Supplementary Table 1. Optimized geometry (Zm matrix is also given) and Mulliken atomic
charges in gas phase and in DMSO of the studies uracil derivatives

A- 5-FU

								Mulliken Charges		
								V	DMSO	
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	S_0	S_0	S_1
1	F							-0.274	-0.381	-0.276
2	C	1			1.351			0.189	0.496	0.192
3	C	2	1		1.453	117.051		0.650	0.505	0.655
4	N	3	2	1	1.399	112.504	-179.963	-0.806	-0.716	-0.814
5	C	4	3	2	1.388	128.019	-0.027	0.903	0.721	0.917
6	N	5	4	3	1.381	113.626	0.004	-0.777	-0.598	-0.786
7	C	2	1	3	1.349	121.047	-179.992	0.105	-0.066	0.109
8	O	5	4	3	1.227	123.074	179.989	-0.488	-0.600	-0.492
9	O	3	2	1	1.229	125.838	0.035	-0.472	-0.584	-0.474
10	H	4	3	2	1.016	116.308	179.990	0.355	0.471	0.357
11	H	6	5	4	1.014	116.336	-179.988	0.353	0.483	0.354
12	H	7	2	1	1.083	122.924	0.007	0.262	0.270	0.260

B- U

								Mulliken Charges		
								V	DMSO	
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	S_0	S_0	S_1
1	C							0.163	0.148	0.172
2	C	1			1.450			0.291	0.327	0.278
3	N	2	1		1.404	114.187		-0.551	-0.527	-0.543
4	C	3	2	1	1.382	127.387	-0.063	0.674	0.700	0.671
5	N	4	3	2	1.383	113.701	0.042	-0.447	-0.418	-0.440
6	C	1	2	3	1.355	119.620	0.037	-0.090	-0.105	-0.092
7	O	4	3	2	1.229	123.307	179.923	-0.520	-0.601	-0.526
8	O	2	1	6	1.234	126.078	179.919	-0.507	-0.608	-0.514
9	H	3	2	1	1.015	116.776	179.877	0.339	0.353	0.342
10	H	5	4	3	1.012	116.116	-179.945	0.333	0.363	0.335
11	H	6	1	2	1.083	122.891	179.928	0.159	0.196	0.159
12	H	1	6	5	1.081	121.492	-179.913	0.158	0.172	0.159

C- TU

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	Mulliken Charges		
								V	DMSO	
								S_0	S_0	S_1
1	C							0.168	0.160	0.171
2	C	1			1.433			-0.195	-0.166	-0.203
3	N	2	1		1.384	114.743		-0.405	-0.368	-0.397
4	C	3	2	1	1.387	127.359	-0.012	0.650	0.675	0.646
5	N	4	3	2	1.383	113.584	0.012	-0.438	-0.400	-0.431
6	C	1	2	3	1.361	119.820	0.010	-0.117	-0.130	-0.120
7	O	4	3	2	1.226	122.977	179.978	-0.515	-0.587	-0.519
8	H	3	2	1	1.015	117.602	179.985	0.347	0.361	0.349
9	H	5	4	3	1.013	116.213	-179.993	0.335	0.369	0.337
10	H	6	1	2	1.083	122.932	-179.992	0.161	0.201	0.162
11	H	1	6	5	1.080	120.734	179.991	0.166	0.180	0.167
12	S	2	1	6	1.682	124.999	179.994	-0.157	-0.294	-0.162

D- DTU

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	Mulliken Charges		
								V	DMSO	
								S_0	S_0	S_1
1	C							0.191	0.194	0.194
2	C	1			1.433			-0.269	-0.250	-0.279
3	N	2	1		1.389	114.493		-0.278	-0.235	-0.272
4	C	3	2	1	1.372	127.474	0.010	0.114	0.127	0.109
5	N	4	3	2	1.368	113.867	-0.019	-0.338	-0.290	-0.332
6	C	1	2	3	1.360	119.654	0.003	-0.148	-0.160	-0.149
7	H	3	2	1	1.015	116.849	179.999	0.355	0.368	0.357
8	H	5	4	3	1.013	116.496	-179.963	0.342	0.375	0.344
9	H	6	1	2	1.083	123.372	-179.997	0.164	0.206	0.165
10	H	1	6	5	1.080	120.857	179.997	0.170	0.187	0.172
11	S	2	1	6	1.677	125.358	179.996	-0.141	-0.264	-0.144
12	S	4	3	2	1.676	123.034	179.975	-0.163	-0.259	-0.164

