Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Regio- and Enantioselective Ring-Opening Reaction of Vinylcyclopropanes with Indoles under Cooperative Catalysis

Xiao Wan,[a] Meng Sun,[a] Jing-Yi Wang,[a] Lei Yu,[a] Qiong Wu,*[b] Yu-Chen Zhang*[a] and Feng Shi*[a]

[a]*School of Chemistry and Materials Science, Jiangsu Normal University, Xuzhou, 221116, China.*

E-mail: fshi@jsnu.edu.cn; zhangyc@jsnu.edu.cn

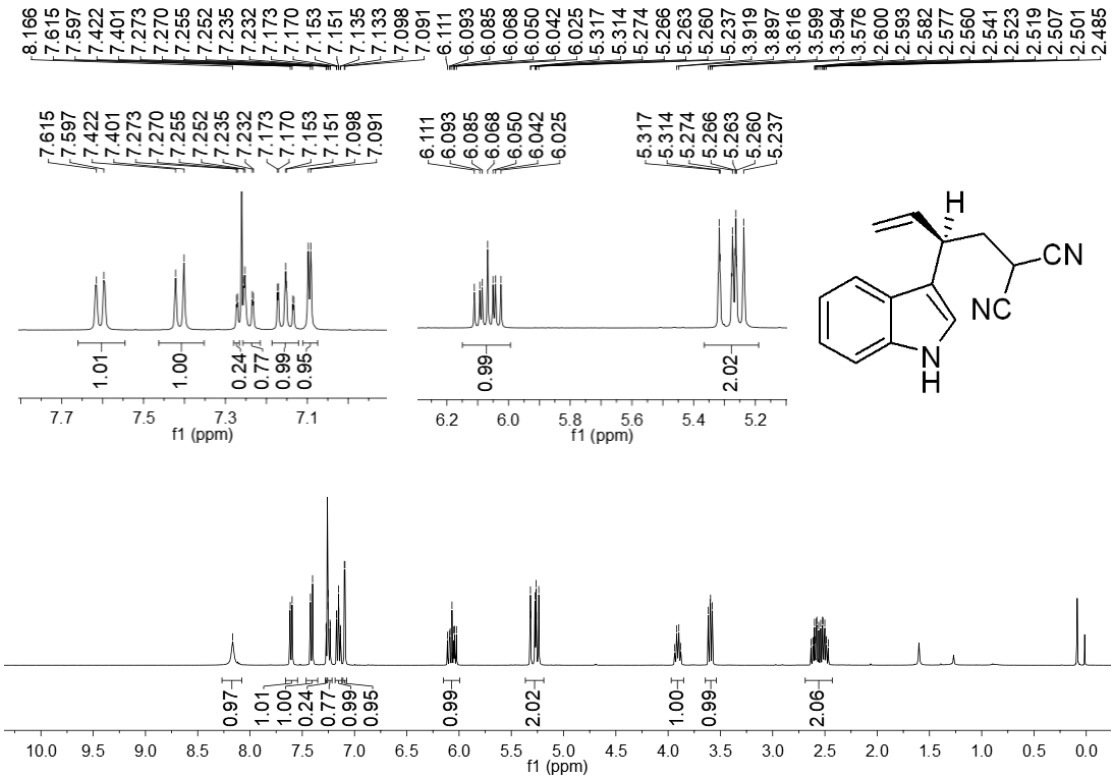
[b]*School of Materials and Chemical Engineering, Xuzhou University of Technology, Xuzhou*

221018, China. E-mail: hgwuqiong@xzit.edu.cn

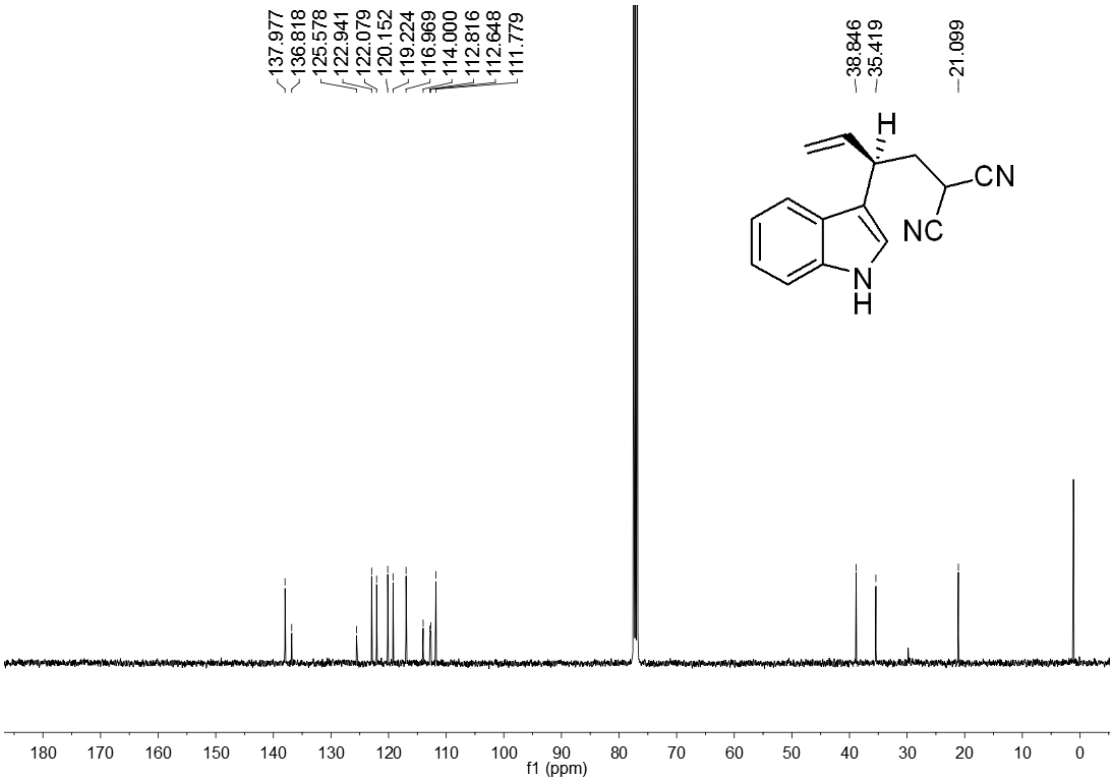
Contents:

1. NMR spectra of products 3 and 5-6

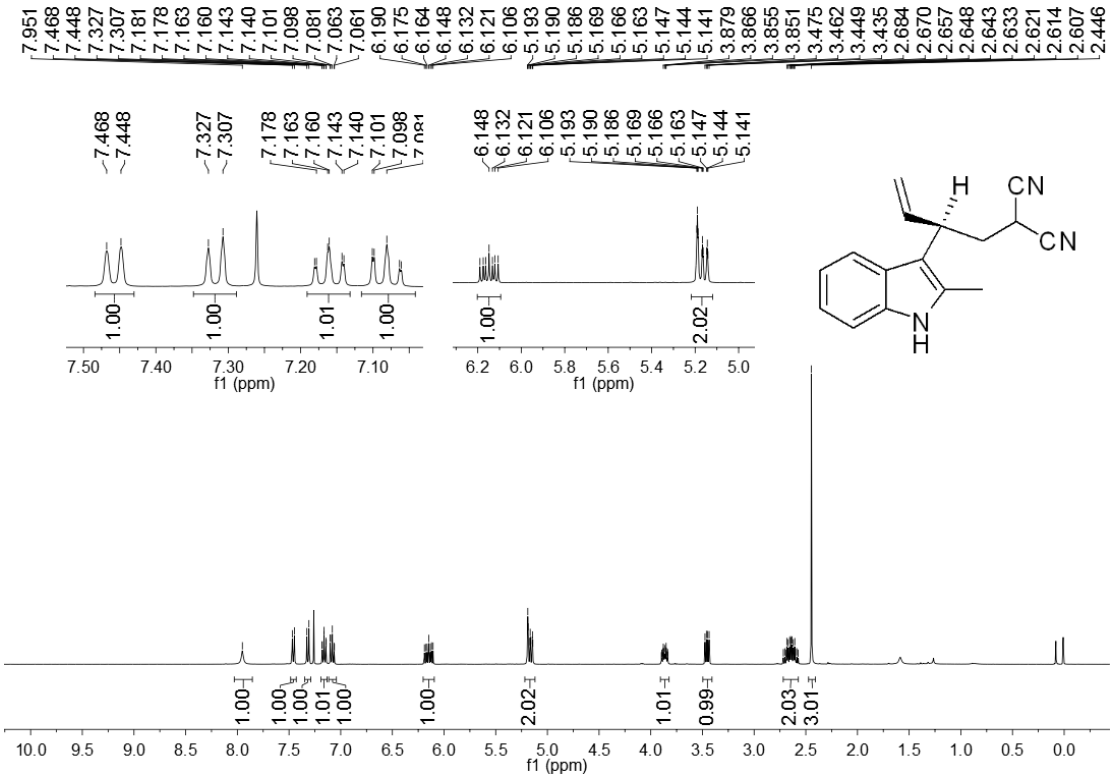
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa**



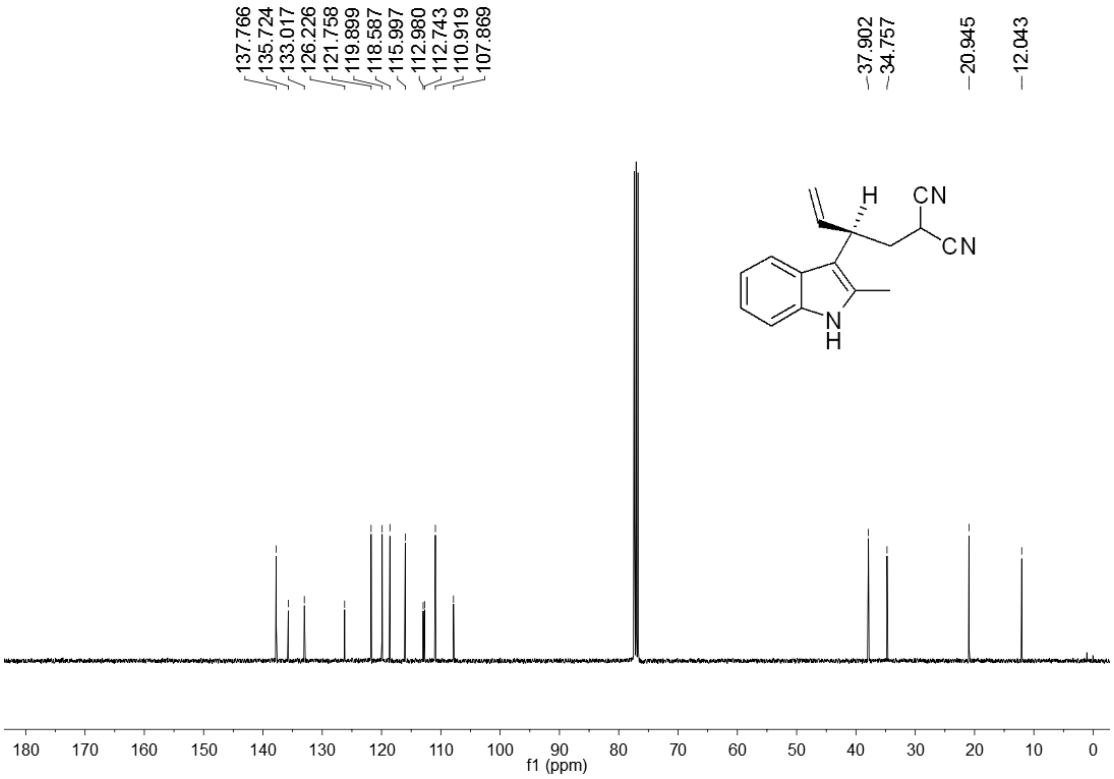
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aa**



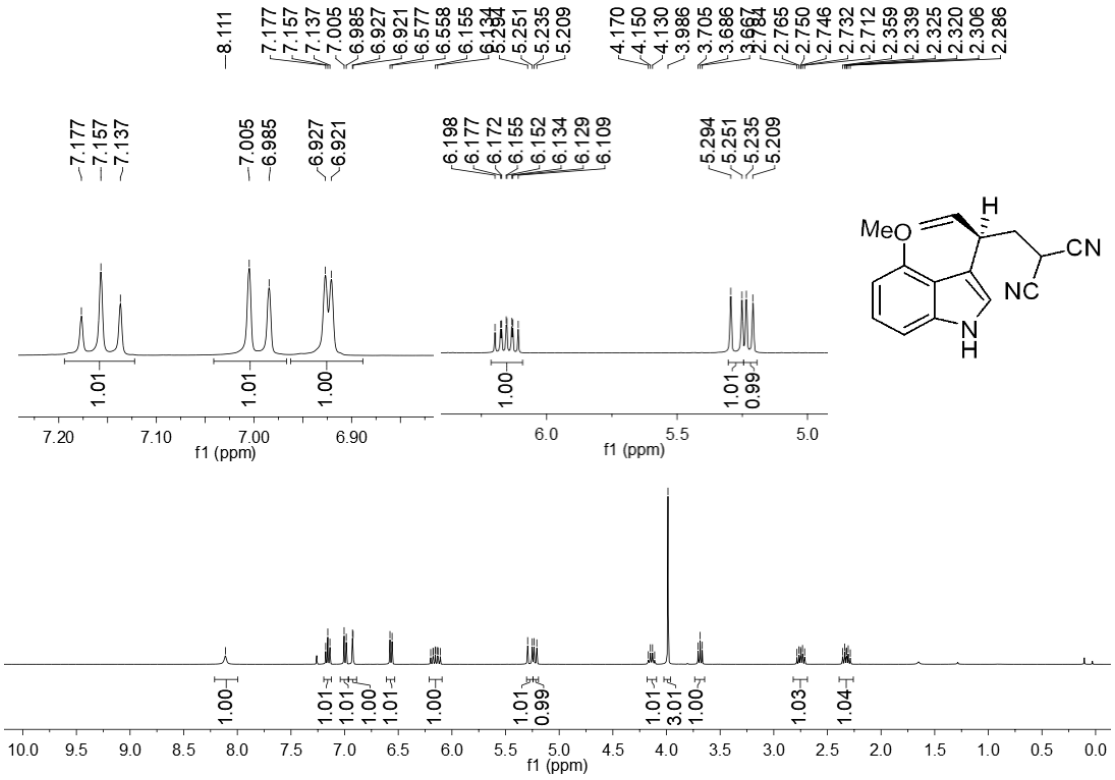
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ba**



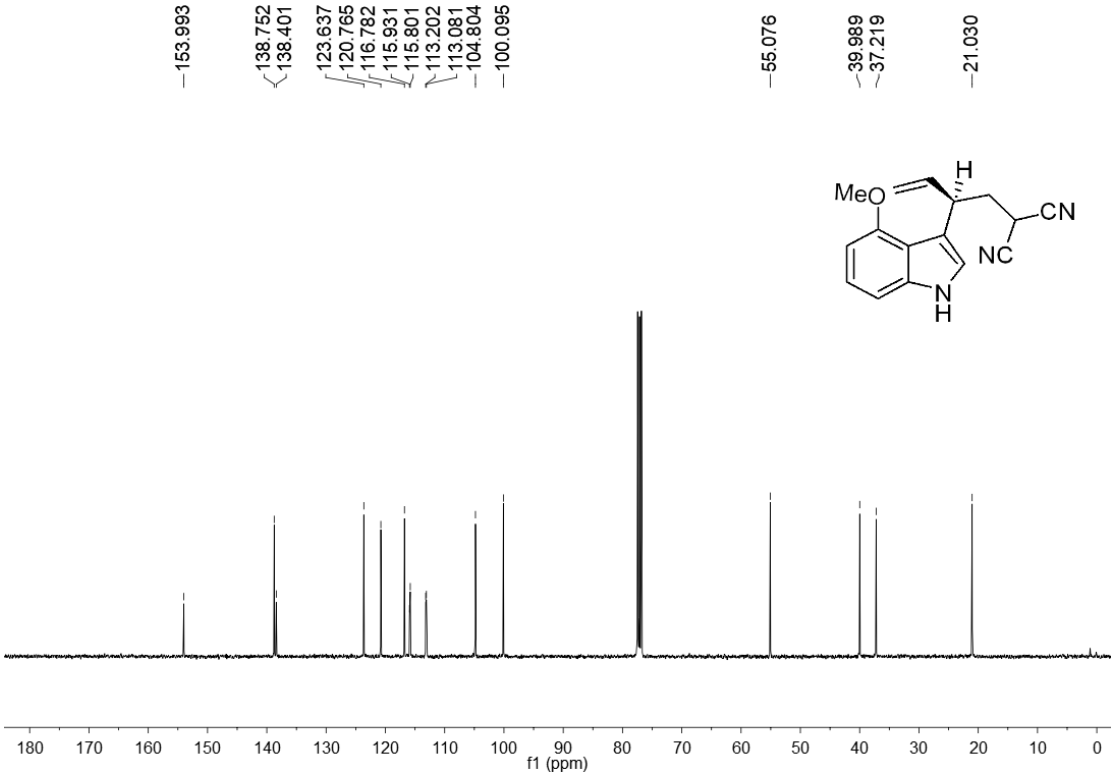
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ba**



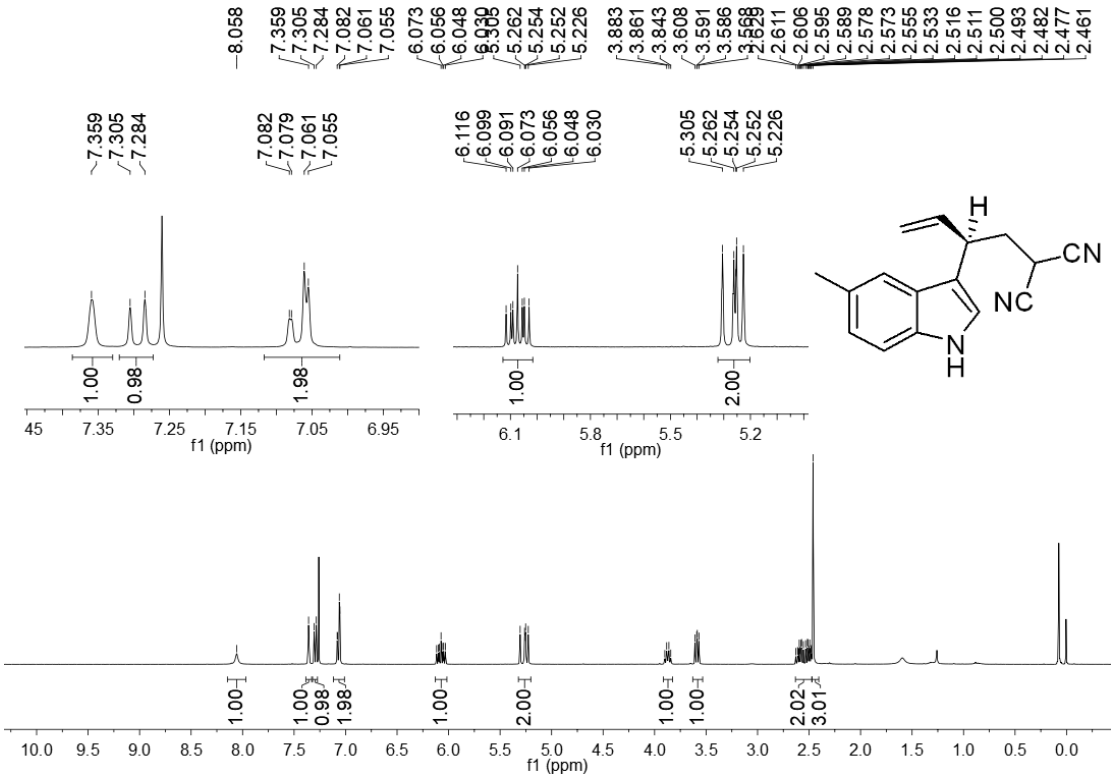
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ca**



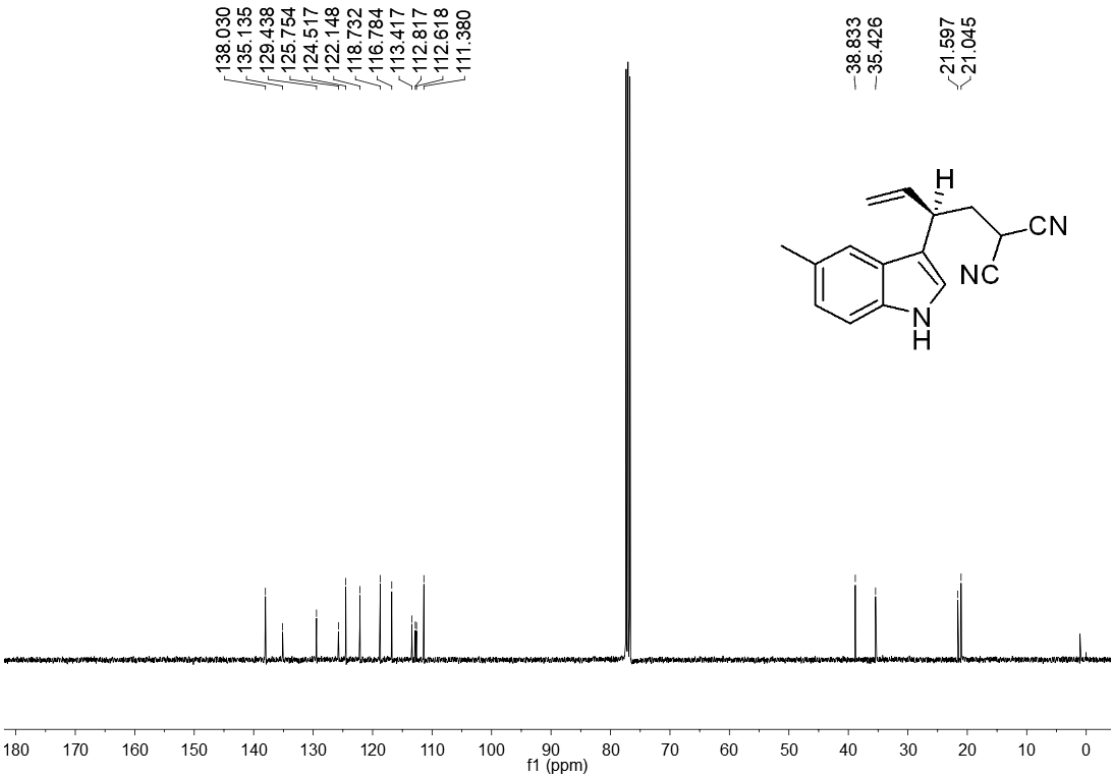
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ca**



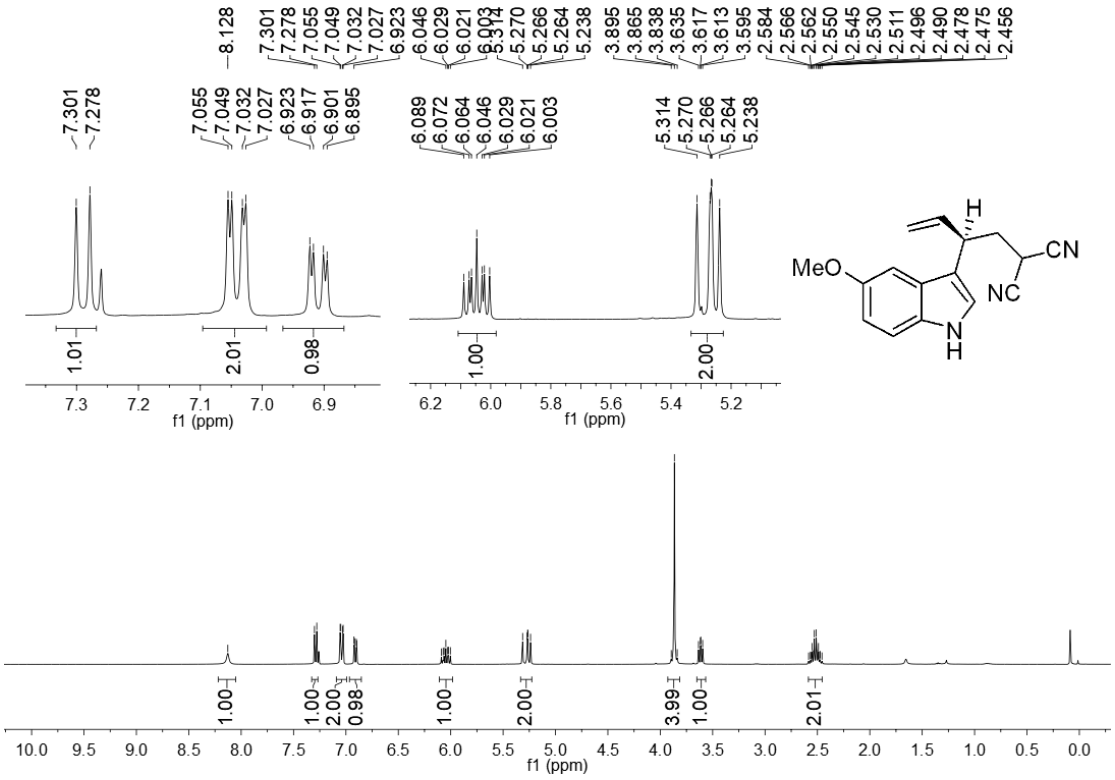
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3da**



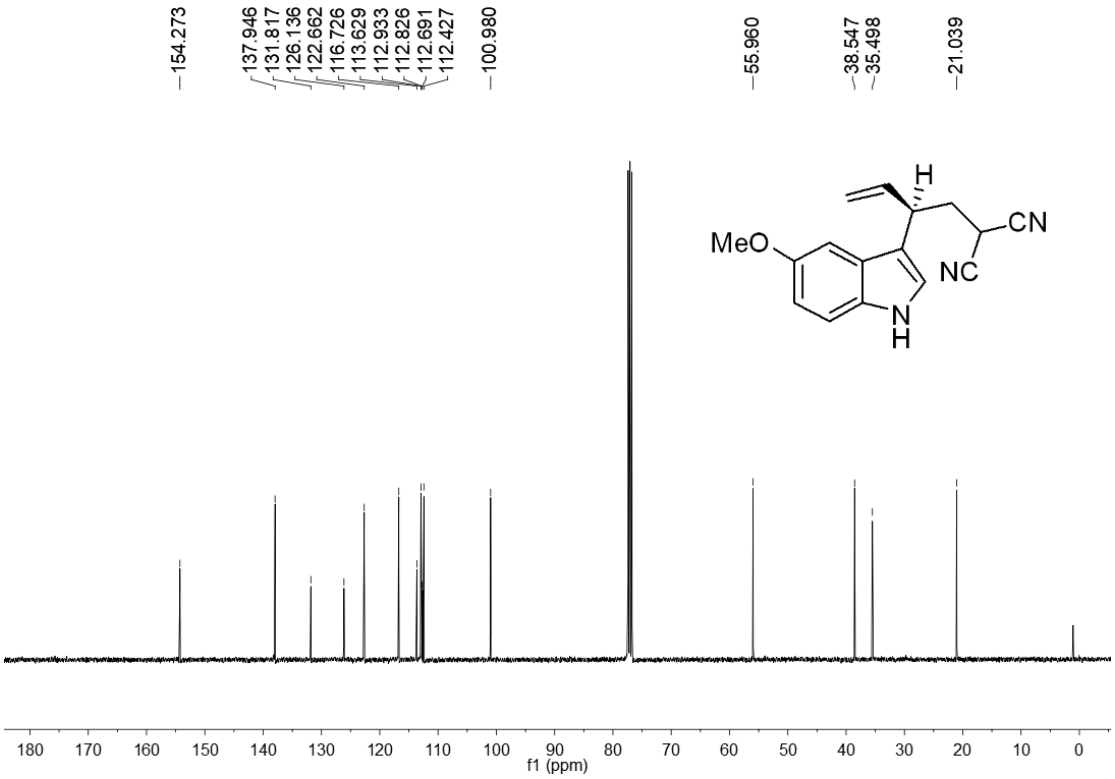
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3da**



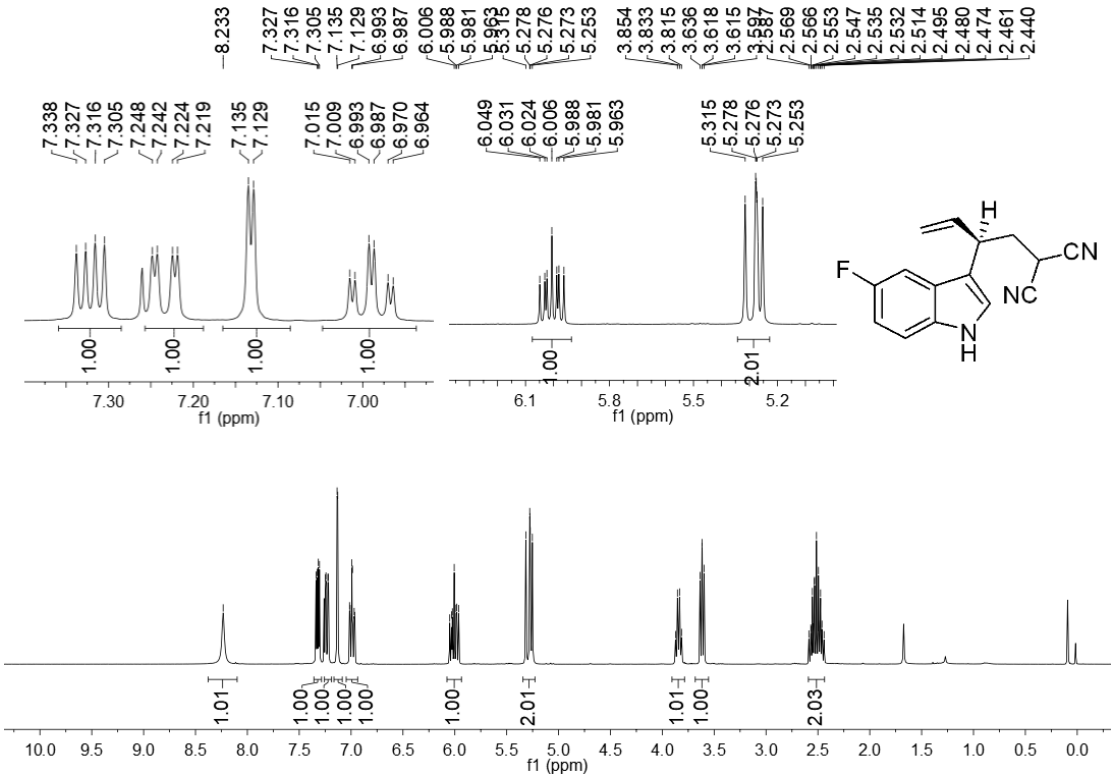
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ea**



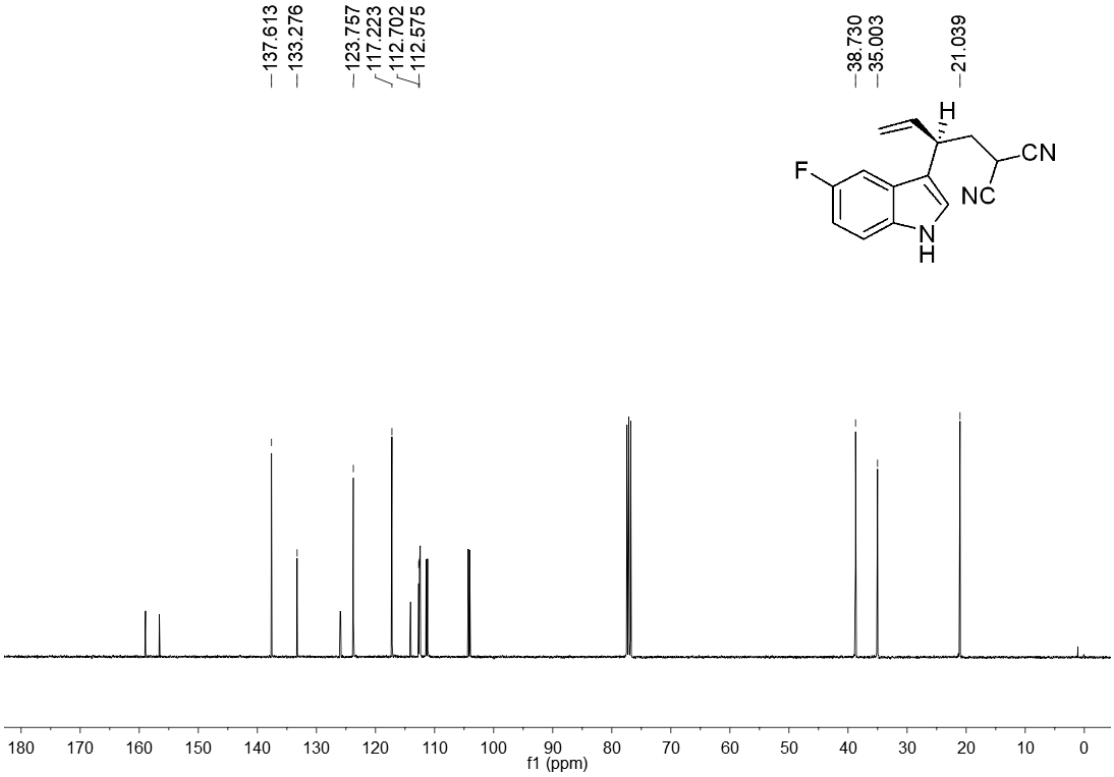
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ea**



