

Supporting Information

Chiral phosphine-squaramide-catalyzed Morita-Baylis-Hillman reaction: Enantioselective synthesis of 3-hydroxy-2-oxindoles

Jing-Ying Qian,^a Ci-Ci Wang,^a Feng Sha^a and Xin-Yan Wu^{*a,b}

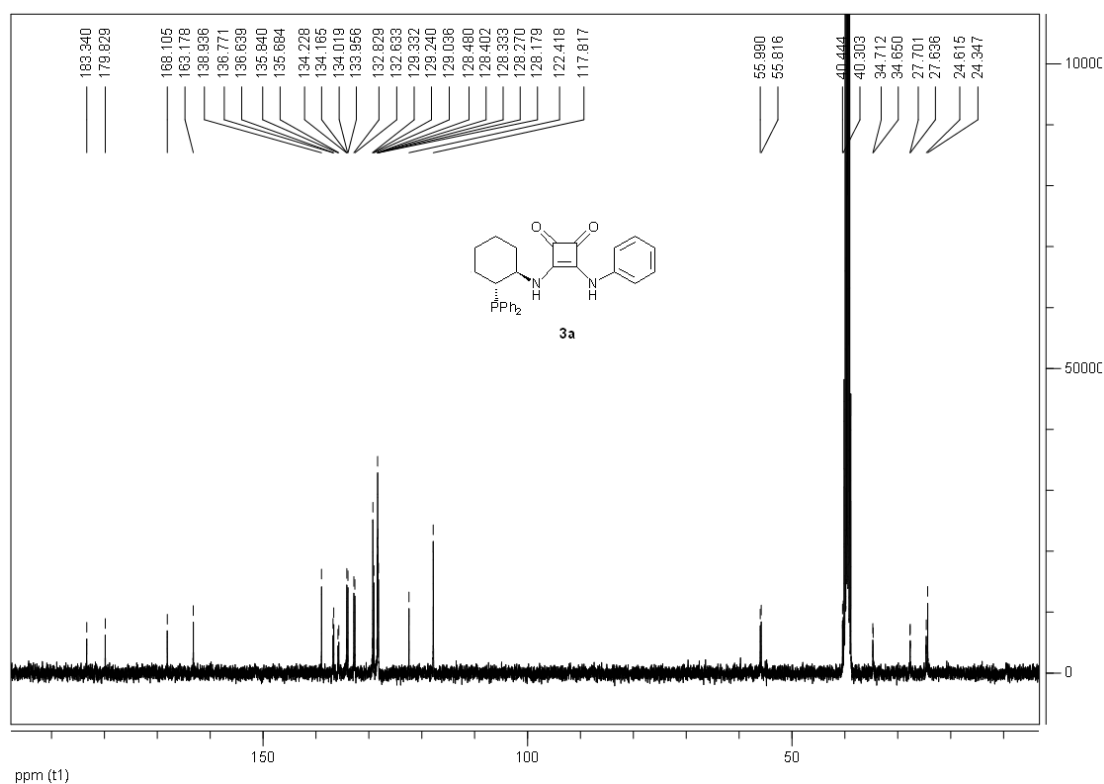
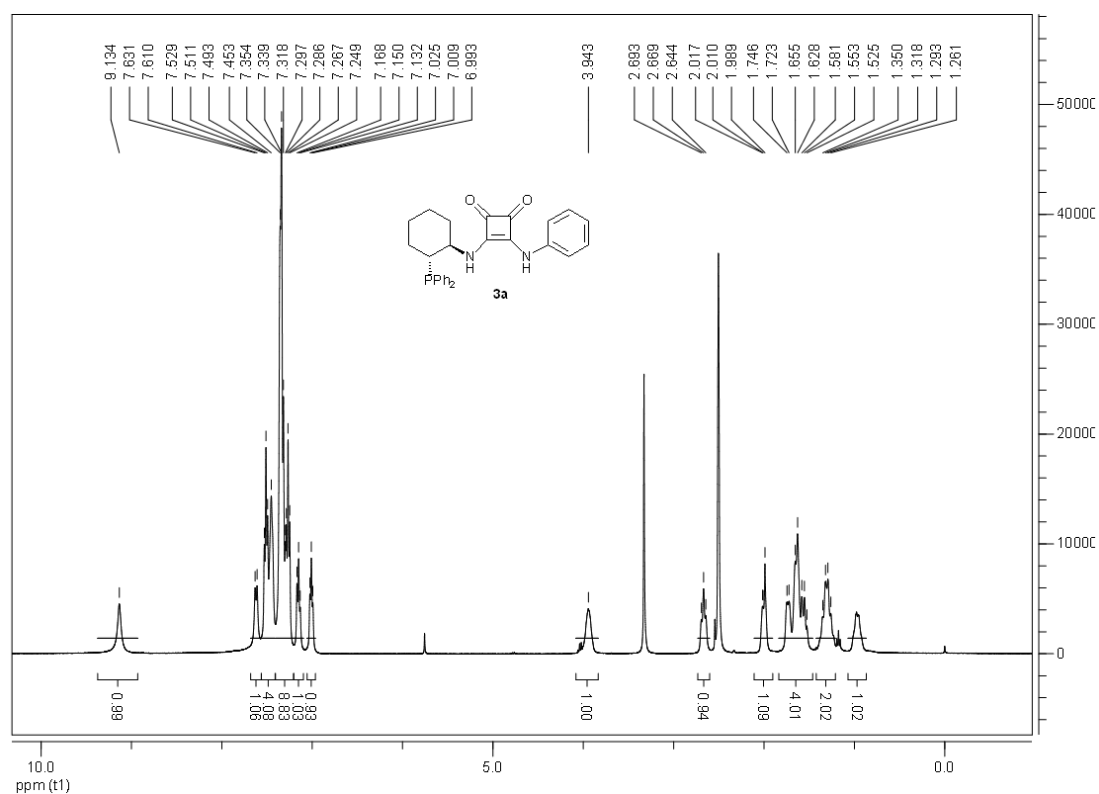
^a*Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science and Technology, Shanghai 200237, P. R. China*

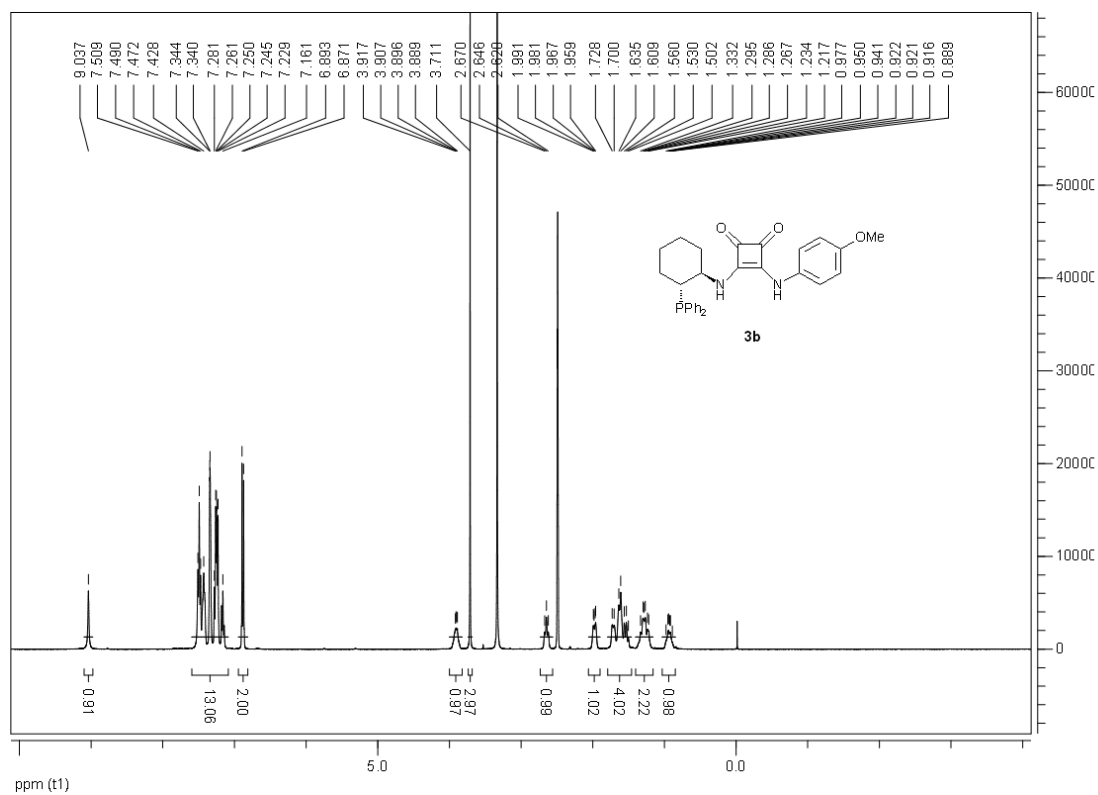
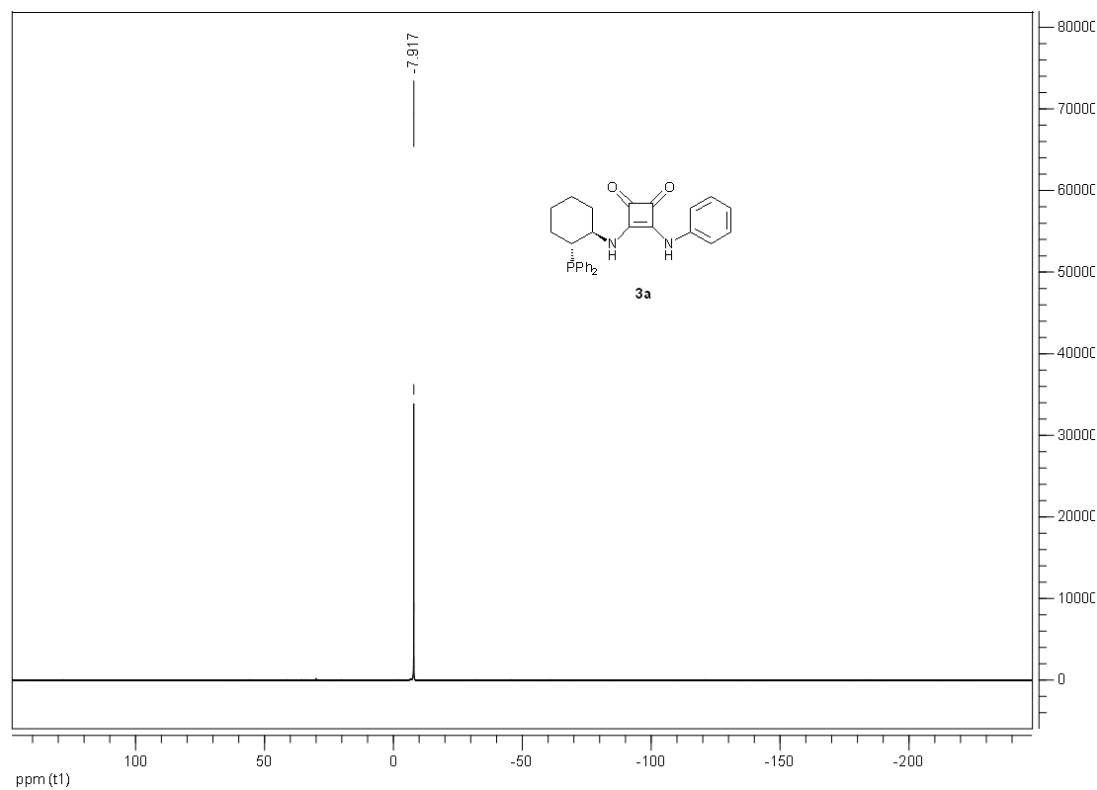
^b*State Key Laboratory of elemento-organic Chemistry, Nankai University, Tianjin 300071, P. R. China*

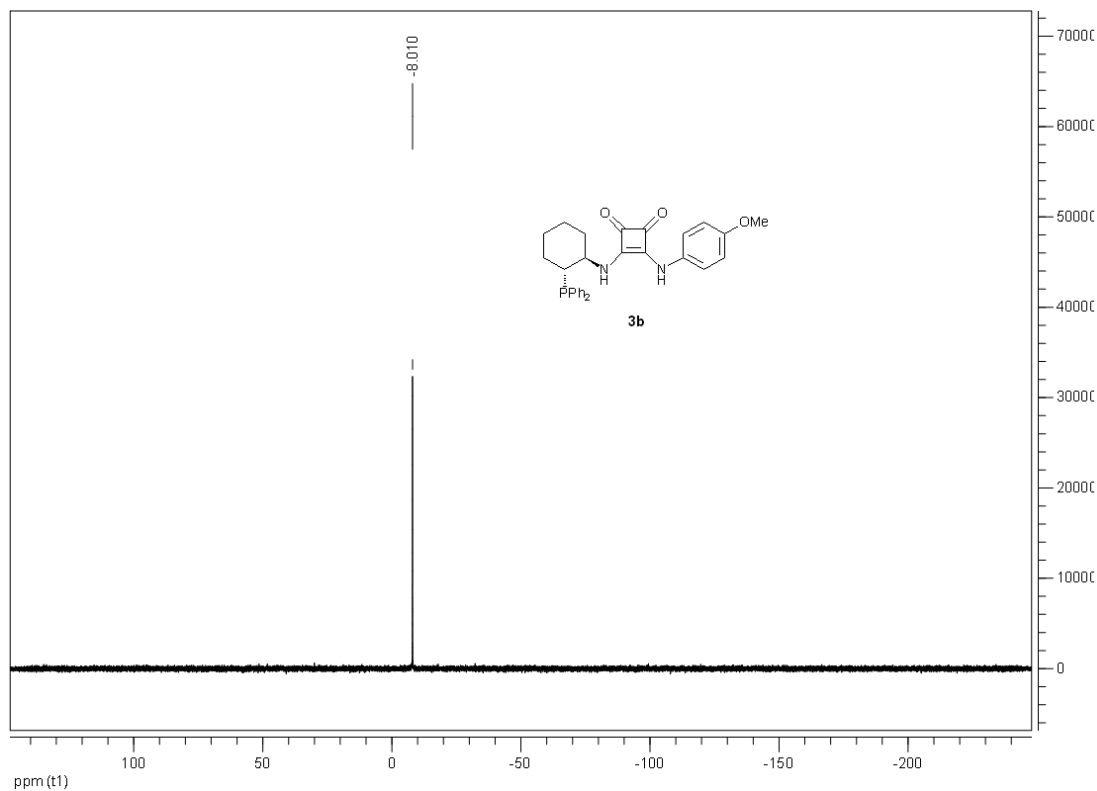
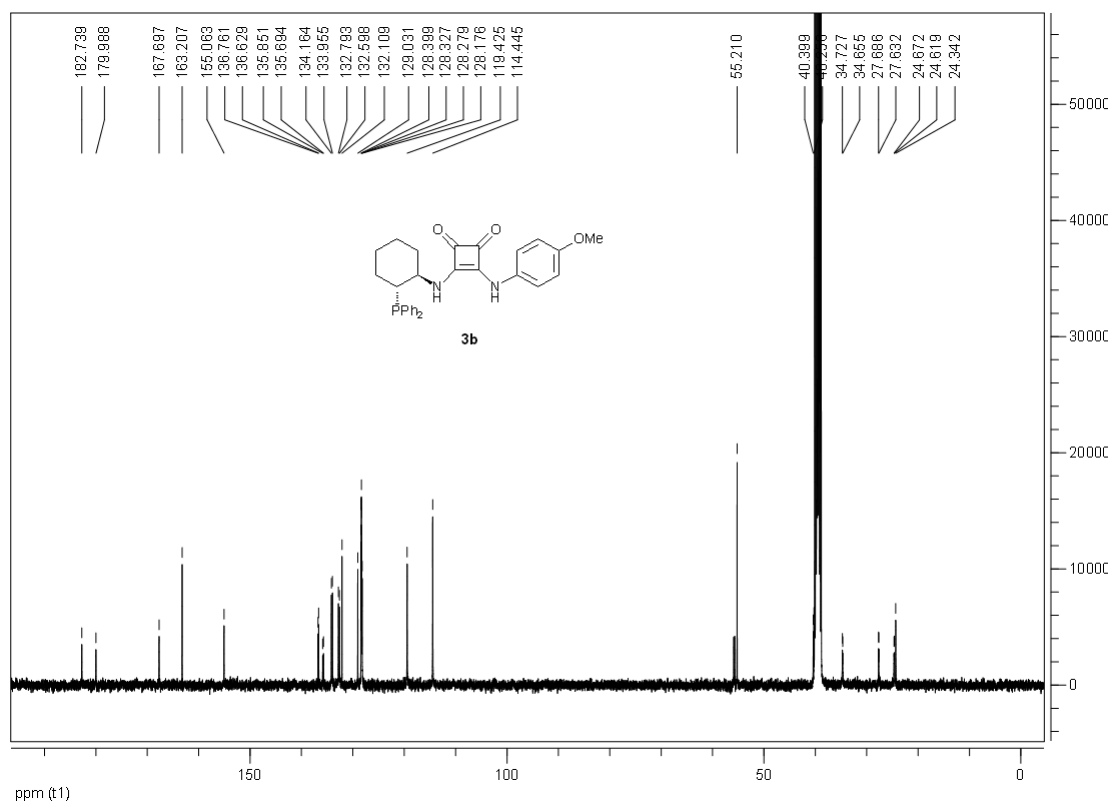
E-mail: xinyanwu@ecust.edu.cn; Tel: 86 21 64252011; Fax: 86 21 64252758

