

Supporting Information

Construction of Highly Enantioselective Spiro-oxindole Derivatives with Fused Chromene via Organocascade Catalysis

Prathibha kumari,^{a, b} Sekhar Nandi,^{a, b} Gaurav Kumar,^{a, b} Noorul H. Khan,*^{a, b} Rukhsana I. Kureshy,^{a, b} Sayed H. R. Abdi^{a, b} E. Suresh,^{b, c} and Hari C. Bajaj^{a, b}

^a Division of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), Council of Scientific & Industrial Research (CSIR), G. B. Marg, Bhavnagar, 364002, Gujarat, India.

^b Academy of Scientific & Innovative Research (AcSIR)

^c Analytical Discipline and Centralised Instrumental Facility, Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), G. B. Marg, Bhavnagar 364 002, Gujarat, India.

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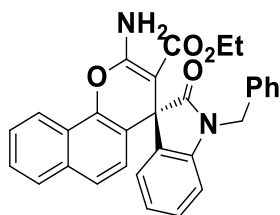
1. General Experimental methods:

Different isatin, naphthols and sesamols (Aldrich, TCI Chemicals and Germany) were used as received. All the solvents used in the present study were dried by known purification technique.¹ NMR spectra were obtained with a Bruker F113V spectrometer (500 MHz / 200 MHz) and are referenced internally with TMS. Splitting patterns were reported as s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet; br, broad. Enantiomeric excess (ee) were determined by HPLC (Shimadzu SCL-10AVP or Shimadzu VP-Prominence) using Daicel Chiralpak IA, IB and IC chiral columns with 2-propanol/hexane as eluent. FT-IR spectra were carried out using KBr (Perkin-Elmer spectrum GX spectrophotometer). High-resolution mass spectra were obtained with a LC-MS (Q-TOF), and for electrolyte quadruple, for calibration leucine was used. All samples were prepared in acetonitrile. Optical rotations were determined by automatic polarimeter (Digipol-781, Rudolph Instrument, USA). For the product purification flash chromatography was performed using silica gel 240-400 mesh.

2. General procedure for asymmetric catalytic reaction:

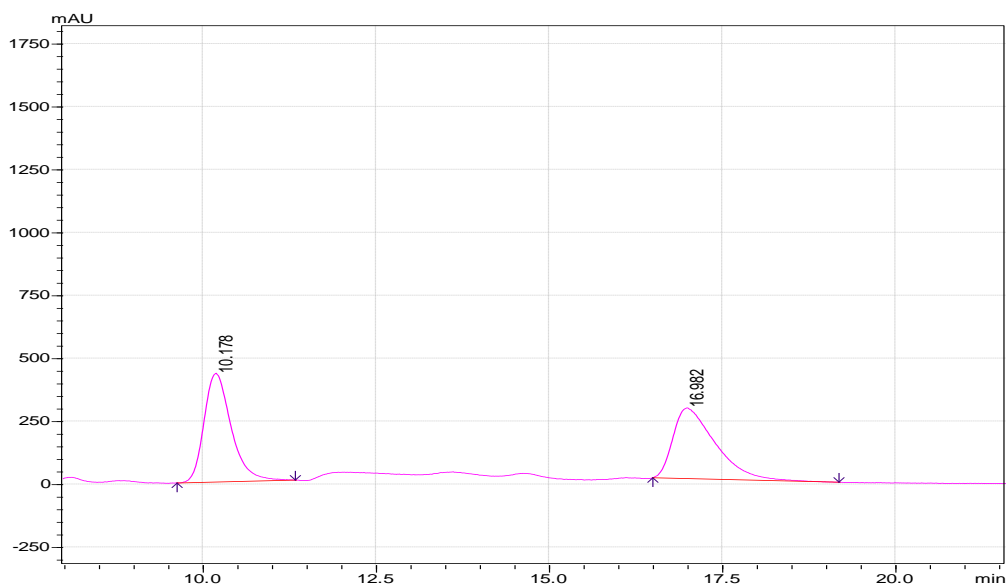
In a reaction vial **Cat. 5** (2 mol%), indonylidene cyanoacetate (0.2 mmol) and 30 mg of 4 ÅMS were dissolved in 2 mL of dry Ph-CF₃ at room temperature and the solution was stirred for 10 mins at RT. After 10 mins 1-naphthol/ sesamol (0.4 mmol) was added slowly over a period of 30 mins. The reaction was stirred at room temperature till the reaction was completed (TLC). Finally the reaction mixture was subjected to column chromatography, using 9:1 (DCM/ EtOAc) as eluent to efford desired product and enantiomeric excess was determined by HPLC.

3. Characterization data for products

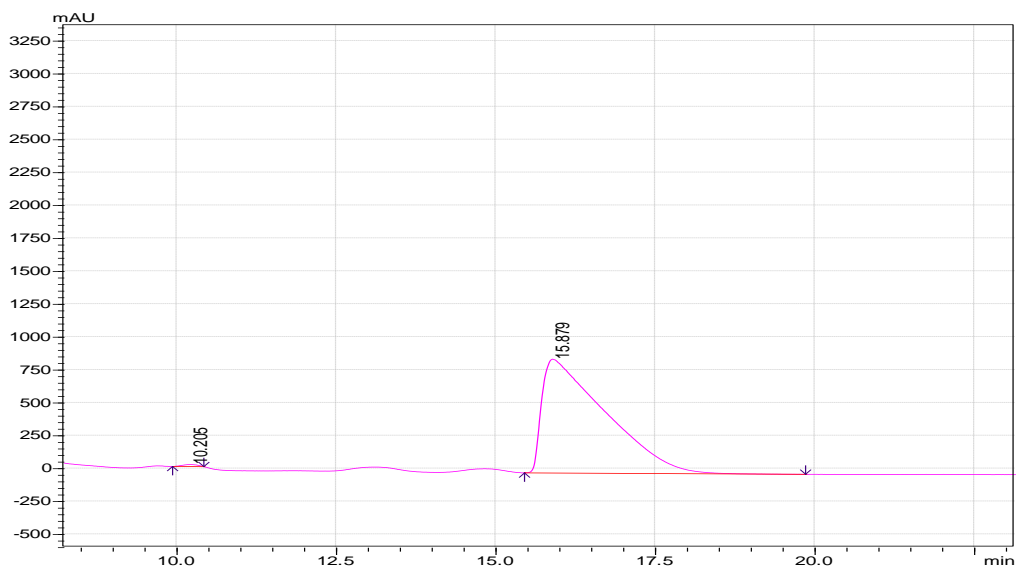


3a; Enantiomeric excess (99%) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 15.87$ min, minor enantiomer $t_r = 10.2$ min.

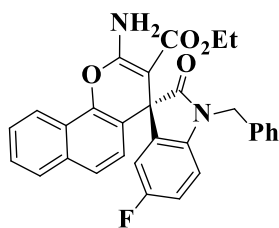
$[\alpha]_D^{20} -58$ ($c = 1$) (99% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.15 (d, $J = 8$ Hz, 1H), 7.68 (d, $J = 7$ Hz, 1H), 7.49-7.45 (m, 5H), 7.35 (t, $J = 14.5$ Hz, 3H), 7.34-7.32 (m, 2H), 7.13-7.15 (m, 1H), 6.98 (s, 1H), 6.53 (d, $J = 8.5$ Hz, 1H), 5.26 (d, $J = 15$, 1H), 4.67 (d, $J = 15.5$ Hz, 1H), 3.97-3.66 (m, 2H), 0.70 (t, $J = 13$ Hz, 3H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 141.3, 140.0, 136.1, 133.4, 128.8, 128.2, 127.9, 127.7, 127.4, 127.0, 126.6, 124.6, 124.2, 122.9, 121.0, 109.3, 96.1, 59.4, 50.5, 44.6, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{25}\text{N}_2\text{O}_4$ ($\text{M}+1$)⁺ 477.1800 found 477.1804, error 0.8 ppm.



Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.178	9.621	11.328	49.7249
2	16.982	16.491	19.179	50.2751

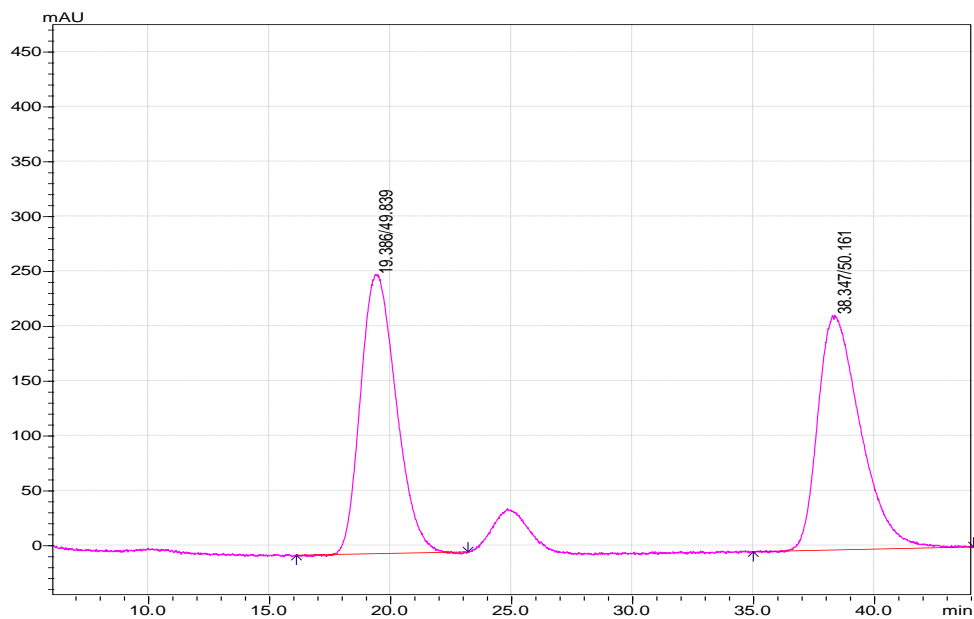


Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.205	9.931	10.421	0.4318
2	15.879	15.445	19.851	99.5682

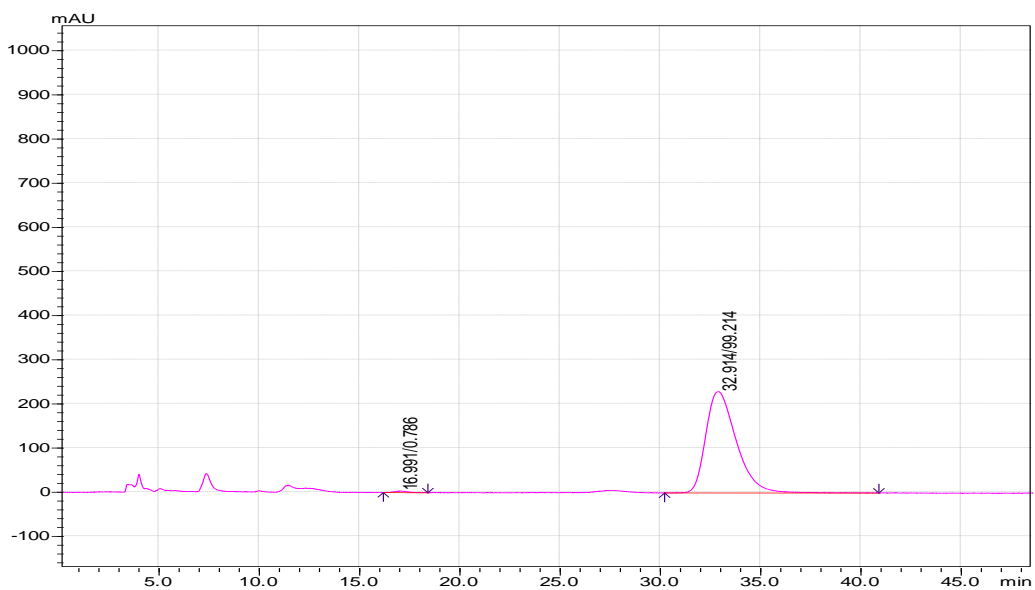


3b; Enantiomeric excess (98%) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 32.9$ min, minor enantiomer $t_r = 16.9$ min.

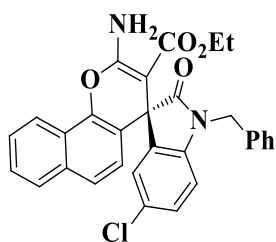
$[\alpha]_D^{20} -58.1$ ($c = 1$) (98% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.12–8.11 (m, 1H), 7.66–7.65 (m, 1H), 7.49 (d, $J = 7$ Hz, 3H), 7.46–7.44 (m, 2H), 7.39 (t, $J = 14.5$, 3H), 7.33 (t, $J = 14.5$ Hz, 2H), 6.89–6.85 (m, 1H), 6.81–6.79 (m, 1H), 6.77–6.75 (m, 1H), 6.54 (d, $J = 8.5$ Hz, 1H), 5.26 (d, $J = 15$ Hz, 1H), 4.68 (d, $J = 15.5$ Hz, 1H), 3.98–3.64 (m, 2H), 0.68 (t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.8, 168.2, 161.0, 160.6, 158.7, 143.1, 140.17, 140.12, 138.7, 136.3, 133.4, 128.8, 128.2, 127.9, 127.4, 127.0, 126.5, 124.5, 123.3, 122.9, 121.0, 115.4, 114.1, 113.9, 111.9, 11.7, 108.9, 108.8, 74.8, 59.4, 50.8, 44.7, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_4\text{F}$ ($\text{M}+1$) $^+$ 495.1714 found 495.1705, error -1.81 ppm.



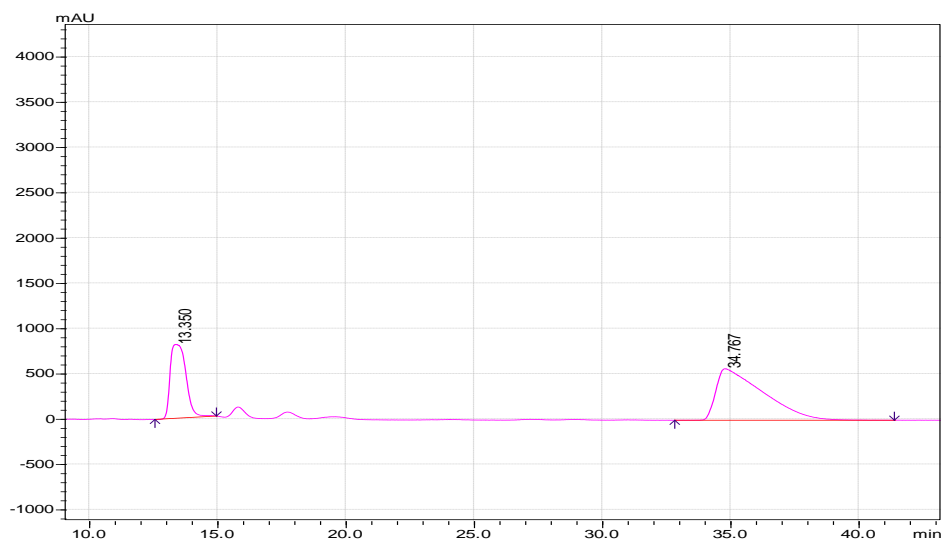
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	19.386	25923330	16.107	23.200	49.8392
2	38.347	26090612	34.987	44.085	50.1608



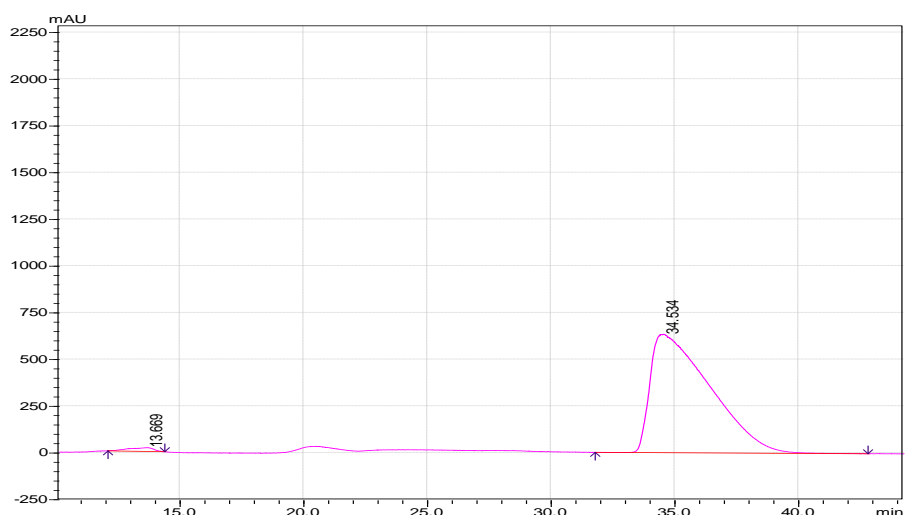
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	16.991	192533	16.181	18.400	0.7863
2	32.914	24293390	30.208	40.896	99.2137



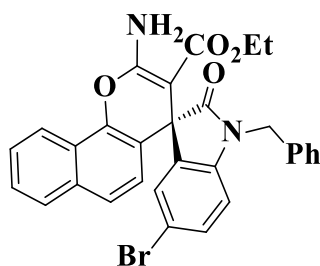
3c; Enantiomeric excess (97%) was determined by chiral HPLC (chiralpak IC), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 34.534$ min, minor enantiomer $t_r = 13.66$ min. $[\alpha]_D^{20} -40.2$ ($c = 1$) (97% *ee*); ^1H NMR (500 MHz, CDCl_3) δ 8.11–8.09 (m, 1H), 7.65–7.64 (m, 1H), 7.49 (d, $J = 7$ Hz, 3H), 7.44-7.42 (m, 2H), 7.40-7.37 (m, 2H), 7.34-7.31 (m, 3H), 6.88-6.84 (m, 1H), 6.81-6.79 (m, 1H), 6.77-6.75 (m, 1H), 6.54 (d, $J = 8.5$ Hz, 1H), 5.26 (d, $J = 15$ Hz, 1H), 4.69 (d, $J = 15$ Hz, 1H), 3.97-3.64 (m, 2H), 0.68 (t, $J = 14$ Hz, 3 H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.8, 168.2, 161.1, 143.2, 140.2, 138.7, 136.3, 133.4, 128.8, 128.2, 127.9, 127.3, 127.0, 126.5, 124.5, 123.3, 122.9, 121.0, 115.3, 114.1, 113.9, 111.9, 108.9, 108.8, 74.7, 59.4, 50.9, 44.7, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_4\text{Cl}$ ($\text{M}+1$) $^+$ 511.1419 found 511.1405, error -2.73 ppm.



Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	13.350	62850036	12.544	14.944	50.7564
2	34.767	60976824	32.811	41.376	49.2436

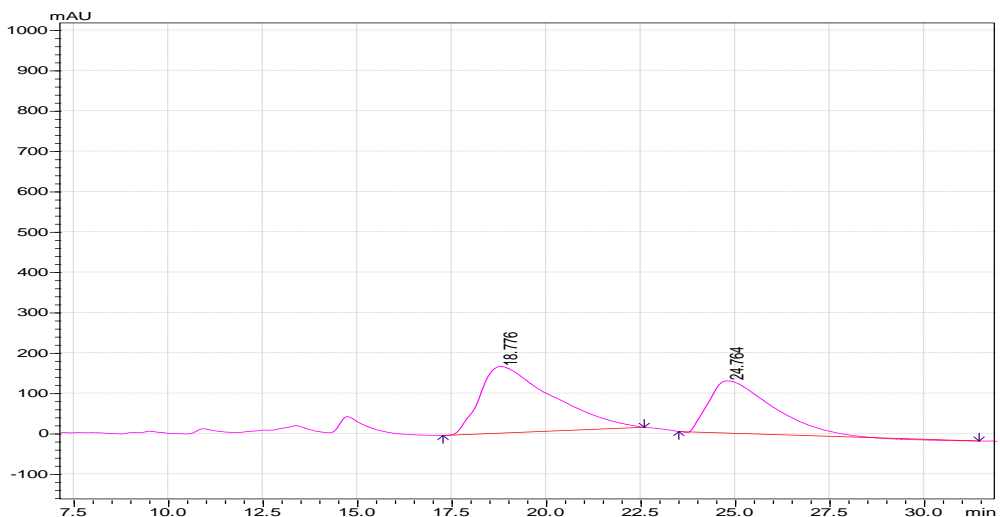


Peak#	Ret. Time	Peak Start	Peak End	Area%
1	13.669	12.085	14.379	1.2917
2	34.534	31.776	42.805	98.7083

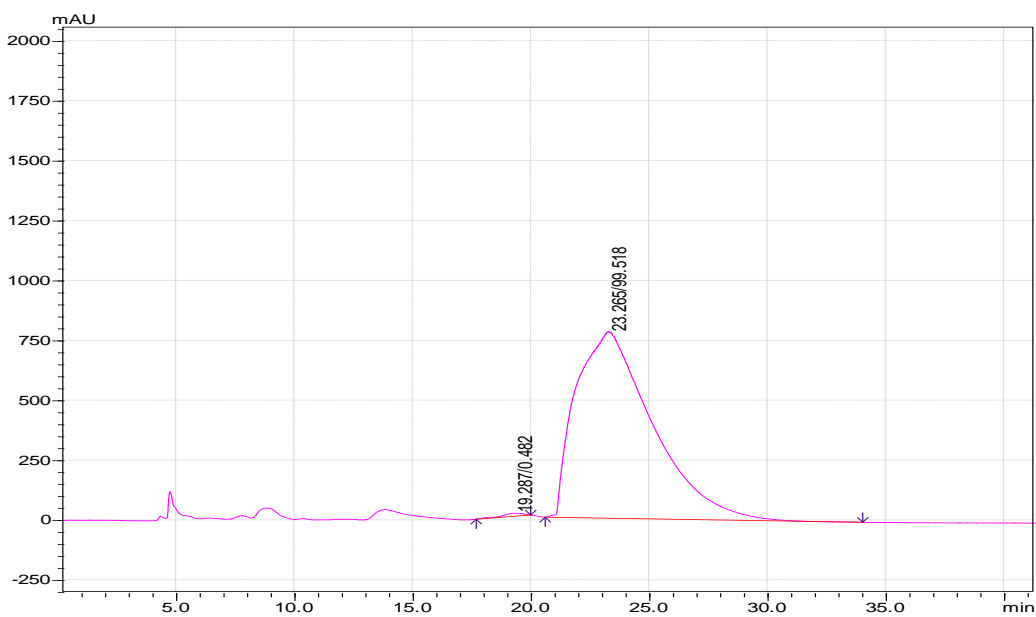


3d; Enantiomeric excess (99 %) was determined by chiral HPLC (chiralpak IB), hexane-*i*-PrOH 80:20, 0.7 mL/min, major enantiomer $t_r = 23.2$ min, minor enantiomer $t_r = 19.2$ min.

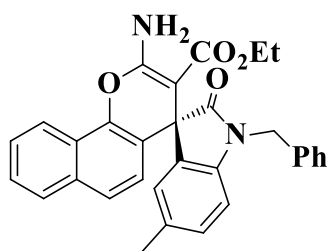
$[\alpha]_D^{20} -23.5$ ($c = 1$) (99 % *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.22 (d, $J = 8.5$ Hz, 1H), 7.73 (d, $J = 8$ Hz, 1H), 7.57 (t, $J = 15$ Hz, 1H), 7.52 (t, $J = 15$ Hz, 1H), 7.47 (d, $J = 7.5$ Hz, 1H), 7.38 (t, $J = 15.5$ Hz, 2H), 7.34 (d, $J = 8.5$ Hz, 3H), 7.29 (d, $J = 8$ Hz, 1H), 7.11 (s, 1H), 6.76 (d, $J = 8$ Hz, 1H), 6.54 (d, $J = 8.5$ Hz, 1H), 5.24 (d, $J = 15$ Hz, 1H), 4.66 (d, $J = 15$ Hz, 1H), 3.97-3.66 (m, 2H), 0.70 (t, $J = 14$ Hz, 3H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.8, 168.1, 160.9, 144.1, 143.1, 137.3, 135.9, 133.4, 130.8, 128.89, 128.80, 127.4, 127.0, 126.6, 125.8, 125.0, 124.5, 123.2, 122.9, 121.0, 115.3, 111.6, 74.7, 59.4, 44.6, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_4\text{Br}$ ($\text{M}+1$) $^+$ 554.0914 found 555.0941, error 4.86 ppm



Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	18.776	21973239	17.259	22.581	59.1268
2	24.764	15189646	23.499	31.445	40.8732

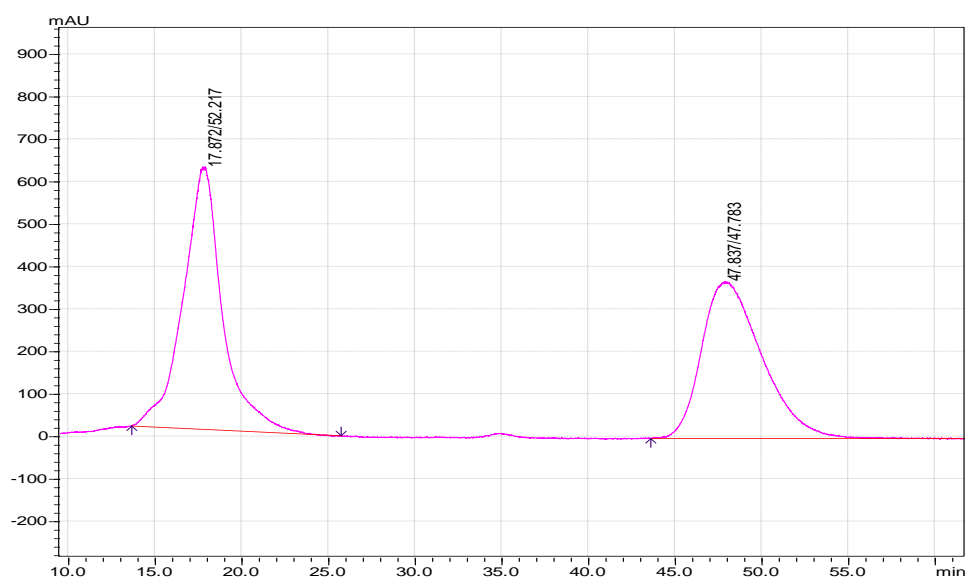


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	19.287	846995	17.664	19.968	0.4816
2	23.265	175024311	20.576	34.005	99.5184

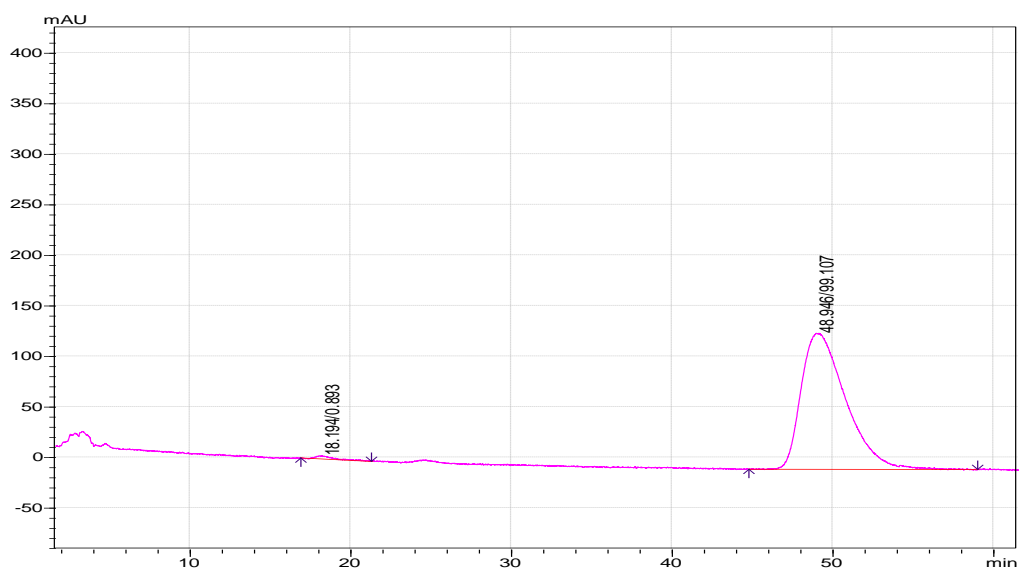


3e; Enantiomeric excess (98%) was determined by chiral HPLC (chiralpak IC), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 48.9$ min, minor enantiomer $t_r = 18.19$ min.

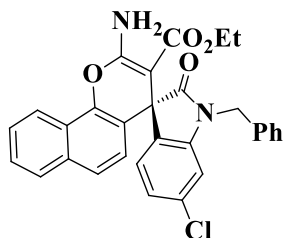
$[\alpha]_D^{25} = +17.5$ ($c = 1$) (98% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.10 (d, $J = 9.5$ Hz, 1H), 7.62(m, 1H), 7.49 (d, $J = 7.5$ Hz, 2H), 7.43-7.40(m, 3H), 7.35(t, $J = 15$ Hz, 2H), 7.31-7.23(m, 3H), 6.93(d, $J = 8$ Hz, 1H), 6.79 (s, 1H), 6.75(d, $J = 8$ Hz, 1H), 6.55(d, $J = 8.5$, 1H), 5.25(d, $J = 15$, 1H), 4.64(d, $J = 15$ Hz, 1H), 3.93-3.66(m, 1H), 3.70-3.64(m, 1H), 2.13(s, 3H), 0.66(t, $J = 14.5$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) .180.01, 168.6, 161.0, 143.1, 140.4, 138.5, 136.7, 133.3, 132.6, 128.8, 128.0, 127.8, 127.4, 126.5, 124.6, 124.4, 23.4, 121.08, 116.3, 108.2, 75.5, 59.4, 50.5, 44.6, 29.7, 21.0, 13.7. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{O}_4$ ($\text{M}+1$)⁺ 491.1965 found 491.1972, error 1.42 ppm.



Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	17.872	97679043	13.643	25.717	52.2175
2	47.837	89382955	43.584	63.872	47.7825

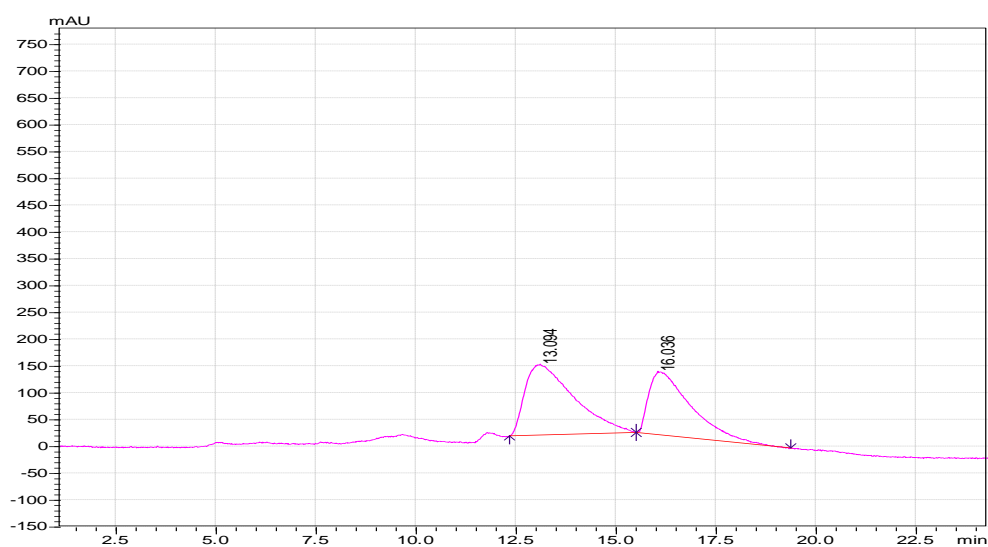


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	18.194	232620	16.885	21.280	0.8930
2	48.946	25817315	44.768	58.997	99.1070

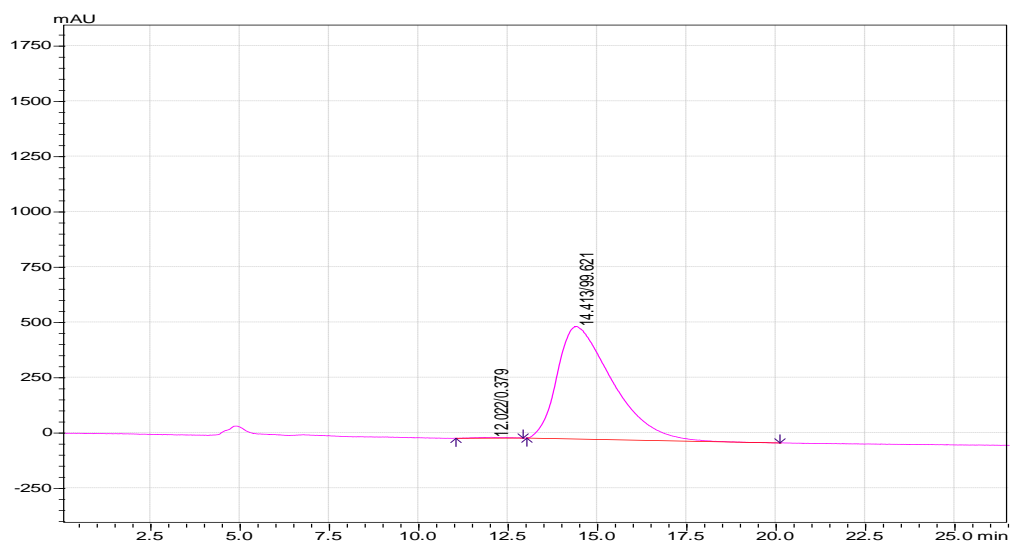


3f; Enantiomeric excess (99%) was determined by chiral HPLC (chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 14.4$ min, minor enantiomer $t_r = 12.0$ min.; $[\alpha]_D^{20} -62$ ($c = 1$) (99% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.15–8.14 (m, 1H), 7.68 (d, $J = 7$ Hz, 1H), 7.50-7.47(m, 5H), 7.40 (*t*, $J = 14.5$ Hz, 2H), 7.35-7.31 (m, 2H), 6.90 (m, 4H), 6.52 (d, $J = 8.5$ Hz, 1H), 5.24 (d, $J = 15$ Hz, 1H), 4.66 (d, $J = 15$ Hz, 1H), 3.95-3.65 (m, 2H), 0.70 (*t*, $J = 14$ Hz, 3H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.9, 168.2, 144.0, 143.1, 136.0, 136.0, 133.4, 133.3, 128.9, 128.2, 128.0, 127.4, 127.0, 126.6, 124.7, 124.6, 123.3, 122.93, 122.91,

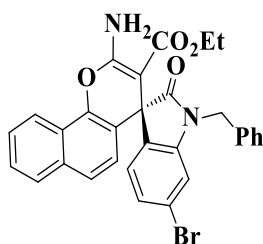
121.1, 115.4, 108.0, 74.8, 59.5, 50.1, 44.7, 13.7. HRMS (TOF ES): Calcd for C₃₀H₂₄N₂O₄Cl (M⁺) 511.1425 found 511.1419, error -1.17 ppm.



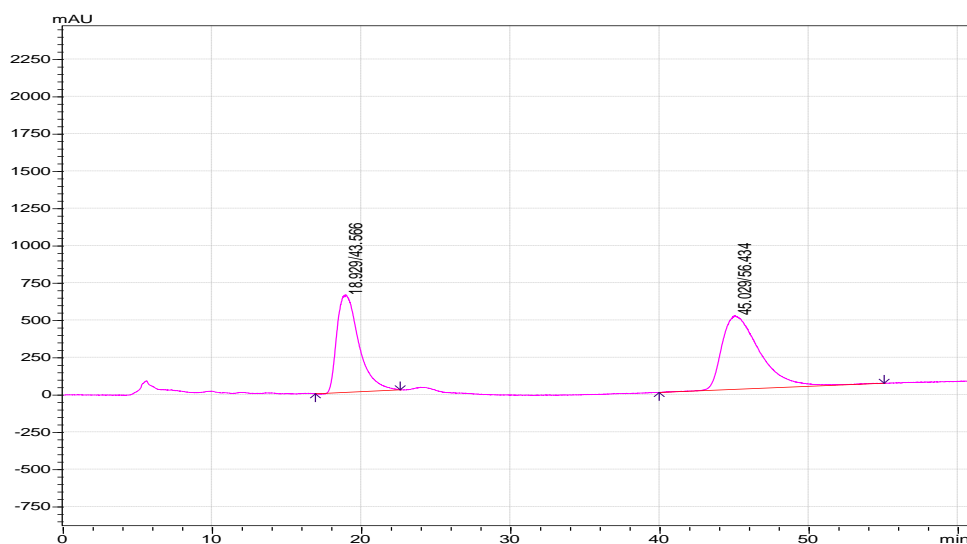
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	13.094	11197558	12.331	15.499	56.2887
2	16.036	8695525	15.499	19.360	43.7113



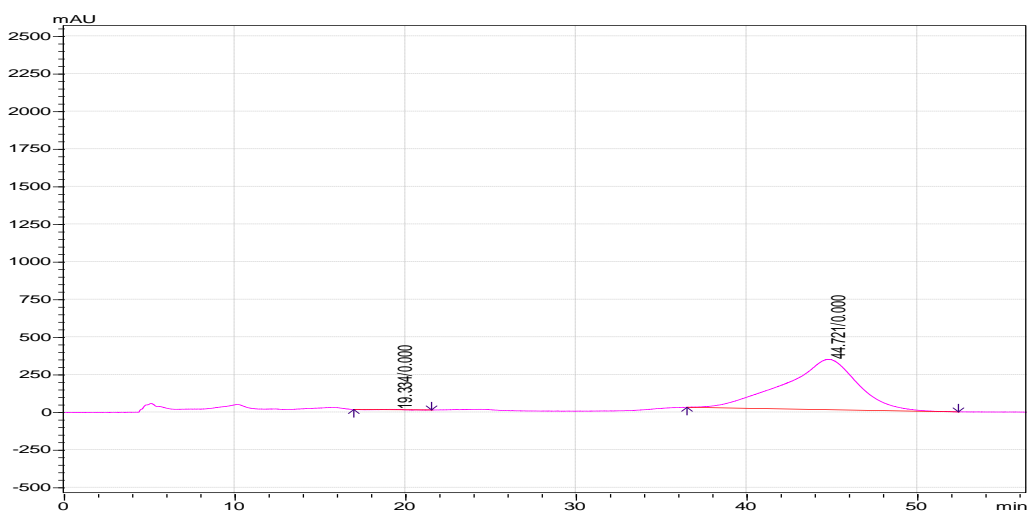
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	12.022	208137	11.040	12.917	0.3792
2	14.413	54683924	13.024	20.107	99.6208



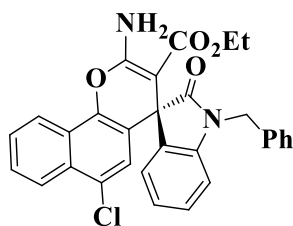
3g; Enantiomeric excess (99.8%) was determined by chiral HPLC (chiralpak IB), hexane-*i*-PrOH 80:20, 0.7 mL/min, major enantiomer $t_r = 44.7$ min, minor enantiomer $t_r = 19.3$ min.; $[\alpha]_D^{20} -72$ ($c = 1$) (99.8 % *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.20 (d, $J = 8$ Hz, 1H), 7.72 (d, $J = 8$ Hz, 1H), 7.55 (t, $J = 15$ Hz, 1H), 7.51 (d, $J = 7$ Hz, 1H), 7.48 (d, $J = 7.5$ Hz, 3H), 7.40 (t, $J = 15$ Hz, 3H), 7.36-7.33 (m, 2H), 7.07-7.05 (m, 1H), 7.03 (d, $J = 1.5$ Hz, 1H), 6.87 (d, $J = 8$ Hz, 1H), 6.53 (d, $J = 8.5$ Hz, 1H), 5.23 (d, $J = 15.5$ Hz, 1H), 4.65 (d, $J = 15$ Hz, 1H), 3.96-3.66 (m, 2H), 0.71 (t, $J = 14$ Hz, 3H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.8, 168.1, 160.9, 144.1, 143.1, 137.3, 135.9, 133.4, 130.8, 128.89, 128.80, 127.4, 127.0, 126.6, 125.8, 125.0, 124.5, 123.2, 122.9, 121.0, 115.3, 111.6, 74.7, 59.4, 44.6, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_4\text{Br}$ ($\text{M}+1$) $^+$ 555.0914 found 555.0938, error 4.32 ppm.



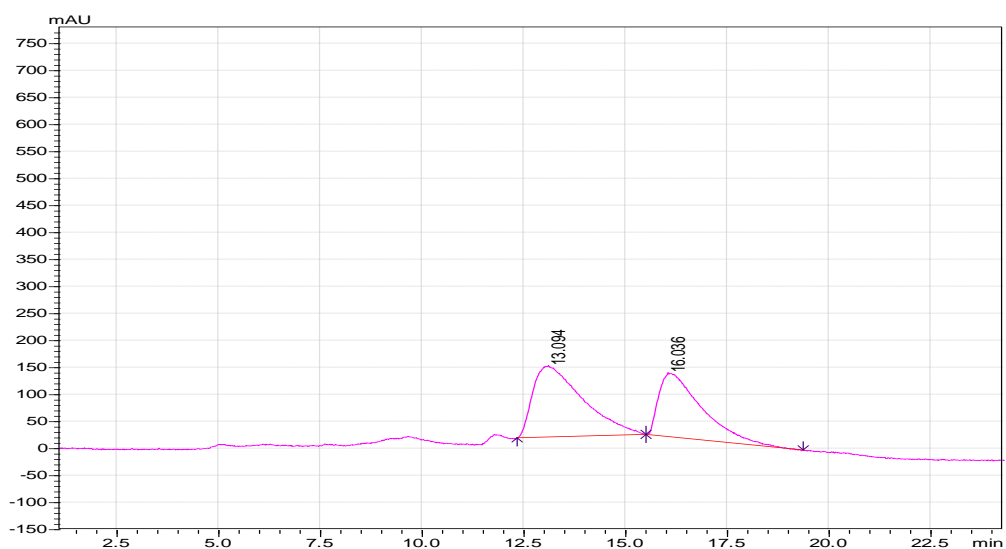
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	18.929	67005902	16.907	22.581	43.5665
2	45.029	86795701	39.947	55.029	56.4335



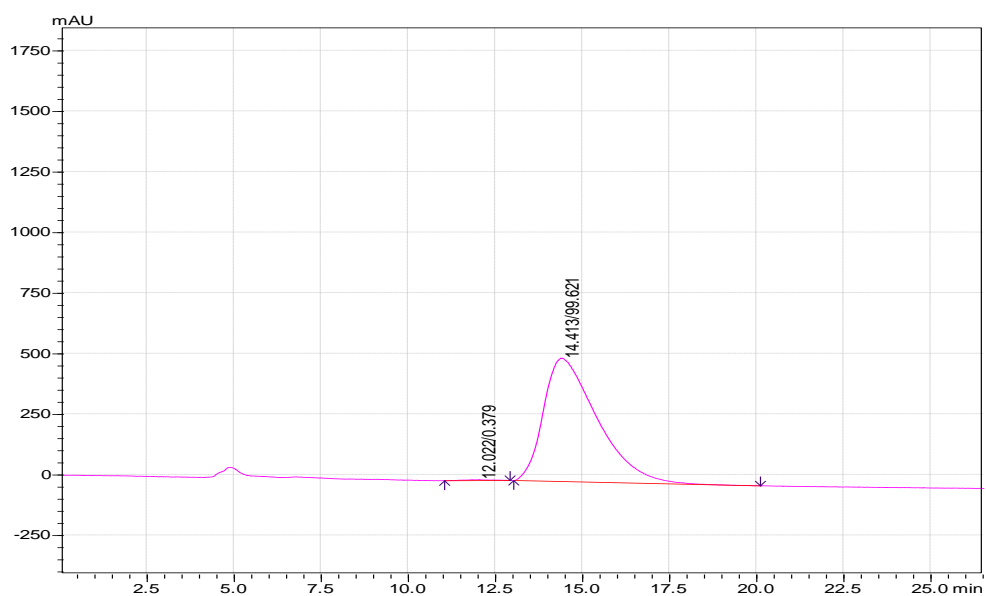
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	19.334	14633	16.960	21.515	0.0147
2	44.721	99580844	36.480	52.384	99.9853



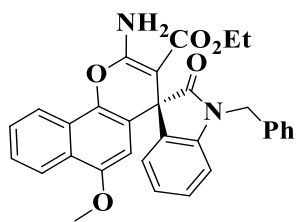
3h; Enantiomeric excess (99%) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 14.4$ min, minor enantiomer $t_r = 12.0$ min.; $[\alpha]_D^{20} -56.02$ ($c = 1$) (99% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.90 (d, $J = 8.5$ Hz, 1H), 7.82 (d, $J = 8.5$ Hz, 1H), 7.54 (*t*, $J = 16.5$ Hz, 2H), 7.45-7.39 (m, 4H), 7.35 (*t*, $J = 14.5$ Hz, 1H), 7.28 (*t*, $J = 15$ Hz, 1H), 6.96 (d, $J = 7.5$ Hz, 2H), 6.91 (d, $J = 7.5$ Hz, 2H), 6.62 (d, $J = 19.5$ Hz, 1H), 5.37 (d, $J = 15.5$ Hz, 1H), 4.69 (d, $J = 15$ Hz, 1H), 3.94-3.64 (m, 2H), 0.68 (*t*, $J = 14.5$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 180.2, 168.2, 161.1, 142.4, 142.2, 138.1, 136.4, 130.0, 129.0, 128.1, 128.0, 127.5, 127.0, 124.1, 124.0, 123.3, 122.8, 121.2, 116.1, 108.6, 74.4, 59.3, 50.5, 44.5, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_4\text{Cl}$ ($\text{M}+1$)⁺ 511.1419 found 511.1425, error 1.17 ppm.



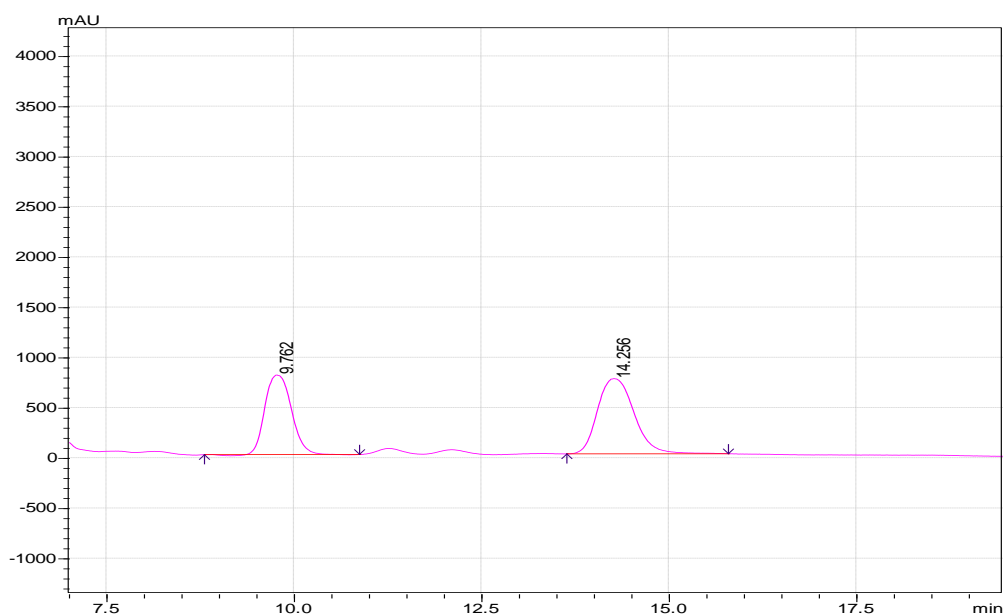
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	13.094	11197558	12.331	15.499	56.2887
2	16.036	8695525	15.499	19.360	43.7113



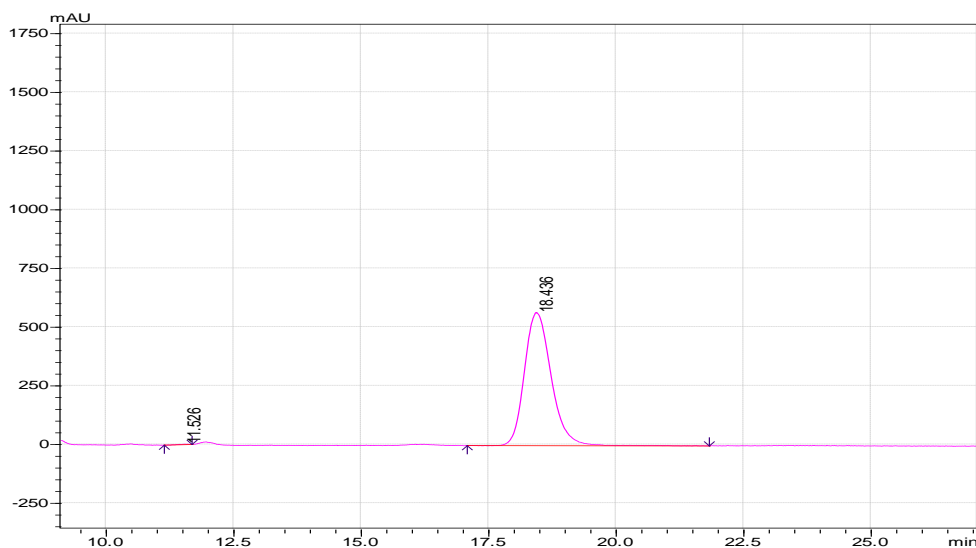
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	12.022	208137	11.040	12.917	0.3792
2	14.413	54683924	13.024	20.107	99.6208



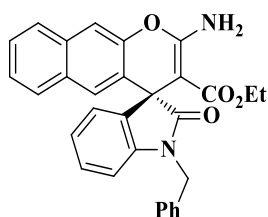
3i; (*S*) Enantiomeric excess (99%) was determined by chiral HPLC (chiralpak IC), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 18.4$ min, minor enantiomer $t_r = 11.5$ min.; $[\alpha]_D^{20} -78.5$ ($c = 1$) (99% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.09 (d, $J = 8$ Hz, 1H), 8.03 (d, $J = 8$ Hz, 1H), 7.56 (d, $J = 7.5$ Hz, 2H), 7.49-7.43 (m, 3H), 7.35 (t, $J = 15$ Hz, 2H), 7.31 (d, $J = 7.5$ Hz, 1H), 7.01 (d, $J = 7$ Hz, 1H), 6.94 (d, $J = 7.5$ Hz, 3H), 5.77 (d, $J = 3$ Hz, 1H), 5.41 (d, $J = 15$ Hz, 1H), 4.56 (d, $J = 15$ Hz, 1H), 3.92-3.76 (m, 2H), 3.41 (s, 3H), 0.77 (t, $J = 7$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.8, 168.3, 160.9, 152.0, 142.4, 138.0, 137.1, 136.6, 128.6, 128.1, 127.6, 126.8, 126.0, 123.6, 122.8, 121.6, 120.5, 115.3, 107.0, 99.7, 74.8, 59.1, 55.0, 50.6, 44.3, 13.5. HRMS (TOF ES): Calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{O}_4$ ($\text{M}+1$) $^+$ 507.1914 found 507.1925, error 2.16 ppm.



Peak#	Ret. Time	Peak Start	Peak End	Area%
1	9.762	8.800	10.869	43.1674
2	14.256	13.632	15.787	56.8326

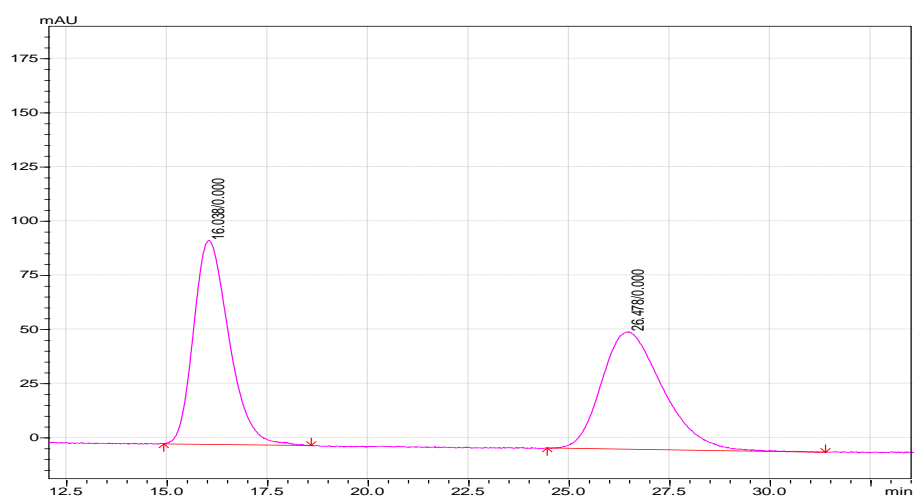


Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.526	11.136	11.680	0.1535
2	18.436	17.077	21.824	99.8465

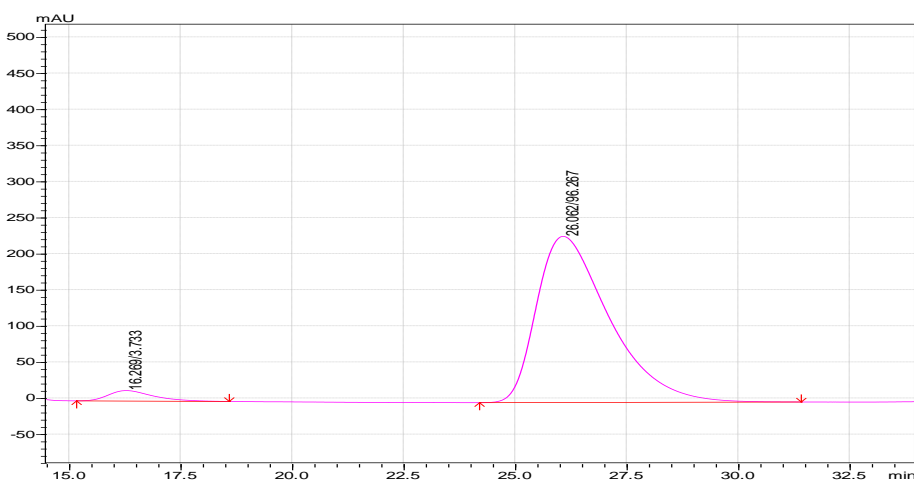


3j; Enantiomeric excess (92%) was determined by chiral HPLC (chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 26.0$ min, minor enantiomer $t_r = 16.2$ min.; $[\alpha]_D^{20} - 64$ ($c = 1$) (92% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.71 (d, $J = 9$ Hz, 1H), 7.65 (d, $J = 8$ Hz, 1H), 7.58 (d, $J = 6.5$ Hz, 2H), 7.36 (d, $J = 7.5$, 3H), 7.28 (d, $J = 9$ Hz, 1H), 7.19-7.15 (m, 3H), 6.99 (t, $J = 14.5$ Hz, 2H), 6.87 (t, $J = 14.5$ Hz, 1H), 6.70 (t, $J = 15$ Hz, 2H), 5.42 (d, $J = 15$ Hz, 1H), 4.62 (d, $J = 15$ Hz, 1H), 3.92-3.67 (m 2H), 0.82 (t, $J = 14$ Hz, 3H).; $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.5, 168.3, 159.7, 147.2, 144.0, 136.5, 135.8, 131.6, 130.9, 129.2, 128.7, 127.9, 127.0, 124.4, 124.3, 123.6, 123.0, 117.1, 113.4, 108.0, 78.2, 59.4, 50.4, 45.3,

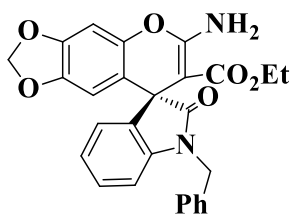
29.6, 14.0. HRMS (TOF ES): Calcd for $C_{30}H_{25}N_2O_4$ (M+1)⁺ 477.1808 found 477.1825, error 3.56 ppm.



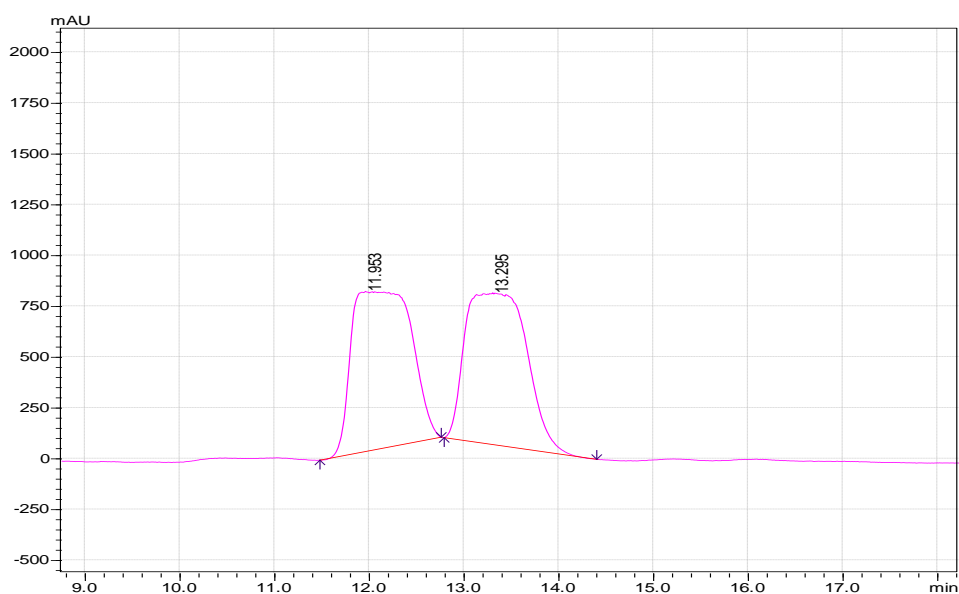
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	16.038	14.912	18.581	50.1661
2	26.478	24.448	31.371	49.8339



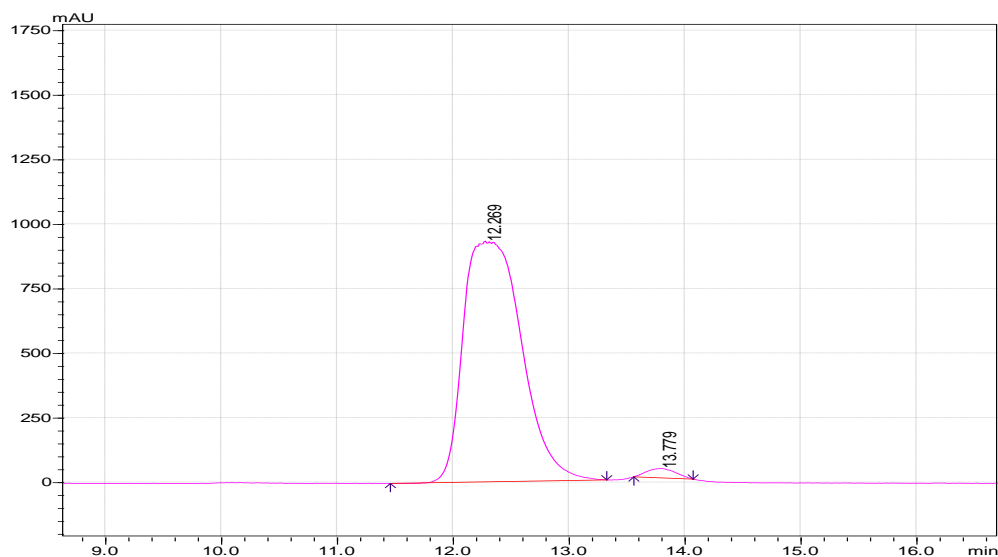
Peak#	Ret. Time	Peak Start	Peak End	Area %
1	16.269	15.157	18.581	3.7328
2	26.062	24.192	31.403	96.2672



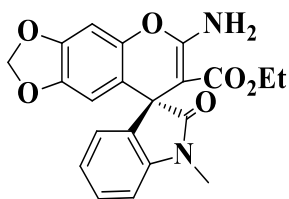
4a; Enantiomeric excess (94%) was determined by chiral HPLC (chiralpak IB), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 12.2$ min, minor enantiomer $t_r = 13.7$ min.; $[\alpha]_D^{20} - 34$ ($c = 1$) (92% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.47 (d, $J = 7.5$ Hz, 2H), 7.35 (t, $J = 15$ Hz, 2H), 7.29 (t, $J = 15$ Hz, 1H), 7.14 (t, $J = 15$ Hz, 1H), 6.99 (d, $J = 7.5$ Hz, 1H), 6.93 (t, $J = 14.5$ Hz, 1H), 6.84 (d, $J = 8$ Hz, 1H), 6.50 (s, 1H), 5.94 (s, 1H), 5.84 (d, $J = 12$ Hz, 2H), 5.15 (d, $J = 15$ Hz, 1H), 4.70 (d, $J = 15$ Hz, 1H), 3.90-3.83 (m, 1H), 3.59-3.53 (m, 1H), 0.56 (t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) 179.8, 168.3, 161.0, 147.6, 144.7, 142.9, 142.5, 138.3, 136.4, 128.7, 128.1, 127.7, 127.6, 123.3, 122.9, 113.5, 108.4, 105.1, 101.6, 97.9, 74.6, 60.3, 59.1, 53.3, 50.1, 44.4, 21.3, 13.4. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_6$ ($\text{M}+1$) $^+$ 471.1550 found 471.1538, error 0.5 ppm.



