Supplementary Information for

Highly diastereoselective Friedel-Crafts reaction of indoles with isatin-derived *N*-sulfinyl ketimines towards the efficient synthesis of chiral tetrasubstituted 3-indolyl-3-aminooxindoles

Jian-Ping Chen, Wen-Wen Chen, Yi Li and Ming-Hua Xu*

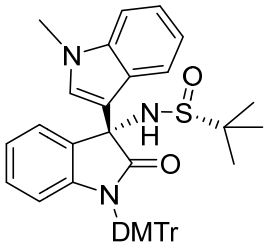
State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203, China

E-mail: xumh@simm.ac.cn

Table of Contents

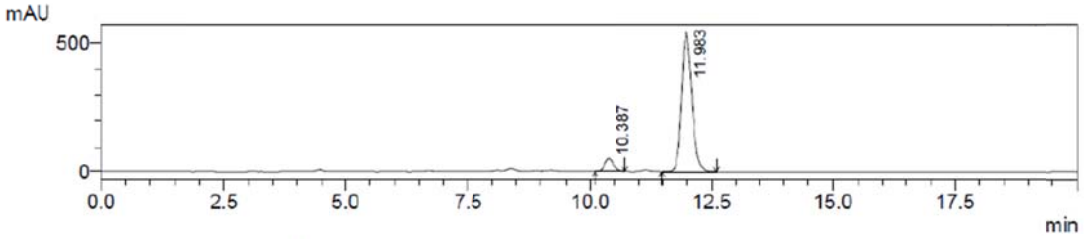
Copies of the HPLC Chromatograms of product 3, 5 and 6

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3g): 96% de



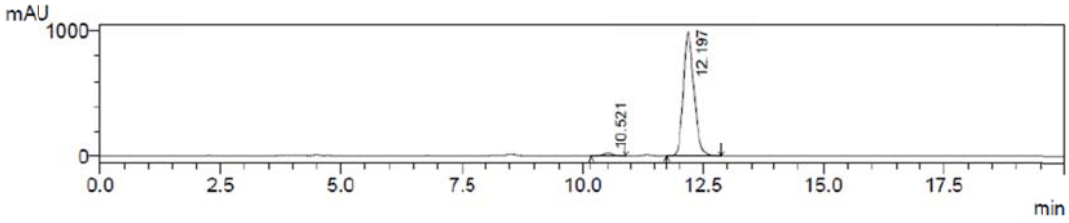
3g

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 10.52 min, 12.19 min (major).



PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	10.387	653222	50442	7.547
2	11.983	8002471	541814	92.453
Totals		8655693	592256	100.000

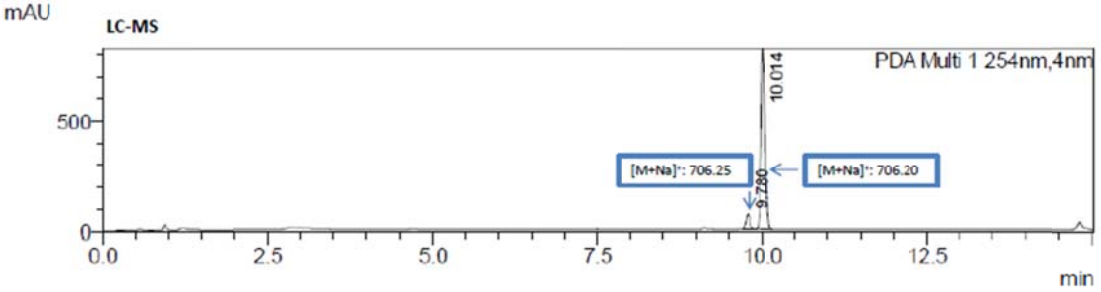


PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	10.521	320480	21622	2.053
2	12.197	15289276	992770	97.947
Totals		15609755	1014392	100.000

Analytical LC-MS of reference compound **3g**: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm;

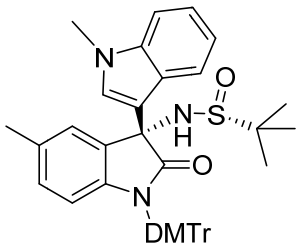
Retention time: 9.78 min, 10.01 min (major).



PDA Ch1 254nm

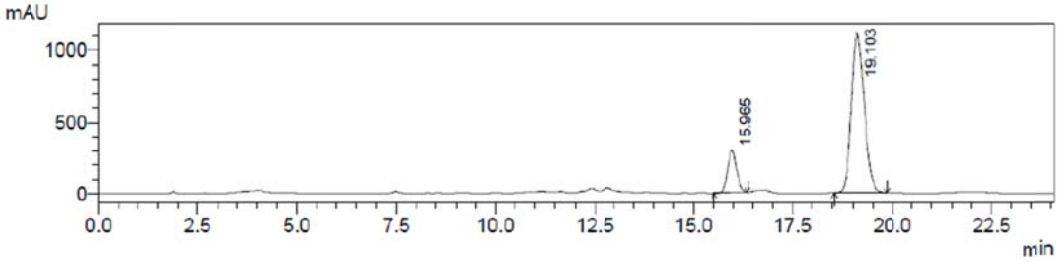
Peak#	Ret. Time	Area	Height	Area%
1	9.780	282257	69232	7.684
2	10.014	3391081	816367	92.316
Total		3673338	885599	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-methyl-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3h): 98% de



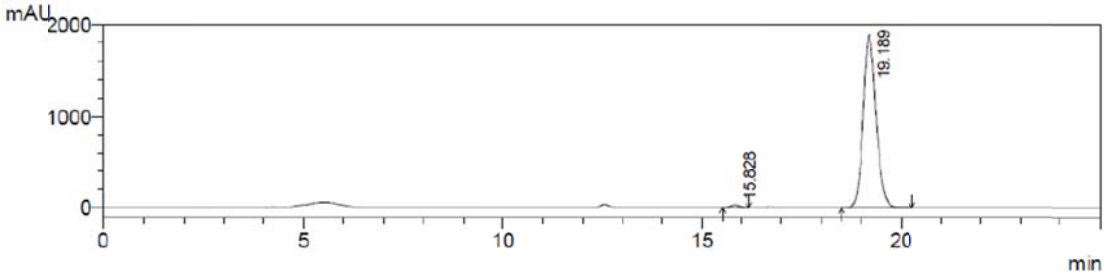
3h

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 15.82min, 19.18min (major).



PDA Ch1 254nm 4nm

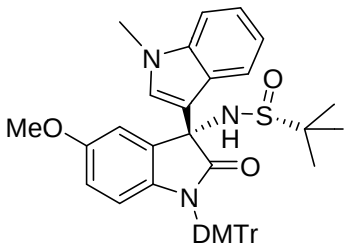
Peak#	RetTime	Area	Height	Area %
1	15.965	4759933	303189	15.784
2	19.103	25396394	1117090	84.216
Totals		30156326	1420279	100.000



PDA Ch1 254nm 4nm

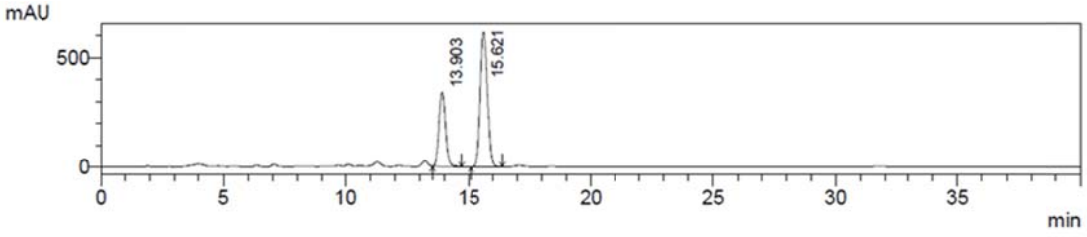
Peak#	RetTime	Area	Height	Area %
1	15.828	524999	31485	1.232
2	19.189	42104345	1888064	98.768
Totals		42629344	1919549	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-methoxy-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3i): 98% de



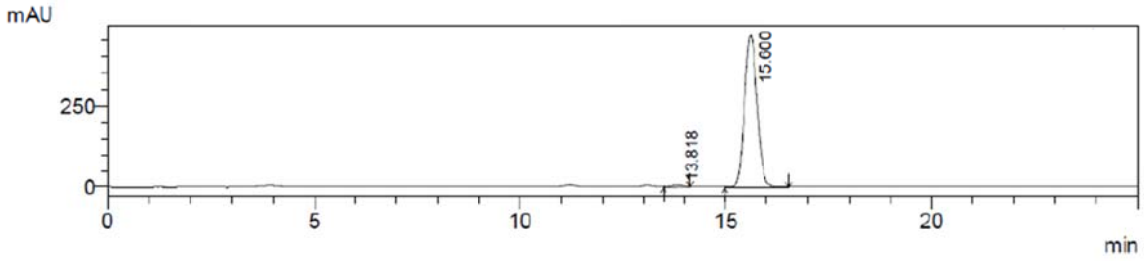
3i

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 70:30; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 13.81 min, 15.60 min (major).



PDA Ch1 254nm 4nm

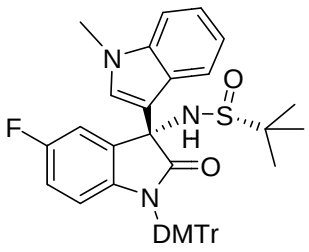
Peak#	RetTime	Area	Height	Area %
1	13.903	6439284	341217	33.625
2	15.621	12710836	618282	66.375
Totals		19150120	959499	100.000



PDA Ch1 254nm 4nm

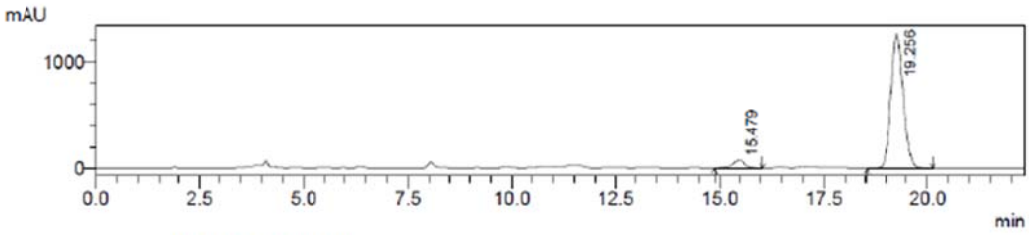
Peak#	RetTime	Area	Height	Area %
1	13.818	82646	4631	0.827
2	15.600	9909327	462076	99.173
Totals		9991973	466707	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-fluoro-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3j): 97% de



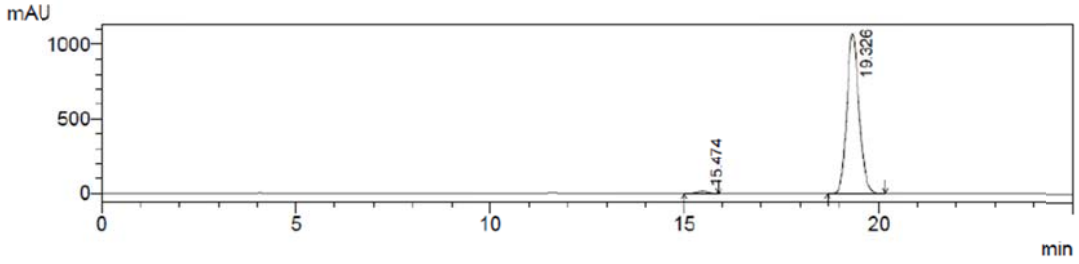
3j

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 70:30; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 15.47 min, 19.32 min (major).



PDA Ch1 254nm 4nm

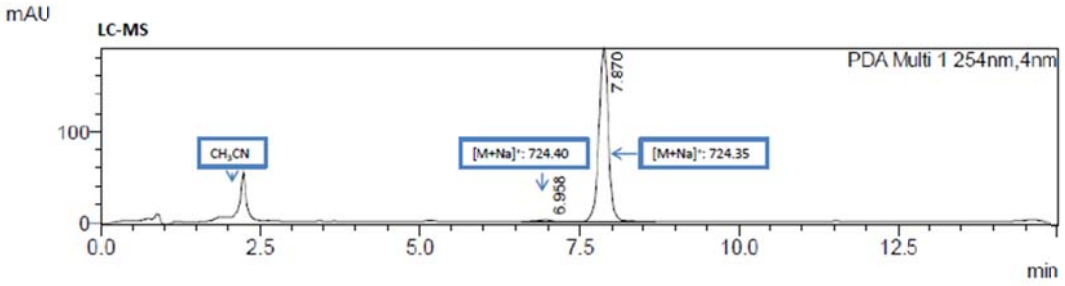
Peak#	RetTime	Area	Height	Area %
1	15.479	1733299	79434	6.257
2	19.256	25968684	1256676	93.743
Totals		27701983	1336110	100.000



PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	15.474	329503	15102	1.396
2	19.326	23267034	1067237	98.604
Totals		23596537	1082339	100.000

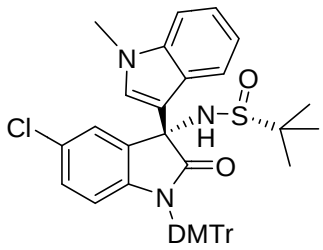
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15 min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 6.96 min, 7.87 min (major).



PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	6.958	25463	2061	1.314
2	7.870	1912752	187778	98.686
Total		1938216	189839	100.000

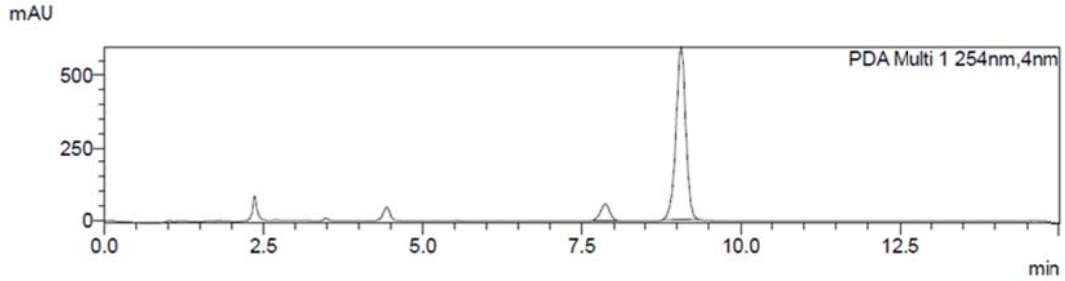
(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-chloro-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3k): 98% de



3k

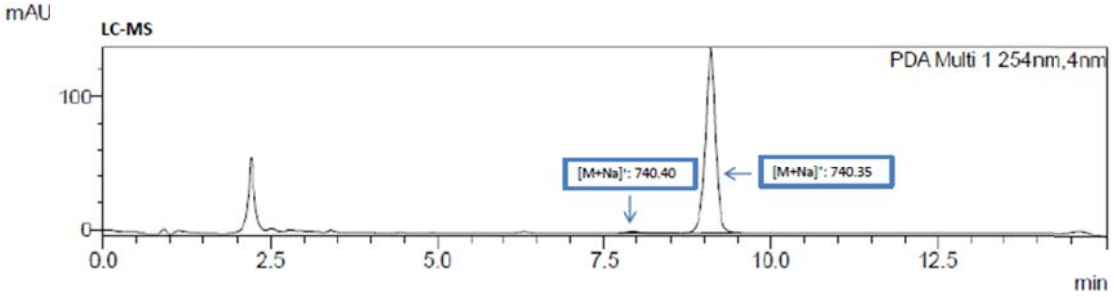
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 20min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm;

Retention time: 7.94 min, 9.10 min (major).



PDA Ch1 254nm

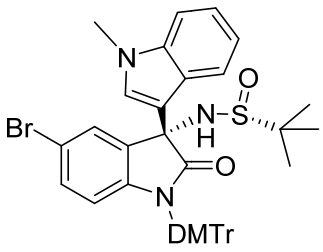
Peak#	Ret. Time	Area	Height	Area%
1	7.866	545476	55660	7.886
2	9.068	6371965	593929	92.114
Total		6917441	649589	100.000



PDA Ch1 254nm

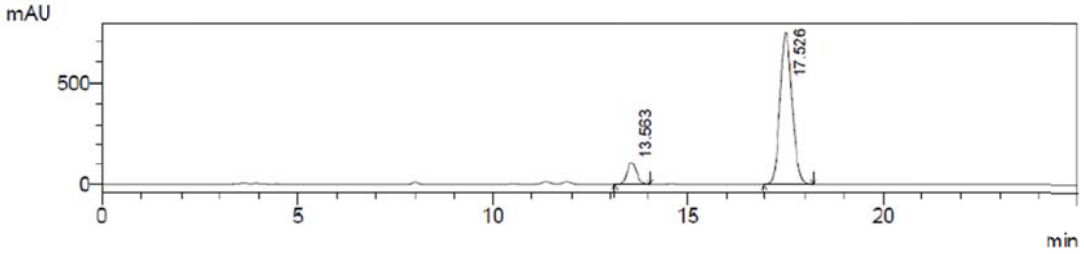
Peak#	Ret. Time	Area	Height	Area%
1	7.939	17136	1451	1.155
2	9.105	1466399	137547	98.845
Total		1483535	138999	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-bromo-3-(1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3l): 94% de



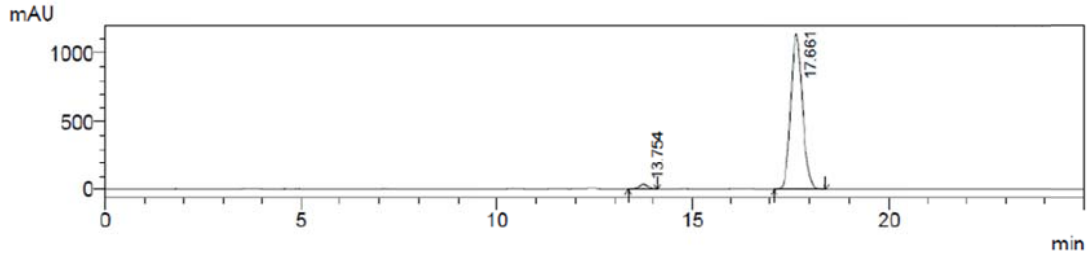
3l

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 13.75 min, 17.66 min (major).



PDA Ch1 254nm 4nm

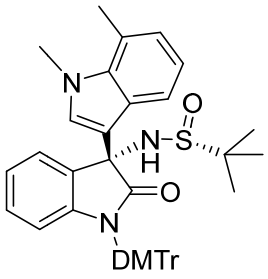
Peak#	RetTime	Area	Height	Area %
1	13.563	1822184	109125	10.315
2	17.526	15843976	743084	89.685
Totals		17666161	852210	100.000



PDA Ch1 254nm 4nm

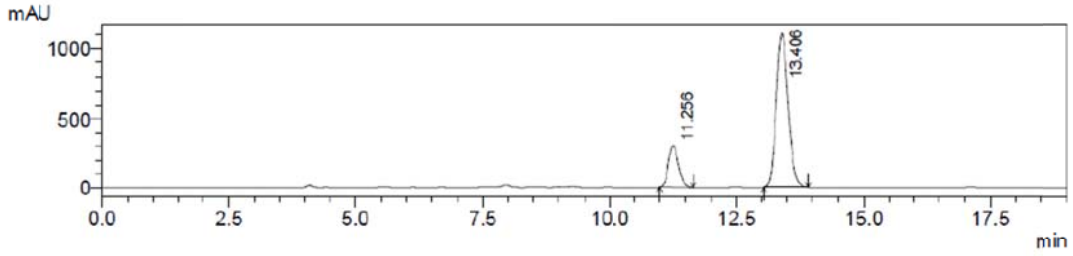
Peak#	RetTime	Area	Height	Area %
1	13.754	677236	39313	2.801
2	17.661	23500965	1133623	97.199
Totals		24178201	1172936	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(1,7-dimethyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3m): 90% de



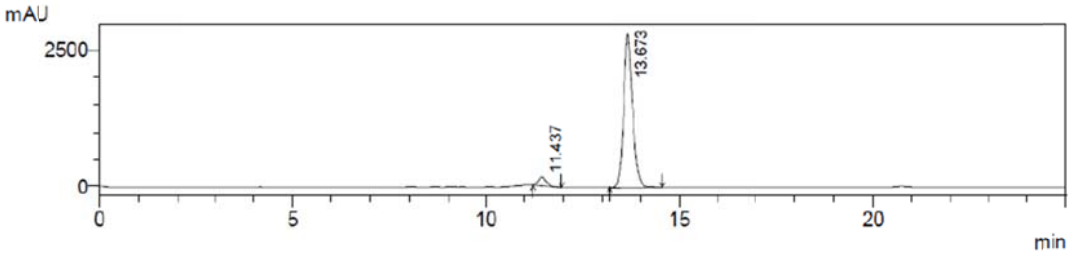
3m

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 70:30; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 11.43 min, 13.67 min (major).



