On extension of the current biomolecular empirical force field for the description of halogen bonds

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Supplementary Information

Table S1: CCSD(T)/CBS interaction energies E_{int} of the complexes.

Filename	Br...Y distance [Å]	E_{int} [kcal/mol]
br2f_o_25.xyz	2.5	0.45
br2f_o_27.xyz	2.7	–2.13
br2f_o_29.xyz	2.9	–2.95
br2f_o_31.xyz	3.1	–2.96
br2f_o_33.xyz	3.3	–2.65
br2f_o_35.xyz	3.5	–2.24
br2f_o_40.xyz	4.0	–1.34
br2f_o_45.xyz	4.5	–0.78
br2f_o_60.xyz	6.0	–0.19
br2f_o_70.xyz	7.0	–0.09
br_o_27.xyz	2.7	–1.10
br_o_29.xyz	2.9	–2.22
br_o_31.xyz	3.1	–2.42
br_o_33.xyz	3.3	–2.23
br_o_35.xyz	3.5	–1.91
br_o_40.xyz	4.0	–1.10
br_o_45.xyz	4.5	–0.59
br_o_60.xyz	6.0	–0.07
br_o_70.xyz	7.0	0.00
br_n_25.xyz	2.5	0.11
br_n_27.xyz	2.7	–2.74
br_n_29.xyz	2.9	–3.62
br_n_31.xyz	3.1	–3.57
br_n_33.xyz	3.3	–3.15
br_n_35.xyz	3.5	–2.62
br_n_45.xyz	4.5	–0.78
br_n_60.xyz	6.0	–0.12

Figure S1: Error analysis of the gas phase dissociation curves of 1-bromo-3,5-difluorobenzene...acetone complex (Br2F_O). Mean unsigned absolute errors (MUAE) are plotted in green and mean unsigned relative errors (MURE) are in grey. Two charge sets are compared: RESP charges based on B3LYP/cc-ptvz electrostatic potential grid and on HF/6-31G* electrostatic potential grid. Three explicit sigma-hole construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Note the different color ranges of the plots.

