

Supporting Information

for

**Aromatization of IMDAF Adducts in Aqueous Alkaline
Medium (Full paper, RSC Advances,
DOI:10.1039/C2RA20295F)**

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Analytical data for compounds **2c-l**

(3aS*,6R*,7S*,7aR*)-2-Methyl-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (2c)

Yield: 89%; mp 177.5-178.9 °C

This compound was obtained earlier^{5d} [lit.^{5d}: 172-173 °C, yield and other characteristics are not given].

IR (KBr): 1726, 1643 cm⁻¹

¹H NMR (600 MHz, DMSO-*d*₆): δ = 2.46 and 2.74 (two d, ³*J*_{7a,7} = 9.5 Hz, 1 H and 1 H, H-7 and H-7a), 2.74 (s, 3 H, NMe), 3.55 (d, ²*J*_{3,3} = 11.8 Hz, 1 H, H-3B), 3.99 (d, ²*J*_{3,3} = 11.8 Hz, 1 H, H-3A), 4.97 (d, ³*J*_{6,5} = 1.9 Hz, 1 H, H-6), 6.42 (dd, ³*J*_{5,6} = 1.9, ³*J*_{5,4} = 5.7 Hz, 1 H, H-5), 6.57 (d, ³*J*_{4,5} = 5.7 Hz, 1 H, H-4), 12.08 (s, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 29.3 (NMe), 44.4 (C₇), 49.8 (C₃), 50.0 (C_{7a}), 81.1 (C₆), 88.3 (C_{3a}), 135.6 and 136.7 (C₄ and C₅), 170.2 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 209 (15) [M]⁺, 191 (20), 164 (50), 110 (100), 96 (27), 80 (90), 68 (20), 53 (80), 42 (93).

Anal. Calcd for C₁₀H₁₁NO₄: C, 57.41; H, 5.30; N, 6.70. Found: C, 57.21; H, 5.48; N, 6.32.

(3aS*,6R*,7S*,7aR*)-2-Ethyl-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2d)

Yield: 86%; mp 158.7-159.5 °C.

IR (KBr): 1732, 1664 cm⁻¹

¹H NMR (400 MHz, DMSO-*d*₆): δ = 1.02 (t, ³*J* = 7.3 Hz, 3 H, CH₂Me), 2.45 and 2.73 (two d, ³*J*_{7a,7} = 9.5 Hz, 1 H and 1 H, H-7 and H-7a), 3.11 (m, 1 H, CH_BH_AMe), 3.32 (m, 1 H, CH_AH_BMe), 3.55 (d, ³*J*_{3,3} = 11.4 Hz, 1 H, H-3B), 4.01 (d, ³*J*_{3,3} = 11.4 Hz, 1 H, H-3A), 4.96 (d, ³*J*_{6,5} = 1.9 Hz, 1 H, H-6), 6.43 (dd, ³*J*_{5,6} = 1.9, ³*J*_{5,4} = 5.7 Hz, 1 H, H-5), 6.56 (d, ³*J*_{4,5} = 5.7 Hz, 1 H, H-4), 12.07 (s, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 12.3 (CH₂Me), 36.6 (CH₂Me), 44.5, 47.1, 50.3 (C₇, C₃, C_{7a}), 81.1 (C₆), 88.3 (C_{3a}), 135.6 and 136.7 (C₅ and C₄), 169.8 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 223 (11) [M]⁺, 205 (25), 178 (36), 125 (47), 96 (74), 80 (46), 72 (23), 55 (100), 43 (54).

Anal. Calcd for C₁₁H₁₃NO₄: C, 59.19; H, 5.87; N, 6.27. Found: C, 59.31; H, 5.67; N, 6.43.

(3aS*,6R*,7S*,7aR*)-2-Allyl-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2e)

Yield: 75%; mp 122.1-123.4 °C.