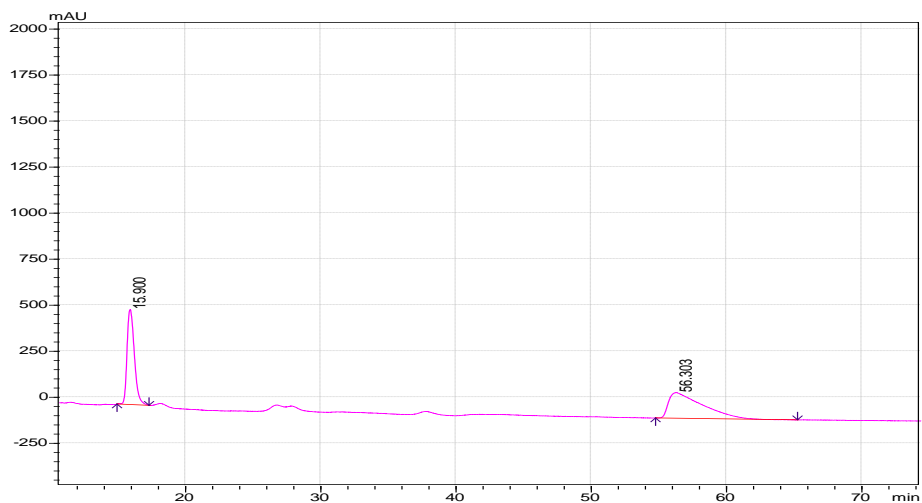
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.953	11.521	12.655	49.8962
2	13.296	12.823	14.457	50.1038



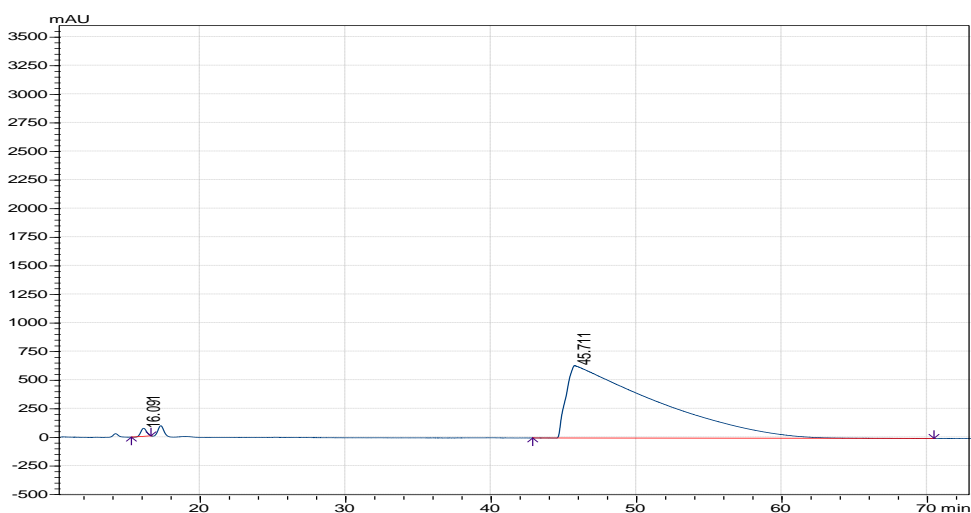
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	12.269	11.521	12.655	97.2345
2	13.779	12.823	14.457	2.7655



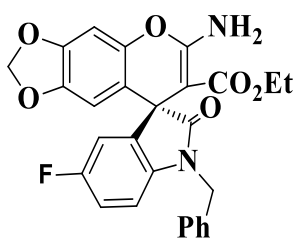
4b; Enantiomeric excess (98%) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 45.71$ min, minor enantiomer $t_r = 16.09$ min.; $[\alpha]_D^{25} = 68$ ($c = 1$) (98% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.17–7.13 (m, 1H), 6.91–6.86 (m, 2H), 6.77 (d, $J = 7.5$ Hz, 1H), 6.4 (s, 1H), 5.8 (s, 1H), 5.75 (s, 2H), 3.72–3.68 (q, 2H), 3.20 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 180.1, 168.4, 161.0, 147.6, 144.7, 143.3, 142.9, 138.3, 127.9, 123.3, 123.0, 13.5, 107.6, 105.1, 106.6, 98.0, 74.6, 59.3, 50.3, 26.6, 13.7. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{19}\text{N}_2\text{O}_6$ ($\text{M}+1$) $^+$, 395.1237 found 395.1266, error 7.33 ppm.



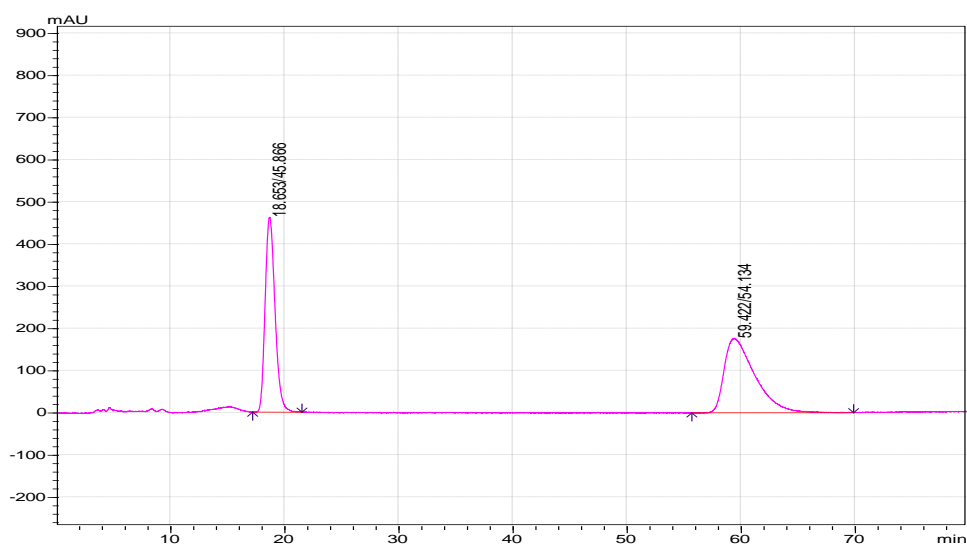
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	15.900	14.933	17.301	50.0005
2	56.303	54.752	65.248	49.9995



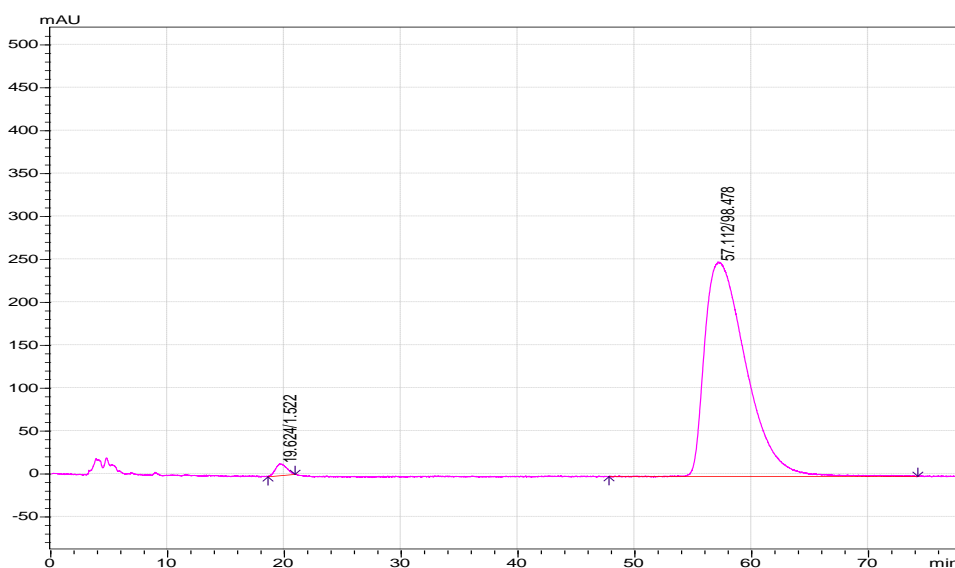
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	16.091	15.264	16.608	0.6996
2	45.711	42.859	70.453	99.3004



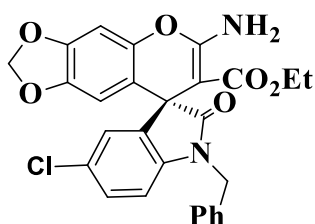
4c; Enantiomeric excess (97 %) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 57.1$ min, minor enantiomer $t_r = 19.6$ min.; $[\alpha]_D^{25} = -17.4$ ($c = 1$) (97% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.43 (d, $J = 8$ Hz, 2H), 7.31 (t, $J = 15$ Hz, 2H), 7.24 (d, $J = 12$ Hz, 1H), 6.90 (d, $J = 7.5$ Hz, 1H), 6.76(s, 1H), 6.69(d, $J = 8$ Hz, 1H), 6.47(s, 1H), 5.91(s, 1H), 5.81(d, $J = 9.5$ Hz, 2H), 5.11(d, $J = 15$ Hz, 1H), 4.62(d, $J = 15.5$ Hz, 1H), 3.86-3.80(m, 1H), 3.60-3.53(m, 1H), 0.57(t, $J = 14$ Hz, 3H). $^{13}\text{C NMR}$ 125MHz, CDCl_3) δ 179.9, 168.5, 161.0, 147.6, 144.8, 142.9, 140.2, 138.3, 136.6, 132.5, 128.7, 128.2, 127.9, 127.8, 124.2, 113.9, 108.2, 105.3, 101.1, 98.0, 74.9, 59.3, 53.4, 50.3, 44.5, 39.7, 21.0, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_6$ ($\text{M}+1$) $^+$ 489.1456 found 489.1487, error 6.3 ppm



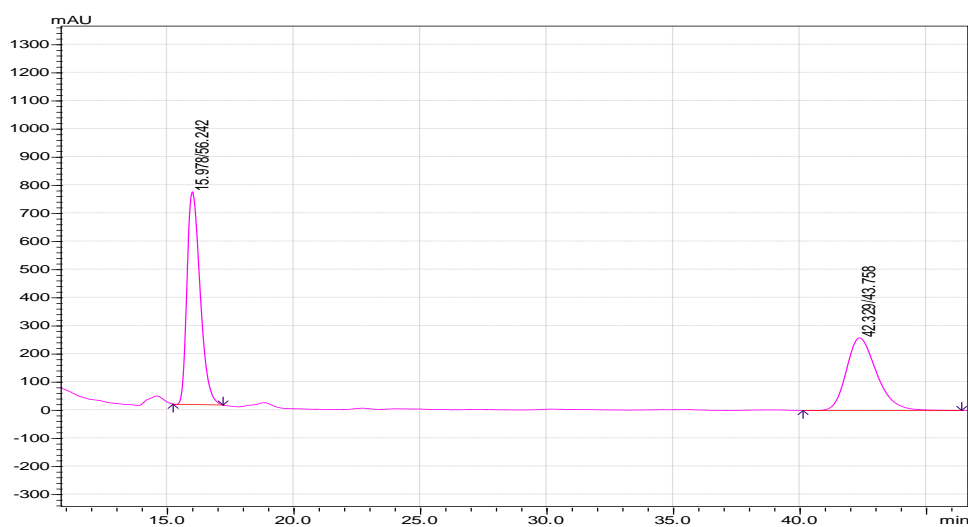
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	18.653	27870737	17.163	21.493	45.8658
2	59.422	32895061	55.669	69.856	54.1342



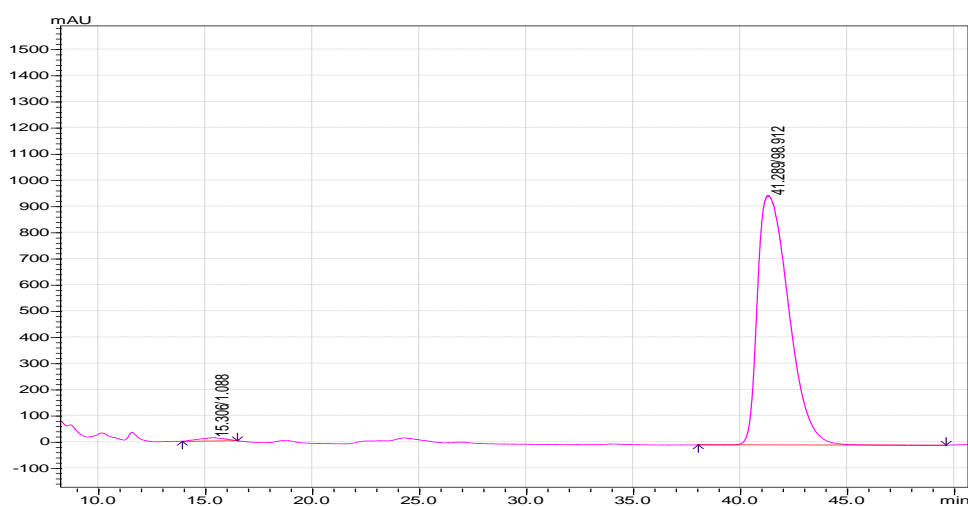
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	19.624	945443	18.592	20.917	1.5222
2	57.112	61166462	47.787	74.229	98.4778



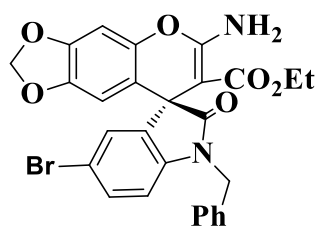
4d; Enantiomeric excess (98%) was determined by chiral HPLC (chiralpak IA), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 41.2$ min, minor enantiomer $t_r = 15.3$ min.; $[\alpha]_D^{25} = -19$ ($c = 1$) (98% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.41(d, $J = 7.5$ Hz, 2H), 7.33(t, $J = 14.5$ Hz, 2H), 7.30(d, $J = 7.5$ Hz, 1H), 7.10-7.08 (m, 1H), 6.94 (d, $J = 2$ Hz, 1H), 6.73(d, $J = 8.5$, 1H), 6.49(s, 1H), 5.88 (s, 1H), 5.85 (d, $J = 1.5$ Hz, 1H), 5.43 (d, $J = 1.5$ Hz, 1H), 5.11 (d, $J = 15$ Hz, 1H), 4.64 (d, $J = 15$ Hz, 1H), 3.90-3.84 (m, 1H), 3.61-3.55(m, 1H), 0.60 (t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) 179.5, 168.2, 161.1, 147.9, 144.9, 142.9, 141.2, 139.9, 126.1, 128.9, 128.4, 128.2, 128.0, 127.7, 124.0, 112.8, 109.4, 105.0, 101.8, 98.2, 74.2, 59.4, 50.5, 46.6, 31.6, 29.7, 22.7, 14.1. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{22}\text{N}_2\text{O}_6\text{Cl}$ ($\text{M}+1$)⁺ 505.1160 found 505.1155, error -1.18 ppm



Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	15.978	27435477	15.221	17.195	56.2420
2	42.329	21345642	40.117	46.389	43.7580

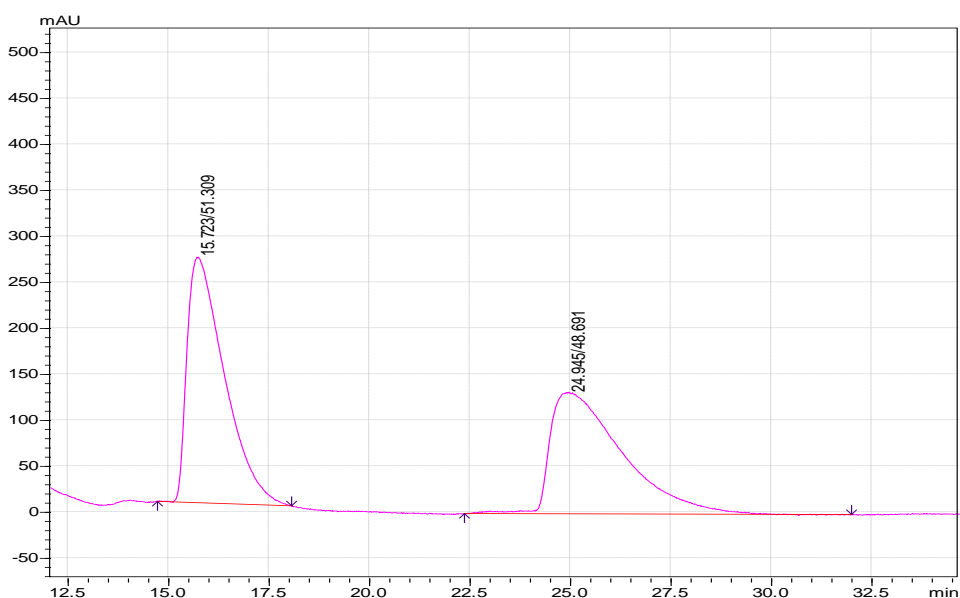


Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	15.306	1061986	13.909	16.480	1.0883
2	41.289	96519695	38.027	49.611	98.9117

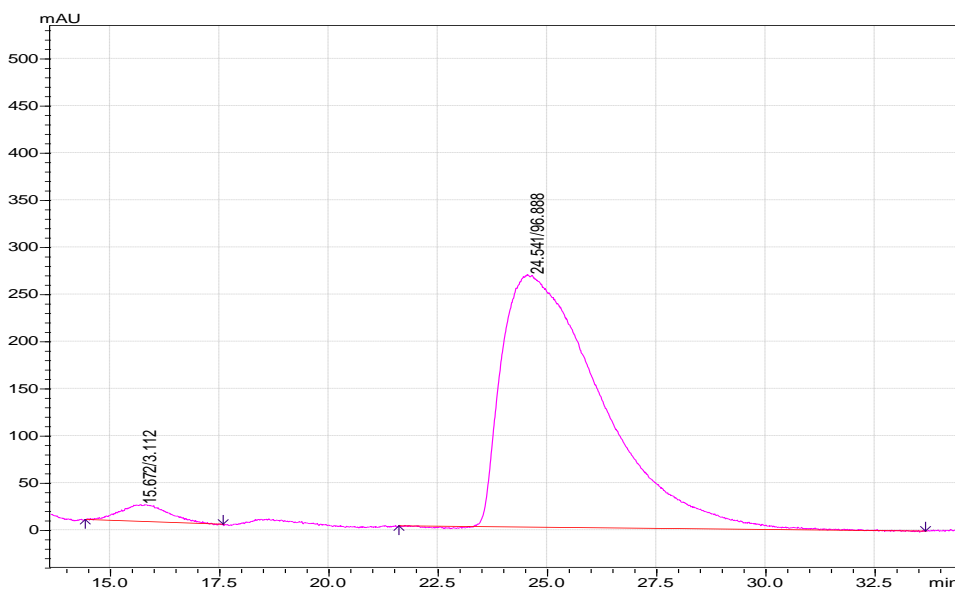


4e; Enantiomeric excess (93%) was determined by chiral HPLC (chiralpak IC), hexane-*i*PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 24.5$ min, minor enantiomer $t_r = 15.6$ min.;

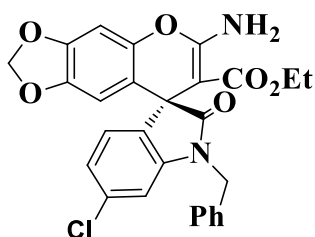
$[\alpha]_D^{25} = -52$ ($c = 1$) (93% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.43(d, $J = 7.5$ Hz, 2H), 7.35(t, $J = 14.5$ Hz, 2H), 7.31(d, $J = 7$ Hz, 1H), 7.28-7.26(m, 2H), 7.10(d, $J = 2$ Hz, 1H), 6.71(d, $J = 8.5$ Hz, 1H), 6.52(s, 1H), 5.90 (s, 1H), 5.87(d, $J = 8$ Hz, 2H), 5.13(d, $J = 15.5$ Hz, 1H), 4.66 (d, $J = 15$ Hz, 1H), 3.92-3.60(m, 1H), 3.67-3.60 (m, 1H), 0.63(t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125MHz, CDCl_3) δ 179.9, 168.8, 161.0, 147.9, 144.9, 142.9, 141.6, 140.2, 136.0, 130.5, 128.8, 128.0, 126.7, 115.6, 112.6, 109.9, 104.9, 101.7, 98.16, 74.1, 59.4, 50.3, 44.6, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{21}\text{N}_2\text{O}_6\text{Br}$ ($\text{M}+1$) $^+$ 549.0655 found 549.0619, error 6.5 ppm.



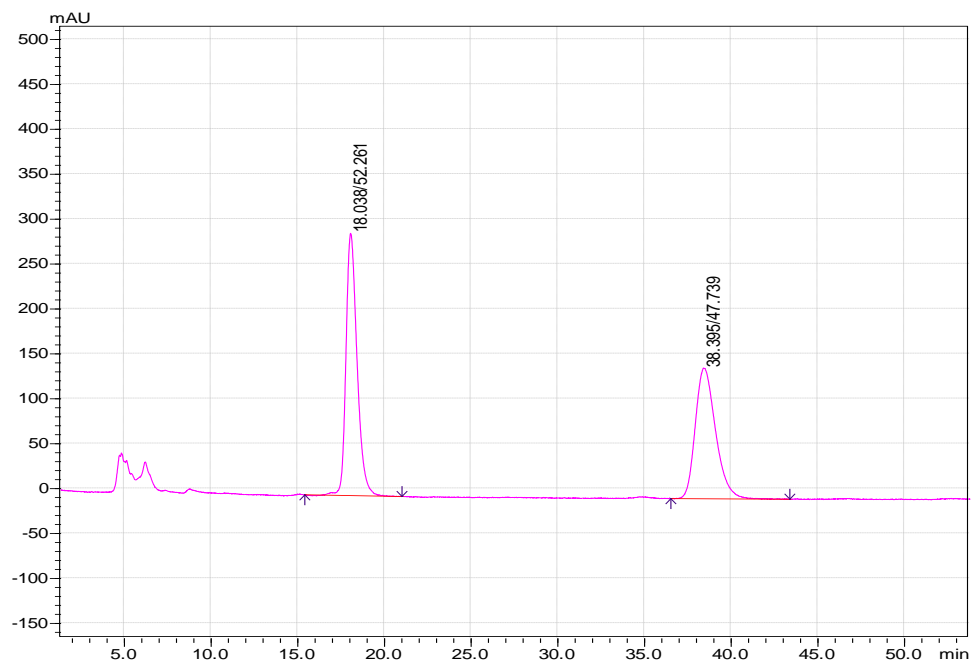
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	15.723	17284176	14.720	18.059	51.3086
2	24.945	16402542	22.357	31.989	48.6914



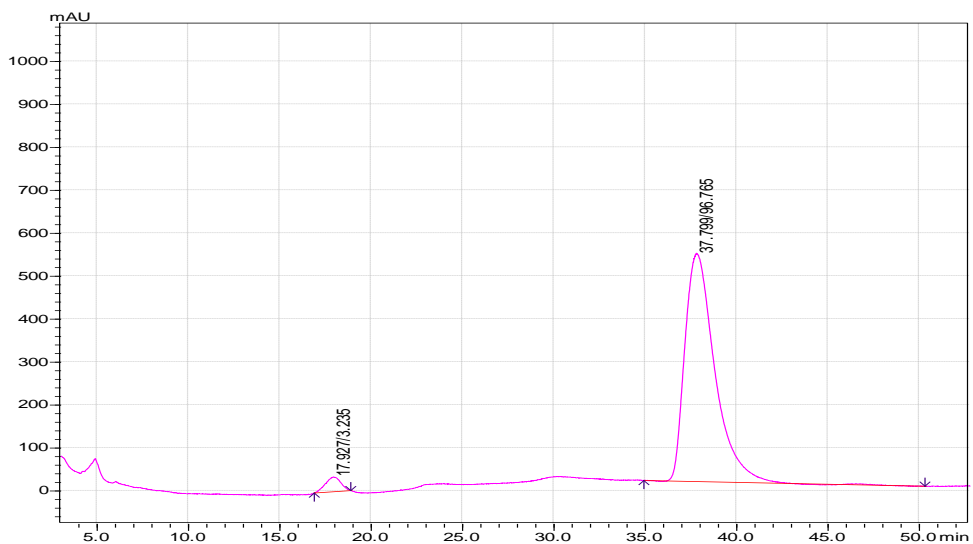
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	15.672	1355339	14.421	17.579	3.1115
2	24.541	42203552	21.600	33.653	96.8885



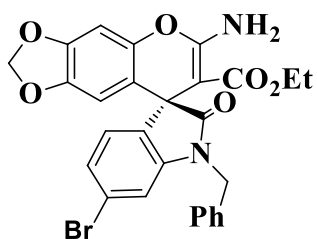
4f; Enantiomeric excess (95%) was determined by chiral HPLC (chiralpak IC), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 37.7$ min, minor enantiomer $t_r = 17.9$ min.; $[\alpha]_D^{25} = -44$ ($c = 1$) (95% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.37(d, $J = 7$ Hz, 2H), 7.29 (t, $J = 15$ Hz, 2H), 7.23 (t, $J = 14.5$ Hz, 1H), 6.83 (s, 2H), 6.76 (s, 1H), 6.41 (s, 1H), 5.82 (s, 1H), 5.75 (d, $J = 1.5$ Hz, 1H), 5.05 (d, $J = 15$ Hz, 1H), 4.58 (d, $J = 15$ Hz, 1H), 3.83-3.77 (m, 1H), 3.56-3.50 (m, 1H), 0.56 (t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) 179.9, 168.2, 161.1, 147.9, 144.9, 143.8, 142.9, 136.8, 135.9, 133.3, 128.2, 128.1, 124.4, 122.9, 113.0, 109.0, 104.9, 101.8, 98.1, 74.1, 59.4, 44.6, 13.7. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{22}\text{N}_2\text{O}_6\text{Cl}$ ($\text{M}+1$) $^+$ 505.1161 found 505.1162, error 0.19 ppm.



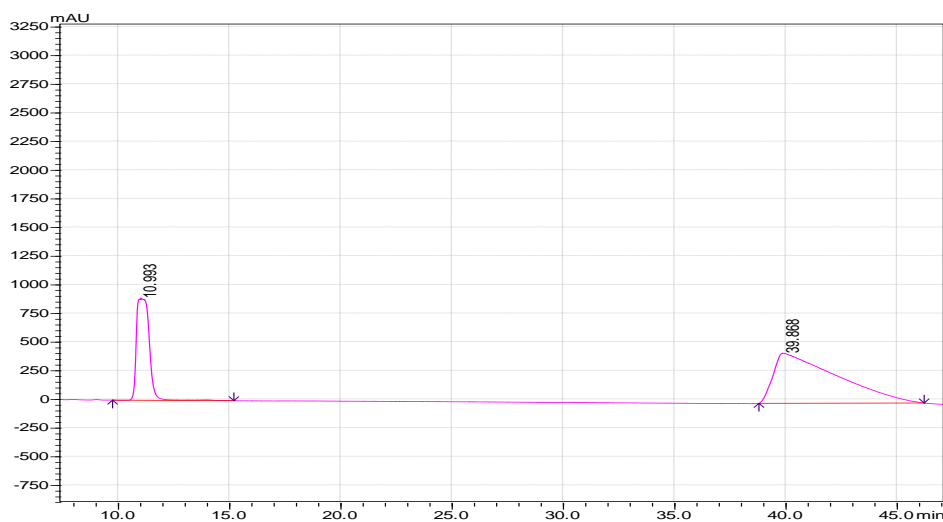
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	18.038	12970155	15.403	21.013	52.2614
2	38.395	11847714	36.523	43.381	47.7386



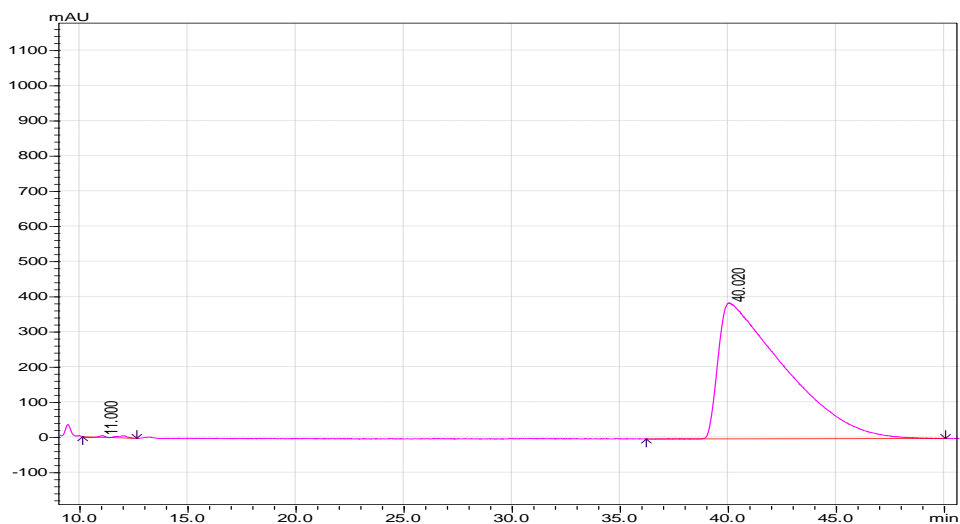
Peak#	Ret. Time	Area	Peak Start	Peak End	Area%
1	17.927	2022961	16.885	18.880	3.2347
2	37.799	60515725	34.923	50.304	96.7653



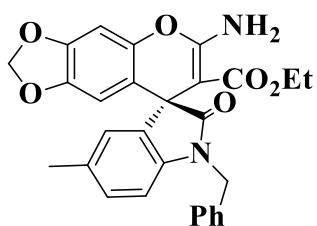
4g; Enantiomeric excess (99%) was determined by chiral HPLC (chiralpak IA), hexane-*i*-PrOH 70:30, 0.7 mL/min, major enantiomer $t_r = 40$ min, minor enantiomer $t_r = 11$ min.; $[\alpha]_D^{25} = -28$ ($c = 1$) (99% ee); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.45(d, $J = 9$ Hz, 2H), 7.37(t, $J = 15$ Hz, 2H), 7.31(t, $J = 14.5$ Hz, 1H), 6.91(s, 2H), 6.84(s, 1H), 6.50(s, 1H), 5.90(s, 1H), 5.86(d, $J = 10$ Hz, 2H), 5.13(d, $J = 15$ Hz, 1H), 4.65(d, $J = 15.5$ Hz, 1H), 3.911-3.59(m, 2H), 0.64(t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 179.8, 168.2, 161.0, 147.8, 144.9, 143.8, 142.9, 136.7, 135.9, 133.2, 124.3, 122.8, 113.0, 108.9, 104.9, 101.7, 98.1, 74.2, 59.4, 49.9, 44.6, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{27}\text{H}_{21}\text{N}_2\text{O}_6\text{Br}$ ($\text{M}+1$) $^+$ 549.0655 found 549.0706, error 9.2 ppm.



