Enantioselective Synthesis of Dihydrocoumarin Derivatives by Chiral Scandium(III)-complex Catalyzed Inverse-Electron-Demand Hetero-Diels–Alder Reaction

Supporting Information

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I. General information.

^{1}H NMR spectra were recorded on commercial instruments (400 MHz). Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26; DMSO, δ = 2.49). Spectra were reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration and assignment. ^{13}C NMR spectra were collected on commercial instruments (100 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 77.0; DMSO, δ = 39.6). Enantiomeric excesses (*ee*) were determined by HPLC analysis using the corresponding commercial chiralpak column as stated in the experimental procedures at 25 ºC. Optical rotations were reported as follows: $[a]^{T}{}_{D}$ (*c* g/100 mL, in solvent). HRMS was recorded on a commercial apparatus (ESI Source). All reagents and solvents were obtained from commercial suppliers and used without further purification except as indicated below. All catalytic reactions were run in dried glassware. THF was distilled from sodium benzophenone ketyl.

II. Optimization of other reaction conditions.

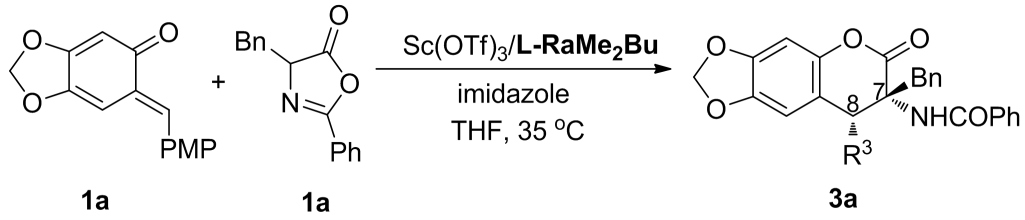


Table S1: **Optimization for the amount of imidazole.**

Entry[a]	Imidazole[b] (eq.)	Yield %[c]	*Ee* %[d]
1	0.1	67	90
2	0.15	67	91
3	0.2	67	91
4	0.5	68	73
5	1.0	86	77
6	1.2	10	ND

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), metal/ligand (1:1, 10 mol%), in THF (1.0 mL) under N_2 at 35 °C for 0.5 h. Then imidazole, azlactone **2a** (0.1 mmol) were added successively and kept stirring at 35 °C for 72 h. [b] The quantity of the additive. [c] Isolated yield. [d] Determined by chiral HPLC analysis. The diastereoselectivities were all over 19:1 determined by ^{1}H NMR spectra.

Table S2: Optimization for the ratio of substrates.

Entry[a]	Ratio(**1a**:**2a**)[b]	Yield %[d]	*Ee* %[c]
1	1.5:1	44	91
2	1.2:1	88	91
3	1:1	67	91
4	1:1.2	67	77
5	1:1.5	78	75

[a] Unless otherwise noted, all reactions were carried out with **1a**, metal/ligand (1:1, 10 mol%), in THF (1.0 mL) under N_2 at 35 °C for 0.5 h. Then imidazole (0.15 eq.), azlactones (0.1 eq.) were added successively and kept stirring at 35 °C for 72 h. [b] The ratio of substrates **1a** to **2a**. [c] Determined by chiral HPLC analysis. [d] Isolated yield. The diastereoselectivities were all over 19:1 determined by ^{1}H NMR spectra.

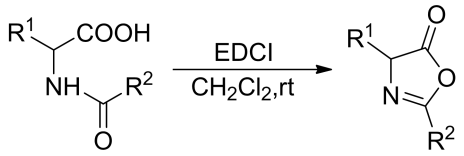
Table S3: **Optimization for the ratio of ligand and metal.**

Entry[a]	M:L	Yield %[b]	*Ee* %[c]
1	1.5：1	38	62
2	1.2：1	82	77
3	1：1	88	91
4	1:1.05	90	91
5	1:1.1	88	90
6	1：1.2	83	90
7	1:1.5	92	84

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.12 mmol), metal/ligand in THF (1.0 mL) under N_2 at 35 °C for 0.5 h. Then imidazole (0.15 eq.), azlactones (0.1 mmol) were added successively and kept stirring at 35 °C for 72 h. [b] Isolated yield. [c] Determined by chiral HPLC analysis. The diastereoselectivities were over 19:1 determined by ^{1}H NMR spectra.

III. Synthesis of substrates.

1. *O*-quinone methides (**1a-1b**) were prepared as previously described by Jurd.[1]
2. Procedure for preparation of azlactones.



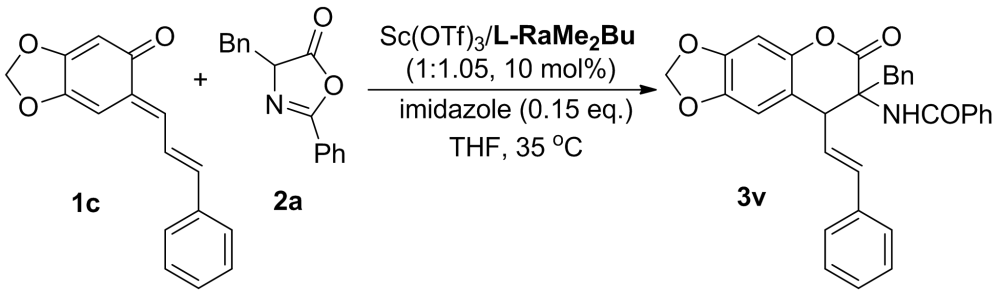
To a solution of amide (8 mmol) in CH_2Cl_2 (25 mL) was added the solution of EDCI (1.56 g) in CH_2Cl_2 (10 mL) at 0 ˚C. After being stirred at room temperature for 2 h, the reaction mixture was diluted with H_2O for twice and extracted with CH_2Cl_2. Organic phase was dried over Na_2SO_4 and then filtered. After being concentrated, recrystallized with CH_2Cl_2 and *n*-hexane, the azlactone was obtained.

IV. General procedure of the catalytic reactions.

A dry reaction tube was charged with substrate **1** (0.12 mmol), $Sc(OTf)_3$ (4.90 mg, 10 mol%), and the ligand **L-RaMe$_2$Bu** (7.40 mg, 10.5 mol%) under nitrogen. Then, THF (1.0 mL) and imidazole (0.15 eq, 20 uL, 0.75 mmol/mL in THF) were added successively. The mixture was stirred at 35 ^{o}C for 0.5 h. Finally, the substrate **2** (0.1 mmol) was added one-pot at the indicated temperature. The reaction was performed at 35 ^{o}C for 72 h. The residue was purified by flash chromatography on silica gel (1/6, Etheyl acetate/petroleum ether) to afford the desired product.

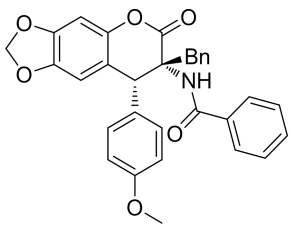
1. L. Jurd, *Tetrahedron,* 1977, **33**, 163.

V. Failed substrates scope of the IEDDA reaction.



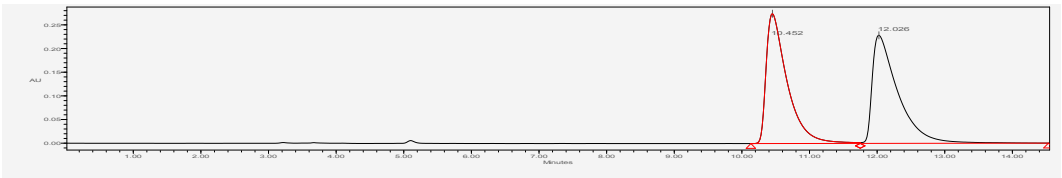
Substrate **1c** was also attempted, 34% *ee*, 25% yield was obtained.

VI. Product characterization data.



***N*-((7*R*,8*R*)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6*H*-[1,3]dioxolo[4,5-*g*]chromen-7-yl)benzamide (3a)**

Result: 90% Yield, 91% *ee*; $[\alpha]^{21}_{D} = -203.2$ (*c* 0.19, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 95/5, 1.0 mL/min) $t_{R(major)}$ = 10.29 min, $t_{R(minor)}$ = 12.09 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 14, 7.2 Hz, 3H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.19 (dd, *J* = 7.0, 3.6 Hz, 3H), 7.06 (d, *J* = 8.7 Hz, 4H), 6.85 – 6.60 (m, 5H), 5.95 (d, *J* =17.4 Hz, 2H), 5.29 (s, 1H), 4.14 (d, *J* = 14.0 Hz, 1H), 3.66 (d, *J* = 11.0 Hz, 3H), 3.17 (d, *J* = 13.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.40, 167.98, 159.01, 148.03, 145.32, 144.30, 135.17, 135.01, 131.61, 130.19, 129.91, 128.97, 128.63, 128.42, 127.40, 126.74, 117.75, 114.15, 108.61, 102.03, 98.49, 65.92, 55.15, 49.17, 38.17. ESI-HRMS calcd for $[C_{31}H_{25}NO_6+Na^+]$: 530.1580, found 530.1588.



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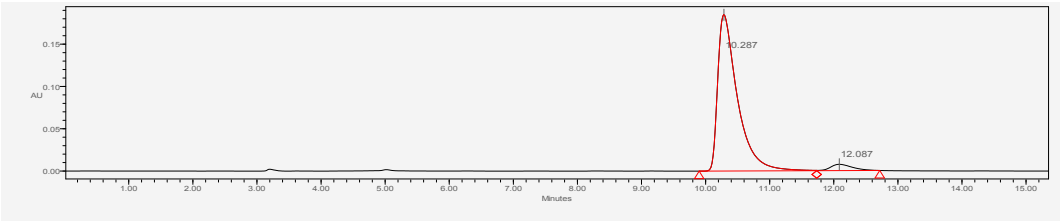

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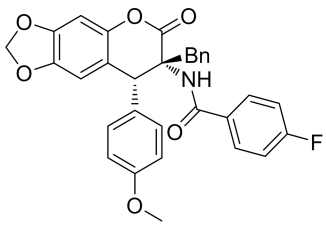
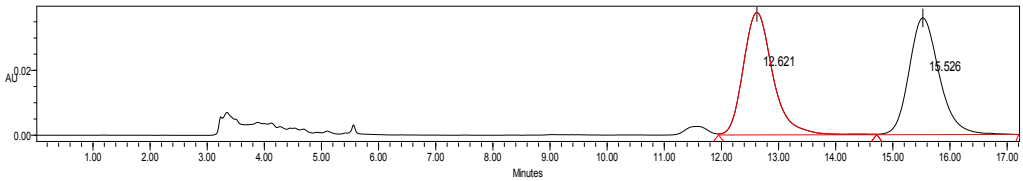


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-fluorobenzamide (3b)

Result: 84% Yield, 92% *ee*; $[\alpha]^{21}_{D}$ = −184.7 (*c* 0.14, CH_2Cl_2); HPLC (Daicel chiralcel IC, *n*-hexane/*i*-PrOH 95/5, 1.0 mL/min) $t_{R(major)}$ = 12.99 min, $t_{R(minor)}$ = 15.97 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.23 – 7.15 (m, 3H), 7.02 (dd, *J* = 19.2, 8.7 Hz, 6H), 6.81 (s, 1H), 6.69 (t, *J* = 7.5 Hz, 4H), 6.06 – 5.91 (m, 2H), 5.26 (s, 1H), 4.11 (d, *J* = 14.0 Hz, 1H), 3.67 (s, 3H), 3.17 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.40, 166.80, 166.03, 163.52, 159.02, 148.05, 145.34, 144.25, 134.93, 131.26, 131.23, 130.14, 129.85, 129.77, 129.12, 129.03, 128.91, 128.41, 127.42, 117.65, 115.78, 115.56, 114.14, 108.59, 102.03, 98.49, 65.90, 55.15, 49.19, 38.21. ESI-HRMS calcd for $[C_{31}H_{24}FNO_6+Na^+]$: 548.1485, found 548.1482.



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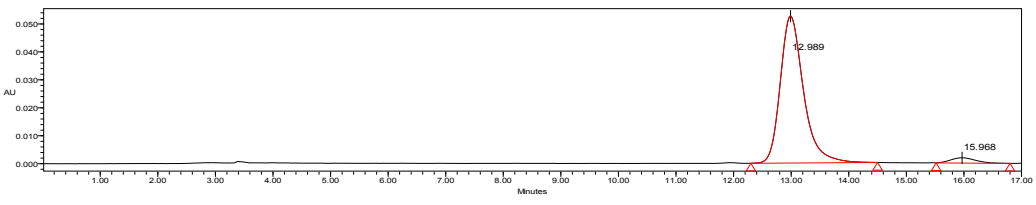
2	15.526	49.34



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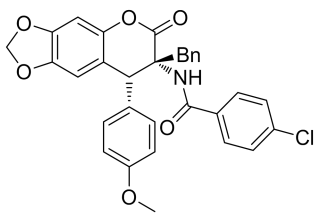
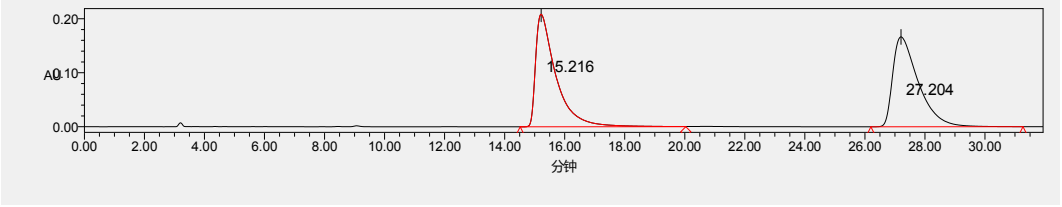
2	15.968	3.75



_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-chlorobenzamide(3c)

Result: 89% Yield, 94% *ee*; $[\alpha]^{25}_{D}$ = −106.2 (*c* 1.3, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 14.84 min, $t_{R(minor)}$ = 27.29 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.34 – 7.27 (m, 2H), 7.19 (dd, *J* = 6.4, 3.6 Hz, 3H), 7.03 (dd, *J* = 6.6, 2.1 Hz, 4H), 6.81 (s, 1H), 6.75 – 6.55 (m, 4H), 5.99 (dd, *J* = 16.3, 1.2 Hz, 2H), 5.25 (s, 1H), 4.09 (d, *J* = 14.0 Hz, 1H), 3.68 (s, 3H), 3.17 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.36, 166.77, 159.03, 148.05, 145.35, 144.22, 137.89, 134.86, 133.38, 130.07, 129.82, 128.88, 128.43, 128.17, 127.45, 117.59, 114.14, 108.58, 102.04, 98.49, 65.91, 55.17, 49.17, 38.19. ESI-HRMS calcd for [$C_{31}H_{24}{}^{35}ClNO_6$+$Na^+$]: 564.1190, found 564.1189.



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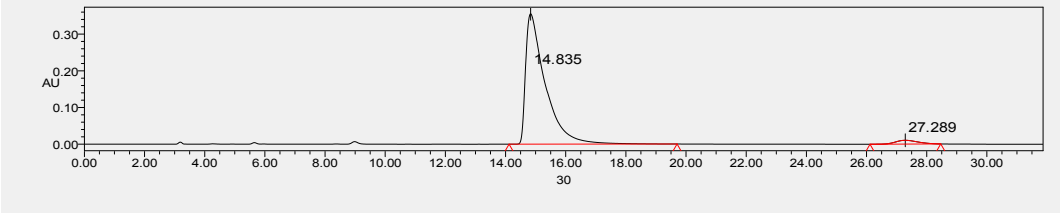
2	27.204	50.05



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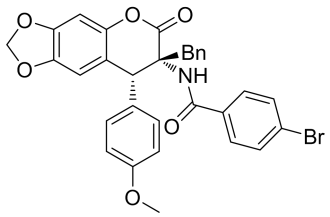
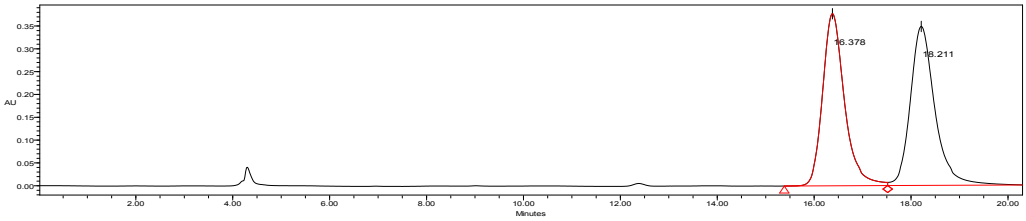
1	14.835	96.81
2	27.289	3.19



_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-bromobenzamide (3d)

Result: 90% Yield, 91% *ee*; $[\alpha]^{21}_{D}$ = −118.0 (*c* 0.2, CH_2Cl_2); HPLC (Daicel chiralcel IC, *n*-hexane/*i*-PrOH 95/5, 0.8 mL/min) $t_{R(major)}$ = 16.86 min, $t_{R(minor)}$ = 19.09 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.5Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.23 – 7.15 (m, 3H), 7.03 (d, *J* = 8.8 Hz, 4H), 6.80 (s, 1H), 6.69 (d, *J* = 8.5 Hz, 4H), 5.97 (d, *J* = 17.0 Hz, 2H), 5.25 (s, 1H), 4.10 (t, *J* = 9.1 Hz, 1H), 3.68 (d, *J* = 13.3 Hz, 3H), 3.17 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.35, 166.85, 159.04, 148.06, 145.35, 144.23, 134.87, 133.85, 131.86, 130.07, 129.82, 128.89, 128.44, 128.35, 127.46, 126.35, 117.59, 114.16, 108.59, 102.04, 98.50, 65.91, 55.16, 49.17, 38.20. ESI-HRMS calcd for $[C_{31}H_{24}{}^{80}BrNO_6+Na^+]$: 608.0685, found 608.0688.



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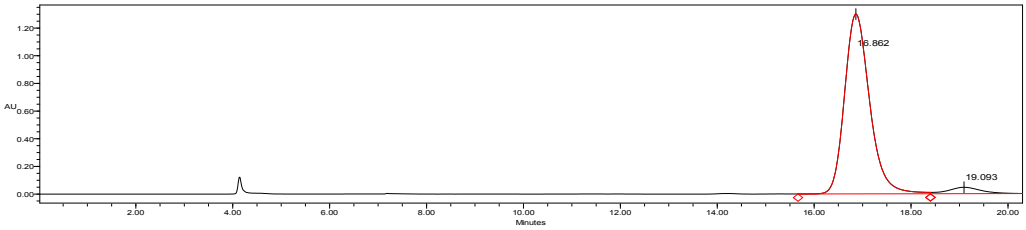
1	16.378	49.15
2	18.211	50.85



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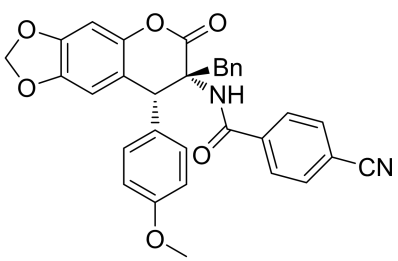
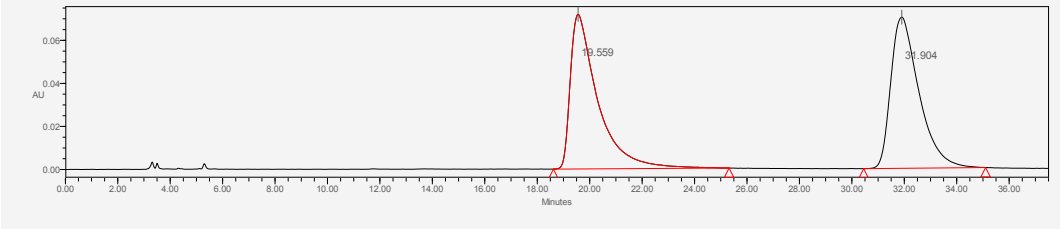
2	19.093	4.44



_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-cyanobenzamide (3e)

Result: 64% Yield, 94% *ee*; $[\alpha]^{21}_D$ = −185.7 (*c* 0.17, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 70/30, 1.0 mL/min) $t_{R(major)}$ = 20.49 min, $t_{R(minor)}$ = 34.27 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 56.3, 7.7 Hz, 4H), 7.24 – 6.97 (m, 7H), 6.74 (dd, *J* = 28.0, 20.6 Hz, 5H), 6.00 (d, *J* = 15.9 Hz, 2H), 5.22 (s, 1H), 4.06 (d, *J* = 14.0 Hz, 1H), 3.68 (s, 3H), 3.20 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.26, 166.05, 159.12, 148.14, 145.43, 144.13, 138.83, 134.68, 132.52, 129.97, 129.76, 128.82, 128.49, 127.56, 127.39, 117.89, 117.35, 115.25, 114.21, 108.55, 102.08, 98.54, 65.99, 55.19, 49.24, 38.29. ESI-HRMS calcd for [$C_{32}H_{24}N_2O_6$+Na^+]: 555.1532, found 555.1535.



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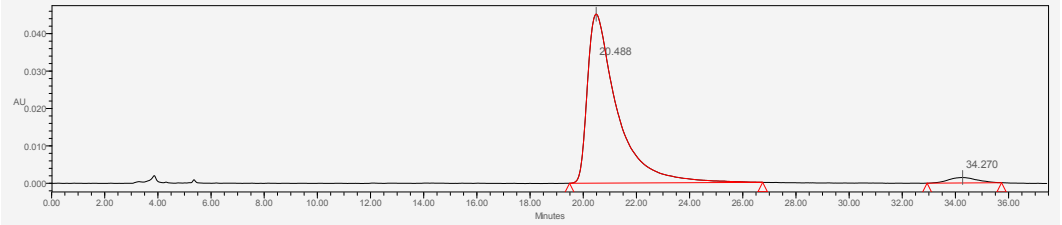
2	31.904	50.13



	Retention Time	% Area
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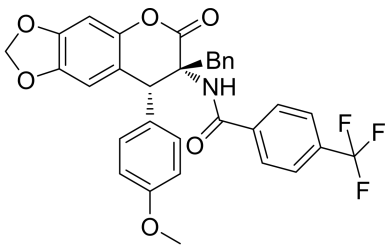
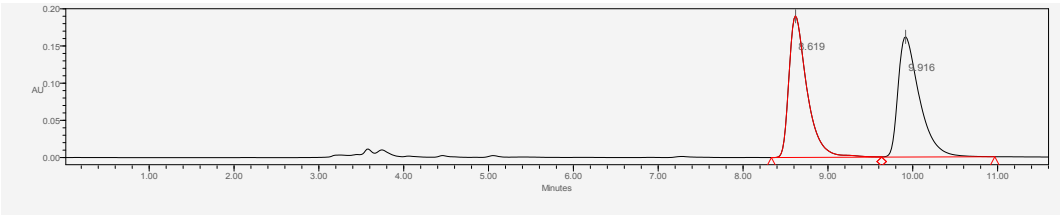
2	34.270	2.98



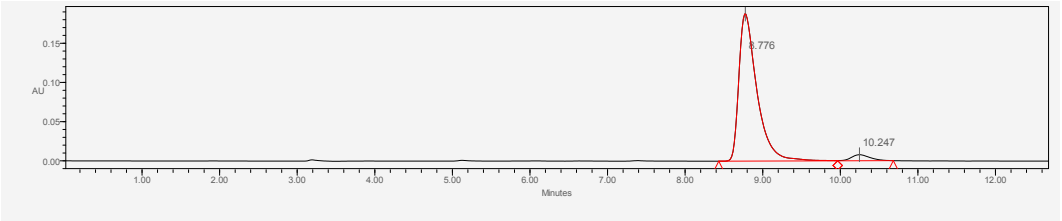
_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-(trifluoromethyl)benzamide (3f)

Result: 68% Yield, 92% *ee*; $[\alpha]^{21}_D$ = −100.6 (*c* 0.36, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 8.78 min, $t_{R(minor)}$ = 10.25 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 6.4 Hz, 2H),

7.46 (dt, J = 15.0, 7.4 Hz, 2H), 7.24 – 6.95 (m, 7H), 6.86 – 6.60 (m, 5H), 5.99 (d, J = 16.7 Hz, 2H), 5.25 (s, 1H), 4.10 (d, J = 14.0 Hz, 1H), 3.71 (d, J = 30.7 Hz, 3H), 3.20 (d, J = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.32, 166.57, 159.15, 148.11, 145.40, 144.18, 135.99, 134.77, 131.86, 131.72, 131.40, 131.07, 130.93, 130.74, 130.06, 129.81, 129.68, 129.23, 128.86, 128.47, 128.20, 128.16, 127.53, 124.94, 124.03, 124.00, 122.23, 117.46, 114.23, 108.59, 102.06, 98.51, 65.98, 55.14, 49.29, 38.34. ESI-HRMS calcd for [$C_{32}H_{24}F_3NO_6$+Na^+]: 598.1453, found 598.1452.



