

Electronic supplementary information

Internal electric fields in methanol [MeOH]₂₋₆ clusters

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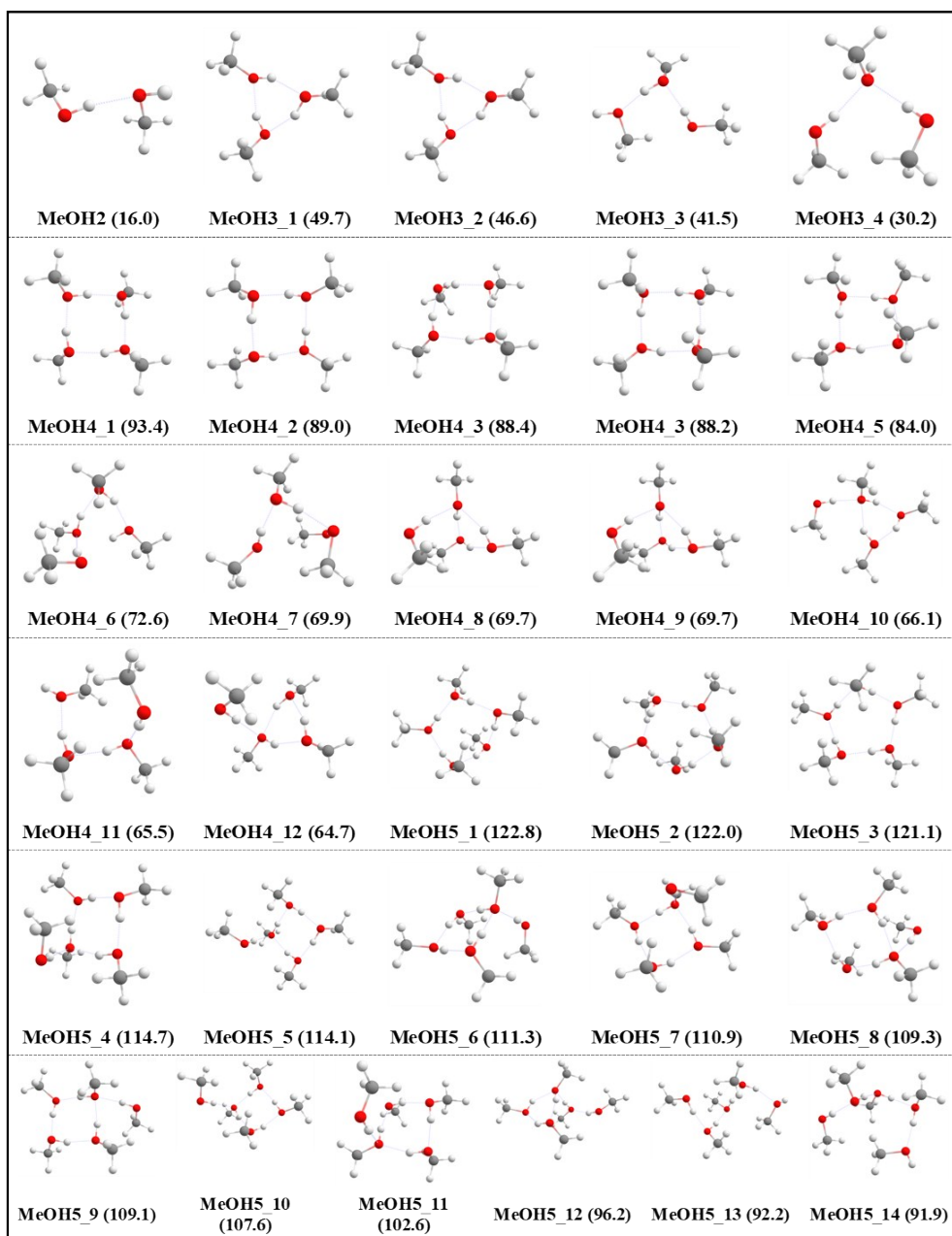


Fig. S1. Structures of [MeOH]_n [*n*=2-5] clusters calculated at MP2/aug-cc-pVDZ level. The ZPE and BSSE corrected stabilization energies (kJ mol⁻¹) are shown in parenthesis.

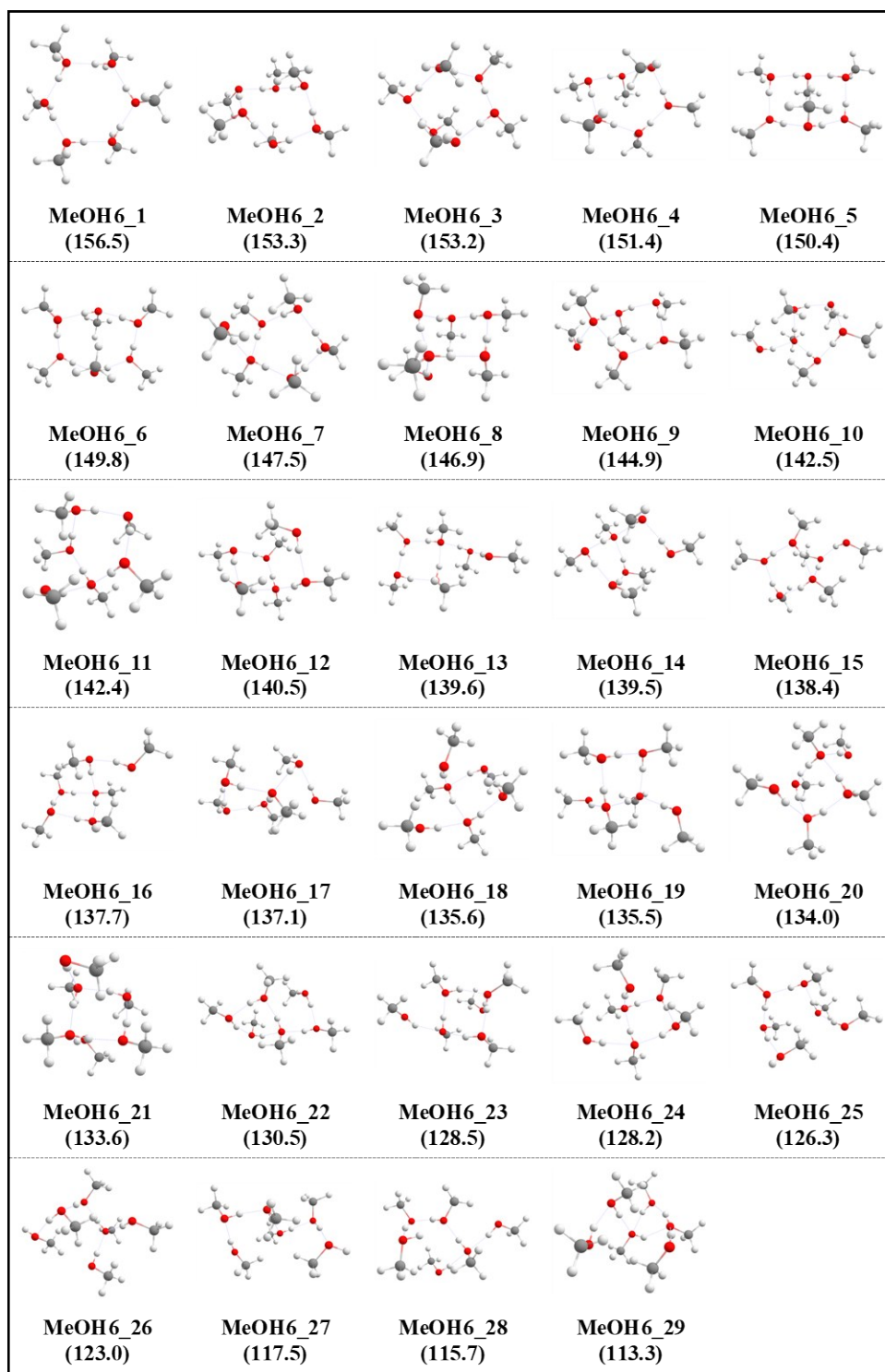


Fig. S2. Structures of $[\text{MeOH}]_6$ cluster calculated at MP2/aug-cc-pVDZ level. The ZPE and BSSE corrected stabilization energies (kJ mol^{-1}) are shown in parenthesis.

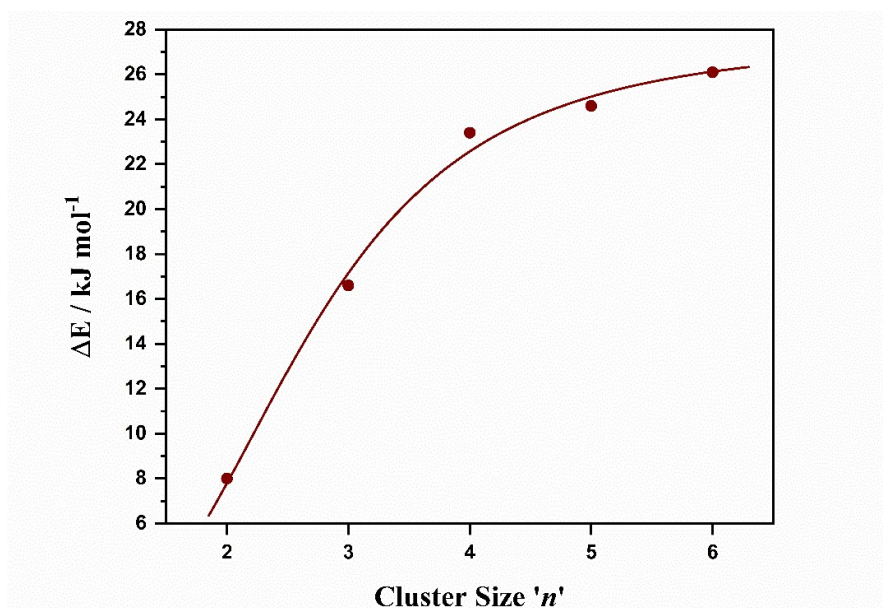


Fig. S3. Plot of stabilization energy per each methanol molecule for the most stable structure for a given cluster size. The solid line is a non-linear least square fit to the data points using a Hill equation [$\Delta E = \Delta E_{max} \cdot [n^l / (n^l + k^l)]$]. Where ΔE is the stabilization energy; ΔE_{max} is the maximum stabilization energy; n is the cluster size; l is Hill-coefficient. The R^2 value is 0.989 with ΔE_{max} value of 27.5 kJ mol⁻¹.

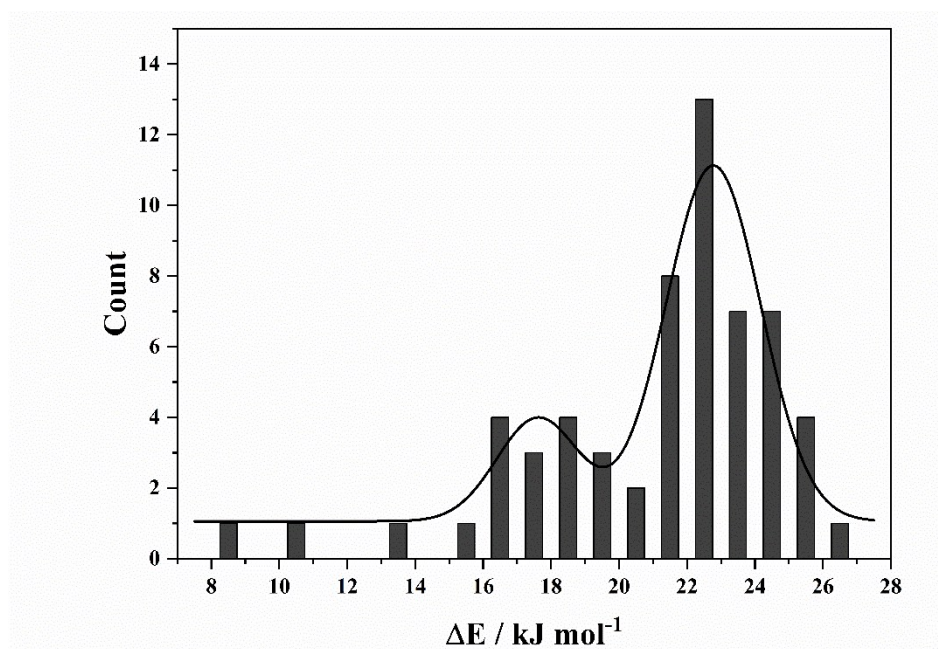


Fig. S4. Distribution plot of stabilization energy per methanol molecule for cluster sizes up to six. Note the bimodal distribution in the stabilization energies.

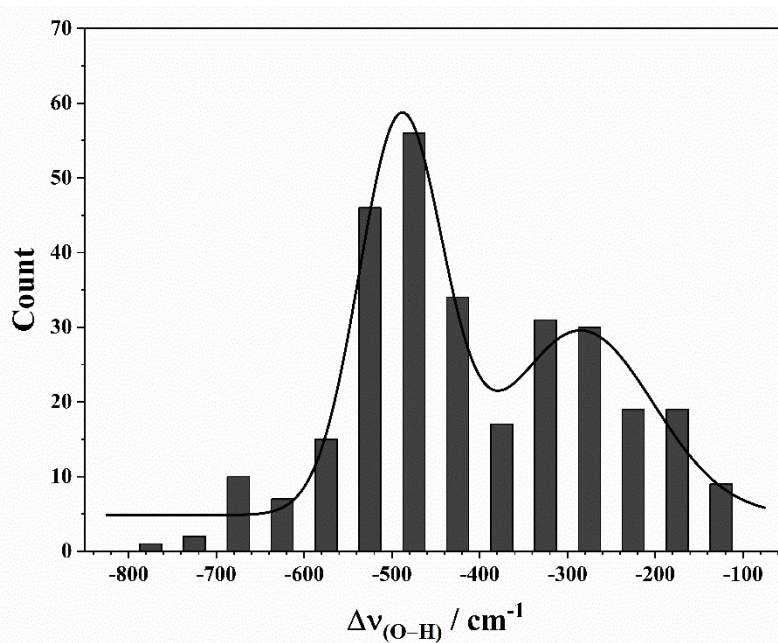


Fig. S5. Distribution plot of shifts (unscaled) in the hydrogen bonded O–H stretching frequencies for all the methanol clusters considered. Note the bimodal distribution in the frequency shifts.

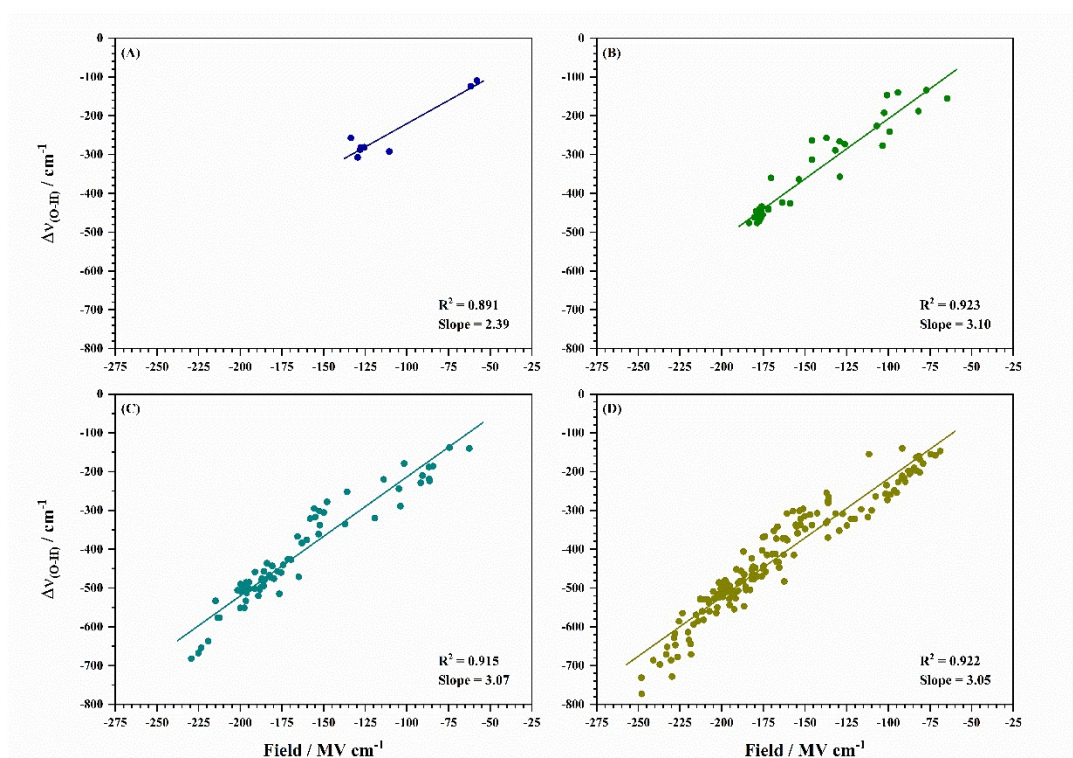


Fig. S6. Plot of the red-shift in the O–H stretching frequencies against the corresponding electric fields for (A) trimer, (B) tetramer, (C) pentamer and (D) hexamer. The straight lines are linear fits to the data

points with Stark tuning rates of 2.39, 3.10, 3.07 and 3.05 $\text{cm}^{-1} (\text{MV cm}^{-1})^{-1}$ and residuals 46, 85, 89 and 114 cm^{-1} , for trimer, tetramer, pentamer and hexamer, respectively.

