# Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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2-Benzylsulfonyl-1-(2-chlorophenyl)-7a-(toluene-4-sulfonyl)-2,3,3a,4,5,7a-hexahydro-1H-isoinodole (11b). Colourless crystals, mp 168-170 °C (from ethyl acetate); IR (film) 1348, 1309, 1170, 1139 cm\(^{-1}\); \(^1\)H NMR (400 MHz) \(\delta 7.91 (d, J = 7.7 \text{ Hz}, 2 \text{ H}), 7.69-7.65 (m, 5 \text{ H}), 7.37-7.30 (m, 3 \text{ H}), 7.22-7.10 (m, 2 \text{ H}), 5.81 (s, 1 \text{ H}), 5.80 (m, 1 \text{ H}), 5.22 (dd, \(J = 10.2, 2.3 \text{ Hz}, 1 \text{ H}), 3.97 (dd, \(J = 9.0, 7.9 \text{ Hz}, 1 \text{ H}), 3.65 (dd, \(J = 9.2, 1.9 \text{ Hz}, 1 \text{ H}), 2.77 (\text{ crude q, } J = 9.2 \text{ Hz}, 1 \text{ H}), 2.42 (s, 3 \text{ H}), 1.91-1.82 (m, 1 \text{ H}), 1.75-1.68 (m, 2 \text{ H}), 1.49-1.40 (m, 1 \text{ H}); \(^{13}\)C NMR (50 MHz) \(\delta 145.2, 136.9, 136.3, 135.7, 133.3, 132.3, 131.4, 129.7, 129.3, 129.1, 128.5, 126.5, 121.5, 77.9, 63.3, 54.6, 26.0, 22.8, 21.8; \text{ MS} (m/z, \%) 527 (<1), 372 (100), 230 (88), 77 (53); HRMS calc’d for \(C_{20}H_{19}ClNO_2S\) (M\(^+\) - Ts): 372.0825. Found: 372.0805. Anal. calc’d for \(C_{27}H_{26}ClNO_4S_2\): C, 61.4; H, 5.0; N, 2.65. Found: C, 61.4; H, 5.0; N, 2.5.

2-Benzylsulfonyl-1-(4-methoxyphenyl)-7a-(toluene-4-sulfonyl)-2,3,3a,4,5,7a-hexahydro-1H-isoinodole (11c). White solid, mp 179-181 °C (from ethyl acetate); IR (film) 1352, 1248, 1165, 1143 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta 7.68 (d, J = 7.1 \text{ Hz}, 2 \text{ H}), 7.60-7.50 (m, 4 \text{ H}), 7.25 (d, \(J = 7.9 \text{ Hz}, 2 \text{ H}), 7.08 (d, \(J = 8.5 \text{ Hz}, 2 \text{ H}), 6.75 (d, \(J = 8.9 \text{ Hz}, 2 \text{ H}), 5.76 (\text{ ddd, } J = 10.1, 5.6, 2.6 \text{ Hz}, 1 \text{ H}), 5.20 (s, 1 \text{ H}), 4.92 (dd, \(J = 10.2, 1.6 \text{ Hz}, 1 \text{ H}), 3.77 (s, 3 \text{ H}), 3.73 (dd, \(J = 9.3, 2.4 \text{ Hz}, 1 \text{ H}), 3.52 (dd, \(J = 9.4, 3.0 \text{ Hz}, 1 \text{ H}), 2.60-2.52 (m, 1 \text{ H}), 2.40 (s, 3 \text{ H}), 1.90-1.79 (m, 1 \text{ H}), 1.69-1.57 (m, 2 \text{ H}), 1.45-1.34 (m, 1 \text{ H}); \(^{13}\)C NMR (75 MHz) \(\delta 159.0, 145.0, 135.8, 134.5, 133.0, 132.1, 130.7, 129.9, 129.7, 129.1, 128.9, 128.3, 122.5, 113.3, 76.3, 66.2, 55.1, 53.9, 37.8, 24.8, 22.0, 21.6; \text{ MS} (m/z, \%) 523 (10), 368 (100), 367 (85). HRMS calc’d for \(C_{28}H_{29}ClNO_5S_2\): 523.1487. Found: 523.1519. Anal. calc’d for \(C_{28}H_{29}NO_5S_2\): C, 64.2; H, 5.6; N, 2.7. Found: C, 64.1; H, 5.8; N, 2.6.