PDA Ch1 254nm 4nm

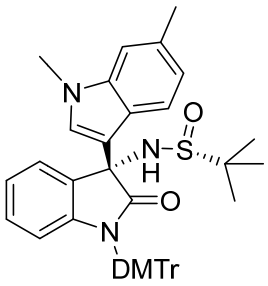
Peak#	RetTime	Area	Height	Area %
1	11.256	12484474	853845	16.305
2	13.406	64082632	3996253	83.695
Totals		76567106	4850098	100.000



PDA Ch1 254nm 4nm

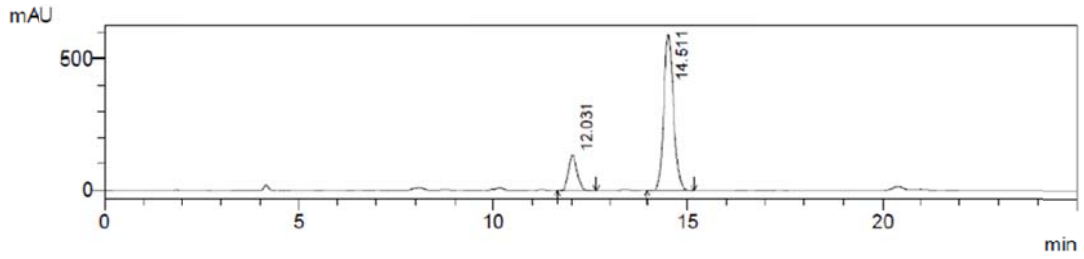
Peak#	RetTime	Area	Height	Area %
1	11.437	2355446	163927	5.012
2	13.673	44641522	2802128	94.988
Totals		46996967	2966056	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(1,6-dimethyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3n): 93% de



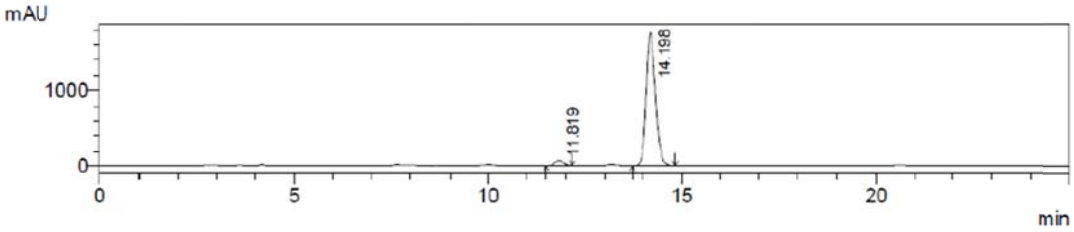
3n

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 11.81 min, 14.19 min (major).



PDA Ch1 254nm 4nm

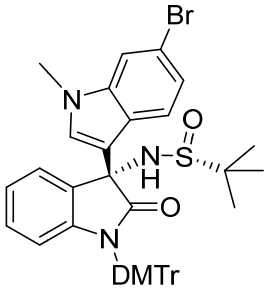
Peak#	RetTime	Area	Height	Area %
1	12.031	2122486	137731	17.175
2	14.511	10235671	588182	82.825
Totals		12358157	725913	100.000



PDA Ch1 254nm 4nm

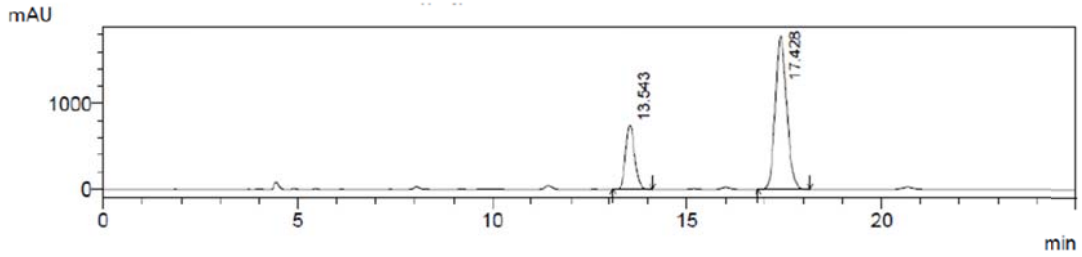
Peak#	RetTime	Area	Height	Area %
1	11.819	1106576	74379	3.650
2	14.198	29206808	1761723	96.350
Totals		30313384	1836101	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(6-bromo-1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3o): 95% de



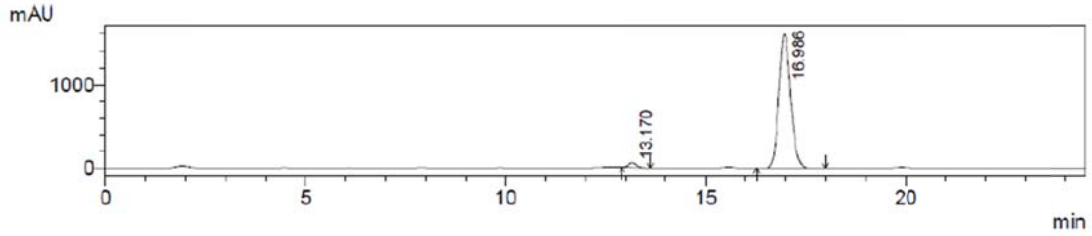
3o

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 13.17 min, 16.98 min (major).



PDA Ch1 254nm 4nm

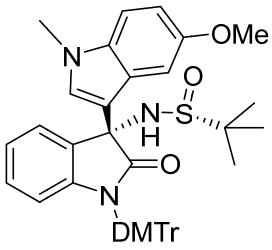
Peak#	RetTime	Area	Height	Area %
1	13.543	11923984	749021	25.043
2	17.428	35690992	1785964	74.957
Totals		47614976	2534985	100.000



PDA Ch1 254nm 4nm

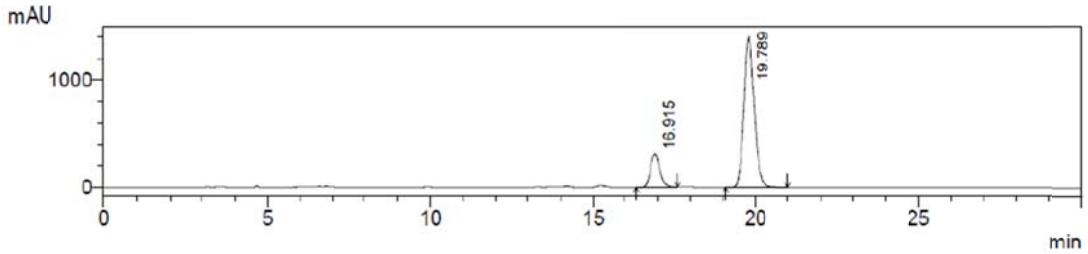
Peak#	RetTime	Area	Height	Area %
1	13.170	825110	53399	2.513
2	16.986	32002995	1599808	97.487
Totals		32828105	1653207	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(5-methoxy-1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3p): 92% de



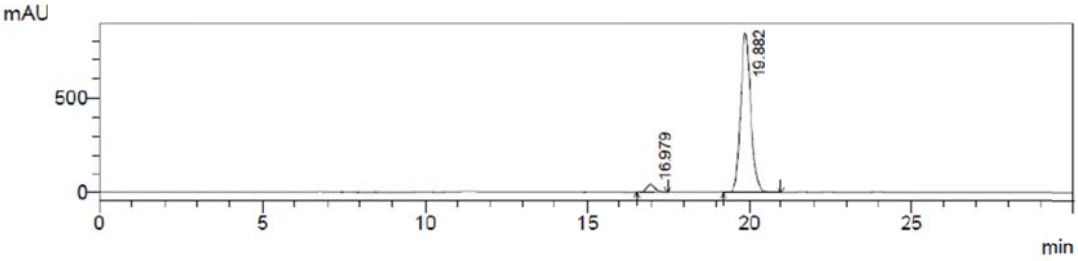
3p

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 85:15; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 16.97 min, 19.88 min (major).



PDA Ch1 254nm 4nm

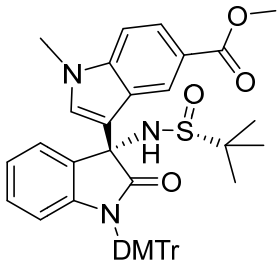
Peak#	RetTime	Area	Height	Area %
1	16.915	6388828	320769	16.972
2	19.789	31254071	1409178	83.028
Totals		37642899	1729947	100.000



PDA Ch1 254nm 4nm

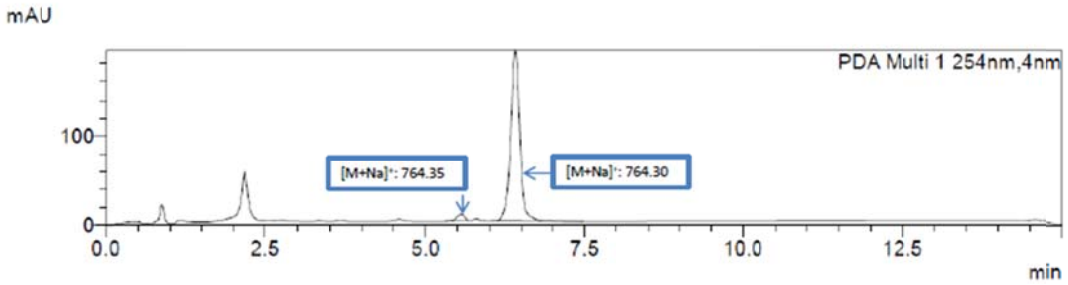
Peak#	RetTime	Area	Height	Area %
1	16.979	787902	41271	4.111
2	19.882	18375877	836458	95.889
Totals		19163779	877728	100.000

methyl 3-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(((*R*)-*tert*-butylsulfinyl)amino)-2-oxoindolin-3-yl)-1 -methyl-*1H*-indole-5-carboxylate (3q): 94% de



3q

Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 5.54 min, 6.41 min (major).

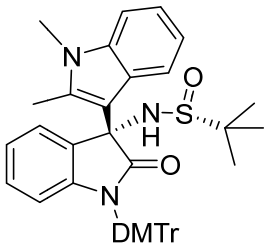


Peak Table

PDA Ch1 254nm

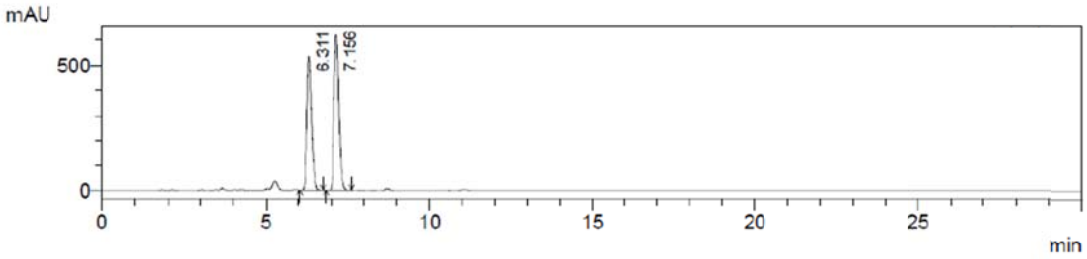
Peak#	Ret. Time	Area	Height	Area%
1	5.545	57750	7201	2.952
2	6.411	1898456	189616	97.048
Total		1956206	196817	100.000

(*R*)-*N*-((*R*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(1,2-dimethyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3r): 90% de



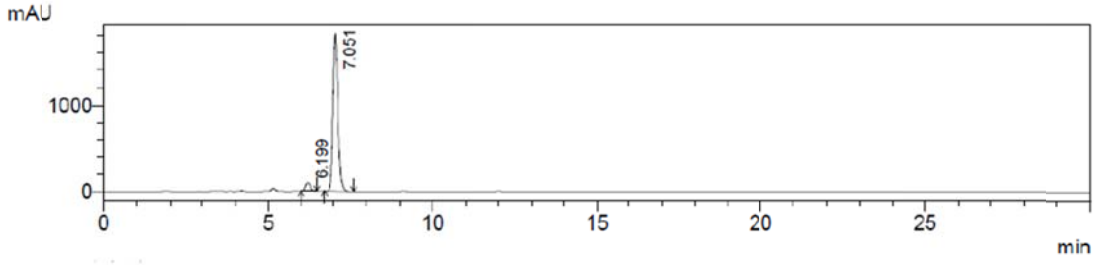
3r

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 85:15; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 6.19 min, 7.05 min (major).



PDA Ch1 254nm 4nm

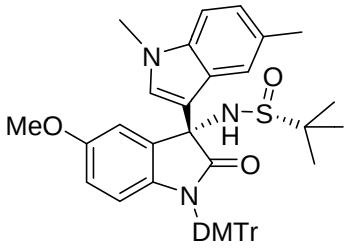
Peak#	RetTime	Area	Height	Area %
1	6.311	5252328	535402	45.051
2	7.156	6406404	617002	54.949
Totals		11658732	1152404	100.000



PDA Ch1 254nm 4nm

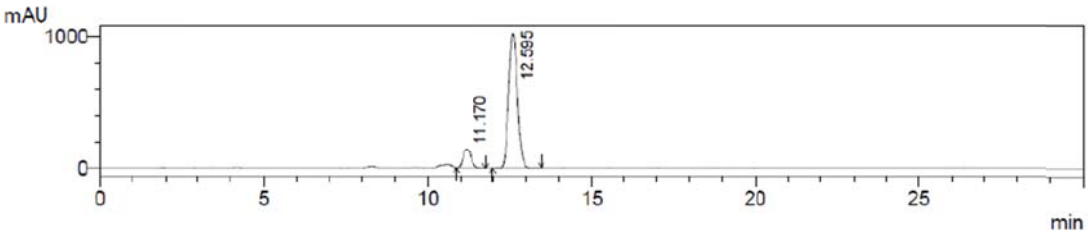
Peak#	RetTime	Area	Height	Area %
1	6.199	974501	93923	4.860
2	7.051	19076611	1818451	95.140
Totals		20051112	1912374	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(1,5-dimethyl-1*H*-indol-3-yl)-5-methoxy-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3s): 96% de



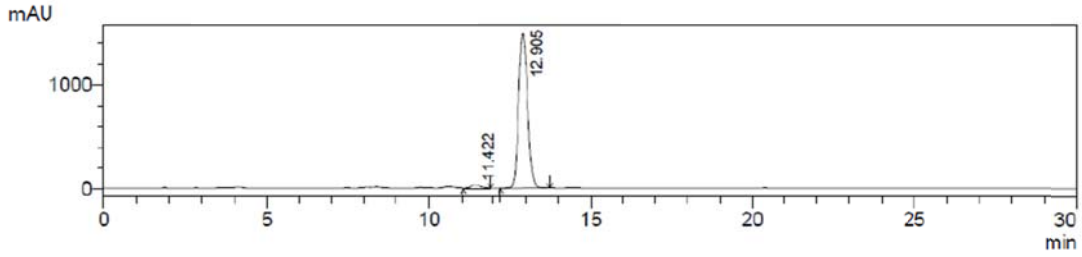
3s

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = **1**.0 mL / min; Detected by UV at 254nm; Retention time: 11.42 min, 12.90 min (major).



PDA Ch1 254nm 4nm

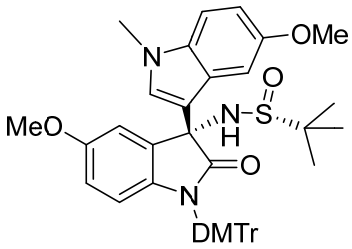
Peak#	RetTime	Area	Height	Area %
1	11.170	2550579	147512	12.001
2	12.595	18702141	1015958	87.999
Totals		21252719	1163469	100.000



PDA Ch1 254nm 4nm

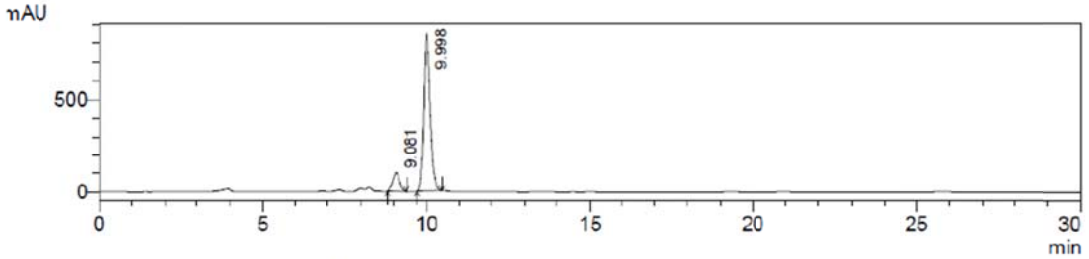
Peak#	RetTime	Area	Height	Area %
1	11.422	654531	31882	2.254
2	12.905	28380192	1486900	97.746
Totals		29034723	1518782	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-methoxy-3-(5-methoxy-1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3t): 93% de



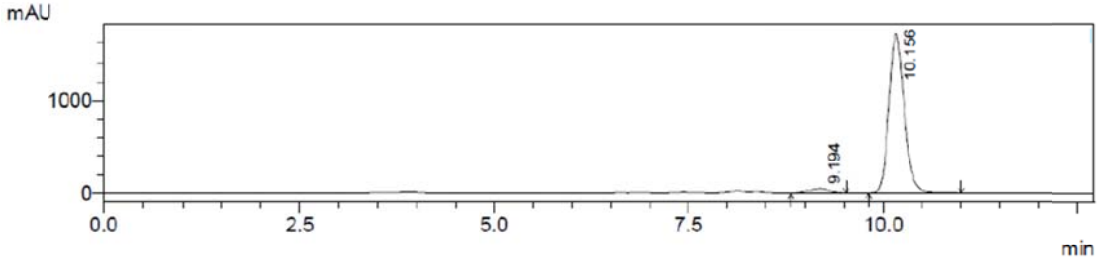
3t

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 9.19 min, 10.15 min (major).



PDA Ch1 254nm 4nm

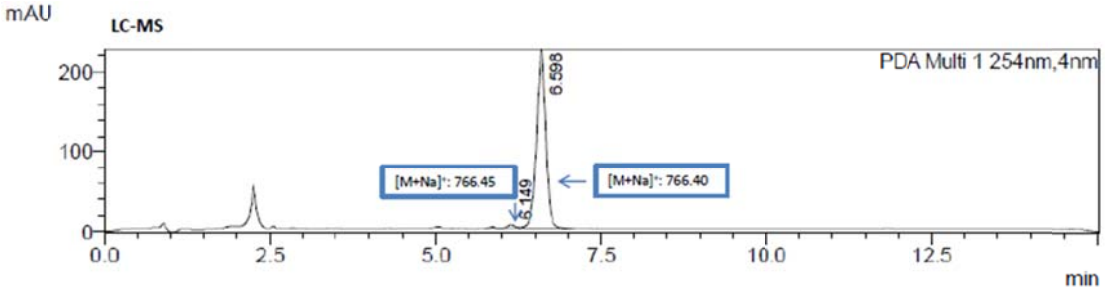
Peak#	RetTime	Area	Height	Area %
1	9.081	1352043	100821	10.508
2	9.998	11515141	849938	89.492
Totals		12867184	950759	100.000



PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	9.194	904889	51055	3.692
2	10.156	23601678	1703879	96.308
Totals		24506567	1754934	100.000

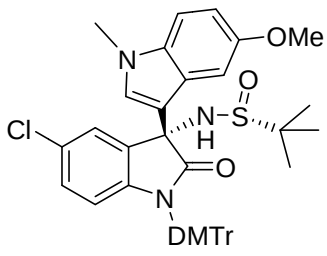
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 6.15 min, 6.60 min (major).



PDA Ch1 254nm

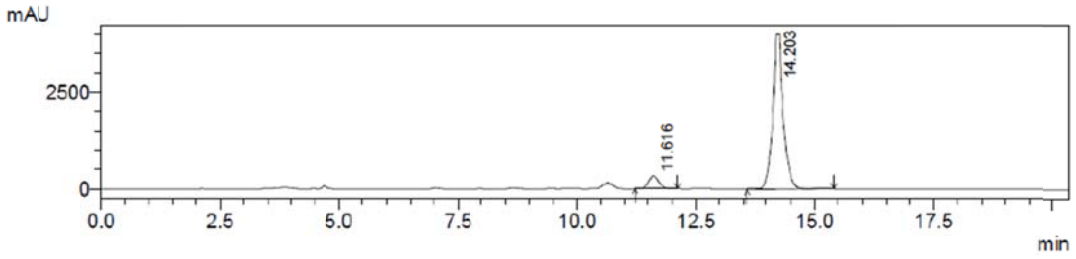
Peak#	Ret. Time	Area	Height	Area%
1	6.149	68035	4825	2.977
2	6.598	2217118	224919	97.023
Total		2285153	229745	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-chloro-3-(5-methoxy-1-methyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3u): 97% de



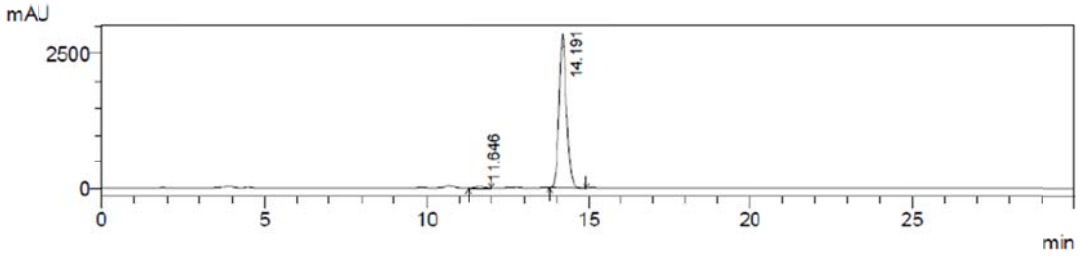
3u

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 11.64 min, 14.19 min (major).



