Supporting Information:

Synthesis and Enantioselective Hydrogenation of Seven-membered Cyclic Imines: Substituted Dibenzo[*b*,*f*][1,4]oxazepines

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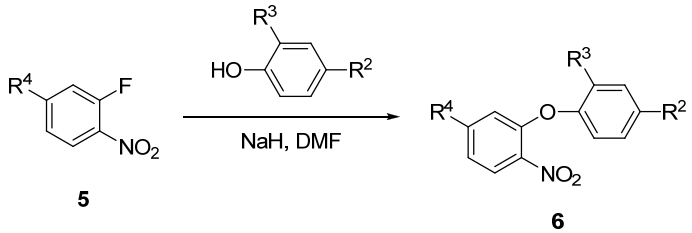
1. General and Materials

General: All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques, unless otherwise noted. ^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature in $CDCl_3$ on 400 MHz instrument with tetramethylsilane (TMS) as internal standard. Enantiomeric excess was determined by HPLC analysis, using chiral column described below in detail. Optical rotations were measured by polarimeter. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis. The configuration was determined by X-ray crystallographic analysis.

Materials: Commercially available reagents were used throughout without further purification other than those detailed below. The solvents for asymmetric hydrogenation reaction were purchased without further purification.

2. Typical Procedure for the Preparation of Diaryl Ether

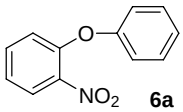


5 **6**

Typical Procedure for the Preparation of Diphenyl Ether 6a: To a reaction mixture of

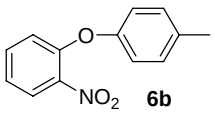
NaH (0.32 g, 8 mmol) and DMF (10 mL) was added dropwise a solution of phenol (0.71 g, 7.5 mmol) in DMF, it was stirred for 1 h at room temperature. Subsequently, *o*-fluoro nitrobenzene (0.71 g, 5 mmol) in DMF (2 mL) was dropped slowly to the mixture above and stirred for another 1 h at room temperature, then stirred for 12 h at 50 ^{o}C. After routine workup, the crude product was purified by flash chromatography on silica gel using petroleum ether and EtOAc to give **6a**.

1-nitro-2-phenoxybenzene (6a).[1] 92% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00-7.06 (m, 3H), 7.17-7.21 (m, 2H), 7.36-7.40 (m, 2H), 7.48-7.49 (m, 1H), 7.95 (dd, *J* = 8.2, 1.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.1, 119.4, 120.7, 123.3, 124.8, 125.9, 130.3, 134.3, 150.9, 156.0.



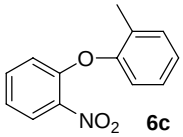
6a

1-nitro-2-(*p*-tolyloxy)benzene (6b).[2] 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 3H), 6.96 (dd, *J* = 8.0, 5.0 Hz, 3H), 7.16 (dd, *J* = 14.6, 8.0 Hz, 3H), 7.44-7.49 (m, 1H), 7.92 (dd, *J* = 8.0, 1.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 119.6, 120.0, 122.8, 125.8, 130.7, 134.2, 134.6, 141.2, 151.5, 153.4.



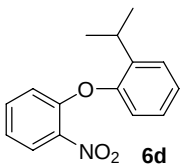
6b

1-methyl-2-(2-nitrophenoxy)benzene (6c).[3] 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.23 (s, 3H), 6.80 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 7.9 Hz, 1H), 7.12-7.15 (m, 2H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 1.6 Hz, 1H), 7.93 (dd, *J* = 8.0, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 118.5, 120.0, 122.3, 125.5, 125.9, 127.6, 130.2, 132.0, 134.3, 140.5, 151.3, 153.1.



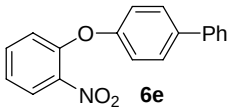
6c

1-isopropyl-2-(2-nitrophenoxy)benzene (6d). 75% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (d, *J* = 8.0 Hz, 3 H), 1.26 (d, *J* = 4.7 Hz, 3H), 3.21-3.28 (m, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.91 (t, *J* = 4.9 Hz, 1H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.19-7.21 (m, 2H), 7.39 (t, *J* = 4.4 Hz, 1H), 7.44 (t, *J* = 1.1 Hz, 1H), 7.95 (dd, *J* = 8.0, 1.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.1, 27.4, 118.7, 120.0, 122.3, 125.6, 125.9, 127.3, 127.6, 134.2, 140.5, 140.7, 151.7, 152.2; HRMS Calculated for $C_{15}H_{15}NO_3Na[M+Na]^{+}$280.0950, found 280.0948.



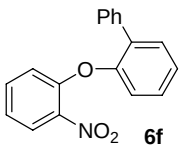
6d

4-(2-nitrophenoxy)biphenyl (6e).[3] 81% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09-7.13 (m, 3H), 7.18-7.22 (m, 1H), 7.29-7.36 (m, 1H), 7.45 (t, *J* = 7.3 Hz, 2H), 7.53-7.61 (m, 5H), 7.98 (dd, *J* = 8.2, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.6, 120.9, 123.5, 126.0, 127.2, 127.5, 128.9, 129.0, 134.4, 137.9, 140.4, 141.6, 150.8, 155.5.



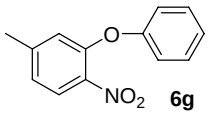
6e

2-(2-nitrophenoxy)biphenyl (6f).[4] 83% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (d, *J* = 8.4 Hz, 1H), 7.00 (t, *J* = 7.8 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 6.8 Hz, 1H), 7.30-7.38 (m, 5H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.0, 120.8, 122.4, 125.8, 127.7, 128.4, 129.2, 131.8, 134.1, 137.0, 140.5, 151.2, 152.0.



6f

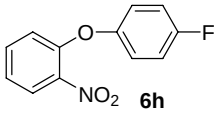
4-methyl-1-nitro-2-phenoxybenzene (6g).[5] 27% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 6.80 (s, 1H), 6.98-7.05 (m, 3H), 7.18 (dd, *J* = 7.4, 1.0 Hz, 1H), 7.35-7.40 (m, 2H), 7.89 (dd, *J*



6g

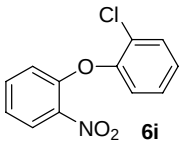
= 8.4, 1.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8, 119.3, 121.2, 124.2, 124.6, 126.0, 130.2, 139.2, 146.2, 150.9, 156.1.

1-(4-fluorophenoxy)-2-nitrobenzene (6h).[6] 81% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (d, *J* = 8.4 Hz, 1H), 6.99-7.08 (m, 4H), 7.19 (dd, *J* = 13.6, 7.9 Hz, 1H), 7.50 (t, *J* = 7.9 Hz, 1H), 7.92 (t, *J* = 3.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.7, 117.0, 120.0, 121.0, 123.3, 125.9, 134.4, 141.3, 151.4 (d, $J_{C\text{-}F}$ = 65 Hz), 159.6 (d, $J_{C\text{-}F}$ = 242 Hz).



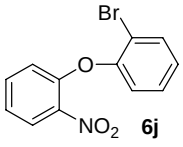
6h

1-chloro-2-(2-nitrophenoxy)benzene (6i).[7] 81% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (d, *J* = 8.4 Hz, 1H), 6.99 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.10-7.14 (m, 2H), 7.18-7.21 (m, 1H), 7.39-7.43 (m, 2H), 7.90 (dd, *J* = 8.2, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.1, 121.6, 123.4, 126.1, 126.4, 128.5, 131.3, 134.5, 140.6, 150.5, 151.0.



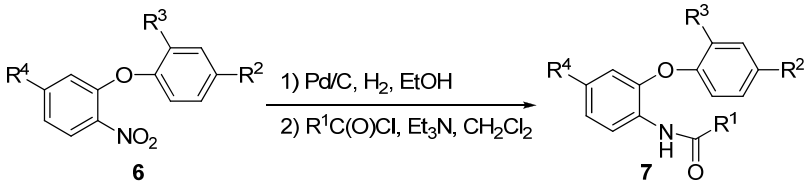
6i

1-bromo-2-(2-nitrophenoxy)benzene (6j).[8] 82% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (d, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 7.11 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.20 (t, *J* = 8.1 Hz, 1H), 7.33 (t, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 8.3 Hz, 1H), 7.65 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.98 (d, *J* = 8.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.3, 119.3, 121.4, 123.4, 126.1, 126.6, 129.2, 134.3, 134.5, 150.4, 152.3.



6j

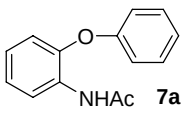
3. Typical Procedure for the Reduction of Nitro Group and Acylation



6 **7**

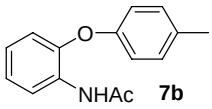
Typical Procedure for the Preparation of Intermediate 7a: Compound **6a** (2.0 g, 9.3 mmol) was dissolved in 5 mL of EtOH, 5% palladium on charcoal (0.10 g) and 0.25 ml of AcOH were added to the solution, the reduction was carried out with hydrogen gas at an initial pressure of 60 psi for 12 h. The catalyst was filtered off. Then concentration in vacuo and purification by flash chromatography afforded aniline derivative. Subsequently, the product was dissolved in 20 mL of CH_2Cl_2 and cooled to 0 ^{o}C, then acetyl chloride (0.70 g, 8.9 mmol) was added slowly to the solution, the temperature increased spontaneous to ambient temperature, and monitored by TLC. Then water (20 mL) was added to the mixture. The organic layers was washed by brine (1×30 mL), dried by anhydrous Na_2SO_4, concentrated in vacuo. The residue was purified by flash chromatography on silica gel using petroleum ether and EtOAc to give **7a**.

***N*-(2-phenoxyphenyl)acetamide** (7**a**).[5] White solid, mp = 74-76 ^{o}C, 89% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.16 (s, 3H), 6.83 (d, *J* = 8.1 Hz, 1H), 7.01 (dd, *J* = 14.0, 8.1 Hz, 3H), 7.09-7.17 (m, 2H), 7.36 (t, *J* = 8.4 Hz, 2H), 7.77 (br, 1H), 8.43 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 117.8, 118.8, 121.1, 124.1, 124.2, 130.0, 130.2, 145.7, 156.6, 168.5.



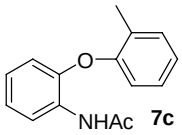
7a

***N*-(2-(*p*-tolyloxy)phenyl)acetamide (7b).**[5] White solid, mp = 74-75 °C, 92% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H), 2.35 (s, 3H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.91-6.99 (m, 3H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 7.79 (br, 1H), 8.43 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 25.1, 117.2, 119.0, 120.9, 123.8, 124.0, 129.7, 130.6, 133.8, 146.2, 154.1, 168.5.



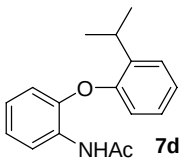
7b

***N*-(2-(*o*-tolyloxy)phenyl)acetamide (7c).**[5] White solid, mp = 79-82 °C, 92% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H), 2.24 (s, 3H), 6.59 (d, *J* = 8.1 Hz, 1H), 6.91 (dd, *J* = 16.7, 7.9 Hz, 2H), 7.03 (t, *J* = 7.8 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.89 (br, 1H), 8.43 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.2, 25.0, 115.5, 119.9, 120.8, 123.1, 123.9, 124.8, 127.6, 128.9, 129.9, 131.8, 146.3, 153.8, 168.5.



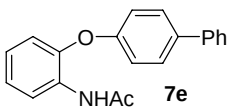
7c

***N*-(2-(2-isopropylphenoxy)phenyl)acetamide (7d)**. White solid, mp = 63-66 °C, 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.26 (s, 3H), 1.27 (s, 3H), 2.20 (s, 3H), 3.24-3.31 (m, 1H), 6.66 (d, *J* = 8.1 Hz, 1 H), 6.86 (t, *J* = 5.6 Hz, 1H), 6.95 (t, *J* = 8.0 Hz, 1H), 7.06 (t, *J* = 7.7 Hz, 1H), 7.18 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.39 (dd, *J* = 5.4, 3.6 Hz, 1H), 7.88 (br, 1H), 8.44 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.2, 25.0, 27.2, 116.0, 119.7, 120.8, 123.2, 124.0, 125.0, 127.3, 129.1, 140.1, 146.7, 152.9, 168.4; HRMS Calculated for $C_{17}H_{19}NO_2Na$ $[M+Na]^+$ 292.1313, found 292.1317.



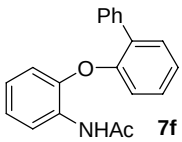
7d

***N*-(2-(biphenyl-4-yloxy)phenyl)acetamide (7e)**. White solid, mp = 136-138 °C, 94% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H), 6.92 (d, *J* = 8.0 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 7.09-7.16 (m, 3H), 7.36 (t, *J* = 6.9 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.58-7.60 (m, 4H), 7.80 (br, 1H), 8.47 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 118.0, 119.0, 121.2, 124.2, 124.3, 127.1, 127.4, 128.8, 129.0, 130.1, 137.2, 140.4, 145.6, 156.1, 168.5; HRMS Calculated for $C_{20}H_{18}NO_2$ $[M+H]^+$ 304.1338, found 304.1347.



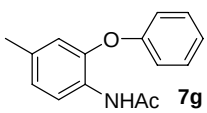
7e

***N*-(2-(biphenyl-2-yloxy)phenyl)acetamide (7f).** 95% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04 (s, 3H), 6.83 (d, *J* = 8.1 Hz, 1H), 6.99-7.03 (m, 3H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.29-7.38 (m, 4H), 7.46 (t, *J* = 5.8 Hz, 3H), 7.49 (br, 1H), 8.34 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.9, 117.1, 120.1, 121.0, 123.7, 123.9, 124.9, 127.7, 128.5, 129.1, 129.2, 129.6, 131.6, 133.9, 137.6, 146.3, 153.0, 168.4; HRMS Calculated for $C_{20}H_{18}NO_2$ $[M+H]^+$ 304.1338, found 304.1345.



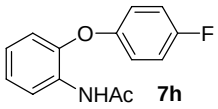
7f

***N*-(4-methyl-2-phenoxyphenyl)acetamide (7g).**[5] White solid, mp = 59-60 °C, 83% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.14 (s, 3H), 2.24 (s, 3H), 6.66 (s, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 7.01 (d, *J* = 7.9 Hz, 2H), 7.15 (t , *J* = 7.3 Hz, 1H), 7.36 (t, *J* = 8.2 Hz, 2H), 7.65 (br, 1H), 8.27 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 25.0, 118.5, 118.7, 121.1, 123.9, 124.8, 127.4, 130.1, 134.2, 145.6, 156.7, 168.4.



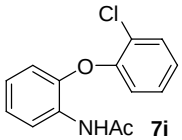
7g

***N*-(2-(4-fluorophenoxy)phenyl)acetamide (7h).** White solid, mp = 76-78 °C, 89% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H), 6.76 (d, *J* = 8.1 Hz, 1H), 6.97-7.00 (m, 3H), 7.03-7.11 (m, 3H), 7.76 (br, 1H), 8.42 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 116.6, 116.9, 120.5, 120.6, 121.2, 124.1, 129.6, 146.2, 152.2, 159.3 (d, $J_{C\text{-}F}$ = 241 Hz), 168.5; HRMS Calculated for $C_{14}H_{13}NO_2F$ $[M+H]^+$ 246.0930, found 246.0924.



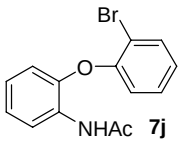
7h

***N*-(2-(2-chlorophenoxy)phenyl)acetamide (7i).**[9] White solid, mp = 82-84 °C, 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.16 (s, 3H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.98-7.03 (m, 2H), 7.09-7.17 (m, 2H), 7.36 (t, *J* = 8.3 Hz, 2H), 7.76 (br, 1H), 8.43 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 117.9, 118.8, 121.1, 124.1, 124.2, 125.6, 128.4, 130.2, 131.1, 145.7, 156.6, 168.5.



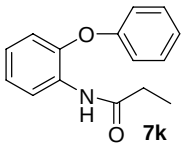
7i

***N*-(2-(2-bromophenoxy)phenyl)acetamide (7j)**.[9] White solid, mp = 90-92 °C, 91% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.19 (s, 3H), 6.75 (t, *J* = 1.0 Hz, 1H), 6.98-7.00 (m, 2H), 7.04-7.12 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.65 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.82 (br, 1H), 8.42 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 114.8, 117.1, 120.6, 121.4, 124.0, 124.4, 125.9, 129.1, 129.5, 134.1, 145.4, 152.9, 168.6.



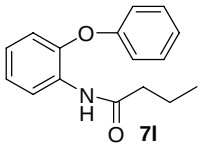
7j

***N*-(2-phenoxyphenyl)propionamide (7k).**[5] 75% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17-1.22 (m, 3H), 2.35-2.42 (m, 2H), 6.86 (t, *J* = 1.3 Hz, 1H), 7.01-7.03 (m, 3H), 7.10-7.15 (m, 2H), 7.34-7.38 (m, 2H), 7.74 (br, 1H), 8.47 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.8, 31.1, 118.0, 118.7, 121.0, 124.0, 124.3, 130.2, 145.5, 156.7, 172.2.



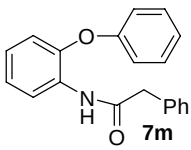
7k

***N*-(2-phenoxyphenyl)butyramide (7l).**[5] White solid, mp = 65-66 °C, 85% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.96 (t, *J* = 7.4 Hz, 3H), 1.68-1.75 (m, 2H), 2.33 (t, *J* = 7.4 Hz, 2H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.98-7.02 (m, 3H), 7.13 (dd, *J* = 17.8, 7.4 Hz, 2H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.72 (br, 1H), 8.47 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 19.2, 40.1, 118.0, 118.7, 121.1, 124.0, 124.3, 130.2, 145.6, 156.7, 171.5.



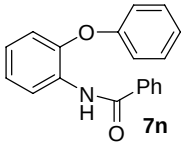
7l

***N*-(2-phenoxyphenyl)-2-phenylacetamide (7m).** White solid, mp = 134-136 °C, 78% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.68 (s, 2H), 6.76 (d, *J* = 7.9 Hz, 2H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 7.06-7.17 (m, 4H), 7.23-7.29 (m, 5H), 7.68 (br, 1H), 8.41 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 45.2, 117.6, 119.0, 121.0, 123.6, 124.4, 124.8, 127.7, 129.3, 129.6, 130.0, 130.4, 134.3, 144.9, 156.8, 169.3; HRMS Calculated for $C_{20}H_{18}NO_2$ $[M+H]^+$ 304.1338, found 304.1344.



7m

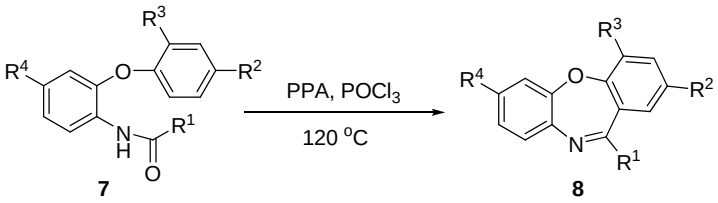
***N*-(2-phenoxyphenyl)benzamide (7n).**[10] White solid, mp = 72-74 °C, 86% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, *J* = 1.2 Hz, 1H), 7.07-7.10 (m, 3H), 7.17-7.20 (m, 2H), 7.37-7.52 (m, 5H), 7.82 (t, *J* = 7.8 Hz, 2H), 8.57 (br, 1H), 8.67 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.0, 118.6, 121.0, 124.1, 124.3, 127.1,



7n

128.8, 130.0, 130.1, 131.9, 135.0, 146.0, 156.5, 165.4.

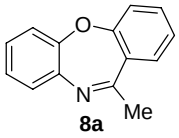
4. Typical Procedure for Cyclization to Seven-membered Cyclic Imines



7 **8**

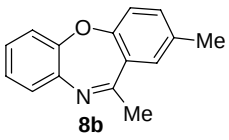
Typical Procedure for the Preparation of Cyclic Imine 8a: To a mixture of polyphosphoric acid (PPA) (7.0 g) and phosphorus oxychloride (2.1 g, 13.5 mmol) was added amido derivative of diphenyl ether **7a** (0.62 g, 2.7 mmol). The reaction mixture was heated at 120 °C for 3 h and poured into ice-cold water, then treated with aqueous ammonia and extracted with CH_2Cl_2 (3×50 mL), dried with anhydrous Na_2SO_4, concentrated under vacuum, the crude product was purified by flash chromatography on silica gel eluted by petroleum ether and EtOAc to give **8a**.

(*Z*)-11-methyldibenzo[*b*,*f*][1,4]oxazepine (8a).[11] Yellow solid, mp = 82-84 °C, 88% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 3H), 7.13-7.15 (m, 3H), 7.16-7.20 (m, 2H), 7.26-7.29 (m, 1H), 7.41 (dd, *J* = 15.8, 7.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.8, 120.8, 121.0, 125.2, 125.7, 127.4, 127.8, 128.6, 129.2, 132.9, 140.8, 152.7, 161.0, 167.5.



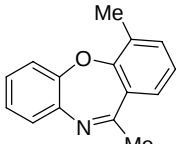
8a

(*Z*)-2,11-dimethyldibenzo[*b*,*f*][1,4]oxazepine (8b). 89% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H), 2.63 (s, 3H), 7.06 (d, *J* = 8.8 Hz, 1H), 7.14 (dd, *J* = 3.7, 1.8 Hz, 3H), 7.19-7.20 (m, 2H), 7.29-7.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 27.6, 120.4, 120.6, 125.5, 127.2, 127.6, 128.7, 133.3, 134.6, 140.8, 152.7, 158.8, 167.4; HRMS Calculated for $C_{15}H_{14}NO$ $[M+H]^+$ 224.1075, found 224.1086.



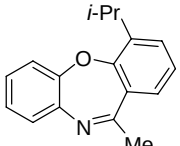
8b

(*Z*)-4,11-dimethyldibenzo[*b*,*f*][1,4]oxazepine (8c). Yellow solid, mp = 49-52 °C, 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.46 (s, 3H), 2.61 (s, 3H), 7.05 (t, *J* = 7.6 Hz, 1H), 7.11-7.15 (m, 3H), 7.23-7.27 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.5, 27.9, 121.0, 124.7, 125.5, 126.2, 127.0, 127.7, 129.1, 130.2, 134.0, 141.1, 152.5, 158.8, 167.9; HRMS Calculated for $C_{15}H_{14}NO$ $[M+H]^+$ 224.1075, found 224.1082.



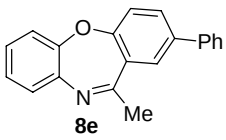
8c

(*Z*)-4-isopropyl-11-methyldibenzo[*b*,*f*][1,4]oxazepine (8d). White solid, mp = 46-48 °C, 89% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27 (s, 3H), 1.29 (s, 3H), 2.63 (s, 3H), 3.76-3.82 (m, 1H), 7.12-7.17 (m, 4H), 7.24-7.29 (m, 2H), 7.38 (dd, *J* = 7.6, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.6, 26.5, 28.1, 121.0, 125.1, 125.6, 126.0, 127.1, 127.8, 129.3, 129.6, 140.8, 141.3, 152.7, 157.9, 168.2; HRMS Calculated for $C_{17}H_{18}NO$ $[M+H]^+$ 252.1388, found 252.1394.



8d

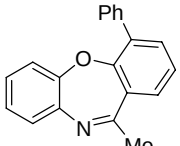
(*Z*)-11-methyl-2-phenyldibenzo[*b*,*f*][1,4]oxazepine (8e). White solid, mp = 83-84 °C, 91% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.71 (s, 3H), 7.17-7.19 (m, 3H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.33-7.39



8e

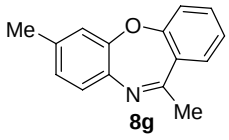
(m, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.52 (t, J = 1.2 Hz, 2H), 7.63 (t, J = 2.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.8, 120.8, 121.3, 125.8, 127.2, 127.3, 127.5, 127.8, 127.9, 129.1, 129.4, 131.5, 138.6, 140.0, 140.8, 152.6, 160.5, 167.4; HRMS Calculated for $C_{20}H_{16}NO$ $[M+H]^+$ 286.1232, found 286.1236.

(*Z*)-11-methyl-4-phenyldibenzo[*b*,*f*][1,4]oxazepine (8f). Yellow solid, mp = 152-154 °C, 87% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.70 (s, 3H), 6.33 (d, J = 8.0 Hz, 1H), 6.91 (t, J = 8.0Hz, 1H), 7.06 (t, J = 7.9 Hz, 1H), 7.23-7.26 (m, 2H), 7.42-7.44 (m, 2H), 7.45-7.49 (m, 3H), 7.59 (d, J = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.0, 120.9, 125.1, 125.5, 127.1, 127.4, 127.6, 127.8, 128.2, 129.9, 130.1, 133.5, 134.9, 137.1, 141.0, 152.3, 157.3, 167.6; HRMS Calculated for $C_{20}H_{16}NO$ $[M+H]^+$ 286.1232, found 286.1235.



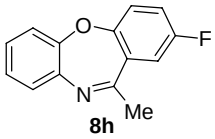
8f

(*Z*)-7,11-dimethyldibenzo[*b*,*f*][1,4]oxazepine (8g). 91% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (s, 3H), 2.63 (s, 3H), 6.96 (d, J = 7.6 Hz, 2H), 7.16-7.19 (m, 3H), 7.39-7.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 27.6, 120.9, 121.2, 125.1, 126.4, 127.5, 128.6, 129.2, 132.7, 137.8, 138.3, 152.3, 160.8, 166.6; HRMS Calculated for $C_{15}H_{14}NO$ $[M+H]^+$ 224.1075, found 224.1081.



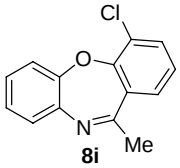
8g

(*Z*)-2-fluoro-11-methyldibenzo[*b*,*f*][1,4]oxazepine (8h). Yellow solid, mp = 72-74 °C, 95% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 3H), 7.08-7.17 (m, 6H), 7.27 (dd, J = 2.8, 1.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.6, 114.9 (d, $J_{C\text{-}F}$ = 24 Hz), 119.5 (d, $J_{C\text{-}F}$ = 23 Hz), 120.7, 122.3, 125.9, 127.7, 128.0, 130.1, 140.5, 152.5, 156.9, 159.6 (d, $J_{C\text{-}F}$ = 243 Hz), 165.9; HRMS Calculated for $C_{14}H_{11}NOF$ $[M+H]^+$ 228.0825, found 228.0823.



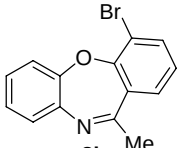
8h

(*Z*)-4-chloro-11-methyldibenzo[*b*,*f*][1,4]oxazepine (8i). 87% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 3H), 7.13 (t, J = 7.9 Hz, 1H), 7.17 (dd, J = 5.9, 3.6 Hz, 2H), 7.27-7.31 (m, 1H), 7.35 (dd, J = 5.8, 3.6 Hz, 2H), 7.49 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.8, 121.5, 125.6, 126.1, 126.6, 126.8, 127.6, 127.7, 130.7, 132.7, 140.5, 151.9, 155.6, 166.5；HRMS Calculated for $C_{14}H_{11}NOCl$ $[M+H]^+$ 244.0529, found 244.0527.



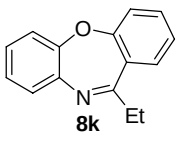
8i

(*Z*)-4-bromo-11-methyldibenzo[*b*,*f*][1,4]oxazepine (8j).[11] 96% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 3H), 7.05 (t, J = 7.9 Hz, 1H), 7.18 (dd, J = 6.0, 3.6 Hz, 2H), 7.28-7.31 (m, 1H), 7.36 (dd, J = 7.8, 1.4 Hz, 1H), 7.43 (t, J = 3.6 Hz, 1H), 7.66 (dd, J = 7.9, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.9, 115.7, 121.7, 126.1, 127.5, 127.6, 127.7, 130.6, 135.8, 140.4, 152.0, 156.6, 166.4.



8j

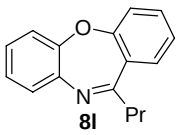
(*Z*)-11-ethyldibenzo[*b*,*f*][1,4]oxazepine (8k). 91% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.32 (t, J = 7.4 Hz, 3H), 2.95 (dd, J = 14.8, 7.4 Hz, 2H), 7.14-7.21 (m, 5H), 7.30 (dd, J = 4.3, 1.0 Hz, 1H), 7.42 (t, J = 7.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.9, 33.4, 120.7, 121.0, 125.3, 125.7, 127.2, 127.9, 128.2, 128.6, 132.6, 141.0, 152.7,



8k

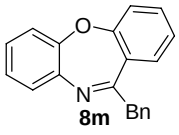
161.6, 171.6; HRMS Calculated for $C_{15}H_{14}NO$ $[M+H]^+$ 224.1075, found 224.1085.

(*Z*)-11-propyldibenzo[*b,f*][1,4]oxazepine (8l).[11] Yellow solid, mp = 65-67 °C, 92% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.4 Hz, 3H), 1.72-1.77(m, 2H), 2.90 (t, *J* = 7.4 Hz, 2H), 7.13-7.20 (m, 5H), 7.26 (t, *J* = 8.2 Hz, 1H), 7.39-7.43(m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 21.1, 42.3, 120.7, 121.0, 125.2, 125.7, 127.2, 127.9, 128.4, 128.6, 132.7, 140.9, 152.8, 161.6, 171.0.



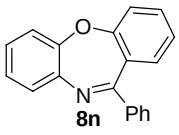
8l

(*Z*)-11-benzyldibenzo[*b,f*][1,4]oxazepine (8m). Yellow solid, mp = 92-95 °C, 81% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.29 (s, 2H), 7.12-7.20 (m, 6H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.35-7.39 (m, 4H), 7.46 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.0, 120.8, 121.1, 125.2, 125.8, 126.8, 127.7, 128.0, 128.4, 128.5, 128.8, 129.0, 132.8, 137.6, 140.8, 152.7, 161.7, 168.8; HRMS Calculated for $C_{20}H_{16}NO$ $[M+H]^+$ 286.1232, found 286.1234.



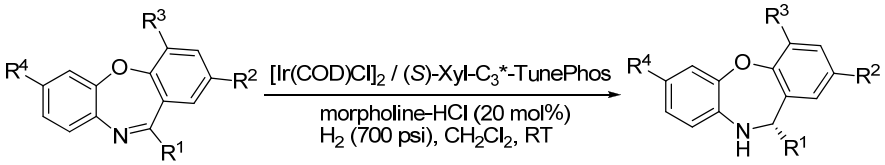
8m

(*Z*)-11-phenyldibenzo[*b,f*][1,4]oxazepine (8n).[11] Yellow solid, mp = 105-107 °C, 71% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12-7.19 (m, 5H), 7.27-7.33 (m, 1H), 7.42-7.47 (m, 5H), 7.82 (dd, *J* = 7.7, 1.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.9, 121.2, 124.7, 125.8, 127.6, 127.7, 128.4, 129.9, 130.6, 131.5, 133.2, 140.3, 141.1, 152.6, 162.2, 167.3.



8n

5. General Procedure for Ir-catalyzed Asymmetric Hydrogenation of Cyclic Imines

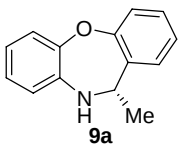


8 **9**

A mixture of $[Ir(COD)Cl]_2$ (1.7 mg, 0.0025 mmol) and (*S*)-Xyl-C_3*-TunePhos (4.0 mg, 0.0055 mmol) in 1 mL CH_2Cl_2 was stirred at room temperature for 10 min in a glovebox, then morpholine-HCl salt (6.2 mg, 0.05 mmol) and substrate **8** (0.25 mmol) together with 2 mL of CH_2Cl_2 were added and the solution was stirred for another 10 min. The hydrogenation was performed at room temperature under H_2 (700 psi) for 20 h. After the hydrogen gas was carefully released, the reaction mixture was purified with a silica gel column eluted with petroleum ether and EtOAc to give pure product **9**.

Racemates of **9** were prepared by $NaBH_4$ reduction of the corresponding hydrogen substrates **8** in MeOH.

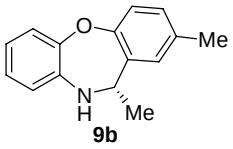
(-)-(*S*)-11-methyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepine (9a).[12] 98% yield, 94% ee, $[\alpha]^{30}_D$ = -109.1 (*c* 1.26, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.63 (d, *J* = 6.8 Hz, 3H), 3.67 (br, 1H), 5.05 (dd, *J* = 13.6, 6.8 Hz, 1H), 6.53 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.67 (t, *J* = 7.8 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H), 7.10 (t, *J* = 7.0 Hz, 2H), 7.15-7.24 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.1, 50.1, 118.6, 119.1, 121.0, 122.0, 124.6, 124.7, 125.5, 129.0, 135.4, 138.4, 144.5, 157.8; HPLC (AD-H, elute:



9a

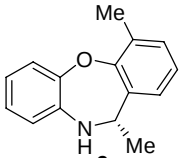
Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 7.9 min (major), t_2 = 9.2 min (minor).

(-)-(*S*)-2,11-dimethyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9b). 96% yield, 90% ee, $[\alpha]^{30}_D$ = -149.2 (*c* 1.22, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.63 (d, *J* = 6.8 Hz, 3H), 2.32 (s, 3H), 3.71 (br, 1H), 5.03 (dd, *J* = 13.6, 6.8 Hz, 1H), 6.53 (d, *J* = 7.9 Hz, 1H), 6.66 (t, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 7.05-7.09 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 21.2, 50.1, 118.6, 119.1, 120.7, 121.9, 124.6, 126.0, 129.3, 134.1, 134.9, 138.4, 144.7, 155.6; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 8.3 min (major), t_2 = 9.4 min (minor); HRMS Calculated for $C_{15}H_{16}NO$ $[M+H]^+$ 226.1232, found 226.1232.



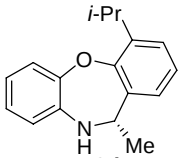
9b

(-)-(*S*)-4,11-dimethyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9c). Yellow solid, mp = 52-55 °C, 98% yield, 91% ee, $[\alpha]^{30}_D$ = -73.6 (*c* 1.12, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64 (d, *J* = 6.8 Hz, 3H), 2.43 (s, 3H), 3.72 (br, 1H), 5.11 (dd, *J* = 13.7, 6.8 Hz, 1H), 6.53 (d, *J* = 7.9 Hz, 1H), 6.66 (t, *J* = 7.7 Hz, 1H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.99-7.06 (m, 2H), 7.14 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.4, 19.9, 49.6, 118.4, 118.7, 122.3, 122.7, 124.3, 124.7, 130.4, 130.6, 135.5, 138.9, 143.8, 156.0; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.5 mL/min), t_1 = 9.7 min (major), t_2 = 10.3 min (minor); HRMS Calculated for $C_{15}H_{16}NO$ $[M+H]^+$ 226.1232, found 226.1238.



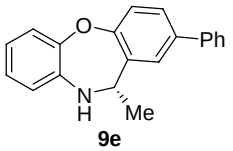
9c

(-)-(*S*)-4-*iso*-propyl-11-methyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9d). Yellow solid, mp = 97-99 °C, 97% yield, 93% ee, $[\alpha]^{30}_D$ = -99.7 (*c* 1.52, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (d, *J* = 6.8 Hz, 3H), 1.27 (d, *J* = 7.2 Hz, 3H), 1.63 (d, *J* = 6.8 Hz, 3H), 3.62-3.70 (m, 2H), 5.12 (dd, *J* = 13.6, 6.8 Hz, 1H), 6.52 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.64-6.69 (m, 1H), 6.83-6.87 (m, 1H), 7.05-7.13 (m, 3H), 7.22 (dd, *J* = 14.4, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 23.5, 26.9, 49.7, 118.4, 118.8, 122.2, 122.5, 124.6, 125.9, 135.7, 138.9, 140.9, 144.2, 155.0; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 99/1, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 12.4 min (minor), t_2 = 13.8 min (major); HRMS Calculated for $C_{17}H_{20}NO$ $[M+H]^+$ 254.1545, found 254.1541.

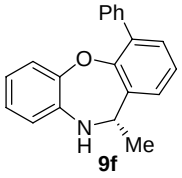


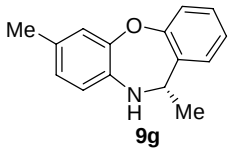
9d

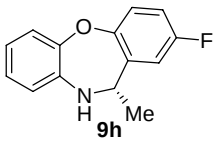
(-)-(*S*)-11-methyl-2-phenyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9e). Yellow solid, mp = 70-71 °C, 94% yield, 86% ee, $[\alpha]^{30}_D$ = -179.2 (*c* 1.40, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (d, *J* = 6.8 Hz, 3H), 3.75 (br, 1H), 5.07 (dd, *J* = 13.6, 6.8 Hz, 1H), 6.55 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.63-6.65 (m, 1H), 6.78-6.81 (m, 1H), 7.11 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.23 (t, *J* = 8.2 Hz, 1H), 7.32 (t, *J* = 8.2 Hz, 1H), 7.38-7.45 (m, 4H), 7.53 (t, *J* = 1.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.3, 50.5, 118.7, 119.3, 121.4, 122.0, 124.5, 124.7, 127.3, 127.7, 128.7, 129.0, 135.5, 137.8, 138.2, 141.1, 144.5, 157.2; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 24.9 min (minor), t_2 = 26.2 min (major); HRMS Calculated for $C_{20}H_{18}NO$ $[M+H]^+$ 288.1388, found 288.1385.

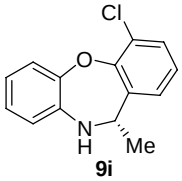


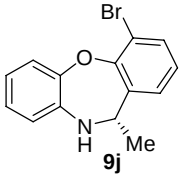
9e

(+)-(*S*)-11-methyl-4-phenyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9f). 98% yield, 90% ee, 
9f
$[\alpha]^{30}_{D}$ = + 87.4 (*c* 1.12, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.66 (d, *J* = 6.8 Hz, 3H), 3.71 (br, 1H), 5.16 (dd, *J* = 13.3, 6.6 Hz, 1H), 6.47-6.49 (m, 3H), 6.77 (dd, *J* = 11.4, 7.2 Hz, 1H), 7.14-7.21 (m, 2H), 7.30 (d, *J* = 7.3 Hz, 1H), 7.38-7.46 (m, 3H), 7.53 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.9, 49.8, 118.2, 118.8, 122.3, 124.4, 124.5, 124.6, 127.4, 128.1, 130.2, 130.4, 135.0, 136.4, 138.2, 138.7, 144.0, 154.7; HPLC (OD-H, elute: Hexanes/*i*-PrOH = 99/1, detector: 254 nm, flow rate: 0.8 mL/min), t_1 = 15.9 min (minor), t_2 = 21.5 min (major); HRMS Calculated for $C_{20}H_{18}NO$ $[M+H]^+$ 288.1388, found 288.1378.

(-)-(*S*)-7,11-dimethyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9g). Yellow solid, mp = 62-64 
9g
°C, 93% yield, 92% ee, $[\alpha]^{30}_{D}$ = -144.2 (*c* 0.66, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.59 (d, *J* = 6.8 Hz, 3H), 2.21 (s, 3H), 3.57 (br, 1H), 4.97 (dd, *J* = 13.6, 6.8 Hz, 1H), 6.45 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.92 (s, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 7.13-7.24 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 20.4, 50.4, 118.9, 120.9, 122.3, 124.4, 125.2, 125.6, 128.9, 129.1, 135.3, 135.6, 144.5, 157.7; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 70/30, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 8.5 min (major), t_2 = 9.8 min (minor); HRMS Calculated for $C_{15}H_{16}NO$ $[M+H]^+$ 226.1232, found 226.1228.

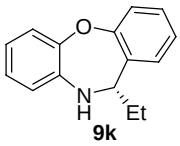
(-)-(*S*)-2-fluoro-11-methyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9h). White solid, mp= 
9h
73-74 °C, 98% yield, 90% ee, $[\alpha]^{30}_{D}$ = -180.1 (*c* 1.34, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.62 (d, *J* = 6.8 Hz, 3H), 3.69 (br, 1H), 5.09 (dd, *J* = 13.5, 6.7 Hz, 1H), 6.54 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.68 (t, *J* = 1.1 Hz, 1H), 6.87-6.94 (m, 3H), 7.08-7.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.6, 49.4, 112.2 (d, J_{C-F} = 24Hz), 115.1 (d, J_{C-F} = 23 Hz), 118.6, 119.3, 121.9, 122.2, 124.9, 137.2, 138.2, 144.4, 153.7, 159.4 (d, J_{C-F} = 241 Hz); HPLC (OD-H, elute: Hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 10.9 min (minor), t_2 = 13.0 min (major); HRMS Calculated for $C_{14}H_{13}NOF$ $[M+H]^+$ 230.0981, found 230.0986.

(+)-(*S*)-4-chloro-11-methyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9i). 95% yield, 90% ee, 
9i
$[\alpha]^{30}_{D}$ = +60.3 (*c* 0.88, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64 (d, *J* = 6.8 Hz, 3H), 3.73 (br, 1H), 5.13 (dd, *J* = 13.2, 6.5 Hz, 1H), 6.53 (d, *J* = 8.0 Hz, 1H), 6.69 (t, *J* = 7.6 Hz, 1H), 6.88 (t, *J* = 7.5 Hz, 1H), 7.03-7.12 (m, 2H), 7.26-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 49.7, 118.2, 119.0, 122.8, 123.6, 125.2, 125.3, 126.5, 129.6, 137.5, 138.3, 143.3, 153.3; HPLC (OD-H, elute: Hexanes/*i*-PrOH = 95/5, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 12.0 min (maj.), t_2 = 13.0 min (min.); HRMS Calculated for $C_{14}H_{13}NOCl$ $[M+H]^+$ 246.0686, found 246.0691.

(+)-(*S*)-4-bromo-11-methyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9j). 97% yield, 87% ee, 
9j
$[\alpha]^{30}_{D}$ = +110.7 (*c* 0.63, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64 (d, *J* = 6.8 Hz, 3H), 3.73 (br, 1H), 5.12 (dd, *J* = 13.7, 6.8 Hz, 1H), 6.53 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.70 (t, *J* = 7.7 Hz, 1H), 6.87 (t, *J* = 7.7 Hz, 1H), 6.98 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.35 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.50 (dd, *J* =

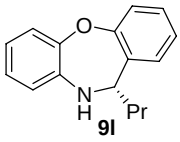
8.0, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 49.8, 115.8, 118.2, 119.0, 123.0, 124.4, 125.3, 125.7, 132.6, 137.4, 138.2, 143.2; HPLC (OD-H, elute: Hexanes/*i*-PrOH = 97/3, detector: 254 nm, flow rate: 0.8 mL/min), t_1 = 13.8 min (minor), t_2 = 14.7 min (major); HRMS Calculated for $C_{14}H_{13}NOBr$ $[M+H]^+$ 290.0181, found 290.0184.

(-)-(*S*)-11-ethyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9k).[13] Yellow solid, mp = 41-43 °C, 98% yield, 83% ee, $[\alpha]^{30}_D$ = -40.9 (*c* 1.22, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.03 (t, *J* = 7.3 Hz, 3H), 2.01-2.15 (m, 2H), 3.49 (br, 1H), 4.33 (t, *J* = 7.5 Hz, 1H), 6.57 (d, *J* = 7.9 Hz, 1H), 6.67 (t, *J* = 7.7 Hz, 1H), 6.86 (t, *J* = 7.6 Hz, 1H), 7.08 (t, *J* = 7.9 Hz, 2H), 7.16 (t, *J* = 8.2 Hz, 2H), 7.22-7.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.6, 28.0, 59.0, 118.7, 119.0, 121.2, 121.9, 124.3, 124.6, 127.3, 128.9, 134.2, 137.9, 144.2, 157.4; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.5 mL/min), t_1 = 11.0 min (major), t_2 = 11.8 min (minor).



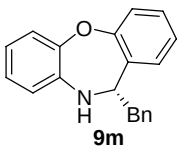
9k

(-)-(*S*)-11-propyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9l). 97% yield, 81% ee, $[\alpha]^{30}_D$ = -87.7 (*c* 1.58, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.98 (t, *J* = 7.2 Hz, 3H), 1.33-1.42 (m, 1H), 1.47-1.56 (m, 1H), 2.00-2.08 (m, 2H), 3.95 (br, 1H), 4.46 (t, *J* = 7.4 Hz, 1H), 6.56 (d, *J* = 7.9 Hz, 1H), 6.66 (t, *J* = 7.4 Hz, 1H), 6.85 (t, *J* = 7.3 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.6 Hz, 2H), 7.22-7.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 20.2, 37.1, 56.9, 118.7, 118.9, 121.2, 121.9, 124.4, 124.6, 127.2, 128.9, 134.5, 137.9, 144.1, 157.5; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 7.4 min (major), t_2 = 8.3 min (minor); HRMS Calculated for $C_{16}H_{18}NO$ $[M+H]^+$ 240.1388, found 240.1389.



