

Table S1: Compounds identified by perivious

No	Compound name
1	2-Amino-3,4-dihydroxypentanedioic acid
2	Benzyl glucosinolate
3	Benzyl isothiocyanate
4	Benzyl thiocyanate
5	3,5,7,8-teta methyl ether of 3,4,5,5',7,8-hexahydroxyflavone
6	O-beta-D-Galactopyranoside of 2-(4-Hydroxybenzyl)imidazole
7	3-Methoxy,O-beta-D-Galactopyranoside of 2-(4-Hydroxybenzyl)imidazole
8	Lepidimoic acid
9	Lepidine
10	O-De-Methyl of lepidine
11	8-Demethoxy,10-hydroxy of lepidine
12	8-Demethoxy,10-methoxy of lepidine
13	Lepidine E
14	Lepidine F
15	Lepidiumterpenoid
16	2,6,10,14,18-Pentamethyl-15-eicosene-2,13-diol
17	Diethylamide of phenylacetic acid
18	Nitrile of phenylacetic acid
19	26-Benzoyl of Stigmast-5-ene-3,26-diol
20	1-(6-Heptenyl)ester of 2,6,10-Trimethyltridecanedioic acid
21	$\alpha$ -D-Xylopyranosyl-(1 $\rightarrow$ 3)- $\alpha$ -L-arabinofuranosyl-(1 $\rightarrow$ 3)-L-arabinose
22	3-O- $\alpha$ -D-Xylopyranosyl-L-arabinose
23	5-(Isothiocyanatomethyl)-1,2,3-trimethoxybenzene
24	7,10-hexadecadienoic acid
25	7,10,13-hexadecatrienoic acid
26	11-octadecaenoic acid
27	behenic acid

28	alpha-linolenic acid
29	9,12-hexadecadienoic acid
30	heneicosanoic acid
31	hexadecanoic acid
32	10-octadecenoic acid
33	15-tetracosenoic acid
34	stearic acid
35	beta-amyrin
36	9,12,15-octadecatrienoic acid methyl ester
37	9-octadecennoic acid methyl ester
38	alpha-amyrin
39	11-eicosenoic acid methyl ester
40	9,12-octadecadienoic acid
41	hexadecanoic acid methyl ester
42	Glucopaoline
43	Sinapoyl malate
44	Ferulic acid
45	Sinapic acid
46	sinapoyl di-glucose
47	Sinapine
48	Quercetin di-hexose rhamnose
49	Oleic acid
50	beta-sitosterol
51	palmitoleic acid
52	Heptadecanoic acid
53	arachidic acid
54	campesterol
55	erucic acid
56	benzoic acid
57	3-methoxy-4-hydroxybenzoic acid
58	Niacin

59	syringaldehyde
60	2-phenylacetamide
61	Kaempferol-7-O-alpha-L-rhamnopyranoside
62	Rutin
63	Quercetin 7-O-L-rhamnoside
64	Aegicin; (7''R*,8''R*)-form, 3''-Methoxy, 7''-Me ether
65	Aegicin; (7''R*,8''S*)-form, 3''-Methoxy
66	Benzylamine
67	Benzylamine; N-Heptadecanoyl
68	Benzylamine; N-(9Z,12Z-Octadecadienoyl)
69	Benzylamine; N-Octadecanoyl
70	Benzylamine; N-(9Z,12Z,15Z-Octadecatrienoyl)
71	Benzylamine; N-(9Z-Octadecenoyl)
72	Benzylamine; N-Pentadecanoyl
73	Benzylamine; N-Tetracosanoyl
74	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
75	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
76	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
77	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
78	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
79	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
80	2-Benzylhexahydro-7a-hydroxy-3-thioxo-1H-pyrrolo[1,2-c]imidazol-
81	3-Benzyl-2-thioxo-1,3-diazabicyclo[3.3.1]nonan-4-one; (±)-form
82	N,N'-Bis(3-methoxybenzyl)urea
83	Desulfoglucosinolate sulfotransferase
84	1,3-Dibenzyl-5-hydroxy-5-methyl-2-thioxo-4-imidazolidinone; (±)-fc
85	1,3-Dibenzyl-5-hydroxy-5-methyl-2-thioxo-4-imidazolidinone; (±)-fc
86	1,3-Dibenzyl-5-hydroxy-5-methyl-2-thioxo-4-imidazolidinone; (±)-fc
87	1,3-Dibenzyl-5-hydroxy-5-methyl-2-thioxo-4-imidazolidinone; (±)-fc
88	N,N'-Dibenzylurea

