Supplementary Information

The study of force fields molecular mechanics and molecular quantum on the interaction with drugs of the alkylating agent with SWCNT-BNNT in different solvents and at different temperatures

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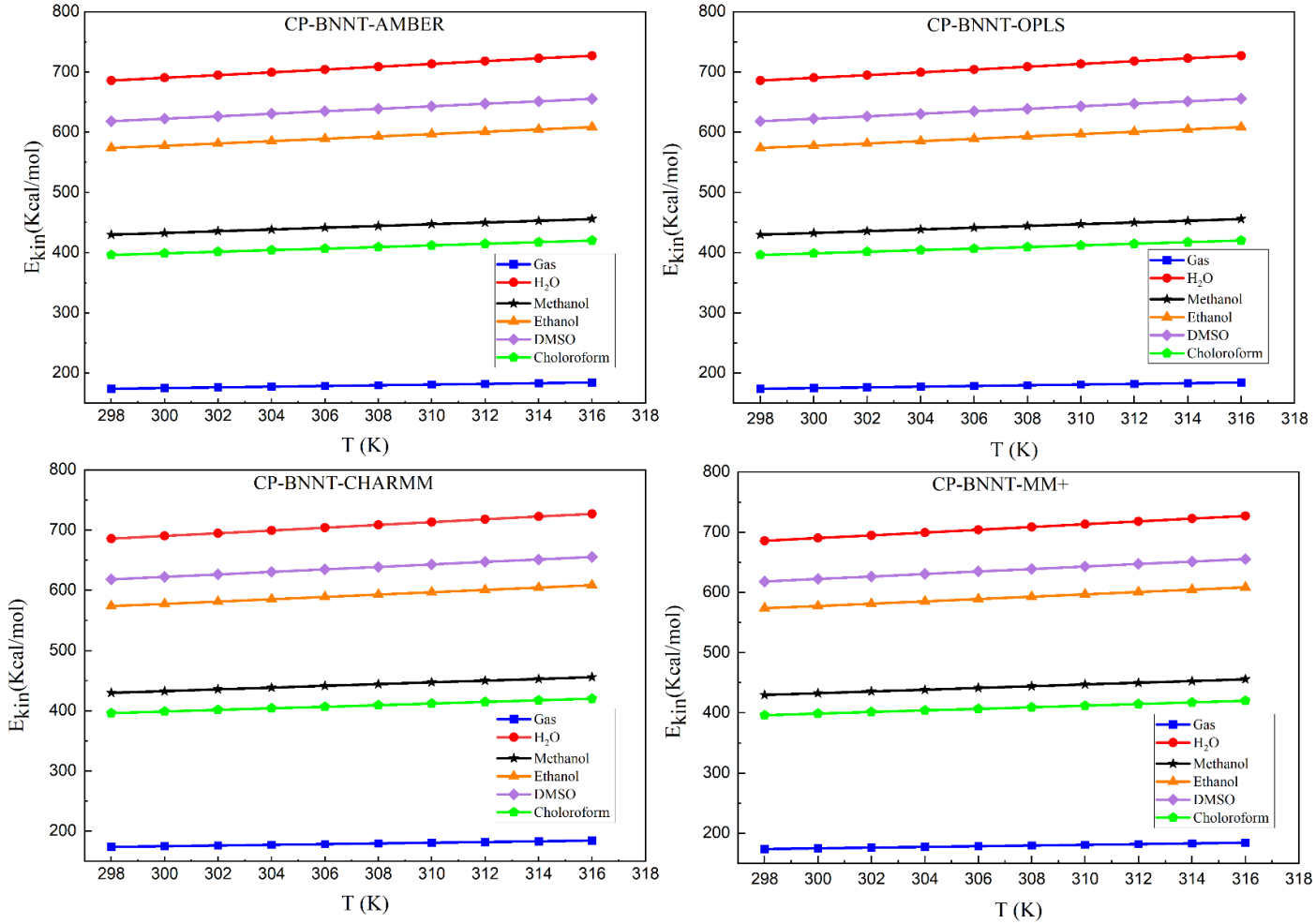

Figure S1. Kinetic energies (E_{Kin}) (kcal/mol) calculated versus temperature at different dielectric constants through Monte Carlo simulation in the AMBER, OPLS, CHARMM and MM^{+} force field for CP- BNNT.

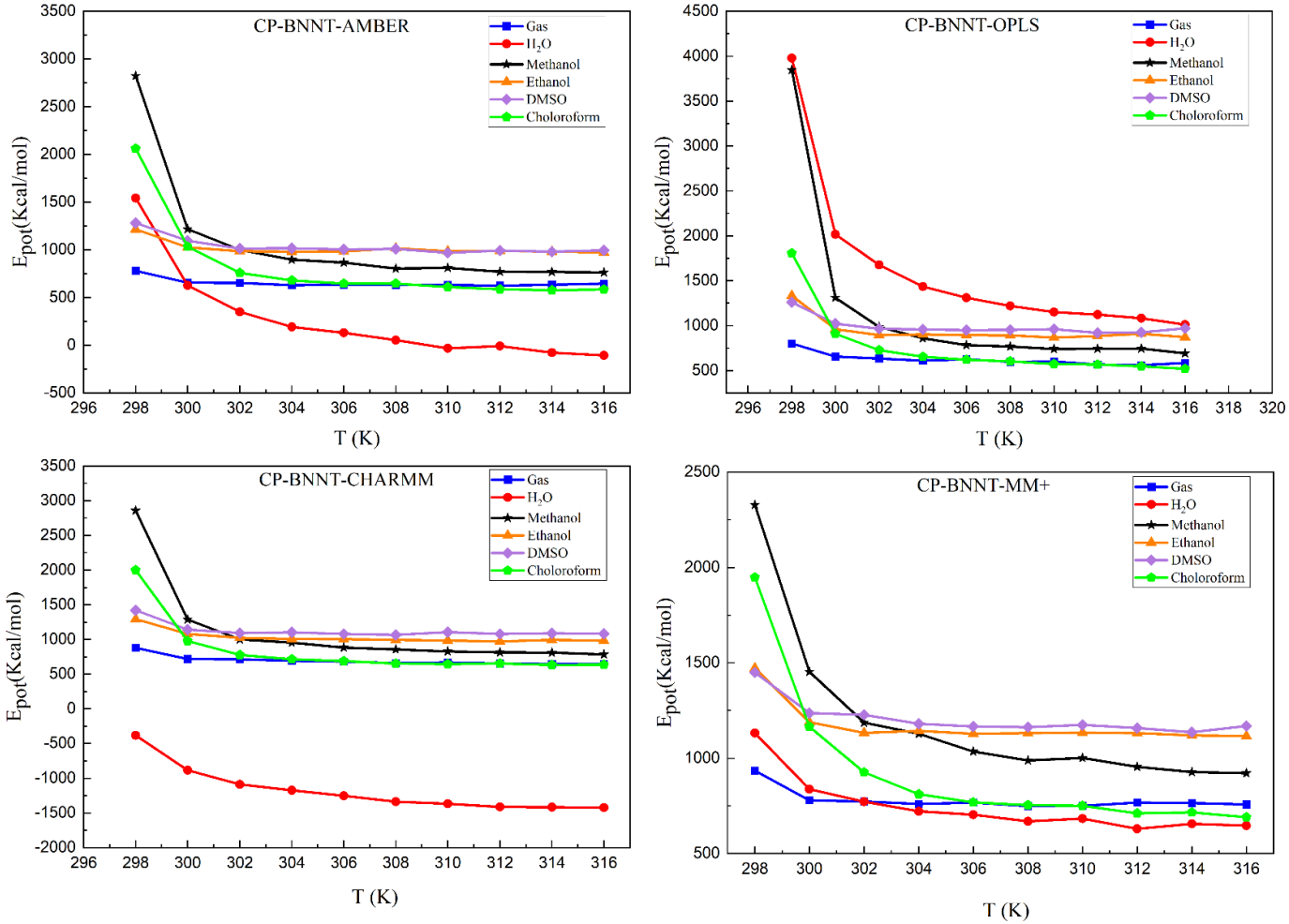

Figure S2. Potential energies (E_{pot}) (kcal/mol) calculated versus temperature at different dielectric constants through Monte Carlo simulation in the AMBER, OPLS, CHARMM and MM+ force field for CP- BNNT.