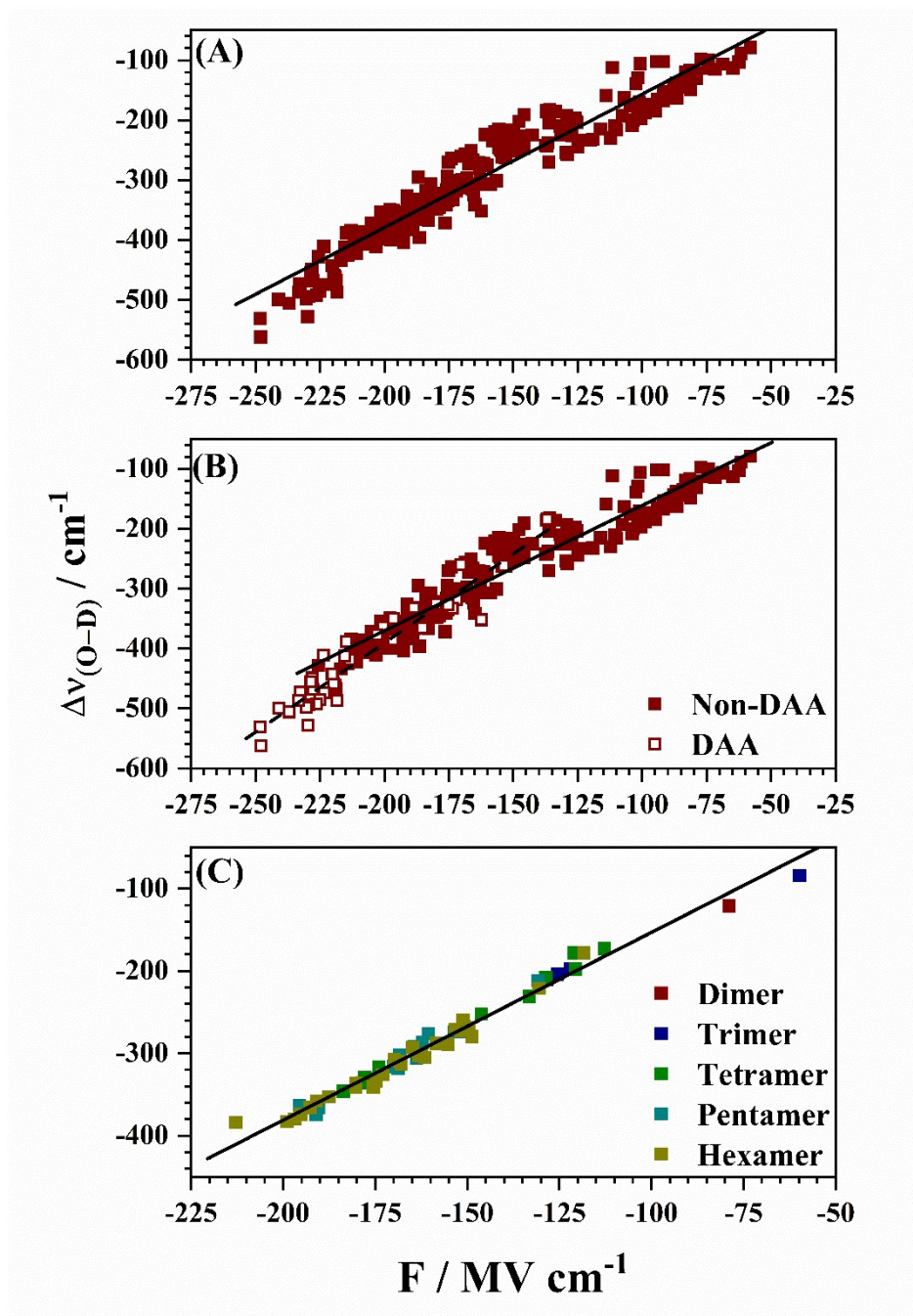


Fig. S7. (A) Plot of the red-shift in the individual O–D stretching frequencies against the corresponding electric fields. The solid is a linear fit to the data points with R^2 value of 0.927 with slope of 2.23 and residuals of 82 cm^{-1} . (B) Plot of the red-shift in the individual O–D stretching frequencies against the corresponding electric fields for non-DAA (solid circles) and DAA (open circles). The solid and dashed lines are linear fits to the non-DAA and DAA data points with R^2 value, slope and residuals of 0.925, 2.09, 73 cm^{-1} and 0.903, 2.97, 73 cm^{-1} , respectively. (C) Plot of the average red-shift in the O–D stretching frequency for each cluster

against the average electric field. The solid line is a linear fit to the data points with R^2 value of 0.980 with slope of 2.28 and residuals of 26 cm^{-1} .

Table S1 ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), total OH only and total OH + CH electric fields and average OH electric field (MV cm⁻¹) for neutral methanol clusters (n=2-6) calculated at MP2/aug-cc-pVDZ level of theory. Vibrational frequency shifts listed in Columns (a) and (b) are the average of selectively labelled hydrogen bonded O–H group in the deuterated methanol cluster and O–D group in the methanol cluster at the same level of theory.

Structure	ΔE	Total field		Average	Average	Average OH Field
		OH only	OH + CH	$ \Delta\nu_{\text{O-H}} _{\text{H-bond}}$	$ \Delta\nu_{\text{O-D}} _{\text{H-bond}}$	
MeOH2	-16.0	-78.90	-78.90	167	121	-78.90
MeOH3_1	-49.7	-464.07	-464.07	292	211	-128.39
MeOH3_2	-46.6	-376.53	-376.53	281	204	-125.51
MeOH3_3	-41.5	-244.16	-293.46	275	198	-122.08
MeOH3_4	-30.2	-119.67	-119.67	116	84	-59.84
MeOH4_1	-93.4	-734.37	-734.37	476	346	-183.59
MeOH4_2	-89.0	-713.95	-713.95	462	336	-178.49
MeOH4_3	-88.4	-711.50	-711.50	453	329	-177.88
MeOH4_4	-88.2	-709.16	-709.16	456	331	-177.29
MeOH4_5	-84.0	-696.15	-696.15	436	317	-174.04
MeOH4_6	-72.6	-514.54	-562.17	287	208	-128.64
MeOH4_7	-69.9	-438.56	-498.95	348	252	-146.19
MeOH4_8	-69.7	-482.48	-482.48	274	198	-120.62
MeOH4_9	-69.7	-482.55	-482.55	274	198	-120.64
MeOH4_10	-66.1	-483.74	-483.74	246	178	-120.94
MeOH4_11	-65.5	-399.56	-437.26	320	231	-133.19
MeOH4_12	-64.7	-450.99	-450.99	239	173	-112.75
MeOH5_1	-122.8	-955.18	-955.18	503	374	-191.04
MeOH5_2	-122.0	-951.97	-951.97	504	366	-190.39
MeOH5_3	-121.1	-977.65	-977.65	499	363	-195.53
MeOH5_4	-114.7	-841.84	-897.90	416	302	-168.37
MeOH5_5	-114.1	-849.70	-849.70	435	316	-169.94
MeOH5_6	-111.3	-843.74	-843.74	437	318	-168.75
MeOH5_7	-110.9	-822.61	-822.61	402	292	-164.52
MeOH5_8	-109.3	-803.08	-803.08	381	276	-160.62
MeOH5_9	-109.1	-810.76	-810.76	394	287	-162.15
MeOH5_10	-107.6	-819.17	-819.17	420	306	-163.83
MeOH5_11	-102.6	-768.20	-768.20	376	274	-153.64
MeOH5_12	-96.2	-653.93	-653.93	293	212	-130.79
MeOH5_13	-92.2	-602.33	-645.72	378	274	-150.58
MeOH5_14	-91.9	-599.72	-644.93	377	273	-149.93
MeOH6_1	-156.5	-1277.19	-1277.19	528	384	-212.86
MeOH6_2	-153.3	-1193.73	-1193.73	526	383	-198.96
MeOH6_3	-153.2	-1182.48	-1182.48	521	380	-196.91
MeOH6_4	-151.4	-1171.22	-1171.22	514	374	-195.20
MeOH6_5	-150.4	-1156.36	-1156.36	504	366	-192.73
MeOH6_6	-149.8	-1145.45	-1145.45	492	358	-190.91
MeOH6_7	-147.5	-1125.56	-1172.63	485	353	-187.59
MeOH6_8	-146.9	-1081.75	-1131.01	468	341	-180.29
MeOH6_9	-144.9	-1081.98	-1090.66	462	337	-180.33

MeOH6_10	-142.5	-1048.22	-1048.22	459	334	-174.70
MeOH6_11	-142.4	-1053.17	-1053.17	467	341	-175.53
MeOH6_12	-140.5	-1008.00	-1070.72	430	313	-168.00
MeOH6_13	-139.6	-1019.34	-1128.60	422	307	-169.89
MeOH6_14	-139.5	-1010.03	-1130.95	427	310	-168.34
MeOH6_15	-138.4	-989.21	-989.21	404	293	-164.87
MeOH6_16	-137.7	-978.96	-1014.76	417	303	-163.16
MeOH6_17	-137.1	-974.37	-974.37	417	303	-162.39
MeOH6_18	-135.6	-906.91	-1000.43	358	260	-151.15
MeOH6_19	-135.5	-949.79	-949.79	395	288	-158.30
MeOH6_20	-134.0	-919.44	-990.99	374	271	-153.24
MeOH6_21	-133.6	-905.80	-951.31	368	267	-150.97
MeOH6_22	-130.5	-931.23	-970.99	397	289	-155.20
MeOH6_23	-128.5	-897.55	-941.23	370	269	-149.59
MeOH6_24	-128.2	-892.68	-892.68	384	280	-148.78
MeOH6_25	-126.3	-864.90	-864.90	450	326	-172.98
MeOH6_26	-123.0	-807.74	-899.41	419	305	-161.55
MeOH6_27	-117.5	-758.84	-837.80	377	273	-151.77
MeOH6_28	-115.7	-783.02	-875.90	305	221	-130.50
MeOH6_29	-113.3	-709.78	-770.12	246	178	-118.30

Table S2 Unscaled vibrational frequencies (cm^{-1}) listed in Columns (a) and (b) are the selectively labelled hydrogen bonded O–H group in the deuterated methanol cluster and O–D group in the methanol cluster with their corresponding shifts and electric field (MV cm^{-1}) calculated at the MP2/aug-cc-pVDZ level of theory. The entries in red are due to DAA configuration.

Structure	$\nu_{\text{O-H}} _{\text{H-bond}}$ (a)	$\Delta\nu_{\text{O-H}} _{\text{H-bond}}$	$\nu_{\text{O-D}} _{\text{H-bond}}$ (b)	$\Delta\nu_{\text{O-D}} _{\text{H-bond}}$	Elec. Field
MeOH	3843		2798		
MeOH2	3675	-167	2677	-121	-78.90
MeOH3_1	3536	-307	2576	-222	-129.56
	3555	-287	2590	-208	-127.96
	3560	-282	2593	-205	-127.65
MeOH3_2	3561	-282	2594	-204	-125.50
	3562	-281	2595	-203	-125.52
	3561	-281	2594	-204	-125.52
MeOH3_3	3550	-292	2587	-210	-110.58
	3586	-257	2612	-186	-133.58
MeOH3_4	3719	-124	2709	-89	-61.66
	3734	-109	2719	-79	-58.02
MeOH4_1	3366	-476	2452	-346	-183.59
	3367	-476	2452	-346	-183.57
	3366	-476	2452	-346	-183.60
	3366	-476	2452	-346	-183.61
MeOH4_2	3394	-449	2471	-327	-178.20
	3366	-476	2453	-345	-178.77
	3394	-448	2471	-327	-178.20
	3366	-476	2452	-346	-178.78
MeOH4_3	3397	-446	2474	-324	-179.35
	3402	-441	2476	-322	-177.55
	3371	-472	2456	-342	-177.62
	3388	-455	2468	-330	-176.99
MeOH4_4	3379	-464	2462	-336	-176.56
	3381	-462	2462	-336	-180.30

	3386	-457	2466	-332	-176.12
	3401	-441	2476	-322	-176.18
MeOH4_5	3409	-434	2482	-316	-175.95
	3405	-438	2480	-318	-172.13
	3409	-434	2482	-316	-175.94
	3405	-438	2480	-318	-172.13
MeOH4_6	3703	-140	2696	-102	-94.28
	3602	-241	2624	-174	-99.12
	3530	-313	2571	-227	-145.77
	3388	-455	2471	-327	-175.38
MeOH4_7	3419	-424	2491	-307	-163.63
	3580	-263	2607	-191	-145.85
	3485	-357	2540	-258	-129.07
MeOH4_8	3401	-442	2480	-318	-172.02
	3655	-188	2661	-137	-81.93
	3651	-192	2659	-139	-102.47
	3570	-273	2601	-197	-126.06
MeOH4_9	3401	-442	2480	-318	-172.04
	3654	-188	2661	-137	-81.95
	3650	-192	2659	-139	-102.48
	3570	-273	2600	-198	-126.08
MeOH4_10	3576	-266	2605	-193	-129.20
	3709	-134	2700	-98	-77.20
	3483	-360	2538	-260	-170.36
	3617	-226	2635	-163	-106.98
MeOH4_11	3566	-277	2598	-200	-103.51
	3417	-426	2491	-307	-158.91
	3586	-257	2612	-186	-137.14
MeOH4_12	3696	-147	2691	-106	-100.82
	3554	-289	2588	-210	-131.80
	3478	-364	2536	-262	-153.59
	3688	-155	2685	-113	-64.78
MeOH5_1	3351	-491	2400	-398	-199.32
	3322	-520	2420	-378	-189.09
	3366	-476	2450	-348	-186.98
	3292	-551	2399	-399	-199.98
	3366	-476	2450	-348	-179.82
MeOH5_2	3341	-502	2432	-366	-194.66
	3291	-551	2398	-400	-197.62
	3339	-504	2432	-366	-188.34
	3383	-460	2463	-335	-175.53
	3341	-501	2433	-365	-195.81
MeOH5_3	3352	-490	2440	-358	-199.91
	3341	-502	2434	-364	-191.22
	3343	-500	2435	-363	-199.02
	3348	-495	2438	-360	-185.95
	3336	-506	2430	-368	-201.55
MeOH5_4	3329	-513	2425	-373	-196.21
	3266	-577	2380	-418	-213.53
	3521	-321	2564	-234	-158.08
	3362	-480	2449	-349	-187.15
	3654	-188	2660	-138	-86.87
MeOH5_5	3189	-654	2324	-474	-223.45
	3537	-305	2575	-223	-149.92
	3364	-478	2451	-347	-185.20
	3333	-509	2426	-372	-199.42
	3614	-229	2631	-167	-91.71

MeOH5_6	3459	-384	2517	-280	-163.01
	3386	-457	2467	-331	-177.74
	3383	-459	2463	-335	-191.20
	3174	-668	2313	-485	-225.14
	3624	-219	2638	-160	-86.64
MeOH5_7	3161	-682	2304	-494	-229.35
	3633	-210	2645	-153	-90.64
	3505	-338	2553	-245	-152.28
	3357	-485	2444	-354	-194.74
	3547	-295	2583	-215	-155.60
MeOH5_8	3525	-317	2568	-230	-154.89
	3476	-367	2532	-266	-165.66
	3386	-457	2465	-333	-185.85
	3265	-577	2380	-418	-212.39
	3657	-186	2663	-135	-84.29
MeOH5_9	3399	-443	2476	-322	-180.87
	3345	-498	2437	-361	-187.67
	3310	-533	2410	-388	-214.87
	3482	-361	2535	-263	-152.97
	3705	-138	2698	-100	-74.38
MeOH5_10	3206	-637	2336	-462	-219.26
	3467	-376	2523	-275	-160.11
	3416	-427	2488	-309	-169.51
	3406	-436	2480	-318	-183.91
	3618	-224	2635	-163	-86.40
MeOH5_11	3375	-467	2457	-340	-182.41
	3310	-533	2413	-385	-196.66
	3541	-302	2578	-220	-152.48
	3402	-440	2479	-319	-174.14
	3702	-140	2695	-103	-62.51
MeOH5_12	3357	-486	2448	-350	-196.45
	3507	-335	2555	-243	-137.08
	3664	-179	2669	-129	-101.64
	3623	-220	2638	-159	-113.98
	3599	-244	2622	-176	-104.78
MeOH5_13	3372	-471	2457	-341	-164.86
	3372	-471	2457	-341	-182.42
	3591	-252	2616	-182	-135.84
	3522	-320	2566	-232	-119.20
	MeOH5_14	3417	-426	2489	-309
3565		-278	2596	-202	-147.87
3328		-515	2426	-372	-176.51
3553		-289	2589	-209	-103.89
MeOH6_1		3314	-528	2414	-384
	3315	-528	2414	-384	-212.82
	3314	-529	2413	-385	-212.86
	3314	-529	2413	-384	-212.84
	3314	-529	2414	-384	-212.90
	3314	-529	2414	-384	-212.90
	MeOH6_2	3314	-528	2414	-384
3315		-527	2415	-383	-191.67
3319		-523	2417	-381	-199.31
3261		-582	2376	-422	-210.89
3377		-465	2459	-339	-186.40
3314		-529	2412	-386	-210.10
MeOH6_3		3374	-468	2456	-342
	3314	-528	2413	-385	-204.59

