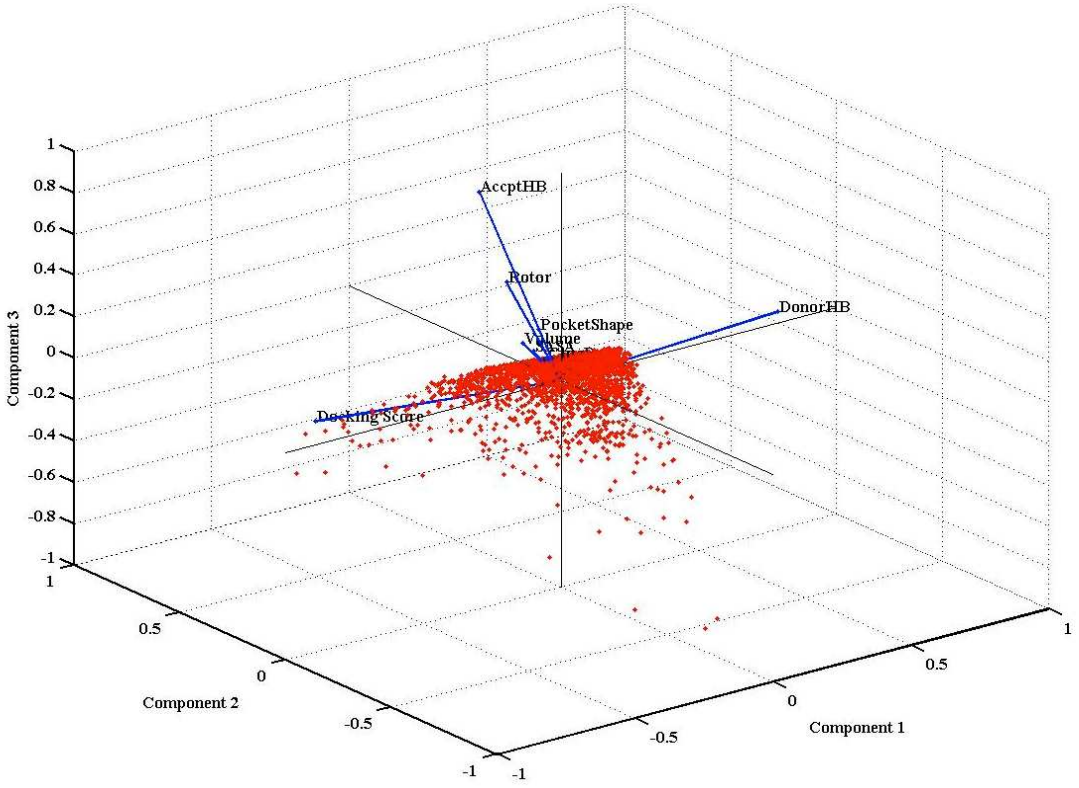
Supplemental.

Supplemental Figure 1. Three-dimensional PCA plot of transformed eigenvalue coefficients of the aforementioned descriptor variables against the first three principal components. The red dots represent individual descriptor observations (i.e. normalized score for each protein- and ligand-based descriptor variable), and corresponding vectors are shown as black arrowheads whose direction and length indicate how that variable contributes to the three principal components. With the exception of docking score and hydrogen bond donor (DonorHB), all descriptor variables exhibit positive correlation coefficients across all three components.



Supplemental Table 1. Tabular depiction of PDB IDs within the protein target collection that correspond to protein targets found in the Directory of Useful Decoys (DUD).

