Supporting Information-I:

Synthesis of Dihydrofuroaporphine Derivatives: Identification of a Potent and Selective Serotonin 5-HT_{1A} Receptor Agonist

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Table 3. Binding affinity of aporphines for DA (D_1, D_2) and 5-HT (5-HT_{1A}) receptors from HEK293 or CHO cells[a]

compd	$K_i \pm$ SEM (nM)		
	D_1([^{3}H]SCH23390)	D_2([^{3}H]Spiperone)	5-HT_{1A} ([^{3}H]8-OH-DPAT)
buspirone	-	-	20.0±1.8 (24[b])
1(8-OH-DPAT)	-	-	1.2 (3.1[c])
10c	>10,000	>10,000	>10,000
10e	>10,000	>10,000	11±2
11e	>10,000	>10,000	>10,000
12a	>10,000	>10,000	340±91
12c	>10,000	>10,000	90±10
13	>10,000	>10,000	626±197
24	>10,000	>10,000	12.0±2.0

[a]Values are means of five to six experiments. Dash lines denote that no experiment was conducted.

[b]Data from ref 17; [c]Data from ref 14.

Experimental Section

General Methods. ^{1}H NMR spectral data were recorded in $CDCl_3$ on Varian Mercury 300 NMR spectrometer and ^{13}C NMR were recorded in $CDCl_3$ on Varian Mercury 400 NMR spectrometer. Low-resolution mass spectra (MS) and high-resolution mass spectra (HRMS) were recorded at an ionizing voltage of 70 eV on a Finnigan/MAT95 spectrometer. Elemental analyses were performed on a CE 1106 elemental analyzer. Optical rotations were determined with a JASCO DCP-1000 digital polarimeter and were the average of 3 measurements. Column chromatography was carried out on silica gel (200–300 mesh). All reactions were monitored using thin-layer chromatography (TLC) on silica gel plates. Yields were of purified compounds and were not optimized. Compounds **4a**[21,28], **4b**[21,28] and **4c**[35] were prepared according to corresponding literature procedures. HPLC analysis was conducted for all compounds listed in Table 1 on an Agilent 1100 series LC system (Agilent ChemStation Rev.A.10.02; ZORBAX Eclipse XDB-C8, 4.8 mm x150 mm, 5 μM, 1.0 mL/min, uv 254 nM , rt) with two solvent systems (MeCN/H_2O, and MeOH/H_2O). All the assayed compounds displayed a purity of 95%-99% in both solvent systems, and the diastereomeric mixtures of **10c**, **10e**, **11e**, **12a**, **12c**, **13**, **19** and **24** were inseparable and displayed one peak with >95% purity in both systems.

General Procedure for the preparation of ethers 10a-d. To a solution of 11-hydroxyaporphine **4a** (1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol) and a catalytic amount of KI (5 mg) in anhydrous DMF (10 mL) at 0 ^{o}C, an appropriate allyl bromide (1.0 mmol) was added. After stirred for 1h at 0 ^{o}C, the reaction mixture was warmed

to rt, and then diluted with Et_2O (30 mL) and H_2O (20 mL). The organic layer was separated, washed with brine, dried over anhydrous Na_2SO_4, and evaporated. The residue was purified by silica gel chromatography (petroleum:ethyl acetate = 3:1, 1% Et_3N) to give a pure oily product.

11-Allyloxy-*N*-methylaporphine (10a): colorless liquid (310 mg, 97%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, *J* = 7.8 Hz, 1H), 7.20 (m, 2H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.91 (dd, *J* = 8.7, 7.8 Hz, 2H), 6.10 (m, 1H), 5.46 (dd, *J* = 17.4, 1.2 Hz, 1H), 5.28 (m, 1H), 4.61 (m, 2H), 3.37 (dd, *J* = 13.8, 3.0 Hz, 1H), 3.14 (m, 3H), 2.92 (m, 1H), 2.50 (m, 4H), 1.62 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.7, 138.6, 135.4, 133.4, 132.9, 131.6, 127.8, 127.4, 126.4, 125.7, 123.7, 121.0, 117.1, 112.1, 69.5, 59.6, 56.5, 49.0, 35.3, 29.3, 19.7, 12.1; EI (MS) 319 (M^+); HRMS calcd for $C_{22}H_{25}NO_2$: 319.1936. Found: 319.1931.

11-(2-Methylallyloxy)-*N*-methylaporphine (10b). Brown oil (306 mg, 92%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, 1H, *J* = 8.1 Hz), 7.18 (m, 2H), 7.05 (d, 1H, *J* = 7.5 Hz), 6.91 (m, 2H), 5,14 (s, 1H), 4.98 (s, 1H), 4.55 (q, 2H, *J* = 12.6 Hz), 3.37 (d, 1H, *J* = 14.7 Hz), 3.18 (m, 3H), 2.91 (m, 1H), 2.76 (dd, 1H, *J* = 16.2, 3.9 Hz), 2.51 (m, 3H), 1.85 (s, 3H), 1.64 (m, 2H), 0.97 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.7, 140.8, 138.4, 135.3, 132.8, 131.5, 127.8, 127.4, 126.5, 125.6, 123.5, 120.9, 112.4, 111.7, 72.3, 59.5, 56.5, 49.0, 35.3, 29.3, 19.6, 19.5, 12.1; EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO_2$: 333.2093. Found: 333.2090.

11-(1-Methylallyloxy)-*N*-methylaporphine (10c). Brown oil (147 mg, 44%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, 1H, *J* = 8.1 Hz), 7.18 (m, 2H), 7.05 (d, 1H, *J*

= 7.5 Hz), 6.91 (m, 2H), 5.82 (m, 2H), 4.57 (m, 1H), 4.51 (m, 1H), 3.39 (d, 1H, *J* = 12.9 Hz), 3.18 (m, 3H), 2.91 (m, 1H), 2.76 (m, 1H), 2.53 (m, 3H), 1.75 (m, 3H), 1.66 (m, 2H), 0.98 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.7, 140.6, 138.4, 135.3, 132.7, 131.5, 127.7, 127.3, 126.4, 125.6, 123.4, 120.8, 112.4, 111.7, 72.3, 59.5, 56.5, 48.9, 35.2, 29.3, 19.6, 19.5, 12.0; EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO_2$: 333.2093. Found: 333.2095.

11-(3,3-Bismethylallyloxy)-*N*-methylaporphine (10d). Brown oil (177 mg, 51%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, 1H, *J* = 8.1 Hz), 7.18 (m, 2H), 7.04 (d, 1H, *J* = 7.5 Hz), 6.91 (dd, 2H, *J* = 7.2, 2.1 Hz), 5.53 (m, 1H), 4.60 (m, 2H), 3.37 (dd, 1H, *J* = 12.3, 2.4 Hz), 3.14 (m, 3H), 2.91 (m, 1H), 2.76 (dd, 1H, *J* = 15.9, 5.4 Hz), 2.50 (m, 3H), 1.78 (s, 3H), 1.73(s, 3H), 1.64 (m, 2H), 0.97 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.9, 138.2, 137.0, 132.5, 131.6, 127.6, 127.3, 126.3, 125.8, 123.4, 120.7, 120.0, 112.0, 65.6, 59.5, 56.4, 48.9, 35.1, 29.1, 25.6, 19.4, 18.2, 12.0; EI (MS) 347 (M^+); HRMS calcd for $C_{24}H_{29}NO_2$: 347.2249. Found: 347.2248.

Preparation of 11-(2-butenyloxy)-*N*-propylnoraporphine (10e). A solution of **15b** (38 mg, 0.11 mmol), Lindar reagent (5 mg) and quinoline (40 μL) in EtOH (10 mL) was stirred for 1 h at rt under H_2. The reaction mixture was filtered. The solvent was removed to yield quantitative crude product **10e** which was purified by silica gel chromatography (petroleum:ethyl acetate = 3:1) to yield a pure oily product (32.9 mg, 90%). ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, 1H, *J* = 8.1 Hz), 7.19 (m, 2H), 7.05 (d, 1H, *J* = 7.5 Hz), 6.92 (m, 2H), 5.75 (m, 2H), 4.67 (m, 2H), 3.37 (dd, 1H, *J* = 3.0, 13.5 Hz), 3.15 (m, 3H), 2.93 (m, 1H), 2.76 (m, 1H), 2.50 (m, 3H), 1.74 (d, 3H, *J* = 5.4 Hz),

1.61 (m, 2H), 0.98 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.7, 138.4, 135.3, 132.8, 131.6, 129.6, 128.0, 127.4, 126.3, 125.9, 125.7, 123.5, 120.8, 111.9, 69.3, 59.6, 56.6, 49.0, 35.3, 29.4, 19.6, 17.8, 12.0; EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO_2$: 333.2093. Found: 333.2091.

General Procedure for the preparation of aporphine derivatives 11a,b and 11e by Cope-rearrangement. A solution of 11-allyloxy-*N*-methylaporphines **10a,b** or **10e** (1.0 mmol) in *N,N*-diethylaniline (10 mL) was refluxed for 1.5 h under N_2. After cooling to rt, the reaction mixture was purified by silica gel chromatography (petroleum:ethyl acetate = 2:1) to yield the rearranged products.

10-Allyl-11-hydroxy-*N*-propylnoraporphine (11a). Off-white solid (303 mg, 95%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.92 (d, 1H, *J* = 7.5 Hz), 7.22 (m, 1H), 7.07 (d, 1H, *J* = 7.5 Hz), 7.00 (d, 1H, *J* = 7.5 Hz), 6.84 (d, 1H, *J* = 7.5 Hz), 6.05 (m, 1H), 5.66 (brs, 1H), 5.18 (m, 2H), 3.46 (d, 2H, *J* = 6.3 Hz), 3.36 (dd, 1H, *J* = 13.8, 3.0 Hz), 3.14 (m, 3H), 2.91 (m, 1H), 2.77 (dd, 1H, *J* = 16.5, 4.2 Hz), 2.49 (m, 3H), 1.65 (m, 2H), 0.97 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 151.0, 136.6, 136.5, 135.9, 133.9, 131.6, 129.0, 127.6, 126.2, 125.2, 124.1, 121.7, 120.3, 116.5, 59.7, 56.4, 48.9, 35.4, 35.0, 29.3, 19.4, 12.1; MS (EI) 319 (M^+); HRMS calcd for $C_{22}H_{25}NO_2$: 319.1936. Found: 319. 1933.

10-(2-Methylallyl)-11-hydroxy-*N*-propylnoraporphine (11b). Brown solid (273 mg, 82%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.99 (d, 1H, *J* = 7.8 Hz), 7.22 (t, 1H, *J* = 7.8 Hz), 7.06 (d, 1H, *J* = 7.8 Hz), 6.98 (d, 1H, *J* = 7.8 Hz), 6.83 (d, 1H, *J* = 7.2 Hz), 4.93 (d, 2H, *J* = 8.1 Hz), 3.43 (d, 2H, *J* = 7.5 Hz), 3.36 (dd, 1H, *J* = 10.8, 2.1 Hz),

3.14 (m, 3H), 2.91 (m, 1H), 2.75 (dd, 1H, *J* = 16.8, 5.7 Hz), 2.49 (m, 3H), 1.77 (s, 3H), 1.62 (m, 2H), 0.97 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 151.7, 144.7, 136.8, 135.6, 133.5, 131.6, 129.5, 127.5, 126.1, 124.9, 124.3, 121.7, 120.2, 112.5, 59.7, 56.5, 49.0, 40.3, 35.0, 29.3, 22.0, 19.4, 12.9; EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO_2$: 333.2093. Found: 333.2086.

10-(2-Butenyl)-11-hydroxy-*N*-propylnoraporphine (11e). This compound was prepared from aporphine **10e** as pale solid (90%) following a similar procedure used for the preparation of compounds **11a,b**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.91 (d, 1H, *J* = 7.8 Hz), 7.25 (t, 1H, *J* = 7.5 Hz), 7.04 (m, 2H), 6.87 (dd, 1H, *J* = 2.7, 1.8 Hz), 6.05 (m, 1H), 5.92 (brs, 1H), 5.19 (m, 2H), 3.80 (m, 1H), 3.36 (dd, 1H, *J* = 9.3, 1.8 Hz), 3.15 (m, 3H), 2.91 (m, 1H), 2.78 (m, 1H), 2.54 (m, 3H), 1.62 (m, 2H), 1.43 (dd, 3H, *J* = 6.9, 3.0 Hz), 0.97 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 150.6, 142.6, 142.4, 136.4, 136.1, 134.1, 131.7, 127.6, 126.8, 126.3, 124.1, 121.8, 120.3, 114.3, 59.8, 56.5, 49.0, 37.6, 35.1, 29.4, 19.6, 19.0, 12.1; EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO_2$: 333.2093. Found: 333.2097.

General Procedure for the synthesis of dihydrofuranoaporphines derivatives 12a-c. A solution of 11-hydroxy-10-substituted-aporphines **11a,b** or **11e** (0.10 mmol) in glacial acetic acid (6 mL) and concentrated HBr (2 mL) was refluxed for 3 h and then evaporated to dryness. The residue was cooled and treated with NH_4OH (5 mL). The solution was extracted with CH_2Cl_2 (4 × 20 mL). The combined organic layer was washed with brine, dried by Na_2SO_4 and evaporated. The residue was purified by silica gel chromatography (petroleum:ethyl acetate = 2:1) to give the title compounds.

***N*-Propyl-2'-methyl-2',3'-dihydrofuro[*m*]noraporphine (12a).** Pale yellow solid (28 mg, 88%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.09 (d, 1H, *J* = 8.7 Hz, H-1), 7.22 (t, 1H, *J* = 7.8 Hz, H-2), 7.02 (m, 2H, H-3, H-8), 6.76 (d, 1H, *J* = 7.2 Hz, H-9), 5.09 and 4.96 (m, 1H, 1:1, H-2'), 3.30 (m, 5H, H-7, H-3', H-6a), 2.82 (m, 3H, H-4, H-5α), 2.55 (m, 3H, H-5β, $\underline{CH_2}CH_2CH_3$), 1.62 (m, 2H, $CH_2\underline{CH_2}CH_3$), 1.60 and 1.44 (d, 3H, *J* = 6.3 Hz, 1:1, 2'-Me), 0.97 (t, 3H, *J* = 7.5 Hz, $CH_2CH_2\underline{CH_3}$); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 156.3 (2), 135.9, 134.3, 133.0, 131.4 (2), 127.3, 126.6 (2), 126.1, 125.0 (2), 123.3 (2), 119.9, 117.5, 80.0 (2), 59.6 (2), 56.3, 49.2, 36.7 (2), 34.4, 29.2, 22.0 (2), 19.3, 12.0; EI (MS) 319 (M^+); Anal. ($C_{22}H_{25}NO\cdot 1/3H_2O$) Calcd: C, 81.19; H, 7.95; N, 4.30; Found: C, 81.43; H, 7.82; N, 4.06.

***N*-Propyl-2',2'-bismethyl-2',3'-dihydrofuro[*m*]noraporphine (12b).** Yellow solid (31 mg, 93%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.15 (d, 1H, *J* = 7.8 Hz), 7.22 (d, 1H, *J* = 7.8 Hz), 7.02 (m, 2H), 6.77 (d, 1H, *J* = 7.2 Hz), 3.47 (dd, 1H, *J* = 14.1, 3.0 Hz), 3.17 (m, 3H), 3.05 (m, 2H), 2.96 (m, 1H), 2.78 (m, 1H), 2.63 (m, 1H), 2.50 (m, 2H), 1.62 (m, 5H), 1.48 (s, 3H), 0.99 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.7, 135.9, 134.3, 133.0, 131.6, 127.2, 126.7, 126.1, 125.0, 123.5, 119.6, 117.5, 86.9, 59.6, 56.4, 49.2, 42.4, 34.5, 29.3, 28.5, 28.3, 19.3, 12.0; EI (MS) 333 (M^+); Anal. ($C_{23}H_{27}NO\cdot 0.3H_2O$) Calcd: C, 81.52; H, 8.21; N, 4.13; Found: C, 81.52; H, 8.13; N, 3.81.

***N*-Propyl-2',3'-bismethyl-2',3'-dihydrofuro[*m*]noraporphine (12c).** Brown oil (27 mg, 82%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 and 8.09 (d, 1H, *J* = 7.8 Hz, 1:1), 7.25 (t, 1H, *J* = 7.8 Hz), 7.00 (m, 2H), 6.80 (d, 1H, *J* = 7.2 Hz), 5.06, 4.92, 4.54 and

4.38 (m, 1H, 1.5:1.7:1:1.3), 3.45 (m, 1H), 3.15 (m, 4H), 2.93 (m, 1H), 2.76 (m, 1H), 2.54 (m, 3H), 1.64 (m, 2H), 1.59 and 1.48 (m, 3H, 1:1), 1.34 and 1.21 (dd, 3H, *J* = 8.1, 6.9 Hz, 1:1), 0.98 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.6 (2), 135.9, 134.2, 133.0 (2), 132.3 (2), 131.5 (2), 127.3, 126.1, 125.1, 122.1 (2), 120.1, 117.6, 87.5 and 82.8 (4), 59.6 (2), 56.3, 49.2, 43.4 (2), 38.8 (2), 34.4, 29.2, 20.3 (2), 18.2 and 14.8 (4), 15.6 and 12.0 (2); EI (MS) 333 (M^+); HRMS calcd for $C_{23}H_{27}NO$: 333.2093. Found: 333.2087.

8-(1-Buten-3-yl)-11-hydroxy-*N*-propylnoraporphine (13). This compound was prepared as brown solid (59%) from ether **10c** following a similar procedure used for the preparation of compounds **11a,b**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.98 (d, 1H, *J* = 7.5 Hz), 7.25 (t, 1H, *J* = 7.8 Hz), 7.03 (m, 2H), 6.84 (dd, 1H, *J* = 7.5, 3.9 Hz), 6.11 (m, 1H), 5.22 (m, 2H), 3.77 (m, 1H), 3.60 (m, 1H), 3.32 (m, 2H), 3.11 (m, 2H), 2.72 (m, 4H), 1.71 (m, 2H), 1.41 (d, 3H, *J* = 7.2 Hz), 0.97 (t, 3H, *J* = 7.2 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 150.7, 142.3, 142.2, 135.1, 132.5, 131.8, 130.2, 127.5, 127.1, 126.7, 125.0, 121.4, 120.3, 114.6, 59.6, 48.4, 37.9, 37.6, 34.0, 27.9, 18.8, 18.7, 11.8; MS (EI) 333 (M^+); Anal. ($C_{23}H_{27}NO{\cdot}1.2H_2O$) Calcd: C, 77.80; H, 8.35; N, 3.94; Found: C, 78.02; H, 8.34; N, 3.64.

8-(2-Methyl-2-buten-4-yl)-11-hydroxy-*N*-propylnoraporphine (14). This compound was prepared as brown solid (31%) from ether **10d** following a similar procedure used for the preparation of compounds **11a,b**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.86 (d, 1H, *J* = 8.1 Hz), 7.21 (d, 1H, *J* = 7.5 Hz), 7.06 (d, 1H, *J* = 7.5 Hz), 6.97 (d, 1H, *J* = 8.1 Hz), 6.74 (d, 1H, *J* = 8.4 Hz), 5.18 (t, 1H, *J* = 6.6 Hz), 3.23 (m, 6H), 2.84

(m, 1H), 2.77 (dd, 1H, *J* = 16.2, 2.8 Hz), 2.47 (m, 2H), 2.23 (t, 1H, *J* = 14.4 Hz), 1.76 (s, 3H), 1.71 (s, 3H), 1.62 (m, 2H), 0.97 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 151.0, 136.3, 135.5, 133.4, 131.7, 131.6, 130.8, 129.2, 127.3, 126.2, 124.2, 123.4, 121.6, 114.8, 59.3, 56.5, 48.9, 32.5, 30.3, 29.0, 25.6, 19.3, 17.8, 12.1; MS (EI) 347 (M^+); Anal. ($C_{24}H_{29}NO{\cdot}0.5H_2O$) Calcd: C, 80.86; H, 8.48; N, 3.93; Found: C, 80.95; H, 8.45; N, 3.53.

11-Propargyloxy-*N*-propylnoraporphine (15a). This compound was prepared as brown oil (90%) from phenol **4a** following a similar procedure used for the preparation of compounds **10a-d**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.10 (d, 1H, *J* = 7.5 Hz), 7.20 (m, 2H), 7.05 (t, 2H, *J* = 6.9 Hz), 6.97 (d, 1H, *J* = 7.5 Hz), 4.74 (m, 2H), 3.36 (dd, 1H, *J* = 13.5, 3.0 Hz), 3.14 (m, 3H), 2.91 (m, 1H), 2.76 (m, 1H), 2.50 (m, 4H), 1.61 (m, 2H), 0.97 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 154.6, 138.6, 132.8, 131.2, 127.7, 127.6, 126.3, 125.8, 123.9, 121.8, 112.5, 78.7, 75.5, 59.4, 56.4, 56.3, 48.9, 35.1, 29.2, 19.5, 12.1; EI (MS) 317 (M^+); HRMS calcd for $C_{22}H_{23}NO_2$: 317.1780. Found: 317.1767.

11-(2-Butynyloxy)-*N*-propylnoraporphine (15b). This compound was prepared as brown oil (98%) from phenol **4a** following a similar procedure used for the preparation of compounds **10a-d**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.12 (d, 1H, *J* = 7.8 Hz), 7.20 (m, 2H), 7.04 (m, 2H), 6.94 (d, 1H, *J* = 7.5 Hz), 4.70 (m, 2H), 3.36 (dd, 1H, *J* = 12.6, 1.2 Hz), 3.14 (m, 3H), 2.91 (m, 1H), 2.75 (m, 1H), 2.50 (m, 3H), 1.85 (t, 3H, *J* = 2.1 Hz), 1.61 (m, 2H), 0.96 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 154.8, 138.4, 135.2, 132.7, 131.3, 127.6, 127.4, 126.3, 125.8, 123.8, 121.3, 112.4,

83.5, 74.2, 59.5, 56.8, 56.4, 48.9, 35.2, 29.2, 19.5, 12.0, 3.7; EI (MS) 331 (M^+); HRMS calcd for $C_{23}H_{25}NO_2$: 331.1936. Found: 331.1944.

General Procedure for the synthesis of furoaporphine derivatives 16a,b: A solution of 11-propargyloxyaporphine derivatives **15a** or **15b** (0.08 mmol) and CsF (20 mg, 0.13 mmol) in *N,N*-diethyl aniline (5 mL) was refluxed for 3h under N_2. After cooling to rt, the reaction mixture was purified by silica gel chromatography (petroleum:ethyl acetate = 5:1 to 1:1) to afford the title compounds.

***N*-Propyl-2'-methyl-furo[*m*]noraporphine (16a):** brown oil (13 mg, 53%); ^{1}H-NMR (300 MHz, CDC1$_3$) δ 8.30 (d, 1H, *J* = 7.8 Hz), 7.32 (t, 2H, *J* = 7.5 Hz), 7.11 (dd, 2H, *J* = 7.8, 4.8 Hz), 6.39 (s, 1H), 3.56 (dd, 1H, *J* = 13.8, 4.2 Hz), 3.20 (m, 3H), 2.96 (m, 1H), 2.78 (m, 2H), 2.52 (s, 3H), 2.50 (m, 2H), 1.64 (m, 2H), 0.99 (t, 3H, *J* = 7.5 Hz); ^{13}C-NMR (100 MHz, CDC1$_3$) δ 155.0, 151.4, 134.7, 133.5, 131.2, 130.8, 129.0, 127.8, 126.3, 125.1, 123.0, 118.7, 102.6, 59.6, 56.4. 49.2, 34.2, 29.3, 19.3, 14.2, 12.0; EI (MS) 317 (M^+); HRMS calcd for $C_{22}H_{23}NO$: 317.1780. Found: 317.1773.

***N*-Propyl-2',3'-bismethyl-furo[*m*]noraporphine (16b).** brown oil (16 mg, 60%); ^{1}H-NMR (300 MHz, CDC1$_3$) δ 8.31 (d, 1H, *J* = 7.5 Hz), 7.29 (m, 2H), 7.13 (d, 1H, *J* = 7.8 Hz), 7.09 (d, 1H, *J* = 7.5 Hz), 3.45 (dd, 1H, *J* = 10.5, 3.9 Hz), 3.21 (m, 3H), 2.97 (m, 1H), 2.80 (m, 2H), 2.52 (m, 2H), 2.44 (s, 3H), 2,17 (s, 3H), 1.64 (m, 2H), 0.98 (t, 3H, *J* = 7.5 Hz). ^{13}C-NMR (100 MHz, CDC1$_3$) δ 150.5, 150.2, 131.0, 130.4, 127.8, 127.6, 126.4, 125.2, 122.5, 122.3, 117.3, 109.6, 59.6, 56.4, 49.2, 34.1, 29.6, 19.3, 12.0, 11.9, 7.9; EI (MS) 331 (M^+); HRMS calcd for $C_{23}H_{25}NO$: 331.1936, Found: 331.1928.

