Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Electronic Supplementary Information

Design, synthesis and antiproliferative activity of indole analogues of indanocine

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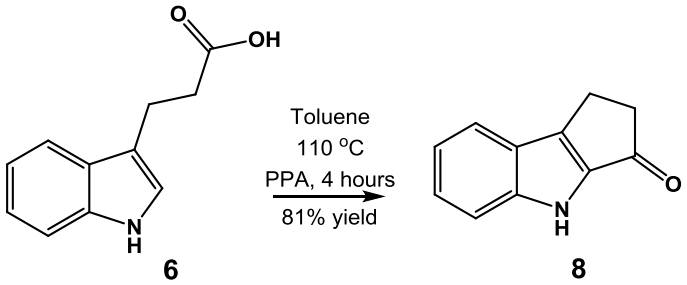
General Experimental

Chemicals, solvents and reagents used are commercially available and were used without further purification.

TLCs were carried out on Merck Aluminium backed TLC plates Silica Gel 60 F254 and viewed using UV light of wavelength 254 nm and then stained with potassium permanganate or 2,4-dinitrophenylhydrazine (DNP). Merck Silica Gel (0.040-0.063 mm) was used for column chromatography. Compounds were loaded as an oil, $CHCl_3$ solution or dry loaded by adsorption onto silica. Melting points were obtained using a Reichert-Jung heated-stage microscope. Infrared spectra were recorded on a Perkin-Elmer Spectrum RXI FT-IR system and all values are recorded in cm^{-1}.

NMR spectra were obtained on a Bruker Avance III (400 MHz) spectrometer. The chemical shifts are recorded in parts per million (ppm) with reference to tetramethylsilane. The coupling constants *J* are quoted to the nearest 0.5 Hz and are not corrected. The multiplicities are assigned as a singlet (s), doublet (d), triplet (t), doublet of doublets (dd), quartet (q) and multiplet (m). The symbols + and – after the carbon NMR chemical shifts indicate odd (CH and CH_3) and even (C and CH_2) numbers of attached protons respectively. Mass spectra and high resolution mass spectra were obtained on a micrOTOF™ from Bruker Daltonics (Bremen, Germany) coupled with an electrospray source (ESI-TOF) using an autosampler in an Agilent 1100 LC system. Data was processed using external calibration with the Bruker Daltonics software, DataAnalysis™ as part of the overall hardware control software, Compass 1.1™.

1,4-Dihydrocyclopenta[*b*]indol-3(*2H*)-one 8



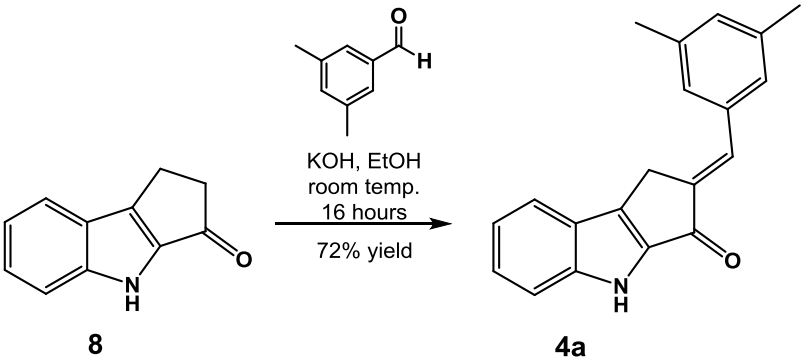
6 8

Following a previously reported procedure,[1] 3-(indole-3-yl)propanoic acid **6** (378 mg, 2 mmol, 1 eq.) was added to PPA (3.5 g, 35.7 mmol, 17.9 eq.) in toluene (20 mL) and the mixture was stirred at 110 °C for 4 hours. On cooling, ice water (80 mL) was added and the purple aqueous layer was extracted using CH_2Cl_2 (3 x 50 mL). The combined organic layers were washed with brine (30 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure to afford, without further purification, the desired compound **8** (278 mg, 81 % yield) as a beige solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.6. **IR** ν_{max}(liquid film): 3466 (NH), 3031 (CH) and 1682 (C=O). **m.p.** 255-258 °C [lit.[2] 250-252 °C]. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 8.98 (1H, br. s. N*H*), 7.75 (1H, dd, *J* = 8.0, 1.0 Hz, ArC*H*), 7.52 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.44 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.23 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 3.17-3.14 (2H, m, $COCH_2CH_2$) and 3.08-3.05 (2H, m, $COCH_2CH_2$). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 194.5− (*C*=O), 147.2− (*C*), 143.8− (*C*), 137.4− (*C*), 127.4+ (Ar*C*H), 123.6− (*C*), 121.6+ (Ar*C*H), 120.8+ (Ar*C*H), 113.5+ (Ar*C*H), 41.0− ($COCH_2CH_2$) and 20.1− ($COCH_2CH_2$). **MS** *m/z* (+ESI) 172 (82 %, MH^+) and 194 (100 %, MNa^+). **HRMS** (+ESI) Found MH^+ 172.0755, $C_{11}H_{10}NO$ requires *MH* 172.0762 and found MNa^+ 194.0572, $C_{11}H_9NNaO$ requires *MNa* 194.0582.

Consistent with the spectroscopic data previously reported for this compound.[3]

***(E)*-2-(3,5-Dimethylbenzylidene)-1,4-dihydrocyclopenta[*b*]indol-3(*2H*)-one 4a**

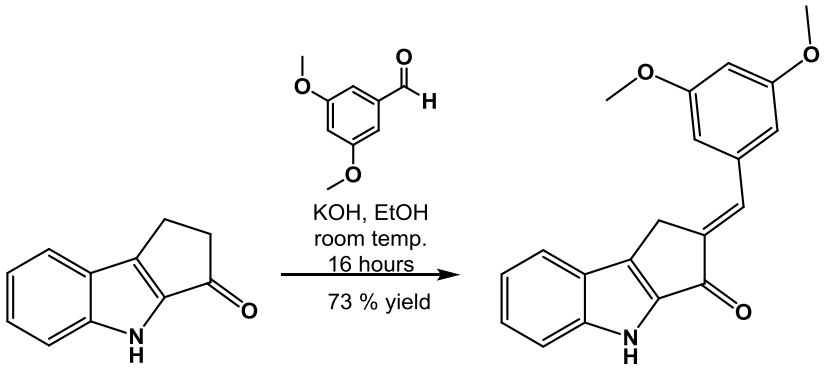


8 **4a**

A mixture of ketone **8** (171 mg, 1 mmol, 1 eq.) and 3,5-dimethylbenzaldehyde (0.15 mL, 1.1 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (10 mL) and stirred at room temperature for 16 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (20 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **4a** (206 mg, 72 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.5. **IR** ν_{max}(liquid film): 3464 (NH), 3028 (CH), 1678 (C=O) and 1627 (C=C). **m.p.** 288-292 °C. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ_H 11.90 (1H, br.s, N*H*), 7.80 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.45 (1H, d, *J* = 8.5 Hz, ArC*H*), 7.37-7.33 (3H, m, ArC*H* and Ar'C*H*), 7.29 (1H, br.s, alkene C*H*), 7.14 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.05 (1H, s, Ar'C*H*), 4.04 (2H, s, CH_2) and 2.33 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $(CD_3)_2SO$): δ_C 181.8− (*C*O), 143.5− (*C*), 140.5− (*C*), 139.9− (*C*), 139.6− (*C*), 138.0− (*C*), 134.9− (*C*), 130.8+ (alkene *C*H), 130.8+ (Ar'*C*H), 128.1+ (Ar*C*H or Ar'*C*H), 126.8+ (Ar'*C*H or Ar*C*H), 122.7− (*C*), 121.7+ (Ar*C*H), 120.3+ (Ar*C*H), 113.6+ (Ar*C*H), 26.3− (*C*H_2) and 20.9+ (Ar'*C*H_3). **MS** *m/z* (+ESI) 288 (100 %, MH^+) and 310 (14 %, MNa^+). **HRMS** (+ESI) Found MH^+ 288.1369, $C_{20}H_{18}NO$ requires *MH* 288.1388 and found MNa^+ 310.1190, $C_{20}H_{17}NNaO$ requires *MNa* 310.1208. **Analysis** (Found: H, 5.92; N, 4.86. $C_{20}H_{17}NO$ requires H, 5.96; N, 4.87 %).

_(E)_-2-(3,5-Dimethoxybenzylidene)-1,4-dihydrocyclopenta[_b_]indol-3(_2H_)-one 4b

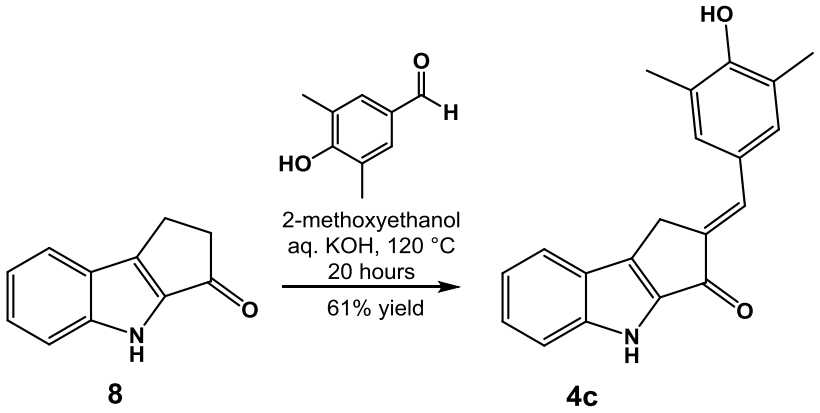


8 **4b**

A mixture of ketone **8** (171 mg, 1 mmol, 1eq.) and 3,5-dimethoxybenzaldehyde (183 mg, 1.1 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (10 mL) and stirred at room temperature for 16 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (15 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **4b** (232 mg, 73 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.3. **IR** ν_{max}(liquid film): 3464 (NH), 3026 (CH), 1674 (C=O) and 1624 (C=C). **m.p.** >220 °C. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ_H 11.86 (1H, br.s, N*H*), 7.80 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.45 (1H, d, *J* = 8.5 Hz, ArC*H*), 7.36 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.30 (1H, m, alkene C*H*), 7.14 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 6.90 (2H, d, *J* = 2.0 Hz, Ar'C*H*), 6.57 (1H, t, *J* = 2.0 Hz, Ar'C*H*), 4.03 (2H, d, *J* = 1.5 Hz, CH_2) and 3.81 (6H, s, Ar'OCH_3). **^{13}C NMR** (100 MHz; $(CD_3)_2SO$): δ_C 181.7− (*C*O), 160.7− (*C*), 143.5− (*C*), 140.7− (*C*), 140.4− (*C*), 139.8− (*C*), 136.8− (*C*), 130.6+ (alkene *C*H), 126.9+ (Ar*C*H), 122.6− (*C*), 121.8+ (Ar*C*H), 120.3+ (Ar*C*H), 113.6+ (Ar*C*H), 108.3+ (Ar'*C*H), 101.3+ (Ar'*C*H), 55.4+ (Ar'O*C*H_3) and 26.2− (CH_2). **MS** *m/z* (+ESI) 320 (100 %, MH^+) and 342 (9 %, MNa^+). **HRMS** (+ESI) Found MH^+ 320.1281, $C_{20}H_{18}NO_3$ requires *MH* 320.1287.

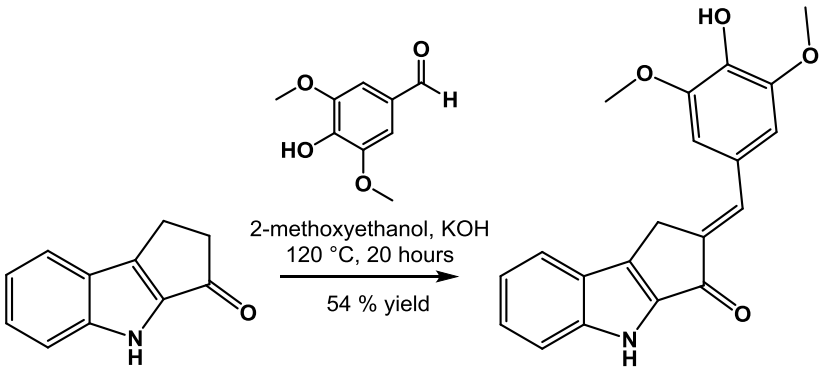
_(E)_-2-(4-Hydroxy-3,5-dimethylbenzylidene)-1,4-dihydrocyclopenta[_b_]indol-3(_2H_)-one 4c



Ketone **8** (128 mg, 0.75 mmol, 1 eq.) and 3,5-dimethyl-4-hydroxybenzaldehyde (123 mg, 0.82 mmol, 1.1 eq.) were dissolved in 2-methoxyethanol (1 mL), followed by the addition of 1 % aqueous KOH solution (0.5 mL). The reaction mixture was heated at 120 °C for 20 hours. The mixture was cooled in an ice bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (15 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10mL: 10mL) to afford compound **4c** (139 mg, 61 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.2. **IR** ν_{max}(liquid film): 3605 (OH), 3463 (NH), 3036 (CH), 1677 (C=O) and 1601 (C=C). **m.p.** > 330 °C. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ_H 11.80 (1H, br.s, N*H*), 8.78 (1H, br.s, O*H*), 7.79 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.44 (1H, d, *J* = 8.5 Hz, ArC*H*), 7.35-7.32 (3H, m, Ar'C*H* and ArC*H*), 7.22 (1H, br.s, alkene C*H*), 7.13 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 3.97 (2H, s, CH_2) and 2.22 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $(CD_3)_2SO$): δ_C 182.1− (*C*O), 155.0− (*C*), 143.3− (*C*), 140.8− (*C*), 138.8− (*C*), 136.7− (*C*), 131.2+ (alkene *C*H), 131.0+ (Ar'*C*H), 126.5+ (Ar*C*H), 126.1− (*C*), 124.7− (*C*), 121.5+ (Ar*C*H), 120.2+ (Ar*C*H), 118.0− (*C*), 113.6+ (Ar*C*H), 26.3− (*C*H_2) and 16.6+ (Ar'*C*H_3). **MS** *m/z* (+ESI) 304 (100 %, MH^+) and 326 (11 %, MNa^+). **HRMS** (+ESI) Found MH^+ 304.1334, $C_{20}H_{18}NO_2$ requires *MH* 304.1338 and found MNa^+ 326.1170, $C_{20}H_{17}NNaO_2$ requires *MNa* 326.1157.

***(E)*-2-(4-Hydroxy-3,5-dimethoxybenzylidene)-1,4-dihydrocyclopenta[*b*]indol-3(2*H*)-one 4d**

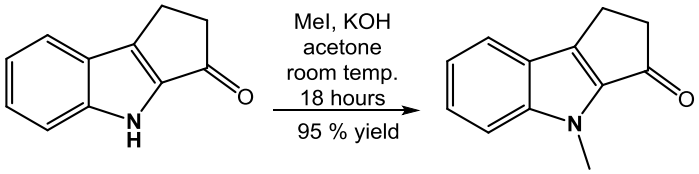


8 **4d**

Ketone **8** (171 mg, 1 mmol, 1 eq.) and 3,5-dimethoxy-4-hydroxybenzaldehyde (200 mg, 1.1 mmol, 1.1 eq.) were dissolved in 2-methoxyethanol (1 mL), followed by the addition of 1 % aqueous KOH solution (0.5 mL). The reaction mixture was heated at 120 °C for 20 hours. The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (15 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **4d** (182 mg, 54 % yield) as a yellow solid.

R_f (70 % EtOAc in light petroleum (b.p. 40-60 °C) 0.6. **IR** ν_{max}(liquid film): 3529 (OH), 3011 (CH), 1673 (C=O) and 1624 (C=C). **m.p.** 237-239 °C. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ_H 11.86 (1H, br.s. N*H*), 8.94 (1H, s, O*H*), 7.80 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.55 (1H, d, *J* = 8.5 Hz, ArC*H*), 7.40 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.29 (1H, br.s, alkene C*H*), 7.17 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.02 (2H, s, Ar'C*H*), 4.03 (2H, s, CH_2) and 3.85 (6H, s, Ar'OCH_3). **^{13}C NMR** (100 MHz; $(CD_3)_2SO$): δ_C 182.0− (*C*=O), 148.1− (*C*), 143.3− (*C*), 140.7− (*C*), 139.0− (*C*), 137.7− (*C*), 137.3− (C), 131.6+ (alkene *C*H), 126.6+ (Ar*C*H), 125.4− (*C*), 122.7− (*C*), 121.6+ (Ar*C*H), 120.2+ (Ar*C*H), 113.6+ (Ar*C*H), 108.5+ (Ar'*C*H), 56.2+ (Ar'OCH_3) and 26.1− (CH_2). **MS** *m/z* (+ESI) 336 (100 %, MH^+) and 358 (12 %, MNa^+). **HRMS** (+ESI) Found MH^+ 336.1228, $C_{20}H_{18}NO_4$ requires *MH* 336.1236 and found MNa^+ 358.1050, $C_{20}H_{17}NNaO_4$ requires *MNa* 358.1055.

4-Methyl-1,4-dihydrocyclopenta[*b*]indol-3(*2H*)-one 10



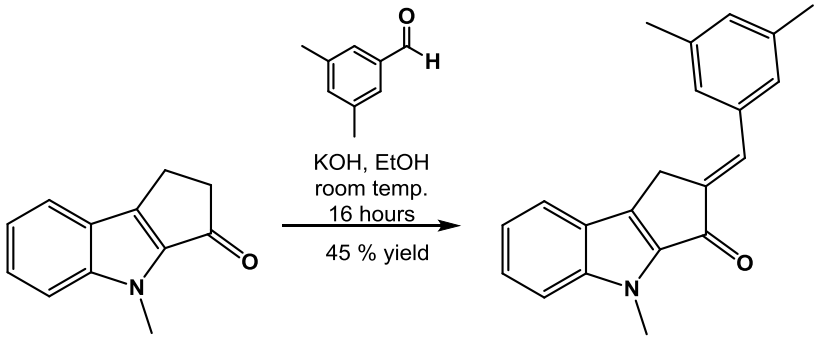
8 **10**

Following the procedure previously reported,[5] MeI (2.4 eq.) was added to a rapidly stirred solution of the indole **8** (6.37 mmol) and KOH (2.9 eq.) in acetone (10 mL/ 1 mmol). After 18 hours at room temperature, the solvent was removed under reduced pressure and H_2O added and acidified to pH 1 with 6M $HCl_{(aq.)}$. The aqueous layer was extracted three times with CH_2Cl_2 and the combined organic layers washed with brine, dried with Na_2SO_4, filtered and concentrated under reduced pressure to afford, without the need for further purification, the methylated product **10** (1.12 g, 95 % yield) as a beige solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.4. **m.p.** 138-142 °C [lit.[6] 135.1-136.1 °C]. **IR** ν_{max}(liquid film): 3033 (CH), 1681 (C=O). **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.69 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.41 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.36 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.17 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 3.91 (3H, s, NCH_3), 3.07-3.05 (2H, m, $COCH_2CH_2$) and 2.99-2.97 (2H, m, $COCH_2CH_2$). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 194.8− (*C*=O), 145.0− (*C*), 144.8− (*C*), 138.9− (*C*), 126.8+ (Ar*C*H), 123.1− (*C*), 121.7+ (Ar*C*H), 120.2+ (Ar*C*H), 110.9+ (Ar*C*H), 41.5− ($COCH_2CH_2$), 30.0+ (NCH_3) and 19.6− ($COCH_2CH_2$). **MS** *m/z* (+ESI) 186 (100 %, MH^+). **HRMS** (+ESI) Found MH^+ 186.0914, $C_{12}H_{12}NO$ requires *MH* 186.0919 and found MNa^+ 208.0736, $C_{12}H_{11}NNaO$ requires *MNa* 208.0738.

Consistent with the spectroscopic data previously reported for this compound.[1,6]

_(E)_-2-(3,5-Dimethylbenzylidene)-4-methyl-1,4-dihydrocyclopenta[_b_]indol-3(_2H_)-one 4e

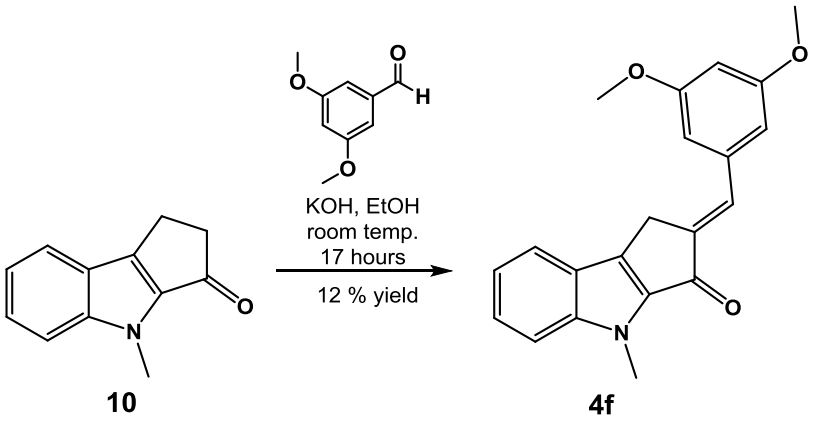


10 **4e**

A mixture of ketone **10** (185 mg, 1 mmol, 1 eq.) and 3,5-dimethylbenzaldehyde (0.15 mL, 1.1 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (10 mL) and stirred at room temperature for 16 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (20 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **4e** (135 mg, 45 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.8. **IR** ν_{max}(liquid film): 3029 (CH), 1678 (C=O) and 1628 (C=C). **m.p.** 174-177 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.76 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.47 (1H, t, *J* = 1.5 Hz, alkene C*H*), 7.42 (1H, ddd, *J* = 8.5, 6.5, 1.0 Hz, ArC*H*), 7.38 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.28 (2H, s, Ar'C*H*), 7.20 (1H, ddd, *J* = 8.0, 6.5, 1.0 Hz, ArC*H*), 7.02 (1H, s, Ar'C*H*), 4.00 (3H, s, NCH_3), 3.95 (2H, d, *J* = 1.5 Hz, CH_2) and 2.39 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 183.4− (*C*=O), 144.6− (*C*), 140.9− (*C*), 139.8− (*C*), 138.6− (*C*), 138.3− (*C*), 135.5− (*C*), 132.0+ (alkene *C*H), 131.0+ (Ar'*C*H), 128.3+ (Ar'*C*H), 126.8+ (Ar*C*H), 123.0− (*C*), 121.9+ (Ar*C*H), 120.5+ (Ar*C*H), 111.0+ (Ar*C*H), 30.3+ (N*C*H_3), 26.5− (*C*H_2) and 21.4+ (Ar'*C*H_3). **MS** *m/z* (+ESI) 302 (100 %, MH^+). **HRMS** (+ESI) Found MH^+ 302.1535, $C_{21}H_{20}NO$ requires *MH* 302.1545 and found MNa^+ 324.1353, $C_{21}H_{19}NNaO$ requires *MNa* 324.1364. **Analysis** (Found: H, 6.47; N, 4.29. $C_{21}H_{19}NO$ requires H, 6.35; N, 4.65 %).

