APPENDICES

Appendix A

The molecular energy

Appendix Table A1 The molecular energy from molecular optimization; Molecular Structure

Structure	Method	Molecular energy	
		(a.u.)	(kcal/mol)
Doxorubicin	B3LYP/6-31G//AM1	-1,927.88	-1,209,764.28
	B3LYP/6-31G//PM3	-1,927.88	-1,209,761.75
	B3LYP/6-31G//HF/6-31G	-1,927.91	-1,209,783.00
Glucosamine-mono(ethylene glycol)	B3LYP/6-31G//AM1	-820.83	-515,081.07
	B3LYP/6-31G//PM3	-820.82	-515,075.50
	B3LYP/6-31G//HF/6-31G	-820.85	-515,088.67
Glucosamine-di(ethylene glycol)	B3LYP/6-31G//AM1	-974.61	-611,579.71
	B3LYP/6-31G//PM3	-974.61	-611,574.40
Glucosamine-tri(ethylene glycol)	B3LYP/6-31G//AM1	-1,128.39	-708,078.36
	B3LYP/6-31G//PM3	-1,128.39	-708,073.33
Glucosamine-penta(ethylene glycol)	B3LYP/6-31G//AM1	-1,435.95	-901,075.52
	B3LYP/6-31G//PM3	-1,435.95	-901,071.33

Appendix Table A2 The molecular energy from molecular optimization; Glucosamine-mono(ethylene glycol) compound

Structure	Method	Molecular energy	
		(a.u.)	(kcal/mol)
Di glucosamine-mono(ethylene glycol)	B3LYP/6-31G//AM1	-1,565.28	-982,229.58
	B3LYP/6-31G//PM3	-1,565.23	-982,198.76
Di glucosamine-mono(ethylene glycol) anion	B3LYP/6-31G//AM1	-1,564.66	-981,840.58
	B3LYP/6-31G//PM3	-1,564.65	-981,832.99
Glucosamine-mono(ethylene glycol) cation	B3LYP/6-31G//AM1	-744.71	-467,314.20
	B3LYP/6-31G//PM3	-744.71	-467,314.20
Glucosamine-mono(ethylene glycol) anion	B3LYP/6-31G//AM1	-820.24	-514,706.50
	B3LYP/6-31G//PM3	-820.25	-514,717.11

Appendix Table A3 The molecular energy from molecular optimization; Glucosamine-di(ethylene glycol) compound and solution structure

Structure	Method	Molecular energy	
		(a.u.)	(kcal/mol)
Glucosamine-di(ethylene glycol) compound			
Di glucosamine-di(ethylene glycol)	B3LYP/6-31G//AM1	-1,872.83	-1,175,219.88
	B3LYP/6-31G//PM3	-1,872.80	-1,175,202.55
Di glucosamine-di(ethylene glycol) anion	B3LYP/6-31G//AM1	-1,872.26	-1,174,864.86
	B3LYP/6-31G//PM3	-1,872.17	-1,174,807.15
Glucosamine-di(ethylene glycol) cation	B3LYP/6-31G//AM1	-898.56	-563,855.93
	B3LYP/6-31G//PM3	-898.54	-563,843.52
Glucosamine-di(ethylene glycol) anion	B3LYP/6-31G//AM1	-974.02	-611,208.95
	B3LYP/6-31G//PM3	-974.04	-611,218.09
Solution structure			
Water	B3LYP/6-31G//AM1	-76.38	-47,932.31
	B3LYP/6-31G//PM3	-76.38	-47,932.31
Hydronium ion	B3LYP/6-31G//AM1	-76.68	-48,116.58
	B3LYP/6-31G//PM3	-76.68	-48,115.95
Hydroxide anion	B3LYP/6-31G//AM1	-75.70	-47,504.69
	B3LYP/6-31G//PM3	-75.70	-47,504.52

Appendix Table A4 The molecular energy from molecular optimization; Micelle Structure

