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Supporting information

Asymmetric Transfer Hydrogenation of Seven Membered Tricyclic Ketones: *N*-Substituted dibenzo[*b,e*]azepine-6,11-dione driven by nonclassical CH/O interaction

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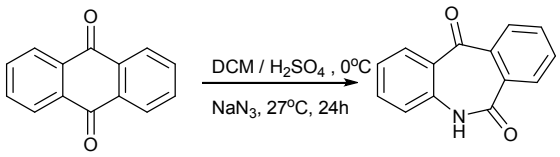
1. General materials and methods

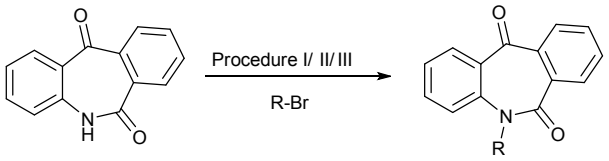
The RuCl(arene)(Ts-DPEN) complexes were commercially purchased from Sigma-Aldrich and used as received. All reactions were carried out under a nitrogen atmosphere, unless otherwise stated, and at the temperature specified in experimental procedures. Yields refer to isolated yields of compounds estimated to be >95 % pure as determined by ^{1}H NMR. All other chemicals and solvents were purchased from different sources and used as received without further purification. Melting points were recorded using Analab melting point apparatus by using open capillary method. ^{1}H NMR and ^{13}C NMR spectra were recorded at 24 °C in $CDCl_3$ & DMSO on 400 MHz, 500 MHz and 101 MHz, 126 MHz instrument respectively with tetramethylsilane (TMS) as internal standard in case of $CDCl_3$. Enantiomeric excess was determined by HPLC analysis, using chiral column described below in detail. Optical rotation was measured by polarimeter. Column chromatography was performed on silica gel (100-200 mesh). Progress of reaction was monitored by TLC analysis. The configuration was determined by X-ray crystallographic analysis.

2. Typical procedure for the preparation of 5*H*-dibenzo[*b,e*]azepine-6,11-dione



Typical procedure for the preparation of 5*H*-dibenzo[*b,e*]azepine-6,11-dione (6). Mixture of Conc. H_2SO_4 (50 mL) and CH_2Cl_2 (16 mL) was taken in round bottom flask and kept in ice to maintain temperature between 0 to 5 °C. Commercially available anthraquinone (10 g, 48 mmol) was introduced to a mixture at once followed by portion wise addition of NaN_3 (3.7 g, 57 mmol) for the period of one hour with vigorous stirring at 0 to 5 °C. After the complete addition, whole mixture was stirred at RT for 12 h. The precipitate was obtained by adding ice water (200 mL) to reaction mixture which was collected by filtration and dried to afford title compound (97% yield).[1]

3. Procedures for the preparation of *N*-substituted 5*H*-dibenzo[*b,e*]azepine-6,11-dione (7a-7l)



Procedure I

Preparation of *N*-substituted 5*H*-dibenzo[*b,e*]azepine-6,11-dione (7d, 7e, 7f, 7g, 7h,). The 5*H*-dibenz[*b,e*]azepine-6,11-dione (1.0 g, 4.48 mmol) was dissolved in DMSO (10 mL) at 10 °C under the N_2. At the same temperature KO*t*Bu (0.9 g, 8.03 mmol) was added and mixture was stirred for 15 min. After the addition of respective alkyl bromide (8 mmol), the mixture was allowed to stirr for 2 h. 1 M HCl (10 mL) and ethyl acetate (10 mL) was added to get biphasic system which was extracted with DCM (2 x 75 mL) . The combined organic phase was washed with H_2O (50 mL), brine (50 mL), dried over $NaSO_4$ and concentrated. The residue was purified by chromatography on silica (EtOAc/pet ether) to afford the title compound (55-80% yield).[2]

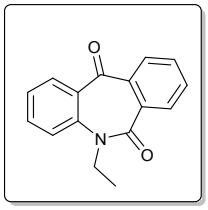
Procedure II

Preparation of *N*-substituted 5*H*-dibenzo[*b,e*]azepine-6,11-dione (7a, 7b, 7c, 7j, 7k, 7l). Solution of 5*H*-dibenz[*b,e*]azepine-6,11-dione (1.0 g, 4.48 mmol) in dry *N,N*-dimethylformamide (10 mL) stirred for 15 minutes under the N_2, sodium hydride (0.25 g, 9 mmol, 60% dispersion in mineral oil) was added in portions and the reaction mixture was stirred for 3 hour. Corresponding alkyl halide (10 mmol) was dissolved in *N,N*-dimethylformamide (5 mL) was slowly added and the mixture was stirred overnight. Ammonium chloride (1.0 g, 20 mmol) was added and stirring was continued for 30 min. The solution was poured onto water (100 mL) and the mixture was extracted with dichloromethane (2 x 75 ml). The combined organic extracts were dried ($NaSO_4$), filtered and the solvent was evaporated in vacuum. The residue was purified by chromatography on silica (EtOAc/pet ether) to afford the title compound of *N*-substituted-5*H*-dibenz[*b,e*]azepine-6,11-dione (78-90% yield).[3]

Procedure III

Preparation of *N*-substituted 5*H*-dibenzo[*b,e*]azepine-6,11-dione (7i). Solution of 5*H*-dibenz[*b,e*]azepine-6,11-dione (1.0 g, 4.48 mmol) in dry *N,N*-dimethylformamide (10 mL) stirred for 15 minutes under the N_2 at 90 °C, sodium hydride (0.25 g, 9 mmol, 60% dispersion in mineral oil) was added in portions and the reaction mixture was stirred for 1 hour at same temperature. The solution was allowed to cool at RT and ethyl bromoacetate (1.67 g, 10 mmol) was added and the mixture was further heated at 90 °C for 2 hours. The solution was poured into water (100 ml) and the mixture was extracted with dichloromethane (2 x 75 mL). The combined organic extracts were dried ($NaSO_4$), filtered and the solvent was evaporated in vacuum. The residue was purified by chromatography on silica (EtOAc/pet ether) to afford the title compound of Ethyl 2-(6,11-dioxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)acetate (65% yield).[4]

5-ethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7a)



Yellow crystalline solid, mp = 93-95 °C (From *n*-hexane/DCM), 85% yield.

MS (EI, 70 eV) *m/z* l;(%): 251(M^+, 100), 222(35.27), 208(57.60), 180(39.11), 77(32.13).

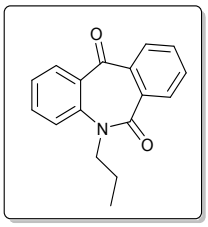
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2920, 1677, 1629, 1590.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.07 (m, 1H), 7.65 – 7.56 (m, 4H), 7.51 (ddt, J = 8.6, 7.3, 1.4 Hz, 1H), 7.41 (dd, J = 8.4, 1.1 Hz, 1H), 7.28 – 7.23 (m, 1H), 4.19 (qd, J = 7.1, 1.1 Hz, 2H), 1.37 (td, J = 7.1, 1.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.44, 166.12, 140.23, 139.38, 137.54, 132.40, 132.34, 132.02, 131.75, 131.70, 128.11, 125.88, 125.73, 122.64, 46.32, 13.80.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 252.1019, found 252.1027.

5-propyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7b)



Pale yellow crystalline solid, mp = 120-125 °C (From *n*-hexane/DCM), 82% yield.

MS (EI, 70 eV) *m/z* (%): 265(M^+ 40.68), 223(94.32), 208(100), 180(32.33), 77(32.13)

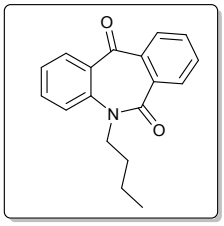
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2972, 1674, 1632, 1593.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (dt, J = 7.0, 1.1 Hz, 1H), 7.67 – 7.54 (m, 4H), 7.51 (ddt, J = 8.5, 7.1, 1.2 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.27 (dd, J = 4.2, 3.3 Hz, 1H), 4.15 – 4.10 (m, 2H), 1.76 – 1.68 (m, 2H), 0.89 (td, J = 7.4, 0.9 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.54, 166.33, 140.32, 139.23, 137.89, 132.41, 132.24, 132.03, 131.78, 131.67, 128.01, 125.85, 125.80, 123.12, 52.24, 21.28, 11.28.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 266.1176, found 266.1175.

5-butyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7c)



Yellow viscous oil, 90% yield.

MS (EI, 70 eV) *m/z* (%): 279(M^+, 43.62), 223(83.04), 208(100), 180(32.34), 77(30.68).

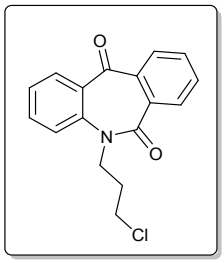
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2962, 1674, 1635, 1593.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (dt, J = 7.9, 1.2 Hz, 1H), 7.66 – 7.55 (m, 4H), 7.51 (ddt, J = 8.5, 7.2, 1.3 Hz, 1H), 7.40 (dt, J = 8.2, 1.0 Hz, 1H), 7.29 – 7.25 (m, 1H), 4.15 (t, J = 7.5 Hz, 2H), 1.72 – 1.65 (m, 2H), 1.32 (hept, J = 7.4, 7.0 Hz, 2H), 0.89 (td, J = 7.3, 1.0 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.52, 166.26, 140.32, 139.27, 137.87, 132.41, 132.25, 132.02, 131.77, 131.68, 128.01, 125.86, 125.79, 123.11, 50.48, 30.06, 20.08, 13.70.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 280.1332, found 280.1337.

5-(3-chloropropyl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7d)[3]



Yellow oil, 80% yield.

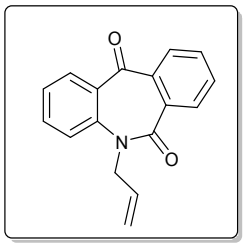
MS (EI, 70 eV) *m/z* (%): 299(M^+, 27.86), 264(52.89), 208(100), 180(32.34), 77(56.60).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2958, 1664, 1615, 1593.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 1H), 7.66 – 7.47 (m, 5H), 7.40 (d, J = 8.2 Hz, 1H), 7.24 (dd, J = 4.6, 3.0 Hz, 1H), 4.28 (td, J = 7.2, 1.6 Hz, 2H), 3.55 (td, J = 6.1, 1.6 Hz, 2H), 2.28 – 2.19 (m, 2H)**.**

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.31, 166.43, 140.27, 139.23, 137.49, 132.48, 132.46, 132.24, 131.72, 131.26, 128.16, 126.02, 125.98, 122.77, 48.75, 42.47, 30.81.

5-allyl-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7e)



Yellow amorphous solid, mp = 88-90 °C (From *n*-hexane/DCM), 77% yield.

MS (EI, 70 eV) *m/z* (%):263(M^+,91.56), 248(100), 206(51.41), 180(29.26), 77(42.68).

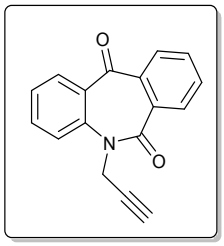
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2923, 1674, 1635, 1590.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.07 (m, 1H), 7.67 – 7.55 (m, 4H), 7.50 – 7.43 (m, 2H), 7.24 (h, J = 1.7 Hz, 1H), 6.16 – 6.05 (m, 1H), 5.33 – 5.26 (m, 2H), 4.66 (dt, J = 5.1, 1.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.33, 166.16, 140.13, 139.89, 136.61, 133.53, 132.46, 132.39, 132.25, 131.89, 131.14, 128.18, 126.06, 125.71, 122.26, 116.98, 54.36.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 264.1019, found 264.1023.

5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7f)[4]



White amorphous solid, mp = 105-107 °C (From *n*-hexane/DCM), 75% yield.

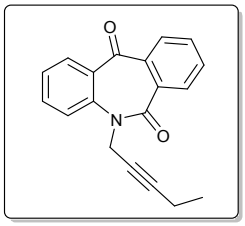
MS (EI, 70 eV) *m/z* (%):261(M^+, 100), 232(37.35), 204(45.54), 180(26.39), 77(28.19).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3256, 2916, 1667, 1639, 1589.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (dt, J = 8.2, 1.3 Hz, 1H), 7.79 (dd, J = 8.2, 1.1 Hz, 1H), 7.70 – 7.54 (m, 5H), 7.30 (td, J = 7.6, 1.2 Hz, 1H), 4.73 (dd, J = 2.5, 1.2 Hz, 2H), 2.45 (dt, J = 3.6, 1.7 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.03, 166.01, 140.13, 139.26, 136.27, 132.64, 132.62, 132.57, 132.24, 130.33, 128.27, 126.48, 126.08, 121.74, 79.45, 72.85, 41.20.

5-(pent-2-yn-1-yl)-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7g)



White amorphous solid, mp = 125-127 °C (From *n*-hexane/DCM), 73% yield.

MS (EI, 70 eV) *m/z* (%): 289(M^+, 22.26), 274(100), 260(45.47), 180(21.06), 77(13.36).

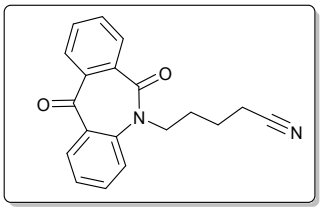
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2920, 1667, 1635, 1593.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.05 (m, 1H), 7.64 – 7.44 (m, 5H), 7.35 (d, J = 8.2 Hz, 1H), 7.24 (t, J = 3.6 Hz, 1H), 4.07 (d, J = 6.9 Hz, 2H), 1.04 (t, J = 8.0 Hz, 3H), 0.84 (q, J = 13.3, 11.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.62, 166.43, 140.43, 139.26, 138.36, 132.42, 132.10, 132.04, 131.81, 131.61, 127.80, 125.87, 125.84, 123.83, 55.61, 35.93, 30.63, 26.25, 25.55.

HRMS Calculated for $C_{18}H_{19}NO_2$ $[M+H]^+$ 290.1176, found 290.1179.

5-(6,11-dioxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (7h)



Colourless viscous oil, 55% yield.

MS (EI, 70 eV) *m/z* (%): 304(M^+, 13.43), 223(62.83), 208(100), 180(42.20), 77(34.67).

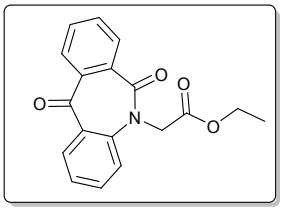
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2911, 2239, 1671, 1625, 1591.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.99 – 7.95 (m, 1H), 7.88 (dt, J = 7.9, 1.5 Hz, 1H), 7.76 – 7.66 (m, 2H), 7.57 (ddt, J = 8.7, 7.2, 1.6 Hz, 1H), 7.42 (dd, J = 8.1, 1.3 Hz, 1H), 7.32 – 7.27 (m, 1H), 4.50 (td, J = 6.2, 1.3 Hz, 2H), 2.49 (td, J = 7.0, 1.3 Hz, 2H), 2.09 – 2.01 (m, 2H), 1.96 – 1.89 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 193.24, 160.87, 143.16, 141.40, 133.39, 132.98, 132.29, 132.20, 128.58, 128.38, 128.32, 127.32, 125.42, 119.44, 65.17, 29.70, 27.75, 22.61, 17.10.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 305.1285, found 305.1286

Ethyl 2-(6,11-dioxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)acetate (7i)[5]



Pale yellow crystalline solid, mp = 113-115 °C (From *n*-hexane/DCM), 65% yield.

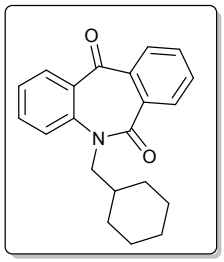
MS (EI, 70 eV) *m/z* (%):309(M^+, 26.85), 235(69.03), 208(100), 180(24.96), 77(25.50).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2930, 1730, 1674, 1639, 1597.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (ddd, J = 6.9, 1.9, 0.8 Hz, 1H), 7.69 – 7.57 (m, 4H), 7.52 – 7.47 (m, 1H), 7.35 – 7.26 (m, 2H), 4.66 – 4.63 (m, 2H), 4.30 (qd, J = 7.1, 1.0 Hz, 2H), 1.32 (td, J = 7.1, 1.0 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.06, 168.95, 166.53, 140.30, 139.50, 136.70, 132.61, 132.59, 132.50, 132.01, 130.28, 128.18, 126.38, 126.10, 122.32, 61.74, 53.78, 14.15.

5-(cyclohexylmethyl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7j)



White crystalline solid, mp = 138-140 °C (From *n*-hexane/DCM), 78% yield.

MS (EI, 70 eV) *m/z* (%):319(M^+, 5.78), 236(39.57), 223(100), 207(52.78), 77(14.12).

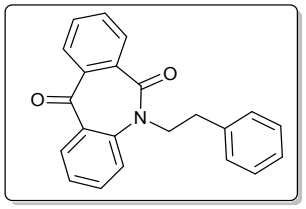
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2919, 2849, 1678, 1625, 1593.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (dd, J = 7.8, 1.7 Hz, 1H), 7.64 – 7.47 (m, 5H), 7.37 (dd, J = 8.2, 1.2 Hz, 1H), 7.29 – 7.25 (m, 1H), 4.09 (d, J = 7.0 Hz, 2H), 1.69 – 1.58 (m, 6H), 1.11 – 1.04 (m, 3H), 0.91 – 0.82 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.63, 166.45, 140.46, 139.29, 138.39, 132.43, 132.11, 132.05, 131.83, 131.64, 127.82, 125.88, 125.86, 123.85, 55.63, 35.96, 30.66, 26.28, 25.57.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 320.1645, found 320.1650.

5-phenethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7k)gbf



Yellow amorphous solid, mp = 100-102 °C (From *n*-hexane/DCM), 82% yield.

MS (EI, 70 eV) *m/z* (%):327(M^+, 1.64), 236(50.06), 223(100), 208(81.01), 77(28.53).

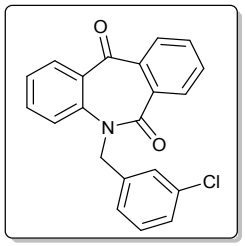
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2958, 1677, 1635, 1597.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 7.6 Hz, 1H), 7.64 – 7.45 (m, 5H), 7.36 (d, J = 8.2 Hz, 1H), 7.27 – 7.11 (m, 6H), 4.41 – 4.36 (m, 2H), 3.01 (t, J = 7.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.98, 166.33, 140.19, 139.20, 138.10, 137.76, 132.41, 132.29, 132.10, 131.71, 131.46, 128.69, 128.60, 128.13, 126.56, 125.99, 125.84, 122.93, 52.16, 34.14.

HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 328.1332, found 328.1336.

5-(3-chlorobenzyl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7l)



White amorphous solid, mp = 155-157 °C (From *n*-hexane/DCM), 85% yield.

MS (EI, 70 eV) *m/z* (%):347(M^+, 100), 318(26.49), 209(45.36), 180(20.80), 77(19.45).

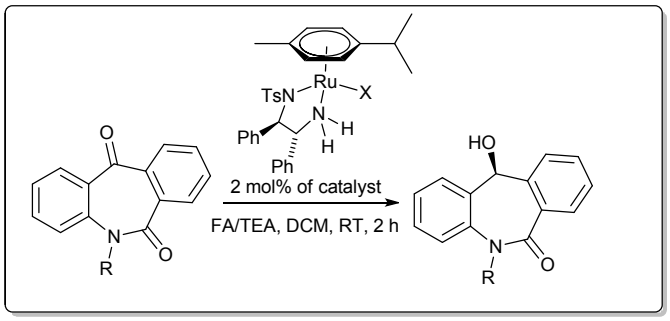
IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2920, 1674, 1642, 1597.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 – 8.14 (m, 1H), 7.73 – 7.58 (m, 4H), 7.43 (ddt, J = 8.3, 7.2, 1.4 Hz, 1H), 7.31 – 7.23 (m, 5H), 7.16 (dq, J = 7.5, 1.4 Hz, 1H), 5.28 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.11, 166.69, 140.21, 139.57, 139.22, 136.76, 134.72, 132.57, 132.56, 132.52, 132.03, 130.89, 130.11, 128.42, 127.56, 126.84, 126.22, 126.03, 124.66, 122.22, 54.68.

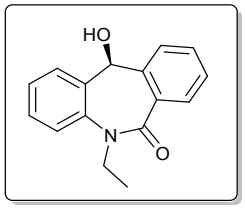
HRMS Calculated for $C_{18}H_{17}NO_4$ $[M+H]^+$ 348.0786, found 348.0789.

4. General procedure for Ruthenium catalyzed asymmetric transfer hydrogenation (8a-8l)



The *N*-substituted dibenzo [*b,e*] azepin-6-11-dione (0.5 mmol), catalyst (5 mg, 7.9 x 10^{-3} mmol), DCM (5 mL) and FA/TEA (5:2, 420 mg) azeotrope was added sequentially to the reaction tube and stirred at 27 °C. Reaction was monitored by TLC. After the completion of reaction it was quenched by water (20 mL) and extracted with ethyl acetate (2 x 20 mL). Organic layer was dried with Na_2SO_4 and concentrated to get residue. The residue was purified with a silica gel column eluted with pet ether and ethyl acetate to get pure desired product (yield 80-99%).

(S)-5-ethyl-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8a)



White crystalline solid, mp = 185-187 °C (From *n*-hexane/DCM), 98% yield, 97% ee, $[\alpha]_D^{25}$ = -213 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):253(M^+, 56.70), 224(100), 208(21.00), 165(23.16), 77(19.45).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3260 (broad), 2965, 1611, 1590, 1060.

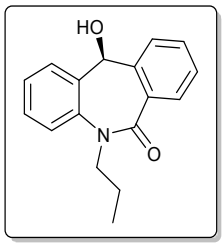
^{1}H NMR (400 MHz, DMSO) δ 7.56 – 7.48 (m, 3H), 7.44 – 7.36 (m, 2H), 7.25 – 7.14 (m, 3H), 6.39 (d, J = 4.2 Hz, 1H), 5.75 (d, J = 4.0 Hz, 1H), 4.46 (dq, J = 14.2, 7.1 Hz, 1H), 3.77 (dq, J = 13.9, 7.0 Hz, 1H), 1.15 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.07, 146.89, 142.68, 137.12, 131.42, 130.17, 129.86, 127.58, 127.13, 126.04, 123.45, 122.48, 120.75, 67.22, 43.85, 14.18.

HPLC (OD-H elute: Hexanes/*i*-PrOH = 97/03, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 66.5 min (major), t_2 = 80.9 min (minor).

HRMS Calculated for $C_{16}H_{15}NO_2$ $[M+H]^+$ 254.1176, found 254.1174.

(S)-11-hydroxy-5-propyl-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8b)



White crystalline solid, mp = 173-175 °C (From *n*-hexane/DCM), 97% yield, 96% ee, $[\alpha]_D^{25}$ = -180 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):267(M^+, 54.89), 236(53.98), 220(100), 165(35.51), 77(20.55).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3348(broad), 2963, 1611, 1593, 1064.

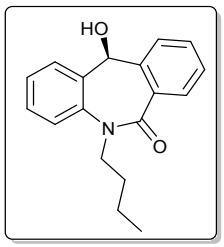
^{1}H NMR (400 MHz, DMSO) δ 7.56 – 7.49 (m, 3H), 7.44 – 7.36 (m, 2H), 7.25 – 7.13 (m, 3H), 6.41 (d, J = 4.4 Hz, 1H), 5.76 (d, J = 4.3 Hz, 1H), 4.53 – 4.43 (m, 1H), 3.66 (ddd, J = 13.6, 8.1, 5.5 Hz, 1H), 1.59 – 1.44 (m, 2H), 0.82 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 167.32, 146.89, 142.61, 137.13, 131.44, 130.19, 129.94, 127.54, 127.13, 126.01, 123.56, 122.52, 120.75, 67.29, 50.04, 21.53, 11.88.

HPLC (OD-H elute: Hexanes/*i*-PrOH = 92/08, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 14.4 min (major), t_2 = 20.0 min (minor).

HRMS Calculated for $C_{17}H_{17}NO_2$ $[M+H]^+$ 268.1332, found 268.1331

(S)-5-butyl-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8c)



White crystalline solid, mp = 143-145 °C (From *n*-hexane/DCM), 98% yield, 96% ee, $[\alpha]_D^{25}$ = -120 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):281(M^+, 52.40), 238(58.94), 220(100), 165(35.51), 77(20.55).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3372(broad), 2951, 1607, 1593, 1065.

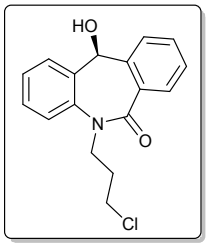
^{1}H NMR (400 MHz, DMSO) δ 7.55 – 7.50 (m, 3H), 7.45 – 7.36 (m, 2H), 7.25 – 7.14 (m, 3H), 6.41 (d, J = 4.3 Hz, 1H), 5.75 (d, J = 4.3 Hz, 1H), 4.55 (dt, J = 13.6, 7.6 Hz, 1H), 3.72 – 3.63 (m, 1H), 1.50 (dtd, J = 15.0, 7.5, 1.5 Hz, 2H), 1.24 (dt, J = 14.9, 7.5 Hz, 2H), 0.82 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 167.26, 146.88, 142.66, 137.12, 131.43, 130.18, 129.92, 127.55, 127.13, 126.02, 123.56, 122.51, 120.75, 67.28, 47.94, 30.38, 20.13, 14.05.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 99/01, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 55.5 min (minor), t_2 = 60.1 min (major).

HRMS Calculated for $C_{18}H_{19}NO_2$ $[M+H]^+$ 282.1489, found 282.1487

(S)-5-(3-chloropropyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8d).



White crystalline solid, mp = 175-177 °C (From *n*-hexane/DCM), 98% yield, 99% ee, $[\alpha]_D^{25}$ = -176 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):301(M^+, 15.56), 265(54.98), 224(100), 165(25.71), 77(29.80).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3407(broad), 2965, 1611, 1593, 1060.

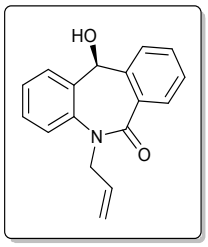
^{1}H NMR (400 MHz, DMSO) δ 7.58 – 7.50 (m, 3H), 7.46 – 7.37 (m, 2H), 7.25 – 7.14 (m, 3H), 6.41 (d, J = 4.3 Hz, 1H), 5.77 (s, 1H), 4.67 – 4.56 (m, 1H), 3.88 – 3.79 (m, 1H), 3.62 (td, J = 6.4, 3.5 Hz, 2H), 2.02 (qd, J = 8.1, 6.3 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ 167.40, 146.90, 142.54, 137.05, 131.60, 130.00, 129.92, 127.64, 127.16, 126.19, 123.47, 122.60, 120.83, 67.27, 46.24, 43.41, 31.33.

HPLC (OD-H elute: Hexanes/*i*-PrOH = 92/08, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 24.9 min (major), t_2 = 40.7 min (minor).

HRMS Calculated for $C_{17}H_{16}ClNO_2$ $[M+H]^+$ 309.0942, found 309.0944.

(S)-5-allyl-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8e)



White crystalline solid, mp = 184-186 °C (From *n*-hexane/DCM), > 99% yield, 97% ee, $[\alpha]_D^{25}$ = -205 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):265(M^+, 40.99), 250(11.11), 224(100), 165(18.92), 77(22.74).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3340(broad), 3063, 1611, 1590, 1565.

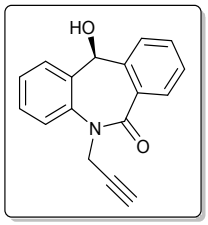
^{1}H NMR (400 MHz, DMSO) δ 7.57 – 7.50 (m, 3H), 7.43 (td, *J* = 7.6, 1.4 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.26 – 7.13 (m, 3H), 6.40 (d, *J* = 4.3 Hz, 1H), 5.95 – 5.86 (m, 1H), 5.78 (d, *J* = 4.3 Hz, 1H), 5.21 – 5.10 (m, 2H), 4.85 (ddt, *J* = 15.7, 5.2, 1.6 Hz, 1H), 4.53 (ddt, *J* = 15.6, 6.2, 1.4 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 167.25, 146.87, 142.05, 137.40, 134.58, 131.62, 129.99, 129.85, 127.45, 127.16, 125.99, 123.10, 122.50, 120.85, 117.79, 67.24, 51.58.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 97/03, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 69.8 min (minor), t_2 = 73.8 min (major).

HRMS Calculated for $C_{17}H_{15}NO_2$ $[M+H]^+$ 266.1176, found 266.1181.

(S)-11-hydroxy-5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8f)



White crystalline solid, mp = 170-172 °C (From *n*-hexane/DCM), > 99% yield, 97% ee, $[\alpha]_D^{25}$ = -176 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):263(M^+, 20.05), 246(49.33), 224(100), 165(18.85), 77(13.39).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3308(broad),, 3238, 2958, 1635,1593, 1316.

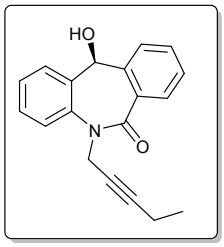
^{1}H NMR (400 MHz, DMSO) δ 7.60 – 7.50 (m, 4H), 7.46 (td, J = 7.6, 1.4 Hz, 1H), 7.29 – 7.18 (m, 3H), 6.47 (d, J = 4.4 Hz, 1H), 5.80 (d, J = 4.3 Hz, 1H), 4.89 (dd, J = 17.6, 2.5 Hz, 1H), 4.75 (dd, J = 17.6, 2.5 Hz, 1H), 3.23 (t, J = 2.4 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 167.02, 146.99, 141.93, 137.01, 132.01, 130.17, 129.14, 127.60, 127.29, 126.39, 122.68, 122.60, 121.05, 80.73, 74.95, 67.11, 38.52.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 32.2 min (minor), t_2 = 36.3 min (major).

HRMS Calculated for $C_{17}H_{13}NO_2$ $[M+H]^+$ 264.1019, found 2641022.

(S)-11-hydroxy-5-(pent-2-yn-1-yl)-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8g)



White crystalline solid, mp = 133-137 °C (From *n*-hexane/DCM), > 99% yield, > 99% ee, $[\alpha]_D^{25}$ = -205 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):291(M^+, 32.34), 262(11.48), 224(100), 165(21.96), 77(11.50).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3319(broad), 2920, 1618, 1593, 1060.

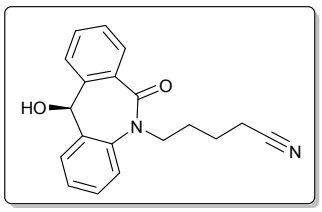
^{1}H NMR (400 MHz, DMSO) δ 7.59 – 7.50 (m, 4H), 7.45 (td, J = 7.6, 1.4 Hz, 1H), 7.27 – 7.16 (m, 3H), 6.42 (d, J = 4.4 Hz, 1H), 5.78 (d, J = 4.2 Hz, 1H), 4.82 (dt, J = 17.3, 2.2 Hz, 1H), 4.71 (dt, J = 17.3, 2.2 Hz, 1H), 2.11 (qt, J = 7.5, 2.1 Hz, 2H), 0.97 (t, J = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 166.99, 147.02, 141.98, 137.21, 131.87, 130.10, 129.35, 127.47, 127.22, 126.26, 122.82, 122.49, 120.99, 85.52, 76.31, 67.15, 39.01, 14.10, 12.09.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 16.1 min (minor), t_2 = 20.4 min (major).

HRMS Calculated for $C_{19}H_{17}NO_2$ $[M+H]^+$ 292.1332, found 292.1330.

(S)-5-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (8h)



Colourless semi-solid, 80% yield, 43% ee, $[\alpha]_D^{25}$ = -55 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):306(M^+, 9.43), 225(100), 208(32.45), 165(11.16), 77(24.56).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3342(broad), 2958, 2242, 1625,1590, 1056.

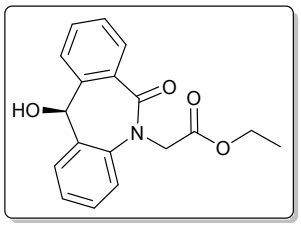
^{1}H NMR (400 MHz, DMSO) δ 7.66 – 7.48 (m, 4H), 7.32 (d, J = 7.6 Hz, 1H), 7.17 – 7.02 (m, 3H), 6.30 (s, 1H), 5.19 (s, 1H), 4.52 – 4.42 (m, 1H), 4.34 (s, 1H), 2.57 (t, J = 7.0 Hz, 2H), 1.92 – 1.84 (m, 2H), 1.79 – 1.70 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 159.75, 146.50, 141.33, 136.53, 136.53, 131.95, 127.36, 127.11, 125.18, 124.81, 122.47, 121.77, 121.08, 67.83, 65.18, 55.33, 27.82, 22.33, 16.50.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 90.2 min (major), t_2 = 111.8 min (minor).

HRMS Calculated for $C_{19}H_{18}N_2O_2$ $[M+H]^+$ 307.1441, found 307.1442.

(S)-ethyl 2-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)acetate (8i)



White crystalline solid, mp = 131-133 °C (From *n*-hexane/DCM), 96% yield, 96% ee, $[\alpha]_D^{25}$ = -160 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):311(M^+, 31.27), 238(80.00), 220(100), 165(36.99), 77(1374).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3340(broad), 2986, 1744, 1618, 1592, 1207, 1063.

^{1}H NMR (400 MHz, DMSO) δ 7.60 – 7.51 (m, 3H), 7.46 (td, J = 7.6, 1.4 Hz, 1H), 7.31 –

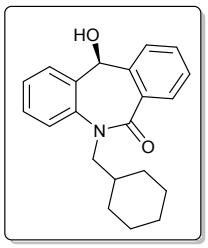
7.17 (m, 4H), 6.43 (dd, J = 4.5, 1.5 Hz, 1H), 6.04 (d, J = 4.4 Hz, 1H), 4.82 (d, J = 17.1 Hz, 1H), 4.65 (d, J = 17.1 Hz, 1H), 4.12 (qd, J = 7.1, 2.6 Hz, 2H), 1.18 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 169.37, 167.73, 147.30, 141.84, 137.71, 131.98, 129.89, 129.13, 127.62, 127.21, 126.26, 123.00, 122.49, 121.08, 67.01, 61.26, 52.41, 14.47.

HPLC (OD-H elute: Hexanes/*i*-PrOH = 95/05, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 26.3 min (major), t_2 = 34.3 min (minor).

HRMS Calculated for $C_{18}H_{17}NaNO_4$ $[M+Na]^+$ 334.1050, found 334.1047.

(S)-5-(cyclohexylmethyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8j)



White crystalline solid, mp = 178-180 °C (From *n*-hexane/DCM), 85% yield, 95% ee, $[\alpha]_D^{25}$ = -114 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):321(M^+, 32.26), 238(100), 220(91.28), 208(43.02), 165(27.48).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3340(broad), 2923, 2850, 1607, 1593, 1064.