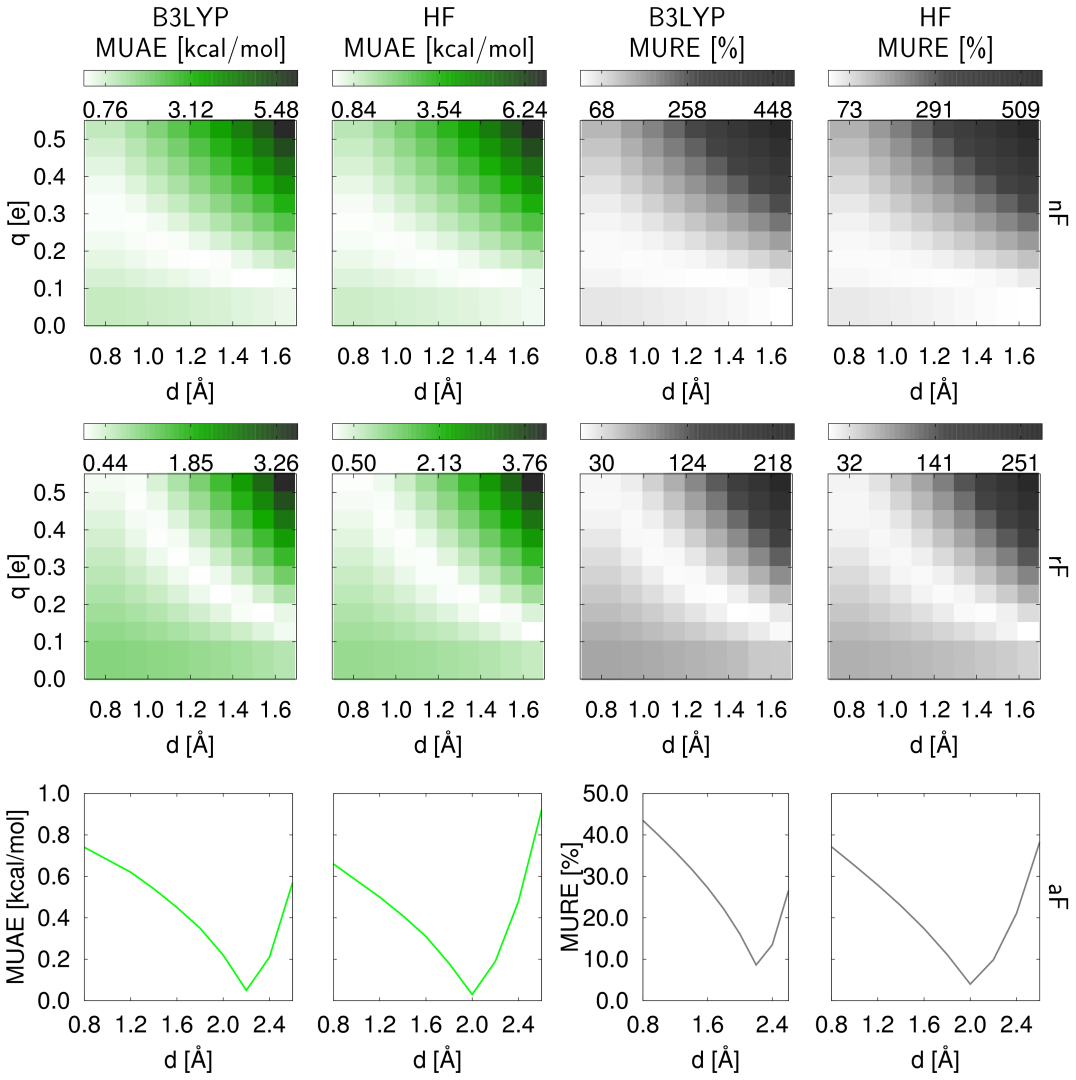

Figure S2: Error analysis of the gas phase dissociation curves of bromobenzene...acetone complex (Br_O). Mean unsigned absolute errors (MUAE) are plotted in green and mean unsigned relative errors (MURE) are in grey. Two charge sets are compared: RESP charges based on B3LYP/cc-ptvz electrostatic potential grid and on HF/6-31G* electrostatic potential grid. Three explicit sigma-hole construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Note the different color ranges of the plots.