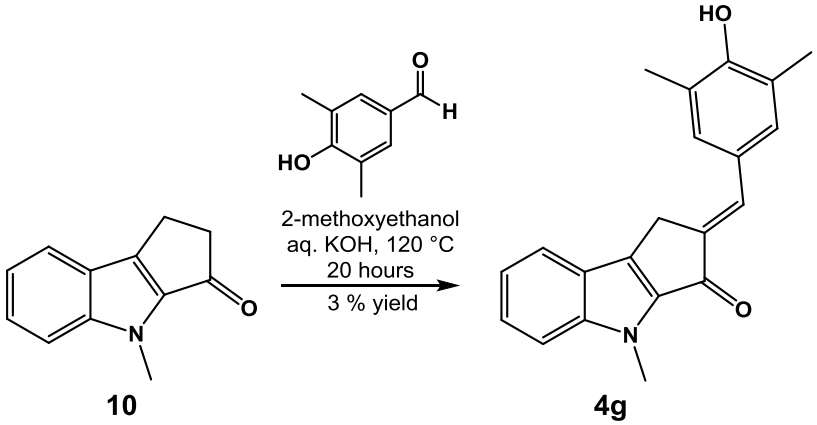
_(E)_-2-(3,5-Dimethoxybenzylidene)-4-methyl-1,4-dihydrocyclopenta[_b_]indol-3(2_H_)-one 4f



A mixture of ketone **10** (185 mg, 1 mmol, 1 eq.) and 3,5-dimethoxybenzaldehyde (183 mg, 1.1 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (10 mL) and stirred at room temperature for 17 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (15 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to collect 301 mg of crude product. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **4f** (40 mg, 12 % yield) as a yellow solid.

R_f (40 % EtOAc in light petroleum (b.p. 40-60 °C) 0.4. **IR** ν_{max}(liquid film): 3014 (CH), 1677 (C=O) and 1592 (C=C). **m.p.** 178-180 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.73 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.44-7.37 (3H, m, ArC*H* and alkene C*H*), 7.20 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 6.81 (2H, d, *J* = 2.0 Hz, Ar'C*H*), 6.51 (1H, t, *J* = 2.0 Hz, Ar'C*H*), 4.01 (3H, s, NCH_3), 3.97 (2H, d, *J* = 1.5 Hz, CH_2) and 3.86 (6H, s, Ar'OCH_3). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 183.1− (*C*=O), 161.0− (*C*), 144.7− (*C*), 140.8− (*C*), 140.7− (*C*), 138.7− (*C*), 137.3− (*C*), 131.6+ (alkene *C*H), 127.0+ (Ar*C*H), 122.9− (*C*), 121.9+ (Ar*C*H), 120.6+ (Ar*C*H), 111.0+ (Ar*C*H), 108.5+ (Ar'*C*H), 101.2+ (Ar'*C*H), 55.5+ (Ar'O*C*H_3), 30.3+ (N*C*H_3) and 26.4− (*C*H_2). **MS** *m/z* (+ESI) 334 (100 %, MH^+) and 356 (8 %, MNa^+). **HRMS** (+ESI) Found MH^+ 334.1445, $C_{21}H_{20}NO_3$ requires *MH* 334.1443 and found MNa^+ 356.1270, $C_{21}H_{19}NNaO_3$ requires *MNa* 356.1263.

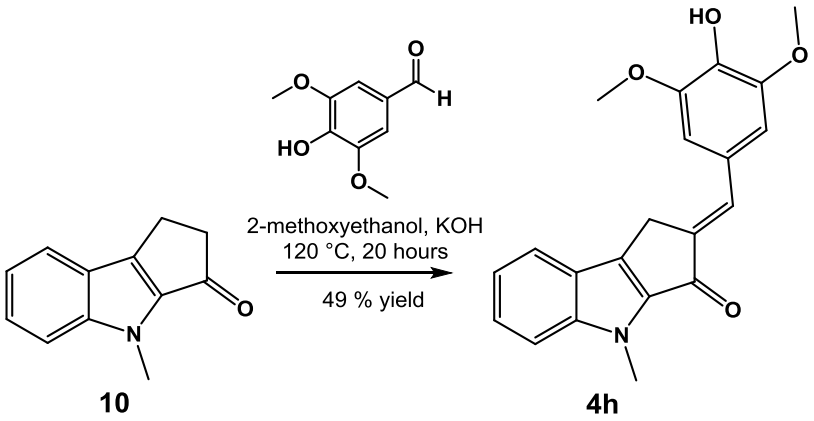
***(E)*-2-(4-Hydroxy-3,5-dimethylbenzylidene)-4-methyl-1,4-dihydrocyclopenta[*b*]indol-3(*2H*)-one 4g**



Ketone **10** (226 mg, 1.22 mmol, 1 eq.) and 3,5-dimethyl-4-hydroxybenzaldehyde (201 mg, 1.34 mmol, 1.1 eq.) were dissolved in 2-methoxyethanol (1.2 mL), followed by the addition of 1 % aqueous KOH solution (0.6 mL). The reaction mixture was heated at 120 °C for 20 hours. The mixture was cooled, H_2O (10 mL) was added and the mixture was neutralised using AcOH. The product was extracted using $CHCl_3$ (3 x 20 mL), the combined organic layers were washed with brine (20 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **4g** (13 mg, 3 % yield) as yellow crystals.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.5. **IR** ν_{max}(liquid film): 3387 (OH), 3022 (CH), 1671 (C=O) and 1600 (C=C). **m.p.** 221-224 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.77 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.42-7.40 (3H, m, ArC*H* and alkene C*H*), 7.34 (2H, s, Ar'C*H*), 7.20 (1H, ddd, *J* = 8.0, 6.5, 1.0 Hz, ArC*H*), 4.86 (1H, s, O*H*), 4.02 (3H, s, NCH_3), 3.95 (2H, d, *J* = 1.5 Hz, CH_2) and 2.32 (6H, s, Ar'CH_3). **MS** *m/z* (+ESI) 318 (100 %, MH^+) and 340 (34 %. MNa^+). **HRMS** Found MH^+ 318.1499, $C_{21}H_{20}NO_2$ requires *MH* 318.1494.

***(E)*-2-(4-Hydroxy-3,5-dimethoxybenzylidene)-4-methyl-1,4-dihydrocyclopenta[*b*]indol-3(*2H*)-one 4h**

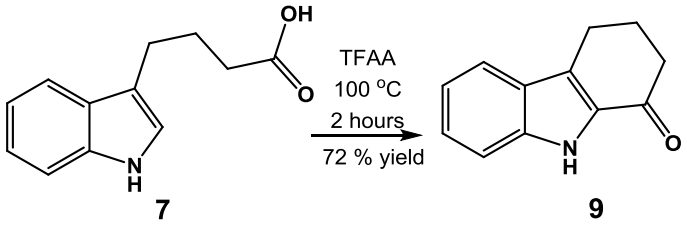


10 **4h**

Ketone **10** (185 mg, 1 mmol, 1 eq.) and 3,5-dimethoxy-4-hydroxybenzaldehyde (200 mg, 1.1 mmol, 1.1 eq.) were dissolved in 2-methoxyethanol (1 mL), followed by the addition of 1 % aqueous KOH solution (0.5 mL). The reaction mixture was heated at 120 °C for 20 hours. The mixture was cooled in an ice-bath and the solid filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (15 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **4h** (171 mg, 49 % yield) as a yellow solid.

IR ν_{max}(liquid film): 3690 (OH), 3464 (NH), 1677 (C=O) and 1627 (C=C). **m.p.** 191-194 °C. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ_H 8.97 (1H, br.s. O*H*), 7.80 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.55 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.40 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.29 (1H, br.s, alkene C*H*), 7.17 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.02 (2H, s, Ar'C*H*), 4.00 (2H, s, CH_2), 3.91 (3H, s, NCH_3) and 3.85 (6H, s, Ar'OCH_3). **^{13}C NMR** (100 MHz; $(CD_3)_2SO$): δ_C 182.3− (*C*=O), 148.1− (*C*), 144.1− (*C*), 140.2− (*C*), 137.8− (*C*), 137.8− (*C*), 137.3− (C), 131.7+ (alkene *C*H), 126.6+ (Ar*C*H), 125.2− (*C*), 122.3− (*C*), 121.8+ (Ar*C*H), 120.3+ (Ar*C*H), 111.5+ (Ar*C*H), 108.5+ (Ar'*C*H), 56.2+ (Ar'O*C*H_3), 30.0+ (NCH_3) and 25.8− (CH_2). **MS** *m/z* (+ESI) 350 (100 %, MH^+) and 372 (12 %, MNa^+). **HRMS** (+ESI) Found MH^+ 350.1376, $C_{21}H_{20}NO_4$ requires *MH* 350.1392 and found MNa^+ 372.1189, $C_{21}H_{19}NNaO_4$ requires *MNa* 372.1212.

2,3,4,9-Tetrahydro-1*H*-carbazol-1-one 9



Method A

4-(Indol-3-yl)butanoic acid **7** (1.22 g, 6 mmol, 1 eq.) in TFAA (0.92 mL, 6.6 mmol, 1.1 eq.) was heated at 100 °C in a sealed pressure tube for 4 hours. On cooling, $CHCl_3$ was added and the solvent was removed under reduced pressure. H_2O (20 mL) and EtOAc (20 mL) were added, the reaction mixture was adjusted to pH 7 using 2M $NaOH_{(aq.)}$ and stirred at room temperature for 16 hours. The layers were separated and the aqueous layer extracted with EtOAc (2 x 20 mL). The combined organic layers were washed with brine (20 mL), dried on Na_2SO_4 and filtered and the solvent was removed under reduced pressure. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column] followed by recrystallisation (EtOAc), gave compound **9** (592 mg, 53 % yield) as a yellow solid.

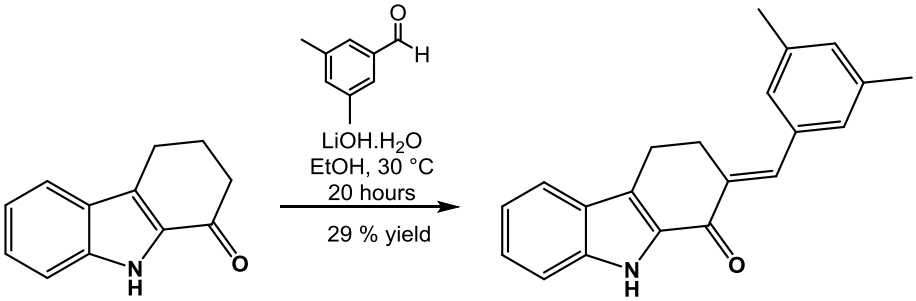
Method B

As above, except on a 2 mmol scale, heated for 2 hours and purification of the crude reaction mixture by column chromatography [silica, CH_2Cl_2 – MeOH gradient column] without aqueous work up, gave compound **9** (268 mg, **72 % yield**) as a pale yellow solid.

R_f (50 % EtOAc in light petroleum (b.p. 40-60 °C) 0.5. **IR** ν_{max}(liquid film): 3450 (NH), 3054 (CH) and 1666 (C=O). **m.p.** 170-172 °C [lit.[7] 168-170 °C]. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 9.31 (1H, br. s, N*H*), 7.66 (1H, d, *J* = 8.0 Hz, ArC*H*), 7.45 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.37 (1H, t, *J* = 8.0 Hz, ArC*H*), 7.15 (1H, t, *J* = 7.5 Hz, ArC*H*), 3.01 (2H, t, *J* = 6.0 Hz, $COCH_2CH_2CH_2$), 2.68 (2H, t, *J* = 6.0 Hz, $COCH_2CH_2CH_2$) and 2.27 (2H, quint, *J* = 6.0 Hz, $COCH_2CH_2CH_2$). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 191.5− (*C*=O), 137.9− (*C*), 131.2− (*C*), 129.6− (*C*), 127.0+ (Ar*C*H), 125.8− (*C*), 121.3+ (Ar*C*H), 120.3+ (Ar*C*H), 112.6+ (Ar*C*H), 38.2− ($COCH_2CH_2CH_2$), 25.0− ($COCH_2CH_2CH_2$) and 21.4− ($COCH_2CH_2CH_2$). **MS** *m/z* (+ESI) 186 (43 %, MH^+) and 208 (100 %, MNa^+). **HRMS** (+ESI) Found MH^+ 186.0909, $C_{12}H_{12}NO$ requires *MH* 186.0919 and found MNa^+ 208.0726, $C_{12}H_{11}NNaO$ requires *MNa* 208.0738.

Consistent with the spectroscopic data previously reported for this compound.[7,8]

***(E)*-2-(3,5-Dimethylbenzylidene)-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5a**

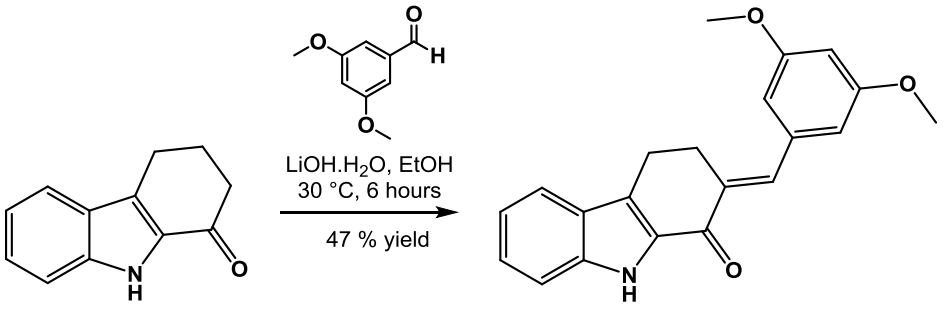


9 **5a**

Following a previously reported procedure,[9] ketone **9** (203 mg, 1.1 mmol, 1 eq.) and $LiOH.H_2O$ (51 mg, 1.21 mmol, 1.1 eq.) in EtOH (3 mL) were stirred for 10 minutes, followed by the addition of 3,5-dimethylbenzaldehyde (0.15 mL, 1.1 mmol, 1.1 eq.). The reaction mixture was stirred at 30 °C for 20 hours. The solvent was removed under reduced pressure and the yellow residue was diluted with H_2O (10 mL) and EtOAc (10 mL). The mixture was neutralised with 6M $HCl_{(aq.)}$ followed by extraction with EtOAc (2 x 10 mL). The combined organic layers were washed with brine (10 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5a** (95 mg, 29 % yield) as a pale yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.8. **IR** ν_{max}(liquid film): 3460 (NH), 3046 (CH), 1651 (C=O) and 1601 (C=C). **m.p.** 209-211 °C (recrystallised from EtOAc). **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 9.21 (1H, br.s, N*H*), 7.80 (1H, br.s, alkene C*H*), 7.70 (1H, dd, *J* = 8.0, 1.0 Hz, ArC*H*), 7.48 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.41 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.20 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.11 (2H, s, Ar'C*H*), 7.04 (1H, s, Ar'C*H*), 3.30 (2H, td, *J* = 6.5, 1.5 Hz, CH_2CH_2C=CH), 3.11 (2H, t, *J* = 6.5 Hz, CH_2CH_2C=CH), 2.41 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 181.1− (*C*=O), 138.6− (*C*), 138.0− (*C*), 136.1− (*C*), 136.0− (*C*), 135.7+ (alkene *C*H), 132.4− (*C*), 130.1+ (Ar'*C*H), 128.3− (*C*), 127.6+ (Ar'*C*H), 127.2+ (Ar*C*H), 126.0− (*C*), 121.4+ (Ar*C*H), 120.5+ (Ar*C*H), 112.5+ (Ar*C*H), 27.7− (CH_2CH_2C=CH), 21.4+ (Ar'CH_3) 20.9− (CH_2CH_2C=CH). **MS** *m/z* (+ESI) 302 (100 %, MH^+) and 324 (32 %, MNa^+). **HRMS** (+ESI) Found MH^+, 302.1546, $C_{21}H_{20}NO$ requires *MH* 302.1545 and found MNa^+ 324.1363, $C_{21}H_{19}NNaO$ requires *MNa* 324.1364.

***(E)*-2-(3,5-Dimethoxybenzylidene)-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5b**



9 **5b**

Method A

A mixture of ketone **9** (260 mg, 1.40 mmol, 1 eq.) and 3,5-dimethoxybenzaldehyde (256 mg, 1.54 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (10 mL) and stirred at room temperature for 16 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (20 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford compound **5b** (158 mg, 34 % yield) as a yellow solid.

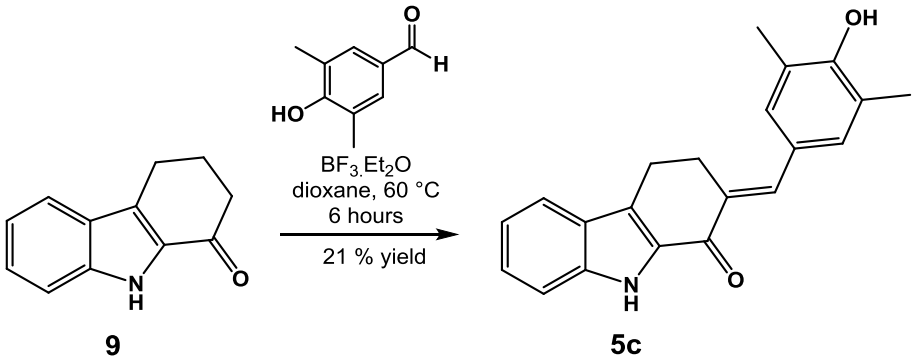
Method B

Following a previously reported procedure,[9] ketone **9** (235 mg, 1.27 mmol, 1 eq.) and $LiOH.H_2O$ (133 mg, 3.18 mmol, 2.5 eq.) in EtOH (2 mL) were stirred for 10 minutes, followed by the addition of 3,5-dimethoxybenzaldehyde (318 mg, 1.91 mmol, 1.5 eq.). The reaction mixture was stirred at 30 °C for 6 hours. The solvent was removed under reduced pressure and the yellow residue was diluted with water (20 mL) and EtOAc (20 mL). The mixture was neutralised with 6M $HCl_{(aq.)}$ followed by extraction with EtOAc (2 x 10 mL). The combined organic layers were washed with brine (20 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure to collect 456 mg of crude product. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5b** (197 mg, **47 % yield**) as a yellow solid.

R_f (70 % EtOAc in light petroleum (b.p. 40-60 °C) 0.9. **IR** ν_{max}(liquid film): 3460 (NH), 3026 (CH), 1652 (C=O) and 1597 (C=C). **m.p.** 168-170 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 8.96 (1H, br.s, N*H*), 7.76 (1H, br.s, alkene C*H*), 7.70 (1H, dd, *J* = 8.0, 1.0 Hz, ArC*H*), 7.48 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.42 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.20 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 6.63 (2H, dd, *J* = 2.5, 0.5 Hz, Ar'C*H*), 6.51 (1H, t, *J* = 2.5 Hz,

Ar'C*H*), 3.87 (6H, s, Ar'OCH_3), 3.30 (2H, td, *J* = 6.5, 2.0 Hz, CH_2CH_2C=CH) and 3.11 (2H, t, *J* = 6.5 Hz, CH_2CH_2C=CH). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 181.7− (*C*=O), 160.8− (*C*), 140.0− (*C*), 138.1− (*C*), 138.0− (*C*), 135.4− (*C*), 135.3+ (alkene *C*H), 132.3− (*C*), 127.3+ (Ar*C*H), 128.0− (*C*), 127.3+ (Ar*C*H), 121.5+ (Ar*C*H), 120.6+ (Ar*C*H), 112.5+ (Ar*C*H), 107.8+ (Ar'CH), 100.4+ (Ar'CH), 55.4+ (OCH_3), 27.7− (CH_2CH_2C=CH) and 20.9− (CH_2CH_2C=CH). **MS** *m/z* (+ESI) 334 (100 %, MH^+) and 356 (9 %, MNa^+). **HRMS** (+ESI) Found MH^+ 334.1433, $C_{21}H_{20}NO_3$ requires *MH* 334.1443 and found MNa^+ 356.1249, $C_{21}H_{19}NNaO_3$ requires *MNa* 356.1263. **Analysis** (Found: H, 5.74; N, 4.20. $C_{21}H_{19}NO_3$ requires H, 5.74; N, 4.20 %).

***(E)*-2-(4-Hydroxy-3,5-dimethylbenzylidene)-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5c**

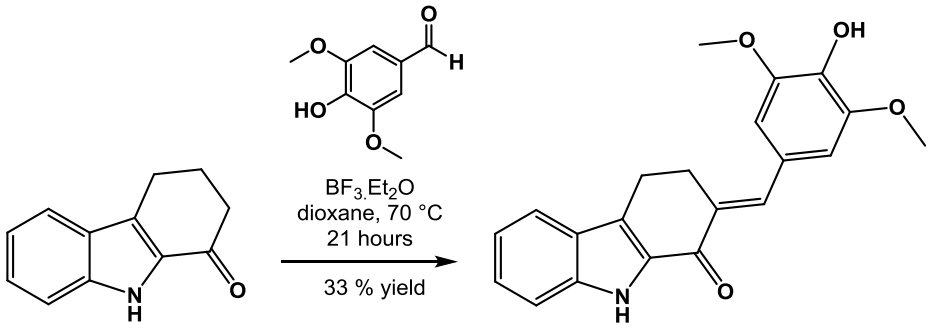


9 **5c**

All glassware was dried under N_2 using a heatgun. Ketone **9** (192 mg, 1.04 mmol, 1 eq.) and 3,5-dimethyl-4-hydroxybenzaldehyde (156 mg, 1.04 mmol, 1 eq.) were added to the flask followed by anhydrous dioxane (2 mL). $BF_3{\cdot}Et_2O$ (0.4 mL, 3.12 mmol, 3 eq.) was added slowly and the reaction mixture was heated at 60 °C for 6 hours.[10] On cooling, H_2O (60 mL), 2M $NaOH_{(aq.)}$ (20 mL) and EtOAc (60 mL) were added to the reaction mixture. The layers were separated and the aqueous layer was extracted with EtOAc (2 x 60 mL). The combined organic layers were washed with brine (60 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure to collect 343 mg of crude product. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5c** (70 mg, 21 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.5. **IR** ν_{max}(liquid film): 3605 (OH), 3460 (NH), 3042 (CH), 1648 (C=O) and 1599 (C=C). **m.p.** 186-188 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 8.80 (1H, br.s, N*H*), 7.73 (1H, br.s, alkene C*H*), 7.70 (1H, dd, *J* = 8.0, 1.0 Hz, ArC*H*), 7.46 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.41 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.20 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.17 (2H, s, Ar'C*H*), 4.84 (1H, br.s, O*H*), 3.32 (2H, td, *J* = 6.5, 1.5 Hz, CH_2CH_2C=CH), 3.11 (2H, t, *J* = 6.5 Hz, CH_2CH_2C=CH) and 2.35 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 181.1− (*C*=O), 152.8− (*C*), 138.4− (*C*), 135.8+ (alkene *C*H), 134.1− (*C*), 132.5− (*C*), 130.7+ (Ar'*C*H), 128.2− (*C*), 127.9− (*C*), 127.0+ (ArCH), 126.0− (*C*), 123.2− (*C*), 121.3+ (ArCH), 120.4+ (ArCH), 112.5+ (ArCH), 27.7− (CH_2CH_2C=CH), 20.8− (CH_2CH_2C=CH) and 16.0+ (Ar'CH_3). **MS** *m/z* (+ESI) 318 (100 %, MH^+) and 340 (19 %, MNa^+). **HRMS** (+ESI) Found MH^+ 318.1486, $C_{21}H_{20}NO_2$ requires *MH* 318.1494 and found MNa^+ 340.1302, $C_{21}H_{19}NNaO_2$ requires *MNa*, 340.1313. **NOESY NMR** Interaction observed between 7.17 (2H, s, Ar'C*H*) and 3.32 (2H, td, *J* = 6.5, 1.5 Hz, CH_2CH_2C=CH) to confirm *E* configuration.