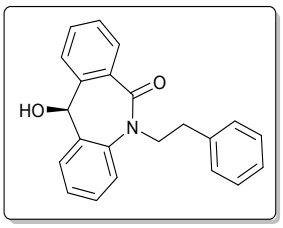
^{1}H NMR (400 MHz, DMSO) δ 7.55 – 7.50 (m, 3H), 7.44 – 7.38 (m, 2H), 7.25 – 7.12 (m, 3H), 6.44 (d, J = 4.4 Hz, 1H), 5.79 (d, J = 4.4 Hz, 1H), 4.54 (dd, J = 13.7, 7.7 Hz, 1H), 3.51 (dd, J = 13.7, 6.0 Hz, 1H), 1.66 – 1.49 (m, 6H), 1.07 (d, J = 8.8 Hz, 3H), 0.89 (dd, J = 25.7, 11.5 Hz, 2H).

^{13}C NMR (101 MHz, dmso) δ 167.48, 146.85, 142.35, 137.47, 131.47, 130.18, 130.03, 127.52, 127.12, 125.89, 123.53, 122.60, 120.76, 67.37, 55.34, 53.99, 36.66, 31.09, 30.89, 26.32, 25.67.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 99/01, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 40.9 min (minor), t_2 = 46.6 min (major).

HRMS Calculated for $C_{21}H_{23}NO_2$ $[M+H]^+$ 322.1802, found 322.1797.

(S)-11-hydroxy-5-phenethyl-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8k)



White crystalline solid, mp = 183-185 °C (From *n*-hexane/DCM), 88% yield, 96% ee, $[\alpha]_D^{25}$ = -161 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):329(M^+, 10.03), 238(100), 208(40.54), 165(37.28), 77(17.05).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3316(broad), 2923, 1607, 1593, 1063.

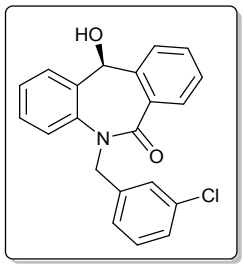
^{1}H NMR (400 MHz, DMSO) δ 7.55 – 7.39 (m, 5H), 7.27 – 7.11 (m, 8H), 6.28 (d, J = 4.2 Hz, 1H), 5.47 (d, J = 4.2 Hz, 1H), 4.77 (dt, J = 13.5, 8.0 Hz, 1H), 3.97 (ddd, J = 13.7, 8.3, 5.5 Hz, 1H), 2.92 – 2.80 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 167.35, 147.01, 142.60, 139.05, 136.86, 131.50, 130.00, 129.98, 128.98, 128.83, 127.57, 127.09, 126.77, 126.09, 123.44, 122.55, 120.79, 67.13, 49.57, 34.07.

HPLC (OD-H elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 15.9 min (major), t_2 = 34.8 min (minor).

HRMS Calculated for $C_{22}H_{19}NO_2$ $[M+H]^+$ 330.1489, found 330.1381.

(S)-5-(3-chlorobenzyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8l)



White crystalline solid, mp = 190-194 °C (From *n*-hexane/DCM), 89% yield, 99% ee, $[\alpha]_D^{25}$ = -251 (c = 0.1 in $CHCl_3$).

MS (EI, 70 eV) *m/z* (%):349(M^+, 100), 224(57.68), 208(34.34), 165(33.83), 77(15.35).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3337(broad), 2923, 1611, 1595, 1067.

^{1}H NMR (400 MHz, DMSO) δ 7.59 (dd, J = 7.7, 1.3 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.34 (ddd, J = 9.5, 7.8, 6.4 Hz, 3H), 7.28 – 7.21 (m, 3H), 7.13 (qd, J = 7.2, 1.8 Hz, 2H), 6.41 (d, J = 4.3 Hz, 1H), 5.74 (d, J = 4.4 Hz, 1H), 5.55 (d, J = 15.6 Hz, 1H), 5.09 (d, J = 15.5 Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 167.83, 146.95, 141.92, 140.93, 137.00, 133.47, 131.84, 130.84, 130.09, 129.54, 127.90, 127.57, 127.57, 127.28, 126.49, 126.19, 123.05, 122.65, 120.92, 67.22, 51.39.

HPLC (OJ-H elute: Hexanes/*i*-PrOH = 96/04, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 90.1 min (minor), t_2 = 95.9 min (major).

HRMS Calculated for $C_{21}H_{16}ClNO_2$ $[M+H]^+$ 350.0942, found 350.0944.

5. DFT Calculation Method and Cartesian Coordinates for transition states Ts-Si and Ts-Re

The ORCA 3.0.3 program[6] was used for all calculations. The co-ordinates for transition states were referred to from Ikariya et. al.[7] and the transition state geometry was modified for our substrate based on these co-ordinates. These geometries were used as input for subsequent optimizations. All the geometries i.e. A, and TSs Si and Re were optimized at the PBE-D3[8] level of density functional theory using the Effective Core Potential for LANL2DZ[9] basis set for Ru and 6-31G* for rest of the atoms. Cartesian Coordinates for transition states Ts-Si and Ts-Re is given in supporting information.

Cartesian Coordinates for transition states Ts-Si and Ts-Re

Ts-Re

N	-0.618451	1.602236	1.482959
H	-0.916155	2.108569	2.329585
H	-1.349742	1.974788	0.566148
C	1.223293	0.997454	0.039273
H	0.651709	1.296934	-0.860698
C	0.803042	1.916739	1.202698
H	1.399841	1.604596	2.081641
C	-1.918140	-2.466753	1.817312
C	-2.893432	-1.478295	2.212467
C	-0.628484	-2.476163	2.398721
C	-1.197608	-0.480663	3.723572
C	-0.218245	-1.466748	3.346451
C	1.210295	-1.463045	3.863100
H	1.856671	-1.533095	2.968676
N	0.834561	-0.370389	0.479315
S	1.240232	-1.592475	-0.592122
O	1.238924	-1.086375	-1.992165
O	0.436922	-2.793675	-0.239889
C	2.705763	1.173471	-0.234149
C	3.137837	1.660939	-1.477186
C	3.659193	0.900449	0.764227
C	4.501648	1.881683	-1.717393
H	2.395121	1.854340	-2.258125
C	5.020245	1.118868	0.527346
H	3.328453	0.485794	1.721920
C	5.445252	1.614073	-0.715539
H	4.827890	2.262028	-2.690581
H	5.752832	0.890779	1.308229
H	6.510139	1.786052	-0.903282
C	1.079750	3.386170	0.949269
C	2.159964	4.003769	1.605343
C	0.310523	4.138761	0.041220
C	2.476012	5.345668	1.357404
H	2.771295	3.417266	2.300162
H	3.324574	5.808892	1.870640
H	0.015689	6.059390	-0.905760
H	1.950925	7.138697	0.255009
C	1.706845	6.090002	0.451659
C	-2.522551	-0.504382	3.184543
Ru	-0.939188	-0.432040	1.576712
H	-1.801293	0.103137	-0.239087
C	2.948937	-2.060697	-0.237874
C	3.960137	-1.723058	-1.143618
C	3.247646	-2.776798	0.929726
C	5.284807	-2.067152	-0.851114
C	4.576027	-3.106967	1.213472
C	5.618305	-2.745408	0.335639
C	-2.306505	0.941758	-0.947775
O	-2.112800	2.166962	-0.409372
C	7.055597	-3.061198	0.671846
H	7.513860	-2.243160	1.259091
H	7.137964	-3.980951	1.274743
H	7.664727	-3.189514	-0.237738
H	6.077681	-1.789188	-1.553594
H	3.702807	-1.177022	-2.053294
H	2.442976	-3.094855	1.596553
H	4.811218	-3.665458	2.126719
H	-0.906638	0.338361	4.387150
H	0.114762	-3.166516	1.997293
C	-3.775929	0.550456	-1.040062
C	-4.757540	1.500770	-0.715302
C	-4.165686	-0.732089	-1.469689
C	-6.116735	1.188959	-0.831770
H	-4.414018	2.481510	-0.377104
C	-5.536525	-1.045960	-1.563764
C	-3.217516	-1.871298	-1.684016
C	-3.217516	-1.871298	-1.684016
C	-6.509117	-0.088513	-1.265594

C	0.623243	5.483057	-0.200236
H	-0.540308	3.668418	-0.461723
H	-7.570420	-0.339634	-1.360227
C	1.456969	-2.711333	4.735151
H	2.513230	-2.754801	5.049728
H	1.225459	-3.641087	4.188183
H	0.829590	-2.689005	5.642789
C	1.596469	-0.185041	4.616086
H	2.667401	-0.211222	4.874910
H	1.031996	-0.081470	5.559478
H	1.418917	0.713856	4.002326
C	-4.291285	-1.517914	1.667174
H	-4.683532	-0.509097	1.464937
H	-4.944690	-1.989502	2.425647
H	-4.344146	-2.119307	0.748862
C	-1.673494	0.757912	-2.331149
C	-1.632411	-0.476948	-3.023770
C	-1.051817	-0.518284	-4.309939
C	-0.520962	0.627574	-4.903752
C	-0.568686	1.852466	-4.224183
C	-1.150795	1.903217	-2.955046
N	-2.076972	-1.699988	-2.447033
H	-1.016579	-1.465533	-4.851080
H	-0.077768	0.560040	-5.901456
H	-0.165459	2.761274	-4.681041
H	-1.214223	2.841543	-2.399648
C	-1.346582	-2.948647	-2.776240
O	-3.511223	-2.995865	-1.226027
H	-3.231563	0.287873	3.442140
H	-2.155007	-3.146124	0.994088
H	-0.338284	-2.649421	-3.090836
H	-1.239148	-3.506123	-1.836384
C	-2.062181	-3.804879	-3.823603
H	-1.467197	-4.711535	-4.025388
H	-2.203407	-3.268336	-4.776488
H	-3.048062	-4.117599	-3.449066
H	-6.872332	1.941538	-0.583391
H	-5.816261	-2.061430	-1.856736

Ts-Si

N	-0.632423	1.743823	1.427723
H	-0.882497	2.215578	2.307945
H	-1.307406	2.130148	0.663701
C	1.184762	1.052448	-0.037412
H	0.636037	1.378685	-0.940995
C	0.798467	1.999306	1.121694
H	1.374144	1.668937	2.006225
C	-2.257905	-2.172206	1.754152
C	-3.024411	-1.079158	2.309247
C	-0.926069	-2.412703	2.165140
C	-1.015698	-0.462127	3.646890
C	-0.260785	-1.553954	3.118230
C	1.207410	-1.783986	3.426160
H	1.714215	-1.811979	2.443425
N	0.758566	-0.305530	0.392053
S	1.031834	-1.500880	-0.769192
O	1.259810	-0.880826	-2.098989
O	0.004147	-2.559090	-0.581520
C	2.675278	1.172172	-0.301765
C	3.135989	1.670955	-1.530814
C	3.609970	0.824396	0.689807
C	4.509477	1.829701	-1.761734
H	2.406980	1.912314	-2.310589
C	4.982323	0.988614	0.465142
H	3.255375	0.393827	1.632181
C	5.435954	1.494226	-0.762759
H	4.857822	2.213882	-2.725667
H	5.699333	0.705114	1.242237
H	6.508629	1.619550	-0.943457
C	1.109331	3.461101	0.853980
C	2.329123	4.002056	1.301877
C	0.218644	4.286237	0.141042
C	2.661948	5.335342	1.032386
H	3.032861	3.362260	1.843865
C	0.549832	5.623243	-0.120146
H	3.617902	5.736815	1.382452
H	-0.154980	6.254385	-0.671187
H	2.028769	7.194247	0.109325
C	-2.382964	-0.242207	3.261731
Ru	-1.056985	-0.299215	1.453567
H	-1.808906	0.217579	-0.175016
C	2.593489	-2.300074	-0.320669
C	3.792608	-1.869376	-0.900964
C	2.590325	-3.376620	0.579720
C	4.993347	-2.492005	-0.538114
C	3.797092	-3.985299	0.937195
C	5.021195	-3.544553	0.394477
C	-2.428805	1.127206	-0.978911
O	-2.376041	2.294291	-0.383418
C	6.324022	-4.185738	0.807486
H	6.665834	-3.800446	1.785571
H	6.222384	-5.279742	0.909363
H	7.122853	-3.980870	0.075950
H	5.929719	-2.148572	-0.990273
H	3.781656	-1.055817	-1.630073
H	1.641650	-3.755458	0.965330
H	3.788537	-4.830427	1.635441
H	-0.531928	0.254465	4.316410
H	-0.353990	-3.181326	1.644978
C	-3.821276	0.521692	-1.090933
C	-4.885584	1.362143	-0.718305
C	-4.102475	-0.789111	-1.552437
C	-6.215838	0.939689	-0.764525
H	-4.610350	2.362203	-0.374496
C	-5.454948	-1.209487	-1.586845
N	-3.100531	-1.729430	-1.906548
C	-6.496266	-0.363208	-1.197611
H	-7.022267	1.616707	-0.467598
H	-5.694033	-2.213118	-1.940883
H	-7.528246	-0.725083	-1.249482

H	-0.738905	3.886202	-0.204779
C	1.771804	6.151417	0.319258
C	1.408696	-3.149776	4.111450
H	2.484974	-3.355703	4.236893

H	0.974829	-3.971899	3.517759
H	0.933941	-3.165250	5.107645
C	1.856696	-0.662891	4.244298
H	2.933128	-0.867102	4.366927
H	1.417079	-0.581987	5.254396
H	1.756010	0.314010	3.741073
C	-4.463656	-0.864433	1.941864
H	-4.733038	0.202208	1.963742
H	-5.109029	-1.399014	2.662856
H	-4.689438	-1.248325	0.937921
C	-1.662282	1.034179	-2.299736
C	-1.552843	-0.124208	-3.099879
C	-0.849952	-0.053086	-4.321459
C	-0.286183	1.139933	-4.769832
C	-0.406653	2.295360	-3.982506
C	-1.087110	2.233320	-2.764387
C	-1.997052	-1.507168	-2.744693
H	-0.736964	-0.979869	-4.888151
H	0.248807	1.168359	-5.723611
H	0.023531	3.244944	-4.317458
H	-1.206938	3.120574	-2.141338
O	-1.406845	-2.482588	-3.224622
C	-3.339001	-3.160975	-1.615201
H	-2.359575	-3.566684	-1.315336
H	-4.018425	-3.195085	-0.747073
C	-3.894695	-4.000938	-2.772533
H	-4.044150	-5.038557	-2.428122
H	-3.174036	-4.006698	-3.601827
H	-4.860004	-3.624570	-3.147920
H	-2.917988	0.633712	3.642597
H	-2.691019	-2.786399	0.963158

6. Determination of absolute configuration

Determination of the absolute configuration of compound 8d (CCDC 1444009)

To determine the absolute configuration of the *N*-Substituted dibenzo [*b,e*] azepin-6-11-dione products, a single crystal of the **8d** was grown from its solution in dichloromethane and hexane, which is suitable for X-ray diffraction analysis. The structure in Figure 1 showed the absolute configuration of **8d** is ***S.***

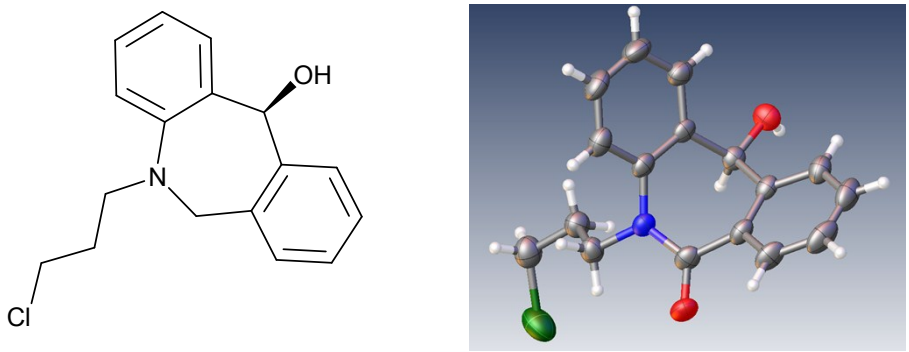


Figure 1. X-ray crystallographic analysis of (***S***) **8d**

Table 1 Crystal data and structure refinement for **(*S*)-8d**

Identification code	**8d**	
Bond precision: C-C	0.0061 Å	
Moiety formula	C17 H16 Cl N O2	
Sum formula	C17 H16 Cl N O2	
Formula weight	301.76	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Crystal description	Needle	
Crystal colour	Colorless	
Space group	P 21 21 21	
Hall group	P 2ac 2ab	
Cell	a=8.1449(2) Å	alpha = 90°
	b=10.8999(4) Å	beta = 90°
	c=16.4545(6) Å	gamma = 90°
Volume	1460.82(8) $Å^3$	

Z	4
Density (Calculated)	1.372 Mg/m^3
Absorption coefficient	2.344 mm^{-1}
F (000)	632.0
Theta range for data collection	4.867 to 72.871 deg
Limiting indices	-9<=h<=9, -11<=k<=13, -19<=l<=18
Reflection collected	2749
Independent reflections	2829 [R(int) = 0.0644]
Completeness to theta = 67.684deg	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.862 and 0.522
Refinement method	'SHELXL-2014/7 (Sheldrick 2014'
Data / restraints / parameters	2829/0/192
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0619
R indices (all data)	R1 = 0.0500
Absolute structure parameter	-0.03(3)
Extinction coefficient	0.0138(11)
Largest diff. peak and hole	0.173 and -0.195 e.$Å^{-3}$

7. References

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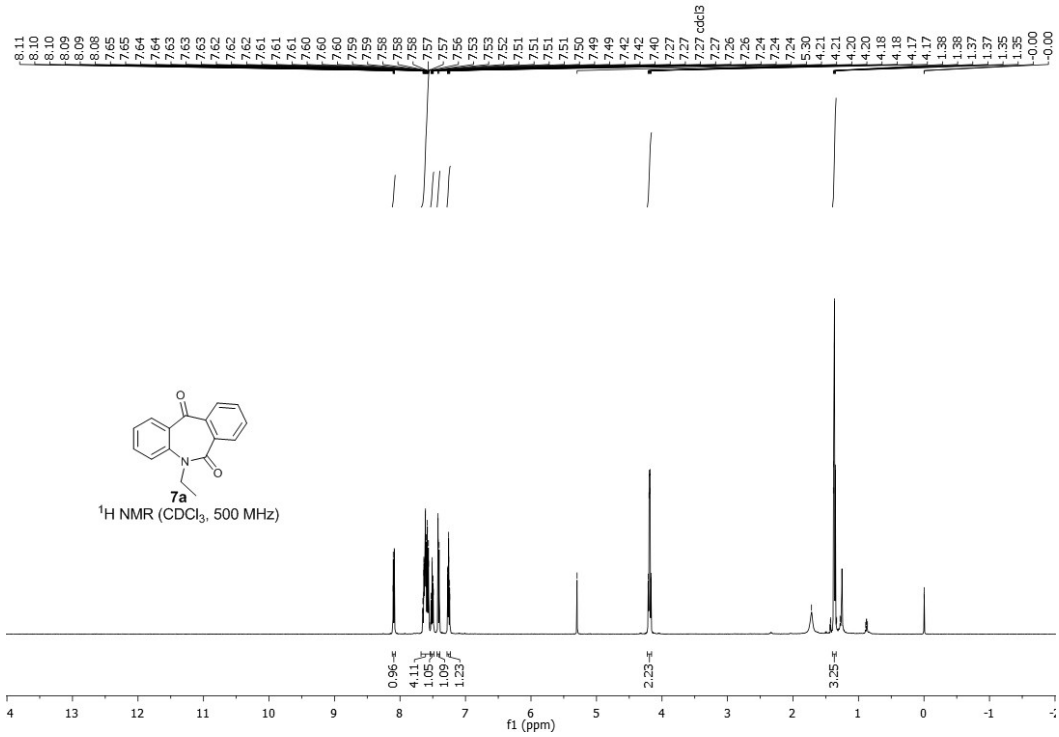
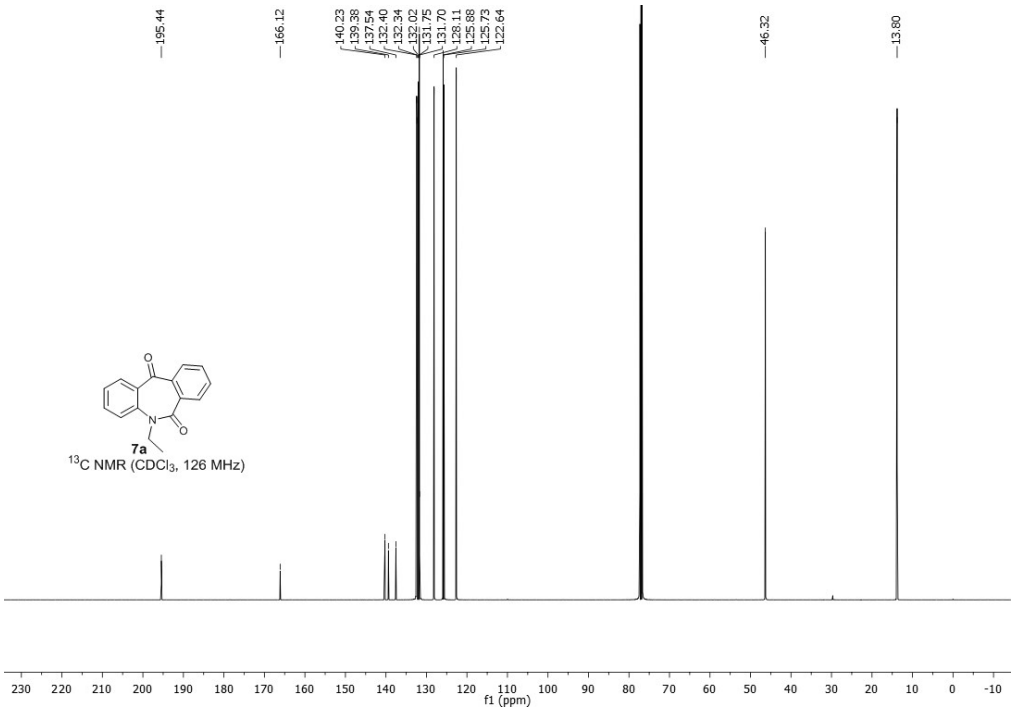
8. Copy of NMR, HRMS and HPLC for Chiral and Racemic compounds

5-ethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7a) (^{1}H NMR).



5-ethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7a) (^{13}C NMR).



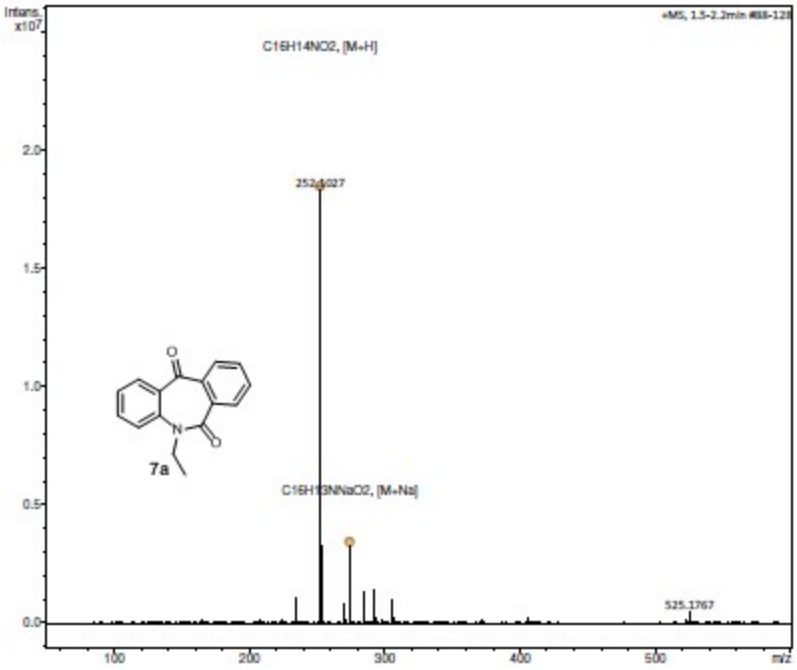
5-ethyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7a) (HRMS)

Analysis Info

Analysis Name	D:\Data\Installation_2014-06-19\ICT\BhanageBM1_RC1_01_2216.d	Acquisition Date	2/27/2016 1:47:51 PM
Method	dic-ms600mz_10min.m	Operator	CIF
Sample Name	1	Instrument	impact HD 1819696.00184
Comment			

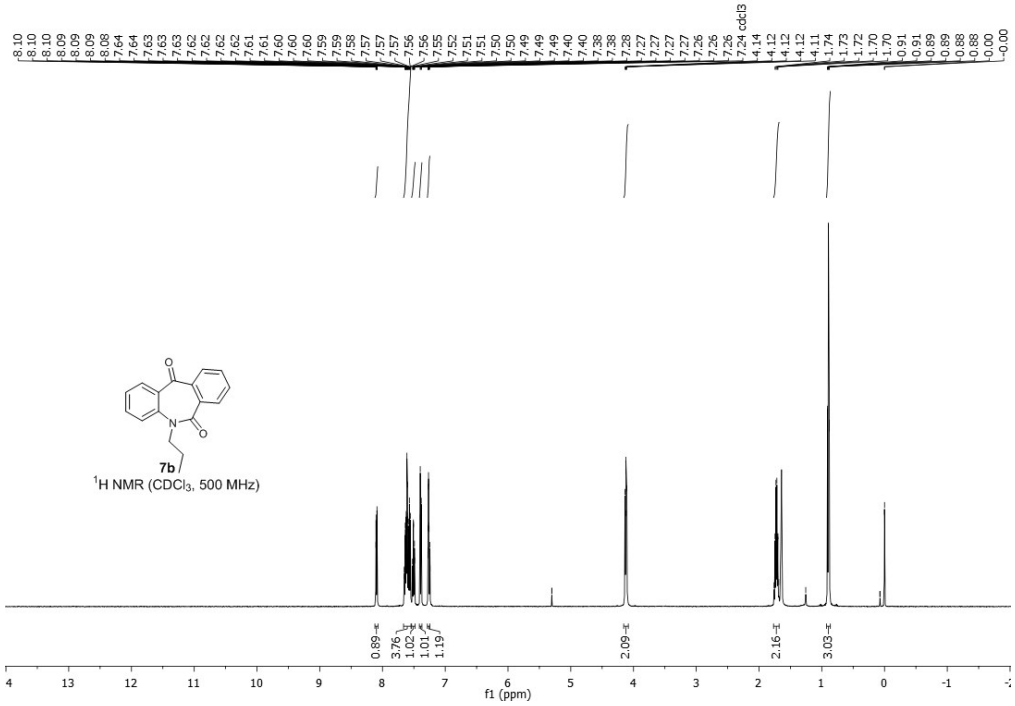
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

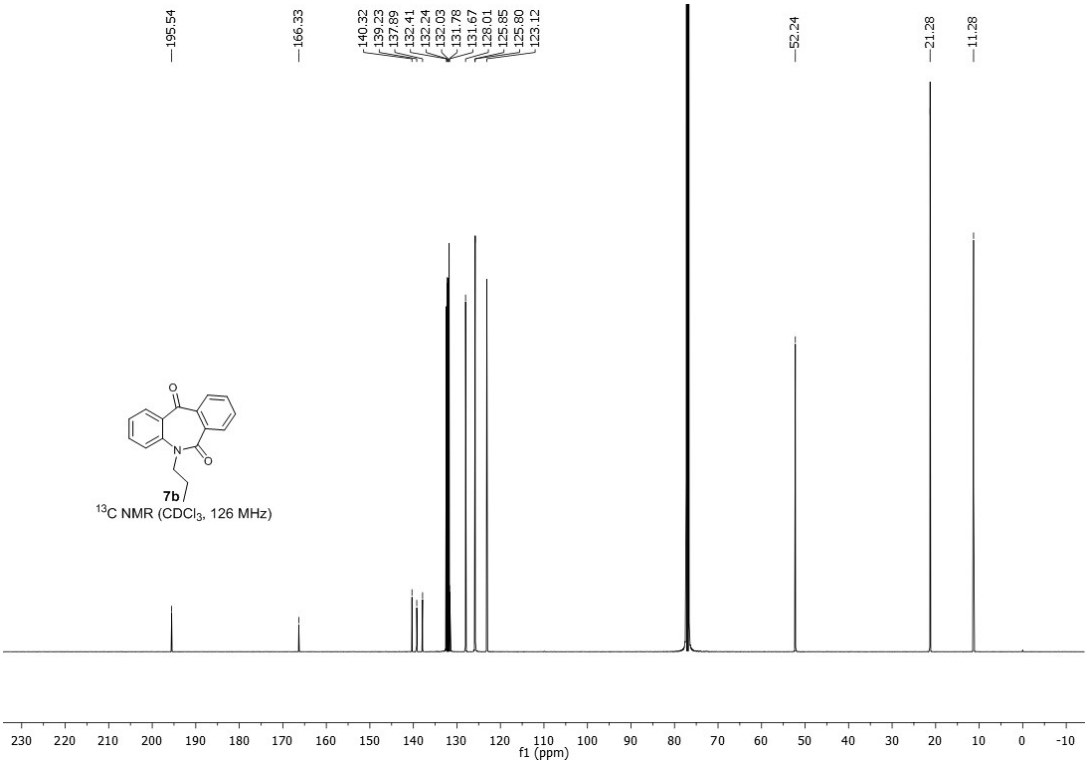


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
252.1027	1	C16H14NO2	252.1019	-3.3	2.5	1	100.00	10.5	even	ok	M+H
274.0846	1	C16H13NNaO2	274.0838	-2.6	12.9	1	100.00	10.5	even	ok	M+Na

5-propyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7b) (^{1}H NMR).



5-propyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7b) (^{13}C NMR).



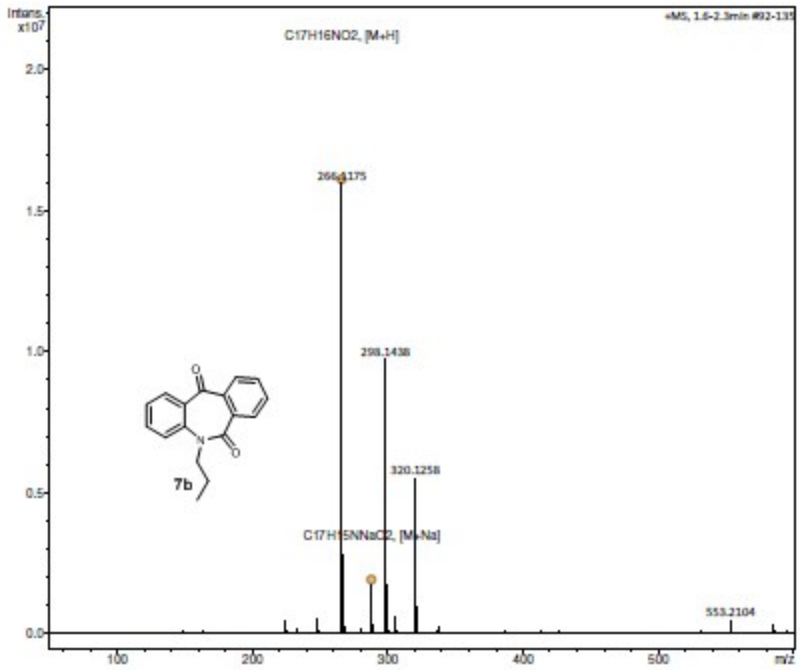
5-propyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7b) (HRMS)

Analysis Info

Analysis Name	D:\Data\Installation_2014-06-19\CT\BhanageBM2_RC2_01_2218.d	Acquisition Date	2/27/2016 3:46:24 PM
Method	dic-ms600mz_10min.m	Operator	CIF
Sample Name	2	Instrument	impact HD 1819696.00184
Comment			

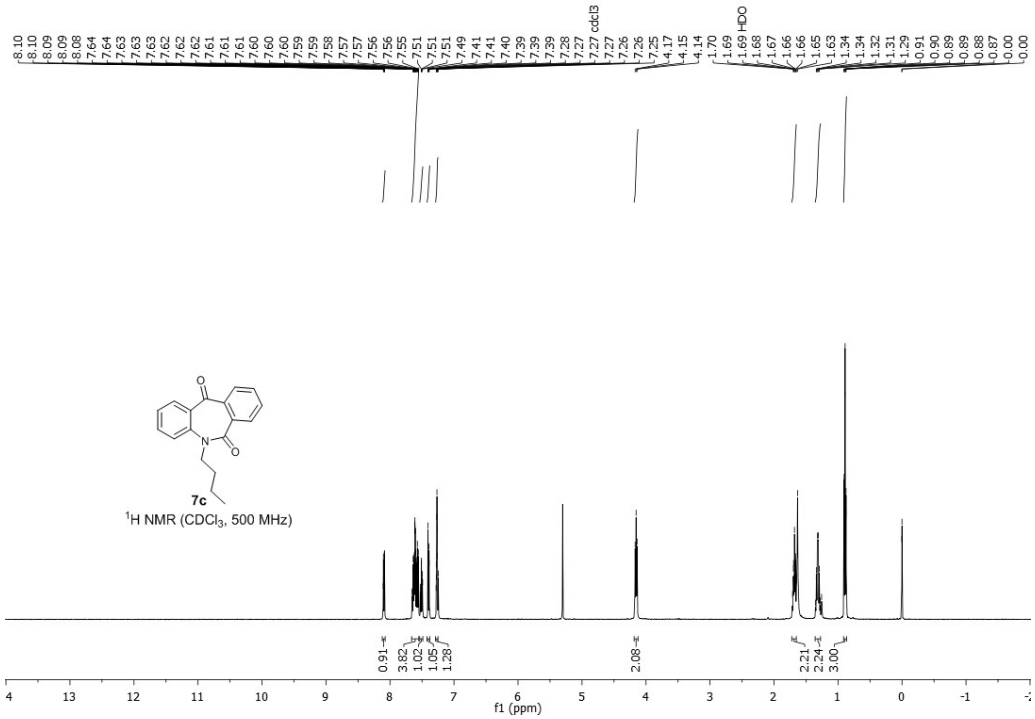
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

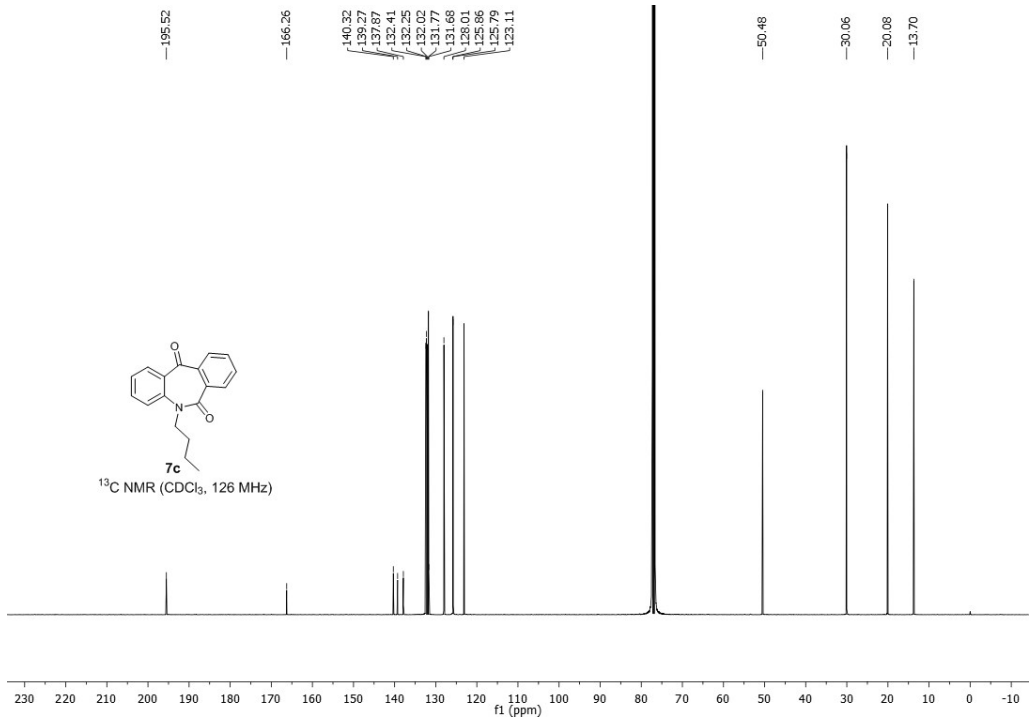


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
266.1175	1	C17H16NO2	266.1176	0.3	9.9	1	100.00	10.5	even	ok	M+H
288.0994	1	C17H15NNaO2	288.0995	0.4	10.2	1	100.00	10.5	even	ok	M+Na

5-butyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7c) (^{1}H NMR).



