

## Supporting Information

### Structural Investigation of Coal Humic Substances by Selective Isotopic Exchange and High-Resolution Mass Spectrometry

Alexander Zhrebker<sup>1,2\*</sup>, Irina V. Perminova<sup>2</sup>, Yury Kostyukevich<sup>1,3</sup>, Alexey S. Kononikhin<sup>3,4</sup>,  
Oleg Kharybin<sup>1</sup>, Eugene Nikolaev<sup>1</sup>

<sup>1</sup>Skolkovo Institute of Science and Technology, 143025, Skolkovo, Moscow region, Russia, e-mail: [a.zhrebker@skoltech.ru](mailto:a.zhrebker@skoltech.ru)

<sup>2</sup>Department of Chemistry, Lomonosov Moscow State University, Leninskie Gory 1-3, Moscow, Russia

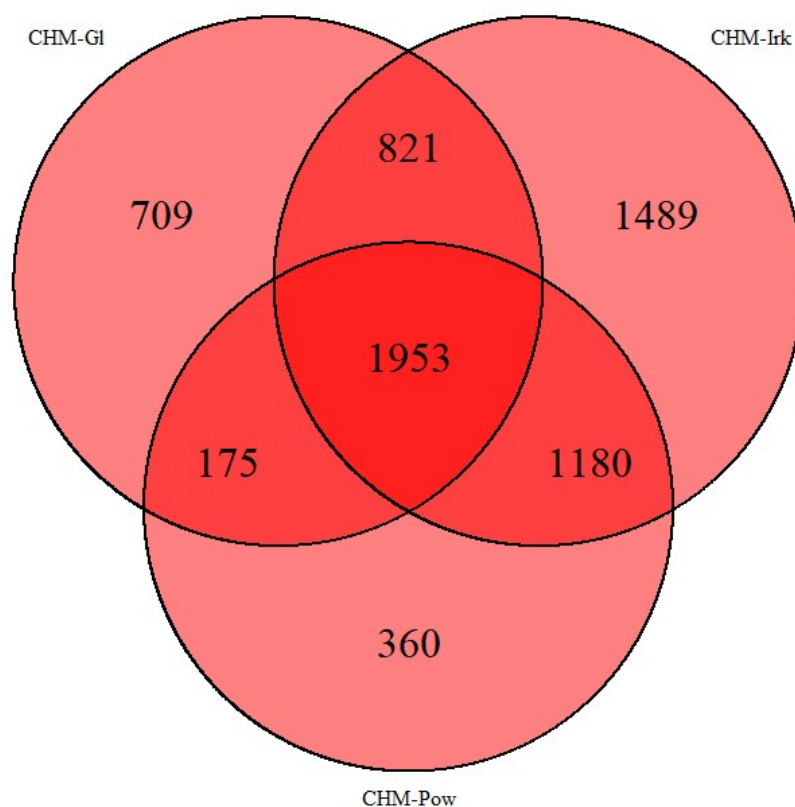
<sup>3</sup>Moscow Institute of Physics and Technology, Dolgoprudnyi, 141700 Moscow Region, Russia

<sup>4</sup>V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Science, Moscow, Russia

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**Figure S1.** Venn diagram for molecular compositions of three coal humatomelanolic acids determined by FTICR MS.

**Table S1.** Results of HDX FTICR MS for 800 most abundant compounds in CHM-Pow

M, Da	Intensity	Formulae	HDX results	
			NaOD	DCl
304.07357	0.025	H12_C19_O4	1	0
308.03213	0.059	H8_C17_O6	1	1
310.12039	0.028	H18_C19_O4	1	0
312.13592	0.035	H20_C19_O4	1	0
318.08924	0.020	H14_C20_O4	1	0
322.12053	0.027	H18_C20_O4	1	0
332.03209	0.040	H8_C19_O6	1	1
346.12648	0.017	H22_C15_O9	1	1
326.00620	0.063	H6_C16_O8	1	0
326.06375	0.057	H14_C14_O9	1	0
328.07351	0.020	H12_C21_O4	1	0
328.20385	0.014	H28_C21_O3	1	0
332.01671	0.099	H8_C15_O9	1	0
356.06838	0.035	H12_C22_O5	1	1
358.04774	0.065	H10_C21_O6	1	1
340.11581	0.055	H20_C16_O8	1	0

344.06834	0.035	H12_C21_O5	1	0
360.01170	0.192	H8_C16_O10	1	1
376.02185	0.119	H8_C20_O8	1	1
348.02703	0.051	H8_C19_O7	1	0
348.13607	0.024	H20_C22_O4	1	0
354.00116	0.090	H6_C17_O9	1	0
382.08395	0.024	H14_C24_O5	1	1
354.24057	0.015	H34_C20_O5	1	0
384.01173	0.205	H8_C18_O10	1	1
386.04264	0.092	H10_C22_O7	1	1
356.11075	0.040	H20_C16_O9	1	0
396.01181	0.219	H8_C19_O10	1	1
398.11545	0.025	H18_C25_O5	1	1
400.00658	0.359	H8_C18_O11	1	1
400.13090	0.039	H20_C25_O5	1	1
362.15174	0.026	H22_C23_O4	1	0
364.02197	0.044	H8_C19_O8	1	0
368.06844	0.022	H12_C23_O5	1	0
372.13624	0.020	H20_C24_O4	1	0
408.09964	0.019	H16_C26_O5	1	1
380.00175	0.026	H8_C15_O12	1	0
410.11552	0.017	H18_C26_O5	1	1
412.09462	0.054	H16_C25_O6	1	1
422.11556	0.018	H18_C27_O5	1	1
384.14201	0.081	H24_C18_O9	1	0
426.11036	0.052	H18_C26_O6	1	1
388.00667	0.262	H8_C17_O11	1	0
432.23006	0.027	H32_C28_O4	1	1
444.15725	0.063	H24_C27_O6	1	1
396.09978	0.019	H16_C25_O5	1	0
450.02233	0.300	H10_C22_O11	1	1
456.12088	0.079	H20_C27_O7	1	1
462.02237	0.311	H10_C23_O11	1	1
466.25661	0.078	H38_C25_O8	1	1
468.08457	0.114	H16_C27_O8	1	1
402.14672	0.037	H22_C25_O5	1	0
474.02231	0.264	H10_C24_O11	1	1
486.05869	0.306	H14_C26_O10	1	1
490.01715	0.275	H10_C24_O12	1	1
412.13116	0.021	H20_C26_O5	1	0
421.99106	0.019	H6_C20_O11	1	0
428.12604	0.064	H20_C26_O6	1	0
438.02229	0.441	H10_C21_O11	1	0
438.07391	0.057	H14_C26_O7	1	0
444.19371	0.027	H28_C28_O5	1	0

