

**Liquid-Liquid Extraction of Furfural from Water by Hydrophobic Deep  
Eutectic Solvents: Improvement of Density Function Theory Modeling with  
Experimental Validations**

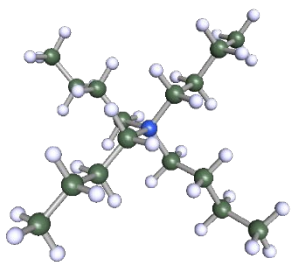
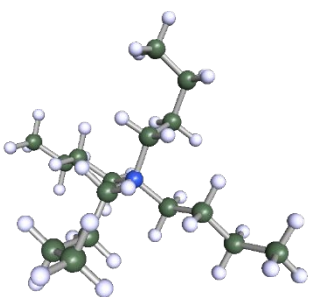
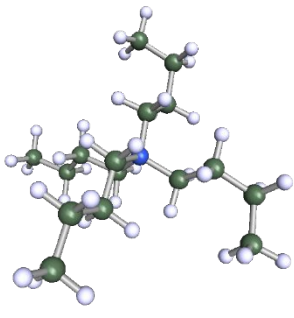
Kyle McGaughy<sup>1</sup> and M. Toufiq Reza<sup>1\*</sup>

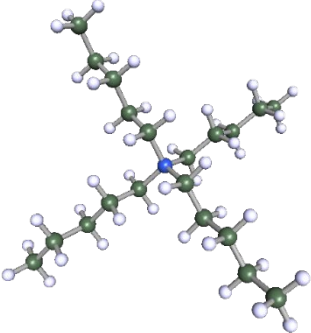
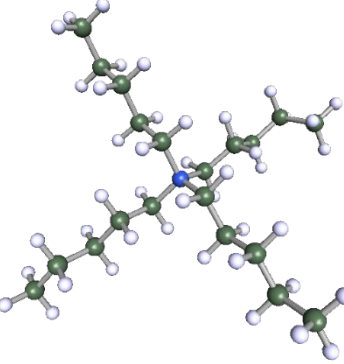
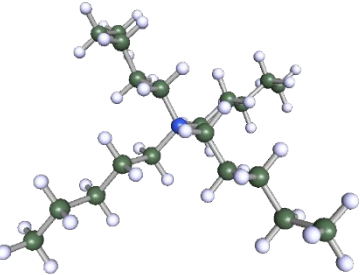
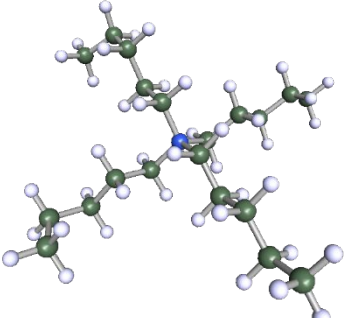
<sup>1</sup> Department of Biomedical and Chemical Engineering and Sciences, Florida Institute of Technology,  
150 W University Blvd, Melbourne, FL 32901

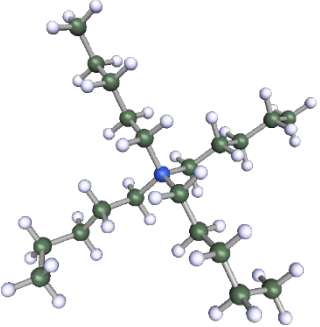
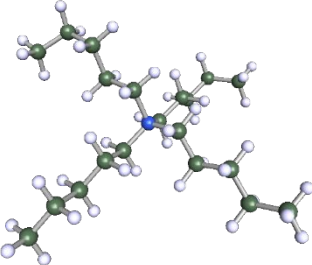
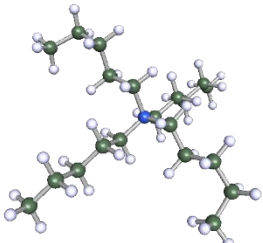
\* Corresponding Author: Email: [treza@fit.edu](mailto:treza@fit.edu), Tel: +1 321 674 8578