Structure	Method	Molecular energy	
		(a.u.)	(kcal/mol)
Doxorubicin-1 Glucosamine-mono(ethylene glycol)	B3LYP/6-31G//PM3	-2,748.71	-1,724,844.23
Doxorubicin-2 Glucosamine-mono(ethylene glycol)	B3LYP/6-31G//PM3	-3,569.55	-2,239,925.40
Doxorubicin-3 Glucosamine-mono(ethylene glycol)	B3LYP/6-31G//PM3	-4,390.37	-2,755,003.57
Doxorubicin-1 Glucosamine-di(ethylene glycol)	B3LYP/6-31G//PM3	-2,902.49	-1,821,343.24
Doxorubicin-2 Glucosamine-di(ethylene glycol)	B3LYP/6-31G//PM3	-3,877.11	-2,432,923.06
Doxorubicin-3 Glucosamine-di(ethylene glycol)	B3LYP/6-31G//PM3	-4,851.71	-3,044,499.51
Doxorubicin-1 Glucosamine-tri(ethylene glycol)	B3LYP/6-31G//PM3	-3,056.27	-1,917,842.05
Doxorubicin-2 Glucosamine-tri(ethylene glycol)	B3LYP/6-31G//PM3	-4,184.67	-2,625,921.11
Doxorubicin-3 Glucosamine-tri(ethylene glycol)	B3LYP/6-31G//PM3	-5,313.06	-3,333,997.29
Doxorubicin-1 Glucosamine-penta(ethylene glycol)	B3LYP/6-31G//PM3	-3,363.83	-2,110,839.45
Doxorubicin-2 Glucosamine-penta(ethylene glycol)	B3LYP/6-31G//PM3	-4,799.79	-3,011,917.85
Doxorubicin-3 Glucosamine-penta(ethylene glycol)	B3LYP/6-31G//PM3	-6,235.75	-3,912,992.39

Appendix B

The molecular energy of transition state in capsule glucosamine(ethylene glycol) interacted by solution reaction

Appendix Table B1 The molecular energy of mechanism in capsule glucosamine(ethylene glycol) with solution reaction; Di glucosamine-mono(ethylene glycol) in solution

Structure	Method	Molecular energy			
		Reactant complex		Product complex	
		(a.u.)	(kcal/mol)	(a.u.)	(kcal/mol)
Di glucosamine-mono(ethylene glycol)--H_3O^+ --> Glucosamine-mono(ethylene glycol) cation---Glucosamine-mono(ethylene glycol)---H_2O					
	B3LYP/6-31G//AM1	-1641.68	-1,030,169.59	-1642.038574	-1,030,395.63
	B3LYP/6-31G//PM3	-1641.68	-1,030,169.21	-1642.057218	-1,030,407.32
Di glucosamine-mono(ethylene glycol)--H_2O --> Glucosamine-mono(ethylene glycol) cation---Glucosamine-mono(ethylene glycol)					
	B3LYP/6-31G//AM1	-1641.40	-1,029,995.29	-1641.681429	-1,030,171.51
	B3LYP/6-31G//PM3	-1641.40	-1,029,995.29	-1641.64432	-1,030,148.23
Di glucosamine-mono(ethylene glycol)--OH^- --> Glucosamine-mono(ethylene glycol) anion---Glucosamine-mono(ethylene glycol)					
	B3LYP/6-31G//AM1	-1640.48	-1,029,415.68	-1641.11	-1,029,811.72
	B3LYP/6-31G//PM3	-1640.48	-1,029,415.68	-1641.11	-1,029,811.72
Di glucosamine-mono(ethylene glycol)--OH^- --> Di glucosamine-mono(ethylene glycol) cation---H_2O					
	B3LYP/6-31G//AM1	-1641.06	-1,029,782.11	-1641.11	-1,029,812.60
	B3LYP/6-31G//PM3	-1641.06	-1,029,782.11	-1641.07	-1,029,785.93

Appendix Table B2 The molecular energy of mechanism in capsule glucosamine(ethylene glycol) with solution reaction; Di glucosamine-di(ethylene glycol) in solution