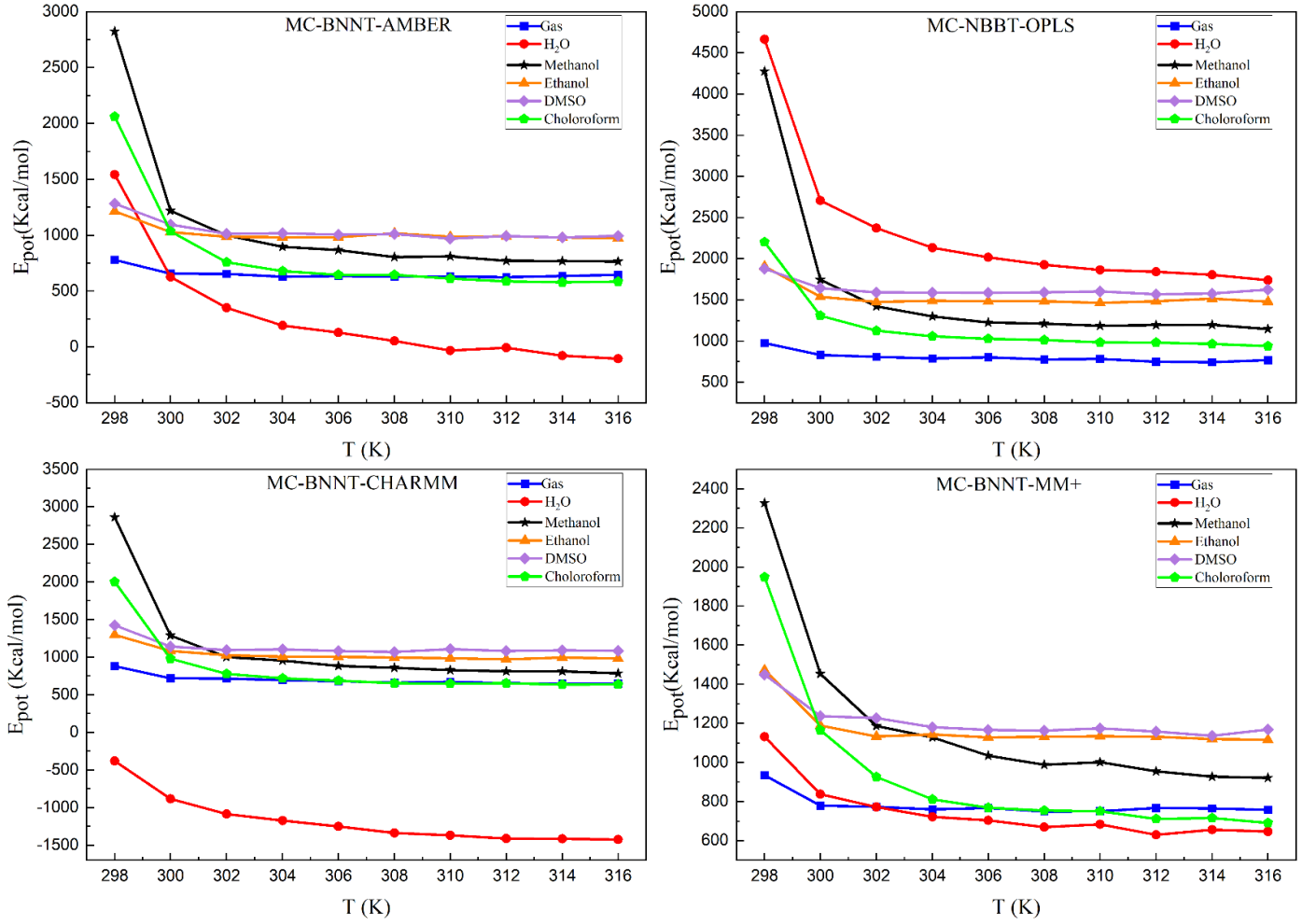

Figure S3. Kinetic energies (E_{kin}) (Kcal/mol) calculated versus temperature at different dielectric constants through Monte Carlo simulation in the AMBER, OPLS, CHARMM and MM^{+} force field for MC-BNNT.

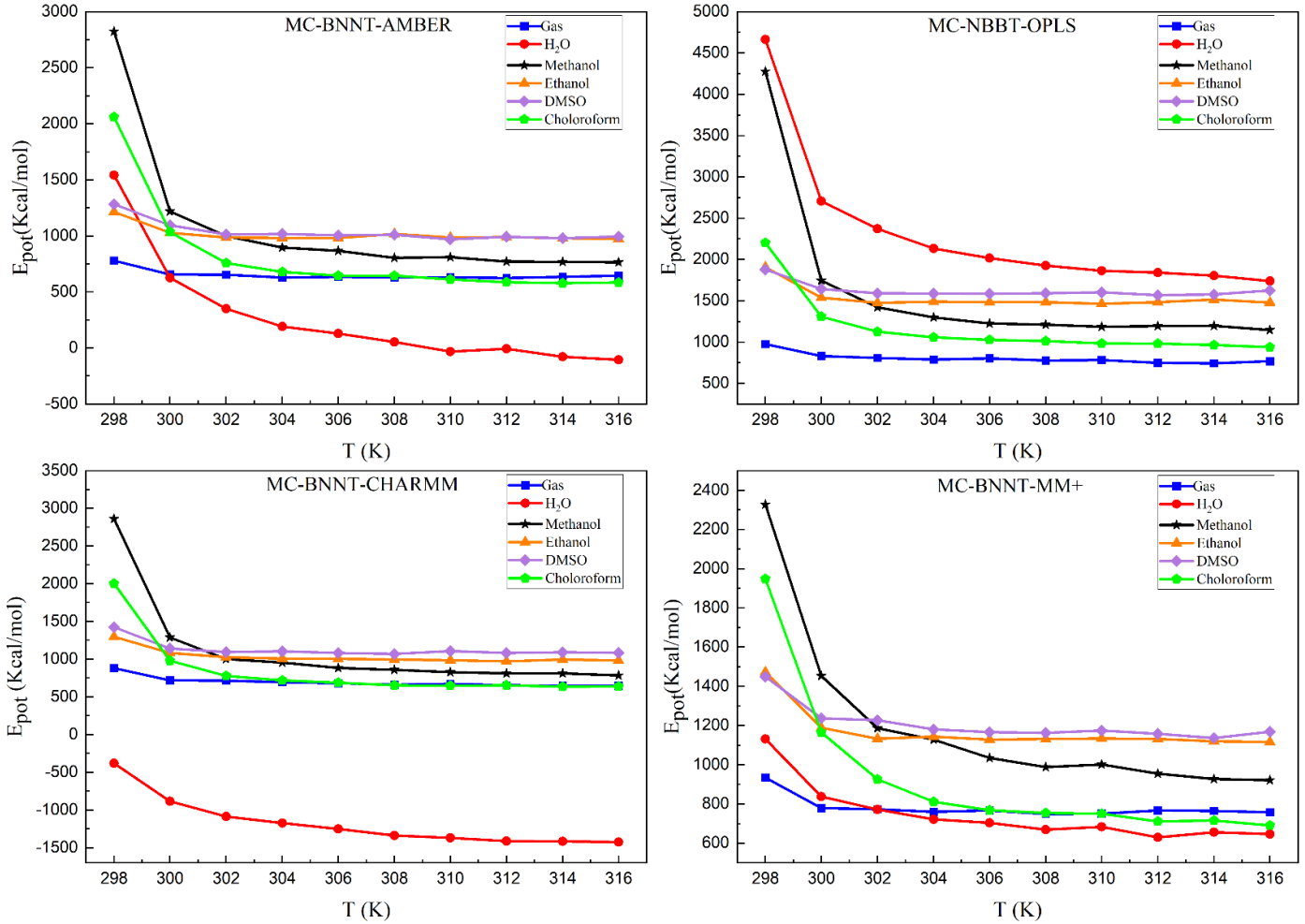

Figure S4. Potential energies (E_{pot}) (Kcal/mol) calculated versus temperature at different dielectric constants through Monte Carlo simulation in the AMBER, OPLS, CHARMM and MM^{+} force field for MC-BNNT.

Table S1. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- BNNT through Monte Carlo Simulation in different solvents in the AMBER force field.