5-butyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7c) (^{13}C NMR).



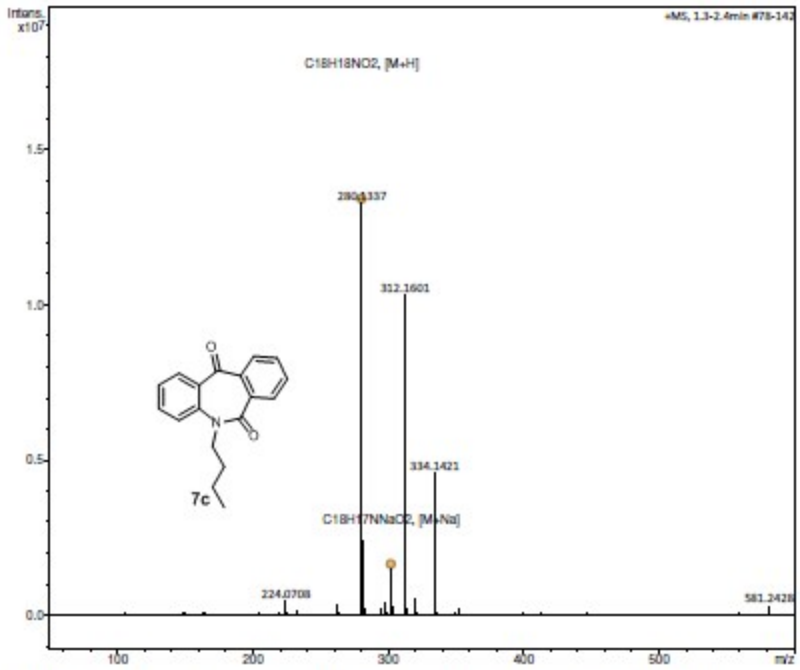
5-butyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7c) (HRMS)

Analysis Info

Analysis Name	D:\Data\Installation_2014-06-19\ICT\BhanagoBM3_RC3_01_2220.d	Acquisition Date	2/27/2016 4:20:45 PM
Method	dlc-ms600mz_10min.m	Operator	CIF
Sample Name	3	Instrument	impact HD 1819696.00184
Comment			

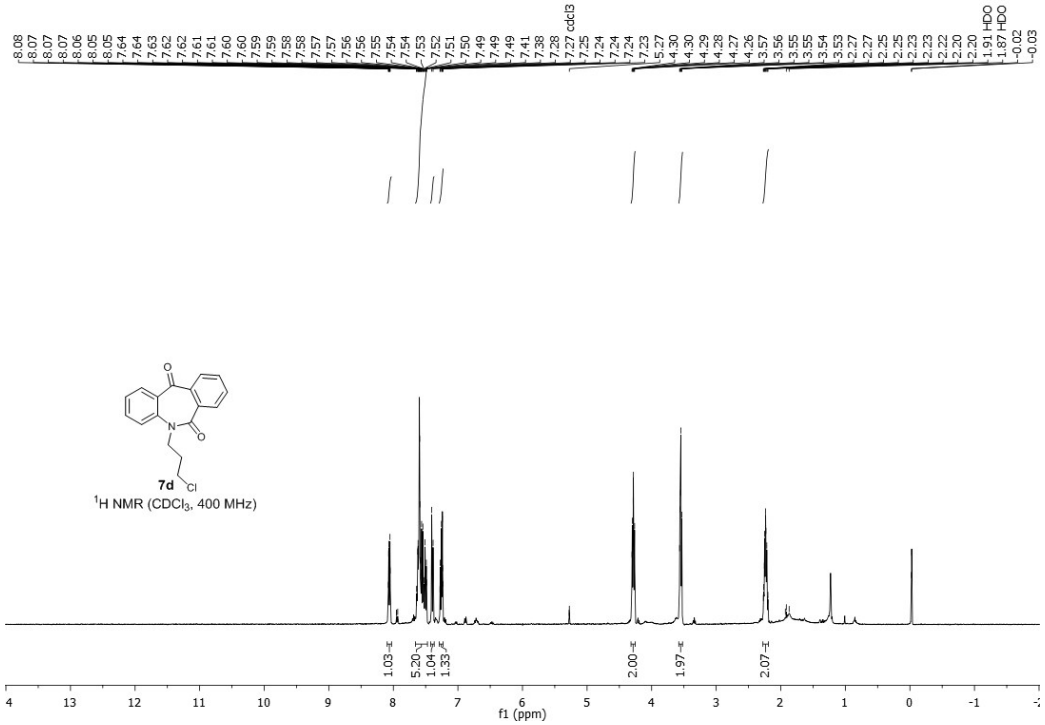
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

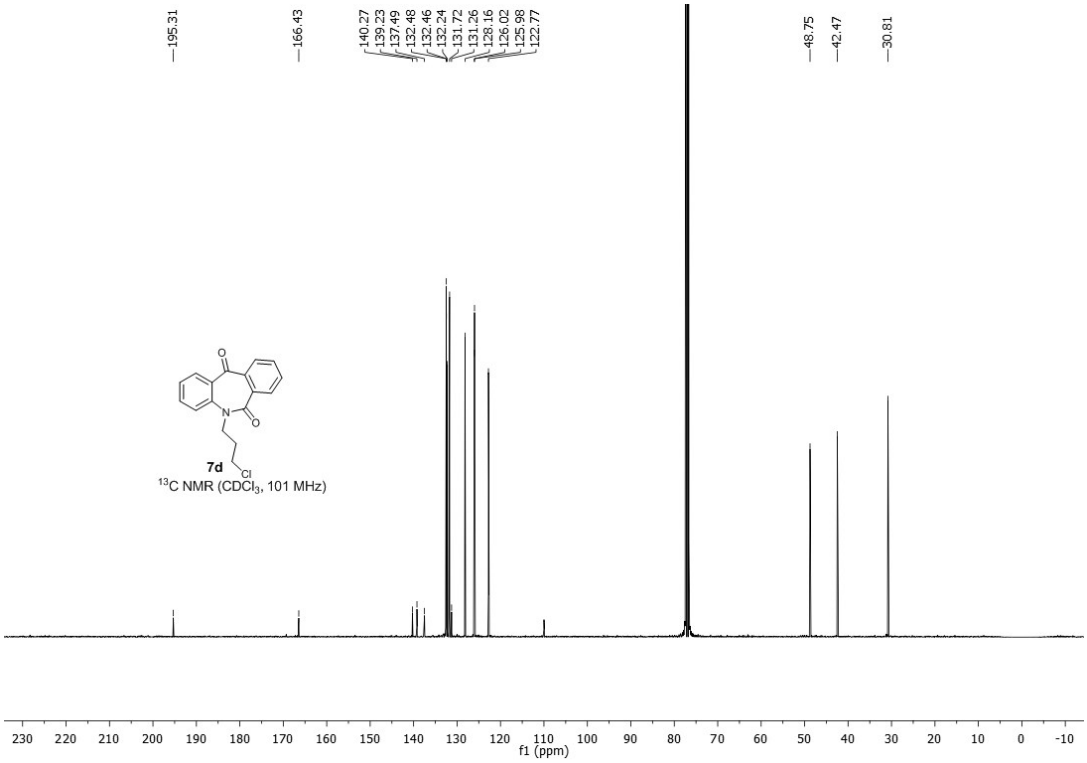


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	Adduct
280.1337	1	C18H18NO2	280.1332	-1.8	12.2	1	100.00	10.5	even	M+H
302.1158	1	C18H17NNaO2	302.1151	-2.0	11.0	1	100.00	10.5	even	M+Na

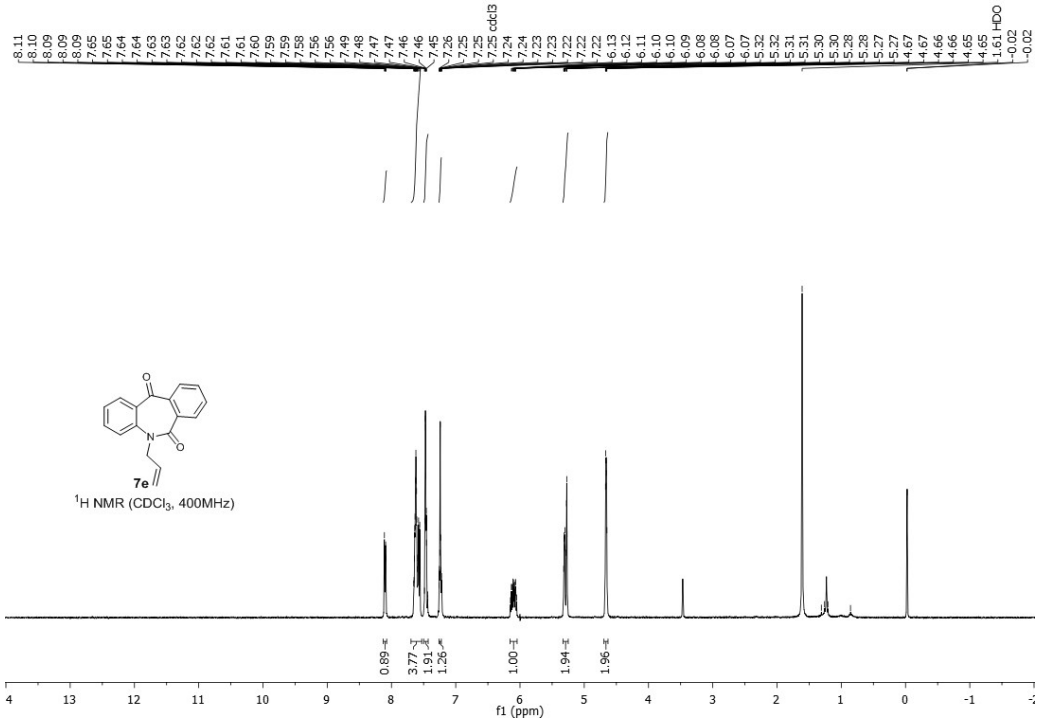
5-(3-chloropropyl)-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7d) (^{1}H NMR).



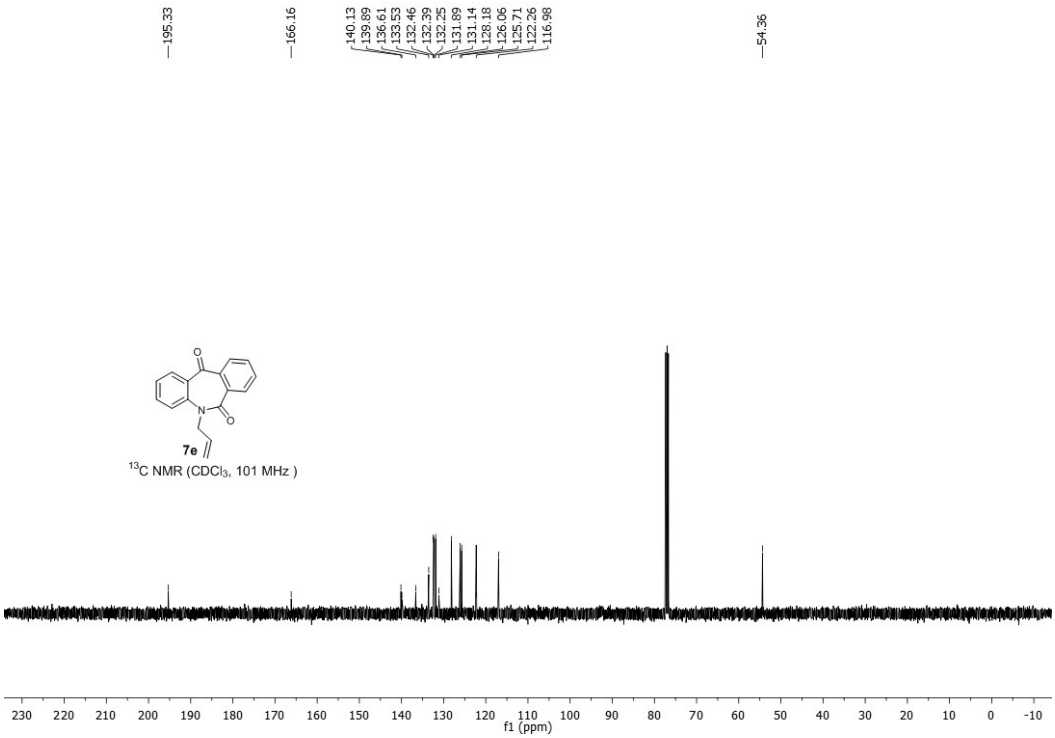
5-(3-chloropropyl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7d) (^{13}C NMR).



5-allyl-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7e) (^{1}H NMR).



5-allyl-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7e) (^{13}C NMR).



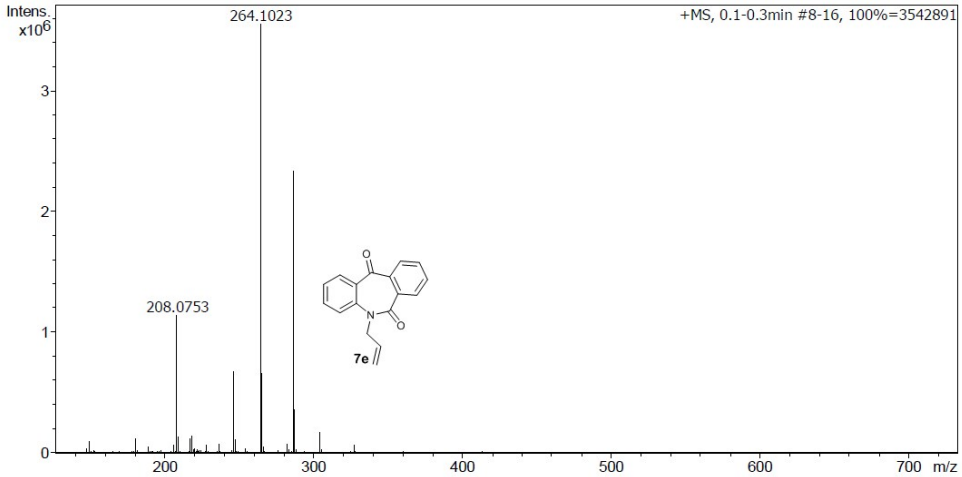
5-allyl-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7e) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-15.d	Acquisition Date	9/3/2015 11:20:24 AM
Method	Tune_pos_NAICSI-1000.m	Operator	MR OUT
Sample Name	EXT-ICT-BMB-VKV-15	Instrument	maXis impact 282001.00081
Comment	C17H13NO2		

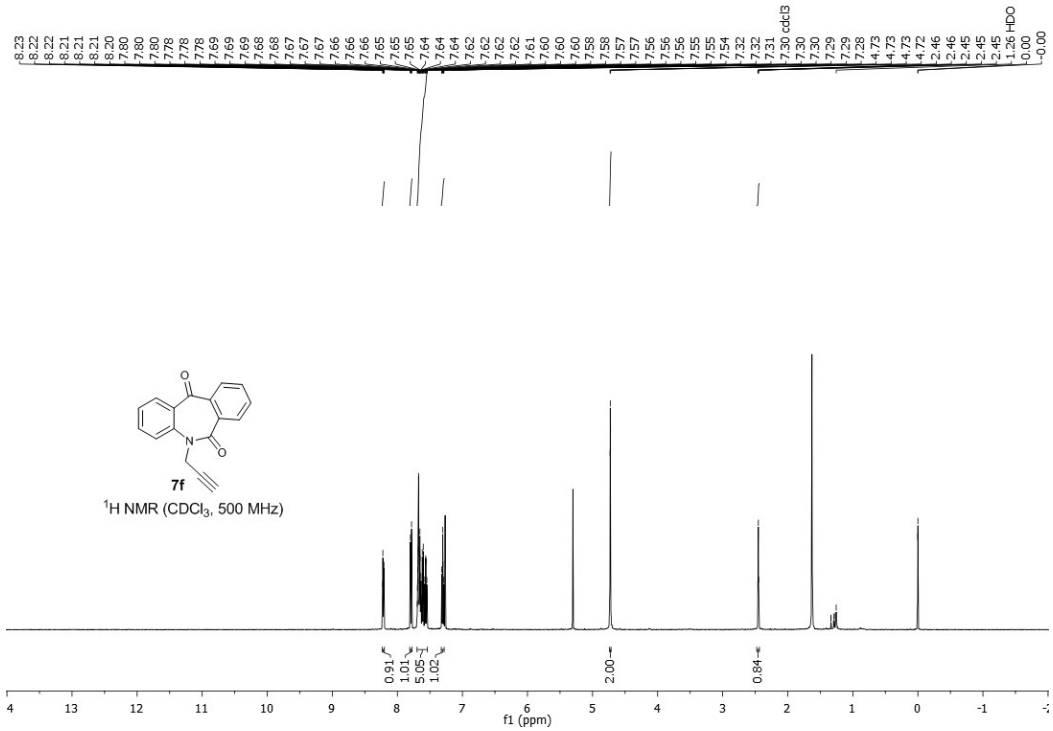
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

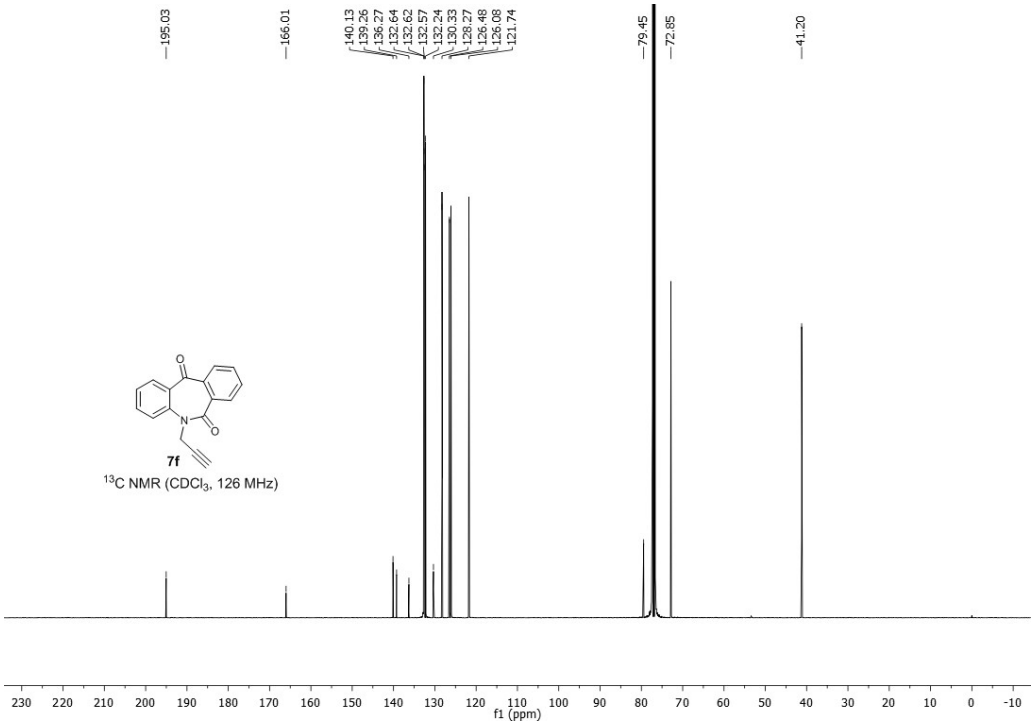


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
264.1023	1	C17H14NO2	264.1019	1.4	4.6	1	100.00	11.5	even	ok

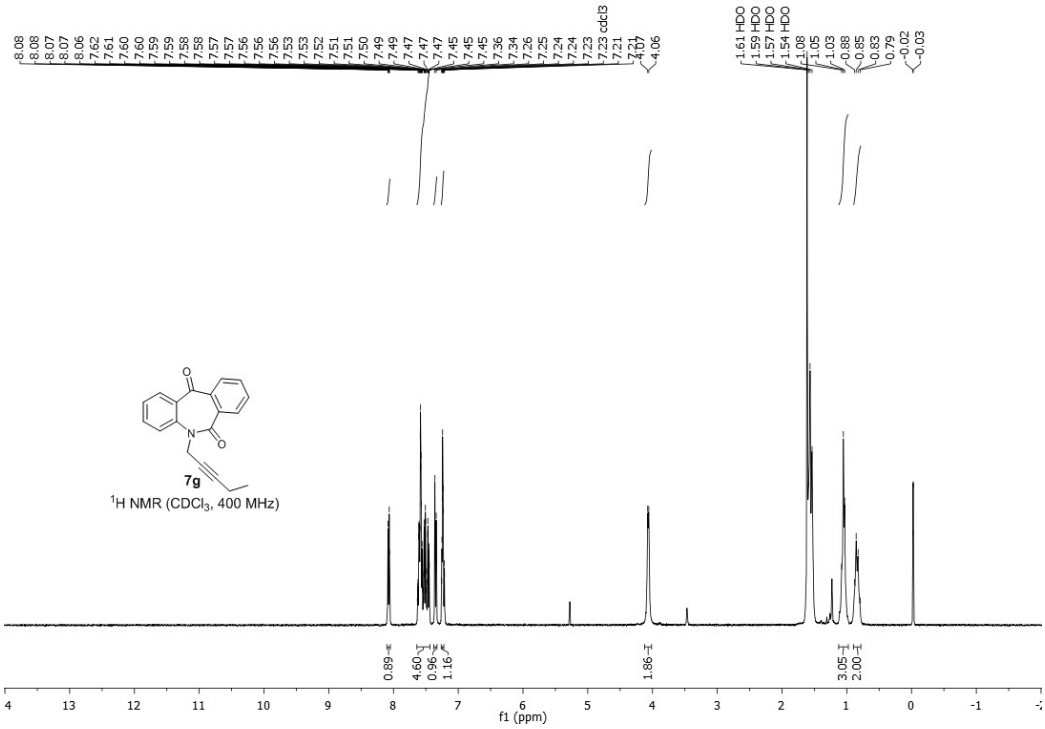
5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7f) (^{1}H NMR).



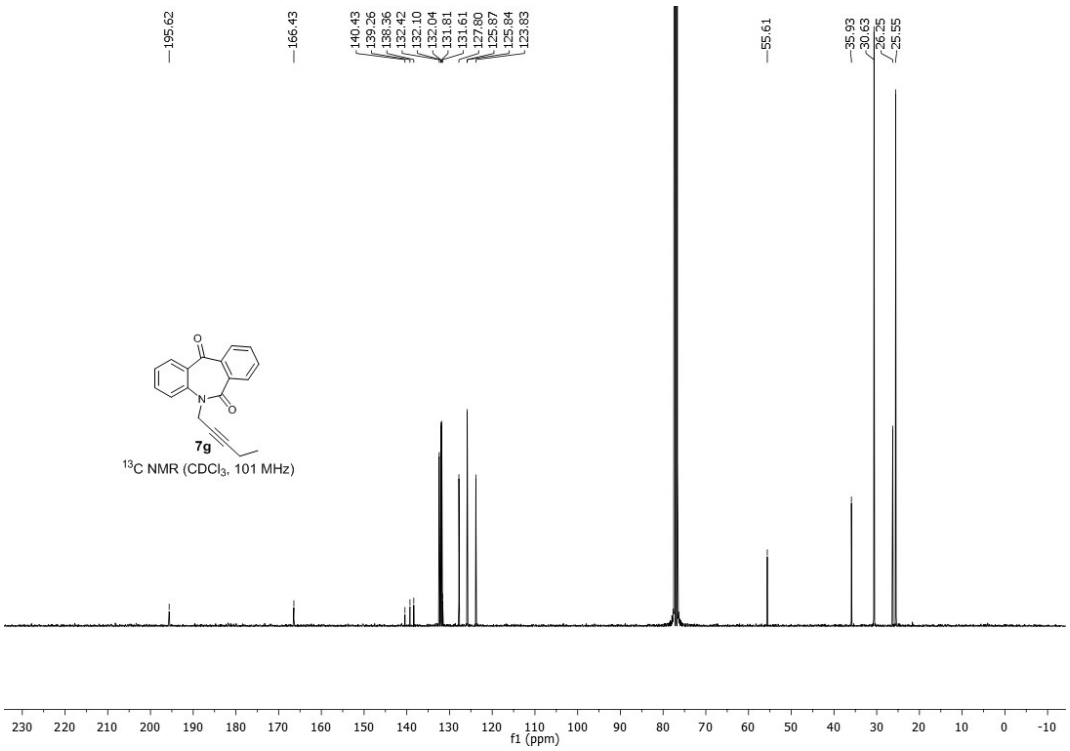
5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7f) (^{13}C NMR).



5-(pent-2-yn-1-yl)-*5H*-dibenzo[*b*,*e*]azepine-6,11-dione (7g) (^{1}H NMR).



5-(pent-2-yn-1-yl)-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7g) (^{13}C NMR).



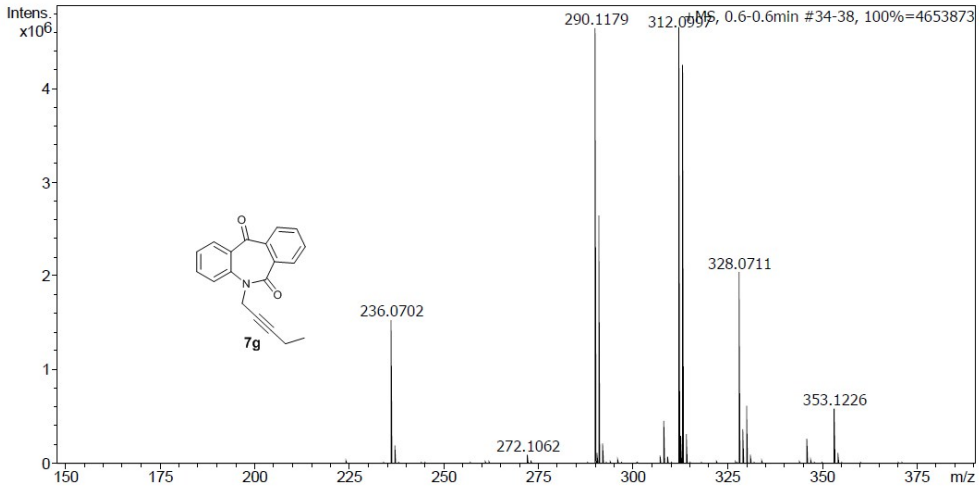
5-(pent-2-yn-1-yl)-*5H*-dibenzo[*b,e*]azepine-6,11-dione (7g) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV- 12.d	Acquisition Date	9/24/2015 3:55:47 PM
Method	Tune_pos_NAF_1000.m	Operator	SJG OUT
Sample Name	EXT-ICT-BMB-VKV-12	Instrument	maXis impact 282001.00081
Comment	C19H15NO2		

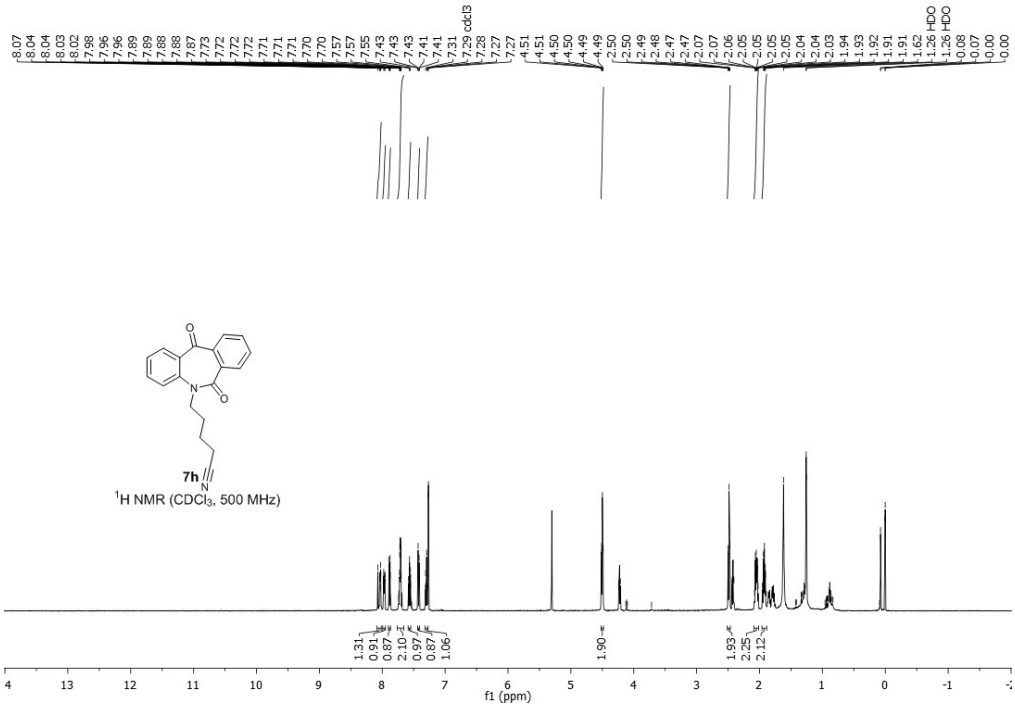
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source

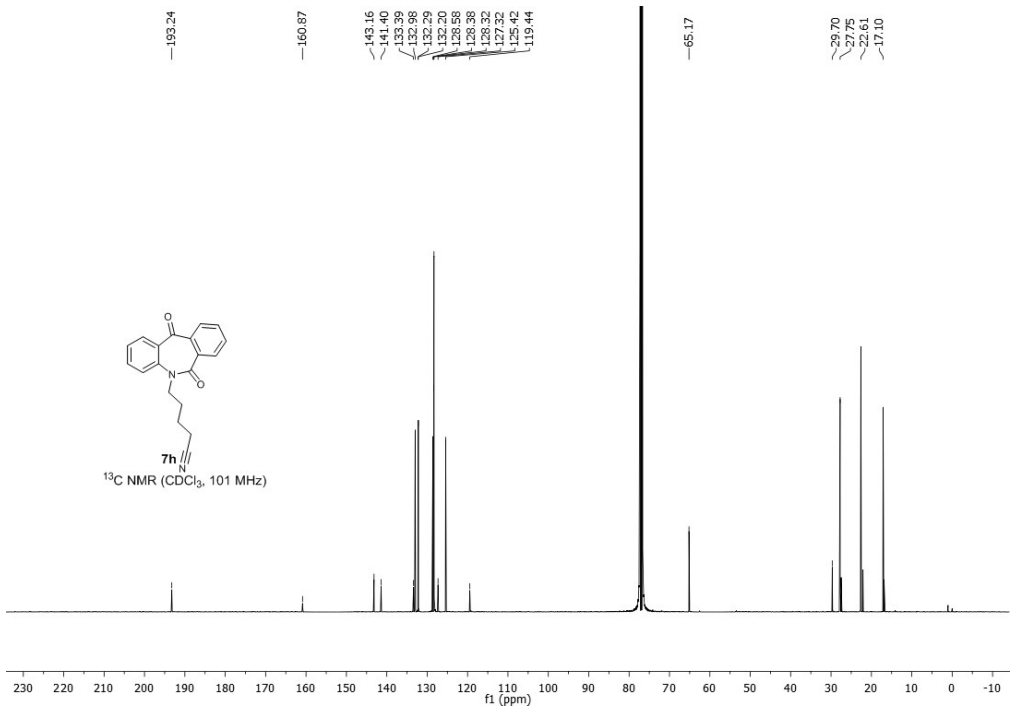


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
290.1179	1	C19H16NO2	290.1176	1.2	207.2	1	100.00	12.5	even	ok

5-(6,11-dioxo-6,11-dihydro-5H-dibenzo[b,e]azepin-5-yl)pentanenitrile (7h) (^{1}H NMR).



5-(6,11-dioxo-6,11-dihydro-5H-dibenzo[b,e]azepin-5-yl)pentanenitrile (7h) (^{13}C NMR).