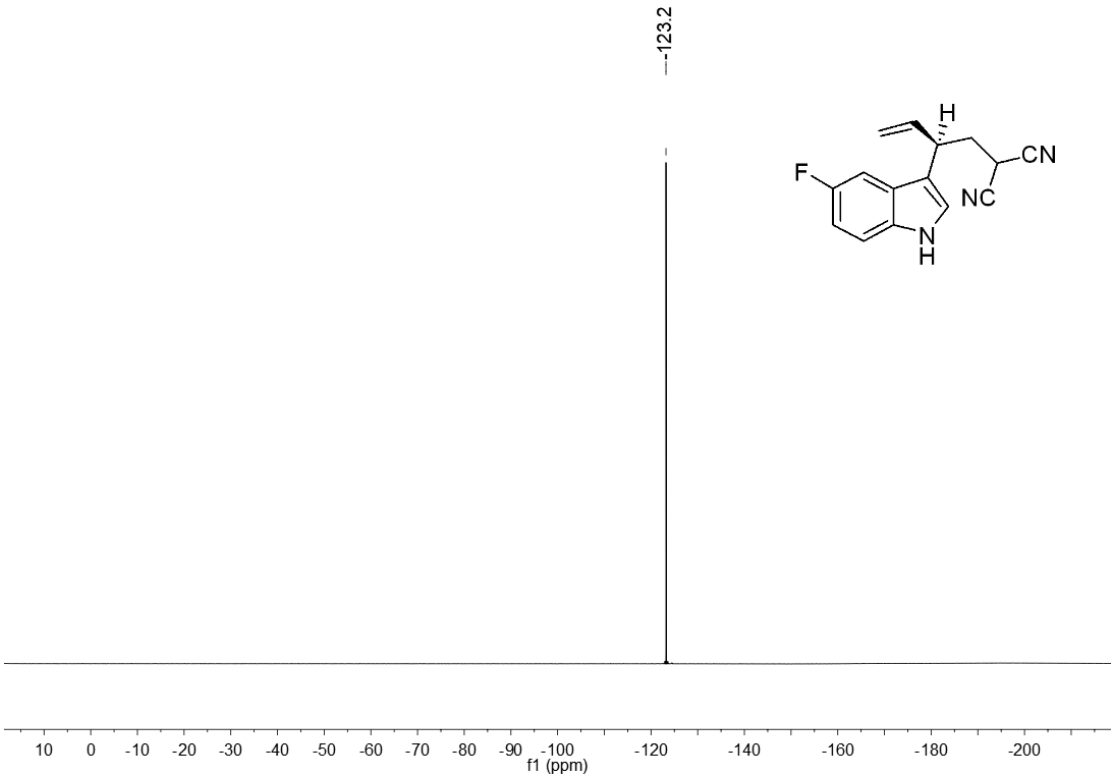
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3fa**



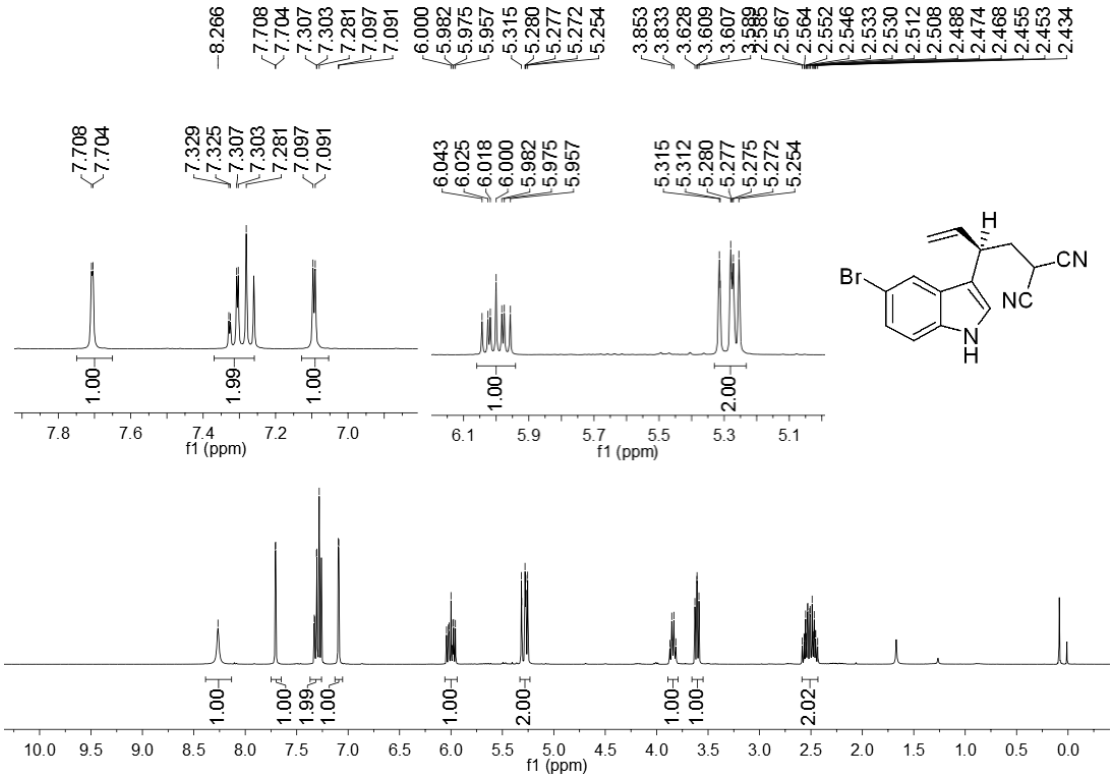
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3fa**



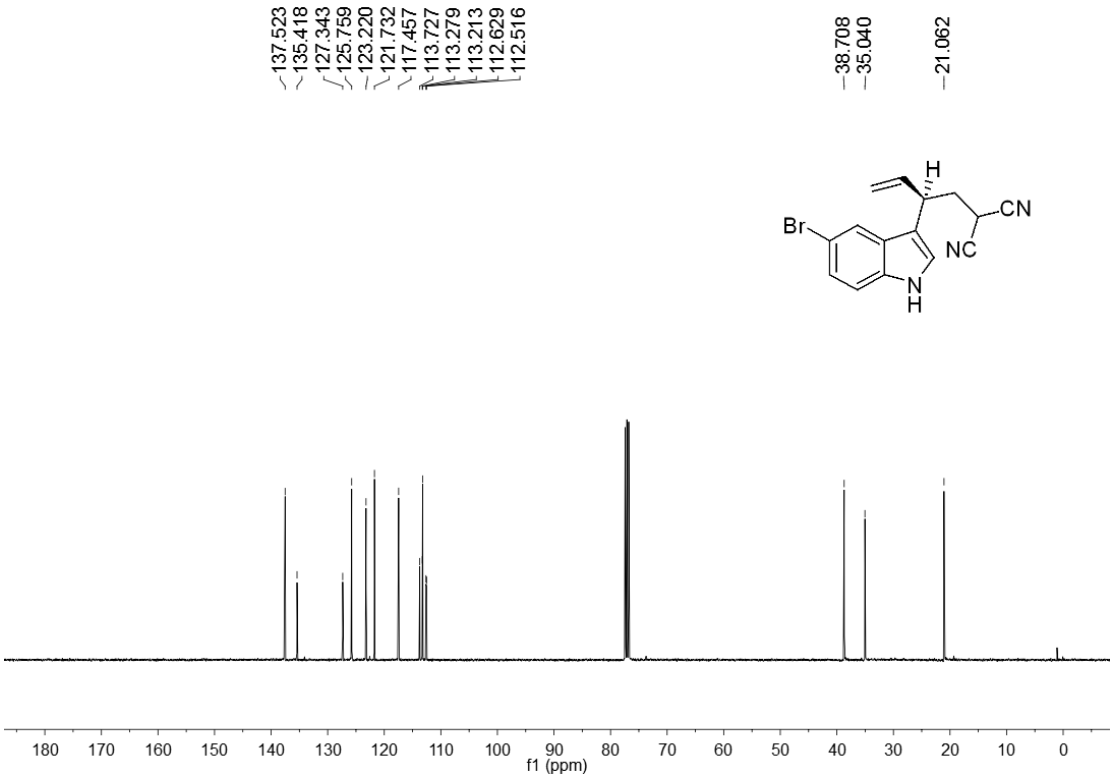
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3fa**



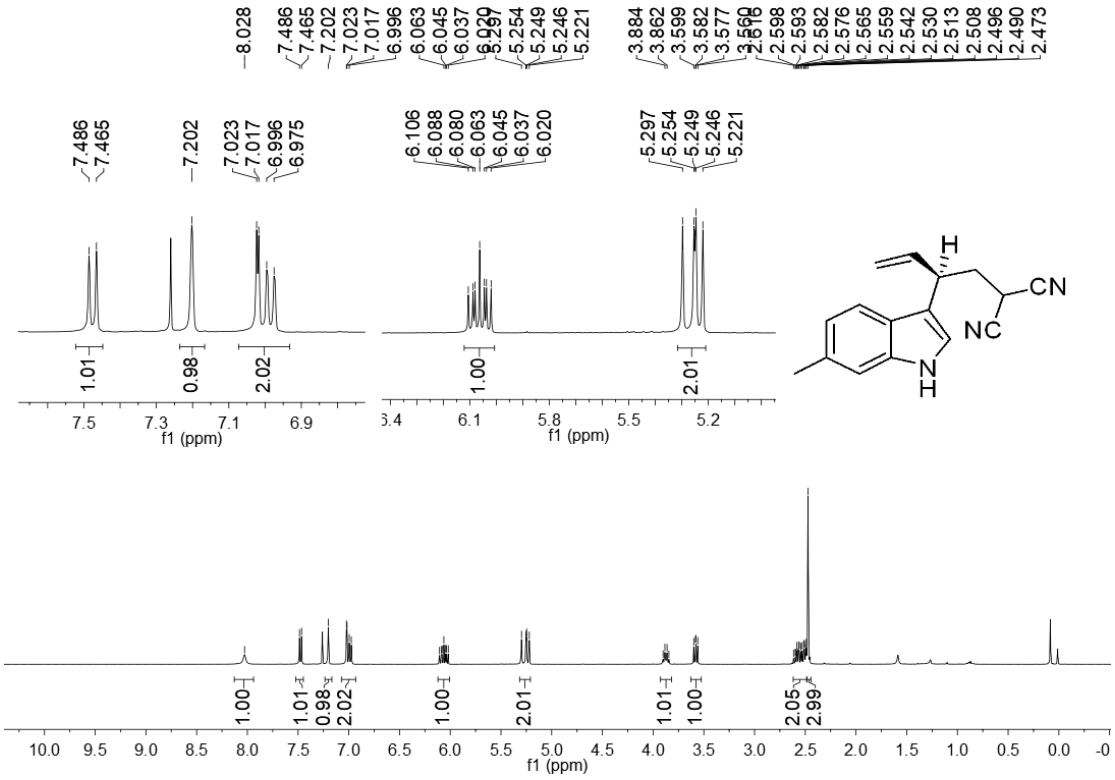
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ga**



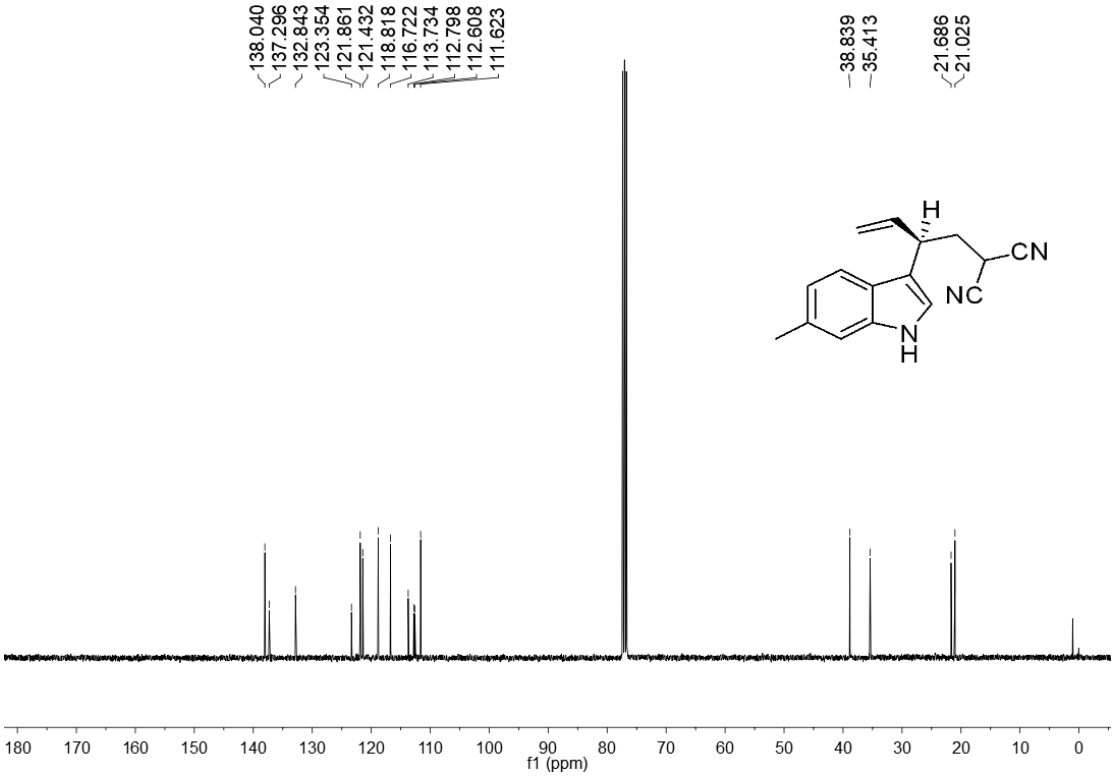
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ga**



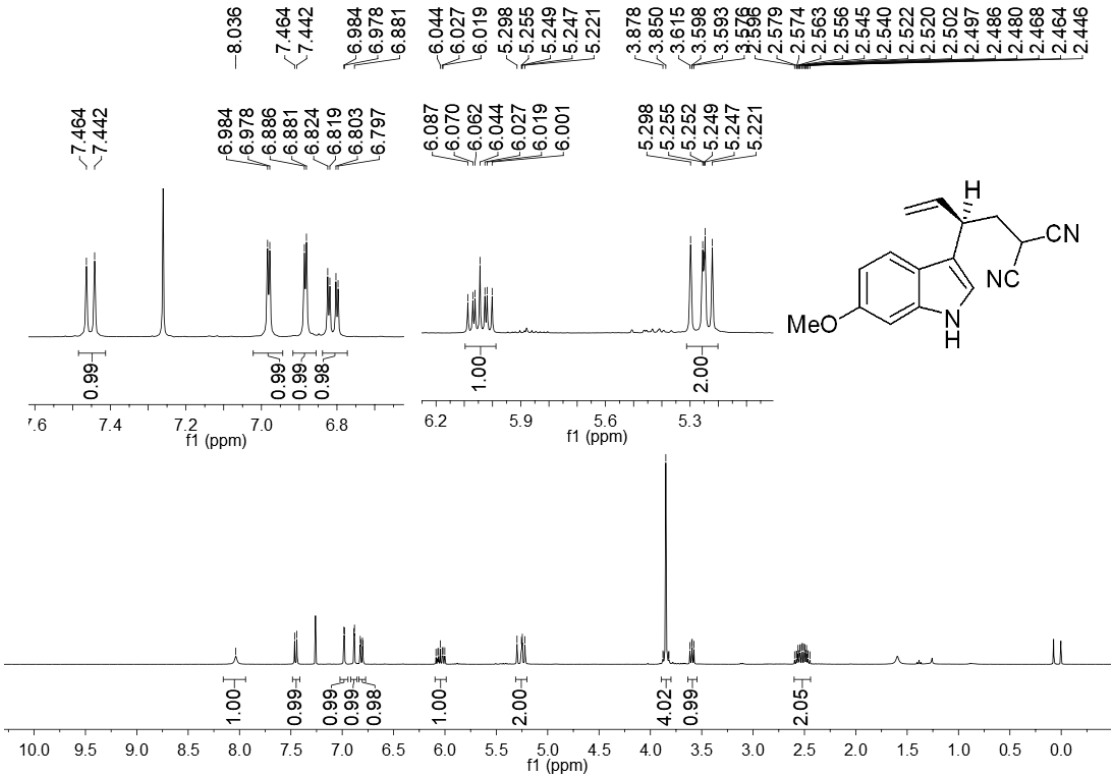
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ha**



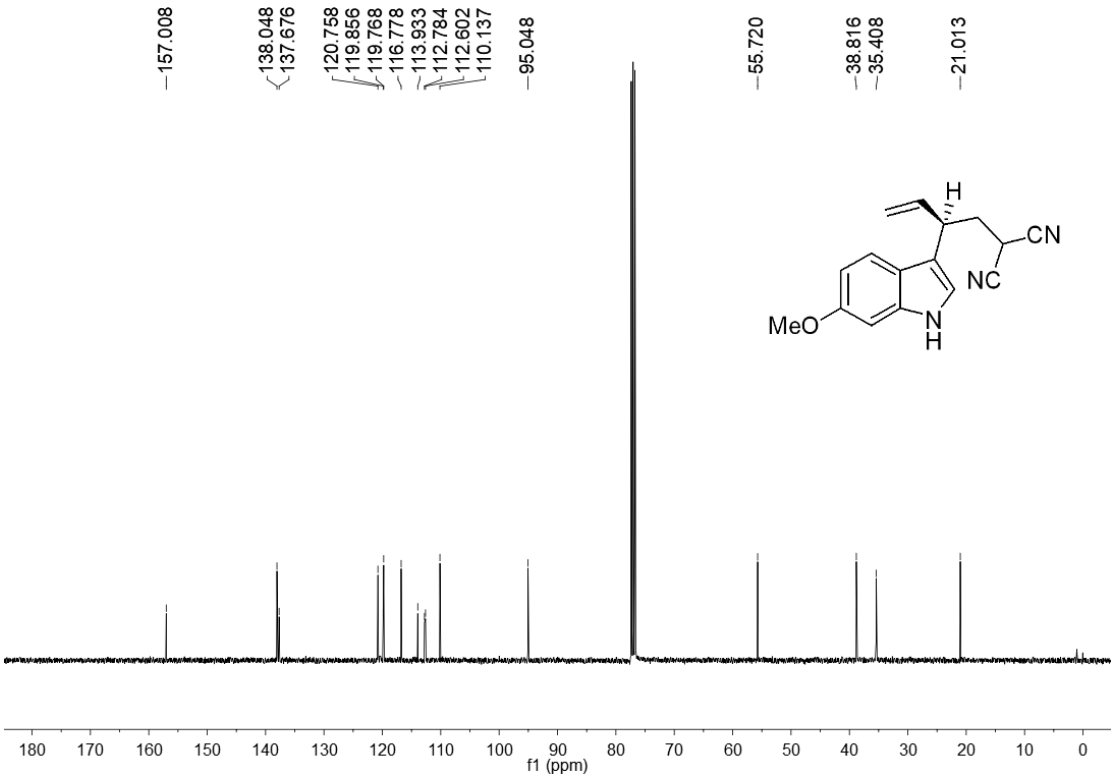
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ha**



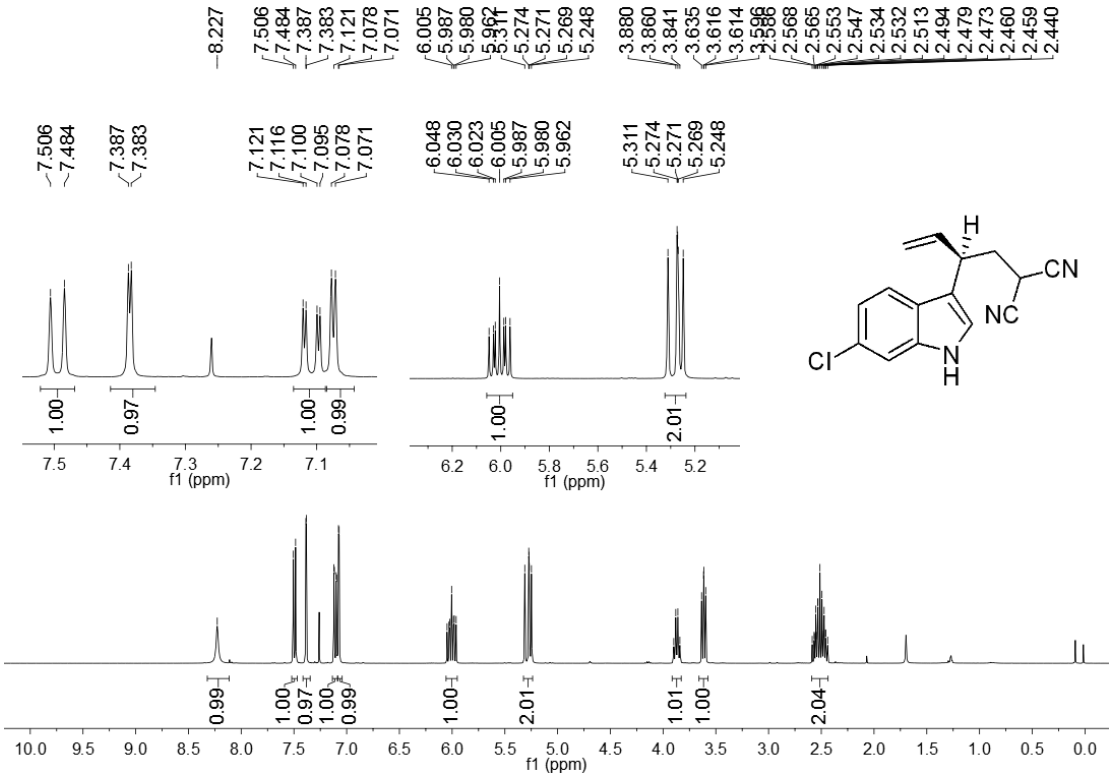
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ia**



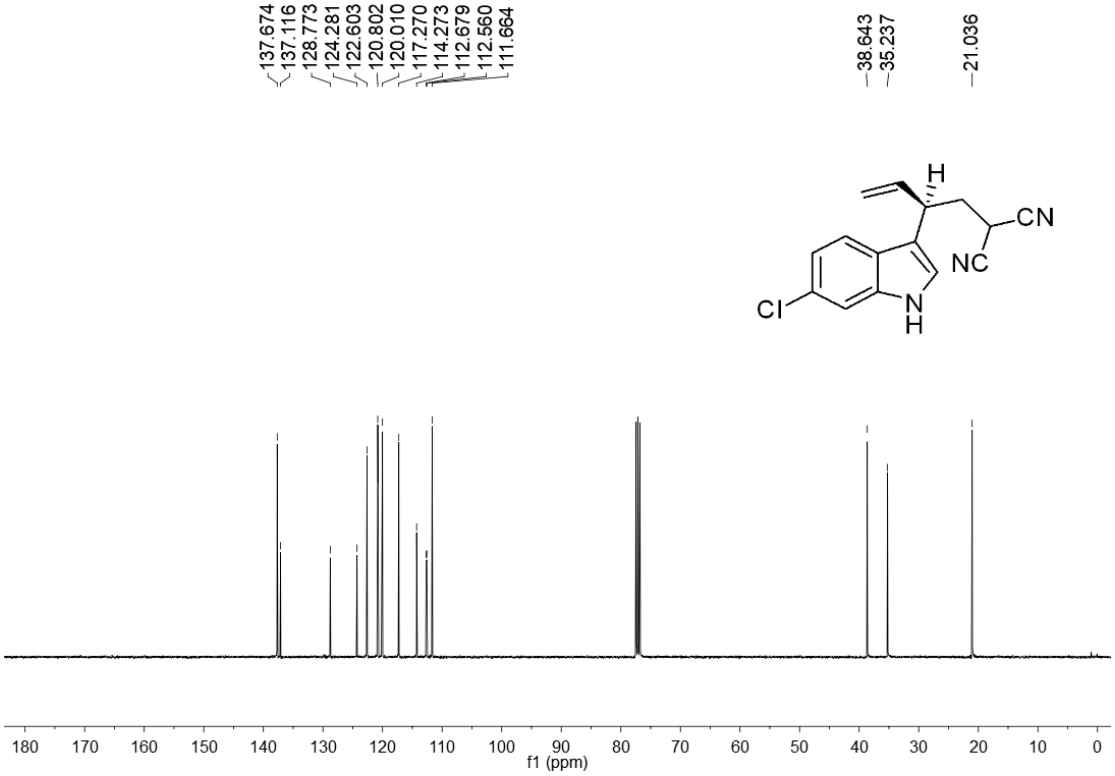
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ia**



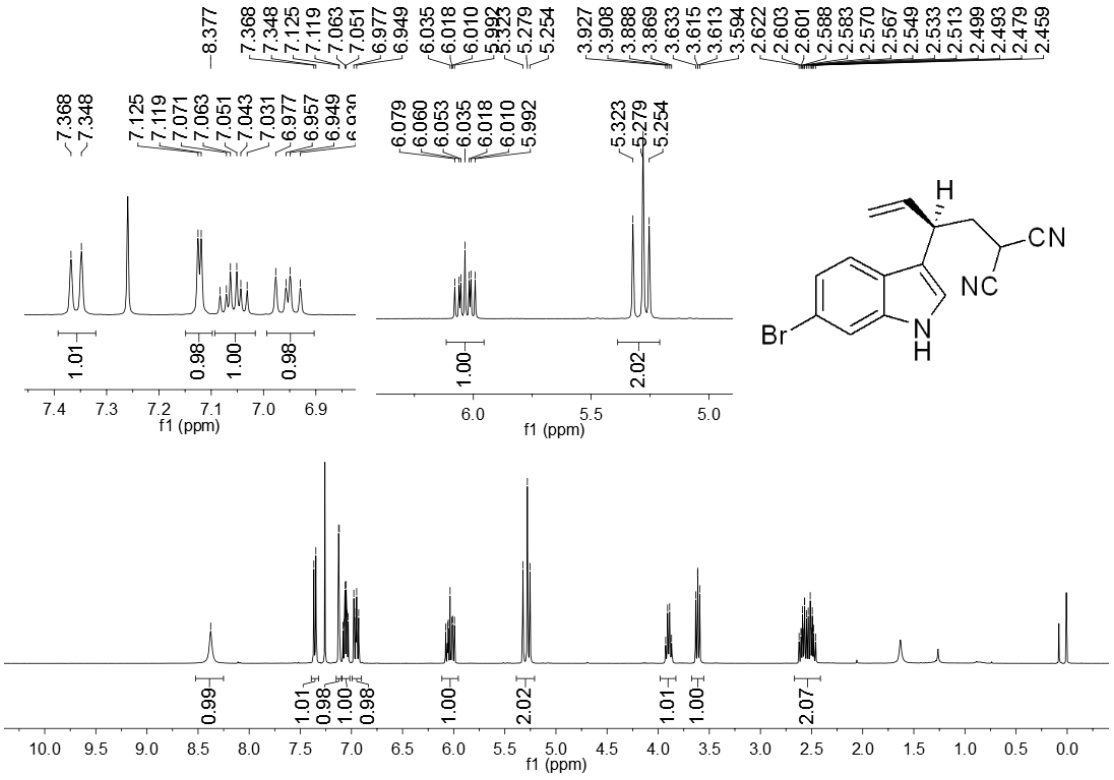
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ja**



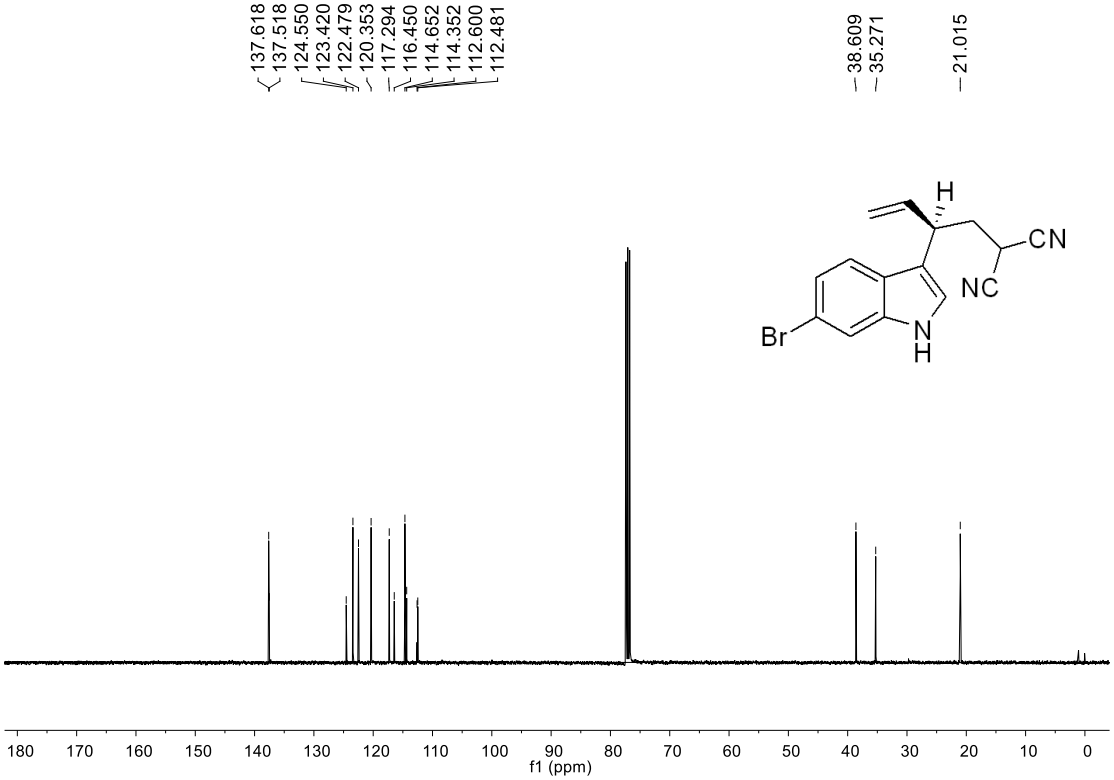
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ja**



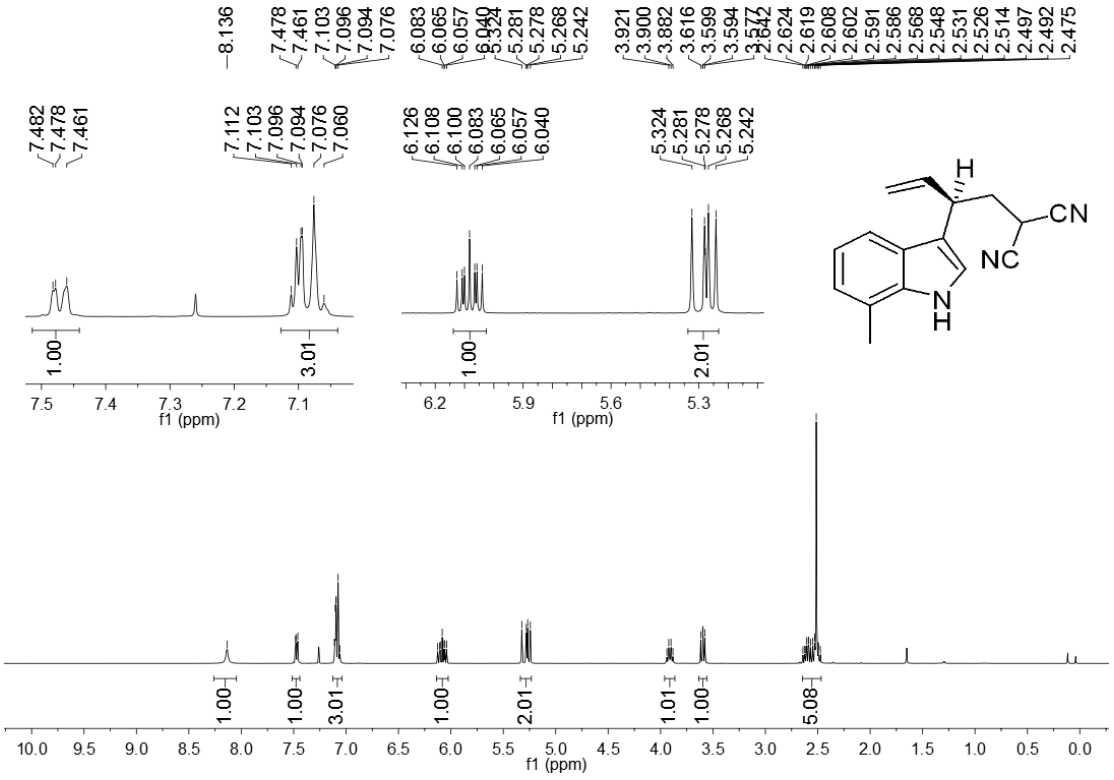
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ka**



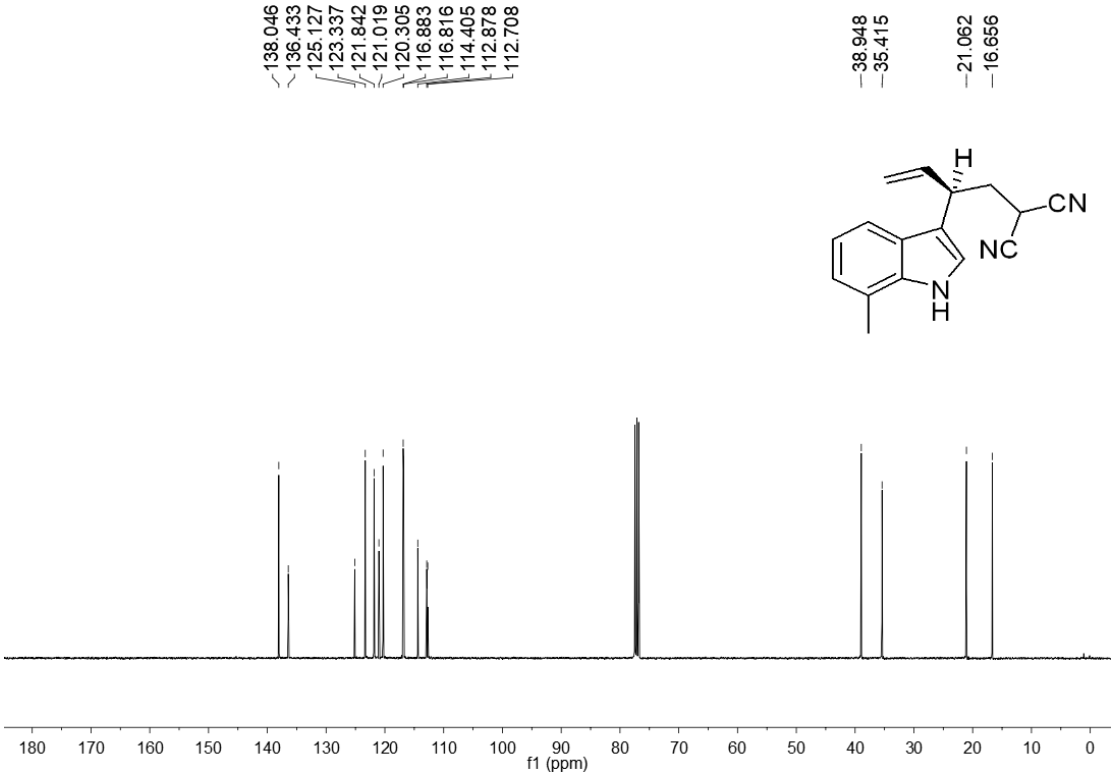
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ka**