89	3,4-Dihydroxybenzyl glucosinolate; Di-Me ether
90	3,4-Dihydroxybenzyl glucosinolate; 3-Me ether
91	3,4-Dihydroxybenzylamine; Di-Me ether, N-hexadecanoyl
92	3,14-Dihydroxycard-20(22)-enolide; (3 $\beta$ ,5 $\beta$ ,14 $\beta$ ,17 $\beta$ )-form, 3-O- $\alpha$ -L-
93	4,5-Dimethylimidazole; N1,N3-Dibenzyl
94	4,5-Dimethylimidazole; N1-(4-Methoxybenzyl), N3-benzyl
95	Ethyl glucosinolate
96	Ethyl isothiocyanate
97	7-C-Glucosyl-2',3',5,6-tetrahydroxyisoflavone; 2',3'-Methylene, 5,6-d
98	Hexadecanoic acid; Benzylamide
99	Hexahydro-7a-(hydroxymethyl)-2-(3-methoxybenzyl)-3-thioxo-1H-p
100	3',4',5,5',7,8-Hexahydroxyflavone; 3',5',7,8-Tetra-Me ether
101	3-Hydroxybenzyl glucosinolate
102	3-Hydroxybenzyl glucosinolate; Me ether
103	3-Hydroxybenzyl isothiocyanate
104	3-Hydroxybenzyl isothiocyanate; Me ether
105	4-Hydroxybenzyl isothiocyanate; Me ether
106	3-Hydroxybenzylamine; Me ether, N-hexadecanoyl
107	3-Hydroxybenzylamine; Me ether, N-(9Z,12Z-octadecadienoyl)
108	3-Hydroxybenzylamine; Me ether, N-(9Z,12Z,15Z-octadecatrienoyl)
109	3-Hydroxybenzylamine; Me ether, N-(9Z-octadecenoyl)
110	2-(4-Hydroxybenzyl)imidazole; O- $\beta$ -D-Galactopyranoside
111	2-(4-Hydroxybenzyl)imidazole; 3'-Methoxy, O- $\beta$ -D-galactopyranosid
112	3-Hydroxyphenylacetic acid; Methylamide
113	Isorhamnetin 3-glycosides; Trisaccharides, 3-O-[ $\beta$ -D-Glucopyranosyl
114	Isorhamnetin 3-glycosides; Trisaccharides, 3-O-[4-Hydroxy-3,5-dime
115	1-Isothiocyanato-4-(methylsulfinyl)butane; (R)-form
116	Kaempferol 3,7-diglycosides; Bis(monosaccharides), 3-O- $\beta$ -D-Xylop
117	Kaempferol 3,7-diglycosides; Tetrasaccharides, 3-O-[3,4-Dihydroxy-
118	Kaempferol 3,7-diglycosides; Trisaccharides, 3-O-[4-Hydroxy-3,5-di
119	Kaempferol 3-glycosides; Triglycosides, 3-O-[4-Hydroxy-3,5-dimeth

120	Macaridine
121	4-(Methylthio)butyl glucosinolate; S-Oxide
122	Meyeniin B
123	Meyeniin B; 3'-Methoxy
124	Meyeniin B; 3',4'-Methylenedioxy
125	5-Oxo-6,8-octadecadienoic acid; (E,E)-form
126	5-Oxo-6,8-octadecadienoic acid; (E,E)-form, Benzylamide
127	9-Oxo-12,15-octadecadienoic acid; (12Z,15Z)-form, Benzylamide
128	13-Oxo-9,11-octadecadienoic acid; (9E,11E)-form, Benzylamide
129	9-Oxo-12-octadecenoic acid; (Z)-form, Benzylamide
130	3,3',4',5,7-Pentahydroxyflavone; 3-O-[6-O-Benzoyl- $\beta$ -D-glucopyranoside]
131	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[3,4-Dihydroxy-E-pyrano]
132	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[ $\beta$ -D-Glucopyranoside]
133	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[ $\beta$ -D-Glucopyranoside]
134	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[ $\beta$ -D-Glucopyranoside]
135	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[4-Hydroxy-3,5-dihydroxy]
136	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[4-Hydroxy-3,5-dihydroxy]
137	Quercetin 3,7-diglycosides; Tetrasaccharides, 3-O-[4-Hydroxy-3-methoxy]
138	Quercetin 3,7-diglycosides; Trisaccharides, 3-O-[ $\alpha$ -L-Rhamnopyranoside]
139	Quercetin 3-glycosides; Trisaccharides, 3-O-[4-Hydroxy-3,5-dimethoxy]
140	Quercetin 3-glycosides; Trisaccharides, 3-O-[4-Hydroxy-3,5-dimethoxy]
141	Quercetin 3-glycosides; Trisaccharides, 3-O-[4-Hydroxy-3-methoxy]
142	Quercetin 3-glycosides; Trisaccharides, 3-O-[4-Hydroxy-3-methoxy]
143	15-Tetracosenoic acid; (Z)-form, Benzylamide
144	2,3,4,9-Tetrahydro-1-methyl-1H-pyrido[3,4-b]indole-3-carboxylic acid
145	3,4,5-Trimethoxybenzyl glucosinolate
146	3,4,5-Trimethoxybenzyl glucosinolate; 4-O-De-Me
147	2,4,5-Trimethyl-1H-imidazole; N1,N3-Dibenzyl
148	2,4,5-Trimethyl-1H-imidazole; N1-(4-Methoxybenzyl), N3-benzyl
149	3-methoxybenzylamide derivative of hexadecanoic acid
150	Apetalumoside D
151	N,N'-Dibenzylurea 3''-Methoxy

