

Supporting Information for

Drug-like Bioactive Structures and Conformational Coverage with the
LigPrep/ConfGen Suite: Comparison to Programs MOE and Catalyst

Table S1. List of proteins-ligand complexes for the Vernalis generic and folded compound sets. 17 compounds from the generic set are also part of the folded set. Entries within a dataset are sorted on the PDB ID. For all complexes, the structures were obtained by X-ray crystallography.

PDB ID	Protein (or RNA for 1HNX)	X-ray Resolution (Å)	Generic set	Folded set
13GS	GLUTATHIONE S-TRANSFERASE	1.9	Yes	
1A28	PROGESTERONE RECEPTOR	1.8	Yes	
1A42	CARBONIC ANHYDRASE II	2.25	Yes	
1A4K	ANTIBODY FAB	2.4	Yes	
1A8T	METALLO-BETA-LACTAMASE	2.55	Yes	
1AFQ	BOVINE GAMMA-CHYMOTRYPSIN	1.8	Yes	
1AOE	DIHYDROFOLATE REDUCTASE	1.6	Yes	
1ATL	ATROLYSIN C	1.8	Yes	
1AZM	LYASE(OXO-ACID)	2	Yes	
1BJU	BETA-TRYPSIN	1.8	Yes	
1BL6	P38 MAP KINASE	2.5	Yes	
1BMK	P38 MAP KINASE	2.4	Yes	
1BNW	CARBONIC ANHYDRASE	2.25	Yes	
1BQO	STROMELYSIN-1	2.3	Yes	
1BR6	RICIN	2.3	Yes	
1BX6	C-AMP DEPENDENT KINASE	2.1	Yes	
1BZS	NEUTROPHIL COLLAGENASE (MMP8)	1.7	Yes	
1C1C	HIV-1 REVERSE TRANSCRIPTASE	2.5	Yes	
1C83	TYROSINE PHOSPHATASE 1B	1.8	Yes	
1CAQ	STROMELYSIN	1.8	Yes	
1CBS	RETINOIC-ACID-BINDING PROTEIN	1.8	Yes	
1CBX	CARBOXYPEPTIDASE A	2	Yes	
1CET	L-LACTATE DEHYDROGENASE	2.05	Yes	
1CIM	LYASE(OXO-ACID)	2.1	Yes	
1D3G	DIHYDROOROTATE DEHYDROGENASE	1.6	Yes	
1D3P	ALPHA-THROMBIN	2.1	Yes	
1D4P	ALPHA-THROMBIN	2.07	Yes	
1D6V	CATALYTIC ANTIBODY AZ-28	2	Yes	
1DAM	DETHIOBIOTIN SYNTHETASE	1.8	Yes	
1DI8	CYCLIN-DEPENDENT KINASE II	2.2	Yes	
1DIB	METHYLENETETRAHYDROFOLATE	2.7	Yes	
1DLR	OXIDO-REDUCTASE	2.3	Yes	
1DYR	DIHYDROFOLATE REDUCTASE	1.86	Yes	
1E1V	CYCLIN-DEPENDENT KINASE II	1.95	Yes	
1E9H	CYCLIN-DEPENDENT KINASE II-CYCLIN	2.5	Yes	
1ECV	TYROSINE PHOSPHATASE 1B	1.95	Yes	
1EFY	POLY (ADP-RIBOSE) POLYMERASE	2.2	Yes	
1EJN	UROKINASE	1.8	Yes	
1ELA	HYDROLASE(SERINE PROTEINASE)	1.8	Yes	
1EP4	HIV-1 REVERSE TRANSCRIPTASE	2.5	Yes	