***(E)*-2-(4-Hydroxy-3,5-dimethoxybenzylidene)-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5d**

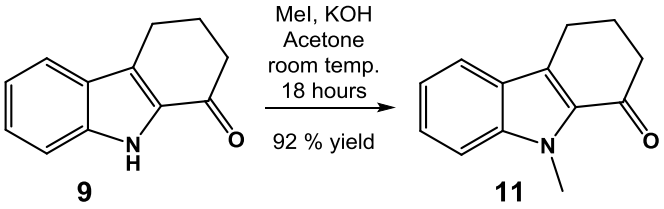


9 **5d**

All glassware was dried under N_2 using a heatgun. Ketone **9** (309 mg, 1.67 mmol, 2.5 eq.) and syringaldehyde (122 mg, 0.67 mmol, 1 eq.) were added to the flask followed by anhydrous dioxane (4 mL). $BF_3{\cdot}Et_2O$ (0.25 mL, 2.01 mmol, 3 eq.) was added slowly and the reaction mixture was heated at 70 °C for 21 hours.[10] On cooling, H_2O (30 mL), 2M $NaOH_{(aq.)}$ (10 mL) and EtOAc (30 mL) were added to the reaction mixture. The layers were separated and the aqueous layer was extracted with EtOAc (2 x 30 mL). The combined organic layers were washed with brine (30 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure to collect 465 mg of crude product. Column chromatography [silica, light petroleum (b.p. 40-60 °C) EtOAc gradient column], gave the product **5d** (78 mg, 33 % yield) as a yellow solid.

R_f (70 % EtOAc in light petroleum (b.p. 40-60 °C) 0.7. **IR** ν_{max}(liquid film): 3534 (OH), 3460 (NH), 3033 (CH), 1649 (C=O) and 1612 (C=C). **m.p.** 155-157 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 9.09 (1H, br.s, N*H*), 7.78 (1H, br.s, alkene C*H*), 7.70 (1H, dd, *J* = 8.0, 1.0 Hz, ArC*H*), 7.47 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.42 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.20 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 6.76 (2H, s, Ar'C*H*), 5.72 (1H, s, O*H*), 3.97 (6H, s, Ar'OCH_3), 3.35 (2H, td, *J* = 6.5, 1.5 Hz, CH_2CH_2CH=CH) and 3.13 (2H, t, *J* = 6.5 Hz, CH_2CH_2CH=CH). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 180.7− (*C*O), 147.0− (*C*), 138.5− (*C*), 135.9+ (alkene *C*H), 135.6− (*C*), 134.7− (*C*), 132.4− (*C*), 128.0− (*C*), 127.4− (*C*), 127.2+ (Ar*C*H), 126.0− (*C*), 121.4+ (Ar*C*H), 120.5+ (Ar*C*H), 112.5+ (Ar*C*H), 107.2+ (Ar'*C*H), 56.5+ (Ar'O*C*H_3), 27.7− (CH_2CH_2CH=CH) and 20.8− (CH_2CH_2CH=CH). **MS** *m/z* (+ESI) 350 (100 %, MH^+). **HRMS** (+ESI) Found MH^+ 350.1394, $C_{21}H_{20}NO_4$ requires *MH*, 350.1392.

9-Methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 11

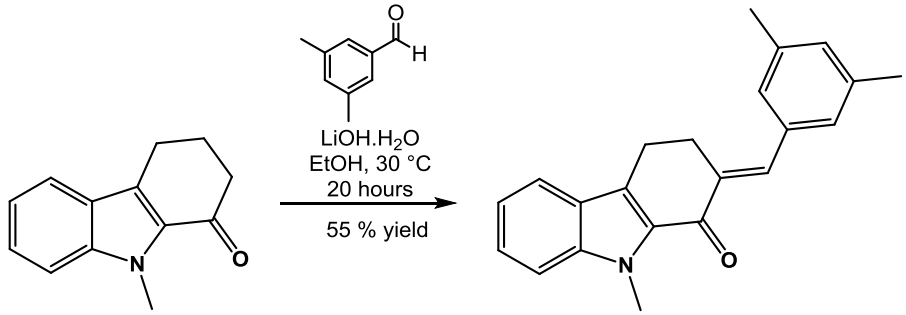


Following the procedure previously reported,[5] MeI (2.4 eq.) was added to a rapidly stirred solution of the indole **9** (1.95 mmol) and KOH (2.9 eq.) in acetone (10 mL/ 1 mmol). After 18 hours at room temperature, the solvent was removed under reduced pressure and H_2O added and acidified to pH 1 with 6M $HCl_{(aq.)}$. The aqueous layer was extracted three times with CH_2Cl_2 and the combined organic layers washed with brine, dried with Na_2SO_4, filtered and concentrated under reduced pressure to afford, without the need for further purification, the methylated product **11** (358 mg, 92 % yield) as a beige solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.8. **IR** ν_{max}(liquid film): 3031 (CH) and 1662 (C=O). **m.p.** 96-99 °C [lit.[11] 100-101 °C]. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.69 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.44 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 7.38 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.18 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz, ArC*H*), 4.11 (3H, s, NCH_3), 3.06 (2H, t, *J* = 6.0 Hz, $COCH_2CH_2CH_2$), 2.69 (2H, t, *J* = 6.0 Hz, $COCH_2CH_2CH_2$) and 2.26 (2H, quint, *J* = 6.0 Hz, $COCH_2CH_2CH_2$). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 192.3− (*C*=O), 139.7− (*C*), 130.5− (*C*), 129.2− (*C*), 126.7+ (Ar*C*H), 124.8− (*C*), 121.3+ (Ar*C*H), 120.0+ (Ar*C*H), 110.3+ (Ar*C*H), 40.0− ($COCH_2CH_2CH_2$), 31.5+ (N*C*H_3), 24.8− ($COCH_2CH_2CH_2$) and 21.9− ($COCH_2CH_2CH_2$). **MS** *m/z* (+ESI) 200 (100 %, MH^+) and 222 (29 %, MNa^+). **HRMS** (+ESI) Found MH^+ 200.1068, $C_{13}H_{14}NO$ requires *MH* 200.1075 and found MNa^+ 222.0886, $C_{13}H_{13}NNaO$ requires *MNa* 222.0895.

Consistent with the spectroscopic data previously reported for this compound.[1,11]

***(E)*-2-(3,5-Dimethylbenzylidene)-9-methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5e**

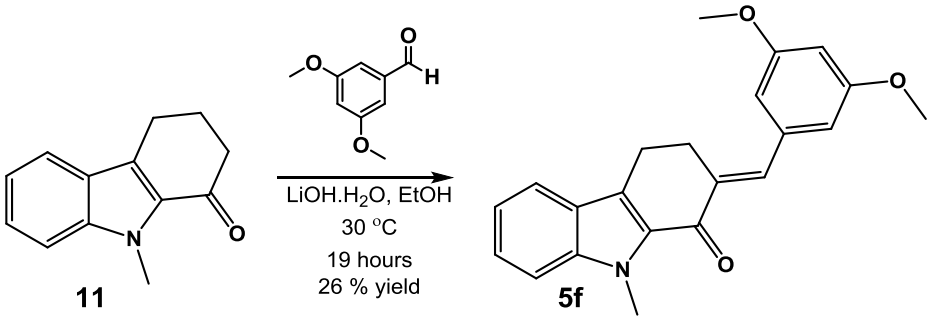


11 **5e**

Following a previously reported procedure,[9] ketone **11** (172 mg, 0.86 mmol, 2 eq.) and $LiOH.H_2O$ (54 mg, 1.29 mmol, 3 eq.) in EtOH (2 mL) were stirred for 10 minutes, followed by the addition of 3,5-dimethylbenzaldehyde (58 mg, 0.43 mmol, 1 eq.). The reaction mixture was stirred at 30 °C for 20 hours and the solvent was removed under reduced pressure. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5e** (75 mg, 55 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.9. **IR** ν_{max}(liquid film): 3027 (CH), 1651 (C=O) and 1613 (C=C). **m.p.** 96-98 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.77 (1H, br.s, alkene C*H*), 7.69 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.45 (1H, td, *J* = 8.5, 1.0 Hz, ArC*H*), 7.41 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.19 (1H, ddd, *J* = 8.0, 6.5, 1.0 Hz, ArC*H*), 7.09 (2H, s, Ar'C*H*), 7.03 (1H, s, Ar'C*H*), 4.20 (3H, s, NCH_3), 3.24 (2H, td, *J* = 6.0, 1.0 Hz, CH_2CH_2C=C), 3.09 (2H, t, *J* = 6.0 Hz, CH_2CH_2C=C) and 2.40 (6H, s, Ar'CH_3). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ_C 181.9− (*C*=O), 140.4− (*C*), 137.9− (*C*), 137.2− (*C*), 136.3− (*C*), 135.4+ (alkene *C*H), 131.6− (*C*), 129.9+ (Ar'*C*H), 128.3− (*C*), 127.5+ (Ar'*C*H), 126.8+ (Ar*C*H), 124.7− (*C*), 121.3+ (Ar*C*H), 120.1+ (Ar*C*H), 110.3+ (Ar*C*H), 31.7+ (N*C*H_3), 27.7− (CH_2CH_2C=C), 21.4+ (Ar'*C*H_3) and 21.1− (CH_2CH_2C=C). **MS** *m/z* (+ESI) 316 (100 %, MH^+) and 338 (15 %, MNa^+). **HRMS** (+ESI) Found MH^+ 316.1701, $C_{22}H_{22}NO$ requires *MH* 316.1701 and found MNa^+ 338.1517, $C_{22}H_{21}NNaO$ requires *MNa* 338.1521.

***(E)*-2-(3,5-Dimethoxybenzylidene)-9-methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one 5f**



Method A

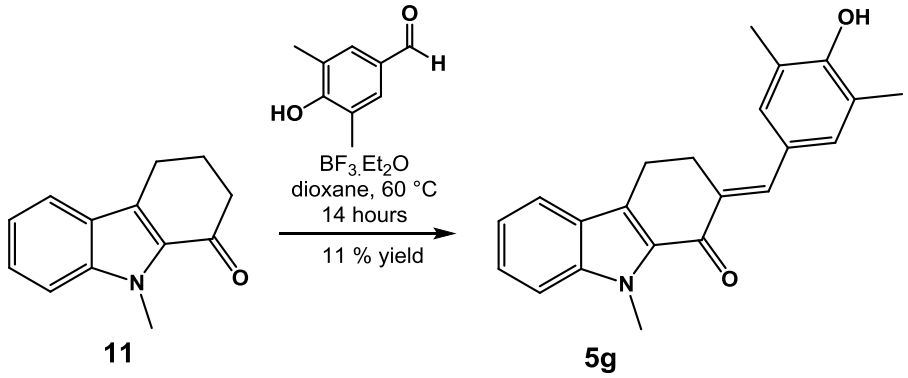
A mixture of ketone **11** (229 mg, 1.15 mmol, 1 eq.) and 3,5-dimethoxybenzaldehyde (211 mg, 1.27 mmol, 1.1 eq.) were treated with 4 % (w/v) ethanolic KOH (11.5 mL) and stirred at room temperature for 16 hours.[4] The mixture was cooled in an ice-bath and the solid was filtered and washed with EtOH: H_2O (10 mL: 10 mL). H_2O (20 mL) was added to the filtrate which was then neutralised using AcOH, followed by a second filtration. The solid was again washed with EtOH: H_2O (10 mL: 10 mL) to afford **5f** (97 mg, 24 % yield) as a yellow solid.

Method B

Following a previously reported procedure,[9] ketone **11** (139 mg, 0.70 mmol, 2 eq.) and $LiOH.H_2O$ (44 mg, 1.05 mmol, 3 eq.) in EtOH (2 mL) were stirred for 10 minutes, followed by the addition of 3,5-dimethoxybenzaldehyde (58 mg, 0.35 mmol, 1 eq.). The reaction mixture was stirred at 30 °C for 19 hours and the solvent was removed under reduced pressure. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5f** (31 mg, **26 % yield**) as yellow crystals.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.8. **IR** ν_{max}(liquid film): 3026 (CH), 1652 (C=O) and 1594 (C=C). **m.p.** 134-135 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.74 (1H, br.s, alkene C*H*), 7.69 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.46 (1H, ddd, *J* = 8.5, 6.5, 1.0 Hz, ArC*H*), 7.41 (1H, dt, *J* = 8.5, 1.0 Hz, ArC*H*), 7.19 (1H, ddd, *J* = 8.0, 6.5, 1.0 Hz, ArC*H*), 6.61 (2H, dd, *J* = 2.5, 0.5 Hz, Ar'C*H*), 6.50 (1H, t, *J* = 2.5 Hz, Ar'C*H*), 4.19 (3H, s, NCH_3), 3.86 (6H, s, Ar'OCH_3), 3.24 (2H, td, *J* = 6.5, 1.0 Hz, CH_2CH_2C=CH) and 3.09 (2H, t, *J* = 6.5 Hz, CH_2CH_2C=CH). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 181.7− (*C*=O), 160.7− (*C*), 140.5− (*C*), 138.3− (*C*), 138.0− (*C*), 134.9+ (alkene *C*H), 131.5− (*C*), 128.6− (*C*), 126.9+ (Ar*C*H), 124.6− (*C*), 121.4+ (Ar*C*H), 120.2+ (Ar*C*H), 110.4+ (Ar*C*H), 107.7+ (Ar'*C*H), 100.2+ (Ar'*C*H), 55.4+ (Ar'O*C*H_3), 31.7+ (N*C*H_3), 27.7− (CH_2CH_2C=CH) and 21.1− (*C*H_2CH_2C=CH). **MS** *m/z* (+ESI) 348 (100 %, MH^+) and 370 (18 %, MNa^+) **HRMS** (+ESI) Found MH^+ 348.1606, $C_{22}H_{22}NO_3$ requires *MH* 348.1600 and found MNa^+ 370.1423, $C_{22}H_{21}NNaO_3$ requires *MNa* 370.1419. **Analysis** (Found: H, 6.06; N, 3.93. $C_{22}H_{21}NO_3$ requires H, 6.09; N, 4.03 %).

_(E)_-2-(4-Hydroxy-3,5-dimethylbenzylidene)-9-methyl-2,3,4,9-tetrahydro-1_H_-carbazol-1-one 5g



11 **5g**

All glassware was dried under N_2 using a heatgun. Ketone **11** (106 mg, 0.53 mmol, 2 eq.) and 3,5-dimethyl-4-hydroxybenzaldehyde (41 mg, 0.27 mmol, 1 eq.) were added to the flask followed by anhydrous dioxane (2 mL). $BF_3{\cdot}Et_2O$ (0.1 mL, 0.8 mmol, 2.3 eq.) was added slowly and the reaction mixture was heated at 60 °C for 14 hours.[10] On cooling, H_2O (40 mL), 2M $NaOH_{(aq.)}$ (20 mL) and EtOAc (40 mL) were added to the reaction mixture. The layers were separated and the aqueous layer was extracted with EtOAc (2 x 40 mL). The combined organic layers were washed with brine (40 mL), dried on Na_2SO_4, filtered and concentrated under reduced pressure to collect 139 mg of crude product. Column chromatography [silica, light petroleum (b.p. 40-60 °C) - EtOAc gradient column], gave the product **5g** (10 mg, 11 % yield) as a yellow solid.

R_f (30 % EtOAc in light petroleum (b.p. 40-60 °C) 0.8. **IR** ν_{max}(liquid film): 3608 (OH), 3038 (CH), 1648 (C=O) and 1601 (C=C). **m.p.** 203-205 °C. **^{1}H NMR** (400 MHz; $CDCl_3$): δ_H 7.72 (1H, br.s, alkene C*H*), 7.69 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.47-7.43 (1H, m, ArC*H*), 7.41 (1H, dt, *J* = 8.0, 1.0 Hz, ArC*H*), 7.19 (1H, ddd, *J* = 8.0, 6.5, 1.0 Hz, ArC*H*), 7.15 (2H, s, Ar'C*H*), 4.81 (1H, br.s, O*H*), 4.19 (3H, s, NCH_3), 3.26 (2H, td, *J* = 6.5, 1.0 Hz, CH_2CH_2C=CH), 3.09 (2H, t, *J* = 6.5 Hz, CH_2CH_2C=CH) and 2.33 (6H, s, Ar'CH_3). **^{13}C NMR** (100 MHz; $CDCl_3$): δ_C 181.9− (*C*O), 152.6− (*C*), 140.4− (*C*), 135.5− (*C*), 135.4+ (alkene *C*H), 131.6− (*C*), 130.5+ (Ar'*C*H), 128.5− (*C*), 127.9− (*C*), 126.7+ (Ar*C*H), 124.7− (*C*), 123.0− (*C*), 121.3+ (Ar*C*H), 120.1+ (Ar*C*H), 110.3+ (Ar*C*H), 31.6+ (N*C*H_3), 27.6− (CH_2CH_2C=CH), 21.0− (CH_2CH_2C=CH) and 15.9+ (Ar'*C*H_3). **MS** *m/z* (+ESI) 332 (100 %, MH^+) and 354 (28 %, MNa^+). **HRMS** (+ESI) Found MH^+ 332.1634, $C_{22}H_{22}NO_2$ requires *MH* 332.1651 and found MNa^+ 354.1453, $C_{22}H_{21}NNaO_2$ requires *MNa* 354.1470. **NOESY NMR** Interaction observed between 7.15 (2H, s, Ar'C*H*) and 3.26 (2H, td, *J* = 6.5, 1.0 Hz, CH_2CH_2C=CH) to confirm *E* configuration.

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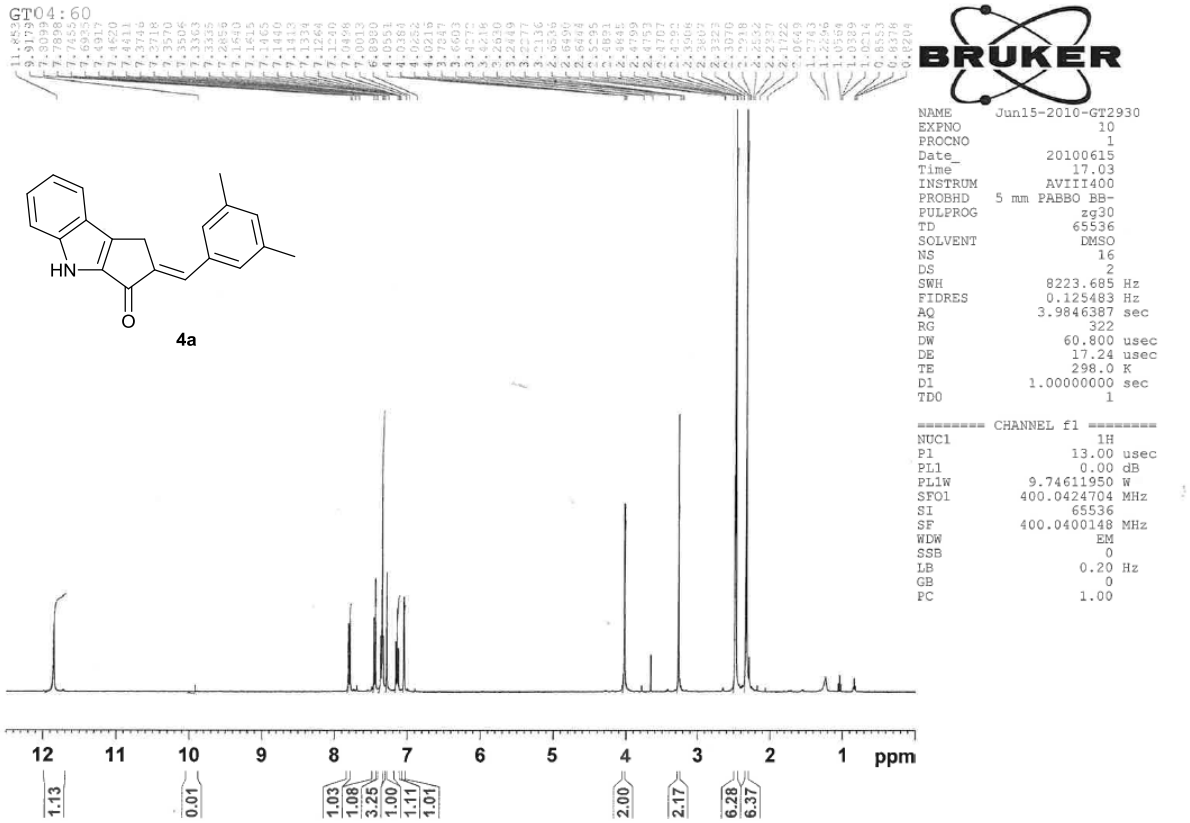
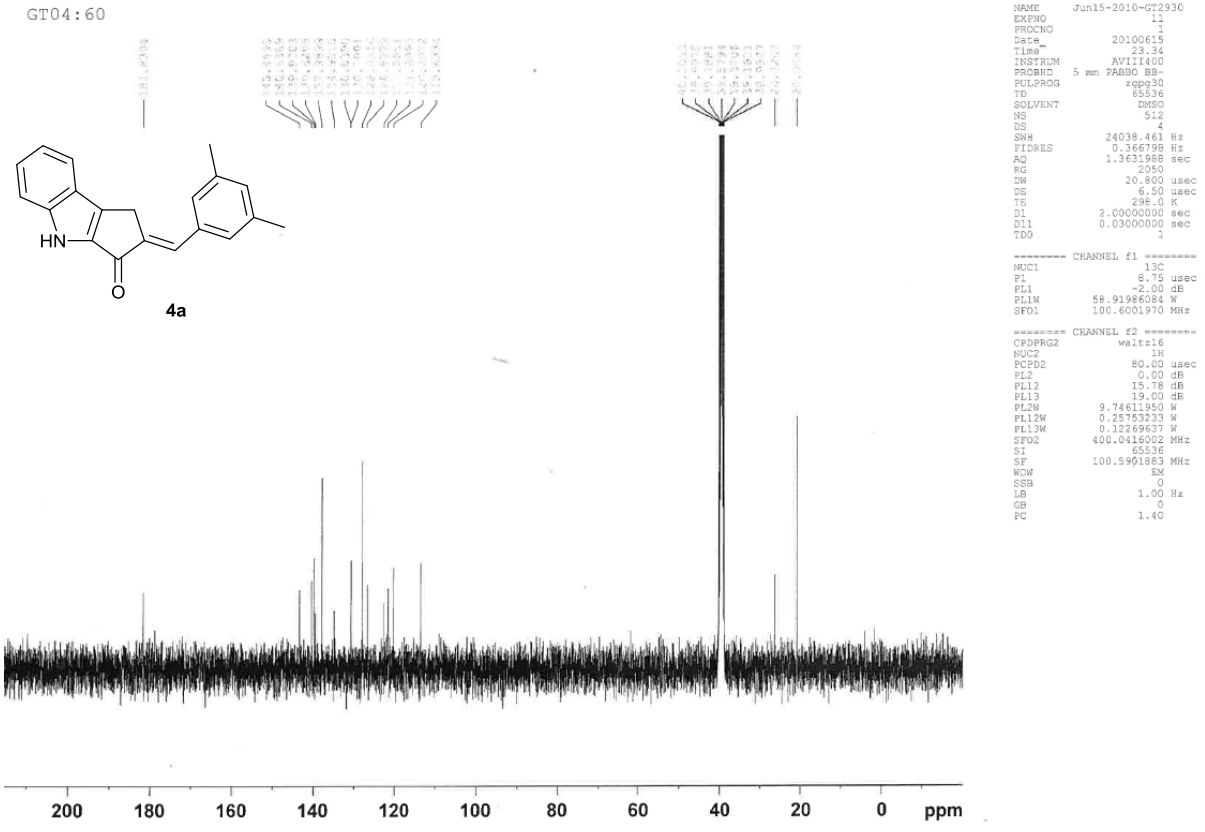
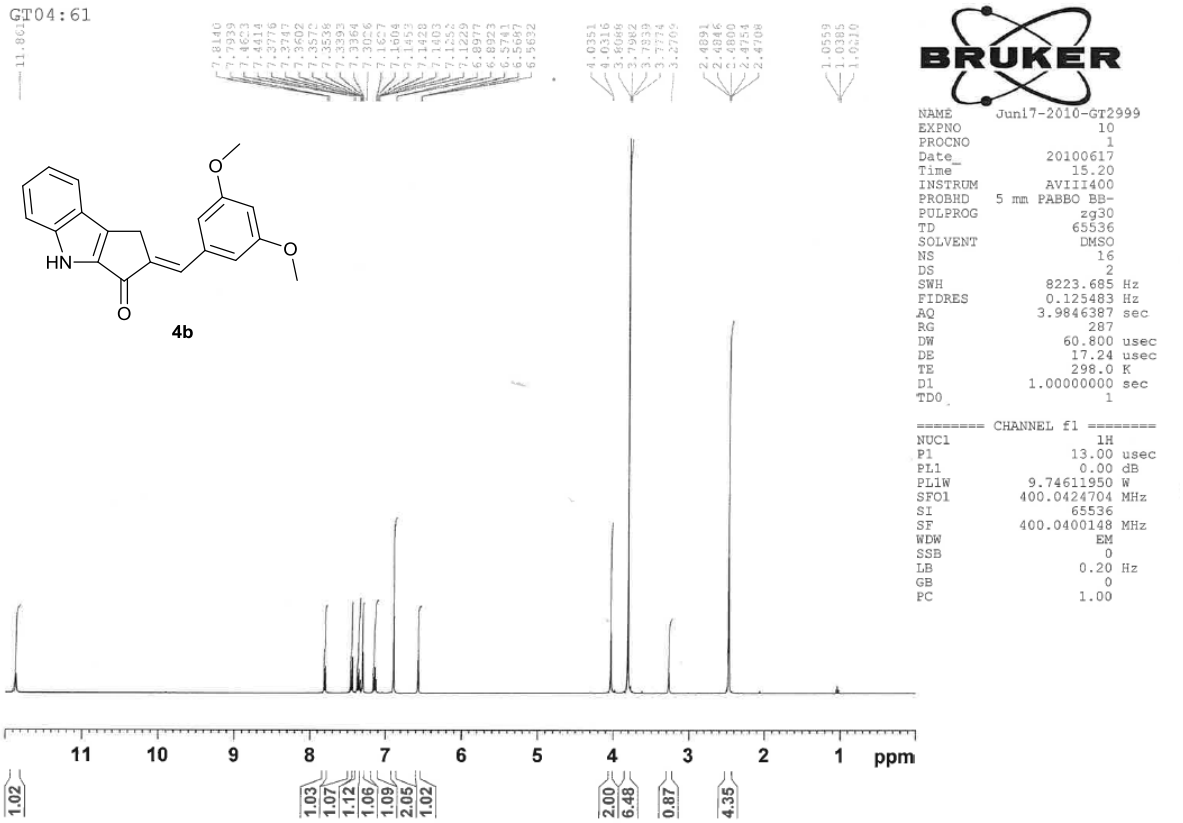
^{1}H and ^{13}C NMR Spectra



