Electronic Supplementary Material (ESI) for RSC Advances

Molecular Structure and Stability of Complexes of Charged Structural Units of Heparin with Arginine and Lysine

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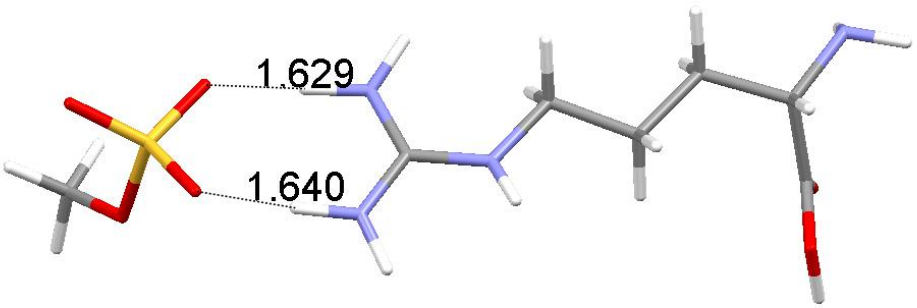
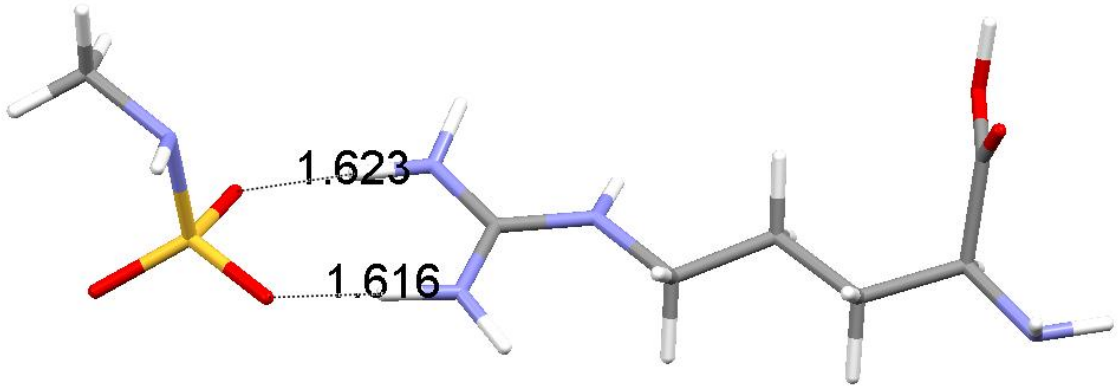
Supporting Information

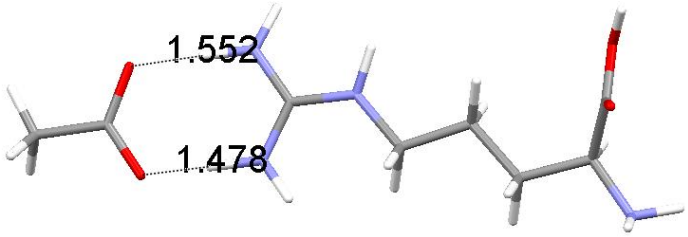
Overall shape of the fourteen complexes investigated computed at the Becke3LYP/6-31+G(d,p) level of theory (bond lengths are in Angstroms).