DUD Protein Target Name	PDB ID
Adenosine Deaminase	3IAR, 3LGG
Aldose Reductase	2QXW, 1EL3, 1IEI, 1PWM, 1T41, 1X97, 1Z89, 1Z8A, 2ACQ, 2IKG, 2IKH, 2IKI, 2NVC, 2NVD, 2PDG, 2PDI, 2PDL, 2PDW, 2PZN, 2R24, 3BCJ, 3DN5, 3G5E
Androgen Receptor	1GS4, 1T65, 1XOW, 1Z95, 2AX6, 2AX8, 2AX9, 2OZ7, 2PIT, 2PIV, 2PNU, 2Q7I, 2Q7K, 3B5R, 3B65, 3B66, 3B67, 3B68, 3L3X, 3L3Z
Cyclin Dependent Kinase 2	1AQ1, 1E1X, 1E9H, 1G5S, 1GII, 1GIJ, 1KE5, 1P2A, 1PXL, 1PXM, 1PXN, 1PXO, 1PYE, 1R78, 1URW, 1V1K, 1W0X, 1Y8Y, 1Y91, 1YKR, 2A0C, 2B52, 2B54, 2B55, 2BTR, 2BTS, 2C5N, 2C5X, 2C68, 2C69, 2C6I, 2C6K, 2C6L, 2C6M, 2CCH, 2DS1, 2DUV, 2J9M, 2UZB, 2UZD, 2UZE, 2UZL, 2UZN, 2UZO, 2VV9, 2W05, 2W06, 2W17, 3LFN, 3LFQ, 3LFS
Dihydrofolate Reductase	1DRF, 1HFR, 1MVT, 1OHK, 1S3U, 1S3V, 1S3W, 1U71, 2DHF, 3EIG
Epidermal Growth Factor Receptor	1XKK, 1Y6A, 1Y6B, 2EB3, 2ITP, 2ITX, 2OH4, 2P2H, 2P2I, 2QU5, 2QU6, 2RGP, 2RL5, 3B8Q, 3B8R, 3BE2, 3BEL, 3CJF, 3CJG, 3CP9, 3CPB, 3CPC, 3DTW
Factor Xa	1EZQ, 1F0R, 1F0S, 1FJS, 1G2L, 1IOE, 1IQG, 1IQH, 1IQI, 1IQJ, 1IQL, 1IQM, 1IQN, 1KSN, 1LPG, 1LPK, 1LPZ, 1LQD, 1MQ5, 1MQ6, 1NFU, 1NFW, 1NFX, 1NFY, 1V3X, 1XKA, 1Z6E, 2BMG, 2BOH, 2BOK, 2BQ6, 2BQW, 2EI6, 2EI7, 2EI8, 2J2U, 2J34, 2J38, 2J4I, 2J94, 2J95, 2JKH, 2P16, 2P3T, 2P3U, 2P93, 2P94, 2P95, 2PHB, 2PR3, 2Q1J, 2RA0, 2UWL, 2UWO, 2UWP, 2VH0, 2VH6, 2W26, 2W3I, 2W3K, 3CEN, 3CS7, 3ENS, 3KL6, 3K9X, 3KQB, 3KQC, 3KQD, 3KQE, 3LIW, 3M36, 3M37
Glycinamide Ribonucleotide Transformylase	1ZLY