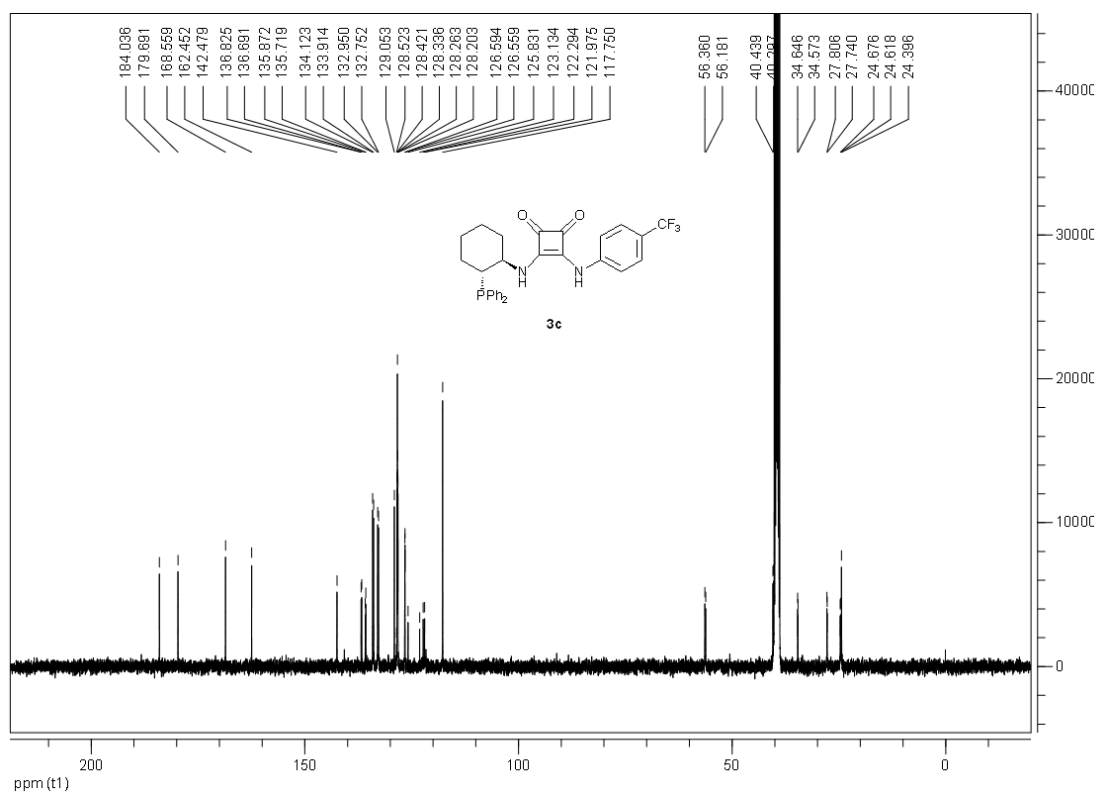
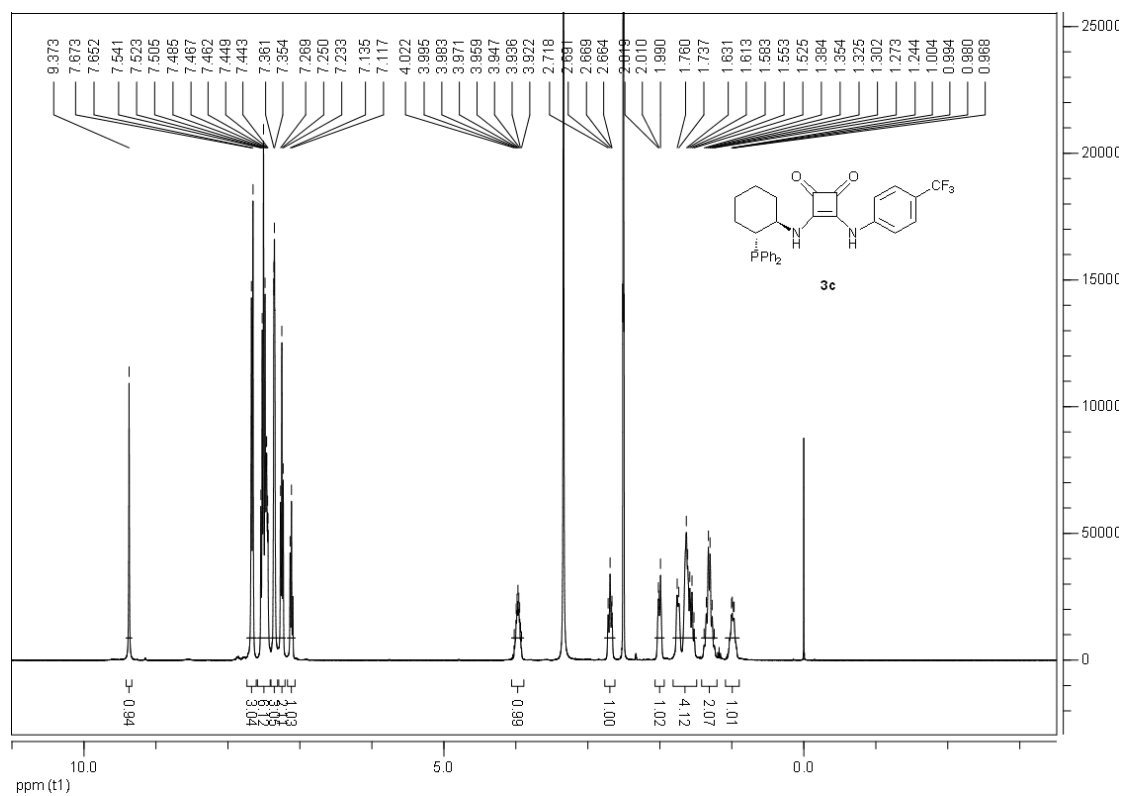
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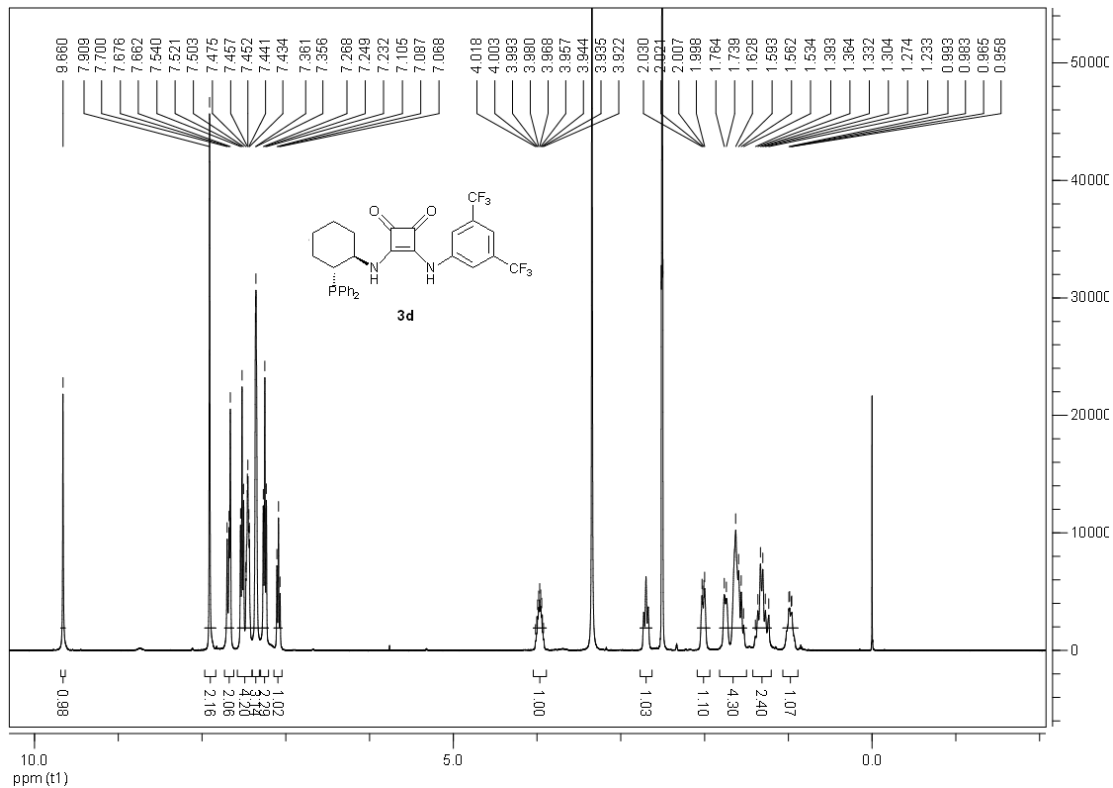
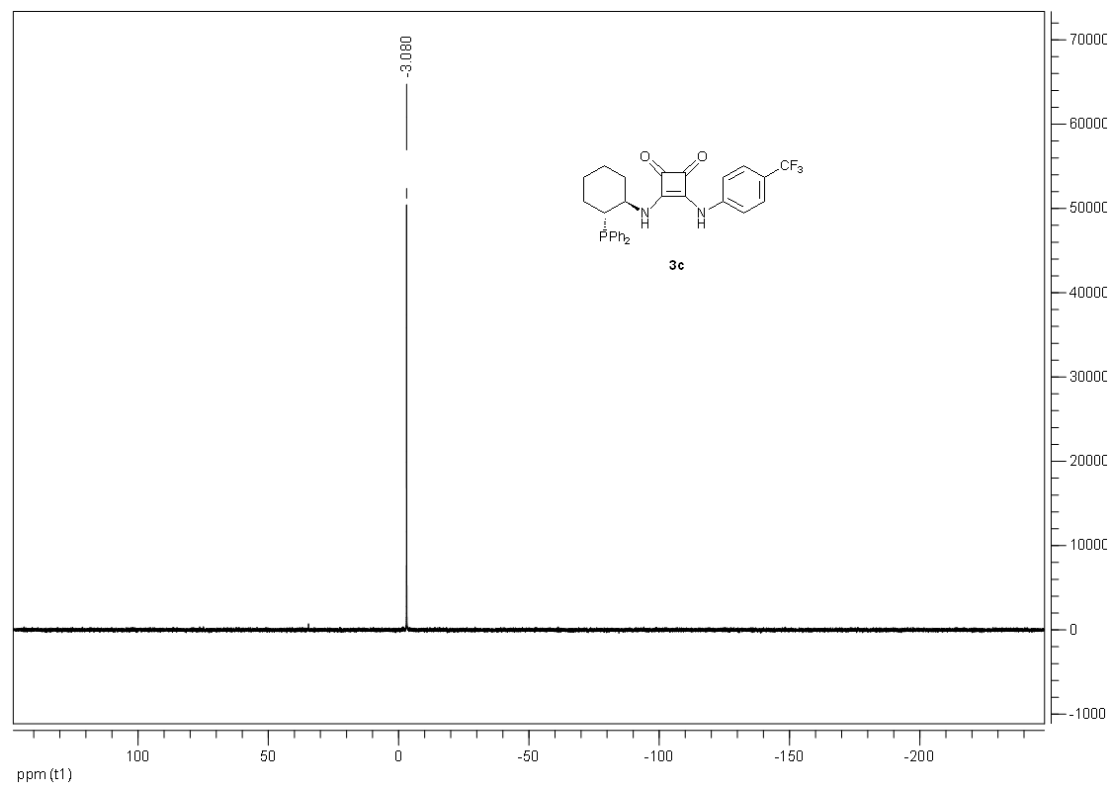
1. ^1H NMR, ^{13}C NMR and ^{31}P NMR Spectra of Catalyst 3a-h