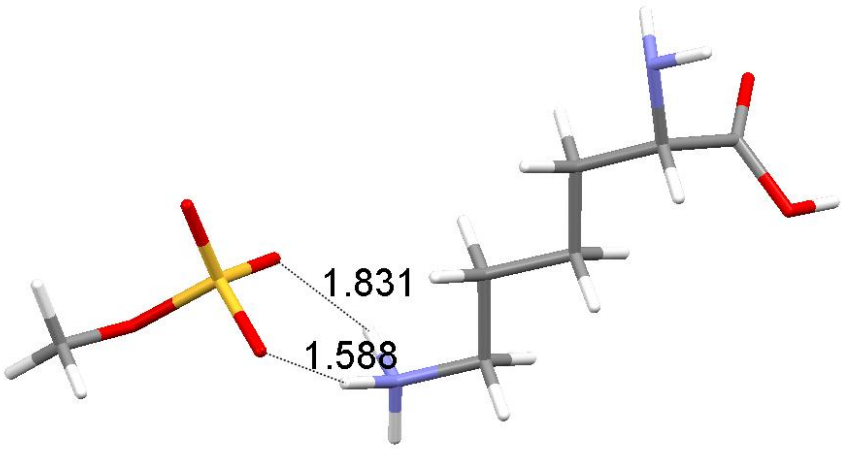
$CH_3OSO_3(-) \cdots Arg(+)$



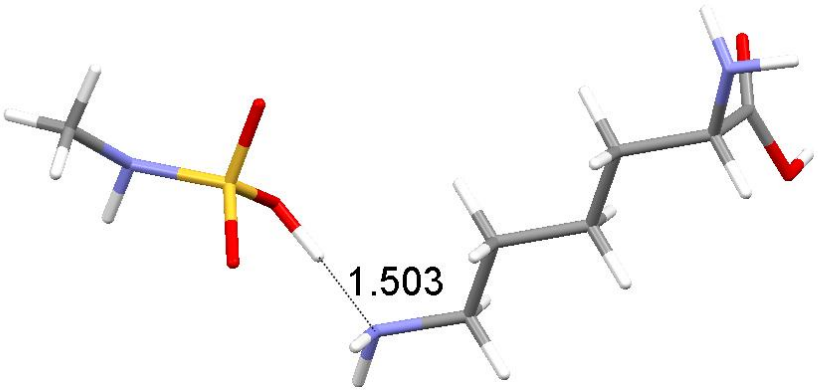
$CH_3NHSO_3(-)\cdots Arg(+)$



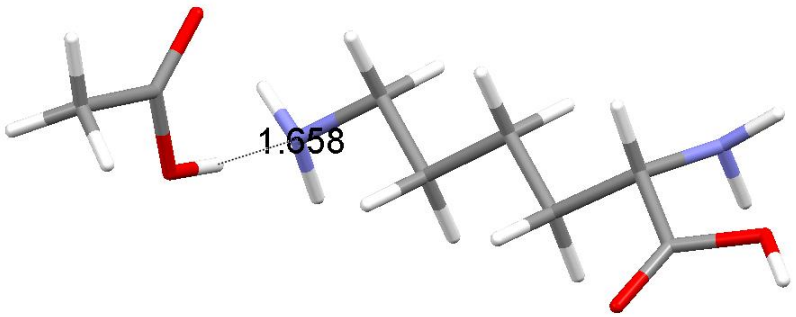
$CH_3CO_2(-)\cdots Arg(+)$



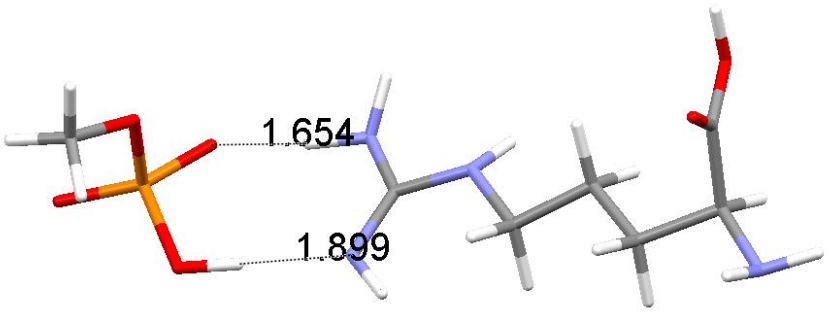
$CH_3OSO_3(-)\cdots Lys(+)$



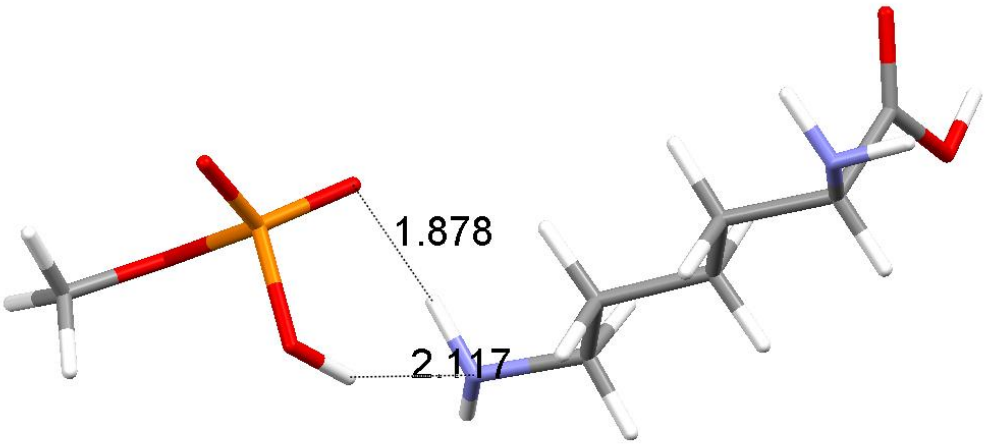
