Cinchona Alkaloid-based Phosphoramide Catalyzed Highly Enantioselective Michael Addition of Unprotected 3-Substituted Oxindoles to Nitroolefins**

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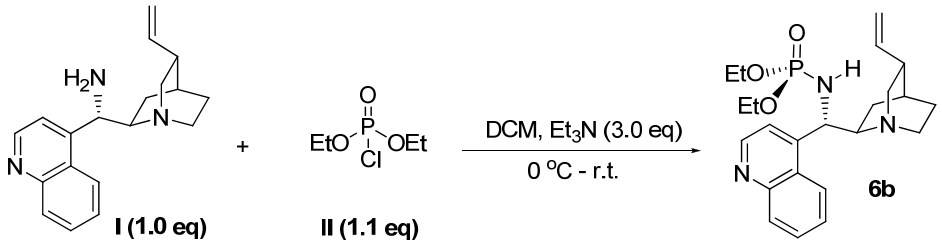
General: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields refer to pure isolated substances. ^{1}H and ^{13}C NMR spectra were obtained using a Bruker DPX-400 spectrometer. The $[\alpha]_D$ was recorded using PolAAr 3005 High Accuracy Polarimeter. Chemical shifts are reported in ppm from $CDCl_3$ or $(CD_3)_2SO$ with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift mutiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad.

All reactions were carried out in air except noted. Anhydrous CH_2Cl_2 was prepared by first distillation over P_2O_5 and then from CaH_2. Anhydrous Et_2O was distilled by distillation over sodium-benzophenone ketyl prior to use. Powdered MS 5Å was purchased from Aldrich and dried under vacuum at 120 ^{o}C for 12 hours, and then stored under nitrogen. Cinchonidine, quinine and cinchonine were purchased from Aldrich and used as received. Cinchona alkaloid derived primary amine was prepared according to literature method.[1]

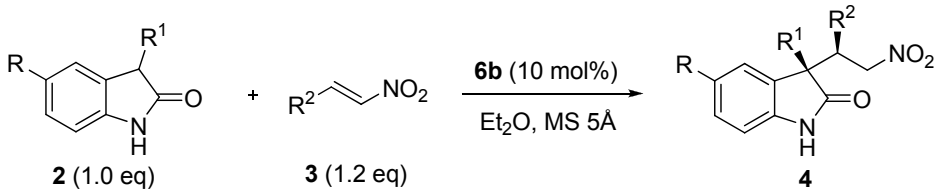
[1] a) X. Liu, H. Li, L. Deng, *Org. Lett.* **2005,** *7*, 167-169; b) B.Vakulya, S. Varga, A. Csámpai, T. Soós, *Org. Lett.* **2005,** *7*, 1967-1969.

1) Synthesis of cinchonidine-derived phosphoramides 6b

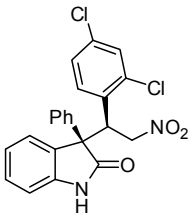


Under an atmosphere of N_2, to a flame-dried three-necked flask were added cinchonidine-derived primary amine **I** (439.2 mg, 1.5 mmol) and 8.0 mL of anhydrous CH_2Cl_2, followed by the addition of Et_3N (0.6 mL, 4.5 mmol). And then diethyl phosphorochloridate **II** (292.4 mg, 1.7 mmol) was added dropwise to the solution of **I** at 0 ^oC over 10 minutes. The resulting mixture was stirred at room temperature overnight. Then 30 mL of H_2O was added. The organic layer was separated, and the aqueous phase was extracted with dichloromethane (25 mL×4). The combined organic phase was dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash chromatography on silica gel using EtOAc:$NH_3 \cdot H_2O$ (200:1, v/v) as eluent to give product **6b** (366 mg, 57% yield) as yellowish oil. (Due to the distinct presence of rotameric isomers, the ^1H NMR and ^{13}C NMR contained extra peaks, so we did not designate the data, and attached the spectrum behind), ^1H NMR (400 MHz, $CDCl_3$): see below; ^{13}C NMR (100 MHz, $CDCl_3$): see below; MS (EI): 429 (M^+, 0.05), 136 (100), 81 (11), 137 (11), 42 (8), 157 (8), 41 (8), 79 (7), 155 (6); HRMS (EI): Exact mass calcd for $C_{23}H_{32}N_3O_3P$: 429.2181, Found: 429.2184.

2) General procedure for the Michael addition of unprotected 3-substituted oxindoles 2 to nitroolefin 3.

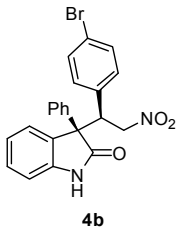


To a 5.0 mL vial were added 3-substituted oxindole **2** (0.25 mmol), catalyst **6b** (10.8 mg, 0.025 mmol) and MS 5Å (250.0 mg), followed by 2.5 mL of anhydrous Et_2O. The reaction mixture was stirred vigorously at room temperature for about half an hour, and then cooled down to the specific temperature for half an hour. Then nitroolefin **3** (0.30 mmol) was added. The resulting mixture was stirring at the specific temperature till full conversion of oxindole **2** by TLC analysis. The solvent was carefully removed under reduced pressure, and then the residue was directly subjected to column chromatography to afford the desired product **4**, using DCM as eluent.



4a

Product **4a** was obtained in 96% yield as white powder.[2] (dr = 21:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +97.9 (c = 0.38, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.30-8.12 (m, 1H), 7.64-7.62 (m, 2H), 7.42-7.25 (m, 7H), 6.87-6.86 (m, 2H), 6.39-6.37 (d, *J* = 8.4 Hz, 1H), 5.24 (t, *J* = 6.8 Hz, 1H), 4.78 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.0, 141.8, 137.0, 135.3, 134.6., 131.2, 129.8, 129.0, 128.7, 128.5, 127.6, 127.4, 126.7, 126.4, 122.7, 111.1, 76.9, 58.9, 44.6; HPLC analysis: Daicel Chiralcel OD-H/OD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 23.1 min (minor) and 28.7 min (major), minor diastereomer: 20.6 min (minor) and 32.2 min (major).

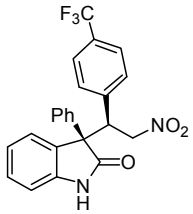


4b

Product **4b** was obtained in 89% yield as white powder. (dr = 13:1, 99% ee for the major diastereomer); $[\alpha]_D^{20}$ = +120.8 (c = 0.75, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.62-7.60 (m, 2H), 7.44-7.35 (m, 6H), 7.22-7.20 (m, 3H), 6.75-6.74 (m, 3H), 4.94 (t, *J* = 12.0 Hz, 1H), 4.80-4.69 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.2, 146.6, 141.6,

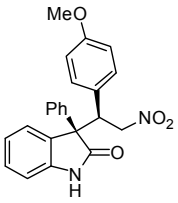
[2] M. Ding, F. Zhou, Z.-Q. Qian, J. Zhou, *Org. Biomol. Chem.* **2010**, *8*, 2912-2914.

135.4, 132.7, 131.0, 130.5, 129.4, 129.1, 128.3, 127.4, 127.2, 126.1, 122.4, 122.3, 110.9, 85.1, 75.9, 59.6, 49.7, 27.2; IR (neat): 3140, 3035, 2923, 1704, 1541, 1472, 1208, 1077, 744, 699; MS (EI): 436 (M^+, 2.88), 208 (100), 43 (24), 209 (22), 91 (19), 180 (19), 57 (19), 41 (15), 77 (14); HRMS (EI): Exact mass calcd for $C_{22}H_{17}N_2O_3Br$: 436.0423, Found: 436.0417; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 20.9 min (minor) and 28.6 min (major), minor diastereomer: 18.8 min (major) and 22.0 min (minor).



4c

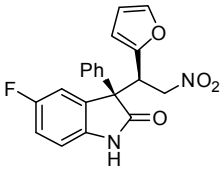
Product **4c** was obtained in 92% yield as white powder.[2] (dr = 13:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +215.8 (c = 0.46, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.62-7.60 (m, 2H), 7.39-7.32 (m, 7H), 7.27-7.23 (m, 1H), 7.05-7.00 (m, 2H), 6.74-6.73 (m, 1H), 4.99 (t, *J* = 12.4 Hz, 1H), 4.89-4.72 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.0, 176.9, 141.4, 137.9, 135.2, 129.8, 129.5, 129.3, 128.6, 127.5, 127.1, 126.4, 125.0, 124.9, 122.7, 110.9, 75.9, 59.7, 50.1; IR (neat): 3250, 3063, 2925, 1714, 1555, 1324, 1118, 846, 744, 697; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 15.2 min (minor) and 19.6 min (major), minor diastereomer: 12.0 min (major) and 16.5 min (minor).



4d

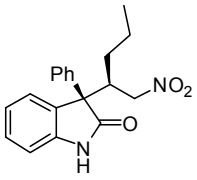
Product **4d** was obtained in 85% yield as white powder. (dr = 7:1, 97% ee for the major diastereomer); $[\alpha]_D^{20}$ = +168.7 (c = 0.52, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.90-7.51 (m, 3H), 7.41-7.20 (m, 6H), 6.79-6.71 (m, 3H), 6.61-6.56 (m, 2H), 5.00-4.90 (m, 1H), 4.88-4.72 (m, 2H), 3.67 (s, 3H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.4, 159.2, 141.7, 135.8, 130.0, 129.3, 129.1, 128.3, 127.8, 127.5, 126.4, 125.4, 122.3, 113.4, 110.7, 76.5, 60.0, 55.0, 49.8; IR (neat): 3194, 3073, 1699, 1552, 1474, 1253, 834, 750, 694, 657; MS (EI): 180 (100), 209 (88), 132 (21), 179 (16), 210 (12), 181 (13), 152 (10), 208 (9); HRMS (EI): Exact mass calcd for $C_{23}H_{20}N_2O_4$: 388.1423, Found: 388.1426; HPLC analysis: Daicel Chiralcel OD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 12.0 min (minor) and 17.9 min (major), minor diastereomer: 13.6 min (minor) and 21.0 min

(major).



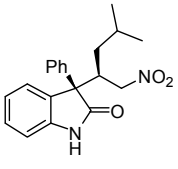
4e

Product **4e** was obtained in 84% yield as white powder. (dr = 3:1, 96% ee for the major diastereomer); $[\alpha]_D^{20}$ = +161.0 (c = 0.82, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.74 (s, 1H), 7.53-7.31 (m, 6H), 7.14-6.80 (m, 3H), 6.12 (s, 1H), 6.03 (s, 1H), 5.12-4.99 (m, 2H), 4.66-4.58 (m, 1H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 179.2, 178.5, 159.8, 157.4, 148.2, 148.1, 142.6, 142.4, 137.4, 136.4, 136.1, 134.7, 131.5, 131.4, 129.7, 129.6, 129.3, 129.2, 128.7, 128.3, 127.2, 126.6, 116.0, 115.7, 115.5, 115.3, 114.1, 113.9, 113.5, 113.2, 111.4, 111.3, 111.2, 111.1, 110.4, 110.3, 109.7, 109.1, 74.3, 59.9, 44.1, 43.8; IR (neat): 3648, 3220, 2988, 1712, 1555, 1485, 1375, 817, 739, 696; MS (EI): 366 (M^+, 0.37), 94 (100), 226 (74), 198 (39), 65 (36), 170 (29), 66 (28), 227 (28), 197 (17); HRMS (EI): Exact mass calcd for $C_{20}H_{15}N_2O_4F$: 366.1016, Found: 366.1013; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 11.4 min (minor) and 24.9 min (major), minor diastereomer: 13.4 min (minor) and 18.3 min (major).



4f

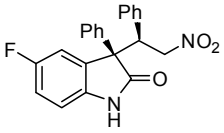
Product **4f** was obtained in 76% yield as white powder.[2] (dr = 6:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +207.4 (c = 0.48, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.65-8.62 (m, 1H), 7.46-7.26 (m, 6H), 7.18-7.14 (m, 2H), 7.02-7.00 (m, 1H), 4.46-4.38 (m, 2H), 3.73 (s, 1H), 1.31-1.10 (m, 4H), 0.78-0.75 (m, 3H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 179.6, 141.5, 137.2, 129.2, 129.1, 128.9, 128.3, 127.5, 125.6, 122.8, 111.0, 77.9, 60.0, 43.6, 32.9, 20.5, 14.2; HPLC analysis: Daicel Chiralcel IC, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 6.1 min (minor) and 6.9 min (major), minor diastereomer: 15.2 min (major) and 18.8 min (minor).



4g

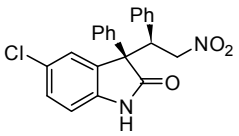
Product **4g** was obtained in 84% yield as white powder.[2] (dr = 6:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +211.4 (c = 0.64, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 9.23 (s, 1H), 7.48-7.46 (m, 2H), 7.34-7.26 (m, 4H), 7.15 (m, 2H), 7.02-7.00 (m, 1H), 4.49-4.35 (m, 2H), 3.79 (m, 1H), 1.45 (m, 1H), 1.13-1.00 (m, 2H), 0.88 (d, *J* = 5.6 Hz, 3H), 0.78 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR for major

diastereomer (100 MHz, $CDCl_3$): δ 179.4, 141.4, 137.1, 129.1, 129.0, 128.8, 128.2, 127.4, 125.5, 122.7, 111.9, 78.4, 60.0, 41.6, 40.1, 25.7, 23.7, 21.6; HPLC analysis: Daicel Chiralcel IC, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 5.3 min (minor) and 5.6 min (major), minor diastereomer: 13.3 min (major) and 15.9 min (minor).



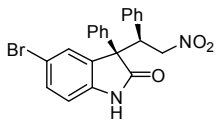
4h

Product **4h** was obtained in 84% yield as white powder.[2] (dr = 10:1, 96% ee for the major diastereomer); $[\alpha]_D^{20}$ = +207.7 (c = 0.52, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.31-8.13 (m, 1H), 7.58-7.57 (m, 2H), 7.39-7.33 (m, 3H), 7.18-7.06 (m, 5H), 6.90-6.88 (m, 2H), 6.68-6.66 (m, 1H), 5.00 (t, *J* = 12.0 Hz, 1H), 4.82-4.70 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.6, 159.8, 157.4, 137.7, 135.1, 133.2, 129.6, 129.3, 129.2, 128.8, 128.6, 128.4, 128.2, 128.1, 127.4, 126.4, 116.2, 115.9, 114.2, 114.0, 111.4, 111.3, 75.9, 60.6, 50.0; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 11.4 min (minor) and 17.2 min (major), minor diastereomer: 13.0 min (major) and 14.2 min (minor).



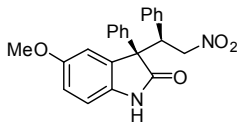
4i

Product **4i** was obtained in 92% yield as white powder. (dr = 8:1, 97% ee for the major diastereomer); $[\alpha]_D^{20}$ = +143.2 (c = 0.51, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.54-8.46 (m, 1H), 7.55-7.53 (m, 2H), 7.37-7.29 (m, 5H), 7.18-7.11 (m, 3H), 6.99-6.97 (m, 2H), 6.65-6.63 (m, 1H), 4.97 (t, *J* = 12.0 Hz, 1H), 4.80-4.69 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.6, 140.3, 134.9, 133.1, 129.6, 129.4, 129.2, 128.8, 128.6, 128.4, 128.1, 127.7, 127.3, 126.3, 111.8, 75.8, 60.4, 49.9; IR (neat): 3207, 2882, 2719, 1719, 1557, 1374, 896, 817, 738, 694; MS (EI): 392 (M^+, 5.46), 242 (100), 243 (46), 244 (38), 207 (36), 104 (18), 245 (15), 152 (15), 214 (14); HRMS (EI): Exact mass calcd for $C_{22}H_{17}N_2O_3Cl$: 392.0928, Found: 392.0929; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 11.0 min (minor) and 16.2 min (major), minor diastereomer: 12.7 min (major) and 13.6 min (minor).



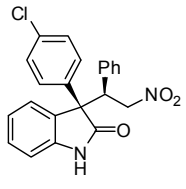
4j

Product **4j** was obtained in 78% yield as white powder.[2] (dr = 7:1, 97% ee for the major diastereomer); $[\alpha]_D^{20}$ = +93.9 (c = 0.56, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.25 (s, 1H), 7.58-7.56 (m, 2H), 7.46-7.35 (m, 5H), 7.20-7.06 (m, 3H), 6.89-6.88 (m, 2H), 6.64-6.62 (m, 1H), 4.97 (t, *J* = 12 Hz, 1H), 4.89-4.74 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.3, 140.7, 135.0, 133.1, 132.4, 130.1, 129.3, 129.2, 128.9, 128.7, 128.4, 128.2, 127.4, 115.0, 112.2, 75.9, 60.3, 50.1; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 11.7 min (minor) and 20.0 min (major), minor diastereomer: 13.4 min (major) and 14.7 min (minor).



4k

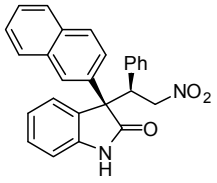
Product **4k** was obtained in 83% yield as white powder. (dr = 11:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +78.0 (c = 0.50, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.65-7.63 (m, 2H), 7.43-7.35 (m, 4H), 7.17-7.05 (m, 4H), 6.94-6.86 (m, 4H), 6.66-6.64 (m, 1H), 5.40 (t, *J* = 12.4 Hz, 1H), 4.83-4.71 (m, 2H), 3.90 (s, 3H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 176.9, 155.6, 135.7, 135.0, 133.6, 129.5, 129.2, 129.1, 129.1, 129.0, 128.4, 128.2, 128.1, 127.6, 126.5, 114.2, 113.2, 110.8, 76.2, 60.4, 56.0, 50.2; MS (EI): 388 (M^+, 4.17), 238 (100), 239 (25), 167 (17), 104 (13), 195 (11), 207 (10), 166 (7), 77 (6); HRMS (EI): Exact mass calcd for $C_{23}H_{20}N_2O_4$: 388.1423, Found: 388.1425; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 17.1 min (minor) and 29.4 min (major), minor diastereomer: 23.1min (major) and 24.3 min (minor).



4l

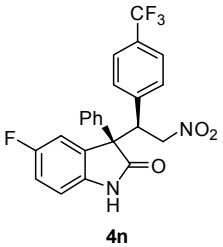
Product **4l** was obtained in 84% yield as white powder.[2] (dr = 18:1, 97% ee for the major diastereomer); $[\alpha]_D^{20}$ = +54.7 (c = 0.72, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.56-7.54 (m, 2H), 7.34-7.32 (m, 4H), 7.25-7.22 (m, 1H), 7.16-7.13 (m, 1H), 7.04-7.00 (m, 2H), 6.83-6.81 (m, 2H), 6.73-6.71 (m, 1H), 4.97 (t, *J* = 12.0 Hz, 1H), 4.73-4.66 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.2, 141.6, 134.6, 134.2, 133.2, 129.6, 129.3, 129.0, 128.8, 128.3, 128.0, 127.2, 126.2, 122.6, 110.9, 76.1, 59.5, 50.4; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer:

21.0 min (minor) and 29.0 min (major), minor diastereomer: 16.6 min (major) and 25.1 min (minor).



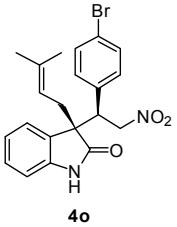
4m

Product **4m** was obtained in 77% yield as white powder.[2] (dr = 11:1, 99% ee for the major diastereomer); $[\alpha]_D^{20}$ = +16.8 (c = 0.59, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.82-7.76 (m, 6H), 7.48-7.42 (m, 3H), 7.37-7.26 (m, 2H), 7.17-7.04 (m, 3H), 6.92-6.90 (m, 2H), 6.75-6.73 (m, 1H), 5.06-4.94 (m, 2H), 4.82-4.66 (m, 1H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.2, 141.6, 133.6, 133.1, 133.1, 132.9, 129.5, 129.2, 129.0, 128.3, 128.1, 127.8, 127.5, 127.3, 126.8, 126.5, 124.6, 122.5, 110.7, 76.3, 60.1, 50.4; HPLC analysis: Daicel Chiralcel OD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 35.9 min (major) and 48.5 min (minor), minor diastereomer: 12.3 min (minor) and 24.2 min (major).



4n

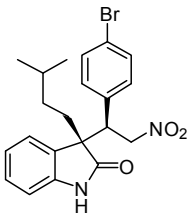
Product **4n** was obtained in 85% yield as white powder. (dr = 9:1, 98% ee for the major diastereomer); $[\alpha]_D^{20}$ = +167.6 (c = 0.68, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.65-7.52 (m, 2H), 7.44-7.36 (m, 5H), 7.15-7.04 (m, 4H), 6.77-6.70 (m, 1H), 4.97 (t, *J* = 12.0 Hz, 1H), 4.91-4.66 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.2, 159.9, 157.5, 137.6, 137.5, 134.7, 130.4, 129.4, 128.8, 128.7, 128.6, 127.3, 125.1, 125.0, 125.0, 116.5, 116.3, 114.2, 114.0, 111.8, 111.7, 75.5, 60.3, 49.8; IR (neat): 3198, 2988, 1713, 1560, 1487, 1325, 1119, 853, 820, 694; MS (EI): 444 (M^+, 2.53), 226 (100), 172 (56), 198 (43), 170 (29), 151 (29), 171 (19), 227 (18), 103 (18); HRMS (EI): Exact mass calcd for $C_{23}H_{16}N_2O_3F_4$: 444.1097, Found: 444.1095; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 11.3 min (minor) and 20.9 min (major), minor diastereomer: 9.4 min (major) and 12.3 min (minor).



4o

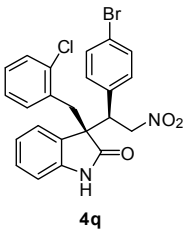
Product **4o** was obtained in 78% yield as white powder. (dr = 8:1, 94% ee for the major diastereomer); $[\alpha]_D^{20}$ = −19.5 (c = 0.86, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.61-7.47 (m, 1H), 7.29-7.27 (m, 3H),

7.14-7.09 (m, 2H), 6.86-6.85 (m, 2H), 6.77-6.75 (m, 1H), 4.96-4.84 (m, 2H), 4.67 (m, 1H), 4.01-3.99 (m, 1H), 2.87-2.54 (m, 2H), 1.49 (s, 6H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 178.6, 141.0, 136.4, 133.8, 131.3, 130.8, 129.2, 129.0, 123.9, 122.6, 122.4, 116.2, 110.0, 76.0, 55.2, 49.3, 33.6, 25.8, 18.1; IR (neat): 3065, 2924, 2854, 1708, 1556, 1472, 1074, 1010, 828, 755; MS (EI): 430 (M^+, 2.83), 69 (100), 41 (95), 200 (51), 55 (36), 77 (34), 184 (33), 43 (31), 360 (29); HRMS (EI): Exact mass calcd for $C_{21}H_{21}N_2O_3Br$: 430.0715, Found: 430.0719; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 16.2 min (minor) and 17.6 min (major), minor diastereomer: 10.0 min (minor) and 18.4 min (major).



4p

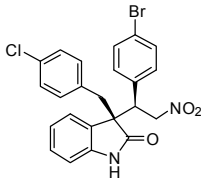
Product **4p** was obtained in 89% yield as white powder. (dr = 8:1, 95% ee for the major diastereomer); $[\alpha]_D^{20}$ = −136.4 (c = 0.51, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.52-7.24 (m, 6H), 6.92-6.66 (m, 3H), 5.00-4.83 (m, 2H), 3.94-3.81 (m, 1H), 2.04-1.74 (m, 2H), 1.43-1.40 (m, 1H), 0.91-0.90 (m, 1H), 0.80-0.76 (m, 6H), 0.69-0.62 (m, 1H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 178.5, 140.1, 133.3, 132.0, 131.5, 131.4, 130.6, 126.8, 122.6, 115.4, 111.6, 75.6, 55.8, 49.6, 32.8, 32.5, 28.0, 22.3, 22.2; IR (neat): 3130, 2926, 2853, 1712, 1555, 1010, 828, 609; MS (EI): 509 (M^+, 2.04), 41 (100), 43 (84), 182 (72), 69 (69), 184 (63), 103 (38), 77 (36), 226 (30); HRMS (EI): Exact mass calcd for $C_{21}H_{22}N_2O_3Br_2$: 511.9956, Found: 511.9956; HPLC analysis: Daicel Chiralcel IC, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 6.5 min (minor) and 8.0 min (major), minor diastereomer: 5.7 min (minor) and 9.3 min (major).



4q

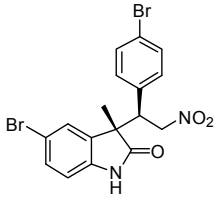
Product **4q** was obtained in 95% yield as white powder. (dr = 7:1, 96% ee for the major diastereomer); $[\alpha]_D^{20}$ = −89.7 (c = 1.22, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.52 (s, 1H), 7.39-7.26 (m, 2H), 7.18-7.10 (m, 2H), 7.06-6,84 (m, 7H), 6.58-6.56 (m, 1H), 5.08-4.92 (m, 2H), 4.11-4.08 (m, 1H), 3.69-3.65 (m, 1H), 3.35-3.32 (m, 1H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 178.4, 140.6, 134.2, 133.6, 133.0, 131.4, 131.4, 130.9, 130.5, 129.5, 129.4, 129.3, 128.8, 128.3, 127.5, 126.5, 126.4, 125.3, 122.6, 122.4, 122.1, 109.8, 76.2, 56.6, 56.5, 49.8, 49.7,

37.1, 36.3; IR (neat): 3213, 1709, 1620, 1553, 1472, 1375, 1011, 821, 755, 658; MS (EI): 486(M^+, 2.09), 125 (100), 256 (66), 182 (42), 89 (40), 77 (37), 220 (36), 127 (33), 257 (32); HRMS (EI): Exact mass calcd for $C_{23}H_{18}N_2O_3ClBr$: 486.0169, Found: 486.0170; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 23.7 min (major) and 31.4 min (minor), minor diastereomer: 19.5 min (minor) and 29.9 min (major).



4r

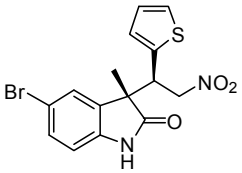
Product **4r** was obtained in 95% yield as white powder. (dr = 8:1, 91% ee for the major diastereomer); $[\alpha]_D^{20}$ = +14.9 (c = 0.54, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.35-7.26 (m, 3H), 7.23-7.15 (m, 2H), 7.04-6.91 (m, 6H), 6.80-6.78 (m, 1H), 6.72-6.70 (m, 1H), 6.57-6.51 (m, 1H), 5.07-4.91 (m, 2H), 4.17-4.09 (m, 1H), 3.25-3.11 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$-DMSO-d_6): δ 176.0, 175.9, 140.9, 140.8, 133.8, 133.3, 133.2, 132.7, 130.3, 130.0, 129.5, 129.2, 128.4, 127.4, 127.2, 126.6, 126.3, 125.9, 124.8, 123.2, 120.2, 120.0, 108.3, 108.1, 75.0, 74.9, 55.3, 55.2, 48.2, 48.0; IR (neat): 3214, 2923, 1905, 1710, 1551, 1472, 1376, 1012, 821, 753; MS (EI): 486 (M^+, 0.02), 43 (100), 57 (90), 55 (55), 41 (49), 71 (46), 91 (43), 69 (40), 125 (37); HRMS (EI): Exact mass calcd for $C_{23}H_{18}N_2O_3ClBr$: 486.0169, Found: 486.0167; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 30.9 min (minor) and 42.8 min (major), minor diastereomer: 22.2 min (minor) and 51.3 min (major).



4s

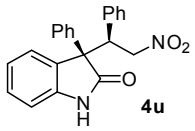
Product **4s** was obtained in 77% yield as white powder. (dr = 9:1, 95% ee for the major diastereomer); $[\alpha]_D^{20}$ = −140.0 (c = 0.72, $CHCl_3$). ^1H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.29 (s, 1H), 7.42-7.40 (m, 1H), 7.34-7.32 (m, 2H), 7.12 (s, 1H), 6.87-6.85 (m, 2H), 6.74-6.72 (m, 1H), 5.05-4.85 (m, 2H), 3.92-3.89 (m, 1H), 1.49-1.45 (m, 3H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 179.7, 139.3, 133.4, 133.1, 132.0, 131.5, 131.5, 130.5, 127.0, 122.7, 115.4, 111.8, 75.4, 50.8, 49.2, 20.7; IR (neat): 3196, 2917, 2340, 1712, 1554, 1474, 1183, 1010, 817, 781; MS (EI): 454 (M^+, 0.57), 103 (100), 117 (94), 77 (78), 184 (77), 89 (73), 182 (72), 102 (71), 145 (69); HRMS (EI): Exact mass calcd for $C_{17}H_{14}N_2O_3Br_2$: 451.9371, Found: 451.9372; HPLC analysis: Daicel

Chiralcel IC, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 230 nm, retention time: major diastereomer: 10.6 min (major) and 15.7 min (minor), minor diastereomer: 8.2 min (minor) and 11.3 min (major).



4t

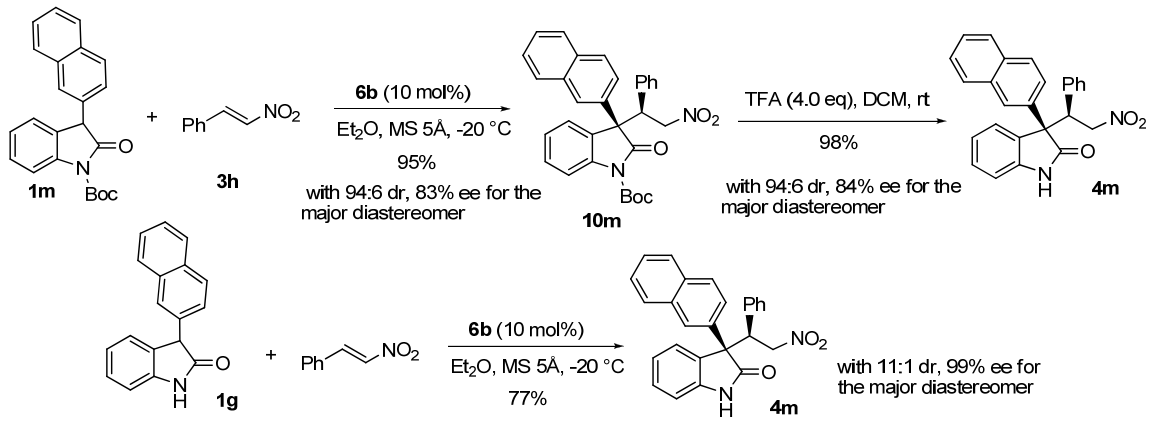
Product **4t** was obtained in 86% yield as white powder. (dr = 12:1, 95% ee for the major diastereomer); $[\alpha]_D^{20}$ = −140.3 (c = 1.04, $CHCl_3$). ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 8.96-8.11 (m, 1H), 7.42-7.40 (m, 1H), 7.16-7.13 (m, 1H), 7.01 (s, 1H), 6.86-6.75 (m, 3H), 5.12-5.09 (m, 1H), 4.84-4.78 (m, 1H), 4.26-4.23 (m, 1H), 1.51 (s, 3H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 180.0, 139.6, 136.5, 133.3, 132.0, 128.2, 127.4, 126.6, 125.8, 115.4, 111.7, 51.0, 45.3, 20.3; IR (neat): 3218, 2924, 1709, 1554, 1475, 1376, 1190, 1063, 816, 703; MS (EI): 225 (100), 227 (87), 110 (78), 224 (43), 117 (37), 197 (24), 199 (21), 156 (22); HRMS (EI): Exact mass calcd for $C_{15}H_{13}N_2O_3BrS$: 379.9830, Found: 379.9829; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ= 205 nm, retention time: major diastereomer: 14.6 min (minor) and 16.9 min (major), minor diastereomer: 12.7 min (minor) and 13.4 min (major).



4u

Product **4u** was obtained in 95% yield as white powder.[2] (dr = 11:1, determined by ^{1}H NMR analysis of the crude reaction mixture. The enantioselectivity can not be determined by HPLC analysis); ^{1}H NMR for major diastereomer (400 MHz, $CDCl_3$): δ 7.68-7.61 (m, 2H), 7.40-7.32 (m, 6H), 7.16-7.03 (m, 4H), 6.87-6.86 (m, 2H), 6.74-6.72 (m, 1H), 5.00 (t, J = 12.0 Hz, 1H), 4.84-4.72 (m, 2H); ^{13}C NMR for major diastereomer (100 MHz, $CDCl_3$): δ 177.1, 177.0, 141.6, 135.7, 133.6, 129.4, 129.2, 129.0, 128.4, 128.2, 128.0, 127.7, 127.6, 126.6, 126.5, 122.4, 110.6, 76.3, 50.4.

3) The determination of absolute configuration of product 4m.



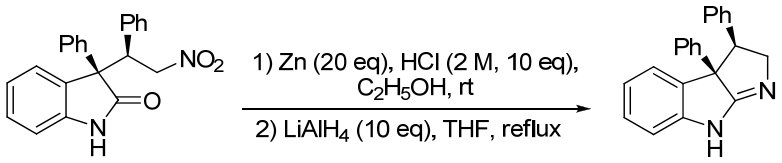
To a 5.0 mL vial were added *N*-Boc protected 3-substituted oxindole **1m** (23 mg, 0.06 mmol), catalyst **6b** (2.8 mg, 0.006 mmol) and MS 5Å (64.0 mg), followed by 1.1 mL of anhydrous Et_2O. The reaction mixture was stirred vigorously at room temperature for about half an hour, and then cooled down to -20°C for half an hour. Then nitrostyrene **3h** (10 mg, 0.07 mmol) was added. The resulting mixture was stirring at -20°C until the full conversion of oxindole **1m** by TLC analysis. The solvent was carefully removed under reduced pressure then the residue was directly subjected to column chromatography (DCM as eluent) to afford the desired product **10m** as white solid in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$): see below; ^{13}C NMR (100 MHz, $CDCl_3$): see below; Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: major diastereomer: 12.1 min (minor) and 15.2 min (major), minor diastereomer: 10.1 min (minor) and 38.0 min (major). By comparing the HPLC performance of product **10m** with Prof. Maruoka' product,[3] the configuration of the stereogenic center of the major diasteromer of product **10m** at C3 position was also assigned to be *R* and that at the remaining stereocenter was *R*.

Compound **4m**: To a solution of compound **10m** (20 mg, 0.04 mmol) in 1.0 mL of CH_2Cl_2 was added TFA (13.0 uL, 4.0 eq). The resulting mixture was stirred at room temperature for 24 h till the full disappearance of compound **10m**. The mixture was directly subjected to column chromatography (DCM as eluent) to afford the desired product **4m** as white solid in 98% yield. Daicel Chiralcel OD-H, hexane/*iso*-PrOH = 9:1, flow rate = 1.0 mL/min, λ = 230 nm, retention time: major diastereomer: 35.4 min (major) and 48.8 min (minor), minor diastereomer: 12.2 min

[3] R. He, S. Shirakawa, K. Maruoka, *J. Am. Chem. Soc.* **2009**, *131*, 16620-16621.

(minor) and 24.9 min (major).

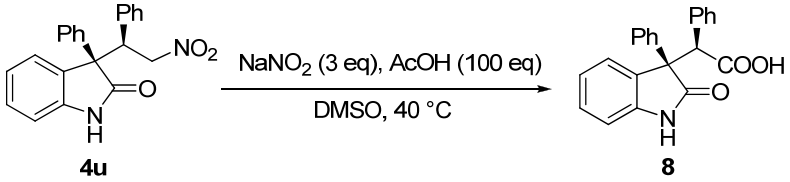
The HPLC performance of compound **4m** obtained from the deprotection of product **10m** was in accordance with that of compound **4m** obtained by the Michael addition of oxindole **1g** to nitrostyrene catalyzed by **6b**. By both methods, the configuration of the stereogenic center of the major diasteromer of product **4m**, at C3 position was assigned to be *R* and that at the remaining stereocenter was *R*.



4u **9**

A mixture of compound **4u** (35.8 mg, 0.1 mmol), Zn (130.0 mg, 2 mmol), HCl (2 M, 5.0 ml, 1 mmol), EtOH (1.5 mL) was stirred at room temperature for 4 h, then it was filtered through celite and washed with DCM. Adding $NH_3 \cdot H_2O$ to make the pH value of the filtrate above 7 and then extracted with DCM (10 mL×4). The combined organic phase was then dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The resulting residue was dissolved again in anhydrous THF (2 mL), and $LiAlH_4$ (38 mg, 1 mmol) was added under N_2, and then the mixture was heated at 75 ℃ for 2 h. After cooling to room temperature, the reaction was quenched with 3 mL of ethyl acetate and 0.5 mL H_2O, and the resulting mixture was filtered through celite and washed with ethyl acetate and MeOH. The filtrates were concentrated and the residue was purified by column chromatography (hexane:ethyl-acetate, 1/1, and then CH_2Cl_2-MeOH, 10/1) to afford **9** as a white solid in 65% yield and 95% ee. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.39 (m, 1H), 7.24-7.14 (m, 9H), 7.00-6.91 (m, 5H), 4.11-3.95 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 182.9, 152.74, 136.7, 135.8, 135.4, 129.1, 128.3, 128.0, 128.0, 127.9, 127.8, 127.5, 127.0, 124.1, 121.0, 113.3, 66.0, 58.8, 57.8. Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 85:15, flow rate = 1.0 mL/min, λ = 230 nm, retention time: 11.5 min (minor) and 20.1 min (major). $[\alpha]_D^{20}$ = −496.6 (c = 0.52, $CHCl_3$); reported rotation for (S, S)-**9**: $[\alpha]_D^{20}$ = +309.7 (c = 0.30, $CHCl_3$, 90% ee).[3]

4) Product elaboration.