11-Allyloxy-*N*-methylaporphine (17). This compound was prepared from phenol **4b** as light brown oil (48%) following a similar procedure used for the preparation of compounds **10a-d**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.19 (d, 1H, *J* = 7.8 Hz), 7.20 (m, 2H), 7.06 (d, 1H, *J* = 7.5 Hz), 6.91 (m, 2H), 6.10 (m, 1H), 5.45 (dd, 1H, *J* = 17.4, 1.5 Hz), 5.27 (dd, 1H, *J* = 10.8, 1.5 Hz), 4.61 (m, 2H), 3.13 (m, 4H), 2.76 (dd, 1H, *J* = 16.2, 2.4 Hz), 2.55 (s, 3H), 2.53 (m, 2H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.6, 138.1, 134.6, 133.2, 132.3, 131.3, 127.8, 127.4, 126.4, 125.8, 123.3, 121.0, 117.1, 111.8, 69.3, 62.0, 52.9, 43.9, 35.1, 29.1; EI (MS) 291 (M^+); HRMS calcd for $C_{20}H_{21}NO_2$: 291.1623. Found: 291.1620.

10-Allyl-11-hydroxy-*N*-methylaporphine (18). This compound was prepared as pale solid (88%) from ether **17** following a similar procedure used for the preparation of compounds **11a,b**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.95 (d, 1H, *J* = 7.5 Hz), 7.25 (m, 1H), 7.07 (d, 1H, *J* = 7.5 Hz), 7.00 (d, 1H, *J* = 7.8 Hz), 6.82 (d, 1H, *J* = 7.8 Hz), 6.05 (m, 1H), 5.17 (m, 2H), 3.46 (d, 2H, *J* = 6.0 Hz), 3.08 (m, 4H), 2.75 (d, 1H, *J* = 16.5 Hz), 2.57 (s, 3H), 2.52 (m, 2H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 151.1, 136.5, 136.3, 135.0, 133.3, 131.4, 129.0, 127.5, 126.4, 125.2, 124.4, 121.7, 120.3, 116.5, 62.2, 52.8, 43.9, 35.4, 34.8, 28.9; EI (MS) 291 (M^+); HRMS calcd for $C_{20}H_{21}NO_2$: 291.1623. Found: 291.1607.

***N*-Methyl-2'-methyl-2',3'-dihydrofuro[*m*]aporphine (19).** This compound was prepared as yellow solid in 91% yield from phenol **18** following a similar procedure used for the preparation of compounds **12a-c**. This compound was purified by preparative TLC with MeCN/TFA (0.05%) as the eluents. ^{1}H-NMR (300 MHz,

$CDC1_3$) δ 8.09 (dd, 1H, *J* = 8.1, 9.0 Hz), 7.23 (t, 1H, *J* = 7.8 Hz), 7.02 (t, 2H, *J* = 7.5 Hz), 6.76 (d, 1H, *J* = 7.5 Hz), 5.09 and 4.96 (m, 1H, 1:1), 3.20 (m, 5H), 2.78 (m, 4H), 2.51 (s, 3H), 1.59 and 1.44 (d, 3H, *J* = 6.3 Hz, 1:1); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 156.3 (2), 135.6, 133.6, 132.6, 131.3 (2), 127.3, 126.7 (2), 126.3, 125.1 (2), 123.3 (2), 119.9, 117.4, 80.0 (2), 62.2, 53.3, 43.9, 36.6 (2), 34.3, 29.0, 21.9 (2); EI (MS) 291 (M^+). Anal. ($C_{20}H_{21}NO.0.4TFA.1.5H_2O$) Calcd: C, 68.63; H, 6.76; N, 3.85; Found: C, 68.81; H, 7.04; N, 3.44.

Chiral HPLC resolution of *N*-methyl-2'-methyl-2',3'-dihydrofuro[*m*]aporphine 19 (*cis/trans*-19). The chiral HPLC of *cis/trans*-**19** was carried out on a Chiracel OD column (25×0.46 cm, Daicel, Japan) under the following conditions: flow rate 1.0 ml/ min, hexane/isopropanol/diethylamine (99/1/0.1) as the eluent. The retention times were 10.1 and 12.3 min.

***trans*-19:** MS (EI) 291 (M^+); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.13 (d, 1H, *J* = 7.8 Hz), 7.26 (t, 1H, *J* = 7.8 Hz), 7.04 (t, 2H, *J* = 7.8 Hz), 6.76 (dd, 1H, *J* = 7.5, 0.9 Hz), 4.97 (m, 1H), 3.20 (m, 5H), 2.80 (m, 1H), 2.64 (m, 3H), 2.58 (s, 3H), 1.62 (d, 3H, *J* = 6.3 Hz); $[\alpha]_D^{20}$ −30° (*c* 0.071, EtOH, 20 °C).

***cis*-19:** MS (EI) 291 (M^+); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.16 (d, 1H, *J* = 7.5 Hz), 7.24 (t, 1H, *J* = 7.8 Hz), 7.02 (t, 2H, *J* = 7.8 Hz), 6.76 (dd, 1H, *J* = 7.5, 1.2 Hz), 5.09 (m, 1H), 3.38 (m, 1H), 3.14 (m, 4H), 2.78 (m, 3H), 2.58 (s, 3H), 2.56 (m, 1H), 1.44 (d, 3H, *J* = 6.3 Hz); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 156.3, 135.6, 133.7, 132.6, 131.3, 127.3, 126.5, 126.3, 125.1, 123.4, 119.9, 117.4, 79.6, 62.2, 53.3, 44.0, 36.6, 34.4, 29.1, 22.0; $[\alpha]_D^{20}$ −109° (*c* 0.075, EtOH, 20 °C).

11-Propargyloxy-*N*-methylaporphine (20). This compound was prepared from phenol **4b** as brown oil (85%) following a similar procedure used for the preparation of compounds **10a-d**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.13 (d, 1H, *J* = 8.1 Hz), 7.22 (m, 2H), 7.06 (dd, 2H, *J* = 9.3, 8.4 Hz), 6.96 (d, 1H, *J* = 7.2 Hz), 4.74 (m, 2H), 3.13 (m, 4H), 2.28 (m, 2H), 2.58 (s, 3H), 2.52 (m, 2H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 154.5, 138.2, 134.7, 132.4, 130.9, 127.7, 127.5, 126.3, 125.9, 123.7, 121.8, 112.4, 78.6, 75.4, 61.9, 56.2, 52.9, 43.9, 35.0, 29.1; EI (MS) 289 (M^+); HRMS calcd for $C_{20}H_{19}NO_2$: 289.1467. Found: 289.1448.

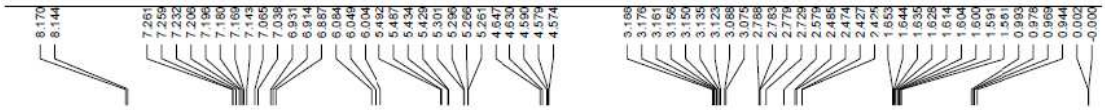
***N*-Methyl-2'-methyl-furo[*m*]aporphine (21).** This compound was prepared as brown oil (29%) from ether **20** following a similar procedure used for the preparation of compounds **16a,b**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 8.33 (d, 1H, *J* = 8.1 Hz), 7.33 (m, 2H), 7.11 (d, 2H, *J* = 7.8 Hz), 6.39 (d, 1H, *J* = 1.2 Hz), 3.29 (m, 3H), 3.10 (m, 1H), 2.78 (t, 1H, *J* = 14.7 Hz), 2.57 (s, 3H), 2.55 (m, 2H), 2.52 (s, 3H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 155.0, 151.4, 133.9, 133.1, 130.8, 130.6, 129.0, 127.9, 126.5, 125.2, 123.0, 118.8, 118.5, 102.6, 62.2, 53.2, 44.0, 34.1, 29.1, 14.2; EI (MS) 289 (M^+); HRMS calcd for $C_{20}H_{19}NO$: 289.1467. Found: 289.1441.

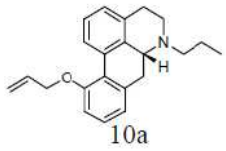
2-Methoxy-11-allyloxy-*N*-methylaporphine (22). This compound was prepared from phenol **4c** as brown oil (34%) following a similar procedure used for the preparation of compounds **10a-d**. ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.85 (d, 1H, *J* = 2.4 Hz), 7.17 (t, 1H, *J* = 7.5 Hz), 6.91 (d, 1H, *J* = 2.1 Hz), 6.89 (d, 1H, *J* = 3.6 Hz), 6.62 (d, 1H, *J* = 2.7 Hz), 6.11 (m, 1H), 5.47 (dd, 1H, *J* = 1.5, 17.1 Hz), 5.29 (dd, 1H, *J* = 1.2, 10.5 Hz), 4.61 (m, 2H), 3.81 (s, 3H), 3.10 (m, 4H), 2.75 (m, 1H), 2.54 (s, 3H),

2.51 (m, 2H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 157.5, 155.6, 138.5, 133.5, 133.2, 132.4, 127.9, 127.3, 123.3, 121.1, 117.6, 112.6, 112.4, 111.9, 69.5, 61.7, 55.2, 53.1, 43.9, 35.5, 29.3; EI (MS) 321 (M^+); HRMS calcd for $C_{21}H_{23}NO_2$: 321.1729. Found: 321.1716.

2-Methoxy-10-allyl-11-hydroxy-*N*-methylaporphine (23). This compound was prepared as brown solid (59%) from ehter **22** following a similar procedure used for the preparation of compounds **11a,b**. pale solid (47%); ^{1}H-NMR (300 MHz, $CDC1_3$) δ 7.58 (d, 1H, *J* = 2.4 Hz), 6.99 (d, 1H, *J* = 7.5 Hz), 6.82 (d, 1H, *J* = 7.5 Hz), 6.60 (d, 1H, *J* = 2.1 Hz), 6.05 (m, 1H), 5.19 (m, 2H), 3.81 (s, 3H), 3.45 (d, 2H, *J* = 6.3 Hz), 3.19 (m, 1H), 3.05 (m, 3H), 2.71 (d, 1H, *J* = 16.5 Hz), 2.52 (s, 3H), 2.50 (m, 2H); ^{13}C-NMR (100 MHz, $CDC1_3$) δ 157.9, 151.1, 136.6, 136.4, 134.5, 132.6, 129.1, 127.6, 125.1, 121.4, 120.4, 116.6, 111.9, 111.1, 61.9, 55.2, 53.0, 43.9, 35.4, 35.2, 29.3; EI (MS) 321 (M^+); HRMS calcd for $C_{21}H_{23}NO_2$: 321.1729. Found: 321.1713.

***N*-Methyl-2-hydroxy-2'-methyl-2',3'-dihydrofuro[*m*]aporphine (24).** This compound was prepared as yellow solid (76%) from phenol **23** following a similar procedure used for the preparation of compounds **12a-c**. ^{1}H-NMR (300 MHz, CD_3OD) δ 7.79 (dd, 1H, *J* = 5.7 Hz, 2.4 Hz), 7.08 (m, 1H), 6.84 (d, 1H, *J* = 6.6 Hz), 6.58 (d, 1H, *J* = 1.2 Hz), 5.15 (m, 1H), 4.24 (m, 1H), 3.78 (m, 1H), 4.45 (m, 1H), 3.43 (m, 3H), 3.16 (s, 3H), 3.05 (m, 1H), 2.84 (m, 2H), 1.58 and 1.40 (d, 3H, *J* = 6.0 Hz, 1:1); ^{13}C-NMR (100 MHz, CD_3OD) δ 159.0, 158.1, 134.8, 133.6 (2), 132.5, 130.0 (2), 126.1, 122.1, 119.9, 117.8 (2), 115.7, 114.9, 82.2 (2), 64.2, 54.4, 42.4, 37.9 (2), 33.2, 27.7, 22.6; EI (MS) 307 (M^+); HRMS calcd for $C_{20}H_{21}NO_2$: 307.1572. Found: 307.1561.





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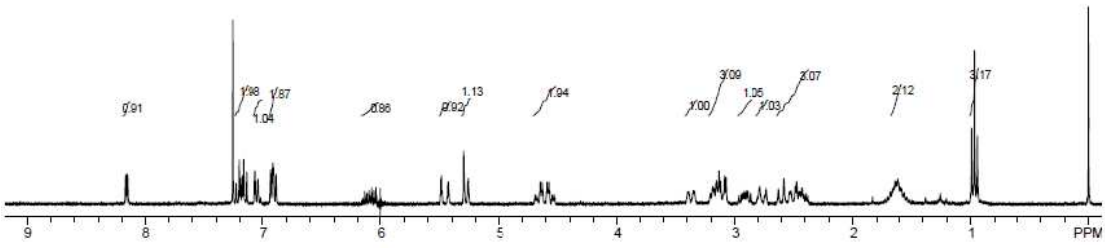
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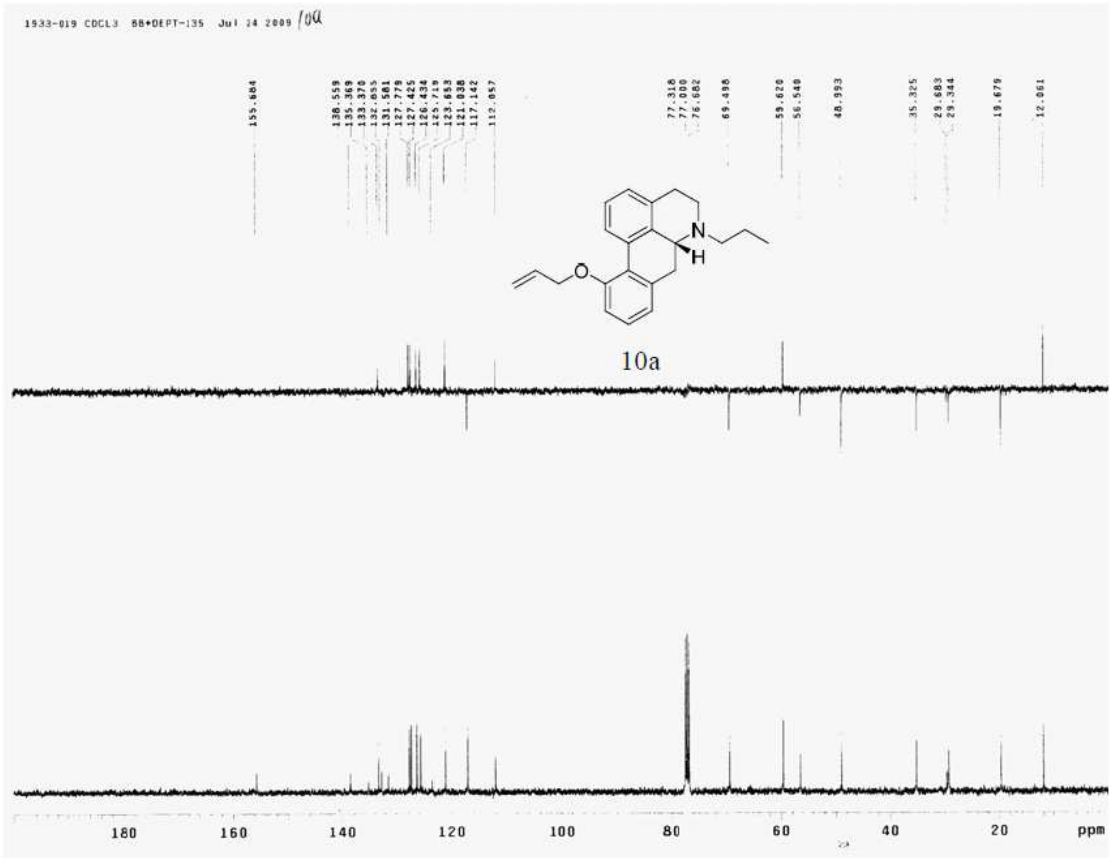
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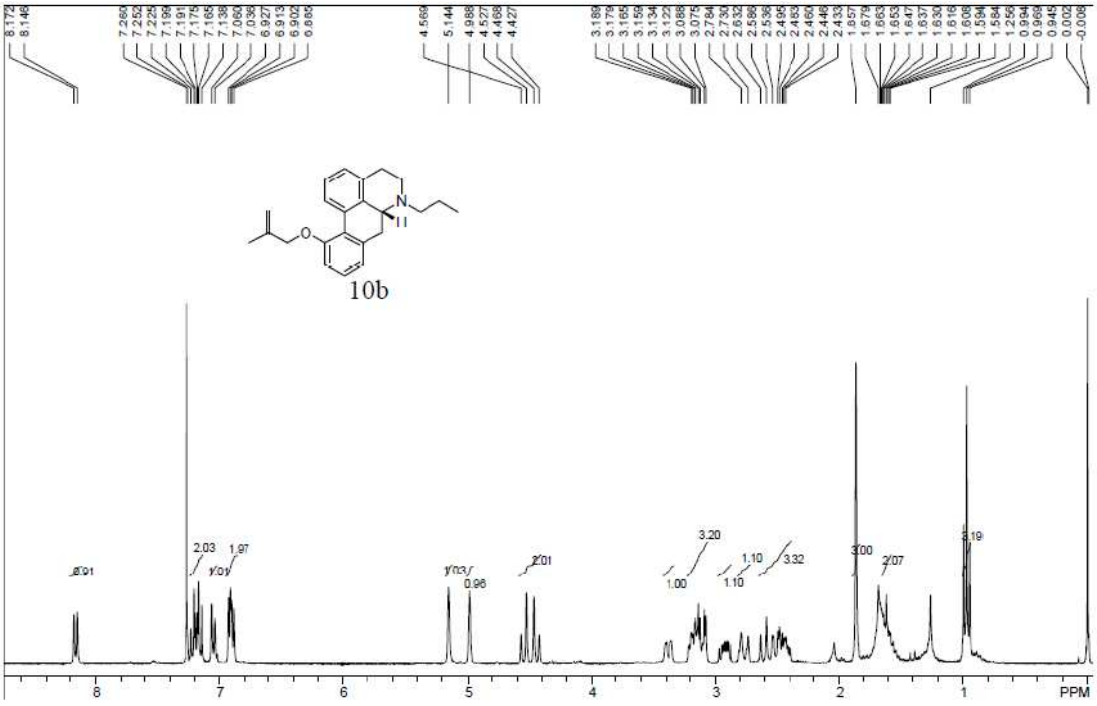
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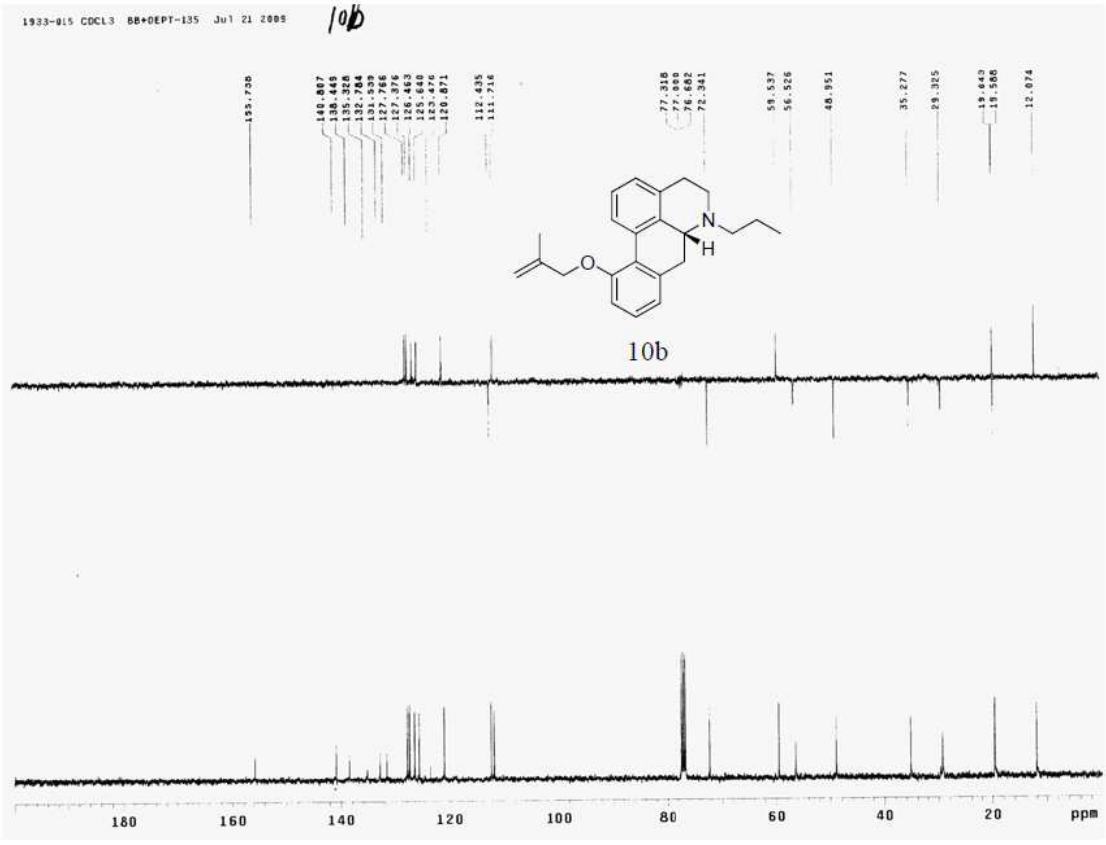
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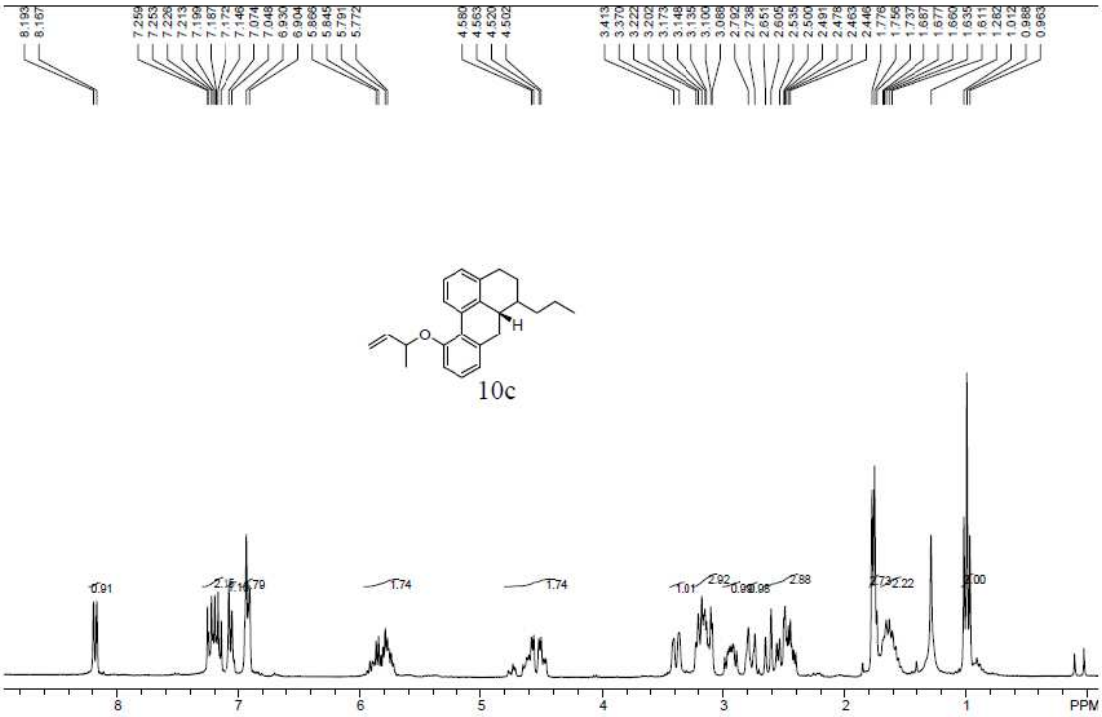
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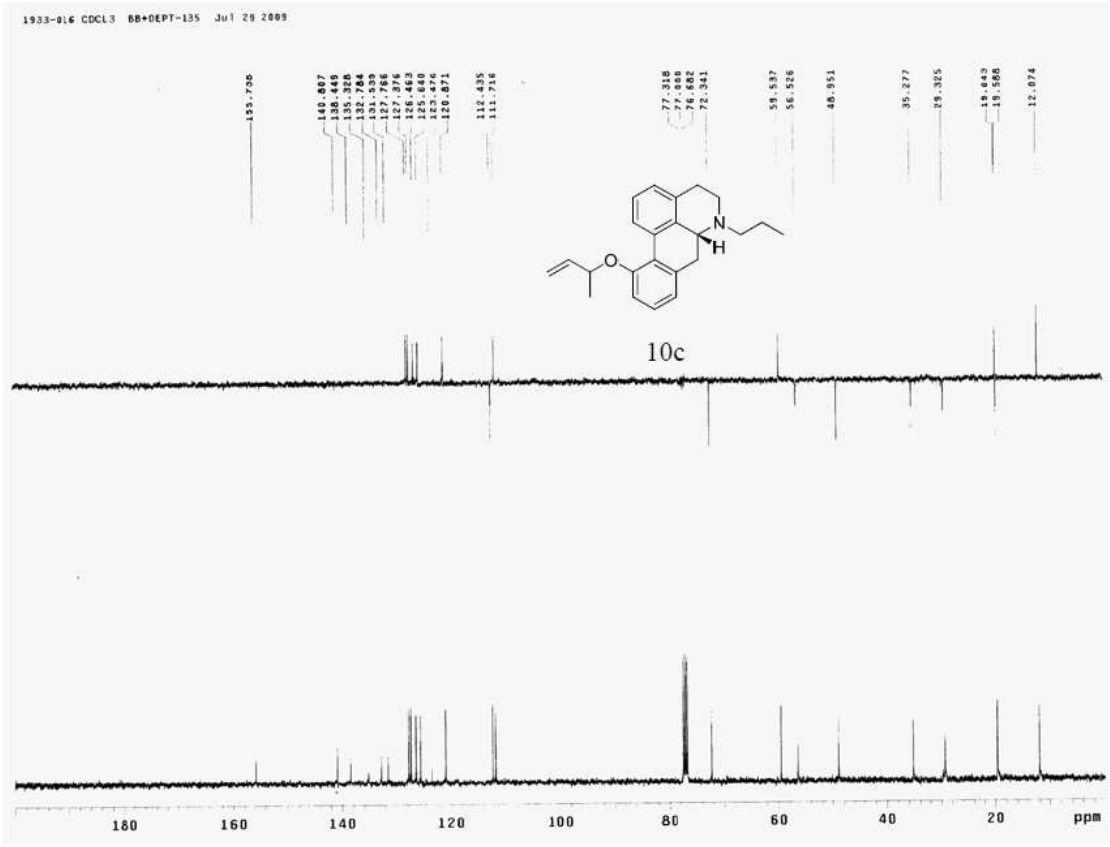
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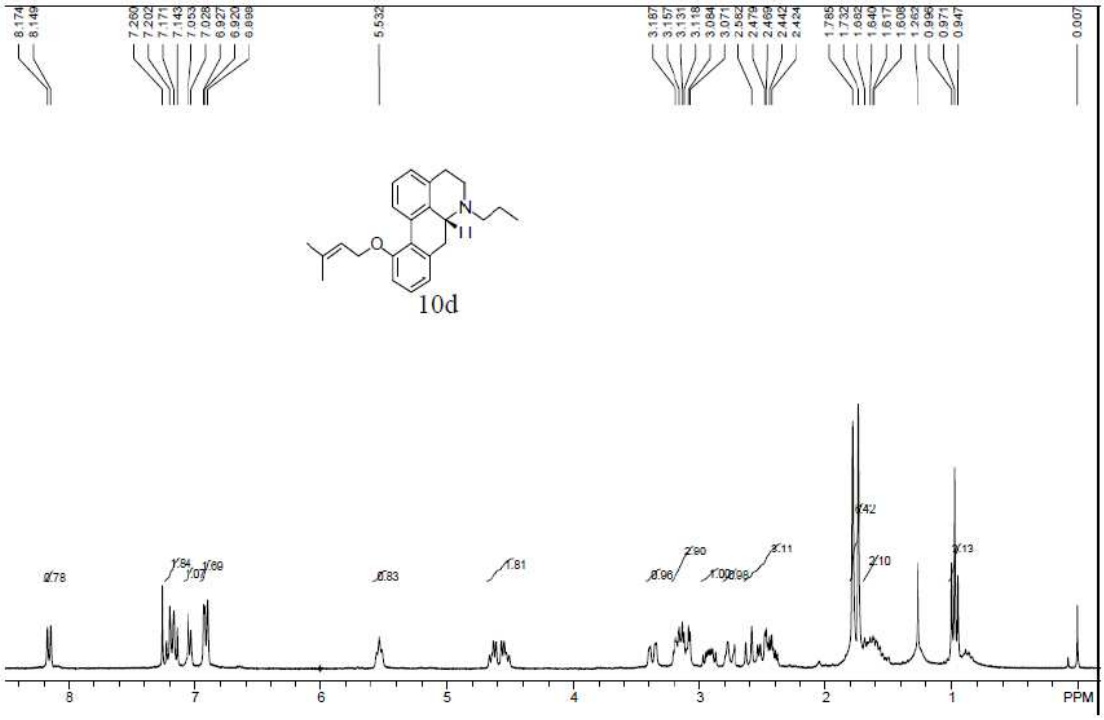
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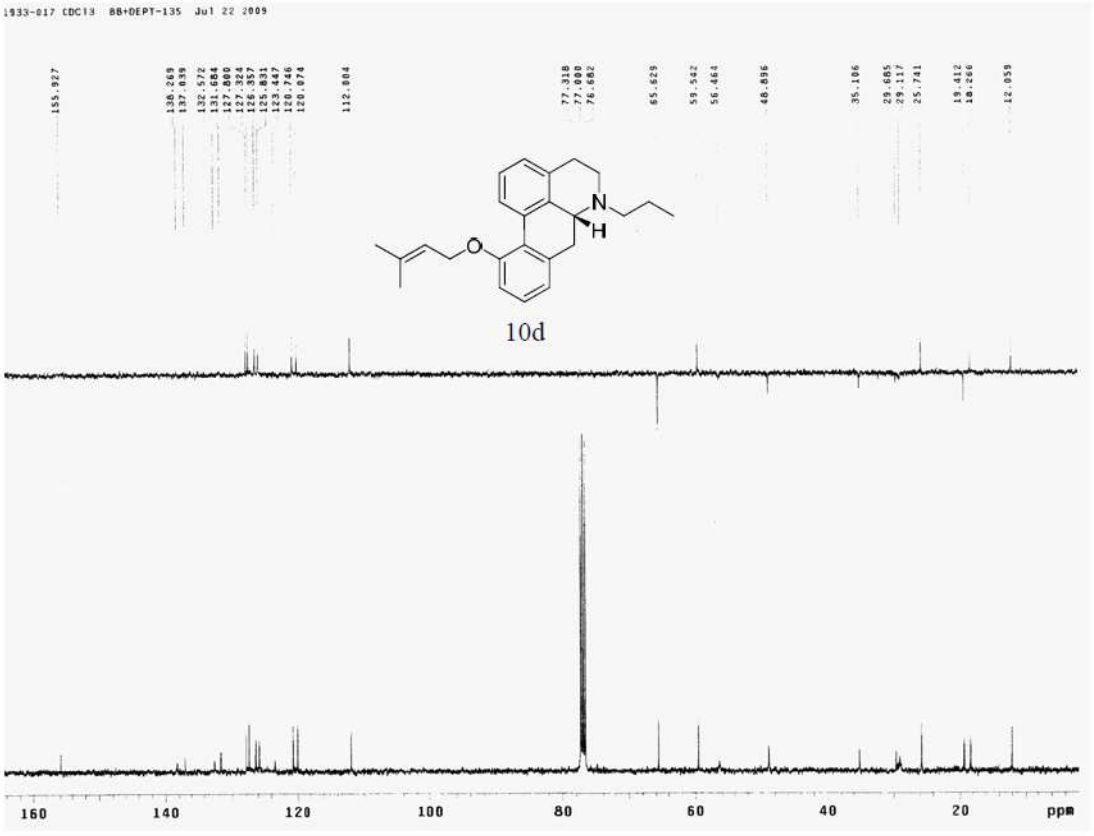
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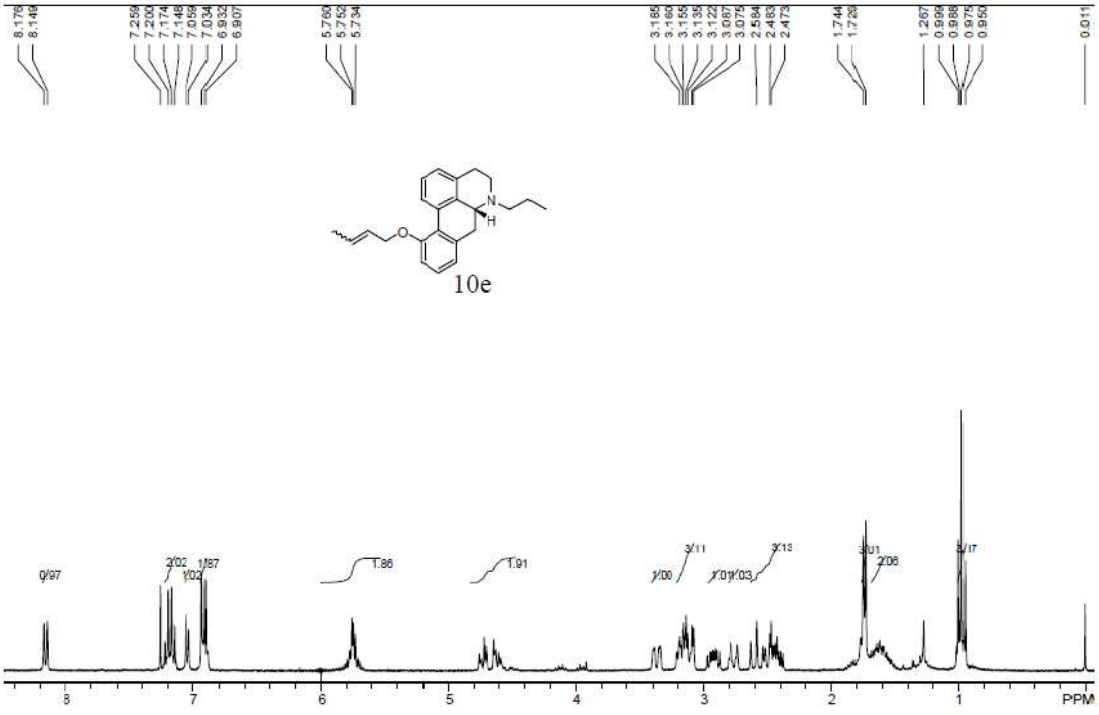
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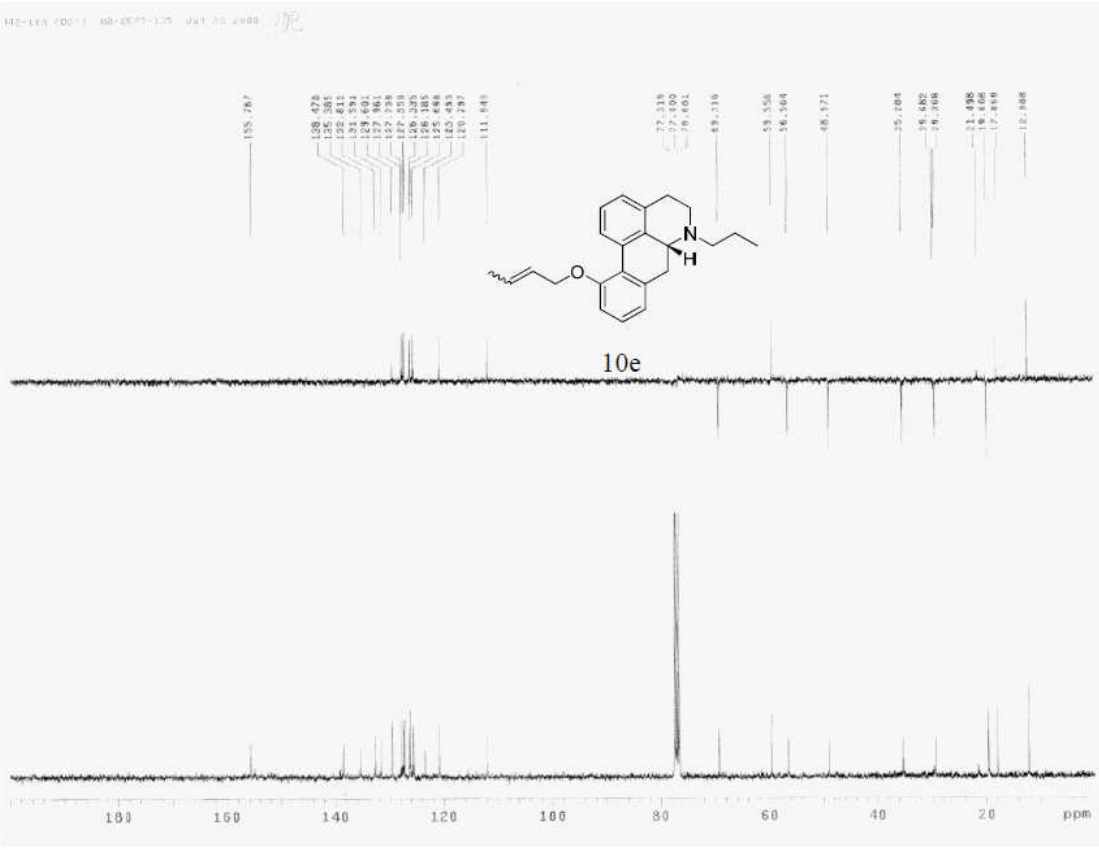
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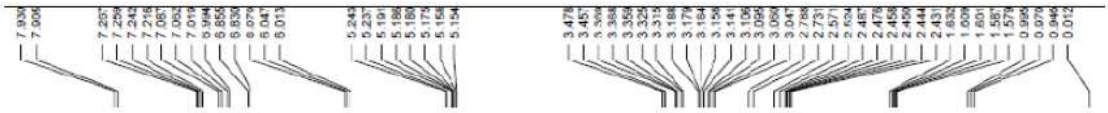

