

Annotation project

Meeeee!

October 27, 2025

Matching overview

name	mode	msLevel		pcgroup	rtime	error	rel. error	#	sim	rev_sim
Choline	pos	1	✓	76	0.47	0.02	3.3%	1	0.92	0.92
N-Methylnicotinamide	pos	1	✓	190	0.47	-0.49	-50.9%	1	0.77	0.77
Dimethylarginine	neg	1	✗							
Dimethylarginine	pos	1	✓	231	0.48	-0.02	-3.4%	1	0.80	0.80
Creatinine	neg	1	✗							
Creatinine	pos	1	✓	3	0.48	0.01	2.2%	1	0.90	0.93
Trigonelline	neg	1	✗							
Trigonelline	pos	1	✓	2	0.49	-0.04	-8.1%	1	1.00	1.00
D-(-)-Quinic acid	neg	1	✓	9	0.51	-0.04	-7.6%	2	0.84	0.84
D-(-)-Quinic acid	pos	1	✗							
stachydrine	neg	1	✗							
stachydrine	pos	1	✓	4	0.52	-0.02	-4.2%	2	0.96	0.96
stachydrine	pos	1	✓	34	0.59	0.05	9.1%	1	0.91	0.91
D-(-)-Ribose	neg	1	✓	90	0.53	0.00	0.9%	1	1.00	1.00
D-(-)-Ribose	pos	1	✗							
-Pseudouridine	neg	1	✓	136	0.58	-0.04	-6.4%	3	0.94	0.94
-Pseudouridine	neg	1	✓	136	0.58	-0.03	-5.2%	3	0.94	0.94
-Pseudouridine	pos	1	✗							
Uridine	neg	1	✓	136	0.58	-0.32	-35.6%	3	0.74	0.74
Uridine	pos	1	✗							
N-Acetylcarnitine	neg	1	✗							
N-Acetylcarnitine	pos	1	✓	213	0.60	0.00	0.7%	1	0.74	0.74
Leucine	neg	1	✗							
Leucine	pos	1	✓	11	0.60	-0.33	-35.2%	1	0.72	0.72
Leucine	pos	1	✓	69	0.97	0.04	3.9%	1	0.72	0.72
AAMU	neg	1	✗							
AAMU	pos	1	✓	91	0.65	0.01	1.2%	1	0.74	0.74
Hypoxanthine	neg	1	✗							

Hypoxanthine	pos	1	✓	24	0.68	-0.04	-6.1%	1	0.94	0.94
Citric acid	neg	1	✓	12	0.69	-0.04	-5.2%	2	0.83	0.84
Citric acid	pos	1	✗							
Citric acid	neg	1	✓	12	0.69	-0.02	-2.5%	2	0.83	0.84
Citric acid	pos	1	✗							
L-2-Pyrrolidon-5-carboxylsyre	neg	1	✓	62	0.73	-0.02	-3.3%	1	0.86	0.86
L-2-Pyrrolidon-5-carboxylsyre	pos	1	✗							
cis-aconitic acid	neg	1	✓	33	0.77	-0.07	-8.8%	3	0.90	0.90
cis-aconitic acid	pos	1	✗							
Tyrosine	neg	1	✗							
Tyrosine	pos	1	✓	50	0.78	-0.06	-6.8%	3	0.71	0.71
propionyl-L-carnitine	pos	1	✓	79	0.99	0.04	4.5%	1	0.76	0.76
N-Isobutyrylglycine	neg	1	✓	160	1.06	-0.31	-22.5%	1	0.38	0.72
N-Isobutyrylglycine	pos	1	✗							
7-Methylxanthine	neg	1	✓	31	1.49	-0.01	-0.8%	1	1.00	1.00
7-Methylxanthine	pos	1	✓	12	1.48	0.04	2.6%	1	0.74	0.74
7-Methylxanthine	pos	1	✓	25	1.16	-0.29	-19.7%	1	0.74	0.74
1-Metyluric acid	neg	1	✗							
1-Metyluric acid	pos	1	✓	48	1.18	-0.39	-24.8%	2	1.00	1.00
3-Methylxanthine	neg	1	✓	31	1.49	-0.12	-7.6%	1	0.91	0.91
3-Methylxanthine	pos	1	✗							
3-Methylxanthine	neg	1	✓	31	1.49	-0.13	-7.8%	1	1.00	1.00
3-Methylxanthine	pos	1	✗							
L-Phenylalanine	neg	1	✗							
L-Phenylalanine	pos	1	✓	22	1.60	0.03	2.0%	2	0.91	0.96
Methyl-2-pyrrolidone	pos	1	✓	142	1.84	0.16	9.6%	1	0.93	0.93
2-Furoylglycine	neg	1	✓	23	1.89	0.11	6.3%	3	0.78	0.78
2-Furoylglycine	pos	1	✓	64	1.89	0.11	6.1%	5	0.83	0.87
3,7-Dimethyluric acid	neg	1	✓	101	1.92	0.24	14.4%	1	0.78	0.78
3,7-Dimethyluric acid	pos	1	✓	95	1.91	0.20	11.8%	1	0.78	0.78

Butyrylcarnitine	neg	1	✗								
Butyrylcarnitine	pos	1	✓	23	1.95	0.16	9.1%	2	0.85	0.85	
Theobromine	pos	1	✓	29	2.52	0.30	13.8%	1	1.00	1.00	
Theobromine	pos	1	✓	51	2.04	-0.17	-7.7%	1	1.00	1.00	
4-Hydroxy-hippuric acid	neg	1	✓	41	2.08	-0.02	-1.0%	3	0.76	0.76	
4-Hydroxy-hippuric acid	pos	1	✓	37	2.39	0.29	13.7%	3	0.81	0.81	
4-Hydroxy-hippuric acid	pos	1	✓	57	2.07	-0.03	-1.3%	2	0.84	0.84	
3-Hydroxyanthranilic acid	neg	1	✗								
3-Hydroxyanthranilic acid	pos	1	✓	166	2.10	0.12	6.1%	1	0.76	0.76	
	neg	1	✓	317	2.18	-0.17	-7.2%	1	0.80	0.80	
	pos	1									
Paracetamol	neg	1	✓	20	2.40	0.38	18.6%	1	0.06	1.00	
Paracetamol	pos	1	✗								
Xanthurenic acid	neg	1	✗								
Xanthurenic acid	pos	1	✓	132	2.57	-0.45	-14.8%	1	0.82	0.82	
Hydroxyphenyllactic acid	neg	1	✓	30	2.57	-0.13	-4.9%	2	0.45	0.70	
Hydroxyphenyllactic acid	pos	1	✗								
DL-P-Hydroxy Phenyl lactic acid	neg	1	✓	30	2.57	-0.10	-3.7%	1	0.46	0.74	
DL-P-Hydroxy Phenyl lactic acid	pos	1	✗								
Tiglyl glycine	neg	1	✓	110	2.59	0.01	0.6%	1	0.74	0.74	
Tiglyl glycine	pos	1	✗								
Tiglyl glycine	neg	1	✓	110	2.59	-0.01	-0.4%	1	0.87	0.87	
N-Acetyltyrosine	neg	1	✓	293	2.65	-0.19	-6.7%	1	0.72	0.72	
N-Acetyltyrosine	pos	1	✗								
2,6-Dihydroxybenzoic acid	neg	1	✓	181	2.72	-0.42	-13.5%	1	0.79	0.79	
2,6-Dihydroxybenzoic acid	pos	1	✗								
2,4-Dihydroxybenzoic acid	neg	1	✓	181	2.72	-0.48	-15.0%	1	0.77	0.77	
2,4-Dihydroxybenzoic acid	pos	1	✗								
Kynurenic acid	neg	1	✓	225	2.75	-0.35	-11.4%	2	0.82	0.82	
Kynurenic acid	pos	1	✓	71	2.75	-0.36	-11.5%	1	0.77	0.77	

Valerylcarnitine	neg	1	✗								
Valerylcarnitine	pos	1	✓	8	2.77	-0.07	-2.6%	1	0.78	0.78	
Valerylcarnitine	pos	1	✓	59	2.84	0.00	0.1%	1	0.78	0.78	
Valerylcarnitine	pos	1	✓	67	2.92	0.08	2.9%	1	0.78	0.78	
Isovaleryl-L-carnitine	neg	1	✗								
Isovaleryl-L-carnitine	pos	1	✓	8	2.77	0.00	0.1%	1	0.74	0.74	
Isovaleryl-L-carnitine	pos	1	✓	59	2.84	0.08	2.8%	1	0.74	0.74	
Isovaleryl-L-carnitine	pos	1	✓	67	2.92	0.16	5.7%	1	0.74	0.74	
Indoxyl sulfate	neg	1	✓	2	2.78	0.24	9.6%	5	0.78	0.79	
3-indoxyl sulfate	neg	1	✓	2	2.78	0.37	15.2%	5	0.78	0.79	
3-indoxyl sulfate	pos	1	✗								
2-Isopropylmalic acid	neg	1	✓	59	2.84	-0.31	-9.8%	1	0.72	0.72	
2-Isopropylmalic acid	pos	1	✗								
2,6-dihydroxyquinoline	neg	1	✗								
2,6-dihydroxyquinoline	pos	1	✓	5	3.06	0.13	4.4%	1	0.02	0.82	
4-Acetamidobenzoic acid	neg	1	✓	3	3.06	-0.21	-6.5%	3	0.85	0.93	
4-Acetamidobenzoic acid	pos	1	✓	5	3.06	-0.22	-6.6%	3	0.31	0.87	
Hippuric acid	neg	1	✓	3	3.06	-0.02	-0.5%	3	0.90	0.91	
Hippuric acid	pos	1	✓	5	3.06	-0.03	-0.8%	5	0.84	0.85	
Caffeine	pos	1	✓	1	3.09	-0.14	-4.3%	2	0.95	0.95	
3-Hydroxyphenylacetic acid	neg	1	✓	112	3.40	0.16	5.0%	1	0.66	0.73	
3-Hydroxyphenylacetic acid	neg	1	✓	169	3.25	0.00	0.1%	1	0.73	0.73	
3-Hydroxyphenylacetic acid	pos	1	✗								
2-oxo-2,3-dihydro-1H-indol-3-yl-acetic acid	neg	1	✗								
2-oxo-2,3-dihydro-1H-indol-3-yl-acetic acid	pos	1	✓	186	3.39	0.03	0.9%	1	0.79	0.79	
p-Cresol sulfate	neg	1	✓	1	3.41	0.16	5.0%	4	0.88	0.88	
p-Cresol sulfate	pos	1	✗								
Urolithin A	neg	1	✓	46	3.89	0.14	3.7%	1	0.05	0.79	
Urolithin A	pos	1	✓	157	3.42	-0.32	-8.7%	1	0.97	0.97	
P-cresol glucuronide	neg	1	✓	76	3.43	0.06	1.7%	2	0.72	0.72	

-Methyl-L-DOPA	pos	1	✘
3-Methylhistidine	neg	1	✘
3-Methylhistidine	pos	1	✘
N-Methyl-4-tyramine	pos	1	✘
Tyramine	pos	1	✘
4-Aminobenzoic acid	neg	1	✘
5-Hydroxydopamine	neg	1	✘
5-Hydroxydopamine	pos	1	✘
Acetylornithine	neg	1	✘
Acetylornithine	pos	1	✘
Alanine	neg	1	✘
Alanine	pos	1	✘
Anserine	neg	1	✘
Arginine	neg	1	✘
Arginine	pos	1	✘
Arginine-13C6	neg	1	✘
Arginine-13C6	pos	1	✘
Arsenobetaine	pos	1	✘
Asp-Phe	neg	1	✘
Asp-Phe	pos	1	✘
Betaine; N,N,N-trimethyllysine	neg	1	✘
Betaine; N,N,N-trimethyllysine	pos	1	✘
Carnitine	neg	1	✘
Carnitine	pos	1	✘
Carnosine	neg	1	✘
Citrulline	neg	1	✘
Citrulline	pos	1	✘
Cortisol 21-sulfate	neg	1	✘
Cortisol 21-sulfate	pos	1	✘
(-)-Cotinine	pos	1	✘

Creatine	neg	1	✘
(L)-Cystine	neg	1	✘
(L)-Cystine	pos	1	✘
Dehydroepiandrosterone 3-sulfate	neg	1	✘
Dehydroepiandrosterone 3-sulfate	pos	1	✘
Dimethyl glycine	pos	1	✘
Disodium hydrogen phosphate	neg	1	✘
Disodium hydrogen phosphate	pos	1	✘
Dopamine	pos	1	✘
Estrone-3 sulfate	neg	1	✘
Estrone-3 sulfate	pos	1	✘
Fructose	neg	1	✘
Fructose	pos	1	✘
Galactitol	neg	1	✘
Galactosamine	neg	1	✘
Galactosamine	pos	1	✘
Glucose 6-phosphate	neg	1	✘
Glucose 6-phosphate	pos	1	✘
Glutamic acid	neg	1	✘
Glutamic acid	pos	1	✘
Glutamine	neg	1	✘
Glutamine	pos	1	✘
Glycine	neg	1	✘
Glycine	pos	1	✘
Hepes	neg	1	✘
Hepes	pos	1	✘
Homocysteine	neg	1	✘
H-Pro-Ile-OH	neg	1	✘
H-Pro-Ile-OH	pos	1	✘
H-Pro-Pro-OH	pos	1	✘

Hypotaurine	neg	1	✘
Hypotaurine	pos	1	✘
Indoxyl -D-glucuronide	neg	1	✘
Indoxyl -D-glucuronide	pos	1	✘
Inositol	neg	1	✘
Inositol	pos	1	✘
Leu-Pro	neg	1	✘
Leu-Pro	pos	1	✘
L-Tyrosine-13C10	neg	1	✘
L-Tyrosine-13C10	pos	1	✘
DL-Methionine sulfoxid	neg	1	✘
DL-Methionine sulfoxid	pos	1	✘
N-Methyl-D-aspartic acid	neg	1	✘
N-Methyl-D-aspartic acid	pos	1	✘
N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimide	pos	1	✘
N-Methyl-cis-4-hydroxy-L-proline	neg	1	✘
N-Methyl-cis-4-hydroxy-L-proline	pos	1	✘
N,N,N-Trimethyllysine	neg	1	✘
N,N,N-Trimethyllysine	pos	1	✘
O-(4-Nitrobenzyl)hydroxylamine	pos	1	✘
Palmitoyl-DL-carnitine	neg	1	✘
Palmitoyl-DL-carnitine	pos	1	✘
Pantothenic acid	pos	1	✘
Phenylalanyl glycine	neg	1	✘
Phenylalanyl glycine	pos	1	✘
Phenylvaline	neg	1	✘
Phenylvaline	pos	1	✘
Phosphoryl choline	pos	1	✘
Pipecolic acid	neg	1	✘
Pipecolic acid	pos	1	✘

L-Proline	neg	1	✗
L-Proline	pos	1	✗
Raffinose	neg	1	✗
Raffinose	pos	1	✗
S-(5'-Adenosyl)-L-methionine	pos	1	✗
salsolinol	neg	1	✗
salsolinol	pos	1	✗
Sarcosine	neg	1	✗
Sarcosine	pos	1	✗
3-methyl-2-oxobutyric acid	neg	1	✗
Sodium fluorescein	neg	1	✗
Sodium fluorescein	pos	1	✗
Glycochenodeoxycholic acid, Sodium salt	neg	1	✗
Glycochenodeoxycholic acid, Sodium salt	pos	1	✗
Glycocholic acid, Sodium salt	neg	1	✗
Glycocholic acid, Sodium salt	pos	1	✗
Glycodeoxycholic acid, Sodium salt	neg	1	✗
Glycodeoxycholic acid, Sodium salt	pos	1	✗
Taurochenodeoxycholic acid, Sodium salt	neg	1	✗
Taurochenodeoxycholic acid, Sodium salt	pos	1	✗
Taurochenodeoxycholic acid, Sodium salt	pos	1	✗
Tauroursodeoxycholic acid, Sodium salt	neg	1	✗
Tauroursodeoxycholic acid, Sodium salt	pos	1	✗
Tauroursodeoxycholic acid, Sodium salt	pos	1	✗
Tartaric acid	neg	1	✗
Taurine	neg	1	✗
Taurine	pos	1	✗
Thiamine	neg	1	✗
Thiamine	neg	1	✗
Thiamine	pos	1	✗

Threonine	neg	1	✘
Threonine	pos	1	✘
Trimethylamine-N-Oxide (TMAO)	pos	1	✘
Tryptamine	pos	1	✘
Ursodeoxycholic Acid -13C4	neg	1	✘
Ursodeoxycholic Acid -13C4	pos	1	✘
Valine	neg	1	✘
Valine	pos	1	✘
Val-Thr	neg	1	✘
Val-Thr	pos	1	✘
GSSG	neg	1	✘
GSSG	pos	1	✘
Indoxylglucoside	neg	1	✘
Indoxylglucoside	pos	1	✘
Dihydrokaempferol	neg	1	✘
Dihydrokaempferol	pos	1	✘
FMOC-(L)-4-hydroxyproline	neg	1	✘
FMOC-(L)-4-hydroxyproline	pos	1	✘
FMOC-(L)-isoleucine	neg	1	✘
FMOC-(L)-isoleucine	pos	1	✘
FMOC-(L)-leucine	neg	1	✘
FMOC-(L)-leucine	pos	1	✘
FMOC-(L)-methionine	neg	1	✘
FMOC-(L)-methionine	pos	1	✘
FMOC-(L)-proline	neg	1	✘
FMOC-(L)-proline	pos	1	✘
12-Hydroxydodecanoic acid	neg	1	✘
12-Hydroxydodecanoic acid	pos	1	✘
1-Methyl-L-Histidine	neg	1	✘
1-Methyl-L-Histidine	pos	1	✘

Metronidazole-1-acetic acid	neg	1	✘
Luteolin	neg	1	✘
Luteolin	pos	1	✘
2,2-Dimethylglutaric acid	neg	1	✘
2,2-Dimethylglutaric acid	pos	1	✘
2,3-Dihydroxybenzoic acid	neg	1	✘
2,3-Dihydroxybenzoic acid	pos	1	✘
2,3-Dimethylphenol	pos	1	✘
2,4,5-Trimethoxycinnamic acid	neg	1	✘
2,4,5-Trimethoxycinnamic acid	pos	1	✘
Mesifurane	pos	1	✘
Mesifurane	pos	1	✘
2-Aminophenol	neg	1	✘
2-Aminophenol	pos	1	✘
2'-Deoxycytidine	neg	1	✘
2'-Deoxycytidine	pos	1	✘
2-ethylmaltol	pos	1	✘
2-Hydroxyisovaleric acid	neg	1	✘
2-(L-)Hydroxyisovaleric acid	neg	1	✘
2-Hydroxybutyric acid	neg	1	✘
o-coumaric acid	neg	1	✘
o-coumaric acid	pos	1	✘
2-Hydroxyhexanoic acid	neg	1	✘
2-Methylactic acid	neg	1	✘
Hydroxymetronidazole	neg	1	✘
Hydroxymetronidazole	pos	1	✘
2-Hydroxyphenylacetic acid	neg	1	✘
2-Hydroxyphenylacetic acid	pos	1	✘
2-Methylhippuric acid	neg	1	✘
2-Methylhippuric acid	pos	1	✘

2-ketovaleric acid	neg	1	✗
2-propylvaleric acid	neg	1	✗
2,4-Dihydroxycinnamic acid	pos	1	✗
Hydrocinnamic acid	neg	1	✗
3,3-Dimethylglutaric acid	neg	1	✗
3,3-Dimethylglutaric acid	pos	1	✗
Trimethylgallic acid	neg	1	✗
3,4,5-Trimethoxycinnamic acid	neg	1	✗
3,4,5-Trimethoxycinnamic acid	pos	1	✗
3,4-Dihydroxybenzene propanoic acid	neg	1	✗
3,4-Dihydroxybenzene propanoic acid	pos	1	✗
3,4-Dihydroxybenzoic acid	neg	1	✗
Caffeic acid	neg	1	✗
Caffeic acid	pos	1	✗
3,4-Dihydroxyphenylacetic acid	neg	1	✗
Isorhamnetin	pos	1	✗
3,5-Dihydroxyhydrocinnamic acid	neg	1	✗
3,5-Dihydroxyhydrocinnamic acid	pos	1	✗
3-Ethylmalic acid	neg	1	✗
3-Ethylmalic acid	pos	1	✗
3-Hydroxy-3-methylglutaric acid	neg	1	✗
3-Hydroxy-3-methylglutaric acid	pos	1	✗
3-Hydroxybenzoic acid	neg	1	✗
3-Hydroxycinnamic acid	neg	1	✗
3-Hydroxycinnamic acid	pos	1	✗
3-hydroxycoumarin	neg	1	✗
3-hydroxycoumarin	pos	1	✗
3-Hydroxykynurenine	neg	1	✗
3-Hydroxykynurenine	pos	1	✗
3-Hydroxymandelic acid	neg	1	✗

3-Hydroxymandelic acid	pos	1	✗
3-Nitrotyrosine	neg	1	✗
3-Nitrotyrosine	pos	1	✗
3-Phenoxybenzoic acid	neg	1	✗
3-Phenoxybenzoic acid	pos	1	✗
3-L-Phenyllactic acid	neg	1	✗
3-L-Phenyllactic acid	pos	1	✗
3-DL-Phenyllactic acid	neg	1	✗
3-DL-Phenyllactic acid	pos	1	✗
3-Phenylpropionic acid	neg	1	✗
3,4-Dihydroxyphenylglycol	neg	1	✗
3,4-Dihydroxyphenylglycol	pos	1	✗
Hordenine	pos	1	✗
5-ketohexanoic acid	neg	1	✗
5-ketohexanoic acid	pos	1	✗
4-Aminobenzoic acid-13C6	neg	1	✗
Syringic acid	neg	1	✗
Syringic acid	pos	1	✗
Sinapic acid	neg	1	✗
Sinapic acid	pos	1	✗
Ferulic acid	neg	1	✗
Ferulic acid	pos	1	✗
4-Hydroxy-3-methoxymandelic acid	neg	1	✗
4-Hydroxy-3-methoxymandelic acid	pos	1	✗
Homovanillic acid	neg	1	✗
Homovanillic acid	pos	1	✗
4-Hydroxybenzaldehyde	neg	1	✗
4-Hydroxybenzaldehyde	pos	1	✗
4-Hydroxybenzoic acid	neg	1	✗
4-Hydroxycinnamic acid	neg	1	✗

4-Hydroxycinnamic acid	pos	1	✘
4-Hydroxyproline	neg	1	✘
4-Hydroxyproline	pos	1	✘
4-Hydroxyphenylacetic acid	neg	1	✘
4-Hydroxyphenylpyruvic acid	neg	1	✘
4-Imidazole-2-acetic acid	neg	1	✘
4-Imidazole-2-acetic acid	pos	1	✘
Perillic acid	neg	1	✘
4-Methyl-2-oxovaleric acid	neg	1	✘
Sulfurol	pos	1	✘
Sulfurol	pos	1	✘
Sulfurol	pos	1	✘
5-Hydroxy-3-indoleacetic acid	neg	1	✘
5-Hydroxy-3-indoleacetic acid	pos	1	✘
5-hydroxymethyl-2-furanecarboxylic acid	neg	1	✘
5-hydroxymethyl-2-furanecarboxylic acid	pos	1	✘
5-Hydroxytryptamine	pos	1	✘
5-Hydroxytryptophan	neg	1	✘
5-Hydroxytryptophan	pos	1	✘
5-Methoxy-DL-tryptophan	neg	1	✘
5-Methoxy-DL-tryptophan	pos	1	✘
5-Methoxysalicylic acid	neg	1	✘
5-Methoxysalicylic acid	pos	1	✘
5-Methyluracil	pos	1	✘
6-Hydroxydopamine	neg	1	✘
6-Hydroxydopamine	pos	1	✘
6-Hydroxymelatonin	neg	1	✘
6-Hydroxymelatonin	pos	1	✘
7-Hydroxycumarin	neg	1	✘
7-Hydroxycumarin	pos	1	✘

8-Hydroxy-2'-deoxyguanosine	neg	1	✗
8-Hydroxy-2'-deoxyguanosine	pos	1	✗
9-hydroxydecanoic acid	neg	1	✗
9-hydroxydecanoic acid	pos	1	✗
Abscisic acid	neg	1	✗
Abscisic acid	pos	1	✗
Acetanilide	pos	1	✗
N-Acetyl-5-hydroxytryptamine	neg	1	✗
N-Acetyl-5-hydroxytryptamine	pos	1	✗
N-Acetylmethionine	neg	1	✗
N-Acetylmethionine	pos	1	✗
N-Acetyltryptophan	neg	1	✗
N-Acetyltryptophan	pos	1	✗
N-Acetylmannosamine	neg	1	✗
N-Acetylmannosamine	pos	1	✗
N-Acetyl-Asp-Glu	neg	1	✗
N-Acetyl-Asp-Glu	pos	1	✗
N-Acetylcysteine	neg	1	✗
N-Acetylcysteine	pos	1	✗
N-Acetylglutamic acid	neg	1	✗
N-Acetylglutamic acid	pos	1	✗
Adenine	neg	1	✗
Adenine	pos	1	✗
Adenosine	neg	1	✗
Adenosine	pos	1	✗
Adipic acid	neg	1	✗
Adipic acid	pos	1	✗
Epinephrine	neg	1	✗
Epinephrine	pos	1	✗
Ala-Gly	neg	1	✗

Ala-Gly	pos	1	✗
Allantoin	neg	1	✗
Allantoin	pos	1	✗
4-Aminohippuric acid	neg	1	✗
4-Aminohippuric acid	pos	1	✗
Androstanolone	pos	1	✗
Androsteron	pos	1	✗
Ascorbic acid	neg	1	✗
Biotin	neg	1	✗
Biotin	pos	1	✗
Biotinamidohexanoic acid hydrazide	neg	1	✗
Biotinamidohexanoic acid hydrazide	pos	1	✗
Biotinamidohexanoic acid hydrazide	pos	1	✗
Cafestol acetate	pos	1	✗
Octanoic acid	neg	1	✗
Catechin	neg	1	✗
Catechin	pos	1	✗
Chenodeoxycholic acid 13C1	neg	1	✗
Chenodeoxycholic acid 13C1	pos	1	✗
Cholic acid-13C1	neg	1	✗
Cholic acid-13C1	pos	1	✗
Trans-cinnamic acid	neg	1	✗
Trans-cinnamic acid	pos	1	✗
Corticosterone	neg	1	✗
Corticosterone	pos	1	✗
Noradrenaline-HCl	neg	1	✗
Noradrenaline-HCl	pos	1	✗
Cortisone	neg	1	✗
Cortisone	pos	1	✗
11-Deoxy-17-hydroxy corticosterone	neg	1	✗

11-Deoxy-17-hydroxy corticosterone	pos	1	✗
Dehydroascorbic acid	neg	1	✗
Dehydrocholic acid	neg	1	✗
Dehydrocholic acid	pos	1	✗
Deoxycholic acid (24-13C)	neg	1	✗
Deoxycholic acid (24-13C)	pos	1	✗
Deoxycholic acid D4	neg	1	✗
Deoxycholic acid D4	pos	1	✗
Hyodeoxycholic acid	neg	1	✗
Hyodeoxycholic acid	pos	1	✗
Diosmetin	neg	1	✗
Diosmetin	pos	1	✗
dithiopyridine	pos	1	✗
Dithiothreitol	neg	1	✗
3-hydroxydecanoic acid	neg	1	✗
3-hydroxydecanoic acid	pos	1	✗
Enterolactone	neg	1	✗
Enterolactone	pos	1	✗
Epicatechin	neg	1	✗
Epicatechin	pos	1	✗
Fumaric acid	neg	1	✗
Gentistic acid	neg	1	✗
Glutaric acid	neg	1	✗
Heptanedioic acid	neg	1	✗
Heptanedioic acid	pos	1	✗
Hydrocortisone	neg	1	✗
Hydrocortisone	pos	1	✗
DL-3-Indole Lactic acid	neg	1	✗
DL-3-Indole Lactic acid	pos	1	✗
3-Hydroxyisovaleric acid	neg	1	✗

3-Hydroxyisovaleric acid	pos	1	✘
3-Hydroxyisovaleric acid	pos	1	✘
3-Hydroxyisovaleric acid	pos	1	✘
17-Hydroxyprogesterone	neg	1	✘
17-Hydroxyprogesterone	pos	1	✘
3-Indole-acetic acid	neg	1	✘
3-Indole-acetic acid	pos	1	✘
Indole-3-carboxaldehyde	neg	1	✘
Indole-3-carboxaldehyde	pos	1	✘
Indole-3-Carboxylic acid	neg	1	✘
Indole-3-Carboxylic acid	pos	1	✘
3-Indole-Propionic acid	neg	1	✘
3-Indole-Propionic acid	pos	1	✘
Inosine	neg	1	✘
Inosine	pos	1	✘
-Ketoglutarsyre	neg	1	✘
Kynurenine	neg	1	✘
Kynurenine	pos	1	✘
Lactic acid	neg	1	
Levulinic acid	neg	1	✘
Levulinic acid	pos	1	✘
Malic acid	neg	1	✘
DL-Mandelic acid	neg	1	✘
Melatonine	neg	1	✘
Melatonine	pos	1	✘
Methylmalonic acid	neg	1	✘
Methylsuccinic acid	neg	1	✘
trans-trans muconic acid	neg	1	✘
N'-Methylnicotinamide	pos	1	✘
Naringenin	neg	1	✘

Naringenin	pos	1	✘
Nicotinamide	pos	1	✘
Nicotinuric acid	neg	1	✘
Nicotinuric acid	pos	1	✘
Orotic acid	neg	1	✘
Orotic acid	pos	1	✘
Perfluorovaleric acid	neg	1	✘
Phenylacetylglycine	neg	1	✘
Phenylacetylglycine	pos	1	✘
D-(-)-Phenylglycine	neg	1	✘
D-(-)-Phenylglycine	pos	1	✘
Phenyllactic acid	neg	1	✘
Phenyllactic acid	pos	1	✘
Prednisolone	neg	1	✘
Prednisolone	pos	1	✘
Pyrogallol	neg	1	✘
Pyrrole-2-carboxylic acid	neg	1	✘
Quinaldic acid	pos	1	✘
LPC(16:0)	neg	1	✘
Lithocholic acid	neg	1	✘
Lithocholic acid	pos	1	✘
Retinol acetate	pos	1	✘
Limonene-1,2-diol	pos	1	✘
LPC(17:1)	neg	1	✘
LPC(17:1)	pos	1	✘
LPC(17:1)	pos	1	✘
PPrp(16:0/18:1)	neg	1	✘
PPrp(16:0/18:1)	pos	1	✘
PC(18:0/14:0)	neg	1	✘
PC(18:0/14:0)	pos	1	✘

PC(18:0/14:0)	pos	1	✗
2,3-dinor-8-iso Prostaglandin F2	neg	1	✗
2,3-dinor-8-iso Prostaglandin F2	pos	1	✗
2-Hydroxyauric acid	neg	1	✗
2-Hydroxyauric acid	pos	1	✗
3alpha-Hydroxy-7-oxo-5beta-cholanic Acid	neg	1	✗
3alpha-Hydroxy-7-oxo-5beta-cholanic Acid	pos	1	✗
4,6-androstadien-17-ol-3-one	pos	1	✗
4-Methylmorpholine	pos	1	✗
8-IsoPGF2 -d5	neg	1	✗
8-IsoPGF2 -d5	pos	1	✗
8-Isoprostane	neg	1	✗
8-Isoprostane	pos	1	✗
Kinetin	neg	1	✗
Kinetin	pos	1	✗
Lauric acid	neg	1	✗
Launoyl L-carnitine	neg	1	✗
Launoyl L-carnitine	pos	1	✗
Lithocholic acid d4	neg	1	✗
Lithocholic acid d4	neg	1	✗
Stearic acid (FA18:0)	neg	1	✗
Testosterone	pos	1	✗
Tetradecanedioic acid (FA14:0)	neg	1	✗
Tetradecanedioic acid (FA14:0)	pos	1	✗
Tocopherol	neg	1	✗
Tocopherol	pos	1	✗
Undecanedioic acid	neg	1	✗
Undecanedioic acid	pos	1	✗
Tetradecanoic acid (FA(14:0)	neg	1	✗
Vaccenic acid (trans FA(18:1))	neg	1	✗

Phenolphthalein	neg	1	✘
Phenolphthalein	pos	1	✘
Pentadecanoic acid (C15:0)	neg	1	✘
EPA (FA20:5 3Z,6Z,9Z,12Z,15Z)	neg	1	✘
16-O-Methylcafestol	pos	1	✘
Undecanoic acid (FA11:0)	neg	1	✘
Elaidic acid (FA18:1 9E)	neg	1	✘
Oleic acid (FA18:1 9Z)	neg	1	✘
Behenic acid (FA22:0)	neg	1	✘
Erucic acid (FA22:1 9Z)	neg	1	✘
Glycocholic acid	neg	1	✘
Glycocholic acid	pos	1	✘
POV-PC	neg	1	✘
POV-PC	pos	1	✘
LPC(17:1)	pos	1	✘
Ursodeoxycholic acid	neg	1	✘
Ursodeoxycholic acid	pos	1	✘
Stearidonic acid (FA18:4 6Z,9Z,12Z,15Z)	neg	1	✘
Stearidonic acid (FA18:4 6Z,9Z,12Z,15Z)	pos	1	✘
2'-0-methyluridine	neg	1	✘
2'-0-methyluridine	neg	1	✘
2'-0-methyluridine	pos	1	✘
2'-0-methyluridine	pos	1	✘
Henaicosanoic acid (FA21:0)	neg	1	✘
Methyltyrosine	pos	1	✘
Methyltyrosine	pos	1	✘
Taurocholate	neg	1	✘
Taurocholate	pos	1	✘
Glycodeoxycholic acid	neg	1	✘
Glycodeoxycholic acid	pos	1	✘

Palmitoleic acid (FA16:1 9Z)	neg	1	✘
Linoleic acid (FA18:2 9Z,12Z)	neg	1	✘
Daidzein	neg	1	✘
Daidzein	pos	1	✘
Hexadecanoic acid (FA16:0)	neg	1	✘
Arachidonic acid (FA20:4 5Z,8Z,11Z,14Z)	neg	1	✘
Palmitic acid (C16:0)	neg	1	✘
Petroselinic acid (FA18:1 12Z)	neg	1	✘
3'-O-Methyluridine	neg	1	✘
3'-O-Methyluridine	pos	1	✘
Chorismic acid	neg	1	✘
Chorismic acid	pos	1	✘
DHA (FA22:6 3Z,6Z,9Z,12Z,15Z,18Z)	neg	1	✘
Nonadecanoic acid (FA19:0)	neg	1	✘
4-Allyl-2,6-dimethoxyphenol	pos	1	✘
Isoxanthohumol	neg	1	✘
Isoxanthohumol	pos	1	✘
PS(17:0/17:0)	pos	1	✘
PG(17:0/17:0)	neg	1	✘
PG(17:0/17:0)	pos	1	✘
Grifolic acid	neg	1	✘
Grifolic acid	pos	1	✘
Solanidine	pos	1	✘
Leu-Enk	neg	1	✘
Leu-Enk	pos	1	✘
Hexestrol	neg	1	✘
1-Dehydrotestosterone	neg	1	✘
1-Dehydrotestosterone	pos	1	✘
Diisobutylphthalate	pos	1	✘
PGPC	neg	1	✘

PGPC	pos	1	✗
3-hydroxypalmitic acid	pos	1	✗
3-Methoxycatechol	pos	1	✗
Equol	pos	1	✗
Oleoyl carnitine	neg	1	✗
Oleoyl carnitine	pos	1	✗
LPC(20:0)	neg	1	✗
LPC(20:0)	pos	1	✗
LPC (22:0)	neg	1	✗
LPC (22:0)	pos	1	✗
PE(16:0/18:1)	neg	1	✗
PE(16:0/18:1)	pos	1	✗
Octadecanedioic acid	neg	1	✗
Octadecanedioic acid	pos	1	✗
PC(20:5/20:5)	neg	1	✗
PC(20:5/20:5)	pos	1	✗
Peth(16:0/18:1)	neg	1	✗
Peth(16:0/18:1)	pos	1	✗
LPC(18:0)	neg	1	✗
LPC(18:0)	pos	1	✗
PC(16:0/18:1; 9Z)	neg	1	✗
PC(16:0/18:1; 9Z)	pos	1	✗
Cer(d18:1/17:0)	pos	1	✗
LPC(18:1)	neg	1	✗
LPC(18:1)	pos	1	✗
Olkeamide	pos	1	✗
Oleoyl-L-Carnitine	neg	1	✗
Oleoyl-L-Carnitine	pos	1	✗
Sphingomyelin	neg	1	✗
Lyso PE (18:1)	neg	1	✗

Lyso PE (18:1)	pos	1	✘
LPC (18:1)	neg	1	✘
LPC (18:1)	pos	1	✘
Phosphatidylcholine (PC(0:0/0:0))	neg	1	✘
Phosphatidylcholine (PC(0:0/0:0))	pos	1	✘
SM (18:1/18:1)	pos	1	✘
Nervonic acid (FA24:1 15Z)	neg	1	✘
Tricosanic acid (FA23:0)	neg	1	✘
Tricosanic acid (FA23:0)	pos	1	✘
5-Nonadecylresorcinol	neg	1	✘
5-Nonadecylresorcinol	pos	1	✘
Arachidic acid (FA20:0)	neg	1	✘
Arachidic acid (FA20:0)	pos	1	✘
Lignoceric acid (FA24:0)	neg	1	✘
Lignoceric acid (FA24:0)	pos	1	✘
5-Heneicosylresorcinol	neg	1	✘
5-Heneicosylresorcinol	pos	1	✘
6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	neg	1	✘
6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	pos	1	✘
1-stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine	pos	1	✘
Kahweol	pos	1	✘
Cyclo (Val-Phe) ether phase	pos	1	✘
Cyclo (Val-Leu) ether phase	pos	1	✘
Propylparabene	neg	1	✘
Propylparabene	pos	1	✘
Pyridine	pos	1	✘
Quercetin 3-glucuronide	neg	1	✘
Quercetin 3-glucuronide	pos	1	✘
Taurocholic acid, Sodium salt	neg	1	✘
Taurodeoxycholic acid, Sodium salt	neg	1	✘

Taurodeoxycholic acid, Sodium salt	pos	1	✗
Resveratrol	neg	1	✗
Resveratrol	pos	1	✗
Salicylic acid	neg	1	✗
Salicylic acid	pos	1	✗
Sebacic acid	neg	1	✗
Sebacic acid	pos	1	✗
Deoxycholic acid, Sodium salt	neg	1	✗
Deoxycholic acid, Sodium salt	pos	1	✗
Glycoursodeoxycholic acid, Sodium salt	neg	1	✗
Glycoursodeoxycholic acid, Sodium salt	pos	1	✗
Trolox	neg	1	✗
Trolox	pos	1	✗
Uracil	neg	1	✗
Uracil	pos	1	✗
Uric acid	neg	1	✗
Vanillic acid	neg	1	✗
Vanillic acid	pos	1	✗
Vanillin	neg	1	✗
Vanillin	pos	1	✗
Glycocholic acid	neg	1	✗
Glycocholic acid	pos	1	✗
Glycodeoxycholic-2,2,4,4-d4acid	neg	1	✗
Glycodeoxycholic-2,2,4,4-d4acid	pos	1	✗
Guanine	neg	1	✗
Guanine	pos	1	✗
Uric acid (1,3-15N2)	neg	1	✗
Uric acid (1,3-15N2)	pos	1	✗
Imidazolepropionic acid	neg	1	✗
Imidazolepropionic acid	pos	1	✗

Heptanoic acid (FA7:0)	neg	1	✘
Heptanoic acid (FA7:0)	pos	1	✘
Nonanoic acid (FA9:0)	neg	1	✘
Triethylamine	pos	1	✘
Phenol Red	neg	1	✘
Phenol Red	pos	1	✘
3,4-dihydroxymandelic acid	neg	1	✘
N-Isovalerylglycine	neg	1	✘
N-Isovalerylglycine	pos	1	✘
Cyclo-(Glu-Glu)	neg	1	✘
Cyclo-(Glu-Glu)	pos	1	✘
L-phenylalanine D8, 98%	neg	1	✘
L-phenylalanine D8, 98%	pos	1	✘
Asparagine	neg	1	✘
Asparagine	pos	1	✘
p-hydroxyphenylacetyl glycine	neg	1	✘
p-hydroxyphenylacetyl glycine	pos	1	✘
3-Methyladipic acid	neg	1	✘
3-Methyladipic acid	pos	1	✘
Piperidin-2-carboxylic acid	pos	1	✘
Serine	neg	1	✘
Serine	pos	1	✘
leucine	pos	1	
Decanoic acid (FA10:0)	neg	1	✘
Proline	neg	1	✘
Proline	pos	1	✘
Guanidinoacetic acid	neg	1	✘
Guanidinoacetic acid	pos	1	✘
perfluoroheptanoic acid	neg	1	✘
Val-Phe-OH	neg	1	✘

Val-Phe-OH	pos	1	✘
4-hydroxyproline methyl ester	pos	1	✘
(2-ethyl-5-oxohexyl)-hydrogenphthalate	neg	1	✘
(2-ethyl-5-oxohexyl)-hydrogenphthalate	pos	1	✘
(2-ethyl-5-hydroxohexyl)-hydrogenphthalate	neg	1	✘
(2-ethyl-5-hydroxohexyl)-hydrogenphthalate	pos	1	✘
Ile-Pro-OH	neg	1	✘
Ile-Pro-OH	pos	1	✘
(2-Ethylhexyl)hydrogenphthalate	neg	1	✘
(2-Ethylhexyl)hydrogenphthalate	pos	1	✘
Hypaphorine	neg	1	✘
Hypaphorine	pos	1	✘
3-amino-3-methoxybenzoic acid	neg	1	✘
3-amino-3-methoxybenzoic acid	pos	1	✘
Coenzyme Q1	neg	1	✘
Coenzyme Q1	pos	1	✘
Tetrahydro-beta-carboline-3-carboxylic acid	neg	1	✘
Tetrahydro-beta-carboline-3-carboxylic acid	pos	1	✘
Mevalonic acid (sælges som lacton)	pos	1	✘
Mevalonic acid (sælges som lacton)	pos	1	✘
Oxfenicine	neg	1	✘
Oxfenicine	pos	1	✘
Phenylacetic acid	neg	1	✘
Phloretin	neg	1	✘
Phloretin	pos	1	✘
Quercetin	neg	1	✘
Quercetin	pos	1	✘
-CEHC	neg	1	✘
-CEHC	pos	1	✘
2-ketocaproic acid	neg	1	✘

