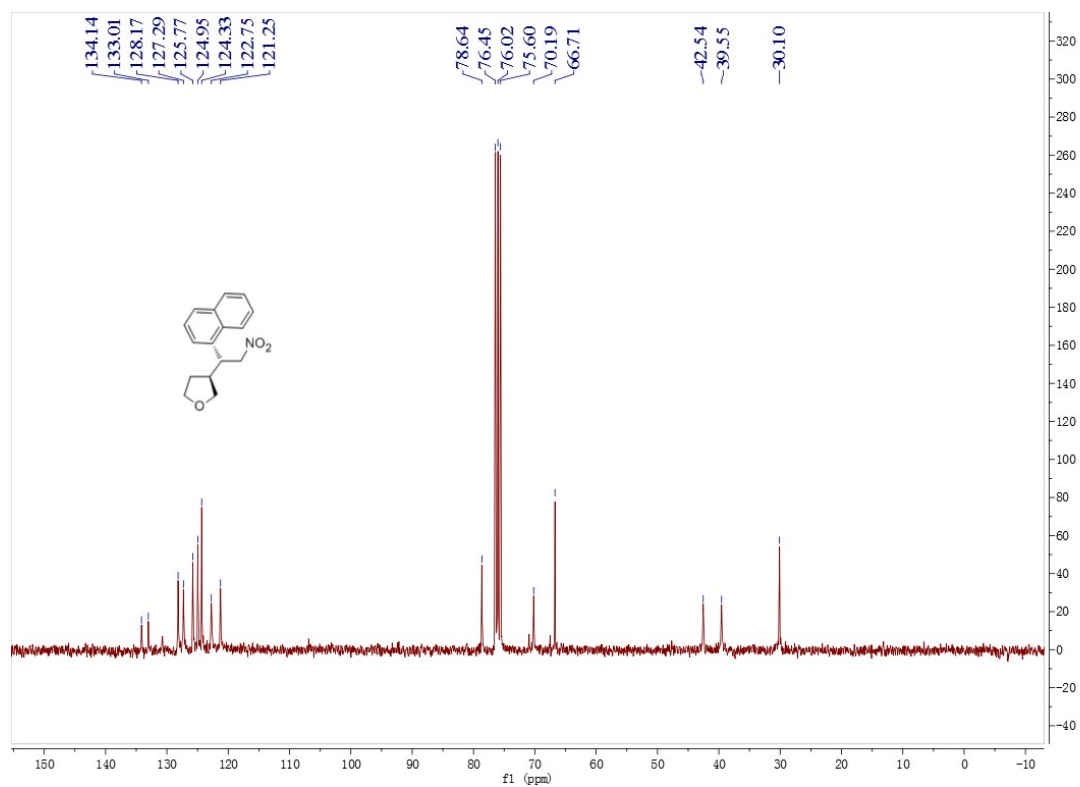
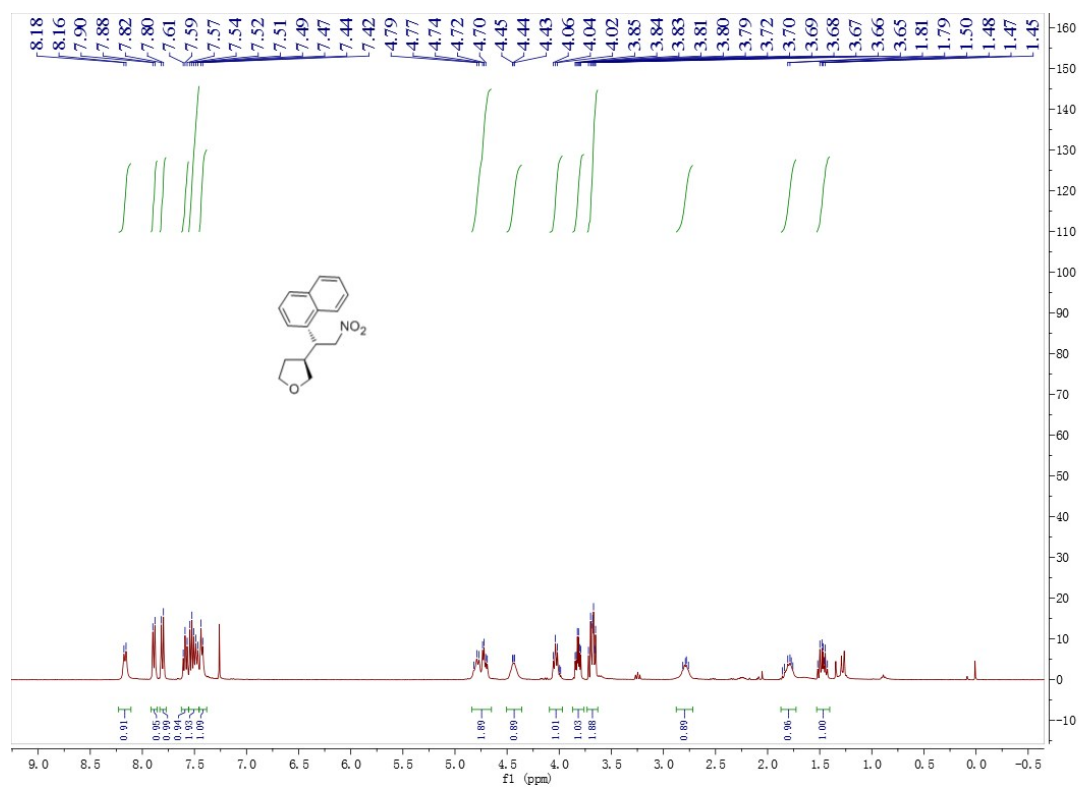


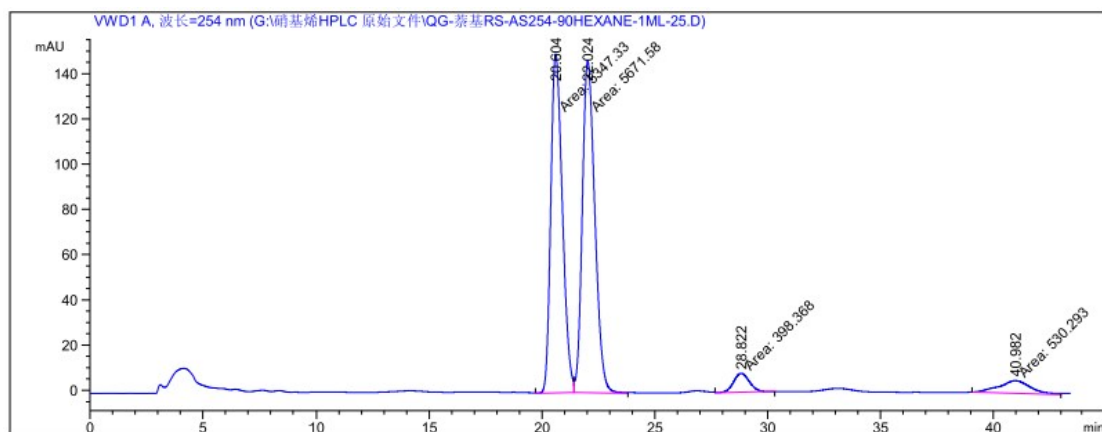
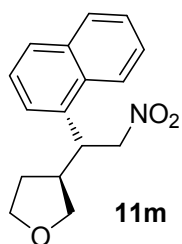


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.969	MM	0.4423	118.20686	4.45442	2.7348
2	22.144	MM	0.5211	111.41585	3.56337	2.5777
3	54.420	MM	1.3217	2049.38501	25.84217	47.4145
4	71.073	MM	1.8694	2043.27161	18.21692	47.2730