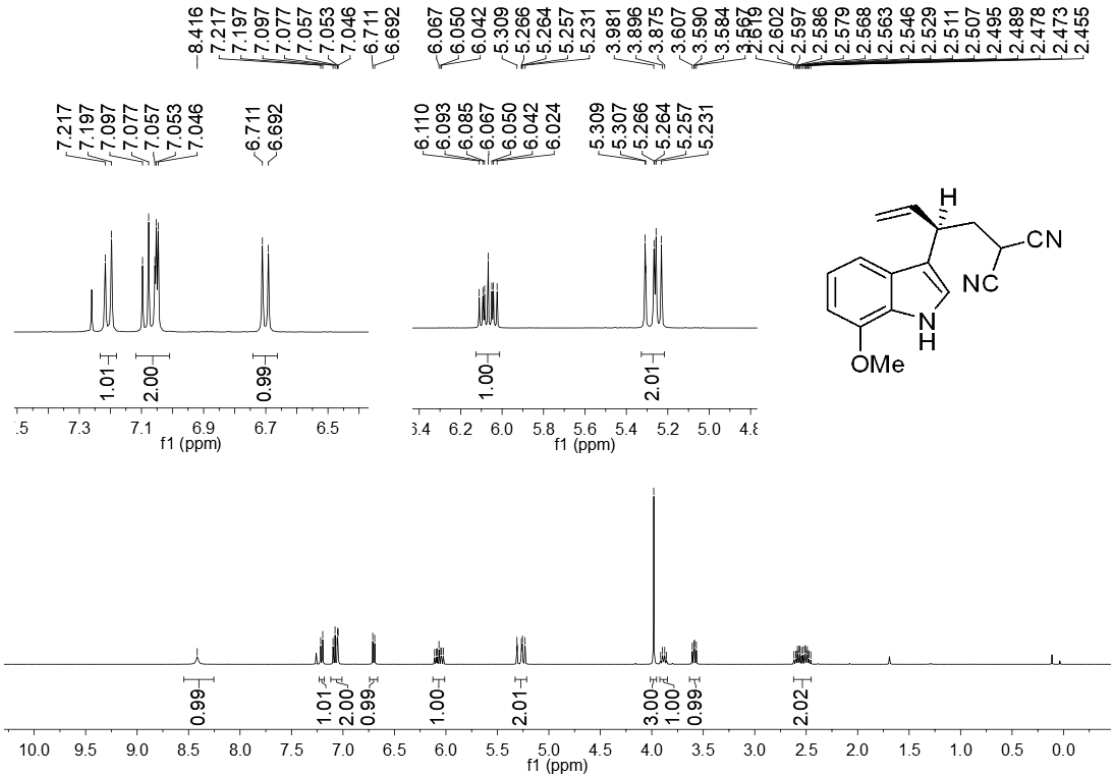
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3la**



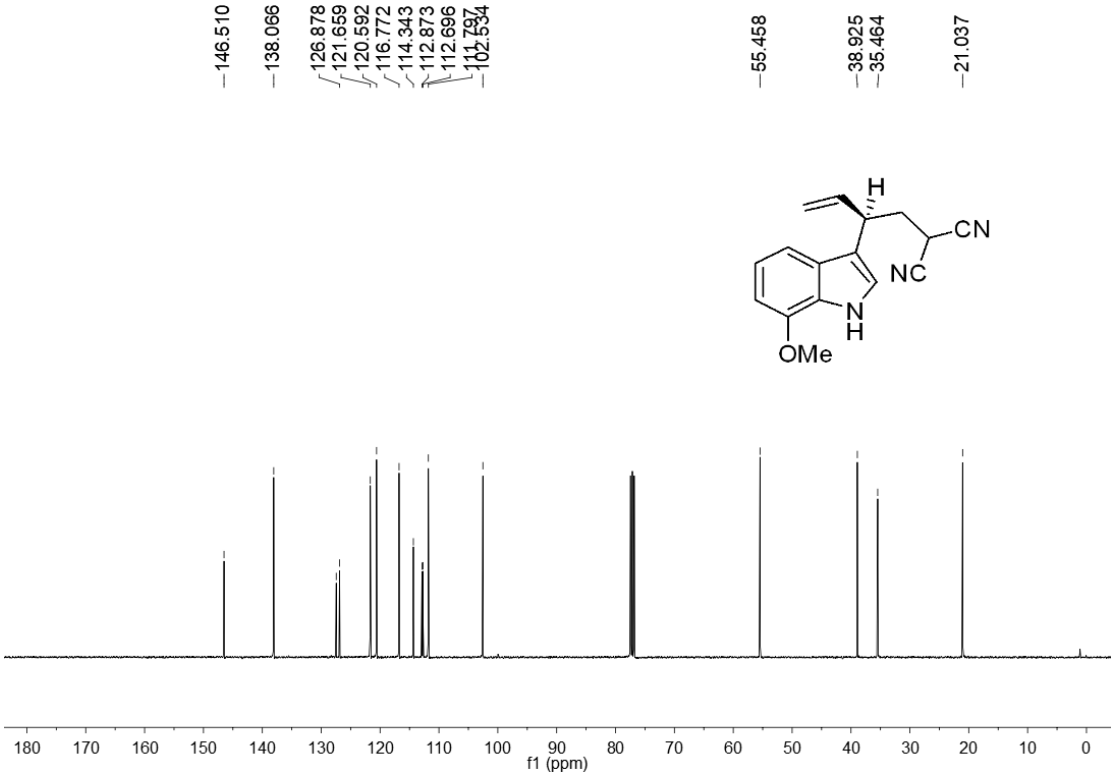
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3la**



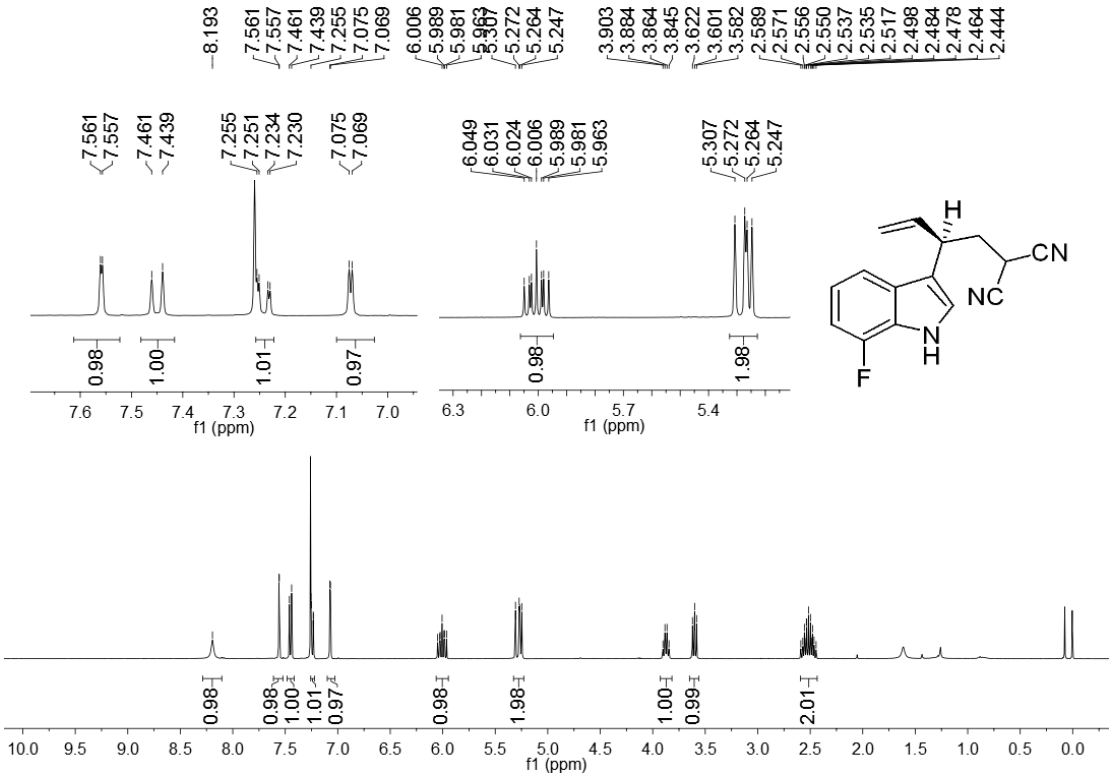
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ma**



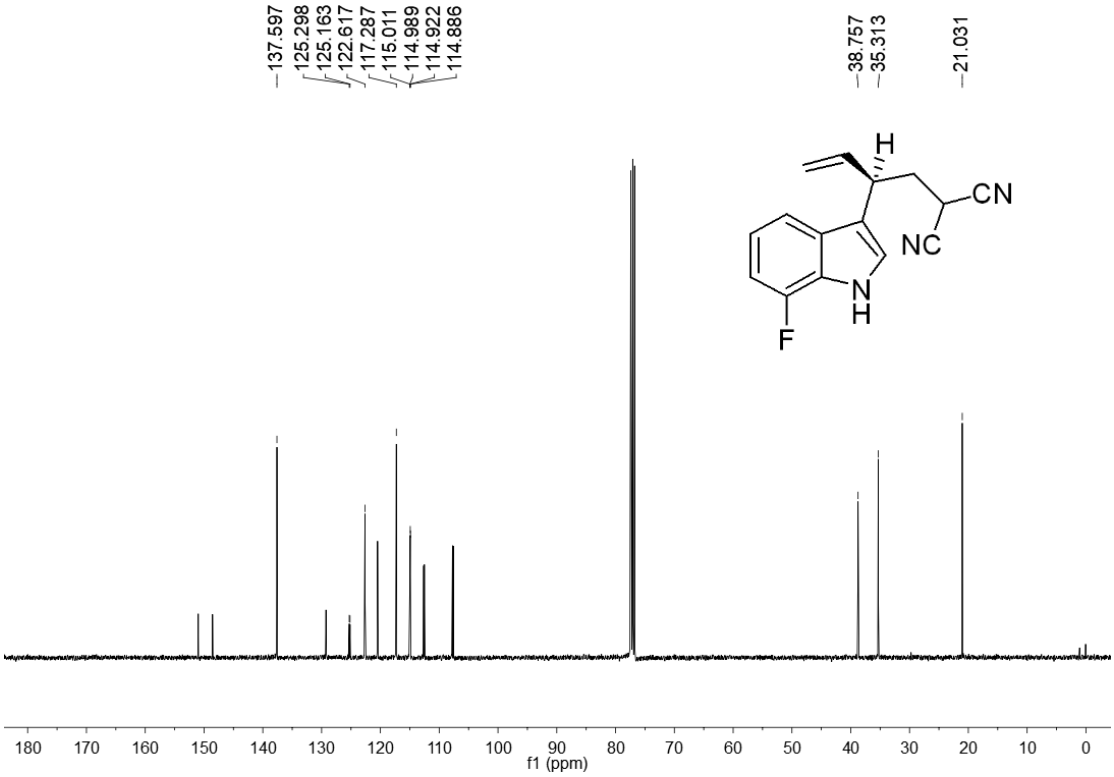
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ma**



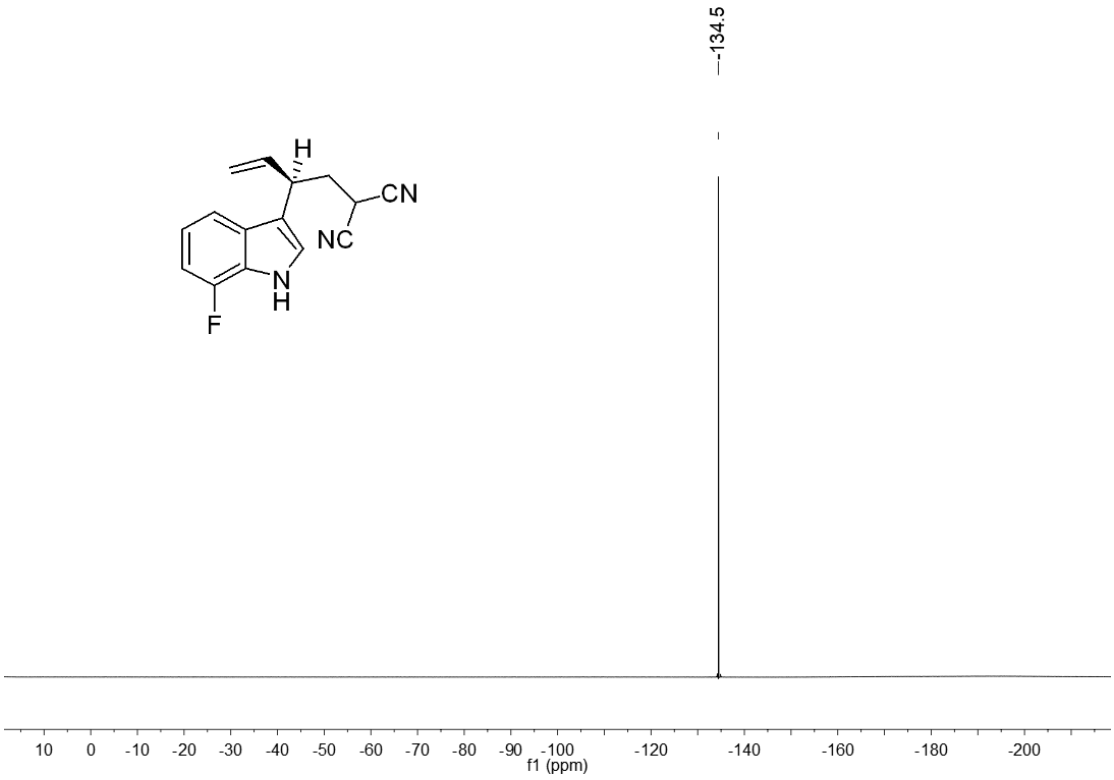
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3na**



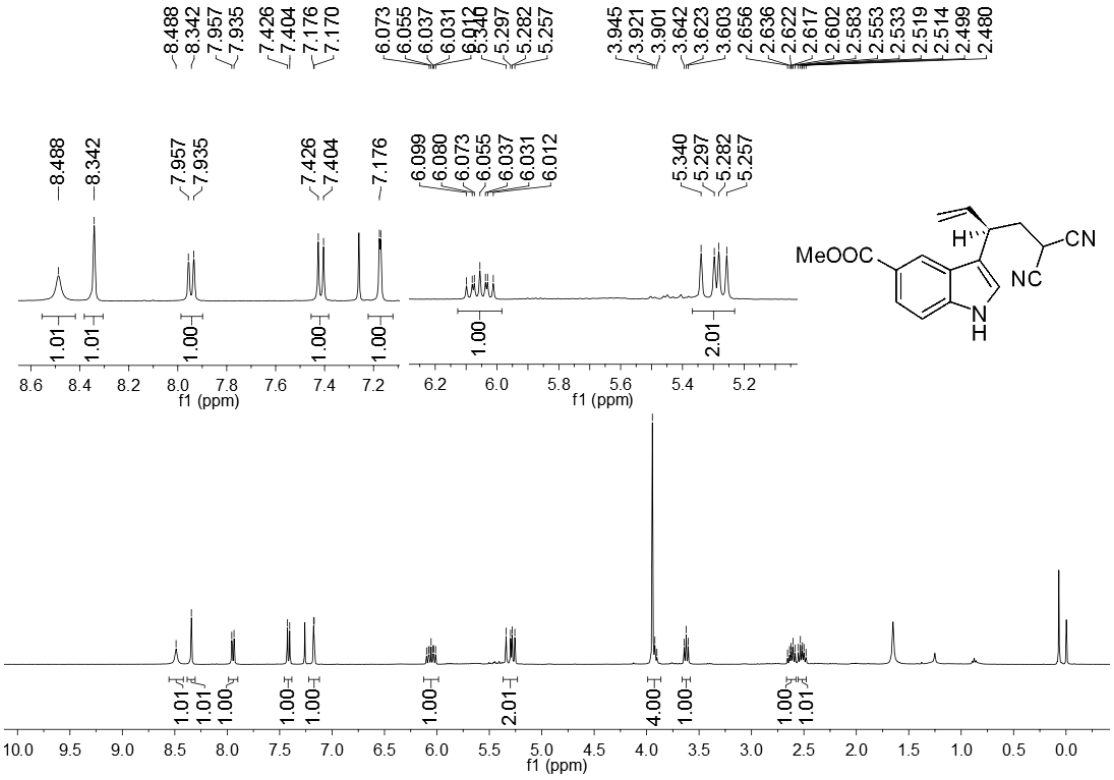
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3na**



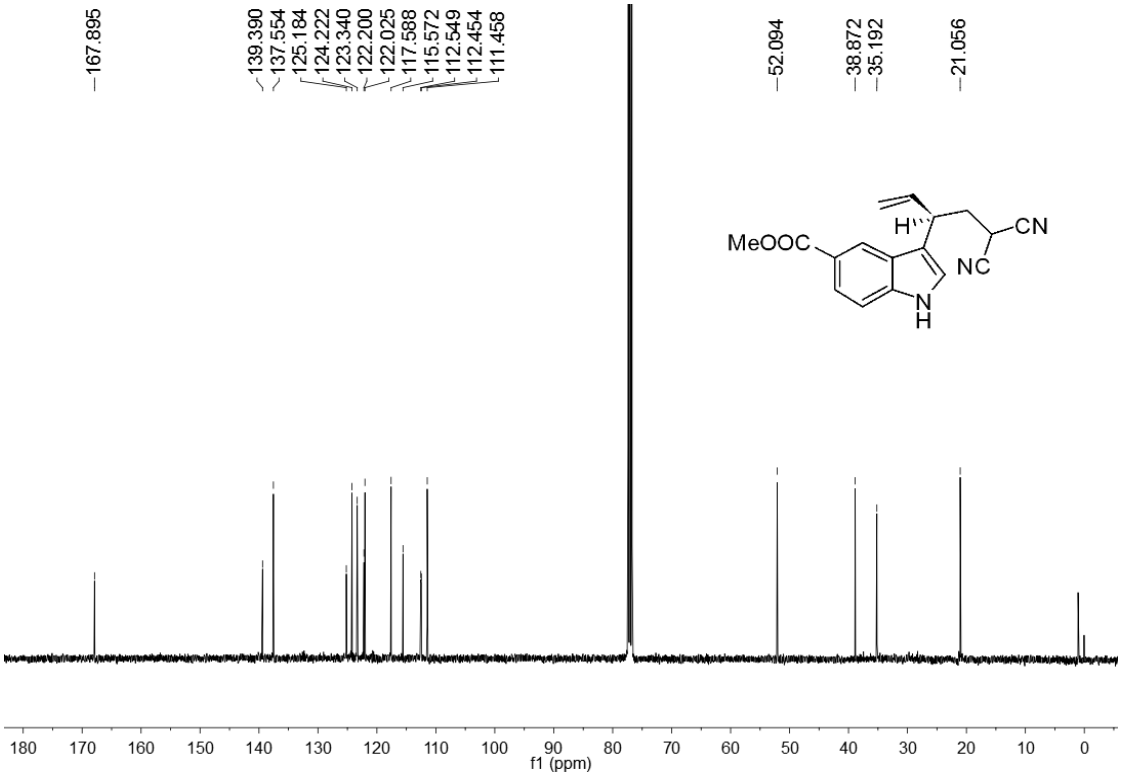
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3na**



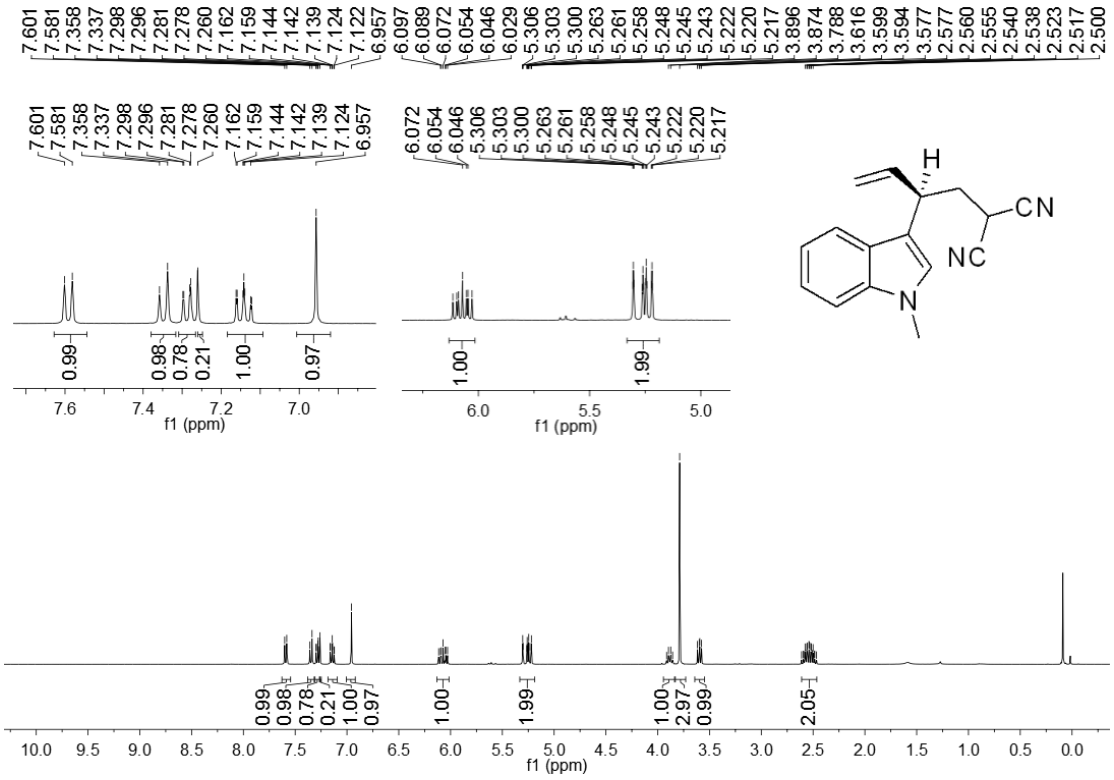
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3oa**



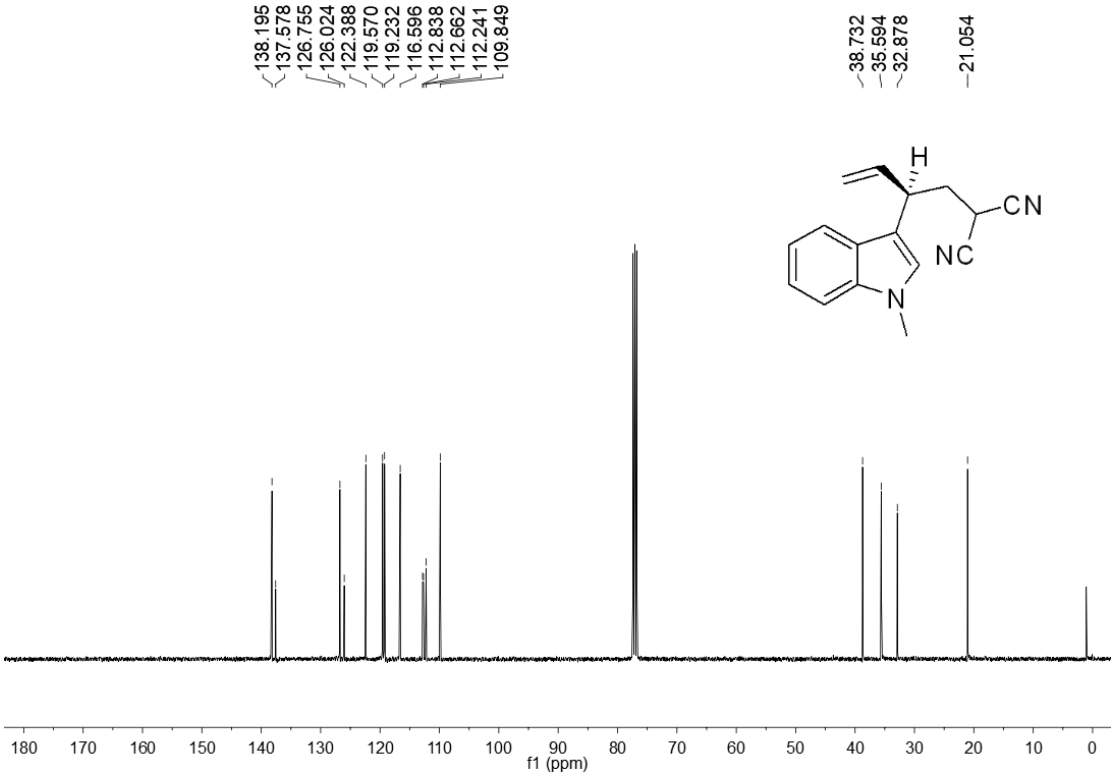
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3oa**



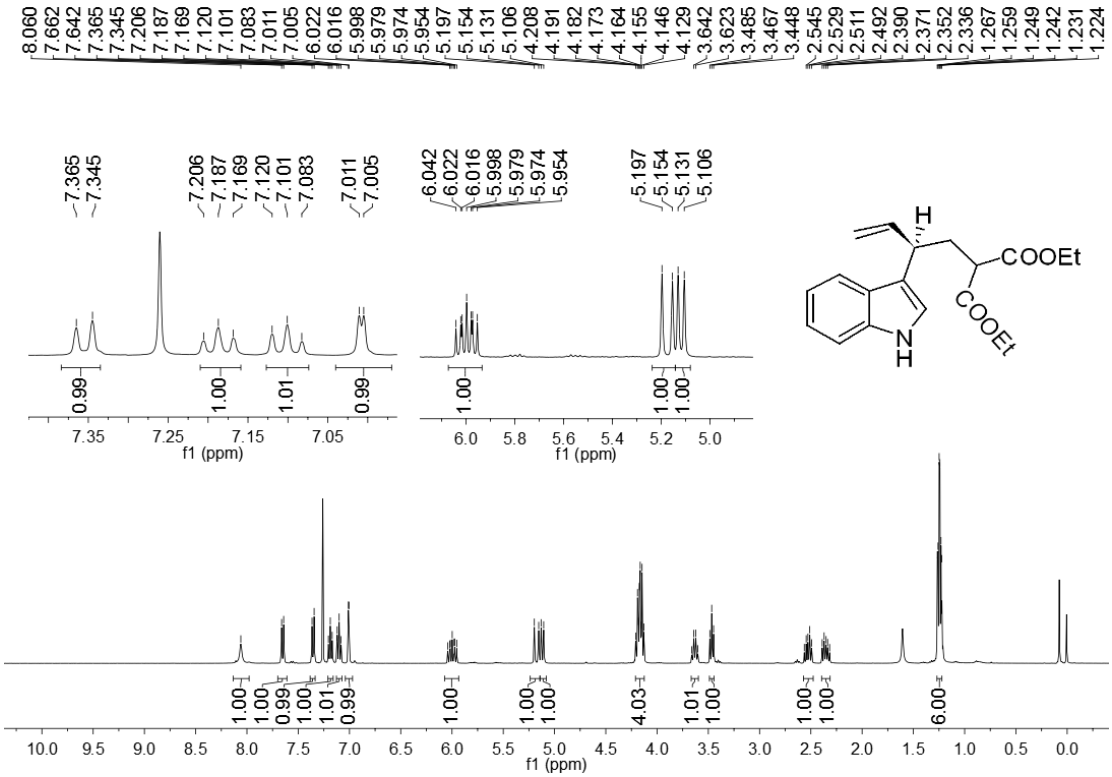
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3qa**



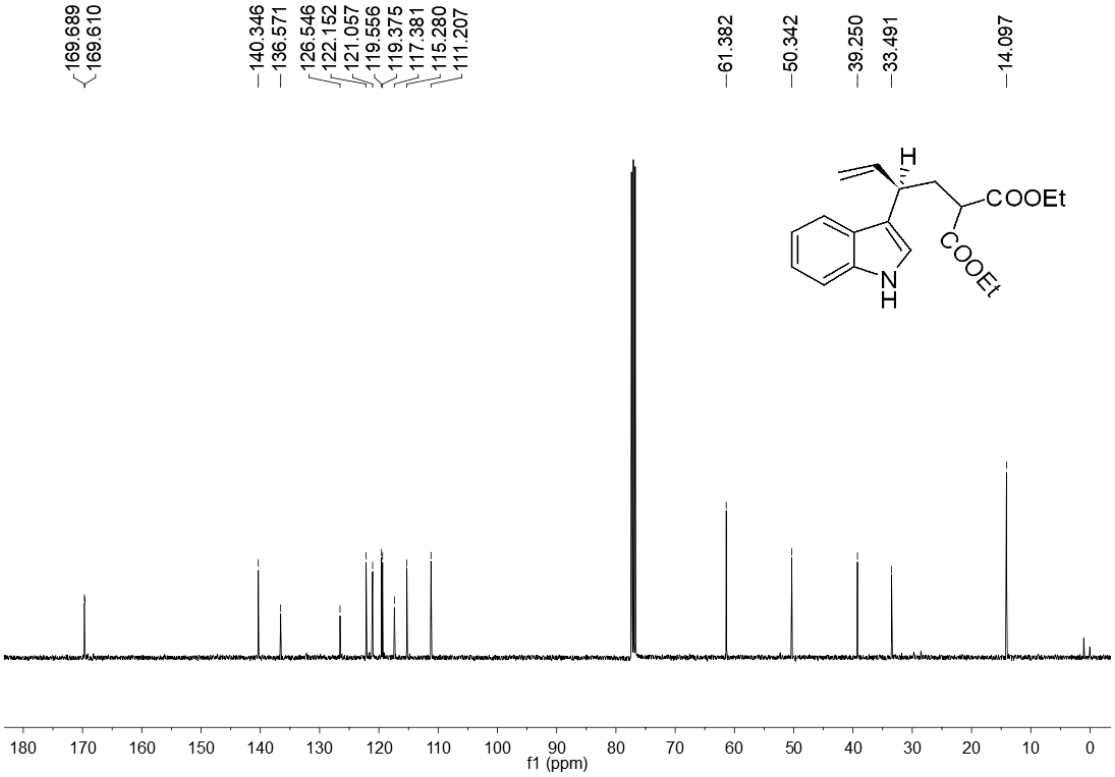
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3qa**



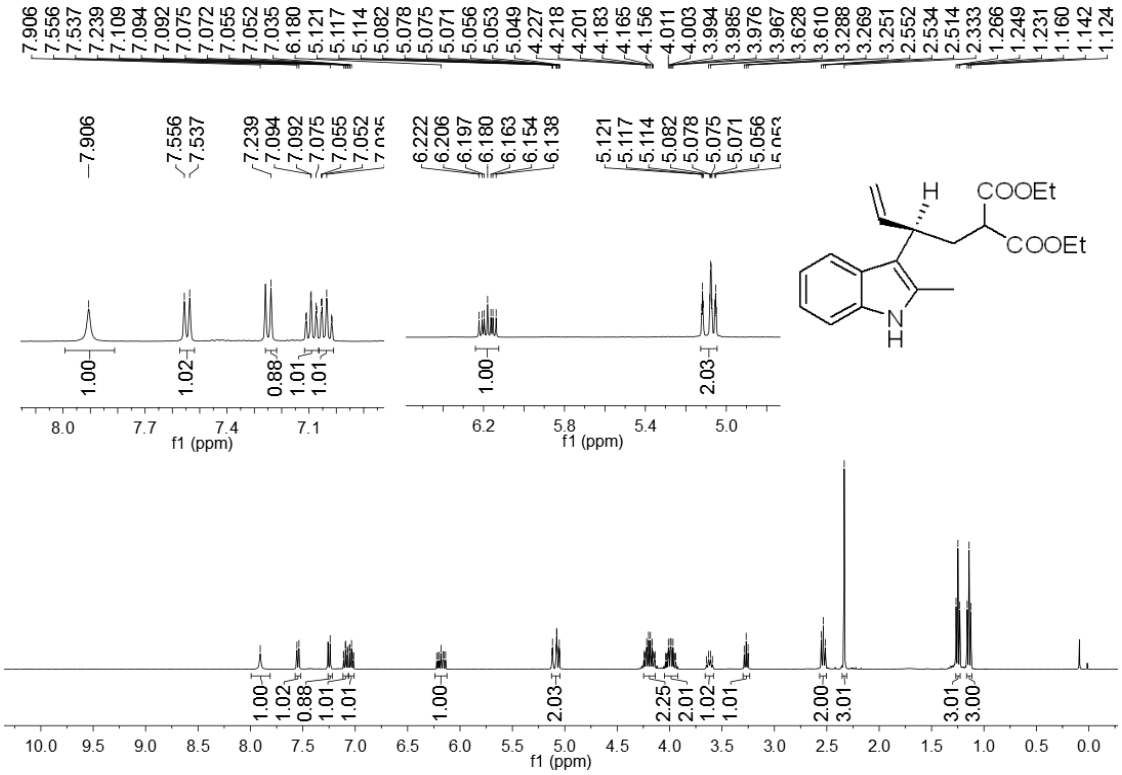
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab**