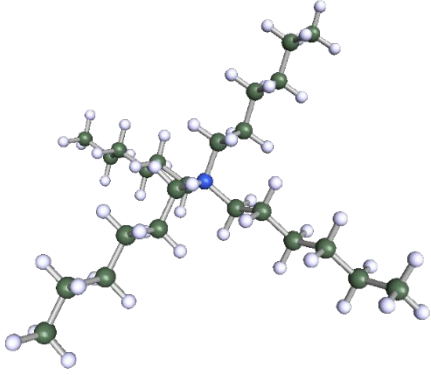
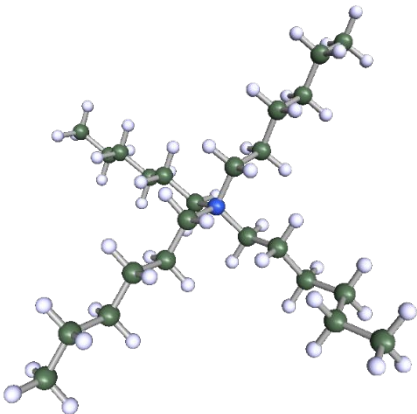
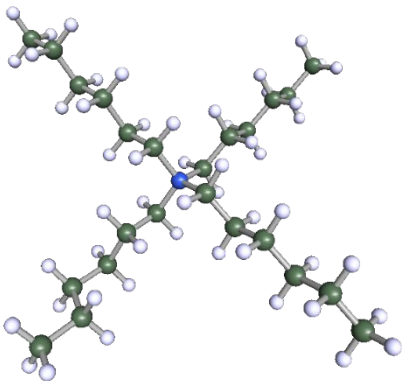
## Supplementary Information and Figures

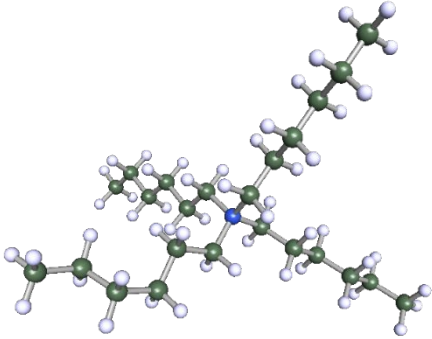
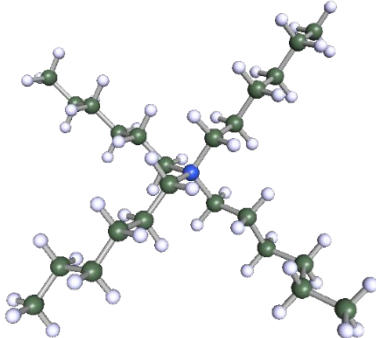
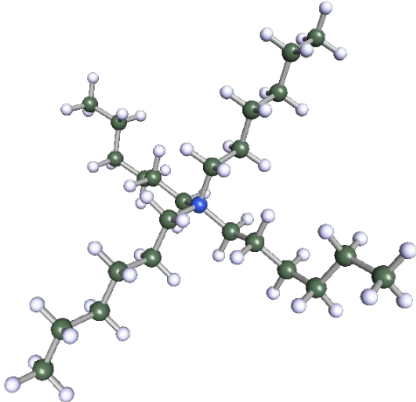
Table S1. Conformers and Relative Energies for Ammonium Cations