	3343	-499	2434	-364	-197.97
	3288	-555	2394	-404	-192.52
	3326	-517	2423	-375	-192.61
	3281	-561	2390	-408	-211.81
MeOH6_4	3376	-467	2457	-341	-179.63
	3282	-560	2391	-407	-211.47
	3329	-514	2425	-373	-199.40
	3278	-564	2387	-411	-203.24
	3343	-499	2433	-365	-195.56
	3366	-477	2451	-347	-181.92
MeOH6_5	3356	-487	2443	-355	-201.58
	3338	-505	2431	-367	-182.93
	3323	-519	2421	-377	-193.69
	3338	-505	2431	-367	-182.94
	3323	-519	2421	-377	-193.67
	3356	-486	2444	-354	-201.55
MeOH6_6	3393	-450	2471	-327	-175.23
	3393	-449	2471	-327	-175.22
	3304	-539	2407	-391	-207.54
	3356	-487	2443	-355	-190.02
	3303	-539	2407	-391	-207.50
	3356	-487	2443	-355	-189.95
MeOH6_7	3584	-259	2610	-188	-98.73
	3502	-341	2549	-249	-155.01
	3363	-480	2449	-349	-197.86
	3157	-686	2299	-499	-241.01
	3283	-560	2391	-407	-207.37
	3257	-586	2370	-428	-225.58
MeOH6_8	3314	-529	2411	-387	-208.59
	3145	-697	2292	-506	-237.03
	3292	-550	2399	-399	-202.68
	3397	-445	2475	-323	-181.15
	3631	-211	2644	-154	-91.62
	3466	-377	2522	-276	-160.67
MeOH6_9	3637	-206	2647	-151	-87.26
	3333	-509	2426	-372	-205.08
	3327	-516	2424	-374	-202.43
	3474	-369	2528	-270	-175.21
	3164	-678	2306	-492	-226.31
	3346	-496	2437	-361	-185.68
MeOH6_10	3347	-496	2435	-363	-199.00
	3333	-509	2429	-369	-191.07
	3366	-477	2450	-348	-180.73
	3640	-202	2649	-149	-81.18
	3501	-342	2547	-251	-166.48
	3115	-728	2270	-528	-229.77
MeOH6_11	3664	-179	2667	-131	-79.15
	3070	-773	2236	-562	-248.01
	3410	-433	2482	-315	-165.86
	3249	-594	2364	-434	-216.84
	3470	-373	2526	-272	-161.56
	3390	-452	2468	-330	-181.74
MeOH6_12	3527	-315	2567	-231	-150.17
	3400	-443	2477	-321	-174.80
	3111	-731	2267	-531	-248.13
	3570	-273	2601	-197	-100.47
	3357	-486	2444	-354	-197.12

	3511	-332	2556	-242	-137.31
MeOH6_13	3483	-359	2536	-262	-154.49
	3278	-565	2387	-411	-223.53
	3329	-513	2425	-373	-193.21
	3503	-339	2553	-244	-124.90
	3361	-481	2448	-349	-187.09
	3568	-274	2597	-200	-136.14
MeOH6_14	3318	-524	2415	-383	-201.54
	3535	-307	2573	-225	-142.74
	3491	-352	2544	-254	-129.41
	3172	-671	2311	-487	-218.39
	3419	-424	2491	-307	-181.93
	3562	-281	2593	-205	-136.03
MeOH6_15	3274	-569	2386	-412	-215.32
	3540	-302	2578	-220	-157.22
	3608	-235	2628	-170	-101.05
	3515	-328	2560	-238	-136.51
	3335	-507	2429	-369	-190.08
	3360	-483	2448	-350	-189.03
MeOH6_16	3473	-370	2528	-270	-136.26
	3372	-471	2456	-342	-179.09
	3429	-413	2498	-300	-169.81
	3191	-652	2325	-473	-232.74
	3547	-296	2582	-216	-151.10
	3543	-300	2582	-216	-109.96
MeOH6_17	3411	-432	2485	-313	-167.19
	3502	-340	2548	-250	-154.82
	3199	-644	2331	-467	-218.67
	3388	-454	2468	-330	-181.87
	3520	-322	2565	-233	-120.19
	3535	-308	2573	-225	-131.63
MeOH6_18	3624	-219	2639	-159	-90.72
	3214	-628	2343	-455	-228.51
	3674	-168	2676	-122	-81.10
	3532	-311	2572	-226	-146.98
	3436	-406	2503	-295	-186.86
	3428	-415	2497	-301	-172.75
MeOH6_19	3521	-322	2563	-235	-152.62
	3386	-456	2466	-332	-188.45
	3172	-671	2311	-487	-233.18
	3627	-216	2641	-157	-90.61
	3645	-198	2654	-144	-87.87
	3333	-510	2427	-371	-197.06
MeOH6_20	3653	-190	2660	-138	-84.46
	3506	-337	2553	-245	-152.89
	3340	-502	2434	-364	-200.54
	3229	-614	2354	-443	-220.22
	3470	-373	2525	-273	-167.25
	3615	-227	2633	-165	-94.08
MeOH6_21	3394	-448	2472	-326	-179.87
	3683	-160	2681	-117	-81.58
	3471	-372	2526	-271	-163.30
	3323	-520	2421	-377	-202.75
	3298	-544	2404	-394	-195.20
	3680	-163	2679	-119	-83.09
MeOH6_22	3226	-617	2349	-449	-228.10
	3504	-338	2550	-248	-145.80

	3534	-309	2572	-226	-127.32
	3586	-257	2612	-186	-101.76
	3396	-447	2474	-324	-165.45
	3429	-414	2498	-300	-162.80
MeOH6_23	3337	-505	2432	-366	-185.36
	3541	-301	2580	-218	-153.36
	3208	-634	2339	-459	-219.63
	3624	-218	2639	-159	-91.70
	3684	-158	2682	-115	-71.78
	3439	-403	2504	-294	-175.72
MeOH6_24	3505	-337	2552	-246	-155.53
	3695	-147	2691	-107	-68.83
	3360	-483	2446	-352	-162.40
	3645	-198	2654	-144	-83.16
	3196	-647	2330	-468	-227.80
	3348	-495	2438	-360	-194.98
MeOH6_25	3525	-317	2568	-230	-112.28
	3295	-547	2402	-396	-186.47
	3332	-511	2426	-372	-197.65
	3322	-521	2420	-378	-199.78
	3490	-353	2542	-256	-168.73
MeOH6_26	3258	-585	2373	-425	-214.02
	3156	-686	2300	-498	-230.37
	3579	-264	2605	-193	-107.64
	3535	-308	2574	-224	-160.85
	3825	-17	2785	-13	-40.75
	3589	-254	2613	-185	-94.86
MeOH6_27	3427	-415	2497	-301	-156.60
	3372	-470	2457	-341	-176.03
	3430	-412	2501	-297	-167.95
	3577	-266	2605	-193	-135.87
	3521	-322	2565	-233	-122.38
MeOH6_28	3702	-140	2696	-102	-91.70
	3385	-458	2465	-333	-173.55
	3639	-204	2650	-148	-86.83
	3391	-452	2472	-326	-191.20
	3494	-348	2546	-252	-149.89
	3616	-226	2635	-163	-89.86
MeOH6_29	3595	-248	2619	-179	-96.43
	3545	-297	2583	-215	-116.23
	3688	-155	2686	-112	-111.57
	3476	-367	2534	-264	-174.08
	3688	-155	2685	-113	-74.46
	3587	-255	2614	-184	-137.01

Cartesian coordinates of neutral methanol clusters optimized at the MP2/aug-cc-pVDZ level of theory

MeOH C 0.67255400 -0.02009800 0.00000000 O -0.75529900 0.12250400 0.00000000 H -1.14214600 -0.76229900 0.00001000 H 1.08381100 0.99739000 -0.00031200 H 1.03267600 -0.54753400 -0.89931800 H 1.03272300 -0.54699800 0.89961600	MeOH2 C 2.03080900 0.51052100 0.18555800 O 1.32896700 -0.73756000 0.00043000 H 1.75371000 -1.21612900 -0.72410200 H 1.52331100 1.02509100 1.01034200 H 1.97600700 1.14091300 -0.71575900 H 3.08305300 0.33728500 0.45935700 H -0.41803700 -0.14550000 -0.39889500 O -1.23654800 0.34882000 -0.58332900 C -2.22312200 -0.08722700 0.35434400 H -3.13343400 0.49628900 0.16037400 H -1.90810200 0.09089300 1.39782800 H -2.46198900 -1.15868300 0.23464500
MeOH3_1 C 2.77420600 0.35942600 -0.04667500 O 1.44686000 0.24457600 0.48840000 H 1.03205200 -0.56309300 0.11558700 H 3.20353500 1.28726100 0.35366400 H 2.76449200 0.41528600 -1.14796900 H 3.40548700 -0.48743500 0.26733300 H -0.01005500 1.18362800 -0.18747700 O -0.89273800 1.22820500 -0.61243800 C -1.80111700 1.83733800 0.31637900 H -2.79737400 1.81551700 -0.14495100 H -1.52664500 2.88598100 0.51595000 H -1.83621300 1.28734200 1.27237800 H -0.78711000 -0.64017800 -0.80162400 O -0.36777600 -1.51183800 -0.64013800 C -1.13445000 -2.16580200 0.38350400 H -2.17146900 -2.34339300 0.05542000 H -1.14456300 -1.58006900 1.31889400 H -0.65474000 -3.13416400 0.57695500	MeOH3_2 C -1.89521700 -1.36318000 0.56484300 O -1.24390800 -1.02437100 -0.66732000 H -1.19365600 -0.04628100 -0.71442400 H -1.90302200 -2.45880200 0.63651500 H -2.93598700 -1.00050100 0.58216100 H -1.35830600 -0.95320300 1.43836100 H 0.63882000 -1.01146000 -0.71234200 O 1.51055900 -0.56491700 -0.66728900 C 2.13053200 -0.95478400 0.56595600 H 3.08159300 -0.41065200 0.63662200 H 2.34012000 -2.03678000 0.58584200 H 1.50596500 -0.69468500 1.43868200 H 0.55727100 1.05869600 -0.71633300 O -0.26460900 1.59135800 -0.66974000 C -0.23706000 2.31634000 0.56758600 H 0.59644600 3.03723400 0.59246100 H -0.15218300 1.64041600 1.43668100 H -1.18292400 2.86919700 0.64026200
MeOH3_3 C -2.79887200 -0.86154600 -0.06370900 O -1.38937300 -0.94768900 0.15321900 H -0.98014200 -0.14701600 -0.23620500 H -3.25302500 -1.76111400 0.37418900 H -3.04806300 -0.83058500 -1.13888100 H -3.23746900 0.02559900 0.42725400 H -1.10630600 2.66825400 0.34672100 C -0.12554200 2.18472600 0.45006900 O 0.02725400 1.29986200 -0.67224000 H 0.65427900 2.96330700 0.45487400 H -0.09578500 1.63329200 1.40473200 H 0.90257300 0.87149700 -0.57895300 H 0.88336800 -1.50968700 0.52083300 C 1.92214300 -1.53117200 0.17079000	MeOH3_4 C -1.13456200 1.92610500 -0.52111200 O -0.66885800 1.31370800 0.71037100 H -0.86632000 1.91238100 1.44321500 H -0.85521200 1.23464900 -1.32416700 H -0.64217100 2.89589000 -0.68529900 H -2.22744800 2.04829100 -0.50671000 H 1.07928300 0.72322500 0.14892200 O 1.78936200 0.46298500 -0.46124600 C 2.65417100 -0.44447600 0.22850500 H 3.43462700 -0.74587800 -0.48288500 H 2.11756400 -1.34832900 0.56542300 H 3.13856700 0.02975900 1.09965900 O -1.90115500 -1.23858000 0.16928800 C -0.81793300 -2.08746800 -0.22977400

O	2.30759900	-0.15392200	-0.06165800	H	-1.50920100	-0.43887400	0.55599600
H	2.56524700	-1.98794800	0.93847000	H	-1.25628500	-2.92002300	-0.79618000
H	1.97405200	-2.11877300	-0.75860800	H	-0.28280100	-2.50329800	0.64261300
H	3.19106100	-0.14487800	-0.45189600	H	-0.09544300	-1.55765900	-0.87360900
MeOH4_1				MeOH4_2			
C	2.67298600	-0.29317600	1.23582100	C	1.73298600	2.23380100	0.30317200
O	1.88645100	-0.29432300	0.03460000	O	0.86721400	1.60162000	-0.65361100
H	1.39798000	0.56545900	-0.00618400	H	1.16072500	0.66028300	-0.72446600
H	3.17541800	-1.26780100	1.29904600	H	1.43095200	3.28717600	0.37226700
H	2.04465500	-0.15490000	2.13169700	H	2.78461800	2.18763200	-0.02289300
H	3.43775300	0.49940100	1.20689100	H	1.64094700	1.77119300	1.30088500
H	0.56541500	-1.39823700	0.00676000	H	-0.67274300	1.34799800	0.08144900
O	-0.29440200	-1.88660400	-0.03421200	O	-1.48297700	1.04380700	0.56137400
C	-0.29357700	-2.67208000	-1.23615100	C	-2.62794000	1.42381100	-0.21549300
H	-1.26839400	-3.17408600	-1.29979500	H	-3.51709800	1.03690900	0.30080100
H	0.49872000	-3.43715800	-1.20790600	H	-2.58972600	0.99857800	-1.23290100
H	-0.15508500	-2.04298700	-2.13145500	H	-2.71148600	2.52004400	-0.28905700
H	-2.04363000	0.15527700	2.13173600	H	-1.64039700	-1.77075100	-1.30147600
C	-2.67243100	0.29360900	1.23620300	C	-1.73287400	-2.23361500	-0.30392400
O	-1.88656300	0.29418900	0.03451500	O	-0.86729000	-1.60184600	0.65332100
H	-3.17443300	1.26845000	1.29949900	H	-1.43102100	-3.28702900	-0.37319100
H	-3.43751600	-0.49867600	1.20785400	H	-2.78460000	-2.18731300	0.02181100
H	-1.39813700	-0.56563100	-0.00615800	H	-1.16082800	-0.66055000	0.72448300
O	0.29409900	1.88633400	-0.03446200	O	1.48308700	-1.04393700	-0.56109900
C	0.29337000	2.67199500	-1.23627900	C	2.62781600	-1.42369200	0.21625100
H	-0.56571200	1.39788400	0.00634800	H	0.67269100	-1.34816700	-0.08145300
H	1.26795900	3.17450500	-1.29944400	H	3.51711800	-1.03666300	-0.29970100
H	-0.49932300	3.43667100	-1.20824400	H	2.71152000	-2.51990600	0.28990400
H	0.15556700	2.04297500	-2.13174300	H	2.58911700	-0.99841300	1.23362000
MeOH4_3				MeOH4_4			
C	-0.43093900	-2.99589200	-0.16736500	C	-3.11411300	0.05481400	-0.71466200
O	-0.33079300	-1.73140500	0.50831900	O	-1.97991000	0.11121800	0.16446400
H	0.53603200	-1.32941100	0.25614400	H	-1.44073800	-0.70621800	0.02593400
H	-1.41542100	-3.41839500	0.07478900	H	-3.68941200	0.97804100	-0.56422100
H	0.34888800	-3.69228600	0.18005000	H	-3.75648400	-0.80749900	-0.47507500
H	-0.34911000	-2.87680400	-1.26040400	H	-2.80529100	-0.00684700	-1.77144900
H	-0.53943700	1.29702900	-0.84475300	H	-0.78390400	1.33278400	-0.09748500
O	0.31760000	1.78914900	-0.82769700	O	0.03692800	1.87546600	-0.19858800
C	0.34655200	2.48572800	0.42767500	C	0.43506500	2.27878400	1.11989200
H	1.29988100	3.02878600	0.48100400	H	1.38561700	2.82154400	1.02499200
H	0.28313400	1.78740000	1.28105500	H	0.58216600	1.40940900	1.78446200
H	-0.47808700	3.21350800	0.49880800	H	-0.31230900	2.94910400	1.57349800
O	-1.88621400	0.22807500	-0.52243000	H	2.79407600	-0.03039800	0.60527300
C	-2.87061400	0.67632400	0.41963000	C	2.88065100	-0.08102000	-0.49433700
H	-1.41116100	-0.54297200	-0.12400200	O	1.59520600	-0.14907700	-1.12628900
H	-3.33852500	1.57784300	0.00089500	H	3.42856600	-0.99359900	-0.76530900
H	-2.41814000	0.92632400	1.39454900	H	3.45249500	0.79176100	-0.84938900
H	-3.65062300	-0.08699000	0.57309000	H	1.09304900	0.66350400	-0.87091100
H	2.70215700	0.45145900	1.31750700	O	-0.21124500	-1.91750300	-0.12897500
C	2.99437000	-0.05301400	0.38063100	C	0.27639000	-2.18419700	1.19510300