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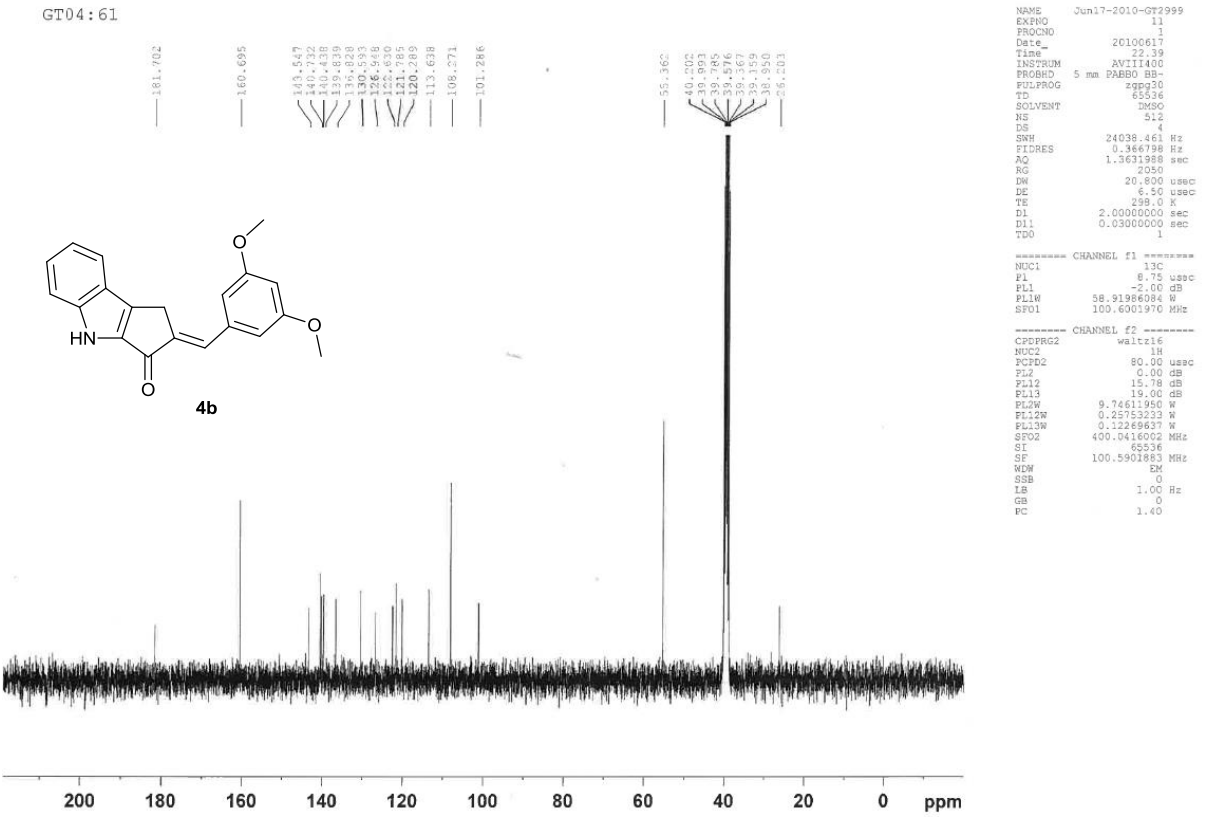
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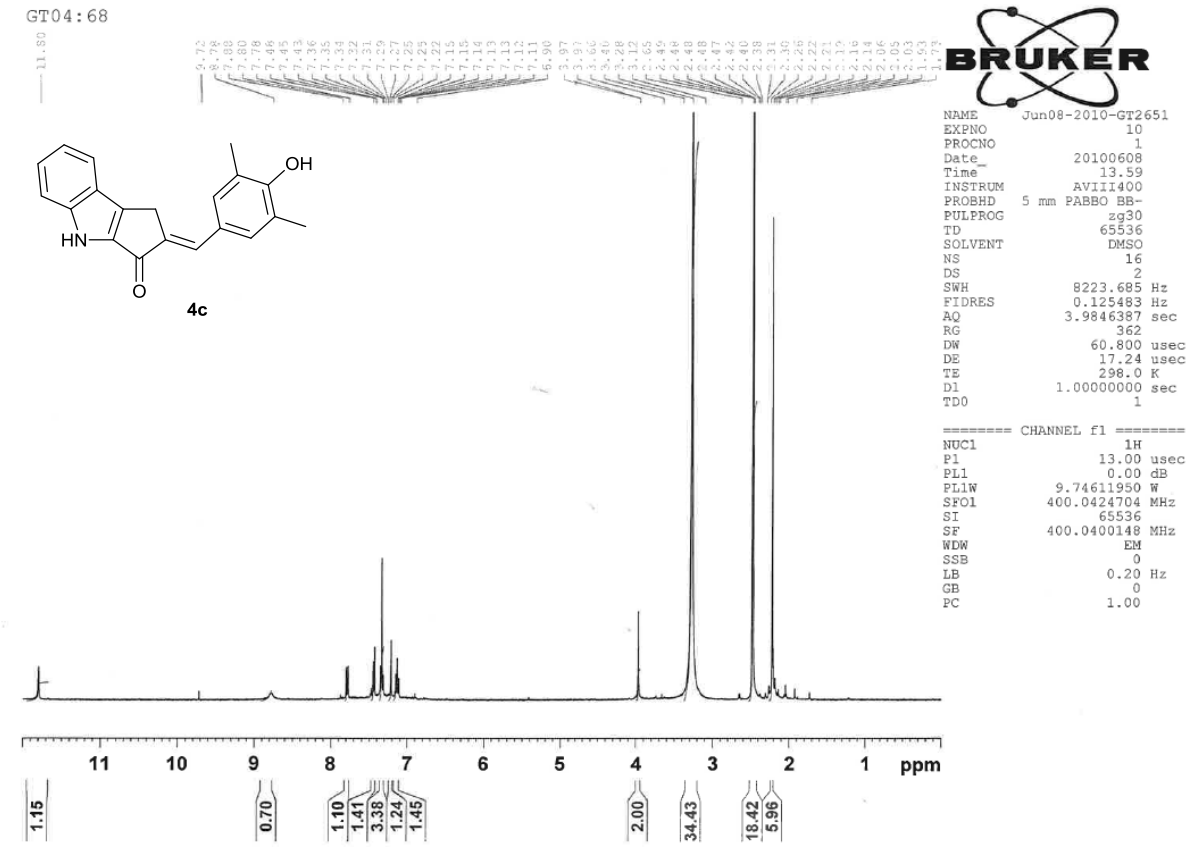
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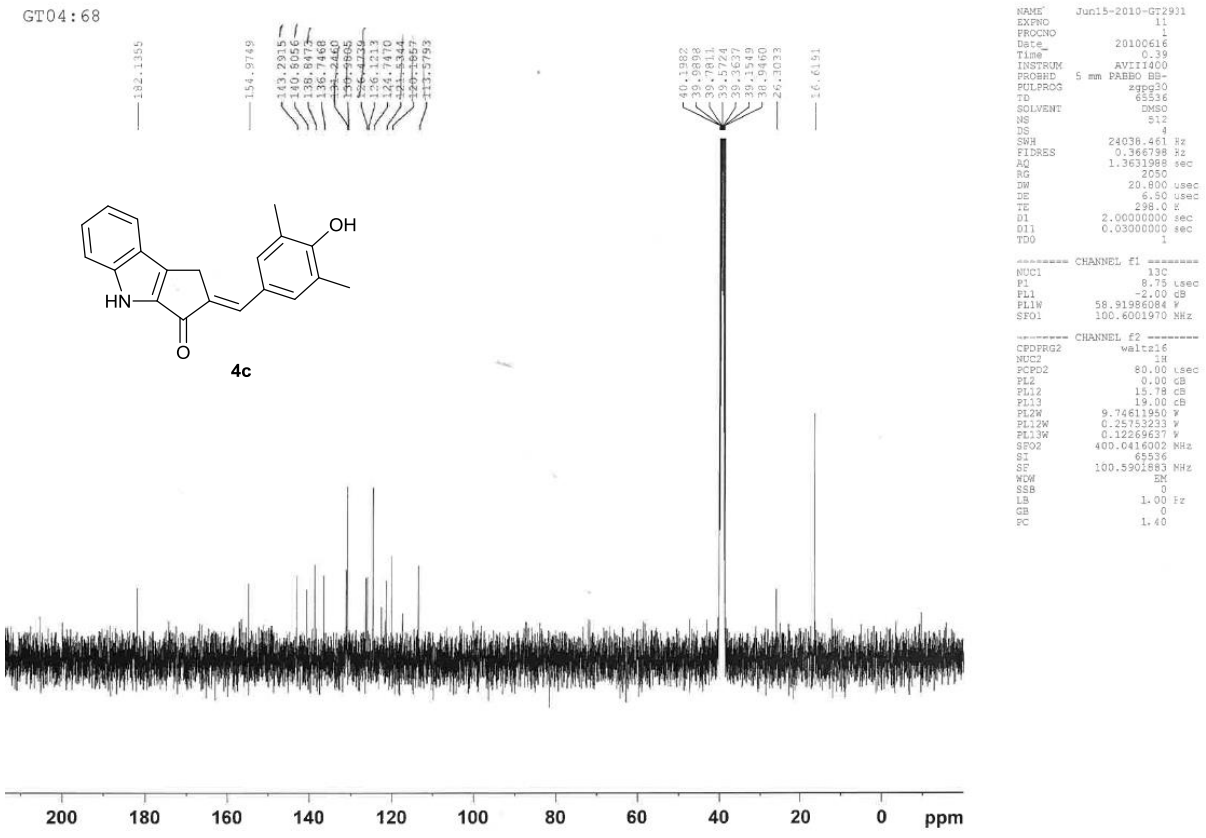
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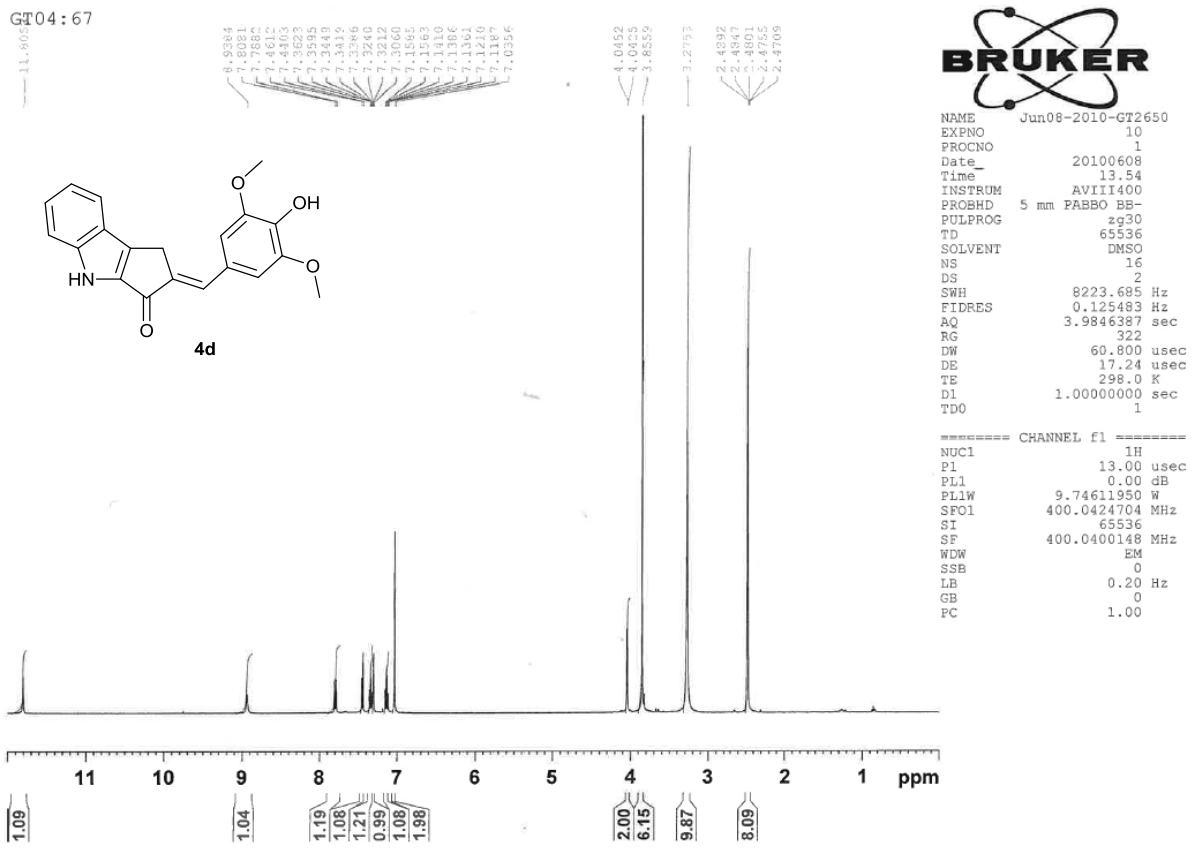
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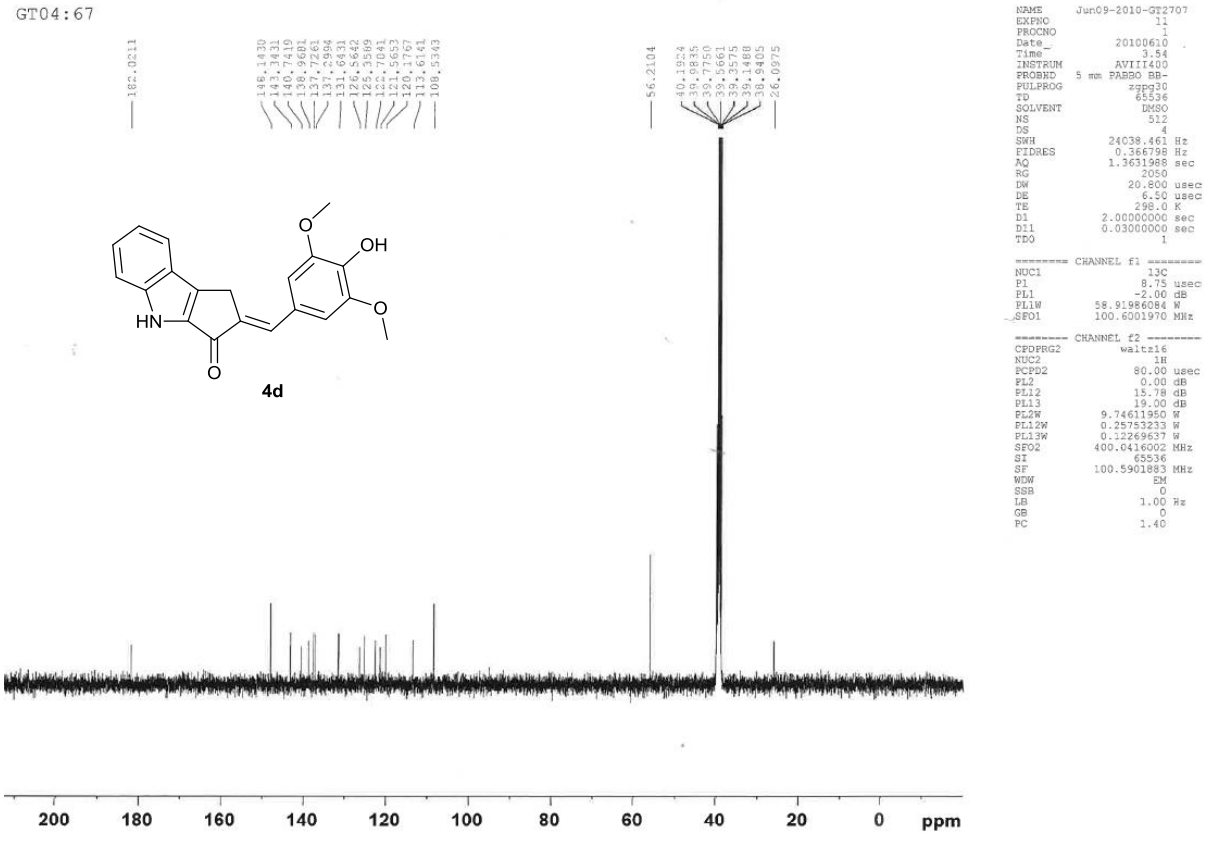
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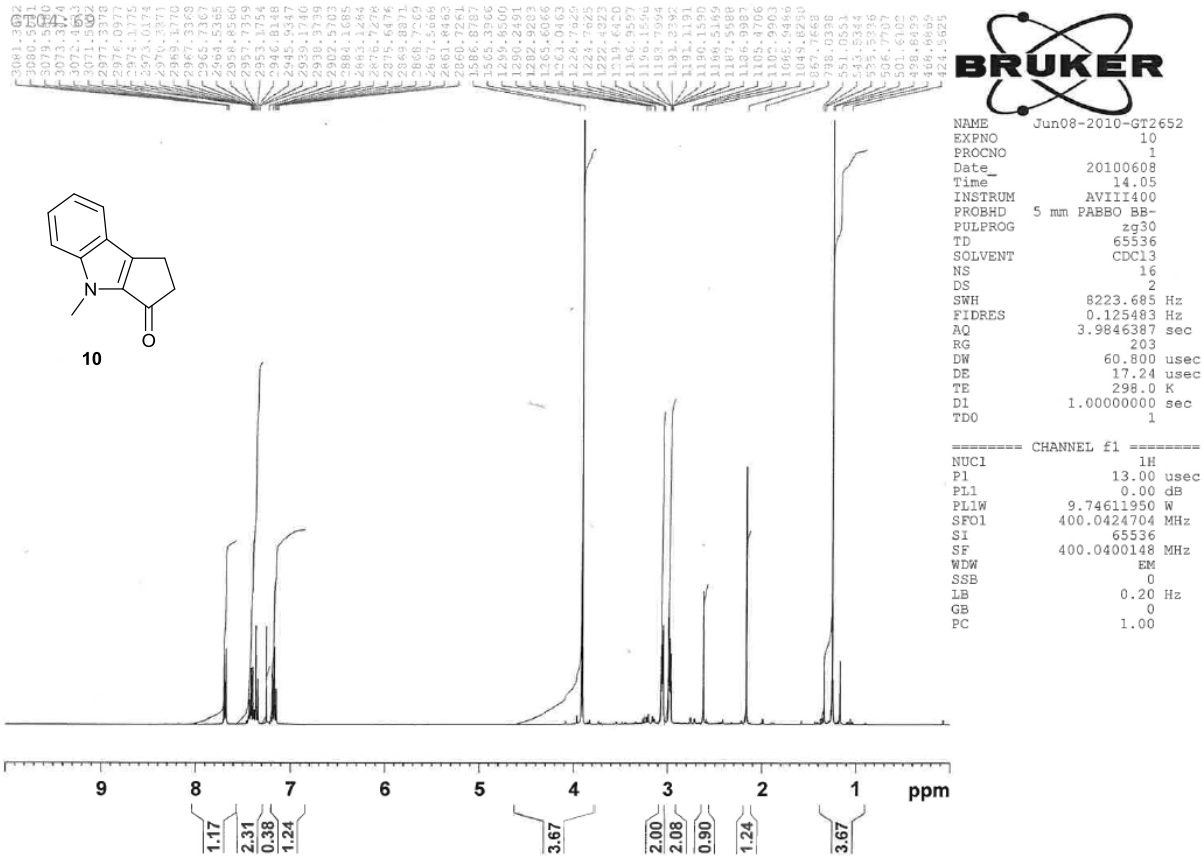
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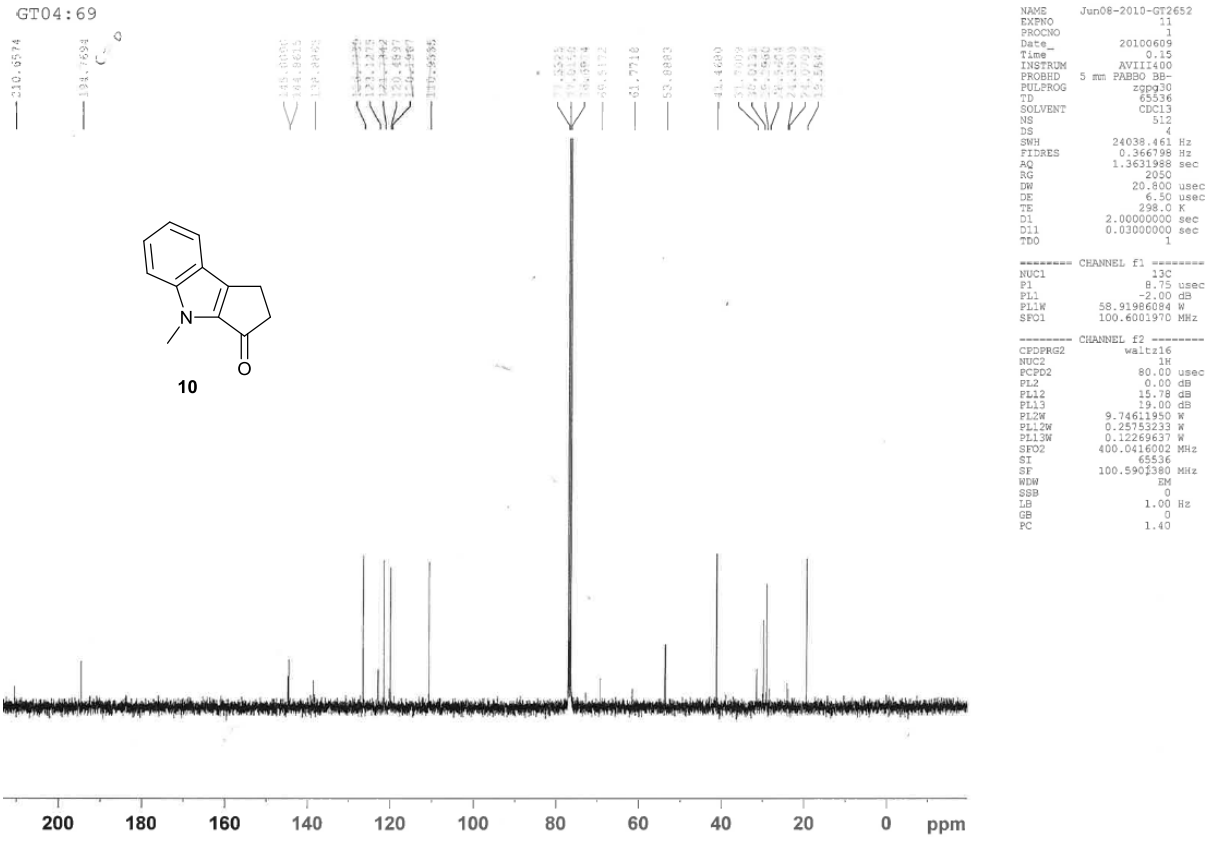
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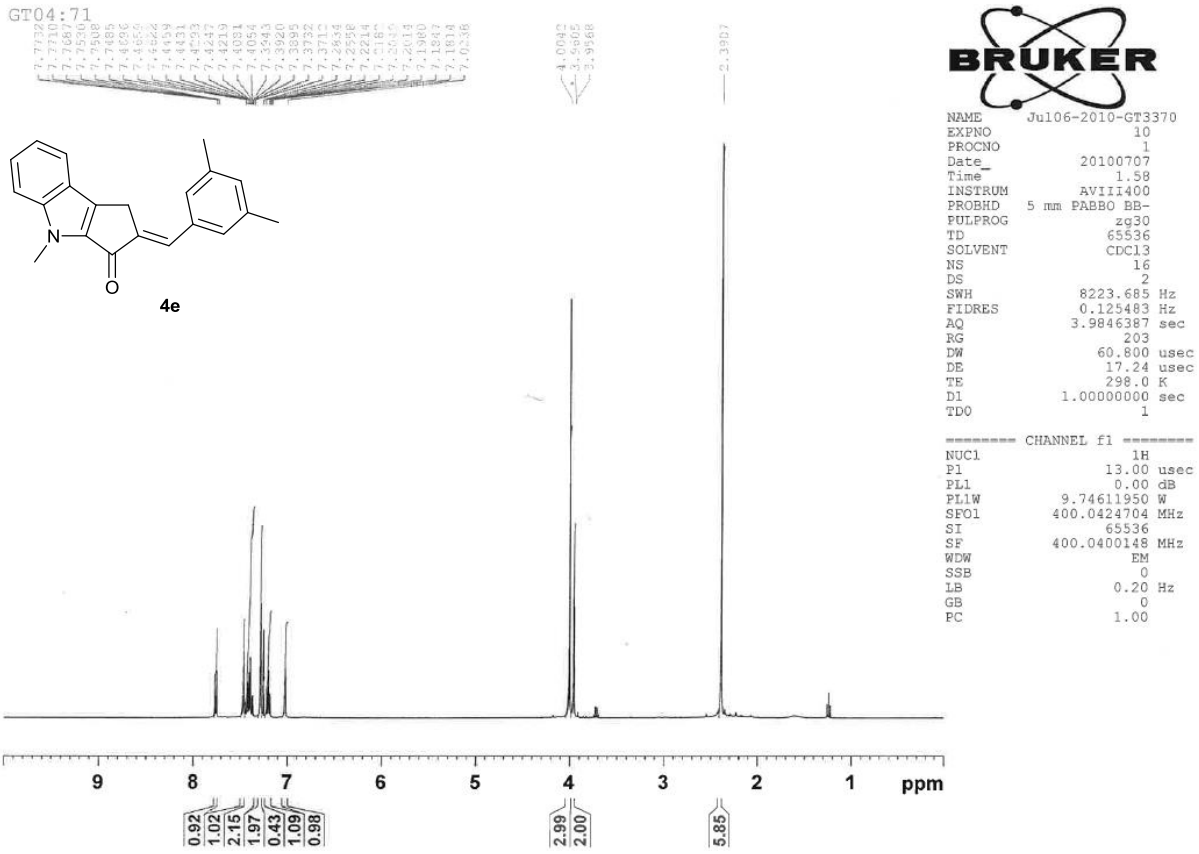
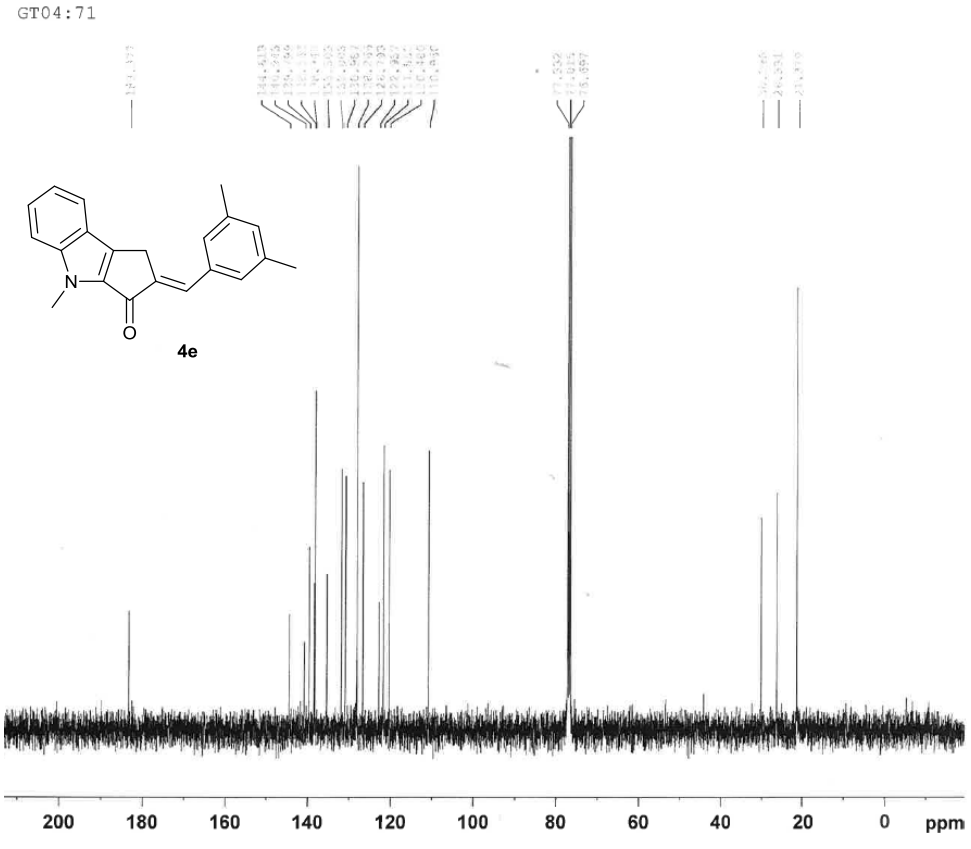
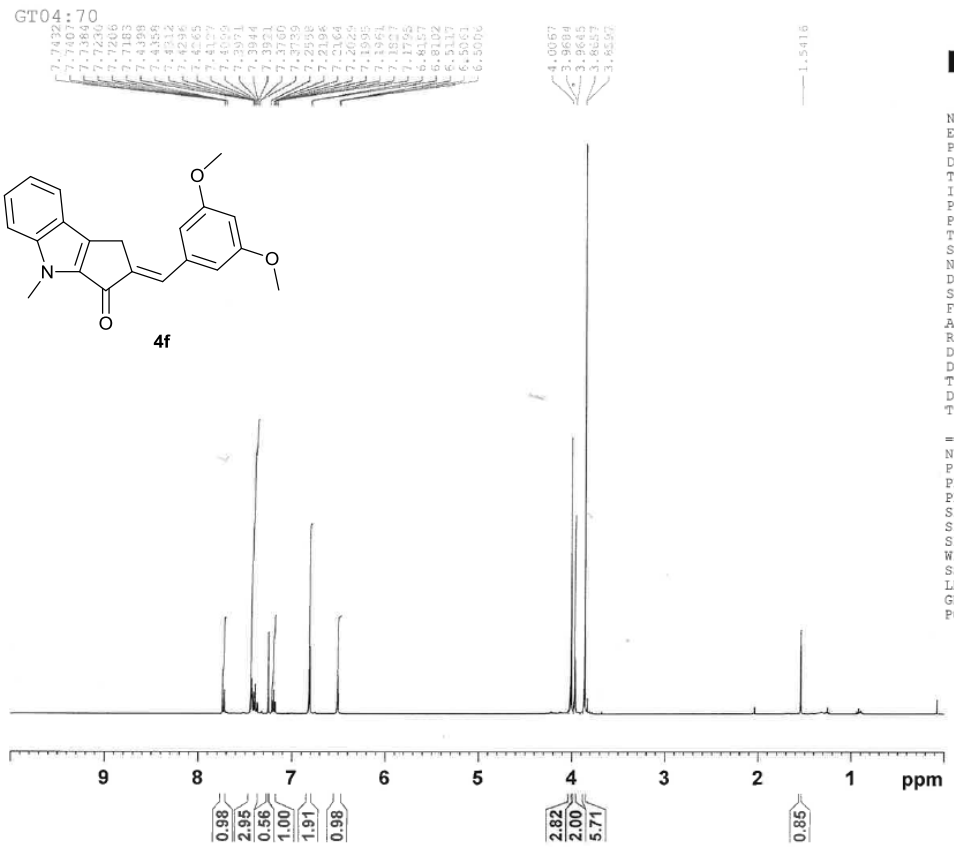
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5902380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
O
10
200
180
160
140
120
100
80
60
40
20
0
ppm




```
NAME          Jul06-2010-GT3370
EXPNO                       10
PROCNO                       1
Date_                 20100707
Time                      1.58
INSTRUM                AVIII400
PROBHD    5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9846387 sec
RG                         203
DW                      60.800 usec
DE                      17.24 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      13.00 usec
PL1                      0.00 dB
PL1W                9.74611950 W
SFO1               400.0424704 MHz
SI                       65536
SF                 400.0400148 MHz
WDW                         EM
SSB                          0
LB                      0.20 Hz
GB                           0
PC                       1.00
```

