CALCULATION OF MOLECULAR FORMULAS IN HIGH-RESOLUTION MASS SPECTROMETRY

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An appendix to

STRUCTURE ELUCIDATION OF NATURAL PRODUCTS BY MASS SPECTROMETRY

Volume II: Steroids, terpenoids, sugars, and miscellaneous classes

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Appendix

Calculation of Molecular Formulas in High-resolution Mass Spectrometry

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The advent of commercial instruments for high resolution work introduces a new dimension into mass spectrometry, as pioneered by Beynon.[1] The high resolution measurement of a molecular mass must then be interpreted as a consistent formula. For example, given a reading of 718.3743 ± .0060, what formulas should be considered to account for it? Few chemists will have the patience and calculating skill to wish to do this by arithmetic trial and error; accordingly, extensive tables[2] and other algorithms[3,4,5] have been presented to aid in this task. At one extreme, one might imagine a complete directory in which every formula is listed — and the chemist need only look up his answer — but he might also need a large library in which to store the necessary number of volumes. To greater advantage, the calculations can be programmed on a computer[3] and this may be the most constructive direction of future work. Alternatively, procedures involving a modest amount of arithmetic can be applied with the help of an abbreviated table. A related procedure and more extensive tables have been presented more fully elsewhere.[3] The present account is confined to compounds containing C, H, O and N, and may be used independently, although reference 3 might be consulted for further clarification if necessary.

Instead of listing all formulas one by one, we note that ^{12}C by definition has a mass of precisely 12. Hence, the fractional part of the mass number is not attributable to C, but only to H, O, and N. A comprehensive table (see for example, ref. 3, Table 2) can be seen to go through a repeating cycle every 12H atoms. Table 3 in this appendix is, in fact, just the basic block also covering the ranges of oxygen up to 11, nitrogen up to 7, and any value of carbon.

To encompass larger values of H in a compressed version of the tables for the purposes of this appendix, the calculation includes a step (Table 2) of figuratively extracting some multiple of 12H from the molecule, as necessary.

For example, to analyze an intact molecule whose mass is determined as 718.3743 ± .0060, we follow these steps:

1. According to the fifth entry of Table 2, a decimal of .30000 - .40000 calls for the subtraction of 36H (=36.28170). We therefore calculate the molecule as (718.37430 - 36.28170) =682.09260.

2. Divide 682 by 12 through the use of Table 1.

Quotient = 56

Integer residue = 10

Decimal = .09260 ± .00600 (expressed as 5 decimal places)

3. Look up in Table 3 integer residue class 10 for 09260 ± 00600, i.e., values in the range 08660 to 09860. Since the molecule is stated to be intact, ignore lines marked with an asterisk (*), which refer to free radicals or protonated species.

4. The following values will be noted as candidates:

DECML	H	N	O	=C	WMIN
08731	14	6	8	18	262
09000	18	0	10	14	274
09134	14	4	6	13	214
09536	14	2	4	8	166
09669	10	6	0	7	106
09721	18	4	11	20	322

Other criteria will have to be used to choose among them, as illustrated in steps 5 and 6.

5. Check that the formula weight, i.e., 682, is not less than the WMIN given in each case.

6. To illustrate further interpretation, suppose that analytical data call for 4 to 5 nitrogens and 6 to 8 oxygens. Then the only solution is listed as

DECML	H	N	O	=C
09134	14	4	6	13

=C stands for the mass of the H+N+O expressed in units of carbon mass, i.e., $H_{14}N_4O_6 \equiv C_{13}$. Thus, 13 is subtracted from the quotient of step 2, (56-13=43) to give the value of the answer: $C_{43}H_{14}N_4O_6 = 682.09134$.

7. Restore 36H (=36.28170 — see Table 2) subtracted in step 1 to give the final answer:

$C_{43}H_{14}N_4O_6$	682.09134
H_{36}	36.28170
$C_{43}H_{50}N_4O_6$	718.37304

REFERENCES

1. J. H. Beynon, Mass Spectrometry and Its Applications to Organic Chemistry, Elsevier, Amsterdam, 1960.

2. J. H. Beynon and A. E. Williams, Mass and Abundance Tables for Use in Mass Spectrometry, Elsevier, Amsterdam, 1963.

3. J. Lederberg, Computation of Molecular Formulas for Mass Spectrometry, Holden-Day, San Francisco, 1964.

4. J. Lederberg, Tables and An Algorithm for Calculating Functional Groups of Organic Molecules in High Resolution Mass Spectrometry, NASA Sci. Techn. Aerosp. Rep., N64-21426 (1964).

5. E. Kendrick, A Mass Scale Based on CH_2 = 14.0000 for High-Resolution Mass Spectrometry of Organic Compounds, Analytical Chemistry, 35, 2146 (1963).

TABLE 1. DIVISION BY 12

(Integers from 0 to 611)

	0	1	2	3	4	5	6	7	8	9	10	11
0	0	1	2	3	4	5	6	7	8	9	10	11
1	12	13	14	15	16	17	18	19	20	21	22	23
2	24	25	26	27	28	29	30	31	32	33	34	35
3	36	37	38	39	40	41	42	43	44	45	46	47
4	48	49	50	51	52	53	54	55	56	57	58	59
5	60	61	62	63	64	65	66	67	68	69	70	71
6	72	73	74	75	76	77	78	79	80	81	82	83
7	84	85	86	87	88	89	90	91	92	93	94	95
8	96	97	98	99	100	101	102	103	104	105	106	107
9	108	109	110	111	112	113	114	115	116	117	118	119
10	120	121	122	123	124	125	126	127	128	129	130	131
11	132	133	134	135	136	137	138	139	140	141	142	143
12	144	145	146	147	148	149	150	151	152	153	154	155
13	156	157	158	159	160	161	162	163	164	165	166	167
14	168	169	170	171	172	173	174	175	176	177	178	179
15	180	181	182	183	184	185	186	187	188	189	190	191
16	192	193	194	195	196	197	198	199	200	201	202	203
17	204	205	206	207	208	209	210	211	212	213	214	215
18	216	217	218	219	220	221	222	223	224	225	226	227
19	228	229	230	231	232	233	234	235	236	237	238	239
20	240	241	242	243	244	245	246	247	248	249	250	251
21	252	253	254	255	256	257	258	259	260	261	262	263
22	264	265	266	267	268	269	270	271	272	273	274	275
23	276	277	278	279	280	281	282	283	284	285	286	287
24	288	289	290	291	292	293	294	295	296	297	298	299
25	300	301	302	303	304	305	306	307	308	309	310	311
26	312	313	314	315	316	317	318	319	320	321	322	323
27	324	325	326	327	328	329	330	331	332	333	334	335
28	336	337	338	339	340	341	342	343	344	345	346	347
29	348	349	350	351	352	353	354	355	356	357	358	359
30	360	361	362	363	364	365	366	367	368	369	370	371
31	372	373	374	375	376	377	378	379	380	381	382	383
32	384	385	386	387	388	389	390	391	392	393	394	395
33	396	397	398	399	400	401	402	403	404	405	406	407
34	408	409	410	411	412	413	414	415	416	417	418	419
35	420	421	422	423	424	425	426	427	428	429	430	431
36	432	433	434	435	436	437	438	439	440	441	442	443
37	444	445	446	447	448	449	450	451	452	453	454	455
38	456	457	458	459	460	461	462	463	464	465	466	467
39	468	469	470	471	472	473	474	475	476	477	478	479
40	480	481	482	483	484	485	486	487	488	489	490	491
41	492	493	494	495	496	497	498	499	500	501	502	503
42	504	505	506	507	508	509	510	511	512	513	514	515
43	516	517	518	519	520	521	522	523	524	525	526	527
44	528	529	530	531	532	533	534	535	536	537	538	539
45	540	541	542	543	544	545	546	547	548	549	550	551
46	552	553	554	555	556	557	558	559	560	561	562	563
47	564	565	566	567	568	569	570	571	572	573	574	575
48	576	577	578	579	580	581	582	583	584	585	586	587
49	588	589	590	591	592	593	594	595	596	597	598	599
50	600	601	602	603	604	605	606	607	608	609	610	611

Table 1. Division by 12

(Integers from 612 to 1211)