	Retention Time	% Area
1	8.619	50.03
2	9.916	49.97



	Retention Time	% Area
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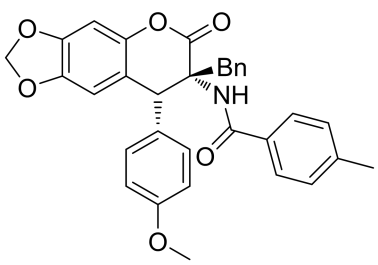
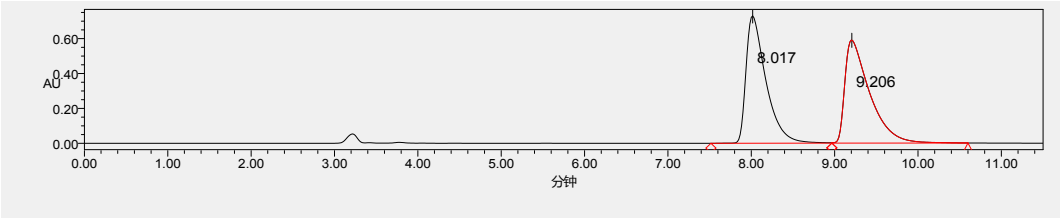
2	10.247	4.08



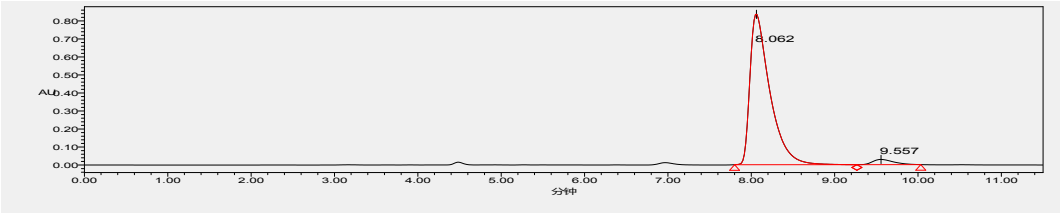
N-((7R,8R)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6H-[1,3]dioxolo[4,5-g]chromen-7-yl)-4-methylbenzamide (3g)

Result: 90% Yield, 93% *ee*; $[\alpha]^{21}_D$ = −101.9 (*c* 1.61, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 8.06 min, $t_{R(minor)}$ = 9.56 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 8.1 Hz, 1H), 7.21 – 7.10 (m, 2H), 7.05 (dd, J = 6.5, 2.3 Hz, 1H), 6.80 (s, 1H), 6.68 (dd, J = 5.6, 2.9 Hz, 1H), 5.98 (dd, J = 16.4, 1.1 Hz, 1H), 5.28 (s, 1H), 4.14 (d, J = 14.0 Hz, 1H), 3.66 (d, J = 5.9 Hz, 3H), 3.15 (d, J = 13.9 Hz, 1H), 2.34 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.43, 167.85, 158.94, 147.99, 145.28, 144.31, 142.06, 135.04, 132.30, 130.19, 129.89, 129.24, 128.96, 128.37, 127.34, 126.76, 117.82,

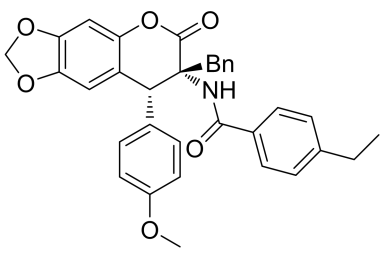
114.10, 108.61, 102.00, 98.46, 65.86, 55.14, 49.14, 38.13, 21.45. ESI-HRMS calcd for [$C_{32}H_{27}NO_6$+Na^+]: 544.1736, found 544.1738.



	Retention Time	% Area
1	8.017	49.69
2	9.206	50.31

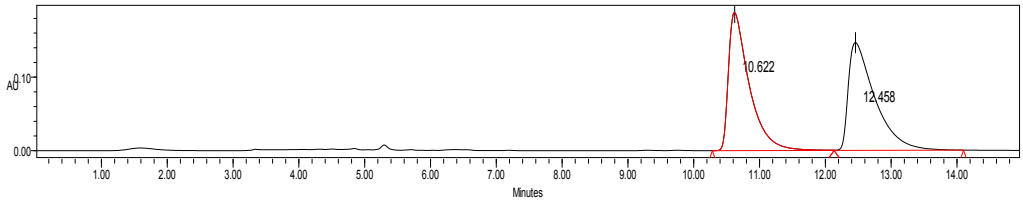


	Retention Time	% Area
1	8.062	96.49
2	9.557	3.51

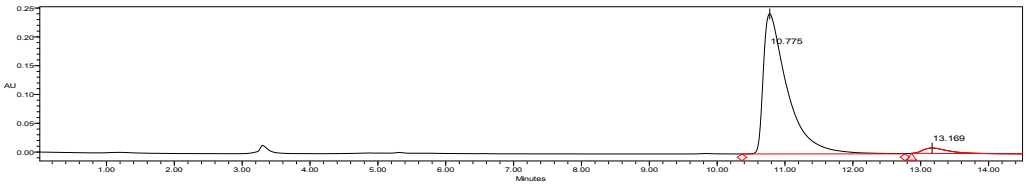


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-ethylbenzamide (3h)

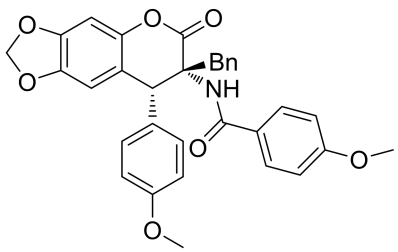
Result: 87% Yield, 92% *ee*; $[\alpha]^{20}_D$ = −133.6 (*c* 0.28, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 95/5, 1.0 mL/min) $t_{R(major)}$ = 10.78 min, $t_{R(minor)}$ = 13.17 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.1 Hz, 2H), 7.23 – 7.13 (m, 5H), 7.05 (dd, *J* = 6.6, 2.2 Hz, 4H), 6.81 (s, 1H), 6.69 (dd, *J* = 6.3, 2.3 Hz, 4H), 5.98 (dd, *J* = 16.3, 1.1 Hz, 2H), 5.28 (s, 1H), 4.14 (d, *J* = 14.0 Hz, 1H), 3.67 (s, 3H), 3.15 (d, *J* = 13.9 Hz, 1H), 2.64 (q, *J* = 7.6 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.42, 167.94, 158.94, 148.25, 147.98, 145.28, 144.31, 135.04, 132.58, 130.21, 129.90, 128.96, 128.38, 128.08, 127.33, 126.84, 117.83, 114.11, 108.61, 102.00, 98.46, 65.86, 55.15, 49.15, 38.13, 28.78, 15.28. ESI-HRMS calcd for [$C_{33}H_{29}NO_6$+Na^+]: 558.1893, found 558.1893.



	Retention Time	% Area
1	10.622	50.12
2	12.458	49.88

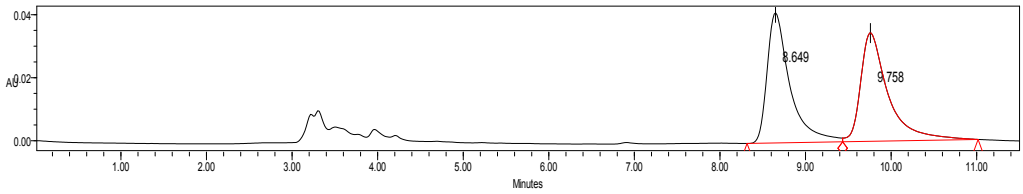


	Retention Time	% Area
1	10.775	96.02
2	13.169	3.98

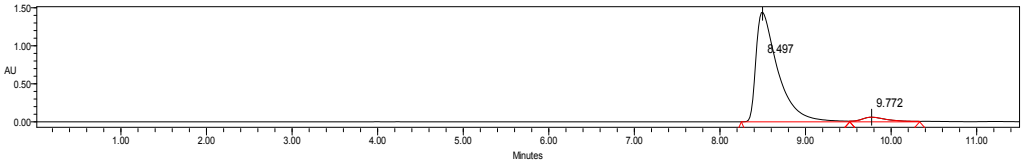


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-methoxybenzamide (3i)

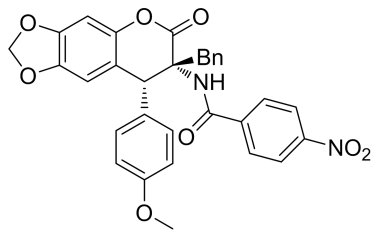
Result: 85% Yield, 90% *ee*; $[\alpha]^{21}_{D}$ = −114.6 (*c* 0.44, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 8.50 min, $t_{R(minor)}$ = 9.77 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.7 Hz, 2H), 7.24 – 7.11 (m, 3H), 7.04 (d, *J* = 8.6 Hz, 4H), 6.88 – 6.75 (m, 3H), 6.68 (dd, *J* = 12.7, 6.7 Hz, 4H), 5.99 (d, *J* = 15.9 Hz, 2H), 5.28 (s, 1H), 4.14 (d, *J* = 13.9 Hz, 1H), 3.84 – 3.75 (m, 3H), 3.67 (s, 3H), 3.14 (d, *J* = 13.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.48, 167.34, 162.29, 158.92, 147.98, 145.27, 144.32, 135.08, 130.22, 129.89, 128.96, 128.58, 128.34, 127.39, 127.30, 117.86, 114.07, 113.77, 108.61, 101.98, 98.44, 77.37, 77.05, 76.74, 65.84, 55.39, 55.14, 49.16, 38.15. ESI-HRMS calcd for [$C_{32}H_{27}NO_7$+Na^+]: 560.1687, found 560.1685.



	Retention Time	% Area
1	8.649	49.91
2	9.758	50.09

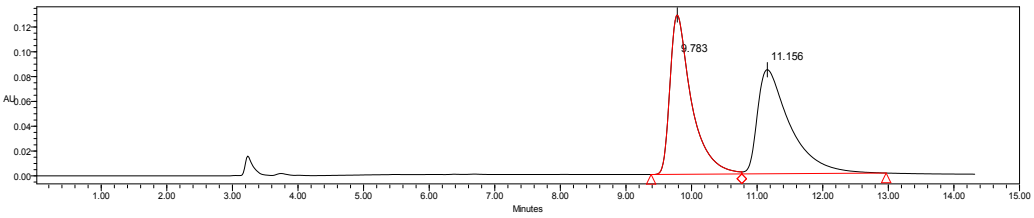


	Retention Time	% Area
1	8.497	95.09
2	9.772	4.91

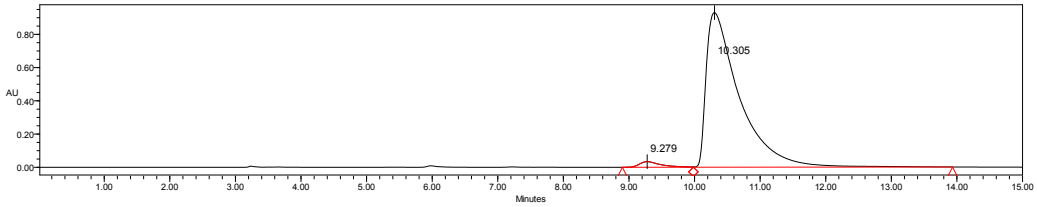


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-4-nitrobenzamide (3j)

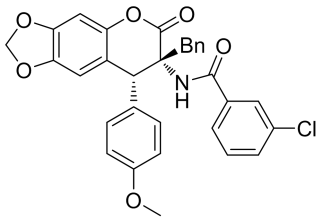
Result: 94% Yield, 96% *ee*; $[\alpha]^{25}_{D}$ = −84.2 (*c* 0.91, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 70/30, 1.0 mL/min) $t_{R(major)}$ = 10.31 min, $t_{R(minor)}$ = 9.28 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.7 Hz, 2H), 7.55 (d, *J* = 8.7 Hz, 2H), 7.25 – 7.12 (m, 3H), 7.04 (d, *J* = 8.6 Hz, 4H), 6.75 (dd, *J* = 32.1, 15.9 Hz, 5H), 6.01 (dd, *J* = 15.9, 1.1 Hz, 2H), 5.23 (s, 1H), 4.07 (d, *J* = 14.1 Hz, 1H), 3.69 (s, 3H), 3.22 (d, *J* = 14.0 Hz, 1H). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.7 Hz, 2H), 7.55 (d, *J* = 8.7 Hz, 2H), 7.25 – 7.12 (m, 3H), 7.04 (d, *J* = 8.6 Hz, 4H), 6.75 (dd, *J* = 32.1, 15.9 Hz, 5H), 6.01 (dd, *J* = 15.9, 1.1 Hz, 2H), 5.23 (s, 1H), 4.07 (d, *J* = 14.1 Hz, 1H), 3.69 (s, 3H), 3.22 (d, *J* = 14.0 Hz, 1H). ESI-HRMS calcd for [$C_{31}H_{24}N_2O_8$+Na^+]: 575.1430, found 575.1428.



	Retention Time	% Area
1	9.783	50.26
2	11.156	49.74

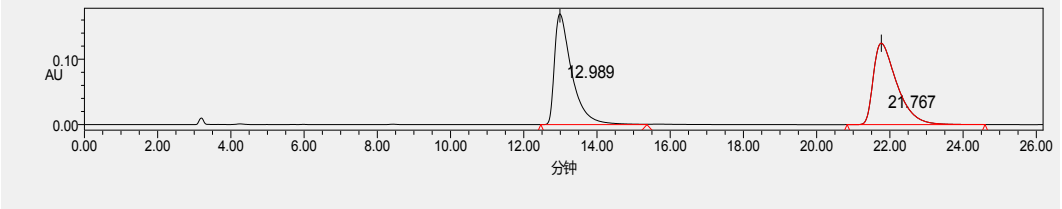


	Retention Time	% Area
1	9.279	2.28
2	10.305	97.72

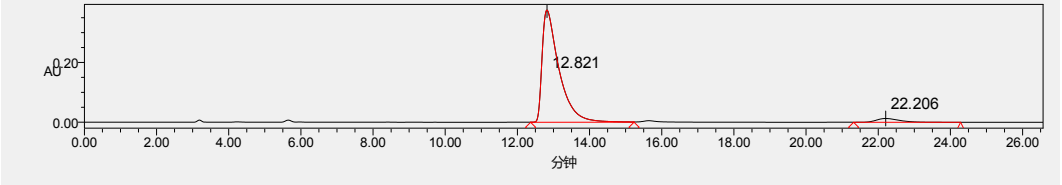


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-3-chlorobenzamide (3k)

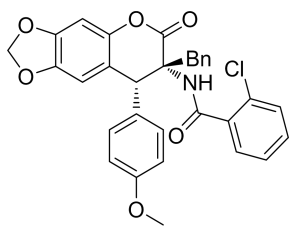
Result: 88% Yield, 91% *ee*; $[\alpha]^{20}_{D}$ = −99.0 (*c* 1.66, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 12.82 min, $t_{R(minor)}$ = 22.21 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.35 (m, 2H), 7.25 – 7.17 (m, 5H), 7.04 (d, *J* = 8.2 Hz, 4H), 6.81 (s, 1H), 6.77 – 6.60 (m, 4H), 5.98 (d, *J* = 16.6 Hz, 2H), 5.24 (s, 1H), 4.09 (d, *J* = 14.0 Hz, 1H), 3.68 (s, 3H), 3.18 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.31, 166.49, 159.08, 148.07, 145.36, 144.20, 136.77, 134.83, 134.81, 131.70, 130.05, 129.92, 129.82, 128.88, 128.47, 127.50, 127.20, 124.64, 117.55, 114.22, 108.59, 102.05, 98.50, 65.94, 55.19, 49.20, 38.22. ESI-HRMS calcd for $[C_{31}H_{24}{}^{35}ClNO_6+Na^+]$: 564.1190, found 564.1187.



	Retention Time	% Area
1	12.989	49.91
2	21.767	50.09

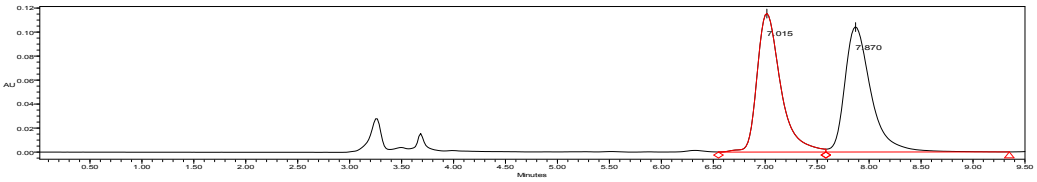


	Retention Time	% Area
1	12.821	95.66
2	22.206	4.34

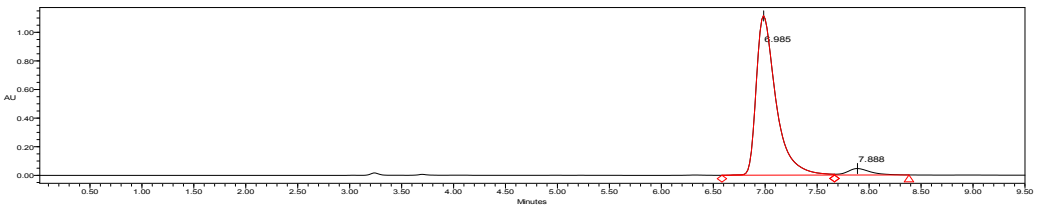


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-2-chlorobenzamide (3l)

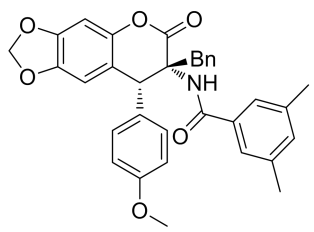
Result: 85% Yield, 91% *ee*; $[\alpha]^{25}_{D} = -75.8$ (*c* 1.49, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 6.99 min, $t_{R(minor)}$ = 7.89 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 2H), 7.25 (s, 1H), 7.24 – 7.21 (m, 2H), 7.15 (m, *J* = 18.0, 9.7, 2.5 Hz, 5H), 6.97 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.82 – 6.65 (m, 5H), 5.97 (dd, *J* = 17.7, 1.2 Hz, 2H), 5.26 (s, 1H), 4.11 (d, *J* = 14.1 Hz, 1H), 3.71 (s, 3H), 3.21 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.23, 166.23, 159.18, 148.01, 145.32, 144.05, 134.77, 134.54, 131.50, 131.48, 130.66, 130.38, 130.11, 129.53, 129.19, 128.43, 127.45, 126.82, 117.72, 114.31, 108.57, 102.03, 98.51, 66.05, 55.27, 49.50, 38.51. ESI-HRMS calcd for $[C_{31}H_{24}{}^{35}ClNO_6+Na^+]$: 564.1190, found 564.1188.



	Retention Time	% Area
1	7.015	50.07
2	7.870	49.93

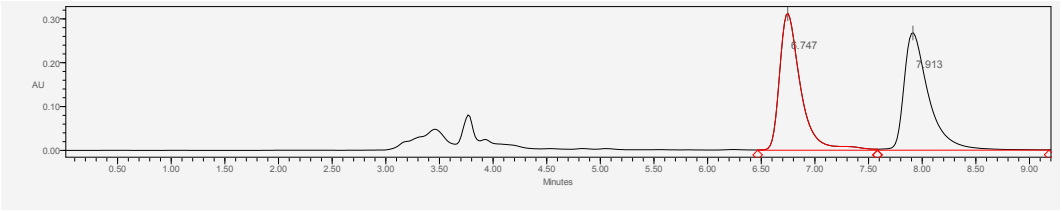


	Retention Time	% Area
1	6.985	95.48
2	7.888	4.52

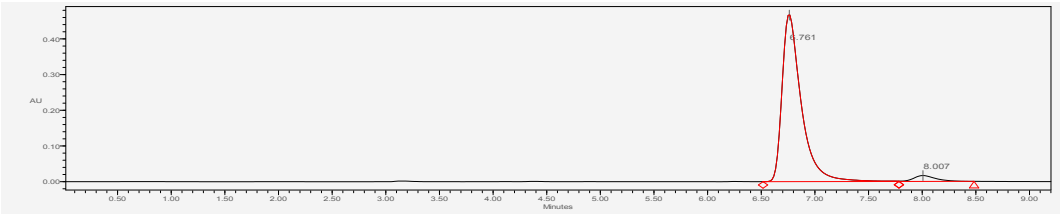


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-3,5-dimethylbenzamide (3m)

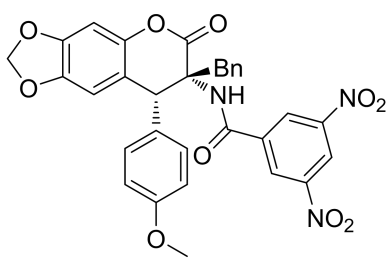
Result: 80% Yield, 92% *ee*; $[\alpha]^{21}_{D}$ = −122.6 (*c* 0.23, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 6.76 min, $t_{R(minor)}$ = 8.01 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 3H), 7.14 – 6.88 (m, 7H), 6.81 (s, 1H), 6.64 (dd, *J* = 47.8, 8.4 Hz, 4H), 5.94 (t, *J* = 31.8 Hz, 2H), 5.28 (s, 1H), 4.12 (t, *J* = 14.5 Hz, 1H), 3.72 (d, *J* = 32.1 Hz, 3H), 3.15 (d, *J* = 13.9 Hz, 1H), 2.19 (d, *J* = 64.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.44, 168.27, 158.97, 147.99, 145.28, 144.29, 138.30, 135.13, 135.04, 133.24, 130.25, 129.92, 128.98, 128.37, 127.34, 124.48, 117.83, 114.14, 108.62, 101.99, 98.45, 68.89, 65.86, 55.16, 49.17, 38.15, 21.18. ESI-HRMS calcd for [$C_{33}H_{29}NO_6$+Na^+]:558.1893, found 558.1894.



	Retention Time	% Area
1	7.264	49.76
2	8.576	50.24



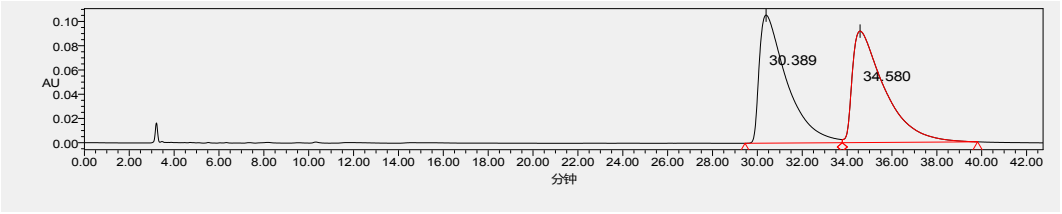
	Retention Time	% Area
1	6.761	96.10
2	8.007	3.90



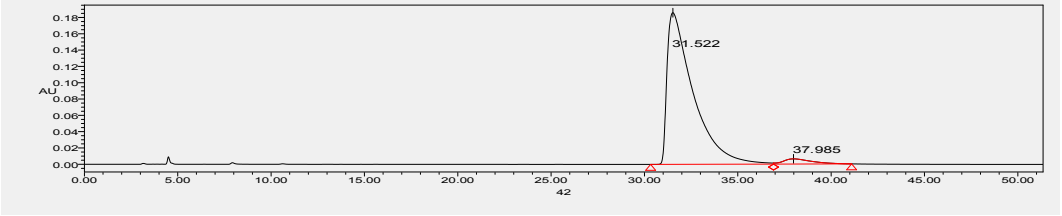
_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-3,5-dinitrobenzamide (3n)

Result: 94% Yield, 93% *ee*; $[\alpha]^{25}_{D}$ = −72.4 (*c* 1.91, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 31.52 min,

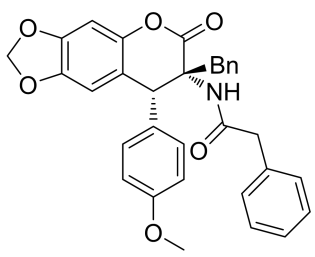
$t_{R(minor)}$ = 37.99 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (t, *J* = 2.0 Hz, 1H), 8.41 (d, *J* = 2.0 Hz, 2H), 7.22 (dd, *J* = 6.2, 3.7 Hz, 3H), 7.10 – 6.97 (m, 4H), 6.89 – 6.58 (m, 5H), 6.01 (dd, *J*=16.5, 1.1 Hz, 2H), 5.19 (s, 1H), 4.02 (d, *J* = 14.2 Hz, 1H), 3.69 (s, 3H), 3.26 (d, *J* = 14.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.19, 168.09, 163.38, 159.38, 148.56, 148.26, 145.54, 143.96, 138.48, 134.38, 129.84, 129.65, 128.69, 128.64, 127.81, 126.84, 121.09, 116.94, 114.42, 108.53, 102.16, 98.61, 66.16, 55.22, 49.47, 38.63. ESI-HRMS calcd for [$C_{31}H_{23}N_3O_{10}$+Na^+]: 620.1281, found 620.1278.