Cafestol	pos	1	✘
Dihydro kaempferol	neg	1	✘
Dihydro kaempferol	pos	1	✘
PGF1	neg	1	✘
PGF1	pos	1	✘
3,5 dihydroxy benzoic acid	neg	1	✘
3-(2-hydroxyphenyl)propionic acid	neg	1	✘
3-(2-hydroxyphenyl)propionic acid	pos	1	✘
Pro-Leu	pos	1	✘
EDTA	neg	1	✘
EDTA	pos	1	✘
creatine	neg	1	✘
creatine	pos	1	✘
Lactulose	neg	1	✘
Lactulose	pos	1	✘
Dimethylsulphoxide	pos	1	✘
Isoleucine	pos	1	✘
Phosphoric acid	neg	1	✘
Phosphoric acid	pos	1	✘
N-Acetyl-D-phenylalanine	neg	1	✘
N-Acetyl-D-phenylalanine	pos	1	✘
Sulfadiazine-d5	neg	1	✘
Sulfadiazine-d5	pos	1	✘
Cyclo (ple-Val) waterphase	pos	1	✘
β-Asp-Leu	neg	1	✘
β-Asp-Leu	pos	1	✘
DL-Indole-3-Lactic acid	neg	1	✘
DL-Indole-3-Lactic acid	pos	1	✘
5-Hydroxydopamine	neg	1	✘
5-Hydroxydopamine	pos	1	✘

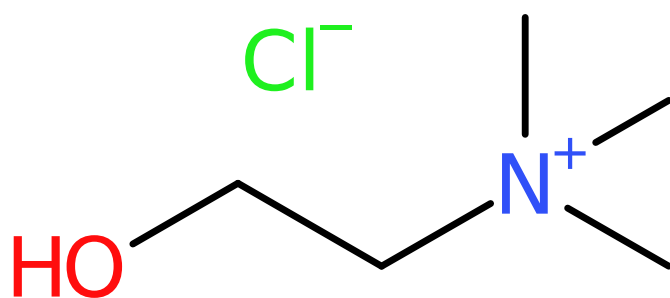
p-Acetylaminohippuric acid	neg	1	✗
p-Acetylaminohippuric acid	pos	1	✗
Cyclo (pro-thr)	pos	1	✗
Palmitoyl-L-Carnitine	neg	1	✗
Palmitoyl-L-Carnitine	pos	1	✗
Cyclo (pro-Val)	pos	1	✗
Asp-Leu	neg	1	✗
Asp-Leu	neg	1	
Asp-Leu	pos	1	✗
Asp-Leu	pos	1	
Galactose	neg	1	✗
Galactose	pos	1	✗
DL-Kynurenin	neg	1	✗
DL-Kynurenin	pos	1	✗
3-Nitro-tyrosine	neg	1	✗
3-Nitro-tyrosine	pos	1	✗
Racemic lactic acid	neg	1	✗
(+)-Alliin	neg	1	✗
(+)-Alliin	pos	1	✗
3(2,4-dihydroxy-phenyl) propionic acid	neg	1	✗
3(2,4-dihydroxy-phenyl) propionic acid	pos	1	✗
N-Acetyl-L-methionine	neg	1	✗
N-Acetyl-L-methionine	pos	1	✗
L-Glutathione-Reduced	neg	1	✗
L-Glutathione-Reduced	pos	1	✗
L-Glutathione-Reduced	pos	1	✗
L-Glutathione-Reduced	pos	1	✗
Sodium dihydrogen phosphate	neg	1	✗
Sodium dihydrogen phosphate	pos	1	✗
Sodium bromide	neg	1	✗
Argininosuccinic acid disodium salt hydrate	neg	1	✗

Argininosuccinic acid disodium salt hydrate	pos	1	✘
Arginine	neg	1	✘
Arginine	pos	1	✘
Thr-Ala-OH	neg	1	✘
Thr-Ala-OH	pos	1	✘
D-glutamine	neg	1	✘
D-glutamine	pos	1	✘
3,5-dinitrosalicylic acid	neg	1	✘
3-(3-hydroxyphenyl)propionic acid	neg	1	✘
3-(3-hydroxyphenyl)propionic acid	pos	1	✘
Beta-cyano-L-Alanine	neg	1	✘
Beta-cyano-L-Alanine	pos	1	✘
Bromophenol blue	neg	1	✘
Bromophenol blue	pos	1	✘
Tridecanoic acid (FA13:0)	neg	1	✘
Benzoic acid	neg	1	✘
Ampicillinic acid	neg	1	✘
Ampicillinic acid	pos	1	✘
N-Acetyl-S-(carbamoylethyl)-L-cysteine	neg	1	✘
N-Acetyl-S-(carbamoylethyl)-L-cysteine	pos	1	✘
trans Resveratrol-3,4',5-trisulfate	neg	1	✘
trans Resveratrol-3,4',5-trisulfate	pos	1	✘
CMPF	neg	1	✘
CMPF	pos	1	✘
Furane-2-carboxylic acid	neg	1	✘
Furane-2-carboxylic acid	pos	1	✘
N-Acetyl-S-(2-carboxypropyl)-L-cysteine	neg	1	✘
N-Acetyl-S-(2-carboxypropyl)-L-cysteine	pos	1	✘
Cinnamic acid D6	neg	1	✘
1,5-anhydro-D-sorbitol	neg	1	✘

1,5-anhydro-D-sorbitol	pos	1	✘
Acarbose	neg	1	✘
Acarbose	pos	1	✘
Acarbose	pos	1	✘
CMC	neg	1	✘
CMC	pos	1	✘
Furosine	neg	1	✘
Furosine	pos	1	✘
Valproic acid glucuronide	neg	1	✘
Valproic acid glucuronide	pos	1	✘
Hecogenin	pos	1	✘
SFN	neg	1	✘
SFN	pos	1	✘
Homostachydrine	pos	1	✘
5-Hydroxydecanoic acid	neg	1	✘
5-Hydroxydecanoic acid	pos	1	✘
4-Hydroxybenzaldehyde	neg	1	✘
3-Hydroxycinnamic acid	neg	1	✘
Hydroferulic acid	neg	1	✘
Hydroferulic acid	pos	1	✘
Val-Phe	neg	1	✘
Val-Phe	pos	1	✘
alpha-Ketoisovaleric acid	neg	1	✘
Enterodiol	neg	1	✘
Enterodiol	pos	1	✘
Epigallocatechin	neg	1	✘
Epigallocatechin	pos	1	✘
Isovalerylglutamic acid	neg	1	✘
Isovalerylglutamic acid	pos	1	✘
4-O-methyl gallic acid	neg	1	✘

trans-Resveratrol 3-O-glucuronide	neg	1	✘
trans-Resveratrol 3-O-glucuronide	pos	1	✘
Resveratrol-3-O-Sulfate	neg	1	✘
Resveratrol-3-O-Sulfate	pos	1	✘
trans-Resveratrol 4'-O-glucuronide	pos	1	✘

Choline



User identifiers

localidentifier	38
dataOrigin	12062019Q-062.mzML
CAS	67-48-1
inchi	InChI=1S/C5H14NO.ClH/c1-6(2,3)4-5-7;/h7H,4-5H2,1-3H3;1H/q+1;/p-1

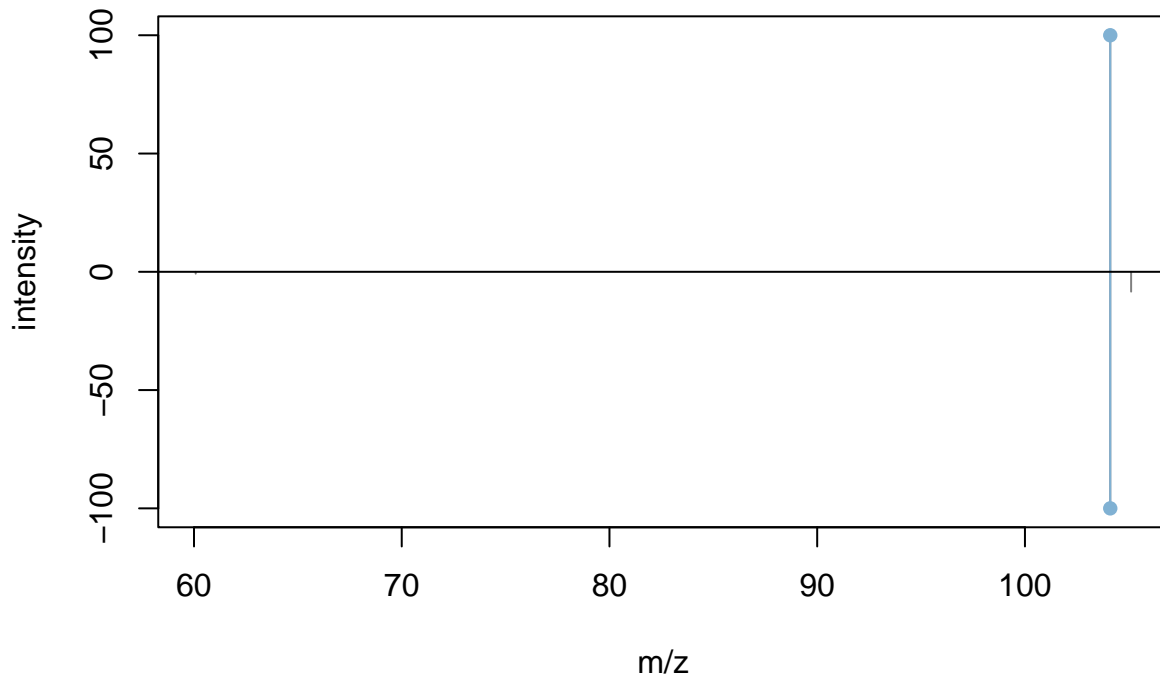
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C5H14NO/c1-6(2,3)4-5-7/h7H,4-5H2,1-3H3/q+1
inchikey	SGMZJAMFUVOLNK-UHFFFAOYSA-M	OEYIOHPDSNJKLS-UHFFFAOYSA-N
smiles	[Cl-].OCC[N+](C)(C)C	OCC[N+](C)(C)C
formula	C5H14ClNO	[C5H14NO] ⁺

Retention time match

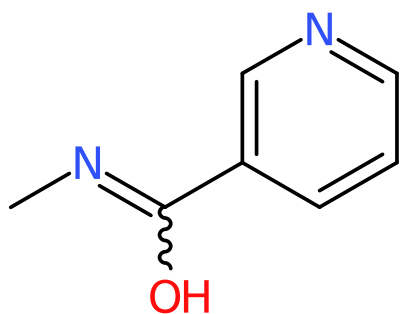
	DB	hit	error	rel. error	pcgroup
Retention time	0.45	0.47	0.02	3.3%	76

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
60.0810	0.8		[M+H-C ₂ H ₄ O] ⁺ (McLafferty)	✗	✗
104.1069	100.0	[M] ⁺	[M+H] ⁺	104.1067	100.0
105.1118	8.4	[M+1] ⁺		✗	✗

N-Methylnicotinamide



User identifiers

localidentifier	610
dataOrigin	20190723Q-043.mzML
CAS	114-33-0
inchi	InChI=1S/C7H8N2O/c1-8-7(10)6-3-2-4-9-5-6/h2-5H,1H3,(H,8,10)

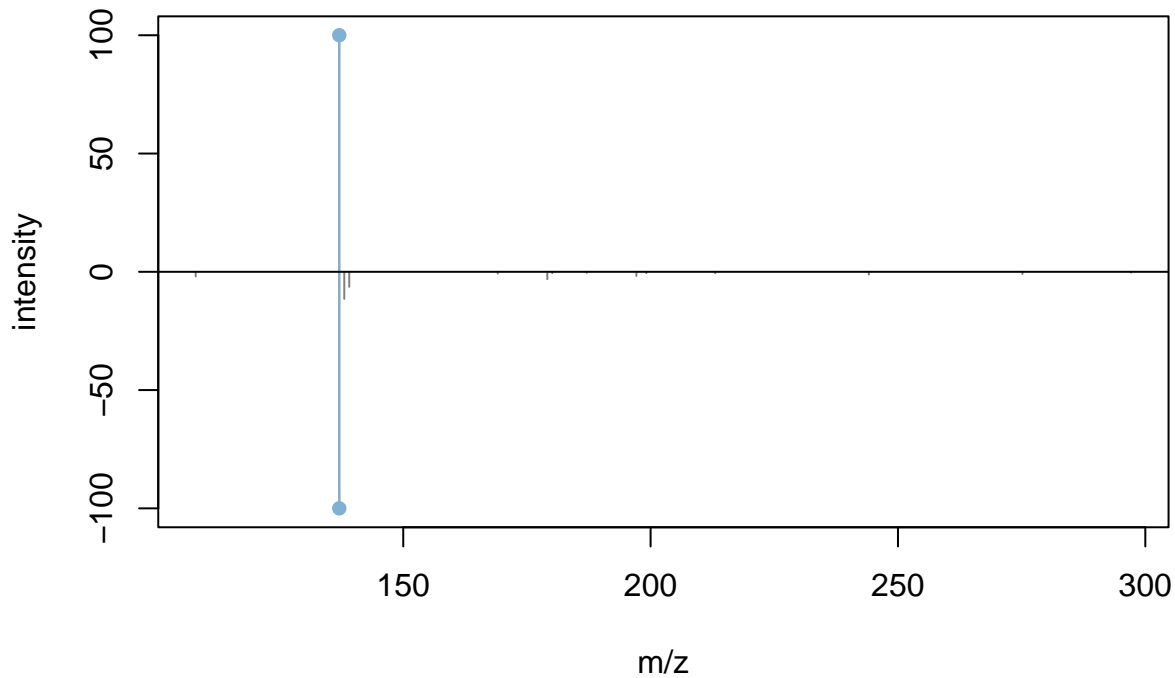
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8N2O/c1-8-7(10)6-3-2-4-9-5-6/h2-5H,1H3,(H,8,10)
inchikey	ZYVXHFWBYUDDBM-UHFFFAOYSA-N	ZYVXHFWBYUDDBM-UHFFFAOYSA-N
smiles	OC(=NC)C=1C=NC=CC1	OC(=NC)C=1C=NC=CC1
formula	C7H8N2O	C7H8N2O

Retention time match

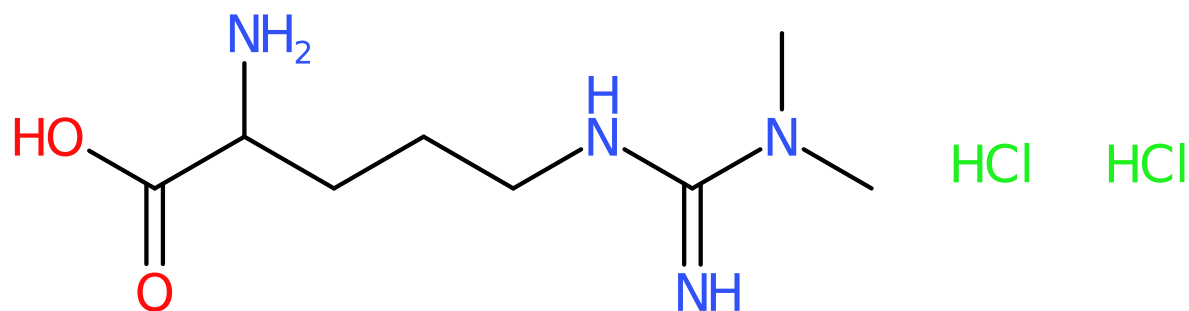
	DB	hit	error	rel. error	pcgroup
Retention time	0.96	0.47	-0.49	-50.9%	190

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
108.0433	2.0			✗	✗
137.0708	100.0	[M] ⁺	[M+H] ⁺	137.0712	100.0
138.0777	11.5	[M+1] ⁺		✗	✗
139.0838	6.4	[M+2] ⁺		✗	✗
169.0956	0.7			✗	✗
179.1188	3.1	[M] ⁺		✗	✗
180.1216	0.6	[M+1] ⁺		✗	✗
187.0865	0.4			✗	✗
197.1310	1.7			✗	✗
199.1424	0.6			✗	✗
213.0656	0.6			✗	✗
244.1138	1.2			✗	✗
275.1501	0.9			✗	✗
297.1309	0.4			✗	✗

Dimethylarginine



User identifiers

localidentifier	82
dataOrigin	12062019Q-110.mzML
CAS	220805-22-1
inchi	InChI=1S/C8H18N4O2.2ClH/c1-12(2)8(10)11-5-3-4-6(9)7(13)14;:/h6H,3-5,9H2,1-2H3,(H2,10,11)(H,13,14);2*1H

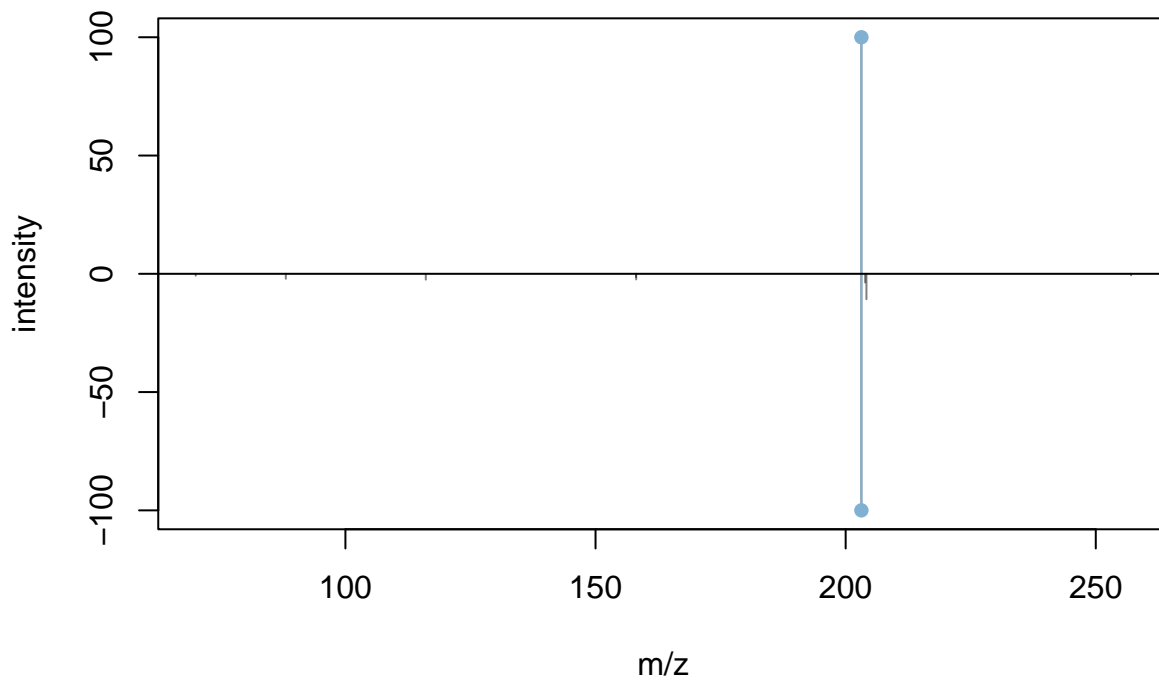
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H18N4O2/c1-12(2)8(10)11-5-3-4-6(9)7(13)14/h6H,3-5,9H2,1-2H3,(H2,10,11)(H,13,14)
inchikey	SYLNVYJOPZWPJL-UHFFFAOYSA-N	YDGMGEXADBMOMJ-UHFFFAOYSA-N
smiles	Cl.Cl.O=C(O)C(N)CCCNC(=N)N(C)C	O=C(O)C(N)CCCNC(=N)N(C)C
formula	C8H20Cl2N4O2	C8H18N4O2

Retention time match

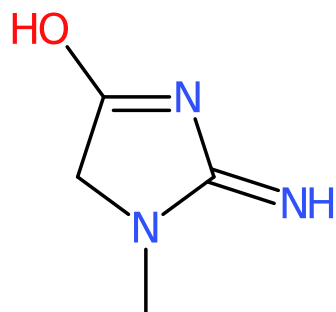
	DB	hit	error	rel. error	pcgroup
Retention time	0.50	0.48	-0.02	-3.4%	231

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
70.0679	0.8			✗	✗
88.0863	2.1			✗	✗
116.0711	2.5			✗	✗
158.0920	1.4			✗	✗
158.1286	2.4			✗	✗
203.1498	100.0	[M] ⁺	[M+H] ⁺	203.1508	100.0
203.9010	3.7			✗	✗
204.1557	10.8	[M+1] ⁺		✗	✗
257.0694	0.7			✗	✗

Creatinine



User identifiers

localidentifier	177
dataOrigin	14062019Q-090.mzML
CAS	60-27-5
inchi	InChI=1S/C4H7N3O/c1-7-2-3(8)6-4(7)5/h2H2,1H3,(H2,5,6,8)

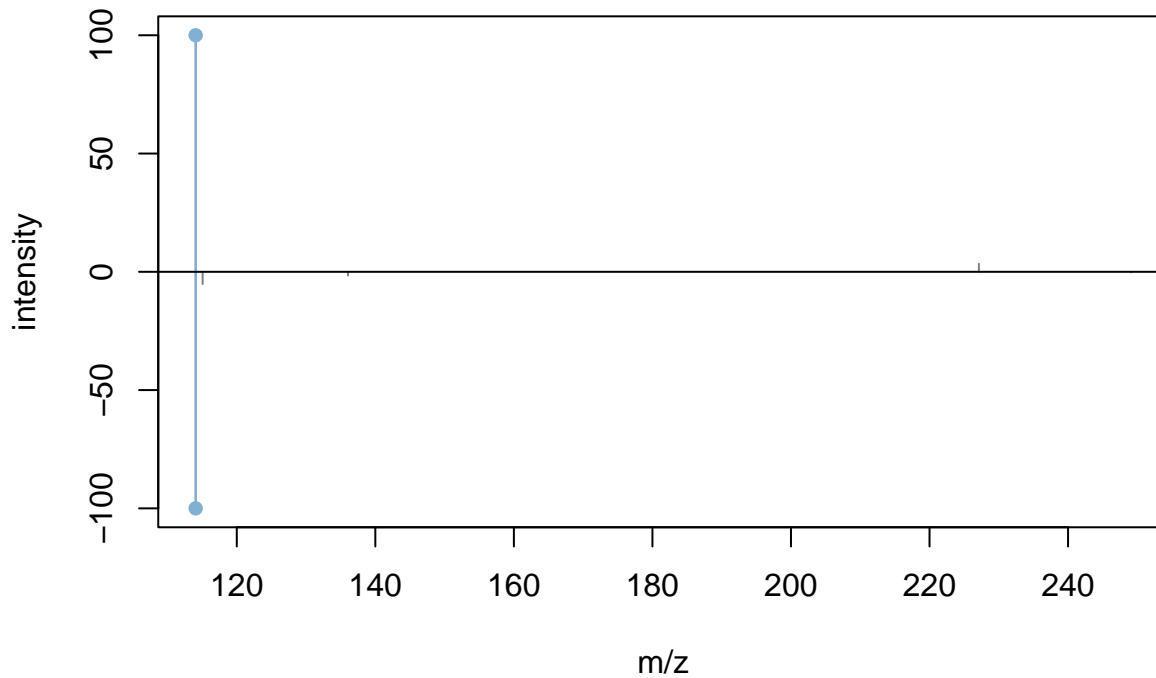
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C4H7N3O/c1-7-2-3(8)6-4(7)5/h2H2,1H3,(H2,5,6,8)
inchikey	DDRJAANPRJIHGJ-UHFFFAOYSA-N	DDRJAANPRJIHGJ-UHFFFAOYSA-N
smiles	N=C1N=C(O)CN1C	N=C1N=C(O)CN1C
formula	C4H7N3O	C4H7N3O

Retention time match

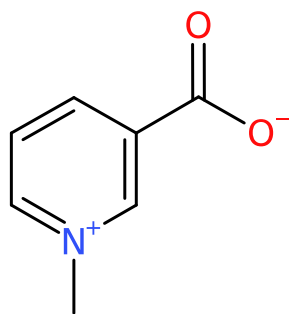
	DB	hit	error	rel. error	pcgroup
Retention time	0.47	0.48	0.01	2.2%	3

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
114.0659	100.0	[M] ⁺	[M+H] ⁺	114.0662	100.0
115.0709	5.2	[M+1] ⁺		✘	✘
136.0500	1.6		[M+Na] ⁺	✘	✘
✘	✘			227.1254	3.4
249.1030	0.2		[2M+Na] ⁺	✘	✘

Trigonelline



User identifiers

localidentifier	855
dataOrigin	20191206Q-058.mzML
CAS	535-83-1
inchi	InChI=1S/C7H7NO2/c1-8-4-2-3-6(5-8)7(9)10/h2-5H,1H3

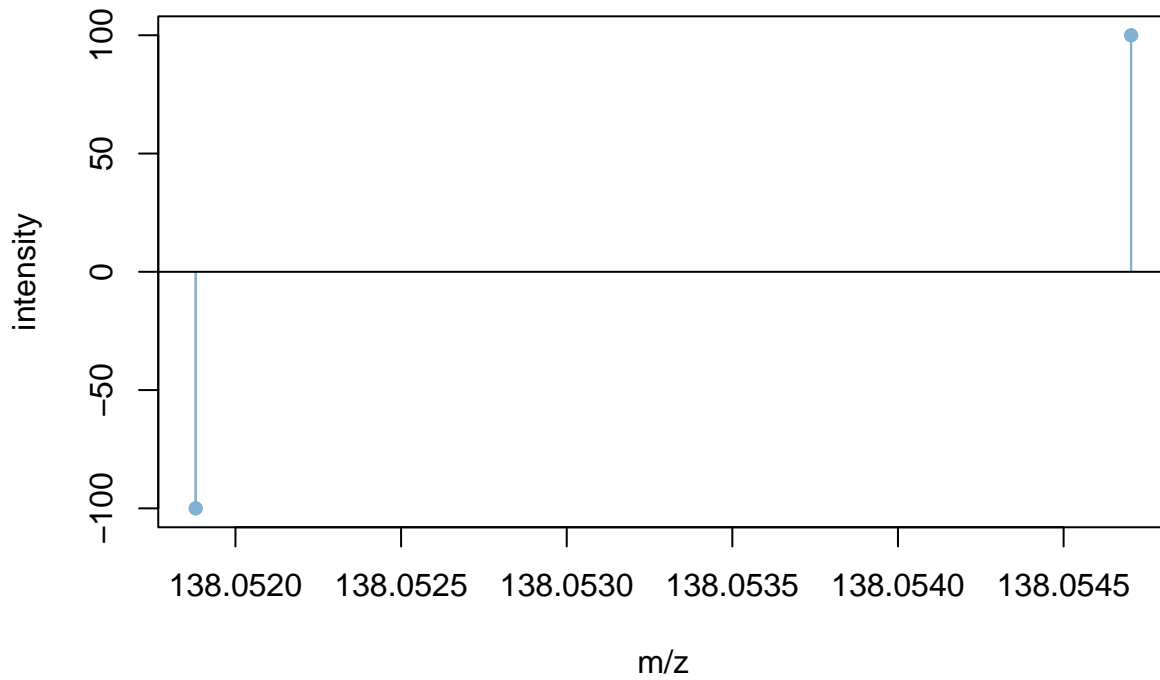
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H7NO2/c1-8-4-2-3-6(5-8)7(9)10/h2-5H,1H3
inchikey	WWNNZCOKKKDOPX-UHFFFAOYSA-N	WWNNZCOKKKDOPX-UHFFFAOYSA-N
smiles	O=C([O-])C1=CC=C[N+](=C1)C	O=C([O-])C1=CC=C[N+](=C1)C
formula	C7H7NO2	C7H7NO2

Retention time match

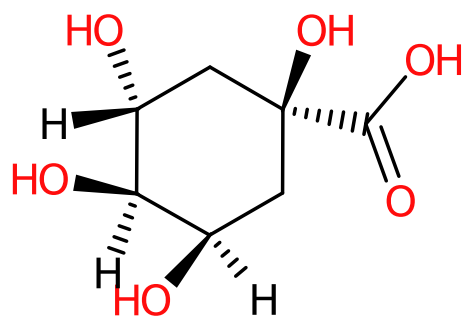
	DB	hit	error	rel. error	pcgroup
Retention time	0.54	0.49	-0.04	-8.1%	2

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
138.0519	100.0		[M+H] ⁺	138.0547	100.0

D-(-)-Quinic acid



User identifiers

localidentifier	101
dataOrigin	14062019Q-115.mzML
CAS	77-95-2
inchi	InChI=1S/C7H12O6/c8-3-1-7(13,6(11)12)2-4(9)5(3)10/h3-5,8-10,13H,1-2H2,(H,11,12)/t3-4-,5-,7+/m1/s1

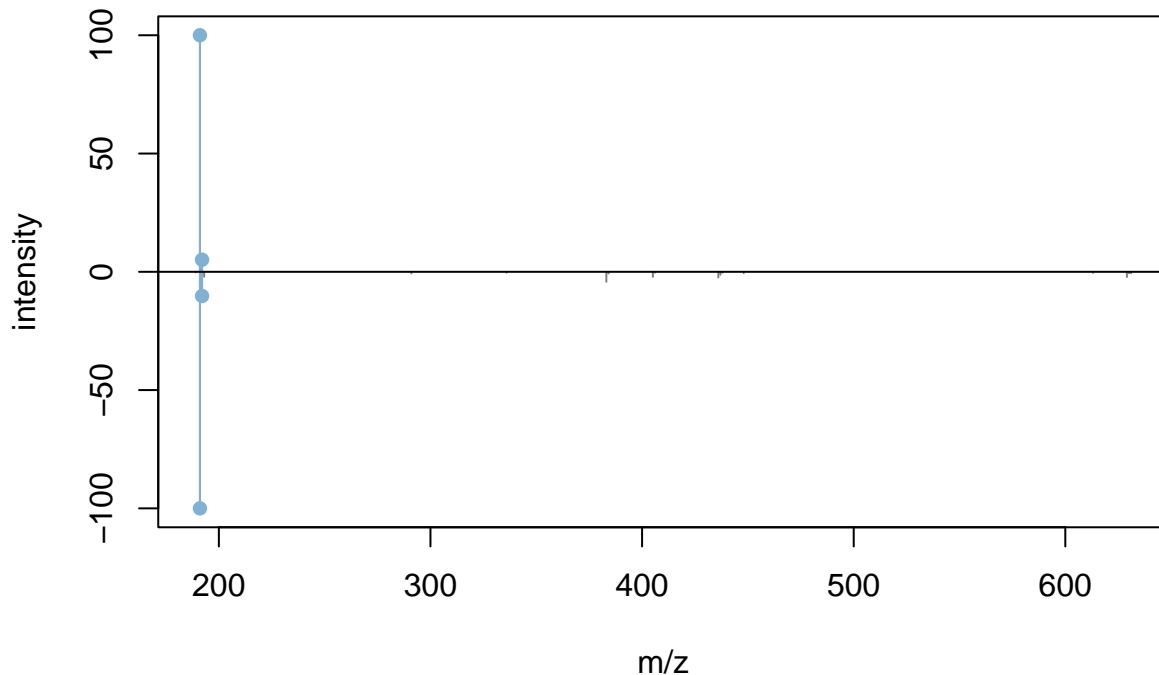
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H12O6/c8-3-1-7(13,6(11)12)2-4(9)5(3)10/h3-5,8-10,13H,1-2H2,(H,11,12)/t3-4-,5-,7+/m1/s1
inchikey	AAWZDTNXLSGCEK-WYWMIBKRSA-N	AAWZDTNXLSGCEK-WYWMIBKRSA-N
smiles	[H]C1(O)CC(O)(C(=O)O)CC([H])(O)C1([H])O	[H]C1(O)CC(O)(C(=O)O)CC([H])(O)C1([H])O
formula	C7H12O6	C7H12O6

Retention time match

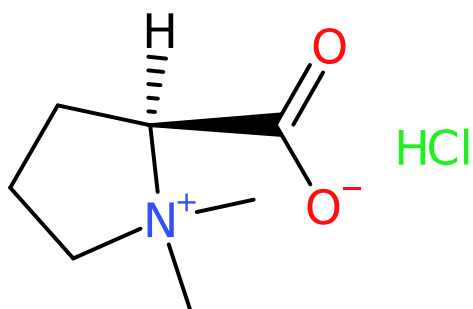
	DB	hit	error	rel. error	pcgroup
Retention time	0.55	0.51	-0.04	-7.6%	9

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
189.0415	0.3			✗	✗
191.0546	100.0	[M] ⁺	[M-H] ⁻	191.0542	100.0
192.0608	10.2	[M+1] ⁺		192.0607	5.1
193.0532	2.1	[M+2] ⁺		✗	✗
290.9837	0.7			✗	✗
335.9833	0.4			✗	✗
383.1191	4.2	[M] ⁺	[2M-H] ⁻	✗	✗
384.1320	0.7	[M+1] ⁺		✗	✗
405.1021	2.1	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
406.1034	0.4	[M+1] ⁺		✗	✗
436.0318	2.4		[2M-4H+Fe3+] ⁻	✗	✗
437.0397	1.3	[M] ⁺	[2M-3H+Fe2+] ⁻	✗	✗
438.0404	0.4	[M+1] ⁺		✗	✗
448.0295	0.6			✗	✗
613.1315	0.4		[3M-2H+K] ⁻	✗	✗
629.1025	2.2	[M] ⁺	[3M-3H+Fe2+] ⁻	✗	✗
630.1003	0.6	[M+1] ⁺		✗	✗
631.1027	0.6	[M+2] ⁺		✗	✗

stachydrine



User identifiers

localidentifier	115
dataOrigin	14062019Q-022.mzML
CAS	4136-37-2
inchi	InChI=1S/C7H13NO2.ClH/c1-8(2)5-3-4-6(8)7(9)10;/h6H,3-5H2,1-2H3;1H/t6-;/m0./s1

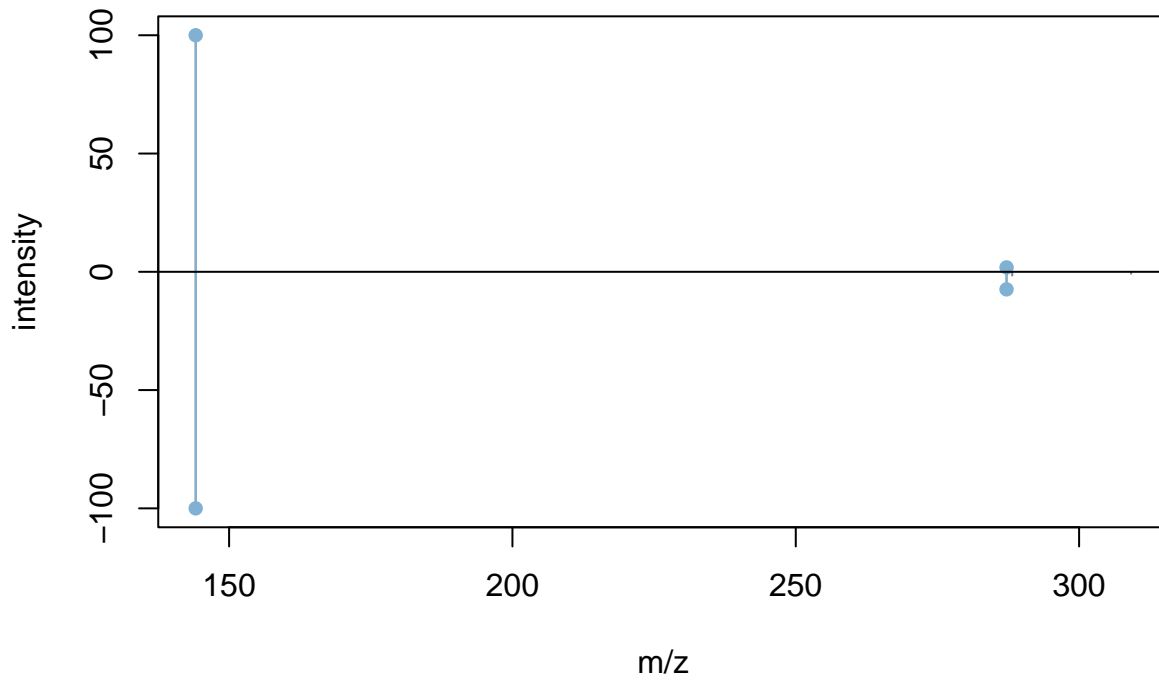
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H13NO2/c1-8(2)5-3-4-6(8)7(9)10/h6H,3-5H2,1-2H3/t6-/m0/s1
inchikey	DUNMULOWUUIQIL-RGMNGODLSA-N	CMUNUTVVVOOHQPW-LURJTMIESA-N
smiles	Cl.[H]C1(C(=O)[O-])CCC[N+]1(C)C	[H]C1(C(=O)[O-])CCC[N+]1(C)C
formula	C7H14ClNO2	C7H13NO2

Retention time match

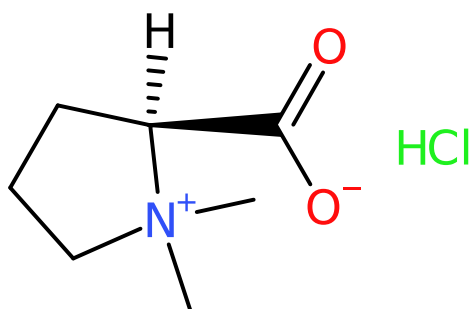
	DB	hit	error	rel. error	pcgroup
Retention time	0.54	0.52	-0.02	-4.2%	4

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
144.1029	100.0		[M+H] ⁺	144.1020	100.0
287.1959	7.4	[M] ⁺	[2M+H] ⁺	287.1982	1.9
288.2009	1.6	[M+1] ⁺		✗	✗
309.1807	0.8		[2M+Na] ⁺	✗	✗

stachydrine



User identifiers

localidentifier	115
dataOrigin	14062019Q-022.mzML
CAS	4136-37-2
inchi	InChI=1S/C7H13NO2.ClH/c1-8(2)5-3-4-6(8)7(9)10;/h6H,3-5H2,1-2H3;1H/t6-;/m0./s1

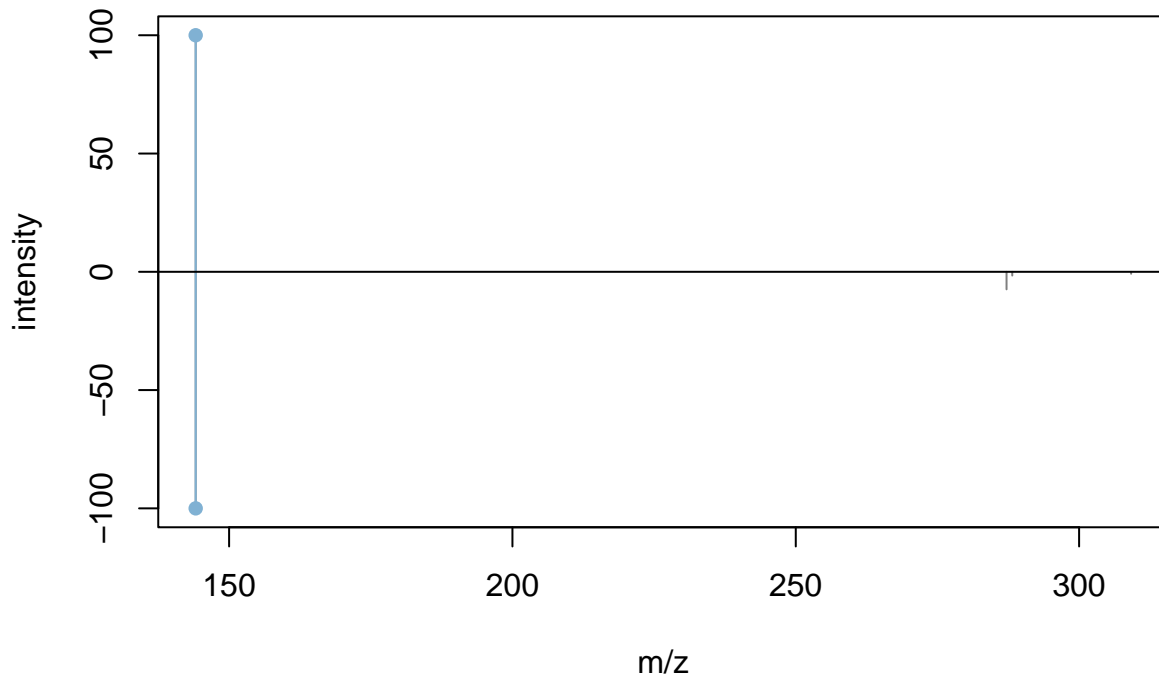
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H13NO2/c1-8(2)5-3-4-6(8)7(9)10/h6H,3-5H2,1-2H3/t6-/m0/s1
inchikey	DUNMULOWUUIQIL-RGMNGODLSA-N	CMUNUTVVOOHQPW-LURJTMIESA-N
smiles	Cl.[H]C1(C(=O)[O-])CCC[N+]1(C)C	[H]C1(C(=O)[O-])CCC[N+]1(C)C
formula	C7H14ClNO2	C7H13NO2

Retention time match

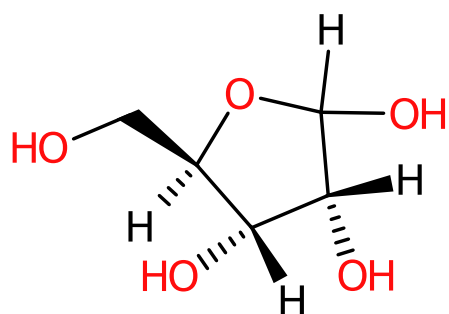
	DB	hit	error	rel. error	pcgroup
Retention time	0.54	0.59	0.05	9.1%	34

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
144.1029	100.0		[M+H] ⁺	144.1013	100.0
287.1959	7.4	[M] ⁺	[2M+H] ⁺	✗	✗
288.2009	1.6	[M+1] ⁺		✗	✗
309.1807	0.8		[2M+Na] ⁺	✗	✗

D-(-)-Ribose



User identifiers

localidentifier	103
dataOrigin	14062019Q-117.mzML
CAS	50-69-1
inchi	InChI=1S/C5H10O5/c6-1-2-3(7)4(8)5(9)10-2/h2-9H,1H2/t2-,3-,4-,5?/m1/s1