Quotient	0	1	2	3	4	5	6	7	8	9	10	11
51	612	613	614	615	616	617	618	619	620	621	622	623
52	624	625	626	627	628	629	630	631	632	633	634	635
53	636	637	638	639	640	641	642	643	644	645	646	647
54	648	649	650	651	652	653	654	655	656	657	658	659
55	660	661	662	663	664	665	666	667	668	669	670	671
56	672	673	674	675	676	677	678	679	680	681	682	683
57	684	685	686	687	688	689	690	691	692	693	694	695
58	696	697	698	699	700	701	702	703	704	705	706	707
59	708	709	710	711	712	713	714	715	716	717	718	719
60	720	721	722	723	724	725	726	727	728	729	730	731
61	732	733	734	735	736	737	738	739	740	741	742	743
62	744	745	746	747	748	749	750	751	752	753	754	755
63	756	757	758	759	760	761	762	763	764	765	766	767
64	768	769	770	771	772	773	774	775	776	777	778	779
65	780	781	782	783	784	785	786	787	788	789	790	791
66	792	793	794	795	796	797	798	799	800	801	802	803
67	804	805	806	807	808	809	810	811	812	813	814	815
68	816	817	818	819	820	821	822	823	824	825	826	827
69	828	829	830	831	832	833	834	835	836	837	838	839
70	840	841	842	843	844	845	846	847	848	849	850	851
71	852	853	854	855	856	857	858	859	860	861	862	863
72	864	865	866	867	868	869	870	871	872	873	874	875
73	876	877	878	879	880	881	882	883	884	885	886	887
74	888	889	890	891	892	893	894	895	896	897	898	899
75	900	901	902	903	904	905	906	907	908	909	910	911
76	912	913	914	915	916	917	918	919	920	921	922	923
77	924	925	926	927	928	929	930	931	932	933	934	935
78	936	937	938	939	940	941	942	943	944	945	946	947
79	948	949	950	951	952	953	954	955	956	957	958	959
80	960	961	962	963	964	965	966	967	968	969	970	971
81	972	973	974	975	976	977	978	979	980	981	982	983
82	984	985	986	987	988	989	990	991	992	993	994	995
83	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007
84	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019
85	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031
86	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043
87	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055
88	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067
89	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079
90	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091
91	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103
92	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115
93	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127
94	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139
95	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151
96	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163
97	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175
98	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187
99	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199
100	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211

TABLE 2

If decimal fraction is	Use Table 1 after subtracting	
Negative (Shown as Complement e.g., -.04979 = .95021)	Mass	H Atoms
	0	0
.00000 - .10000	0	0
.10000 - .20000	12.09390	(12H)
.20000 - .30000	24.18780	(24H)
.30000 - .40000	36.28170	(36H)
.40000 - .50000	48.37560	(48H)
.50000 - .60000	60.46950	(60H)
.60000 - .70000	72.56340	(72H)
.70000 - .80000	84.65730	(84H)
.80000 - .90000	96.75120	(96H)

TABLE 3

DECIMAL WEIGHTS OF (H,O,N) COMBINATIONS OF ORGANIC MOLECULES

Each page is an integer residue class (0,1,.....11) corresponding to the residue after dividing the non-decimal part of the formula weight by 12 through the use of Table 1.

=C stands for the mass of the combination of the non-carbon atoms in units of 12, i.e., equivalent number of carbon atoms.

WMIN is the lowest formula weight to be considered for each specification of (H,O,N), taking account of the number of carbons needed to bind the given number of hydrogens.

Asterisk (*) marks molecules of odd parity, i.e., mono-radicals or species with an extra proton. WMIN allows for an extra proton; where this is implausible, WMIN should be increased by 12.

TABLE 3. DECIMAL WEIGHTS OF (H,O,N) COMBINATIONS OF ORGANIC MOLECULES

Integer Residue Class

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95021	0	2	11	17	204	02968	6	1	4	7	96*	08452	16	0	8	12	228
95424	0	0	9	12	144	03019	8	6	10	21	252	08586	12	4	4	11	168
96145	0	4	10	18	216	03102	2	5	0	6	72*	08720	14	1	5	9	168*
96279	2	1	11	16	192*	03154	10	3	11	19	252*	08771	16	6	11	23	324
96547	0	2	8	13	156	03236	4	2	1	4	48	08854	10	5	1	8	108*
96949	0	0	6	8	96	03422	8	4	8	16	204	08988	12	2	2	6	120
97268	0	6	9	19	228	03556	10	1	9	14	204*	09173	16	4	9	18	276
97402	2	3	10	17	204*	03690	6	5	5	13	156*	09307	18	1	10	16	276*
97537	4	0	11	15	192	03824	8	2	6	11	156	09390	12	0	0	1	72
97670	0	4	7	14	168	03957	4	6	2	10	120	09441	14	5	6	15	216*
97804	2	1	8	12	144*	04092	6	3	3	8	96*	09575	16	2	7	13	228
98072	0	2	5	9	108	04226	8	0	4	6	108	09709	12	6	3	12	168
98475	0	0	3	4	48	04277	10	5	10	20	252*	09843	14	3	4	10	168*
98526	2	5	9	18	216*	04360	4	4	0	5	60	09978	16	0	5	8	180
98660	4	2	10	16	192	04411	12	2	11	18	264	10029	18	5	11	22	324*
98793	0	6	6	15	180	04494	6	1	1	3	48*	10111	12	4	1	7	120
98928	2	3	7	13	156*	04545	8	6	7	17	204	10245	14	1	2	5	120*
99062	4	0	8	11	144	04679	10	3	8	15	204*	10296	16	6	8	19	276
99196	0	4	4	10	120	04814	12	0	9	13	216	10431	18	3	9	17	276*
99330	2	1	5	8	96*	04947	8	4	5	12	156	10565	20	0	10	15	288
99381	4	6	11	22	264	05081	10	1	6	10	156*	10699	16	4	6	14	228
99598	0	2	2	5	60	05215	6	5	2	9	108*	10833	18	1	7	12	228*
99783	4	4	9	17	204	05349	8	2	3	7	108	10967	14	5	3	11	168*
99917	6	1	10	15	192*	05535	12	4	10	19	264	11101	16	2	4	9	180
00000	0	0	0	0	0	05617	6	3	0	4	48*	11234	12	6	0	8	120
00051	2	5	6	14	168*	05669	14	1	11	17	264*	11286	20	4	11	21	336
00185	4	2	7	12	144	05752	8	0	1	2	60	11369	14	3	1	6	120*
00319	0	6	3	11	132	05803	10	5	7	16	204*	11503	16	0	2	4	132
00453	2	3	4	9	108*	05937	12	2	8	14	216	11554	18	5	8	18	276*
00588	4	0	5	7	96	06070	8	6	4	13	156	11688	20	2	9	16	288
00639	6	5	11	21	252*	06205	10	3	5	11	156*	11822	16	6	5	15	228
00721	0	4	1	6	72	06339	12	0	6	9	168	11956	18	3	6	13	228*
00855	2	1	2	4	48*	06473	8	4	2	8	108	12091	20	0	7	11	240
00906	4	6	8	18	216	06607	10	1	3	6	108*	12224	16	4	3	10	180
01041	6	3	9	16	192*	06658	12	6	9	20	264	12358	18	1	4	8	180*
01175	8	0	10	14	204	06792	14	3	10	18	264*	12409	20	6	10	22	336
01309	4	4	6	13	156	06875	8	2	0	3	60	12492	14	5	0	7	120*
01443	6	1	7	11	144*	06927	16	0	11	16	276	12544	22	3	11	20	336*
01577	2	5	3	10	120*	07060	12	4	7	15	216	12626	16	2	1	5	132
01711	4	2	4	8	96	07194	14	1	8	13	216*	12812	20	4	8	17	288
01844	0	6	0	7	84	07328	10	5	4	12	156*	12946	22	1	9	15	288*
01896	8	4	11	20	252	07462	12	2	5	10	168	13080	18	5	5	14	228*
01979	2	3	1	5	60*	07596	8	6	1	9	108	13214	20	2	6	12	240
02113	4	0	2	3	48	07730	10	3	2	7	108*	13347	16	6	2	11	180
02164	6	5	8	17	204*	07865	12	0	3	5	120	13482	18	3	3	9	180*
02298	8	2	9	15	204	07916	14	5	9	19	264*	13616	20	0	4	7	192
02432	4	6	5	14	168	08050	16	2	10	17	276	13667	22	5	10	21	336*
02566	6	3	6	12	144*	08132	10	1	0	2	60*	13750	16	4	0	6	132
02701	8	0	7	10	156	08183	12	6	6	16	216	13801	24	2	11	19	348
02834	4	4	3	9	108	08318	14	3	7	14	216*	13884	18	1	1	4	132*
DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class 1