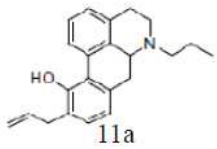
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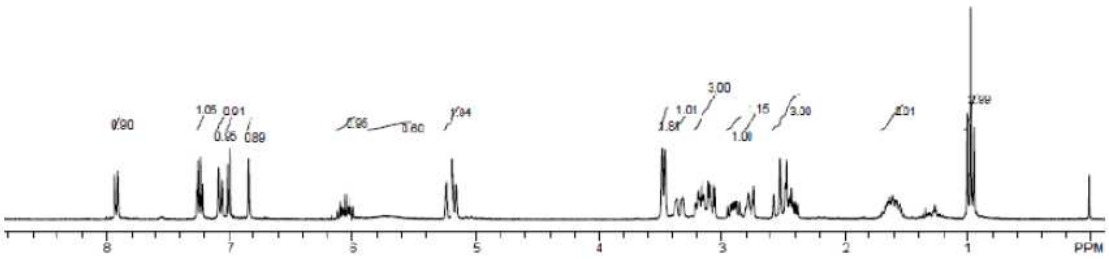
11a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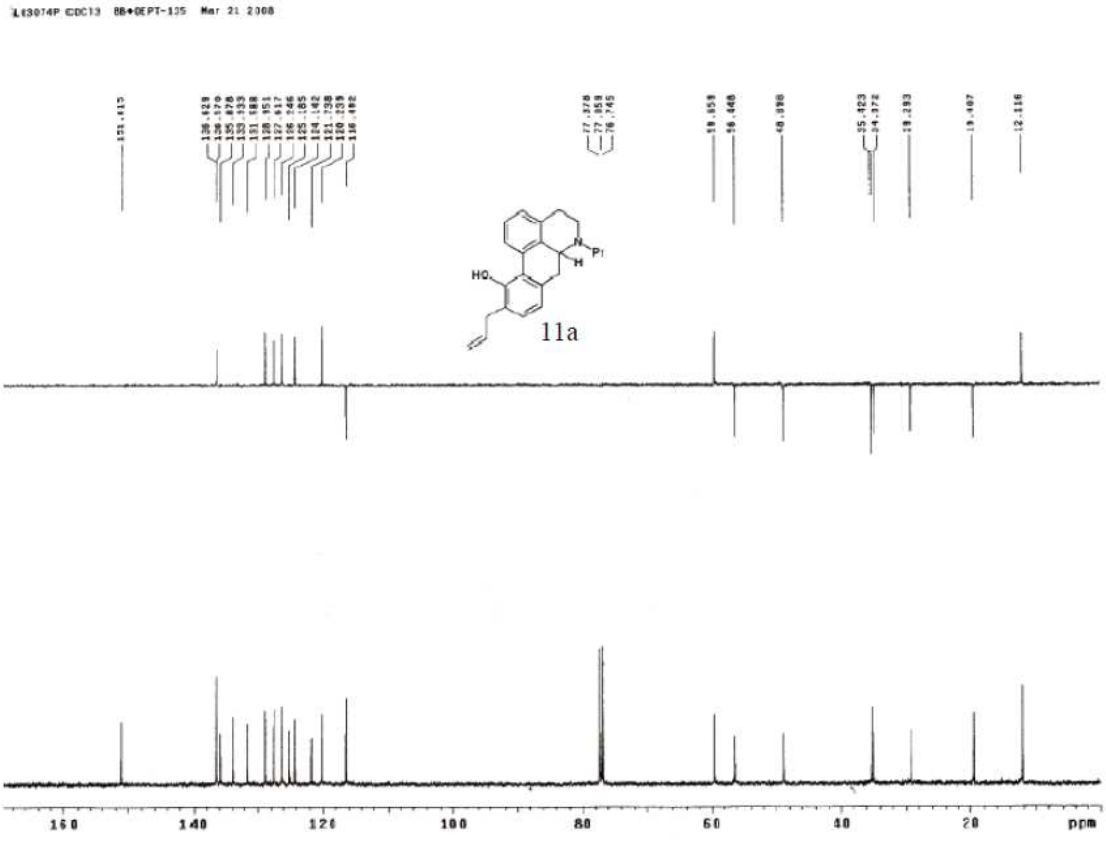
2.96
3.60
1.04
3.00
1.01
1.00
1.15
3.00
2.01
2.99
8
7
6
5
4
3
2
1
PPM


HO
N
H
11a
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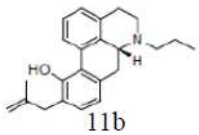
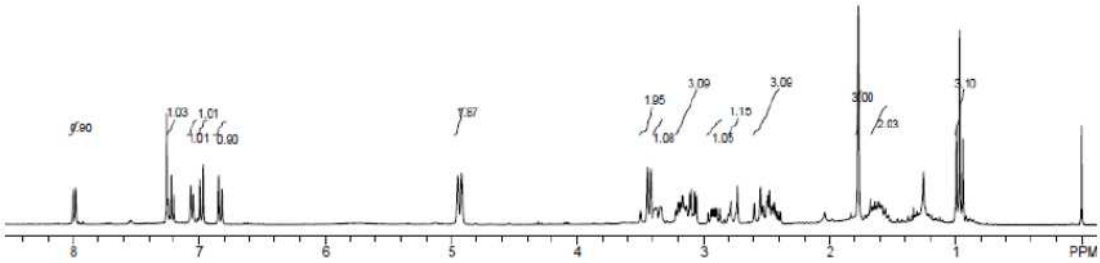
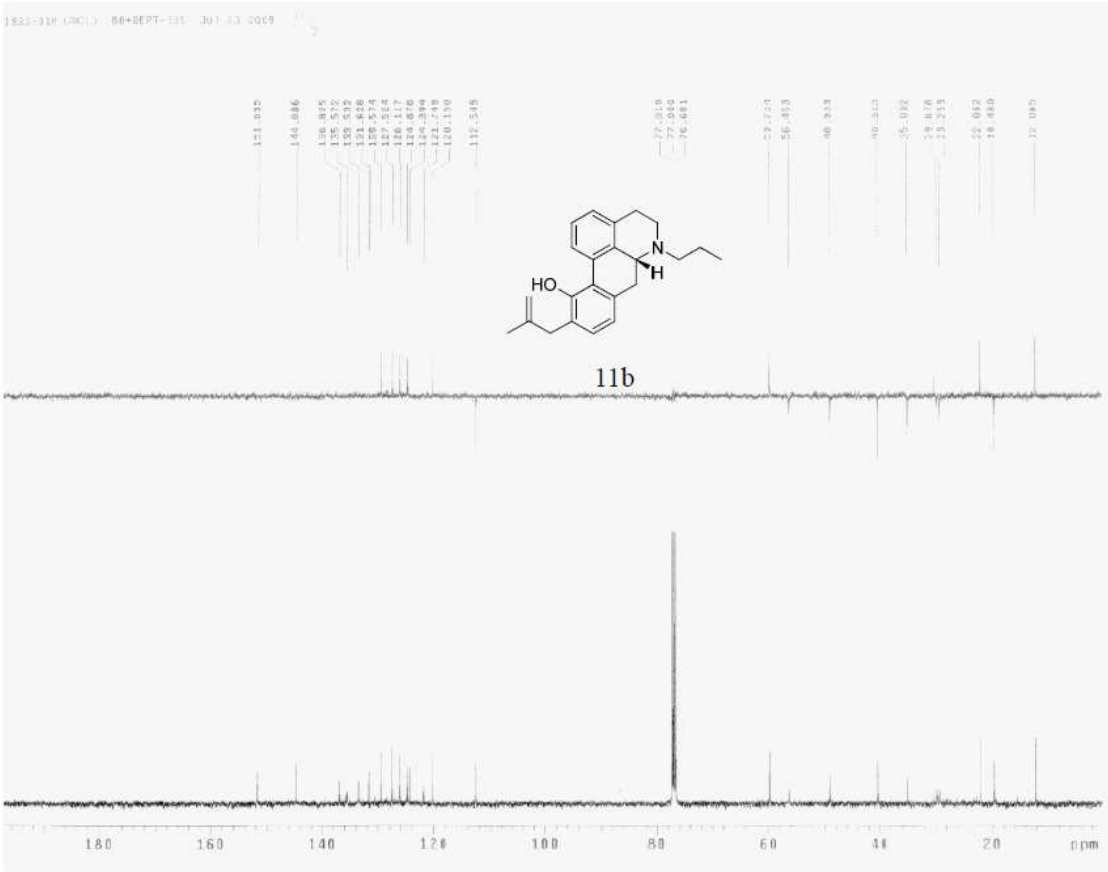
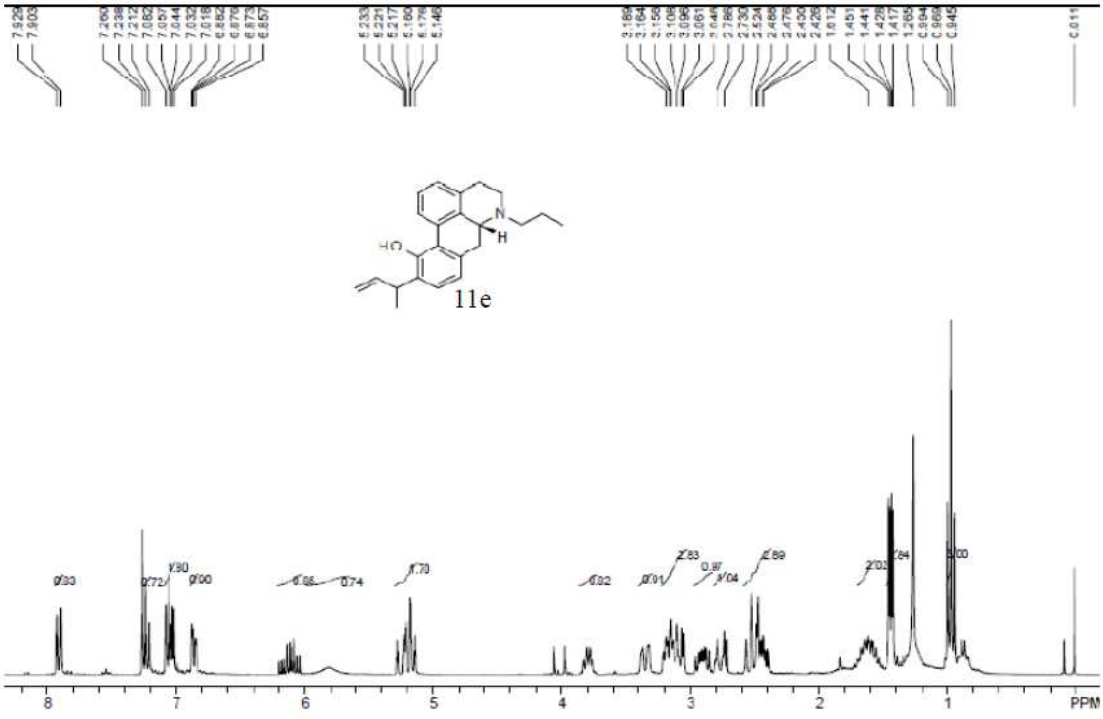
140
120
100
80
60
40
20
ppm