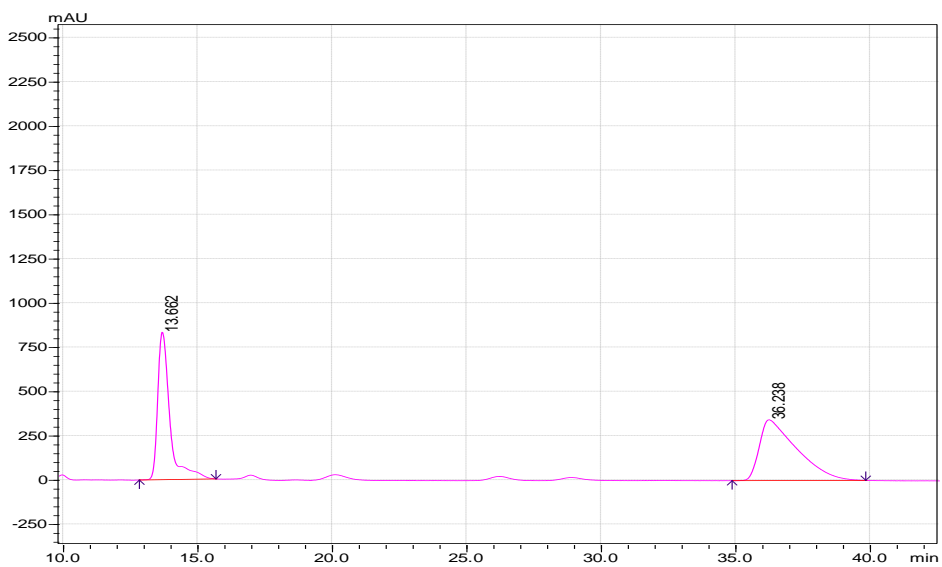
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	10.993	9.739	15.189	49.8962
2	39.868	38.784	46.208	50.1038



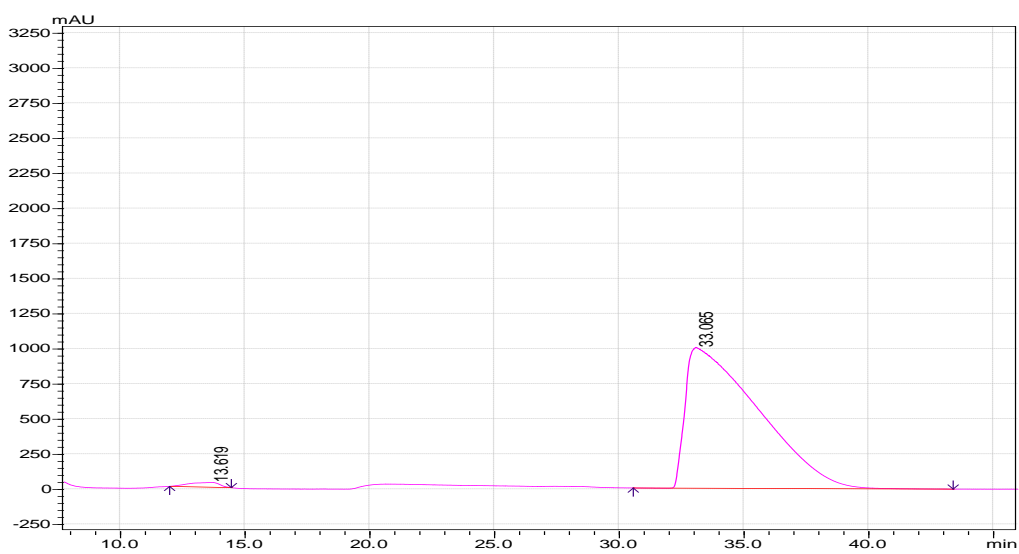
Peak#	Ret. Time	Peak Start	Peak End	Area%
1	11.000	10.123	12.629	0.2725
2	40.020	36.203	50.048	99.7275



4h; Enantiomeric excess (97%) was determined by chiral HPLC (chiralpak IC), hexane-*i*-PrOH 60:40, 0.8 mL/min, major enantiomer $t_r = 15.879$ min, minor enantiomer $t_r = 10.205$ min.; $[\alpha]_D^{25} = 68$ ($c = 1$) (97% *ee*); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.71(d, $J = 8$ Hz, 2H), 7.43(d, $J = 8$ Hz, 2H), 7.31(t, $J = 15$ Hz, 2H), 7.24(d, $J = 12$ Hz, 1H), 6.90(d, $J = 7.5$ Hz, 1H), 6.76(s, 1H), 6.69(d, $J = 8$ Hz, 1H), 6.47(s, 1H), 5.91(s, 1H), 5.81(d, $J = 9.5$ Hz, 2H), 5.11(d, $J = 15$ Hz, 1H), 4.62(d, $J = 15.5$ Hz, 1H), 3.86-3.80 (m, 1H), 3.60-3.53 (m, 1H), 2.16 (s, 3H), 0.575 (t, $J = 14$ Hz, 3H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) 179.9, 168.5, 161.0, 147.6, 144.8, 142.9, 140.2, 140.2, 138.3, 136.6, 132.5, 128.7, 128.2, 127.9, 127.8, 124.2, 113.9, 108.2, 105.3, 101.1, 98.0, 74.9, 59.3, 53.4, 50.3, 44.5, 29.9, 21.0, 13.6. HRMS (TOF ES): Calcd for $\text{C}_{28}\text{H}_{25}\text{N}_2\text{O}_6$ ($\text{M}+1$)⁺ 485.1707 found 485.1731, error 4.9 ppm

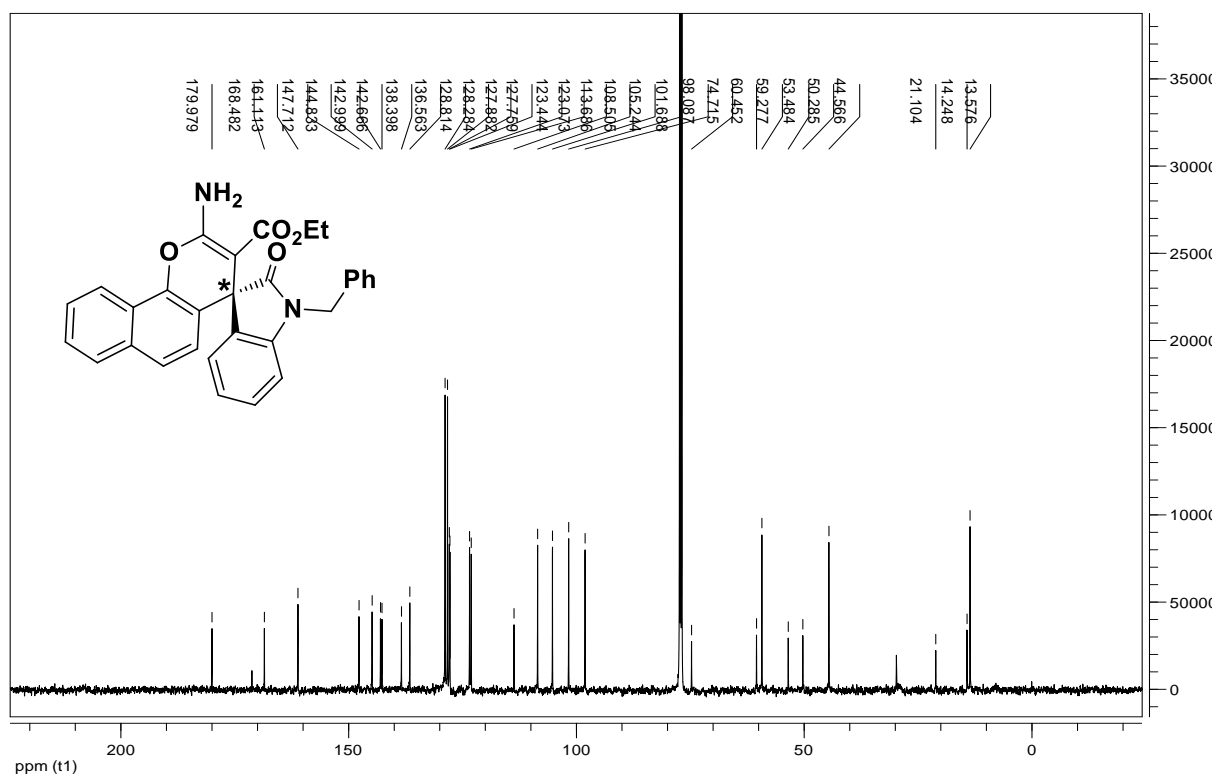
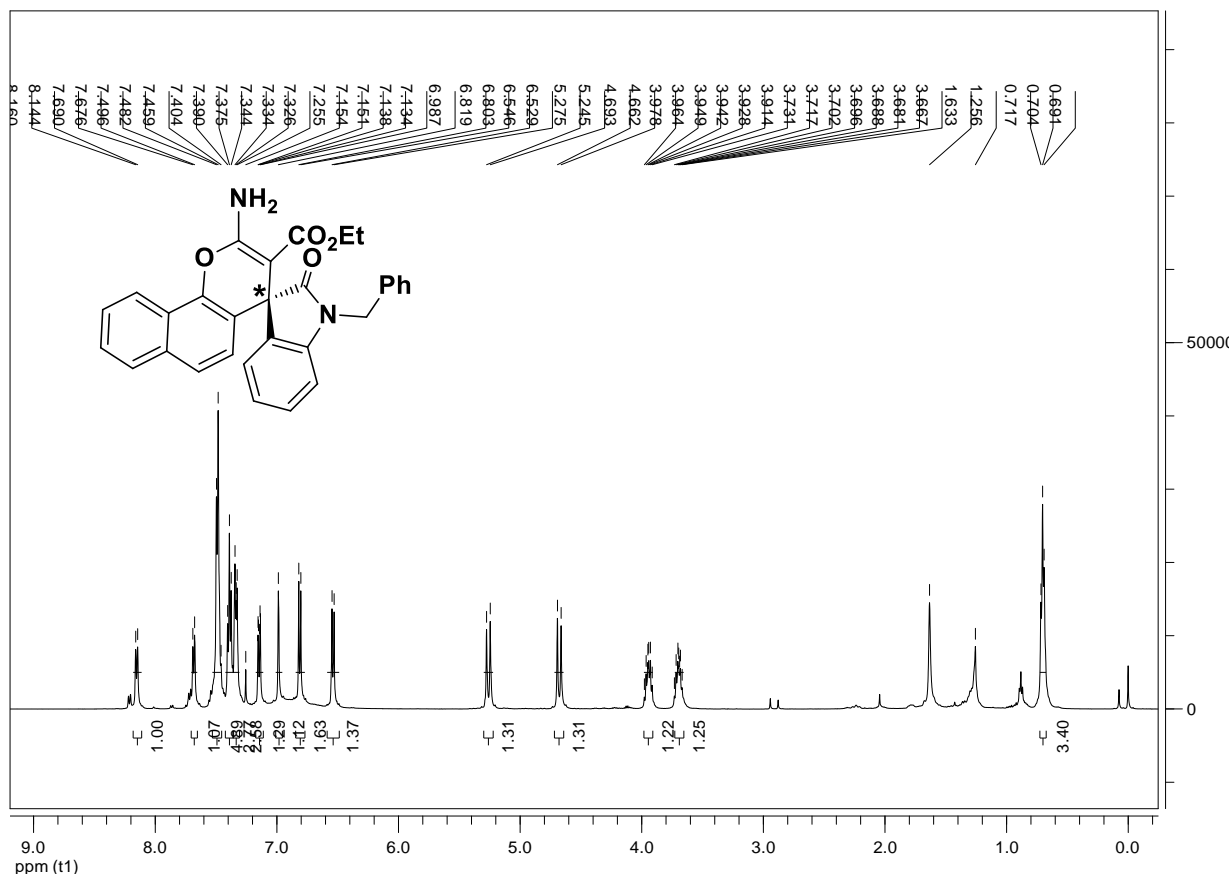


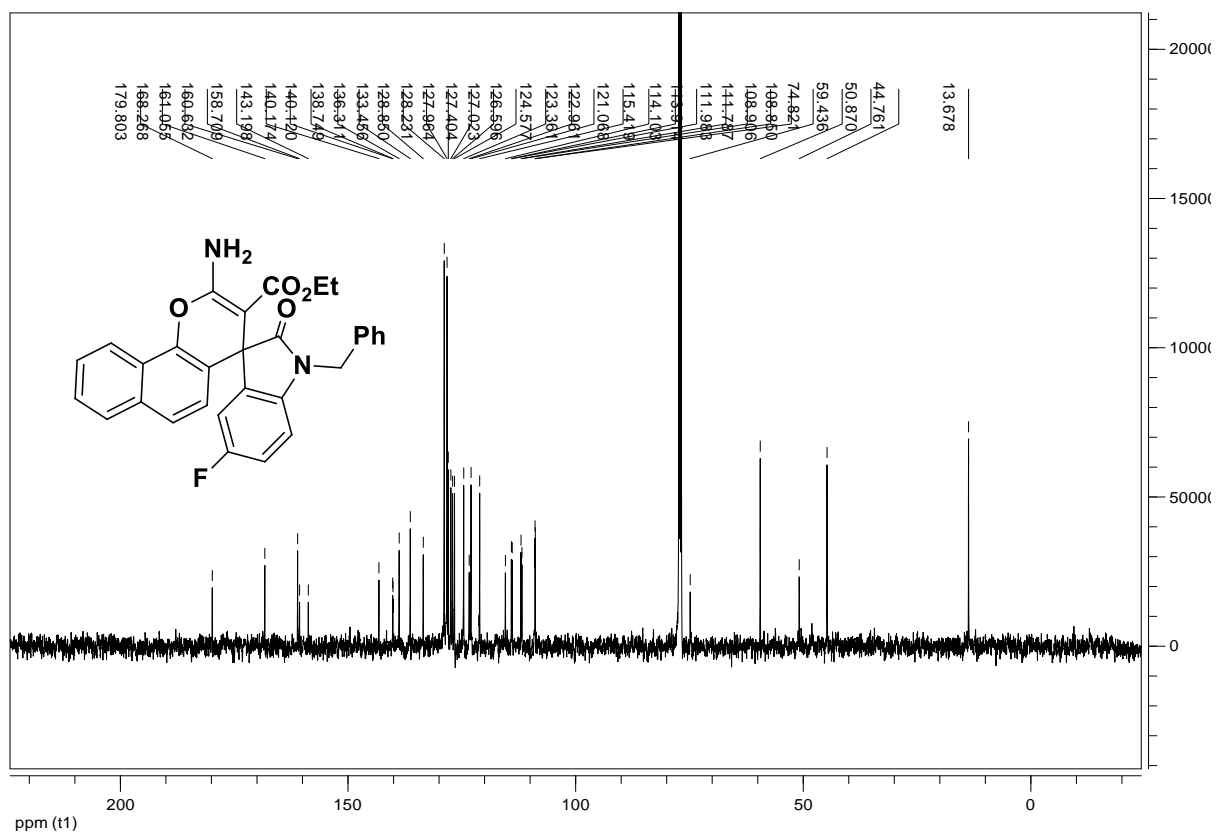
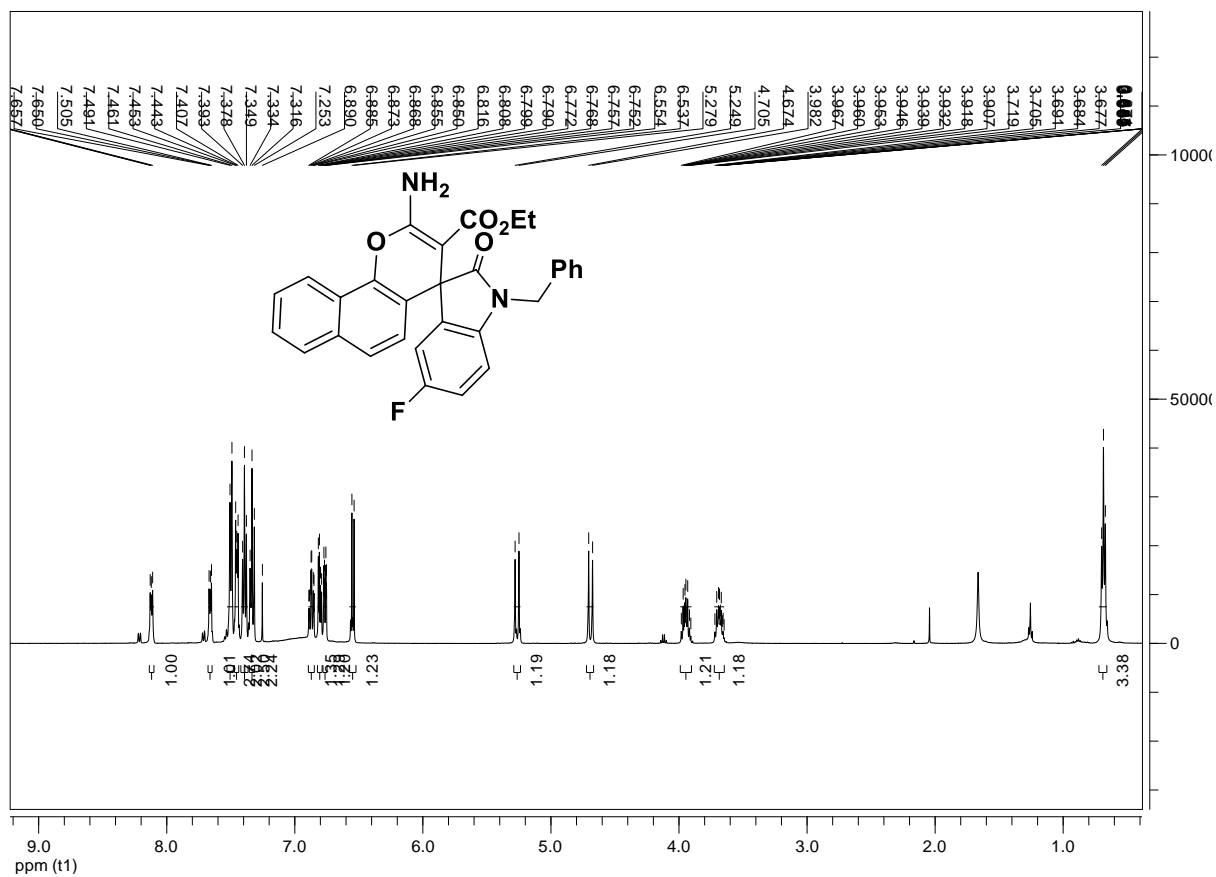
Peak	Ret. Time	Peak Start	Peak End	Area%
1	13.662	12.821	15.669	44.2722
2	36.238	34.859	39.829	55.7278

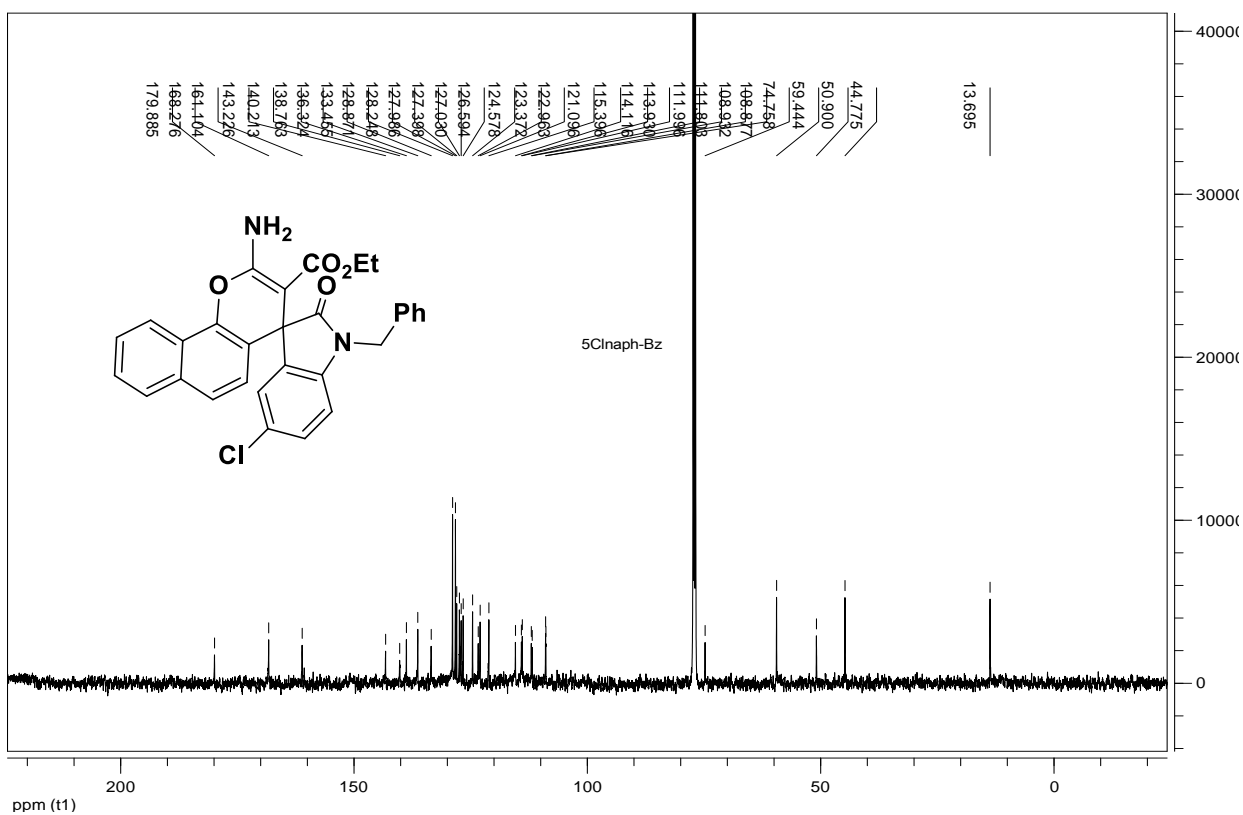
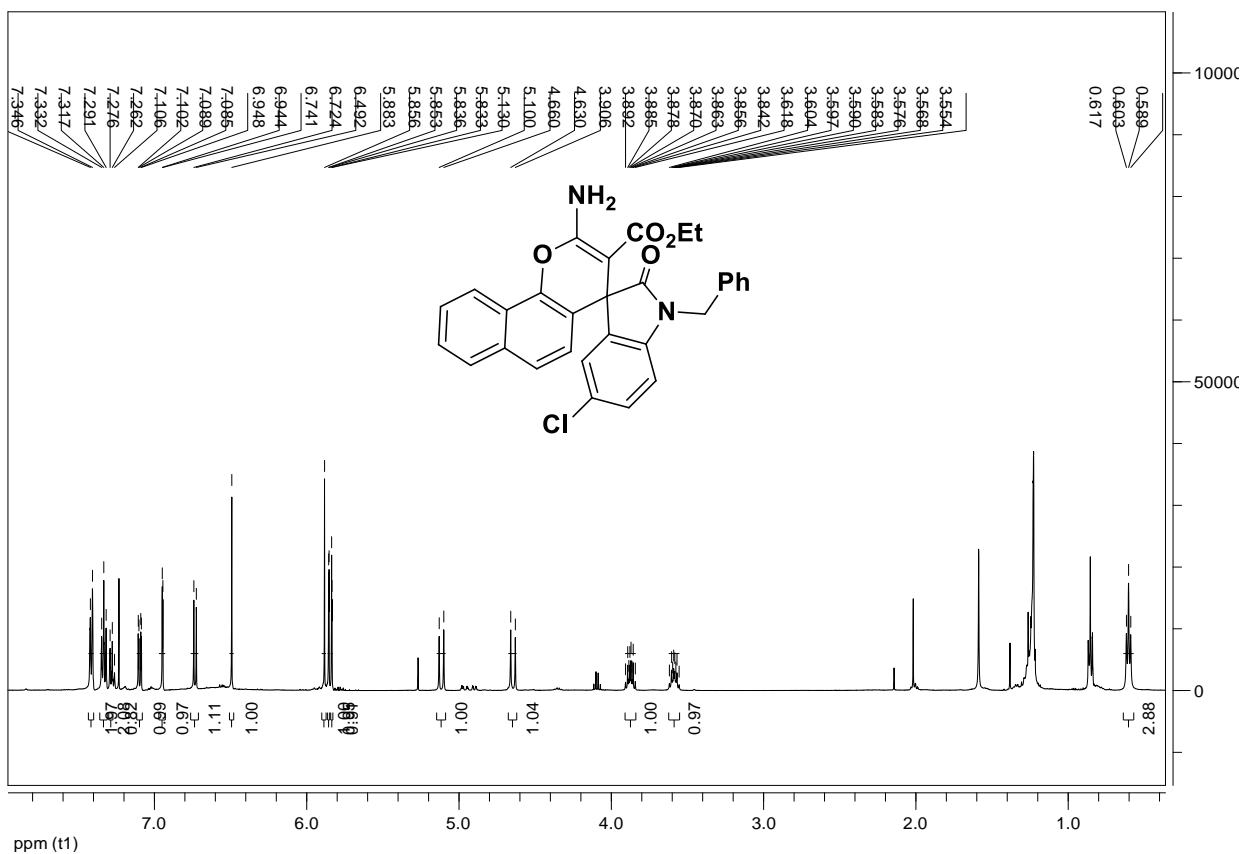


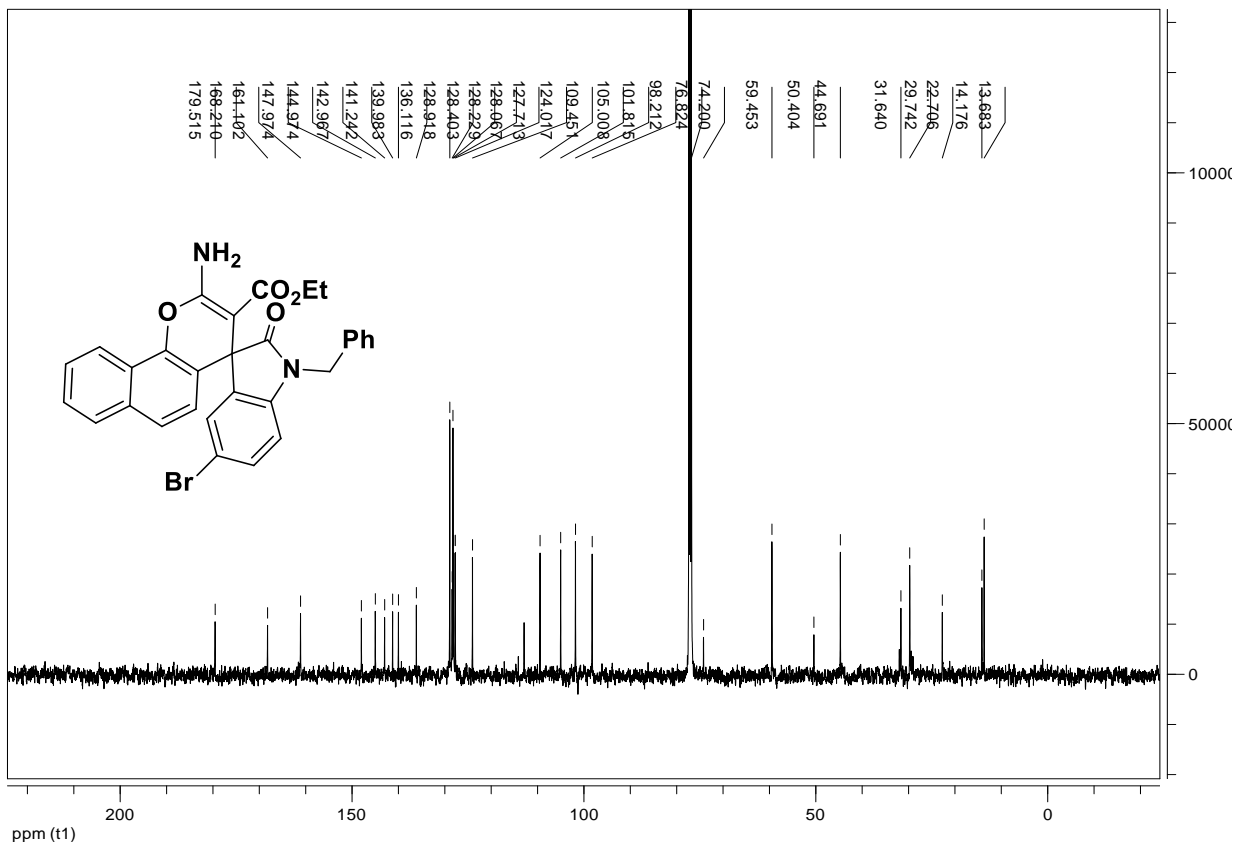
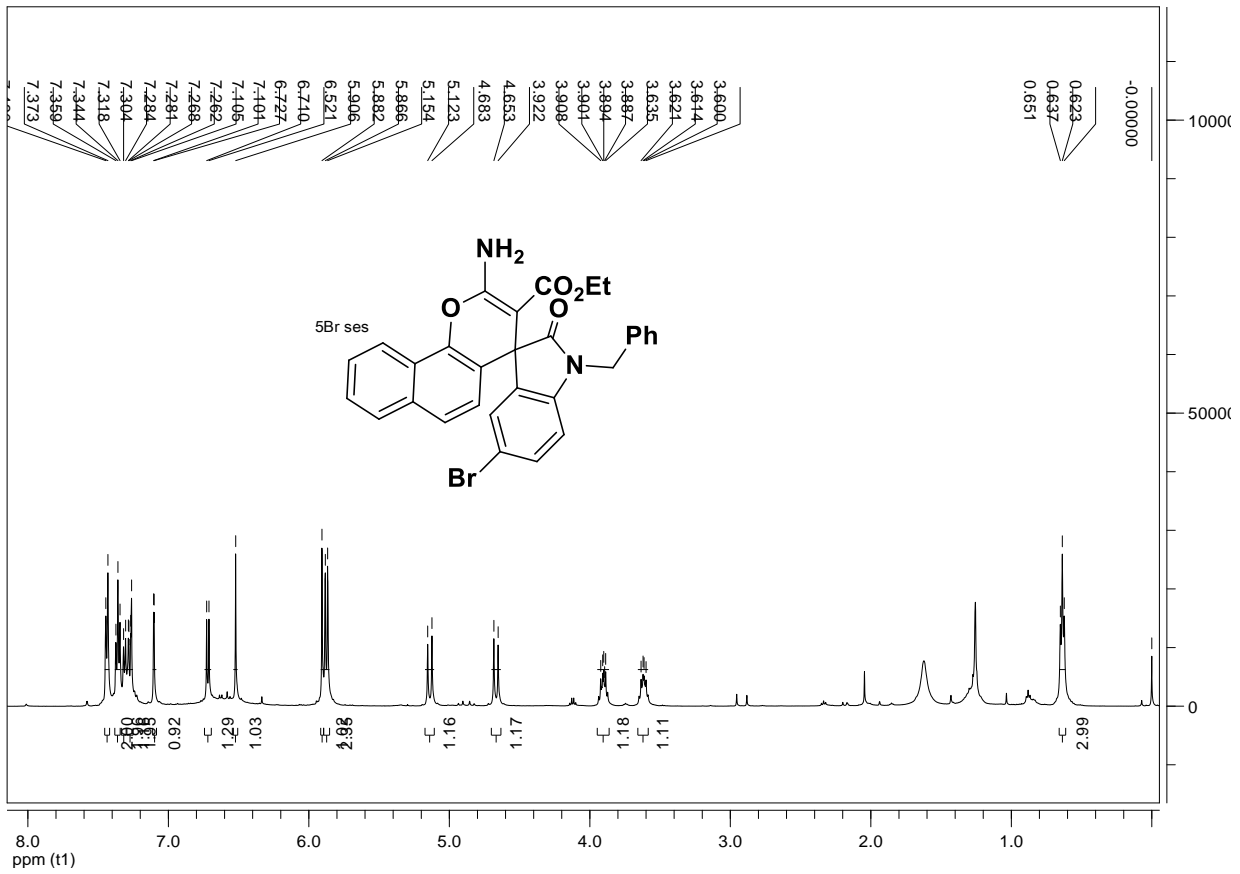
Peak	Ret. Time	Peak Start	Peak End	Area %
1	13.619	11.968	14.443	1.3680
2	33.065	30.560	43.381	98.6320