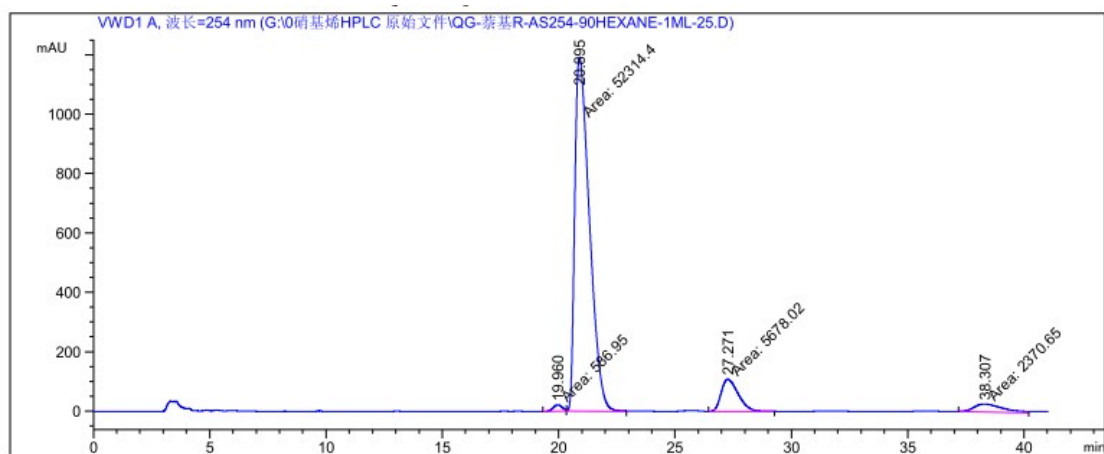


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.059	MM	0.4418	114.62480	4.32452	2.1668
2	22.182	MM	0.5278	269.00717	8.49531	5.0851
3	54.313	MM	1.4065	4906.51514	58.14243	92.7482

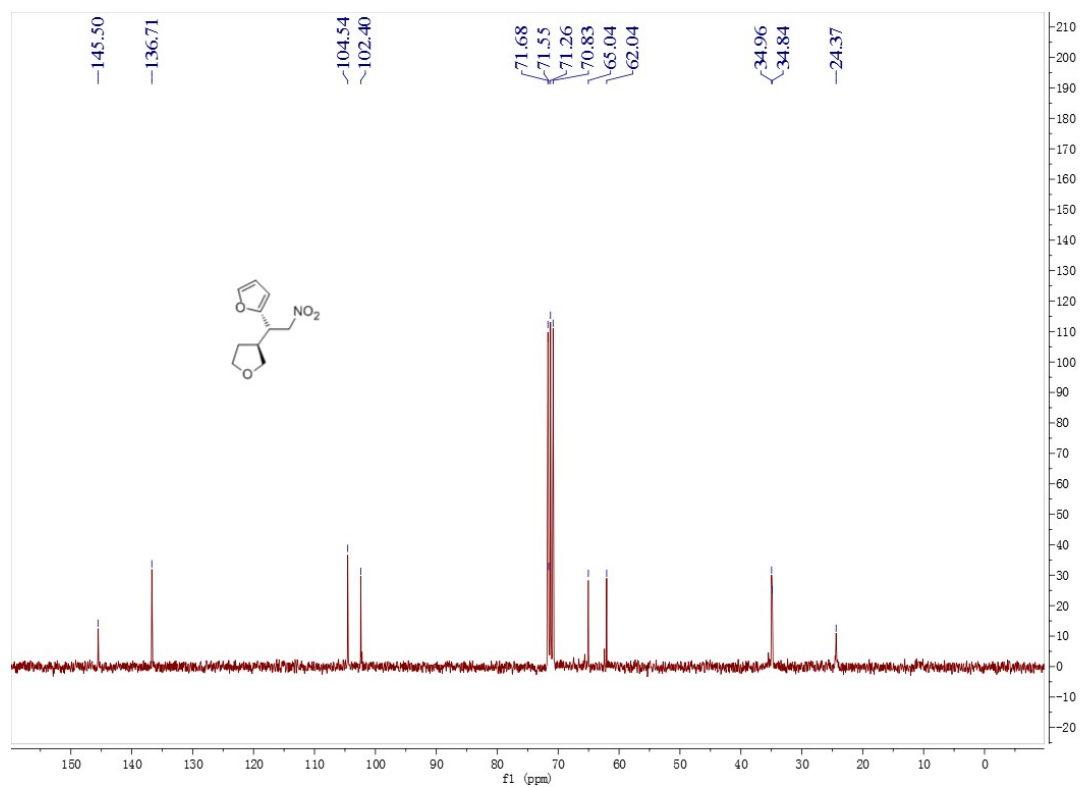
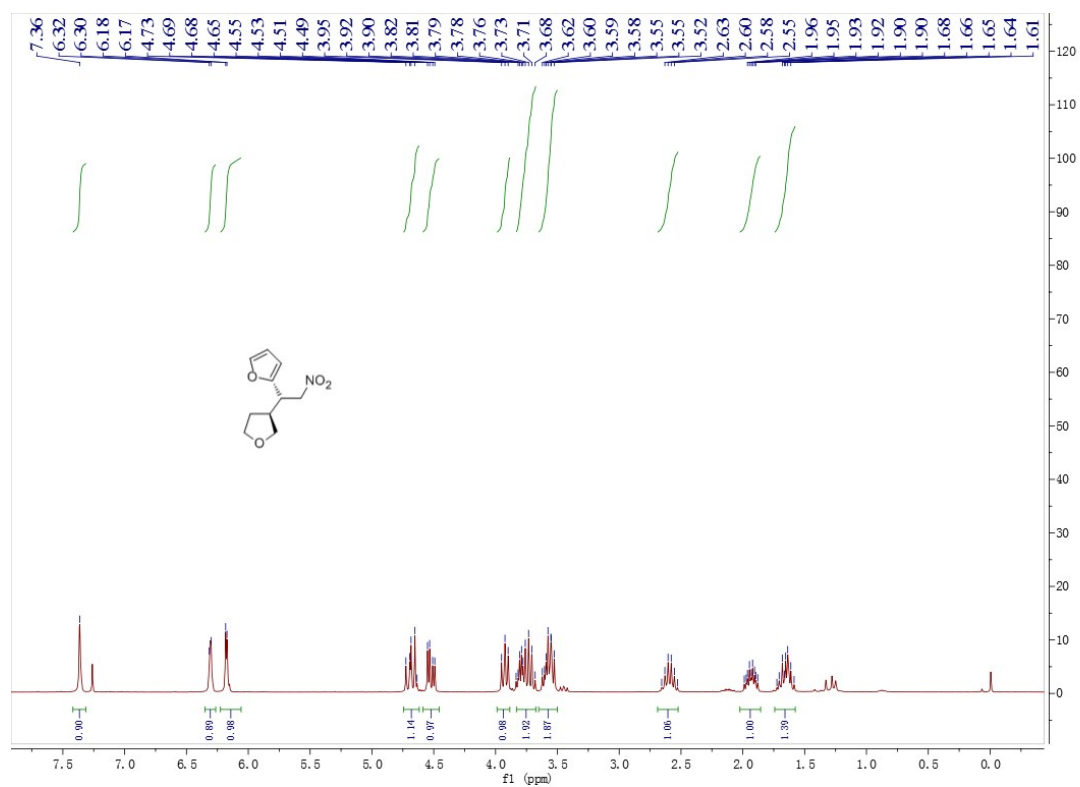