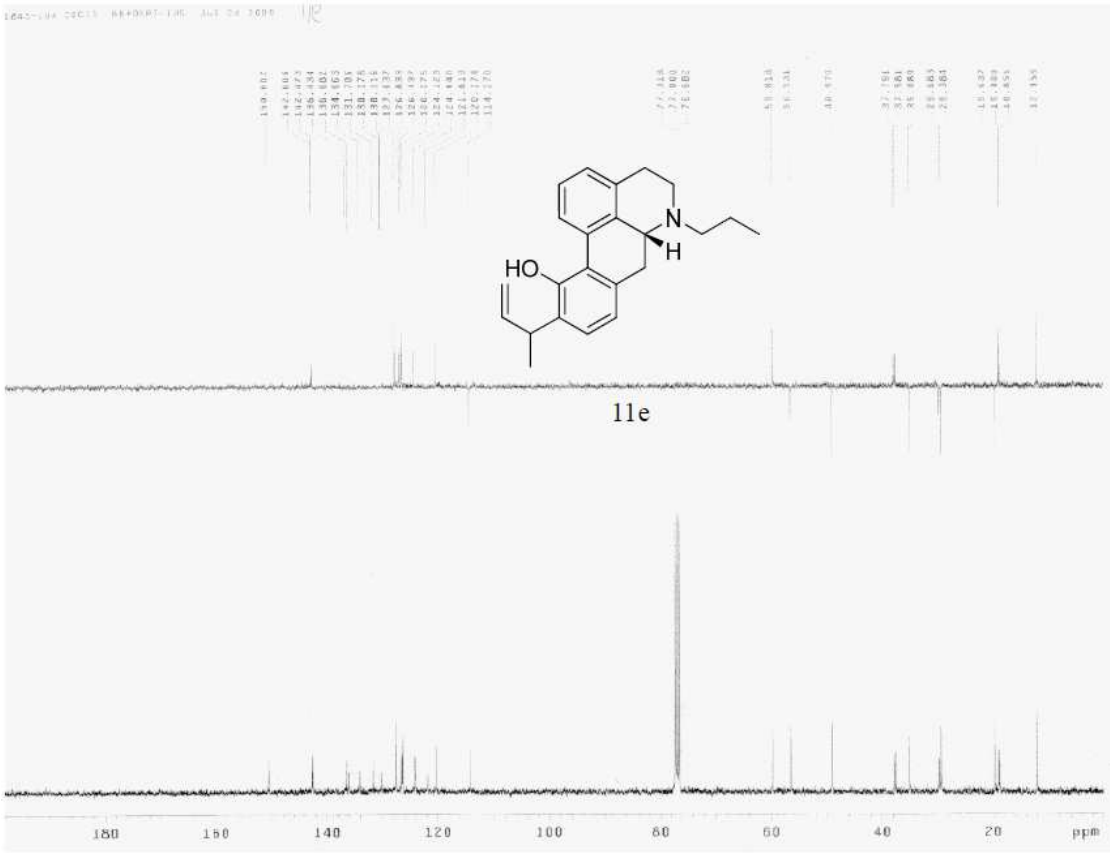


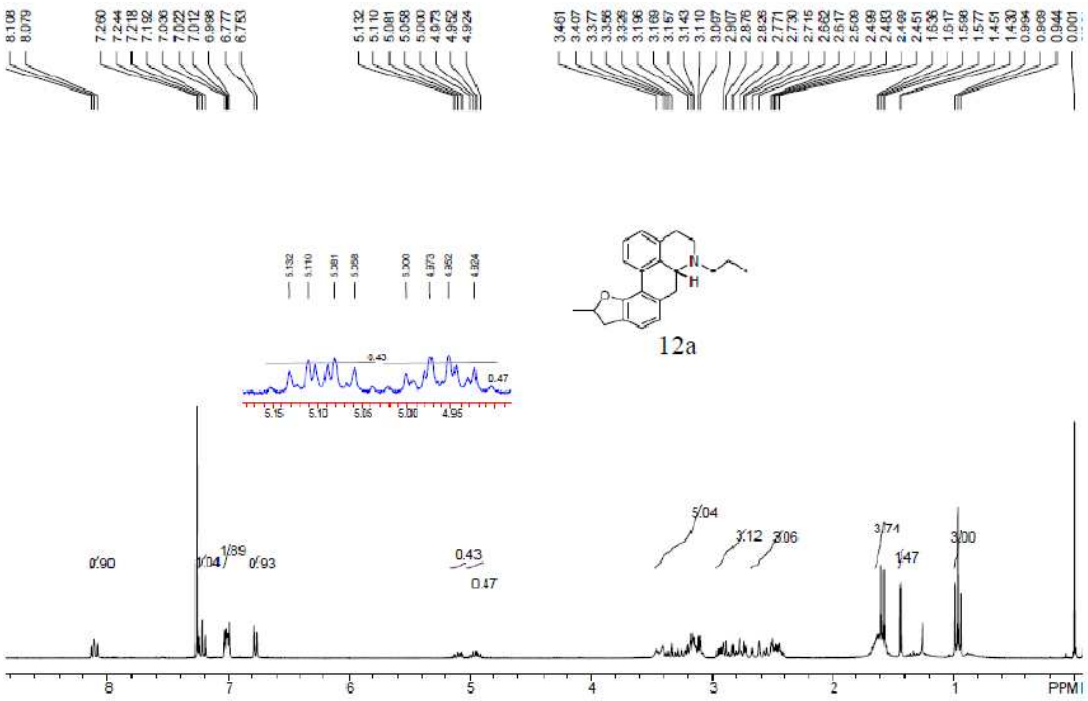
11b

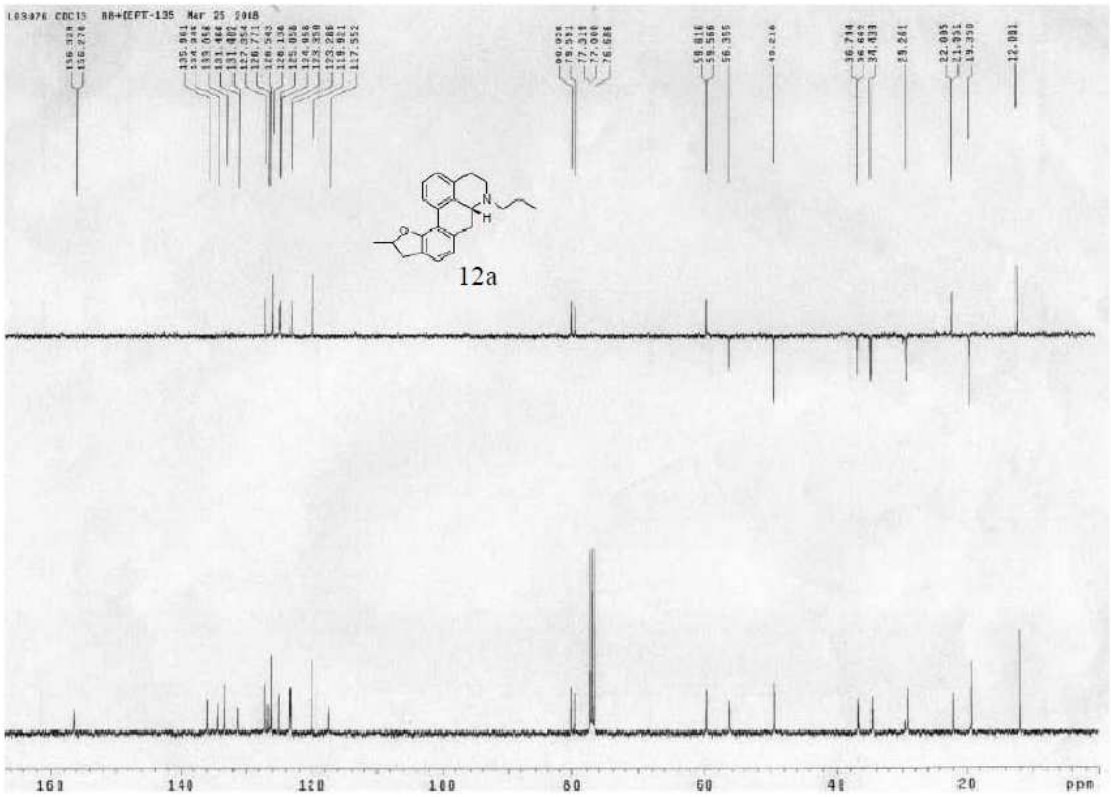

1.03
1.01
1.01
0.90
1.87
1.95
3.09
1.08
1.15
1.05
3.09
3.00
2.03
3.10
8
7
6
5
4
3
2
1
PPM

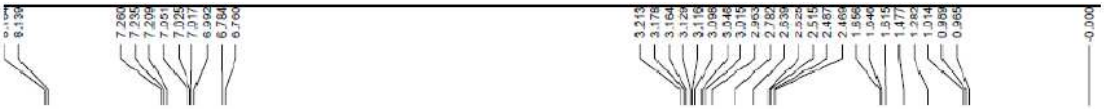

HO
N
H
11b
180
160
140
120
100
80
60
40
20
ppm

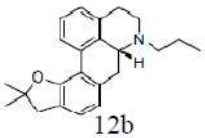

HO
N
H
11e
PPM


HO
N
H
11e
ppm

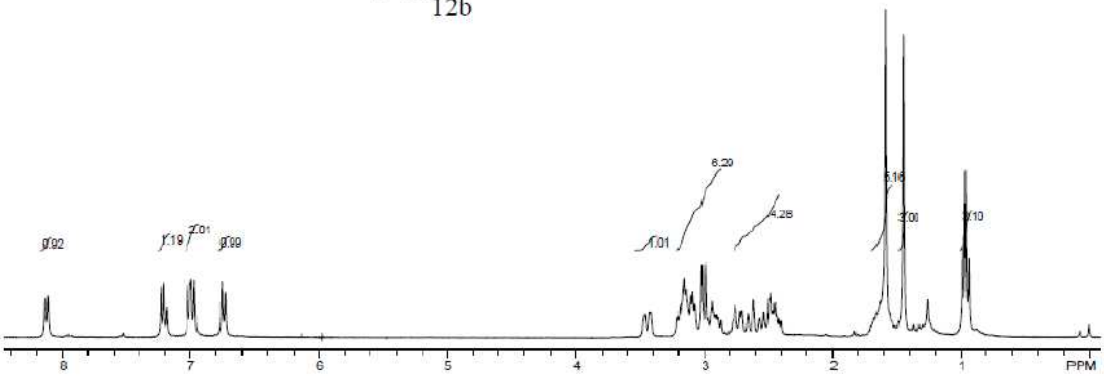

12a
0.90
1.04
1.89
0.93
0.43
0.47
5.04
3.12
3.06
3.74
1.47
3.00
PPM

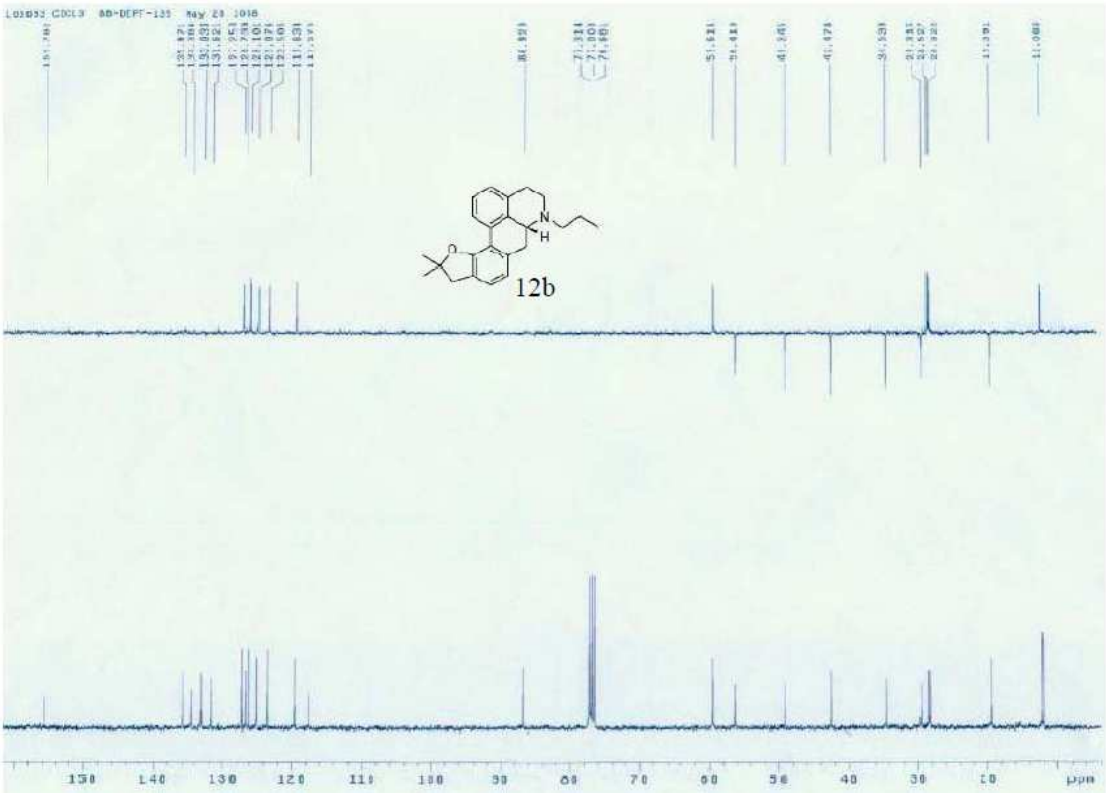

12a
ppm



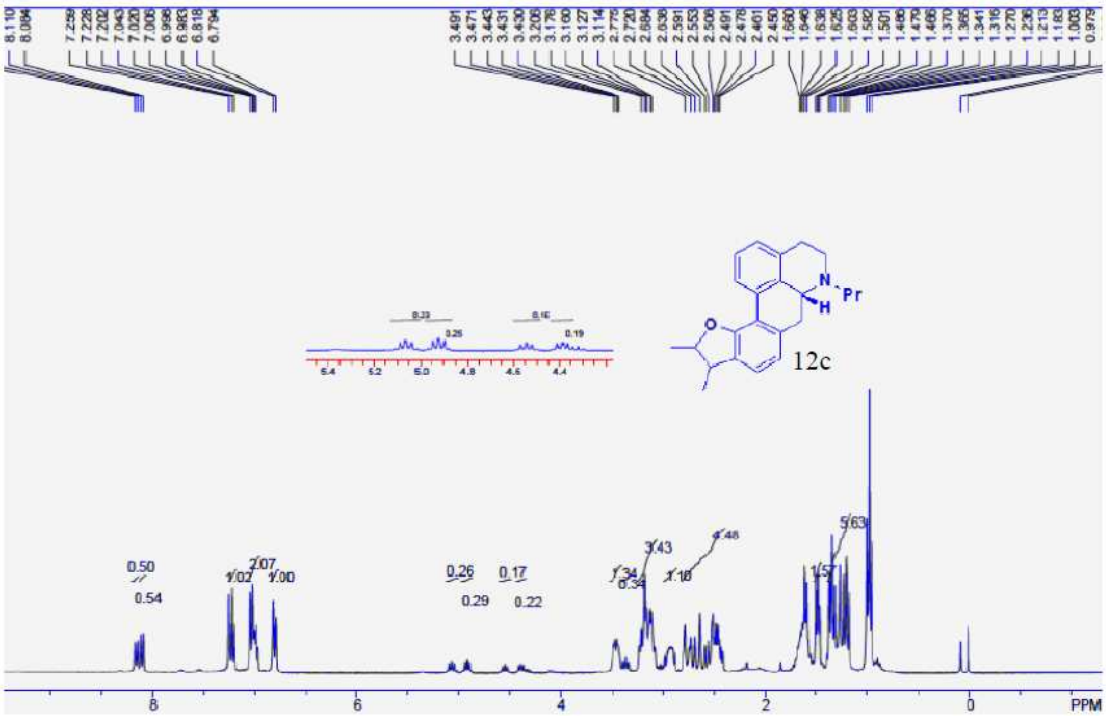


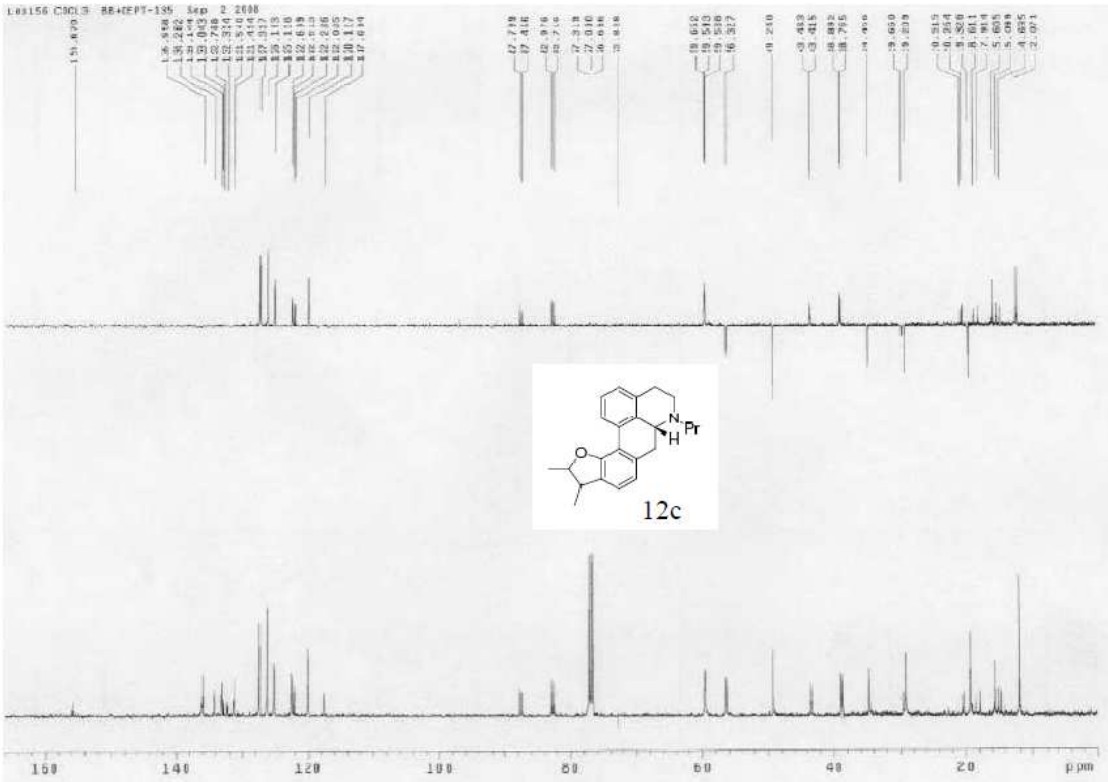
12b

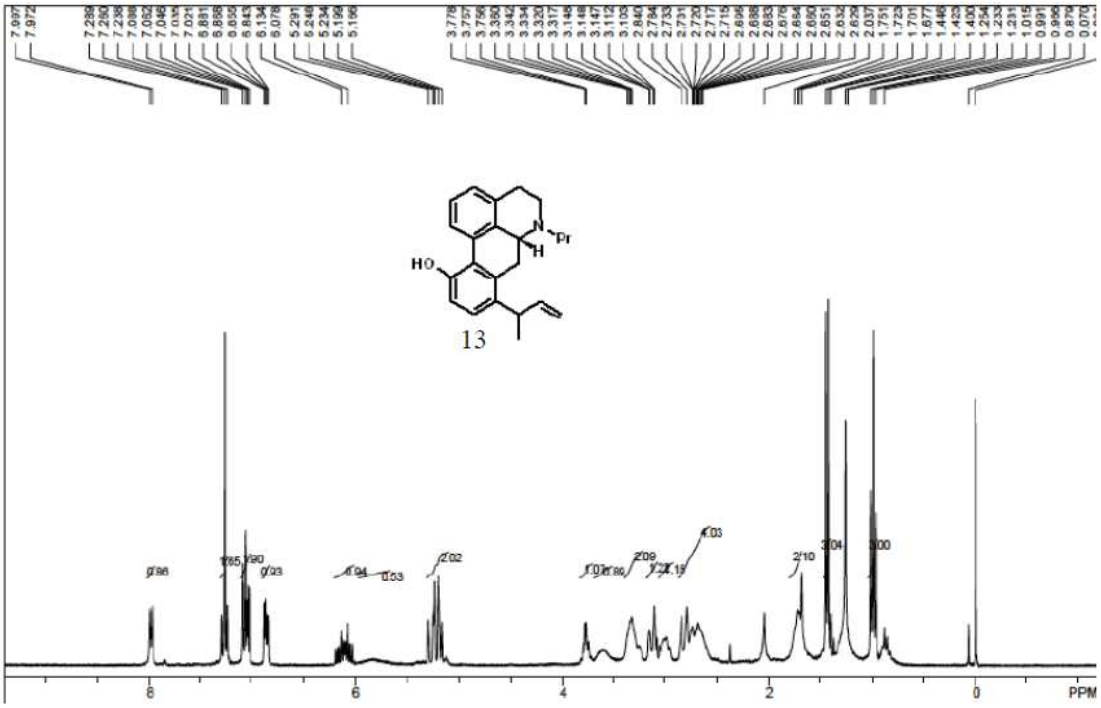


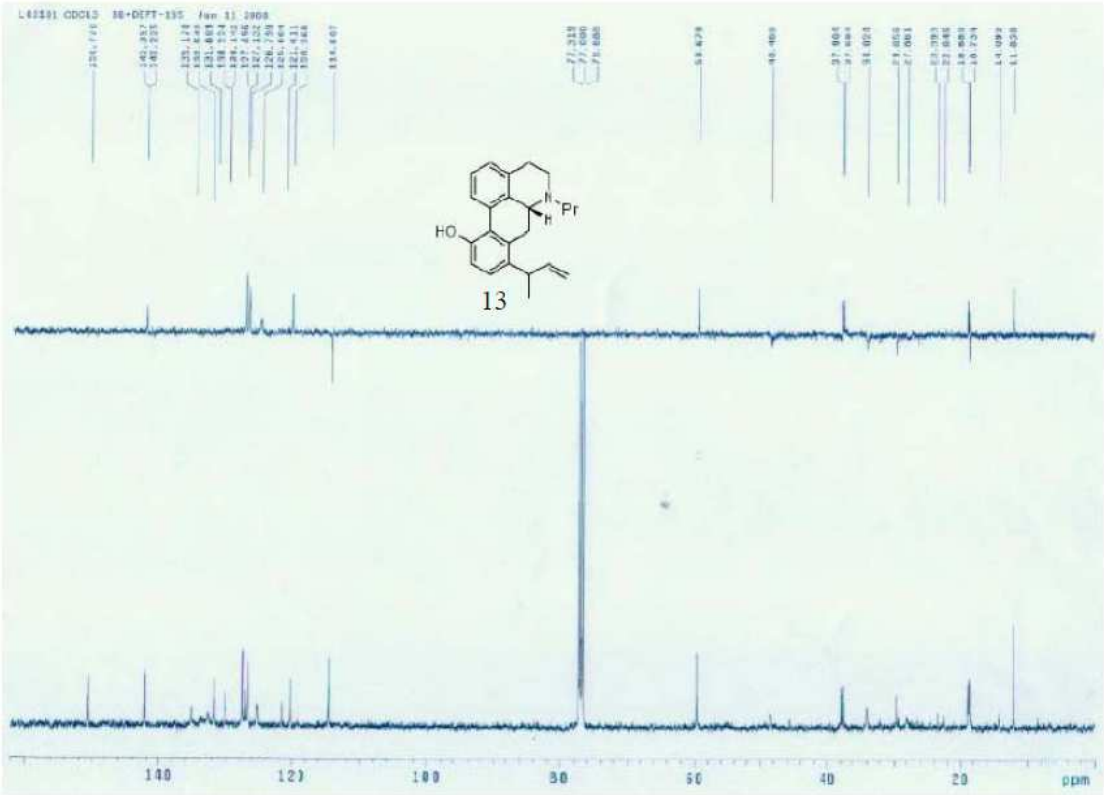


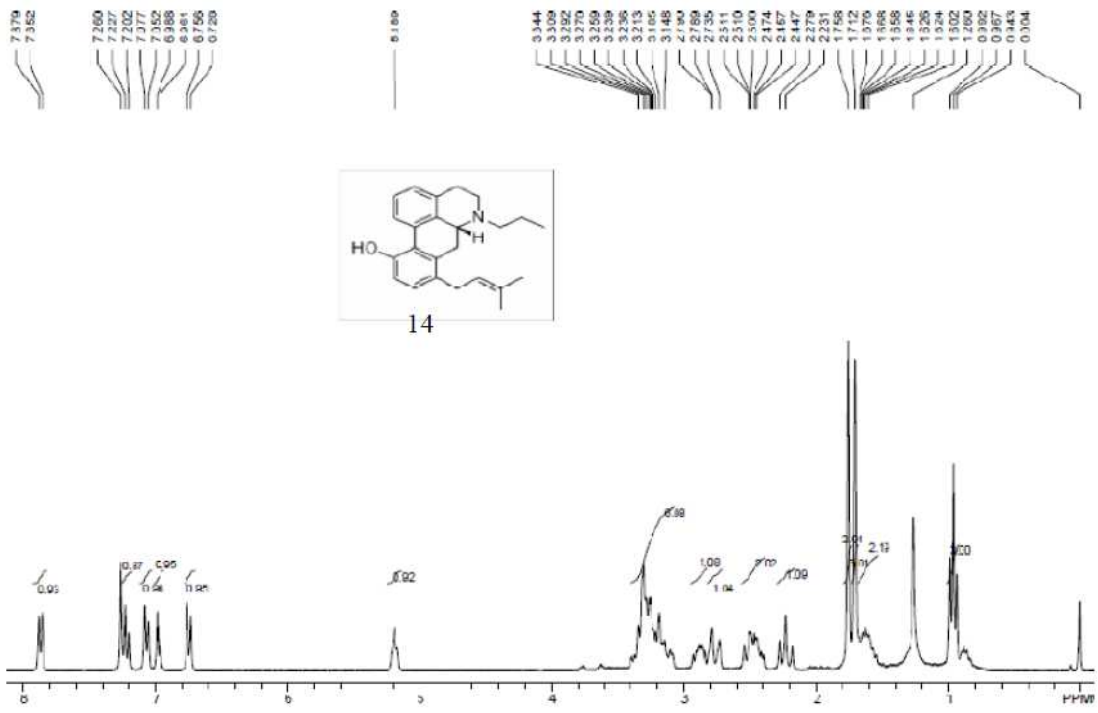
12b

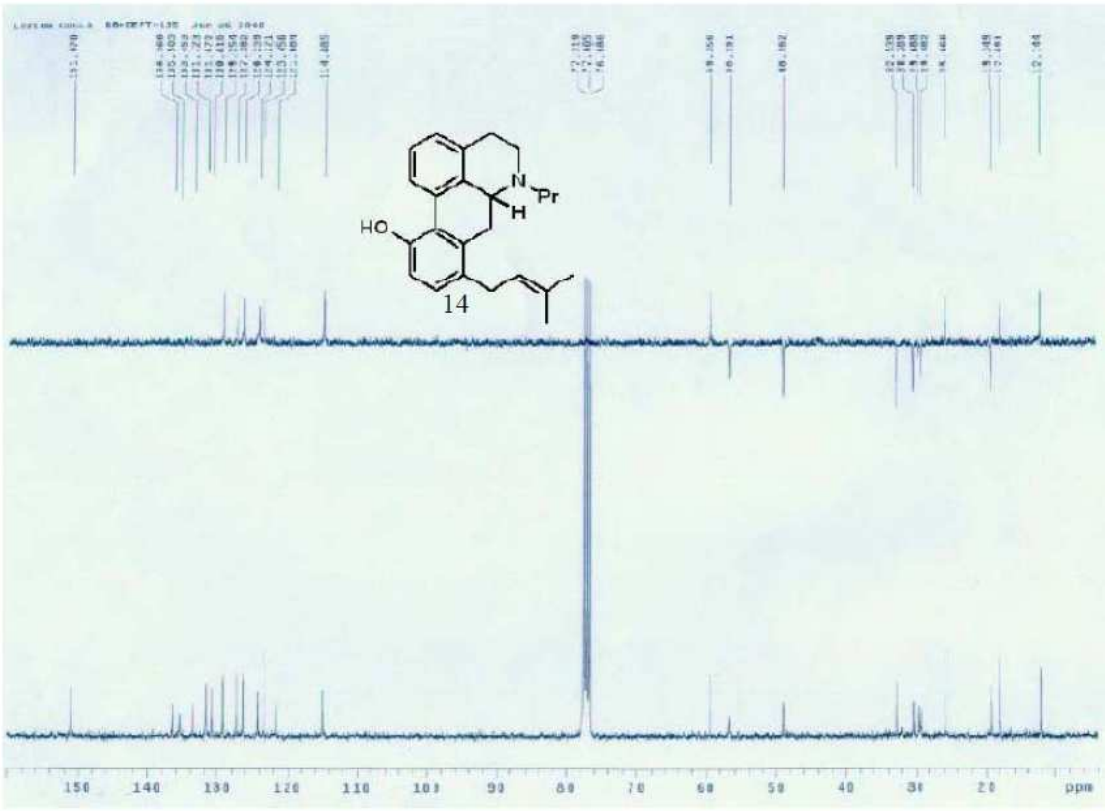

12c
0.50
0.54
2.07
1.02
1.00
0.26
0.29
0.17
0.22
3.43
1.34
0.34
1.18
1.57
5.63
8
6
4
2
0
PPM