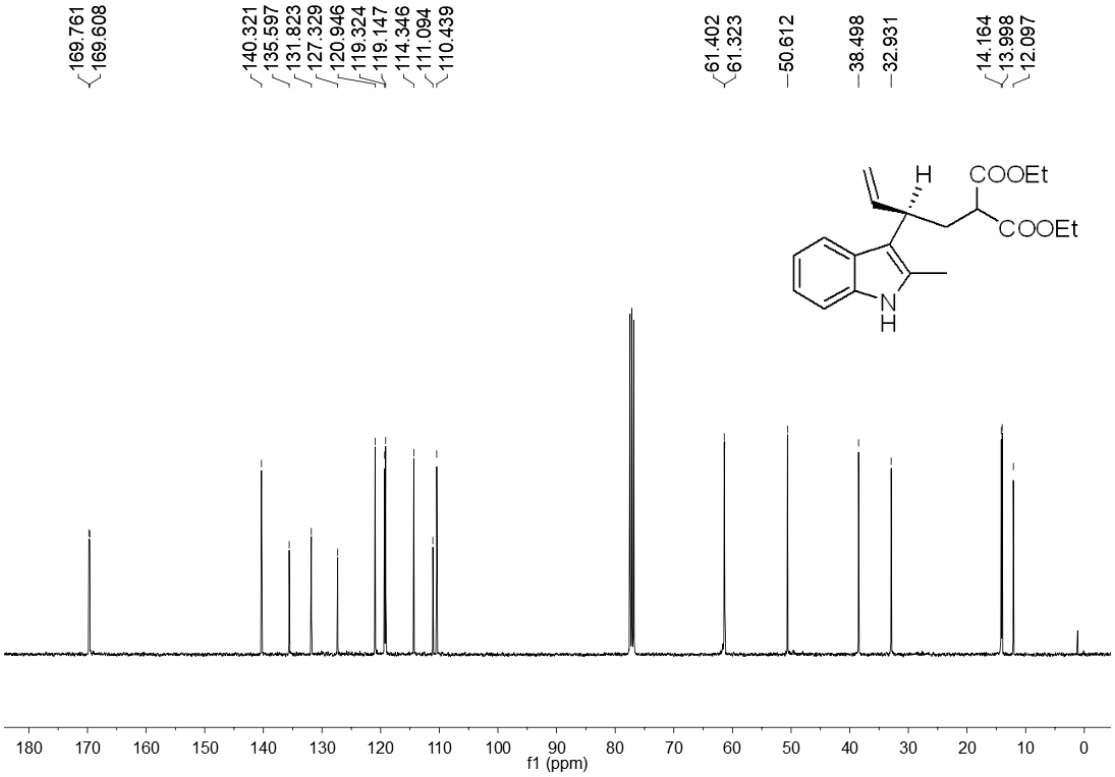
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab**



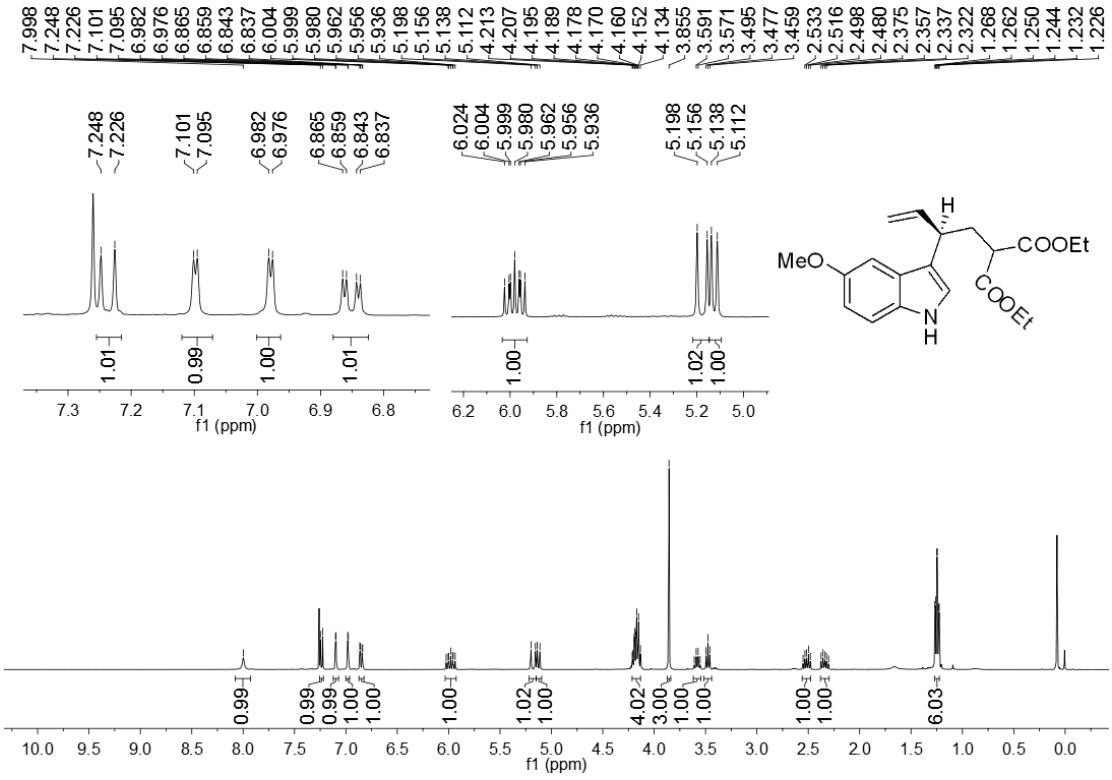
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3bb**



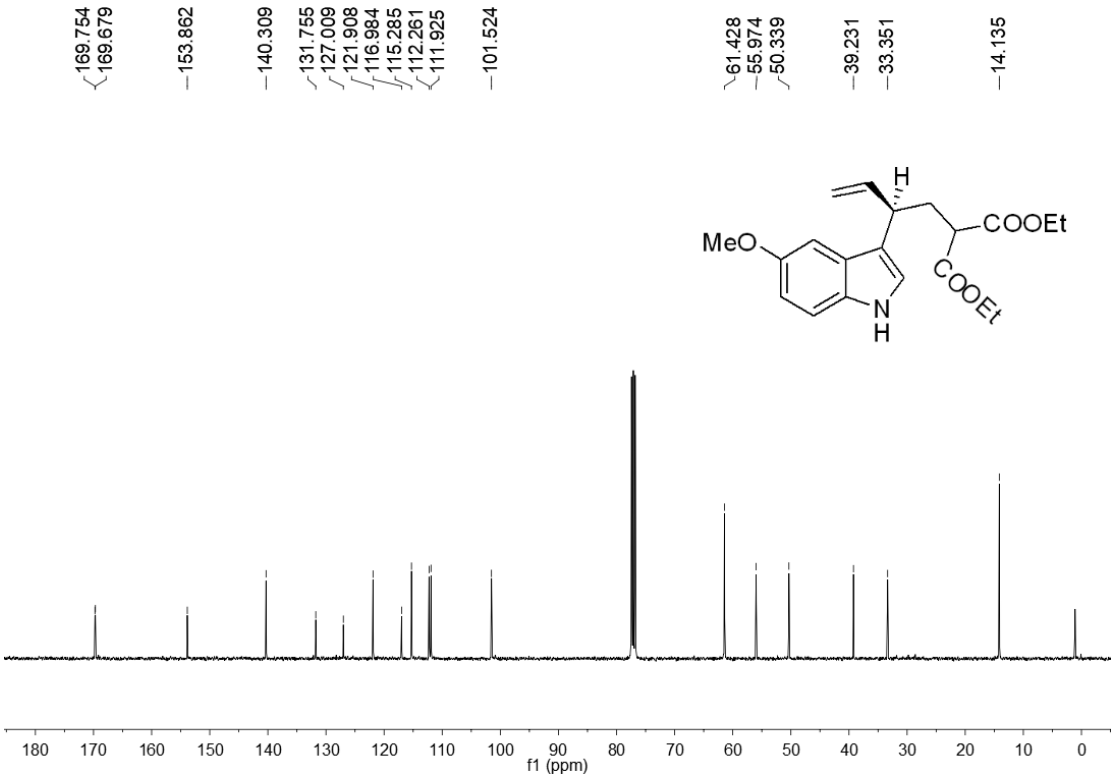
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3bb**



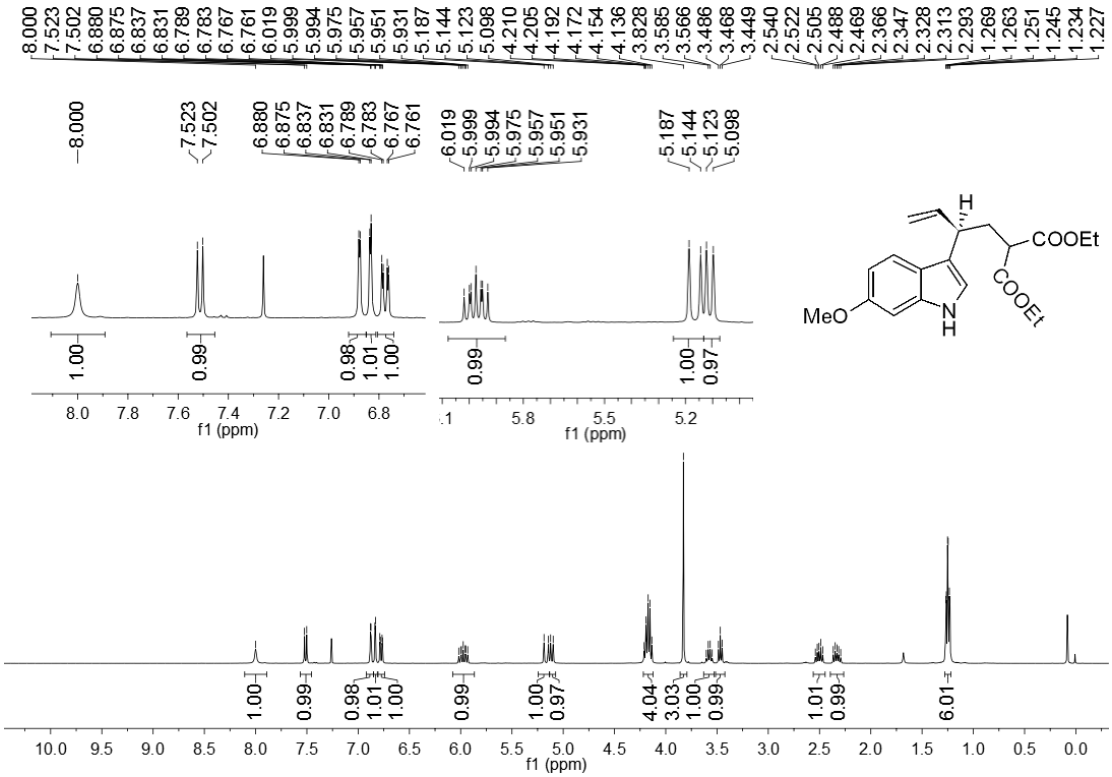
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3eb**



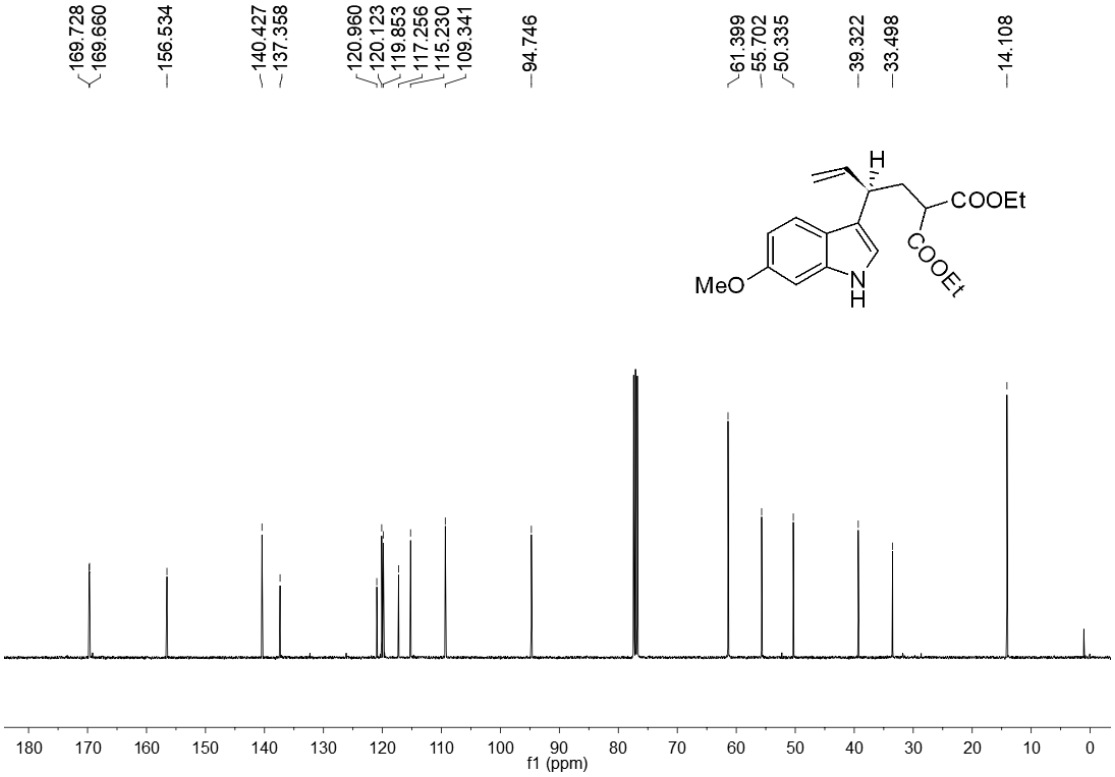
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3eb**



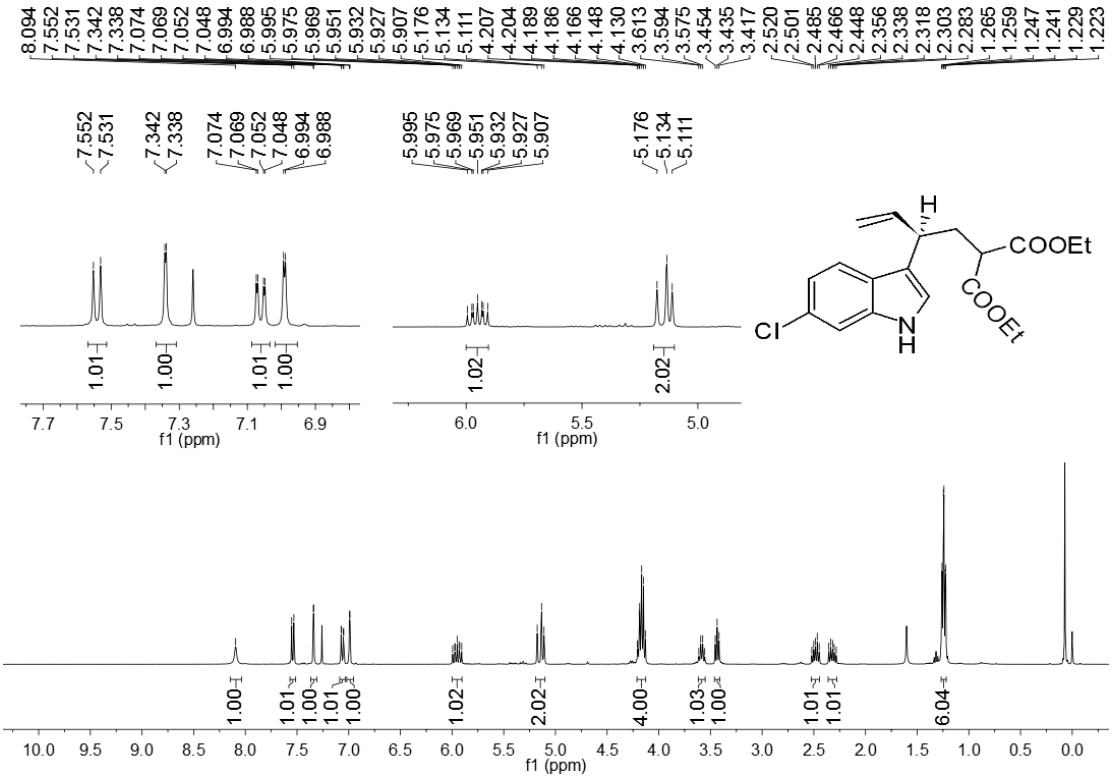
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ib**



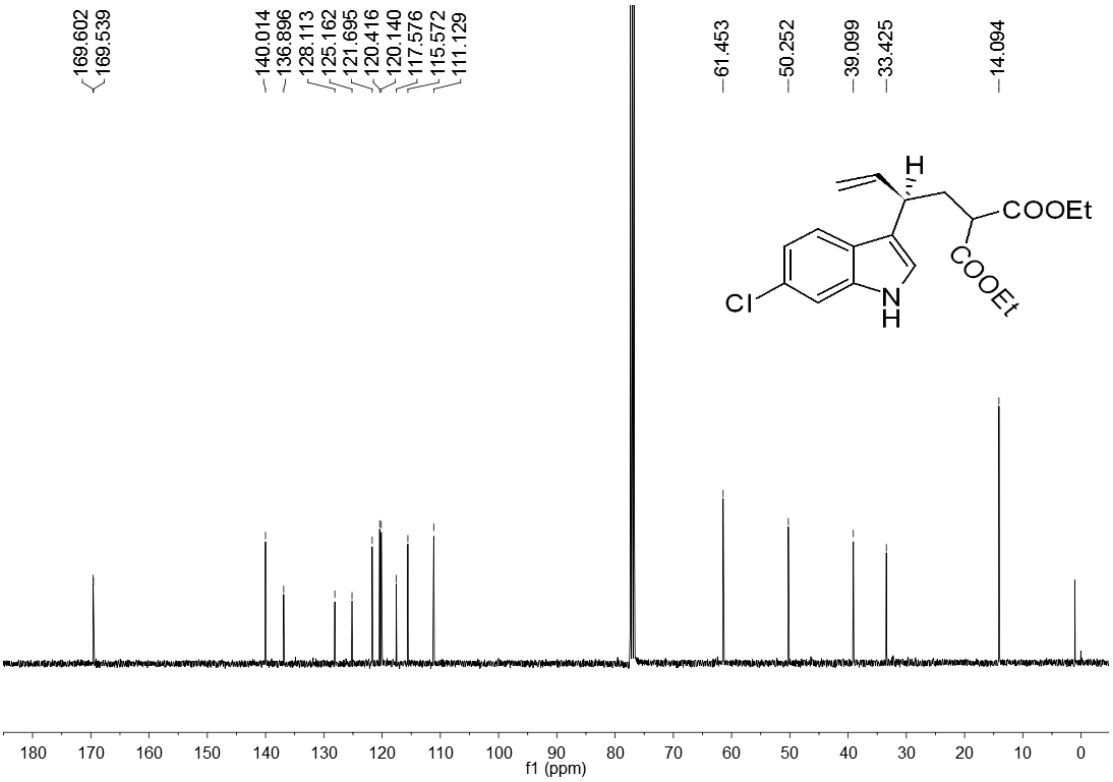
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ib**



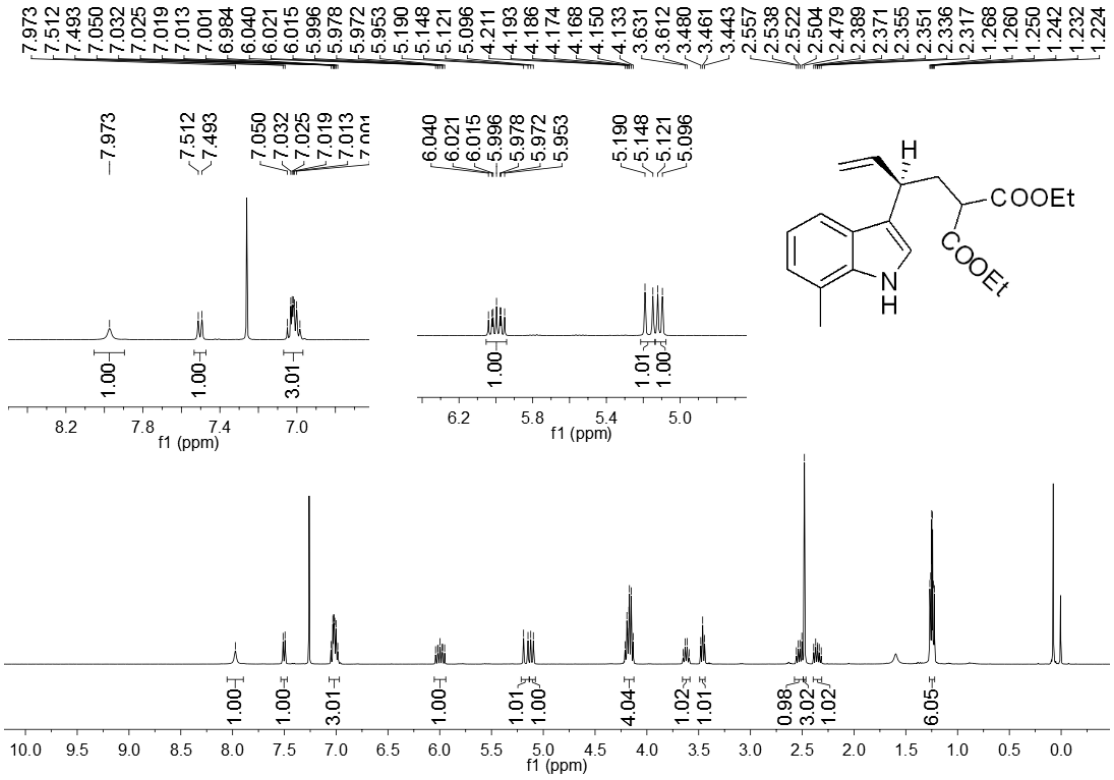
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3jb**



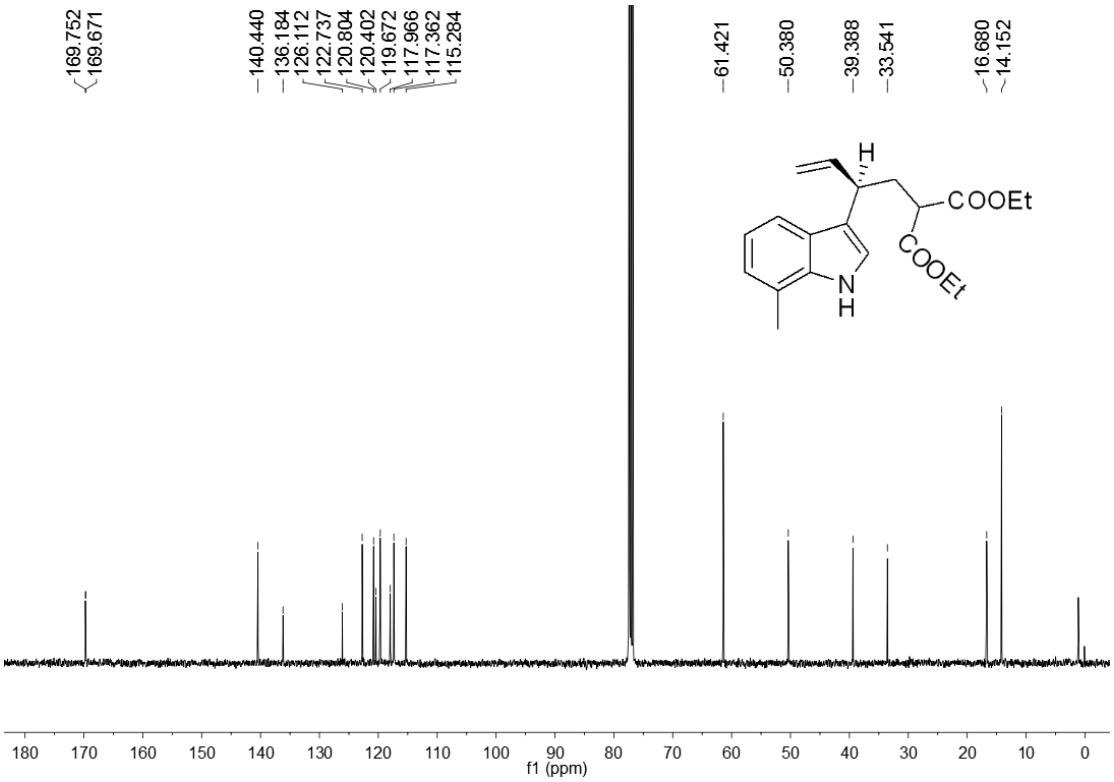
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3jb**



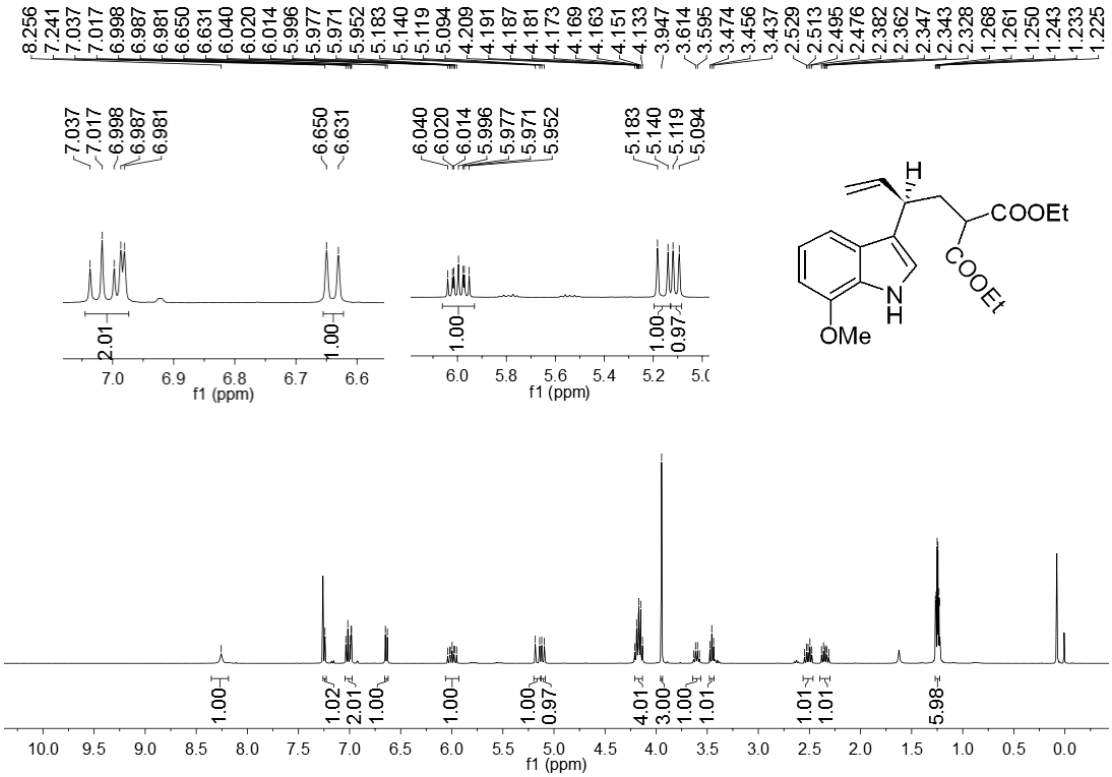
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3lb**



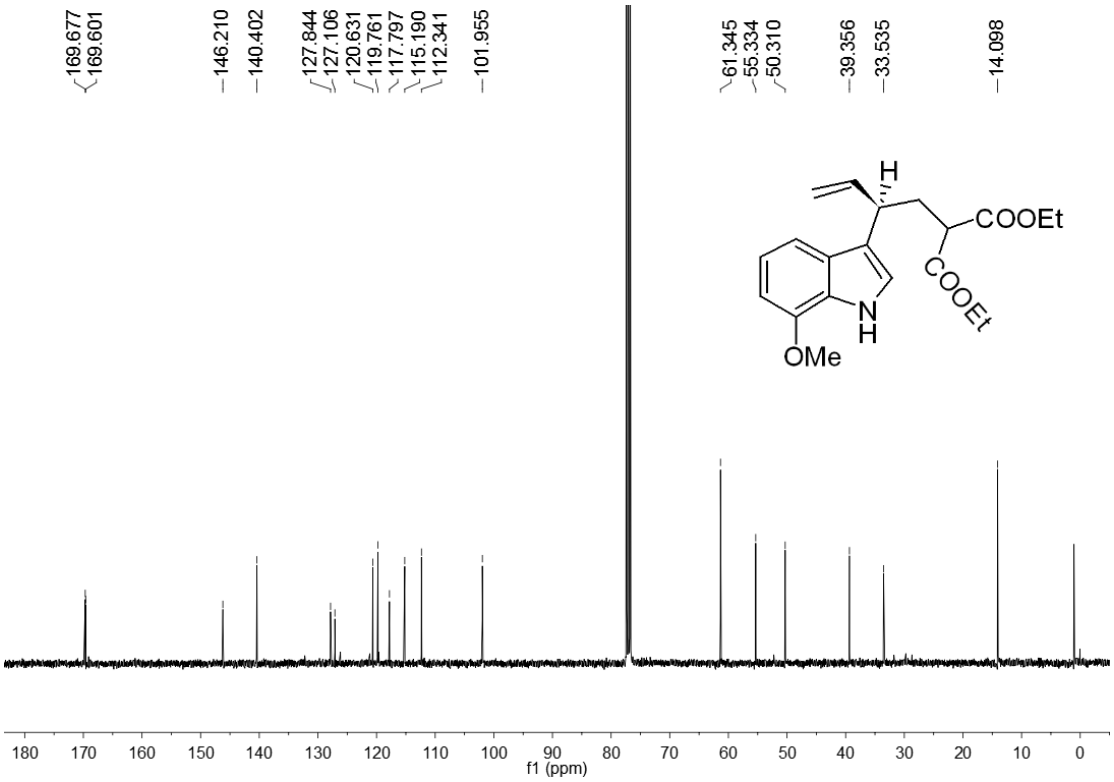
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3lb**



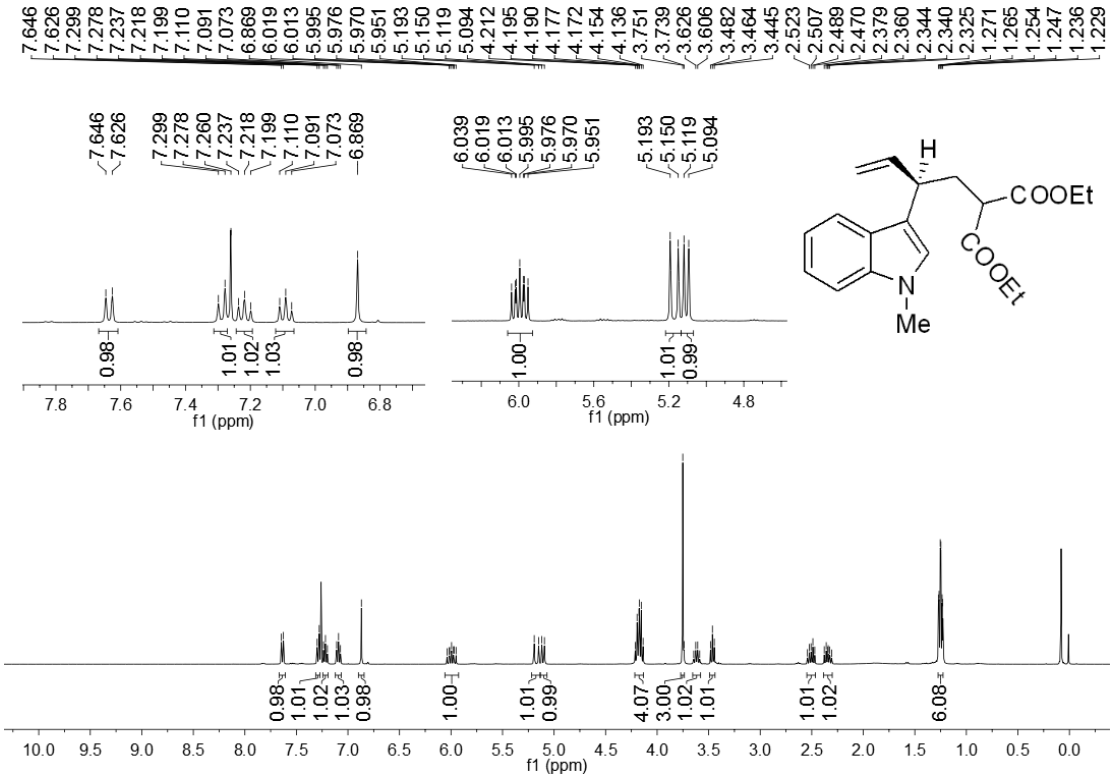
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3mb**



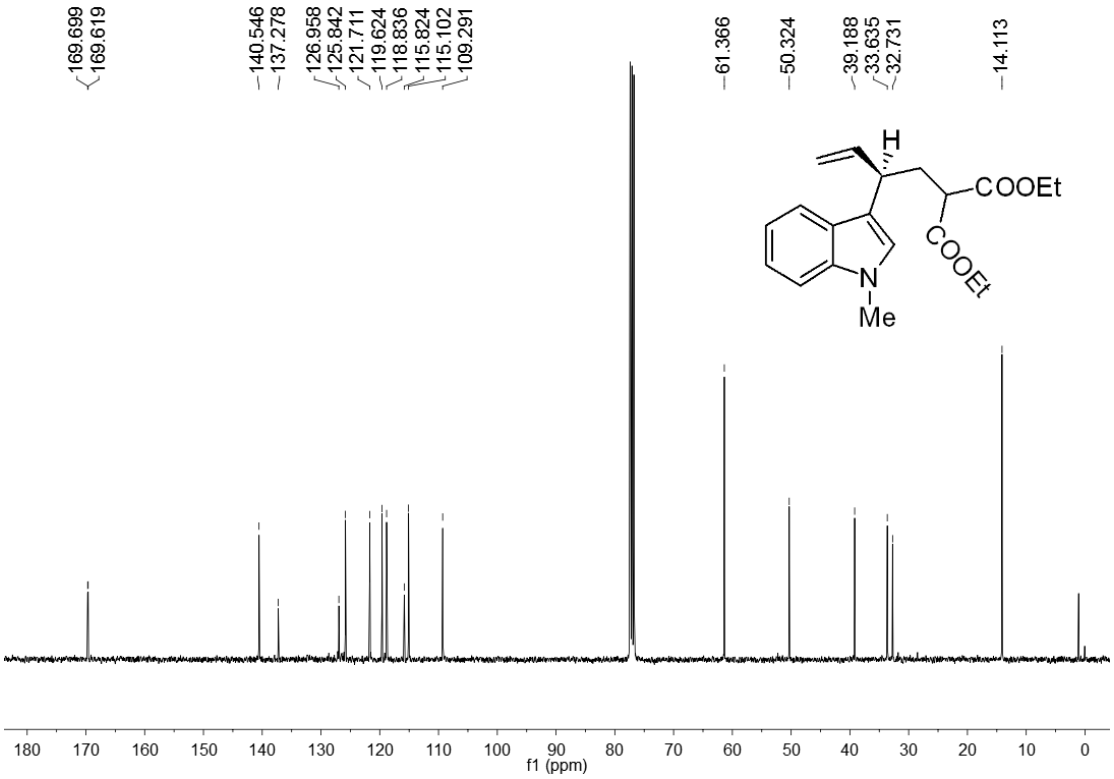
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3mb**



