Can we visually predict binding energies?

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Part 1 Na^+ DF-HF/6-31G**

SCF Energy (Hartrees)	-161.659
SCF Energy (kcal/mol)	-101442.5757

Part 2 Benzene Ring

Molecule Name: Benzene

System (DF-HF/STO-3G)	SCF Energy (Hartrees)	SCF Energy (kcal/mol)	Binding Energy
Benzene	-227.892046	-143002.259	1152.562528
Benzene – Na^+	-387.716768	-243292.272	

Part 3 Other Aromatics

Molecule Name: Chlorobenzene

System (DF-HF/STO-3G)	SCF Energy (Hartrees)	SCF Energy (kcal/mol)	Binding Energy
Aromatic	-681.897	-427890.121	1153.3448
Aromatic – Na^+	-841.72	-528179.352	

Molecule Name: Fluorobenzene

System (DF-HF/STO-3G)	SCF Energy (Hartrees)	SCF Energy (kcal/mol)	Binding Energy
Aromatic	-325.352	-204158.412	1156.2594
Aromatic – Na^+	-485.171	-304444.728	

Molecule Name: 1,3,5-trifluorobenzene

System (DF-HF/ STO-3G)	SCF Energy (Hartrees)	SCF Energy (kcal/mol)	Binding Energy
Aromatic	-520.271	-326470.294	1163.3413
Aromatic – Na^+	-680.079	-426749.528	

1. What atoms or functional groups most significantly changed the π-cloud and, hence, location of the sodium cation as compared to benzene? Why? Please use complete and grammatically correct sentences.

Chloro functional group has the most significant change to the π-cloud because it withdraws the most electron density from the π-cloud.

2. **Discuss** the trends that you observe between the visual depiction of the electrostatic potentials for your four aromatic compounds and the strength of the binding energies. Please use complete and grammatically correct sentences.

The binding energies are close to each other, but we can observe that the π-cloud becomes more reddish, which mean more electron density, the higher the binding energy gets.