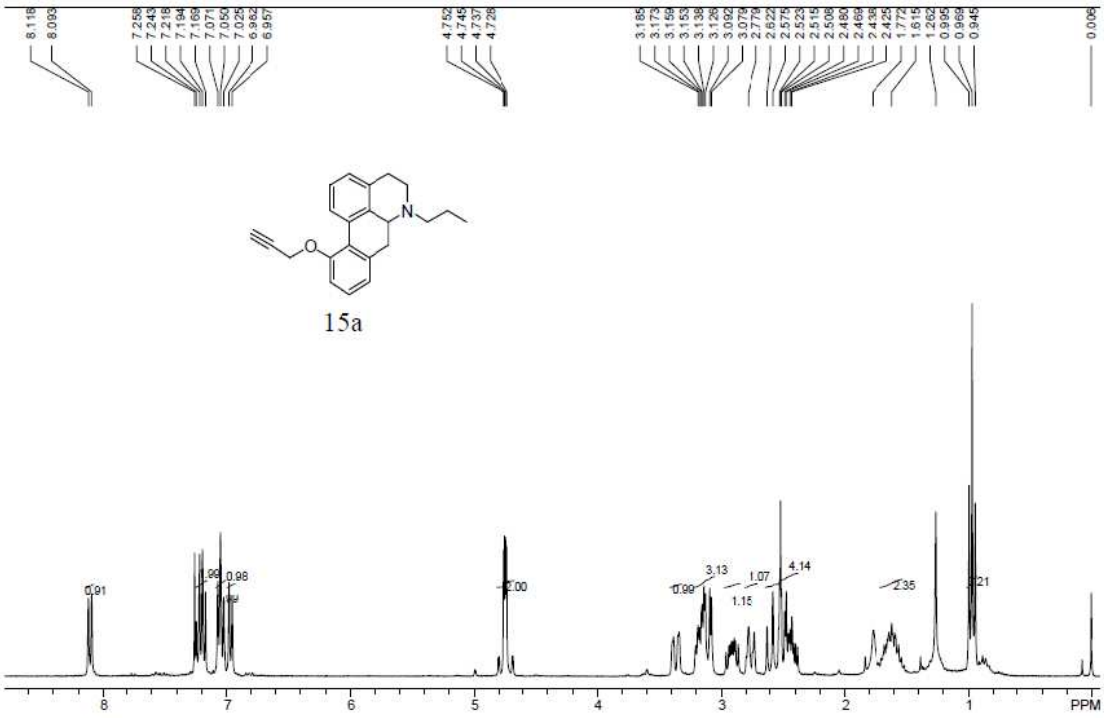

12c
160
140
120
100
80
60
40
20
ppm

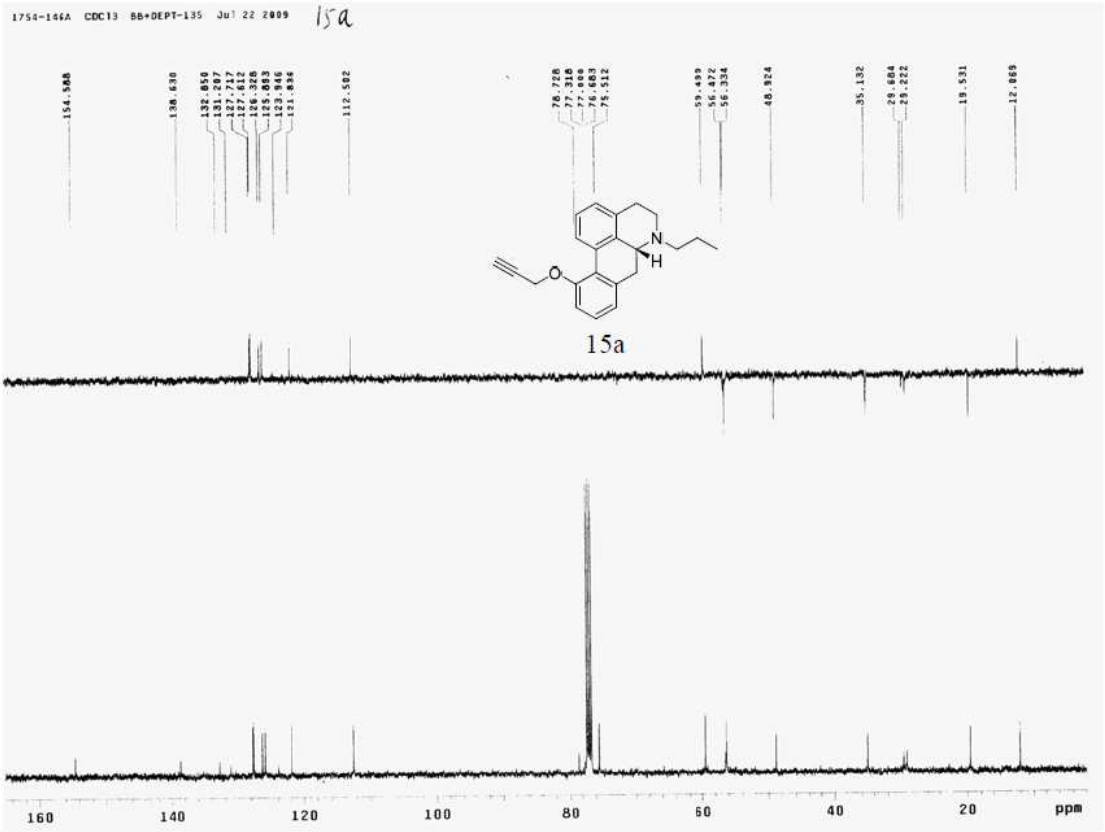

HO
N
Pr
H
13
PPM

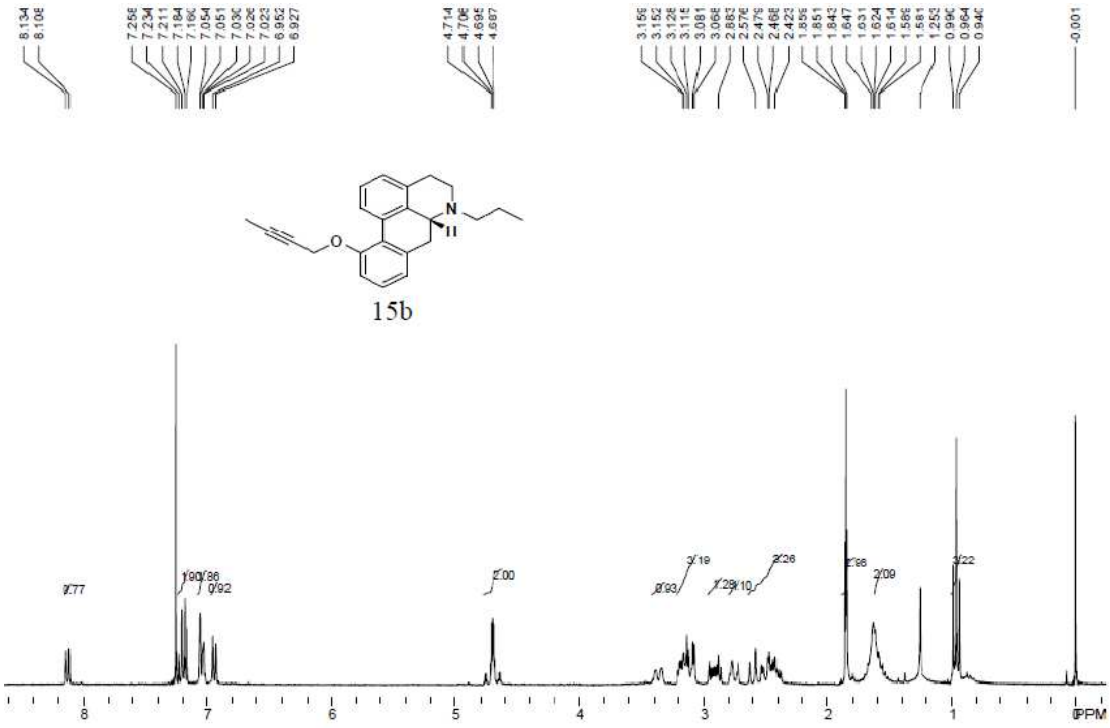

HO
N
Pr
H
13
ppm


HO
N
H
14
PPM

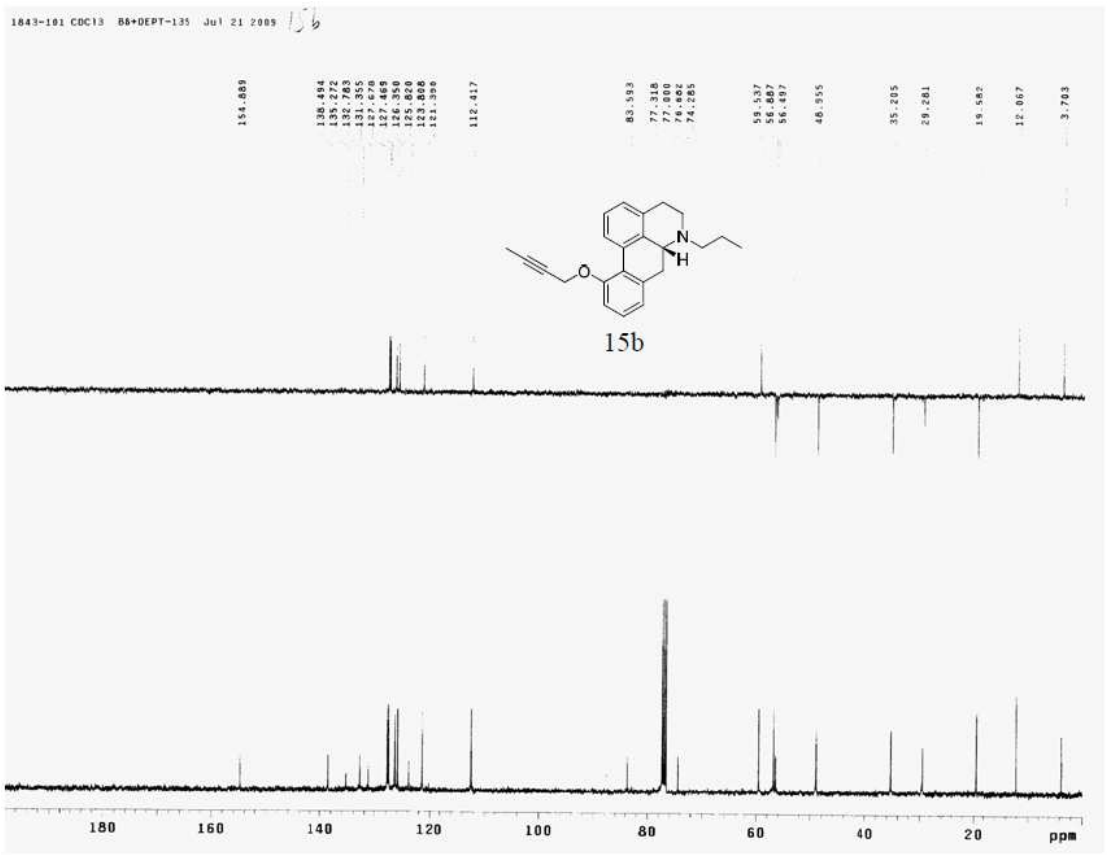

HO
N
Pr
H
14
ppm


8.116
8.093
7.258
7.243
7.218
7.194
7.169
7.071
7.050
7.025
6.982
6.957
4.752
4.745
4.737
4.728
3.185
3.173
3.159
3.153
3.138
3.126
3.092
3.079
2.779
2.622
2.575
2.523
2.515
2.508
2.480
2.469
2.438
2.425
1.772
1.615
1.262
0.995
0.969
0.945
0.006
O
N
15a
0.91
1.99
0.98
2.00
0.99
3.13
1.07
1.15
4.14
2.35
3.21
8
7
6
5
4
3
2
1
PPM

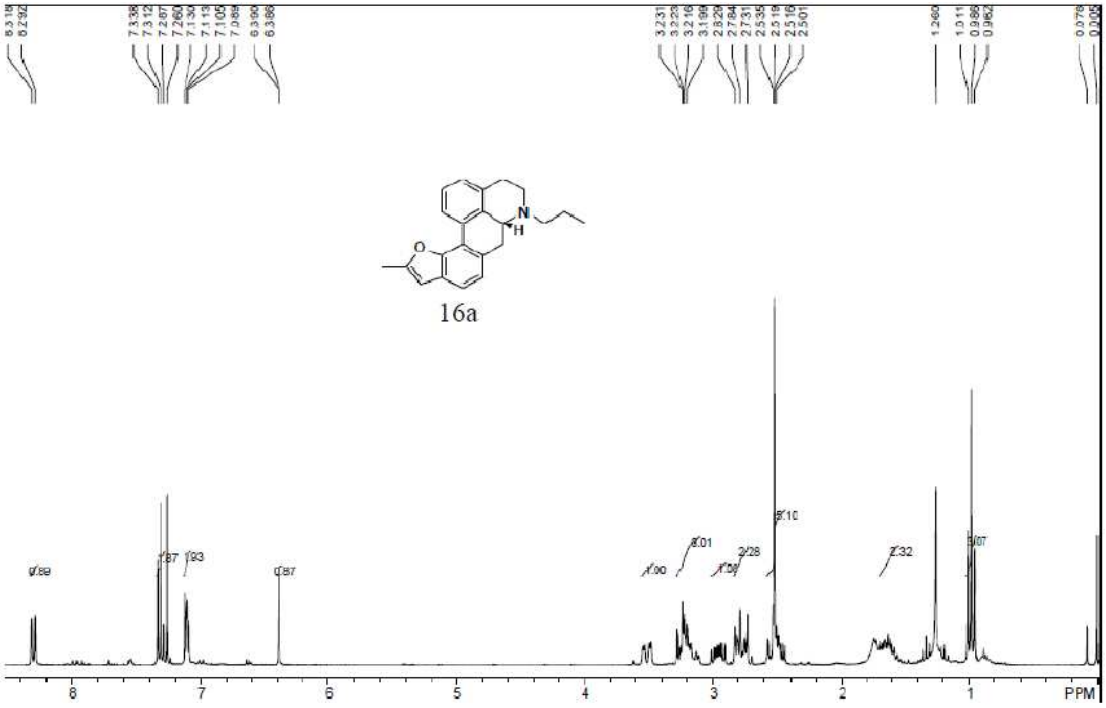

1754-146A CDCl3 BB+DEPT-135 Jul 22 2009
15a
154.588
136.630
132.850
131.287
127.717
127.612
126.326
125.883
123.946
121.854
112.502
78.728
77.316
77.000
76.683
75.512
59.499
56.472
56.334
48.924
35.132
29.684
29.222
19.531
12.869
O
N
H
15a
160
140
120
100
80
60
40
20
ppm