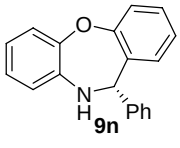
9l

(-)-(*S*)-11-benzyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9m). 90% conv., 52% ee, $[\alpha]^{30}_D$ = -100.3 (*c* 1.02, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.30-3.34 (m, 1H), 3.41-3.47 (m, 1H), 3.97 (br, 1H), 4.58 (dd, *J* = 9.8, 4.7 Hz, 1H), 6.46 (d, *J* = 7.9 Hz, 1H), 6.73 (t, *J* = 7.4 Hz, 1H), 6.86 (t, *J* = 7.8 Hz, 1H), 7.08 (t, *J* = 7.2 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 2H), 7.20-7.27 (m, 5H), 7.31 (dd, *J* = 14.5, 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 41.7, 59.5, 119.0, 119.2, 121.4, 122.0, 124.4, 124.6, 126.8, 127.7, 128.8, 129.2, 129.6, 133.7, 137.6, 138.9, 144.1, 157.3; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 80/20, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 8.9 min (major), t_2 =10.4 min (minor); HRMS Calculated for $C_{20}H_{18}NO$ $[M+H]^+$ 288.1388, found 288.1388.



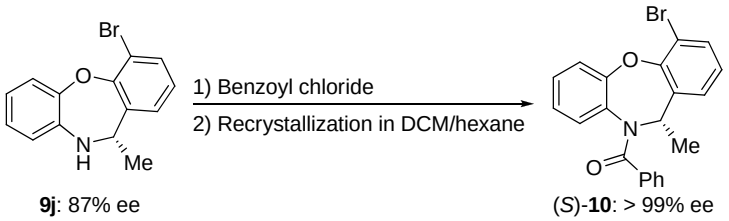
9m

(-)-(*S*)-11-phenyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (9n).[13] 12% conv., 78% ee, $[\alpha]^{30}_D$ = -16.4 (*c* 0.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.23 (br, 1H), 5.89 (s, 1H), 6.63 (t, *J* = 1.4 Hz, 1H), 6.69-6.71 (m, 1H), 6.88 (t, *J* = 7.6 Hz, 2H), 7.02-7.05 (m, 1H), 7.08-7.10 (m, 1H), 7.18-7.24 (m, 2H), 7.33-7.42 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 60.5, 118.8, 119.6, 121.3, 122.0, 124.4, 124.9, 127.4, 127.9, 128.6, 128.9, 129.4, 134.5, 138.4, 141.9, 144.9, 157.7; HPLC (AD-H, elute: Hexanes/*i*-PrOH = 70/30, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 9.2 min (major), t_2 = 12.4 min (minor).



9n

6. The Determination of the Absolute Configuration



9j: 87% ee (*S*)-**10**: > 99% ee

(+)-(*S*)-4-bromo-10-benzoyl-11-methyl-10,11-dihydrodibenzo[*b*,*f*][1,4]oxazepine (10). To a stirred solution of **9j** (215 mg, 0.74 mmol) in anhydrous benzene (5.0 mL) was added dropwisely a solution of benzoyl chloride (104 mg, 0.74 mmol) at 0 ^{o}C. The mixture was stirred at room temperature for 72 h. Benzene was removed in vacuum, then water (20 mL) was added, which was extracted by CH_2Cl_2 (2×30 mL), the combined organic layer was washed successively with saturated $NaHCO_3$ solution and brine, then dried with anhydrous Na_2SO_4. After removal of the solvent, the residue was subjected to column chromatograph to give the desired white solid **10** (266 mg, 91% yield). The product was finally recrystallized from hexane and dichloromethane to give the colorless crystals with > 99% ee. mp = 129-131 ^{o}C, $[\alpha]^{20}_{D}$ = +526.6 (*c* 1.08, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.35 (d, *J* = 7.0 Hz, 3H), 6.39 (d, *J* = 5.7 Hz, 1H), 6.72 (d, *J* = 7.5 Hz, 1H), 6.88-6.95 (m, 2H), 7.14-7.26 (m, 5H), 7.37-7.43 (m, 3H), 7.51 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 52.0, 115.7, 122.3, 124.4, 125.2, 128.1, 128.5, 129.0, 129.5, 130.4, 130.8, 132.2, 132.4, 133.0, 135.5, 150.0, 153.0, 170.1; HPLC (OD-H, elute: Hexanes/*i*-PrOH = 90/10, detector: 254 nm, flow rate: 0.7 mL/min), t_1 = 9.0 min (minor), t_2 =11.2 min (major); HRMS Calculated for $C_{21}H_{17}NO_2Br$ $[M+H]^+$ 394.0443, found 394.0438.

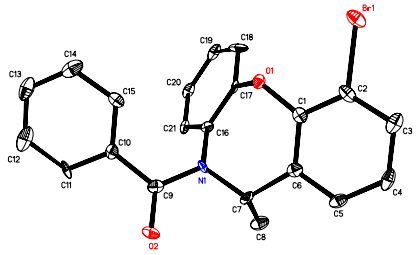


Fig. 1 X-Ray Crystal Structure of (*S*)-**10**.

Table 1 Crystal data and structure refinement for (*S*)-**10**.

Identification code	cd21162
Empirical formula	$C_{21}H_{16}BrNO_2$
Formula weight	394.26
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Tetragonal, P4(3)2(1)2
Unit cell dimensions	a = 8.0493(5) A alpha = 90 deg.
	b = 8.0493(5) A beta = 90 deg.
	c = 54.900(5) A gamma = 90 deg.
Volume	3557.1(4) A^3

Z, Calculated density	8, 1.472 Mg/m^3
Absorption coefficient	2.325 mm^{-1}
F(000)	1600
Crystal size	0.386 x 0.257 x 0.122 mm
Theta range for data collection	2.56 to 25.99 deg.
Limiting indices	-9<=h<=9, -9<=k<=9, -67<=l<=41
Reflections collected / unique	19376 / 3481 [R(int) = 0.0631]
Completeness to theta = 25.99	100.0 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.4536
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3481 / 0 / 228
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0433, wR2 = 0.1064
R indices (all data)	R1 = 0.0667, wR2 = 0.1149
Absolute structure parameter	0.028(14)
Extinction coefficient	0.0000(5)
Largest diff. peak and hole	0.420 and -0.390 $e.A^{-3}$

Table 2 Bond lengths [A] and angles [deg] for (*S*)-**10**.

Br(1)-C(2)	1.893(5)
N(1)-C(9)	1.369(5)
N(1)-C(16)	1.424(4)
N(1)-C(7)	1.458(5)
O(1)-C(1)	1.363(5)
O(1)-C(17)	1.381(4)
O(2)-C(9)	1.217(5)
C(1)-C(2)	1.388(5)
C(1)-C(6)	1.407(6)
C(2)-C(3)	1.367(7)
C(3)-C(4)	1.366(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.381(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.518(5)
C(7)-C(8)	1.537(6)
C(7)-H(7)	0.9800
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(10)	1.496(6)

C(10)-C(15)	1.379(6)
C(10)-C(11)	1.381(6)
C(11)-C(12)	1.385(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.356(8)
C(12)-H(12)	0.9300
C(13)-C(14)	1.369(8)
C(13)-H(13)	0.9300
C(14)-C(15)	1.380(7)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(21)	1.367(5)
C(16)-C(17)	1.375(5)
C(17)-C(18)	1.375(5)
C(18)-C(19)	1.377(6)
C(18)-H(18)	0.9300
C(19)-C(20)	1.364(7)
C(19)-H(19)	0.9300
C(20)-C(21)	1.388(6)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(9)-N(1)-C(16)	121.4(3)
C(9)-N(1)-C(7)	118.4(3)
C(16)-N(1)-C(7)	117.5(3)
C(1)-O(1)-C(17)	118.7(3)
O(1)-C(1)-C(2)	115.9(4)
O(1)-C(1)-C(6)	124.4(3)
C(2)-C(1)-C(6)	119.6(4)
C(3)-C(2)-C(1)	122.5(5)
C(3)-C(2)-Br(1)	118.5(4)
C(1)-C(2)-Br(1)	118.8(3)
C(4)-C(3)-C(2)	118.3(5)
C(4)-C(3)-H(3)	120.9
C(2)-C(3)-H(3)	120.9
C(3)-C(4)-C(5)	120.7(5)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	122.2(5)
C(4)-C(5)-H(5)	118.9
C(6)-C(5)-H(5)	118.9
C(5)-C(6)-C(1)	116.6(4)
C(5)-C(6)-C(7)	116.8(4)
C(1)-C(6)-C(7)	126.6(3)
N(1)-C(7)-C(6)	114.4(3)

N(1)-C(7)-C(8)	110.9(3)
C(6)-C(7)-C(8)	112.0(3)
N(1)-C(7)-H(7)	106.3
C(6)-C(7)-H(7)	106.3
C(8)-C(7)-H(7)	106.3
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(2)-C(9)-N(1)	121.7(4)
O(2)-C(9)-C(10)	121.2(4)
N(1)-C(9)-C(10)	117.0(4)
C(15)-C(10)-C(11)	119.6(4)
C(15)-C(10)-C(9)	122.3(4)
C(11)-C(10)-C(9)	118.0(4)
C(10)-C(11)-C(12)	119.1(5)
C(10)-C(11)-H(11)	120.4
C(12)-C(11)-H(11)	120.4
C(13)-C(12)-C(11)	121.0(5)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(14)	120.1(5)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	119.9(6)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(10)-C(15)-C(14)	120.2(5)
C(10)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(21)-C(16)-C(17)	119.2(3)
C(21)-C(16)-N(1)	121.9(4)
C(17)-C(16)-N(1)	118.9(3)
C(16)-C(17)-C(18)	122.0(4)
C(16)-C(17)-O(1)	119.9(3)
C(18)-C(17)-O(1)	117.8(4)
C(17)-C(18)-C(19)	118.0(4)
C(17)-C(18)-H(18)	121.0
C(19)-C(18)-H(18)	121.0
C(20)-C(19)-C(18)	121.0(4)
C(20)-C(19)-H(19)	119.5
C(18)-C(19)-H(19)	119.5

C(19)-C(20)-C(21)	120.1(4)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(16)-C(21)-C(20)	119.7(4)
C(16)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1

7. References

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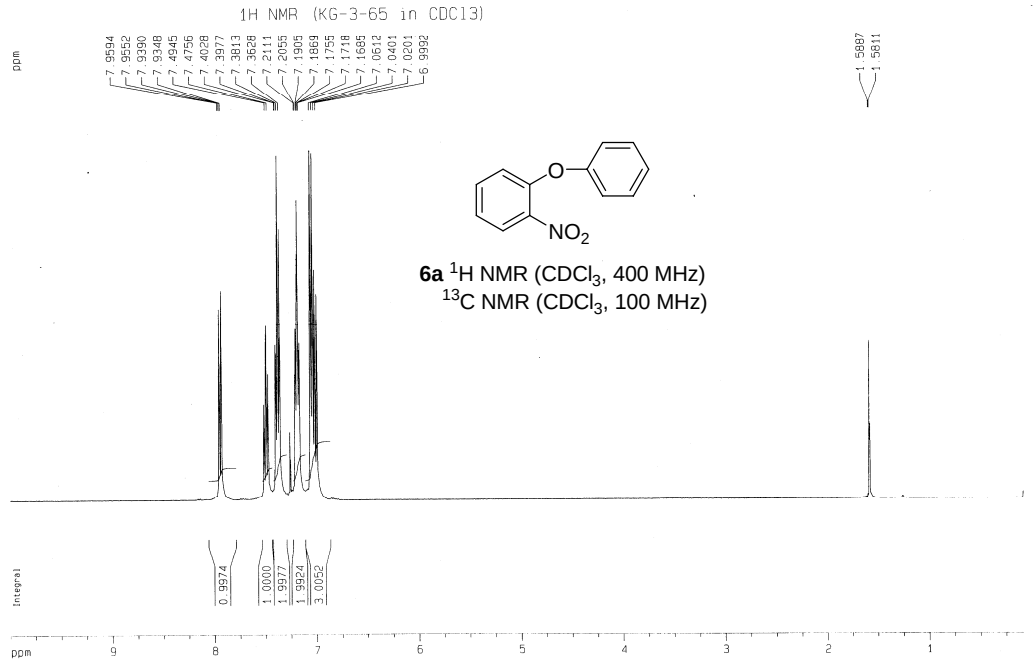
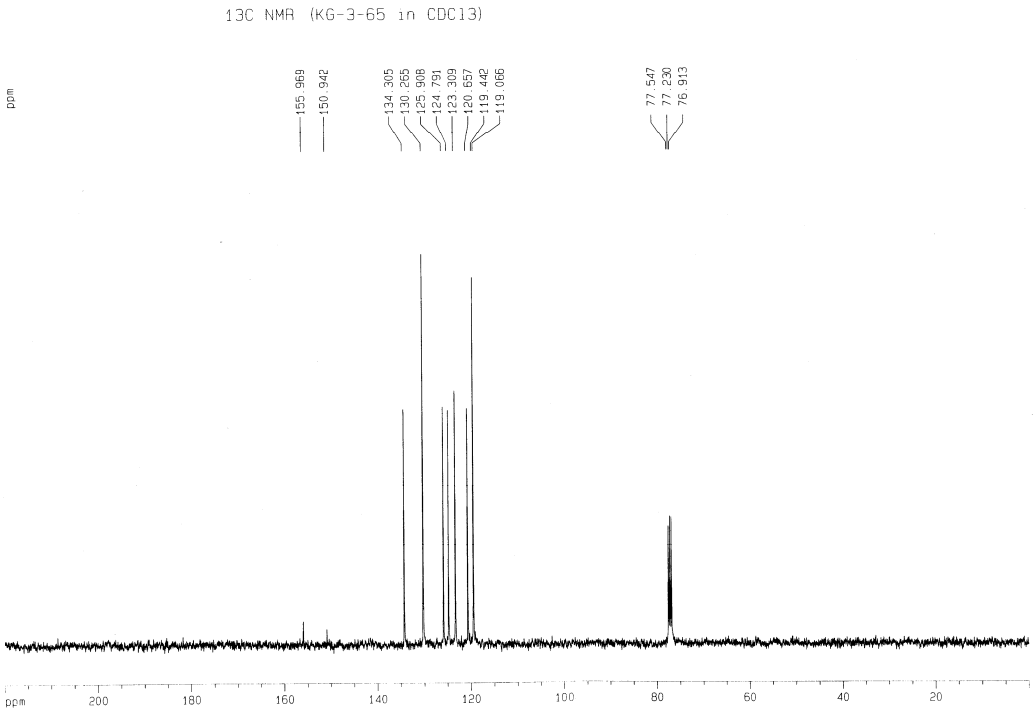
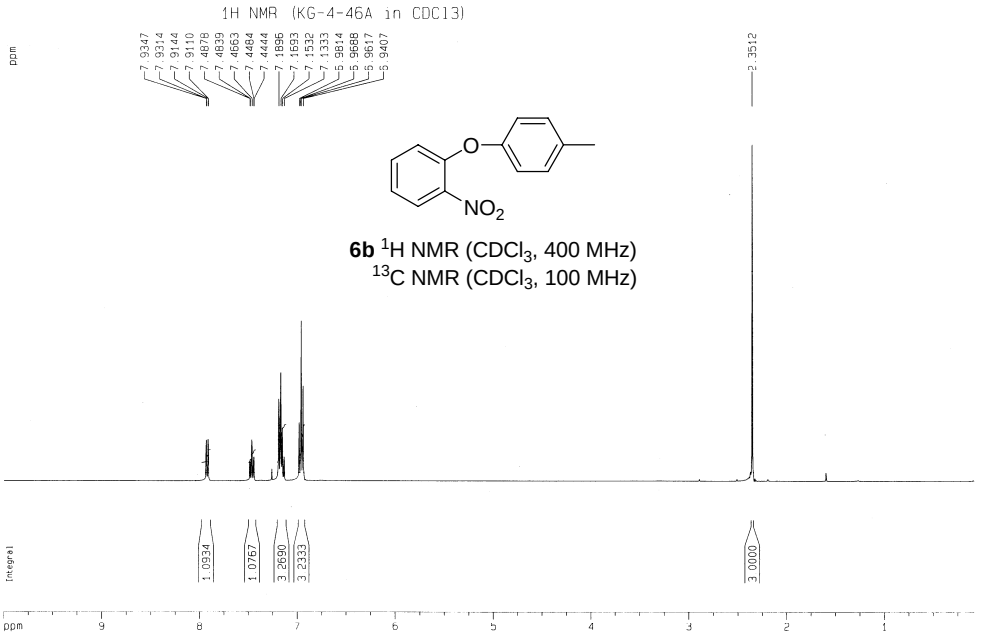
8. Copy of NMR, HRMS and HPLC for Racemic and Chiral Compounds

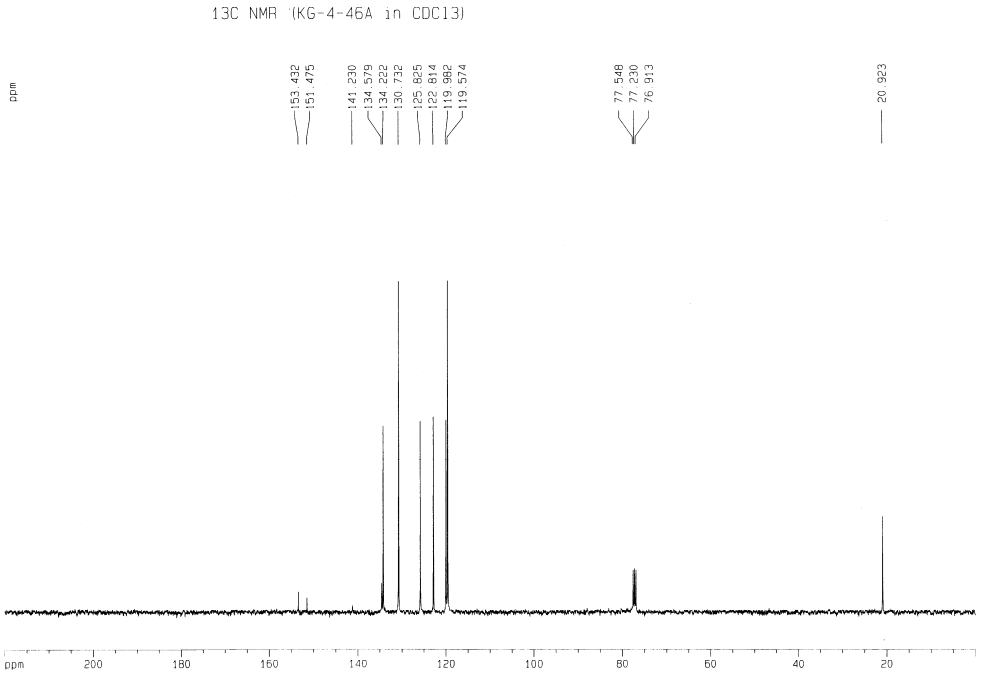


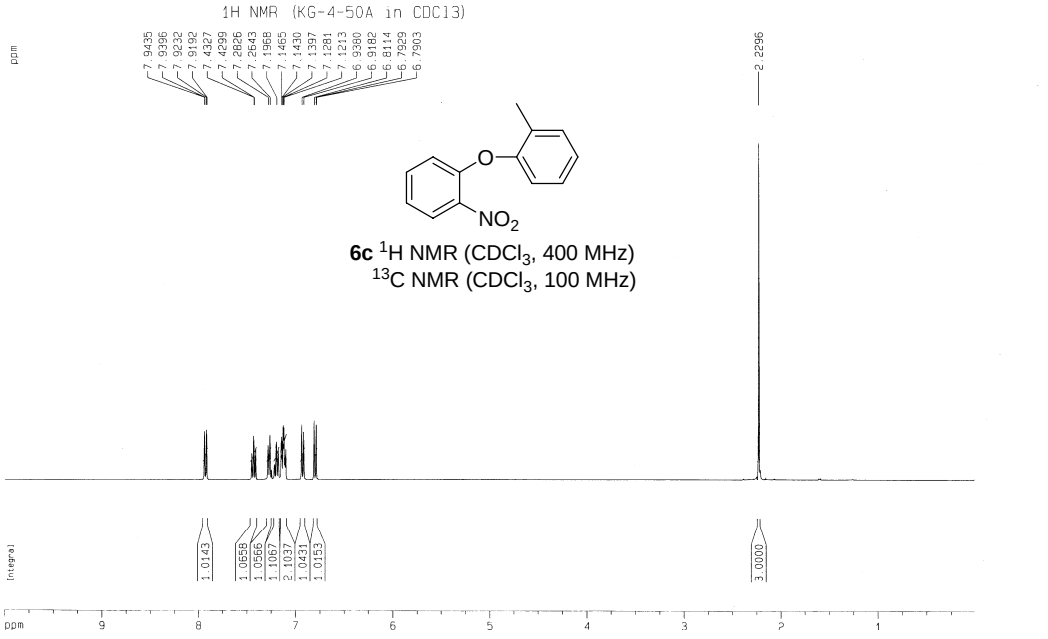
6a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





6b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





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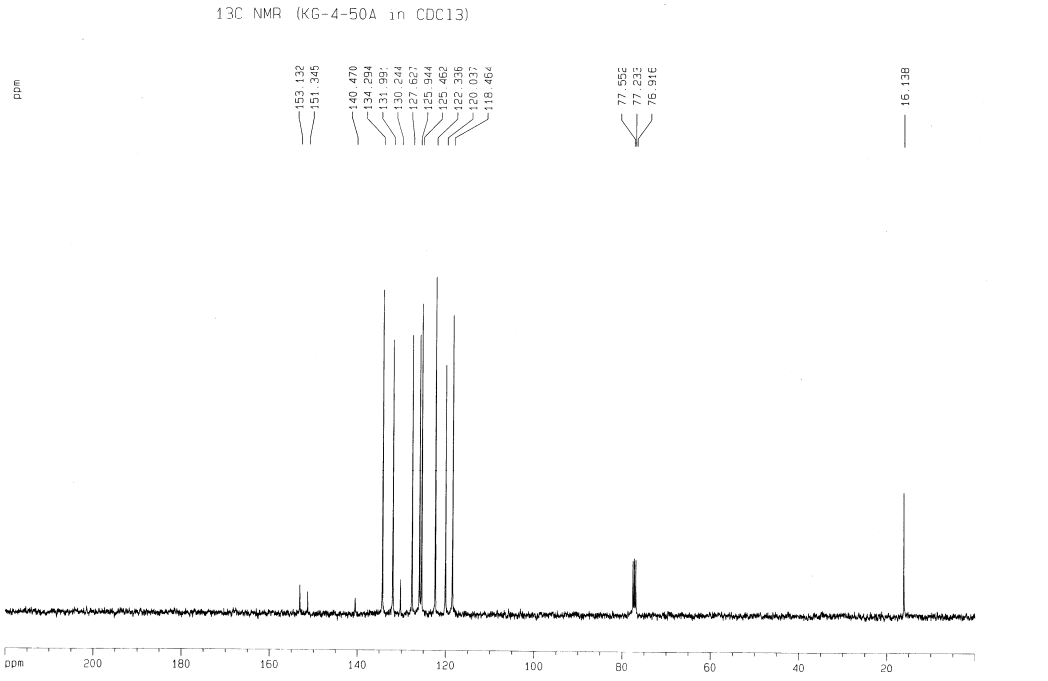
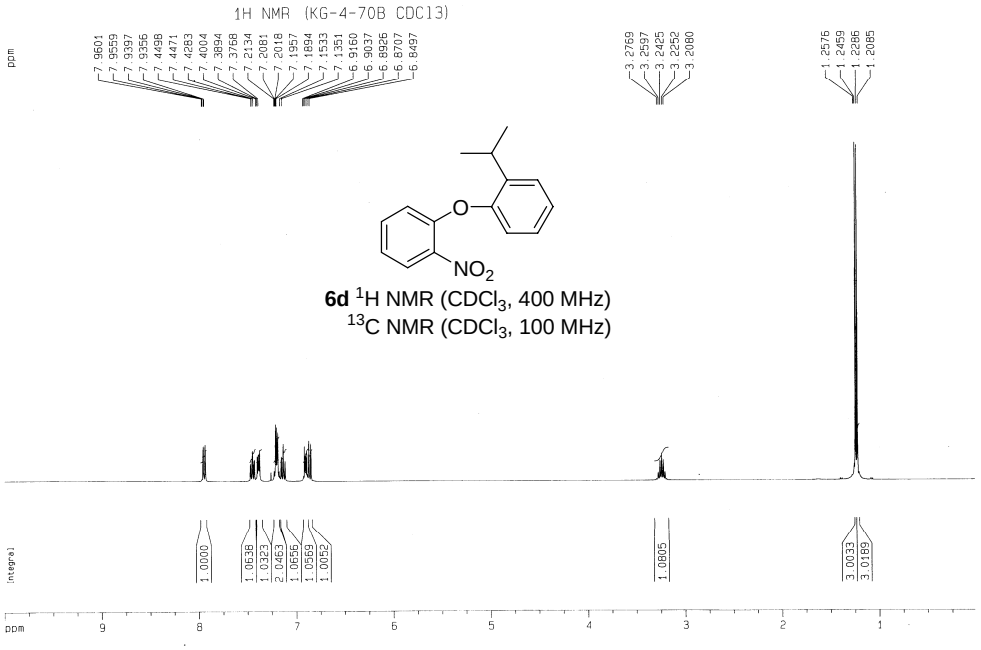
^{13}C NMR ($CDCl_3$, 100 MHz)





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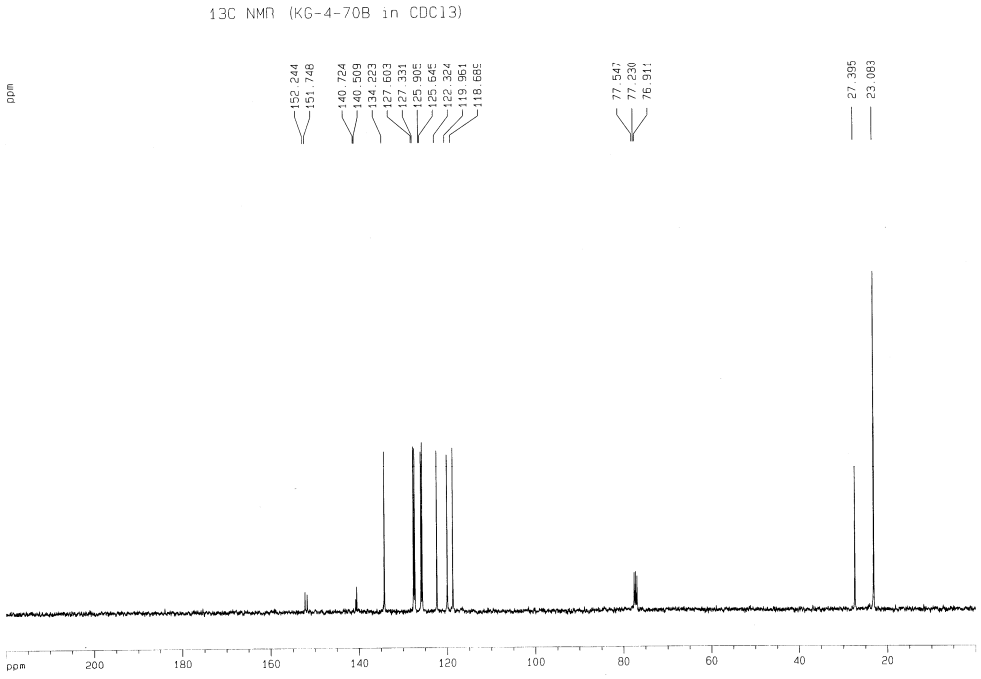
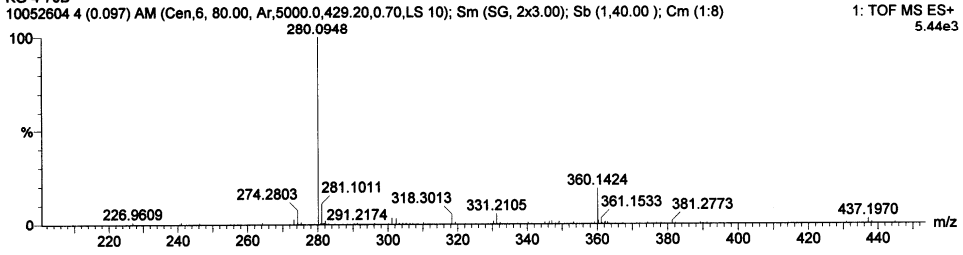


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 3-3 Na: 1-1

KG-4-70B
10052604 4 (0.097) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:8) 1: TOF MS ES+ 5.44e3



Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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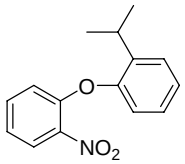
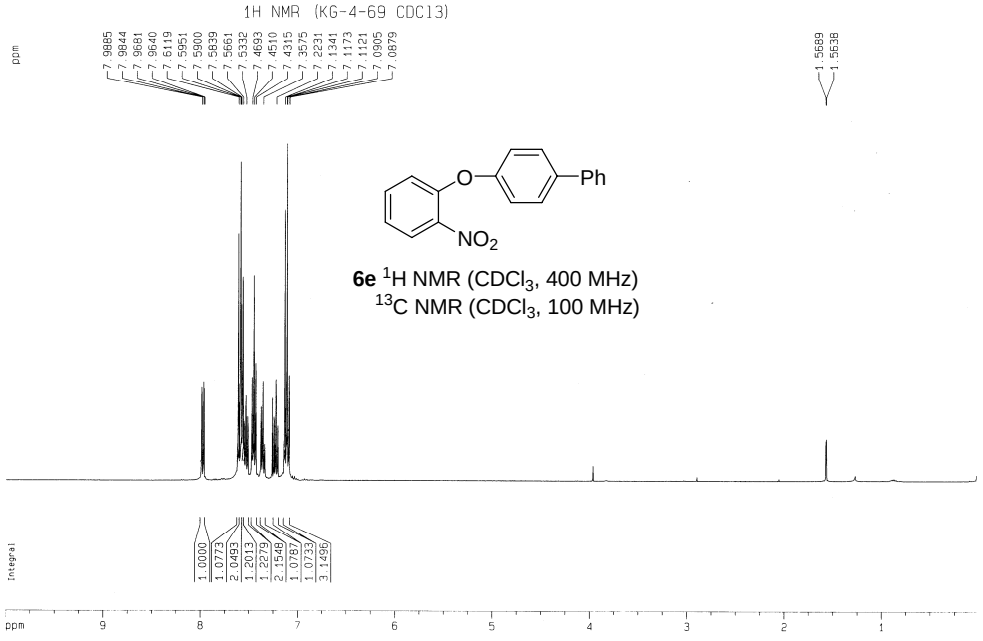


6d HRMS



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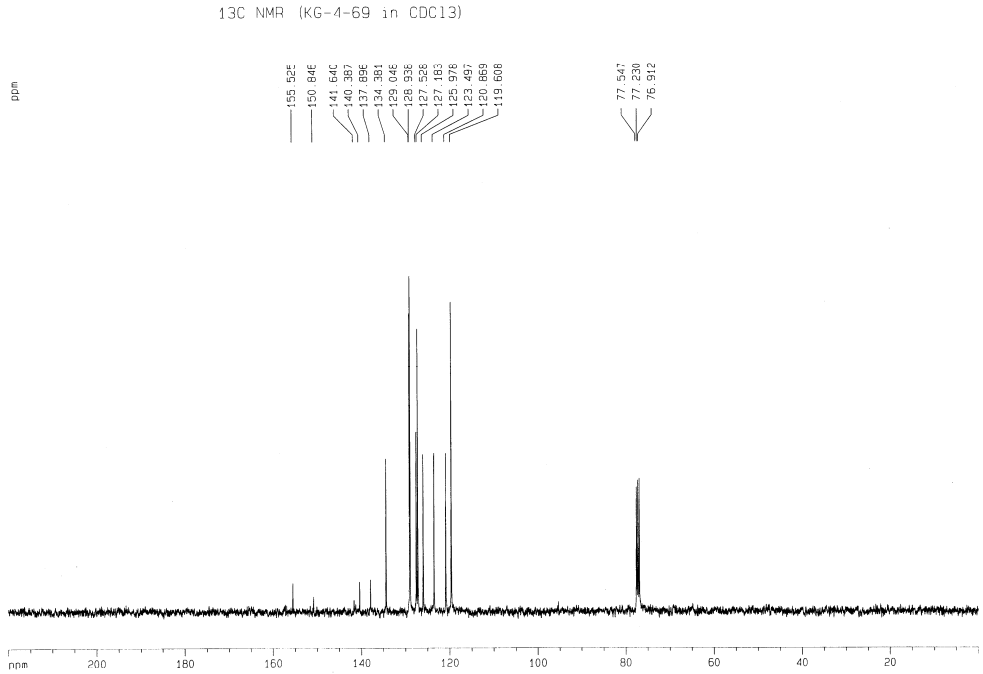
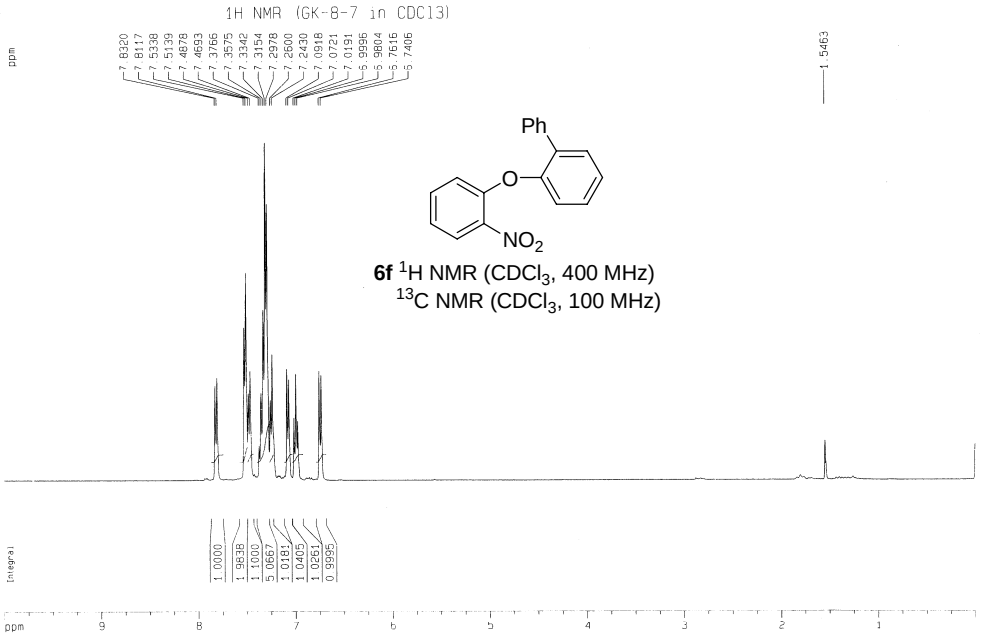
^{13}C NMR ($CDCl_3$, 100 MHz)





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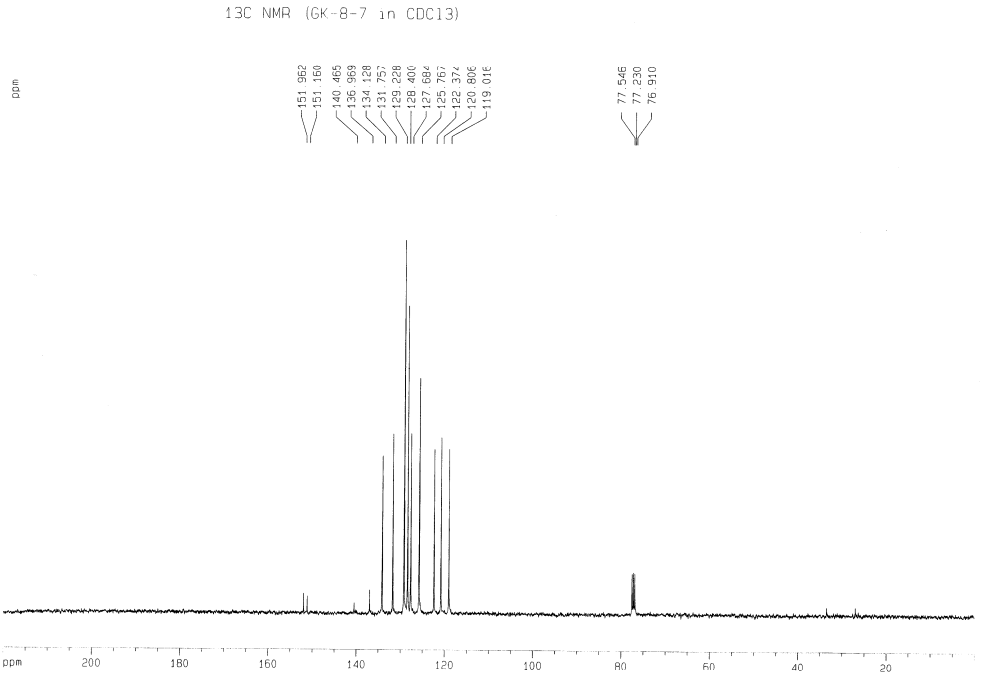

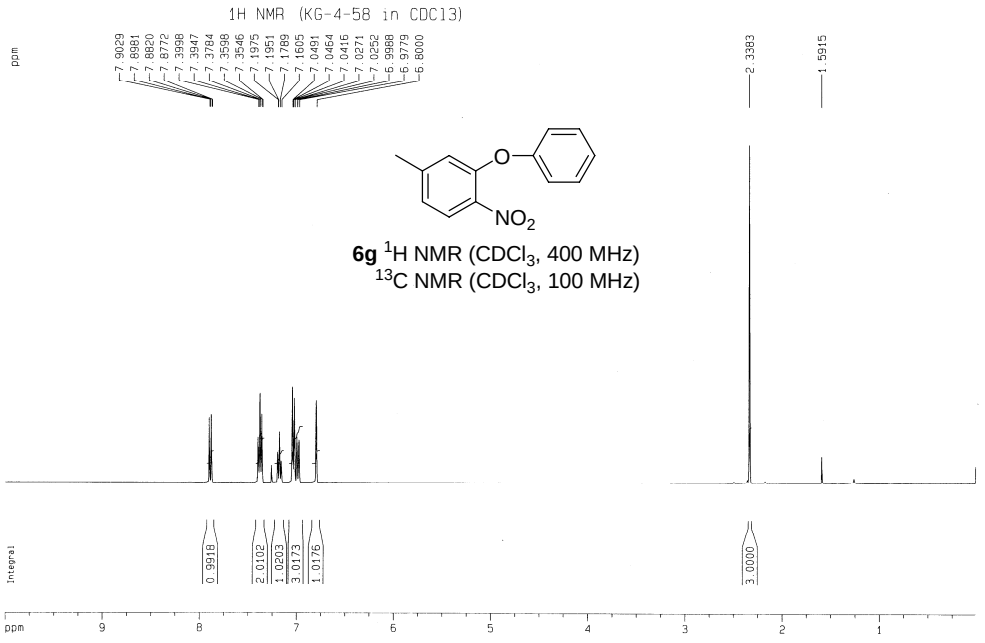

6g ^{1}H NMR ($CDCl_3$, 400 MHz)
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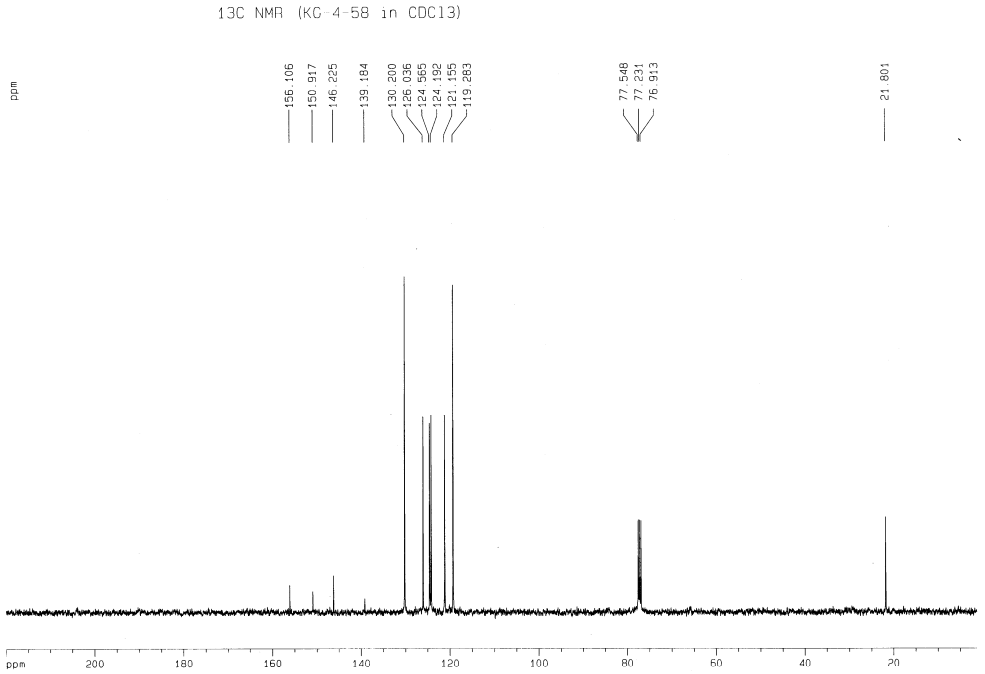

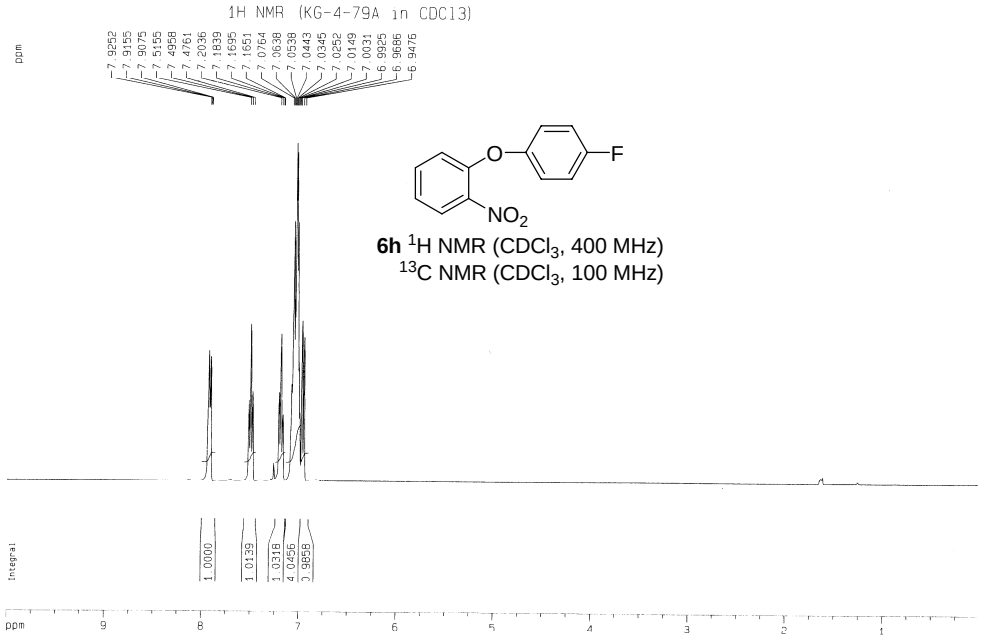

6h ^{1}H NMR ($CDCl_3$, 400 MHz)
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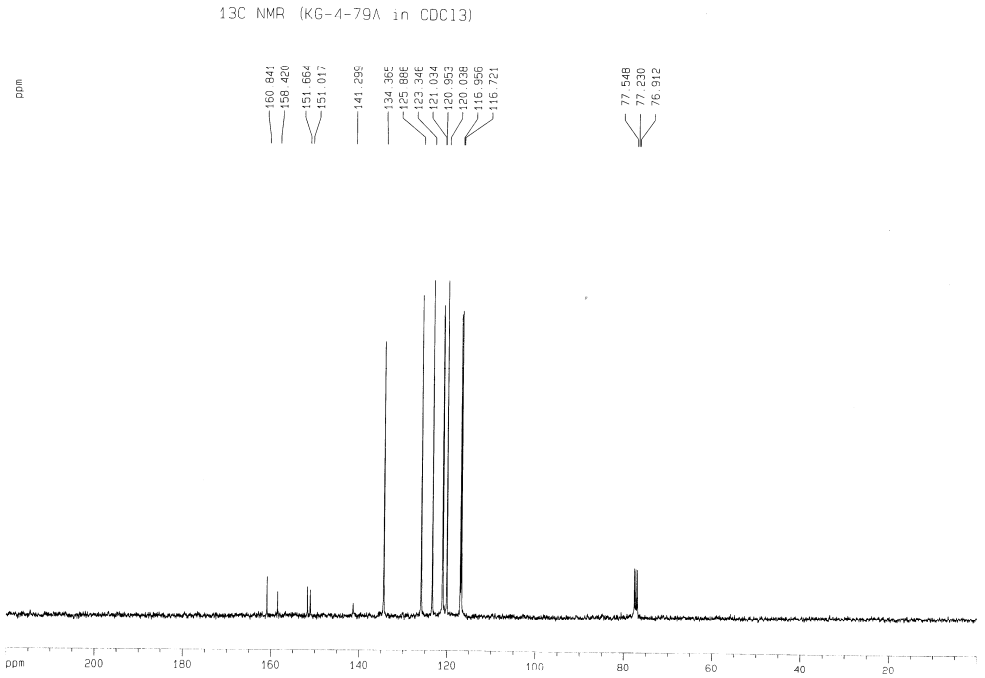