152	N,N'-Dibenzylurea 3'',3'''-Dimethoxy
153	4,5-Dihydro-2-oxo-1 <i>H</i> -imidazole-4,5-dipropanoic acid Dibenzylamide
154	(-)- $\beta$ -thujone
155	Alpha-pinene
156	3,4-Dihydroxybenzylamine Di-Me ether, N-hexadecanoyl
157	3,14-Dihydroxycard-20(22)-enolide 3-O- $\alpha$ -L-Rhamnopyranoside
158	4,5-Dimethyl-1 <i>H</i> -imidazole N1,N3-Dibenzyl
159	4,5-Dimethyl-1 <i>H</i> -imidazole N1-(4-Methoxybenzyl), N3-benzyl
160	3,7'-Epoxy-3',4',5,9'-tetrahydroxy-2,8'-lign-7-en-9-oic acid 3',5-Di-Me ether
161	Ethyl glucosinolater
162	Ethyl isothiocyanate
163	7- <i>C</i> -Glucosyl-2',3',5,6-tetrahydroxyisoflavone;2',3'-Methylene, 5,6-d
164	9-Hexadecenoic acid 3,4-Dimethoxybenzylamide
165	5-(Hydroxymethyl)-1 <i>H</i> -pyrrole-2-carboxaldehyde N-Benzyl
166	5-(Hydroxymethyl)-1 <i>H</i> -pyrrole-2-carboxaldehyde N-Benzyl Me ether
167	5-(Hydroxymethyl)-1 <i>H</i> -pyrrole-2-carboxaldehyde N-Benzyl Me ether
168	1 <i>H</i> -Imidazole-4-carboxylic acid
169	Isorhamnetin 3-glycosides 3-O-[ $\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 2)-[ $\beta$ -D-gl
170	Lepidine E Deoxy, 3-methoxy
171	Lepidiumamide A
172	Macahydantoin A( $\pm$ )-form
173	Macahydantoin B ( $\pm$ )-form
174	Macahydantoin C
175	Macahydantoin C 3'-Methoxy
176	Macahydantoin D
177	Macahydantoin D 3'-Hydroxy
178	Macahydantoin D 3'-Methoxy
179	Macathioamide A
180	Macathiohydantoin D ( $\pm$ )-form
181	Quercetin
182	Kaempferol-3-O- $\alpha$ -L-rhamnopyranoside
183	Kaempferol-3-O- $\beta$ -D-glucopyranoside
184	Quercetin-3-O- $\beta$ -D-galactopyranoside

185	sabinene
186	1,8-cineole
187	Macaurea A
188	3,3',7',8',9'-Pentahydroxy-4,4'-oxylign-7-en-9-oic acid 5'-Methoxy, 3
189	2,3,4,9-Tetrahydro-1 <i>H</i> -pyrido[3,4- <i>b</i> ]indole-3-carboxylic acid (S)-for
190	3,6 <i>a</i> ,8,9-Tetrahydropterocarpan 8,9-Methylene, 3-Me ether
191	1-Thio- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 1)-1-thio- $\alpha$ -D-glucopyranose
192	Uridine-5'-Benzoyl
193	N-acetylbenzylamide
194	N-benzylhexadecanamide
195	$\beta$ -carboline
196	Catechol
197	N-(3,4-dimethoxybenzyl)- hexadecanamide
198	N-benzyl-9 <i>Z</i> -octadecanamide
199	N-benzyl-octanamide
200	N-benzyl-9, 16-dioxo 10 <i>E</i> , 12 <i>E</i> , 14 <i>E</i> -octadecatrieneamide
201	N-benzyl-16-hydroxy-9-oxo 10 <i>E</i> , 12 <i>E</i> , 14 <i>E</i> -octadecatrieneamide
202	Catechin
203	N-benzyl-9-oxo-12 <i>E</i> -octadecenamide
204	D-(+)-Mannose
205	D-(+)-Xylose
206	Tocopherol
207	N-( <i>m</i> -methoxybenzyl)-hexadecanamide
208	N-benzyl-9 <i>E</i> -octadecenamide
209	N-benzyl-9 <i>E</i> , 12 <i>E</i> -octadecadienamide
210	N-benzyl-9 <i>E</i> , 12 <i>E</i> , 15 <i>E</i> octadecatrienamide
211	N-(3, 4-dimethoxybenzyl)-hexadecanamide
212	(S)-(-)-limonene
213	Ellagic
214	(1 <i>R</i> , 3 <i>S</i> )-1-methyltetrahydro- $\beta$ -carboline-3-carboxylic acid
215	1,3-dibenzyl-4, 5-dimethylimidazolium chloride
216	1,3-dibenzyl-2, 4,5-trimethylimidazolium chloride
217	3-benzyl-1-(3-methoxybenzyl)-4, 5-dimethylimidazolium chloride

218	3-benzyl 1-(3-methoxybenzyl)-2, 4, 5-trimethylimidazolium chloride
219	rhamnose
220	galactose
221	glucose
222	arabinose
223	p-methoxybenzylglucosinolate
224	4-methoxyindolyl 3-methoxyglucosinolate
225	indolyl-3-methylglucosinolate
226	Glu 1
227	Glu 2
228	acetyl-benzylglucosinolate
229	indolyl-5-methylglucosinolate
230	indolyl-3-hexyl-4-methyl-cyclohexaneglucosinolate
231	4-methoxyindolyl-3-hexylhydroxyglucosinolate
232	pent-4-enylglucosinolate
233	p-hydroxybenzylglucosinolate
234	o-hydroxybenzylglucosinolate
235	brassicasterol
236	$\beta$ -sitosterol
237	ergosterol
238	$\Delta^7,22$ -ergostadienol
239	stigmasterol
240	3,5-Stigmastadien-7-one
241	caprylic acid
242	capric acid
243	lauric acid
244	myristic acid
245	tricin 40 -O-[threo- $\beta$ -guaiacyl-(700-O-methyl)-glyceryl] ether
246	tricin 40 -O-(erythro- $\beta$ -guaiacyl-glyceryl) ether
247	tricin
248	Isoleucine
249	Leucine
250	Valine