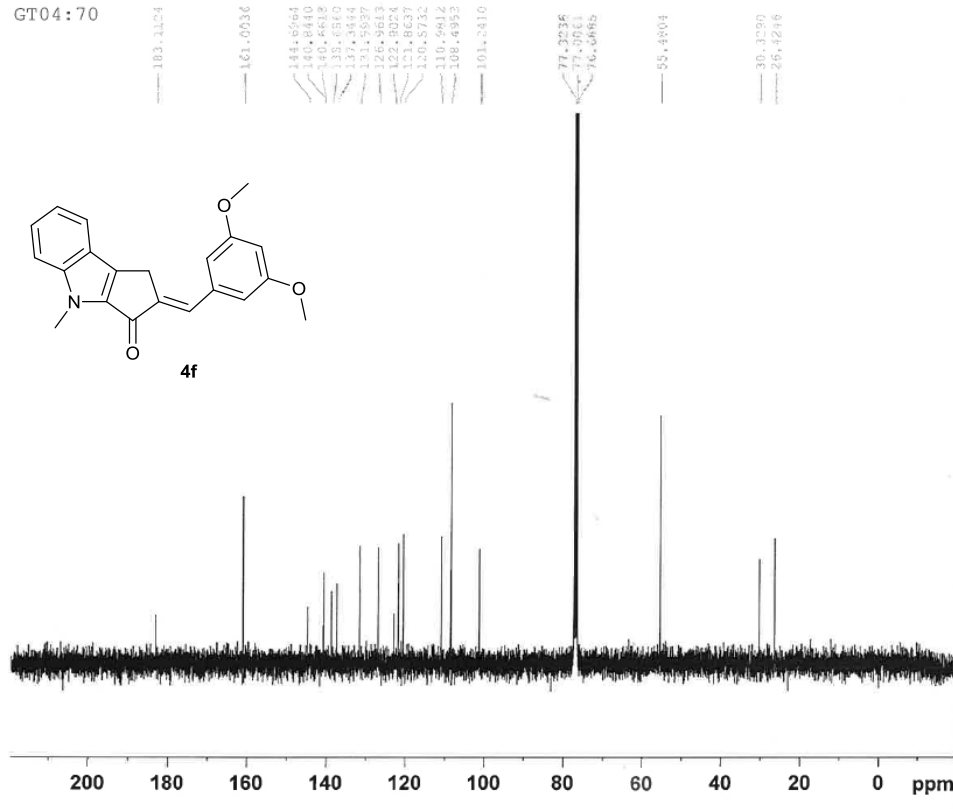



```
NAME          Jul06-2010-GT3370
EXPNO                       11
PROCNO                       1
Date_                 20100707
Time                      2.30
INSTRUM                AVIII400
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         512
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                        2050
DW                      20.800 usec
DE                       6.50 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       8.75 usec
PL1                     -2.00 dB
PL1W               58.91986084 W
SFO1              100.6001970 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.78 dB
PL13                    19.00 dB
PL2W                9.74611950 W
PL12W               0.25753233 W
PL13W               0.12269637 W
SFO2              400.0416002 MHz
SI                       65536
SF                100.5901380 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                       1.40
```



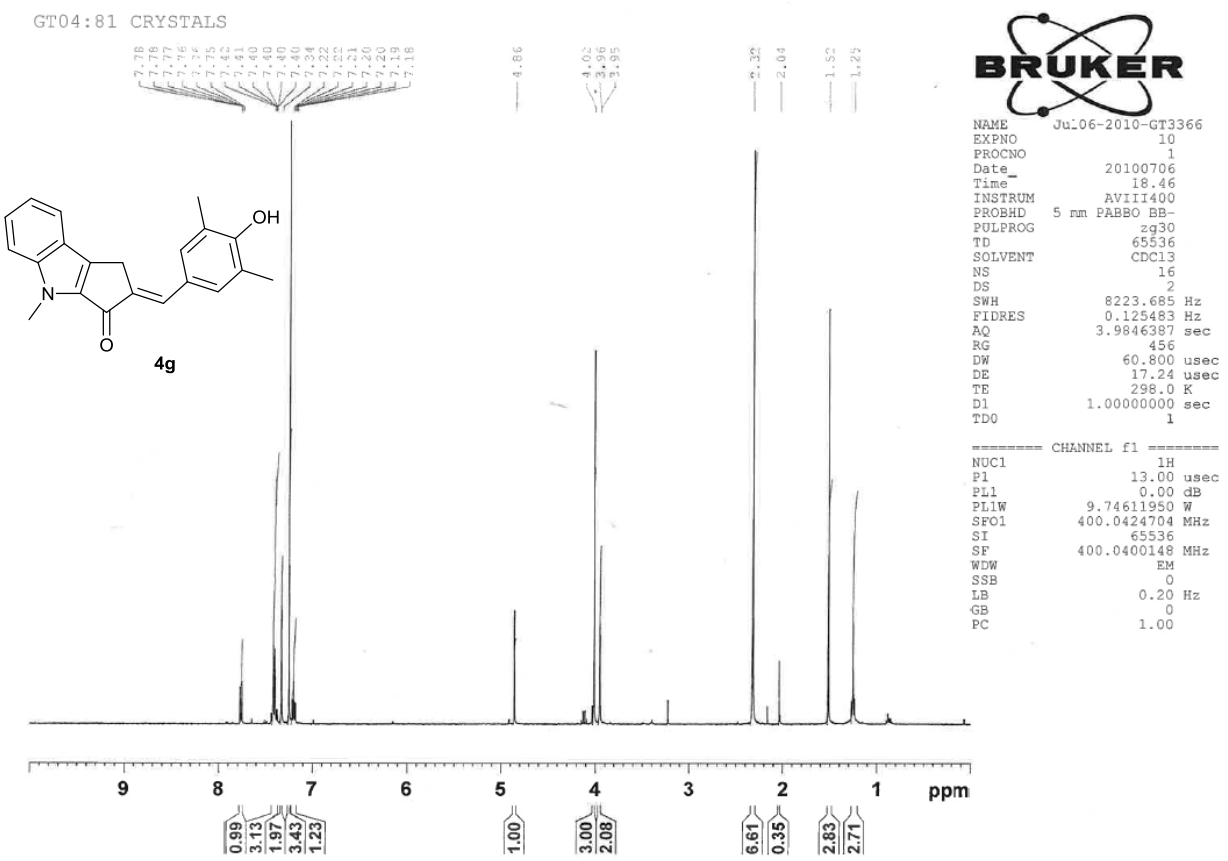
BRUKER

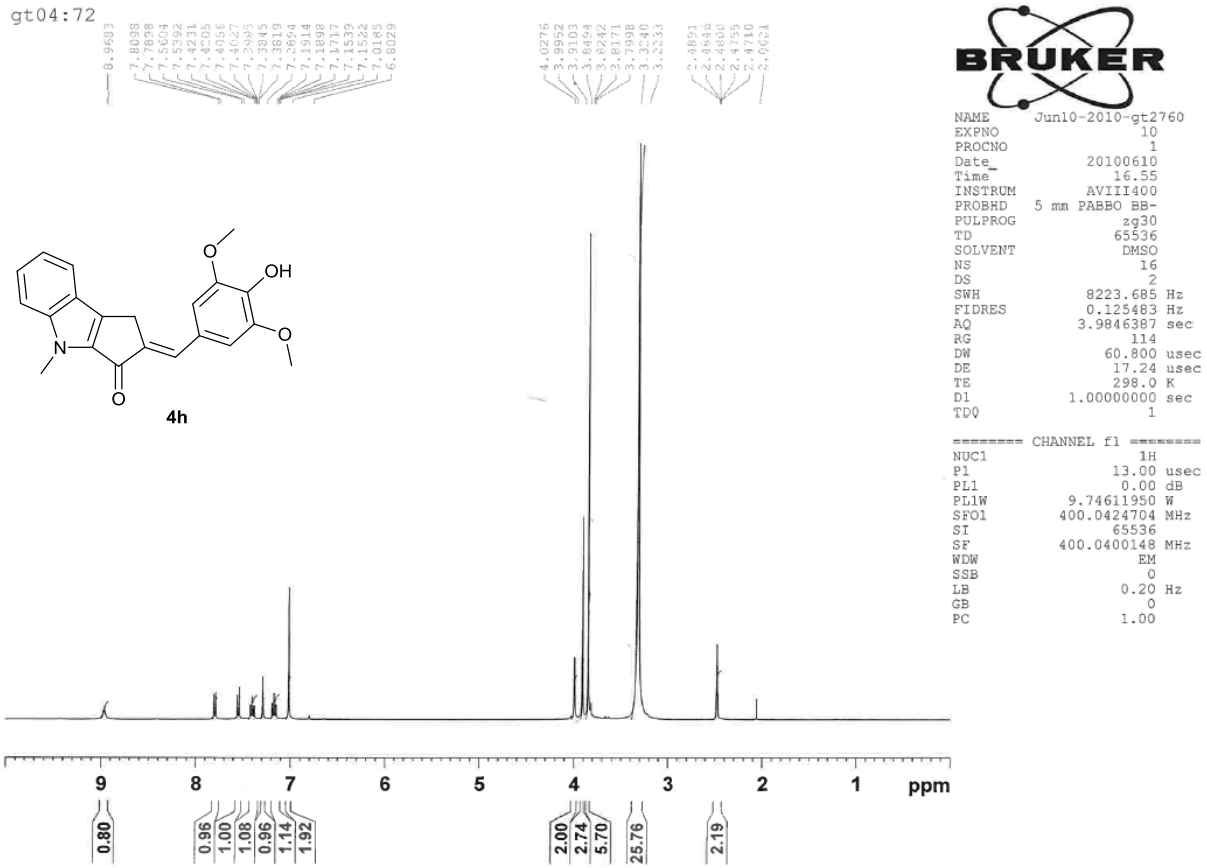
```
NAME          Jul06-2010-GT3369
EXPNO                       10
PROCNO                       1
Date_                 20100707
Time                      0.46
INSTRUM                AVIII400
PROBHD    5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9846387 sec
RG                         287
DW                      60.800 usec
DE                      17.24 usec
TE                      298.0 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      13.00 usec
PL1                      0.00 dB
PL1W                9.74611950 W
SFO1              400.0424704 MHz
SI                       65536
SF                400.0400148 MHz
WDW                         EM
SSB                          0
LB                      0.20 Hz
GB                           0
PC                       1.00
```