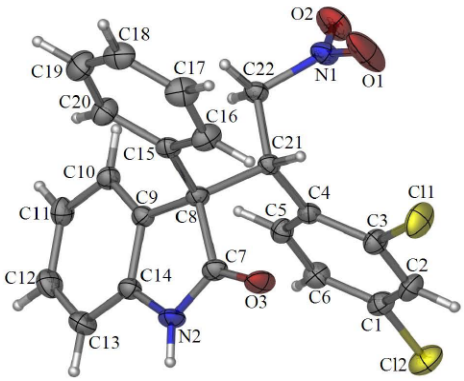
Compound **8** was obtained using a literature method to convert nitro group to carboxylic acid:[4] A mixture of compound **4u** (35.8 mg, 0.1 mmol), $NaNO_2$ (20.7 mg, 0.3 mmol), AcOH (63 μL，10 mmol), DMSO (250 μL) was stirred at 40 □ for 10 h, then the reaction mixture was poured into 10 mL of water and 10 mL of HCl (2 M), and extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4, and then concentrated. The residue was purified by column chromatography (hexane:ethyl-acetate, 1/2) to afford product as pale yellow solid in 75% yield and 95% ee. $[\alpha]_D^{20}$ = ＋335.8 (c = 0.50, CH_3OH). ^1H NMR for major diastereomer (400 MHz, DMSO-d_6): δ 12.57 (s, 1H), 10.26 (s, 1H), 8.09-8.07 (m, 1H), 7.38-7.01 (m, 12H), 6.64-6.62 (m, 1H), 4.90 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 177.7, 172.5, 142.9, 139.6, 134.6, 129.8, 129.2, 129.2, 128.9, 128.6, 128.0, 127.7, 127.4, 127.3, 121.6, 109.8, 60.0, 57.5; HRMS (ESI-TOF) calcd for $C_{22}H_{17}NO_3Na^+$: 366.1101 ($[M+Na]^+$), found: 366.1073; HPLC analysis: Daicel Chiralcel AD-H, hexane/*iso*-PrOH = 85:15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: 11.4 min (minor) and 22.8 min (major).

Single-Crystal X-ray Crystallography of product 4a[5]

Data intensity of **4a** was collected using a Bruker SMART APEX II (Mo radiation). The X-ray condition of was 50 kV × 30 mA. Data collection and reduction were done by using the Bruker ApexII software package. The structure was solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for dimmer of **4a**: $C_{52}H_{48}Cl_4N_4O_{10}$, M = 1030.74, T = 296(2) K, λ = 0.71073 Å, monoclinic, space group P2(1)/n, a = 12.5561(5) Å, b = 12.8030(5) Å, c = 16.3869(7) Å, V = 2521.48(18) Å^3, z = 2, d_{calc} = 1.358 mg/m^3, 29125 reflections measured, 8834 unique [R_{int} = 0.0199], R_1 = 0.0460, wR_2 = 0.1167 ($I > 2\sigma(I)$, final), R_1 = 0.0607, wR_2 = 0.1326 (all data), GOF

[4] C. Matt, A. Wagner, C. Mioskowski, *J. Org. Chem.* **1997**, 62, 234-235.
[5] CCDC number 827254

= 1.048, and 685 parameters.



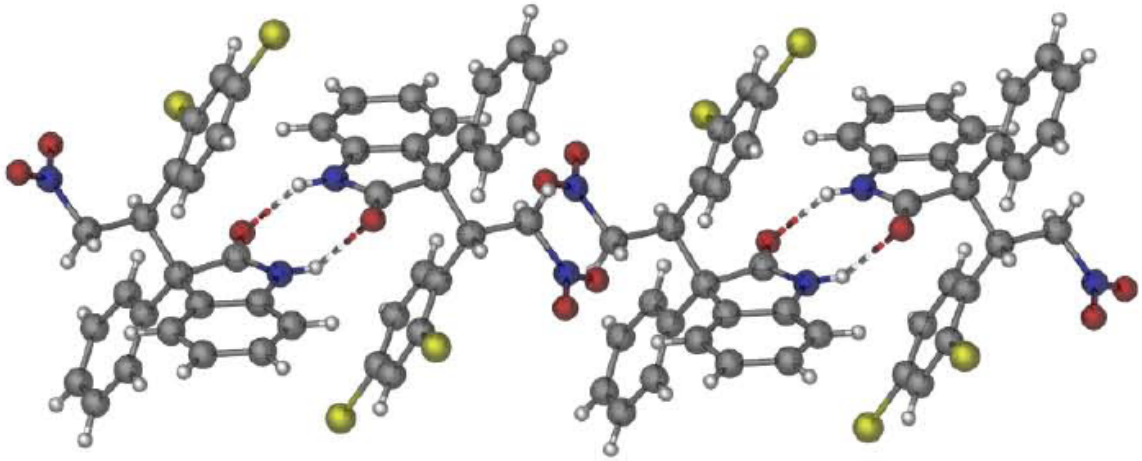


Table 1. Crystal data and structure refinement for z.

Identification code	z
Empirical formula	C52 H48 Cl4 N4 O10
Formula weight	1030.74
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.5561(5) A alpha = 83.5940(10) deg.
	b = 12.8030(5) A beta = 83.9170(10) deg.
	c = 16.3869(7) A gamma = 75.0880(10) deg.
Volume	2521.48(18) A^3
Z, Calculated density	2, 1.358 Mg/m^3
Absorption coefficient	0.297 mm^-1
F(000)	1072
Crystal size	0.49 x 0.42 x 0.22 mm
Theta range for data collection	1.99 to 25.01 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -19<=l<=19

Reflections collected / unique	29125 / 8834 [R(int) = 0.0199]
Completeness to theta = 25.01	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9376 and 0.8682
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8834 / 30 / 685
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1167
R indices (all data)	R1 = 0.0607, wR2 = 0.1326
Largest diff. peak and hole	0.438 and -0.314 e.A^-3

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

	x	y	z	U(eq)
Cl(1)	2802(1)	3689(1)	1876(1)	76(1)
Cl(2)	553(1)	715(1)	2898(1)	75(1)
O(1)	5246(2)	2319(2)	927(2)	119(1)
O(2)	5555(2)	667(2)	740(2)	79(1)
O(3)	1474(1)	4778(1)	151(1)	57(1)
N(1)	5096(2)	1597(2)	588(1)	50(1)
N(2)	662(2)	3786(2)	-548(1)	48(1)
C(1)	1335(2)	1281(2)	2116(2)	51(1)
C(2)	1690(2)	2168(2)	2254(2)	56(1)
C(3)	2323(2)	2608(2)	1637(2)	48(1)
C(4)	2588(2)	2200(2)	867(1)	39(1)
C(5)	2223(2)	1285(2)	771(1)	43(1)
C(6)	1600(2)	825(2)	1379(2)	50(1)
C(7)	1525(2)	4039(2)	-274(1)	43(1)
C(8)	2603(2)	3229(2)	-587(1)	38(1)
C(9)	2130(2)	2467(2)	-1008(1)	38(1)
C(10)	2613(2)	1524(2)	-1373(1)	43(1)
C(11)	1953(2)	971(2)	-1686(2)	52(1)
C(12)	821(2)	1372(2)	-1646(2)	62(1)
C(13)	318(2)	2320(2)	-1290(2)	59(1)
C(14)	985(2)	2847(2)	-967(1)	43(1)
C(15)	3303(2)	3860(2)	-1178(1)	40(1)
C(16)	3583(2)	4744(2)	-927(2)	57(1)
C(17)	4245(2)	5298(2)	-1437(2)	65(1)
C(18)	4639(2)	4984(2)	-2204(2)	60(1)
C(19)	4363(3)	4119(2)	-2465(2)	65(1)

C(20)	3696(2)	3566(2)	-1960(2)	55(1)
C(21)	3262(2)	2697(2)	180(1)	37(1)
C(22)	4328(2)	1880(2)	-83(1)	42(1)
Cl(3)	4434(1)	-487(1)	2221(1)	74(1)
Cl(4)	1222(1)	-2498(1)	3103(1)	72(1)
O(4)	4403(2)	-5470(2)	4270(2)	110(1)
O(5)	2881(2)	-4911(2)	3782(2)	95(1)
O(6)	104(1)	-1459(1)	4861(1)	52(1)
N(3)	3478(2)	-4940(2)	4308(2)	54(1)
N(4)	1236(2)	-727(1)	5501(1)	42(1)
C(23)	3818(2)	-1280(2)	2959(2)	50(1)
C(24)	2892(2)	-1553(2)	2785(2)	52(1)
C(25)	2390(2)	-2168(2)	3374(1)	45(1)
C(26)	2796(2)	-2523(2)	4143(1)	37(1)
C(27)	3758(2)	-2244(2)	4278(1)	45(1)
C(28)	4266(2)	-1622(2)	3698(2)	53(1)
C(29)	892(2)	-1550(2)	5258(1)	39(1)
C(30)	1689(2)	-2635(2)	5570(1)	36(1)
C(31)	2465(2)	-2222(2)	6027(1)	38(1)
C(32)	2152(2)	-1095(2)	5960(1)	41(1)
C(33)	2709(2)	-486(2)	6313(2)	58(1)
C(34)	3603(2)	-1031(2)	6743(2)	65(1)
C(35)	3935(2)	-2147(2)	6815(2)	60(1)
C(36)	3365(2)	-2750(2)	6458(1)	48(1)
C(37)	1030(2)	-3356(2)	6104(2)	44(1)
C(38)	218(2)	-3695(2)	5774(2)	59(1)
C(39)	-364(3)	-4372(3)	6245(3)	80(1)
C(40)	-139(3)	-4717(3)	7042(3)	89(1)
C(41)	646(3)	-4379(3)	7377(2)	83(1)
C(42)	1230(2)	-3700(2)	6916(2)	61(1)
C(43)	2258(2)	-3217(2)	4781(1)	37(1)
C(44)	3073(2)	-4281(2)	5032(2)	45(1)
O(01)	2627(4)	8392(2)	707(2)	138(1)
O(02)	2202(2)	7311(2)	-52(2)	94(1)
C(01)	3096(3)	6529(3)	1100(2)	98(1)
C(02)	2636(3)	7509(3)	576(2)	65(1)
C(03)	1756(5)	8227(4)	-623(3)	126(2)
C(04)	1493(5)	7832(5)	-1331(3)	167(3)
O(03)	7871(8)	6330(6)	4796(5)	148(3)
O(04)	7473(14)	7851(13)	4797(9)	143(6)
C(06)	7960(20)	7080(20)	3536(17)	165(11)
C(05)	7540(20)	7127(14)	4299(13)	143(9)
C(07)	6944(13)	7836(8)	5614(9)	115(4)
C(08)	6600(13)	8992(9)	5812(8)	112(4)

O(03')	6696(7)	6765(7)	4359(5)	144(3)
O(04')	7154(14)	8045(8)	4630(9)	137(6)
C(05')	7519(9)	7264(11)	4327(6)	60(3)
C(06')	8343(15)	7180(20)	3614(18)	107(5)
C(07')	6428(12)	8210(14)	5360(9)	123(4)
C(08')	7021(18)	8615(15)	5936(12)	187(9)

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

Cl(1)-C(3)	1.742(2)
Cl(2)-C(1)	1.738(2)
O(1)-N(1)	1.194(3)
O(2)-N(1)	1.194(3)
O(3)-C(7)	1.221(3)
N(1)-C(22)	1.491(3)
N(2)-C(7)	1.341(3)
N(2)-C(14)	1.398(3)
N(2)-H(2B)	0.8600
C(1)-C(2)	1.370(4)
C(1)-C(6)	1.373(3)
C(2)-C(3)	1.380(3)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.395(3)
C(4)-C(5)	1.393(3)
C(4)-C(21)	1.518(3)
C(5)-C(6)	1.374(3)
C(5)-H(5A)	0.9300
C(6)-H(6A)	0.9300
C(7)-C(8)	1.555(3)
C(8)-C(9)	1.521(3)
C(8)-C(15)	1.542(3)
C(8)-C(21)	1.571(3)
C(9)-C(10)	1.375(3)
C(9)-C(14)	1.391(3)
C(10)-C(11)	1.388(3)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.379(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.377(4)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.379(3)
C(13)-H(13A)	0.9300
C(15)-C(20)	1.381(3)

C(15)-C(16)	1.383(3)
C(16)-C(17)	1.385(4)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.365(4)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.365(4)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.383(4)
C(19)-H(19A)	0.9300
C(20)-H(20A)	0.9300
C(21)-C(22)	1.526(3)
C(21)-H(21A)	0.9800
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
Cl(3)-C(23)	1.739(2)
Cl(4)-C(25)	1.740(2)
O(4)-N(3)	1.183(3)
O(5)-N(3)	1.193(3)
O(6)-C(29)	1.216(3)
N(3)-C(44)	1.502(3)
N(4)-C(29)	1.347(3)
N(4)-C(32)	1.392(3)
N(4)-H(4A)	0.8600
C(23)-C(24)	1.364(4)
C(23)-C(28)	1.368(4)
C(24)-C(25)	1.381(3)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.393(3)
C(26)-C(27)	1.390(3)
C(26)-C(43)	1.514(3)
C(27)-C(28)	1.380(3)
C(27)-H(27A)	0.9300
C(28)-H(28A)	0.9300
C(29)-C(30)	1.558(3)
C(30)-C(31)	1.515(3)
C(30)-C(37)	1.537(3)
C(30)-C(43)	1.574(3)
C(31)-C(36)	1.379(3)
C(31)-C(32)	1.390(3)
C(32)-C(33)	1.378(3)
C(33)-C(34)	1.379(4)
C(33)-H(33A)	0.9300
C(34)-C(35)	1.376(4)
C(34)-H(34A)	0.9300

C(35)-C(36)	1.387(3)
C(35)-H(35A)	0.9300
C(36)-H(36A)	0.9300
C(37)-C(42)	1.382(4)
C(37)-C(38)	1.385(4)
C(38)-C(39)	1.393(4)
C(38)-H(38A)	0.9300
C(39)-C(40)	1.366(5)
C(39)-H(39A)	0.9300
C(40)-C(41)	1.358(5)
C(40)-H(40A)	0.9300
C(41)-C(42)	1.389(4)
C(41)-H(41A)	0.9300
C(42)-H(42A)	0.9300
C(43)-C(44)	1.523(3)
C(43)-H(43A)	0.9800
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
O(01)-C(02)	1.172(4)
O(02)-C(02)	1.291(4)
O(02)-C(03)	1.447(4)
C(01)-C(02)	1.461(5)
C(01)-H(01A)	0.9600
C(01)-H(01B)	0.9600
C(01)-H(01C)	0.9600
C(03)-C(04)	1.418(5)
C(03)-H(03A)	0.9700
C(03)-H(03B)	0.9700
C(04)-H(04A)	0.9600
C(04)-H(04B)	0.9600
C(04)-H(04C)	0.9600
O(03)-C(05)	1.243(17)
O(04)-C(05)	1.284(17)
O(04)-C(07)	1.43(2)
C(06)-C(05)	1.31(3)
C(06)-H(06A)	0.9600
C(06)-H(06B)	0.9600
C(06)-H(06C)	0.9600
C(07)-C(08)	1.494(7)
C(07)-H(07A)	0.9700
C(07)-H(07B)	0.9700
C(08)-H(08A)	0.9600
C(08)-H(08B)	0.9600
C(08)-H(08C)	0.9600

O(03')-C(05')	1.341(17)
O(04')-C(05')	1.133(15)
O(04')-C(07')	1.43(2)
C(05')-C(06')	1.47(3)
C(06')-H(06D)	0.9600
C(06')-H(06E)	0.9600
C(06')-H(06F)	0.9600
C(07')-C(08')	1.473(9)
C(07')-H(07C)	0.9700
C(07')-H(07D)	0.9700
C(08')-H(08D)	0.9600
C(08')-H(08E)	0.9600
C(08')-H(08F)	0.9600
O(2)-N(1)-O(1)	123.3(2)
O(2)-N(1)-C(22)	118.5(2)
O(1)-N(1)-C(22)	118.1(2)
C(7)-N(2)-C(14)	112.03(18)
C(7)-N(2)-H(2B)	124.0
C(14)-N(2)-H(2B)	124.0
C(2)-C(1)-C(6)	121.2(2)
C(2)-C(1)-Cl(2)	119.1(2)
C(6)-C(1)-Cl(2)	119.7(2)
C(1)-C(2)-C(3)	119.1(2)
C(1)-C(2)-H(2A)	120.5
C(3)-C(2)-H(2A)	120.5
C(2)-C(3)-C(4)	122.2(2)
C(2)-C(3)-Cl(1)	116.43(18)
C(4)-C(3)-Cl(1)	121.33(19)
C(5)-C(4)-C(3)	115.9(2)
C(5)-C(4)-C(21)	121.71(19)
C(3)-C(4)-C(21)	122.4(2)
C(6)-C(5)-C(4)	123.0(2)
C(6)-C(5)-H(5A)	118.5
C(4)-C(5)-H(5A)	118.5
C(1)-C(6)-C(5)	118.6(2)
C(1)-C(6)-H(6A)	120.7
C(5)-C(6)-H(6A)	120.7
O(3)-C(7)-N(2)	125.8(2)
O(3)-C(7)-C(8)	125.8(2)
N(2)-C(7)-C(8)	108.40(18)
C(9)-C(8)-C(15)	113.85(18)
C(9)-C(8)-C(7)	101.00(17)
C(15)-C(8)-C(7)	108.84(17)
C(9)-C(8)-C(21)	115.29(17)

C(15)-C(8)-C(21)	109.36(17)
C(7)-C(8)-C(21)	107.88(17)
C(10)-C(9)-C(14)	118.9(2)
C(10)-C(9)-C(8)	132.5(2)
C(14)-C(9)-C(8)	108.58(18)
C(9)-C(10)-C(11)	119.6(2)
C(9)-C(10)-H(10A)	120.2
C(11)-C(10)-H(10A)	120.2
C(12)-C(11)-C(10)	120.4(2)
C(12)-C(11)-H(11A)	119.8
C(10)-C(11)-H(11A)	119.8
C(13)-C(12)-C(11)	121.2(2)
C(13)-C(12)-H(12A)	119.4
C(11)-C(12)-H(12A)	119.4
C(12)-C(13)-C(14)	117.7(2)
C(12)-C(13)-H(13A)	121.2
C(14)-C(13)-H(13A)	121.2
C(13)-C(14)-C(9)	122.3(2)
C(13)-C(14)-N(2)	127.9(2)
C(9)-C(14)-N(2)	109.79(19)
C(20)-C(15)-C(16)	117.4(2)
C(20)-C(15)-C(8)	122.4(2)
C(16)-C(15)-C(8)	120.2(2)
C(15)-C(16)-C(17)	121.0(3)
C(15)-C(16)-H(16A)	119.5
C(17)-C(16)-H(16A)	119.5
C(18)-C(17)-C(16)	120.7(3)
C(18)-C(17)-H(17A)	119.6
C(16)-C(17)-H(17A)	119.6
C(19)-C(18)-C(17)	119.0(3)
C(19)-C(18)-H(18A)	120.5
C(17)-C(18)-H(18A)	120.5
C(18)-C(19)-C(20)	120.7(3)
C(18)-C(19)-H(19A)	119.6
C(20)-C(19)-H(19A)	119.6
C(15)-C(20)-C(19)	121.2(2)
C(15)-C(20)-H(20A)	119.4
C(19)-C(20)-H(20A)	119.4
C(4)-C(21)-C(22)	111.41(18)
C(4)-C(21)-C(8)	114.06(17)
C(22)-C(21)-C(8)	110.72(17)
C(4)-C(21)-H(21A)	106.7
C(22)-C(21)-H(21A)	106.7
C(8)-C(21)-H(21A)	106.7

N(1)-C(22)-C(21)	110.94(18)
N(1)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22A)	109.5
N(1)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	108.0
O(4)-N(3)-O(5)	121.5(2)
O(4)-N(3)-C(44)	118.3(2)
O(5)-N(3)-C(44)	120.2(2)
C(29)-N(4)-C(32)	112.25(17)
C(29)-N(4)-H(4A)	123.9
C(32)-N(4)-H(4A)	123.9
C(24)-C(23)-C(28)	121.1(2)
C(24)-C(23)-Cl(3)	118.8(2)
C(28)-C(23)-Cl(3)	120.0(2)
C(23)-C(24)-C(25)	119.0(2)
C(23)-C(24)-H(24A)	120.5
C(25)-C(24)-H(24A)	120.5
C(24)-C(25)-C(26)	122.4(2)
C(24)-C(25)-Cl(4)	116.35(18)
C(26)-C(25)-Cl(4)	121.21(18)
C(27)-C(26)-C(25)	116.0(2)
C(27)-C(26)-C(43)	121.62(19)
C(25)-C(26)-C(43)	122.31(19)
C(28)-C(27)-C(26)	122.3(2)
C(28)-C(27)-H(27A)	118.9
C(26)-C(27)-H(27A)	118.9
C(23)-C(28)-C(27)	119.1(2)
C(23)-C(28)-H(28A)	120.4
C(27)-C(28)-H(28A)	120.4
O(6)-C(29)-N(4)	125.9(2)
O(6)-C(29)-C(30)	126.08(19)
N(4)-C(29)-C(30)	107.98(18)
C(31)-C(30)-C(37)	114.93(18)
C(31)-C(30)-C(29)	101.14(16)
C(37)-C(30)-C(29)	110.00(17)
C(31)-C(30)-C(43)	114.04(17)
C(37)-C(30)-C(43)	109.45(17)
C(29)-C(30)-C(43)	106.65(16)
C(36)-C(31)-C(32)	118.9(2)
C(36)-C(31)-C(30)	132.2(2)
C(32)-C(31)-C(30)	108.80(18)
C(33)-C(32)-C(31)	122.2(2)
C(33)-C(32)-N(4)	128.0(2)

C(31)-C(32)-N(4)	109.81(19)
C(32)-C(33)-C(34)	117.8(2)
C(32)-C(33)-H(33A)	121.1
C(34)-C(33)-H(33A)	121.1
C(35)-C(34)-C(33)	121.2(2)
C(35)-C(34)-H(34A)	119.4
C(33)-C(34)-H(34A)	119.4
C(34)-C(35)-C(36)	120.4(2)
C(34)-C(35)-H(35A)	119.8
C(36)-C(35)-H(35A)	119.8
C(31)-C(36)-C(35)	119.5(2)
C(31)-C(36)-H(36A)	120.3
C(35)-C(36)-H(36A)	120.3
C(42)-C(37)-C(38)	117.8(2)
C(42)-C(37)-C(30)	122.0(2)
C(38)-C(37)-C(30)	120.2(2)
C(37)-C(38)-C(39)	120.8(3)
C(37)-C(38)-H(38A)	119.6
C(39)-C(38)-H(38A)	119.6
C(40)-C(39)-C(38)	120.4(3)
C(40)-C(39)-H(39A)	119.8
C(38)-C(39)-H(39A)	119.8
C(41)-C(40)-C(39)	119.4(3)
C(41)-C(40)-H(40A)	120.3
C(39)-C(40)-H(40A)	120.3
C(40)-C(41)-C(42)	120.9(3)
C(40)-C(41)-H(41A)	119.6
C(42)-C(41)-H(41A)	119.6
C(37)-C(42)-C(41)	120.7(3)
C(37)-C(42)-H(42A)	119.6
C(41)-C(42)-H(42A)	119.6
C(26)-C(43)-C(44)	111.27(18)
C(26)-C(43)-C(30)	114.63(17)
C(44)-C(43)-C(30)	110.02(17)
C(26)-C(43)-H(43A)	106.8
C(44)-C(43)-H(43A)	106.8
C(30)-C(43)-H(43A)	106.8
N(3)-C(44)-C(43)	110.93(19)
N(3)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44A)	109.5
N(3)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	108.0
C(02)-O(02)-C(03)	117.1(3)

C(02)-C(01)-H(01A)	109.5
C(02)-C(01)-H(01B)	109.5
H(01A)-C(01)-H(01B)	109.5
C(02)-C(01)-H(01C)	109.5
H(01A)-C(01)-H(01C)	109.5
H(01B)-C(01)-H(01C)	109.5
O(01)-C(02)-O(02)	122.2(3)
O(01)-C(02)-C(01)	124.8(3)
O(02)-C(02)-C(01)	112.9(3)
C(04)-C(03)-O(02)	108.6(4)
C(04)-C(03)-H(03A)	110.0
O(02)-C(03)-H(03A)	110.0
C(04)-C(03)-H(03B)	110.0
O(02)-C(03)-H(03B)	110.0
H(03A)-C(03)-H(03B)	108.4
C(03)-C(04)-H(04A)	109.5
C(03)-C(04)-H(04B)	109.5
H(04A)-C(04)-H(04B)	109.5
C(03)-C(04)-H(04C)	109.5
H(04A)-C(04)-H(04C)	109.5
H(04B)-C(04)-H(04C)	109.5
C(05)-O(04)-C(07)	124.5(17)
C(05)-C(06)-H(06A)	109.5
C(05)-C(06)-H(06B)	109.5
H(06A)-C(06)-H(06B)	109.5
C(05)-C(06)-H(06C)	109.5
H(06A)-C(06)-H(06C)	109.5
H(06B)-C(06)-H(06C)	109.5
O(03)-C(05)-O(04)	96.2(17)
O(03)-C(05)-C(06)	118(2)
O(04)-C(05)-C(06)	129(2)
O(04)-C(07)-C(08)	105.7(12)
O(04)-C(07)-H(07A)	110.6
C(08)-C(07)-H(07A)	110.6
O(04)-C(07)-H(07B)	110.6
C(08)-C(07)-H(07B)	110.6
H(07A)-C(07)-H(07B)	108.7
C(07)-C(08)-H(08A)	109.5
C(07)-C(08)-H(08B)	109.5
H(08A)-C(08)-H(08B)	109.5
C(07)-C(08)-H(08C)	109.5
H(08A)-C(08)-H(08C)	109.5
H(08B)-C(08)-H(08C)	109.5
C(05')-O(04')-C(07')	128.4(12)

O(04')-C(05')-O(03')	105.9(12)
O(04')-C(05')-C(06')	123.0(17)
O(03')-C(05')-C(06')	120.0(13)
C(05')-C(06')-H(06D)	109.5
C(05')-C(06')-H(06E)	109.5
H(06D)-C(06')-H(06E)	109.5
C(05')-C(06')-H(06F)	109.5
H(06D)-C(06')-H(06F)	109.5
H(06E)-C(06')-H(06F)	109.5
O(04')-C(07')-C(08')	105.8(15)
O(04')-C(07')-H(07C)	110.6
C(08')-C(07')-H(07C)	110.6
O(04')-C(07')-H(07D)	110.6
C(08')-C(07')-H(07D)	110.6
H(07C)-C(07')-H(07D)	108.7
C(07')-C(08')-H(08D)	109.5
C(07')-C(08')-H(08E)	109.5
H(08D)-C(08')-H(08E)	109.5
C(07')-C(08')-H(08F)	109.5
H(08D)-C(08')-H(08F)	109.5
H(08E)-C(08')-H(08F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for z.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	103(1)	74(1)	65(1)	-33(1)	11(1)	-43(1)
Cl(2)	80(1)	72(1)	66(1)	2(1)	25(1)	-21(1)
O(1)	103(2)	84(2)	176(3)	-61(2)	-85(2)	16(1)
O(2)	79(1)	50(1)	102(2)	14(1)	-38(1)	-2(1)
O(3)	44(1)	46(1)	75(1)	-24(1)	0(1)	4(1)
N(1)	39(1)	44(1)	65(1)	-6(1)	-10(1)	-3(1)
N(2)	31(1)	49(1)	59(1)	-13(1)	-4(1)	5(1)
C(1)	49(1)	48(1)	49(1)	1(1)	6(1)	-8(1)
C(2)	64(2)	56(2)	44(1)	-14(1)	9(1)	-9(1)
C(3)	52(1)	44(1)	48(1)	-11(1)	0(1)	-10(1)
C(4)	36(1)	35(1)	42(1)	-5(1)	-4(1)	-1(1)

C(5)	50(1)	39(1)	40(1)	-6(1)	-2(1)	-8(1)
C(6)	55(1)	42(1)	53(2)	-2(1)	-2(1)	-14(1)
C(7)	37(1)	36(1)	48(1)	-3(1)	0(1)	2(1)
C(8)	33(1)	32(1)	44(1)	-7(1)	-2(1)	1(1)
C(9)	37(1)	35(1)	38(1)	0(1)	-4(1)	-4(1)
C(10)	43(1)	41(1)	42(1)	-6(1)	-4(1)	-2(1)
C(11)	66(2)	46(1)	45(1)	-9(1)	-9(1)	-13(1)
C(12)	64(2)	67(2)	63(2)	-12(1)	-14(1)	-26(1)
C(13)	41(1)	72(2)	66(2)	-10(1)	-10(1)	-13(1)
C(14)	37(1)	45(1)	44(1)	-2(1)	-4(1)	-3(1)
C(15)	35(1)	30(1)	49(1)	-1(1)	-3(1)	2(1)
C(16)	62(2)	43(1)	63(2)	-10(1)	5(1)	-13(1)
C(17)	68(2)	42(1)	85(2)	-3(1)	2(2)	-18(1)
C(18)	58(2)	49(2)	66(2)	15(1)	1(1)	-11(1)
C(19)	76(2)	64(2)	51(2)	2(1)	8(1)	-20(2)
C(20)	65(2)	50(1)	52(2)	-6(1)	3(1)	-17(1)
C(21)	33(1)	34(1)	42(1)	-7(1)	-3(1)	-4(1)
C(22)	36(1)	40(1)	47(1)	-3(1)	-4(1)	-2(1)
Cl(3)	75(1)	74(1)	66(1)	8(1)	18(1)	-22(1)
Cl(4)	68(1)	102(1)	58(1)	3(1)	-27(1)	-36(1)
O(4)	55(1)	133(2)	131(2)	-78(2)	-11(1)	24(1)
O(5)	83(2)	97(2)	104(2)	-60(2)	-22(1)	5(1)
O(6)	47(1)	40(1)	66(1)	-6(1)	-20(1)	3(1)
N(3)	42(1)	41(1)	76(2)	-20(1)	1(1)	-4(1)
N(4)	44(1)	26(1)	50(1)	0(1)	-5(1)	0(1)
C(23)	51(1)	47(1)	47(1)	-4(1)	9(1)	-8(1)
C(24)	60(2)	53(1)	37(1)	0(1)	-5(1)	-6(1)
C(25)	45(1)	47(1)	43(1)	-6(1)	-8(1)	-8(1)
C(26)	36(1)	35(1)	38(1)	-7(1)	-4(1)	-2(1)
C(27)	40(1)	51(1)	42(1)	-5(1)	-5(1)	-9(1)
C(28)	43(1)	58(2)	58(2)	-9(1)	1(1)	-15(1)
C(29)	37(1)	33(1)	41(1)	-3(1)	0(1)	0(1)
C(30)	37(1)	29(1)	39(1)	-3(1)	-4(1)	0(1)
C(31)	40(1)	34(1)	35(1)	-4(1)	-2(1)	-3(1)
C(32)	44(1)	36(1)	40(1)	-4(1)	1(1)	-6(1)
C(33)	66(2)	40(1)	70(2)	-12(1)	-9(1)	-14(1)
C(34)	66(2)	67(2)	71(2)	-23(2)	-15(2)	-21(2)
C(35)	55(2)	66(2)	57(2)	-11(1)	-21(1)	-6(1)
C(36)	51(1)	43(1)	45(1)	-4(1)	-11(1)	-3(1)
C(37)	43(1)	29(1)	53(1)	-4(1)	6(1)	-1(1)
C(38)	47(1)	52(2)	76(2)	-7(1)	2(1)	-13(1)
C(39)	57(2)	57(2)	125(3)	-15(2)	15(2)	-22(2)
C(40)	86(2)	53(2)	114(3)	5(2)	39(2)	-19(2)
C(41)	101(3)	63(2)	76(2)	16(2)	18(2)	-19(2)

C(42)	71(2)	51(2)	55(2)	5(1)	4(1)	-13(1)
C(43)	36(1)	33(1)	40(1)	-6(1)	-6(1)	-4(1)
C(44)	45(1)	34(1)	52(1)	-7(1)	-2(1)	1(1)
O(01)	247(4)	80(2)	96(2)	-17(2)	-45(2)	-42(2)
O(02)	128(2)	72(1)	84(2)	-5(1)	-42(2)	-17(1)
C(01)	104(3)	87(3)	90(3)	-6(2)	-31(2)	8(2)
C(02)	70(2)	65(2)	60(2)	-15(1)	-1(1)	-14(2)
C(03)	170(5)	104(3)	98(3)	19(3)	-54(3)	-18(3)
C(04)	177(6)	191(6)	121(4)	-23(4)	-77(4)	9(5)
O(03)	214(9)	104(5)	133(6)	30(4)	-9(6)	-70(5)
O(04)	121(6)	220(15)	112(8)	-102(9)	30(6)	-63(8)
C(06)	270(30)	142(14)	69(8)	-20(8)	6(17)	-30(17)
C(05)	230(20)	65(9)	160(20)	-7(10)	4(15)	-85(11)
C(07)	137(12)	96(8)	104(9)	-34(7)	-16(7)	-5(7)
C(08)	161(11)	91(7)	77(7)	-25(6)	10(7)	-19(8)
O(03')	169(7)	114(5)	167(7)	-23(5)	-13(6)	-62(5)
O(04')	227(16)	57(4)	119(8)	-22(4)	68(9)	-49(6)
C(05')	77(6)	50(6)	52(6)	-10(4)	2(4)	-13(5)
C(06')	97(7)	106(9)	107(14)	-32(7)	24(7)	-7(6)
C(07')	118(10)	142(12)	115(11)	-31(9)	18(8)	-44(8)
C(08')	240(20)	154(18)	157(13)	3(12)	-106(13)	-2(14)

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

	x	y	z	U(eq)
H(2B)	-12	4157	-474	58
H(2A)	1507	2469	2757	67
H(5A)	2408	970	274	52
H(6A)	1364	217	1292	60
H(10A)	3378	1258	-1410	52
H(11A)	2275	325	-1924	62
H(12A)	389	997	-1863	74
H(13A)	-445	2595	-1267	71
H(16A)	3322	4970	-407	68
H(17A)	4424	5890	-1256	78
H(18A)	5089	5354	-2544	72
H(19A)	4626	3900	-2986	78
H(20A)	3509	2985	-2152	66

H(21A)	3479	3280	407	44
H(22A)	4154	1227	-219	51
H(22B)	4687	2185	-571	51
H(4A)	924	-53	5386	50
H(24A)	2602	-1329	2277	62
H(27A)	4071	-2484	4776	54
H(28A)	4903	-1438	3808	63
H(33A)	2490	268	6261	69
H(34A)	3989	-638	6990	78
H(35A)	4544	-2498	7104	71
H(36A)	3589	-3504	6508	57
H(38A)	60	-3468	5231	71
H(39A)	-910	-4590	6016	96
H(40A)	-519	-5179	7353	106
H(41A)	794	-4605	7921	100
H(42A)	1762	-3474	7156	73
H(43A)	1674	-3403	4518	44
H(44A)	3696	-4130	5257	55
H(44B)	2715	-4694	5458	55
H(01A)	3400	6723	1558	147
H(01B)	3668	6049	787	147
H(01C)	2522	6172	1300	147
H(03A)	1097	8689	-366	151
H(03B)	2295	8652	-777	151
H(04A)	1205	8432	-1719	251
H(04B)	948	7425	-1175	251
H(04C)	2148	7372	-1579	251
H(06A)	7905	6425	3335	247
H(06B)	8721	7103	3508	247
H(06C)	7557	7695	3203	247
H(07A)	7452	7402	6000	138
H(07B)	6306	7535	5638	138
H(08A)	6249	9032	6361	168
H(08B)	6091	9407	5428	168
H(08C)	7239	9281	5773	168
H(06D)	8880	7567	3693	161
H(06E)	7982	7486	3124	161
H(06F)	8707	6430	3560	161
H(07C)	6259	7534	5591	148
H(07D)	5742	8736	5242	148
H(08D)	6589	8693	6455	281
H(08E)	7138	9306	5713	281
H(08F)	7722	8109	6014	281

Table 6. Torsion angles [deg] for z.