2-Benzylsulfonyl-3-phenyl-1,2,3,6,7,7a-hexahydroisoindole-3a-carbonitrile (11d). White solid, mp 176-178 °C (from ethyl acetate); IR (film) 2233, 1348, 1171, 1086 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta 7.67 (d, J = 7.6 \text{ Hz}, 2 \text{ H}), 7.53 (t, J = 7.2 \text{ Hz}, 1 \text{ H}), 7.41 (t, \(J = 7.9 \text{ Hz}, 1 \text{ H}), 7.33-7.24 (m, 6 \text{ H}), 5.70 (dt, \(J = 9.8, 3.7 \text{ Hz}, 1 \text{ H}), 5.29 (d, \(J = 10.1 \text{ Hz}, 1 \text{ H}), 4.73 (s, 1 \text{ H}), 3.85 (dd, \(J = 10.1, 7.6 \text{ Hz}, 1 \text{ H}), 3.47 (dd, \(J = 10.1, 7.4 \text{ Hz}, 1 \text{ H}), 2.88-2.79 (m, 1 \text{ H}), 2.07-1.96 (m, 2 \text{ H}), 1.84-1.73 (m, 1 \text{ H}), 1.63-1.54 (m, 1 \text{ H}); \(^{13}\)C NMR (75 MHz) \(\delta 138.0, 137.0, 132.8, 132.0, 128.8, 128.7, 128.4, 127.4, 127.2, 122.7, 118.9, 70.9, 50.0, 48.2, 39.2, 20.9, 19.6; \text{ MS} (m/z, \%) 364 (70), 118 (100), 91 (45). HRMS calc’d for
C\textsubscript{21}H\textsubscript{20}N\textsubscript{2}O\textsubscript{2}S: 364.1245. Found: 364.1252. Anal. calc'd for C\textsubscript{21}H\textsubscript{20}N\textsubscript{2}O\textsubscript{2}S: C, 69.2; H, 5.5; N, 7.7. Found: C, 69.1; H, 5.8; N, 7.6.

2-Benzensulfonyl-3-(2-chlorophenyl)-1,2,3,6,7,7a-hexahydroisoindole-3a-carbonitrile (11e). Obtained as an inseparable mixture of two diastereoisomers (ca. 1:1) that cocrystallized to afford white sugar-like crystals, mp 179-186 °C (from ethyl acetate); IR (film) 2243, 1352, 1176, 752, 714 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta\) 7.9-7.2 (m, 2 x 9 H, both isomers), 5.83 (dt, \(J = 10.1, 3.8, \) Hz, 1 H), 5.58 (m, 1 H), 5.55 (s, 1 H), 5.27 (d, \(J = 7.5\) Hz, 1 H), 5.22 (s, 1 H), 5.12 (d, \(J = 10.1\) Hz, 1 H), 3.88 (dd, \(J = 9.8, 7.8\) Hz, 1 H), 3.73 (dd, \(J = 10.9, 7.3\) Hz, 1 H), 3.62 (dd, \(J = 10.9, 6.9\) Hz, 1 H), 3.32 (t, \(J = 9.7\) Hz, 1 H), 2.92 (m, 1 H), 2.42 (m, 1 H), 2.1-1.65 (m, 2 x 4 H, both isomers); \(^13\)C NMR (75 MHz) both isomers: \(\delta\) 136.2, 136.1, 135.1, 134.5, 133.7, 133.2, 133.0, 132.3, 131.6, 130.4, 129.9, 129.6, 129.5, 129.45, 129.4, 129.1, 128.4, 128.0, 127.7, 127.2, 126.6, 122.5, 120.8, 120.1, 118.5, 67.1, 67.0, 51.5, 49.5, 47.1, 44.4, 41.9, 38.9, 20.93, 20.88, 20.1, 18.4; MS (m/z, %) 398 (14), 152 (100), 125 (55). HRMS calc'd for C\textsubscript{21}H\textsubscript{19}ClN\textsubscript{2}O\textsubscript{2}S: 398.0856. Found: 398.0838. Anal calc'd for C\textsubscript{21}H\textsubscript{19}ClN\textsubscript{2}O\textsubscript{2}S: C, 63.2; H, 4.8; N, 7.0. Found: C, 63.0; H, 4.85; N, 6.8.

2-Benzensulfonyl-3-(4-chlorophenyl)-1,2,3,6,7,7a-hexahydroisoindole-3a-carbonitrile (11f). White solid, mp 178-180 °C (from ethyl acetate); IR (film): 2239, 1343, 1174 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta\) 7.66 (d, \(J = 7.1\) Hz, 2 H), 7.56 (tt, \(J = 7.4, 1.2\) Hz, 1 H), 7.44 (t, \(J = 7.4\) Hz, 2 H), 7.29-7.20 (m, 4 H), 5.69 (dt, \(J = 9.9, 3.7\) Hz, 1 H), 5.24 (d, \(J = 9.9\) Hz, 1 H), 4.66 (s, 1 H), 3.86 (dd, \(J = 10.3, 7.5\) Hz, 1 H), 3.44 (dd, \(J = 10.3, 7.2\) Hz, 1 H), 2.78 (m, 1 H), 2.12-1.90 (m, 2 H), 1.81-1.70 (m, 1 H), 1.56-1.46 (m, 1 H); \(^13\)C NMR (75 MHz) \(\delta\) 137.5, 135.7, 134.7, 133.1, 132.3, 129.0, 128.7, 128.6, 127.7, 127.4, 122.1, 118.8, 70.3, 50.1, 48.1, 39.2, 21.0, 19.6; MS (m/z, %) 398 (14), 152 (100), 125 (55). HRMS calc'd for C\textsubscript{21}H\textsubscript{19}ClN\textsubscript{2}O\textsubscript{2}S: 398.0856. Found: 398.0838. Anal calc'd for C\textsubscript{21}H\textsubscript{19}ClN\textsubscript{2}O\textsubscript{2}S: C, 63.2; H, 4.8; N, 7.0. Found: C, 63.0; H, 4.85; N, 6.8.

