LIST OF TABLES

Table		Page
1	The optimised structure of propylene oxide for the six levels of theory	
	MP2, RHF, DFT/B3LYP, AM1, PM3 and SCC-TB together with the	
	experimental structure	10
2	Constants for the Vosko-Wilk-Nusair parameterizations	30
3	Equilibrium geometrical parameters of doxorubicin molecule	
	from Figure 15 in the ground state.	52
4	Dihedral angle of doxorubicin structure optimized by	
	AM1, PM3 and HF/6-31G methods	53
5	Equilibrium geometrical parameters of glucosamine(ethylene glycol)	
	molecule from Figure 20 in the ground state	59
6	Dihedral angle of glucosamine(ethylene glycol) structure optimized	
	by AM1, PM3 and HF/6-31G methods	60
7	Relative energy of di glucosamine(ethylene glycol) in acid solution	64
8	Relative energy of di glucosamine(ethylene glycol) in water solution	68
9	Relative energy of di glucosamine(ethylene glycol) in base solution	72
10	Relative energy of di glucosamine(ethylene glycol) in base solution	76
11	Relative energy of poly(ethylene glycol) in glucosamine molecule	79
12	Relative energy of micelle formation by B3LYP/6-31G//PM3 method	
	calculation	83
13	The relative energy of di glucosamine-mono(ethylene glycol), di	
	glucosamine- di(ethylene glycol), and di glucosamine-tri(ethylene	
	glycol) in acid solution	87
14	The relative energy of di glucosamine-mono(ethylene glycol) and di	
	glucosamine-di(ethylene glycol)in normal solution	88
15	The relative energy of di glucosamine-mono(ethylene glycol) and di	
	glucosamine-di(ethylene glycol) in base solution	89

LIST OF TABLES (Continued)

Appen	Appendix Table	
A1	The molecular energy from molecular optimization;	
	Molecular Structure	104
A2	The molecular energy from molecular optimization;	
	Glucosamine-mono(ethylene glycol) compound	105
A3	The molecular energy from molecular optimization;	
	Glucosamine-di(ethylene glycol) compound and solution structure	106
A4	The molecular energy from molecular optimization;	
	Micelle Structure	107
B1	The molecular energy of mechanism in capsule glucosamine	
	(ethylene glycol) with solution reaction; Di glucosamine-mono(ethylene	
	glycol) in solution	109
B2	The molecular energy of mechanism in capsule glucosamine	
	(ethylene glycol) with solution reaction; Di glucosamine-di(ethylene	
	glycol) in solution	110
C1	The relative energy of reaction in acid solution; Di glucosamine-mono	
	(ethylene glycol)	112
C2	The relative energy of reaction in acid solution; Di glucosamine-di	
	(ethylene glycol)	113
C3	The relative energy of reaction in acid solution; Di glucosamine-tri	
	(ethylene glycol)	114
C4	The relative energy of reaction in normal solution; Di glucosamine-mono	
	(ethylene glycol)	115
C5	The relative energy of reaction in normal solution; Di glucosamine-di	
	(ethylene glycol)	116
C6	The relative energy of reaction in base solution; Di glucosamine-mono	
	(ethylene glycol) attracted at polymer bonding	117
C7	The relative energy of reaction in base solution; Di glucosamine-mono	
	(ethylene glycol) attracted at ethylene glycol group	118

LIST OF TABLES (Continued)

Appendix Table		Page
C8	The relative energy of reaction in base solution; Di glucosamine-di	
	(ethylene glycol)	119
D	Molecular energy of water	121
E	Relative energy of micelle formation by the B3LYP/6-31G//PM3	
	method simulation	123