PDA Ch1 254nm 4nm

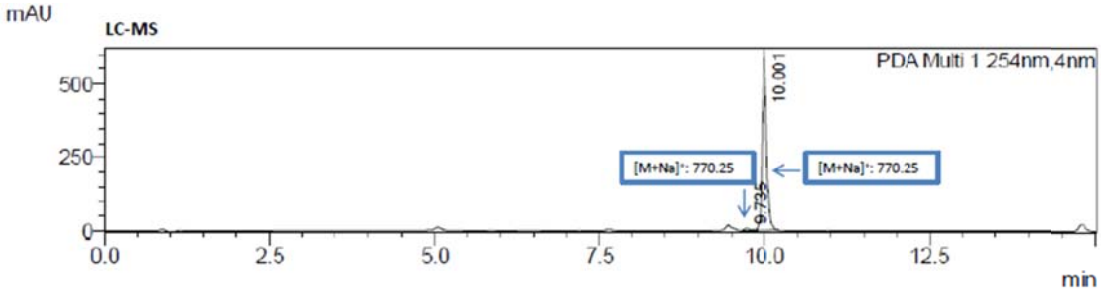
Peak#	RetTime	Area	Height	Area %
1	11.616	4792701	319036	7.505
2	14.203	59068317	4003928	92.495
Totals		63861019	4322964	100.000



PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	11.646	672847	39787	1.458
2	14.191	45488839	2854610	98.542
Totals		46161686	2894398	100.000

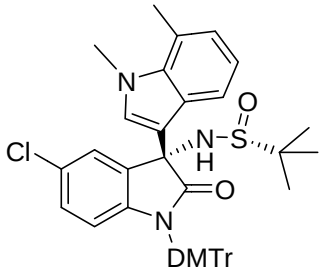
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 5% to 100% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time**:** 9.74 min, 10.00 min (major).



PDA Ch1 254nm

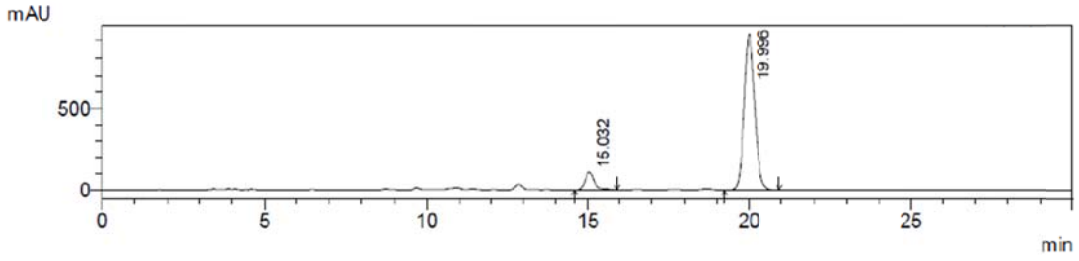
Peak#	Ret. Time	Area	Height	Area%
1	9.735	39203	6494	1.304
2	10.001	2966340	617626	98.696
Total		3005544	624120	100.000

(*R*)-*N*-((*S*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-chloro-3-(1,7-dimethyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3v): 96% de



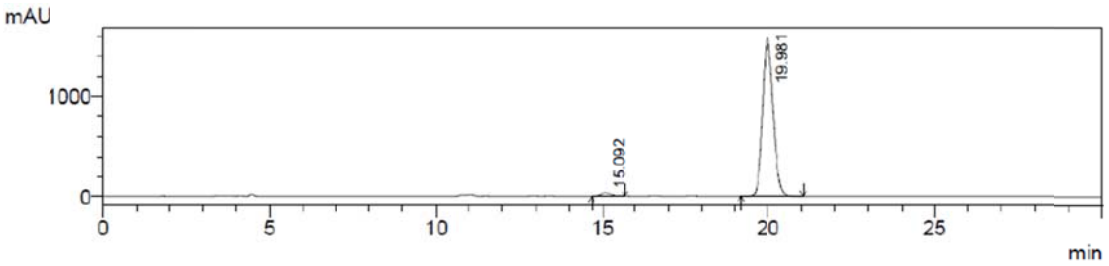
3v

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 75:25; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 15.09min, 19.98 min (major).



PDA Ch1 254nm 4nm

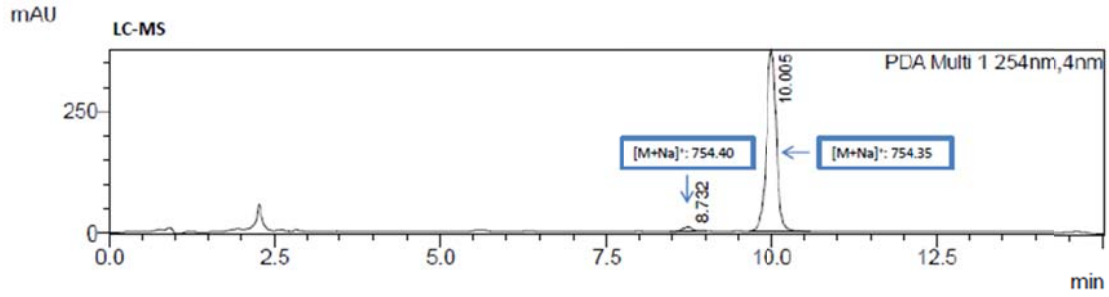
Peak#	RetTime	Area	Height	Area %
1	15.032	2243246	112134	9.322
2	19.996	21821394	941923	90.678
Totals		24064640	1054057	100.000



PDA Ch1 254nm 4nm

Peak#	RetTime	Area	Height	Area %
1	15.092	795069	39629	2.155
2	19.981	36102449	1589477	97.845
Totals		36897518	1629106	100.000

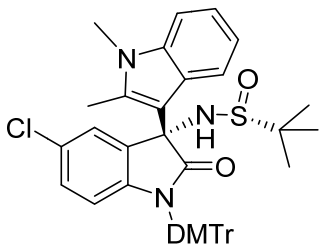
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time**:** 8.73 min, 10.00 min (major).



PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%
1	8.732	72064	7358	1.784
2	10.005	3967335	372744	98.216
Total		4039398	380103	100.000

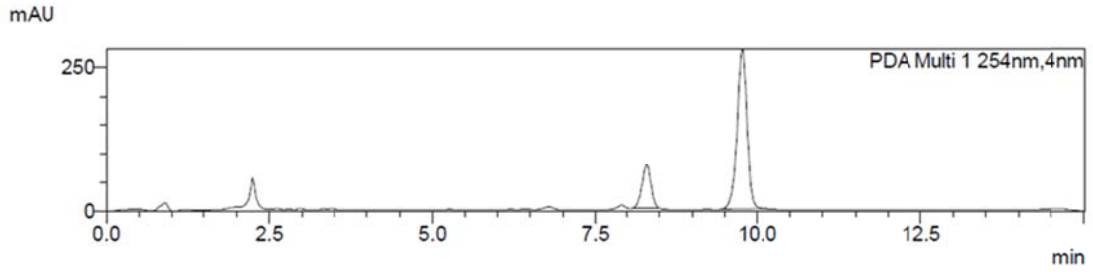
(*R*)-*N*-((*R*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-5-chloro-3-(1,2-dimethyl-1*H*-indol-3-yl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3w): 95% de



3w

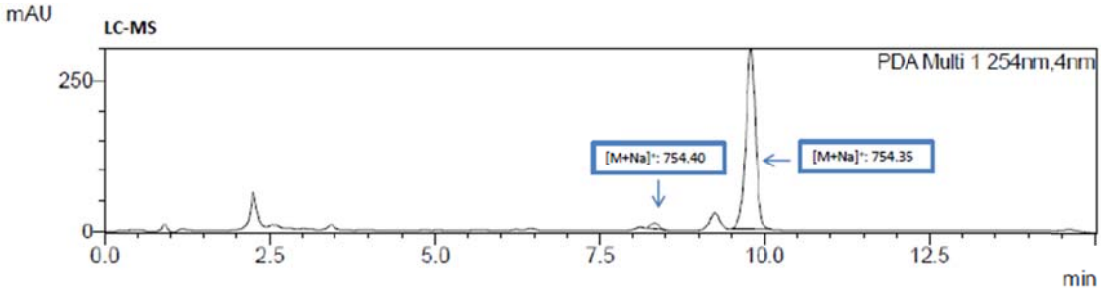
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over

15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 8.34 min, 9.80min (major).



PDA Ch1 254nm

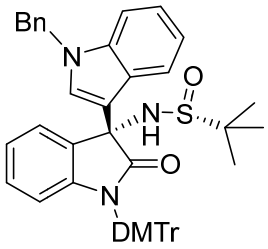
Peak#	Ret. Time	Area	Height	Area%
1	8.301	718696	74962	19.729
2	9.764	2924229	276920	80.271
Total		3642926	351882	100.000



PDA Ch1 254nm

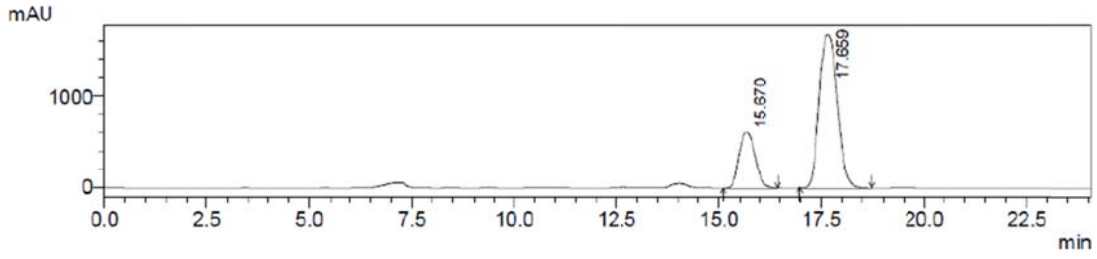
Peak#	Ret. Time	Area	Height	Area%
1	8.339	77544	9838	2.447
2	9.793	3091411	297287	97.553
Total		3168954	307125	100.000

(*R*)-*N*-((*S*)-3-(1-benzyl-1*H*-indol-3-yl)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-2-oxoindolin-3-yl)-2-methylpropane-2-sulfinamide (3x): 98% de



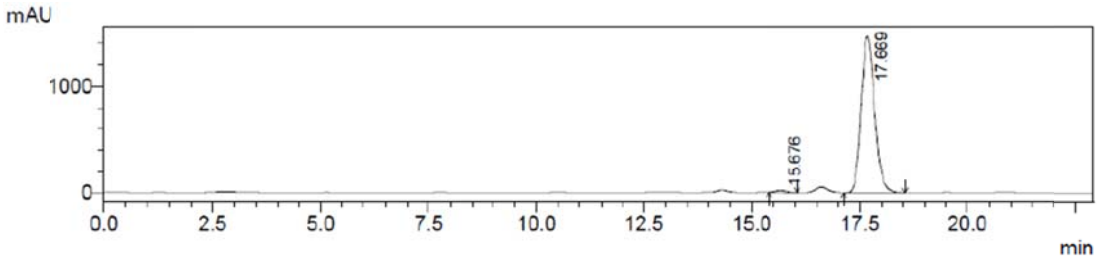
3x

Analytical HPLC: C18 Column (4.6×150mm, 5 micron particle size), mobile phase aqueous CH_3CN/H_2O = 90:10; Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 15.67 min, 17.67 min (major).



PDA Ch1 254nm 4nm

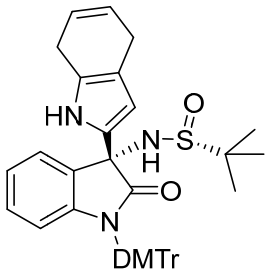
Peak#	RetTime	Area	Height	Area %
1	15.670	16707311	607348	24.691
2	17.659	50958197	1680749	75.309
Totals		67665508	2288097	100.000



PDA Ch1 254nm 4nm

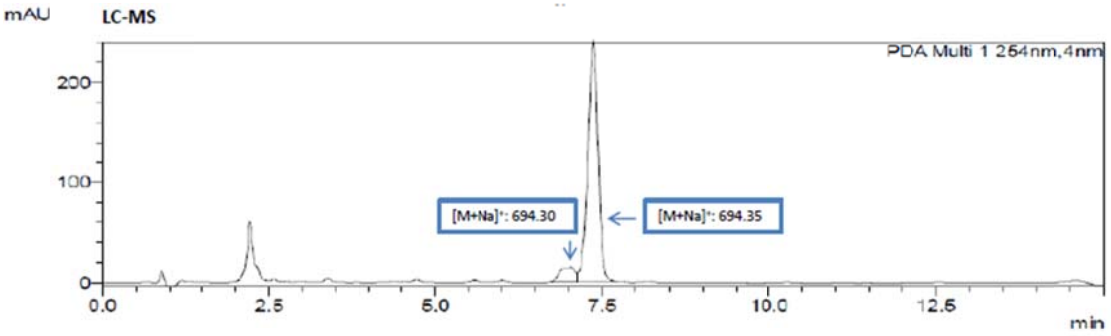
Peak#	RetTime	Area	Height	Area %
1	15.676	378839	19822	1.159
2	17.669	32313286	1524471	98.841
Totals		32692125	1544293	1.159

(*R*)-*N*-((*R*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-3-(4,7-dihydro-1*H*-indol-2-yl)-2-oxo indolin-3-yl)-2-methylpropane-2-sulfinamide (5a): 84% de



5a

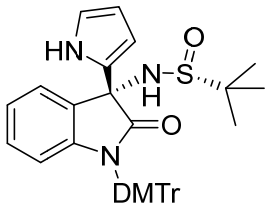
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 7.02 min, 7.37 min (major).



PDA Ch1 254nm

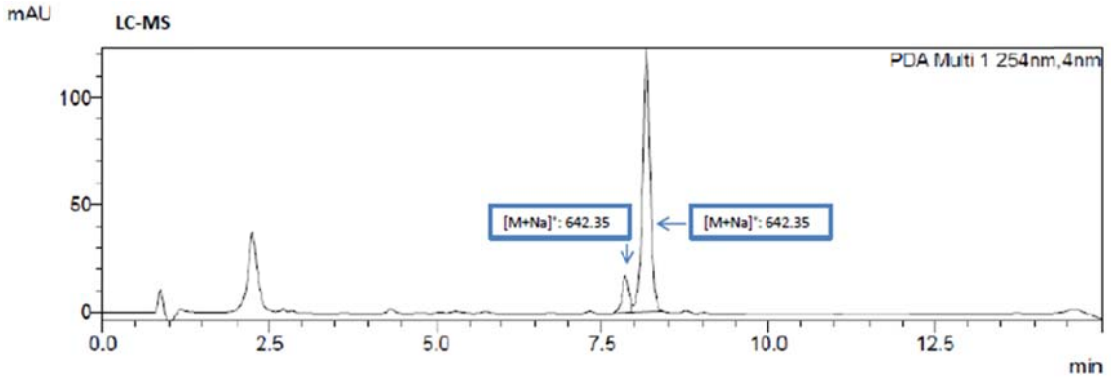
Peak#	Ret. Time	Area	Area%
1	7.029	227478	8.232
2	7.370	2535953	91.768
Total		2763431	100.000

(*R*)-*N*-((*R*)-1-(bis(4-methoxyphenyl)(phenyl)methyl)-2-oxo-3-(1*H*-pyrrol-2-yl)indolin-3-yl)-2-methylpropane-2-sulfinamide (5b): 77% de



5b

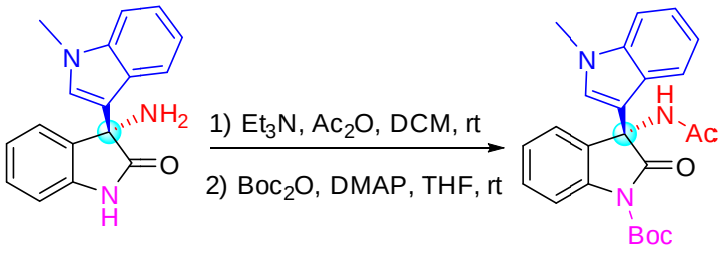
Analytical LC-MS: C18-WP Column (2.1×50mm, 3 micron particle size), mobile phase H_2O/CH_3CN linear gradient over 15min (the gradient of CH_3CN is from 50% to 75% during 3-15min); Flow = 1.0 mL / min; Detected by UV at 254nm; Retention time: 7.87 min, 8.19 min (major).



PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	7.866	131825	11.672
2	8.185	997585	88.328
Total		1129410	100.000

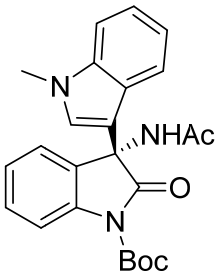
Determination of the enantioselectivity of compound 6



6 **7**

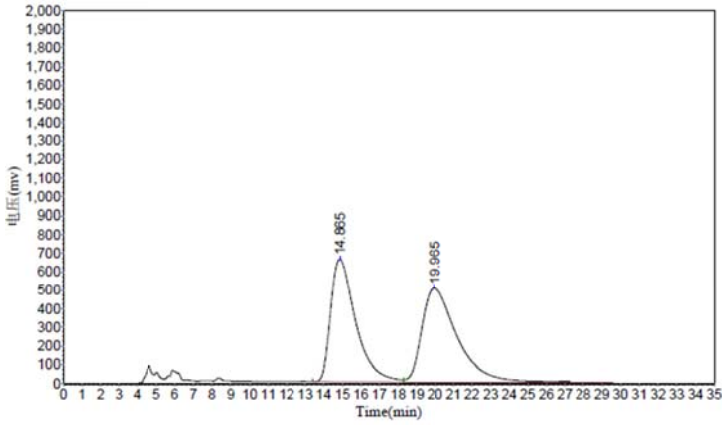
96% ee

The enantiomeric excess of compound **6** were measured by chiral HPLC analysis of its *N*-Boc-*N'*-Ac-derivative **7**, *tert*-butyl (S)-3-acetamido-3-(1-methyl-1H-indol-3-yl)-2-oxoind -oline-1-carboxylate. The HPLC reference compound was a mixture of related product consisting of *R* and *S* enantiomer.



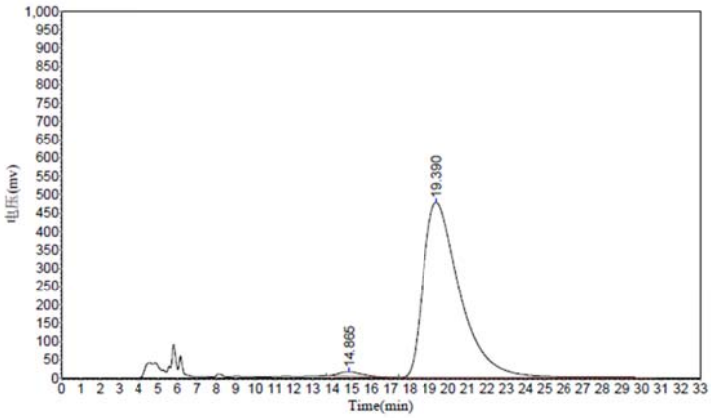
7

96% ee. Analytical HPLC: Chiralcel OD-H column (250 mm); detected at 220 nm; hexane/i-propanol = 85/15; flow = 0.7 mL/min; Retention time: 14.87 min, 19.39 min (major).