C(6)-C(1)-C(2)-C(3)	0.2(4)
Cl(2)-C(1)-C(2)-C(3)	179.1(2)
C(1)-C(2)-C(3)-C(4)	1.9(4)
C(1)-C(2)-C(3)-Cl(1)	-176.8(2)
C(2)-C(3)-C(4)-C(5)	-3.2(3)
Cl(1)-C(3)-C(4)-C(5)	175.47(18)
C(2)-C(3)-C(4)-C(21)	178.6(2)
Cl(1)-C(3)-C(4)-C(21)	-2.7(3)
C(3)-C(4)-C(5)-C(6)	2.6(3)
C(21)-C(4)-C(5)-C(6)	-179.2(2)
C(2)-C(1)-C(6)-C(5)	-0.8(4)
Cl(2)-C(1)-C(6)-C(5)	-179.73(19)
C(4)-C(5)-C(6)-C(1)	-0.6(4)
C(14)-N(2)-C(7)-O(3)	-175.5(2)
C(14)-N(2)-C(7)-C(8)	4.3(3)
O(3)-C(7)-C(8)-C(9)	175.5(2)
N(2)-C(7)-C(8)-C(9)	-4.4(2)
O(3)-C(7)-C(8)-C(15)	-64.4(3)
N(2)-C(7)-C(8)-C(15)	115.7(2)
O(3)-C(7)-C(8)-C(21)	54.1(3)
N(2)-C(7)-C(8)-C(21)	-125.72(19)
C(15)-C(8)-C(9)-C(10)	68.3(3)
C(7)-C(8)-C(9)-C(10)	-175.2(2)
C(21)-C(8)-C(9)-C(10)	-59.2(3)
C(15)-C(8)-C(9)-C(14)	-113.5(2)
C(7)-C(8)-C(9)-C(14)	3.0(2)
C(21)-C(8)-C(9)-C(14)	119.0(2)
C(14)-C(9)-C(10)-C(11)	-0.5(3)
C(8)-C(9)-C(10)-C(11)	177.6(2)
C(9)-C(10)-C(11)-C(12)	1.2(4)
C(10)-C(11)-C(12)-C(13)	-0.6(4)
C(11)-C(12)-C(13)-C(14)	-0.6(4)
C(12)-C(13)-C(14)-C(9)	1.4(4)
C(12)-C(13)-C(14)-N(2)	-176.9(3)
C(10)-C(9)-C(14)-C(13)	-0.8(4)
C(8)-C(9)-C(14)-C(13)	-179.3(2)
C(10)-C(9)-C(14)-N(2)	177.7(2)
C(8)-C(9)-C(14)-N(2)	-0.7(3)
C(7)-N(2)-C(14)-C(13)	176.1(2)
C(7)-N(2)-C(14)-C(9)	-2.4(3)

C(9)-C(8)-C(15)-C(20)	-15.6(3)
C(7)-C(8)-C(15)-C(20)	-127.4(2)
C(21)-C(8)-C(15)-C(20)	115.0(2)
C(9)-C(8)-C(15)-C(16)	165.9(2)
C(7)-C(8)-C(15)-C(16)	54.1(3)
C(21)-C(8)-C(15)-C(16)	-63.5(3)
C(20)-C(15)-C(16)-C(17)	-1.0(4)
C(8)-C(15)-C(16)-C(17)	177.6(2)
C(15)-C(16)-C(17)-C(18)	0.0(4)
C(16)-C(17)-C(18)-C(19)	0.5(4)
C(17)-C(18)-C(19)-C(20)	-0.1(4)
C(16)-C(15)-C(20)-C(19)	1.4(4)
C(8)-C(15)-C(20)-C(19)	-177.2(2)
C(18)-C(19)-C(20)-C(15)	-0.9(4)
C(5)-C(4)-C(21)-C(22)	-58.5(3)
C(3)-C(4)-C(21)-C(22)	119.6(2)
C(5)-C(4)-C(21)-C(8)	67.7(3)
C(3)-C(4)-C(21)-C(8)	-114.2(2)
C(9)-C(8)-C(21)-C(4)	-59.2(2)
C(15)-C(8)-C(21)-C(4)	171.03(16)
C(7)-C(8)-C(21)-C(4)	52.8(2)
C(9)-C(8)-C(21)-C(22)	67.4(2)
C(15)-C(8)-C(21)-C(22)	-62.4(2)
C(7)-C(8)-C(21)-C(22)	179.39(18)
O(2)-N(1)-C(22)-C(21)	135.8(2)
O(1)-N(1)-C(22)-C(21)	-46.6(3)
C(4)-C(21)-C(22)-N(1)	-67.3(2)
C(8)-C(21)-C(22)-N(1)	164.67(18)
C(28)-C(23)-C(24)-C(25)	1.3(4)
Cl(3)-C(23)-C(24)-C(25)	-178.94(18)
C(23)-C(24)-C(25)-C(26)	-0.2(4)
C(23)-C(24)-C(25)-Cl(4)	-179.26(19)
C(24)-C(25)-C(26)-C(27)	-1.4(3)
Cl(4)-C(25)-C(26)-C(27)	177.60(17)
C(4)-C(25)-C(26)-C(43)	-178.7(2)
Cl(4)-C(25)-C(26)-C(43)	0.4(3)
C(25)-C(26)-C(27)-C(28)	2.0(3)
C(43)-C(26)-C(27)-C(28)	179.3(2)
C(24)-C(23)-C(28)-C(27)	-0.8(4)
Cl(3)-C(23)-C(28)-C(27)	179.51(18)
C(26)-C(27)-C(28)-C(23)	-1.0(4)
C(32)-N(4)-C(29)-O(6)	179.0(2)
C(32)-N(4)-C(29)-C(30)	-1.5(2)
O(6)-C(29)-C(30)-C(31)	-179.0(2)

N(4)-C(29)-C(30)-C(31)	1.5(2)
O(6)-C(29)-C(30)-C(37)	-57.1(3)
N(4)-C(29)-C(30)-C(37)	123.46(19)
O(6)-C(29)-C(30)-C(43)	61.5(3)
N(4)-C(29)-C(30)-C(43)	-117.94(19)
C(37)-C(30)-C(31)-C(36)	61.2(3)
C(29)-C(30)-C(31)-C(36)	179.6(2)
C(43)-C(30)-C(31)-C(36)	-66.3(3)
C(37)-C(30)-C(31)-C(32)	-119.5(2)
C(29)-C(30)-C(31)-C(32)	-1.0(2)
C(43)-C(30)-C(31)-C(32)	113.0(2)
C(36)-C(31)-C(32)-C(33)	-0.3(3)
C(30)-C(31)-C(32)-C(33)	-179.7(2)
C(36)-C(31)-C(32)-N(4)	179.7(2)
C(30)-C(31)-C(32)-N(4)	0.2(2)
C(29)-N(4)-C(32)-C(33)	-179.2(2)
C(29)-N(4)-C(32)-C(31)	0.9(3)
C(31)-C(32)-C(33)-C(34)	-0.1(4)
N(4)-C(32)-C(33)-C(34)	-180.0(2)
C(32)-C(33)-C(34)-C(35)	0.5(4)
C(33)-C(34)-C(35)-C(36)	-0.6(5)
C(32)-C(31)-C(36)-C(35)	0.2(3)
C(30)-C(31)-C(36)-C(35)	179.5(2)
C(34)-C(35)-C(36)-C(31)	0.2(4)
C(31)-C(30)-C(37)-C(42)	-7.2(3)
C(29)-C(30)-C(37)-C(42)	-120.5(2)
C(43)-C(30)-C(37)-C(42)	122.6(2)
C(31)-C(30)-C(37)-C(38)	173.7(2)
C(29)-C(30)-C(37)-C(38)	60.4(3)
C(43)-C(30)-C(37)-C(38)	-56.4(3)
C(42)-C(37)-C(38)-C(39)	-0.8(4)
C(30)-C(37)-C(38)-C(39)	178.3(2)
C(37)-C(38)-C(39)-C(40)	-0.3(4)
C(38)-C(39)-C(40)-C(41)	1.1(5)
C(39)-C(40)-C(41)-C(42)	-0.8(5)
C(38)-C(37)-C(42)-C(41)	1.1(4)
C(30)-C(37)-C(42)-C(41)	-177.9(2)
C(40)-C(41)-C(42)-C(37)	-0.3(5)
C(27)-C(26)-C(43)-C(44)	-54.7(3)
C(25)-C(26)-C(43)-C(44)	122.4(2)
C(27)-C(26)-C(43)-C(30)	71.0(3)
C(25)-C(26)-C(43)-C(30)	-111.9(2)
C(31)-C(30)-C(43)-C(26)	-58.1(2)
C(37)-C(30)-C(43)-C(26)	171.55(17)

C(29)-C(30)-C(43)-C(26)	52.6(2)
C(31)-C(30)-C(43)-C(44)	68.1(2)
C(37)-C(30)-C(43)-C(44)	-62.2(2)
C(29)-C(30)-C(43)-C(44)	178.88(18)
O(4)-N(3)-C(44)-C(43)	145.2(3)
O(5)-N(3)-C(44)-C(43)	-33.7(3)
C(26)-C(43)-C(44)-N(3)	-61.6(2)
C(30)-C(43)-C(44)-N(3)	170.26(18)
C(03)-O(02)-C(02)-O(01)	3.7(6)
C(03)-O(02)-C(02)-C(01)	-178.1(4)
C(02)-O(02)-C(03)-C(04)	170.2(4)
C(07)-O(04)-C(05)-O(03)	-49(3)
C(07)-O(04)-C(05)-C(06)	177(2)
C(05)-O(04)-C(07)-C(08)	-154(2)
C(07')-O(04')-C(05')-O(03')	42(2)
C(07')-O(04')-C(05')-C(06')	-174.1(18)
C(05')-O(04')-C(07')-C(08')	119.6(19)

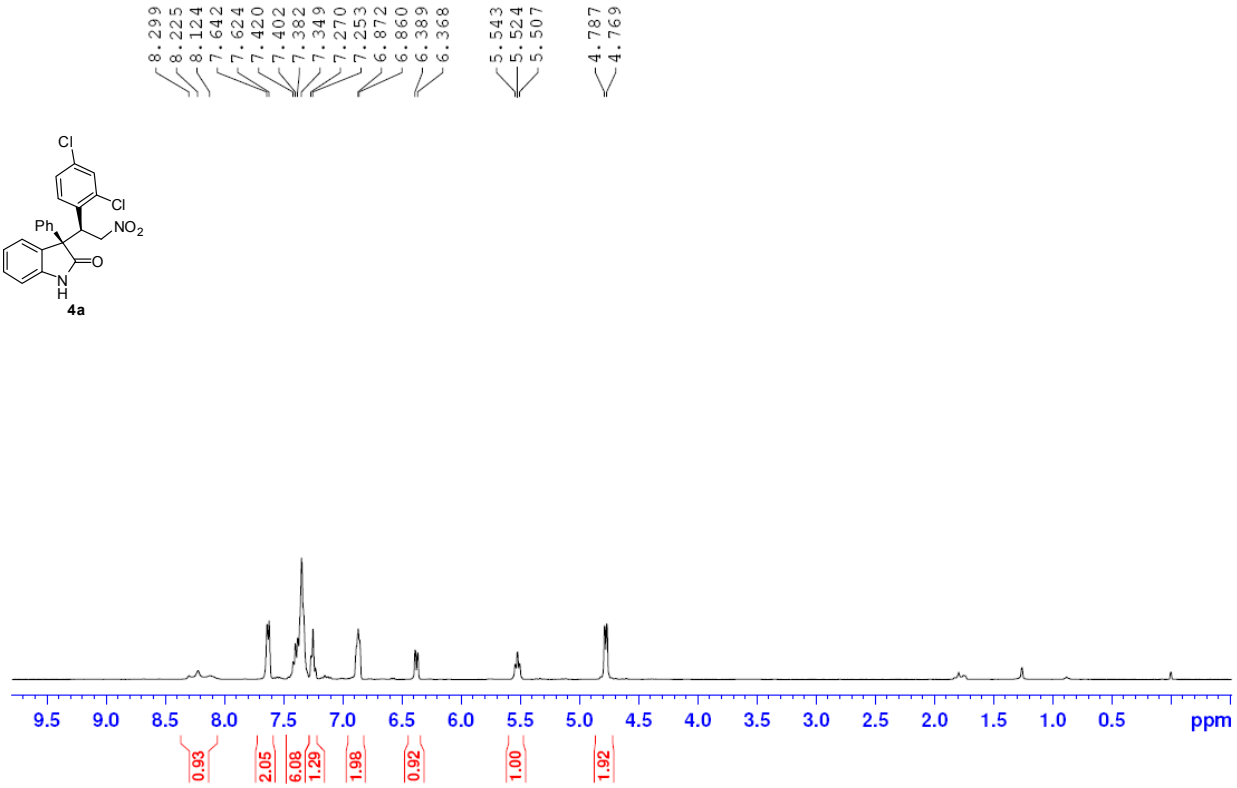
Symmetry transformations used to generate equivalent atoms:

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

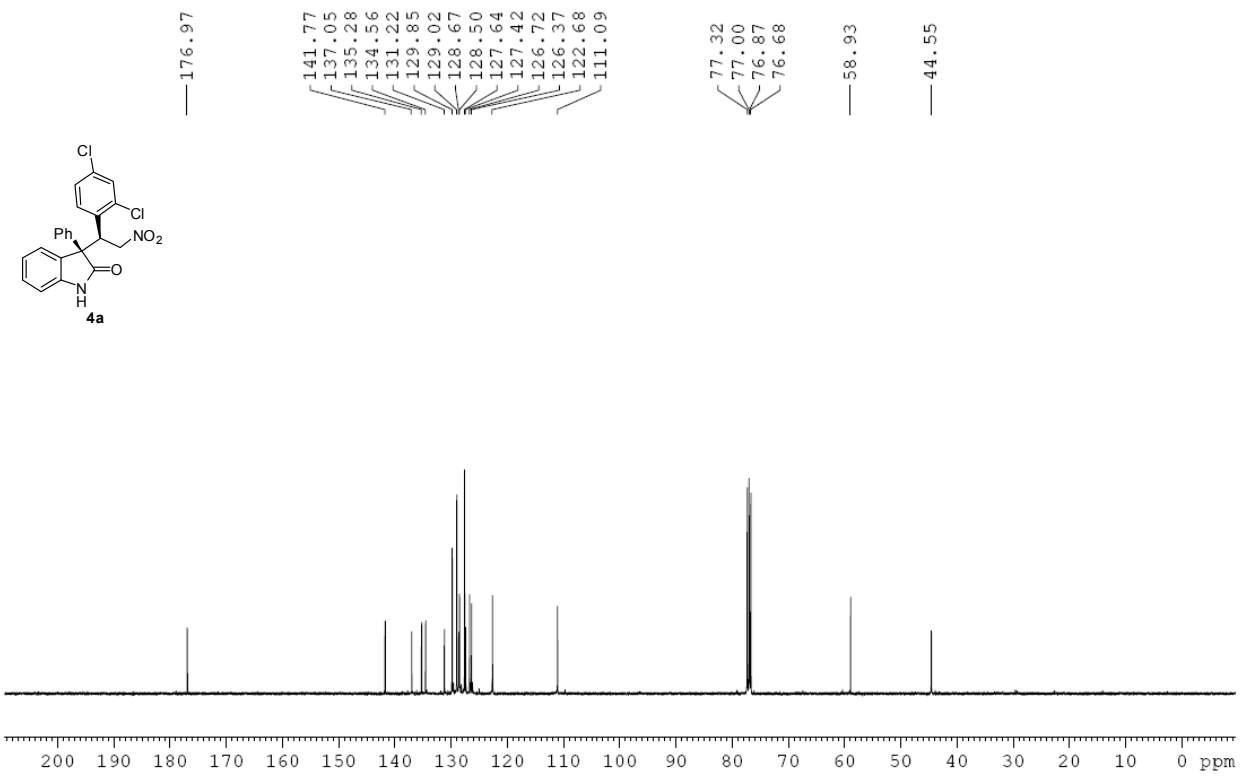
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2B)...O(3)#1	0.86	2.04	2.891(2)	167.9
N(4)-H(4A)...O(6)#2	0.86	2.06	2.904(2)	168.7

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z #2 -x,-y,-z+1

DIM-DE-55 H



DIM-DE-55 C



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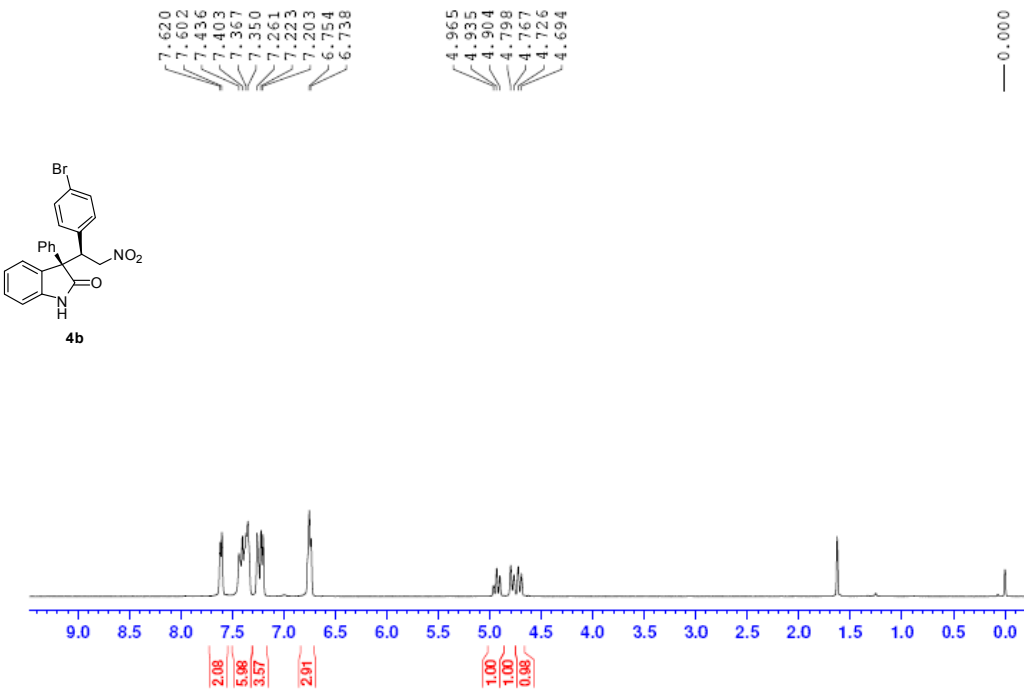

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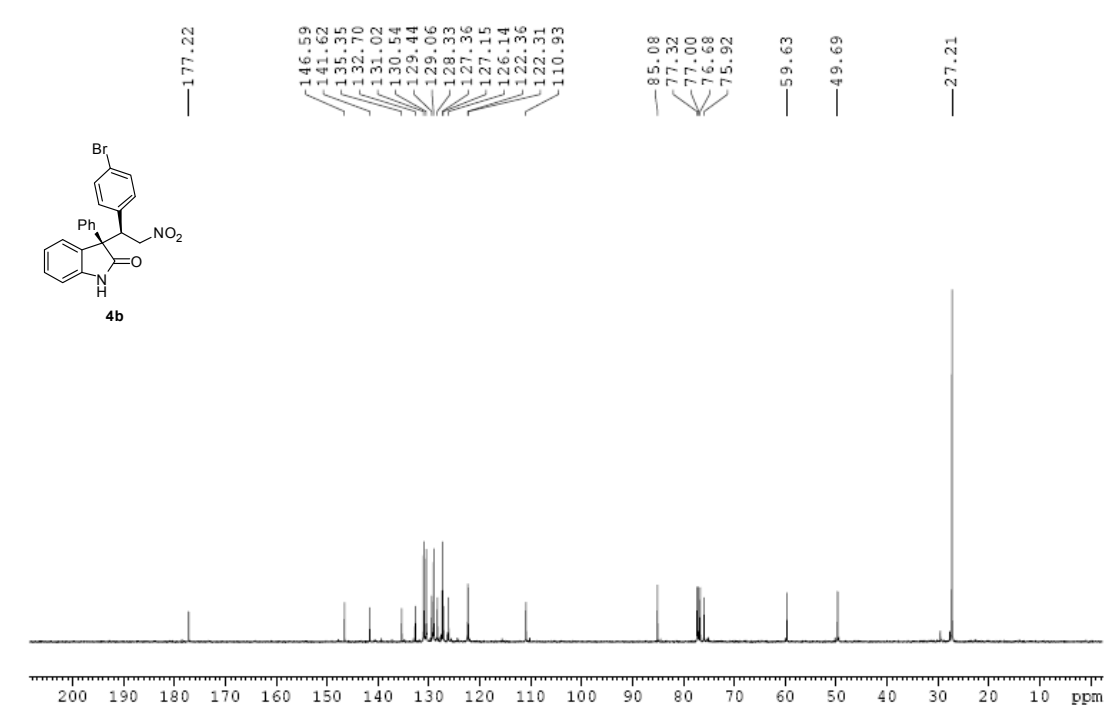

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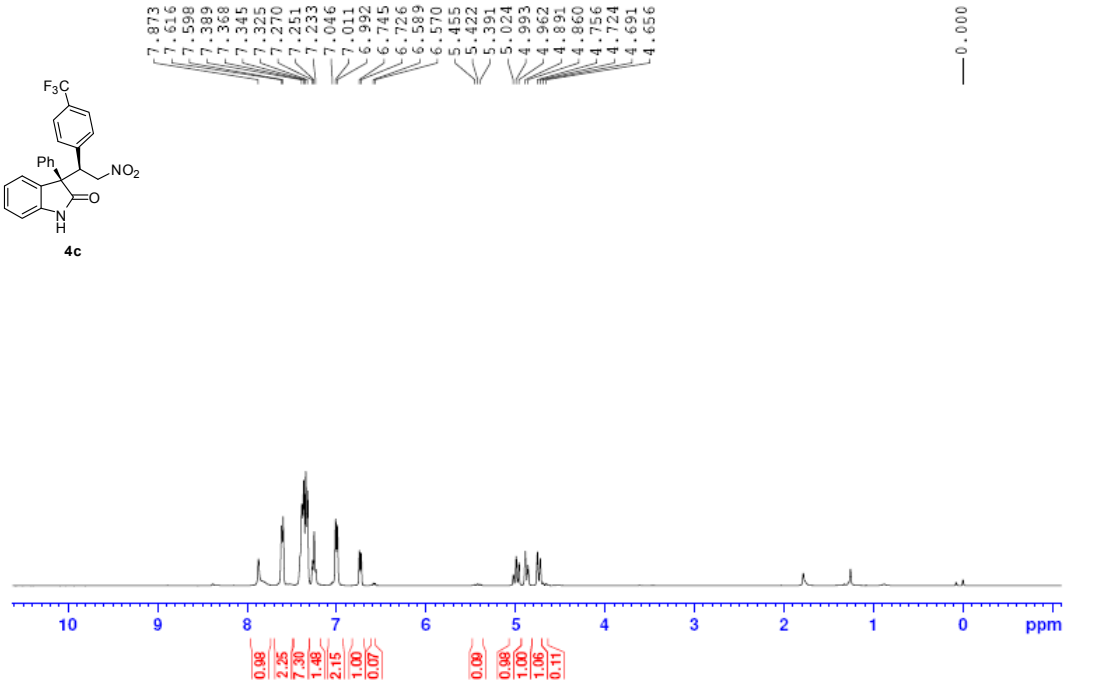

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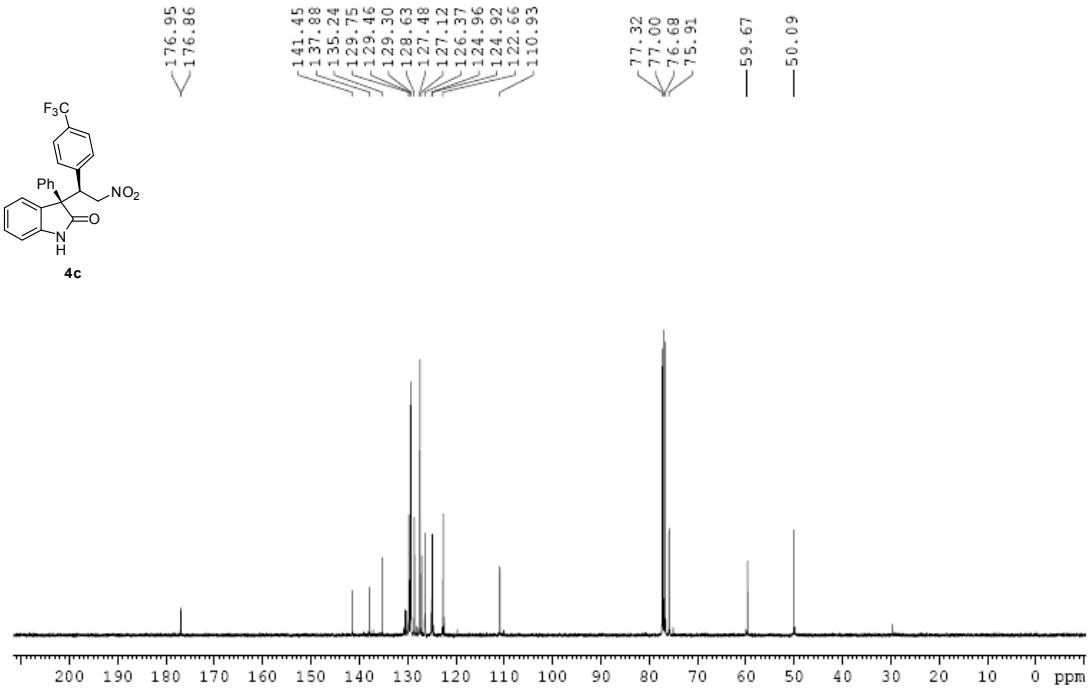
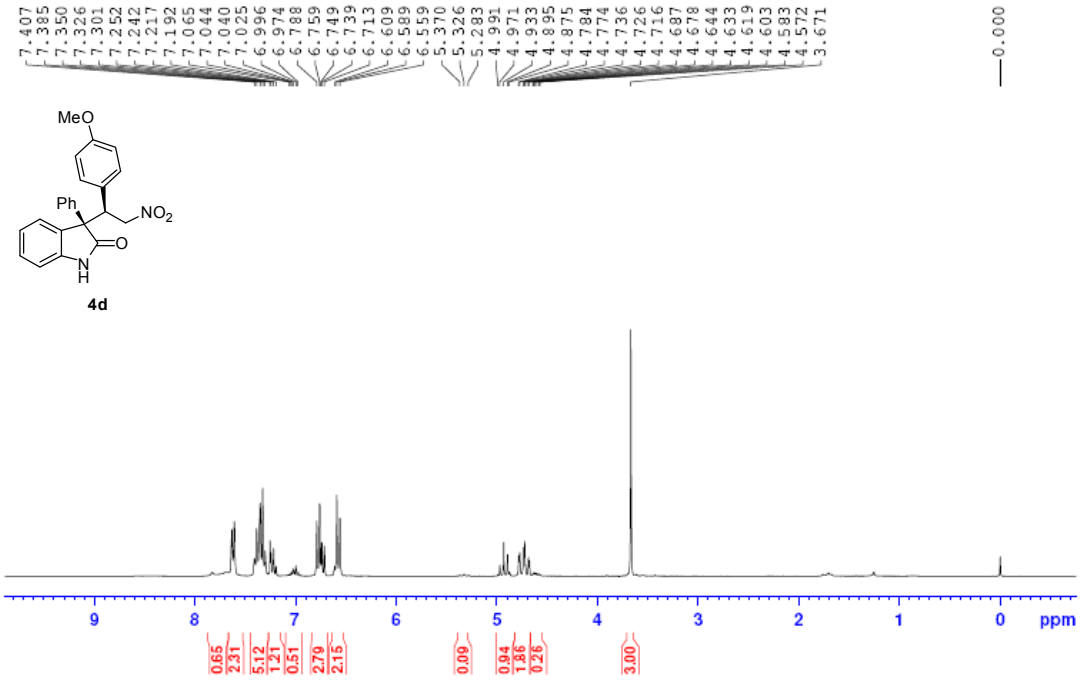
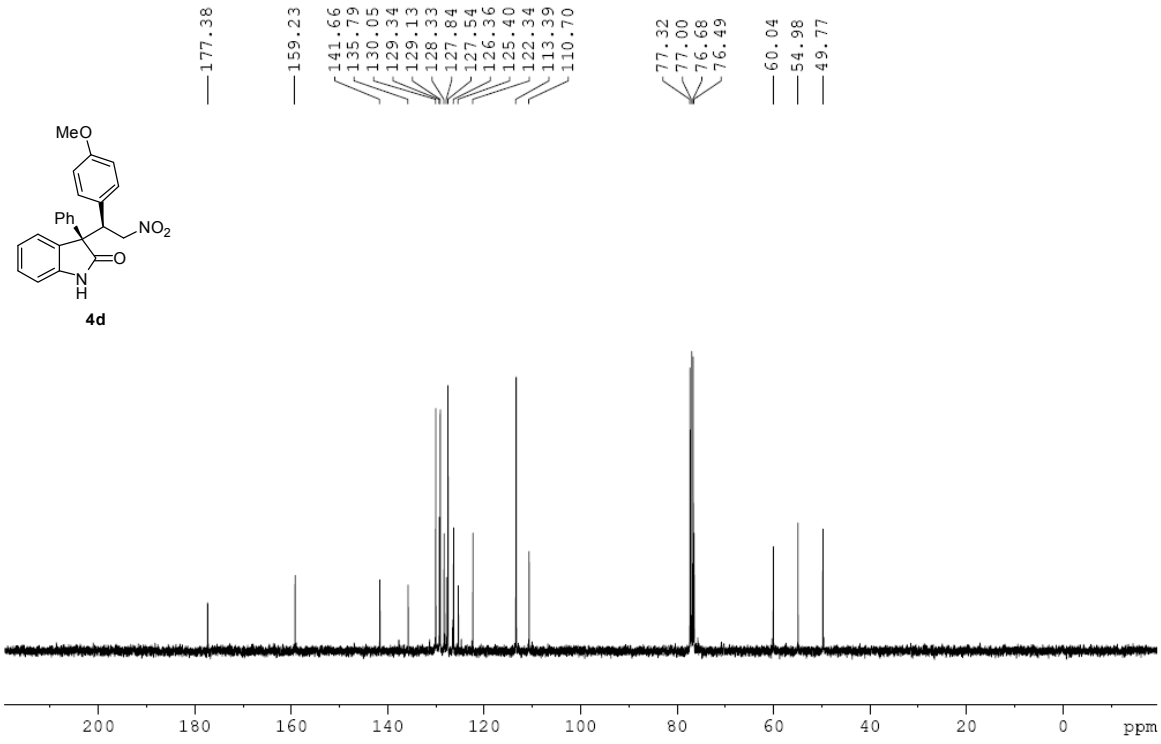


DIM-DD-138 H



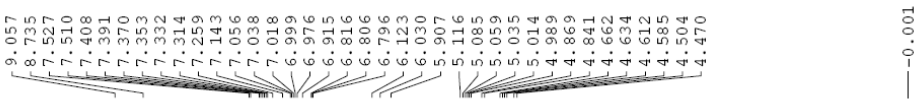
4d

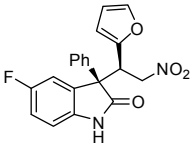
DIM-DD-138 C



4d

DIM-DC-85 H





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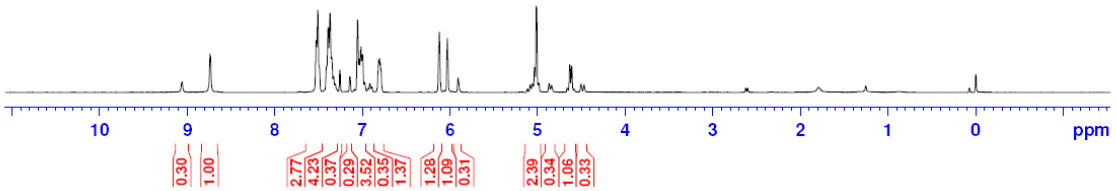

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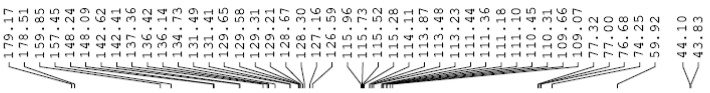

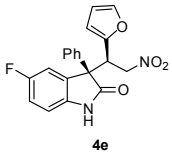

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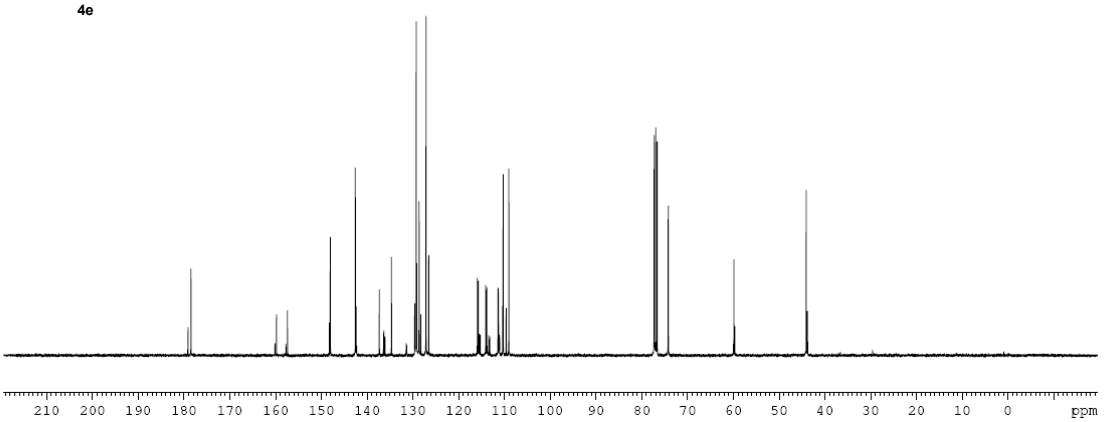
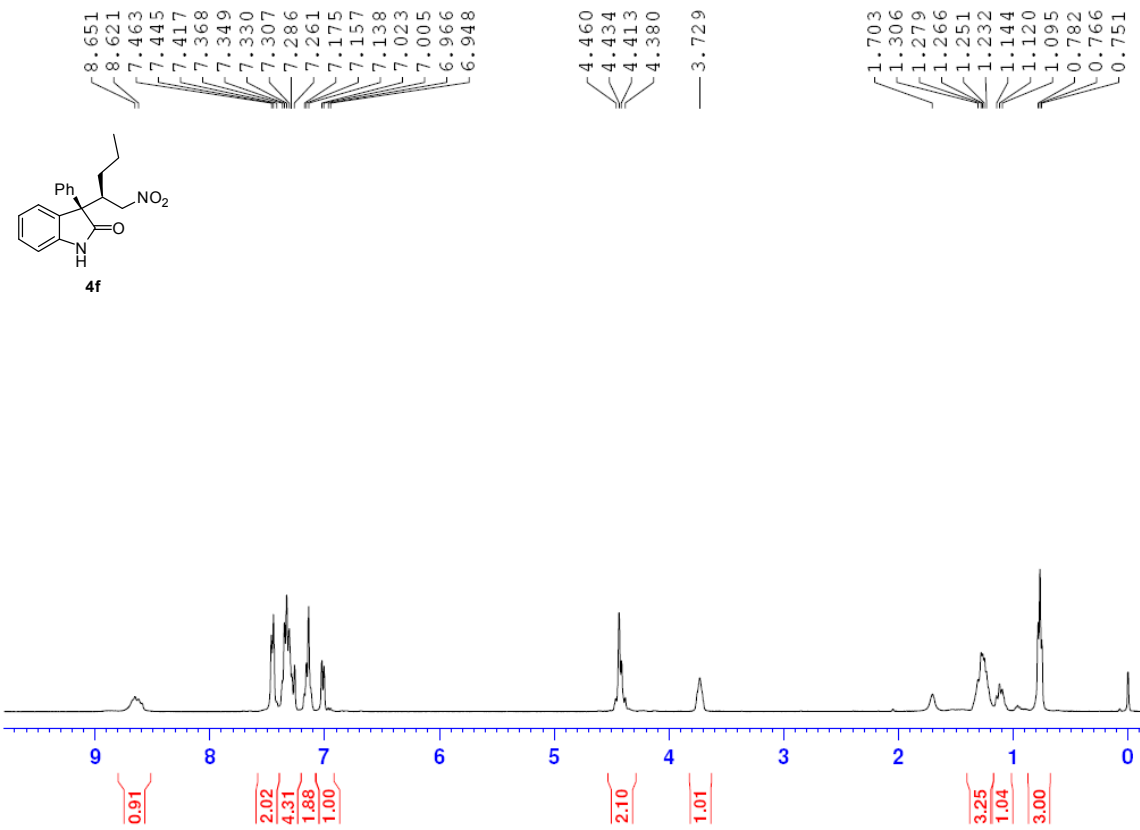
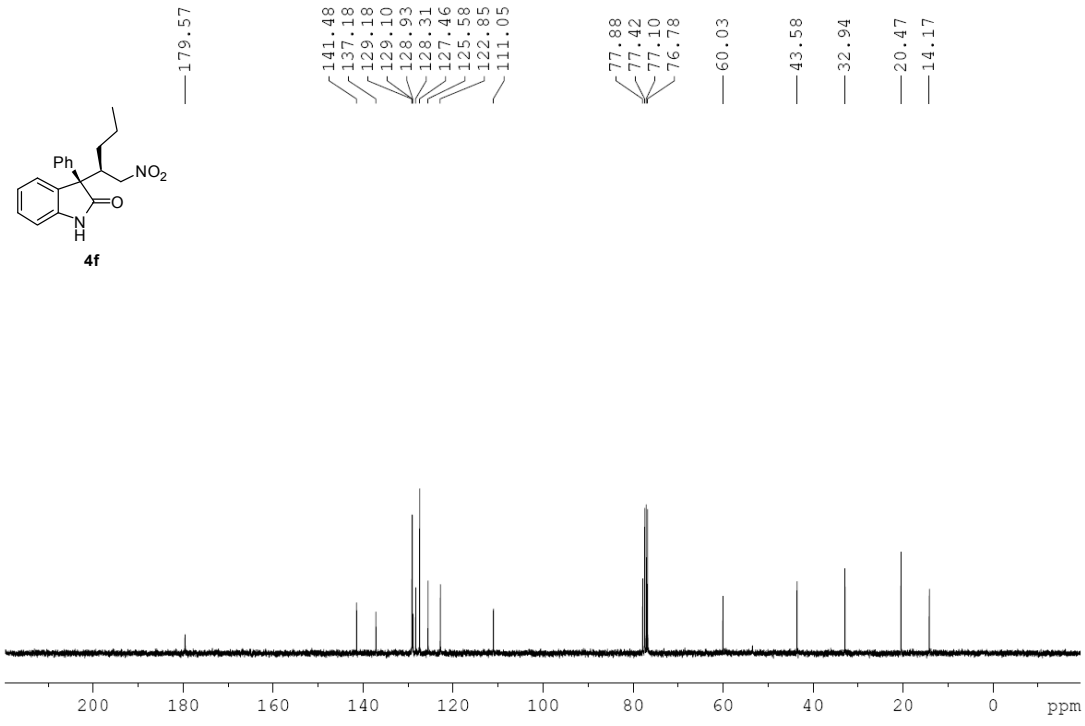


