Electronic Supplementary Material (ESI) for RSC Advances

Effect of metal ions (Li^+, Na^+, K^+, Mg^{2+} and Ca^{2+}) and water on the conformational changes of glycosidic bonds in heparin oligosaccharides

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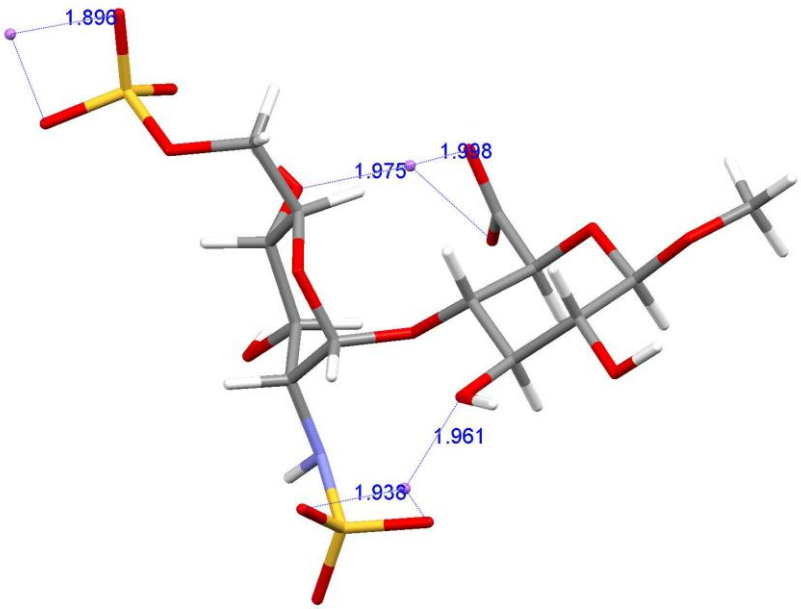
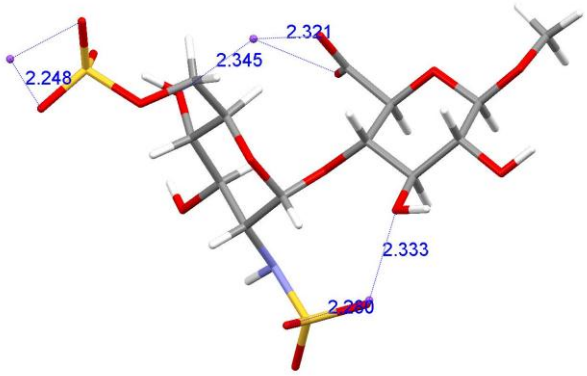
Supporting Information

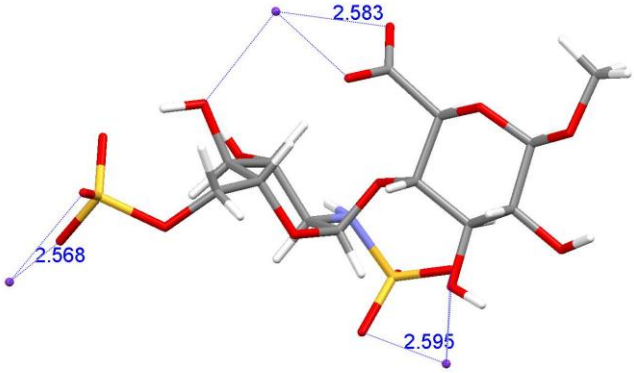
Overall shape of the Li^+, Na^+, K^+, Mg^{2+} and Ca^{2+} salts of dimeric and pentameric structural units of heparin (bond lengths are in Angstroms).