251	Lysine
252	Phenylalanine
253	tyrosine
254	Threonine
255	Methionine
256	Glucosinabin
257	4-Hydroxyglucobrassicin
258	4-Methoxyglucobrassicin
259	5-methylsulfinylpentyl glucosinolate
260	Sitosteryl acetate
261	Campesteryl acetate
262	Ergosteryl acetate
263	3,5-Dimethylpyrazole
264	2-Hexenal
265	p-Xylene
266	Hexanoic acid
267	Benzyl alcohol
268	Heptanoic acid
269	3-Methoxybenzaldehyde
270	1-Phenylmethyl-pyrrole
271	(3-Methoxyphenyl)acetonitrile
272	Dimethyl phthalate
273	9-oxo-10E,12E-octadecadienoic acid
274	4-Phenylamino-phenol
275	Diphenylamine
276	9-Tetradecenoic acid
277	Pentadecanoic acid
278	Diisobutyl phthalate
279	9-Hexadecenoic acid
280	Methyl hexadecenoate
281	Methyl linoleate
282	Methyl linolenate
283	9,11,14-Eicosatrienoic acid

284	cis-10-Heptadecenoic acid
285	9,12,15-Octadecatrienoic acid
286	cis-10-Nonadecenoic acid
287	6,9,12-Octadecatrienoic acid
288	9c,11t,13t-Octadecatrienoic acid
289	6c,9c,11t-Octadecatrienoic acid
290	10,13-Eicosadienoic acid
291	13-Eicosenoic acid
292	10,13-Octadecadienoic acid
293	9c,11t,13t,15c-Parinaric acid
294	11-Docosenoic acid
295	22-Tricosenoic acid
296	21-Methyldocosanoic acid
297	Tetracosanoic acid
298	16-Pentacosenic acid
299	Pentacosanic acid
300	Hexacosanoic acid
301	macahydantoins C
302	macahydantoins D
303	(9E)-N-benzyl octadecenamide
304	Propanoate
305	Kaempferol
306	octadecadienamide
307	N-(3,4-dimethoxybenzyl)hexadecanamide
308	Furfuranol
309	gamma-Terpinen
310	9-oxo-10E,12Z-octadecadienoic acid
311	N-benzyl-9,16-dioxo 10E,12E,14E-octadecatriene amide
312	N-Benzyl oleamide
313	N-(3,4-dimethoxybenzyl)- 9Z oleamide
314	(1R,3S)-1-methyltetrahydro- $\beta$ carboline-3-carboxylic acid
315	Terpineol
316	Cholesterol

317	(+)-alpha-Phellandrene
318	Ascorbic acid
319	Apigenin
320	3',5'-dimethoxyacetophenone
321	Luteolin
322	6-prenylnaringenin
323	Hexose rhamnose 1
324	Benzaldehyde
325	Benzonitrile
326	Cysteine
327	6-Heptenoic acid, methyl ester
328	Capric acid methyl ester
329	(+)-Meyeniin A
330	(+)-Meyeniin B
331	(+)-Meyeniin C
332	Avenasterol
333	Gallocatechin
334	Epigallocatechin gallate
335	Mandelic acid
336	3,4-Dihydroxybenzoic acid
337	p-coumaric acid
338	3,5-Stigmastadiene
339	Nonadecanoic Acid
340	Docosanoic acid
341	(E)-octadec-9-enoic acid
342	2-oxononadecanoic acid
343	Anandamide
344	Gallic acid
345	Gentisic acid
346	Chlorogenic acid
347	4-Hydroxy benzoic acid
348	Caffeic acid
349	Hesperidin

350	Apigenin-7-glucoside
351	Rosmarinic acid
352	Salicylic acid
353	Chicoric acid
354	Quercetin-3-O- $\beta$ -D-sophoroside-7-O- $\alpha$ -L-rhamnoside
355	Kaempferol-3-O- $\beta$ -D-glucopyranosyl-(1-2)- $\beta$ -D-glucopyranoside-7-O-
356	Kaempferol-3-O- $\beta$ -D-glucopyranoside-7-O- $\alpha$ -L-rhamnopyranoside
357	Kaempferol-3-O-(2-O-feruloyl- $\beta$ -D-glucopyranosyl-(1-2)- $\beta$ -D-glucop
358	Kaempferol-3-O- $\beta$ -D-sophoroside-7-O- $\alpha$ -L-rhamnoside
359	Kaempferol-3-O-robinoside-7-O-(2''''-(E)-feruloyl)-sophoroside
360	Quercetin-3-O-(2,6-di-O- $\beta$ -D-glucopyranosyl)- $\beta$ -D-glucopyranoside-
361	Serine
362	Aspartic acid
363	Glutamic acid
364	Glycine
365	alanine
366	Proline
367	Histidine
368	Arginine
369	Geraniol
370	citronellol
371	triacontane
372	1,6-octadien-3-ol, 3,7-dimethyl
373	Pyrogallol
374	4-Aminobenzoic
375	Quercitrin
376	8-Nonynoic acid, methyl ester
377	Cyclopropanepentanoic acid, 2-undecyl-, methyl ester, trans-
378	Behenic acid, methyl ester
379	Eicosanoic acid, methyl ester
380	9,12-Hexadecadienoic acid, methyl ester
381	7,10-Hexadecadienoic acid, methyl ester
382	7,10,13-Hexadecatrienoic acid, methyl ester