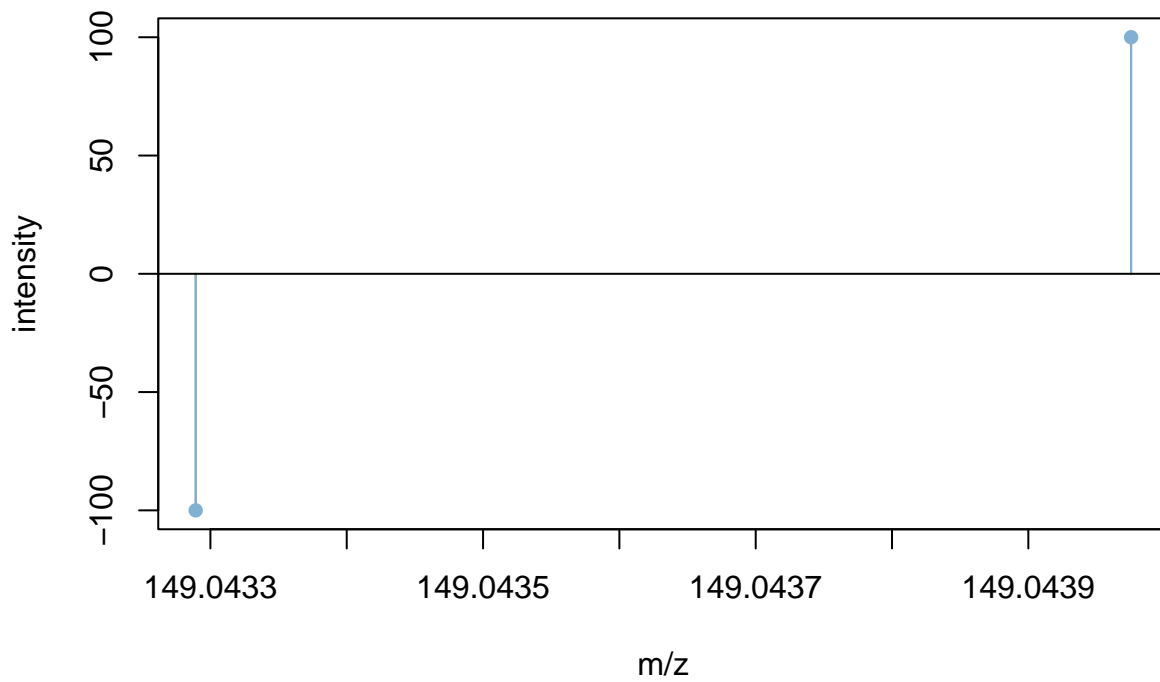
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C5H10O5/c6-1-2-3(7)4(8)5(9)10-2/h2-9H,1H2/t2-,3-,4-,5?/m1/s1
inchikey	HMFHBZSHGGEWLO-SOOFDHNKSA-N	HMFHBZSHGGEWLO-SOOFDHNKSA-N
smiles	[H]C1(O)OC([H])(CO)C([H])(O)C1([H])O	[H]C1(O)OC([H])(CO)C([H])(O)C1([H])O
formula	C5H10O5	C5H10O5

Retention time match

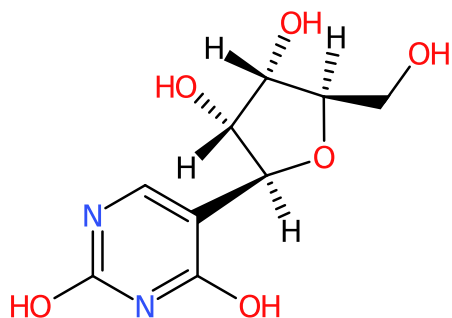
	DB	hit	error	rel. error	pcgroup
Retention time	0.52	0.53	0.00	0.9%	90

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
149.0433	100.0		[M-H]-	149.0440	100.0

-Pseudouridine



User identifiers

localidentifier	380
dataOrigin	20190710Q-212.mzML
CAS	1445-07-4
inchi	InChI=1S/C9H12N2O6/c12-2-4-5(13)6(14)7(17-4)3-1-10-9(16)11-8(3)15/h1,4-7,12-14H,2H2,(H2,10,11,15,16)/t4-,5-,6-,7+/m1/s1

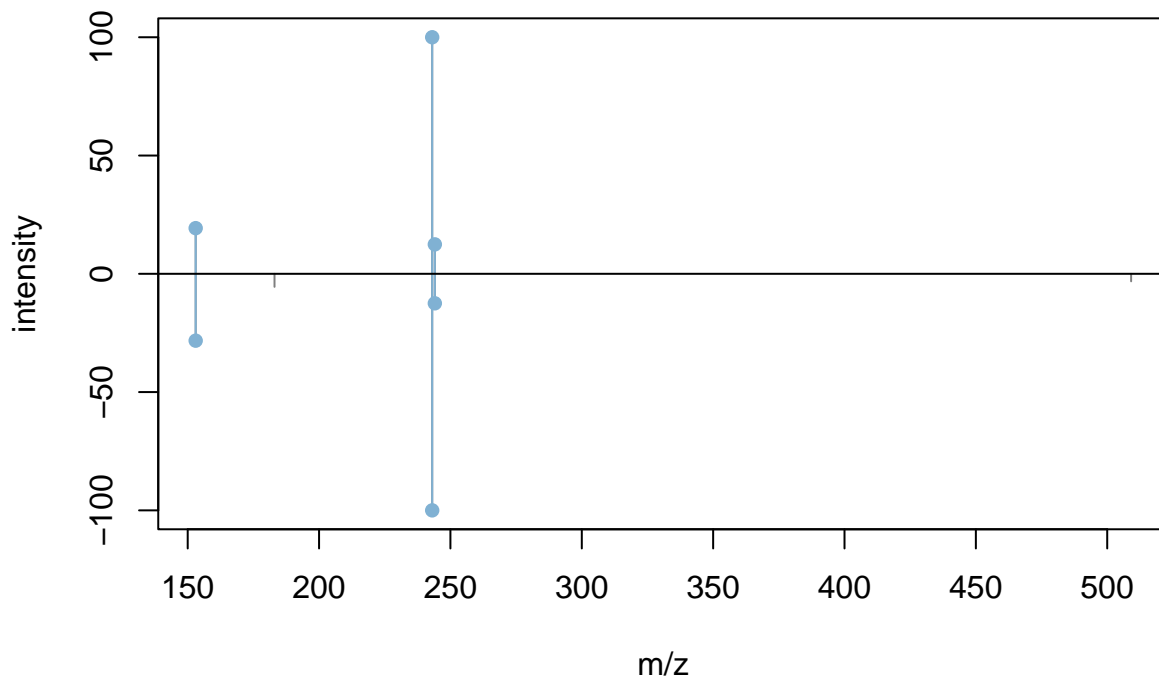
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H12N2O6/c12-2-4-5(13)6(14)7(17-4)3-1-10-9(16)11-8(3)15/h1,4-7,12-14H,2H2,(H2,10,11,15,16)/t4-,5-,6-,7+/m1/s1
inchikey	PTJWIQPHWPFNBW-GBNDHIKLSA-N	PTJWIQPHWPFNBW-GBNDHIKLSA-N
smiles	[H]C1(O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C	[H]C1(O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C
formula	C9H12N2O6	C9H12N2O6

Retention time match

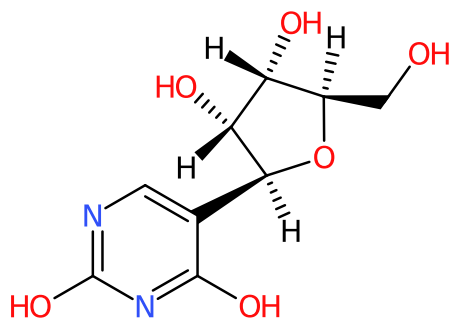
	DB	hit	error	rel. error	pcgroup
Retention time	0.62	0.58	-0.04	-6.4%	136

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
153.0293	28.3			153.0302	19.3
183.0401	5.5		[M-H-C ₂ H ₄ O ₂]-	✘	✘
243.0617	100.0	[M] ⁺	[M-H] ⁻	243.0602	100.0
244.0652	12.5	[M+1] ⁺		244.0662	12.4
509.1036	3.2		[2M-2H+Na] ⁻	✘	✘

-Pseudouridine



User identifiers

localidentifier	380
dataOrigin	20190710Q-212.mzML
CAS	1445-07-4
inchi	InChI=1S/C9H12N2O6/c12-2-4-5(13)6(14)7(17-4)3-1-10-9(16)11-8(3)15/h1,4-7,12-14H,2H2,(H2,10,11,15,16)/t4-,5-,6-,7+/m1/s1

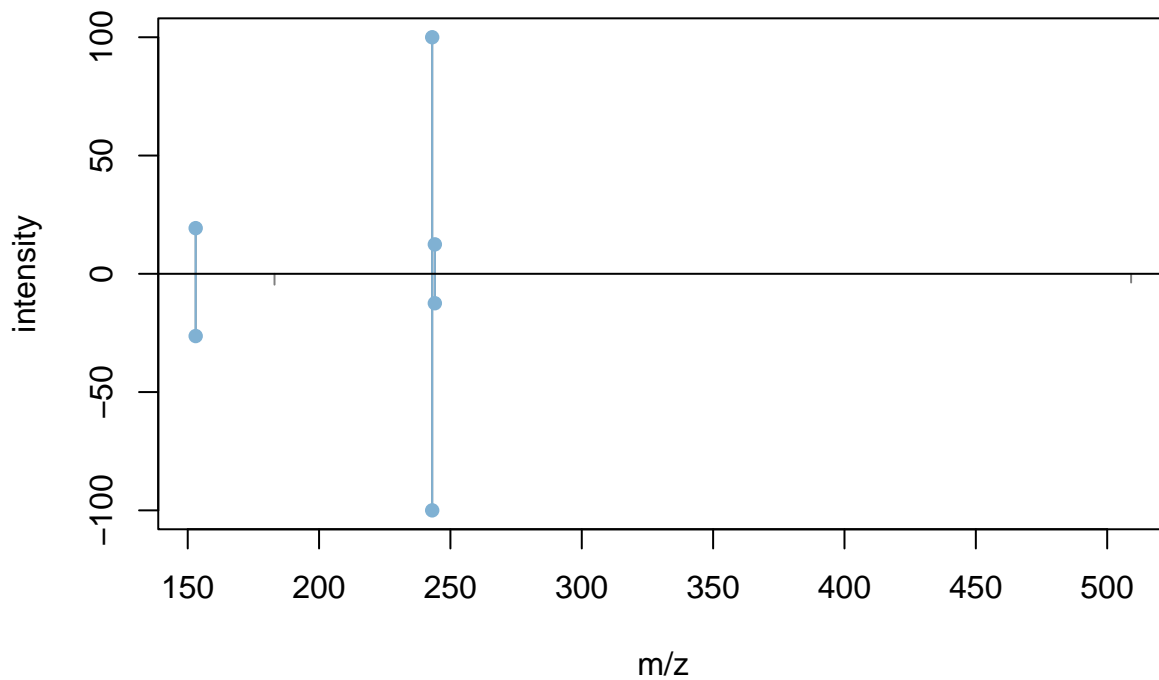
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H12N2O6/c12-2-4-5(13)6(14)7(17-4)3-1-10-9(16)11-8(3)15/h1,4-7,12-14H,2H2,(H2,10,11,15,16)/t4-,5-,6-,7+/m1/s1
inchikey	PTJWIQPHWPFNBW-GBNDHIKLSA-N	PTJWIQPHWPFNBW-GBNDHIKLSA-N
smiles	[H]C1(O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C	[H]C1(O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C([H])(O)C([H])(OC1([H])C2=CN=C(O)N=C2O)C
formula	C9H12N2O6	C9H12N2O6

Retention time match

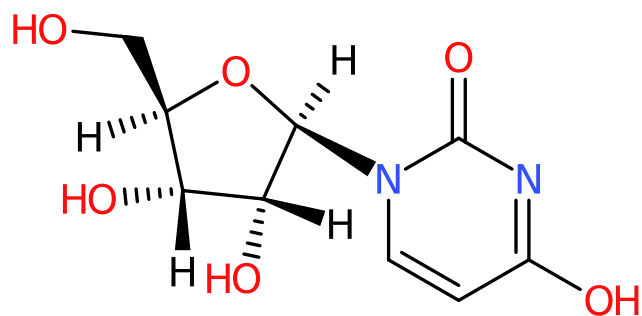
	DB	hit	error	rel. error	pcgroup
Retention time	0.62	0.58	-0.03	-5.2%	136

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
153.0276	26.3			153.0302	19.3
183.0386	4.6		[M-H-C2H4O2]-	✘	✘
243.0593	100.0	[M] ⁺	[M-H] ⁻	243.0602	100.0
244.0636	12.4	[M+1] ⁺		244.0662	12.4
509.1169	3.7		[2M-2H+Na] ⁻	✘	✘

Uridine



User identifiers

localidentifier	596
dataOrigin	20190723Q-134.mzML
CAS	58-96-8
inchi	InChI=1S/C9H12N2O6/c12-3-4-6(14)7(15)8(17-4)11-2-1-5(13)10-9(11)16/h1-2,4,6-8,12,14-15H,3H2,(H,10,13,16)/t4-,6-,7-,8-/m1/s1

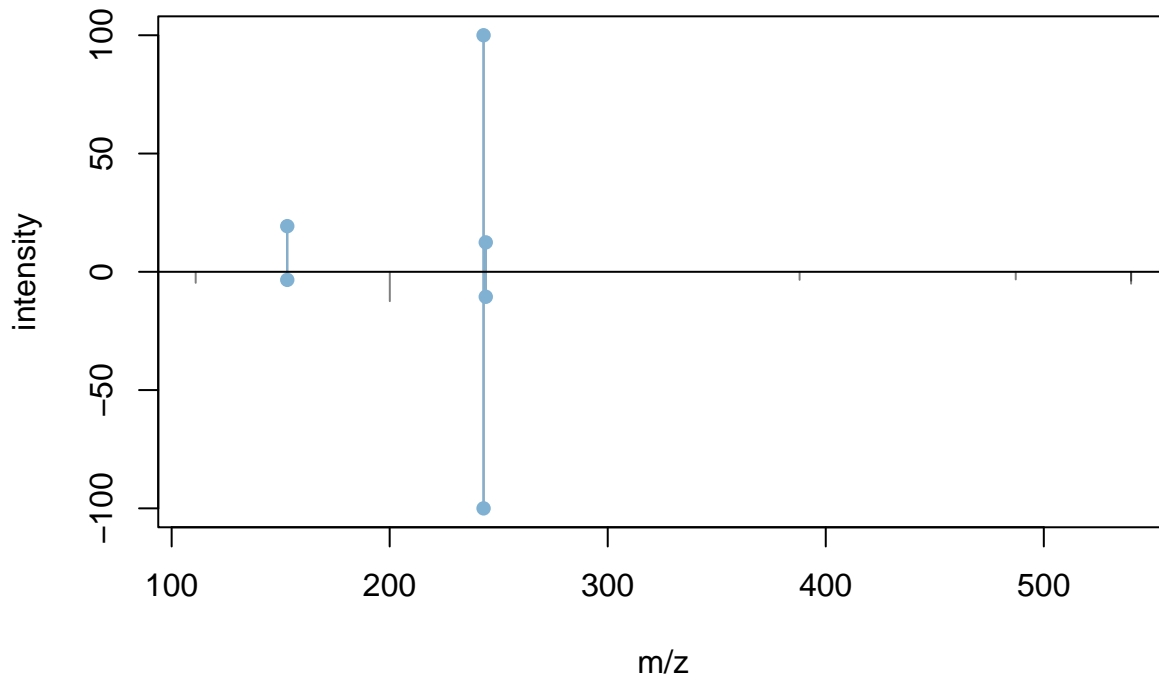
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H12N2O6/c12-3-4-6(14)7(15)8(17-4)11-2-1-5(13)10-9(11)16/h1-2,4,6-8,12,14-15H,3H2,(H,10,13,16)/t4-,6-,7-,8-/m1/s1
inchikey	DRTQHJPMGBCF-XVFCMESISA-N	DRTQHJPMGBCF-XVFCMESISA-N
smiles	[H]C1(O)C([H])(O)C([H])(OC1([H])N2C=CC(O)=NC2=O)C	[H]C1(O)C([H])(O)C([H])(OC1([H])N2C=CC(O)=NC2=O)C
formula	C9H12N2O6	C9H12N2O6

Retention time match

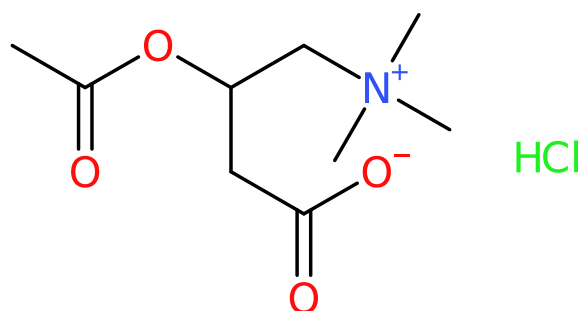
	DB	hit	error	rel. error	pcgroup
Retention time	0.91	0.58	-0.32	-35.6%	136

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
111.0221	4.7			✗	✗
153.0302	3.4			153.0302	19.3
200.0550	12.4			✗	✗
243.0608	100.0	[M] ⁺	[M-H] ⁻	243.0602	100.0
244.0659	10.6	[M+1] ⁺		244.0662	12.4
387.9917	3.4			✗	✗
487.1393	3.2		[2M-H] ⁻	✗	✗
540.0436	5.0		[2M-4H+Fe3+] ⁻	✗	✗
540.0546	3.8		[2M-4H+Fe3+] ⁻	✗	✗

N-Acetylcarnitine



User identifiers

localidentifier	24
dataOrigin	12062019Q-046.mzML
CAS	2504-11-2
inchi	InChI=1S/C9H17NO4.ClH/c1-7(11)14-8(5-9(12)13)6-10(2,3)4;/h8H,5-6H2,1-4H3;1H

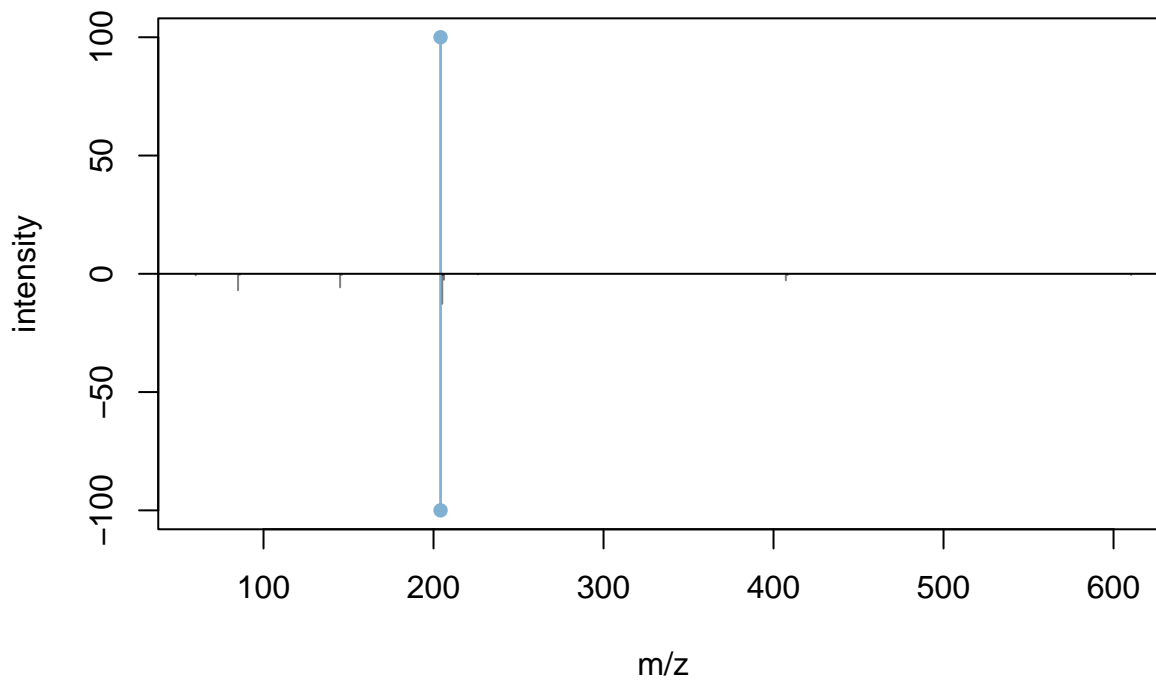
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H17NO4/c1-7(11)14-8(5-9(12)13)6-10(2,3)4/h8H,5-6H2,1-4H3
inchikey	JATPLOXBFFRHDN-UHFFFAOYSA-N	RDHQFKQIGNGIED-UHFFFAOYSA-N
smiles	Cl.O=C(OC(CC(=O)[O-])C[N+](C)(C)C)C	O=C(OC(CC(=O)[O-])C[N+](C)(C)C)C
formula	C9H18ClNO4	C9H17NO4

Retention time match

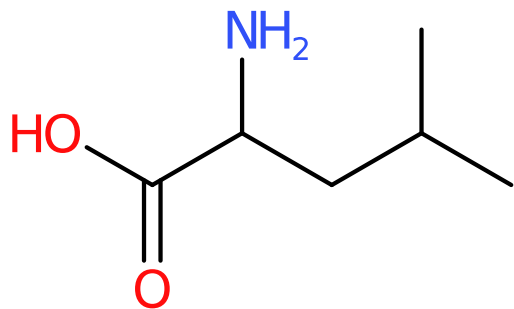
	DB	hit	error	rel. error	pcgroup
Retention time	0.60	0.60	0.00	0.7%	213

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
60.0827	0.6			✗	✗
85.0275	6.9	[M] ⁺	[M+H-C ₃ H ₉ N-C ₂ H ₄ O ₂] ⁺	✗	✗
86.0322	0.4	[M+1] ⁺		✗	✗
145.0495	5.7	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✗	✗
146.0537	0.5	[M+1] ⁺		✗	✗
204.1249	100.0	[M] ⁺	[M+H] ⁺	204.1228	100.0
205.1284	12.7	[M+1] ⁺		✗	✗
205.4111	0.6			✗	✗
206.1286	2.5	[M+2] ⁺		✗	✗
226.1023	0.3		[M+Na] ⁺	✗	✗
226.1041	0.2		[M+Na] ⁺	✗	✗
407.2399	2.8	[M] ⁺	[2M+H] ⁺	✗	✗
408.2461	0.6	[M+1] ⁺		✗	✗
610.3522	0.5		[3M+H] ⁺	✗	✗

Leucine



User identifiers

localidentifier	73
dataOrigin	12062019Q-101.mzML
CAS	61-90-5
inchi	InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)

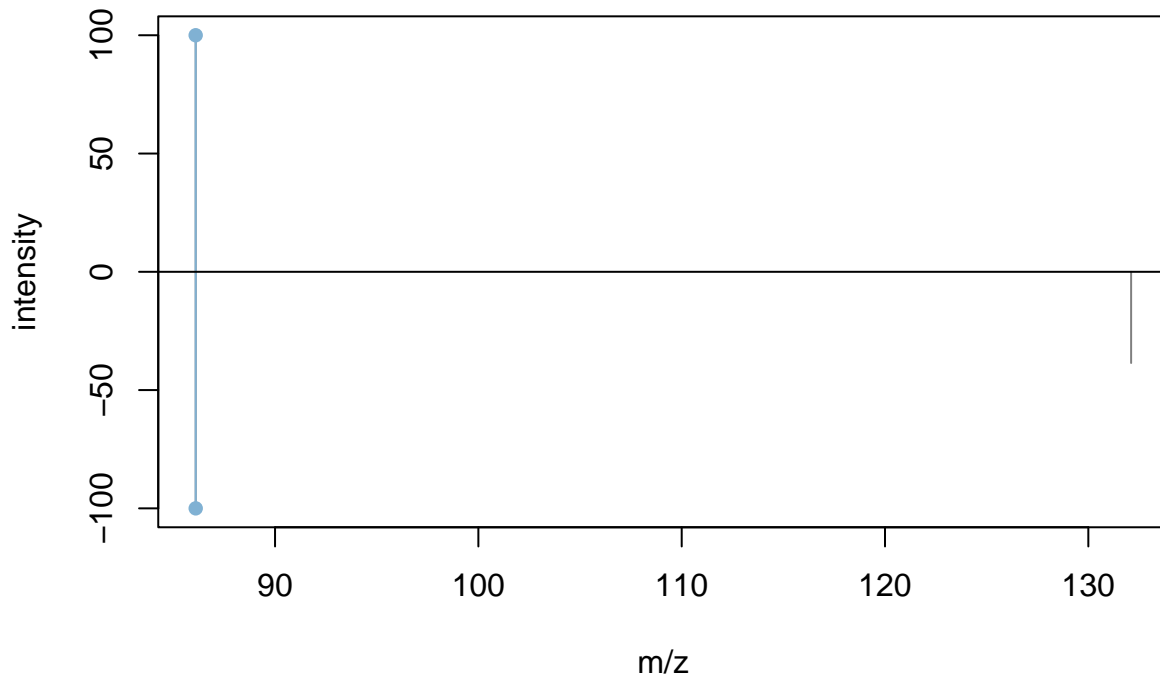
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)
inchikey	ROHFNLRQFUQHCH-UHFFFAOYSA-N	ROHFNLRQFUQHCH-UHFFFAOYSA-N
smiles	O=C(O)C(N)CC(C)C	O=C(O)C(N)CC(C)C
formula	C6H13NO2	C6H13NO2

Retention time match

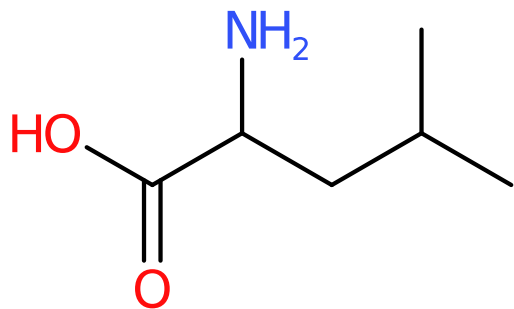
	DB	hit	error	rel. error	pcgroup
Retention time	0.93	0.60	-0.33	-35.2%	11

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
86.0972	100.0		[M+H-HCOOH] ⁺	86.0959	100.0
132.1047	38.6		[M+H] ⁺	✗	✗

Leucine



User identifiers

localidentifier	73
dataOrigin	12062019Q-101.mzML
CAS	61-90-5
inchi	InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)

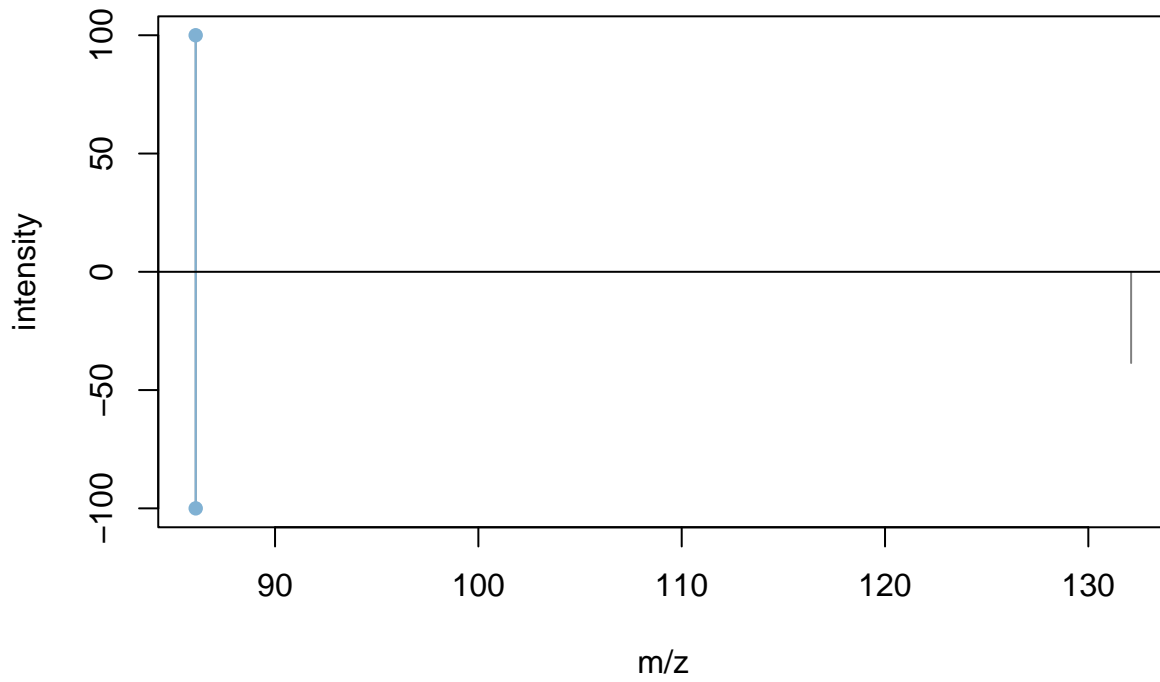
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)
inchikey	ROHFNLRQFUQHCH-UHFFFAOYSA-N	ROHFNLRQFUQHCH-UHFFFAOYSA-N
smiles	O=C(O)C(N)CC(C)C	O=C(O)C(N)CC(C)C
formula	C6H13NO2	C6H13NO2

Retention time match

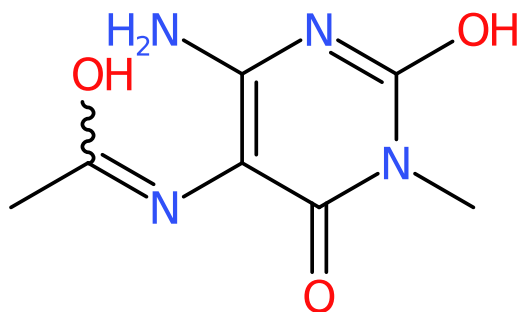
	DB	hit	error	rel. error	pcgroup
Retention time	0.93	0.97	0.04	3.9%	69

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
86.0972	100.0		[M+H-HCOOH] ⁺	86.0956	100.0
132.1047	38.6		[M+H] ⁺	✗	✗

AAMU



User identifiers

localidentifier	698
dataOrigin	20190725Q-035.mzML
CAS	19893-78-8
inchi	InChI=1S/C7H10N4O3/c1-3(12)9-4-5(8)10-7(14)11(2)6(4)13/h8H2,1-2H3,(H,9,12)(H,10,14)

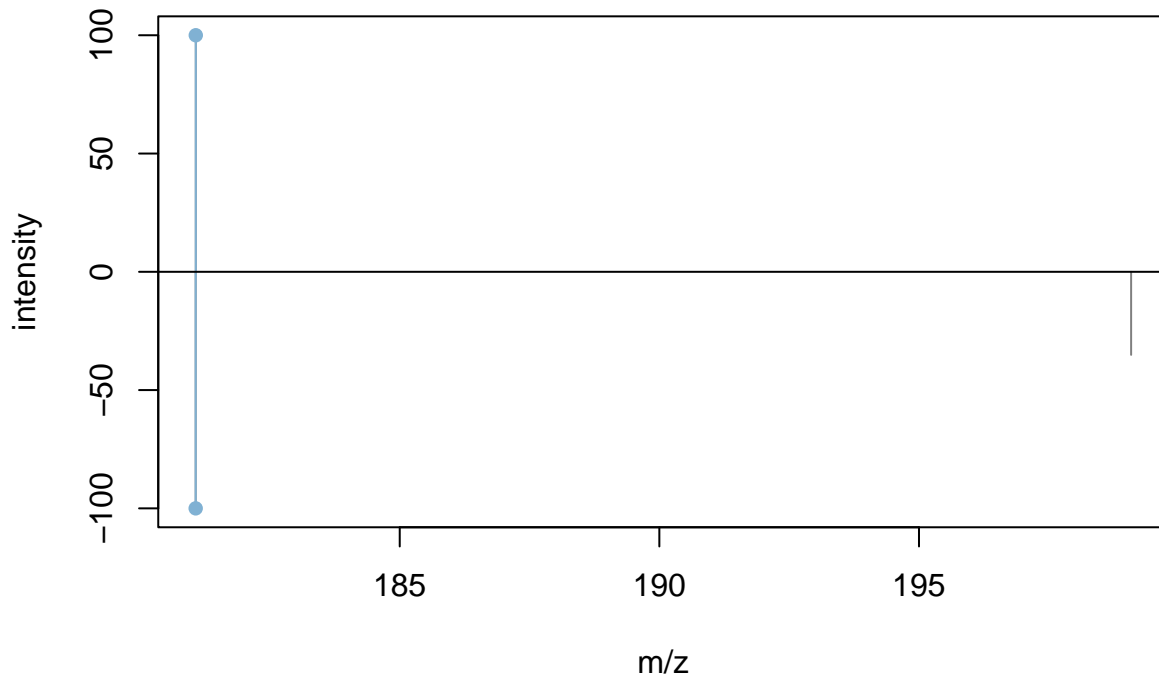
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H10N4O3/c1-3(12)9-4-5(8)10-7(14)11(2)6(4)13/h8H2,1-2H3,(H,9,12)(H,10,14)
inchikey	POQOTWQIYYNXAT-UHFFFAOYSA-N	POQOTWQIYYNXAT-UHFFFAOYSA-N
smiles	O=C1C(N=C(O)C)=C(N=C(O)N1C)N	O=C1C(N=C(O)C)=C(N=C(O)N1C)N
formula	C7H10N4O3	C7H10N4O3

Retention time match

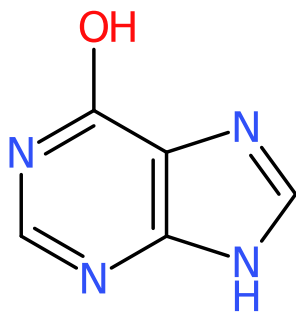
	DB	hit	error	rel. error	pcgroup
Retention time	0.64	0.65	0.01	1.2%	91

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
181.0704	100.0		[M+H-H ₂ O] ⁺	181.0724	100.0
199.0854	35.1		[M+H] ⁺	✗	✗

Hypoxanthine



User identifiers

localidentifier	348
dataOrigin	20190710Q-071.mzML
CAS	68-94-0
inchi	InChI=1S/C5H4N4O/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)

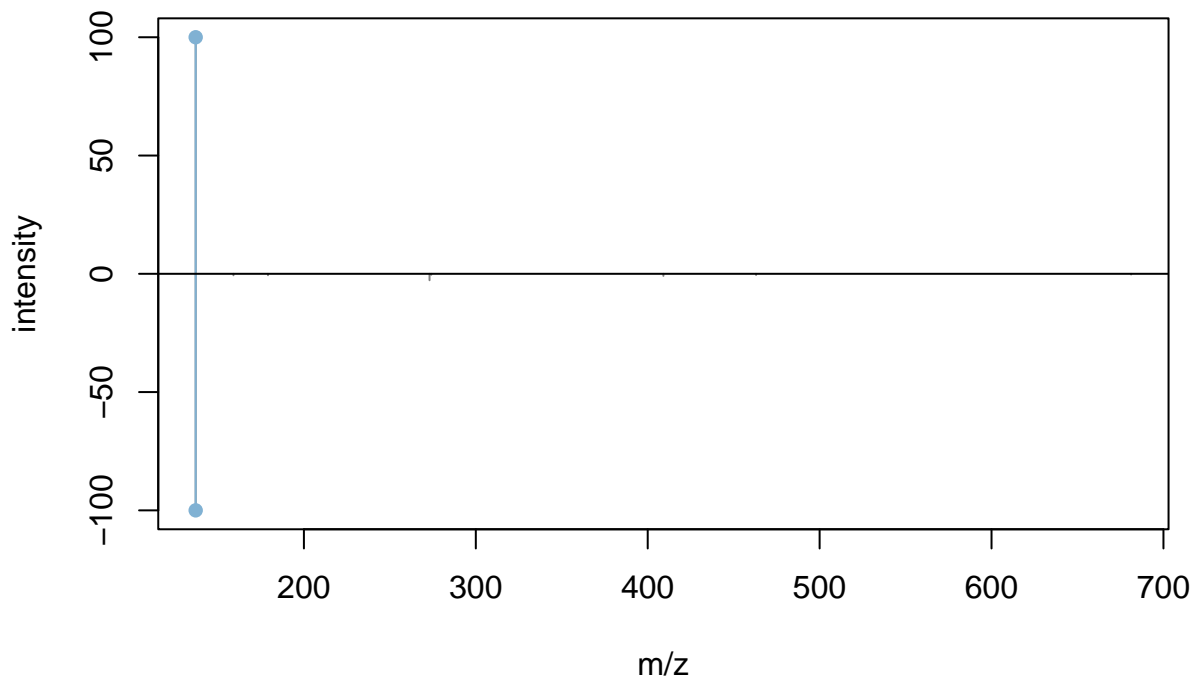
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C5H4N4O/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)
inchikey	FDGQSTZJBFJUBT-UHFFFAOYSA-N	FDGQSTZJBFJUBT-UHFFFAOYSA-N
smiles	OC1=NC=NC=2NC=NC12	OC1=NC=NC=2NC=NC12
formula	C5H4N4O	C5H4N4O

Retention time match

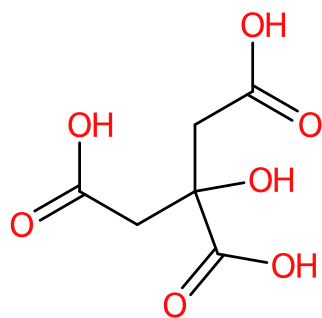
	DB	hit	error	rel. error	pcgroup
Retention time	0.73	0.68	-0.04	-6.1%	24

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
137.0438	100.0		[M+H] ⁺	137.0457	100.0
159.0295	0.6		[M+Na] ⁺	✗	✗
179.0947	0.6			✗	✗
273.0848	2.7	[M] ⁺	[2M+H] ⁺	✗	✗
274.0859	0.4	[M+1] ⁺		✗	✗
409.1278	0.9		[3M+H] ⁺	✗	✗
463.0319	0.5			✗	✗
681.2029	0.3			✗	✗

Citric acid



User identifiers

localidentifier	39
dataOrigin	12062019Q-170.mzML
CAS	77-92-9
inchi	InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)

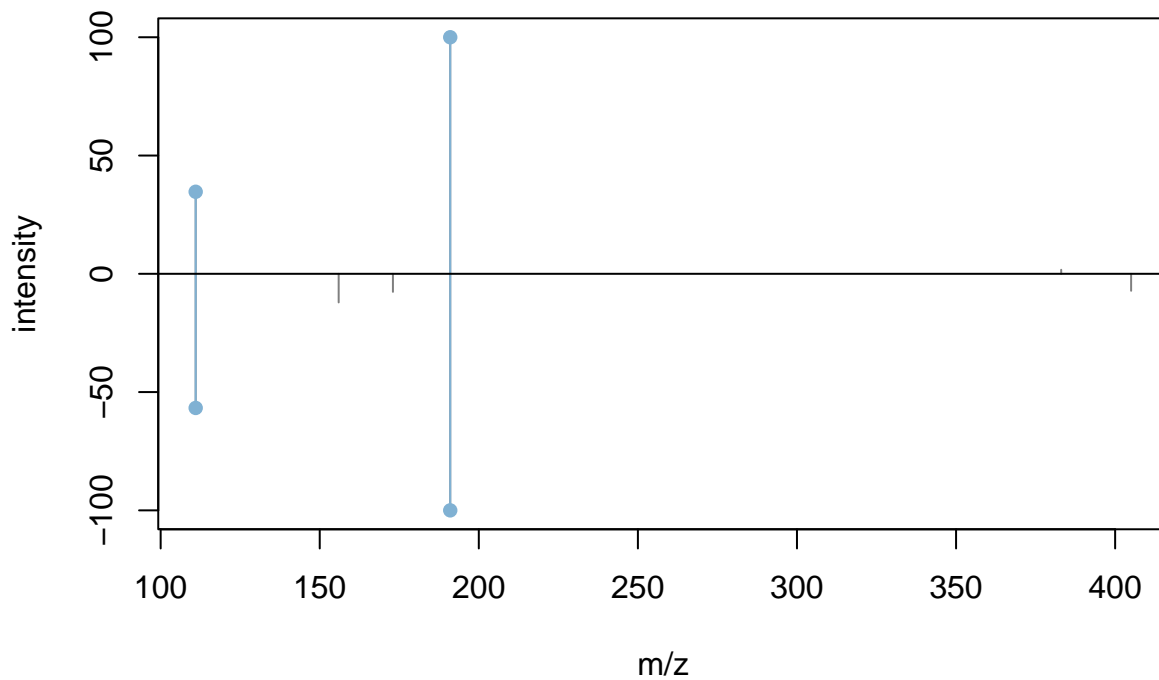
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
inchikey	KRKNYBCHXYNGOX-UHFFFAOYSA-N	KRKNYBCHXYNGOX-UHFFFAOYSA-N
smiles	O=C(O)CC(O)(C(=O)O)CC(=O)O	O=C(O)CC(O)(C(=O)O)CC(=O)O
formula	C6H8O7	C6H8O7

Retention time match

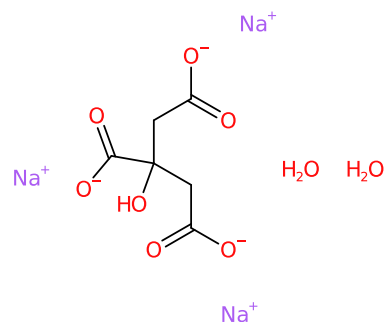
	DB	hit	error	rel. error	pcgroup
Retention time	0.73	0.69	-0.04	-5.2%	12

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
111.0092	56.7			111.0088	34.7
155.9505	12.1			×	×
173.0029	7.6			×	×
191.0186	100.0		[M-H]-	191.0193	100.0
×	×			383.0459	1.7
405.0262	7.2		[2M-2H+Na]-	×	×

Citric acid



User identifiers

localidentifier	675
dataOrigin	20190725Q-117.mzML
CAS	6132-04-3
inchi	InChI=1S/C6H8O7.3Na.2H2O/c7-3(8)1-6(13,5(11)12)2-4(9)10;;;;;/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12);;;2*1H2/q;3*+1;;/p-3