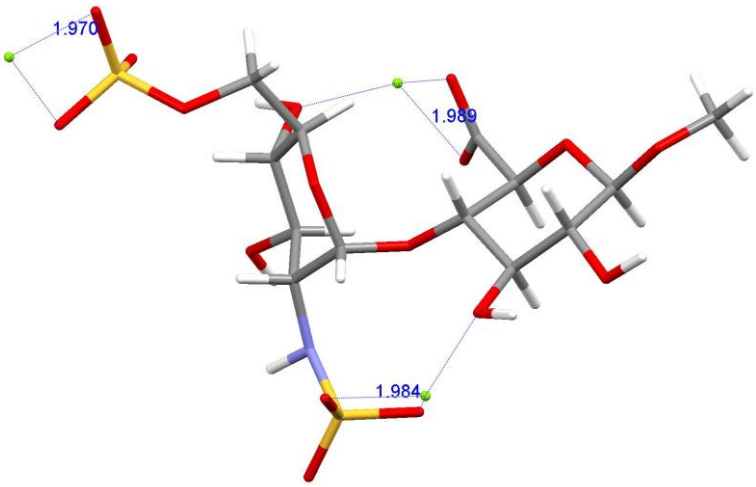
D-E·Li^+



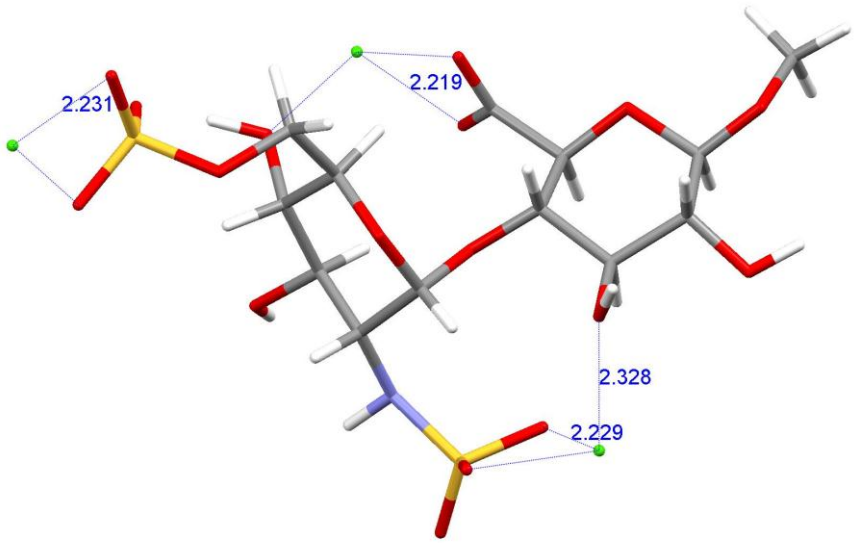
D-E·Na^+



D-E·K^+

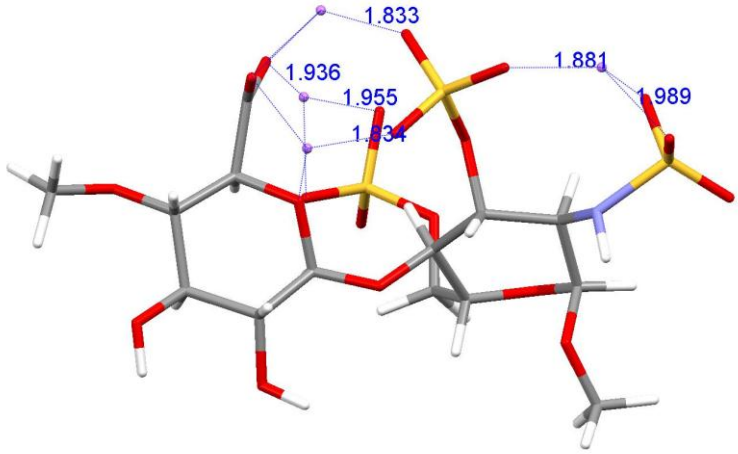


D-E·Mg^{2+}

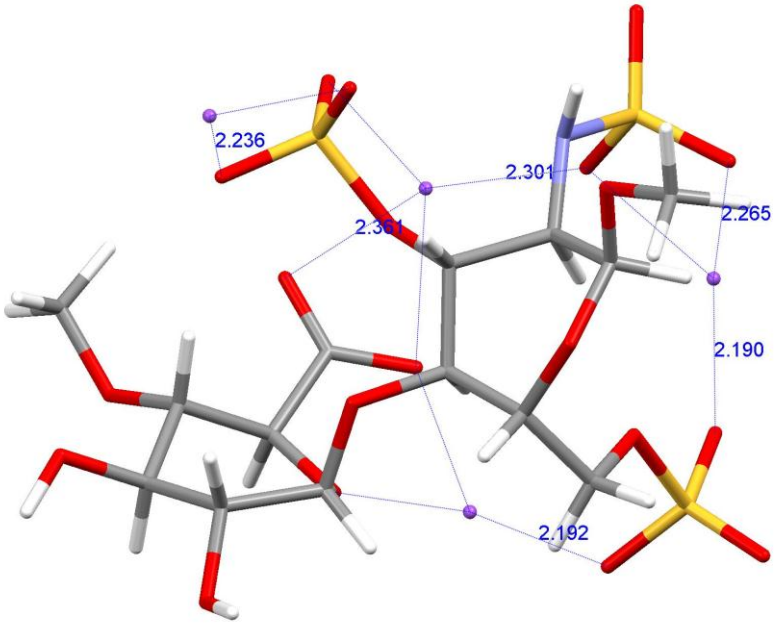


D-E·Ca^{2+}

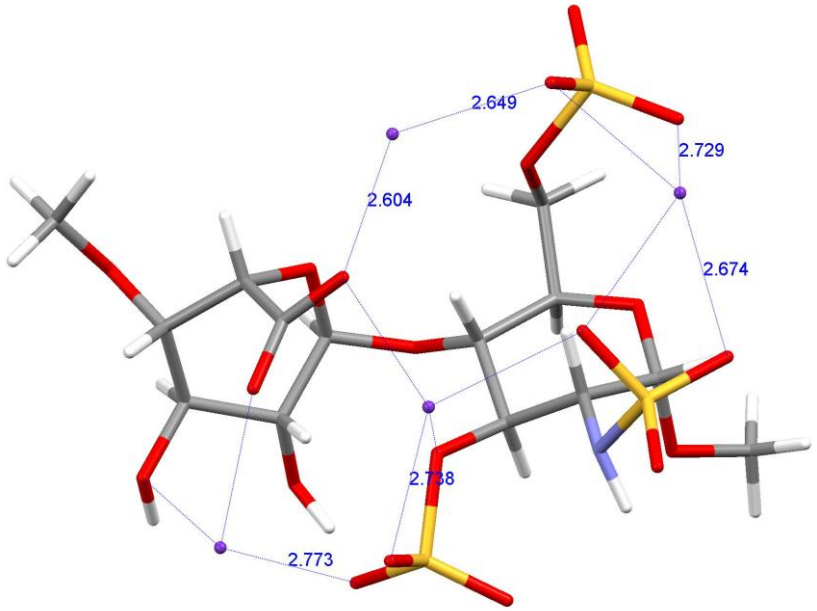
Fig. 1A: B3LYP/6–311+G(d,p) optimized structures of the Li^{+}, Na^{+}, K^{+}, Mg^{2+} and Ca^{2+} salts of D–E dimeric unit of heparin.