448.26138	0.027	H36_C29_O4	1	0
462.07397	0.023	H14_C28_O7	1	0
464.08967	0.032	H16_C28_O7	1	0
464.29270	0.022	H40_C30_O4	1	0
466.01721	0.300	H10_C22_O12	1	0
466.06877	0.062	H14_C27_O8	1	0
470.02748	0.092	H10_C25_O10	1	0
474.24058	0.023	H34_C30_O5	1	0
478.32939	0.025	H46_C28_O6	1	0
480.08452	0.068	H16_C28_O8	1	0
483.99142	0.044	H8_C21_O14	1	0
484.02784	0.329	H12_C22_O13	1	0
484.15231	0.039	H24_C29_O7	1	0
484.18858	0.020	H28_C30_O6	1	0
492.25113	0.072	H36_C30_O6	1	0
494.13673	0.022	H22_C30_O7	1	0
494.26688	0.090	H38_C30_O6	1	0
494.28798	0.057	H42_C27_O8	1	0
368.01684	0.189	H8_C18_O9	2	1
384.09974	0.033	H16_C24_O5	2	1
400.09467	0.093	H16_C24_O6	2	1
402.02227	0.367	H10_C18_O11	2	1
406.21444	0.027	H30_C26_O4	2	1
414.14677	0.028	H22_C26_O5	2	1
416.16238	0.043	H24_C26_O5	2	1
418.21440	0.027	H30_C27_O4	2	1
440.08966	0.084	H16_C26_O7	2	1
460.18865	0.075	H28_C28_O6	2	1
328.16750	0.046	H24_C20_O4	3	1
346.04767	0.059	H10_C20_O6	3	1
350.15169	0.032	H22_C22_O4	3	1
352.20377	0.018	H28_C23_O3	3	1
374.24562	0.027	H34_C23_O4	3	1
376.13111	0.057	H20_C23_O5	3	1
376.16744	0.027	H24_C24_O4	3	1
386.11525	0.036	H18_C24_O5	3	1
390.14671	0.058	H22_C24_O5	3	1
390.18286	0.019	H26_C25_O4	3	1
402.18315	0.023	H26_C26_O4	3	1
416.12600	0.087	H20_C25_O6	3	1
418.05358	0.441	H14_C19_O11	3	1
428.31394	0.023	H44_C24_O6	3	1
430.21450	0.019	H30_C28_O4	3	1
434.24561	0.028	H34_C28_O4	3	1
458.17301	0.048	H26_C28_O6	3	1

478.25670	0.128	H38_C26_O8	3	1
492.27232	0.103	H40_C27_O8	3	1
324.19361	0.041	H28_C18_O5	4	1
338.15172	0.037	H22_C21_O4	4	1
358.21437	0.039	H30_C22_O4	4	1
378.18318	0.034	H26_C24_O4	4	1
380.19866	0.039	H28_C24_O4	4	1
384.23007	0.050	H32_C24_O4	4	1
394.21444	0.042	H30_C25_O4	4	1
396.23003	0.047	H32_C25_O4	4	1
410.24559	0.042	H34_C26_O4	4	1
306.03756	0.048	H10_C14_O8	2	0
312.12092	0.036	H20_C15_O7	2	0
314.18806	0.031	H26_C20_O3	2	0
360.09961	0.052	H16_C22_O5	2	0
372.09972	0.041	H16_C23_O5	2	0
374.15180	0.022	H22_C24_O4	2	0
386.15184	0.017	H22_C25_O4	2	0
388.26146	0.031	H36_C24_O4	2	0
392.19871	0.037	H28_C25_O4	2	0
422.24563	0.036	H34_C27_O4	4	1
404.03797	0.361	H12_C18_O11	2	0
464.21990	0.126	H32_C28_O6	4	1
464.25630	0.055	H36_C29_O5	4	1
472.28246	0.096	H40_C28_O6	4	1
442.17800	0.022	H26_C28_O5	2	0
456.32403	0.026	H44_C29_O4	2	0
460.22495	0.034	H32_C29_O5	2	0
466.27189	0.066	H38_C29_O5	2	0
488.18354	0.070	H28_C29_O7	2	0
492.30868	0.042	H44_C28_O7	2	0
494.01219	0.183	H10_C23_O13	2	0
474.16780	0.099	H26_C28_O7	4	1
478.23555	0.088	H34_C29_O6	4	1
478.27190	0.048	H38_C30_O5	4	1
490.23551	0.048	H34_C30_O6	4	1
390.24071	0.060	H34_C23_O5	5	1
408.25115	0.060	H36_C23_O6	5	1
420.25108	0.086	H36_C24_O6	5	1
438.24071	0.097	H34_C27_O5	5	1
442.27191	0.066	H38_C27_O5	5	1
484.28248	0.113	H40_C29_O6	5	1
490.25663	0.154	H38_C27_O8	5	1
446.26683	0.102	H38_C26_O6	6	1
324.02702	0.112	H8_C17_O7	1	2

324.13605	0.034	H20_C20_O4	1	2
334.04769	0.154	H10_C19_O6	1	2
356.01677	0.307	H8_C17_O9	1	2
362.02730	0.218	H10_C16_O10	1	2
362.04264	0.130	H10_C20_O7	1	2
384.06340	0.064	H12_C23_O6	1	2
390.02227	0.319	H10_C17_O11	1	2
400.05831	0.176	H12_C23_O7	1	2
402.03756	0.201	H10_C22_O8	1	2
406.03245	0.274	H10_C21_O9	1	2
430.01726	0.381	H10_C19_O12	1	2
430.17791	0.043	H26_C27_O5	1	2
442.01723	0.385	H10_C20_O12	1	2
446.02737	0.310	H10_C23_O10	1	2
454.06879	0.137	H14_C26_O8	1	2
480.03292	0.623	H12_C23_O12	1	2
306.05282	0.077	H10_C18_O5	2	2
312.02700	0.155	H8_C16_O7	2	2
350.11542	0.065	H18_C21_O5	2	2
364.13105	0.062	H20_C22_O5	2	2
372.01174	0.452	H8_C17_O10	2	2
418.14165	0.111	H22_C25_O6	2	2
330.18313	0.055	H26_C20_O4	3	2
332.06838	0.086	H12_C20_O5	3	2
338.04254	0.162	H10_C18_O7	3	2
344.01680	0.352	H8_C16_O9	3	2
352.13102	0.080	H20_C21_O5	3	2
352.16759	0.031	H24_C22_O4	3	2
358.08412	0.053	H14_C22_O5	3	2
366.18300	0.033	H26_C23_O4	3	2
388.22489	0.084	H32_C23_O5	3	2
398.07892	0.071	H14_C24_O6	3	2
492.23599	0.169	H36_C26_O9	3	2
316.16754	0.037	H24_C19_O4	4	2
338.06372	0.103	H14_C15_O9	4	2
340.16743	0.047	H24_C21_O4	4	2
346.08408	0.050	H14_C21_O5	4	2
354.18304	0.046	H26_C22_O4	4	2
370.21445	0.043	H30_C23_O4	4	2
376.04309	0.206	H12_C17_O10	4	2
378.14662	0.065	H22_C23_O5	4	2
402.24059	0.079	H34_C24_O5	4	2
404.16240	0.054	H24_C25_O5	4	2
416.08963	0.215	H16_C24_O7	4	2
430.10525	0.152	H18_C25_O7	4	2