IR (KBr): 1713, 1634 cm⁻¹

¹H NMR (400 MHz, DMSO-*d*₆): δ = 2.48 and 2.81 (two d, ³J = 9.5 Hz, 1 H and 1 H, H-7 and H-7a), 3.51 (d, ²J = 12.0 Hz, 1 H, H-3B), 3.82 (m, 2 H, H-1'), 3.97 (d, ²J = 12.0 Hz, 1 H, H-3A), 4.99 (d, ³J_{5,6} = 1.9 Hz, 1 H, H-6), 5.14 (dd, ²J_{3',3'} = 1.9, ³J_{3'cis,2'} = 10.2 Hz, 1 H, H-3'cis), 5.21 (dd, ²J_{3',3'} = 1.9, ³J_{3'trans,2'} = 17.2 Hz, 1 H, H-3'trans), 5.72 (ddt, ³J_{1',2'} = 5.1, ³J_{3'cis,2'} = 10.2, ³J_{3'trans,2'} = 17.2 Hz, 1 H, H-2'), 6.43 (dd, 1 H, ³J_{5,6} = 1.9, ³J_{5,4} = 5.7 Hz, H-5), 6.58 (d, ³J_{4,5} = 5.7 Hz, 1 H, H-6), 12.06 (brs, 1 H, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 44.1 (C_{7a}), 44.6 (C₃), 47.6 (C₇), 50.1 (C_{1'}), 81.2 (C₆), 88.4 (C_{3a}), 116.8 (C_{3'}), 132.5, 135.6, 136.7 (C_{2'}, C₄, C₅), 170.3 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 235 (35) [M]⁺, 219 (60), 194 (78), 176 (63), 162 (25), 136 (85), 108 (55), 96 (65), 80 (100), 53 (86), 43 (31).

Anal. Calcd for C₁₂H₁₃NO₄: C, 61.27; H, 5.57; N, 5.95. Found: C, 61.41; H, 5.18; N, 6.12.

(3aS*,6R*,7S*,7aR*)-2-(2-Furylmethyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2f)

Yield: 83%; mp 144.8-146.3 °C.

This compound was obtained and described earlier^{3d} [lit.^{3d}: 146-148 °C, yield 95%].

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 38.8 (C_{1''}), 44.5 and 49.9 (C_{7a} and C₇), 47.8 (C₃), 81.1 (C₆), 88.2 (C_{3a}), 107.8 and 110.5 (C_{4'} and C_{3'}), 135.5 and 136.6 (C₄ and C₅), 142.6 (C_{5'}), 150.0 (C_{2'}), 170.1 and 172.7 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 275 (3) [M]⁺, 231 (2), 194 (47), 176 (31), 150 (18), 121 (12), 109 (64), 99 (61), 80 (100), 69 (24), 54 (94), 43 (63).

Anal. Calcd for C₁₄H₁₃NO₅: C, 61.09; H, 4.76; N, 5.09. Found: C, 61.31; H, 4.48; N, 5.31.

(3aS*,6R*,7S*,7aR*)-1-Oxo-2-pentyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2g)

Yield: 80%; mp 129.8-130.8 °C.

IR (KBr): 1722, 1643 cm⁻¹

¹H NMR (600 MHz, DMSO-*d*₆): δ = 0.86 (t, ³J = 7.5 Hz, 3 H, Me-5'), 1.17–1.30 (m, 4 H, H-3' and H-4'), 1.41–1.49 (m, 2 H, H-2'), 2.45 and 2.75 (two d, ³J_{7a,7} = 9.3 Hz, 1 H and 1

H, H-7 and H-7a), 3.10 (m, H-1'B), 3.25 (m, H-1'A), 3.55 (d, $^2J_{3,3} = 11.8$ Hz, 1 H, H-3B), 3.98 (d, $^2J_{3,3} = 11.8$ Hz, 1 H, H-3A), 4.97 (d, $^3J_{6,5} = 1.5$ Hz, 1 H, H-6), 6.42 (dd, $^3J_{5,6} = 1.5$, $^3J_{5,4} = 6.2$ Hz, 1 H, H-5), 6.57 (d, $^3J_{4,5} = 6.2$ Hz, 1 H, H-4), 12.04 (brs, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): $\delta = 13.9$ (C_{5'}), 21.8 (C_{4'}), 26.3 (C_{2'}), 28.2 (C_{3'}), 41.6 (C_{1'}), 44.6 (C_{7a}), 47.6 (C₃), 50.3 (C₇), 81.1 (C₆), 88.4 (C_{3a}), 135.6 and 136.7 (C₄ and C₅), 170.1 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 265 (46) [M]⁺, 247 (25), 220 (40), 166 (80), 134 (31), 110 (64), 100 (65), 96 (84), 80 (100), 53 (90), 43 (66).