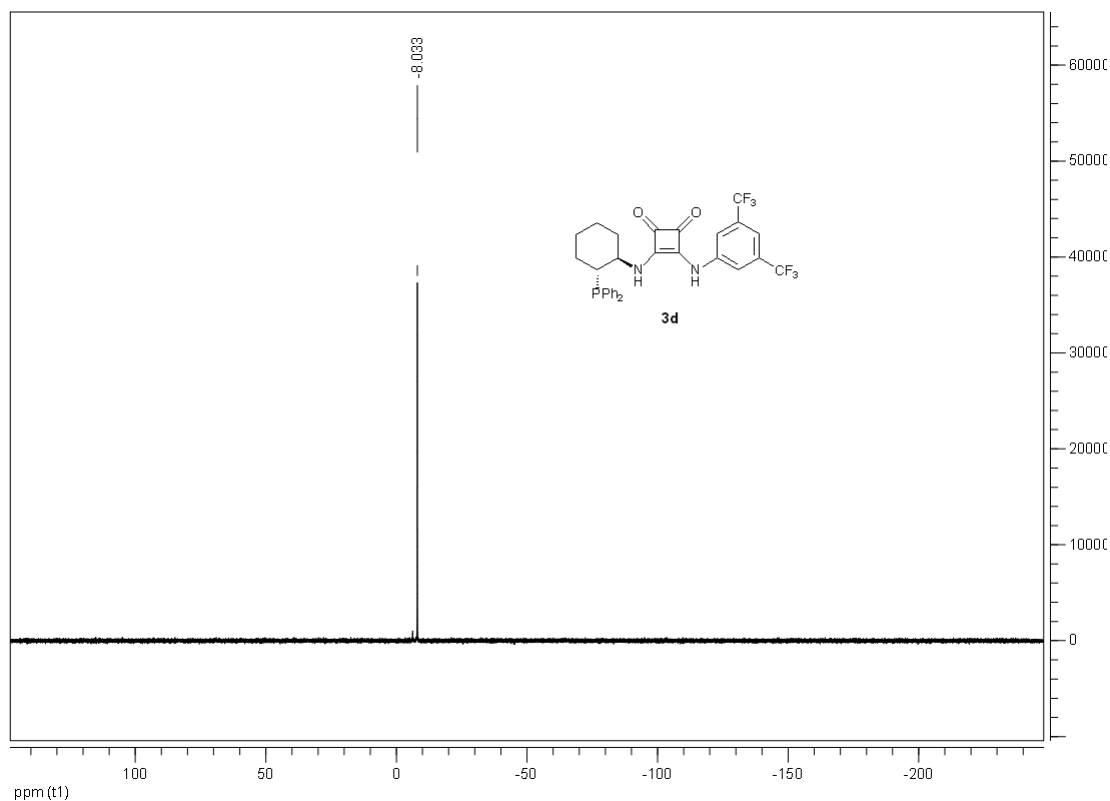
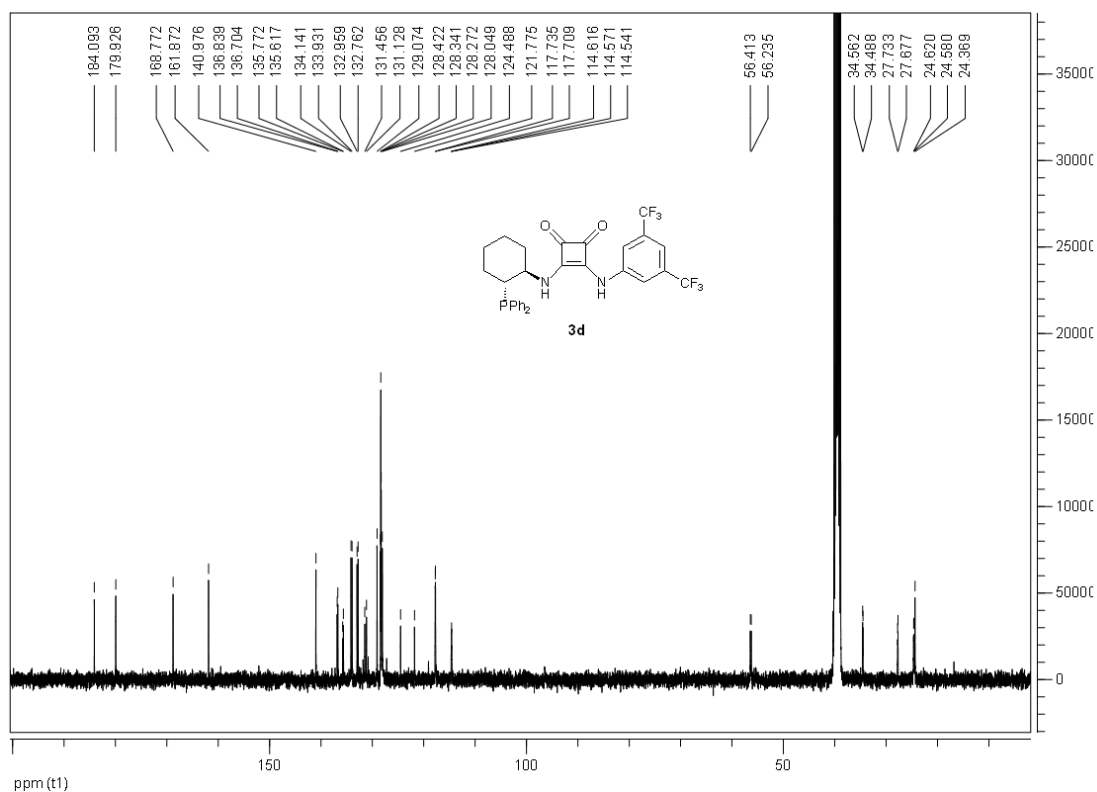


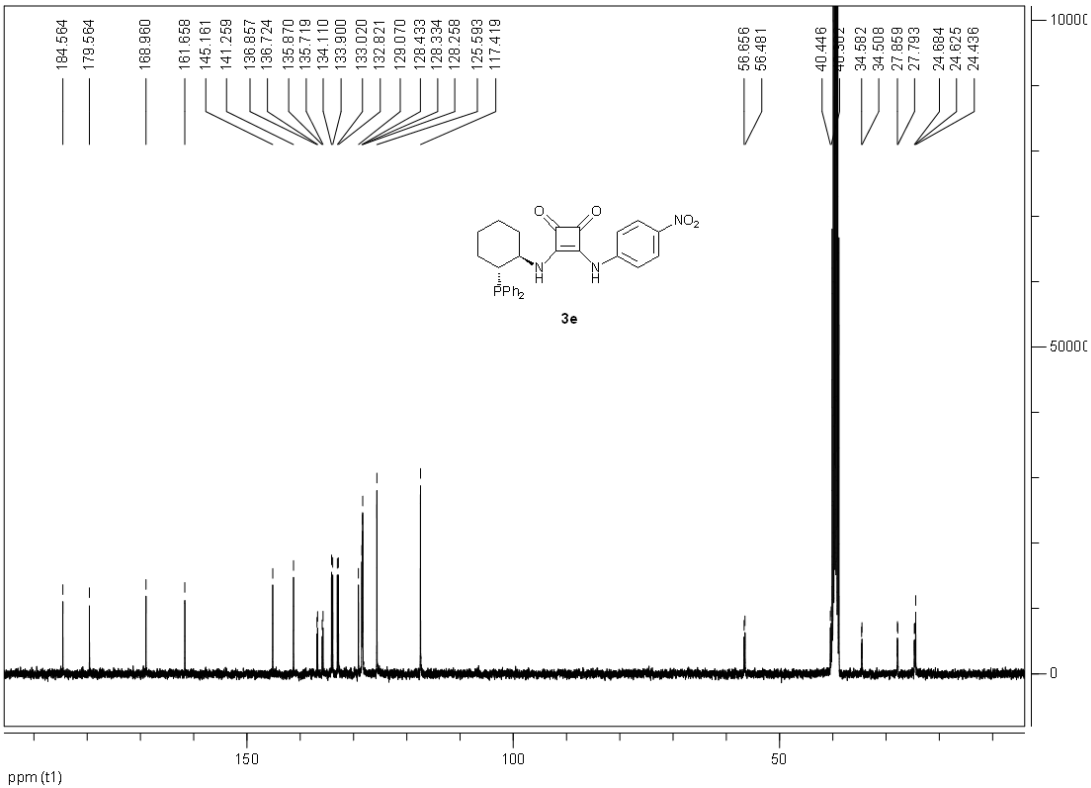
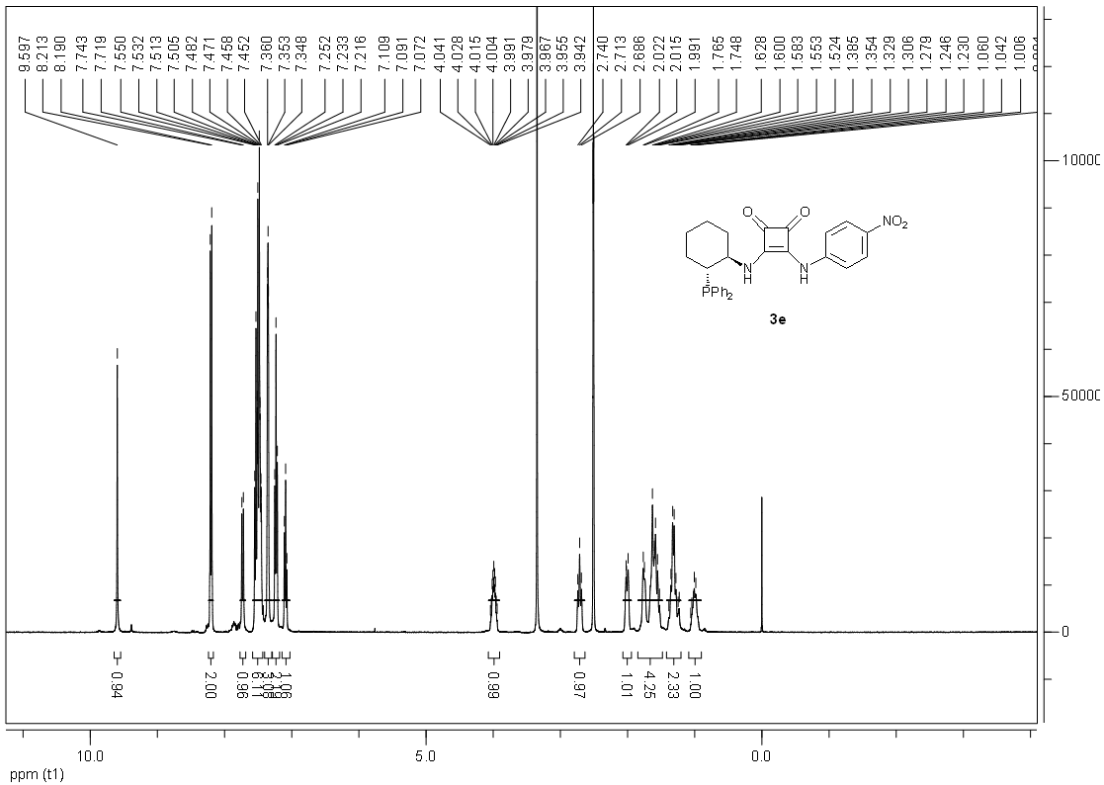


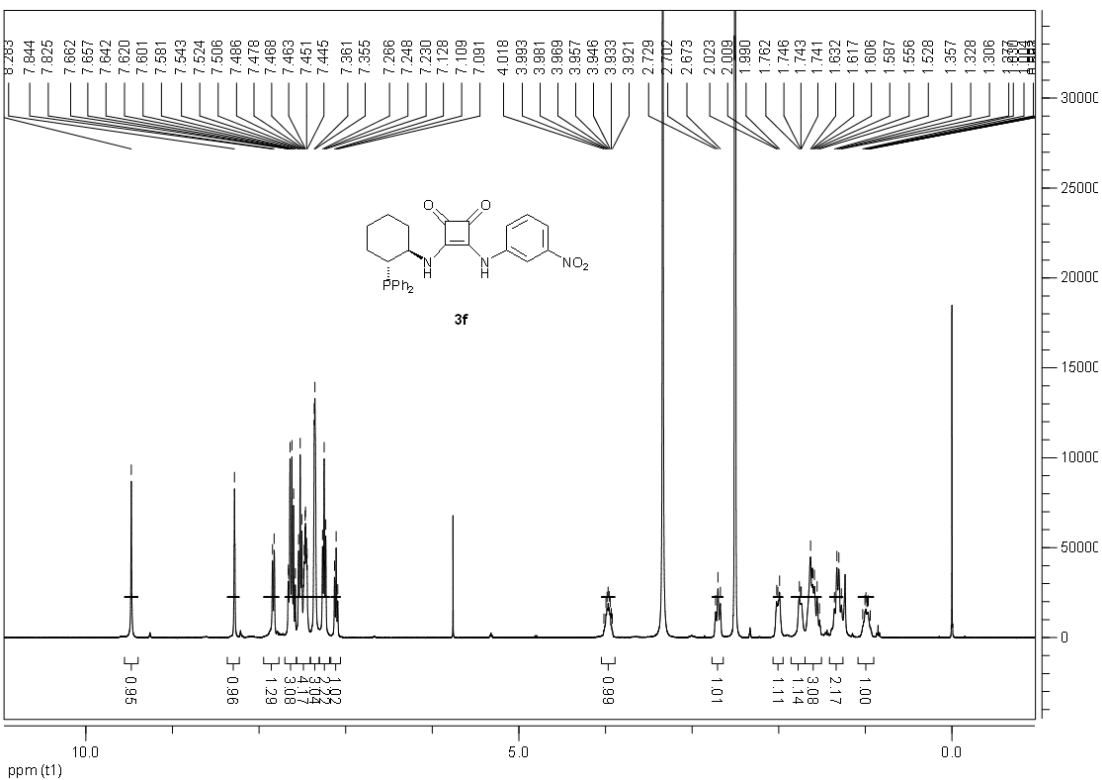
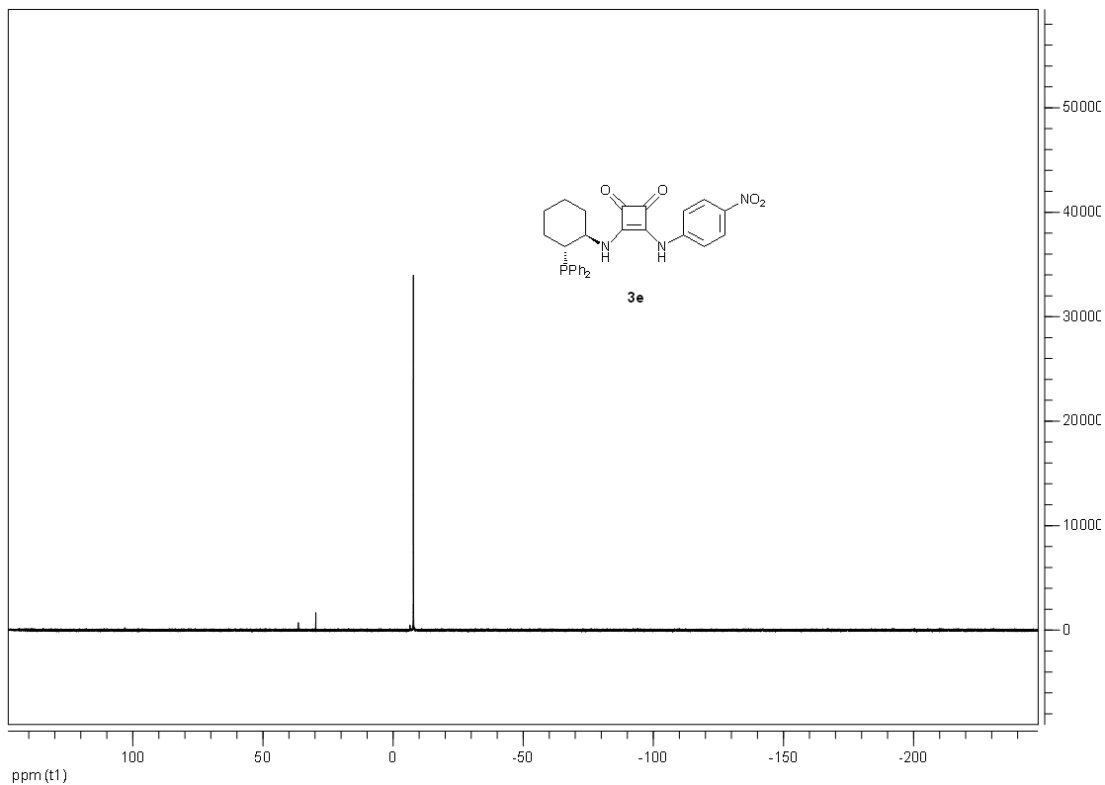