432.15725	0.109	H24_C26_O6	4	2
448.22493	0.069	H32_C28_O5	4	2
460.24601	0.166	H36_C26_O7	4	2
340.13103	0.080	H20_C20_O5	5	2
394.23556	0.086	H34_C22_O6	5	2
408.19368	0.084	H28_C25_O5	5	2
420.15728	0.130	H24_C25_O6	5	2
422.20937	0.083	H30_C26_O5	5	2
434.26678	0.080	H38_C25_O6	5	2
464.24103	0.164	H36_C25_O8	5	2
486.26179	0.157	H38_C28_O7	5	2
488.27737	0.104	H40_C28_O7	5	2
418.23553	0.135	H34_C24_O6	6	2
454.23548	0.160	H34_C27_O6	6	2
470.26683	0.131	H38_C28_O6	6	2
414.07391	0.139	H14_C24_O7	1	3
426.02230	0.362	H10_C20_O11	1	3
426.07395	0.118	H14_C25_O7	1	3
430.03253	0.211	H10_C23_O9	1	3
430.14167	0.069	H22_C26_O6	1	3
440.03800	0.687	H12_C21_O11	1	3
446.17294	0.089	H26_C27_O6	1	3
458.10014	0.214	H18_C26_O8	1	3
458.13658	0.099	H22_C27_O7	1	3
466.05356	0.772	H14_C23_O11	1	3
472.07944	0.294	H16_C26_O9	1	3
476.03797	0.553	H12_C24_O11	1	3
488.03794	0.432	H12_C25_O11	1	3
302.18824	0.016	H26_C19_O3	3	0
304.16748	0.021	H24_C18_O4	3	0
306.18317	0.022	H26_C18_O4	3	0
308.19874	0.024	H28_C18_O4	3	0
310.06879	0.069	H14_C14_O8	3	0
312.01176	0.024	H8_C12_O10	3	0
312.19371	0.015	H28_C17_O5	3	0
318.18315	0.035	H26_C19_O4	3	0
318.21956	0.014	H30_C20_O3	3	0
328.22479	0.014	H32_C18_O5	3	0
334.21429	0.027	H30_C20_O4	3	0
336.13621	0.028	H20_C21_O4	3	0
336.23016	0.017	H32_C20_O4	3	0
494.23045	0.144	H34_C29_O7	1	3
302.11546	0.049	H18_C17_O5	2	3
340.22486	0.014	H32_C19_O5	3	0
346.21444	0.027	H30_C21_O4	3	0

316.02182	0.168	H8_C15_O8	2	3
348.04805	0.166	H12_C16_O9	3	0
318.03761	0.218	H10_C15_O8	2	3
350.24549	0.016	H34_C21_O4	3	0
354.21944	0.015	H30_C23_O3	3	0
364.16742	0.028	H24_C23_O4	3	0
364.20376	0.017	H28_C24_O3	3	0
364.26120	0.019	H36_C22_O4	3	0
368.23528	0.022	H32_C24_O3	3	0
372.23017	0.031	H32_C23_O4	3	0
380.23523	0.016	H32_C25_O3	3	0
382.25079	0.019	H34_C25_O3	3	0
388.13109	0.049	H20_C24_O5	3	0
388.16748	0.022	H24_C25_O4	3	0
390.27686	0.018	H38_C24_O4	3	0
392.29257	0.021	H40_C24_O4	3	0
396.25113	0.033	H36_C22_O6	3	0
398.26672	0.018	H38_C22_O6	3	0
404.19868	0.030	H28_C26_O4	3	0
408.26629	0.017	H36_C27_O3	3	0
412.26131	0.035	H36_C26_O4	3	0
414.11034	0.070	H18_C25_O6	3	0
420.23011	0.042	H32_C27_O4	3	0
426.27687	0.029	H38_C27_O4	3	0
322.04781	0.107	H10_C18_O6	2	3
434.30310	0.024	H42_C26_O5	3	0
436.26135	0.031	H36_C28_O4	3	0
438.27707	0.038	H38_C28_O4	3	0
440.29258	0.027	H40_C28_O4	3	0
442.30833	0.025	H42_C28_O4	3	0
450.27694	0.030	H38_C29_O4	3	0
450.29823	0.026	H42_C26_O6	3	0
452.20458	0.155	H32_C23_O9	3	0
452.29263	0.025	H40_C29_O4	3	0
454.30819	0.031	H42_C29_O4	3	0
462.29811	0.057	H42_C27_O6	3	0
462.33467	0.020	H46_C28_O5	3	0
464.31365	0.027	H44_C27_O6	3	0
466.22020	0.129	H34_C24_O9	3	0
466.30840	0.021	H42_C30_O4	3	0
474.20414	0.056	H30_C29_O6	3	0
476.21989	0.085	H32_C29_O6	3	0
476.27737	0.112	H40_C27_O7	3	0
480.27234	0.059	H40_C26_O8	3	0
488.31373	0.068	H44_C29_O6	3	0



488.35025	0.033	H48_C30_O5	3	0
490.03843	0.090	H14_C21_O14	3	0
346.03240	0.380	H10_C16_O9	2	3
360.06337	0.138	H12_C21_O6	2	3
362.11535	0.056	H18_C22_O5	2	3
372.06336	0.091	H12_C22_O6	2	3
374.02737	0.423	H10_C17_O10	2	3
386.07901	0.096	H14_C23_O6	2	3
418.17800	0.062	H26_C26_O5	2	3
444.03288	0.563	H12_C20_O12	2	3
450.24059	0.069	H34_C28_O5	2	3
472.04305	0.328	H12_C25_O10	2	3
474.05869	0.491	H14_C25_O10	2	3
478.22023	0.204	H34_C25_O9	2	3
492.06928	0.665	H16_C25_O11	2	3
492.21483	0.142	H32_C29_O7	2	3
302.07906	0.078	H14_C16_O6	3	3
308.05312	0.077	H12_C14_O8	3	3
312.09976	0.073	H16_C18_O5	3	3
320.06852	0.053	H12_C19_O5	3	3
326.15171	0.044	H22_C20_O4	3	3
328.02186	0.364	H8_C16_O8	3	3
330.03754	0.248	H10_C16_O8	3	3
332.05318	0.177	H12_C16_O8	3	3
334.08414	0.055	H14_C20_O5	3	3
336.06335	0.111	H12_C19_O6	3	3
342.18299	0.043	H26_C21_O4	3	3
348.09972	0.064	H16_C21_O5	3	3
358.03251	0.407	H10_C17_O9	3	3
378.03754	0.366	H10_C20_O8	3	3
388.09473	0.106	H16_C23_O6	3	3
396.14201	0.142	H24_C19_O9	3	3
416.19889	0.019	H28_C27_O4	3	3
438.22540	0.138	H34_C23_O8	3	3
444.08446	0.295	H16_C25_O8	3	3
446.20932	0.056	H30_C28_O5	3	3
458.06380	0.312	H14_C25_O9	3	3
464.07435	0.706	H16_C24_O10	3	3
470.10012	0.128	H18_C27_O8	3	3
474.13150	0.184	H22_C27_O8	3	3
476.14712	0.235	H24_C27_O8	3	3
482.19409	0.328	H30_C27_O8	3	3
488.11068	0.236	H20_C27_O9	3	3
488.14708	0.141	H24_C28_O8	3	3
488.16830	0.380	H28_C25_O10	3	3