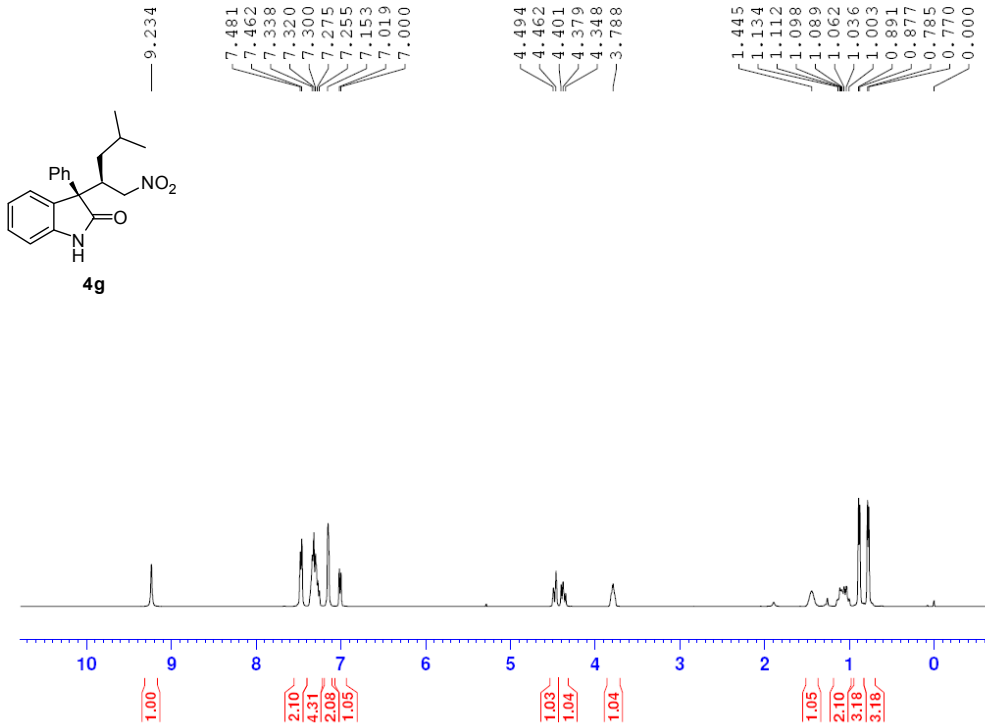
DIM-DC-104 H



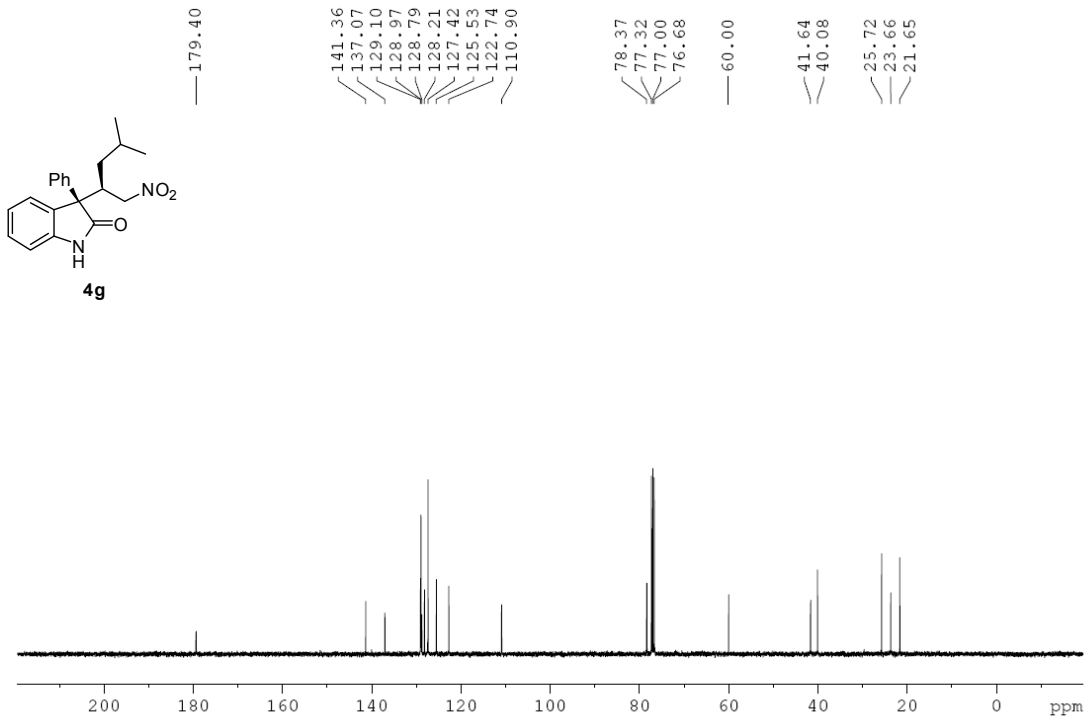
DIM-DC-104 C



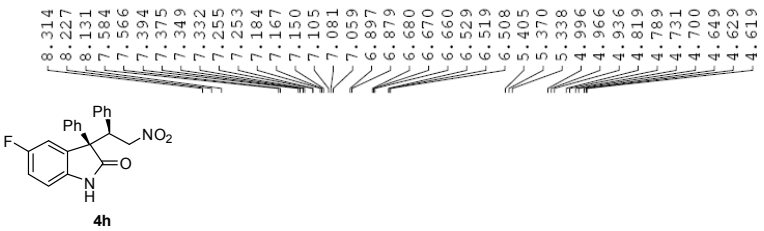
DIM-DC-105 H



DIM-DC-105 C



DIM-DC-94 H



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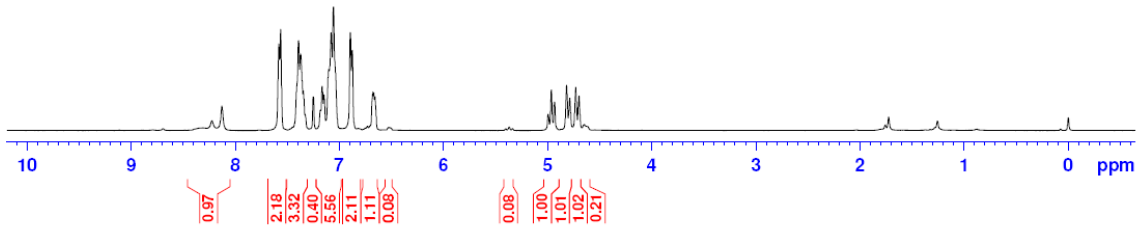

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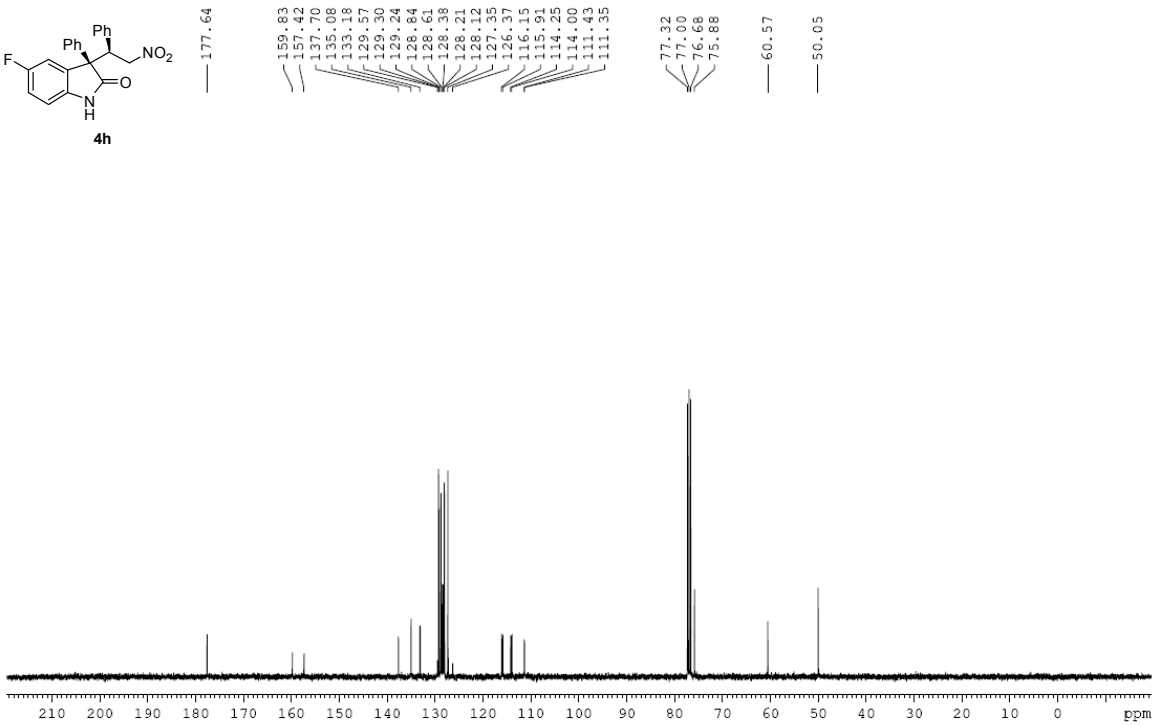
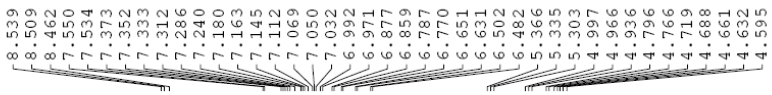
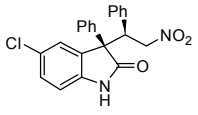
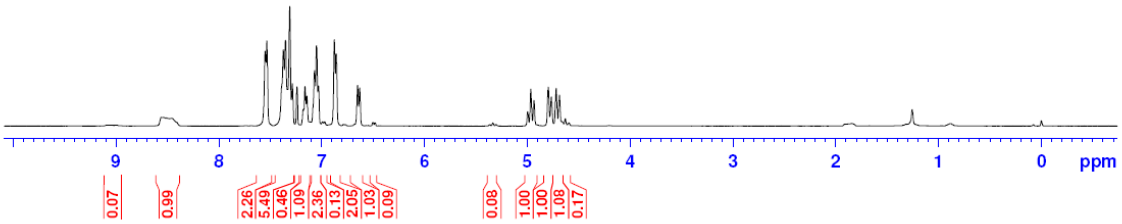


DIM-DC-95 H

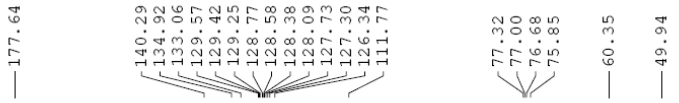


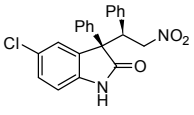


4i



DIM-DC-95 C





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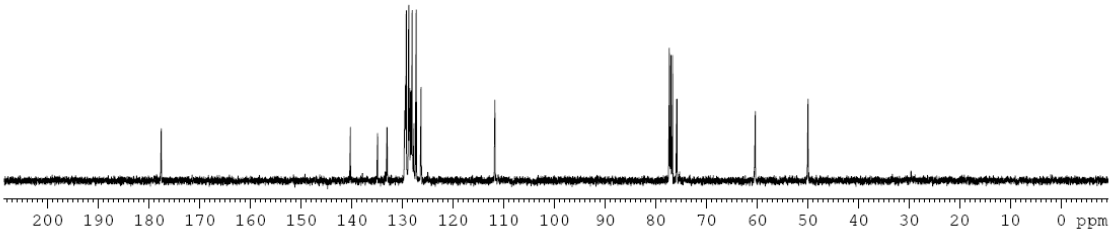
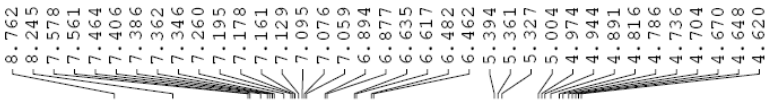
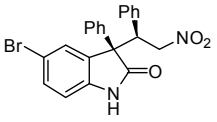


DIM-DE-57 H





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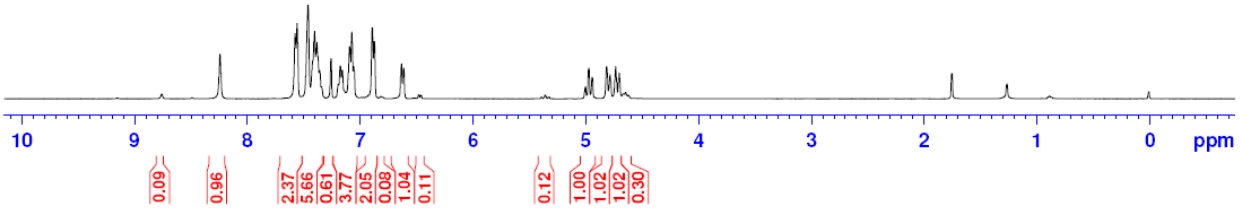

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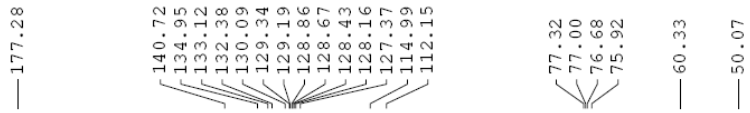

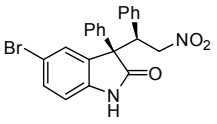

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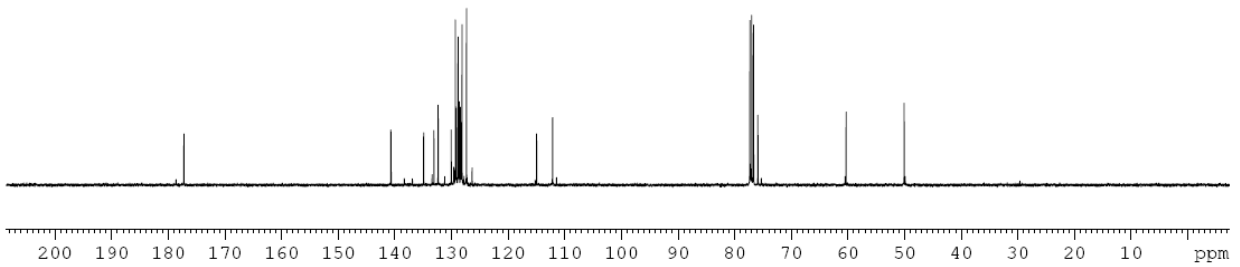
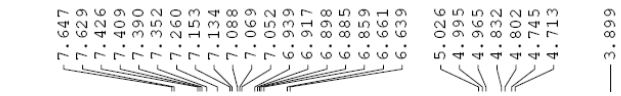
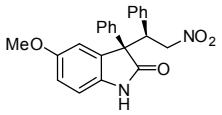


DIM-DE-28 H





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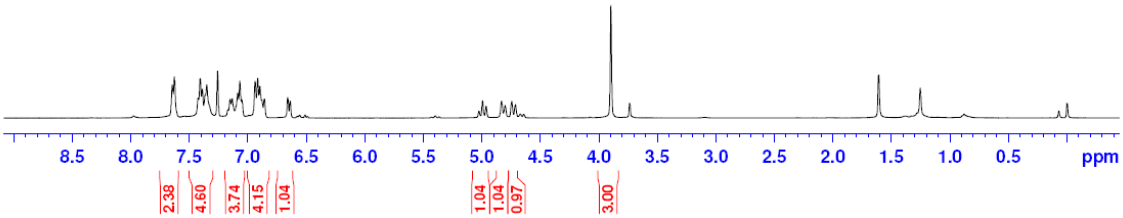

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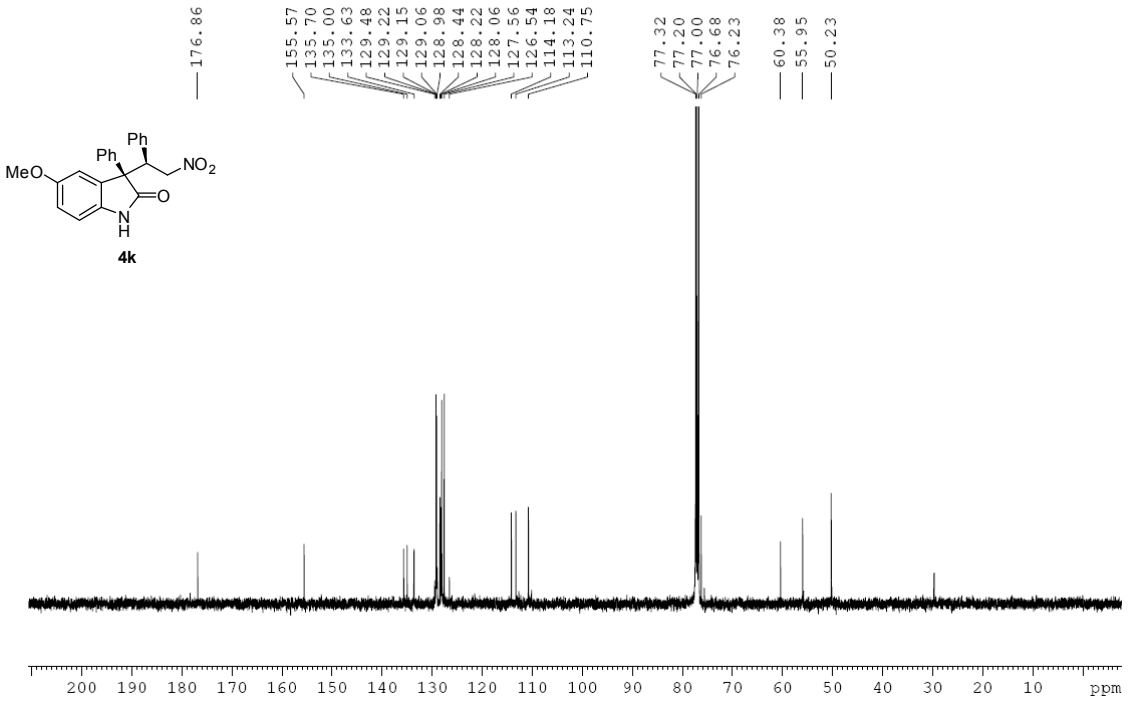

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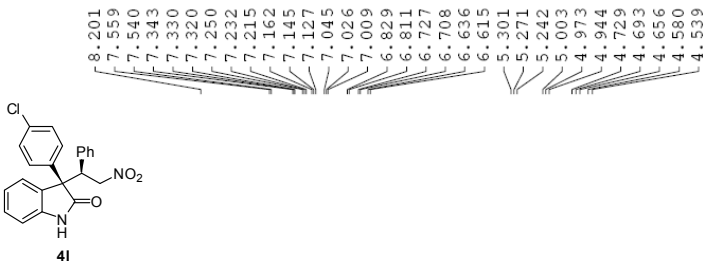
DIM-DC-98 H



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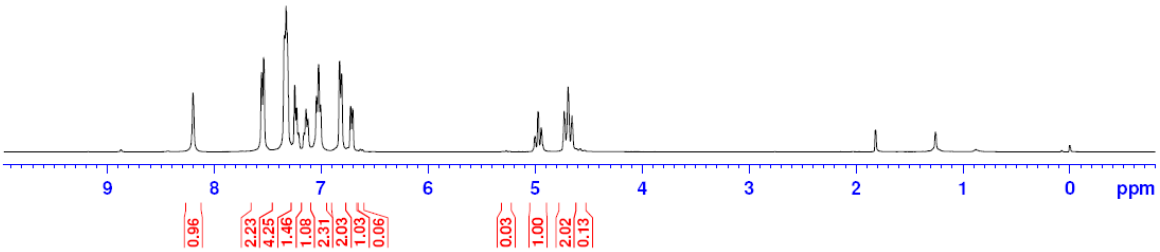

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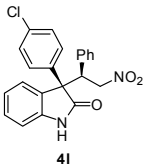

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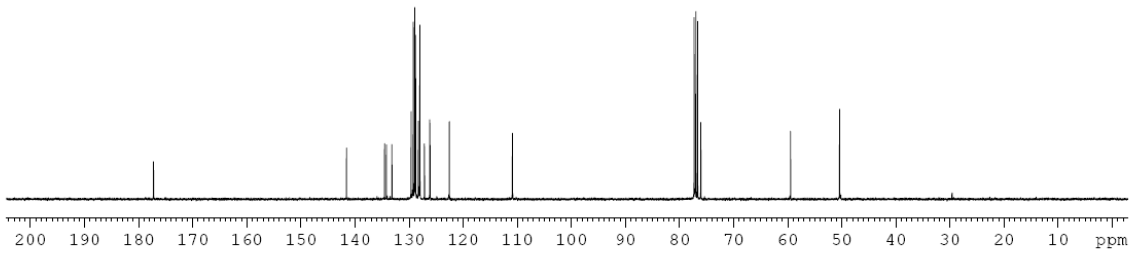
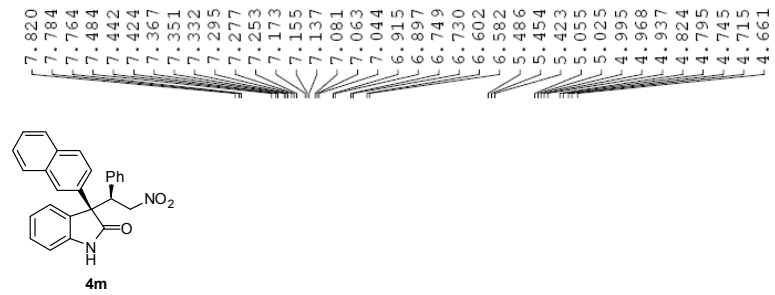


DIM-DE-54 H



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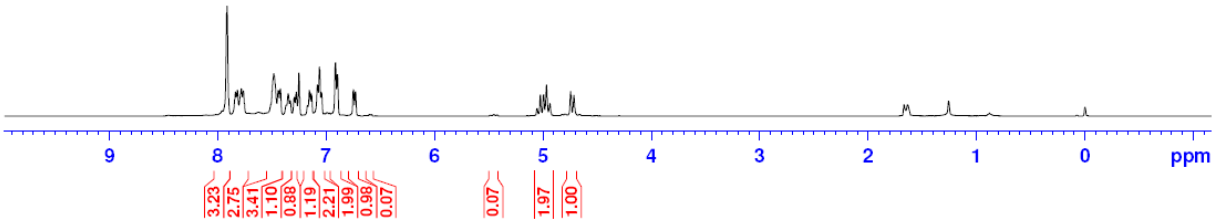
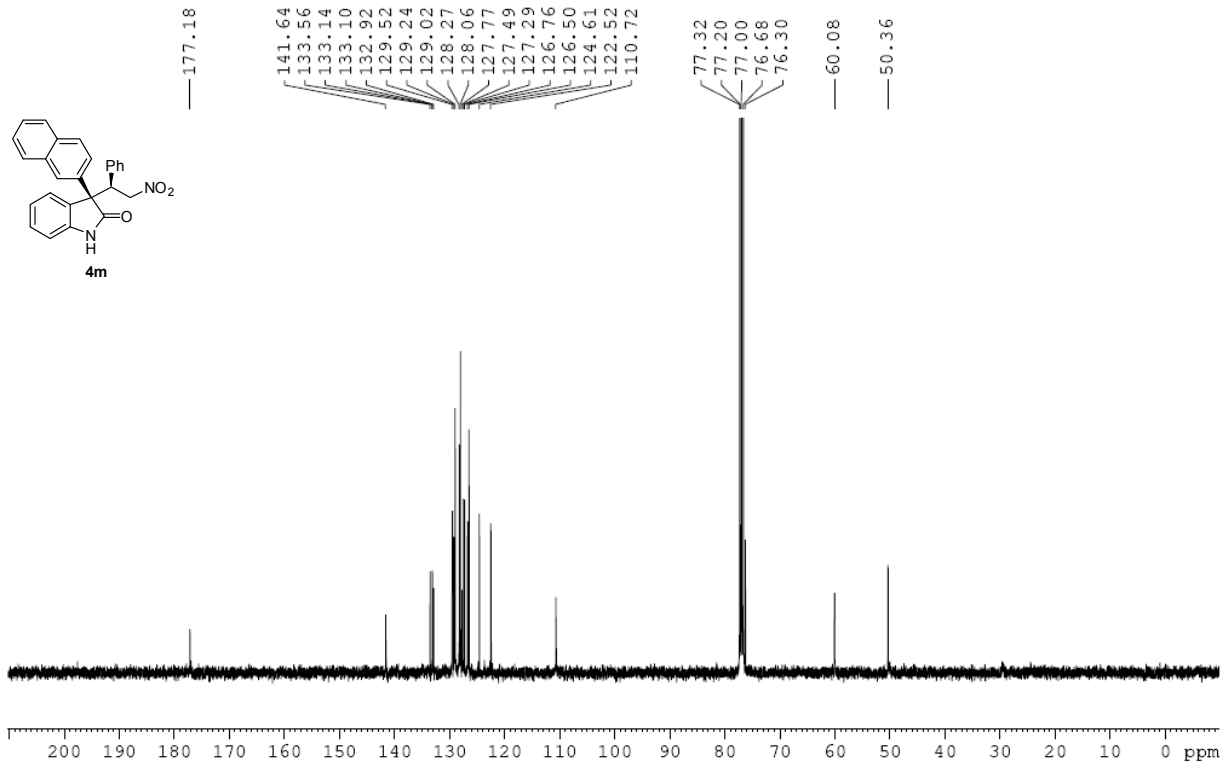
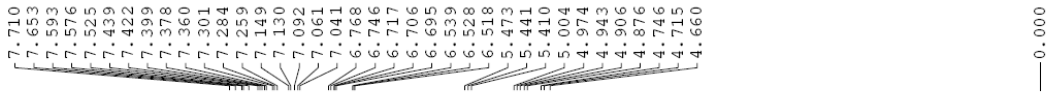


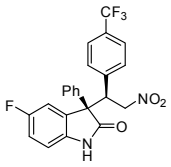
DIM-DE-54 C



4m

DIM-DC-84 H





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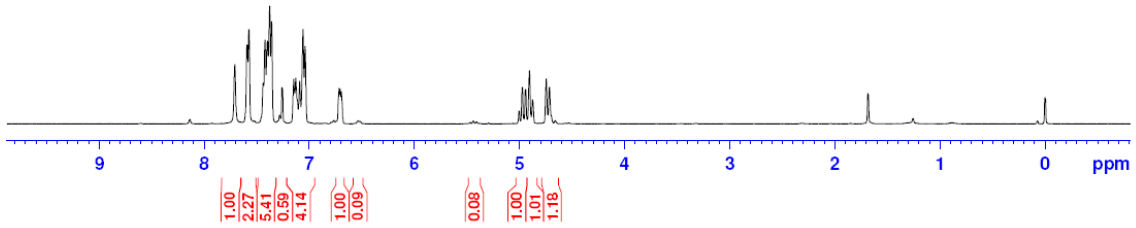
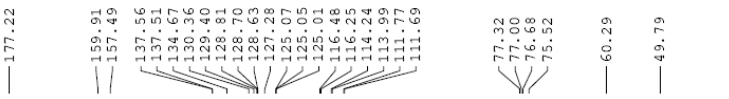
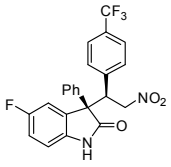


DIM-DC-84 C





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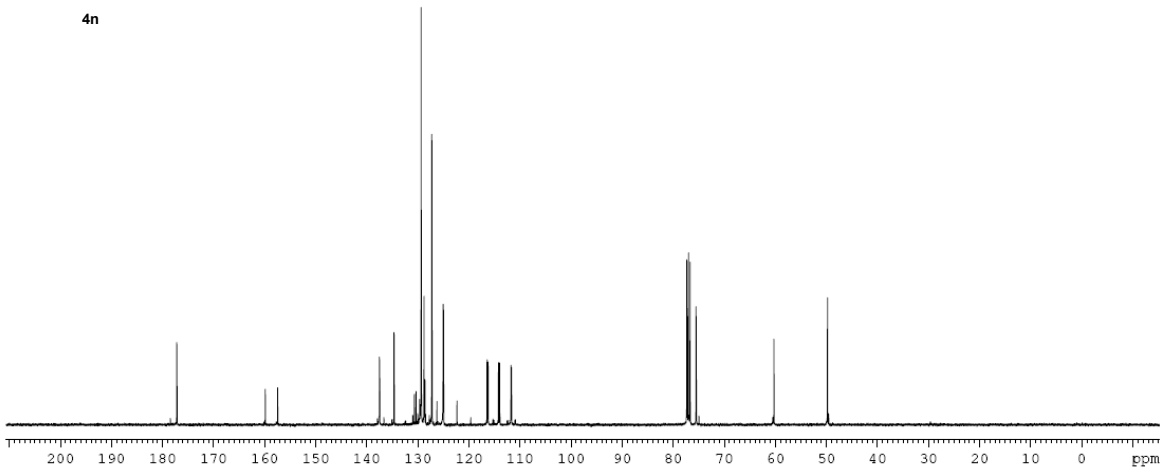
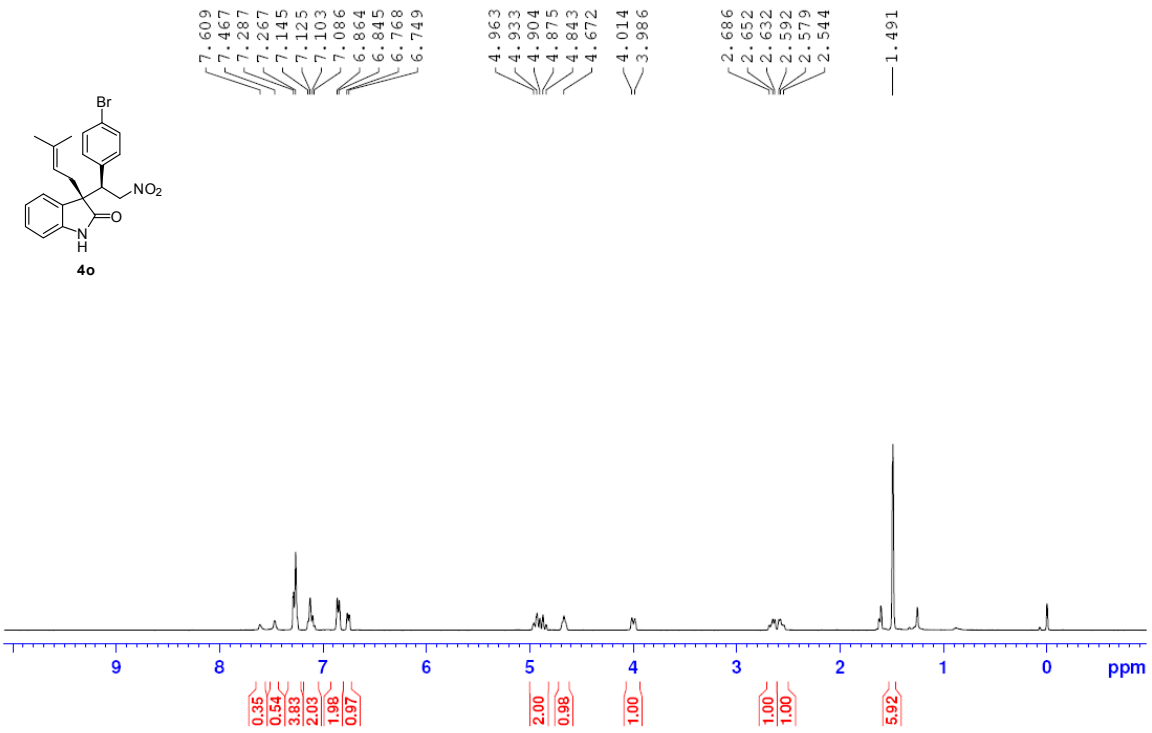
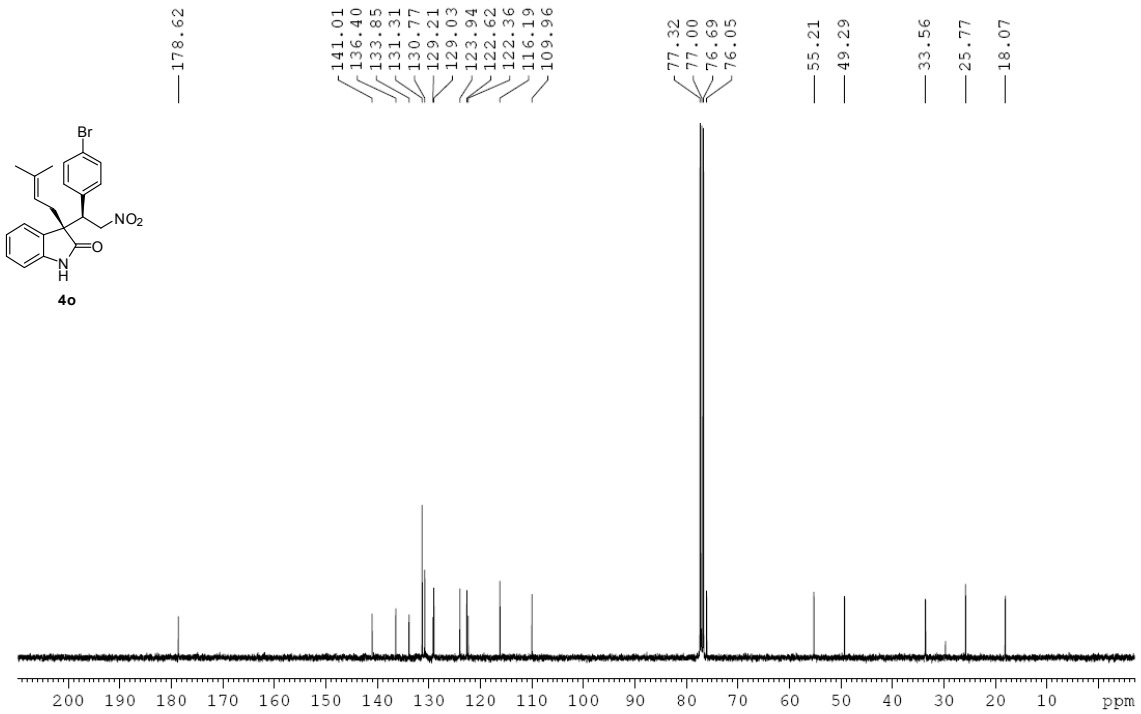