O	1.85069700	-0.41769100	-0.40454700	H	0.48505300	-1.38079500	-0.58038600
H	3.53018900	-0.97884100	0.62898400	H	-0.47972300	-2.79370500	1.70722400
H	3.67081600	0.60529900	-0.18807200	H	0.42703200	-1.25209500	1.76777700
H	1.38287900	0.41415900	-0.66222900	H	1.22401200	-2.74610000	1.16419100
MeOH4_5				MeOH4_6			
C	0.07825200	2.16818400	0.96527300	C	2.17185700	-1.08801100	-1.31379600
O	0.13993200	1.91147400	-0.44440700	O	2.05917800	0.27344000	-0.84608700
H	-0.66460100	1.38194500	-0.66465600	H	1.21617200	0.63234000	-1.17558500
H	0.97726500	2.73786500	1.23683300	H	3.06436800	-1.50969200	-0.83338500
H	0.05968800	1.23143600	1.55069000	H	2.31118800	-1.11557800	-2.40613600
H	-0.81011100	2.76707700	1.22415000	H	1.28441400	-1.67889000	-1.03985800
H	1.34596400	0.67646900	-0.76843500	H	-1.09345700	-0.49140600	-0.69198900
O	1.88920200	-0.14551100	-0.83857400	O	-1.15757600	-1.46632800	-0.66501300
C	2.94491400	-0.05569400	0.12733300	C	-2.36721400	-1.78963000	0.02509000
H	3.54755800	-0.96979800	0.04028900	H	-2.41738700	-2.88443600	0.10027700
H	2.55309000	0.01620100	1.15721400	H	-3.25975200	-1.43519600	-0.51940700
H	3.59252300	0.81368700	-0.07122600	H	-2.38410500	-1.36706900	1.04603900
H	-0.05985500	-1.23031800	1.55042700	O	0.95419100	0.81747500	1.63319200
C	-0.07775600	-2.16744700	0.96559400	C	0.56932800	-0.42233000	2.26071800
O	-0.13988700	-1.91165600	-0.44423600	H	1.58765400	0.58930900	0.91788700
H	-0.97626400	-2.73768500	1.23765500	H	-0.20544500	-0.17952900	3.00018600
H	0.81113500	-2.76546000	1.22469200	H	1.42487700	-0.87830100	2.78399900
H	0.66447100	-1.38208000	-0.66500900	H	0.16420300	-1.13400300	1.52283500
O	-1.88919600	0.14533500	-0.83809800	H	-0.83701600	3.35662000	-0.53416900
C	-2.94543200	0.05525800	0.12720900	C	-1.44055600	2.44043900	-0.63225900
H	-1.34602700	-0.67669200	-0.76798500	O	-0.62192700	1.26658400	-0.50756100
H	-3.54803300	0.96938200	0.04007900	H	-1.89295400	2.41524900	-1.63219600
H	-2.55416200	-0.01690500	1.15728200	H	-2.24205000	2.45038100	0.12399500
H	-3.59292400	-0.81407500	-0.07193300	H	-0.19212200	1.25802200	0.38272900
MeOH4_7				MeOH4_7			
C	-0.44580500	2.47961000	-0.69157100	C	0.24287200	2.81272200	0.23832800
O	-1.02737200	1.61614200	0.29464800	O	0.14340300	1.40660100	-0.04533300
H	-0.28791400	1.27884300	0.85483000	H	-0.04827300	0.91630200	0.79104700
H	-1.25821900	2.82531500	-1.34480900	H	0.42189600	3.32332700	-0.71669300
H	0.30157800	1.94786800	-1.30636700	H	1.08370200	3.02128200	0.91883900
H	0.03190100	3.35598000	-0.22372200	H	-0.68958400	3.19583300	0.68242400
H	-0.31268600	-0.51794900	2.92957700	H	1.71393800	0.45042100	-0.50001300
C	0.40721100	-0.81411500	2.15483000	O	2.40793300	-0.21922100	-0.64277100
O	0.99708000	0.39854500	1.64575300	C	1.90164600	-1.13913000	-1.61629400
H	1.17340300	-1.46168500	2.60955500	H	2.65951600	-1.92429600	-1.74191900
H	-0.11817200	-1.36517200	1.35800100	H	1.73662200	-0.65304600	-2.59375800
H	1.61067600	0.13410800	0.92996600	H	0.95561400	-1.60723300	-1.29251900
H	0.68795400	-0.96828500	-1.37698300	O	-1.55180800	-0.70773000	-0.82761700
C	1.72692000	-0.81390200	-1.69315500	C	-2.95574200	-0.43620200	-0.98186300
O	2.48794800	-0.52699400	-0.49495800	H	-1.07512900	0.14041800	-0.90706800
H	2.10108700	-1.72761600	-2.17979400	H	-3.47998200	-1.39201100	-0.85431300
H	1.77535100	0.02752100	-2.40214400	H	-3.17736700	-0.03980300	-1.98555500
H	3.40687200	-0.36118200	-0.74124500	H	-3.31646800	0.27505700	-0.21996700
O	-1.51414800	-0.85363300	-0.82127500	H	1.30722200	-1.33101100	1.35602100
C	-2.71098100	-1.43226900	-0.29653600	C	0.53001600	-1.32008100	2.13663800

H	-1.43970100	0.05331400	-0.44916100	O	-0.56704600	-0.45401900	1.77079200
H	-2.78027400	-2.45660500	-0.68858200	H	0.95513800	-0.91448900	3.06378800
H	-3.60949300	-0.87388300	-0.61114500	H	0.17110900	-2.34322600	2.32909500
H	-2.69450700	-1.47898300	0.80726200	H	-0.99056300	-0.82642900	0.96916100
MeOH4_9				MeOH4_10			
C	0.24077600	2.81266300	0.23676200	C	-3.46871500	-0.48428000	-0.04903200
O	0.14340100	1.40607200	-0.04538600	O	-2.31821600	-0.10970500	-0.82405400
H	-0.04979100	0.91660600	0.79114400	H	-1.91913800	0.68436400	-0.41152300
H	0.42178100	3.32223200	-0.71844100	H	-3.86159000	-1.41198800	-0.48527800
H	1.07963700	3.02288100	0.91918500	H	-4.25073600	0.29010900	-0.09826900
H	-0.69321100	3.19540400	0.67795400	H	-3.20552300	-0.66502300	1.00690200
H	1.71424800	0.44995400	-0.49787000	H	1.99472400	-1.18245800	-0.77957000
O	2.40869700	-0.21926200	-0.64041600	O	2.94156900	-1.01725700	-0.62994500
C	1.90390000	-1.13868800	-1.61511100	C	3.02830700	0.26947700	-0.01980500
H	2.66252200	-1.92309700	-1.74095700	H	4.09012200	0.46181500	0.18545200
H	1.73913200	-0.65187100	-2.59226900	H	2.47666600	0.31292500	0.93806900
H	0.95804500	-1.60792400	-1.29244200	H	2.65198700	1.06853800	-0.68373800
O	-1.55000400	-0.70913200	-0.82885200	O	0.16089800	-1.12902300	-0.25006500
C	-2.95380100	-0.43748200	-0.98418000	C	0.06271800	-1.86863300	0.98255400
H	-1.07321300	0.13897200	-0.90821200	H	-0.75220500	-0.98926700	-0.58937800
H	-3.47821800	-1.39325700	-0.85709100	H	1.08903800	-2.05592800	1.32462900
H	-3.17462200	-0.04100300	-1.98802000	H	-0.44367300	-2.83406800	0.82648900
H	-3.31505900	0.27376600	-0.22251700	H	-0.47642900	-1.28897200	1.75051900
H	1.30479300	-1.33078500	1.35749200	H	0.47707400	2.75116400	-0.92193200
C	0.52790200	-1.31813800	2.13839500	C	0.21482200	2.71254700	0.14797900
O	-0.56956400	-0.45326100	1.77092100	O	-0.48900700	1.50403000	0.47655600
H	0.95333300	-0.91011800	3.06433900	H	-0.46010800	3.54623000	0.38021100
H	0.16933800	-2.34089200	2.33356100	H	1.13015100	2.81681800	0.75190800
H	-0.99161700	-0.82632900	0.96881500	H	0.07488700	0.73671600	0.25540500
MeOH4_11				MeOH4_12			
C	-0.26332400	2.42878500	0.65089200	C	-2.09878400	-1.78092300	-1.26461500
O	1.05270200	1.89527200	0.80221200	O	-0.97490700	-1.38957900	-0.45849000
H	1.16850500	1.21372200	0.10873300	H	-0.39461000	-0.82600900	-1.00123300
H	-0.39267500	3.19994200	1.42301500	H	-2.75162000	-2.38817100	-0.62437800
H	-1.04354700	1.65874100	0.79237500	H	-1.77798100	-2.38946900	-2.12477000
H	-0.40619700	2.90062600	-0.33802900	H	-2.66296200	-0.90555100	-1.62778000
H	3.06967800	0.15923100	-1.92300600	H	-1.08387900	-0.13915500	0.91933100
C	2.62084200	-0.60066900	-1.26954400	O	-0.96448400	0.74772600	1.32151800
O	1.25890400	-0.21053700	-1.03707700	C	-2.23416600	1.41609000	1.24336100
H	2.67472700	-1.58004200	-1.77204800	H	-2.09810900	2.41828300	1.67035600
H	3.19583300	-0.64377400	-0.32895500	H	-3.00199300	0.88358500	1.82720200
H	0.83641100	-0.89669900	-0.46730400	H	-2.57655600	1.51497600	0.19865200
H	1.11918400	-1.81962900	2.27095800	H	0.10686000	1.12048500	-0.08168100
C	0.17811700	-1.33534000	1.97840000	O	0.56728700	0.91112400	-0.92601300
O	-0.14148300	-1.81374500	0.65384200	C	1.31812600	2.05953000	-1.35940700
H	-0.60471100	-1.62308000	2.69775600	H	2.08408900	2.33495700	-0.61711800
H	0.31679100	-0.24233500	1.98848100	H	0.65525800	2.91973400	-1.54443000
H	-1.01939500	-1.45089500	0.41719700	H	1.81535700	1.78274100	-2.29788200
H	-1.04411200	0.29186500	-1.54139200	H	1.65750400	-0.47469200	2.00009500
C	-2.12764700	0.12833300	-1.50410700	C	2.02317100	-1.29182100	1.35393000

O	-2.40845000	-0.46191700	-0.21203000	O	2.62751000	-0.79268600	0.15401200
H	-2.65053600	1.09064100	-1.61387300	H	2.80027400	-1.84683100	1.89659500
H	-2.41886800	-0.55035600	-2.32035300	H	1.18541000	-1.97586700	1.13499100
H	-3.34238800	-0.70720800	-0.18297700	H	1.94962200	-0.25894400	-0.29578800
MeOH5_1				MeOH5_2			
C	0.18199800	2.97837900	0.40436800	C	0.77739800	-0.97410200	2.18994000
O	0.35488100	1.86014900	-0.48116500	O	0.93247200	-1.77051700	1.00237900
H	-0.53003900	1.42600100	-0.57592100	H	0.01654100	-1.95897300	0.67343100
H	1.17368700	3.41958200	0.57426300	H	1.76900600	-0.58187400	2.45635800
H	-0.24208200	2.66422200	1.37270900	H	0.40348400	-1.58636200	3.02577300
H	-0.47504900	3.73921100	-0.04582300	H	0.08302000	-0.13311000	2.02427000
H	1.50592000	0.76030500	0.08128700	H	1.54742800	-0.84313600	-0.26373200
O	2.15697500	0.07973900	0.39174000	O	1.80359600	-0.22151400	-0.99476800
C	3.33340700	0.20680200	-0.42149400	C	3.23208000	-0.09336800	-0.99622900
H	4.01462000	-0.60918200	-0.14429400	H	3.49935300	0.59963900	-1.80566800
H	3.83899000	1.16899200	-0.23961900	H	3.71519500	-1.06506800	-1.18603400
H	3.09352600	0.12618800	-1.49535600	H	3.60591500	0.31271200	-0.04024300
H	-0.05228500	0.01039300	2.15335400	H	-3.05634000	1.27664200	-1.27600200
C	-0.93233700	-0.60097700	2.41656200	C	-3.12506500	1.33928200	-0.17685600
O	-1.45403700	-1.29288500	1.26719400	O	-1.97208200	0.76462000	0.45686700
H	-1.72947600	0.05367900	2.79419300	H	-4.00206700	0.77025400	0.16038200
H	-0.64916800	-1.31338800	3.20729100	H	-3.25266500	2.39443300	0.11429200
H	-0.68437600	-1.74567700	0.84022000	H	-1.17005000	1.22512100	0.10159500
O	-2.03394400	0.65954400	-0.45688500	O	-1.56038000	-1.86938400	-0.01015200
C	-2.84687300	0.22978200	-1.55622300	C	-1.41053000	-1.93895900	-1.43990400
H	-1.90384300	-0.10785300	0.15987300	H	-1.78757000	-0.93013600	0.20033400
H	-2.94224700	1.07824000	-2.24727100	H	-1.15401800	-2.97686400	-1.69077800
H	-3.85140500	-0.06449700	-1.21238200	H	-0.60500900	-1.27450200	-1.79650800
H	-2.38874100	-0.61781300	-2.09380700	H	-2.35270500	-1.67566100	-1.94767900
H	-0.32011800	-2.79319800	-1.66930500	H	0.30676500	3.46320900	0.83945600
C	0.45993500	-2.05829500	-1.42738600	C	0.98090400	2.67969600	0.46784600
O	0.74746300	-2.17907400	-0.02518900	O	0.25794400	1.91367900	-0.50702800
H	1.35255100	-2.27896700	-2.03545200	H	1.86560900	3.15872700	0.01738800
H	0.09493500	-1.04733600	-1.67918100	H	1.30261700	2.05439300	1.31812300
H	1.34712100	-1.42282800	0.19470000	H	0.84438000	1.16018400	-0.77192000
MeOH5_3				MeOH5_4			
C	0.27638500	-1.74652600	1.36556400	C	-1.16331300	-2.68242300	0.82453700
O	0.28767300	-2.07244600	-0.03292800	O	-1.07355800	-1.77956800	-0.28942300
H	-0.60353900	-1.80993300	-0.37687400	H	-1.54878500	-0.94493600	-0.04318200
H	1.30268000	-1.86111100	1.74191200	H	-0.46361800	-3.50852800	0.63834200
H	-0.37978900	-2.43203700	1.92635400	H	-2.18168000	-3.09304200	0.91397400
H	-0.05848400	-0.70902200	1.53668000	H	-0.89071100	-2.18397900	1.76840100
H	1.44637700	-1.07823600	-0.79381900	H	0.42155600	-1.19415700	-0.75925200
O	2.10105400	-0.40637500	-1.11286500	O	1.24547500	-0.70074300	-1.01861300
C	3.41277000	-0.86688000	-0.76307300	C	1.77093100	-1.28929500	-2.22082700
H	4.13390600	-0.13981700	-1.16068100	H	2.66417100	-0.71643100	-2.50263100
H	3.61853000	-1.85191100	-1.21143000	H	1.03553300	-1.23905300	-3.03951900
H	3.54411100	-0.93672100	0.33124700	H	2.05776700	-2.33940100	-2.05286500
H	-1.78190200	2.47052700	-1.70653200	H	1.54672700	3.26701600	-0.94647500
C	-2.14584900	2.48930600	-0.66604700	C	0.88658100	2.80732900	-0.19365400

O	-1.55973600	1.43591800	0.11582200	O	0.06130500	1.79085100	-0.79792700
H	-3.23327100	2.33299600	-0.66440300	H	0.20965700	3.57738000	0.20018700
H	-1.92758000	3.47504700	-0.22530300	H	1.49576300	2.39031900	0.62199100
H	-0.57858600	1.57208300	0.10593700	H	0.61487800	0.99851500	-0.97086700
O	-2.12676000	-1.07246600	-0.67001200	O	-2.06457400	0.62647200	0.36432700
C	-3.16482500	-1.53888700	0.20417100	C	-3.26247500	1.08415700	-0.28390200
H	-1.94982300	-0.12626800	-0.43635000	H	-1.30873300	1.15282700	0.00153400
H	-3.25857500	-2.62348000	0.05575400	H	-4.08848200	0.45365000	0.07169500
H	-4.12970500	-1.06393000	-0.03735000	H	-3.18759300	0.99544700	-1.38031200
H	-2.92362700	-1.33935800	1.26217000	H	-3.47725000	2.13204100	-0.02023200
H	1.26618600	2.71178500	1.86604200	H	1.16626000	-1.06908200	2.50855700
C	1.78508800	1.93626100	1.28648800	C	1.29859600	-0.00275300	2.25373200
O	1.09940900	1.80091200	0.03458200	O	2.41956900	0.20056400	1.38910400
H	2.83090700	2.24920000	1.13304000	H	1.49989200	0.55087200	3.18111400
H	1.77220300	0.99471300	1.86171800	H	0.35899600	0.37817800	1.81480300
H	1.51544300	1.04150100	-0.44752700	H	2.18799500	-0.21033200	0.53568600
MeOH5_5				MeOH5_6			
C	-1.26408500	-0.05747600	2.65761100	C	0.43538700	2.60719900	-0.71937200
O	-0.82144100	0.11858700	1.30141300	O	1.02570500	1.84559200	0.34816300
H	-0.36159200	-0.71443500	0.99750300	H	0.30207100	1.33497600	0.77944200
H	-1.78741900	0.86114300	2.95406300	H	1.23782800	3.20145100	-1.17576700
H	-0.41062900	-0.22004600	3.33479800	H	-0.33904400	3.29011900	-0.33591200
H	-1.95845200	-0.90887400	2.73897200	H	-0.00658500	1.95130400	-1.48757200
H	0.37899400	1.36419600	0.74848100	H	2.02005700	0.56581900	-0.26782400
O	1.09023600	1.83932200	0.26778400	O	2.43196400	-0.26718200	-0.60528300
C	0.46324700	2.65835900	-0.74235800	C	3.78531400	-0.32681600	-0.12944600
H	1.26992900	3.07120000	-1.36212900	H	4.21778800	-1.26806200	-0.49389600
H	-0.09135100	3.48932300	-0.27883700	H	3.82924000	-0.31494700	0.97232500
H	-0.22235200	2.06890300	-1.37001700	H	4.37962000	0.51307000	-0.52317300
H	3.73725500	-0.30265300	0.98851400	H	0.12700700	-3.37621800	-1.21783600
C	3.74270000	-0.38183100	-0.11154300	C	-0.23158200	-2.36495300	-0.97128500
O	2.41413400	-0.32454800	-0.65231900	O	0.43449200	-1.87115600	0.20942900
H	4.17084400	-1.35187300	-0.39773300	H	-1.30960100	-2.39675700	-0.76355200
H	4.37258000	0.42096000	-0.52688900	H	-0.05046500	-1.69944500	-1.83026200
H	2.00416800	0.52973400	-0.36633000	H	1.26370900	-1.41880100	-0.08263200
O	0.46305600	-1.93728000	0.24835300	O	-0.88851200	0.13134400	1.29042100
C	-0.28041000	-2.36700200	-0.91012000	C	-1.20023000	-0.07446700	2.68203800
H	1.25268300	-1.43788100	-0.08398300	H	-0.41145600	-0.67862200	0.94945600
H	-1.11716100	-2.98017400	-0.54855400	H	-1.70751000	0.83038100	3.04134900
H	0.35073200	-2.98266500	-1.56927000	H	-0.28453300	-0.23459900	3.27273400
H	-0.67465600	-1.50629400	-1.47487100	H	-1.87231100	-0.93767900	2.80831300
H	-4.20126400	0.19180000	-0.35045800	H	-1.82679700	0.16275000	-2.05321200
C	-3.45656300	-0.13217100	-1.09872300	C	-2.79307200	0.47874600	-1.61893200
O	-2.26361200	0.65244000	-1.03903100	O	-3.10360600	-0.24157500	-0.42636000
H	-3.88713500	0.00505500	-2.09993600	H	-3.58595400	0.26073200	-2.34727800
H	-3.25073800	-1.20759800	-0.95107200	H	-2.76505400	1.56979800	-1.44892200
H	-1.86274600	0.50273100	-0.16105500	H	-2.39325400	-0.04970400	0.21523800
MeOH5_7				MeOH5_8			
C	0.33683200	3.09616200	-0.35536200	C	-0.74942100	2.48020100	-1.04856300
O	0.22760600	1.68896000	-0.08231700	O	0.05239100	1.34424900	-0.68023900