E- Uridines (I)

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	MM Charge
1	C							-0.314
2	C	1			1.454			0.181
3	N	2	1		1.409	112.960		-0.532
4	C	3	2	1	1.382	128.495	-0.874	0.775
5	N	4	3	2	1.408	114.326	1.200	0.042
6	C	1	2	3	1.352	120.192	0.360	0.174
7	O	4	3	2	1.222	122.413	-179.513	-0.503
8	O	2	1	6	1.224	126.687	-179.880	-0.510
9	H	3	2	1	1.014	116.469	179.930	0.337
10	H	6	1	2	1.084	121.214	-179.574	0.193
11	H	1	6	5	1.082	121.384	179.340	0.155
12	C	5	4	3	1.474	116.494	-174.760	-0.387
13	O	12	5	4	1.424	112.022	95.796	-0.240
14	C	12	5	4	1.538	114.863	-144.543	0.012
15	H	12	5	4	1.087	104.613	-19.312	0.182
16	C	13	12	5	1.432	110.673	96.174	0.094
17	C	14	12	5	1.540	105.739	-99.647	-0.068
18	H	14	12	5	1.093	107.971	142.424	0.171
19	H	14	12	5	1.092	114.044	22.829	0.193
20	H	16	13	12	1.101	109.715	-94.631	0.143
21	H	17	14	12	1.096	111.170	-130.088	0.138
22	C	16	13	12	1.531	107.584	146.620	-0.323
23	H	22	16	13	1.097	108.880	50.893	0.167
24	H	22	16	13	1.092	109.214	-65.925	0.155
25	N	22	16	13	1.458	110.430	173.516	-0.395
26	H	25	22	16	1.015	116.941	-63.937	0.316
27	O	17	14	12	1.430	109.020	109.611	-0.513
28	H	27	17	14	0.967	109.140	170.962	0.371
29	C	25	22	16	1.379	128.394	136.699	0.276
30	O	29	25	22	1.227	120.065	169.419	-0.468
31	C	29	25	22	1.519	118.013	-11.450	-0.347
32	H	31	29	25	1.095	112.116	-54.660	0.159
33	H	31	29	25	1.096	111.071	66.030	0.173
34	H	31	29	25	1.090	107.720	-174.748	0.193

F- deoxyuridines (II)

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	MM Charge
1	C							-0.289
2	C	1			1.453			0.191
3	N	2	1		1.408	112.944		-0.529
4	C	3	2	1	1.383	128.500	-0.944	0.766
5	N	4	3	2	1.407	114.356	1.059	0.004
6	C	1	2	3	1.353	120.162	0.469	0.168
7	O	4	3	2	1.222	122.361	-179.670	-0.501
8	O	2	1	6	1.224	126.695	-179.805	-0.514
9	H	3	2	1	1.014	116.486	179.742	0.337
10	H	6	1	2	1.084	121.060	-179.660	0.192
11	H	1	6	5	1.081	121.369	179.396	0.154
12	C	5	4	3	1.479	116.492	-174.697	-0.259

13	O	12	5	4	1.423	111.803	92.346	-0.232
14	C	12	5	4	1.541	114.003	-148.554	-0.032
15	H	12	5	4	1.087	104.983	-22.879	0.176
16	C	13	12	5	1.431	108.574	89.976	0.134
17	C	14	12	5	1.542	105.136	-100.929	0.069
18	H	14	12	5	1.092	108.223	140.854	0.169
19	H	14	12	5	1.092	114.032	21.332	0.185
20	H	16	13	12	1.102	109.750	-83.896	0.142
21	H	17	14	12	1.097	110.824	-121.118	0.138
22	C	16	13	12	1.523	110.395	156.423	-0.523
23	H	22	16	13	1.099	109.923	52.981	0.150
24	H	22	16	13	1.095	109.059	-64.467	0.149
25	N	22	16	13	1.475	107.579	177.769	-0.693
26	H	25	22	16	1.015	111.259	157.678	0.298
27	H	25	22	16	1.017	110.964	-83.490	0.293
28	O	17	14	12	1.426	110.388	117.675	-0.517
29	H	28	17	14	0.970	106.430	178.852	0.375