2-Benzensulfonyl-3-(4-cyanophenyl)-1,2,3,6,7,7a-hexahydroisoindole-3a-carbonitrile (11g). White solid, mp 160-164 °C (from ethyl acetate); IR (film): 2228, 1357, 1174 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta\) 7.72-7.60 (m, 5 H), 7.52-7.45 (m, 4 H), 5.77 (dt, \(J = 9.8, 3.7\) Hz, 1 H), 5.27 (d, \(J = 9.9\) Hz, 1 H), 4.73 (s, 1 H), 3.92 (dd, \(J = 10.4, 7.3\) Hz, 1 H), 3.48 (dd, \(J = 10.4, 6.9\) Hz, 1 H), 2.82-2.74 (m, 1 H), 2.15-1.94 (m, 2 H), 1.84-1.73
(m, 1 H), 1.56-1.41 (m, 1 H); $^{13}$C NMR (75 MHz) δ 142.4, 137.3, 133.3, 132.7, 132.2, 129.1, 128.1, 127.4, 121.7, 118.5, 118.3, 112.8, 70.5, 50.5, 48.2, 39.5, 21.1, 19.7; MS (m/z, %) 389 (20), 248 (25), 143 (100), 116 (51). HRMS calc’d for C$_{22}$H$_{19}$N$_3$O$_2$: 389.1198. Found: 389.1187.

4-(2-Benzenesulfonyl-7a-cyano-2,3,3a,4,5,7a-hexahydro-1H-isouindol-1-yl)-benzoic acid methyl ester (11h). White solid, mp 176-179 ºC (from ethyl acetate); IR (film) 2226, 1717, 1283, 1165 cm$^{-1}$; $^1$H NMR (400 MHz) δ 8.02 (d, $J$ = 8.4 Hz, 2 H), 7.70 (d, $J$ = 7.3 Hz, 1 H), 7.59 (t, $J$ = 7.3 Hz, 2 H), 7.38 (d, $J$ = 8.3 Hz, 2 H), 5.77 (dd, $J$ = 9.8, 3.8 Hz, 1 H), 5.32 (d, $J$ = 9.3 Hz, 1 H), 4.79 (s, 1 H), 3.93 (s, 3 H), 3.91 (dd, $J$ = 10.3, 7.4 Hz, 1 H), 3.52 (dd, $J$ = 10.3, 7.1 Hz, 1 H), 2.87-2.79 (m, 1 H), 2.15-1.96 (m, 2 H), 1.84-1.76 (m, 1 H), 1.63-1.54 (m, 1 H); $^{13}$C NMR (75 MHz) δ 166.5, 142.0, 137.8, 135.9, 133.0, 132.3, 130.6, 129.7, 128.9, 127.4, 127.3, 122.3, 70.7, 52.1, 50.2, 48.2, 39.5, 21.0, 19.7; MS (m/z, %) 422 (67), 281 (21), 176 (100). HRMS calc’d for C$_{23}$H$_{22}$N$_2$O$_4$S: 422.1300. Found: 422.1283. Anal calc’d for C$_{23}$H$_{22}$N$_2$O$_4$S: C, 65.4; H, 5.25; N, 6.6. Found: C, 65.0; H, 5.3; N, 6.5.

2-Benzenesulfonyl-3-(1-naphthyl)-1,2,3,6,7,7a-hexahydroisoindole-3a-carbonitrile (11i). White solid, mp 199-201 ºC (from ethyl acetate); IR (film): 2235, 1348, 1162, 959 cm$^{-1}$; $^1$H NMR (300 MHz) δ 7.95 (d, $J$ = 8.4 Hz, 1 H), 7.91 (d, $J$ = 8.2 Hz, 1 H), 7.83 (d, $J$ = 8.2 Hz, 1 H), 7.69 (d, $J$ = 7.5 Hz, 2 H), 7.60-7.50 (m, 4 H), 7.46-7.33 (m, 7 H), 6.07-6.03 (m, 1 H), 5.82 (s, 1 H), 5.60 (d, $J$ = 9.7 Hz, 1 H), 4.52-4.35 (m, 2 H), 4.29 (s, 1 H), 3.00-2.94 (m, 2 H); $^{13}$C NMR (75 MHz) δ 137.9, 133.7, 132.8, 131.9, 131.0, 129.24, 129.20, 128.8, 127.4, 126.4, 125.8, 125.4, 125.0, 122.9, 119.0, 66.3, 50.0, 48.2, 39.8, 20.9, 19.4; MS (m/z, %) 414 (20), 168 (100), 141 (45). HRMS calc’d for C$_{25}$H$_{22}$N$_2$O$_2$: 414.1402. Found: 414.1387. Anal calc’d for C$_{25}$H$_{22}$N$_2$O$_2$: C, 72.4; H, 5.35; N, 6.8. Found: C, 72.4; H, 5.5; N, 6.7.

