

Supplementary Information

An Investigation on the Weak Interactions Assembling the Crystal Structures of Betti Bases

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Table A. Dihedral angles (°) between mean aryl planes.

	<u><i>naphthyl/phenyl</i></u>	<u><i>naphthyl/ aryl^(B)</i></u>	<u><i>phenyl/ aryl^(B)</i></u>
(<i>S, S</i>)-1	74.06(13) 75.18(11)	35.51(12) 26.01(11)	45.11(14) 55.10(11)
(<i>S, S</i>)-2	81.33(9)	45.05(10)	64.50(11)
(<i>S, S</i>)-3	81.61(9)	43.93(11)	66.59(11)
(<i>S, S</i>)-4	82.82(9)	44.09(12)	68.94(12)
(<i>S, S</i>)-5	71.70(9)	71.20(6)	17.10(9)
(<i>S, S</i>)-6	73.10(8)	75.35(6)	17.95(8)
(<i>S, S</i>)-7	77.66(12)	47.02(10)	59.10(13)
(<i>S, S</i>)-8	77.44(17)	45.97(15)	59.63(19)
(<i>S, S</i>)-9	80.79(11) 77.13(11)	45.27(10) 28.83(12)	43.93(13) 56.20(15)

Spectra of already reported compounds

1-[(S)-(Phenyl)-((1'S)-1'-phenylethylamino)-methyl]-naphthalen-2-ol (1).

¹H-NMR (500MHz, CDCl₃) δ_H 14.04-13.48 (1H, br s, OH), 7.76-7.72 (2H, m, H_{Ar}), 7.44-7.35 (3H, m, H_{Ar}), 7.28-7.17 (11H, m, H_{Ar}), 5.46 (1H, s, CHAr₂), 3.90 (1H, q, ³J_{HH} 6.7 Hz, CHMe), 2.50-2.06 (1H, br s, NH), 1.51 (3H, d, ³J_{HH} 6.7 Hz, CH₃). ¹³C-NMR (125 MHz, CDCl₃) δ_C 157.3 (C_{Ar}), 143.1 (C_{Ar}), 141.5 (C_{Ar}), 132.6 (C_{Ar}), 129.7 (C_{Ar}), 129.0 (C_{Ar}), 128.9 (C_{Ar}), 128.7 (C_{Ar}), 128.0 (C_{Ar}), 127.9 (C_{Ar}), 127.7 (C_{Ar}), 126.9 (C_{Ar}), 126.4 (C_{Ar}), 122.4 (C_{Ar}), 121.1 (C_{Ar}), 120.0 (C_{Ar}), 113.1 (C_{Ar}), 60.3 (CHAr₂), 56.6 (CHMe), 23.0 (CH₃). IR (KBr) 3770m, 3272s, 3056m, 3048m, 3034m, 3023m, 2961m, 2924m, 2367m, 2344m, 1600m, 1439m, 1269s, 1230s, 1076m, 1015s, 946m, 813m, 764s, 742s, 696s.

1-[(R)-(Phenyl)-((1'S)-1'-phenylethylamino)-methyl]-naphthalen-2-ol (1).

¹H-NMR (500MHz, CDCl₃) δ_H 7.74-7.70 (2H, m, H_{Ar}), 7.68 (1H, d, ³J_{HH} 8.9 Hz, H_{Ar}), 7.42-7.39 (2H, m, H_{Ar}), 7.36-7.20 (10H, m, H_{Ar}), 7.13 (1H, d, ³J_{HH} 8.9 Hz, H_{Ar}), 5.87 (1H, s, CHAr₂), 3.98 (1H, q, ³J_{HH} 6.7 Hz, CHMe), 1.59 (3H, d, ³J_{HH} 6.7 Hz, CH₃), 1.60-1.48 (2H, br s, OH and NH). ¹³C-NMR (125 MHz, CDCl₃) δ_C 156.7 (C_{Ar}), 143.0 (C_{Ar}), 141.3 (C_{Ar}), 132.3 (C_{Ar}), 129.7 (C_{Ar}), 129.0 (C_{Ar}), 128.8 (C_{Ar}), 128.7 (C_{Ar}), 128.6 (C_{Ar}), 128.0 (C_{Ar}), 127.9 (C_{Ar}), 127.5 (C_{Ar}), 126.6 (C_{Ar}), 126.5 (C_{Ar}), 122.4 (C_{Ar}), 121.0 (C_{Ar}), 120.3 (C_{Ar}), 114.3 (C_{Ar}), 60.1 (CHAr₂), 55.4 (CHMe), 21.0 (CH₃).