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95804	1	2	11	17	205*	03751	7	1	4	7	109	09235	17	0	8	12	229*
96206	1	0	9	12	145*	03802	9	6	10	21	253*	09368	13	4	4	11	169*
96927	1	4	10	18	217*	03885	3	5	0	6	73	09502	15	1	5	9	181
97061	3	1	11	16	193	03936	11	3	11	19	265	09553	17	6	11	23	325*
97329	1	2	8	13	157*	04019	5	2	1	4	49*	09636	11	5	1	8	121
97732	1	0	6	8	97*	04204	9	4	8	16	205*	09770	13	2	2	6	121*
98050	1	6	9	19	229*	04338	11	1	9	14	217	09956	17	4	9	18	277*
98185	3	3	10	17	205	04472	7	5	5	13	157	10090	19	1	10	16	289
98319	5	0	11	15	193*	04606	9	2	6	11	157*	10173	13	0	0	1	73*
98453	1	4	7	14	169*	04740	5	6	2	10	121*	10224	15	5	6	15	229
98587	3	1	8	12	145	04874	7	3	3	8	109	10358	17	2	7	13	229*
98855	1	2	5	9	109*	05009	9	0	4	6	109*	10491	13	6	3	12	169*
99257	1	0	3	4	49*	05060	11	5	10	20	265	10626	15	3	4	10	181
99308	3	5	9	18	217	05142	5	4	0	5	61*	10760	17	0	5	8	181*
99442	5	2	10	16	193*	05194	13	2	11	18	265*	10811	19	5	11	22	337
99576	1	6	6	15	181*	05276	7	1	1	3	61	10894	13	4	1	7	121*
99710	3	3	7	13	157	05327	9	6	7	17	205*	11028	15	1	2	5	133
99845	5	0	8	11	145*	05462	11	3	8	15	217	11079	17	6	8	19	277*
99978	1	4	4	10	121*	05596	13	0	9	13	217*	11213	19	3	9	17	289
00112	3	1	5	8	97	05730	9	4	5	12	157*	11348	21	0	10	15	289*
00163	5	6	11	22	265*	05864	11	1	6	10	169	11481	17	4	6	14	229*
00380	1	2	2	5	61*	05998	7	5	2	9	109	11615	19	1	7	12	241
00566	5	4	9	17	205*	06132	9	2	3	7	109*	11749	15	5	3	11	181
00700	7	1	10	15	205	06317	13	4	10	19	265*	11883	17	2	4	9	181*
00783	1	0	0	0	1*	06400	7	3	0	4	61	12017	13	6	0	8	121*
00834	3	5	6	14	169	06451	15	1	11	17	277	12069	21	4	11	21	337*
00968	5	2	7	12	145*	06534	9	0	1	2	61*	12151	15	3	1	6	133
01101	1	6	3	11	133*	06585	11	5	7	16	217	12286	17	0	2	4	133*
01236	3	3	4	9	109	06719	13	2	8	14	217*	12337	19	5	8	18	289
01370	5	0	5	7	97*	06853	9	6	4	13	157*	12471	21	2	9	16	289*
01421	7	5	11	21	253	06987	11	3	5	11	169	12604	17	6	5	15	229*
01504	1	4	1	6	73*	07122	13	0	6	9	169*	12739	19	3	6	13	241
01638	3	1	2	4	49	07255	9	4	2	8	109*	12873	21	0	7	11	241*
01689	5	6	8	18	217*	07389	11	1	3	6	121	13007	17	4	3	10	181*
01823	7	3	9	16	205	07440	13	6	9	20	265*	13141	19	1	4	8	193
01958	9	0	10	14	205*	07575	15	3	10	18	277	13192	21	6	10	22	337*
02091	5	4	6	13	157*	07657	9	2	0	3	61*	13275	15	5	0	7	133
02225	7	1	7	11	157	07709	17	0	11	16	277*	13326	23	3	11	20	349
02359	3	5	3	10	121	07843	13	4	7	15	217*	13409	17	2	1	5	133*
02493	5	2	4	8	97*	07977	15	1	8	13	229	13594	21	4	8	17	289*
02627	1	6	0	7	85*	08111	11	5	4	12	169	13728	23	1	9	15	301
02679	9	4	11	20	253*	08245	13	2	5	10	169*	13862	19	5	5	14	241
02761	3	3	1	5	61	08378	9	6	1	9	109*	13996	21	2	6	12	241*
02896	5	0	2	3	49*	08513	11	3	2	7	121	14130	17	6	2	11	181*
02947	7	5	8	17	205	08647	13	0	3	5	121*	14264	19	3	3	9	193
03081	9	2	9	15	205*	08698	15	5	9	19	277	14399	21	0	4	7	193*
03214	5	6	5	14	169*	08832	17	2	10	17	277*	14450	23	5	10	21	349
03349	7	3	6	12	157	08915	11	1	0	2	73	14532	17	4	0	6	133*
03483	9	0	7	10	157*	08966	13	6	6	16	217*	14584	25	2	11	19	349*
03617	5	4	3	9	109*	09100	15	3	7	14	229	14666	19	1	1	4	145

DECML H N O =C WMIN DECML H N O =C WMIN DECML H N O =C WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

2

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95329	0	3	11	18	218*	03142	4	5	3	10	122*	08625	14	4	7	15	230
95731	0	1	9	13	158*	03276	6	2	4	8	110	08759	16	1	8	13	230*
96452	0	5	10	19	230*	03409	2	6	0	7	86	08893	12	5	4	12	170*
96586	2	2	11	17	206	03461	10	4	11	20	266	09027	14	2	5	10	182
96854	0	3	8	14	170*	03544	4	3	1	5	62*	09161	10	6	1	9	122
96989	2	0	9	12	146	03678	6	0	2	3	62	09295	12	3	2	7	122*
97256	0	1	6	9	110*	03729	8	5	8	17	206*	09430	14	0	3	5	134
97710	2	4	10	18	218	03863	10	2	9	15	218	09481	16	5	9	19	278*
97844	4	1	11	16	194*	03997	6	6	5	14	170	09615	18	2	10	17	290
97978	0	5	7	15	182*	04131	8	3	6	12	158*	09697	12	1	0	2	74*
98112	2	2	8	13	158	04266	10	0	7	10	170	09748	14	6	6	16	230
98380	0	3	5	10	122*	04399	6	4	3	9	110	09883	16	3	7	14	230*
98514	2	0	6	8	98	04533	8	1	4	7	110*	10017	18	0	8	12	242
98782	0	1	3	5	62*	04584	10	6	10	21	266	10151	14	4	4	11	182
98833	2	6	9	19	230	04667	4	5	0	6	74*	10285	16	1	5	9	182*
98967	4	3	10	17	206*	04719	12	3	11	19	266*	10336	18	6	11	23	338
99102	6	0	11	15	206	04801	6	2	1	4	62	10419	12	5	1	8	122*
99235	2	4	7	14	170	04987	10	4	8	16	218	10553	14	2	2	6	134
99369	4	1	8	12	146*	05121	12	1	9	14	218*	10738	18	4	9	18	290
99503	0	5	4	11	134*	05255	8	5	5	13	158*	10872	20	1	10	16	290*
99637	2	2	5	9	110	05389	10	2	6	11	170	10955	14	0	0	1	86
99905	0	3	2	6	74*	05522	6	6	2	10	122	11006	16	5	6	15	230*
00040	2	0	3	4	50	05657	8	3	3	8	110*	11140	18	2	7	13	242
00091	4	5	9	18	218*	05791	10	0	4	6	122	11274	14	6	3	12	182
00225	6	2	10	16	206	05842	12	5	10	20	266*	11408	16	3	4	10	182*
00307	0	1	0	1	14*	05925	6	4	0	5	62	11543	18	0	5	8	194
00358	2	6	6	15	182	05976	14	2	11	18	278	11594	20	5	11	22	338*
00493	4	3	7	13	158*	06059	8	1	1	3	62*	11676	14	4	1	7	134
00627	6	0	8	11	158	06110	10	6	7	17	218	11810	16	1	2	5	134*
00761	2	4	4	10	122	06244	12	3	8	15	218*	11861	18	6	8	19	290
00895	4	1	5	8	98*	06379	14	0	9	13	230	11996	20	3	9	17	290*
00946	6	6	11	22	266	06512	10	4	5	12	170	12130	22	0	10	15	302
01029	0	5	1	7	86*	06646	12	1	6	10	170*	12264	18	4	6	14	242
01163	2	2	2	5	62	06780	8	5	2	9	110*	12398	20	1	7	12	242*
01348	6	4	9	17	206	06914	10	2	3	7	122	12532	16	5	3	11	182*
01482	8	1	10	15	206*	07100	14	4	10	19	278	12666	18	2	4	9	194
01565	2	0	0	0	2	07182	8	3	0	4	62*	12799	14	6	0	8	134
01616	4	5	6	14	170*	07234	16	1	11	17	278*	12851	22	4	11	21	350
01750	6	2	7	12	158	07317	10	0	1	2	74	12934	16	3	1	6	134*
01884	2	6	3	11	134	07368	12	5	7	16	218*	13068	18	0	2	4	146
02018	4	3	4	9	110*	07502	14	2	8	14	230	13119	20	5	8	18	290*
02153	6	0	5	7	110	07635	10	6	4	13	170	13253	22	2	9	16	302
02204	8	5	11	21	254*	07770	12	3	5	11	170*	13387	18	6	5	15	242
02286	2	4	1	6	74	07904	14	0	6	9	182	13521	20	3	6	13	242*
02420	4	1	2	4	50*	08038	10	4	2	8	122	13656	22	0	7	11	254
02471	6	6	8	18	218	08172	12	1	3	6	122*	13789	18	4	3	10	194
02606	8	3	9	16	206*	08223	14	6	9	20	278	13923	20	1	4	8	194*
02740	10	0	10	14	218	08357	16	3	10	18	278*	13974	22	6	10	22	350
02874	6	4	6	13	158	08440	10	2	0	3	74	14057	16	5	0	7	134*
03008	8	1	7	11	158*	08492	18	0	11	16	290	14109	24	3	11	20	350*
DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