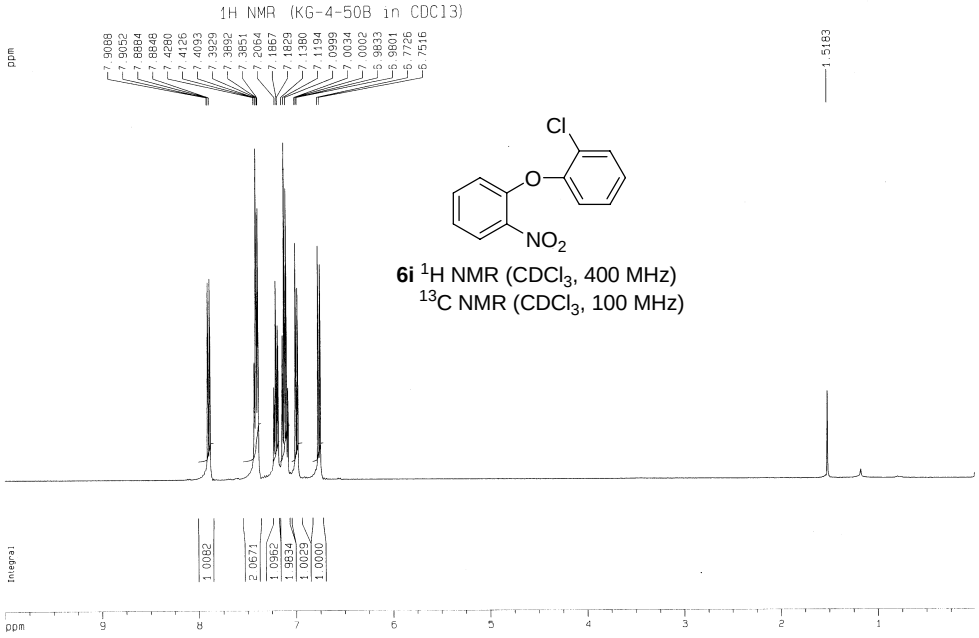

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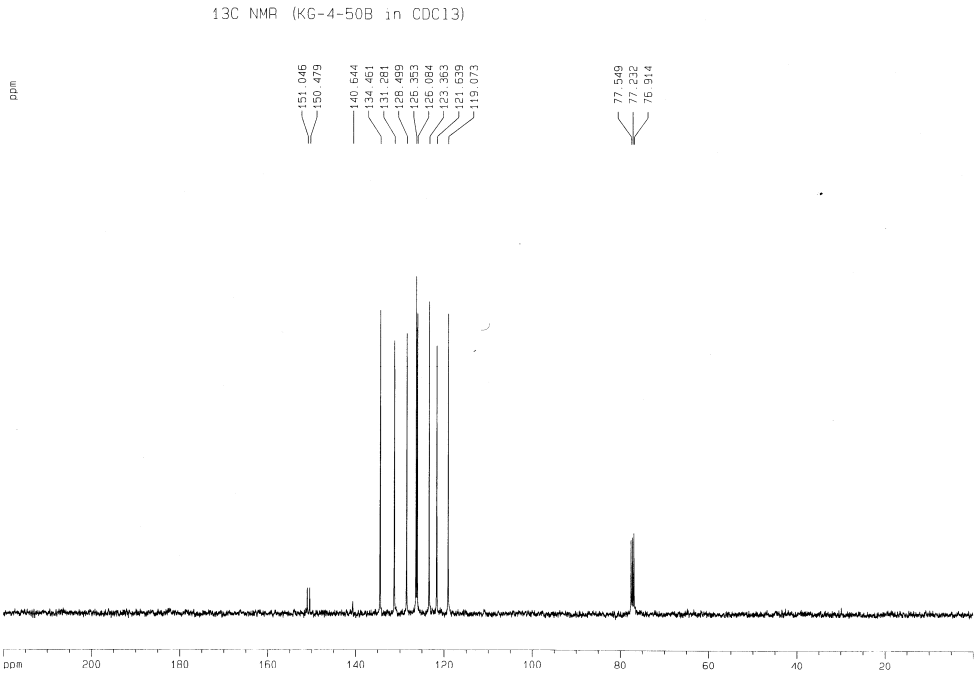
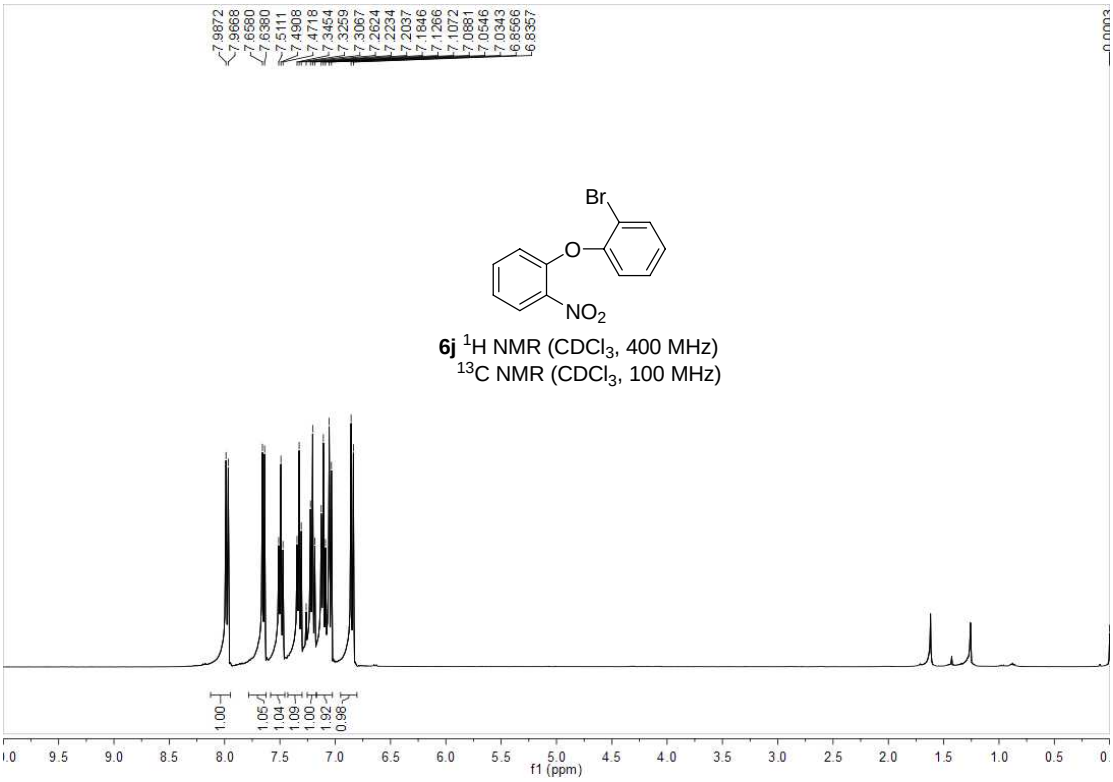
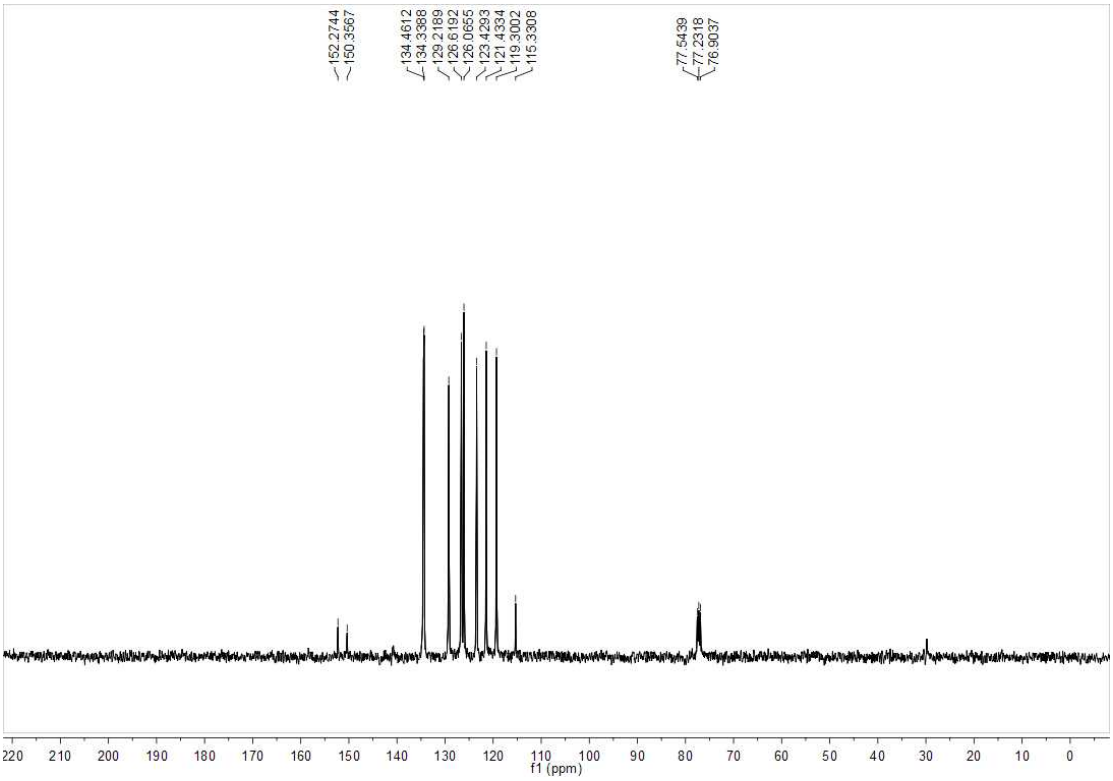
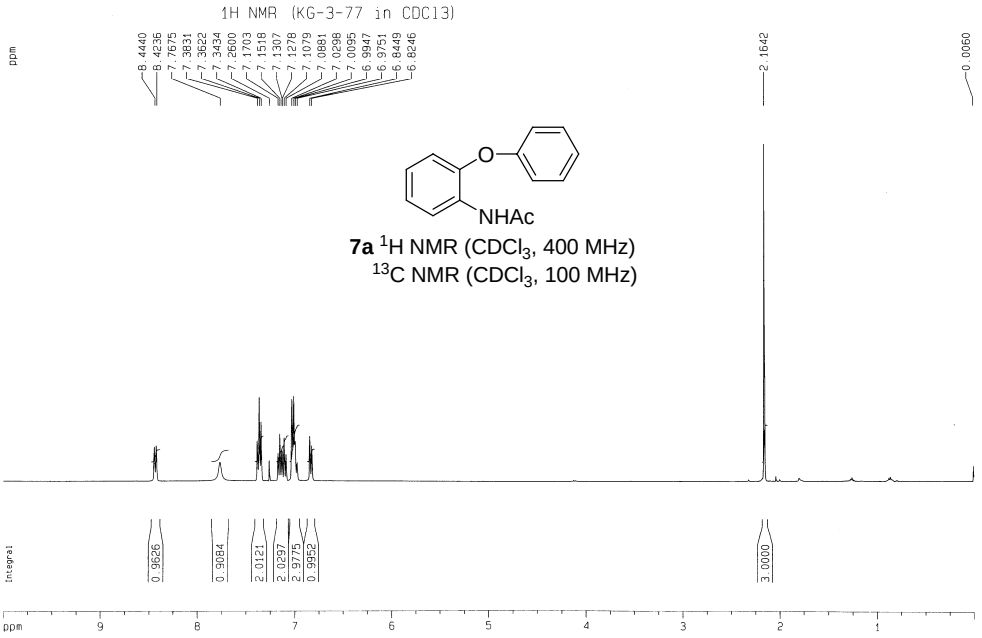


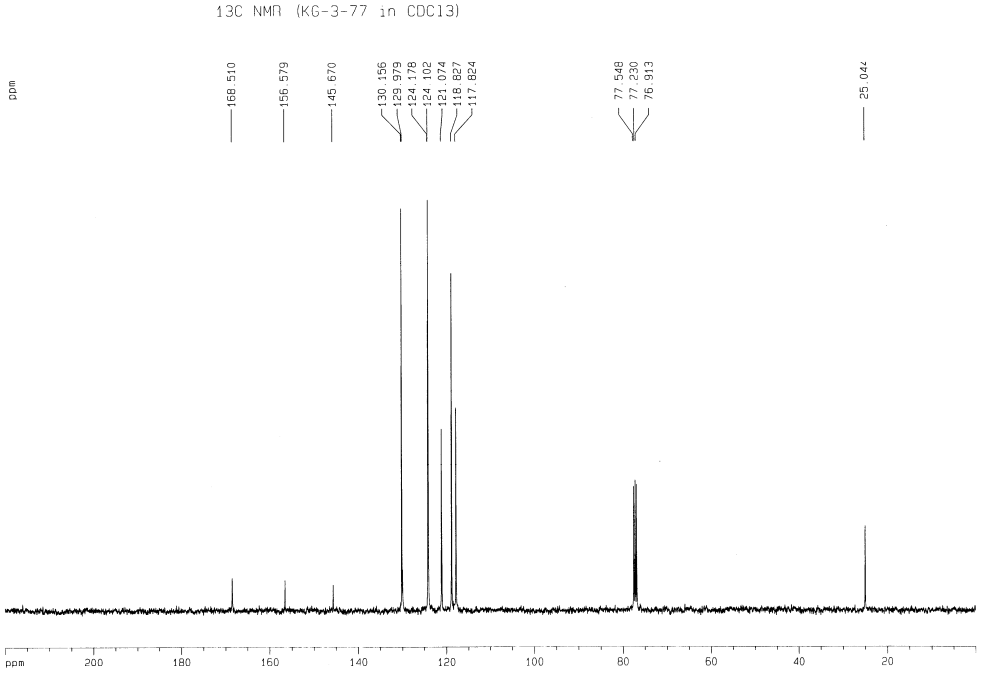


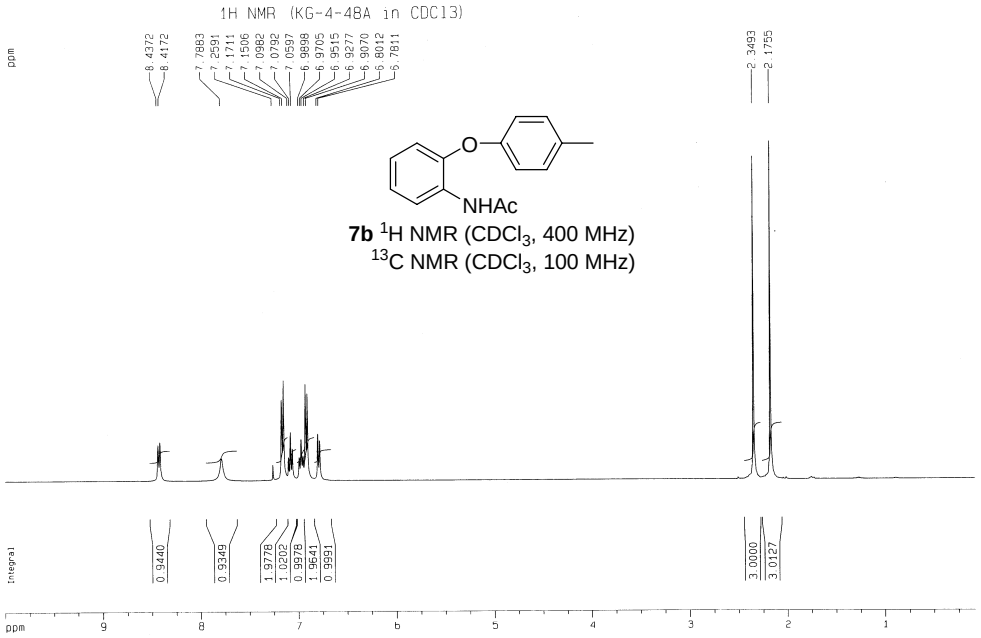
6j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





7a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





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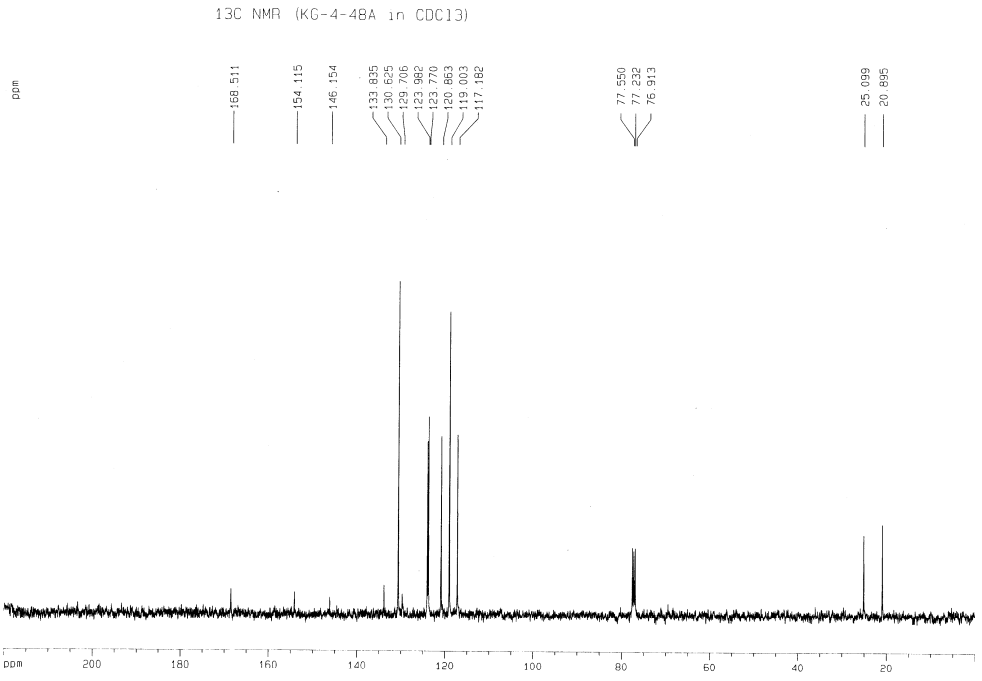
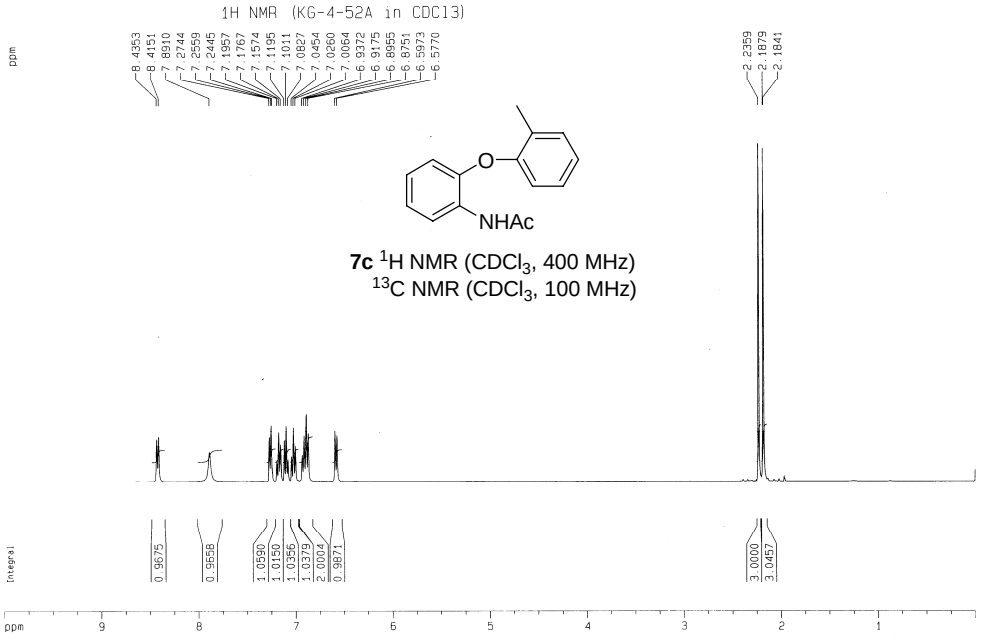
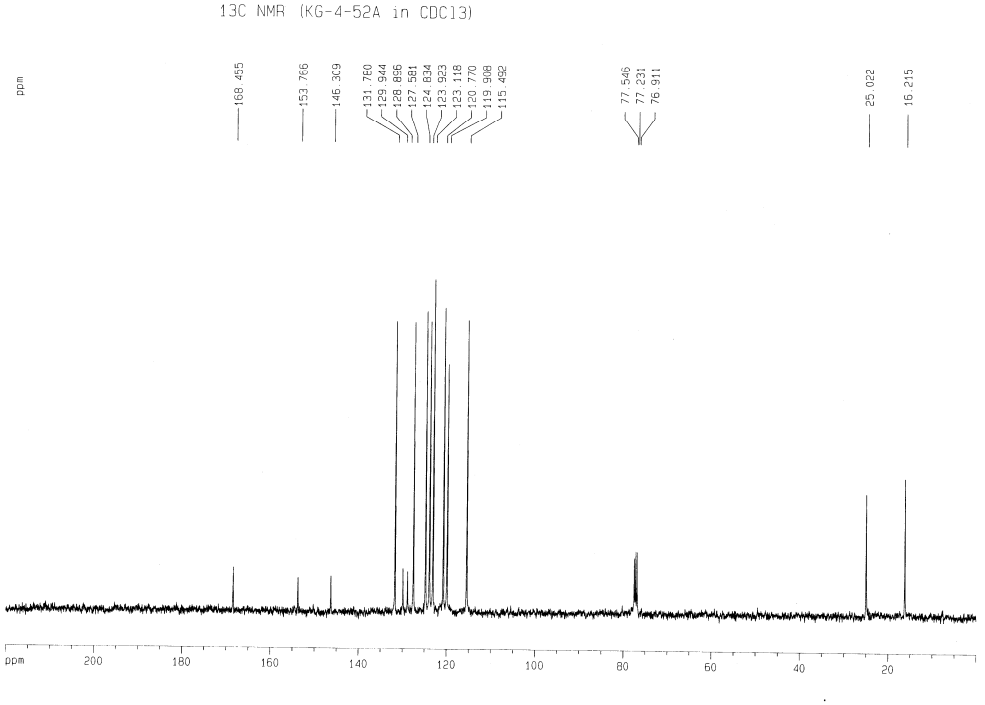
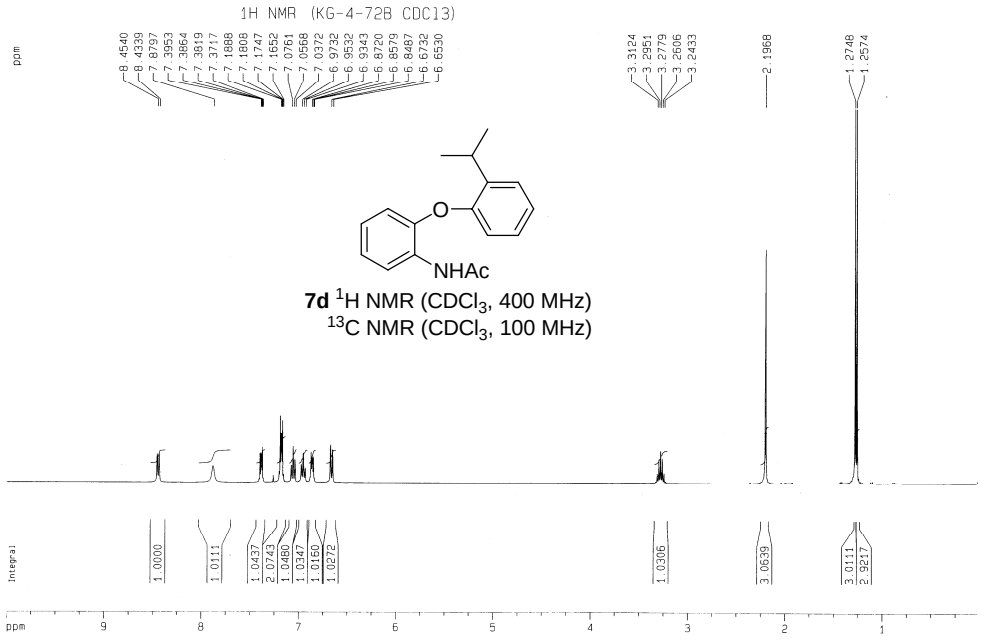
^{13}C NMR ($CDCl_3$, 100 MHz)



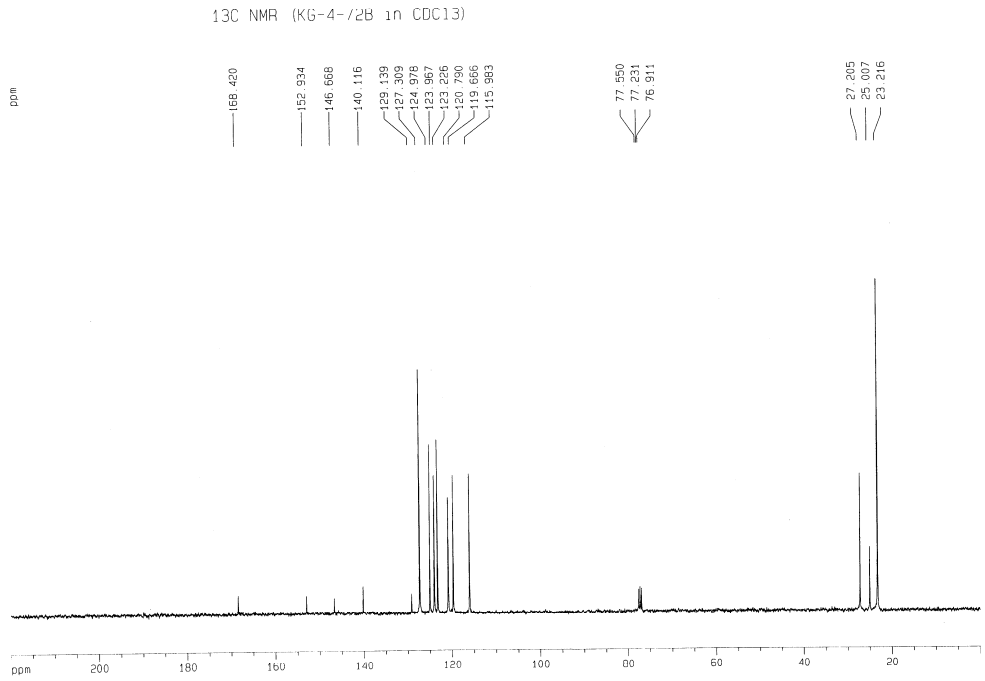


7c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





7d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

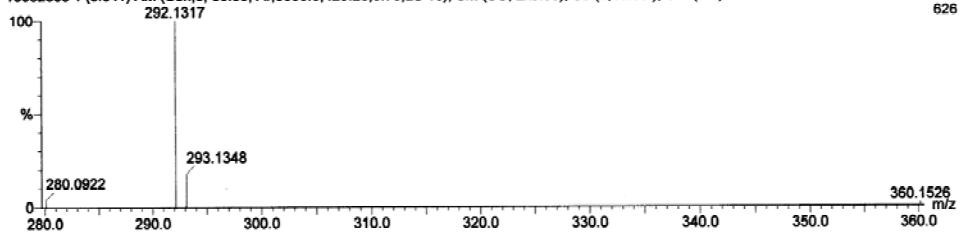


Elemental Composition Report **Page 1**

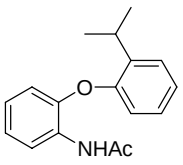
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 2-2 Na: 1-1

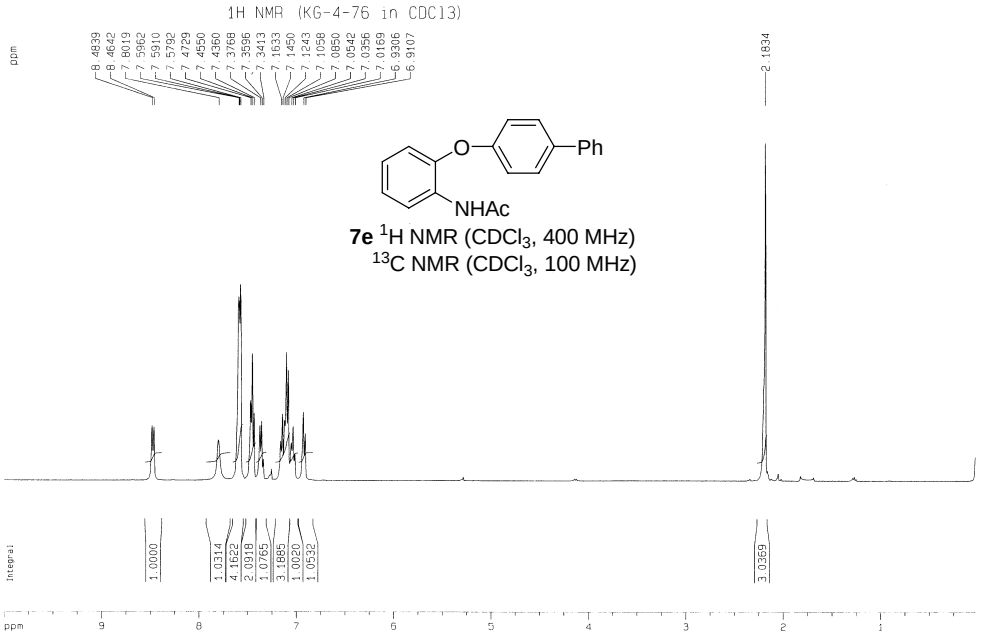
KG-4-72B
10052605 1 (0.041) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:4) 1: TOF MS ES+ 626



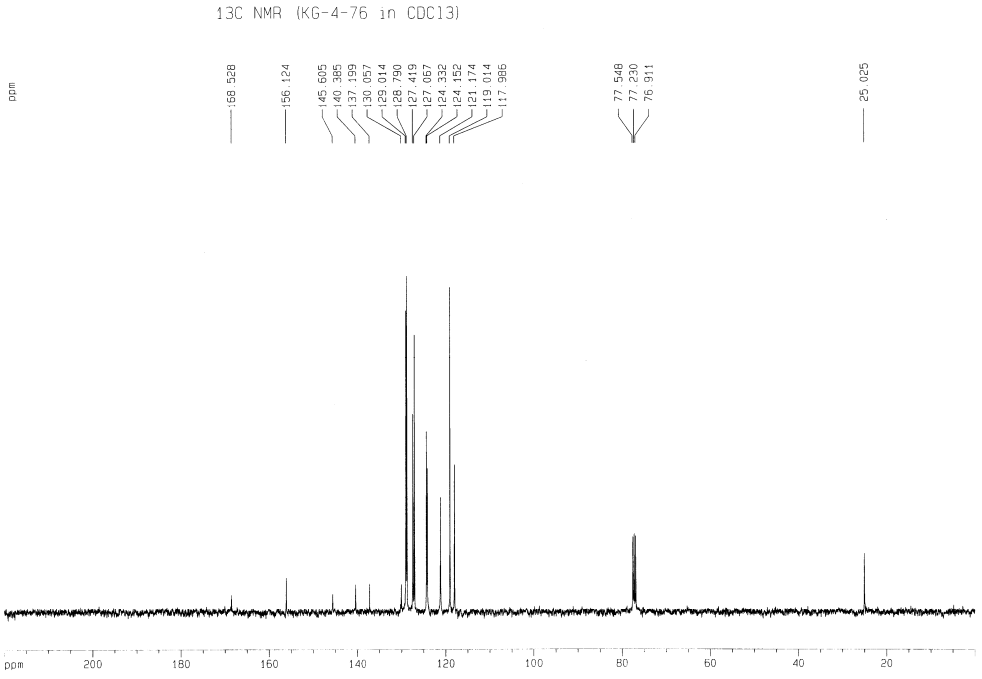
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.1317	292.1313	0.4	1.4	8.5	2773077.0	C17 H19 N O2 Na



7d HRMS



7e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

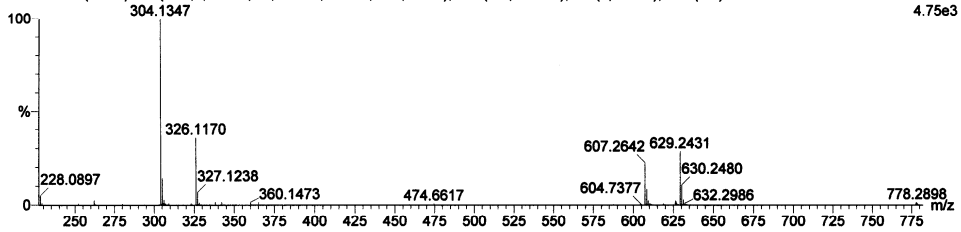


Elemental Composition Report **Page 1**

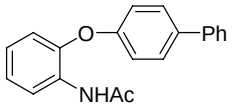
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 2-2

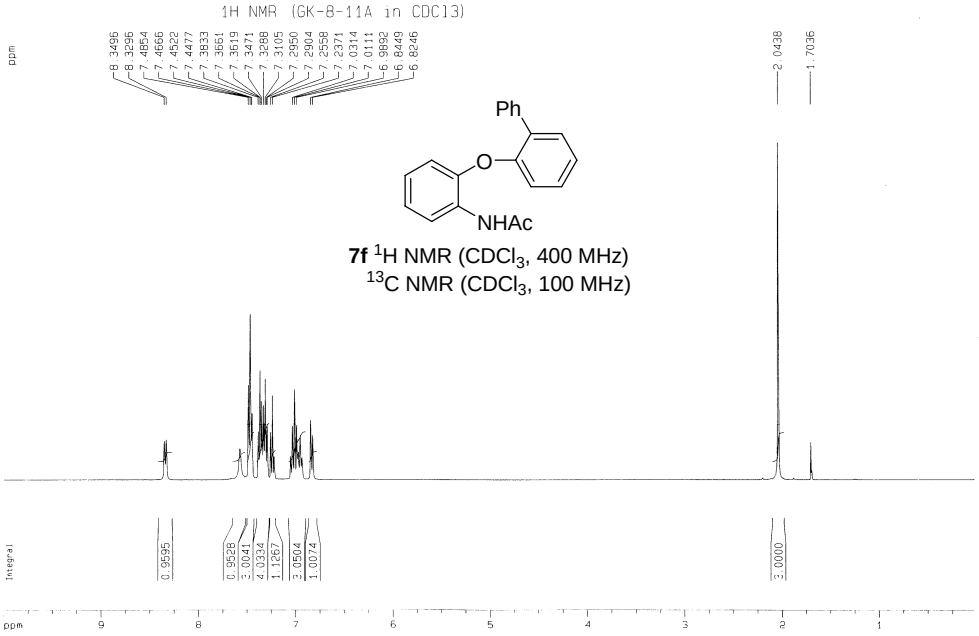
KG-4-76
10052912 7 (0.194) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:9) 1: TOF MS ES+ 4.75e3



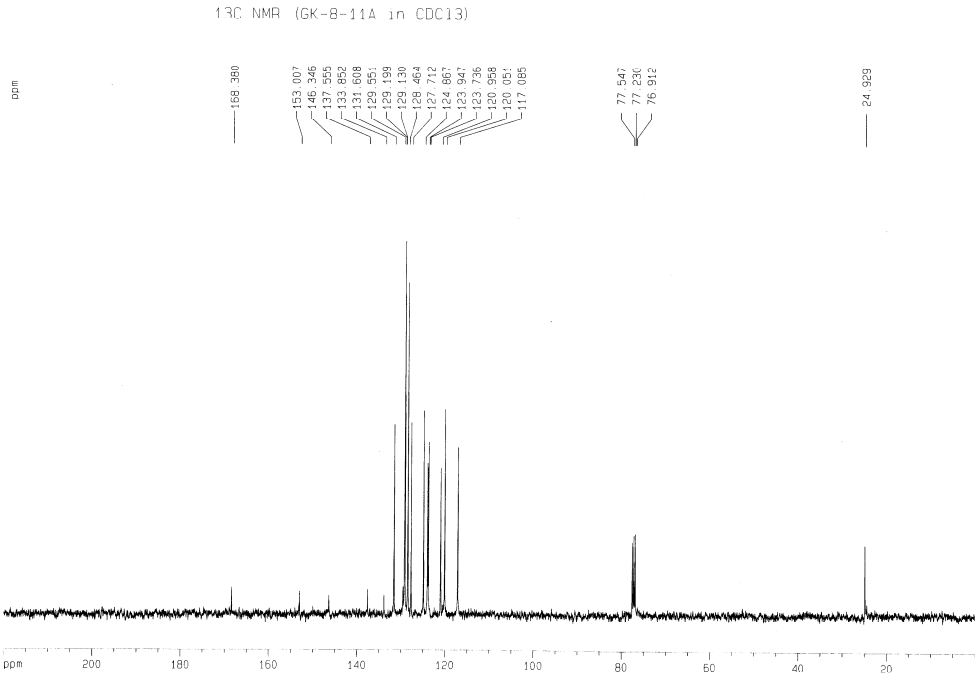
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.1347	304.1338	0.9	3.0	12.5	95.7	C20 H18 N O2



7e HRMS



7f ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

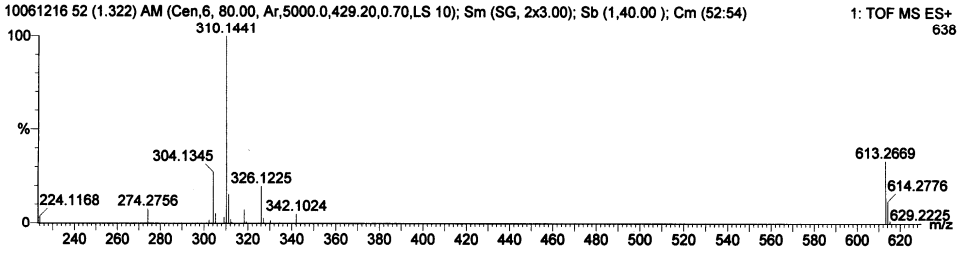


Elemental Composition Report **Page 1**

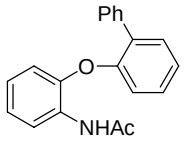
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 2-2

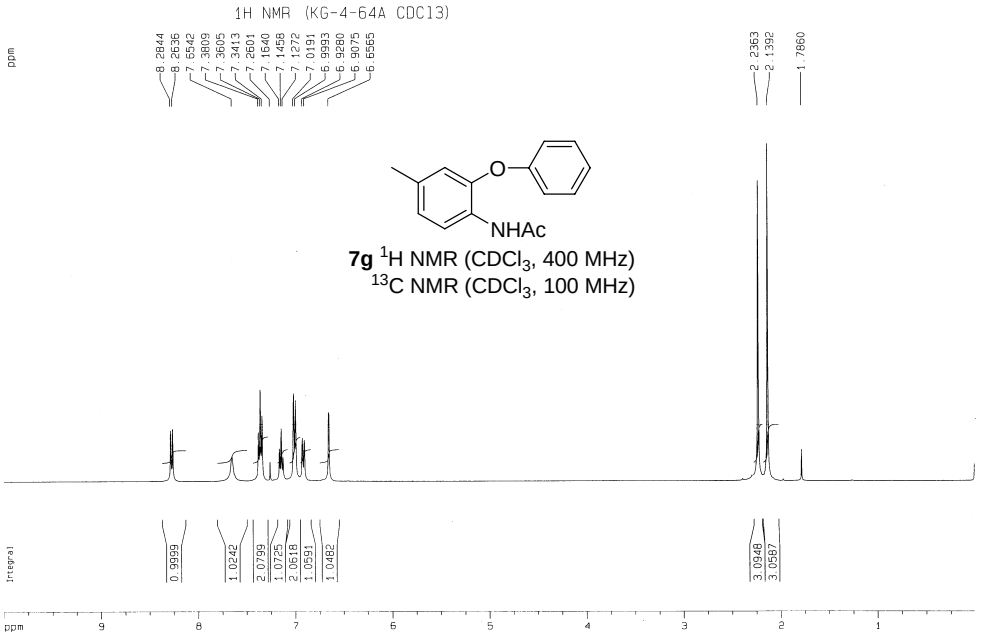
KG-8-11A
10061216 52 (1.322) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (52:54) 1: TOF MS ES+ 638



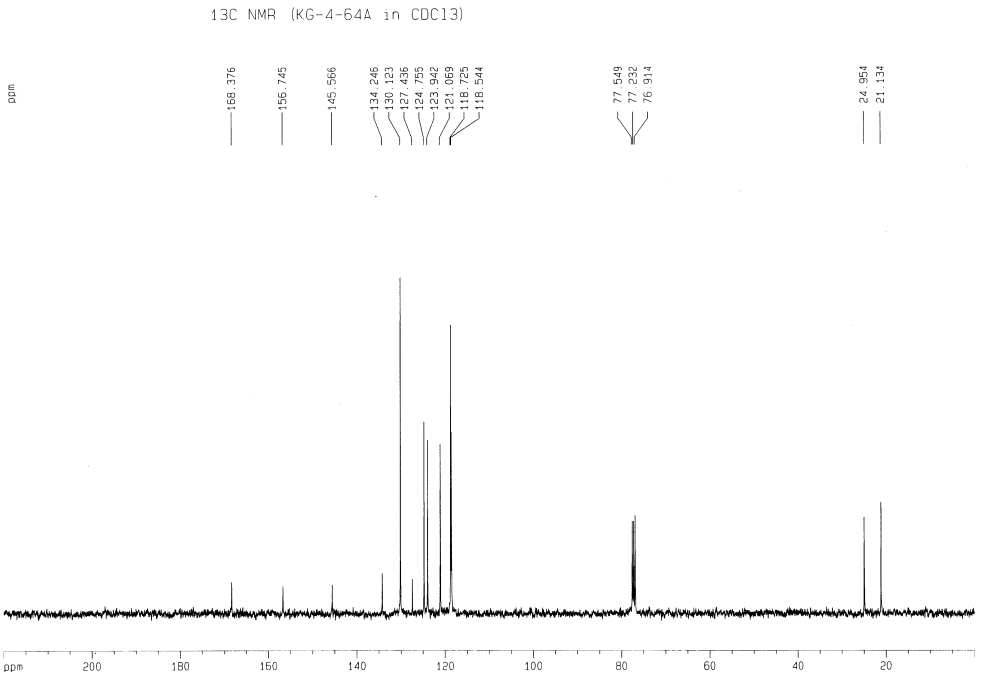
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.1345	304.1338	0.7	2.3	12.5	2773019.8	C20 H18 N O2

