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Supporting information for article:

The evaluation of QM/MM-driven molecular docking combined with MM/GBSA calculations as a halogen bond scoring strategy

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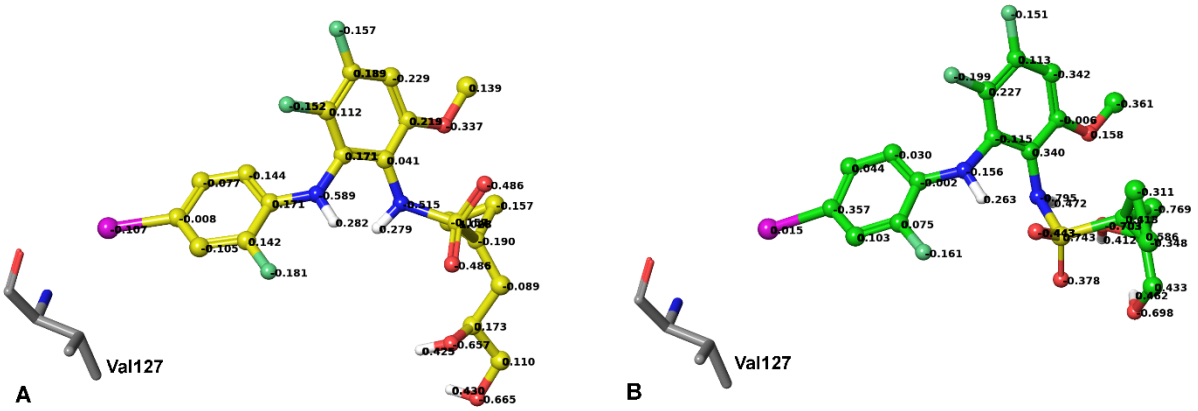

Figure S1 Comparison of atomic partial charges assigned by OPLS3 force field (A) and calculated using quantum mechanics at the B3PW91/cc-pVTZ-pp level of theory in the field of protein (B) for top ranked complexes for PDB 3E8N obtained by Glide and QPLD docking, respectively. For iodine atom, involved in halogen bonding with carbonyl oxygen of Val127, the significant change of charge value was noted – according to the XB theory, charge located on iodine substituent in case (A) should rather prevent the halogen bonding formation, mainly due to the electrostatic repulsion with acceptor group (O=C).

Table S1 The comparison of median, 95% confidence interval (CI) and standard deviation (SD) calculated for differences between estimated halogen bonding geometry (XB distance and angle) by the given docking/scoring procedure and crystallographic structure.

		XB distance [Å]			XB angle [º]		
		Median	95% CI	SD	Median	95% CI	SD
QPLD	RMSD	-0.11	-0.52; -0.11	0.90	8.8	10.58; 18.68	17.84
	GScore	-0.14	-1.52; -0.63	1.96	13.63	23.39; 42.22	41.49
	GBSA	-0.05	-0.81; -0.20	1.35	7.58	10.55; 22.88	27.16
	XBSF	-0.13	-1.51; -0.52	2.19	9.99	16.91; 33.38	36.28
Glide_SP	RMSD	-0.14	-2.18; -0.76	3.13	11.06	18.89; 38.12	42.36
	GScore	-0.32	-3.38; -1.72	3.66	19.44	37.42; 62.51	55.27
	XBSF	-0.66	-3.46; -1.87	3.50	25.99	41.36; 66.74	55.89
Glide_XP	RMSD	-0.09	-1.50; -0.53	2.15	10.97	18.67; 36.94	40.23
	GScore	-0.21	-2.05; -0.91	2.51	13.59	26.32; 48.26	48.31
	XBSF	-0.17	-1.93; -0.82	2.45	11.81	24.01; 44.69	45.55