490.09001	0.472	H18_C26_O10	3	3
492.10565	0.488	H20_C26_O10	3	3
302.15189	0.034	H22_C18_O4	4	3
308.08949	0.083	H16_C15_O7	4	3
308.12586	0.056	H20_C16_O6	4	3
310.04774	0.123	H10_C17_O6	4	3
310.08413	0.078	H14_C18_O5	4	3
310.14162	0.058	H22_C16_O6	4	3
314.15176	0.047	H22_C19_O4	4	3
316.05824	0.197	H12_C16_O7	4	3
318.14667	0.077	H22_C18_O5	4	3
356.19876	0.045	H28_C22_O4	4	3
368.19868	0.060	H28_C23_O4	4	3
368.21980	0.068	H32_C20_O6	4	3
382.23552	0.042	H34_C21_O6	4	3
386.02733	0.760	H10_C18_O10	4	3
392.16237	0.079	H24_C24_O5	4	3
398.24561	0.038	H34_C25_O4	4	3
402.11028	0.092	H18_C24_O6	4	3
428.25625	0.068	H36_C26_O5	4	3
432.25124	0.124	H36_C25_O6	4	3
436.22491	0.080	H32_C27_O5	4	3
442.10527	0.105	H18_C26_O7	4	3
444.12090	0.120	H20_C26_O7	4	3
446.13655	0.152	H22_C26_O7	4	3
456.06926	0.872	H16_C22_O11	4	3
460.15219	0.132	H24_C27_O7	4	3
474.09512	0.325	H18_C26_O9	4	3
482.30324	0.051	H42_C30_O5	4	3
488.07429	0.467	H16_C26_O10	4	3
490.12643	0.285	H22_C27_O9	4	3
490.16277	0.169	H26_C28_O8	4	3
490.19902	0.099	H30_C29_O7	4	3
304.09471	0.086	H16_C16_O6	5	3
306.07393	0.105	H14_C15_O7	5	3
306.11028	0.077	H18_C16_O6	5	3
312.15729	0.045	H24_C16_O6	5	3
316.13112	0.105	H20_C18_O5	5	3
320.16242	0.059	H24_C18_O5	5	3
324.12092	0.068	H20_C16_O7	5	3
326.13644	0.058	H22_C16_O7	5	3
326.17294	0.055	H26_C17_O6	5	3
338.11532	0.073	H18_C20_O5	5	3
340.18858	0.056	H28_C18_O6	5	3
350.06379	0.190	H14_C16_O9	5	3

350.20933	0.061	H30_C20_O5	5	3
354.20427	0.061	H30_C19_O6	5	3
364.09464	0.166	H16_C21_O6	5	3
374.20934	0.093	H30_C22_O5	5	3
386.20931	0.106	H30_C23_O5	5	3
394.17796	0.096	H26_C24_O5	5	3
400.22488	0.106	H32_C24_O5	5	3
404.21981	0.149	H32_C23_O6	5	3
404.25632	0.077	H36_C24_O5	5	3
410.20928	0.109	H30_C25_O5	5	3
414.24058	0.087	H34_C25_O5	5	3
420.19361	0.068	H28_C26_O5	5	3
422.17293	0.154	H26_C25_O6	5	3
426.24072	0.096	H34_C26_O5	5	3
430.05360	0.719	H14_C20_O11	5	3
434.17295	0.128	H26_C26_O6	5	3
434.20934	0.111	H30_C27_O5	5	3
440.25618	0.090	H36_C27_O5	5	3
442.23551	0.168	H34_C26_O6	5	3
444.25115	0.122	H36_C26_O6	5	3
448.24609	0.148	H36_C25_O7	5	3
450.18893	0.218	H30_C23_O9	5	3
450.22530	0.178	H34_C24_O8	5	3
452.25631	0.084	H36_C28_O5	5	3
454.27192	0.086	H38_C28_O5	5	3
458.26683	0.104	H38_C27_O6	5	3
466.23549	0.137	H34_C28_O6	5	3
470.12125	0.538	H22_C24_O10	5	3
308.16235	0.041	H24_C17_O5	4	0
310.10524	0.043	H18_C15_O7	4	0
314.13643	0.025	H22_C15_O7	4	0
320.19879	0.028	H28_C19_O4	4	0
322.21431	0.017	H30_C19_O4	4	0
330.13144	0.022	H22_C15_O8	4	0
332.19887	0.046	H28_C20_O4	4	0
340.09459	0.175	H16_C19_O6	4	0
342.16782	0.043	H26_C17_O7	4	0
344.19863	0.051	H28_C21_O4	4	0
348.23002	0.025	H32_C21_O4	4	0
352.22501	0.028	H32_C20_O5	4	0
356.21979	0.016	H32_C19_O6	4	0
360.22998	0.033	H32_C22_O4	4	0
362.24581	0.016	H34_C22_O4	4	0
366.24053	0.027	H34_C21_O5	4	0
374.11541	0.048	H18_C23_O5	4	0

380.25623	0.019	H36_C22_O5	4	0
386.24577	0.030	H34_C24_O4	4	0
392.25616	0.038	H36_C23_O5	4	0
400.26144	0.030	H36_C25_O4	4	0
474.26174	0.148	H38_C27_O7	5	3
402.27691	0.026	H38_C25_O4	4	0
406.27172	0.031	H38_C24_O5	4	0
408.22993	0.044	H32_C26_O4	4	0
414.27702	0.020	H38_C26_O4	4	0
420.28756	0.026	H40_C25_O5	4	0
424.26137	0.038	H36_C27_O4	4	0
428.29254	0.025	H40_C27_O4	4	0
480.25123	0.112	H36_C29_O6	5	3
430.30838	0.023	H42_C27_O4	4	0
484.17334	0.399	H28_C26_O9	5	3
340.15210	0.077	H24_C17_O7	6	3
406.23550	0.108	H34_C23_O6	6	3
436.28263	0.030	H40_C25_O6	4	0
430.23554	0.142	H34_C25_O6	6	3
460.17336	0.435	H28_C24_O9	6	3
438.26195	0.041	H38_C24_O7	4	0
442.22007	0.035	H34_C22_O9	4	0
474.22537	0.239	H34_C26_O8	6	3
354.16779	0.098	H26_C18_O7	7	3
406.17801	0.071	H26_C25_O5	1	4
448.31887	0.020	H44_C27_O5	4	0
418.03245	0.272	H10_C22_O9	1	4
454.05358	0.802	H14_C22_O11	4	0
434.02740	0.274	H10_C22_O10	1	4
456.03283	0.595	H12_C21_O12	1	4
460.11582	0.230	H20_C26_O8	4	0
460.31900	0.031	H44_C28_O5	4	0
456.08451	0.162	H16_C26_O8	1	4
460.04307	0.445	H12_C24_O10	1	4
462.24062	0.052	H34_C29_O5	4	0
462.26166	0.132	H38_C26_O7	4	0
464.27729	0.061	H40_C26_O7	4	0
476.25625	0.043	H36_C30_O5	4	0
476.31379	0.045	H44_C28_O6	4	0
478.29309	0.064	H42_C27_O7	4	0
480.28747	0.047	H40_C30_O5	4	0
490.32940	0.042	H46_C29_O6	4	0
472.11578	0.162	H20_C27_O8	1	4
492.03287	0.690	H12_C24_O12	1	4
314.11537	0.063	H18_C18_O5	2	4