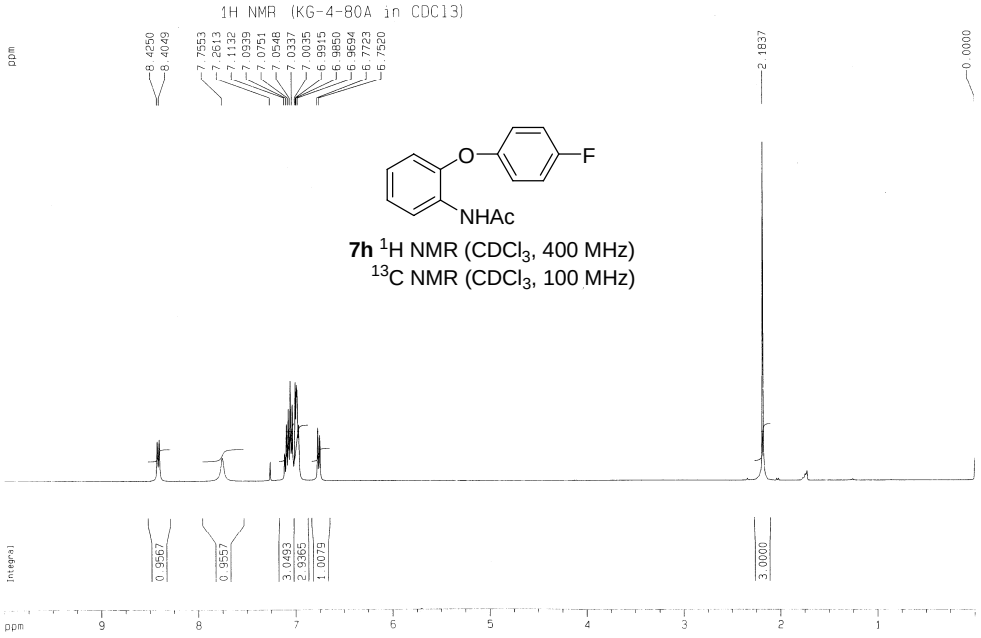


7f HRMS

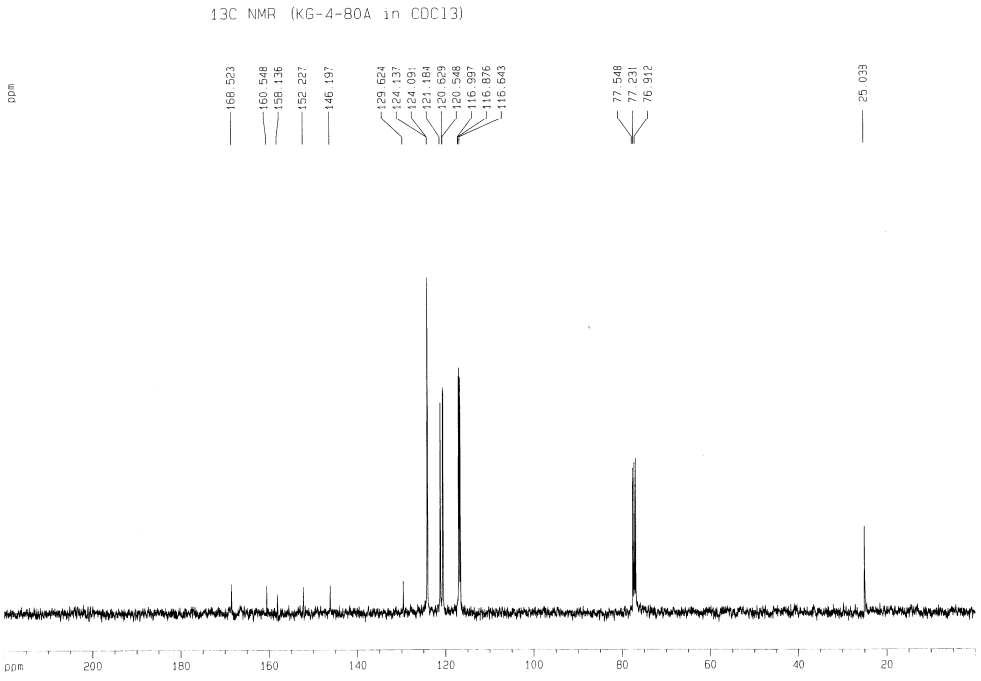


7g ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





7h ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

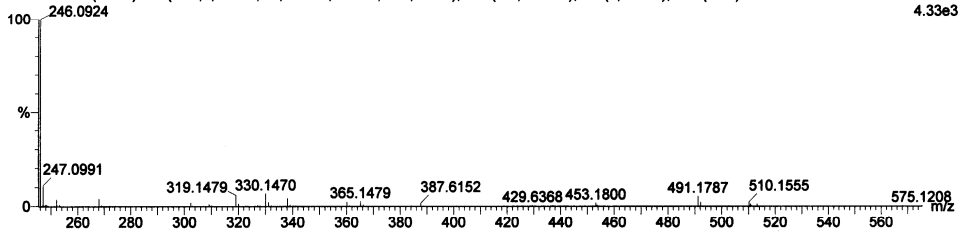


Elemental Composition Report **Page 1**

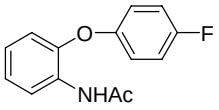
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 2-2 F: 1-1

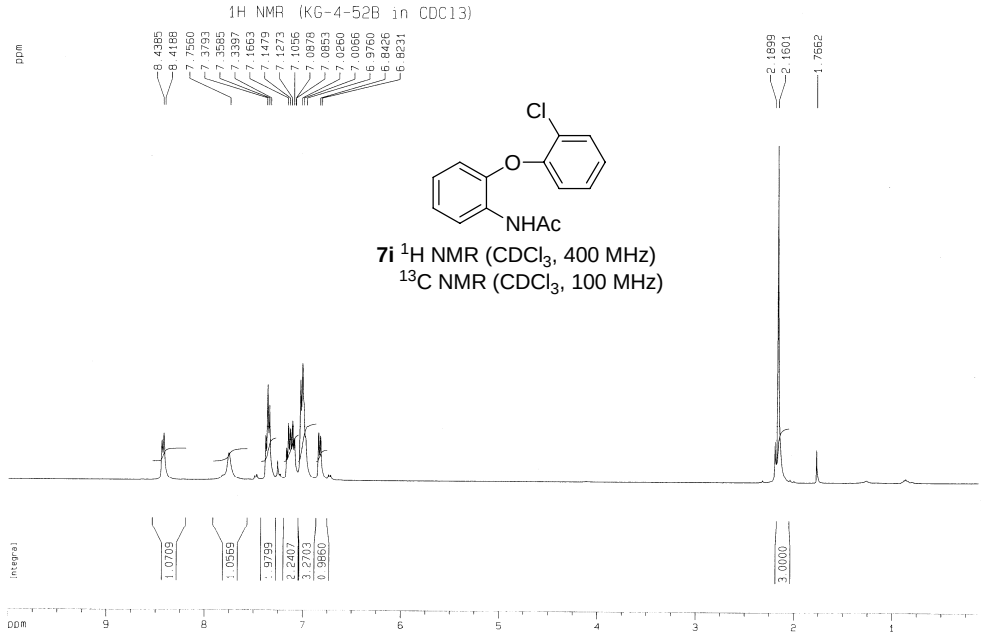
KG-4-80A
10052910 14 (0.366) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (7:14) 1: TOF MS ES+ 4.33e3



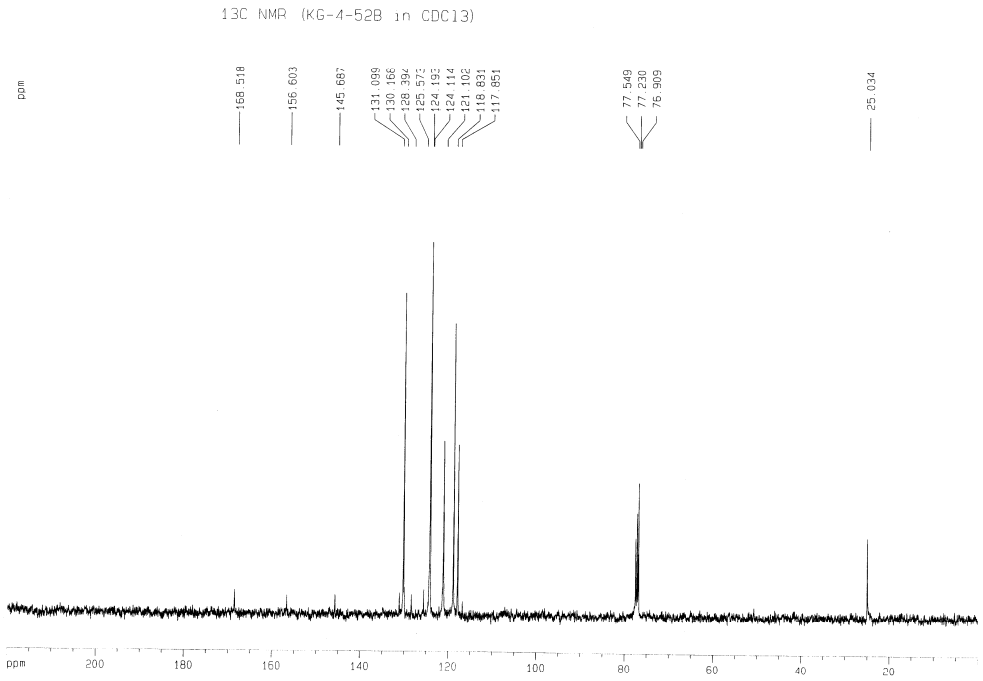
Minimum:				-10.0		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0924	246.0930	-0.6	-2.4	8.5	58.2	C14 H13 N O2 F

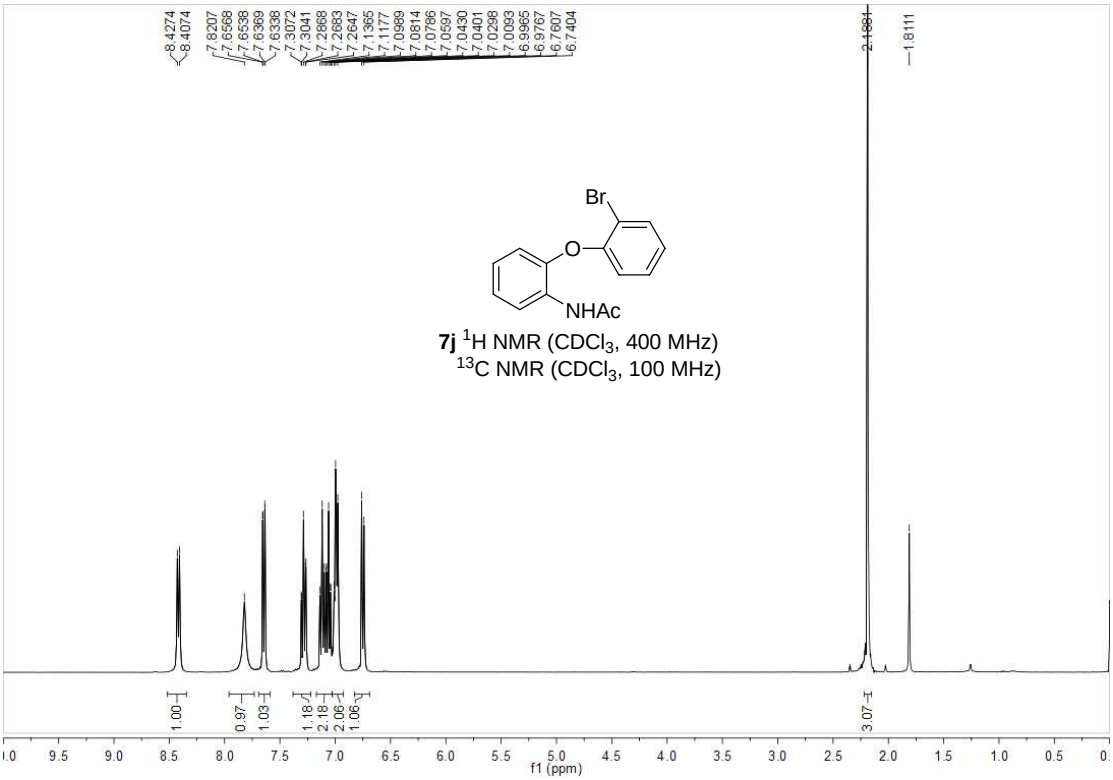


7h HRMS

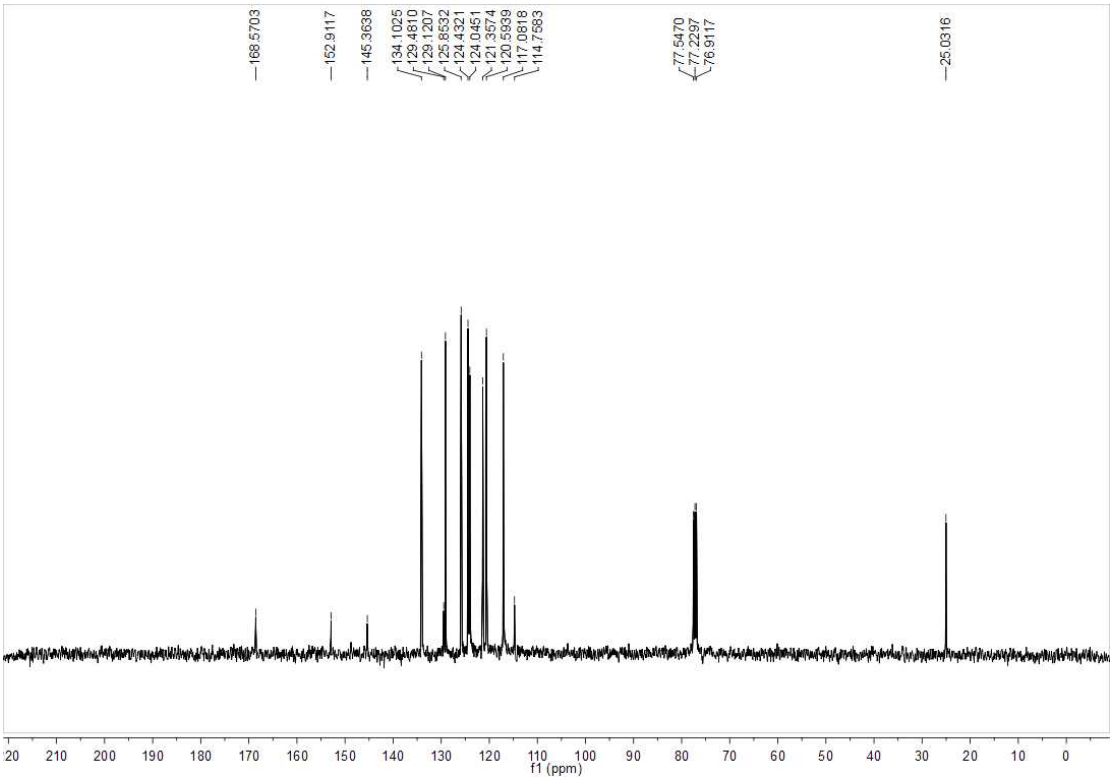


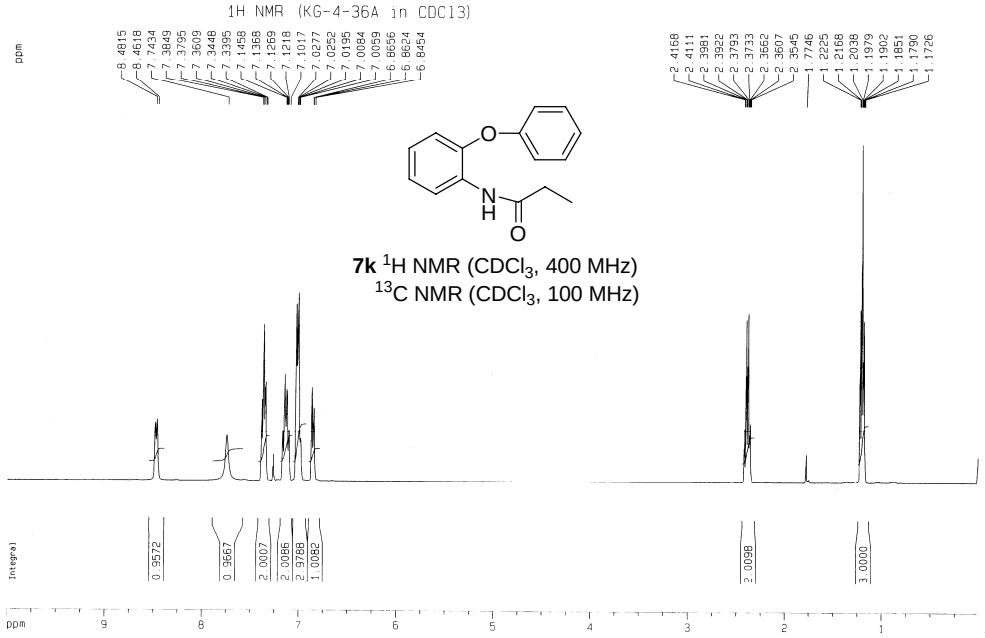
7i ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



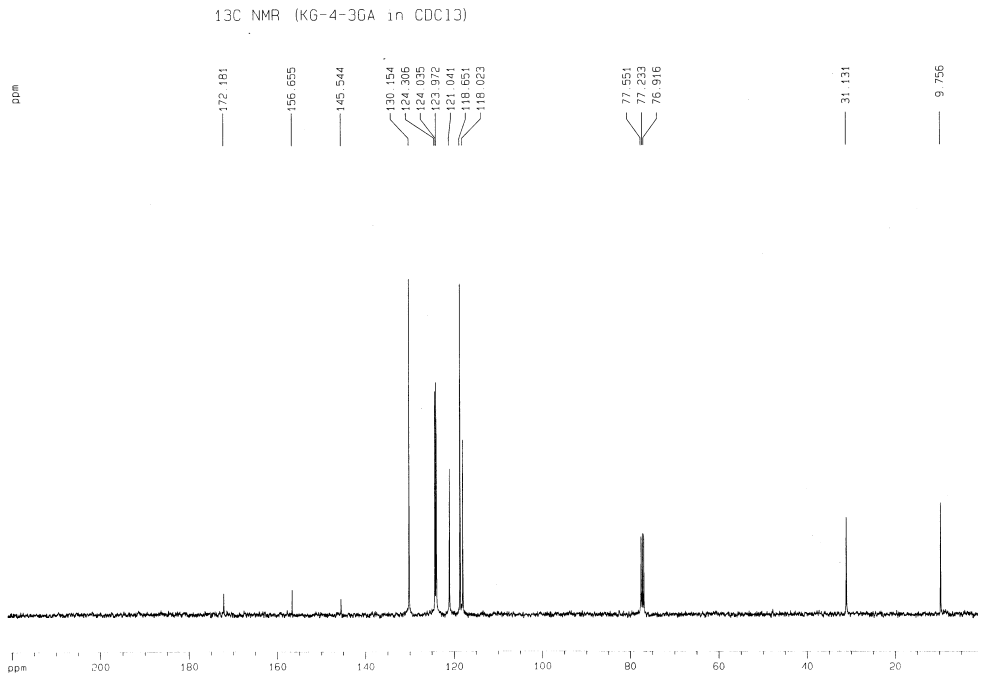


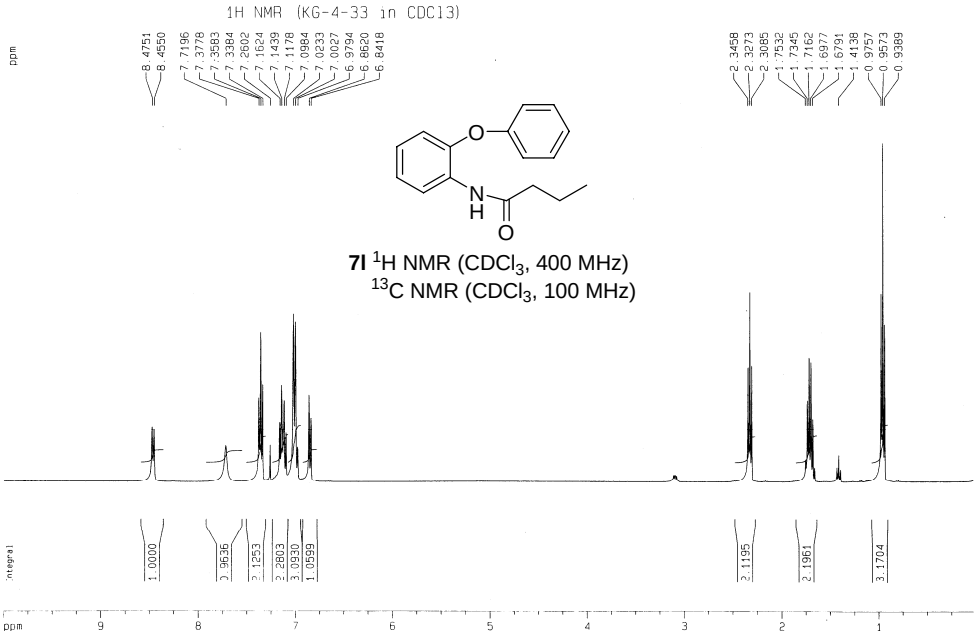
7j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



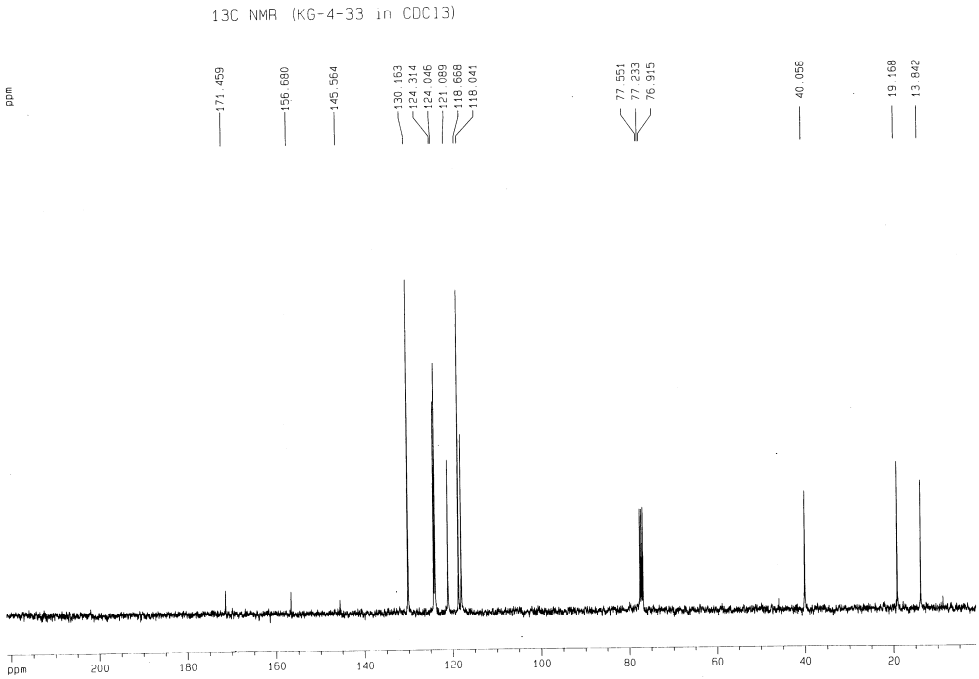


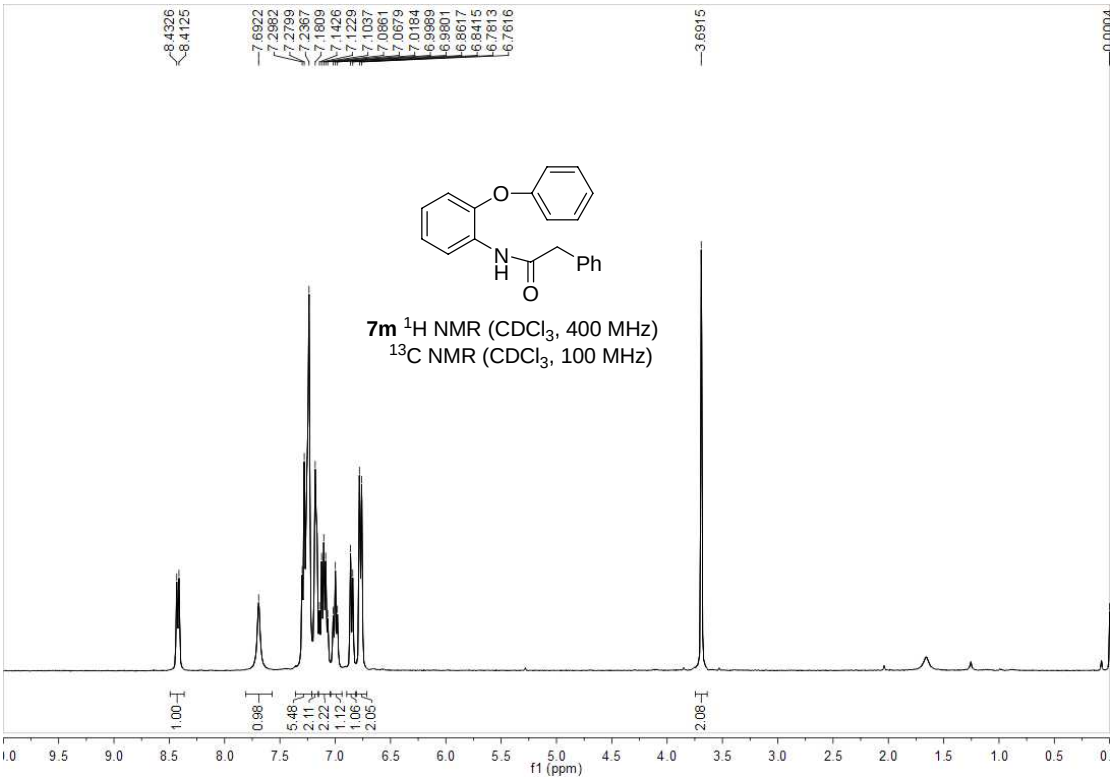
7k ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



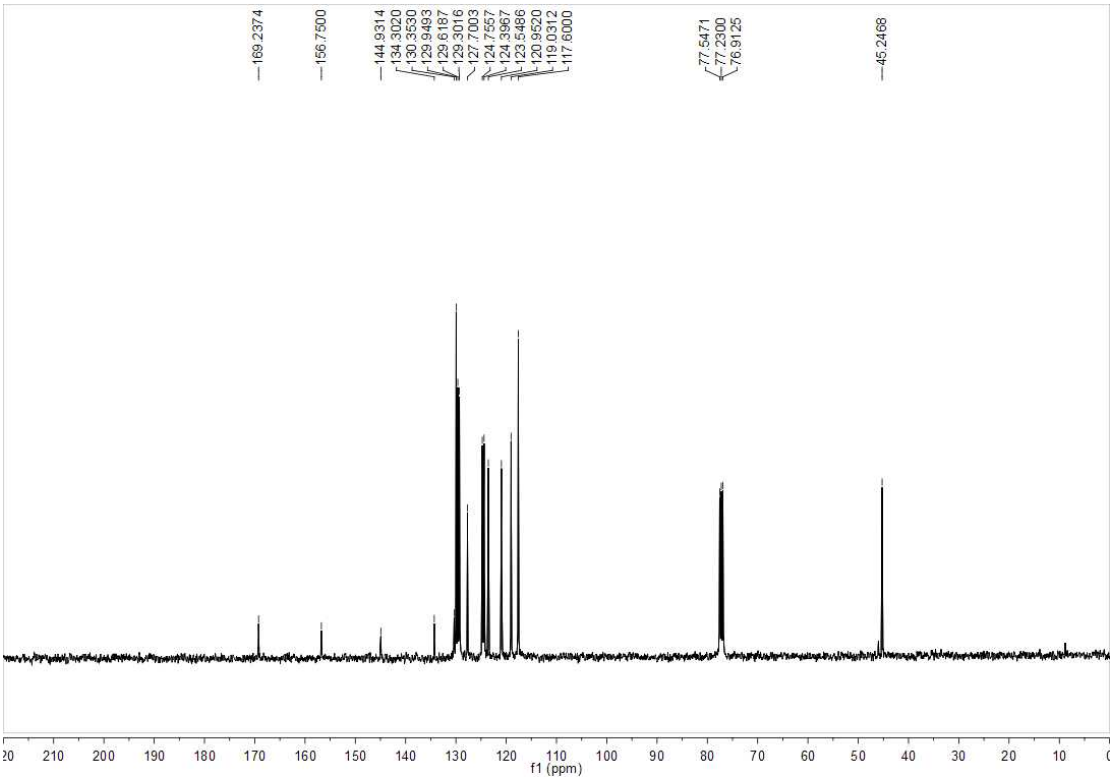


7l ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





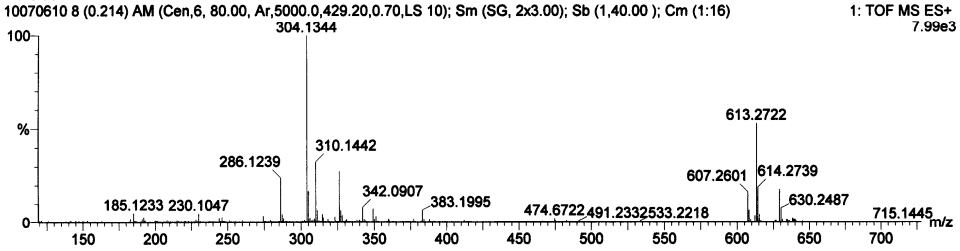
7m ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



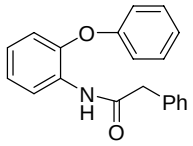
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

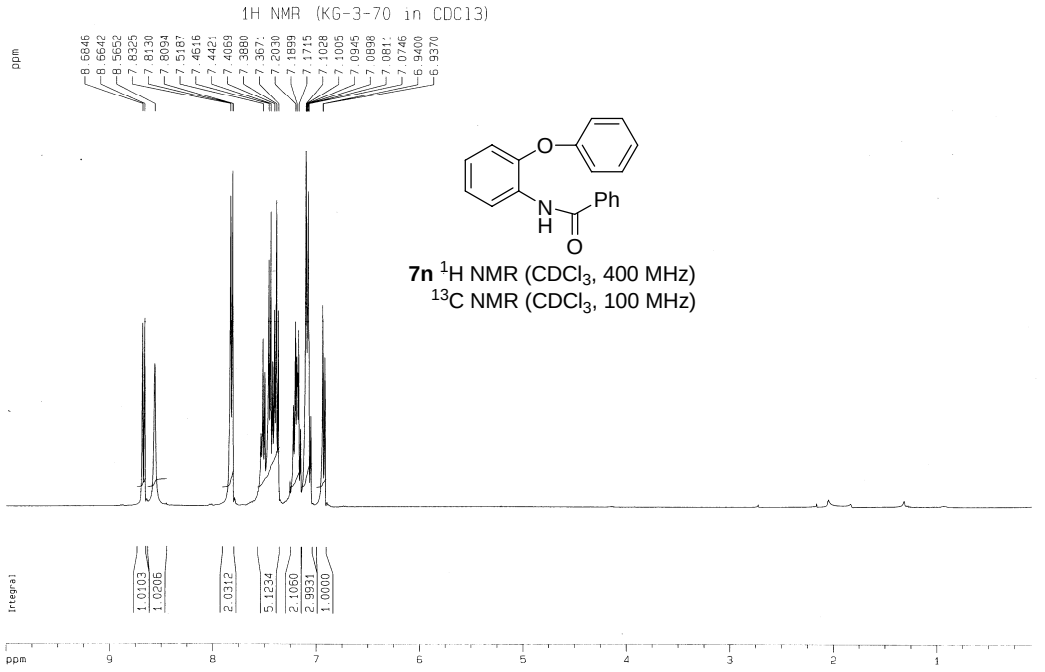
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 2-2
KG-3-93
10070610 8 (0.214) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:16) 1: TOF MS ES+ 7.99e3



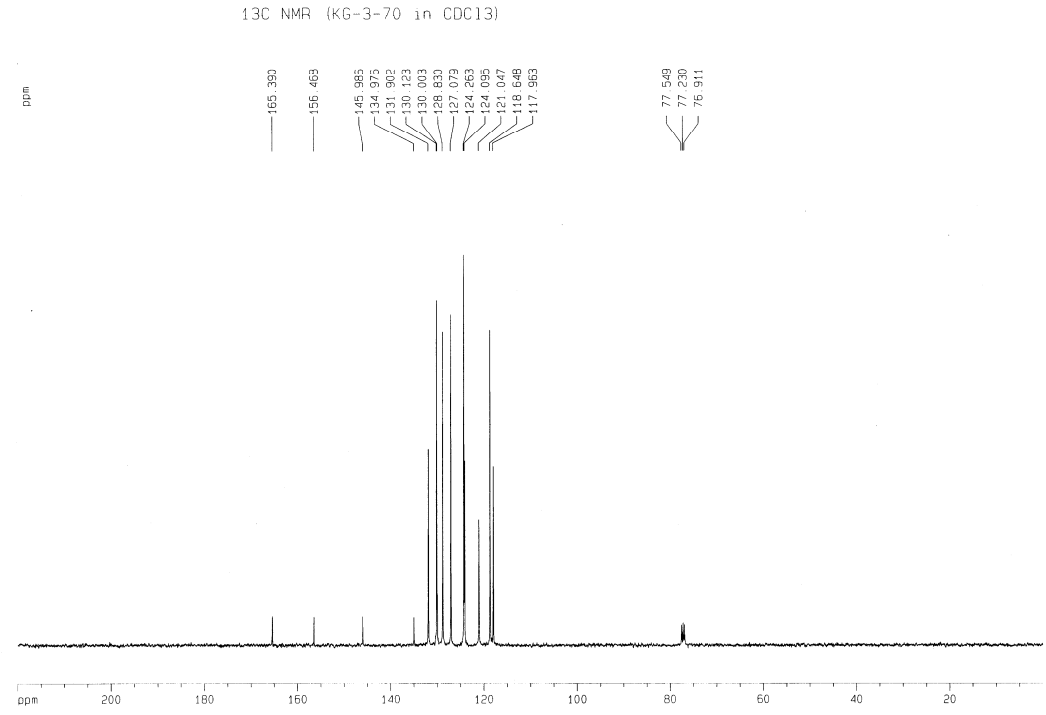
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.1344	304.1338	0.6	2.0	12.5	70.9	C20 H18 N O2

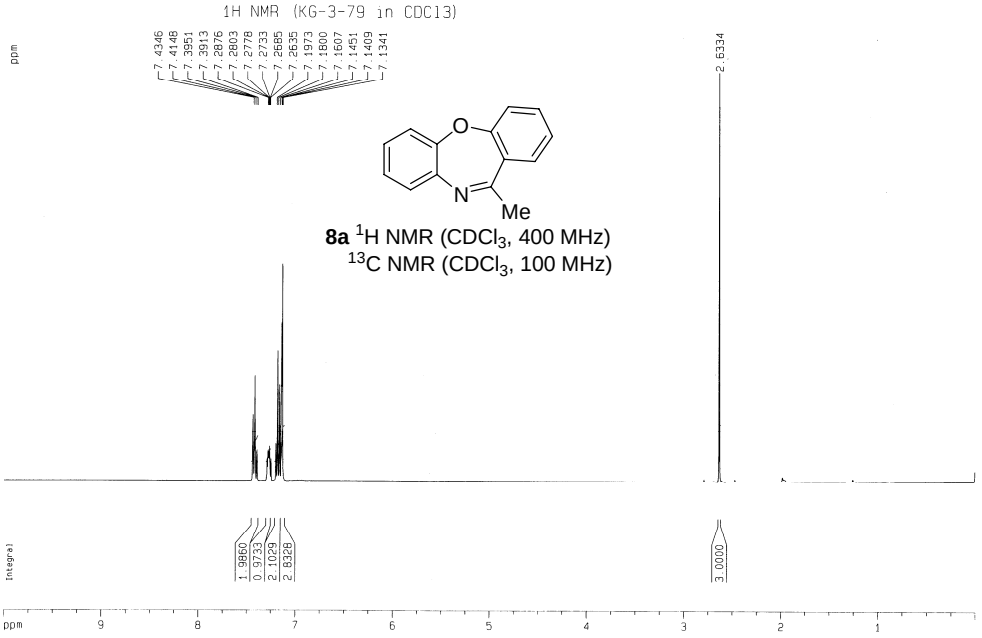


7m HRMS

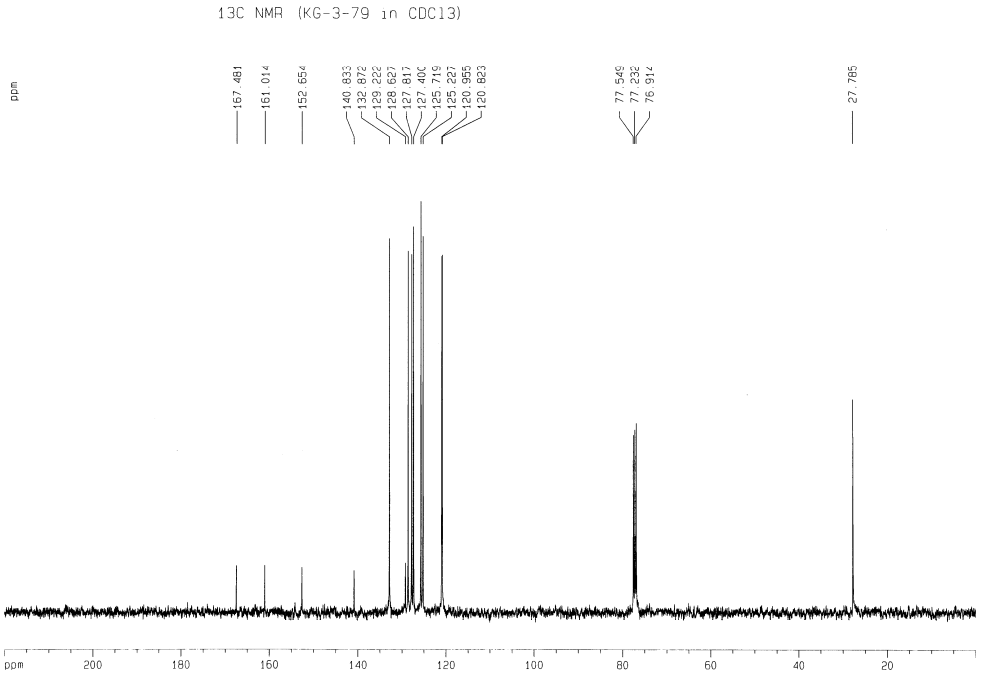


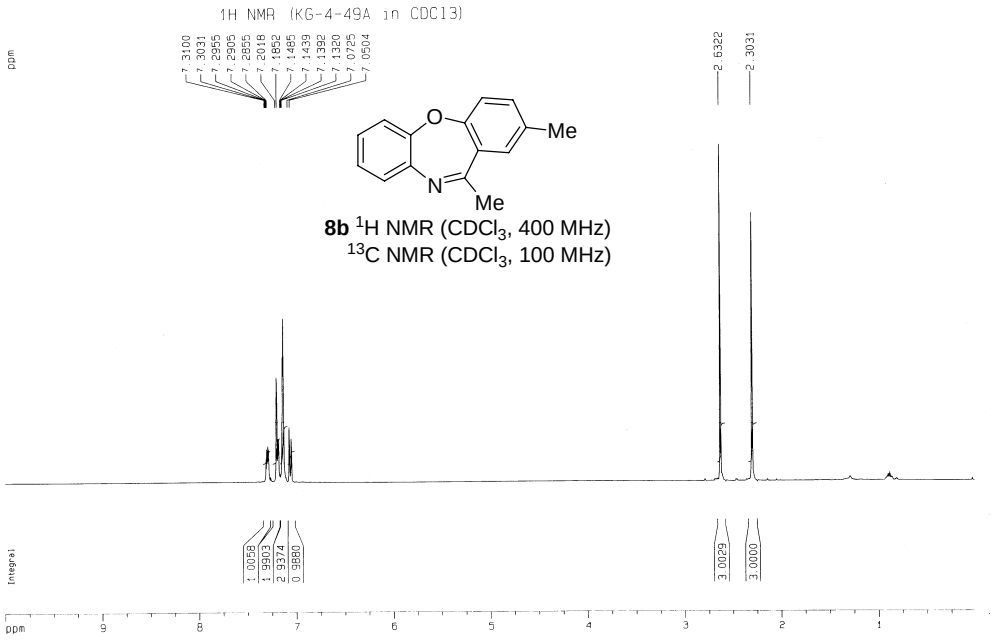
7n ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



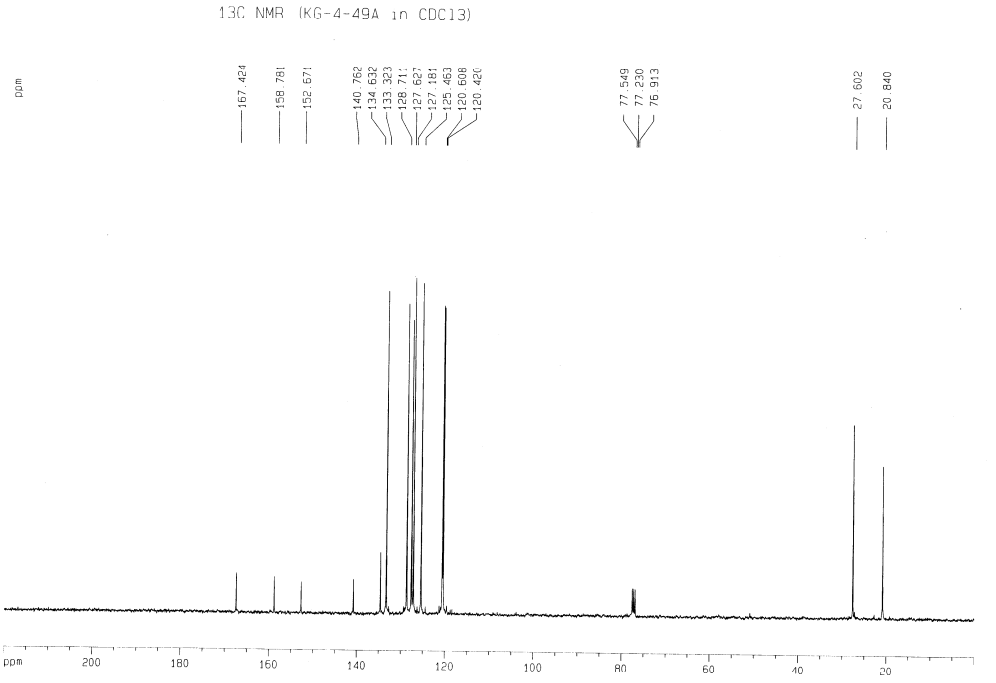


8a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





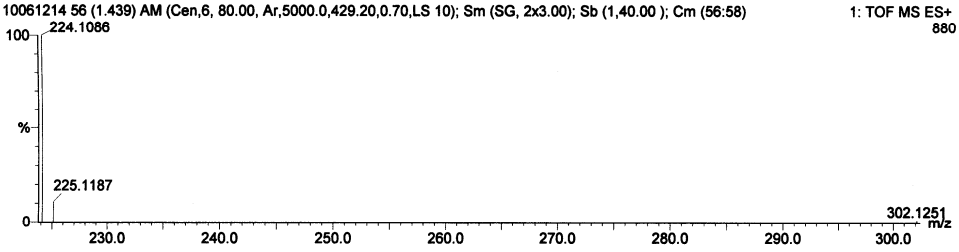
8b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



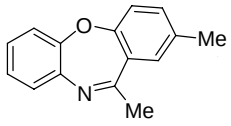
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

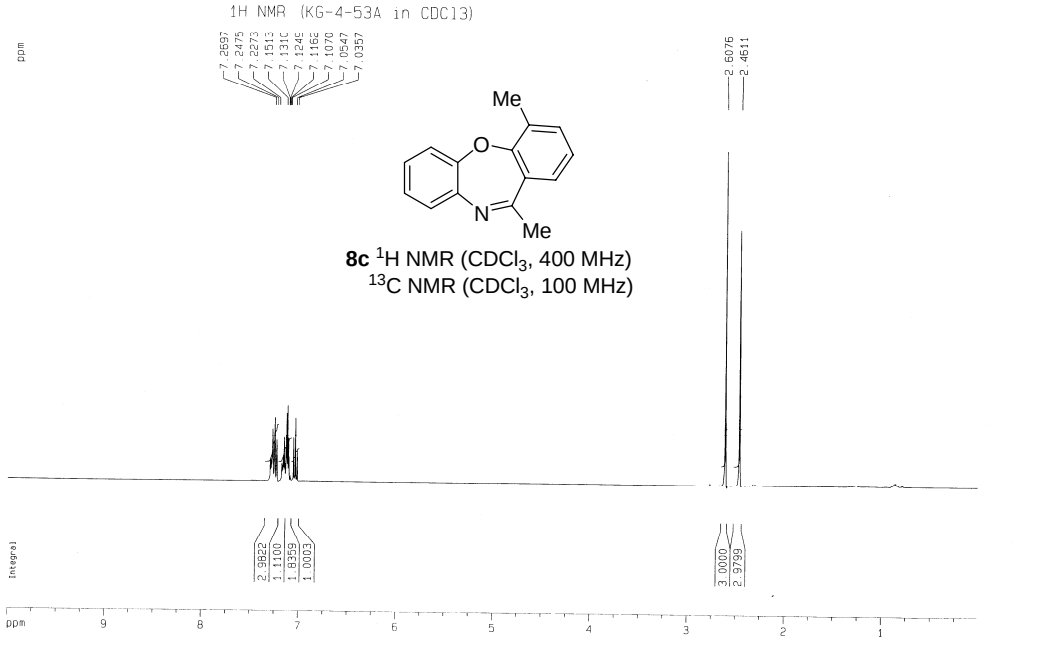
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-49A
10061214 56 (1.439) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (56:58) 1: TOF MS ES+
880