$CH_3NHSO_3H\cdots Lys$



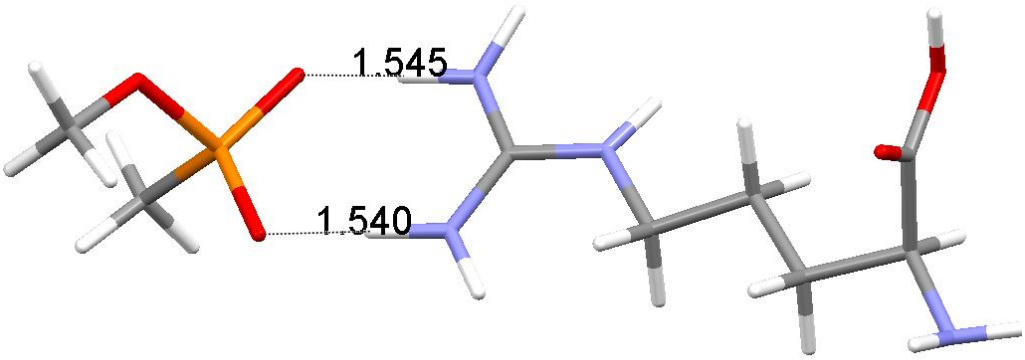
$CH_3CO_2H\cdots Lys$



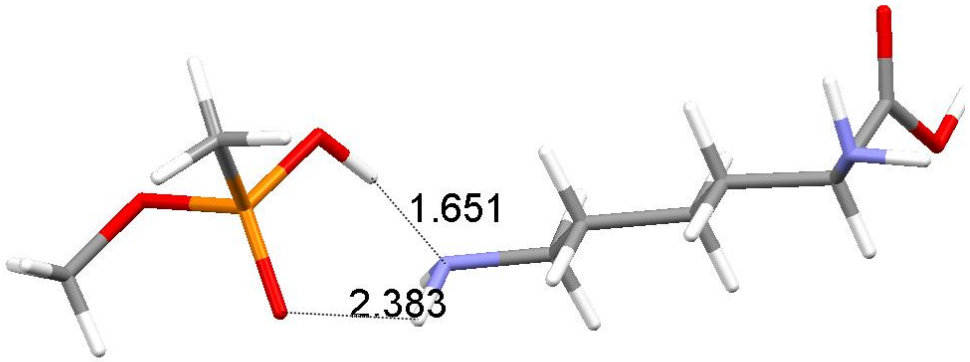
$CH_3OPO_3H(-)\cdots Arg$



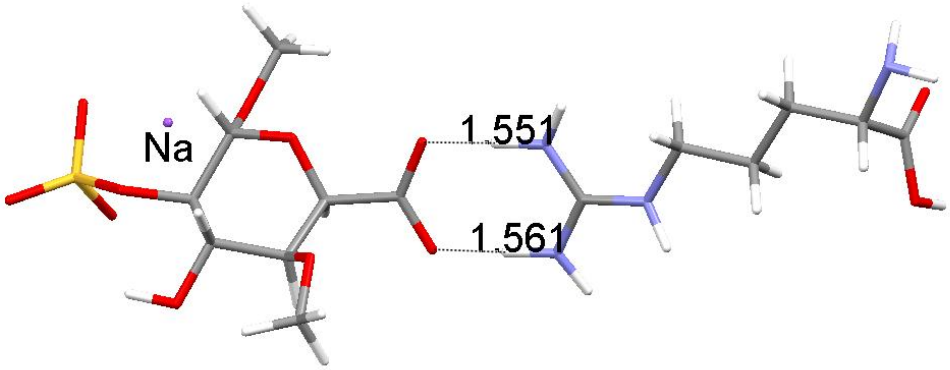
$CH_3OPO_3H(-)\cdots Lys$



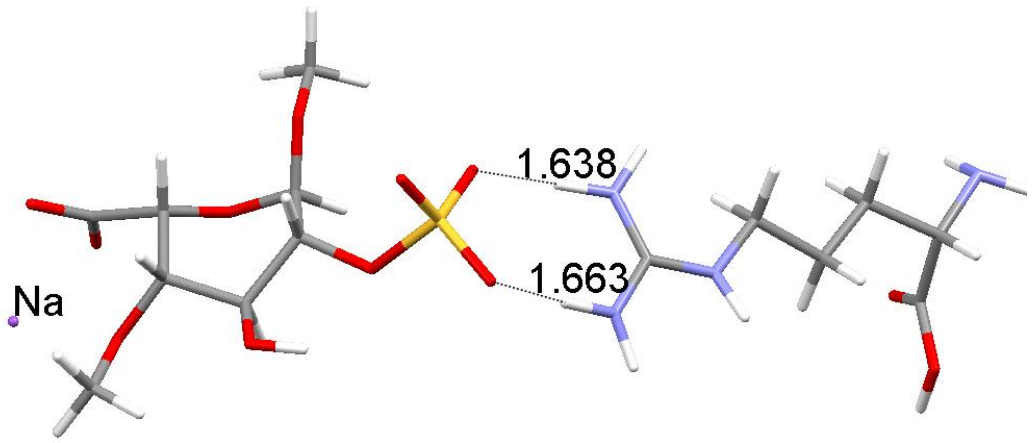
$CH_3O(CH_3)PO_2(-)\cdots Arg(+)$