Structure	Method	Molecular energy			
		Reactant complex		Product complex	
		(a.u.)	(kcal/mol)	(a.u.)	(kcal/mol)
Di glucosamine-di(ethylene glycol)--H_3O^+ --> Glucosamine-di(ethylene glycol) cation---Glucosamine-di(ethylene glycol)---H_2O					
	B3LYP/6-31G//AM1	-1949.32	-1,223,217.33	-1949.602109	-1,223,394.82
	B3LYP/6-31G//PM3	-1947.94	-1,222,353.78	-1949.551462	-1,223,363.04
Di glucosamine-di(ethylene glycol)--H_2O --> Glucosamine-di(ethylene glycol) cation---Glucosamine-di(ethylene glycol)					
	B3LYP/6-31G//AM1	-1948.92	-1,222,967.97	-1949.246936	-1,223,171.94
	B3LYP/6-31G//PM3	-1947.53	-1,222,096.02	-1949.209819	-1,223,148.65
Di glucosamine-di(ethylene glycol)--OH^- --> Di glucosamine-di(ethylene glycol) cation---H_2O					
	B3LYP/6-31G//AM1	-1946.61	-1,221,516.64	-1948.640107	-1,222,791.15
	B3LYP/6-31G//PM3	-1948.00	-1,222,388.88	-1948.640107	-1,222,791.15

Appendix C

The relative energy of reaction

Appendix Table C1 The relative energy of reaction in acid solution; Di glucosamine-mono(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)			Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method					
Reactant	Di glucosamine-mono(ethylene glycol)	H_3O^+			
	-982,229.58	-48,116.58		-1,030,346.16	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--H_3O^+				
	-1,030,169.59			-1030169.585	176.58
Product complex	Glucosamine-mono(ethylene glycol) cation---Glucosamine-mono(ethylene glycol)---H_2O				
	-1030395.625			-1,030,395.63	-49.46
Product	Glucosamine-mono(ethylene glycol) cation	Glucosamine-mono(ethylene glycol)	H_2O		
	-467,314.20	-515,081.07	-47,932.31	-1,030,327.58	18.58
Simulation by B3LYP/6-31G//PM3 method					
Reactant	Di glucosamine-mono(ethylene glycol)	H_3O^+			
	-982,198.76	-48,115.95		-1,030,314.72	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--H_3O^+				
	-1,030,169.21			-1030169.211	145.51
Product complex	Glucosamine-mono(ethylene glycol) cation---Glucosamine-mono(ethylene glycol)---H_2O				
	-1,030,407.32			-1,030,407.32	-92.61
Product	Glucosamine-mono(ethylene glycol) cation	Glucosamine-mono(ethylene glycol)	H_2O		
	-467,314.20	-515,075.50	-47,932.31	-1,030,322.01	-7.29

Appendix Table C2 The relative energy of reaction in acid solution; Di glucosamine-di(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)			Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method					
Reactant	Di glucosamine-di(ethylene glycol)	H_3O^+			
	-1,175,219.88	-48,116.58		-1,223,336.46	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--H_3O^+				
	-1,223,217.33			-1,223,217.33	119.13
Product complex	Glucosamine-di(ethylene glycol) cation---Glucosamine-di(ethylene glycol)---H_2O				
	-1,223,394.82			-1,223,394.82	-58.36
Product	Glucosamine-di(ethylene glycol) cation	Glucosamine-di(ethylene glycol)	H_2O		
	-563855.9263	-611579.7127	-47,932.31	-1,223,367.95	-31.48
Simulation by B3LYP/6-31G//PM3 method					
Reactant	Di glucosamine-di(ethylene glycol)	H_3O^+			
	-1,175,219.88	-48,115.95		-1,223,335.84	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--H_3O^+				
	-1,223,217.33			-1,223,217.33	118.50
Product complex	Glucosamine-di(ethylene glycol) cation---Glucosamine-di(ethylene glycol)---H_2O				
	-1,223,363.04			-1,223,363.04	-27.20
Product	Glucosamine-di(ethylene glycol) cation	Glucosamine-di(ethylene glycol)	H_2O		
	-611579.7127	-563843.5194	-47,932.31	-1,223,355.54	-19.70