Results

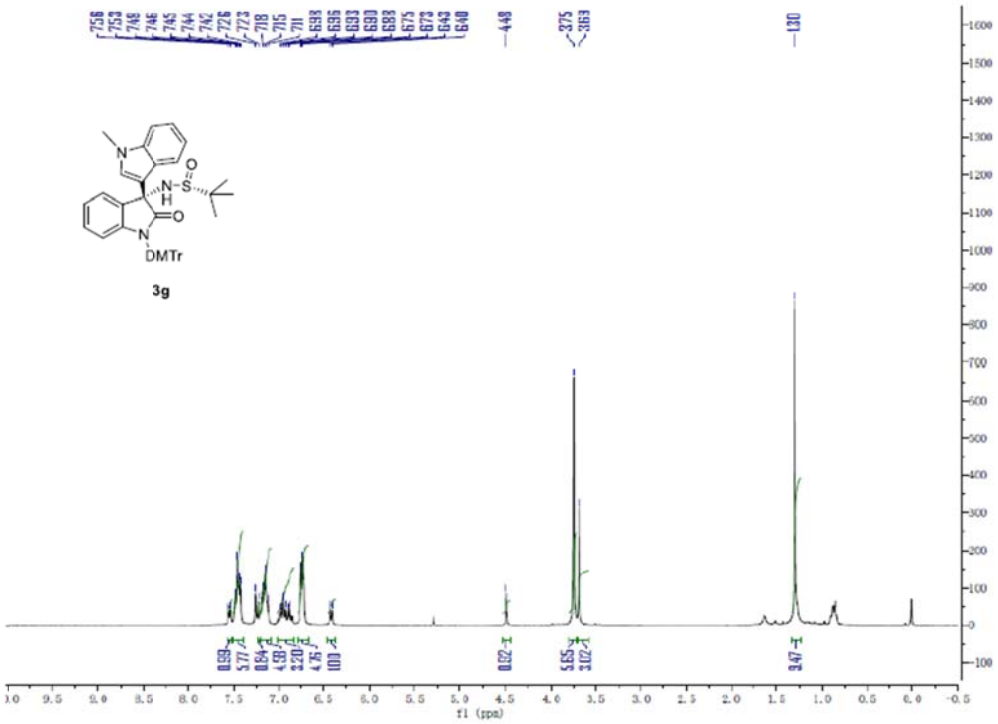
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.865	657760.813	61268404.000	47.8914
2		19.965	502539.219	66663468.000	52.1086
Total			1160300.031	127931872.000	100.0000

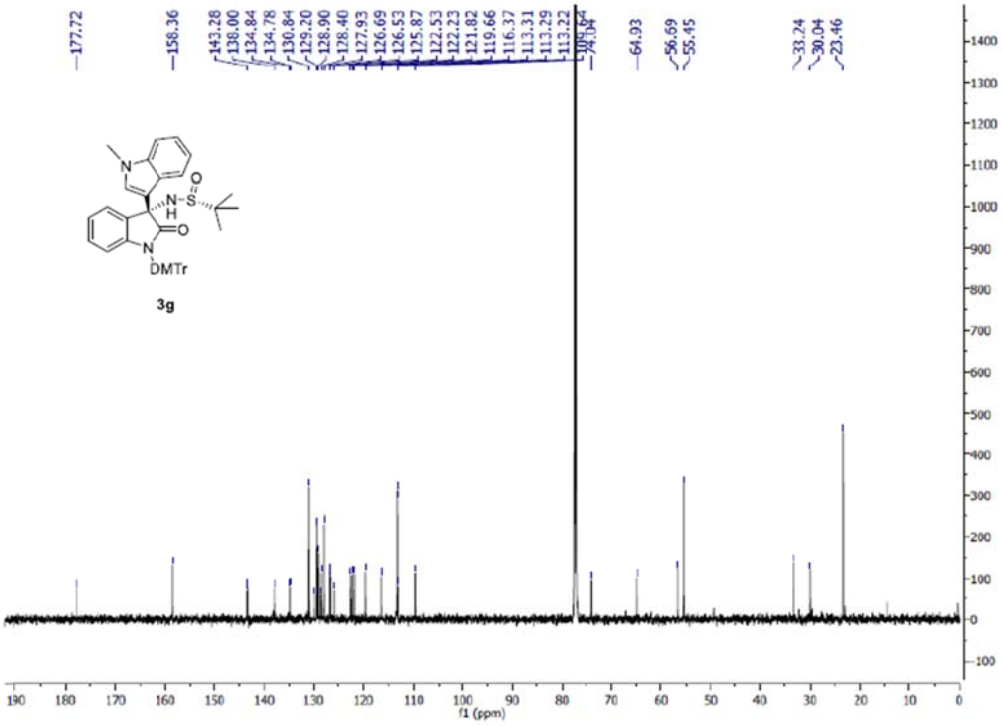


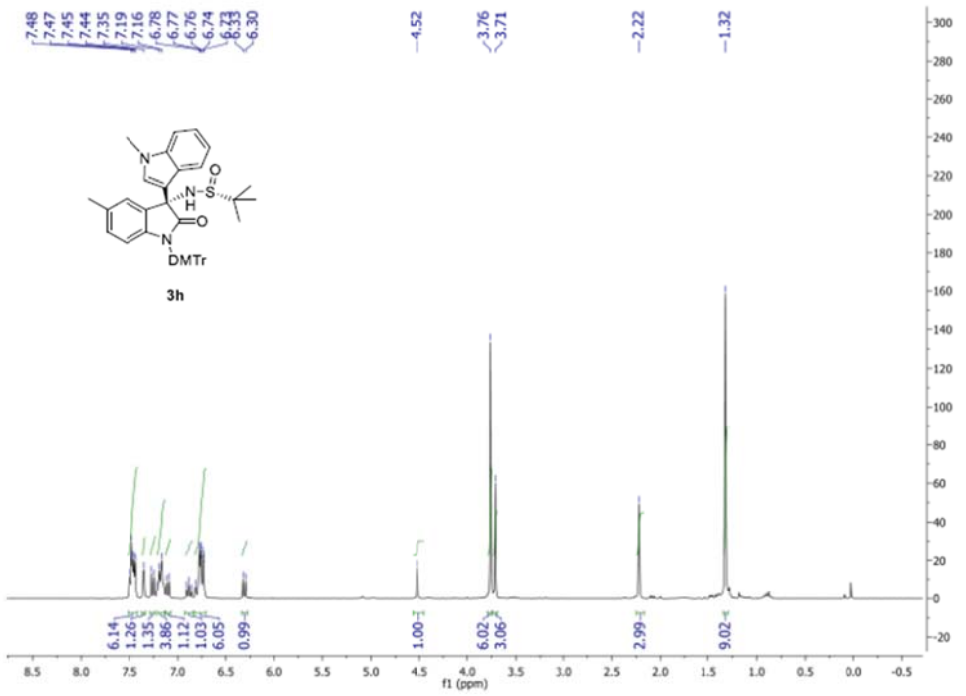
Results

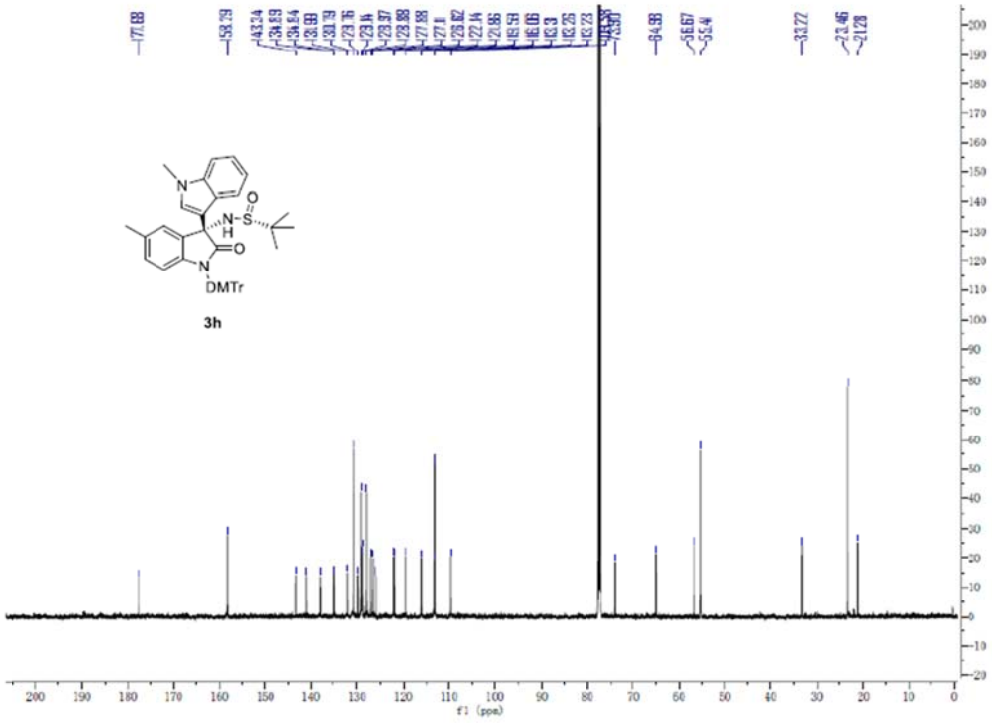
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		14.865	14606.226	1389762.875	2.1413
2		19.390	477822.531	63512788.000	97.8587
Total			492428.757	64902550.875	100.0000

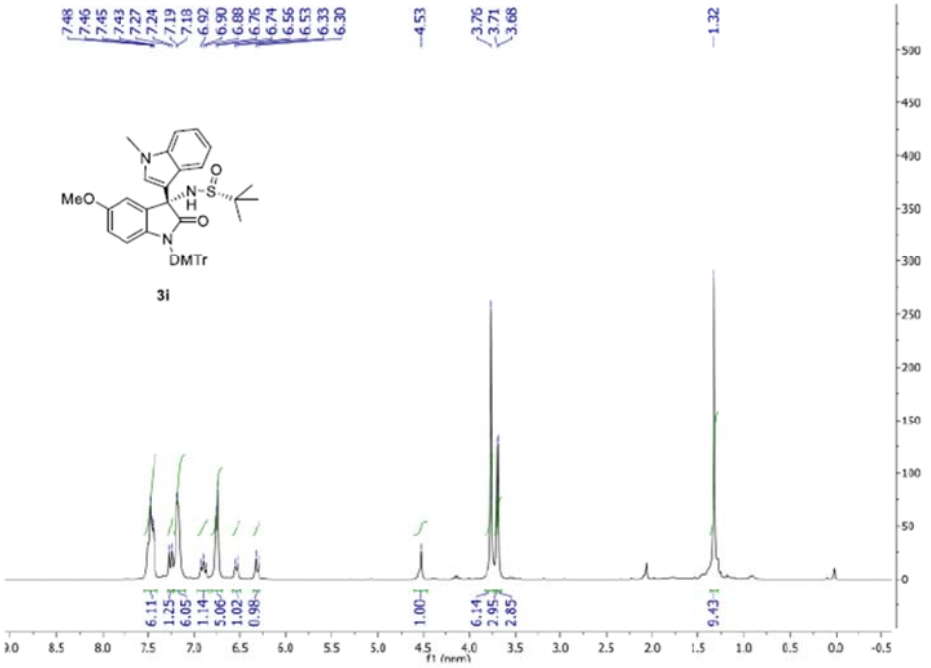
Copies of ^{1}H NMR and ^{13}C NMR spectra

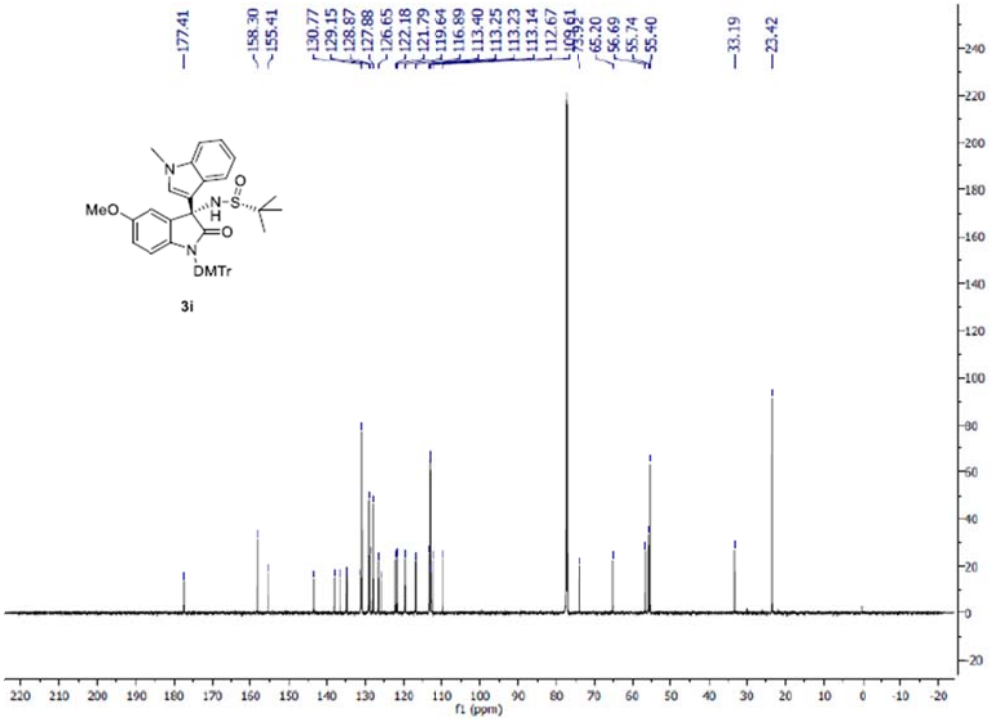


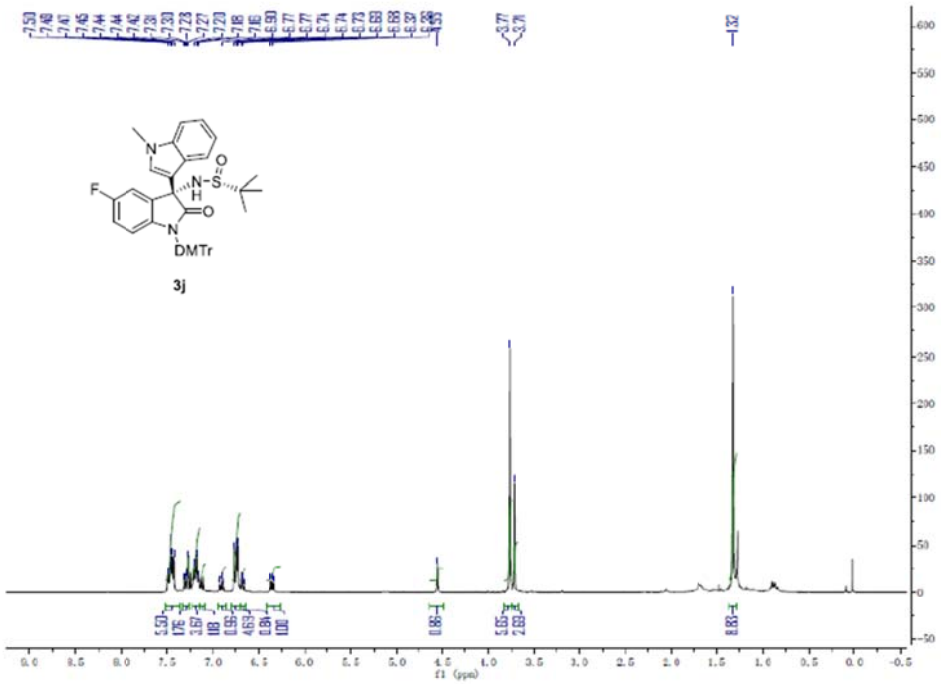



7.48
7.47
7.45
7.44
7.35
7.19
7.16
6.78
6.77
6.76
6.74
6.73
6.33
6.30
4.52
3.76
3.71
2.22
1.32
DMTr
3h
6.14
1.26
1.35
3.86
1.12
1.03
6.05
0.99
1.00
6.02
3.06
2.99
9.02
f1 (ppm)

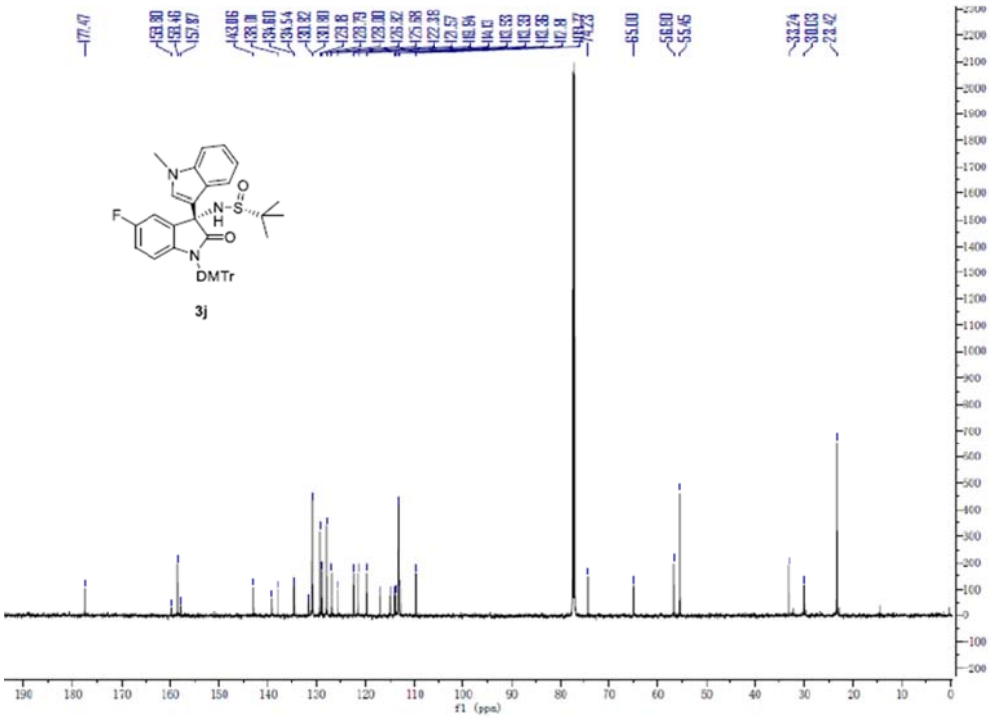

177.88
153.79
84.58
56.67
55.44
33.72
23.46
21.28
DMTr
3h
f1 (ppm)


7.48
7.46
7.45
7.43
7.27
7.24
7.19
7.18
6.92
6.90
6.88
6.76
6.74
6.56
6.53
6.33
6.30
4.53
3.76
3.71
3.68
1.32
MeO
DMTr
3i
6.11
1.25
6.05
1.14
5.06
1.02
0.98
1.00
6.14
2.95
2.85
9.43
f1 (ppm)

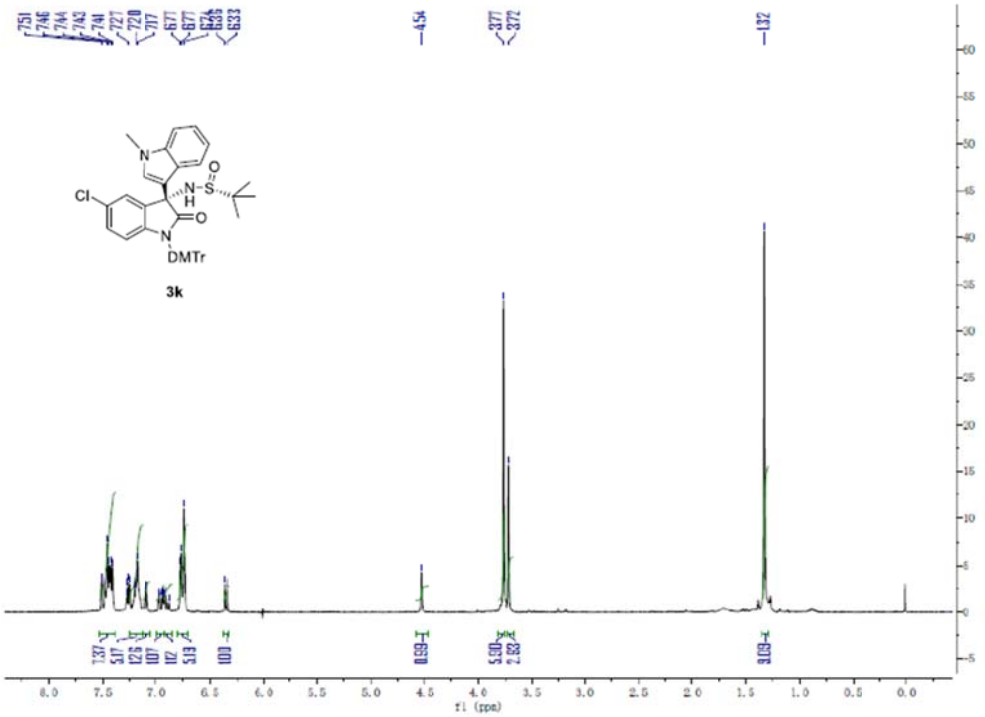

177.41
158.30
155.41
130.77
129.15
128.87
127.88
126.65
122.18
121.79
119.64
116.89
113.40
113.25
113.23
113.14
112.67
109.61
79.92
65.20
56.69
55.74
55.40
33.19
23.42
MeO
DMTr
3i
f1 (ppm)