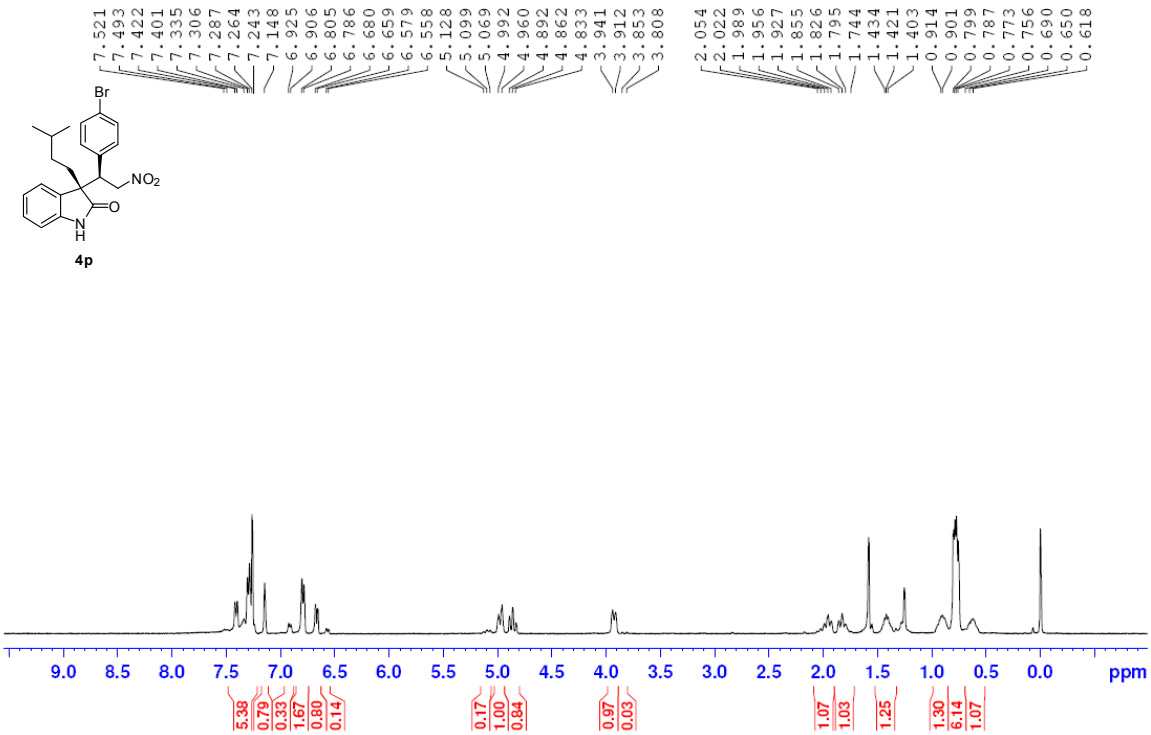
DIM-DD-51 H



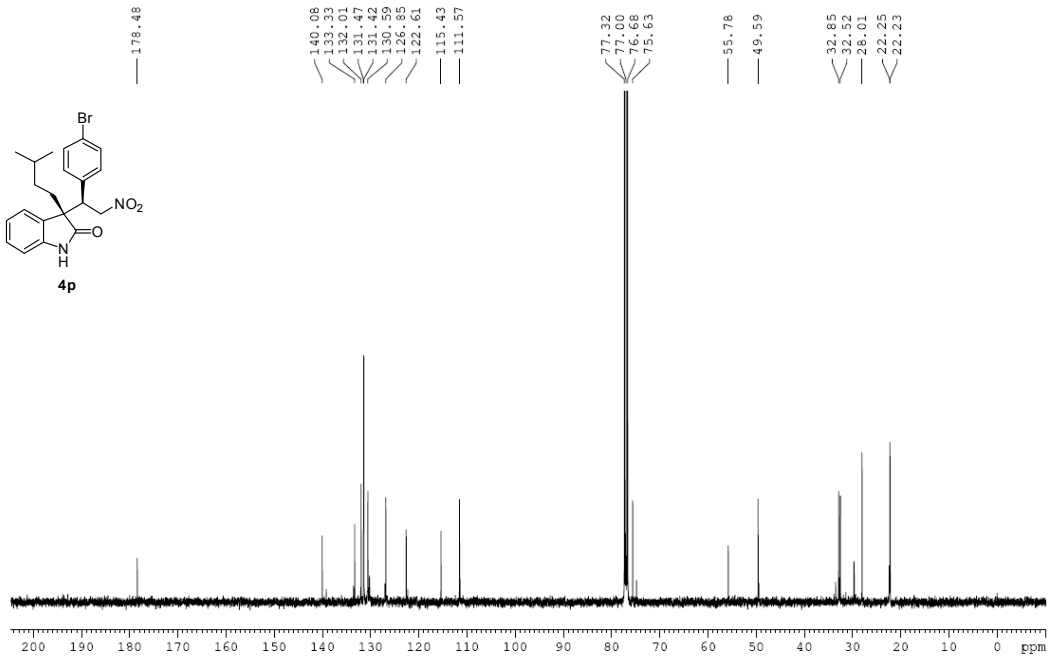
DIM-DD-51 C



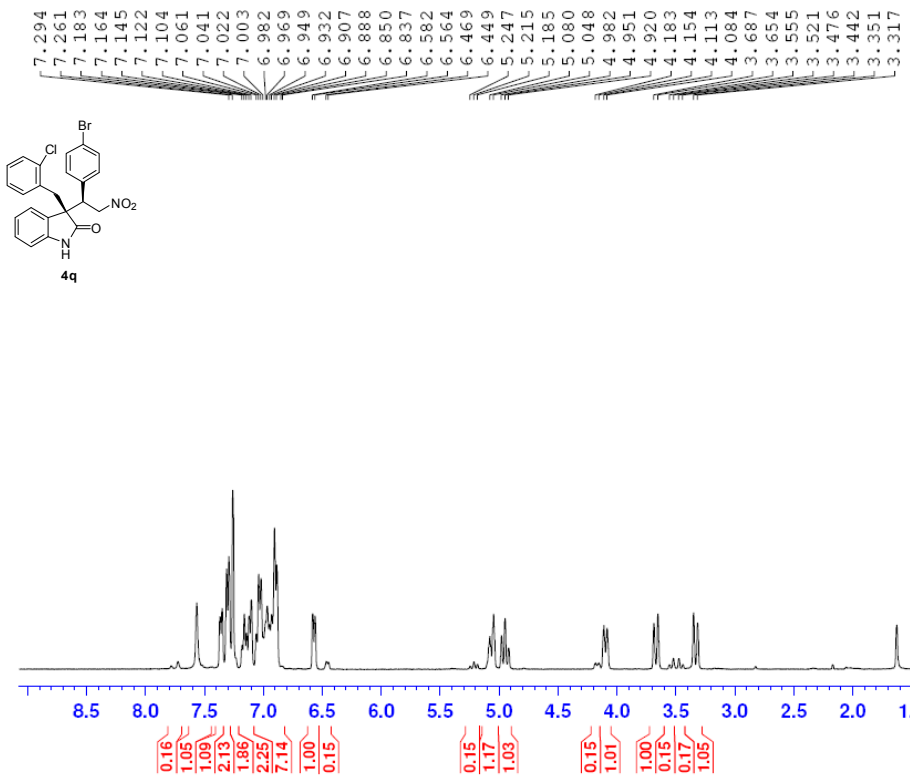
DIM-DD-12 H



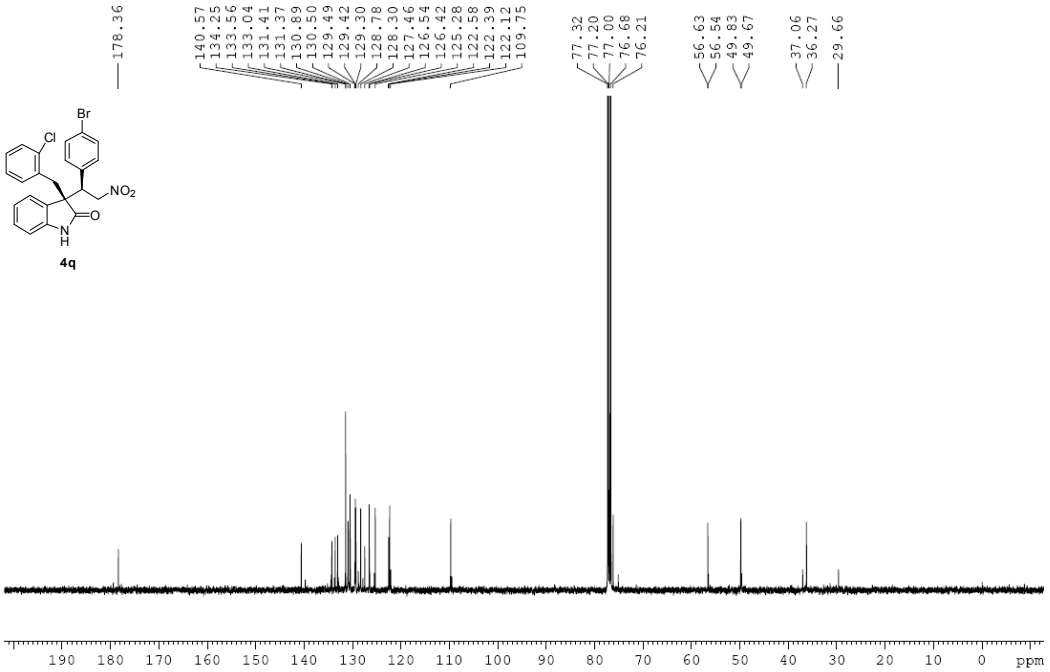
DIM-DD-12 C



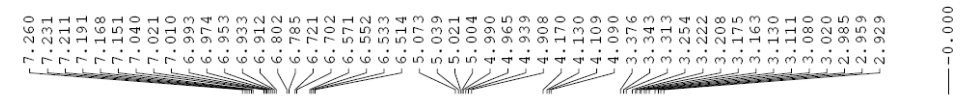
DIM-DD-65 H

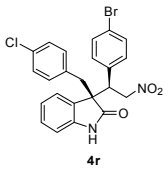


DIM-DD-65 C

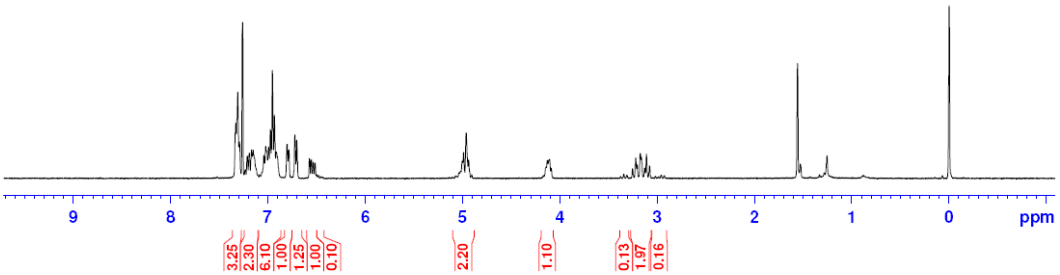


DIM-DC-134 H

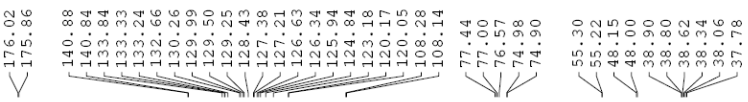


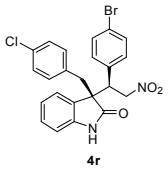


4r

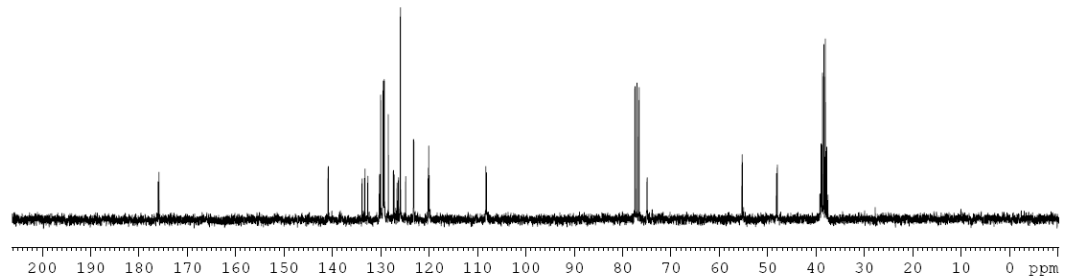


DIM-DC-134 C

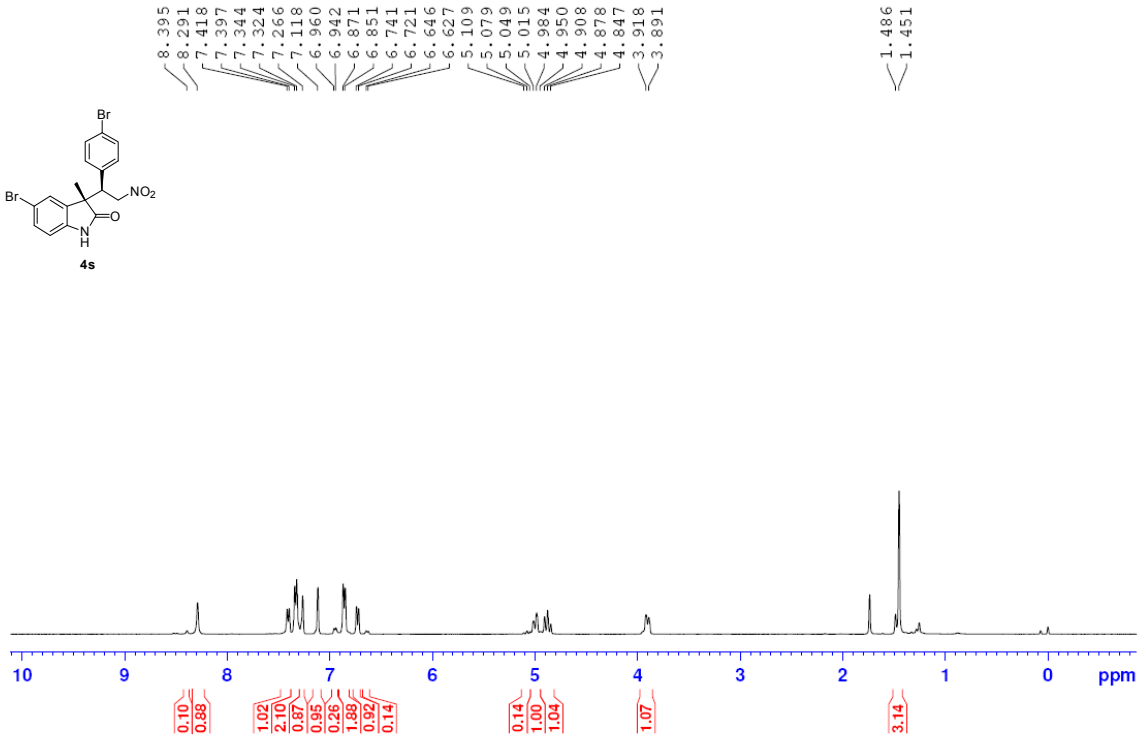




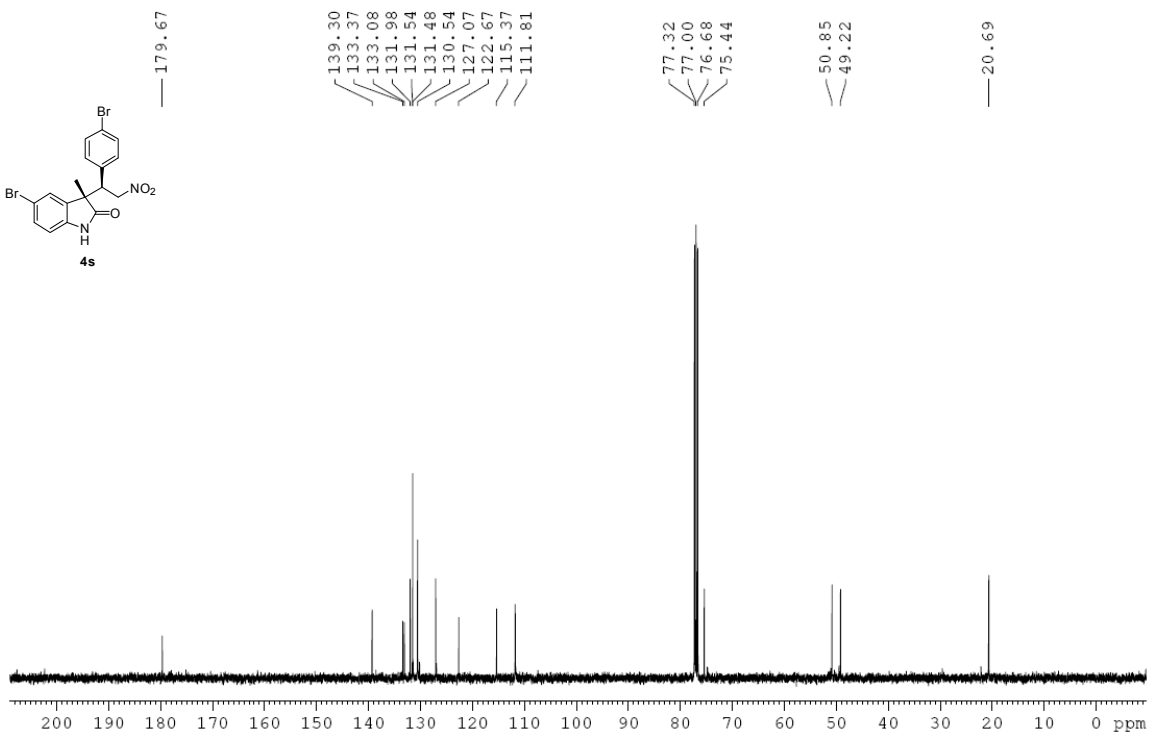
4r



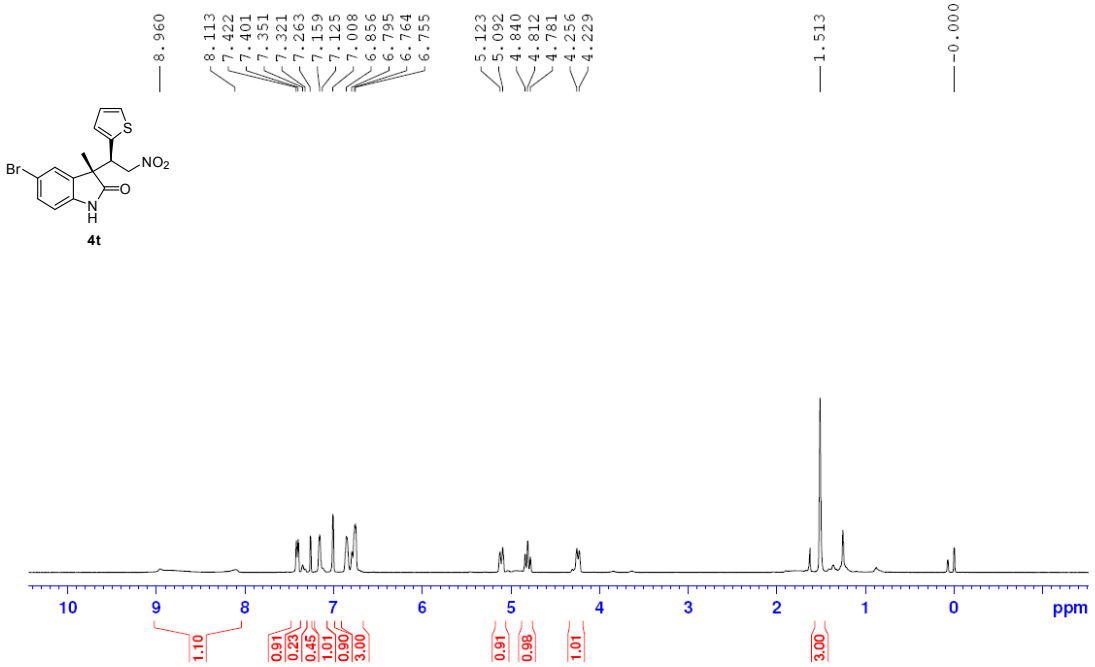
DIM-DD-127 H



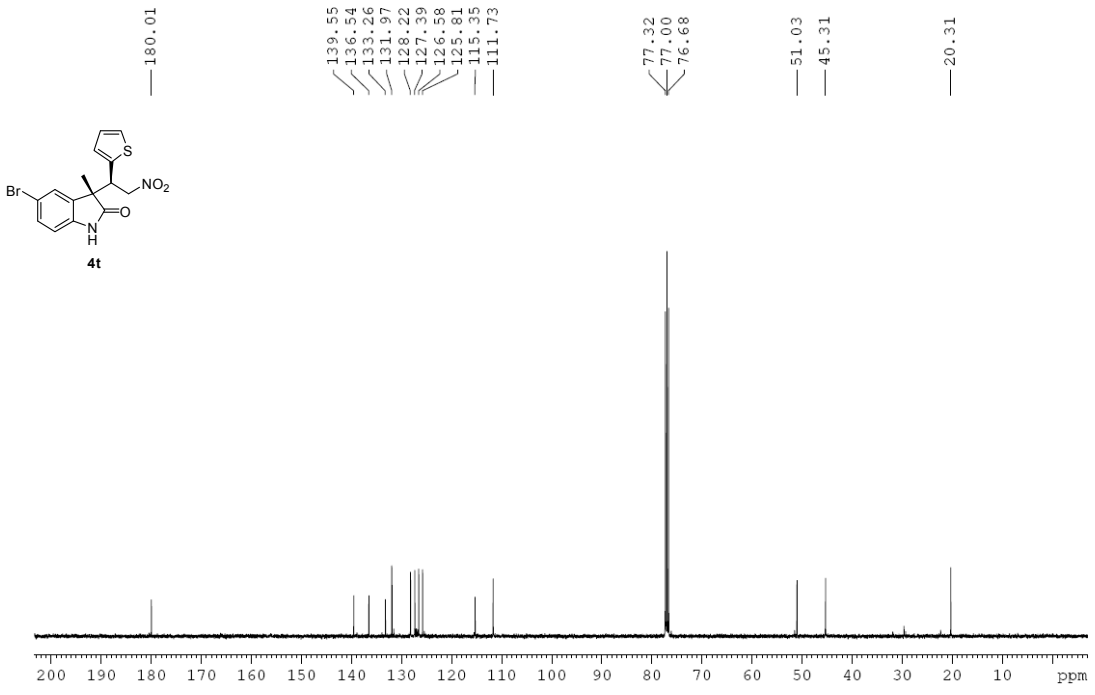
DIM-DD-127 C



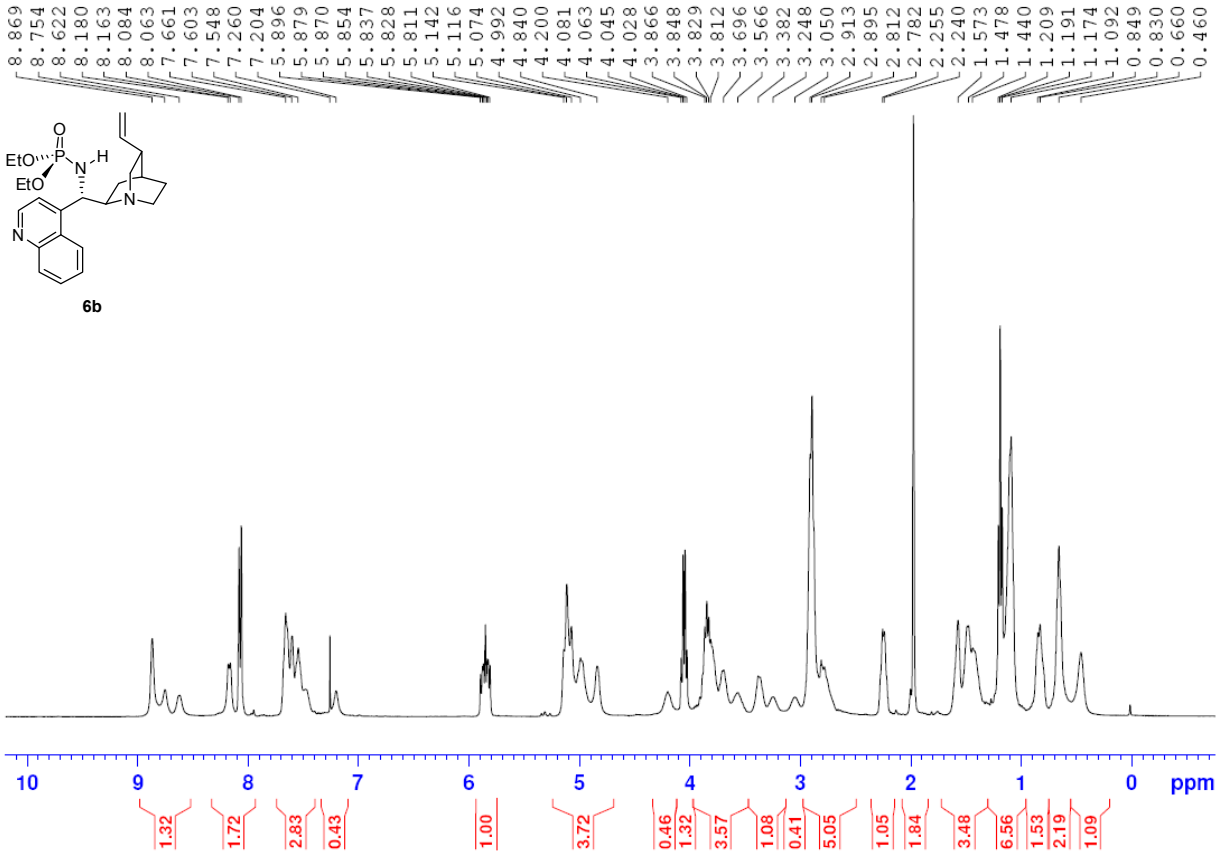
DIM-DD-144 H



DIM-DD-144 C

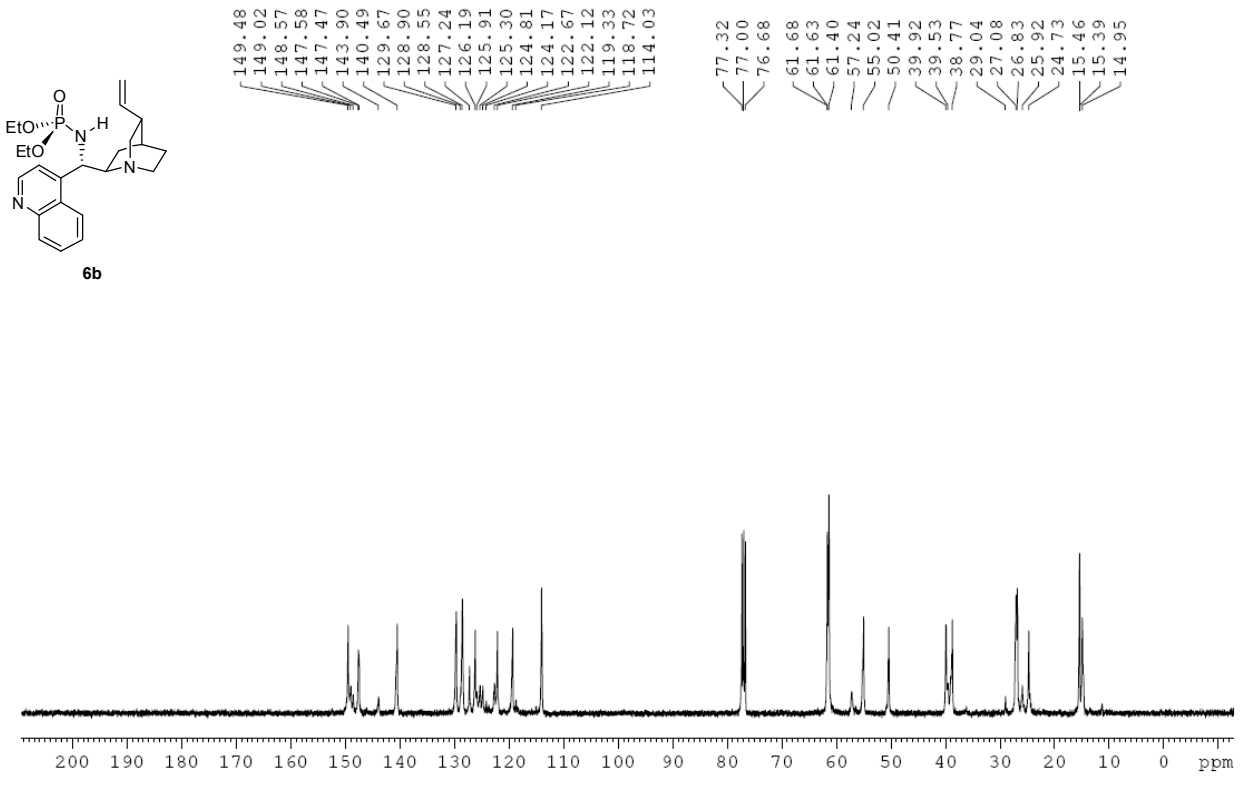


DIM-DB-96 H



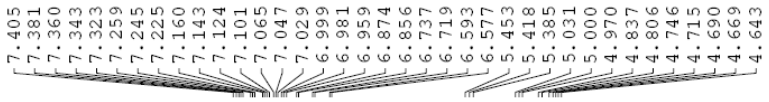
6b

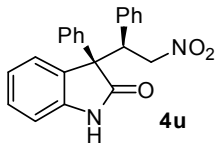
DIM-DB-96 C



6b

DIM-DD-90 H





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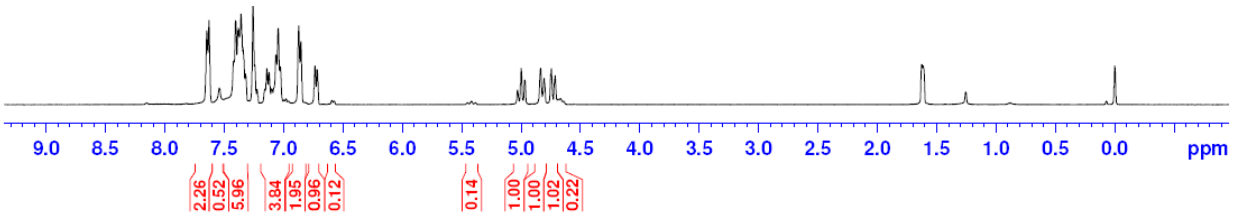
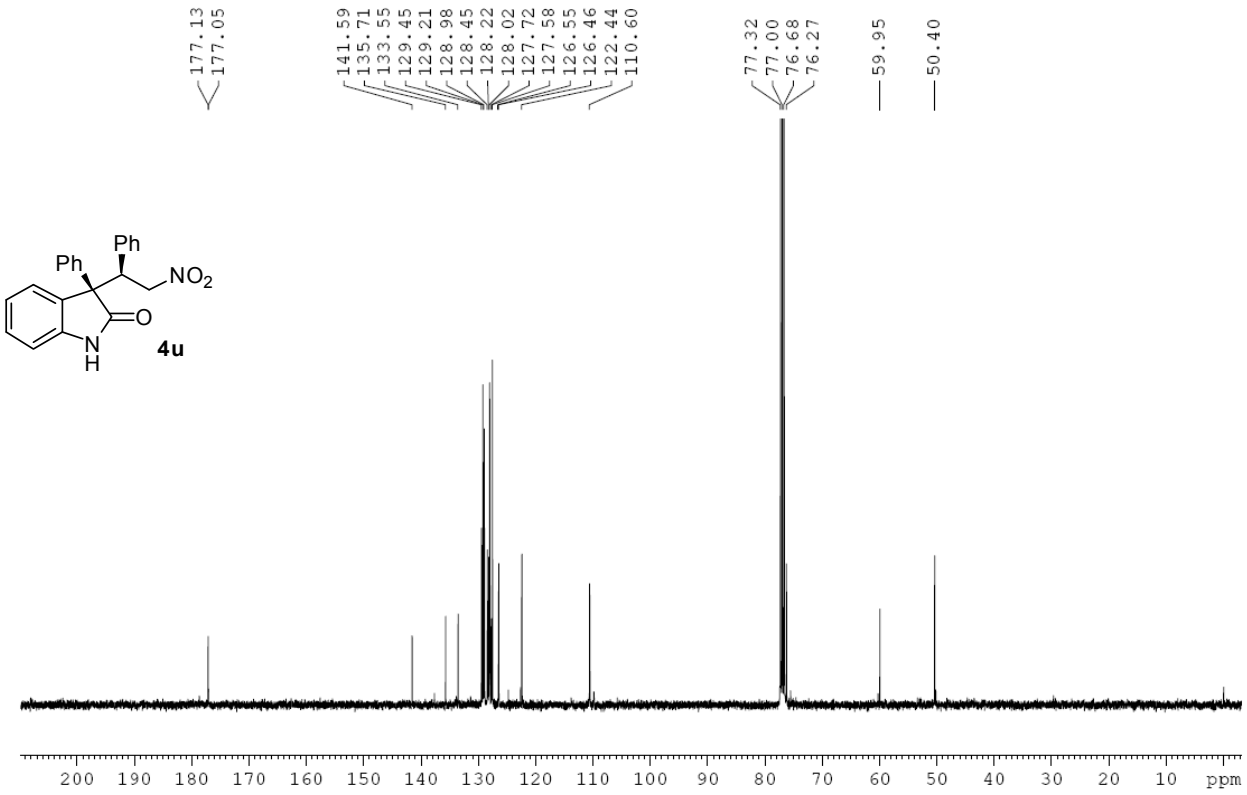
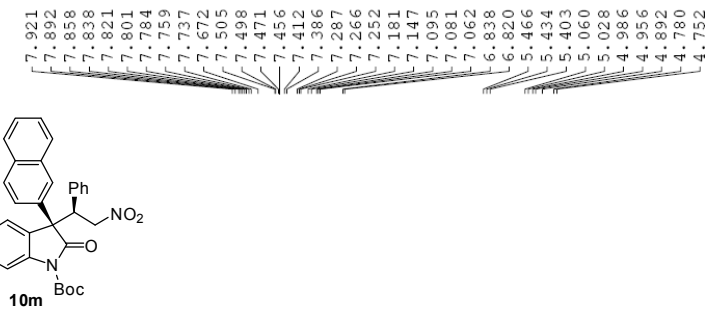