Glucocorticoid Receptor	1L2I, 1M2Z, 1NHZ, 1T65, 1ZKY, 1ZN8, 2G0G, 2H79, 2PZN, 2VKM, 3BQD, 3CLD, 3E7C, 3ERD, 3HZF, 3ILZ, 3K23, 3LGG
HSP90	1BYQ, 1OSF, 1YET, 2BSM, 2BSM, 2BT0, 2BT0, 2BYH, 2BYH, 2BYI, 2BYI, 2BZ5, 2CCS, 2CCT, 2CCU, 2QG0, 2QG2, 2UWD, 2UWD, 2VCI, 2VCJ, 3EKR, 3K97, 3K98, 3K99
P38	1DI9, 1KV1, 1KV2, 1M7Q, 1OVE, 1OZ1, 1PME, 1W82, 1W83, 1WBN, 1WBS, 1WBT, 1WBV, 1WBW, 1YQJ, 1ZYJ, 1ZZL, 2GFS, 2QD9, 2RG5, 2RG6, 2ZAZ, 2ZB0, 2ZB1, 3BV2, 3BV3, 3BX5, 3CTQ, 3D7Z, 3D83, 3DS6, 3DT1, 3FC1, 3GCQ, 3GCS, 3GCU, 3GCV, 3HUB, 3HUC, 3HV6, 3HV7, 3IPH, 3IW5, 3IW6, 3IW7, 3IW8, 3L8S, 3L8X, 3MPT
Poly(ADP-ribose) Polymerase	2RCW,3KR8,3L3M,3MHJ,3MHK
Phosphodiesterase V	2H42
Purine Nucleoside Phosphorylase	1PF7, 1RCT, 1RFG, 1RSZ, 1V45, 1YRY, 2EB3, 2ITX, 2ON6, 2Q7O, 3BGS, 3GGS, 3K8O, 3K8Q
Peroxisome Proliferator Activated Receptor Gamma	1KNU, 1NYX, 3CS8, 3FUR, 3K8S
Progesterone Receptor	1A28, 1SQN, 1SR7, 2OVH, 2W8Y, 3D90, 3KBA
SRC	1BYG, 1QCF, 1QPD, 1QPE, 1YOL, 1YOM, 2BDJ, 2C0O, 2H8H, 2P54
Thrombin	1A2C, 1A46, 1A4W, 1A5G, 1B5G, 1BHX, 1C4U, 1C4V, 1CA8, 1D3D, 1D3T, 1D4P, 1D6W, 1D9I, 1EB1, 1FPC, 1G30, 1G32, 1H8D, 1JWT, 1K21, 1K22, 1KTS, 1KTT, 1MU6, 1MU8, 1MUE, 1NM6, 1NT1, 1NZQ, 1O0D, 1OYT, 1RIW, 1SB1, 1SL3, 1T4U, 1T4V, 1TA2, 1TA6, 1VZQ, 1WAY, 1YPE, 1YPG, 1YPJ, 1YPK, 1YPL, 1YPM, 1Z71, 1ZGI, 1ZGV, 2BXU, 2FES, 2JH0, 2JH5, 2JH6, 2PKS, 2R2M, 2UUJ, 2UUK, 2UWL, 2UWO, 2V3H, 2V3O, 2ZC9, 2ZDA, 2ZDV, 2ZF0, 2ZFF, 2ZFP, 2ZFQ, 2ZFR, 2ZG0, 2ZGB, 2ZGX, 2ZHE, 2ZHF, 2ZHQ, 2ZHW, 2ZI2, 2ZIQ, 2ZNK, 2ZO3, 3BIU, 3C27, 3DA9, 3DHK
Thymidine Kinase	1W4R, 2WVJ
Trypsin	1GJ7, 1GJ8, 1GJ9, 1GJA, 1GJC, 1GJD

Vascular Endothelial Growth Factor Receptor 2	1Y6A, 1Y6B, 2OH4, 2P2H, 2P2I, 2QU5, 2QU6, 2RL5, 3B8Q, 3B8R, 3BE2, 3CJF, 3CJG, 3CP9, 3CPB, 3CPC, 3DTW

Supplemental Table 2. Raw score values for each descriptor as noted in the Methods section and Z-rank score for protein targets that were considered to be the Top 1 hit for staurosporine (DB2010) using the TMFS approach. Furthermore, each protein-ligand complex has a line similar to those below (not shown). Thus, it can be extrapolated that the raw data of all protein-ligand interaction permutations total to 2,335 targets X 3,671 ligands = 8,204,685 lines of descriptor scores.