CP- BNNT - AMBER											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	174.1018	175.2703	176.4388	177.6072	178.7757	179.9442	181.1126	182.2811	183.4496	184.6181
	E_{pot}	780.4289	656.7158	654.3474	629.1282	634.9758	631.6799	631.5763	624.9368	634.3217	645.7903
	E_{tot}	954.5307	831.9861	830.7862	806.7354	813.7515c	811.6241	812.6889	807.2179	817.7713	830.4084
Water	E_{kin}	685.7481	690.3504	694.9527	699.5551	704.1574	708.7597	713.3621	717.9644	722.5667	727.1691
	E_{pot}	1542.074	627.4249	350.6378	192.7839	130.2594	53.93935	-31.75732	-7.084021	-76.92163	-105.7628
	E_{tot}	2227.822	1317.775	1045.591	892.339	834.4168	762.6991	681.6048	710.8804	645.6451	621.4063
Methanol	E_{kin}	429.9249	432.8103	435.6958	438.5812	441.4666	444.352	447.2374	450.1228	453.0082	455.8936
	E_{pot}	2823.612	1219.122	999.8655	897.3593	867.6917	804.1025	811.6258	770.7018	768.7778	763.9504
	E_{tot}	3253.537	1651.932	1435.561	1335.94	1309.158	1248.454	1258.863	1220.825	1221.786	1219.844
Ethanol	E_{kin}	573.8254	577.6766	581.5278	585.379	589.2302	593.0813	596.9325	600.7837	604.6349	608.486
	E_{pot}	1215.368	1028.071	986.4902	982.0223	983.3978	1017.459	986.9392	991.4577	981.0263	974.0756
	E_{tot}	1789.193	1605.748	1568.018	1567.401	1572.628	1610.54	1583.872	1592.241	1585.661	1582.562
DMSO	E_{kin}	618.2392	622.3884	626.5377	630.6869	634.8362	638.9855	643.1347	647.284	651.4332	655.5825
	E_{pot}	1282.991	1095.393	1014.267	1018.136	1005.123	1010.801	969.8135	992.6684	981.2798	995.7768
	E_{tot}	1901.23	1717.782	1640.804	1648.823	1639.959	1649.786	1612.948	1639.952	1632.713	1651.359
Chloroform	E_{kin}	396.1705	398.8294	401.4882	404.1471	406.806	409.4648	412.1237	414.7825	417.4414	420.1003
	E_{pot}	2060.59	1034.154	758.9589	679.4744	645.8084	646.4915	612.2791	588.2267	578.6951	585.5439
	E_{tot}	2456.76	1432.983	1160.447	1083.621	1052.614	1055.956	1024.403	1003.009	996.1365	1005.644

Table S2. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- BNNT through Monte Carlo Simulation in different solvents in the OPLS force field.

CP- BNNT- OPLS											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	174.1018	175.2703	176.4388	177.6072	178.7757	179.9442	181.1126	182.2811	183.4496	184.6181
	E_{pot}	801.2443	655.0223	633.4982	610.6473	625.7887	598.6333	601.4306	568.2771	560.436	584.0494
	E_{tot}	975.3461	830.2926	809.937	788.2545	804.5644	778.5775	782.5432	750.5582	743.8856	768.6674
Water	E_{kin}	685.7481	690.3504	694.9527	699.5551	704.1574	708.7597	713.3621	717.9644	722.5667	727.1691
	E_{pot}	3980.595	2016.792	1676.828	1435.086	1312.28	1219.153	1150.51	1124.463	1081.522	1011.997
	E_{tot}	4666.343	2707.143	2371.78	2134.641	2016.438	1927.913	1863.872	1842.428	1804.089	1739.166
Methanol	E_{kin}	429.9249	432.8103	435.6958	438.5812	441.4666	444.352	447.2374	450.1228	453.0082	455.8936
	E_{pot}	3846.81	1312.221	985.2574	859.937	784.021	766.8108	738.8702	743.6135	745.5486	691.4171
	E_{tot}	4276.735	1745.031	1420.953	1298.518	1225.488	1211.163	1186.108	1193.736	1198.557	1147.311
Ethanol	E_{kin}	573.8254	577.6766	581.5278	585.379	589.2302	593.0813	596.9325	600.7837	604.6349	608.486
	E_{pot}	1334.249	960.0039	894.9921	903.3132	895.661	891.0787	866.455	884.7291	910.8879	871.5624
	E_{tot}	1908.074	1537.681	1476.52	1488.692	1484.891	1484.16	1463.388	1485.513	1515.523	1480.048
DMSO	E_{kin}	618.2392	622.3884	626.5377	630.6869	634.8362	638.9855	643.1347	647.284	651.4332	655.5825
	E_{pot}	1260.346	1021.718	965.6231	959.4017	950.9126	954.3765	960.8885	921.3327	926.5292	970.1498
	E_{tot}	1878.585	1644.107	1592.161	1590.089	1585.749	1593.362	1604.023	1568.617	1577.962	1625.732
Chloroform	E_{kin}	396.1705	398.8294	401.4882	404.1471	406.806	409.4648	412.1237	414.7825	417.4414	420.1003
	E_{pot}	1806.203	910.2487	726.3885	654.2333	620.7026	602.7251	572.1709	566.617	547.0449	520.2759
	E_{tot}	2202.374	1309.078	1127.877	1058.38	1027.509	1012.19	984.2945	981.3995	964.4863	940.3761

Table S3. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- BNNT through Monte Carlo Simulation in different solvents in the CHARMM force field.

CP- BNNT- CHARMM											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	174.1018	175.2703	176.4388	177.6072	178.7757	179.9442	181.1126	182.2811	183.4496	184.6181
	E_{pot}	881.5012	721.0639	715.848	694.6572	682.991	661.613	672.6855	655.1084	647.091	648.6454
	E_{tot}	1055.603	896.3342	892.2868	872.2645	861.7667	841.5572	853.7981	837.3895	830.5406	833.2634
Water	E_{kin}	685.7481	690.3504	694.9527	699.5551	704.1574	708.7597	713.3621	717.9644	722.5667	727.1691
	E_{pot}	-380.8562	-882.76	-1085.395	-1171.327	-1250.139	-1337.836	-1367.442	-1410.707	-1415.052	-1422.935
	E_{tot}	304.8918	-192.4096	-390.4421	-471.7715	-545.9812	-629.0766	-654.0796	-692.7424	-692.4854	-695.7659
Methanol	E_{kin}	429.9249	432.8103	435.6958	438.5812	441.4666	444.352	447.2374	450.1228	453.0082	455.8936
	E_{pot}	2858.699	1287.704	1003.932	956.754	884.085	858.1788	828.9782	814.3154	811.6709	786.4296
	E_{tot}	3288.624	1720.515	1439.628	1395.335	1325.552	1302.531	1276.216	1264.438	1264.679	1242.323
Ethanol	E_{kin}	573.8254	577.6766	581.5278	585.379	589.2302	593.0813	596.9325	600.7837	604.6349	608.486
	E_{pot}	1296.527	1083.129	1026.767	1008.74	1005.832	996.0251	987.0698	972.5854	995.7	983.6429
	E_{tot}	1870.353	1660.806	1608.295	1594.119	1595.062	1589.106	1584.002	1573.369	1600.335	1592.129
DMSO	E_{kin}	618.2392	622.3884	626.5377	630.6869	634.8362	638.9855	643.1347	647.284	651.4332	655.5825
	E_{pot}	1423.592	1142.718	1095.583	1104.819	1082.444	1069.531	1107.357	1082.969	1091.301	1086.061
	E_{tot}	2041.831	1765.106	1722.121	1735.506	1717.281	1708.517	1750.491	1730.253	1742.734	1741.643
Chloroform	E_{kin}	396.1705	398.8294	401.4882	404.1471	406.806	409.4648	412.1237	414.7825	417.4414	420.1003
	E_{pot}	2002.106	980.4152	779.3257	718.5622	689.677	654.4424	648.8769	653.7351	634.93	638.3029
	E_{tot}	2398.277	1379.245	1180.814	1122.709	1096.483	1063.907	1061.001	1068.518	1052.371	1058.403

Table S4. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- BNNT through Monte Carlo Simulation in different solvents in the MM+ force field.