H	-0.64740500	1.36148000	-0.44046700	H	-0.47145600	0.52880200	-0.83384600
H	1.31268800	3.43071700	0.02099900	H	-0.21408700	3.37697100	-0.70929800
H	-0.45690200	3.65992700	0.15982500	H	-1.73377100	2.43038900	-0.55873400
H	0.27966500	3.29403300	-1.43755100	H	-0.88427300	2.53706900	-2.14128700
H	0.10678000	0.73979700	1.52279500	H	1.72571600	0.83639400	-0.81331900
O	-0.05246500	0.05560400	2.20042600	O	2.55374700	0.31726400	-0.69430200
C	1.19012700	-0.61692000	2.42672700	C	3.35721800	1.01017500	0.27337500
H	1.01148300	-1.37417700	3.20250300	H	4.21734600	0.36729100	0.50464500
H	1.97070600	0.07418200	2.79011400	H	2.79342400	1.20658800	1.20109800
H	1.55274900	-1.12242800	1.51471400	H	3.72862300	1.96564400	-0.13085200
O	1.61877500	-0.42083100	-1.13174900	H	0.65442900	-0.47650700	1.77495100
C	3.04571800	-0.44515100	-1.02015400	C	1.10342600	-1.48053000	1.68994800
H	1.27831100	0.42991700	-0.77824300	O	1.27562000	-1.86191800	0.31217500
H	3.38465400	-1.42409400	-1.38406900	H	0.43004900	-2.21553600	2.15034200
H	3.37146700	-0.32257100	0.02664100	H	2.06598300	-1.49634800	2.22555100
H	3.50999500	0.34132600	-1.63766400	H	1.84649500	-1.16602600	-0.09797000
H	-2.37496100	0.03873000	1.06638200	O	-1.06271200	-1.17027200	-0.74833900
C	-2.90875000	0.38518000	0.16678100	C	-1.52155900	-1.96232300	-1.85764900
O	-2.00317200	0.57532400	-0.94006200	H	-0.21466400	-1.55684400	-0.40092600
H	-3.37590900	1.35750000	0.37272600	H	-2.45294800	-1.50698200	-2.21943600
H	-3.69863100	-0.33492100	-0.09911200	H	-1.72722000	-2.99710600	-1.54255100
H	-1.62611600	-0.31300100	-1.16338700	H	-0.78090400	-1.96895900	-2.67325200
H	-0.19339000	-3.41506300	-0.05849000	H	-2.06486200	-0.02560400	2.62200200
C	-0.88598400	-2.55828400	-0.07322500	C	-2.20412300	0.81912700	1.92439700
O	-0.74328500	-1.80602000	-1.29492800	O	-2.87626600	0.41672100	0.72802500
H	-1.91543200	-2.94065500	-0.05232600	H	-2.83898900	1.57045600	2.41364600
H	-0.71415500	-1.92441800	0.81150300	H	-1.22053600	1.27255400	1.70811900
H	0.17707100	-1.46650000	-1.31646200	H	-2.31383700	-0.25049400	0.29350500
MeOH5_9				MeOH5_10			
C	2.52486800	2.41671600	-0.64273600	C	1.67755300	-0.85367200	2.39797800
O	2.09719200	1.37712500	0.25326700	O	1.06468500	-0.29566800	1.21795700
H	1.12167600	1.47531800	0.37588500	H	0.51865700	-1.00516900	0.77645800
H	3.59920400	2.27352200	-0.82001800	H	2.25633400	-0.05198100	2.87465600
H	2.36856000	3.41118600	-0.19550900	H	2.35660600	-1.67834300	2.13126800
H	1.99035500	2.36410100	-1.60555900	H	0.91461600	-1.21877200	3.10304700
H	2.18783400	-0.19706900	-0.42090700	H	-0.18006400	0.96586700	1.30560700
O	2.07087000	-1.11456100	-0.77617400	O	-0.95440300	1.55147400	1.14021600
C	3.00262900	-1.97483900	-0.10306200	C	-0.61112600	2.38750900	0.02368600
H	2.81374100	-2.99917400	-0.45201200	H	-1.47808600	3.02990100	-0.18062900
H	2.87310400	-1.93724000	0.99192300	H	-0.38527400	1.79099100	-0.87701500
H	4.04110600	-1.70283100	-0.35050500	H	0.25624300	3.02559400	0.25576000
H	0.20560400	-1.32422600	1.84942100	H	-2.90893700	0.54282700	-1.55003800
C	-0.46699800	-1.91795400	1.20706900	C	-3.49944300	0.07441700	-0.74348600
O	-0.51249000	-1.38286400	-0.12959400	O	-2.66136500	-0.41442000	0.31312000
H	-1.48703900	-1.86962100	1.61144300	H	-4.04252700	-0.78651900	-1.15557100
H	-0.13206400	-2.96705300	1.20032000	H	-4.23174300	0.80497800	-0.36333400
H	0.41895000	-1.38144000	-0.47309400	H	-2.15264200	0.35031100	0.67493000
O	-0.60294500	1.33889200	0.33511300	O	-0.47684400	-1.94367000	-0.15889400
C	-1.47069300	1.63756500	1.44467800	C	-0.12691800	-1.69086400	-1.53330500
H	-0.69593300	0.38110800	0.13164600	H	-1.36258500	-1.53215600	-0.00949300
H	-1.50891800	2.73073400	1.54019200	H	0.94044200	-1.91687600	-1.65207800
H	-1.08145600	1.21009400	2.38434700	H	-0.29696800	-0.63355700	-1.80016500

H	-2.48201600	1.24629400	1.25918900	H	-0.71581600	-2.33082400	-2.20902700
H	-3.57159300	-0.15964600	-2.34025400	H	2.68168400	2.00824800	-1.04932600
C	-3.51908200	0.28017200	-1.32971400	C	2.67485800	1.07498600	-1.63986500
O	-3.23605600	-0.71029000	-0.33367100	O	2.98515600	-0.06691900	-0.84264800
H	-4.50075600	0.70822800	-1.08522200	H	3.44768300	1.15027300	-2.41689400
H	-2.76648600	1.08774800	-1.32794200	H	1.69253200	0.97811400	-2.13817600
H	-2.35078000	-1.06641500	-0.52228600	H	2.34246600	-0.09354600	-0.10804000
MeOH5_11				MeOH5_12			
C	0.98750700	0.11018800	2.59302800	C	-0.55985700	-1.64034700	-1.87798500
O	0.03786200	-0.56421000	1.75294900	O	0.33472000	-0.79702500	-1.12481600
H	0.55506700	-0.96683100	1.01131800	H	0.32202700	-1.09063500	-0.17862300
H	0.43186600	0.54447300	3.43478300	H	-0.59186100	-1.24544600	-2.90194900
H	1.50626100	0.92076200	2.05161400	H	-1.56808400	-1.61657500	-1.43733200
H	1.73613600	-0.59405900	2.98997800	H	-0.19044900	-2.67740100	-1.90253300
H	-0.86243400	0.53079500	0.81201000	H	-0.40645300	0.81245000	-0.88800400
O	-1.25866700	1.10928400	0.10981100	O	-0.92833600	1.58634200	-0.58237200
C	-2.31600700	1.89467900	0.68944800	C	-0.01073800	2.62672300	-0.21488900
H	-2.72544500	2.52855000	-0.10779200	H	-0.58837100	3.39995600	0.30924100
H	-1.93446000	2.53679700	1.49946400	H	0.45727500	3.07659600	-1.10614700
H	-3.11700100	1.24603200	1.07758700	H	0.78460500	2.25290900	0.45060200
H	1.90413500	2.07345900	-0.14264600	O	2.68588500	0.24445100	-0.03778900
C	1.75515300	2.08240100	-1.23646000	C	4.05128400	-0.04239300	-0.38182500
O	0.83515400	1.06154200	-1.65315600	H	2.11098900	-0.09867400	-0.74711800
H	2.71424800	1.87749000	-1.73088700	H	4.67314900	0.35040800	0.43281600
H	1.40601300	3.08153300	-1.54173500	H	4.33949000	0.45636900	-1.32096500
H	-0.00232000	1.21701200	-1.16560600	H	4.22649900	-1.12677800	-0.47558900
O	1.48997500	-1.27967800	-0.41540900	H	-0.09896300	0.61332500	2.05383400
C	2.91834900	-1.36957300	-0.30872500	C	0.03076300	-0.42284800	2.40518300
H	1.28030300	-0.49410500	-0.97648500	O	0.82673500	-1.19253600	1.47934100
H	3.14549200	-2.24969100	0.30761300	H	-0.95430000	-0.90042700	2.45454400
H	3.34926600	-0.47468100	0.17346800	H	0.49560500	-0.41741700	3.40355300
H	3.38119100	-1.50260000	-1.29970500	H	1.64406100	-0.69143700	1.28802100
H	-0.98886600	-2.25340900	-0.96950500	H	-3.68360100	-0.08649600	-1.23818800
C	-2.02818600	-2.17943600	-0.60575600	C	-3.86703600	-0.15566600	-0.15117100
O	-2.71173700	-1.04750200	-1.15923000	O	-2.64749500	-0.26200500	0.58788400
H	-2.57823800	-3.07336300	-0.92930000	H	-4.45096900	-1.06458700	0.05072600
H	-2.01745800	-2.15322300	0.49808400	H	-4.46199600	0.72027500	0.16040000
H	-2.22533600	-0.25998000	-0.86119700	H	-2.09723100	0.50694900	0.33885100
MeOH5_13				MeOH5_14			
C	0.40325700	-2.43357800	-0.79437400	C	-0.33969000	-0.35712400	2.34039500
O	1.22821700	-1.73819900	0.14533500	O	0.40715800	-1.22831800	1.47281900
H	0.64140400	-1.17340300	0.70685600	H	1.28782400	-0.81350700	1.30942300
H	1.06108900	-3.06914700	-1.40220500	H	-1.39755100	-0.64230500	2.26530500
H	-0.12813400	-1.73736200	-1.46746900	H	-0.23433200	0.69804900	2.03524700
H	-0.33291600	-3.07779900	-0.28419200	H	-0.00396400	-0.46255000	3.38412300
H	1.34642200	0.09579100	2.96290600	H	3.15925400	-1.94533600	-0.18907900
C	0.84797700	0.78422300	2.26685100	C	2.94699000	-0.93559600	-0.56488100
O	-0.19311100	0.03949100	1.60421400	O	2.70400700	-0.10157400	0.58543500
H	0.42401400	1.62535600	2.83809700	H	3.81760600	-0.57513600	-1.13462000
H	1.58314300	1.16677000	1.54030700	H	2.06513200	-0.96972800	-1.22591600

H	-0.58104300	0.64009000	0.92058600	H	2.46005800	0.78306500	0.24197800
H	0.51031200	1.51884400	-1.39397100	H	0.03675700	1.18655300	-0.88887300
C	-0.56975700	1.49611300	-1.58647600	C	0.34338300	2.22608900	-0.72062200
O	-1.24061900	1.61853000	-0.31382800	O	1.78691400	2.21719700	-0.60979500
H	-0.84805100	2.32890800	-2.25105100	H	0.02304500	2.83997500	-1.57632400
H	-0.82778000	0.54440200	-2.07999100	H	-0.12232600	2.60657300	0.20137200
H	-2.16923000	1.33461400	-0.43184000	H	2.08962000	3.12133900	-0.45374700
H	-2.37465100	-1.31044200	-0.35334900	O	-0.71399300	-1.01318200	-0.94732300
C	-3.20157200	-0.92586500	0.25544800	C	-0.93100800	-2.28171400	-1.58476300
O	-3.66224300	0.27681500	-0.40657900	H	-0.29150800	-1.18382500	-0.06695700
H	-4.00113800	-1.68099400	0.29316900	H	-1.36631400	-2.08097000	-2.57287800
H	-2.82906700	-0.71341400	1.26878100	H	-1.63020100	-2.90928900	-1.00745600
H	-4.42040400	0.61914400	0.08600300	H	0.01790900	-2.82773500	-1.71704100
O	2.56977500	0.47866700	-0.83936800	O	-3.16419100	-0.07564600	0.00720300
C	3.91190000	0.47511700	-0.34901300	C	-3.09668400	1.34514400	0.08740200
H	2.15516700	-0.36394800	-0.55456400	H	-2.31296100	-0.38887200	-0.36280400
H	4.36517200	1.43690800	-0.62697100	H	-4.09674500	1.70772900	0.36306700
H	4.51136400	-0.33769400	-0.79472100	H	-2.81566700	1.80369300	-0.87819800
H	3.94734400	0.37487600	0.75081300	H	-2.38273700	1.68367300	0.86148900
MeOH6_1				MeOH6_2			
C	-1.61904000	2.94601800	-1.38019800	H	2.44282400	0.03048700	0.55463400
O	-1.34700000	2.28049500	-0.13847600	O	2.87629400	-0.78136100	0.18360200
H	-0.36224900	2.25530200	-0.02173800	C	3.82483000	-0.35050800	-0.80273400
H	-2.70730700	2.93058600	-1.53003400	H	3.34934200	0.27599400	-1.57725300
H	-1.13388100	2.43509100	-2.22866000	H	4.23962400	-1.25085100	-1.27656700
H	-1.27718700	3.99293000	-1.34911700	H	4.64693400	0.21761800	-0.33860900
H	-2.13544700	0.81371900	0.02097700	H	-1.19320500	1.55585200	-0.38714600
O	-2.65007800	-0.02621500	0.13770200	O	-0.38062700	2.07482400	-0.62023300
C	-3.36083200	0.07052700	1.38039400	C	-0.69308100	3.46734500	-0.45523200
H	-3.89262100	-0.87913900	1.52985300	H	0.23565500	4.03272900	-0.61054600
H	-4.09555500	0.89099700	1.35107200	H	-1.07635100	3.67832300	0.55715300
H	-2.67454800	0.23345600	2.22820900	H	-1.43866600	3.79573900	-1.19749900
H	2.67641900	-0.23588900	-2.22902800	H	-2.08997200	-0.21683900	0.44486400
C	3.36160700	-0.07155500	-1.38060000	O	-2.50888200	0.59796500	0.06436900
O	2.64935300	0.02617400	-0.13886700	C	-3.29427200	0.17946500	-1.06160600
H	3.89298400	0.87826900	-1.53054400	H	-4.08947000	-0.51807700	-0.75208600
H	4.09681300	-0.89153200	-1.34948100	H	-2.67173400	-0.30219200	-1.83472100
H	2.13486100	-0.81384500	-0.02184400	H	-3.76145000	1.07649200	-1.49027600
O	1.30210600	2.30708000	0.13800800	H	-0.50148100	-1.78293700	0.32716200
C	1.74138500	2.87352300	1.38097100	O	-1.25067200	-1.58320300	0.95022800
H	1.77256100	1.44168900	0.02056700	C	-1.95821600	-2.80483000	1.20539400
H	1.18517600	3.80903600	1.53081900	H	-2.81844300	-2.55998900	1.84353300
H	2.81937800	3.09919400	1.35182600	H	-1.31720500	-3.52806000	1.73417600
H	1.53904900	2.19742000	2.22848300	H	-2.32281700	-3.26504800	0.27139000
H	2.70669000	-2.92857000	1.53170300	H	0.87800800	1.61944100	0.45134000
C	1.61843900	-2.94374600	1.38173200	O	1.55901300	1.35251400	1.11665800
O	1.34691000	-2.28045300	0.13871500	C	0.84940900	1.01021800	2.32321300
H	1.27607400	-3.99054600	1.35260000	H	0.32251300	1.88971400	2.72777400
H	1.13341700	-2.43097100	2.22916300	H	1.59747300	0.67956800	3.05607900
H	0.36219700	-2.25530300	0.02158000	H	0.12648900	0.19622600	2.15101800
H	-1.18204200	-3.80889800	-1.53098100	H	1.54760100	-1.64392400	-0.41887300
C	-1.74103100	-2.87508900	-1.38082500	O	0.70558700	-2.00230200	-0.80304800