PDB ID	Docking Score	AccpHB	ClogP	DonorHB	Electron Affinity	Globularity	# Rot. Bonds	SASA	Volume	Ligand Shape	Pocket Shape	Z-Rank Score
2HY8	0.672449808	0.9453	1	0.9444	0.9999	0.9919	1	0.9999	0.9996	0.768584	0.761536	13.631
1YVJ	0.875028394	1	1	0.9989	0.9999	0.9998	1	0.9995	0.9988	0.775387	0.760643	14.5691
3FQS	0.522309759	0.8682	0.95	0.9965	0.9719	1	0.95	0.991	0.9978	0.819295	0.689066	12.8314
2VWV	0.442048898	0.9933	1	1	0.9927	1	1	0.9738	0.9726	0.827829	0.685366	12.727
1R0P	0.822706452	0.9948	1	1	0.9998	0.9952	1	0.9988	0.9986	0.83525	0.77387	14.4963
3EQF	0.821345165	0.9948	1	0.9965	0.9943	0.9952	1	0.9961	0.9982	0.787755	0.797516	14.431
2VTQ	0.537657029	0.9925	0.95	0.9998	0.9759	0.9872	0.95	0.9955	0.9999	0.783797	0.770382	13.1098
2VU3	0.562129482	1	1	0.9996	0.9835	0.9808	1	0.9706	0.9733	0.797526	0.758176	13.2677
2RKU	0.46518681	0.9928	0.9875	0.9988	0.8716	0.999	0.9875	0.9552	0.9678	0.74663	0.751712	12.6176
1AQ1	0.885652795	1	1	0.9978	0.9971	1	1	0.9999	0.9998	0.767904	0.746055	14.5651
1BYG	0.697023234	1	1	0.9994	0.991	1	1	0.9981	0.9999	0.822882	0.698677	13.8196
1OKY	0.863962184	1	1	0.9998	0.9924	1	1	0.9973	0.9995	0.774026	0.763875	14.5207
1Q3D	0.73634797	1	1	0.9991	1	1	1	0.9994	0.999	0.761905	0.677498	13.8217
1QPD	0.816816505	1	1	0.9985	0.9946	1	1	0.9985	0.9998	0.787755	0.749288	14.3328
1SM2	0.830555037	1	1	0.9996	0.9991	1	1	0.9999	1	0.76141	0.763237	14.3701
1U59	0.865553676	1	1	0.9996	1	1	1	0.9991	0.9983	0.735931	0.714668	14.3604
1XBC	0.893880093	1	1	0.9999	0.9836	1	1	0.996	0.9998	0.817378	0.7384	14.6664
1XJD	0.86133885	0.9986	1	0.9942	0.9987	1	1	0.9966	0.9965	0.778912	0.748139	14.4841
1YHS	0.773450912	1	1	1	0.9995	1	1	0.9999	0.9995	0.761472	0.731255	14.0782
2BUJ	0.466999409	1	1	0.9992	0.9856	1	1	0.9944	0.9988	0.780519	0.710628	12.8283
2DQ7	0.722714629	1	1	1	0.9867	1	1	0.9963	0.9997	0.828881	0.734913	14.0011
2HW7	0.822767946	1	1	0.9996	0.9971	1	1	0.9993	0.9999	0.804515	0.754264	14.4045
2NRY	0.901679547	1	1	0.9993	0.9933	1	1	0.998	0.9997	0.838033	0.748565	14.7702
2OIC	0.878598722	1	1	0.9998	0.9878	1	1	0.9955	0.9991	0.773346	0.743589	14.5305
2Z7R	0.779119528	1	1	0.9978	0.9999	1	1	0.9998	0.9994	0.756895	0.715179	14.0575
3A4O	0.72635619	0.9979	1	0.9993	0.9995	1	1	0.9999	1	0.820779	0.690044	13.9237
3A60	0.786378855	1	1	0.9977	0.9997	1	1	0.9986	0.9985	0.750897	0.754008	14.1498
3A62	0.81615076	1	1	0.9988	0.9999	1	1	0.9992	0.9989	0.741868	0.699613	14.1444
3BKB	0.856501308	1	1	0.9999	0.9968	1	1	0.999	0.9999	0.746815	0.793008	14.5013
3FME	0.88065962	1	1	1	0.9881	1	1	0.996	0.9991	0.796475	0.775996	14.6508
1PKD	0.811851111	0.9479	0.95	0.9982	0.9839	0.9967	0.95	0.9982	0.9999	0.78491	0.74193	14.1259
3DTC	0.724582576	0.9935	0.95	0.9557	0.9821	0.9997	0.95	0.999	0.9995	0.713234	0.706886	13.5681