Anal. Calcd for C₁₄H₁₉NO₄: C, 63.38; H, 7.22; N, 5.28. Found: C, 63.71; H, 7.39; N, 5.12.

(3aS*,6R*,7S*,7aR*)-2-(2,3-Dichlorobenzyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2h)

Yield: 87%; mp 196.6-197.9 °C.

IR (KBr): 1736, 1671 cm⁻¹

¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 2.54$ and 2.91 (two d, $^3J_{7,7a} = 9.2$ Hz, 1 H and 1 H, H-7 and H-7a), 3.59 (d, $^2J_{3,3} = 12.1$ Hz, 1 H, H-3B), 4.03 (d, $^2J_{3,3} = 12.1$ Hz, 1 H, H-3A), 4.48 (d, $^2J = 16.5$ Hz, 1 H, CH₂A_{Ar}), 4.56 (d, $^2J = 16.5$ Hz, 1 H, CH₂B_{Ar}), 5.05 (d, $^3J_{5,6} = 1.6$ Hz, 1 H, H-6), 6.45 (dd, $^3J_{5,6} = 1.6$, $^3J_{4,5} = 5.7$ Hz, 1 H, H-5), 6.60 (d, $^3J_{4,5} = 5.7$ Hz, 1 H, H-4), 7.33 (d, $^3J_{4',5'} = ^3J_{6',5'} = 5.1$ Hz, 2 H, H-4' and H-6'), 7.57 (t, $^3J_{4',5'} = ^3J_{6',5'} = 5.1$ Hz, 1 H, H-5'), 12.14 (brs, 1 H, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): $\delta = 44.0$ (CH₂Ar), 44.6 (C_{7a}), 48.2 (C₃), 50.0 (C₇), 81.2 (C₆), 88.5 (C_{3a}), 127.0 (C_{5'}), 128.2 (C_{4'}), 129.2 (C_{6'}), 130.0 (C_{2'}), 131.8 (C_{3'}), 135.6 and 136.63 (C₄ and C₅), 136.68 (C_{1'}), 170.9 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 355 (5), 353 (7) [M]⁺, 318 (60), 274 (14), 254 (55), 194 (66), 174 (54), 161 (91), 150 (55), 96 (100), 80 (96), 53 (95), 43 (65).

Anal. Calcd for C₁₆H₁₃Cl₂NO₄: C, 54.26; H, 3.70; N, 3.95. Found: C, 55.41; H, 3.52; N, 4.21.

(3aS*,6R*,7S*,7aR*)-2-[2-(3,4-Dimethoxyphenyl)ethyl]-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2i)

Yield: 78%; mp 153.5-154.2 °C.

This compound was obtained and described earlier^{5b,7a,7b} [lit.^{5b}: 134-135 °C, yield 85%; lit.^{7a}: 134-135 °C, yield 84%; lit.^{7b}: 134-135 °C, yield 85%].

¹³C NMR (100.6 MHz, DMSO-*d*₆): $\delta = 32.7$ (CH₂Ar), 43.8 (NCH₂), 44.5 (C_{7a}), 48.2 (C₃), 50.2 (C₇), 55.42 and 55.53 (OCH₃), 81.1 (C₆), 88.4 (C_{3a}), 112.0 and 112.7 (C_{2'} and C_{5'}),

120.4 (C₆), 131.5 (C₁'), 135.6 and 136.7 (C₄ and C₅), 147.3 and 148.7 (C₃' and C₄'), 170.2 and 172.8 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 359 (10) [M]⁺, 315 (5), 164 (80), 152 (65), 110 (76), 98 (44), 80 (100), 65 (19), 53 (67), 43 (64).