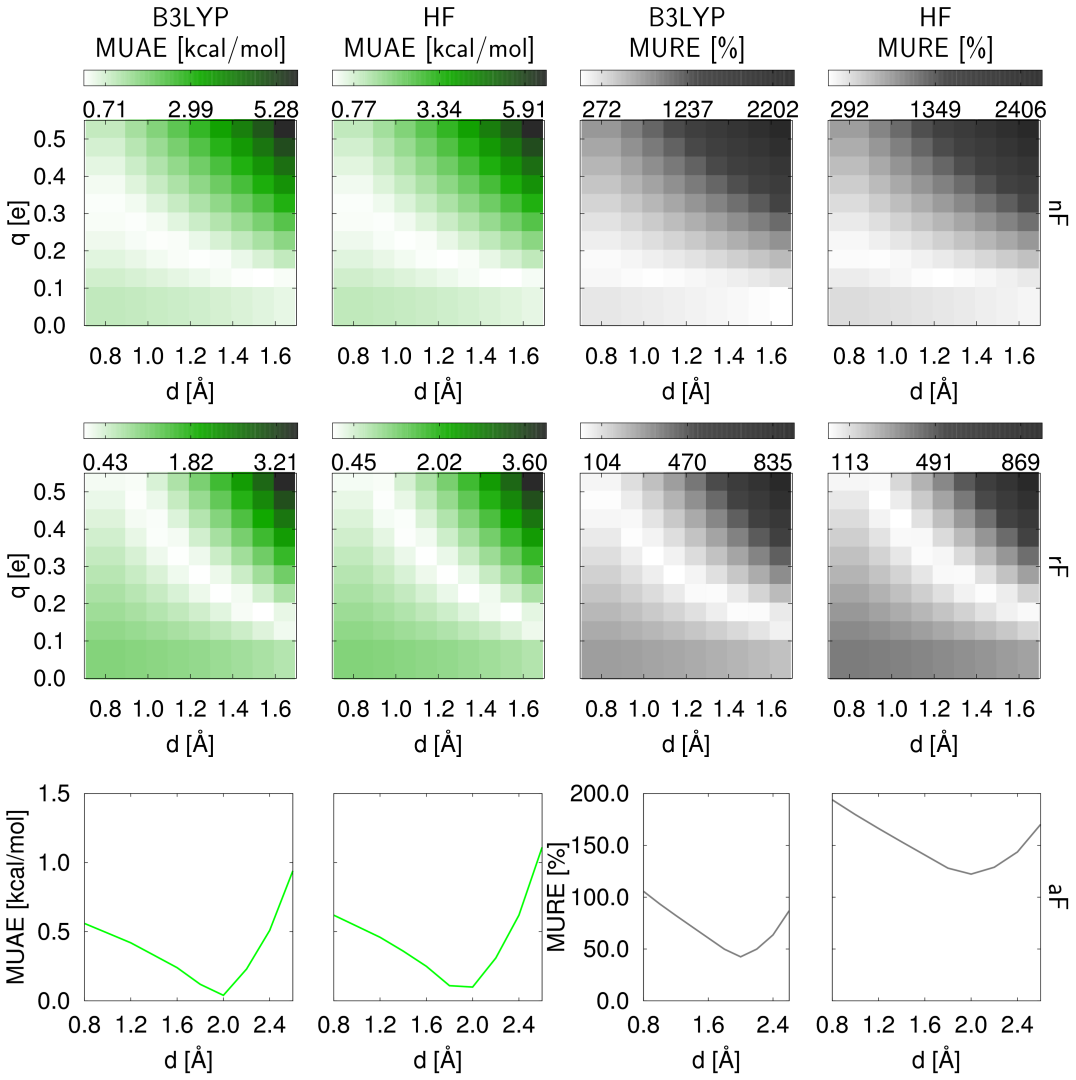

Figure S3: Error analysis of the gas phase dissociation curves of bromobenzene...trimethylammonia complex (Br_N). Mean unsigned absolute errors (MUAE) are plotted in green and mean unsigned relative errors (MURE) are in grey. Two charge sets are compared: RESP charges based on B3LYP/cc-ptvz electrostatic potential grid and on HF/6-31G* electrostatic potential grid. Three explicit sigma-hole construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Note the different color ranges of the plots.

