The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents

Gábor Paragi, [a,c][1] Zoltán Kupihár, [b] Gábor Endre, [b] Célia Fonseca Guerra, *[a]
Lajos Kovács * [b]

Supporting Information

[1] [a] Dr. G. Paragi, Dr. C. Fonseca Guerra. Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, Vrije Universiteit Amsterdam (VU). De Boelelaan 1083, 1081 HV Amsterdam (The Netherlands) E-mail: c.fonsecaguerra@vu.nl
[b] Dr. Z. Kupihár, G. Endre, Dr. L. Kovács. Department of Medicinal Chemistry, University of Szeged. Dóm tér 8, 6720 Szeged (Hungary). E-mail: kovacs.lajos@med.u-szeged.hu
[c] Dr. G. Paragi. MTA-SZTE Supramolecular and Nanostructured Materials Research Group, University of Szeged. Dóm tér 8, 6720 Szeged (Hungary)

Table SI-1. Stacking energies between layers (in kcal/mol) based on ho^{5}U and X units (without cation) in different geometries. The geometries were taken from Scheme 1 in the manuscript according to arrangements O4-O9

Geometry	O4	O5	O6	O7	O8	O9
Stacking energy	-48.4	-50.0	-48.1	-47.9	-49.7	-51.1

Table SI-2. Coordinates (in Å) of optimized X_4 tetramer in C(4h) symmetry

number	atom	x	y	z
1	N	4.887	4.879	0.000
2	N	-4.887	-4.879	0.000
3	N	4.879	-4.887	0.000
4	N	-4.879	4.887	0.000
5	N	3.369	1.119	0.000
6	N	-3.369	-1.119	0.000
7	N	1.119	-3.369	0.000
8	N	-1.119	3.369	0.000
9	N	5.329	2.451	0.000
10	N	-5.329	-2.451	0.000
11	N	2.451	-5.329	0.000
12	N	-2.451	5.329	0.000
13	N	2.631	4.747	0.000
14	N	-2.631	-4.747	0.000
15	N	4.747	-2.631	0.000
16	N	-4.747	2.631	0.000
17	O	5.464	0.149	0.000
18	O	-5.464	-0.149	0.000
19	O	0.149	-5.464	0.000
20	O	-0.149	5.464	0.000
21	O	1.227	1.967	0.000
22	O	-1.227	-1.967	0.000
23	O	1.967	-1.227	0.000
24	O	-1.967	1.227	0.000
25	H	3.646	6.635	0.000
26	H	-3.646	-6.635	0.000
27	H	6.635	-3.646	0.000
28	H	-6.635	3.646	0.000
29	H	2.940	0.166	0.000
30	H	-2.940	-0.166	0.000
31	H	0.166	-2.940	0.000
32	H	-0.166	2.940	0.000
33	C	3.115	3.448	0.000
34	C	3.727	5.556	0.000
35	C	2.447	2.185	0.000
36	C	4.502	3.568	0.000
37	C	-3.115	-3.448	0.000
38	C	-3.727	-5.556	0.000
39	C	-2.447	-2.185	0.000
40	C	-4.502	-3.568	0.000
41	C	3.448	-3.115	0.000
42	C	5.556	-3.727	0.000
43	C	2.185	-2.447	0.000
44	C	3.568	-4.502	0.000
45	C	6.800	2.572	0.000
46	C	-6.800	-2.572	0.000
47	C	2.572	-6.800	0.000
48	C	-2.572	6.800	0.000
49	H	1.629	5.019	0.000
50	H	-1.629	-5.019	0.000
51	H	5.019	-1.629	0.000
52	H	-5.019	1.629	0.000
53	C	-3.448	3.115	0.000
54	C	-5.556	3.727	0.000
55	C	-2.185	2.447	0.000
56	C	-3.568	4.502	0.000
57	C	4.756	1.176	0.000
58	C	-4.756	-1.176	0.000
59	C	1.176	-4.756	0.000
60	C	-1.176	4.756	0.000
61	H	-7.047	-3.634	0.000
62	H	-7.212	-2.085	-0.889
63	H	-7.212	-2.085	0.889
64	H	-2.085	7.212	0.889
65	H	-3.634	7.047	0.000
66	H	-2.085	7.212	-0.889
67	H	7.212	2.085	0.889
68	H	7.047	3.634	0.000
69	H	7.212	2.085	-0.889
70	H	3.634	-7.047	0.000
71	H	2.085	-7.212	-0.889
72	H	2.085	-7.212	0.889

Table SI-3. Coordinates (in Å) of optimized n^5U_4 tetramer in C(4h) symmetry

number	atom	x	y	z
1	H	-4.873	5.775	0.887
2	H	5.081	6.262	0.000
3	H	-4.873	5.775	-0.887
4	H	6.262	-5.081	0.000
5	N	2.567	2.611	0.000
6	N	-2.567	-2.611	0.000
7	N	2.611	-2.567	0.000
8	N	-2.611	2.567	0.000
9	N	3.882	4.543	0.000
10	N	-3.882	-4.543	0.000
11	N	4.543	-3.882	0.000
12	N	-4.543	3.882	0.000
13	N	0.294	5.482	0.000
14	N	-0.294	-5.482	0.000
15	N	5.482	-0.294	0.000
16	N	-5.482	0.294	0.000
17	O	4.883	2.475	0.000
18	O	-4.883	-2.475	0.000
19	O	2.475	-4.883	0.000
20	O	-2.475	4.883	0.000
21	O	0.272	2.677	0.000
22	O	-0.272	-2.677	0.000
23	O	2.677	-0.272	0.000
24	O	-2.677	0.272	0.000
25	H	-6.262	5.081	0.000
26	H	5.775	4.873	-0.887
27	H	5.775	4.873	0.887
28	H	4.873	-5.775	-0.887
29	H	2.534	1.578	0.000
30	H	-2.534	-1.578	0.000
31	H	1.578	-2.534	0.000
32	H	-1.578	2.534	0.000
33	C	1.461	4.766	0.000
34	H	6.390	-2.871	0.000
35	C	1.348	3.293	0.000
36	C	2.715	5.316	0.000
37	C	-1.461	-4.766	0.000
38	H	-6.390	2.871	0.000
39	C	-1.348	-3.293	0.000
40	C	-2.715	-5.316	0.000
41	C	4.766	-1.461	0.000
42	H	-2.871	-6.390	0.000
43	C	3.293	-1.348	0.000
44	C	5.316	-2.715	0.000
45	C	5.211	5.178	0.000
46	C	-5.211	-5.178	0.000
47	C	5.178	-5.211	0.000
48	C	-5.178	5.211	0.000
49	H	-0.625	5.032	0.000
50	H	0.625	-5.032	0.000
51	H	5.032	0.625	0.000
52	H	-5.032	-0.625	0.000
53	C	-4.766	1.461	0.000
54	H	4.873	-5.775	0.887
55	C	-3.293	1.348	0.000
56	C	-5.316	2.715	0.000
57	C	3.846	3.162	0.000
58	C	-3.846	-3.162	0.000
59	C	3.162	-3.846	0.000
60	C	-3.162	3.846	0.000
61	H	-5.081	-6.262	0.000
62	H	-5.775	-4.873	-0.887
63	H	-5.775	-4.873	0.887
64	H	2.871	6.390	0.000
65	H	-0.315	-6.490	0.000
66	H	6.490	-0.315	0.000
67	H	0.315	6.490	0.000
68	H	-6.490	0.315	0.000