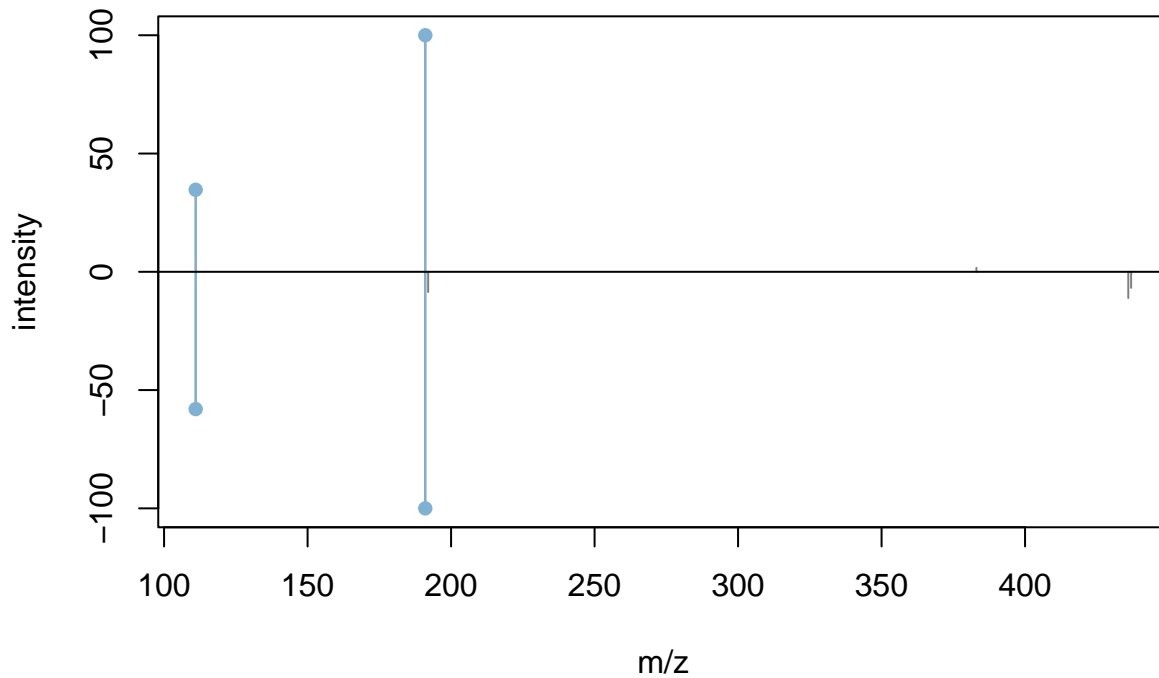
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/p-3
inchikey	NLJMYIDDQXHKNR-UHFFFAOYSA-K	KRKNYBCHXYNGOX-UHFFFAOYSA-K
smiles	[Na+].[Na+].[Na+].O=C([O-])CC(O)(C(=O)[O-])CC(=O)[O-].O.O	O=C([O-])CC(O)(C(=O)[O-])CC(=O)[O-]
formula	C6H9Na3O9	[C6H5O7]3-

Retention time match

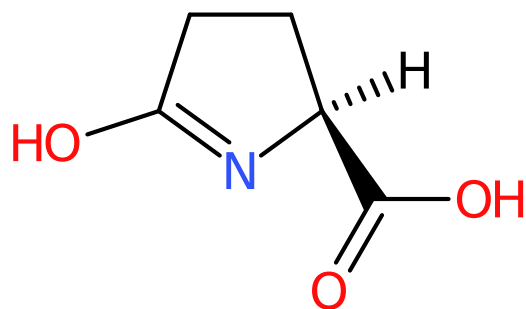
	DB	hit	error	rel. error	pcgroup
Retention time	0.71	0.69	-0.02	-2.5%	12

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
111.0075	58.0			111.0088	34.7
191.0183	100.0	[M] ⁺	[M-H] ⁻	191.0193	100.0
192.0219	8.6	[M+1] ⁺		✗	✗
✗	✗			383.0459	1.7
435.9685	11.1		[2M-4H+Fe3 ⁺] ⁻	✗	✗
436.9592	6.8		[2M-3H+Fe2 ⁺] ⁻	✗	✗

L-2-Pyrrolidon-5-carboxylsyre



User identifiers

localidentifier	378
dataOrigin	20190710Q-210.mzML
CAS	98-79-3
inchi	InChI=1S/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)/t3-/m0/s1

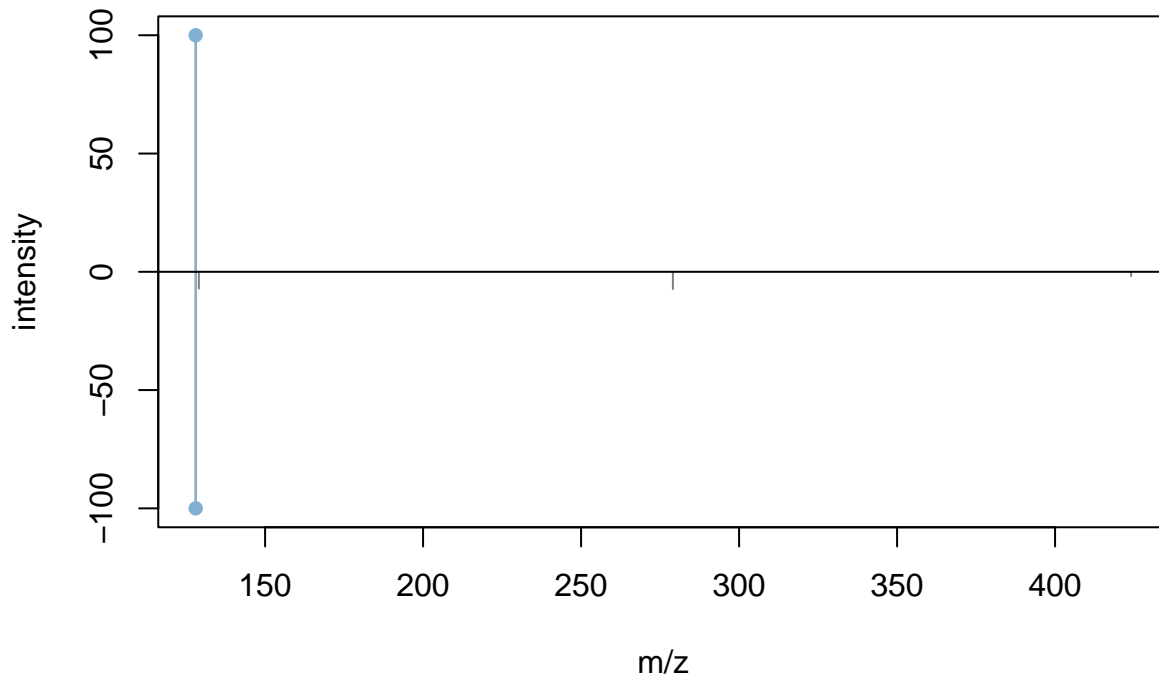
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)/t3-/m0/s1
inchikey	ODHCTXKNWHHXJC-VKHMYHEASA-N	ODHCTXKNWHHXJC-VKHMYHEASA-N
smiles	[H]C1(N=C(O)CC1)C(=O)O	[H]C1(N=C(O)CC1)C(=O)O
formula	C5H7NO3	C5H7NO3

Retention time match

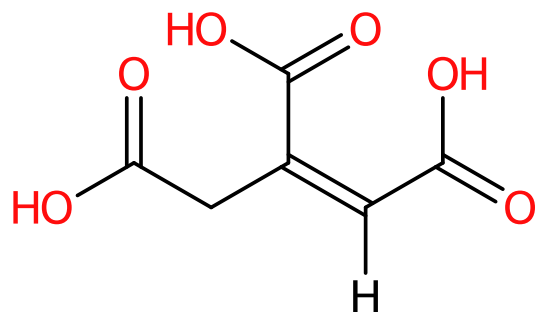
	DB	hit	error	rel. error	pcgroup
Retention time	0.76	0.73	-0.02	-3.3%	62

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
128.0335	100.0	[M] ⁺	[M-H] ⁻	128.0341	100.0
129.0374	7.1	[M+1] ⁺		✗	✗
279.0564	7.3		[2M-2H+Na] ⁻	✗	✗
424.0677	1.8		[3M-2H+K] ⁻	✗	✗

cis-aconitic acid



User identifiers

localidentifier	270
dataOrigin	20190701Q-198.mzML
CAS	585-84-2
inchi	InChI=1S/C6H6O6/c7-4(8)1-3(6(11)12)2-5(9)10/h1H,2H2,(H,7,8)(H,9,10)(H,11,12)/b3-1-

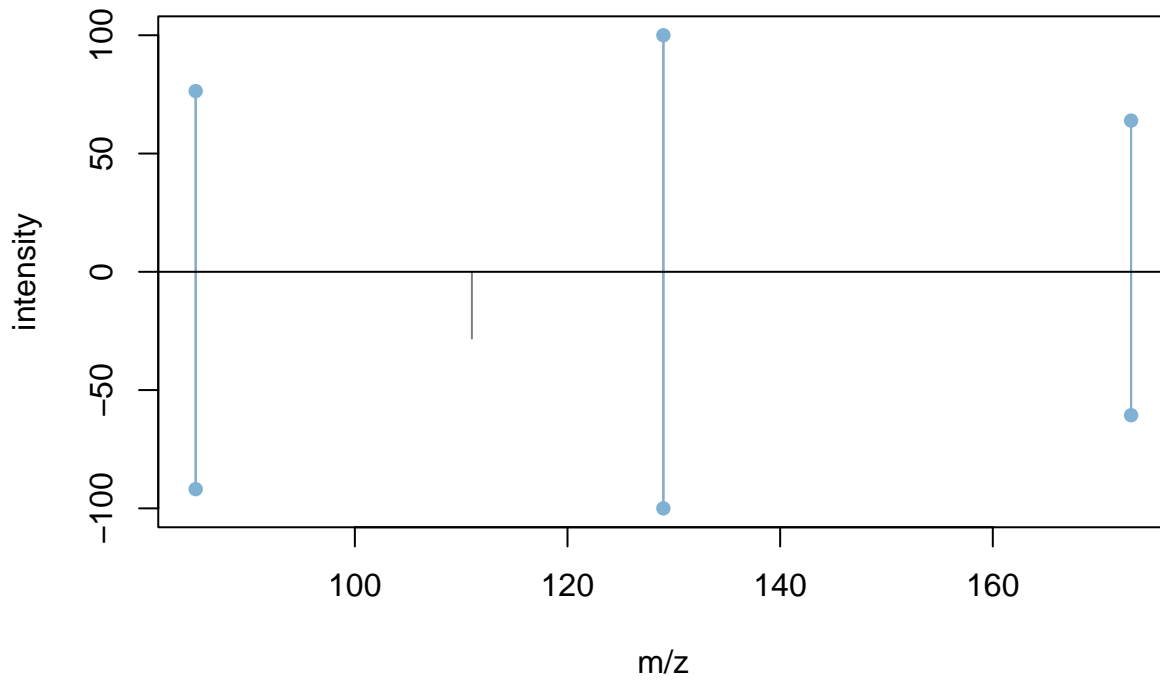
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6O6/c7-4(8)1-3(6(11)12)2-5(9)10/h1H,2H2,(H,7,8)(H,9,10)(H,11,12)/b3-1-
inchikey	GTZCVFVGUGFEME-IWQZZHSRSA-N	GTZCVFVGUGFEME-IWQZZHSRSA-N
smiles	[H]C(C(=O)O)=C(C(=O)O)CC(=O)O	[H]C(C(=O)O)=C(C(=O)O)CC(=O)O
formula	C6H6O6	C6H6O6

Retention time match

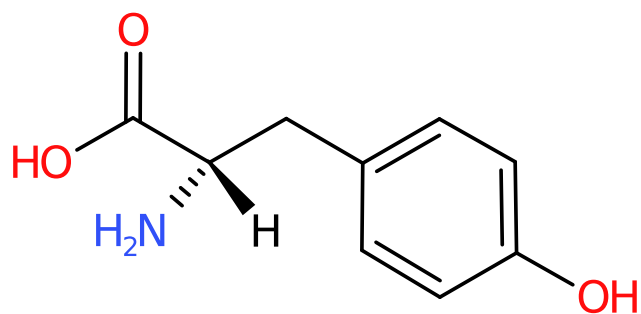
	DB	hit	error	rel. error	pcgroup
Retention time	0.84	0.77	-0.07	-8.8%	33

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0299	91.9			85.0285	76.4
111.0067	28.3		[M-H-H ₂ O-CO ₂]-	✘	✘
129.0170	100.0		[M-H-CO ₂]-	129.0183	100.0
173.0098	60.6		[M-H]-	173.0073	63.9

Tyrosine



User identifiers

localidentifier	602
dataOrigin	20190723Q-035.mzML
CAS	60-18-4
inchi	InChI=1S/C9H11NO3/c10-8(9(12)13)5-6-1-3-7(11)4-2-6/h1-4,8,11H,5,10H2,(H,12,13)/t8-/m0/s1

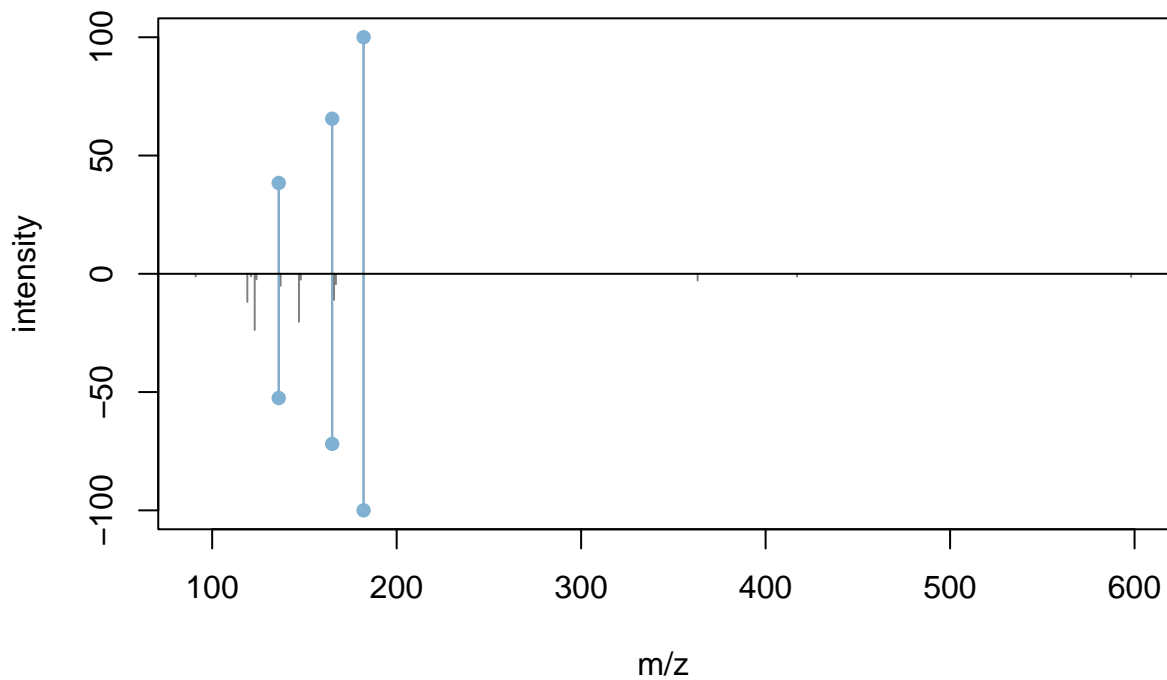
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H11NO3/c10-8(9(12)13)5-6-1-3-7(11)4-2-6/h1-4,8,11H,5,10H2,(H,12,13)/t8-/m0/s1
inchikey	OUYCCASQSFEME-QMMMGPBSA-N	OUYCCASQSFEME-QMMMGPBSA-N
smiles	[H]C(N)(C(=O)O)CC1=CC=C(O)C=C1	[H]C(N)(C(=O)O)CC1=CC=C(O)C=C1
formula	C9H11NO3	C9H11NO3

Retention time match

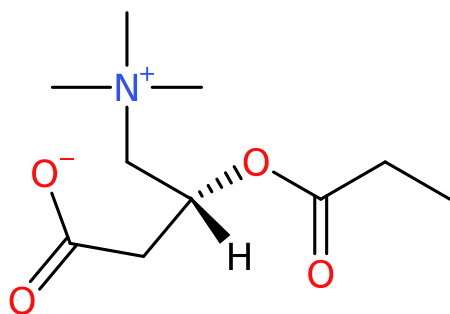
	DB	hit	error	rel. error	pcgroup
Retention time	0.84	0.78	-0.06	-6.8%	50

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
91.0554	1.1		[M+H-NH3-CO2-CH2O]+	✗	✗
119.0492	11.9		[M+H-NH3-HCOOH]+	✗	✗
121.0620	1.1		[M+H-NH3-CO2]+	✗	✗
123.0439	23.8		[M+H-NH3-COCH2]+	✗	✗
124.0505	2.3			✗	✗
136.0744	52.5		[M+H-HCOOH]+	136.0756	38.4
137.0796	5.1			✗	✗
147.0450	20.3	[M]+	[M+H-NH3-H2O]+	✗	✗
148.0492	2.5	[M+1]+		✗	✗
165.0554	71.9		[M+H-NH3]+	165.0542	65.6
166.0584	11.0	[M]+		✗	✗
167.0637	4.4	[M+1]+		✗	✗
182.0824	100.0		[M+H]+	182.0803	100.0
363.1564	2.8		[2M+H]+	✗	✗
417.0660	1.2			✗	✗
598.1419	1.4			✗	✗

propionyl-L-carnitine



User identifiers

localidentifier	622
dataOrigin	20190723Q-055.mzML
CAS	20064-19-1
inchi	InChI=1S/C10H19NO4/c1-5-10(14)15-8(6-9(12)13)7-11(2,3)4/h8H,5-7H2,1-4H3/t8-/m1/s1

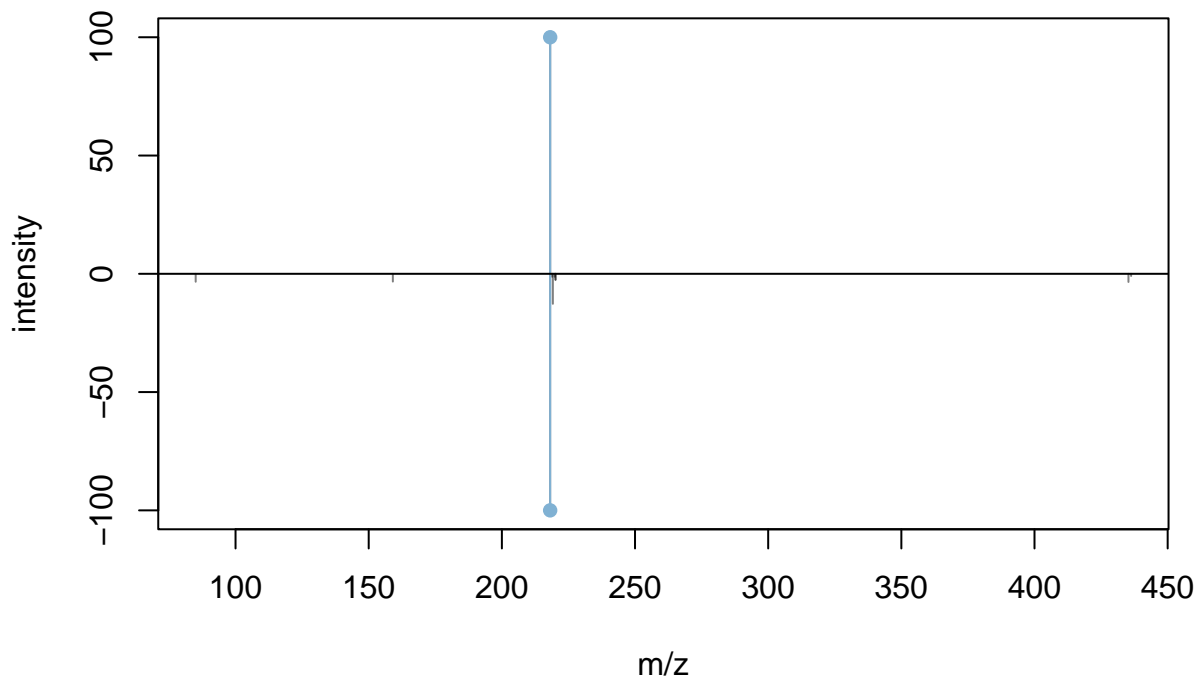
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C10H19NO4/c1-5-10(14)15-8(6-9(12)13)7-11(2,3)4/h8H,5-7H2,1-4H3/t8-/m1/s1
inchikey	UFAHZIUFPNSHSL-MRVPVSSYSA-N	UFAHZIUFPNSHSL-MRVPVSSYSA-N
smiles	[H]C(OC(=O)CC)(CC(=O)[O-])C[N+](C)(C)C	[H]C(OC(=O)CC)(CC(=O)[O-])C[N+](C)(C)C
formula	C10H19NO4	C10H19NO4

Retention time match

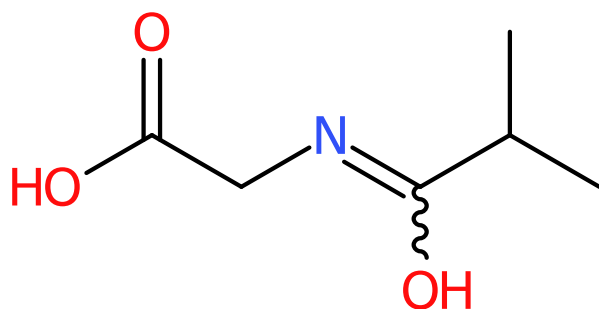
	DB	hit	error	rel. error	pcgroup
Retention time	0.94	0.99	0.04	4.5%	79

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0276	3.4			✗	✗
159.0667	3.3		[M+H-C ₃ H ₉ N] ⁺	✗	✗
218.1378	100.0	[M] ⁺	[M+H] ⁺	218.1386	100.0
218.8906	1.3			✗	✗
219.1464	12.7	[M+1] ⁺		✗	✗
219.8869	1.3			✗	✗
220.1370	2.5	[M+2] ⁺		✗	✗
220.1492	2.5			✗	✗
435.2728	3.5	[M] ⁺	[2M+H] ⁺	✗	✗
436.2805	0.9	[M+1] ⁺		✗	✗

N-Isobutyrylglycine



User identifiers

localidentifier	617
dataOrigin	20190723Q-157.mzML
CAS	15926-18-8
inchi	InChI=1S/C6H11NO3/c1-4(2)6(10)7-3-5(8)9/h4H,3H2,1-2H3,(H,7,10)(H,8,9)

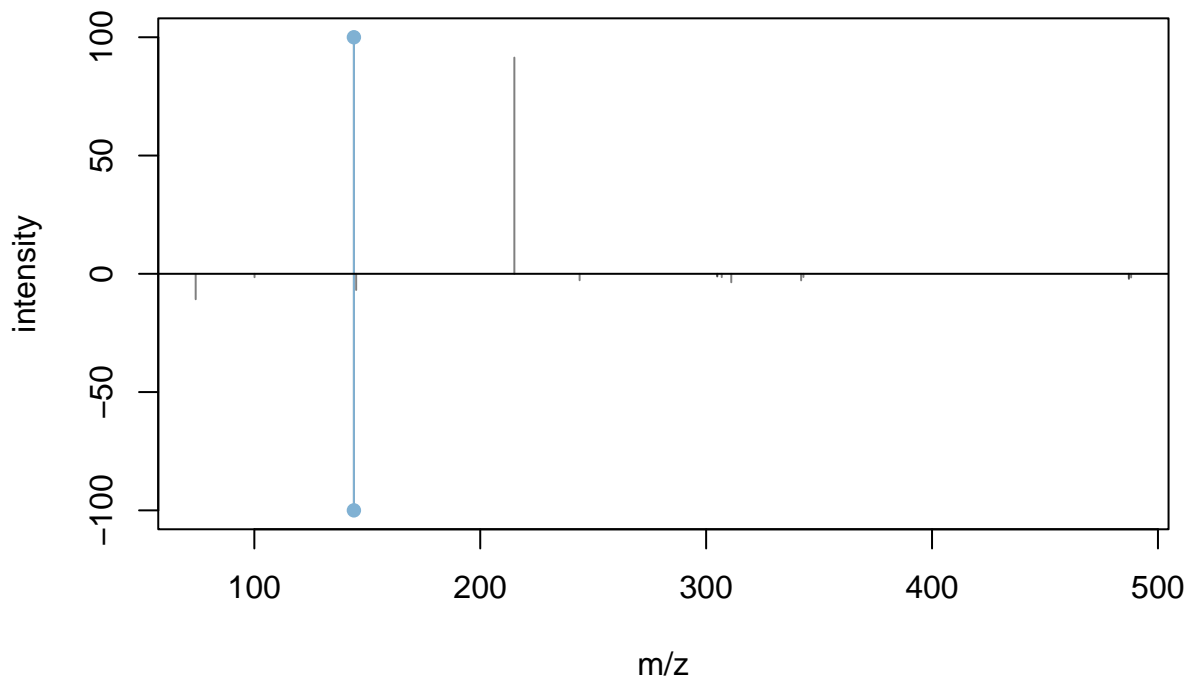
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H11NO3/c1-4(2)6(10)7-3-5(8)9/h4H,3H2,1-2H3,(H,7,10)(H,8,9)
inchikey	DCICDMMXFIELDF-UHFFFAOYSA-N	DCICDMMXFIELDF-UHFFFAOYSA-N
smiles	O=C(O)CN=C(O)C(C)C	O=C(O)CN=C(O)C(C)C
formula	C6H11NO3	C6H11NO3

Retention time match

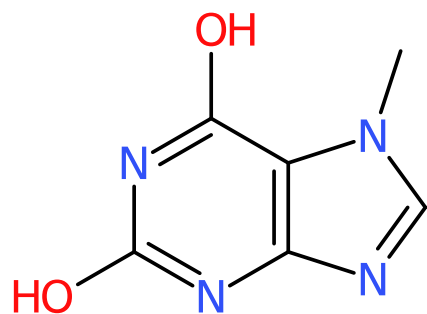
	DB	hit	error	rel. error	pcgroup
Retention time	1.37	1.06	-0.31	-22.5%	160

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
74.0263	10.8		[M-H-C4H6O]-	✗	✗
100.0762	1.4		[M-H-CO2]-	✗	✗
144.0664	100.0	[M] ⁺	[M-H] ⁻	144.0658	100.0
145.0688	6.8	[M+1] ⁺		✗	✗
✗	✗			215.1032	91.4
243.9908	2.7			✗	✗
304.9039	1.2			✗	✗
304.9063	1.0			✗	✗
306.9062	1.4			✗	✗
311.1245	3.6		[2M-2H+Na]-	✗	✗
342.0525	2.8		[2M-4H+Fe3+] ⁻	✗	✗
343.0621	1.3		[2M-3H+Fe2+] ⁻	✗	✗
487.1306	1.8		[3M-4H+Fe3+] ⁻	✗	✗
487.1330	2.2		[3M-4H+Fe3+] ⁻	✗	✗
488.1299	1.5		[3M-3H+Fe2+] ⁻	✗	✗

7-Methylxanthine



User identifiers

localidentifier	256
dataOrigin	20190701Q-182.mzML
CAS	552-62-5
inchi	InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)

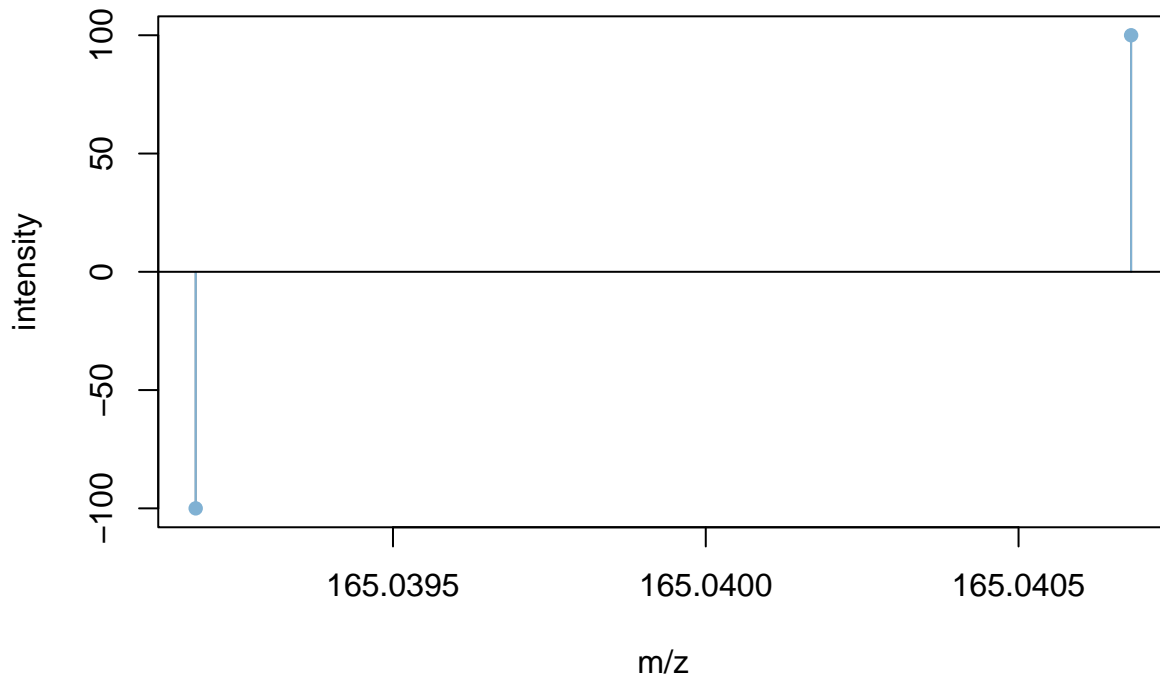
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
inchikey	PFWLFWPASULGAN-UHFFFAOYSA-N	PFWLFWPASULGAN-UHFFFAOYSA-N
smiles	OC=1N=C(O)C2=C(N=CN2C)N1	OC=1N=C(O)C2=C(N=CN2C)N1
formula	C6H6N4O2	C6H6N4O2

Retention time match

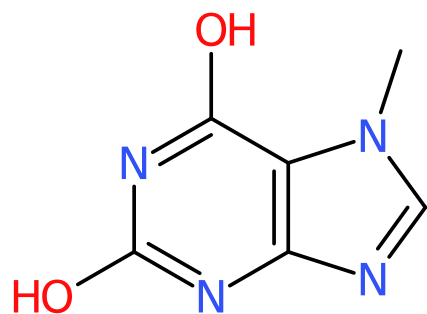
	DB	hit	error	rel. error	pcgroup
Retention time	1.50	1.49	-0.01	-0.8%	31

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
165.0392	100.0		[M-H]-	165.0407	100.0

7-Methylxanthine



User identifiers

localidentifier	256
dataOrigin	20190701Q-075.mzML
CAS	552-62-5
inchi	InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)

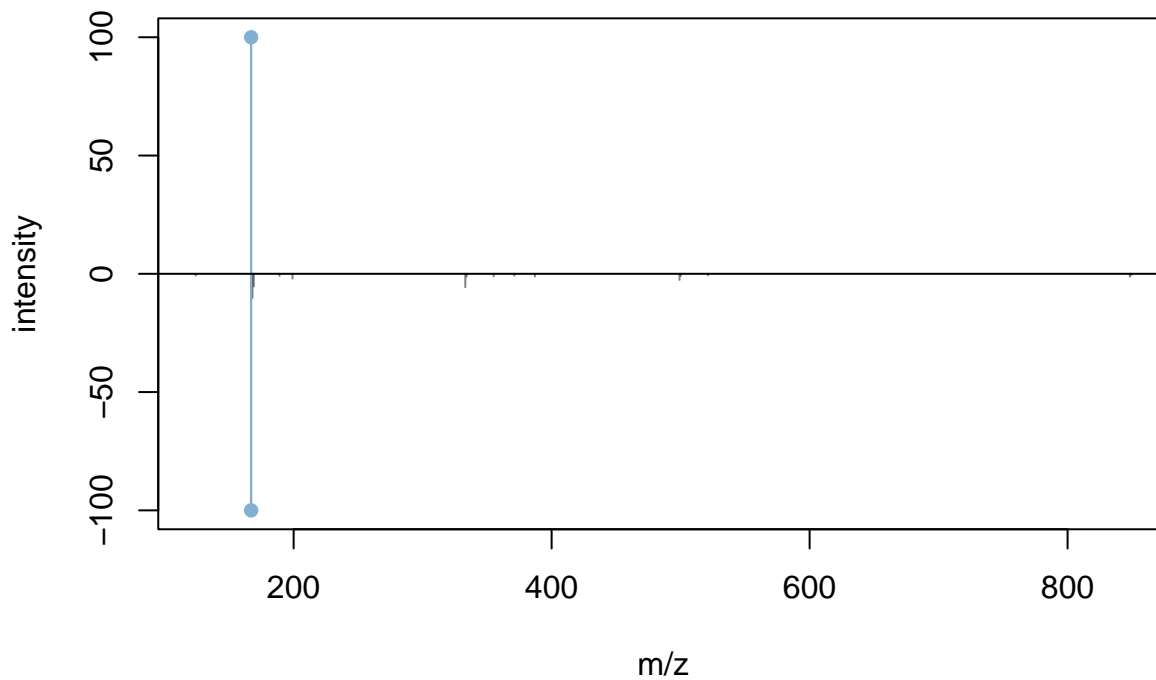
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
inchikey	PFWLFWPASULGAN-UHFFFAOYSA-N	PFWLFWPASULGAN-UHFFFAOYSA-N
smiles	OC=1N=C(O)C2=C(N=CN2C)N1	OC=1N=C(O)C2=C(N=CN2C)N1
formula	C6H6N4O2	C6H6N4O2

Retention time match

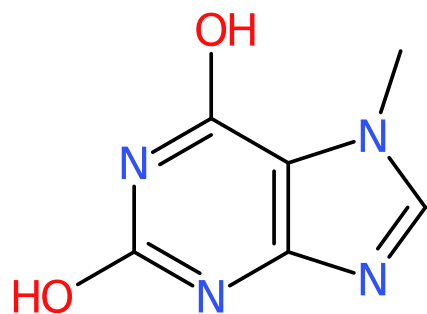
	DB	hit	error	rel. error	pcgroup
Retention time	1.45	1.48	0.04	2.6%	12

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
124.0500	0.8			✗	✗
167.0570	100.0	[M] ⁺	[M+H] ⁺	167.0561	100.0
168.0605	10.2	[M+1] ⁺		✗	✗
169.0749	5.3	[M+2] ⁺		✗	✗
189.0368	0.9		[M+Na] ⁺	✗	✗
199.0860	2.0			✗	✗
333.1055	5.7	[M] ⁺	[2M+H] ⁺	✗	✗
334.1093	1.2	[M+1] ⁺		✗	✗
355.0941	1.0		[2M+Na] ⁺	✗	✗
371.0525	0.8		[2M+K] ⁺	✗	✗
387.0207	1.1			✗	✗
499.1599	2.6	[M] ⁺	[3M+H] ⁺	✗	✗
500.1619	0.9	[M+1] ⁺		✗	✗
521.1400	0.6		[3M+Na] ⁺	✗	✗
848.2678	1.3	[M] ⁺		✗	✗
849.2600	0.5	[M+1] ⁺		✗	✗

7-Methylxanthine



User identifiers

localidentifier	256
dataOrigin	20190701Q-075.mzML
CAS	552-62-5
inchi	InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)

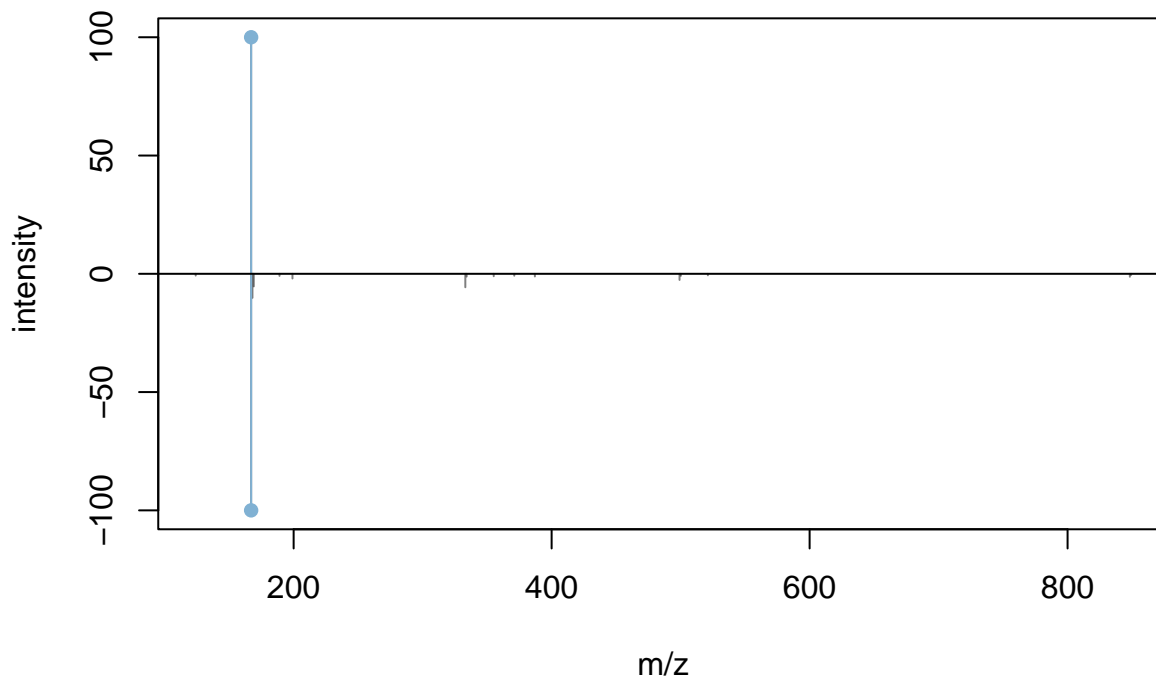
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
inchikey	PFWLFWPASULGAN-UHFFFAOYSA-N	PFWLFWPASULGAN-UHFFFAOYSA-N
smiles	OC=1N=C(O)C2=C(N=CN2C)N1	OC=1N=C(O)C2=C(N=CN2C)N1
formula	C6H6N4O2	C6H6N4O2

Retention time match

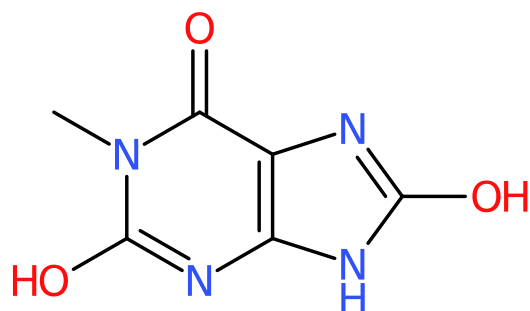
	DB	hit	error	rel. error	pcgroup
Retention time	1.45	1.16	-0.29	-19.7%	25

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
124.0500	0.8			✗	✗
167.0570	100.0	[M] ⁺	[M+H] ⁺	167.0557	100.0
168.0605	10.2	[M+1] ⁺		✗	✗
169.0749	5.3	[M+2] ⁺		✗	✗
189.0368	0.9		[M+Na] ⁺	✗	✗
199.0860	2.0			✗	✗
333.1055	5.7	[M] ⁺	[2M+H] ⁺	✗	✗
334.1093	1.2	[M+1] ⁺		✗	✗
355.0941	1.0		[2M+Na] ⁺	✗	✗
371.0525	0.8		[2M+K] ⁺	✗	✗
387.0207	1.1			✗	✗
499.1599	2.6	[M] ⁺	[3M+H] ⁺	✗	✗
500.1619	0.9	[M+1] ⁺		✗	✗
521.1400	0.6		[3M+Na] ⁺	✗	✗
848.2678	1.3	[M] ⁺		✗	✗
849.2600	0.5	[M+1] ⁺		✗	✗

1-Metyluric acid



User identifiers

localidentifier	148
dataOrigin	14062019Q-059.mzML
CAS	708-79-2
inchi	InChI=1S/C6H6N4O3/c1-10-4(11)2-3(9-6(10)13)8-5(12)7-2/h1H3,(H,9,13)(H2,7,8,12)

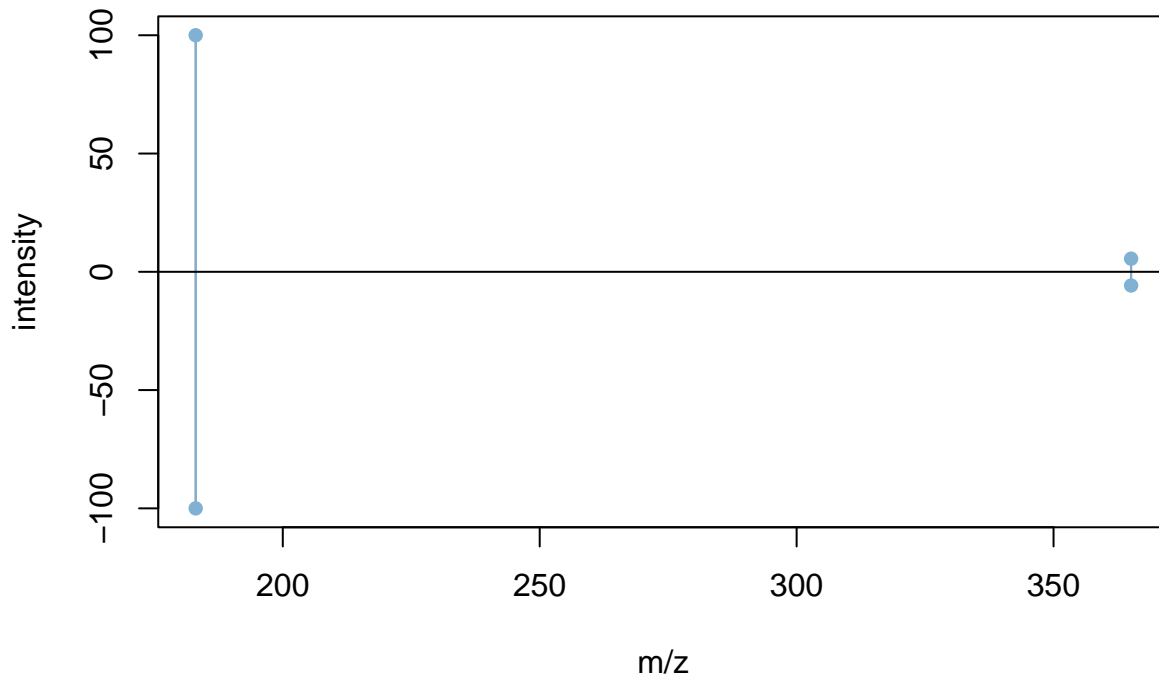
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O3/c1-10-4(11)2-3(9-6(10)13)8-5(12)7-2/h1H3,(H,9,13)(H2,7,8,12)
inchikey	QFDRTQONISXGJA-UHFFFAOYSA-N	QFDRTQONISXGJA-UHFFFAOYSA-N
smiles	O=C1C=2N=C(O)NC2N=C(O)N1C	O=C1C=2N=C(O)NC2N=C(O)N1C
formula	C6H6N4O3	C6H6N4O3