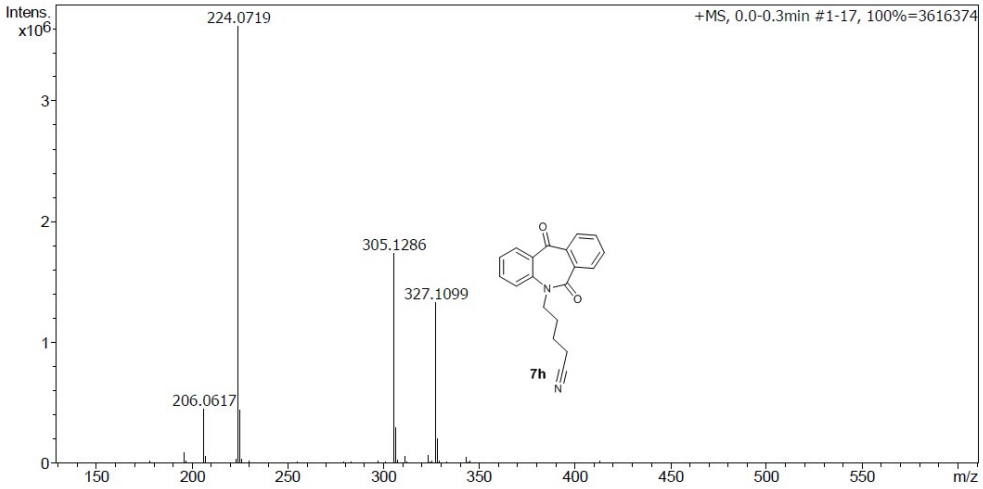
5-(6,11-dioxo-6,11-dihydro-5H-dibenzo[b,e]azepin-5-yl)pentanenitrile (7h) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-13.d	Acquisition Date	9/3/2015 11:55:24 AM
Method	Tune_pos_NAICSI-1000.m	Operator	MR OUT
Sample Name	EXT-ICT-BMB-VKV-13	Instrument	maXis impact 282001.00081
Comment	C19H16N2O2		

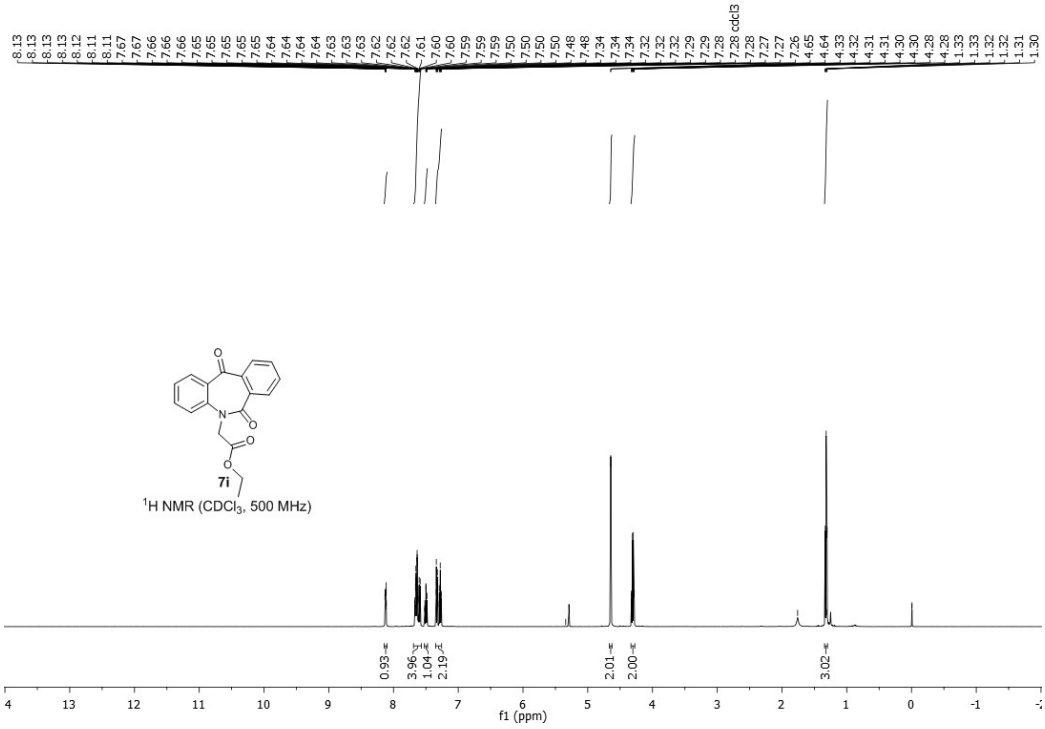
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

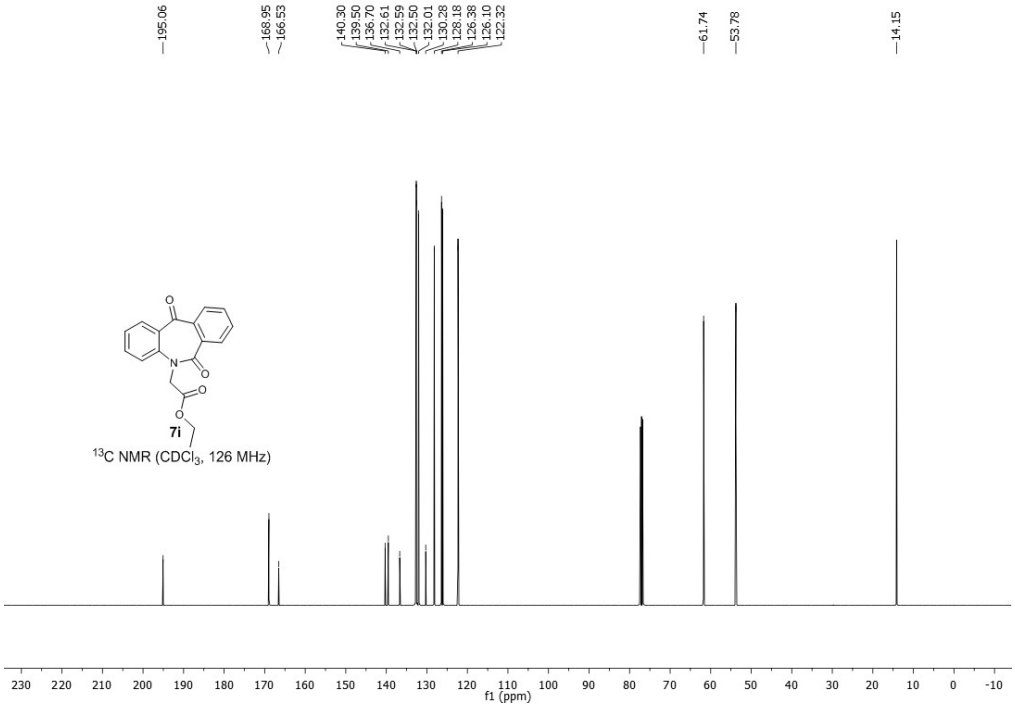


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
305.1286	1	C19H17N2O2	305.1285	0.4	28.4	1	100.00	12.5	even	ok

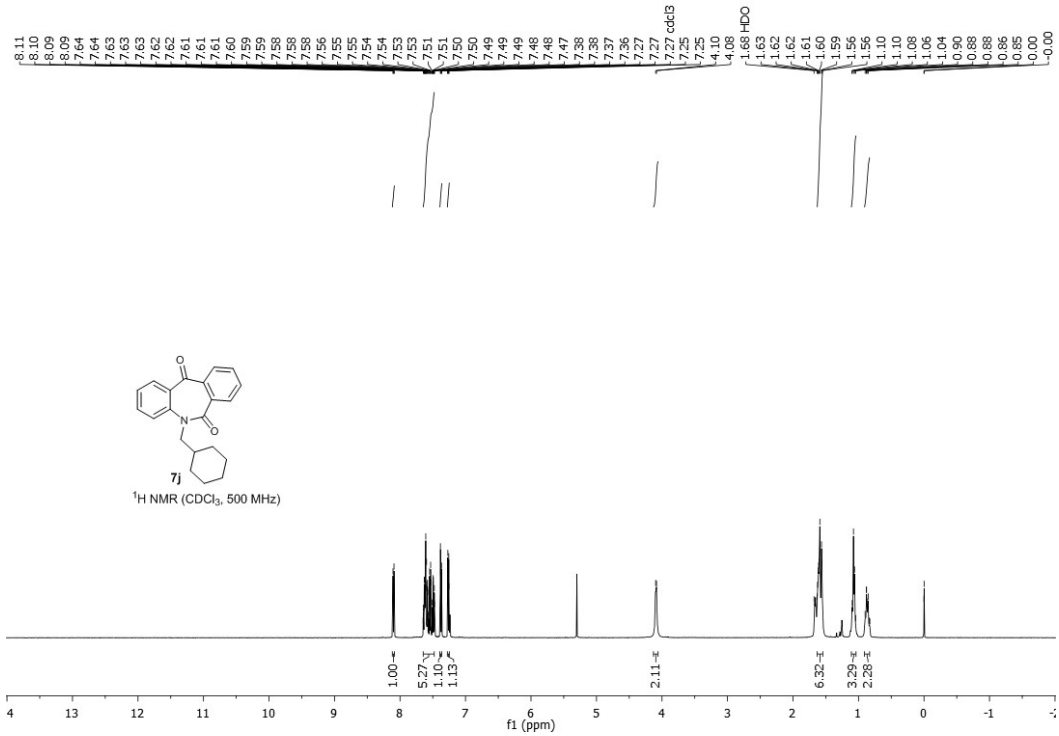
Ethyl 2-(6,11-dioxo-6,11-dihydro-5H-dibenzo[b,e]azepin-5-yl)acetate (7i) (^{1}H NMR).



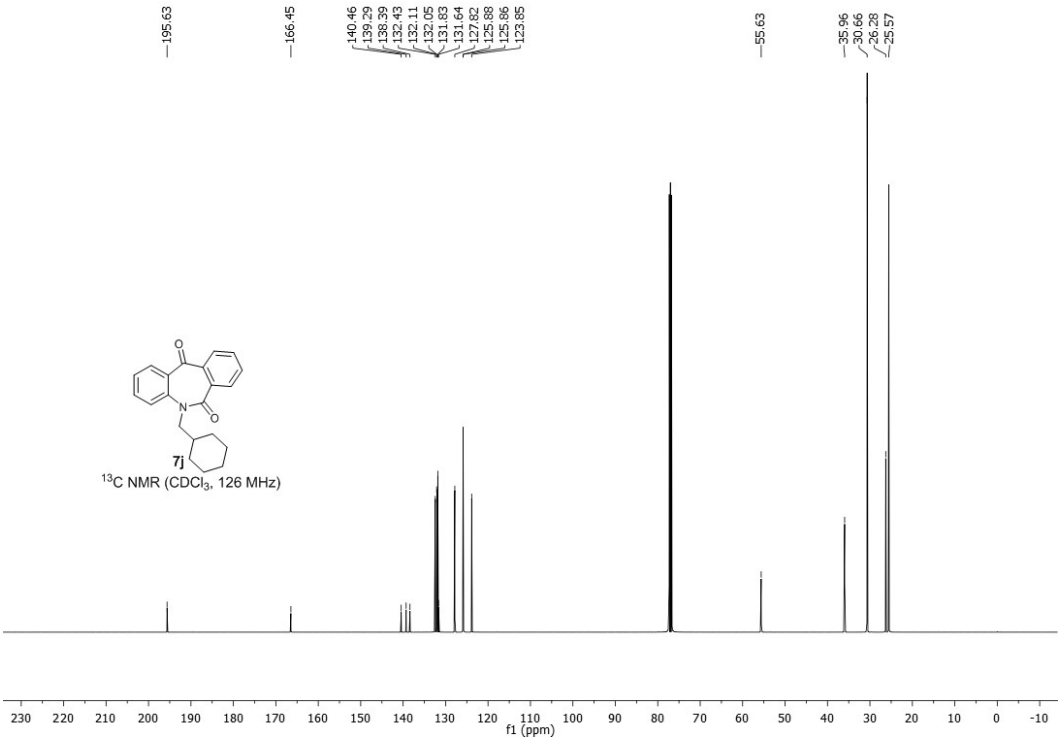
Ethyl 2-(6,11-dioxo-6,11-dihydro-5H-dibenzo[b,e]azepin-5-yl)acetate (7i) (^{13}C NMR).



5-(cyclohexylmethyl)-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7j) (^{1}H NMR).



5-(cyclohexylmethyl)-5H-dibenzo[b,e]azepine-6,11-dione (7j) (^{13}C NMR).



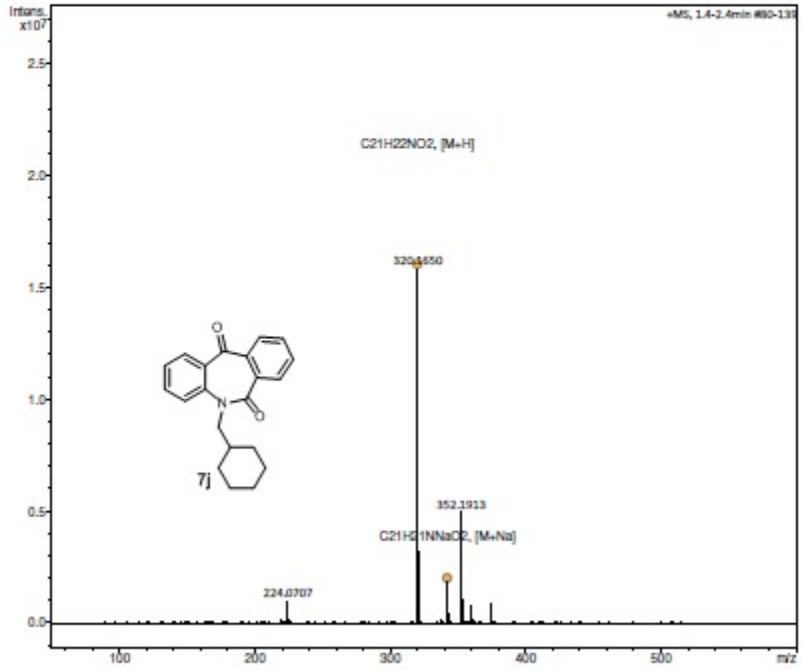
5-(cyclohexylmethyl)-5H-dibenzo[b,e]azepine-6,11-dione (7j) (HRMS)

Analysis Info

Analysis Name	D:\Data\Installation_2014-06-19\ICT\BhanageBM4_RC4_01_2221.d	Acquisition Date	2/27/2016 4:31:28 PM
Method	dic-ms600mz_10min.m	Operator	CIF
Sample Name	4	Instrument	impact HD 1819696.00184
Comment			

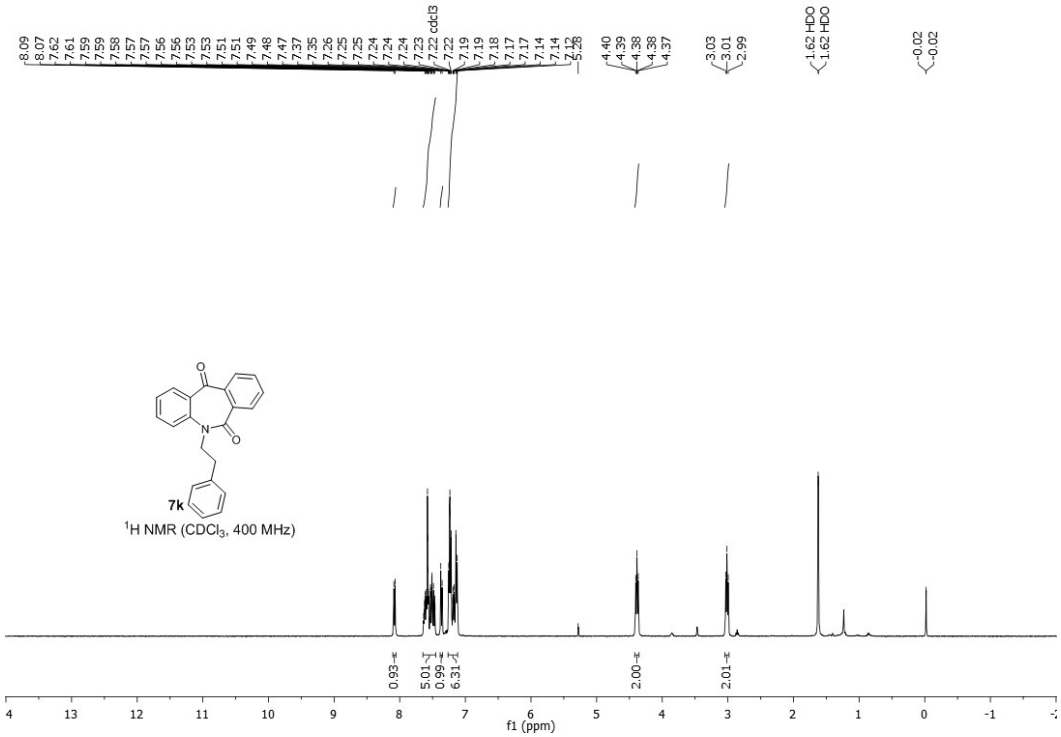
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

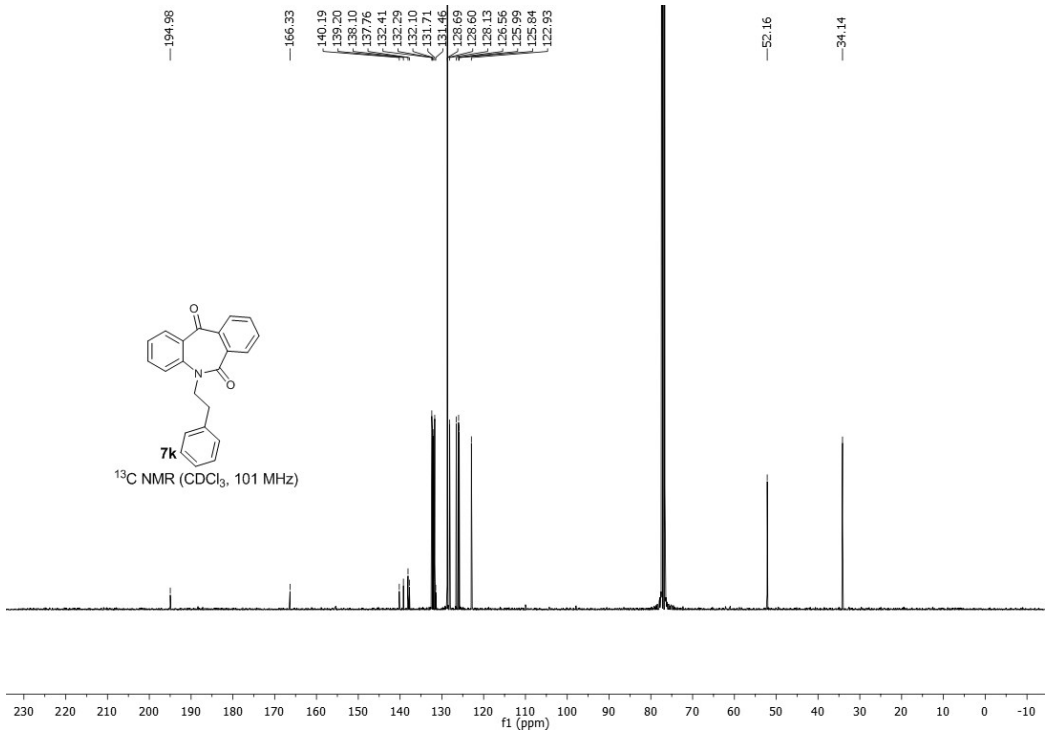


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	Adduct
320.1650	1	C21H22NO2	320.1645	-1.7	20.4	1	100.00	11.5	even	M+H
342.1470	1	C21H21NNaO2	342.1464	-1.6	12.4	1	100.00	11.5	even	M+Na

5-phenethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7k) (^{1}H NMR).



5-phenethyl-5*H*-dibenzo[*b,e*]azepine-6,11-dione (7k) (^{13}C NMR).



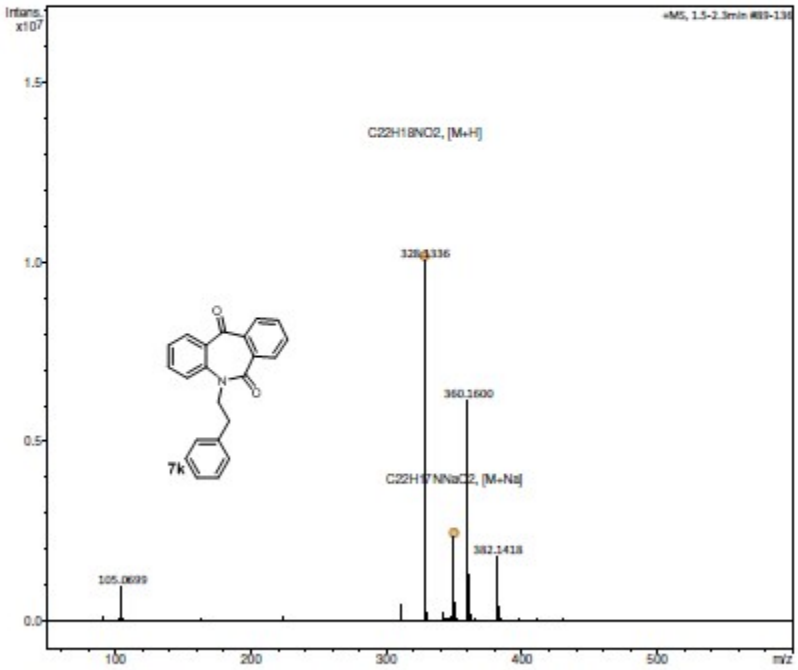
5-phenethyl-5*H*-dibenzo[*b*,*e*]azepine-6,11-dione (7k) (HRMS)

Analysis Info

Analysis Name	D:\Data\Installation_2014-06-19\ICT\BhanagaBM5_RC5_01_2223.d	Acquisition Date	2/27/2016 5:48:30 PM
Method	dlc-ms600mz_10min.m	Operator	CIF
Sample Name	5	Instrument	impact HD 1819696.00184
Comment			

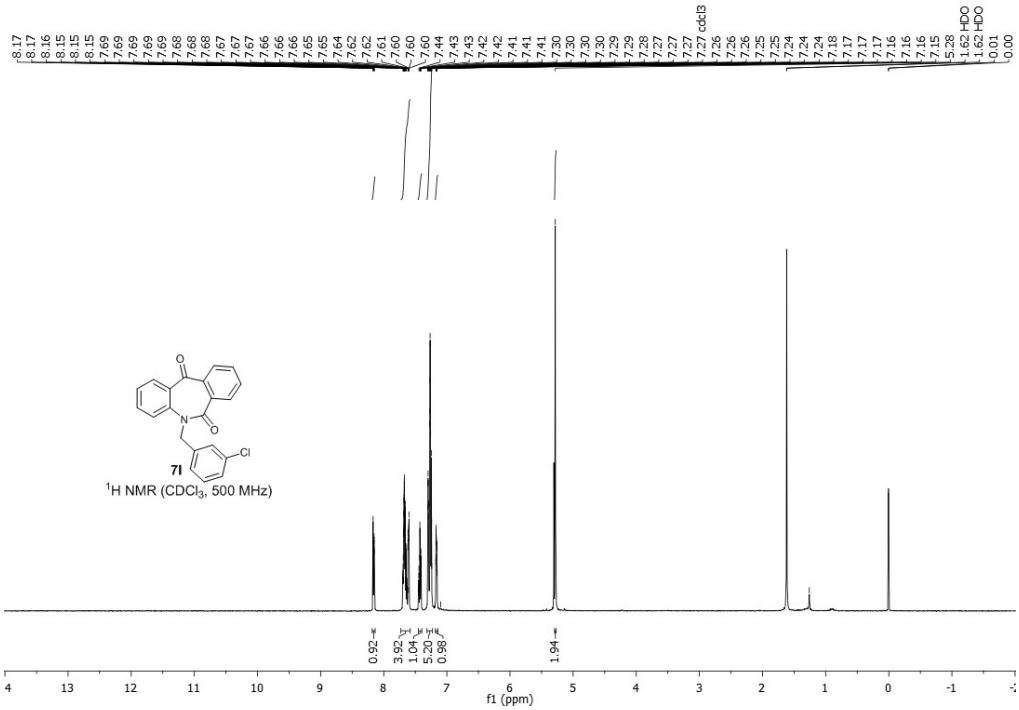
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

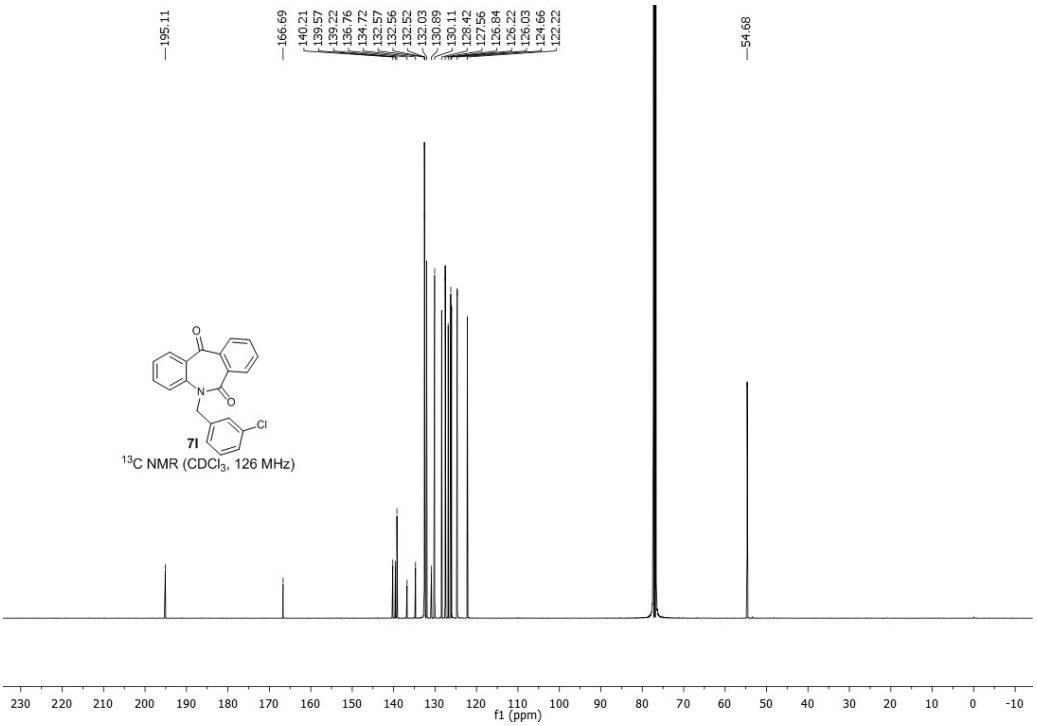


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Adduct
328.1336	1	C22H18NO2	328.1332	-1.1	23.2	1	100.00	14.5	even	ok	M+H
350.1155	1	C22H17NNaO2	350.1151	-1.1	16.5	1	100.00	14.5	even	ok	M+Na

5-(3-chlorobenzyl)-5H-dibenzo[b,e]azepine-6,11-dione (7l) (^{1}H NMR).



5-(3-chlorobenzyl)-5H-dibenzo[b,e]azepine-6,11-dione (7l) (^{13}C NMR).



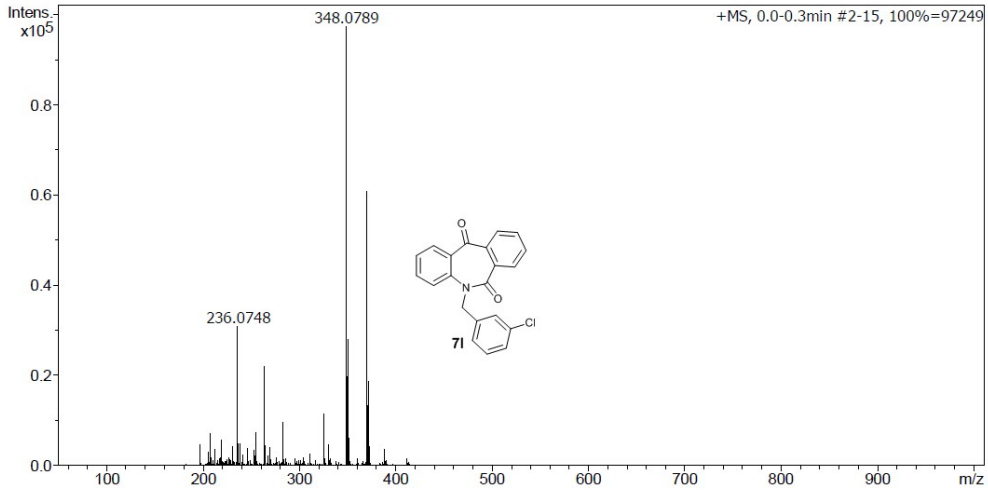
5-(3-chlorobenzyl)-5H-dibenzo[b,e]azepine-6,11-dione (7l) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-14.d	Acquisition Date	9/3/2015 11:37:53 AM
Method	Tune_pos_NAICSI-1000.m	Operator	MR OUT
Sample Name	EXT-ICT-BMB-VKV-14	Instrument	maXis impact 282001.00081
Comment	C21H14NO2Cl		

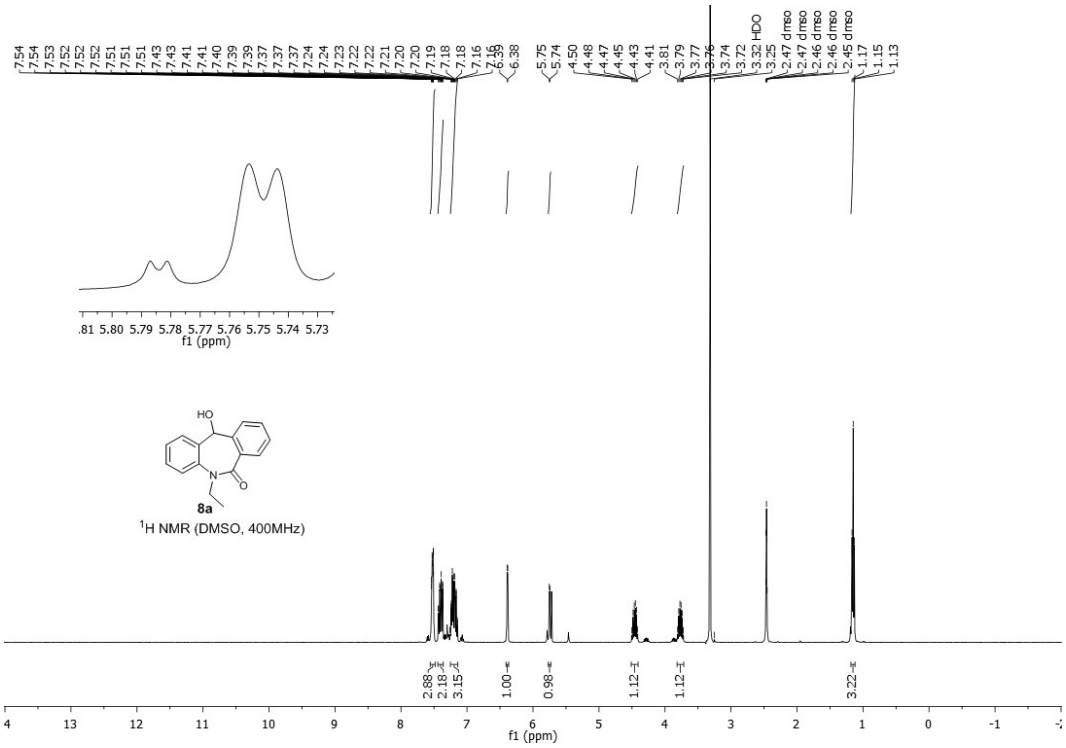
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

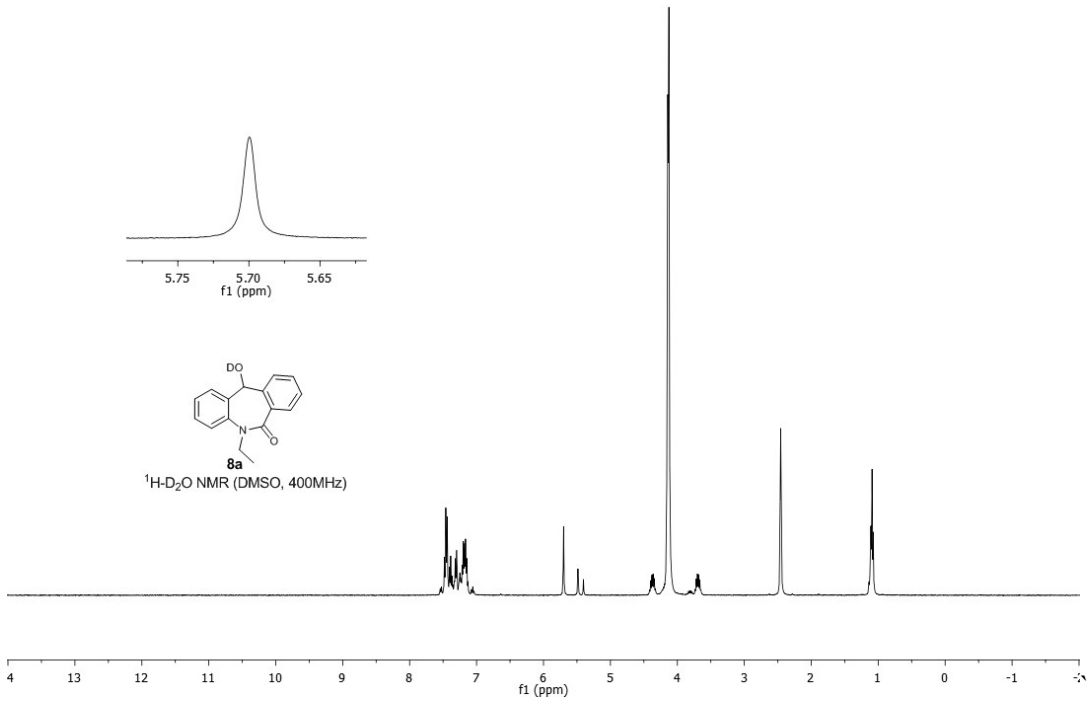


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
348.0789	1	C21H15ClNO2	348.0786	1.0	32.7	1	100.00	14.5	even	ok

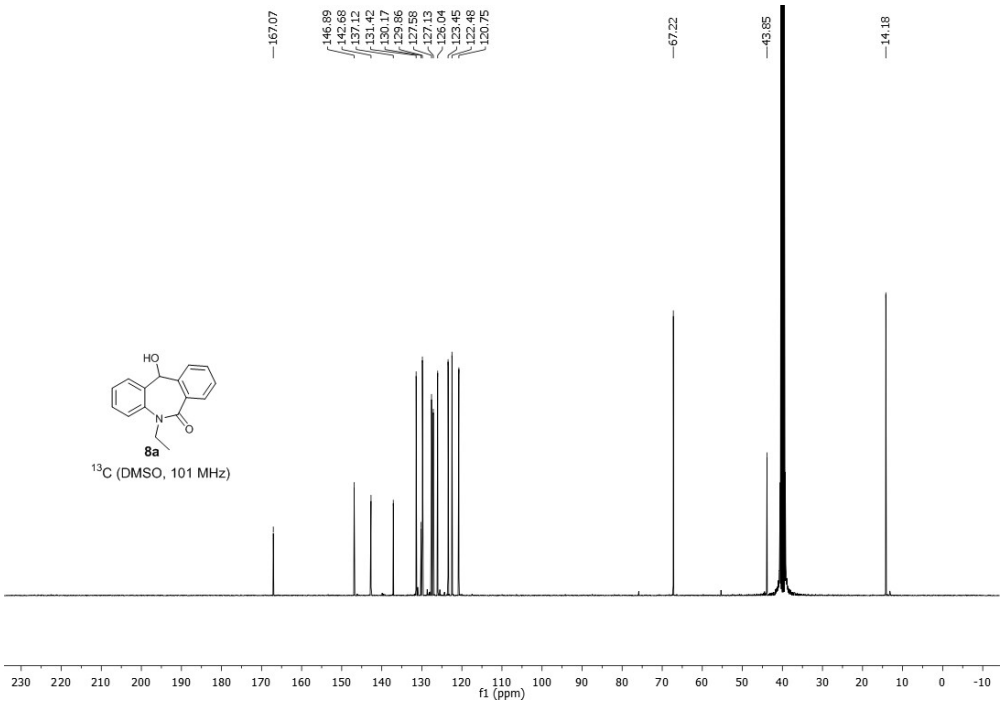
(S)-5-ethyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8a) (^{1}H NMR)