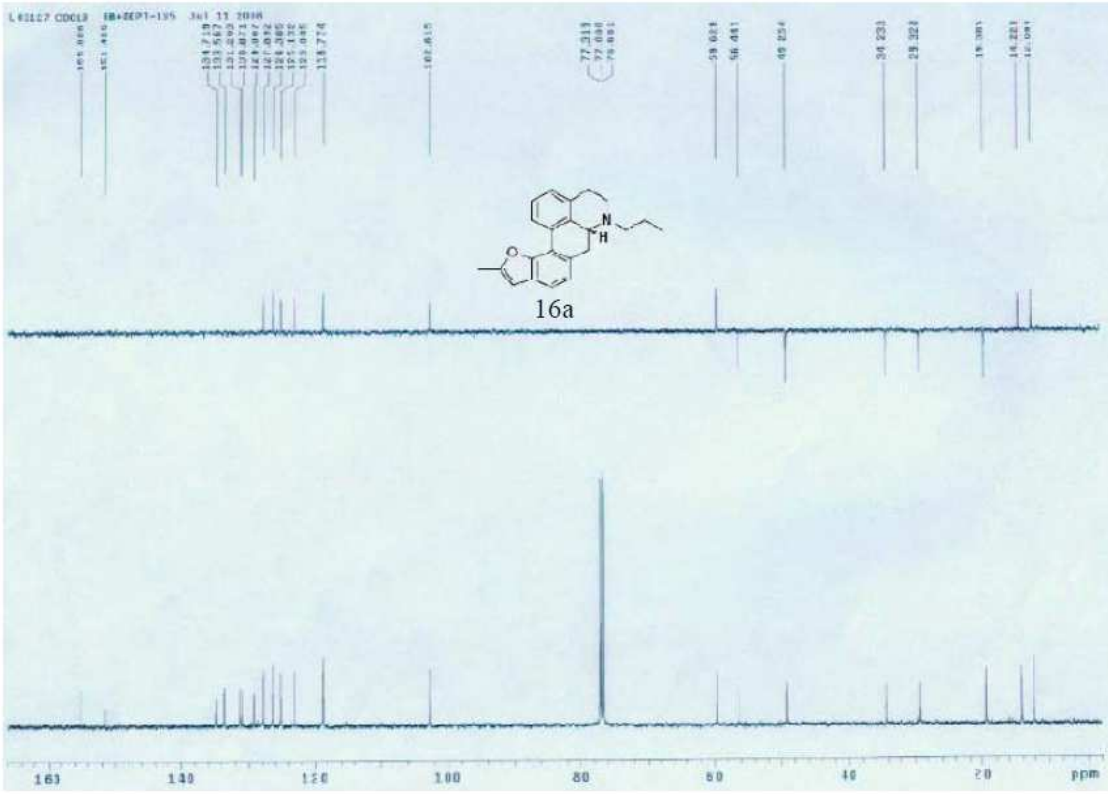


15b



15b


16a
PPM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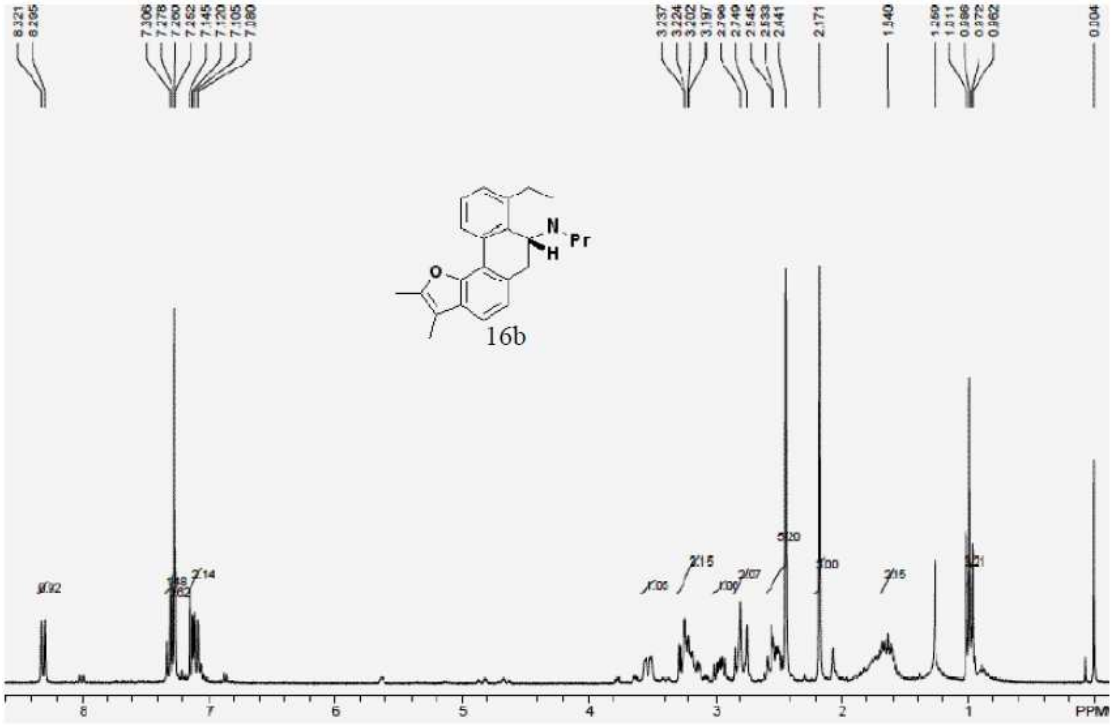
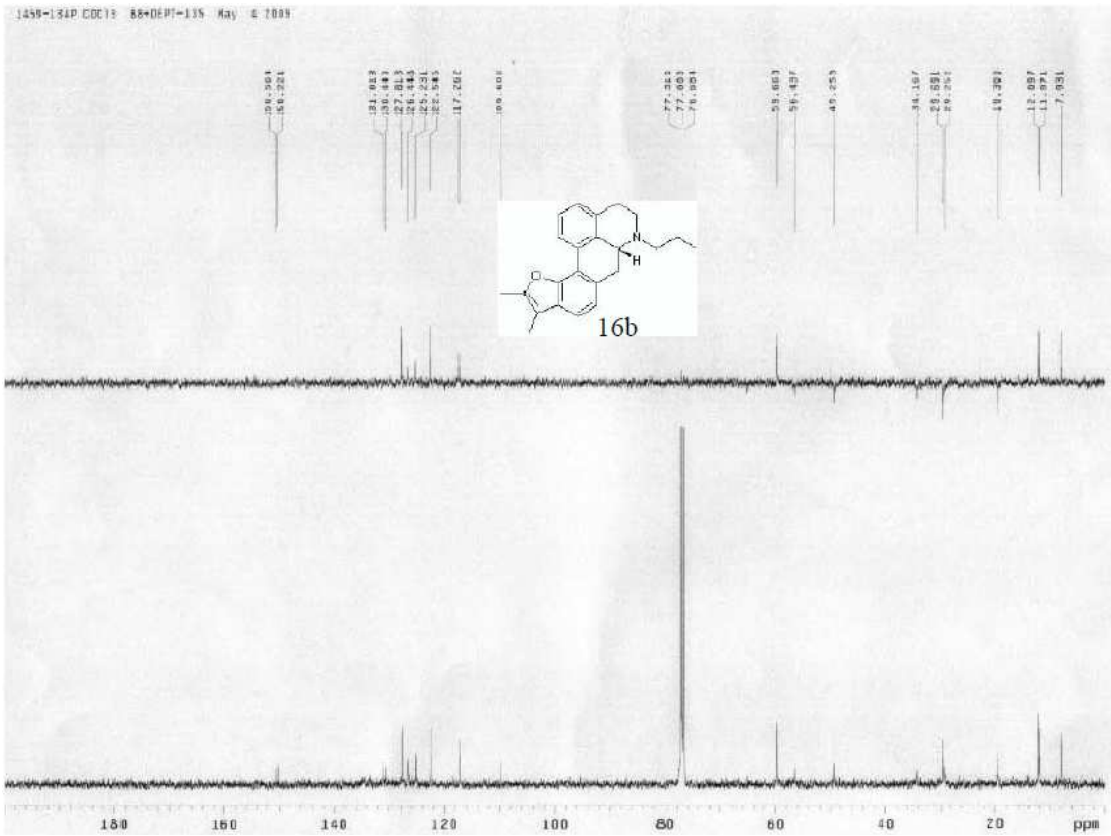
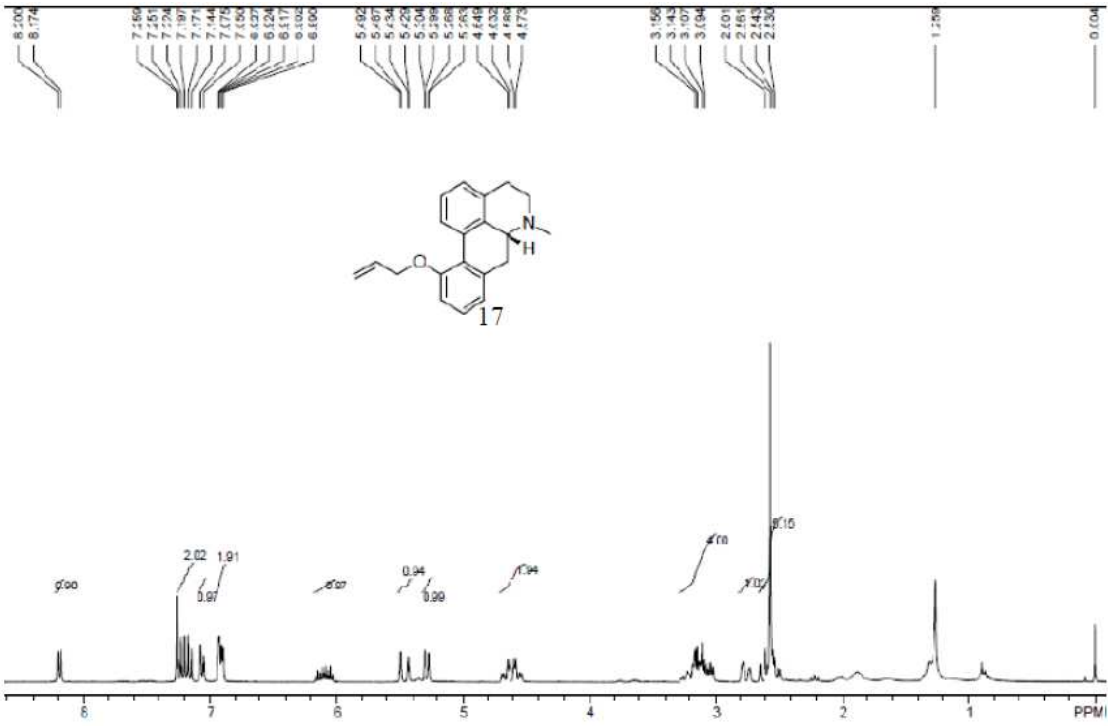
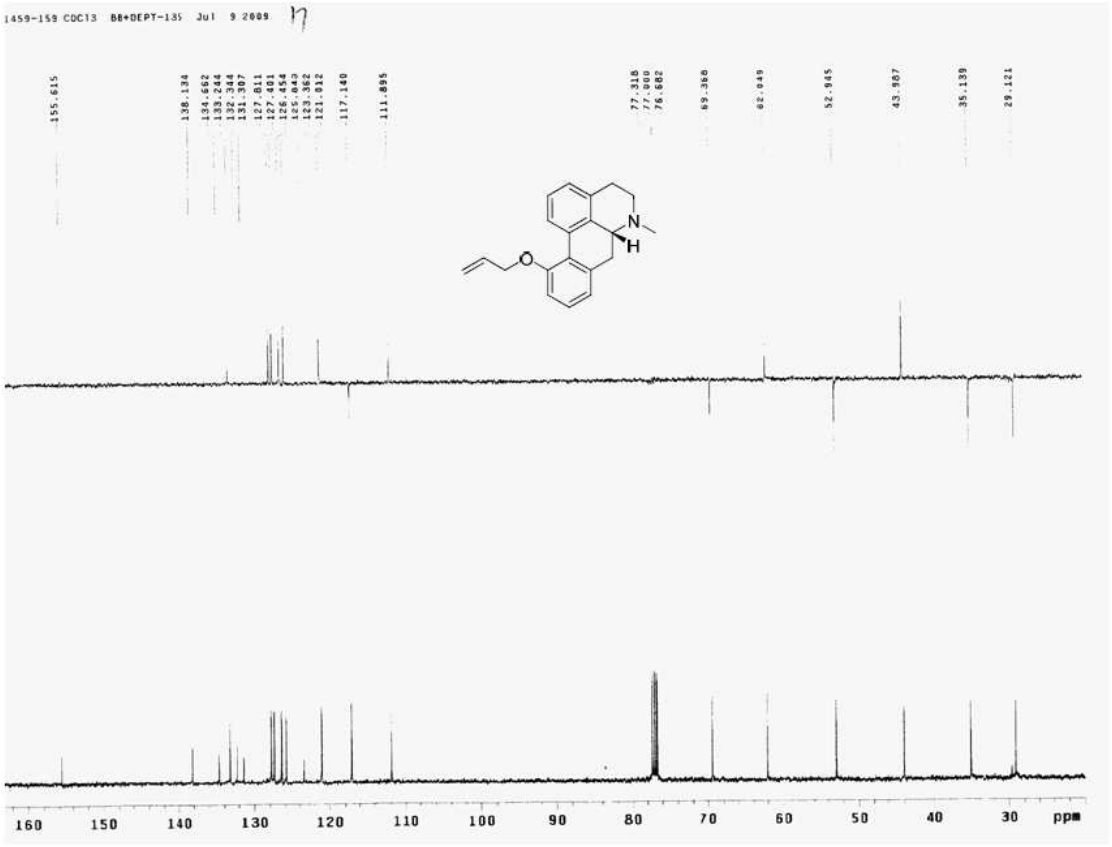
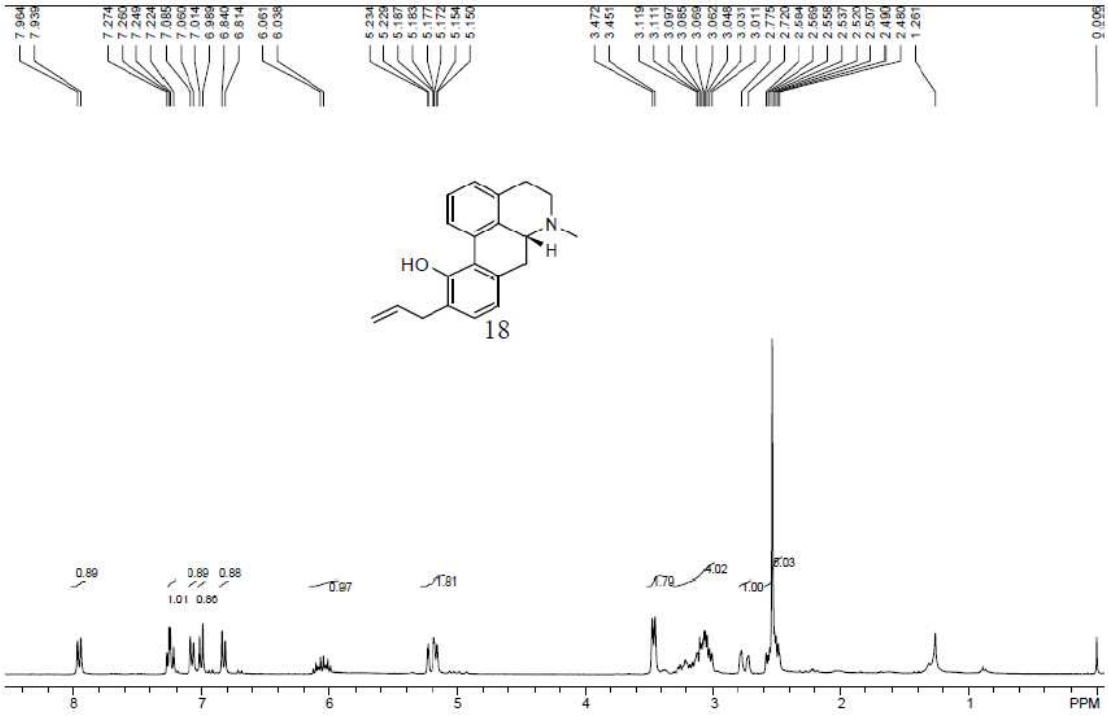
ppm

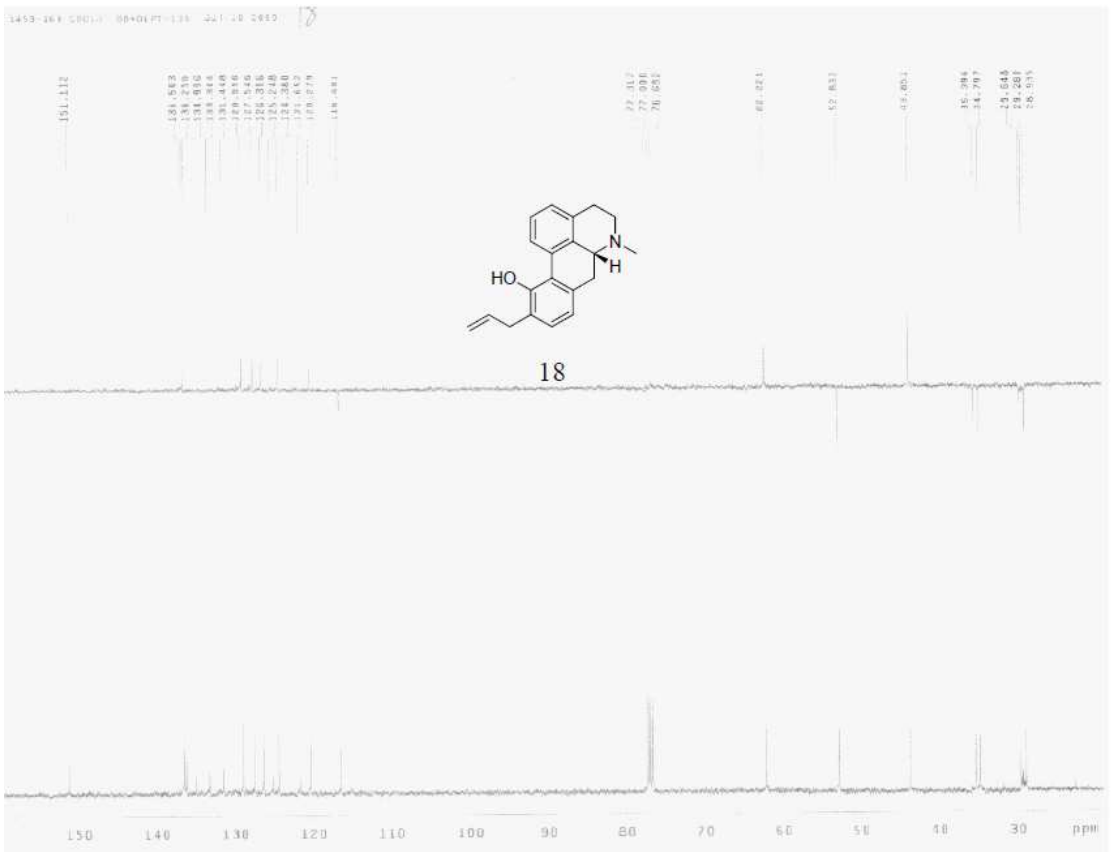

16b
PPM

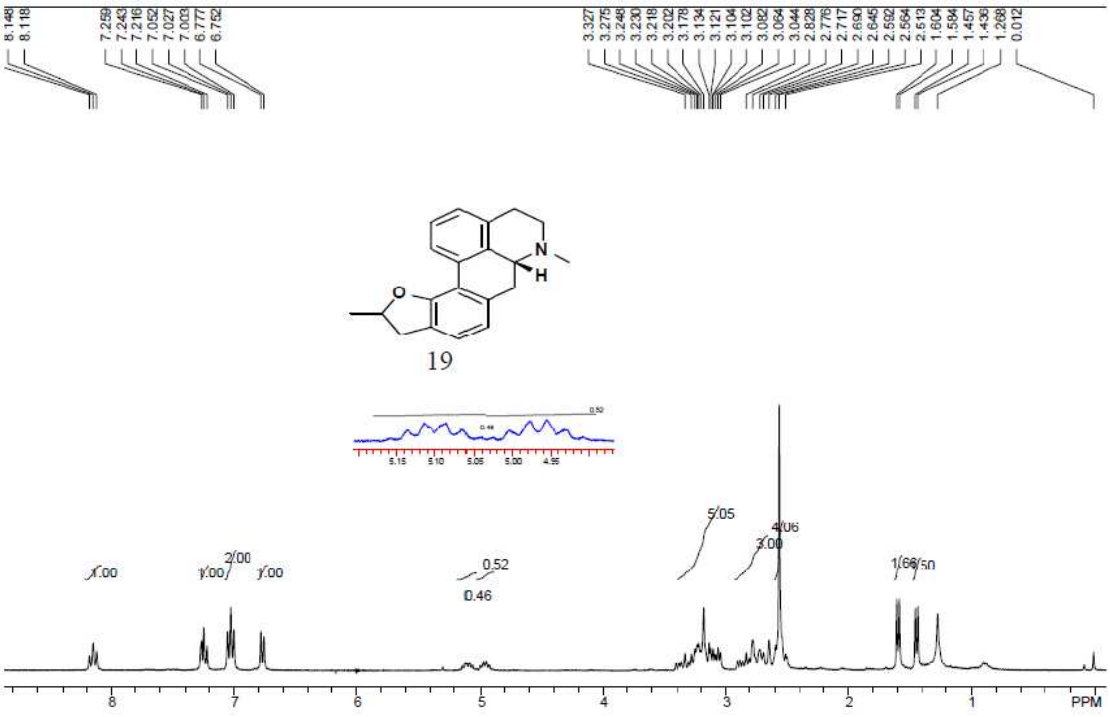

16b
ppm


N
H
O
17
2.02
1.91
0.97
0.94
0.99
PPM


1459-159 CDCl3 BB+DEPT-135 Jul 9 2009
155.615
138.134
134.662
133.244
132.344
131.307
127.811
127.401
126.454
125.043
123.462
121.012
117.140
111.895
77.318
77.000
76.682
69.368
62.049
52.945
43.987
35.139
29.121
N
H
O
ppm


HO
N
H
18
0.89
0.89
0.88
1.01
0.86
0.97
1.81
1.79
4.02
1.00
6.03
8
7
6
5
4
3
2
1
PPM


HO
N
H
18
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm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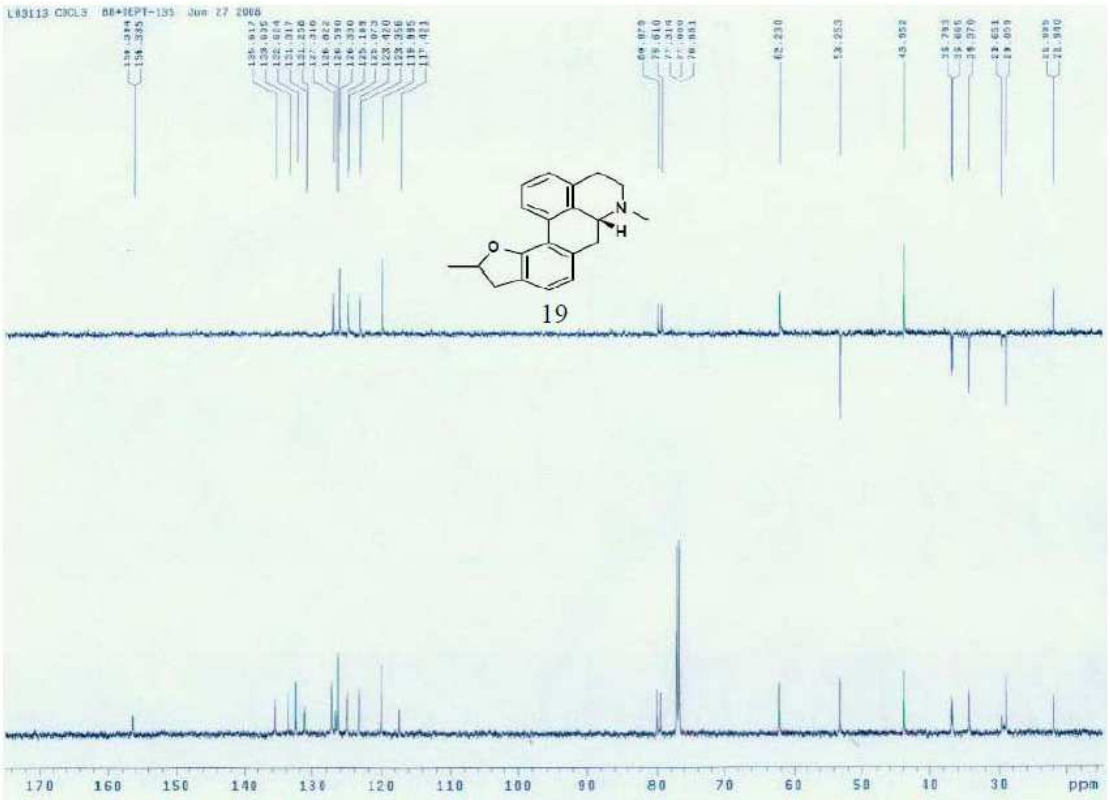
8.118
7.259
7.243
7.216
7.052
7.027
7.003
6.777
6.752
3.327
3.275
3.246
3.230
3.218
3.202
3.178
3.134
3.121
3.104
3.102
3.082
3.064
3.044
2.828
2.776
2.717
2.690
2.645
2.592
2.564
2.513
1.604
1.584
1.457
1.436
1.268
0.012
N
H
O
19
1.00
2.00
1.00
1.00
0.52
0.46
5.05
4.06
3.00
1.66
1.50
8
7
6
5
4
3
2
1
PPM


L83113 CDCL3 BB+DEPT-135 Jun 27 2008
N
H
O
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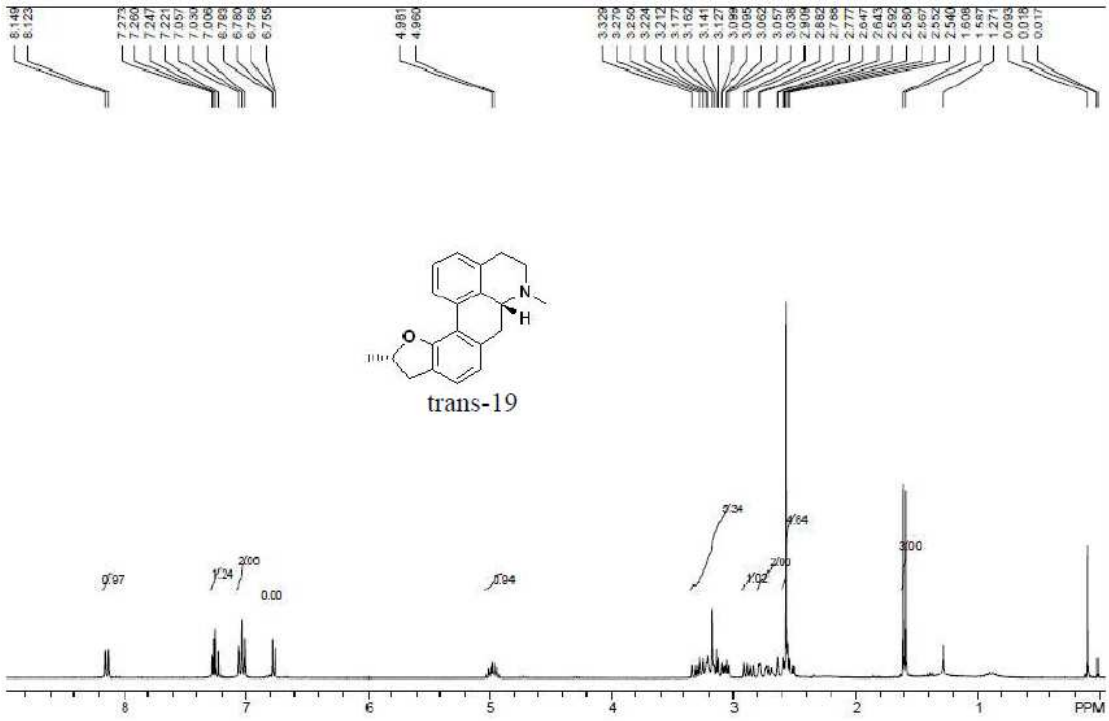
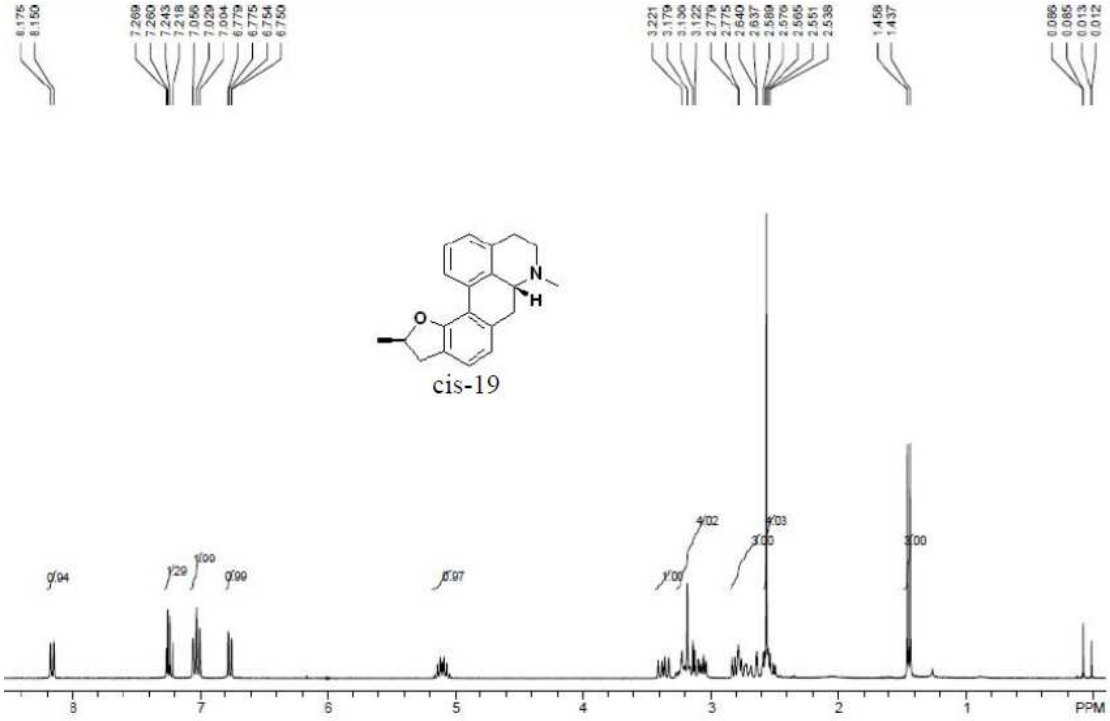
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