	Retention Time	% Area
1	30.389	49.59
2	34.580	50.41

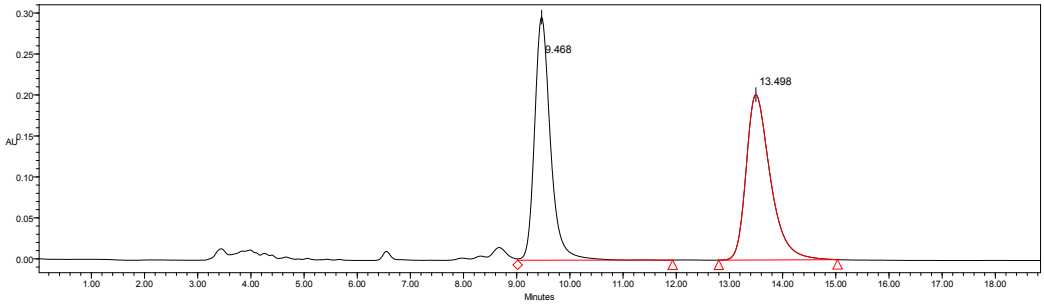


	Retention Time	% Area
1	31.522	96.44
2	37.985	3.56

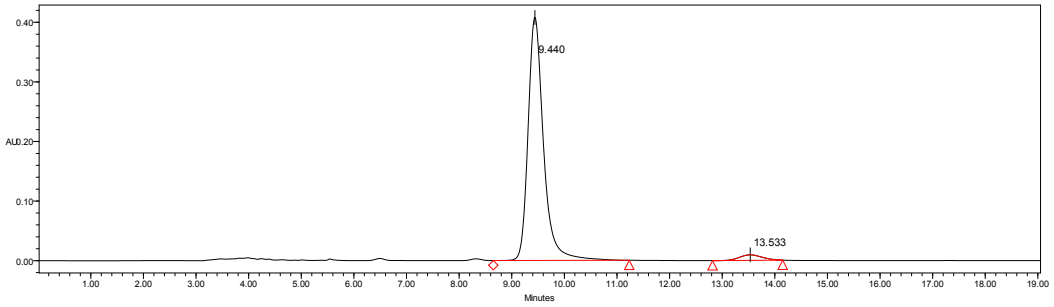


_N_-((7_R_,8_R_)-7-benzyl-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)-2-phenylacetamide (3o)

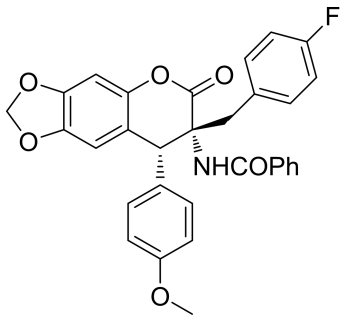
Result: 63% Yield, 94% *ee*; $[\alpha]^{20}_D$ = −56.1 (*c* 0.28, CH_2Cl_2); HPLC (Daicel chiralcel IC, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 9.47 min, $t_{R(minor)}$ = 13.50 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.13 (m, 6H), 7.00 – 6.87 (m, 6H), 6.69 (dd, *J* = 28.7, 20.0 Hz, 4H), 6.13 (s, 1H), 6.02 – 5.91 (m, 2H), 5.08 (s, 1H), 3.91 (d, *J* = 14.0 Hz, 1H), 3.75 (s, 3H), 3.32 (s, 2H), 3.04 (d, *J* = 13.9 Hz, 1H). ^{13}C NMR (100MHz, $CDCl_3$) δ 170.69, 168.08, 158.97, 147.90, 145.19, 144.06, 134.84, 134.04, 130.32, 129.80, 129.26, 128.88, 128.68, 128.31, 127.28, 127.17, 117.67, 114.09, 108.52, 101.94, 98.42, 65.21, 55.21, 49.21, 44.46, 38.21. ESI-HRMS calcd for [$C_{32}H_{27}NO_6$+Na^+]: 544.1736, found 544.1736.



	Retention Time	% Area
1	9.468	49.10
2	13.498	50.90

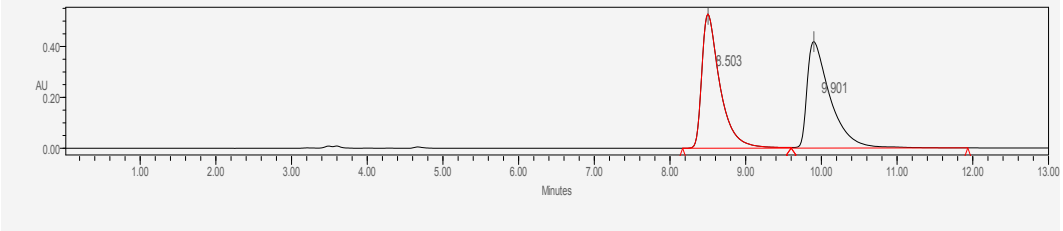


	Retention Time	% Area
1	9.440	96.78
2	13.533	3.22

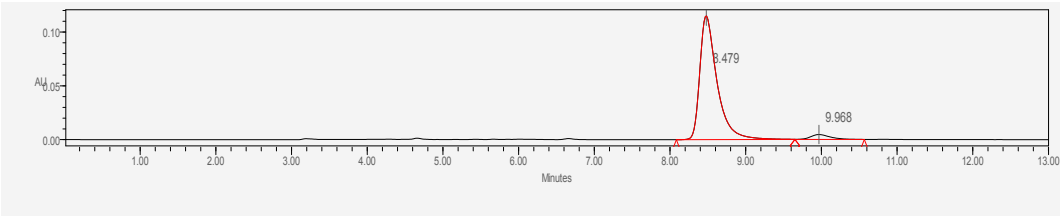


_N_-((7_R_,8_R_)-7-(4-fluorobenzyl)-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3p)

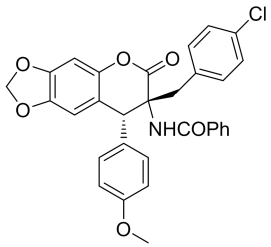
Result: 42% Yield, 91% *ee*; $[\alpha]^{22}_{D}$ = −106.6 (*c* 0.30, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 8.48 min, $t_{R(minor)}$ = 9.97 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 34.6, 6.5 Hz, 5H), 7.16 – 6.46 (m, 11H), 5.99 (d, *J* = 15.1 Hz, 2H), 5.26 (s, 1H), 4.12 (d, *J* = 14.0 Hz, 1H), 3.67 (s, 3H), 3.14 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.33, 167.93, 163.38, 160.94, 159.02, 148.06, 145.36, 144.21, 134.95, 131.71, 131.42, 131.34, 130.73, 130.70, 130.04, 128.91, 128.67, 126.68, 117.61, 115.44, 115.23, 114.16, 108.60, 102.04, 98.45, 65.84, 55.16, 49.08, 37.36. ESI-HRMS calcd for $[C_{31}H_{24}FO_6+Na^+]$: 548.1485, found 548.1489.



	Retention Time	% Area
1	8.503	49.84
2	9.901	50.16

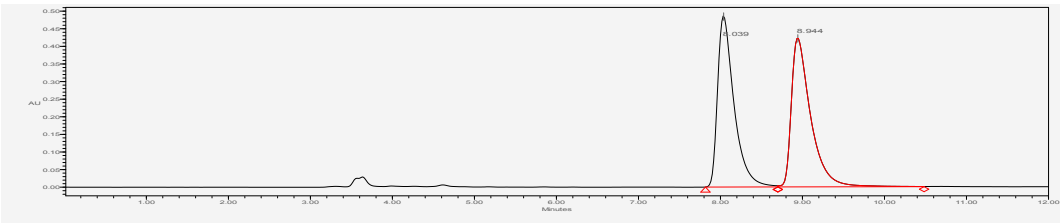


	Retention Time	% Area
1	8.479	95.61
2	9.968	4.39

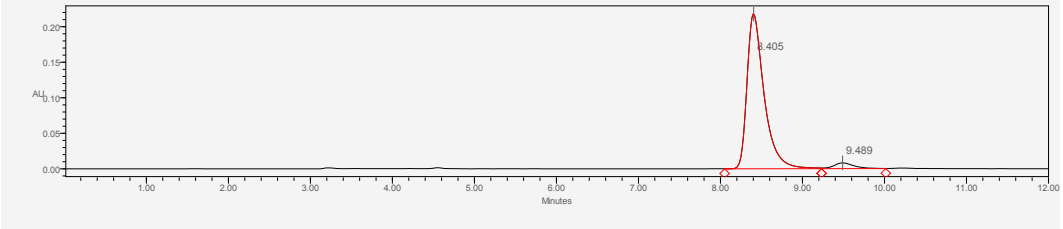


_N_-((7_R_,8_R_)-7-(4-chlorobenzyl)-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3q)

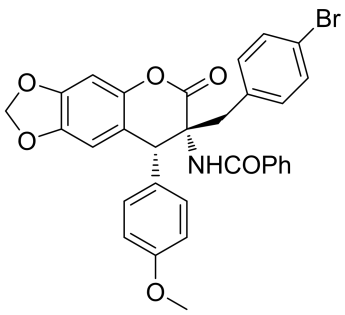
Result: 70% Yield, 92% *ee*; $[\alpha]^{21}_{D}$ = −95.4 (*c* 0.35, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 8.41 min, $t_{R(minor)}$ = 9.49 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 6.7 Hz, 3H), 7.36 (d, *J* = 6.7 Hz, 2H), 7.17 (d, *J* = 7.4 Hz, 2H), 7.01 (dd, *J* = 19.2, 7.7 Hz, 4H), 6.86 – 6.62 (m, 5H), 5.98 (d, *J* = 14.7 Hz, 2H), 5.25 (s, 1H), 4.13 (d, *J* = 13.9 Hz, 1H), 3.71 (d, *J* = 33.2 Hz, 3H), 3.14 (d, *J* = 13.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.23, 167.96, 159.05, 148.08, 145.38, 144.19, 134.89, 133.48, 133.37, 131.75, 131.18, 129.96, 128.91, 128.69, 128.60, 126.68, 117.56, 114.18, 108.59, 102.05, 98.46, 65.74, 55.16, 49.10, 37.51. ESI-HRMS calcd for $[C_{31}H_{24}{}^{35}ClNO_6+Na^+]$: 564.1184, found 564.1187.



	Retention Time	% Area
1	8.039	49.53
2	8.944	50.47

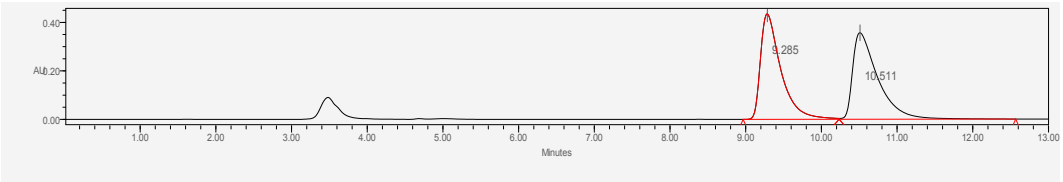


	Retention Time	% Area
1	8.405	95.78
2	9.489	4.22

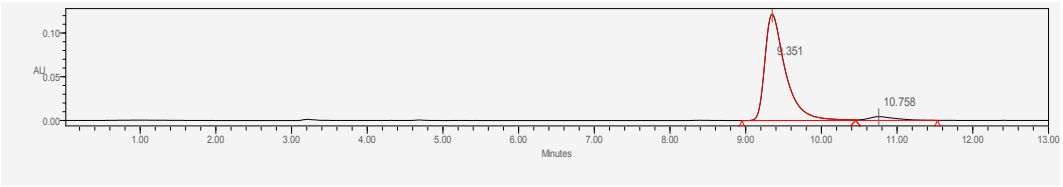


_N_-((7_R_,8_R_)-7-(4-bromobenzyl)-8-(4-methoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3r)

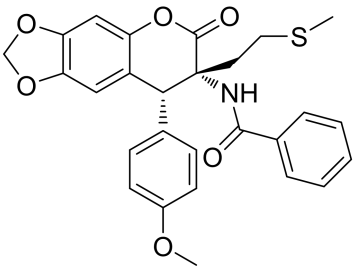
Result: 91% Yield, 91% *ee*; $[\alpha]^{22}_{D}$ = −205.9 (*c* 0.12, CH_2Cl_2); HPLC (Daicel chiralcel IB, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min) $t_{R(major)}$ = 9.35 min, $t_{R(minor)}$ = 10.76 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.41 (m, 3H), 7.34 (dd, *J* = 15.8, 7.8 Hz, 4H), 6.98 (dd, *J* = 42.5, 8.3 Hz, 4H), 6.85 – 6.58 (m, 5H), 5.99 (d, *J* = 14.4 Hz, 2H), 5.25 (s, 1H), 4.11 (d, *J* = 14.0 Hz, 1H), 3.67 (s, 3H), 3.12 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.20, 167.96, 159.05, 148.08, 145.39, 144.19, 134.87, 133.98, 131.75, 131.54, 129.94, 128.91, 128.69, 126.68, 121.55, 117.55, 114.18, 108.58, 102.05, 98.46, 65.67, 55.16, 49.10, 37.58. ESI-HRMS calcd for $[C_{31}H_{24}{}^{80}BrNO_6+Na^+]$: 608.0685, found 608.0687.



	Retention Time	% Area
1	9.285	49.66
2	10.511	50.34

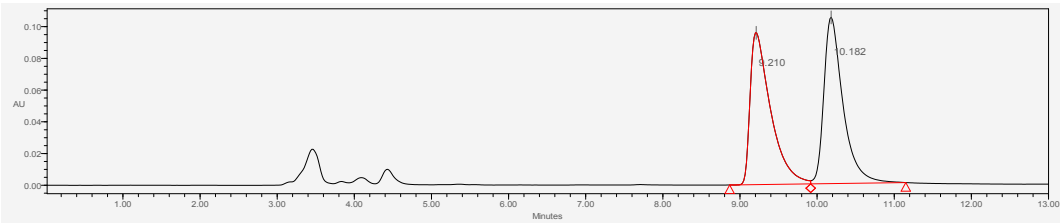


	Retention Time	% Area
1	9.351	95.56
2	10.758	4.44

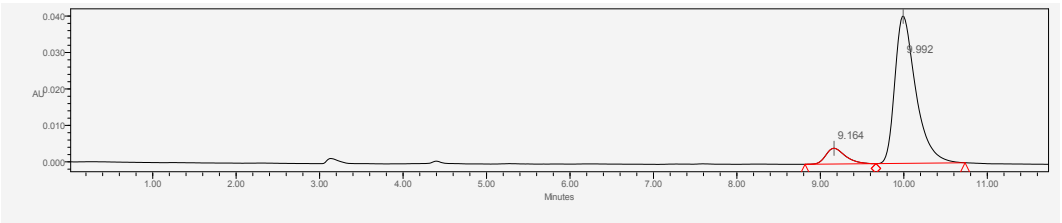


_N_-((7_R_,8_R_)-8-(4-methoxyphenyl)-7-(2-(methylthio)ethyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3s)

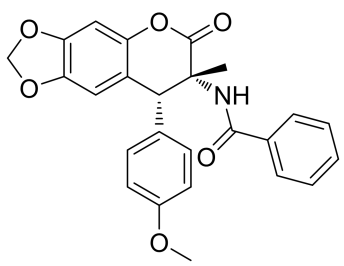
Result: 75% Yield, 82% *ee*; $[\alpha]^{22}_{D}$ = −159.1 (*c* 0.97, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 9.16 min, $t_{R(minor)}$ = 9.99 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (ddd, *J* = 39.3, 19.2, 7.4 Hz, 5H), 7.05 – 6.88 (m, 3H), 6.77 – 6.48 (m, 4H), 5.97 (d, *J* = 15.3 Hz, 2H), 5.09 (s, 1H), 3.68 (s, 3H), 3.30 – 3.12 (m, 1H), 2.51 (td, *J* = 12.7, 5.0 Hz, 1H), 2.35 (td, *J* = 12.4, 4.9 Hz, 1H), 2.19 – 2.07 (m, 1H), 2.01 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ 169.12, 167.27, 159.03, 147.93, 145.30, 144.21, 134.55, 131.79, 129.94, 128.86, 128.66, 126.78, 117.29, 114.17, 108.49, 101.99, 98.45, 64.08, 55.17, 49.01, 32.58, 28.92, 15.60. ESI-HRMS calcd for [$C_{27}H_{25}NO_6S$+Na^+]: 514.1300, found 514.1299.



	Retention Time	% Area
1	9.210	49.41
2	10.182	50.59

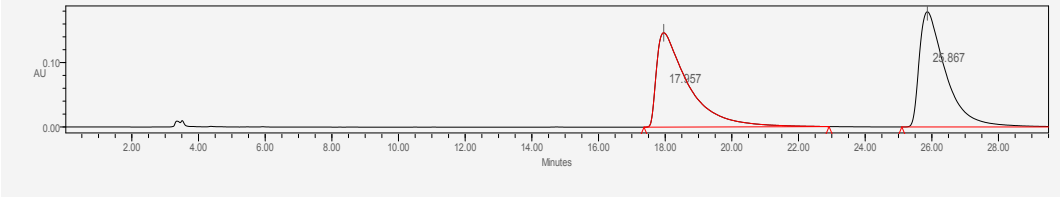


	Retention Time	% Area
1	9.164	9.03
2	9.992	90.97

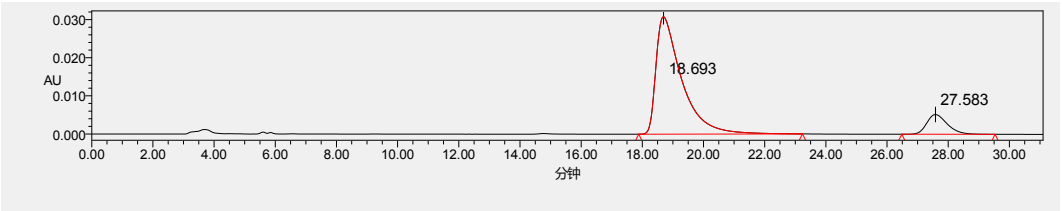


_N_-((7_R_,8_R_)-8-(4-methoxyphenyl)-7-methyl-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3t)

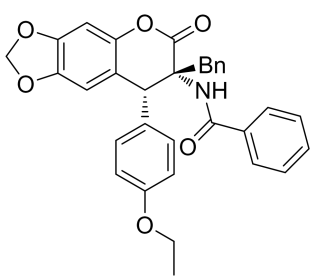
Result: 71% Yield, 77% *ee*; $[\alpha]^{22}_{D}$ = −190.3 (*c* 0.25, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 17.82 min, $t_{R(minor)}$ = 26.39 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.4 Hz, 2H), 7.42 (dt, *J* = 37.3, 7.4 Hz, 3H), 7.13 – 6.92 (m, 3H), 6.79 – 6.57 (m, 4H), 5.97 (d, *J* = 15.4 Hz, 2H), 5.10 (s, 1H), 3.68 (s, 3H), 1.90 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ 170.55, 167.25, 158.95, 147.80, 145.18, 144.31, 134.84, 131.60, 130.39, 128.71, 128.57, 126.79, 117.73, 114.10, 108.50, 101.92, 98.45, 60.50, 55.16, 48.90, 21.91. ESI-HRMS calcd for [$C_{25}H_{21}NO_6$+Na^+]: 454.1267, found 454.1267.



	Retention Time	% Area
1	17.957	49.63
2	25.867	50.37

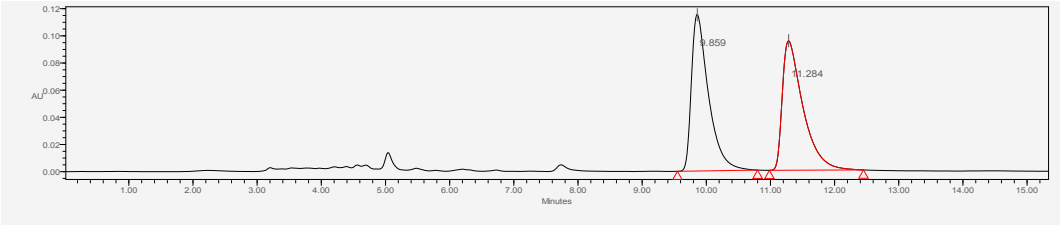


	Retention Time	% Area
1	18.693	88.55
2	27.583	11.45

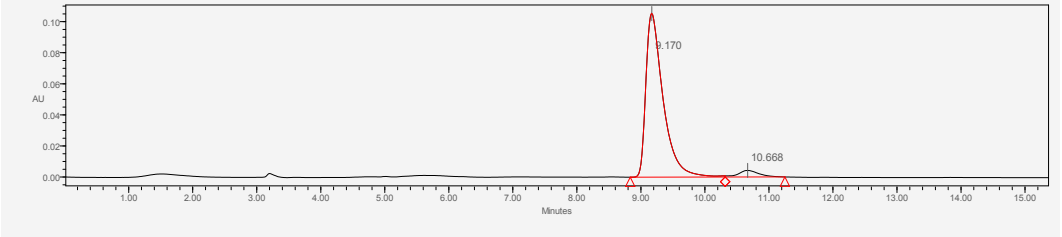


_N_-((7_R_,8_R_)-7-benzyl-8-(4-ethoxyphenyl)-6-oxo-7,8-dihydro-6_H_-[1,3]dioxolo[4,5-_g_]chromen-7-yl)benzamide (3u)

Result: 70% Yield, 91% *ee*; $[\alpha]^{20}_{D}$ = −207.9 (*c* 0.04, CH_2Cl_2); HPLC (Daicel chiralcel IE, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min) $t_{R(major)}$ = 9.17 min, $t_{R(minor)}$ = 10.67 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.39 (m, 3H), 7.37 – 7.29 (m, 2H), 7.23 – 7.13 (m, 3H), 7.10 – 6.98 (m, 4H), 6.81 (s, 1H), 6.69 (t, *J* = 7.6 Hz, 4H), 5.99 (dd, *J* = 15.5, 1.2 Hz, 2H), 5.28 (d, *J* = 5.2 Hz, 1H), 4.21 – 4.03 (m, 1H), 4.02 – 3.76 (m, 2H), 3.11 (t, *J* = 32.7 Hz, 1H), 1.31 (t, *J* = 7.0 Hz, 4H), 1.25 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.39, 167.98, 158.36, 147.99, 145.29, 144.28, 135.19, 134.99, 131.55, 129.97, 129.88, 128.92, 128.59, 128.38, 127.36, 126.71, 117.77, 114.64, 108.62, 102.00, 98.46, 65.90, 63.31, 49.16, 38.14, 14.74. ESI-HRMS calcd for [$C_{32}H_{27}NO_6$+Na^+]: 544.1736, found 544.1734.

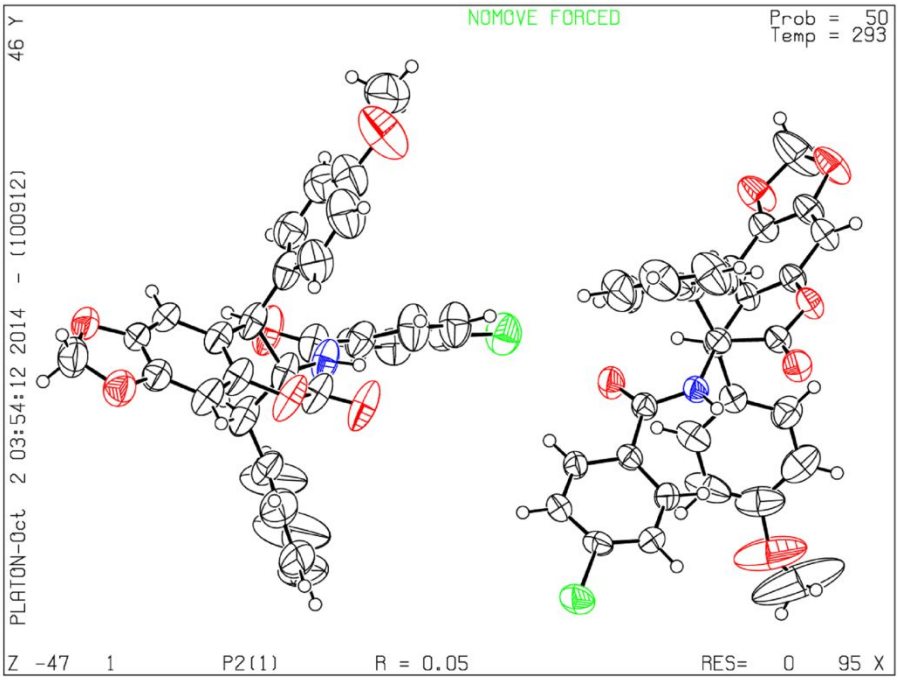


	Retention Time	% Area
1	9.859	50.08
2	11.284	49.92



	Retention Time	% Area
1	9.170	95.45
2	10.668	4.55

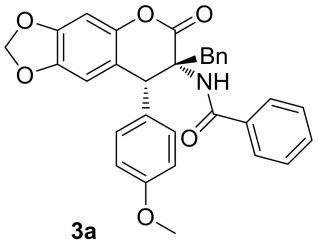
VII. Crystal data of compound 3d.