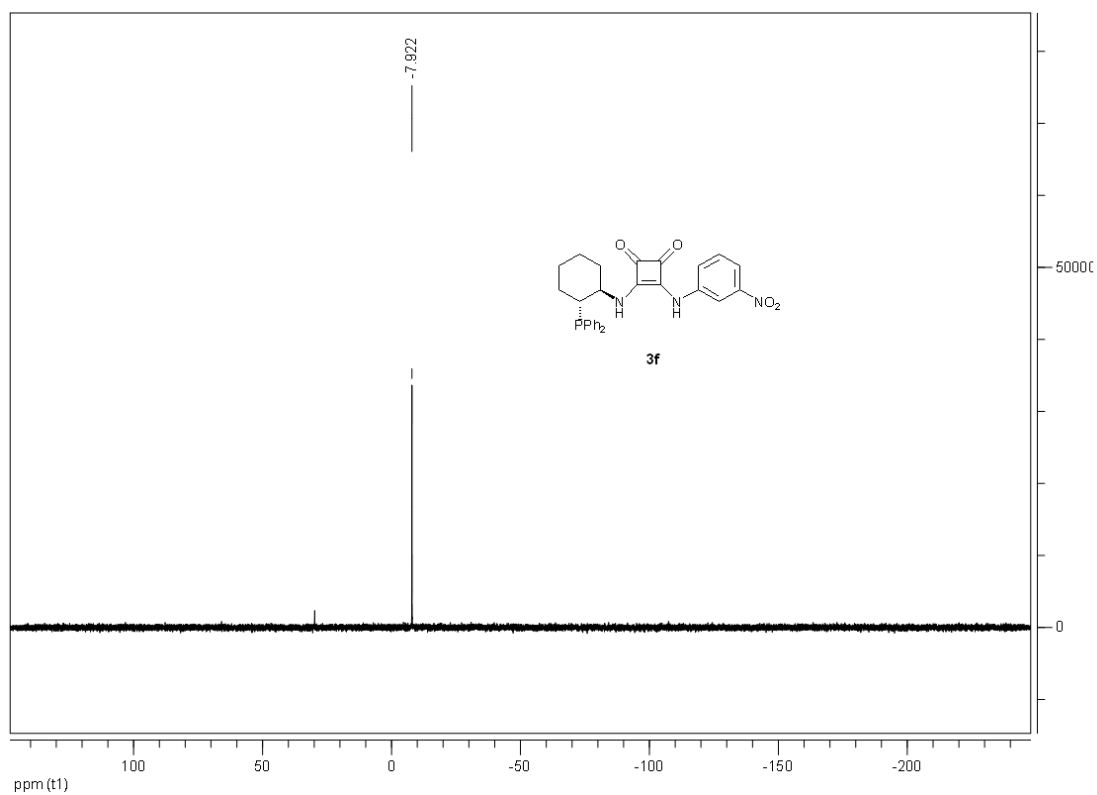
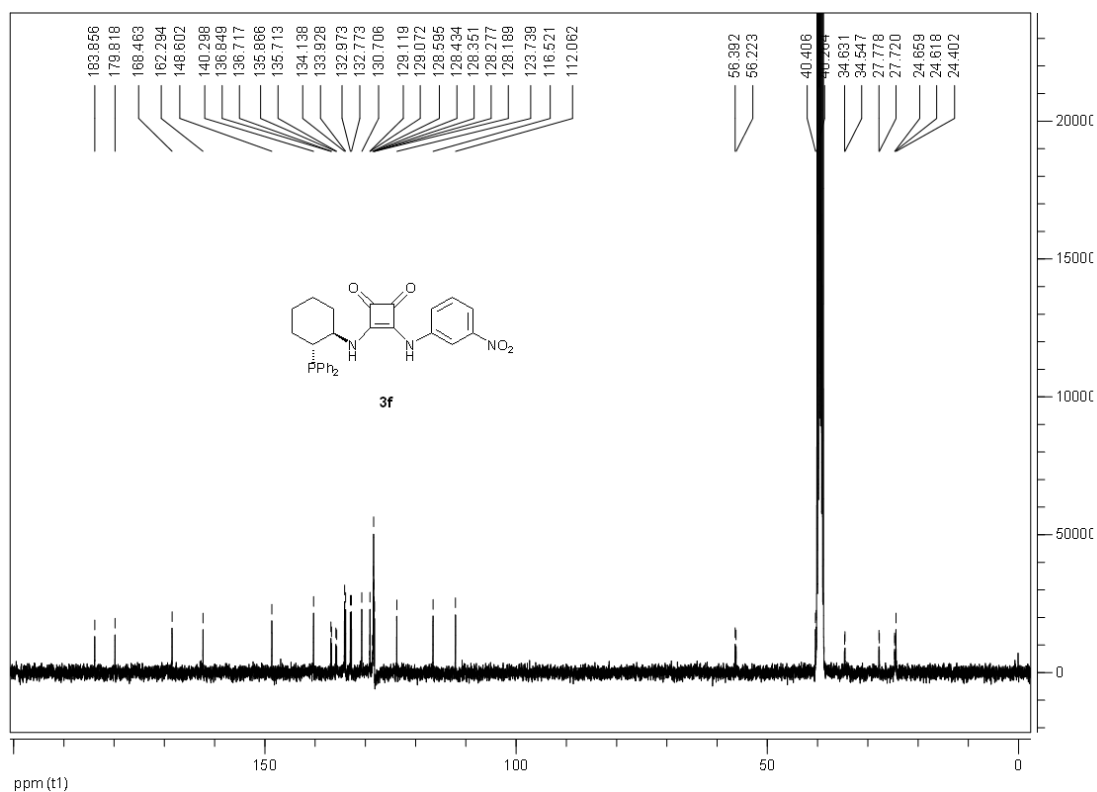


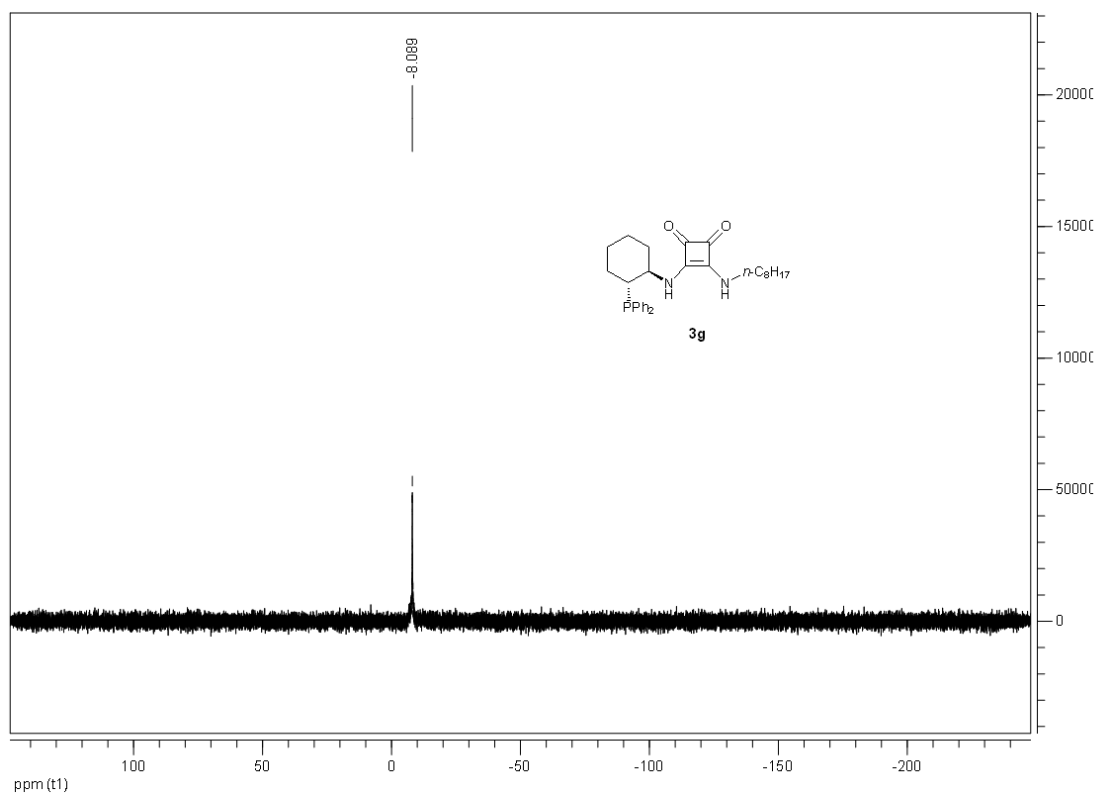
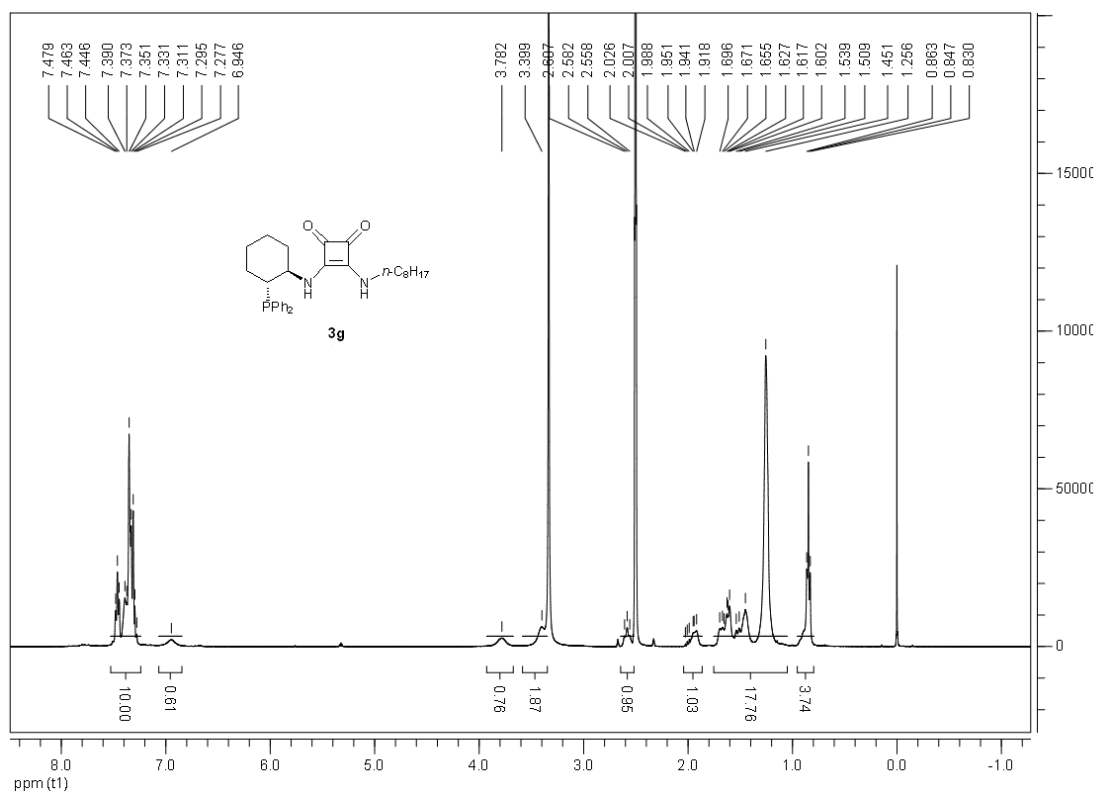


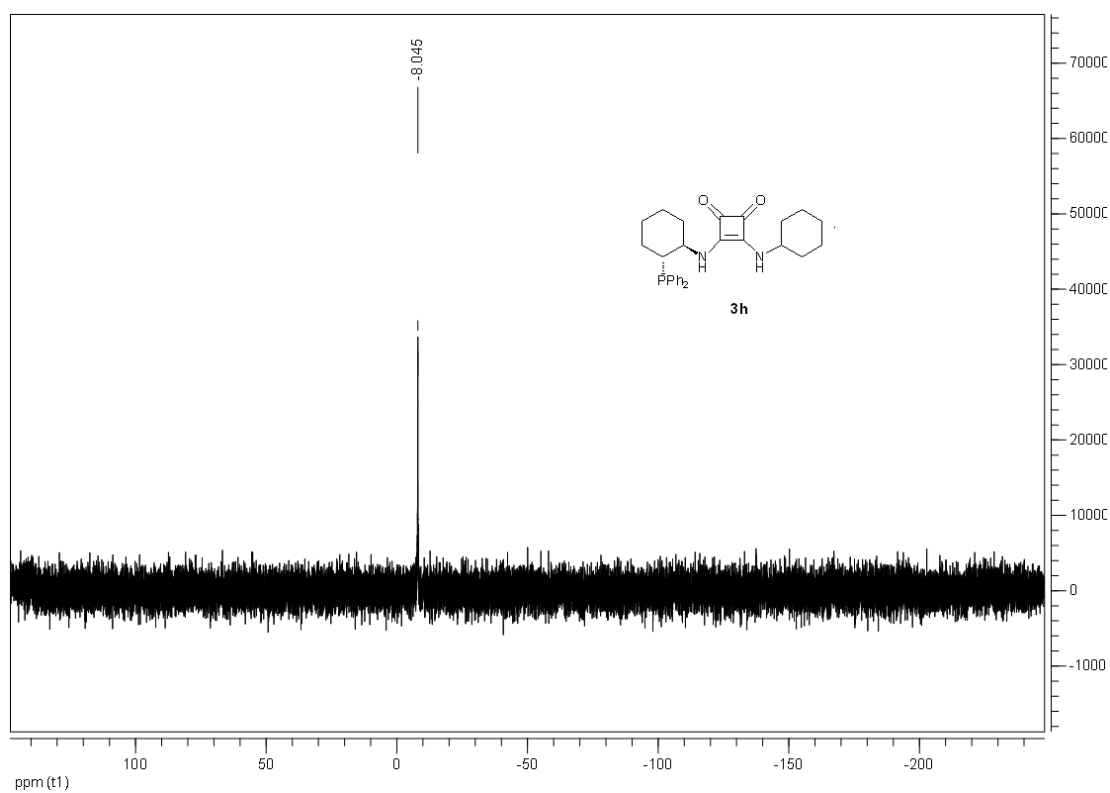
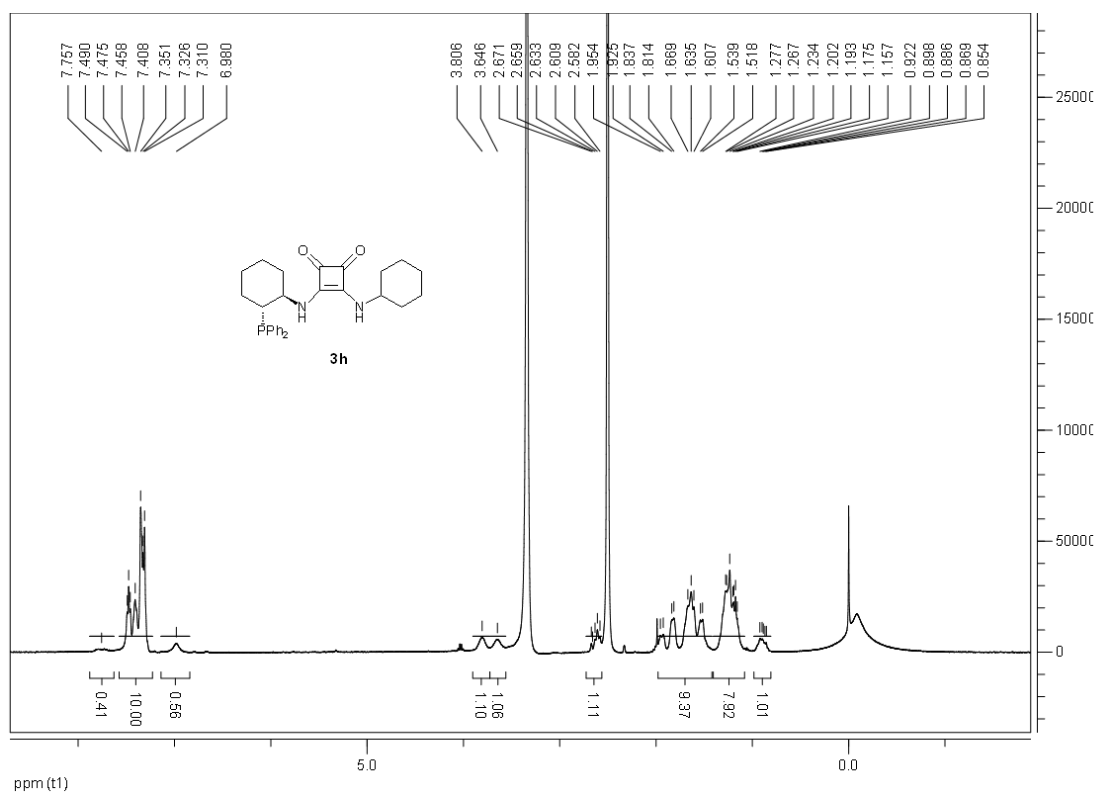