3

DECML	H	N	O	=C	WMIN
96111	1	3	11	18	219
96513	1	1	9	13	159
97235	1	5	10	19	231
97369	3	2	11	17	207*
97637	1	3	8	14	171
97771	3	0	9	12	147*
98039	1	1	6	9	111
98492	3	4	10	18	219*
98626	5	1	11	16	207
98760	1	5	7	15	183
98894	3	2	8	13	159*
99162	1	3	5	10	123
99297	3	0	6	8	99*
99564	1	1	3	5	63
99615	3	6	9	19	231*
99750	5	3	10	17	207
99884	7	0	11	15	207*
00018	3	4	7	14	171*
00152	5	1	8	12	159
00286	1	5	4	11	135
00420	3	2	5	9	111*
00688	1	3	2	6	75
00822	3	0	3	4	51*
00873	5	5	9	18	219
01007	7	2	10	16	207*
01090	1	1	0	1	15
01141	3	6	6	15	183*
01275	5	3	7	13	159
01410	7	0	8	11	159*
01543	3	4	4	10	123*
01677	5	1	5	8	111
01728	7	6	11	22	267*
01811	1	5	1	7	87
01945	3	2	2	5	63*
02131	7	4	9	17	207*
02265	9	1	10	15	219
02348	3	0	0	0	3*
02399	5	5	6	14	171
02533	7	2	7	12	159*
02666	3	6	3	11	135*
02801	5	3	4	9	111
02935	7	0	5	7	111*
02986	9	5	11	21	267
03069	3	4	1	6	75*
03203	5	1	2	4	63
03254	7	6	8	18	219*
03388	9	3	9	16	219
03523	11	0	10	14	219*
03656	7	4	6	13	159*
03790	9	1	7	11	171

DECML	H	N	O	=C	WMIN
03924	5	5	3	10	123
04058	7	2	4	8	111*
04192	3	6	0	7	87*
04244	11	4	11	20	267*
04326	5	3	1	5	63
04461	7	0	2	3	63*
04512	9	5	8	17	219
04646	11	2	9	15	219*
04779	7	6	5	14	171*
04914	9	3	6	12	171
05048	11	0	7	10	171*
05182	7	4	3	9	111*
05316	9	1	4	7	123
05367	11	6	10	21	267*
05450	5	5	0	6	75
05501	13	3	11	19	279
05584	7	2	1	4	63*
05769	11	4	8	16	219*
05903	13	1	9	14	231
06037	9	5	5	13	171
06171	11	2	6	11	171*
06305	7	6	2	10	123*
06439	9	3	3	8	123
06574	11	0	4	6	123*
06625	13	5	10	20	279
06707	7	4	0	5	63*
06759	15	2	11	18	279*
06841	9	1	1	3	75
06892	11	6	7	17	219*
07027	13	3	8	15	231
07161	15	0	9	13	231*
07295	11	4	5	12	171*
07429	13	1	6	10	183
07563	9	5	2	9	123
07697	11	2	3	7	123*
07832	15	4	10	19	279*
07965	9	3	0	4	75
08016	17	1	11	17	291
08099	11	0	1	2	75*
08150	13	5	7	16	231
08284	15	2	8	14	231*
08418	11	6	4	13	171*
08552	13	3	5	11	183
08687	15	0	6	9	183*
08820	11	4	2	8	123*
08954	13	1	3	6	135
09005	15	6	9	20	279*
09140	17	3	10	18	291
09222	11	2	0	3	75*
09274	19	0	11	16	291*

DECML	H	N	O	=C	WMIN
09408	15	4	7	15	231*
09542	17	1	8	13	243
09676	13	5	4	12	183
09810	15	2	5	10	183*
09943	11	6	1	9	123*
10078	13	3	2	7	135
10212	15	0	3	5	135*
10263	17	5	9	19	291
10397	19	2	10	17	291*
10480	13	1	0	2	87
10531	15	6	6	16	231*
10665	17	3	7	14	243
10800	19	0	8	12	243*
10933	15	4	4	11	183*
11067	17	1	5	9	195
11118	19	6	11	23	339*
11201	13	5	1	8	135
11335	15	2	2	6	135*
11521	19	4	9	18	291*
11655	21	1	10	16	303
11738	15	0	0	1	87*
11789	17	5	6	15	243
11923	19	2	7	13	243*
12056	15	6	3	12	183*
12191	17	3	4	10	195
12325	19	0	5	8	195*
12376	21	5	11	22	351
12459	15	4	1	7	135*
12593	17	1	2	5	147
12644	19	6	8	19	291*
12778	21	3	9	17	303
12913	23	0	10	15	303*
13046	19	4	6	14	243*
13180	21	1	7	12	255
13314	17	5	3	11	195
13448	19	2	4	9	195*
13582	15	6	0	8	135*
13634	23	4	11	21	351*
13716	17	3	1	6	147
13851	19	0	2	4	147*
13902	21	5	8	18	303
14036	23	2	9	16	303*
14169	19	6	5	15	243*
14304	21	3	6	13	255
14438	23	0	7	11	255*
14572	19	4	3	10	195*
14706	21	1	4	8	207
14757	23	6	10	22	351*
14840	17	5	0	7	147
14891	25	3	11	20	363

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

4

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
94915	0	0	10	13	160	02913	8	4	9	17	220	08479	12	2	3	7	136
95636	0	4	11	19	232	03047	10	1	10	15	220*	08665	16	4	10	19	292
96038	0	2	9	14	172	03130	4	0	0	0	16	08747	10	3	0	4	76*
96441	0	0	7	9	112	03181	6	5	6	14	172*	08799	18	1	11	17	292*
96759	0	6	10	20	244	03315	8	2	7	12	172	08882	12	0	1	2	88
96894	2	3	11	18	220*	03449	4	6	3	11	136	08933	14	5	7	16	232*
97162	0	4	8	15	184	03583	6	3	4	9	112*	09067	16	2	8	14	244
97296	2	1	9	13	160*	03718	8	0	5	7	124	09200	12	6	4	13	184
97564	0	2	6	10	124	03769	10	5	11	21	268*	09335	14	3	5	11	184*
97966	0	0	4	5	64	03851	4	4	1	6	76	09469	16	0	6	9	196
98017	2	5	10	19	232*	03985	6	1	2	4	64*	09603	12	4	2	8	136
98151	4	2	11	17	208	04036	8	6	8	18	220	09737	14	1	3	6	136*
98285	0	6	7	16	196	04171	10	3	9	16	220*	09788	16	6	9	20	292
98419	2	3	8	14	172*	04305	12	0	10	14	232	09922	18	3	10	18	292*
98554	4	0	9	12	160	04439	8	4	6	13	172	10005	12	2	0	3	88
98687	0	4	5	11	136	04573	10	1	7	11	172*	10057	20	0	11	16	304
98821	2	1	6	9	112*	04707	6	5	3	10	124*	10190	16	4	7	15	244
99089	0	2	3	6	76	04841	8	2	4	8	124	10324	18	1	8	13	244*
99275	4	4	10	18	220	04974	4	6	0	7	88	10458	14	5	4	12	184*
99409	6	1	11	16	208*	05026	12	4	11	20	280	10592	16	2	5	10	196
99492	0	0	1	1	16	05109	6	3	1	5	64*	10726	12	6	1	9	136
99543	2	5	7	15	184*	05243	8	0	2	3	76	10860	14	3	2	7	136*
99677	4	2	8	13	160	05294	10	5	8	17	220*	10995	16	0	3	5	148
99810	0	6	4	12	148	05428	12	2	9	15	232	11046	18	5	9	19	292*
99945	2	3	5	10	124*	05562	8	6	5	14	172	11180	20	2	10	17	304
00079	4	0	6	8	112	05696	10	3	6	12	172*	11262	14	1	0	2	88*
00213	0	4	2	7	88	05831	12	0	7	10	184	11313	16	6	6	16	244
00347	2	1	3	5	64*	05964	8	4	3	9	124	11448	18	3	7	14	244*
00398	4	6	9	19	232	06098	10	1	4	7	124*	11582	20	0	8	12	256
00532	6	3	10	17	208*	06149	12	6	10	21	280	11716	16	4	4	11	196
00615	0	2	0	2	28	06232	6	5	0	6	76*	11850	18	1	5	9	196*
00667	8	0	11	15	220	06284	14	3	11	19	280*	11901	20	6	11	23	352
00800	4	4	7	14	172	06366	8	2	1	4	76	11984	14	5	1	8	136*
00934	6	1	8	12	160*	06552	12	4	8	16	232	12118	16	2	2	6	148
01068	2	5	4	11	136*	06686	14	1	9	14	232*	12303	20	4	9	18	304
01202	4	2	5	9	112	06820	10	5	5	13	172*	12437	22	1	10	16	304*
01336	0	6	1	8	100	06954	12	2	6	11	184	12520	16	0	0	1	100
01470	2	3	2	6	76*	07087	8	6	2	10	124	12571	18	5	6	15	244*
01605	4	0	3	4	64	07222	10	3	3	8	124*	12705	20	2	7	13	256
01656	6	5	9	18	220*	07356	12	0	4	6	136	12839	16	6	3	12	196
01790	8	2	10	16	220	07407	14	5	10	20	280*	12973	18	3	4	10	196*
01872	2	1	0	1	16*	07490	8	4	0	5	76	13108	20	0	5	8	208
01923	4	6	6	15	184	07541	16	2	11	18	292	13159	22	5	11	22	352*
02058	6	3	7	13	160*	07624	10	1	1	3	76*	13241	16	4	1	7	148
02192	8	0	8	11	172	07675	12	6	7	17	232	13375	18	1	2	5	148*
02326	4	4	4	10	124	07809	14	3	8	15	232*	13426	20	6	8	19	304
02460	6	1	5	8	112*	07944	16	0	9	13	244	13561	22	3	9	17	304*
02511	8	6	11	22	268	08077	12	4	5	12	184	13695	24	0	10	15	316
02594	2	5	1	7	88*	08211	14	1	6	10	184*	13829	20	4	6	14	256
02728	4	2	2	5	64	08345	10	5	2	9	124*	13963	22	1	7	12	256*

| DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN |

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

5

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95698	1	0	10	13	161*	03696	9	4	9	17	221*	09262	13	2	3	7	137*
96419	1	4	11	19	233*	03830	11	1	10	15	233	09447	17	4	10	19	293*
96821	1	2	9	14	173*	03913	5	0	0	0	17*	09530	11	3	0	4	89
97223	1	0	7	9	113*	03964	7	5	6	14	173	09581	19	1	11	17	305
97542	1	6	10	20	245*	04098	9	2	7	12	173*	09664	13	0	1	2	89*
97676	3	3	11	18	221	04231	5	6	3	11	137*	09715	15	5	7	16	245
97944	1	4	8	15	185*	04366	7	3	4	9	125	09849	17	2	8	14	245*
98078	3	1	9	13	161	04500	9	0	5	7	125*	09983	13	6	4	13	185*
98346	1	2	6	10	125*	04551	11	5	11	21	281	10117	15	3	5	11	197
98749	1	0	4	5	65*	04634	5	4	1	6	77*	10252	17	0	6	9	197*
98800	3	5	10	19	233	04768	7	1	2	4	77	10385	13	4	2	8	137*
98934	5	2	11	17	209*	04819	9	6	8	18	221*	10519	15	1	3	6	149
99067	1	6	7	16	197*	04953	11	3	9	16	233	10570	17	6	9	20	293*
99202	3	3	8	14	173	05088	13	0	10	14	233*	10705	19	3	10	18	305
99336	5	0	9	12	161*	05221	9	4	6	13	173*	10787	13	2	0	3	89*
99470	1	4	5	11	137*	05355	11	1	7	11	185	10839	21	0	11	16	305*
99604	3	1	6	9	113	05489	7	5	3	10	125	10973	17	4	7	15	245*
99872	1	2	3	6	77*	05623	9	2	4	8	125*	11107	19	1	8	13	257
00057	5	4	10	18	221*	05757	5	6	0	7	89*	11241	15	5	4	12	197
00191	7	1	11	16	221	05809	13	4	11	20	281*	11375	17	2	5	10	197*
00274	1	0	1	1	17*	05891	7	3	1	5	77	11508	13	6	1	9	137*
00325	3	5	7	15	185	06026	9	0	2	3	77*	11643	15	3	2	7	149
00459	5	2	8	13	161*	06077	11	5	8	17	233	11777	17	0	3	5	149*
00593	1	6	4	12	149*	06211	13	2	9	15	233*	11828	19	5	9	19	305
00727	3	3	5	10	125	06344	9	6	5	14	173*	11962	21	2	10	17	305*
00862	5	0	6	8	113*	06479	11	3	6	12	185	12045	15	1	0	2	101
00995	1	4	2	7	89*	06613	13	0	7	10	185*	12096	17	6	6	16	245*
01129	3	1	3	5	65	06747	9	4	3	9	125*	12230	19	3	7	14	257
01180	5	6	9	19	233*	06881	11	1	4	7	137	12365	21	0	8	12	257*
01315	7	3	10	17	221	06932	13	6	10	21	281*	12498	17	4	4	11	197*
01397	1	2	0	2	29*	07015	7	5	0	6	77	12632	19	1	5	9	209
01449	9	0	11	15	221*	07066	15	3	11	19	293	12683	21	6	11	23	353*
01583	5	4	7	14	173*	07149	9	2	1	4	77*	12766	15	5	1	8	149
01717	7	1	8	12	173	07334	13	4	8	16	233*	12900	17	2	2	6	149*
01851	3	5	4	11	137	07468	15	1	9	14	245	13086	21	4	9	18	305*
01985	5	2	5	9	113*	07602	11	5	5	13	185	13220	23	1	10	16	317
02118	1	6	1	8	101*	07736	13	2	6	11	185*	13303	17	0	0	1	101*
02253	3	3	2	6	77	07870	9	6	2	10	125*	13354	19	5	6	15	257
02387	5	0	3	4	65*	08004	11	3	3	8	137	13488	21	2	7	13	257*
02438	7	5	9	18	221	08139	13	0	4	6	137*	13621	17	6	3	12	197*
02572	9	2	10	16	221*	08190	15	5	10	20	293	13756	19	3	4	10	209
02655	3	1	0	1	17	08272	9	4	0	5	77*	13890	21	0	5	8	209*
02706	5	6	6	15	185*	08324	17	2	11	18	293*	13941	23	5	11	22	365
02840	7	3	7	13	173	08406	11	1	1	3	89	14024	17	4	1	7	149*
02975	9	0	8	11	173*	08457	13	6	7	17	233*	14158	19	1	2	5	161
03108	5	4	4	10	125*	08592	15	3	8	15	245	14209	21	6	8	19	305*
03242	7	1	5	8	125	08726	17	0	9	13	245*	14343	23	3	9	17	317
03293	9	6	11	22	269*	08860	13	4	5	12	185*	14478	25	0	10	15	317*
03376	3	5	1	7	89	08994	15	1	6	10	197	14611	21	4	6	14	257*
03510	5	2	2	5	65*	09128	11	5	2	9	137	14745	23	1	7	12	269
DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

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DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95222	0	1	10	14	174*	03170	6	0	3	4	78	08787	12	3	3	8	138*
95944	0	5	11	20	246*	03221	8	5	9	18	222*	08921	14	0	4	6	150
96346	0	3	9	15	186*	03355	10	2	10	16	234	08972	16	5	10	20	294*
96480	2	0	10	13	162	03437	4	1	0	1	18*	09055	10	4	0	5	90
96748	0	1	7	10	126*	03488	6	6	6	15	186	09106	18	2	11	18	306
97201	2	4	11	19	234	03623	8	3	7	13	174*	09189	12	1	1	3	90*
97469	0	5	8	16	198*	03757	10	0	8	11	186	09240	14	6	7	17	246
97603	2	2	9	14	174	03891	6	4	4	10	126	09374	16	3	8	15	246*
97871	0	3	6	11	138*	04025	8	1	5	8	126*	09509	18	0	9	13	258
98006	2	0	7	9	114	04076	10	6	11	22	282	09642	14	4	5	12	198
98273	0	1	4	6	78*	04159	4	5	1	7	90*	09776	16	1	6	10	198*
98324	2	6	10	20	246	04293	6	2	2	5	78	09910	12	5	2	9	138*
98459	4	3	11	18	222*	04478	10	4	9	17	234	10044	14	2	3	7	150
98727	2	4	8	15	186	04612	12	1	10	15	234*	10230	18	4	10	19	306
98861	4	1	9	13	162*	04695	6	0	0	0	30	10312	12	3	0	4	90*
98995	0	5	5	12	150*	04746	8	5	6	14	174*	10364	20	1	11	17	306*
99129	2	2	6	10	126	04880	10	2	7	12	186	10447	14	0	1	2	102
99397	0	3	3	7	90*	05014	6	6	3	11	138	10498	16	5	7	16	246*
99531	2	0	4	5	66	05148	8	3	4	9	126*	10632	18	2	8	14	258
99582	4	5	10	19	234*	05283	10	0	5	7	138	10765	14	6	4	13	198
99716	6	2	11	17	222	05334	12	5	11	21	282*	10900	16	3	5	11	198*
99799	0	1	1	2	30*	05416	6	4	1	6	78	11034	18	0	6	9	210
99850	2	6	7	16	198	05550	8	1	2	4	78*	11168	14	4	2	8	150
99984	4	3	8	14	174*	05601	10	6	8	18	234	11302	16	1	3	6	150*
00119	6	0	9	12	174	05736	12	3	9	16	234*	11353	18	6	9	20	306
00252	2	4	5	11	138	05870	14	0	10	14	246	11487	20	3	10	18	306*
00386	4	1	6	9	114*	06004	10	4	6	13	186	11570	14	2	0	3	102
00520	0	5	2	8	102*	06138	12	1	7	11	186*	11622	22	0	11	16	318
00654	2	2	3	6	78	06272	8	5	3	10	126*	11755	18	4	7	15	258
00840	6	4	10	18	222	06406	10	2	4	8	138	11889	20	1	8	13	258*
00922	0	3	0	3	42*	06539	6	6	0	7	90	12023	16	5	4	12	198*
00974	8	1	11	16	222*	06591	14	4	11	20	294	12157	18	2	5	10	210
01057	2	0	1	1	18	06674	8	3	1	5	78*	12291	14	6	1	9	150
01108	4	5	7	15	186*	06808	10	0	2	3	90	12425	16	3	2	7	150*
01242	6	2	8	13	174	06859	12	5	8	17	234*	12560	18	0	3	5	162
01375	2	6	4	12	150	06993	14	2	9	15	246	12611	20	5	9	19	306*
01510	4	3	5	10	126*	07127	10	6	5	14	186	12745	22	2	10	17	318
01644	6	0	6	8	126	07261	12	3	6	12	186*	12827	16	1	0	2	102*
01778	2	4	2	7	90	07396	14	0	7	10	198	12878	18	6	6	16	258
01912	4	1	3	5	66*	07529	10	4	3	9	138	13013	20	3	7	14	258*
01963	6	6	9	19	234	07663	12	1	4	7	138*	13147	22	0	8	12	270
02097	8	3	10	17	222*	07714	14	6	10	21	294	13281	18	4	4	11	210
02180	2	2	0	2	30	07797	8	5	0	6	78*	13415	20	1	5	9	210*
02232	10	0	11	15	234	07849	16	3	11	19	294*	13466	22	6	11	23	366
02365	6	4	7	14	174	07931	10	2	1	4	90	13549	16	5	1	8	150*
02499	8	1	8	12	174*	08117	14	4	8	16	246	13683	18	2	2	6	162
02633	4	5	4	11	138*	08251	16	1	9	14	246*	13868	22	4	9	18	318
02767	6	2	5	9	126	08385	12	5	5	13	186*	14002	24	1	10	16	318*
02901	2	6	1	8	102	08519	14	2	6	11	198	14085	18	0	0	1	114
03035	4	3	2	6	78*	08652	10	6	2	10	138	14136	20	5	6	15	258*

| DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN |

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

7

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
96005	1	1	10	14	175	03952	7	0	3	4	79*	09569	13	3	3	8	151
96726	1	5	11	20	247	04003	9	5	9	18	235	09704	15	0	4	6	151*
97128	1	3	9	15	187	04137	11	2	10	16	235*	09755	17	5	10	20	307
97263	3	0	10	13	163*	04220	5	1	0	1	31	09837	11	4	0	5	91*
97530	1	1	7	10	127	04271	7	6	6	15	187*	09889	19	2	11	18	307*
97984	3	4	11	19	235*	04405	9	3	7	13	187	09971	13	1	1	3	103
98252	1	5	8	16	199	04540	11	0	8	11	187*	10022	15	6	7	17	247*
98386	3	2	9	14	175*	04673	7	4	4	10	127*	10157	17	3	8	15	259
98654	1	3	6	11	139	04807	9	1	5	8	139	10291	19	0	9	13	259*
98788	3	0	7	9	115*	04858	11	6	11	22	283*	10425	15	4	5	12	199*
99056	1	1	4	6	79	04941	5	5	1	7	91	10559	17	1	6	10	211
99107	3	6	10	20	247*	05075	7	2	2	5	79*	10693	13	5	2	9	151
99241	5	3	11	18	223	05261	11	4	9	17	235*	10827	15	2	3	7	151*
99509	3	4	8	15	187*	05395	13	1	10	15	247	11012	19	4	10	19	307*
99643	5	1	9	13	175	05478	7	0	0	0	31*	11095	13	3	0	4	103
99777	1	5	5	12	151	05529	9	5	6	14	187	11146	21	1	11	17	319
99911	3	2	6	10	127*	05663	11	2	7	12	187*	11229	15	0	1	2	103*
00179	1	3	3	7	91	05796	7	6	3	11	139*	11280	17	5	7	16	259
00314	3	0	4	5	67*	05931	9	3	4	9	139	11414	19	2	8	14	259*
00365	5	5	10	19	235	06065	11	0	5	7	139*	11548	15	6	4	13	199*
00499	7	2	11	17	223*	06116	13	5	11	21	295	11682	17	3	5	11	211
00581	1	1	1	2	31	06199	7	4	1	6	79*	11817	19	0	6	9	211*
00632	3	6	7	16	199*	06333	9	1	2	4	91	11950	15	4	2	8	151*
00767	5	3	8	14	175	06384	11	6	8	18	235*	12084	17	1	3	6	163
00901	7	0	9	12	175*	06518	13	3	9	16	247	12135	19	6	9	20	307*
01035	3	4	5	11	139*	06653	15	0	10	14	247*	12270	21	3	10	18	319
01169	5	1	6	9	127	06786	11	4	6	13	187*	12352	15	2	0	3	103*
01303	1	5	2	8	103	06920	13	1	7	11	199	12404	23	0	11	16	319*
01437	3	2	3	6	79*	07054	9	5	3	10	139	12538	19	4	7	15	259*
01622	7	4	10	18	223*	07188	11	2	4	8	139*	12672	21	1	8	13	271
01705	1	3	0	3	43	07322	7	6	0	7	91*	12806	17	5	4	12	211
01756	9	1	11	16	235	07374	15	4	11	20	295*	12940	19	2	5	10	211*
01839	3	0	1	1	19*	07456	9	3	1	5	91	13073	15	6	1	9	151*
01890	5	5	7	15	187	07591	11	0	2	3	91*	13208	17	3	2	7	163
02024	7	2	8	13	175*	07642	13	5	8	17	247	13342	19	0	3	5	163*
02158	3	6	4	12	151*	07776	15	2	9	15	247*	13393	21	5	9	19	319
02292	5	3	5	10	127	07909	11	6	5	14	187*	13527	23	2	10	17	319*
02427	7	0	6	8	127*	08044	13	3	6	12	199	13610	17	1	0	2	115
02560	3	4	2	7	91*	08178	15	0	7	10	199*	13661	19	6	6	16	259*
02694	5	1	3	5	79	08312	11	4	3	9	139*	13795	21	3	7	14	271
02745	7	6	9	19	235*	08446	13	1	4	7	151	13930	23	0	8	12	271*
02880	9	3	10	17	235	08497	15	6	10	21	295*	14063	19	4	4	11	211*
02962	3	2	0	2	31*	08580	9	5	0	6	91	14197	21	1	5	9	223
03014	11	0	11	15	235*	08631	17	3	11	19	307	14248	23	6	11	23	367*
03148	7	4	7	14	175*	08714	11	2	1	4	91*	14331	17	5	1	8	163
03282	9	1	8	12	187	08899	15	4	8	16	247*	14465	19	2	2	6	163*
03416	5	5	4	11	139	09033	17	1	9	14	259	14651	23	4	9	18	319*
03550	7	2	5	9	127*	09167	13	5	5	13	199	14785	25	1	10	16	331
03683	3	6	1	8	103*	09301	15	2	6	11	199*	14868	19	0	0	1	115*
03818	5	3	2	6	79	09435	11	6	2	10	139*	14919	21	5	6	15	271

DECML H N O =C WMIN DECML H N O =C WMIN DECML H N O =C WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class 8