Retention time match

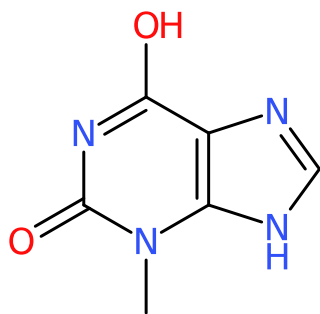
	DB	hit	error	rel. error	pcgroup
Retention time	1.57	1.18	-0.39	-24.8%	48

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
183.0501	100.0		[M+H] ⁺	183.0502	100.0
365.0975	5.8		[2M+H] ⁺	365.0958	5.5

3-Methylxanthine



User identifiers

localidentifier	210
dataOrigin	20190701Q-132.mzML
CAS	1076-22-8
inchi	InChI=1S/C6H6N4O2/c1-10-4-3(7-2-8-4)5(11)9-6(10)12/h2H,1H3,(H,7,8)(H,9,11,12)

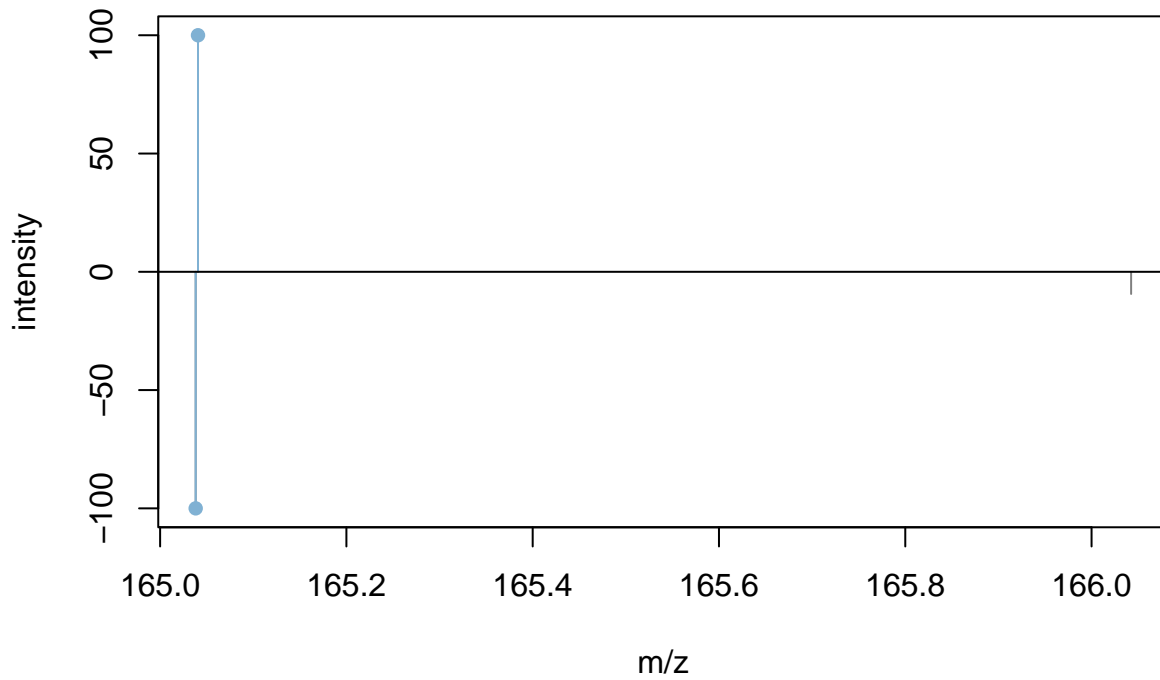
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O2/c1-10-4-3(7-2-8-4)5(11)9-6(10)12/h2H,1H3,(H,7,8)(H,9,11,12)
inchikey	GMSNIKWVOQH ZGF-UHFFFAOYSA-N	GMSNIKWVOQH ZGF-UHFFFAOYSA-N
smiles	O=C1N=C(O)C=2N=CNC2N1C	O=C1N=C(O)C=2N=CNC2N1C
formula	C6H6N4O2	C6H6N4O2

Retention time match

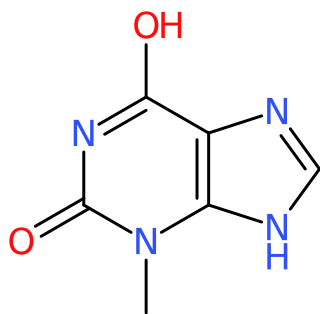
	DB	hit	error	rel. error	pcgroup
Retention time	1.61	1.49	-0.12	-7.6%	31

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
165.0382	100.0	[M] ⁺	[M-H] ⁻	165.0407	100.0
166.0425	9.4	[M+1] ⁺		✗	✗

3-Methylxanthine



User identifiers

localidentifier	211
dataOrigin	20190701Q-133.mzML
CAS	1076-22-8
inchi	InChI=1S/C6H6N4O2/c1-10-4-3(7-2-8-4)5(11)9-6(10)12/h2H,1H3,(H,7,8)(H,9,11,12)

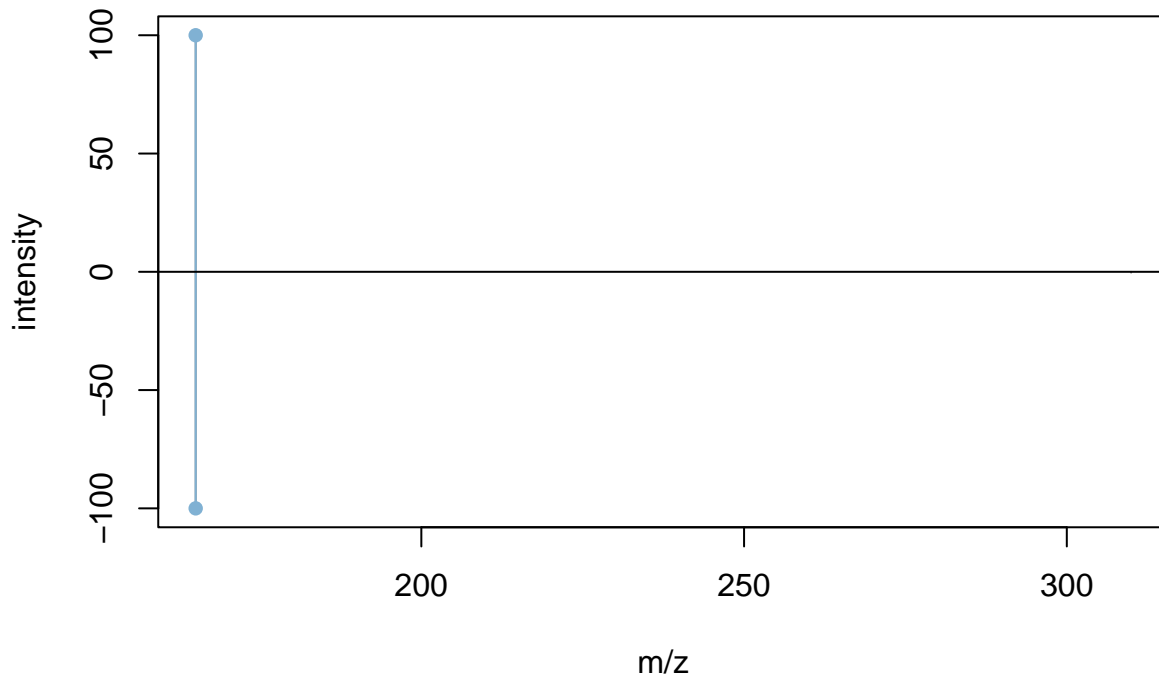
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C6H6N4O2/c1-10-4-3(7-2-8-4)5(11)9-6(10)12/h2H,1H3,(H,7,8)(H,9,11,12)
inchikey	GMSNIKWVOQHZGF-UHFFFAOYSA-N	GMSNIKWVOQHZGF-UHFFFAOYSA-N
smiles	O=C1N=C(O)C=2N=CNC2N1C	O=C1N=C(O)C=2N=CNC2N1C
formula	C6H6N4O2	C6H6N4O2

Retention time match

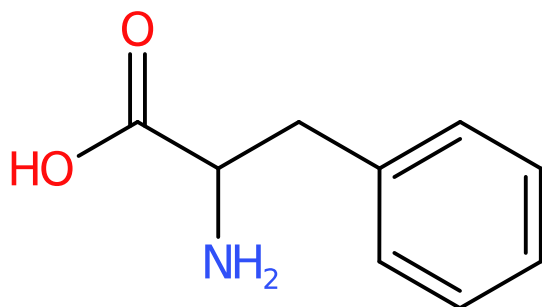
	DB	hit	error	rel. error	pcgroup
Retention time	1.62	1.49	-0.13	-7.8%	31

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
165.0408	100.0		[M-H]-	165.0407	100.0
309.9659	0.3			×	×

L-Phenylalanine



User identifiers

localidentifier	92
dataOrigin	12062019Q-120.mzML
CAS	63-91-2
inchi	InChI=1S/C9H11NO2/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5,8H,6,10H2,(H,11,12)

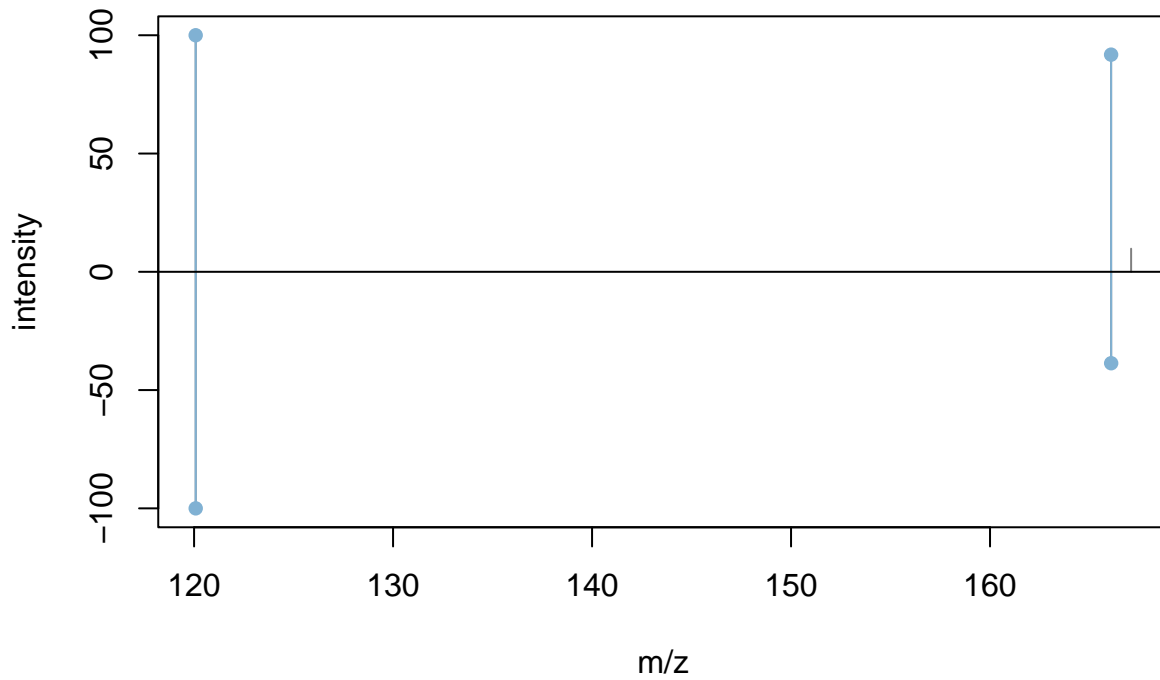
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H11NO2/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5,8H,6,10H2,(H,11,12)
inchikey	COLNVLDHVKWLRT-UHFFFAOYSA-N	COLNVLDHVKWLRT-UHFFFAOYSA-N
smiles	O=C(O)C(N)CC=1C=CC=CC1	O=C(O)C(N)CC=1C=CC=CC1
formula	C9H11NO2	C9H11NO2

Retention time match

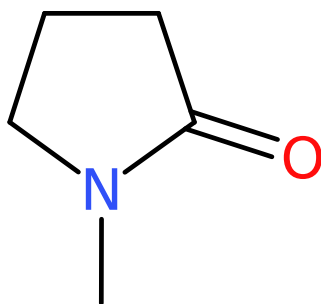
	DB	hit	error	rel. error	pcgroup
Retention time	1.57	1.60	0.03	2.0%	22

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
120.0819	100.0		[M+H-HCOOH] ⁺	120.0802	100.0
166.0876	38.6		[M+H] ⁺	166.0853	91.8
✘	✘			167.0906	9.8

Methyl-2-pyrrolidone



User identifiers

localidentifier	475
dataOrigin	20190715Q-104.mzML
CAS	872-50-4
inchi	InChI=1S/C5H9NO/c1-6-4-2-3-5(6)7/h2-4H2,1H3

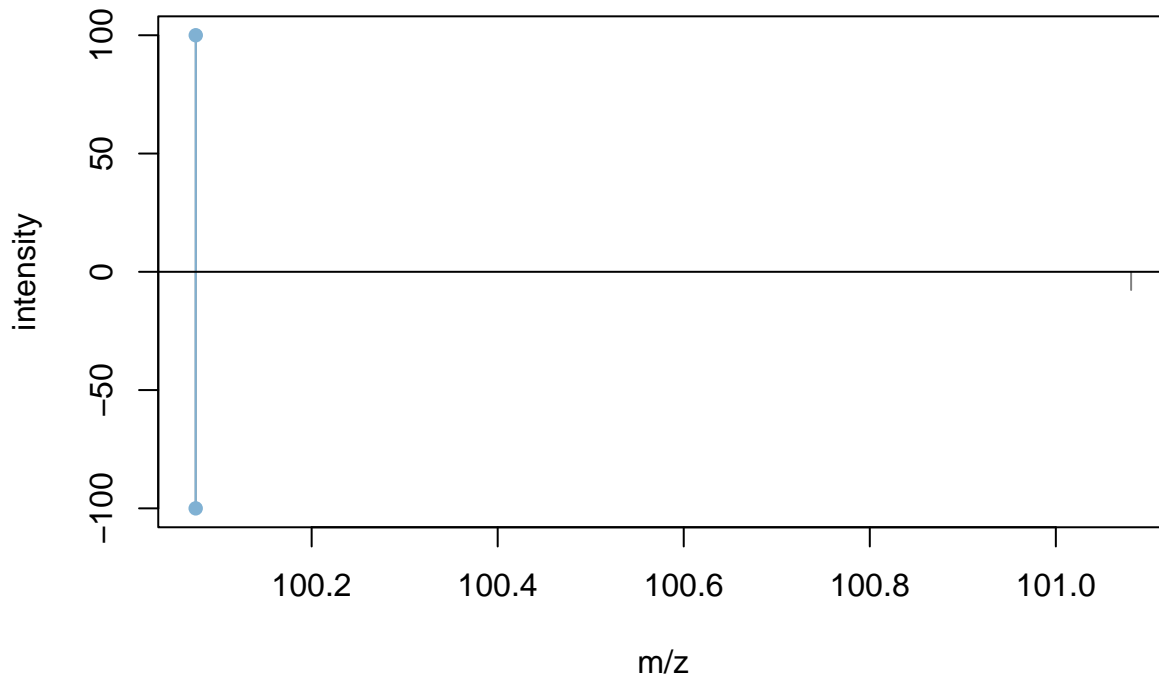
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C5H9NO/c1-6-4-2-3-5(6)7/h2-4H2,1H3
inchikey	SECXISVLQFMRJM-UHFFFAOYSA-N	SECXISVLQFMRJM-UHFFFAOYSA-N
smiles	O=C1N(C)CCC1	O=C1N(C)CCC1
formula	C5H9NO	C5H9NO

Retention time match

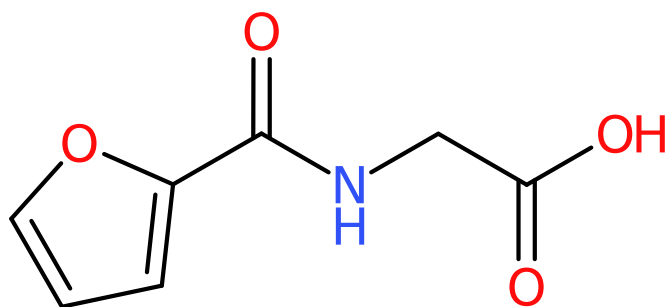
	DB	hit	error	rel. error	pcgroup
Retention time	1.68	1.84	0.16	9.6%	142

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
100.0753	100.0	[M] ⁺	[M+H] ⁺	100.0754	100.0
101.0809	7.7	[M+1] ⁺		✗	✗

2-Furoylglycine



User identifiers

localidentifier	2
dataOrigin	12062019Q-131.mzML
CAS	5657-19-2
inchi	InChI=1S/C7H7NO4/c9-6(10)4-8-7(11)5-2-1-3-12-5/h1-3H,4H2,(H,8,11)(H,9,10)

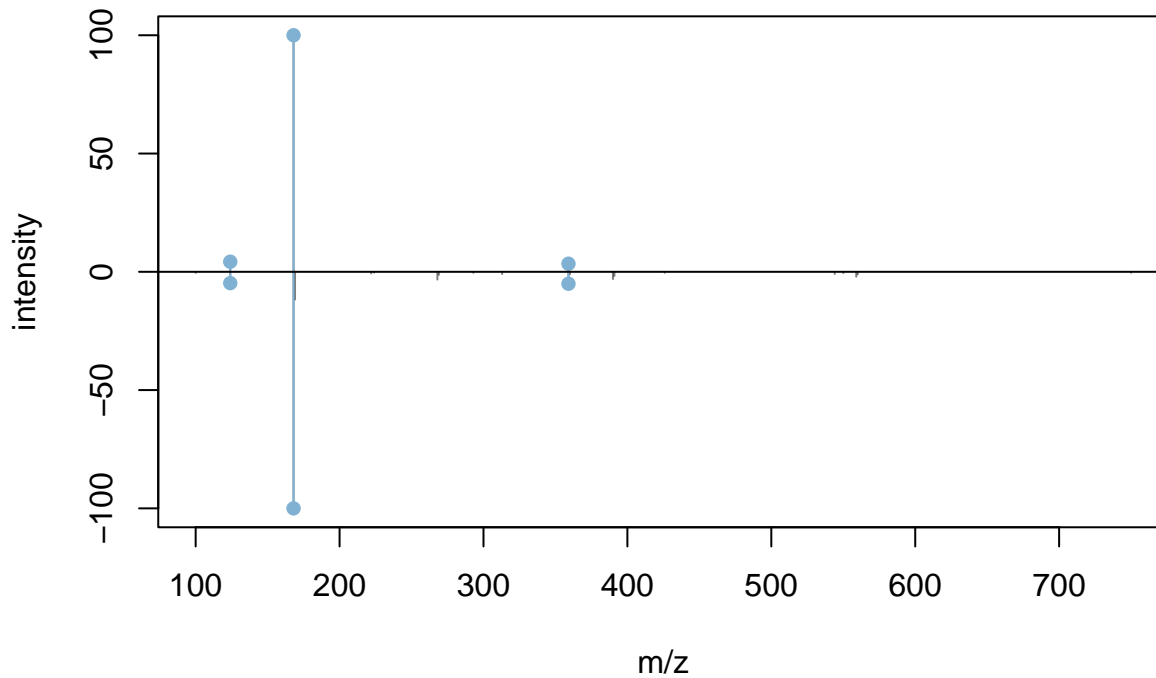
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H7NO4/c9-6(10)4-8-7(11)5-2-1-3-12-5/h1-3H,4H2,(H,8,11)(H,9,10)
inchikey	KSPQDMRTZZYQLM-UHFFFAOYSA-N	KSPQDMRTZZYQLM-UHFFFAOYSA-N
smiles	O=C(O)CNC(=O)C=1OC=CC1	O=C(O)CNC(=O)C=1OC=CC1
formula	C7H7NO4	C7H7NO4

Retention time match

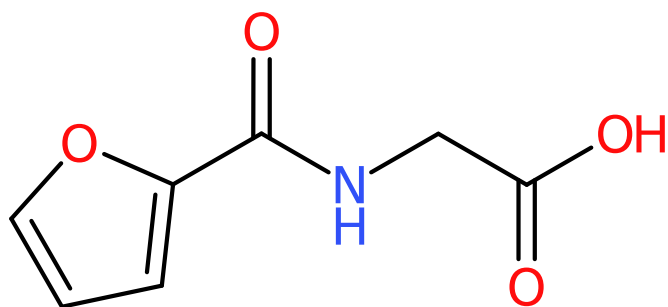
	DB	hit	error	rel. error	pcgroup
Retention time	1.78	1.89	0.11	6.3%	23

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
100.0037	0.5			✗	✗
124.0414	4.8		[M-H-CO ₂]-	124.0409	4.3
168.0297	100.0	[M] ⁺	[M-H]-	168.0299	100.0
169.0326	11.8	[M+1] ⁺		✗	✗
221.9514	0.7			✗	✗
223.9661	0.4			✗	✗
267.9556	3.3			✗	✗
268.9576	1.3			✗	✗
292.8997	0.4			✗	✗
312.9542	0.9			✗	✗
359.0534	5.0	[M] ⁺	[2M-2H+Na]-	359.0516	3.4
360.0564	1.1	[M+1] ⁺		✗	✗
389.9814	3.1		[2M-4H+Fe ³⁺]-	✗	✗
390.9892	1.7		[2M-3H+Fe ²⁺]-	✗	✗
425.9562	0.4			✗	✗
544.0565	0.9		[3M-2H+K]-	✗	✗
550.0610	0.5			✗	✗
559.0166	2.1	[M] ⁺	[3M-4H+Fe ³⁺]-	✗	✗
560.0256	1.1	[M+1] ⁺		✗	✗
750.0310	0.4			✗	✗

2-Furoylglycine



User identifiers

localidentifier	2
dataOrigin	12062019Q-024.mzML
CAS	5657-19-2
inchi	InChI=1S/C7H7NO4/c9-6(10)4-8-7(11)5-2-1-3-12-5/h1-3H,4H2,(H,8,11)(H,9,10)

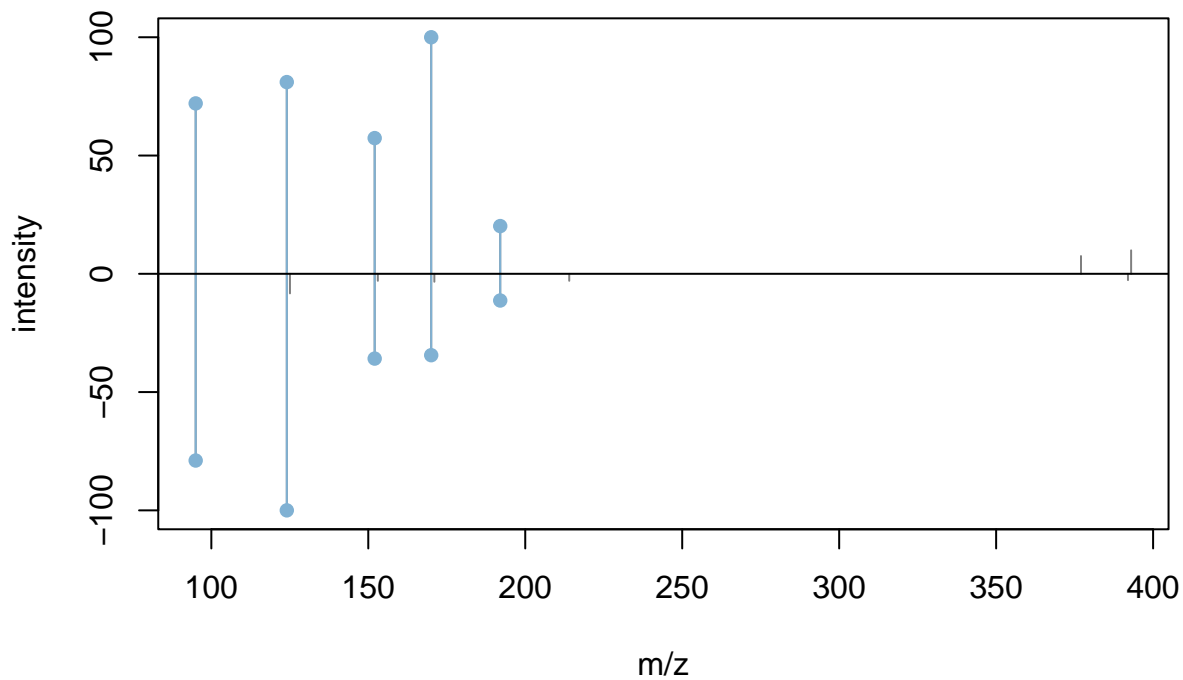
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H7NO4/c9-6(10)4-8-7(11)5-2-1-3-12-5/h1-3H,4H2,(H,8,11)(H,9,10)
inchikey	KSPQDMRTZZYQLM-UHFFFAOYSA-N	KSPQDMRTZZYQLM-UHFFFAOYSA-N
smiles	O=C(O)CNC(=O)C=1OC=CC1	O=C(O)CNC(=O)C=1OC=CC1
formula	C7H7NO4	C7H7NO4

Retention time match

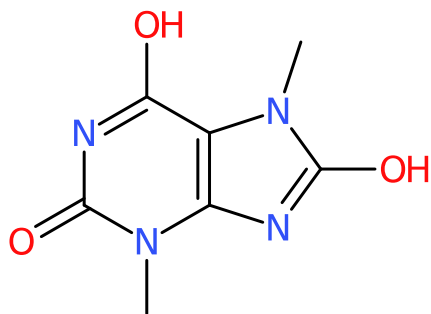
	DB	hit	error	rel. error	pcgroup
Retention time	1.78	1.89	0.11	6.1%	64

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
95.0129	78.9			95.0124	72.0
124.0398	100.0	[M] ⁺	[M+H-HCOOH] ⁺	124.0392	81.0
125.0431	8.3	[M+1] ⁺		✗	✗
152.0353	35.8	[M] ⁺	[M+H-H ₂ O] ⁺	152.0342	57.4
153.0360	3.0	[M+1] ⁺		✗	✗
170.0448	34.4	[M] ⁺	[M+H] ⁺	170.0445	100.0
171.0456	3.4	[M+1] ⁺		✗	✗
192.0288	11.3		[M+Na] ⁺	192.0275	20.2
214.0123	3.0		[M+2Na-H] ⁺	✗	✗
✗	✗			377.0300	7.5
391.9956	2.7		[2M-2H+Fe ₃] ⁺	✗	✗
✗	✗			393.0019	9.9

3,7-Dimethyluric acid



User identifiers

localidentifier	196
dataOrigin	20190701Q-118.mzML
CAS	13087-49-5
inchi	InChI=1S/C7H8N4O3/c1-10-3-4(8-6(10)13)11(2)7(14)9-5(3)12/h1-2H3,(H,8,13)(H,9,12,14)

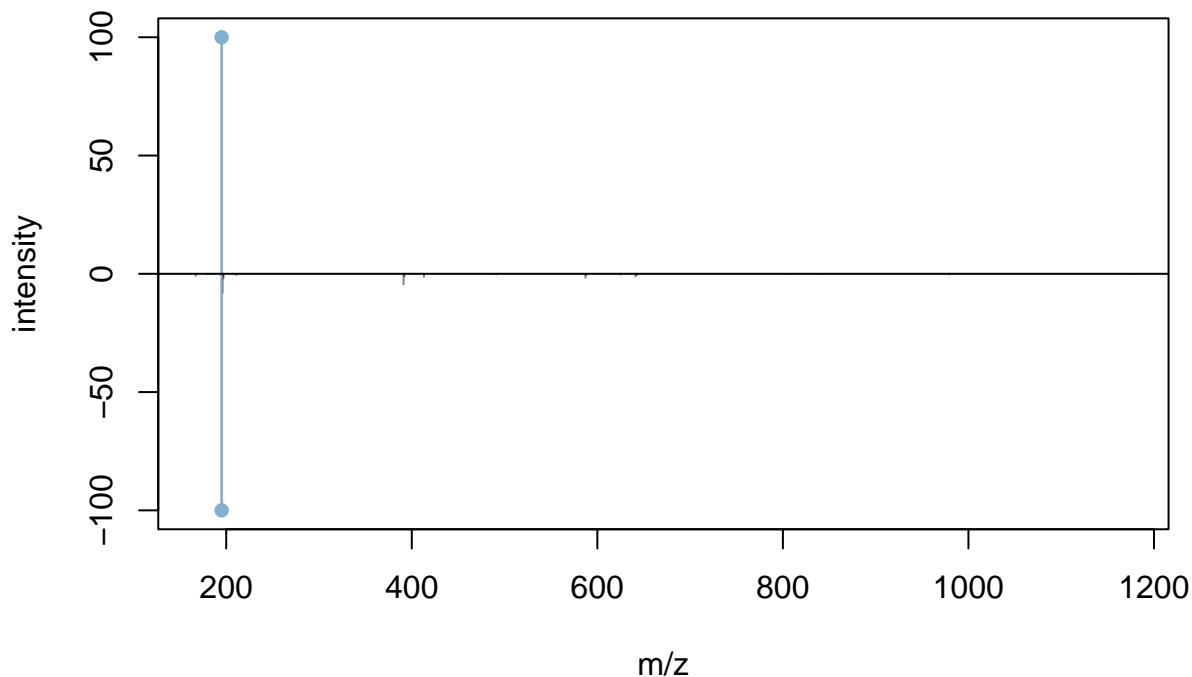
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8N4O3/c1-10-3-4(8-6(10)13)11(2)7(14)9-5(3)12/h1-2H3,(H,8,13)(H,9,12,14)
inchikey	HMLZLHKHNBLJJD-UHFFFAOYSA-N	HMLZLHKHNBLJJD-UHFFFAOYSA-N
smiles	O=C1N=C(O)C2=C(N=C(O)N2C)N1C	O=C1N=C(O)C2=C(N=C(O)N2C)N1C
formula	C7H8N4O3	C7H8N4O3

Retention time match

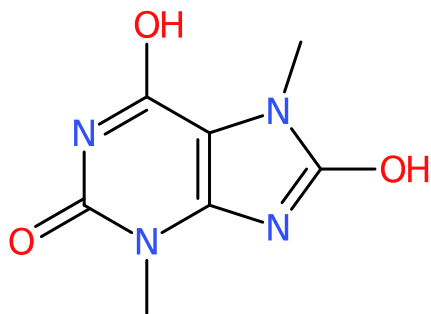
	DB	hit	error	rel. error	pcgroup
Retention time	1.67	1.92	0.24	14.4%	101

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
167.0585	0.8		[M-H-CO]-	✗	✗
180.0277	0.3			✗	✗
194.0480	0.3			✗	✗
195.0517	100.0	[M] ⁺	[M-H] ⁻	195.0508	100.0
195.7653	1.3			✗	✗
195.9022	0.6			✗	✗
195.9687	0.6			✗	✗
196.0522	8.1	[M+1] ⁺		✗	✗
196.2151	0.6			✗	✗
197.0545	1.9	[M+2] ⁺		✗	✗
211.0480	0.5			✗	✗
391.1105	4.4	[M] ⁺	[2M-H] ⁻	✗	✗
392.1151	1.0	[M+1] ⁺		✗	✗
413.1007	1.3		[2M-2H+Na] ⁻	✗	✗
491.0472	0.3			✗	✗
587.1668	1.6	[M] ⁺	[3M-H] ⁻	✗	✗
588.1673	0.6	[M+1] ⁺		✗	✗
625.1250	0.3		[3M-2H+K] ⁻	✗	✗
641.0874	1.2	[M] ⁺	[3M-3H+Fe2 ⁺] ⁻	✗	✗
642.0823	0.5	[M+1] ⁺		✗	✗
643.0828	0.4	[M+2] ⁺		✗	✗
807.1742	0.2		[4M-4H+Al3 ⁺] ⁻	✗	✗
837.1379	0.1		[4M-3H+Fe2 ⁺] ⁻	✗	✗
979.2953	0.3			✗	✗
1175.3555	0.2			✗	✗

3,7-Dimethyluric acid



User identifiers

localidentifier	196
dataOrigin	20190701Q-011.mzML
CAS	13087-49-5
inchi	InChI=1S/C7H8N4O3/c1-10-3-4(8-6(10)13)11(2)7(14)9-5(3)12/h1-2H3,(H,8,13)(H,9,12,14)

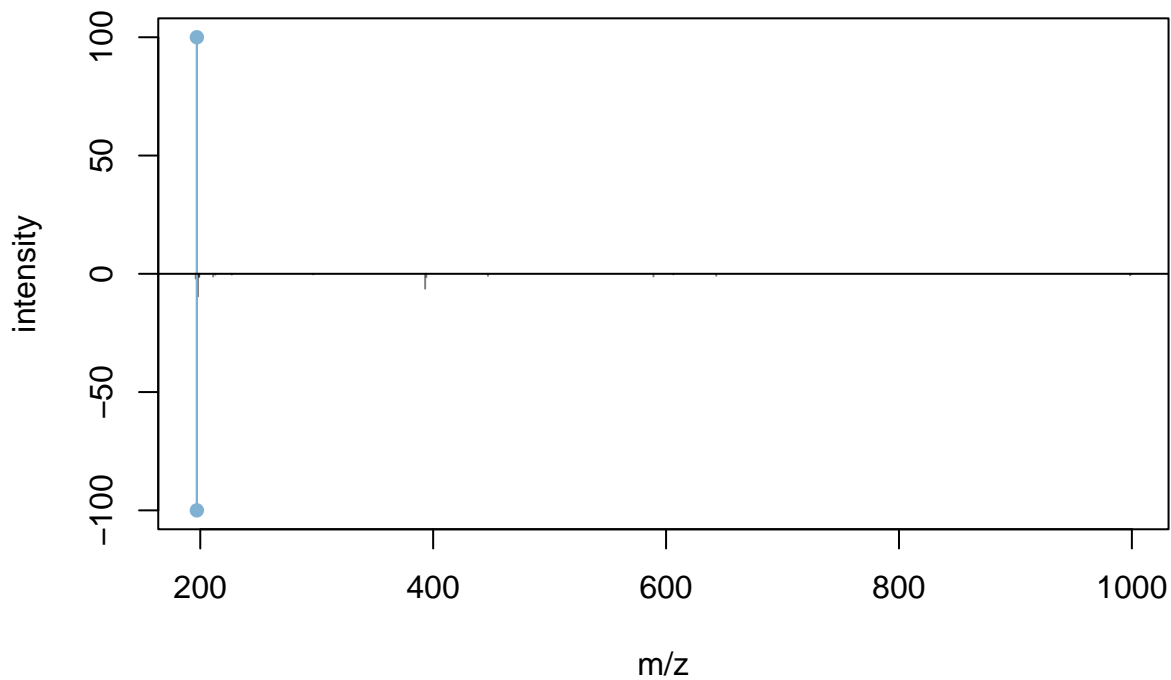
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8N4O3/c1-10-3-4(8-6(10)13)11(2)7(14)9-5(3)12/h1-2H3,(H,8,13)(H,9,12,14)
inchikey	HMLZLHKHNBLJJD-UHFFFAOYSA-N	HMLZLHKHNBLJJD-UHFFFAOYSA-N
smiles	O=C1N=C(O)C2=C(N=C(O)N2C)N1C	O=C1N=C(O)C2=C(N=C(O)N2C)N1C
formula	C7H8N4O3	C7H8N4O3

Retention time match

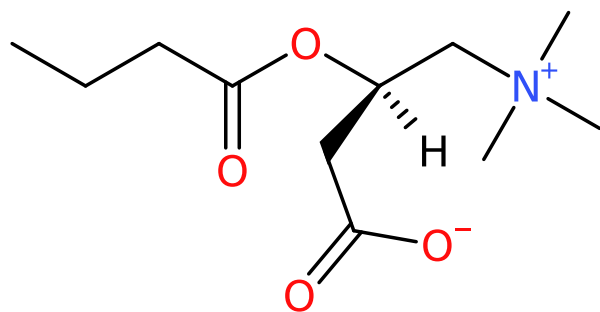
	DB	hit	error	rel. error	pcgroup
Retention time	1.71	1.91	0.20	11.8%	95

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
196.0596	2.0			✗	✗
197.0693	100.0	[M] ⁺	[M+H] ⁺	197.0668	100.0
198.0671	9.6	[M+1] ⁺		✗	✗
198.9510	1.0			✗	✗
199.0808	1.4	[M+2] ⁺		✗	✗
211.0866	1.2			✗	✗
213.0656	0.4			✗	✗
227.0789	0.4			✗	✗
296.9912	0.3			✗	✗
393.1248	6.3	[M] ⁺	[2M+H] ⁺	✗	✗
394.1294	1.4	[M+1] ⁺		✗	✗
447.0467	0.8			✗	✗
589.1823	1.1		[3M+H] ⁺	✗	✗
606.2250	0.3			✗	✗
643.1093	0.8			✗	✗
998.3433	0.6	[M] ⁺		✗	✗
999.3561	0.3	[M+1] ⁺		✗	✗

Butyrylcarnitine



User identifiers

localidentifier	35
dataOrigin	12062019Q-059.mzML
CAS	25576-40-3
inchi	InChI=1S/C11H21NO4/c1-5-6-11(15)16-9(7-10(13)14)8-12(2,3)4/h9H,5-8H2,1-4H3/t9-/m1/s1

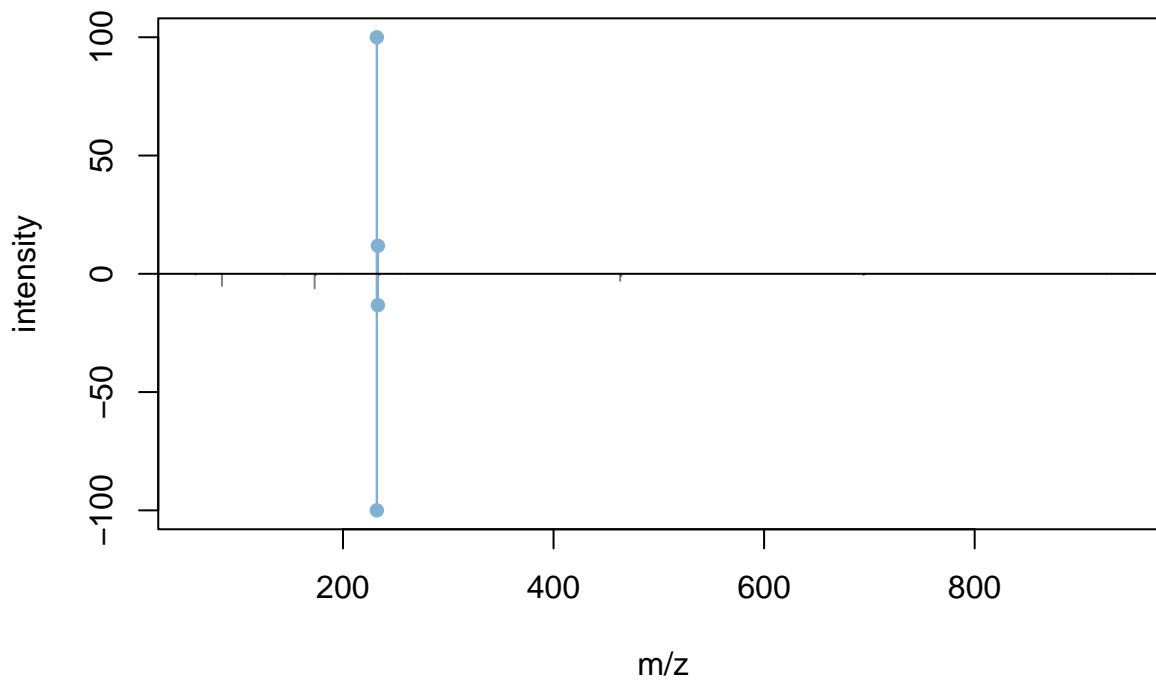
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C11H21NO4/c1-5-6-11(15)16-9(7-10(13)14)8-12(2,3)4/h9H,5-8H2,1-4H3/t9-/m1/s1
inchikey	QWYFHHGCZUCMBN-SECBINFHSA-N	QWYFHHGCZUCMBN-SECBINFHSA-N
smiles	[H]C(OC(=O)CCC)(CC(=O)[O-])C[N+](C)(C)C	[H]C(OC(=O)CCC)(CC(=O)[O-])C[N+](C)(C)C
formula	C11H21NO4	C11H21NO4

Retention time match

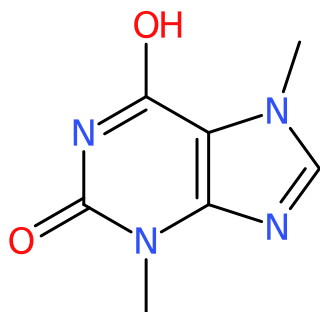
	DB	hit	error	rel. error	pcgroup
Retention time	1.79	1.95	0.16	9.1%	23

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
60.0812	0.4			✗	✗
85.0278	5.1			✗	✗
144.1017	0.2		[M+H-C4H8O2]+	✗	✗
173.0796	6.2	[M]+	[M+H-C3H9N]+	✗	✗
174.0852	0.6	[M+1]+		✗	✗
195.0650	0.1			✗	✗
232.0162	0.2			✗	✗
232.1549	100.0	[M]+	[M+H]+	232.1543	100.0
232.8848	0.4			✗	✗
233.1568	13.3	[M+1]+		233.1586	11.8
233.3313	1.5			✗	✗
233.3687	0.4			✗	✗
234.8417	0.4			✗	✗
254.1456	0.2			✗	✗
463.3007	3.0	[M]+	[2M+H]+	✗	✗
464.3104	0.8	[M+1]+		✗	✗
694.4503	0.5	[M]+	[3M+H]+	✗	✗
695.4453	0.2	[M+1]+		✗	✗
925.6074	0.1		[4M+H]+	✗	✗
948.6128	0.1			✗	✗

Theobromine



User identifiers

localidentifier	592
dataOrigin	20190723Q-023.mzML
CAS	83-67-0
inchi	InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)