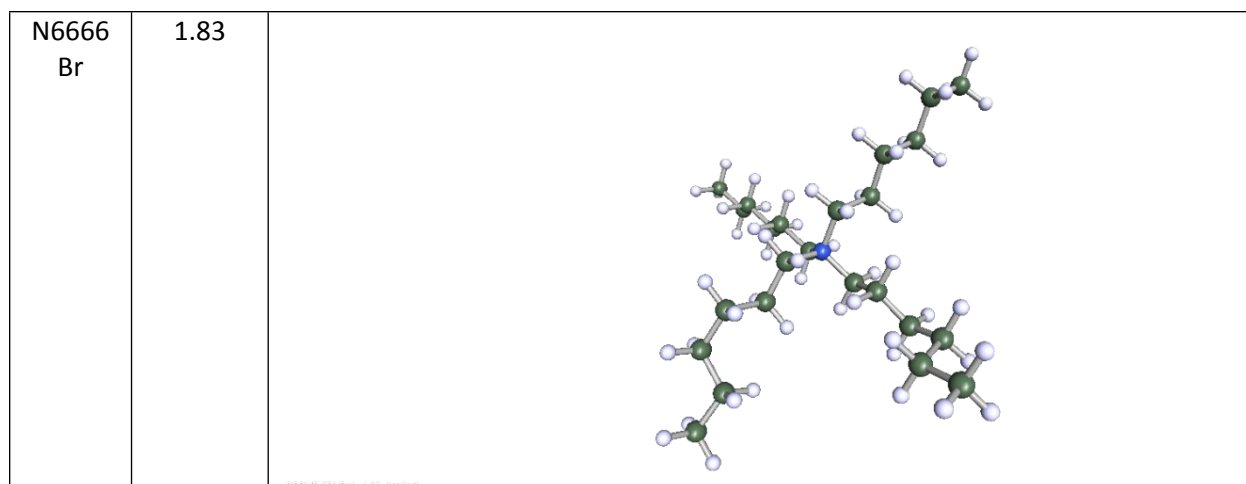
Species	Relative Energy (kcal/mol)	Conformer
N4444Br	0	
N4444Br	2.04	
N4444Br	2.06	

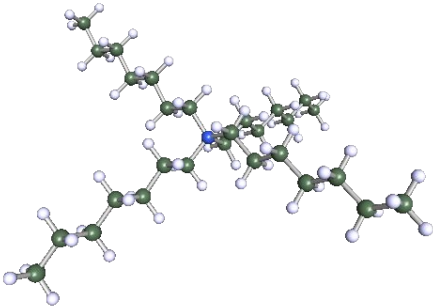
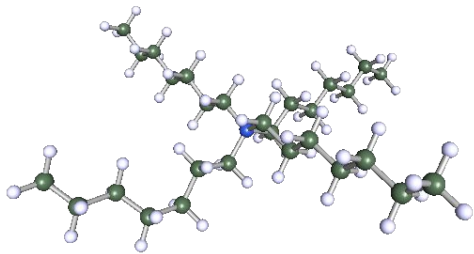
Species	Relative Energy (kcal/mol)	Conformer
N5555Br	0	
N5555Br	0.83	
N5555Br	0.89	
N5555Br	1.71	

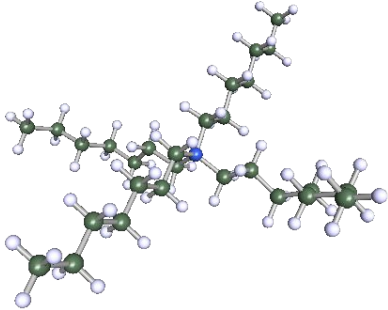
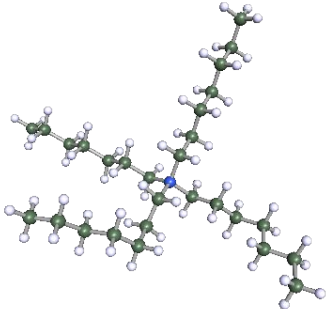
N5555Br	1.72	 <small>CCDC 1000000, 1.72 Å</small>
N5555Br	1.8	 <small>CCDC 1000000, 1.8 Å</small>
N5555Br	1.82	 <small>CCDC 1000000, 1.82 Å</small>

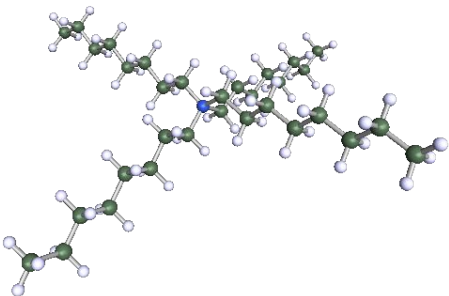
Species	Relative Energy (kcal/mol)	Conformer
N6666 Br	0	 <p style="text-align: center; font-size: small;">P0007-001-001-001-001</p>
N6666 Br	0.78	 <p style="text-align: center; font-size: small;">P0007-001-001-001-001</p>
N6666 Br	0.84	 <p style="text-align: center; font-size: small;">P0007-001-001-001-001</p>