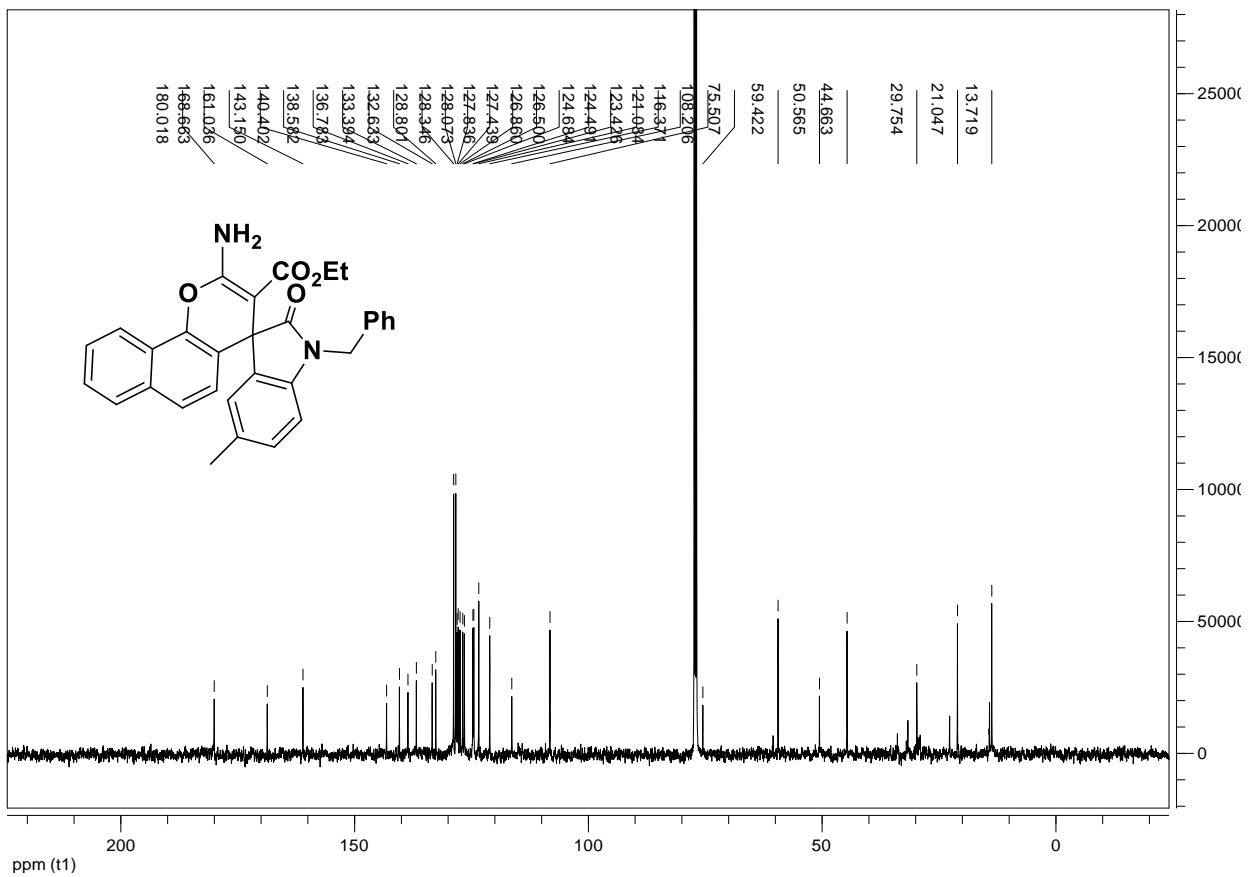
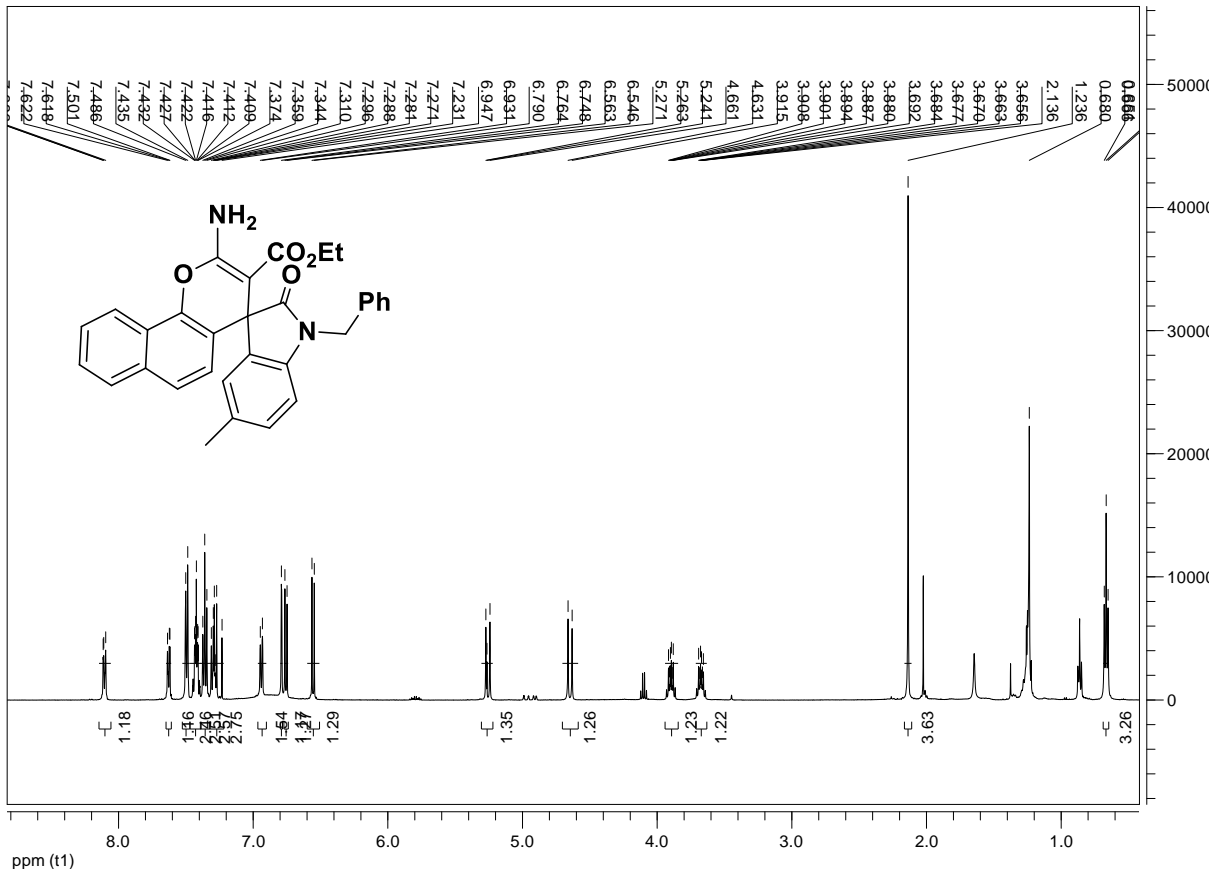
¹H NMR and ¹³C NMR spectrum of compounds

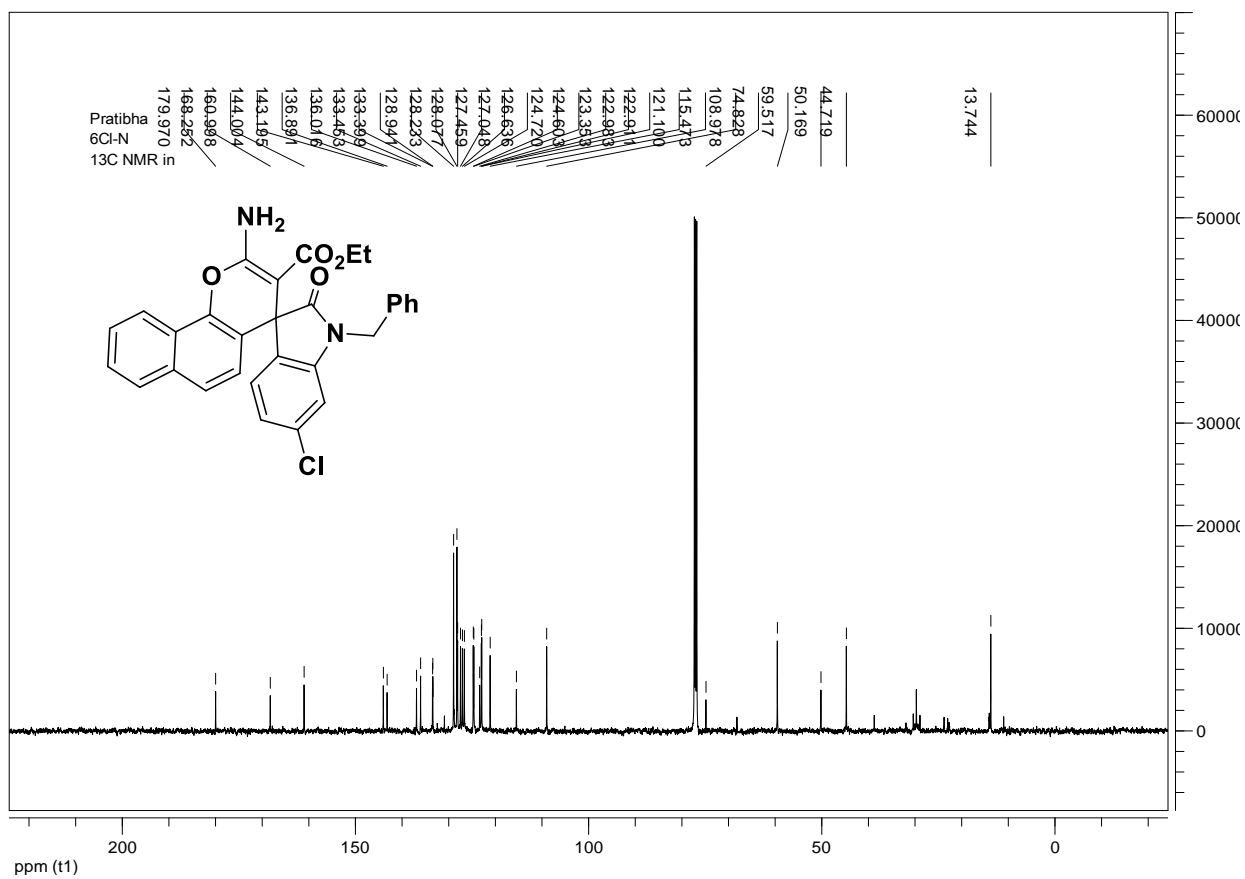
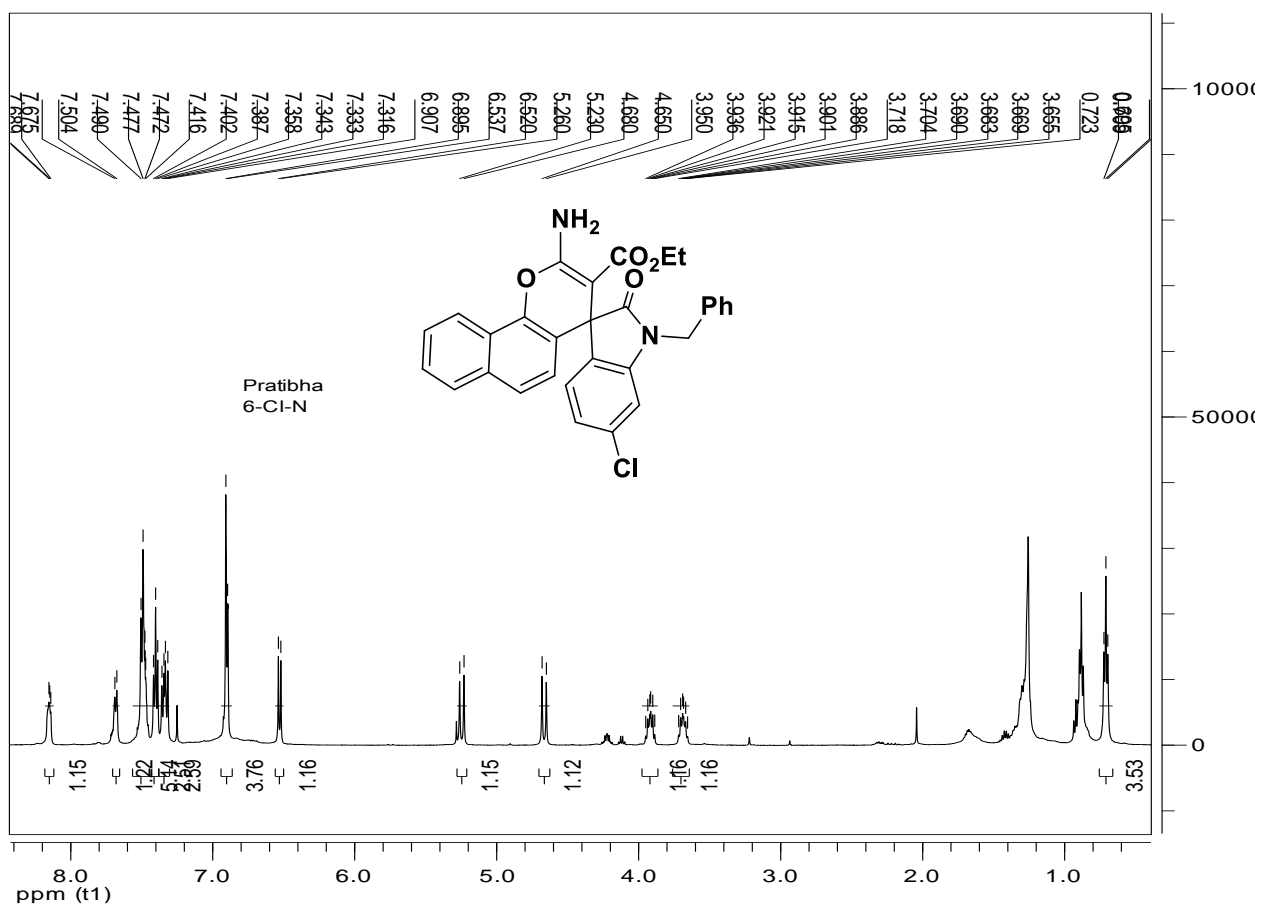


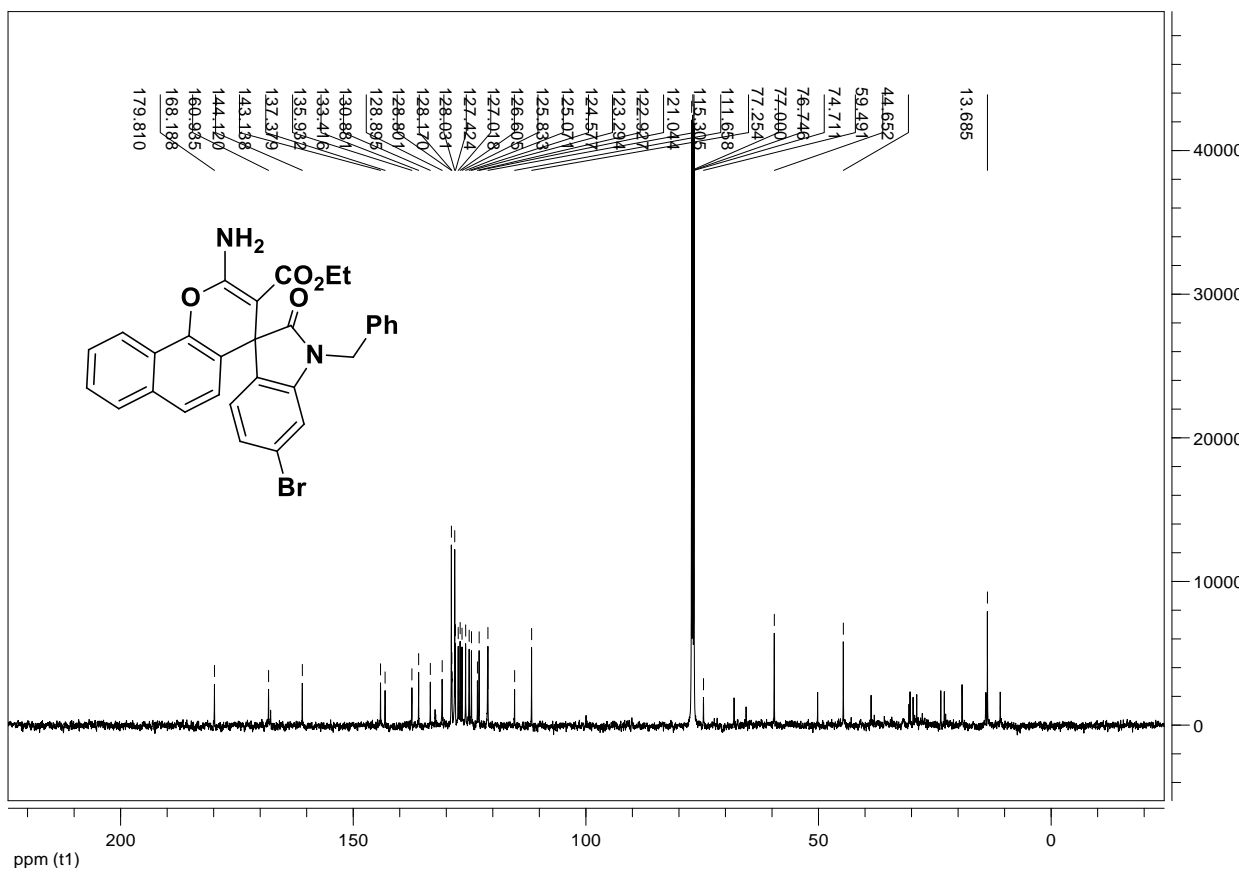
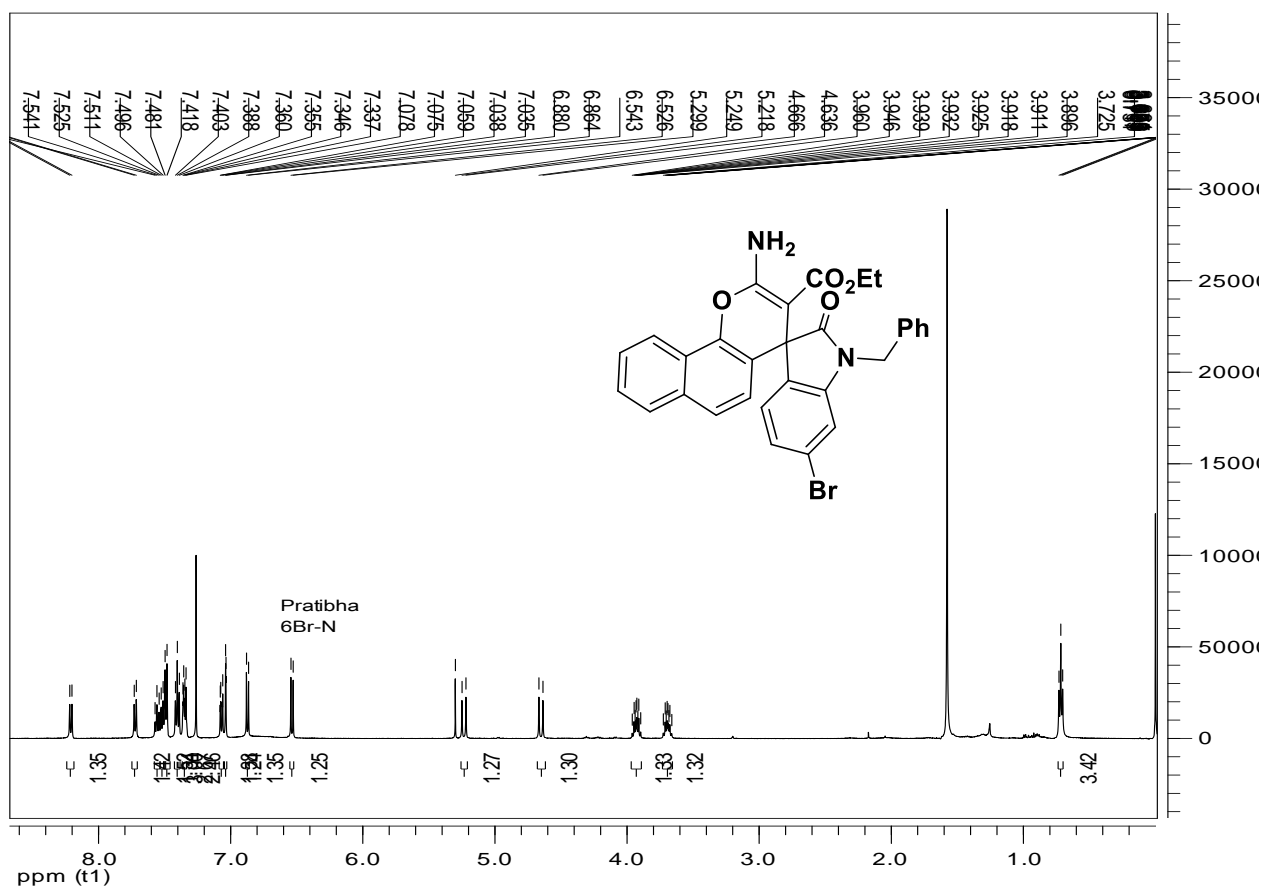


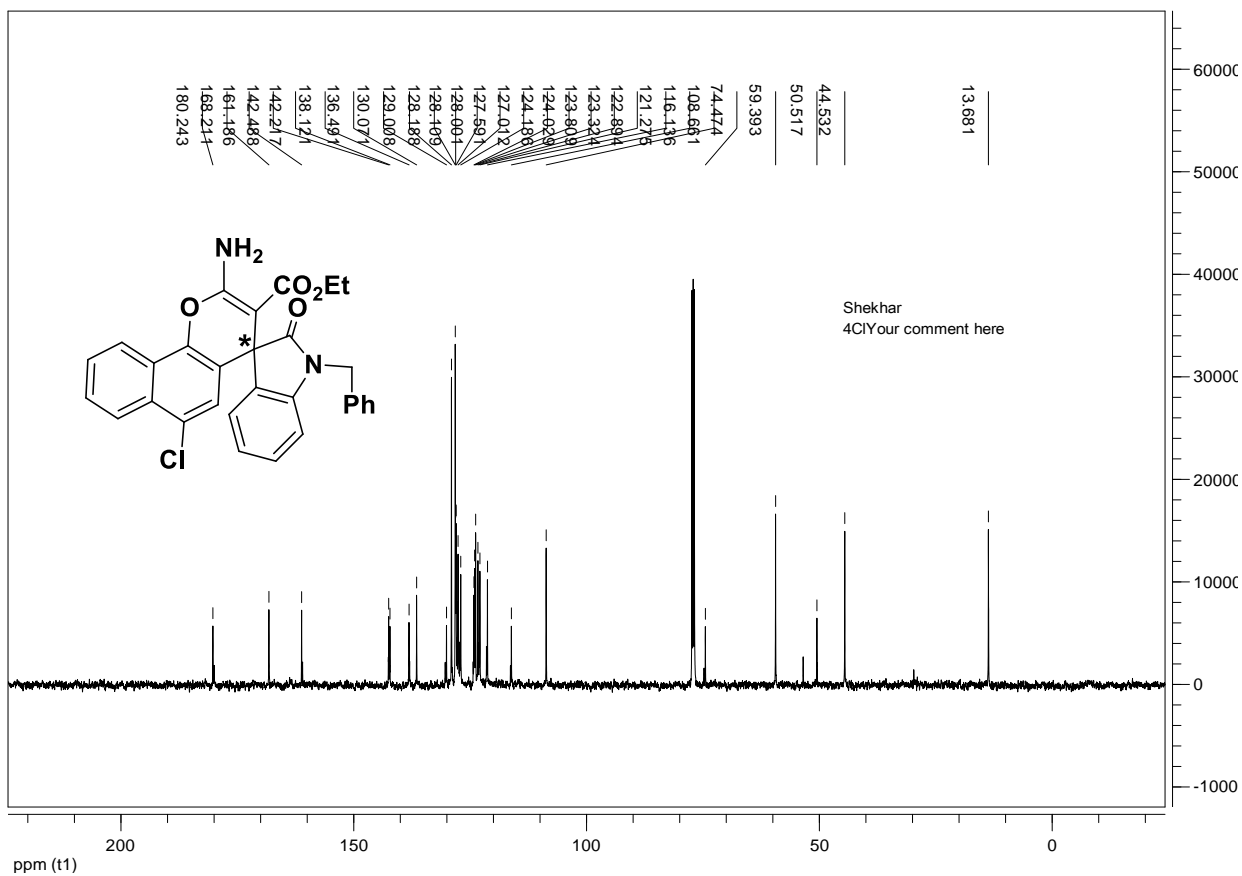
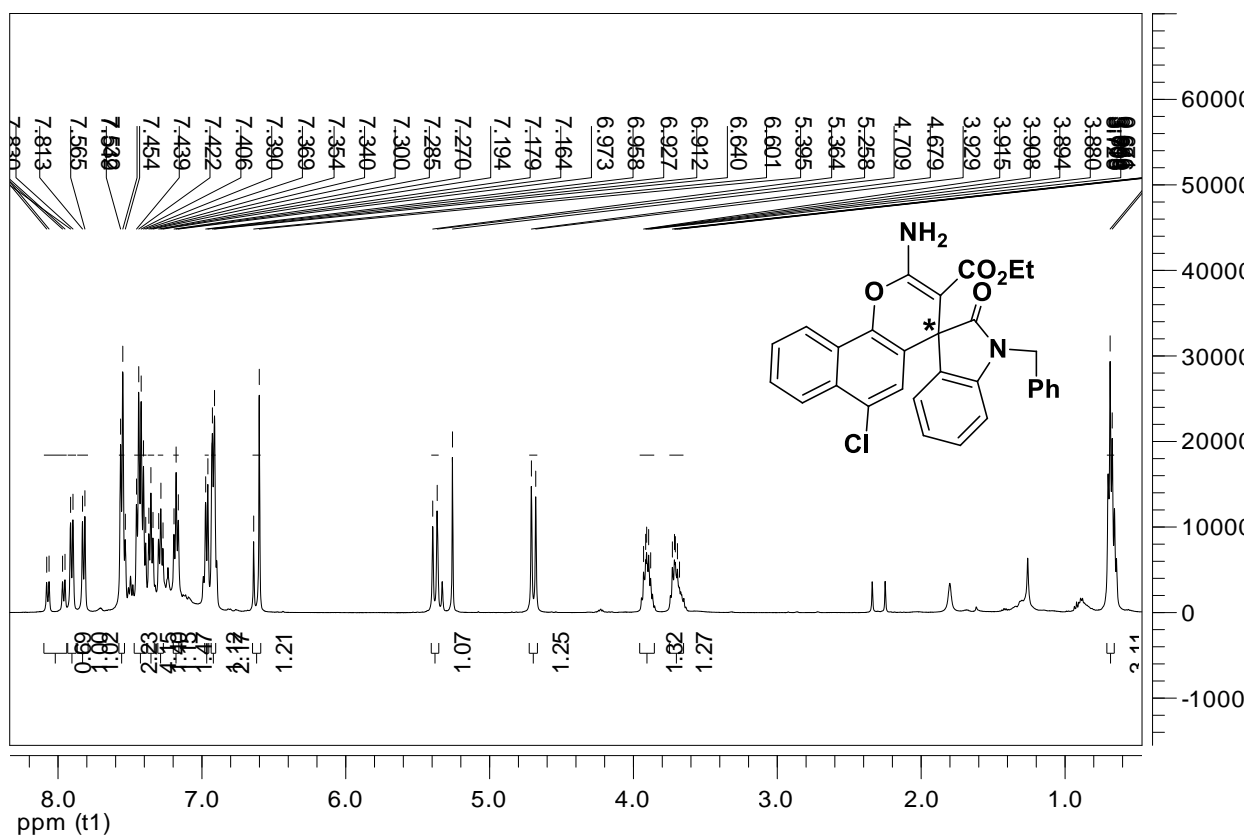