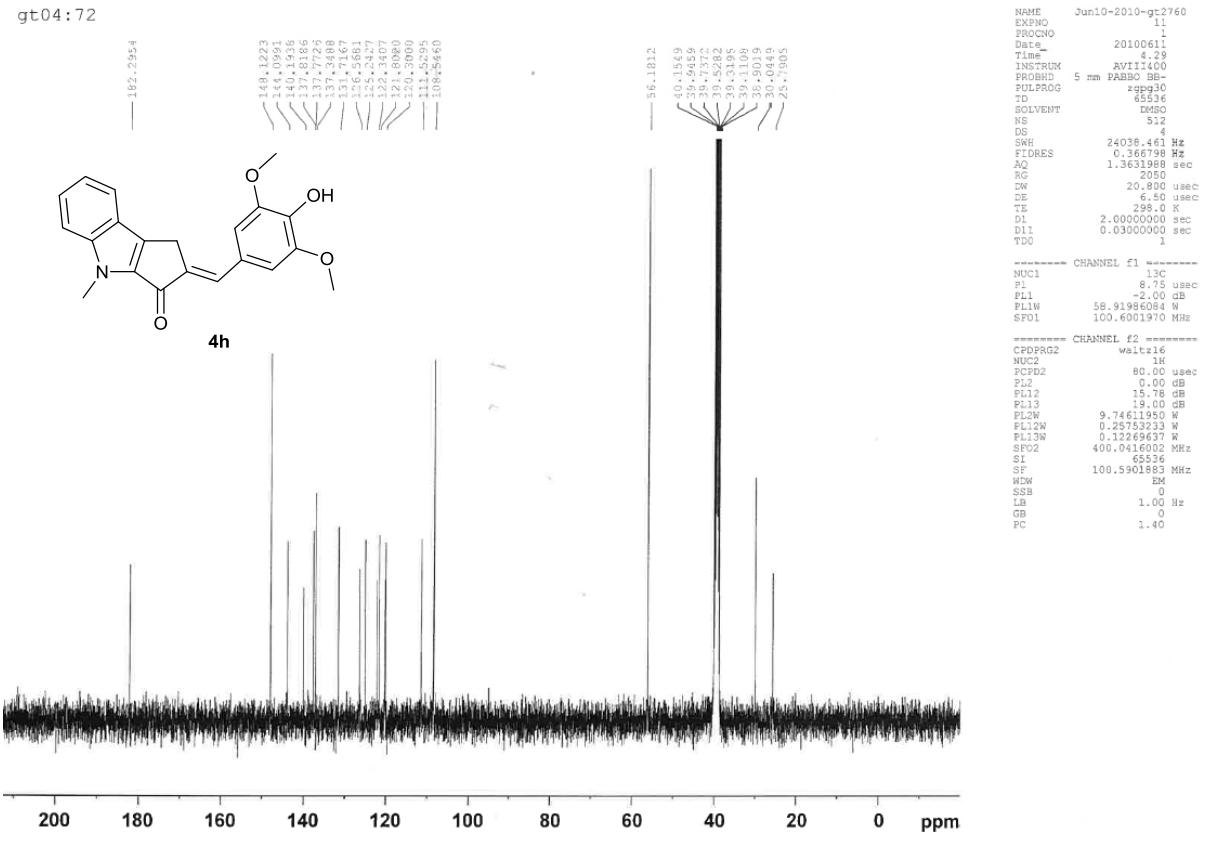


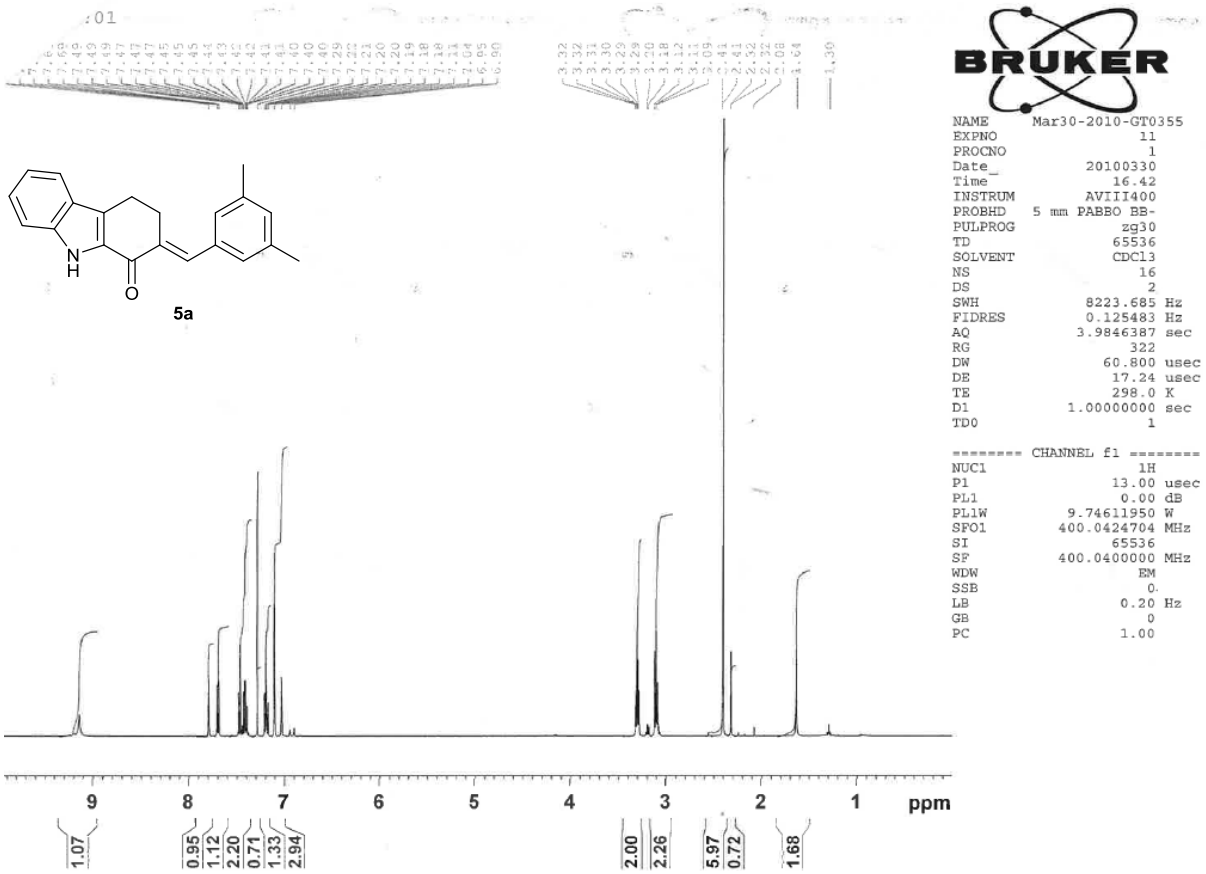
BRUKER

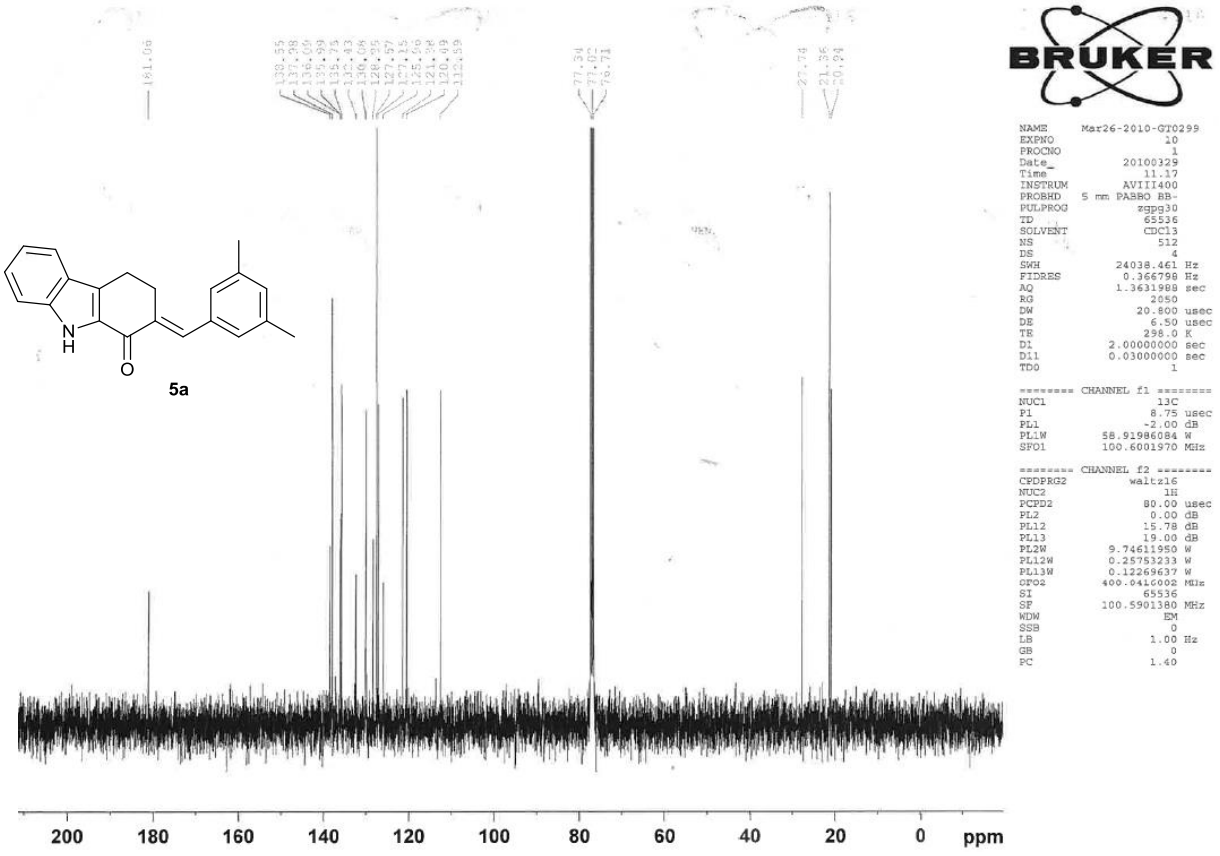
```
NAME          Jul06-2010-GT3369
EXPNO                       11
PROCNO                       1
Date_                 20100707
Time                      1.17
INSTRUM                AVIII400
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         512
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                        2050
DW                      20.800 usec
DE                       6.50 usec
TE                      298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       8.75 usec
PL1                     -2.00 dB
PL1W               58.91986084 W
SFO1              100.6001970 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.78 dB
PL13                    19.00 dB
PL2W                9.74611950 W
PL12W               0.25753233 W
PL13W               0.12269637 W
SFO2              400.0416002 MHz
SI                       65536
SF                100.5901380 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                       1.40
```

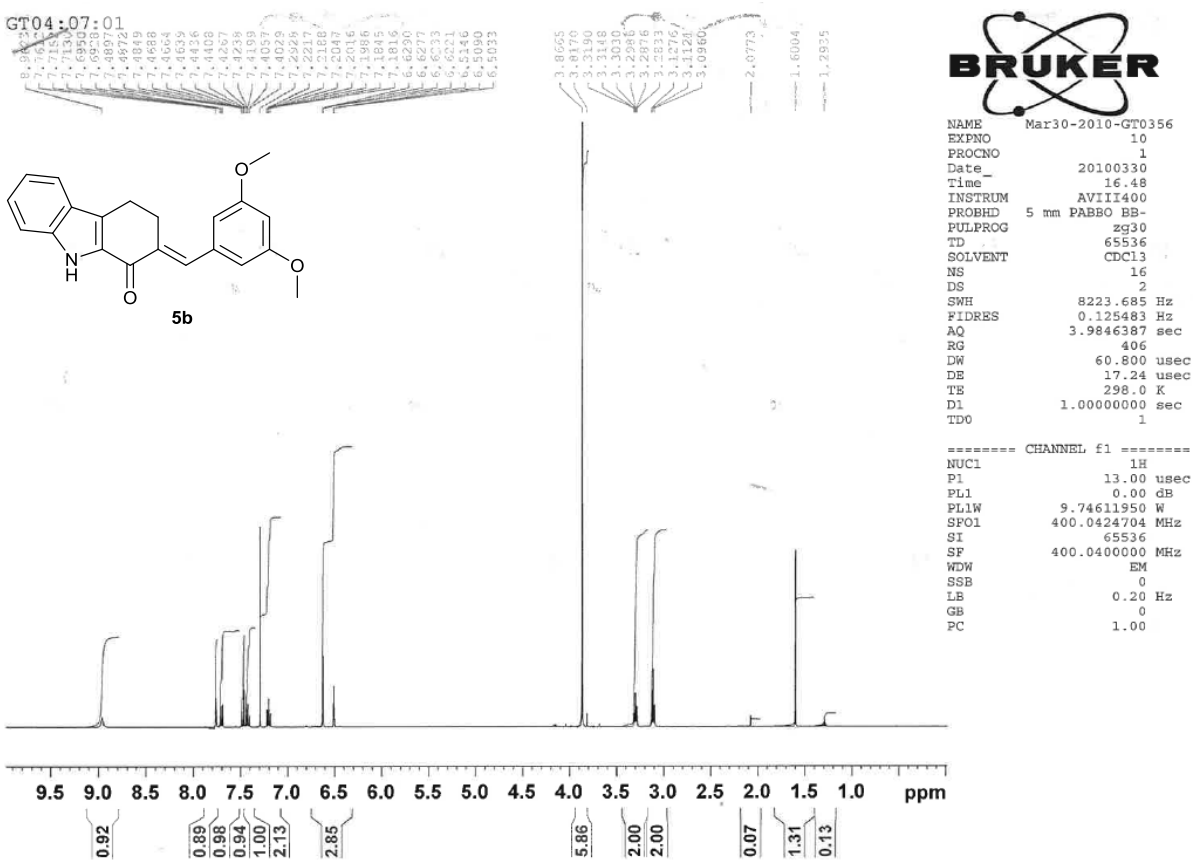

GT04:81 CRYSTALS
7.78
7.78
7.77
7.77
7.76
7.76
7.75
7.75
7.42
7.41
7.40
7.40
7.40
7.40
7.34
7.22
7.21
7.20
7.20
7.19
7.18
4.86
4.02
3.96
3.95
2.32
2.04
1.52
1.25
OH
N
O
4g
BRUKER
NAME Jul06-2010-GT3366
EXPNO 10
PROCNO 1
Date_ 20100706
Time 18.46
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400148 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
0.99
3.13
1.97
3.43
1.23
1.00
3.00
2.08
6.61
0.35
2.83
2.71

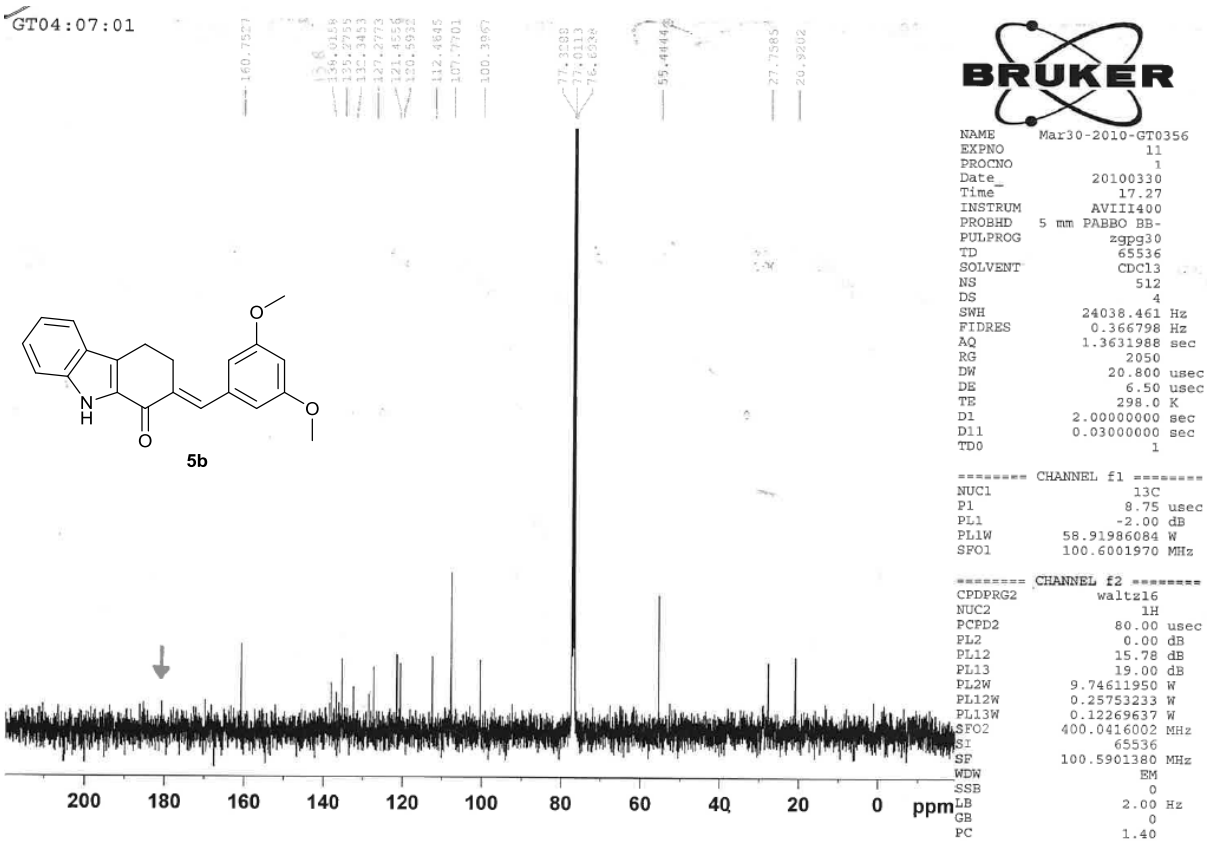

gt04:72
4h
NAME Jun10-2010-gt2760
EXPNO 10
PROCNO 1
Date_ 20100610
Time 16.55
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400148 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
ppm

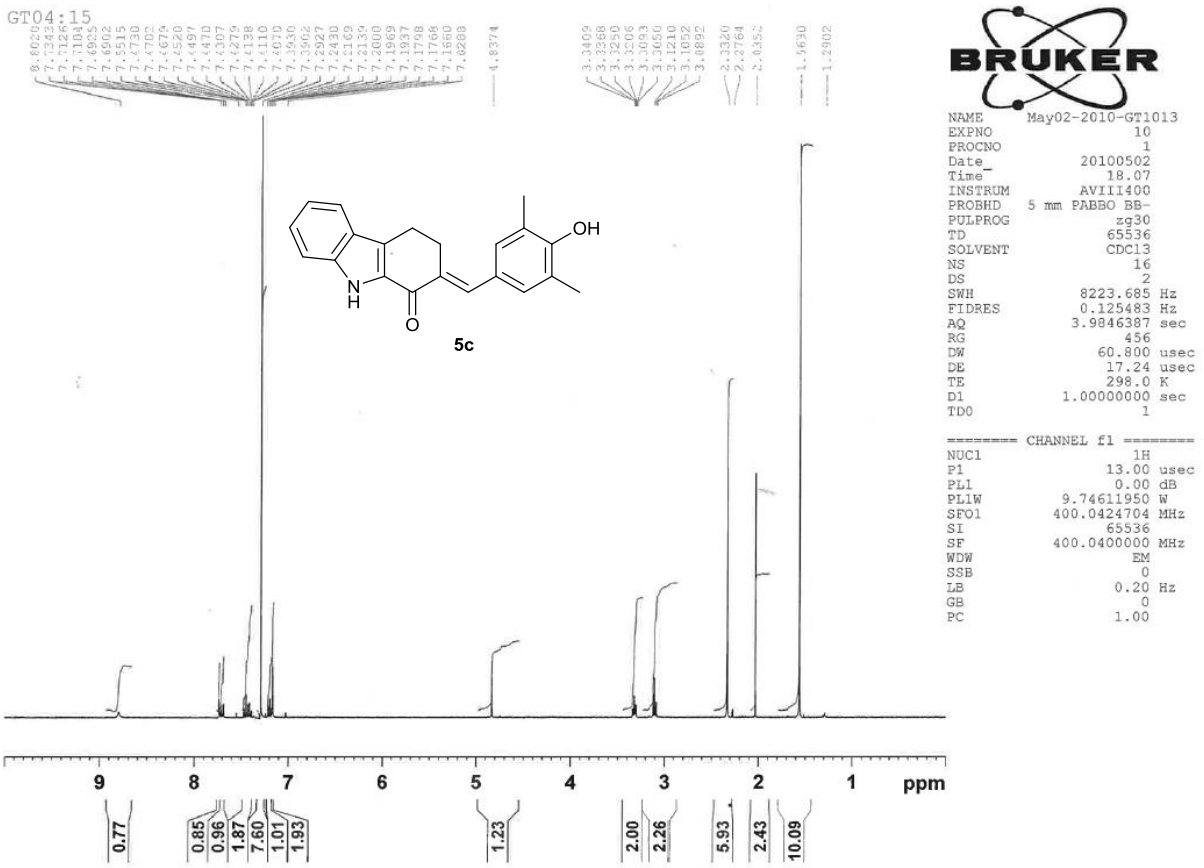

gt04:72
4h
NAME Jun10-2010-gt2760
EXPNO 11
PROCNO 1
Date_ 20100611
Time 4.29
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.76 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5901883 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm


5a
NAME Mar30-2010-GT0355
EXPNO 11
PROCNO 1
Date_ 20100330
Time_ 16.42
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 ppm
1.07 0.95 1.12 2.20 0.71 1.33 2.94 2.00 2.26 5.97 0.72 1.68


5a
NAME Mar26-2010-GT0299
EXPNO 10
PROCNO 1
Date_ 20100329
Time_ 11.17
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

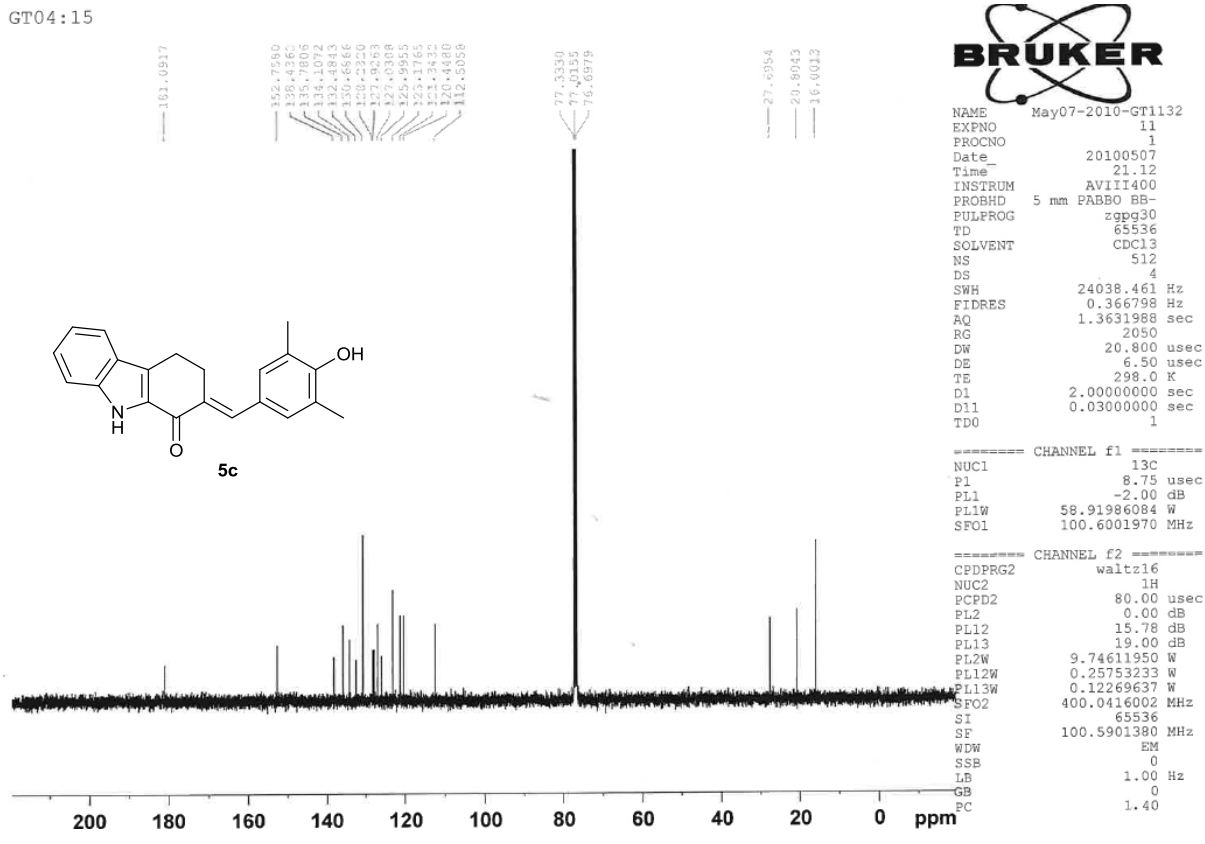

GT04:07:01
5b
BRUKER
NAME Mar30-2010-GT0356
EXPNO 10
PROCNO 1
Date_ 20100330
Time 16.48
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.92 0.89 0.98 0.94 1.00 2.13 2.85 5.86 2.00 2.00 0.07 1.31 0.13