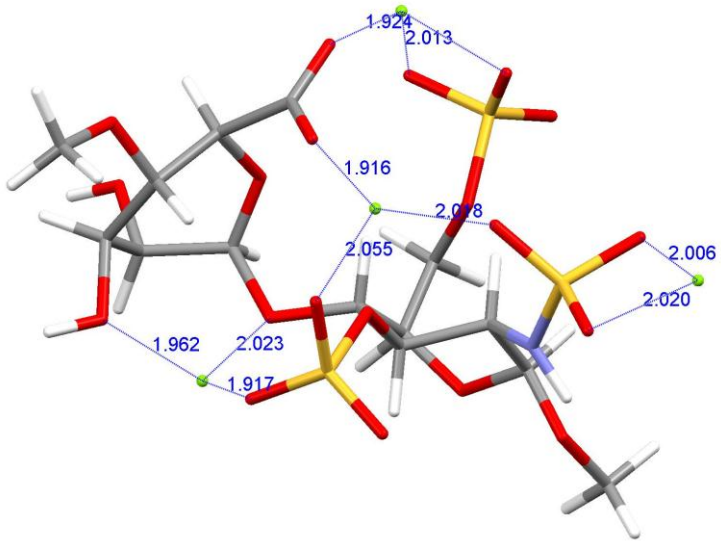
E-F·Li^+



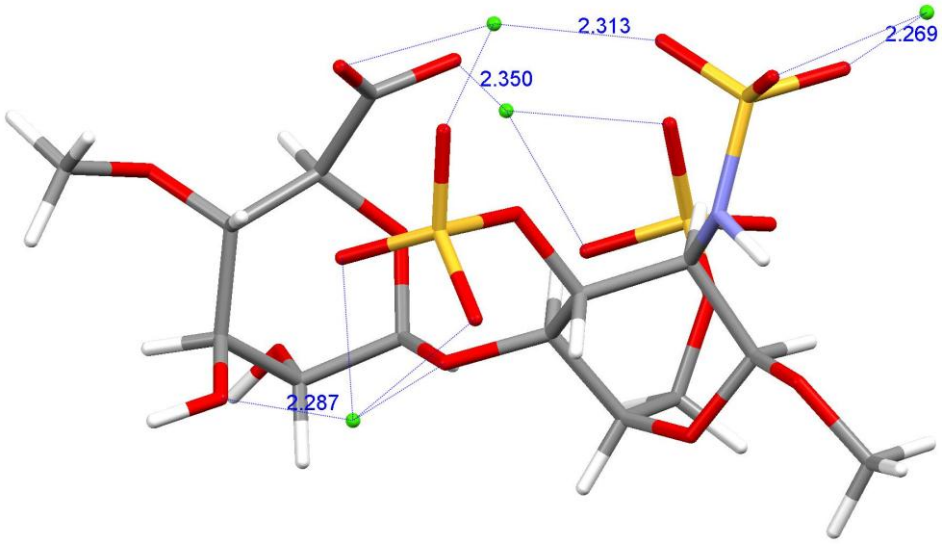
E-F·Na^+



E-F·K^+

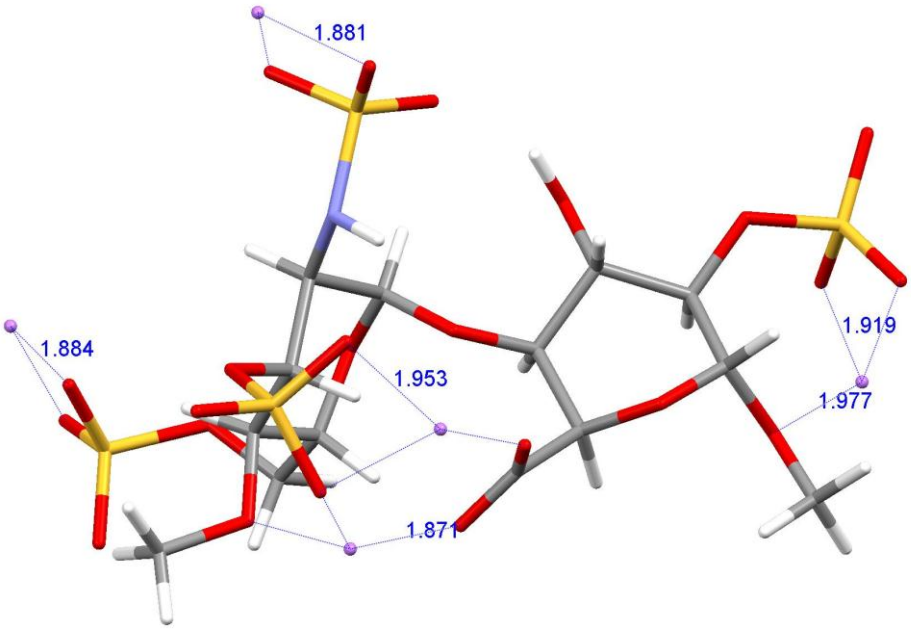


E-F·Mg^{2+}

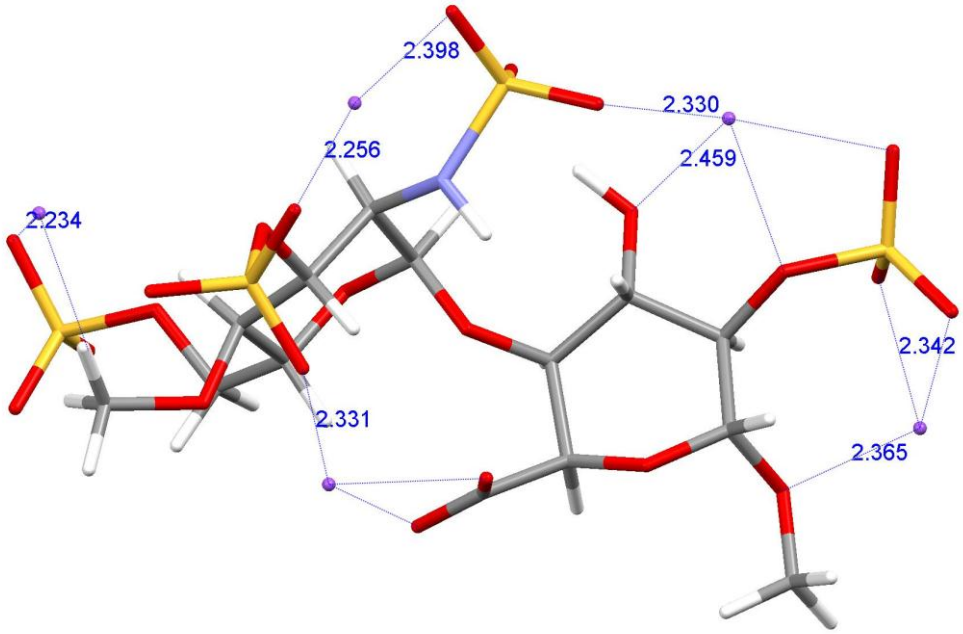