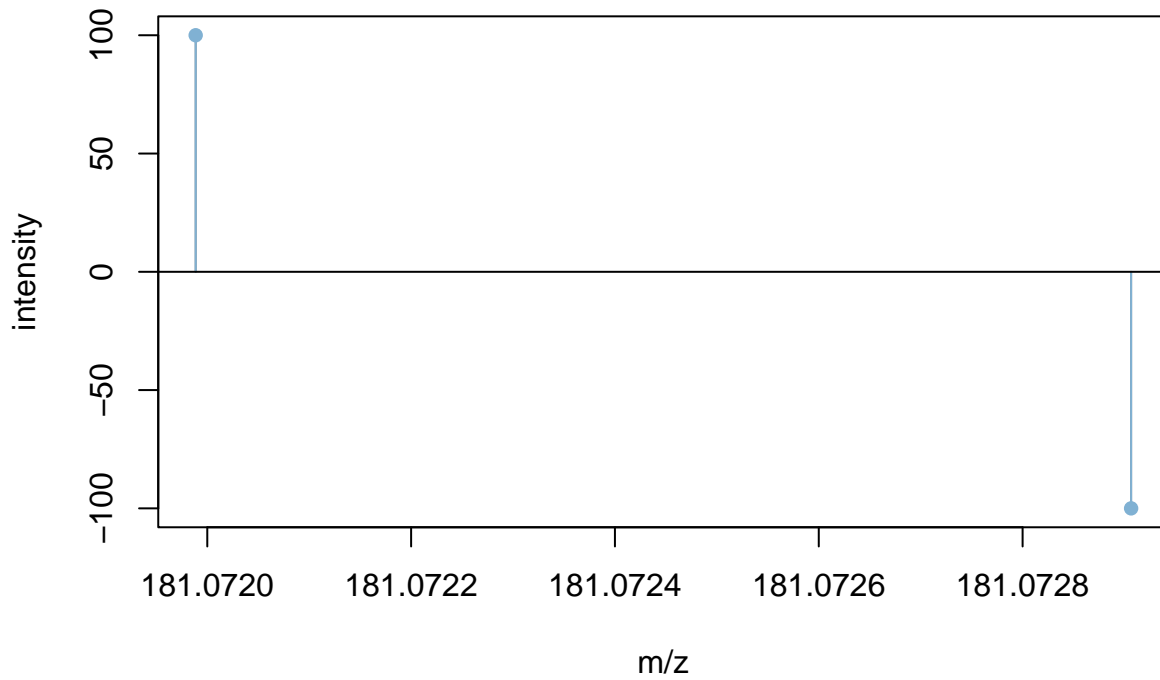
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)
inchikey	YAPQBXQYLJRXSA-UHFFFAOYSA-N	YAPQBXQYLJRXSA-UHFFFAOYSA-N
smiles	O=C1N=C(O)C2=C(N=CN2C)N1C	O=C1N=C(O)C2=C(N=CN2C)N1C
formula	C7H8N4O2	C7H8N4O2

Retention time match

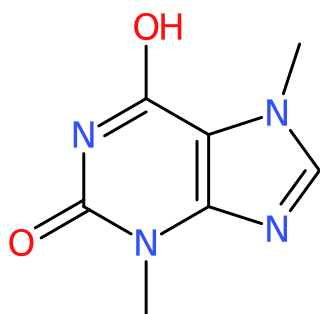
	DB	hit	error	rel. error	pcgroup
Retention time	2.21	2.52	0.30	13.8%	29

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
181.0729	100.0		[M+H] ⁺	181.0720	100.0

Theobromine



User identifiers

localidentifier	592
dataOrigin	20190723Q-023.mzML
CAS	83-67-0
inchi	InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)

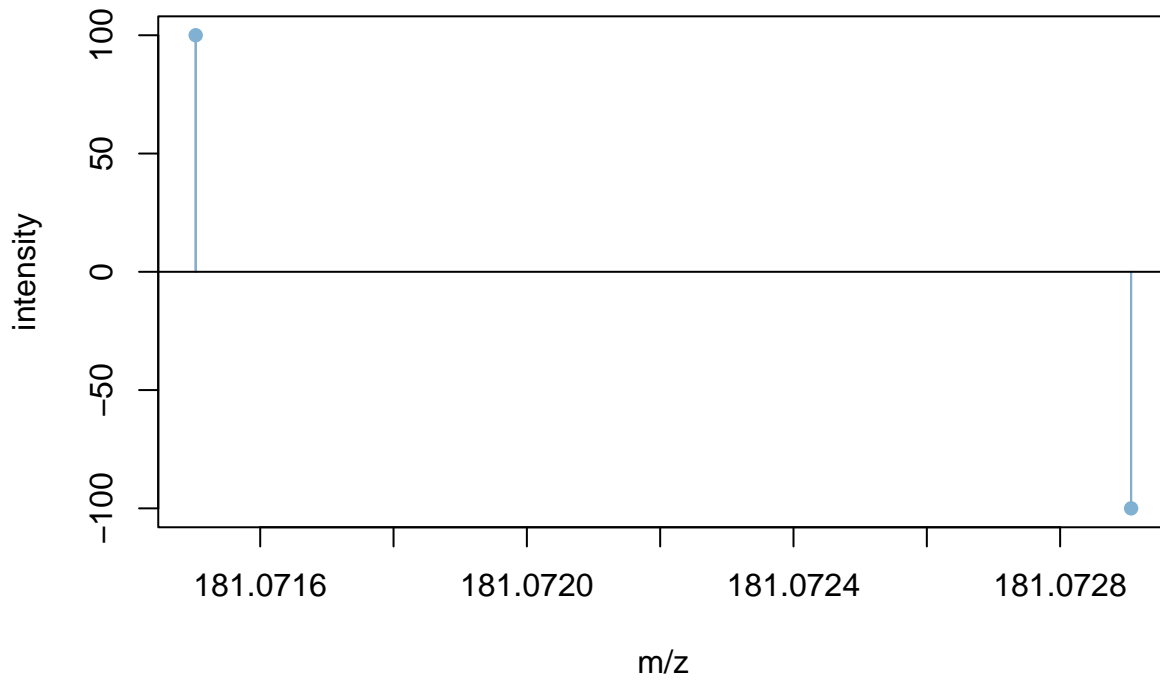
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)
inchikey	YAPQBXQYLJRXSA-UHFFFAOYSA-N	YAPQBXQYLJRXSA-UHFFFAOYSA-N
smiles	O=C1N=C(O)C2=C(N=CN2C)N1C	O=C1N=C(O)C2=C(N=CN2C)N1C
formula	C7H8N4O2	C7H8N4O2

Retention time match

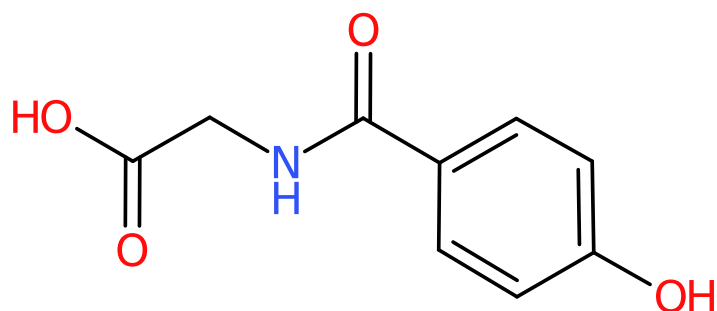
	DB	hit	error	rel. error	pcgroup
Retention time	2.21	2.04	-0.17	-7.7%	51

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
181.0729	100.0		[M+H] ⁺	181.0715	100.0

4-Hydroxy-hippuric acid



User identifiers

localidentifier	235
dataOrigin	20190701Q-159.mzML
CAS	2482-25-9
inchi	InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)

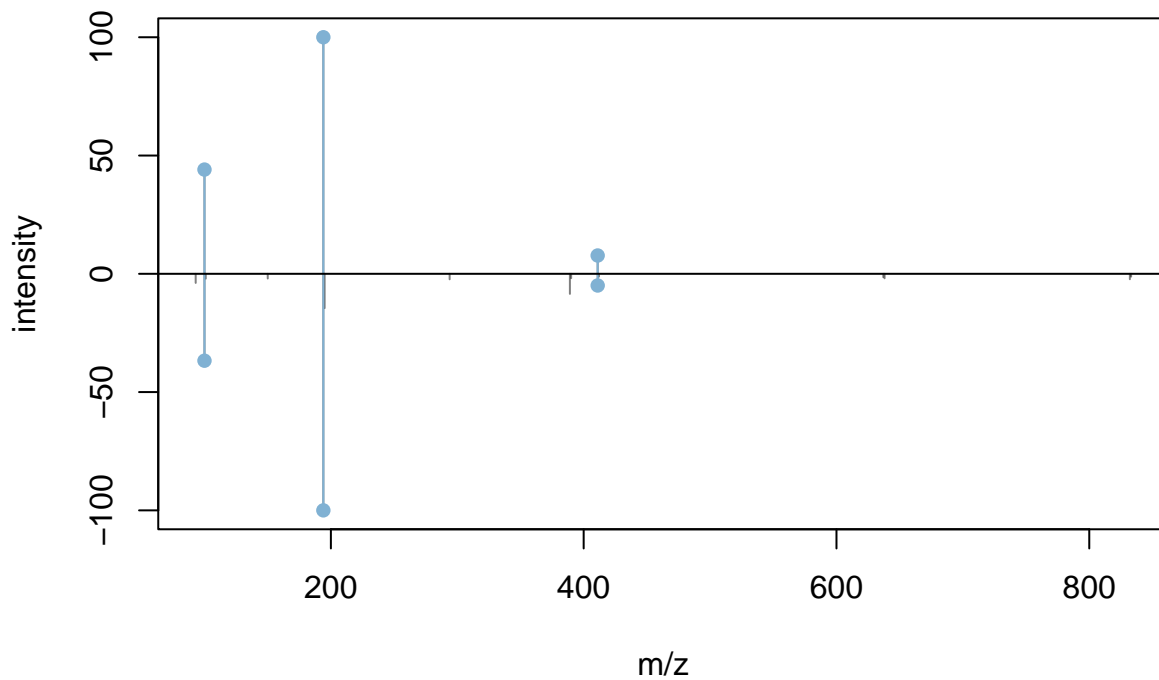
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)
inchikey	ZMHLUFWWPBTIU-UHFFFAOYSA-N	ZMHLUFWWPBTIU-UHFFFAOYSA-N
smiles	O=C(O)CNC(=O)C1=CC=C(O)C=C1	O=C(O)CNC(=O)C1=CC=C(O)C=C1
formula	C9H9NO4	C9H9NO4

Retention time match

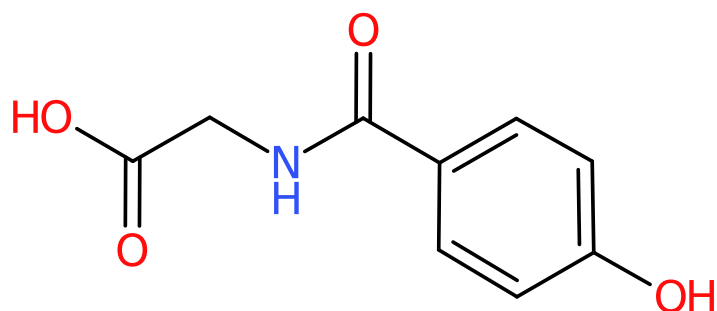
	DB	hit	error	rel. error	pcgroup
Retention time	2.10	2.08	-0.02	-1.0%	41

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
93.0347	3.9			✗	✗
100.0017	36.7	[M] ⁺		100.0034	44.1
101.0083	2.1	[M+1] ⁺		✗	✗
150.0540	2.0		[M-H-CO ₂] ⁻	✗	✗
194.0460	100.0	[M] ⁺	[M-H] ⁻	194.0443	100.0
195.0436	14.5	[M+1] ⁺		✗	✗
293.9672	2.3			✗	✗
389.0983	8.5	[M] ⁺	[2M-H] ⁻	✗	✗
390.1039	1.9	[M+1] ⁺		✗	✗
411.0845	4.9	[M] ⁺	[2M-2H+Na] ⁻	411.0815	7.7
412.0918	1.2	[M+1] ⁺		✗	✗
637.0640	1.5		[3M-4H+Fe ³⁺] ⁻	✗	✗
638.0659	1.9		[3M-3H+Fe ²⁺] ⁻	✗	✗
832.1155	2.3	[M] ⁺	[4M-4H+Fe ³⁺] ⁻	✗	✗
833.1182	1.2	[M+1] ⁺		✗	✗

4-Hydroxy-hippuric acid



User identifiers

localidentifier	235
dataOrigin	20190701Q-052.mzML
CAS	2482-25-9
inchi	InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)

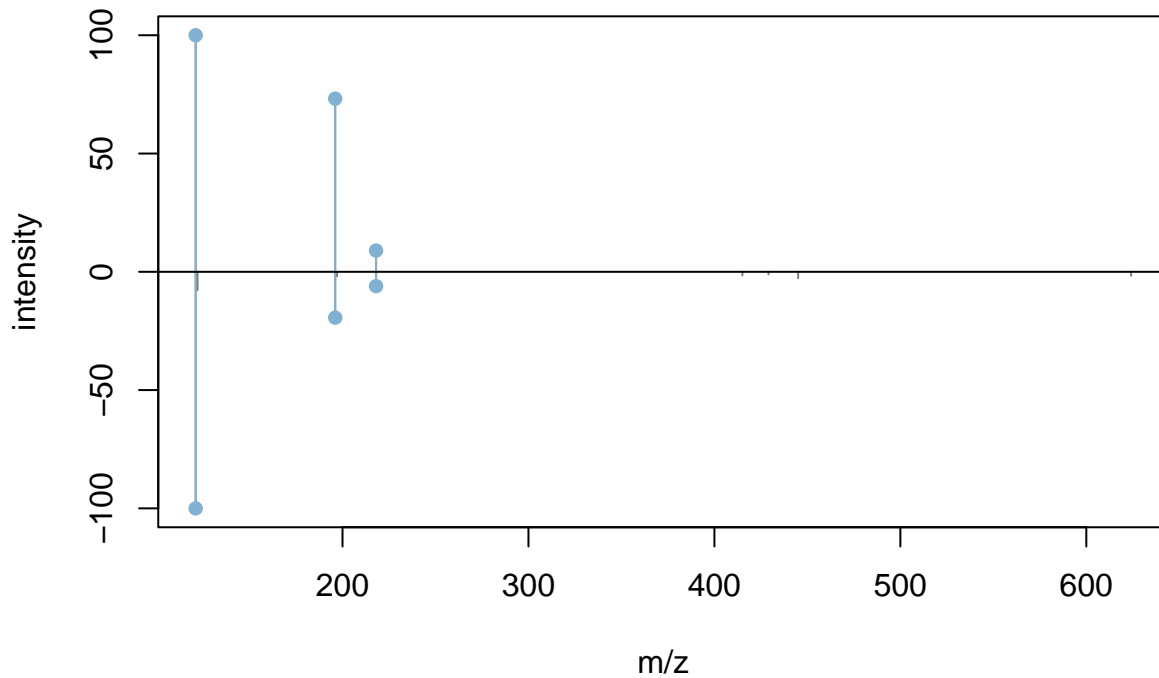
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)
inchikey	ZMHLUFWWPBTIU-UHFFFAOYSA-N	ZMHLUFWWPBTIU-UHFFFAOYSA-N
smiles	O=C(O)CNC(=O)C1=CC=C(O)C=C1	O=C(O)CNC(=O)C1=CC=C(O)C=C1
formula	C9H9NO4	C9H9NO4

Retention time match

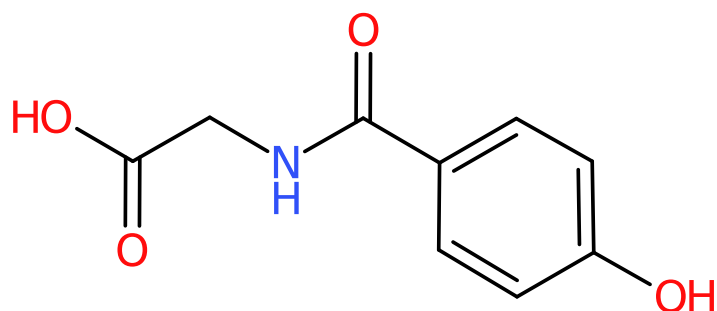
	DB	hit	error	rel. error	pcgroup
Retention time	2.10	2.39	0.29	13.7%	37

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
121.0298	100.0	[M] ⁺		121.0279	100.0
122.0333	7.8	[M+1] ⁺		✗	✗
196.0617	19.4	[M] ⁺	[M+H] ⁺	196.0600	73.2
197.0651	1.9	[M+1] ⁺		✗	✗
218.0422	6.1		[M+Na] ⁺	218.0434	9.0
415.0793	1.6		[2M-2H+Al ₃] ⁺	✗	✗
429.0574	1.1		[2M+K] ⁺	✗	✗
445.0277	2.8			✗	✗
624.1069	1.7		[3M+K] ⁺	✗	✗

4-Hydroxy-hippuric acid



User identifiers

localidentifier	235
dataOrigin	20190701Q-052.mzML
CAS	2482-25-9
inchi	InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)

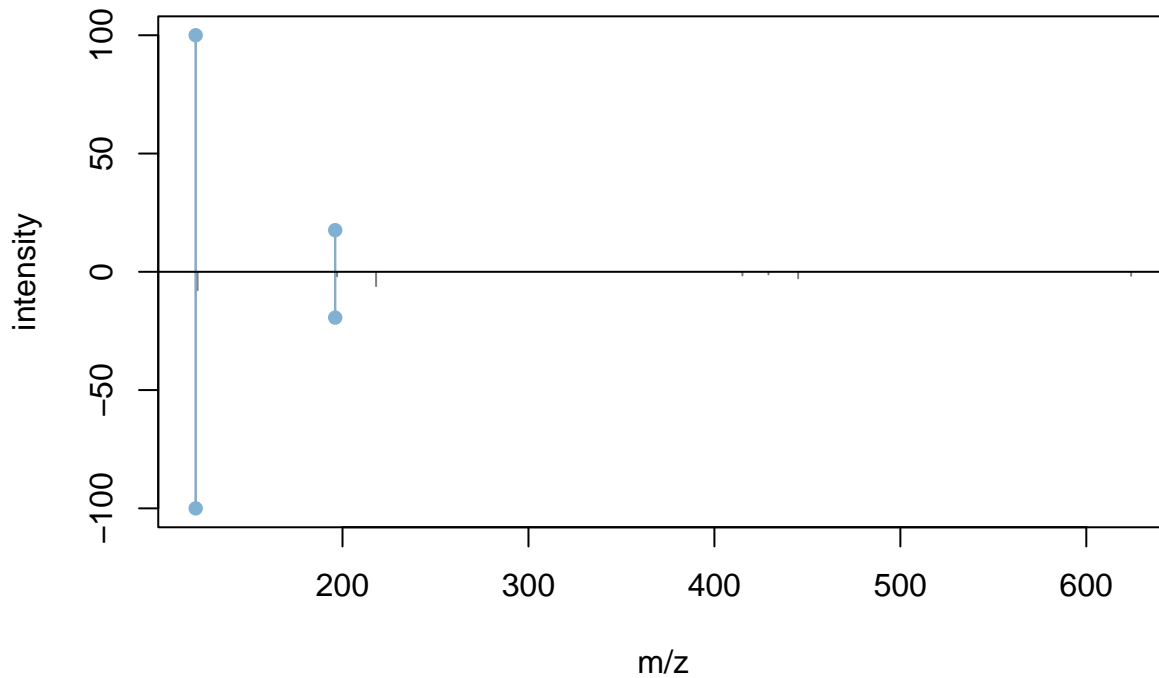
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO4/c11-7-3-1-6(2-4-7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)
inchikey	ZMHLUFWWPBTIU-UHFFFAOYSA-N	ZMHLUFWWPBTIU-UHFFFAOYSA-N
smiles	O=C(O)CNC(=O)C1=CC=C(O)C=C1	O=C(O)CNC(=O)C1=CC=C(O)C=C1
formula	C9H9NO4	C9H9NO4

Retention time match

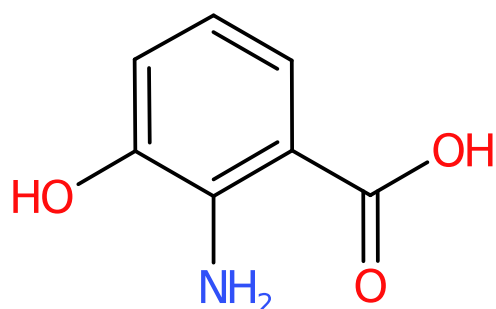
	DB	hit	error	rel. error	pcgroup
Retention time	2.10	2.07	-0.03	-1.3%	57

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
121.0298	100.0	[M] ⁺		121.0280	100.0
122.0333	7.8	[M+1] ⁺		✗	✗
196.0617	19.4	[M] ⁺	[M+H] ⁺	196.0612	17.6
197.0651	1.9	[M+1] ⁺		✗	✗
218.0422	6.1		[M+Na] ⁺	✗	✗
415.0793	1.6		[2M-2H+Al ₃] ⁺	✗	✗
429.0574	1.1		[2M+K] ⁺	✗	✗
445.0277	2.8			✗	✗
624.1069	1.7		[3M+K] ⁺	✗	✗

3-Hydroxyanthranilic acid



User identifiers

localidentifier	163
dataOrigin	14062019Q-074.mzML
CAS	548-93-6
inchi	InChI=1S/C7H7NO3/c8-6-4(7(10)11)2-1-3-5(6)9/h1-3,9H,8H2,(H,10,11)

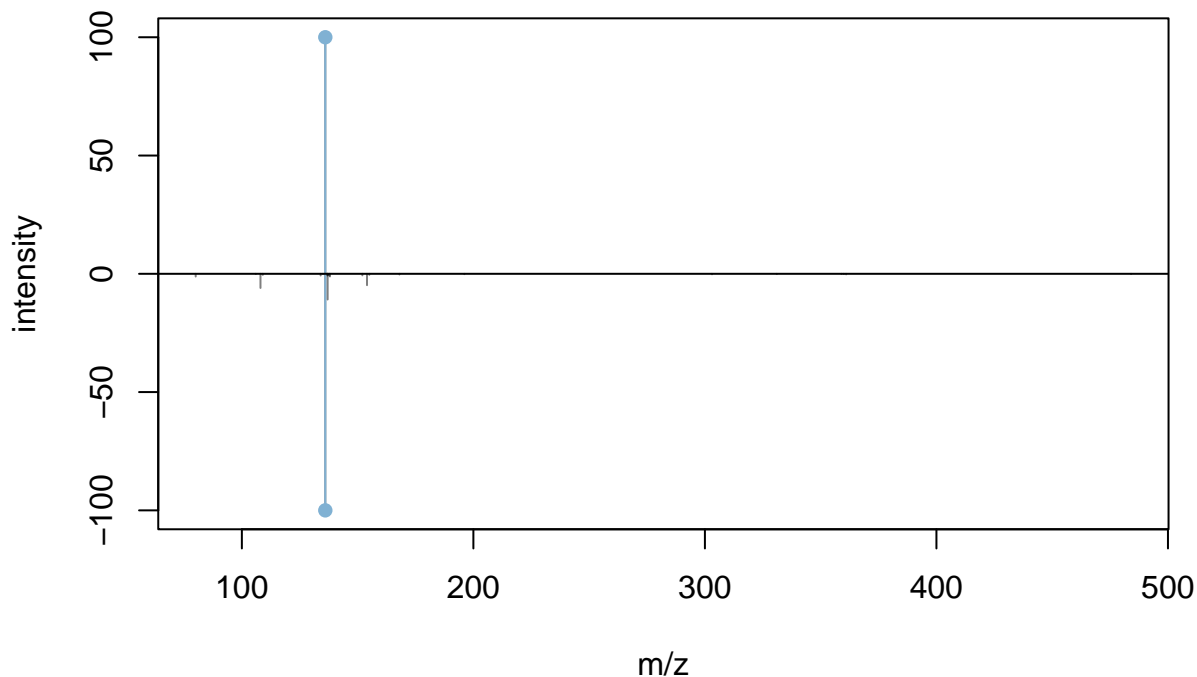
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H7NO3/c8-6-4(7(10)11)2-1-3-5(6)9/h1-3,9H,8H2,(H,10,11)
inchikey	WJXSWCUQABXPFS-UHFFFAOYSA-N	WJXSWCUQABXPFS-UHFFFAOYSA-N
smiles	O=C(O)C=1C=CC=C(O)C1N	O=C(O)C=1C=CC=C(O)C1N
formula	C7H7NO3	C7H7NO3

Retention time match

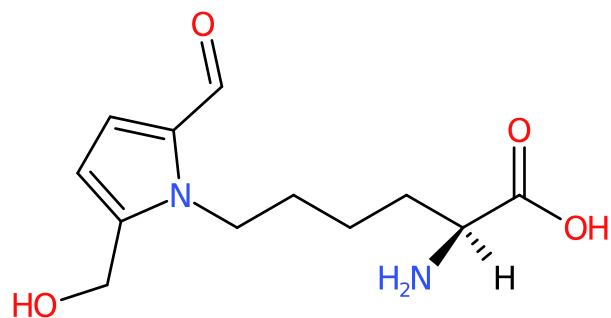
	DB	hit	error	rel. error	pcgroup
Retention time	1.98	2.10	0.12	6.1%	166

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
80.0501	1.2			✗	✗
106.0296	0.1			✗	✗
108.0433	6.0	[M] ⁺	[M+H-HCOOH] ⁺	✗	✗
109.0490	0.5	[M+1] ⁺		✗	✗
134.0227	0.7			✗	✗
135.0316	0.1			✗	✗
135.9621	0.2			✗	✗
136.0397	100.0	[M] ⁺	[M+H-H ₂ O] ⁺	136.0397	100.0
136.5631	0.4			✗	✗
136.9864	0.8			✗	✗
137.0415	10.9	[M+1] ⁺		✗	✗
137.1300	0.4			✗	✗
137.2124	0.4			✗	✗
137.7995	0.8			✗	✗
138.0455	1.1	[M+2] ⁺		✗	✗
152.0395	0.7			✗	✗
154.0504	4.8	[M] ⁺	[M+H] ⁺	✗	✗
155.0560	0.5	[M+1] ⁺		✗	✗
168.0700	0.3			✗	✗
196.0949	0.2			✗	✗
303.0627	0.2			✗	✗
331.0522	0.1		[2M-2H+Al ₃] ⁺	✗	✗
359.0000	0.1			✗	✗
359.9990	0.1		[2M-2H+Fe ₃] ⁺	✗	✗
361.0128	0.2			✗	✗
484.0939	0.1		[3M-2H+Al ₃] ⁺	✗	✗

NA



User identifiers

localidentifier	100
dataOrigin	14062019Q-114.mzML
CAS	74509-14-1
inchi	InChI=1S/C12H18N2O4/c13-11(12(17)18)3-1-2-6-14-9(7-15)4-5-10(14)8-16/h4-5,7,11,16H,1-3,6,8,13H2,(H,17,18)/t11-/m0/s1

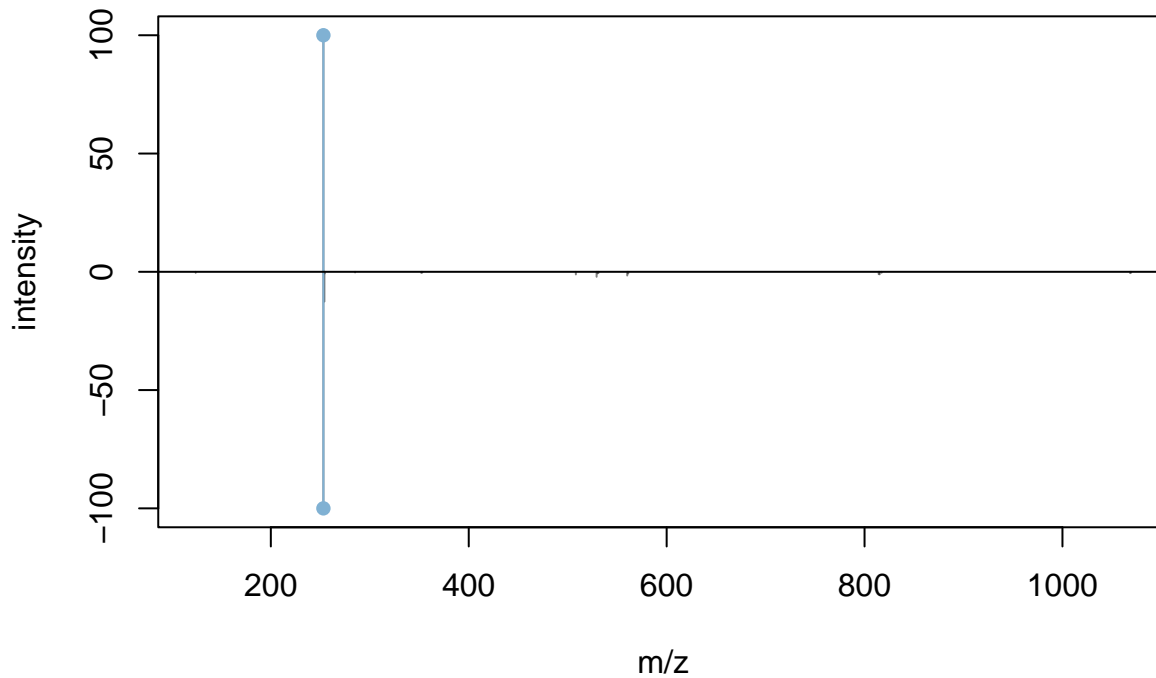
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C12H18N2O4/c13-11(12(17)18)3-1-2-6-14-9(7-15)4-5-10(14)8-16/h4-5,7,11,16H,1-3,6,8,13H2,(H,17,18)/t11-/m0/s1
inchikey	VTYFITADLSVOAS-NSHDSACASA-N	VTYFITADLSVOAS-NSHDSACASA-N
smiles	[H]C(N)(C(=O)O)CCCCN1C(C=O)=CC=C1CO	[H]C(N)(C(=O)O)CCCCN1C(C=O)=CC=C1CO
formula	C12H18N2O4	C12H18N2O4

Retention time match

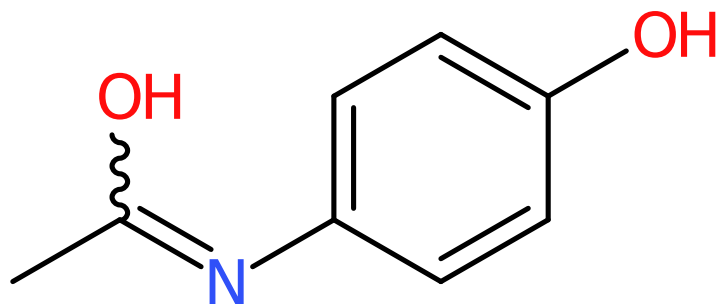
	DB	hit	error	rel. error	pcgroup
Retention time	2.35	2.18	-0.17	-7.2%	317

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
124.0405	0.4		[M-H-NH3-CO2-C5H8]-	✗	✗
253.1184	100.0	[M] ⁺	[M-H] ⁻	253.1195	100.0
254.1238	12.6	[M+1] ⁺		✗	✗
254.4538	0.7	[M+2] ³⁺		✗	✗
285.1447	0.3			✗	✗
352.0422	0.5			✗	✗
353.0440	0.3			✗	✗
508.2496	1.1			✗	✗
529.2241	2.1	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
530.2328	0.7	[M+1] ⁺		✗	✗
531.2225	0.4	[M+2] ⁺		✗	✗
560.1627	1.6	[M] ⁺	[2M-4H+Fe3 ⁺] ⁻	✗	✗
561.1655	0.7	[M+1] ⁺		✗	✗
814.2939	1.0		[3M-4H+Fe3 ⁺] ⁻	✗	✗
815.2869	1.1		[3M-3H+Fe2 ⁺] ⁻	✗	✗
817.2845	0.4			✗	✗
1068.4039	0.6	[M] ⁺	[4M-4H+Fe3 ⁺] ⁻	✗	✗
1069.4052	0.4	[M+1] ⁺		✗	✗

Paracetamol



User identifiers

localidentifier	814
dataOrigin	20191206Q-082.mzML
CAS	103-90-2
inchi	InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)

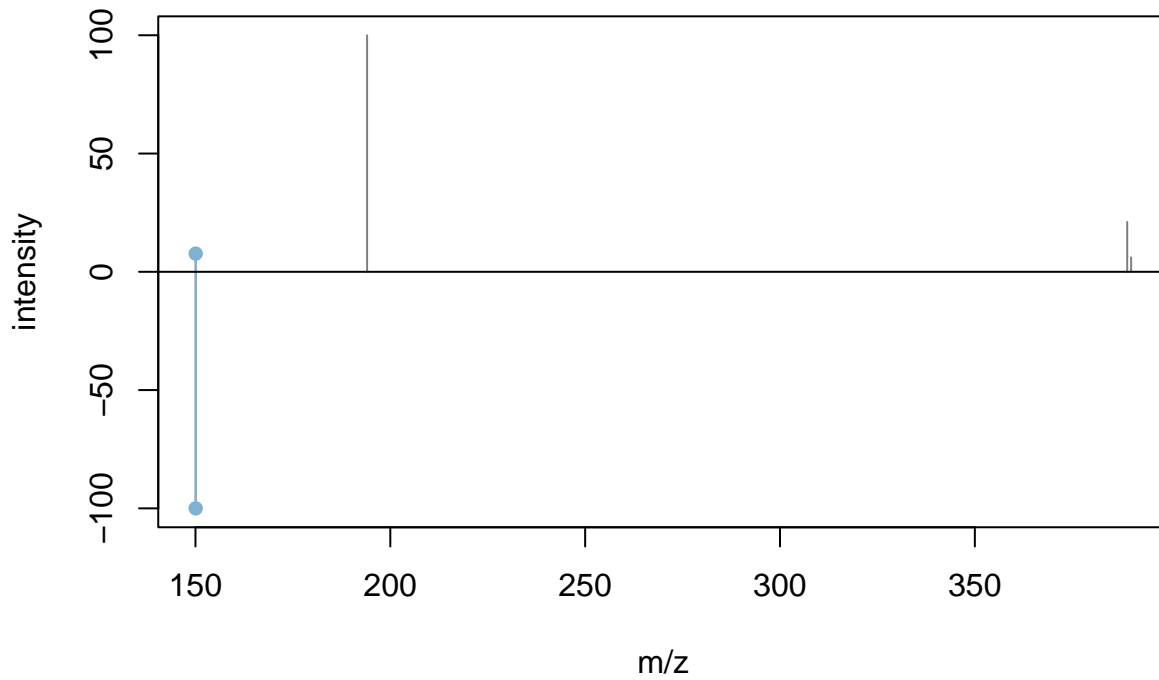
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)
inchikey	RZVAJINKPMORJF-UHFFFAOYSA-N	RZVAJINKPMORJF-UHFFFAOYSA-N
smiles	OC1=CC=C(N=C(O)C)C=C1	OC1=CC=C(N=C(O)C)C=C1
formula	C8H9NO2	C8H9NO2

Retention time match

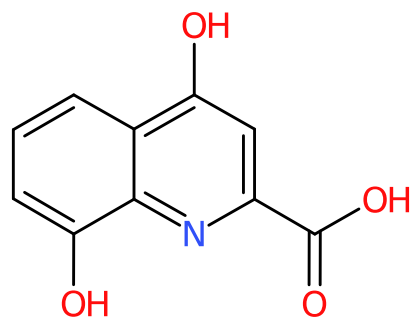
	DB	hit	error	rel. error	pcgroup
Retention time	2.02	2.40	0.38	18.6%	20

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
150.0561	100.0		[M-H]-	150.0556	7.7
×	×			194.0455	100.0
×	×			389.0983	21.1
×	×			390.1039	6.1

Xanthurenic acid



User identifiers

localidentifier	219
dataOrigin	20190701Q-036.mzML
CAS	59-00-7
inchi	InChI=1S/C10H7NO4/c12-7-3-1-2-5-8(13)4-6(10(14)15)11-9(5)7/h1-4,12H,(H,11,13)(H,14,15)

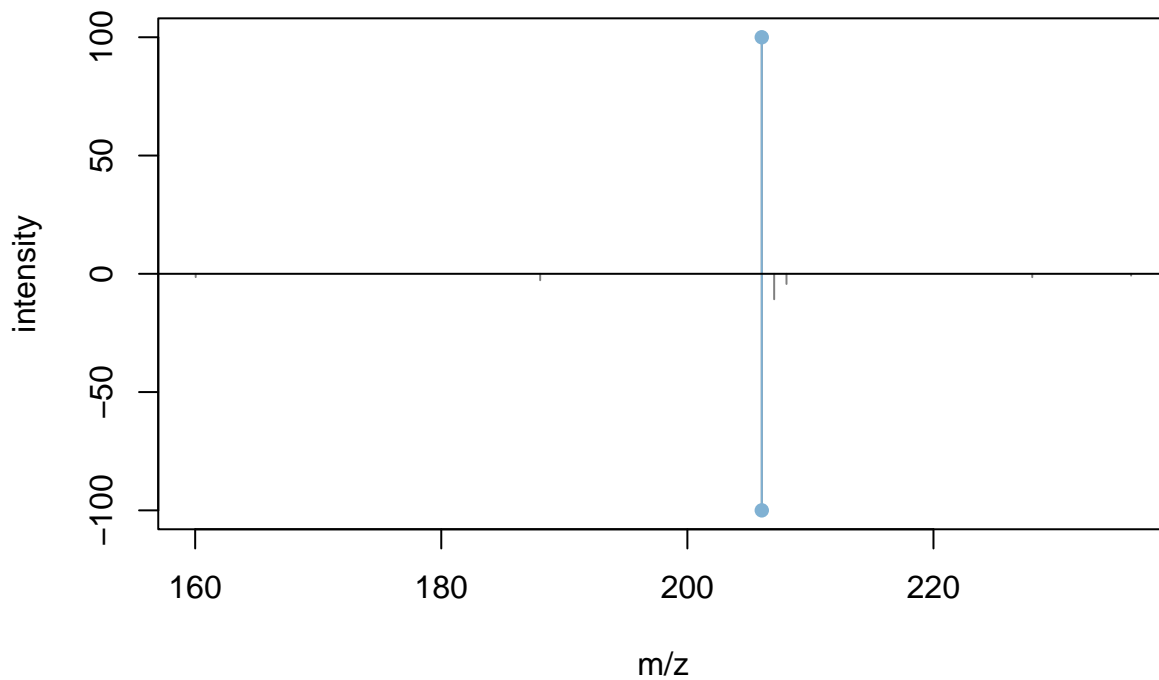
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C10H7NO4/c12-7-3-1-2-5-8(13)4-6(10(14)15)11-9(5)7/h1-4,12H,(H,11,13)(H,14,15)
inchikey	FBZONXHGGPHHIY-UHFFFAOYSA-N	FBZONXHGGPHHIY-UHFFFAOYSA-N
smiles	O=C(O)C=1N=C2C(O)=CC=CC2=C(O)C1	O=C(O)C=1N=C2C(O)=CC=CC2=C(O)C1
formula	C10H7NO4	C10H7NO4

Retention time match

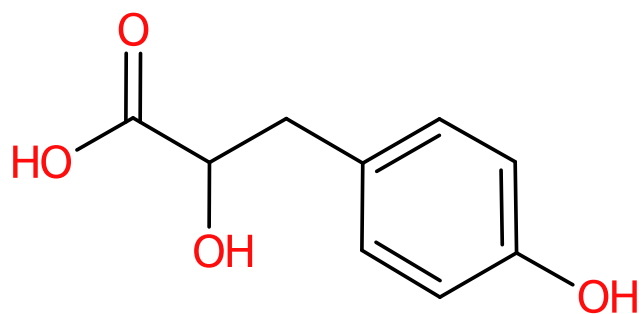
	DB	hit	error	rel. error	pcgroup
Retention time	3.02	2.57	-0.45	-14.8%	132

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
160.0403	1.4		[M+H-HCOOH]+	✗	✗
188.0377	2.7		[M+H-H ₂ O]+	✗	✗
206.0474	100.0	[M]+	[M+H]+	206.0449	100.0
207.0522	10.8	[M+1]+		✗	✗
208.0553	4.3	[M+2]+		✗	✗
228.0279	1.4		[M+Na]+	✗	✗
236.0631	0.8			✗	✗

Hydroxyphenyllactic acid



User identifiers

localidentifier	346
dataOrigin	20190710Q-176.mzML
CAS	6482-98-0
inchi	InChI=1S/C9H10O4/c10-7-3-1-6(2-4-7)5-8(11)9(12)13/h1-4,8,10-11H,5H2,(H,12,13)

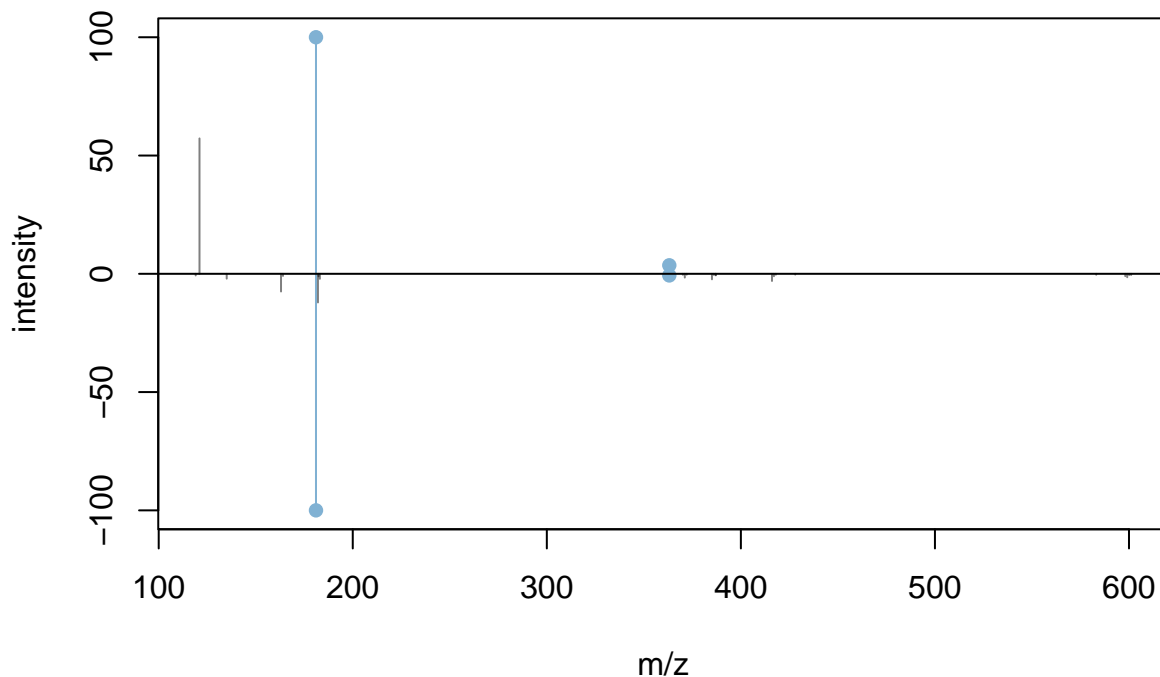
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H10O4/c10-7-3-1-6(2-4-7)5-8(11)9(12)13/h1-4,8,10-11H,5H2,(H,12,13)
inchikey	JVGVDSSUAVXRDY-UHFFFAOYSA-N	JVGVDSSUAVXRDY-UHFFFAOYSA-N
smiles	O=C(O)C(O)CC1=CC=C(O)C=C1	O=C(O)C(O)CC1=CC=C(O)C=C1
formula	C9H10O4	C9H10O4