383	Stearic acid, methyl ester
384	4-Tridecen-6-yne, (Z)-
385	9,12-Octadecadienoic acid, methyl ester
386	13,16-Octadecadienoic acid, methyl ester
387	Tetradecanoic acid, 12-methyl-, methyl ester
388	11-Octadecenoic acid, methyl ester
389	Hexadecanoic acid, 15-methyl-, methyl ester
390	7-Octadecynoic acid, methyl ester
391	15-Tetracosenoic acid, methyl ester
392	Heneicosanoic acid, methyl ester
393	13-Docosenoic acid, methyl ester
394	Triacontanoic acid, methyl ester
395	10-Octadecenoic acid, methyl ester
396	Tetracosanoic acid, methyl ester
397	24-methylenecholesterol
398	Clerosterol

literature in *lepidium* species

Molecular formula	Molecular weight
$C_5H_9NO_6$	179.129
$C_{14}H_{18}NO_9S_2$	409.437
$C_8H_7NS$	149.216
$C_8H_7NS$	149.216
$C_{19}H_{18}O_8$	374.346
$C_{16}H_{20}N_2O_6$	336.344
$C_{17}H_{22}N_2O_7$	366.37
$C_{12}H_{18}O_{10}$	322.268
$C_{21}H_{20}N_4O_2$	360.415
$C_{20}H_{18}N_4O_2$	346.388
$C_{20}H_{18}N_4O_2$	346.388
$C_{21}H_{20}N_4O_2$	360.415
$C_{20}H_{18}N_4O_2$	346.388
$C_{20}H_{18}N_4O_2$	346.388
$C_{27}H_{48}O_2$	404.675
$C_{25}H_{50}O_2$	382.669
$C_{12}H_{17}NO$	191.272
$C_8H_7N$	117.15
$C_{36}H_{54}O_3$	534.821
$C_{23}H_{42}O_4$	382.582
$C_{15}H_{26}O_{13}$	414.363
$C_{10}H_{18}O_9$	282.247
$C_{11}H_{13}NO_3S$	239.29
$C_{16}H_{28}O_2$	252.39
$C_{16}H_{26}O_2$	250.38
$C_{18}H_{34}O_2$	282.5
$C_{22}H_{44}O_2$	340.6

$C_{18}H_{30}O_2$	278.4
$C_{16}H_{28}O_2$	252.39
$C_{21}H_{42}O_2$	326.6
$C_{16}H_{32}O_2$	256.42
$C_{18}H_{34}O_2$	282.5
$C_{24}H_{46}O_2$	366.6
$C_{18}H_{36}O_2$	284.5
$C_{30}H_{50}O$	426.7
$C_{19}H_{32}O_2$	292.5
$C_{19}H_{36}O_2$	296.5
$C_{30}H_{50}O$	426.7
$C_{21}H_{40}O_2$	324.5
$C_{18}H_{32}O_2$	280.4
$C_{17}H_{34}O_2$	270.5
$C_{14}H_{19}NO_9S_2$	409.4
$C_{15}H_{16}O_9$	340.28
$C_{10}H_{10}O_4$	194.18
$C_{11}H_{12}O_5$	224.21
$C_{28}H_{32}O_{14}$	592.5
$C_{16}H_{24}NO_5^+$	310.36
$C_{33}H_{40}O_{21}$	772.66
$C_{18}H_{34}O_2$	282.5
$C_{29}H_{50}O$	414.7
$C_{16}H_{30}O_2$	254.41
$C_{17}H_{34}O_2$	270.5
$C_{20}H_{40}O_2$	312.5
$C_{28}H_{48}O$	400.7
$C_{22}H_{42}O_2$	338.6
$C_7H_6O_2$	122.12
$C_8H_8O_4$	168.15
$C_6H_5O_2N$	123.11

$C_9H_{10}O_4$	182.17
$C_8H_9NO$	135.16
$C_{21}H_{20}O_{10}$	432.38
$C_{27}H_{30}O_{16}$	610.5
$C_{21}H_{20}O_{11}$	448.38
$C_{28}H_{28}O_{11}$	540.51
$C_{27}H_{26}O_{11}$	526.49
$C_7H_9N$	107.15
$C_{24}H_{41}NO$	359.59
$C_{25}H_{39}NO$	369.6
$C_{25}H_{43}NO$	373.6
$C_{25}H_{37}NO$	367.6
$C_{25}H_{41}NO$	371.6
$C_{22}H_{37}NO$	331.53
$C_{31}H_{55}NO$	457.77
$C_{13}H_{14}N_2O_2S$	262.33
$C_{13}H_{14}N_2OS$	246.33
$C_{13}H_{14}N_2O_2S$	262.33
$C_{14}H_{16}N_2O_2S$	276.35
$C_{13}H_{14}N_2O_3S$	278.33
$C_{14}H_{16}N_2O_2S$	276.35
$C_{14}H_{16}N_2O_3S$	292.35
$C_{14}H_{16}N_2OS$	260.35
$C_{17}H_{20}N_2O_3$	300.35
enzyme	
$C_{18}H_{18}N_2O_2S$	326.41
$C_{19}H_{20}N_2O_2S$	340.44
$C_{19}H_{20}N_2O_2S$	340.44
$C_{19}H_{20}N_2O_3S$	356.44
$C_{15}H_{16}N_2O$	240.3