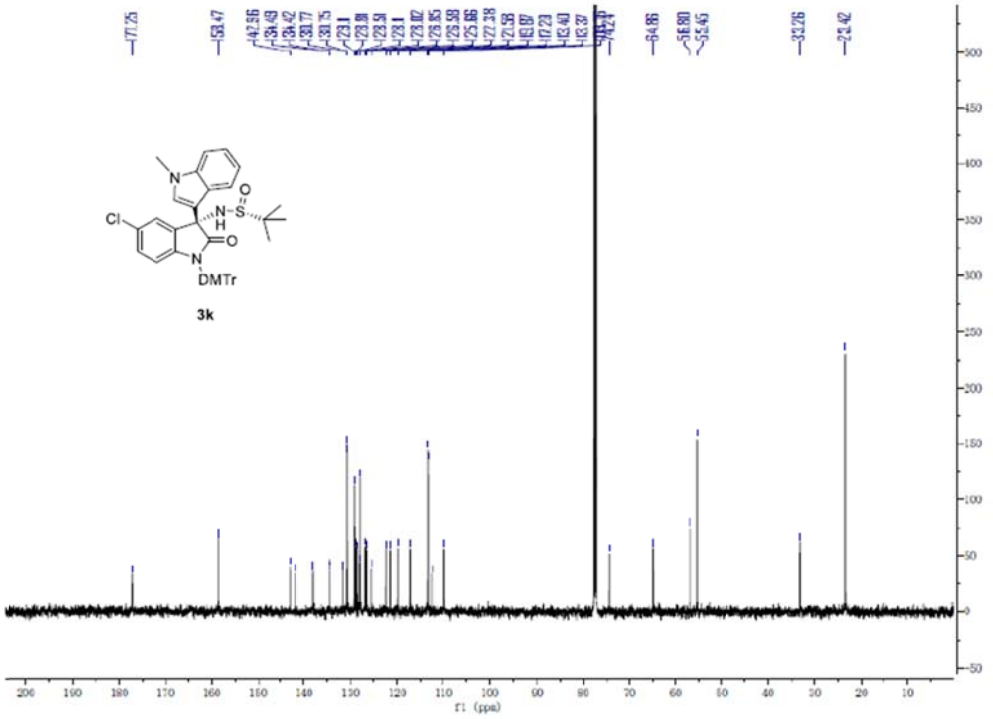
3j



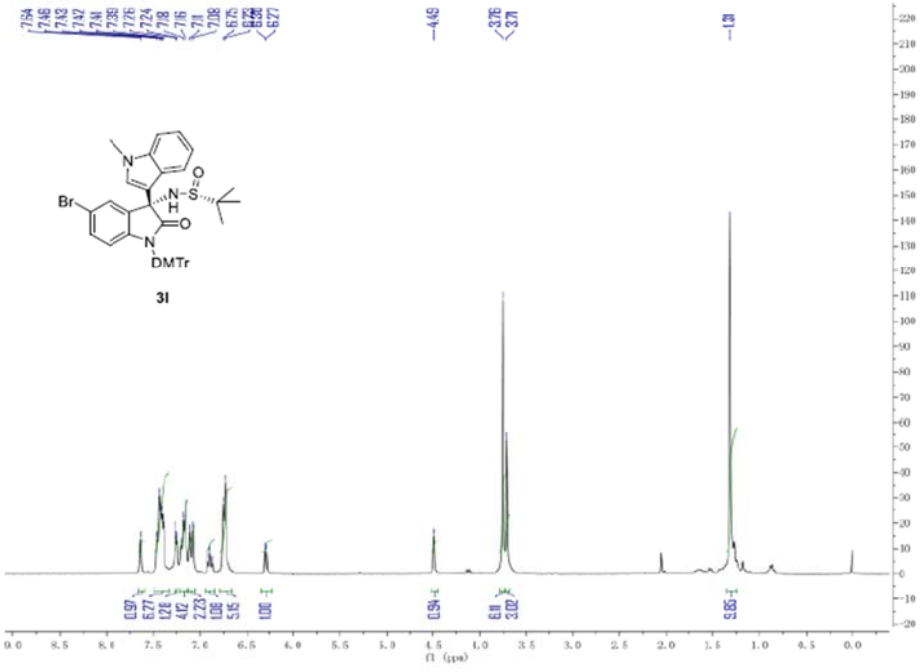
3j

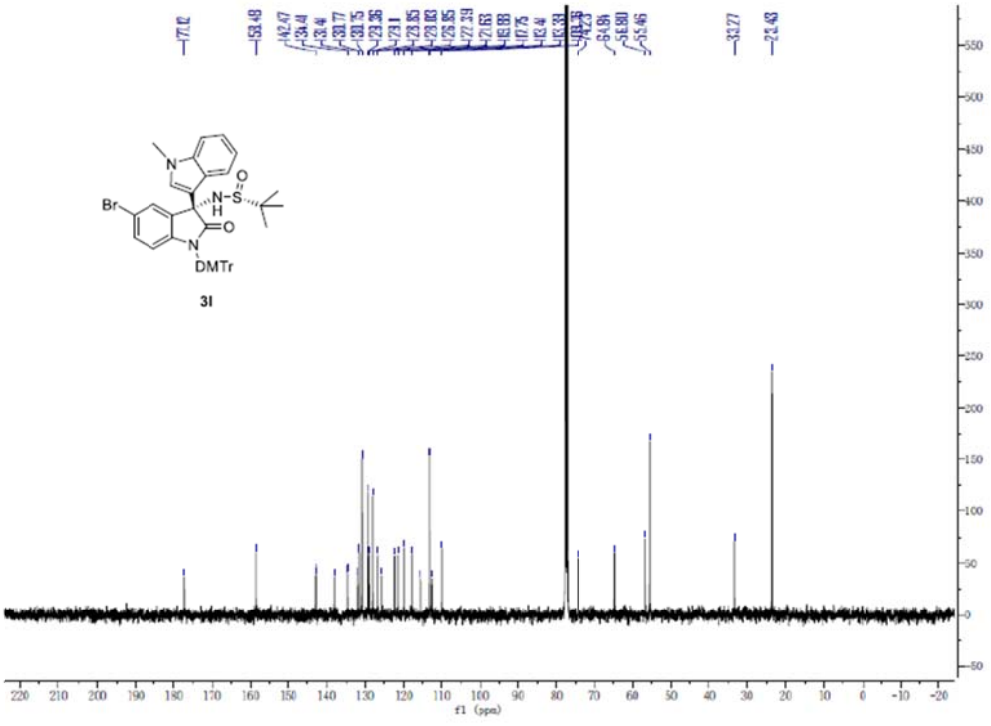


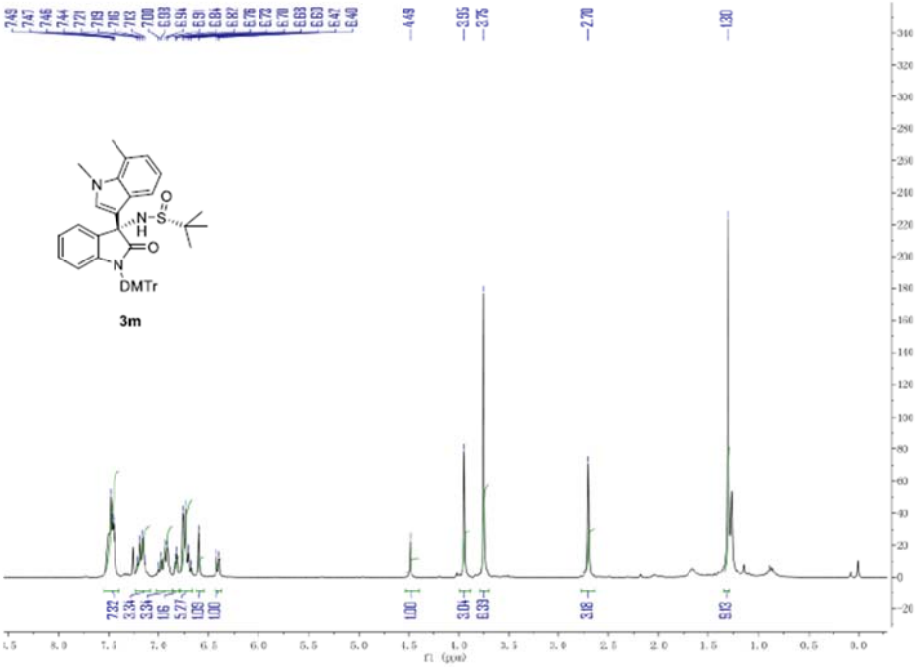
3k

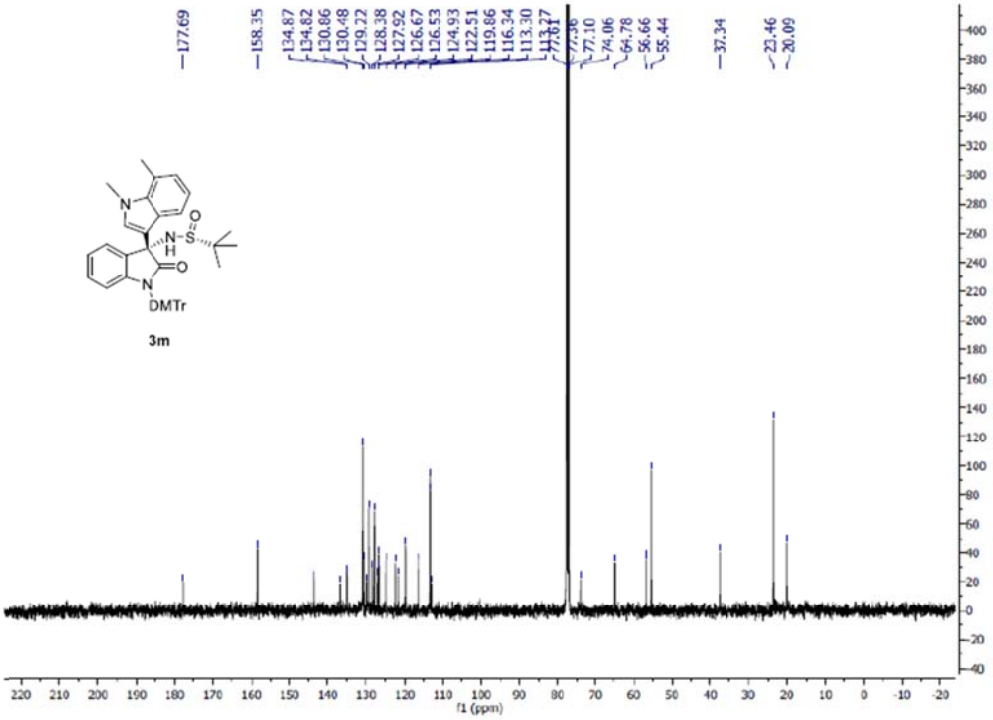


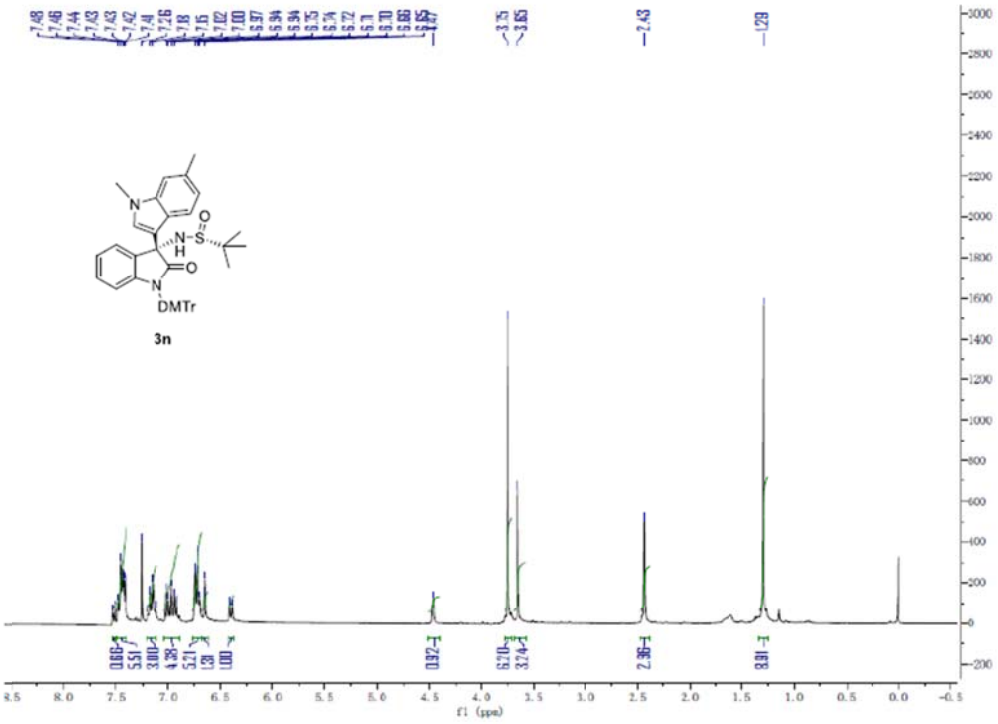
3k

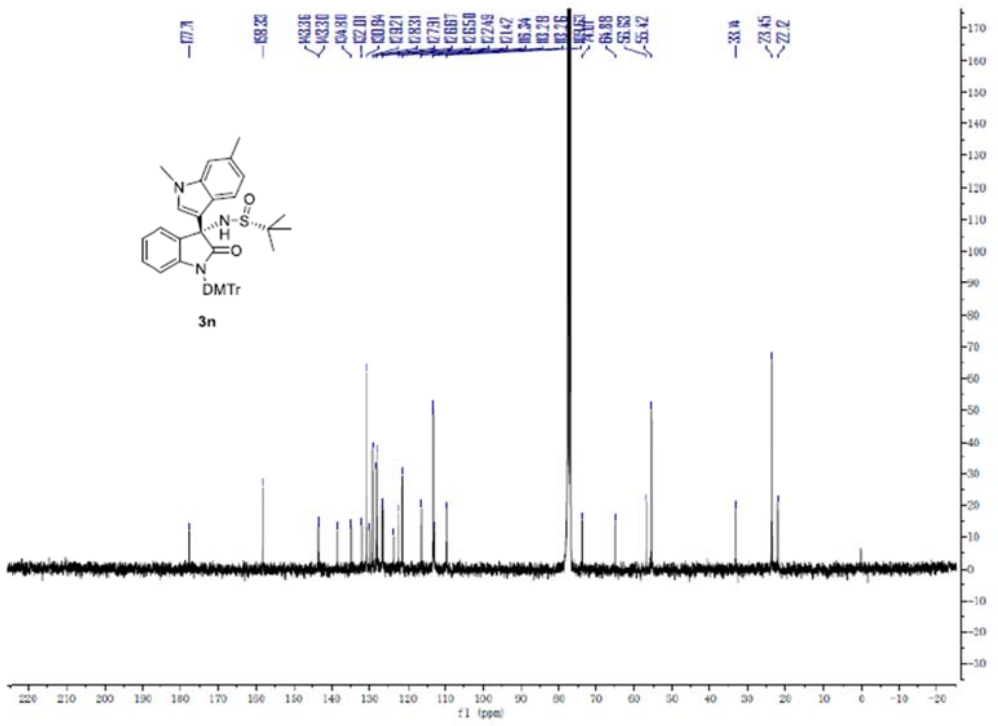

Br
N
S
O
H
O
N
DMTr
3l
f1 (ppm)

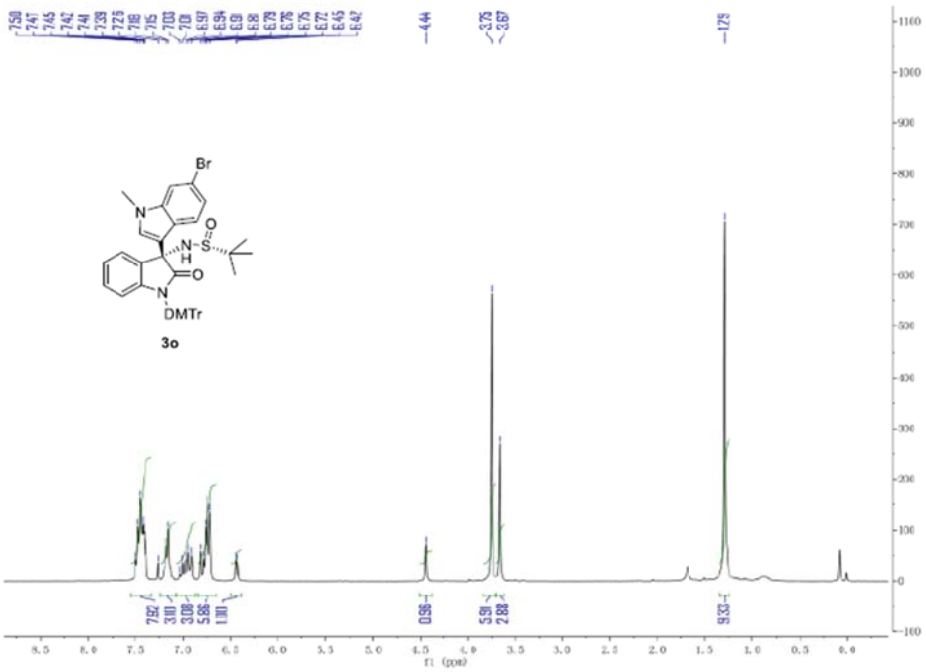

Br
N
S
O
H
O
N
DMTr
3l
f1 (ppm)

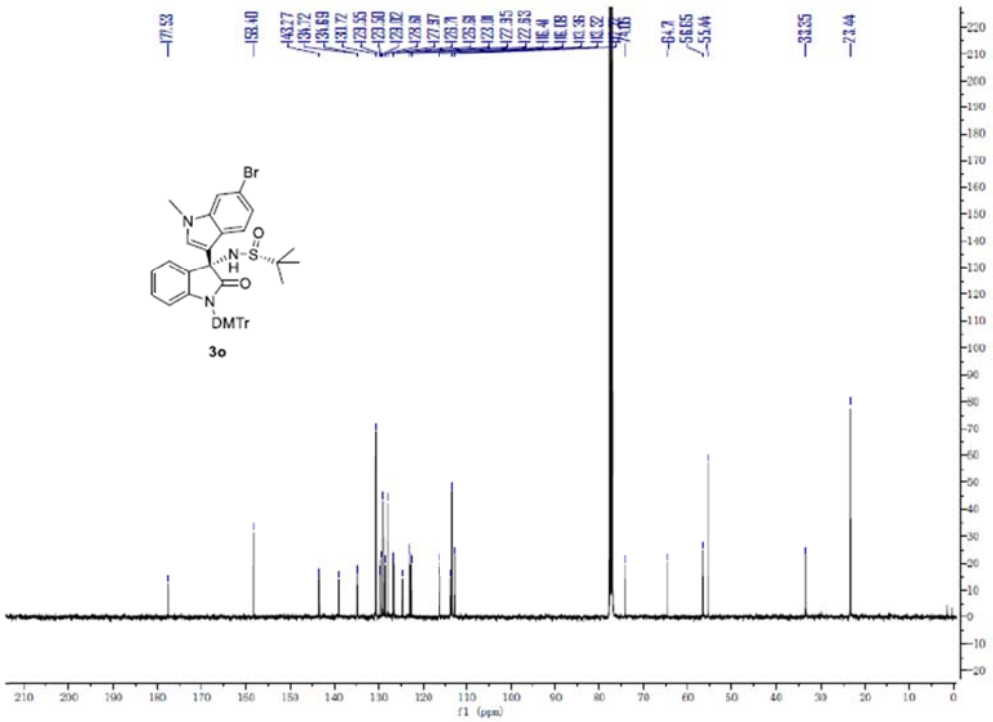

DMTr
3m

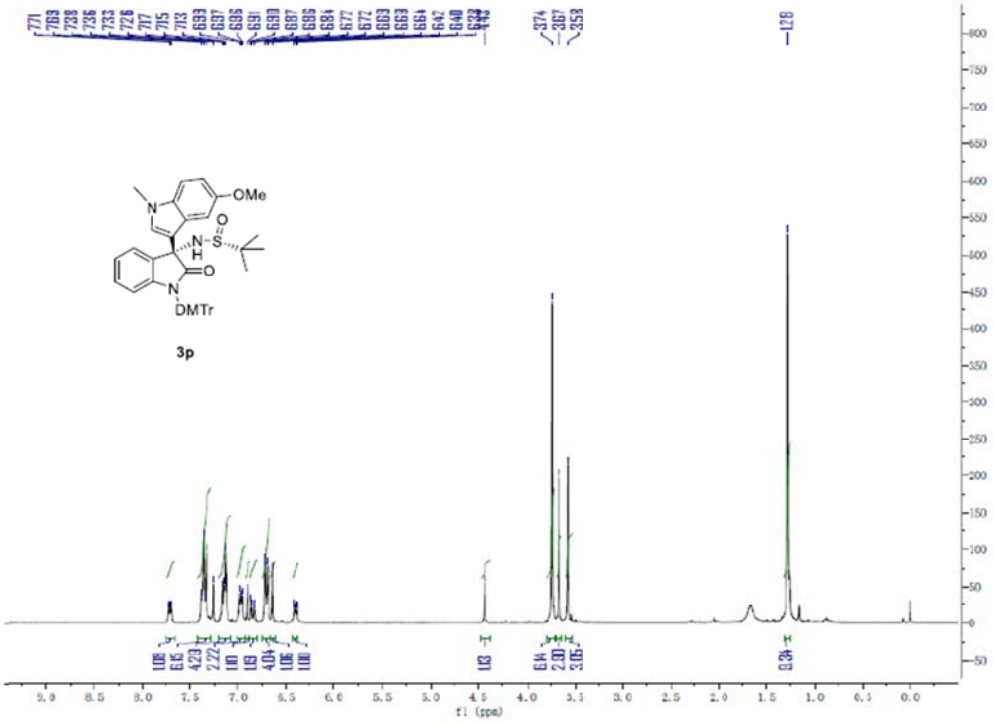

DMTr
3m

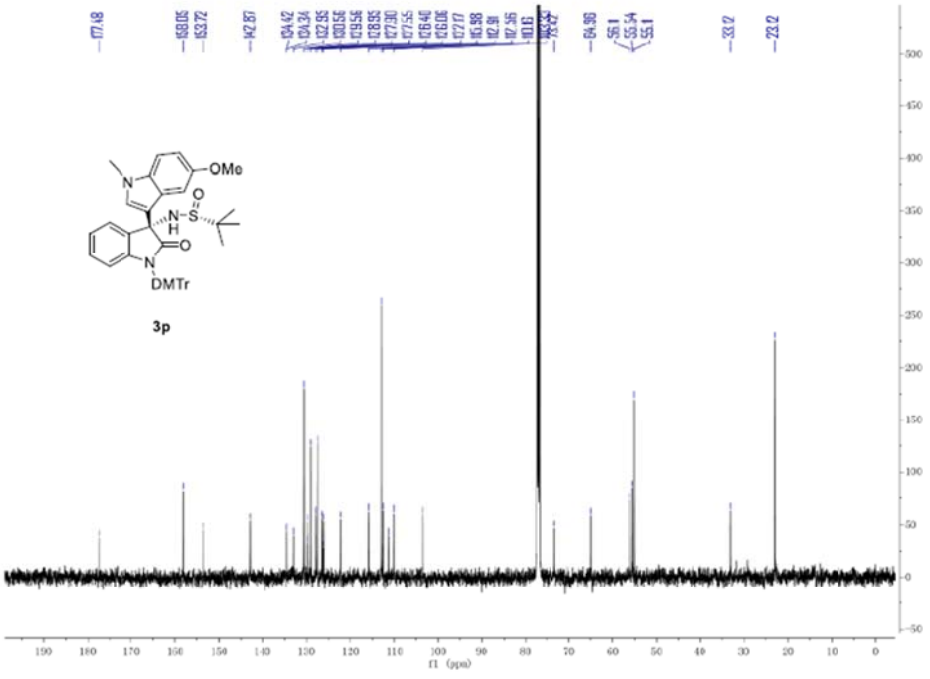

DMTr
3n
f1 (ppm)