E-F·Ca^{2+}

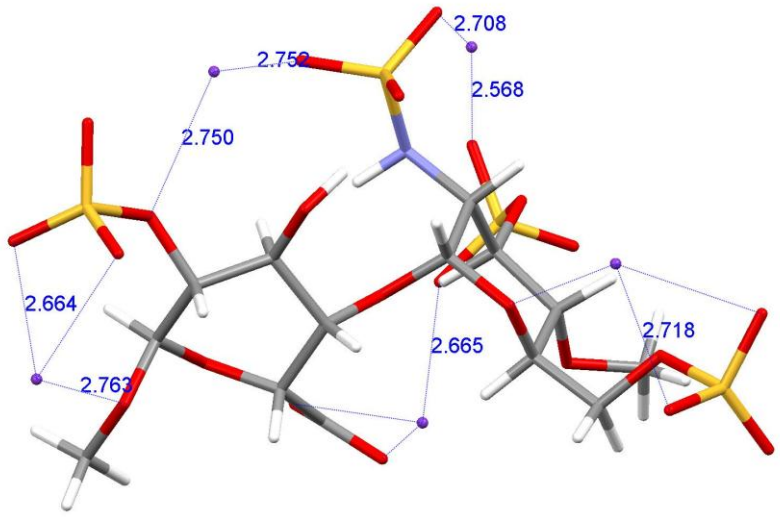
Fig. 2A: B3LYP/6–311+G(d,p) optimized structures of the Li^{+}, Na^{+}, K^{+}, Mg^{2+} and Ca^{2+} salts of E–F dimeric unit of heparin.