O	-1.30187000	-2.30665000	-0.13873200	C	0.41950000	-1.20453300	-1.96559300
H	-1.54198100	-2.19874200	-2.22890800	H	0.30137300	-0.13767600	-1.71184100
H	-2.81826000	-3.10419800	-1.35012100	H	-0.51816600	-1.58082500	-2.39776600
H	-1.77308100	-1.44157900	-0.02204200	H	1.21638600	-1.31219600	-2.71919100
MeOH6_3				MeOH6_4			
H	1.98705600	-0.98328900	0.84432600	O	0.88067500	-2.18676800	-0.91229400
O	1.43652700	-1.69385800	1.25781700	H	1.61985100	-1.70914400	-0.46017300
C	0.60702500	-1.05213900	2.24291900	O	-1.17358600	1.78501900	-0.43357300
H	-0.01025100	-0.25199100	1.80223600	H	-1.75527100	0.98333200	-0.35722900
H	1.21825200	-0.62655500	3.05516100	O	1.34411500	1.71332500	0.44347200
H	-0.05034400	-1.82323200	2.66767500	H	0.41127400	1.70886100	0.10882700
H	0.45056700	-2.09879400	-0.06567800	O	-2.68102900	-0.40739100	-0.29276500
O	-0.14300100	-2.16271300	-0.85789800	H	-2.11957000	-1.10263800	0.14226400
C	0.68054900	-1.99142600	-2.02370300	O	-1.03742400	-2.09038000	0.96971800
H	1.24823000	-2.91135800	-2.23646800	H	-0.34655900	-2.28432600	0.28589800
H	1.38584000	-1.15460100	-1.89553400	O	2.70240400	-0.60025500	0.28653100
H	0.01486200	-1.78152000	-2.87247900	H	2.19918300	0.24720500	0.37407400
H	-0.14183100	1.84215700	0.02880800	C	1.34292400	2.36547900	1.72188900
O	0.62468600	1.93205700	-0.59204200	H	0.70940500	1.83031300	2.44971900
C	0.10779200	1.70311800	-1.91385000	H	2.37810500	2.37064800	2.08933200
H	0.96441500	1.53617600	-2.58111900	H	0.98826100	3.40455200	1.63401000
H	-0.45432000	2.58100300	-2.27195700	C	-1.31220300	2.29958900	-1.76658200
H	-0.54885000	0.81814600	-1.94099700	H	-0.55352100	3.08334500	-1.89810600
H	-1.89053900	0.68082100	0.45240800	H	-1.14982200	1.51211500	-2.52133500
O	-1.58969800	1.52944100	0.87235900	H	-2.31071900	2.74034400	-1.91757600
C	-2.57786500	2.52689300	0.56895400	C	-3.89285400	-0.29454000	0.46947000
H	-2.18127200	3.49613200	0.90052700	H	-3.69290300	0.03711300	1.50273400
H	-3.51984300	2.32600700	1.10471100	H	-4.52619800	0.45307500	-0.02706600
H	-2.78435700	2.57387600	-0.51373700	H	-4.43011700	-1.25551800	0.49682400
H	1.93131600	0.94314000	-0.22389700	C	-0.40342600	-1.23018600	1.93393000
O	2.67530300	0.31567600	-0.03495300	H	-0.11006500	-0.26730300	1.48279800
C	3.75835900	1.06762200	0.53126800	H	-1.13128200	-1.04594800	2.73594300
H	4.13552900	1.81626500	-0.18390200	H	0.49018400	-1.70848500	2.36440300
H	4.56468500	0.35835400	0.76173300	C	3.86461200	-0.32590600	-0.51083600
H	3.45518800	1.57994500	1.45991900	H	4.38653500	-1.27936000	-0.66892100
H	-1.49628500	-1.22315700	-0.61358900	H	3.59202000	0.10132400	-1.49086800
O	-2.31361400	-0.70619000	-0.38474500	H	4.54447800	0.37060000	0.00593900
C	-3.17192700	-1.58660000	0.35809800	C	0.37371200	-1.27453800	-1.90231500
H	-2.70148900	-1.90649300	1.30342400	H	-0.55789300	-1.69921800	-2.30014300
H	-3.42866700	-2.47768100	-0.23564200	H	0.15503800	-0.28681900	-1.46359000
H	-4.09311200	-1.03346200	0.58766400	H	1.09175700	-1.15185000	-2.72980400
MeOH6_5				MeOH6_6			
O	-0.12794800	1.95641400	0.20943500	O	0.15826000	2.44298500	0.91057500
H	0.72992400	1.73852500	-0.23407200	H	0.87960800	1.84074400	0.60355000
O	-2.29122800	-1.24064300	0.73776300	O	-0.15815000	-2.44207700	0.91136600
H	-2.43369800	-0.38362000	0.26102500	H	-0.87953200	-1.84013400	0.60388300
O	-2.47782600	1.04682700	-0.65875400	O	-2.01658900	-0.77823300	-0.08123600
H	-1.58409800	1.42702400	-0.45810600	H	-1.79027500	0.10021700	-0.48282000
O	2.29132400	1.24088000	-0.73784000	O	-1.46337300	1.63477800	-1.07863200
H	2.43398000	0.38371300	-0.26144700	H	-0.92280900	2.07027100	-0.37267500

O	2.47807100	-1.04683100	0.65821000	O	2.01613000	0.77835600	-0.08147900
H	1.58423000	-1.42687700	0.45782100	H	1.78868200	-0.10025700	-0.48210000
O	0.12802200	-1.95646400	-0.20956400	O	1.46424200	-1.63526100	-1.07775700
H	-0.72989100	-1.73885100	0.23392500	H	0.92361200	-2.07055000	-0.37173200
C	3.45417700	-2.03167800	0.28670600	C	-0.41215700	1.86202400	2.09392100
H	3.40685400	-2.26445100	-0.79098000	H	-1.15466400	2.57309500	2.48014200
H	4.44470400	-1.61652300	0.51779000	H	-0.91165800	0.90265000	1.87349500
H	3.31534500	-2.96122300	0.86105300	H	0.35623500	1.69884000	2.86721800
C	3.27879900	2.16543300	-0.25546000	C	3.35887400	0.70388700	0.41622900
H	3.05455200	3.14606700	-0.69633300	H	3.59489000	1.67560600	0.87134400
H	3.24978200	2.25162200	0.84412800	H	3.46235500	-0.08526600	1.18021900
H	4.29170600	1.86034600	-0.56488600	H	4.07333800	0.50869100	-0.39935200
C	-0.05374900	1.39423500	1.53328100	C	0.71510400	-1.73064900	-2.30189100
H	-1.01489600	1.58945200	2.02779200	H	1.20525700	-1.08051300	-3.03933600
H	0.11655400	0.30655400	1.50378700	H	0.71978300	-2.76505600	-2.68053500
H	0.74951200	1.87106300	2.11726400	H	-0.32733900	-1.40237600	-2.15938100
C	-3.27914100	-2.16505000	0.25600300	C	0.41190900	-1.86042600	2.09456100
H	-3.05514200	-3.14557900	0.69723400	H	1.15455700	-2.57111300	2.48122000
H	-4.29187500	-1.85948000	0.56553000	H	0.91115800	-0.90100200	1.87379900
H	-3.25041500	-2.25170900	-0.84355900	H	-0.35666100	-1.69711900	2.86765100
C	-3.45418400	2.03116100	-0.28650000	C	-3.35973000	-0.70525300	0.41575900
H	-4.44452600	1.61668000	-0.51957400	H	-3.59478400	-1.67710700	0.87107700
H	-3.40809900	2.26181800	0.79170100	H	-3.46453800	0.08403300	1.17942300
H	-3.31446000	2.96179500	-0.85886000	H	-4.07399400	-0.51123900	-0.40027300
C	0.05374100	-1.39423400	-1.53338800	C	-0.71433000	1.72998500	-2.30281300
H	-0.11725200	-0.30666600	-1.50383300	H	-1.20408300	1.07918000	-3.03993800
H	1.01511900	-1.58880100	-2.02770000	H	-0.71963500	2.76419100	-2.68200600
H	-0.74909800	-1.87154000	-2.11755500	H	0.32831300	1.40241100	-2.16016200
MeOH6_7				MeOH6_8			
H	1.74559000	-1.44065000	-2.21486100	O	0.53336300	-2.19352100	-0.47681400
C	2.74821700	-1.19421100	-1.82137100	H	1.24931100	-1.63754200	-0.07265200
H	3.18438800	-2.10261100	-1.37015400	O	-1.69850500	-1.12487100	0.40335200
H	3.38354400	-0.88475400	-2.66228100	H	-0.86623400	-1.60051900	0.11488300
O	2.70667800	-0.10507200	-0.89749300	O	2.38615800	-0.55102900	0.52822700
H	2.17707100	-0.39146000	-0.12658400	H	2.04523100	0.37462900	0.41378300
H	2.23622000	2.18586600	-0.03866200	O	1.32573200	1.88482700	0.25269900
C	1.73094100	2.69285600	0.79834900	H	0.45435300	1.72430000	0.69011000
H	2.41693500	2.75483500	1.65839500	O	-1.78866300	0.60884700	-1.81009800
H	1.45032800	3.71148600	0.49839200	H	-1.91930800	-0.04585400	-1.09819500
O	0.51297500	2.01310000	1.16554800	O	-0.85813900	1.14435400	1.67499800
H	0.73147500	1.06522700	1.30485500	H	-1.22133500	0.33338400	1.25120200
H	0.42839900	0.74348300	-1.65327000	C	3.71485100	-0.60554400	-0.00946600
C	-0.38905300	1.40227700	-1.98787600	H	4.07271000	-1.63823100	0.10100600
H	0.04871400	2.27866500	-2.49245000	H	3.73194800	-0.33418300	-1.07920300
H	-1.02819400	0.86594500	-2.70392700	H	4.39110300	0.06678800	0.54239700
O	-1.22133700	1.81374800	-0.88696800	C	0.56326800	-1.92990300	-1.89476100
H	-0.62142800	1.97523500	-0.11674700	H	1.54992700	-2.18324600	-2.31395300
H	1.66225500	-2.41163500	2.30552000	H	-0.19426700	-2.57238100	-2.36289700
C	1.52251300	-1.33153000	2.46892600	H	0.32207200	-0.87741800	-2.11477700
H	0.81451600	-1.17916900	3.29877800	C	-0.20772100	0.72045700	2.88880800
H	2.48895000	-0.88031000	2.73061500	H	0.24282300	1.61303400	3.34239800
O	1.05630900	-0.68762100	1.26921600	H	-0.93549400	0.29040000	3.59553000

H	0.22714300	-1.15727700	0.96512600	H	0.58643900	-0.01691900	2.68372300
H	-4.58425900	1.03575200	0.11643700	C	-2.43927400	1.81678800	-1.39541400
C	-3.93415800	0.29769400	0.61236800	H	-2.21459200	2.58105200	-2.15225000
H	-3.50939100	0.74713300	1.52570400	H	-3.53446300	1.69210200	-1.34189300
H	-4.53734200	-0.57682500	0.89131500	H	-2.07129300	2.16592200	-0.41528000
O	-2.90476600	-0.15627000	-0.27936800	C	1.08499700	2.33436400	-1.09450500
H	-2.32942200	0.62210400	-0.50487800	H	2.06011500	2.37486700	-1.59925300
H	-0.68063200	-1.92538200	-1.65360400	H	0.41347100	1.64891000	-1.63471100
C	-0.82356200	-2.63581300	-0.82241700	H	0.64927300	3.34643600	-1.09331600
H	-1.65281900	-3.31615200	-1.07108900	C	-2.61812900	-2.08420200	0.95131100
H	0.09447500	-3.22509700	-0.68998800	H	-3.49698100	-1.53098100	1.30846600
O	-1.08162200	-1.94961400	0.41387000	H	-2.93641400	-2.80750400	0.18396900
H	-1.82180800	-1.30821700	0.23703600	H	-2.16591000	-2.62766300	1.79616100
MeOH6_9				MeOH6_10			
O	-3.32147700	-0.23238900	-0.91794000	O	-0.51843700	-1.42888100	-1.12735200
H	-2.80669800	-0.43032100	-0.11297500	H	0.42044600	-1.72493600	-1.01641100
O	-0.29868500	1.66668900	0.06031200	O	2.56081000	0.78101400	-0.59817300
H	0.64437700	1.74434000	0.35576700	H	1.86090000	1.15680700	-0.00566600
O	2.49734200	-0.91052300	-0.36063400	O	2.07604000	-1.86768300	-0.56677800
H	1.62833200	-1.36890700	-0.22790500	H	2.35037200	-0.91977100	-0.64622200
O	0.16399300	-2.16012600	0.04726200	O	-3.16921200	1.04616000	-0.34458200
H	-0.42736500	-1.60453100	0.60373800	H	-2.52124100	0.70970100	0.30236800
O	-1.49883500	-0.35996400	1.22812200	O	0.62669800	1.72066600	1.01072600
H	-1.03798700	0.45063300	0.86598500	H	0.02465100	0.97603700	1.23178000
O	2.32239500	1.58149600	0.62586800	O	-1.18294300	-0.30872100	1.14478900
H	2.45114700	0.64681600	0.32366400	H	-0.93396100	-0.79791000	0.30565700
C	3.09673800	2.41949400	-0.24635600	C	2.10240700	-2.17283400	0.83668100
H	2.85716600	3.46256100	0.00109800	H	1.48559200	-1.46338100	1.41604500
H	4.17635100	2.25820200	-0.09457700	H	1.69841000	-3.18681900	0.96141400
H	2.85196500	2.23496500	-1.30617000	H	3.13246300	-2.15267300	1.22807200
C	-0.25346200	1.35145200	-1.34847300	C	3.83201200	1.26707200	-0.14062300
H	0.53242200	0.60827400	-1.56170400	H	4.60664000	0.78757800	-0.75420200
H	-1.22973000	0.93487100	-1.62874900	H	3.90546800	2.35944200	-0.26528900
H	-0.06139300	2.26157100	-1.93871000	H	4.00438300	1.01448700	0.91915900
C	-1.80519700	-0.13230500	2.61477400	C	-0.50913400	-0.39137900	-2.13515100
H	-2.32352300	-1.02532700	2.98799300	H	-0.50881200	-0.83884600	-3.14086400
H	-0.88672700	0.02414100	3.20284300	H	-1.41773200	0.21045800	-2.00039500
H	-2.46466700	0.74245000	2.73129600	H	0.37676800	0.25491600	-2.02553000
C	-3.91871400	1.05161900	-0.70482700	C	-1.66847100	-1.26280800	2.10386500
H	-4.41180500	1.34045400	-1.64302600	H	-1.99005800	-0.70416800	2.99270400
H	-4.67955300	1.02204000	0.09476500	H	-2.52722900	-1.82226200	1.69897900
H	-3.16483600	1.81789700	-0.45002000	H	-0.87754100	-1.97419800	2.39248000
C	-0.59022800	-2.54000200	-1.12088200	C	-0.18618500	2.73831900	0.38993200
H	-1.09629900	-1.67344200	-1.57405800	H	-0.91189700	3.14998200	1.10815100
H	0.12088400	-2.96543100	-1.84177500	H	0.49215900	3.53929900	0.06769700
H	-1.34294200	-3.30262300	-0.86686700	H	-0.72941200	2.34539000	-0.48381500
C	3.52619200	-1.78911000	0.12126300	C	-3.98101700	-0.07413700	-0.71416400
H	3.52945400	-2.73696400	-0.44013100	H	-4.63225500	0.25313900	-1.53590500
H	4.48915400	-1.28312700	-0.03242100	H	-3.37105700	-0.92594500	-1.06460800
H	3.40243800	-2.00688700	1.19502300	H	-4.61838100	-0.41215200	0.12211600

