

**The Energetics of Covalent and Non-covalent Binding in Complexes Containing Phosphate and Cationic Amino Groups**

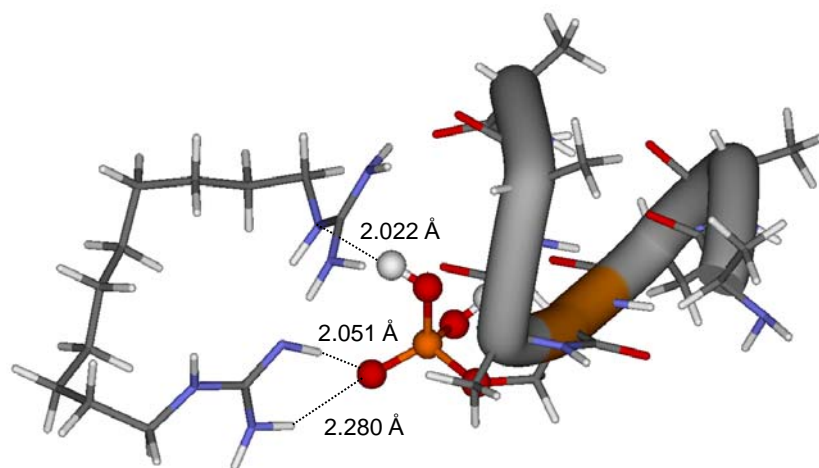
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**Supporting Information**

Complete reference 41:

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Figure S1



[DGD+H][A<sub>3</sub>pSA<sub>3</sub>-NH<sub>2</sub>]

16.8 kcal/mol

B3LYP/6-31++G(d,p)//B3LYP/6-31G(d) with ZPE correction

Figure S1. The canonical structure [DGD+H]<sup>+</sup>[A<sub>3</sub>pSA<sub>3</sub>-NH<sub>2</sub>]<sup>-</sup>, of the DGD- A<sub>3</sub>pSA<sub>3</sub>-NH<sub>2</sub> complex.