Anal. Calcd for C₁₉H₂₁NO₆: C, 63.50; H, 5.89; N, 3.90. Found: C, 63.31; H, 5.73; N, 4.09.

(3aS*,6R*,7S*,7aR*)-2-(3-Chloro-4-methylphenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2j)

Yield: 73%; mp 189.9-191.2 °C.

IR (KBr): 1745, 1691 cm⁻¹

¹H NMR (400 MHz, DMSO-*d*₆): δ = 2.26 (s, 3 H, Me-4), 2.56 and 3.05 (two d, ³J_{7,7a} = 9.2 Hz, 1 H and 1 H, H-7 and H-7a), 4.03 (d, ²J_{3,3} = 11.7 Hz, 1 H, H-3B), 4.48 (d, ²J_{3,3} = 11.7 Hz, 1 H, H-3A), 5.01 (d, ³J_{6,5} = 1.4 Hz, 1 H, H-6), 6.45 (dd, ³J_{5,6} = 1.4, ³J_{5,4} = 5.5 Hz, 1 H, H-5), 6.59 (d, ³J_{4,5} = 5.5 Hz, 1 H, H-4), 7.32 (d, ³J_{5',6'} = 8.2 Hz, 1 H, H-5'), 7.40 (dd, ⁴J_{6',2'} = 2.0, ³J_{6',5'} = 8.2 Hz, 1 H, H-6'), 7.85 (d, ⁴J_{6',2'} = 2.0 Hz, 1 H, H-2'), 12.26 (br.s, 1H, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 18.6 (Me-4), 45.3 and 51.3 (C₇ and C_{7a}), 49.0 (C₃), 81.3 (C₆), 87.1 (C_{3a}), 117.6 and 119.5 (C₂' and C₆'), 130.6 and 133.0 (C₃' and C₄'), 130.9 (C₅'), 135.0 and 136.8 (C₄ and C₅), 138.4 (C₁'), 170.3 and 172.4 (CO₂H and C₁).

MS (EI, 70 eV): *m/z* (%) = 319 (34) [M]⁺, 275 (20), 220 (95), 152 (17), 125 (15), 101 (26), 89 (30), 80 (100), 53 (56), 43 (83).

Anal. Calcd for C₁₆H₁₄ClNO₄: C, 60.10; H, 4.41; N, 4.38. Found: C, 60.31; H, 4.54; N, 4.57.

(3aS*,6R*,7S*,7aR*)-2-Cyclohexyl-4-methylphenyl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindol-7-carboxylic acid (2k)

Yield: 83%; mp 193.7-195.7 °C.

This compound was obtained and described earlier^{3d} [lit.^{3d}: 191-192 °C, yield 90%].

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 24.94, 24.99, 25.13 (C₃', C₄', C₅'), 29.43 and 29.65 (C₂' and C₆'), 43.8 (C₃), 44.6 (C_{7a}), 50.0 and 50.6 (C₇ and C₁'), 81.0 (C₆), 88.3 (C_{3a}), 135.6 and 136.7 (C₅ and C₄), 169.6 and 172.7 (C₁ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 277 (15) [M]⁺, 248 (20), 232 (35), 177 (63), 150 (30), 136 (28), 96 (80), 80 (100), 53 (65), 43 (27).

Anal. Calcd for C₁₅H₁₉NO₄: C, 64.97; H, 6.91; N, 5.05. Found: C, 64.76; H, 6.87; N, 5.22.

(3aS*,6R*,7S*,7aR*)-2-(5-Methylisoxazol-3-yl)-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (2l)

Yield: 83%; mp 205.9-207.4 °C.