$C_{16}H_{23}NO_{11}S_2$	469.48
$C_{15}H_{21}NO_{11}S_2$	455.46
$C_{25}H_{43}NO_3$	405.61
$C_{29}H_{44}O_8$	520.65
$C_{19}H_{21}N_2$	277.38
$C_{20}H_{23}N_2O$	307.41
$C_9H_{17}NO_9S_2$	347.4
$C_3H_5NS$	87.15
$C_{24}H_{24}O_{11}$	488.44
$C_{23}H_{39}NO$	345.567
$C_{15}H_{18}N_2O_3S$	306.38
$C_{19}H_{18}O_8$	374.34
$C_{14}H_{19}NO_{10}S_2$	425.437
$C_{15}H_{21}NO_{10}S_2$	439.464
$C_8H_7NOS$	165.21
$C_9H_9NOS$	179.24
$C_9H_9NOS$	179.24
$C_{24}H_{41}NO_2$	375.59
$C_{26}H_{41}NO_2$	399.61
$C_{26}H_{39}NO_2$	397.59
$C_{26}H_{43}NO_2$	401.62
$C_{16}H_{20}N_2O_6$	336.34
$C_{17}H_{22}N_2O_7$	366.36
$C_9H_{11}NO_2$	165.19
$C_{34}H_{42}O_{22}$	802.68
$C_{56}H_{62}O_{30}$	1215.07
$C_6H_{11}NOS_2$	177.291
$C_{26}H_{28}O_{14}$	564.499
$C_{48}H_{56}O_{29}$	1096.94
$C_{44}H_{50}O_{24}$	962.85
$C_{55}H_{60}O_{29}$	1185.05

$C_{13}H_{13}NO_2$	215.25
$C_{12}H_{23}NO_{10}S_3$	437.5
$C_{13}H_{14}N_2OS_2$	278.39
$C_{14}H_{16}N_2O_2S_2$	308.42
$C_{14}H_{14}N_2O_3S_2$	322.4
$C_{18}H_{30}O_3$	294.433
$C_{25}H_{37}NO_2$	383.573
$C_{25}H_{37}NO_2$	383.573
$C_{25}H_{37}NO_2$	383.57
$C_{25}H_{39}NO_2$	385.589
$C_{40}H_{44}O_{22}$	876.76
$C_{48}H_{56}O_{30}$	1112.94
$C_{39}H_{50}O_{27}$	950.8
$C_{48}H_{56}O_{29}$	1096.94
$C_{49}H_{58}O_{30}$	1126.96
$C_{50}H_{60}O_{31}$	1156.99
$C_{61}H_{70}O_{35}$	1363.18
$C_{49}H_{58}O_{30}$	1126.96
$C_{33}H_{40}O_{20}$	756.667
$C_{44}H_{50}O_{26}$	994.85
$C_{55}H_{60}O_{30}$	1201.04
$C_{49}H_{60}O_{30}$	1128.98
$C_{43}H_{48}O_{25}$	964.82
$C_{31}H_{53}NO$	455.766
$C_{13}H_{14}N_2O_2$	230.266
$C_{17}H_{25}NO_{12}S_2$	499.516
$C_{16}H_{23}NO_{12}S_2$	485.48
$C_{20}H_{23}N_2$	291.415
$C_{21}H_{25}N_2O$	321.43
$C_{24}H_{41}NO_2$	375.6
$C_{22}H_{34}O_{13}S_2$	570.63
$C_{16}H_{18}N_2O_2$	270.33

$C_{17}H_{20}N_2O_3$	300.35
$C_{23}H_{28}N_4O_3$	408.49
$C_{10}H_{16}O$	152.23
$C_{10}H_{16}$	136.23
$C_{25}H_{43}NO_3$	405.61
$C_{29}H_{44}O_8$	520.7
$C_{19}H_{21}N_{21}^+$	312.8
$C_{20}H_{23}N_2O_1^+$	342.9
$C_{20}H_{20}O_7$	372.37
$C_9H_{17}NO_9S_2$	347.36
$C_3H_5NS$	87.15
$C_{24}H_{24}O_{11}$	488.44
$C_{25}H_{41}NO_3$	403.6
$C_{13}H_{13}NO_2$	215.25
$C_{14}H_{15}NO_2$	229.27
$C_{14}H_{15}NO_3$	245.27
$C_4H_4N_2O_2$	112.09
$C_{34}H_{42}O_{22}$	802.68
$C_{21}H_{20}N_4O_2$	360.41
$C_{15}H_{16}N_2O$	240.3
$C_{14}H_{16}N_2OS$	260.35
$C_{15}H_{18}N_2O_3S$	306.38
$C_{13}H_{14}N_2O_3$	246.26
$C_{14}H_{16}N_2O_4$	276.29
$C_{13}H_{14}N_2O_2$	230.26
$C_{13}H_{14}N_2O_3$	246.26
$C_{14}H_{16}N_2O_3$	260.29
$C_{16}H_{16}N_2OS$	284.38
$C_{13}H_{14}N_2O_2S$	262.33
$C_{15}H_{10}O_7$	302.23
$C_{21}H_{22}O_{10}$	434.39
$C_{21}H_{22}O_{11}$	450.39
$C_{21}H_{20}O_{12}$	464.3763