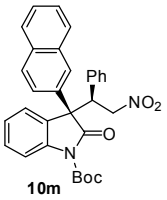
DIM-DD-90 C



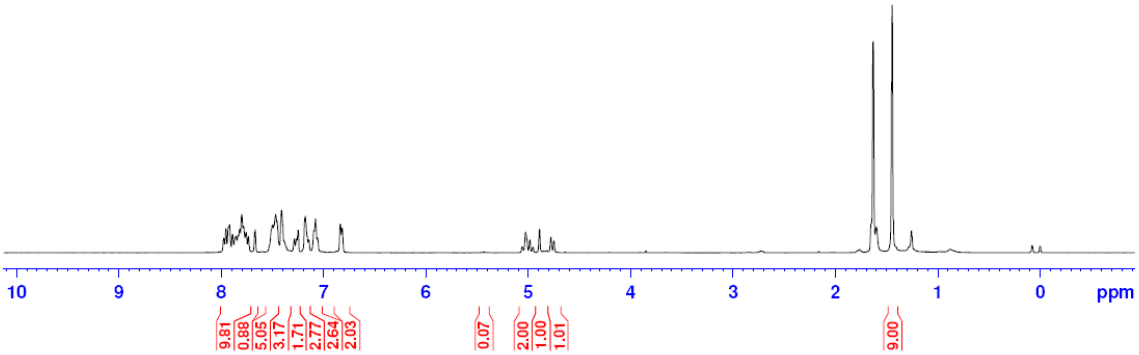
4u

DIM-DD-143 H

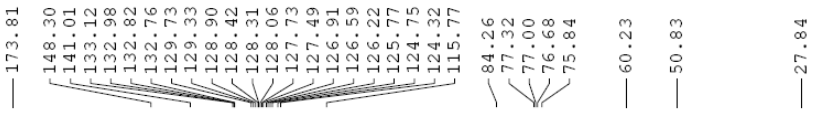


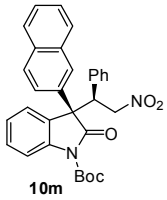


10m

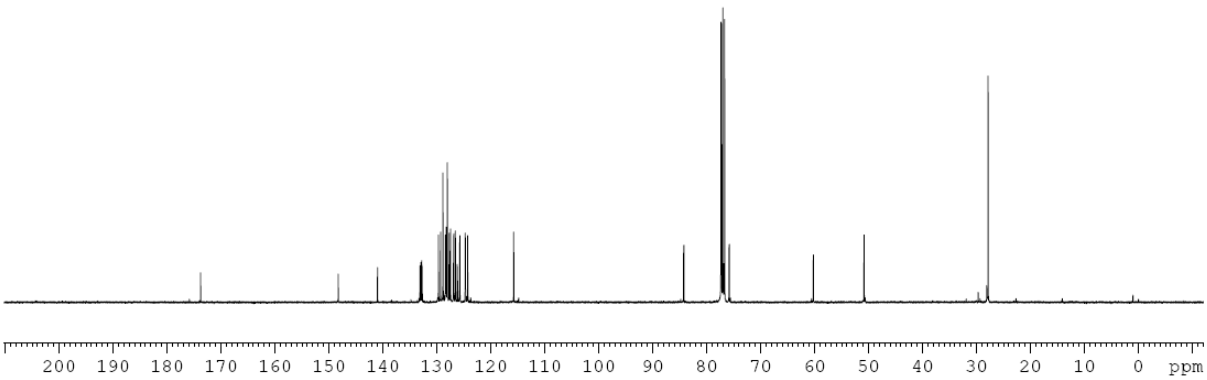


DIM-DD-149(2) C

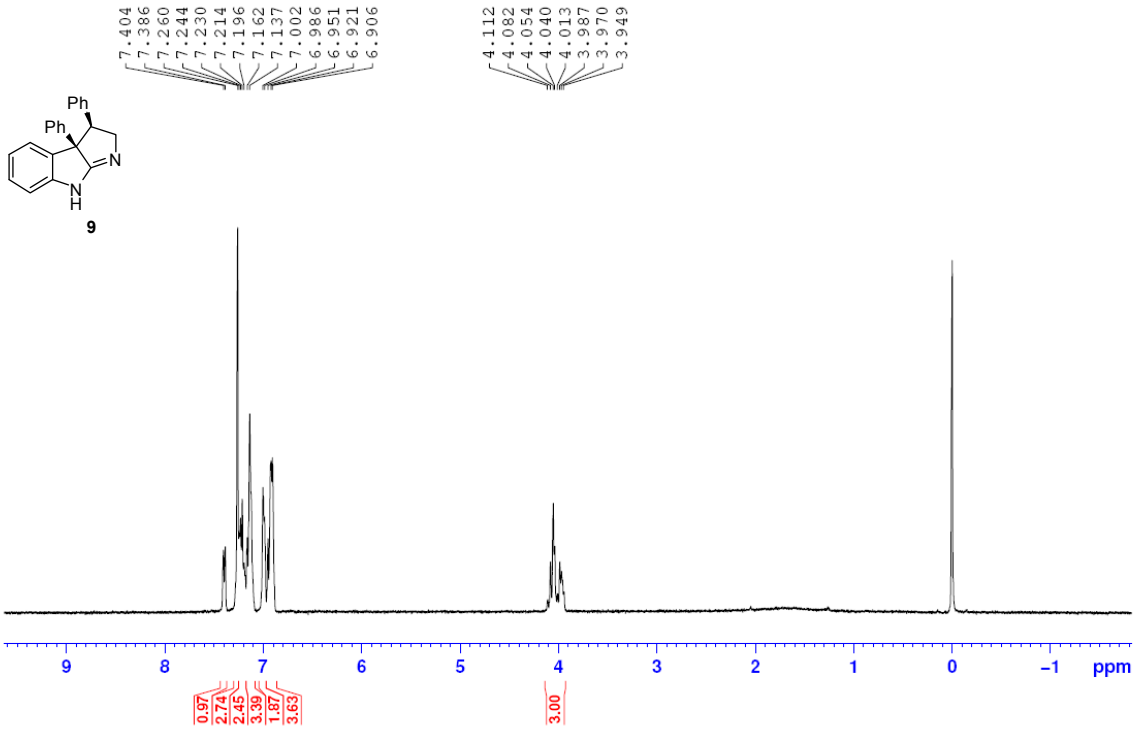




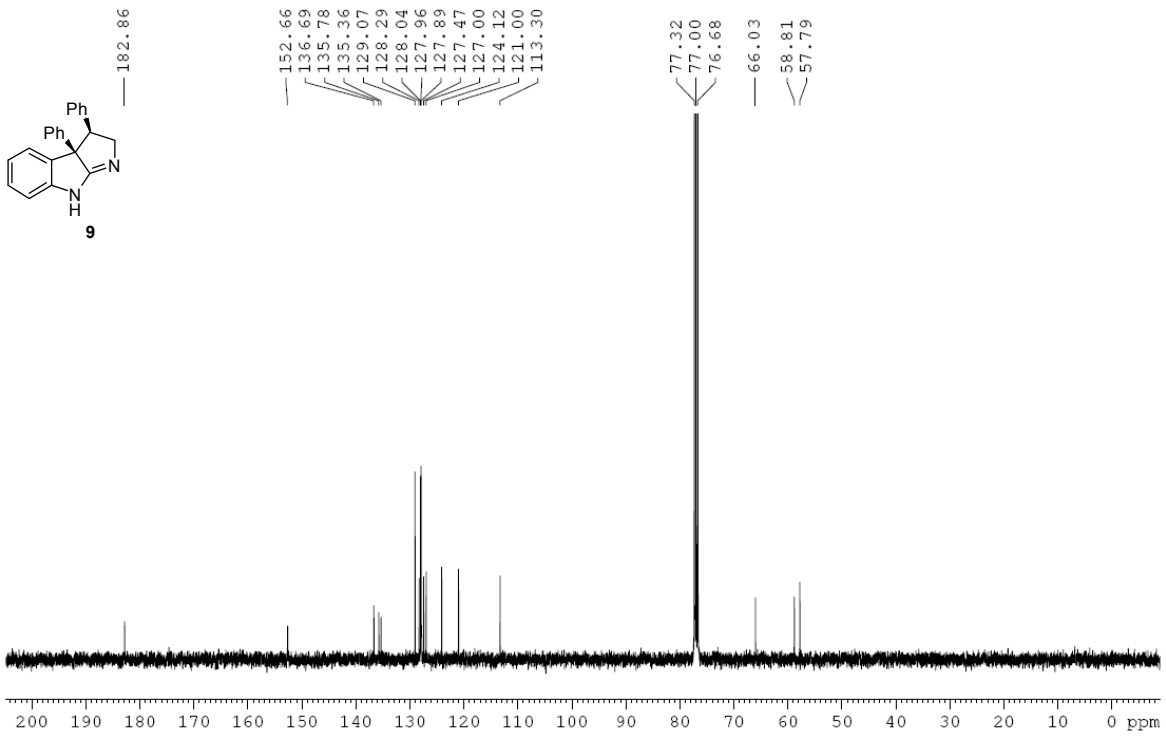
10m

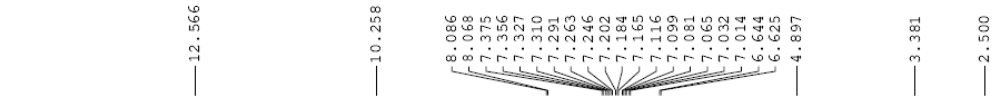


DIM-DD-81 CRS H

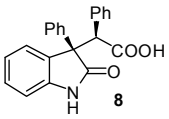


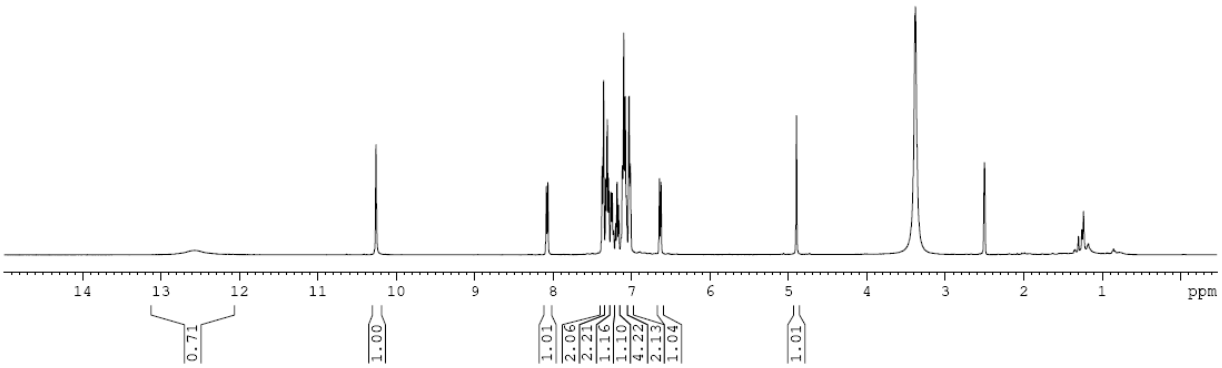
DIM-DD-81 CRS C



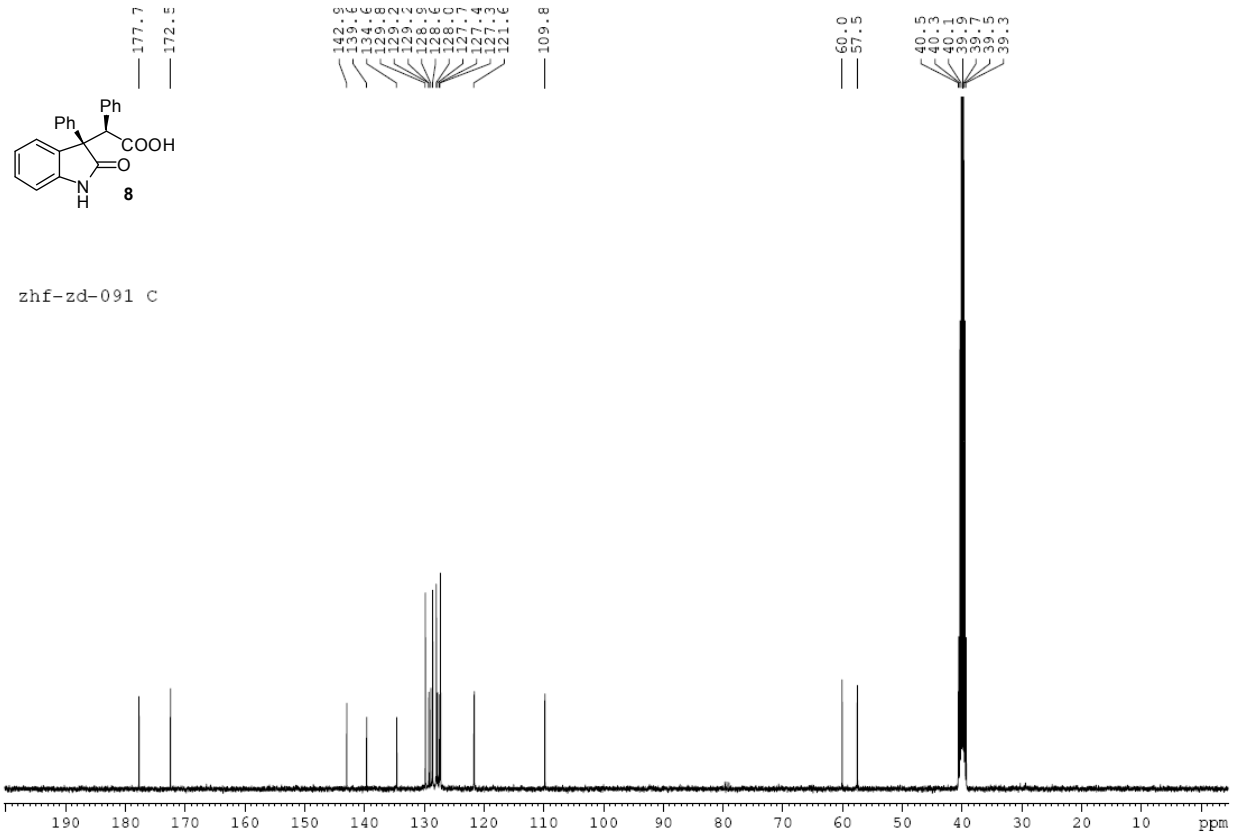


zhf-zd-091 H



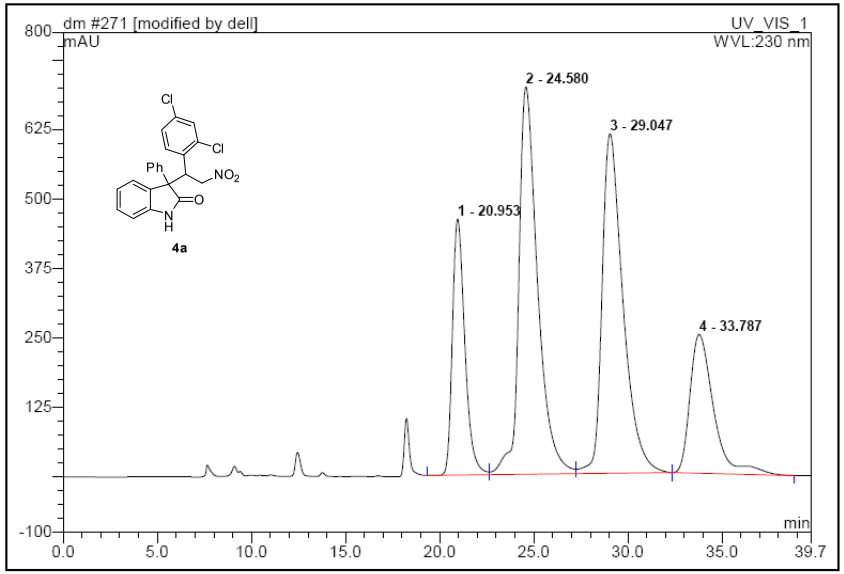


zhf-zd-091 C



271 DIM-Da-88-rac-ODH(Z)-ODH(J)-90/10-230

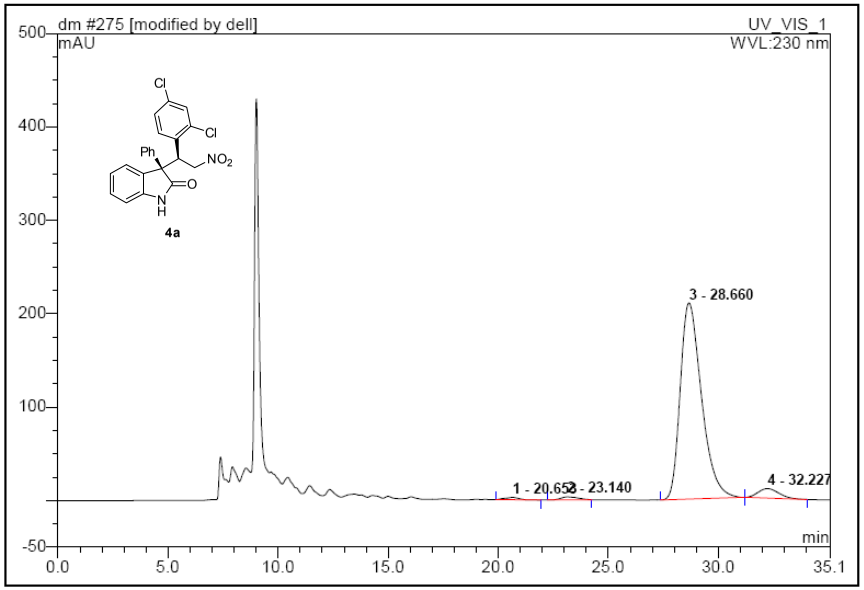
Sample Name:	**DIM-Da-88-rac-ODH(Z)-ODH(J)-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**282**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-7-13 21:51**	*Sample Weight:*	**1.0000**
Run Time (min):	**39.72**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.95	n.a.	460.351	353.163	15.28	n.a.	BM *
2	24.58	n.a.	697.140	805.809	34.85	n.a.	M *
3	29.05	n.a.	610.769	789.116	34.13	n.a.	Mb*
4	33.79	n.a.	249.746	363.888	15.74	n.a.	bMB
Total:			2018.007	2311.975	100.00	0.000	

275 DIM-DB-117-D-ODH(Z)-ODH(J)-90/10-230

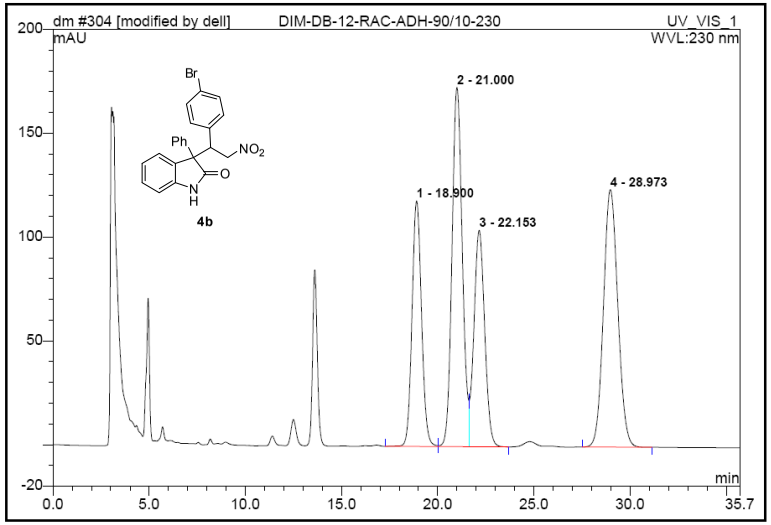
Sample Name:	**DIM-DB-117-D-ODH(Z)-ODH(J)-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**286**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-7-17 10:59**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.07**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.65	n.a.	2.347	1.741	0.69	n.a.	BMB*
2	23.14	n.a.	3.140	2.755	1.10	n.a.	BMB*
3	28.66	n.a.	210.104	235.773	93.76	n.a.	BMB
4	32.23	n.a.	10.199	11.188	4.45	n.a.	BMB*
Total:			225.790	251.457	100.00	0.000	

304 DIM-DB-12-RAC-ADH-90/10-230

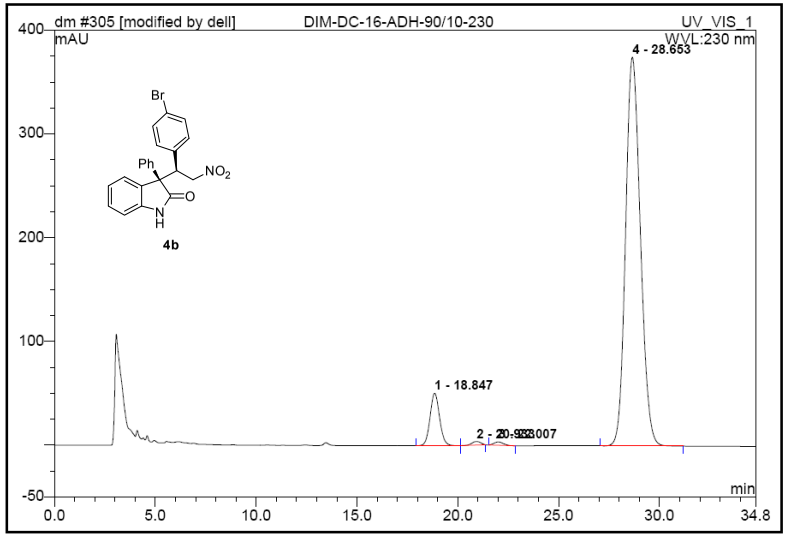
Sample Name:	**DIM-DB-12-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**311**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-23 11:02**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.71**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.90	n.a.	118.212	67.687	19.37	n.a.	BM
2	21.00	n.a.	172.923	106.899	30.59	n.a.	M
3	22.15	n.a.	104.198	67.625	19.35	n.a.	MB
4	28.97	n.a.	124.028	107.190	30.68	n.a.	BMB
Total:			519.361	349.401	100.00	0.000	

305 DIM-DC-16-ADH-90/10-230

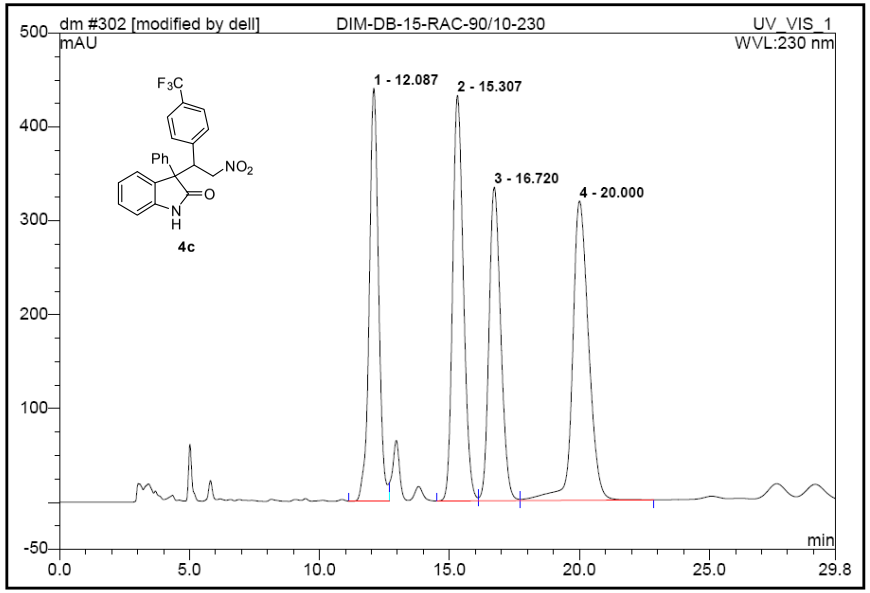
Sample Name:	**DIM-DC-16-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**312**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-23 11:38**	*Sample Weight:*	**1.0000**
Run Time (min):	**34.77**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.85	n.a.	50.457	27.644	7.90	n.a.	BMb*
2	20.93	n.a.	3.487	1.734	0.50	n.a.	bMB*
3	22.01	n.a.	3.100	1.674	0.48	n.a.	BMB*
4	28.65	n.a.	374.739	319.040	91.13	n.a.	BMB
Total:			431.782	350.093	100.00	0.000	

302 DIM-DB-15-RAC-90/10-230

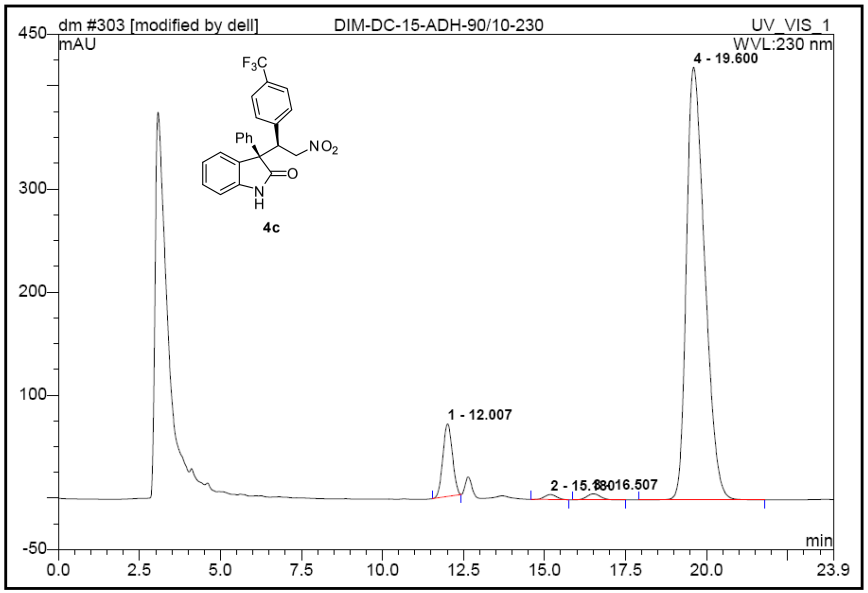
Sample Name:	**DIM-DB-15-RAC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**309**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-23 10:07**	*Sample Weight:*	**1.0000**
Run Time (min):	**29.83**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.09	n.a.	439.965	182.723	22.99	n.a.	BM *
2	15.31	n.a.	432.266	207.755	26.14	n.a.	BM
3	16.72	n.a.	334.245	175.376	22.07	n.a.	M
4	20.00	n.a.	318.959	228.816	28.79	n.a.	MB
Total:			1525.434	794.671	100.00	0.000	

303 DIM-DC-15-ADH-90/10-230

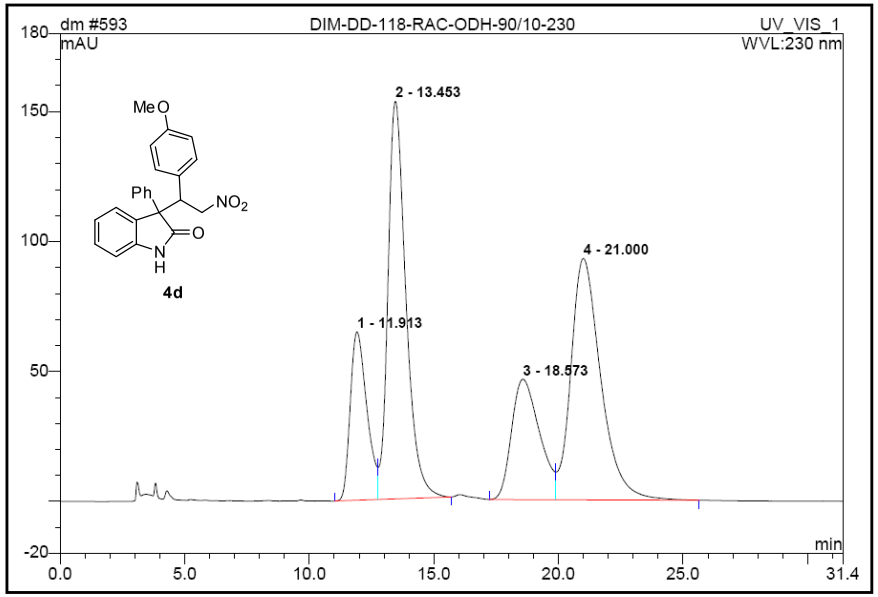
Sample Name:	**DIM-DC-15-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**310**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-23 10:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.91**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.01	n.a.	70.383	24.093	7.93	n.a.	BMB
2	15.18	n.a.	4.793	2.046	0.67	n.a.	BMB*
3	16.51	n.a.	5.847	2.794	0.92	n.a.	BMB*
4	19.60	n.a.	419.739	274.887	90.48	n.a.	BMB
Total:			500.762	303.819	100.00	0.000	

593 DIM-DD-118-RAC-ODH-90/10-230

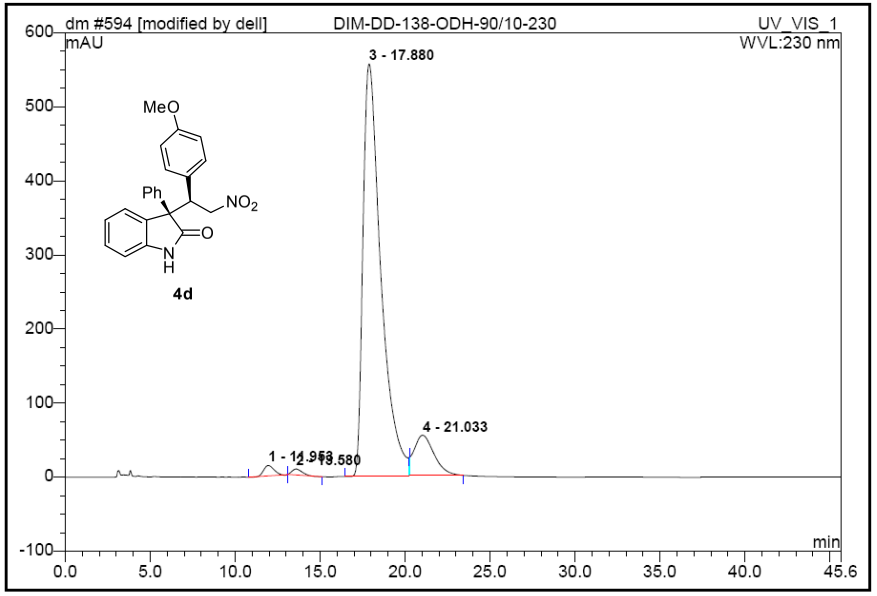
Sample Name:	**DIM-DD-118-RAC-ODH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**587**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-23 12:39**	*Sample Weight:*	**1.0000**
Run Time (min):	**31.41**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.91	n.a.	64.776	50.192	13.67	n.a.	BM
2	13.45	n.a.	153.012	127.601	34.74	n.a.	MB
3	18.57	n.a.	46.308	60.305	16.42	n.a.	BM
4	21.00	n.a.	92.855	129.192	35.17	n.a.	MB
Total:			356.950	367.290	100.00	0.000	

594 DIM-DD-138-ODH-90/10-230

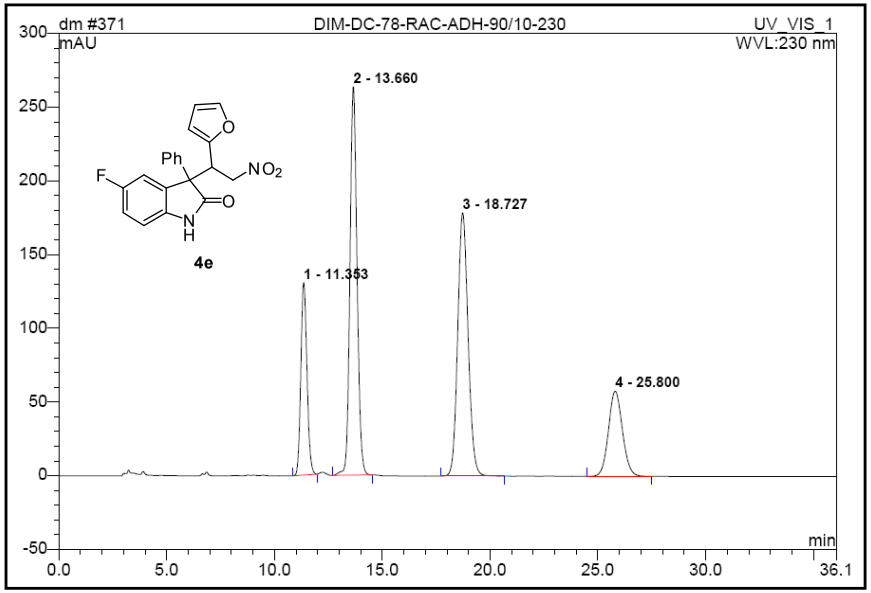
Sample Name:	**DIM-DD-138-ODH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**588**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-23 13:11**	*Sample Weight:*	**1.0000**
Run Time (min):	**45.64**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.95	n.a.	13.978	9.551	1.24	n.a.	BMB*
2	13.58	n.a.	8.021	5.387	0.70	n.a.	BMB*
3	17.88	n.a.	556.806	682.630	88.55	n.a.	BM *
4	21.03	n.a.	54.169	73.334	9.51	n.a.	MB*
Total:			632.974	770.902	100.00	0.000	

371 DIM-DC-78-RAC-ADH-90/10-230

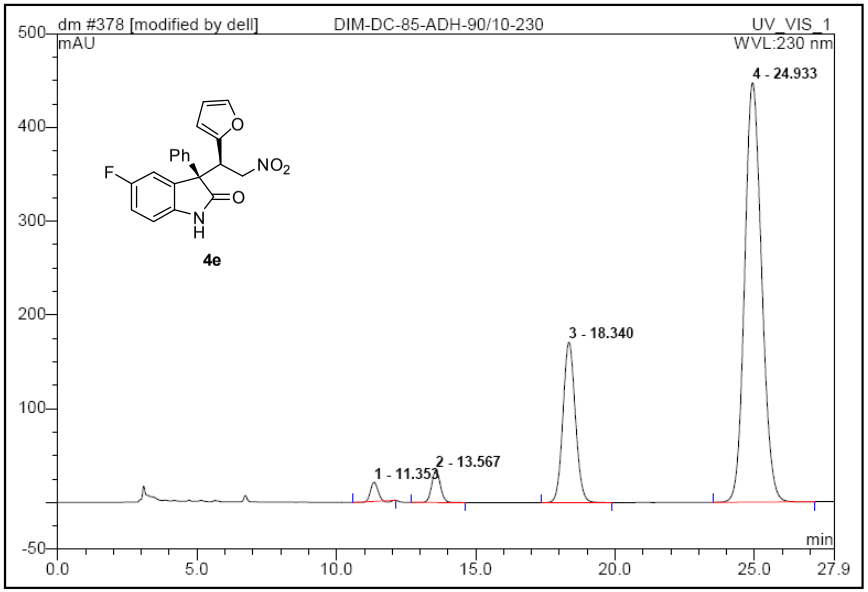
Sample Name:	**DIM-DC-78-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**375**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-6 15:06**	*Sample Weight:*	**1.0000**
Run Time (min):	**36.06**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.35	n.a.	130.526	42.773	14.94	n.a.	BMB
2	13.66	n.a.	263.267	100.692	35.17	n.a.	BMB
3	18.73	n.a.	178.455	99.583	34.78	n.a.	BMB
4	25.80	n.a.	57.696	43.282	15.12	n.a.	BMB
Total:			629.945	286.331	100.00	0.000	

378 DIM-DC-85-ADH-90/10-230

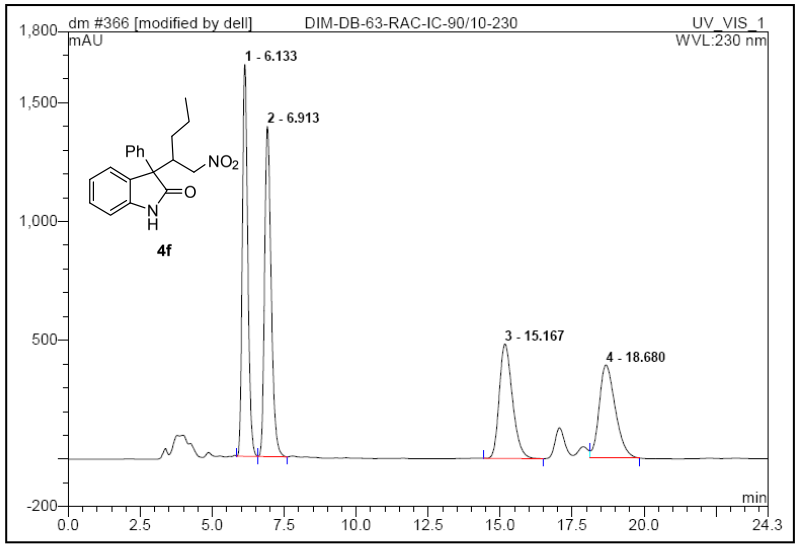
Sample Name:	**DIM-DC-85-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**382**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-11 13:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**27.86**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.35	n.a.	20.338	5.628	1.33	n.a.	BMB*
2	13.57	n.a.	34.179	12.296	2.91	n.a.	BMB*
3	18.34	n.a.	171.027	88.631	20.96	n.a.	BMB
4	24.93	n.a.	447.592	316.282	74.80	n.a.	BMB
Total:			673.137	422.836	100.00	0.000	

366 DIM-DB-63-RAC-IC-90/10-230

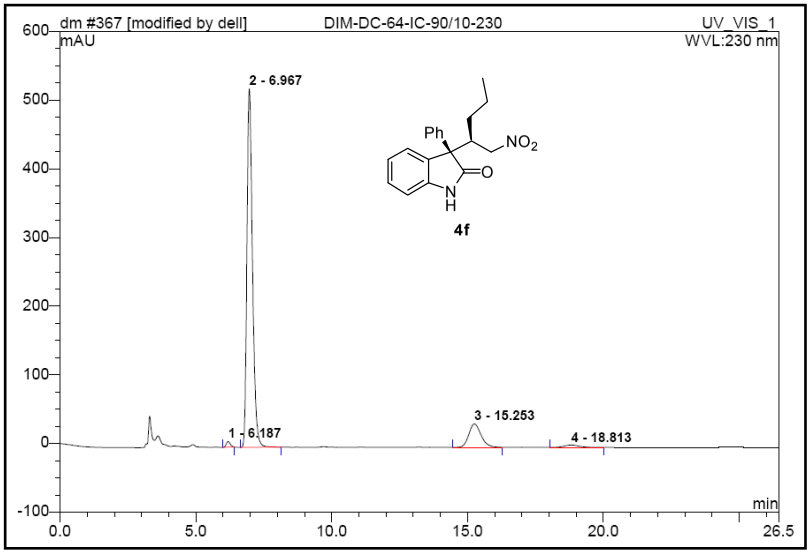
Sample Name:	**DIM-DB-63-RAC-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**370**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-6 11:48**	*Sample Weight:*	**1.0000**
Run Time (min):	**24.30**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.13	n.a.	1649.198	362.890	29.17	n.a.	BM
2	6.91	n.a.	1389.368	369.060	29.67	n.a.	MB
3	15.17	n.a.	481.586	256.004	20.58	n.a.	BMB
4	18.68	n.a.	391.957	256.062	20.58	n.a.	MB*
Total:			3912.109	1244.017	100.00	0.000	

367 DIM-DC-64-IC-90/10-230

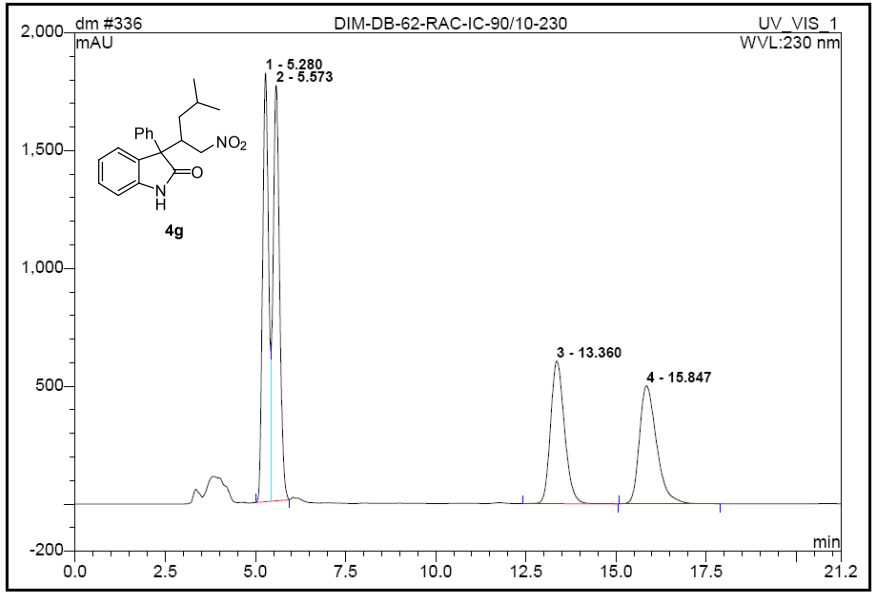
Sample Name:	**DIM-DC-64-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**371**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-6 12:36**	*Sample Weight:*	**1.0000**
Run Time (min):	**26.45**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.19	n.a.	8.160	1.409	0.98	n.a.	BMB*
2	6.97	n.a.	522.143	123.266	85.45	n.a.	BMB
3	15.25	n.a.	34.018	17.574	12.18	n.a.	BMB*
4	18.81	n.a.	3.251	2.008	1.39	n.a.	BMB*
Total:			567.572	144.256	100.00	0.000	

336 DIM-DB-62-RAC-IC-90/10-230

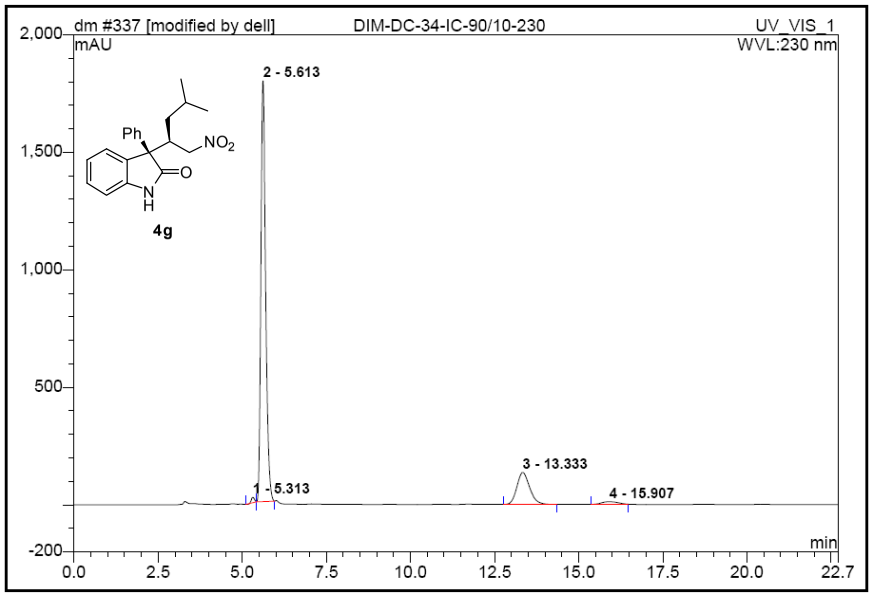
Sample Name:	**DIM-DB-62-RAC-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**343**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-10-15 21:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.24**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.28	n.a.	1818.355	349.464	27.53	n.a.	BM
2	5.57	n.a.	1762.788	372.228	29.33	n.a.	MB
3	13.36	n.a.	604.727	270.900	21.34	n.a.	BMB
4	15.85	n.a.	500.939	276.668	21.80	n.a.	BMB
Total:			4686.809	1269.260	100.00	0.000	

337 DIM-DC-34-IC-90/10-230

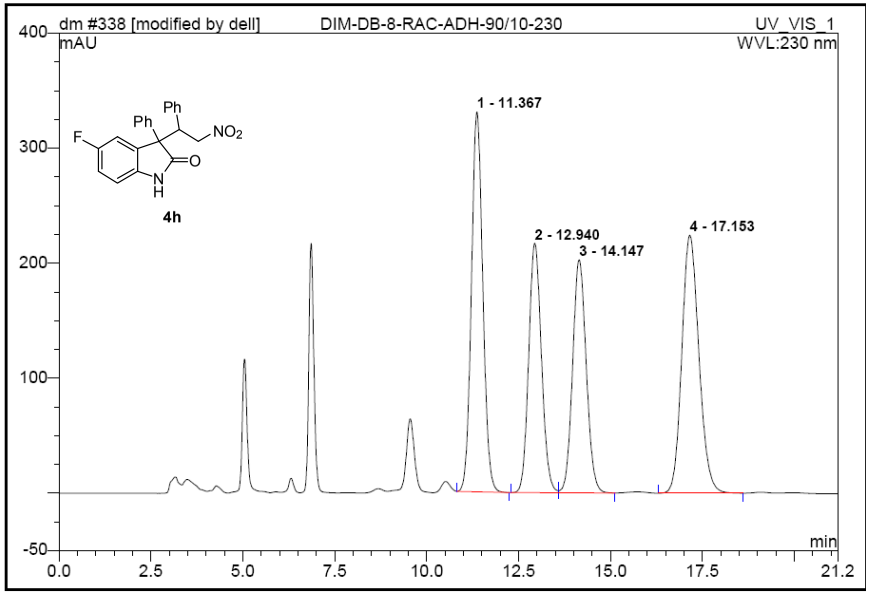
Sample Name:	**DIM-DC-34-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**344**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-10-15 21:59**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.71**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.31	n.a.	22.200	2.287	0.63	n.a.	BMb*
2	5.61	n.a.	1789.632	296.534	81.30	n.a.	bMB*
3	13.33	n.a.	136.071	59.741	16.38	n.a.	BMB
4	15.91	n.a.	11.614	6.197	1.70	n.a.	BMB*
Total:			1959.518	364.760	100.00	0.000	