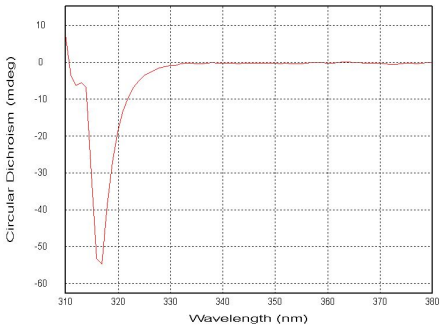
Datablock:

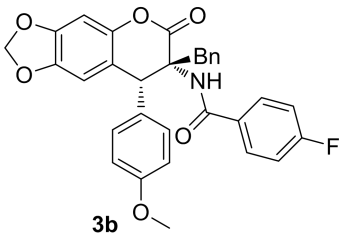
Empirical formula	$C_{31}H_{24}BrNO_6$
Formula weight	586.41
Temperature	293
Crystal system	monoclinic
Unit cell dimensions	a= 9.4993 (3) Å
	b= 18.9341(3) Å
	c= 15.0393(2) Å
	α= 90° β= 97.203(6)°γ= 90°
Cell Volume	2683.64(9)
Z	2
F(000)	1200
CCDC deposition number	1039793

VIII. Copies of CD spectra for dihydrocoumarins.

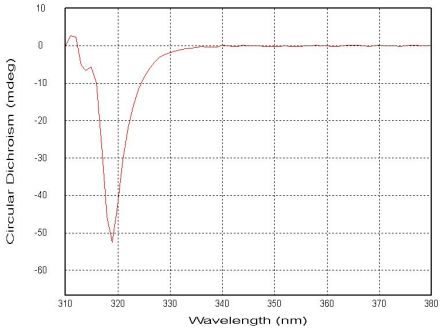


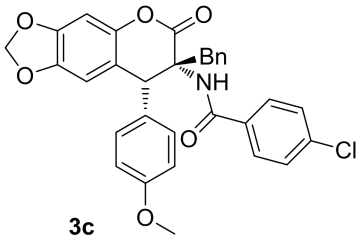
3a



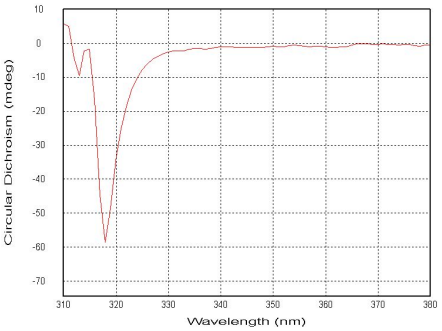


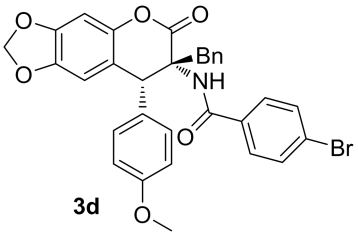
3b



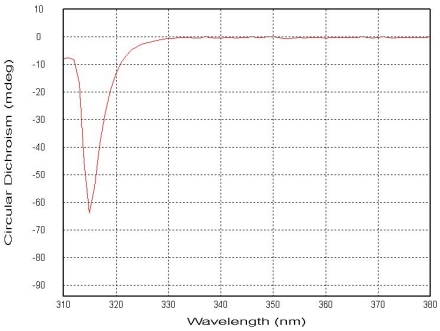


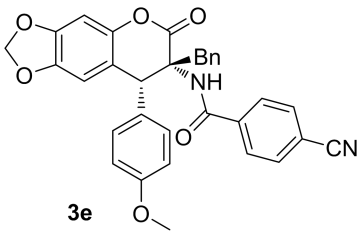
3c



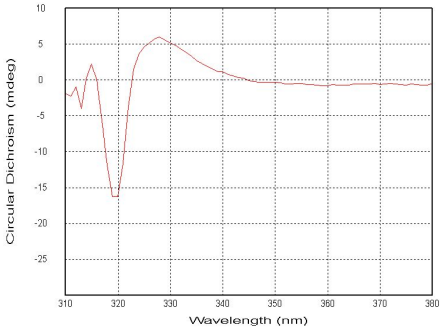


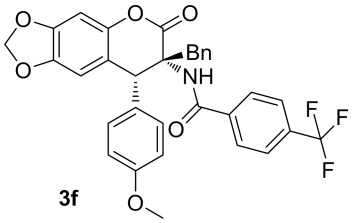
3d



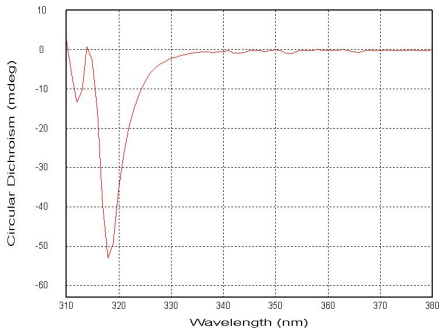

O
O
O
O
Bn
NH
O
CN
O

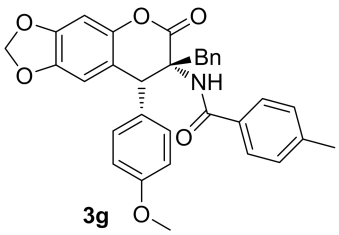
3e


Circular Dichroism (mdeg)
Wavelength (nm)

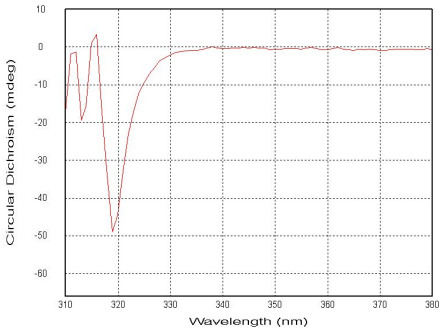

O
O
O
O
Bn
NH
O
F
F
F
O

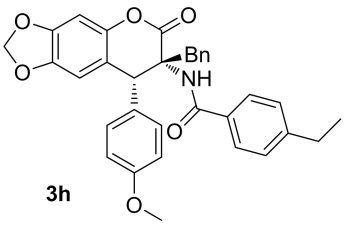
3f


Circular Dichroism (mdeg)
Wavelength (nm)

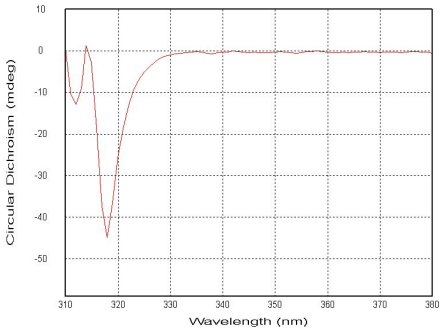

O
O
O
O
Bn
NH
O
O

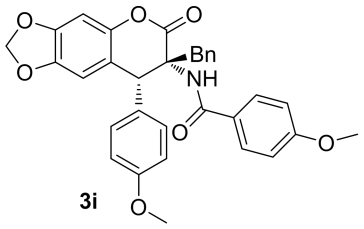
3g


Circular Dichroism (mdeg)
Wavelength (nm)

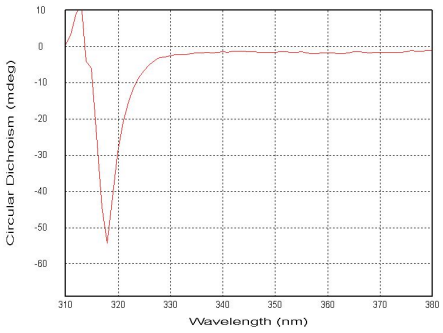

O
O
O
O
Bn
NH
O
O

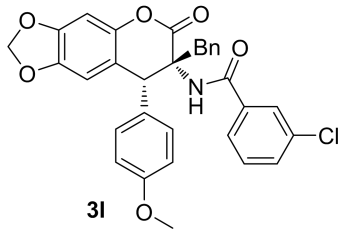
3h


Circular Dichroism (mdeg)
Wavelength (nm)

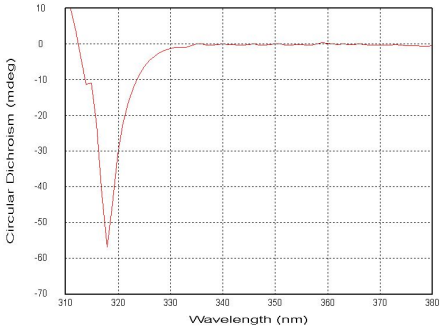

Bn
NH
O
O
O
O
O
O
O

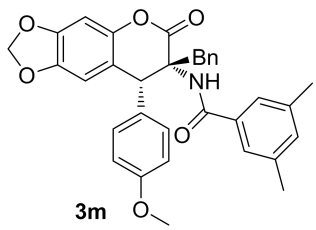
3i


Circular Dichroism (mdeg)
Wavelength (nm)
10
0
-10
-20
-30
-40
-50
-60
310
320
330
340
350
360
370
380

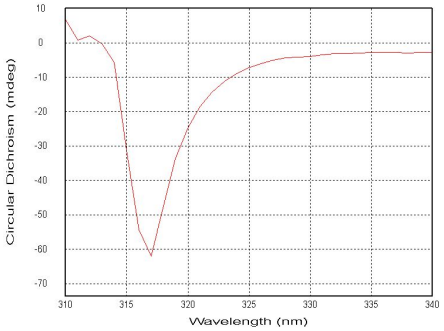

Bn
O
N
H
Cl
O
O
O
O

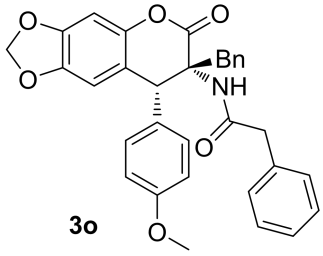
3l


Circular Dichroism (mdeg)
Wavelength (nm)
10
0
-10
-20
-30
-40
-50
-60
-70
310
320
330
340
350
360
370
380

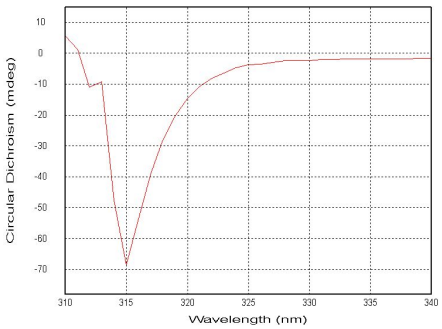

Bn
NH
O
O
O
O
O

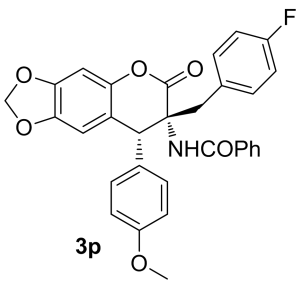
3m


Circular Dichroism (mdeg)
Wavelength (nm)
10
0
-10
-20
-30
-40
-50
-60
-70
310
315
320
325
330
335
340

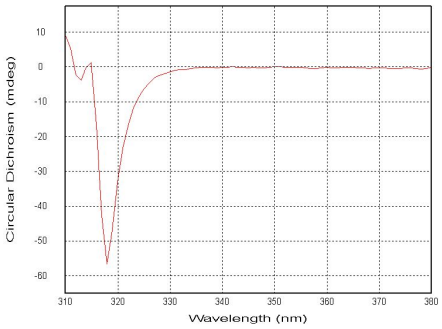

Bn
NH
O
O
O
O
O

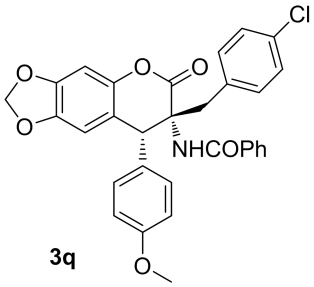
3o


Circular Dichroism (mdeg)
Wavelength (nm)
10
0
-10
-20
-30
-40
-50
-60
-70
310
315
320
325
330
335
340

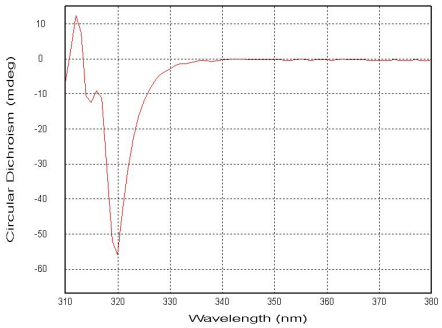

F
O
O
O
NHCOPh
O

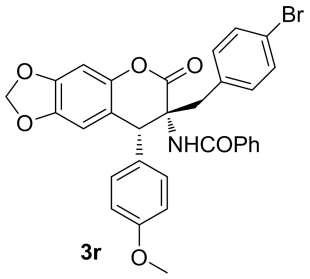
3p


Circular Dichroism (mdeg)
10
0
-10
-20
-30
-40
-50
-60
310
320
330
340
350
360
370
380
Wavelength (nm)

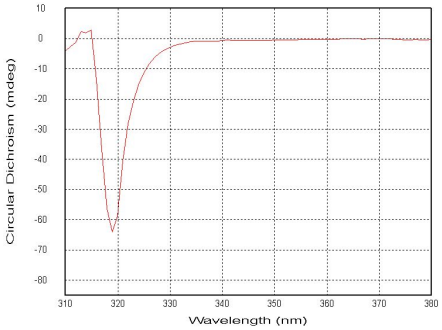

Cl
O
O
O
NHCOPh
O

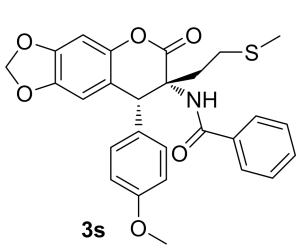
3q


Circular Dichroism (mdeg)
10
0
-10
-20
-30
-40
-50
-60
310
320
330
340
350
360
370
380
Wavelength (nm)

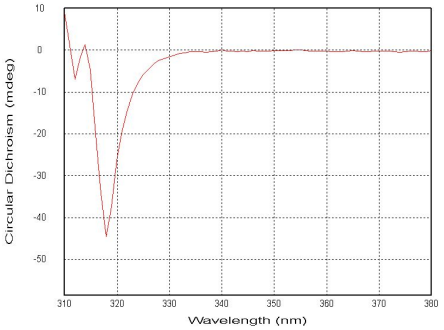

Br
O
O
O
NHCOPh
O

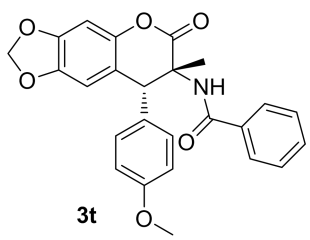
3r


Circular Dichroism (mdeg)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
310
320
330
340
350
360
370
380
Wavelength (nm)

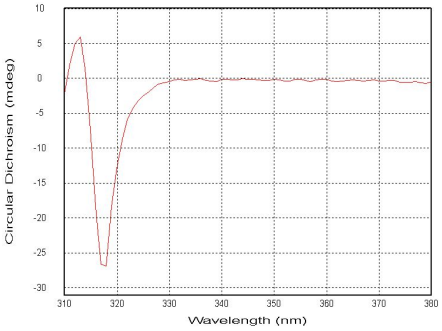

O
O
O
S
NH
O
O

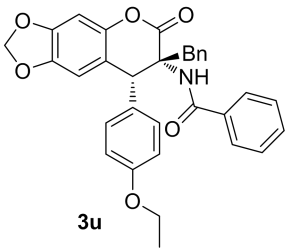
3s


Circular Dichroism (mdeg)
10
0
-10
-20
-30
-40
-50
310
320
330
340
350
360
370
380
Wavelength (nm)

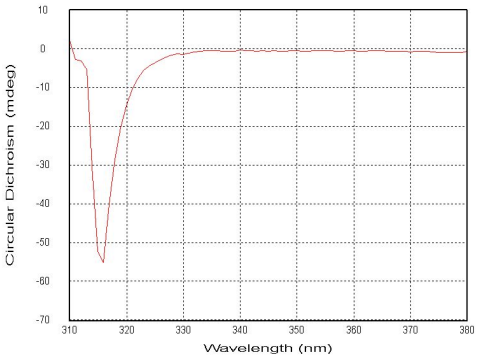

O
O
O
O
NH
O
O

3t

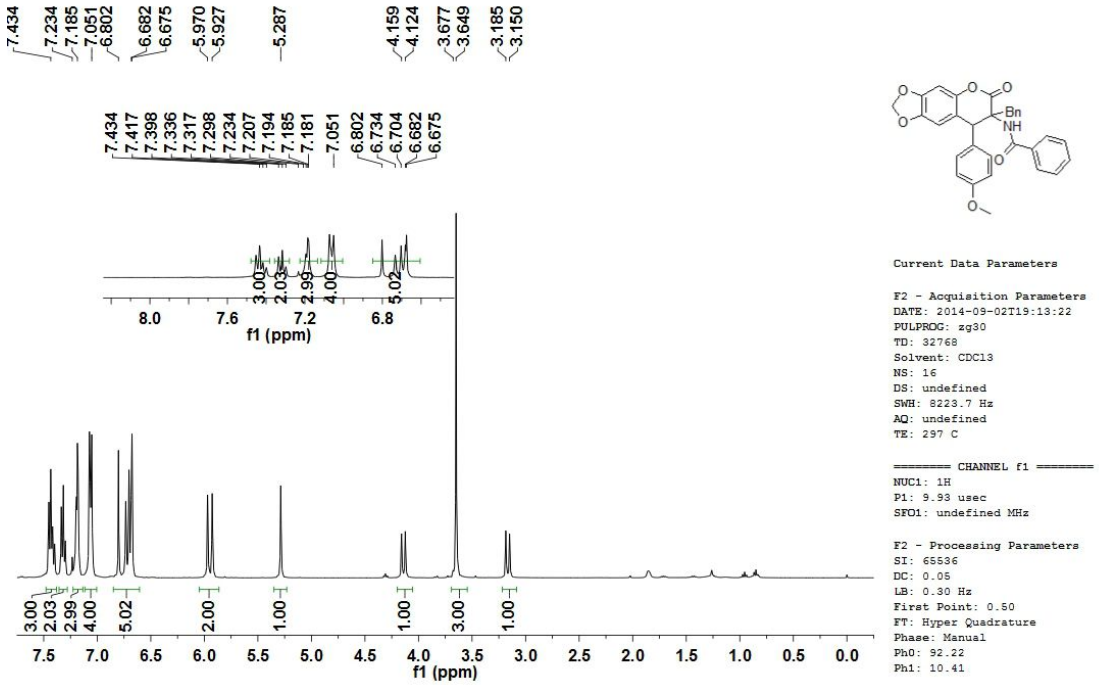

Circular Dichroism (mdeg)
10
5
0
-5
-10
-15
-20
-25
-30
310
320
330
340
350
360
370
380
Wavelength (nm)

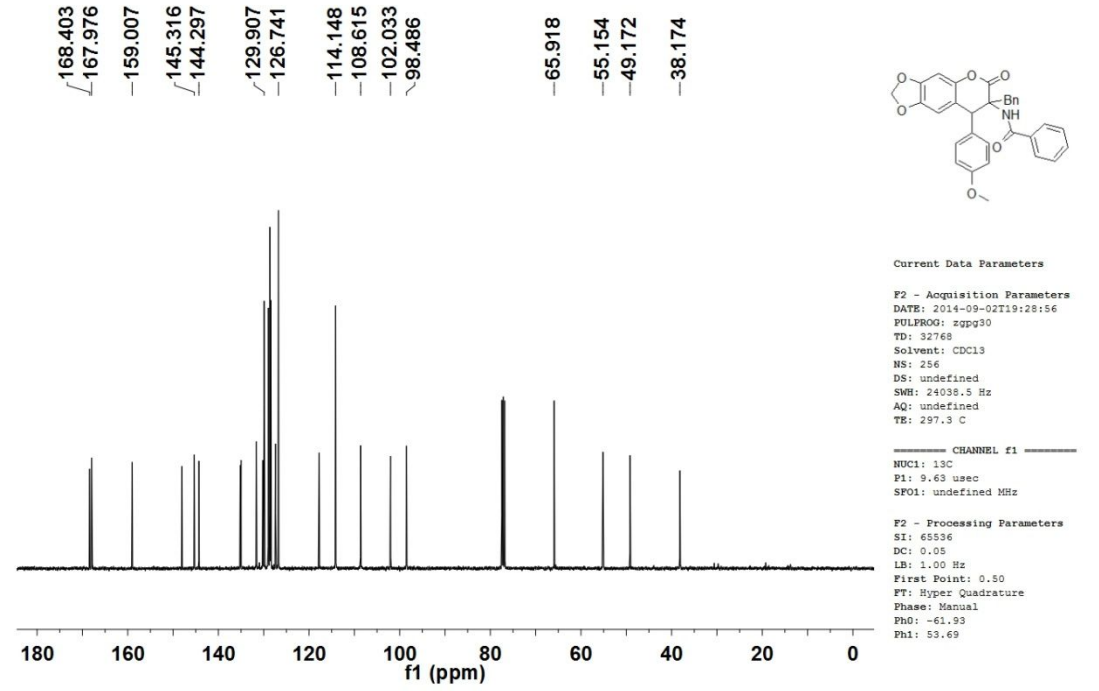

O
O
O
O
Bn
NH
O
O

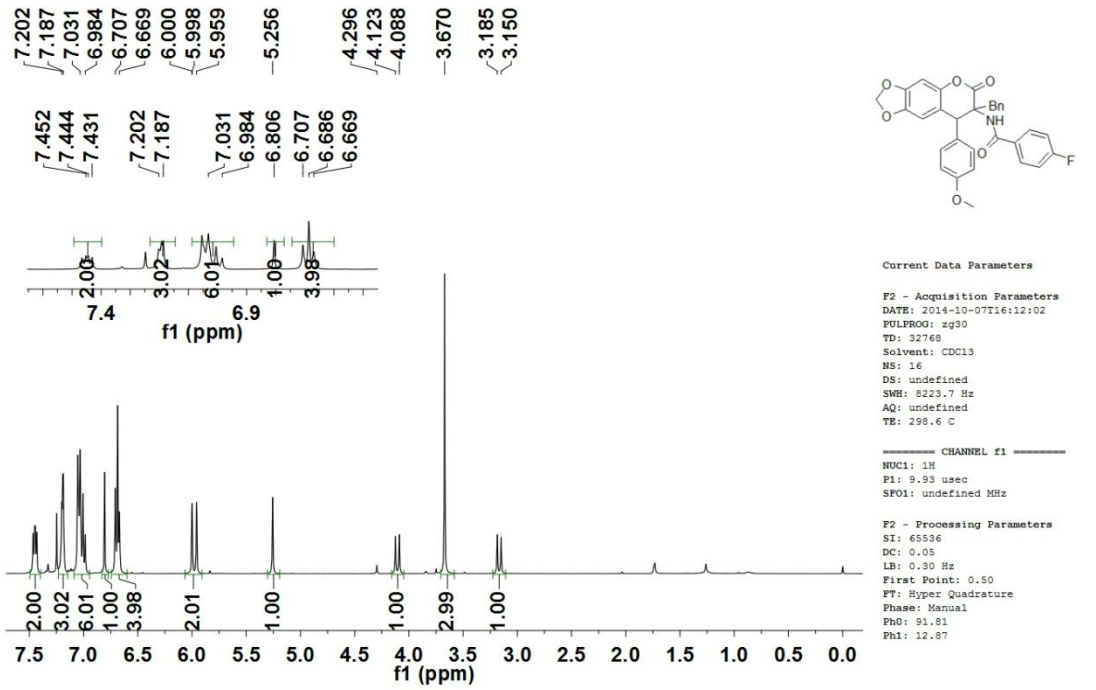
3u

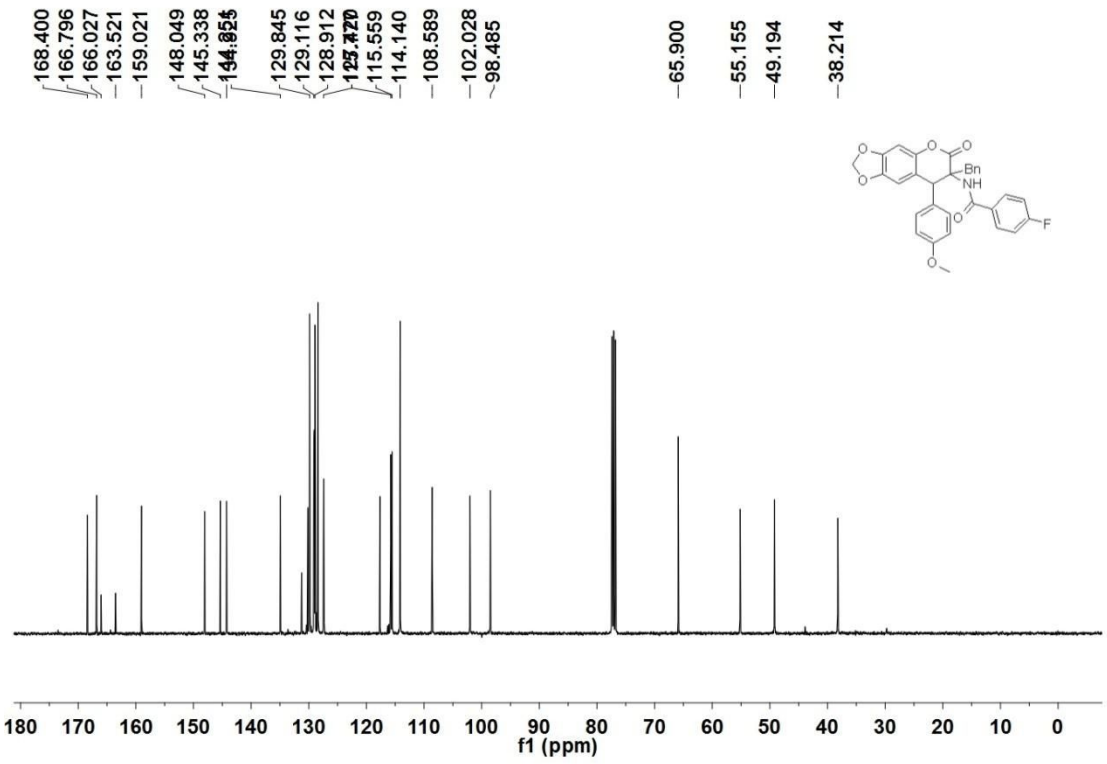

Circular Dichroism (mdeg)
10
0
-10
-20
-30
-40
-50
-60
-70
310
320
330
340
350
360
370
380
Wavelength (nm)

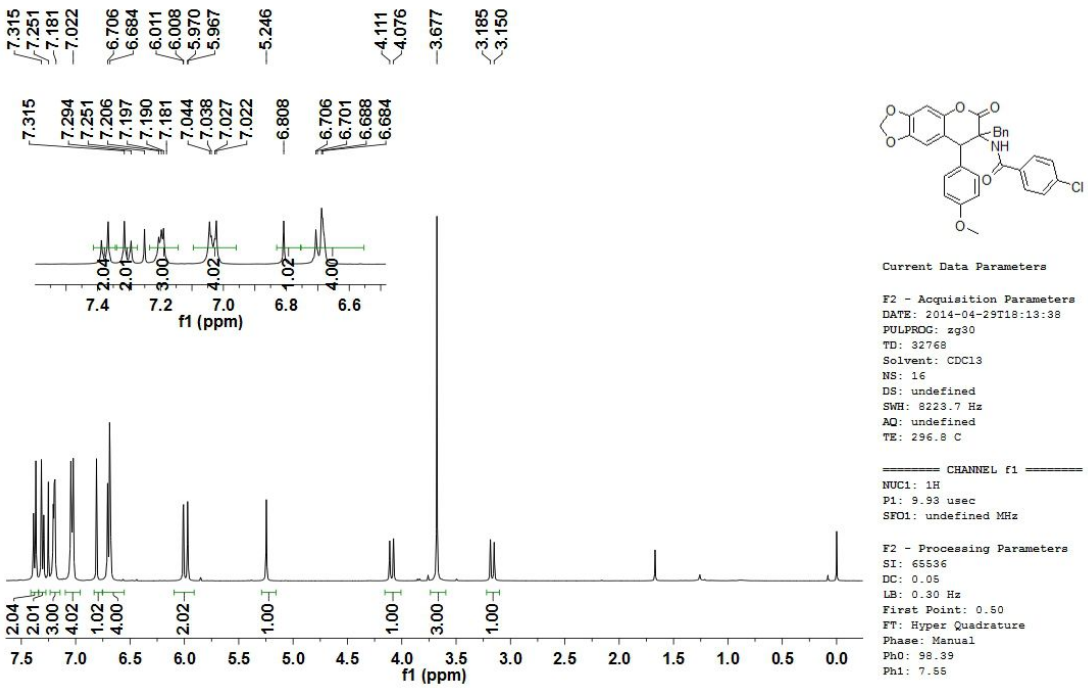
IX. Copies of NMR spectra for dihydrocoumarins.