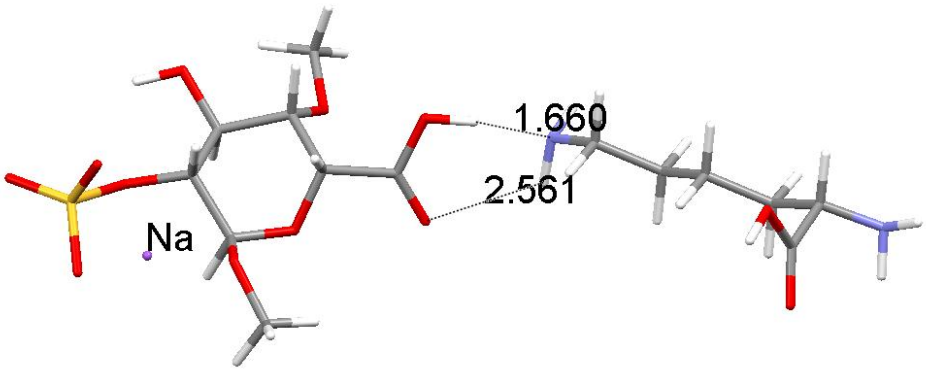
$CH_3O(CH_3)PO_2H \cdots Lys$



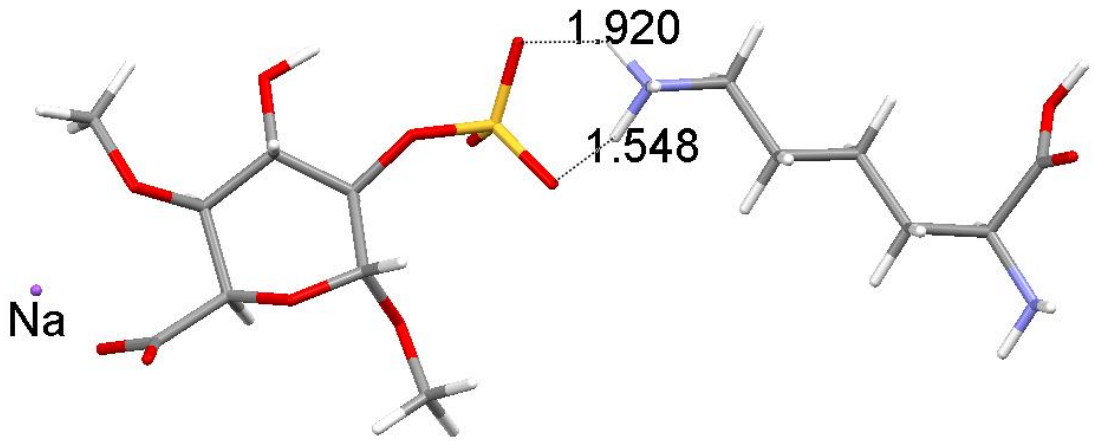
1,4-DiOMeIdoA2SNa(-)···Arg(+)



1,4-DiOMeIdoA2SNa(-)···Arg(+)



1,4-DiOMeIdoA2SNaH···Lys



1,4-DiOMeIdoA2SNa(-)···Lys(+)

Fig. A: B3LYP optimized structures of the systems studied