IR (KBr): brd 1725 cm⁻¹

¹H NMR (400 MHz, DMSO-*d*₆): δ = 2.40 (br.s, 3 H, Me-5'), 2.62 and 3.10 (two d, ³J_{7,7a} = 8.9 Hz, 1 H and 1 H, H-7 and H-7a), 4.05 (d, ²J_{3,3} = 12.1 Hz, 1 H, H-3B), 4.39 (d, ²J_{3,3} = 12.1 Hz, 1 H, H-3A), 5.05 (d, ³J_{6,5} = 1.7 Hz, 1 H, H-6), 6.49 (dd, ³J_{5,6} = 1.7, ³J_{5,4} = 5.7 Hz, 1 H, H-5), 6.63 (d, ³J_{4,5} = 5.7 Hz, 1 H, H-4), 6.73 (q, ⁴J_{4',Me-5'} = 1.3 Hz, 1 H, H-4'), 12.28 (br.s, 1H, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 12.2 (Me-5'), 45.4 and 50.6 (C₇ and C_{7a}), 47.6 (C₃), 81.5 (C₆), 88.4 (C_{3a}), 94.8 (C_{4'}), 135.1 and 137.2 (C₄ and C₅), 157.9 (br.s, C_{3'} and C_{5'}), 170.3 and 172.6 (CO₂H and C₁).

MS (EI, 70 eV): *m/z* (%) = 276 (10) [M]⁺, 233 (6), 232 (12), 231 (77), 178 (12), 177 (100), 163 (5), 161 (4), 135 (8), 125 (4), 109 (9), 99 (8), 96 (8), 81 (51), 68 (4), 53 (13), 52 (4), 27 (7).

Anal. Calcd for C₁₃H₁₂N₂O₅: C, 56.52; H, 4.38; N, 10.14. Found: C, 56.49; H, 4.50; N, 10.33.

Data for compounds 3c-l

2-Methyl-3-oxoisoindoline-4-carboxylic acid (3c)

This compound was obtained earlier^{5b} [lit.^{5b}: 203-204 °C, yield 58 and 67%, other characteristics are not given].

¹H NMR (600 MHz, DMSO-*d*₆): δ = 3.21 (s, 3 H, NMe), 4.70 (s, 2 H, H-1), 7.80 (t, ³J_{6,5} = ³J_{6,7} = 7.6 Hz, 1 H, H-6), 7.89 (d, ³J_{6,7} = 7.6 Hz, 1 H, H-7), 8.15 (d, ³J_{5,6} = 7.6 Hz, 1 H, H-5), 15.99 (s, CO₂H).

¹³C NMR (100.6 MHz, DMSO-*d*₆): δ = 29.6 (NMe), 52.6 (C₁), 127.2, 131.4, 131.8 (C₅, C₆, C₇), 128.0 and 128.9 (C_{3a} and C₄), 142.8 (C_{7a}), 164.5 and 168.7 (C₃ and CO₂H).

MS (EI, 70 eV): *m/z* (%) = 191 (16) [M]⁺, 147 (100), 118 (97), 110 (41), 89 (55), 80 (30), 76 (66), 63 (85), 51 (45), 43 (63).

2-Ethyl-3-oxoisoindoline-4-carboxylic acid (3d)

¹H NMR (400 MHz, DMSO-*d*₆): δ = 1.26 (t, ³J_{CH₂,Me} = 7.0 Hz, 3 H, CH₂Me), 3.68 (q, ³J_{CH₂,Me} = 7.0 Hz, 2 H, CH₂Me), 4.72 (m, 2 H, H-1), 7.80 (t, ³J_{6,7} = ³J_{6,5} = 7.6 Hz, 1 H, H-6), 7.89 (d, ³J_{7,6} = 7.6 Hz, 1 H, H-7), 8.15 (d, ³J_{5,6} = 7.6 Hz, 1 H, H-5), 16.09 (s, CO₂H).