390.11028	0.122	H18_C23_O6	2	4
394.03251	0.496	H10_C20_O9	2	4
398.02744	0.573	H10_C19_O10	2	4
410.02740	0.440	H10_C20_O10	2	4
420.04814	0.809	H12_C22_O9	2	4
432.19377	0.053	H28_C27_O5	2	4
448.04306	0.760	H12_C23_O10	2	4
470.08491	0.725	H18_C23_O11	2	4
494.15761	0.343	H26_C27_O9	2	4
494.19408	0.262	H30_C28_O8	2	4
302.04265	0.182	H10_C15_O7	3	4
322.08412	0.074	H14_C19_O5	3	4
324.06338	0.221	H12_C18_O6	3	4
334.06877	0.215	H14_C16_O8	3	4
336.09968	0.069	H16_C20_O5	3	4
350.04258	0.264	H10_C19_O7	3	4
352.02191	0.158	H8_C18_O8	3	4
362.06376	0.248	H14_C17_O9	3	4
388.04303	0.687	H12_C18_O10	3	4
388.05824	0.181	H12_C22_O7	3	4
406.08999	0.401	H18_C19_O10	3	4
418.08999	0.469	H18_C20_O10	3	4
420.08457	0.451	H16_C23_O8	3	4
422.12129	0.258	H22_C20_O10	3	4
428.03796	0.831	H12_C20_O11	3	4
428.08967	0.143	H16_C25_O7	3	4
430.06883	0.295	H14_C24_O8	3	4
432.04811	0.414	H12_C23_O9	3	4
452.03791	0.583	H12_C22_O11	3	4
462.20424	0.110	H30_C28_O6	3	4
478.09001	0.599	H18_C25_O10	3	4
304.13099	0.074	H20_C17_O5	4	4
306.14667	0.046	H22_C17_O5	4	4
312.06338	0.128	H12_C17_O6	4	4
314.04265	0.178	H10_C16_O7	4	4
324.09970	0.083	H16_C19_O5	4	4
336.08443	0.184	H16_C16_O8	4	4
348.06334	0.159	H12_C20_O6	4	4
348.19369	0.086	H28_C20_O5	4	4
354.03753	0.381	H10_C18_O8	4	4
356.14715	0.067	H24_C17_O8	4	4
358.17803	0.118	H26_C21_O5	4	4
376.05838	0.345	H12_C21_O7	4	4
382.21434	0.061	H30_C24_O4	4	4
390.05869	0.336	H14_C18_O10	4	4

398.20938	0.161	H30_C24_O5	4	4
404.12597	0.107	H20_C24_O6	4	4
416.03799	0.633	H12_C19_O11	4	4
416.07438	0.677	H16_C20_O10	4	4
428.07437	0.887	H16_C21_O10	4	4
442.05359	0.942	H14_C21_O11	4	4
444.04816	0.356	H12_C24_O9	4	4
446.06378	0.607	H14_C24_O9	4	4
448.18853	0.116	H28_C27_O6	4	4
458.08488	0.625	H18_C22_O11	4	4
462.05870	0.808	H14_C24_O10	4	4
464.11069	0.472	H20_C25_O9	4	4
476.07429	0.595	H16_C25_O10	4	4
480.14199	0.422	H24_C26_O9	4	4
482.08494	0.700	H18_C24_O11	4	4
484.13694	0.460	H24_C25_O10	4	4
486.09516	0.243	H18_C27_O9	4	4
320.12599	0.120	H20_C17_O6	5	4
322.10529	0.092	H18_C16_O7	5	4
322.14169	0.080	H22_C17_O6	5	4
322.17803	0.053	H26_C18_O5	5	4
324.15726	0.077	H24_C17_O6	5	4
328.05831	0.263	H12_C17_O7	5	4
328.13095	0.093	H20_C19_O5	5	4
330.14670	0.127	H22_C19_O5	5	4
332.08961	0.186	H16_C17_O7	5	4
332.16235	0.085	H24_C19_O5	5	4
334.17798	0.077	H26_C19_O5	5	4
336.12092	0.128	H20_C17_O7	5	4
336.19362	0.058	H28_C19_O5	5	4
338.10002	0.105	H18_C16_O8	5	4
344.08965	0.218	H16_C18_O7	5	4
344.16238	0.118	H24_C20_O5	5	4
346.17805	0.108	H26_C20_O5	5	4
348.08450	0.280	H16_C17_O8	5	4
354.14676	0.086	H22_C21_O5	5	4
356.16238	0.103	H24_C21_O5	5	4
362.20923	0.089	H30_C21_O5	5	4
364.22509	0.057	H32_C21_O5	5	4
366.14674	0.098	H22_C22_O5	5	4
370.03238	0.893	H10_C18_O9	5	4
370.17789	0.127	H26_C22_O5	5	4
372.19362	0.113	H28_C22_O5	5	4
376.22496	0.101	H32_C22_O5	5	4
380.16243	0.102	H24_C23_O5	5	4

384.19359	0.132	H28_C23_O5	5	4
406.06881	0.441	H14_C22_O8	5	4
412.22496	0.138	H32_C25_O5	5	4
416.21986	0.181	H32_C24_O6	5	4
424.22491	0.101	H32_C26_O5	5	4
436.18859	0.140	H28_C26_O6	5	4
448.13695	0.384	H24_C22_O10	5	4
450.16783	0.219	H26_C26_O7	5	4
460.07940	0.452	H16_C25_O9	5	4
462.13146	0.289	H22_C26_O8	5	4
462.16788	0.174	H26_C27_O7	5	4
468.25119	0.144	H36_C28_O6	5	4
474.15254	0.429	H26_C24_O10	5	4
476.18359	0.143	H28_C28_O7	5	4
478.19913	0.179	H30_C28_O7	5	4
480.21482	0.206	H32_C28_O7	5	4
482.15763	0.402	H26_C26_O9	5	4
482.26688	0.119	H38_C29_O6	5	4
488.24094	0.209	H36_C27_O8	5	4
490.18388	0.273	H30_C25_O10	5	4
350.13658	0.144	H22_C18_O7	6	4
352.11579	0.114	H20_C17_O8	6	4
352.18853	0.127	H28_C19_O6	6	4
370.16268	0.096	H26_C18_O8	6	4
376.18854	0.158	H28_C21_O6	6	4
380.21981	0.117	H32_C21_O6	6	4
396.21477	0.120	H32_C21_O7	6	4
398.19408	0.095	H30_C20_O8	6	4
416.14715	0.490	H24_C22_O8	6	4
428.21992	0.208	H32_C25_O6	6	4
434.19410	0.255	H30_C23_O8	6	4
446.23047	0.214	H34_C25_O7	6	4
450.20419	0.150	H30_C27_O6	6	4
456.21483	0.291	H32_C26_O7	6	4
456.25122	0.147	H36_C27_O6	6	4
458.23044	0.218	H34_C26_O7	6	4
462.18902	0.297	H30_C24_O9	6	4
470.15763	0.456	H26_C25_O9	6	4
470.19406	0.373	H30_C26_O8	6	4
470.23051	0.236	H34_C27_O7	6	4
474.18894	0.354	H30_C25_O9	6	4
380.18346	0.211	H28_C20_O7	7	4
384.17834	0.097	H28_C19_O8	7	4
408.17839	0.265	H28_C21_O8	7	4
410.15761	0.191	H26_C20_O9	7	4