$C_{10}H_{16}$	136.23
$C_{10}H_{18}O$	154.25
$C_{20}H_{23}N_3O_2$	337.41
$C_{22}H_{26}O_9$	434.44
$C_{12}H_{12}N_2O_2$	216.24
$C_{17}H_{14}O_6$	314.29
$C_{12}H_{22}O_{10}S_2$	390.43
$C_{16}H_{16}N_2O_7$	348.31
$C_9H_9NO_2$	163.17
$C_{23}H_{39}NO$	345.6
$C_{11}H_8N_2$	168.19
$C_6H_6O_2$	110.11
$C_{25}H_{43}NO_3$	405.6
$C_{25}H_{41}NO$	371.6
$C_{15}H_{23}NO$	233.35
$C_{25}H_{33}NO_3$	395.53
$C_{25}H_{35}NO_3$	397.55
$C_{15}H_{14}O_6$	290.27
$C_{25}H_{39}NO_2$	385.58
$C_6H_{12}O_6$	180.16
$C_5H_{10}O_5$	150.13
$C_{29}H_{50}O_2$	430.7
$C_{24}H_{41}NO_2$	375.59
$C_{25}H_{41}NO$	371.6
$C_{25}H_{39}NO$	369.6
$C_{25}H_{37}NO$	367.57
$C_{25}H_{43}NO_3$	405.61
$C_{10}H_{16}$	136.23
$C_{14}H_6O_8$	302.19
$C_{13}H_{16}N_2O_2$	232.28
$C_{19}H_{21}ClN_2$	312.8
$C_{20}H_{23}ClN_2$	326.9
$C_{20}H_{23}ClN_2O$	342.86

$C_{21}H_{25}ClN_2O$	356.89
$C_6H_{12}O_5$	164.16
$C_6H_{12}O_6$	180.16
$C_6H_{12}O_6$	180.16
$C_5H_{10}O_5$	150.13
$C_{15}H_{21}NO_{10}S_2$	439.46
$C_{17}H_{22}N_2O_{10}S_2$	478.49
$C_{16}H_{20}N_2O_9S_2$	448.47
$C_{14}H_{19}NO_9S_2$	409.43
$C_{15}H_{21}NO_{10}S_2$	439.46
$C_{16}H_{11}NO_{21}S_2$	617.38
$C_{16}H_{20}N_2O_9S_2$	448.47
$C_{22}H_{32}N_2O_{11}S_2$	564.63
$C_{22}H_{32}N_2O_9S_2$	532.63
$C_{12}H_{20}NO_9S_2^-$	386.4
$C_{14}H_{19}NO_7S$	345.37
$C_{14}H_{19}NO_{10}S_2$	425.43
$C_{28}H_{46}O$	398.7
$C_{29}H_{50}O$	414.7
$C_{28}H_{44}O$	396.6
$C_{28}H_{46}O$	398.66
$C_{29}H_{48}O$	412.7
$C_{29}H_{46}O$	410.7
$C_8H_{16}O_2$	144.21
$C_{10}H_{20}O_2$	172.26
$C_{12}H_{24}O_2$	200.32
$C_{14}H_{28}O_2$	228.37
$C_{28}H_{28}O_{10}$	524.51
$C_{27}H_{26}O_{10}$	510.49
$C_{17}H_{14}O_7$	330.29
$C_6H_{13}NO_2$	131.17
$C_6H_{13}NO_2$	131.17
$C_5H_{11}NO_2$	117.15

$C_6H_{14}N_2O_2$	146.19
$C_9H_{11}NO_2$	165.19
$C_9H_{11}NO_3$	181.19
$C_4H_9NO_3$	119.12
$C_5H_{11}NO_2S$	149.21
$C_{14}H_{19}NO_{10}S_2$	425.4
$C_{16}H_{20}N_2O_{10}S_2$	464.5
$C_{17}H_{22}N_2O_{10}S_2$	478.5
$C_{13}H_{25}NO_{10}S_3$	451.5
$C_{31}H_{52}O_2$	456.7
$C_{30}H_{50}O_2$	442.7
$C_{30}H_{46}O_2$	438.7
$C_5H_8N_2$	96.13
$C_6H_{10}O$	98.14
$C_8H_{10}$	106.16
$C_6H_{12}O_2$	116.16
$C_7H_8O$	108.14
$C_7H_{14}O_2$	130.18
$C_8H_8O_2$	136.15
$C_{11}H_{11}N$	157.21
$C_9H_9NO$	147.17
$C_{10}H_{10}O_4$	194.18
$C_{18}H_{30}O_3$	294.43
$C_{12}H_{11}NO$	185.22
$C_{12}H_{11}N$	169.22
$C_{14}H_{26}O_2$	226.35
$C_{15}H_{30}O_2$	242.4
$C_{16}H_{22}O_4$	278.34
$C_{16}H_{30}O_2$	254.41
$C_{17}H_{32}O_2$	268.4
$C_{19}H_{34}O_2$	294.5
$C_{19}H_{32}O_2$	292.5
$C_{20}H_{34}O_2$	302.25