Appendix Table C3 The relative energy of reaction in acid solution; Di glucosamine-tri(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)			Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method					
Reactant	Di glucosamine-tri(ethylene glycol)	H_3O^+			
	-1,368,221.12	-48,116.58		-1,416,335.96	0.00
Reactant complex	Di glucosamine-tri(ethylene glycol)--H_3O^+				
	-1,416,225.97			-1416225.968	111.73
Product complex	Glucosamine-tri(ethylene glycol) cation---Glucosamine-tri(ethylene glycol)---H_2O				
	-1,416,387.18			-1,416,387.18	-49.48
Product	Glucosamine-tri(ethylene glycol) cation	Glucosamine-tri(ethylene glycol)	H_2O		
	-708,071.16	-660,355.04	-47,932.31	-1,416,358.51	-20.81
Simulation by B3LYP/6-31G//PM3 method					
Reactant	Di glucosamine-tri(ethylene glycol)	H_3O^+			
	-1,368,200.64	-48,115.95		-1,416,316.59	0.00
Reactant complex	Di glucosamine-tri(ethylene glycol)--H_3O^+				
	-1,416,186.42			-1416186.417	135.02
Product complex step1	Glucosamine-tri(ethylene glycol) cation---Glucosamine-tri(ethylene glycol)---H_2O				
	-1,416,238.35			-1,416,238.35	83.09
Product complex step2	Di glucosamine-tri(ethylene glycol)---H^+ ---Water				
	-1,416,369.40			-1,416,369.40	-47.96
Product	Glucosamine-tri(ethylene glycol) cation	Glucosamine-tri(ethylene glycol)	H_2O		
	-708,064.55	-660,342.88	-47,932.31	-1,416,339.74	-18.30

Appendix Table C4 The relative energy of reaction in normal solution; Di glucosamine-mono(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)		Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method				
Reactant	Di glucosamine-mono(ethylene glycol)	H_2O		
	-982,229.58	-47,932.31	-1,030,161.89	0.00
Reactant complex	Di glucosamine (monoethyleneglycol)---H_2O			
	-1,030,085.94		-1,029,995.29	166.60
Product complex	Glucosamine-mono(ethylene glycol)---Glucosamine-mono(ethylene glycol)			
	-1,030,171.51		-1,030,171.51	-9.62
Product	Glucosamine-mono(ethylene glycol)	Glucosamine-mono(ethylene glycol)		
	-515,081.07	-515,081.07	-1,030,162.14	-0.25
Simulation by B3LYP/6-31G//PM3 method				
Reactant	Di glucosamine-mono(ethylene glycol)	H_2O		
	-982,198.76	-47,932.31	-1,030,131.07	0.00
Reactant complex	Di glucosamine (monoethyleneglycol)---H_2O			
	-1,029,995.29		-1,029,995.29	135.78
Product complex	Glucosamine-mono(ethylene glycol)---Glucosamine-mono(ethylene glycol)			
	-1,030,148.23		-1,030,148.23	-17.16
Product	Glucosamine-mono(ethylene glycol)	Glucosamine-mono(ethylene glycol)		
	-515,075.50	-515,075.50	-1,030,151.00	-19.93

Appendix Table C5 The relative energy of reaction in normal solution; Di glucosamine-di(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)		Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method				
Reactant	Di glucosamine-di(ethylene glycol)	H_2O		
	-1,175,219.88	-47,932.31	-1,223,152.19	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--H_2O			
	-1,222,967.97		-1,222,967.97	184.22
Product complex	Glucosamine-di(ethylene glycol)---Glucosamine-di(ethylene glycol)			
	-1,223,171.94		-1,223,171.94	-19.75
Product	Glucosamine-di(ethylene glycol)	Glucosamine-di(ethylene glycol)		
	-611,579.7127	-611,579.7127	-1,223,159.43	-7.24
Simulation by B3LYP/6-31G//PM3 method				
Reactant	Di glucosamine-di(ethylene glycol)	H_2O		
	-1,175,202.55	-47,932.31	-1,223,134.85	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--H_2O			
	-1,222,981.49		-1,222,981.49	153.37
Product complex	Glucosamine-di(ethylene glycol)---Glucosamine-di(ethylene glycol)			
	-1,223,148.65		-1,223,148.65	-13.80
Product	Glucosamine-di(ethylene glycol)	Glucosamine-di(ethylene glycol)		
	-611574.3952	-611574.3952	-1,223,148.79	-13.94

Appendix Table C6 The relative energy of reaction in base solution; Di glucosamine-mono(ethylene glycol) attracted at polymer bonding

