Supporting Information

Diastereotopic and Deuterium Effects in Gemini

Hubert Maehr, Natacha Rochel, Hong Jin Lee, Nanjoo Suh, Milan Radoje Uskokovic

Elemental Analyses

Compound **6**: Anal calcd for C₃₁H₄₂D₁₂O₄ (502.83) C, 74.05; found C, 73.70

Compound **7a**: Anal calcd for C₃₂H₄₈D₆O₄ (508.81) C, 75.54; found C, 75.22

Compound **7b**: Anal calcd for C₃₁H₄₈D₆O₄ (496.44) C, 74.95; found C, 74.53

Compound **8a**: Anal calcd for C₃₂H₄₈D₆O₄ (508.81) C, 75.54; found C, 75.18

Compound **8b**: Anal calcd for C₃₁H₄₈D₆O₄ (496.44) C, 75.95; found C, 74.59

Crystal data. Data collection and refinement statistics are summarized below.

Compound	7a	7b	8a	8b
PDB ID	4IA2	4IA1	4IA3	4IA7
Resolution (Å)	25.0-2.95 (3.06-2.95)	25.0-2.44 (2.53-2.44)	25.0-2.70 (2.80-2.70)	25.0-2.70 (2.80-2.70)
Crystal space group	P6 ₅ 22	P6 ₅ 22	P6 ₅ 22	P6 ₅ 22
Cell parameters (Å)	a=b=65.770 ; c=266.421	a=b=66.893 ; c=266.886	a=b=66.178 ; c=266.412	a=b=66.044 ; c=266.634
Unique reflections	7983	13792	10366	10345
Mean redundancy	5.7	5.9	8.9	6.3
Rsym (%) [*]	11.6 (37.1)	8.6 (35.0)	9.4 (47.2)	8.9 (43.9)
Completeness (%)	99.8 (99.6)	96.1 (92.5)	98.8 (97.2)	100 (100)
R.m.s.d. bond length (Å) ¶	0.007	0.006	0.007	0.006
R.m.s.d. bond angles (°)	1.18	1.14	1.19	1.14
R _{cryst} (%)§	20.4	21.7	21.0	20.7
R _{free} (%)	25.6	25.6	25.5	25.6

Values in parentheses correspond to the highest resolution shell

^{*}R_{sym} (I) = $\sum_{hkl} \sum_i |I_{hkl,i} - \langle I_{hkl} \rangle| / \sum_{hkl} \sum_i I_{hkl,i}$ with $\langle I_{hkl} \rangle$ the mean intensity of the multiple $I_{hkl,i}$ observations for symmetry-related reflections.

¶Root-mean-squared deviations (R.m.s.d.) are given from ideal values.

§R_{cryst} = $\sum_{hkl} |F_{obs} - F_{calc}| / \sum_{hkl} |F_{obs}|$, where F_{obs} and F_{calc} are the observed and calculated structure amplitudes, respectively. R_{free} is the same as R_{cryst}, but calculated on the 10% of data excluded from refinement.