引用文献について

本ソフトウェアの使用時には、以下の文献を引用してください。

myPresto 全体及び Filling potential 法について

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11) "Noise reduction method for molecular interaction energy: application to in silico drug screening and in silico target protein screening", Y. Fukunishi, S. Kubota, H. Nakamura, Journal of Chemical Information and Modeling, 46, 2071-2084 (2006).
12) "Improvement of protein-compound docking scores by using amino-acid sequence similarities of proteins", Y. Fukunishi, H. Nakamura, Journal of chemical information and modeling, 48, 148-156 (2008)
Docking Score Index (DSI)法について
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14) "An efficient in silico screening method based on the protein-compound affinity matrix and its application to the design of a focused library for cytochrome P450 (CYP) ligands", Y. Fukunishi, S. Hojo, H.Nakamura, Journal of chemical information and modeling, 46, 2610-22 (2006).
Maximum Volume Overlap (MVO)法について
15) "Prediction of protein-ligand complex by docking software guided by other complex structures", Y. Fukunishi, H. Nakamura, Journal of Molecular Graphics and Modelling, 26 (2008) 1030-1033.