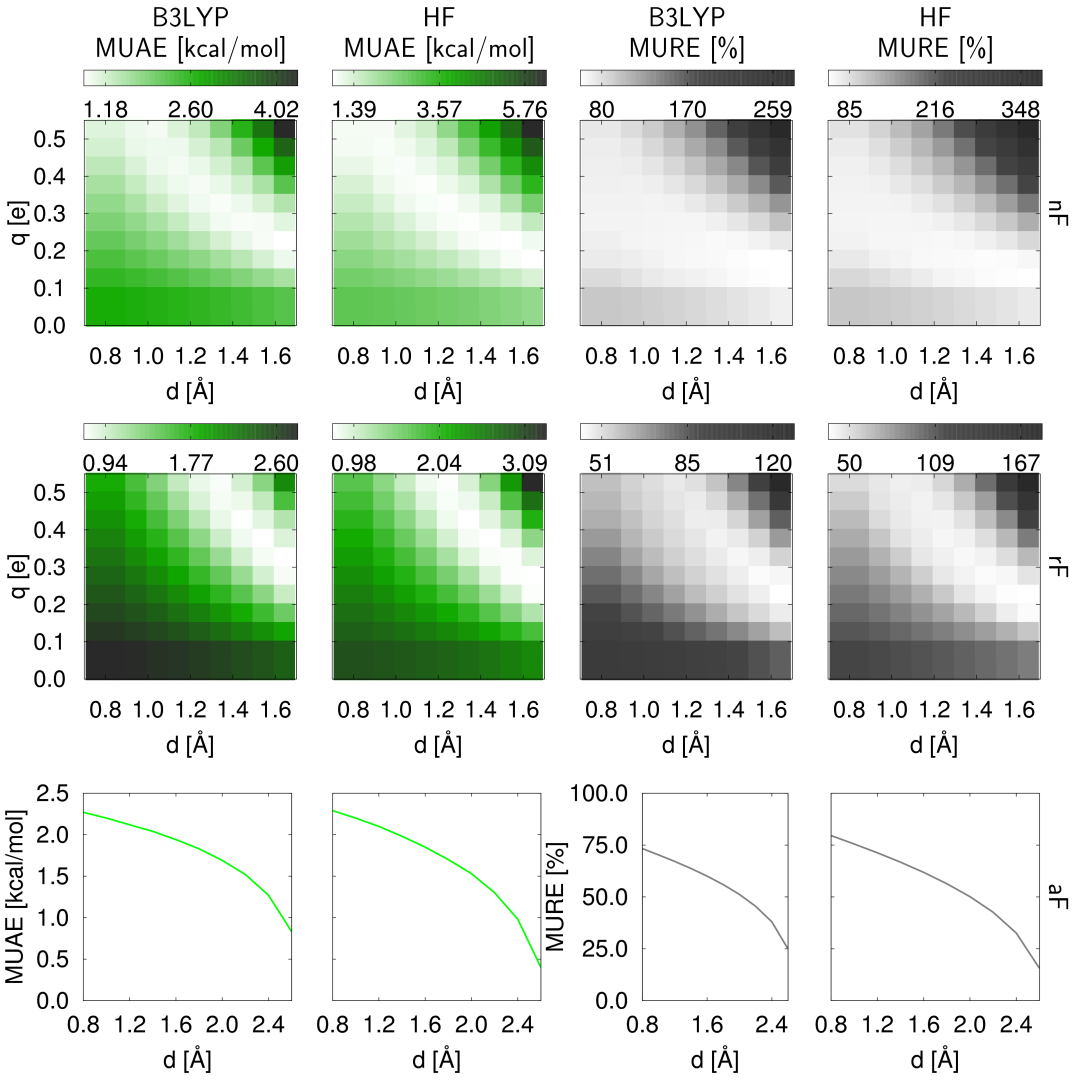

Figure S4: Root mean square deviations (RMSD) with respect to the X-ray geometry. PDB codes were calculated for seven casein kinase 2 inhibitors. Three explicit sigma-hole construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Note the different color ranges of the plots.

