

Supplementary Table 1

Octane	Chemical Structure	Octane	Chemical Structure
1		9	
2		10	
3		11	
4		12	
5		13	
6		14	
7		15	
8		16	

Supplementary Table 1. Sixteen structural isomers of octane used in conformational comparisons. Isomers **5**, **12** (and its enantiomer **12***), and **13** were investigated in detail in this study.