488.20464	0.303	H32_C26_O9	7	4
428.05319	0.213	H12_C24_O8	1	5
458.19409	0.413	H30_C25_O8	1	5
478.05361	0.761	H14_C24_O11	1	5
318.07389	0.115	H14_C16_O7	2	5
362.07894	0.147	H14_C21_O6	2	5
364.05821	0.241	H12_C20_O7	2	5
374.04267	0.135	H10_C21_O7	2	5
390.03749	0.180	H10_C21_O8	2	5
390.07399	0.282	H14_C22_O7	2	5
396.19374	0.113	H28_C24_O5	2	5
418.10523	0.208	H18_C24_O7	2	5
492.17836	0.215	H28_C28_O8	2	5
494.12121	0.484	H22_C26_O10	2	5
316.09470	0.097	H16_C17_O6	3	5
326.04257	0.426	H10_C17_O7	3	5
364.07940	0.299	H16_C17_O9	3	5
382.03247	0.310	H10_C19_O9	3	5
388.07939	0.497	H16_C19_O9	3	5
404.05325	0.453	H12_C22_O8	3	5
408.14195	0.242	H24_C20_O9	3	5
416.05326	0.259	H12_C23_O8	3	5
424.04310	0.571	H12_C21_O10	3	5
434.10015	0.374	H18_C24_O8	3	5
442.06884	0.197	H14_C25_O8	3	5
446.10019	0.295	H18_C25_O8	3	5
478.12640	0.424	H22_C26_O9	3	5
480.06930	0.764	H16_C24_O11	3	5
482.23054	0.211	H34_C28_O7	3	5
320.08951	0.149	H16_C16_O7	4	5
326.07899	0.165	H14_C18_O6	4	5
326.11540	0.063	H18_C19_O5	4	5
340.02188	0.153	H8_C17_O8	4	5
352.09472	0.170	H16_C20_O6	4	5
360.04809	0.394	H12_C17_O9	4	5
374.07900	0.145	H14_C22_O6	4	5
376.07940	0.388	H16_C18_O9	4	5
376.09458	0.150	H16_C22_O6	4	5
378.07393	0.282	H14_C21_O7	4	5
392.05318	0.517	H12_C21_O8	4	5
392.12596	0.148	H20_C23_O6	4	5
400.04300	0.875	H12_C19_O10	4	5
402.05869	0.601	H14_C19_O10	4	5
406.10526	0.255	H18_C23_O7	4	5
310.17805	0.035	H26_C17_O5	5	0



314.17271	0.017	H26_C16_O6	5	0
328.15211	0.032	H24_C16_O7	5	0
408.04807	0.541	H12_C21_O9	4	5
338.20927	0.045	H30_C19_O5	5	0
342.11027	0.157	H18_C19_O6	5	0
356.18354	0.038	H28_C18_O7	5	0
366.09505	0.180	H18_C17_O9	5	0
370.19908	0.046	H30_C19_O7	5	0
378.24061	0.054	H34_C22_O5	5	0
384.21480	0.037	H32_C20_O7	5	0
398.15763	0.110	H26_C19_O9	5	0
416.25628	0.061	H36_C25_O5	5	0
418.27181	0.063	H38_C25_O5	5	0
422.23050	0.128	H34_C23_O7	5	0
422.26683	0.037	H38_C24_O6	5	0
424.24607	0.054	H36_C23_O7	5	0
426.22543	0.068	H34_C22_O8	5	0
430.27201	0.056	H38_C26_O5	5	0
432.28759	0.040	H40_C26_O5	5	0
436.24604	0.113	H36_C24_O7	5	0
444.28761	0.058	H40_C27_O5	5	0
446.30325	0.038	H42_C27_O5	5	0
448.28253	0.059	H40_C26_O6	5	0
450.11622	0.254	H22_C21_O11	5	0
450.26174	0.081	H38_C25_O7	5	0
452.24100	0.092	H36_C24_O8	5	0
422.06376	0.693	H14_C22_O9	4	5
430.08997	0.608	H18_C21_O10	4	5
434.15766	0.340	H26_C22_O9	4	5
456.28754	0.065	H40_C28_O5	5	0
436.04303	0.759	H12_C22_O10	4	5
440.07437	0.924	H16_C22_O10	4	5
458.30309	0.051	H42_C28_O5	5	0
446.15767	0.468	H26_C23_O9	4	5
448.07940	0.518	H16_C24_O9	4	5
450.05863	0.696	H14_C23_O10	4	5
458.12127	0.556	H22_C23_O10	4	5
464.13182	0.230	H24_C22_O11	5	0
480.10564	0.596	H20_C25_O10	4	5
486.18899	0.374	H30_C26_O9	4	5
492.14195	0.319	H24_C27_O9	4	5
466.12640	0.491	H22_C25_O9	5	0
314.07906	0.107	H14_C17_O6	5	5
318.11026	0.139	H18_C17_O6	5	5
468.28748	0.076	H40_C29_O5	5	0

328.09460	0.154	H16_C18_O6	5	5
470.30324	0.061	H42_C29_O5	5	0
330.07388	0.196	H14_C17_O7	5	5
330.11025	0.164	H18_C18_O6	5	5
334.14167	0.122	H22_C18_O6	5	5
472.31885	0.051	H44_C29_O5	5	0
474.29814	0.075	H42_C28_O6	5	0
474.33463	0.033	H46_C29_O5	5	0
476.09546	0.248	H20_C22_O12	5	0
484.31879	0.041	H44_C30_O5	5	0
486.33458	0.068	H46_C30_O5	5	0
490.22022	0.208	H34_C26_O9	5	0
336.15724	0.096	H24_C18_O6	5	5
490.29313	0.089	H42_C28_O7	5	0
338.07904	0.203	H14_C19_O6	5	5
338.17290	0.113	H26_C18_O6	5	5
342.03756	0.532	H10_C17_O8	5	5
342.14670	0.112	H22_C20_O5	5	5
344.05319	0.429	H12_C17_O8	5	5
348.15728	0.152	H24_C19_O6	5	5
350.07903	0.166	H14_C20_O6	5	5
354.11025	0.165	H18_C20_O6	5	5
356.08961	0.299	H16_C19_O7	5	5
360.19376	0.083	H28_C21_O5	5	5
366.11031	0.178	H18_C21_O6	5	5
366.13149	0.140	H22_C18_O8	5	5
366.20427	0.150	H30_C20_O6	5	5
368.14712	0.129	H24_C18_O8	5	5
368.16240	0.094	H24_C22_O5	5	5
372.04805	0.686	H12_C18_O9	5	5
376.11581	0.448	H20_C19_O8	5	5
378.09512	0.350	H18_C18_O9	5	5
378.11030	0.150	H18_C22_O6	5	5
380.11071	0.204	H20_C18_O9	5	5
380.12592	0.169	H20_C22_O6	5	5
382.17805	0.109	H26_C23_O5	5	5
386.06381	0.777	H14_C19_O9	5	5
394.06886	0.546	H14_C21_O8	5	5
398.17289	0.239	H26_C23_O6	5	5
402.07392	0.262	H14_C23_O7	5	5
404.07437	0.417	H16_C19_O10	5	5
404.08960	0.230	H16_C23_O7	5	5
406.19920	0.248	H30_C22_O7	5	5
408.15722	0.177	H24_C24_O6	5	5
410.17287	0.203	H26_C24_O6	5	5