MeOH6_11				MeOH6_12			
O	2.76264100	-0.19849600	-0.51250800	C	0.19460500	-0.47243300	2.79622400
H	2.20224500	-0.43348600	0.24927900	O	1.01745100	0.35407900	1.94949400
O	0.70651200	-0.54545600	1.39428000	H	0.42749300	0.94182600	1.43023600
H	0.47358900	0.43030200	1.33078600	H	0.82272600	-1.30143900	3.14814400
O	-0.70700000	-1.81243600	-0.53463500	H	-0.66984300	-0.87521500	2.24719900
H	-0.18145800	-1.38729200	0.18405200	H	-0.16363800	0.10003000	3.66632000
O	0.16533900	1.99458100	1.12589700	H	2.06630700	-0.30284900	0.74214600
H	-0.34682200	2.05764800	0.27431800	O	2.58909500	-0.53192400	-0.06431600
O	-2.76877500	-0.06293600	-0.70167500	C	3.90024000	0.03549300	0.09093000
H	-2.12450400	-0.80747400	-0.71895600	H	4.46158800	-0.18656200	-0.82639900
O	-1.06870900	1.99014900	-1.23874900	H	4.42554300	-0.41446800	0.94824100
H	-1.74898800	1.28013800	-1.13744700	H	3.85476900	1.12869900	0.22849800
C	0.50432600	-0.97026400	2.75268600	H	0.00777400	1.38536400	-0.68085400
H	0.83967400	-2.01363200	2.82771200	O	-0.52938600	1.70776800	0.10246200
H	1.09471800	-0.35432600	3.44858000	C	-0.68374100	3.13454500	-0.00269000
H	-0.56076200	-0.91214600	3.03168700	H	-1.22613800	3.40491200	-0.92241000
C	1.40466600	2.70715300	0.92088500	H	0.29610600	3.63705300	0.00148900
H	1.20279600	3.73725500	0.58894700	H	-1.26346000	3.46836500	0.86819000
H	1.92415600	2.74211200	1.88791700	H	0.54039200	-2.05174400	0.05325600
H	2.04240500	2.19336600	0.18353100	C	-0.25517900	-2.80416900	-0.08258800
C	-3.10923200	0.14996500	0.67870600	O	-1.41501800	-2.25822100	-0.71801800
H	-2.22732300	0.44509700	1.27406000	H	0.13054600	-3.59640300	-0.73904300
H	-3.84486400	0.96427100	0.71104400	H	-0.49654400	-3.25288400	0.89699100
H	-3.55965300	-0.75395700	1.11966500	H	-1.77105500	-1.55492400	-0.13768300
C	2.68525200	-1.27879000	-1.44947300	H	1.12541900	-0.57558900	-3.41663700
H	1.64485100	-1.47925500	-1.75833600	C	0.36685600	-0.11119400	-2.76774600
H	3.26612800	-0.98070700	-2.33281500	O	0.99768600	0.77286400	-1.81355500
H	3.12520200	-2.20619600	-1.04214200	H	-0.29283400	0.50960500	-3.38911600
C	-0.56416000	-3.23349200	-0.41146100	H	-0.22674400	-0.89006500	-2.26412900
H	-1.12173400	-3.69218700	-1.23858600	H	1.63001000	0.23929000	-1.26933900
H	0.49458200	-3.53198000	-0.48874700	H	-4.39488300	-0.67438900	0.06121000
H	-0.97484200	-3.60320700	0.54347000	C	-3.67768500	0.12374200	-0.17053000
C	-0.07266900	1.49583200	-2.15796500	O	-2.52354000	-0.08934100	0.65963500
H	-0.54816200	1.07959900	-3.05951000	H	-3.41980700	0.06802800	-1.24177400
H	0.55241800	2.35079600	-2.44871500	H	-4.14806700	1.09779200	0.04235700
H	0.56717400	0.72957800	-1.69094800	H	-1.87653500	0.61787200	0.44588600
MeOH6_13				MeOH6_14			
O	-0.26027100	1.53592300	-0.32615800	O	-2.41885700	-0.03359300	1.00069100
H	-0.04530900	0.59310300	-0.14685200	H	-1.75506900	-0.76624500	1.08993600
O	0.01907500	-1.17348000	0.12823600	O	1.02324100	1.98487800	0.84390900
H	-0.94090700	-1.35059000	0.31681300	H	0.32066200	1.85671900	0.17118000
O	-2.62099800	-1.36676900	0.45312400	O	2.79701500	-0.02784600	0.24919300
H	-2.84493100	-0.43830300	0.18639200	H	2.22738100	0.75128600	0.43469800
O	3.19226600	0.00341300	-0.74152100	O	-1.06540600	1.30285800	-0.83628000
H	2.96787500	-0.27219500	0.17415100	H	-1.62914400	0.86021800	-0.13930700
O	-2.93262800	1.18950300	-0.31997600	O	-0.66679000	-2.02553300	0.76754100
H	-1.97351400	1.42610300	-0.38422900	H	-0.45119400	-1.85635200	-0.18062800
O	2.22047400	-0.74842100	1.73060500	O	-0.28324000	-1.19513300	-1.79801100
H	1.39297900	-1.05706300	1.30599500	H	-0.45103700	-0.24620000	-1.61980200
C	-3.34471300	-2.26270600	-0.40464500	C	-1.88987300	2.24659700	-1.54423500
H	-3.12999200	-2.06839200	-1.46905400	H	-2.33281800	2.98003100	-0.85184800

H	-3.02769000	-3.28429000	-0.15458900	H	-1.24628900	2.77434000	-2.26016800
H	-4.43013600	-2.17814400	-0.23684400	H	-2.69355500	1.73169700	-2.09504700
C	-3.53863900	2.08841500	0.62307600	C	-3.60028300	-0.62502400	0.42714000
H	-3.49491300	3.12769200	0.26055300	H	-4.34238200	0.17637000	0.30837700
H	-4.59159400	1.79374200	0.72635600	H	-3.38654400	-1.07437600	-0.55754300
H	-3.04989600	2.02863000	1.60969200	H	-4.01300800	-1.39794900	1.09328900
C	0.46590800	1.93076800	-1.51051700	C	4.06816200	0.45985800	-0.18610400
H	0.01508500	1.49132400	-2.41650100	H	4.55450500	1.08307700	0.58389700
H	0.40041000	3.02481300	-1.57681800	H	4.70548400	-0.41412500	-0.38114200
H	1.51897200	1.62301300	-1.43639300	H	3.98643500	1.04923000	-1.11683400
C	1.89313500	0.45948600	2.44165300	C	1.02400900	-1.32154600	-2.39693700
H	2.82466600	0.83025500	2.88961800	H	1.18396500	-2.39269000	-2.57911300
H	1.48420000	1.22817300	1.76518200	H	1.06186000	-0.79254500	-3.36296500
H	1.16849600	0.26046600	3.24780600	H	1.80644800	-0.93989800	-1.72305600
C	4.61733100	0.07948500	-0.83397200	C	0.55416900	-2.35928600	1.45753000
H	5.09490600	-0.89051700	-0.61261900	H	1.37218600	-1.67511300	1.18462400
H	4.86378400	0.36315000	-1.86665000	H	0.35102900	-2.28131000	2.53454900
H	5.03250300	0.84271300	-0.15268500	H	0.85160400	-3.39589100	1.23066100
C	0.33266000	-1.77257600	-1.14945300	C	0.47119000	1.53924000	2.09706300
H	-0.36154800	-1.41236400	-1.92670000	H	1.22375300	1.74284200	2.86975700
H	1.35610400	-1.46946500	-1.40491300	H	-0.45346300	2.08505900	2.34160700
H	0.27300900	-2.87043500	-1.08905300	H	0.25722800	0.45775300	2.08179400
MeOH6_15				MeOH6_16			
O	-0.31584500	1.01570500	0.81028100	O	-1.08868600	1.35820600	-1.01157600
H	0.61409600	1.36751800	0.81454600	H	-0.70862300	1.12886800	-0.13315900
O	0.26008200	-1.69061400	0.74775800	O	0.47800000	-1.93156700	0.76655800
H	-0.15239700	-0.80329700	0.82121600	H	1.17401600	-1.66187900	0.11747700
O	-3.19999000	-0.62588600	0.22472100	O	2.45408900	-0.94299300	-0.78603100
H	-2.64175600	-0.43615400	-0.55479200	H	2.42439400	-0.02070100	-0.43675300
O	-1.40502900	0.44182600	-1.62224700	O	-0.15983000	0.53781500	1.44694800
H	-1.00296700	0.81124000	-0.80620000	H	0.00627200	-0.43198500	1.27503000
O	2.24673600	1.64604600	0.51168100	O	2.22650700	1.45778700	0.47934600
H	2.50389800	0.71871800	0.27280200	H	1.43597600	1.27091700	1.02884000
O	2.65823600	-0.92359500	-0.18633000	O	-3.13033500	-0.37415000	-0.28453900
H	1.79337000	-1.31170900	0.09880200	H	-2.52802800	0.31811000	-0.62920600
C	2.40120100	2.44763500	-0.67185400	C	2.05758400	2.76234400	-0.10488500
H	2.11385800	3.47509300	-0.41138100	H	2.83826500	2.87806100	-0.86857000
H	3.44787100	2.44706000	-1.01444000	H	1.06723200	2.86661400	-0.57626800
H	1.75427200	2.08861500	-1.49000900	H	2.18523200	3.55007800	0.65462900
C	3.70159000	-1.65304200	0.48052200	C	3.70977300	-1.51192900	-0.37363700
H	3.72583400	-2.70186100	0.14412400	H	3.81231000	-1.50822200	0.72400200
H	4.65489900	-1.17506700	0.21780400	H	3.72910600	-2.54970000	-0.73223000
H	3.57529400	-1.62705400	1.57537500	H	4.55548000	-0.96472800	-0.81917100
C	-1.07735600	1.59639800	1.88656400	C	-1.19295200	0.65418500	2.44806000
H	-1.23662600	2.67345600	1.71903700	H	-0.87597600	0.17639400	3.38788700
H	-2.04334800	1.07635200	1.90306200	H	-1.35391700	1.72579100	2.62634600
H	-0.56503900	1.44784200	2.84975000	H	-2.12723100	0.19782900	2.08646800
C	-0.33387500	-0.00628000	-2.46519200	C	-4.46855600	0.00828900	-0.61310300
H	-0.76361700	-0.68965900	-3.21017100	H	-5.13743400	-0.76154100	-0.20417600
H	0.13382900	0.83971400	-2.99631000	H	-4.73838100	0.98144600	-0.16690700
H	0.44067500	-0.54192000	-1.89152500	H	-4.62405100	0.06372500	-1.70460300
C	-4.29704200	0.29107800	0.17914800	C	-0.32749000	0.64646200	-2.00322700

H	-4.88439400	0.14179300	1.09602500	H	-0.79181100	0.85539600	-2.97605900
H	-3.95394200	1.34052100	0.14480500	H	0.72019100	0.98597000	-2.02912100
H	-4.95062000	0.10702500	-0.69061300	H	-0.34349400	-0.44132200	-1.82593600
C	-0.68737100	-2.60775600	0.16761400	C	-0.53803100	-2.69258700	0.07634600
H	-0.89954900	-2.35358300	-0.88347500	H	-0.10517500	-3.21530700	-0.79030900
H	-0.23001800	-3.60499400	0.21184600	H	-0.92806800	-3.43975900	0.78108900
H	-1.63002300	-2.60570100	0.73199400	H	-1.36619900	-2.04543300	-0.25227500
MeOH6_17				MeOH6_18			
O	3.05090400	1.17730900	0.29113200	O	0.56462000	2.13813900	-0.25549300
O	2.38449500	-1.36640200	1.03592100	H	0.49142300	1.45825700	0.44143300
O	-0.26600100	-0.66589900	1.19334600	O	0.50348100	-1.61151600	-0.50673400
O	0.47517500	1.20872500	-0.51140300	H	-0.25098000	-1.23824200	-1.04162100
O	-3.12416100	0.81574200	-0.25758900	O	3.02442200	-0.53295300	0.09804800
O	-1.98776600	-1.67087600	-0.73568200	H	2.20804800	-0.85366000	-0.32504600
H	2.92845100	0.27092400	0.66377600	O	-2.48613600	0.29833500	0.75318400
H	1.45487500	-1.19858300	1.30882600	H	-1.62998400	0.29448700	1.23342400
H	-0.06229900	0.10488900	0.59193000	O	0.10284000	0.04071500	1.60566600
H	1.42807200	1.35322600	-0.29193300	H	0.35107600	-0.67468600	0.97377900
H	-2.81493000	-0.08426900	-0.49740900	O	-1.59195800	-0.51625100	-1.69756800
H	-1.35737600	-1.50046100	-0.00313900	H	-1.97590200	-0.09922500	-0.88987300
C	-4.47142200	0.69249200	0.20552600	C	-3.23619900	-0.83454600	1.22581900
H	-4.80558100	1.69390500	0.51085900	H	-3.48040800	-0.72975500	2.29475900
H	-5.14622500	0.32306600	-0.58567600	H	-4.16885700	-0.86895600	0.64784800
H	-4.54588200	0.01637000	1.07607300	H	-2.68361400	-1.77694800	1.07024300
C	-1.23533900	-1.59317200	-1.96009400	C	-0.50865300	3.06573800	-0.05290200
H	-1.95831900	-1.64343700	-2.78490700	H	-0.45648400	3.80155900	-0.86731000
H	-0.67331100	-0.64696100	-2.02622200	H	-1.49434700	2.57018100	-0.08288800
H	-0.53837900	-2.44282900	-2.05064600	H	-0.40945400	3.60146500	0.90696800
C	2.29974200	-2.04371800	-0.23143200	C	0.44968600	-3.04700200	-0.56884100
H	3.32718900	-2.25921100	-0.55378000	H	1.30006300	-3.43062300	0.01043500
H	1.75046600	-2.99365100	-0.13564000	H	-0.48863300	-3.42898600	-0.13456000
H	1.80508600	-1.41434700	-0.99135900	H	0.53658400	-3.39837700	-1.60868800
C	4.08096600	1.09861100	-0.70639500	C	1.01042200	0.01176000	2.72923400
H	4.26219300	2.11892700	-1.06941400	H	0.79979800	0.90432400	3.33278300
H	5.01634300	0.70321500	-0.27908500	H	0.84050000	-0.88634300	3.34384500
H	3.77479000	0.46586000	-1.55707400	H	2.05026400	0.03245800	2.37265200
C	-1.02303500	-0.15841100	2.31464800	C	3.55329400	0.52051700	-0.72228000
H	-1.32559900	-1.02281900	2.92014300	H	2.81993600	1.33080700	-0.86271200
H	-0.40408700	0.51315300	2.93101600	H	4.43310600	0.91986300	-0.19932500
H	-1.91499400	0.37909300	1.95829200	H	3.87686300	0.14143000	-1.70730700
C	-0.20207700	2.48313700	-0.55105400	C	-1.27345500	0.52767200	-2.64328300
H	0.12463900	3.06496200	-1.42731400	H	-0.49553400	1.19645600	-2.24409100
H	-1.27620300	2.27188600	-0.62420100	H	-0.90641000	0.03200600	-3.55162300
H	-0.00310900	3.06466200	0.36388400	H	-2.17577600	1.10593300	-2.89643300
MeOH6_19				MeOH6_20			
O	0.74239000	2.21970000	-0.88913000	H	-2.07474500	-2.28144000	0.85904900
H	0.79111700	1.27991300	-1.16970100	C	-2.94912300	-2.19008500	0.19229700
O	0.77811300	-0.52518500	-1.21721900	H	-3.13594600	-3.16086600	-0.28743700
H	0.20770400	-0.71575600	-0.43250800	H	-3.83386500	-1.92779100	0.79818900

O	-0.64483700	-0.73785600	1.08072900	O	-2.72358600	-1.24153000	-0.85754200
H	-0.76170800	0.24604000	1.21468300	H	-2.54018300	-0.38116100	-0.43733200
O	3.07767100	-0.51449600	0.38149100	H	0.33735300	0.53792400	3.27046100
H	2.38599400	-0.58108700	-0.30415300	C	0.78574100	-0.04106800	2.44819600
O	-2.65979200	-1.24471000	-0.77006300	H	1.46175000	0.60209100	1.86147600
H	-2.06403800	-1.20847300	0.00127100	H	1.36434500	-0.86999300	2.87678100
O	-0.99084300	1.87587900	1.13898600	O	-0.23839900	-0.62856900	1.61939100
H	-0.34455200	2.11007400	0.42428500	H	-0.86393000	0.08493400	1.36321500
C	-4.00145700	-1.31640600	-0.27956500	H	-0.62267000	-2.13585400	-1.71096400
H	-4.66631200	-1.32144800	-1.15389500	C	0.46844300	-2.11510200	-1.57559900
H	-4.17808200	-2.23806700	0.30139200	H	0.80717200	-3.02910800	-1.06301300
H	-4.25588800	-0.44524900	0.34968900	H	0.96537400	-2.04722800	-2.55204100
C	2.07549900	2.63512000	-0.52333200	O	0.85567400	-0.94169300	-0.82500100
H	2.72187600	2.69192800	-1.41320900	H	0.41508700	-0.96948100	0.06231500
H	1.98703000	3.63702900	-0.08340500	H	-3.33818700	2.53880300	-0.24153800
H	2.52519500	1.94702000	0.20914300	C	-2.75960100	2.27583700	0.65799100
C	-2.30982800	2.12738900	0.61488600	H	-2.21436000	3.16443800	1.01459400
H	-2.52956900	1.47628600	-0.24760900	H	-3.45016400	1.94106200	1.44319300
H	-3.02439500	1.91506700	1.42170100	O	-1.85826900	1.18937300	0.38671800
H	-2.41434800	3.18164800	0.31576800	H	-1.22798400	1.45936100	-0.33671900
C	3.59070900	-1.83218000	0.59363900	H	1.84412300	2.35964200	-1.95974000
H	4.09168300	-2.22889700	-0.30642800	C	1.03781600	2.46814300	-1.21924700
H	4.32956000	-1.76691000	1.40388600	H	1.45530400	2.29143000	-0.21564000
H	2.79789300	-2.53900200	0.89812000	H	0.63015400	3.48603000	-1.27823100
C	0.13149900	-1.26528500	2.17666500	O	-0.04949300	1.56492500	-1.50961800
H	0.16826800	-2.35594800	2.05313700	H	0.30094900	0.64787400	-1.43119300
H	1.15435600	-0.85815200	2.15852200	H	4.54602200	-1.36096500	-0.15786800
H	-0.34931000	-1.03029000	3.13845400	C	4.12415000	-0.63265400	0.55656200
C	0.27076500	-1.25898300	-2.35425200	H	3.61642100	-1.18607000	1.36694200
H	0.83004900	-0.91275500	-3.23286400	H	4.94985500	-0.05458400	0.99344700
H	0.43581200	-2.33982000	-2.22301900	O	3.24745400	0.29714300	-0.08395800
H	-0.80305900	-1.06772900	-2.48985500	H	2.49653300	-0.21666200	-0.43906200
MeOH6_21				MeOH6_22			
C	0.20650600	-2.94187800	-0.30288800	C	-0.37985700	-1.84994100	-1.40968200
O	-0.58278500	-1.73239600	-0.34165500	O	-0.55548700	-1.13831500	-0.16560600
H	-0.37031600	-1.19503200	0.46024200	H	-0.23996500	-0.20620900	-0.33093000
H	0.05294100	-3.45446300	-1.26167200	H	-0.66133100	-2.89620900	-1.23144500
H	-0.13162600	-3.60022200	0.51264000	H	0.67049800	-1.80813500	-1.74065500
H	1.27263800	-2.70420000	-0.17005600	H	-1.02649400	-1.42996300	-2.19667100
H	-2.48118100	-1.41555200	-0.18537800	H	0.89362900	-1.54773500	0.84743600
O	-3.27051300	-0.86202400	-0.04732400	O	1.79658300	-1.54185600	1.23595900
C	-2.99395200	0.38774900	-0.68553000	C	1.78566900	-0.54592900	2.27789400
H	-3.88385700	1.01927100	-0.55745600	H	2.78223200	-0.55279500	2.73906200
H	-2.79626800	0.26896200	-1.76476800	H	1.03771900	-0.79049700	3.04830700
H	-2.12963900	0.89951200	-0.22691000	H	1.57731900	0.45789300	1.87046900
O	0.30975100	0.21715900	-2.07064000	O	-3.22722400	-0.91030900	0.53862100
C	1.66589600	-0.16521700	-2.38518500	C	-3.89183500	-1.06882800	-0.72413700
H	-0.08201800	-0.53384600	-1.56875700	H	-2.27695400	-1.09441200	0.37638900
H	2.15498100	0.71467500	-2.82380500	H	-4.95848100	-0.86990300	-0.55697000
H	1.67664100	-0.98109000	-3.12544800	H	-3.78053400	-2.09518400	-1.11243900
H	2.20772600	-0.47831200	-1.47899700	H	-3.51128500	-0.35281500	-1.47398600
H	-2.15943600	0.11717100	2.10905800	H	-0.93066900	1.13305400	1.80909700