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 12.5 (CH_2Me), 37.5 (CH_2Me), 50.1 (C_1), 127.3, 131.5, 131.7 (C_5 , C_6 , C_7), 128.1 and 129.0 (C_4 and C_{3a}), 142.9 (C_{7a}), 164.4 and 168.3 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 205 (7) $[\text{M}]^+$, 190 (70), 161 (97), 146 (100), 132 (56), 117 (35), 105 (38), 89 (89), 77 (50), 51 (52), 43 (56).

2-Allyl-3-oxoisindoline-4-carboxylic acid (3e)

^1H NMR (600 MHz, DMSO- d_6): δ = 4.20 (d, $^3J_{1',2'} = 5.5$ Hz, 1 H, H-1'), 4.59 (s, 2 H, H-1), 5.19 (dd, $^2J_{3',3'} = 1.6$, $^3J_{3'\text{cis},2'} = 9.6$ Hz, 1 H, H-1'*cis*), 5.22 (dd, $^2J_{3',3'} = 1.6$, $^3J_{3'\text{trans},2'} = 17.2$ Hz, 1 H, H-1'*trans*), 5.86 (ddt, $^3J_{1',2'} = 5.5$, $^3J_{3'\text{cis},2'} = 9.6$, $^3J_{3'\text{trans},2'} = 17.2$ Hz, 1 H, H-2'), 7.72 (t, $^3J_{6,5} = ^3J_{6,7} = 7.6$ Hz, 1 H, H-6), 7.83 (d, $^3J_{6,7} = 7.6$ Hz, 1 H, H-7), 8.06 (d, $^3J_{5,6} = 7.6$ Hz, 1 H, H-5), 15.99 (br.s, 1 H, CO_2H).

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 45.0 ($\text{C}_{1'}$), 50.6 (C_1), 118.2 ($\text{C}_{3'}$), 128.8 and 128.2 (C_{3a} and C_4), 127.33, 127.42, 131.5, 132.0 ($\text{C}_{2'}$, C_5 , C_6 , C_7), 143.0 (C_{7a}), 164.5 and 168.5 (C_1 and CO_2H).

MS (EI, 70 eV): m/z (%) = 217 (46) $[\text{M}]^+$, 199 (135), 176 (65), 171 (87), 118 (65), 90 (100), 76 (70), 63 (77), 51 (40), 43 (36).

2-(2-Furfurylmethyl)-3-oxoisindoline-4-carboxylic acid (3f)

^1H NMR (600 MHz, DMSO- d_6): δ = 4.60 (s, 2 H, CH_2Furyl), 4.84 (s, 2 H, H-1), 6.43 (dd, $^3J_{4',5'} = 1.8$, $^3J_{3',4'} = 3.4$ Hz, 1 H, H-4'), 6.49 (dd, $^4J_{3',5'} = 0.8$, $^3J_{3',4'} = 3.4$ Hz, H-3'), 7.63 (br.d, $^3J_{4',5'} = 1.8$ Hz, 1 H, H-5'), 7.76 (t, $^3J_{6,7} = ^3J_{6,5} = 7.6$ Hz, 1 H, H-6), 7.84 (d, $^3J_{7,6} = 7.6$ Hz, 1 H, H-7), 8.08 (d, $^3J_{5,6} = 7.6$ Hz, 1 H, H-5).

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 39.0 (CH_2Furyl), 50.4 (C_1), 108.6 and 110.2 ($\text{C}_{3'}$ and C_4'), 127.1, 131.3, 131.8 (C_5 , C_6 , C_7), 128.30 and 128.34 (C_{3a} and C_4), 142.65 (C_{7a}), 142.70 (C_5), 148.6 ($\text{C}_{2'}$), 164.1 and 168.4 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 257 (24) $[\text{M}]^+$, 211 (100), 145 (15), 89 (17), 80 (54), 65 (5), 53 (46), 43 (47).