CP- BNNT - MM+											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	174.1018	175.2703	176.4388	177.6072	178.7757	179.9442	181.1126	182.2811	183.4496	184.6181
	E_{pot}	934.8133	780.0572	773.4157	760.2885	767.4363	750.0041	750.8583	767.0763	765.6463	757.4773
	E_{tot}	1108.915	955.3276	949.8545	937.8958	946.212	929.9483	931.971	949.3574	949.0959	942.0954
Water	E_{kin}	685.7481	690.3504	694.9527	699.5551	704.1574	708.7597	713.3621	717.9644	722.5667	727.1691
	E_{pot}	1131.707	838.4981	772.2717	722.5751	704.5421	670.2468	683.6235	629.6526	656.5519	647.0533
	E_{tot}	1817.455	1528.848	1467.224	1422.13	1408.7	1379.007	1396.986	1347.617	1379.119	1374.222
Methanol	E_{kin}	429.9249	432.8103	435.6958	438.5812	441.4666	444.352	447.2374	450.1228	453.0082	455.8936
	E_{pot}	2327.936	1453.737	1186.758	1128.346	1035.393	988.4023	1001.284	955.4717	927.4787	922.3295
	E_{tot}	2757.861	1886.548	1622.453	1566.927	1476.86	1432.754	1448.521	1405.594	1380.487	1378.223
Ethanol	E_{kin}	573.8254	577.6766	581.5278	585.379	589.2302	593.0813	596.9325	600.7837	604.6349	608.486
	E_{pot}	1472.504	1189.148	1132.855	1143.715	1128.228	1132.16	1134.325	1132.274	1120.493	1116.651
	E_{tot}	2046.329	1766.824	1714.383	1729.094	1717.458	1725.242	1731.258	1733.058	1725.128	1725.137
DMSO	E_{kin}	618.2392	622.3884	626.5377	630.6869	634.8362	638.9855	643.1347	647.284	651.4332	655.5825
	E_{pot}	1449.292	1237.169	1227.148	1180.662	1166.455	1163.659	1174.789	1158.531	1137.168	1168.871
	E_{tot}	2067.531	1859.557	1853.686	1811.349	1801.292	1802.644	1817.923	1805.815	1788.601	1824.454
Chloroform	E_{kin}	396.1705	398.8294	401.4882	404.1471	406.806	409.4648	412.1237	414.7825	417.4414	420.1003
	E_{pot}	1947.998	1165.471	926.0517	812.0209	769.0256	753.9332	750.4723	711.9727	715.7445	691.3131
	E_{tot}	2344.168	1564.301	1327.54	1216.168	1175.832	1163.398	1162.596	1126.755	1133.186	1111.413

Table S5. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (Kcal/mol) calculated for MC- BNNT through Monte Carlo Simulation in different solvents in the AMBER force field.

MC- BNN - AMBER											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	178.5432	179.7415	180.9398	182.138	183.3363	184.5346	185.7329	186.9311	188.1294	189.3277
	E_{pot}	735.2401	678.9404	648.2992	627.5908	621.9662	624.4696	629.9878	616.595	633.7851	612.0243
	E_{tot}	913.7833	858.6819	829.239	809.7289	805.3025	809.0042	815.7207	803.5261	821.9146	801.352
Water	E_{kin}	687.5246	692.1389	696.7531	701.3674	705.9816	710.5959	715.2102	719.8244	724.4387	729.0529
	E_{pot}	1466.331	653.0162	369.8994	180.4423	111.7671	42.99988	-44.73044	-80.36586	-114.3651	-124.7911
	E_{tot}	2153.856	1345.155	1066.653	881.8097	817.7487	753.5958	670.4797	639.4586	610.0736	604.2618
Methanol	E_{kin}	439.696	442.6469	445.5979	448.5489	451.4999	454.4509	457.4018	460.3528	463.3038	466.2548
	E_{pot}	2594.296	1194.565	1012.905	903.6215	844.879	808.8698	790.9671	770.9939	791.6163	755.5514
	E_{tot}	3033.992	1637.212	1458.503	1352.17	1296.379	1263.321	1248.369	1231.347	1254.92	1221.806
Ethanol	E_{kin}	578.2668	582.1478	586.0288	589.9098	593.7908	597.6717	601.5527	605.4337	609.3147	613.1957
	E_{pot}	1086.999	1015.323	997.0792	962.0238	951.2279	941.1858	952.2196	943.8936	971.934	975.9758
	E_{tot}	1665.266	1597.471	1583.108	1551.934	1545.019	1538.858	1553.772	1549.327	1581.249	1589.172
DMSO	E_{kin}	631.5633	635.802	640.0407	644.2793	648.518	652.7567	656.9954	661.2341	665.4727	669.7114
	E_{pot}	1291.606	1135.724	1077.44	1056.412	1072.718	1027.072	997.9215	983.059	994.4728	980.9639
	E_{tot}	1923.17	1771.526	1717.481	1700.692	1721.236	1679.829	1654.917	1644.293	1659.946	1650.675
Chloroform	E_{kin}	400.6119	403.3006	405.9892	408.6779	411.3666	414.0552	416.7439	419.4326	422.1212	424.8099
	E_{pot}	1716.983	976.9383	758.0947	680.3906	637.3741	616.6887	582.4572	597.8527	583.9084	586.0028
	E_{tot}	2117.595	1380.239	1164.084	1089.068	1048.741	1030.744	999.2011	1017.285	1006.03	1010.813

Table S6. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (Kcal/mol) calculated for MC- BNNT through Monte Carlo Simulation in different solvents in the OPLS force field.

MC- BNNT - OPLS											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	178.5432	179.7415	180.9398	182.138	183.3363	184.5346	185.7329	186.9311	188.1294	189.3277
	E_{pot}	686.091	627.4769	601.4566	591.9451	577.6154	574.5441	557.3809	565.6874	569.0432	581.1652
	E_{tot}	864.6342	807.2184	782.3964	774.0831	760.9517	759.0787	743.1138	752.6186	757.1726	770.4929
Water	E_{kin}	687.5246	692.1389	696.7531	701.3674	705.9816	710.5959	715.2102	719.8244	724.4387	729.0529
	E_{pot}	3500.131	1964.593	1627.002	1339.839	1183.617	1131.047	1041.262	988.0189	922.085	907.3972
	E_{tot}	4187.656	2656.732	2323.755	2041.206	1889.598	1841.643	1756.472	1707.843	1646.524	1636.45
Methanol	E_{kin}	439.696	442.6469	445.5979	448.5489	451.4999	454.4509	457.4018	460.3528	463.3038	466.2548
	E_{pot}	2656.534	1183.884	961.3807	855.0993	771.8229	742.4123	706.8102	694.2534	690.7072	661.935
	E_{tot}	3096.23	1626.531	1406.979	1303.648	1223.323	1196.863	1164.212	1154.606	1154.011	1128.19
Ethanol	E_{kin}	578.2668	582.1478	586.0288	589.9098	593.7908	597.6717	601.5527	605.4337	609.3147	613.1957
	E_{pot}	965.5823	913.4932	889.5104	892.0736	853.2403	892.2204	851.8678	825.0999	865.8156	892.2722
	E_{tot}	1543.849	1495.641	1475.539	1481.983	1447.031	1489.892	1453.421	1430.534	1475.13	1505.468
DMSO	E_{kin}	631.5633	635.802	640.0407	644.2793	648.518	652.7567	656.9954	661.2341	665.4727	669.7114
	E_{pot}	1193.065	1058.587	1000.698	928.4133	955.2872	947.4693	923.875	948.9928	924.927	915.8402
	E_{tot}	1824.629	1694.389	1640.739	1572.693	1603.805	1600.226	1580.87	1610.227	1590.4	1585.552
Chloroform	E_{kin}	400.6119	403.3006	405.9892	408.6779	411.3666	414.0552	416.7439	419.4326	422.1212	424.8099
	E_{pot}	1547.941	897.2164	697.6932	653.9817	621.2777	572.5888	551.9577	548.5288	526.0667	508.6087
	E_{tot}	1948.553	1300.517	1103.682	1062.66	1032.644	986.644	968.7016	967.9614	948.1879	933.4186

Table S7. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (Kcal/mol) calculated for MC- BNNT through Monte Carlo Simulation in different solvents in the CHARMM force field.

