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Theoritical study of diffusion flow of anticancer medicines through single-wall armchair (10, 10) carbon nanotube

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Table 1. *The energies of the flow process of Carmustine (1) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Carmustine from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube(10,10)		
			Dipole moment vector (°)		
			0°	90°	180°
Carmustine	0	34.99	14744.22	14746.05	14747.66
	1	32.02	14735.43	14745.96	14746.14
	2	29.7	14930.93	14742.83	14730.60
	3	27.46	15895.54	14732.58	14774.95
	4	25.11	16472.25	14721.05	16018.34
	5	22.69	16659.20	14711.44	16762.13
	6	20.25	16623.73	14701.76	17304.00
	7	17.85	16558.84	14696.71	16838.81
	8	15.62	16605.80	14697.09	16845.22
	9	13.30	16593.43	14695.01	17213.01
	10	11.08	16680.46	14696.64	17134.33
	11	9.02	16780.11	14697.26	17062.35
	12	7.20	16819.83	14697.37	17229.79
	13	0.00	15698.96	14701.09	16866.32
	14	7.35	14721.08	14727.04	16001.06
	15	8.46	14741.05	14731.86	14917.66
	16	10.02	14747.33	14739.48	14734.94
	17	11.74	14747.75	14745.09	14734.29
	18	13.44	14747.24	14747.02	14744.62

Table 2*. The energies of the flow process of Lomustine (2) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Lomustine from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube (10,10)		
			Dipole moment vector (°)		
			0°	90°	180°
Lomustine	0	34.99	14699.88	14700.25	14700.64
	1	32.02	14700.57	14699.80	14698.06
	2	29.7	14698.11	14690.15	14686.78
	3	27.46	14689.27	14779.87	14668.25
	4	25.11	14679.42	15519.59	14653.51
	5	22.69	14661.58	15884.12	14644.23
	6	20.25	14638.62	16376.87	14634.21
	7	17.85	14627.54	15946.82	14632.14
	8	15.62	14624.08	15837.97	14631.34
	9	13.30	14623.96	16162.89	14631.69
	10	11.08	14624.84	15926.45	14629.28
	11	9.02	14624.97	15503.24	14630.83
	12	7.20	14625.58	15514.49	14631.95
	13	0.00	14627.29	15947.85	14635.75
	14	7.35	14634.76	14851.89	14649.56
	15	8.46	14645.85	14697.66	14673.19
	16	10.02	14661.45	14681.52	14683.40
	17	11.74	14681.22	14693.16	14694.47
	18	13.44	14694.76	14698.49	14699.45

Table 3. *The energies of the flow process of Ifosfamide (3) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Ifosfamide from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube(10,10)		
			Dipole moment vector (°)		
			0°	90°	180°
Ifosffamide	0	34.99	14354.93	14358.93	14360.46
	1	32.02	14347.22	14359.82	14350.61
	2	29.7	14907.56	14358.02	14320.14
	3	27.46	16044.45	14348.40	15029.63
	4	25.11	17153.07	14331.63	16988.65
	5	22.69	17509.84	14316.31	17718.53
	6	20.25	17489.66	14298.13	17978.79
	7	17.85	17473.86	14290.83	17699.93
	8	15.62	17617.66	14289.36	17599.57
	9	13.30	17723.73	14287.86	17521.58
	10	11.08	17856.27	14288.02	17648.93
	11	9.02	17756.97	14286.48	17679.35
	12	7.20	16527.24	14286.26	17816.58
	13	0.00	16024.84	14287.67	17490.08
	14	7.35	14978.78	14314.71	14620.09
	15	8.46	14316.49	14324.70	14350.09
	16	10.02	14350.16	14338.56	14353.76
	17	11.74	14359.24	14351.26	14355.70
	18	13.44	14360.68	14356.41	14356.05