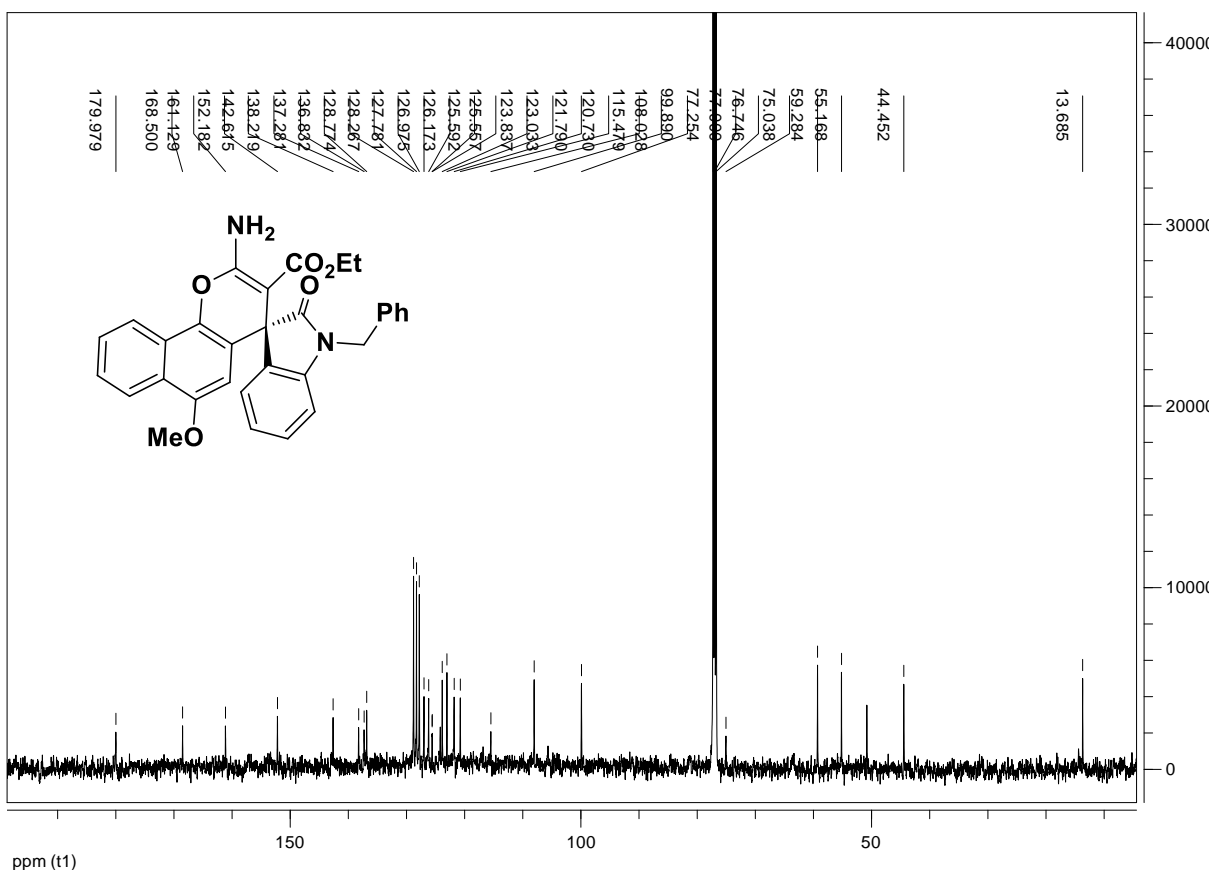
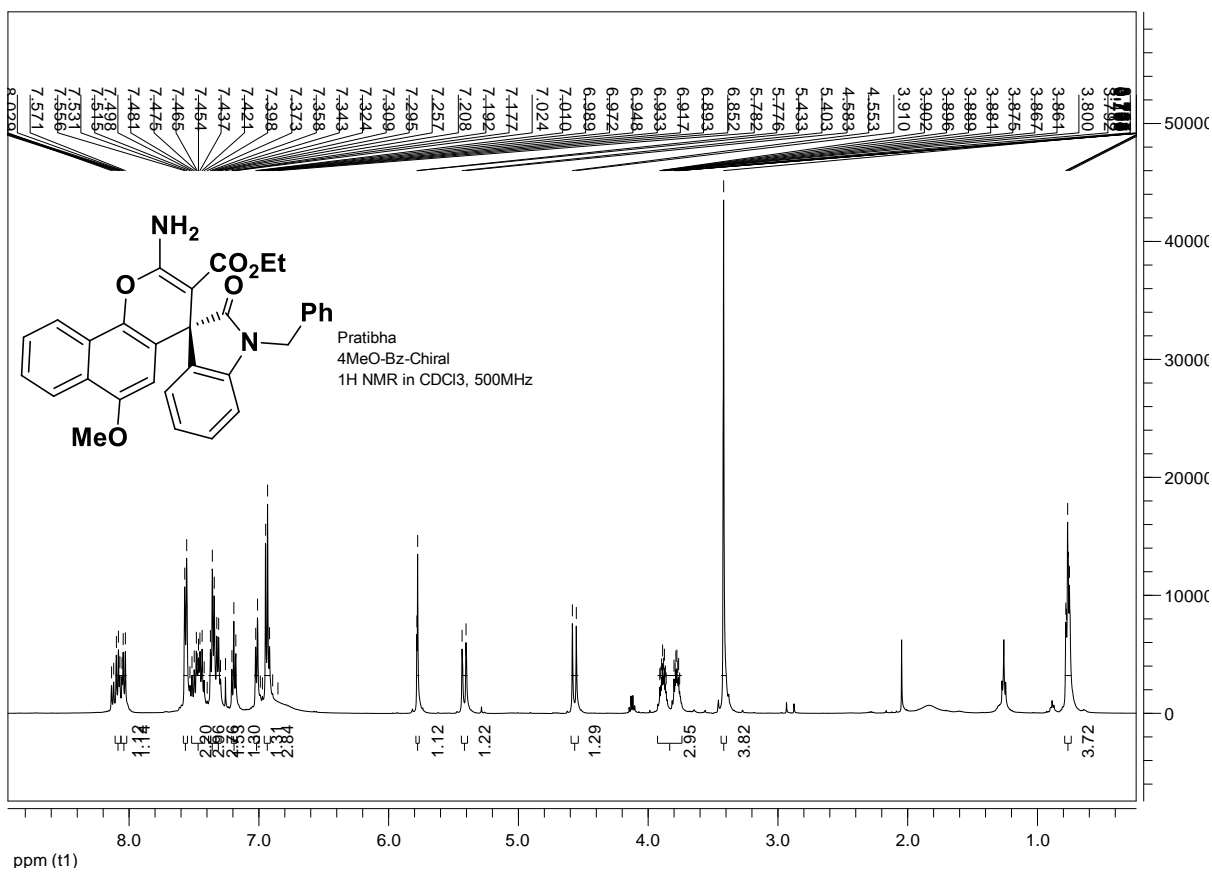


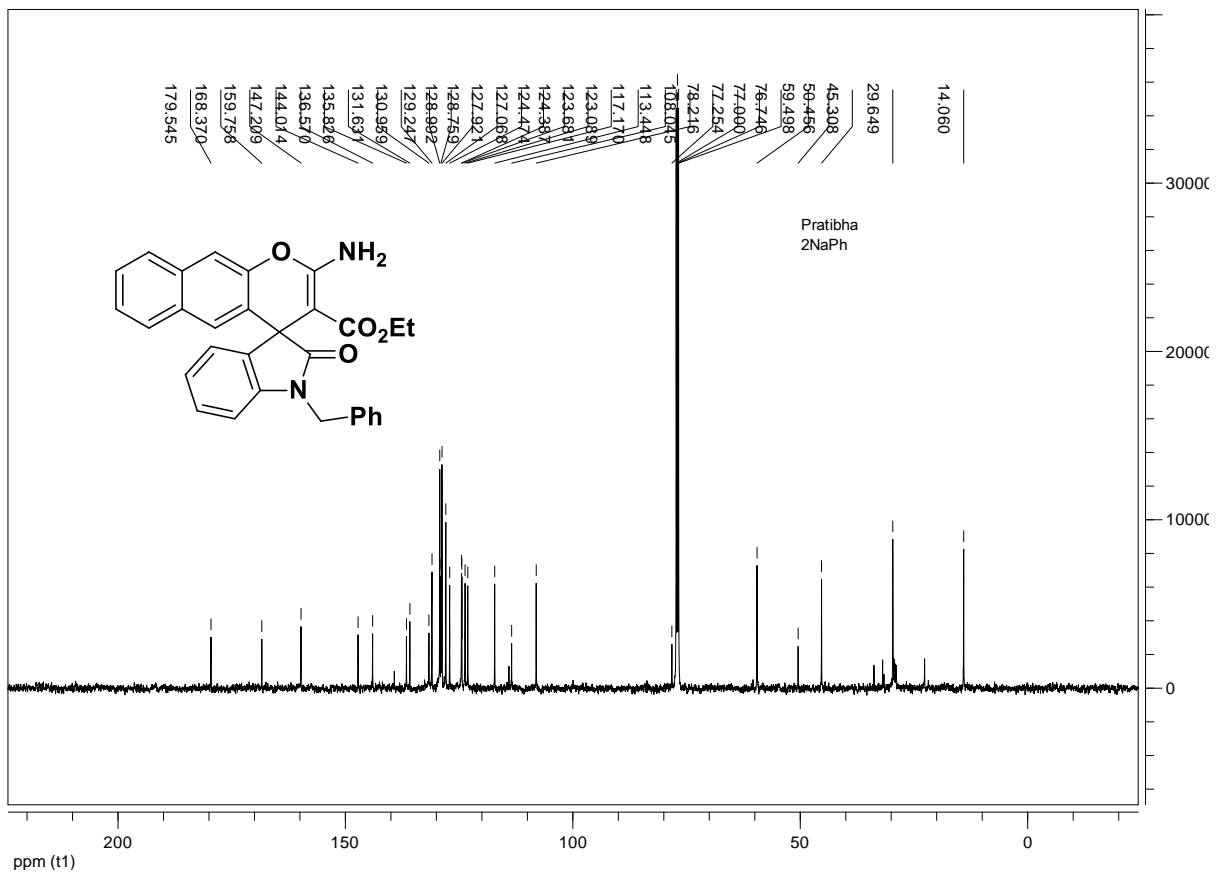
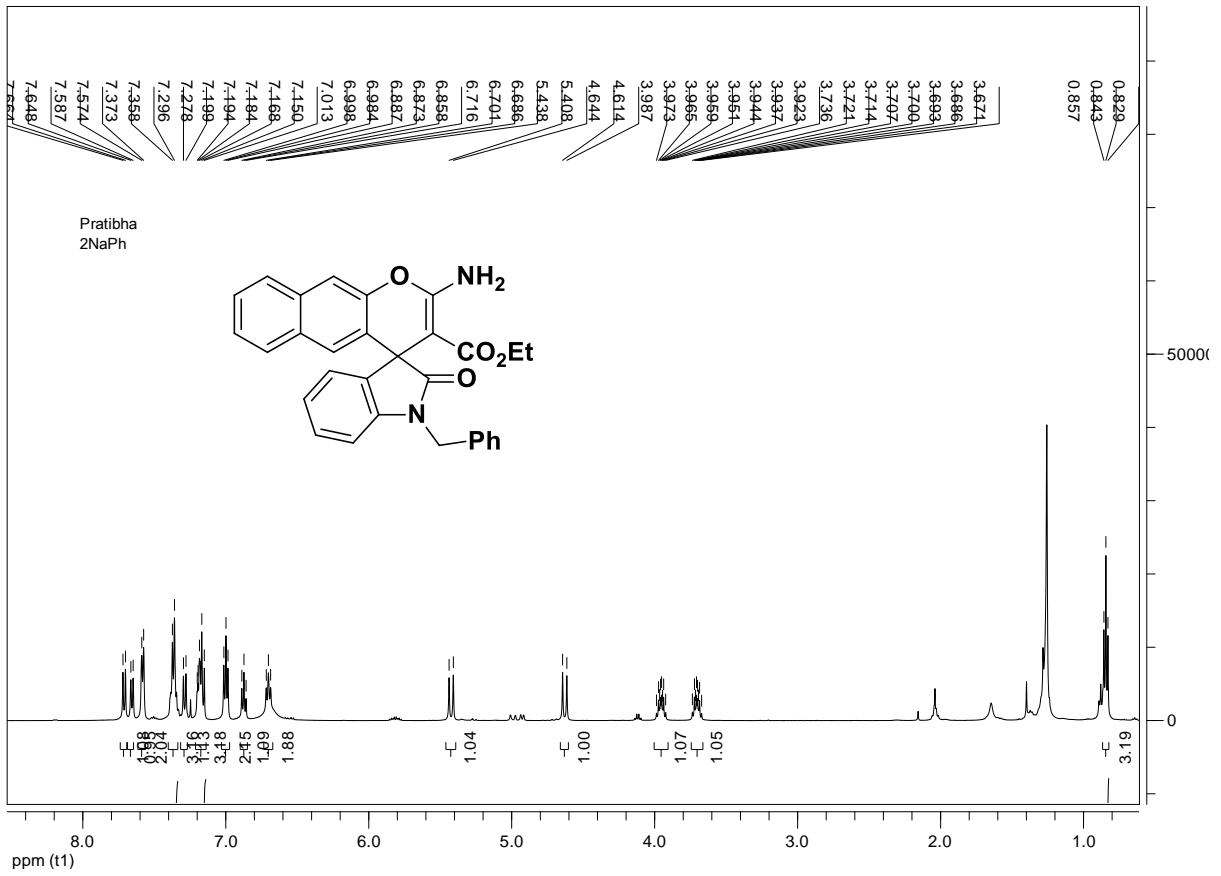


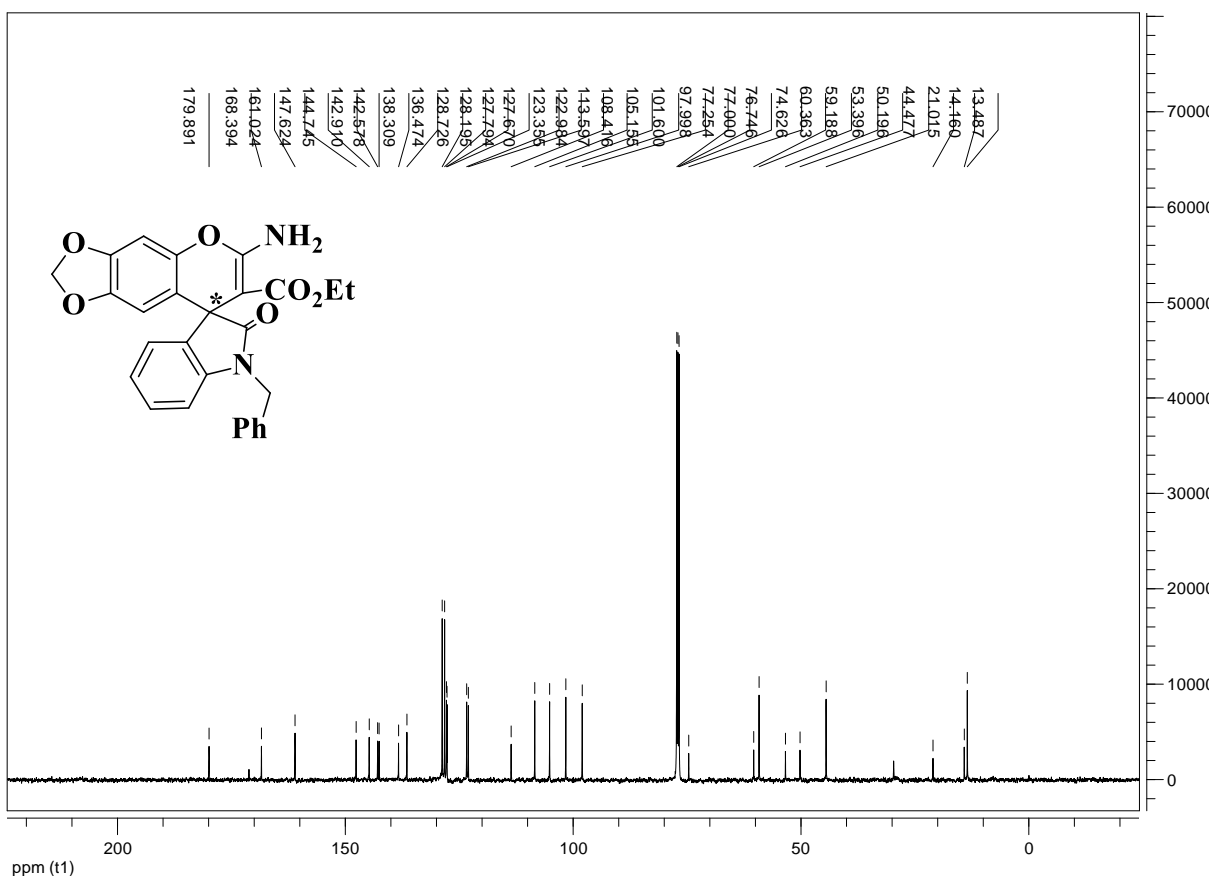
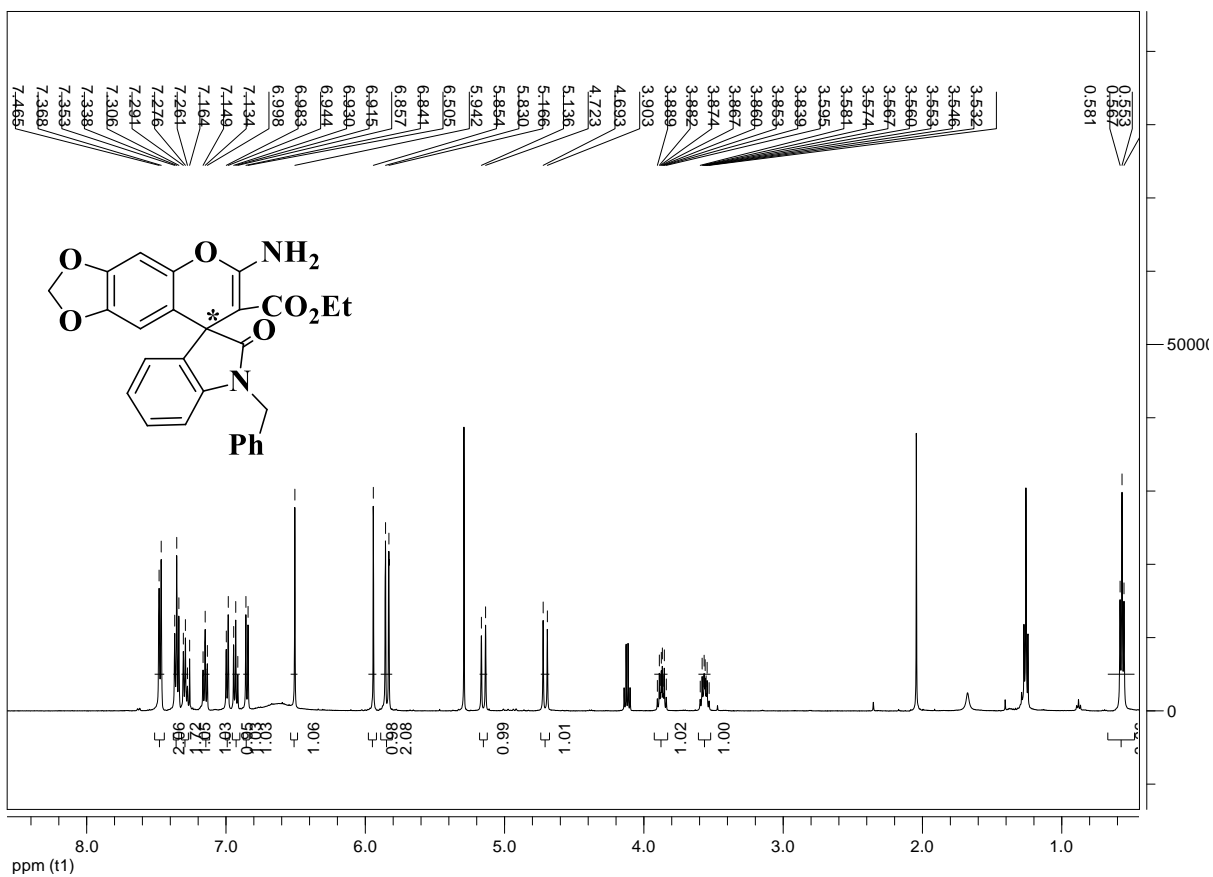


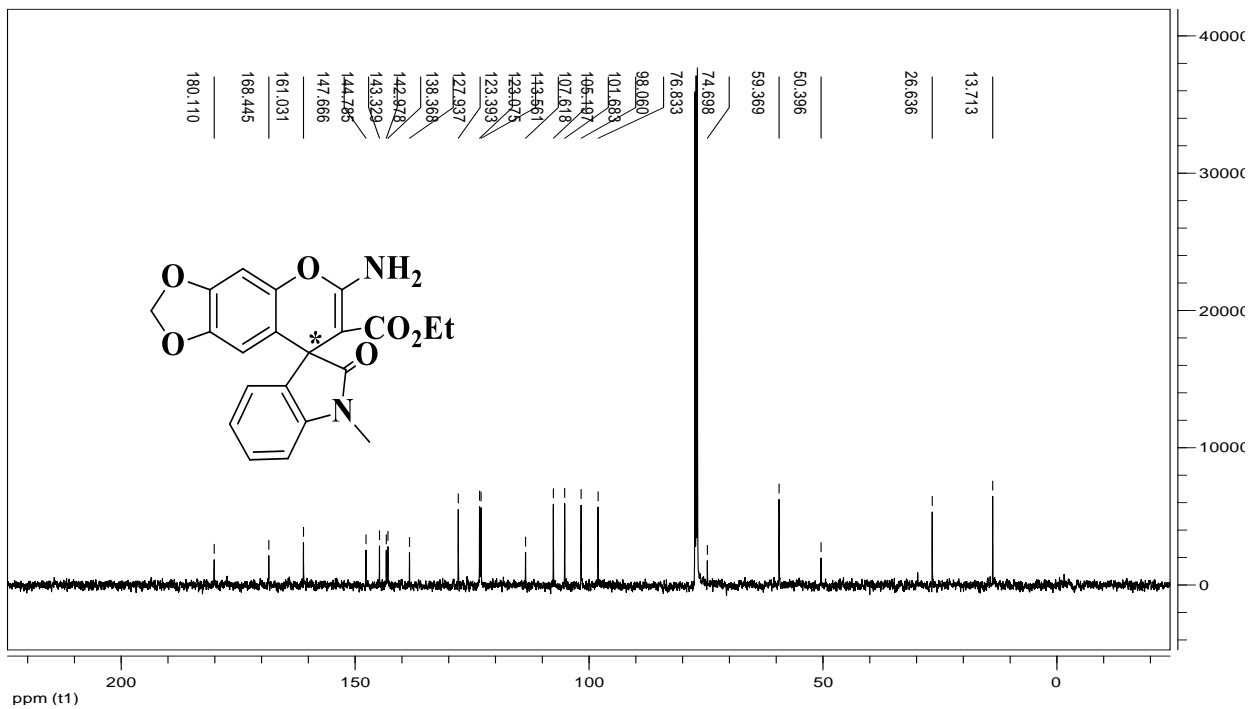
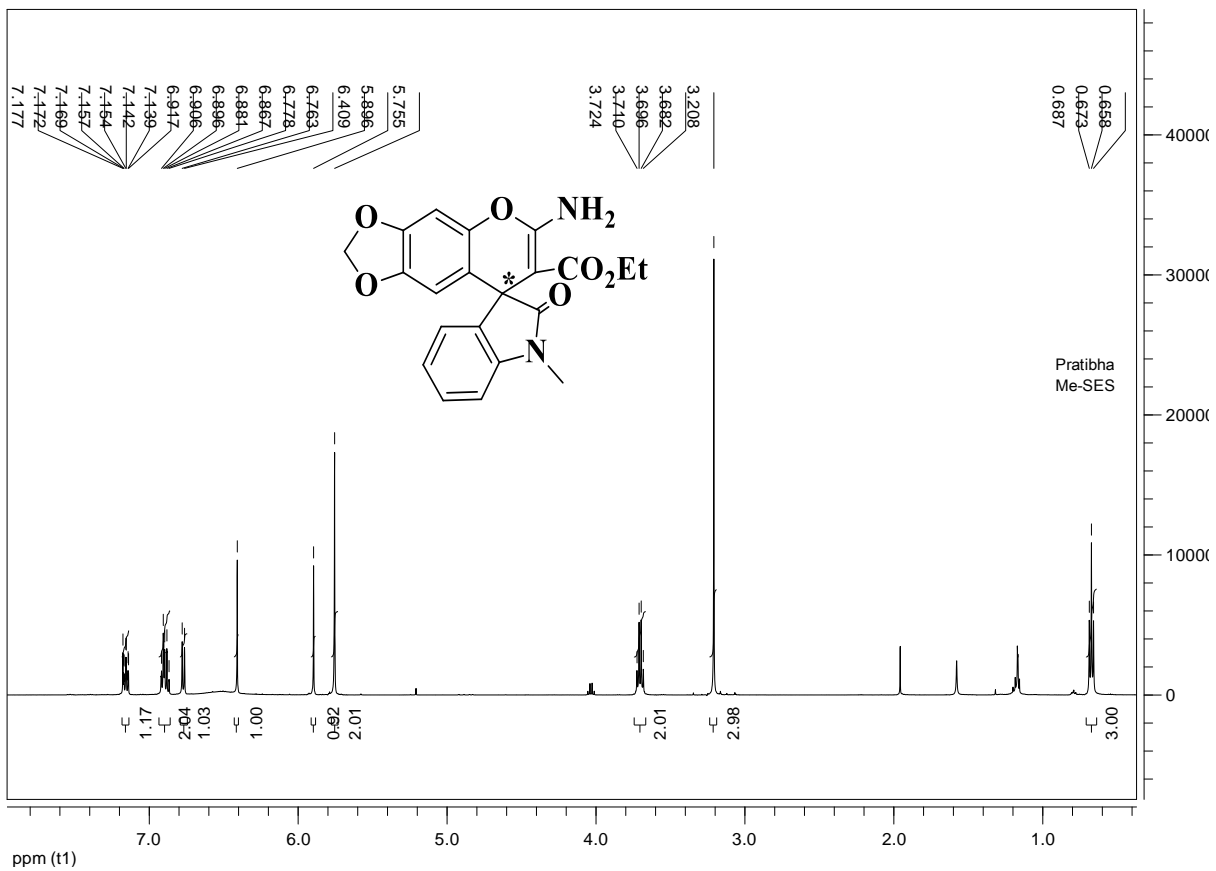


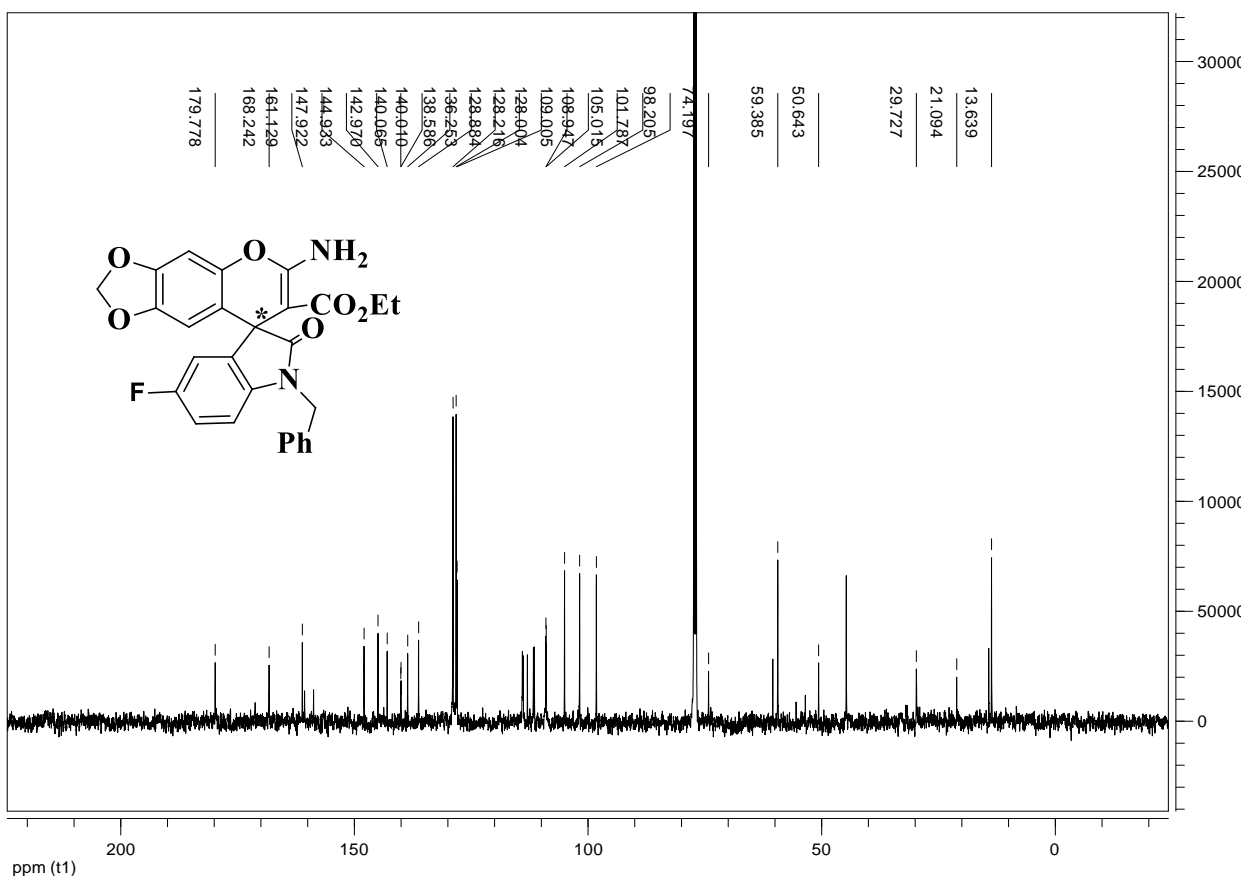
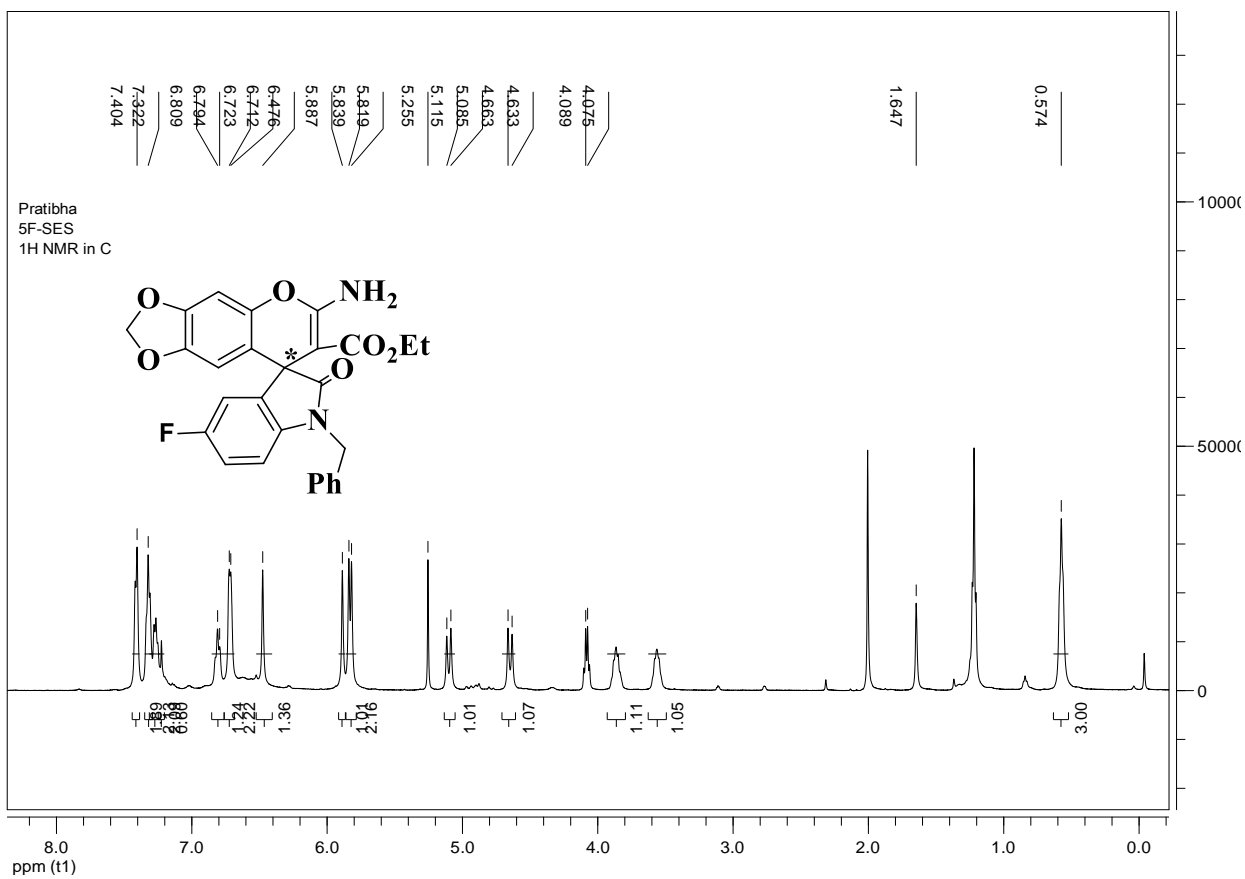