Reaction step	Molecular energy (kcal/mol)		Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method				
Reactant	Di glucosamine-mono(ethylene glycol)	OH^-		
	-982,229.58	-47,504.69	-1,029,734.27	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--OH^-			
	-1,029,476.70		-1,029,476.70	257.57
Product complex	Glucosamine-mono(ethylene glycol) anion---Glucosamine-mono(ethylene glycol)			
	-1,029,811.716		-1029811.716	-77.45
Product	Glucosamine-mono(ethylene glycol) anion	Glucosamine-mono(ethylene glycol)		
	-514,706.50	-515,081.07	-1,029,787.56	-53.29
Simulation by B3LYP/6-31G//PM3 method				
Reactant	Di glucosamine-mono(ethylene glycol)	OH^-		
	-982,198.76	-47,504.52	-1,029,703.29	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--OH^-			
	-1,029,415.68		-1,029,415.68	287.60
Product complex	Glucosamine-mono(ethylene glycol) anion---Glucosamine-mono(ethylene glycol)			
	-1,029,811.716		-1029811.716	-108.43
Product	Glucosamine-mono(ethylene glycol) anion	Glucosamine-mono(ethylene glycol)		
	-514,717.1136	-515,075.50	-1,029,792.61	-89.33

Appendix Table C7 The relative energy of reaction in base solution; Di glucosamine-mono(ethylene glycol) attracted at ethylene glycol group

Reaction step	Molecular energy (kcal/mol)		Total energy (kcal/mol)	Relative energy (kcal/mol)
Simulation by B3LYP/6-31G//AM1method				
Reactant	Di glucosamine-mono(ethylene glycol)	OH^-		
	-982,229.58	-47,504.69	-1,029,734.27	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--OH^-			
	-1,029,782.11		-1,029,782.11	-47.84
Product complex	Glucosamine-mono(ethylene glycol) cation---H_2O			
	-1,029,812.60		-1,029,812.60	-78.33
Product	Glucosamine-mono(ethylene glycol) cation	H_2O		
	-981,840.58	-47,932.31	-1,029,772.89	-38.62
Simulation by B3LYP/6-31G//PM3 method				
Reactant	Di glucosamine-mono(ethylene glycol)	OH^-		
	-982,198.76	-47,504.52	-1,029,703.29	0.00
Reactant complex	Di glucosamine-mono(ethylene glycol)--OH^-			
	-1,029,782.11		-1,029,782.11	-78.83
Product complex	Glucosamine-mono(ethylene glycol) cation---H_2O			
	-1,029,785.93		-1,029,785.93	-82.64
Product	Glucosamine-mono(ethylene glycol) cation	H_2O		
	-981,832.9944	-47,932.31	-1029765.301	-62.01

Appendix Table C8 The relative energy of reaction in base solution; Di glucosamine-di(ethylene glycol)

Reaction step	Molecular energy (kcal/mol)		Total energy (kcal/mol)	Relative energy (kcal/mol)
OH^- Solution by method B3LYP/6-31G//AM1				
Reactant	Di glucosamine-di(ethylene glycol)	OH^-		
	-1,175,219.88	-47,504.69	-1,222,724.57	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--OH^-			
	-1,222,401.89		-1,222,401.89	322.68
Product complex	Di glucosamine-di(ethylene glycol) anion--- Di glucosamine-di(ethylene glycol)			
	-1,222,791.15		-1,222,791.15	-66.58
Product	Di glucosamine-di(ethylene glycol) anion	Di glucosamine-di(ethylene glycol)		
	-611,579.7127	-611,208.9465	-1,222,788.66	-64.09
OH^- Solution by method B3LYP/6-31G//PM3				
Reactant	Di glucosamine-di(ethylene glycol)	OH^-		
	-1,175,202.55	-47,504.52	-1,222,707.07	0.00
Reactant complex	Di glucosamine-di(ethylene glycol)--OH^-			
	-1,222,388.88		-1,222,388.88	318.19
Product complex	Di glucosamine-di(ethylene glycol) anion--- Di glucosamine-di(ethylene glycol)			
	-1,222,791.15		-1,222,791.15	-84.08
Product	Di glucosamine-di(ethylene glycol) anion	Di glucosamine-di(ethylene glycol)		
	-611,574.3952	-611,218.0875	-1,222,792.48	-85.41