2-Benzenesulfonyl-3-phenyl-1,2,3,6-tetrahydroisoindole-3a-carbonitrile (12d). White solid, mp 185-187 ºC (from ethyl acetate); IR (film): 2217 1344, 1162, 959 cm$^{-1}$; $^1$H NMR (300 MHz) δ 7.62-7.53 (m, 3 H), 7.46-7.33 (m, 7 H), 6.07-6.03 (m, 1 H), 5.82 (s, 1 H), 5.60 (d, $J$ = 9.7 Hz, 1 H), 4.52-4.35 (m, 2 H), 4.29 (s, 1 H), 2.87-2.69 (m, 2 H); $^{13}$C NMR (75 MHz) δ 137.5, 133.7, 133.0, 129.9, 129.3, 129.1, 128.9, 128.3, 128.1,
127.7, 121.1, 119.2, 117.3, 72.0, 51.3, 47.8, 26.5; MS (m/z, %) 362 (28), 246 (62), 221 (80), 219 (80), 116 (100). HRMS calc’d for C_{21}H_{18}N_{2}O_{2}S: 362.1089. Found: 362.1076. Anal calc’d for C_{21}H_{18}N_{2}O_{2}S: C, 69.6; H, 5.0; N, 7.7. Found: C, 69.25; H, 5.05; N, 7.6.

2-Benzensulfonyl-3-(2-chlorophenyl)-1,2,3,6-tetrahydroisoindole-3a-carbonitrile (12e). Colourless needles; mp 228-229 °C (from ethyl acetate); IR (film) 2224, 1352, 1167, 1081, 1038 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta\) 7.85-7.82 (m, 1 H), 7.72 (d, \(J = 7.3\) Hz, 2 H), 7.49 (t, \(J = 7.5\) Hz, 2 H), 7.40-7.37 (m, 3 H), 6.09-5.97 (m, 1 H), 5.57 (d, \(J = 9.3\) Hz, 2 H), 5.02 (s, 1 H), 4.58-4.45 (m, 1 H), 4.33 (d, \(J = 14.0\) Hz, 1 H), 2.88-2.58 (m, 2 H); \(^{13}\)C NMR (50 MHz) \(\delta\) 136.2, 133.3, 132.8, 132.7, 131.0, 129.4, 129.2, 129.09, 129.05, 128.0, 126.9, 121.5, 119.6, 117.2, 66.6, 51.6, 48.4, 26.3; MS (m/z, %) 396 (4), 280 (17), 219 (100), 116 (100). HRMS calc’d for C_{21}H_{17}ClN_{2}O_{2}S: 396.0699. Found: 396.0704. Anal calc’d for C_{21}H_{17}ClN_{2}O_{2}S: C, 63.55; H, 4.3; N, 7.1. Found: C, 63.3; H, 4.35; N, 6.9.

2-Benzensulfonyl-3-(4-chlorophenyl)-1,2,3,6-tetrahydroisoindole-3a-carbonitrile (12f). White solid, mp 181-183 °C (from ethyl acetate); IR (film) 2230, 1350, 1167, 1091 cm\(^{-1}\); \(^1\)H NMR (400 MHz) \(\delta\) 7.65-7.55 (m, 3 H), 7.46 (t, \(J = 7.7\) Hz, 2 H), 6.10-5.99 (m, 1 H), 5.81 (s, 1 H), 5.55 (d, \(J = 9.6\) Hz, 1 H), 4.47 (dd, \(J = 13.7,\) 2.5 Hz, 1 H), 4.38 (d, \(J = 13.7\) Hz, 1 H), 4.23 (s, 1 H), 2.75 (m, 2 H); \(^{13}\)C NMR (75MHz) \(\delta\) 137.1, 135.1, 133.3, 133.0, 130.2, 129.4, 128.9, 128.6, 127.8, 121.4, 118.9, 117.1, 71.3, 51.4, 47.6, 26.5; MS (m/z, %) 396 (17), 280 (51), 255 (100), 116 (75). HRMS calc’d for C_{21}H_{17}ClN_{2}O_{2}S: 396.0699. Found: 396.0704. Anal calc’d for C_{21}H_{17}ClN_{2}O_{2}S: C, 63.55; H, 4.3; N, 7.1. Found: C, 63.3; H, 4.35; N, 6.9.