Table SI-4. Coordinates (in Å) of optimized ho^5U_4 tetramer in C(4h) symmetry

number	atom	x	y	z
1	H	-1.978	7.184	0.887
2	H	7.140	3.531	0.000
3	H	-1.978	7.184	-0.887
4	H	3.531	-7.140	0.000
5	N	3.326	1.275	0.000
6	N	-3.326	-1.275	0.000
7	N	1.275	-3.326	0.000
8	N	-1.275	3.326	0.000
9	N	5.328	2.474	0.000
10	N	-5.328	-2.474	0.000
11	N	2.474	-5.328	0.000
12	N	-2.474	5.328	0.000
13	O	2.561	4.863	0.000
14	O	-2.561	-4.863	0.000
15	O	4.863	-2.561	0.000
16	O	-4.863	2.561	0.000
17	O	5.353	0.165	0.000
18	O	-5.353	-0.165	0.000
19	O	0.165	-5.353	0.000
20	O	-0.165	5.353	0.000
21	O	1.272	2.284	0.000
22	O	-1.272	-2.284	0.000
23	O	2.284	-1.272	0.000
24	O	-2.284	1.272	0.000
25	H	-3.531	7.140	0.000
26	H	7.184	1.978	-0.887
27	H	7.184	1.978	0.887
28	H	1.978	-7.184	-0.887
29	H	2.863	0.347	0.000
30	H	-2.863	-0.347	0.000
31	H	0.347	-2.863	0.000
32	H	-0.347	2.863	0.000
33	C	3.226	3.678	0.000
34	H	4.580	-5.161	0.000
35	C	2.506	2.403	0.000
36	C	4.590	3.657	0.000
37	C	-3.226	-3.678	0.000
38	H	-4.580	5.161	0.000
39	C	-2.506	-2.403	0.000
40	C	-4.590	-3.657	0.000
41	C	3.678	-3.226	0.000
42	H	-5.161	-4.580	0.000
43	C	2.403	-2.506	0.000
44	C	3.657	-4.590	0.000
45	C	6.803	2.493	0.000
46	C	-6.803	-2.493	0.000
47	C	2.493	-6.803	0.000
48	C	-2.493	6.803	0.000
49	H	1.570	4.758	0.000
50	H	-1.570	-4.758	0.000
51	H	4.758	-1.570	0.000
52	H	-4.758	1.570	0.000
53	C	-3.678	3.226	0.000
54	H	1.978	-7.184	0.887
55	C	-2.403	2.506	0.000
56	C	-3.657	4.590	0.000
57	C	4.709	1.229	0.000
58	C	-4.709	-1.229	0.000
59	C	1.229	-4.709	0.000
60	C	-1.229	4.709	0.000
61	H	-7.140	-3.531	0.000
62	H	-7.184	-1.978	-0.887
63	H	-7.184	-1.978	0.887
64	H	5.161	4.580	0.000

Table SI-5. Coordinates (in Å) of optimized ho^5U_2-X_2 tetramer in C(4h) symmetry and in T2 arrangement. The definition of T2 arrangement can be found in Scheme 1 in the manuscript

1	H	5.084	-5.121	0.000
2	N	4.435	5.024	0.000
3	N	-5.284	3.997	0.000
4	H	-1.063	-5.217	0.000
5	N	-3.156	-1.906	0.000
6	N	3.296	1.142	0.000
7	N	-1.397	2.849	0.000
8	N	1.633	-3.572	0.000
9	N	-5.026	-3.307	0.000
10	N	5.118	2.654	0.000
11	N	-2.913	4.672	0.000
12	N	2.999	-5.464	0.000
13	O	-2.042	-5.409	0.000
14	N	2.203	4.670	0.000
15	N	-4.933	1.766	0.000
16	O	5.145	-2.500	0.000
17	O	-5.300	-1.023	0.000
18	O	5.459	0.364	0.000
19	O	-0.638	5.031	0.000
20	O	0.700	-5.685	0.000
21	O	-1.010	-2.721	0.000
22	O	1.082	1.753	0.000
23	O	-2.032	0.629	0.000
24	O	2.465	-1.445	0.000
25	H	-2.736	6.581	0.889
26	H	3.029	6.650	0.000
27	H	-6.912	2.593	0.000
28	H	-2.736	6.581	-0.889
29	H	-2.767	-0.936	0.000
30	H	2.992	0.151	0.000
31	H	-0.402	2.524	0.000
32	H	0.672	-3.185	0.000
33	C	-2.817	-4.296	0.000
34	H	4.954	-1.525	0.000
35	C	-2.227	-2.955	0.000
36	C	-4.176	-4.413	0.000
37	C	2.812	3.425	0.000
38	C	3.214	5.583	0.000
39	C	2.274	2.102	0.000
40	C	4.183	3.681	0.000
41	C	-3.688	2.371	0.000
42	C	-5.845	2.777	0.000
43	C	-2.367	1.825	0.000
44	C	-3.943	3.740	0.000
45	C	-6.492	-3.477	0.000
46	C	6.569	2.920	0.000
47	C	-3.180	6.123	0.000
48	C	3.144	-6.933	0.000
49	H	-4.653	-5.387	0.000
50	H	1.179	4.834	0.000
51	H	-5.095	0.740	0.000
52	H	-6.924	-3.006	-0.888
53	C	4.022	-3.268	0.000
54	H	-4.261	6.262	0.000
55	C	2.690	-2.663	0.000
56	C	4.117	-4.629	0.000
57	C	-4.535	-2.010	0.000
58	C	4.673	1.326	0.000
59	C	-1.589	4.225	0.000
60	C	1.706	-4.953	0.000
61	H	6.709	4.002	0.000
62	H	7.027	2.476	-0.889
63	H	7.027	2.476	0.889
64	H	2.663	-7.356	0.888
65	H	4.207	-7.181	0.000
66	H	2.663	-7.356	-0.888
67	H	-6.924	-3.006	0.888
68	H	-6.720	-4.545	0.000

Table SI-6. Coordinates (in Å) of optimized ho^5U_2-X_2 tetramer in C(4h) symmetry and in T3 arrangement. The definition of T3 arrangement can be found in Scheme 1 in the manuscript

1	H	6.369	4.451	0.000
2	H	5.052	5.284	-0.889
3	N	6.523	1.962	0.000
4	N	-6.523	-1.962	0.000
5	N	2.518	-2.756	0.000
6	N	-2.518	2.756	0.000
7	N	2.485	2.266	0.000
8	N	-2.485	-2.266	0.000
9	N	3.686	-4.777	0.000
10	N	-3.686	4.777	0.000
11	N	4.547	3.435	0.000
12	N	-4.547	-3.435	0.000
13	O	0.105	-5.522	0.000
14	O	-0.105	5.522	0.000
15	N	5.405	-0.002	0.000
16	N	-5.405	0.002	0.000
17	O	4.833	-2.777	0.000
18	O	-4.833	2.777	0.000
19	O	2.539	4.570	0.000
20	O	-2.539	-4.570	0.000
21	O	0.231	-2.662	0.000
22	O	-0.231	2.662	0.000
23	O	2.282	-0.029	0.000
24	O	-2.282	0.029	0.000
25	H	5.550	-5.243	0.888
26	H	5.052	5.284	0.889
27	H	7.548	0.072	0.000
28	H	-7.548	-0.072	0.000
29	H	2.522	-1.708	0.000
30	H	-2.522	1.708	0.000
31	H	1.454	2.346	0.000
32	H	-1.454	-2.346	0.000
33	C	1.266	-4.820	0.000
34	H	5.550	-5.243	-0.888
35	C	1.256	-3.355	0.000
36	C	2.469	-5.462	0.000
37	C	-1.266	4.820	0.000
38	H	4.760	-6.579	0.000
39	C	-1.256	3.355	0.000
40	C	-2.469	5.462	0.000
41	C	4.454	1.007	0.000
42	C	6.615	0.622	0.000
43	C	3.025	0.969	0.000
44	C	5.178	2.198	0.000
45	C	4.968	-5.507	0.000
46	C	-4.968	5.507	0.000
47	C	5.307	4.700	0.000
48	C	-5.307	-4.700	0.000
49	H	-0.702	-4.937	0.000
50	H	0.702	4.937	0.000
51	H	5.205	-1.021	0.000
52	H	-5.205	1.021	0.000
53	C	-4.454	-1.007	0.000
54	C	-6.615	-0.622	0.000
55	C	-3.025	-0.969	0.000
56	C	-5.178	-2.198	0.000
57	C	3.745	-3.390	0.000
58	C	-3.745	3.390	0.000
59	C	3.150	3.489	0.000
60	C	-3.150	-3.489	0.000
61	H	-4.760	6.579	0.000
62	H	-5.550	5.243	0.888
63	H	-5.550	5.243	-0.888
64	H	-5.052	-5.284	-0.889
65	H	-6.369	-4.451	0.000
66	H	-5.052	-5.284	0.889
67	H	2.528	-6.545	0.000
68	H	-2.528	6.545	0.000

Table SI-7. Coordinates (in Å) of optimized $X_8 + NH_4^+$ octamer.