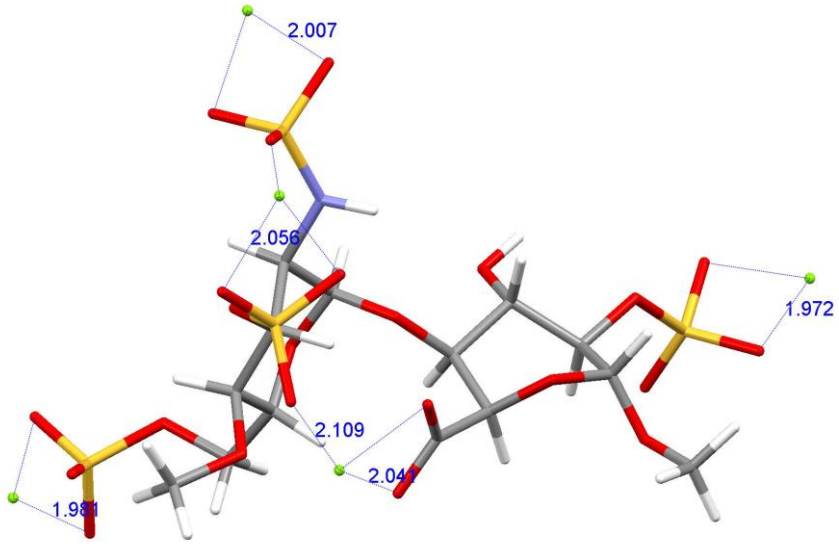
F–G·Li^{+}



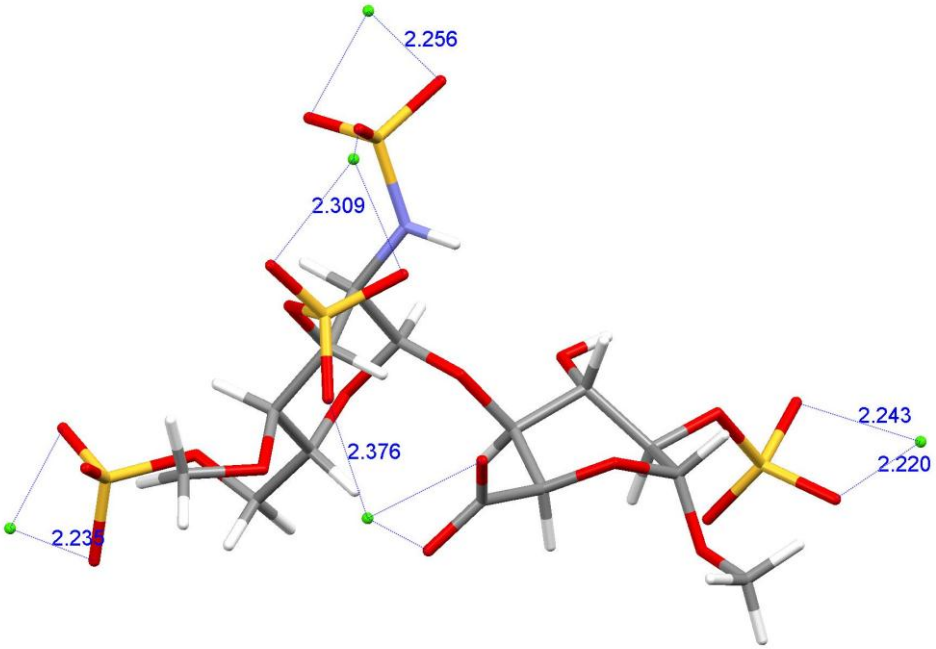
F–G·Na$^+$



F–G·K$^+$

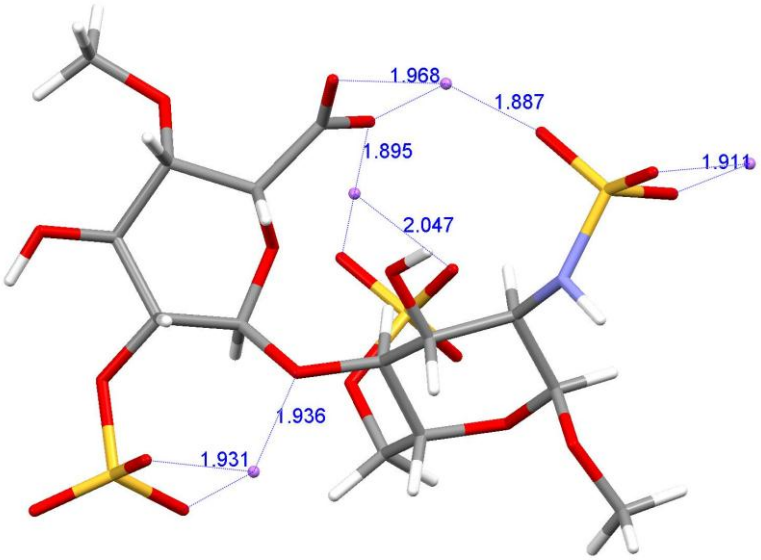


F–G·Mg^{2+}

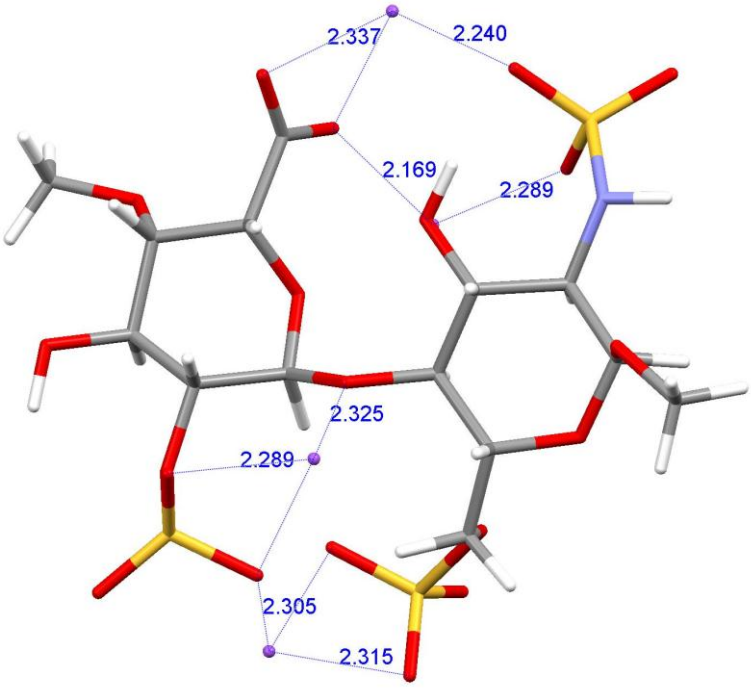