2-Benzensulfonyl-3-(1-naphthyl)-1,2,3,6-tetrahydroisoindole-3a-carbonitrile (12i). White solid, mp 225-227 °C (from ethyl acetate); IR (film) 2243, 1357, 1171 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta\) 7.91-7.85 (m, 3 H), 7.81 (d, \(J = 8.2\) Hz, 1 H), 7.54-7.48 (m, 5 H), 7.41-7.31 (m, 3 H), 5.99 (dt, \(J = 9.8, 2.8\) Hz, 1 H), 5.85 (m, 1 H), 5.51 (d, \(J = 9.8\) Hz, 1 H), 5.37 (s, 1 H), 4.55 (s, 2 H), 2.77 (m, 2 H); \(^{13}\)C NMR (75MHz) \(\delta\) 137.4, 133.7, 133.0, 131.1, 129.74, 129.72, 129.5, 129.4, 128.9, 128.7, 128.6, 127.8, 121.1, 119.7, 117.4, 66.0, 51.5, 49.3, 26.4; MS (m/z, %) 412 (6), 296 (33), 269 (55), 154 (77), 116 (100). HRMS calc’d for C_{25}H_{20}N_{2}O_{2}S: 412.1245. Found 412.1241. Anal calc’d for C_{25}H_{20}N_{2}O_{2}S: C, 72.8; H, 4.9; N, 6.8. Found: C, 72.5; H, 5.0; N, 6.6.
2-Benzylsulfonyl-7-methyl-3-phenyl-1,2,3,6-tetrahydroisoindole-3-carbonitrile (13d). White solid, mp 189-191 °C (from ethyl acetate); IR (film) 2227, 1360, 1167 cm\(^{-1}\); \(^1\)H NMR (400 MHz) \(\delta 7.62 (d, J = 7.3 \text{ Hz}, 2 \text{ H}), 7.55 (t, J = 7.5 \text{ Hz}, 1 \text{ H}), 7.44 (d, J = 7.8 \text{ Hz}, 2 \text{ H}), 7.40 (d, J = 8.3 \text{ Hz}, 2 \text{ H}), 7.32 (t, J = 7.1 \text{ Hz}, 3 \text{ H}), 6.03 (ddd, J = 9.6, 4.5, 2.3 \text{ Hz}, 1 \text{ H}), 5.58 (d, J = 9.6 \text{ Hz}, 1 \text{ H}), 4.55 (d, J = 13.9 \text{ Hz}, 1 \text{ H}), 4.40 (d, J = 13.9 \text{ Hz}, 1 \text{ H}), 4.19 (s, 1 \text{ H}), 2.84 (d, J = 22.8 \text{ Hz}, 1 \text{ H}), 2.57 (dd, J = 22.6, 4.2 \text{ Hz}, 1 \text{ H}), 1.73 (s, 3 \text{ H}); \(^{13}\)C NMR (75 MHz) \(\delta 137.5, 134.2, 133.0, 130.1, 129.1, 129.0, 128.8, 128.3, 128.2, 127.8, 119.4, 117.7, 71.6, 49.3, 48.9, 32.1, 18.9; MS (m/z, %) 376 (2), 246 (75), 141 (50), 130 (72), 91 (49), 77 (100). HRMS calc’d for C\(_{22}\)H\(_{20}\)N\(_2\)O\(_2\)S: 376.1245. Found: 376.1236.

2-Benzylsulfonyl-1-(2-chlorophenyl)-2,3-dihydro-1\(H\)-isoindole (14e). White solid, mp 164-167 °C (from ethyl acetate); IR (film): 1350, 1167, 1094 cm\(^{-1}\); \(^1\)H NMR (400 MHz) \(\delta 7.83 (d, J = 7.4 \text{ Hz}, 2 \text{ H}), 7.55-7.53 (m, 1 \text{ H}), 7.51-7.42 (m, 2 \text{ H}), 7.40-7.29 (m, 2 \text{ H}), 7.23-7.15 (m, 5 \text{ H}), 7.00(d, J = 7.6 \text{ Hz}, 1 \text{ H}), 6.45 (d, J = 2.4 \text{ Hz}, 1 \text{ H}), 4.99 (dd, J = 13.4, 2.9 \text{ Hz}, 1 \text{ H}), 4.84 (d, J = 13.4 \text{ Hz}, 1 \text{ H}); \(^{13}\)C NMR (75 MHz) \(\delta 140.1, 139.7, 137.3, 134.8, 132.8, 132.1, 129.9, 129.6, 129.1, 128.9, 128.2, 127.7, 127.3, 123.4, 122.5, 65.9, 54.3; MS (m/z, %) 369 (2), 258 (52), 228 (100). HRMS calc’d for C\(_{20}\)H\(_{16}\)ClNO\(_2\)S: 369.0590. Found: 369.0574.