1ETR	HYDROLASE(SERINE PROTEINASE)	2.2	Yes	Yes
1ETT	HYDROLASE(SERINE PROTEINASE)	2.5	Yes	Yes
1EVE	ACETYLCHOLINESTERASE	2.5	Yes	
1EXA	RETINOIC ACID RECEPTOR GAMMA-2	1.59	Yes	
1F0R	COAGULATION FACTOR XA	2.1	Yes	
1F0T	TRYPSIN	1.8	Yes	
1F0U	TRYPSIN	1.9	Yes	
1F4E	THYMIDYLATE SYNTHASE	1.9	Yes	
1F4F	THYMIDYLATE SYNTHASE	2	Yes	
1F4G	THYMIDYLATE SYNTHASE	1.75	Yes	
1FCX	RETINOIC ACID RECEPTOR GAMMA-1	1.47	Yes	
1FCZ	RETINOIC ACID NUCLEAR RECEPTOR	1.38	Yes	
1FCZ	RETINOIC ACID RECEPTOR GAMMA-1	1.38	Yes	
1FJS	COAGULATION FACTOR XA	1.92	Yes	
1FK9	HIV-1 REVERSE TRANSCRIPTASE	2.5	Yes	
1FKG	FK506 BINDING PROTEIN	2	Yes	
1FKG	CIS-TRANS ISOMERASE	2	Yes	
1FM6	RETINOIC ACID RECEPTOR RXR-ALPHA	2.1	Yes	
1FM9	RETINOIC ACID RECEPTOR RXR-ALPHA	2.1	Yes	
1FPU	ABL KINASE	2.4	Yes	
1FRB	FR-1 PROTEIN	1.7	Yes	
1FRB	FR-1 PROTEIN	1.7	Yes	
1FTM	GLUTAMATE RECEPTOR-2	1.7	Yes	
1FVT	CYCLIN-DEPENDENT KINASE II	2.2	Yes	
1G4O	CARBONIC ANHYDRASE II	1.96	Yes	
1GII	CYCLIN-DEPENDENT KINASE II	2	Yes	
1GIJ	CYCLIN-DEPENDENT KINASE II	2.2	Yes	
1GR2	GLUTAMATE RECEPTOR-2	1.9	Yes	
1GWX	PPAR-DELTA	2.5	Yes	
1GZ8	CYCLIN-DEPENDENT KINASE II	1.3	Yes	
1H07	CYCLIN-DEPENDENT KINASE II	1.85	Yes	Yes
1H0V	CYCLIN-DEPENDENT KINASE II	1.9	Yes	
1H0W	CYCLIN-DEPENDENT KINASE II	2.1	Yes	
1H1R	CYCLIN-DEPENDENT KINASE II-CYCLIN	2	Yes	
1H1S	CYCLIN-DEPENDENT KINASE II	2	Yes	
1H9U	RETINOID X RECEPTOR	2.7	Yes	
1HDQ	CARBOXYPEPTIDASEA	2.3	Yes	
1HFC	METALLOPROTEASE	1.56	Yes	
1HPV	HYDROLASE (ACID PROTEINASE)	1.9	Yes	
1HTF	HYDROLASE(ACID PROTEINASE)	2.2	Yes	
1I7Z	ANTIBODY GNC92H2	2.3	Yes	
1I8Z	CARBONIC ANHYDRASE II	1.93	Yes	
1IAN	P38 MAP KINASE	2	Yes	
1IEP	ABL KINASE	2.1	Yes	
1IF7	CARBONIC ANHYDRASE II	1.98	Yes	
1IY7	CARBOXYPEPTIDASE A	2	Yes	
1JLA	HIV-1 REVERSE TRANSCRIPTASE	2.5	Yes	
1JSV	CYCLIN-DEPENDENT KINASE II	1.96	Yes	