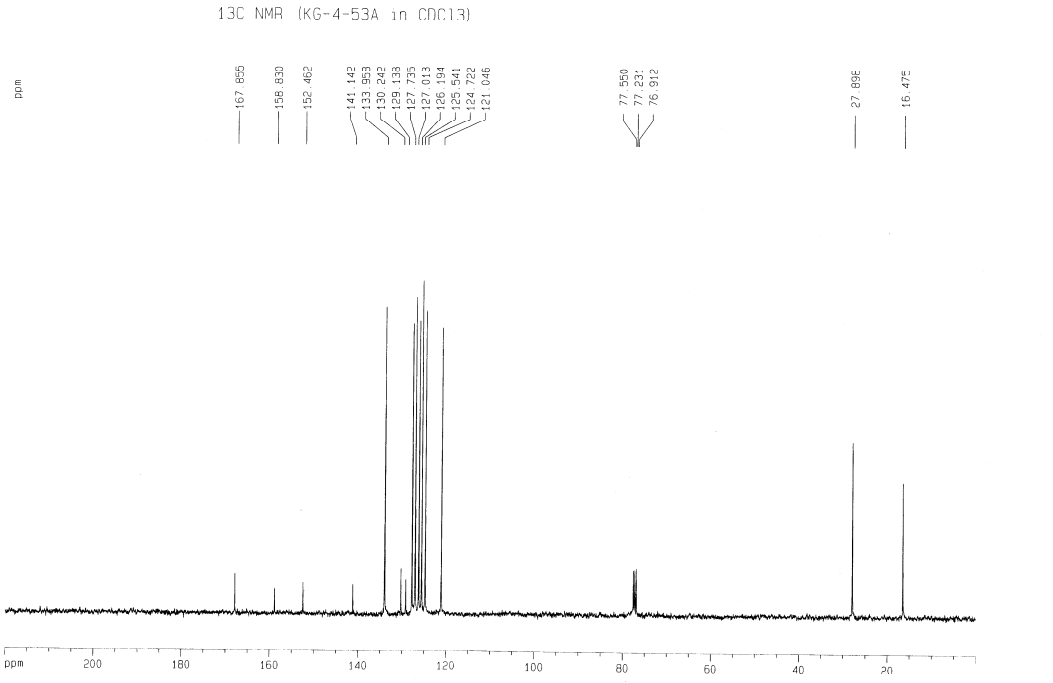
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1086	224.1075	1.1	4.9	9.5	2773087.5	C15 H14 N O



8b HRMS



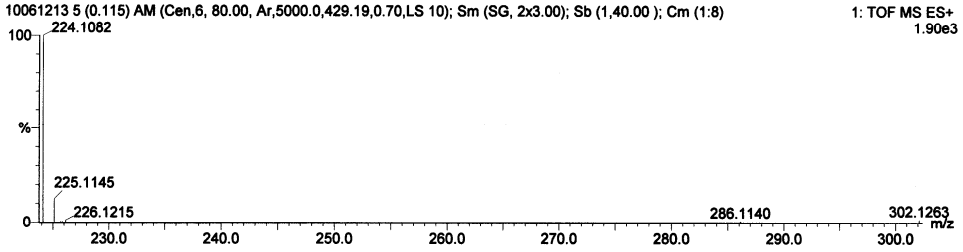
8c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



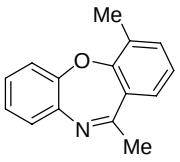
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

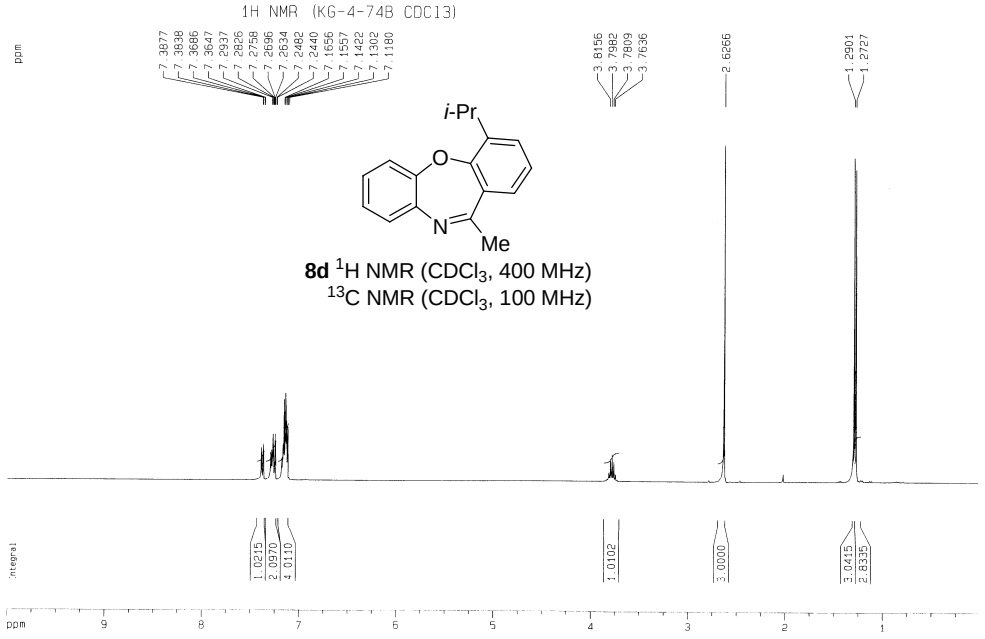
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-53A
10061213 5 (0.115) AM (Cen,6, 80.00, Ar,5000.0,429.19,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:8) 1: TOF MS ES+ 1.90e3



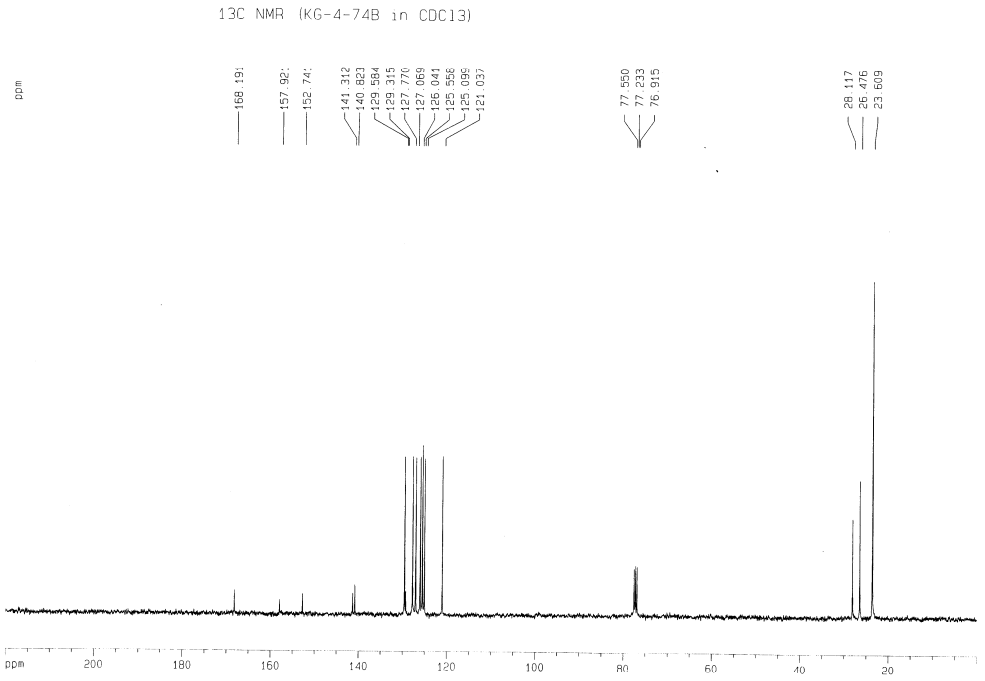
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1082	224.1075	0.7	3.1	9.5	19.1	C15 H14 N O



8c HRMS



8d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

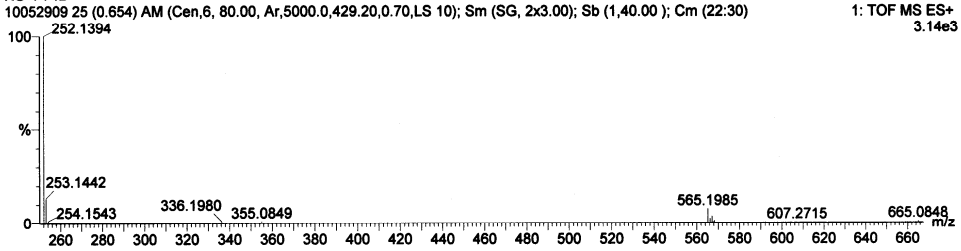


Elemental Composition Report **Page 1**

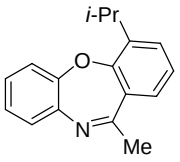
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 1-1

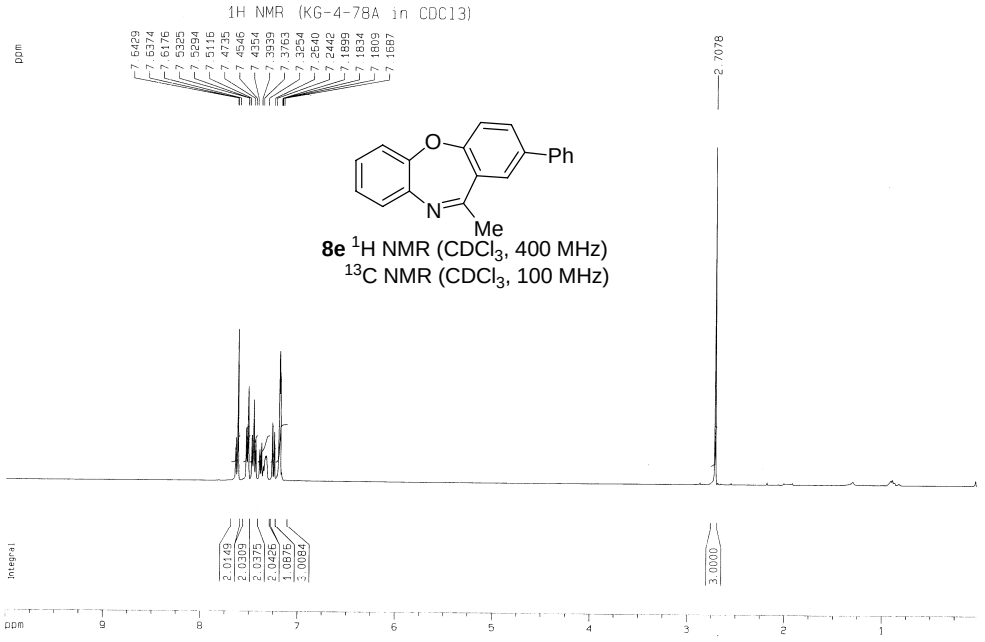
KG-4-74B
10052909 25 (0.654) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (22:30) 1: TOF MS ES+ 3.14e3



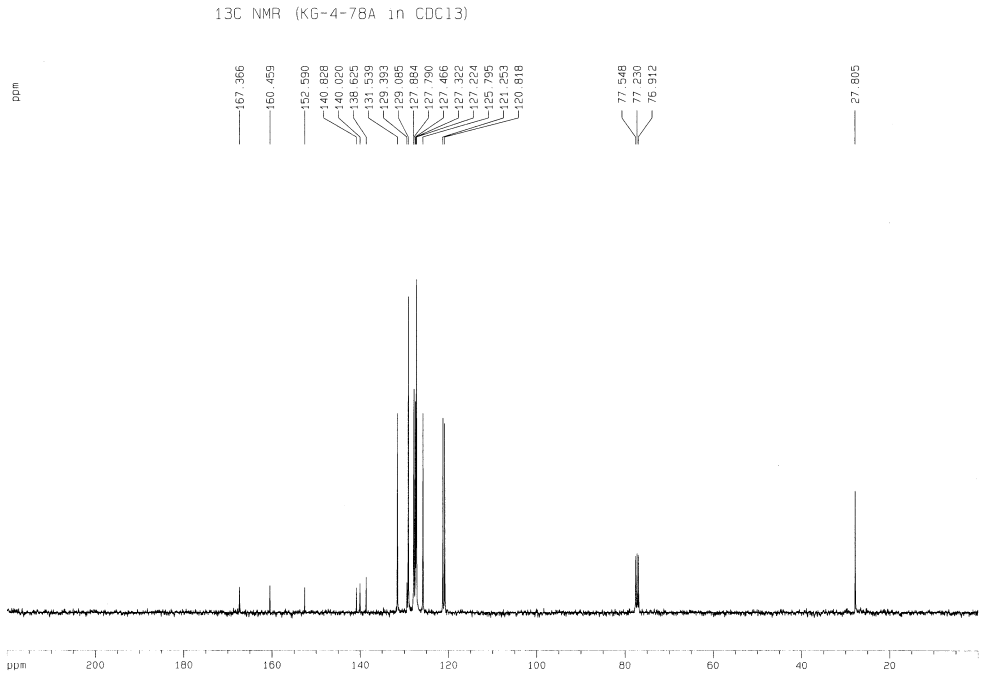
Minimum:				-10.0		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.1394	252.1388	0.6	2.4	9.5	45.9	C17 H18 N O



8d HRMS



8e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

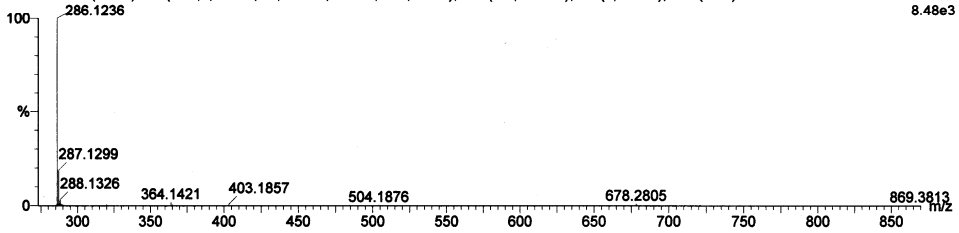


Elemental Composition Report **Page 1**

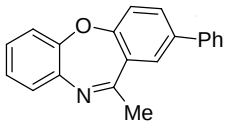
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1

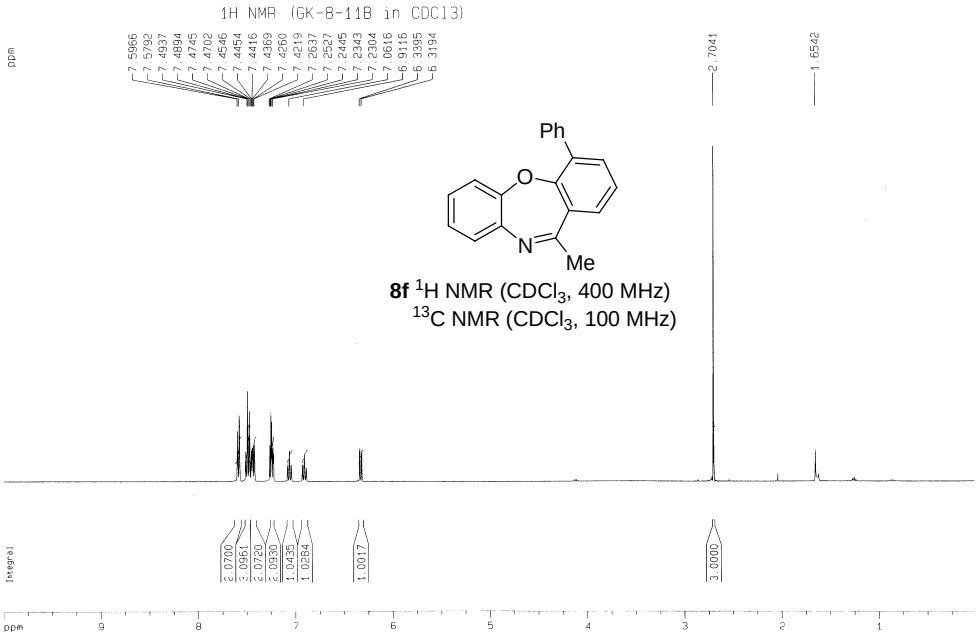
KG-4-78A
10061211 37 (0.960) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (9:46) 1: TOF MS ES+ 8.48e3



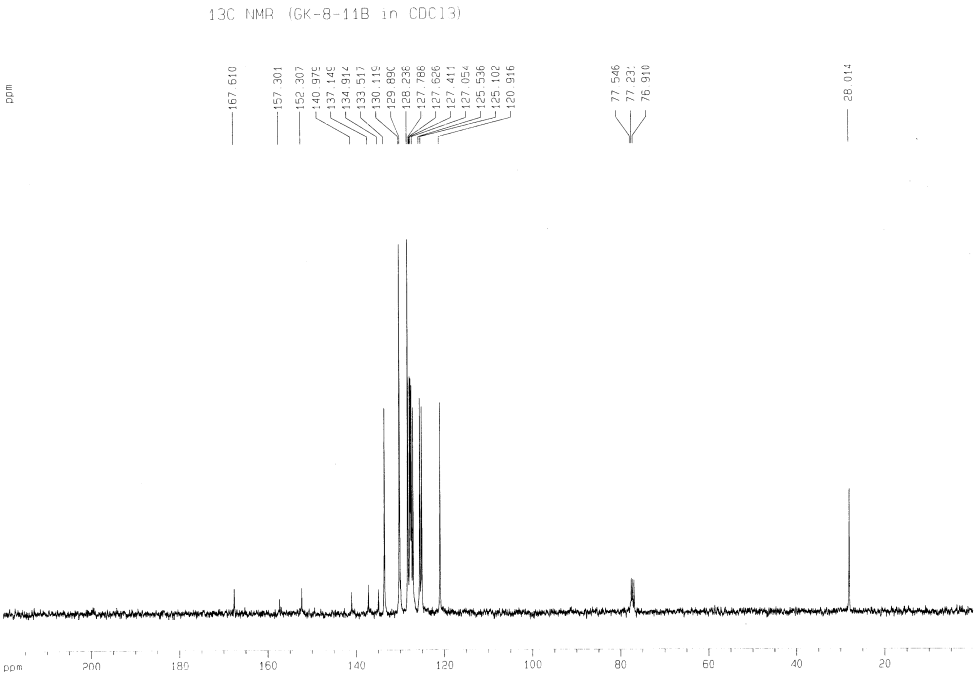
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.1236	286.1232	0.4	1.4	13.5	35.8	C20 H16 N O



8e HRMS



8f ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

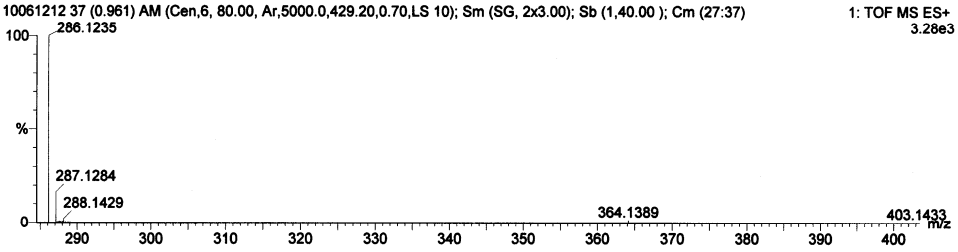


Elemental Composition Report **Page 1**

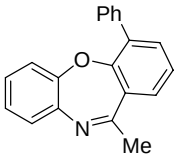
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1

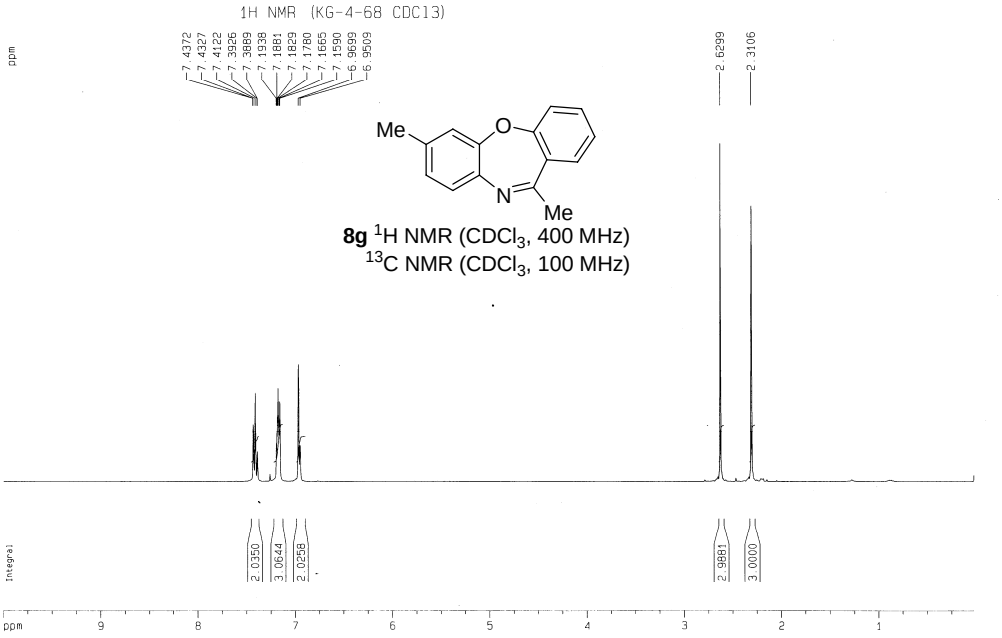
GK KS-8-11B
10061212 37 (0.961) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (27:37) 1: TOF MS ES+ 3.28e3



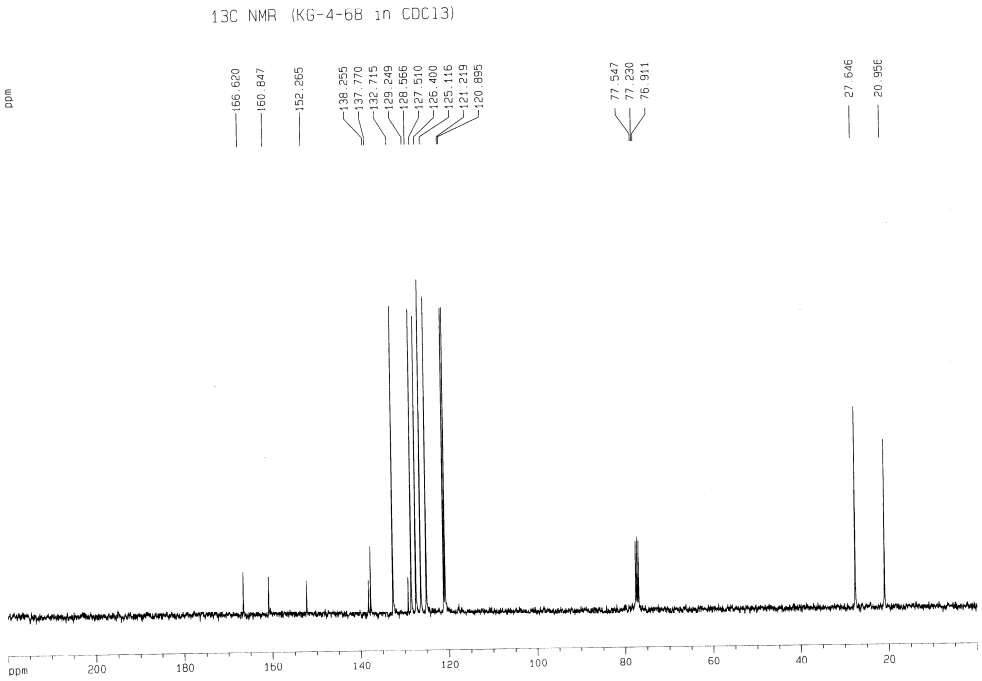
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.1235	286.1232	0.3	1.0	13.5	38.6	C20 H16 N O



8f HRMS



8g ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

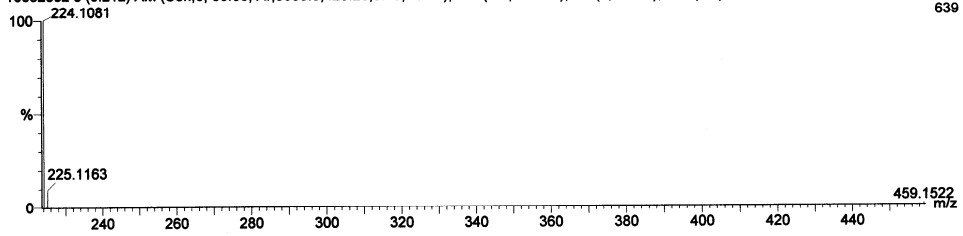


Elemental Composition Report **Page 1**

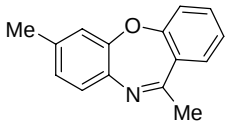
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 1-1

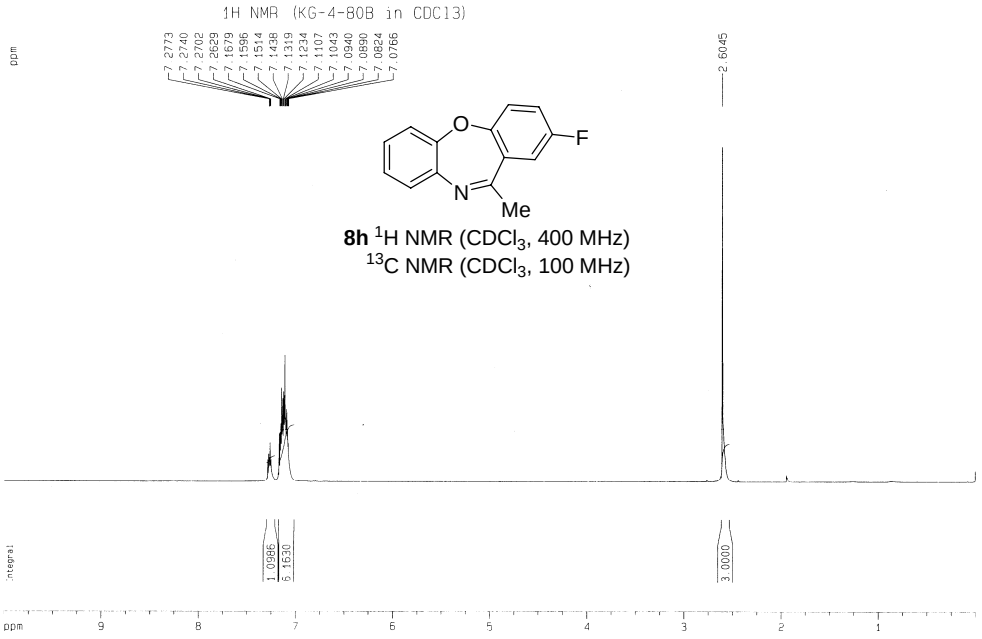
KG-4-6B
10052602 8 (0.212) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (8:9) 1: TOF MS ES+ 639



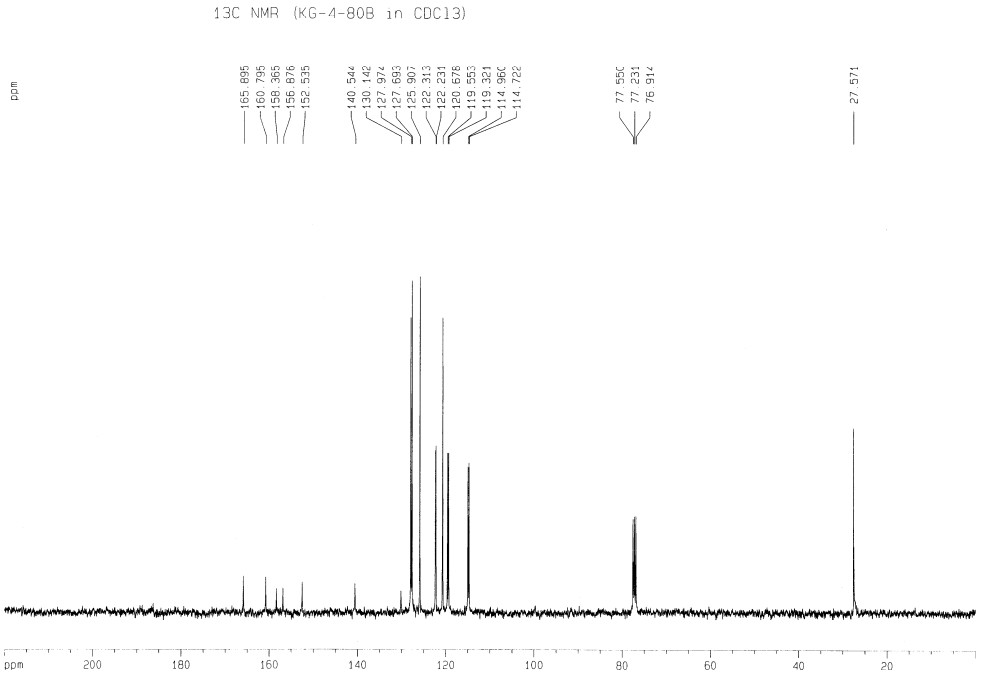
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1081	224.1075	0.6	2.7	9.5	2773058.0	C15 H14 N O



8g HRMS



8h ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

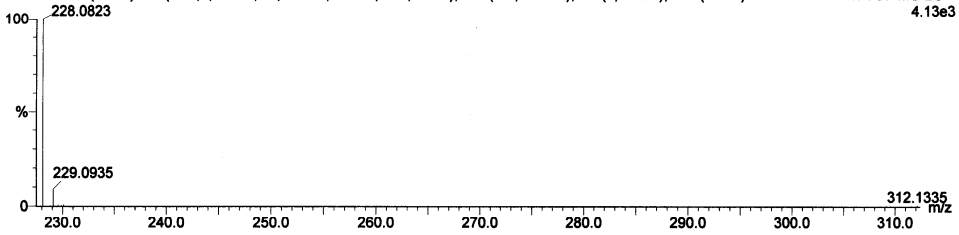


Elemental Composition Report **Page 1**

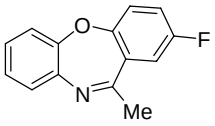
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 1-1 F: 1-1

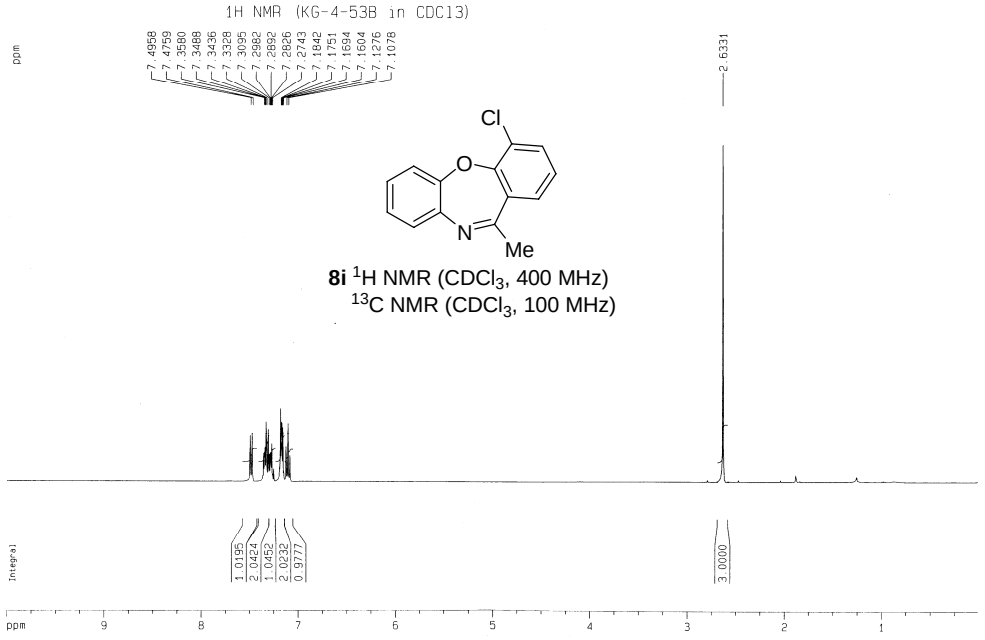
KG-4-80B
10052911 22 (0.557) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (22:24) 1: TOF MS ES+
4.13e3



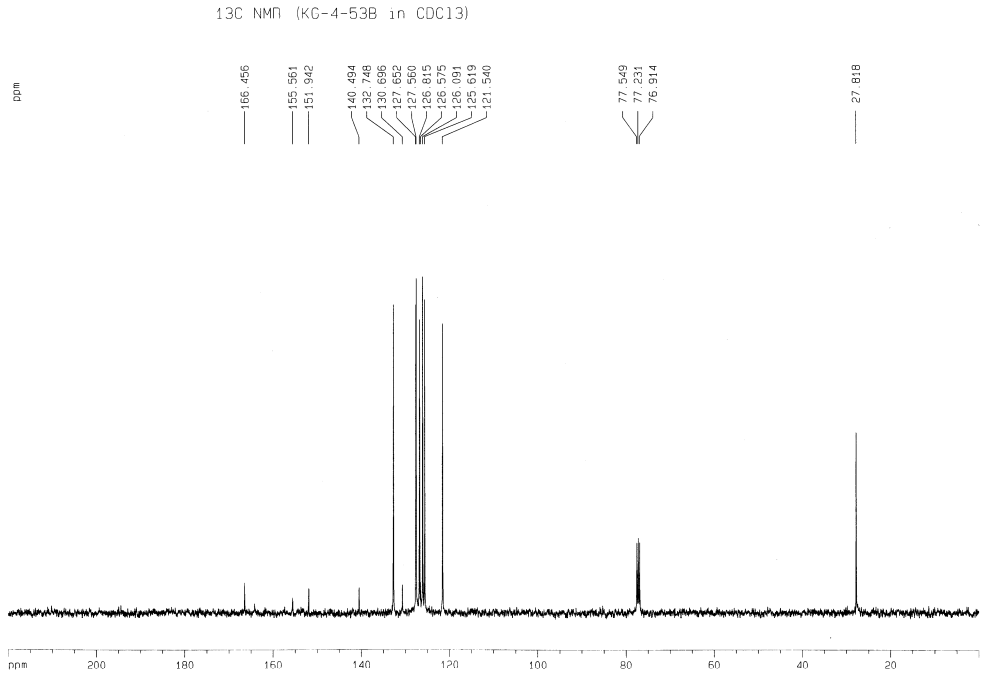
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
228.0823	228.0825	-0.2	-0.9	9.5	112.9	C14 H11 N O F



8h HRMS



8i ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

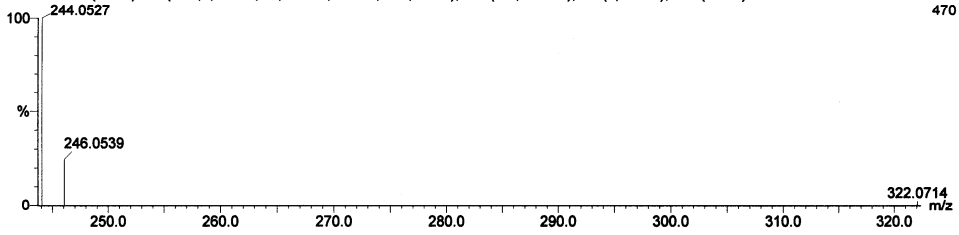


Elemental Composition Report **Page 1**

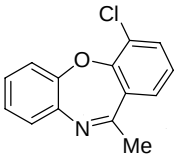
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1 Cl: 1-1

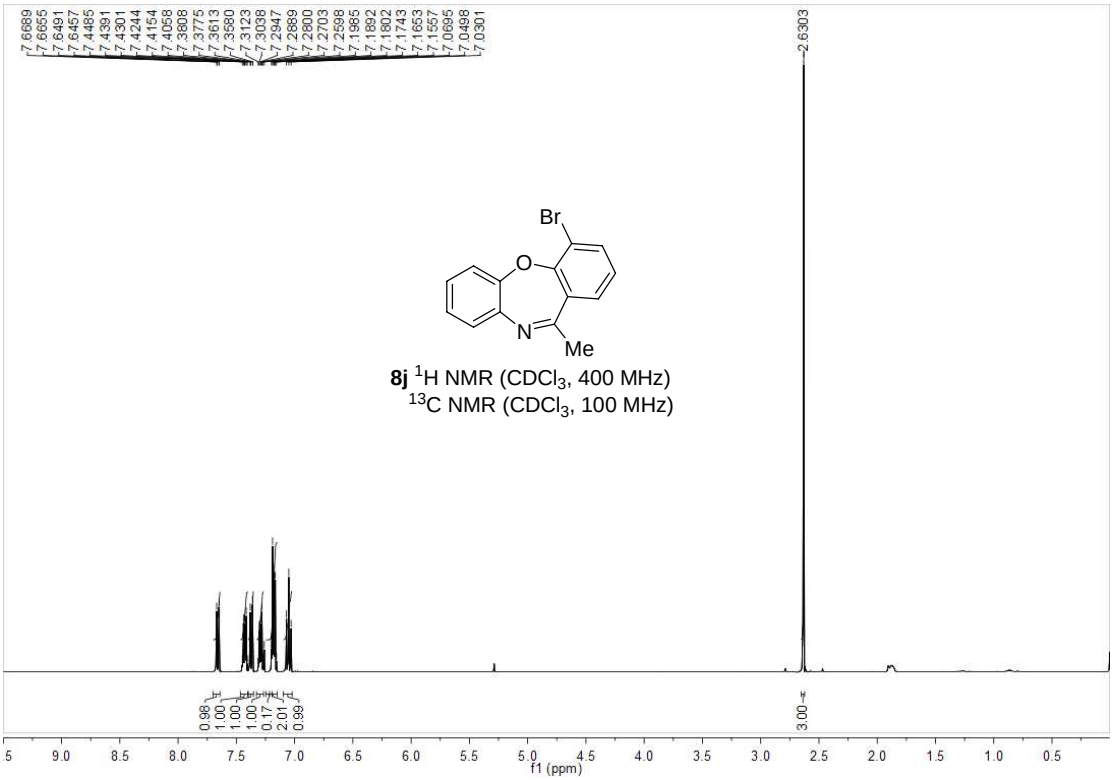
KG-4-53B
10061215 36 (0.899) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (36:38) 1: TOF MS ES+ 470



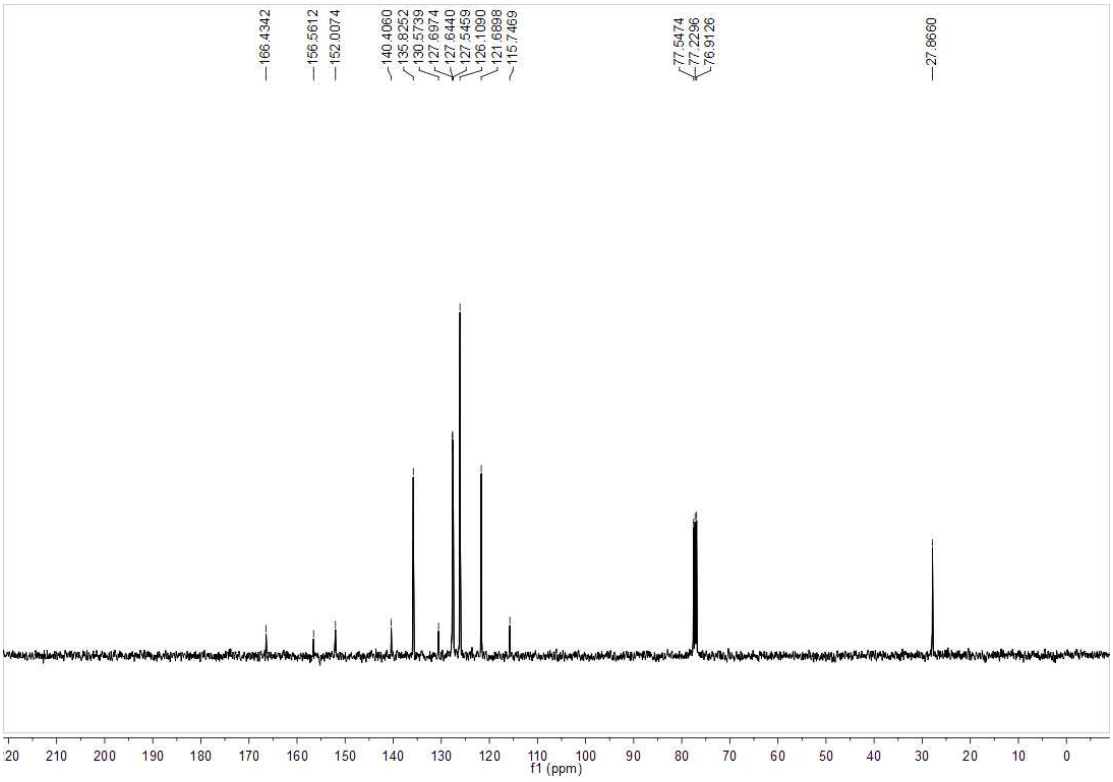
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.0527	244.0529	-0.2	-0.8	9.5	2773266.8	C14 H11 N O Cl

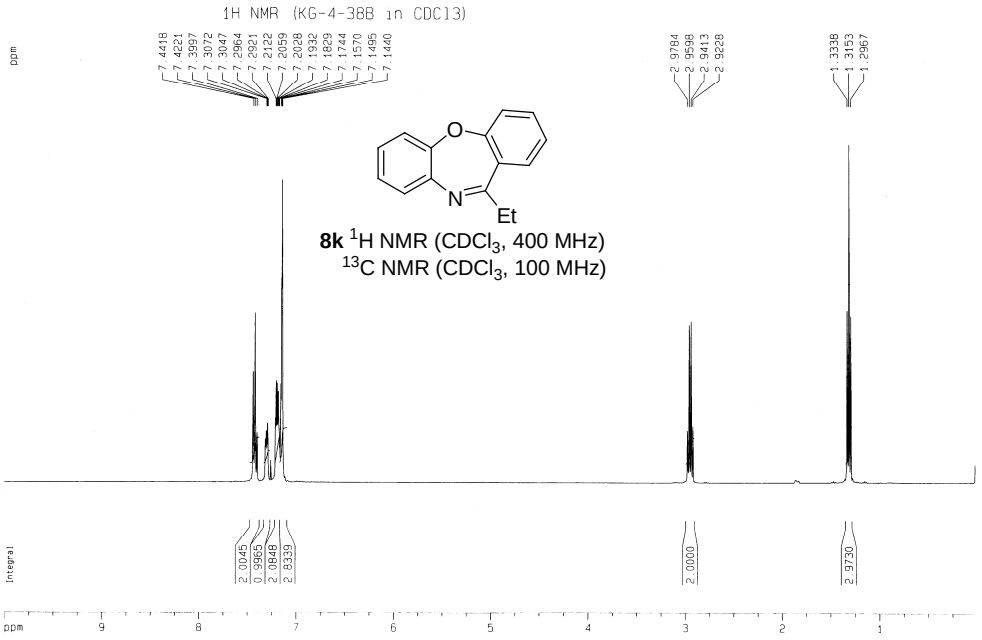


8i HRMS

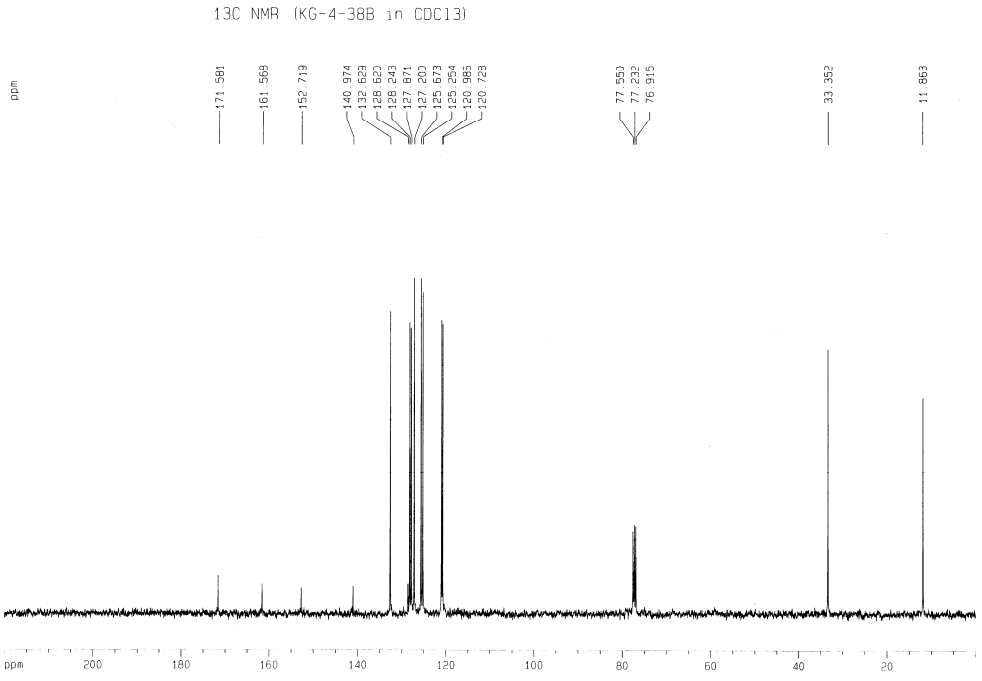


8j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





8k ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

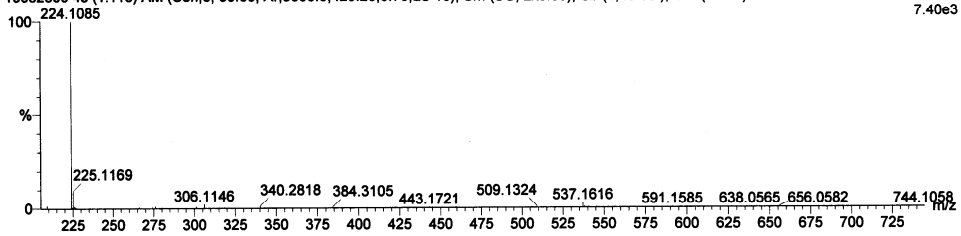


Elemental Composition Report **Page 1**

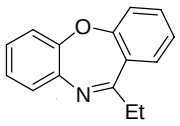
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 1-1 O: 1-1