2-Benzylsulfonyl-1-(4-chlorophenyl)-2,3-dihydro-1\(H\)-isoindole (14f). Off white solid, mp 119-121 °C (from ethyl acetate); IR (film) 1356, 1164, 1097 cm\(^{-1}\); \(^1\)H NMR (300 MHz) \(\delta 7.63 (d, J = 7.2 \text{ Hz}, 2 \text{ H}), 7.51-7.46 (m, 1 \text{ H}), 7.40-7.35 (m, 2 \text{ H}), 7.22-7.10 (m, 5 \text{ H}), 7.00(d, J = 7.6 \text{ Hz}, 1 \text{ H}), 6.45 (d, J = 2.4 \text{ Hz}, 1 \text{ H}), 4.99 (dd, J = 13.4, 2.9 \text{ Hz}, 1 \text{ H}), 4.84 (d, J = 13.4 \text{ Hz}, 1 \text{ H}); \(^{13}\)C NMR (75 MHz) \(\delta 140.4, 140.2, 138.3, 135.0, 133.7, 132.6, 129.0, 128.9, 128.7, 128.2, 128.1, 127.2, 123.6, 68.7, 54.0; MS (m/z, %) 369 (1), 258 (33), 228 (100), 77 (93). HRMS calc’d for C\(_{20}\)H\(_{16}\)ClNO\(_2\)S: 369.0590. Found 369.0580.

2-Benzylsulfonyl-1-(1-naphthyl)-2,3-dihydro-1\(H\)-isoindole (14i). White solid, mp 159-161 °C (from ethyl acetate); IR (film) 1356, 1164, 1097 cm\(^{-1}\); \(^1\)H NMR (400 MHz) \(\delta 7.93 (d, J = 8.0 \text{ Hz}, 1 \text{ H}), 7.83 (d, J = 7.9 \text{ Hz}, 1 \text{ H}), 7.75 (d, J = 8.1 \text{ Hz}, 1 \text{ H}), 7.55 (d, J = 8.1 \text{ Hz}, 2 \text{ H}), 7.44 (t, J = 8.1 \text{ Hz}, 2 \text{ H}), 7.41-7.32 (m, 3 \text{ H}), 7.29-7.19 (m, 4 \text{ H}), 7.09 (t, J = 7.4 \text{ Hz}, 1 \text{ H}), 6.85 (d, J = 7.7 \text{ Hz}, 1 \text{ H}), 6.67 (s, 1 \text{ H}), 5.10 (d, J = 14.6 \text{ Hz}, 1 \text{ H}), 5.05 (d, J = 14.6 \text{ Hz}, 1 \text{ H}); \(^{13}\)C NMR \(\delta 141.3, 138.1, 136.5, 134.6, 134.1, 132.3, 132.0, 129.1, 128.9, 128.2, 128.1, 127.2, 123.6, 68.7, 54.0; MS (m/z, %) 369 (1), 258 (33), 228 (100), 77 (93). HRMS calc’d for C\(_{20}\)H\(_{16}\)ClNO\(_2\)S: 369.0590. Found 369.0580.
130.8, 128.9, 128.7, 128.5, 128.12, 128.08, 127.2, 126.2, 125.5, 125.3, 123.14, 123.11, 122.6, 67.1, 54.2; MS (m/z, %) 385 (21), 258 (53), 242 (85), 77 (100). HRMS calc’d for C$_{24}$H$_{19}$NO$_2$S: 385.1137. Found: 385.1121. Anal calc’d for C$_{24}$H$_{19}$NO$_2$S: C, 74.8; H, 5.0; N, 3.6. Found: C, 74.65; H, 5.0; N, 3.7.

2-Benzensulfonyl-4-methyl-1-phenyl-2,3-dihydro-1H-isooindole (15d). White solid, mp 180-182 °C (from ethyl acetate); IR (film) 1337, 1167, 1094 cm$^{-1}$; $^1$H NMR (400 MHz) $\delta$ 7.65 (d, $J = 8.5$ Hz, 2 H), 7.49 (t, $J = 7.4$ Hz, 1 H), 7.38 (t, $J = 7.7$ Hz, 2 H), 7.28-7.18 (m, 5 H), 7.11 (t, $J = 7.5$ Hz, 1 H), 7.05 (d, $J = 7.3$ Hz, 1 H), 6.73 (d, $J = 7.4$ Hz, 1 H), 5.98 (s, 1 H), 4.89-4.76 (m, 2 H), 2.30 (s, 3 H); $^{13}$C NMR (75 MHz) $\delta$ 141.8, 140.7, 138.6, 134.1, 132.5, 132.4, 128.8, 128.7, 128.5, 128.4, 127.7, 127.2, 120.9, 69.9, 53.4, 18.7; MS (m/z, %) 349 (2), 272 (47), 208 (100), 77 (85). HRMS calc’d for C$_{21}$H$_{19}$NO$_2$S: 349.1137. Found: 349.1125. Anal calc’d for C$_{21}$H$_{19}$NO$_2$S: C, 72.2; H, 5.5; N, 4.0. Found: C, 71.7; H, 5.2; N, 4.0.