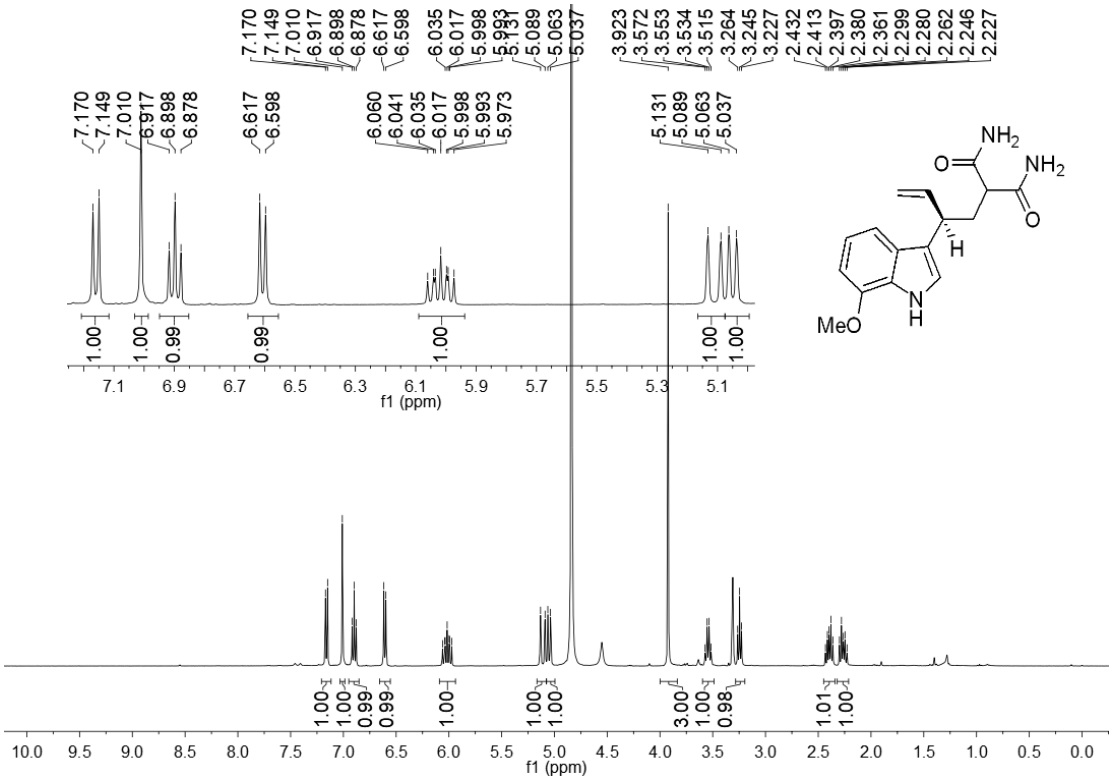
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3qb**



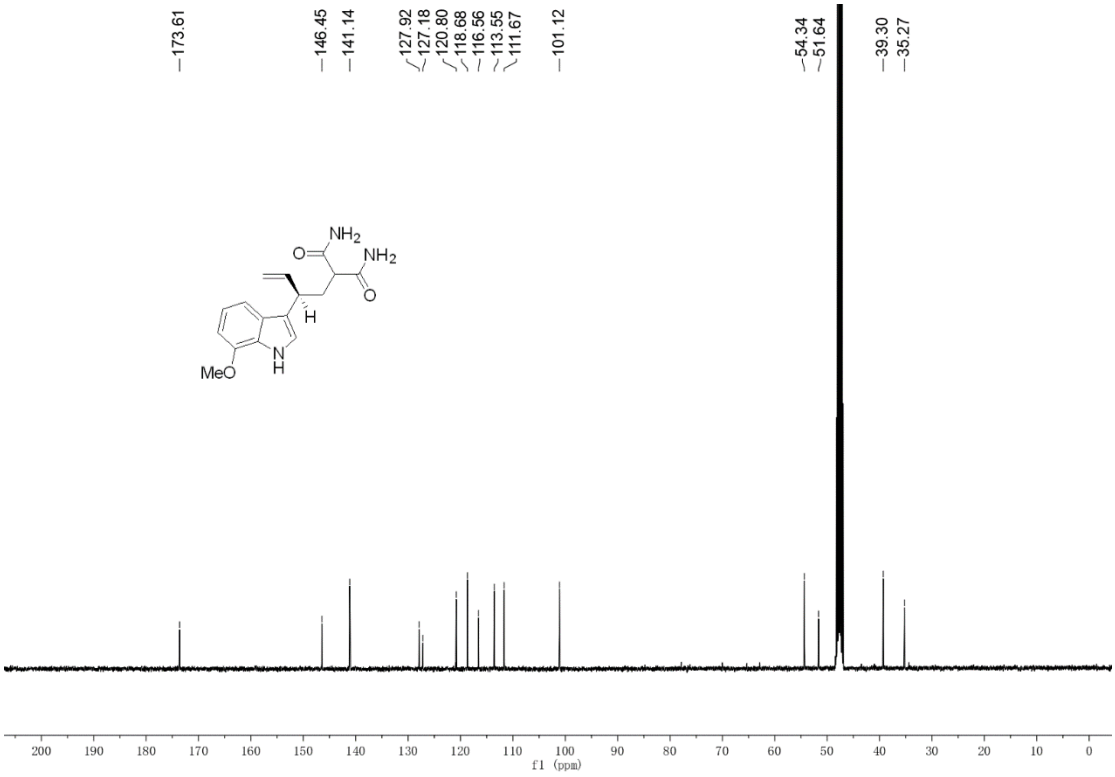
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3qb**



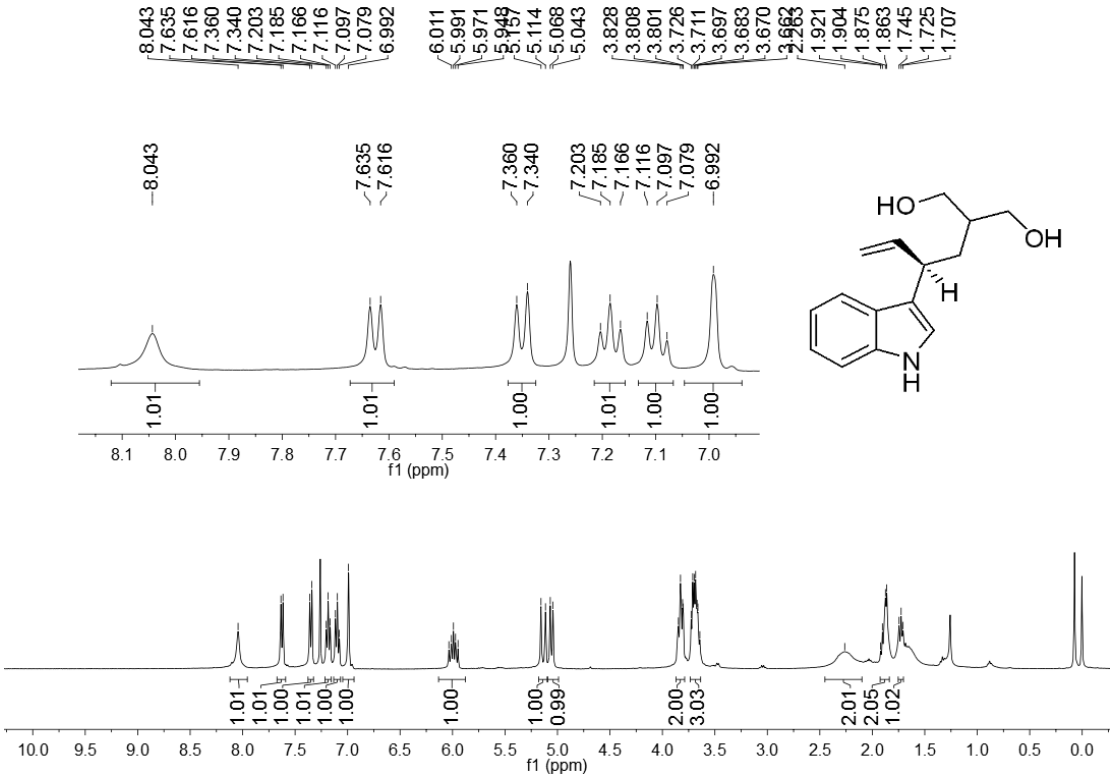
^{1}H NMR (400 MHz, CD_3OD) of compound **5**



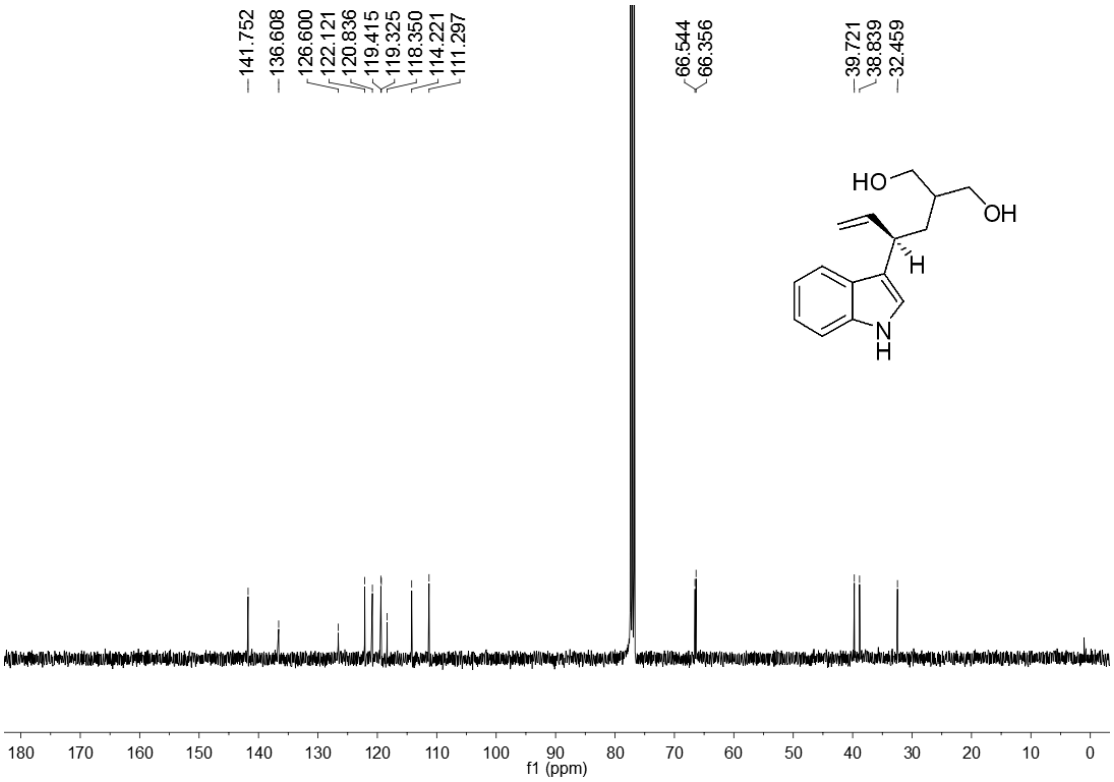
^{13}C NMR (100 MHz, CD_3OD) of compound **5**



^{1}H NMR (400 MHz, $CDCl_3$) of compound **6**

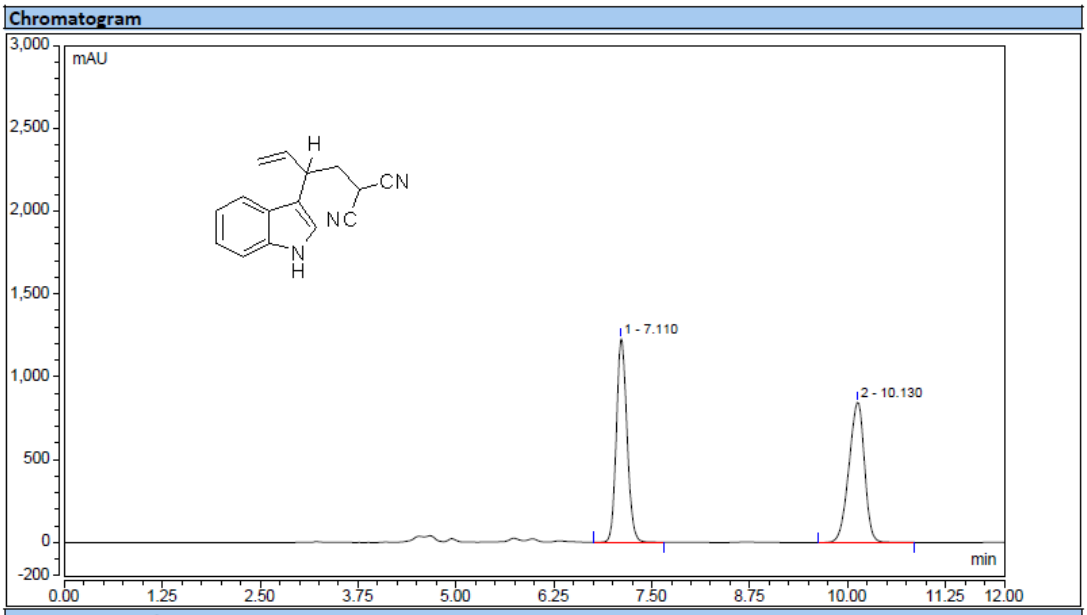


^{13}C NMR (100 MHz, $CDCl_3$) of compound **6**



2. HPLC spectra of product 3 and 5-6

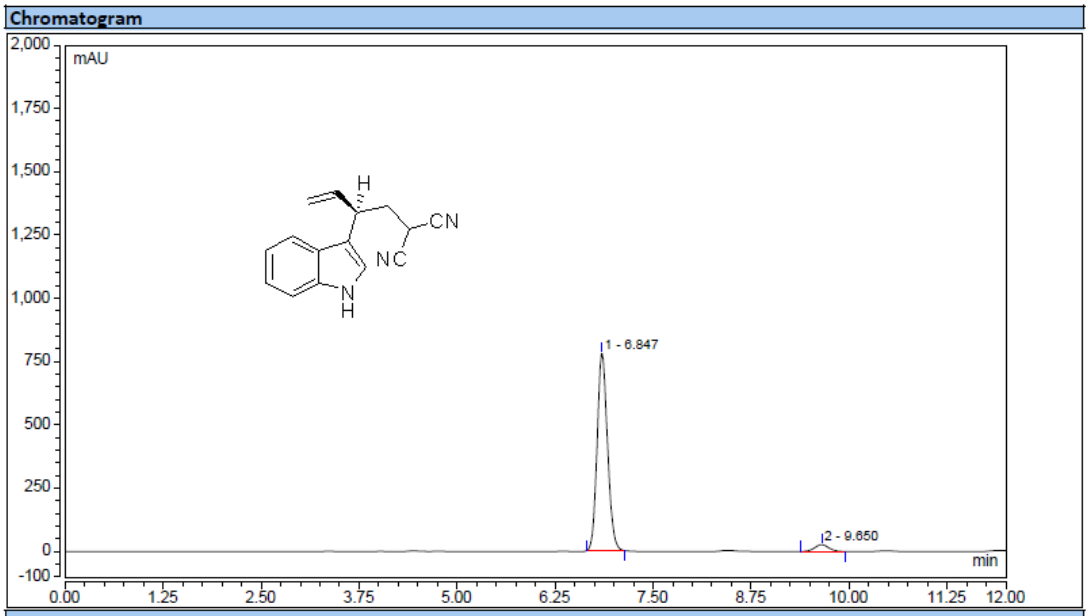
3aa Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.110	194.042	1230.089	49.77	59.20	n.a.
2		10.130	195.832	847.590	50.23	40.80	n.a.
Total:			**389.874**	**2077.679**	**100.00**	**100.00**	

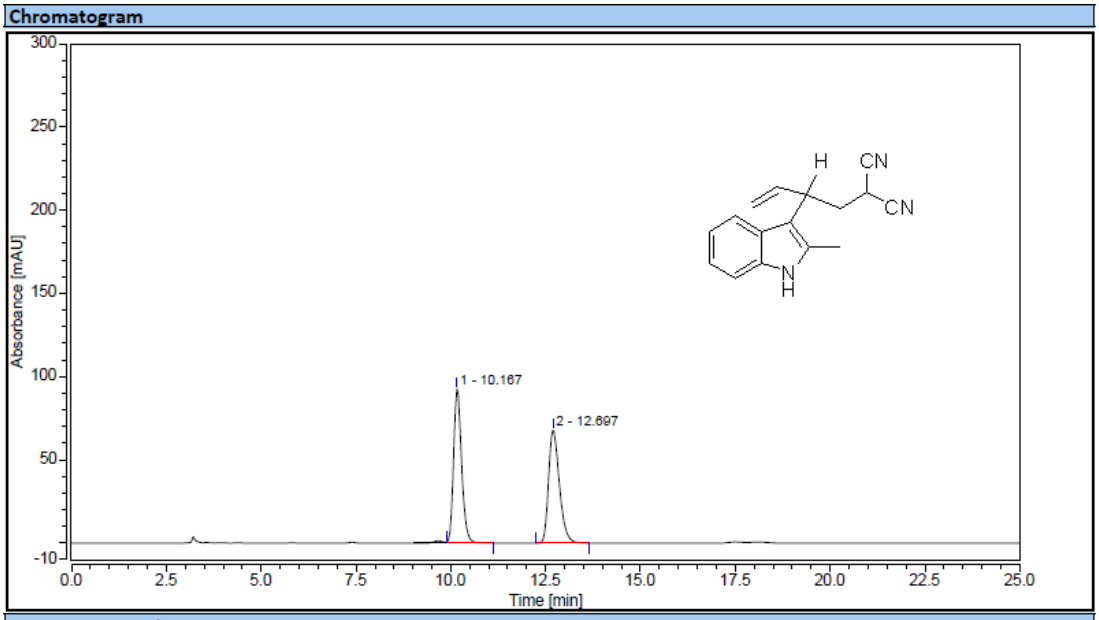
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.847	119.940	779.734	95.49	96.67	n.a.
2		9.650	5.662	26.884	4.51	3.33	n.a.
Total:			**125.602**	**806.618**	**100.00**	**100.00**	

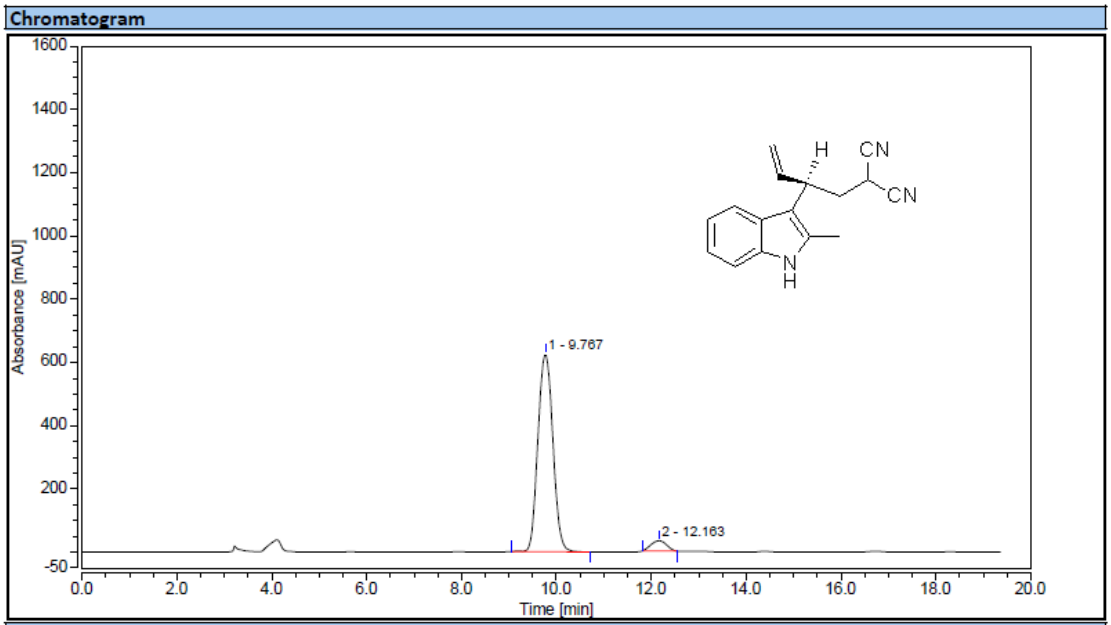
3ba Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.167	22.759	92.575	50.48	57.65	n.a.
2		12.697	22.330	68.007	49.52	42.35	n.a.
Total:			**45.089**	**160.582**	**100.00**	**100.00**	

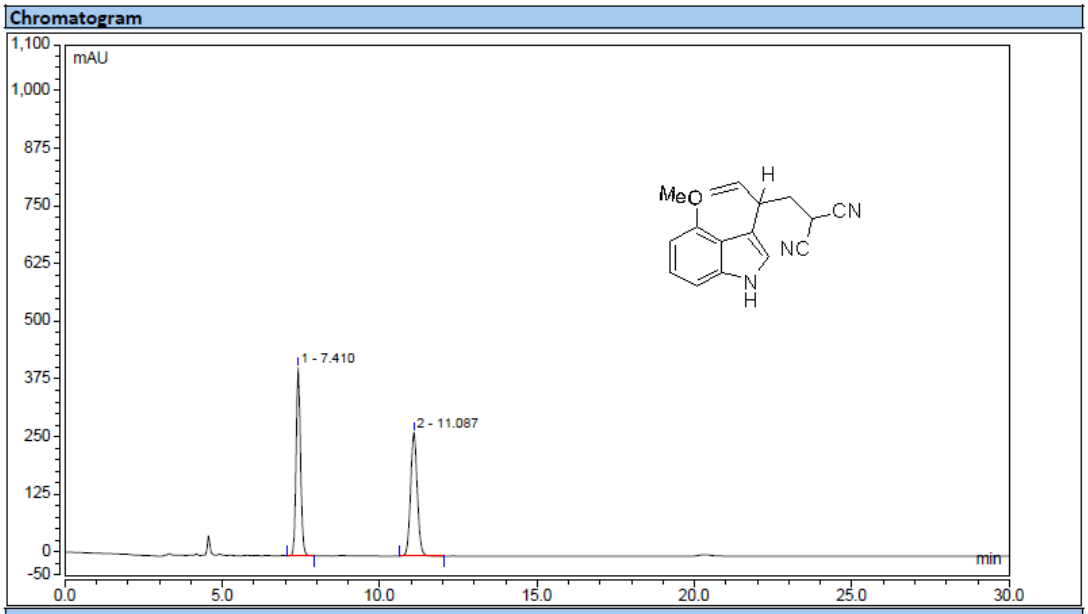
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.767	228.240	623.740	94.84	95.06	n.a.
2		12.163	12.429	32.420	5.16	4.94	n.a.
Total:			**240.669**	**656.160**	**100.00**	**100.00**	

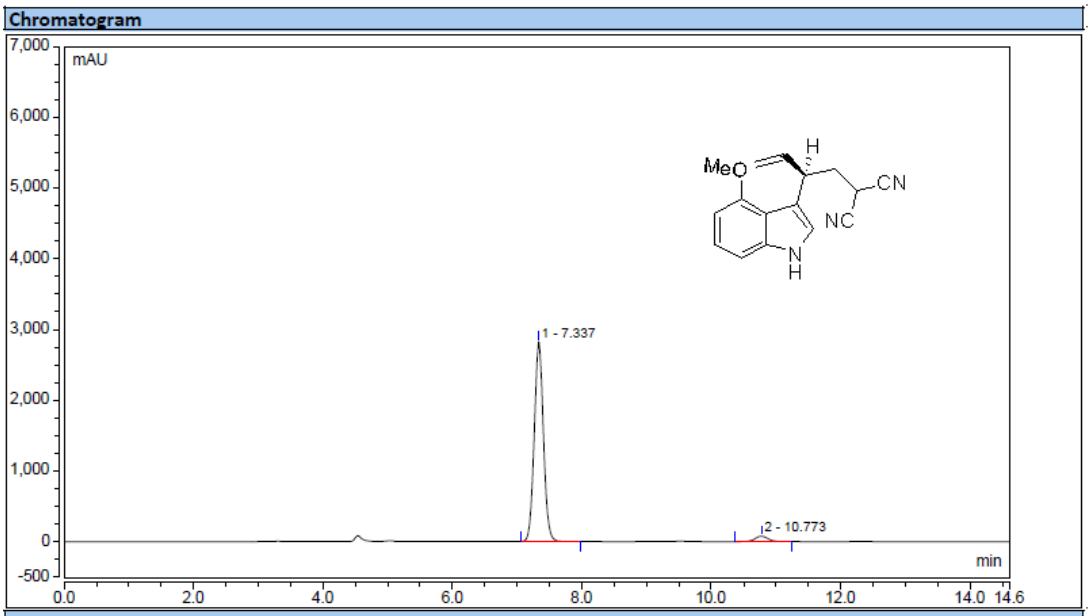
3ca Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.410	65.873	407.456	49.90	60.30	n.a.
2		11.087	66.133	268.293	50.10	39.70	n.a.
Total:			**132.006**	**675.750**	**100.00**	**100.00**	

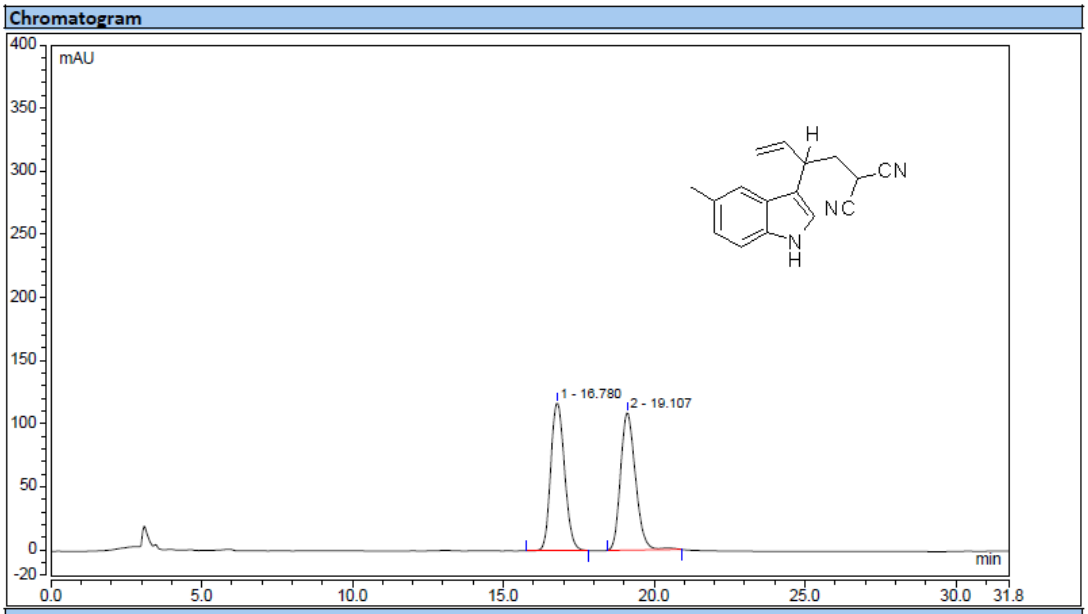
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.337	460.399	2822.218	96.05	97.34	n.a.
2		10.773	18.952	77.269	3.95	2.66	n.a.
Total:			**479.351**	**2899.487**	**100.00**	**100.00**	

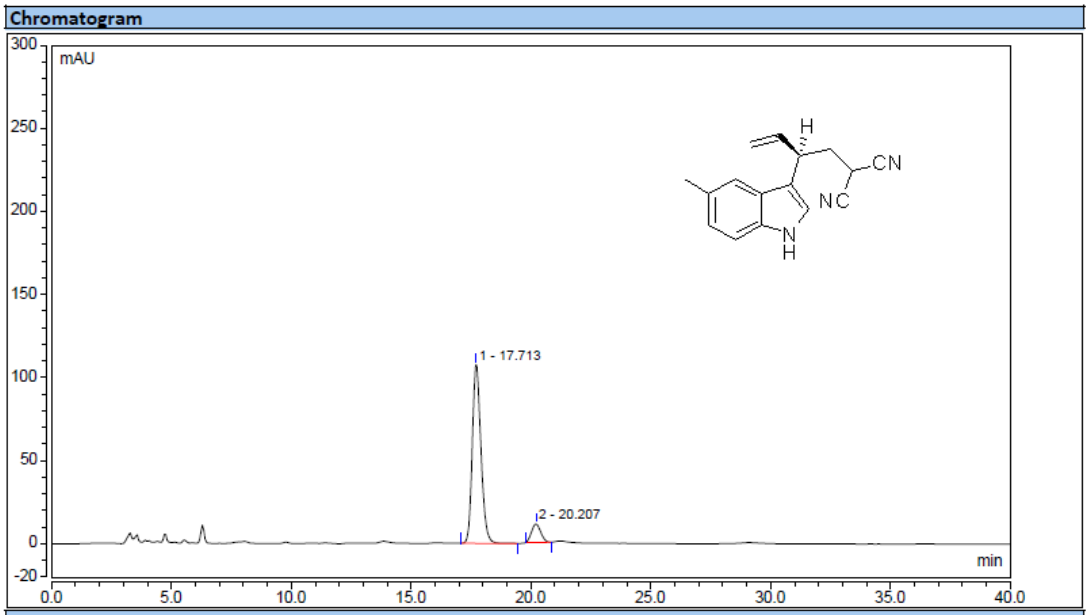
3da Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.780	62.419	117.062	49.87	51.82	n.a.
2		19.107	62.752	108.839	50.13	48.18	n.a.
Total:			**125.171**	**225.901**	**100.00**	**100.00**	

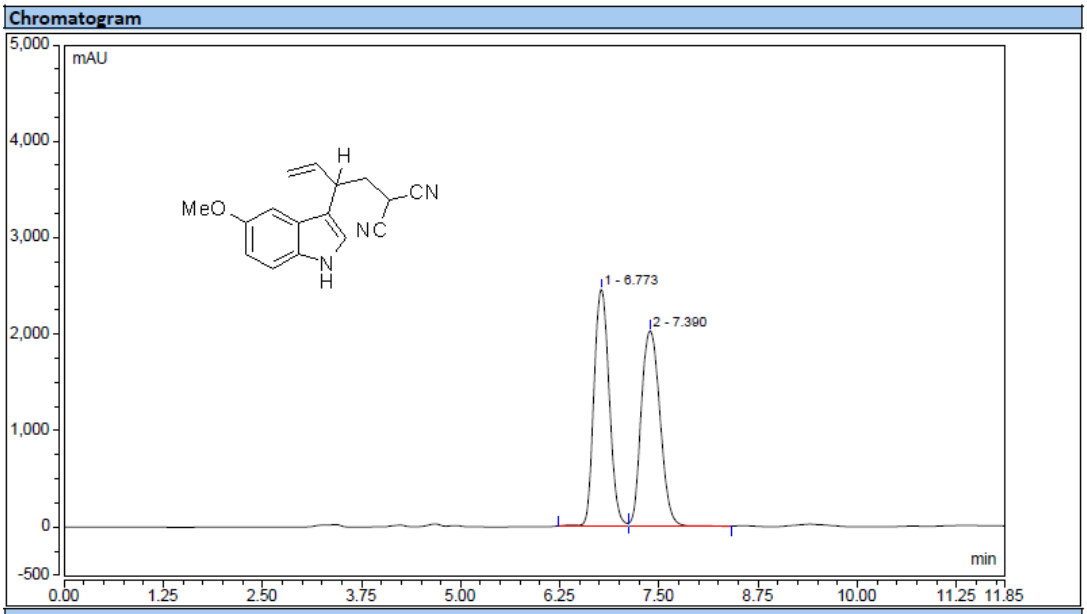
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.713	45.274	107.692	90.26	90.67	n.a.
2		20.207	4.885	11.077	9.74	9.33	n.a.
Total:			**50.159**	**118.769**	**100.00**	**100.00**	

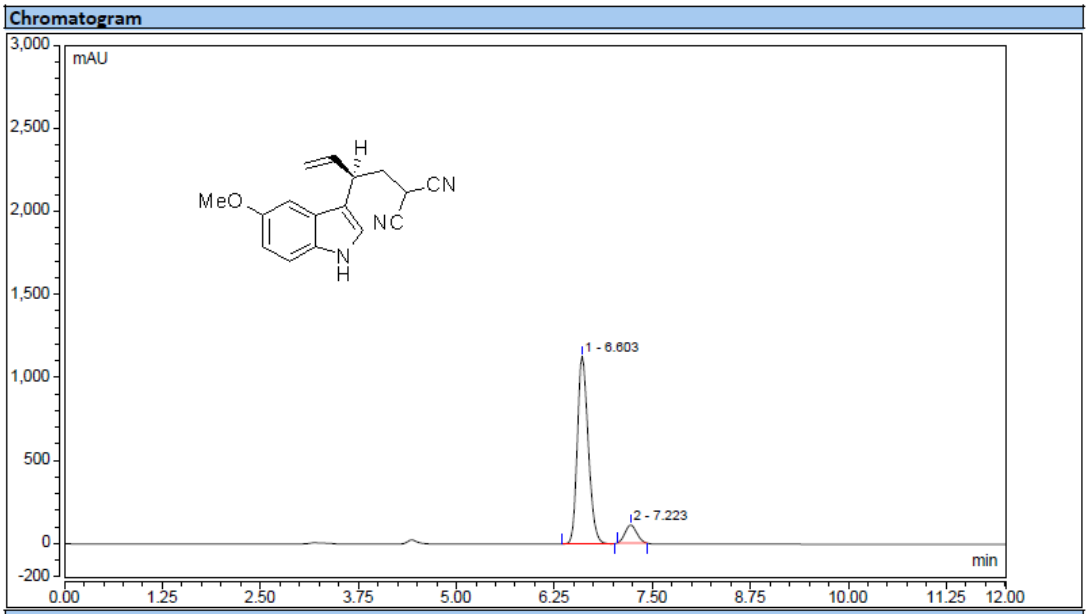
3ea Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.773	546.774	2456.630	49.49	54.81	n.a.
2		7.390	557.944	2025.181	50.51	45.19	n.a.
Total:			**1104.718**	**4481.811**	**100.00**	**100.00**	