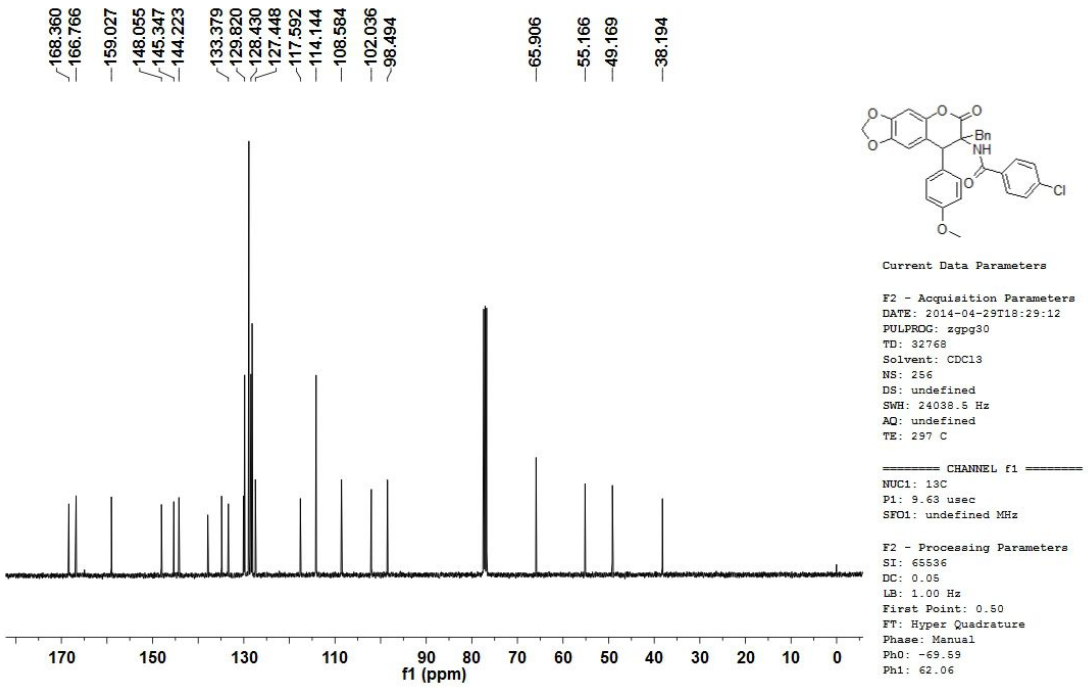


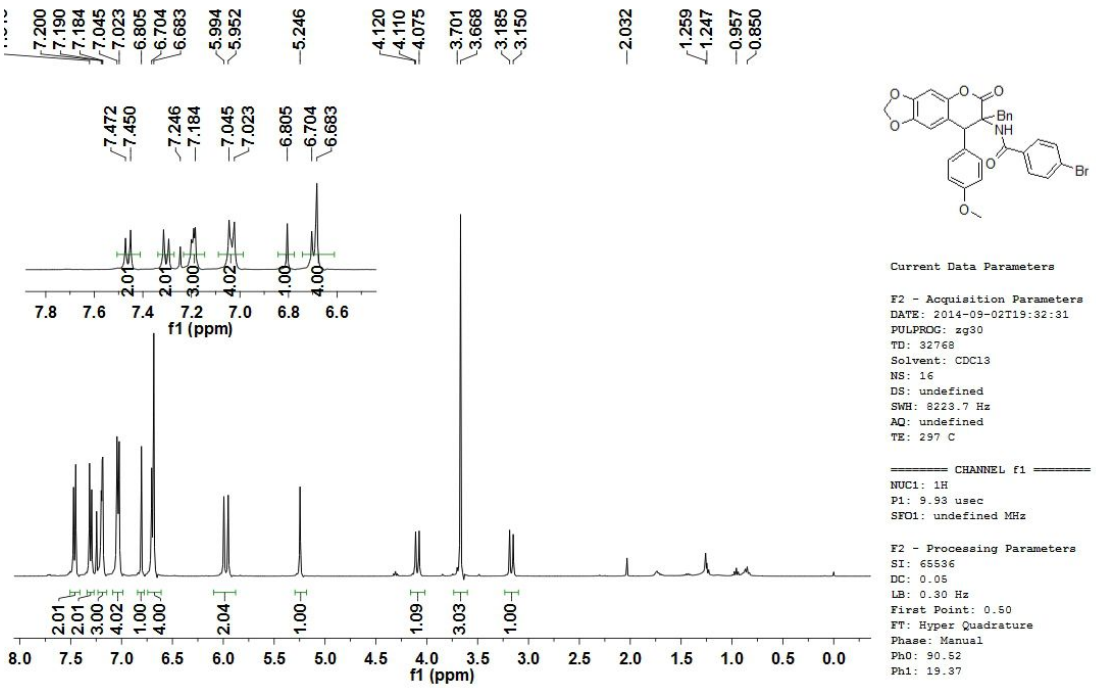


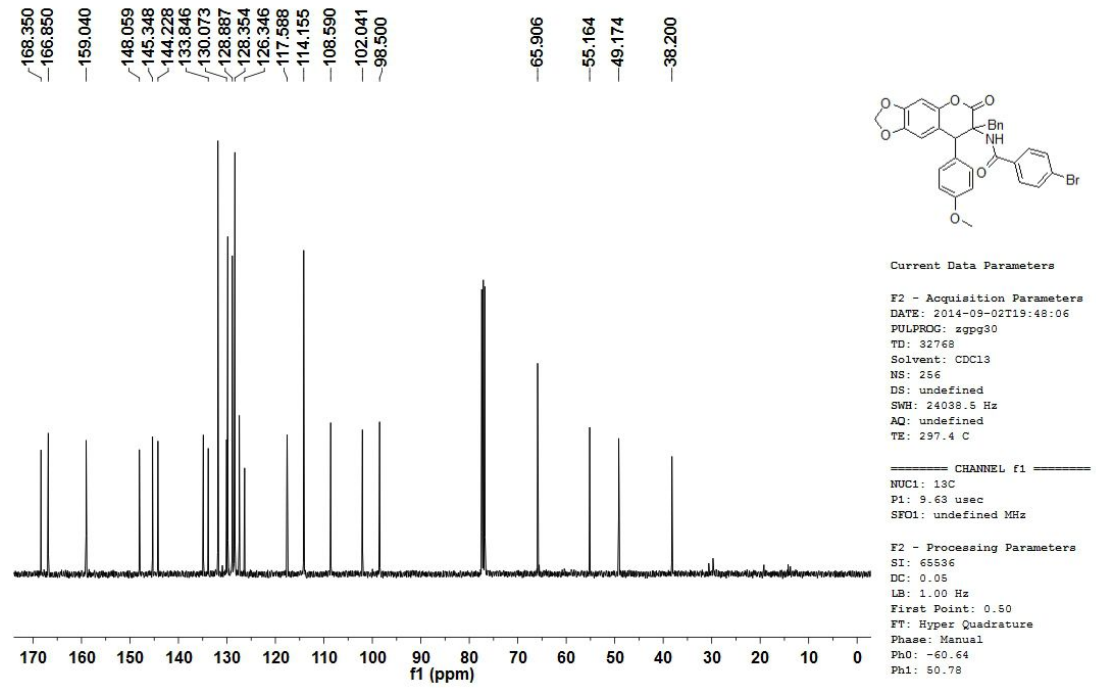

7.202
7.187
7.031
6.984
6.707
6.669
6.000
5.998
5.959
5.256
4.296
4.123
4.088
3.670
3.185
3.150
7.452
7.444
7.431
7.202
7.187
7.031
6.984
6.806
6.707
6.686
6.669
2.00
3.02
6.01
1.00
3.98
7.4
6.9
f1 (ppm)
Bn
NH
F
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-07T16:12:02
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.6 C
CHANNEL f1
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 91.81
Ph1: 12.87
2.00
3.02
6.01
1.00
3.98
2.01
1.00
1.00
2.99
1.00
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 0.5 0.0
f1 (ppm)

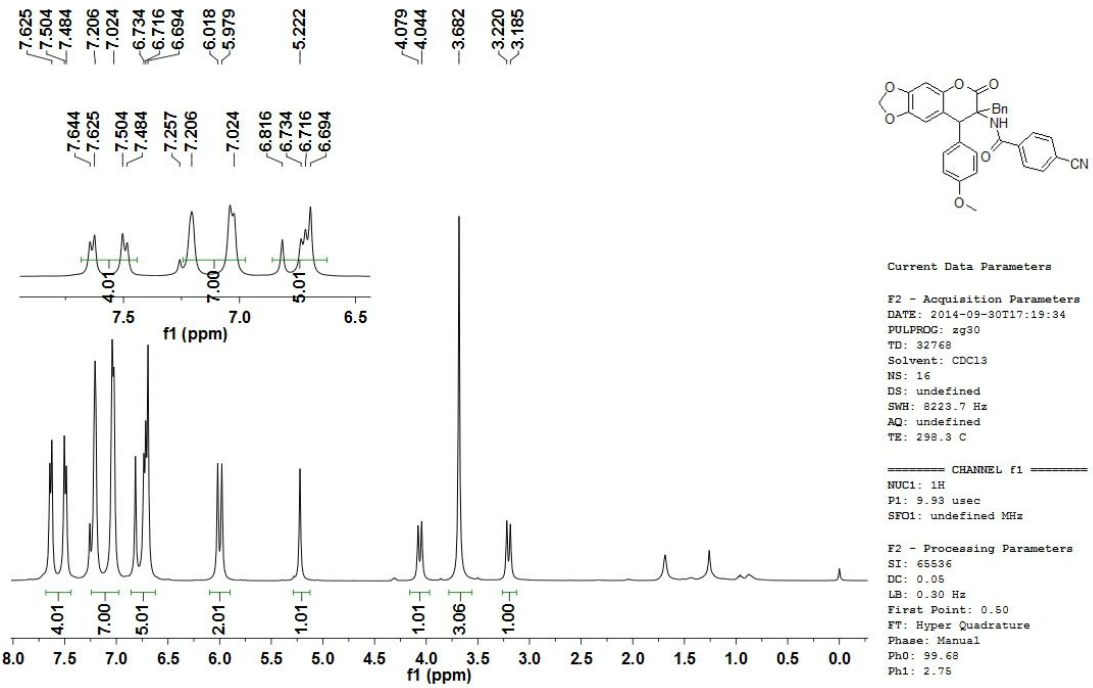

168.400
166.796
166.027
163.521
159.021
148.049
145.338
129.845
129.116
128.912
115.559
114.140
108.589
102.028
98.485
65.900
55.155
49.194
38.214
Bn
NH
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

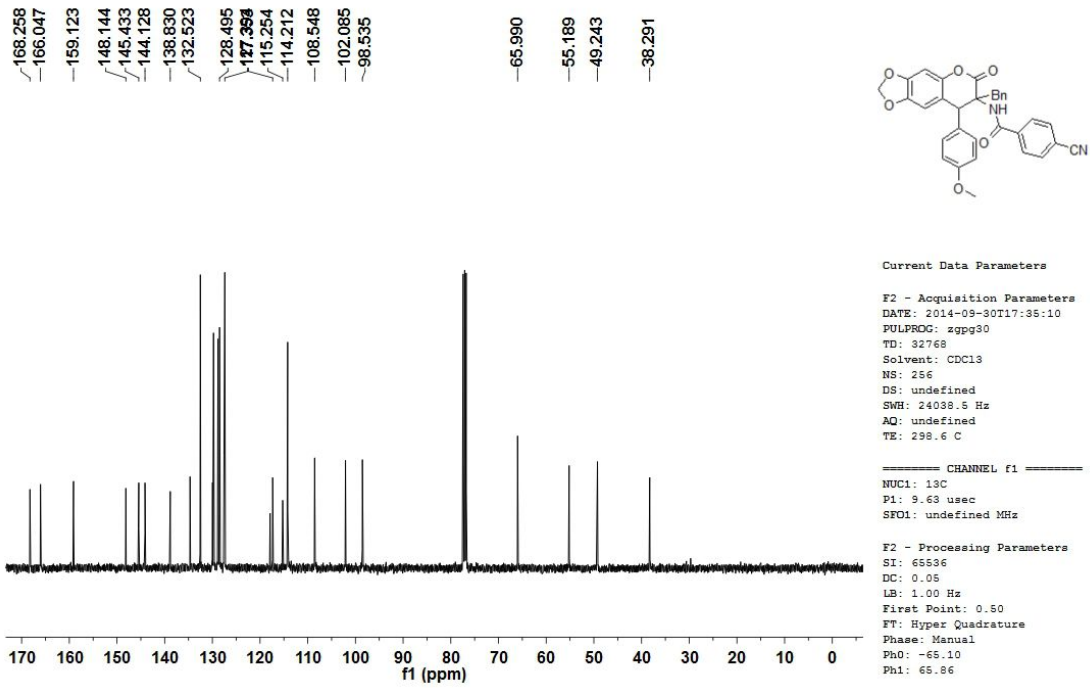

7.315
7.251
7.181
7.022
6.706
6.684
6.011
6.008
5.970
5.967
5.246
4.111
4.076
3.677
3.185
3.150
2.04
2.01
3.00
4.02
1.02
4.00
2.02
1.00
1.00
3.00
1.00
f1 (ppm)
Bn
NH
O
Cl
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-04-29T18:13:38
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 296.8 C
CHANNEL f1
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 98.39
Ph1: 7.55

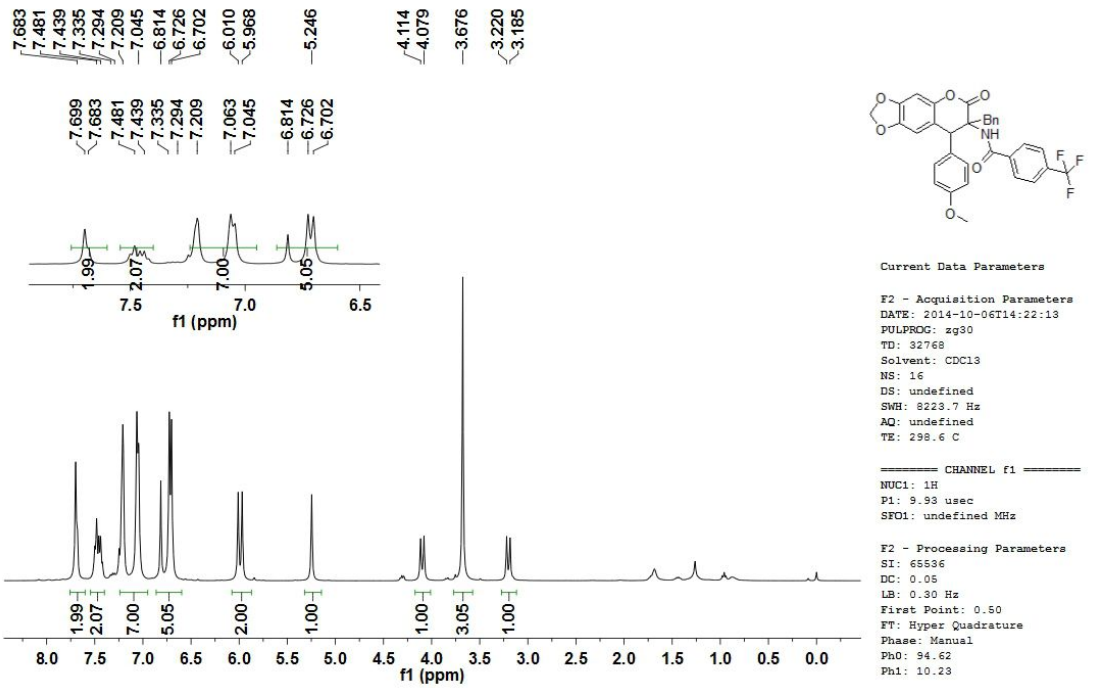

168.360
166.766
159.027
148.055
145.347
144.223
133.379
129.820
128.430
127.448
117.592
114.144
108.584
102.036
98.494
65.906
55.166
49.169
38.194
f1 (ppm)
Bn
NH
O
Cl
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-04-29T18:29:12
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297 C
CHANNEL f1
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -69.59
Ph1: 62.06

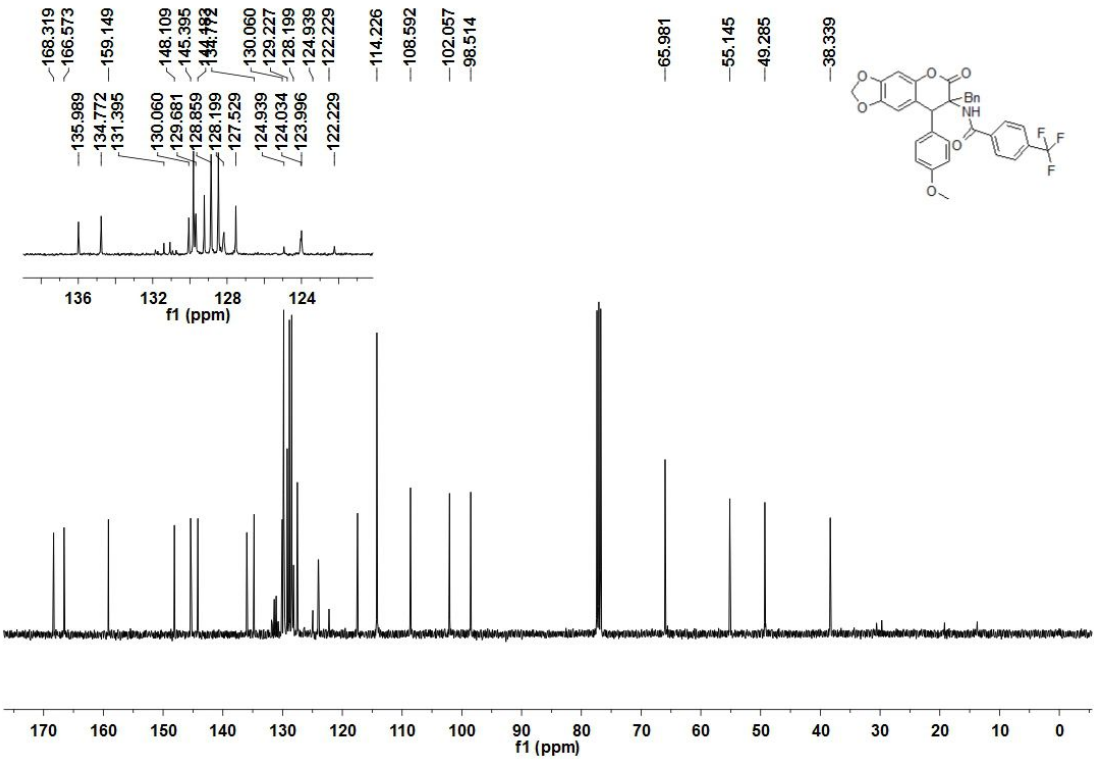

7.200
7.190
7.184
7.045
7.023
6.805
6.704
6.683
5.994
5.952
5.246
4.120
4.110
4.075
3.701
3.668
3.185
3.150
2.032
1.259
1.247
0.957
0.850
7.472
7.450
7.246
7.184
7.045
7.023
6.805
6.704
6.683
2.01
2.01
3.00
4.02
1.00
4.00
7.8 7.6 7.4 7.2 7.0 6.8 6.6
f1 (ppm)
2.01
2.01
3.00
4.02
1.00
4.00
2.04
1.00
1.09
3.03
1.00
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 0.5 0.0
f1 (ppm)
Bn
NH
Br
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-02T19:32:31
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 90.52
Ph1: 19.37

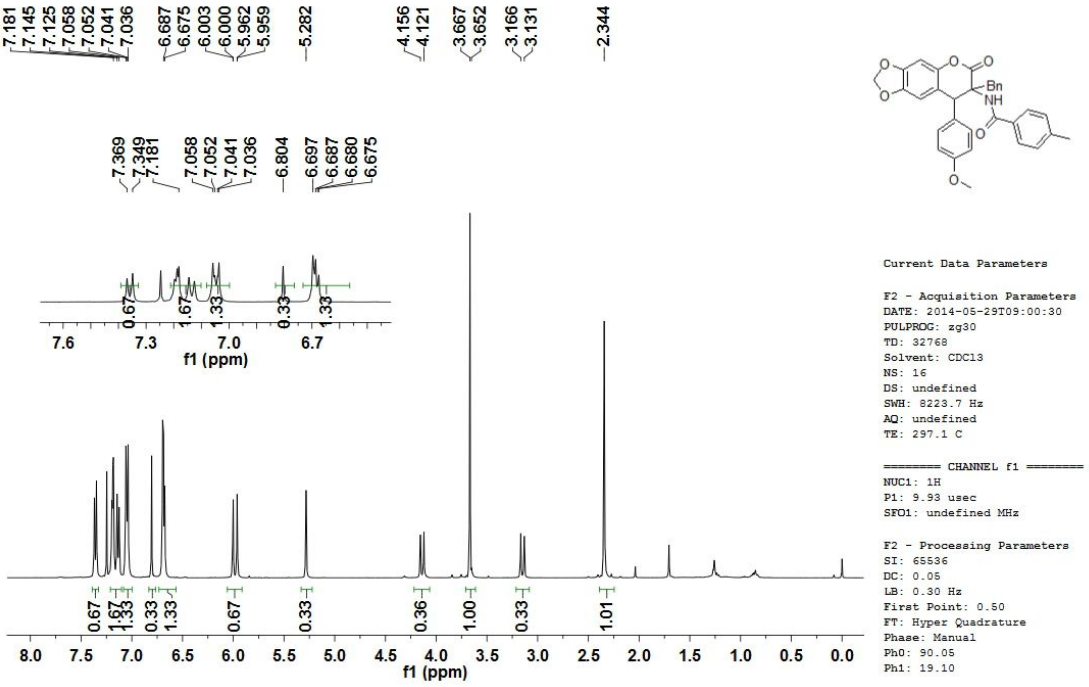

168.350
166.850
159.040
148.059
145.348
144.228
133.846
130.073
128.887
128.354
126.346
117.588
114.155
108.590
102.041
98.500
65.906
55.164
49.174
38.200
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Bn
NH
Br
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-02T19:48:06
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.4 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -60.64
Ph1: 50.78


7.625
7.504
7.484
7.206
7.024
6.734
6.716
6.694
6.018
5.979
5.222
4.079
4.044
3.682
3.220
3.185
7.644
7.625
7.504
7.484
7.257
7.206
7.024
6.816
6.734
6.716
6.694
4.01
7.00
5.01
7.5
7.0
6.5
f1 (ppm)
4.01
7.00
5.01
2.01
1.01
1.01
3.06
1.00
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 0.5 0.0
f1 (ppm)
Bn
NH
O
CN
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-30T17:19:34
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.3 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 99.68
Ph1: 2.75


168.258
166.047
159.123
148.144
145.433
144.128
138.830
132.523
128.495
115.254
114.212
108.548
102.085
98.535
65.990
55.189
49.243
38.291
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Bn
NH
O
CN
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-30T17:35:10
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 298.6 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -65.10
Ph1: 65.86


7.683
7.481
7.439
7.335
7.294
7.209
7.045
6.814
6.726
6.702
6.010
5.968
5.246
4.114
4.079
3.676
3.220
3.185
1.99
2.07
7.00
5.05
2.00
1.00
1.00
3.05
1.00
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-06T14:22:13
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.6 C
CHANNEL f1
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 94.62
Ph1: 10.23
Bn
NH
O
F
F
F


168.319
166.573
159.149
148.109
145.395
130.060
129.227
128.199
124.939
122.229
114.226
108.592
102.057
98.514
65.981
55.145
49.285
38.339
135.989
134.772
131.395
130.060
129.681
128.859
128.199
127.529
124.939
124.034
123.996
122.229
f1 (ppm)
Bn
NH
O
F
F
F