(S)-5-ethyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8a) (^{1}H-D_2O Experiment)



(S)-5-ethyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8a) (^{13}C NMR)



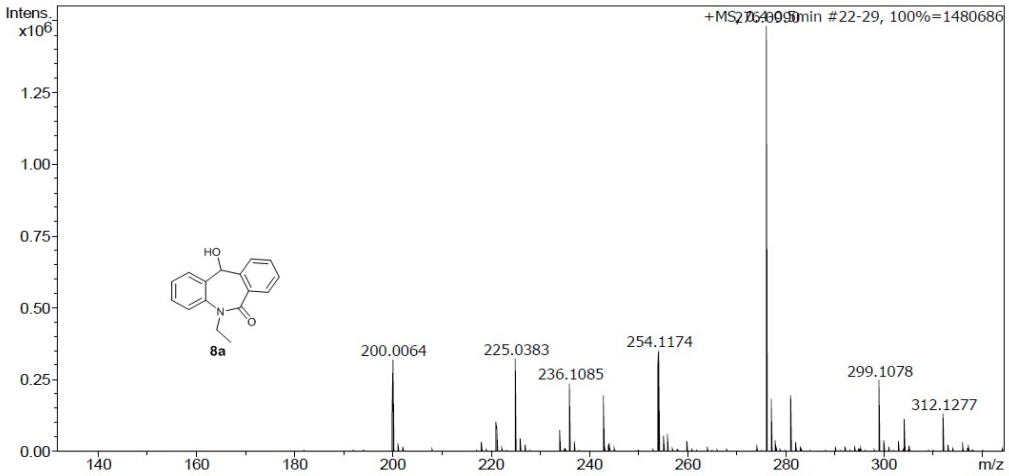
(S)-5-ethyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8a) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-1.d	Acquisition Date	9/11/2015 5:02:40 PM
Method	Tune_pos_NAICSI-1000.m	Operator	RAF IN
Sample Name	EXT-ICT-BMB-VKV-1	Instrument	maXis impact 282001.00081
Comment	C16H15NO2		

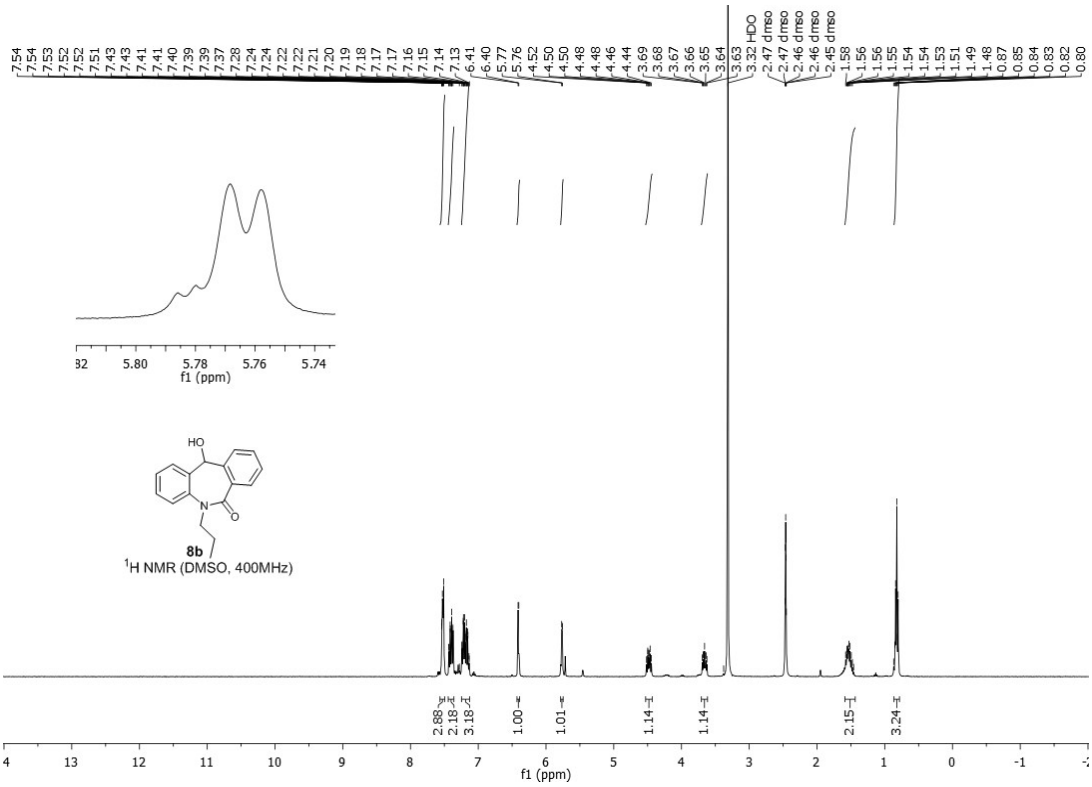
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

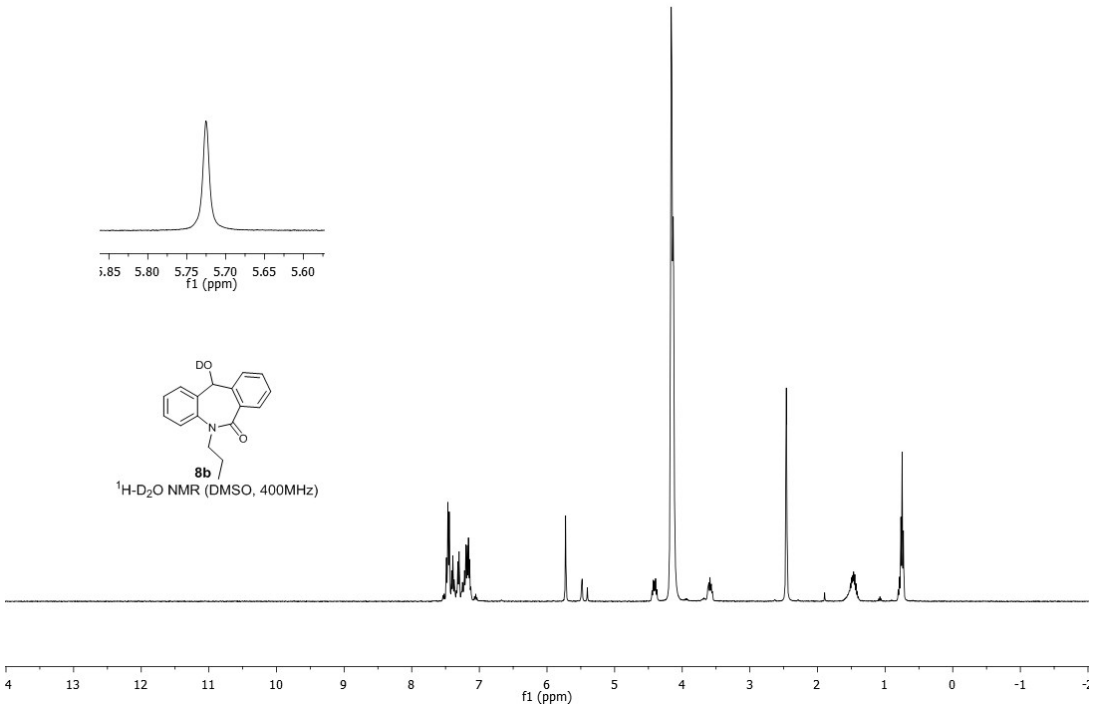


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
254.1174	1	C16H16NO2	254.1176	-0.5	15.1	1	100.00	9.5	even	ok
276.0990	1	C16H15NNaO2	276.0995	1.6	32.9	1	100.00	9.5	even	ok

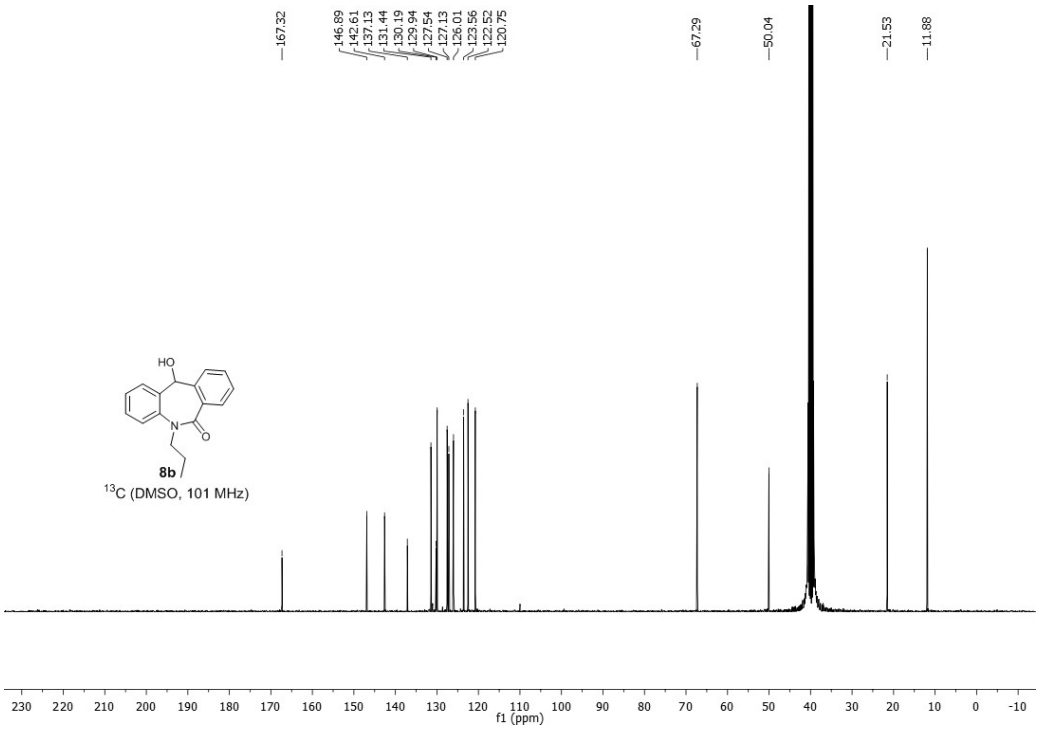
(S)-11-hydroxy-5-propyl-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8b) (^{1}H NMR)



(S)-11-hydroxy-5-propyl-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8b) (^{1}H-D_2O Experiment)



(S)-11-hydroxy-5-propyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8b) (^{13}C NMR)



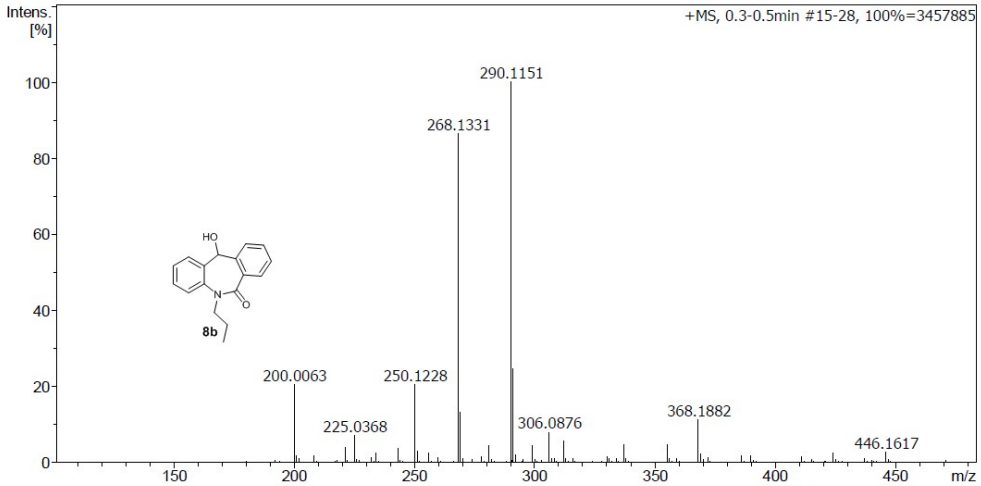
(S)-11-hydroxy-5-propyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8b) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-2.d	Acquisition Date	9/11/2015 4:39:21 PM
Method	Tune_pos_NAICSI-1000.m	Operator	RAF IN
Sample Name	EXT-ICT-BMB-VKV-2	Instrument	maXis impact 282001.00081
Comment	C17H17NO2		

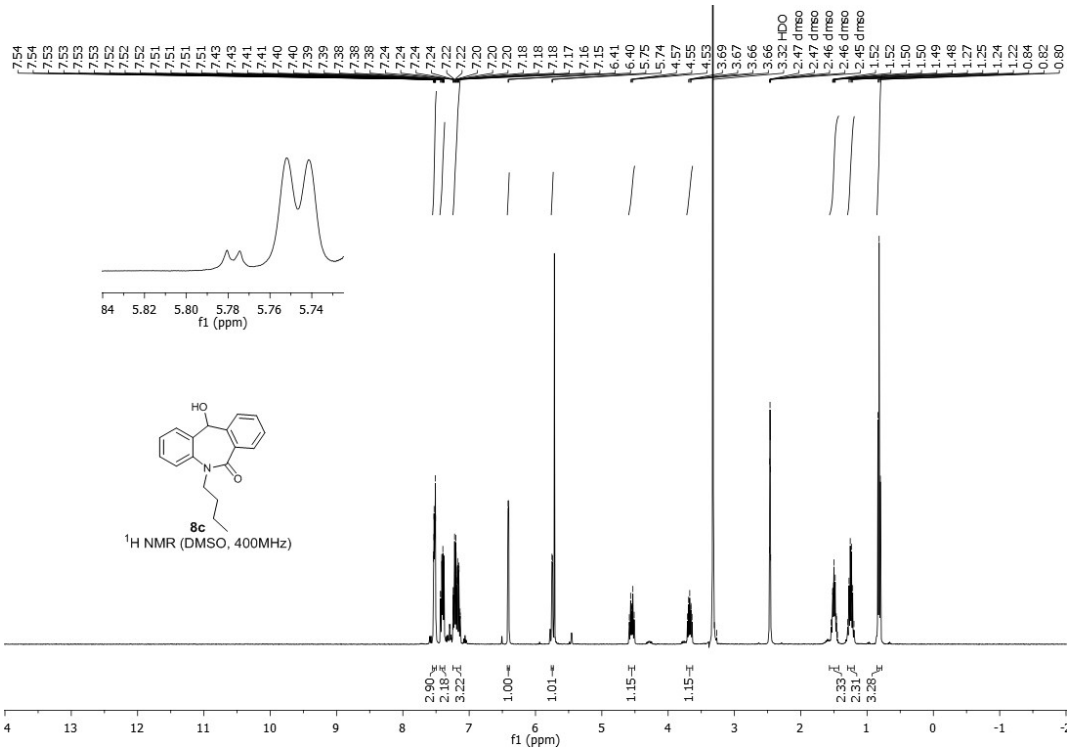
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

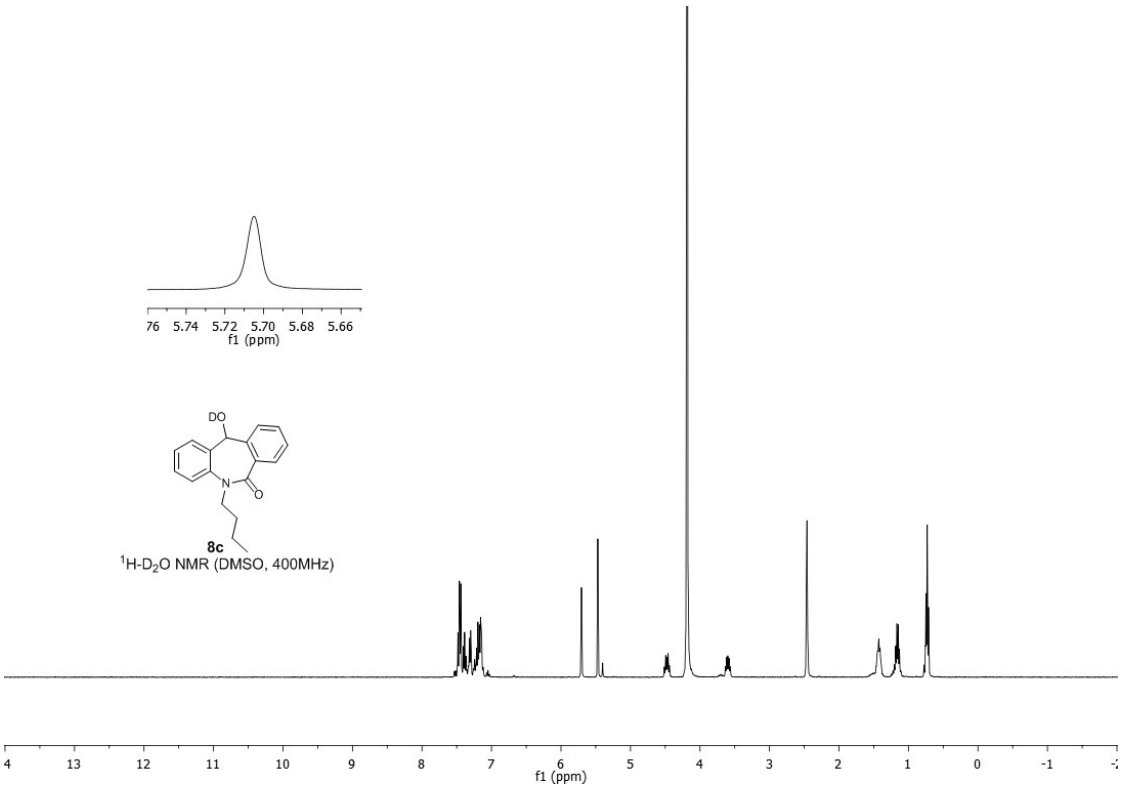


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
268.1331	1	C17H18NO2	268.1332	0.4	21.9	1	100.00	9.5	even	ok

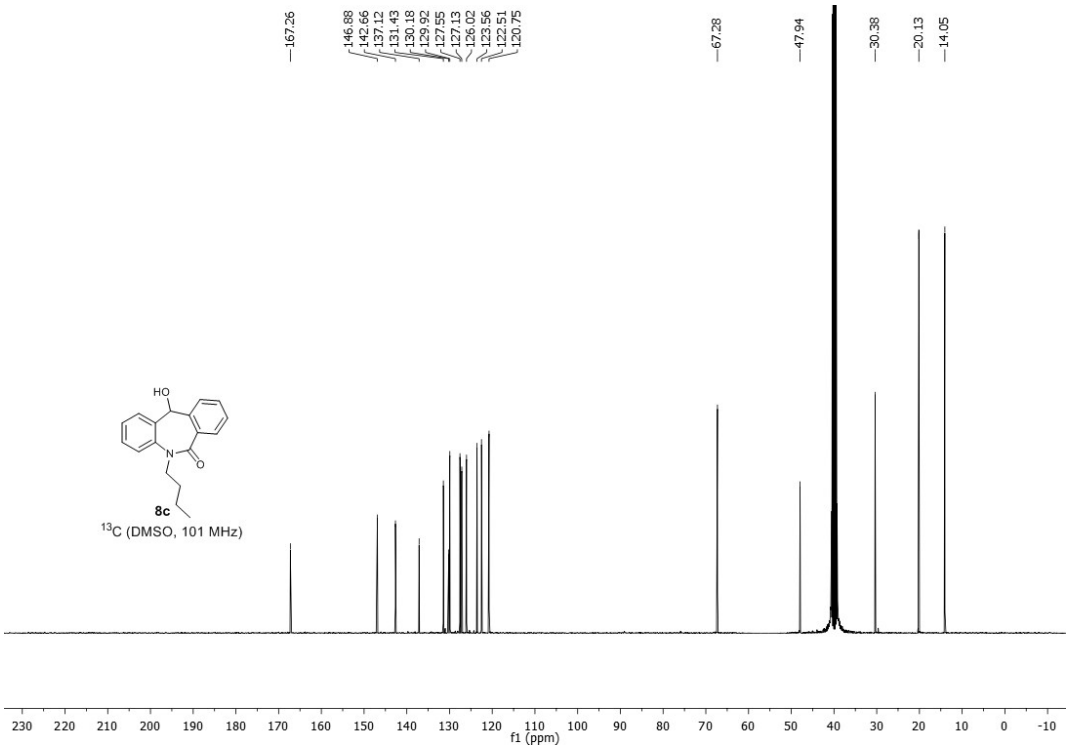
(S)-5-butyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8c) (^{1}H NMR)



(S)-5-butyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8c) (^{1}H-D_2O Experiment)



(S)-5-butyl-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8c) (^{13}C NMR)



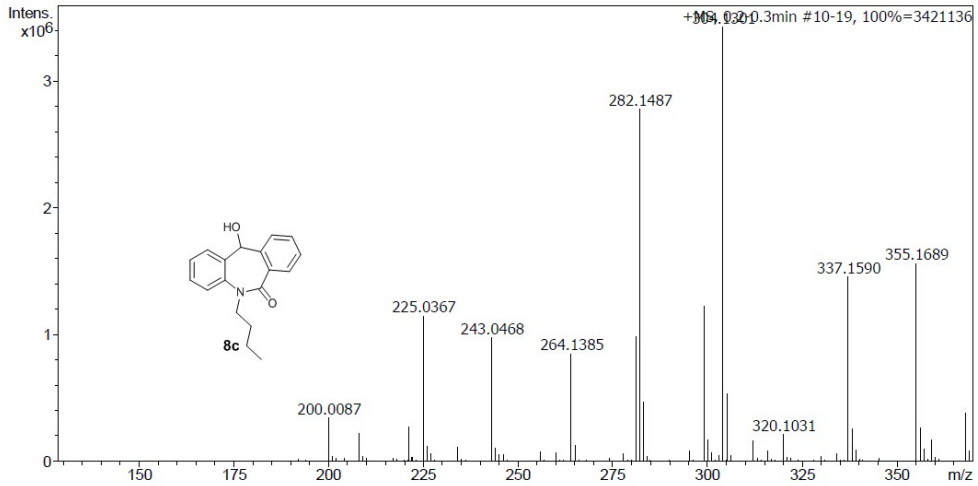
(S)-5-butyl-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8c) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-3.d	Acquisition Date	9/11/2015 4:52:20 PM
Method	Tune_pos_NAICSI-1000.m	Operator	RAF IN
Sample Name	EXT-ICT-BMB-VKV-3	Instrument	maXis impact 282001.00081
Comment	C18H19NO2		

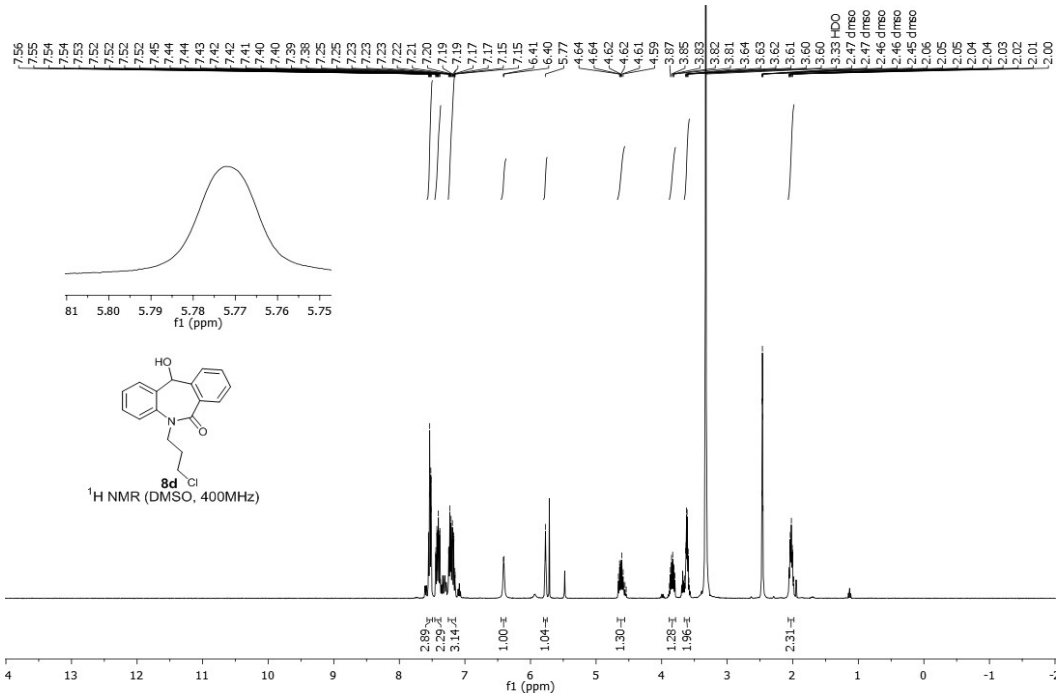
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

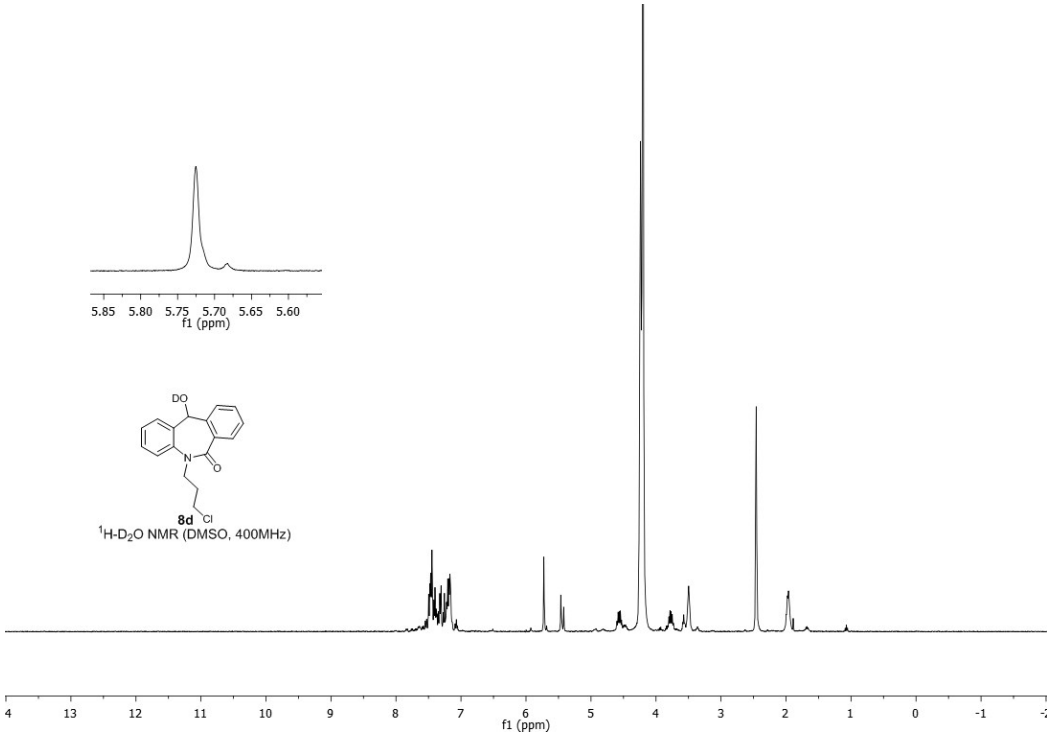


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
282.1487	1	C18H20NO2	282.1489	-0.4	19.8	1	100.00	9.5	even	ok

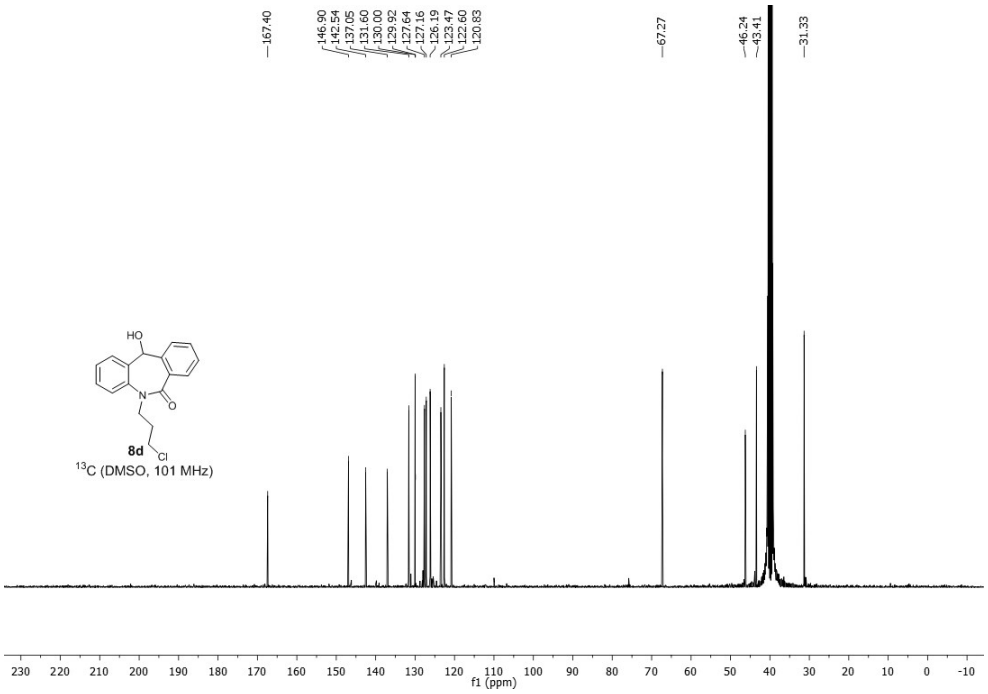
(S)-5-(3-chloropropyl)-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8d) (^{1}H NMR)



(S)-5-(3-chloropropyl)-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8d) (^{1}H-D_2O Experiment)



(S)-5-(3-chloropropyl)-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8d) (^{13}C NMR)



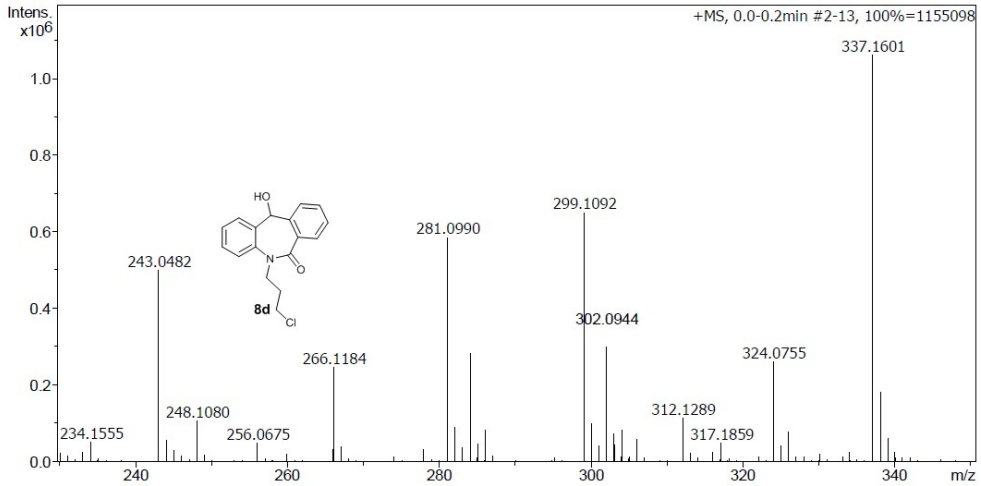
(S)-5-(3-chloropropyl)-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8d) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-4.d	Acquisition Date	9/11/2015 4:13:03 PM
Method	Tune_pos_NAICSI-1000.m	Operator	RAF IN
Sample Name	EXT-ICT-BMB-VKV-4	Instrument	maXis impact 282001.00081
Comment	C17H16ClNO2		

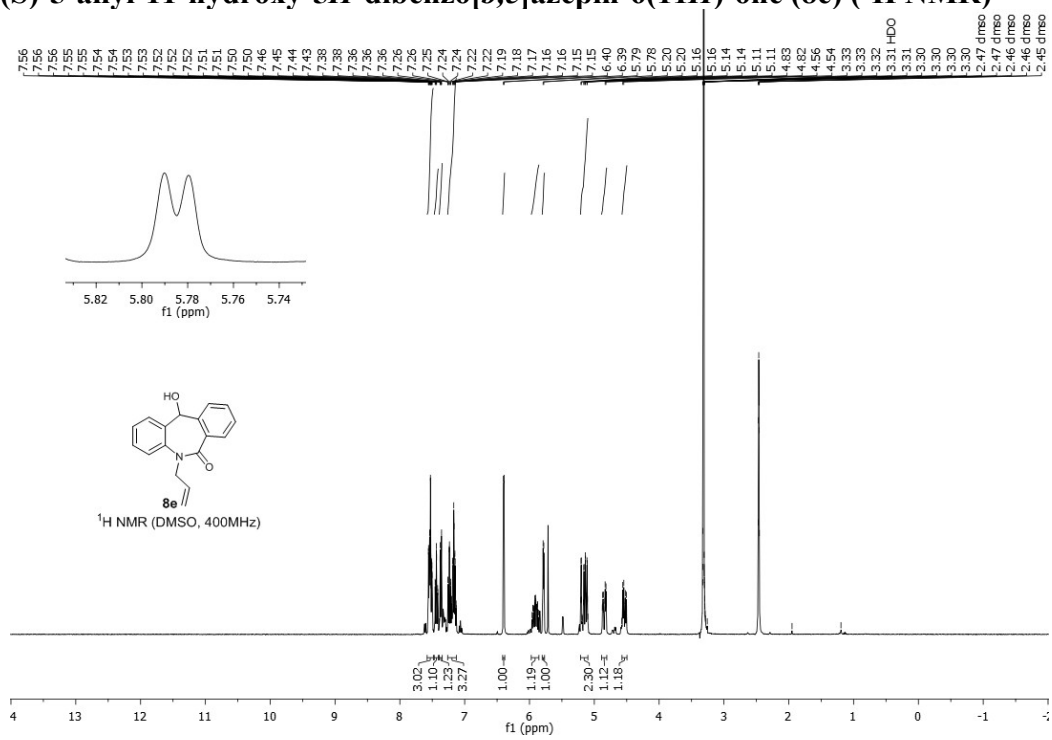
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source