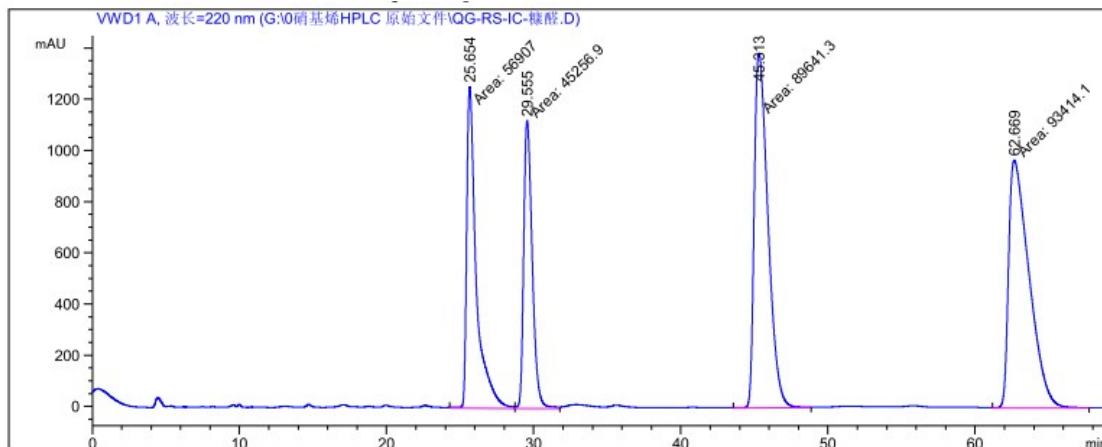
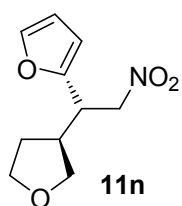


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	20.604	MM	0.5949	5347.33105	149.81253	44.7566
2	22.024	MM	0.6440	5671.58057	146.77705	47.4706
3	28.822	MM	0.8002	398.36755	8.29742	3.3343
4	40.982	MM	1.5978	530.29309	5.53135	4.4385

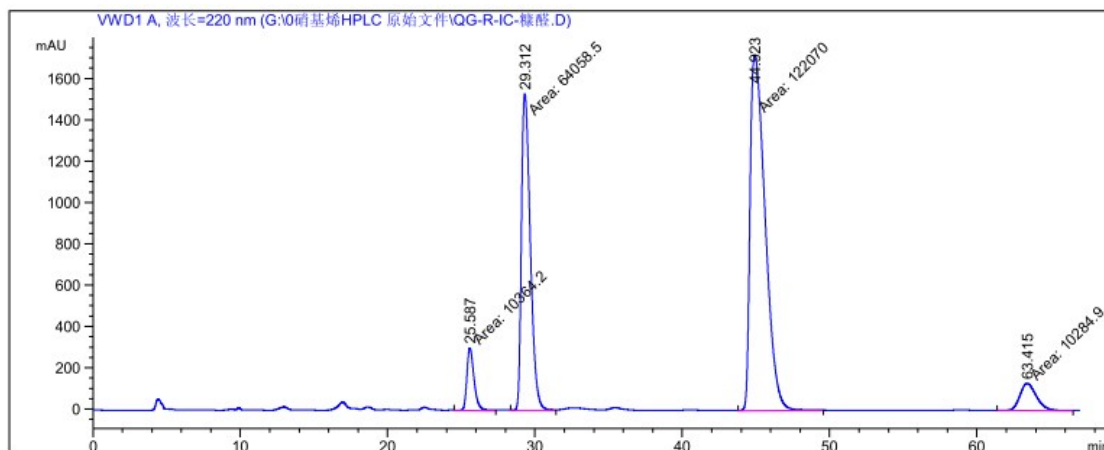


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	19.960	MM	0.4578	586.95026	21.36757	0.9630
2	20.895	MM	0.7312	5.23144e4	1192.45447	85.8316
3	27.271	MM	0.8697	5678.02002	108.81712	9.3159
4	38.307	MM	1.4697	2370.65137	26.88394	3.8895

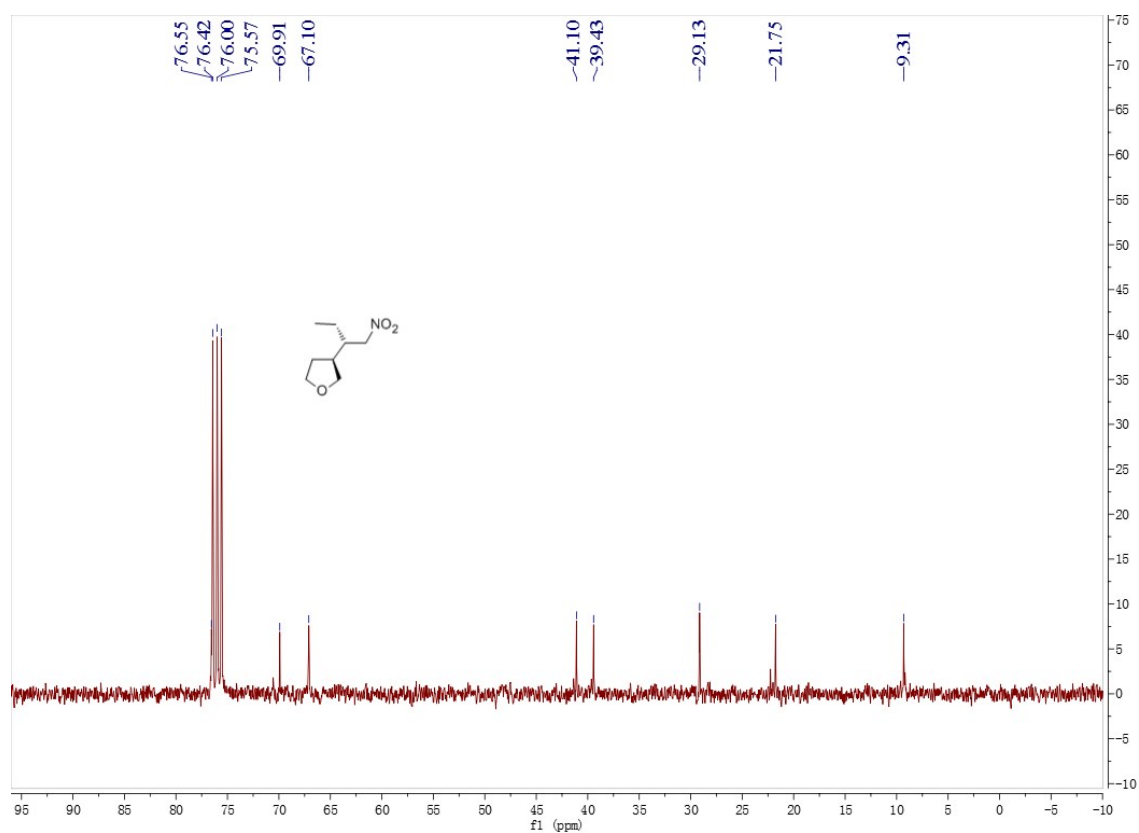
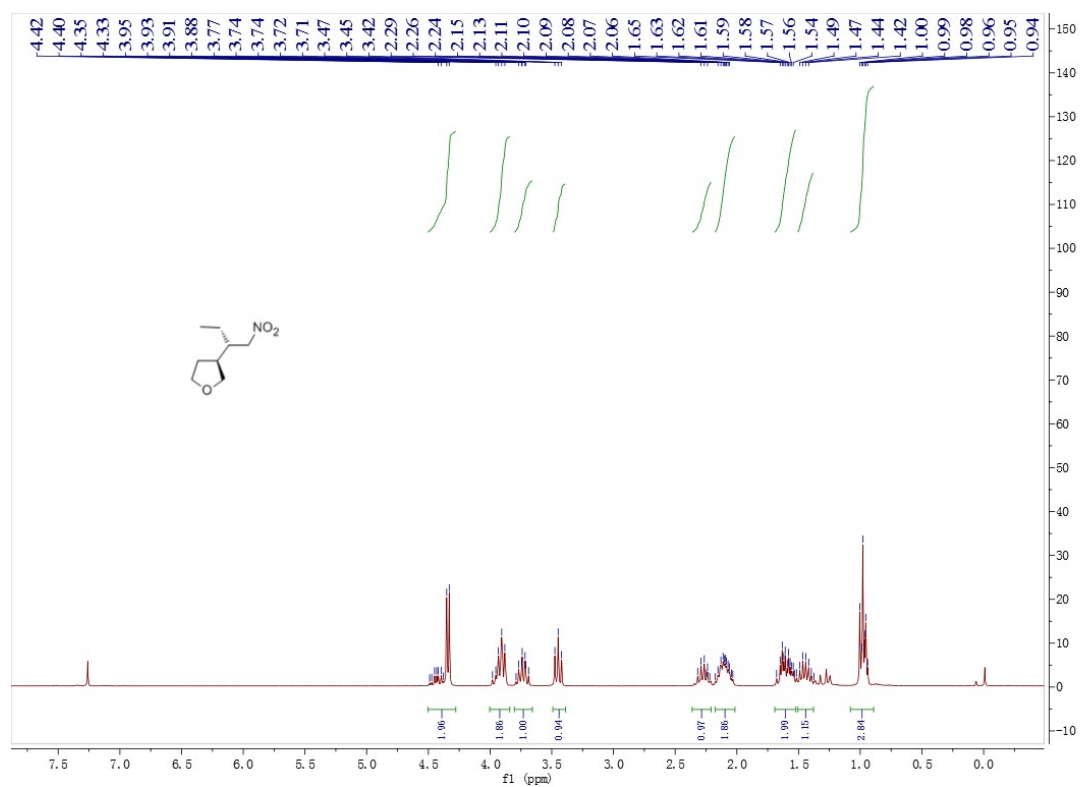