338 DIM-DB-8-RAC-ADH-90/10-230

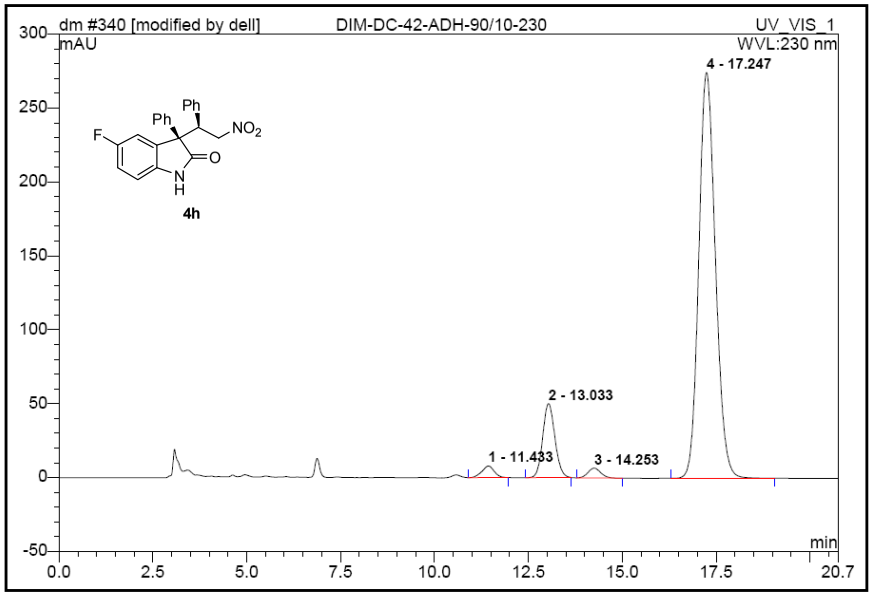
Sample Name:	**DIM-DB-8-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**345**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-10-21 18:08**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.18**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.37	n.a.	330.337	118.677	28.65	n.a.	BMB
2	12.94	n.a.	216.823	87.331	21.09	n.a.	BM
3	14.15	n.a.	202.547	87.183	21.05	n.a.	MB
4	17.15	n.a.	224.307	120.987	29.21	n.a.	BMB
Total:			974.014	414.178	100.00	0.000	

340 DIM-DC-42-ADH-90/10-230

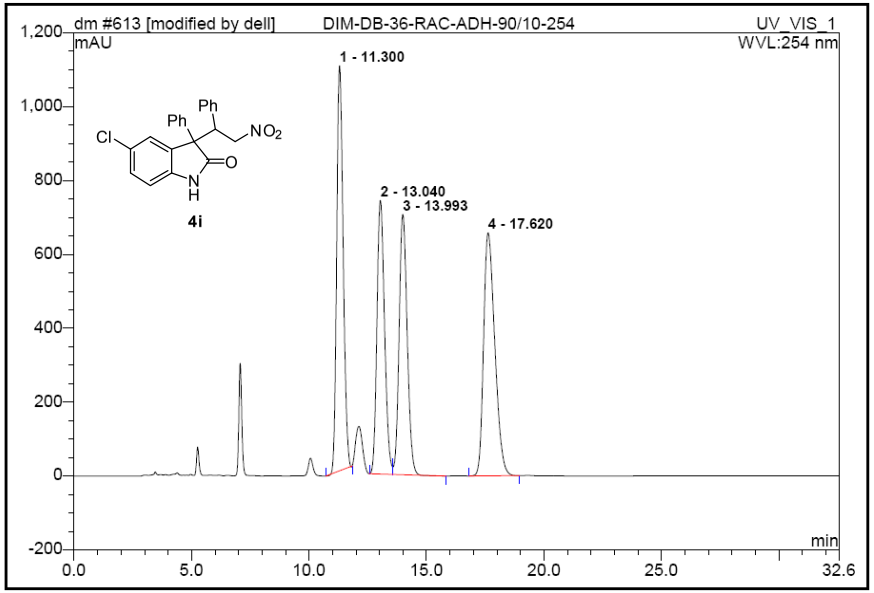
Sample Name:	**DIM-DC-42-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**347**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-10-21 18:56**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.75**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.43	n.a.	7.821	2.955	1.79	n.a.	BMB*
2	13.03	n.a.	50.010	18.803	11.38	n.a.	BMB*
3	14.25	n.a.	6.595	2.609	1.58	n.a.	BMB*
4	17.25	n.a.	274.359	140.881	85.25	n.a.	BMB
Total:			338.786	165.249	100.00	0.000	

613 DIM-DB-36-RAC-ADH-90/10-254

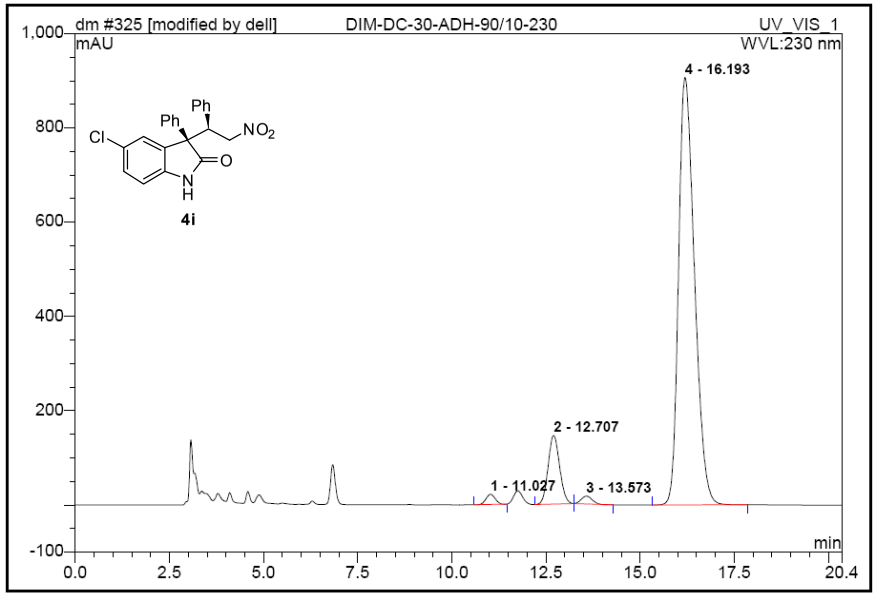
Sample Name:	**DIM-DB-36-RAC-ADH-90/10-254**	*Injection Volume:*	**20.0**
Vial Number:	**607**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-27 15:50**	*Sample Weight:*	**1.0000**
Run Time (min):	**32.55**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.30	n.a.	1096.882	348.674	27.44	n.a.	BMB*
2	13.04	n.a.	740.935	278.868	21.94	n.a.	BM *
3	13.99	n.a.	704.911	280.033	22.03	n.a.	MB*
4	17.62	n.a.	657.776	363.309	28.59	n.a.	BMB
Total:			3200.504	1270.883	100.00	0.000	

325 DIM-DC-30-ADH-90/10-230

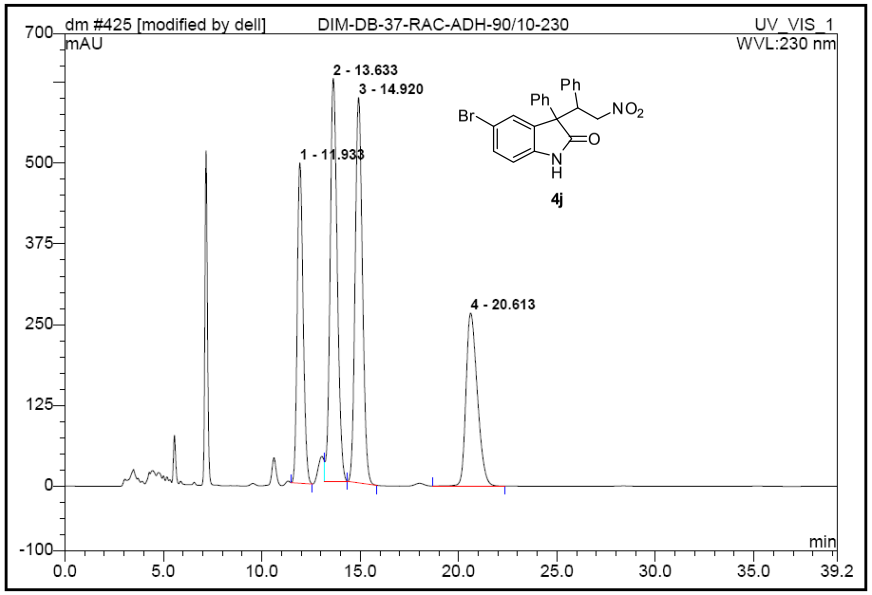
Sample Name:	**DIM-DC-30-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**332**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-10-12 20:49**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.36**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.03	n.a.	21.542	6.053	1.19	n.a.	BMB*
2	12.71	n.a.	145.633	51.453	10.12	n.a.	BMb*
3	13.57	n.a.	16.637	5.554	1.09	n.a.	bMB*
4	16.19	n.a.	907.040	445.412	87.60	n.a.	BMB
Total:			1090.851	508.473	100.00	0.000	

425 DIM-DB-37-RAC-ADH-90/10-230

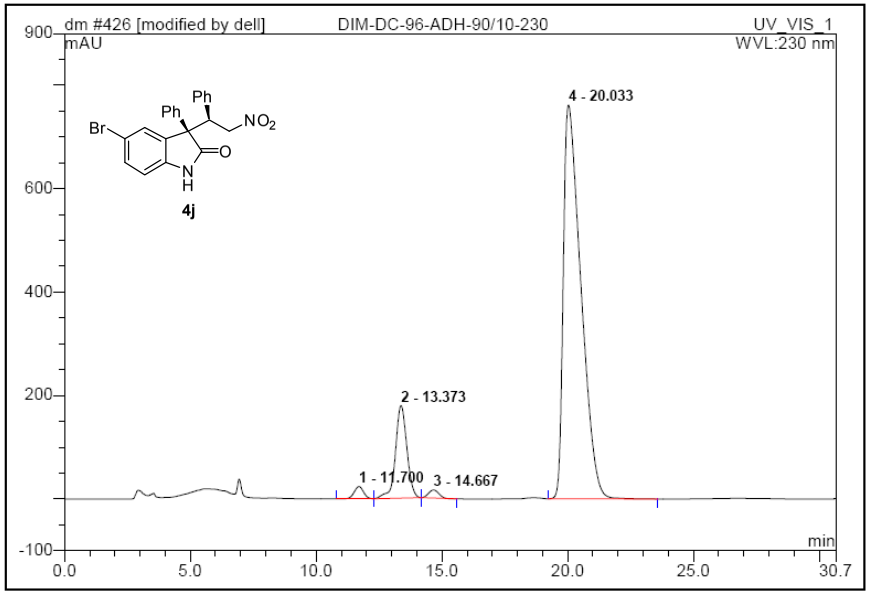
Sample Name:	**DIM-DB-37-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**427**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-12-2 19:36**	*Sample Weight:*	**1.0000**
Run Time (min):	**39.23**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.93	n.a.	495.639	172.944	19.93	n.a.	BMB
2	13.63	n.a.	623.005	260.767	30.04	n.a.	MB*
3	14.92	n.a.	596.076	255.768	29.47	n.a.	BMB
4	20.61	n.a.	267.900	178.478	20.56	n.a.	BMB
Total:			1982.620	867.957	100.00	0.000	

426 DIM-DC-96-ADH-90/10-230

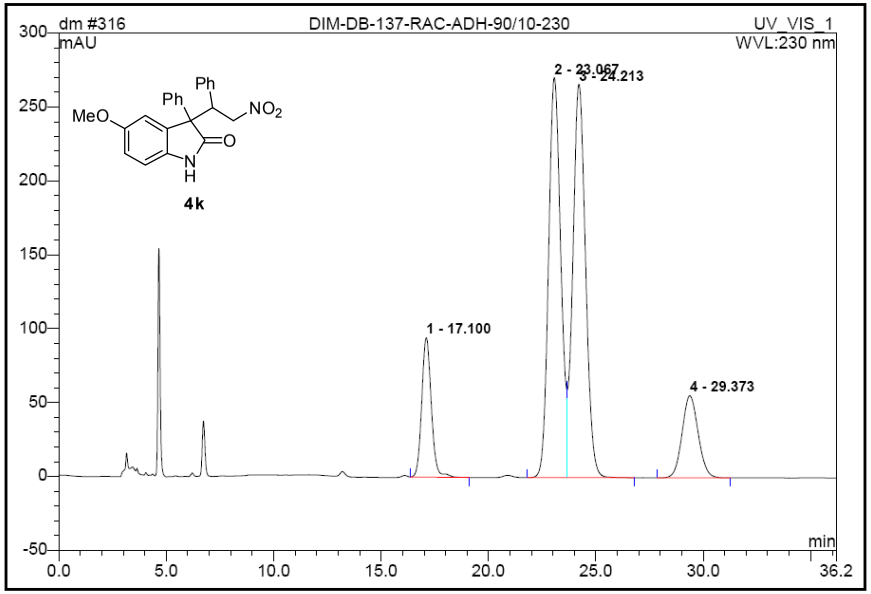
Sample Name:	**DIM-DC-96-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**427**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-12-2 20:17**	*Sample Weight:*	**1.0000**
Run Time (min):	**30.66**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.70	n.a.	23.469	10.043	1.38	n.a.	BMB*
2	13.37	n.a.	178.740	94.111	12.93	n.a.	BMb*
3	14.67	n.a.	15.699	7.264	1.00	n.a.	bMB*
4	20.03	n.a.	761.524	616.645	84.70	n.a.	BMB
Total:			979.433	728.063	100.00	0.000	

316 DIM-DB-137-RAC-ADH-90/10-230

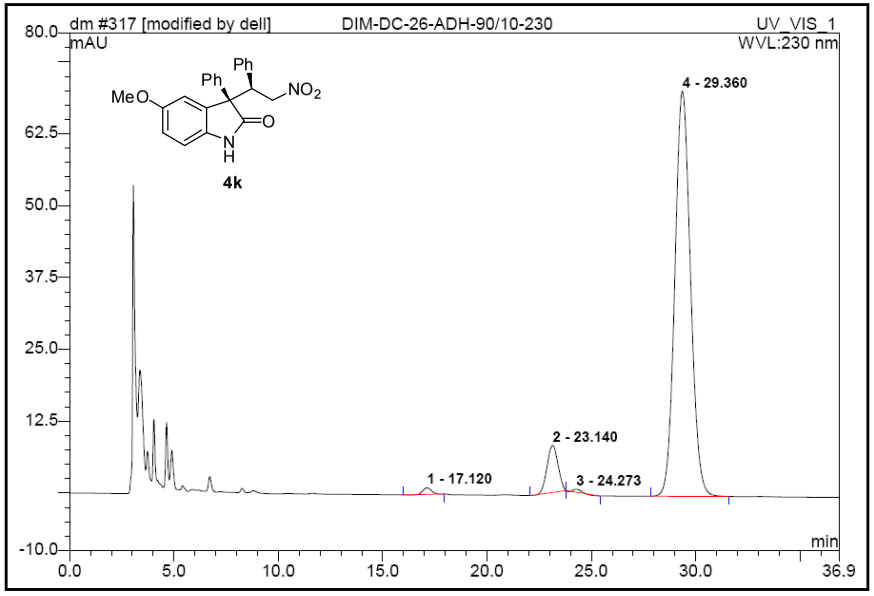
Sample Name:	**DIM-DB-137-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**323**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-30 11:20**	*Sample Weight:*	**1.0000**
Run Time (min):	**36.19**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.10	n.a.	94.200	48.747	10.63	n.a.	BMB
2	23.07	n.a.	270.507	177.943	38.81	n.a.	BM
3	24.21	n.a.	266.046	183.622	40.05	n.a.	MB
4	29.37	n.a.	55.545	48.161	10.50	n.a.	BMB
Total:			686.297	458.473	100.00	0.000	

317 DIM-DC-26-ADH-90/10-230

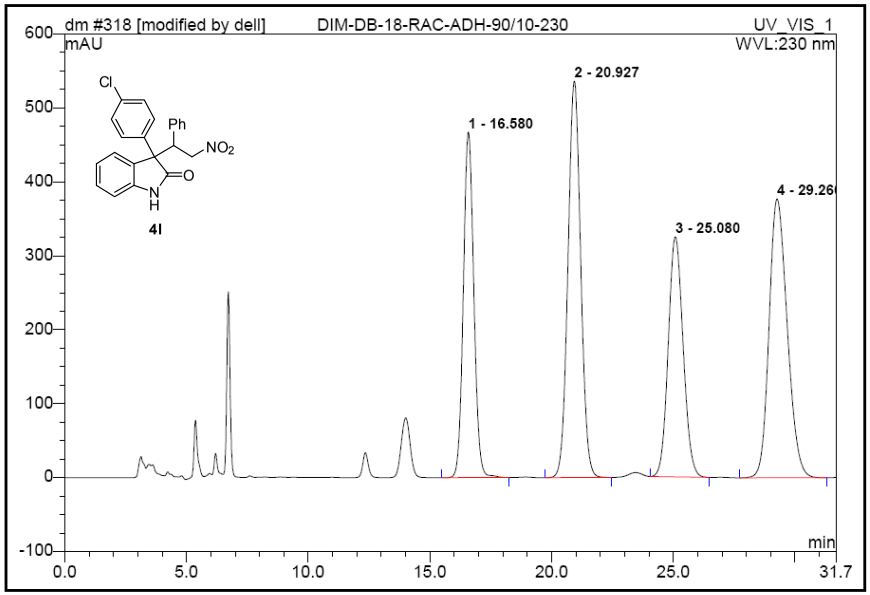
Sample Name:	**DIM-DC-26-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**324**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-30 11:57**	*Sample Weight:*	**1.0000**
Run Time (min):	**36.87**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.12	n.a.	1.129	0.518	0.77	n.a.	BMB*
2	23.14	n.a.	8.159	4.958	7.41	n.a.	BMb*
3	24.27	n.a.	0.487	0.128	0.19	n.a.	bMB*
4	29.36	n.a.	70.478	61.334	91.63	n.a.	BMB
Total:			80.252	66.938	100.00	0.000	

318 DIM-DB-18-RAC-ADH-90/10-230

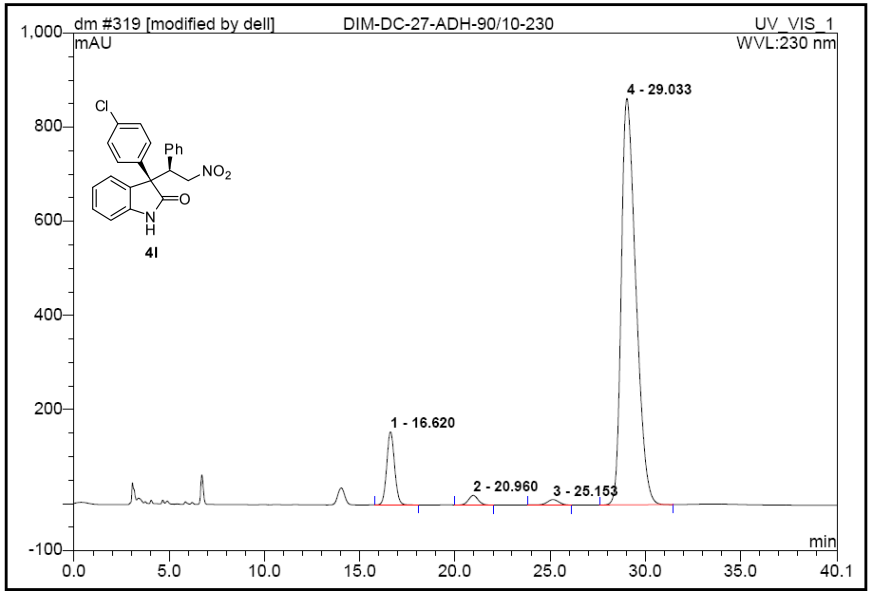
Sample Name:	**DIM-DB-18-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**325**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-30 12:35**	*Sample Weight:*	**1.0000**
Run Time (min):	**31.68**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.58	n.a.	467.312	232.503	20.87	n.a.	BMB
2	20.93	n.a.	536.157	325.453	29.21	n.a.	BMB
3	25.08	n.a.	324.666	230.184	20.66	n.a.	BMB
4	29.26	n.a.	377.026	325.981	29.26	n.a.	BMB
Total:			1705.162	1114.121	100.00	0.000	

319 DIM-DC-27-ADH-90/10-230

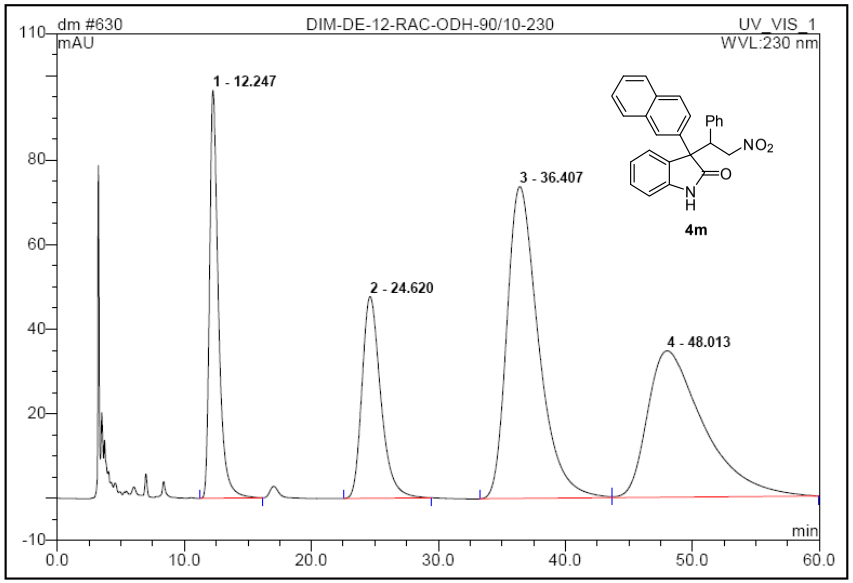
Sample Name:	**DIM-DC-27-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**326**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-9-30 13:07**	*Sample Weight:*	**1.0000**
Run Time (min):	**40.07**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.62	n.a.	155.283	74.032	8.59	n.a.	BMB
2	20.96	n.a.	20.332	11.936	1.38	n.a.	BMB*
3	25.15	n.a.	11.615	8.101	0.94	n.a.	BMB*
4	29.03	n.a.	864.080	768.107	89.09	n.a.	BMB
Total:			1051.309	862.176	100.00	0.000	

630 DIM-DE-12-RAC-ODH-90/10-230

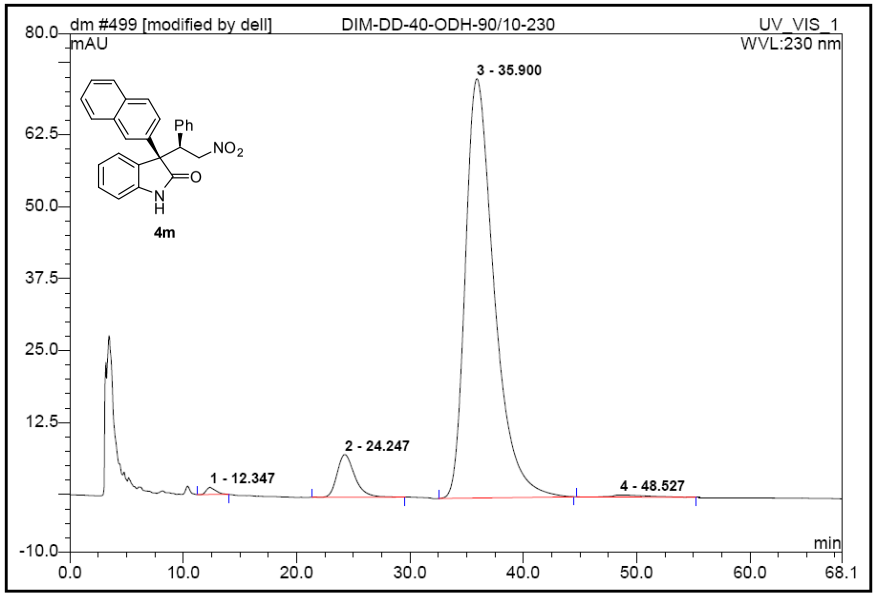
Sample Name:	**DIM-DE-12-RAC-ODH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**625**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-2 22:18**	*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.25	n.a.	96.539	78.450	14.23	n.a.	BMB
2	24.62	n.a.	47.736	81.656	14.81	n.a.	BMB
3	36.41	n.a.	73.834	213.010	38.64	n.a.	BM
4	48.01	n.a.	34.670	178.137	32.31	n.a.	MB
Total:			252.778	551.254	100.00	0.000	

499 DIM-DD-40-ODH-90/10-230

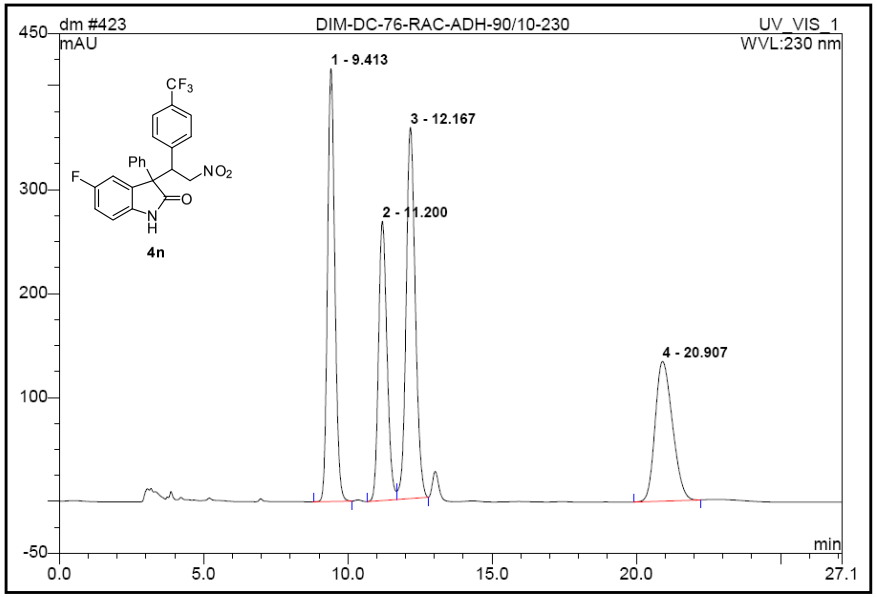
Sample Name:	**DIM-DD-40-ODH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**499**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-19 12:47**	*Sample Weight:*	**1.0000**
Run Time (min):	**68.10**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.35	n.a.	1.248	1.186	0.52	n.a.	BMB*
2	24.25	n.a.	7.408	13.284	5.78	n.a.	BMB*
3	35.90	n.a.	72.801	214.093	93.13	n.a.	BMB
4	48.53	n.a.	0.351	1.329	0.58	n.a.	BMB*
Total:			81.808	229.892	100.00	0.000	

423 DIM-DC-76-RAC-ADH-90/10-230

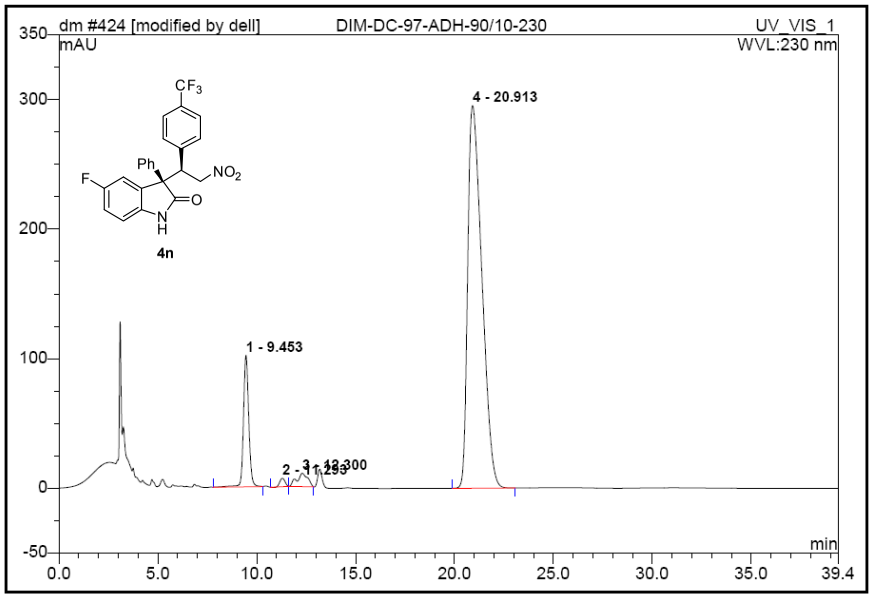
Sample Name:	**DIM-DC-76-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**425**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-30 18:40**	*Sample Weight:*	**1.0000**
Run Time (min):	**27.12**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.41	n.a.	416.225	121.784	27.77	n.a.	BMB
2	11.20	n.a.	268.646	91.683	20.90	n.a.	BM
3	12.17	n.a.	357.032	131.651	30.02	n.a.	MB
4	20.91	n.a.	134.292	93.467	21.31	n.a.	BMB
Total:			1176.194	438.585	100.00	0.000	

424 DIM-DC-97-ADH-90/10-230

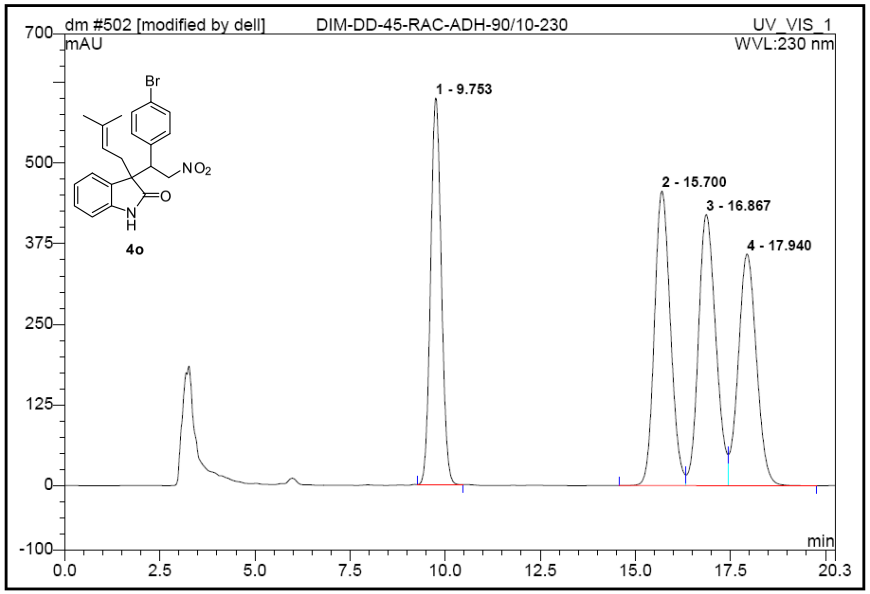
Sample Name:	**DIM-DC-97-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**426**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-11-30 19:09**	*Sample Weight:*	**1.0000**
Run Time (min):	**39.39**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.45	n.a.	101.476	31.197	10.97	n.a.	BMB
2	11.29	n.a.	6.459	1.880	0.66	n.a.	BMb*
3	12.30	n.a.	10.309	6.538	2.30	n.a.	bMB*
4	20.91	n.a.	295.214	244.799	86.07	n.a.	BMB
Total:			413.458	284.414	100.00	0.000	

502 DIM-DD-45-RAC-ADH-90/10-230

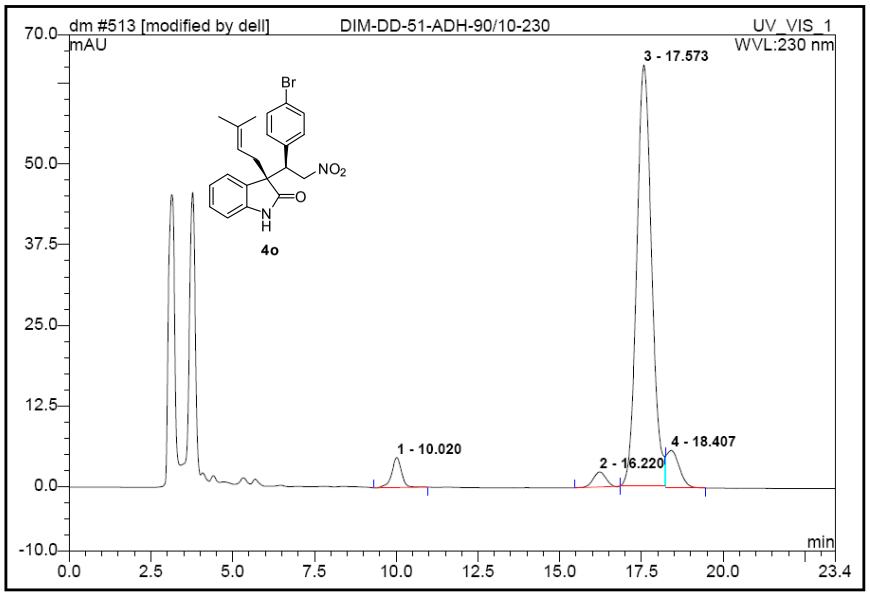
Sample Name:	**DIM-DD-45-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**498**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-19 17:22**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.25**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.75	n.a.	599.101	196.255	23.32	n.a.	BMB
2	15.70	n.a.	456.410	222.629	26.45	n.a.	BM
3	16.87	n.a.	420.226	222.280	26.41	n.a.	M
4	17.94	n.a.	359.250	200.444	23.82	n.a.	MB
Total:			1834.987	841.609	100.00	0.000	

513 DIM-DD-51-ADH-90/10-230

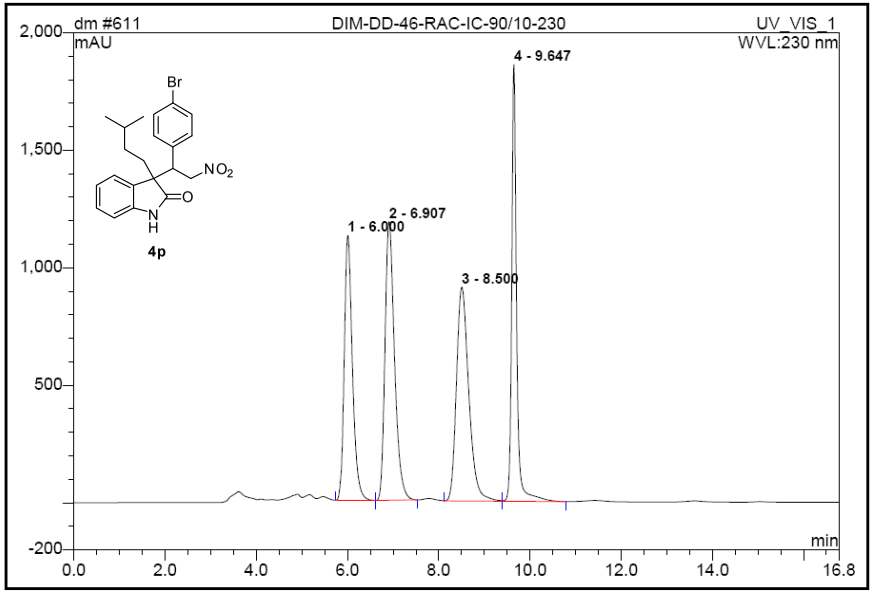
Sample Name:	**DIM-DD-51-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**508**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-21 12:31**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.42**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.02	n.a.	4.637	1.612	4.06	n.a.	BMB*
2	16.22	n.a.	2.307	1.015	2.56	n.a.	BMB*
3	17.57	n.a.	65.218	34.368	86.67	n.a.	BM *
4	18.41	n.a.	5.811	2.659	6.71	n.a.	MB*
Total:			77.973	39.653	100.00	0.000	