2-Benzensulfonyl-3-(4-chlorophenyl)-2,3-dihydro-isooindol-1-one (16f). White solid, mp 166-168 °C (from ethyl acetate); IR (film) 1729, 1362, 1281, 1162, 1086 cm$^{-1}$; $^1$H NMR (300 MHz) $\delta$ 7.89 (d, $J = 7.6$ Hz, 1 H), 7.69 (d, $J = 7.5$ Hz, 2 H), 7.23 (d, $J = 8.4$ Hz, 2 H), 7.16 (d, $J = 7.7$ Hz, 1 H), 7.02 (d, $J = 8.5$ Hz, 2 H), 6.21 (s, 1 H); $^{13}$C NMR (75 MHz) $\delta$ 166.2, 145.9, 138.8, 135.4, 134.5, 133.8, 129.4, 129.3, 129.0, 128.8, 128.6, 127.9, 127.8, 124.9, 123.7, 64.6; MS (m/z, %) 383 (<1), 319 (80), 242 (100). HRMS calc’d for C$_{20}$H$_{14}$ClNO$_3$S: 383.0383. Found: 383.0389.

2-Benzensulfonyl-1-(1-naphthyl)-2,3-dihydro-isooindol-1-one (16i). White solid, mixture of two rotamers, mp 182-183 °C (from ethyl acetate); IR (film): 1729, 1362, 1295, 1176, 1095 cm$^{-1}$; $^1$H NMR (400 MHz; signals from both rotamers are given) $\delta$ 8.54 (d, $J = 8.5$ Hz), 8.03 (m), 7.97 (d, $J = 8.2$ Hz), 7.95-7.87 (m), 7.84-7.68 (m), 7.61 (dt, $J = 14.4$, 7.5 Hz), 7.52 (m), 7.50-7.44 (m), 7.41 (t, $J = 7.8$ Hz), 7.32-7.27 (m), 7.23-7.09 (m), 6.93 (t, $J = 7.8$ Hz), 6.76 (d, $J = 7.2$ Hz), 6.68 (t, $J = 7.6$ Hz), 6.56 (s), 6.50 (d, $J = 8.6$ Hz); when heated to 100 °C, coalescence of numerous signals was observed, while cooling back to room temperature restored the original spectrum; $^{13}$C NMR (75 MHz; signals from both rotamers are given) $\delta$ 166.9, 166.6, 147.2, 145.9, 138.6, 137.9, 134.6, 134.4, 134.11, 134.09, 133.8, 133.1, 133.0, 132.1, 131.2, 130.5, 129.6, 129.3,
2-Benzene sulfonyl-4-methyl-1-phenyl-2,3-dihydro-isoindol-1-one (17d). White solid, mp 162-164 °C (from ethyl acetate); IR (film): 1733, 1362, 1190, 1162, 1100 cm⁻¹; 'H NMR (400 MHz) δ 7.62 (dd, J = 8.5, 1.2 Hz, 2 H), 7.54-7.49 (m, 1 H), 7.41 (t, J = 7.6 Hz, 1 H), 7.36-7.29 (m 3 H), 7.25-7.21 (m, 3 H), 7.09-7.07 (m, 2 H), 6.97 (d, J = 7.6 Hz, 1 H), 6.18 (s, 1 H), 2.71 (s, 3 H); 13C NMR (75 MHz) δ 167.1, 147.0, 139.4, 138.9, 137.1, 133.9, 133.5, 130.9, 128.7, 128.6, 128.5, 128.1, 128.0, 125.9, 121.1, 64.8, 17.5; MS (m/z, %): 363 (<1), 299 (43), 222 (100), 77 (60). HRMS calc’d for C₂₁H₁₇NO₃S: 363.0929. Found: 363.0918.
$^1$H and $^{13}$C NMR Spectra of 11a
$^1$H and $^{13}$C NMR Spectra of 11b
1H and 13C NMR Spectra of 11c
$^1$H and $^{13}$C NMR Spectra of 11d
$^1$H and $^{13}$C NMR Spectra of 11e
$^1$H and $^{13}$C NMR Spectra of 11f
$^1$H and $^{13}$C NMR Spectra of 11g
$^1$H and $^{13}$C NMR Spectra of 11h
$^1$H and $^{13}$C NMR Spectra of 11i
$^1$H and $^{13}$C NMR Spectra of 12d
$^1$H and $^{13}$C NMR Spectra of 12e
$^1$H and $^{13}$C NMR Spectra of 12f
$^1$H and $^{13}$C NMR Spectra of 12i

# Supplementary Material (ESI) for Organic & Biomolecular Chemistry
# This journal is (c) The Royal Society of Chemistry 2009
$^1$H and $^{13}$C NMR Spectra of 13d

# Supplementary Material (ESI) for Organic & Biomolecular Chemistry
# This journal is (c) The Royal Society of Chemistry 2009
$^1$H and $^{13}$C NMR Spectra of 14d
$^1$H and $^{13}$C NMR Spectra of 14e
$^1$H and $^{13}$C NMR Spectra of 14f
$^1$H and $^{13}$C NMR Spectra of 14i
$^1$H and $^{13}$C NMR Spectra of 15d
$^1$H and $^{13}$C NMR Spectra of 16d

# Supplementary Material (ESI) for Organic & Biomolecular Chemistry
# This journal is (c) The Royal Society of Chemistry 2009
$^1$H and $^{13}$C NMR Spectra of 16f
$^1$H and $^{13}$C NMR Spectra of 16i
$^1$H and $^{13}$C NMR Spectra of 17d
X-Ray Crystallographic Data for 11b.