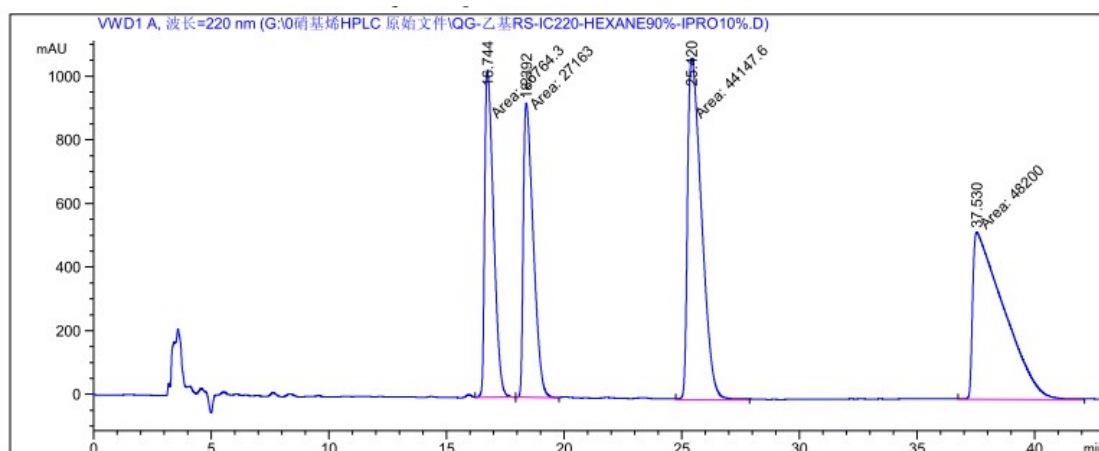
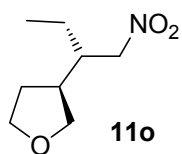


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	25.654	MM	0.7556	5.69070e4	1255.17078	19.9520
2	29.555	MM	0.6710	4.52569e4	1124.07776	15.8674
3	45.313	MM	1.0786	8.96413e4	1385.18958	31.4289
4	62.669	MM	1.6090	9.34141e4	967.59302	32.7517

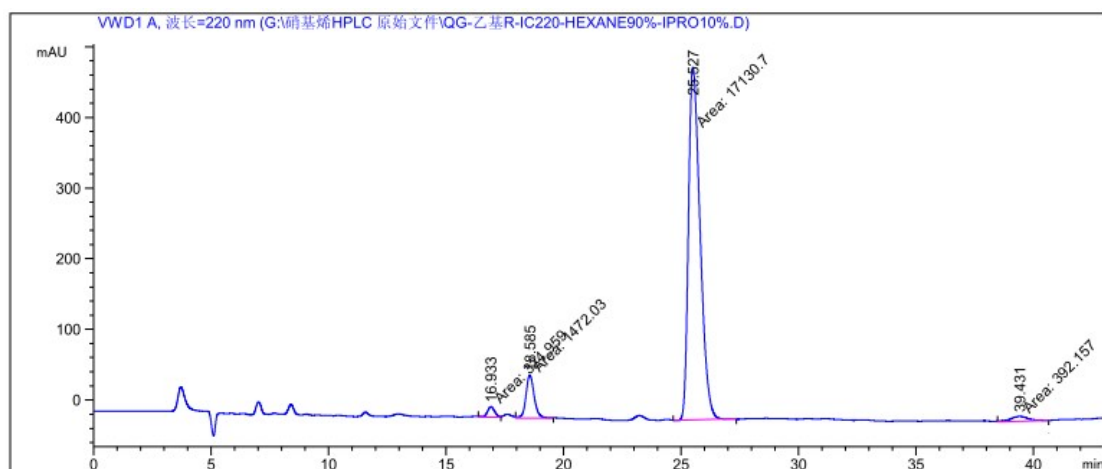


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	25.587	MM	0.5701	1.03642e4	302.98264	5.0123
2	29.312	MM	0.6979	6.40585e4	1529.88464	30.9795
3	44.923	MM	1.1818	1.22070e5	1721.50720	59.0344
4	63.415	MM	1.3093	1.02849e4	130.91922	4.9739