G- deoxyuridines (III)

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	M Charge
1	C							-0.222
2	C	1			1.454			0.183
3	N	2	1		1.410	113.059		-0.516
4	C	3	2	1	1.382	128.460	-0.115	0.724
5	N	4	3	2	1.403	114.071	0.440	-0.033
6	C	1	2	3	1.352	120.033	0.193	0.207
7	O	4	3	2	1.224	122.513	179.824	-0.505
8	O	2	1	6	1.224	126.717	-179.896	-0.511
9	H	3	2	1	1.014	116.427	-179.931	0.339
10	H	6	1	2	1.083	122.104	179.431	0.188
11	H	1	6	5	1.081	121.524	179.721	0.156
12	C	5	4	3	1.468	117.870	-176.714	-0.377
13	O	12	5	4	1.429	108.684	120.843	-0.315
14	C	12	5	4	1.550	115.052	-120.107	-0.244
15	H	12	5	4	1.090	104.551	3.106	0.177
16	C	13	12	5	1.437	111.081	133.534	0.057
17	C	14	12	5	1.525	104.765	-110.070	0.361
18	H	14	12	5	1.094	109.637	131.862	0.176
19	H	14	12	5	1.092	112.983	11.736	0.190
20	H	16	13	12	1.096	107.226	-142.414	0.149
21	H	17	14	12	1.090	115.437	-148.482	0.171
22	C	16	13	12	1.537	110.595	97.956	-0.281
23	H	22	16	13	1.100	107.373	48.886	0.154
24	H	22	16	13	1.097	109.563	-66.756	0.137
25	N	22	16	13	1.465	110.037	174.481	-0.597
26	H	25	22	16	1.015	111.346	166.478	0.291
27	H	25	22	16	1.017	111.453	-73.794	0.288
28	F	17	14	12	1.420	109.202	91.565	-0.345

H- Uridines (IV)

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	Charge
1	F							-0.352
2	C	1			1.344			0.307
3	C	2	1		1.461	117.435		0.327
4	N	3	2	1	1.406	111.501	-179.623	-0.492
5	C	4	3	2	1.388	129.127	0.343	0.562
6	N	5	4	3	1.400	114.149	-1.176	-0.258
7	C	2	1	3	1.347	120.763	-179.644	0.082
8	O	5	4	3	1.222	122.663	179.201	-0.479
9	O	3	2	1	1.218	126.555	0.195	-0.483
10	H	4	3	2	1.015	115.904	179.554	0.344
11	H	7	2	1	1.084	121.428	-0.167	0.175
12	C	6	5	4	1.466	118.665	177.183	-0.258
13	H	12	6	5	1.092	107.296	-15.742	0.223
14	H	12	6	5	1.092	109.592	-133.163	0.183
15	C	12	6	5	1.535	116.474	104.975	0.346
16	O	15	12	6	1.229	118.912	163.233	-0.493
17	N	15	12	6	1.353	117.144	-18.033	-0.222
18	H	17	15	12	1.013	121.318	3.140	0.346
19	C	17	15	12	1.456	122.211	-179.391	-0.440
20	H	19	17	15	1.095	108.447	-41.072	0.189
21	C	19	17	15	1.525	107.147	-158.284	0.614
22	O	21	19	17	1.217	124.164	-12.401	-0.478
23	O	21	19	17	1.339	111.562	168.730	-0.260
24	C	23	21	19	1.446	116.247	178.274	-0.130
25	H	24	23	21	1.089	105.219	179.938	0.157
26	H	24	23	21	1.092	110.168	-60.489	0.167
27	H	24	23	21	1.092	110.138	60.395	0.168
28	C	19	17	15	1.542	112.561	79.059	-0.357
29	H	28	19	17	1.092	108.901	-59.085	0.187
30	H	28	19	17	1.094	110.705	60.641	0.157
31	H	28	19	17	1.093	110.341	-178.512	0.168