List of Figures

Figure Number	Figure Caption	Page Number
2.1	Flow chart for self-consistent density functional calculations.	33
2.2	Different types of interactions observed in system.	38
2.3	General steps involved in MD simulation.	41
3.1	DFT calculated the binding energy curve of SA-Gal complex at 37° C (a) and 42° C (b) temperature and under various pH conditions.	57
3.2	Molecular structure of target olligodaccharide SA and ligand sachharides Monovalent Gal, Man and PBA carries the Carbon (C) with parrot green color, Oxygen (O) is in red, Hydrogen (H) is in grey and Nitrogen (N) is in blue and Boron is in peach color.	57
3.3	Optimized structure of SA-Gal with the least bond distance (d =1.67Å) between O8-H62 which belongs to targeted molecule and ligand molecule respectively.	59
3.4	Calculated Mulliken atomic charge distribution (in atomic unit) throughout the SA-Gal complex.	60
3.5	Density of electrons with red (high electron density (-))and blue (low electron density (+)) surface at different pH and temperature: (a) pH 5.0; 37°C, (b) pH 5.0; 42°C, (c) pH 5.5; 37°C, (d) pH 5.5; 42°C, (e) pH 6.0; 37°C, (f) pH 6.0; 42°C, (g) pH 6.5; 37°C, (h) pH 6.5; 37°C, (i) pH 7.0; 37°C, and (j) pH 7.0; 42°C.	65
4.1	(a) Examples of the structurally diverse SA family. Where, alpha- anomer is the form that is found when sialic acid is bound to glycans and beta- anomeric configuration is in solvent) [5] (b) Specific imaging of glycans on cell surface [6].	85
4.2	Molecular configuration of sialic acid (a) defined as a target structure, where biantennary Gal (b), biantennary Man (c) and biantennary PBA (d) play the role as ligands.	91
4.3	Time course of the root mean square deviation (RMSD) for MD simulations of 5ns (pink) 15ns (blue) and 25ns (orange) of SA with Biantennary PBA. The RMSD of 25ns is very high than 5ns and 15ns.	93

4.4	Atomic orbital HOMO and LUMO composition of frontier molecular orbital at, 5ns, 15ns and 25ns complex frames of SA against Bi- antennary PBA.	95
4.5	Evolution of the predictivity of the Mulliken charge during (a) 5ns (b) 15ns and (c) 25ns complex simulation time frames of SA-Bi-antennary PBA.	96
4.6	MEP of (a) 5ns (b) 15ns (c) 25ns complex of SA-Bi-antennary PBA.	97
5.1	PTX encapsulated SWCNT with (a) $n = 12$, $m = 12$ and (b) $n = 13$, $m = 13$ chirality and length (L) = 2.0 nm.	115
5.2	Time dependent snapshots of PTX encapsulated (15, 15) SWCNT with length (L) = 2.0 nm at temperatures (a) 310.15 K and (b) 315.15 K .	116
5.3	Computed radial distribution function of significant contributing atoms/molecule of PTX loaded SWCNT at temperature 310.15K: (a) PTX, (b) O14, (c) O5 and (d) N1.	117
5.4	Computed radial distribution function of significant contributing atoms/molecule of PTX loaded SWCNT at temperature 315.15K: (a) PTX, (b) O14, (c) O5 and (d) N1.	118
5.5	Temperature dependent interaction energy of the PTX encapsulated SWCNT as a function of time for temperatures (a) 310.15K and (b) 315.15K.	120
5.6	Calculated temperature dependent SASA as a function of time for temperatures (a) 310.15K and (b) 315.15K.	121
5.7	Computed radius of gyration of the system at temperatures a) 310.15K and b) 315.15K.	122
5.8	Temperature dependent root mean square deviation (RMSD) of PTX encapsulated SWCNT at temperatures (a) 310.15K and (b) 315.15K.	124
6.1	Analyzed Electronic properties (a) Mulliken charge (b) molecular electrostatic potential (MEP), (c) molecular structure of galactose and sialic acid (d) orbital data in tabular form (e) fukui indices data base of chapter 3.	132
6.2	These figures depict the (a) Orbital properties, (b) Molecular structure, (c) Electrophilicity and nucleophilicity and (d) shows the mulliken charge.	133
6.3	Minimized distorted (a) (12, 12) and (13, 13) nanotube encapsulated PTX.	135
	Minimized (15, 15) (a) side view (b) Front view of nanotube encapsulated PTX	
6.4		135

х