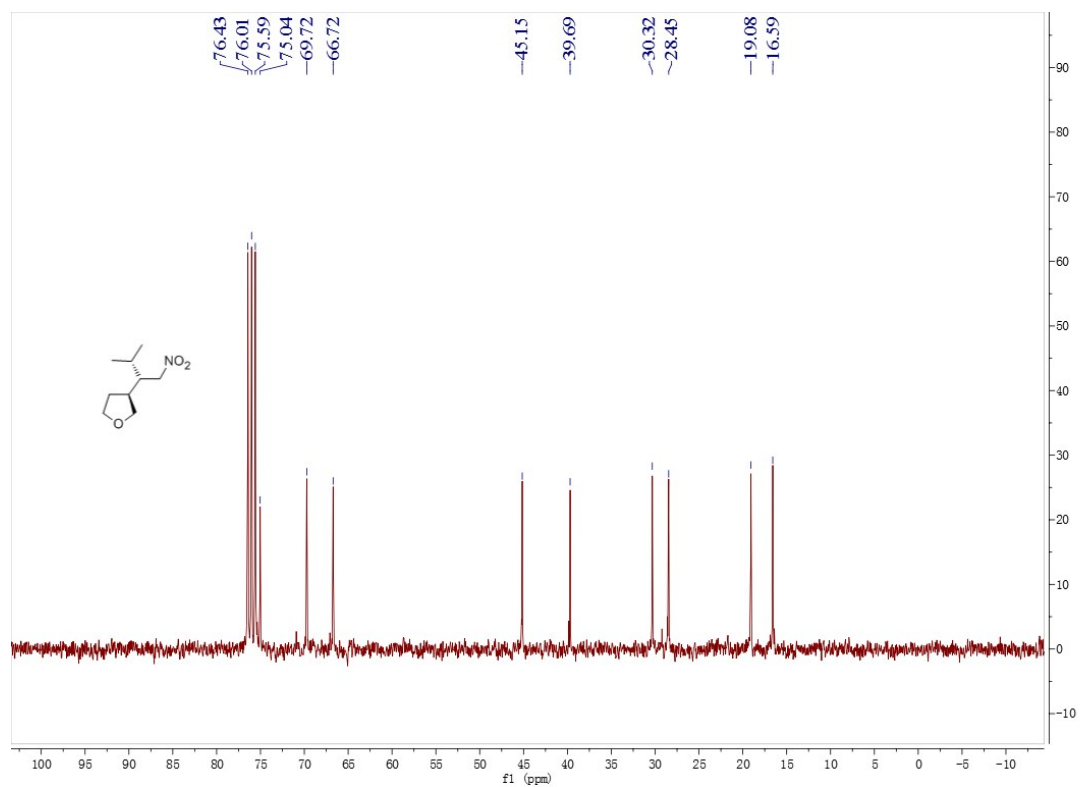
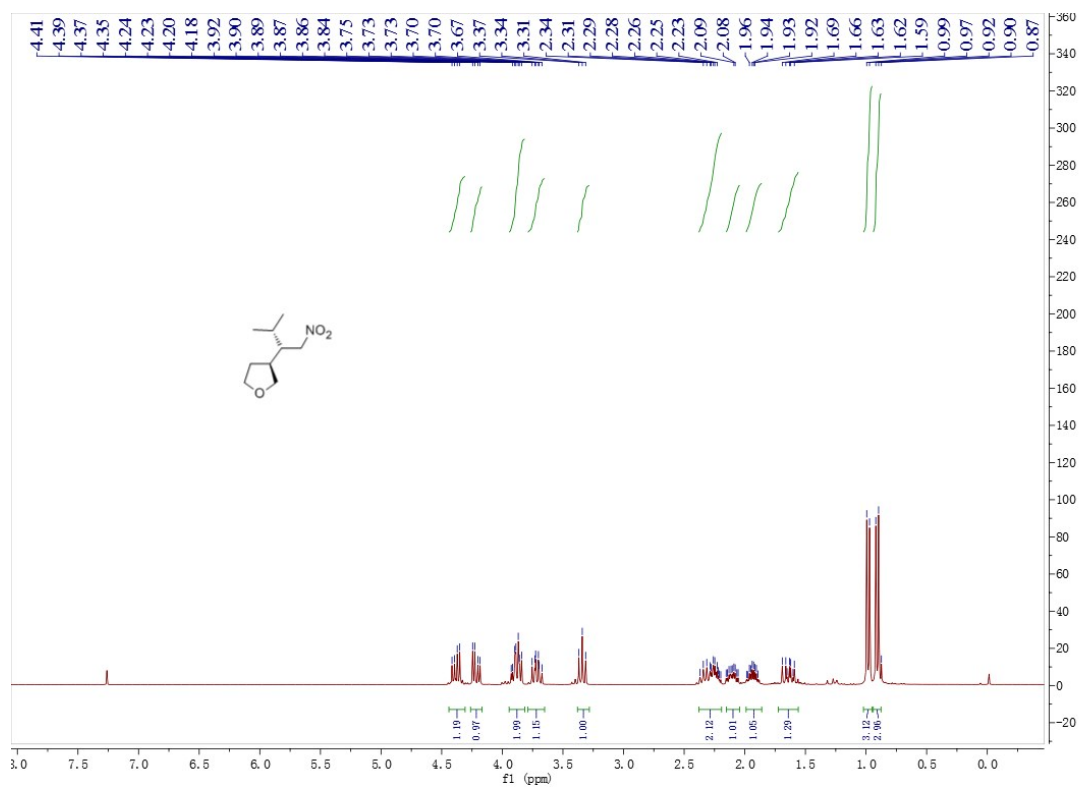


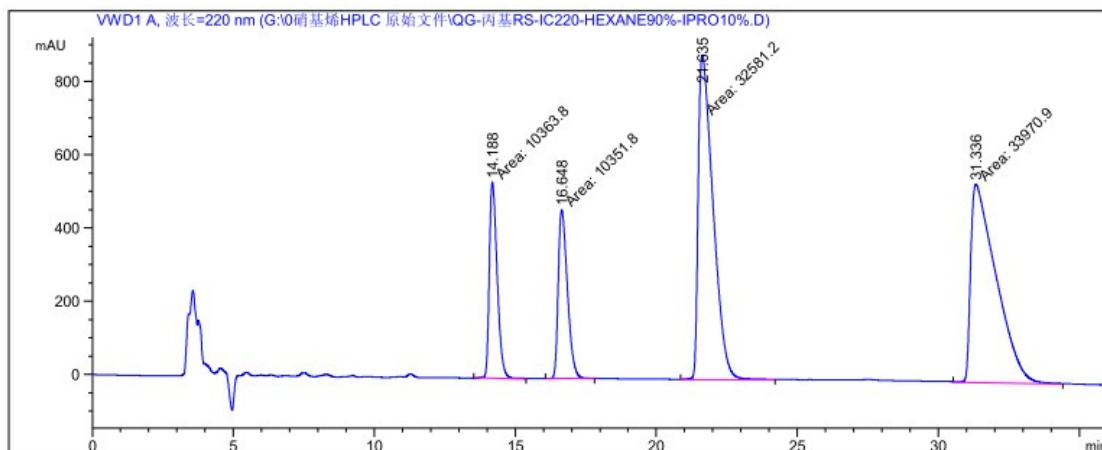
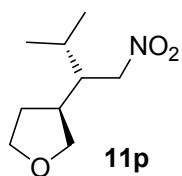


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.744	MM	0.4342	2.67643e4	1027.40820	18.2973
2	18.392	MM	0.4892	2.71630e4	925.44470	18.5698
3	25.420	MM	0.6857	4.41476e4	1073.00500	30.1812
4	37.530	MM	1.5306	4.82000e4	524.84393	32.9517

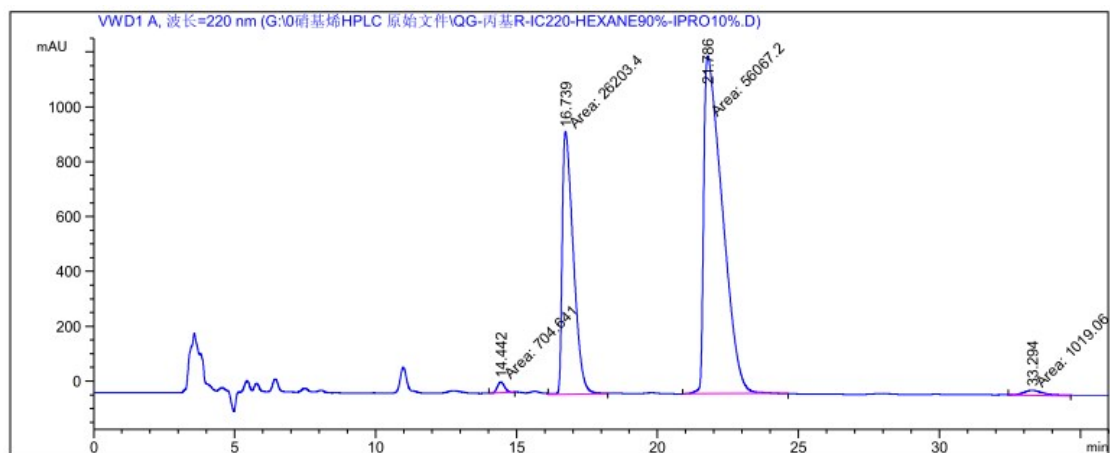


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.933	MM	0.3667	324.95874	14.76833	1.6820
2	18.585	MM	0.4040	1472.02930	60.72160	7.6192
3	25.527	MM	0.5719	1.71307e4	499.22037	88.6689
4	39.431	MM	0.9244	392.15720	7.07036	2.0298