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
94407	0	0	11	14	176	02807	8	2	8	13	188	08424	14	5	8	17	248*
95530	0	2	10	15	188	02940	4	6	4	12	152	08558	16	2	9	15	260
95932	0	0	8	10	128	03075	6	3	5	10	128*	08692	12	6	5	14	200
96251	0	6	11	21	260	03209	8	0	6	8	140	08826	14	3	6	12	200*
96653	0	4	9	16	200	03343	4	4	2	7	92	08961	16	0	7	10	212
96787	2	1	10	14	176*	03477	6	1	3	5	80*	09094	12	4	3	9	152
97055	0	2	7	11	140	03528	8	6	9	19	236	09228	14	1	4	7	152*
97458	0	0	5	6	80	03662	10	3	10	17	236*	09279	16	6	10	21	308
97509	2	5	11	20	248*	03745	4	2	0	2	32	09362	10	5	0	6	92*
97776	0	6	8	17	212	03797	12	0	11	15	248	09414	18	3	11	19	308*
97911	2	3	9	15	188*	03930	8	4	7	14	188	09496	12	2	1	4	104
98045	4	0	10	13	176	04064	10	1	8	12	188*	09682	16	4	8	16	260
98179	0	4	6	12	152	04198	6	5	4	11	140*	09816	18	1	9	14	260*
98313	2	1	7	10	128*	04332	8	2	5	9	140	09950	14	5	5	13	200*
98581	0	2	4	7	92	04466	4	6	1	8	104	10084	16	2	6	11	212
98766	4	4	11	19	236	04600	6	3	2	6	80*	10217	12	6	2	10	152
98983	0	0	2	2	32	04735	8	0	3	4	92	10352	14	3	3	8	152*
99034	2	5	8	16	200*	04786	10	5	9	18	236*	10486	16	0	4	6	164
99168	4	2	9	14	176	04920	12	2	10	16	248	10537	18	5	10	20	308*
99302	0	6	5	13	164	05002	6	1	0	1	32*	10620	12	4	0	5	104
99436	2	3	6	11	140*	05053	8	6	6	15	188	10671	20	2	11	18	320
99571	4	0	7	9	128	05188	10	3	7	13	188*	10754	14	1	1	3	104*
99704	0	4	3	8	104	05322	12	0	8	11	200	10805	16	6	7	17	260
99838	2	1	4	6	80*	05456	8	4	4	10	140	10939	18	3	8	15	260*
99889	4	6	10	20	248	05590	10	1	5	8	140*	11074	20	0	9	13	272
C0024	6	3	11	18	224*	05641	12	6	11	22	296	11207	16	4	5	12	212
C0106	0	2	1	3	44	05724	6	5	1	7	92*	11341	18	1	6	10	212*
C0292	4	4	8	15	188	05858	8	2	2	5	92	11475	14	5	2	9	152*
C0426	6	1	9	13	176*	06043	12	4	9	17	248	11609	16	2	3	7	164
C0560	2	5	5	12	152*	06177	14	1	10	15	248*	11795	20	4	10	19	320
C0694	4	2	6	10	128	06260	8	0	0	0	44	11877	14	3	0	4	104*
C0827	0	6	2	9	116	06311	10	5	6	14	188*	11929	22	1	11	17	320*
C0962	2	3	3	7	92*	06445	12	2	7	12	200	12012	16	0	1	2	116
C1096	4	0	4	5	80	06579	8	6	3	11	140	12063	18	5	7	16	260*
C1147	6	5	10	19	236*	06713	10	3	4	9	140*	12197	20	2	8	14	272
C1230	0	4	0	4	56	06848	12	0	5	7	152	12330	16	6	4	13	212
C1281	8	2	11	17	236	06899	14	5	11	21	296*	12465	18	3	5	11	212*
C1364	2	1	1	2	32*	06981	8	4	1	6	92	12599	20	0	6	9	224
C1415	4	6	7	16	200	07115	10	1	2	4	92*	12733	16	4	2	8	164
C1549	6	3	8	14	176*	07166	12	6	8	18	248	12867	18	1	3	6	164*
C1684	8	0	9	12	188	07301	14	3	9	16	248*	12918	20	6	9	20	320
C1817	4	4	5	11	140	07435	16	0	10	14	260	13052	22	3	10	18	320*
C1951	6	1	6	9	128*	07569	12	4	6	13	200	13135	16	2	0	3	116
C2085	2	5	2	8	104*	07703	14	1	7	11	200*	13187	24	0	11	16	332
C2219	4	2	3	6	80	07837	10	5	3	10	140*	13320	20	4	7	15	272
C2405	8	4	10	18	236	07971	12	2	4	8	152	13454	22	1	8	13	272*
C2487	2	3	0	3	44*	08104	8	6	0	7	92	13588	18	5	4	12	212*
C2539	10	1	11	16	236*	08156	16	4	11	20	308	13722	20	2	5	10	224
C2622	4	0	1	1	32	08239	10	3	1	5	92*	13856	16	6	1	9	164
C2673	6	5	7	15	188*	08373	12	0	2	3	104	13990	18	3	2	7	164*

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class 9

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95189	1	0	11	14	177*	03589	9	2	8	13	189*	09207	15	5	8	17	261
96312	1	2	10	15	189*	03723	5	6	4	12	153*	09341	17	2	9	15	261*
96715	1	0	8	10	129*	03857	7	3	5	10	141	09474	13	6	5	14	201*
97033	1	6	11	21	261*	03992	9	0	6	8	141*	09609	15	3	6	12	213
97436	1	4	9	16	201*	04125	5	4	2	7	93*	09743	17	0	7	10	213*
97570	3	1	10	14	177	04259	7	1	3	5	93	09877	13	4	3	9	153*
97838	1	2	7	11	141*	04310	9	6	9	19	237*	10011	15	1	4	7	165
98240	1	0	5	6	81*	04445	11	3	10	17	249	10062	17	6	10	21	309*
98291	3	5	11	20	249	04527	5	2	0	2	33*	10145	11	5	0	6	105
98559	1	6	8	17	213*	04579	13	0	11	15	249*	10196	19	3	11	19	321
98693	3	3	9	15	189	04713	9	4	7	14	189*	10279	13	2	1	4	105*
98828	5	0	10	13	177*	04847	11	1	8	12	201	10464	17	4	8	16	261*
98961	1	4	6	12	153*	04981	7	5	4	11	141	10598	19	1	9	14	273
99095	3	1	7	10	129	05115	9	2	5	9	141*	10732	15	5	5	13	213
99363	1	2	4	7	93*	05248	5	6	1	8	105*	10866	17	2	6	11	213*
99549	5	4	11	19	237*	05383	7	3	2	6	93	11000	13	6	2	10	153*
99766	1	0	2	2	33*	05517	9	0	3	4	93*	11134	15	3	3	8	165
99817	3	5	8	16	201	05568	11	5	9	18	249	11269	17	0	4	6	165*
99951	5	2	9	14	177*	05702	13	2	10	16	249*	11320	19	5	10	20	321
00084	1	6	5	13	165*	05785	7	1	0	1	45	11402	13	4	0	5	105*
00219	3	3	6	11	141	05836	9	6	6	15	189*	11454	21	2	11	18	321*
00353	5	0	7	9	129*	05970	11	3	7	13	201	11536	15	1	1	3	117
00487	1	4	3	8	105*	06105	13	0	8	11	201*	11587	17	6	7	17	261*
00621	3	1	4	6	81	06238	9	4	4	10	141*	11722	19	3	8	15	273
00672	5	6	10	20	249*	06372	11	1	5	8	153	11856	21	0	9	13	273*
00806	7	3	11	18	237	06423	13	6	11	22	297*	11990	17	4	5	12	213*
00889	1	2	1	3	45*	06506	7	5	1	7	93	12124	19	1	6	10	225
01074	5	4	8	15	189*	06640	9	2	2	5	93*	12258	15	5	2	9	165
01208	7	1	9	13	189	06826	13	4	9	17	249*	12392	17	2	3	7	165*
01342	3	5	5	12	153	06960	15	1	10	15	261	12577	21	4	10	19	321*
01476	5	2	6	10	129*	07043	9	0	0	0	45*	12660	15	3	0	4	117
01610	1	6	2	9	117*	07094	11	5	6	14	201	12711	23	1	11	17	333
01744	3	3	3	7	93	07228	13	2	7	12	201*	12794	17	0	1	2	117*
01879	5	0	4	5	81*	07361	9	6	3	11	141*	12845	19	5	7	16	273
01930	7	5	10	19	237	07496	11	3	4	9	153	12979	21	2	8	14	273*
02012	1	4	0	4	57*	07630	13	0	5	7	153*	13113	17	6	4	13	213*
02064	9	2	11	17	237*	07681	15	5	11	21	309	13247	19	3	5	11	225
02146	3	1	1	2	33	07764	9	4	1	6	93*	13382	21	0	6	9	225*
02197	5	6	7	16	201*	07898	11	1	2	4	105	13515	17	4	2	8	165*
02332	7	3	8	14	189	07949	13	6	8	18	249*	13649	19	1	3	6	177
02466	9	0	9	12	189*	08083	15	3	9	16	261	13700	21	6	9	20	321*
02600	5	4	5	11	141*	08218	17	0	10	14	261*	13835	23	3	10	18	333
02734	7	1	6	9	141	08351	13	4	6	13	201*	13917	17	2	0	3	117*
02868	3	5	2	8	105	08485	15	1	7	11	213	13969	25	0	11	16	333*
03002	5	2	3	6	81*	08619	11	5	3	10	153	14103	21	4	7	15	273*
03187	9	4	10	18	237*	08753	13	2	4	8	153*	14237	23	1	8	13	285
03270	3	3	0	3	45	08887	9	6	0	7	93*	14371	19	5	4	12	225
03321	11	1	11	16	249	08939	17	4	11	20	309*	14505	21	2	5	10	225*
03404	5	0	1	1	33*	09021	11	3	1	5	105	14638	17	6	1	9	165*
03455	7	5	7	15	189	09156	13	0	2	3	105*	14773	19	3	2	7	177
DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class