trans-19
PPM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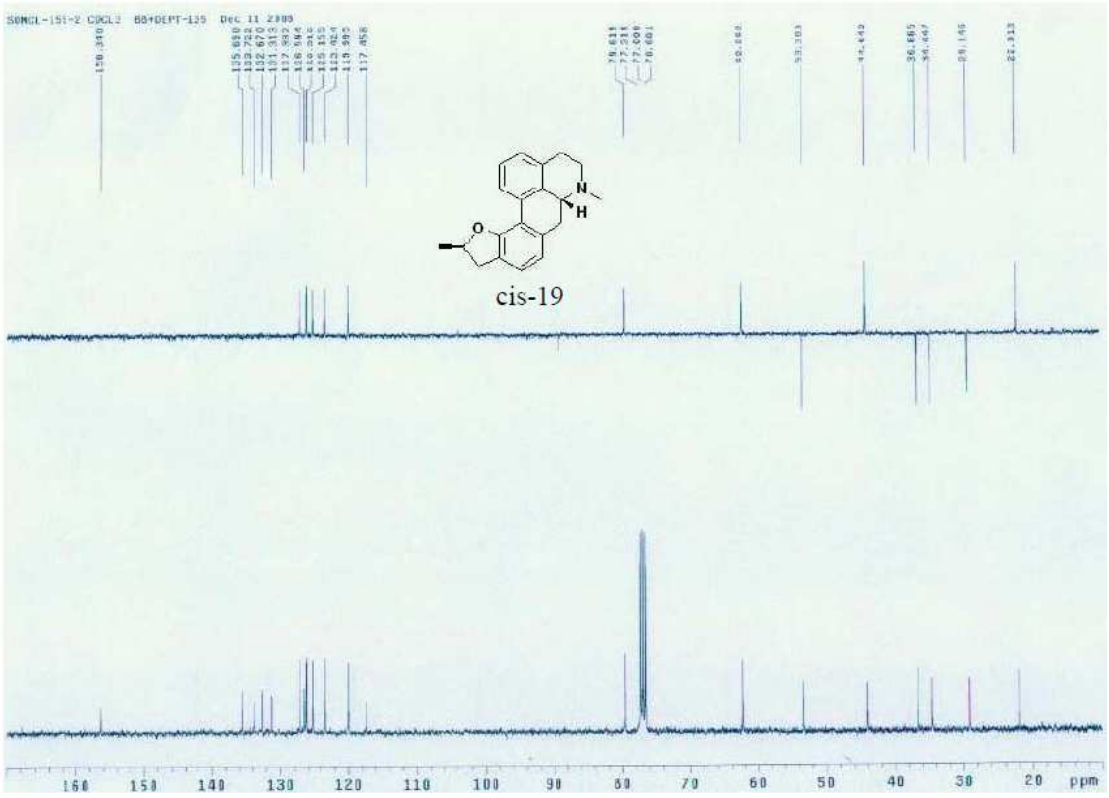
8.150
7.269
7.260
7.243
7.218
7.056
7.029
7.004
6.779
6.775
6.754
6.750
3.221
3.179
3.130
3.122
2.779
2.775
2.640
2.637
2.589
2.579
2.565
2.551
2.538
1.458
1.437
0.086
0.085
0.013
0.012
cis-19
0.94
2.29
1.00
0.99
0.97
1.00
4.02
4.03
3.00
3.00
8
7
6
5
4
3
2
1
PPM


cis-19
160
150
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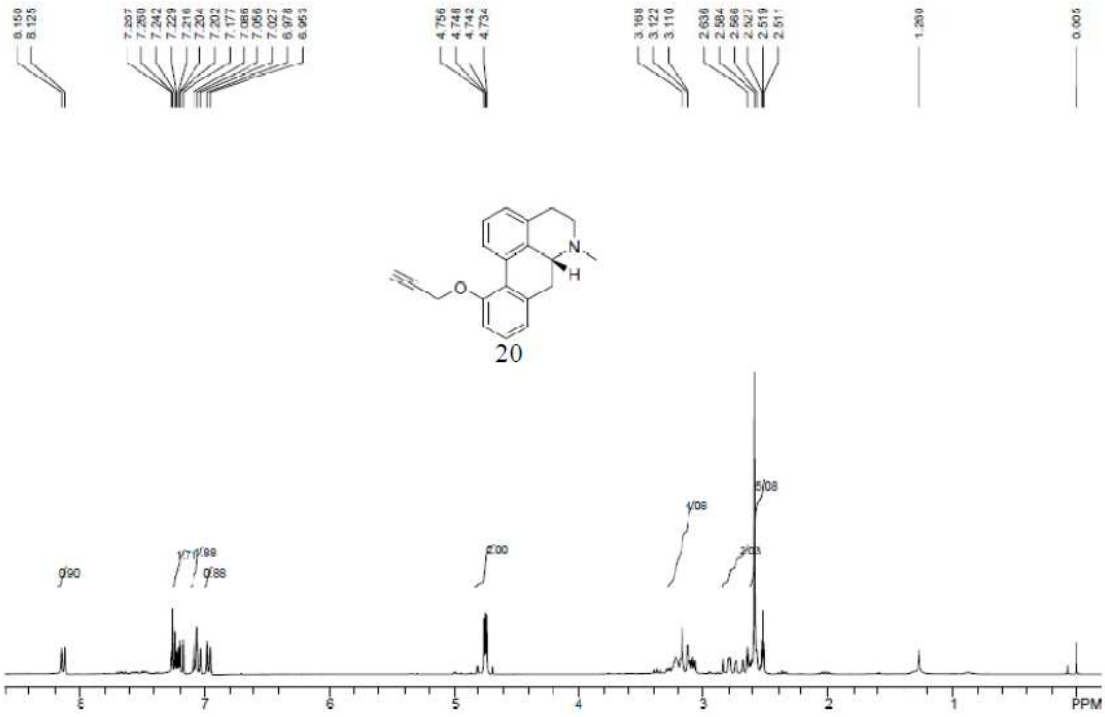
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.159
8.125
7.257
7.250
7.242
7.229
7.216
7.204
7.202
7.177
7.086
7.066
7.027
6.978
6.963
4.756
4.748
4.742
4.734
3.108
3.122
3.110
2.636
2.584
2.566
2.527
2.519
2.511
1.269
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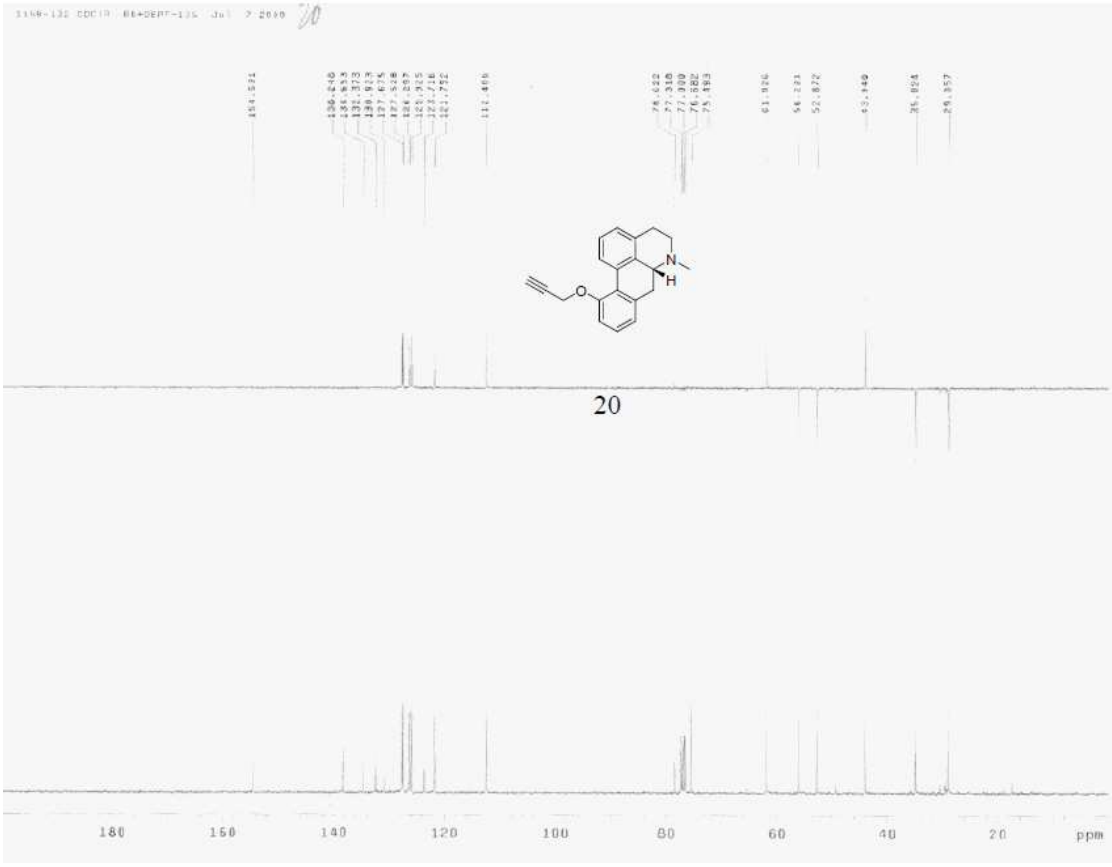
0.90
0.88
2.00
3.08
5.08
PPM

20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132.373
129.023
127.675
127.348
125.325
122.716
121.752
112.469
78.622
77.338
77.000
76.882
75.193
61.926
54.231
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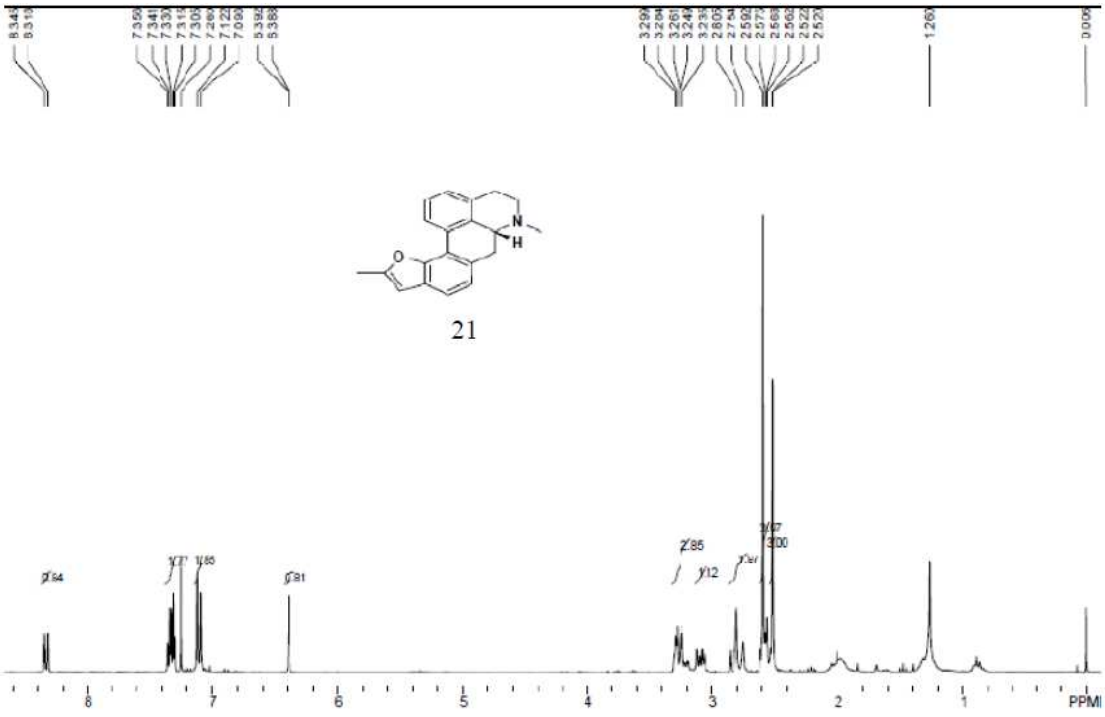
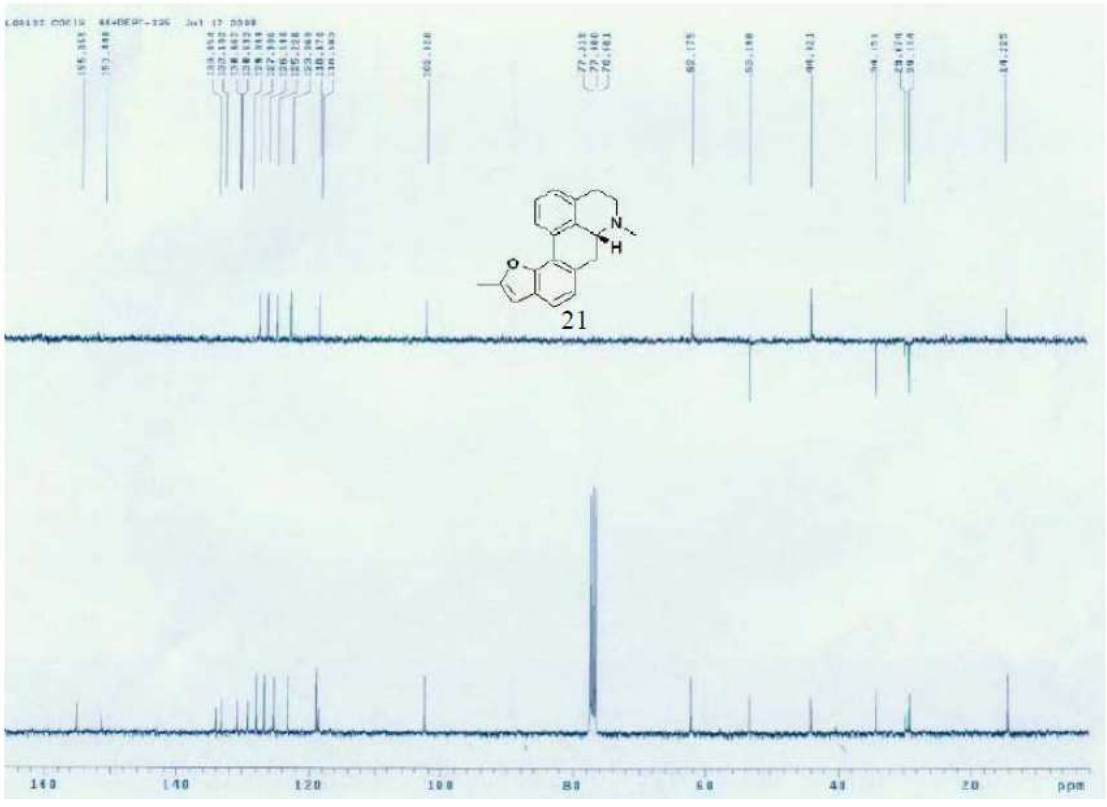
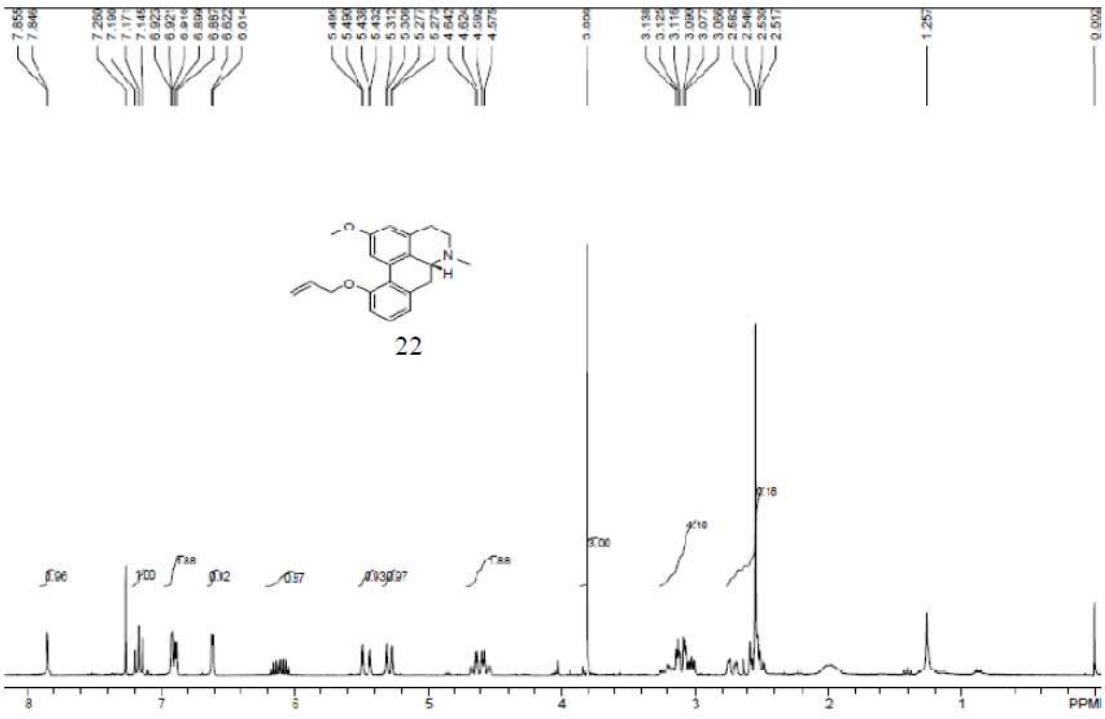
43.149
35.824
24.357
180
160
140
120
100
80
60
40
20
ppm

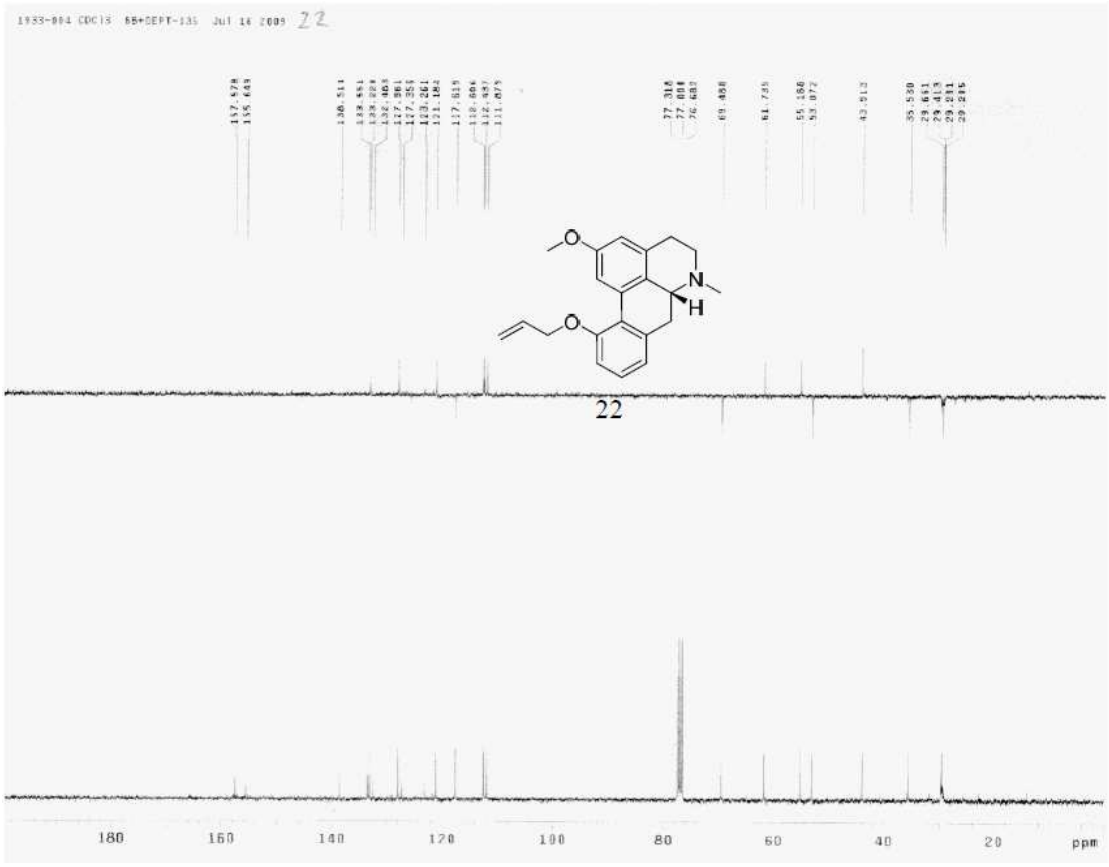
20


21
PPMI

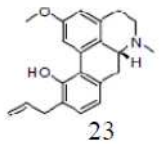

21
ppm



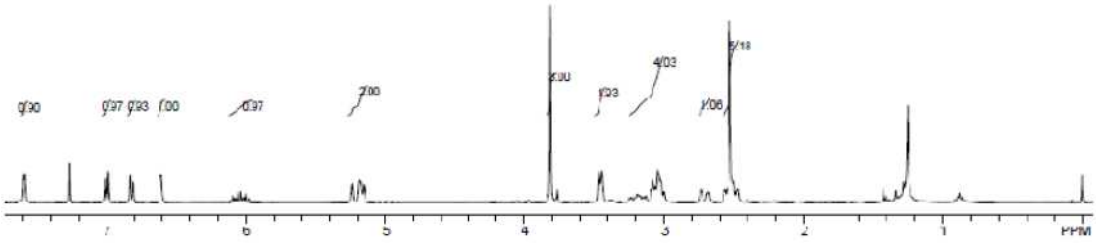
22

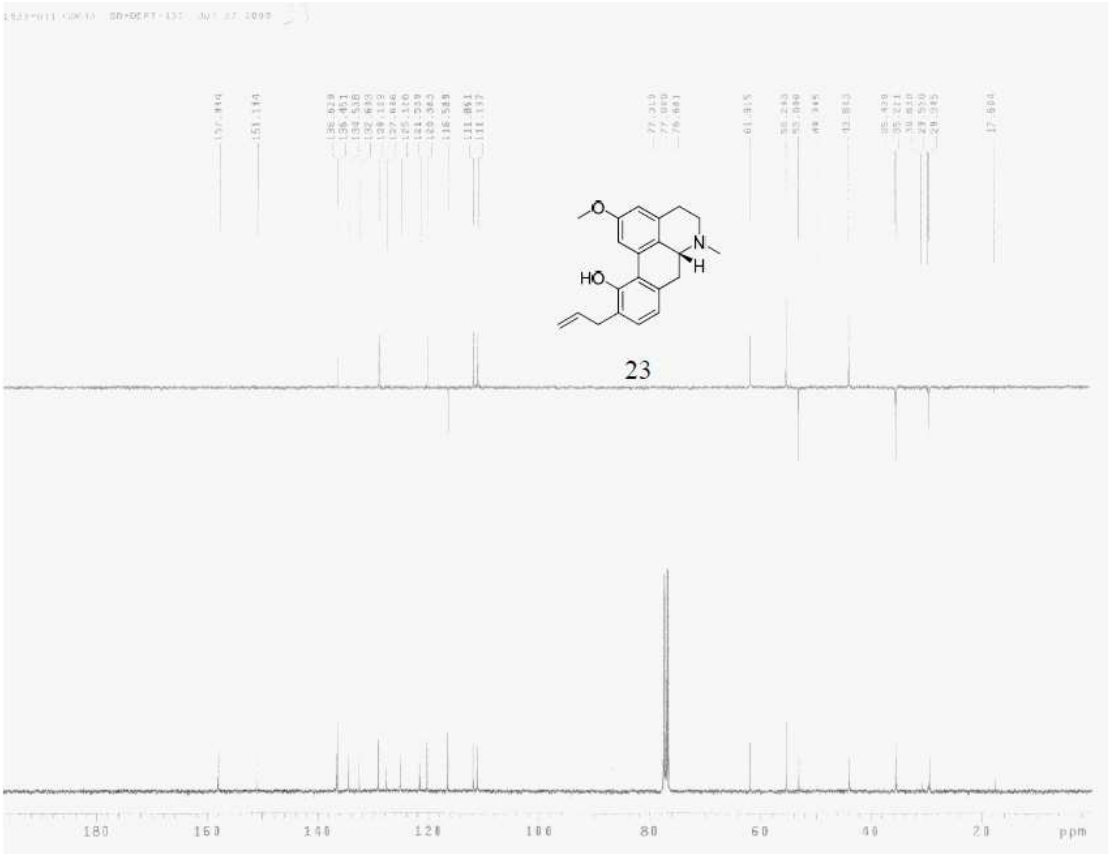


22



23





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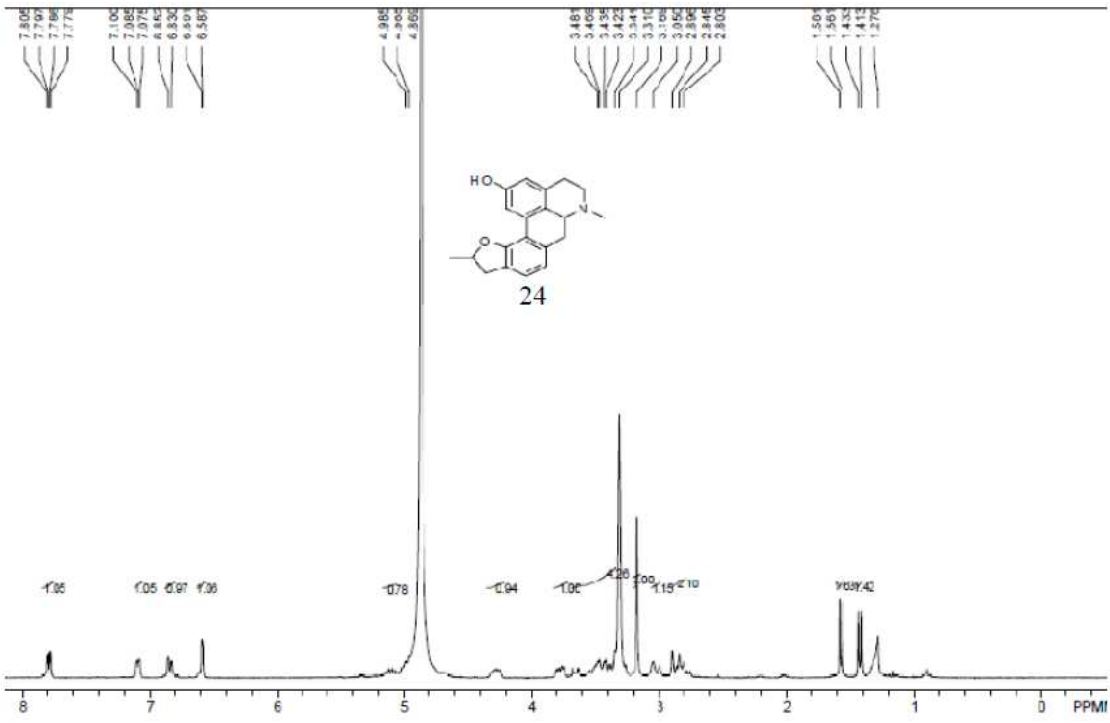