number	atom	x	y	z
1	N	-3.485	0.782	-1.386
2	N	0.796	3.447	-1.430
3	N	-0.796	-3.447	-1.430
4	N	5.537	-1.890	-1.809
5	N	-5.537	1.890	-1.809
6	N	1.898	5.504	-1.836
7	N	-1.898	-5.504	-1.836
8	N	3.094	-4.448	-1.632
9	N	-3.094	4.448	-1.632
10	N	4.473	3.087	-1.561
11	N	-4.473	-3.087	-1.561
12	O	5.451	0.404	-1.534
13	O	-5.451	-0.404	-1.534
14	O	-0.405	5.400	-1.630
15	O	0.405	-5.400	-1.630
16	O	1.466	-1.856	-1.074
17	O	-1.466	1.856	-1.074
18	O	1.867	1.434	-1.081
19	O	-1.867	-1.434	-1.081
20	H	4.277	-6.210	-1.937
21	H	-4.277	6.210	-1.937
22	H	6.232	4.286	-1.827
23	H	-6.232	-4.286	-1.827
24	H	2.986	0.123	-1.248
25	H	-2.986	-0.123	-1.248
26	H	-0.106	2.950	-1.299
27	H	0.106	-2.950	-1.299
28	C	3.440	-3.107	-1.600
29	C	4.251	-5.131	-1.851
30	C	2.688	-1.934	-1.342
31	C	4.823	-3.077	-1.801
32	C	-3.440	3.107	-1.600
33	C	-4.251	5.131	-1.851
34	C	-2.688	1.934	-1.342
35	C	-4.823	3.077	-1.801
36	C	3.127	3.419	-1.570
37	C	5.151	4.249	-1.772
38	C	1.953	2.651	-1.347
39	C	3.090	4.798	-1.785
40	C	7.009	-1.897	-1.971
41	C	-7.009	1.897	-1.971
42	C	1.907	6.974	-2.010
43	C	-1.907	-6.974	-2.010
44	H	2.132	-4.824	-1.551
45	H	-2.132	4.824	-1.551
46	H	4.857	2.130	-1.467
47	H	-4.857	-2.130	-1.467
48	C	-3.127	-3.419	-1.570
49	C	-5.151	-4.249	-1.772
50	C	-1.953	-2.651	-1.347
51	C	-3.090	-4.798	-1.785
52	C	4.864	-0.693	-1.580
53	C	-4.864	0.693	-1.580
54	C	0.699	4.823	-1.638
55	C	-0.699	-4.823	-1.638
56	H	-7.278	2.749	-2.597
57	H	-7.482	2.000	-0.990
58	H	-7.311	0.961	-2.441
59	H	-0.945	-7.279	-2.421
60	H	-2.719	-7.234	-2.691
61	H	-2.077	-7.453	-1.040
62	H	7.311	-0.961	-2.441
63	H	7.278	-2.749	-2.597
64	H	7.482	-2.000	-0.990
65	H	2.719	7.234	-2.691
66	H	2.077	7.453	-1.040
67	H	0.945	7.279	-2.421
68	N	6.421	-2.502	1.352
69	N	-6.421	2.502	1.352
70	N	0.111	5.828	1.466
71	N	-0.111	-5.828	1.466
72	N	4.330	-3.297	1.656
73	N	-4.330	3.297	1.656
74	N	3.304	4.308	1.688
75	N	-3.304	-4.308	1.688
76	O	5.061	2.050	1.606
77	O	-5.061	-2.050	1.606
78	O	-2.043	5.001	1.476
79	O	2.043	-5.001	1.476
80	N	2.504	6.389	1.326
81	O	1.962	-1.316	2.131
82	O	-1.962	1.316	2.131
83	O	1.340	1.940	2.144
84	O	-1.340	-1.940	2.144
85	H	5.986	-4.605	1.269
86	H	-5.986	4.605	1.269
87	H	4.611	5.966	1.309
88	H	-4.611	-5.966	1.309
89	H	2.828	1.024	2.038
90	H	-2.828	-1.024	2.038
91	N	-2.504	-6.389	1.326
92	H	-1.017	2.768	1.961
93	H	1.017	-2.768	1.961
94	C	4.257	-1.914	1.756
95	C	5.637	-3.591	1.413
96	C	3.162	-1.028	1.961
97	C	5.563	-1.460	1.563
98	C	-4.257	1.914	1.756
99	C	-5.637	3.591	1.413
100	C	-3.162	1.028	1.961
101	C	-5.563	1.460	1.563
102	N	3.578	0.316	1.922
103	C	1.919	4.229	1.750
104	C	3.596	5.613	1.431
105	C	1.033	3.137	1.940
106	C	1.463	5.528	1.520
107	C	7.250	0.360	1.268
108	C	-7.250	-0.360	1.268
109	C	-0.365	7.194	1.160
110	C	0.365	-7.194	1.160
111	H	3.520	-3.943	1.669
112	H	-3.520	3.943	1.669
113	N	-3.578	-0.316	1.922
114	H	3.958	3.504	1.734
115	H	-3.958	-3.504	1.734
116	C	-1.919	-4.229	1.750
117	C	-3.596	-5.613	1.431
118	C	-1.033	-3.137	1.940
119	C	-1.463	-5.528	1.520
120	C	4.853	0.826	1.689
121	C	-4.853	-0.826	1.689
122	C	-0.821	4.798	1.589
123	C	0.821	-4.798	1.589
124	N	-0.310	3.526	1.847
125	H	-7.935	0.467	1.459
126	H	-7.478	-1.206	1.919
127	H	-7.315	-0.671	0.221
128	H	0.686	-7.239	0.115
129	H	-0.463	-7.883	1.331
130	H	1.205	-7.433	1.815
131	H	7.315	0.671	0.221
132	H	7.935	-0.467	1.459
133	H	7.478	1.206	1.919
134	H	0.463	7.883	1.331
135	N	0.310	-3.526	1.847
136	H	-1.205	7.433	1.815
137	H	-0.686	7.239	0.115
138	N	5.878	-0.110	1.555
139	N	-5.878	0.110	1.555
140	N	3.485	-0.782	-1.386
141	N	5.327	-4.334	-1.951
142	N	-5.327	4.334	-1.951
143	N	4.346	5.315	-1.905
144	N	-4.346	-5.315	-1.905
145	N	0.000	0.000	0.538
146	H	-0.535	-0.639	1.147
147	H	-0.631	0.551	-0.064
148	H	0.631	-0.551	-0.064
149	H	0.535	0.639	1.147

Table SI-8. Coordinates (in Å) of optimized $(ho^5U)_8 + NH_4^+$ octamer.

number	atom	x	y	z
1	H	7.832	-1.241	2.137
2	H	7.558	-0.140	0.749
3	H	6.228	-2.823	1.715
4	H	-0.500	7.328	2.267
5	C	2.508	4.091	1.458
6	N	0.191	3.493	1.527
7	N	3.576	-0.157	1.562
8	H	2.811	6.198	1.580
9	C	1.501	3.045	1.404
10	N	0.758	5.751	1.663
11	N	5.818	-0.761	1.771
12	C	2.091	5.387	1.573
13	C	4.131	-2.481	1.523
14	O	3.835	3.821	1.314
15	O	3.842	-3.803	1.377
16	H	0.108	7.449	0.591
17	C	3.111	-1.453	1.427
18	O	-1.461	5.091	1.635
19	O	5.192	1.471	1.709
20	C	5.432	-2.087	1.678
21	H	1.203	7.782	1.970
22	O	1.730	1.825	1.250
23	O	1.888	-1.661	1.227
24	C	0.365	7.175	1.620
25	C	7.250	-0.393	1.770
26	H	7.398	0.470	2.420
27	C	-0.252	4.801	1.613
28	C	4.889	0.265	1.684
29	H	4.085	2.873	1.496
30	H	-0.565	2.788	1.464
31	H	2.884	0.613	1.474
32	H	2.878	-4.029	1.508
33	H	-7.832	1.241	2.137
34	H	-7.558	0.140	0.750
35	H	-6.228	2.823	1.715
36	H	0.500	-7.328	2.266
37	C	-2.508	-4.091	1.458
38	N	-0.191	-3.493	1.527
39	N	-3.576	0.157	1.562
40	H	-2.811	-6.198	1.580
41	C	-1.501	-3.045	1.404
42	N	-0.758	-5.751	1.663
43	N	-5.818	0.761	1.771
44	C	-2.091	-5.387	1.573
45	C	-4.131	2.481	1.523
46	O	-3.835	-3.821	1.314
47	O	-3.842	3.803	1.377
48	H	-0.108	-7.449	0.591
49	C	-3.111	1.453	1.427
50	O	1.461	-5.091	1.635
51	O	-5.192	-1.471	1.709
52	C	-5.432	2.087	1.678
53	H	-1.203	-7.782	1.970
54	O	-1.730	-1.825	1.250
55	O	-1.888	1.661	1.227
56	C	-0.365	-7.175	1.620
57	C	-7.250	0.393	1.770
58	H	-7.398	-0.470	2.420
59	C	0.252	-4.801	1.613
60	C	-4.889	-0.265	1.684
61	H	-4.085	-2.873	1.496
62	H	0.565	-2.788	1.464
63	H	-2.884	-0.613	1.474
64	H	-2.878	4.029	1.508
65	H	6.594	4.555	-1.707
66	H	5.128	5.508	-2.077
67	H	6.491	2.279	-1.344
68	H	-5.003	5.336	-0.397
69	C	-0.991	4.672	-1.556
70	N	-2.255	2.651	-1.748
71	N	2.759	2.353	-1.799
72	H	-2.230	6.404	-1.431
73	C	-0.998	3.226	-1.655
74	N	-3.410	4.675	-1.612
75	N	4.789	3.482	-1.620
76	C	-2.192	5.326	-1.538
77	C	4.744	1.063	-1.488
78	O	0.159	5.384	-1.383
79	O	5.422	-0.099	-1.268
80	H	-5.434	4.996	-2.096
81	C	3.299	1.085	-1.637
82	O	-4.557	2.664	-1.657
83	O	2.787	4.650	-1.752
84	C	5.416	2.253	-1.485
85	H	-4.503	6.468	-1.696
86	O	0.027	2.501	-1.645
87	O	2.549	0.085	-1.612
88	C	-4.675	5.422	-1.438
89	C	5.552	4.735	-1.435
90	H	5.482	5.050	-0.388
91	C	-3.483	3.289	-1.672
92	C	3.408	3.573	-1.727
93	H	0.994	4.882	-1.599
94	H	-2.319	1.616	-1.757
95	H	1.728	2.426	-1.839
96	H	4.890	-0.915	-1.485
97	H	-6.594	-4.555	-1.707
98	H	-5.128	-5.508	-2.077
99	H	-6.491	-2.278	-1.344
100	H	5.003	-5.336	-0.397
101	C	0.991	-4.672	-1.556
102	N	2.255	-2.651	-1.748
103	N	-2.759	-2.353	-1.799
104	H	2.230	-6.404	-1.431
105	C	0.998	-3.226	-1.655
106	N	3.410	-4.675	-1.612
107	N	-4.789	-3.482	-1.620
108	C	2.192	-5.326	-1.537
109	C	-4.744	-1.063	-1.488
110	O	-0.159	-5.384	-1.383
111	O	-5.422	0.099	-1.268
112	H	5.434	-4.996	-2.096
113	C	-3.299	-1.085	-1.637
114	O	4.557	-2.664	-1.657
115	O	-2.787	-4.650	-1.752
116	C	-5.416	-2.253	-1.485
117	H	4.503	-6.468	-1.696
118	O	-0.027	-2.501	-1.645
119	O	-2.549	-0.085	-1.612
120	C	4.675	-5.422	-1.438
121	C	-5.552	-4.735	-1.435
122	H	-5.482	-5.050	-0.388
123	C	3.483	-3.289	-1.672
124	C	-3.408	-3.573	-1.727
125	H	-0.994	-4.882	-1.599
126	H	2.319	-1.616	-1.757
127	H	-1.728	-2.426	-1.839
128	H	-4.890	0.915	-1.485
129	N	0.000	0.000	-0.194
130	H	0.270	0.795	-0.789
131	H	0.787	-0.307	0.398
132	H	-0.270	-0.795	-0.789
133	H	-0.787	0.307	0.398