611 DIM-DD-46-RAC-IC-90/10-230

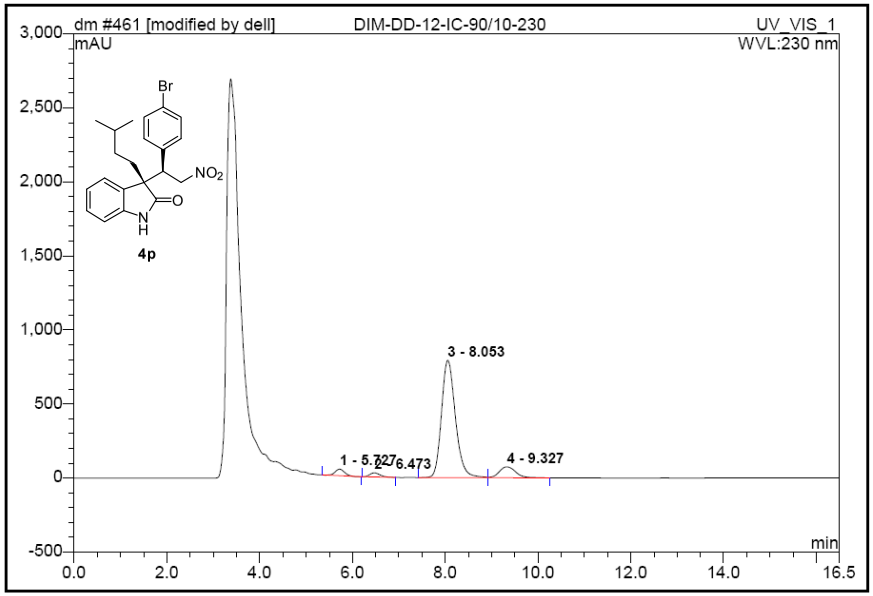
Sample Name:	**DIM-DD-46-RAC-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**605**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-27 14:56**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.77**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.00	n.a.	1126.522	233.188	22.55	n.a.	BMB
2	6.91	n.a.	1185.756	286.653	27.72	n.a.	BMB
3	8.50	n.a.	910.050	285.186	27.58	n.a.	BM
4	9.65	n.a.	1858.996	229.173	22.16	n.a.	MB
Total:			5081.323	1034.200	100.00	0.000	

461 DIM-DD-12-IC-90/10-230

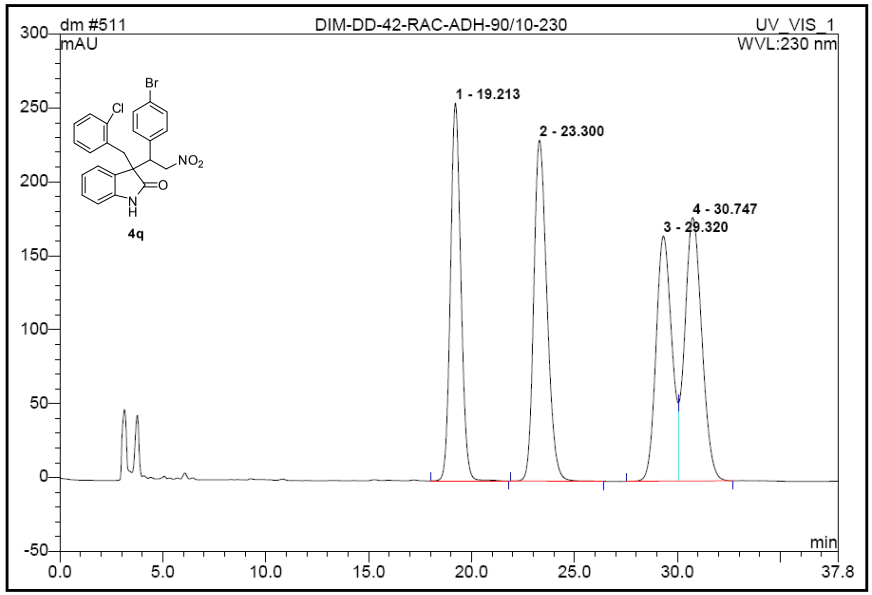
Sample Name:	**DIM-DD-12-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**461**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2010-12-25 13:34**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.49**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.73	n.a.	44.433	10.354	3.21	n.a.	BMB*
2	6.47	n.a.	28.193	7.242	2.24	n.a.	BMB*
3	8.05	n.a.	792.241	275.636	85.33	n.a.	BM
4	9.33	n.a.	73.116	29.800	9.23	n.a.	MB
Total:			937.983	323.032	100.00	0.000	

511 DIM-DD-42-RAC-ADH-90/10-230

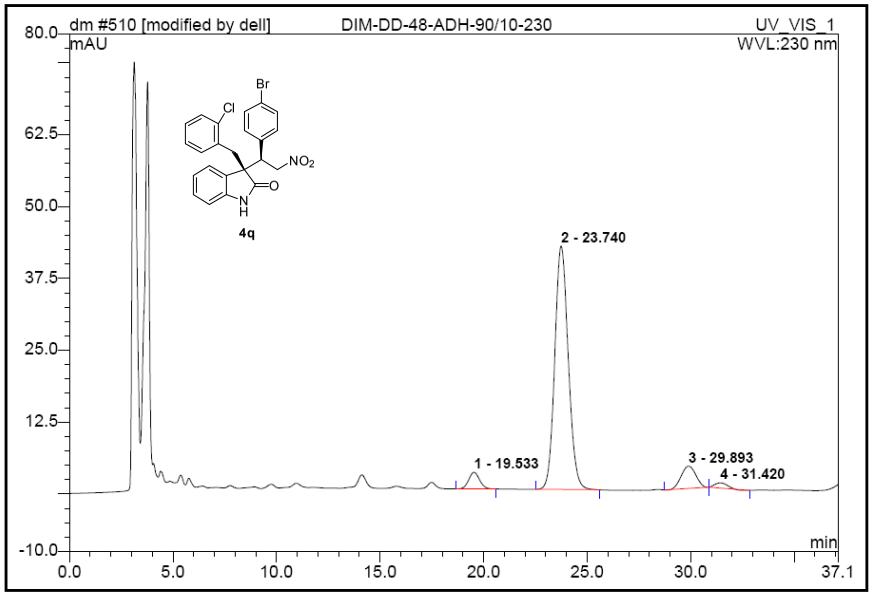
Sample Name:	**DIM-DD-42-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**507**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-21 10:05**	*Sample Weight:*	**1.0000**
Run Time (min):	**37.80**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.21	n.a.	255.527	150.299	23.47	n.a.	BMB
2	23.30	n.a.	230.629	171.173	26.73	n.a.	BMB
3	29.32	n.a.	165.710	146.528	22.88	n.a.	BM
4	30.75	n.a.	178.151	172.457	26.93	n.a.	MB
Total:			830.018	640.458	100.00	0.000	

510 DIM-DD-48-ADH-90/10-230

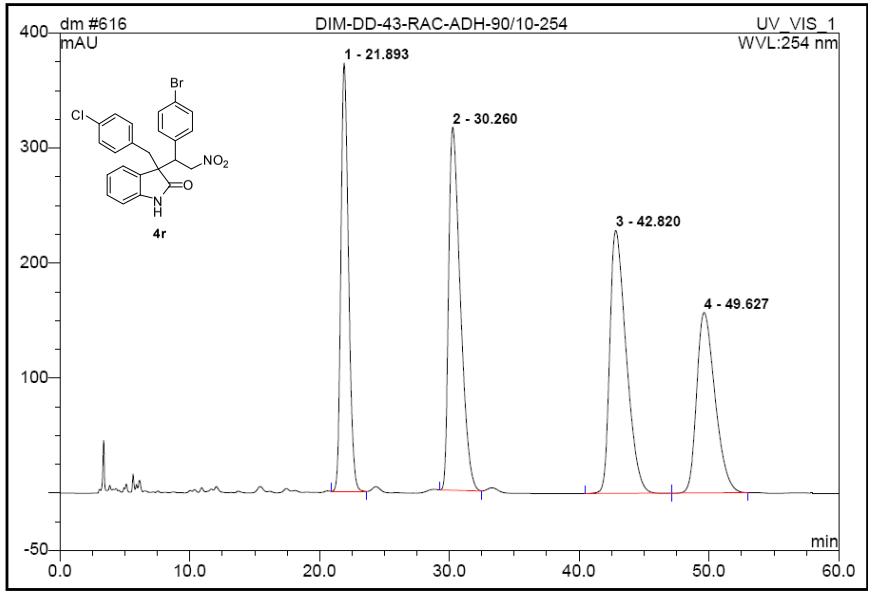
Sample Name:	**DIM-DD-48-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**506**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-21 9:27**	*Sample Weight:*	**1.0000**
Run Time (min):	**37.11**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.53	n.a.	2.882	1.744	4.65	n.a.	BMB*
2	23.74	n.a.	42.322	32.014	85.30	n.a.	BMB
3	29.89	n.a.	3.891	3.170	8.45	n.a.	BMb*
4	31.42	n.a.	0.919	0.604	1.61	n.a.	bMB*
Total:			50.014	37.533	100.00	0.000	

616 DIM-DD-43-RAC-ADH-90/10-254

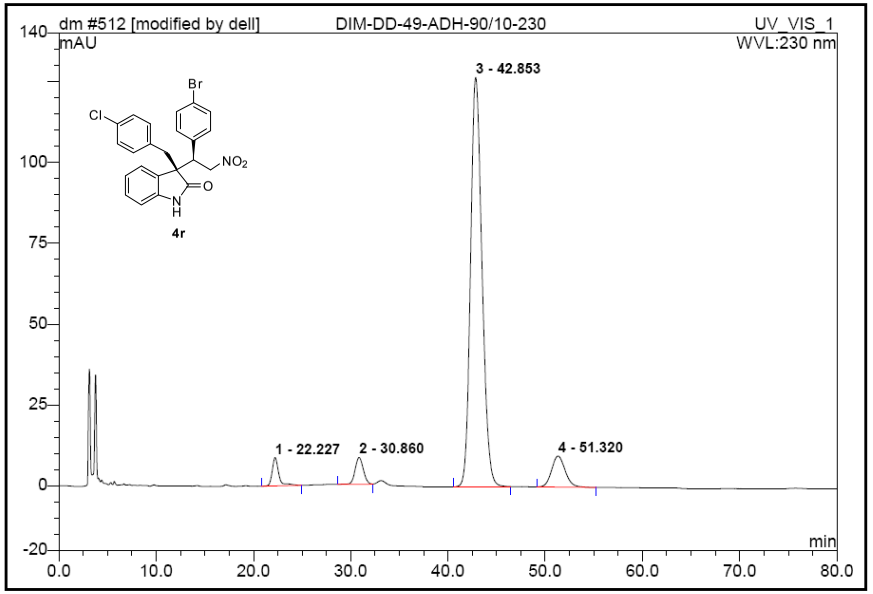
Sample Name:	**DIM-DD-43-RAC-ADH-90/10-254**	*Injection Volume:*	**20.0**
Vial Number:	**610**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-27 17:26**	*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	21.89	n.a.	372.456	254.161	21.62	n.a.	BMB
2	30.26	n.a.	315.765	329.254	28.01	n.a.	BMB
3	42.82	n.a.	228.563	334.919	28.50	n.a.	BM
4	49.63	n.a.	156.873	257.013	21.87	n.a.	MB
Total:			1073.657	1175.347	100.00	0.000	

512 DIM-DD-49-ADH-90/10-230

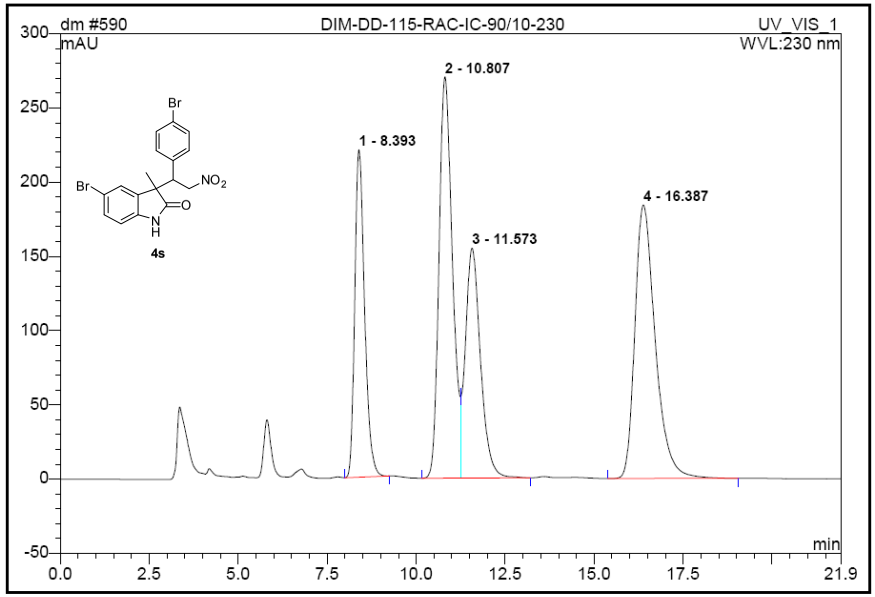
Sample Name:	**DIM-DD-49-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**507**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-1-21 10:43**	*Sample Weight:*	**1.0000**
Run Time (min):	**80.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	22.23	n.a.	8.751	6.797	3.35	n.a.	BMB*
2	30.86	n.a.	8.263	8.046	3.96	n.a.	BMB*
3	42.85	n.a.	126.530	172.645	85.05	n.a.	BMB
4	51.32	n.a.	9.596	15.516	7.64	n.a.	BMB*
Total:			153.139	203.004	100.00	0.000	

590 DIM-DD-115-RAC-IC-90/10-230

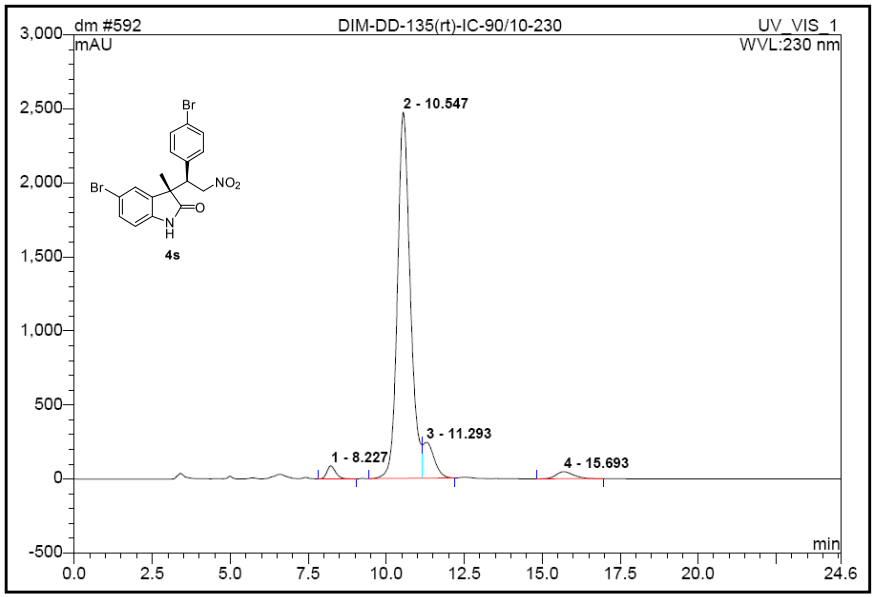
Sample Name:	**DIM-DD-115-RAC-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**584**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-23 10:42**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.93**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.39	n.a.	220.468	70.547	18.20	n.a.	BMB
2	10.81	n.a.	270.248	117.495	30.32	n.a.	BM
3	11.57	n.a.	154.833	77.198	19.92	n.a.	MB
4	16.39	n.a.	184.171	122.313	31.56	n.a.	BMB
Total:			829.720	387.554	100.00	0.000	

592 DIM-DD-135(rt)-IC-90/10-230

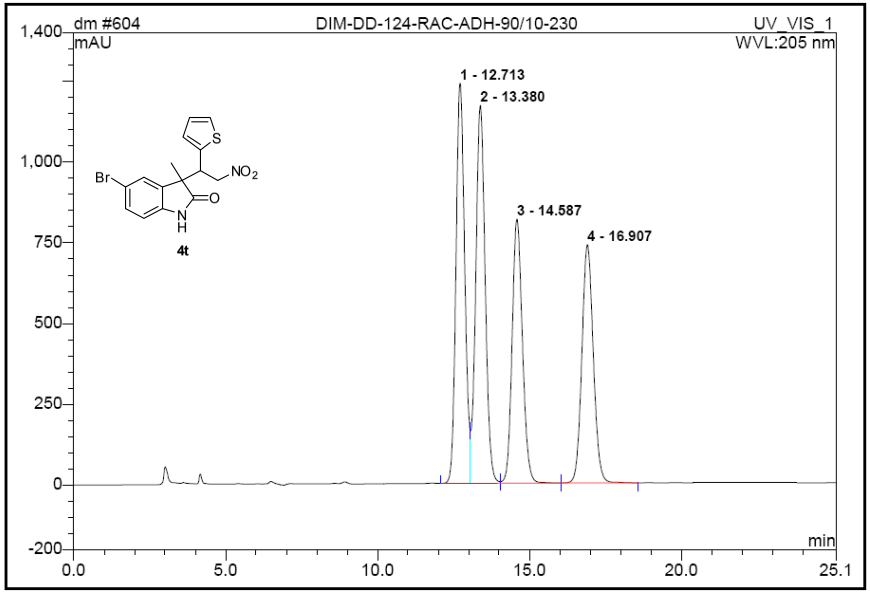
Sample Name:	**DIM-DD-135(rt)-IC-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**586**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-23 11:26**	*Sample Weight:*	**1.0000**
Run Time (min):	**24.57**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.23	n.a.	86.797	27.786	2.08	n.a.	BMB
2	10.55	n.a.	2473.088	1176.907	87.92	n.a.	BM
3	11.29	n.a.	242.488	103.000	7.69	n.a.	MB
4	15.69	n.a.	47.428	30.901	2.31	n.a.	BMB
Total:			2849.802	1338.594	100.00	0.000	

604 DIM-DD-124-RAC-ADH-90/10-230

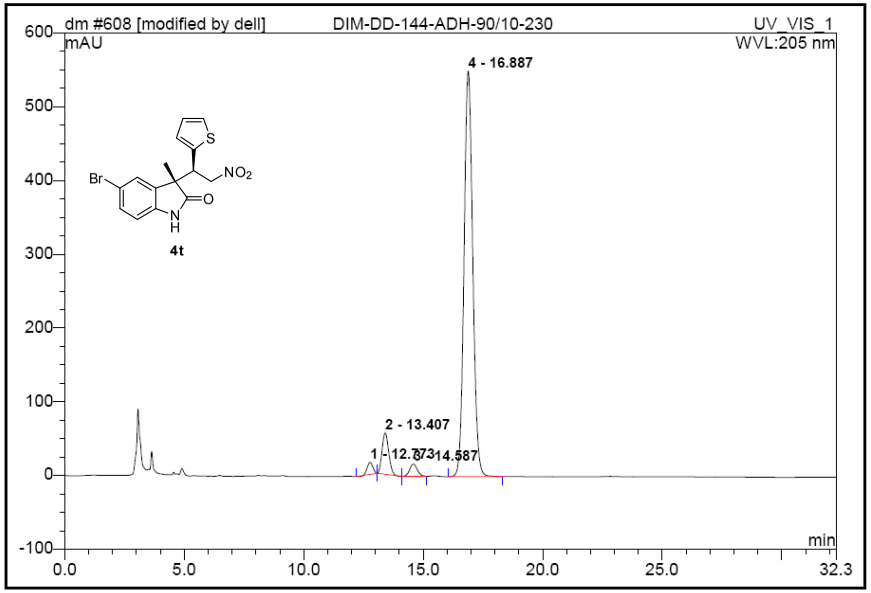
Sample Name:	**DIM-DD-124-RAC-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**598**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**205**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-26 11:45**	*Sample Weight:*	**1.0000**
Run Time (min):	**25.09**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.71	n.a.	1238.689	413.415	28.00	n.a.	BM
2	13.38	n.a.	1169.124	421.012	28.51	n.a.	M
3	14.59	n.a.	816.729	321.269	21.76	n.a.	Mb
4	16.91	n.a.	736.881	320.786	21.73	n.a.	bMB
Total:			3961.423	1476.482	100.00	0.000	

608 DIM-DD-144-ADH-90/10-230

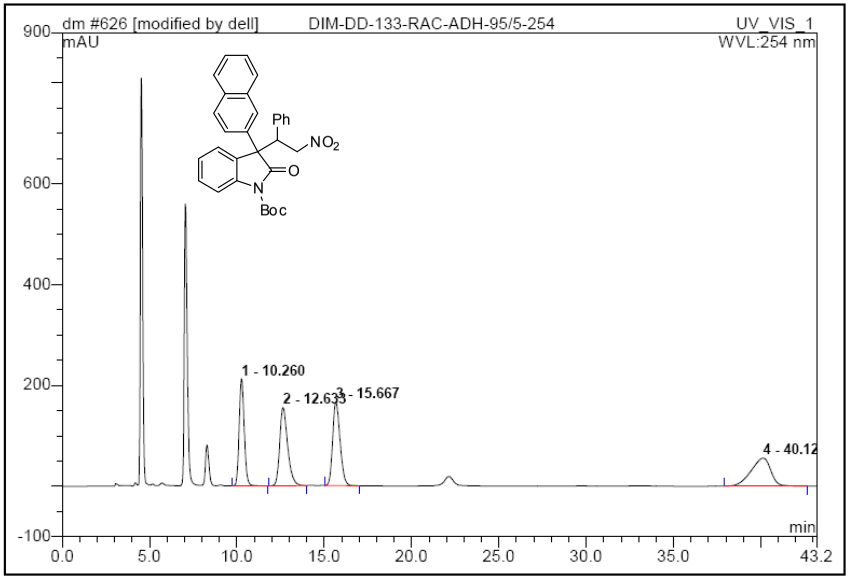
Sample Name:	**DIM-DD-144-ADH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**602**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**205**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-4-26 14:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**32.28**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.77	n.a.	15.985	4.171	1.60	n.a.	BMb*
2	13.41	n.a.	55.910	17.950	6.89	n.a.	bMB*
3	14.59	n.a.	16.538	6.111	2.35	n.a.	BMB*
4	16.89	n.a.	549.845	232.165	89.16	n.a.	BMB
Total:			638.279	260.398	100.00	0.000	

626 DIM-DD-133-RAC-ADH-95/5-254

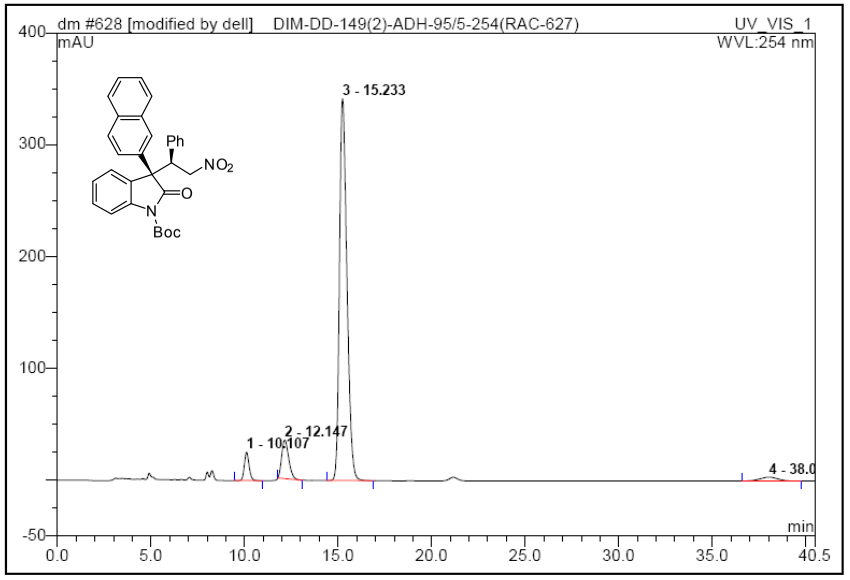
Sample Name:	**DIM-DD-133-RAC-ADH-95/5-254**	*Injection Volume:*	**20.0**
Vial Number:	**621**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-2 9:46**	*Sample Weight:*	**1.0000**
Run Time (min):	**43.20**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.26	n.a.	212.347	71.750	23.29	n.a.	BMB
2	12.63	n.a.	154.827	81.996	26.61	n.a.	BMB
3	15.67	n.a.	165.551	81.428	26.43	n.a.	BMB
4	40.13	n.a.	55.646	72.949	23.68	n.a.	BMB
Total:			588.372	308.123	100.00	0.000	

628 DIM-DD-149(2)-ADH-95/5-254(RAC-627)

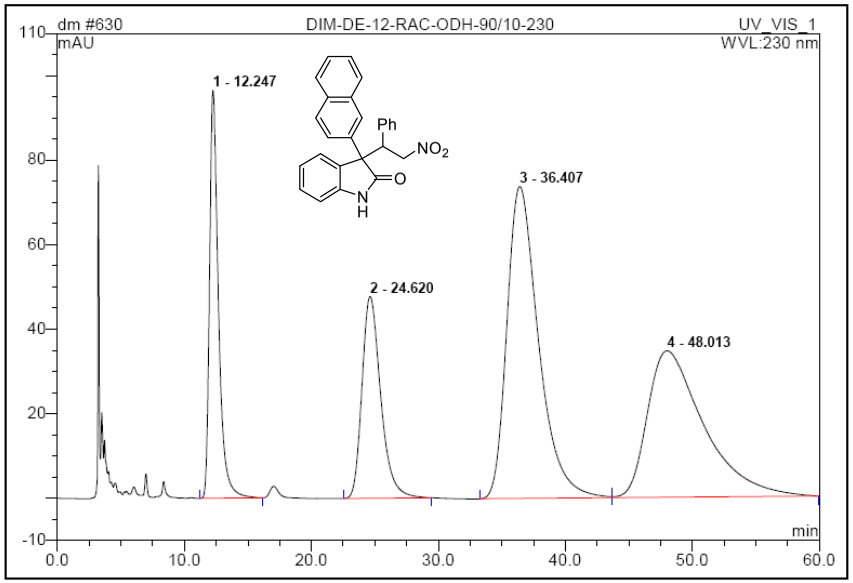
Sample Name:	**DIM-DD-149(2)-ADH-95/5-254(RAC-627)**	*Injection Volume:*	**20.0**
Vial Number:	**623**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-2 11:16**	*Sample Weight:*	**1.0000**
Run Time (min):	**40.48**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.11	n.a.	25.285	7.438	4.03	n.a.	BMB*
2	12.15	n.a.	34.468	14.903	8.08	n.a.	BMB*
3	15.23	n.a.	341.423	158.411	85.86	n.a.	BMB
4	38.02	n.a.	3.393	3.757	2.04	n.a.	BMB*
Total:			404.568	184.508	100.00	0.000	

630 DIM-DE-12-RAC-ODH-90/10-230

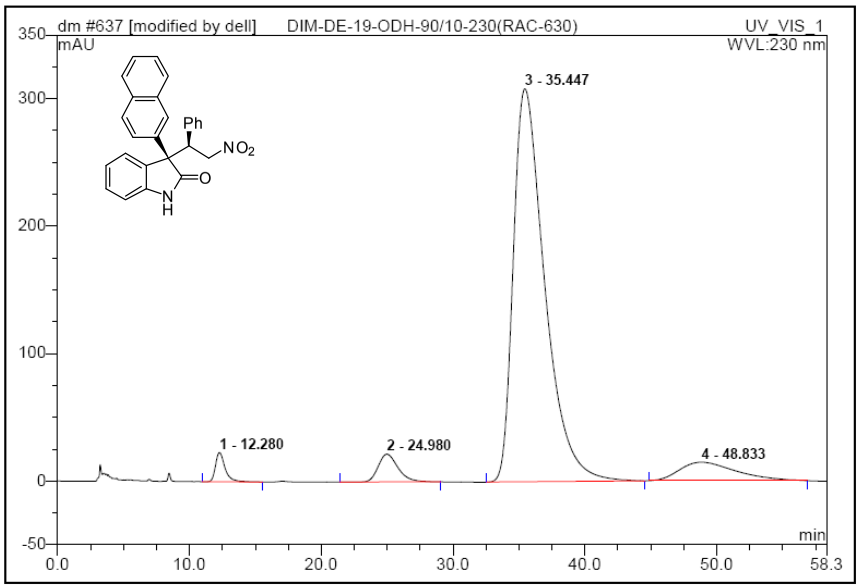
Sample Name:	**DIM-DE-12-RAC-ODH-90/10-230**	*Injection Volume:*	**20.0**
Vial Number:	**625**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-2 22:18**	*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.25	n.a.	96.539	78.450	14.23	n.a.	BMB
2	24.62	n.a.	47.736	81.656	14.81	n.a.	BMB
3	36.41	n.a.	73.834	213.010	38.64	n.a.	BM
4	48.01	n.a.	34.670	178.137	32.31	n.a.	MB
Total:			252.778	551.254	100.00	0.000	

637 DIM-DE-19-ODH-90/10-230(RAC-630)

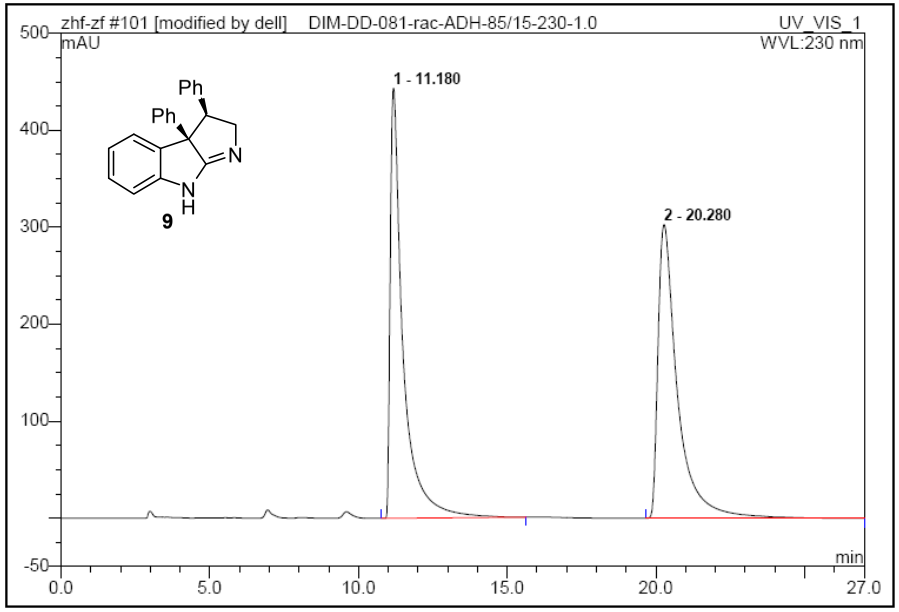
Sample Name:	**DIM-DE-19-ODH-90/10-230(RAC-630)**	*Injection Volume:*	**20.0**
Vial Number:	**632**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**dm**	*Bandwidth:*	**n.a.**
Quantif. Method:	**dm**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-4 21:09**	*Sample Weight:*	**1.0000**
Run Time (min):	**58.34**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.28	n.a.	22.964	19.338	1.97	n.a.	BMB*
2	24.98	n.a.	21.804	38.099	3.89	n.a.	BMB*
3	35.45	n.a.	308.464	851.078	86.81	n.a.	BMB
4	48.83	n.a.	14.481	71.889	7.33	n.a.	BMB*
Total:			367.713	980.405	100.00	0.000	

101 DIM-DD-081-rac-ADH-85/15-230-1.0

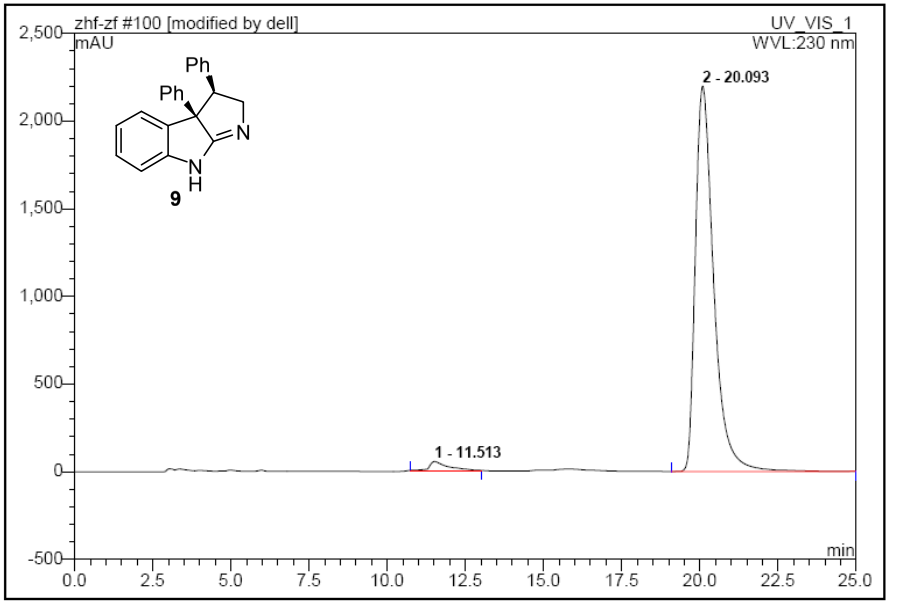
Sample Name:	**DIM-DD-081-rac-ADH-85/15-230-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**190**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-24 16:33**	*Sample Weight:*	**1.0000**
Run Time (min):	**27.01**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.18	n.a.	443.389	221.207	48.83	n.a.	BMB
2	20.28	n.a.	303.024	231.800	51.17	n.a.	BMB
Total:			746.413	453.007	100.00	0.000	

100 zhf-zf-112-P-asy-ADH-85/15-230-1.0

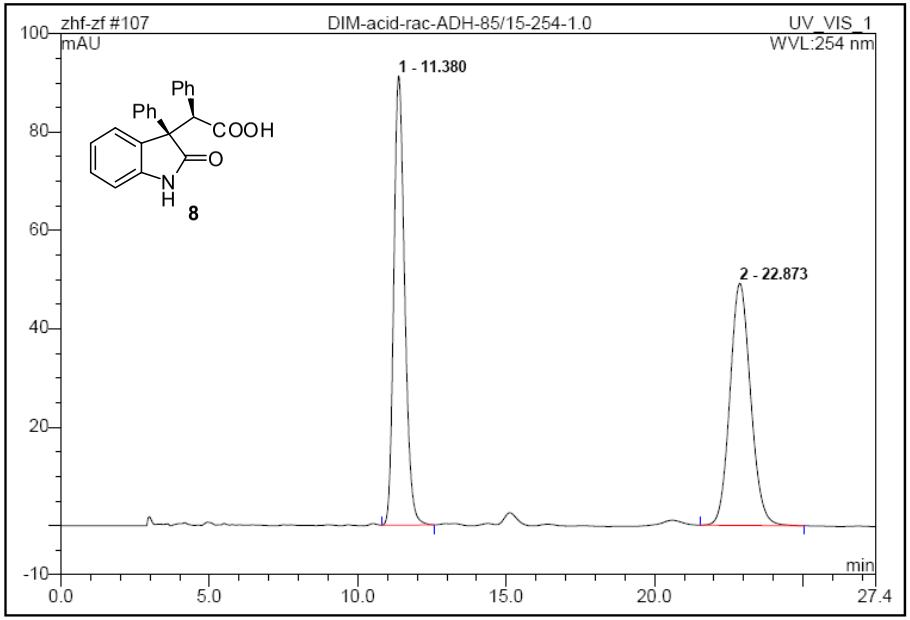
Sample Name:	**zhf-zf-112-P-asy-ADH-85/15-230-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**189**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-24 15:53**	*Sample Weight:*	**1.0000**
Run Time (min):	**24.97**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.51	n.a.	50.922	34.404	2.24	n.a.	BMB*
2	20.09	n.a.	2198.033	1500.028	97.76	n.a.	BMB
Total:			2248.954	1534.432	100.00	0.000	

107 DIM-acid-rac-ADH-85/15-254-1.0

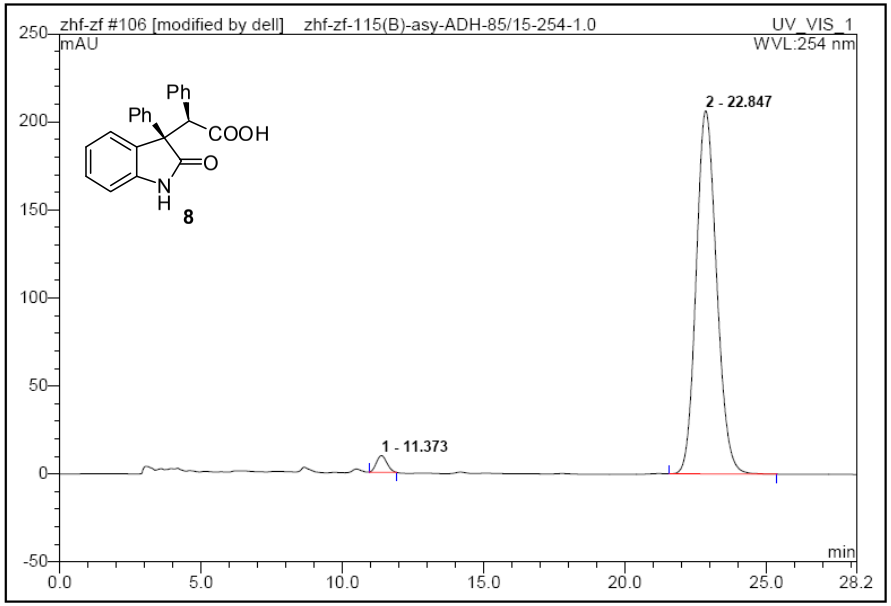
Sample Name:	**DIM-acid-rac-ADH-85/15-254-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**197**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-25 16:30**	*Sample Weight:*	**1.0000**
Run Time (min):	**27.43**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.38	n.a.	91.311	38.657	49.26	n.a.	BMB
2	22.87	n.a.	49.205	39.820	50.74	n.a.	BMB
Total:			140.516	78.477	100.00	0.000	

106 zhf-zf-115(B)-asy-ADH-85/15-254-1.0

Sample Name:	**zhf-zf-115(B)-asy-ADH-85/15-254-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**196**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2011-5-25 15:58**	*Sample Weight:*	**1.0000**
Run Time (min):	**28.18**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.37	n.a.	9.482	4.080	2.30	n.a.	BMB*
2	22.85	n.a.	206.362	173.262	97.70	n.a.	BMB
Total:			215.844	177.342	100.00	0.000	