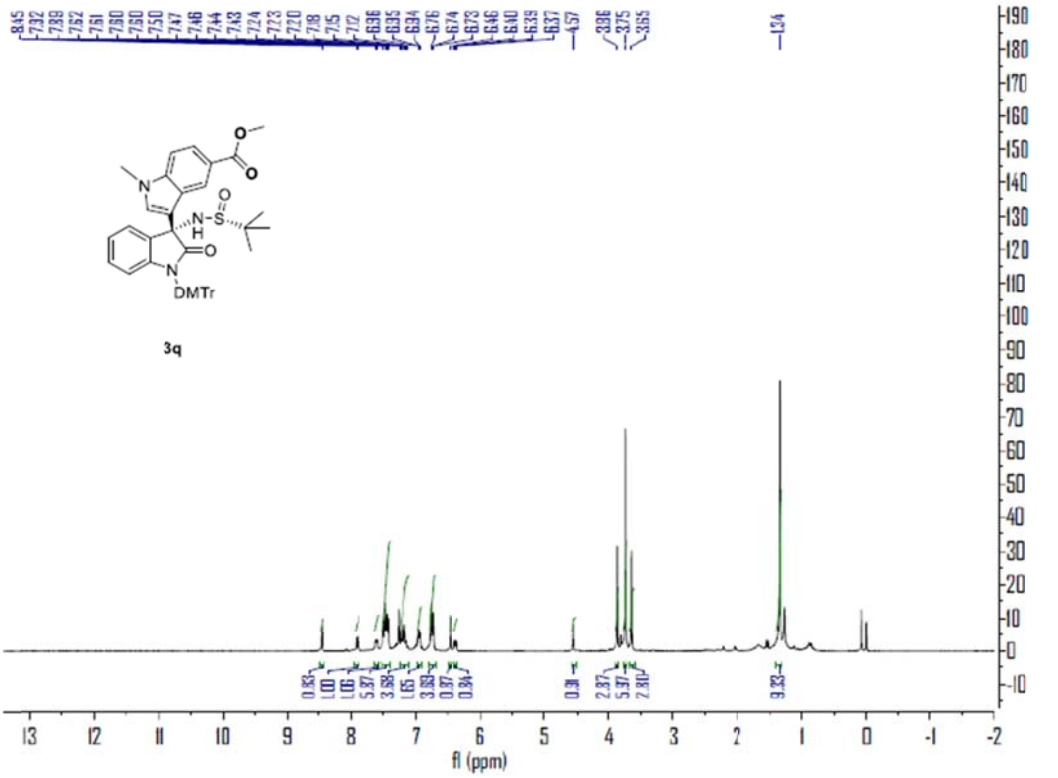

DMTr
3n
f1 (ppm)

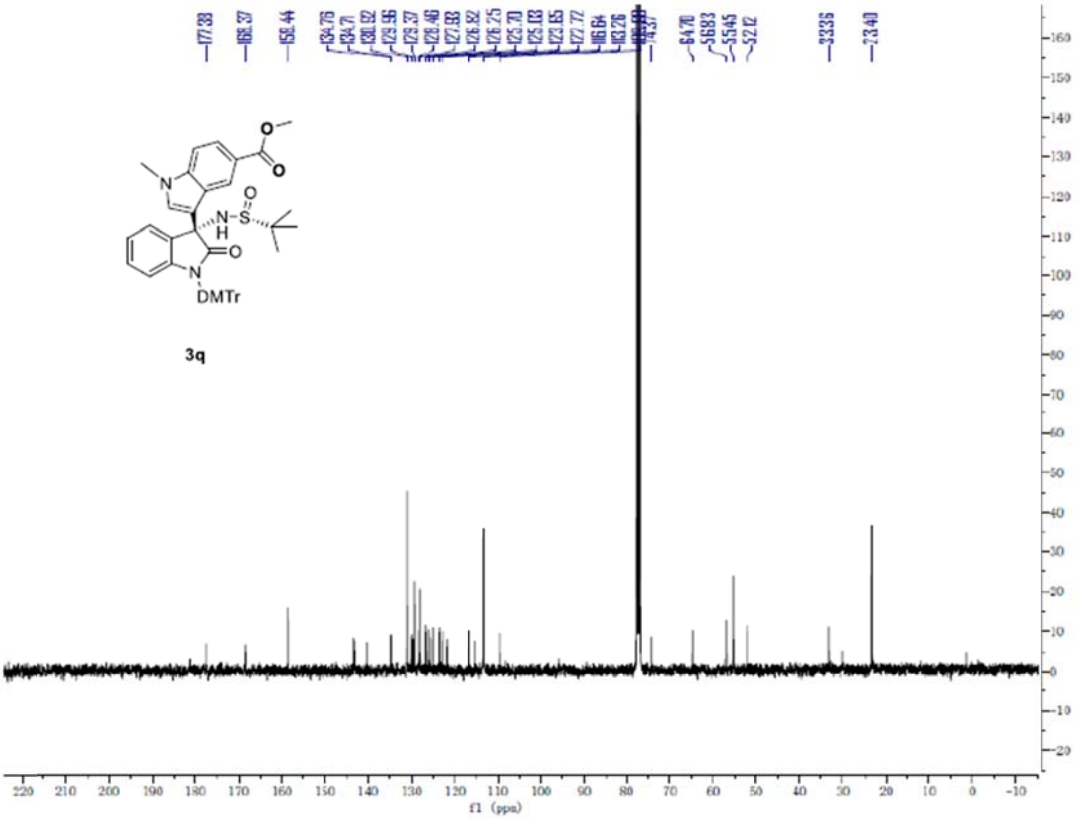

Br
DMTr
3o

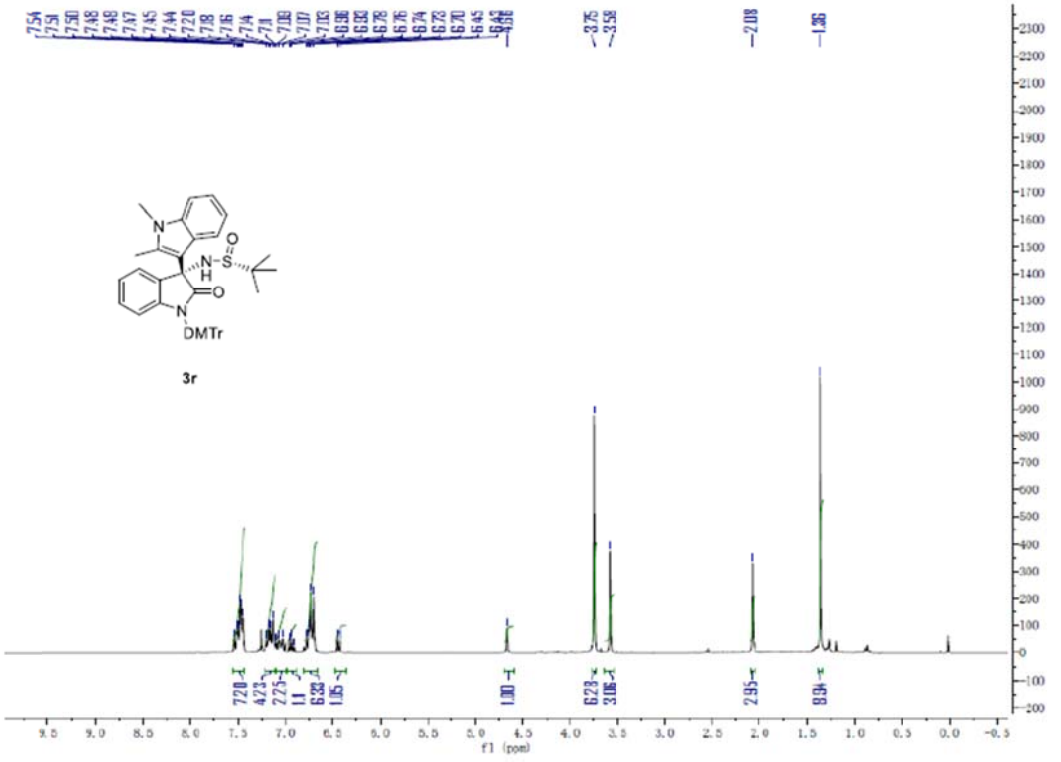

Br
DMTr
3o

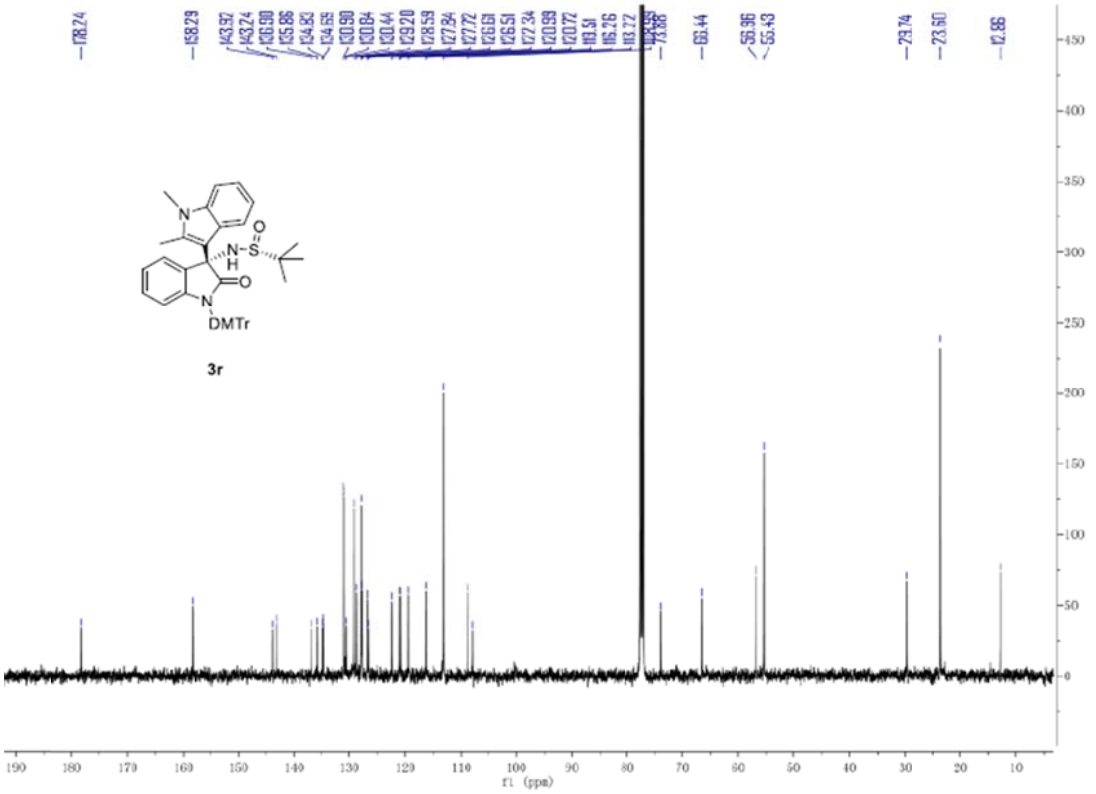

OMe
DMTr
3p
f1 (ppm)

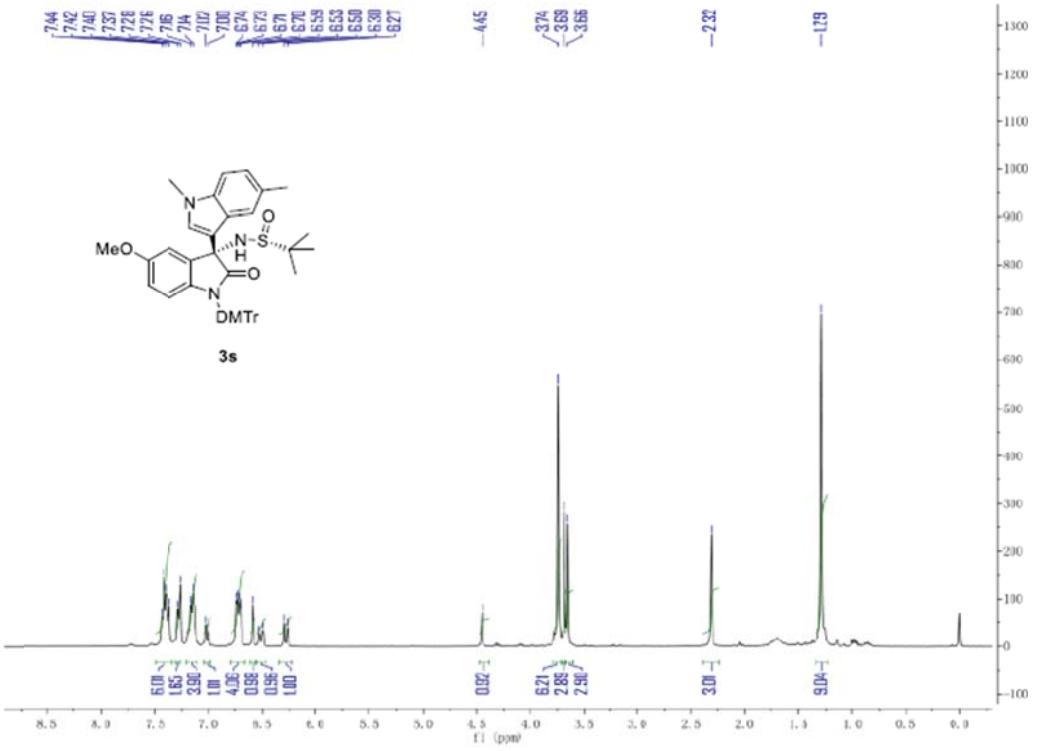

OMe
DMTr
3p
f1 (ppm)

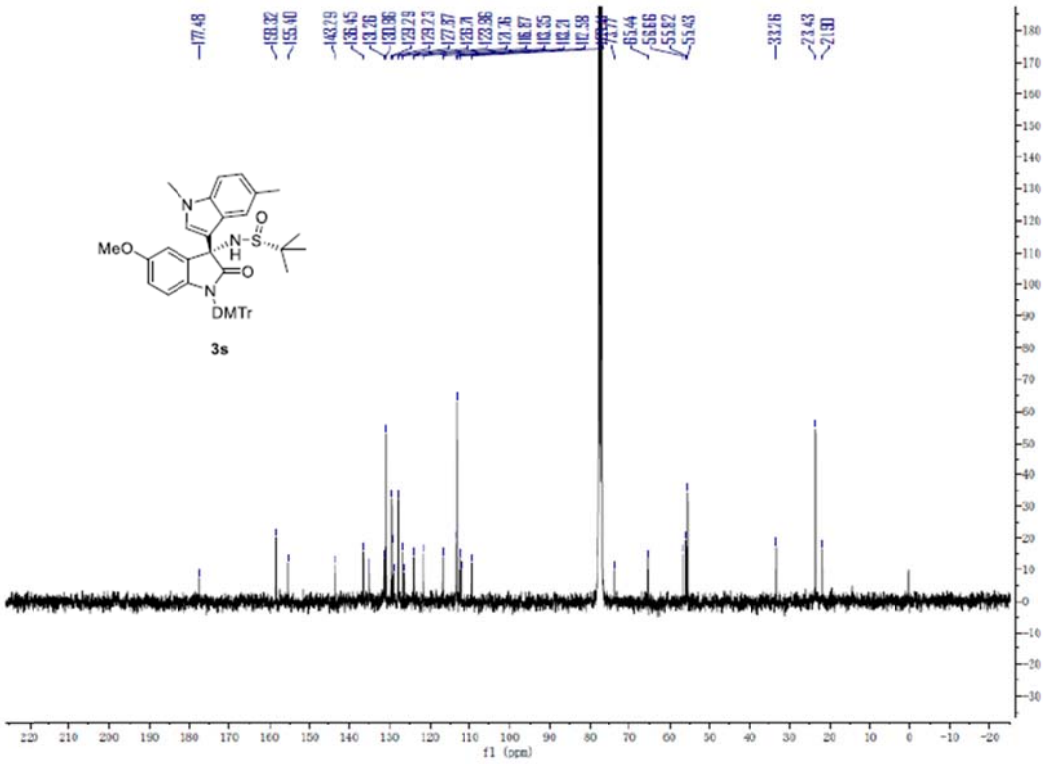

DMTr
3q
f1 (ppm)

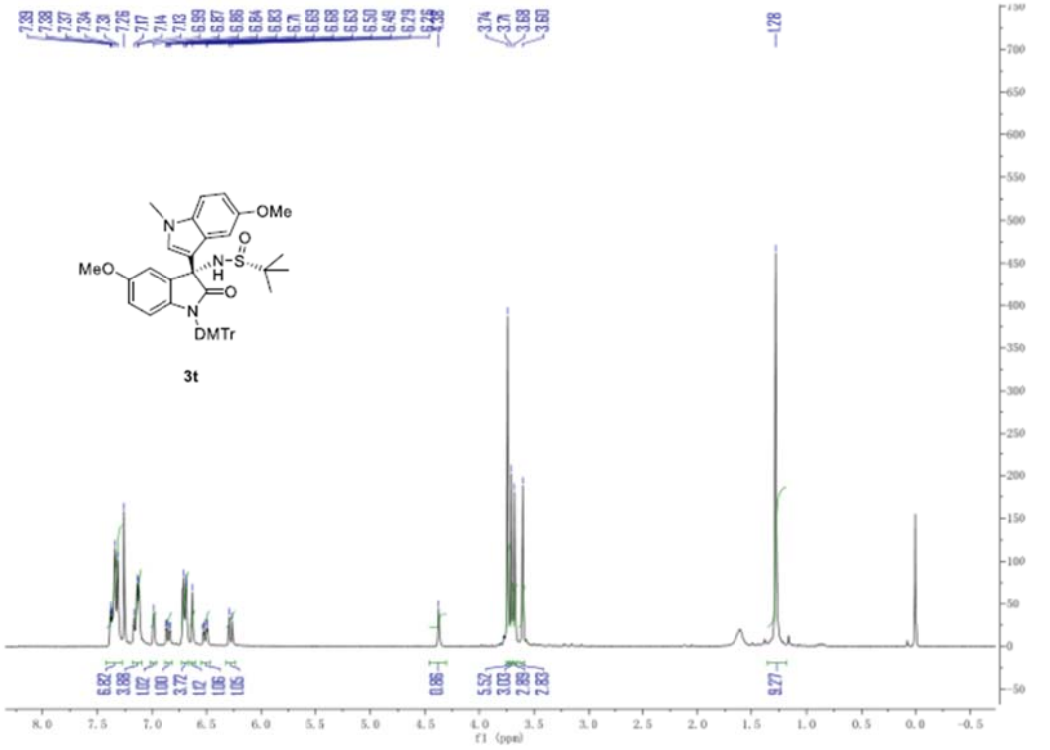

DMTr
3q
f1 (ppm)