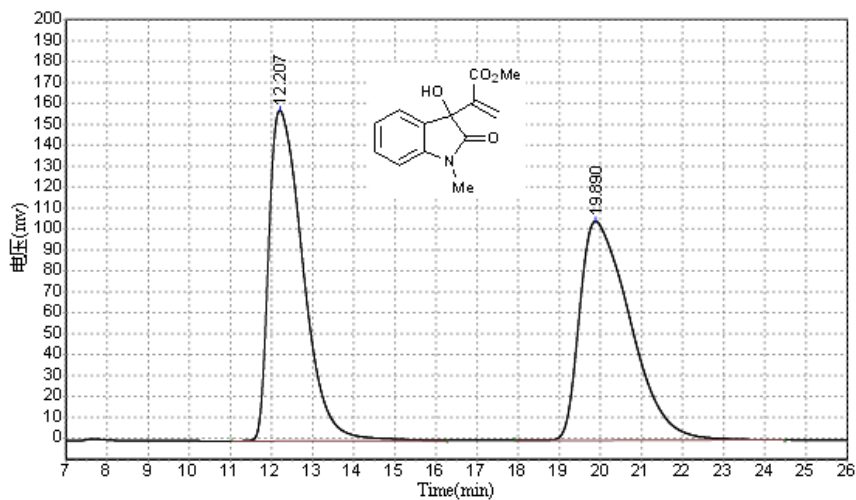




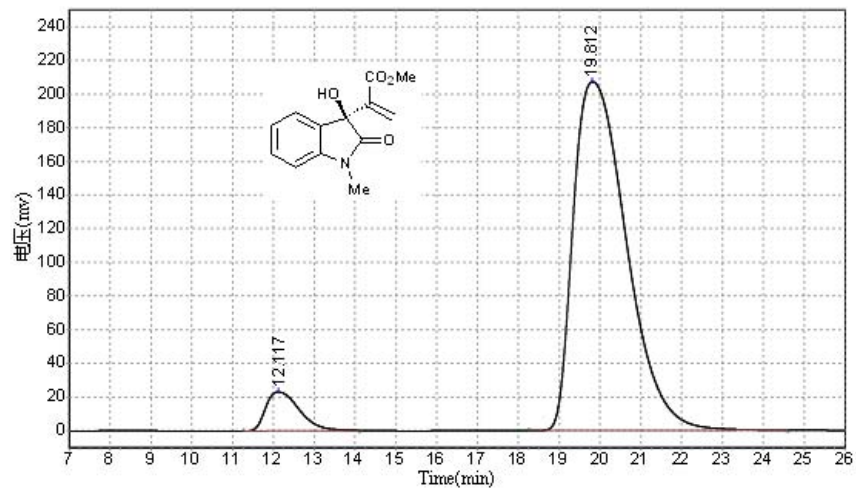




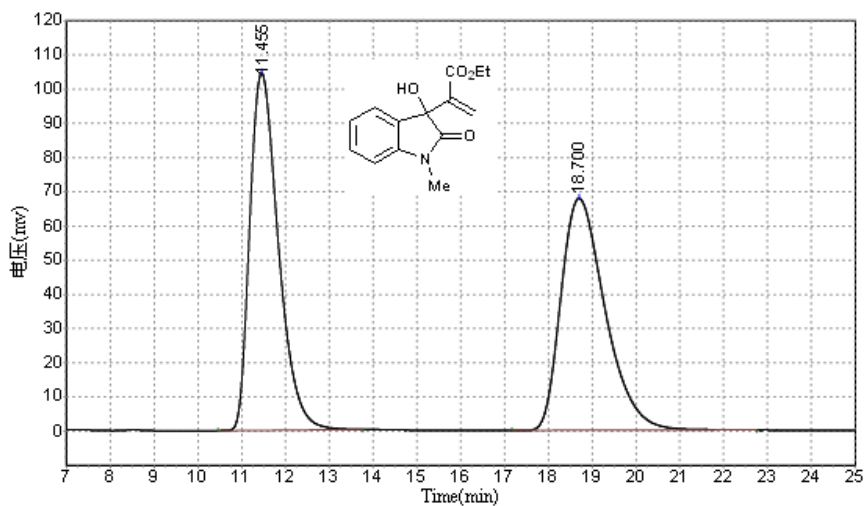
2. HPLC Spectra for the Morita-Baylis-Hillman Products



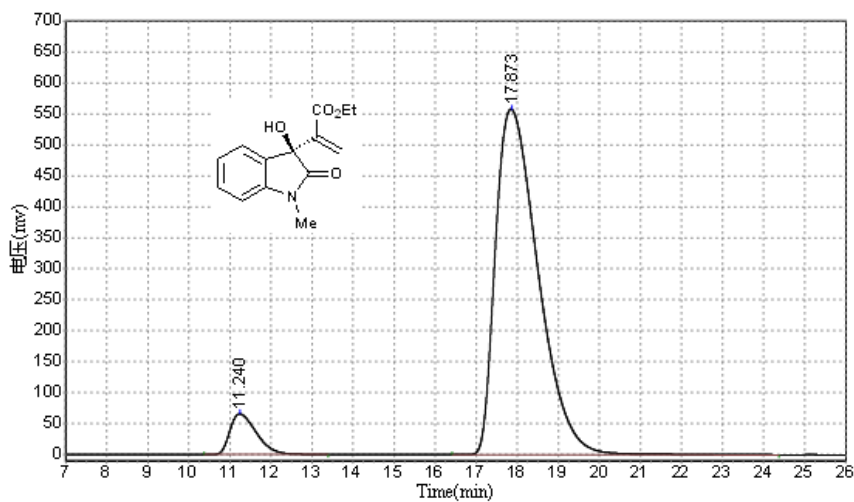
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		12.207	157978.578	9127587.000	50.3639
2		19.890	104714.586	8995686.000	49.6361
Total			262693.164	18123273.000	100.0000



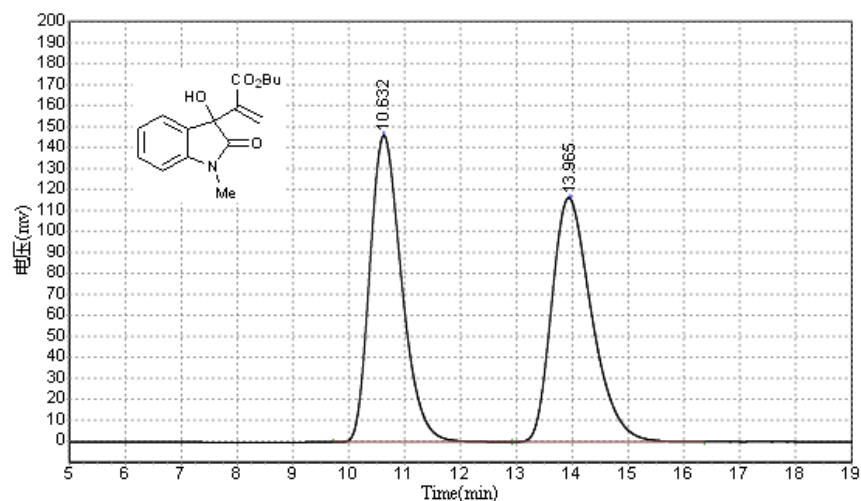
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		12.117	23179.410	1326025.500	6.6089
2		19.812	207192.641	18738218.000	93.3911
Total			230372.051	20064243.500	100.0000



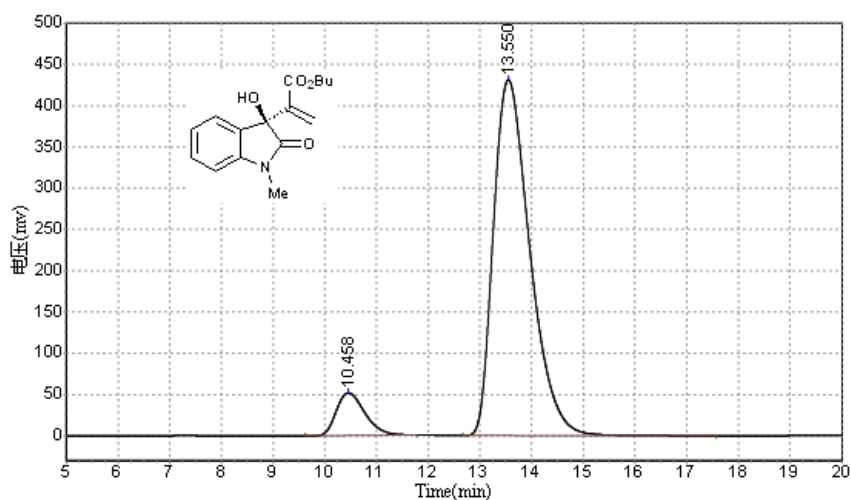
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		11.455	104512.727	4732744.500	49.8311
2		18.700	67888.133	4764818.500	50.1689
Total			172400.859	9497563.000	100.0000



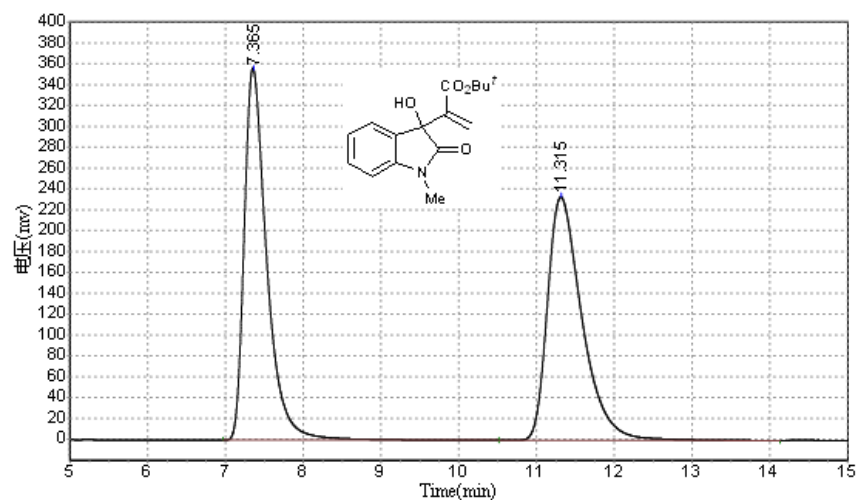
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		11.240	65798.281	2988279.000	6.9069
2		17.873	558054.875	40276756.000	93.0931
Total			623853.156	43265035.000	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		10.632	145982.891	5790629.000	50.0634
2		13.965	116276.047	5775970.000	49.9366
Total			262258.938	11566599.000	100.0000

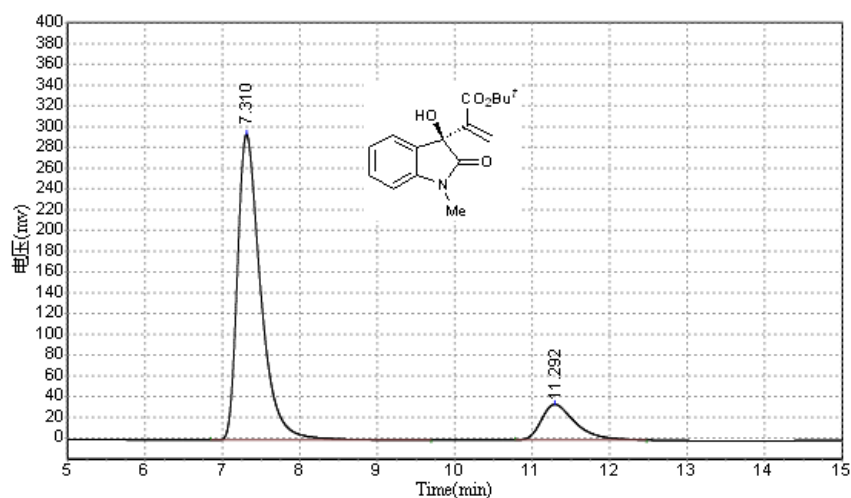


Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		10.458	51587.789	1965414.000	8.5192
2		13.550	431361.063	21104862.000	91.4808
Total			482948.852	23070276.000	100.0000



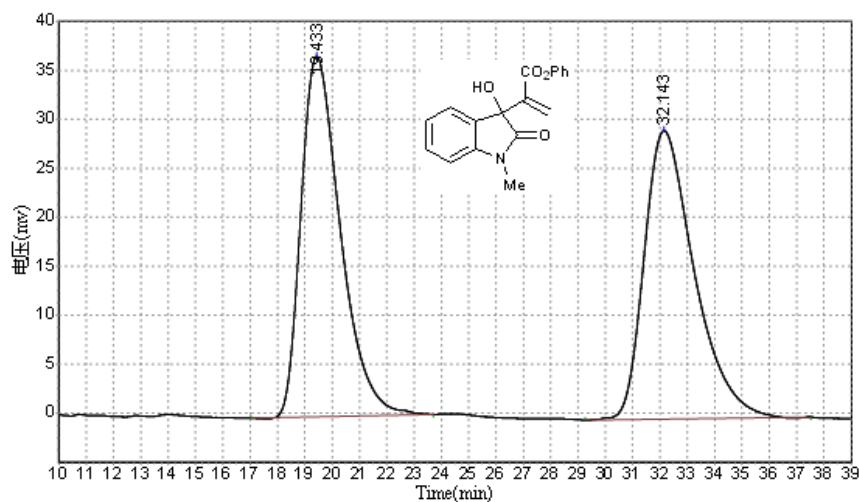
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		7.365	356304.313	7214100.500	50.0367
2		11.315	233157.313	7203517.000	49.9633
Total			589461.625	14417617.500	100.0000