Table 4. *The energies of the flow process of Azathioprine (4) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Azathioprine from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube (10,10)		
			Dipole moment vector (°)		
			0°	90°	180°
Azathioprine	0	34.99	15285.45	15289.23	15292.67
	1	32.02	15290.32	15289.65	15289.15
	2	29.7	15295.69	15283.60	15261.11
	3	27.46	15287.74	15263.04	15214.62
	4	25.11	15250.98	15255.92	15195.99
	5	22.69	15220.34	15293.42	15195.00
	6	20.25	15214.48	15340.14	15199.83
	7	17.85	15210.24	15347.78	15201.44
	8	15.62	15216.46	15332.31	15203.37
	9	13.30	15215.59	15336.71	15201.21
	10	11.08	15212.23	15343.51	15201.25
	11	9.02	15219.34	15330.90	15203.09
	12	7.20	15209.51	15305.28	15200.49
	13	0.00	15206.44	15304.16	15199.47
	14	7.35	15206.86	15276.47	15289.64
	15	8.46	15223.99	15277.06	15296.39
	16	10.02	15266.87	15284.39	15293.43
	17	11.74	15288.47	15287.51	15288.27
	18	13.44	15292.39	15287.65	15285.42

Table 5. *The energies of the flow process of Gemcitabine (5) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Gemcitabine from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube (10,10)		
			Dipole moment vector (°)		
			0°	90°	180°
Gemcitabine	0	34.99	14922.19	14924.59	14927.37
	1	32.02	14925.61	14922.71	14924.79
	2	29.7	14926.71	14917.69	14907.98
	3	27.46	15091.04	14908.19	15090.09
	4	25.11	15779.33	14896.46	15914.28
	5	22.69	16379.25	14886.77	16408.57
	6	20.25	16369.31	14878.59	16537.26
	7	17.85	16290.92	14870.85	16647.58
	8	15.62	16310.06	14866.94	16481.33
	9	13.30	16259.44	14865.33	16531.39
	10	11.08	16170.46	14864.98	16537.13
	11	9.02	16282.93	14864.54	16421.91
	12	7.20	16121.41	14865.07	16660.15
	13	0.00	16091.35	14872.60	16543.65
	14	7.35	14933.69	14897.13	14923.57
	15	8.46	14897.69	14905.56	14923.84
	16	10.02	14921.22	14910.79	14922.63
	17	11.74	14926.76	14915.43	14921.74
	18	13.44	14927.30	14919.53	14921.61

Table 6*. The energies of the flow process of Procarbazine (6) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Procarbazine from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube(10,10)
Procarbazine	0	34.99	15113.17
	1	32.02	15111.80
	2	29.7	15104.53
	3	27.46	15089.13
	4	25.11	15073.16
	5	22.69	15061.38
	6	20.25	15052.18
	7	17.85	15034.64
	8	15.62	15024.87
	9	13.30	15022.09
	10	11.08	15021.98
	11	9.02	15022.12
	12	7.20	15022.71
	13	0.00	15031.53
	14	7.35	15063.43
	15	8.46	15075.40
	16	10.02	15082.65
	17	11.74	15090.11
	18	13.44	15100.38

Table 7. *The energies of the flow process of Methotrexate (7) flow through armchair (10, 10) nanotubes. The flow process was identified by the distances of Methotrexate from the ends of the nanotubes and the direction of the dipole moment vector (in °) related to the flow pathway. Each distance changes were identified by one stage (stages 0-18).*

AC	Stages	Distance (Å)	Energy (kJ mol^{-1}) Armchair Carbon Nanotube(10,10)
Methotrexate	0	34.99	25330.63
	1	32.02	25328.40
	2	29.7	25318.30
	3	27.46	25292.40
	4	25.11	25259.86
	5	22.69	25236.67
	6	20.25	25221.85
	7	17.85	25196.57
	8	15.62	25182.93
	9	13.30	25174.82
	10	11.08	25171.86
	11	9.02	25171.26
	12	7.20	25169.73
	13	0.00	25173.16
	14	7.35	25258,41
	15	8.46	25264.08
	16	10.02	25287.02
	17	11.74	25293.16
	18	13.44	25317.38