Figure SI-1. ^{1}H NMR spectrum of 1-benzyl-5-bromouracil in DMSO-d_6

7/29/2015 4:57:03 PM

Formula $C_{11}H_9BrN_2O_2$	***FW***	281.1054							
Acquisition Time (sec)	1.6384	***Comment***	proton	***Date***	29 Jul 2015 13:16:16			***Date Stamp***	29 Jul 2015 13:16:16
File Name	E:\NMR\KL939\1\fid			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	181.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3068.6233	***Spectrum Type***	STANDARD
Sweep Width (Hz)	9999.39	***Temperature (degree C)***	25.000						

^{1}H NMR (500 MHz): δ = 4.80 (s, 2H, M01), 7.05 - 7.48 (m, 5H, M02), 8.30 (s, 1H, M03), 11.81 (br. s., 1H, M04) ppm

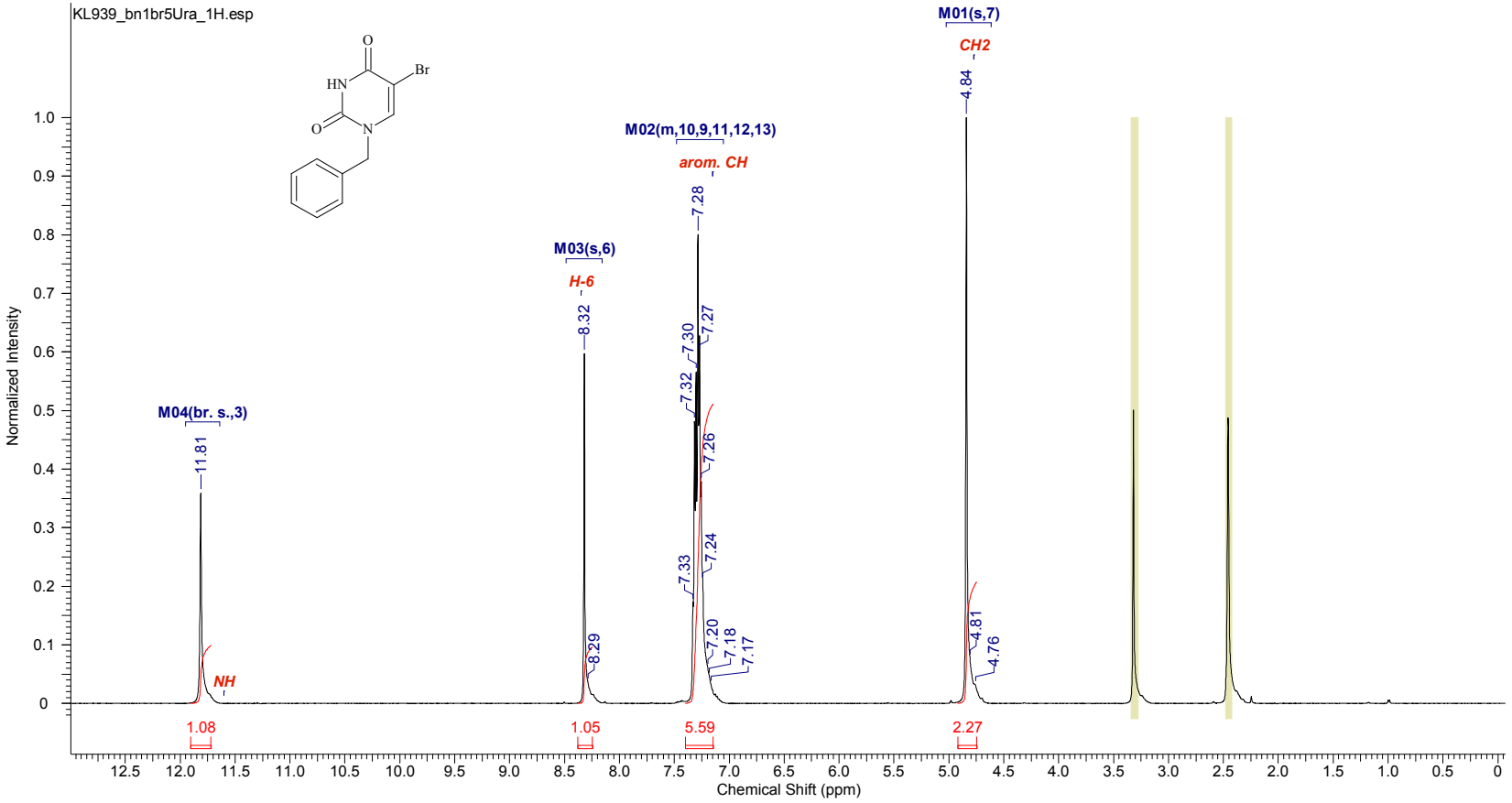


Figure SI-2. ^{1}H NMR spectrum of 1-benzyl-5-bromouracil in DMSO-d_6 after deuteration

Formula $C_{11}H_9BrN_2O_2$	***FW***	281.1054							
Acquisition Time (sec)	1.6384	***Comment***	proton	***Date***	30 Jul 2015 09:23:44			***Date Stamp***	30 Jul 2015 09:23:44
File Name	E:\NMR\KL939D2O\1\fid			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	181.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3077.1682	***Spectrum Type***	STANDARD
Sweep Width (Hz)	9999.39	***Temperature (degree C)***	25.000						

^{1}H NMR (500 MHz): δ = 4.83 (s, 2H, M01), 7.04 - 7.28 (m, 3H, M02), 7.28 - 7.49 (m, 2H, M03), 8.26 (s, 1H, M04) ppm

