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Supporting Information for the manuscript

Conformational Features of 4-(*N*)-Squalenoyl-Gemcitabine in solution: a combined NMR and Molecular Dynamics Investigation

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Table I. List of the 51 conformers obtained from the MD calculations, together with their relative energy (calculated as the difference in energy between the *i*-th conformer and the dominant conformer at 3.8 ns) and the corresponding relative existence probability. The threshold value of about 8 kJ/mol is indicated by a horizontal dividing line. Among the 27 conformers with energy lower than the threshold value, the 4 major conformations chosen for the discussion are in bold type.

snapshot (ns)	relative energy (kcal/mol)	relative energy (kJ/mol)	relative probability (%)
3,8	**0,0000**	**0,0000**	**20,2983**
5,4	0,5686	2,3792	7,8201
1,3	0,6205	2,5963	7,1683
2,1	0,6410	2,6818	6,9268
4,9	0,7897	3,3041	5,3972
5,7	0,8140	3,4058	5,1816
3,6	**1,0800**	**4,5188**	**3,3166**
1,5	1,1314	4,7339	3,0426
4,1	1,1467	4,7978	2,9656
3,0	1,1596	4,8518	2,9020
1,6	1,1602	4,8541	2,8993
2,2	1,3035	5,4539	2,2797
4,2	1,3557	5,6724	2,0885
2,5	1,3920	5,8242	1,9651
2,3	1,3933	5,8297	1,9608
5,0	1,5068	6,3045	1,6210
1,0	**1,5679**	**6,5600**	**1,4631**
5,8	1,6324	6,8301	1,3130
4,6	1,6404	6,8633	1,2956
3,5	1,6525	6,9139	1,2696
1,8	1,7119	7,1627	1,1491
5,5	1,7433	7,2942	1,0901
3,3	1,7460	7,3054	1,0852
2,7	1,7636	7,3788	1,0537
2,9	**1,7782**	**7,4400**	**1,0282**
5,3	1,8170	7,6024	0,9634
2,8	1,8953	7,9301	0,8448
2,6	2,0130	8,4225	0,6934
3,9	2,0238	8,4675	0,6810
4,7	2,0339	8,5098	0,6696
3,1	2,0780	8,6943	0,6218
3,2	2,0780	8,6943	0,6218
2,0	2,1377	8,9440	0,5626
2,4	2,1383	8,9466	0,5620
5,2	2,1531	9,0087	0,5482

1,9	2,2359	9,3550	0,4771
3,7	2,2490	9,4099	0,4667
4,0	2,2704	9,4994	0,4503
3,4	2,3136	9,6802	0,4188
1,7	2,3196	9,7052	0,4146
5,9	2,3286	9,7428	0,4084
5,1	2,4518	10,2585	0,3321
5,6	2,4654	10,3153	0,3247
4,5	2,4777	10,3667	0,3181
4,8	2,4899	10,4178	0,3116
6,0	2,7171	11,3685	0,2128
1,1	2,7551	11,5272	0,1997
1,4	3,0005	12,5541	0,1323
4,3	3,1042	12,9878	0,1112
1,2	3,5024	14,6540	0,0570
4,4	4,3160	18,0581	0,0146

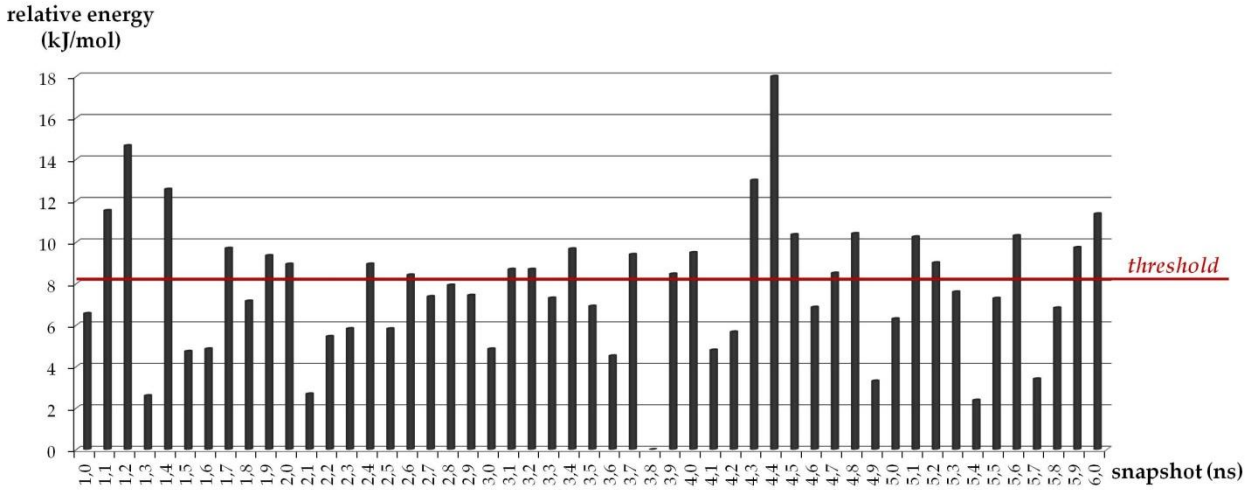

Figure I. Relative energy of the 51 conformers obtained from MD simulations calculated as the difference in energy between the *i*-th conformer and the dominant conformer at 3.8 ns. The red horizontal line indicates the value of the threshold of about 8 kJ/mol above which the conformers have been neglected.