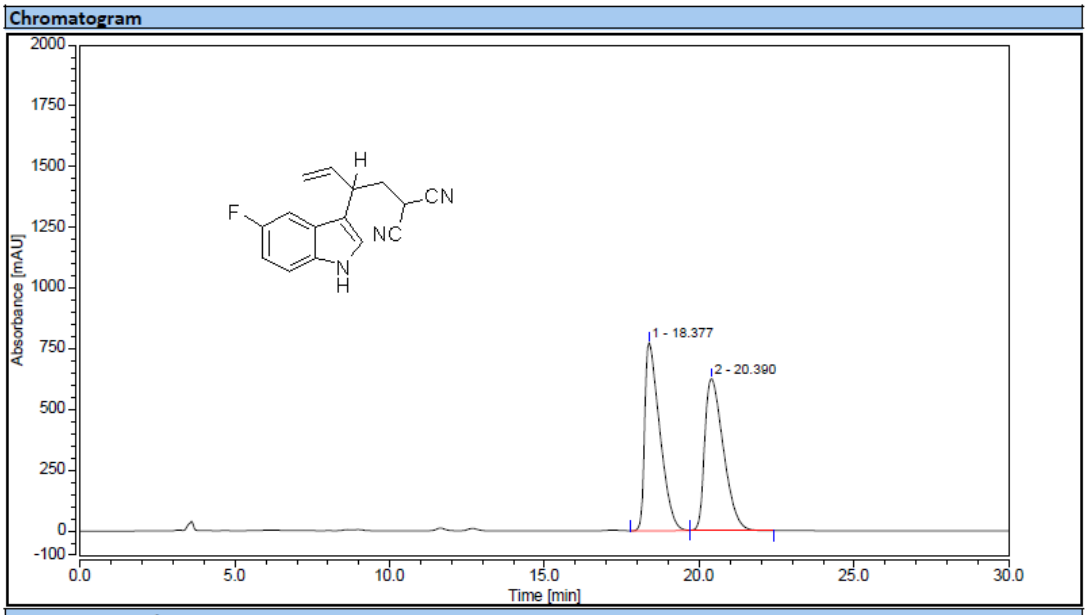
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.603	182.940	1129.520	90.71	91.23	n.a.
2		7.223	18.730	108.606	9.29	8.77	n.a.
Total:			**201.670**	**1238.126**	**100.00**	**100.00**	

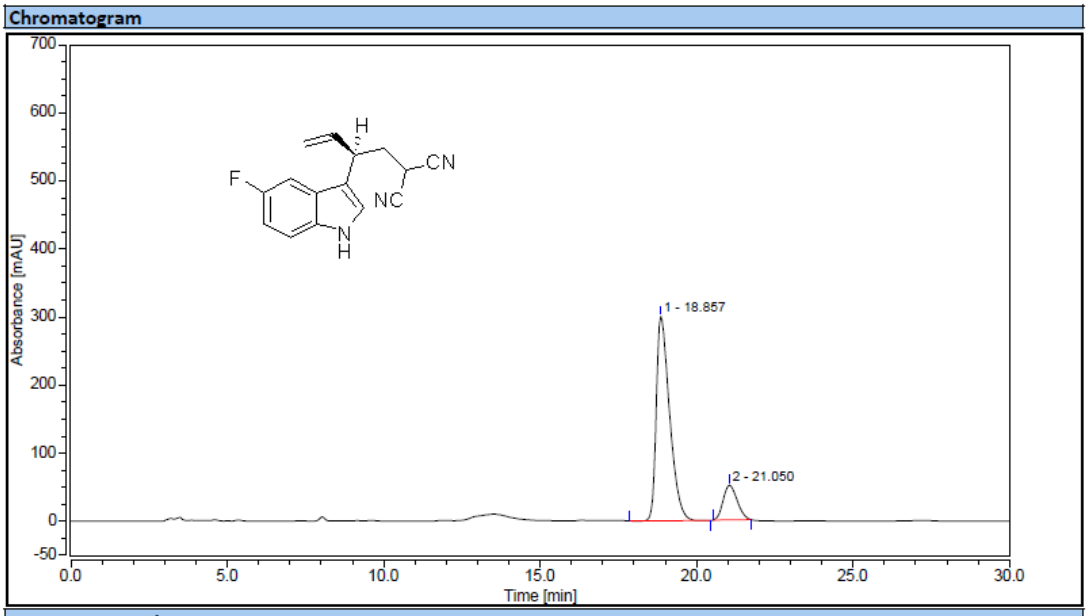
3fa Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.377	436.185	774.610	49.83	55.29	n.a.
2		20.390	439.151	626.273	50.17	44.71	n.a.
Total:			**875.336**	**1400.883**	**100.00**	**100.00**	

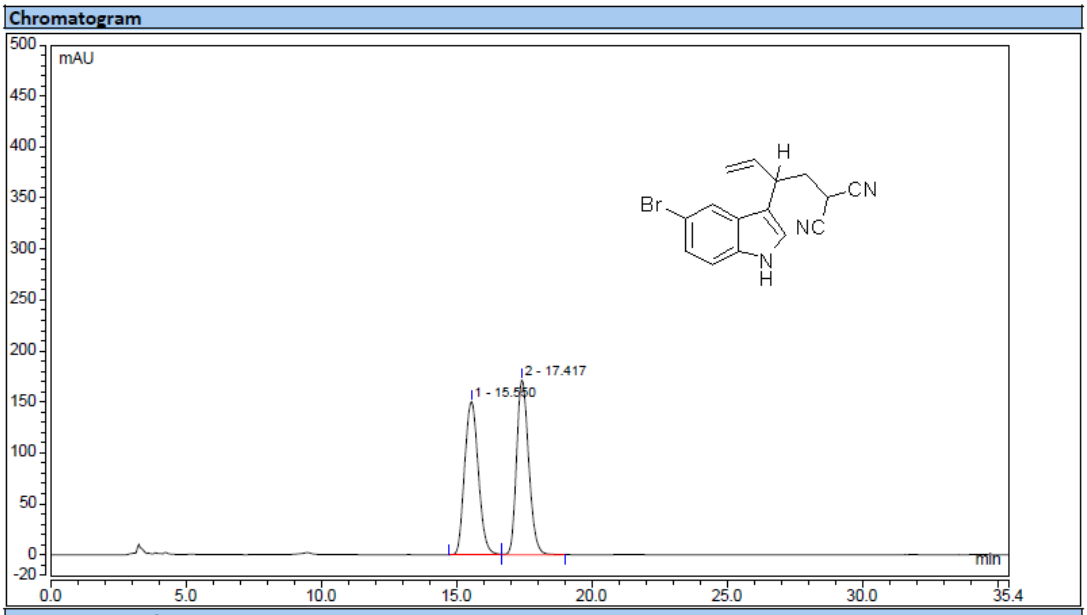
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.857	147.609	300.480	84.90	85.56	n.a.
2		21.050	26.253	50.713	15.10	14.44	n.a.
Total:			**173.862**	**351.193**	**100.00**	**100.00**	

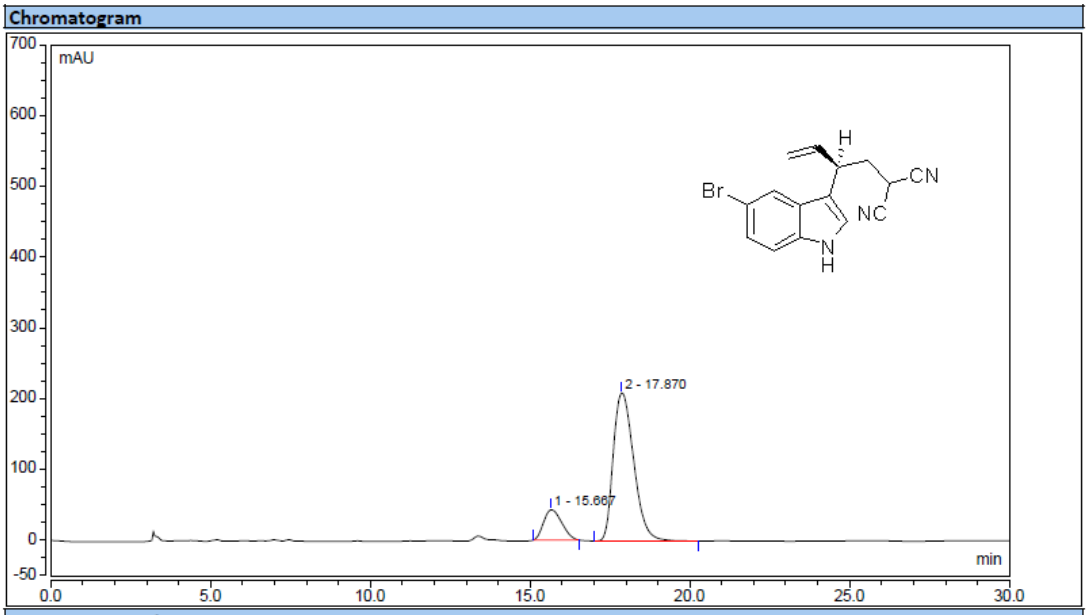
3ga Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.550	88.495	150.489	49.78	46.70	n.a.
2		17.417	89.276	171.785	50.22	53.30	n.a.
Total:			**177.771**	**322.275**	**100.00**	**100.00**	

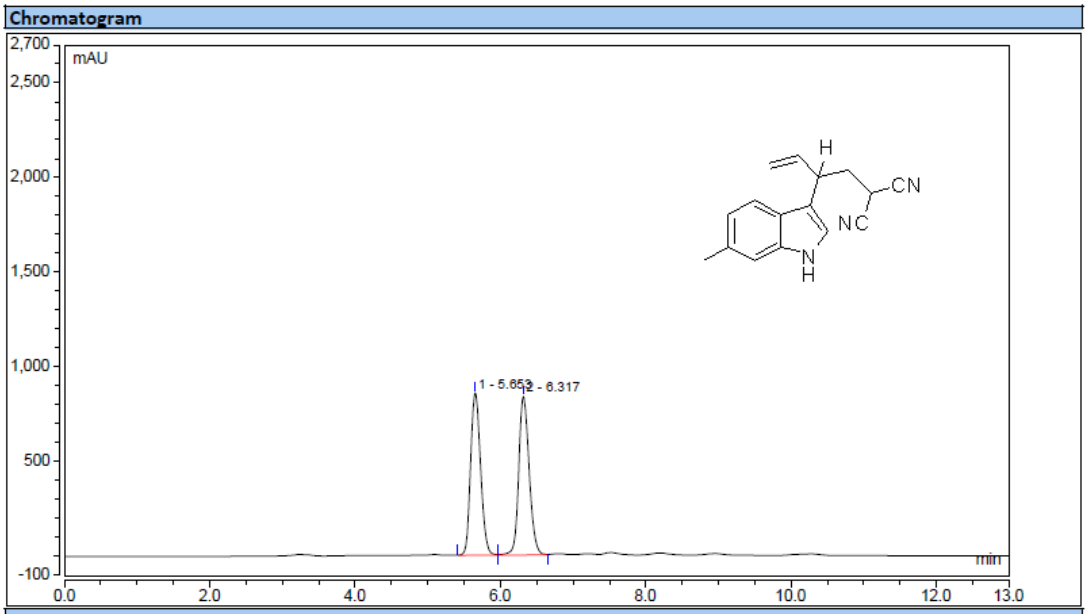
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.667	28.045	42.900	15.24	16.98	n.a.
2		17.870	156.036	209.679	84.76	83.02	n.a.
Total:			**184.081**	**252.579**	**100.00**	**100.00**	

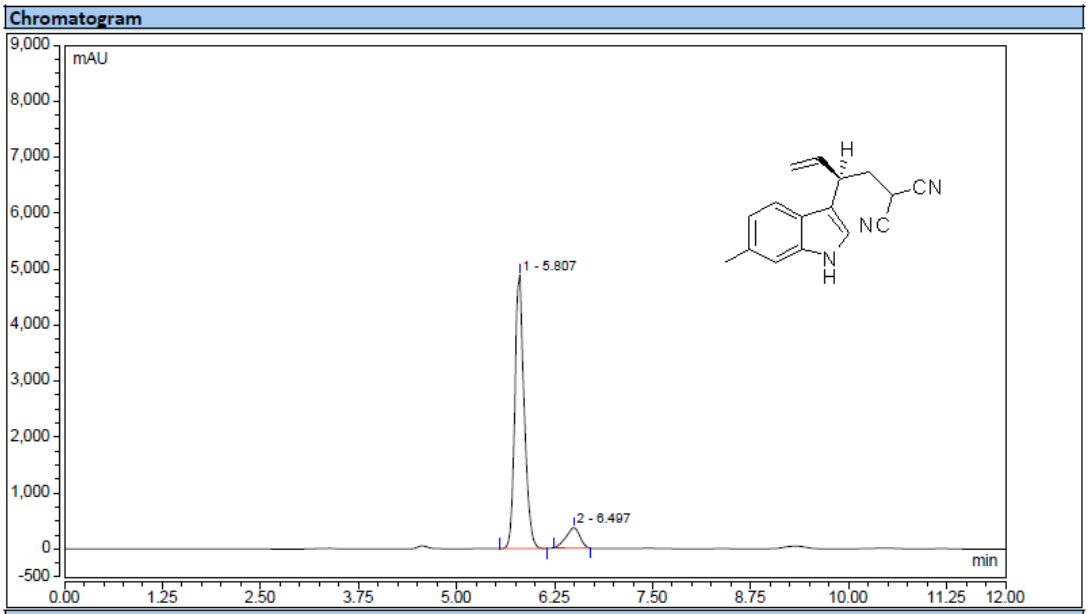
3ha Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.653	136.305	857.157	49.52	50.60	n.a.
2		6.317	138.952	836.987	50.48	49.40	n.a.
Total:			**275.258**	**1694.143**	**100.00**	**100.00**	

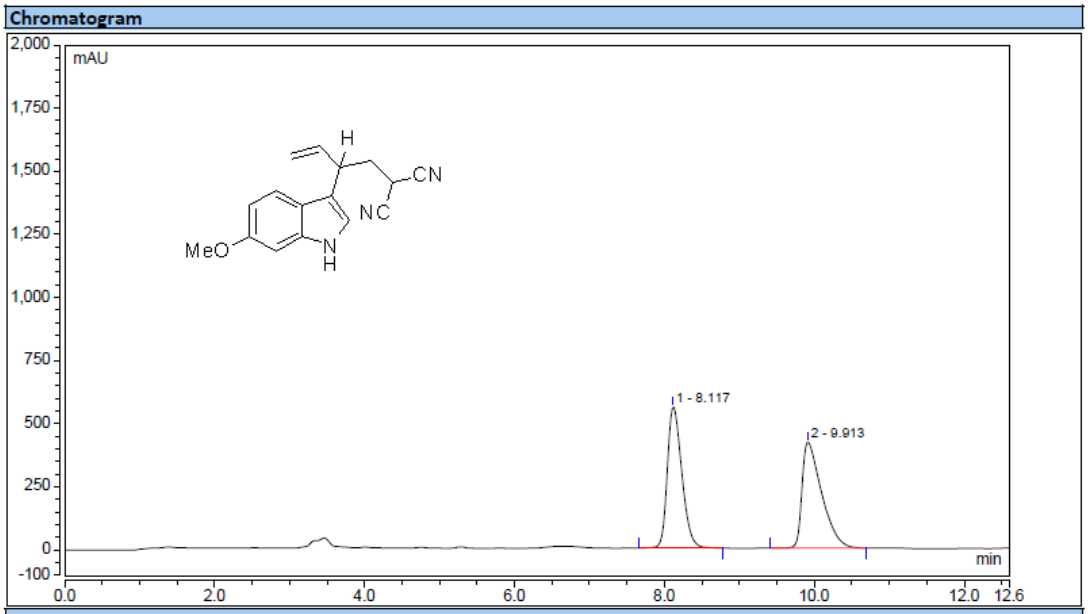
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.807	677.527	4891.934	90.14	93.06	n.a.
2		6.497	74.071	364.548	9.86	6.94	n.a.
Total:			**751.598**	**5256.482**	**100.00**	**100.00**	

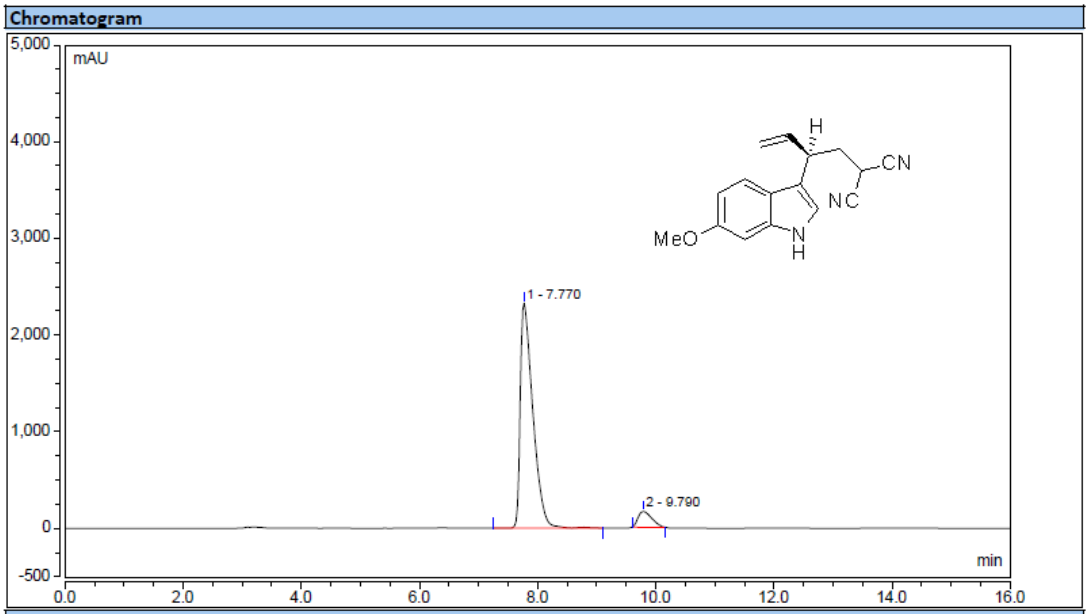
3ia Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.117	126.333	560.257	49.80	57.16	n.a.
2		9.913	127.361	419.899	50.20	42.84	n.a.
Total:			**253.694**	**980.156**	**100.00**	**100.00**	

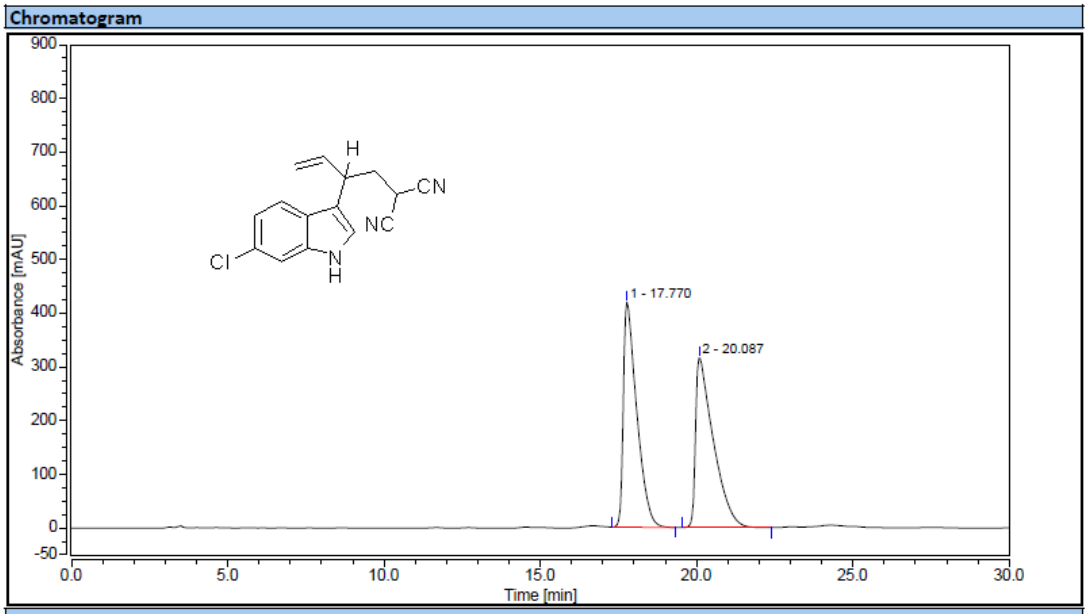
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.770	574.521	2329.749	92.86	93.45	n.a.
2		9.790	44.152	163.290	7.14	6.55	n.a.
Total:			**618.673**	**2493.039**	**100.00**	**100.00**	

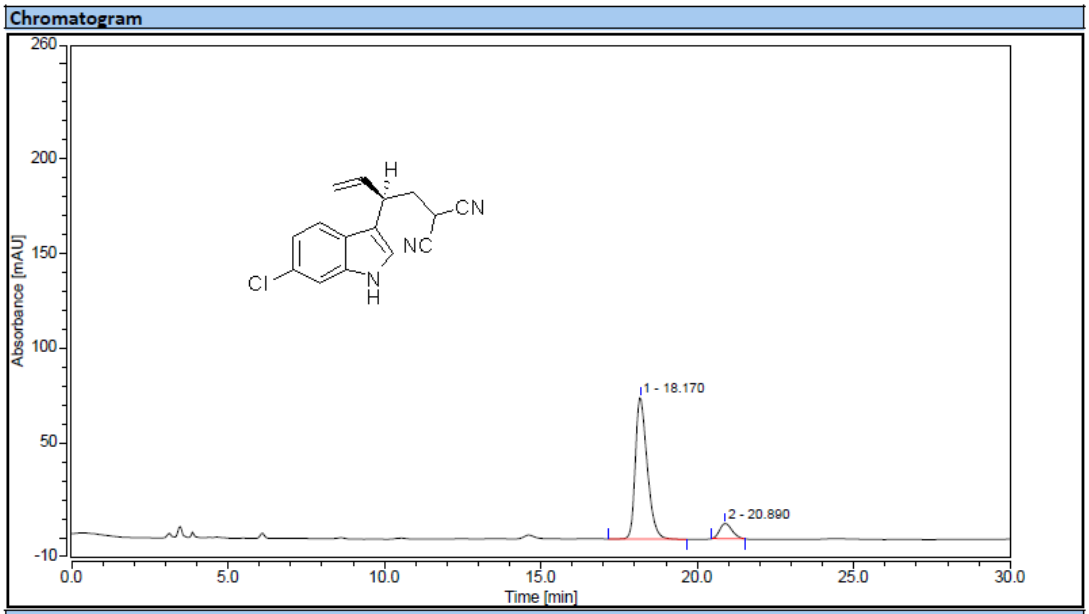
3ja Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.770	207.429	419.077	49.92	56.94	n.a.
2		20.087	208.125	316.937	50.08	43.06	n.a.
Total:			**415.553**	**736.014**	**100.00**	**100.00**	

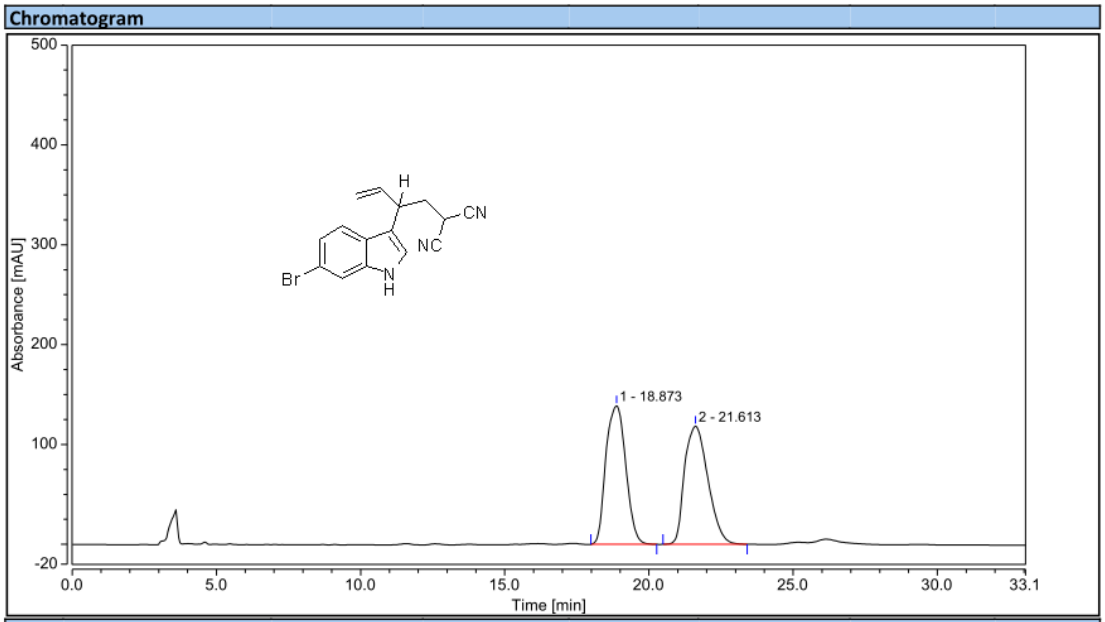
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.170	32.699	74.718	89.94	90.34	n.a.
2		20.890	3.659	7.989	10.06	9.66	n.a.
Total:			**36.358**	**82.708**	**100.00**	**100.00**	

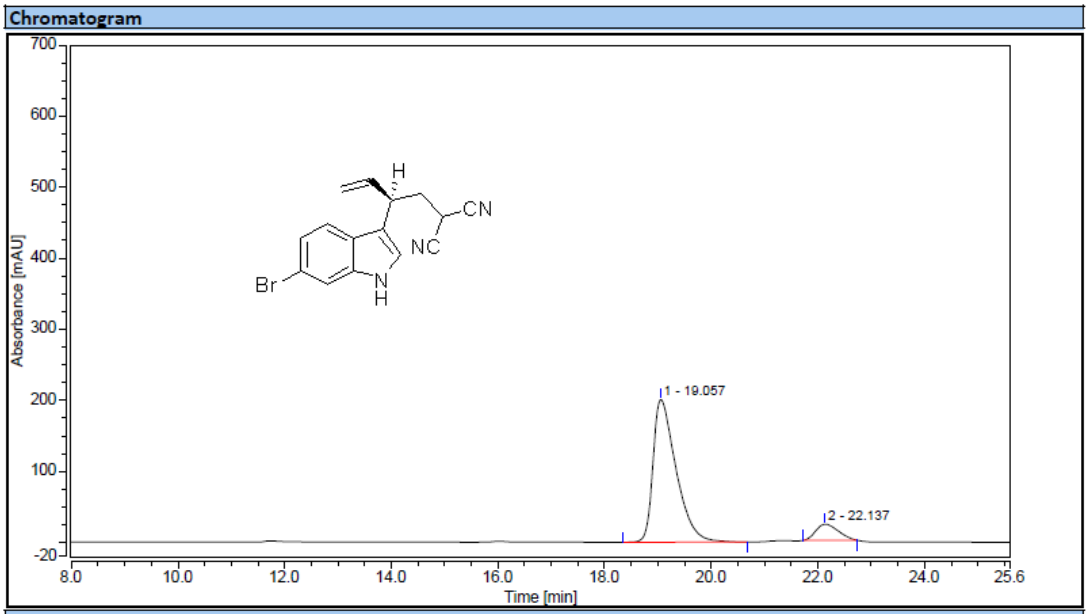
3ka Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.873	111.148	138.809	49.95	53.99	n.a.
2		21.613	111.378	118.314	50.05	46.01	n.a.
Total:			**222.526**	**257.123**	**100.00**	**100.00**	

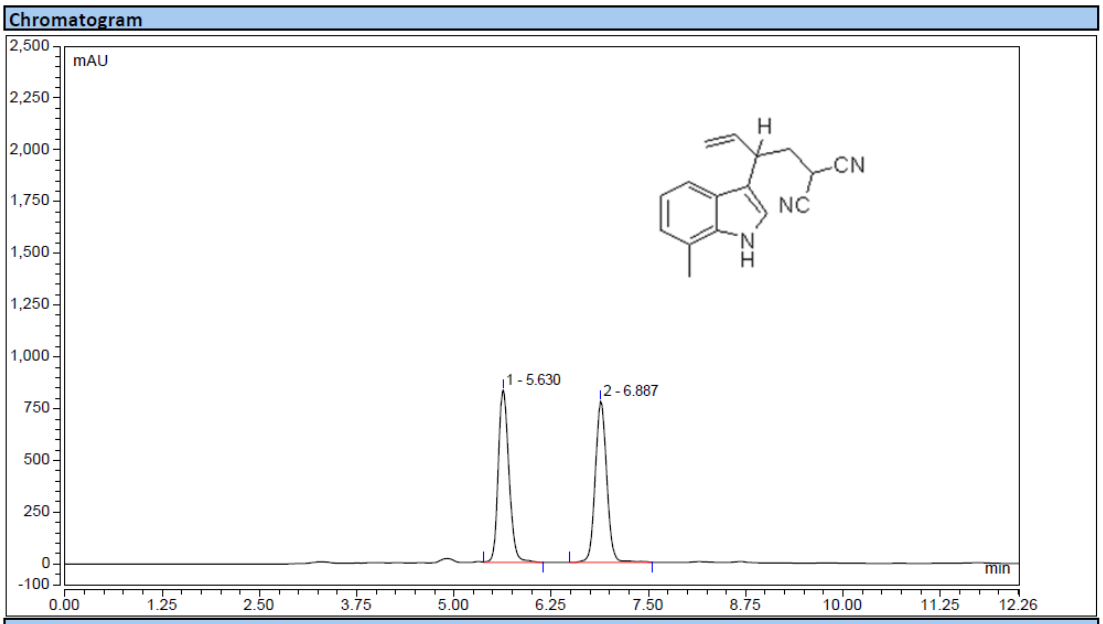
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		19.057	100.247	201.168	89.96	89.81	n.a.
2		22.137	11.193	22.837	10.04	10.19	n.a.
Total:			**111.440**	**224.005**	**100.00**	**100.00**	

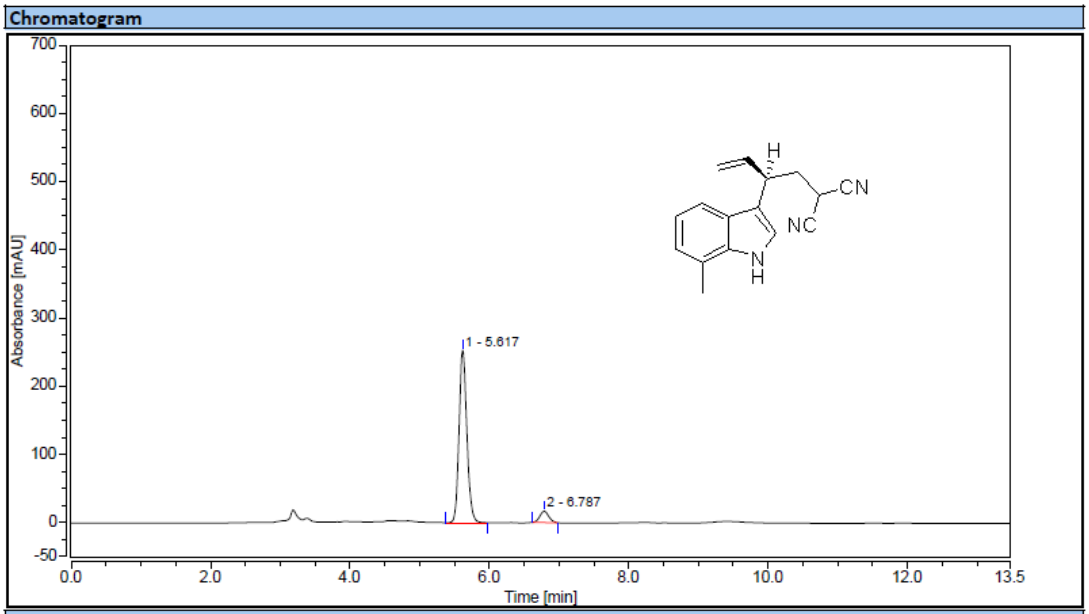
3la Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.630	133.180	832.878	50.00	51.61	n.a.
2		6.887	133.199	780.891	50.00	48.39	n.a.
Total:			**266.379**	**1613.769**	**100.00**	**100.00**	

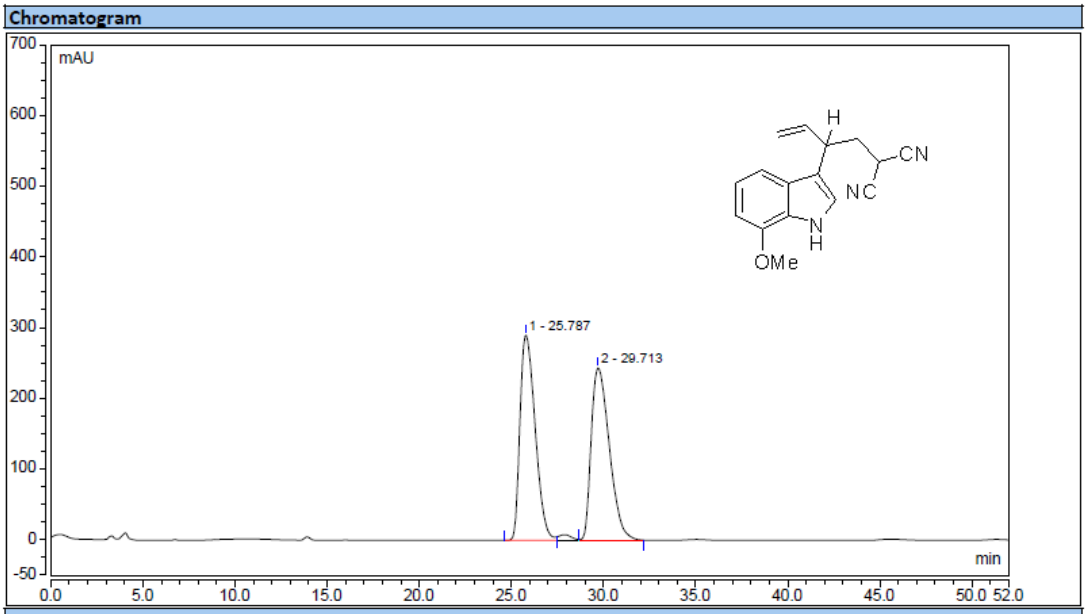
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.617	32.564	252.650	92.94	93.75	n.a.
2		6.787	2.472	16.849	7.06	6.25	n.a.
Total:			**35.036**	**269.500**	**100.00**	**100.00**	