1K1J	TRYPSIN	2.2	Yes	Yes
1K22	PROTHROMBIN	1.93	Yes	
1K7E	TRYPTOPHAN SYNTHASE ALPHA CHAIN	2.3	Yes	
1K7F	TRYPTOPHAN SYNTHASE ALPHA CHAIN	1.9	Yes	
1KE5	CYCLIN-DEPENDENT KINASE II	2.2	Yes	
1KE6	CYCLIN-DEPENDENT KINASE II	2	Yes	
1KE7	CYCLIN-DEPENDENT KINASE II	2	Yes	
1KE8	CYCLIN-DEPENDENT KINASE II	2	Yes	
1KE9	CYCLIN-DEPENDENT KINASE II	2	Yes	
1KV1	P38 MAP KINASE	2.5	Yes	
1KV2	P38 MAP KINASE	2.8	Yes	
1L2S	BETA-LACTAMASE	1.94	Yes	
1L8G	PROTEIN-TYROSINE PHOSPHATASE	2.5	Yes	
1LQD	BLOOD COAGULATION FACTOR XA	2.7	Yes	
1M48	INTERLEUKIN-2	1.95	Yes	
1M7Q	P38 MAP KINASE	2.4	Yes	
1MMB	NEUTROPHIL COLLAGENASE	2.1	Yes	Yes
1MQ5	COAGULATION FACTOR X	2.1	Yes	
1MQ6	COAGULATION FACTOR X	2.1	Yes	
1MTV	TRYPSIN	1.9	Yes	
1MTW	TRYPSIN	1.9	Yes	
1NHU	HCV RNA POLYMERASE	2	Yes	
1NHV	HCV RNA POLYMERASE	2.9	Yes	Yes
1O86	ANGIOTENSIN CONVERTING ENZYME	2	Yes	
1O9U	GLYCOGEN SYNTHASE KINASE 3 BETA	2.4	Yes	
1OHR	ASPARTYLPROTEASE	2.1	Yes	
1OI9	CYCLIN-DEPENDENT KINASE II	2.1	Yes	
1OIQ	CYCLIN-DEPENDENT KINASE II	2.31	Yes	
1OIR	CYCLIN-DEPENDENT KINASE II	1.91	Yes	
1OIT	CYCLIN-DEPENDENT KINASE II	1.6	Yes	
1OPK	ABL KINASE	1.8	Yes	
1OUK	P38 MAP KINASE	2.5	Yes	
1OUY	P38 MAP KINASE	2.5	Yes	
1OVE	P38 MAP KINASE	2.1	Yes	
1OZ1	P38 MAP KINASE	2.1	Yes	
1P2A	CYCLIN-DEPENDENT KINASE II	2.5	Yes	
1PHG	CYTOCHROME P450-CAM	1.6	Yes	
1PMQ	MITOGEN-ACTIVATED PROTEIN KINASE 10	2.2	Yes	
1PPC	TRYPSIN	1.8	Yes	Yes
1PPC	HYDROLASE(SERINE PROTEINASE)	1.8	Yes	Yes
1PPH	TRYPSIN	1.9	Yes	Yes
1PPH	HYDROLASE(SERINE PROTEINASE)	1.9	Yes	Yes
1PXI	CYCLIN-DEPENDENT KINASE II	1.95	Yes	
1PXJ	CYCLIN-DEPENDENT KINASE II	2.3	Yes	
1PXL	CYCLIN-DEPENDENT KINASE II	2.5	Yes	
1PXN	CYCLIN-DEPENDENT KINASE II	2.5	Yes	
1PXP	CYCLIN-DEPENDENT KINASE II	2.3	Yes	
1PY5	TGF-BETA RECEPTOR TYPE I	2.3	Yes	

1PYE	CYCLIN-DEPENDENT KINASE II	2	Yes	Yes
1Q3W	GLYCOGEN SYNTHASE KINASE 3 BETA	2.3	Yes	
1Q5K	GLYCOGEN SYNTHASE KINASE 3 BETA	1.94	Yes	
1Q8T	C-AMP DEPENDENT KINASE	2	Yes	
1Q8W	C-AMP DEPENDENT KINASE	2.2	Yes	
1QBU	HIV-1 PROTEASE	1.8	Yes	Yes
1QFT	HISTAMINE BINDING PROTEIN	1.25	Yes	
1QHI	THYMIDINE KINASE	1.9	Yes	
1QKN	ESTROGEN RECEPTOR BETA	2.25	Yes	
1QL9	TRYPSIN	2.3	Yes	
1QPE	LCK KINASE	2	Yes	
1QS4	HIV-1 INTEGRASE	2.1	Yes	
1R09	RHINOVIRUS COAT PROTEIN	2.9	Yes	
1R0E	GLYCOGEN SYNTHASE KINASE 3 BETA	2.25	Yes	
1R78	CYCLIN-DEPENDENT KINASE II	2	Yes	
1REK	C-AMP DEPENDENT KINASE	2.3	Yes	
1RW8	TGF-BETA RECEPTOR TYPE I	2.4	Yes	
1S1T	HIV-1 REVERSE TRANSCRIPTASE	2.4	Yes	
1S9P	ESTROGEN RECEPTOR GAMMA	2.13	Yes	
1SYN	THYMIDYLATE SYNTHASE	2	Yes	
1THL	THERMOLYSIN	1.7	Yes	
1TNG	TRYPSIN	1.8	Yes	
1TNH	TRYPSIN	1.8	Yes	
1U3Q	ESTROGEN RECEPTOR BETA	2.4	Yes	
1UNG	CYCLIN-DEPENDENT KINASE V	2.3	Yes	
1UNL	CYCLIN-DEPENDENT KINASE V	2.2	Yes	
1UOM	ESTROGEN RECEPTOR	2.28	Yes	
1URW	CYCLIN-DEPENDENT KINASE II	1.6	Yes	
1UVS	THROMBIN	2.8	Yes	Yes
1UVT	THROMBIN	2.5	Yes	
1UY6	HEAT SHOCK PROTEIN 90	1.9	Yes	
1UY7	HEAT SHOCK PROTEIN 90	1.9	Yes	
1UYC	HEAT SHOCK PROTEIN 90	2	Yes	
1UYD	HEAT SHOCK PROTEIN 90	2.2	Yes	
1UYF	HEAT SHOCK PROTEIN 90	2	Yes	
1UYG	HEAT SHOCK PROTEIN 90	2	Yes	
1UYH	HEAT SHOCK PROTEIN 90	2.2	Yes	
1UYI	HEAT SHOCK PROTEIN 90	2.2	Yes	
1UYK	HEAT SHOCK PROTEIN 90	2.2	Yes	
1V0P	P. FALCIPARUM PROTEIN KINASE 5	2	Yes	
1V1K	CYCLIN-DEPENDENT KINASE II	2.31	Yes	
1VJY	TGF-BETA RECEPTOR TYPE I	2	Yes	
1VYW	CYCLIN-DEPENDENT KINASE II	2.3	Yes	
1VYZ	CYCLIN-DEPENDENT KINASE II	2.21	Yes	
1W0X	CYCLIN-DEPENDENT KINASE II	2.2	Yes	
1W83	P38 MAP KINASE	2.5	Yes	
1W84	P38 MAP KINASE	2.2	Yes	Yes
1WBN	P38 MAP KINASE	2.4	Yes	