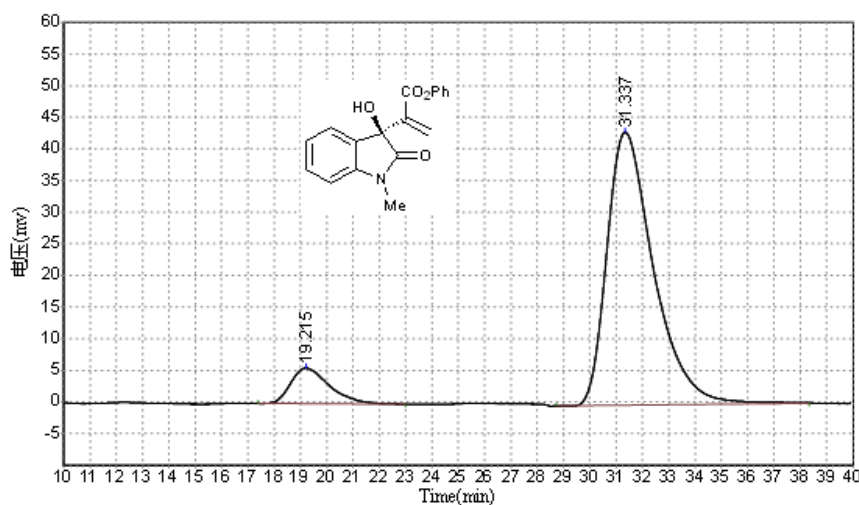


Results

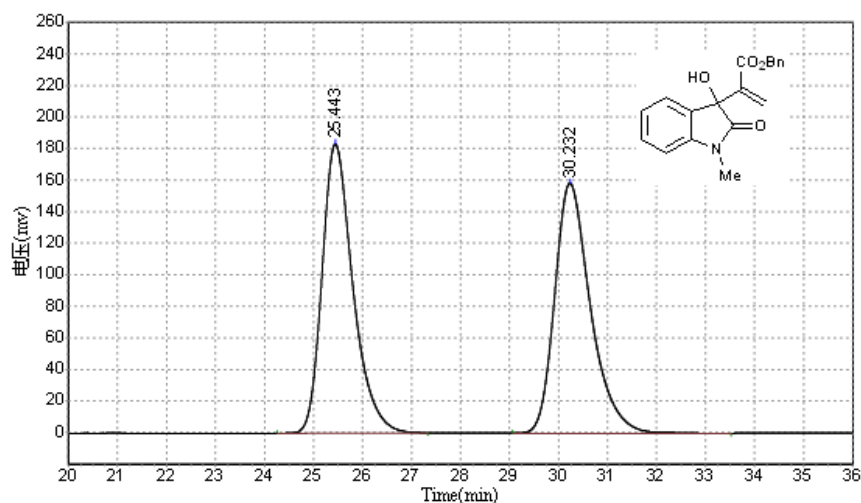
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		7.310	294581.031	6131392.500	85.4088
2		11.292	34323.359	1047482.500	14.5912
Total			328904.391	7178875.000	100.0000



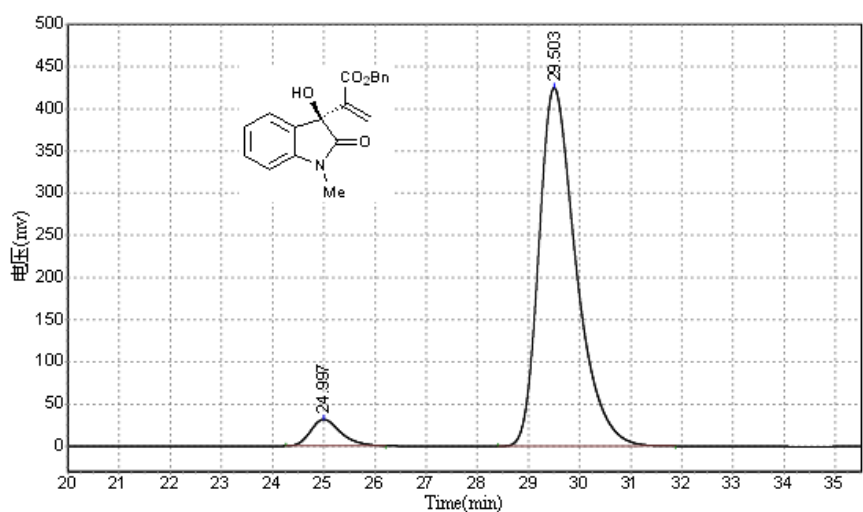
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		19.433	36786.387	3686438.750	49.6135
2		32.143	29453.410	3743873.000	50.3865
Total			66239.797	7430311.750	100.0000



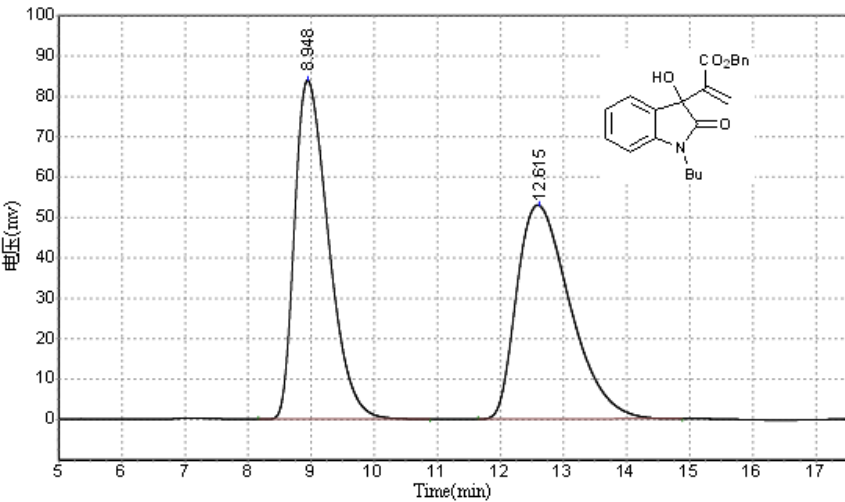
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		19.215	5641.313	577685.438	9.8129
2		31.337	43178.230	5309336.500	90.1871
Total			48819.544	5887021.938	100.0000



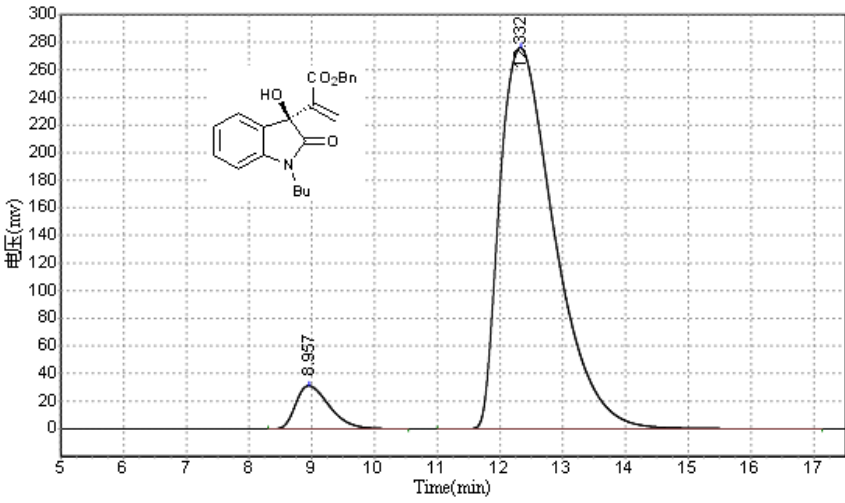
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		25.443	183270.469	8014493.500	49.8892
2		30.232	158570.484	8050090.500	50.1108
Total			341840.953	16064584.000	100.0000



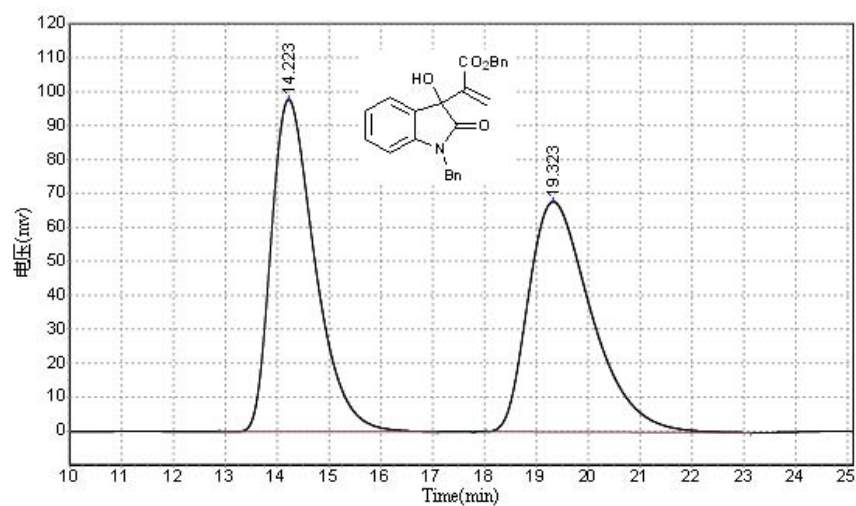
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		24.997	31488.721	1290454.375	5.6808
2		29.503	425013.906	21425612.000	94.3192
Total			456502.627	22716066.375	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		8.948	83991.039	3139415.500	50.1080
2		12.615	52992.875	3125881.750	49.8920
Total			136983.914	6265297.250	100.0000

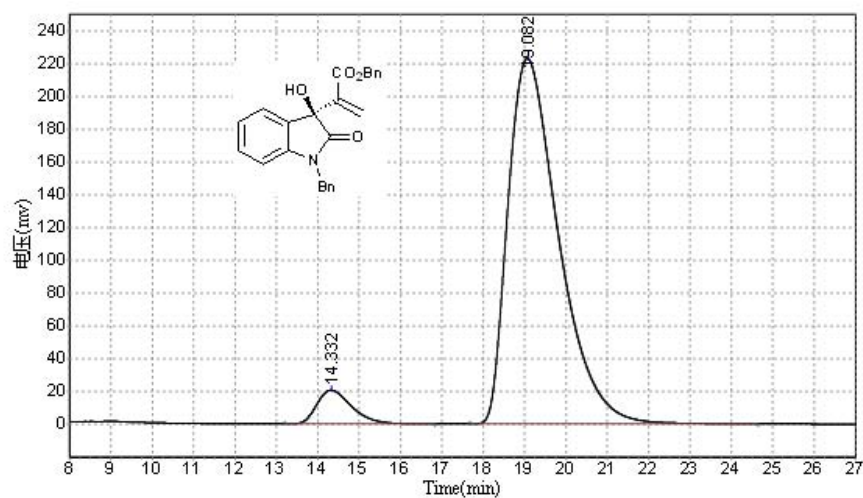


Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		8.957	31323.779	1172340.250	6.5375
2		12.332	276267.031	16760318.000	93.4625
Total			307590.811	17932658.250	100.0000



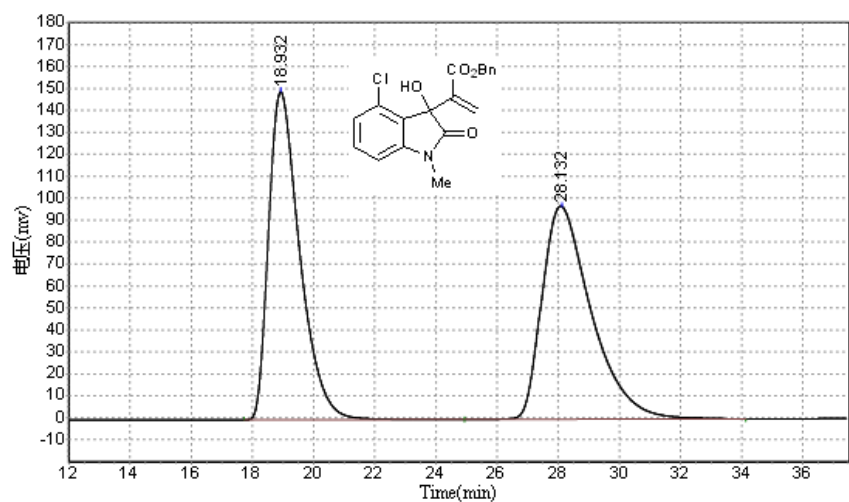
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.223	97976.578	5733076.000	50.0215
2		19.323	67902.172	5728135.500	49.9784
Total			165878.750	11461211.500	100.0000



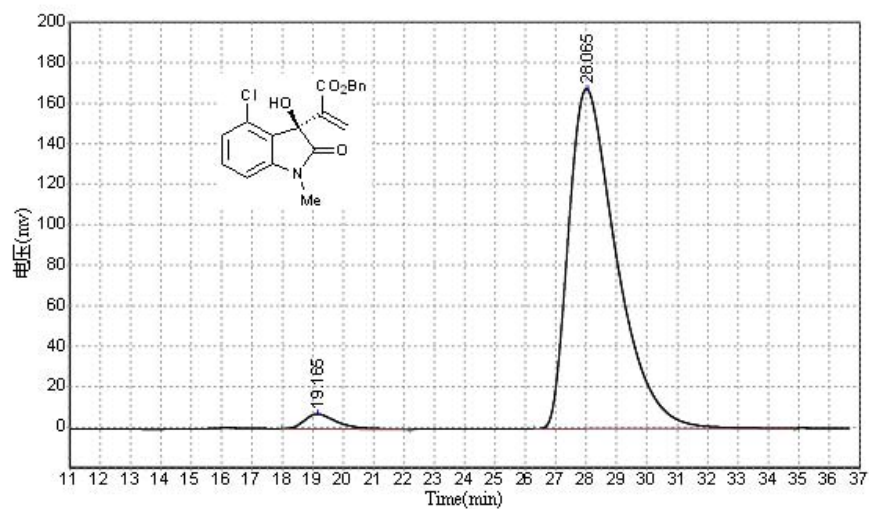
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.332	20620.146	1214902.500	6.0197
2		19.082	222999.141	18967322.000	93.9803
Total			243619.287	20182224.500	100.0000



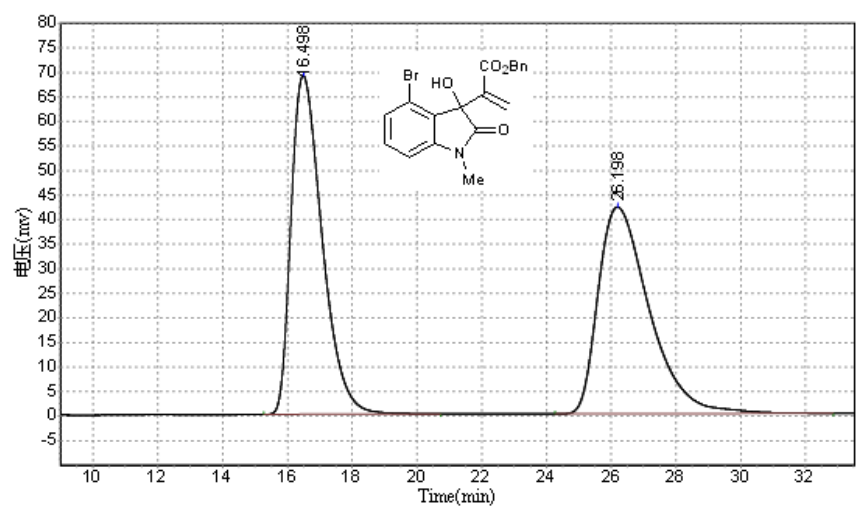
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		18.932	149358.656	10595534.000	49.2213
2		28.132	97143.359	10930805.000	50.7787
Total			246502.016	21526339.000	100.0000