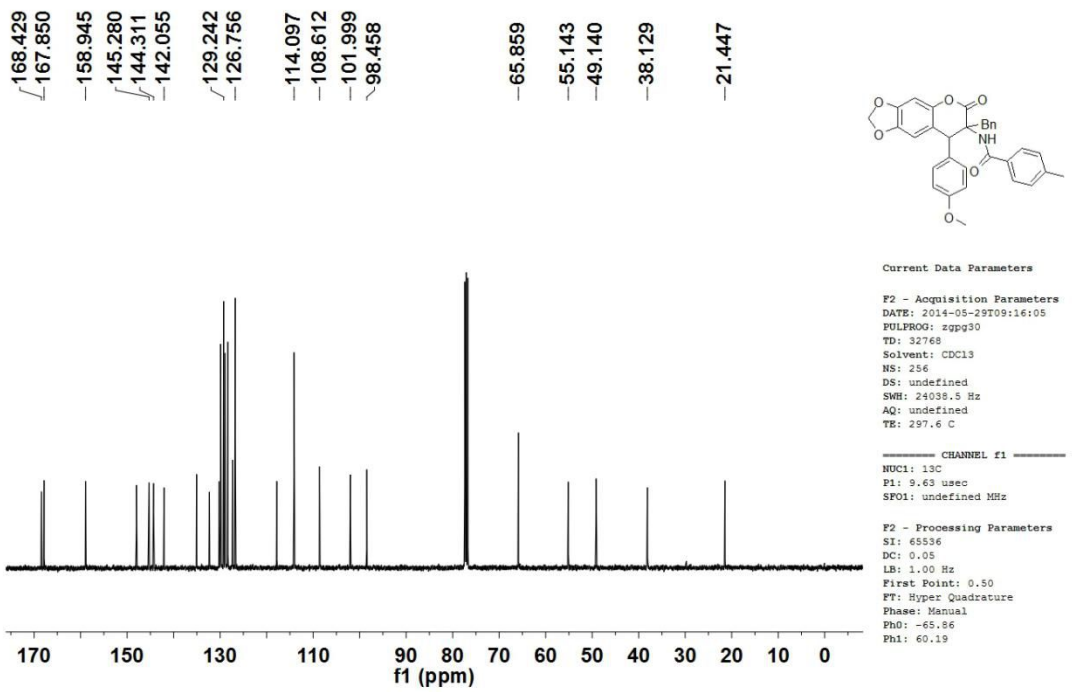


Current Data Parameters

F2 - Acquisition Parameters
DATE: 2014-05-29T09:00:30
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.1 C

======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz

F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 90.05
Ph1: 19.10

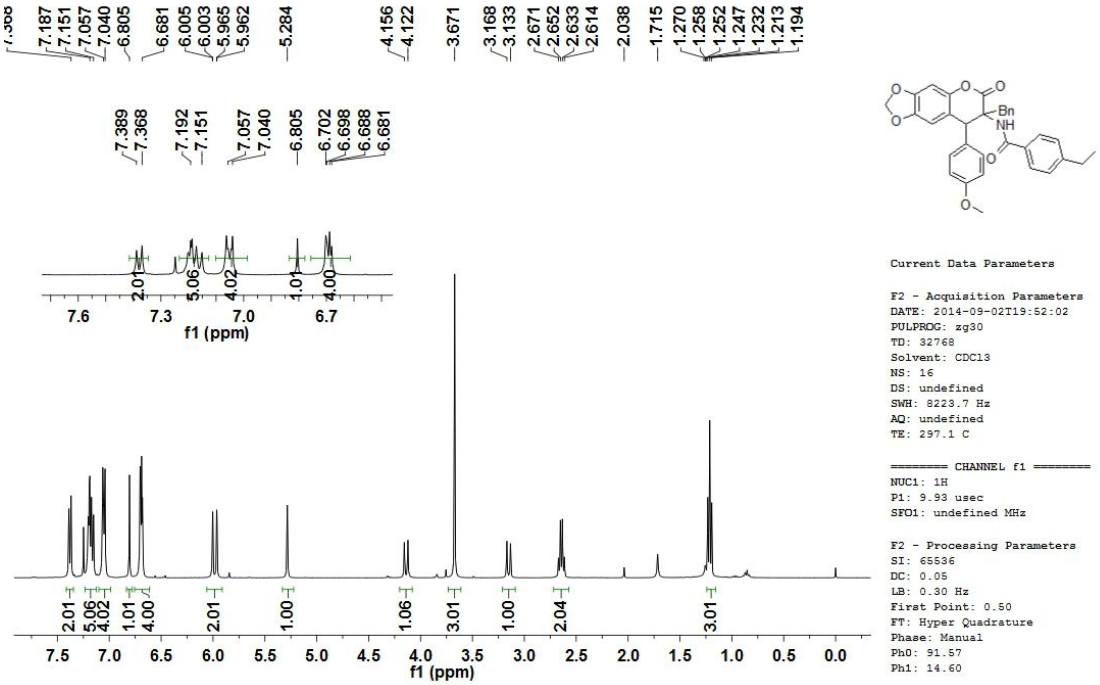


Current Data Parameters

F2 - Acquisition Parameters
DATE: 2014-05-29T09:16:05
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.6 C

======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz

F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -65.86
Ph1: 60.19

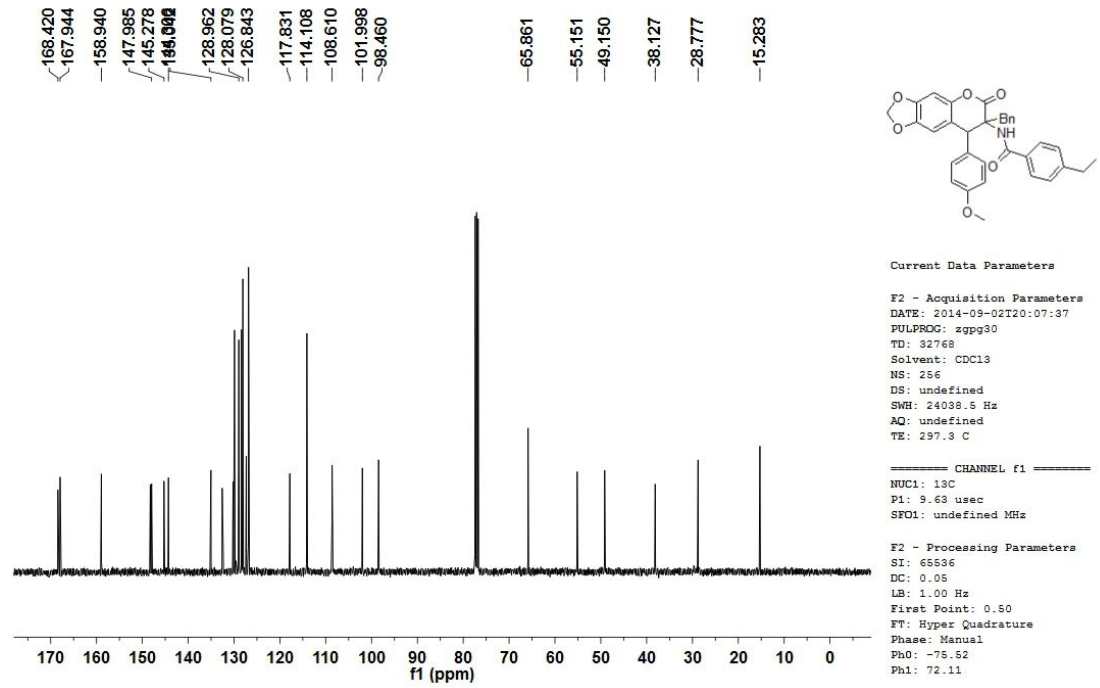


Current Data Parameters

F2 - Acquisition Parameters
DATE: 2014-09-02T19:52:02
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.1 C

======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz

F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 91.57
Ph1: 14.60

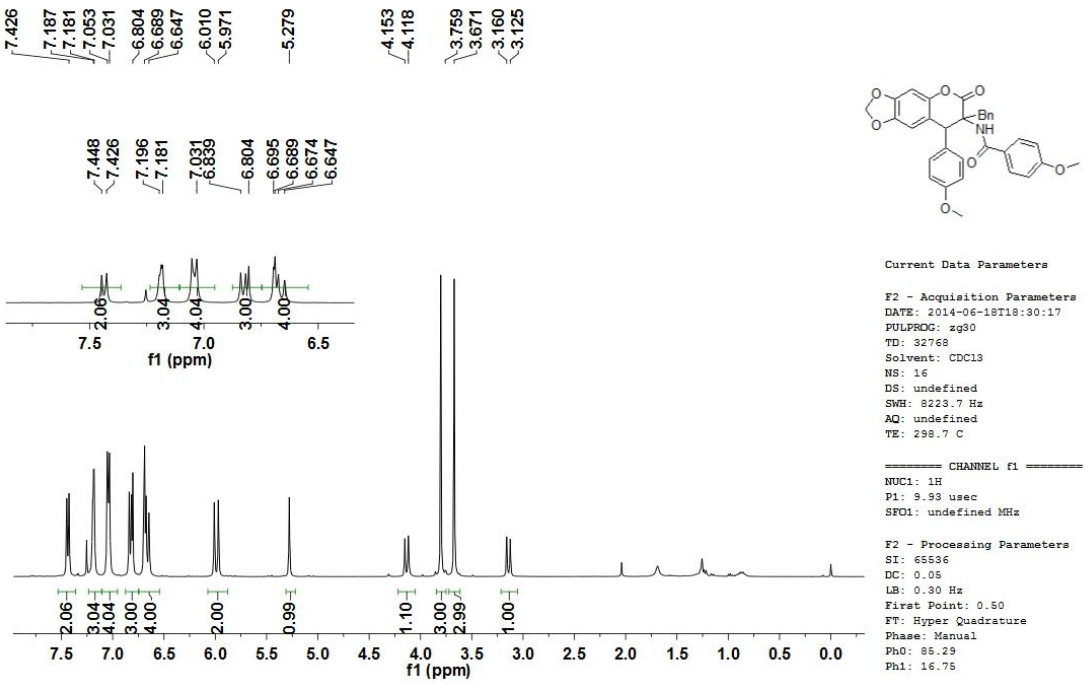


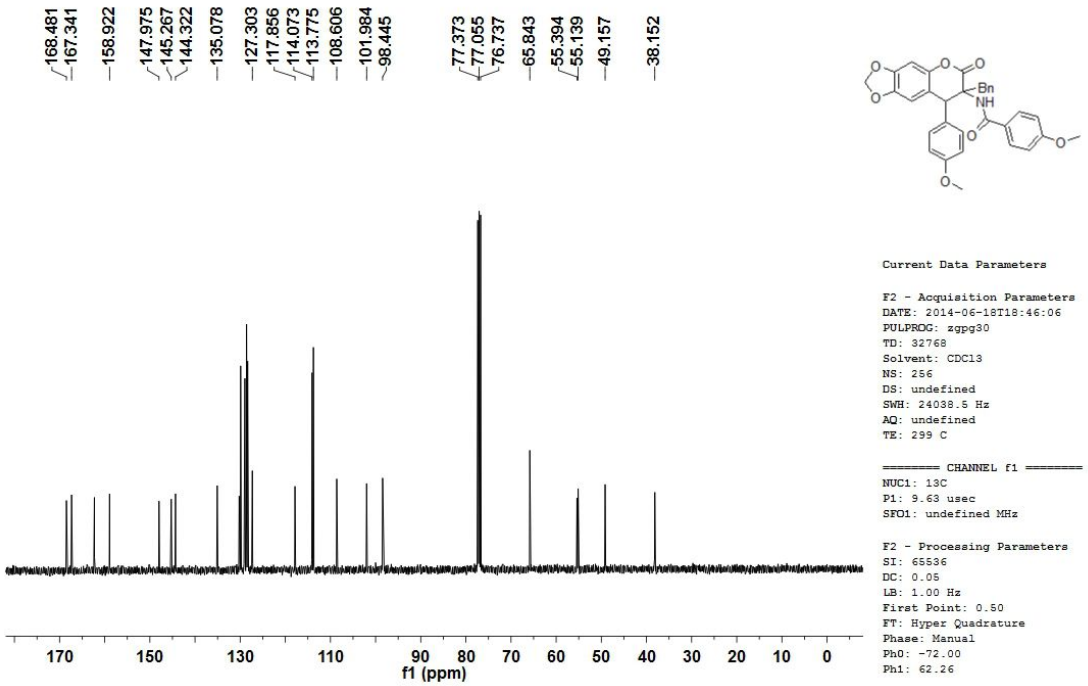
Current Data Parameters

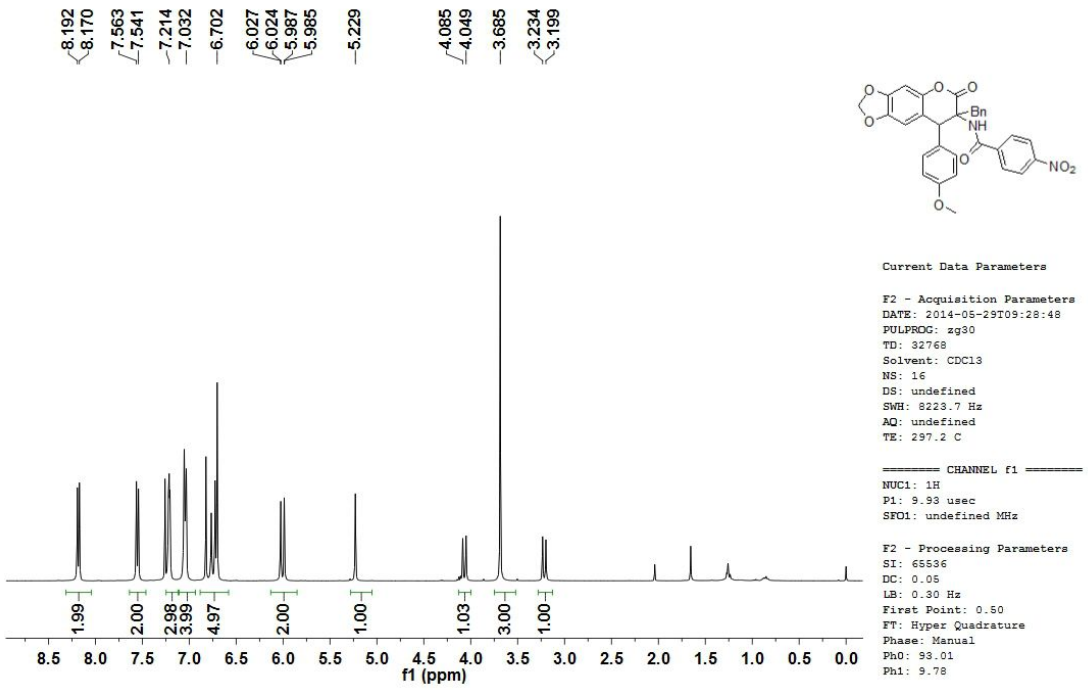
F2 - Acquisition Parameters
DATE: 2014-09-02T20:07:37
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.3 C

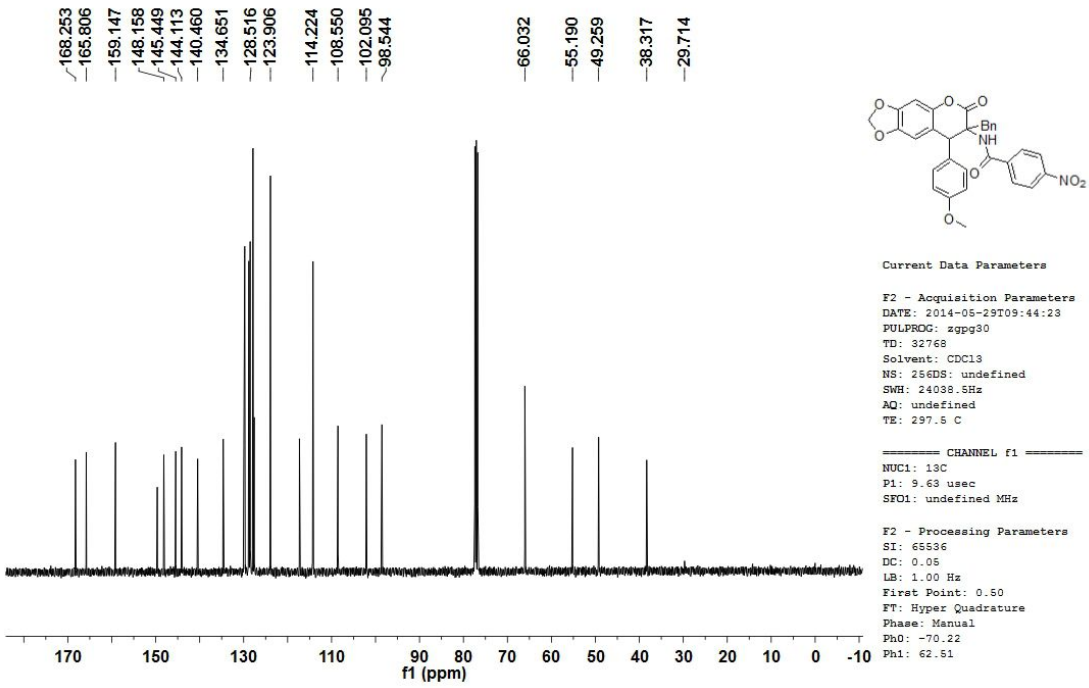
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz

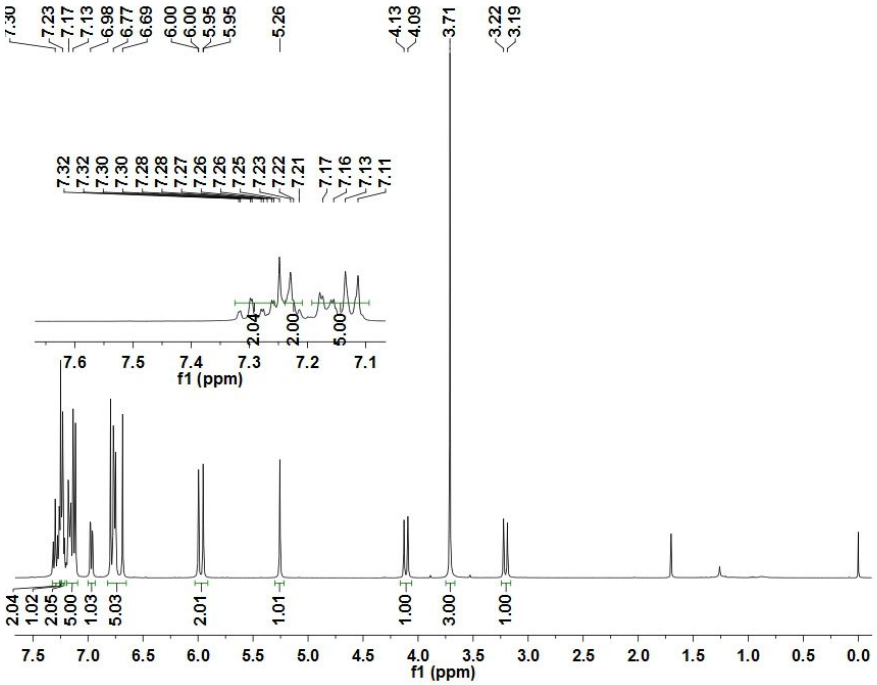
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -75.52
Ph1: 72.11

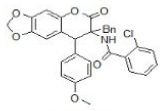

7.426
7.187
7.181
7.053
7.031
6.804
6.689
6.647
6.010
5.971
5.279
4.153
4.118
3.759
3.671
3.160
3.125
Bn
NH
O
O
O
O
O
O
7.448
7.426
7.196
7.181
7.031
6.839
6.804
6.695
6.689
6.674
6.647
2.06
3.04
4.04
3.00
4.00
7.5
7.0
6.5
f1 (ppm)
2.06
3.04
4.04
3.00
4.00
2.00
0.99
1.10
3.00
2.99
1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-06-18T18:30:17
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.7 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 85.29
Ph1: 16.75


168.481
167.341
158.922
147.975
145.267
144.322
135.078
127.303
117.856
114.073
113.775
108.606
101.984
98.445
77.373
77.055
76.737
65.843
55.394
55.139
49.157
38.152
Bn
NH
O
O
O
O
O
O
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-06-18T18:46:06
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 299 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -72.00
Ph1: 62.26


8.192
8.170
7.563
7.541
7.214
7.032
6.702
6.027
6.024
5.987
5.985
5.229
4.085
4.049
3.685
3.234
3.199
Bn
NH
NO2
1.99
2.00
2.98
3.99
4.97
2.00
1.00
1.03
3.00
1.00
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-05-29T09:28:48
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.2 C
CHANNEL f1
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 93.01
Ph1: 9.78


168.253
165.806
159.147
148.158
145.449
144.113
140.460
134.651
128.516
123.906
114.224
108.550
102.095
98.544
66.032
55.190
49.259
38.317
29.714
Bn
NH
NO2
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-05-29T09:44:23
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256DS: undefined
SWH: 24038.5Hz
AQ: undefined
TE: 297.5 C
CHANNEL f1
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -70.22
Ph1: 62.51



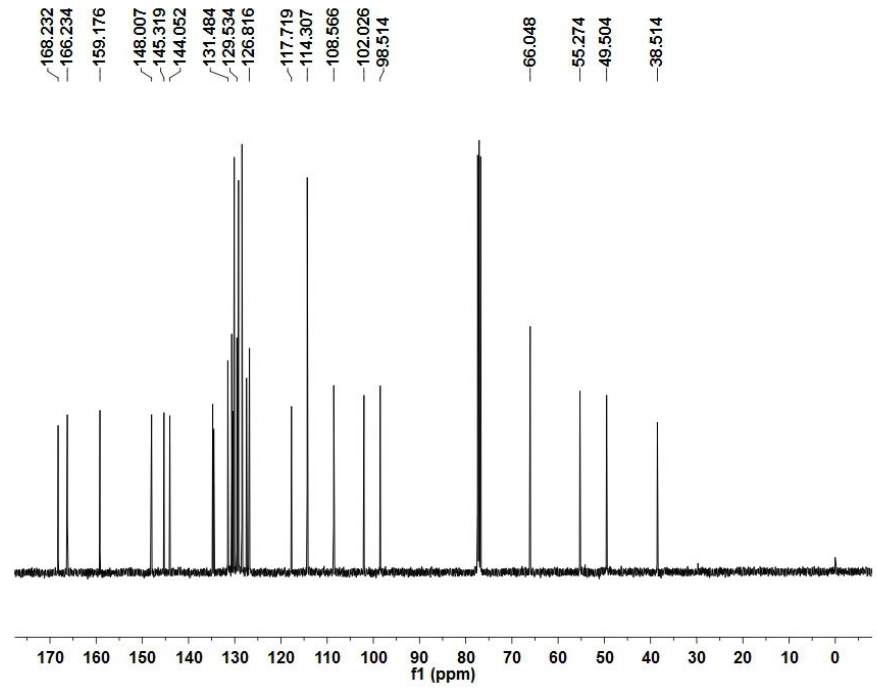


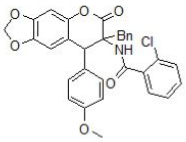
Current Data Parameters

F2 - Acquisition Parameters
DATE: 2014-04-29T17:34:39
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 296.6 C