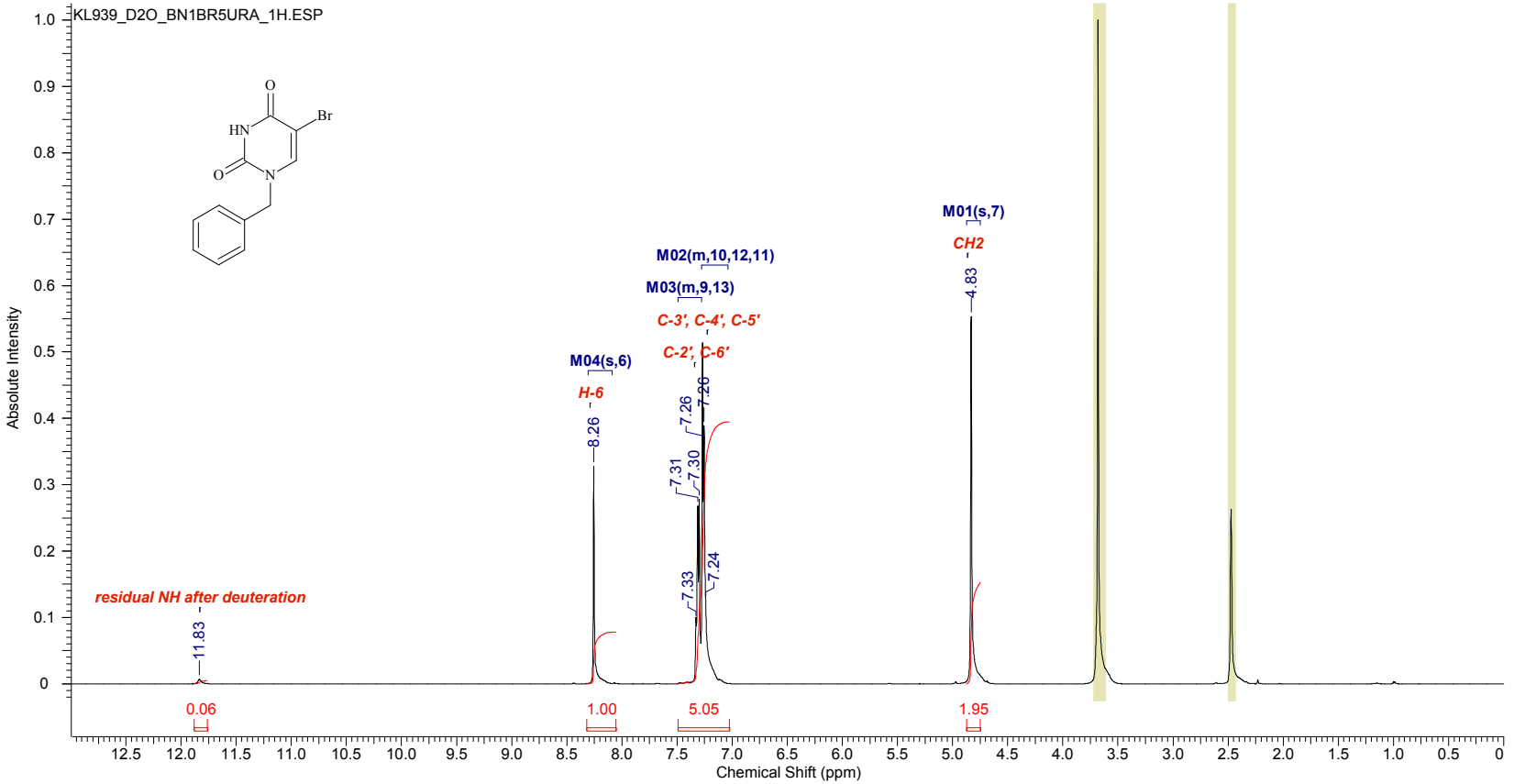


Figure SI-3. ^{13}C NMR spectrum of 1-benzyl-5-bromouracil

Formula $C_{11}H_9BrN_2O_2$	***FW***	281.1054							
Acquisition Time (sec)	1.1108	***Comment***	jmod	***Date***	29 Jul 2015 13:20:32			***Date Stamp***	29 Jul 2015 13:20:32
File Name	E:\NMR\KL939\2\fid			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	316
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	jmod
Receiver Gain	5792.60	***SW(cyclical) (Hz)***	29498.53	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	14093.9150
Spectrum Type	APT	***Sweep Width (Hz)***	29497.63	***Temperature (degree C)***	25.000				

^{13}C NMR (126 MHz): δ = 50.8 (M01), 95.2 (M02), 127.5 (M03), 127.8 (M04), 128.7 (M05), 136.5 (M06), 145.2 (M07), 150.4 (M08), 159.7 (M09) ppm

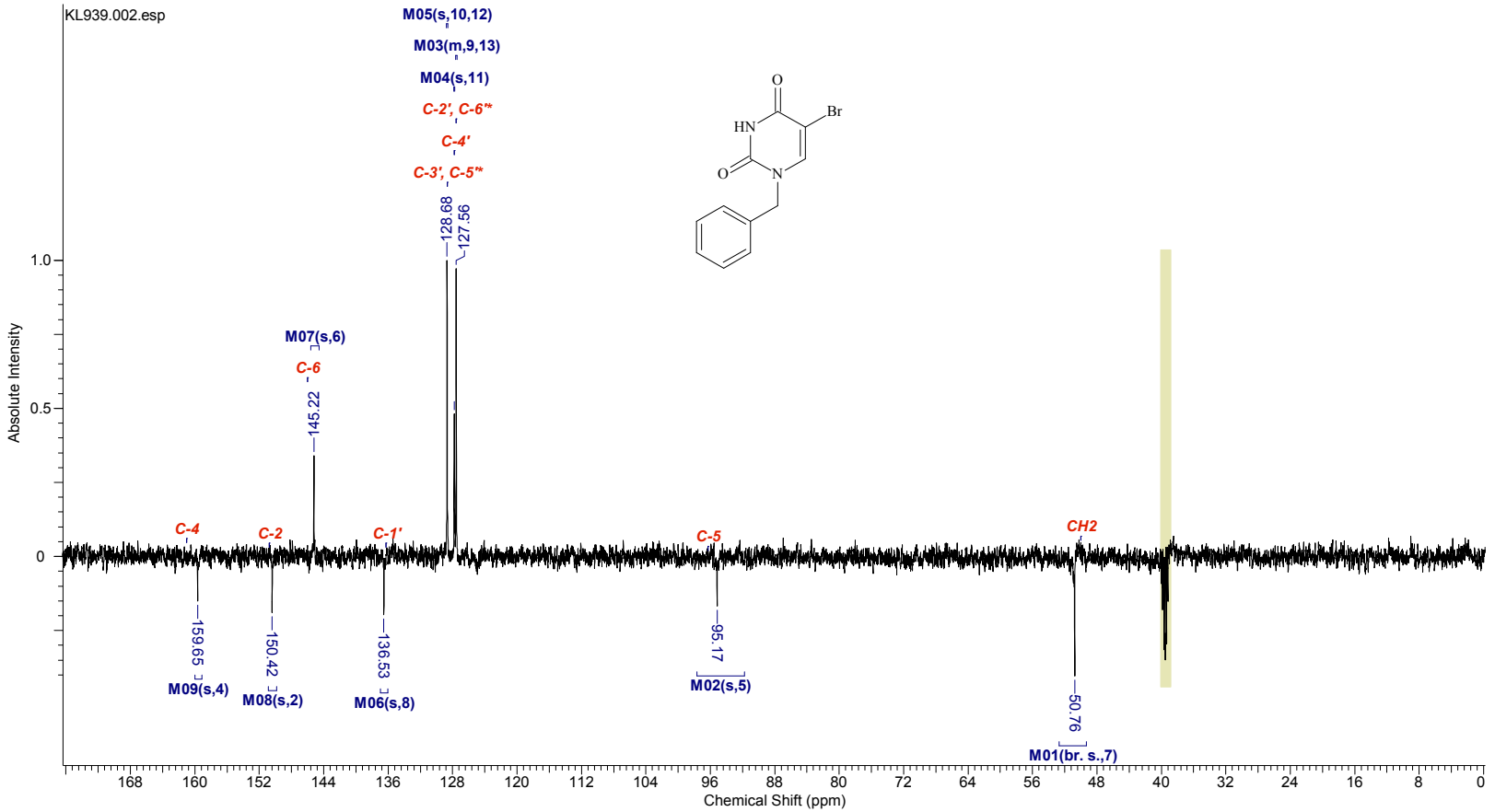


Figure SI-4. ^{1}H NMR spectrum of 1,3-dibenzyl-5-bromouracil in DMSO-d_6

Formula $C_{18}H_{15}BrN_2O_2$				***FW***	371.2279				
Acquisition Time (sec)	1.6384	***Comment***	proton	***Date***	29 Jul 2015 13:56:48			***Date Stamp***	29 Jul 2015 13:56:48
File Name	E:\NMR\EG111 2\1\fid			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	161.30	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3086.9338	***Spectrum Type***	STANDARD
Sweep Width (Hz)	9999.39	***Temperature (degree C)***	25.000						

^{1}H NMR (500 MHz): δ = 4.96 (s, 2H, M01), 5.02 (s, 2H, M02), 7.14 - 7.38 (m, 10H, M03), 8.50 (s, 1H, M04) ppm