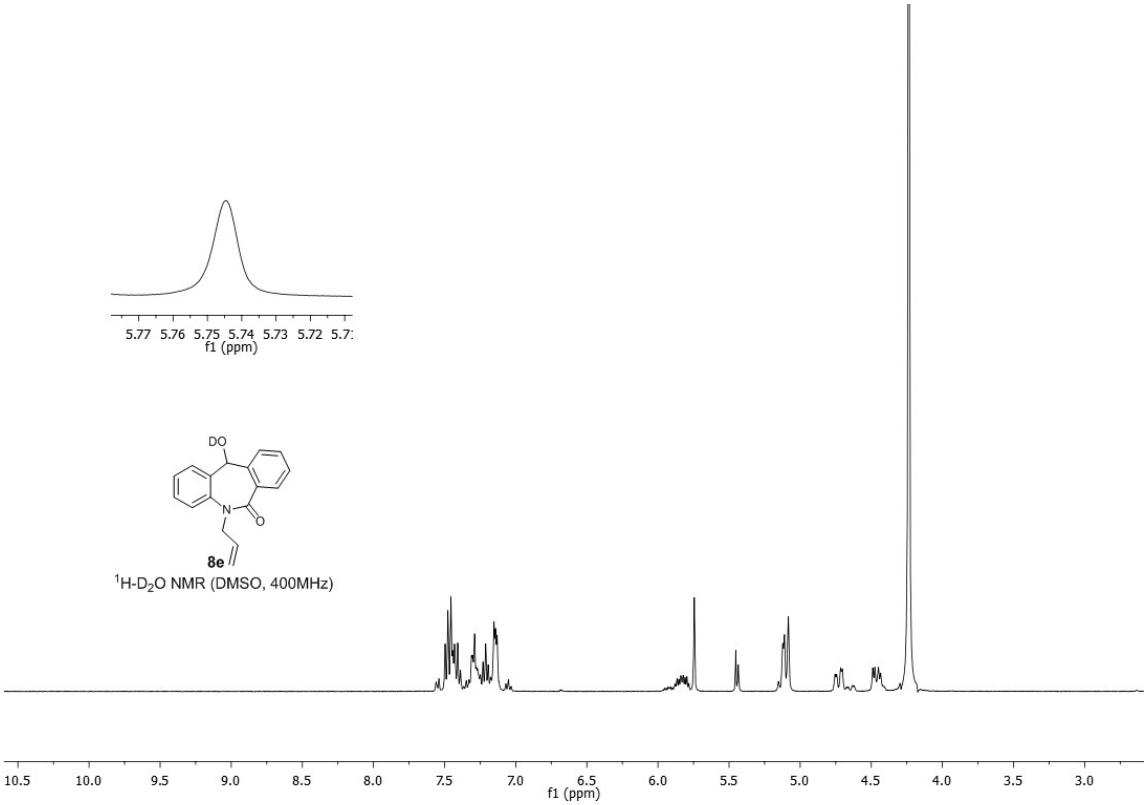


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
302.0944	1	C17H17ClNO2	302.0942	-0.5	27.4	1	100.00	9.5	even	ok

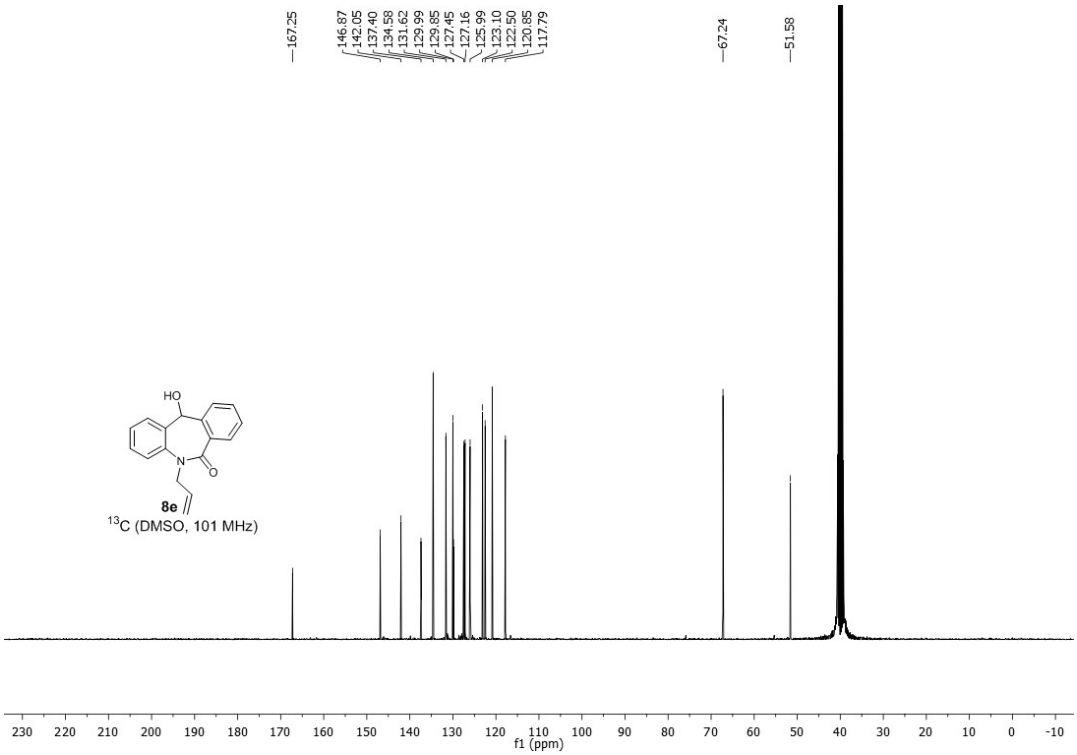
(S)-5-allyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8e) (^{1}H NMR)



(S)-5-allyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8e) (^{1}H-D_2O Experiment)



(S)-5-allyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8e) (^{13}C NMR)



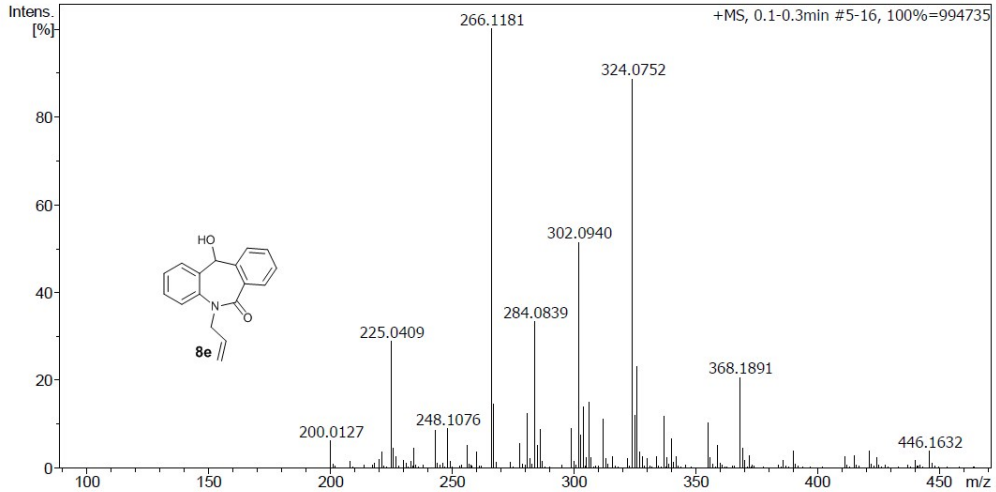
(S)-5-allyl-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8e) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-5.d	Acquisition Date	9/11/2015 4:23:44 PM
Method	Tune_pos_NAICSI-1000.m	Operator	RAF IN
Sample Name	EXT-ICT-BMB-VKV-5	Instrument	maXis impact 282001.00081
Comment	C17H15NO2		

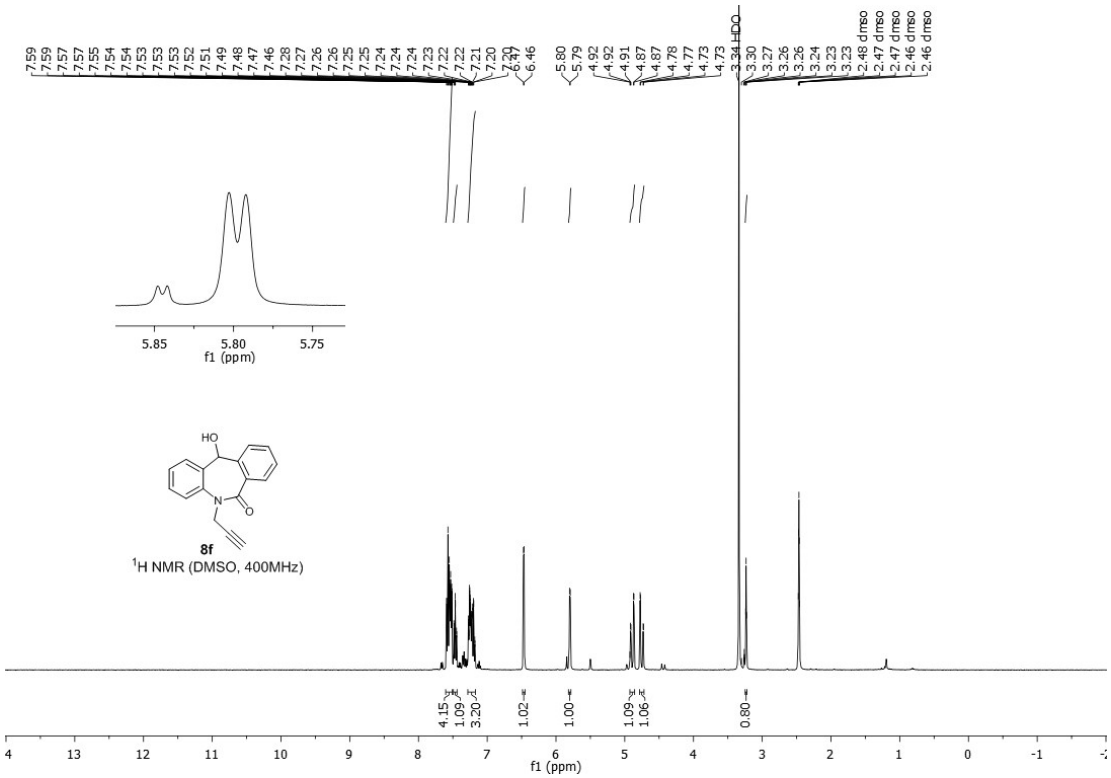
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

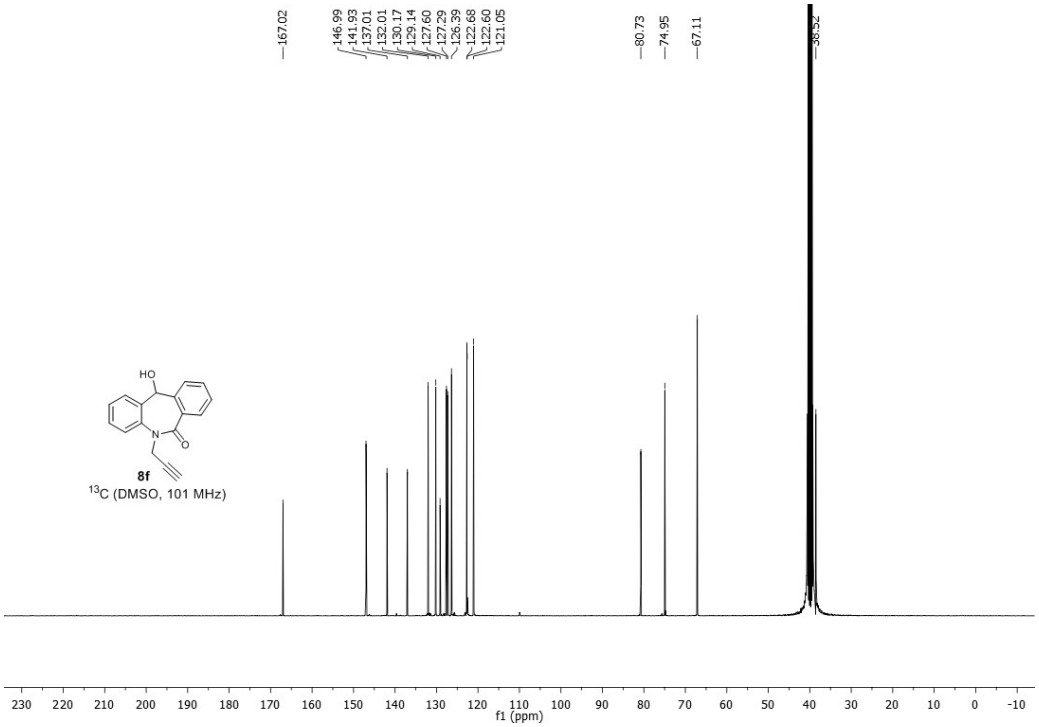


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
266.1181	1	C17H16NO2	266.1176	1.9	26.1	1	100.00	10.5	even	ok

(S)-11-hydroxy-5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8f) (^{1}H NMR)



(S)-11-hydroxy-5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8f) (^{13}C NMR)



(S)-11-hydroxy-5-(prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8f) (HRMS)

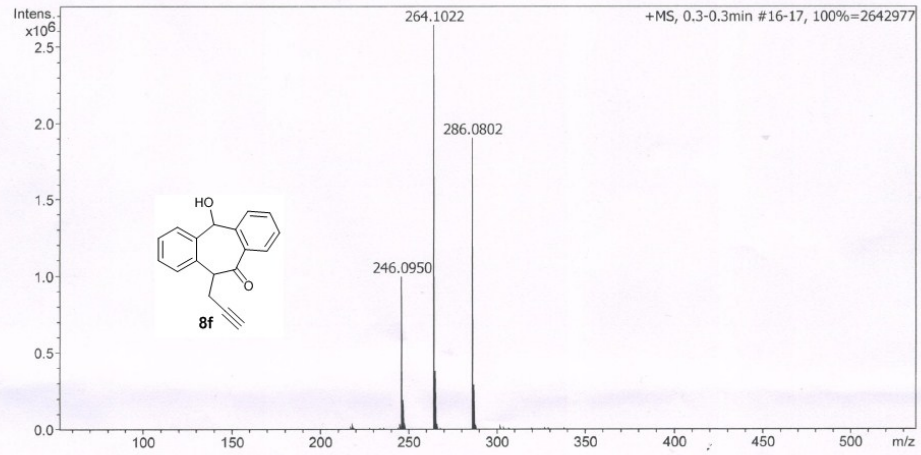
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\APR 15\EXT-ICT-BMB-ART-20.d	Acquisition Date	4/21/2015 12:39:07 PM
Method	Tune_pos_NAICSI_500.m	Operator	iitb
Sample Name	EXT-ICT-BMB-ART-20	Instrument	maXis impact 282001.00081
Comment	C17H13NO2		

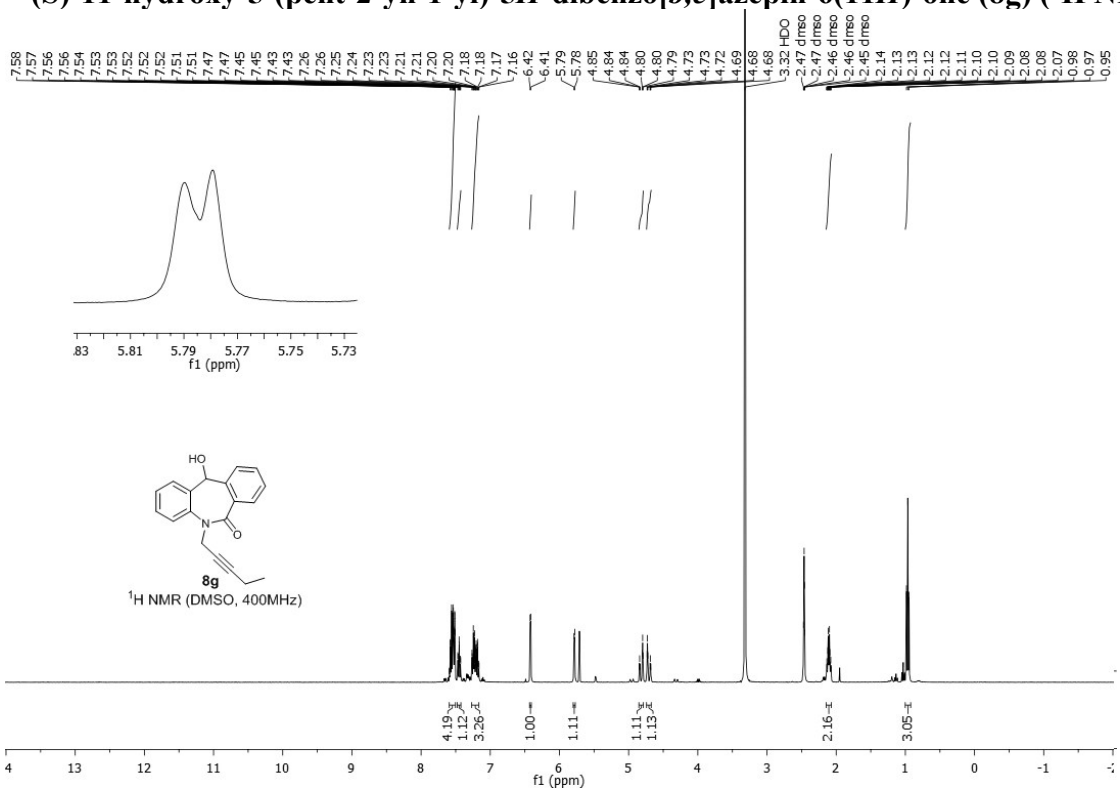
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

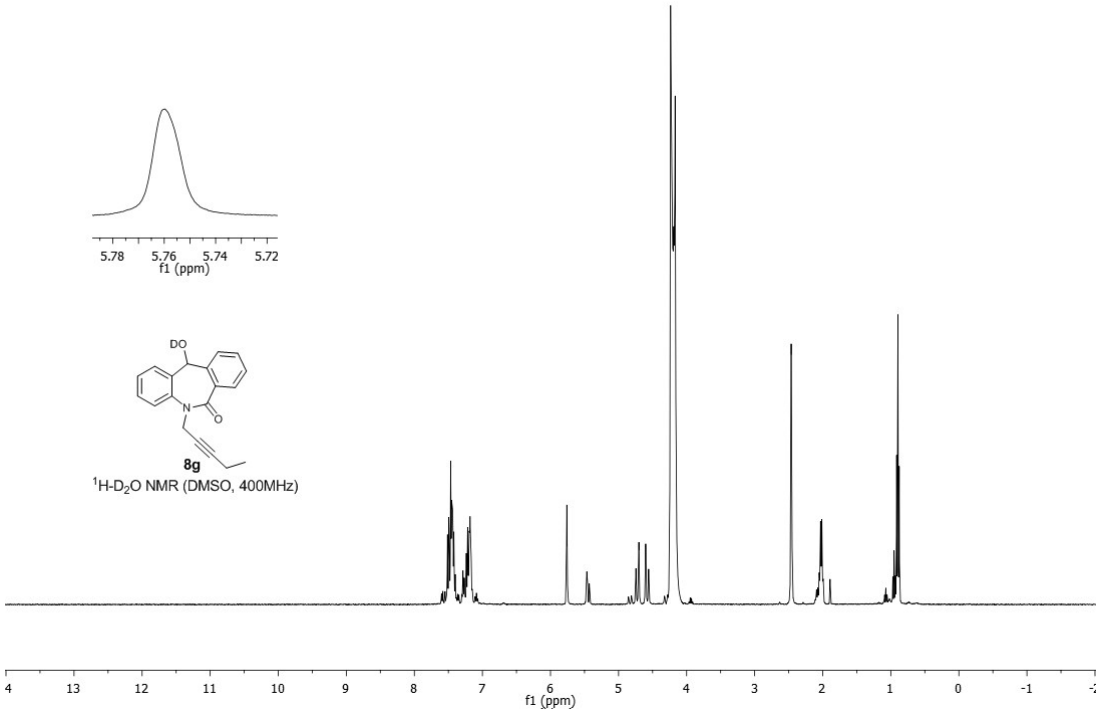


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
264.1022	1	C17H14NO2	264.1019	1.1	26.8	1	100.00	11.5	even	ok

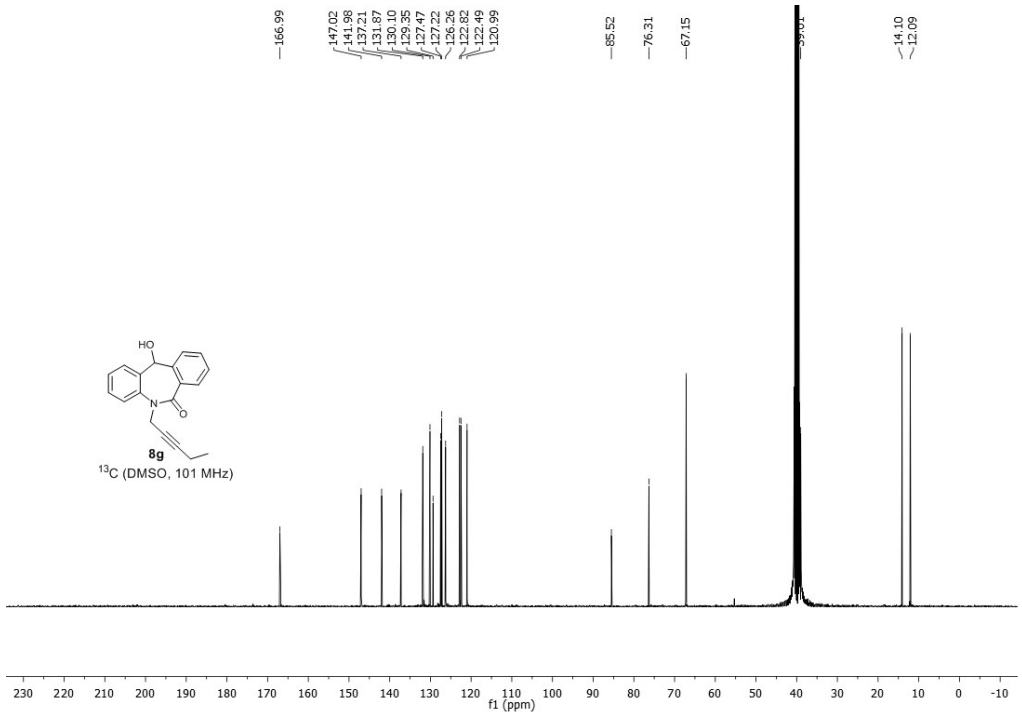
(S)-11-hydroxy-5-(pent-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8g) (^{1}H NMR)



(S)-11-hydroxy-5-(pent-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8g) (^{1}H-D_2O Experiment)



(S)-11-hydroxy-5-(pent-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8g) (^{13}C NMR).



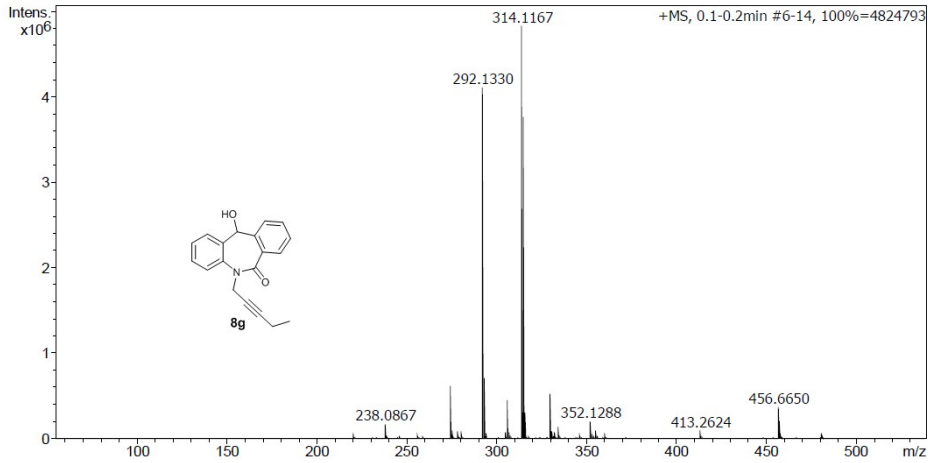
(S)-11-hydroxy-5-(pent-2-yn-1-yl)-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8g) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-8.d	Acquisition Date	9/24/2015 12:39:46 PM
Method	Tune_pos_NAF_1000.m	Operator	PG APP IN
Sample Name	EXT-ICT-BMB-VKV-8	Instrument	maXis impact 282001.00081
Comment	C19H17NO2		

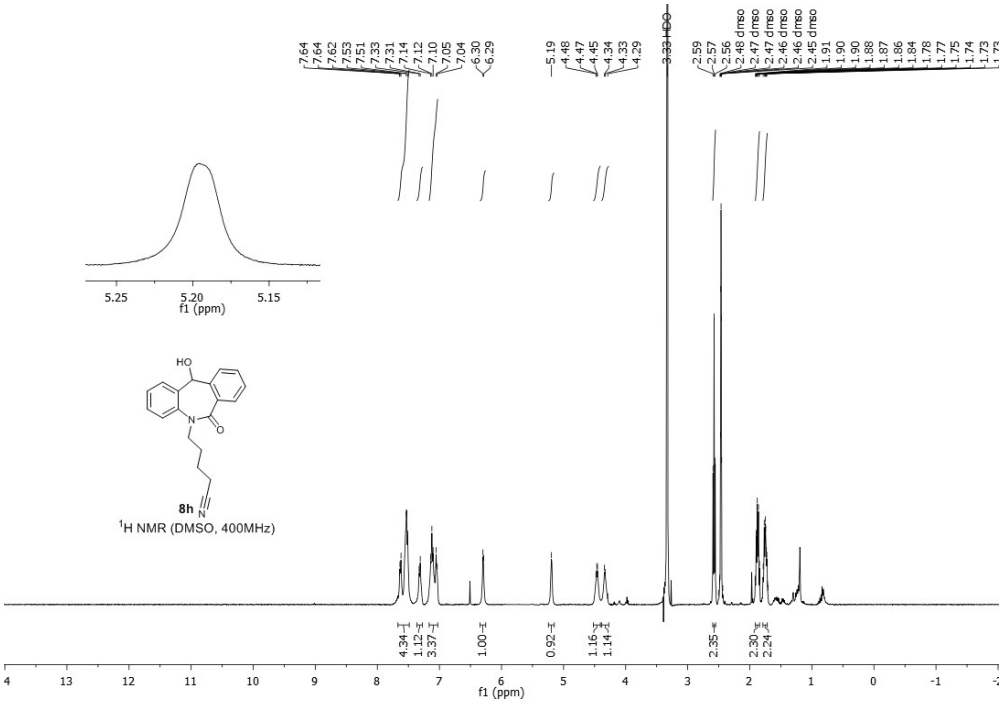
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source

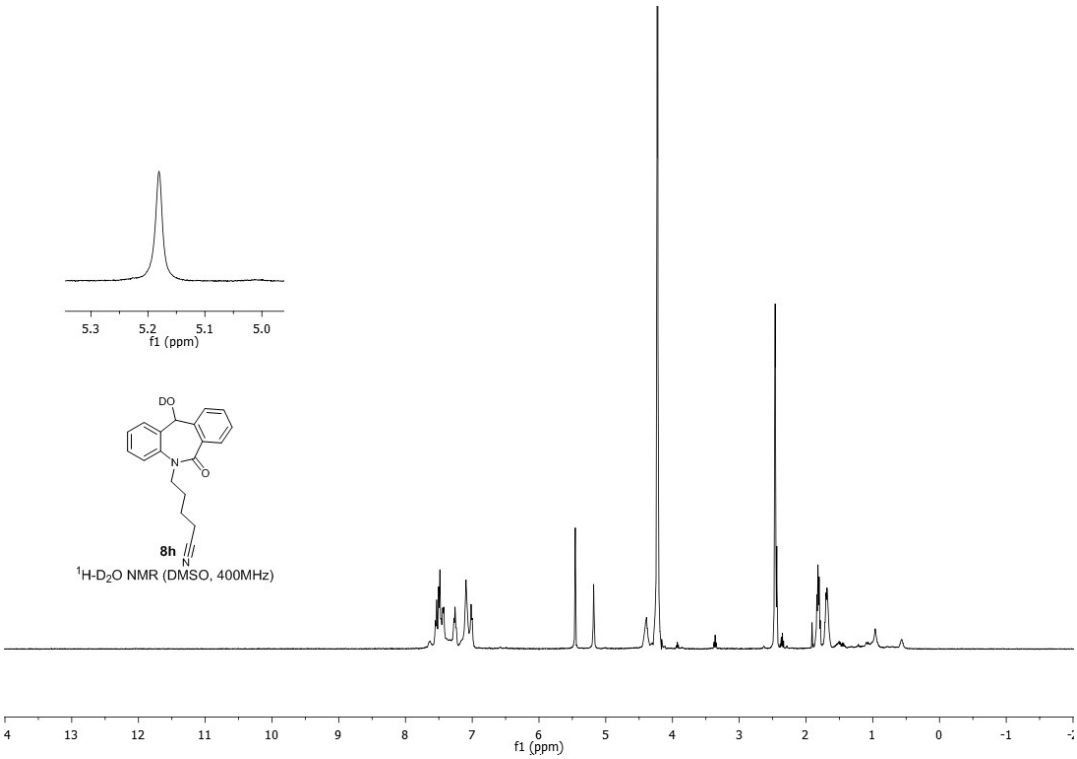


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
292.1330	1	C19H18NO2	292.1332	-0.7	22.8	1	100.00	11.5	even	ok

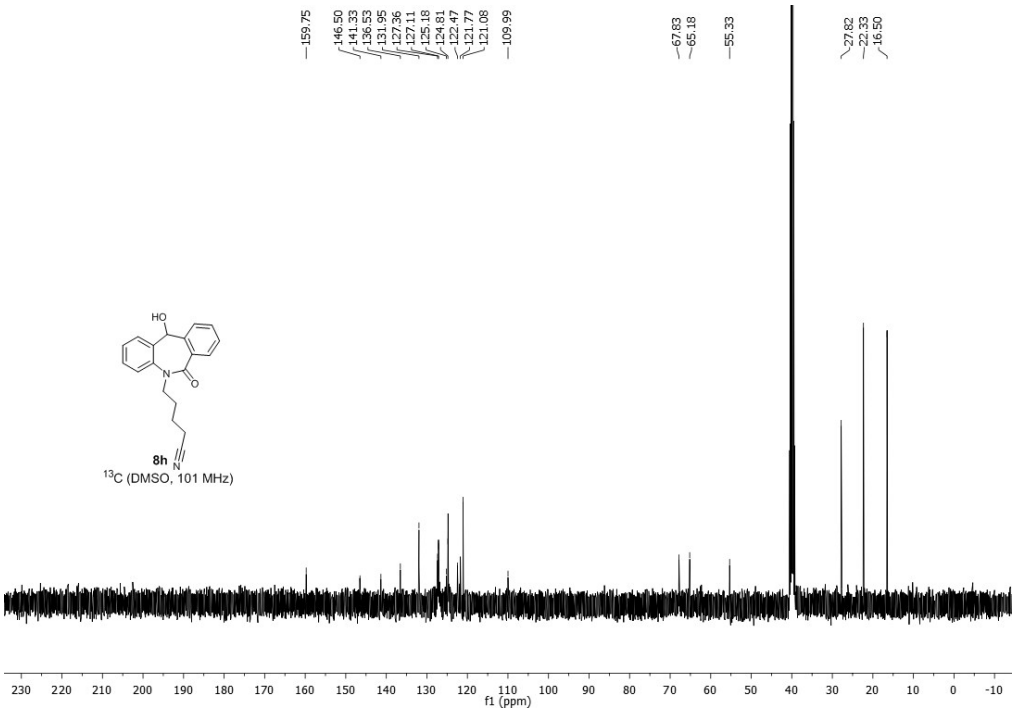
(S)-5-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (8h) (^{1}H NMR).



(S)-5-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (8h) (^{1}H-D_2O Experiment).