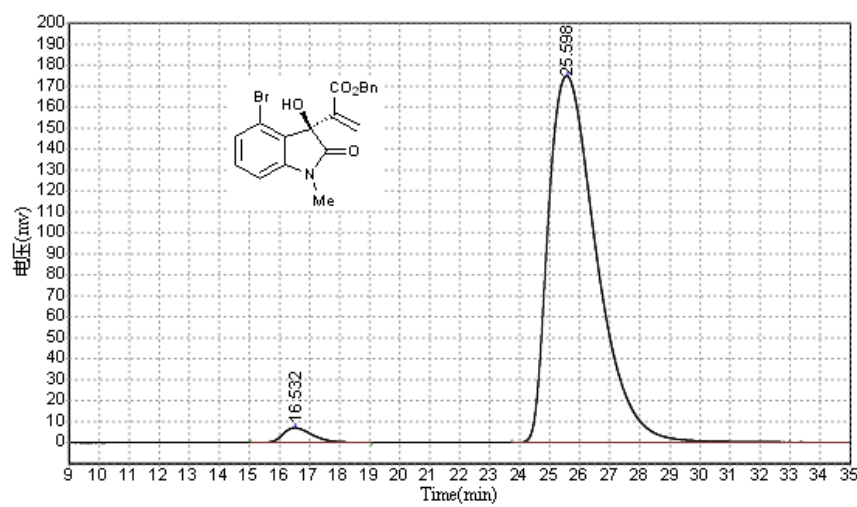
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		19.165	7469.940	569384.375	3.0068
2		28.065	167870.063	18367192.000	96.9932
Total			175340.003	18936576.375	100.0000



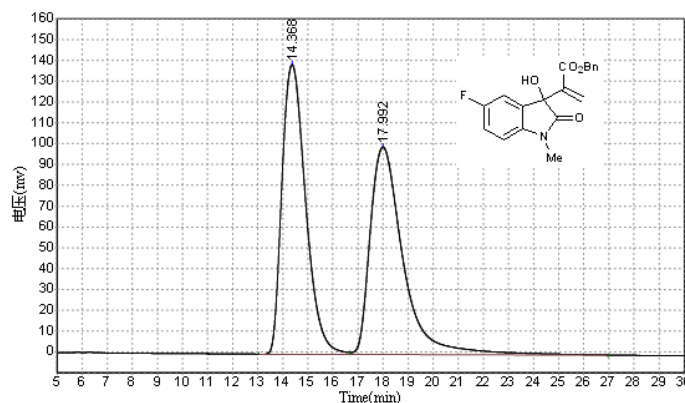
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		16.498	69075.609	4626191.500	50.0385
2		26.198	42061.504	4619074.000	49.9615
Total			111137.113	9245265.500	100.0000

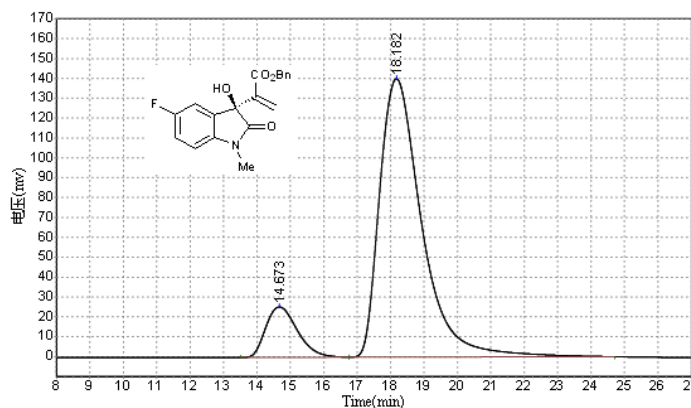


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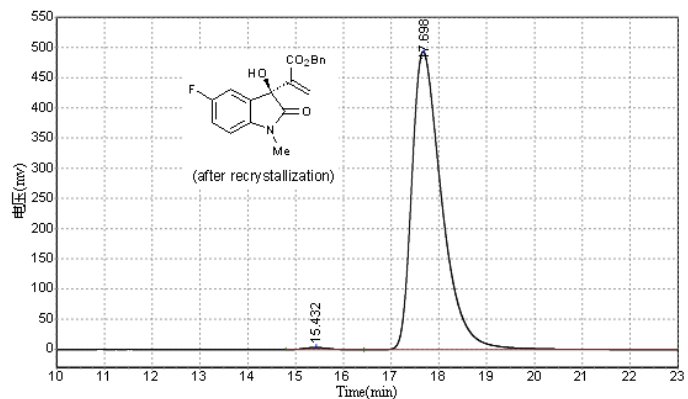
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		16.532	6973.661	471321.688	2.3800
2		25.598	174833.109	19332270.000	97.6200
Total			181806.771	19803591.688	100.0000



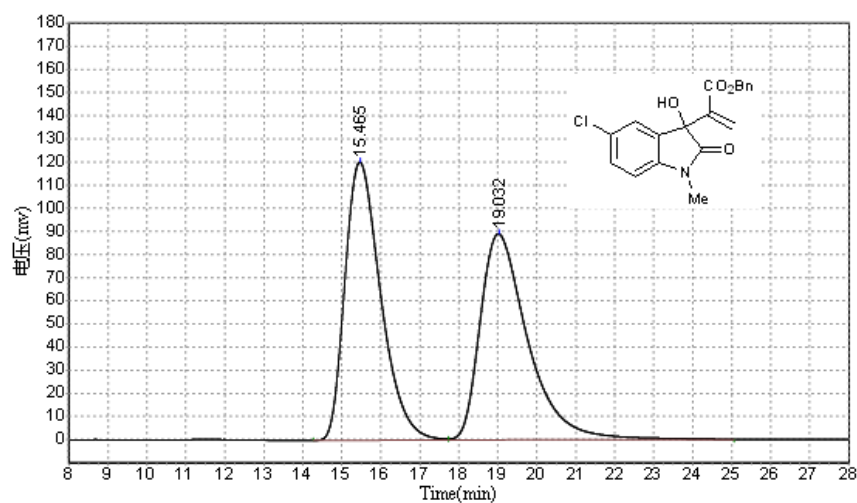
Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.368	139192.734	9099970.000	49.9913
2		17.992	99661.984	9103144.000	50.0087
Total			238854.719	18203114.000	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.673	25445.666	1672743.875	12.0224
2		18.182	140073.000	12240760.000	87.9775
Total			165518.666	13913503.875	100.0000

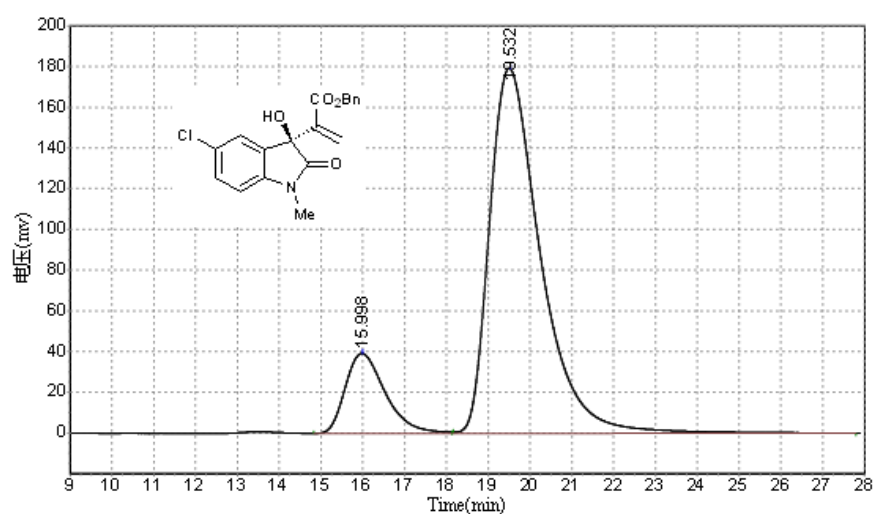


Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		15.432	3736.918	131980.906	0.6101
2		17.698	493424.844	21502210.000	99.3899
Total			497161.762	21634190.906	100.0000



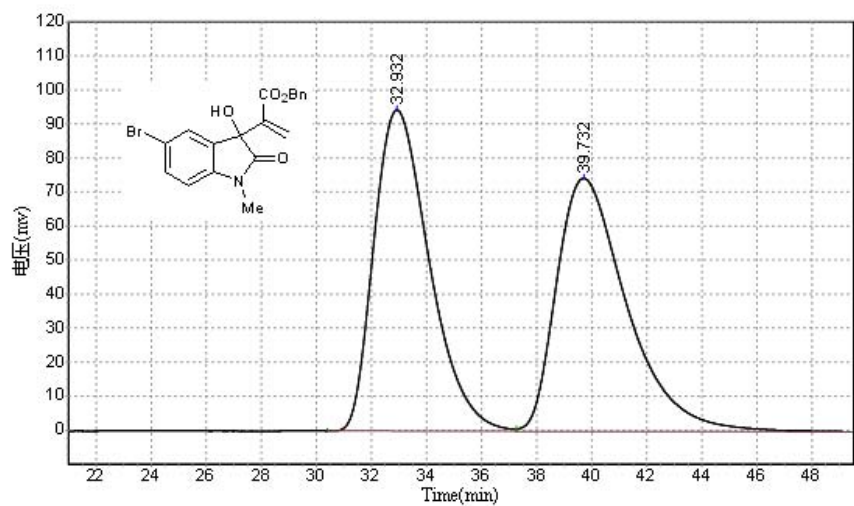
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		15.465	120231.055	7668881.000	50.1151
2		19.032	89148.063	7633644.000	49.8849
Total			209379.117	15302525.000	100.0000

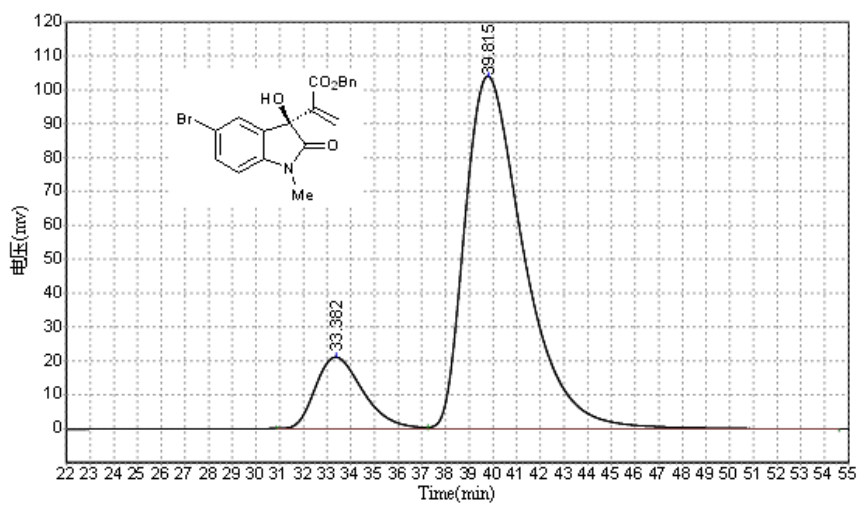


Results

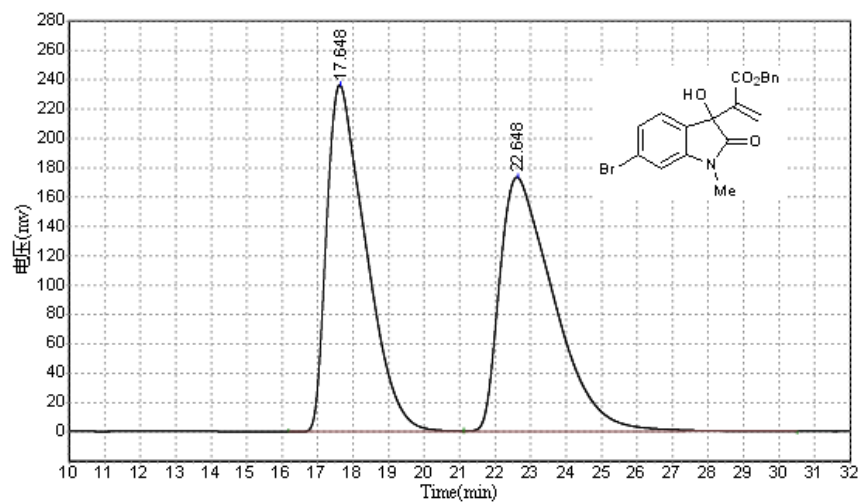
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		15.998	39354.973	2613811.250	14.6935
2		19.532	179372.469	15175131.000	85.3065
Total			218727.441	17788942.250	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		32.932	94444.789	13230509.000	50.0118
2		39.732	74425.242	13224276.000	49.9882
Total			168870.031	26454785.000	100.0000

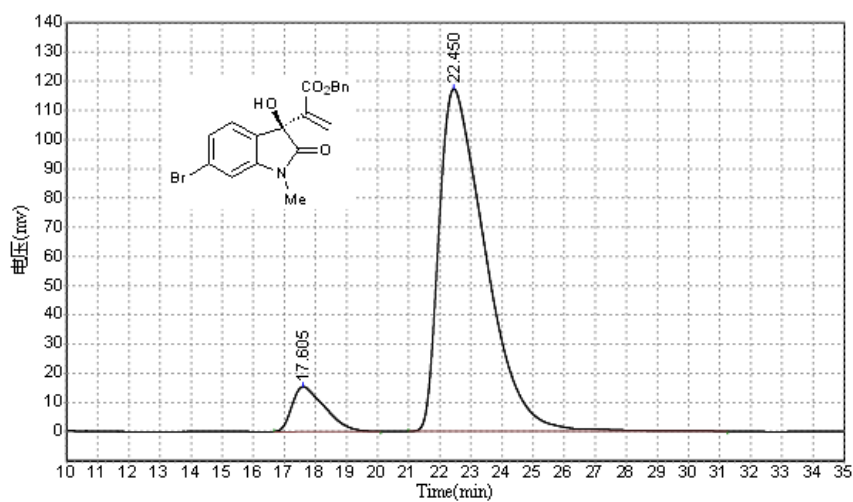


Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		33.382	21189.031	2959736.250	14.1061
2		39.815	104151.617	18022208.000	85.8939
Total			125340.648	20981944.250	100.0000