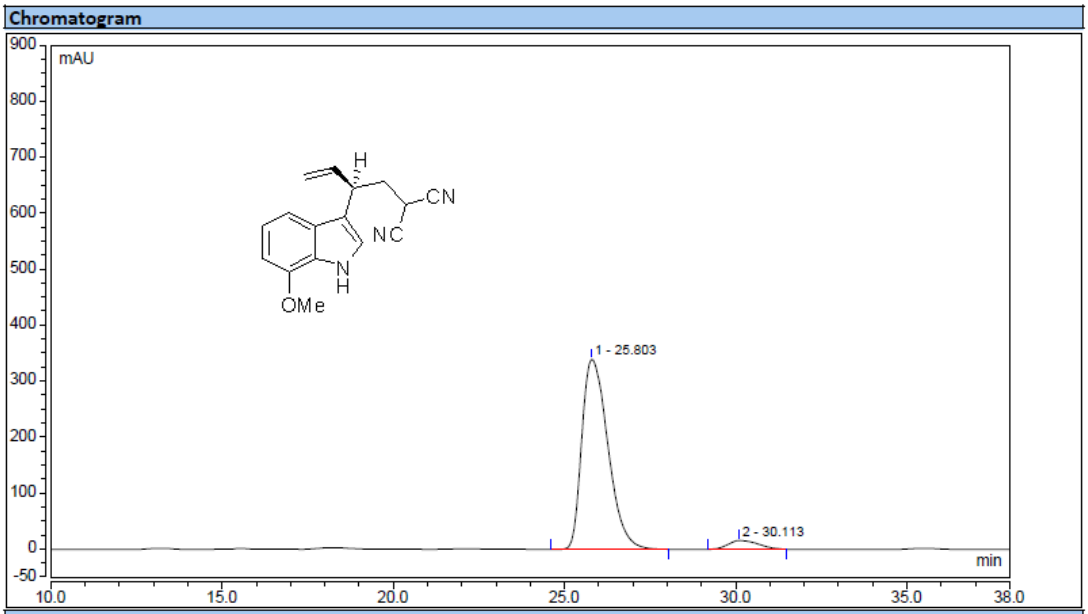
3ma Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		25.787	276.972	290.693	49.92	54.40	n.a.
2		29.713	277.891	243.682	50.08	45.60	n.a.
Total:			**554.863**	**534.376**	**100.00**	**100.00**	

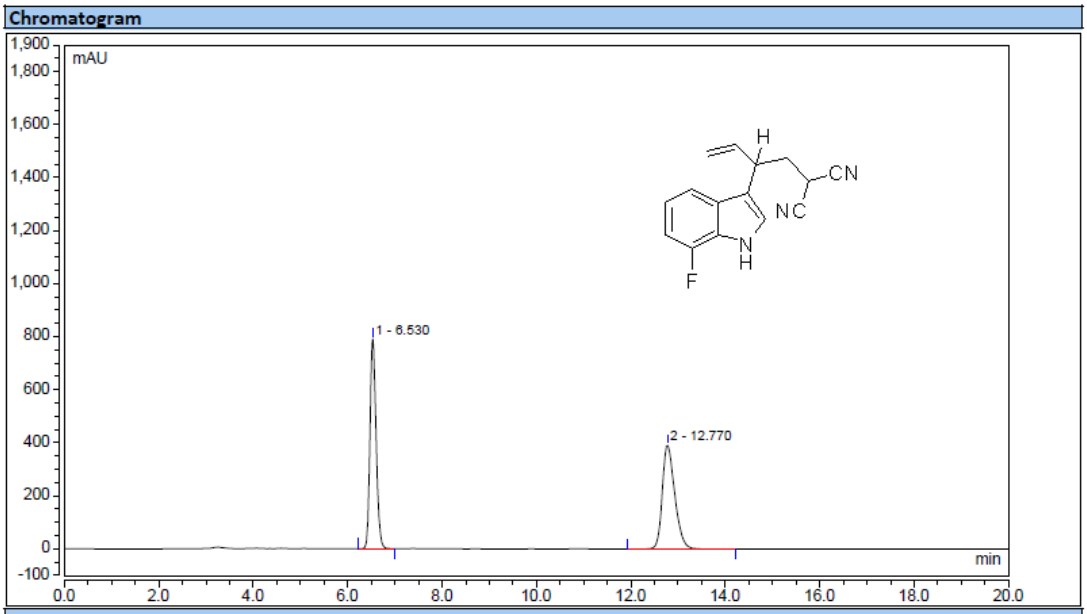
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		25.803	300.639	339.574	94.90	95.55	n.a.
2		30.113	16.144	15.806	5.10	4.45	n.a.
Total:			**316.783**	**355.380**	**100.00**	**100.00**	

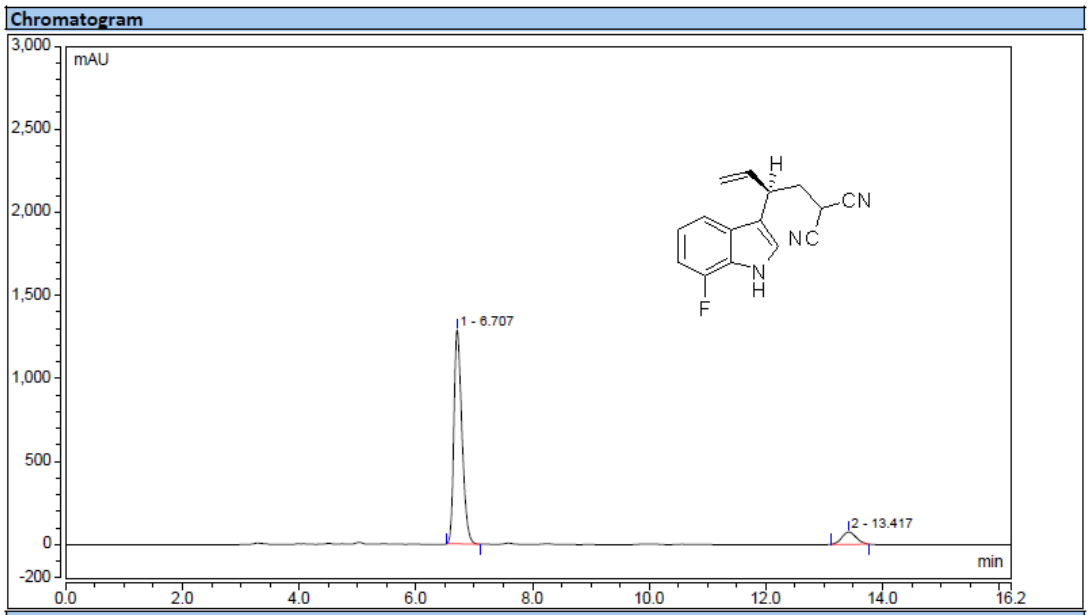
3na Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.530	118.290	791.798	49.80	66.88	n.a.
2		12.770	119.262	392.187	50.20	33.12	n.a.
Total:			**237.552**	**1183.986**	**100.00**	**100.00**	

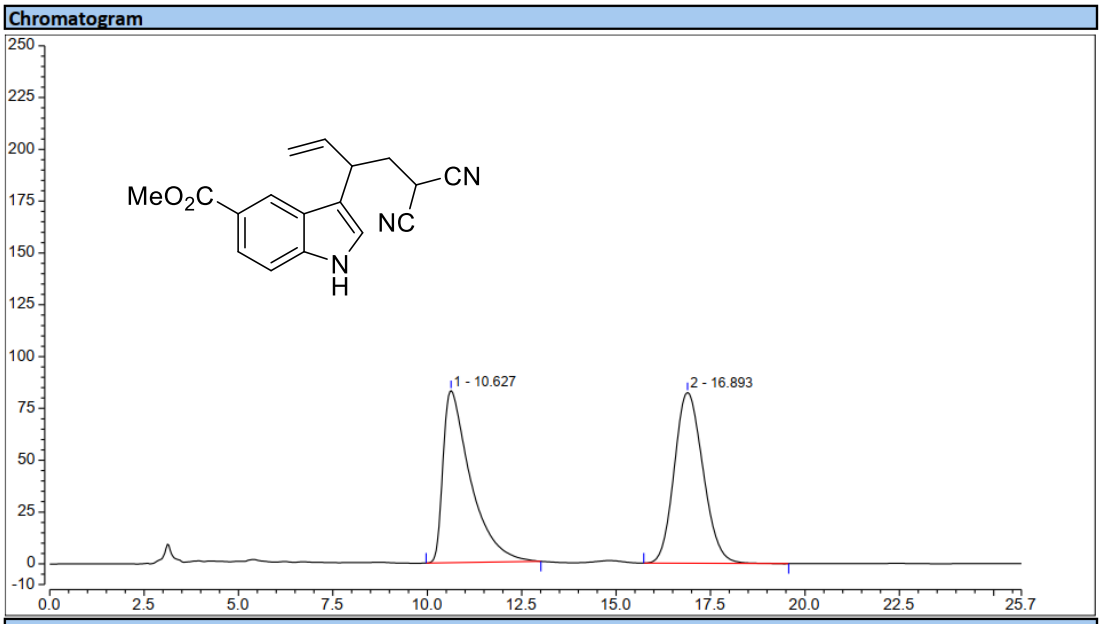
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.707	204.520	1287.230	90.76	94.62	n.a.
2		13.417	20.825	73.139	9.24	5.38	n.a.
Total:			**225.345**	**1360.369**	**100.00**	**100.00**	

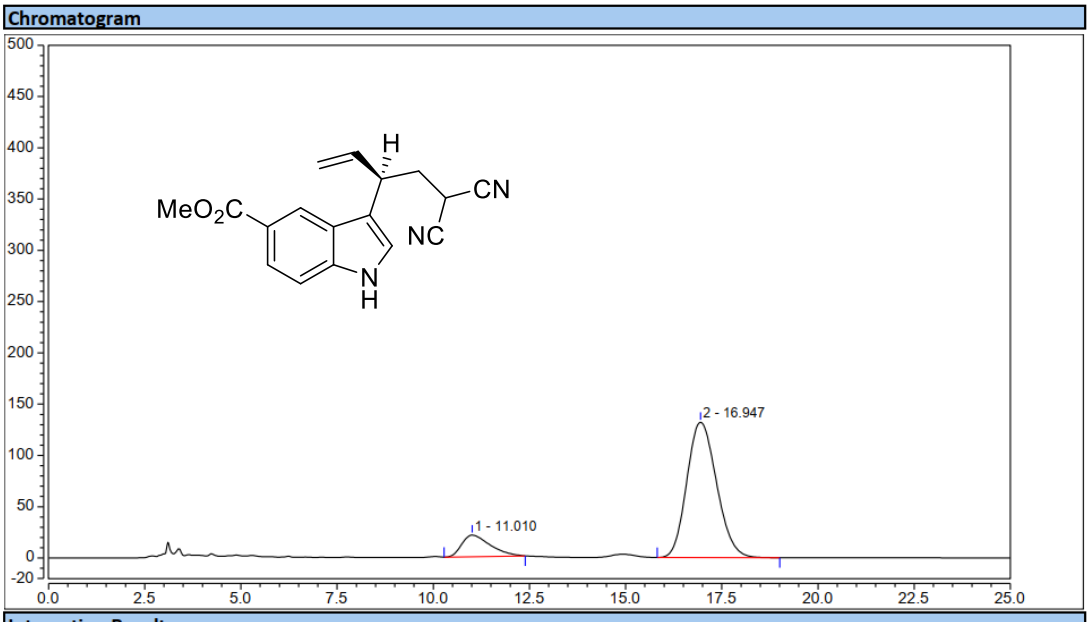
3oa Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.627	70.438	83.053	49.15	50.20	n.a.
2		16.893	72.883	82.377	50.85	49.80	n.a.
Total:			**143.320**	**165.430**	**100.00**	**100.00**	

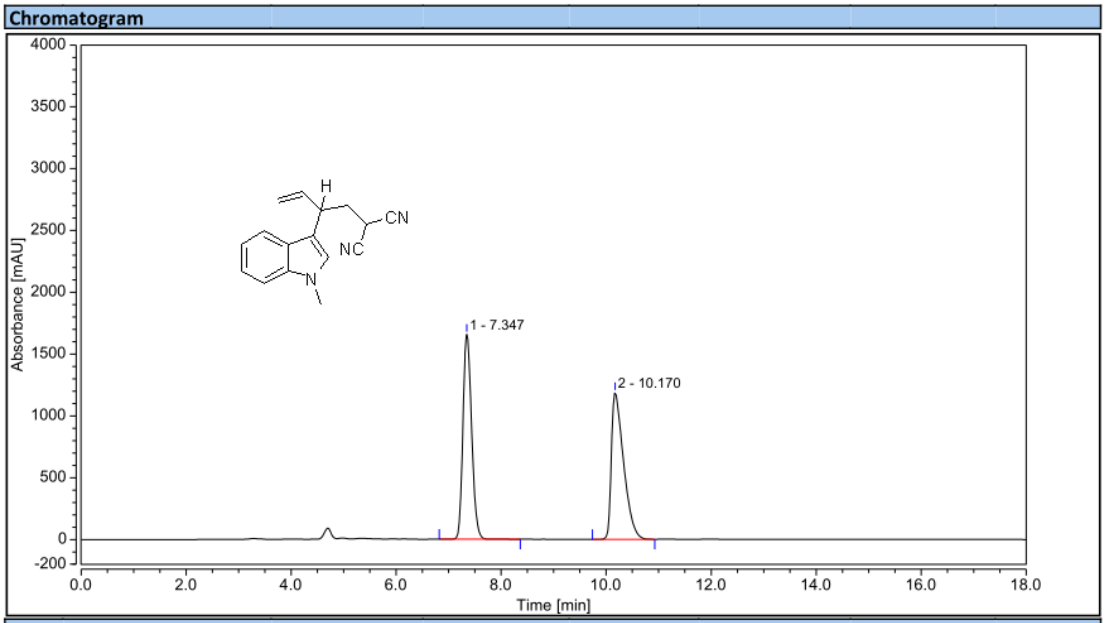
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.010	18.065	21.095	13.21	13.78	n.a.
2		16.947	118.644	132.039	86.79	86.22	n.a.
Total:			**136.709**	**153.134**	**100.00**	**100.00**	

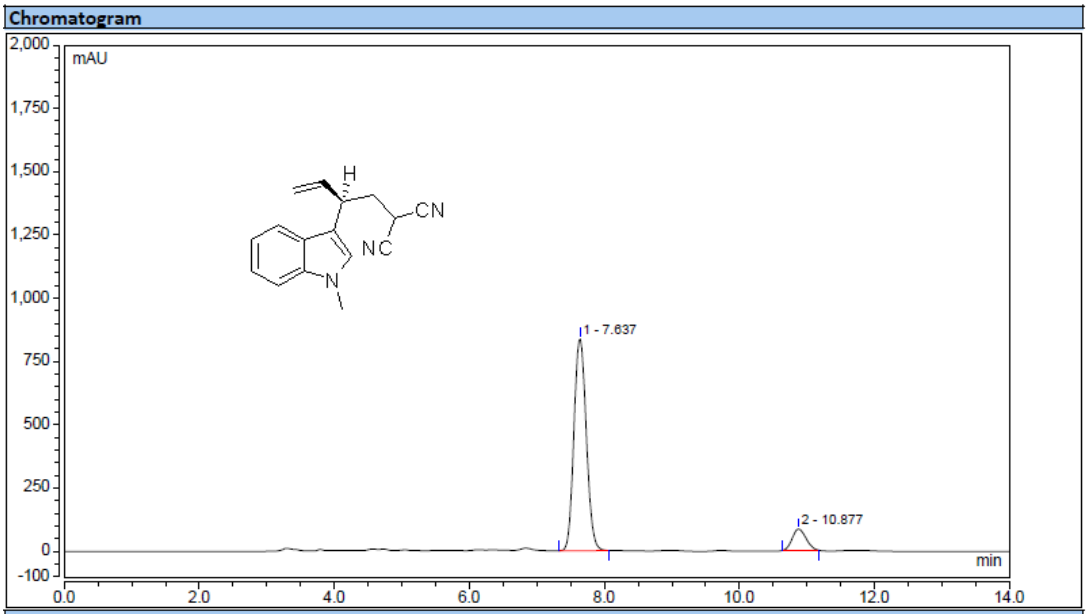
3qa Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.347	317.907	1657.181	49.85	58.24	n.a.
2		10.170	319.867	1188.413	50.15	41.76	n.a.
Total:			**637.774**	**2845.594**	**100.00**	**100.00**	

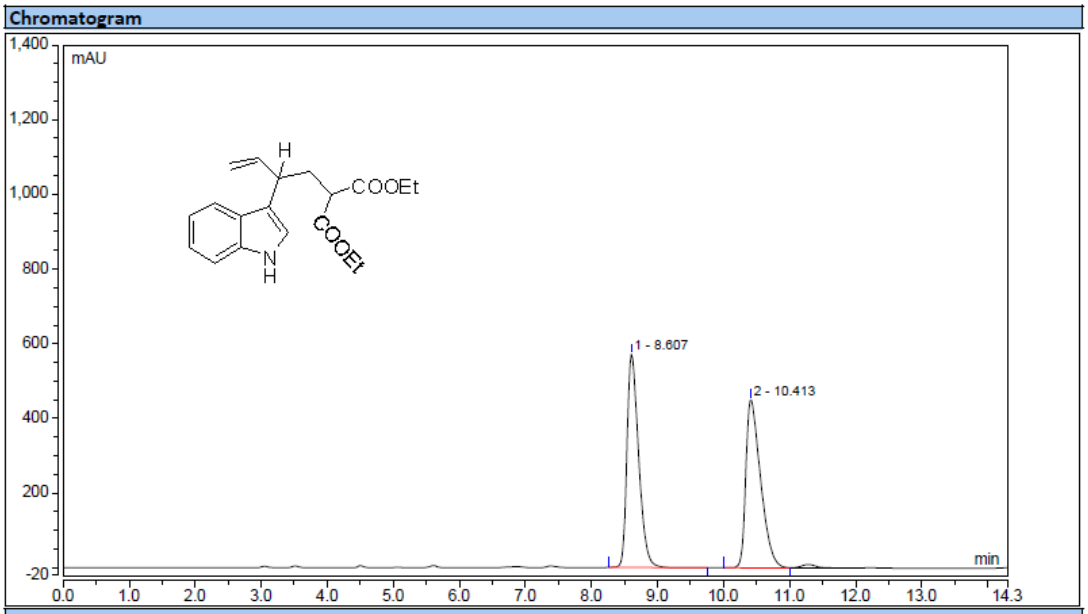
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.637	177.631	838.364	89.90	90.86	n.a.
2		10.877	19.953	84.332	10.10	9.14	n.a.
Total:			**197.583**	**922.696**	**100.00**	**100.00**	

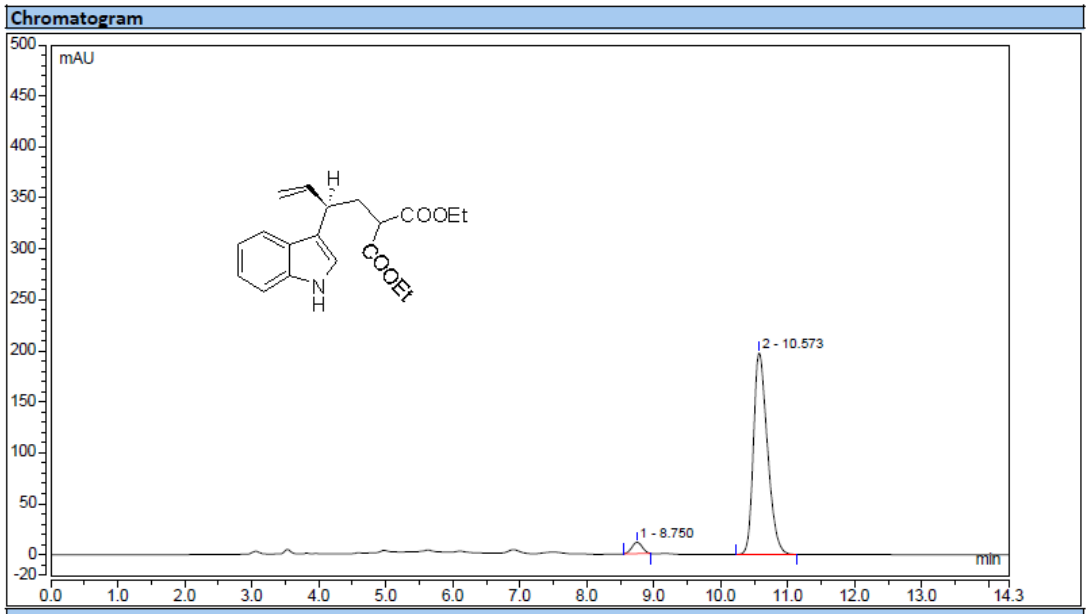
3ab Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.607	116.785	571.033	50.08	55.89	n.a.
2		10.413	116.431	450.712	49.92	44.11	n.a.
Total:			**233.216**	**1021.745**	**100.00**	**100.00**	

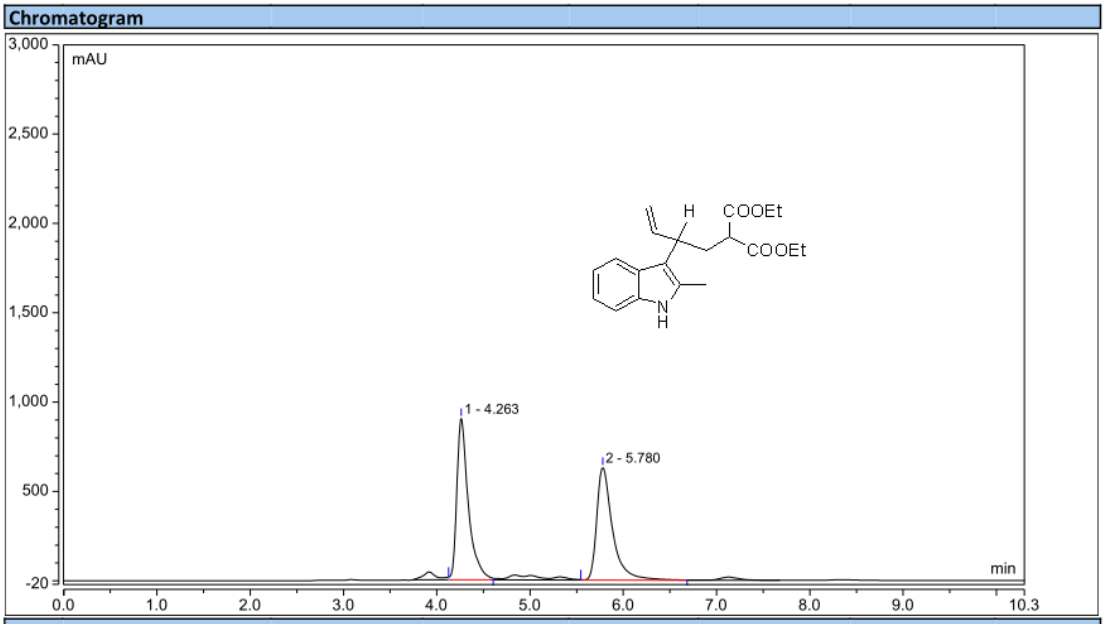
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.750	1.996	11.153	4.00	5.33	n.a.
2		10.573	47.959	198.292	96.00	94.67	n.a.
Total:			**49.956**	**209.445**	**100.00**	**100.00**	

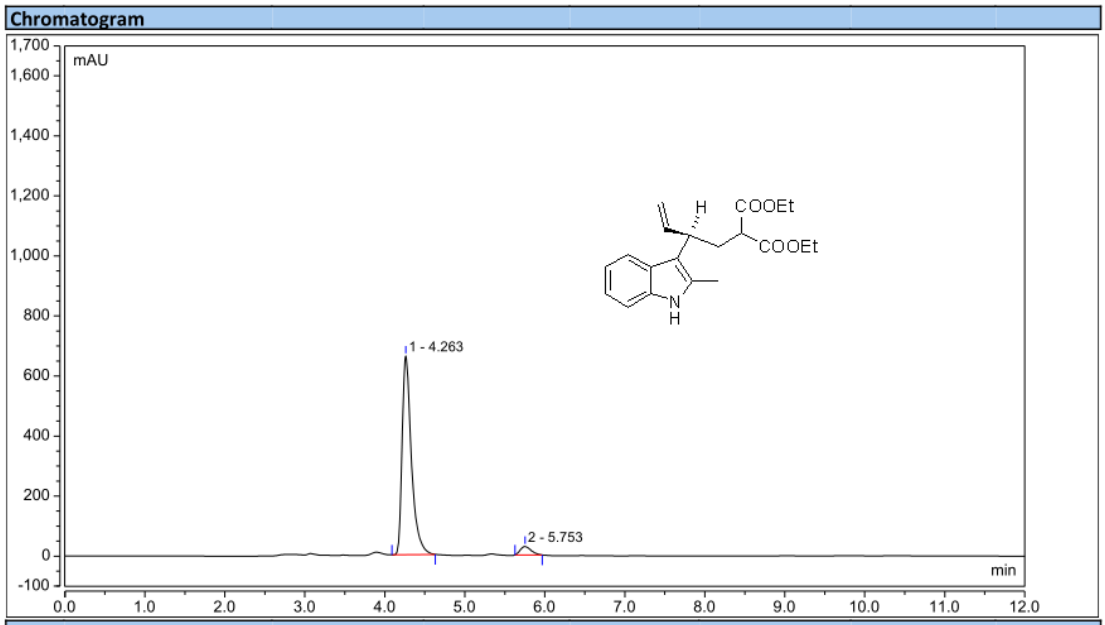
3bb Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.263	129.320	903.444	51.13	58.89	n.a.
2		5.780	123.601	630.732	48.87	41.11	n.a.
Total:			**252.921**	**1534.175**	**100.00**	**100.00**	

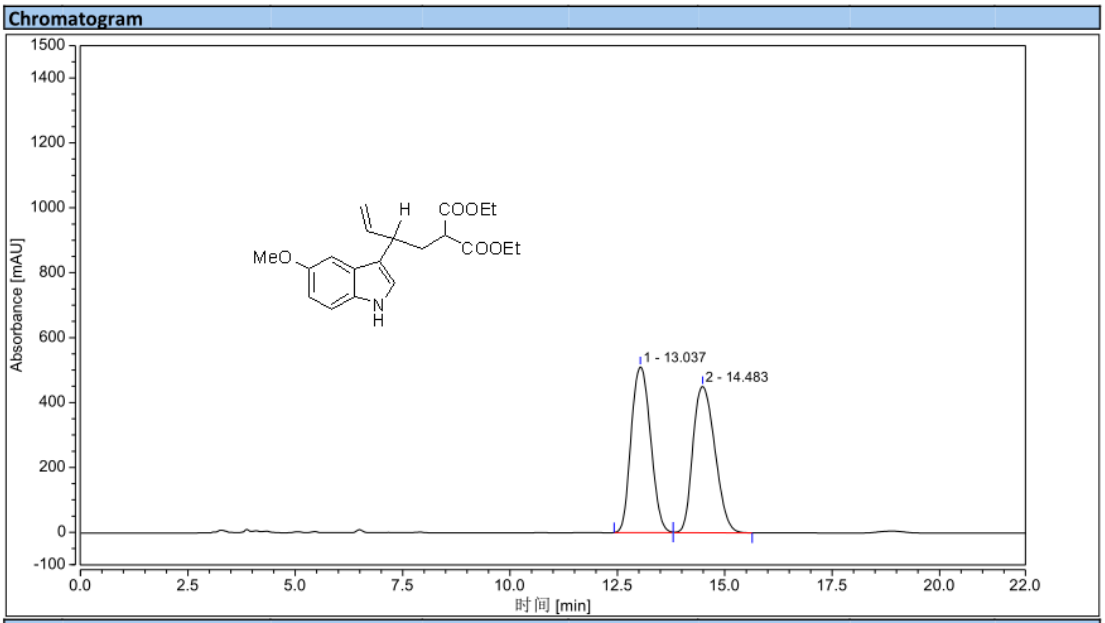
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.263	88.977	662.225	95.29	95.93	n.a.
2		5.753	4.401	28.111	4.71	4.07	n.a.
Total:			**93.378**	**690.336**	**100.00**	**100.00**	

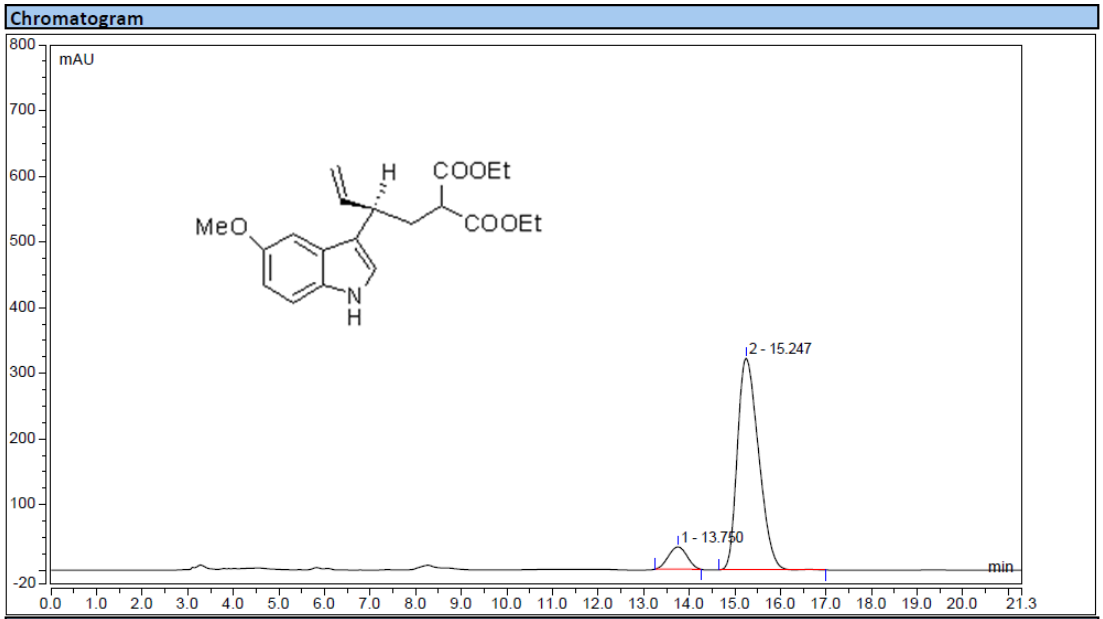
3eb Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.037	268.877	511.025	49.92	53.12	n.a.
2		14.483	269.765	451.067	50.08	46.88	n.a.
Total:			**538.642**	**962.092**	**100.00**	**100.00**	

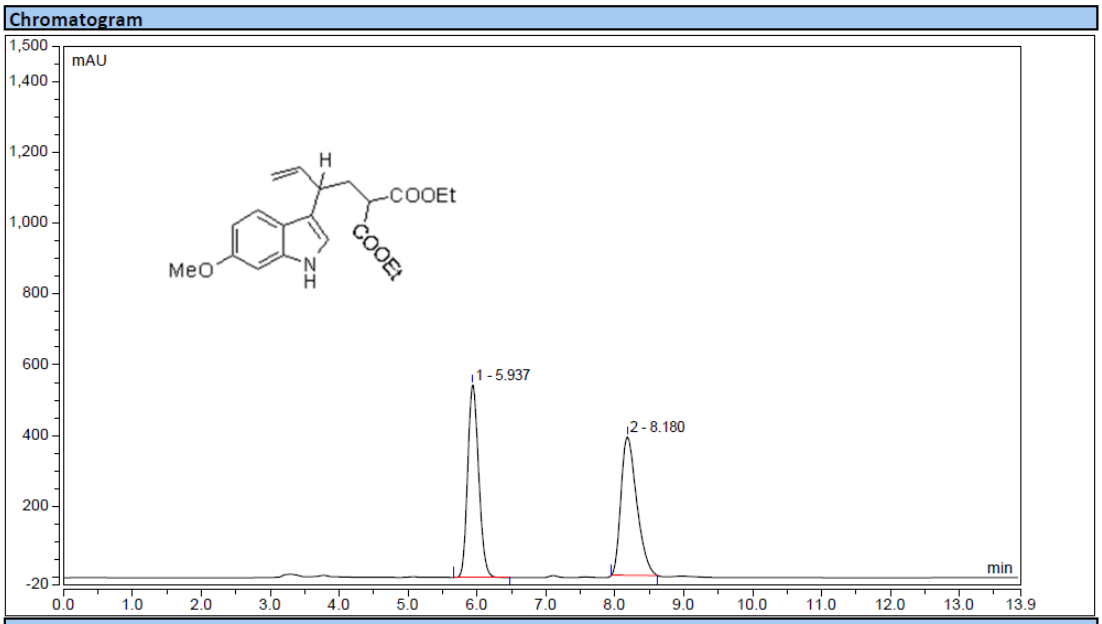
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.750	16.060	33.792	8.43	9.49	n.a.
2		15.247	174.489	322.449	91.57	90.51	n.a.
Total:			**190.549**	**356.240**	**100.00**	**100.00**	

