

# **MovableType Software for Fast Free-Energy based Virtual Screening: Protocol Development, Deployment, Validation and Assessment**

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## Supporting Information

The Homologous Protein Family (HPF) is a set of homologous proteins which were chosen from the PDBbind dataset and clustered according to 90% sequence similarity. Table S1 is included in order to provide a list of PDBid's which make up the HPF.

Table S1: List of PDB ID's included in the Homologous Protein Family (HPF) Benchmark

Abbreviation	Name	Ligand Count	PDBIDs
14-3-3 $\eta$	14-3-3 protein	12	1O9D, 3E6Y, 3T0L, 3T0M, 4DHM, 4DHN, 4DHO, 4DHP, 4DHQ, 4DHR, 4DHS, 4DHT
DHQD	3-Dehydroquinate dehydratase	22	1GUI, 1V1J, 2C4W, 2C57, 2WKS, 2XB8, 2XB9, 2XD9, 2XDA, 2Y71, 2Y76, 2Y77, 3N76, 3N7A, 3N87, 4B6O, 4B6P, 4B6R, 4CIV, 4GUI, 4IJO
PDPK1	3-phosphoinositide-dependent protein kinase-1	26	1UU7, 1UU8, 1UU9, 1UVR, 1Z5M, 2PE0, 2PE1, 2PE2, 2R7B, 2XCH, 2XCK, 3H9O, 3HRF, 3ION, 3IOP, 3QCQ, 3QCS, 3QCX, 3QCY, 3QD0, 3QD3, 3QD4, 3RCJ, 3RWP, 3RWQ, 4RKQ
AChE	Acetylcholine receptor	38	1ACJ, 1E66, 1EVE, 1GPK, 1GQS, 1H23, 1HBJ, 1J07, 1N5R, 1Q84, 1QON, 1QTI, 1U65, 1UV6, 1UW6, 1VOT, 1W76, 2CKM, 2CMF, 2HA0, 2HA2, 2HA3, 2HA4, 2HA5, 2HA6, 2HA7, 2J3Q, 2PGZ, 2PH9, 2W6C, 2W8F, 2W8G, 2WHP, 2WNC, 2WNJ, 2WNL, 2XUP, 2XYS
FUCA-1	Alpha-L-fucosidase	12	2WVT, 2XII, 2ZWZ, 2ZX7, 2ZX8, 2ZX9, 2ZXA, 2ZXB, 2ZXD, 4J28, 4JFS, 4JFT
GBA3	Beta-glucosidase	22	1OIM, 1UZ1, 1W3J, 2CBU, 2CBV, 2CES, 2CET, 2J75, 2J77, 2J78, 2J79, 2J7B, 2J7D, 2J7E, 2J7F, 2J7G, 2JAL, 2WC3, 2WC4, 4IIC, 4IID, 4IIF
BC	Biotin carboxylase	13	2V59, 2V5A, 2W6M, 2W6N, 2W6O, 2W6Q, 2W6Z, 2W70, 2W71, 3EFR, 3JZF, 3JZI, 3V7S
PKA	Protein kinase A	47	1Q8T, 1Q8U, 1Q8W, 1REK, 1SVE, 1SVH, 1VEB, 1XH4, 1XH6, 1XH7, 1YDR, 1YDS, 1YDT, 2C1A, 2C1B, 2ERZ, 2GNF, 2GNH, 2GNI, 2GNJ, 2GU8, 2JDS, 2JDT, 2JDV, 2OH0, 2OJF, 2UW0, 2UW4, 2UW5, 2UW6, 2UW7, 2UW8, 2VO7, 3AMA, 3AMB, 3DND, 3DNE, 3L9L, 3L9M, 3L9N, 3OW3, 3VQH, 3ZO1, 3ZO2, 3ZO4, 4C35, 4C36
Tryp	Trypsin	20	3AAV, 3ATI, 3ATK, 3ATL, 3ATM, 3NK8, 3RXA, 3RXB, 3RXD, 3RXE, 3RXF, 3RXG, 3RXH, 3RXI, 3RXK, 3RXL, 3RXM, 3RXO, 3RXP, 4AB8
DSP	Dual-specificity phosphatase	36	2WU6, 2WU7, 2ZMD, 3ANQ, 3ANR, 3GFW, 3H9F, 3KVW, 3OS3, 3PP1, 3V01, 3V04, 3VQU, 3W1F, 3WIG, 3ZLS, 3ZLW, 3ZLX, 3ZLY, 3ZM4, 4AN2, 4AN3, 4AN9, 4ANB, 4ARK, 4AZE, 4BHZ, 4BI0, 4BI1, 4C4E, 4C4F, 4C4G, 4C4H, 4C4I, 4C4J, 4LMN

All prepared structural files (including input, output, and associated structures) for both the HPF set and the CASF set are available at:

<http://downloads.quantumbioinc.com/media/tutorials/MT/MT-FreeEnergyPaper.tar.bz2>