GT04:07:01
5b
BRUKER
NAME Mar30-2010-GT0356
EXPNO 11
PROCNO 1
Date_ 20100330
Time 17.27
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



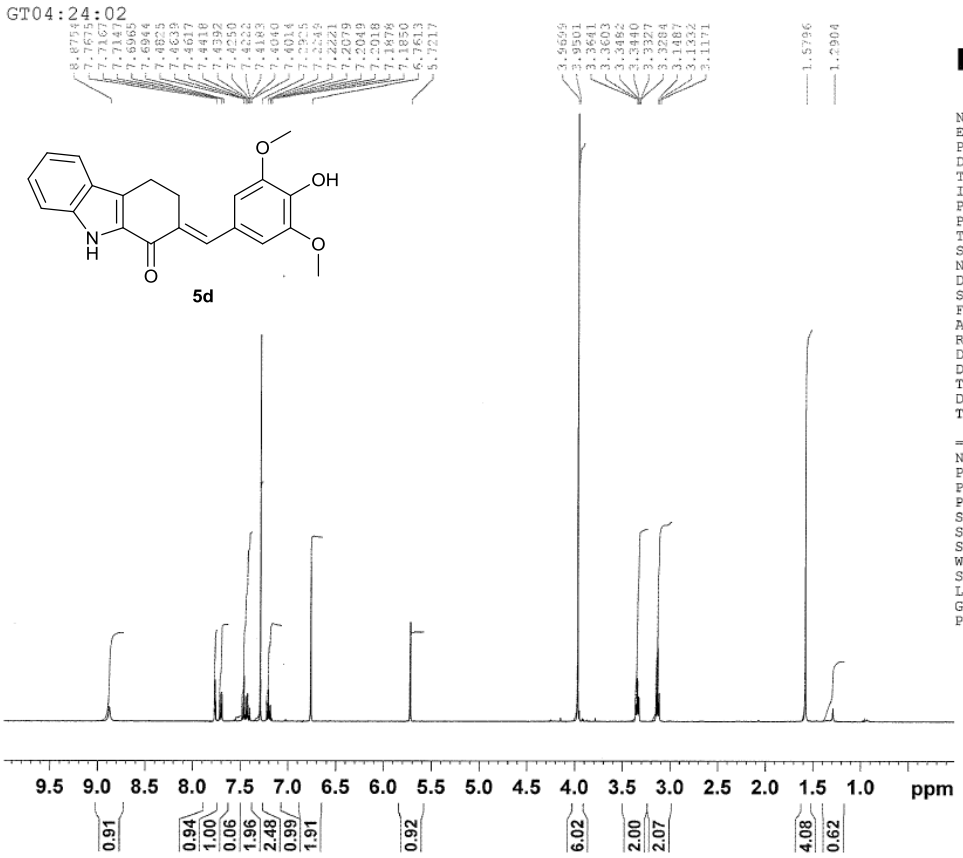
BRUKER

NAME	May02-2010-GT1013
EXPNO	10
PROCNO	1
Date_	20100502
Time	18.07
INSTRUM	AVIII400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	456
DW	60.800 usec
DE	17.24 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	0.00 dB
PL1W	9.74611950 W
SFO1	400.0424704 MHz
SI	65536
SF	400.0400000 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

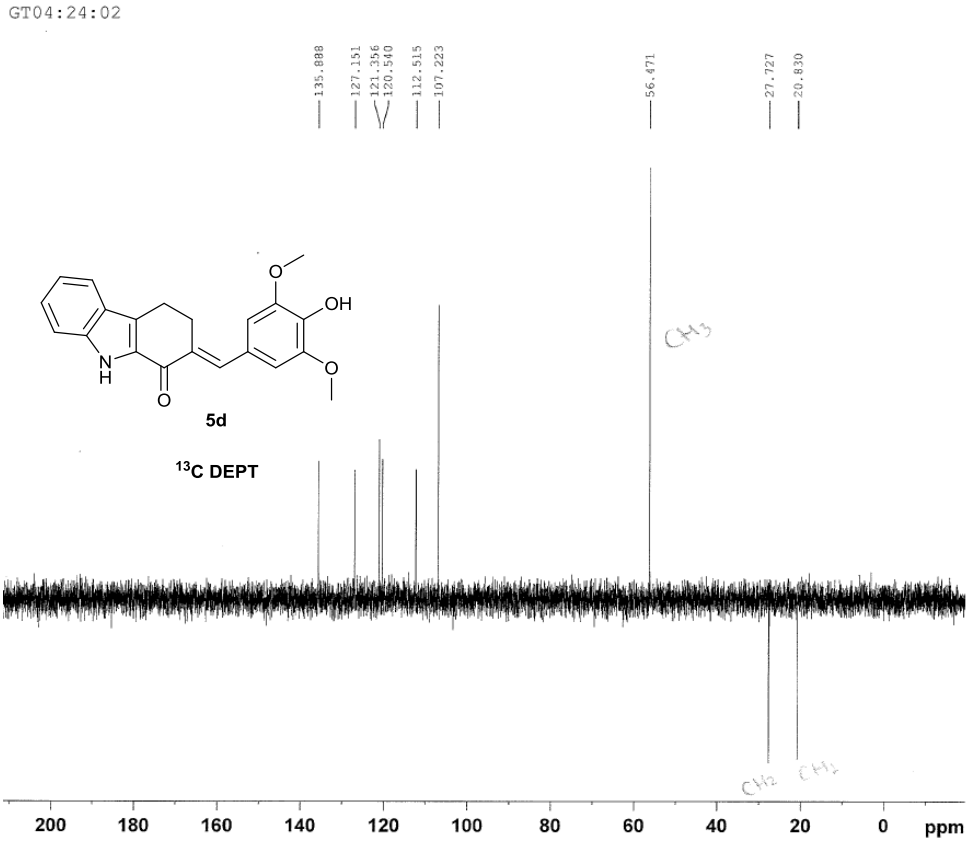


BRUKER

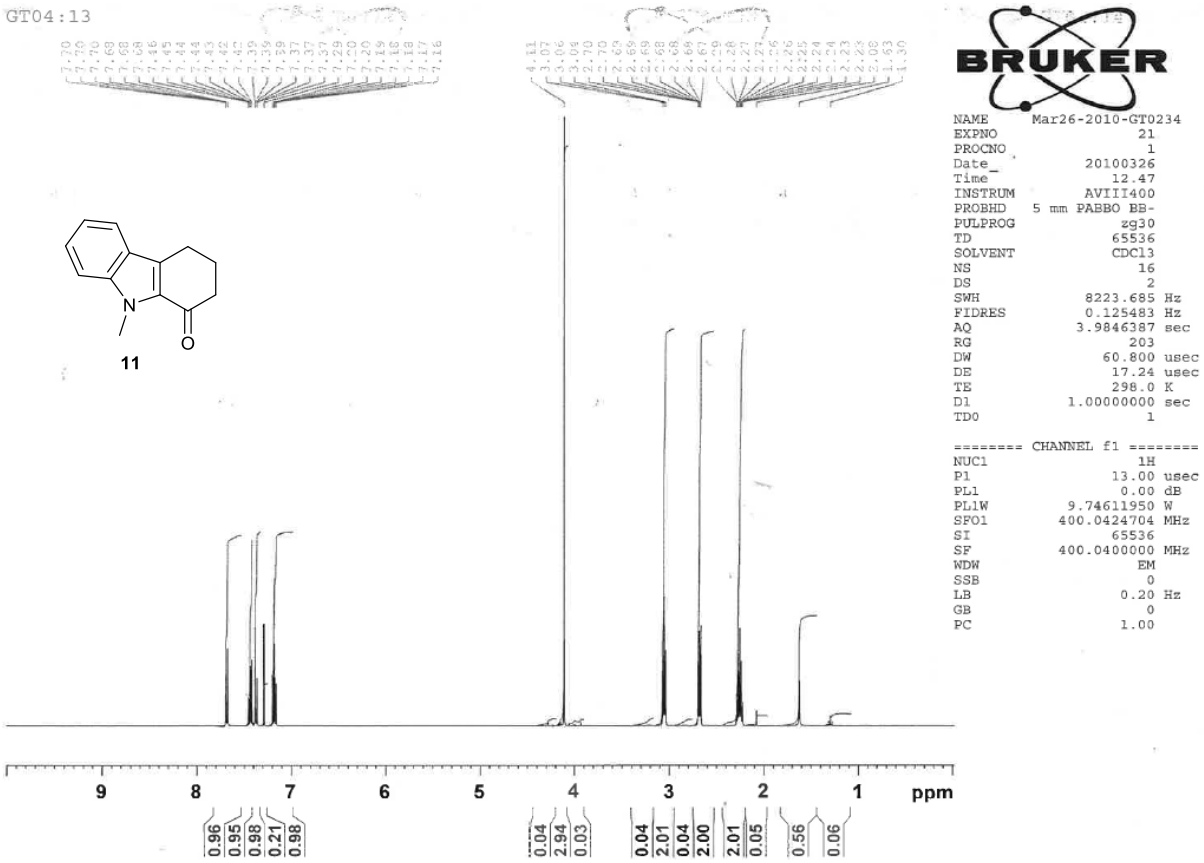
NAME	May07-2010-GT1132
EXPNO	11
PROCNO	1
Date_	20100507
Time	21.12
INSTRUM	AVIII400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
PL1W	58.91986084 W
SFO1	100.6001970 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.78 dB
PL13	19.00 dB
PL2W	9.74611950 W
PL12W	0.25753233 W
PL13W	0.12269637 W
SFO2	400.0416002 MHz
SI	65536
SF	100.5901380 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

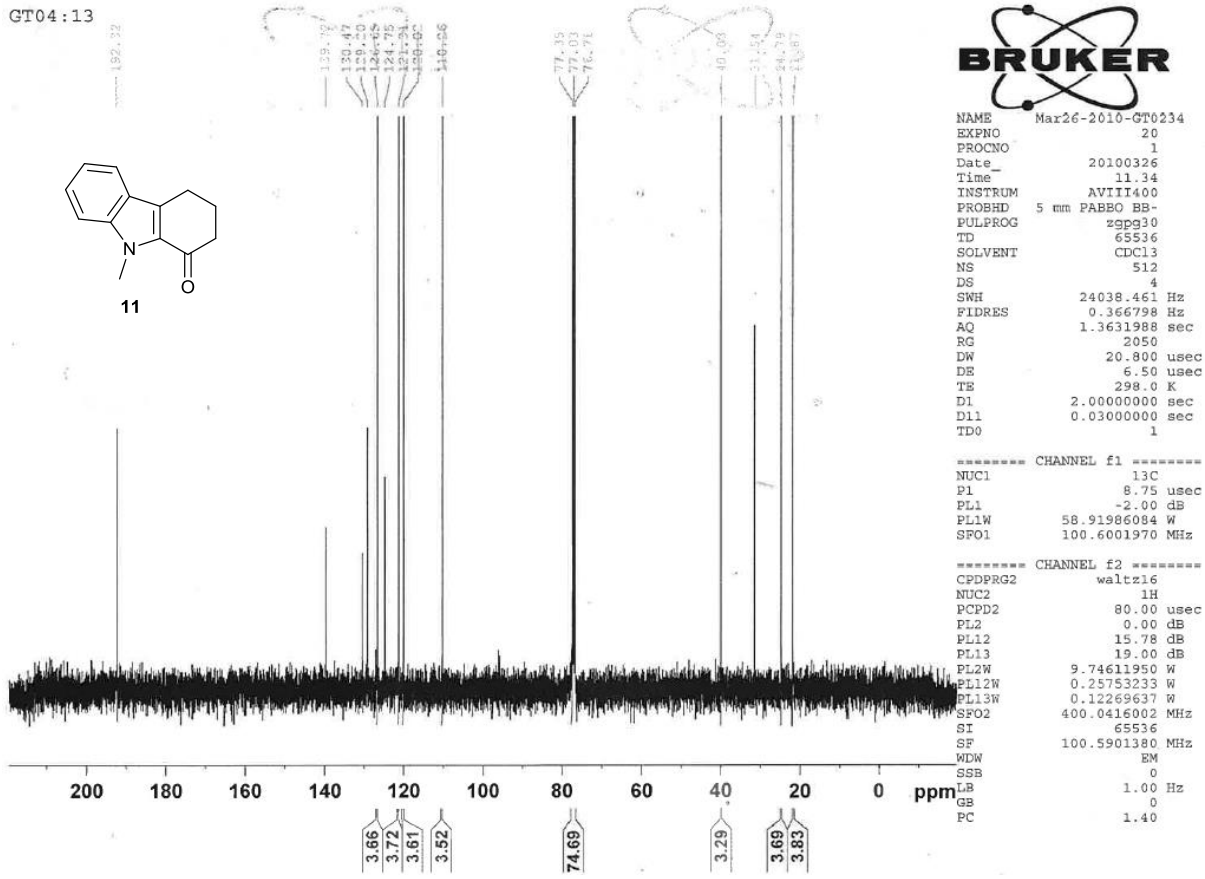


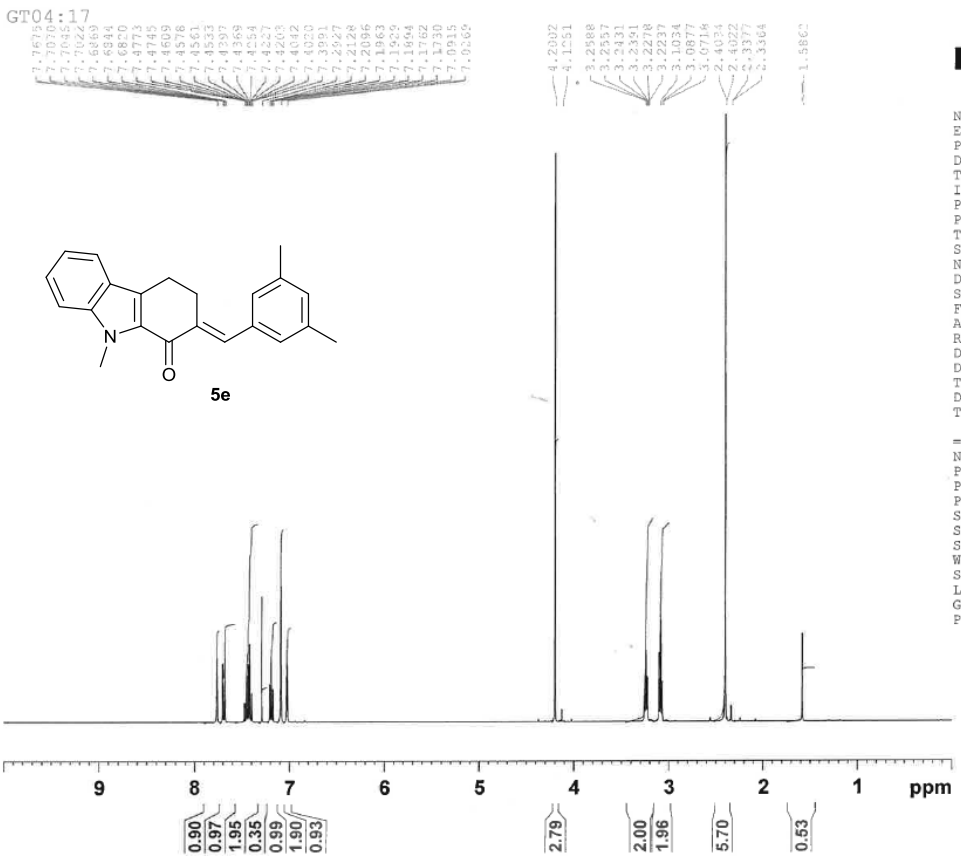

```
NAME          May02-2010-GT1016
EXPNO                       10
PROCNO                       1
Date_                 20100502
Time                     21.36
INSTRUM               AVIII400
PROBHD    5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                         456
DW                    60.800 usec
DE                    17.24 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                    13.00 usec
PL1                    0.00 dB
PL1W                9.74611950 W
SFO1              400.0424704 MHz
SI                       65536
SF                400.0400000 MHz
WDW                         EM
SSB                          0
LB                    0.20 Hz
GB                           0
PC                    1.00
```




```
NAME          Jul21-2010-GT4021
EXPNO                       12
PROCNO                       1
Date_                 20100721
Time                     19.52
INSTRUM               AVIII400
PROBHD    5 mm PABBO BB-
PULPROG              deptsp135
TD                       65536
SOLVENT                  CDCl3
NS                         256
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                        2050
DW                    20.800 usec
DE                     6.50 usec
TE                    298.0 K
CNST2               145.0000000
D1                 2.00000000 sec
D2                 0.00344828 sec
D12                0.00002000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                     8.75 usec
P12                 2000.00 usec
PL0                  120.00 dB
PL1                   -2.00 dB
PL0W           0.00000000 W
PL1W          58.91986084 W
SFO1             100.6001970 MHz
SP2                    7.32 dB
SPNAM2          Crp60comp.4
SPOAL2                0.500
SPOFFS2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                        1H
P3                    13.00 usec
P4                    26.00 usec
PCPD2                 80.00 usec
PL2                    0.00 dB
PL12                  15.78 dB
PL2W           9.74611950 W
PL12W          0.25753233 W
SFO2             400.0416002 MHz
SI                       65536
SF               100.5901380 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

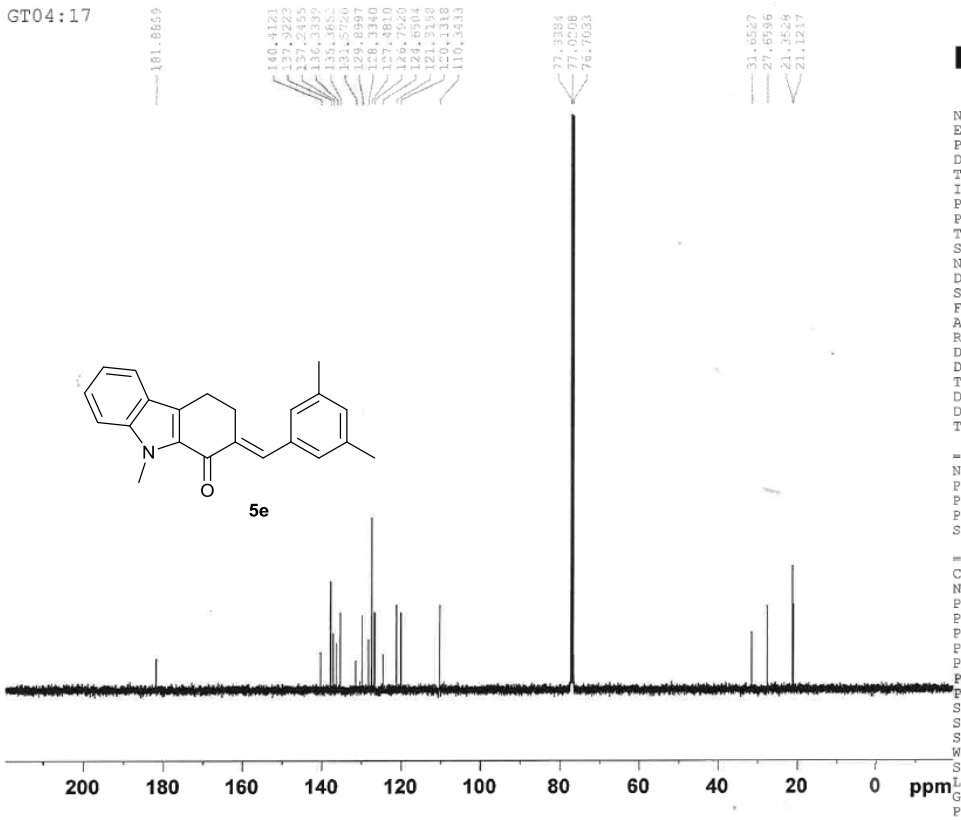

GT04:13
11
BRUKER
NAME Mar26-2010-GT0234
EXPNO 21
PROCNO 1
Date_ 20100326
Time 12.47
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 ppm
0.96 0.95 0.98 0.21 0.98 0.04 2.94 0.03 0.04 2.01 0.04 2.00 2.01 0.05 0.56 0.06


GT04:13
11
BRUKER
NAME Mar26-2010-GT0234
EXPNO 20
PROCNO 1
Date_ 20100326
Time 11.34
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm
3.66 3.72 3.61 3.52 74.69 3.29 3.69 3.83



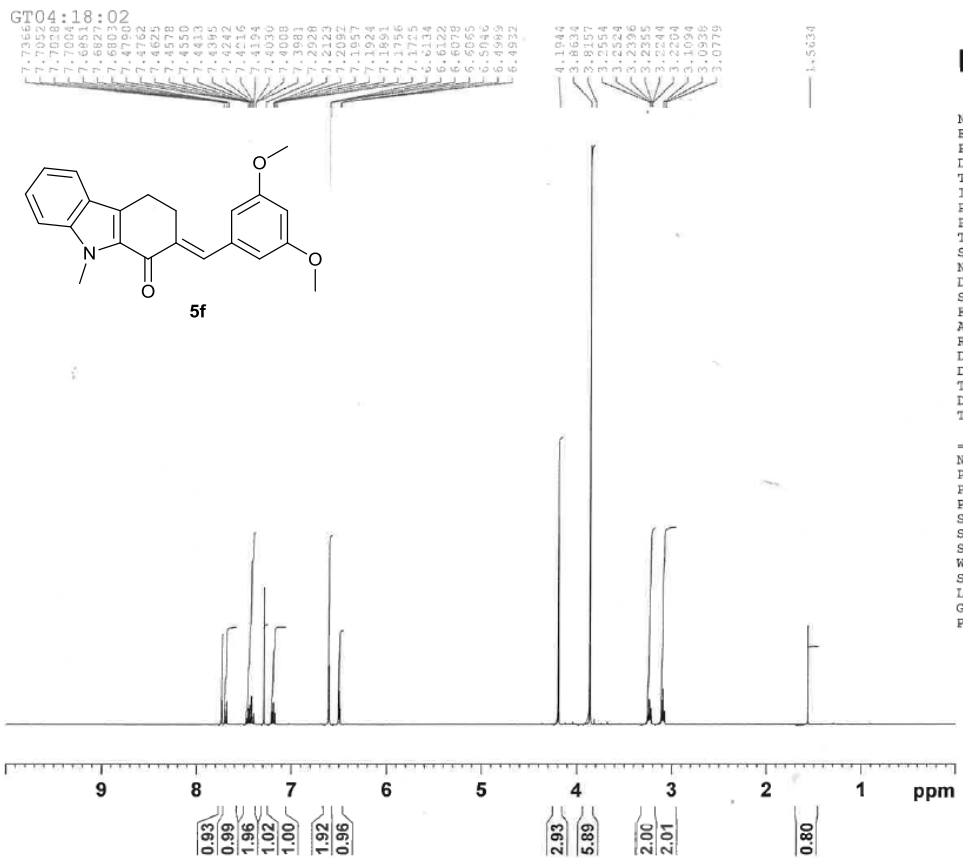
BRUKER