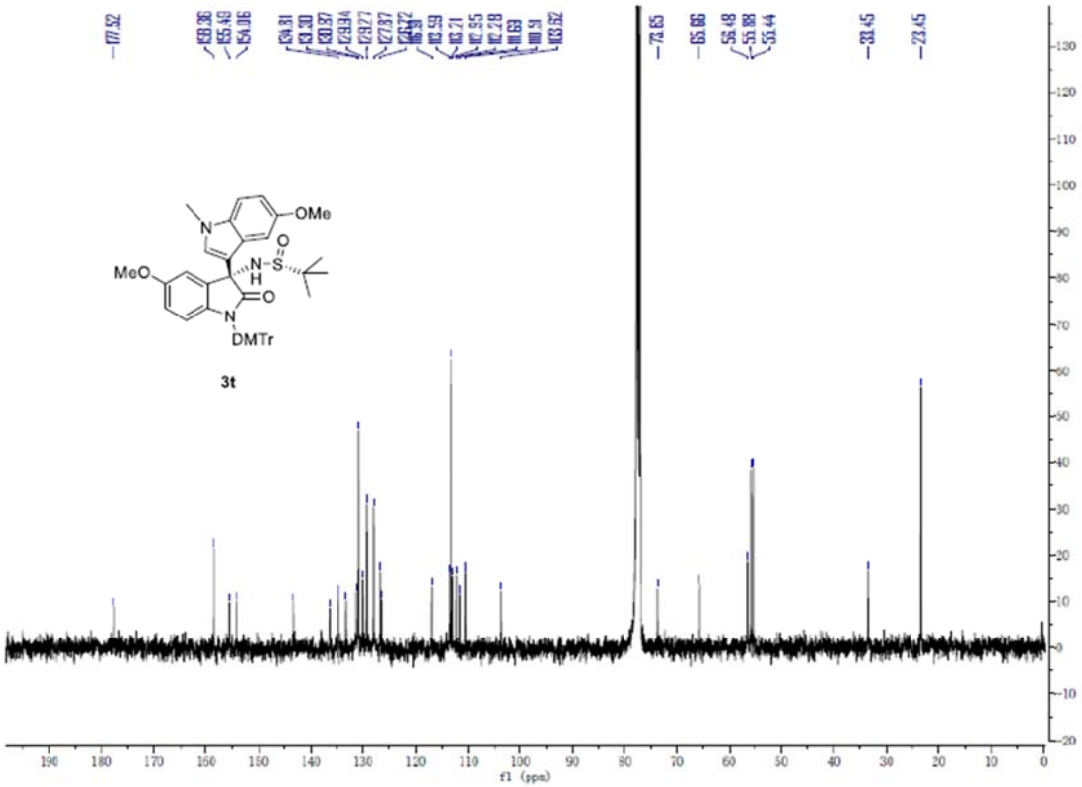

DMTr
3r
f1 (ppm)

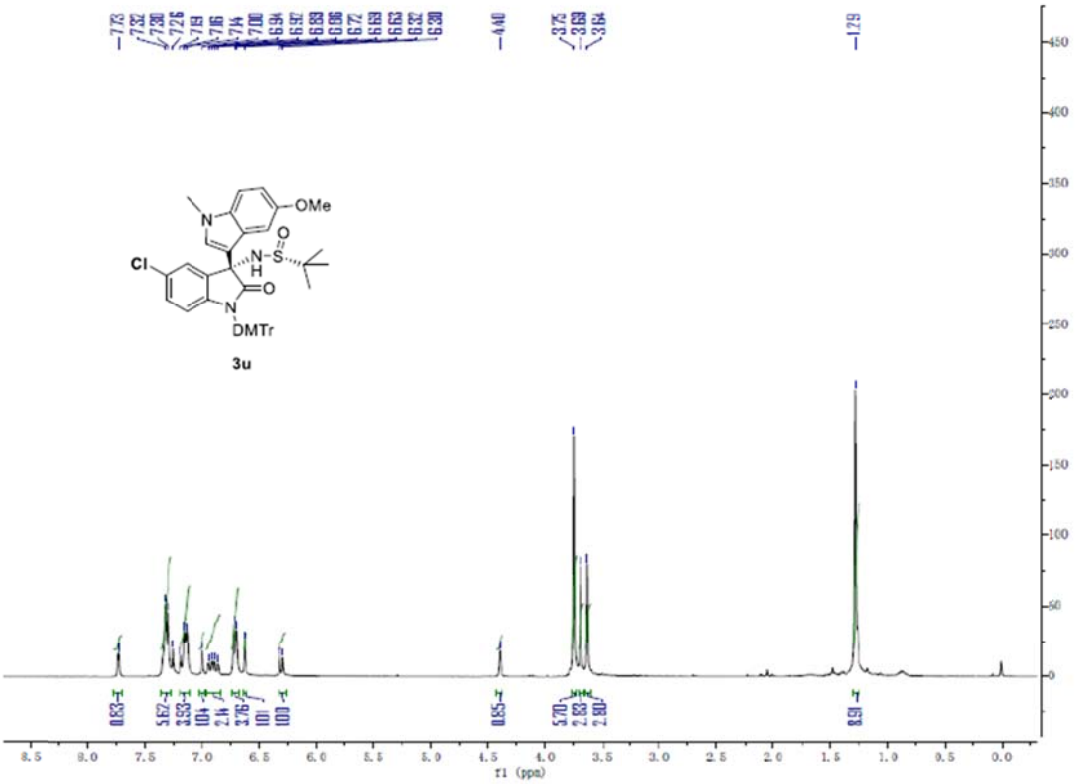

DMTr
3r
f1 (ppm)

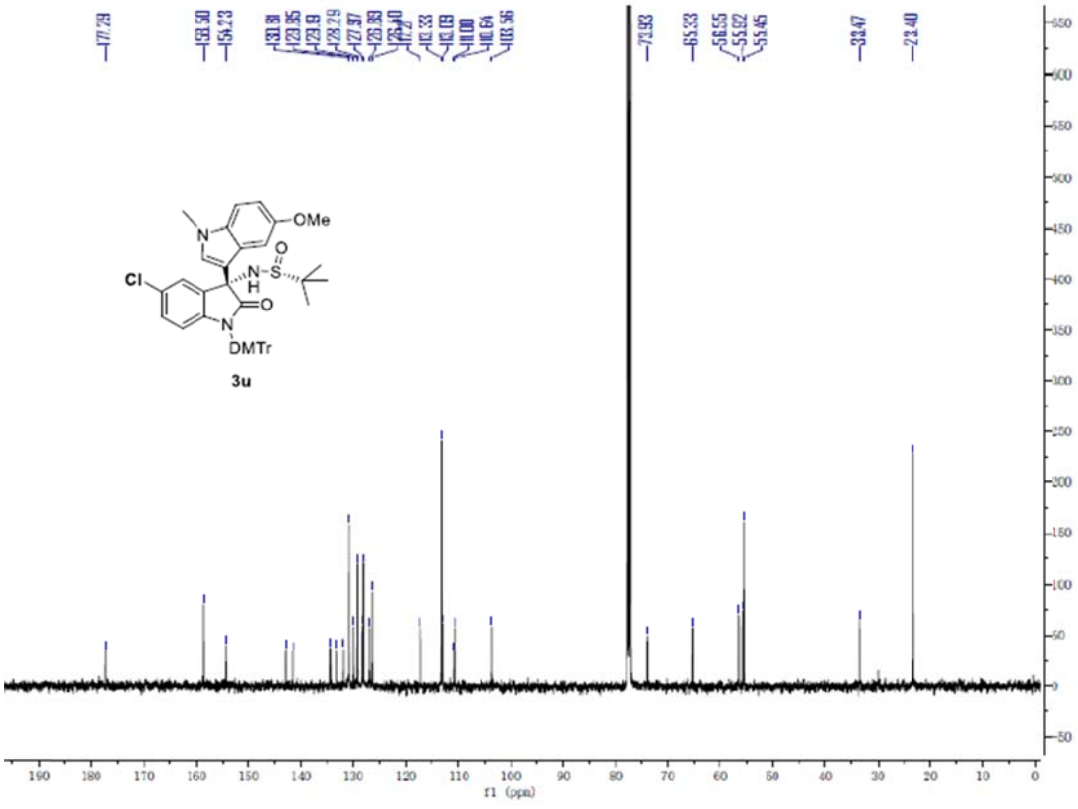

MeO
DMTr
3s
f1 (ppm)

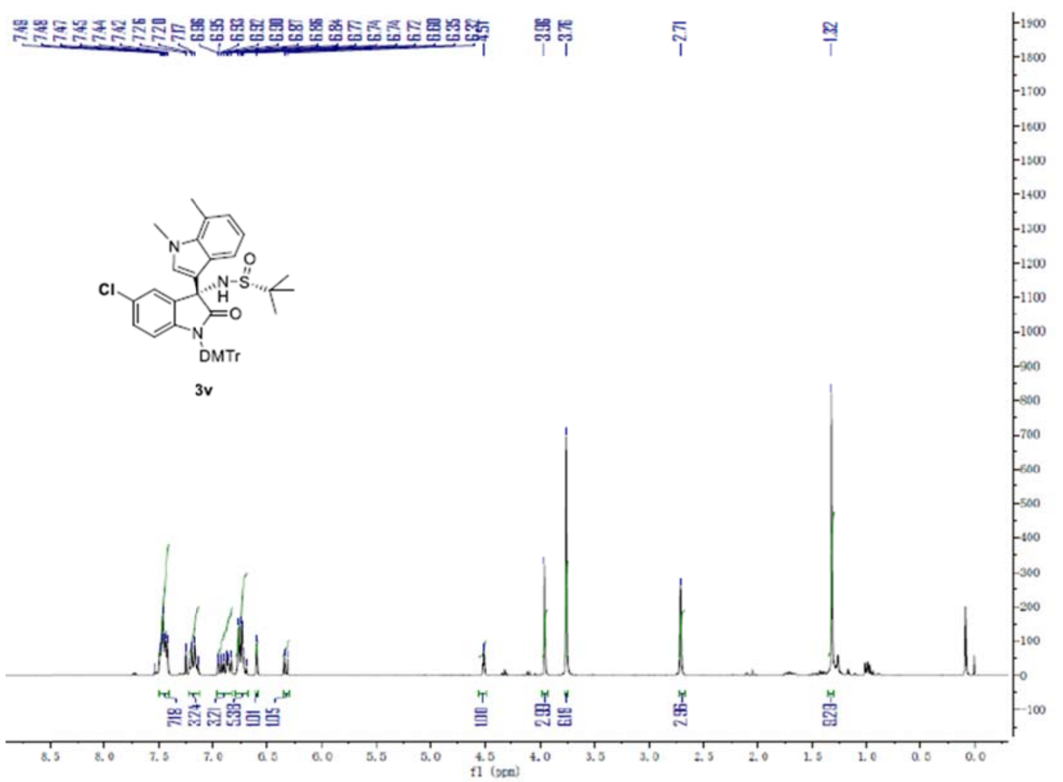

MeO
DMTr
3s
f1 (ppm)

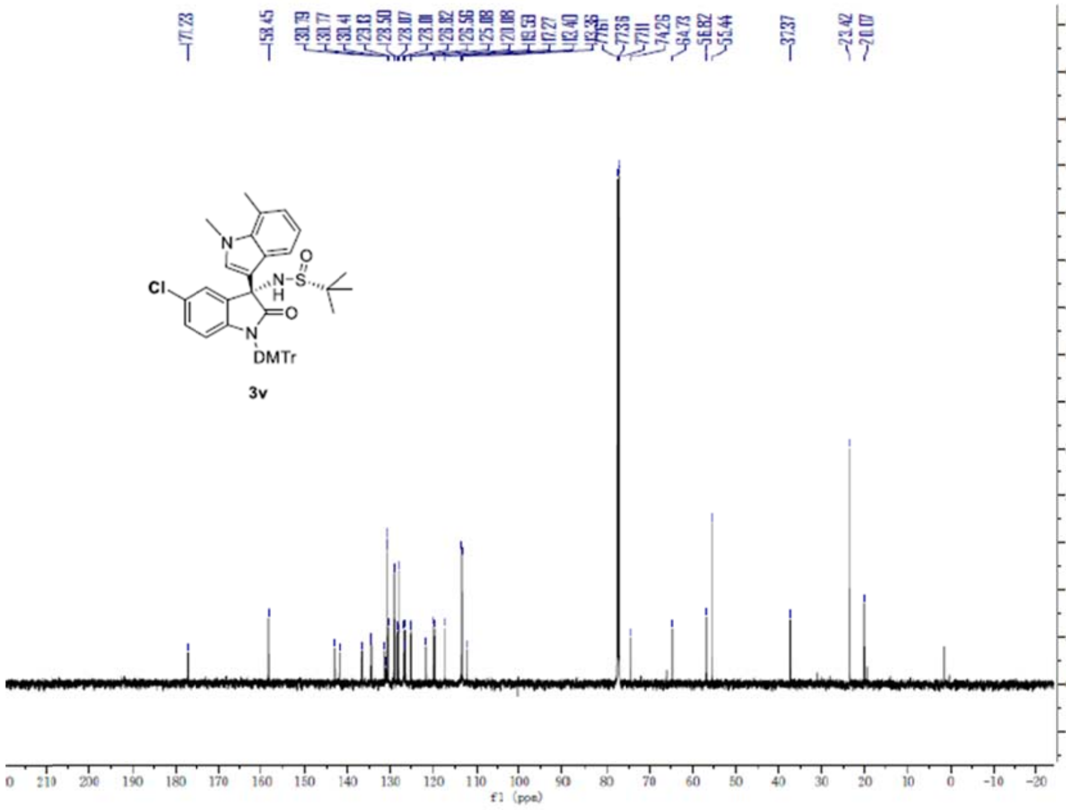

OMe
MeO
N
H
S
O
DMTr
3t
f1 (ppm)

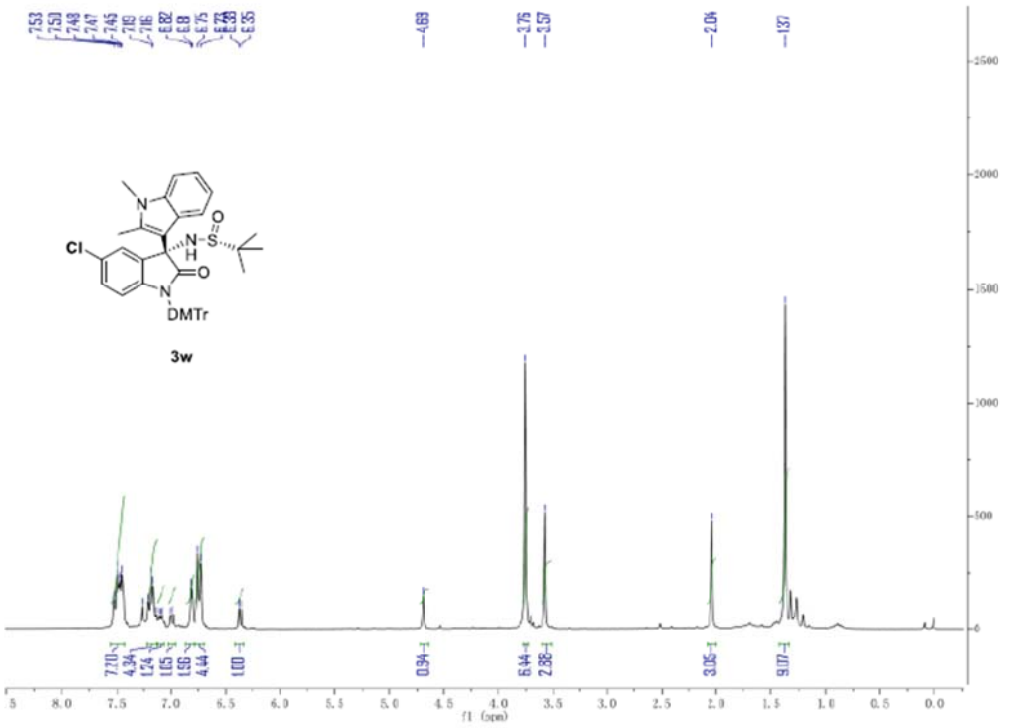

OMe
MeO
N
H
S
O
DMTr
3t
f1 (ppm)

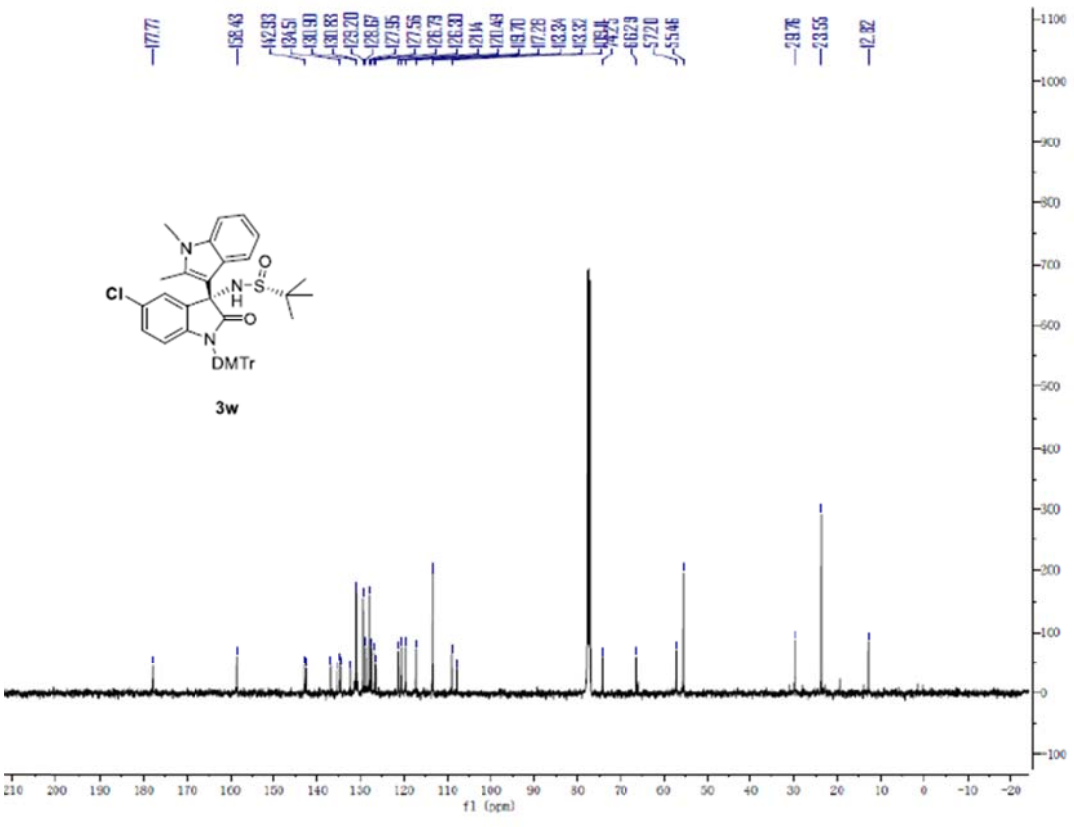

OMe
Cl
DMTr
3u
f1 (ppm)

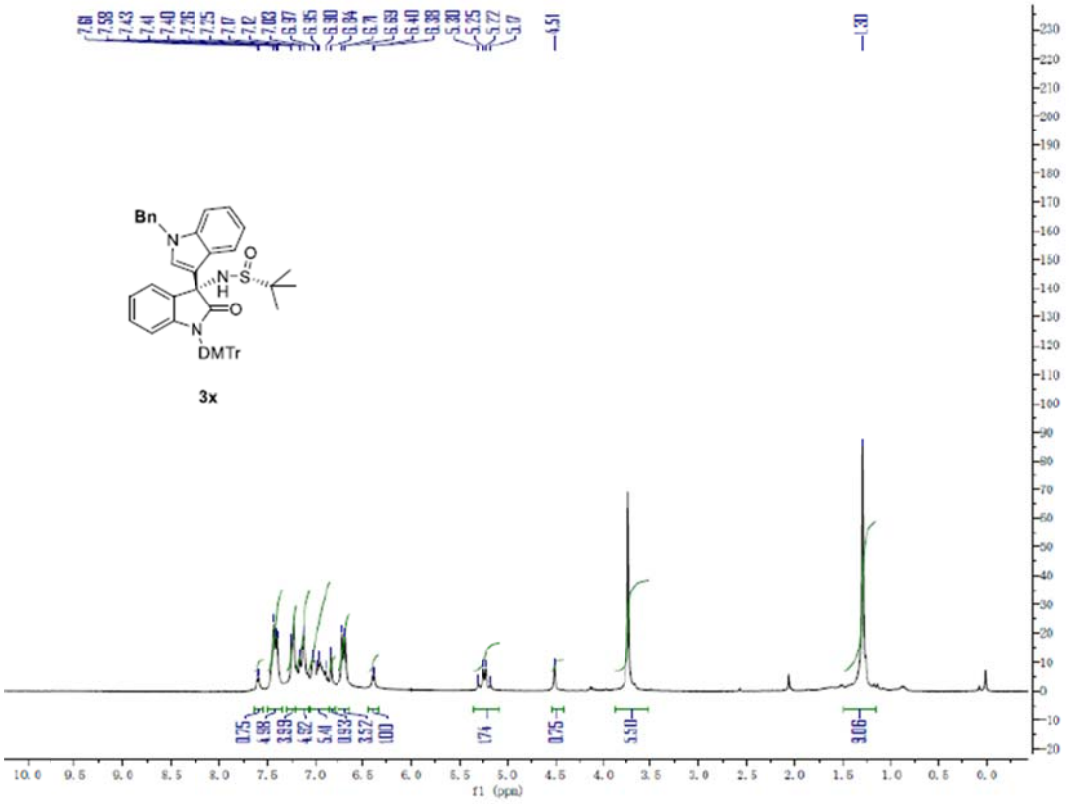

OMe
Cl
DMTr
3u
f1 (ppm)