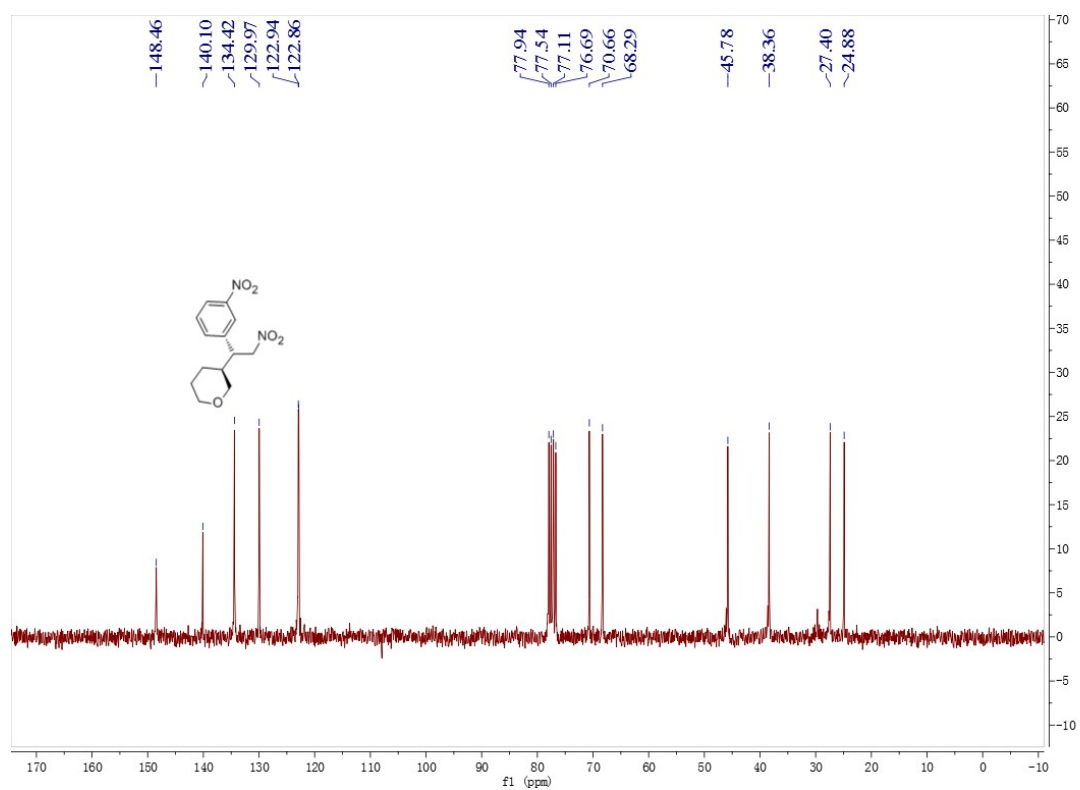
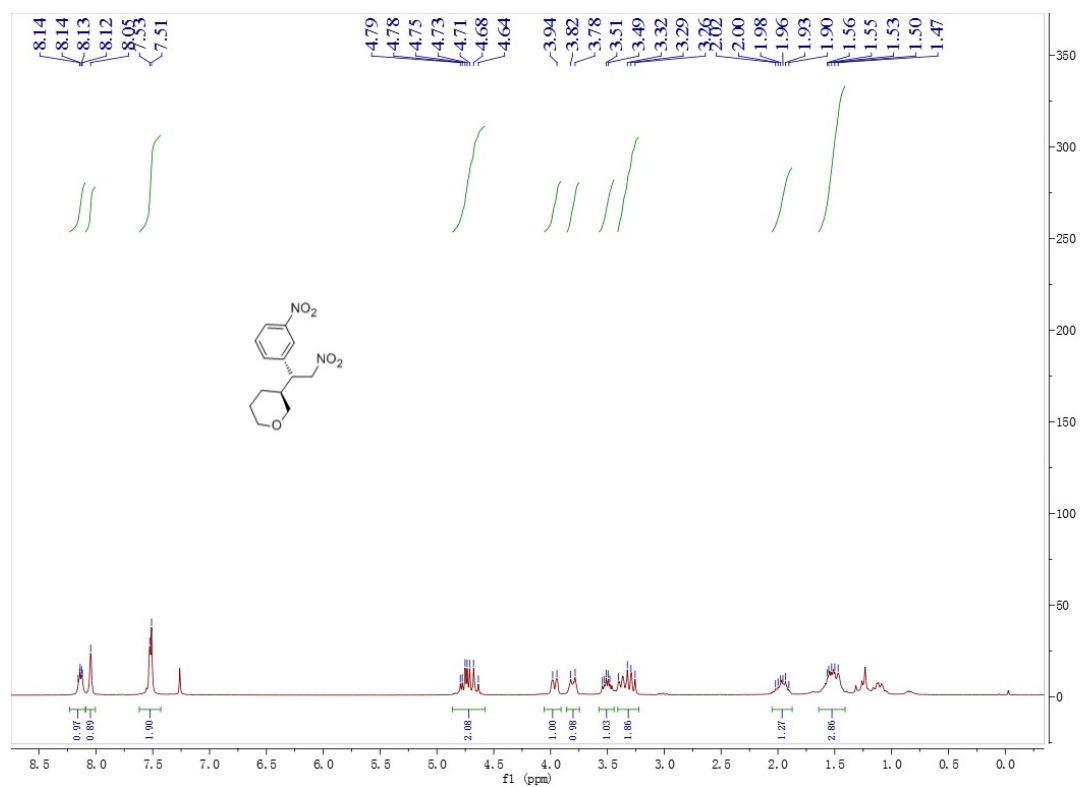


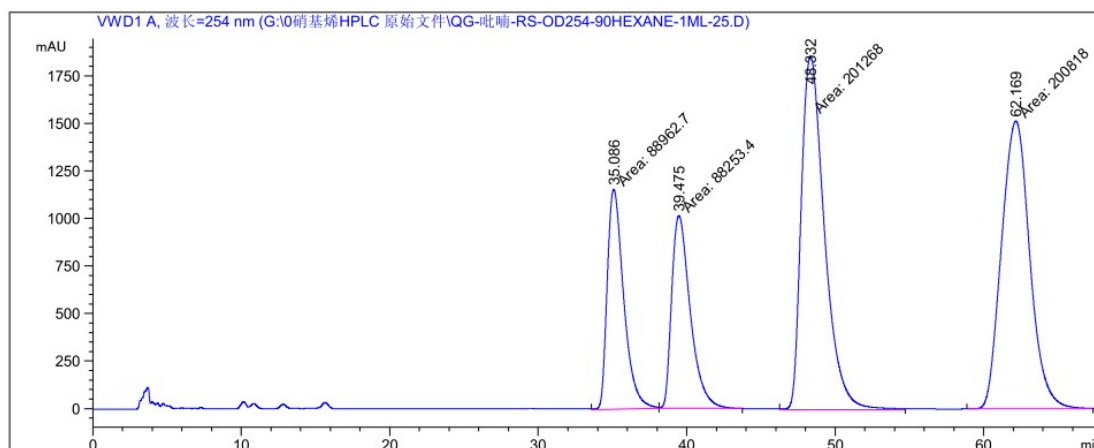
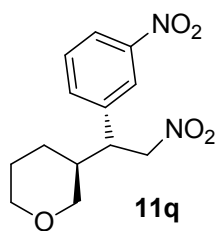