$C_{17}H_{32}O_2$	268.4
$C_{18}H_{30}O_2$	278.4
$C_{19}H_{36}O_2$	296.5
$C_{18}H_{30}O_2$	278.4
$C_{18}H_{30}O_3$	278.4
$C_{18}H_{30}O_4$	278.4
$C_{20}H_{36}O_2$	308.5
$C_{20}H_{38}O_2$	310.5
$C_{18}H_{28}O_2$	276.4
$C_{18}H_{28}O_2$	278.43
$C_{22}H_{42}O_2$	338.6
$C_{23}H_{44}O_2$	352.6
$C_{23}H_{46}O_2$	354.6
$C_{24}H_{48}O_2$	368.6
$C_{25}H_{48}O_2$	380.39
$C_{25}H_{50}O_3$	382.4
$C_{26}H_{52}O_2$	396.7
$C_{13}H_{14}N_2O_3$	246.26
$C_{13}H_{14}N_2O_2$	230.26
$C_{25}H_{41}NO$	371.6
$C_3H_5O_2^-$	73.07
$C_{15}H_{10}O_6$	286.24
$C_{18}H_{33}NO$	279.5
$C_{25}H_{43}NO_3$	405.6
$C_5H_6O_2$	98.1
$C_{10}H_{16}$	136.23
$C_{18}H_{30}O_3$	294.4
$C_{25}H_{33}NO_3$	395.53
$C_{25}H_{41}NO$	371.6
$C_{27}H_{45}NO_3$	431.65
$C_{13}H_{13}N_2O_2$	229.25
$C_{10}H_{18}O$	154.25
$C_{27}H_{46}O$	386.7

$C_{10}H_{16}$	136.23
$C_6H_8O_6$	176.12
$C_{15}H_{10}O_5$	270.24
$C_{10}H_{12}O_3$	180.2
$C_{15}H_{10}O_6$	286.24
$C_{20}H_{20}O_5$	340.4
$C_{18}H_{44}O_5Si_4$	452.9
$C_7H_6O$	106.12
$C_7H_5N$	103.12
$C_3H_7NO_2S$	121.16
$C_8H_{14}O_2$	142.2
$C_{11}H_{22}O_2$	186.29
$C_{14}H_{14}N_2O_3S_2$	322.4
$C_{13}H_{14}N_2OS_2$	278.39
$C_{14}H_{16}N_2O_2S_2$	308.42
$C_{29}H_{48}O$	412.7
$C_{15}H_{14}O_7$	306.27
$C_{22}H_{18}O_{11}$	458.4
$C_8H_8O_3$	152.15
$C_7H_6O_4$	154.12
$C_9H_8O_3$	164.16
$C_{29}H_{48}$	396.69
$C_{19}H_{38}O_2$	298.5
$C_{22}H_{44}O_2$	340.6
$C_{18}H_{34}O_2$	282.5
$C_{19}H_{36}O_3$	312.5
$C_{22}H_{37}NO_2$	347.5
$C_7H_6O_5$	170.12
$C_7H_6O_4$	154.12
$C_{16}H_{18}O_9$	354.31
$C_7H_6O_3$	138.12
$C_9H_8O_4$	180.16
$C_{28}H_{34}O_{15}$	610.6



$C_{21}H_{20}O_{10}$	432.4
$C_{18}H_{16}O_8$	360.3
$C_7H_6O_3$	138.12
$C_{22}H_{18}O_{12}$	474.4
$C_{33}H_{40}O_{21}$	772.66
$C_{32}H_{42}O_{21}$	762.66
$C_{27}H_{30}O_{15}$	594.52
$C_{43}H_{50}O_{24}$	950.84
$C_{33}H_{42}O_{20}$	758.67
$C_{49}H_{58}O_{28}$	1094.97
$C_{39}H_{50}O_{26}$	934.8
$C_3H_7NO_3$	105.09
$C_4H_7NO_4$	133.1
$C_5H_9NO_4$	147.13
$C_2H_5NO_2$	75.07
$C_3H_7NO_2$	89.09
$C_5H_9NO_2$	115.13
$C_6H_9N_3O_2$	155.15
$C_6H_{14}N_4O_2$	174.2
$C_{10}H_{18}O$	154.25
$C_{10}H_{20}O$	156.26
$C_{30}H_{62}$	422.8
$C_{10}H_{18}O$	154.25
$C_6H_6O_3$	126.11
$C_7H_7NO_2$	137.14
$C_{21}H_{20}O_{11}$	448.4
$C_{10}H_{16}O_2$	168.23
$C_{20}H_{38}O_2$	310.5
$C_{23}H_{46}O_2$	354.6
$C_{21}H_{42}O_2$	326.6
$C_{17}H_{30}O_2$	266.4
$C_{17}H_{30}O_2$	266.4
$C_{17}H_{28}O_2$	264.4

$C_{19}H_{38}O_2$	298.5
$C_{13}H_{22}$	178.31
$C_{19}H_{34}O_2$	294.5
$C_{19}H_{34}O_2$	294.5
$C_{16}H_{32}O_2$	256.42
$C_{19}H_{36}O_2$	296.5
$C_{18}H_{36}O_2$	284.5
$C_{19}H_{34}O_2$	294.5
$C_{25}H_{48}O_2$	380.6
$C_{22}H_{44}O_2$	340.6
$C_{23}H_{44}O_2$	352.6
$C_{31}H_{62}O_2$	466.8
$C_{19}H_{36}O_2$	296.5
$C_{25}H_{50}O_2$	382.7
$C_{28}H_{46}O$	398.7
$C_{29}H_{48}O$	412.7