Retention time match

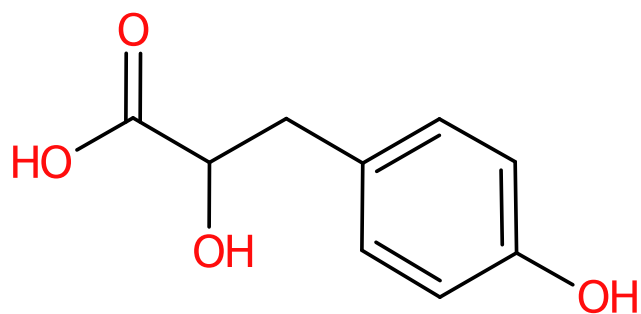
	DB	hit	error	rel. error	pcgroup
Retention time	2.71	2.57	-0.13	-4.9%	30

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
119.0523	0.7		[M-H-H ₂ O-CO ₂]-	✗	✗
✗	✗			121.0287	57.2
135.0451	2.1		[M-H-HCOOH]-	✗	✗
163.0387	7.5	[M] ⁺	[M-H-H ₂ O]-	✗	✗
164.0420	0.9	[M+1] ⁺		✗	✗
181.0508	100.0	[M] ⁺	[M-H]-	181.0502	100.0
182.0553	12.1	[M+1] ⁺		✗	✗
182.3760	1.1			✗	✗
183.0430	2.1	[M+2] ⁺		✗	✗
363.1081	0.7		[2M-H]-	363.1098	3.6
370.0993	0.4			✗	✗
371.0936	1.6	[M] ⁺		✗	✗
372.1037	0.4	[M+1] ⁺		✗	✗
385.0930	2.3	[M] ⁺	[2M-2H+Na]-	✗	✗
386.0924	0.5	[M+1] ⁺		✗	✗
387.0696	0.6	[M+2] ⁺		✗	✗
387.0737	0.7		[2M-4H+Al ³⁺]-	✗	✗
416.0218	3.0		[2M-4H+Fe ³⁺]-	✗	✗
417.0249	1.0	[M] ⁺	[2M-3H+Fe ²⁺]-	✗	✗
418.0207	0.4	[M+1] ⁺		✗	✗
428.0117	0.3			✗	✗
583.1161	0.4		[3M-2H+K]-	✗	✗
598.0767	1.0		[3M-4H+Fe ³⁺]-	✗	✗
599.0807	1.5	[M] ⁺	[3M-3H+Fe ²⁺]-	✗	✗
600.0912	0.5	[M+1] ⁺		✗	✗
601.0980	0.5	[M+2] ⁺		✗	✗

DL-P-Hydroxy Phenyl lactic acid



User identifiers

localidentifier	703
dataOrigin	20190725Q-147.mzML
CAS	306-23-0
inchi	InChI=1S/C9H10O4/c10-7-3-1-6(2-4-7)5-8(11)9(12)13/h1-4,8,10-11H,5H2,(H,12,13)

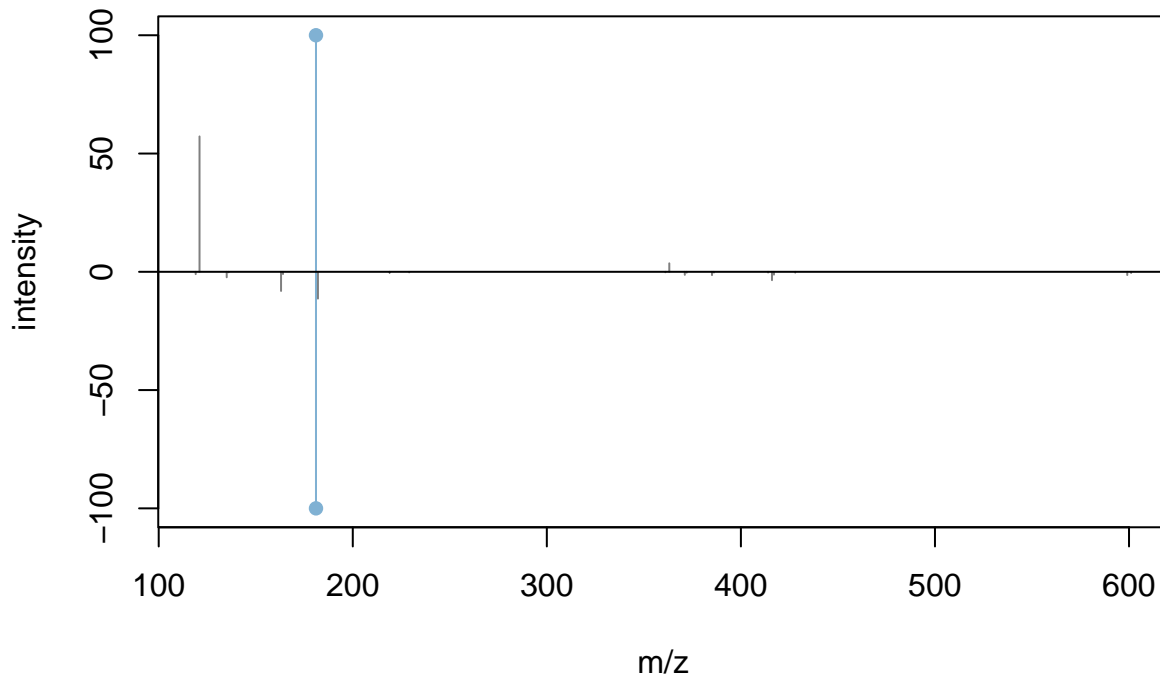
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H10O4/c10-7-3-1-6(2-4-7)5-8(11)9(12)13/h1-4,8,10-11H,5H2,(H,12,13)
inchikey	JVGVDSUAVXRDY-UHFFFAOYSA-N	JVGVDSUAVXRDY-UHFFFAOYSA-N
smiles	O=C(O)C(O)CC1=CC=C(O)C=C1	O=C(O)C(O)CC1=CC=C(O)C=C1
formula	C9H10O4	C9H10O4

Retention time match

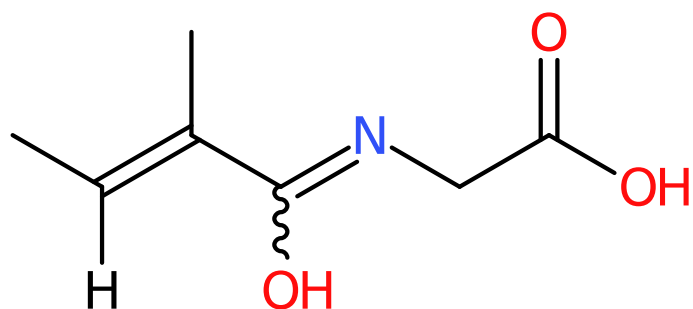
	DB	hit	error	rel. error	pcgroup
Retention time	2.67	2.57	-0.10	-3.7%	30

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
119.0500	1.0		[M-H-H ₂ O-CO ₂]-	✗	✗
✗	✗			121.0287	57.2
135.0434	2.3	[M] ⁺	[M-H-HCOOH]-	✗	✗
136.0478	0.2	[M+1] ⁺		✗	✗
163.0370	8.1	[M] ⁺	[M-H-H ₂ O]-	✗	✗
164.0433	0.9	[M+1] ⁺		✗	✗
181.0498	100.0	[M] ⁺	[M-H]-	181.0502	100.0
182.0531	11.3	[M+1] ⁺		✗	✗
218.9723	0.4			✗	✗
218.9759	0.4			✗	✗
229.0729	0.2			✗	✗
361.0912	0.2			✗	✗
✗	✗			363.1098	3.6
371.0929	1.3	[M] ⁺		✗	✗
372.0948	0.3	[M+1] ⁺		✗	✗
385.0948	1.4	[M] ⁺	[2M-2H+Na]-	✗	✗
386.0912	0.3	[M+1] ⁺		✗	✗
414.0186	0.3			✗	✗
416.0199	3.5	[M] ⁺	[2M-4H+Fe ³⁺]-	✗	✗
417.0295	1.2	[M+1] ⁺		✗	✗
428.0200	0.3			✗	✗
599.0898	1.4		[3M-3H+Fe ²⁺]-	✗	✗
601.0873	0.5			✗	✗

Tiglyl glycine



User identifiers

localidentifier	450
dataOrigin	20190715Q-184.mzML
CAS	35842-45-6
inchi	InChI=1S/C7H11NO3/c1-3-5(2)7(11)8-4-6(9)10/h3H,4H2,1-2H3,(H,8,11)(H,9,10)/b5-3+

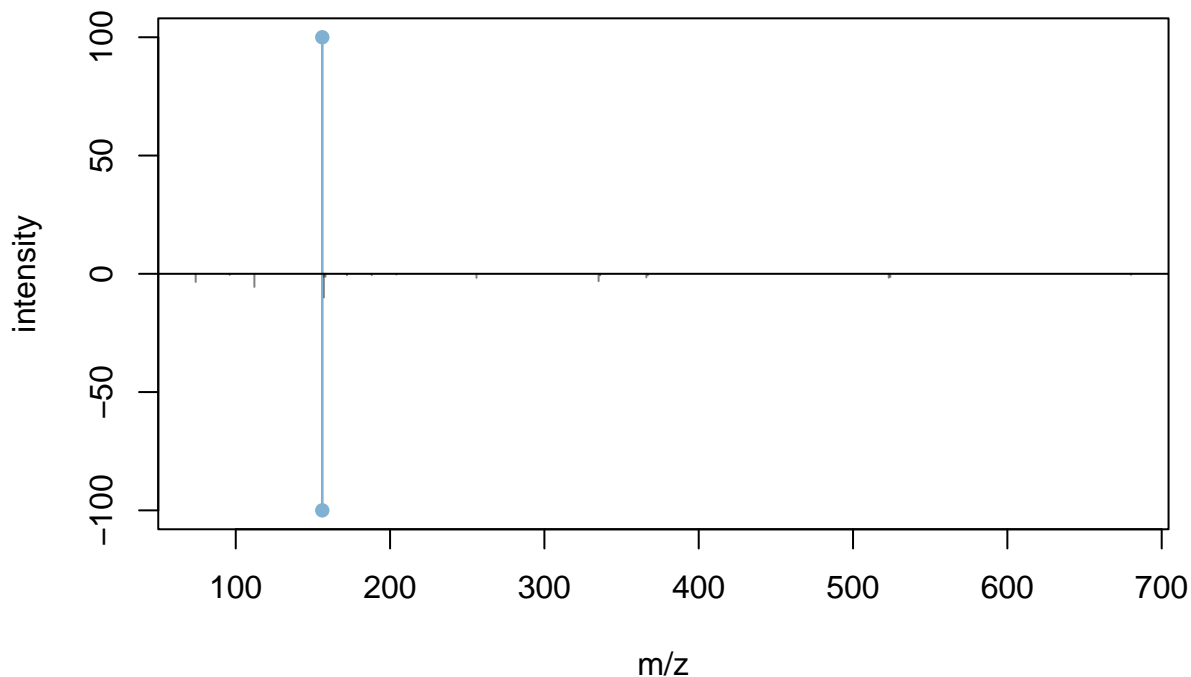
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H11NO3/c1-3-5(2)7(11)8-4-6(9)10/h3H,4H2,1-2H3,(H,8,11)(H,9,10)/b5-3+
inchikey	WRUSVQOKJIDBLP-HWKANZROSA-N	WRUSVQOKJIDBLP-HWKANZROSA-N
smiles	[H]C(=C(C(O)=NCC(=O)O)C)C	[H]C(=C(C(O)=NCC(=O)O)C)C
formula	C7H11NO3	C7H11NO3

Retention time match

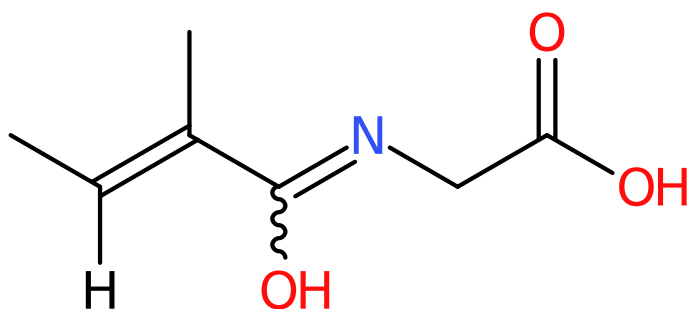
	DB	hit	error	rel. error	pcgroup
Retention time	2.57	2.59	0.01	0.6%	110

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
74.0258	3.4			✗	✗
96.0458	0.5		[M-H-C2H4O2]-	✗	✗
112.0757	5.5		[M-H-CO2]-	✗	✗
156.0657	100.0	[M]+	[M-H]-	156.0654	100.0
156.3543	1.3			✗	✗
156.8753	1.3			✗	✗
157.0718	10.0	[M+1]+		✗	✗
158.0943	1.3	[M+2]+		✗	✗
172.0626	0.6			✗	✗
188.0894	0.6			✗	✗
204.0856	0.3			✗	✗
255.9888	1.7			✗	✗
335.1229	3.1	[M]+	[2M-2H+Na]-	✗	✗
336.1215	0.7	[M+1]+		✗	✗
366.0558	1.5	[M]+	[2M-4H+Fe3+]-	✗	✗
367.0570	0.6	[M+1]+		✗	✗
523.1319	1.7		[3M-4H+Fe3+]-	✗	✗
524.1307	1.4		[3M-3H+Fe2+]-	✗	✗
680.1946	0.4		[4M-4H+Fe3+]-	✗	✗

Tiglyl glycine



User identifiers

localidentifier	857
dataOrigin	20191206Q-129.mzML
CAS	35842-45-6
inchi	InChI=1S/C7H11NO3/c1-3-5(2)7(11)8-4-6(9)10/h3H,4H2,1-2H3,(H,8,11)(H,9,10)/b5-3+

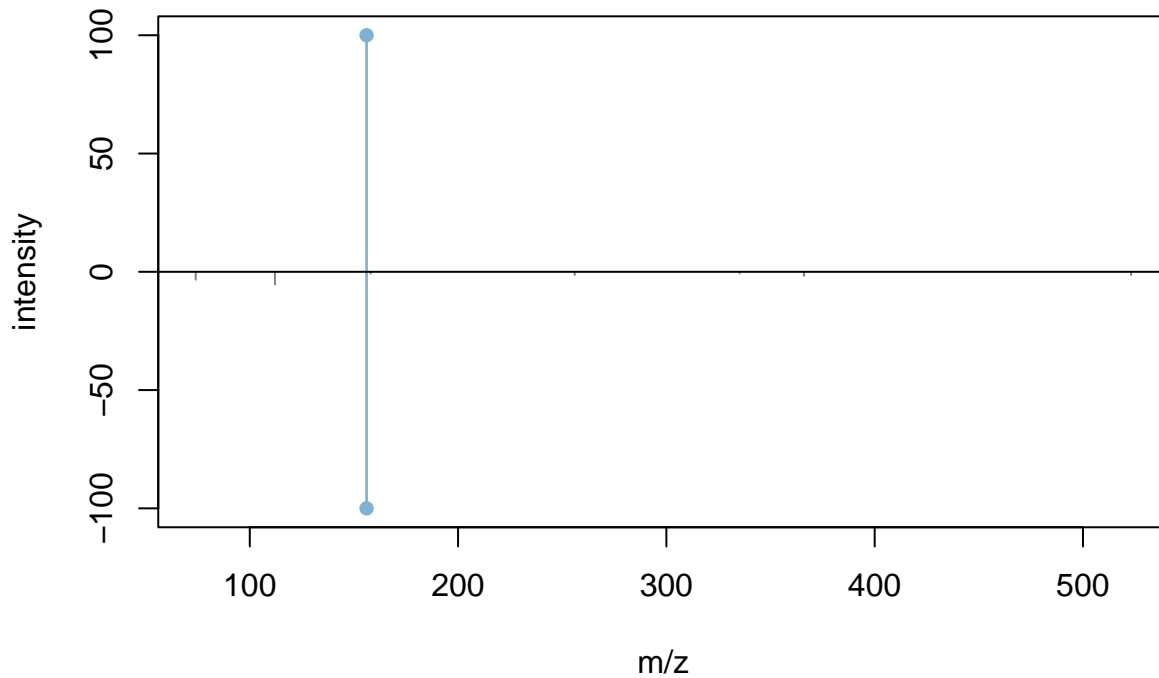
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H11NO3/c1-3-5(2)7(11)8-4-6(9)10/h3H,4H2,1-2H3,(H,8,11)(H,9,10)/b5-3+
inchikey	WRUSVQOKJIDBLP-HWKANZROSA-N	WRUSVQOKJIDBLP-HWKANZROSA-N
smiles	[H]C(=C(C(O)=NCC(=O)O)C)C	[H]C(=C(C(O)=NCC(=O)O)C)C
formula	C7H11NO3	C7H11NO3

Retention time match

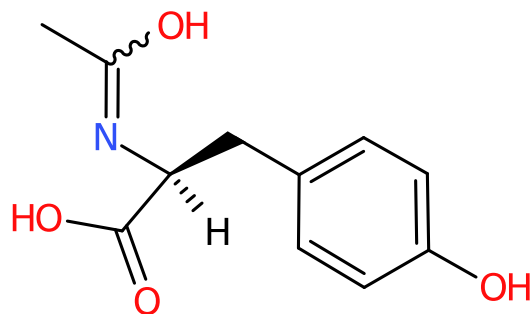
	DB	hit	error	rel. error	pcgroup
Retention time	2.60	2.59	-0.01	-0.4%	110

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
74.0263	3.3			✗	✗
112.0774	5.4		[M-H-CO ₂]-	✗	✗
156.0667	100.0		[M-H]-	156.0654	100.0
158.0750	0.7			✗	✗
255.9883	1.3			✗	✗
335.1203	0.7		[2M-2H+Na]-	✗	✗
366.0530	1.7		[2M-4H+Fe ³⁺]-	✗	✗
523.1151	1.4		[3M-4H+Fe ³⁺]-	✗	✗

N-Acetytyrosine



User identifiers

localidentifier	269
dataOrigin	20190701Q-197.mzML
CAS	537-55-3
inchi	InChI=1S/C11H13NO4/c1-7(13)12-10(11(15)16)6-8-2-4-9(14)5-3-8/h2-5,10,14H,6H2,1H3,(H,12,13)(H,15,16)/t10-/m0/s1

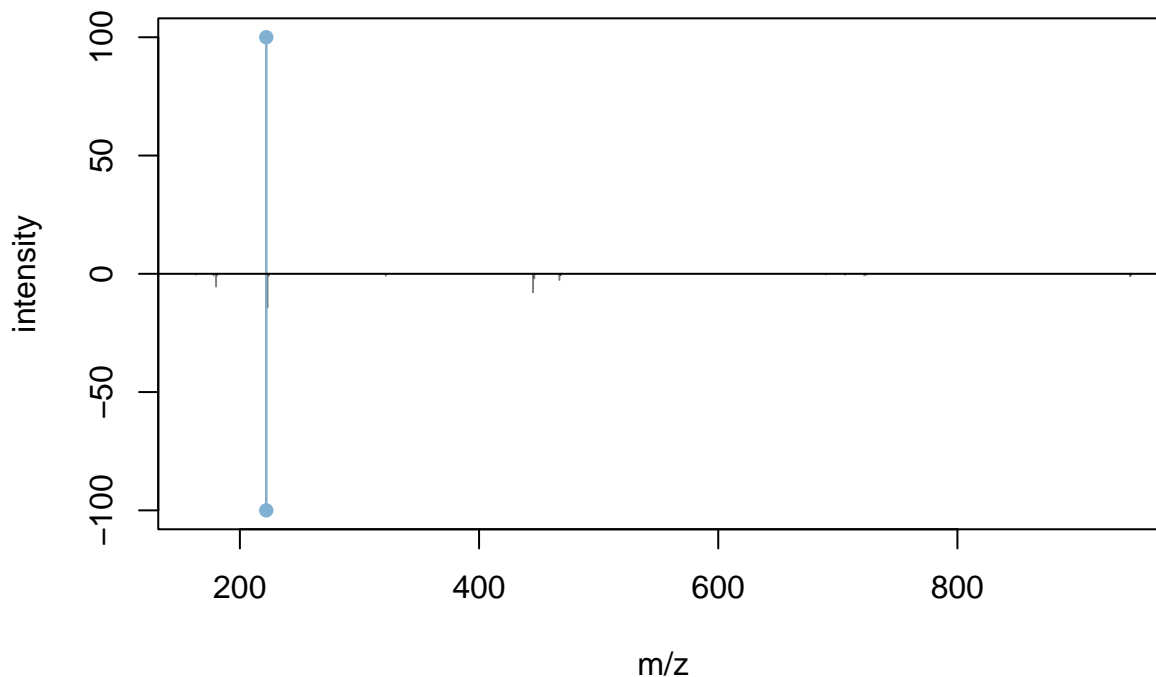
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C11H13NO4/c1-7(13)12-10(11(15)16)6-8-2-4-9(14)5-3-8/h2-5,10,14H,6H2,1H3,(H,12,13)(H,15,16)/t10-/m0/s1
inchikey	CAHKINHBCWCHCF-JTQLQIEISA-N	CAHKINHBCWCHCF-JTQLQIEISA-N
smiles	[H]C(N=C(O)C)(C(=O)O)CC1=CC=C(O)C=C1	[H]C(N=C(O)C)(C(=O)O)CC1=CC=C(O)C=C1
formula	C11H13NO4	C11H13NO4

Retention time match

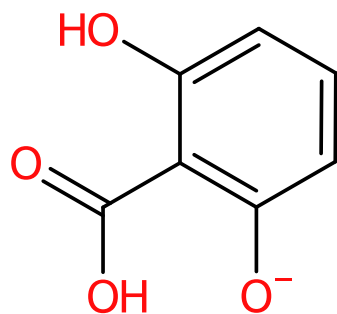
	DB	hit	error	rel. error	pcgroup
Retention time	2.84	2.65	-0.19	-6.7%	293

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
163.0417	0.3		[M-H-NH3-COCH2]-	✗	✗
178.0877	0.7		[M-H-CO2]-	✗	✗
180.0647	5.4	[M]+	[M-H-COCH2]-	✗	✗
181.0676	0.6	[M+1]+		✗	✗
222.0759	100.0	[M]+	[M-H]-	222.0771	100.0
223.0820	14.2	[M+1]+		✗	✗
224.1043	0.8	[M+2]+		✗	✗
321.9971	0.8			✗	✗
445.1608	7.9	[M]+	[2M-H]-	✗	✗
446.1624	1.9	[M+1]+		✗	✗
467.1436	2.6	[M]+	[2M-2H+Na]-	✗	✗
468.1394	0.5	[M+1]+		✗	✗
468.1404	0.5			✗	✗
690.2206	0.3		[3M-2H+Na]-	✗	✗
706.1924	0.4		[3M-2H+K]-	✗	✗
722.1634	0.7	[M]+	[3M-3H+Fe2+]-	✗	✗
723.1589	0.3	[M+1]+		✗	✗
724.1710	0.3	[M+2]+		✗	✗
944.2587	1.0		[4M-4H+Fe3+]-	✗	✗
945.2365	0.6		[4M-3H+Fe2+]-	✗	✗

2,6-Dihydroxybenzoic acid



User identifiers

localidentifier	160
dataOrigin	14062019Q-178.mzML
CAS	303-07-1
inchi	InChI=1S/C7H6O4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,8-9H,(H,10,11)/p-1

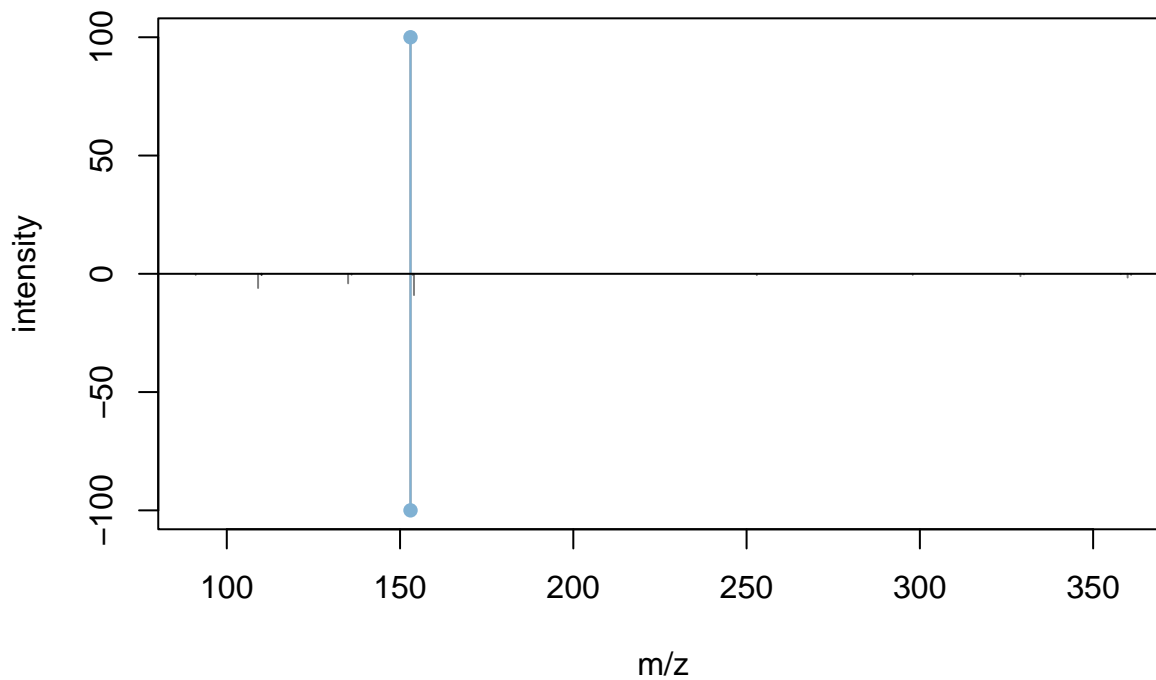
Computed identifiers

	Input as-is	Standardized structure
charge	-1	0
inchi		InChI=1S/C7H6O4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,8-9H,(H,10,11)/p-1
inchikey	AKEUNCKRJATALU-UHFFFAOYSA-M	AKEUNCKRJATALU-UHFFFAOYSA-M
smiles	O=C(O)C=1C([O-])=CC=CC1O	O=C(O)C=1C([O-])=CC=CC1O
formula	[C7H5O4]-	[C7H5O4]-

Retention time match

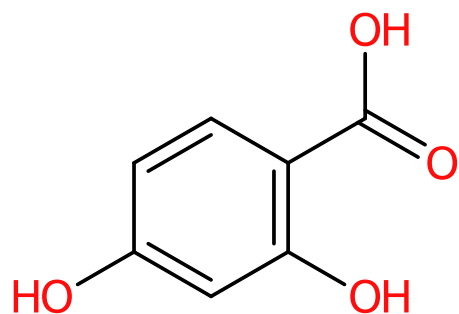
	DB	hit	error	rel. error	pcgroup
Retention time	3.15	2.72	-0.42	-13.5%	181

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
91.0197	0.4		[M-H-H ₂ O-CO ₂]-	✘	✘
109.0290	6.0	[M] ⁺	[M-H-CO ₂]-	✘	✘
110.0316	0.5	[M+1] ⁺		✘	✘
110.0330	0.4			✘	✘
110.0334	0.4			✘	✘
135.0073	4.0	[M] ⁺	[M-H-H ₂ O]-	✘	✘
136.0123	0.4	[M+1] ⁺		✘	✘
153.0177	100.0	[M] ⁺	[M-H]-	153.0187	100.0
153.6383	0.5			✘	✘
154.0192	9.0	[M+1] ⁺		✘	✘
252.9454	0.6			✘	✘
297.9388	0.4			✘	✘
329.0279	1.0	[M] ⁺	[2M-2H+Na]-	✘	✘
330.0339	0.2	[M+1] ⁺		✘	✘
357.9684	0.2			✘	✘
359.9572	1.6	[M] ⁺	[2M-4H+Fe ³⁺]-	✘	✘
360.9678	0.5	[M+1] ⁺		✘	✘

2,4-Dihydroxybenzoic acid



User identifiers

localidentifier	721
dataOrigin	20190725Q-167.mzML
CAS	89-86-1
inchi	InChI=1S/C7H6O4/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,8-9H,(H,10,11)

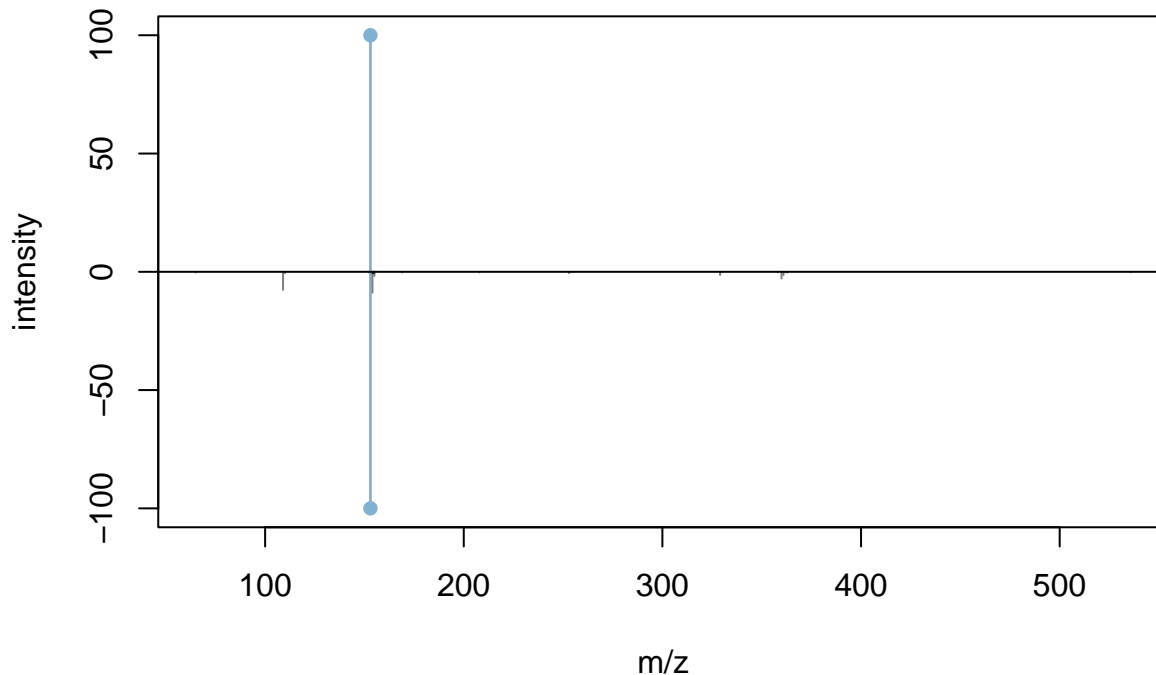
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H6O4/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,8-9H,(H,10,11)
inchikey	UIAFKZKHHVMJGS-UHFFFAOYSA-N	UIAFKZKHHVMJGS-UHFFFAOYSA-N
smiles	O=C(O)C1=CC=C(O)C=C1O	O=C(O)C1=CC=C(O)C=C1O
formula	C7H6O4	C7H6O4

Retention time match

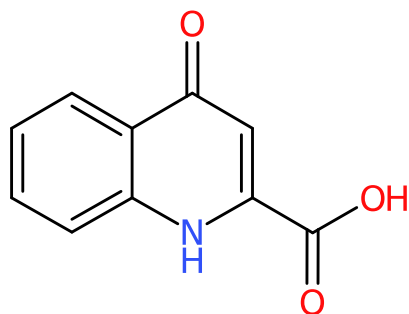
	DB	hit	error	rel. error	pcgroup
Retention time	3.20	2.72	-0.48	-15.0%	181

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
65.0396	0.3			✗	✗
109.0272	7.6	[M] ⁺	[M-H-CO ₂] ⁻	✗	✗
110.0331	0.6	[M+1] ⁺		✗	✗
152.0095	0.2			✗	✗
153.0164	100.0	[M] ⁺	[M-H] ⁻	153.0187	100.0
153.7124	0.6			✗	✗
154.0232	8.8	[M+1] ⁺		✗	✗
154.3469	0.6			✗	✗
154.3879	0.6			✗	✗
154.9003	0.6			✗	✗
155.0219	1.8	[M+2] ⁺		✗	✗
169.0143	0.3			✗	✗
207.9442	0.3			✗	✗
252.9484	0.6	[M] ⁺		✗	✗
253.9453	0.2	[M+1] ⁺		✗	✗
329.0314	1.4	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
330.0305	0.2	[M+1] ⁺		✗	✗
357.9662	0.2			✗	✗
359.9570	2.9	[M] ⁺	[2M-4H+Fe ³⁺] ⁻	✗	✗
360.9639	1.4	[M+1] ⁺		✗	✗
361.9663	0.3	[M+2] ⁺		✗	✗
362.9674	0.4	[M+3] ⁺		✗	✗
535.9694	0.2			✗	✗

Kynurenic acid



User identifiers

localidentifier	239
dataOrigin	20190701Q-163.mzML
CAS	492-27-3
inchi	InChI=1S/C10H7NO3/c12-9-5-8(10(13)14)11-7-4-2-1-3-6(7)9/h1-5H,(H,11,12)(H,13,14)

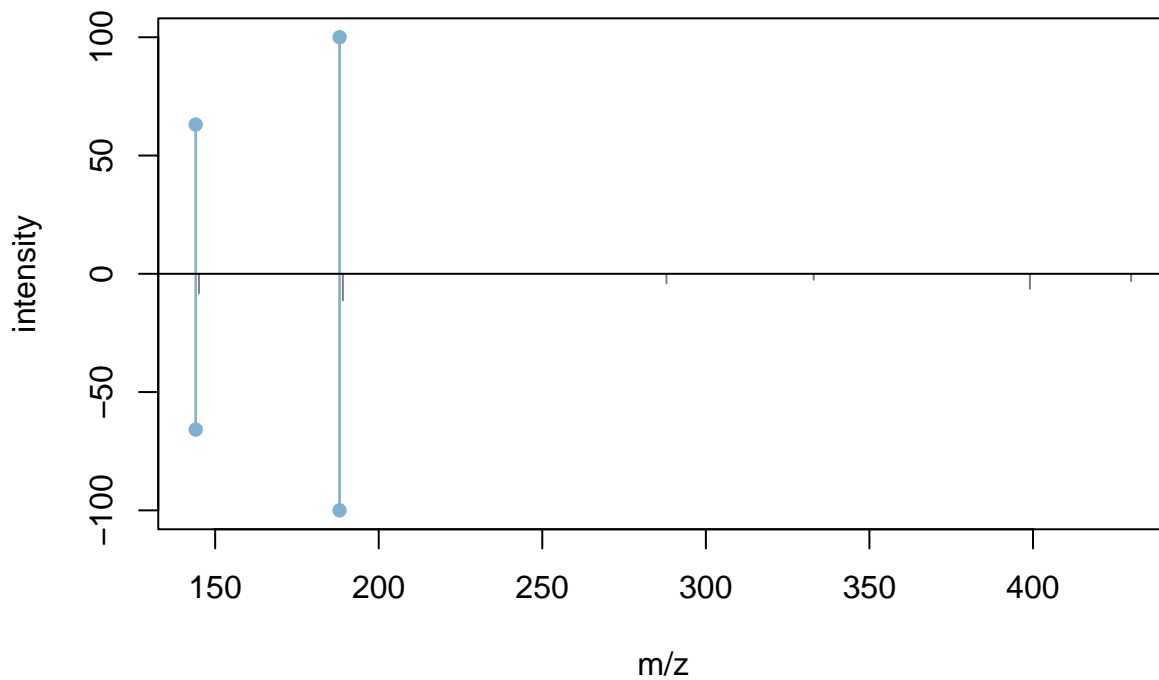
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C10H7NO3/c12-9-5-8(10(13)14)11-7-4-2-1-3-6(7)9/h1-5H,(H,11,12)(H,13,14)
inchikey	HCZHHEIFKROPDY-UHFFFAOYSA-N	HCZHHEIFKROPDY-UHFFFAOYSA-N
smiles	O=C(O)C1=CC(=O)C=2C=CC=CC2N1	O=C(O)C1=CC(=O)C=2C=CC=CC2N1
formula	C10H7NO3	C10H7NO3

Retention time match

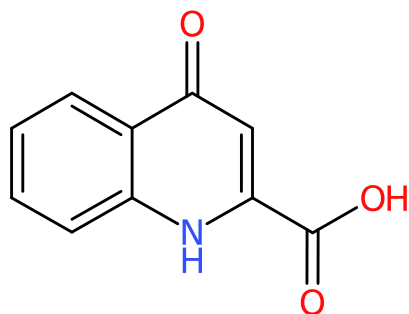
	DB	hit	error	rel. error	pcgroup
Retention time	3.11	2.75	-0.35	-11.4%	225

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
144.0427	65.8	[M] ⁺	[M-H-CO ₂] ⁻	144.0451	63.1
145.0483	8.3	[M+1] ⁺		✗	✗
188.0322	100.0	[M] ⁺	[M-H] ⁻	188.0347	100.0
189.0391	11.3	[M+1] ⁺		✗	✗
287.9630	4.0			✗	✗
332.9557	2.5			✗	✗
399.0507	6.3		[2M-2H+Na] ⁻	✗	✗
429.9957	3.1		[2M-4H+Fe ³⁺] ⁻	✗	✗

Kynurenic acid



User identifiers

localidentifier	239
dataOrigin	20190701Q-056.mzML
CAS	492-27-3
inchi	InChI=1S/C10H7NO3/c12-9-5-8(10(13)14)11-7-4-2-1-3-6(7)9/h1-5H,(H,11,12)(H,13,14)

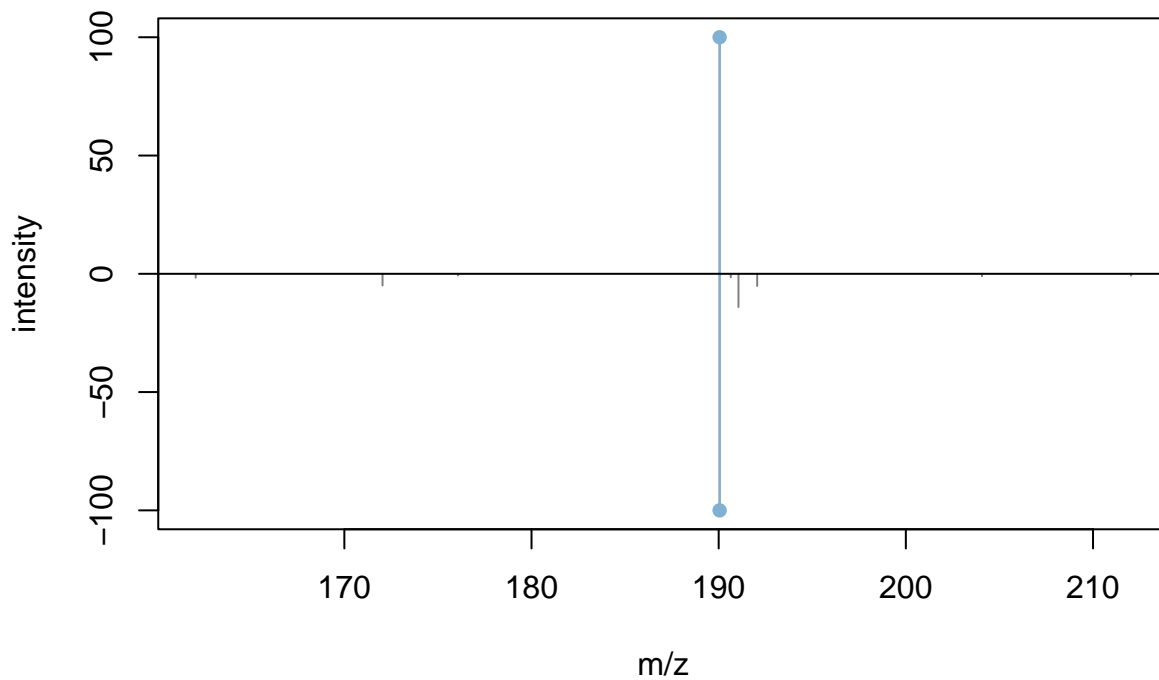
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C10H7NO3/c12-9-5-8(10(13)14)11-7-4-2-1-3-6(7)9/h1-5H,(H,11,12)(H,13,14)
inchikey	HCZHHEIFKROPDY-UHFFFAOYSA-N	HCZHHEIFKROPDY-UHFFFAOYSA-N
smiles	O=C(O)C1=CC(=O)C=2C=CC=CC2N1	O=C(O)C1=CC(=O)C=2C=CC=CC2N1
formula	C10H7NO3	C10H7NO3

Retention time match

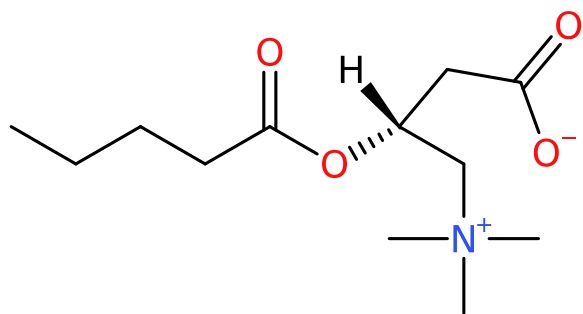
	DB	hit	error	rel. error	pcgroup
Retention time	3.11	2.75	-0.36	-11.5%	71

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
162.0572	1.7		[M+H-CO]+	✗	✗
172.0407	5.0		[M+H-H ₂ O]+	✗	✗
176.0706	0.7			✗	✗
190.0490	100.0	[M]+	[M+H]+	190.0493	100.0
190.6459	1.5			✗	✗
191.0571	14.1	[M+1]+		✗	✗
192.0572	5.2	[M+2]+		✗	✗
204.0665	1.0			✗	✗
212.0361	0.8		[M+Na]+	✗	✗