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	14.188	MM	0.3234	1.03638e4		534.14276	11.8759
2	16.648	MM	0.3749	1.03518e4		460.23706	11.8621
3	21.635	MM	0.6118	3.25812e4		887.51318	37.3348
4	31.336	MM	1.0443	3.39709e4		542.18597	38.9272

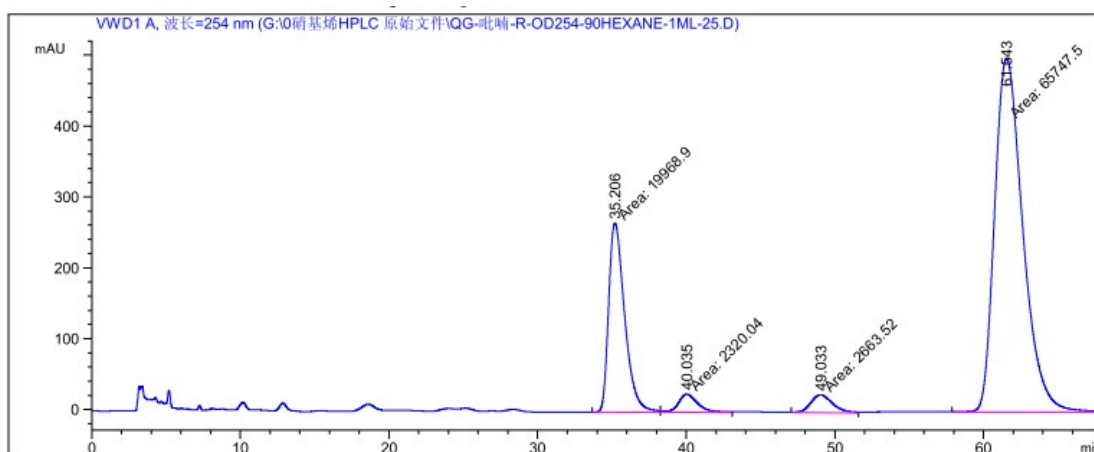


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	14.442	MM	0.2955	704.64069		39.74073	0.8389
2	16.739	MM	0.4559	2.62034e4		957.96661	31.1966
3	21.786	MM	0.7588	5.60672e4		1231.42578	66.7512
4	33.294	MM	0.9167	1019.06354		18.52791	1.2133

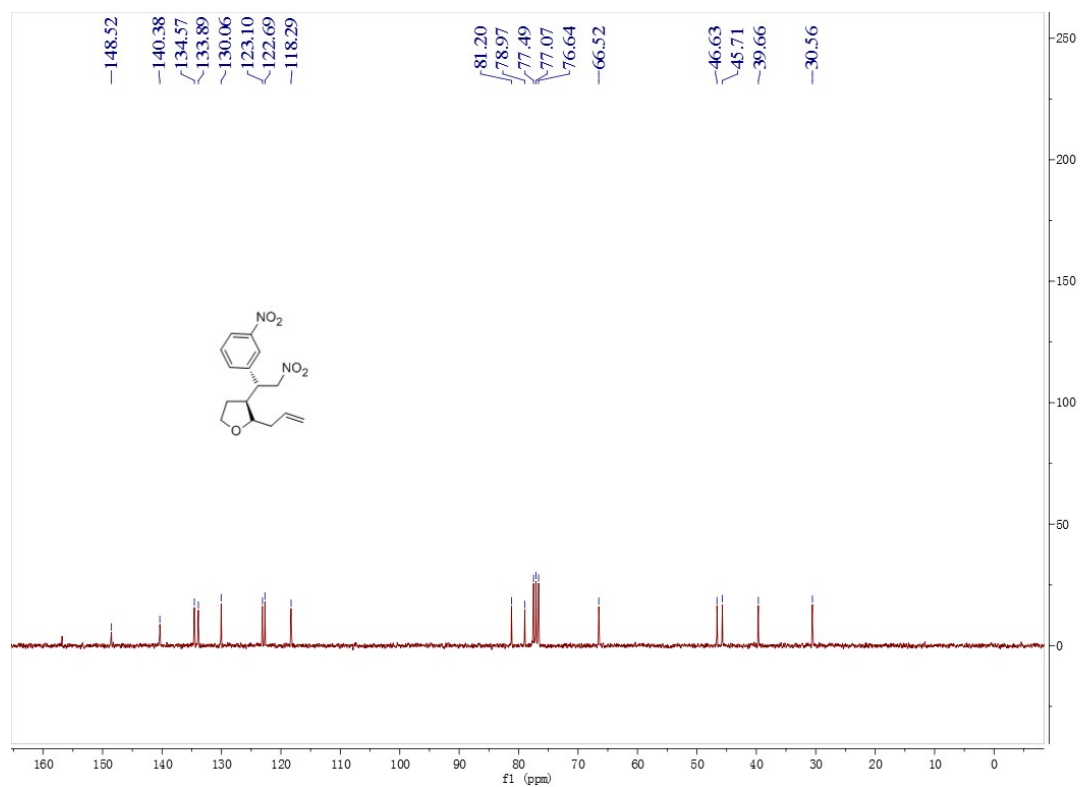
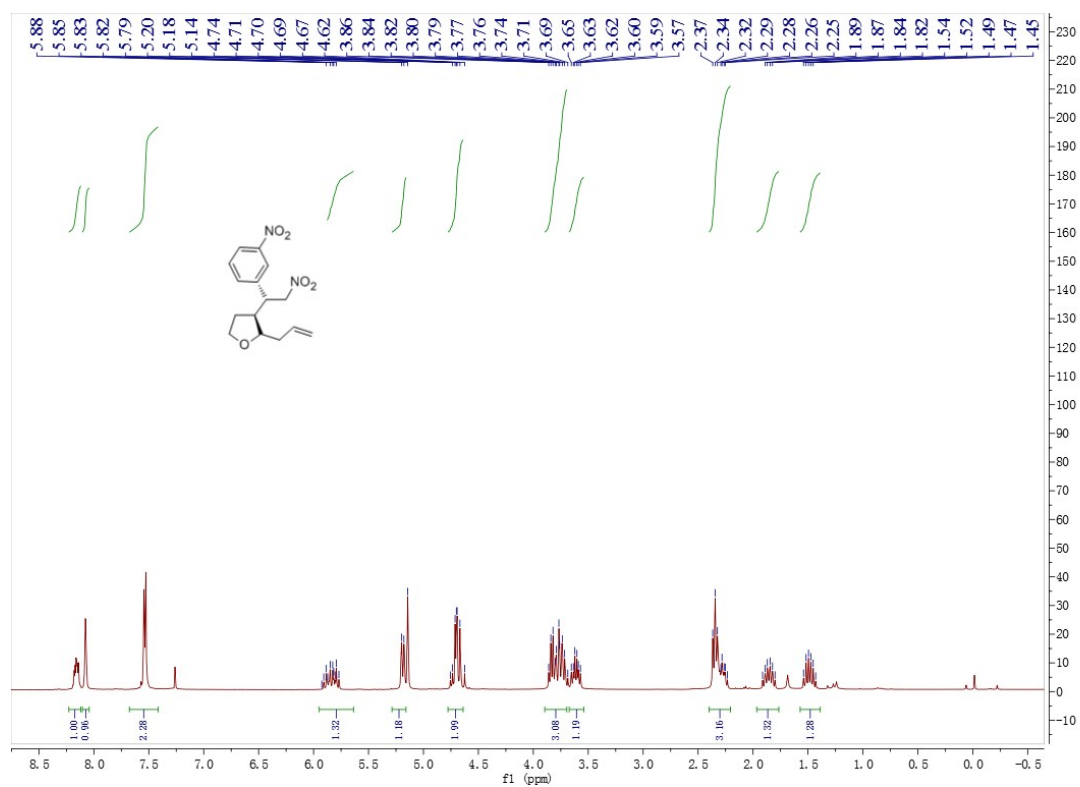