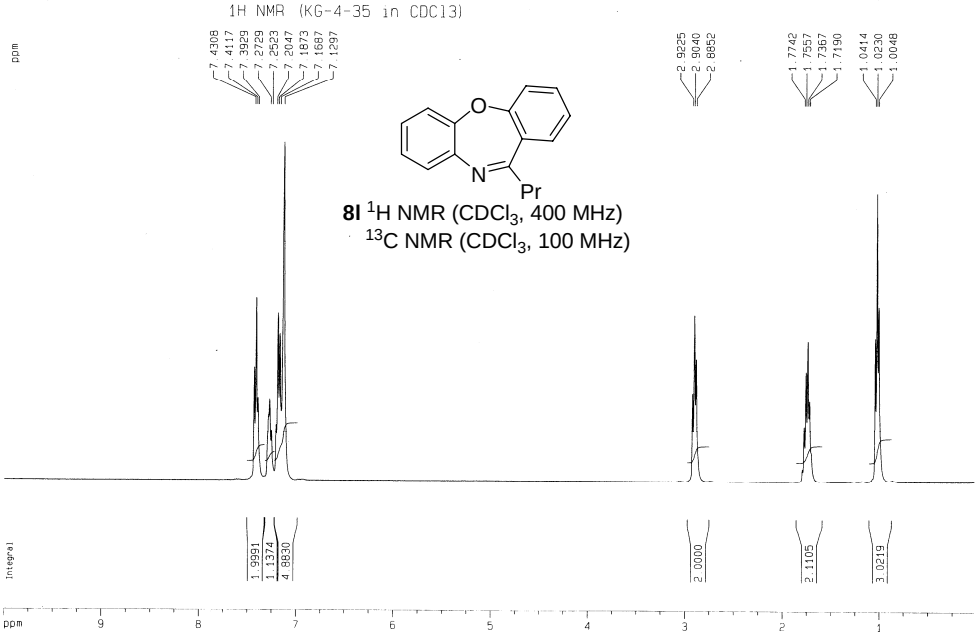
KG-4-38B
10052600 43 (1.113) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (35:51) 1: TOF MS ES+ 7.40e3



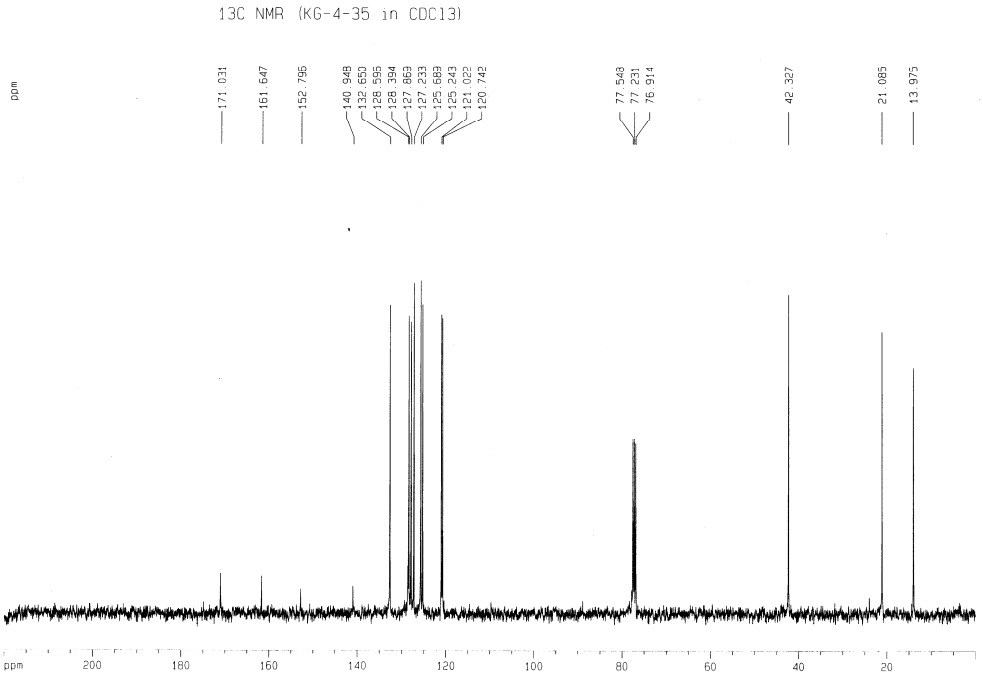
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1085	224.1075	1.0	4.5	9.5	190.3	C15 H14 N O

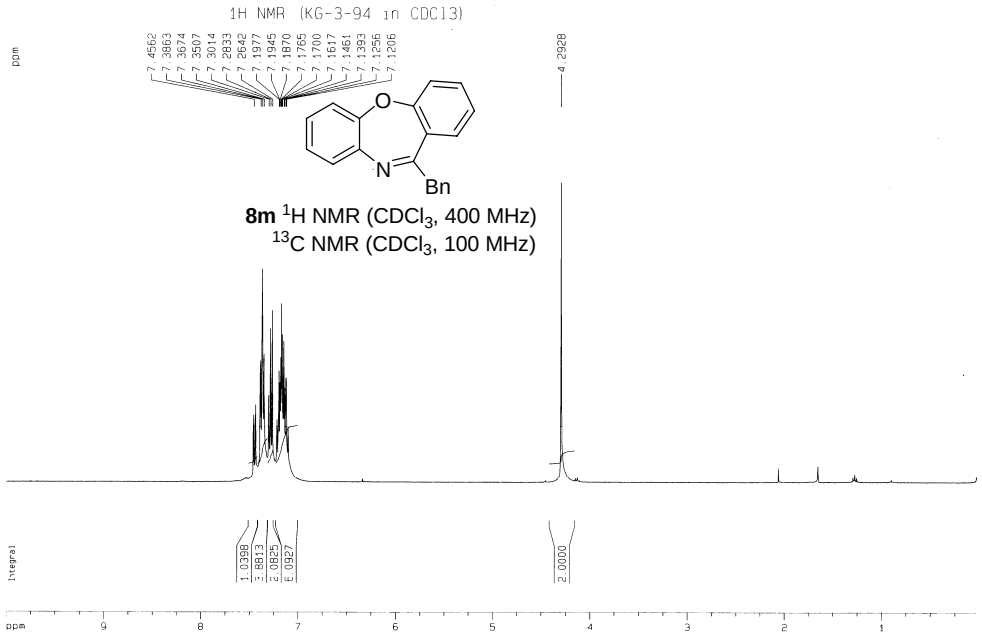


8k HRMS

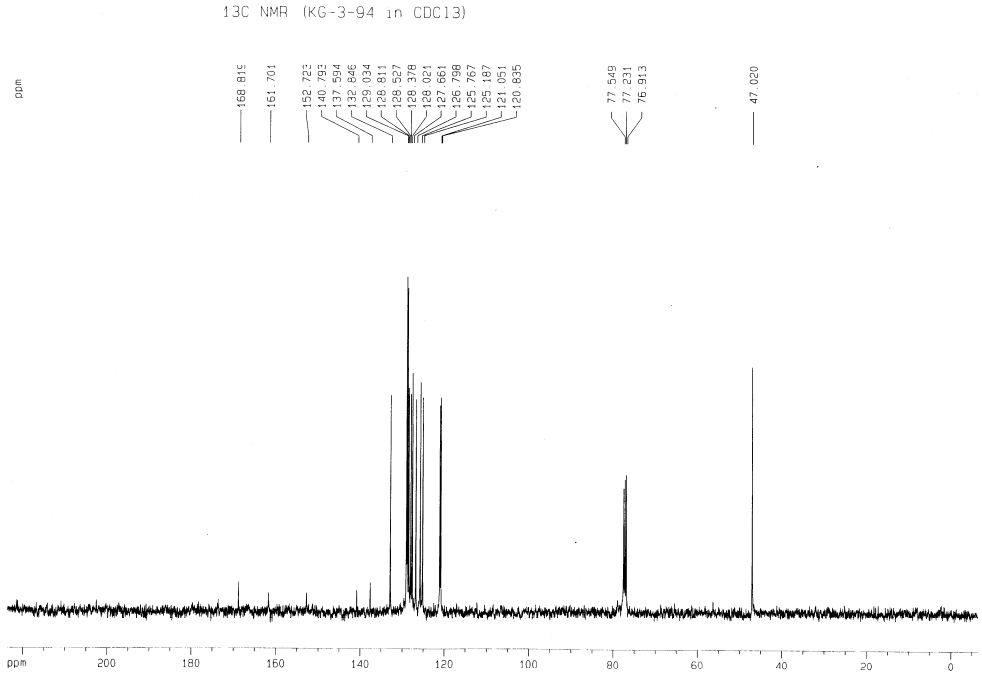


8l ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





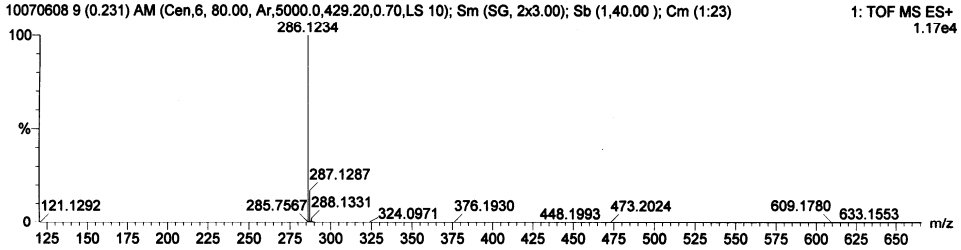
8m ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



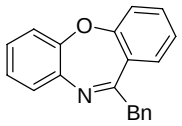
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

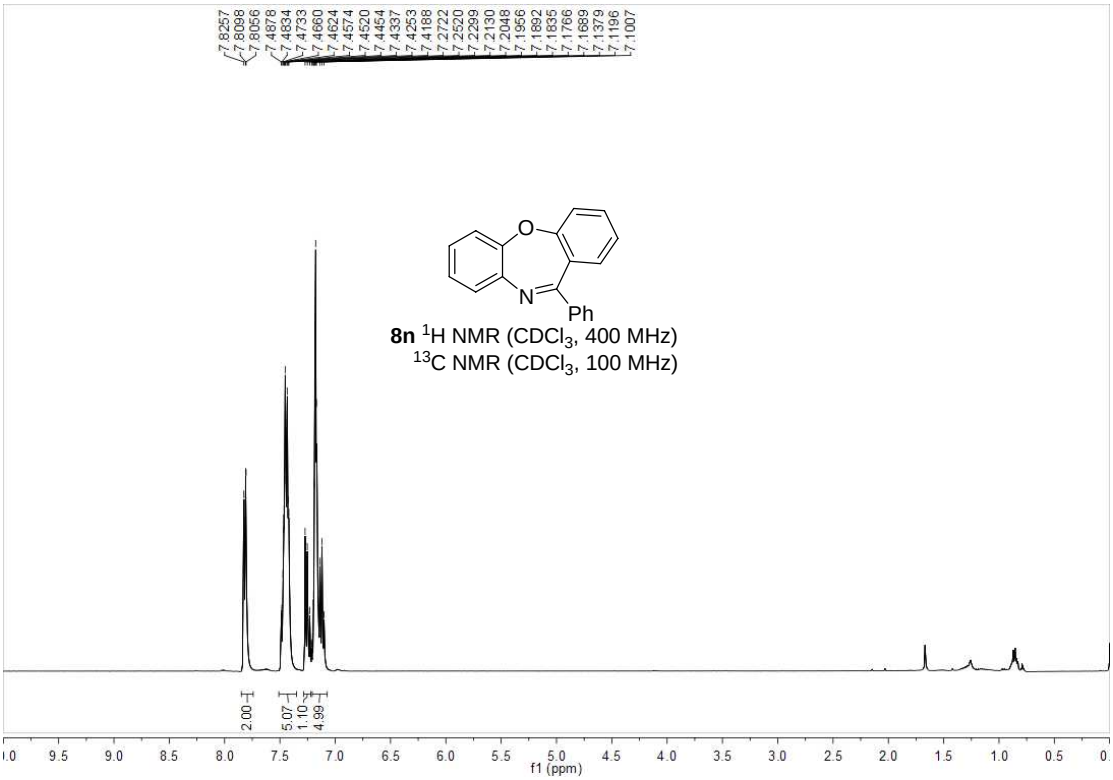
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-3-94
10070608 9 (0.231) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:23) 1: TOF MS ES+ 1.17e4



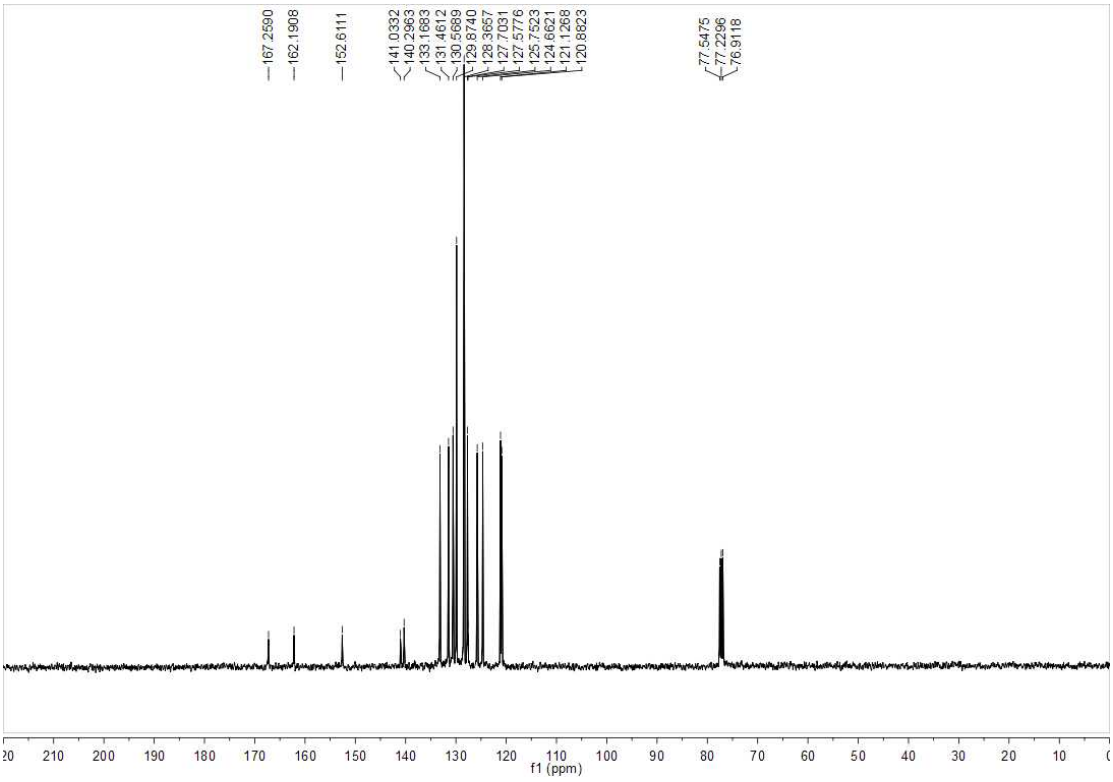
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.1234	286.1232	0.2	0.7	13.5	101.6	C20 H16 N O

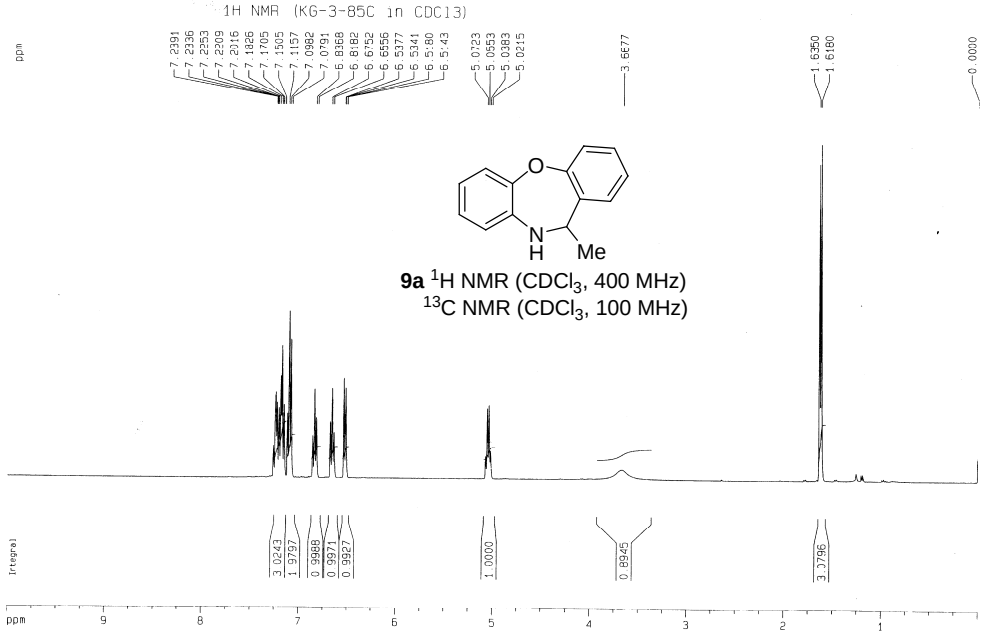


8m HRMS

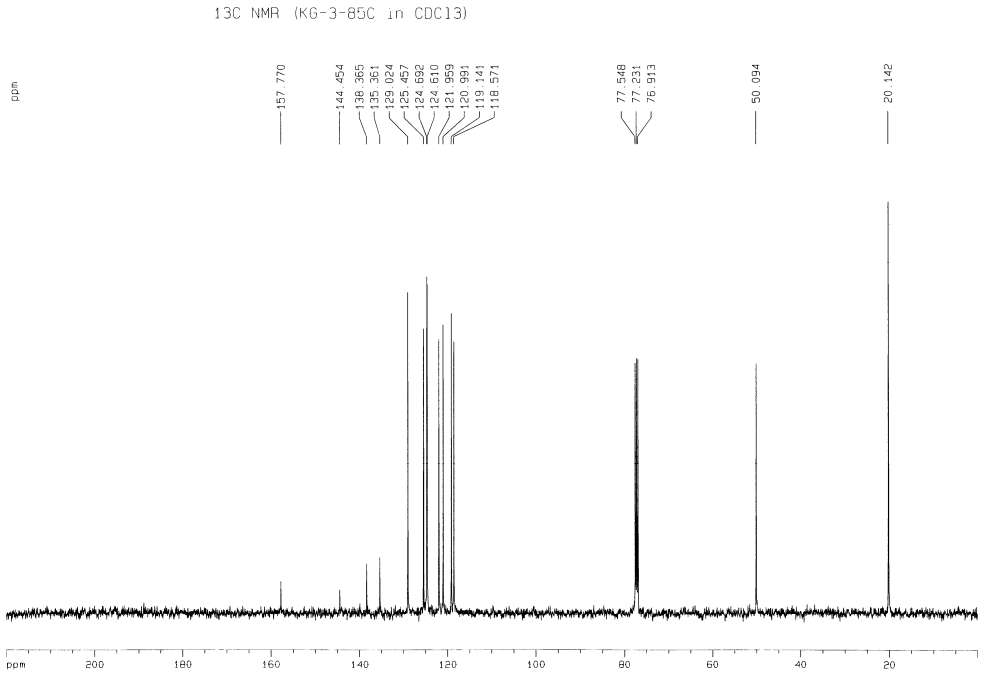


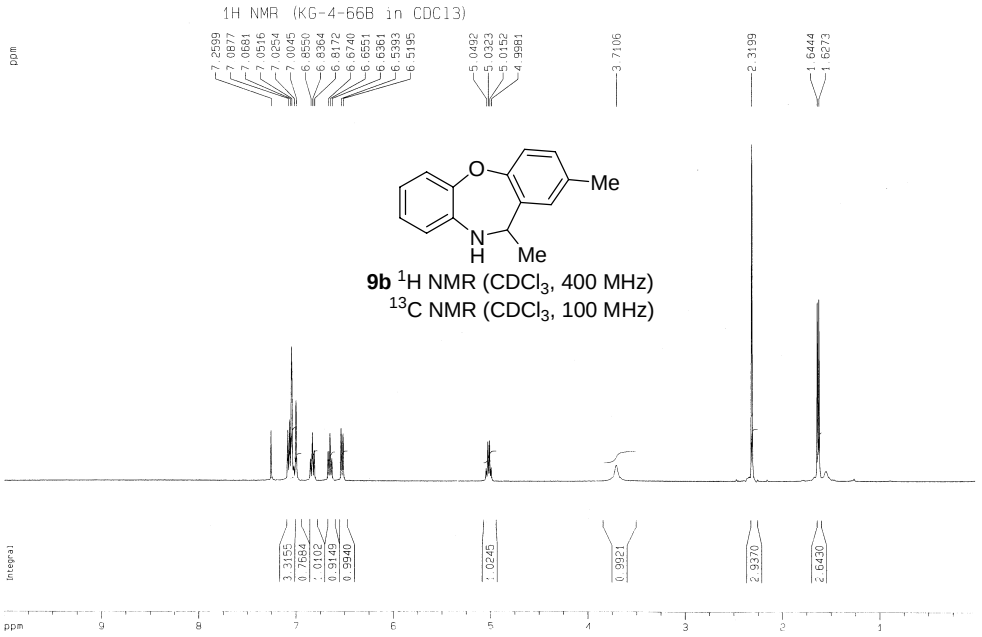
8n ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



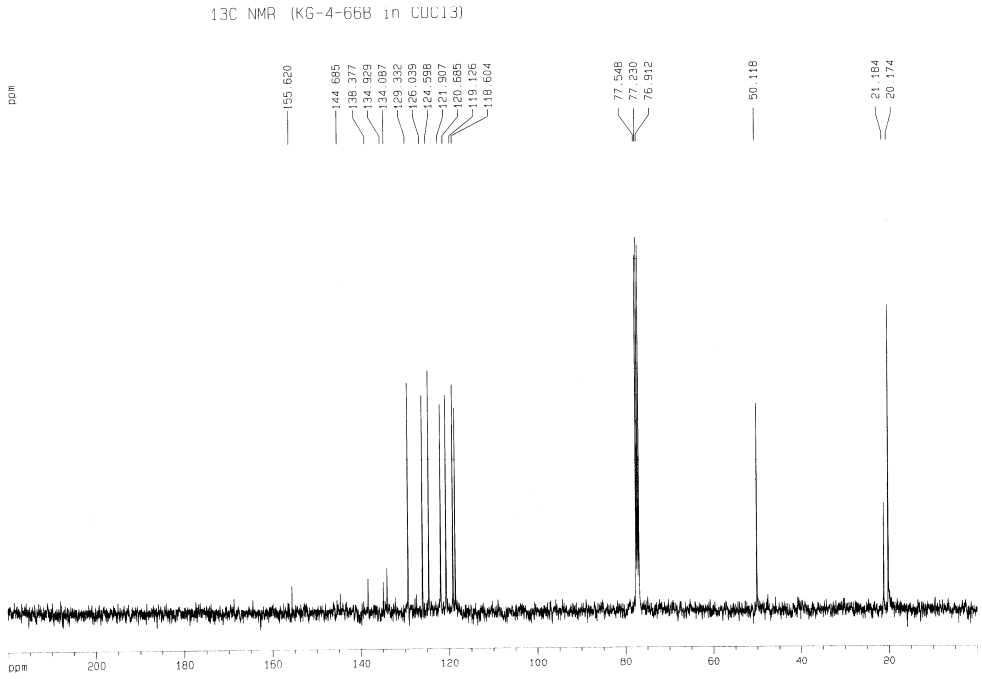


9a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





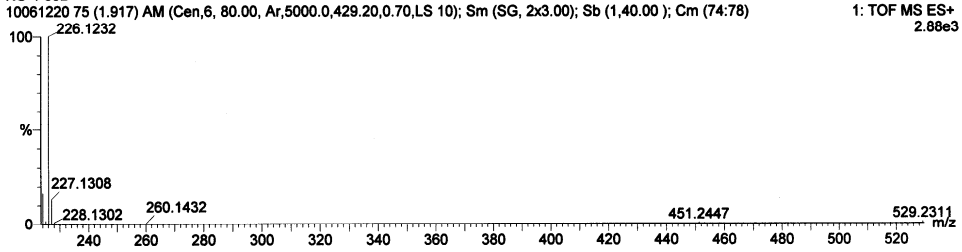
9b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



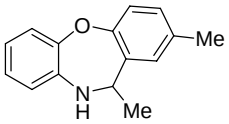
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

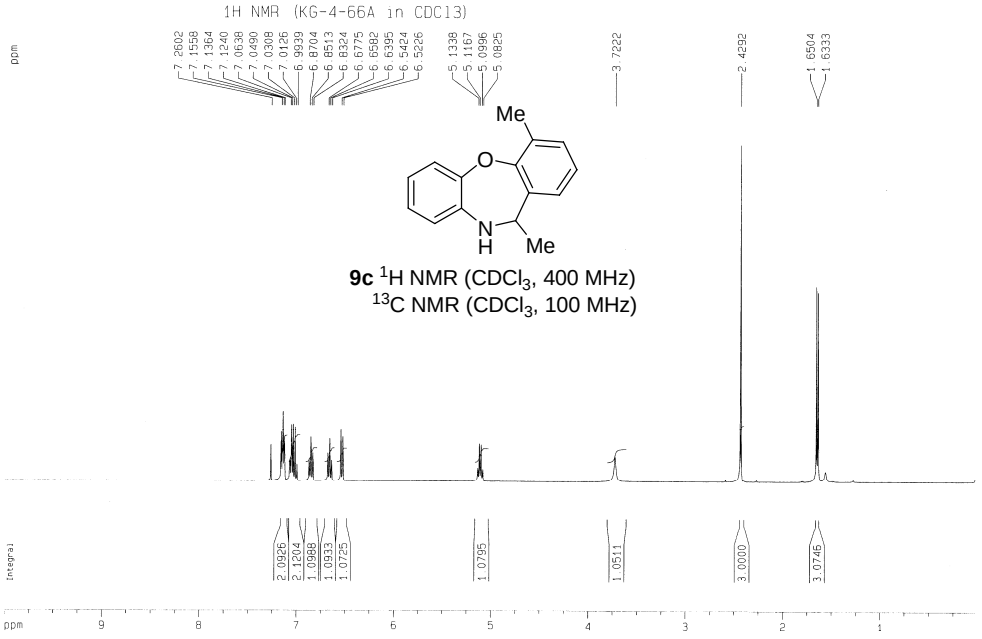
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-66B
10061220 75 (1.917) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (74:78) 1: TOF MS ES+
2.88e3



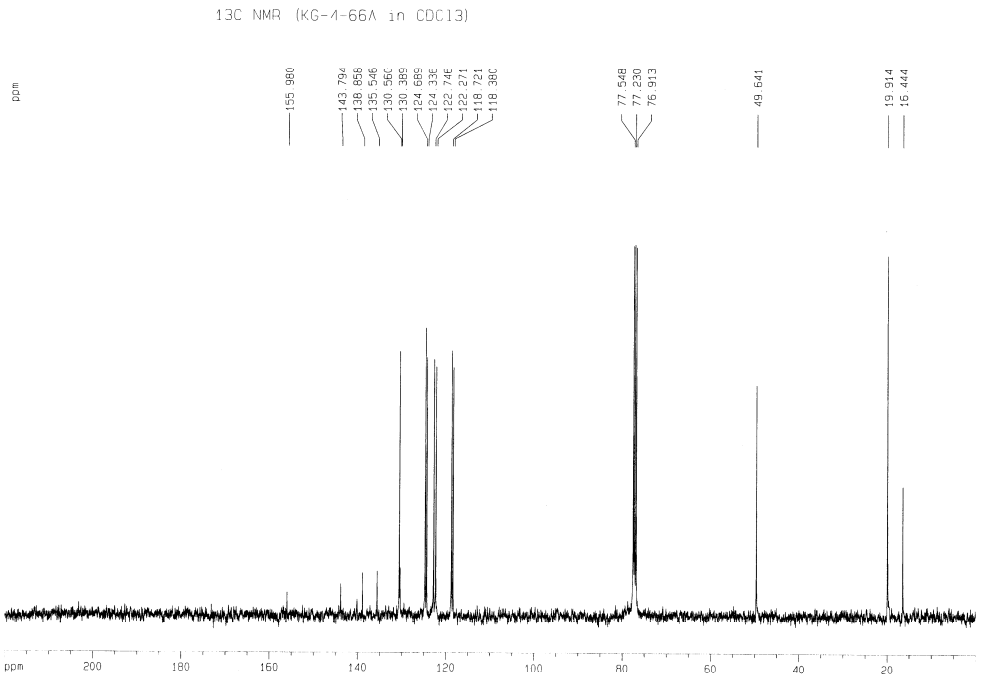
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.1232	226.1232	0.0	0.0	8.5	30.4	C15 H16 N O



9b HRMS



9c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

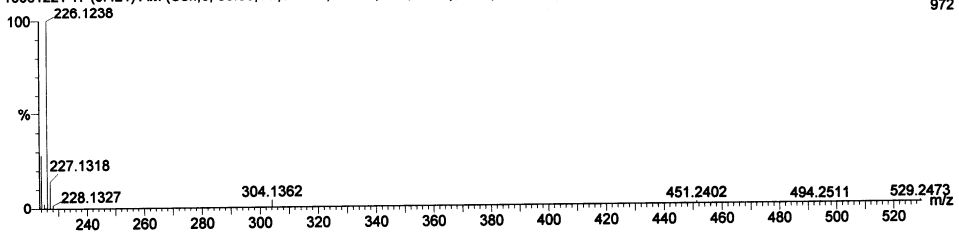


Elemental Composition Report **Page 1**

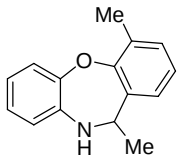
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1

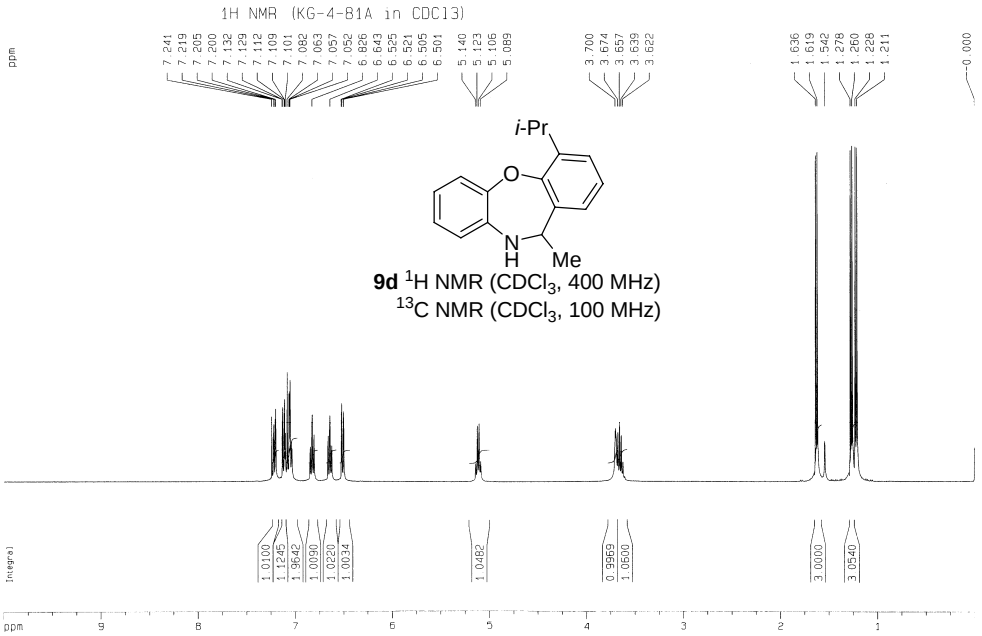
KG-4-66A
10061221 17 (0.421) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (15:17) 1: TOF MS ES+ 972



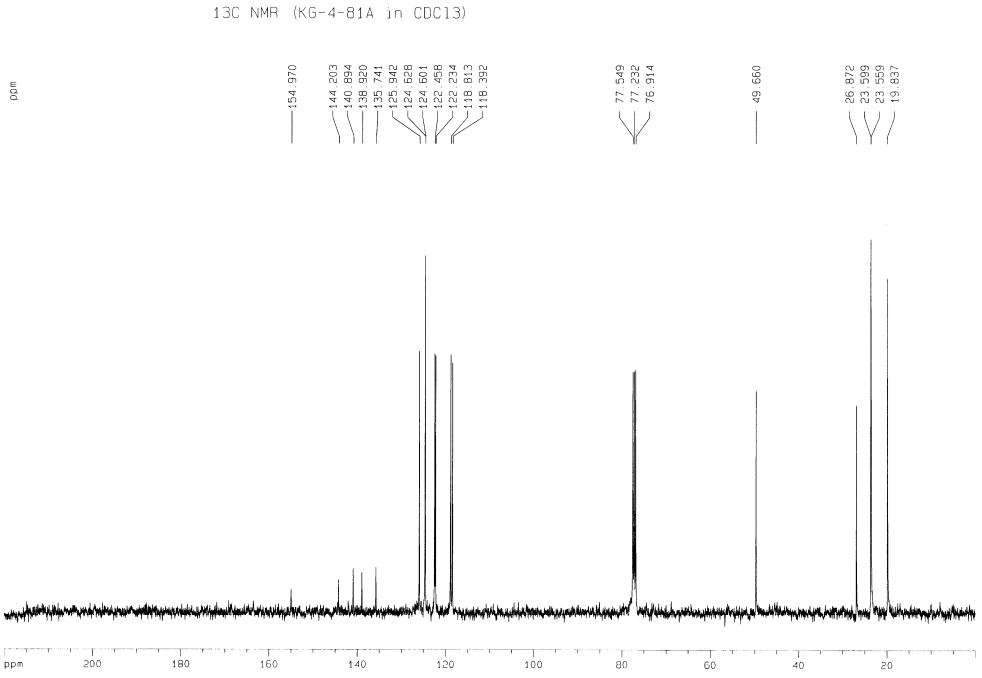
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.1238	226.1232	0.6	2.7	8.5	3.4	C15 H16 N O



9c HRMS



9d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

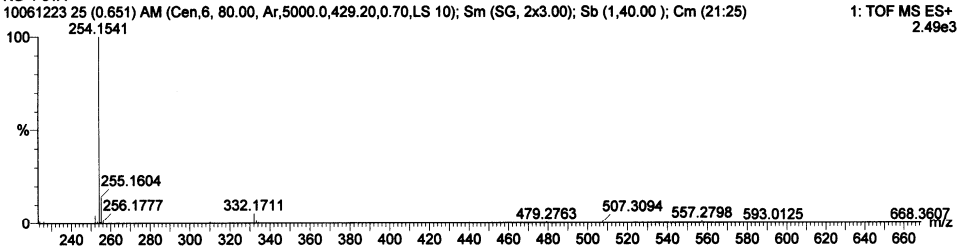


Elemental Composition Report **Page 1**

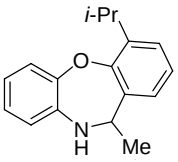
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1

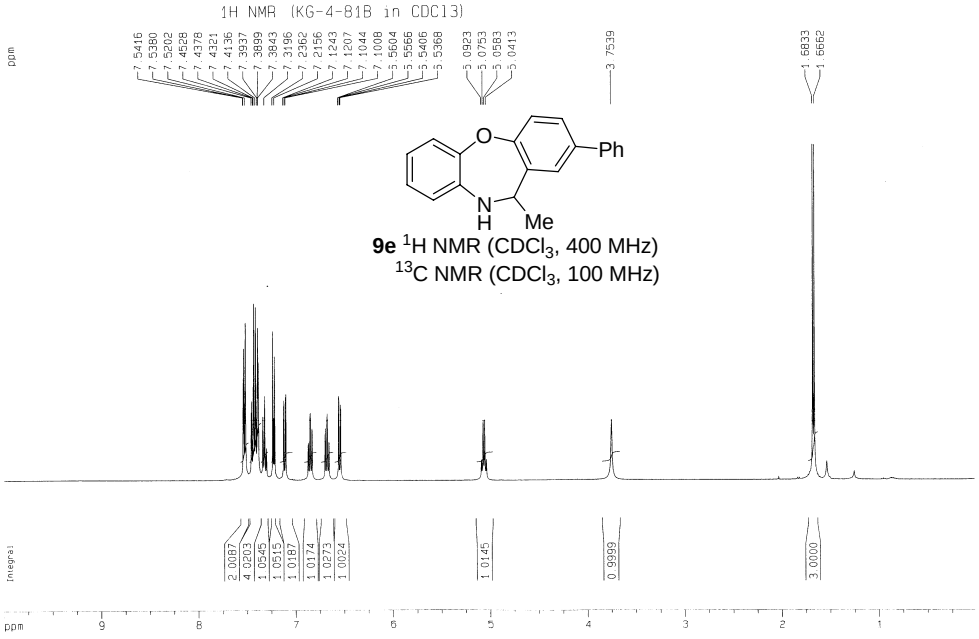
KG-4-81A
10061223 25 (0.651) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (21:25) 1: TOF MS ES+ 2.49e3



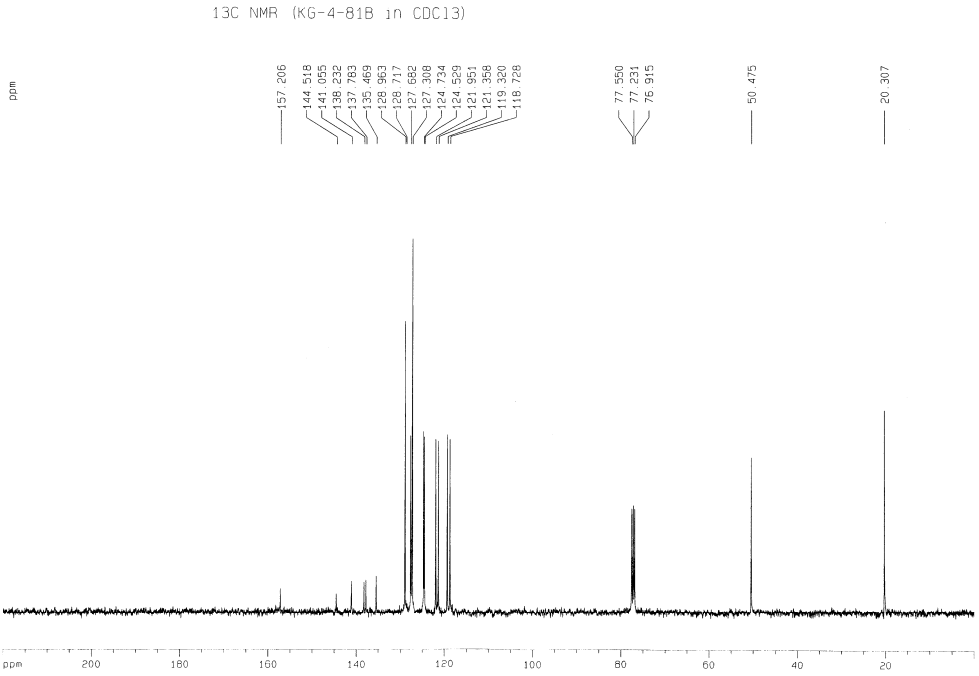
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
254.1541	254.1545	-0.4	-1.6	8.5	28.6	C17 H20 N O



9d HRMS



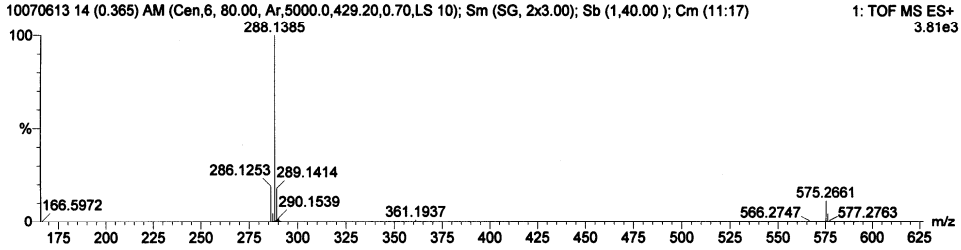
9e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



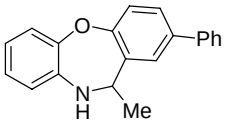
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

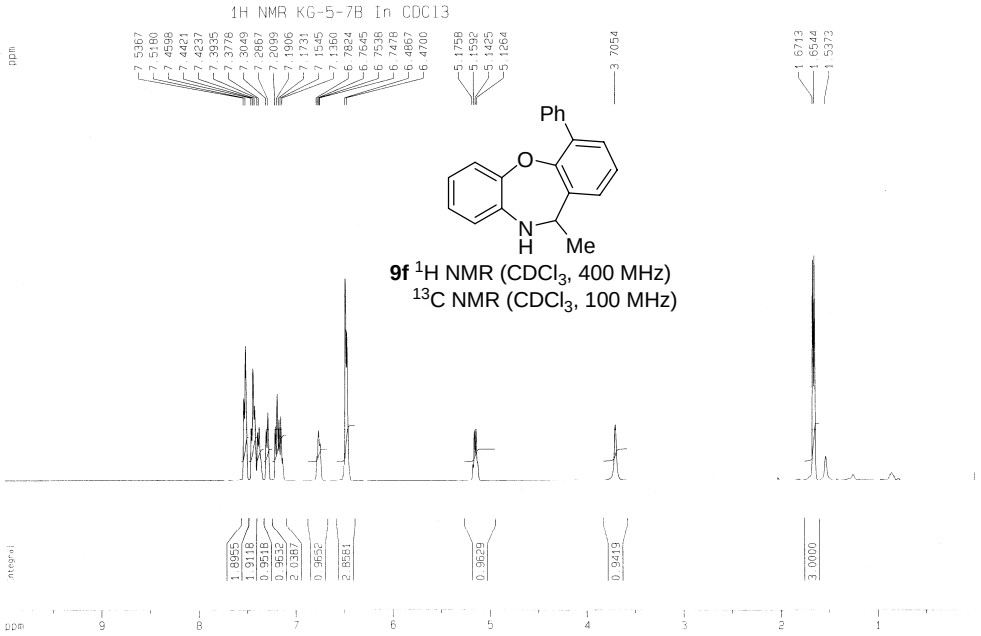
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-81B
10070613 14 (0.365) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (11:17) 1: TOF MS ES+ 3.81e3



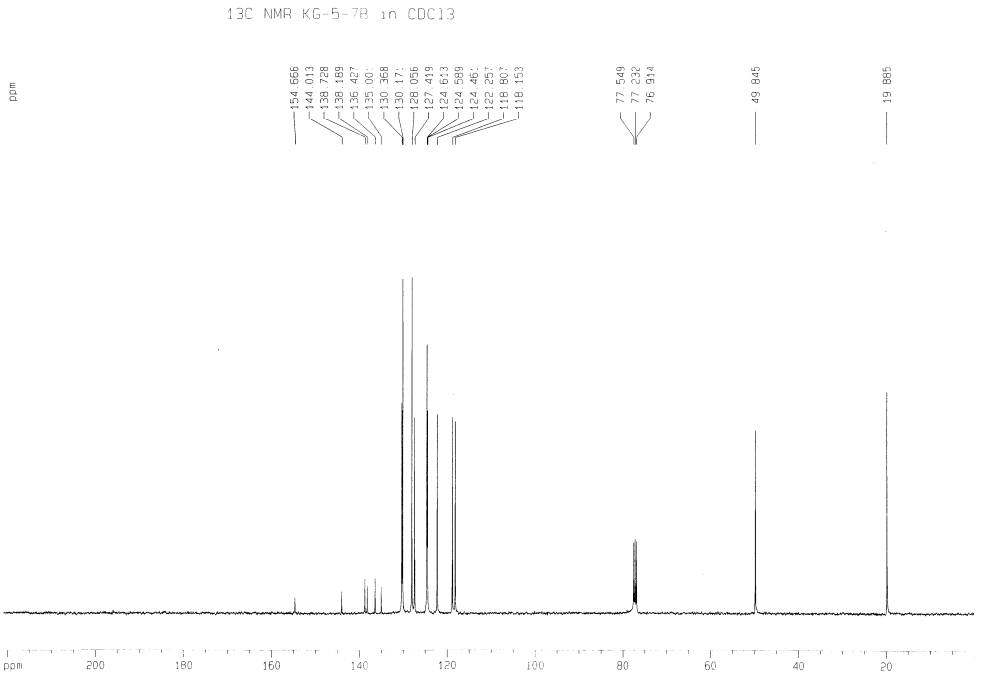
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.1385	288.1388	-0.3	-1.0	12.5	26.7	C20 H18 N O