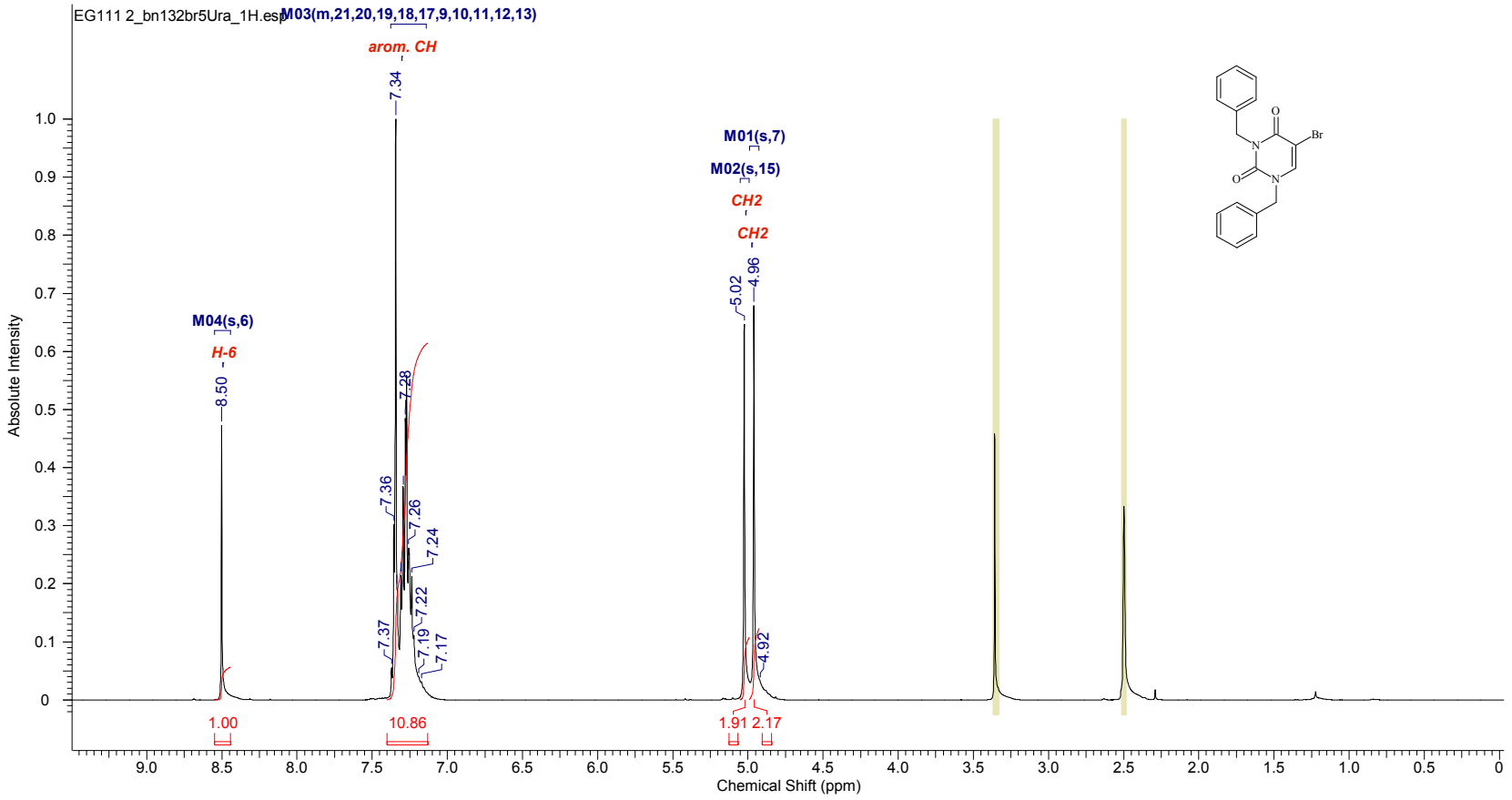


Figure SI-5. ^{13}C NMR spectrum of 1,3-dibenzyl-5-bromouracil in DMSO-d_6

7/29/2015 5:31:07 PM

Formula $C_{18}H_{15}BrN_2O_2$		***FW***	371.2279						
Acquisition Time (sec)	1.1108	***Comment***	jmod	***Date***	29 Jul 2015 13:58:56			***Date Stamp***	29 Jul 2015 13:58:56
File Name	E:\NMR\EG111 2\2\fid			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	437
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	jmod
Receiver Gain	5792.60	***SW(cyclical) (Hz)***	29498.53	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	14093.9150
Spectrum Type	APT	***Sweep Width (Hz)***	29497.63	***Temperature (degree C)***	25.000				

^{13}C NMR (126 MHz): δ = 45.1 (M01), 52.1 (M02), 94.5 (M03), 127.3 (M04), 127.6 (M05), 127.7 (M06), 127.9 (M07), 128.4 (M08), 128.7 (M09), 136.3 (M10), 136.6 (M11), 144.2 (M12), 150.6 (M13), 158.8 (M14) ppm

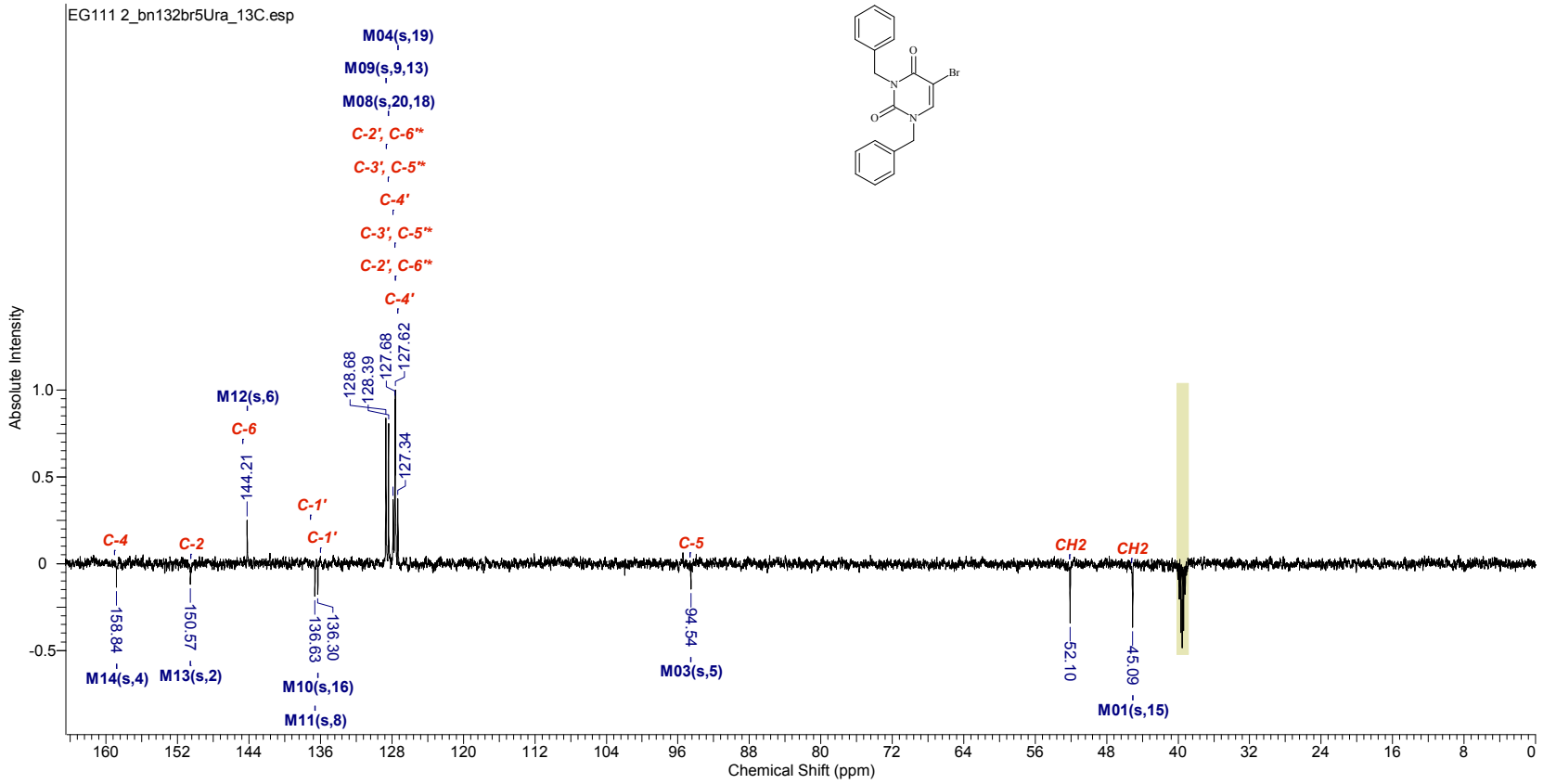


Figure SI-6. ^{1}H NMR spectrum of 1-benzyl-5-hydroxyuracil in DMSO-d_6

Formula $C_{11}H_{10}N_2O_3$	***FW***	218.2087							
Acquisition Time (sec)	1.6384	***Comment***	proton	***Date***	29 Jul 2015 14:33:04			***Date Stamp***	29 Jul 2015 14:33:04
File Name	E:\NMR\EG121\1\fid			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	181.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3080.2202	***Spectrum Type***	STANDARD
Sweep Width (Hz)	9999.39	***Temperature (degree C)***	25.000						