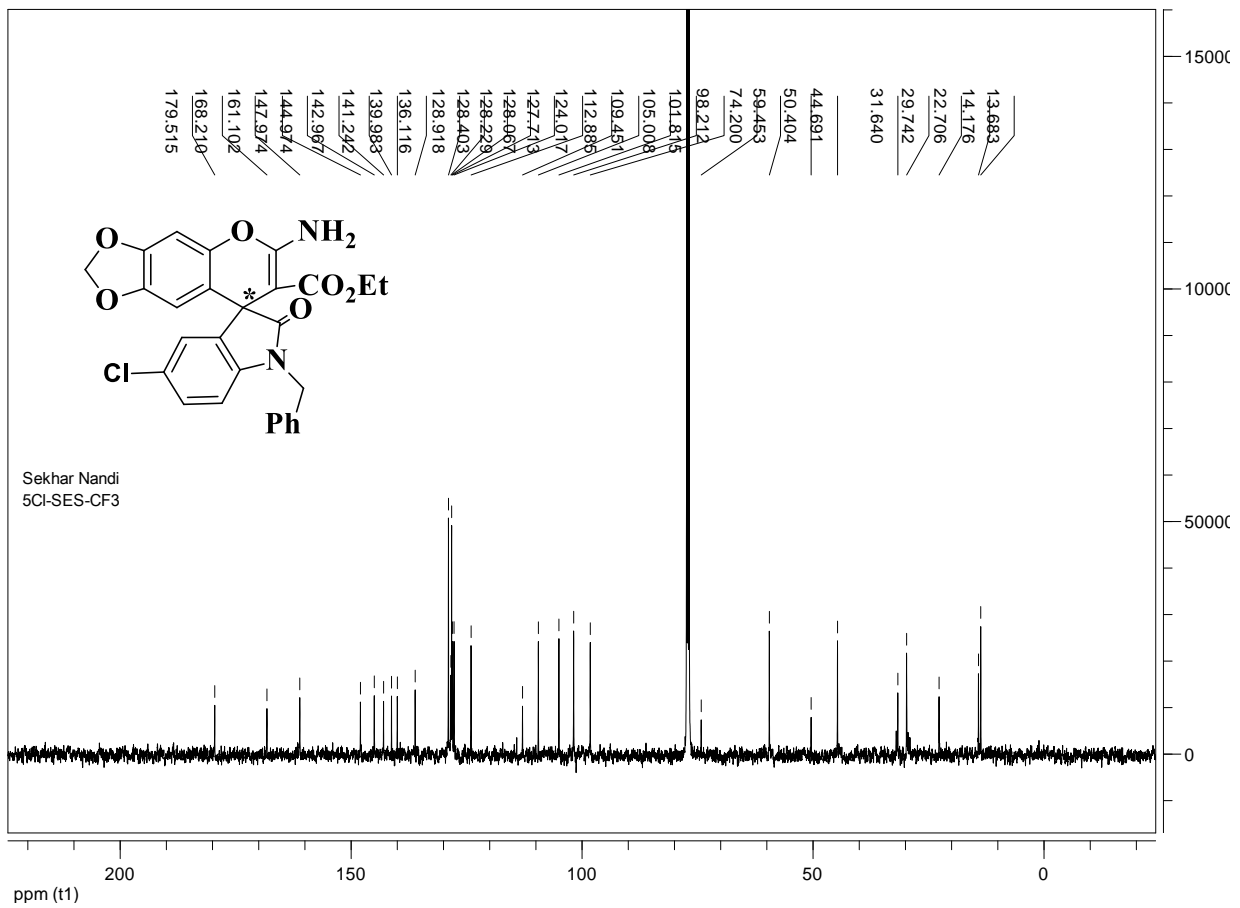
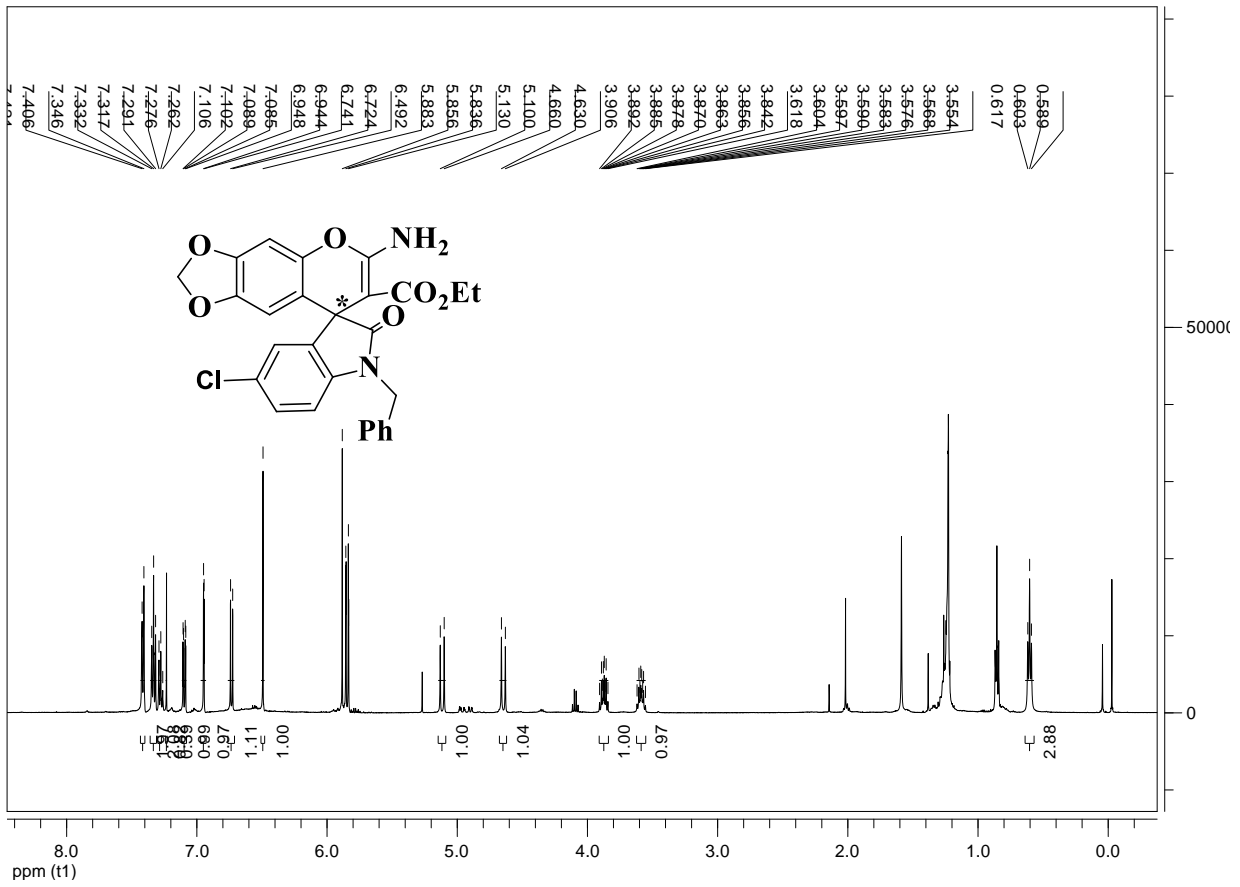


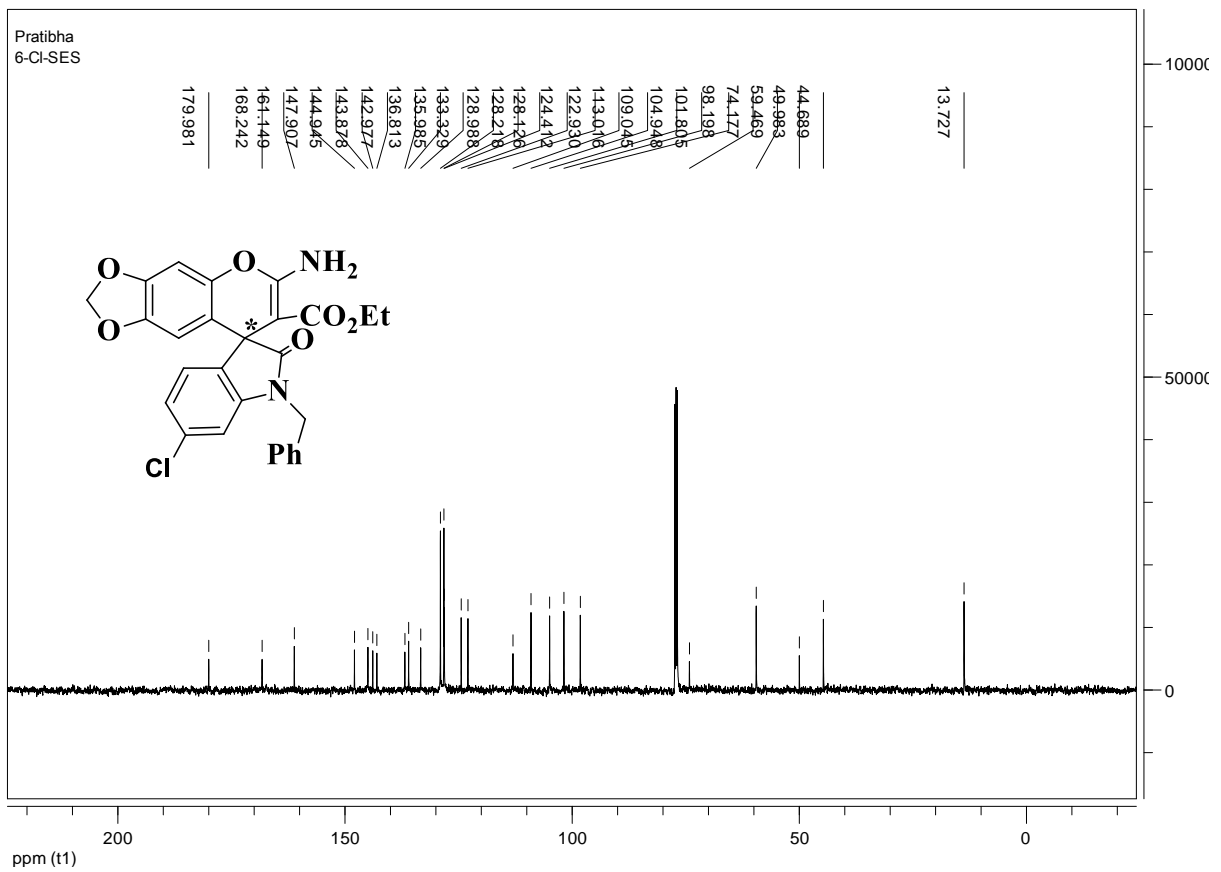
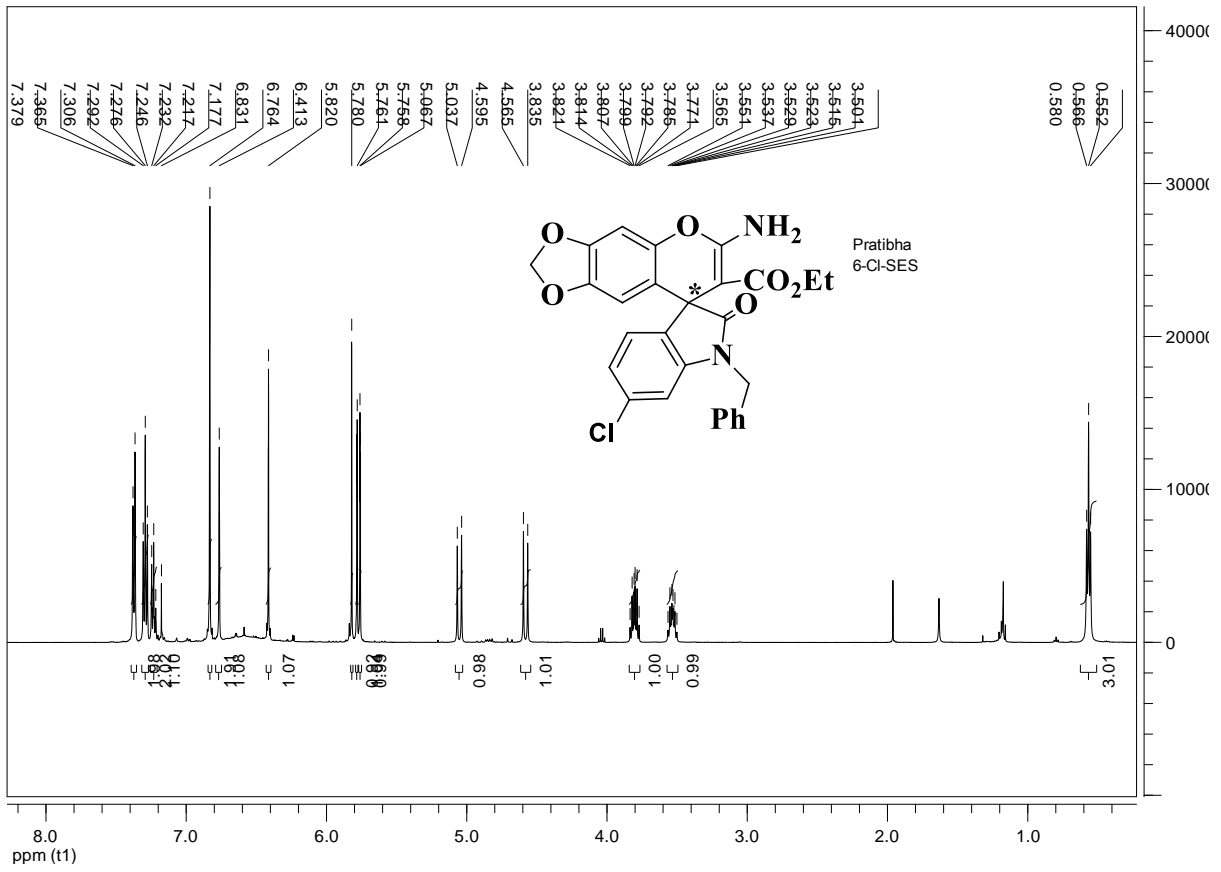


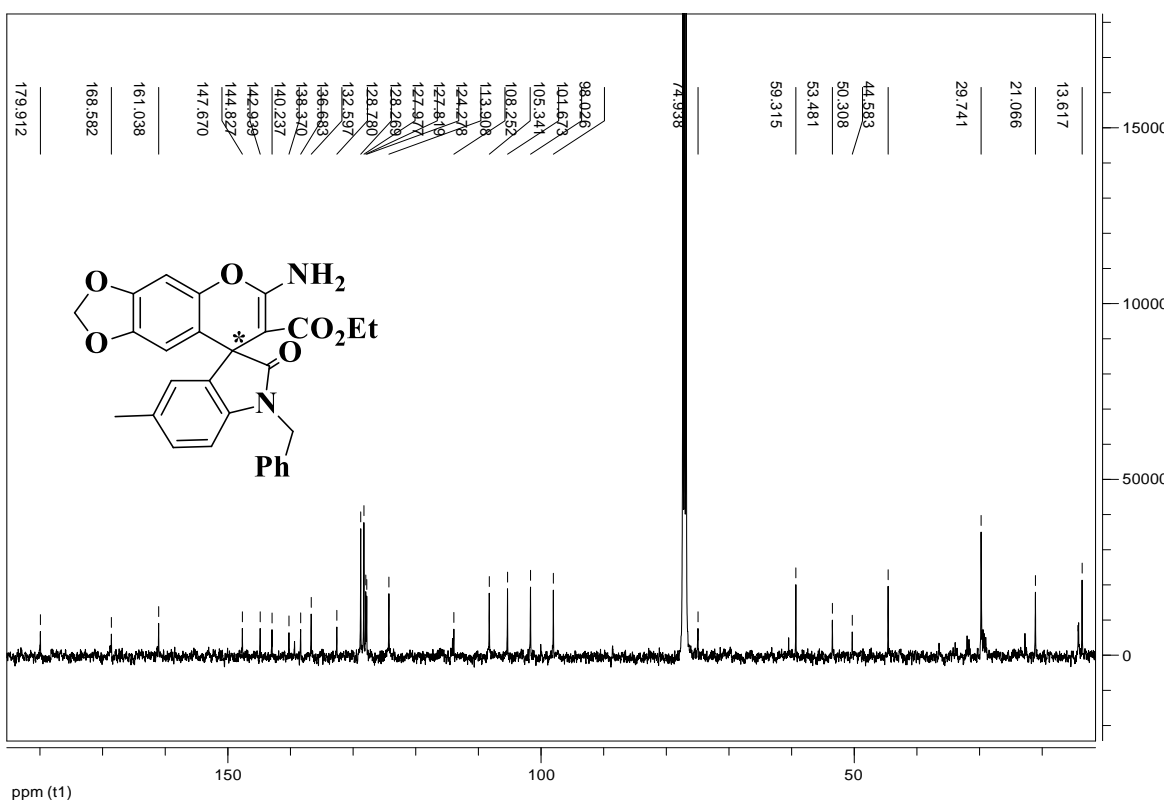
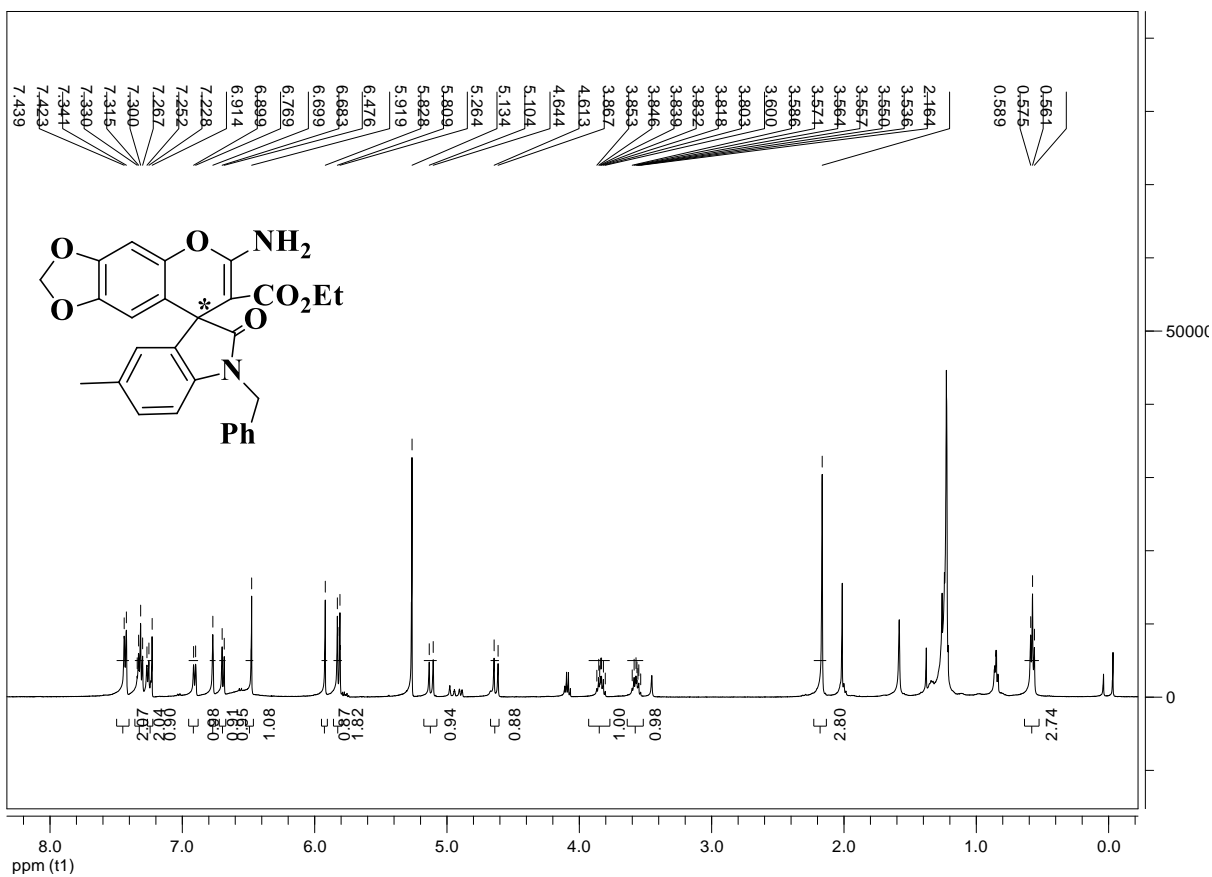




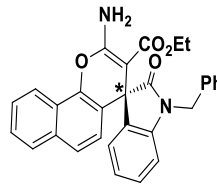








Elemental Composition Report



Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

21717 formula(e) evaluated with 41 results within limits (up to 50 closest results for each mass)

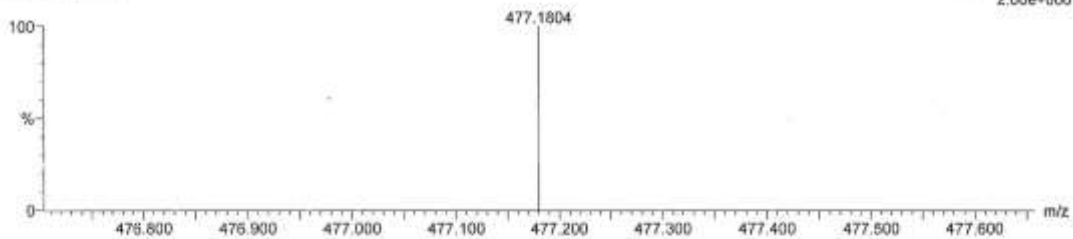
Elements Used:

C: 0-31 H: 0-25 Li: 0-1 B: 0-1 N: 0-2 O: 0-4 Na: 0-1 Si: 0-1 K: 0-1 V: 0-2 Ru: 0-1 I: 0-1

Eu: 0-2

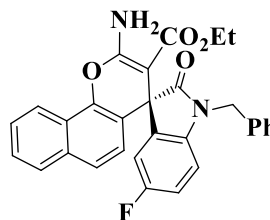
N BZ
N BZ 66 (0.988)

1: TOF MS ES+
2.00e+000



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
477.1804	477.1814	-1.0	-2.1	19.5	n/a	C30 H25 N2 O4
	477.1790	1.4	2.9	21.5	n/a	C31 H22 Li N2 O3
	477.1825	-2.1	-4.4	17.5	n/a	C29 H24 Li B O4 Na
	477.1782	2.2	4.6	20.5	n/a	C29 H23 Li B N2 O2 Si
	477.1766	3.8	8.0	18.5	n/a	C29 H23 Li N2 O3 Na
	477.1849	-4.5	-9.4	20.5	n/a	C31 H23 Li B O4
	477.1758	4.6	9.6	17.5	n/a	C27 H24 Li B N2 O2 Na Si
	477.1750	5.4	11.3	20.5	n/a	C30 H23 B N2 O2 Na
	477.1744	6.0	12.6	18.5	n/a	C31 H25 Li B Na K
	477.1736	6.8	14.3	21.0	n/a	C31 H24 Li N O2 Si
	477.1876	-7.2	-15.1	20.0	n/a	C31 H25 B N O2 Na
	477.1728	7.6	15.9	17.5	n/a	C28 H24 Li B N2 O2 K
	477.1726	7.8	16.3	22.5	n/a	C31 H20 Li B N2 O Na
	477.1724	8.0	16.8	21.0	n/a	C30 H21 Li B N O4
	477.1892	-8.8	-18.4	18.0	n/a	C30 H25 Li N O3 Na
	477.1712	9.2	19.3	18.0	n/a	C29 H25 Li N O2 Na Si
	477.1704	10.0	21.0	14.5	n/a	C26 H25 Li B N2 O2 Na K
	477.1908	-10.4	-21.8	20.0	n/a	C30 H25 Li B N O2 Si
	477.1700	10.4	21.8	18.0	n/a	C28 H22 Li B N O4 Na
	477.1696	10.8	22.6	20.0	n/a	C30 H25 B N O Na Si
	477.1682	12.2	25.6	18.0	n/a	C30 H25 Li N O2 K
	477.1672	13.2	27.7	22.0	n/a	C31 H22 Li B N Na Si
	477.1670	13.4	28.1	20.5	n/a	C30 H23 Li B O3 Si
	477.1938	-13.4	-28.1	17.5	n/a	C28 H24 Li B N2 O3 Na
	477.1666	13.8	28.9	20.0	n/a	C31 H25 B N O K
	477.1654	15.0	31.4	18.5	n/a	C30 H23 Li O4 Na
	477.1646	15.8	33.1	17.5	n/a	C28 H24 Li B O3 Na Si
	477.1962	-15.8	-33.1	20.5	n/a	C30 H23 Li B N2 O3
	477.1638	16.6	34.8	20.5	n/a	C31 H23 B O3 Na
	477.1634	17.0	35.6	19.5	n/a	C29 H25 N2 O3 Si
	477.1618	18.6	39.0	19.0	n/a	C30 H23 Li B N Na K
	477.1616	18.8	39.4	17.5	n/a	C29 H24 Li B O3 K
	477.1611	19.3	40.4	21.5	n/a	C30 H22 Li N2 O2 Si
	477.1598	20.6	43.2	21.5	n/a	C29 H19 Li B N2 O4
	477.1594	21.0	44.0	23.5	n/a	C31 H22 B N2 O Si
	477.1592	21.2	44.4	14.5	n/a	C27 H25 Li B O3 Na K
	477.1587	21.7	45.5	18.5	n/a	C28 H23 Li N2 O2 Na Si
	477.1579	22.5	47.2	21.5	n/a	C31 H22 N2 O2 Na
	477.1574	23.0	48.2	18.5	n/a	C27 H20 Li B N2 O4 Na
	477.1570	23.4	49.0	20.5	n/a	C29 H23 B N2 O Na Si

Elemental Composition Report



Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

43217 formula(e) evaluated with 50 results within limits (up to 50 closest results for each mass)

Elements Used:

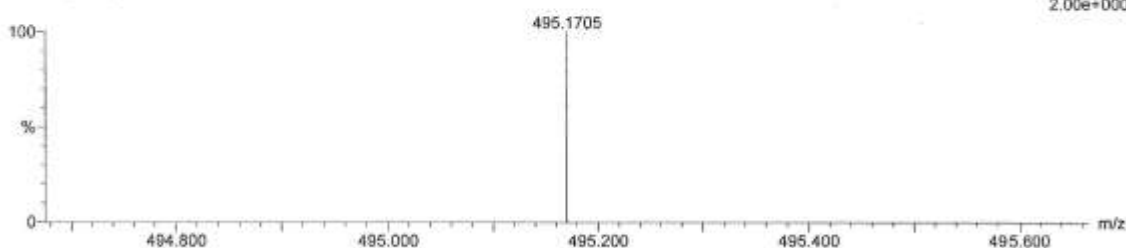
C: 0-31 H: 0-24 Li: 0-1 B: 0-1 N: 0-2 O: 0-4 F: 0-1 Na: 0-1 Si: 0-1 K: 0-1 V: 0-2 Ru: 0-1

I: 0-1 Eu: 0-2

5F N

5F N 51 (0.749)

1: TOF MS ES+
2.00e+000



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
495.1705	495.1700	0.5	1.0	22.5	n/a	C31 H24 B N2 O2 Si
	495.1696	0.9	1.8	21.5	n/a	C31 H21 Li N2 O3 F
	495.1716	-1.1	-2.2	20.5	n/a	C30 H24 Li N2 O3 Si
	495.1720	-1.5	-3.0	19.5	n/a	C30 H24 N2 O4 F
	495.1688	1.7	3.4	20.5	n/a	C29 H22 Li B N2 O2 F Si
	495.1685	2.0	4.0	20.5	n/a	C31 H24 N2 O3 Na
	495.1731	-2.6	-5.3	17.5	n/a	C29 H23 Li B O4 F Na
	495.1672	3.3	6.7	18.5	n/a	C29 H22 Li N2 O3 F Na
	495.1664	4.1	8.3	17.5	n/a	C27 H23 Li B N2 O2 F Na Si
	495.1656	4.9	9.9	20.5	n/a	C30 H22 B N2 O2 F Na
	495.1755	-5.0	-10.1	20.5	n/a	C31 H22 Li B O4 F
	495.1652	5.3	10.7	21.5	n/a	C30 H22 Li B N2 O Na Si
	495.1650	5.5	11.1	18.5	n/a	C31 H24 Li B F Na K
	495.1634	7.1	14.3	17.5	n/a	C28 H23 Li B N2 O2 F K
	495.1632	7.3	14.7	22.5	n/a	C31 H19 Li B N2 O F Na
	495.1622	8.3	16.8	21.5	n/a	C31 H22 Li B N2 O K
	495.1610	9.5	19.2	14.5	n/a	C26 H24 Li B N2 O2 F Na K
	495.1604	10.1	20.4	20.5	n/a	C31 H24 Li O4 Si
	495.1598	10.7	21.6	18.5	n/a	C29 H23 Li B N2 O Na K
	495.1832	-12.7	-25.6	21.5	n/a	C31 H22 Li B N2 O2 Na
	495.1575	13.0	26.3	20.5	n/a	C30 H22 Li B O3 F Si
	495.1844	-13.9	-28.1	17.5	n/a	C28 H23 Li B N2 O3 F Na
	495.1560	14.5	29.3	18.5	n/a	C30 H22 Li O4 F Na
	495.1551	15.4	31.1	17.5	n/a	C28 H23 Li B O3 F Na Si
	495.1551	15.4	31.1	20.5	n/a	C31 H24 Li B N O V
	495.1544	16.1	32.5	20.5	n/a	C31 H22 B O3 F Na
	495.1868	-16.3	-32.9	20.5	n/a	C30 H22 Li B N2 O3 F
	495.1540	16.5	33.3	21.5	n/a	C31 H22 Li B O2 Na Si
	495.1540	16.5	33.3	19.5	n/a	C29 H24 N2 O3 F Si
	495.1524	18.1	36.6	20.5	n/a	C28 H21 Li B N2 O4 Si
	495.1521	18.4	37.2	17.5	n/a	C29 H23 Li B O3 F K
	495.1516	18.9	38.2	23.5	n/a	C31 H20 B N2 O4
	495.1516	18.9	38.2	21.5	n/a	C30 H21 Li N2 O2 F Si
	495.1896	-19.1	-38.6	20.5	n/a	C31 H24 Li N2 O4
	495.1505	20.0	40.4	20.5	n/a	C30 H24 N2 O2 Na Si
	495.1504	20.1	40.6	21.5	n/a	C29 H18 Li B N2 O4 F
	495.1500	20.5	41.4	23.5	n/a	C31 H21 B N2 O F Si
	495.1500	20.5	41.4	17.5	n/a	C26 H22 Li B N2 O4 Na Si
	495.1497	20.8	42.0	14.5	n/a	C27 H24 Li B O3 F Na K
	495.1492	21.3	43.0	20.5	n/a	C29 H21 B N2 O4 Na