3-Oxo-2-pentylisindoline-4-carboxylic acid (3g)

^1H NMR (600 MHz, DMSO- d_6): δ = 0.79 (t, $^3J_{\text{Me},4'} = 7.3$ Hz, 3 H, Me-5'), 1.16–1.27 (m, 4 H, H-3' and H-4'), 1.59 (p, $^3J_{2',1'} = ^3J_{2',3'} = 7.3$ Hz, 2 H, H-2'), 3.54 (t, $^3J_{1',2'} = 7.3$ Hz, 2 H, H-1'), 4.64 (s, 2 H, H-1), 7.72 (t, $^3J_{6,7} = ^3J_{6,5} = 7.7$ Hz, 1 H, H-6), 7.82 (dd, $^4J_{7,5} = 0.9$, $^3J_{7,6} = 7.7$ Hz, 1 H, H-7), 8.06 (dd, $^4J_{7,5} = 0.9$, $^3J_{5,6} = 7.7$ Hz, 1 H, H-5).

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 13.5 (Me-5'), 21.5 ($\text{C}_{4'}$), 26.8 and 28.2 ($\text{C}_{2'}$ and $\text{C}_{3'}$), 42.6 ($\text{C}_{1'}$), 50.8 (C_1), 127.4, 131.6, 131.8, (C_5 , C_6 , C_7), 128.1 and 129.0 (C_{3a} and C_4), 143.0 (C_{7a}), 164.5 and 168.6 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 247 (21) $[M]^+$, 229 (13), 218 (44), 203 (99), 190 (100), 161 (54), 146 (66), 104 (34), 89 (79), 51 (25), 43 (46).

2-(2,3-Dichlorobenzyl)-3-oxoisindoline-4-carboxylic acid (3h)

^1H NMR (400 MHz, DMSO- d_6): δ = 4.66 (s, 2 H, NCH_2Ar), 5.00 (s, 2 H, H-1), 7.37–7.41 (m, 2 H, H-4' and H-6'), 7.64 (dd, $^3J_{4',5'} = 5.7$, $^3J_{6',5'} = 7.0$ Hz, 1 H, H-5'), 7.83 (t, $^3J_{6,7} = ^3J_{6,5} = 7.6$ Hz, 1 H, H-6), 7.86 (br.d, $^3J_{7,6} = 7.6$ Hz, 1 H, H-7), 8.16 (br.d, $^3J_{5,6} = 7.6$ Hz, 1 H, H-5), 15.58 (br.s, 1 H, CO_2H).

^{13}C NMR (100.6 MHz, CDCl_3): δ = 44.8 (CH_2Ar), 50.8 (C_1), 127.3 (C_5), 128.1 and 128.4 ($\text{C}_{5'}$ and $\text{C}_{4'}$), 128.3 and 128.5 (C_{3a} and C_4), 129.8 ($\text{C}_{6'}$), 131.3 and 132.03 (C_6 and C_7), 130.4 and 131.98 ($\text{C}_{2'}$ and $\text{C}_{3'}$), 135.5 ($\text{C}_{1'}$), 143.0 (C_{7a}), 164.4 and 168.9 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 337 (2), 335 (2) $[M]^+$, 300 (94), 291 (50), 256 (15), 173 (12), 159 (70), 101 (47), 63 (100), 51 (46), 43 (57).

2-[2-(3,4-Dimethoxyphenyl)ethyl]-3-oxoisindoline-4-carboxylic acid (3i)

This compound was obtained and described earlier^{7a,7b} [lit.^{7a}: 179-178 °C, yield 44%; lit.^{7b}: 179-178 °C, yield 90%].

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 32.8 (CH_2Ar), 44.1 (NCH_2CH_2), 51.1 (C_1), 55.37 and 55.46 (2×OMe), 112.1 and 112.6 ($\text{C}_{2'}$ and $\text{C}_{5'}$), 120.5 ($\text{C}_{6'}$), 127.4, 131.6, 132.0 (C_5 , C_6 , C_7), 128.1, 128.9, 130.7 ($\text{C}_{1'}$, C_{3a} , C_4), 143.0 (C_{7a}), 147.5 and 148.8 ($\text{C}_{3'}$ and $\text{C}_{4'}$), 164.5 and 168.7 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 341 (8) $[M]^+$, 311 (3), 279 (6), 190 (10), 164 (100), 151 (17), 146 (20), 105 (10), 90 (19), 77 (15), 43 (26).