^{1}H NMR (500 MHz): δ = 4.78 (br. s., 3H, M01), 7.19 (br. s., 2H, M02), 7.22 - 7.36 (m, 6H, M03), 8.66 (br. s., 1H, M04), 11.46 (br. s., 1H, M05) ppm

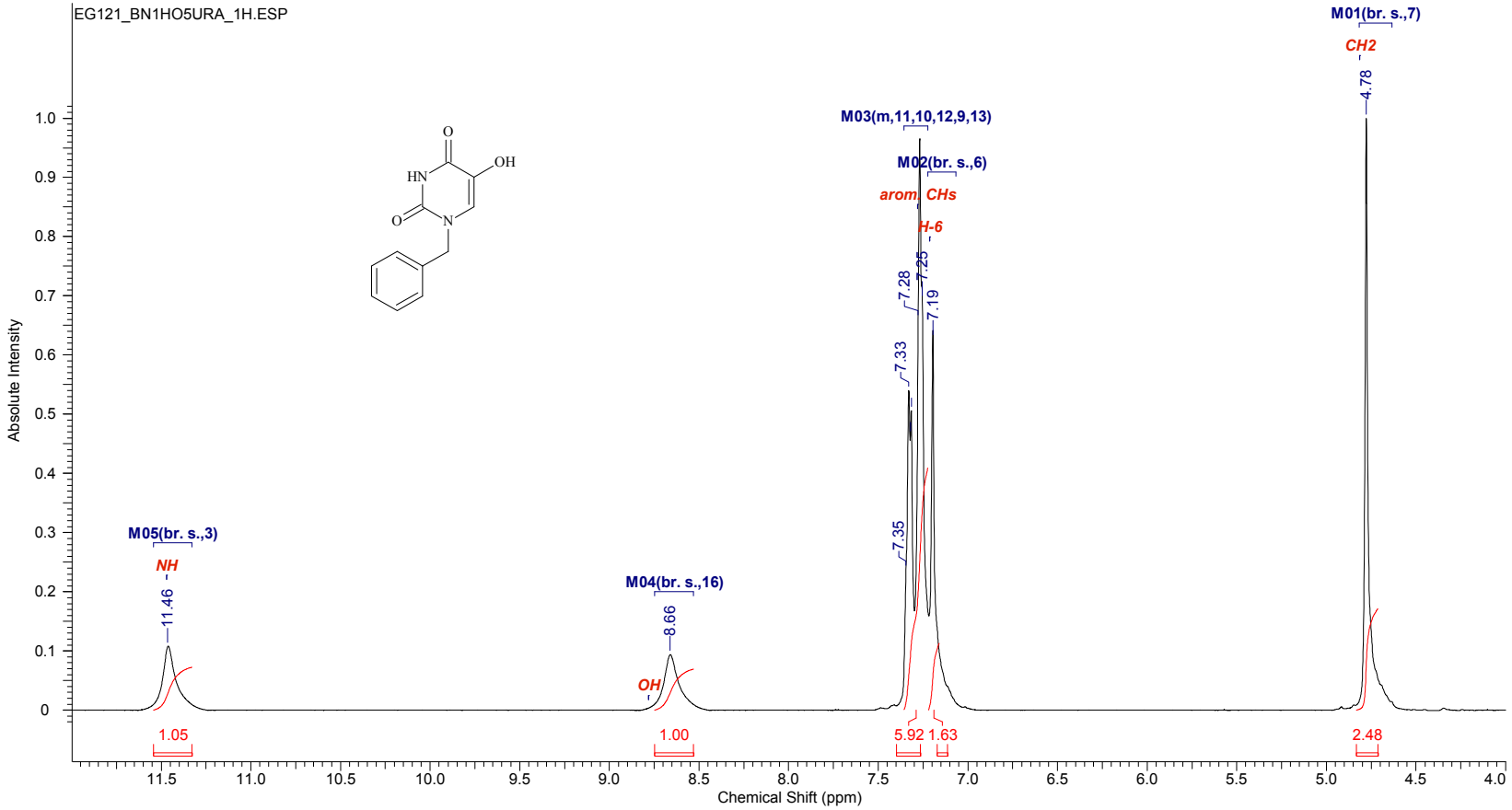


Figure SI-7. ^{1}H NMR spectrum of 1-benzyl-5-hydroxyuracil in DMSO-d_6 after deuteration

Formula $C_{11}H_{10}N_2O_3$	***FW***	218.2087							
Acquisition Time (sec)	1.6384	***Comment***	proton	***Date***	30 Jul 2015 09:13:04			***Date Stamp***	30 Jul 2015 09:13:04
File Name	E:\NMR\EG121D2O\1\fid			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	psm	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	161.30	***SW(cyclical) (Hz)***	10000.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3087.5444	***Spectrum Type***	STANDARD
Sweep Width (Hz)	9999.39	***Temperature (degree C)***	25.000						

^{1}H NMR (500 MHz): δ = 4.77 (s, 2H, M01), 7.17 (s, 1H, M02), 7.20 - 7.37 (m, 5H, M03) ppm

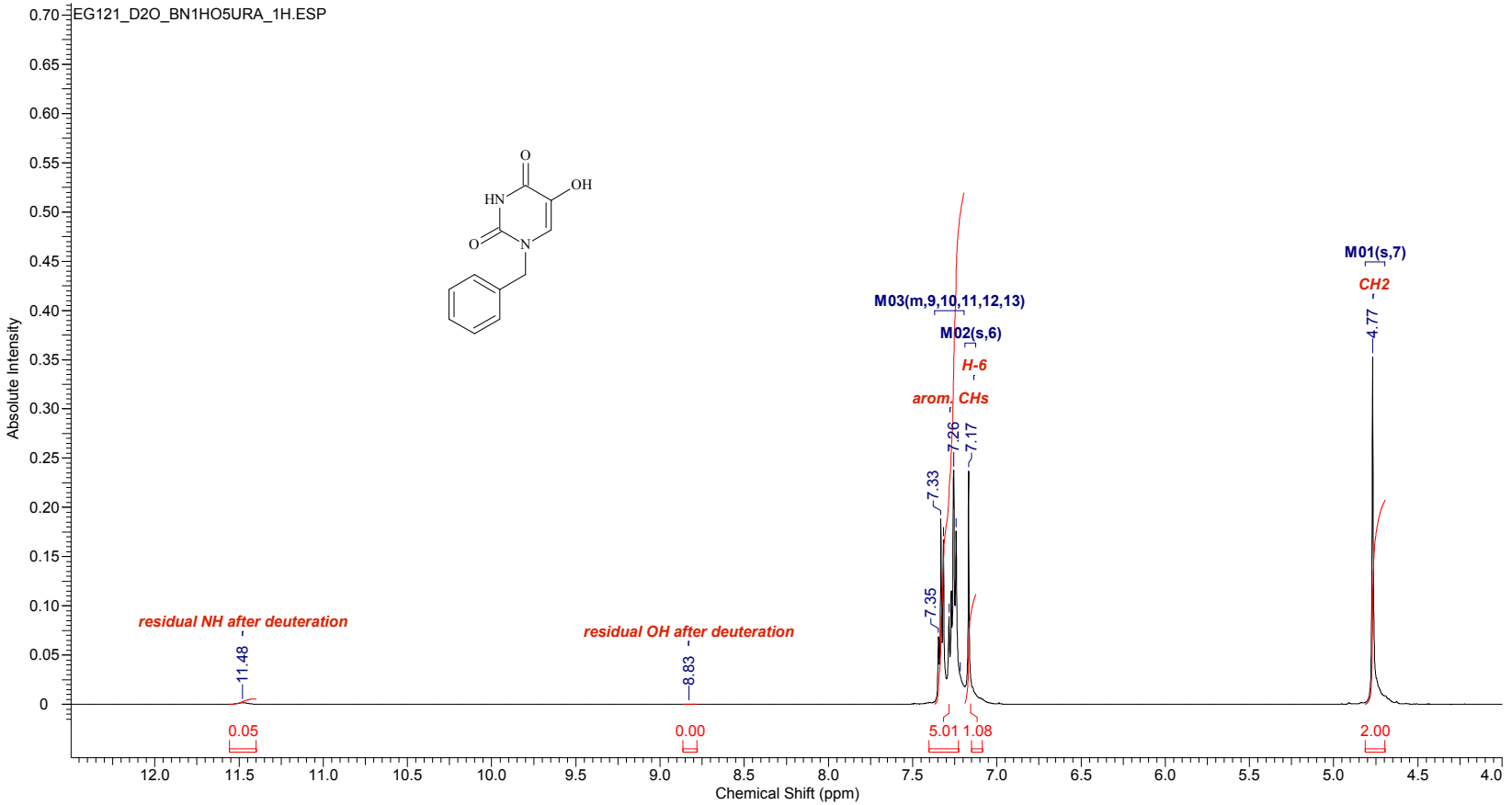
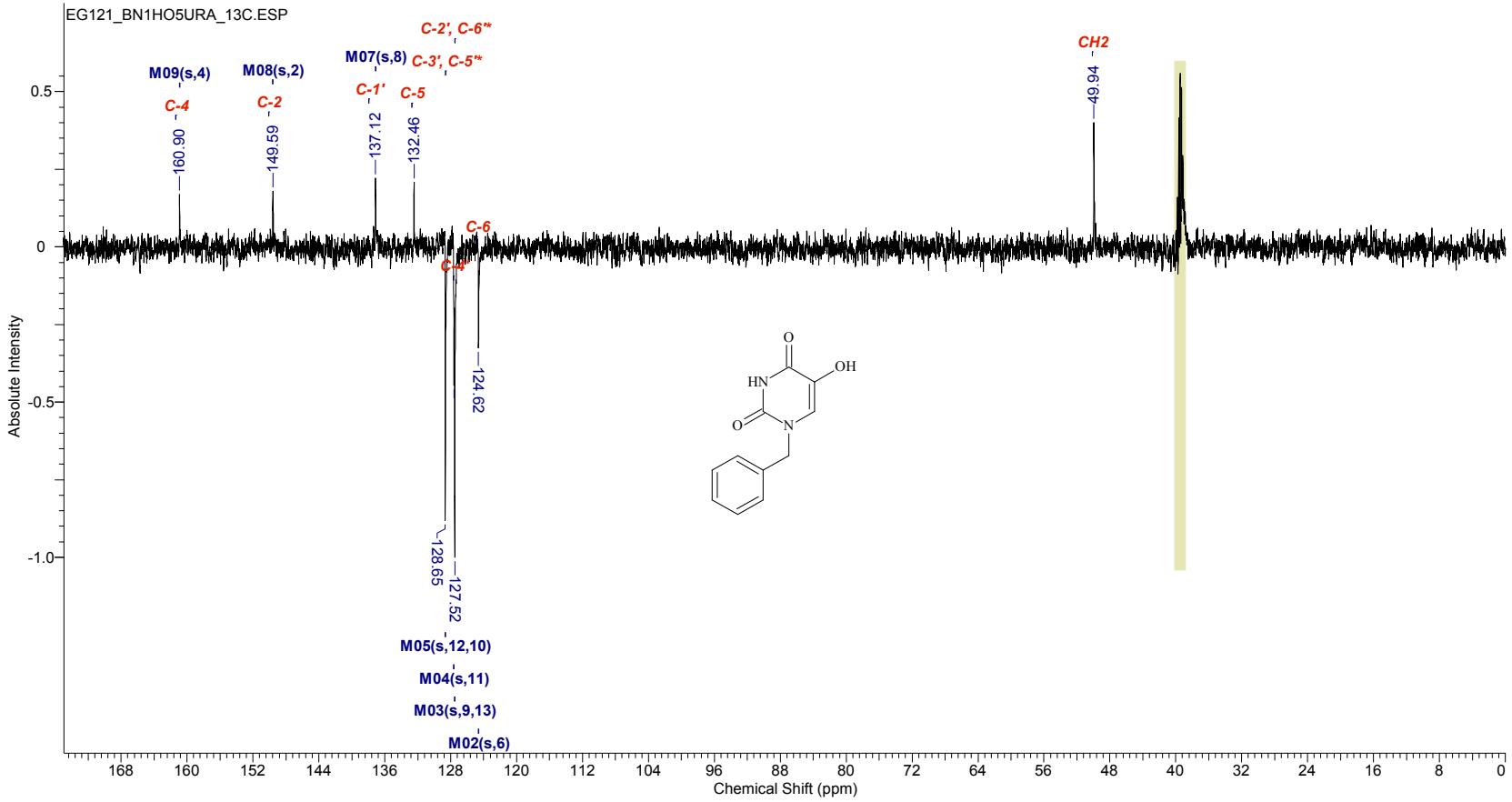