412.04302	1.000	H12_C20_O10	5	5
414.05869	0.936	H14_C20_O10	5	5
414.20418	0.239	H30_C24_O6	5	5
418.12638	0.530	H22_C21_O9	5	5
418.19913	0.251	H30_C23_O7	5	5
420.21483	0.197	H32_C23_O7	5	5
422.15764	0.249	H26_C21_O9	5	5
424.17334	0.209	H28_C21_O9	5	5
424.20970	0.158	H32_C22_O8	5	5
432.08454	0.364	H16_C24_O8	5	5
432.12089	0.181	H20_C25_O7	5	5
432.14199	0.496	H24_C22_O9	5	5
434.23043	0.184	H34_C24_O7	5	5
436.17334	0.255	H28_C22_O9	5	5
436.20972	0.199	H32_C23_O8	5	5
438.18901	0.193	H30_C22_O9	5	5
438.20426	0.166	H30_C26_O6	5	5
440.21987	0.178	H32_C26_O6	5	5
442.19913	0.371	H30_C25_O7	5	5
444.10559	0.555	H20_C22_O10	5	5
448.15225	0.222	H24_C26_O7	5	5
448.20966	0.255	H32_C24_O8	5	5
450.09505	0.552	H18_C24_O9	5	5
452.07428	0.773	H16_C23_O10	5	5
452.18346	0.245	H28_C26_O7	5	5
452.21983	0.173	H32_C27_O6	5	5
454.08991	0.786	H18_C23_O10	5	5
462.22535	0.226	H34_C25_O8	5	5
464.18350	0.195	H28_C27_O7	5	5
468.10564	0.673	H20_C24_O10	5	5
472.13690	0.477	H24_C24_O10	5	5
472.24611	0.183	H36_C27_O7	5	5
476.20466	0.273	H32_C25_O9	5	5
478.16272	0.268	H26_C27_O8	5	5
480.17841	0.312	H28_C27_O8	5	5
482.12128	0.556	H22_C25_O10	5	5
484.20975	0.306	H32_C27_O8	5	5
486.22536	0.274	H34_C27_O8	5	5
334.10519	0.217	H18_C17_O7	6	5
338.13654	0.085	H22_C17_O7	6	5
340.05826	0.403	H12_C18_O7	6	5
344.12591	0.215	H20_C19_O6	6	5
348.12082	0.298	H20_C18_O7	6	5
350.10010	0.212	H18_C17_O8	6	5
352.15226	0.118	H24_C18_O7	6	5

356.05321	0.500	H12_C18_O8	6	5
358.06876	0.430	H14_C18_O8	6	5
362.10011	0.385	H18_C18_O8	6	5
364.11573	0.275	H20_C18_O8	6	5
368.12587	0.182	H20_C21_O6	6	5
368.18345	0.120	H28_C19_O7	6	5
370.10515	0.343	H18_C20_O7	6	5
378.20416	0.155	H30_C21_O6	6	5
382.14155	0.212	H22_C22_O6	6	5
382.19914	0.130	H30_C20_O7	6	5
392.21985	0.148	H32_C22_O6	6	5
394.12642	0.232	H22_C19_O9	6	5
394.14165	0.184	H22_C23_O6	6	5
406.12639	0.414	H22_C20_O9	6	5
408.21479	0.173	H32_C22_O7	6	5
414.09502	0.642	H18_C21_O9	6	5
420.12088	0.230	H20_C24_O7	6	5
420.14201	0.357	H24_C21_O9	6	5
424.07943	0.747	H16_C22_O9	6	5
424.18854	0.177	H28_C25_O6	6	5
426.13147	0.490	H22_C23_O8	6	5
426.16781	0.340	H26_C24_O7	6	5
426.20425	0.232	H30_C25_O6	6	5
428.11080	0.631	H20_C22_O9	6	5
430.19912	0.322	H30_C24_O7	6	5
436.15219	0.263	H24_C25_O7	6	5
438.13147	0.460	H22_C24_O8	6	5
444.21477	0.281	H32_C25_O7	6	5
454.19913	0.269	H30_C26_O7	6	5
466.16277	0.339	H26_C26_O8	6	5
466.19912	0.227	H30_C27_O7	6	5
468.21479	0.248	H32_C27_O7	6	5
360.12091	0.375	H20_C19_O7	7	5
382.16281	0.167	H26_C19_O8	7	5
390.13140	0.481	H22_C20_O8	7	5
394.16273	0.265	H26_C20_O8	7	5
394.19909	0.205	H30_C21_O7	7	5
410.19405	0.200	H30_C21_O8	7	5
424.11582	0.495	H20_C23_O8	7	5
466.10545	0.038	H18_C28_O7	1	6
366.03749	0.303	H10_C19_O8	2	6
368.08962	0.370	H16_C20_O7	3	6
426.05865	0.957	H14_C21_O10	3	6
446.12129	0.507	H22_C22_O10	3	6
486.15262	0.443	H26_C25_O10	3	6