F–G·Ca^{2+}

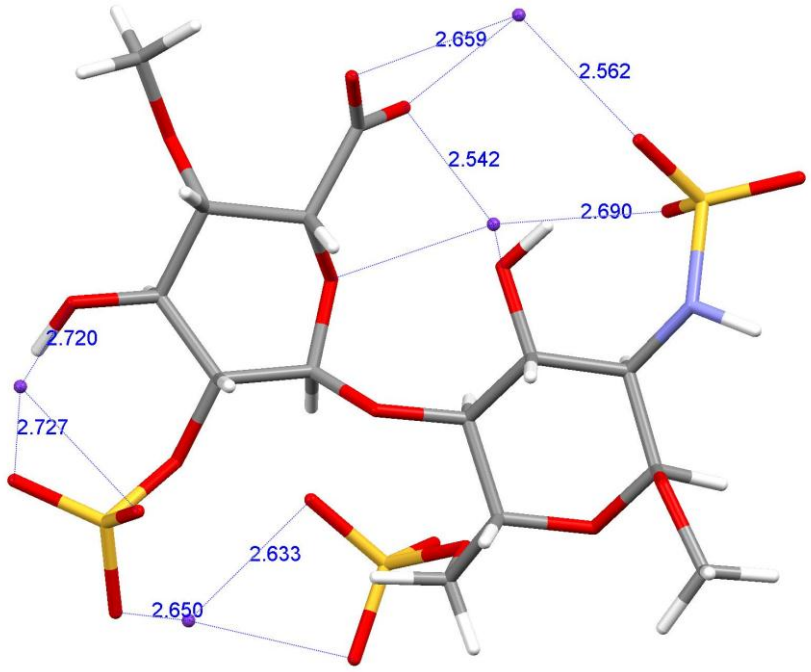
Fig. 3A: B3LYP/6–311+G(d,p) optimized structures of the Li^{+}, Na^{+}, K^{+}, Mg^{2+} and Ca^{2+} salts of F–G dimeric unit of heparin.