1WBS	P38 MAP KINASE	1.8	Yes	
1WBW	P38 MAP KINASE	2.41	Yes	
1WZY	MITOGEN-ACTIVATED PROTEIN KINASE 1	2.5	Yes	
1X76	ESTROGEN RECEPTOR BETA	2.2	Yes	
1X78	ESTROGEN RECEPTOR BETA	2.3	Yes	
1X8B	WEE1-LIKE PROTEIN KINASE	1.81	Yes	
1XP1	ESTROGEN RECEPTOR ALPHA	1.8	Yes	
1XQC	ESTROGEN RECEPTOR ALPHA	2.05	Yes	
1XWS	PIM1 KINASE DOMAIN	1.8	Yes	
1Y8Y	CYCLIN-DEPENDENT KINASE II	2	Yes	
1Y91	CYCLIN-DEPENDENT KINASE II	2.15	Yes	
1YC3	HEAT SHOCK PROTEIN 90	2.12	Yes	
1YDR	C-AMP-DEPENDENT PROTEIN KINASE	2.2	Yes	
1YDS	C-AMP-DEPENDENT PROTEIN KINASE	2.2	Yes	
1YDT	C-AMP-DEPENDENT PROTEIN KINASE	2.3	Yes	
1YI3	PIM1 KINASE DOMAIN	2.5	Yes	
1YIM	ESTROGEN RECEPTOR ALPHA	1.9	Yes	
1YIN	ESTROGEN RECEPTOR ALPHA	2.2	Yes	
1YKR	CYCLIN-DEPENDENT KINASE II	1.8	Yes	
1YQJ	P38 MAP KINASE	2	Yes	Yes
1YW2	P38 MAP KINASE	2.01	Yes	
1YWR	P38 MAP KINASE	1.95	Yes	
1YXX	PIM1 KINASE DOMAIN	2	Yes	
1Z5M	3-PHOSPHOINOSITIDE-DEPENDENT PROTEIN KINASE 1	2.17	Yes	
1ZYJ	P38 MAP KINASE	2	Yes	
1ZZ2	P38 MAP KINASE	2	Yes	
1ZZL	P38 MAP KINASE	2	Yes	
2A0C	CYCLIN-DEPENDENT KINASE II	1.95	Yes	
2AYR	ESTROGEN RECEPTOR	1.9	Yes	
2B52	CYCLIN-DEPENDENT KINASE II	1.88	Yes	
2BAK	P38 MAP KINASE	2.2	Yes	
2BAL	P38 MAP KINASE	2.1	Yes	
2BE2	HIV-1 REVERSE TRANSCRIPTASE	2.43	Yes	
2BFY	AURORA KINASE B	1.8	Yes	
2BR1	CHECKPOINT KINASE 1	2	Yes	
2BRB	CHECKPOINT KINASE 1	2.1	Yes	
2BRC	HEAT SHOCK PROTEIN 90	1.6	Yes	
2BRE	HEAT SHOCK PROTEIN 90	2	Yes	
2BRG	CHECKPOINT KINASE 1	2.1	Yes	
2BRH	CHECKPOINT KINASE 1	2.1	Yes	
2BRM	CHECKPOINT KINASE 1	2.2	Yes	
2BRO	CHECKPOINT KINASE 1	2.2	Yes	
2BSM	HEAT SHOCK PROTEIN 90	2.05	Yes	
2BTR	CYCLIN-DEPENDENT KINASE II	1.85	Yes	
2BTS	CYCLIN-DEPENDENT KINASE II	1.99	Yes	
2BYH	HEAT SHOCK PROTEIN 90	1.9	Yes	
2BYI	HEAT SHOCK PROTEIN 90	1.6	Yes	

