

Complementing Ultrafast Shape Recognition with an Optical Isomerism Descriptor

Ting Zhou, Karine Lafleur, and Amedeo Caflisch*

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*Department of Biochemistry, University of Zurich,
Winterthurerstrasse 190, CH-8057 Zurich, Switzerland*

Phone: (+41 44) 635 55 21, Fax: (+41 44) 635 68 62

Email: caflisch@bioc.uzh.ch

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*To whom correspondence should be addressed.

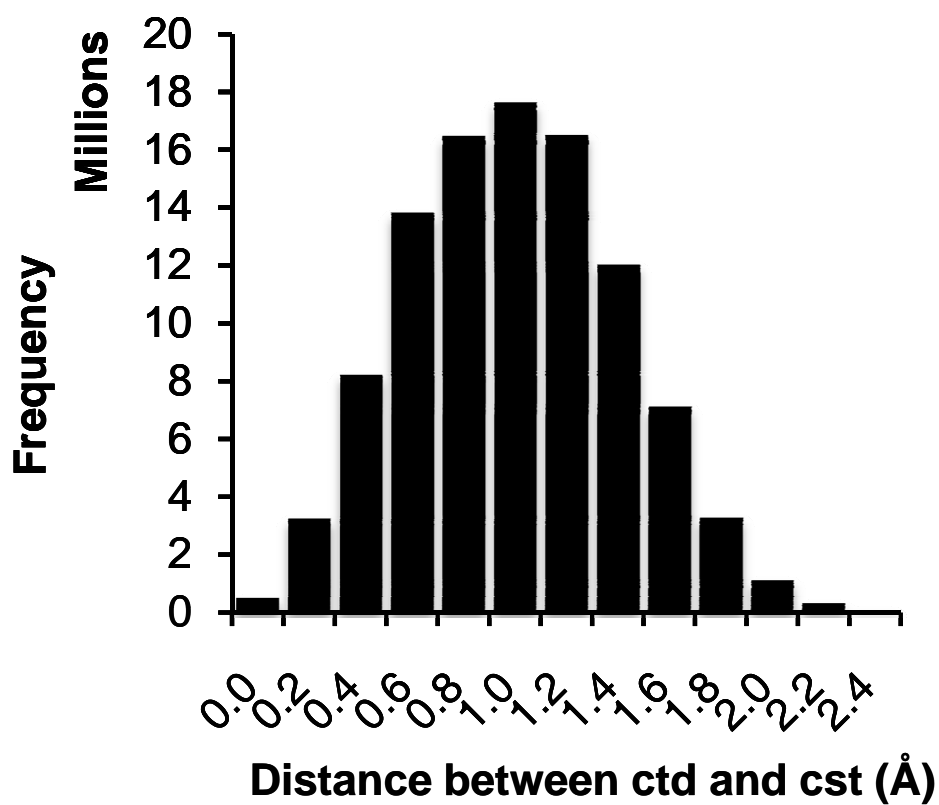


Figure S-1: The distribution of ctd–cst distances of 100 million poses of 2.7 million of molecules. These molecules are from a subset of the ZINC library with molecular weight less than 500 Da.

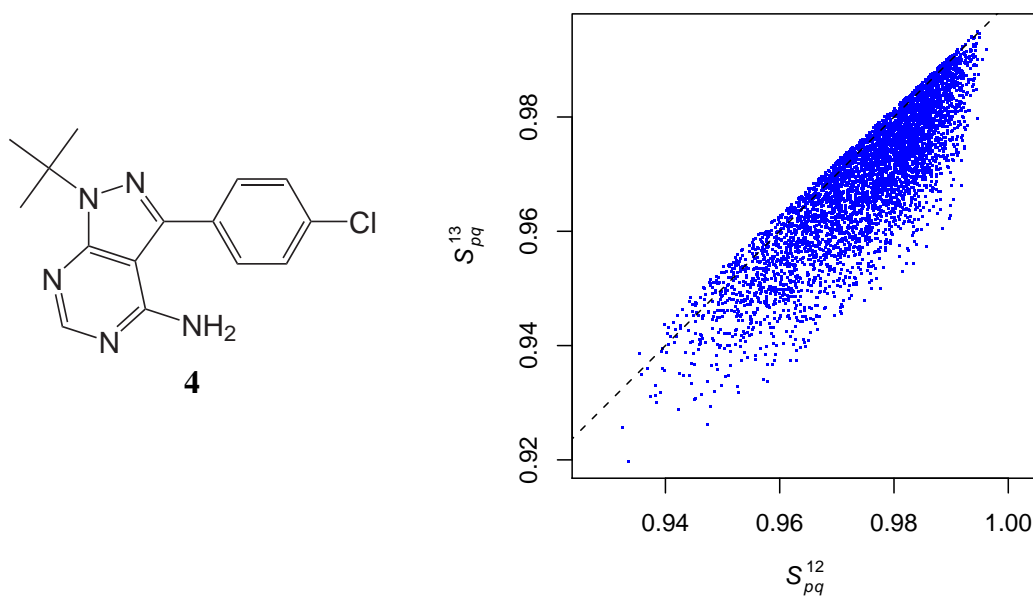


Figure S-2: Pairwise comparison of 100 little fluctuated conformers of compound **4**. The dashed line represents $S_{pq}^{13} = S_{pq}^{12}$.