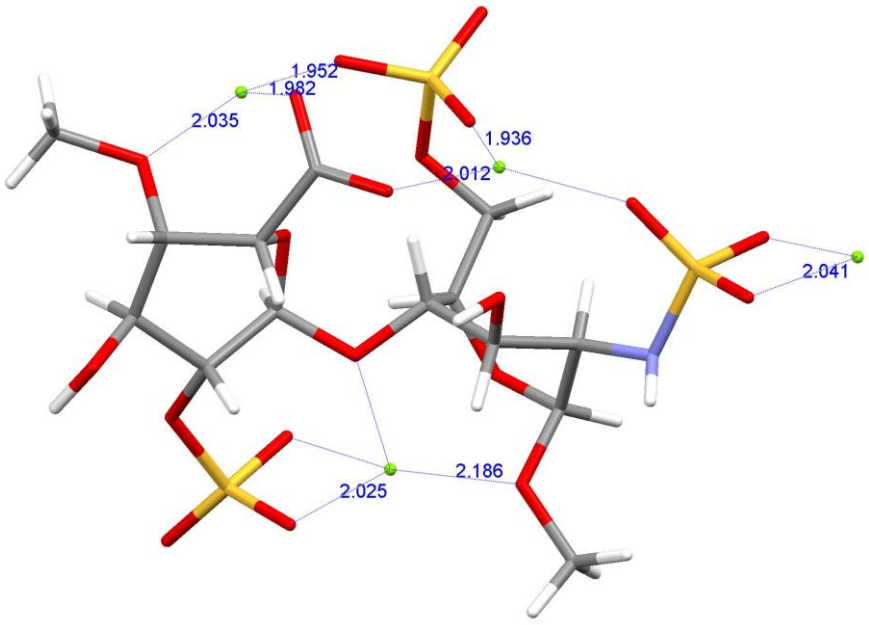
G–H·Li^+



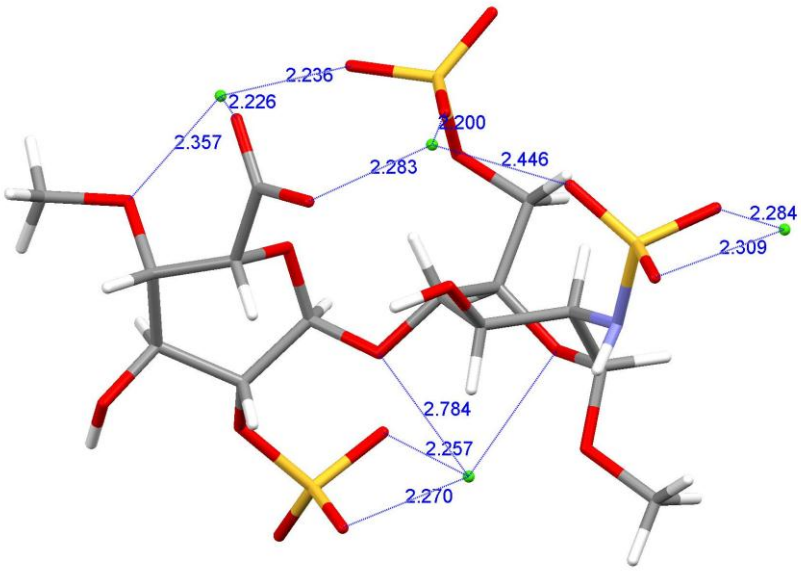
G–H·Na^+



G–H·K^+

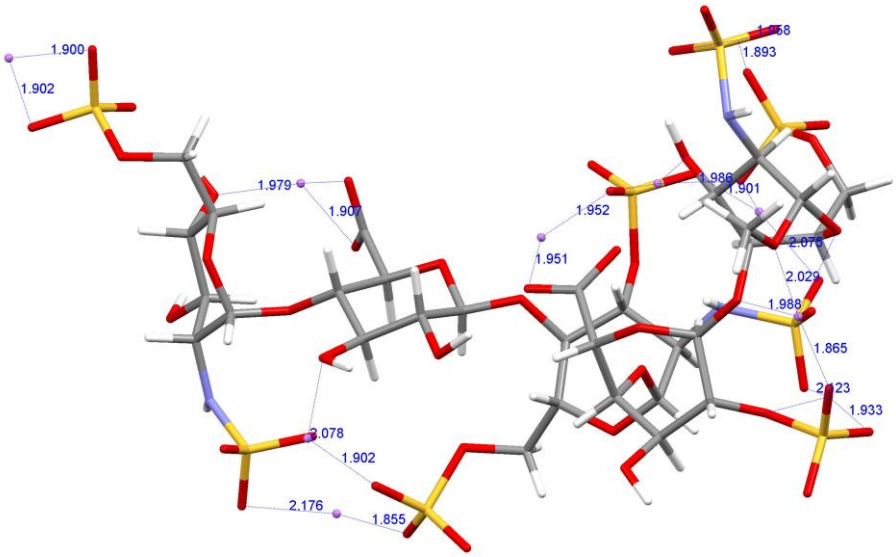


G–H·Mg^{2+}

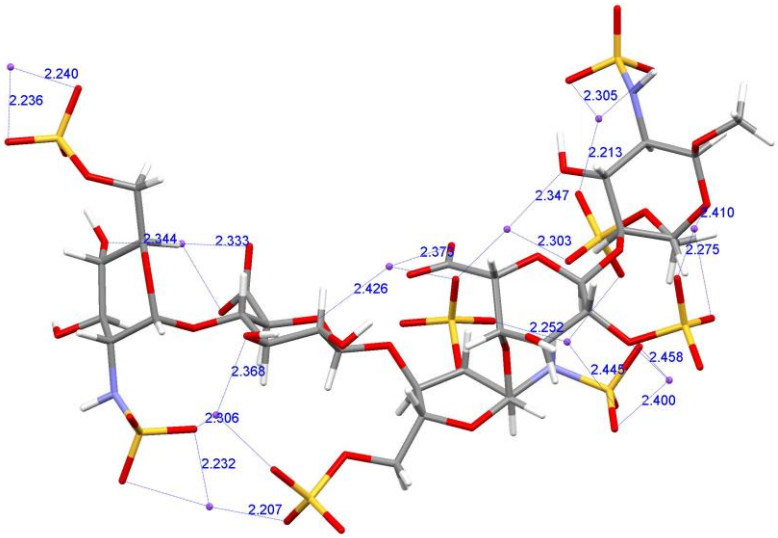


G–H·Ca^{2+}

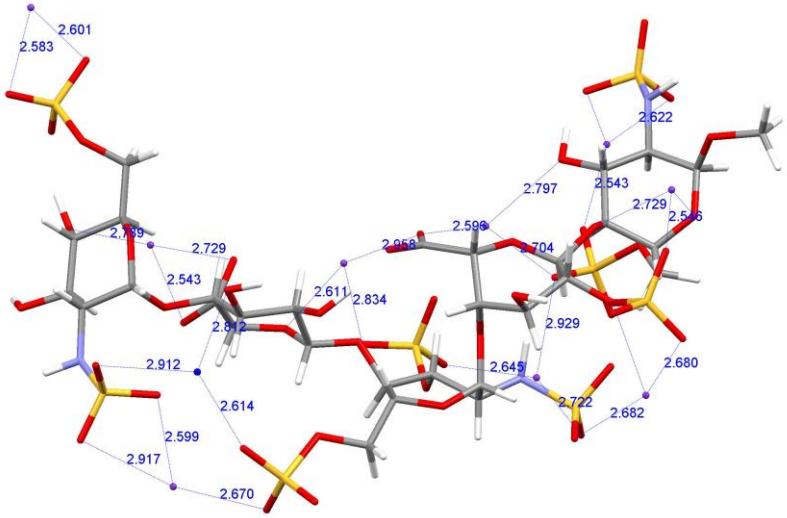
Fig. 4A: B3LYP/6-311+G(d,p) optimized structures of the Li^{+}, Na^{+}, K^{+}, Mg^{2+} and Ca^{2+} salts of G–H dimeric unit of heparin.