```
NAME          May07-2010-GT1133
EXPNO                       10
PROCNO                       1
Date_              20100507
Time                    15.22
INSTRUM              AVIII400
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                        228
DW                     60.800 usec
DE                     17.24 usec
TE                     298.0 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     13.00 usec
PL1                     0.00 dB
PL1W                9.74611950 W
SFO1              400.0424704 MHz
SI                      65536
SF                400.0400000 MHz
WDW                        EM
SSB                         0
LB                      0.20 Hz
GB                          0
PC                      1.00
```

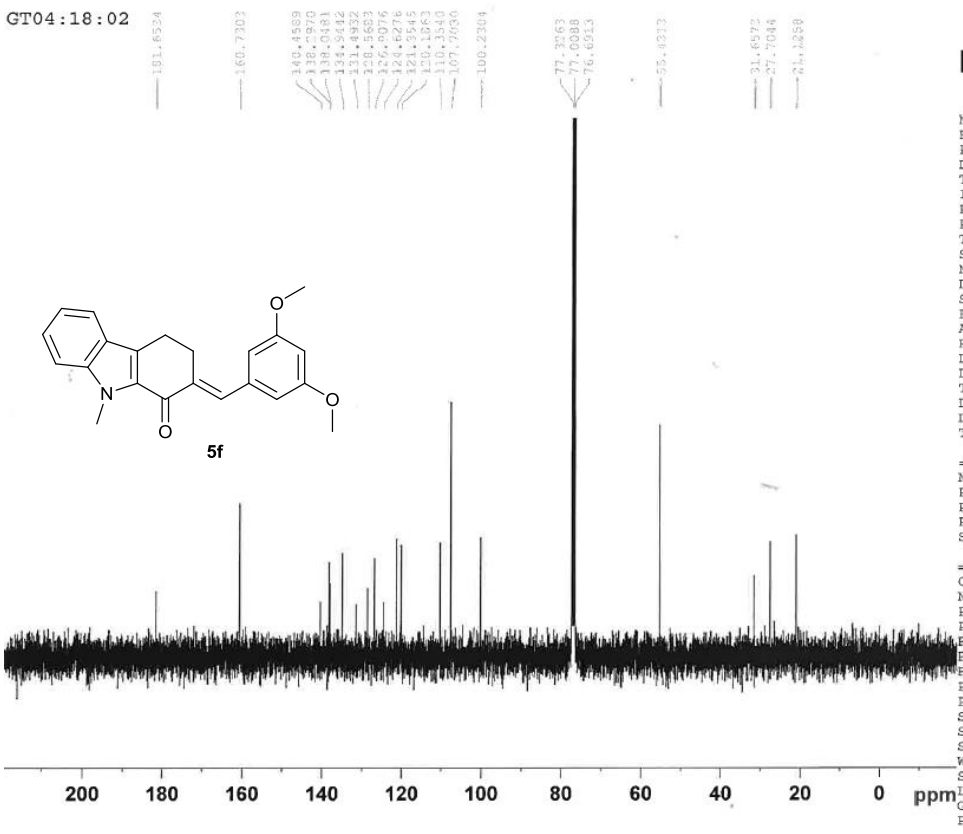


BRUKER

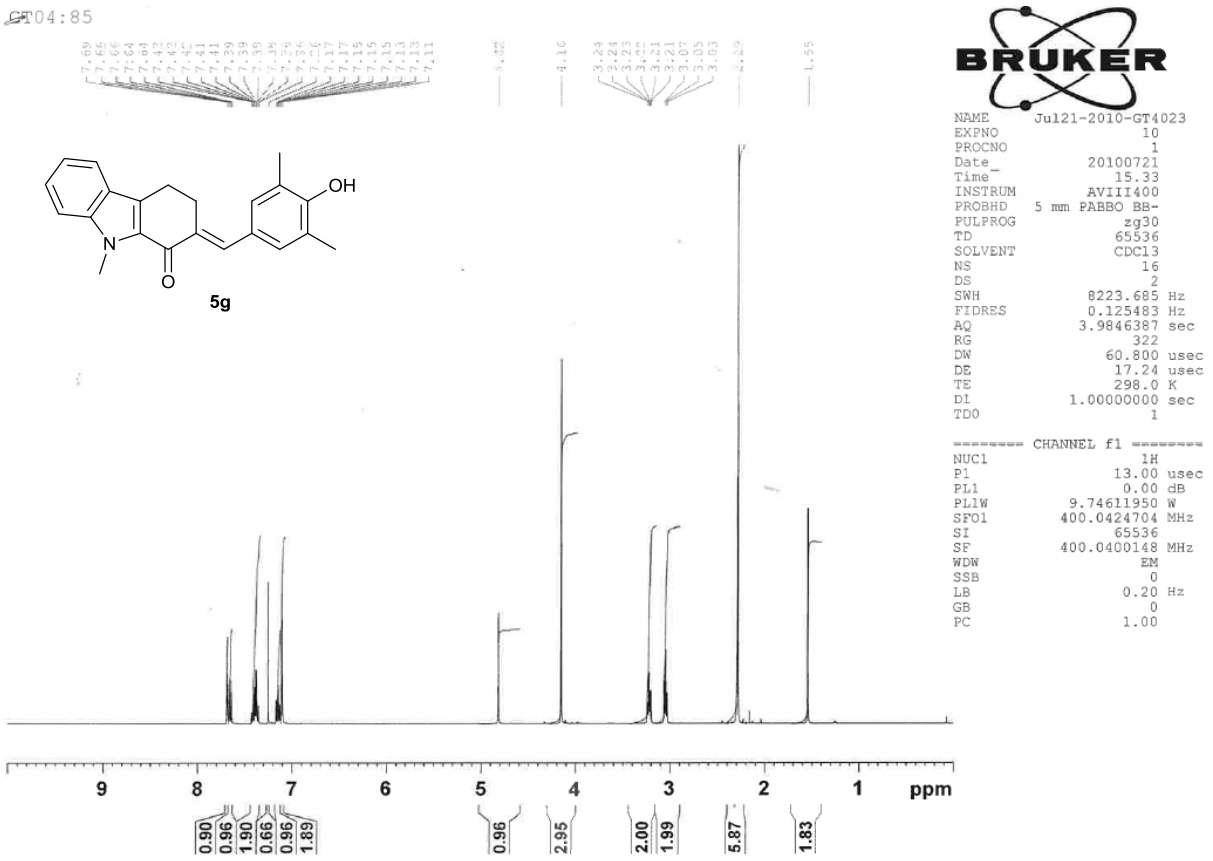
```
NAME          May07-2010-GT1133
EXPNO                       11
PROCNO                       1
Date_              20100507
Time                    22.18
INSTRUM              AVIII400
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        512
DS                          4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                       2050
DW                     20.800 usec
DE                      6.50 usec
TE                     298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      8.75 usec
PL1                    -2.00 dB
PL1W               58.91986084 W
SFO1              100.6001970 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     0.00 dB
PL12                   15.78 dB
PL13                   19.00 dB
PL2W                9.74611950 W
PL12W               0.25753233 W
PL13W               0.12269637 W
SFO2              400.0416002 MHz
SI                      65536
SF                100.5901380 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

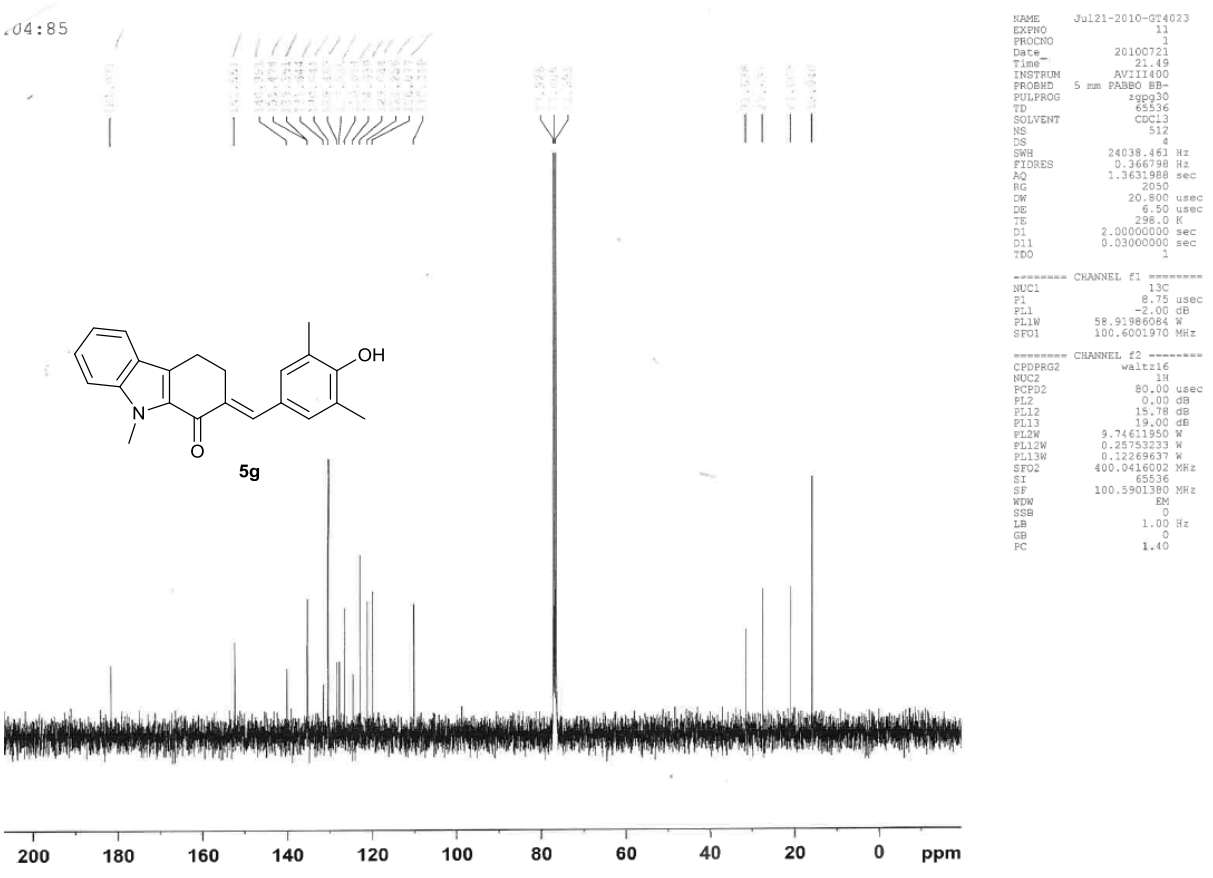



```
NAME        Apr01-2010-GT0430
EXPNO                 10
PROCNO                 1
Date_           20100401
Time              11.52
INSTRUM         AVIII400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                   362
DW                60.800 usec
DE                17.24 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.00 usec
PL1                0.00 dB
PL1W          9.74611950 W
SFO1        400.0424704 MHz
SI                 65536
SF          400.0400000 MHz
WDW                   EM
SSB                    0
LB                 0.20 Hz
GB                     0
PC                 1.00
```




```
NAME        Apr01-2010-GT0430
EXPNO                 11
PROCNO                 1
Date_           20100401
Time              12.37
INSTRUM         AVIII400
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.75 usec
PL1               -2.00 dB
PL1W         58.91986084 W
SFO1        100.6001970 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              15.78 dB
PL13              19.00 dB
PL2W          9.74611950 W
PL12W         0.25753233 W
PL13W         0.12269637 W
SFO2        400.0416002 MHz
SI                 65536
SF          100.5901380 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


GT04:85
OH
N
O
5g
9
8
7
6
5
4
3
2
1
ppm
0.90
0.96
1.90
0.66
0.96
1.89
0.96
2.95
2.00
1.99
5.87
1.83
BRUKER
NAME Jul21-2010-GT4023
EXPNO 10
PROCNO 1
Date_ 20100721
Time_ 15.33
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 17.24 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
PL1W 9.74611950 W
SFO1 400.0424704 MHz
SI 65536
SF 400.0400148 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00


04:85
OH
N
O
5g
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME Jul21-2010-GT4023
EXPNO 11
PROCNO 1
Date_ 20100721
Time_ 21.49
INSTRUM AVIII400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 58.91986084 W
SFO1 100.6001970 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.78 dB
PL13 19.00 dB
PL2W 9.74611950 W
PL12W 0.25753233 W
PL13W 0.12269637 W
SFO2 400.0416002 MHz
SI 65536
SF 100.5901380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COMPARE analyses

Results of the Standard COMPARE analysis of GI_{50} values of compound **4c (**NSC 756592) with Synthetic Compounds.

Rank	Correlatio	namecode	Target Vector ident For Display	Target Vector descript	Common Cell Lines
1	1	--DISCREE	NSC:S756592 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
2	0.842	--DISCREE	NSC:S756590 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	compound **5g**	58
3	0.795	PUBLIC	NSC:S106969 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	CENTAUREIDIN	52
4	0.769	PUBLIC	NSC:S675003 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
5	0.725	PUBLIC	NSC:S750873 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		55
6	0.724	PUBLIC	NSC:S748541 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
7	0.723	PUBLIC	NSC:S748533 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
8	0.722	PUBLIC	NSC:S609397 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	B817373K328	56
9	0.715	--DISCREE	NSC:S756586 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
10	0.713	PUBLIC	NSC:S648581 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		57
11	0.7	PUBLIC	NSC:S119754 Endpt:GI50 ExpId:AVGDATA hiConc:-4.9	COPTISINE CHLORIDE	57
12	0.7	PUBLIC	NSC:S686560 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
13	0.698	PUBLIC	NSC:S656160 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		53
14	0.697	PUBLIC	NSC:S659853 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	PANZEM NCD	58
15	0.695	PUBLIC	NSC:S638389 Endpt:GI50 ExpId:AVGDATA hiConc:2.2		48
16	0.694	PUBLIC	NSC:S695588 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	AMINO MMI-S02 CI	55
17	0.683	PUBLIC	NSC:S680185 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		53
18	0.679	PUBLIC	NSC:S653008 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		41
19	0.679	PUBLIC	NSC:S673787 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		52
20	0.671	PUBLIC	NSC:S720716 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		57
21	0.671	PUBLIC	NSC:S645645 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0	ANTINEOPLASTIC-6456	55
22	0.671	PUBLIC	NSC:S712304 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		51
23	0.669	PUBLIC	NSC:S751957 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
24	0.659	PUBLIC	NSC:S643813 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
25	0.657	PUBLIC	NSC:S681683 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
26	0.646	PUBLIC	NSC:S698666 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	Indanocine **1**	54
27	0.646	PUBLIC	NSC:S642198 Endpt:GI50 ExpId:AVGDATA hiConc:-7.0	ANTINEOPLASTIC-6421	57
28	0.645	PUBLIC	NSC:S645646 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0	ANTINEOPLASTIC-6456	57
29	0.643	PUBLIC	NSC:S113764 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	U 32027	58
30	0.642	PUBLIC	NSC:S671178 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		45
31	0.64	PUBLIC	NSC:S656157 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
32	0.639	PUBLIC	NSC:S642321 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		44
33	0.634	PUBLIC	NSC:S667048 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHYL ESTRADIOL	53
34	0.632	PUBLIC	NSC:S689466 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	DESMETHOXYCENTAUR	56
35	0.631	PUBLIC	NSC:S657275 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
36	0.631	PUBLIC	NSC:S671618 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-IODOESTRADIOL	57
37	0.629	PUBLIC	NSC:S642321 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0		43
38	0.628	PUBLIC	NSC:S684423 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		57
39	0.626	PUBLIC	NSC:S649977 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		46
40	0.626	PUBLIC	NSC:S174589 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
41	0.625	PUBLIC	NSC:S643812 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	ANTINEOPLASTIC-6438	58
42	0.624	PUBLIC	NSC:S667047 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-PROPENYL ESTRADIO	57
43	0.623	PUBLIC	NSC:S123399 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
44	0.621	PUBLIC	NSC:S682429 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-(1-PROPYNYL)-3,17.B	57
45	0.62	PUBLIC	NSC:S702400 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		57
46	0.619	PUBLIC	NSC:S652809 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
47	0.616	PUBLIC	NSC:S281300 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		49
48	0.615	PUBLIC	NSC:S720872 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
49	0.61	PUBLIC	NSC:S671041 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-N-PROPOXYESTRADI	58
50	0.605	PUBLIC	NSC:S136513 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	DIBENZOYLFURAN DER	58

Results of the Standard COMPARE analysis of GI_{50} values of compound **5c (**NSC 756586) with Synthetic Compounds.

Rank	Correlatio	namecode	Target Vector ident For Display	Target Vector descriptor For	Common Cell Lines
1	1	--DISCREE	NSC:S756586 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
2	0.846	--DISCREE	NSC:S756590 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	compound **5g**	60
3	0.788	PUBLIC	NSC:S240579 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
4	0.781	PUBLIC	NSC:S748533 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
5	0.744	PUBLIC	NSC:S642321 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		45
6	0.724	PUBLIC	NSC:S686560 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
7	0.722	PUBLIC	NSC:S638389 Endpt:GI50 ExpId:AVGDATA hiConc:2.2		49
8	0.721	PUBLIC	NSC:S667049 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHENYL ESTRADIOL	53
9	0.715	--DISCREE	NSC:S756592 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
10	0.705	PUBLIC	NSC:S643813 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
11	0.7	PUBLIC	NSC:S659853 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	PANZEM NCD	60
12	0.697	PUBLIC	NSC:S709581 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		51
13	0.695	PUBLIC	NSC:S703321 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
14	0.685	PUBLIC	NSC:S671043 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
15	0.683	PUBLIC	NSC:S681683 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
16	0.674	PUBLIC	NSC:S709566 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		52
17	0.674	PUBLIC	NSC:S675003 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
18	0.674	PUBLIC	NSC:S645620 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		46
19	0.672	PUBLIC	NSC:S123399 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
20	0.67	PUBLIC	NSC:S671041 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-N-PROPOXYESTRADIOL	60
21	0.669	PUBLIC	NSC:S297360 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		50
22	0.662	PUBLIC	NSC:S710266 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
23	0.662	PUBLIC	NSC:S642198 Endpt:GI50 ExpId:AVGDATA hiConc:-7.0	ANTINEOPLASTIC-642198	59
24	0.66	PUBLIC	NSC:S642321 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0		44
25	0.659	PUBLIC	NSC:S648581 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
26	0.653	PUBLIC	NSC:S643812 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	ANTINEOPLASTIC-643812	60
27	0.652	PUBLIC	NSC:S647246 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0	ANTINEOPLASTIC-647246	56
28	0.652	PUBLIC	NSC:S625857 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		48
29	0.651	PUBLIC	NSC:S652890 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
30	0.649	PUBLIC	NSC:S645646 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0	ANTINEOPLASTIC-645646	58
31	0.646	PUBLIC	NSC:S641526 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	4'-HYDROXY-3',8-DIMETHOX'	44
32	0.645	PUBLIC	NSC:S682429 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-(1-PROPYNYL)-3,17.BETA.-	59
33	0.637	PUBLIC	NSC:S628949 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		45
34	0.635	PUBLIC	NSC:S683125 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
35	0.635	PUBLIC	NSC:S131734 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
36	0.634	PUBLIC	NSC:S673787 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
37	0.634	PUBLIC	NSC:S625863 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		46
38	0.634	PUBLIC	NSC:S709567 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		53
39	0.633	PUBLIC	NSC:S674256 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
40	0.631	PUBLIC	NSC:S402590 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
41	0.63	PUBLIC	NSC:S717356 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
42	0.63	PUBLIC	NSC:S709568 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		53
43	0.63	PUBLIC	NSC:S748541 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
44	0.625	PUBLIC	NSC:S667048 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHYL ESTRADIOL	54
45	0.625	PUBLIC	NSC:S716893 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
46	0.624	PUBLIC	NSC:S667047 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-PROPENYL ESTRADIOL	59
47	0.622	PUBLIC	NSC:S179485 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	BREVICID	59
48	0.622	PUBLIC	NSC:S671042 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-I-PROPOXYESTRADIOL	60
49	0.621	PUBLIC	NSC:S119754 Endpt:GI50 ExpId:AVGDATA hiConc:-4.9	COPTISINE CHLORIDE	59
50	0.62	PUBLIC	NSC:S653564 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		41

Results of the Standard COMPARE analysis of GI_{50} values of compound **5g (**NSC 756590) with Synthetic Compounds.

Rank	Correlatio	namecode	Target Vector ident For Display	Target Vector descriptor For Display	Common Cell Lines
1	1	--DISCREE	NSC:S756590 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
2	0.846	--DISCREE	NSC:S756586 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	compound **5c**	60
3	0.842	--DISCREE	NSC:S756592 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	compound **4c**	58
4	0.813	PUBLIC	NSC:S748533 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
5	0.785	PUBLIC	NSC:S675003 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
6	0.728	PUBLIC	NSC:S609397 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	B817373K328	58
7	0.724	PUBLIC	NSC:S751957 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
8	0.724	PUBLIC	NSC:S682429 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-(1-PROPYNYL)-3,17.BETA.-ESTRADIOL	59
9	0.718	PUBLIC	NSC:S748541 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
10	0.717	PUBLIC	NSC:S119754 Endpt:GI50 ExpId:AVGDATA hiConc:-4.9	COPTISINE CHLORIDE	59
11	0.709	PUBLIC	NSC:S680185 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		55
12	0.698	PUBLIC	NSC:S671167 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
13	0.698	PUBLIC	NSC:S686560 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
14	0.697	PUBLIC	NSC:S674263 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
15	0.691	PUBLIC	NSC:S720872 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
16	0.691	PUBLIC	NSC:S695588 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	AMINO MMI-S02 CI	57
17	0.69	PUBLIC	NSC:S679431 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHOXY-6-KETO-ESTRADIOL	59
18	0.69	PUBLIC	NSC:S681684 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
19	0.684	PUBLIC	NSC:S671169 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
20	0.683	PUBLIC	NSC:S106969 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	CENTAUREIDIN	54
21	0.68	PUBLIC	NSC:S710266 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
22	0.679	PUBLIC	NSC:S667048 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHYL ESTRADIOL	54
23	0.678	PUBLIC	NSC:S683125 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		56
24	0.675	PUBLIC	NSC:S659853 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	PANZEM NCD	60
25	0.671	PUBLIC	NSC:S645645 Endpt:GI50 ExpId:AVGDATA hiConc:-6.0	ANTINEOPLASTIC-645645	57
26	0.67	PUBLIC	NSC:S667049 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-ETHENYL ESTRADIOL	53
27	0.664	PUBLIC	NSC:S671041 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-N-PROPOXYESTRADIOL	60
28	0.663	PUBLIC	NSC:S673787 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		54
29	0.662	PUBLIC	NSC:S669229 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-TRANS-N-BUTEN-1-YL-ESTRADIOL	57
30	0.661	PUBLIC	NSC:S638389 Endpt:GI50 ExpId:AVGDATA hiConc:2.2		49
31	0.66	PUBLIC	NSC:S653008 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		42
32	0.659	PUBLIC	NSC:S678473 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
33	0.659	PUBLIC	NSC:S674256 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
34	0.659	PUBLIC	NSC:S671618 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	2-IODOESTRADIOL	59
35	0.659	PUBLIC	NSC:S684423 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
36	0.658	PUBLIC	NSC:S671165 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
37	0.658	PUBLIC	NSC:S720716 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
38	0.656	PUBLIC	NSC:S665694 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
39	0.656	PUBLIC	NSC:S689466 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0	DESMETHOXYCENTAUREIDIN	58
40	0.655	PUBLIC	NSC:S240579 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
41	0.654	PUBLIC	NSC:S681683 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
42	0.654	PUBLIC	NSC:S51361 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
43	0.653	PUBLIC	NSC:S642198 Endpt:GI50 ExpId:AVGDATA hiConc:-7.0	ANTINEOPLASTIC-642198	59
44	0.651	PUBLIC	NSC:S701101 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		58
45	0.651	PUBLIC	NSC:S123399 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
46	0.65	PUBLIC	NSC:S682597 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
47	0.65	PUBLIC	NSC:S648581 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
48	0.649	PUBLIC	NSC:S652893 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		59
49	0.648	PUBLIC	NSC:S746498 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		60
50	0.645	PUBLIC	NSC:S117028 Endpt:GI50 ExpId:AVGDATA hiConc:-4.0		57