======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz

F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 100.03
Ph1: 5.94



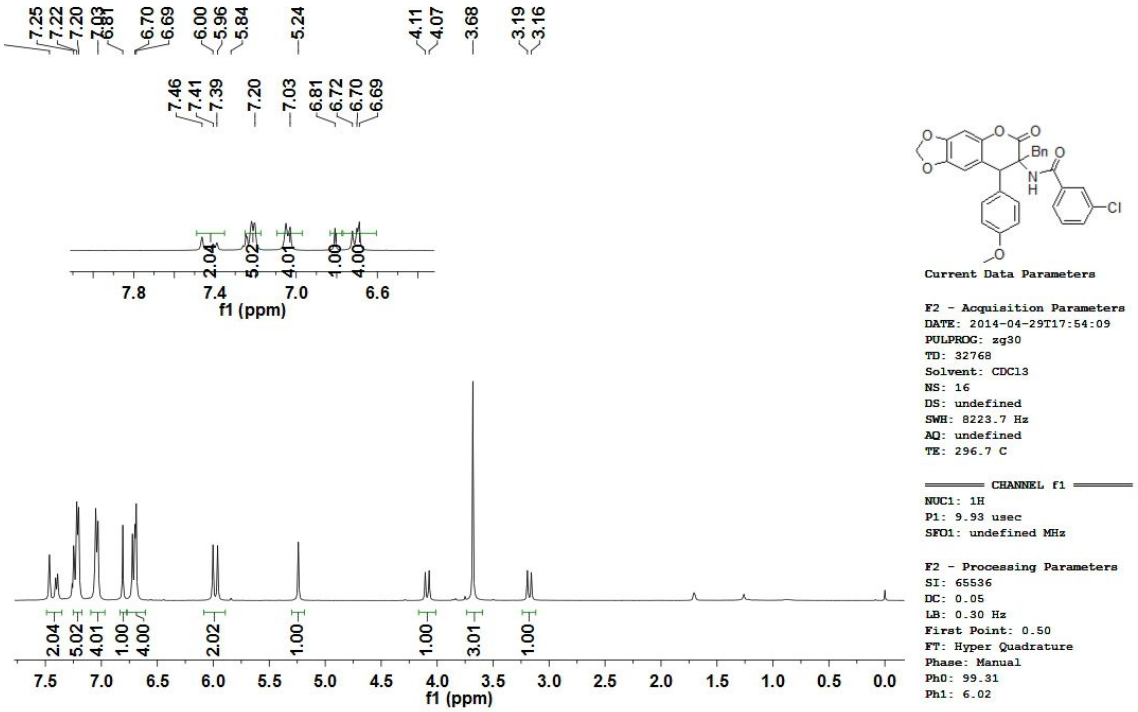


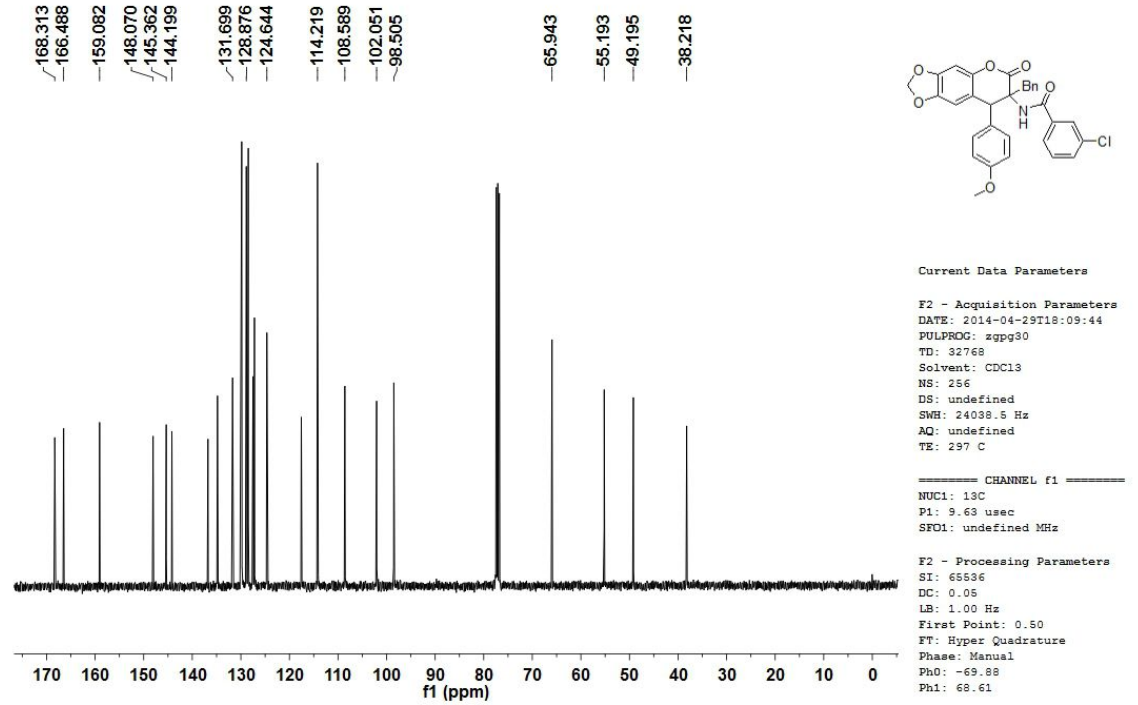
Current Data Parameters

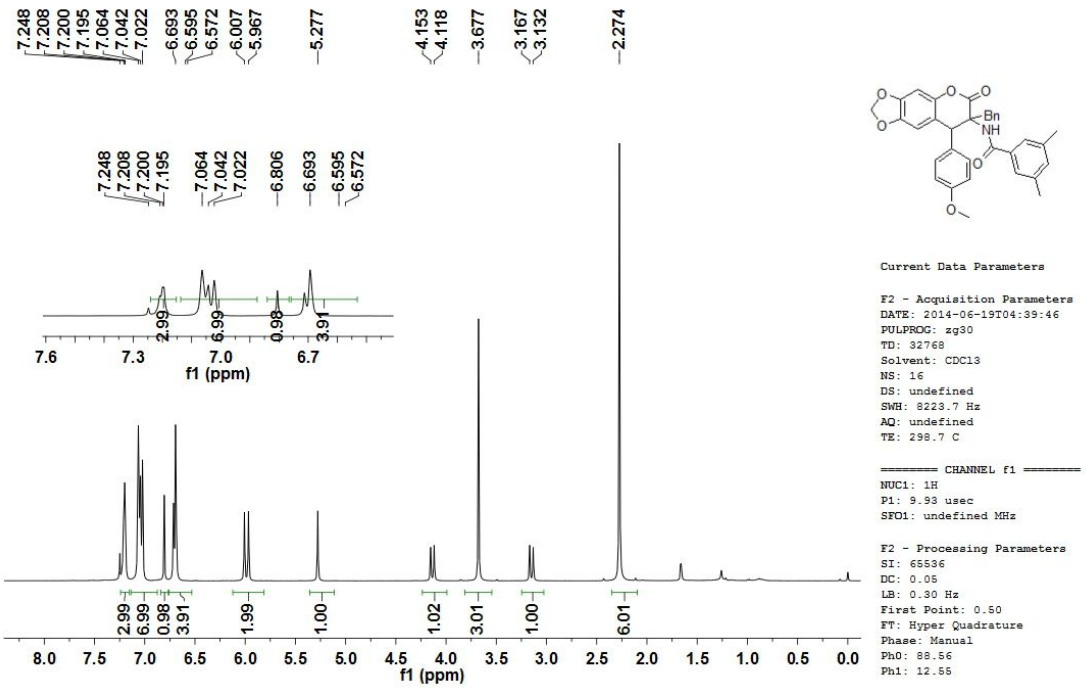
F2 - Acquisition Parameters
DATE: 2014-04-29T17:50:14
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.1 C

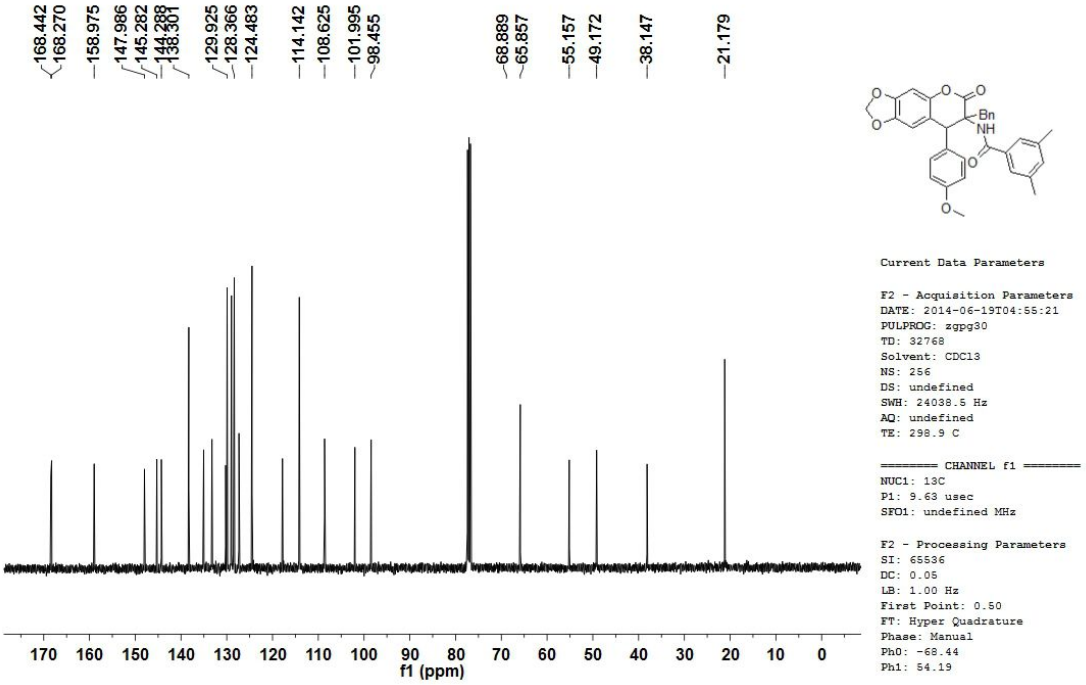
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz

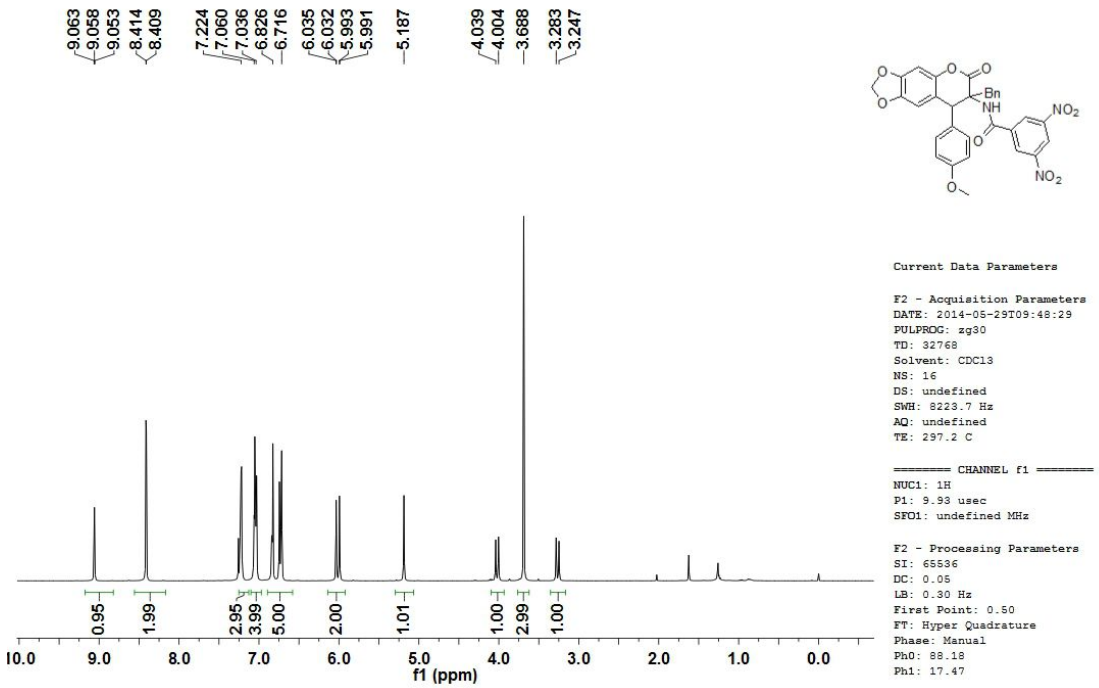
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -64.14
Ph1: 59.68

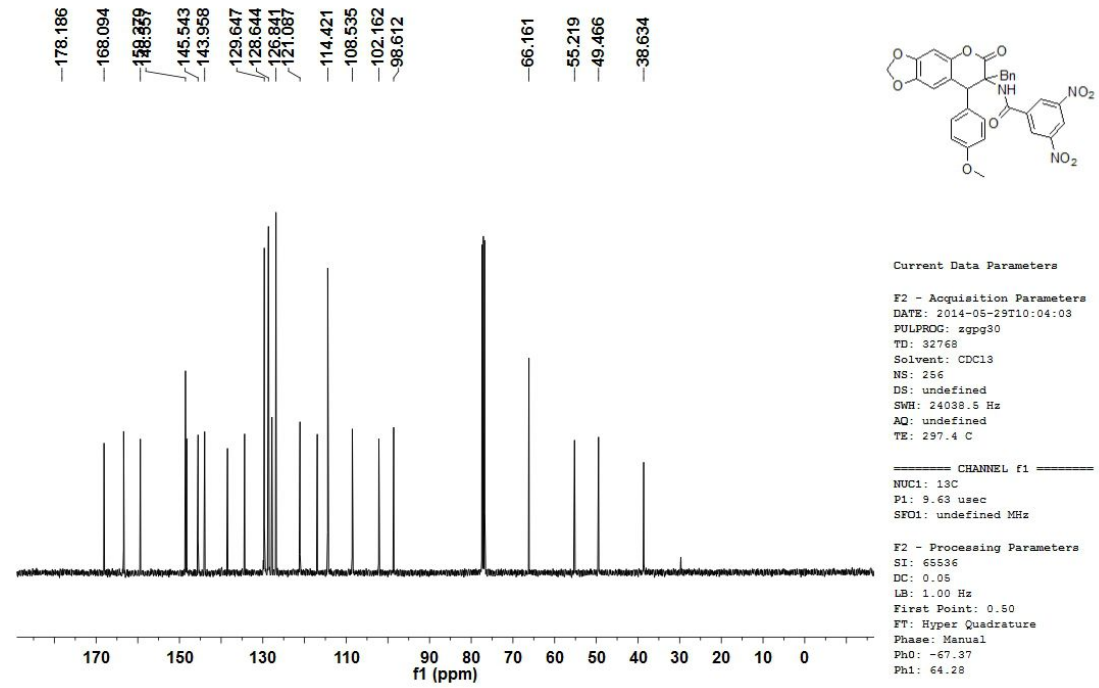

7.25
7.22
7.20
7.03
6.81
6.70
6.69
6.00
5.96
5.84
5.24
4.11
4.07
3.68
3.19
3.16
7.46
7.41
7.39
7.20
7.03
6.81
6.72
6.70
6.69
2.04
5.02
4.01
1.00
4.00
7.8
7.4
7.0
6.6
f1 (ppm)
Bn
N
H
Cl
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-04-29T17:54:09
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 296.7 C
CHANNEL f1
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 99.31
Ph1: 6.02


168.313
166.488
159.082
148.070
145.362
144.199
131.699
128.876
124.644
114.219
108.589
102.051
98.505
65.943
55.193
49.195
38.218
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Bn
N
H
Cl
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-04-29T18:09:44
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297 C
CHANNEL f1
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -69.88
Ph1: 68.61

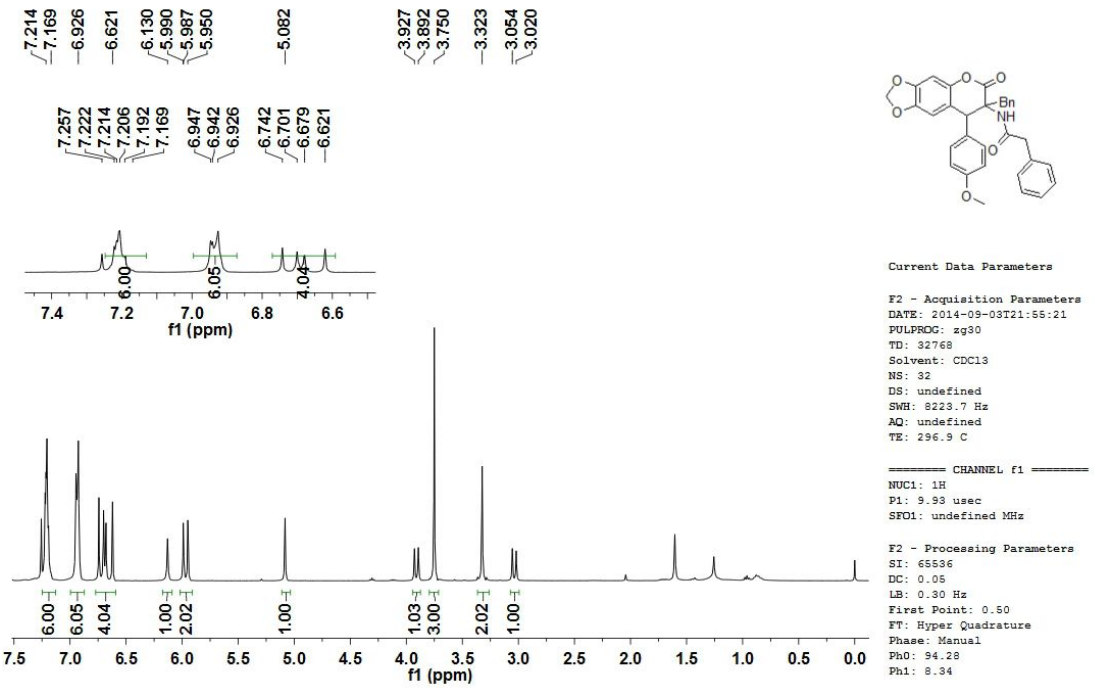

7.248
7.208
7.200
7.195
7.064
7.042
7.022
6.693
6.595
6.572
6.007
5.967
5.277
4.153
4.118
3.677
3.167
3.132
2.274
7.248
7.208
7.200
7.195
7.064
7.042
7.022
6.806
6.693
6.595
6.572
2.99
6.99
0.98
3.91
7.6
7.3
7.0
6.7
f1 (ppm)
2.99
6.99
0.98
3.91
1.99
1.00
1.02
3.01
1.00
6.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
Bn
NH
O
O
O
O
O
O
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-06-19T04:39:46
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.7 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 88.56
Ph1: 12.55

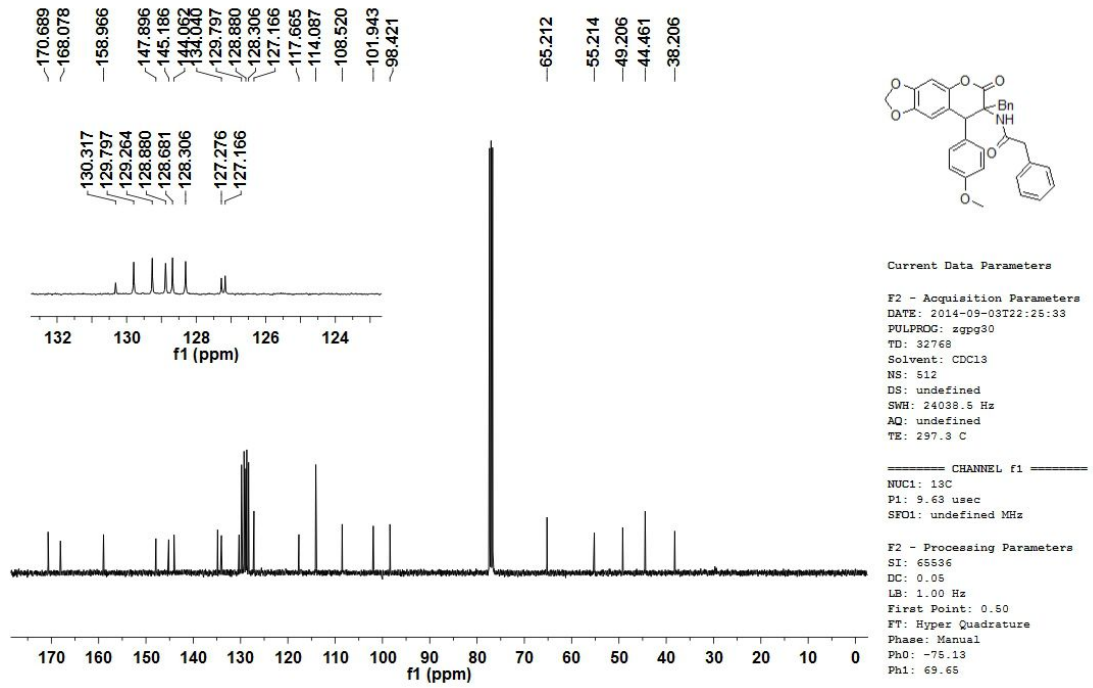

168.442
168.270
158.975
147.986
145.282
144.288
138.301
129.925
128.366
124.483
114.142
108.625
101.995
98.455
68.889
65.857
55.157
49.172
38.147
21.179
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Bn
NH
O
O
O
O
O
O
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-06-19T04:55:21
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 298.9 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -68.44
Ph1: 54.19

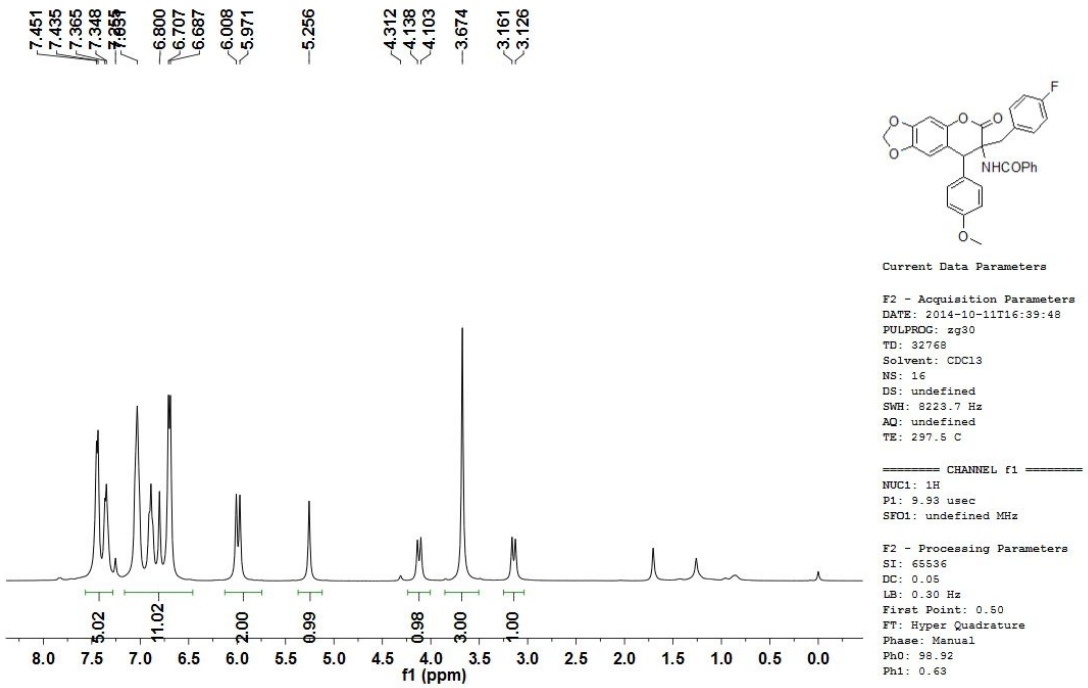

9.063
9.058
9.053
8.414
8.409
7.224
7.060
7.036
6.826
6.716
6.035
6.032
5.993
5.991
5.187
4.039
4.004
3.688
3.283
3.247
Bn
NH
O
NO2
NO2
0.95
1.99
2.95
3.99
5.00
2.00
1.01
1.00
2.99
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-05-29T09:48:29
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.2 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 88.18
Ph1: 17.47

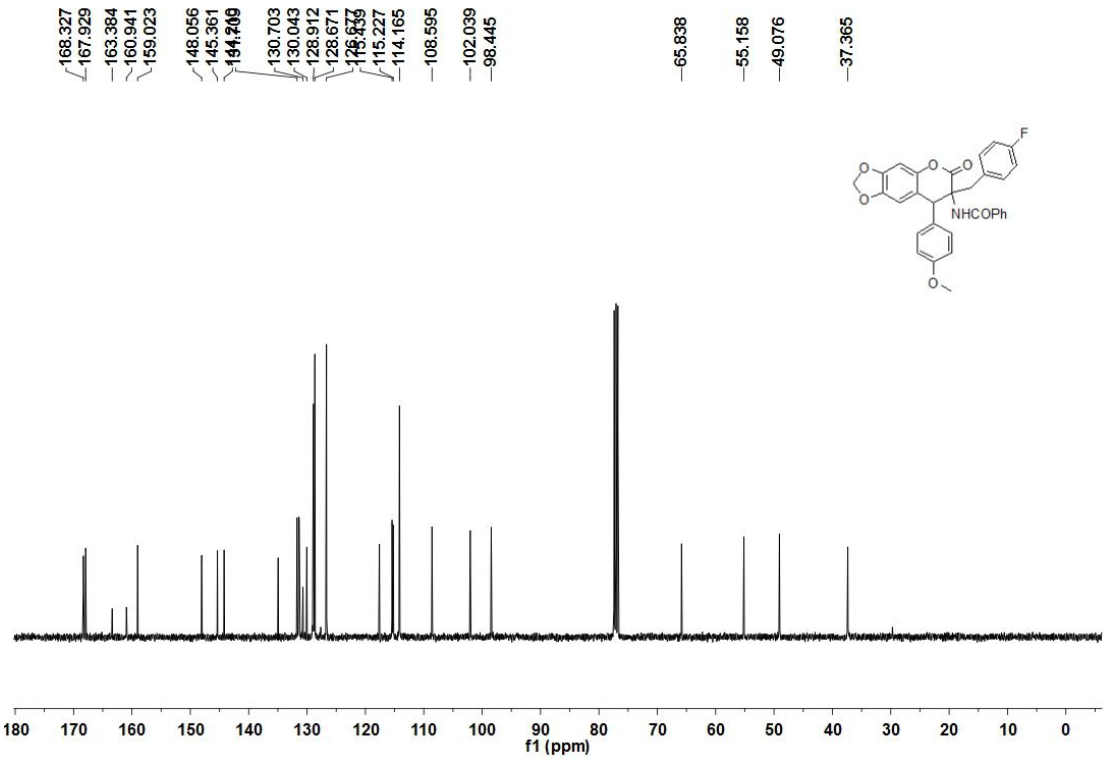

178.186
168.094
145.543
143.958
129.647
128.644
126.841
121.087
114.421
108.535
102.162
98.612
66.161
55.219
49.466
38.634
Bn
NH
O
NO2
NO2
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-05-29T10:04:03
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 256
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.4 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -67.37
Ph1: 64.28

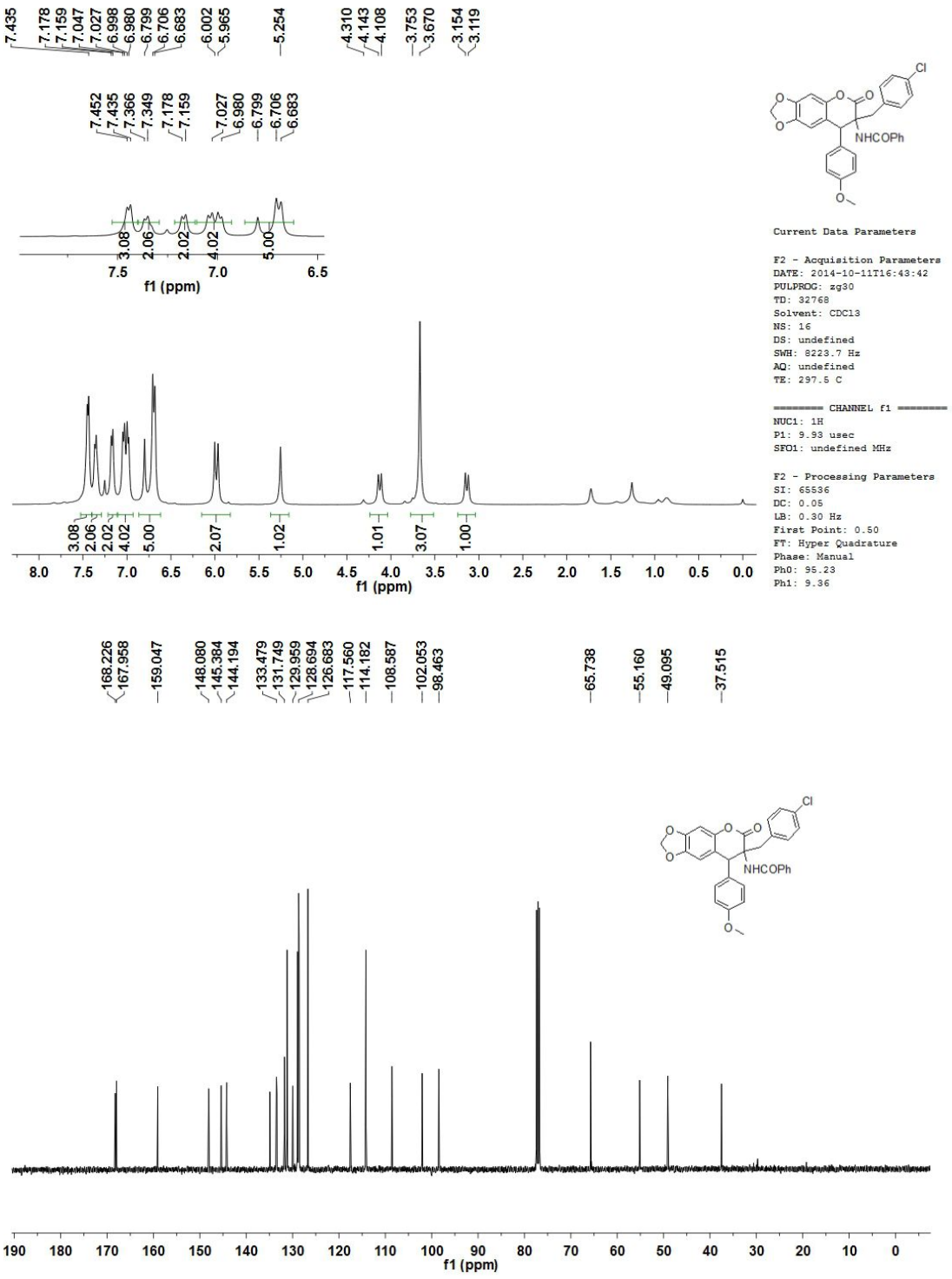
(s, 2H).