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DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
94714	0	1	11	15	190*	02980	6	6	7	16	202	08680	12	1	2	4	106*
95837	0	3	10	16	202*	03114	8	3	8	14	190*	08731	14	6	8	18	262
95972	2	0	11	14	178	03249	10	0	9	12	202	08866	16	3	9	16	262*
96239	0	1	8	11	142*	03382	6	4	5	11	142	09000	18	0	10	14	274
96961	0	5	9	17	214*	03516	8	1	6	9	142*	09134	14	4	6	13	214
97095	2	2	10	15	190	03650	4	5	2	8	106*	09268	16	1	7	11	214*
97363	0	3	7	12	154*	03784	6	2	3	6	94	09402	12	5	3	10	154*
97497	2	0	8	10	130	03970	10	4	10	18	250	09536	14	2	4	8	166
97765	0	1	5	7	94*	04052	4	3	0	3	46*	09669	10	6	0	7	106
97816	2	6	11	21	262	04104	12	1	11	16	250*	09721	18	4	11	20	322
98218	2	4	9	16	202	04187	6	0	1	1	46	09804	12	3	1	5	106*
98352	4	1	10	14	178*	04238	8	5	7	15	190*	09938	14	0	2	3	118
98486	0	5	6	13	166*	04372	10	2	8	13	202	09989	16	5	8	17	262*
98620	2	2	7	11	142	04505	6	6	4	12	154	10123	18	2	9	15	274
98888	0	3	4	8	106*	04640	8	3	5	10	142*	10257	14	6	5	14	214
99023	2	0	5	6	82	04774	10	0	6	8	154	10391	16	3	6	12	214*
99074	4	5	11	20	250*	04908	6	4	2	7	94	10526	18	0	7	10	226
99290	0	1	2	3	46*	05042	8	1	3	5	94*	10659	14	4	3	9	166
99341	2	6	8	17	214	05093	10	6	9	19	250	10793	16	1	4	7	166*
99476	4	3	9	15	190*	05227	12	3	10	17	250*	10844	18	6	10	21	322
99610	6	0	10	13	190	05310	6	2	0	2	46	10927	12	5	0	6	106*
99744	2	4	6	12	154	05362	14	0	11	15	262	10979	20	3	11	19	322*
99878	4	1	7	10	130*	05495	10	4	7	14	202	11061	14	2	1	4	118
00012	0	5	3	9	118*	05629	12	1	8	12	202*	11247	18	4	8	16	274
00146	2	2	4	7	94	05763	8	5	4	11	142*	11381	20	1	9	14	274*
00331	6	4	11	19	238	05897	10	2	5	9	154	11515	16	5	5	13	214*
00414	0	3	1	4	58*	06031	6	6	1	8	106	11649	18	2	6	11	226
00548	2	0	2	2	34	06165	8	3	2	6	94*	11782	14	6	2	10	166
00599	4	5	8	16	202*	06300	10	0	3	4	106	11917	16	3	3	8	166*
00733	6	2	9	14	190	06351	12	5	9	18	250*	12051	18	0	4	6	178
00867	2	6	5	13	166	06485	14	2	10	16	262	12102	20	5	10	20	322*
01001	4	3	6	11	142*	06567	8	1	0	1	46*	12185	14	4	0	5	118
01136	6	0	7	9	142	06618	10	6	6	15	202	12236	22	2	11	18	334
01269	2	4	3	8	106	06753	12	3	7	13	202*	12319	16	1	1	3	118*
01403	4	1	4	6	82*	06887	14	0	8	11	214	12370	18	6	7	17	274
01454	6	6	10	20	250	07021	10	4	4	10	154	12504	20	3	8	15	274*
01537	0	5	0	5	70*	07155	12	1	5	8	154*	12639	22	0	9	13	286
01589	8	3	11	18	238*	07206	14	6	11	22	310	12772	18	4	5	12	226
01671	2	2	1	3	46	07289	8	5	1	7	94*	12906	20	1	6	10	226*
01857	6	4	8	15	190	07423	10	2	2	5	106	13040	16	5	2	9	166*
01991	8	1	9	13	190*	07608	14	4	9	17	262	13174	18	2	3	7	178
02125	4	5	5	12	154*	07742	16	1	10	15	262*	13360	22	4	10	19	334
02259	6	2	6	10	142	07825	10	0	0	0	58	13442	16	3	0	4	118*
02392	2	6	2	9	118	07876	12	5	6	14	202*	13494	24	1	11	17	334*
02527	4	3	3	7	94*	08010	14	2	7	12	214	13577	18	0	1	2	130
02661	6	0	4	5	94	08144	10	6	3	11	154	13628	20	5	7	16	274*
02712	8	5	10	19	238*	08278	12	3	4	9	154*	13762	22	2	8	14	286
02795	2	4	0	4	58	08413	14	0	5	7	166	13895	18	6	4	13	226
02846	10	2	11	17	250	08464	16	5	11	21	310*	14030	20	3	5	11	226*
02929	4	1	1	2	34*	08546	10	4	1	6	106	14164	22	0	6	9	238

| DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN | DECML | H | N | O | =C | WMIN |

Table 3. Decimal Weights of (H,O,N) Combinations of Organic Molecules

Integer Residue Class **11**

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN
95496	1	1	11	15	191	03762	7	6	7	16	203*	09463	13	1	2	4	119
96620	1	3	10	16	203	03897	9	3	8	14	203	09514	15	6	8	18	263*
96754	3	0	11	14	179*	04031	11	0	9	12	203*	09648	17	3	9	16	275
97022	1	1	8	11	143	04165	7	4	5	11	143*	09783	19	0	10	14	275*
97743	1	5	9	17	215	04299	9	1	6	9	155	09916	15	4	6	13	215*
97877	3	2	10	15	191*	04433	5	5	2	8	107	10050	17	1	7	11	227
98145	1	3	7	12	155	04567	7	2	3	6	95*	10184	13	5	3	10	167
98280	3	0	8	10	131*	04752	11	4	10	18	251*	10318	15	2	4	8	167*
98547	1	1	5	7	95	04835	5	3	0	3	47	10452	11	6	0	7	107*
98598	3	6	11	21	263*	04886	13	1	11	16	263	10504	19	4	11	20	323*
99001	3	4	9	16	203*	04969	7	0	1	1	47*	10586	13	3	1	5	119
99135	5	1	10	14	191	05020	9	5	7	15	203	10721	15	0	2	3	119*
99269	1	5	6	13	167	05154	11	2	8	13	203*	10772	17	5	8	17	275
99403	3	2	7	11	143*	05288	7	6	4	12	155*	10906	19	2	9	15	275*
99671	1	3	4	8	107	05422	9	3	5	10	155	11039	15	6	5	14	215*
99805	3	0	5	6	83*	05557	11	0	6	8	155*	11174	17	3	6	12	227
99856	5	5	11	20	251	05690	7	4	2	7	95*	11308	19	0	7	10	227*
00073	1	1	2	3	47	05824	9	1	3	5	107	11442	15	4	3	9	167*
00124	3	6	8	17	215*	05875	11	6	9	19	251*	11576	17	1	4	7	179
00258	5	3	9	15	191	06010	13	3	10	17	263	11627	19	6	10	21	323*
00393	7	0	10	13	191*	06092	7	2	0	2	47*	11710	13	5	0	6	119
00526	3	4	6	12	155*	06144	15	0	11	15	263*	11761	21	3	11	19	335
00660	5	1	7	10	143	06278	11	4	7	14	203*	11844	15	2	1	4	119*
00794	1	5	3	9	119	06412	13	1	8	12	215	12029	19	4	8	16	275*
00928	3	2	4	7	95*	06546	9	5	4	11	155	12163	21	1	9	14	287
01114	7	4	11	19	239*	06680	11	2	5	9	155*	12297	17	5	5	13	227
01196	1	3	1	4	59	06813	7	6	1	8	107*	12431	19	2	6	11	227*
01331	3	0	2	2	35*	06948	9	3	2	6	107	12565	15	6	2	10	167*
01382	5	5	8	16	203	07082	11	0	3	4	107*	12699	17	3	3	8	179
01516	7	2	9	14	191*	07133	13	5	9	18	263	12834	19	0	4	6	179*
01649	3	6	5	13	167*	07267	15	2	10	16	263*	12885	21	5	10	20	335
01784	5	3	6	11	143	07350	9	1	0	1	59	12967	15	4	0	5	119*
01918	7	0	7	9	143*	07401	11	6	6	15	203*	13019	23	2	11	18	335*
02052	3	4	3	8	107*	07535	13	3	7	13	215	13101	17	1	1	3	131
02186	5	1	4	6	95	07670	15	0	8	11	215*	13152	19	6	7	17	275*
02237	7	6	10	20	251*	07803	11	4	4	10	155*	13287	21	3	8	15	287
02320	1	5	0	5	71	07937	13	1	5	8	167	13421	23	0	9	13	287*
02371	9	3	11	18	251	07988	15	6	11	22	311*	13555	19	4	5	12	227*
02454	3	2	1	3	47*	08071	9	5	1	7	107	13689	21	1	6	10	239
02639	7	4	8	15	191*	08205	11	2	2	5	107*	13823	17	5	2	9	179
02773	9	1	9	13	203	08391	15	4	9	17	263*	13957	19	2	3	7	179*
02907	5	5	5	12	155	08525	17	1	10	15	275	14142	23	4	10	19	335*
03041	7	2	6	10	143*	08608	11	0	0	0	59*	14225	17	3	0	4	131
03175	3	6	2	9	119*	08659	13	5	6	14	215	14276	25	1	11	17	347
03309	5	3	3	7	95	08793	15	2	7	12	215*	14359	19	0	1	2	131*
03444	7	0	4	5	95*	08926	11	6	3	11	155*	14410	21	5	7	16	287
03495	9	5	10	19	251	09061	13	3	4	9	167	14544	23	2	8	14	287*
03577	3	4	0	4	59*	09195	15	0	5	7	167*	14678	19	6	4	13	227*
03629	11	2	11	17	251*	09246	17	5	11	21	323	14812	21	3	5	11	239
03711	5	1	1	2	47	09329	11	4	1	6	107*	14947	23	0	6	9	239*

DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN	DECML	H	N	O	=C	WMIN