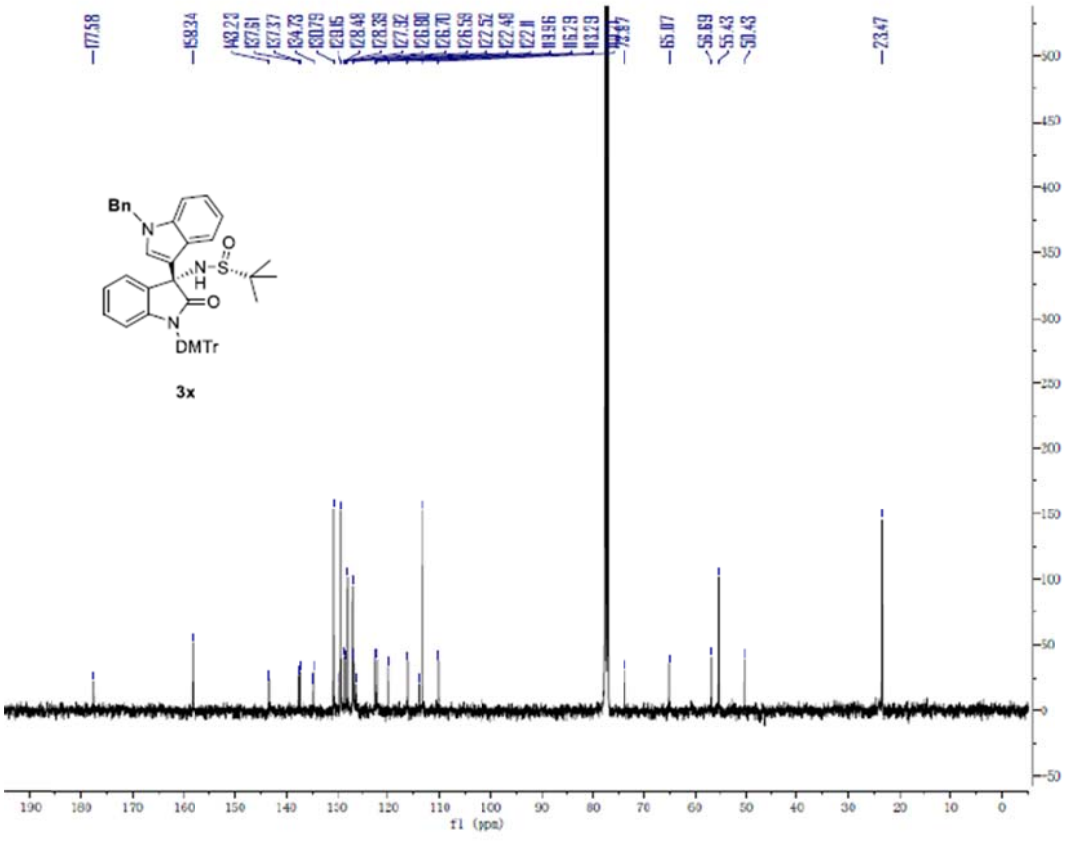

Cl
N
H
O
DMTr
3v
f1 (ppm)

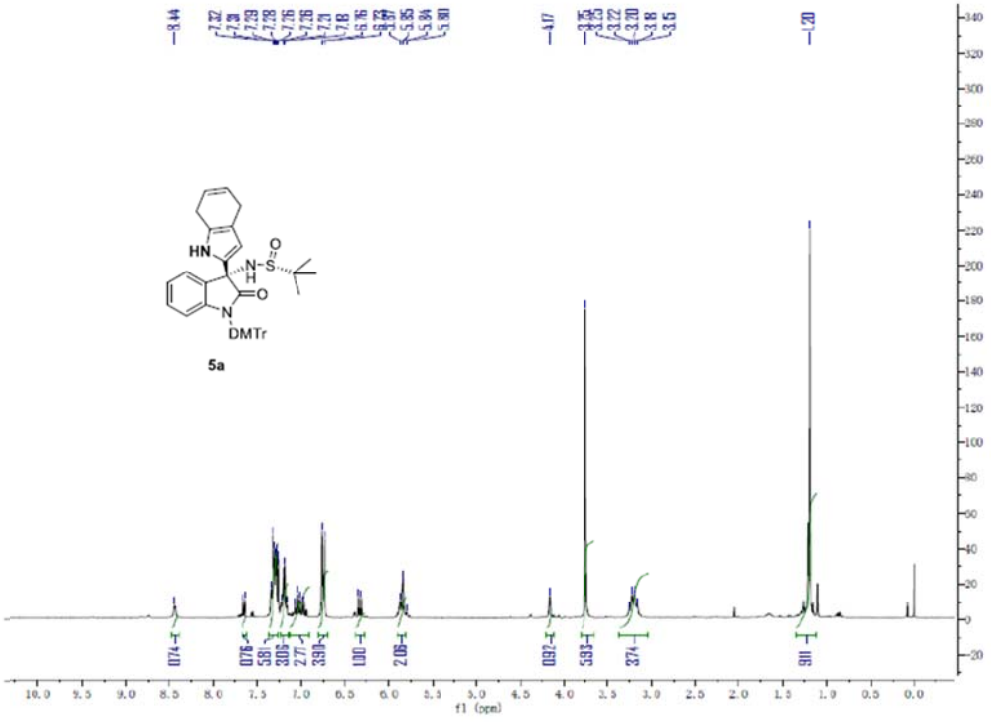

Cl
N
H
O
DMTr
3v
f1 (ppm)

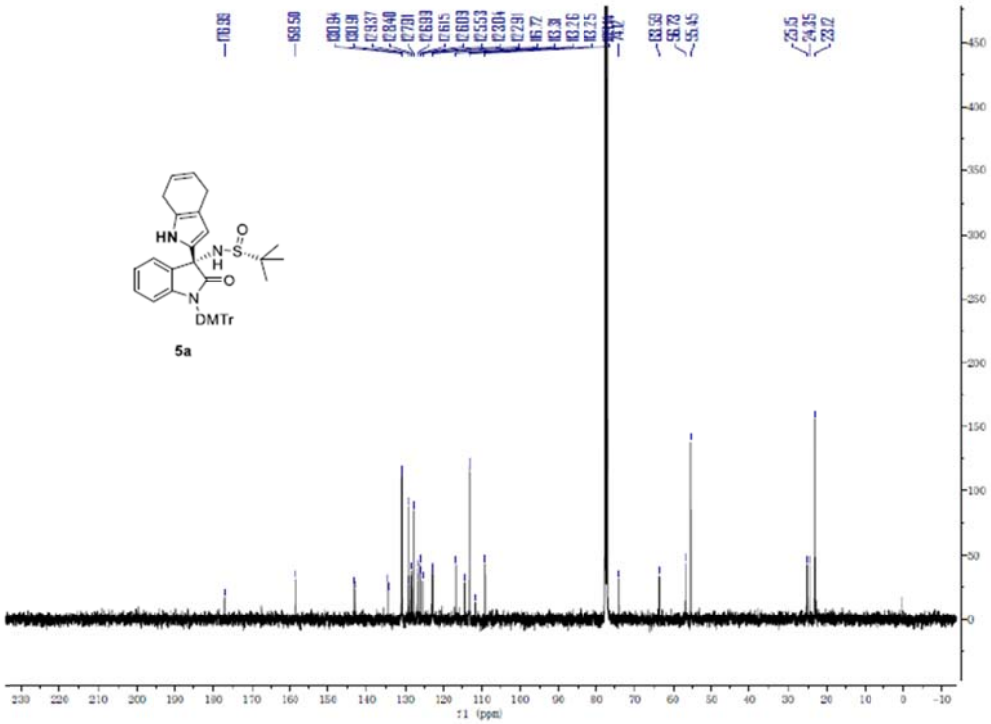

Cl
N
O
N-S
H
O
N
DMTr
3w
f1 (ppm)

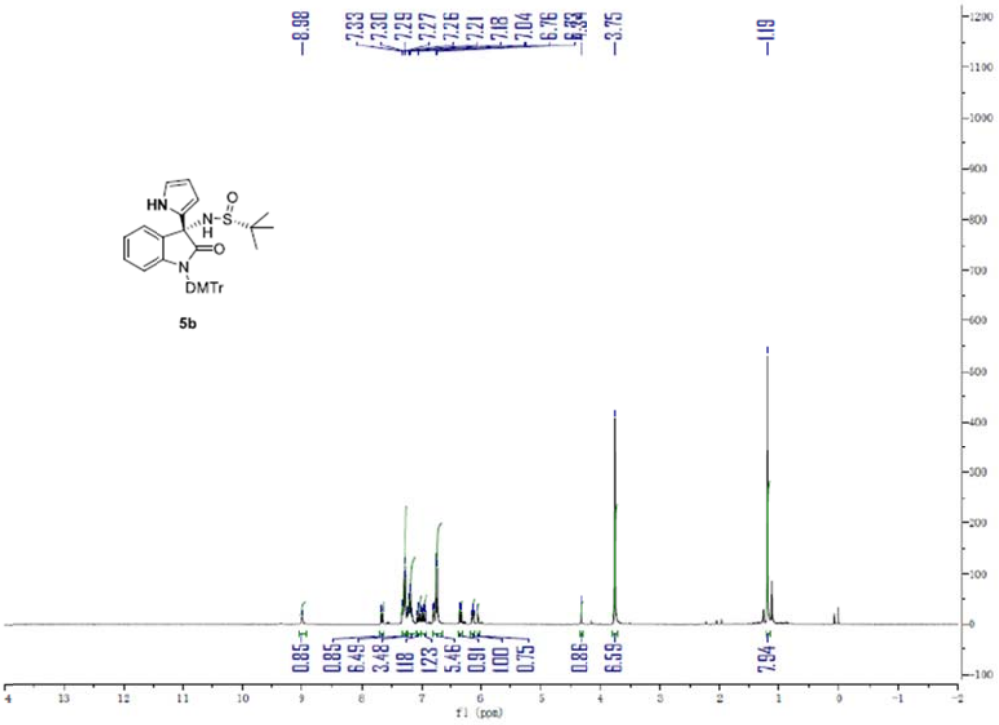

Cl
N
O
N-S
H
O
N
DMTr
3w
f1 (ppm)

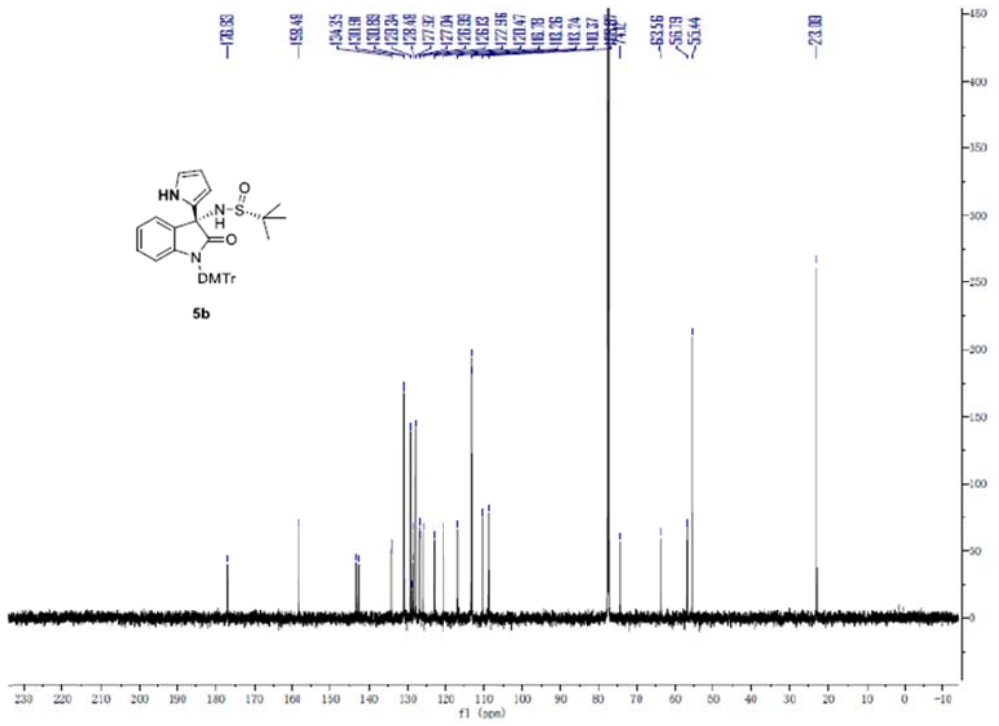

Bn
N
O
N-S
H
O
N
DMTr
3x
f1 (ppm)

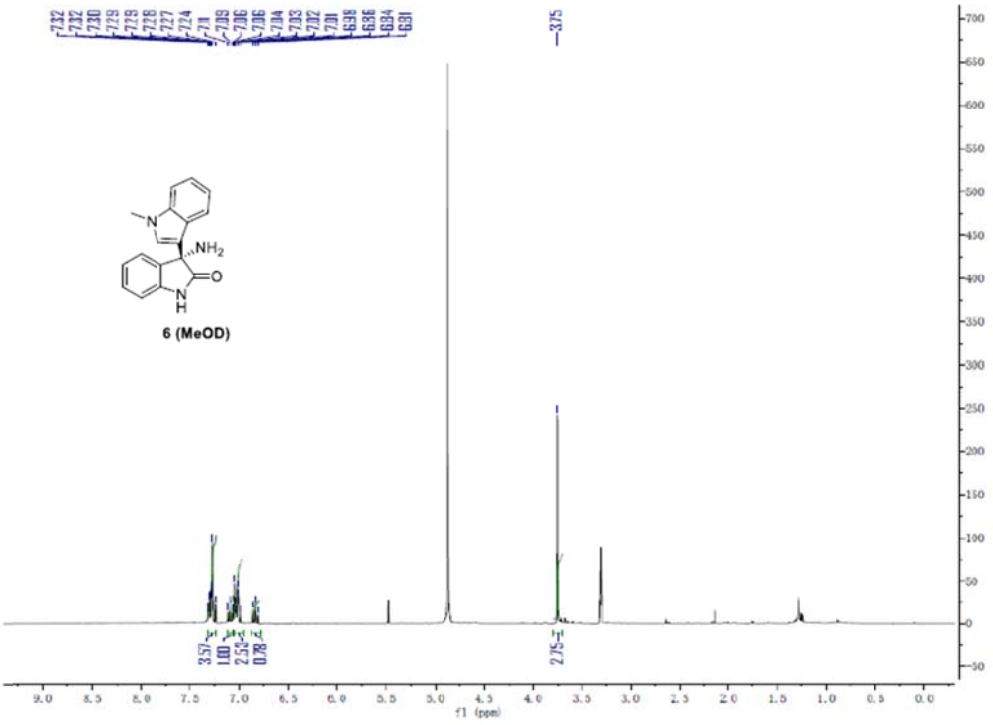

Bn
N
O
N-S
H
O
N
DMTr
3x
f1 (ppm)

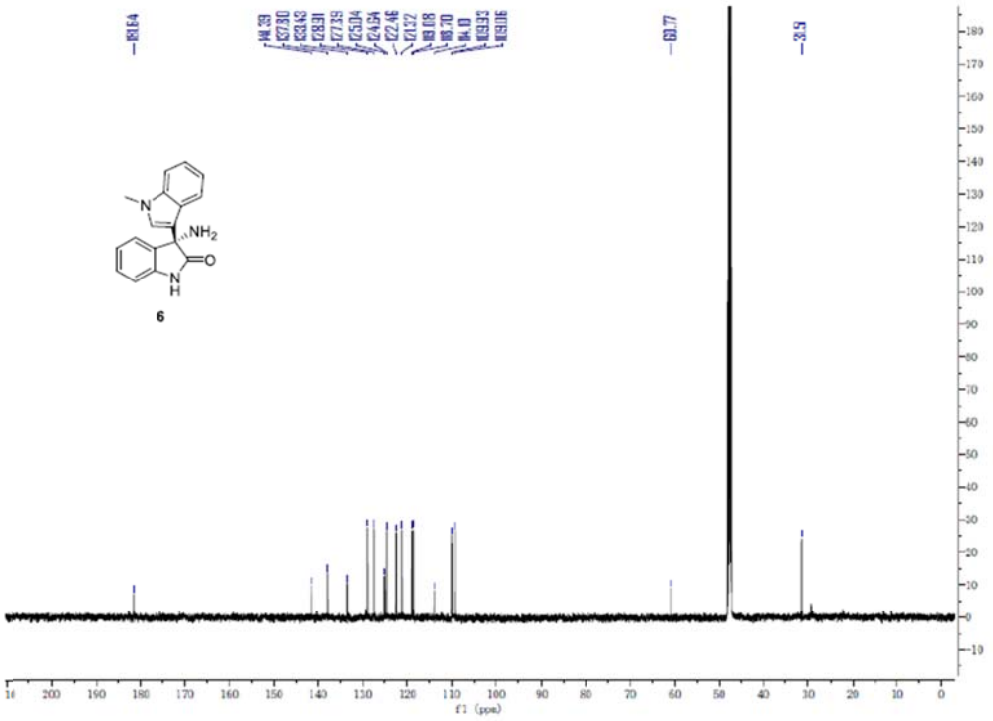

HN
N
S
O
H
O
N
DMTr
5a
f1 (ppm)


HN
N
S
O
H
O
N
DMTr
5a
f1 (ppm)

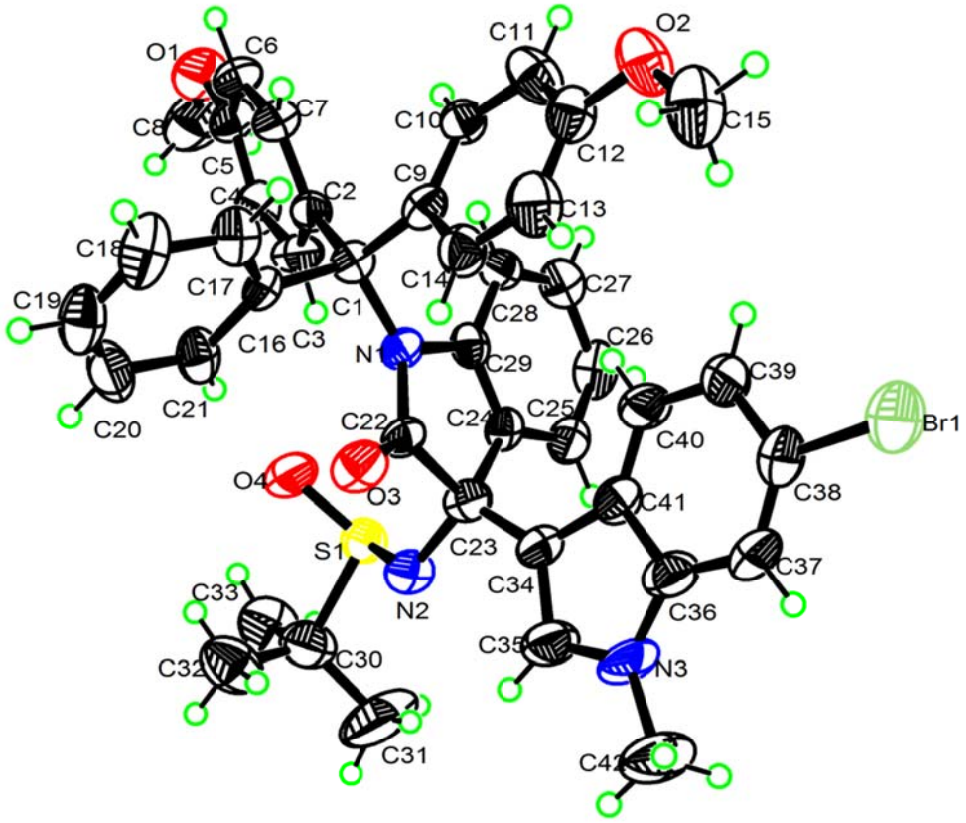

HN
N
H
S
O
O
N
DMTr
5b
8.98
7.33
7.30
7.29
7.27
7.26
7.21
7.18
7.04
6.76
3.75
1.19
0.85
0.85
6.45
3.48
1.18
1.23
5.46
0.91
1.00
0.75
0.86
6.59
7.64
f1 (ppm)


HN
N
H
S
O
O
N
DMTr
5b
f1 (ppm)


6 (MeOD)
f1 (ppm)


6
f1 (ppm)

X-ray of product 3o



CCDC **1043242**. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www. ccdc.cam.ac.uk/data_request/cif.