C	-1.18564000	0.16033000	2.62095400	C	-1.54772400	2.00197100	1.52114300
O	-0.10277000	0.02210000	1.67532800	O	-2.33087800	1.73480900	0.35460600
H	-1.10989100	-0.68077900	3.32221100	H	-0.87402100	2.83646300	1.28160700
H	-1.08975800	1.10246300	3.18226100	H	-2.17965800	2.29055000	2.37884300
H	-0.04141100	0.84796300	1.12916400	H	-2.80422700	0.89484600	0.51960100
H	0.18942600	3.79281800	-1.14042600	H	4.97957500	-0.49371900	-0.23508800
C	-0.34116500	3.22862500	-0.35704400	C	4.24634600	0.29656400	-0.46216300
O	0.33460400	1.99571400	-0.06828200	O	2.98598200	-0.26679100	-0.85903200
H	-0.34706100	3.82360100	0.56613700	H	4.61829500	0.89202200	-1.30649100
H	-1.38123200	3.05626100	-0.68026000	H	4.13694400	0.95314900	0.41802200
H	0.32051700	1.42753800	-0.88261200	H	2.66683200	-0.83351300	-0.11492100
H	4.21732800	0.09399100	0.34935400	H	0.33217100	1.63846300	-2.62698800
C	3.34920000	0.33846800	0.97707500	C	0.27371400	2.08548700	-1.62048400
O	2.49562800	-0.81530600	0.97939600	O	0.69521100	1.15066900	-0.60921600
H	3.70967800	0.57822900	1.99167600	H	-0.76787900	2.34312600	-1.39197500
H	2.83609400	1.22025200	0.55770900	H	0.89713800	2.99365700	-1.59355400
H	1.68932300	-0.56966200	1.46721400	H	1.58776800	0.79626800	-0.83479600
MeOH6_23				MeOH6_24			
O	-0.99540500	1.43011800	-0.05796600	O	-2.00495000	-1.64939900	-0.75290800
O	-0.83077200	-1.21362500	-0.32720000	H	-1.03226100	-1.77049300	-0.82353300
O	1.84138000	-1.08450000	-0.83652700	O	3.24091100	-0.27162800	-0.42820400
O	2.14432600	-0.04898800	1.76833900	H	2.42657800	-0.69039000	-0.75745400
O	-3.68862500	0.45125900	0.14325000	O	0.75684300	-1.74100900	-0.54008000
O	1.36519000	1.45012900	-1.47725100	H	0.65876400	-1.05487300	0.16652300
H	-0.95860300	0.43929500	-0.05191600	O	-0.27455300	1.66103800	-1.10848000
H	0.10224100	-1.45266000	-0.51180300	H	0.10181200	1.26499500	-0.30074900
H	1.70916800	-0.15151700	-1.16581700	O	0.38195300	0.24175100	1.22794200
H	2.14805600	-0.52673800	0.91678200	H	-0.57226400	0.13969600	1.50458600
H	-2.90759200	1.00365700	-0.03741300	O	-2.20300300	-0.15485600	1.50681300
H	0.47991500	1.56474400	-1.05785300	H	-2.22898800	-0.76252000	0.72416300
C	2.28432900	2.31078900	-0.77108800	C	-2.93106400	1.03243300	1.13488000
H	2.39671500	1.99866600	0.27940200	H	-2.87088600	1.72863800	1.98228100
H	3.25379900	2.23186200	-1.28083300	H	-2.49315700	1.50205900	0.23903000
H	1.94674600	3.35792600	-0.81739800	H	-3.99074200	0.79588900	0.94900900
C	2.72929200	-1.76625600	-1.73949700	C	3.14657600	1.13428500	-0.68184100
H	3.71967100	-1.28436800	-1.75692100	H	2.84632700	1.34699000	-1.72087000
H	2.84066000	-2.79627300	-1.37604100	H	2.42879800	1.62492400	-0.00091800
H	2.31513200	-1.78551000	-2.75985400	H	4.14398200	1.55924700	-0.50459300
C	-4.05599500	-0.16732800	-1.09566000	C	1.24383600	0.31181000	2.38138300
H	-3.21755600	-0.73942800	-1.52919700	H	2.27242400	0.17992500	2.02069000
H	-4.88390000	-0.85593300	-0.87750800	H	1.14689900	1.28829500	2.88113800
H	-4.40384200	0.57393700	-1.83530500	H	1.00182400	-0.48843500	3.09817600
C	1.36017600	-0.81460000	2.68777700	C	-0.13096600	3.07910200	-0.99144100
H	1.41815200	-0.31027900	3.66204700	H	-0.61719900	3.52812700	-1.86821400
H	0.30020600	-0.86377400	2.38172400	H	-0.62084800	3.46788100	-0.08071800
H	1.74826100	-1.84123400	2.80395100	H	0.92942600	3.38675600	-0.98299300
C	-1.49724600	-2.25936200	0.39881600	C	1.24531200	-2.93918000	0.09873800
H	-2.45322800	-1.84268800	0.74148900	H	1.34721200	-3.70381200	-0.68180600
H	-1.68790600	-3.12763300	-0.25216200	H	2.22994900	-2.76119600	0.56005700
H	-0.90645400	-2.58310200	1.27063200	H	0.53756600	-3.29823100	0.86399200
C	-0.74895900	1.87837200	1.29500000	C	-2.43137100	-0.91440600	-1.92009100
H	-0.78536900	2.97564500	1.28066700	H	-3.50303300	-0.70893200	-1.79319100

H	-1.53272900	1.50524900	1.97415200	H	-1.87940700	0.03352800	-2.01498600
H	0.24011600	1.54532800	1.64593600	H	-2.29431900	-1.51950300	-2.83005200
MeOH6_25				MeOH6_26			
O	2.83165300	0.85425400	-0.84488700	O	0.58277300	2.05772700	0.53737400
H	2.31190100	0.64738000	-0.03908500	O	-0.97642100	0.08362200	1.30139600
O	1.31447000	0.07346500	1.33647600	O	0.03243000	-2.38366200	0.51701000
H	0.89160100	-0.73249800	0.93937700	O	1.81064000	0.89281700	-1.51616300
O	0.22012400	-2.01532200	0.07965100	O	3.74674100	-0.47219300	-0.10721200
H	-0.68295500	-1.71279600	-0.19491600	O	-2.39869500	0.37216500	-1.09645300
C	4.04175000	0.10179700	-0.75366600	H	1.08074200	1.65159100	-0.22263600
H	3.84831100	-0.98403700	-0.68075500	H	-0.35462400	0.83364900	1.07477300
H	4.61765600	0.28981100	-1.67036400	H	-0.31505300	-1.54280100	0.87725700
H	4.65486500	0.40911300	0.11244800	H	2.59464300	0.42676700	-1.15455200
C	2.03832000	-0.33936300	2.50371600	H	4.51382600	0.05134100	0.16149200
H	1.36119000	-0.76132700	3.26473100	H	-1.96835600	0.22838400	-0.23033300
H	2.81150700	-1.08797000	2.25959800	C	-3.71488000	-0.17938400	-1.01051400
H	2.52711700	0.55246600	2.91956300	H	-4.19459100	-0.03333900	-1.98786300
C	0.98554600	-2.21109500	-1.12466600	H	-3.69323700	-1.26121500	-0.78907600
H	0.38335200	-2.72739900	-1.88839300	H	-4.32535000	0.32766900	-0.24228800
H	1.35064400	-1.25280600	-1.53022500	C	-1.56836500	0.35885800	2.58135100
H	1.84674700	-2.84391300	-0.86858100	H	-2.22945900	1.24001200	2.53184400
O	-2.19465700	-1.18441100	-0.71939000	H	-2.16350200	-0.51934100	2.86598300
H	-2.43327800	-0.33461200	-0.26762300	H	-0.79440500	0.52910600	3.34624100
C	-3.25943500	-2.11882100	-0.48448400	C	-0.98288500	-2.92176200	-0.33730800
H	-2.99841600	-3.05119700	-1.00323100	H	-1.27802500	-2.20552300	-1.12376300
H	-3.38228400	-2.33203600	0.59074400	H	-0.56572000	-3.82014600	-0.81269100
H	-4.21156300	-1.73990000	-0.88836000	H	-1.88240900	-3.21568300	0.23236300
O	-2.74484400	1.13329600	0.50741900	C	-0.26902300	3.07955200	-0.02167000
H	-2.30649600	1.78607100	-0.08334400	H	-0.73378400	3.61278600	0.81905700
C	-2.09348300	1.20958900	1.79221300	H	0.32357400	3.79542700	-0.61173900
H	-1.02875100	0.93268300	1.72531700	H	-1.05686200	2.64050700	-0.65585500
H	-2.18517800	2.22278000	2.21397300	C	0.92899100	-0.11281800	-2.06904800
H	-2.61190300	0.50376900	2.45514100	H	-0.05014000	0.35796300	-2.22756300
O	-1.23630600	2.70820900	-1.15158700	H	1.31944400	-0.47502600	-3.03285000
H	-1.54469400	2.81014500	-2.06200400	H	0.81221100	-0.95952000	-1.37512600
C	0.00407900	1.95153100	-1.17919400	C	2.98044700	-0.79270800	1.08285400
H	-0.16324500	0.92884300	-1.55222900	H	2.55499600	0.11763600	1.53528700
H	0.76269100	2.45441400	-1.79335300	H	2.17101600	-1.45893500	0.76164400
H	0.35699100	1.90524600	-0.14340300	H	3.60961300	-1.31554500	1.81878900
MeOH6_27				MeOH6_28			
C	3.89154800	1.69285100	-0.21996300	O	2.30155500	-0.15209000	-1.52105400
O	3.11416700	0.67076700	-0.85825400	H	1.36711500	0.11407100	-1.45894700
H	2.17696500	0.97698300	-0.88151900	O	-1.57544400	-0.93704400	0.13746100
H	4.93292900	1.34453800	-0.19770200	H	-0.94483700	-0.17555200	0.11333500
H	3.55584200	1.87265400	0.81611000	O	0.52222800	-2.64133000	1.00161300
H	3.84596200	2.63992400	-0.78233800	H	-0.30208800	-2.13361700	0.88042000
H	0.24859600	1.06130300	-2.94030900	O	0.07865000	1.14657900	-0.21342300
C	-0.03612900	0.50580100	-2.03680500	H	0.90430300	1.29519800	0.30860900
O	0.45801300	1.24611800	-0.90789000	O	2.57349100	1.21303400	0.82596200
H	-1.13427100	0.41425400	-2.00475300	H	2.74855400	0.64105800	0.04475600

H	0.41106600	-0.50207400	-2.08454300	O	-3.66413100	0.93757500	-0.01228000
H	0.13244400	0.78299400	-0.09677700	H	-3.05076300	0.20370200	0.18500800
H	1.18006500	-0.56724500	2.22081900	C	1.27711300	-1.98556000	2.02885600
C	0.19185700	-0.14497300	2.44521300	H	0.75996000	-2.02519600	3.00267300
O	-0.53883900	-0.10423000	1.20168600	H	2.23056600	-2.52400500	2.12040900
H	-0.32562500	-0.78543500	3.17669700	H	1.49229800	-0.93206200	1.78048400
H	0.30977900	0.86587000	2.86952500	C	2.36045900	-1.58323300	-1.72068000
H	-1.44030900	0.26398200	1.35805600	H	1.92423700	-1.85657200	-2.69473700
H	-2.66509500	2.88664900	1.27129200	H	3.42498800	-1.84948500	-1.72678200
C	-2.86522700	2.18283700	0.45299100	H	1.84660900	-2.12225200	-0.90994100
O	-3.05043900	0.88480200	1.05359700	C	-1.63041200	-1.45081200	-1.21025300
H	-3.77539100	2.50521000	-0.07674100	H	-0.64825800	-1.84113300	-1.52272400
H	-2.00983500	2.18774100	-0.24253500	H	-2.35493300	-2.27563300	-1.21379400
H	-3.27905100	0.26313200	0.33200400	H	-1.96600000	-0.67281600	-1.91443600
O	2.84174000	-1.55374600	0.78846000	C	-4.97471200	0.53218500	0.39262400
C	1.89093100	-2.38759500	0.12558700	H	-5.02364500	0.32587300	1.47582300
H	3.00255700	-0.78384200	0.20115800	H	-5.65613300	1.36276000	0.16367100
H	1.80074200	-3.31335600	0.71188700	H	-5.31614700	-0.36299700	-0.15634100
H	2.21848600	-2.65415400	-0.89503100	C	3.34967100	2.41426200	0.67235000
H	0.89442300	-1.91251500	0.07162700	H	3.08915700	3.07549800	1.50919200
H	-2.06784000	-2.44638100	-1.84990600	H	4.42814000	2.19512900	0.71381900
C	-2.38739500	-2.04440300	-0.87626600	H	3.12083200	2.92476400	-0.27821300
O	-3.28076900	-0.91770600	-1.05663400	C	-0.63106300	2.40057500	-0.33852500
H	-1.51791700	-1.66120500	-0.32984700	H	-0.10663800	3.07090300	-1.03758600
H	-2.86730100	-2.83855900	-0.28424600	H	-1.63457100	2.17387400	-0.71927600
H	-4.09172200	-1.23560900	-1.47519600	H	-0.72987300	2.89020400	0.64211100
MeOH6_29							
O	-2.79529000	-1.17132800	0.53549100				
H	-2.03322300	-1.64077100	0.14158300				
O	-0.30714300	-2.02676200	-0.50330700				
H	0.06098200	-1.48425700	0.22593100				
O	2.92660500	-0.70862900	0.04817400				
H	2.36578000	-0.91016000	0.81909600				
O	1.36815200	1.48972100	-0.29998300				
H	2.01092800	0.75304200	-0.41493500				
O	-1.19889100	2.19942400	-1.23734300				
H	-0.27670500	1.90323700	-1.14061700				
O	0.61321000	-0.38890300	1.57915700				
H	0.61630600	0.47809500	1.12382000				
C	-3.67649800	-0.80392300	-0.53269500				
H	-4.55036100	-0.31780400	-0.07745300				
H	-3.20246600	-0.09287500	-1.23180500				
H	-4.02344900	-1.68635500	-1.09727200				
C	-1.76396300	2.16819500	0.07899300				
H	-1.19141000	2.79713200	0.78516800				
H	-2.78080200	2.57686300	0.00313800				
H	-1.83247400	1.14111700	0.47636900				
C	2.10656600	2.69911000	-0.03703200				
H	2.76777300	2.94824000	-0.88110900				
H	1.36906400	3.50296700	0.08753800				
H	2.70559500	2.60479000	0.88275400				
C	-0.32775300	-0.36142500	2.67901900				

H	-1.36086300	-0.31351500	2.30538200
H	-0.18495900	-1.29689200	3.23436000
H	-0.11680800	0.48829800	3.34601000
C	-0.24991700	-1.22359300	-1.69807700
H	0.79177300	-0.99845200	-1.98157100
H	-0.71200800	-1.81371800	-2.50045100
H	-0.80185600	-0.27714800	-1.58423900
C	3.19502800	-1.94076400	-0.65226600
H	3.67860900	-1.66708300	-1.59872500
H	3.88192700	-2.57568800	-0.07144000
H	2.26472400	-2.49284300	-0.85669300