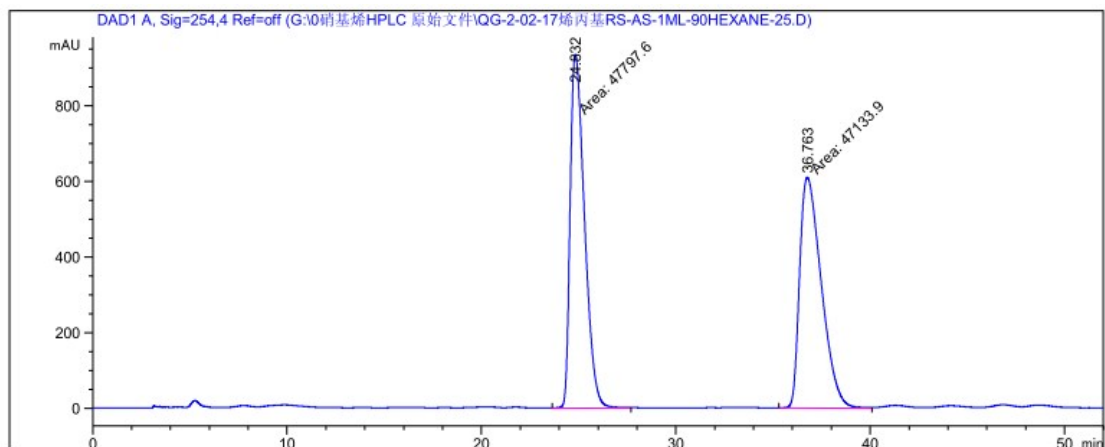
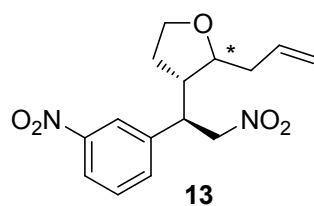


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	35.086	MM	1.2817	8.89627e4	1156.80957	15.3569
2	39.475	MM	1.4522	8.82534e4	1012.88965	15.2344
3	48.332	MM	1.8046	2.01268e5	1858.85779	34.7431
4	62.169	MM	2.2107	2.00818e5	1513.98694	34.6655

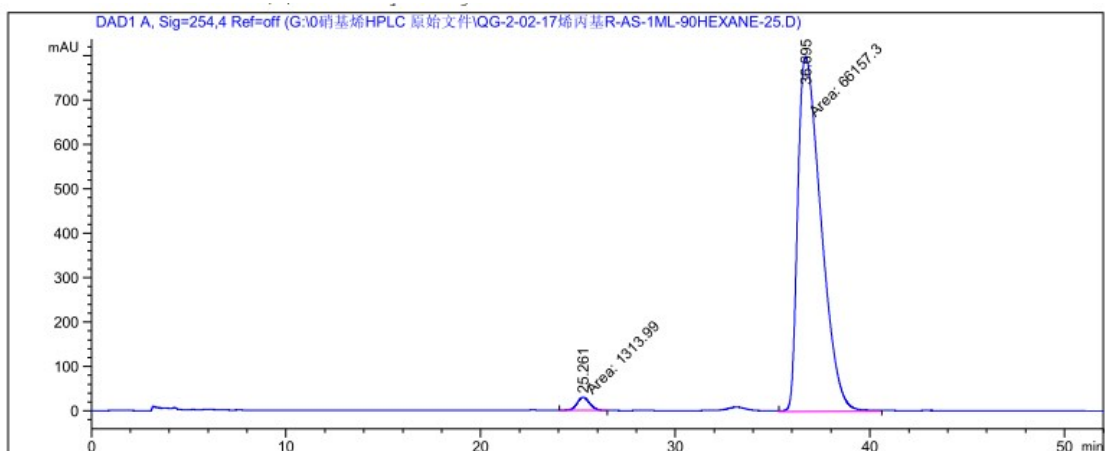


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	35.206	MM	1.2465	1.99689e4	266.99985	22.0164
2	40.035	MM	1.5243	2320.03882	25.36766	2.5579
3	49.033	MM	1.7444	2663.51611	25.44810	2.9366
4	61.543	MM	2.1959	6.57475e4	499.00662	72.4890



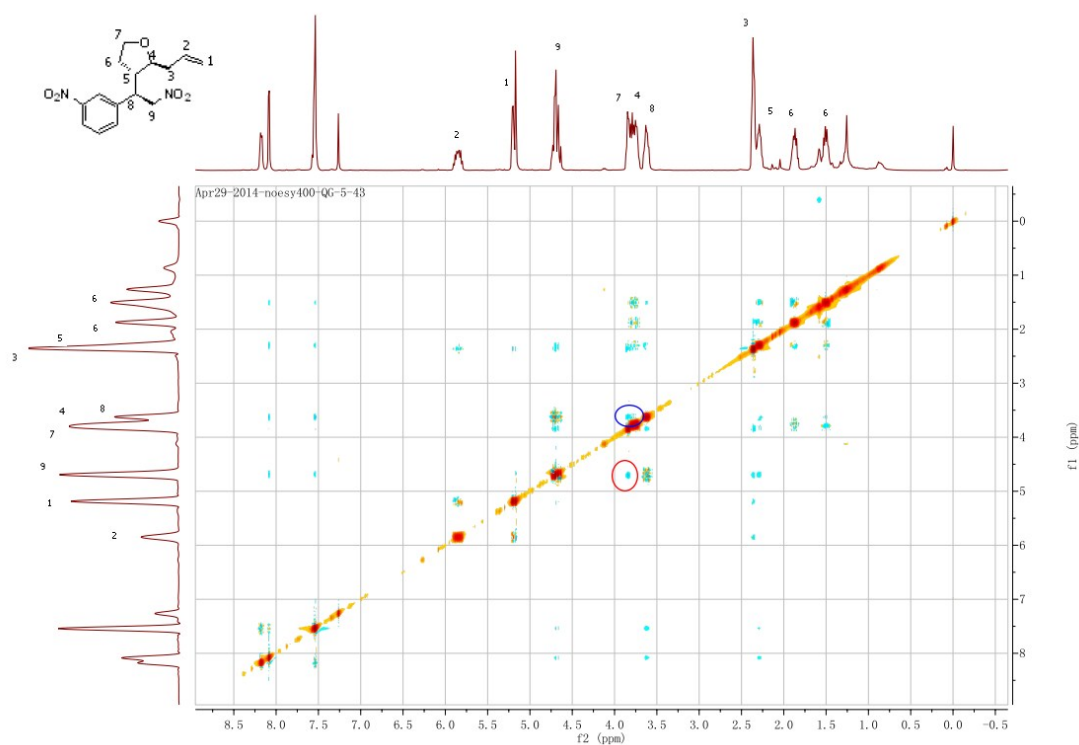


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.832	MM	0.8526	4.77976e4	934.34662	50.3496
2	36.763	MM	1.2897	4.71339e4	609.08789	49.6504



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.261	MM	0.7394	1313.98999	29.61870	1.9475
2	36.695	MM	1.3795	6.61573e4	799.30426	98.0525

NOESY for compound **13**



The signals between H-4 and H-8 (blue circle), H-4 and H-9 (red circle) show that the two substituents of tetrahydrofuran are on *anti*-position.