<p>N6666 Br</p>	<p>1.48</p>	 <p style="font-size: small; text-align: center;">2007 01 25 1.48 kbdm</p>
<p>N6666 Br</p>	<p>1.68</p>	 <p style="font-size: small; text-align: center;">2007 01 25 1.68 kbdm</p>
<p>N6666 Br</p>	<p>1.73</p>	 <p style="font-size: small; text-align: center;">2007 01 25 1.73 kbdm</p>

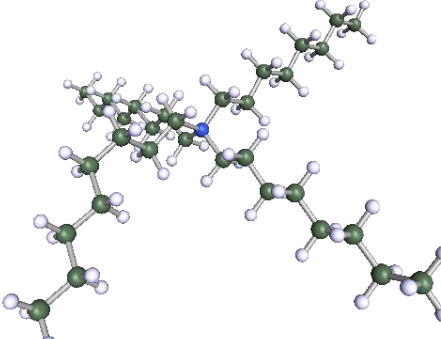
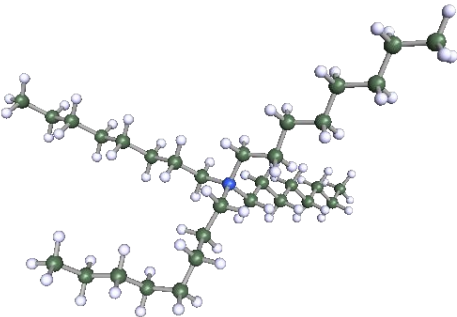
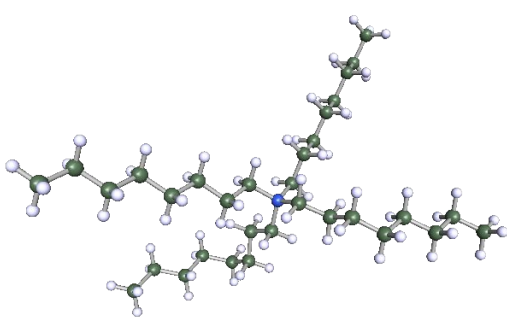


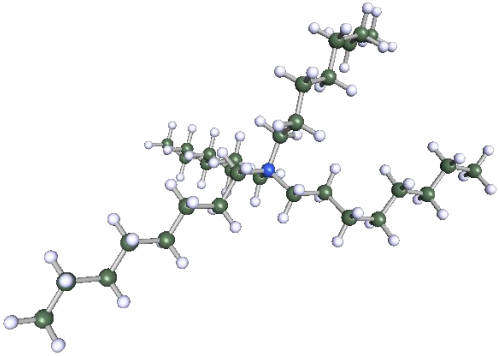
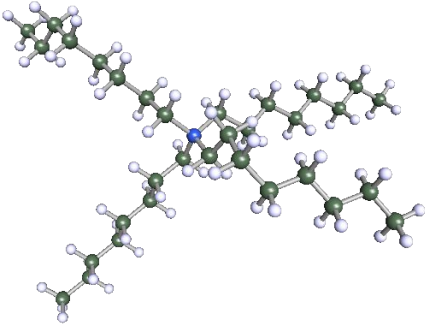
Species	Relative Energy (kcal/mol)	Conformer
N7777Br	0	 <p style="text-align: right; font-size: x-small;">BCONF_235 Brak 0 kcal/mol</p>
N7777Br	0.85	 <p style="text-align: right; font-size: x-small;">BCONF_258 Brak 0.85 kcal/mol</p>

N7777Br	1.69	 <p data-bbox="678 653 829 667">BCONF_751 Erel= 1.69 kcal/mol</p>
N7777Br	3.11	 <p data-bbox="678 1129 829 1144">BCONF_705 Erel= 3.11 kcal/mol</p>

Species	Relative Energy (kcal/mol)	Conformer
N8888Br	0	 <p data-bbox="727 1707 873 1722">BCONF_1159 Erel= 0 kcal/mol</p>



N8888Br	0.89	 <p>8CONF_1203 Enr= 0.89 kcal/mol</p>
N8888Br	2.32	 <p>8CONF_1163 Enr= 2.32 kcal/mol</p>
N8888Br	3.32	 <p>8CONF_1198 Enr= 3.32 kcal/mol</p>