A colorless prismatic crystal of $C_{27}H_{26}ClNO_4S_2$ was coated with Paratone 8277 oil (Exxon) and mounted on a glass fiber. All measurements were made on a Nonius KappaCCD diffractometer with graphite monochromated Mo-$K\alpha$ radiation. Details of crystal data and structure refinement have been provided in Table 1. The data were collected using $\omega$ and $\varphi$ scans. The data were corrected for Lorentz and polarization effects and for absorption using multi-scan method.

The structure was solved by the direct methods and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. The H-atoms were included at geometrically idealized positions and were not refined. The final cycle of full-matrix least-squares refinement using SHELXL97 converged with unweighted and weighted agreement factors, $R = 0.039$ and $wR = 0.103$ (all data), respectively, and goodness of fit, $S = 1.03$. The weighting scheme was based on counting statistics and the final difference Fourier map was essentially featureless. The figure was plotted with the aid of ORTEPII.

Table 1. Crystal data and structure refinement for $C_{27}H_{26}ClNO_4S_2$.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>$C_{27}H_{26}ClNO_4S_2$</td>
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<tr>
<td>Formula weight</td>
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<tr>
<td>Temperature</td>
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<tr>
<td>Wavelength</td>
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<td>Crystal system</td>
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<td></td>
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<td>$b = 11.772(3)$ Å</td>
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<tr>
<td></td>
<td>$\beta = 72.991(15)^\circ$</td>
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<tr>
<td></td>
<td>$c = 12.075(4)$ Å</td>
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<tr>
<td></td>
<td>$\gamma = 65.948(17)^\circ$</td>
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<tr>
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<td>$Z$</td>
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<tr>
<td>Density (calculated)</td>
<td>1.420 Mg/m³</td>
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<tr>
<td>Absorption coefficient</td>
<td>0.359 mm$^{-1}$</td>
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<tr>
<td>$F(000)$</td>
<td>552</td>
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<tr>
<td>Crystal size</td>
<td>0.16 x 0.14 x 0.10 mm$^3$</td>
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</table>
Theta range for data collection  | 3.6 to 27.5°.
Index ranges  | -12≤h≤12, -15≤k≤15, -15≤l≤15
Reflections collected  | 10359
Independent reflections  | 5589 \([R(\text{int}) = 0.026]\)
Completeness to theta = 27.5°  | 98.9 %
Absorption correction  | Multi-scan method
Max. and min. transmission  | 0.9650 and 0.9448
Refinement method  | Full-matrix least-squares on \(F^2\)
Data / restraints / parameters  | 5589 / 0 / 316
Goodness-of-fit on \(F^2\)  | 1.03
Final R indices \([I>2\sigma(I)]\)  | \(R1 = 0.039, \ wR2 = 0.093\)
R indices (all data)  | \(R1 = 0.057, \ wR2 = 0.103\)
Largest diff. peak and hole  | 0.34 and -0.41 e.Å\(^{-3}\)
**X-Ray Crystallographic Data for 11d.**

A colorless prismatic crystal of $C_{21}H_{20}N_2O_2S$ was coated with Paratone 8277 oil (Exxon) and mounted on a glass fiber. All measurements were made on a Nonius KappaCCD diffractometer with graphite monochromated Mo-Kα radiation. Details of crystal data and structure refinement have been provided in Table 1. The data were collected using ω and φ scans. The data were corrected for Lorentz and polarization effects and for absorption using multi-scan method.

The structure was solved by the direct methods and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. The H-atoms were located from a difference map and were included at geometrically idealized positions in a riding mode. The final cycle of full-matrix least-squares refinement using SHELXL97 converged with unweighted and weighted agreement factors, $R = 0.0474$ and $wR = 0.1263$ (all data), respectively, and goodness of fit, $S = 1.016$. The weighting scheme was based on counting statistics and the final difference Fourier map was essentially featureless. The Figure was plotted with the aid of ORTEP-3 for Windows.

Table 2. Crystal data and structure refinement for $C_{21}H_{20}N_2O_2S$.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Empirical formula</td>
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<td>Crystal system</td>
<td>Orthorhombic</td>
</tr>
<tr>
<td>Space group</td>
<td>P b c a</td>
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<td></td>
<td>$b = 9.048(6)$ Å $\beta = 90°$.</td>
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<td></td>
<td>$c = 25.308(9)$ Å $\gamma = 90°$.</td>
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<tr>
<td>Crystal size</td>
<td>0.26 x 0.21 x 0.16 mm³</td>
</tr>
</tbody>
</table>
Theta range for data collection
Index ranges
Reflections collected
Independent reflections
Completeness to theta = 27.48°
Absorption correction
Max. and min. transmission
Refinement method
Data / restraints / parameters
Goodness-of-fit on F^2
Final R indices [I>2sigma(I)]
R indices (all data)
Largest diff. peak and hole

References for X-ray Crystallography