MC- BNNT - CHARMM											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	178.5432	179.7415	180.9398	182.138	183.3363	184.5346	185.7329	186.9311	188.1294	189.3277
	E_{pot}	798.6752	704.3308	680.2462	652.2868	656.3089	649.2045	650.7041	630.7281	634.2377	667.7132
	E_{tot}	977.2184	884.0723	861.1859	834.4249	839.6452	833.7391	836.437	817.6592	822.3672	857.0409
Water	E_{kin}	687.5246	692.1389	696.7531	701.3674	705.9816	710.5959	715.2102	719.8244	724.4387	729.0529
	E_{pot}	-454.3117	-925.1488	-1081.888	-1181.302	-1232.182	-1236.108	-1248.921	-1312.153	-1372.102	-1309.673
	E_{tot}	233.2129	-233.0099	-385.1352	-479.935	-526.2003	-525.512	-533.7109	-592.3281	-647.6636	-580.6201
Methanol	E_{kin}	439.696	442.6469	445.5979	448.5489	451.4999	454.4509	457.4018	460.3528	463.3038	466.2548
	E_{pot}	2827.016	1304.056	1061.386	958.3339	892.8791	848.5104	807.2604	791.3392	793.7274	792.3214
	E_{tot}	3266.712	1746.703	1506.984	1406.883	1344.379	1302.961	1264.662	1251.692	1257.031	1258.576
Ethanol	E_{kin}	578.2668	582.1478	586.0288	589.9098	593.7908	597.6717	601.5527	605.4337	609.3147	613.1957
	E_{pot}	1098.893	1023.842	976.7447	953.4086	945.3489	944.85	940.0149	964.3679	971.6246	967.9815
	E_{tot}	1677.16	1605.99	1562.773	1543.318	1539.14	1542.522	1541.568	1569.802	1580.939	1581.177
DMSO	E_{kin}	631.5633	635.802	640.0407	644.2793	648.518	652.7567	656.9954	661.2341	665.4727	669.7114
	E_{pot}	1376.314	1184.974	1082.075	1122.932	1116.24	1101.61	1093.789	1084.294	1059.624	1086.463
	E_{tot}	2007.878	1820.776	1722.116	1767.212	1764.758	1754.366	1750.784	1745.528	1725.097	1756.174
Chloroform	E_{kin}	400.6119	403.3006	405.9892	408.6779	411.3666	414.0552	416.7439	419.4326	422.1212	424.8099
	E_{pot}	1792.663	981.0325	790.1084	710.3755	664.0537	640.7671	642.3614	628.021	599.0072	615.3709
	E_{tot}	2193.275	1384.333	1196.098	1119.053	1075.42	1054.822	1059.105	1047.454	1021.128	1040.181

Table S8. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (Kcal/mol) calculated for MC- BNNT through Monte Carlo Simulation in different solvents in the MM+ force field.

MC- BNNT - MM+											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	178.5432	179.7415	180.9398	182.138	183.3363	184.5346	185.7329	186.9311	188.1294	189.3277
	E_{pot}	880.6537	807.2383	764.6399	768.4084	771.1425	747.9577	742.6027	761.7283	740.7482	731.225
	E_{tot}	1059.197	986.9798	945.5796	950.5464	954.4788	932.4923	928.3355	948.6595	928.8776	920.5527
Water	E_{kin}	687.5246	692.1389	696.7531	701.3674	705.9816	710.5959	715.2102	719.8244	724.4387	729.0529
	E_{pot}	1047.601	856.0232	802.4788	714.0272	705.9816	668.2977	652.1143	644.6745	621.1557	633.0168
	E_{tot}	1735.125	1548.162	1499.232	1415.395	1410.554	1378.894	1367.324	1364.499	1345.594	1362.07
Methanol	E_{kin}	439.696	442.6469	445.5979	448.5489	451.4999	454.4509	457.4018	460.3528	463.3038	466.2548
	E_{pot}	2111.134	1459.979	1253.256	1121.018	1071.499	1011.516	985.9405	992.8743	934.4407	926.3846
	E_{tot}	2550.83	1902.626	1698.854	1569.567	1522.999	1465.967	1443.342	1453.227	1397.744	1392.639
Ethanol	E_{kin}	578.2668	582.1478	586.0288	589.9098	593.7908	597.6717	601.5527	605.4337	609.3147	613.1957
	E_{pot}	1238.85	1123.802	1140.725	1112.588	1097.207	1068.253	1074.74	1072.092	1074.43	1116.879
	E_{tot}	1817.117	1705.95	1726.754	1702.498	1690.998	1665.924	1676.293	1677.525	1683.745	1730.074
DMSO	E_{kin}	631.5633	635.802	640.0407	644.2793	648.518	652.7567	656.9954	661.2341	665.4727	669.7114
	E_{pot}	1463.704	1325.442	1233.549	1247.161	1200.68	1202.235	1174.472	1191.551	1169.104	1137.312
	E_{tot}	2095.267	1961.244	1873.59	1891.441	1849.198	1854.992	1831.468	1852.785	1834.577	1807.023
Chloroform	E_{kin}	400.6119	403.3006	405.9892	408.6779	411.3666	414.0552	416.7439	419.4326	422.1212	424.8099
	E_{pot}	1609.177	1068.57	880.34	796.2639	745.7688	714.3477	692.1408	679.9914	673.9341	656.3385
	E_{tot}	2009.789	1471.87	1286.329	1204.942	1157.135	1128.403	1108.885	1099.424	1096.055	1081.148

Table S9. Minimum temperature that contain minimum total energy for each solvent and each compound.

Molecule name	Solvent	H_2O	DMSO	Methanol	Ethanol	Chloroform	Gas
MC–SWCNT	**T(K)**	312	306	310	304	312	310
	$E_{tot\ min}$	1285.021	1389.395	1301.977	1222.951	1045.052	867.9545
MC-BNNT	**T(K)**	314	316	316	308	316	316
	$E_{tot\ min}$	1345.594	1807.023	1392.639	1665.924	1081.148	920.5527
CP-SWCNT	**T(K)**	310	308	316	312	312	310
	$E_{tot\ min}$	5003.89	1891.565	1471.364	1206.979	1199.385	1015.171
CP-BNNT	**T (K)**	312	314	316	302	316	308
	$E_{tot\ min}$	1347.617	1788.601	1378.223	1714.383	1111.413	929.9483

Table S10. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- SWCNT through Monte Carlo Simulation in different solvents in the AMBER force field.

CP- SWCNT - AMBER											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	132.3529	133.2412	134.1295	135.0178	135.906	136.7943	137.6826	138.5709	139.4591	140.3474
	E_{pot}	3590.469	1155.749	806.8396	698.8635	707.5618	701.7199	713.1676	694.9904	689.3227	694.1765
	E_{tot}	3722.822	1288.99	940.9691	833.8813	843.4678	838.5142	850.8502	833.5613	828.7818	834.5239
Water	E_{kin}	638.6695	642.9559	647.2422	651.5286	655.815	660.1014	664.3877	668.6741	672.9605	677.2468
	E_{pot}	4316.646	964.4622	324.5848	129.6025	39.69876	32.08561	-47.12459	-76.38422	-55.64763	-75.85215
	E_{tot}	4955.316	1607.418	971.827	781.1311	695.5137	692.187	617.2631	592.2899	617.3128	601.3947
Methanol	E_{kin}	374.8519	377.3677	379.8835	382.3993	384.9151	387.4308	389.9466	392.4624	394.9782	397.494
	E_{pot}	5079.289	1723.445	994.4861	887.0532	856.1911	826.5387	817.8908	840.2115	823.2651	820.0841
	E_{tot}	5454.141	2100.813	1374.37	1269.452	1241.106	1213.97	1207.837	1232.674	1218.243	1217.578
Ethanol	E_{kin}	518.7524	522.234	525.7155	529.1971	532.6787	536.1602	539.6418	543.1233	546.6049	550.0865
	E_{pot}	3665.075	1613.839	1188.527	1057.887	1071.021	1038.368	1017.75	1040.767	1049.291	1039.733
	E_{tot}	4183.827	2136.073	1714.242	1587.084	1603.7	1574.528	1557.392	1583.89	1595.896	1589.819
DMSO	E_{kin}	572.0489	575.8881	579.7274	583.5667	587.4059	591.2452	595.0844	598.9237	602.7629	606.6022
	E_{pot}	3603.665	1594.21	1172.399	1137.573	1073.049	1057.526	1075.253	1092.236	1048.284	1054.653
	E_{tot}	4175.714	2170.098	1752.126	1721.14	1660.455	1648.771	1670.337	1691.16	1651.047	1661.255
Chloroform	E_{kin}	341.0975	343.3867	345.676	347.9652	350.2545	352.5437	354.8329	357.1222	359.4114	361.7007
	E_{pot}	3521.772	1187.879	807.3075	735.2485	694.2313	685.5443	695.6089	664.6177	659.0321	684.3485
	E_{tot}	3862.87	1531.266	1152.983	1083.214	1044.486	1038.088	1050.442	1021.74	1018.444	1046.049

Table S11. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for **CP- SWCNT** through Monte Carlo Simulation in different solvents in the OPLS force field.