9e HRMS



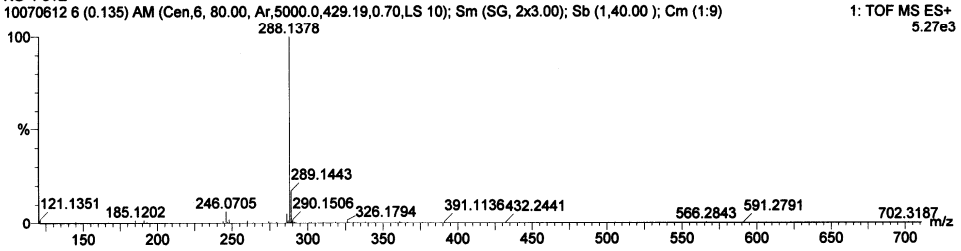
9f ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



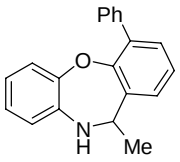
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

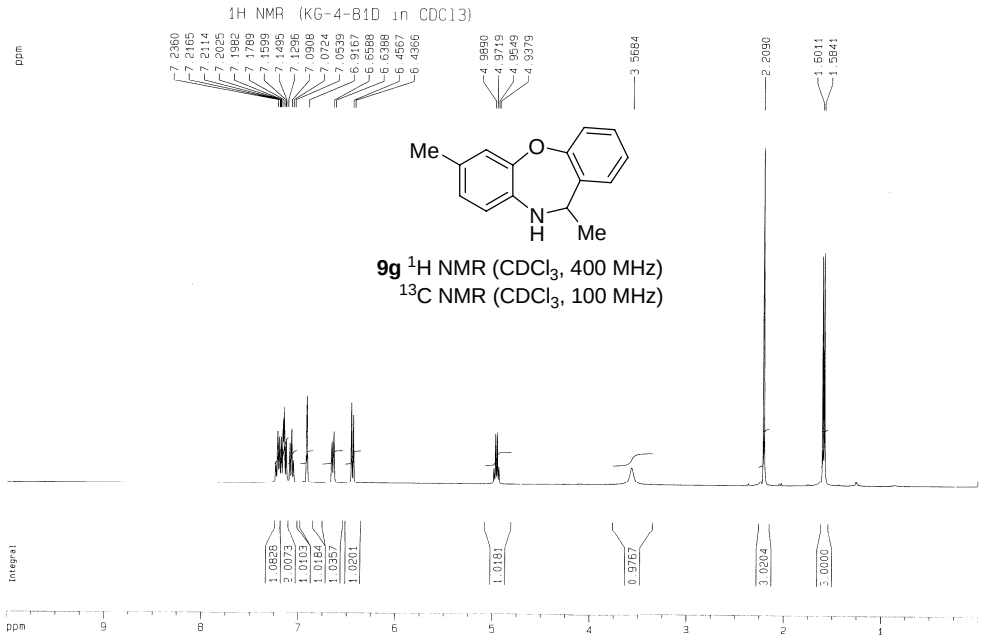
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-81E
10070612 6 (0.135) AM (Cen,6, 80.00, Ar,5000.0,429.19,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:9) 1: TOF MS ES+ 5.27e3



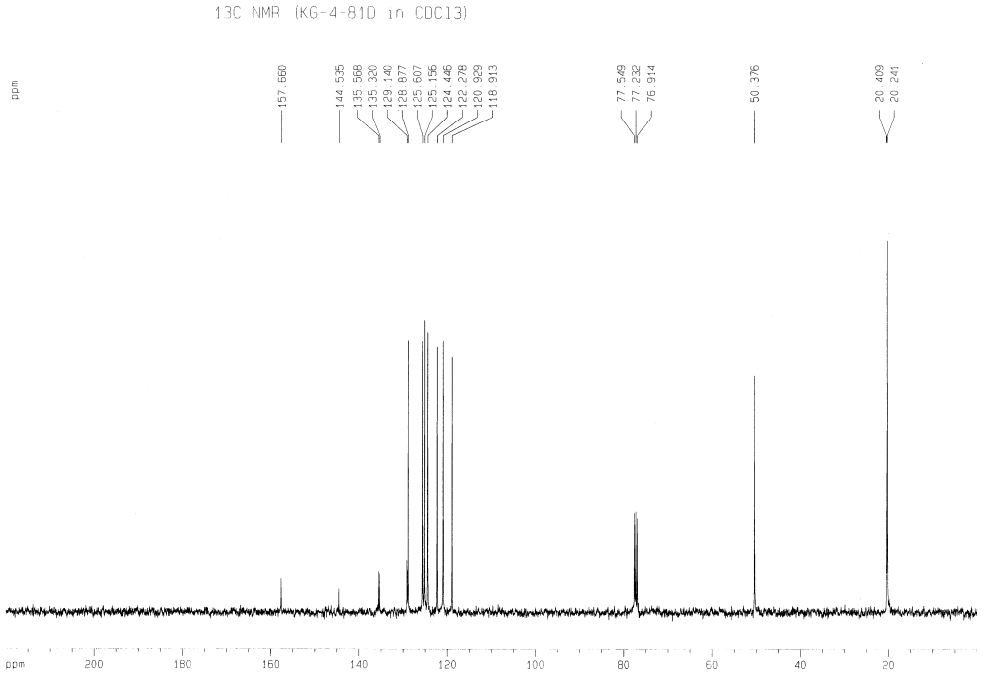
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.1378	288.1388	-1.0	-3.5	12.5	48.1	C20 H18 N O



9f HRMS



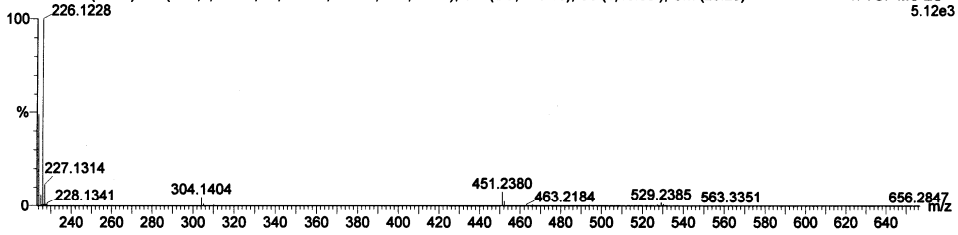
9g ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



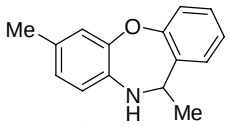
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

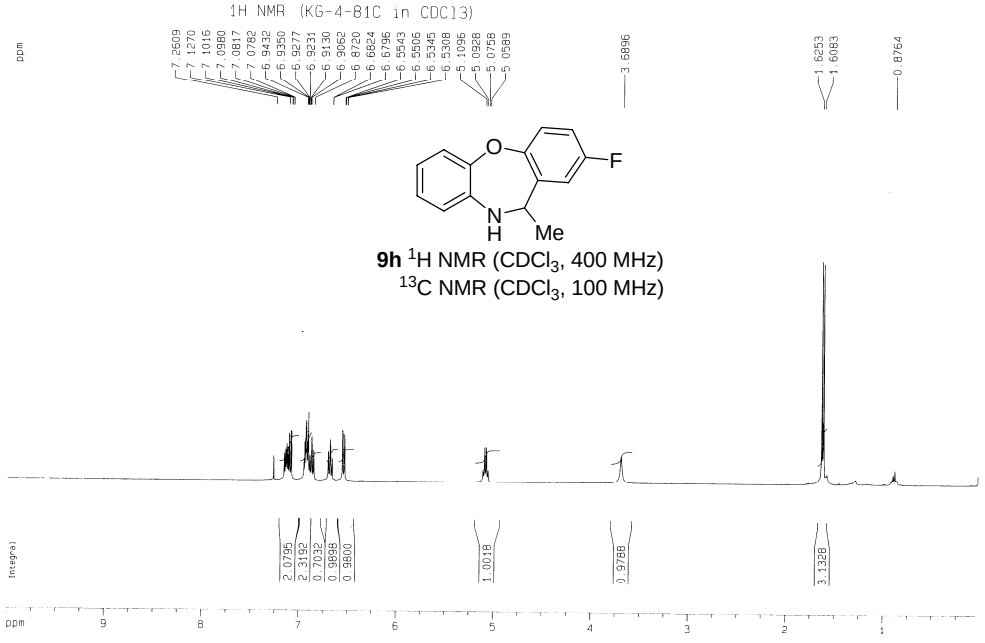
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-81D
10061222 23 (0.577) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (23:29) 1: TOF MS ES+ 5.12e3



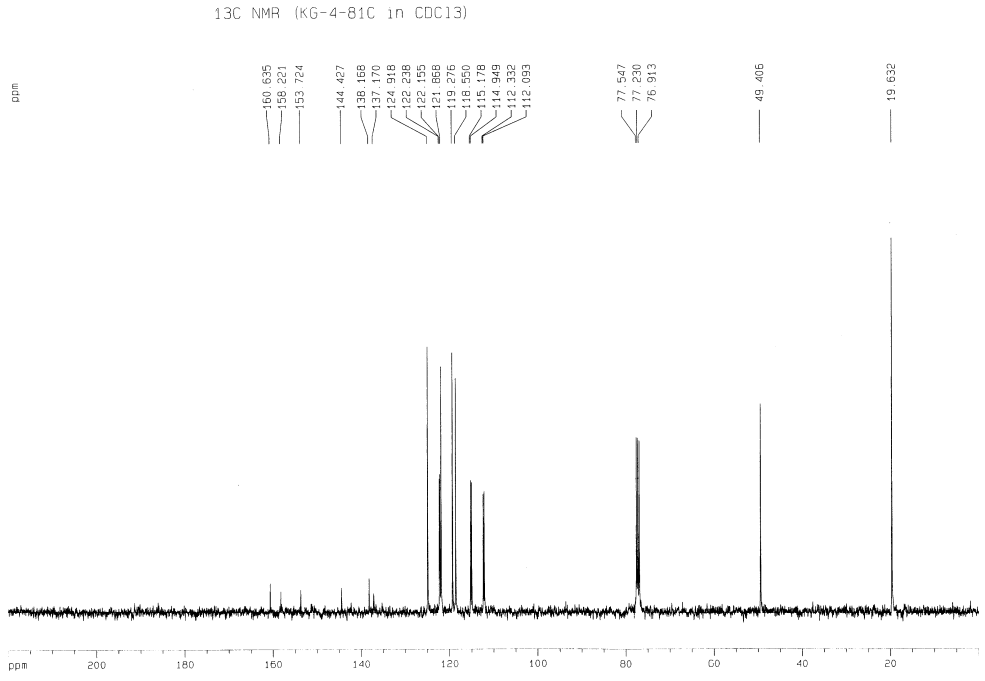
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
226.1228	226.1232	-0.4	-1.8	8.5	61.3	C15 H16 N O



9g HRMS



9h ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

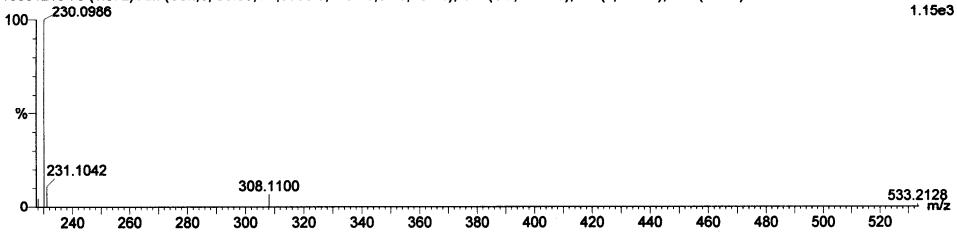


Elemental Composition Report **Page 1**

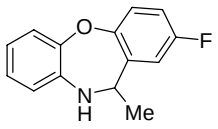
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1 F: 1-1

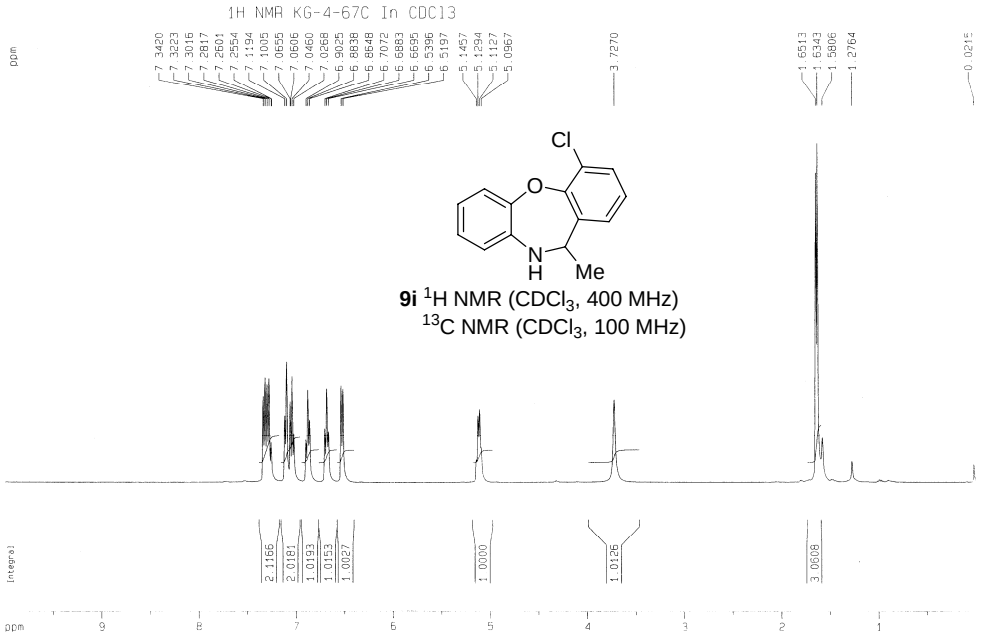
KG-4-81A
10061219 78 (1.972) AM (Cen,6, 80.00, Ar,5000.0,429.19,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (77:78) 1: TOF MS ES+
1.15e3



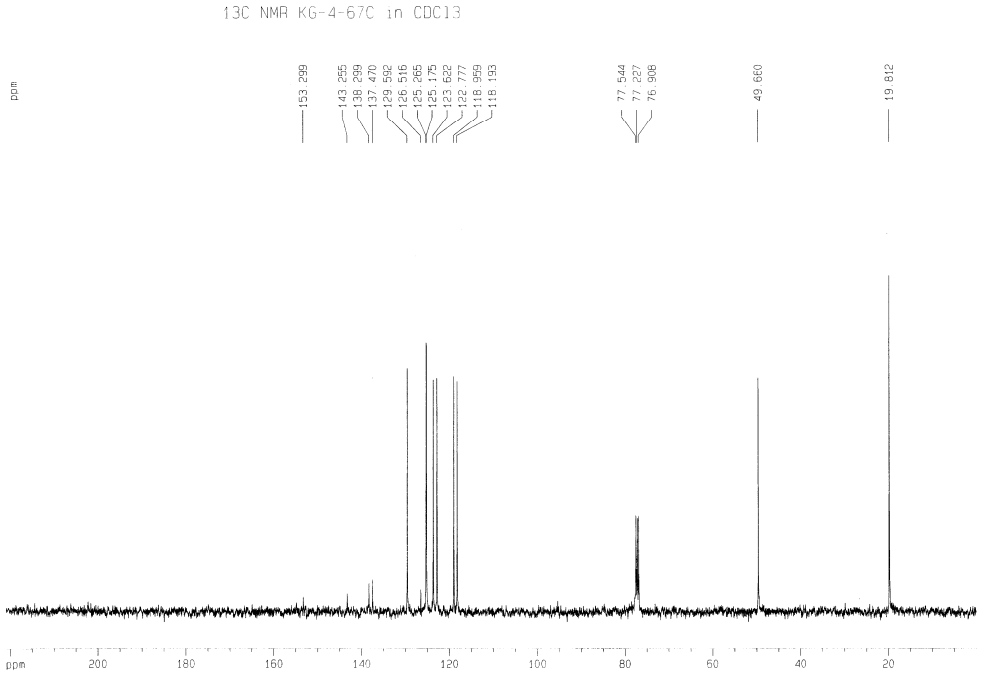
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
230.0986	230.0981	0.5	2.2	8.5	2773110.8	C14 H13 N O F



9h HRMS



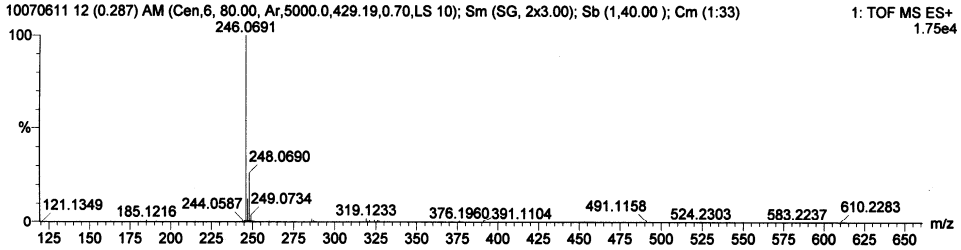
9i ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



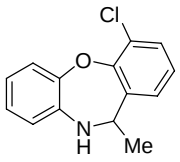
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

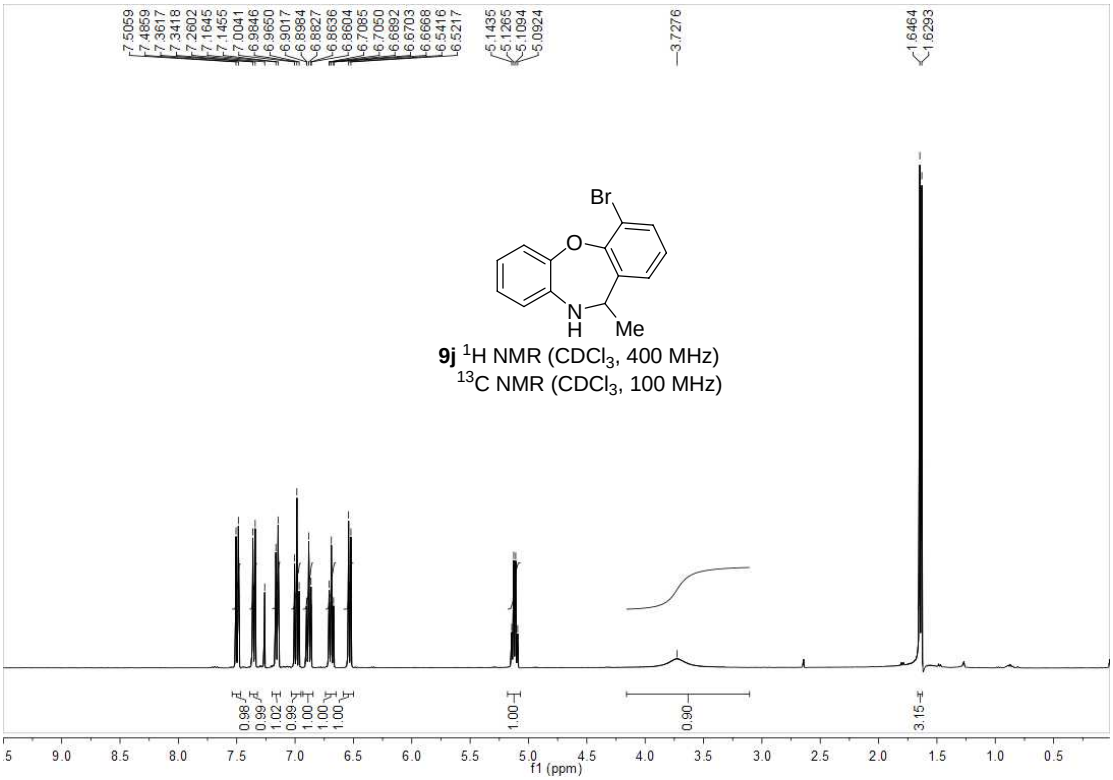
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1 Cl: 1-1
KG-4-67C
10070611 12 (0.287) AM (Cen,6, 80.00, Ar,5000.0,429.19,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:33) 1: TOF MS ES+ 1.75e4



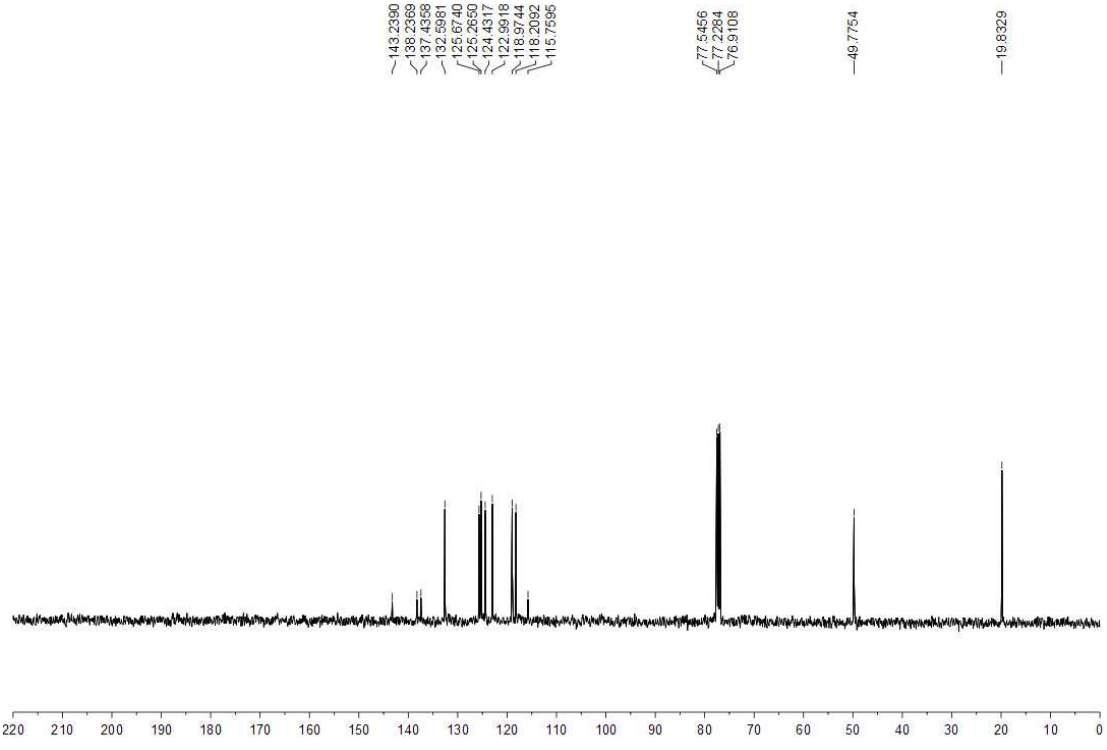
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0691	246.0686	0.5	2.0	8.5	166.0	C14 H13 N O Cl



9i HRMS



9j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

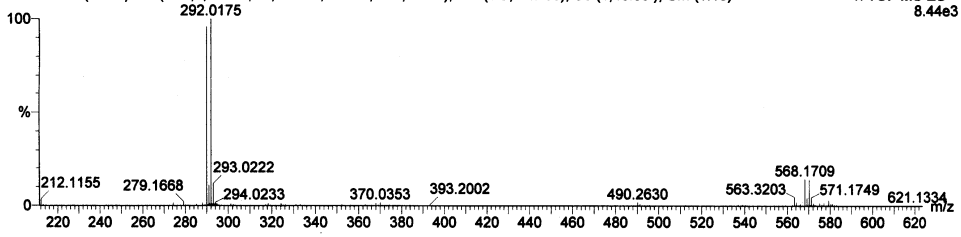


Elemental Composition Report **Page 1**

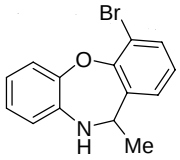
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1 Br: 1-1

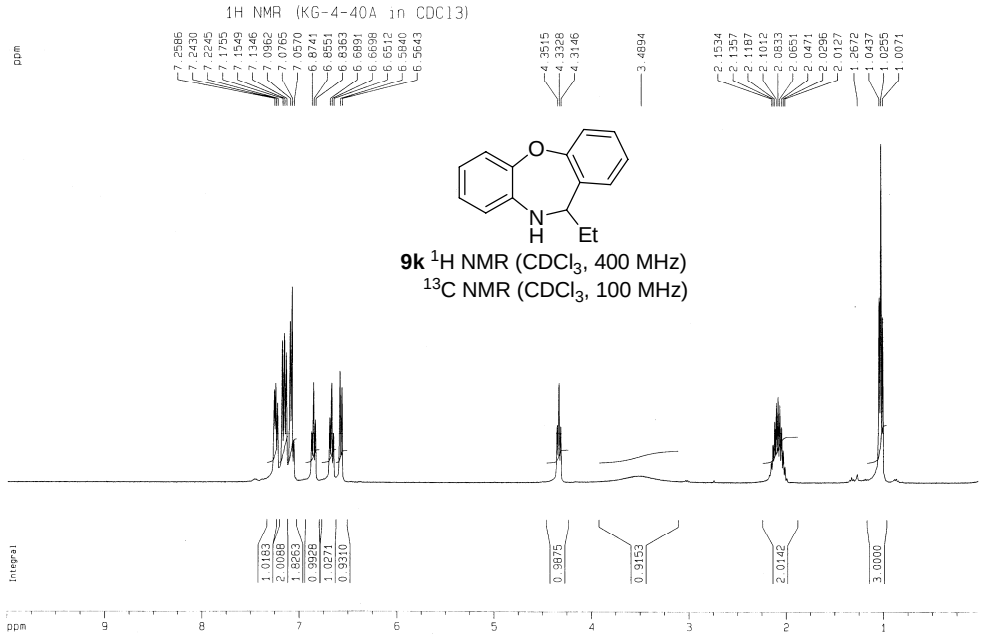
KG-5-14
10071806 5 (0.116) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:15) 1: TOF MS ES+ 8.44e3



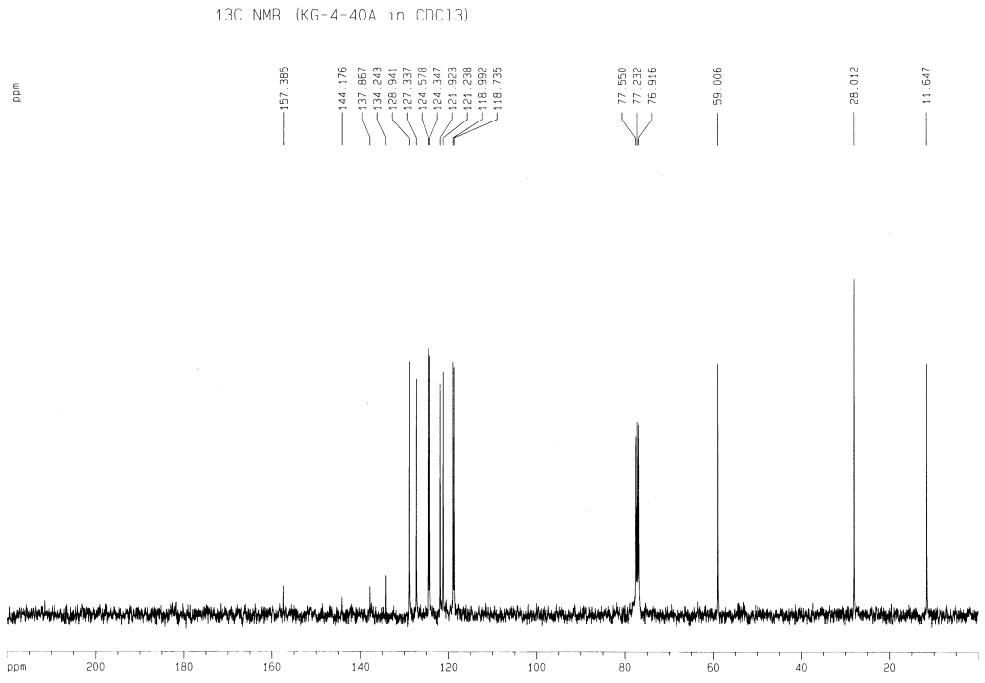
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0184	290.0181	0.3	1.0	8.5	96.9	C14 H13 N O Br

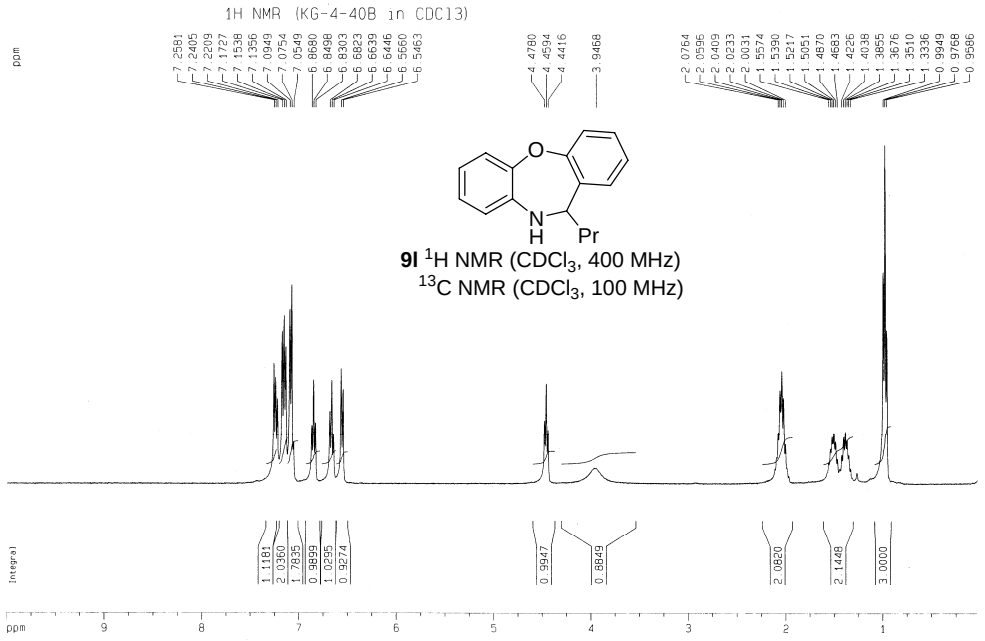


9j HRMS

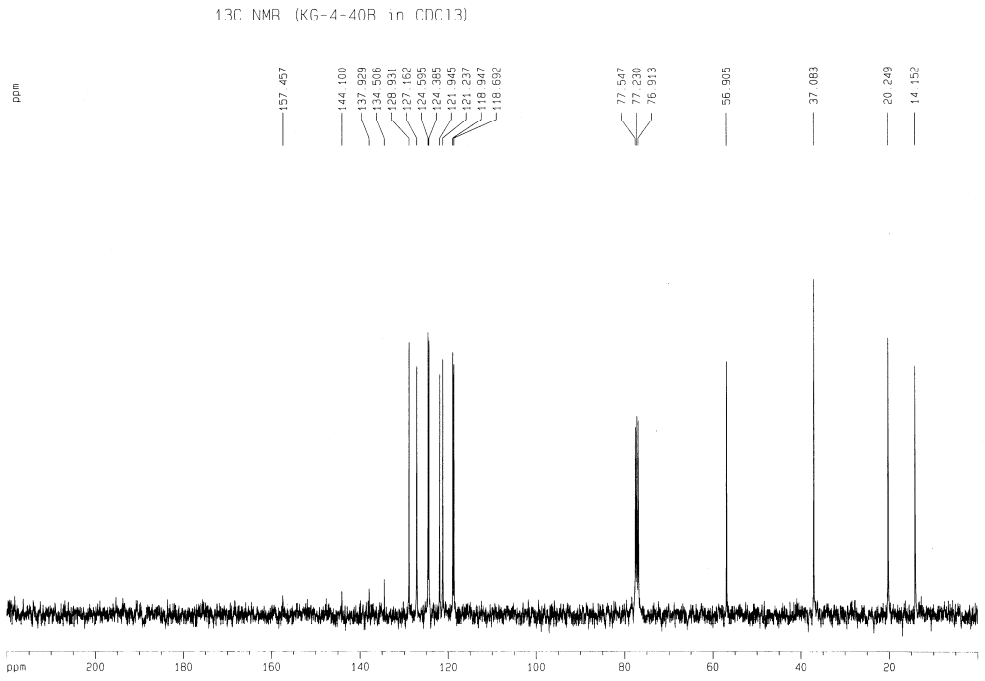


9k ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





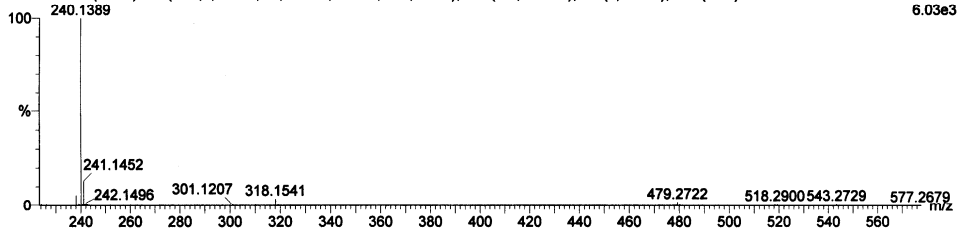
9l ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



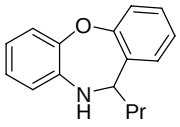
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

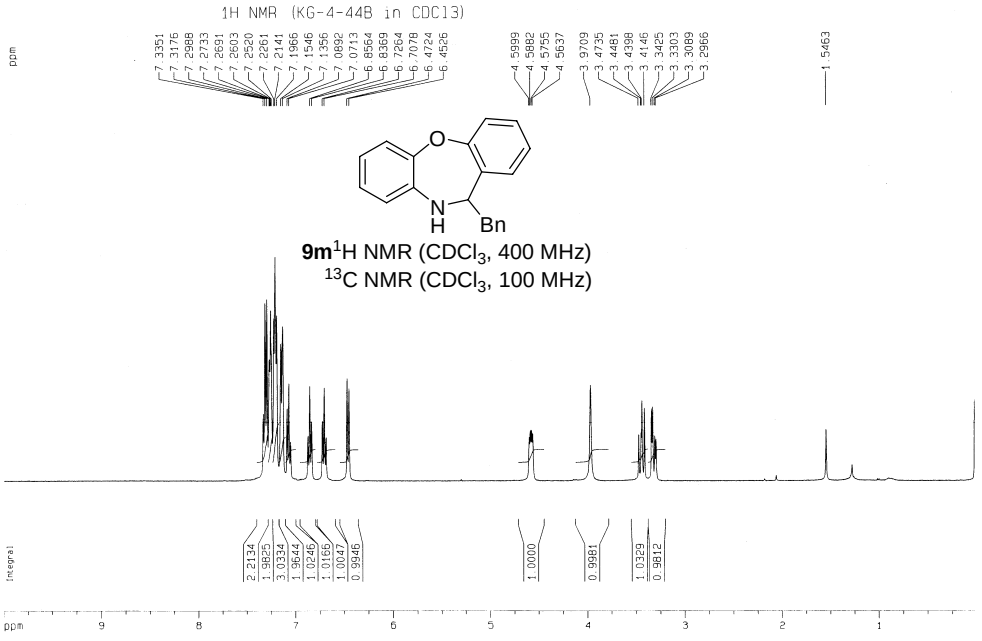
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-80B
10061224 16 (0.403) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (7:18) 1: TOF MS ES+ 6.03e3



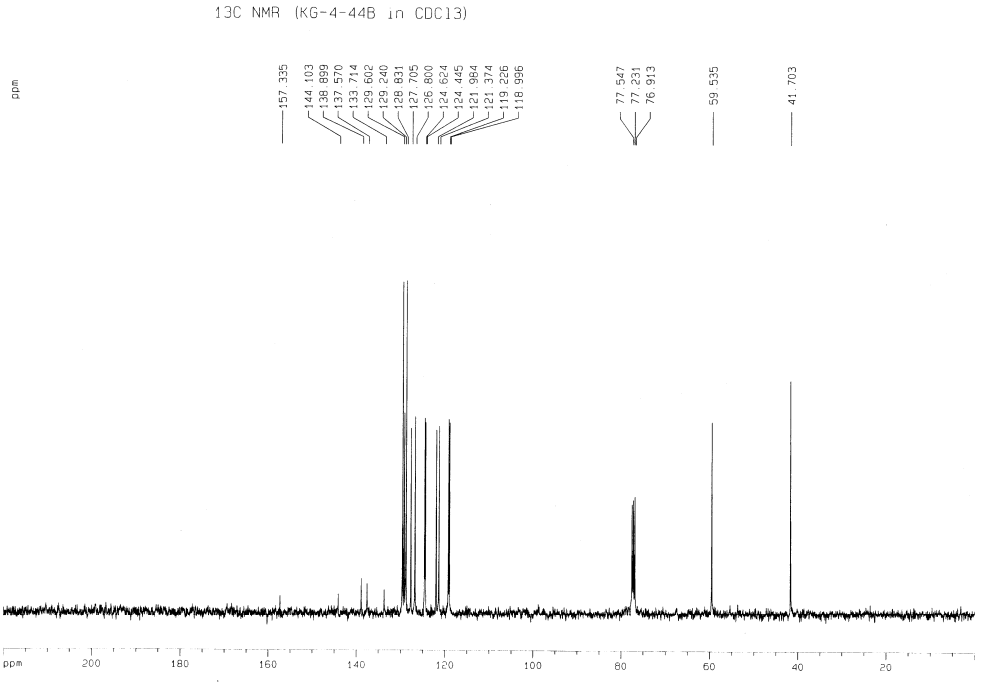
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
240.1389	240.1388	0.1	0.4	8.5	59.8	C16 H18 N O



9l HRMS



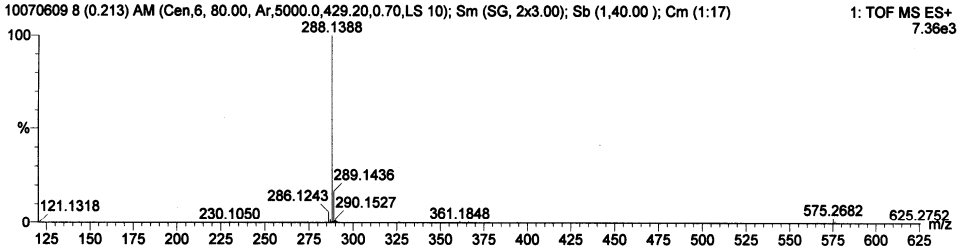
9m ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



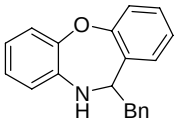
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

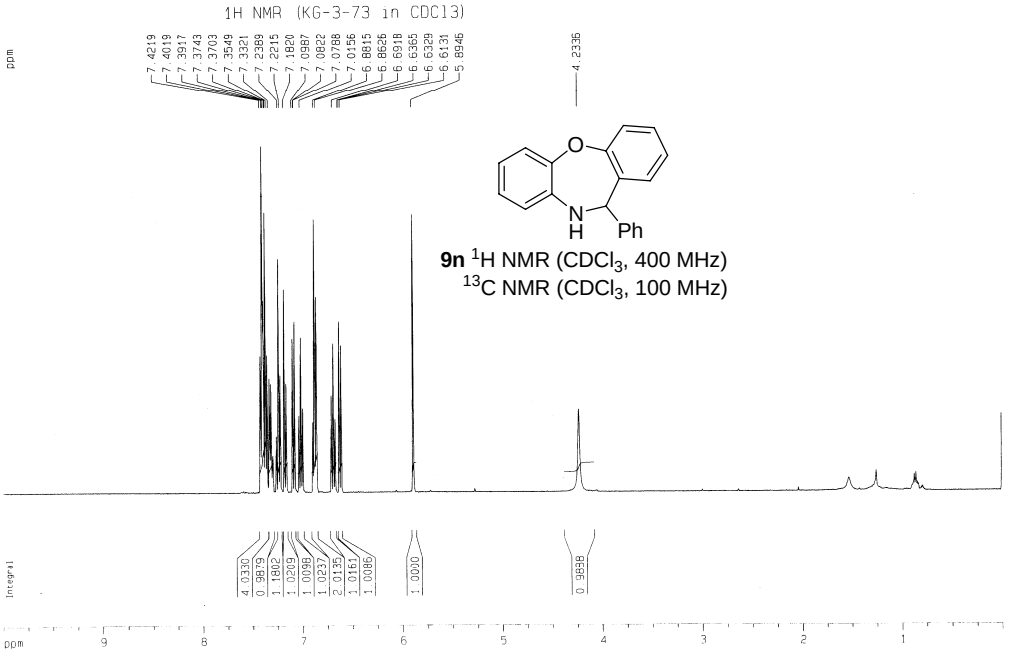
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 1-1
KG-4-44B
10070609 8 (0.213) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:17) 1: TOF MS ES+ 7.36e3



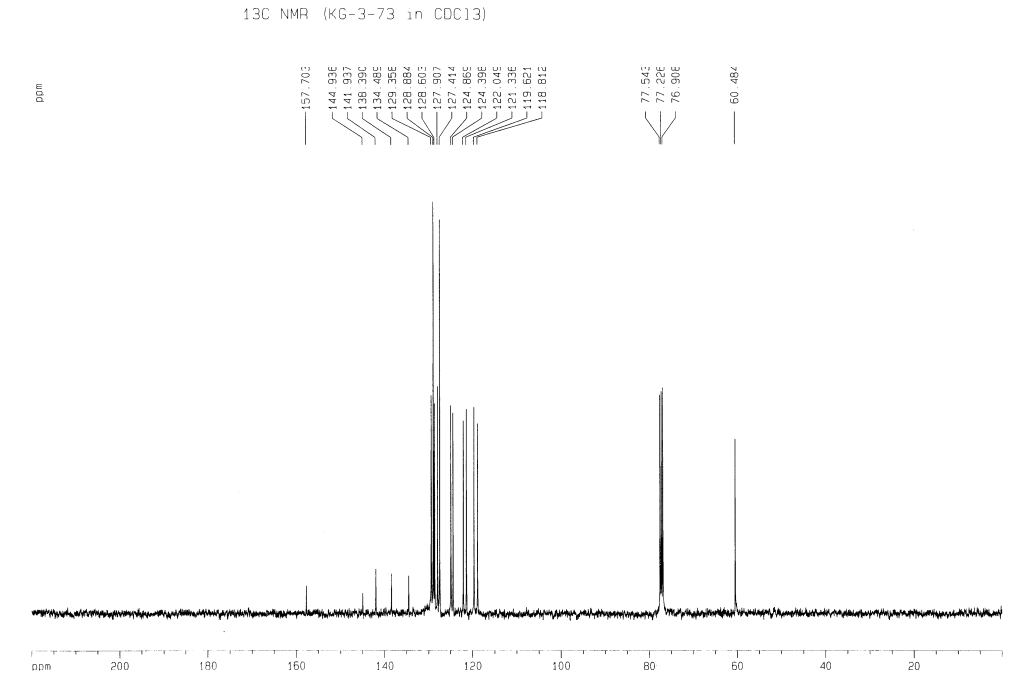
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.1388	288.1388	0.0	0.0	12.5	67.9	C20 H18 N O