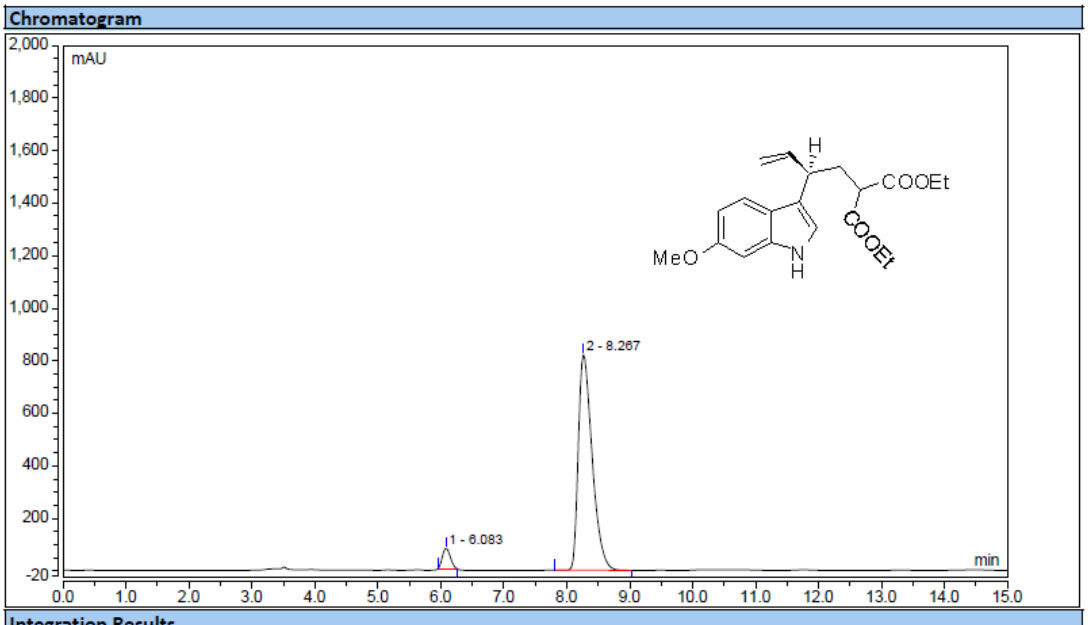
3ib Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.937	101.147	543.679	49.29	58.17	n.a.
2		8.180	104.076	391.027	50.71	41.83	n.a.
Total:			**205.223**	**934.707**	**100.00**	**100.00**	

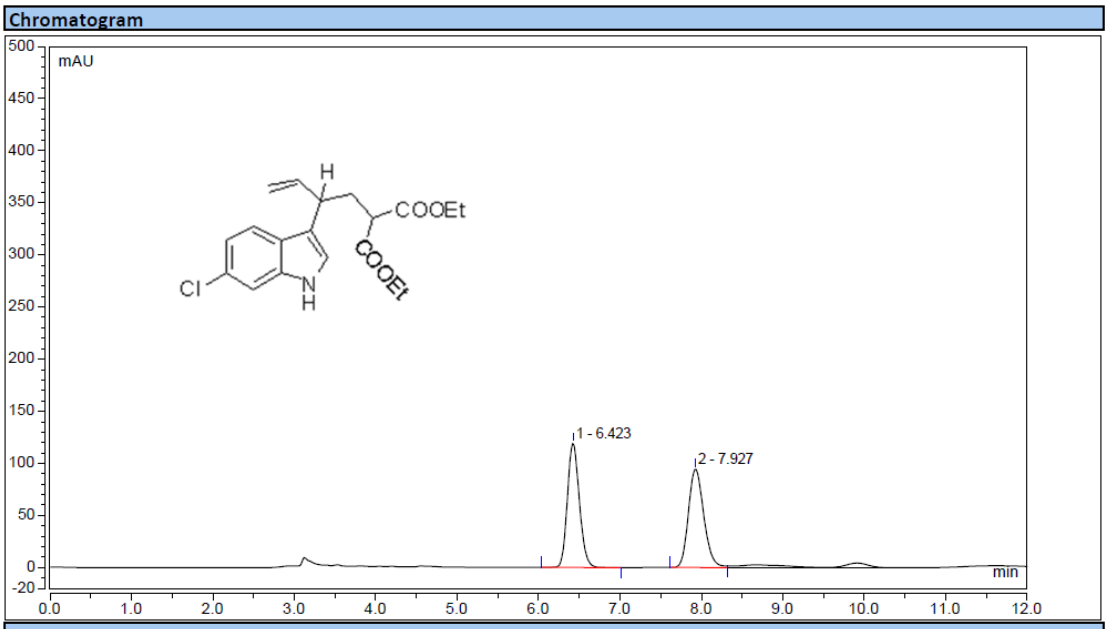
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.083	11.407	78.675	5.19	8.75	n.a.
2		8.267	208.333	820.824	94.81	91.25	n.a.
Total:			**219.740**	**899.499**	**100.00**	**100.00**	

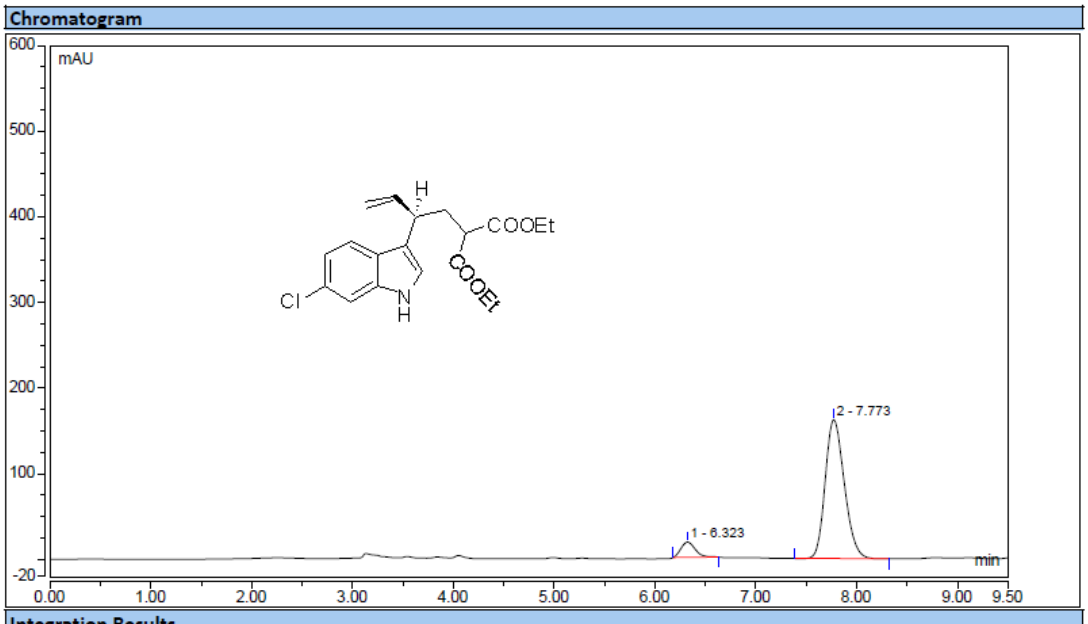
3jb Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.423	20.369	119.224	49.72	55.78	n.a.
2		7.927	20.594	94.509	50.28	44.22	n.a.
Total:			**40.963**	**213.734**	**100.00**	**100.00**	

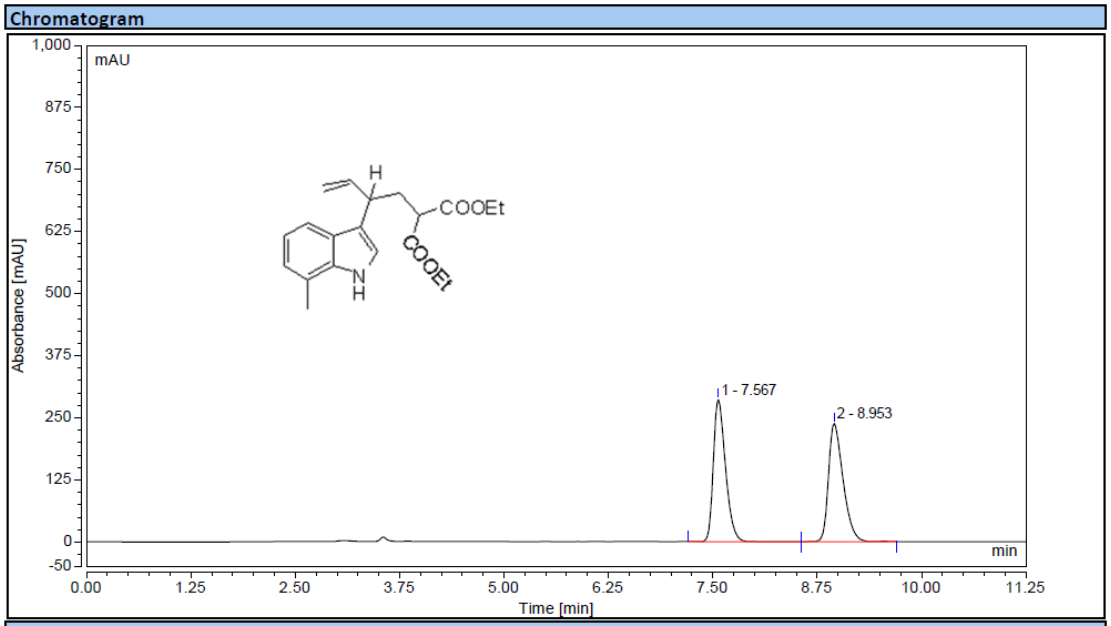
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.323	2.946	17.960	7.65	9.97	n.a.
2		7.773	35.563	162.220	92.35	90.03	n.a.
Total:			**38.509**	**180.179**	**100.00**	**100.00**	

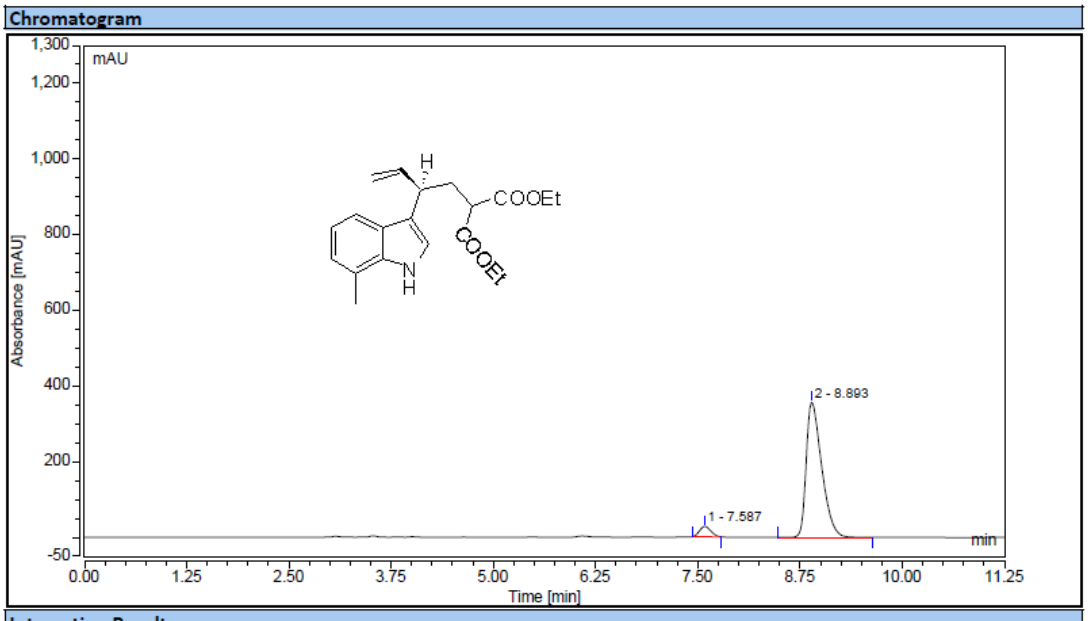
3lb Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.567	48.022	286.505	49.65	54.61	n.a.
2		8.953	48.706	238.177	50.35	45.39	n.a.
Total:			**96.728**	**524.682**	**100.00**	**100.00**	

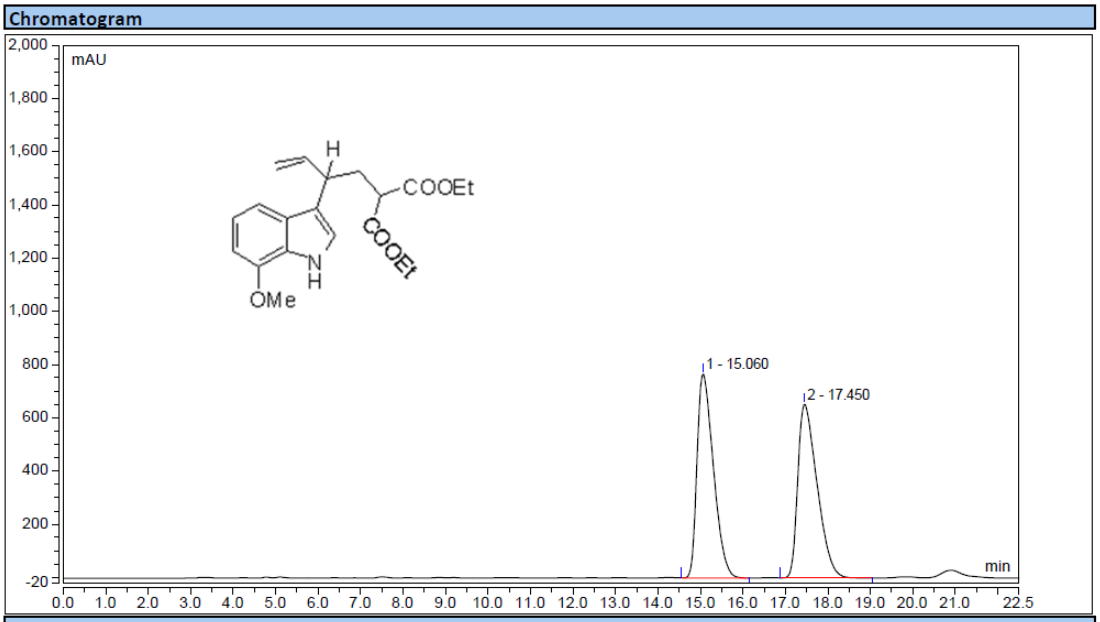
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.587	4.284	27.340	5.17	7.10	n.a.
2		8.893	78.505	357.598	94.83	92.90	n.a.
Total:			**82.789**	**384.937**	**100.00**	**100.00**	

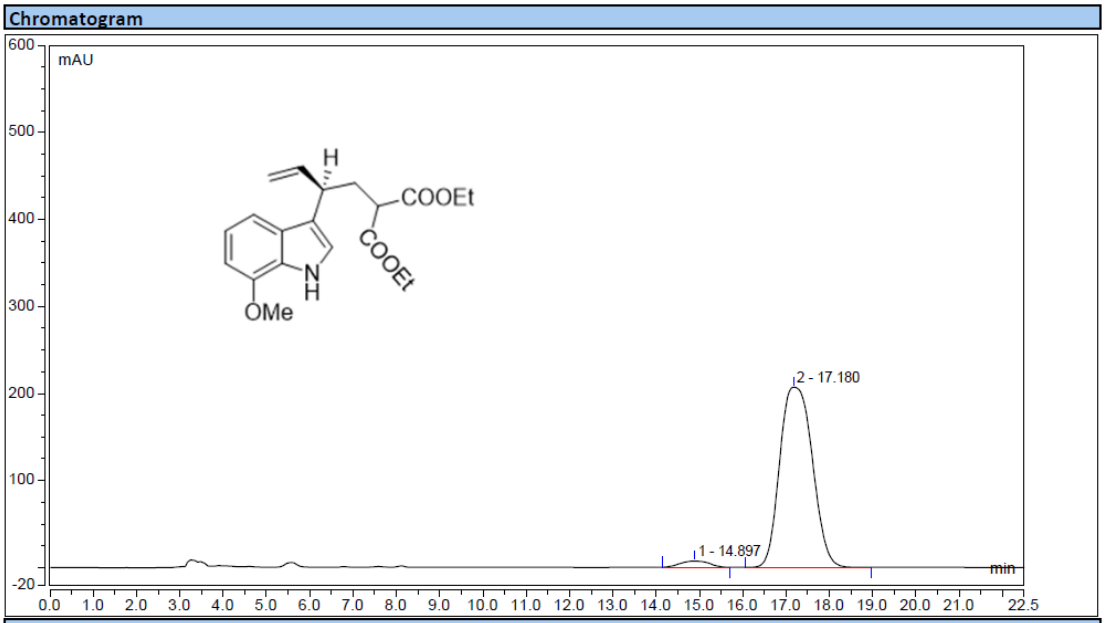
3mb Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.060	342.325	767.431	49.86	54.01	n.a.
2		17.450	344.240	653.507	50.14	45.99	n.a.
Total:			**686.565**	**1420.937**	**100.00**	**100.00**	

Enantioselective

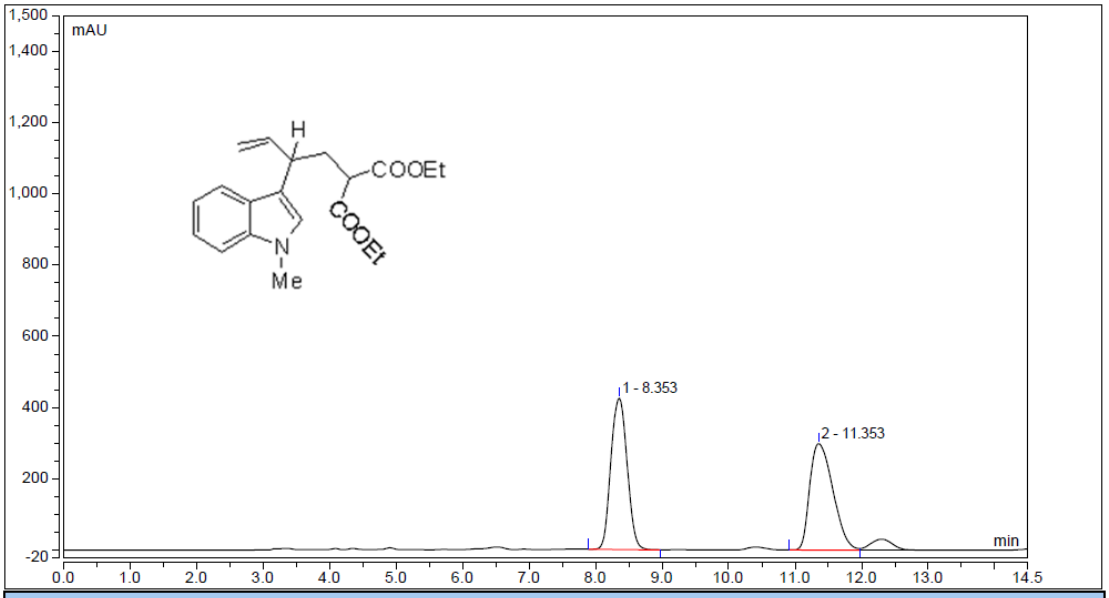


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.897	5.413	6.986	2.91	3.26	n.a.
2		17.180	180.685	206.996	97.09	96.74	n.a.
Total:			**186.098**	**213.982**	**100.00**	**100.00**	

3qb Racemic

Chromatogram

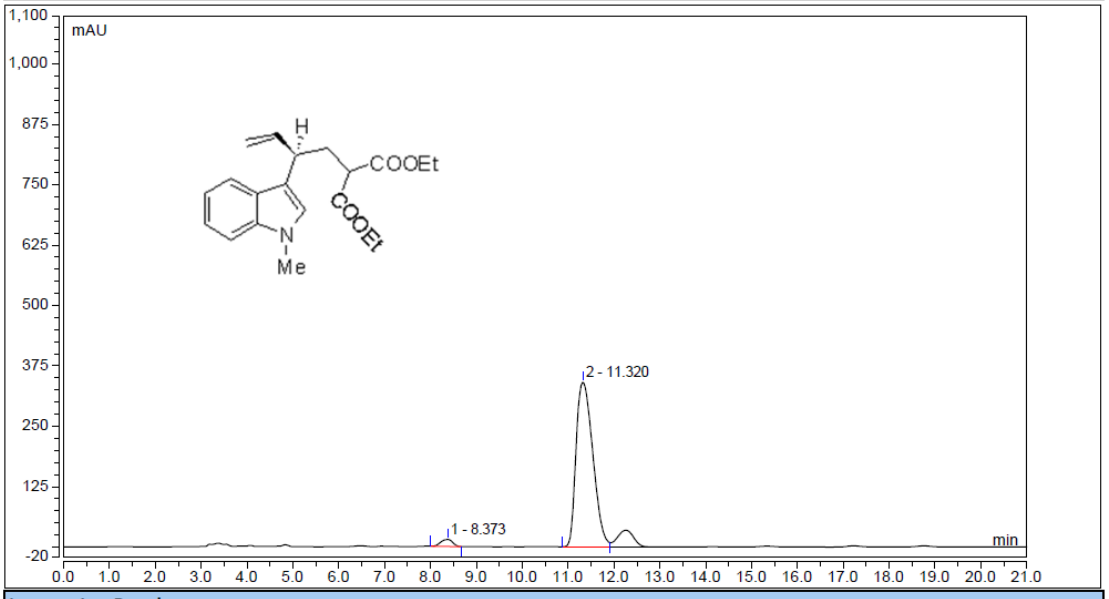


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.353	120.130	424.839	49.92	58.72	n.a.
2		11.353	120.539	298.684	50.08	41.28	n.a.
Total:			**240.669**	**723.523**	**100.00**	**100.00**	

Enantioselective

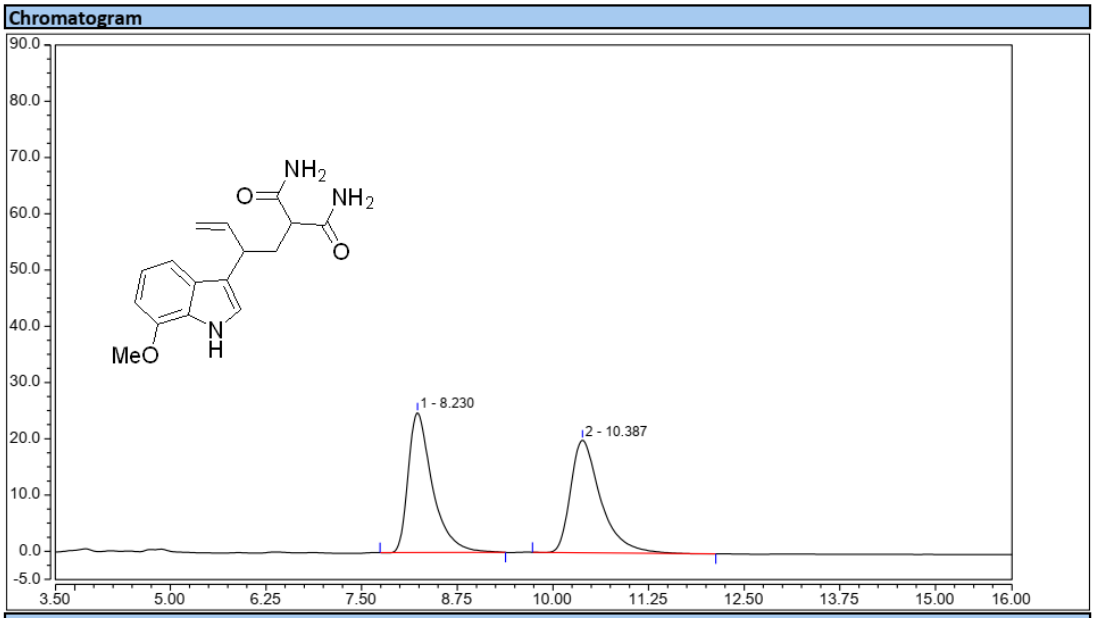
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.373	4.349	14.682	2.92	4.13	n.a.
2		11.320	144.467	340.914	97.08	95.87	n.a.
Total:			**148.816**	**355.596**	**100.00**	**100.00**	

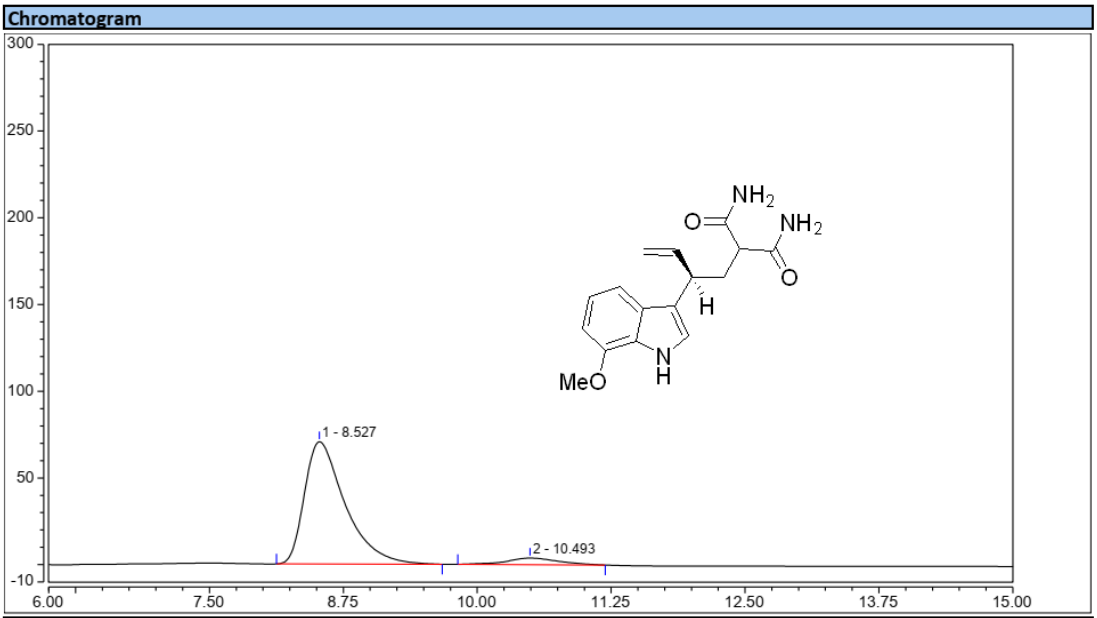
Compound 5: Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.230	9.161	24.846	50.19	55.41	n.a.
2		10.387	9.092	19.993	49.81	44.59	n.a.
Total:			**18.253**	**44.838**	**100.00**	**100.00**	

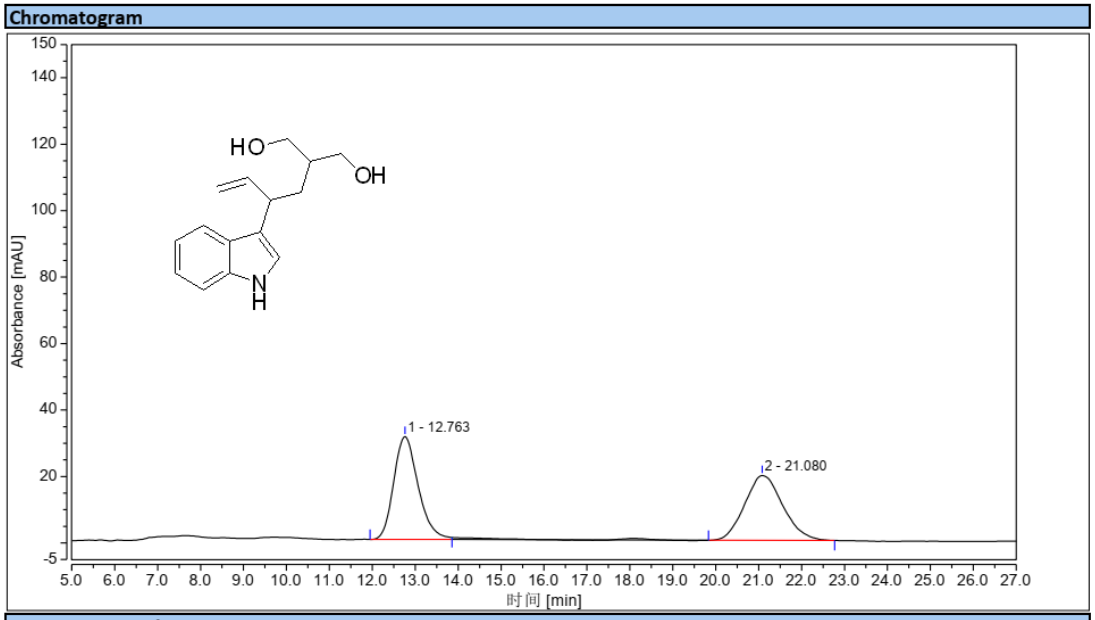
Enantioselective



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.527	31.067	70.521	93.55	94.88	n.a.
2		10.493	2.141	3.808	6.45	5.12	n.a.
Total:			**33.208**	**74.329**	**100.00**	**100.00**	

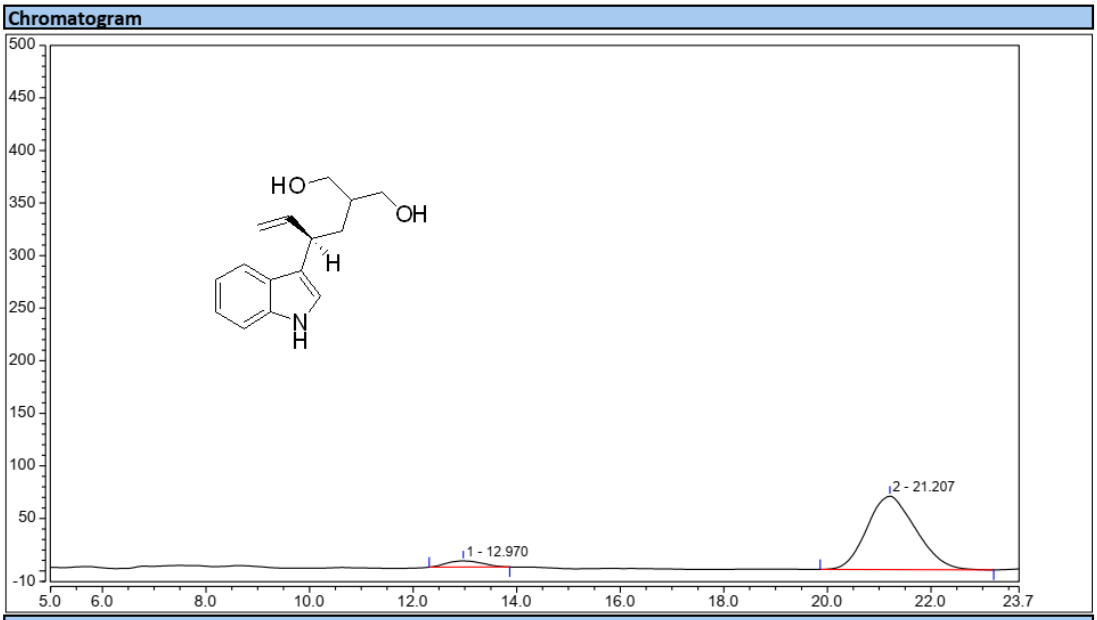
Compound 6: Racemic



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.763	20.417	30.946	50.53	61.36	n.a.
2		21.080	19.985	19.483	49.47	38.64	n.a.
Total:			**40.402**	**50.429**	**100.00**	**100.00**	

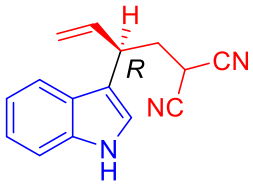
Enantioselective



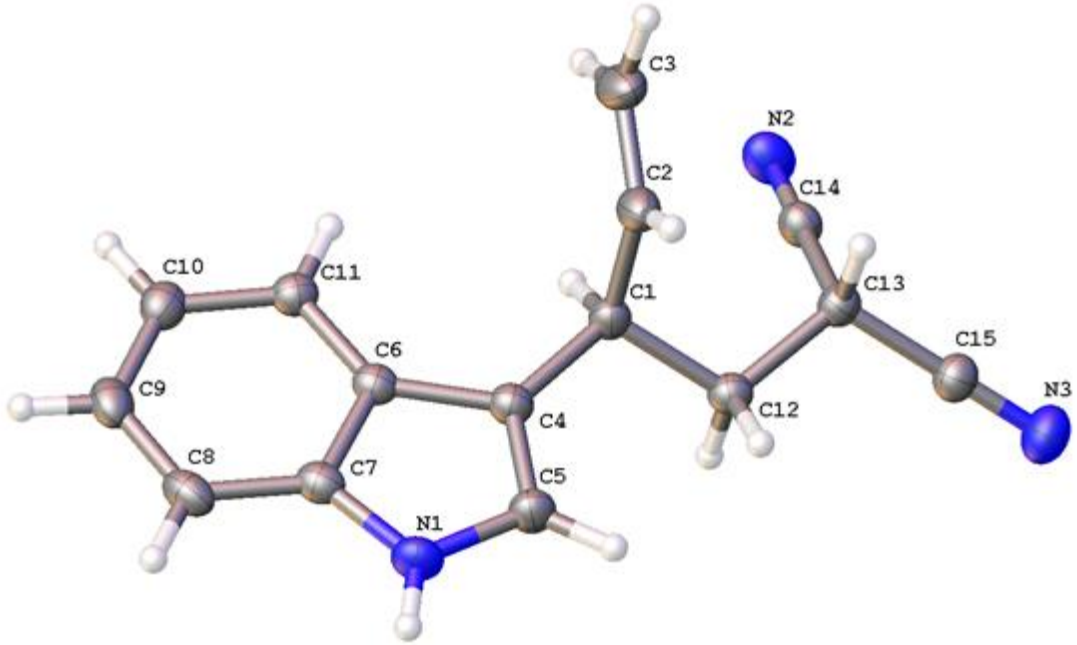
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.970	4.739	5.864	5.85	7.75	n.a.
2		21.207	76.293	69.794	94.15	92.25	n.a.
Total:			**81.032**	**75.658**	**100.00**	**100.00**	

3. X-ray single-crystal data of product 3aa



(*R*)-**3aa**



The thermal ellipsoid was drawn at the 30% probability level.

Identification code	20181217sf_0m	
Empirical formula	C15 H13 N3	
Formula weight	235.28	
Temperature	169.97 K	
Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.6046(4) Å	α= 90 °.
	b = 8.4709(6) Å	β= 90 °.
	c = 27.2897(18) Å	γ = 90 °.
Volume	1295.61(16) $Å^3$	
Z	4	
Density (calculated)	1.206 Mg/m^3	
Absorption coefficient	0.372 mm^{-1}	
F(000)	496	
Crystal size	0.12 x 0.1 x 0.01 mm^3	

Theta range for data collection	4.755 to 54.877 °.
Index ranges	-6<=h<=5, -10<=k<=10, -32<=l<=33
Reflections collected	9001
Independent reflections	2303 [R(int) = 0.0218]
Completeness to theta = 53.594 °	96.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7508 and 0.5269
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2303 / 0 / 171
Goodness-of-fit on F^2	1.205
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0858
R indices (all data)	R1 = 0.0382, wR2 = 0.0869
Absolute structure parameter	0.07(18)
Extinction coefficient	n/a
Largest diff. peak and hole	0.147 and -0.158 e.$Å^{-3}$