CP- SWCNT - OPLS											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	132.3529	133.2412	134.1295	135.0178	135.906	136.7943	137.6826	138.5709	139.4591	140.3474
	E_{pot}	4666.66	2469.749	1961.162	1809.81	1794.402	1760.011	1659.926	1619.59	1579.312	1509.147
	E_{tot}	4799.013	2602.99	2095.291	1944.827	1930.308	1896.806	1797.609	1758.161	1718.771	1649.494
Water	E_{kin}	638.6695	642.9559	647.2422	651.5286	655.815	660.1014	664.3877	668.6741	672.9605	677.2468
	E_{pot}	6012.333	2304.662	1472.421	1092.453	822.236	604.8949	477.714	381.47	296.7668	184.2318
	E_{tot}	6651.003	2947.618	2119.663	1743.981	1478.051	1264.996	1142.102	1050.144	969.7273	861.4786
Methanol	E_{kin}	374.8519	377.3677	379.8835	382.3993	384.9151	387.4308	389.9466	392.4624	394.9782	397.494
	E_{pot}	4022.007	1392.477	1038.736	945.276	901.7485	919.3899	899.5207	907.1472	917.8523	878.4544
	E_{tot}	4396.858	1769.845	1418.619	1327.675	1286.664	1306.821	1289.467	1299.61	1312.83	1275.948
Ethanol	E_{kin}	518.7524	522.234	525.7155	529.1971	532.6787	536.1602	539.6418	543.1233	546.6049	550.0865
	E_{pot}	3884.511	1557.903	1155.264	1107.775	1090.998	1085.64	1102.223	1067.188	1112.05	1068.486
	E_{tot}	4403.263	2080.137	1680.979	1636.972	1623.677	1621.8	1641.865	1610.311	1658.654	1618.573
DMSO	E_{kin}	572.0489	575.8881	579.7274	583.5667	587.4059	591.2452	595.0844	598.9237	602.7629	606.6022
	E_{pot}	3570.559	1683.482	1268.844	1192.442	1219.366	1164.484	1130.208	1173.145	1151.732	1171.271
	E_{tot}	4142.608	2259.37	1848.571	1776.008	1806.771	1755.73	1725.293	1772.069	1754.495	1777.873
Chloroform	E_{kin}	341.0975	343.3867	345.676	347.9652	350.2545	352.5437	354.8329	357.1222	359.4114	361.7007
	E_{pot}	3526.541	1329.666	892.7791	793.6451	794.4743	773.1605	761.0963	763.5919	770.2086	774.5046
	E_{tot}	3867.638	1673.053	1238.455	1141.61	1144.729	1125.704	1115.929	1120.714	1129.62	1136.205

Table S12. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- SWCNT through Monte Carlo Simulation in different solvents in the CHRMM force field.

CP- SWCNT - CHARMM											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	132.3529	133.2412	134.1295	135.0178	135.906	136.7943	137.6826	138.5709	139.4591	140.3474
	E_{pot}	5343.54	2370.549	1912.069	1831.594	1823.08	1810.087	1802.129	1823.85	1807.156	1807.38
	E_{tot}	5475.893	2503.791	2046.199	1966.611	1958.986	1946.882	1939.812	1962.421	1946.615	1947.728
Water	E_{kin}	638.6695	642.9559	647.2422	651.5286	655.815	660.1014	664.3877	668.6741	672.9605	677.2468
	E_{pot}	3872.338	607.9218	112.4541	-85.71316	-140.1905	-242.2188	-259.0313	-224.1094	-264.3325	-254.4148
	E_{tot}	4511.007	1250.878	759.6964	565.8155	515.6245	417.8826	405.3565	444.5647	408.628	422.832
Methanol	E_{kin}	374.8519	377.3677	379.8835	382.3993	384.9151	387.4308	389.9466	392.4624	394.9782	397.494
	E_{pot}	6359.471	2697.295	2095.898	1994.007	1939.814	1940.672	1934.669	1946.667	1933.338	1915.905
	E_{tot}	6734.323	3074.663	2475.782	2376.406	2324.729	2328.103	2324.615	2339.129	2328.316	2313.399
Ethanol	E_{kin}	518.7524	522.234	525.7155	529.1971	532.6787	536.1602	539.6418	543.1233	546.6049	550.0865
	E_{pot}	5572.627	2590.256	2239.056	2170.167	2135.165	2124.983	2130.261	2121.747	2121.953	2109.531
	E_{tot}	6091.379	3112.49	2764.772	2699.364	2667.843	2661.143	2669.903	2664.87	2668.558	2659.617
DMSO	E_{kin}	572.0489	575.8881	579.7274	583.5667	587.4059	591.2452	595.0844	598.9237	602.7629	606.6022
	E_{pot}	5602.668	2654.611	2289.211	2241.188	2212.359	2209.743	2205.405	2227.096	2239.77	2209.206
	E_{tot}	6174.717	3230.5	2868.938	2824.754	2799.765	2800.988	2800.49	2826.02	2842.533	2815.809
Chloroform	E_{kin}	341.0975	343.3867	345.676	347.9652	350.2545	352.5437	354.8329	357.1222	359.4114	361.7007
	E_{pot}	5631.168	2471.012	1954.357	1884.392	1829.618	1829.688	1802.659	1811.898	1800.964	1832.874
	E_{tot}	5972.266	2814.399	2300.033	2232.357	2179.872	2182.232	2157.492	2169.02	2160.375	2194.575

Table S13. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for CP- SWCNT through Monte Carlo Simulation in different solvents in the MM+ force field.

CP- SWCNT - MM+											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	132.3529	133.2412	134.1295	135.0178	135.906	136.7943	137.6826	138.5709	139.4591	140.3474
	E_{pot}	2221.051	1312.854	1051.66	952.3523	908.5644	888.2503	877.4888	895.9343	901.5646	907.1714
	E_{tot}	2353.404	1446.095	1185.789	1087.37	1044.47	1025.045	1015.171	1034.505	1041.024	1047.519
Water	E_{kin}	638.6695	642.9559	647.2422	651.5286	655.815	660.1014	664.3877	668.6741	672.9605	677.2468
	E_{pot}	5143.981	4681.202	4537.869	4442.761	4396.69	4381.241	4339.502	4349.212	4331.741	4364.036
	E_{tot}	5782.651	5324.158	5185.111	5094.289	5052.505	5041.343	5003.89	5017.886	5004.702	5041.283
Methanol	E_{kin}	374.8519	377.3677	379.8835	382.3993	384.9151	387.4308	389.9466	392.4624	394.9782	397.494
	E_{pot}	2789.041	1675.876	1275.006	1147.44	1133.012	1125.759	1087.002	1094.143	1077.353	1073.87
	E_{tot}	3163.893	2053.243	1654.889	1529.84	1517.927	1513.19	1476.948	1486.605	1472.331	1471.364
Ethanol	E_{kin}	518.7524	522.234	525.7155	529.1971	532.6787	536.1602	539.6418	543.1233	546.6049	550.0865
	E_{pot}	2490.299	1041.746	768.6493	707.0849	709.748	698.7631	699.6834	663.8557	708.5042	706.8889
	E_{tot}	3009.051	1563.98	1294.365	1236.282	1242.427	1234.923	1239.325	1206.979	1255.109	1256.975
DMSO	E_{kin}	572.0489	575.8881	579.7274	583.5667	587.4059	591.2452	595.0844	598.9237	602.7629	606.6022
	E_{pot}	2565.845	1707.899	1458.183	1393.821	1321.301	1300.32	1309.753	1293.096	1312.594	1339.034
	E_{tot}	3137.894	2283.787	2037.911	1977.387	1908.706	1891.565	1904.837	1892.02	1915.357	1945.637
Chloroform	E_{kin}	341.0975	343.3867	345.676	347.9652	350.2545	352.5437	354.8329	357.1222	359.4114	361.7007
	E_{pot}	2442.15	1319.331	1006.296	882.1639	884.9643	863.9542	863.8379	842.2629	848.5743	861.5984
	E_{tot}	2783.248	1662.718	1351.972	1230.129	1235.219	1216.498	1218.671	1199.385	1207.986	1223.299

Table S14. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for MC- SWCNT through Monte Carlo Simulation in different solvents in the AMBER force field.