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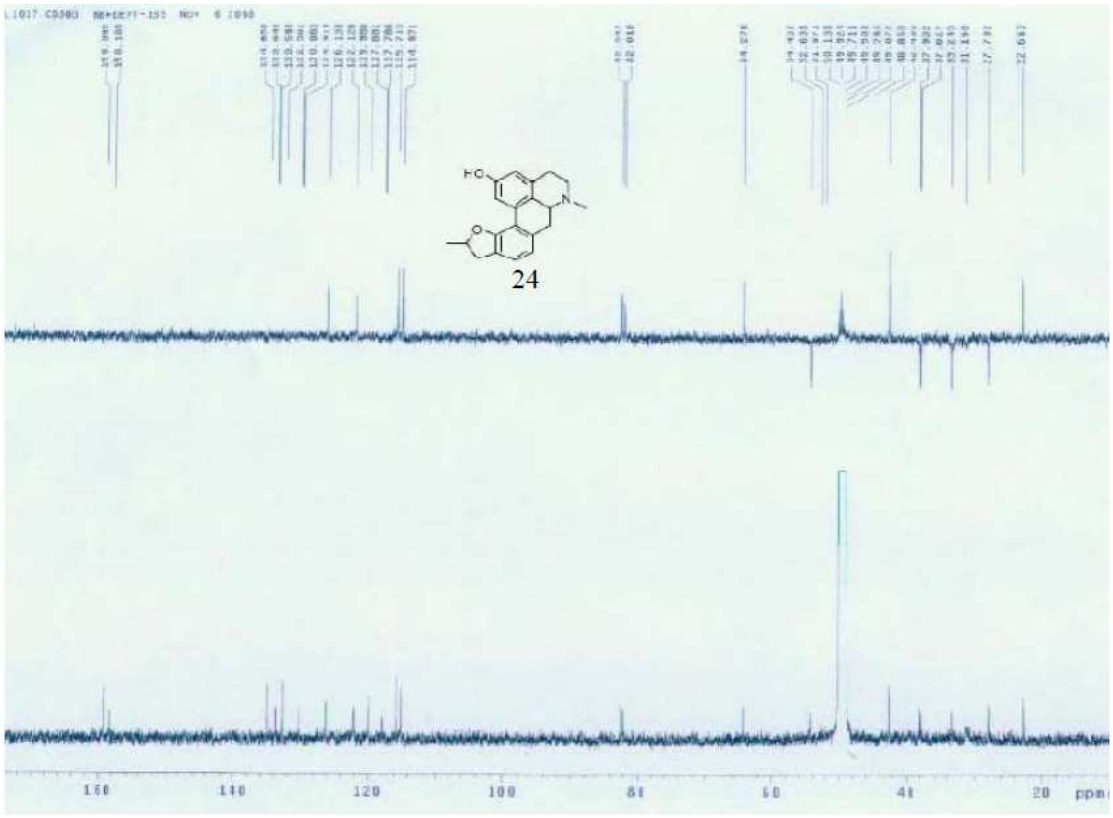
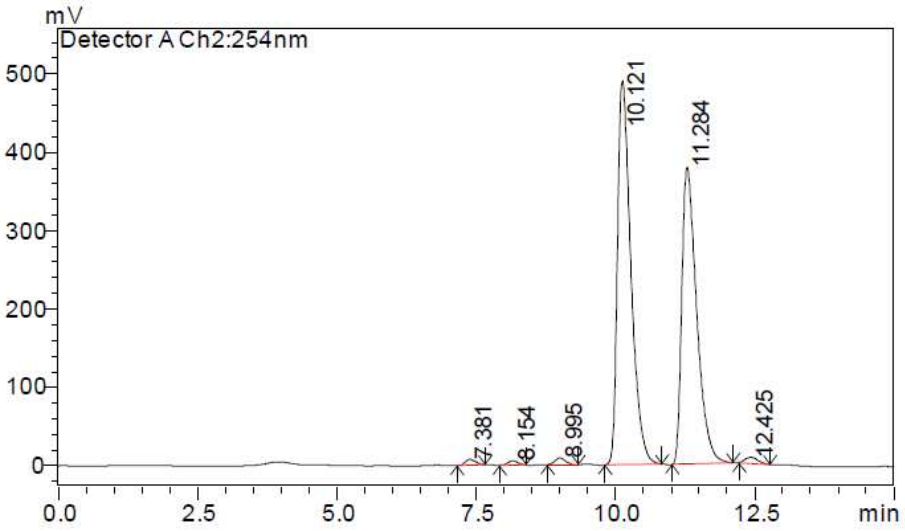
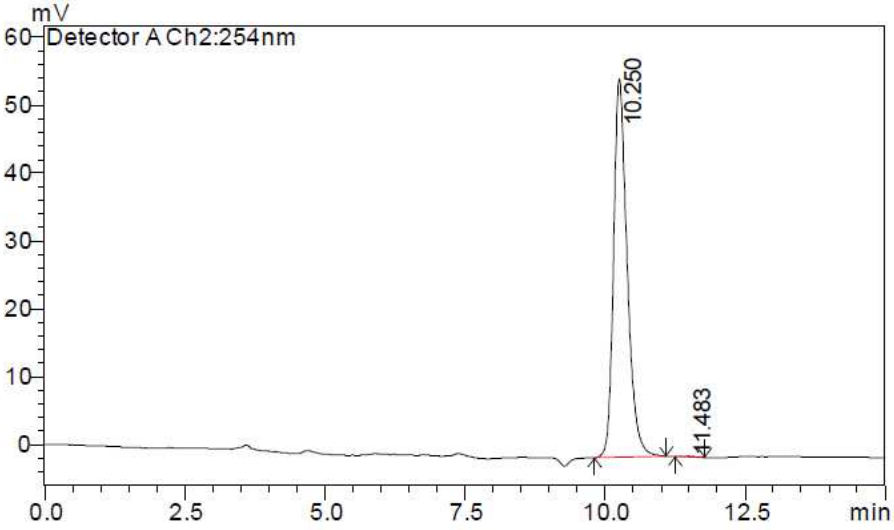


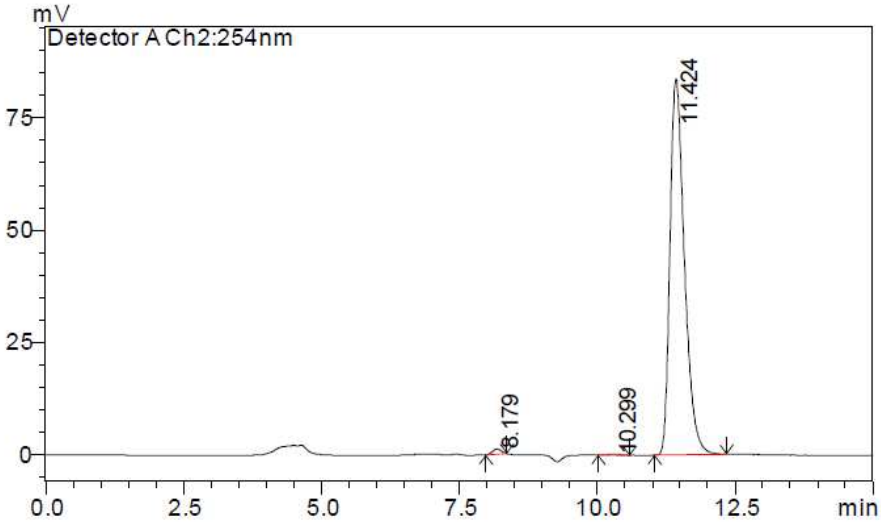
24



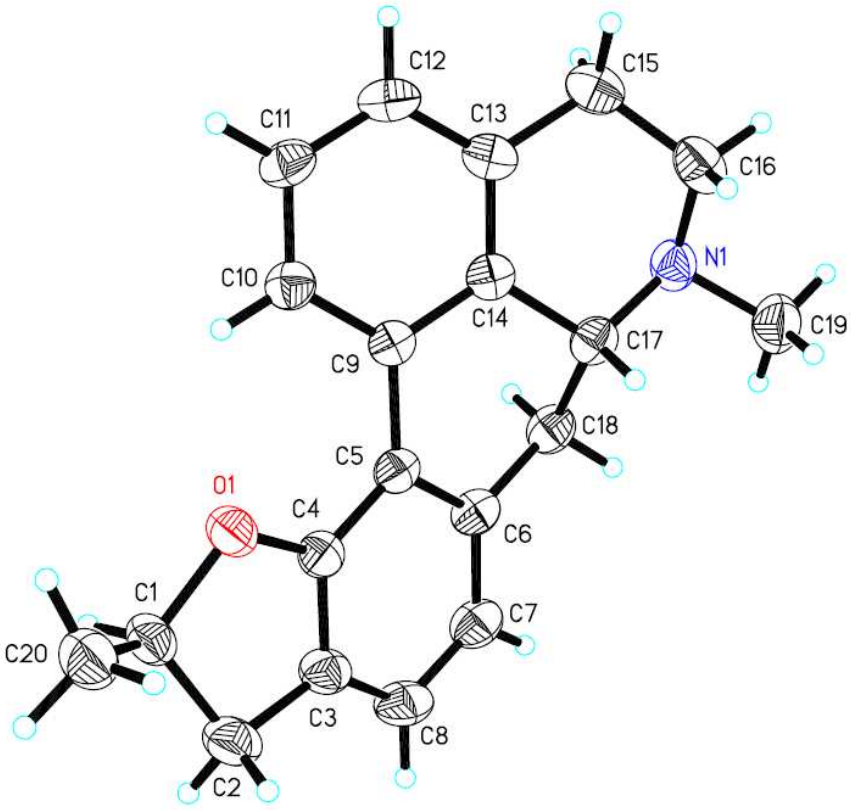
The retention time of compound *cis/trans*-**19**

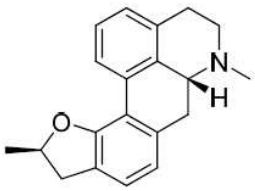


The retention time of compound ***trans*-19**



The retention time of compound ***cis*-19**





cis-19

The crystal structure of compound *cis*-19

Table 1. Crystal data and structure refinement for cd2971.

Identification code	cd2971
Empirical formula	C20 H21 N O
Formula weight	291.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 7.983(3) A alpha = 90 deg. b = 12.721(4) A beta = 90 deg. c = 15.432(5) A gamma = 90 deg.
Volume	1567.0(8) A^3
Z, Calculated density	4, 1.235 Mg/m^3
Absorption coefficient	0.075 mm^-1
F(000)	624
Crystal size	0.411 x 0.369 x 0.237 mm
Theta range for data collection	2.07 to 26.00 deg.
Limiting indices	-9<=h<=9, -15<=k<=11, -19<=l<=15
Reflections collected / unique	8585 / 1782 [R(int) = 0.0817]
Completeness to theta = 26.00	100.0 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.7523
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1782 / 0 / 201

Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.0995
R indices (all data)	R1 = 0.0520, wR2 = 0.1039
Absolute structure parameter	10(10)
Largest diff. peak and hole	0.151 and -0.122 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd2971.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	6575(3)	3253(2)	4090(1)	61(1)
O(1)	7758(2)	2415(1)	-30(1)	59(1)
C(1)	8412(3)	1769(2)	-740(2)	60(1)
C(2)	8478(4)	659(2)	-376(2)	69(1)
C(3)	8601(3)	865(2)	579(2)	56(1)
C(4)	8128(3)	1896(2)	721(1)	48(1)
C(5)	8022(3)	2339(2)	1547(1)	47(1)
C(6)	8414(3)	1668(2)	2243(2)	52(1)
C(7)	8918(3)	641(2)	2097(2)	62(1)
C(8)	9016(3)	236(2)	1267(2)	67(1)
C(9)	7606(2)	3455(2)	1726(1)	44(1)
C(10)	7827(3)	4243(2)	1115(2)	53(1)
C(11)	7442(3)	5269(2)	1301(2)	59(1)
C(12)	6816(3)	5522(2)	2107(2)	60(1)
C(13)	6600(3)	4762(2)	2736(1)	54(1)
C(14)	7010(3)	3731(2)	2551(1)	47(1)
C(15)	5952(4)	5046(2)	3623(2)	70(1)
C(16)	5321(4)	4086(2)	4093(2)	72(1)
C(17)	6805(3)	2852(2)	3212(2)	52(1)
C(18)	8309(3)	2123(2)	3139(2)	58(1)
C(19)	6059(4)	2407(3)	4678(2)	82(1)
C(20)	7318(4)	1924(2)	-1521(2)	74(1)

Table 3. Bond lengths [A] and angles [deg] for cd2971.

N(1)-C(16)	1.458(4)
N(1)-C(17)	1.460(3)
N(1)-C(19)	1.467(3)
O(1)-C(4)	1.366(3)
O(1)-C(1)	1.467(3)
C(1)-C(20)	1.501(4)
C(1)-C(2)	1.521(4)
C(1)-H(1)	0.9800
C(2)-C(3)	1.500(4)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(8)	1.369(3)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.396(3)
C(5)-C(6)	1.407(3)
C(5)-C(9)	1.484(3)
C(6)-C(7)	1.385(3)
C(6)-C(18)	1.501(3)
C(7)-C(8)	1.385(4)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-C(10)	1.387(3)
C(9)-C(14)	1.405(3)
C(10)-C(11)	1.370(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.379(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.381(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.381(3)
C(13)-C(15)	1.507(3)
C(14)-C(17)	1.521(3)
C(15)-C(16)	1.506(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.521(3)
C(17)-H(17)	0.9800
C(18)-H(18A)	0.9700

C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600

C(16)-N(1)-C(17)	110.04(19)
C(16)-N(1)-C(19)	109.8(2)
C(17)-N(1)-C(19)	110.7(2)
C(4)-O(1)-C(1)	106.64(17)
O(1)-C(1)-C(20)	108.6(2)
O(1)-C(1)-C(2)	104.83(19)
C(20)-C(1)-C(2)	116.0(2)
O(1)-C(1)-H(1)	109.0
C(20)-C(1)-H(1)	109.0
C(2)-C(1)-H(1)	109.0
C(3)-C(2)-C(1)	101.74(19)
C(3)-C(2)-H(2A)	111.4
C(1)-C(2)-H(2A)	111.4
C(3)-C(2)-H(2B)	111.4
C(1)-C(2)-H(2B)	111.4
H(2A)-C(2)-H(2B)	109.3
C(8)-C(3)-C(4)	119.9(2)
C(8)-C(3)-C(2)	132.4(2)
C(4)-C(3)-C(2)	107.7(2)
O(1)-C(4)-C(3)	112.5(2)
O(1)-C(4)-C(5)	124.48(19)
C(3)-C(4)-C(5)	123.0(2)
C(4)-C(5)-C(6)	116.0(2)
C(4)-C(5)-C(9)	124.71(19)
C(6)-C(5)-C(9)	119.25(19)
C(7)-C(6)-C(5)	120.9(2)
C(7)-C(6)-C(18)	122.0(2)
C(5)-C(6)-C(18)	117.1(2)
C(8)-C(7)-C(6)	121.2(2)
C(8)-C(7)-H(7)	119.4
C(6)-C(7)-H(7)	119.4
C(3)-C(8)-C(7)	119.0(2)
C(3)-C(8)-H(8)	120.5
C(7)-C(8)-H(8)	120.5
C(10)-C(9)-C(14)	118.6(2)
C(10)-C(9)-C(5)	122.5(2)

C(14)-C(9)-C(5)	118.90(19)
C(11)-C(10)-C(9)	121.2(2)
C(11)-C(10)-H(10)	119.4
C(9)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	119.5(2)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(11)-C(12)-C(13)	121.1(2)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(12)-C(13)-C(14)	119.3(2)
C(12)-C(13)-C(15)	120.9(2)
C(14)-C(13)-C(15)	119.7(2)
C(13)-C(14)-C(9)	120.3(2)
C(13)-C(14)-C(17)	122.3(2)
C(9)-C(14)-C(17)	117.41(19)
C(16)-C(15)-C(13)	111.0(2)
C(16)-C(15)-H(15A)	109.4
C(13)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15B)	109.4
C(13)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
N(1)-C(16)-C(15)	111.0(2)
N(1)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16A)	109.4
N(1)-C(16)-H(16B)	109.4
C(15)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
N(1)-C(17)-C(18)	112.4(2)
N(1)-C(17)-C(14)	112.25(18)
C(18)-C(17)-C(14)	108.30(19)
N(1)-C(17)-H(17)	107.9
C(18)-C(17)-H(17)	107.9
C(14)-C(17)-H(17)	107.9
C(6)-C(18)-C(17)	110.31(19)
C(6)-C(18)-H(18A)	109.6
C(17)-C(18)-H(18A)	109.6
C(6)-C(18)-H(18B)	109.6
C(17)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	108.1
N(1)-C(19)-H(19A)	109.5
N(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(1)-C(19)-H(19C)	109.5

H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(1)-C(20)-H(20A)	109.5
C(1)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(1)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd2971.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	67(1)	66(1)	49(1)	-1(1)	2(1)	-9(1)
O(1)	67(1)	58(1)	51(1)	-3(1)	5(1)	10(1)
C(1)	56(1)	65(2)	59(2)	-12(1)	15(1)	0(1)
C(2)	67(2)	62(2)	79(2)	-17(1)	12(1)	8(2)
C(3)	48(1)	50(1)	71(2)	-7(1)	6(1)	6(1)
C(4)	41(1)	49(1)	55(1)	2(1)	2(1)	4(1)
C(5)	40(1)	44(1)	57(1)	3(1)	-1(1)	0(1)
C(6)	48(1)	48(1)	61(1)	5(1)	-8(1)	0(1)
C(7)	60(1)	51(1)	75(2)	12(1)	-8(1)	7(1)
C(8)	65(2)	46(1)	90(2)	-2(1)	-3(1)	14(1)
C(9)	38(1)	46(1)	48(1)	0(1)	-8(1)	-1(1)
C(10)	55(1)	52(1)	52(1)	3(1)	-5(1)	3(1)
C(11)	70(2)	46(1)	61(2)	6(1)	-13(1)	3(1)
C(12)	70(2)	43(1)	68(2)	-7(1)	-19(1)	8(1)
C(13)	50(1)	55(1)	56(1)	-10(1)	-12(1)	5(1)
C(14)	38(1)	51(1)	51(1)	-3(1)	-10(1)	-4(1)
C(15)	75(2)	69(2)	66(2)	-16(1)	-3(1)	6(2)
C(16)	66(2)	89(2)	62(2)	-17(2)	7(1)	1(2)
C(17)	51(1)	54(1)	53(1)	0(1)	-8(1)	-9(1)
C(18)	63(1)	56(1)	56(1)	10(1)	-8(1)	0(1)
C(19)	93(2)	88(2)	65(2)	1(2)	13(2)	-19(2)
C(20)	81(2)	80(2)	62(2)	-11(1)	7(1)	-6(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd2971.

	x	y	z	U(eq)
H(1)	9552	1999	-879	72
H(2A)	7472	267	-517	83
H(2B)	9449	280	-587	83
H(7)	9197	217	2566	74
H(8)	9358	-455	1176	80
H(10)	8243	4073	570	64
H(11)	7603	5790	887	71
H(12)	6534	6216	2229	72
H(15A)	6842	5369	3958	84
H(15B)	5050	5552	3567	84
H(16A)	5048	4271	4686	87
H(16B)	4307	3835	3815	87
H(17)	5803	2450	3056	63
H(18A)	9326	2511	3265	70
H(18B)	8208	1560	3559	70
H(19A)	6921	1882	4703	123
H(19B)	5040	2095	4469	123
H(19C)	5876	2690	5247	123
H(20A)	7223	2661	-1645	111
H(20B)	6226	1638	-1408	111
H(20C)	7805	1570	-2010	111

Table 6. Torsion angles [deg] for cd2971.

C(4)-O(1)-C(1)-C(20)	149.1(2)
C(4)-O(1)-C(1)-C(2)	24.4(2)
O(1)-C(1)-C(2)-C(3)	-24.5(3)
C(20)-C(1)-C(2)-C(3)	-144.3(2)
C(1)-C(2)-C(3)-C(8)	-165.7(3)
C(1)-C(2)-C(3)-C(4)	16.7(3)
C(1)-O(1)-C(4)-C(3)	-14.4(3)
C(1)-O(1)-C(4)-C(5)	166.6(2)
C(8)-C(3)-C(4)-O(1)	179.9(2)
C(2)-C(3)-C(4)-O(1)	-2.1(3)
C(8)-C(3)-C(4)-C(5)	-1.0(4)
C(2)-C(3)-C(4)-C(5)	176.9(2)
O(1)-C(4)-C(5)-C(6)	178.3(2)
C(3)-C(4)-C(5)-C(6)	-0.6(3)
O(1)-C(4)-C(5)-C(9)	-4.4(3)
C(3)-C(4)-C(5)-C(9)	176.7(2)
C(4)-C(5)-C(6)-C(7)	1.8(3)
C(9)-C(5)-C(6)-C(7)	-175.6(2)
C(4)-C(5)-C(6)-C(18)	-180.0(2)
C(9)-C(5)-C(6)-C(18)	2.6(3)
C(5)-C(6)-C(7)-C(8)	-1.6(4)
C(18)-C(6)-C(7)-C(8)	-179.7(2)
C(4)-C(3)-C(8)-C(7)	1.3(4)
C(2)-C(3)-C(8)-C(7)	-176.0(3)
C(6)-C(7)-C(8)-C(3)	-0.1(4)
C(4)-C(5)-C(9)-C(10)	-22.3(3)
C(6)-C(5)-C(9)-C(10)	154.9(2)
C(4)-C(5)-C(9)-C(14)	159.5(2)
C(6)-C(5)-C(9)-C(14)	-23.3(3)
C(14)-C(9)-C(10)-C(11)	-1.3(3)
C(5)-C(9)-C(10)-C(11)	-179.5(2)
C(9)-C(10)-C(11)-C(12)	-0.4(4)
C(10)-C(11)-C(12)-C(13)	1.3(4)
C(11)-C(12)-C(13)-C(14)	-0.4(3)
C(11)-C(12)-C(13)-C(15)	178.6(2)
C(12)-C(13)-C(14)-C(9)	-1.3(3)
C(15)-C(13)-C(14)-C(9)	179.6(2)
C(12)-C(13)-C(14)-C(17)	-180.0(2)
C(15)-C(13)-C(14)-C(17)	1.0(3)
C(10)-C(9)-C(14)-C(13)	2.2(3)

C(5)-C(9)-C(14)-C(13)	-179.55(19)
C(10)-C(9)-C(14)-C(17)	-179.1(2)
C(5)-C(9)-C(14)-C(17)	-0.8(3)
C(12)-C(13)-C(15)-C(16)	162.3(2)
C(14)-C(13)-C(15)-C(16)	-18.6(3)
C(17)-N(1)-C(16)-C(15)	-68.0(3)
C(19)-N(1)-C(16)-C(15)	169.9(2)
C(13)-C(15)-C(16)-N(1)	51.7(3)
C(16)-N(1)-C(17)-C(18)	169.8(2)
C(19)-N(1)-C(17)-C(18)	-68.7(3)
C(16)-N(1)-C(17)-C(14)	47.4(3)
C(19)-N(1)-C(17)-C(14)	168.9(2)
C(13)-C(14)-C(17)-N(1)	-15.1(3)
C(9)-C(14)-C(17)-N(1)	166.2(2)
C(13)-C(14)-C(17)-C(18)	-139.8(2)
C(9)-C(14)-C(17)-C(18)	41.5(2)
C(7)-C(6)-C(18)-C(17)	-142.7(2)
C(5)-C(6)-C(18)-C(17)	39.1(3)
N(1)-C(17)-C(18)-C(6)	175.64(19)
C(14)-C(17)-C(18)-C(6)	-59.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd2971 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)