2-(3-Chloro-4-methyl)-3-oxoisindoline-4-carboxylic acid (3j)

^1H NMR (400 MHz, DMSO- d_6): δ = 2.30 (s, 3 H, Me-4'), 5.14 (s, 2 H, H-1), 7.42 (d, $^3J_{5',6'} = 8.2$ Hz, 1 H, H-5'), 7.67 (dd, $^3J_{6',5'} = 8.2$, $^4J_{6',2'} = 1.4$ Hz, 1 H, H-6'), 7.80 (t, $^3J_{6,7} = ^3J_{6,5} = 7.7$ Hz, 1 H, H-6), 7.87 (br.d, $^3J_{7,6} = 7.7$ Hz, 1 H, H-7), 7.96 (d, $^4J_{6',2'} = 1.4$ Hz, 1 H, H-2'), 8.00 (d, $^3J_{5,6} = 7.7$ Hz, 1 H, H-5), 14.84 (br.s, 1 H, CO_2H).

^{13}C NMR (100.6 MHz, DMSO- d_6): δ = 18.2 (Me-4'), 51.4 (C_1), 119.1 and 120.8 ($\text{C}_{2'}$ and $\text{C}_{6'}$), 126.3 ($\text{C}_{5'}$), 128.5 and 129.2 (C_{3a} and C_4), 130.6, 130.9, 132.2 (C_5 , C_6 , C_7), 132.5 and 133.1 ($\text{C}_{3'}$ and $\text{C}_{4'}$), 136.5 ($\text{C}_{1'}$), 142.0 (C_{7a}), 164.4 and 167.5 (C_3 and CO_2H).

MS (EI, 70 eV): m/z (%) = 303 (33), 301 (100) $[M]^+$, 272 (9), 256 (54), 228 (40), 190 (12), 152 (36), 125 (21), 105 (13), 89 (45), 59 (34), 51 (17), 43 (57).

2-Cyclohexyl-3-oxoisindoline-4-carboxylic acid (3k)

This compound was obtained and described earlier^{3d} [lit.^{3d}: 245-246 °C, yield 37%].

^{13}C NMR (100.6 MHz, $\text{DMSO-}d_6$): δ = 24.41 ($\text{C}_{4'}$), 24.55 ($\text{C}_{3'}$ and $\text{C}_{5'}$), 29.8 ($\text{C}_{2'}$ and $\text{C}_{6'}$), 47.3 (C_1), 51.9 ($\text{C}_{1'}$), 127.0, 131.3, 131.5 (C_5 , C_6 , C_7), 128.1 and 129.0 (C_{3a} and C_4), 142.9 (C_{7a}), 164.1 and 167.9 (C_3 and CO_2H).

2-(5-Methyl-1,2-oxazol-3-yl)-3-oxoisindoline-4-carboxylic acid (3I)

^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ = 2.45 (s, 3 H, Me-5'), 5.01 (s, 2 H, H-1), 6.95 (s, 1 H, H-4'), 7.80-7.89 (m, 3 H, H-5, H-6, H-7), 13.89 (br.s, 1 H, CO_2H).

^{13}C NMR (100.6 MHz, $\text{DMSO-}d_6$): δ = 12.2 (Me-5'), 49.3 (C_1), 94.9 ($\text{C}_{4'}$), 126.5, 129.0, 133.2 (C_5 , C_6 , C_7), 127.1 and 130.8 (C_{3a} and C_4), 142.8 (C_{7a}), 157.4 ($\text{C}_{3'}$), 166.18, 166.39, 170.8 (C_3 , $\text{C}_{5'}$, CO_2H).

MS (EI, 70 eV): m/z (%) = 258 (5) $[\text{M}]^+$, 215 (15) 214 (100), 212 (12), 171 (10), 161 (7), 158 (8), 134 (7), 130 (7), 118 (9), 116 (7), 104 (6), 90 (7), 89 (13), 77 (9), 63 (7), 43 (12).