MC- SWCNT - AMBER											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	123.4702	124.2988	125.1275	125.9562	126.7848	127.6135	128.4421	129.2708	130.0995	130.9281
	E_{pot}	1332.548	604.7266	501.3847	502.4735	467.5057	466.5256	477.8577	478.3757	490.9937	472.9685
	E_{tot}	1456.018	729.0254	626.5122	628.4296	594.2905	594.139	606.2998	607.6465	621.0931	603.8966
Water	E_{kin}	637.7812	642.0616	646.342	650.6225	654.9029	659.1833	663.4637	667.7441	672.0245	676.3049
	E_{pot}	1826.938	301.1003	-12.22749	-145.5544	-192.0738	-217.1734	-269.7275	-292.4428	-323.1202	-303.1572
	E_{tot}	2464.719	943.1619	634.1146	505.0681	462.8291	442.0099	393.7362	375.3013	348.9043	373.1477
Methanol	E_{kin}	384.6229	387.2043	389.7857	392.367	394.9484	397.5297	400.1111	402.6925	405.2738	407.8552
	E_{pot}	1858.695	843.557	638.0351	603.5731	609.646	587.0507	626.7253	610.5114	591.7176	592.3128
	E_{tot}	2243.318	1230.761	1027.821	995.9402	1004.594	984.5804	1026.836	1013.204	996.9915	1000.168
Ethanol	E_{kin}	523.1938	526.7052	530.2165	533.7279	537.2393	540.7506	544.262	547.7734	551.2847	554.7961
	E_{pot}	1109.375	938.172	919.0059	932.9993	902.656	924.5472	927.5662	931.2511	939.6635	928.3587
	E_{tot}	1632.569	1464.877	1449.222	1466.727	1439.895	1465.298	1471.828	1479.024	1490.948	1483.155
DMSO	E_{kin}	576.4903	580.3593	584.2284	588.0975	591.9665	595.8356	599.7046	603.5737	607.4428	611.3118
	E_{pot}	1171.569	1029.381	968.377	944.2394	966.1399	928.5578	971.2665	974.0044	951.3856	956.9805
	E_{tot}	1748.059	1609.74	1552.605	1532.337	1558.106	1524.393	1570.971	1577.578	1558.828	1568.292
Chloroform	E_{kin}	345.5389	347.8579	350.177	352.496	354.8151	357.1341	359.4532	361.7722	364.0913	366.4103
	E_{pot}	1321.794	589.2145	504.5982	438.4234	431.2828	445.2003	441.843	459.1008	447.6387	446.1226
	E_{tot}	1667.333	937.0724	854.7751	790.9194	786.0979	802.3344	801.2962	820.873	811.73	812.5329

Table S15. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for MC- SWCNT through Monte Carlo Simulation in different solvents in the OPLS force field.

MC- SWCNT - OPLS											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	123.4702	124.2988	125.1275	125.9562	126.7848	127.6135	128.4421	129.2708	130.0995	130.9281
	E_{pot}	1399.179	745.676	599.6582	590.6402	596.2498	589.515	569.6523	575.7761	587.4496	575.4079
	E_{tot}	1522.649	869.9749	724.7857	716.5964	723.0346	717.1285	698.0944	705.0469	717.549	706.3361
Water	E_{kin}	637.7812	642.0616	646.342	650.6225	654.9029	659.1833	663.4637	667.7441	672.0245	676.3049
	E_{pot}	4043.665	1630.176	1031.658	668.006	469.2351	345.0043	190.4576	117.7998	62.78296	-85.34302
	E_{tot}	4681.447	2272.238	1678	1318.628	1124.138	1004.188	853.9213	785.5439	734.8075	590.9619
Methanol	E_{kin}	384.6229	387.2043	389.7857	392.367	394.9484	397.5297	400.1111	402.6925	405.2738	407.8552
	E_{pot}	1983.842	959.2897	794.7558	735.16	733.3629	718.7079	707.1711	723.0295	723.9037	710.9362
	E_{tot}	2368.465	1346.494	1184.541	1127.527	1128.311	1116.238	1107.282	1125.722	1129.178	1118.791
Ethanol	E_{kin}	523.1938	526.7052	530.2165	533.7279	537.2393	540.7506	544.262	547.7734	551.2847	554.7961
	E_{pot}	1041.171	831.6285	838.2177	789.329	761.1094	738.9363	770.4529	749.086	746.1496	755.6098
	E_{tot}	1564.365	1358.334	1368.434	1323.057	1298.349	1279.687	1314.715	1296.859	1297.434	1310.406
DMSO	E_{kin}	576.4903	580.3593	584.2284	588.0975	591.9665	595.8356	599.7046	603.5737	607.4428	611.3118
	E_{pot}	1114.238	930.2528	887.7226	868.2024	883.8317	880.2964	848.3306	826.692	845.6084	847.1276
	E_{tot}	1690.728	1510.612	1471.951	1456.3	1475.798	1476.132	1448.035	1430.266	1453.051	1458.439
Chloroform	E_{kin}	345.5389	347.8579	350.177	352.496	354.8151	357.1341	359.4532	361.7722	364.0913	366.4103
	E_{pot}	1631.107	735.1158	615.0772	577.8313	564.6626	584.6541	581.9693	554.6287	570.4865	559.3119
	E_{tot}	1976.646	1082.974	965.2541	930.3273	919.4777	941.7882	941.4225	916.4009	934.5778	925.7223

Table S16. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for MC- SWCNT through Monte Carlo Simulation in different solvents in the CHARMM force field.

MC- SWCNT - CHARMM											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	123.4702	124.2988	125.1275	125.9562	126.7848	127.6135	128.4421	130.0995	130.0995	130.9281
	E_{pot}	2806.247	1725.294	1636.343	1608.351	1634.037	1622.494	1636.002	1642.069	1639.302	1621.191
	E_{tot}	2929.718	1849.593	1761.471	1734.307	1760.822	1750.107	1764.444	1751.912	1762.875	1752.232
Water	E_{kin}	637.7812	642.0616	646.342	650.6225	654.9029	659.1833	663.4637	667.7441	672.0245	676.3049
	E_{pot}	1212.005	-34.24564	-203.7585	-290.1176	-318.961	-354.5506	-384.8248	-396.3385	-431.9636	-459.7365
	E_{tot}	1855.115	613.1814	447.9847	365.9418	341.4146	310.1411	284.1831	276.9857	245.6767	222.22
Methanol	E_{kin}	384.6229	387.2043	389.7857	392.367	394.9484	397.5297	400.1111	402.6925	405.2738	407.8552
	E_{pot}	3353.277	1937.388	1798.052	1745.996	1753.802	1757.675	1750.169	1724.92	1755.098	1730.726
	E_{tot}	3737.9	2324.592	2187.838	2138.363	2148.751	2155.205	2150.28	2127.612	2160.372	2138.581
Ethanol	E_{kin}	523.1938	526.7052	530.2165	533.7279	537.2393	540.7506	544.262	547.7734	551.2847	554.7961
	E_{pot}	891.9682	663.6169	675.1802	649.9938	656.8362	656.8362	732.8201	716.8341	745.9462	748.9759
	E_{tot}	1415.162	1190.322	1205.397	1183.722	1194.075	1200.449	1277.082	1264.607	1297.231	1303.772
DMSO	E_{kin}	576.4903	580.3593	584.2284	588.0975	591.9665	595.8356	599.7046	603.5737	607.4428	611.3118
	E_{pot}	1072.412	812.0793	802.0336	785.7122	772.6572	768.1914	789.8769	778.3661	811.1743	796.4874
	E_{tot}	1648.902	1392.439	1386.262	1373.81	1364.624	1364.027	1389.582	1381.94	1418.617	1407.799
Chloroform	E_{kin}	345.5389	347.8579	350.177	352.496	354.8151	357.1341	359.4532	361.7722	364.0913	366.4103
	E_{pot}	2789.365	1754.043	1655.732	1639.557	1626.634	1621.21	1624.749	1626.047	1627.121	1610.563
	E_{tot}	3134.904	2101.901	2005.908	1992.053	1981.449	1978.345	1984.202	1987.819	1991.212	1976.974

Table S17. Total (E_{tot}), Potential (E_{pot}), and Kinetic (E_{kin}) energies (kcal/mol) calculated for MC- SWCNT through Monte Carlo Simulation in different solvents in the MM+ force field.