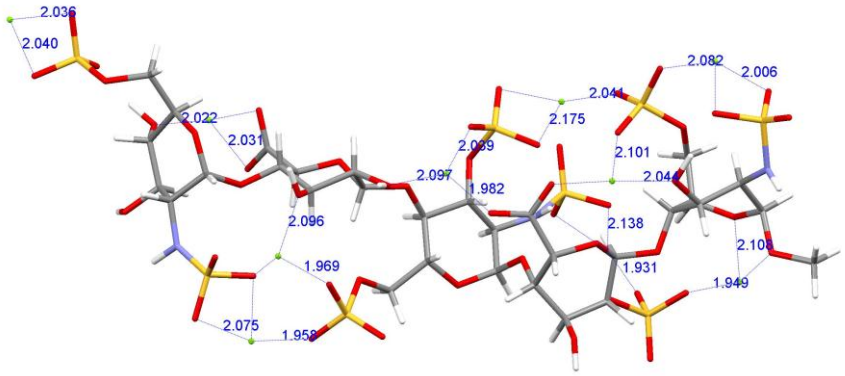
D–E–F–G–H·Li^{+}



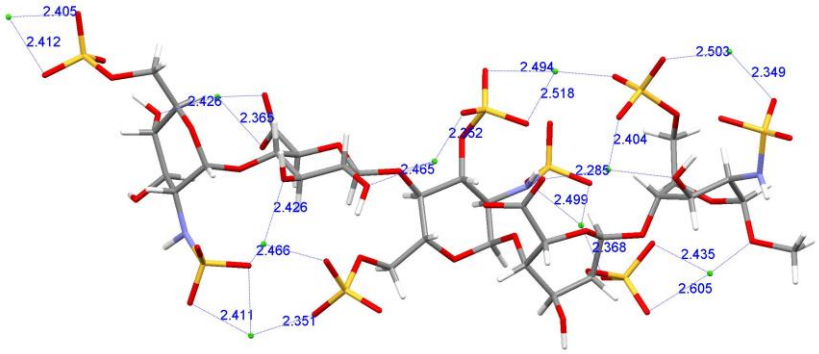
D–E–F–G–H·Na^+



D–E–F–G–H·K^+



D–E–F–G–H·Mg^{2+}



D–E–F–G–H·Ca^{2+}

Fig. 5A: B3LYP/6-31G(d) optimized structures of the Li^{+}, Na^{+}, K^{+}, Mg^{2+} and Ca^{2+} salts of D–E–F–G–H pentameric unit of heparin.