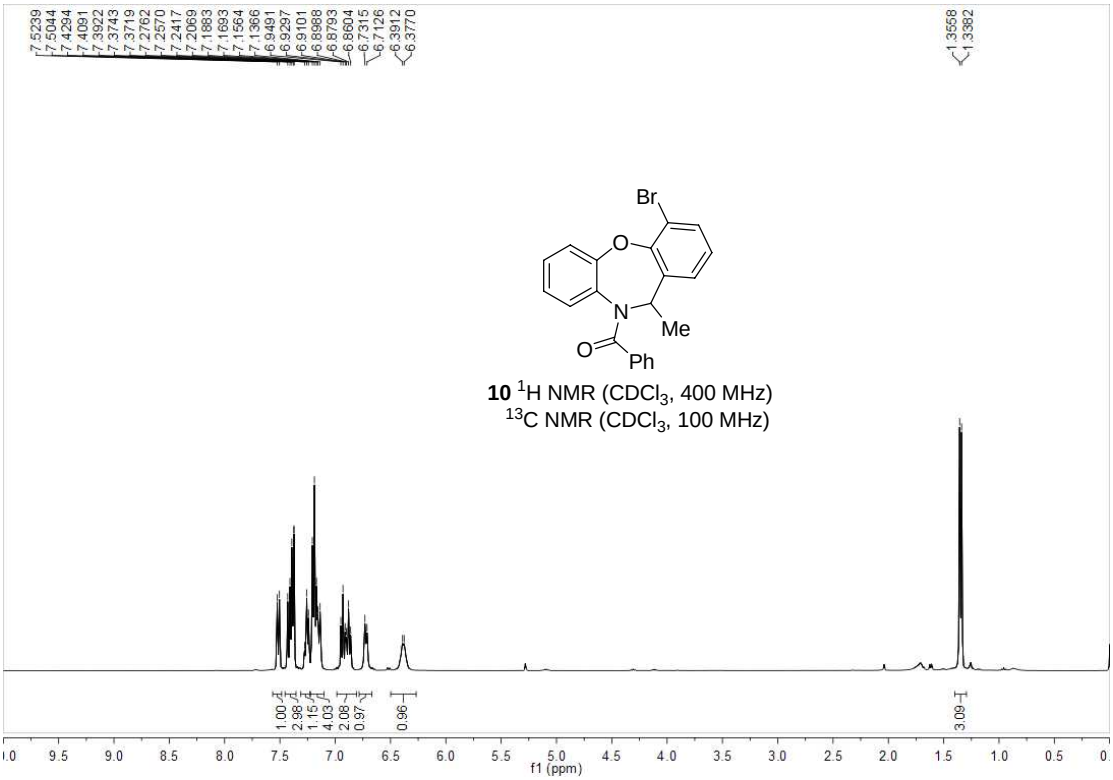


9m HRMS

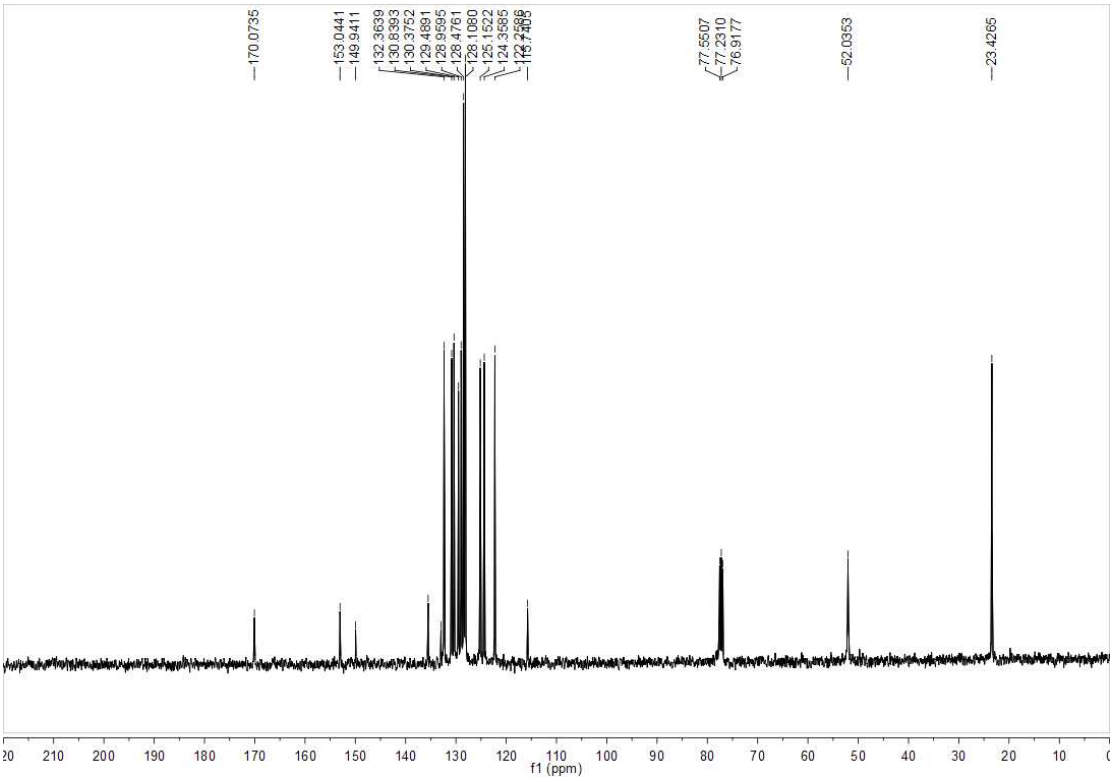


9n ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





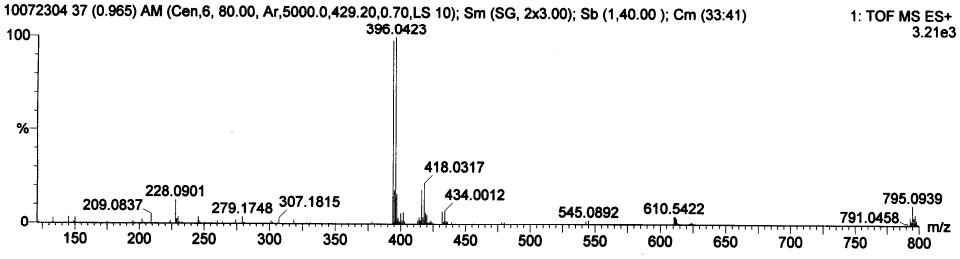
10 ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



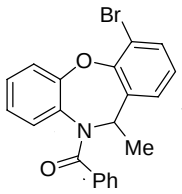
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 2-2 Br: 1-1
KG-5-16
10072304 37 (0.965) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (33:41) 1: TOF MS ES+ 3.21e3



Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
394.0438	394.0443	-0.5	-1.3	13.5	26.3	C21 H17 N O2 Br



10 HRMS

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008612.D Sample Name: KG-3-82
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 4/24/2010 2:05:27 PM
Sample Name     : KG-3-82                       Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 4/24/2010 1:58:11 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:22:57 PM by ZX
                  (modified after loading)
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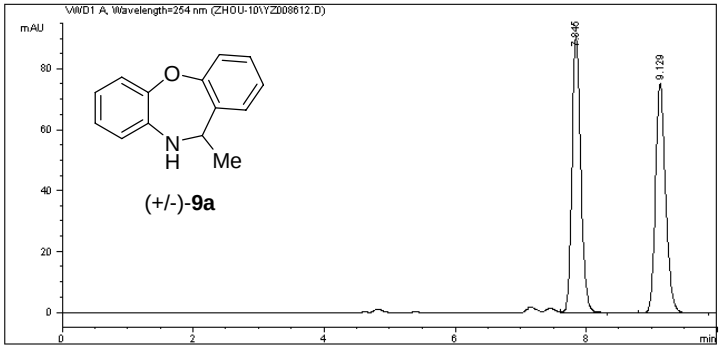

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.845 VV    0.1417  846.14868   91.19021  51.1625
   2   9.129 VV    0.1645  807.69629   75.24200  48.8375

Totals :                  1653.84497  166.43221

 Results obtained with enhanced integrator!
```

*** End of Report ***

Instrument 1 7/9/2010 2:23:03 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008610.D Sample Name: KG-4-63A
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 4/24/2010 1:29:57 PM
Sample Name     : KG-4-63A                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 4/24/2010 1:05:12 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:19:36 PM by ZX
                  (modified after loading)
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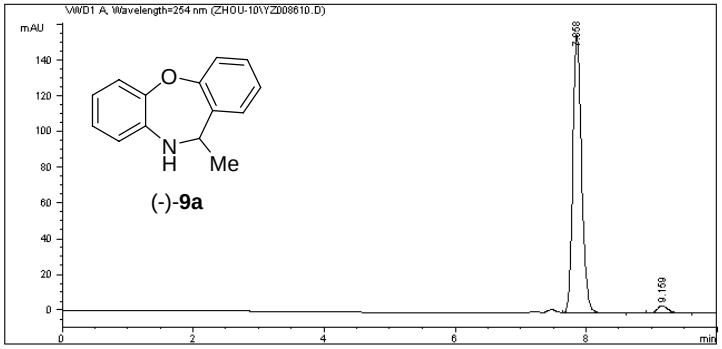


Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.858 VB    0.1416 1436.98572  155.11029  97.1756
   2   9.159 PP    0.1650   41.76616    3.87599   2.8244

Totals :                  1478.75187  158.98628

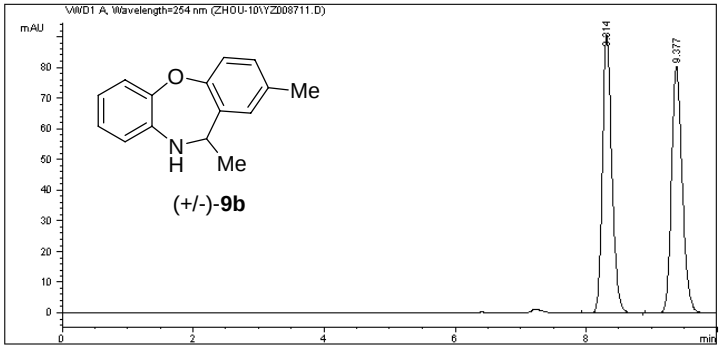
 Results obtained with enhanced integrator!
```

*** End of Report ***

Instrument 1 7/9/2010 2:19:43 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008711.D Sample Name: KG-4-65B
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 10:47:07 AM
Sample Name     : KG-4-65B                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 10:42:44 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:38:14 PM by ZX
                  (modified after loading)
==================================================================
```



(+/-)-**9b**

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   8.314 VB    0.1540  912.40393   90.49643  49.9765
   2   9.377 BB    0.1748  913.26129   80.34127  50.0235

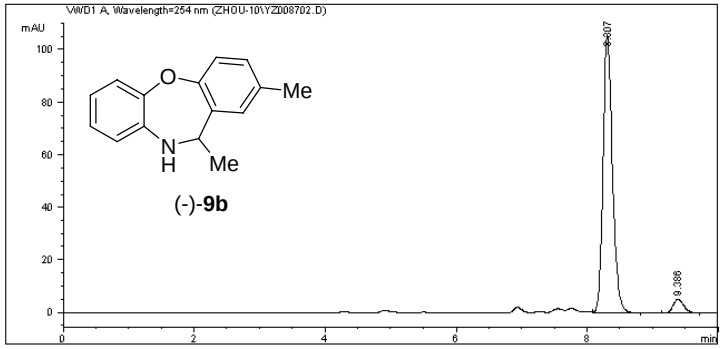
Totals :                  1825.66522  170.83770

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:38:18 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008702.D Sample Name: KG-4-66B
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 8:08:59 AM
Sample Name     : KG-4-66B                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 8:01:22 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:37:33 PM by ZX
                  (modified after loading)
==================================================================
```



(-)-**9b**

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   8.307 VV    0.1549 1059.80334  105.61897  94.7345
   2   9.386 VV    0.1739   58.90525    5.16209   5.2655

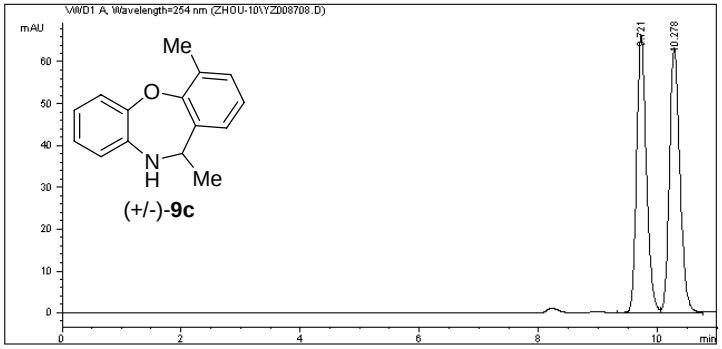
Totals :                  1118.70860  110.78106

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:37:36 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008708.D Sample Name: KG-4-65A
AD-H, H/i-PrOH =80/20, 0.5 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 10:04:03 AM
Sample Name     : KG-4-65A                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 9:59:09 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:35:02 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.721 VV    0.1757  758.59064   66.29560  49.8118
   2  10.278 VV    0.1844  764.32172   63.37954  50.1882

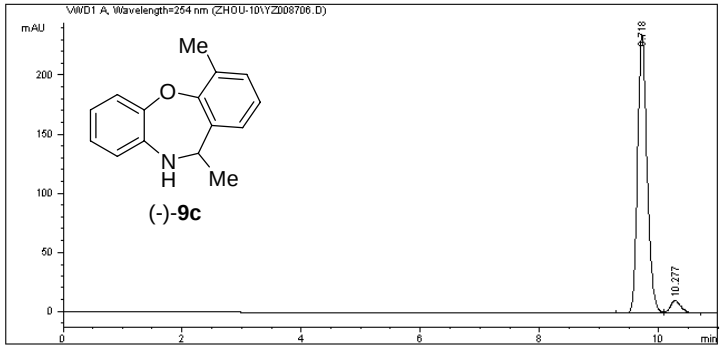
Totals :                  1522.91235  129.67514

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:35:37 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008706.D Sample Name: KG-4-66A
AD-H, H/i-PrOH =80/20, 0.5 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 9:24:41 AM
Sample Name     : KG-4-66A                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 9:20:05 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:34:59 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.718 VV    0.1711 2624.52979  234.86183  95.3931
   2  10.277 VV    0.1858  126.74825   10.40343   4.6069

Totals :                  2751.27804  245.26526

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:35:02 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500425.D Sample Name: KG-4-81A
AD-H, H/i-PrOH =99/1, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 4:33:03 PM
Sample Name     : KG-4-81A                      Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 4:30:13 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:46:45 PM by ZX
                  (modified after loading)
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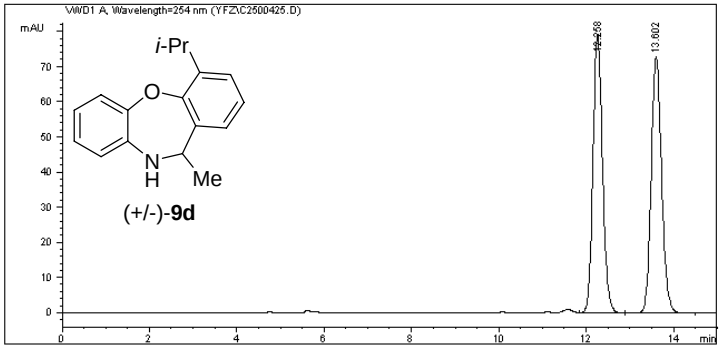



```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  12.258 VV    0.2336 1195.25745   78.87473  49.8936
   2  13.602 VB    0.2567 1200.35400   72.71040  50.1064

Totals :                  2395.61145  151.58514

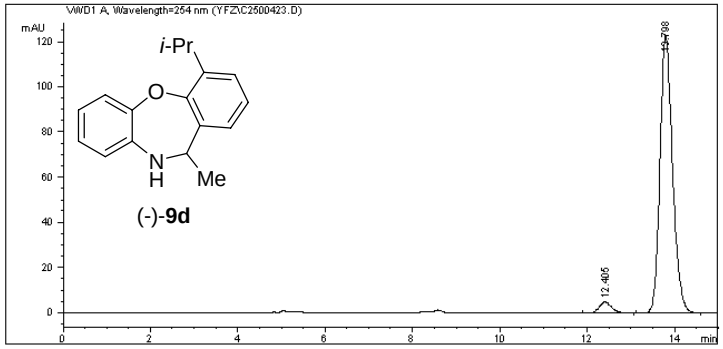
 Results obtained with enhanced integrator!

                        *** End of Report ***
```

Instrument 1 7/9/2010 2:47:15 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500423.D Sample Name: KG-5-7A
AD-H, H/i-PrOH =99/1, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 3:48:04 PM
Sample Name     : KG-5-7A                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 3:15:08 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:46:41 PM by ZX
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  12.405 VB    0.2964   94.78050    4.85119   3.7188
   2  13.798 BV    0.3046 2453.92944  122.74625  96.2812

Totals :                  2548.70995  127.59744

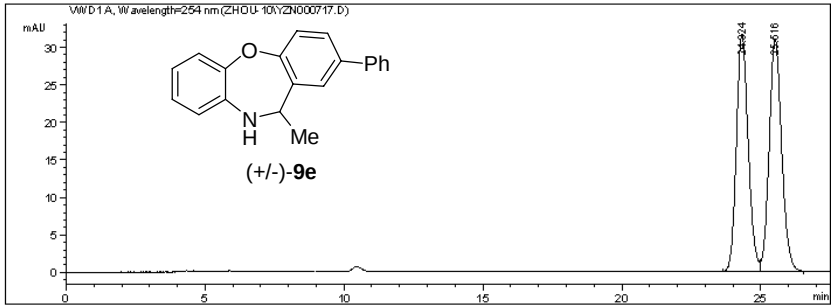
 Results obtained with enhanced integrator!

                        *** End of Report ***
```

Instrument 1 7/9/2010 2:46:45 PM ZX Page 1 of 1

Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000717.D
Sample Name: KG-4-81B

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 7/5/2010 9:39:22 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 9:34:57 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:11:29 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =90/10, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

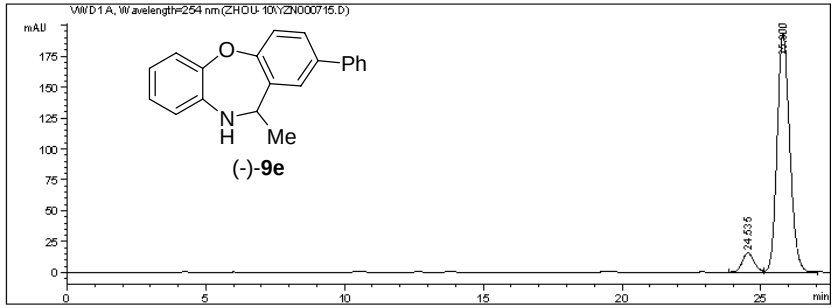
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  24.324 BV    0.4525  928.41504   31.62052  48.9881
   2  25.516 VB    0.4710  966.76935   30.92361  51.0119

Totals :                  1895.18439   62.54412

======================================================================
                          *** End of Report ***
```


Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000715.D
Sample Name: KG-5-8E

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 7/5/2010 8:30:16 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 8:08:56 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:11:29 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =90/10, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

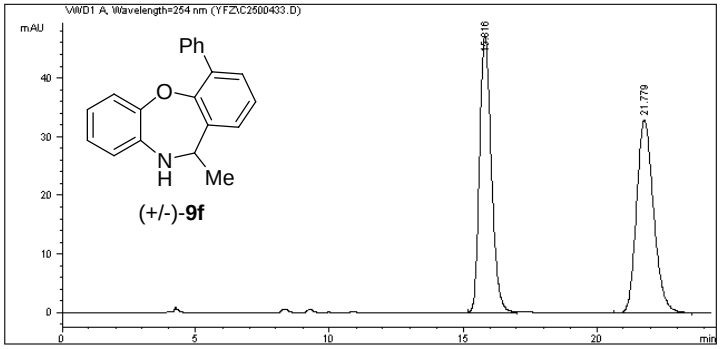
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  24.535 BV    0.4504  460.78754   15.62304   7.0208
   2  25.800 VB    0.4879 6102.41504  192.83282  92.9792

Totals :                  6563.20258  208.45587

======================================================================
                          *** End of Report ***
```

Data File C:\HPCHEM\1\DATA\YFZ\C2500433.D Sample Name: KG-4-81E
OD-H, H/i-PrOH =99/1, 0.8 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 8:19:03 PM
Sample Name     : KG-4-81E                      Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 8:20:06 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:49:46 PM by ZX
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  15.816 BV    0.4739 1447.19617   47.24082  49.9748
   2  21.779 VV    0.6848 1448.65637   32.85302  50.0252

Totals :                  2895.85254   80.09384

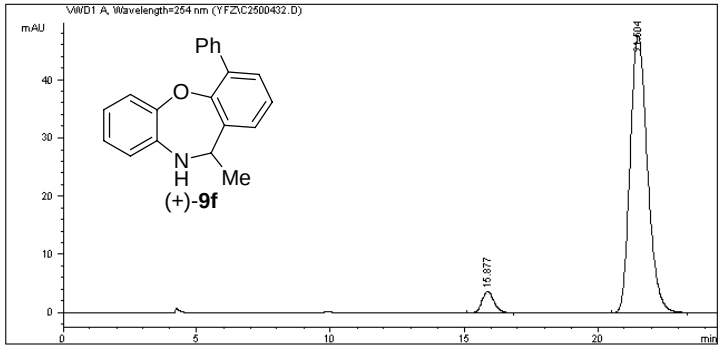
 Results obtained with enhanced integrator!
```

*** End of Report ***

Instrument 1 7/9/2010 2:50:13 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500432.D Sample Name: KG-5-7B
OD-H, H/i-PrOH =99/1, 0.8 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 7:48:51 PM
Sample Name     : KG-5-7B                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 8:08:08 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:49:42 PM by ZX
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  15.877 BB    0.4830  112.59505    3.62699   5.0212
   2  21.504 BB    0.6967 2129.78955   47.60670  94.9788

Totals :                  2242.38460   51.23370

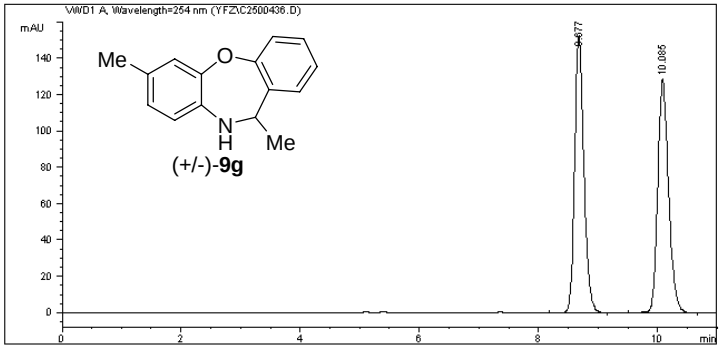
 Results obtained with enhanced integrator!
```

*** End of Report ***

Instrument 1 7/9/2010 2:49:45 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500436.D Sample Name: KG-4-81D
AD-H, H/i-PrOH =70/30, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 9:39:32 PM
Sample Name     : KG-4-81D                      Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 9:40:19 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:53:01 PM by ZX
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1   8.677 VV    0.1663 1661.32886  152.58455  50.2924
   2  10.085 VV    0.1954 1642.00940  128.70866  49.7076

Totals :                  3303.33826  281.29321

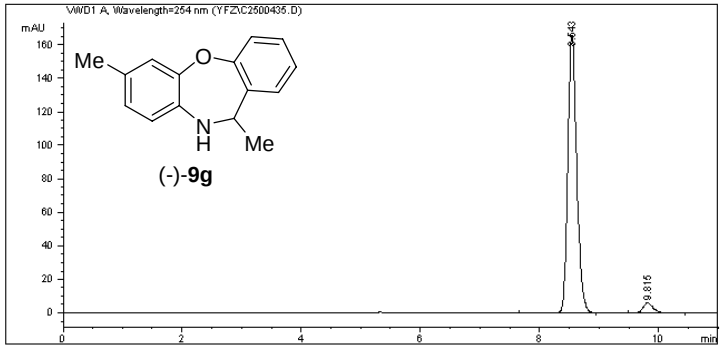
 Results obtained with enhanced integrator!

                        *** End of Report ***
```

Instrument 1 7/9/2010 2:53:34 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500435.D Sample Name: KG-5-8C
AD-H, H/i-PrOH =70/30, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 6/28/2010 9:21:01 PM
Sample Name     : KG-5-8C                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 6/28/2010 9:17:45 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:52:53 PM by ZX
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1   8.543 VV    0.1566 1708.52136  165.77908  96.0213
   2   9.815 VB    0.1848   70.79294    5.79136   3.9787

Totals :                  1779.31430  171.57045

 Results obtained with enhanced integrator!

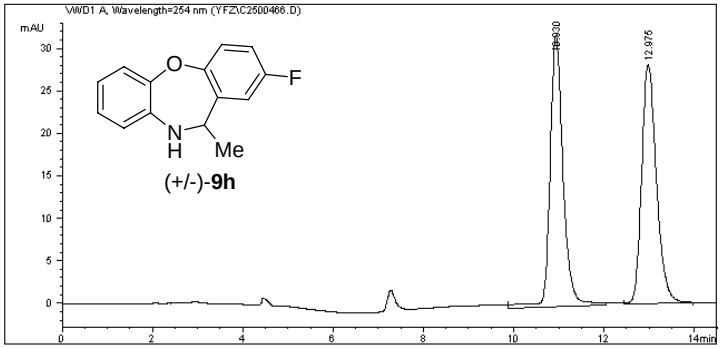
                        *** End of Report ***
```

Instrument 1 7/9/2010 2:53:01 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500466.D Sample Name: KG-4-81C

OD-H, H/i-PrOH =95/5, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 7/3/2010 7:21:45 PM
Sample Name     : KG-4-81C                      Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/3/2010 7:19:16 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:56:13 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  10.930 VV    0.3038  643.73584   31.90368  50.0842
   2  12.975 VB    0.3488  641.57147   28.15842  49.9158

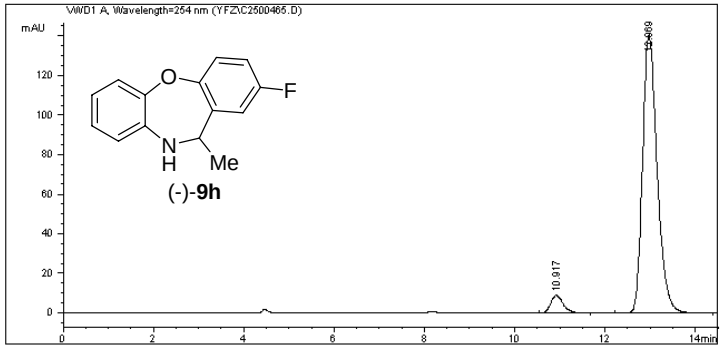
Totals :                  1285.30731   60.06210

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```


Data File C:\HPCHEM\1\DATA\YFZ\C2500465.D Sample Name: KG-5-8D

OD-H, H/i-PrOH =95/5, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 7/3/2010 6:20:03 PM
Sample Name     : KG-5-8D                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/3/2010 6:15:34 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:56:06 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

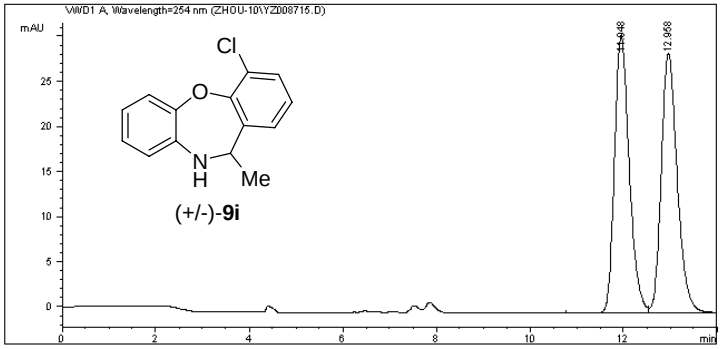
Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  10.917 VP    0.2856  165.44066    8.88727   5.0049
   2  12.969 PB    0.3444 3140.13208  140.15746  94.9951

Totals :                  3305.57274  149.04472

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008715.D Sample Name: KG-4-65C
OD-H, H/i-PrOH =95/5, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 12:56:00 PM
Sample Name     : KG-4-65C                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 12:52:30 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:40:57 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.948 VV    0.3379  676.42719   30.78129  49.8021
   2  12.958 VB    0.3654  681.80359   28.76358  50.1979

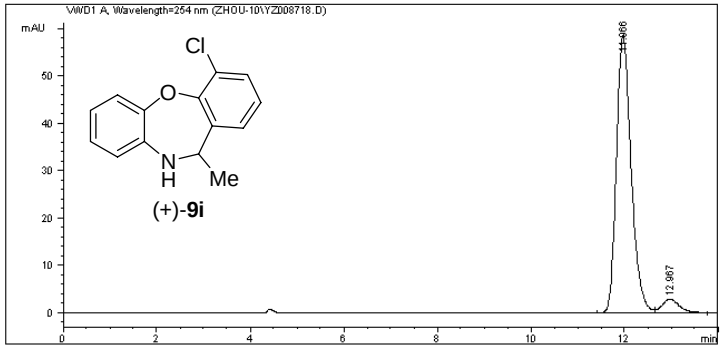
Totals :                  1358.23077   59.54488

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:41:45 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008718.D Sample Name: KG-4-67C
OD-H, H/i-PrOH =95/5, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 4/29/2010 2:07:10 PM
Sample Name     : KG-4-67C                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 4/29/2010 1:59:43 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:40:49 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.966 BV    0.3365 1277.88708   58.46330  94.9067
   2  12.967 VB    0.3710   68.57983    2.82097   5.0933

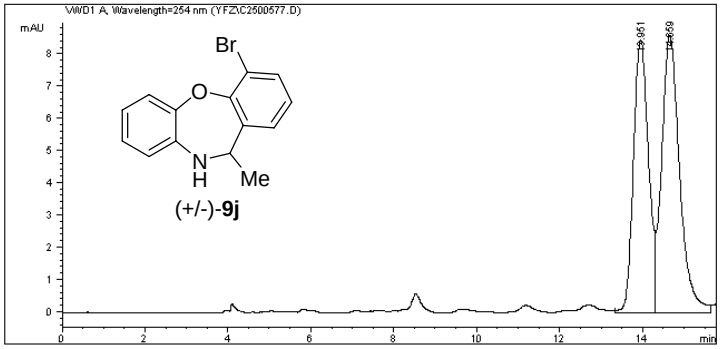
Totals :                  1346.46692   61.28427

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/9/2010 2:40:57 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500577.D Sample Name: KG-5-14
OD-H, H/i-PrOH = 97/3, 0.8 mL/min, 30 oC, 254 nm

```
Injection Date  : 7/21/2010 4:43:20 PM
Sample Name     : KG-5-14                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/21/2010 4:44:10 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/24/2010 4:16:13 PM by ZX
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  13.951 VV    0.3907  213.41322    8.45130  45.1857
   2  14.659 VV    0.4519  258.88928    8.59319  54.8143

Totals :                   472.30251   17.04449

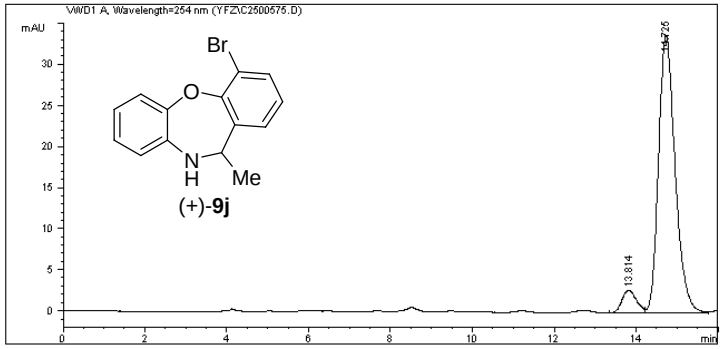
 Results obtained with enhanced integrator!

                        *** End of Report ***
```

Instrument 1 7/24/2010 4:16:22 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500575.D Sample Name: KG-5-21A
OD-H, H/i-PrOH = 97/3, 0.8 mL/min, 30 oC, 254 nm

```
Injection Date  : 7/21/2010 3:50:46 PM
Sample Name     : KG-5-21A                      Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/21/2010 3:56:43 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/24/2010 4:14:47 PM by ZX
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  13.814 VV    0.3821   68.27535    2.75704   6.6614
   2  14.725 VV    0.4348  956.65759   33.82646  93.3386

Totals :                  1024.93295   36.58350

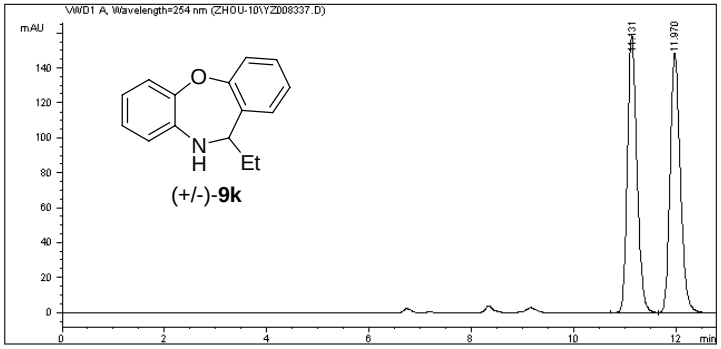
 Results obtained with enhanced integrator!

                        *** End of Report ***
```

Instrument 1 7/24/2010 4:14:52 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008337.D Sample Name: KG-4-40A
AD-H, H/i-PrOH =80/20, 0.5 mL/min, 30 oC, 254 nm

```
==========================================================================
Injection Date  : 3/24/2010 10:59:28 PM
Sample Name     : KG-4-40A                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 3/24/2010 11:02:50 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:30:45 PM by ZX
                  (modified after loading)
==========================================================================
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|---------|---------|-------|
   1  11.131 VV    0.1973 2054.04468  158.98668  49.9304
   2  11.970 VP    0.2126 2059.77393  148.67378  50.0696

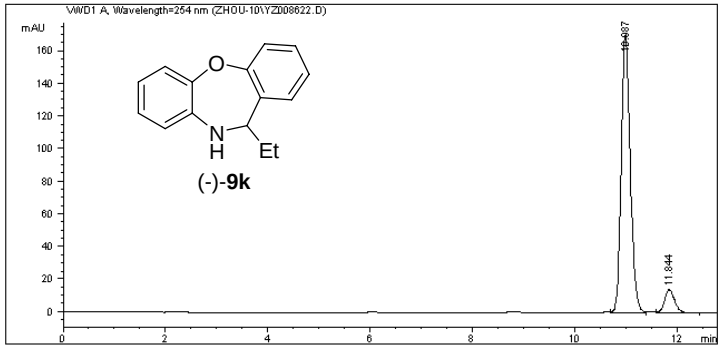
Totals :                  4113.81860  307.66046

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 7/9/2010 2:30:50 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008622.D Sample Name: KG-4-63B
AD-H, H/i-PrOH =80/20, 0.5 mL/min, 30 oC, 254 nm

```
==========================================================================
Injection Date  : 4/25/2010 12:01:24 PM
Sample Name     : KG-4-63B                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 4/25/2010 11:45:11 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:30:51 PM by ZX
                  (modified after loading)
==========================================================================
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|---------|---------|-------|
   1  10.987 VV    0.1911 2107.13794  170.07513  91.7059
   2  11.844 VB    0.2058  190.57419   14.22766   8.2941

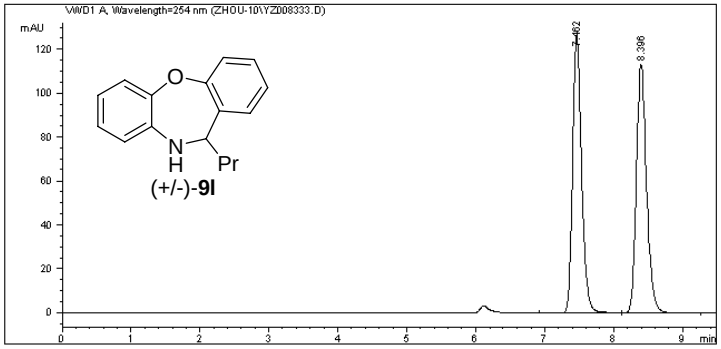
Totals :                  2297.71213  184.30280

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 7/9/2010 2:31:28 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-10\YZ008333.D Sample Name: KG-4-40B
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 3/24/2010 9:08:11 PM
Sample Name     : KG-4-40B                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 3/24/2010 9:03:52 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:59:47 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

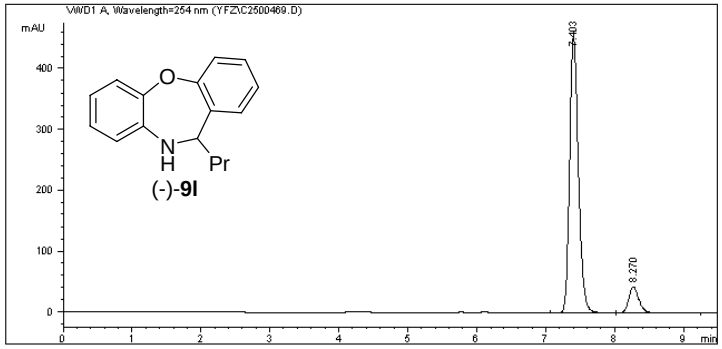
Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.462 VV    0.1389 1158.08008  126.39703  49.9403
   2   8.396 VB    0.1577 1160.84973  113.04852  50.0597

Totals :                  2318.92981  239.44555

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```


Data File C:\HPCHEM\1\DATA\YFZ\C2500469.D Sample Name: KG-5-9F
AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 nm

```
==================================================================
Injection Date  : 7/4/2010 9:48:06 AM
Sample Name     : KG-5-9F                       Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/4/2010 9:29:42 AM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/9/2010 2:59:44 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

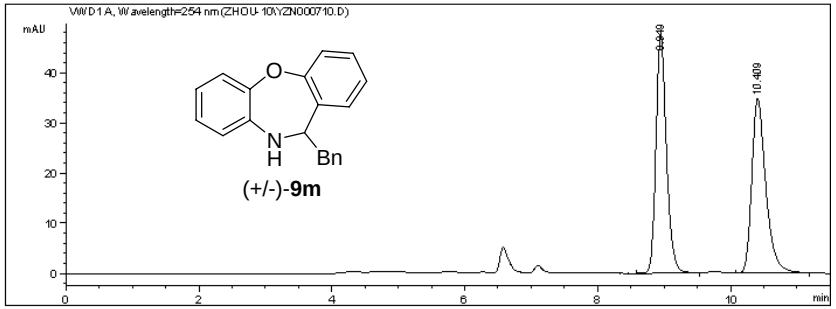
Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min] mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.403 BV    0.1355 4044.57739  456.15140  90.4212
   2   8.270 VP    0.1524  428.46588   43.11025   9.5788

Totals :                  4473.04327  499.26165

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000710.D
Sample Name: KG-4-45

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                  Location : Vial 1
Injection Date  : 7/5/2010 6:28:13 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 6:23:14 PM
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:15:34 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

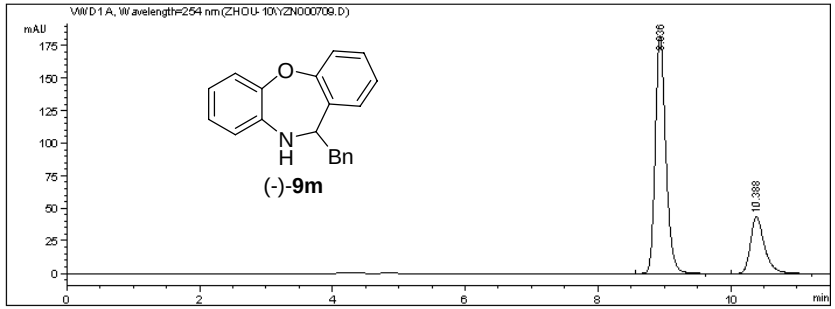
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   8.949 BB    0.1666  523.61438   47.45347  50.4311
   2  10.409 VB    0.2218  514.66266   34.85919  49.5689

Totals :                  1038.27704   82.31266

======================================================================
                        *** End of Report ***
```


Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000709.D
Sample Name: KG-5-9G

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                  Location : Vial 1
Injection Date  : 7/5/2010 6:09:02 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 6:04:40 PM
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:15:34 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =80/20, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

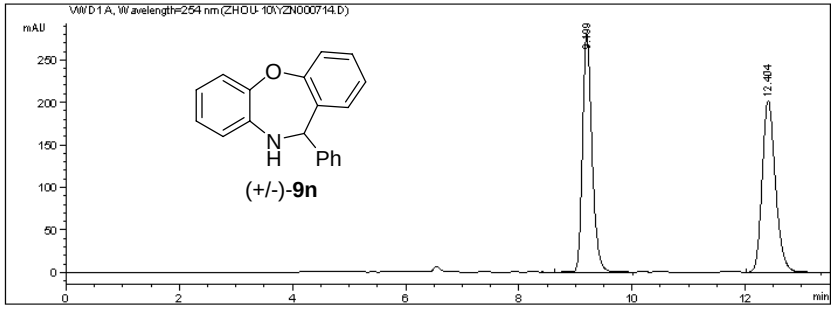
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   8.936 BB    0.1678 2016.64795  183.05724  75.9359
   2  10.388 VB    0.2218  639.07739   43.64631  24.0641

Totals :                  2655.72534  226.70354

======================================================================
                        *** End of Report ***
```

Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000714.D
Sample Name: KG-3-73

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 7/5/2010 7:49:46 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 7:48:49 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:18:33 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =70/30, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

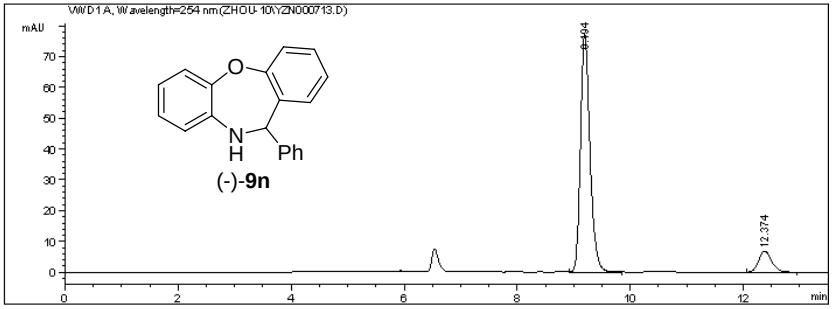
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|---------|---------|--------|
   1   9.199 VB    0.1799 3307.07715  280.24417  50.1566
   2  12.404 VB    0.2481 3286.42676  201.91351  49.8434

Totals :                  6593.50391  482.15768

======================================================================
                        *** End of Report ***
```


Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000713.D
Sample Name: KG-5-9H

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 7/5/2010 7:35:02 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/5/2010 7:29:54 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\SW.M
Last changed    : 7/9/2010 3:18:33 PM
                  (modified after loading)
Sample Info     : AD-H, H/i-PrOH =70/30, 0.7 mL/min, 30 oC, 254 NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

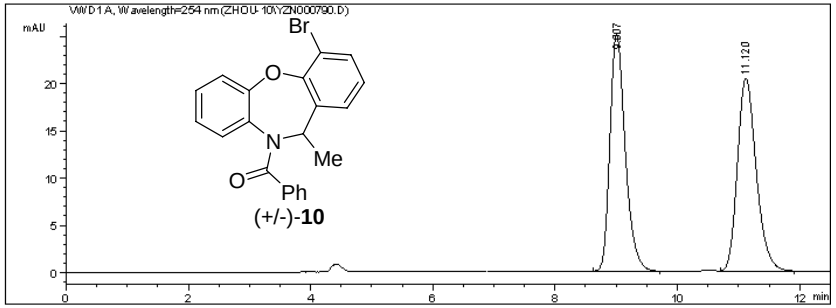
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|---------|---------|--------|
   1   9.194 BB    0.1789  905.23511   77.26433  89.0396
   2  12.374 BB    0.2477  111.43023    6.91412  10.9604

Totals :                  1016.66534   84.17845

======================================================================
                        *** End of Report ***
```

Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000790.D
Sample Name: KG-5-16

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 8/23/2010 10:24:49 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 8/23/2010 10:20:06 PM
                  (modified after loading)
Analysis Method : D:\DY-3-78B.M
Last changed    : 2/21/2011 12:40:26 PM
                  (modified after loading)
Sample Info     : OD-H, H/i-PrOH =90/10, 0.7 mL/min, 30 oC, 254NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

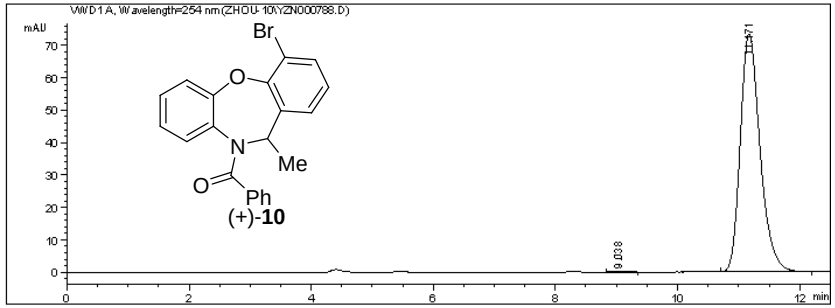
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|---------|---------|--------|
   1   9.007 BB    0.2634  436.59869   25.09956  49.9758
   2  11.120 BB    0.3305  437.02081   20.41703  50.0242

Totals :                   873.61951   45.51659

======================================================================
                          *** End of Report ***
```


Data File C:\CHEM32\1\DATA\ZHOU-10\YZN000788.D
Sample Name: KG-5-22C

```
======================================================================
Acq. Operator   :
Acq. Instrument : Instrument 1                    Location : Vial 1
Injection Date  : 8/23/2010 9:39:54 PM
Acq. Method     : C:\CHEM32\1\METHODS\SW.M
Last changed    : 8/23/2010 9:35:13 PM
                  (modified after loading)
Analysis Method : D:\DY-3-78B.M
Last changed    : 2/21/2011 12:40:26 PM
                  (modified after loading)
Sample Info     : OD-H, H/i-PrOH =90/10, 0.7 mL/min, 30 oC, 254NM
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|---------|---------|--------|
   1   9.038 BB    0.1946    1.80908 1.13537e-1   0.1093
   2  11.171 VB    0.3458 1652.82617   73.37356  99.8907

Totals :                  1654.63525   73.48709

======================================================================
                          *** End of Report ***
```