Appendix D

Study method to use for simulation in micelle formation

Appendix Table D Molecular energy of water

Substances	Method	molecular energy (a.u.)	molecular energy (kcal/mol)	length of H-bonding(Å)
H2O	B3LYP/6-31G//AM1	-76.38	-47932.31	
	B3LYP/6-31G//PM3	-76.38	-47932.31	
	B3LYP/6-31G//HF/6-31G	-76.38	-47932.26	
	B3LYP/6-31G//B3LYP/6-31G	-76.39	-47933.05	
H2O---H2O	B3LYP/6-31G//AM1	-152.78	-95869.32	2.13
	B3LYP/6-31G//PM3	-152.78	-95873.36	1.81
	B3LYP/6-31G//HF/6-31G	-152.78	-95873.43	1.89
	B3LYP/6-31G//B3LYP/6-31G	-152.79	-95875.03	1.79

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Appendix Table D2 Relative energy of water interaction by H-bond

	$2H_2O$ ⟶	**H_2O---H-O-H**	**Relative energy (kcal/mol)**
B3LYP/6-31G//AM1	-47932.31	-95869.32	-4.70
B3LYP/6-31G//PM3	-47932.31	-95873.36	-8.74
B3LYP/6-31G//HF/6-31G	-47932.26	-95873.43	-8.92
B3LYP/6-31G//B3LYP/6-31G	-47933.05	-95875.03	-8.93

From this simulation, micelle simulation should use B3LYP/6-31G//PM3 method to study.

Appendix E

Relative energy of micelle formation

Appendix Table E Relative energy of micelle formation by B3LYP/6-31G//PM3 method simulation

Molecular energy of reactant		→	Molecular energy of micelle formation	Relative energy
Doxorubicin	**1 Glucosamine-mono(ethylene glycol)**		**Doxorubicin(Glucosamine-mono(ethylene glycol))**	**Kcal/mol**
-1,209,761.75	-515,075.50		-1724844.234	-6.99
Doxorubicin	**2 Glucosamine-mono(ethylene glycol)**		**Doxorubicin(Glucosamine-mono(ethylene glycol))$_2$**	
-1,209,761.75	-515,075.50		-2239925.401	-12.65
Doxorubicin	**3 Glucosamine-mono(ethylene glycol)**		**Doxorubicin(Glucosamine-mono(ethylene glycol))$_3$**	
-1,209,761.75	-515,075.50		-2,755,003.57	-15.32
Doxorubicin	**1 Glucosamine-di(ethylene glycol)**		**Doxorubicin(Glucosamine-di(ethylene glycol))**	
-1,209,761.75	-611,574.40		-1,821,343.24	-7.10
Doxorubicin	**2 Glucosamine-di(ethylene glycol)**		**Doxorubicin(Glucosamine-di(ethylene glycol))$_2$**	
-1,209,761.75	-611,574.40		-2432923.061	-12.52
Doxorubicin	**3 Glucosamine-di(ethylene glycol)**		**Doxorubicin(Glucosamine-di(ethylene glycol))$_3$**	
-1,209,761.75	-611,574.40		-3,044,499.51	-14.58
Doxorubicin	**1 Glucosamine-tri(ethylene glycol)**		**Doxorubicin(Glucosamine-tri(ethylene glycol))**	
-1,209,761.75	-708,073.33		-1,917,842.05	-6.97
Doxorubicin	**2 Glucosamine-tri(ethylene glycol)**		**Doxorubicin(Glucosamine-tri(ethylene glycol))$_2$**	
-1,209,761.75	-708,073.33		-2,625,921.11	-12.70
Doxorubicin	**3 Glucosamine-tri(ethylene glycol)**		**Doxorubicin(Glucosamine-tri(ethylene glycol))$_3$**	
-1,209,761.75	-708,073.33		-3,333,997.29	-15.56
Doxorubicin	**1 Glucosamine-penta(ethylene glycol)**		**Doxorubicin(Glucosamine-penta(ethylene glycol))**	
-1,209,761.75	-901,071.33		-2,110,839.45	-6.37
Doxorubicin	**2 Glucosamine-penta(ethylene glycol)**		**Doxorubicin(Glucosamine-penta(ethylene glycol))$_2$**	
-1,209,761.75	-901,071.33		-3,011,917.85	-13.44
Doxorubicin	**3 Glucosamine-penta(ethylene glycol)**		**Doxorubicin(Glucosamine-penta(ethylene glycol))$_3$**	
-1,209,761.75	-901,071.33		-3,912,992.39	-16.65