Figure SI-8. ^{13}C NMR spectrum of 1-benzyl-5-hydroxyuracil in DMSO-d_6

7/30/2015 11:14:24 AM

Formula $C_{11}H_{10}N_2O_3$	***FW***	218.2087							
Acquisition Time (sec)	1.1108	***Comment***	jmod	***Date***	29 Jul 2015 14:37:20			***Date Stamp***	29 Jul 2015 14:37:20
File Name	E:\NMR\EG121\2\fid			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	447
Origin	spect	***Original Points Count***	32768	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	jmod
Receiver Gain	8192.00	***SW(cyclical) (Hz)***	29498.53	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	14093.9150
Spectrum Type	APT	***Sweep Width (Hz)***	29497.63	***Temperature (degree C)***	25.000				

^{13}C NMR (126 MHz): δ = 49.9 (M01), 124.6 (M02), 127.5 (M03), 127.6 (M04), 128.7 (M05), 132.5 (M06), 137.1 (M07), 149.6 (M08), 160.9 (M09) ppm



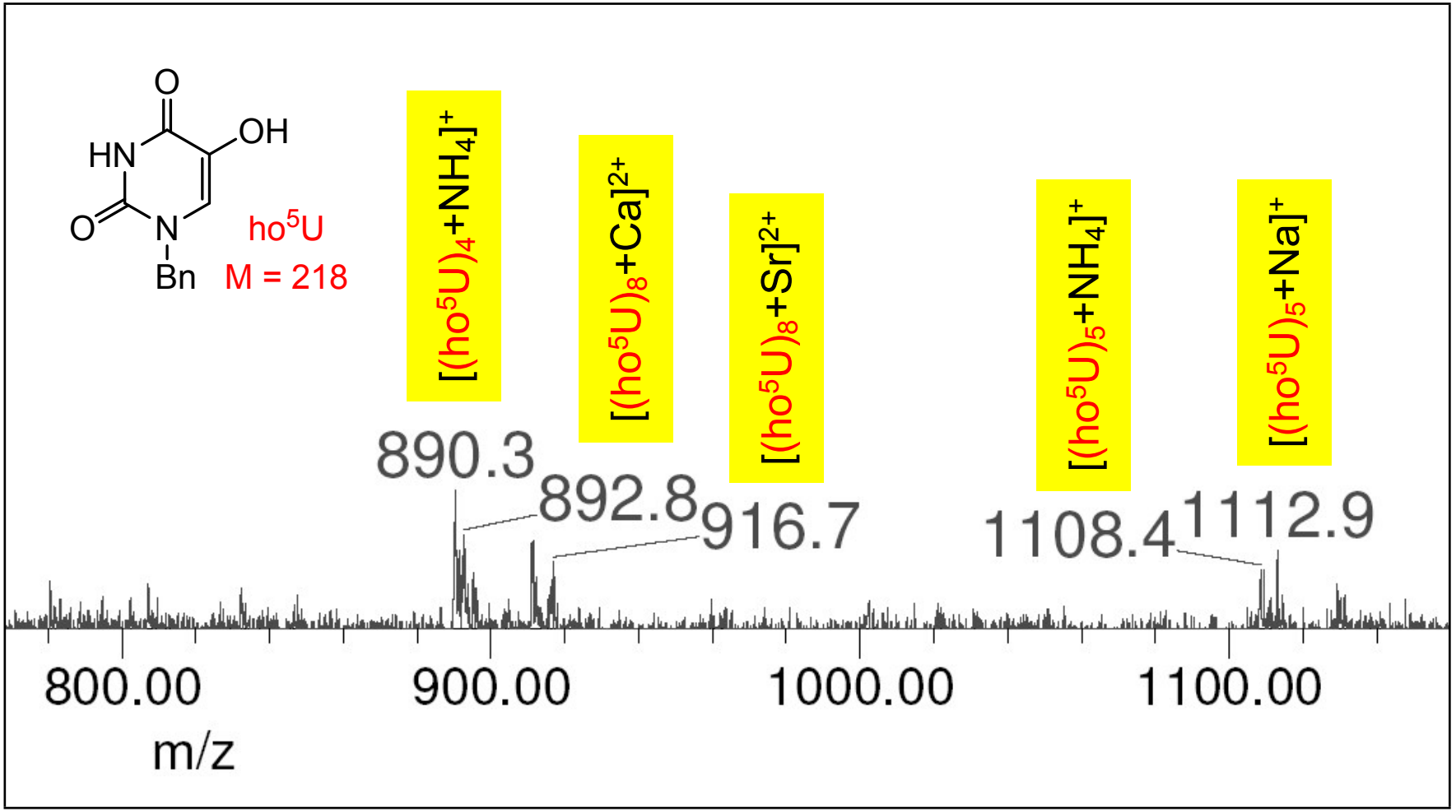


Figure SI-9. Zoomed nano-ESI-MS spectrum of 1-benzyl-5-hydroxyuracil (ho^{5}U, M = 218) in the presence of 100 µM $Sr(NO_3)_2$. The calcium and sodium adducts are contaminants from previous measurements