2BZ5	HEAT SHOCK PROTEIN 90	1.9	Yes	Yes
2C6E	AURORA KINASE A	2.1	Yes	
2CCS	HEAT SHOCK PROTEIN 90	1.79	Yes	
2CCT	HEAT SHOCK PROTEIN 90	2.3	Yes	
2CGR	IMMUNOGLOBULIN	2.2	Yes	
2CSN	CASEIN KINASE-1	2.5	Yes	
2EXM	CYCLIN-DEPENDENT KINASE II	1.8	Yes	
2F4J	ABL KINASE	1.91	Yes	Yes
2IZG	STREPTAVIDIN	1.36	Yes	
2PCP	IMMUNOGLOBULIN	2.2	Yes	
2QWI	NEURAMINIDASE	2	Yes	
3BTO	LIVER ALCOHOL DEHYDROGENASE	1.66	Yes	
3CPA	HYDROLASE (C-TERMINAL PEPTIDASE)	2	Yes	
3ERK	EXTRACELLULAR REGULATED KINASE 2	2.1	Yes	
3ERT	ESTROGEN RECEPTOR ALPHA	1.9	Yes	
3STD	SCYTALONE DEHYDRATASE	1.65	Yes	Yes
3TMN	HYDROLASE (METALLOPROTEINASE)	1.7	Yes	
4DFR	OXIDO-REDUCTASE	1.7	Yes	
4STD	SCYTALONE DEHYDRATASE	2.15	Yes	
5STD	SCYTALONE DEHYDRATASE	1.95	Yes	Yes
5STD	SCYTALONE DEHYDRATASE	1.95	Yes	Yes
5TLN	HYDROLASE (METALLOPROTEINASE)	2.3	Yes	
6STD	SCYTALONE DEHYDRATASE	1.8	Yes	
7DFR	OXIDO-REDUCTASE	2.5	Yes	
7EST	HYDROLASE (SERINE PROTEINASE)	1.8	Yes	
7STD	SCYTALONE DEHYDRATASE	1.8	Yes	
830C	COLLAGENASE-3 (MMP-13)	1.6	Yes	
966C	COLLAGENASE-1 (MMP-1)	1.9	Yes	

1CJ1	SH2	3		Yes
1DTQ	HIV-1 REVERSE TRANSCRIPTASE	2.8		Yes
1GA9	AMPC BETA-LACTAMASE	2.1		Yes
1HNX	30S RIBOSOMAL SUBUNIT	3.4		Yes
1IKY	HIV-1 REVERSE TRANSCRIPTASE	3		Yes
1RV1	MDM2	2.3		Yes
1S6P	HIV-1 REVERSE TRANSCRIPTASE	2.9		Yes
1S9E	HIV-1 REVERSE TRANSCRIPTASE	2.6		Yes
1SUQ	HIV-1 REVERSE TRANSCRIPTASE	3		Yes
1T4E	MDM2	2.6		Yes
1TQF	BETA SECRETASE	1.8		Yes
1YQJ	P38 MAP KINASE	2		Yes
2AZ5	TNF-a	2.1		Yes
2B8V	BETA SECRETASE	1.8		Yes
2I0H	P38 MAP KINASE	2		Yes
2ICA	CD11a	1.56		Yes
2OFU	Lck	2		Yes
2ORS	Nitric Oxide Synthase	2		Yes

2Q15	BETA SECRETASE	2.4	Yes
2R2M	THROMBIN	2.1	Yes
2RFS	c-Met	2.2	Yes
2VG5	HIV-1 REVERSE TRANSCRIPTASE	2.8	Yes
2VIZ	BETA SECRETASE	1.6	Yes
2VJ6	BETA SECRETASE	1.8	Yes
2VWV	EPHB4	1.9	Yes
2YXJ	Bcl-xL	2.2	Yes
2ZD1	HIV-1 REVERSE TRANSCRIPTASE	1.8	Yes
3CIB	BETA SECRETASE	1.72	Yes
3CID	BETA SECRETASE	1.8	Yes
3EQP	Ack1	2.3	Yes
3FKT	BETA SECRETASE	1.9	Yes
3FZM	HEAT SHOCK PROTEIN 70	2.3	Yes
3HA6	AURORA KINASE A	2.36	Yes
3HA8	P38 MAP KINASE	2.48	Yes