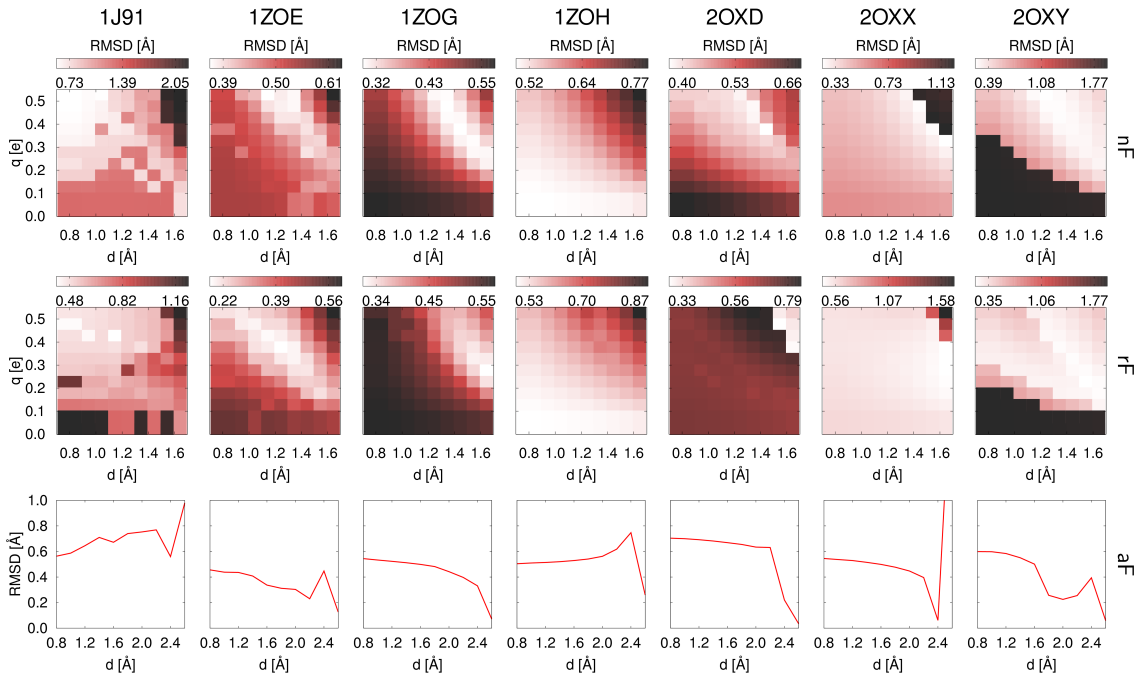

Figure S5: Root mean square deviations (RMSD) with respect to the X-ray geometry. PDB codes were calculated for the active sites of seven casein kinase 2 complexes. Three explicit sigma-hole construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Note the different color ranges of the plots.

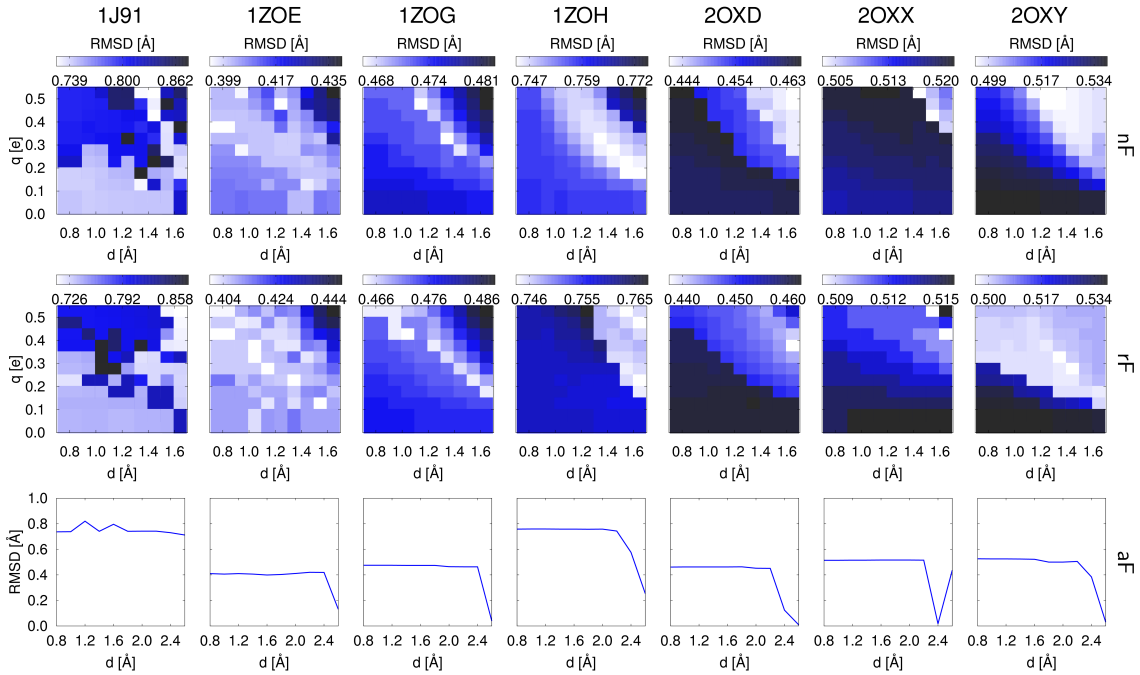

Figure S6: Number of contacts between inhibitor bromines and protein oxygen atoms (xbs). The results for three explicit sigma-hole (ESH) construction schemes are shown: two-parameter models nF and rF, and one-parameter model aF. Fro comparison, the number of bromine-oxygen contacts in experimental X-ray structure (X-ray) and force field without ESH (noESH) are provided as the insets of the last row plots.