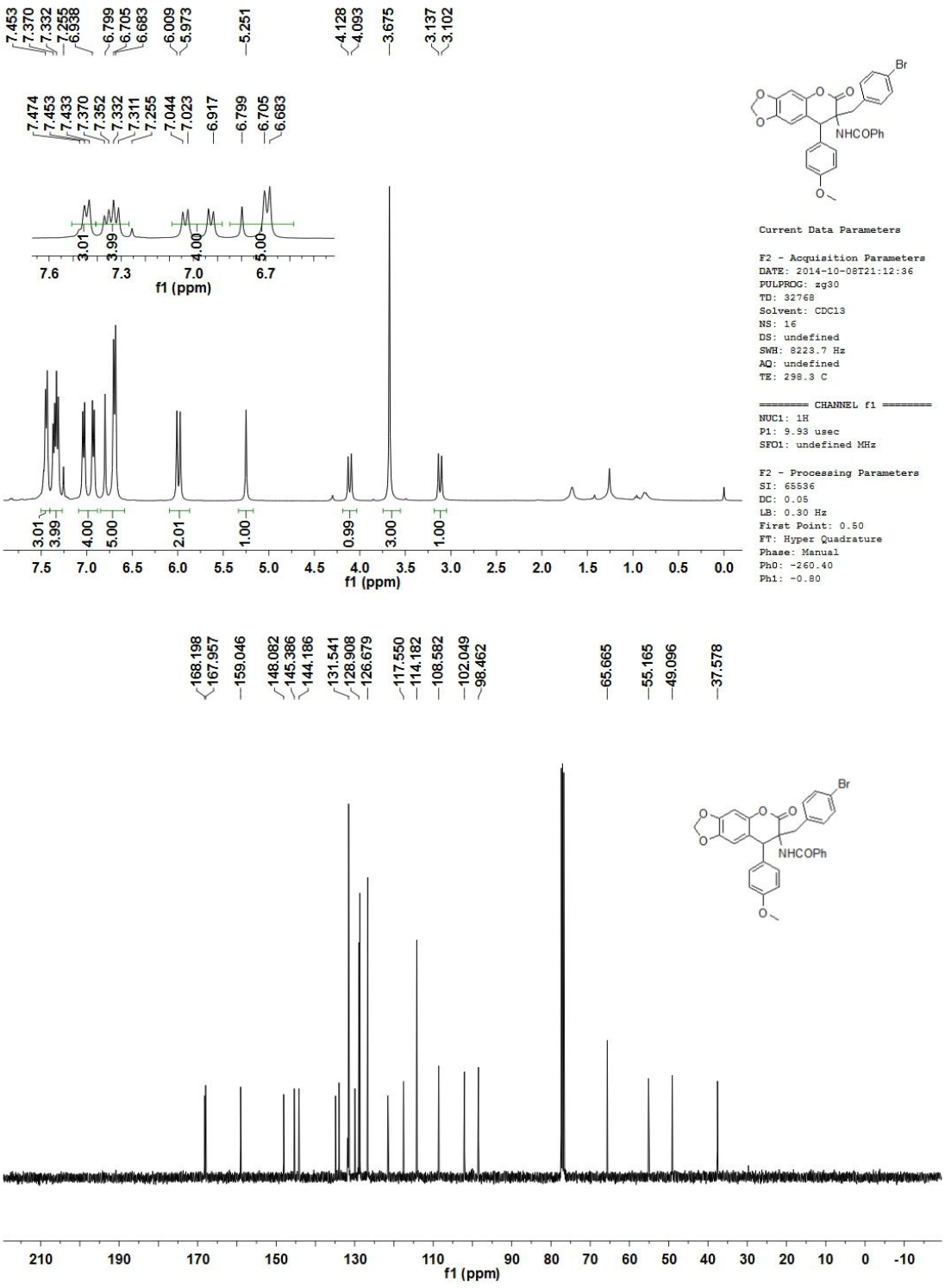

7.214
7.169
6.926
6.621
6.130
5.990
5.987
5.950
5.082
3.927
3.892
3.750
3.323
3.054
3.020
7.257
7.222
7.214
7.206
7.192
7.169
6.947
6.942
6.926
6.742
6.701
6.679
6.621
6.00
6.05
4.04
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
6.00
6.05
4.04
1.00
2.02
1.00
1.03
3.00
2.02
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
Bn
NH
O
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-03T21:55:21
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 32
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 296.9 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 94.28
Ph1: 8.34

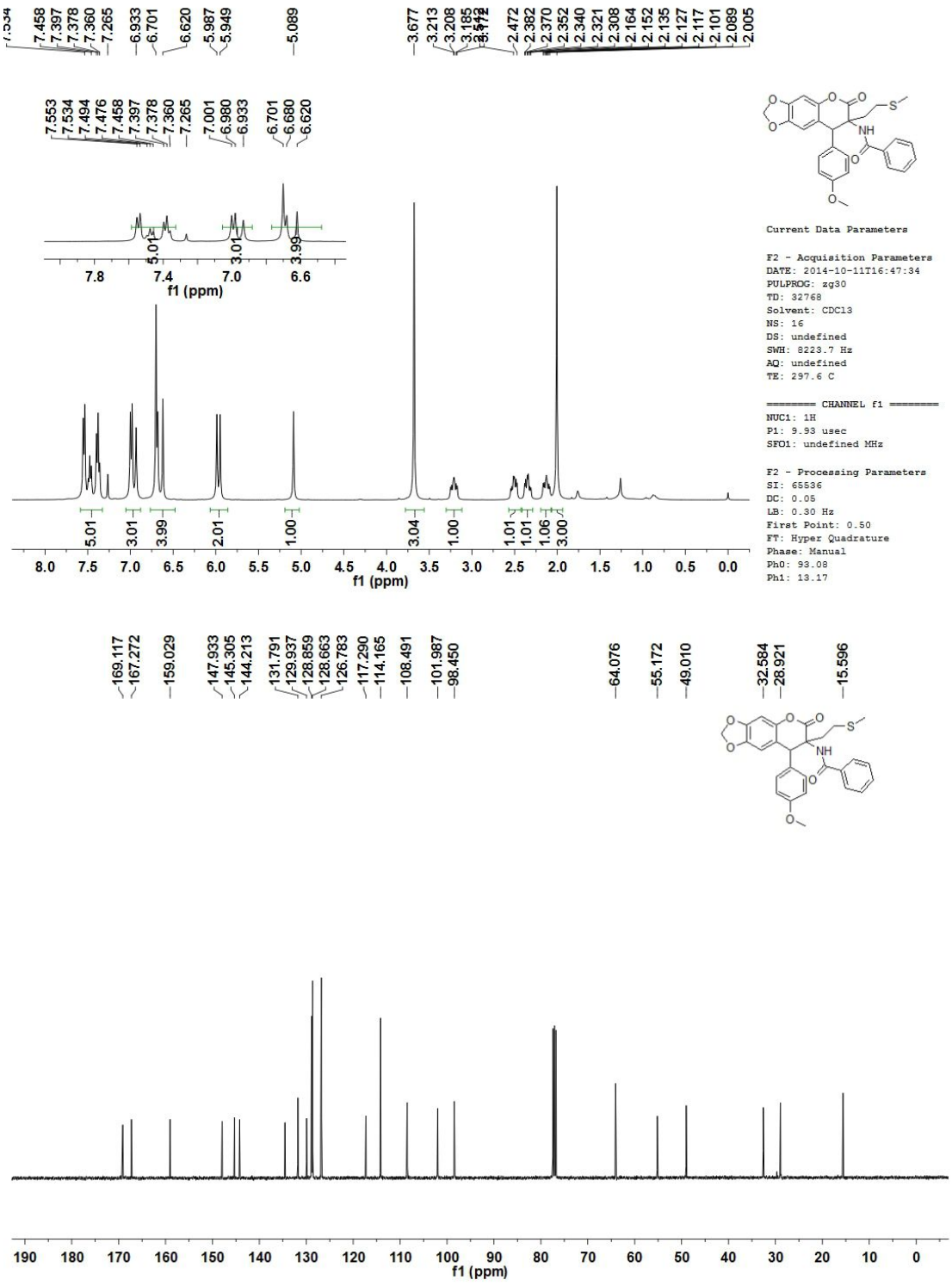

170.689
168.078
158.966
147.896
145.186
144.062
134.040
129.797
128.880
128.306
127.166
117.665
114.087
108.520
101.943
98.421
65.212
55.214
49.206
44.461
38.206
130.317
129.797
129.264
128.880
128.681
128.306
127.276
127.166
132
130
128
126
124
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
Bn
NH
O
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-03T22:25:33
PULPROG: zgpg30
TD: 32768
Solvent: CDCl3
NS: 512
DS: undefined
SWH: 24038.5 Hz
AQ: undefined
TE: 297.3 C
======== CHANNEL f1 ========
NUC1: 13C
P1: 9.63 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 1.00 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -75.13
Ph1: 69.65

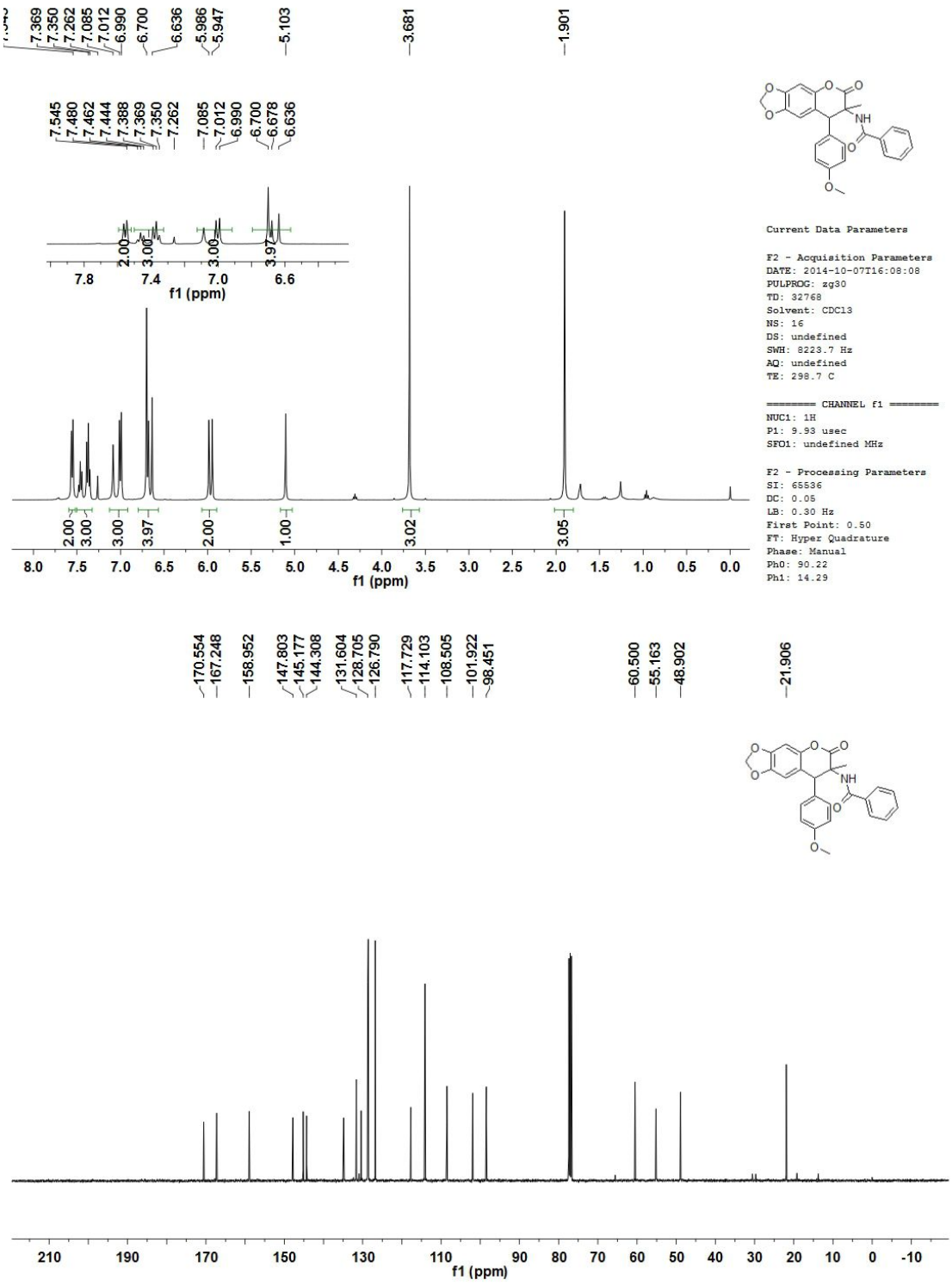

7.451
7.435
7.365
7.348
6.800
6.707
6.687
6.008
5.971
5.256
4.312
4.138
4.103
3.674
3.161
3.126
F
O
O
O
O
NHCOPh
O
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-11T16:39:48
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.5 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 98.92
Ph1: 0.63
5.02
11.02
2.00
0.99
0.98
3.00
1.00
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 0.5 0.0
f1 (ppm)

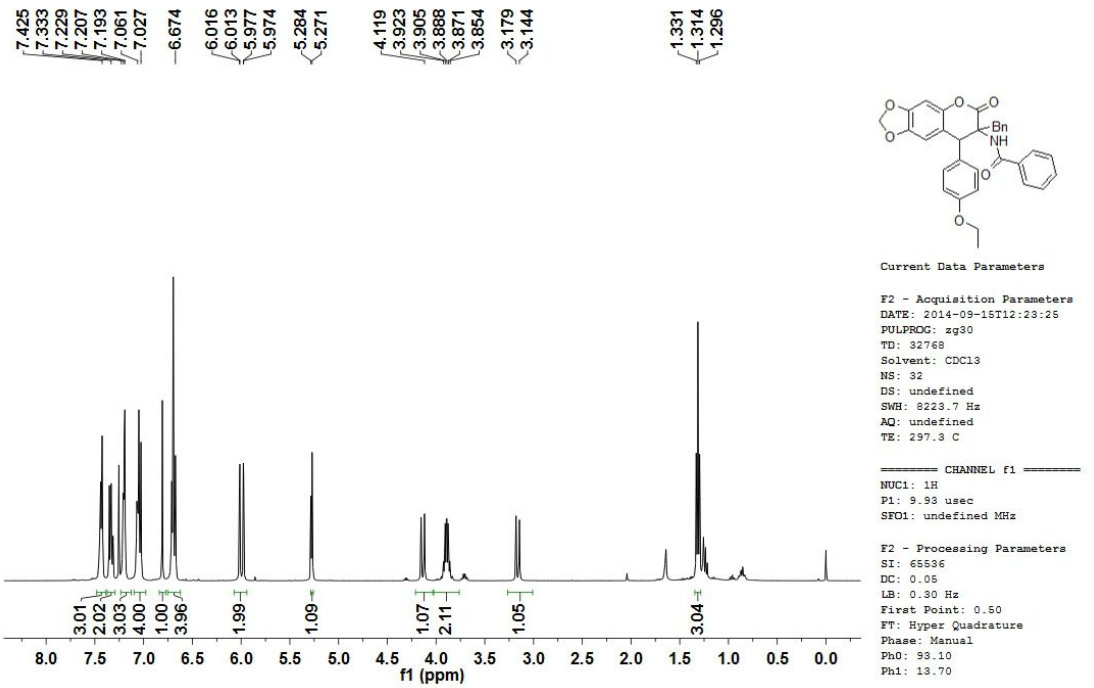

168.327
167.929
163.384
160.941
159.023
148.056
145.361
130.703
130.043
128.912
128.671
115.227
114.165
108.595
102.039
98.445
65.838
55.158
49.076
37.365
F
O
O
O
O
NHCOPh
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

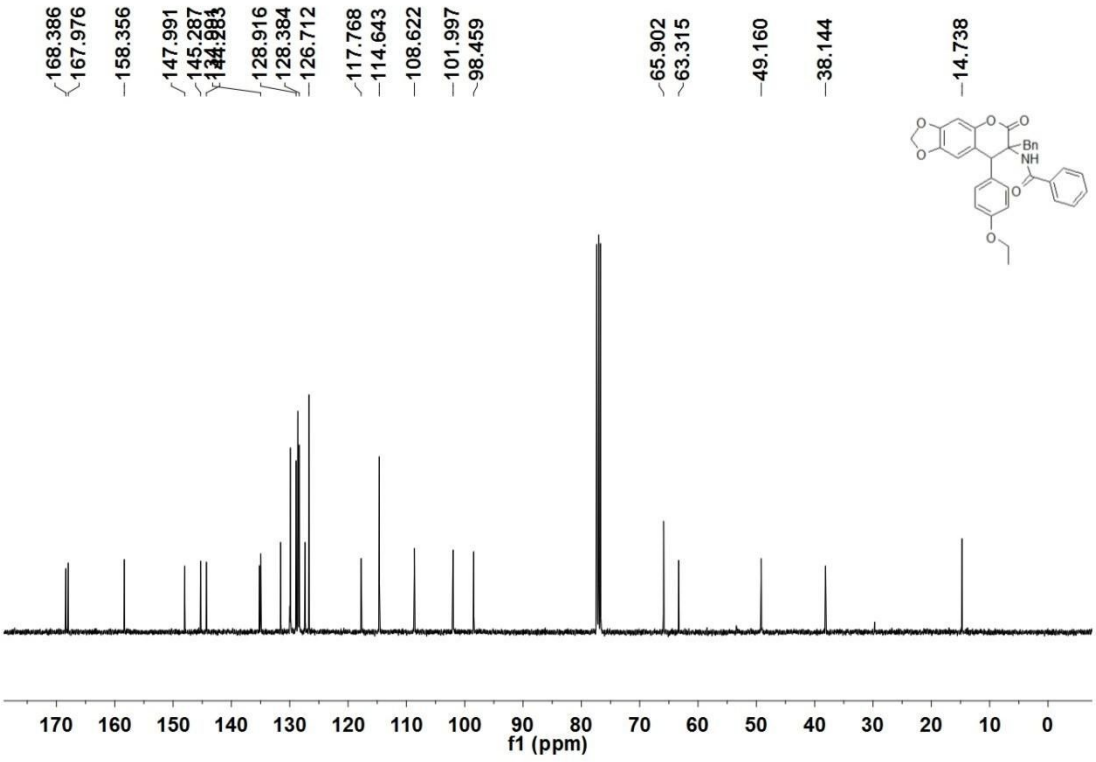

7.435
7.178
7.159
7.047
7.027
6.998
6.980
6.799
6.706
6.683
6.002
5.965
5.254
4.310
4.143
4.108
3.753
3.670
3.154
3.119
7.452
7.435
7.366
7.349
7.178
7.159
7.027
6.980
6.799
6.706
6.683
3.08
2.06
2.02
4.02
5.00
7.5
7.0
6.5
f1 (ppm)
Cl
NHCOPh
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-11T16:43:42
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.5 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 95.23
Ph1: 9.36
3.08
2.06
2.02
4.02
5.00
2.07
1.02
1.01
3.07
1.00
f1 (ppm)
168.226
167.958
159.047
148.080
145.384
144.194
133.479
131.749
129.959
128.694
126.683
117.560
114.182
108.587
102.053
98.463
65.738
55.160
49.095
37.515
Cl
NHCOPh
f1 (ppm)


7.453
7.370
7.332
7.255
6.938
6.799
6.705
6.683
6.009
5.973
5.251
4.128
4.093
3.675
3.137
3.102
7.474
7.453
7.433
7.370
7.352
7.332
7.311
7.255
7.044
7.023
6.917
6.799
6.705
6.683
3.01
3.99
4.00
5.00
7.6
7.3
7.0
6.7
f1 (ppm)
Br
NHCOPh
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-08T21:12:36
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.3 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: -260.40
Ph1: -0.80
3.01
3.99
4.00
5.00
2.01
1.00
0.99
3.00
1.00
f1 (ppm)
168.198
167.957
159.046
148.082
145.386
144.186
131.541
128.908
126.679
117.550
114.182
108.582
102.049
98.462
65.665
55.165
49.096
37.578
Br
NHCOPh
f1 (ppm)


7.458
7.397
7.378
7.360
7.265
6.933
6.701
6.620
5.987
5.949
5.089
3.677
3.213
3.208
2.472
2.382
2.370
2.352
2.340
2.321
2.308
2.164
2.152
2.135
2.127
2.117
2.101
2.089
2.005
7.553
7.534
7.494
7.476
7.458
7.397
7.378
7.360
7.265
7.001
6.980
6.933
6.701
6.680
6.620
5.01
3.01
3.99
7.8
7.4
7.0
6.6
f1 (ppm)
5.01
3.01
3.99
2.01
1.00
3.04
1.00
1.01
1.01
1.06
3.00
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
0.5
0.0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-11T16:47:34
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.6 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 93.08
Ph1: 13.17
169.117
167.272
159.029
147.933
145.305
144.213
131.791
129.937
128.859
128.663
126.783
117.290
114.165
108.491
101.987
98.450
64.076
55.172
49.010
32.584
28.921
15.596
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.369
7.350
7.262
7.085
7.012
6.990
6.700
6.636
5.986
5.947
5.103
3.681
1.901
7.545
7.480
7.462
7.444
7.388
7.369
7.350
7.262
7.085
7.012
6.990
6.700
6.678
6.636
2.00
3.00
3.00
3.97
7.8
7.4
7.0
6.6
f1 (ppm)
2.00
3.00
3.00
3.97
2.00
1.00
3.02
3.05
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
0.5
0.0
f1 (ppm)
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-10-07T16:08:08
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 298.7 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 90.22
Ph1: 14.29
170.554
167.248
158.952
147.803
145.177
144.308
131.604
128.705
126.790
117.729
114.103
108.505
101.922
98.451
60.500
55.163
48.902
21.906
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.425
7.333
7.229
7.207
7.193
7.061
7.027
6.674
6.016
6.013
5.977
5.974
5.284
5.271
4.119
3.923
3.905
3.888
3.871
3.854
3.179
3.144
1.331
1.314
1.296
Bn
NH
Current Data Parameters
F2 - Acquisition Parameters
DATE: 2014-09-15T12:23:25
PULPROG: zg30
TD: 32768
Solvent: CDCl3
NS: 32
DS: undefined
SWH: 8223.7 Hz
AQ: undefined
TE: 297.3 C
======== CHANNEL f1 ========
NUC1: 1H
P1: 9.93 usec
SFO1: undefined MHz
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.30 Hz
First Point: 0.50
FT: Hyper Quadrature
Phase: Manual
Ph0: 93.10
Ph1: 13.70
3.01
2.02
3.03
4.00
1.00
3.96
1.99
1.09
1.07
2.11
1.05
3.04
f1 (ppm)


168.386
167.976
158.356
147.991
145.287
128.916
128.384
126.712
117.768
114.643
108.622
101.997
98.459
65.902
63.315
49.160
38.144
14.738
Bn
NH
f1 (ppm)