

**Dioxygenase-catalysed oxidation of disubstituted benzene substrates: benzylic monohydroxylation *versus* aryl *cis*-dihydroxylation and the *meta* effect**

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**Table S1**  $^1\text{H-NMR}$  spectroscopic data for *cis*-dihydrodiol metabolites **2B–12B**, **14B–17B** and **19B**

<i>cis</i> -Dihydrodiol <sup>a</sup>			Ring protons				Exocyclic protons			
R	R'		H-1	H-2	H-4	H-5	H-6	CH <sub>2</sub> CH <sub>2</sub>	CH <sub>2</sub> Me	Me
Me	4-F	<b>2B</b>	4.35, d, <i>J</i> 5.8	4.05, d, <i>J</i> 5.8		5.77, m	m, 5.77	2.10, m 2.31, m		1.03, t, <i>J</i> 7.6
Me	4-Cl	<b>3B</b>	4.29, m	4.04, d, <i>J</i> 5.8		5.82, m	m, 5.29	2.24, q, <i>J</i> 7.6 2.42, q, <i>J</i> 7.6		1.03, t, <i>J</i> 7.6
Me	4-Br	<b>4B</b>	4.29, d, <i>J</i> 5.8	4.05, d, <i>J</i> 5.8		5.96, d, <i>J</i> 9.8	d, 5.65, <i>J</i> 9.8	2.24, q, <i>J</i> 7.5 2.40, q, <i>J</i> 7.5		1.04, t, <i>J</i> 7.5
Me	4-I	<b>5B</b>	4.33, m	4.10, d, <i>J</i> 5.7		6.22, d, <i>J</i> 9.8	m, 5.56	2.41, m		1.08, m
Me	6-F	<b>6B<sup>b</sup></b>	4.22, m	4.22, m	5.48, m	5.48, m		2.14, q, <i>J</i> 7.4		0.97, t, <i>J</i> 7.4
Me	6-Cl	<b>7B</b>	4.29, d, <i>J</i> 6.2	4.27, d, <i>J</i> 6.2	6.09, d, <i>J</i> 6.1	5.64, d, <i>J</i> 6.1		2.29, q, <i>J</i> 7.4		1.10, t, <i>J</i> 7.4
Me	6-Br	<b>8B</b>	4.25, d, <i>J</i> 6.0	4.21, d, <i>J</i> 6.0	6.26, d, <i>J</i> 6.1	5.50, d, <i>J</i> 6.1		2.17, q, <i>J</i> 7.3		1.02, t, <i>J</i> 7.3
Me	6-I	<b>9B</b>	4.27, d, <i>J</i> 5.7	4.22, d, <i>J</i> 5.7	6.63, d, <i>J</i> 5.9	5.45, d, <i>J</i> 5.9		2.24, q, <i>J</i> 7.0		1.09, t, <i>J</i> 7.0
Me	5-F	<b>10B</b>	4.27, d, <i>J</i> 6.0	4.18, d, <i>J</i> 6.0	5.28, m		m, 5.55	2.26, q, <i>J</i> 7.3		1.04, t, <i>J</i> 7.3
Me	5-Cl	<b>11B</b>	4.31, m	4.31, m	5.63, m		m, 5.85	2.31, q, <i>J</i> 7.4		1.11, t, <i>J</i> 7.4
Me	5-Br	<b>12B</b>	4.27, m	4.05, m	5.69, m		m, 6.02	2.32, q, <i>J</i> 7.3		1.11, t, <i>J</i> 7.3
Et	4-F	<b>14B</b>	4.36, d, <i>J</i> 5.7	4.10, m		5.85, m	m, 5.85	2.13, m 2.34, m	1.5, m	0.95, t, <i>J</i> 7.4
Et	6-F	<b>15B<sup>b</sup></b>	4.34, d, <i>J</i> 6.2	4.31, d, <i>J</i> 6.2	5.53, d, <i>J</i> 6.0	5.58, d, <i>J</i> 6.0		2.18, m 2.34, m	1.51, m	0.94, t, <i>J</i> 7.4
Et	6-Cl	<b>16B</b>	4.27, m	4.27, m		5.64, d, <i>J</i> 6.0	d, 6.08, <i>J</i> 6.0	2.22, m	1.52, m	0.94, t, <i>J</i> 7.4
Et	6-Br	<b>17B</b>	4.30, d, <i>J</i> 5.5	4.26, d, <i>J</i> 5.5		5.58, d, <i>J</i> 6.0	d, 6.32, <i>J</i> 6.0	2.18, m	1.50, m	0.94, t, <i>J</i> 7.4
Et	5-Cl	<b>19B<sup>b</sup></b>	4.22, m	4.13, d, <i>J</i> 5.6	5.82, m		d 6.21, <i>J</i> 4.2	2.12, m	1.48, m	0.93, t, <i>J</i> 7.3

<sup>a</sup> All  $^1\text{H-NMR}$  spectra were recorded in  $\text{CDCl}_3$  solution at 500 MHz except where indicated. Coupling constants, *J*, recorded in Hz.

<sup>b</sup>  $^1\text{H-NMR}$  spectrum recorded at 300 MHz.