346.06891	0.237	H14_C17_O8	4	6
352.05823	0.325	H12_C19_O7	4	6
392.08964	0.300	H16_C22_O7	4	6
392.11069	0.428	H20_C19_O9	4	6
394.10524	0.310	H18_C22_O7	4	6
412.07941	0.855	H16_C21_O9	4	6
432.17844	0.374	H28_C23_O8	4	6
434.12125	0.419	H22_C21_O10	4	6
438.05865	0.872	H14_C22_O10	4	6
438.09508	0.688	H18_C23_O9	4	6
442.08995	0.729	H18_C22_O10	4	6
448.11579	0.297	H20_C25_O8	4	6
456.10562	0.659	H20_C23_O10	4	6
460.13696	0.472	H24_C23_O10	4	6
462.09502	0.455	H18_C25_O9	4	6
332.12589	0.212	H20_C18_O6	5	6
350.17284	0.136	H26_C19_O6	5	6
358.14153	0.277	H22_C20_O6	5	6
360.08447	0.343	H16_C18_O8	5	6
366.07400	0.351	H14_C20_O7	5	6
368.05312	0.804	H12_C19_O8	5	6
374.06382	0.447	H14_C18_O9	5	6
384.08451	0.558	H16_C20_O8	5	6
390.09508	0.485	H18_C19_O9	5	6
390.20414	0.178	H30_C22_O6	5	6
396.04812	0.668	H12_C20_O9	5	6
406.14161	0.135	H22_C24_O6	5	6
410.06373	0.822	H14_C21_O9	5	6
410.13651	0.342	H22_C23_O7	5	6
418.06883	0.480	H14_C23_O8	5	6
422.10017	0.474	H18_C23_O8	5	6
422.13651	0.270	H22_C24_O7	5	6
424.15222	0.326	H24_C24_O7	5	6
430.12641	0.562	H22_C22_O9	5	6
434.06382	0.634	H14_C23_O9	5	6
436.07944	0.648	H16_C23_O9	5	6
436.11579	0.411	H20_C24_O8	5	6
442.12636	0.574	H22_C23_O9	5	6
444.06924	0.683	H16_C21_O11	5	6
448.17333	0.318	H28_C23_O9	5	6
452.14711	0.398	H24_C25_O8	5	6
342.13138	0.046	H22_C16_O8	6	0
358.16277	0.034	H26_C17_O8	6	0
360.15728	0.211	H24_C20_O6	6	0
386.19403	0.036	H30_C19_O8	6	0

412.17335	0.117	H28_C20_O9	6	0
412.20970	0.087	H32_C21_O8	6	0
414.16783	0.388	H26_C23_O7	6	0
454.12635	0.566	H22_C24_O9	5	6
456.14200	0.533	H24_C24_O9	5	6
458.15772	0.526	H26_C24_O9	5	6
466.08997	0.691	H18_C24_O10	5	6
472.17330	0.457	H28_C25_O9	5	6
342.07389	0.352	H14_C18_O7	6	6
346.14167	0.201	H22_C19_O6	6	6
354.07393	0.375	H14_C19_O7	6	6
356.12599	0.186	H20_C20_O6	6	6
362.17287	0.174	H26_C20_O6	6	6
364.18850	0.169	H28_C20_O6	6	6
370.06888	0.588	H14_C19_O8	6	6
370.14165	0.205	H22_C21_O6	6	6
372.08454	0.450	H16_C19_O8	6	6
372.15734	0.246	H24_C21_O6	6	6
458.17913	0.024	H30_C21_O11	6	0
374.17286	0.220	H26_C21_O6	6	6
378.13137	0.285	H22_C19_O8	6	6
380.08961	0.310	H16_C21_O7	6	6
380.14711	0.187	H24_C19_O8	6	6
382.06882	0.638	H14_C20_O8	6	6
382.10527	0.337	H18_C21_O7	6	6
460.28252	0.090	H40_C27_O6	6	0
384.04809	0.876	H12_C19_O9	6	6
384.15732	0.216	H24_C22_O6	6	6
386.17290	0.242	H26_C22_O6	6	6
388.18861	0.195	H28_C22_O6	6	6
396.08450	0.607	H16_C21_O8	6	6
396.12095	0.343	H20_C22_O7	6	6
484.23095	0.038	H36_C24_O10	6	0
396.15722	0.211	H24_C23_O6	6	6
486.29827	0.100	H42_C29_O6	6	0
398.06372	0.948	H14_C20_O9	6	6
400.07944	0.690	H16_C20_O9	6	6
400.18853	0.259	H28_C23_O6	6	6
402.09500	0.554	H18_C20_O9	6	6
402.13146	0.532	H22_C21_O8	6	6
402.20417	0.190	H30_C23_O6	6	6
404.11067	0.557	H20_C20_O9	6	6
408.08451	0.493	H16_C22_O8	6	6
408.12085	0.303	H20_C23_O7	6	6
410.10016	0.568	H18_C22_O8	6	6

412.11577	0.502	H20_C22_O8	6	6
412.15222	0.357	H24_C23_O7	6	6
412.18860	0.262	H28_C24_O6	6	6
416.18351	0.358	H28_C23_O7	6	6
418.16274	0.399	H26_C22_O8	6	6
426.09509	0.734	H18_C22_O9	6	6
432.21484	0.237	H32_C24_O7	6	6
434.13654	0.207	H22_C25_O7	6	6
438.16781	0.284	H26_C25_O7	6	6
440.18353	0.312	H28_C25_O7	6	6
442.16278	0.480	H26_C24_O8	6	6
444.14200	0.547	H24_C23_O9	6	6
444.17843	0.450	H28_C24_O8	6	6
452.11072	0.570	H20_C24_O9	6	6
454.16275	0.393	H26_C25_O8	6	6
456.17839	0.431	H28_C25_O8	6	6
460.20968	0.298	H32_C25_O8	6	6
468.14199	0.483	H24_C25_O9	6	6
468.17837	0.353	H28_C26_O8	6	6
472.20973	0.333	H32_C26_O8	6	6
364.15220	0.192	H24_C19_O7	7	6
384.12083	0.316	H20_C21_O7	7	6
392.18350	0.245	H28_C21_O7	7	6
396.17836	0.203	H28_C20_O8	7	6
420.17844	0.287	H28_C22_O8	7	6
422.19407	0.244	H30_C22_O8	7	6
428.18350	0.409	H28_C24_O7	7	6
446.19408	0.333	H30_C24_O8	7	6
416.11073	0.551	H20_C21_O9	4	7
380.05317	0.365	H12_C20_O8	5	7
388.11583	0.518	H20_C20_O8	5	7
398.10014	0.515	H18_C21_O8	5	7
406.16270	0.301	H26_C21_O8	5	7
346.10521	0.280	H18_C18_O7	6	7
358.10526	0.286	H18_C19_O7	6	7
362.13651	0.296	H22_C19_O7	6	7
372.12082	0.376	H20_C20_O7	6	7
374.10014	0.442	H18_C19_O8	6	7
374.13659	0.428	H22_C20_O7	6	7
376.15216	0.305	H24_C20_O7	6	7
386.13659	0.367	H22_C21_O7	6	7
398.13659	0.356	H22_C22_O7	6	7
400.15220	0.384	H24_C22_O7	6	7
404.14711	0.438	H24_C21_O8	6	7
414.13146	0.526	H22_C22_O8	6	7

428.14714	0.513	H24_C23_O8	6	7
430.16278	0.487	H26_C23_O8	6	7
440.11070	0.666	H20_C23_O9	6	7
440.14709	0.452	H24_C24_O8	6	7
366.16777	0.174	H26_C19_O7	7	7
378.16787	0.229	H26_C20_O7	7	7
386.10010	0.479	H18_C20_O8	7	7
388.15214	0.399	H24_C21_O7	7	7
390.16789	0.297	H26_C21_O7	7	7
392.14708	0.306	H24_C20_O8	7	7
426.18897	0.124	H30_C21_O9	7	0
400.11572	0.536	H20_C21_O8	7	7
402.16781	0.380	H26_C22_O7	7	7
404.18346	0.277	H28_C22_O7	7	7