IR (KBr) 3770m, 3303s, 3065m, 3057m, 3049m, 3031m, 2925s, 2370m, 2344m, 1598m, 1441m, 1269s, 1230s, 1089sm, 961s, 807m, 764s, 741s, 689s.

1-[(S)-(4-Chlorophenyl)-((1'S)-1'-phenylethylamino)-methyl]-naphthalen-2-ol (3).

¹H-NMR (500MHz, CDCl₃) δ_H 13.80-13.12 (1H, br s, OH), 7.77-7.71 (2H, m, H_{Ar}), 7.44-7.29 (4H, m, H_{Ar}), 7.27-7.15 (7H, m, H_{Ar}), 7.14-7.09 (2H, m, H_{Ar}), 5.41 (1H, s, CHAr₂), 3.91-3.84 (1H, m, CHMe), 2.32-2.12 (1H, br s, NH), 1.50 (3H, d, ³J_{HH} 6.9 Hz, CH₃). ¹³C-NMR (125 MHz, CDCl₃) δ_C 157.2 (C_{Ar}), 142.9 (C_{Ar}), 139.9 (C_{Ar}), 133.8 (C_{Ar}), 132.4 (C_{Ar}), 129.9 (C_{Ar}), 129.2 (C_{Ar}), 129.1 (C_{Ar}), 129.0 (C_{Ar}), 128.8 (C_{Ar}), 128.7 (C_{Ar}), 128.0 (C_{Ar}), 126.6 (C_{Ar}), 126.5 (C_{Ar}), 122.5 (C_{Ar}), 120.8 (C_{Ar}), 120.0 (C_{Ar}), 112.6 (C_{Ar}), 59.5 (CHAr₂), 56.6 (CHMe), 22.9 (CH₃).

1-[(S)-(4-Bromophenyl)-((1'S)-1'-phenylethylamino)-methyl]-naphthalen-2-ol (4).

¹H-NMR (500MHz, CDCl₃) δ_H 13.63-13.48 (1H, br s, OH), 7.76-7.71 (2H, m, H_{Ar}), 7.42-7.29 (m, 6H, H_{Ar}), 7.25-7.15 (5H, m, H_{Ar}), 7.07-7.04 (2H, m, H_{Ar}), 5.40 (1H, s, CHAr₂), 3.92-3.84 (1H, m, CHMe), 2.26-2.16 (1H, br s, NH), 1.51 (3H, d, ³J_{HH} 6.9 Hz, CH₃). ¹³C-NMR (125 MHz, CDCl₃) δ_C 157.2 (C_{Ar}), 142.9 (C_{Ar}), 140.5 (C_{Ar}), 132.2 (C_{Ar}), 130.0 (C_{Ar}), 129.4 (C_{Ar}), 129.0 (C_{Ar}), 128.8 (C_{Ar}), 128.7 (C_{Ar}), 128.0 (C_{Ar}), 126.6 (C_{Ar}), 126.5 (C_{Ar}), 122.5 (C_{Ar}), 121.9 (C_{Ar}), 120.8 (C_{Ar}), 120.1 (C_{Ar}), 112.5 (C_{Ar}), 59.6 (CHAr₂), 56.6 (CHMe), 22.9 (CH₃).