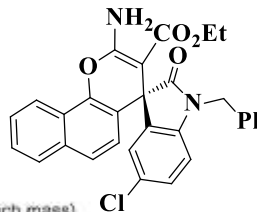
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Odd and Even Electron Ions

35 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

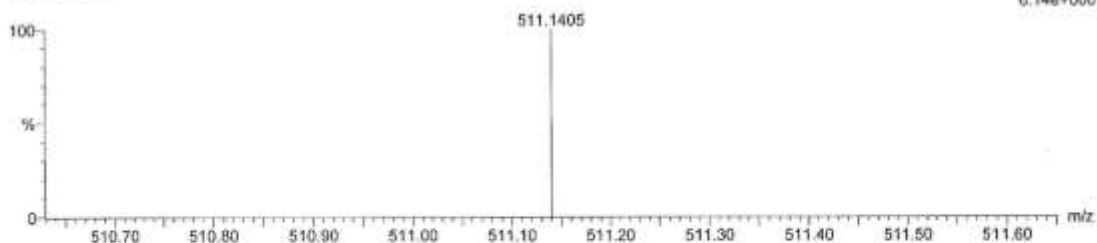
Elements Used:

C: 0-31 H: 0-24 N: 0-2 O: 0-4 Na: 0-1 Cl: 0-1

SCL N 11 (0.204)

1: TOF MS ES+

6.14e+000



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
511.1405	511.1425	-2.0	-3.9	19.5	n/a	C30 H24 N2 O4 Cl
	511.1189	21.6	42.3	21.5	n/a	C31 H21 N2 O2 Na Cl
	511.1634	-22.9	-44.8	20.5	n/a	C31 H24 N2 O4 Na

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

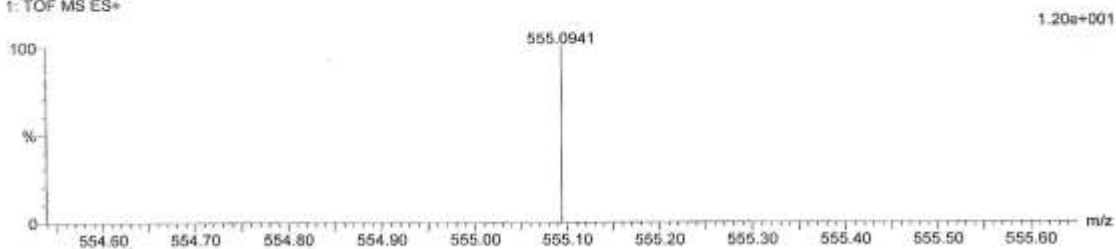
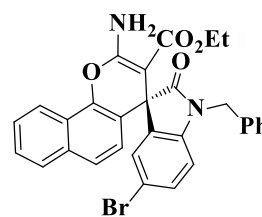
45 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-31 H: 0-24 N: 0-2 O: 0-4 Na: 0-1 Br: 0-1

SBR N 49 (0.909)

1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
555.0941	555.0919	2.2	4.0	19.5	n/a	C30 H24 N2 O4 Br
	555.0684	25.7	46.3	21.5	n/a	C31 H21 N2 O2 Na Br

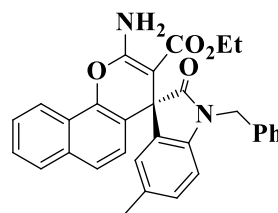
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Odd and Even Electron Ions

24155 formula(e) evaluated with 40 results within limits (up to 50 closest results for each mass)

Elements Used:

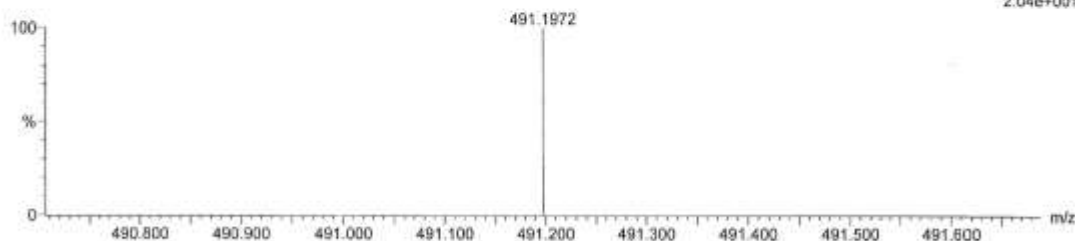
C: 0-32 H: 0-27 Li: 0-1 B: 0-1 N: 0-2 O: 0-4 Na: 0-1 Si: 0-1 K: 0-1 V: 0-2 Ru: 0-1 I: 0-1

Eu: 0-2

SME N

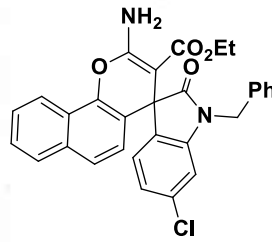
SME N 46 (0.686)

1: TOF MS ES+
2.04e+001



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
491.1972	491.1971	0.1	0.2	19.5	n/a	C31 H27 N2 O4
	491.1982	-1.0	-2.0	17.5	n/a	C30 H26 Li B O4 Na
	491.1947	2.5	5.1	21.5	n/a	C32 H24 Li N2 O3
	491.1938	3.4	6.9	20.5	n/a	C30 H25 Li B N2 O2 Si
	491.2006	-3.4	-6.9	20.5	n/a	C32 H25 Li B O4
	491.1923	4.9	10.0	18.5	n/a	C30 H25 Li N2 O3 Na
	491.1914	5.8	11.8	17.5	n/a	C28 H26 Li B N2 O2 Na Si
	491.2033	-6.1	-12.4	20.0	n/a	C32 H27 B N O2 Na
	491.1907	6.5	13.2	20.5	n/a	C31 H25 B N2 O2 Na
	491.1901	7.1	14.5	18.5	n/a	C32 H27 Li B Na K
	491.2049	-7.7	-15.7	18.0	n/a	C31 H27 Li N O3 Na
	491.1893	7.9	16.1	21.0	n/a	C32 H26 Li N O2 Si
	491.1884	8.8	17.9	17.5	n/a	C29 H26 Li B N2 O2 K
	491.1883	8.9	18.1	22.5	n/a	C32 H22 Li B N2 O Na
	491.1880	9.2	18.7	21.0	n/a	C31 H23 Li B N O4
	491.2064	-9.2	-18.7	20.0	n/a	C31 H27 Li B N O2 Si
	491.1869	10.3	21.0	18.0	n/a	C30 H27 Li N O2 Na Si
	491.1860	11.2	22.8	14.5	n/a	C27 H27 Li B N2 O2 Na K
	491.1856	11.6	23.6	18.0	n/a	C29 H24 Li B N O4 Na
	491.1853	11.9	24.2	20.0	n/a	C31 H27 B N O Na Si
	491.2094	-12.2	-24.8	17.5	n/a	C29 H26 Li B N2 O3 Na
	491.1839	13.3	27.1	18.0	n/a	C31 H27 Li N O2 K
	491.1829	14.3	29.1	22.0	n/a	C32 H24 Li B N Na Si
	491.2118	-14.6	-29.7	20.5	n/a	C31 H25 Li B N2 O3
	491.1826	14.6	29.7	20.5	n/a	C31 H25 Li B O3 Si
	491.1823	14.9	30.3	20.0	n/a	C32 H27 B N O K
	491.1811	16.1	32.8	18.5	n/a	C31 H25 Li O4 Na
	491.1802	17.0	34.6	17.5	n/a	C29 H26 Li B O3 Na Si
	491.1794	17.8	36.2	20.5	n/a	C32 H25 B O3 Na
	491.1791	18.1	36.8	19.5	n/a	C30 H27 N2 O3 Si
	491.1775	19.7	40.1	19.0	n/a	C31 H25 Li B N Na K
	491.1772	20.0	40.7	17.5	n/a	C30 H26 Li B O3 K
	491.1767	20.5	41.7	21.5	n/a	C31 H24 Li N2 O2 Si
	491.1754	21.8	44.4	21.5	n/a	C30 H21 Li B N2 O4
	491.1751	22.1	45.0	23.5	n/a	C32 H24 B N2 O Si
	491.1748	22.4	45.6	14.5	n/a	C28 H27 Li B O3 Na K
	491.1743	22.9	46.6	18.5	n/a	C29 H25 Li N2 O2 Na Si
	491.1735	23.7	48.2	21.5	n/a	C32 H24 H2 O2 Na
	491.1730	24.2	49.3	18.5	n/a	C29 H22 Li B N2 O4 Na
	491.1727	24.5	49.9	20.5	n/a	C30 H25 B N2 O Na Si

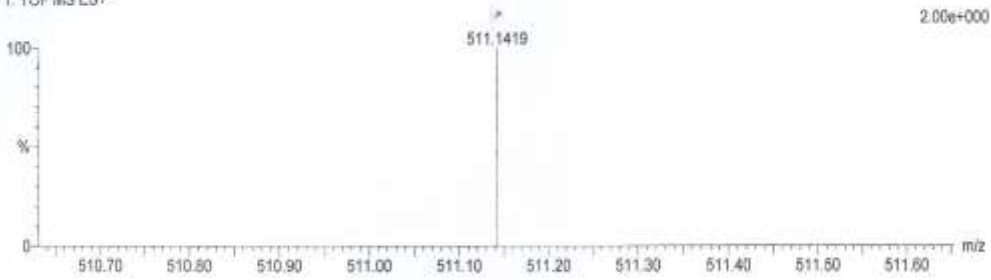
Elemental Composition Report



Single Mass Analysis

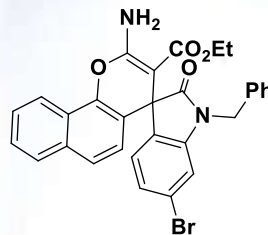
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
 35 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 0-31 H: 0-24 N: 0-2 O: 0-4 Na: 0-1 Cl: 0-1
 6CLN 32 (0.594)
 1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
511.1419	511.1425	-0.6	-1.2	19.5	n/a	C30 H24 N2 O4 Cl
	511.1634	-21.5	-42.1	20.5	n/a	C31 H24 N2 O4 Na
	511.1189	23.0	45.0	21.5	n/a	C31 H21 N2 O2 Na Cl

Elemental Composition Report



Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

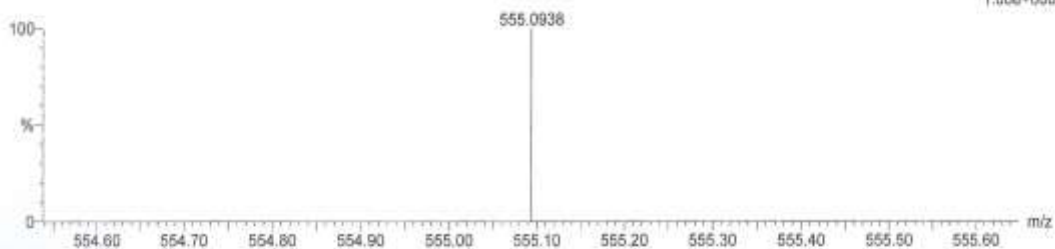
45 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-31 H: 0-24 N: 0-2 O: 0-4 Na: 0-1 Br: 0-1

6BRN 44 (0.816)

1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
555.0938	555.0919	1.9	3.4	19.5	n/a	C30 H24 N2 O4 Br
	555.0684	25.4	45.8	21.5	n/a	C31 H21 N2 O2 Na Br

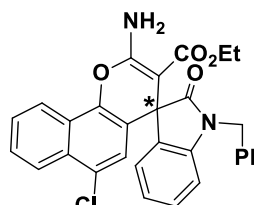
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Odd and Even Electron Ions

34 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

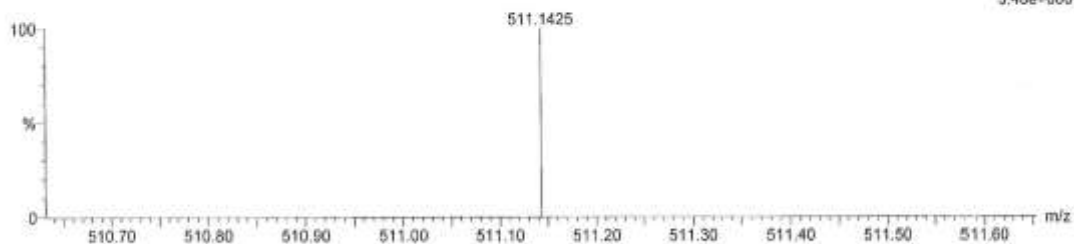
Elements Used:

C: 0-31 H: 0-24 N: 0-2 O: 0-4 F: 0-1 Cl: 0-1

4CLN 49 (0.909)

1: TOF MS ES+

3.48e+000



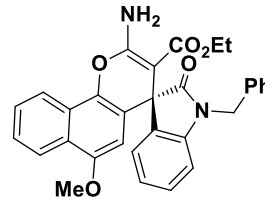
Minimum: -1.5
Maximum: 50.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
511.1425	511.1425	0.0	0.0	19.5	n/a	C30 H24 N2 O4 Cl
	511.1350	7.5	14.7	20.0	n/a	C31 H23 N O3 F Cl
	511.1225	20.0	39.1	20.5	n/a	C30 H21 N2 O3 F Cl

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



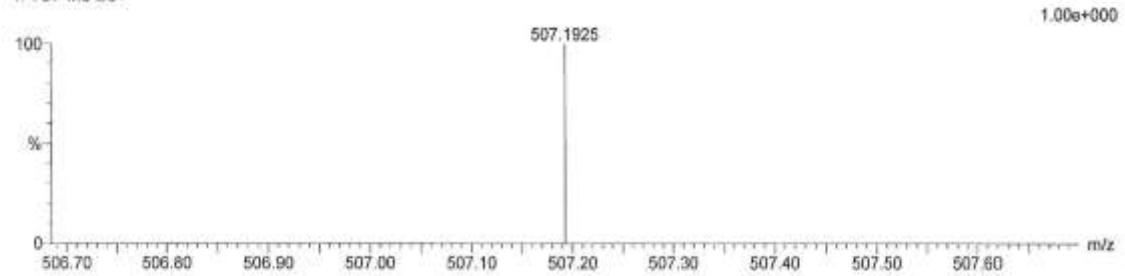
Monoisotopic Mass, Even Electron Ions

29707 formula(e) evaluated with 31 results within limits (up to 50 closest results for each mass)

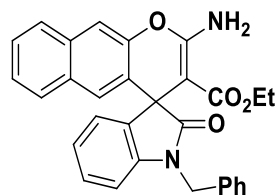
Elements Used:

C: 0-32 H: 0-27 Li: 0-1 B: 0-1 N: 0-2 O: 0-5 Na: 0-1 Si: 0-1 K: 0-1 V: 0-2 Ru: 0-1 I: 0-1
 Eu: 0-2

4MEON 54 (1.001)
 1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
507.1925	507.1920	0.5	1.0	19.5	n/a	C31 H27 N2 O5
	507.1931	-0.6	-1.2	17.5	n/a	C30 H26 Li B O5 Na
	507.1896	2.9	5.7	21.5	n/a	C32 H24 Li N2 O4
	507.1955	-3.0	-5.9	20.5	n/a	C32 H25 Li B O5
	507.1962	-3.7	-7.3	18.5	n/a	C31 H27 Li B N2 Na K
	507.1888	3.7	7.3	20.5	n/a	C30 H25 Li B N2 O3 Si
	507.1872	5.3	10.4	18.5	n/a	C30 H25 Li N2 O4 Na
	507.1864	6.1	12.0	17.5	n/a	C28 H26 Li B N2 O3 Na Si
	507.1856	6.9	13.6	20.5	n/a	C31 H25 B N2 O3 Na
	507.1830	7.5	14.8	18.5	n/a	C32 H27 Li B O Na K
	507.1834	9.1	17.9	17.5	n/a	C29 H26 Li B N2 O3 K
	507.2016	-9.1	-17.9	21.5	n/a	C32 H26 Li B N2 Na Si
	507.1832	9.3	18.3	22.5	n/a	C32 H22 Li B N2 O2 Na
	507.1810	11.5	22.7	14.5	n/a	C27 H27 Li B N2 O3 Na K
	507.2043	-11.8	-23.3	17.5	n/a	C29 H26 Li B N2 O4 Na
	507.1791	13.4	26.4	19.5	n/a	C32 H26 Li N2 Na K
	507.2067	-14.2	-28.0	20.5	n/a	C31 H25 Li B N2 O4
	507.1775	15.0	29.6	20.5	n/a	C31 H25 Li B O4 Si
	507.1760	16.5	32.5	18.5	n/a	C31 H25 Li O5 Na
	507.1751	17.4	34.3	17.5	n/a	C29 H26 Li B O4 Na Si
	507.1744	18.1	35.7	20.5	n/a	C32 H25 B O4 Na
	507.1740	18.5	36.5	19.5	n/a	C30 H27 N2 O4 Si
	507.1721	20.4	40.2	17.5	n/a	C30 H26 Li B O4 K
	507.1716	20.9	41.2	21.5	n/a	C31 H24 Li N2 O3 Si
	507.1704	22.1	43.6	21.5	n/a	C30 H21 Li B N2 O5
	507.1700	22.5	44.4	23.5	n/a	C32 H24 B N2 O2 Si
	507.1697	22.8	45.0	14.5	n/a	C28 H27 Li B O4 Na K
	507.1692	23.3	45.9	18.5	n/a	C29 H25 Li N2 O3 Na Si
	507.1685	24.0	47.3	21.5	n/a	C32 H24 N2 O3 Na
	507.1680	24.5	48.3	18.5	n/a	C28 H22 Li B N2 O5 Na
	507.1676	24.9	49.1	20.5	n/a	C30 H25 B N2 O2 Na Si



Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

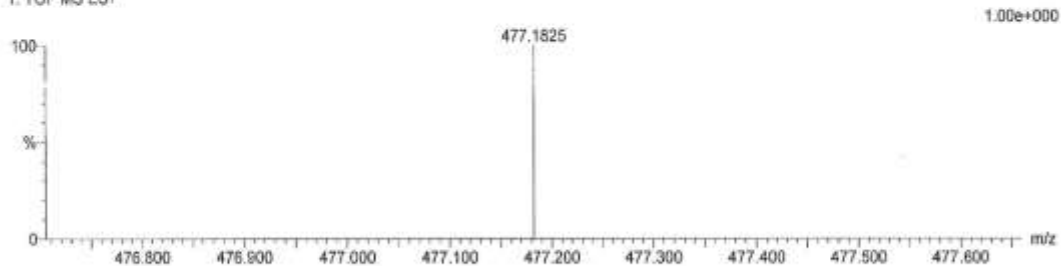
6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

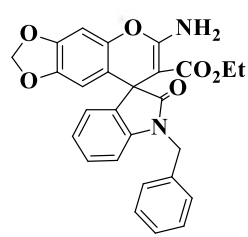
C: 0-31 H: 0-25 N: 0-2 O: 0-4

2NEZ 43 (0.797)

1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
477.1825	477.1814	1.1	2.3	19.5	n/a	C30 H25 N2 O4

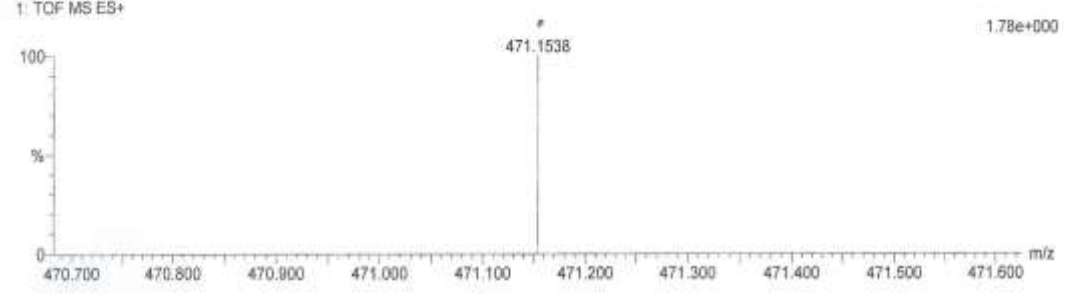


Elemental Composition Report

Single Mass Analysis

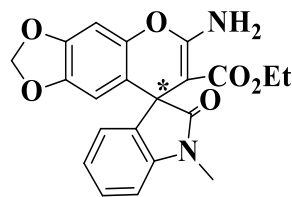
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
 29 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 0-28 H: 0-23 N: 0-2 O: 0-6 Na: 0-1
 S BZ 23 (0.427)
 1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
471.1538	471.1556	-1.8	-3.8	17.5	n/a	C27 H23 N2 O6
	471.1321	21.7	46.1	19.5	n/a	C28 H20 N2 O4 Na

Elemental Composition Report



Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

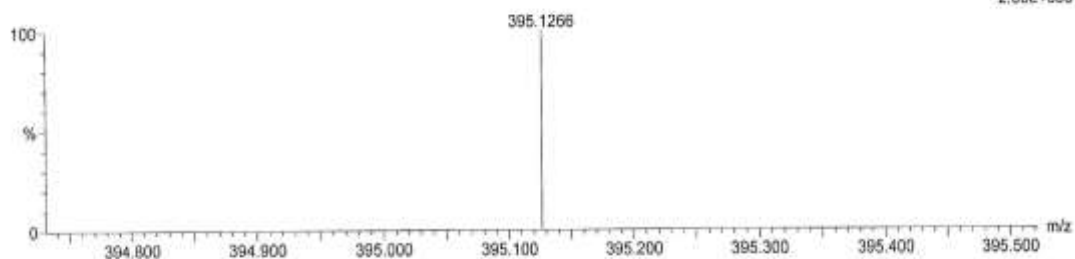
30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-22 H: 0-19 N: 0-2 O: 0-6 Na: 0-1

S ME 44 (0.816)

I: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
395.1266	395.1243	2.3	5.8	13.5	n/a	C21 H19 N2 O6

Elemental Composition Report

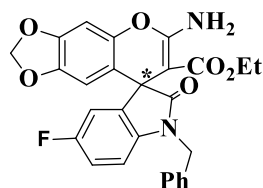
Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Odd and Even Electron Ions

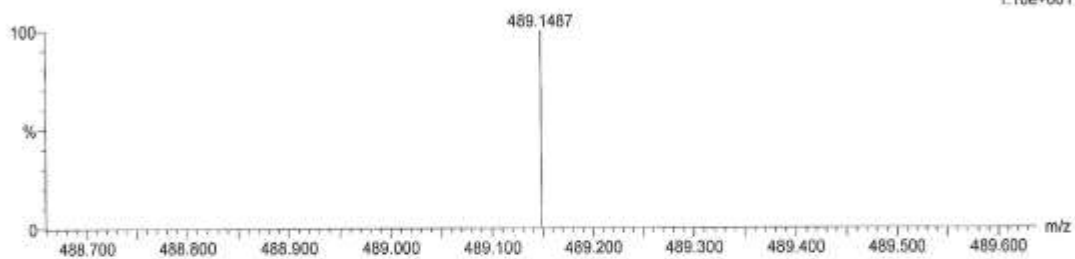
81 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-28 H: 0-22 N: 0-2 O: 0-6 F: 0-1 Br: 0-1

5F S 45 (0.835)

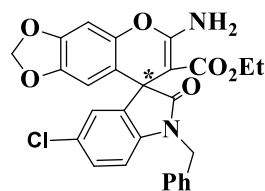
1: TOF MS ES+



Minimum: -1.5
Maximum: 50.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
489.1467	489.1462	2.5	5.1	17.5	n/a	C27 H22 N2 O6 F

Elemental Composition Report



Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

61 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

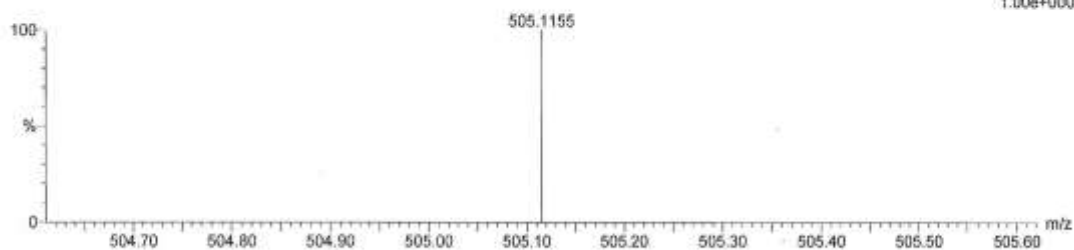
Elements Used:

C: 0-28 H: 0-22 N: 0-2 O: 0-6 Na: 0-1 Cl: 0-1

5CLS

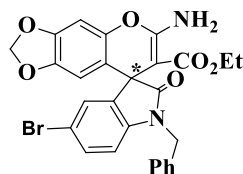
5CLS 31 (0.452)

t: TOF MS ES+
1.00e+000



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
505.1155	505.1166	-1.1	-2.2	17.5	n/a	C27 H22 N2 O6 Cl
	505.1376	-22.1	-43.8	18.5	n/a	C28 H22 N2 O6 Na
	505.0931	22.4	44.3	19.5	n/a	C28 H19 N2 O4 Na Cl

Elemental Composition Report



Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

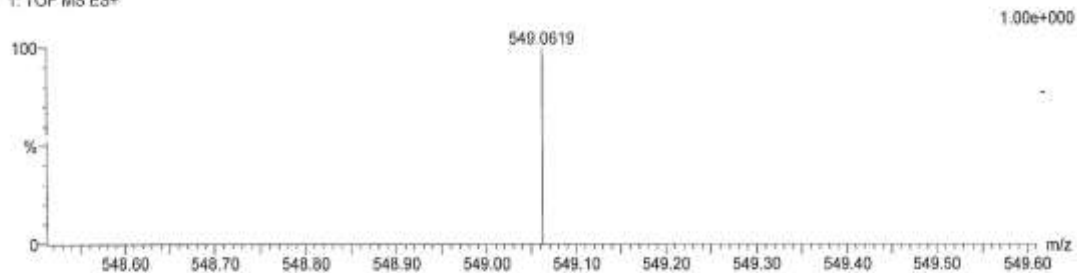
70 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-28 H: 0-22 N: 0-2 O: 0-6 Na: 0-1 Br: 0-1

58R S 13 (0.241)

1: TOF MS ES+

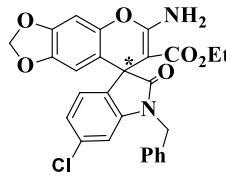


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
549.0619	549.0661	-4.2	-7.6	17.5	n/a	C27 H22 N2 O6 Br
	549.0426	19.3	35.2	19.5	n/a	C28 H19 N2 O4 Na Br

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Odd and Even Electron Ions

61 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

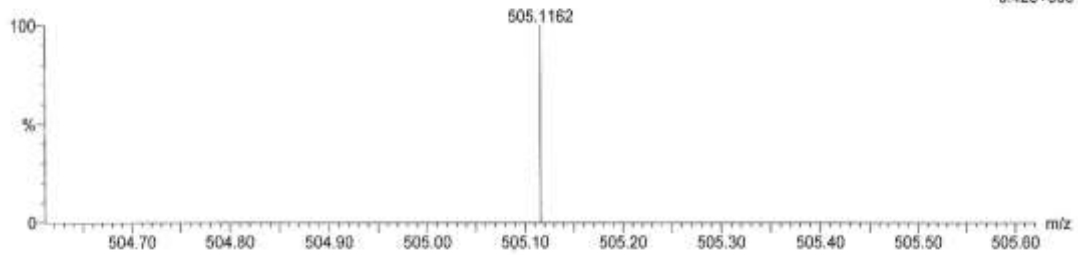
Elements Used:

C: 0-28 H: 0-22 N: 0-2 O: 0-6 Na: 0-1 Cl: 0-1

6CL S 45 (0.834)

1: TOF MS ES+

3.42e+000



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
505.1162	505.1166	-0.4	-0.8	17.5	n/a	C27 H22 N2 O6 Cl
	505.1376	-21.4	-42.4	18.5	n/a	C28 H22 N2 O6 Na
	505.0931	23.1	45.7	19.5	n/a	C28 H19 N2 O4 Na Cl

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

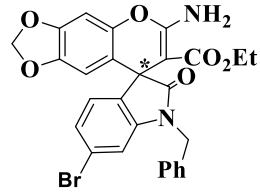
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

70 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

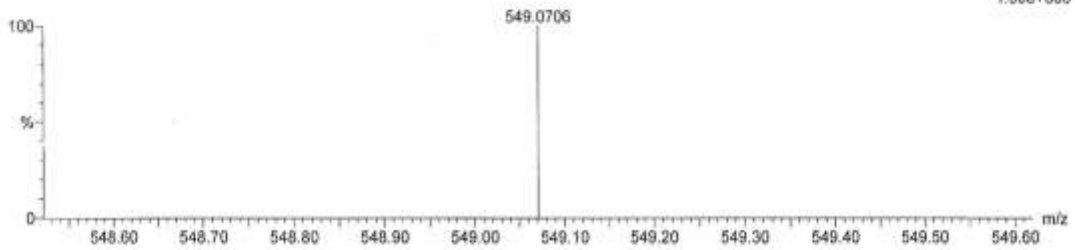
C: 0-26 H: 0-22 N: 0-2 O: 0-6 Na: 0-1 Br: 0-1



Page 1

6BR S 26 (0.482)

1: TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
549.0706	549.0661	4.5	8.2	17.5	n/a	C27 H22 N2 O6 Br

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

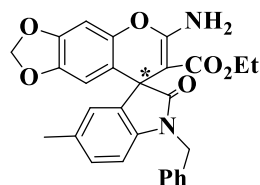
29 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

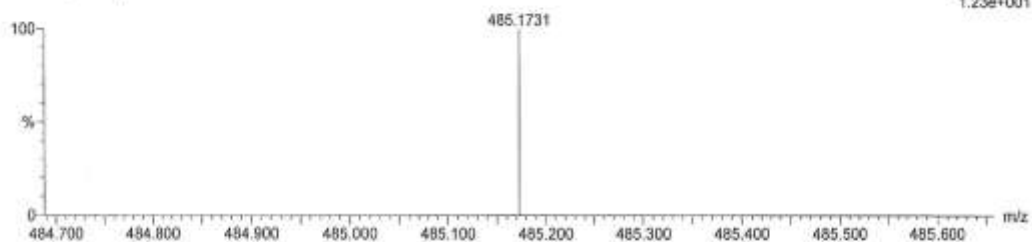
C: 0-29 H: 0-25 N: 0-2 O: 0-6 Na: 0-1

5ME5

5ME5 61 (1.177)



Page 1



Minimum: -1.5

Maximum: 5.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
485.1731	485.1713	1.8	3.7	17.5	n/a	C28 H25 N2 O6