MC- SWCNT - MM+											
Temperature		298	300	302	304	306	308	310	312	314	316
Gas	E_{kin}	123.4702	124.2988	125.1275	125.9562	126.7848	127.6135	128.4421	129.2708	130.0995	130.9281
	E_{pot}	1445.795	913.7254	786.3948	753.9936	751.2879	748.0026	739.5123	743.8458	766.9971	746.4366
	E_{tot}	1569.265	1038.024	911.5223	879.9498	878.0727	875.616	867.9545	873.1166	897.0965	877.3647
Water	E_{kin}	637.7812	642.0616	646.342	650.6225	654.9029	659.1833	663.4637	667.7441	672.0245	676.3049
	E_{pot}	1612.421	1098.681	887.7459	741.0745	685.8826	684.1646	630.8577	620.0669	622.4751	635.3095
	E_{tot}	2247.537	1738.06	1531.387	1388.978	1338.049	1340.594	1291.549	1285.021	1291.692	1308.789
Methanol	E_{kin}	384.6229	387.2043	389.7857	392.367	394.9484	397.5297	400.1111	402.6925	405.2738	407.8552
	E_{pot}	1919.841	1263.121	1025.405	951.5088	949.0932	923.4287	901.8659	901.5261	898.161	907.1176
	E_{tot}	2304.464	1650.325	1415.19	1343.876	1344.042	1320.958	1301.977	1304.219	1303.435	1314.973
Ethanol	E_{kin}	523.1938	526.7052	530.2165	533.7279	537.2393	540.7506	544.262	547.7734	551.2847	554.7961
	E_{pot}	983.9625	762.6992	712.9956	689.2229	697.3007	689.9451	698.5802	709.4153	711.4425	732.5303
	E_{tot}	1507.156	1289.404	1243.212	1222.951	1234.54	1230.696	1242.842	1257.189	1262.727	1287.326
DMSO	E_{kin}	576.4903	580.3593	584.2284	589.0036	592.8786	595.8356	599.7046	603.5737	607.4428	611.3118
	E_{pot}	1105.347	870.6674	821.6058	809.1907	796.5163	804.804	810.7641	837.4092	835.3959	810.6247
	E_{tot}	1681.838	1451.027	1405.834	1398.194	1389.395	1400.64	1410.469	1440.983	1442.839	1421.937
Chloroform	E_{kin}	345.5389	347.8579	350.177	352.496	354.8151	357.1341	359.4532	361.7722	364.0913	366.4103
	E_{pot}	1472.11	895.4624	761.1185	725.4608	702.4683	702.9341	731.4397	683.2797	712.4565	687.0272
	E_{tot}	1817.649	1243.32	1111.295	1077.957	1057.283	1060.068	1090.893	1045.052	1076.548	1053.438

Table S18. QTAIM topological parameters at the BCPs of the studied MC-SWCNT complex.

Bond	ρ	$\nabla^2\rho$	$H_{(r)}$	$\frac{V}{G}$
Cl_{121}-C $_{29}$	0.0127	0.0093	-0.0002	0.9671
H_{129}-C_{34}	0.0173	0.0159	-0.0013	0.9042
H_{131}-C_{48}	0.0307	0.028	-0.0001	0.9970
H_{132}-C_{49}	0.0288	0.025	0.0002	1.0030
H_{133}-C_{68}	0.0306	0.027	0.0001	1.0070
H_{134}-C_{69}	0.0292	0.0252	0.0002	1.0111
H_{135}-C_{80}	0.0124	0.0117	-0.0012	0.8795
H_{136}-C_{76}	0.0244	0.0218	-0.0006	0.9671
H_{137}-C_{66}	0.0307	0.0279	0.0001	1.0010
H_{138}-C_{46}	0.0303	0.0274	0.0006	0.9980
H_{139}-C_{54}	0.0345	0.0286	0.0016	1.0549
CL_{127}-C_{83}	0.0129	0.0098	0.0003	0.9588
N_{124}-C_{57}	0.0192	0.0143	0.0003	1.0256

Table S19. QTAIM topological parameters at the BCPs of the studied MC-BNNT complex.

Bond	**ρ**	$\nabla^2\rho$	$H_{(r)}$	$\frac{V}{G}$
Cl_1-N_{120}	0.0027	0.0027	-0.0006	0.6840
Cl_7-N_{92}	0.0066	0.0068	-0.0009	0.8091
C_{98}-N_{192}	0.0043	0.0042	-0.0008	0.7692
H_9-N_{53}	0.0073	0.022	-0.0006	0.5865
H_{10}-N_{88}	0.0061	0.0062	-0.0015	0.6623
H_{11}-B_{122}	0.0022	0.0018	-0.0006	0.4998
H_{12}-N_{156}	0.0005	0.0005	-0.0001	0.5063
H_{13}-N_{154}	0.0052	0.0051	-0.0014	0.6169
H_{14}-N_{141}	0.0056	0.0052	-0.0012	0.6770
H_{15}-N_{126}	0.0026	0.0024	-0.0007	0.5501
H_{18}-N_{36}	0.0041	0.0042	-0.0011	0.6180
H_{19}-N_{191}	0.0051	0.0045	-0.0013	0.5790

Table S20. QTAIM topological parameters at the BCPs of the studied CP -SWCNT complex.

Bond	ρ	$\nabla^2\rho$	$H_{(r)}$	$\frac{V}{G}$
O_{127}-C_{73}	0.0443	0.0452	0.0041	1.0834
O_{121}-C_{84}	0.0159	0.0163	-0.0001	0.9416
N_{125}-C_{81}	0.0073	0.0069	-0.0007	0.8764
N_{128}-C_{66}	0.0316	0.0279	0.0012	1.0256
C_{131}-C_{47}	0.1989	-0.098	0.1561	3.6900
H_{133}-C_{94}	0.0231	0.019	-0.0011	0.9372
H_{134}-C_{95}	0.0248	0.0216	-0.0011	0.9443
H_{136}-C_{99}	0.0099	0.0084	-0.0010	0.8569
H_{137}-C_{92}	0.0287	0.0235	-0.0002	0.9911
H_{138}-C_{91}	0.0169	0.0135	-0.0012	0.9017
H_{139}-C_{82}	0.0428	0.0307	0.0061	1.1682
H_{141}-C_{70}	0.0484	0.0399	0.0066	1.1442
H_{142}-C_{68}	0.0252	0.0223	-0.0009	0.9560
H_{143}-C_{67}	0.0580	0.0443	0.0132	1.2315
H_{144}-C_{41}	0.0268	0.0248	-0.0004	0.9833
H_{146}-C_{53}	0.0289	0.0278	-0.0014	0.9434
H_{147}-C_{57}	0.0264	0.0247	-0.0015	0.9355

Table S21. QTAIM topological parameters at the BCPs of the studied CP -BNNT complex.

Bond	**ρ**	$\nabla^2\rho$	$H_{(r)}$	$\frac{V}{G}$
O_1-N_{63}	0.0049	-0.0059	-0.0019	0.5356
O_7-N_{46}	0.0147	0.0167	-0.0015	0.9025
Cl_{13}-N_{130}	0.0085	0.0078	-0.0011	0.8230
Cl_{14}-N_{155}	0.0093	0.0082	-0.0010	0.8489
H_{15}-N_{99}	0.0166	0.016	-0.0013	0.9066
H_{17}-N_{102}	0.0046	0.0045	-0.0011	0.6698
H_{18}-N_{83}	0.0084	0.0085	-0.0014	0.7893
H_{19}-N_{50}	0.0079	0.0078	-0.0016	0.7326
H_{21}-N_{34}	0.0244	0.0203	0.00091	1.0431
H_{22}-N_{166}	0.0075	0.0076	-0.0017	0.7087
H_{23}-N_{183}	0.0100	0.0096	-0.0017	0.7716
H_{24}-N_{187}	0.0050	0.0051	-0.0013	0.6518
H_{25}-N_{186}	0.0107	0.011	-0.0019	0.8035
H_{26}-N_{135}	0.0176	0.01569	-0.0009	0.9363