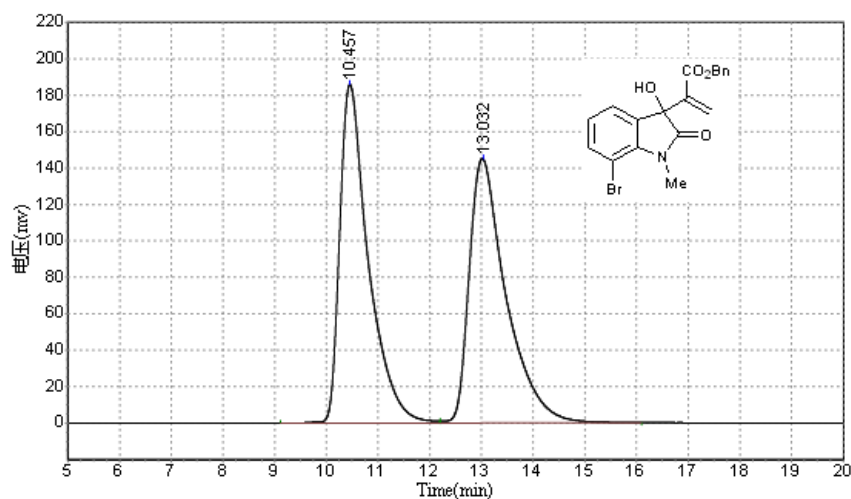
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		17.648	236411.328	18150110.000	49.5287
2		22.648	173465.969	18495516.000	50.4713
Total			409877.297	36645626.000	100.0000



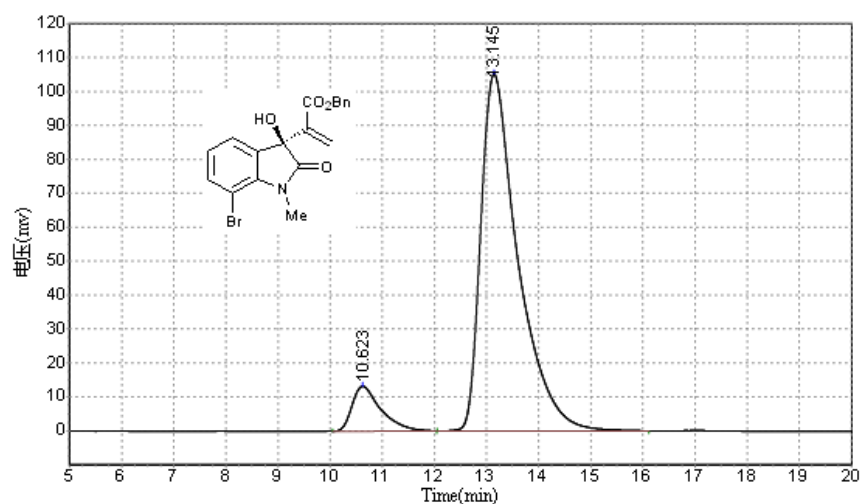
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		17.605	15442.905	1125423.875	8.4687
2		22.450	117371.563	12163828.000	91.5313
Total			132814.468	13289251.875	100.0000



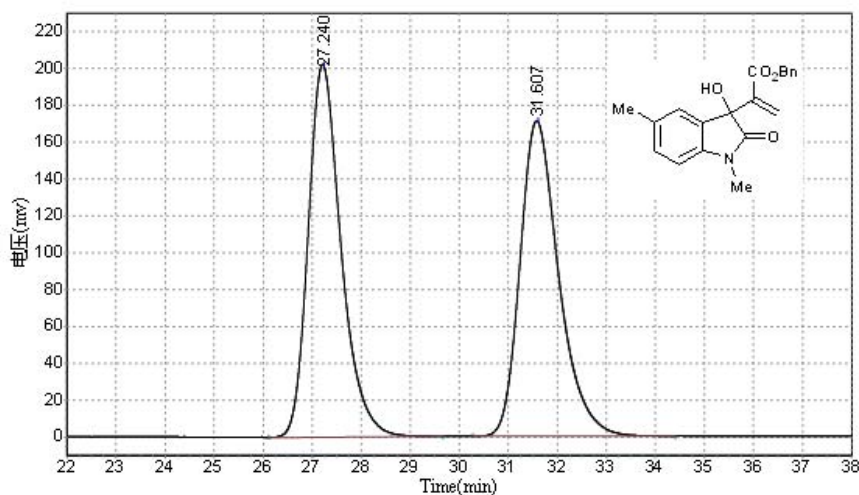
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		10.457	186050.813	7147039.000	49.7175
2		13.032	145308.656	7228251.500	50.2825
Total			331359.469	14375290.500	100.0000

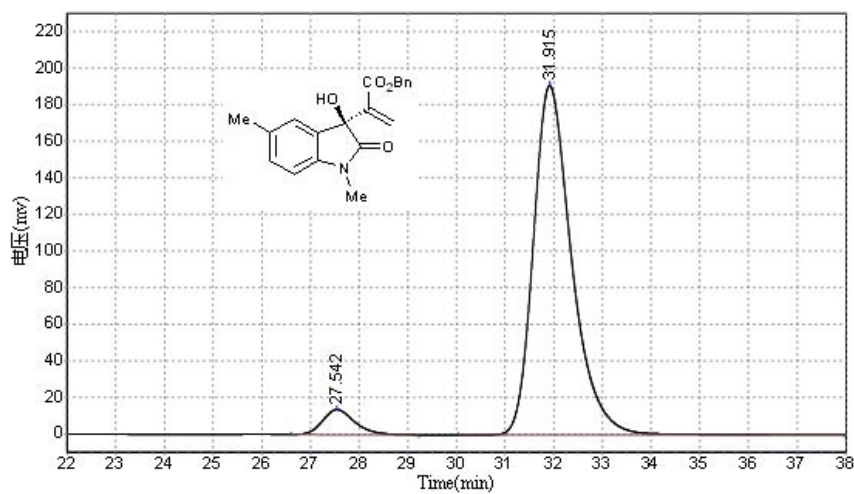


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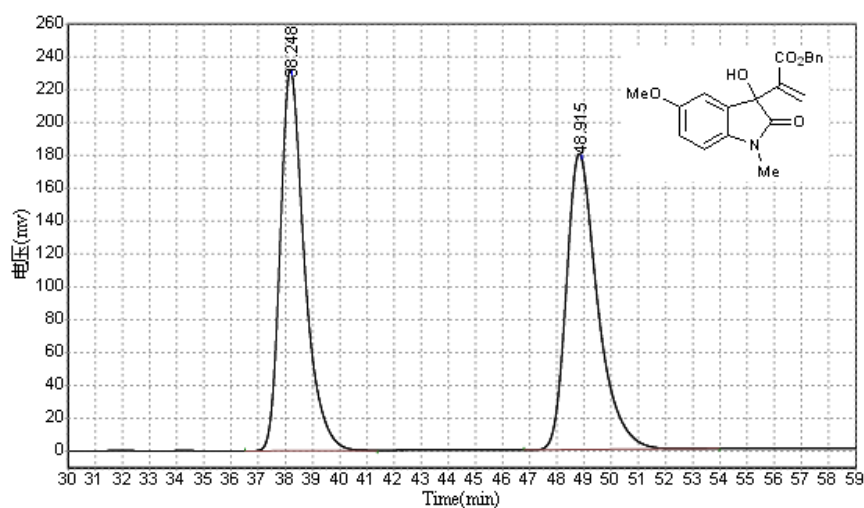
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		10.623	13278.778	507845.125	8.8864
2		13.145	105208.398	5207043.000	91.1136
Total			118487.177	5714888.125	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		27.240	202082.938	9436402.000	50.0973
2		31.607	171120.141	9399759.000	49.9027
Total			373203.078	18836161.000	100.0000

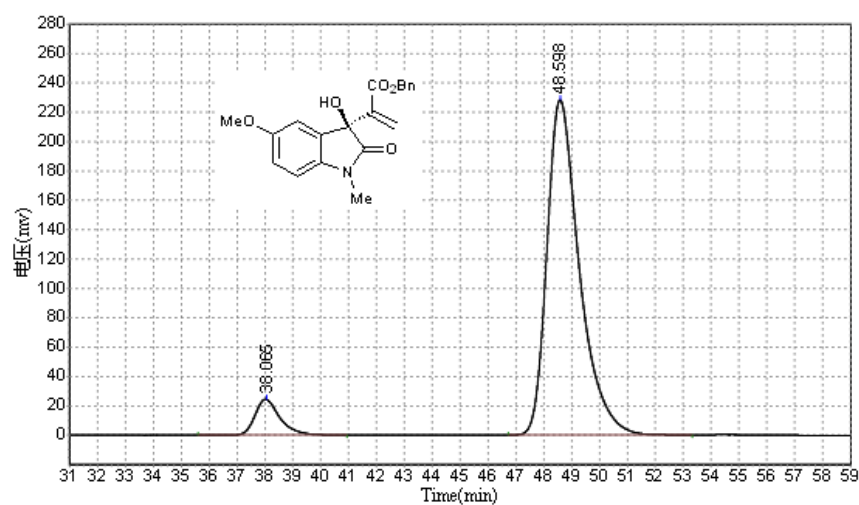


Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		27.542	13647.647	623203.250	5.6261
2		31.915	191149.703	10453784.000	94.3739
Total			204797.351	11076987.250	100.0000



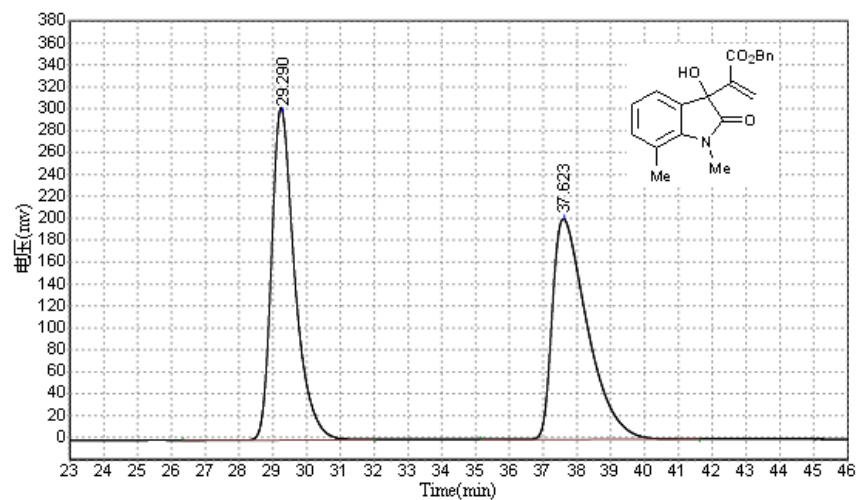
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		38.248	230748.391	14378258.000	49.8685
2		48.915	179338.297	14454069.000	50.1315
Total			410086.688	28832327.000	100.0000

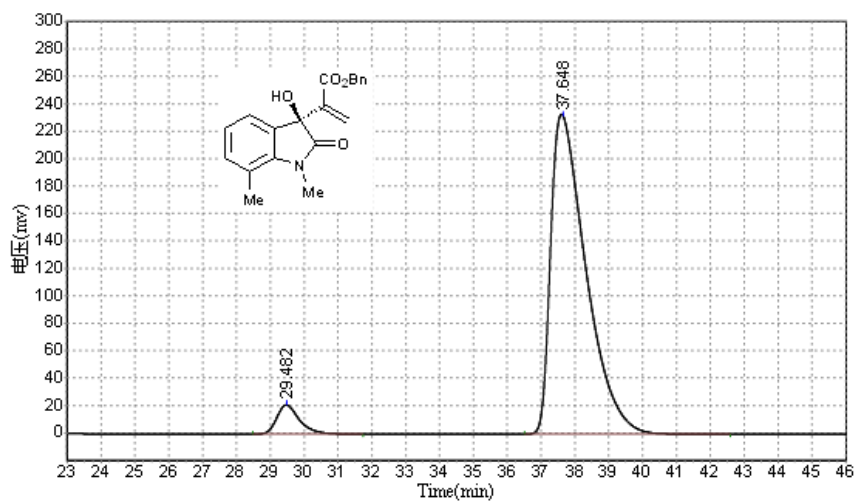


Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		38.065	24384.520	1508491.000	7.5418
2		48.598	228090.359	18493348.000	92.4582
Total			252474.879	20001839.000	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		29.290	302148.906	14462515.000	49.9029
2		37.623	201372.906	14518802.000	50.0971
Total			503521.813	28981317.000	100.0000



Results					
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		29.482	21326.793	1004682.563	5.6207
2		37.648	233115.438	16869930.000	94.3793
Total			254442.230	17874612.563	100.0000

7. Absolute Configuration and X-Ray Analysis Data of **6m**

The crystal data of **6m** have been deposited in CCDC with number 856997.

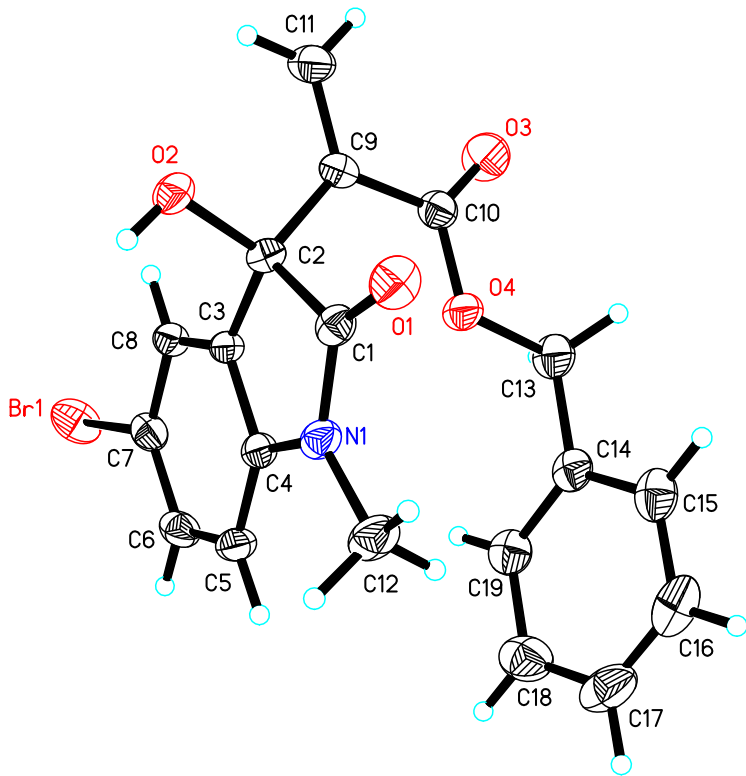


Table 1. Crystal data and structure refinement for cd211247.

Identification code	cd211247
Empirical formula	C ₁₉ H ₁₆ Br N O ₄
Formula weight	402.24
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 7.8115(7) Å alpha = 90 deg. b = 11.8206(11) Å beta = 90 deg. c = 18.4780(17) Å gamma = 90 deg.
Volume	1706.2(3) Å ³
Z, Calculated density	4, 1.566 Mg/m ³
Absorption coefficient	2.433 mm ⁻¹

F(000)	816
Crystal size	0.369 x 0.311 x 0.257 mm
Theta range for data collection	2.05 to 26.00 deg.
Limiting indices	-9<=h<=7, -14<=k<=14, -21<=l<=22
Reflections collected / unique	9218 / 3335 [R(int) = 0.0338]
Completeness to theta = 26.00	100.0 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.28748
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3335 / 0 / 229
Goodness-of-fit on F ²	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.0951
R indices (all data)	R1 = 0.0463, wR2 = 0.0989
Absolute structure parameter	0.002(12)
Extinction coefficient	0.128(4)
Largest diff. peak and hole	0.959 and -0.490 e.A ⁻³