(S)-5-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (8h) (^{13}C NMR)



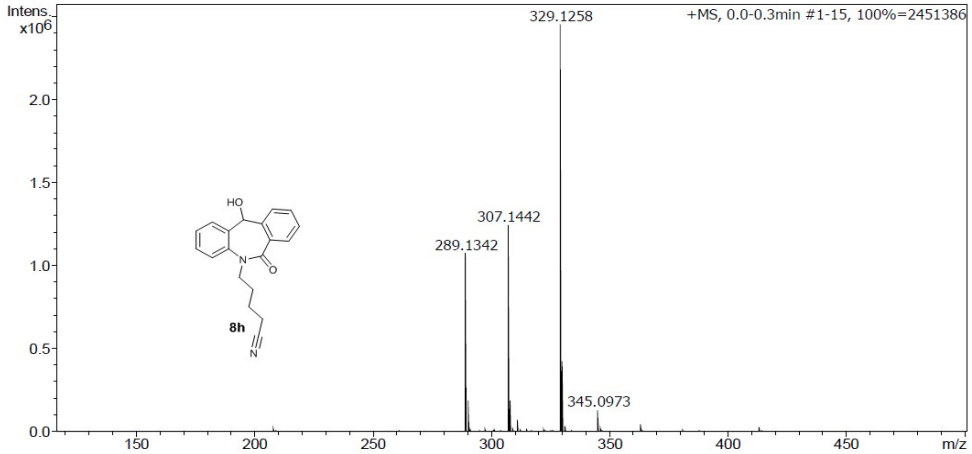
(S)-5-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)pentanenitrile (8h) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-6.d	Acquisition Date	9/24/2015 1:05:32 PM
Method	Tune_pos_NAICSI-1000.m	Operator	PG APP IN
Sample Name	EXT-ICT-BMB-VKV-6	Instrument	maXis impact 282001.00081
Comment	C19H18N2O2		

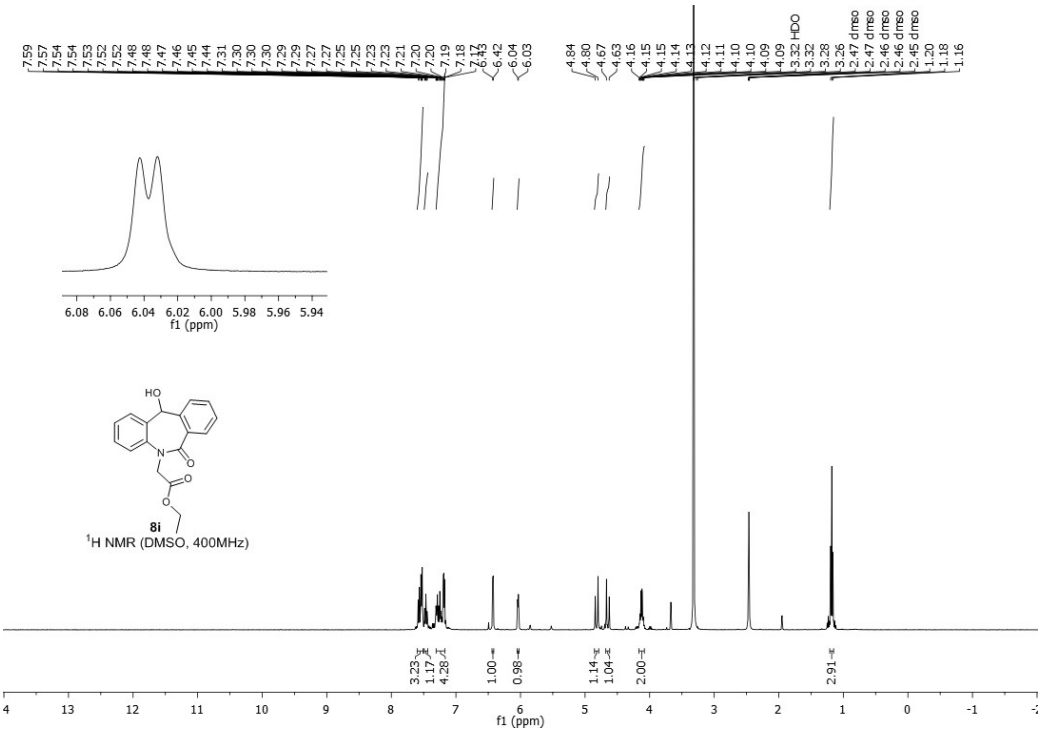
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

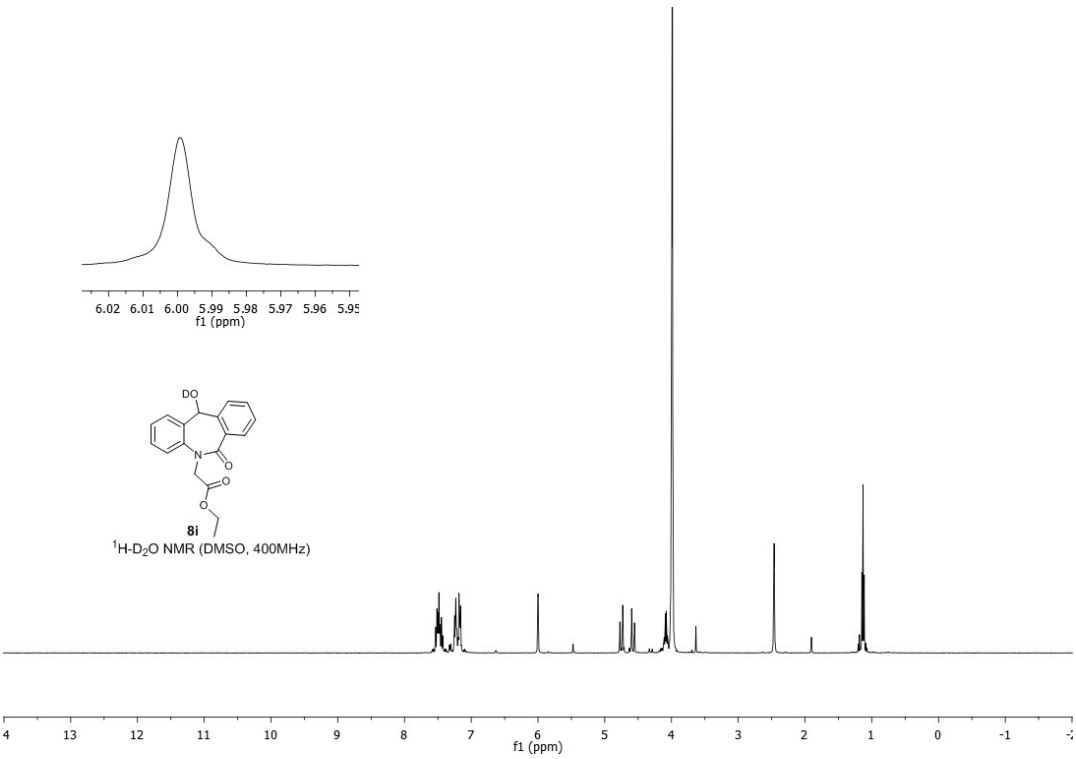


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e$^-$ Conf	N-Rule
307.1442	1	C19H19N2O2	307.1441	0.4	39.6	1	100.00	11.5	even	ok

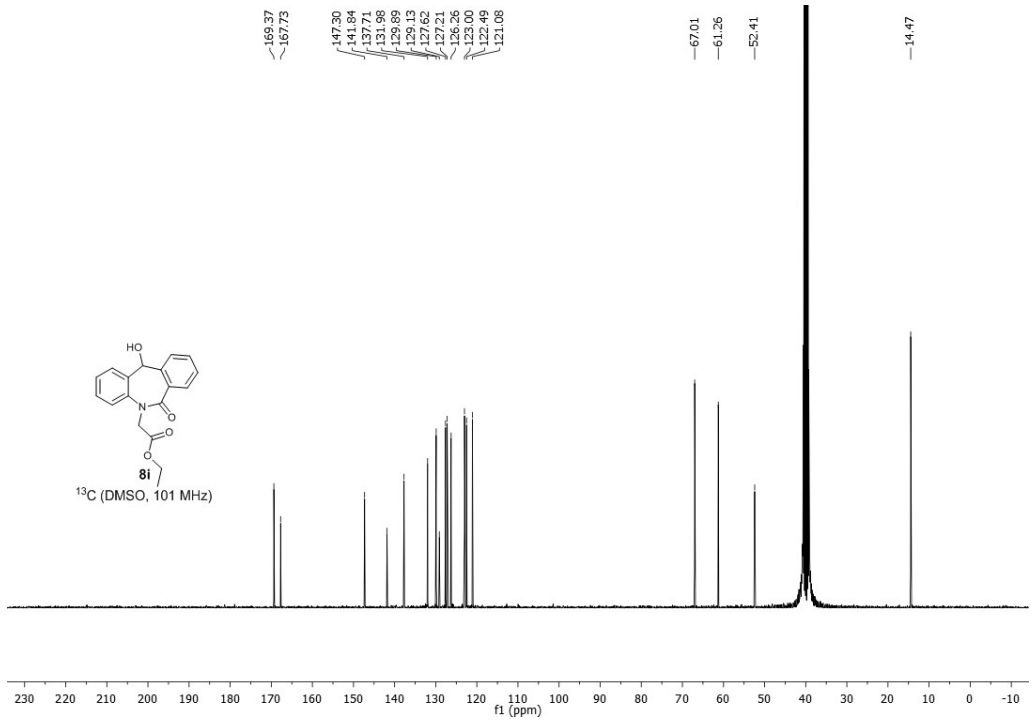
(S)-ethyl 2-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)acetate (8i) (^{1}H NMR)



(S)-ethyl 2-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b,e*]azepin-5-yl)acetate (8i) (^{1}H-D_2O Experiment)



(S)-ethyl 2-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b*,*e*]azepin-5-yl)acetate (8i) (^{13}C NMR)



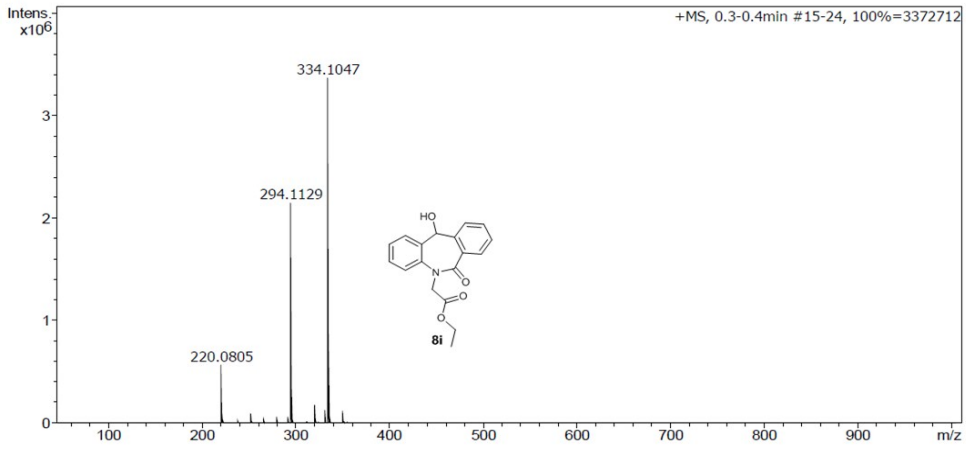
(S)-ethyl 2-(11-hydroxy-6-oxo-6,11-dihydro-5*H*-dibenzo[*b*,*e*]azepin-5-yl)acetate (8i) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-7.d	Acquisition Date	9/24/2015 12:50:15 PM
Method	Tune_pos_NAICSI-1000.m	Operator	PG APP IN
Sample Name	EXT-ICT-BMB-VKV-7	Instrument	maXis impact 282001.00081
Comment	C18H17NO4		

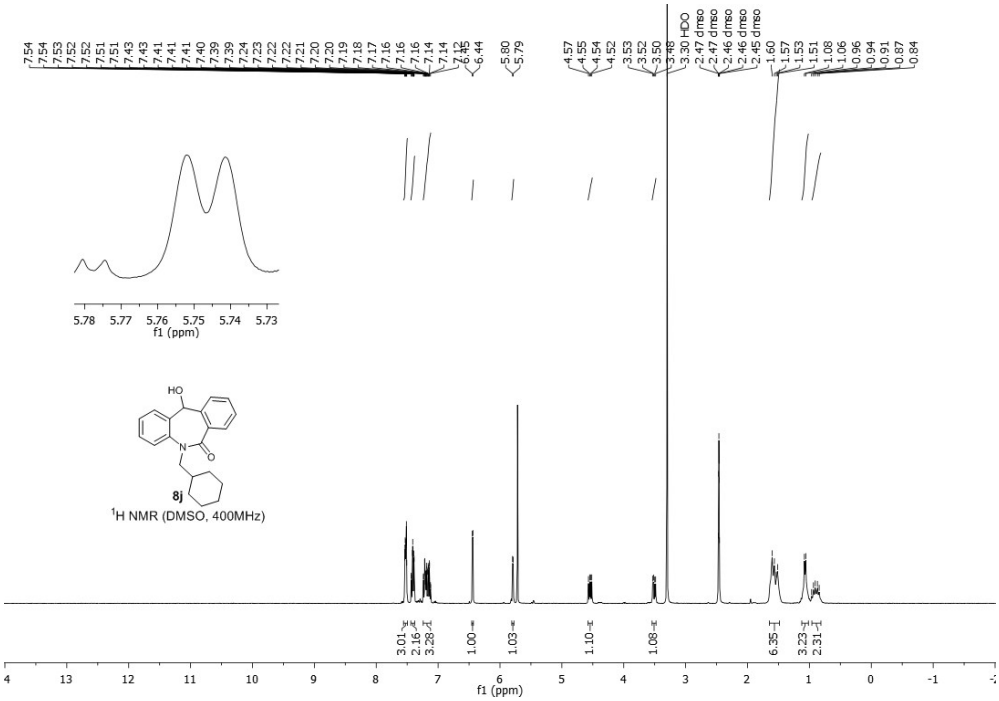
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

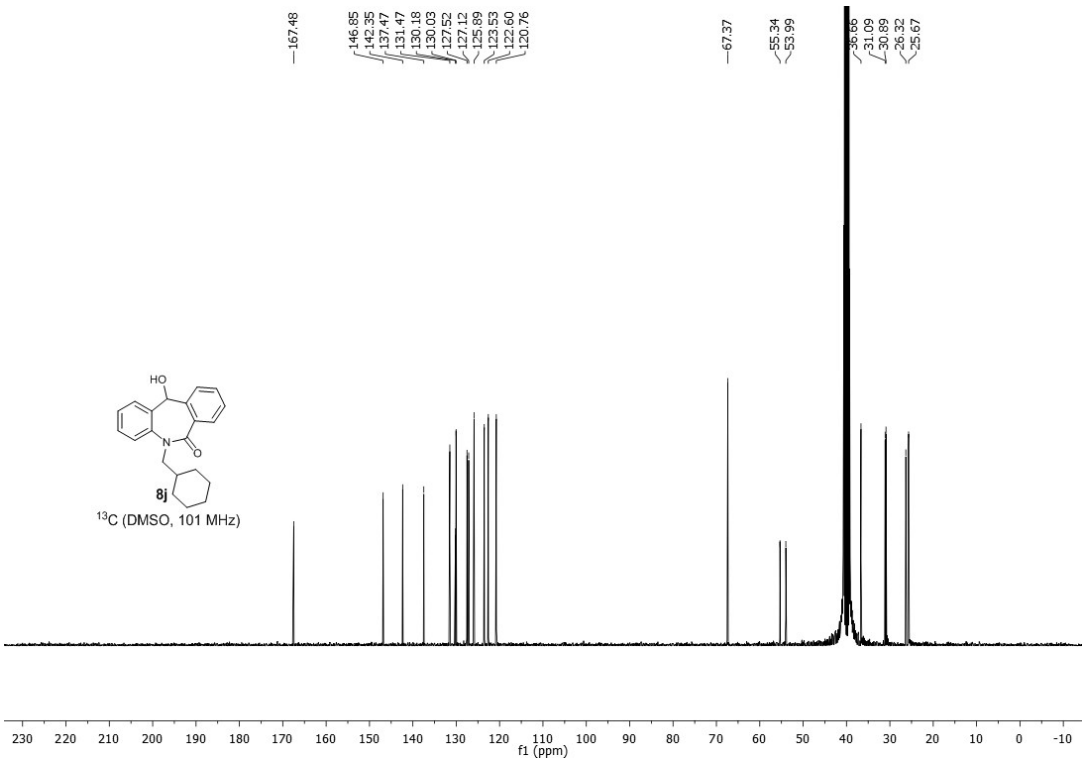


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
334.1047	1	C18H17NNaO4	334.1050	0.7	6.6	1	100.00	10.5	even	ok

(S)-5-(cyclohexylmethyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11H)-one (8j) (^{1}H NMR)



(S)-5-(cyclohexylmethyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8j) (^{13}C NMR)



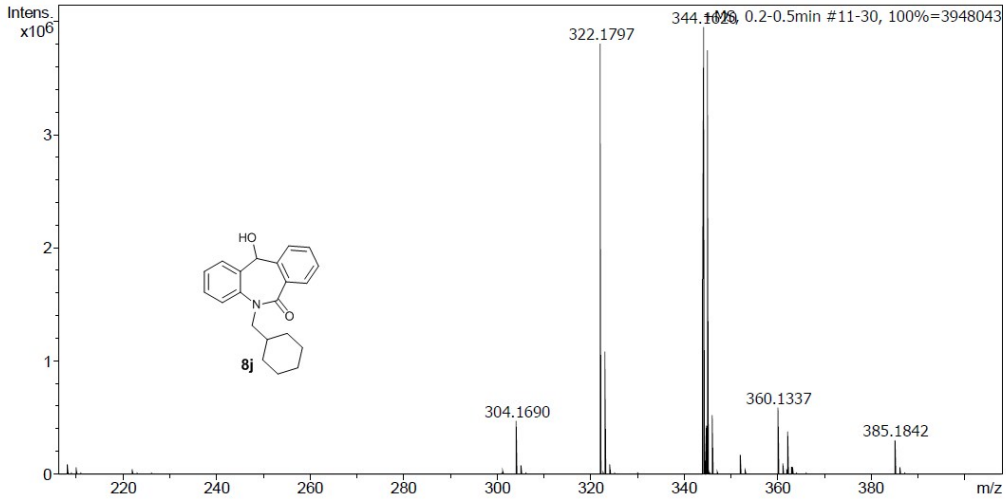
(S)-5-(cyclohexylmethyl)-11-hydroxy-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8j) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-9.d	Acquisition Date	9/24/2015 12:30:44 PM
Method	Tune_pos_NAICSI-1000.m	Operator	PG APP IN
Sample Name	EXT-ICT-BMB-VKV-9	Instrument	maXis impact 282001.00081
Comment	C21H23NO2		

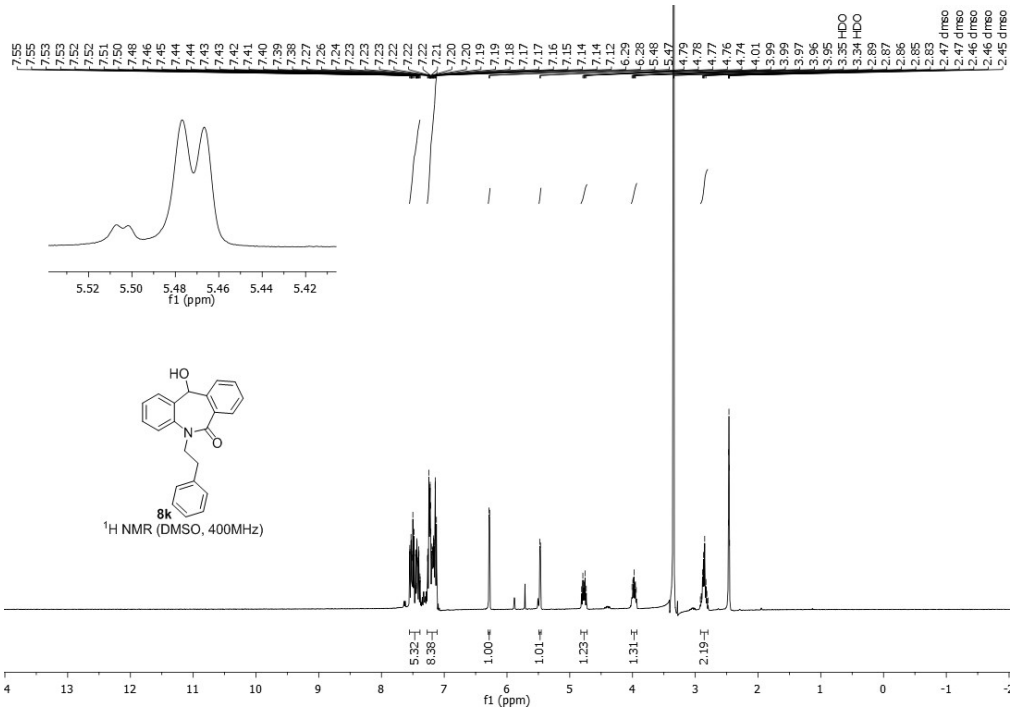
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

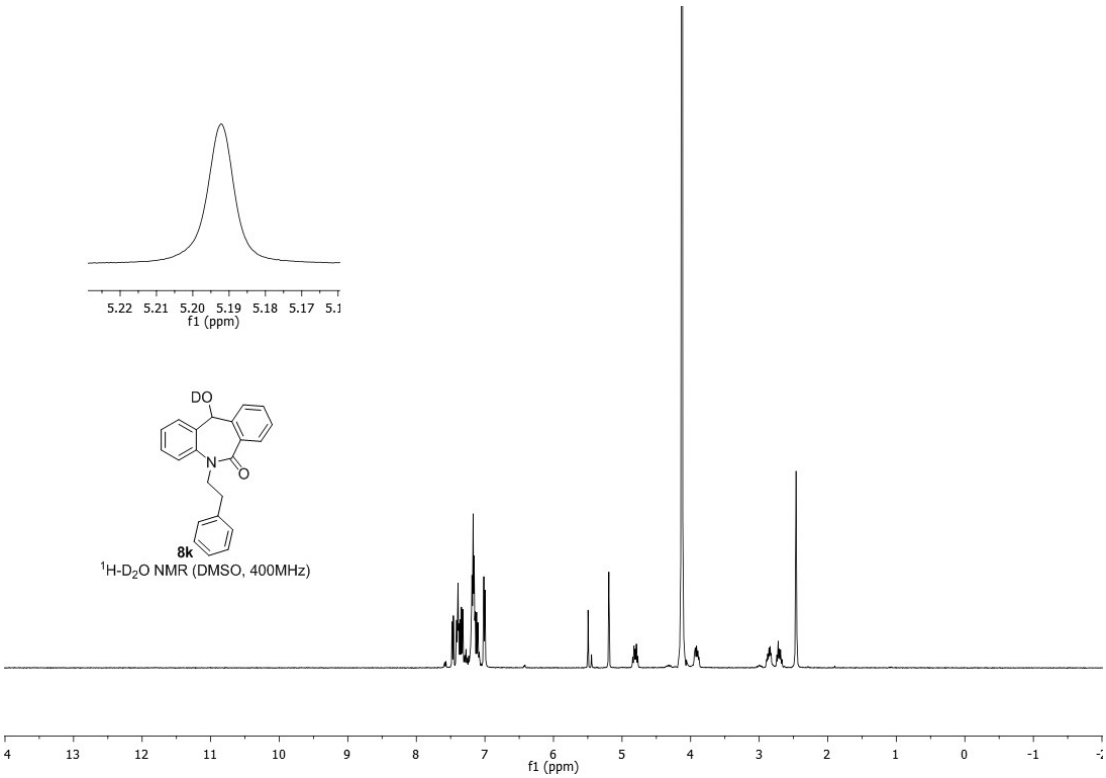


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
322.1797	1	C21H24NO2	322.1802	-1.5	29.6	1	100.00	10.5	even	ok

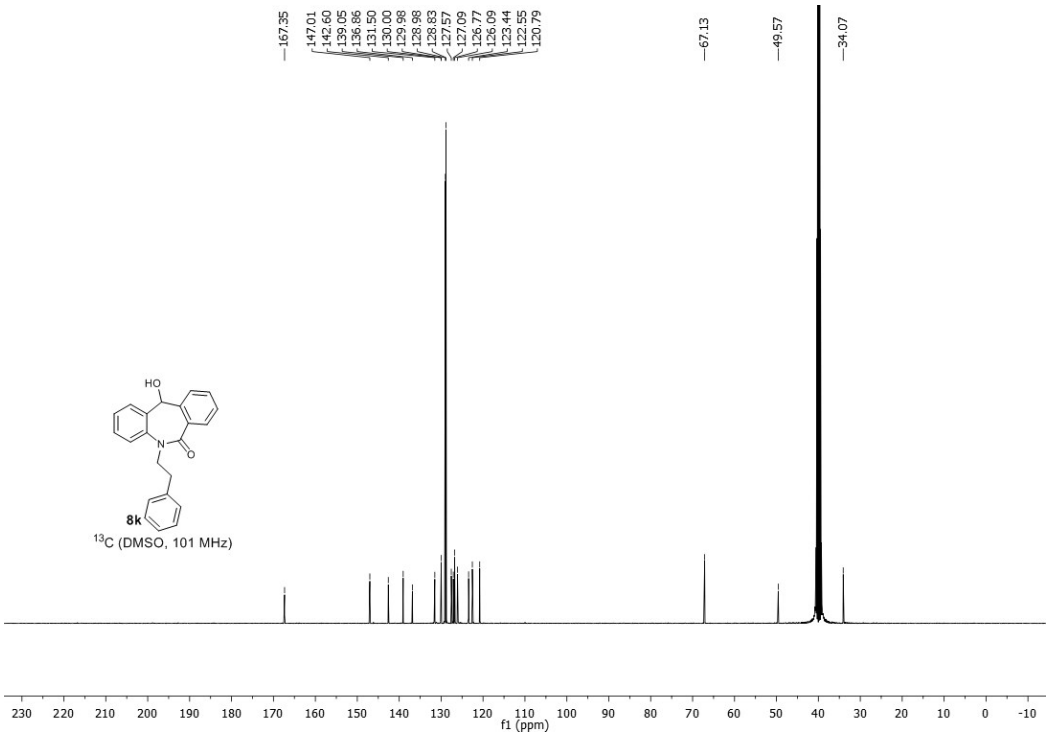
(S)-11-hydroxy-5-phenethyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8k) (^{1}H NMR)



(S)-11-hydroxy-5-phenethyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8k) (^{1}H-D_2O Experiment)



(S)-11-hydroxy-5-phenethyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8k) (^{13}C NMR)



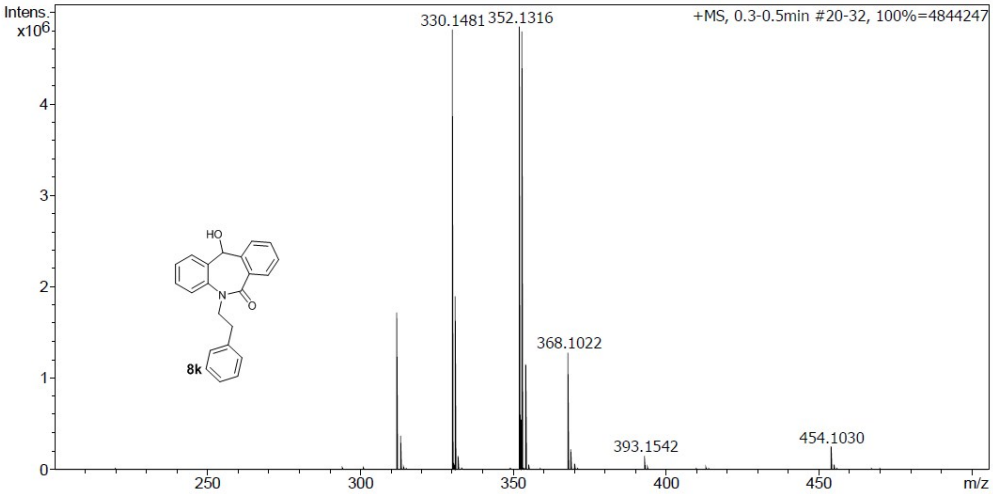
(S)-11-hydroxy-5-phenethyl-5*H*-dibenzo[*b*,*e*]azepin-6(11*H*)-one (8k) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-10.d	Acquisition Date	9/24/2015 12:19:06 PM
Method	Tune_pos_NAF_1000.m	Operator	PG APP IN
Sample Name	EXT-ICT-BMB-VKV-10	Instrument	maXis impact 282001.00081
Comment	C22H19NO2		

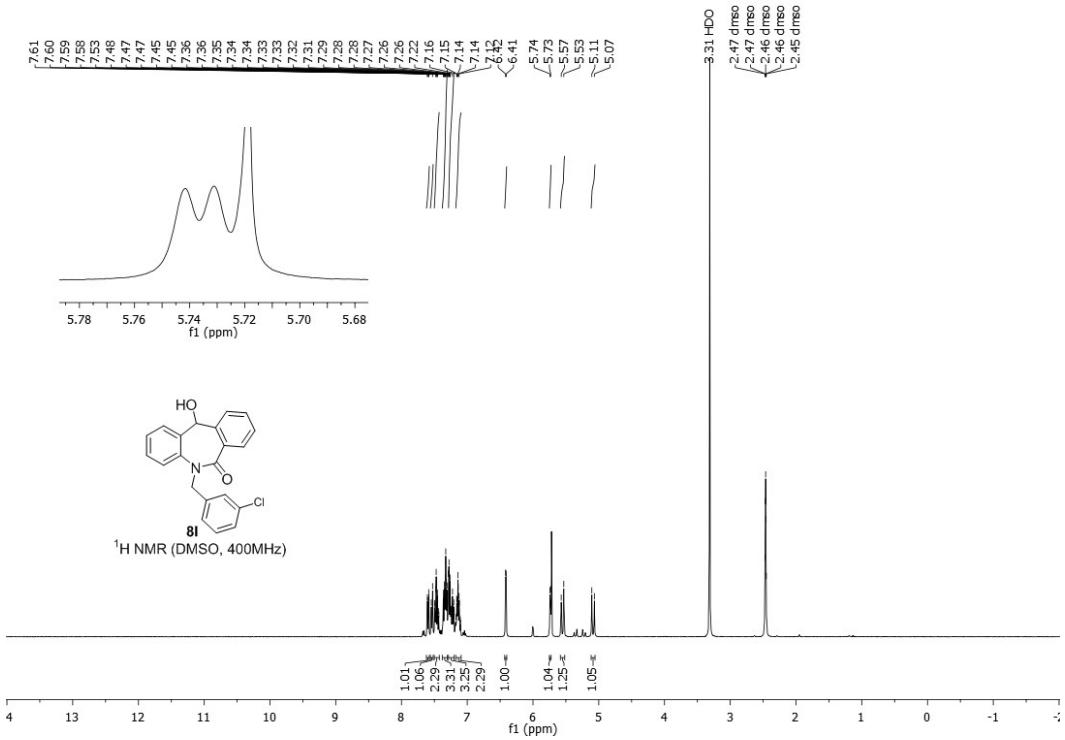
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source

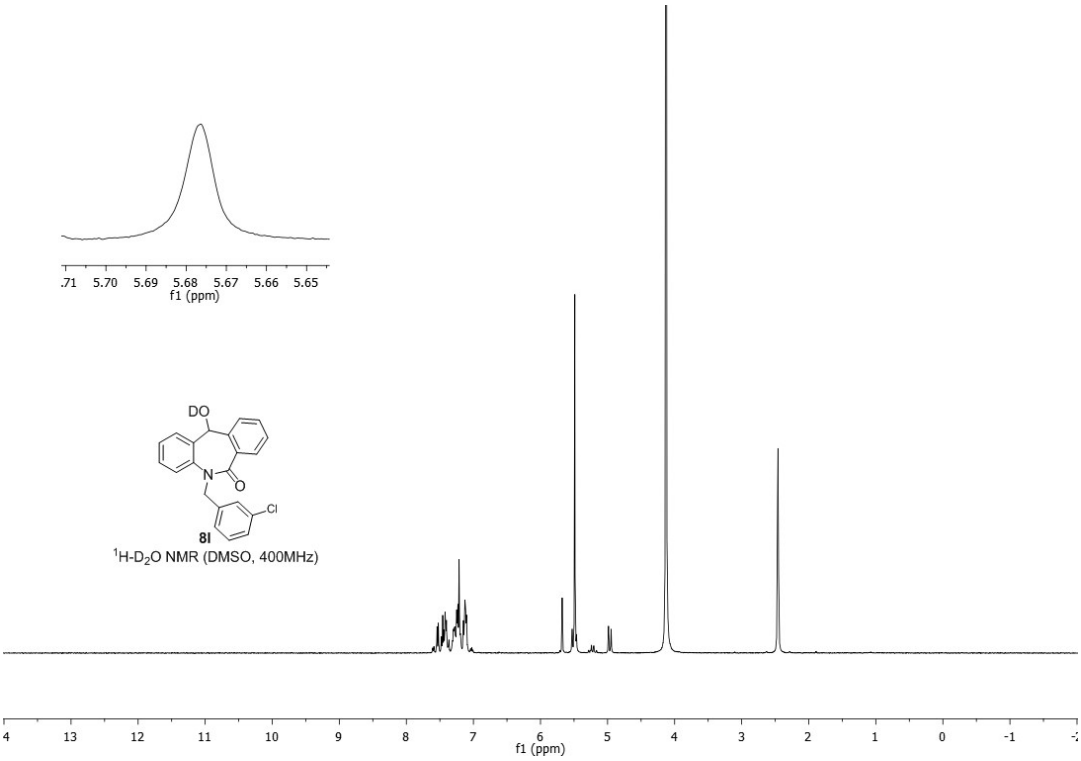


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
330.1481	1	C22H20NO2	330.1489	-2.4	86.0	1	100.00	13.5	even	ok

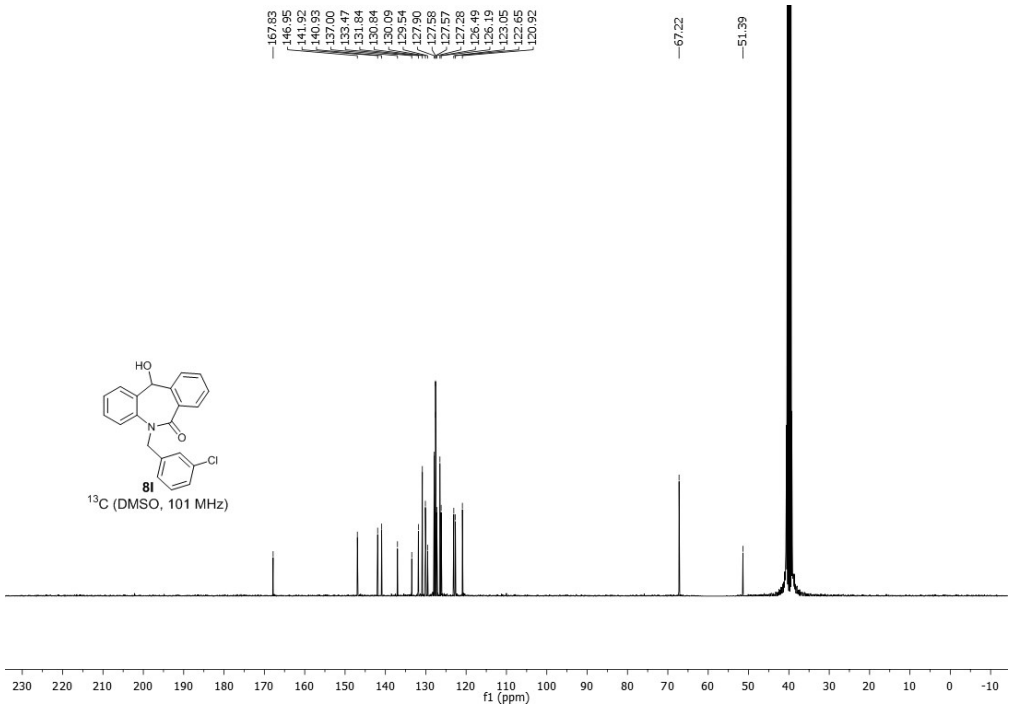
(S)-5-(3-chlorobenzyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8l) (^{1}H NMR)



(S)-5-(3-chlorobenzyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8l) (^{1}H-D_2O Experiment)



(S)-5-(3-chlorobenzyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8l) (^{13}C NMR)