N8888Br	3.35	 <p>8CONF_1408 Enk 3.35 kcal/mol</p>
N8888Br	3.62	 <p>8CONF_717 Enk 3.62 kcal/mol</p>

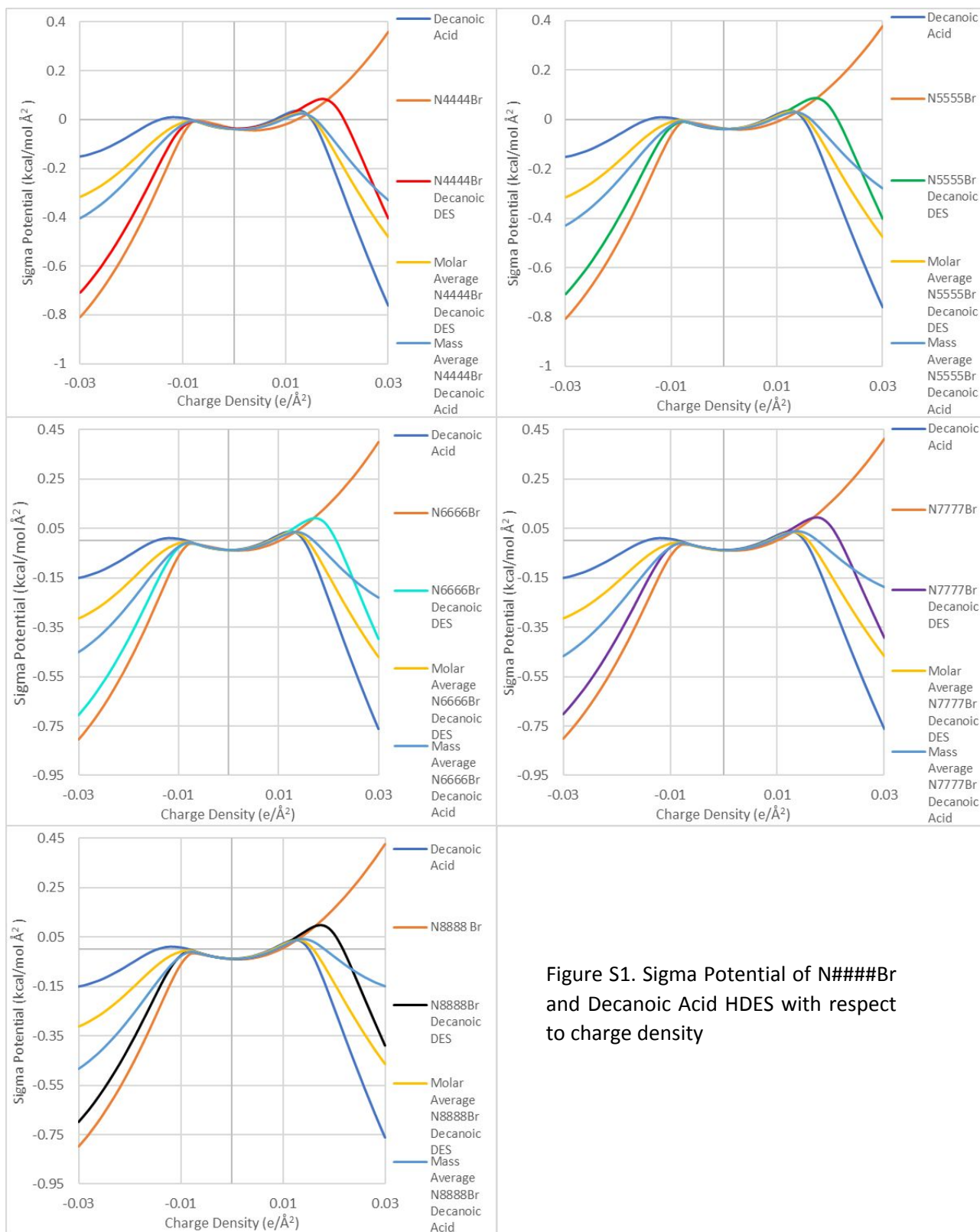
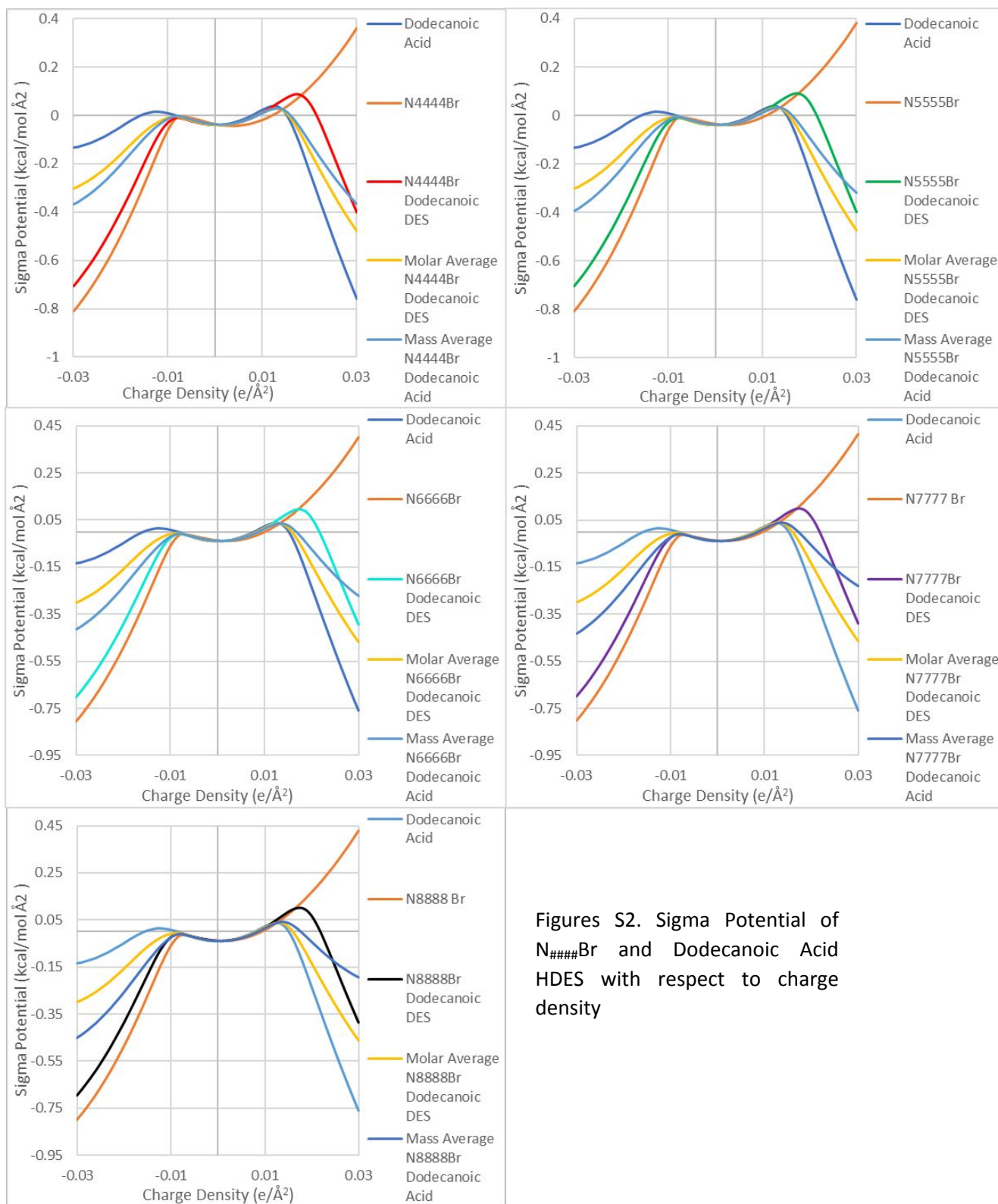


Figure S1. Sigma Potential of N####Br and Decanoic Acid HDES with respect to charge density



Figures S2. Sigma Potential of N####Br and Dodecanoic Acid HDES with respect to charge density