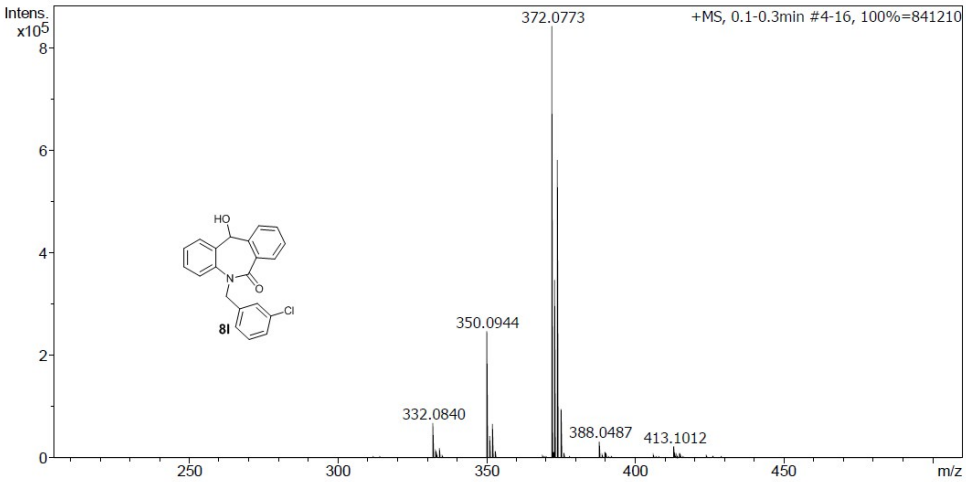
(S)-5-(3-chlorobenzyl)-11-hydroxy-5*H*-dibenzo[*b,e*]azepin-6(11*H*)-one (8l) (HRMS)

Analysis Info

Analysis Name	D:\Data\SEP 15\EXT-ICT-BMB-VKV-11.d	Acquisition Date	9/24/2015 4:10:09 PM
Method	Tune_pos_NAF_1000.m	Operator	SJG OUT
Sample Name	EXT-ICT-BMB-VKV-11	Instrument	maXis impact 282001.00081
Comment	C21H16NO2Cl		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source

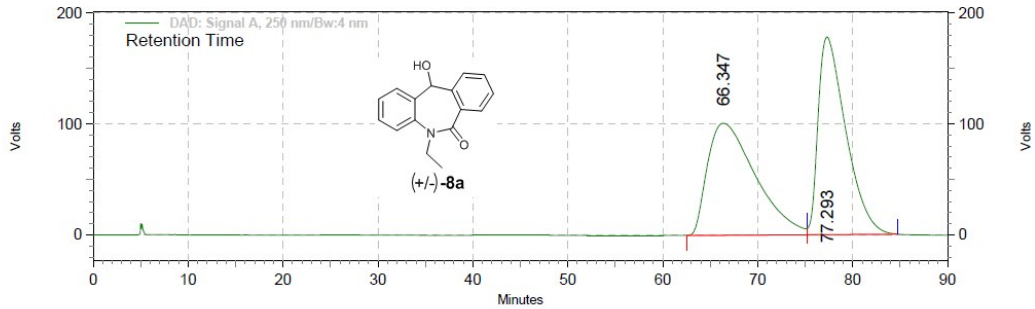


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
350.0944	1	C21H17ClNO2	350.0942	0.5	49.0	1	100.00	13.5	even	ok

HPLC copy of Racemic and chiral compounds (8a-8l)

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Et racemic 97 03 0.6 paper.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/20/2015 10:36:29 AM
Printed: 8/27/2015 4:19:35 PM

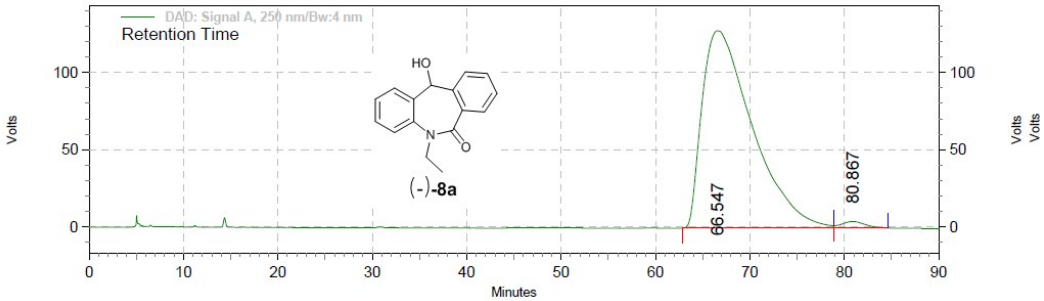


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
66.347	74354780	49.55	211724	36.18
77.293	75696035	50.45	373459	63.82
Totals	150050815	100.00	585183	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Et 97 03 0.6 chiral re.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/18/2015 6:14:23 PM
Printed: 8/27/2015 4:21:06 PM

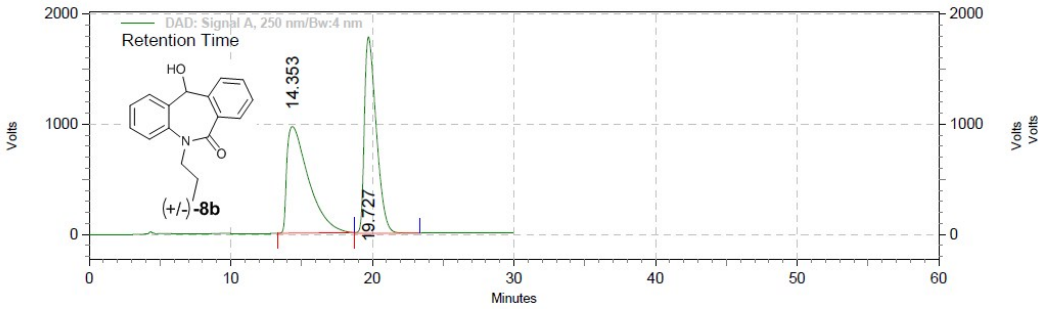


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
66.547	99046666	98.45	267502	96.77
80.867	1554837	1.55	8926	3.23
Totals	100601503	100.00	276428	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Pr 92 08 racemic final.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/17/2015 2:30:55 PM
Printed: 8/27/2015 4:34:55 PM

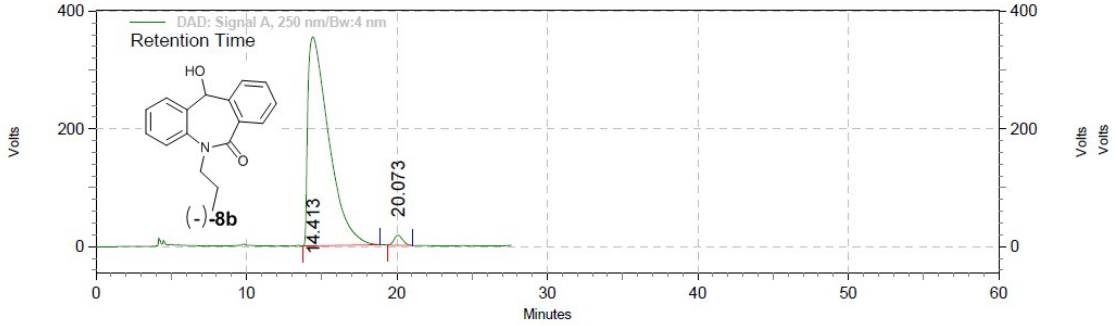


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
14.353	215238814	49.80	2026941	35.20
19.727	216990683	50.20	3731765	64.80
Totals	432229497	100.00	5758706	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Pr 92 08 chiral final.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/17/2015 3:02:56 PM
Printed: 8/27/2015 4:36:25 PM

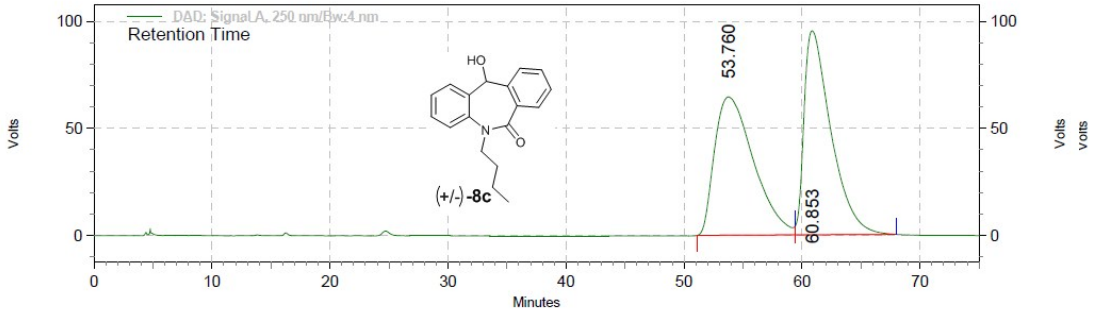


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
14.413	71634762	98.06	743823	95.45
20.073	1416177	1.94	35452	4.55
Totals	73050939	100.00	779275	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Bu Racemic 99 01 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/25/2015 10:09:49 AM
Printed: 8/27/2015 4:50:29 PM

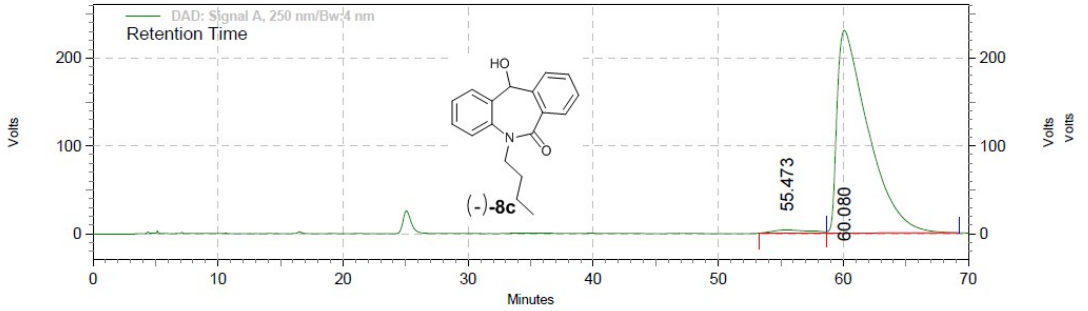


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
53.760	31079274	49.56	135335	40.42
60.853	31625026	50.44	199525	59.58
Totals	62704300	100.00	334860	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Bu chiral 99 01 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/25/2015 11:26:34 AM
Printed: 8/27/2015 4:51:28 PM

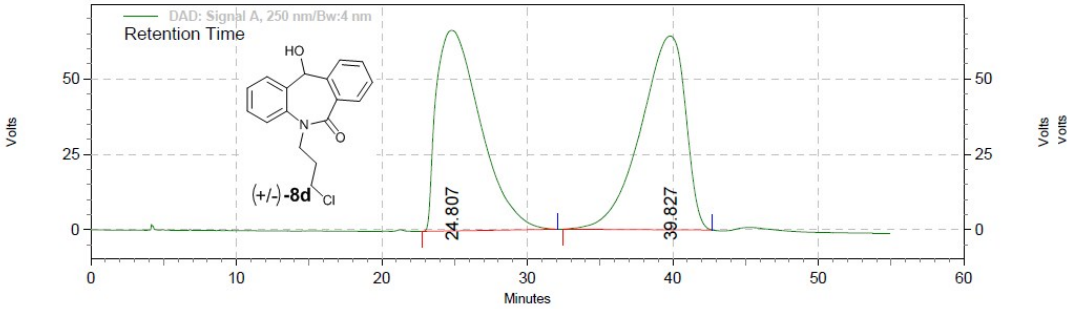


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
55.473	1654901	1.93	7783	1.58
60.080	83967936	98.07	483745	98.42
Totals	85622837	100.00	491528	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Cl racemic 92 08.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/11/2015 1:50:50 PM
Printed: 8/27/2015 4:28:22 PM

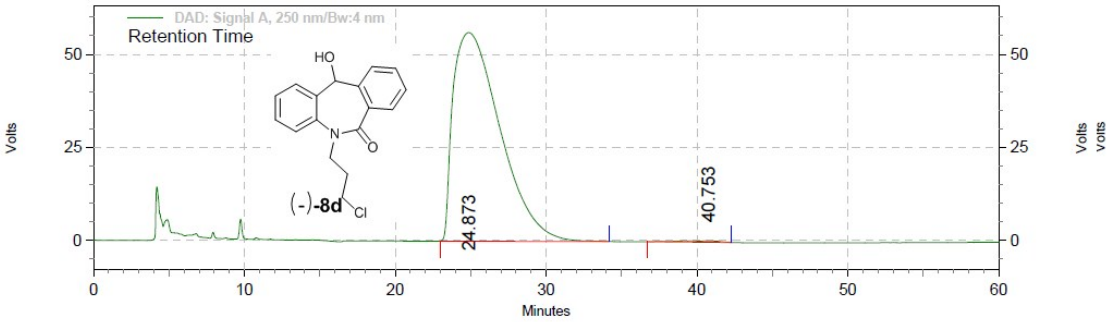


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
24.807	29380661	50.52	139332	50.85
39.827	28777429	49.48	134666	49.15
Totals	58158090	100.00	273998	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N cl 92 08 chiral.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/11/2015 2:47:46 PM
Printed: 8/27/2015 4:32:16 PM



DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
24.873	25472370	99.41	117701	99.30
40.753	150800	0.59	824	0.70
Totals	25623170	100.00	118525	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N allyl 97 03 0.6 racemic.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
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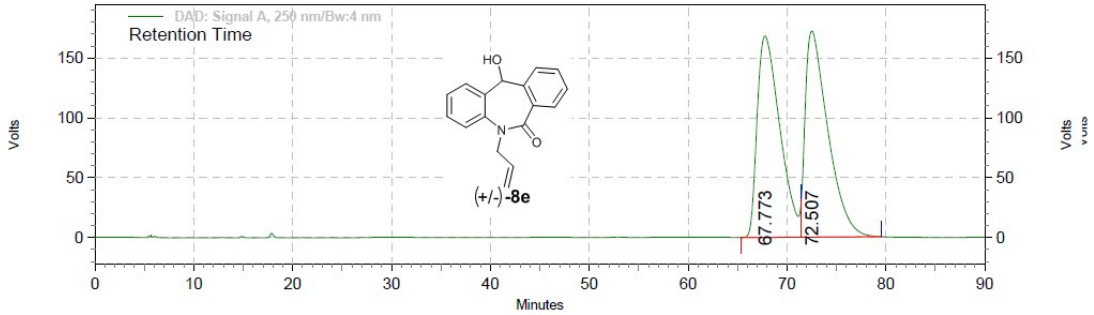
Printed: 8/27/2015 4:49:39 PM



DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
67.773	56600503	49.65	353223	49.44
72.507	57394489	50.35	361262	50.56
Totals	113994992	100.00	714485	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N allyl 97 03 0.6 chiral.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/22/2015 7:23:22 PM
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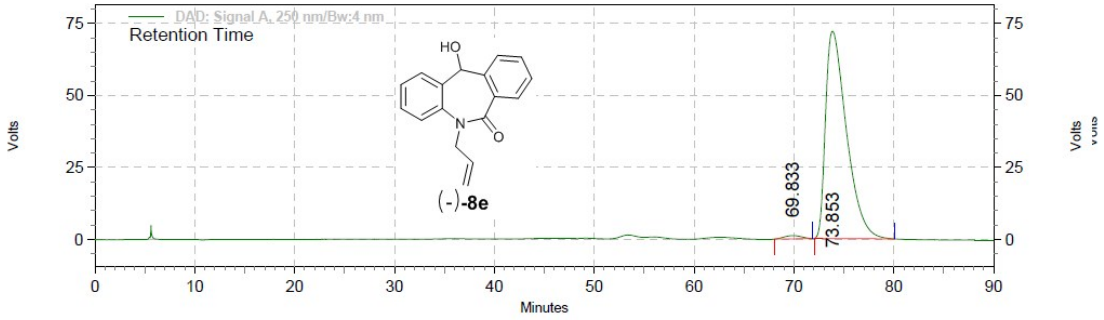
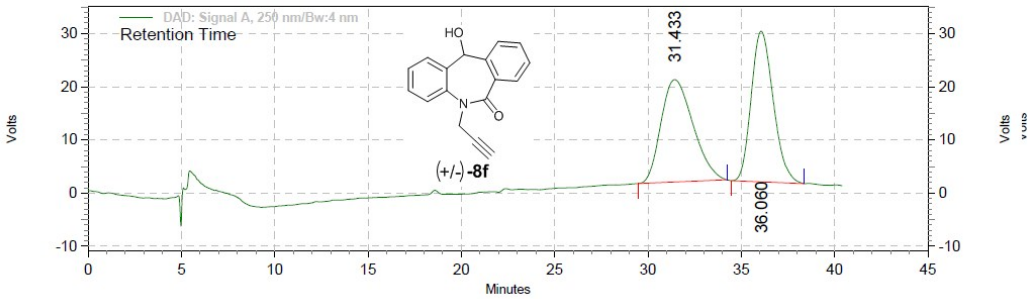


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
69.833	289437	1.30	2408	1.57
73.853	21952837	98.70	150690	98.43
Totals	22242274	100.00	153098	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Propyl\Racemic Propyl nn.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 1/13/2015 2:54:13 PM
Printed: 8/27/2015 5:08:31 PM

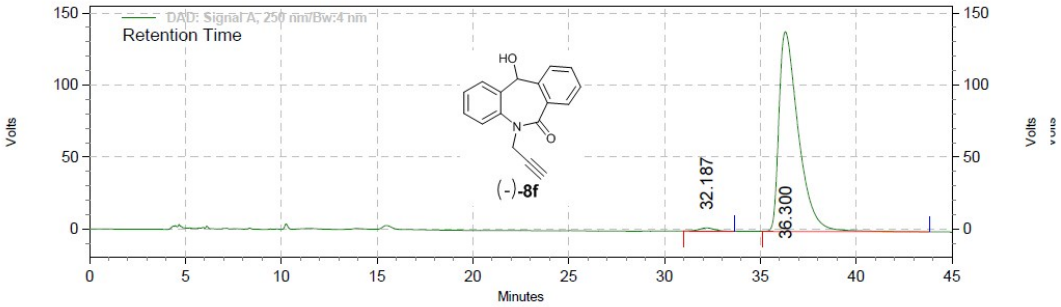


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
31.433	4829342	49.70	40392	40.46
36.060	4888034	50.30	59442	59.54
Totals	9717376	100.00	99834	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Propyl\Chiral confirmation on oj-h.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 3/27/2015 8:29:42 PM
Printed: 8/27/2015 5:19:04 PM

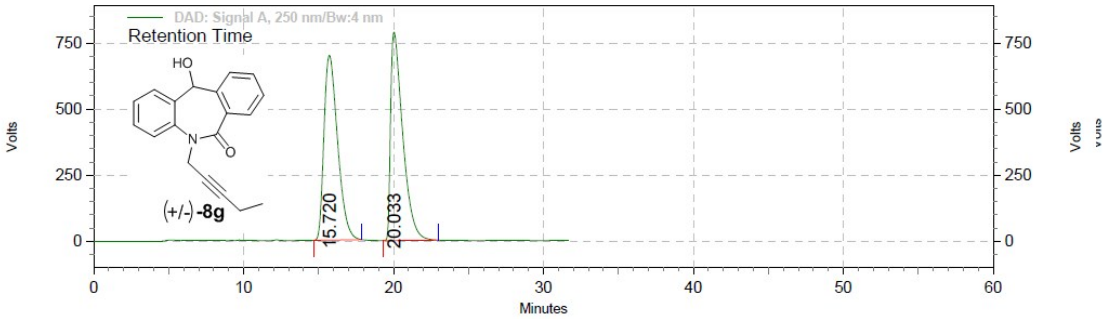


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
32.187	271186	1.31	4833	1.63
36.300	20483472	98.69	291172	98.37
Totals	20754658	100.00	296005	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N internal racemic 90 10 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/22/2015 10:30:44 AM
Printed: 8/27/2015 4:44:16 PM

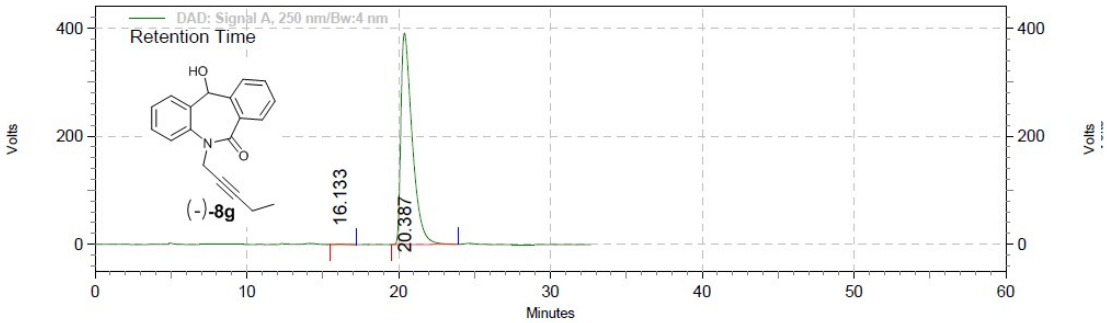


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
15.720	92782920	49.96	1466958	46.99
20.033	92934755	50.04	1654656	53.01
Totals	185717675	100.00	3121614	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N internal chiral 90 10 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/22/2015 11:04:25 AM
Printed: 8/27/2015 4:45:15 PM

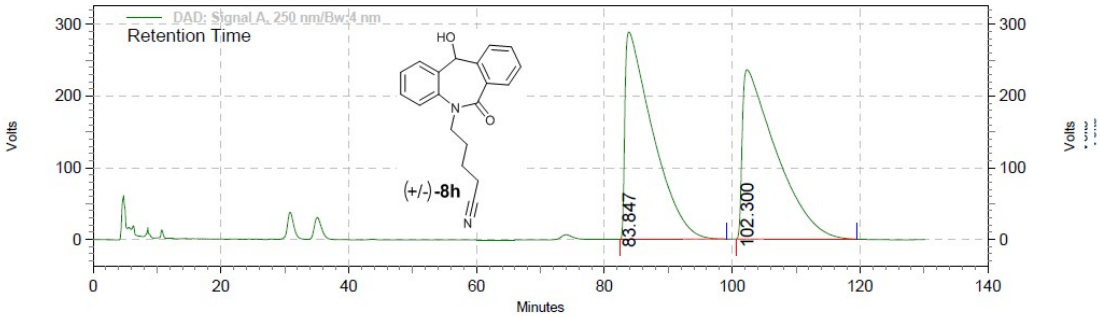


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
16.133	96575	0.23	1876	0.23
20.387	42665754	99.77	821081	99.77
Totals	42762329	100.00	822957	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N CN racemic new 90 10 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/24/2015 1:25:21 PM
Printed: 8/27/2015 5:00:36 PM

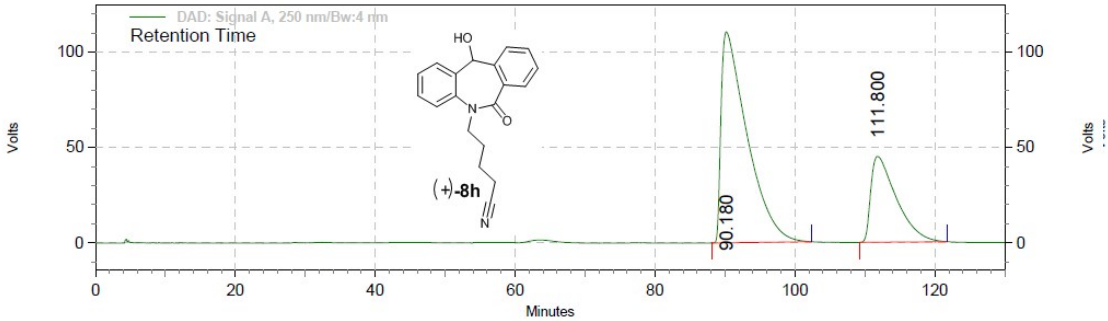


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
83.847	183048665	49.98	606492	55.02
102.300	183179708	50.02	495891	44.98
Totals	366228373	100.00	1102383	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N CN chiral new 90 10 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/24/2015 3:37:34 PM
Printed: 8/27/2015 5:01:17 PM

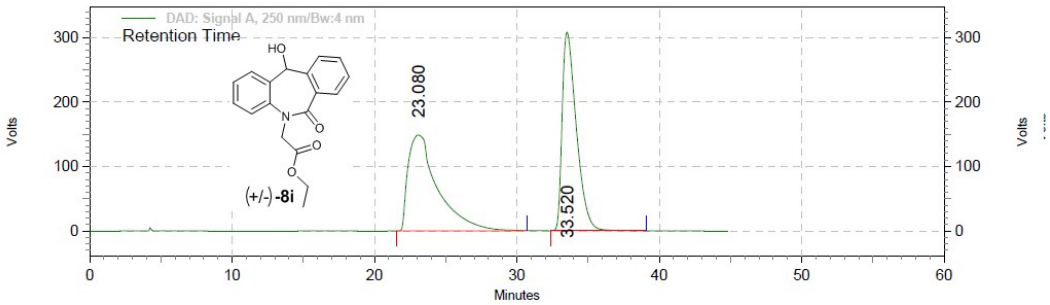


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
90.180	59813866	71.40	231877	71.08
111.800	23954037	28.60	94340	28.92
Totals	83767903	100.00	326217	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Ester 95 05 racemic.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/18/2015 12:44:22 PM
Printed: 8/27/2015 4:41:23 PM

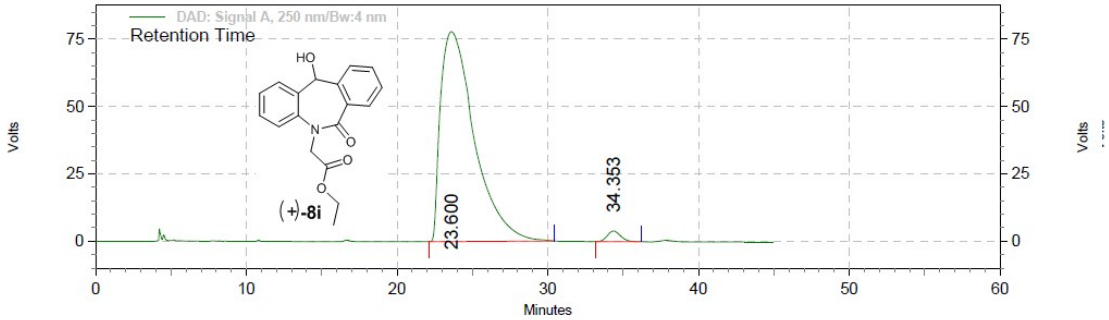


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
23.080	45035383	50.14	311835	32.55
33.520	44781672	49.86	646233	67.45
Totals	89817055	100.00	958068	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Ester 95 05 chiral.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/18/2015 1:31:05 PM
Printed: 8/27/2015 4:42:50 PM

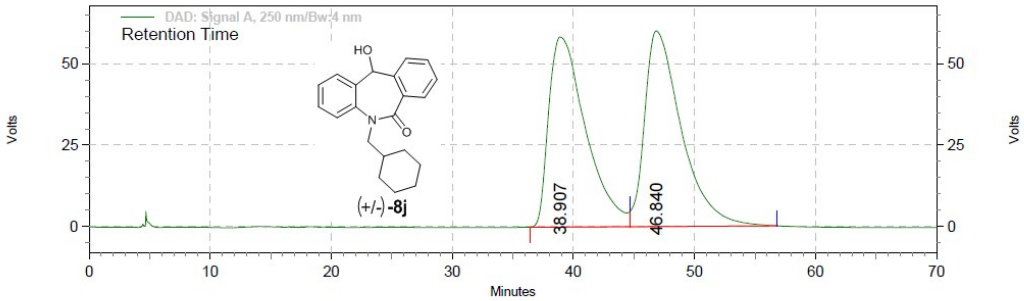


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
23.600	25445181	98.00	163320	95.14
34.353	518066	2.00	8346	4.86
Totals	25963247	100.00	171666	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Cy Racemic 99 01 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/25/2015 12:38:21 PM
Printed: 8/27/2015 4:53:16 PM

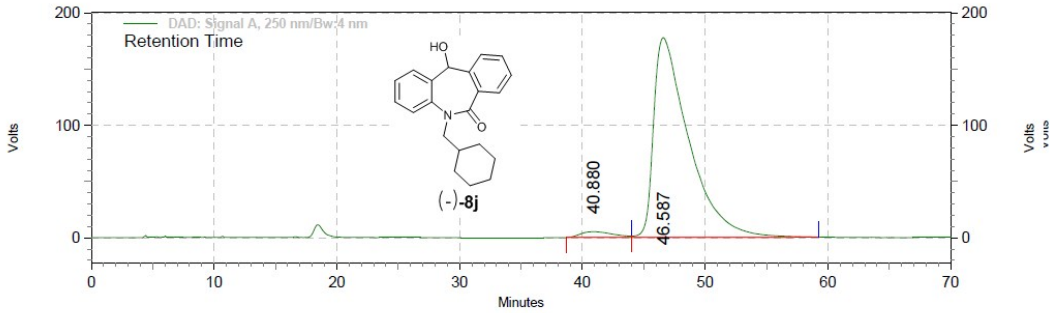


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
38.907	26097057	49.42	122801	49.28
46.840	26708812	50.58	126376	50.72
Totals	52805869	100.00	249177	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Cy chiral 99 01 0.7.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/25/2015 1:50:08 PM
Printed: 8/27/2015 4:54:01 PM

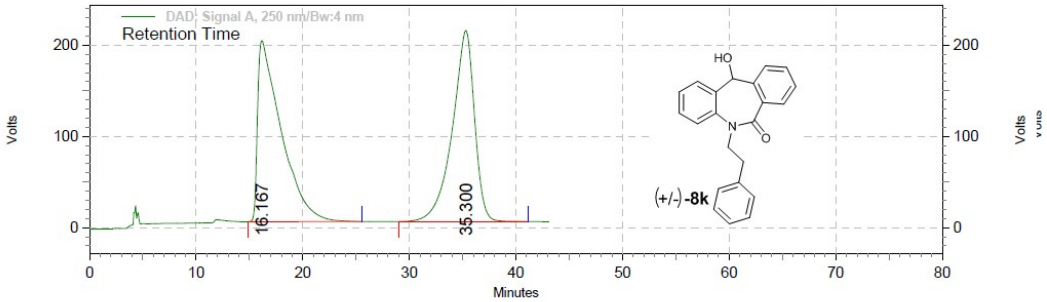


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
40.880	1988923	2.61	10897	2.84
46.587	74131683	97.39	372192	97.16
Totals	76120606	100.00	383089	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Ph 90 10 racemic final.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/17/2015 3:32:42 PM
Printed: 8/27/2015 4:38:44 PM

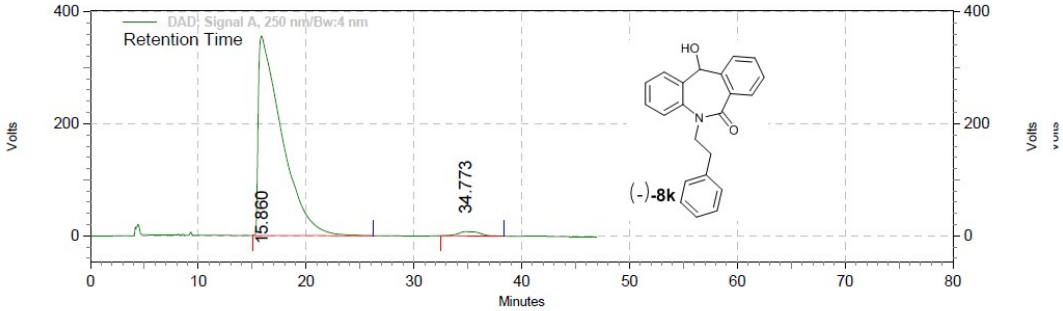


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
16.167	64202368	50.21	416698	48.67
35.300	63656457	49.79	439494	51.33
Totals	127858825	100.00	856192	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\data for manu\N Ph 90 10 chiral final.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/17/2015 4:17:56 PM
Printed: 8/27/2015 4:40:07 PM

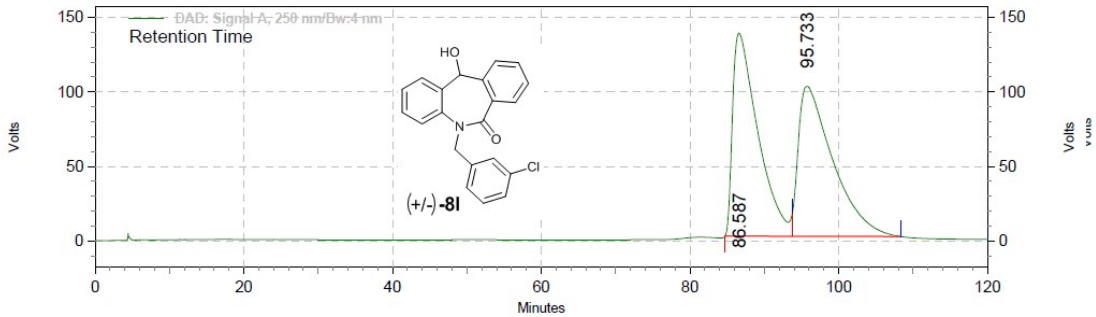


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
15.860	112762783	98.01	745897	97.91
34.773	2290351	1.99	15921	2.09
Totals	115053134	100.00	761818	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Ph Cl 96 04 0.7 racemic.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/24/2015 8:49:31 AM
Printed: 8/27/2015 4:58:31 PM

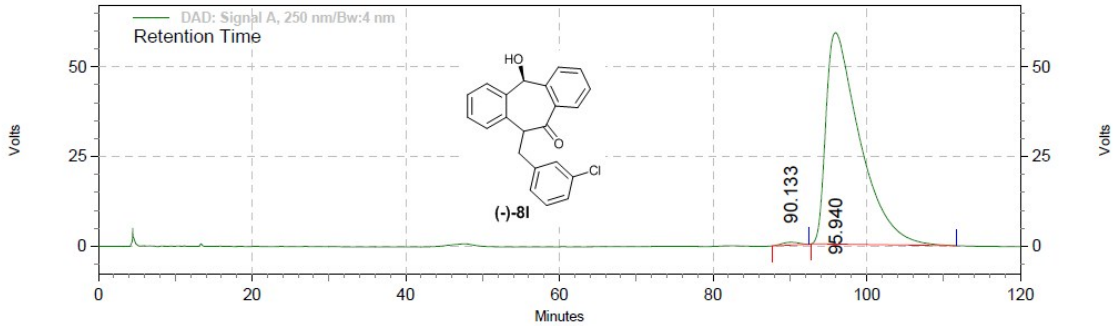


DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
86.587	67403198	49.71	285764	57.54
95.733	68196417	50.29	210844	42.46
Totals	135599615	100.00	496608	100.00

Area % Report

Data File: D:\ICT\Data\vijay\Substrate study\On OD-H Column\110815\N Ph Cl 96 04 0.7 chiral.dat
Method: D:\ICT\Method\VIJAY\rac N-Boc 90 10 0.7ml.met
Acquired: 8/24/2015 10:51:21 AM
Printed: 8/27/2015 4:59:16 PM



DAD: Signal A,
250 nm/Bw:4 nm
Results

Retention Time	Area	Area %	Height	Height %
90.133	258528	0.68	1683	1.35
95.940	37860550	99.32	123447	98.65
Totals	38119078	100.00	125130	100.00