Valerylcarnitine



User identifiers

localidentifier	453
dataOrigin	20190715Q-080.mzML
CAS	40225-14-7
inchi	InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1

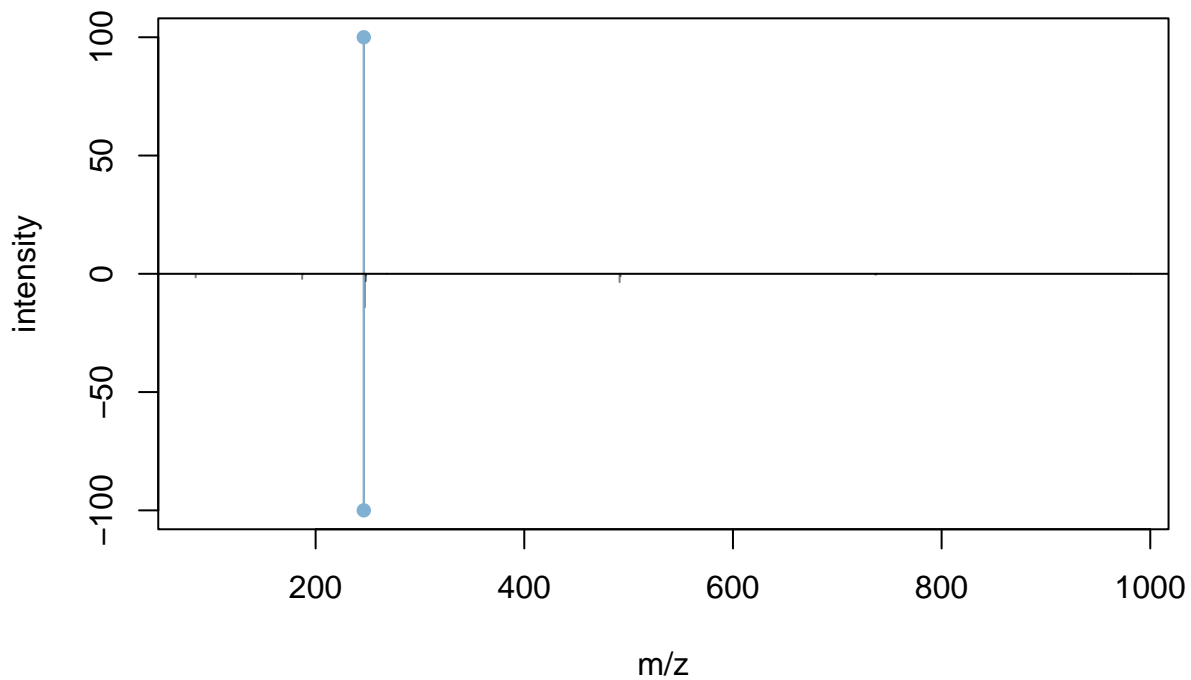
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1
inchikey	VSNFQQXVMPSASB-SNVBAGLBSA-N	VSNFQQXVMPSASB-SNVBAGLBSA-N
smiles	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C
formula	C12H23NO4	C12H23NO4

Retention time match

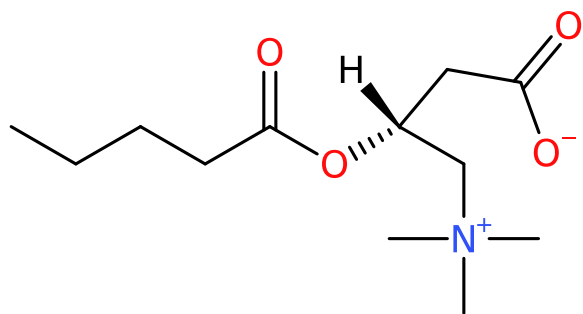
	DB	hit	error	rel. error	pcgroup
Retention time	2.84	2.77	-0.07	-2.6%	8

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0278	1.5			✘	✘
187.0969	2.2	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✘	✘
188.1056	0.2	[M+1] ⁺		✘	✘
246.1696	100.0	[M] ⁺	[M+H] ⁺	246.1689	100.0
246.3190	0.3			✘	✘
246.9140	0.7			✘	✘
247.1761	14.1	[M+1] ⁺		✘	✘
248.1772	3.1	[M+2] ⁺		✘	✘
248.2908	0.7			✘	✘
268.1561	0.1		[M+Na] ⁺	✘	✘
491.3337	3.5	[M] ⁺	[2M+H] ⁺	✘	✘
492.3415	1.1	[M+1] ⁺		✘	✘
736.5054	0.4	[M] ⁺	[3M+H] ⁺	✘	✘
737.5021	0.2	[M+1] ⁺		✘	✘
981.6574	0.1		[4M+H] ⁺	✘	✘

Valerylcarnitine



User identifiers

localidentifier	453
dataOrigin	20190715Q-080.mzML
CAS	40225-14-7
inchi	InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1

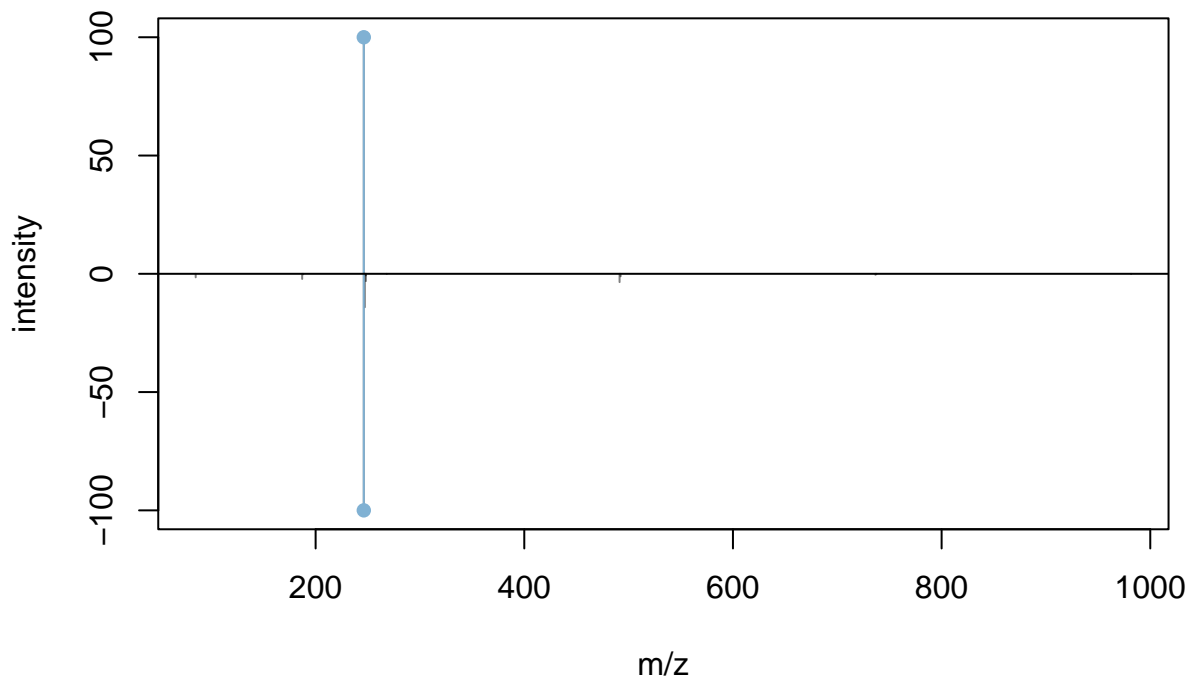
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1
inchikey	VSNFQQXVMPSASB-SNVBAGLBSA-N	VSNFQQXVMPSASB-SNVBAGLBSA-N
smiles	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C
formula	C12H23NO4	C12H23NO4

Retention time match

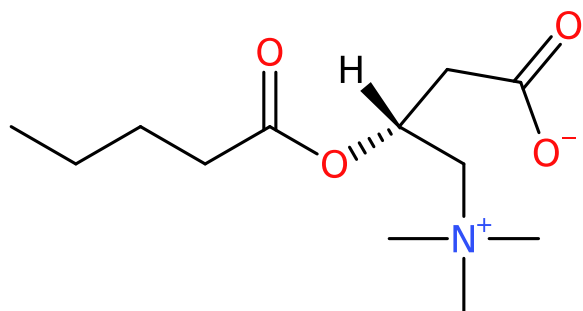
	DB	hit	error	rel. error	pcgroup
Retention time	2.84	2.84	0.00	0.1%	59

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0278	1.5			✘	✘
187.0969	2.2	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✘	✘
188.1056	0.2	[M+1] ⁺		✘	✘
246.1696	100.0	[M] ⁺	[M+H] ⁺	246.1691	100.0
246.3190	0.3			✘	✘
246.9140	0.7			✘	✘
247.1761	14.1	[M+1] ⁺		✘	✘
248.1772	3.1	[M+2] ⁺		✘	✘
248.2908	0.7			✘	✘
268.1561	0.1		[M+Na] ⁺	✘	✘
491.3337	3.5	[M] ⁺	[2M+H] ⁺	✘	✘
492.3415	1.1	[M+1] ⁺		✘	✘
736.5054	0.4	[M] ⁺	[3M+H] ⁺	✘	✘
737.5021	0.2	[M+1] ⁺		✘	✘
981.6574	0.1		[4M+H] ⁺	✘	✘

Valerylcarnitine



User identifiers

localidentifier	453
dataOrigin	20190715Q-080.mzML
CAS	40225-14-7
inchi	InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1

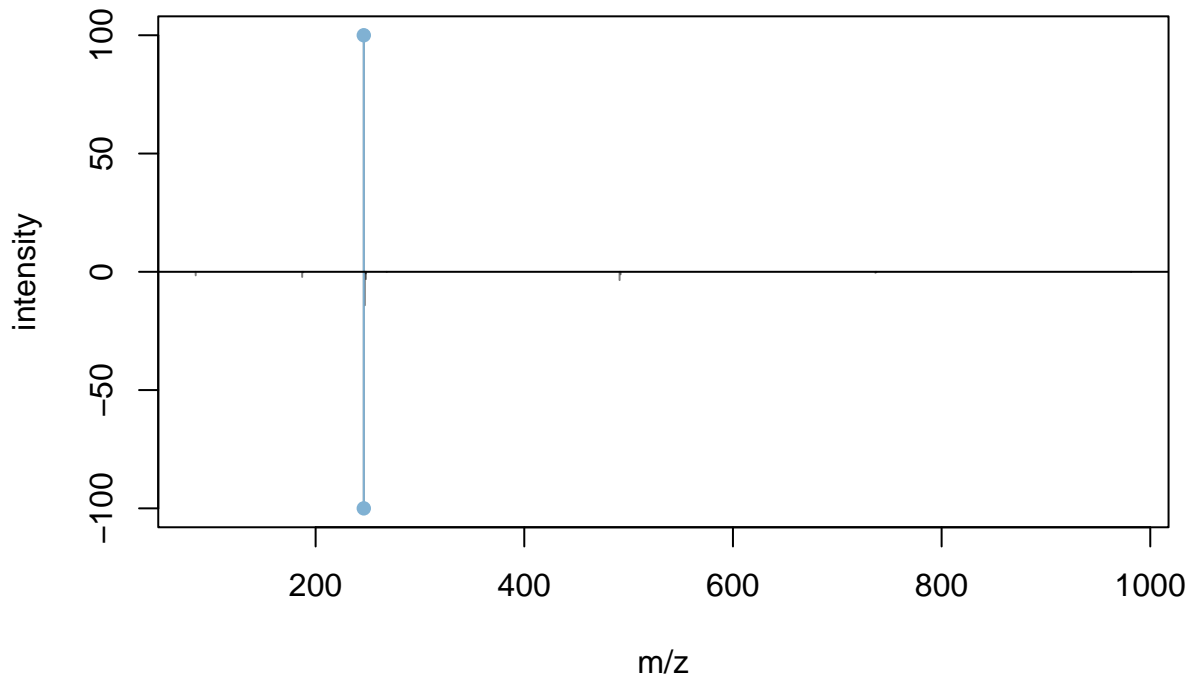
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C12H23NO4/c1-5-6-7-12(16)17-10(8-11(14)15)9-13(2,3)4/h10H,5-9H2,1-4H3/t10-/m1/s1
inchikey	VSNFQQXVMPSASB-SNVBAGLBSA-N	VSNFQQXVMPSASB-SNVBAGLBSA-N
smiles	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C	[H]C(OC(=O)CCCC)(CC(=O)[O-])C[N+](C)(C)C
formula	C12H23NO4	C12H23NO4

Retention time match

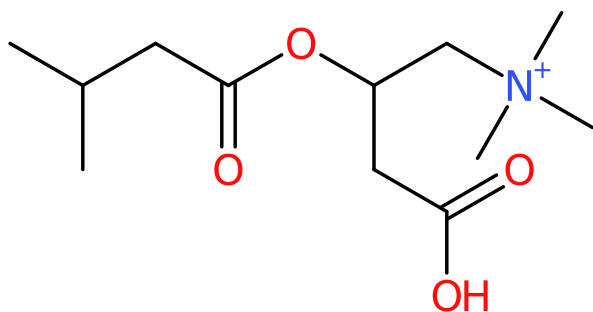
	DB	hit	error	rel. error	pcgroup
Retention time	2.84	2.92	0.08	2.9%	67

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0278	1.5			✘	✘
187.0969	2.2	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✘	✘
188.1056	0.2	[M+1] ⁺		✘	✘
246.1696	100.0	[M] ⁺	[M+H] ⁺	246.1702	100.0
246.3190	0.3			✘	✘
246.9140	0.7			✘	✘
247.1761	14.1	[M+1] ⁺		✘	✘
248.1772	3.1	[M+2] ⁺		✘	✘
248.2908	0.7			✘	✘
268.1561	0.1		[M+Na] ⁺	✘	✘
491.3337	3.5	[M] ⁺	[2M+H] ⁺	✘	✘
492.3415	1.1	[M+1] ⁺		✘	✘
736.5054	0.4	[M] ⁺	[3M+H] ⁺	✘	✘
737.5021	0.2	[M+1] ⁺		✘	✘
981.6574	0.1		[4M+H] ⁺	✘	✘

Isovaleryl-L-carnitine



User identifiers

localidentifier	627
dataOrigin	20190723Q-062.mzML
CAS	31023-24-2
inchi	InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1

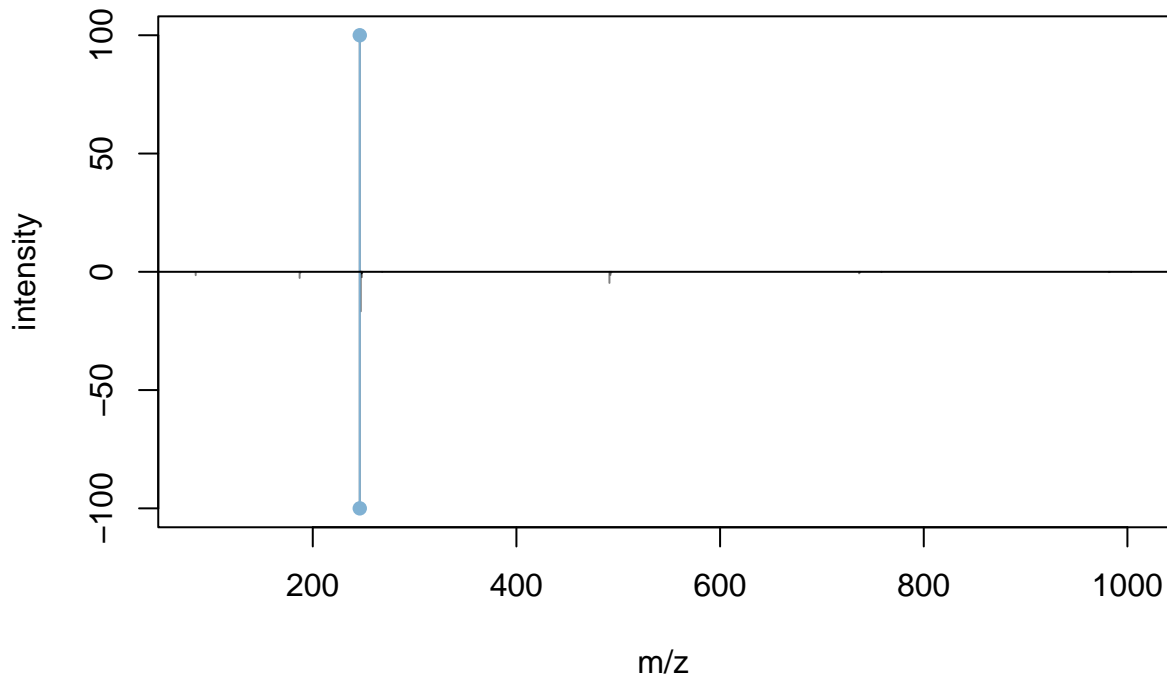
Computed identifiers

	Input as-is	Standardized structure
charge	1	0
inchi		InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1
inchikey	IGQBPDJNUXPEMT-UHFFFAOYSA-O	IGQBPDJNUXPEMT-UHFFFAOYSA-O
smiles	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C
formula	[C12H24NO4] ⁺	[C12H24NO4] ⁺

Retention time match

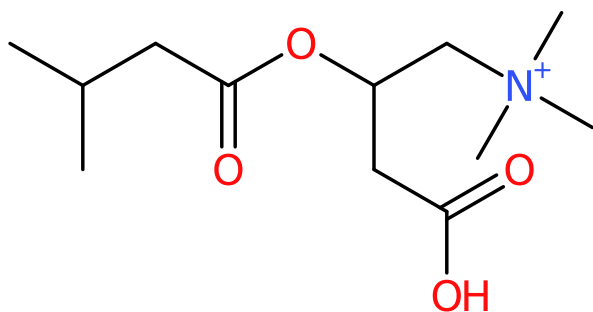
	DB	hit	error	rel. error	pcgroup
Retention time	2.76	2.77	0.00	0.1%	8

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0292	1.4			✗	✗
187.0973	2.6	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✗	✗
188.1010	0.3	[M+1] ⁺		✗	✗
246.1698	100.0	[M] ⁺	[M+H] ⁺	246.1689	100.0
246.7103	0.6			✗	✗
246.9698	0.3			✗	✗
247.0063	1.2			✗	✗
247.1745	16.7	[M+1] ⁺		✗	✗
247.4625	0.6			✗	✗
247.6552	0.4			✗	✗
247.7231	0.6			✗	✗
248.1782	2.3	[M+2] ⁺		✗	✗
248.4072	0.6			✗	✗
248.6134	0.3			✗	✗
268.1548	0.1		[M+Na] ⁺	✗	✗
491.3316	4.7	[M] ⁺	[2M+H] ⁺	✗	✗
492.3414	1.3	[M+1] ⁺		✗	✗
493.3423	0.3	[M+2] ⁺		✗	✗
736.4988	0.7	[M] ⁺	[3M+H] ⁺	✗	✗
737.5002	0.3	[M+1] ⁺		✗	✗
758.4821	0.1		[3M+Na] ⁺	✗	✗
981.6756	0.2	[M] ⁺	[4M+H] ⁺	✗	✗
982.6835	0.1	[M+1] ⁺		✗	✗
1003.6419	0.1		[4M+Na] ⁺	✗	✗

Isovaleryl-L-carnitine



User identifiers

localidentifier	627
dataOrigin	20190723Q-062.mzML
CAS	31023-24-2
inchi	InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1

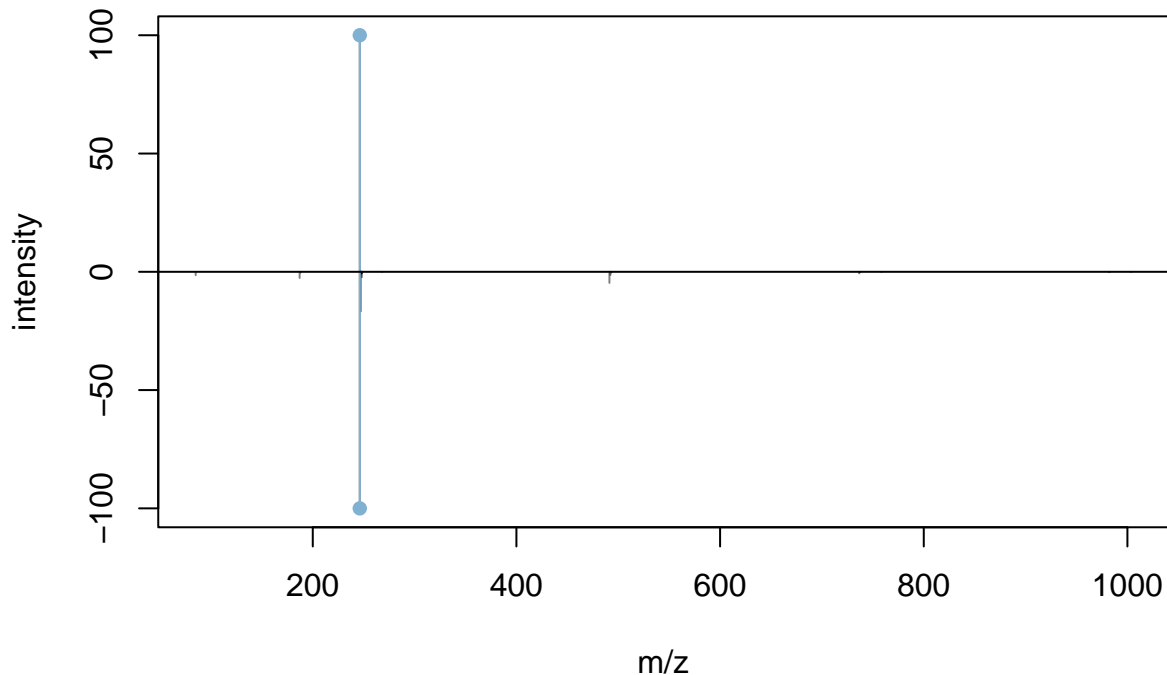
Computed identifiers

	Input as-is	Standardized structure
charge	1	0
inchi		InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1
inchikey	IGQBPDJNUXPEMT-UHFFFAOYSA-O	IGQBPDJNUXPEMT-UHFFFAOYSA-O
smiles	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C
formula	[C12H24NO4] ⁺	[C12H24NO4] ⁺

Retention time match

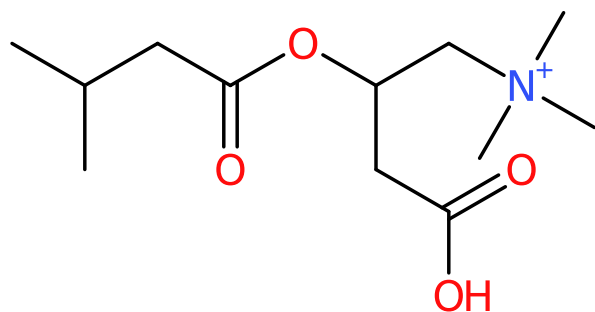
	DB	hit	error	rel. error	pcgroup
Retention time	2.76	2.84	0.08	2.8%	59

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0292	1.4			✗	✗
187.0973	2.6	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✗	✗
188.1010	0.3	[M+1] ⁺		✗	✗
246.1698	100.0	[M] ⁺	[M+H] ⁺	246.1691	100.0
246.7103	0.6			✗	✗
246.9698	0.3			✗	✗
247.0063	1.2			✗	✗
247.1745	16.7	[M+1] ⁺		✗	✗
247.4625	0.6			✗	✗
247.6552	0.4			✗	✗
247.7231	0.6			✗	✗
248.1782	2.3	[M+2] ⁺		✗	✗
248.4072	0.6			✗	✗
248.6134	0.3			✗	✗
268.1548	0.1		[M+Na] ⁺	✗	✗
491.3316	4.7	[M] ⁺	[2M+H] ⁺	✗	✗
492.3414	1.3	[M+1] ⁺		✗	✗
493.3423	0.3	[M+2] ⁺		✗	✗
736.4988	0.7	[M] ⁺	[3M+H] ⁺	✗	✗
737.5002	0.3	[M+1] ⁺		✗	✗
758.4821	0.1		[3M+Na] ⁺	✗	✗
981.6756	0.2	[M] ⁺	[4M+H] ⁺	✗	✗
982.6835	0.1	[M+1] ⁺		✗	✗
1003.6419	0.1		[4M+Na] ⁺	✗	✗

Isovaleryl-L-carnitine



User identifiers

localidentifier	627
dataOrigin	20190723Q-062.mzML
CAS	31023-24-2
inchi	InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1

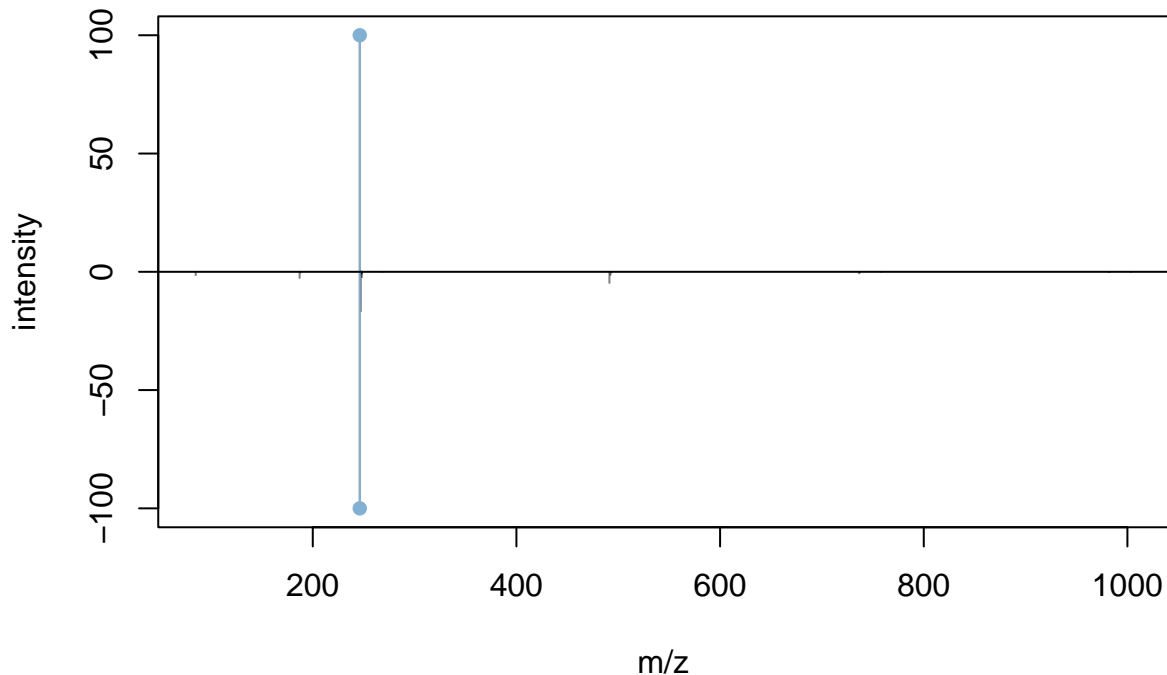
Computed identifiers

	Input as-is	Standardized structure
charge	1	0
inchi		InChI=1S/C12H23NO4/c1-9(2)6-12(16)17-10(7-11(14)15)8-13(3,4)5/h9-10H,6-8H2,1-5H3/p+1
inchikey	IGQBPDJNUXPEMT-UHFFFAOYSA-O	IGQBPDJNUXPEMT-UHFFFAOYSA-O
smiles	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C	O=C(O)CC(OC(=O)CC(C)C)C[N+](C)(C)C
formula	[C12H24NO4] ⁺	[C12H24NO4] ⁺

Retention time match

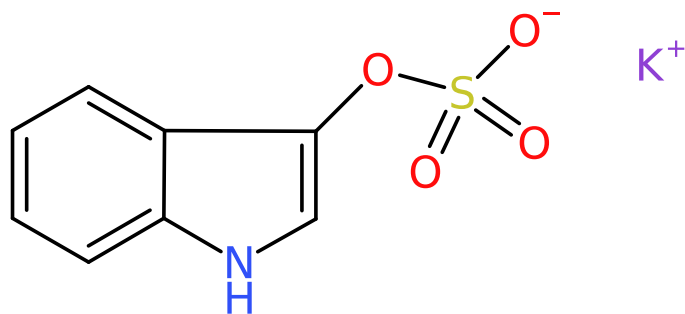
	DB	hit	error	rel. error	pcgroup
Retention time	2.76	2.92	0.16	5.7%	67

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0292	1.4			✗	✗
187.0973	2.6	[M] ⁺	[M+H-C ₃ H ₉ N] ⁺	✗	✗
188.1010	0.3	[M+1] ⁺		✗	✗
246.1698	100.0	[M] ⁺	[M+H] ⁺	246.1702	100.0
246.7103	0.6			✗	✗
246.9698	0.3			✗	✗
247.0063	1.2			✗	✗
247.1745	16.7	[M+1] ⁺		✗	✗
247.4625	0.6			✗	✗
247.6552	0.4			✗	✗
247.7231	0.6			✗	✗
248.1782	2.3	[M+2] ⁺		✗	✗
248.4072	0.6			✗	✗
248.6134	0.3			✗	✗
268.1548	0.1		[M+Na] ⁺	✗	✗
491.3316	4.7	[M] ⁺	[2M+H] ⁺	✗	✗
492.3414	1.3	[M+1] ⁺		✗	✗
493.3423	0.3	[M+2] ⁺		✗	✗
736.4988	0.7	[M] ⁺	[3M+H] ⁺	✗	✗
737.5002	0.3	[M+1] ⁺		✗	✗
758.4821	0.1		[3M+Na] ⁺	✗	✗
981.6756	0.2	[M] ⁺	[4M+H] ⁺	✗	✗
982.6835	0.1	[M+1] ⁺		✗	✗
1003.6419	0.1		[4M+Na] ⁺	✗	✗

Indoxyl sulfate



User identifiers

localidentifier	70
dataOrigin	12062019Q-203.mzML
CAS	2642-37-7
inchi	InChI=1S/C8H7NO4S.K/c10-14(11,12)13-8-5-9-7-4-2-1-3-6(7)8;/h1-5,9H,(H,10,11,12);/q:+1/p-1

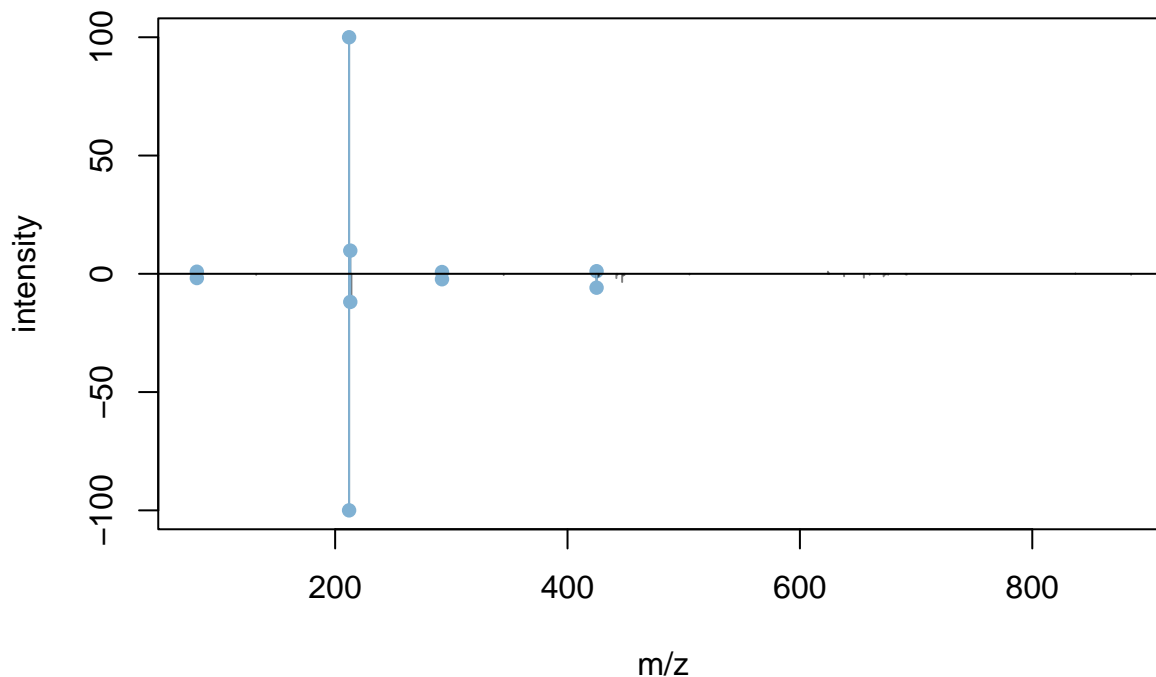
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H7NO4S/c10-14(11,12)13-8-5-9-7-4-2-1-3-6(7)8/h1-5,9H,(H,10,11,12)/p-1
inchikey	MDAWATNFDJIBBD-UHFFFAOYSA-M	BXFFHSIDQOFMLE-UHFFFAOYSA-M
smiles	[K+].O=S(=O)([O-])OC1=CNC=2C=CC=CC12	O=S(=O)([O-])OC1=CNC=2C=CC=CC12
formula	C8H6KNO4S	[C8H6NO4S]-

Retention time match

	DB	hit	error	rel. error	pcgroup
Retention time	2.54	2.78	0.24	9.6%	2

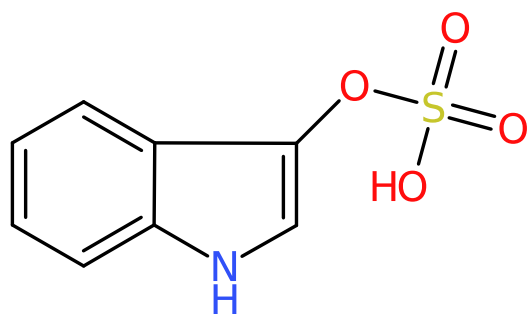
Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
79.9574	0.8			✗	✗
79.9587	0.8			✗	✗
80.9659	1.8			80.9655	0.9
132.0464	0.5		[M-H-SO ₃]-	✗	✗
212.0016	100.0	[M] ⁺	[M-H]-	212.0015	100.0
213.0066	11.9	[M+1] ⁺		213.0060	9.8
213.9969	11.4	[M+2] ⁺		✗	✗
291.9571	2.3			291.9617	0.7
293.9603	0.3			✗	✗
345.0540	0.5			✗	✗
425.0122	5.9	[M] ⁺	[2M-H]-	425.0124	1.1
426.0213	1.3	[M+1] ⁺		✗	✗
427.0160	0.9	[M+2] ⁺		✗	✗
442.0412	1.8	[M] ⁺		✗	✗
443.0338	0.4	[M+1] ⁺		✗	✗
446.9933	3.5	[M] ⁺	[2M-2H+Na]-	✗	✗
447.9982	0.8	[M+1] ⁺		✗	✗
448.9868	0.5	[M+2] ⁺		✗	✗
504.9658	0.3			✗	✗
✗	✗			624.1364	0.9
✗	✗			625.1407	0.3
638.0197	1.0		[3M-H]-	✗	✗
655.0536	1.6			✗	✗
659.9962	0.4		[3M-2H+Na]-	✗	✗
672.0743	1.1	[M] ⁺		✗	✗
673.0706	0.4	[M+1] ⁺		✗	✗
674.0726	0.3	[M+2] ⁺		✗	✗
675.9636	0.4		[3M-2H+K]-	✗	✗
690.9435	0.3		[3M-4H+Fe ³⁺]-	✗	✗
691.9406	0.4		[3M-3H+Fe ²⁺]-	✗	✗

	X	X		837.1468	0.2
885.0814		0.4		X	X

3-indoxyl sulfate



User identifiers

localidentifier	663
dataOrigin	20190723Q-207.mzML
CAS	487-94-5
inchi	InChI=1S/C8H7NO4S/c10-14(11,12)13-8-5-9-7-4-2-1-3-6(7)8/h1-5,9H,(H,10,11,12)

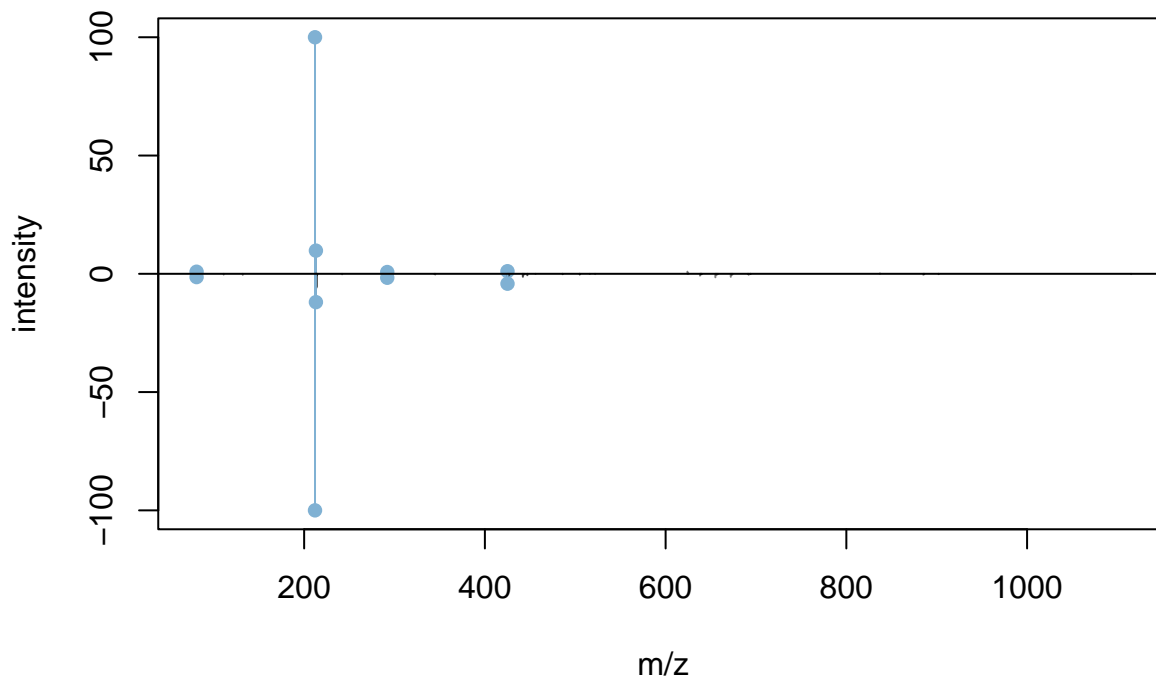
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H7NO4S/c10-14(11,12)13-8-5-9-7-4-2-1-3-6(7)8/h1-5,9H,(H,10,11,12)
inchikey	BXFFHSIDQOFMLE-UHFFFAOYSA-N	BXFFHSIDQOFMLE-UHFFFAOYSA-N
smiles	O=S(=O)(O)OC1=CNC=2C=CC=CC12	O=S(=O)(O)OC1=CNC=2C=CC=CC12
formula	C8H7NO4S	C8H7NO4S

Retention time match

	DB	hit	error	rel. error	pcgroup
Retention time	2.42	2.78	0.37	15.2%	2

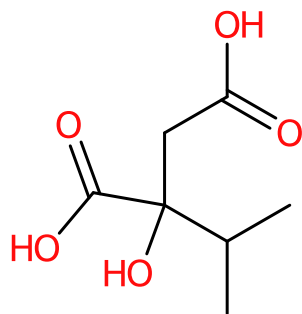
Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
79.9599	0.7			✗	✗
80.9650	1.4			80.9655	0.9
110.9779	0.3			✗	✗
132.0463	0.4		[M-H-SO ₃]-	✗	✗
212.0019	100.0	[M] ⁺	[M-H] ⁻	212.0015	100.0
212.4269	0.3			✗	✗
212.7689	0.5			✗	✗
213.0043	12.0	[M+1] ⁺		213.0060	9.8
213.4798	0.3			✗	✗
214.0015	5.8	[M+2] ⁺		✗	✗
214.0020	5.3			✗	✗
214.0960	0.7			✗	✗
214.6904	0.3			✗	✗
242.0211	0.2			✗	✗
291.9627	1.7	[M] ⁺		291.9617	0.7
292.9626	0.2	[M+1] ⁺		✗	✗
293.9618	0.2	[M+2] ⁺		✗	✗
344.0508	0.1			✗	✗
345.0565	0.3			✗	✗
425.0144	4.2	[M] ⁺	[2M-H] ⁻	425.0124	1.1
426.0175	1.0	[M+1] ⁺		✗	✗
427.0138	0.6	[M+2] ⁺		✗	✗
442.0370	1.0	[M] ⁺		✗	✗
442.0394	1.3			✗	✗
443.0453	0.3	[M+1] ⁺		✗	✗
444.0307	0.3	[M+2] ⁺		✗	✗
446.9938	0.5		[2M-2H+Na] ⁻	✗	✗
446.9969	0.6		[2M-2H+Na] ⁻	✗	✗
456.0500	0.1			✗	✗
486.0638	0.2			✗	✗

486.0698	0.1			×	×
504.9656	0.2			×	×
504.9696	0.3			×	×
504.9748	0.2			×	×
516.0831	0.1			×	×
521.9953	0.2			×	×
×	×			624.1364	0.9
×	×			625.1407	0.3
638.0250	0.8	[M]+	[3M-H]-	×	×
639.0140	0.2	[M+1]+		×	×
639.0240	0.2			×	×
639.0266	0.2			×	×
640.0184	0.2			×	×
640.0223	0.1			×	×
655.0473	1.5	[M]+		×	×
656.0547	0.4	[M+1]+		×	×
657.0465	0.3	[M+2]+		×	×
658.0512	0.1	[M+3]+		×	×
672.0756	1.3	[M]+		×	×
673.0737	0.4	[M+1]+		×	×
674.0778	0.3	[M+2]+		×	×
690.9317	0.2		[3M-4H+Fe3+]-	×	×
691.9392	0.4		[3M-3H+Fe2+]-	×	×
693.9480	0.1			×	×
693.9535	0.1			×	×
×	×			837.1468	0.2
885.0939	0.4	[M]+		×	×
886.0713	0.2	[M+1]+		×	×
886.0761	0.2			×	×
902.0957	0.1			×	×
902.1255	0.2			×	×
1115.1279	0.1			×	×

2-Isopropylmalic acid



User identifiers

localidentifier	178
dataOrigin	14062019Q-198.mzML
CAS	3237-44-3
inchi	InChI=1S/C7H12O5/c1-4(2)7(12,6(10)11)3-5(8)9/h4,12H,3H2,1-2H3,(H,8,9)(H,10,11)

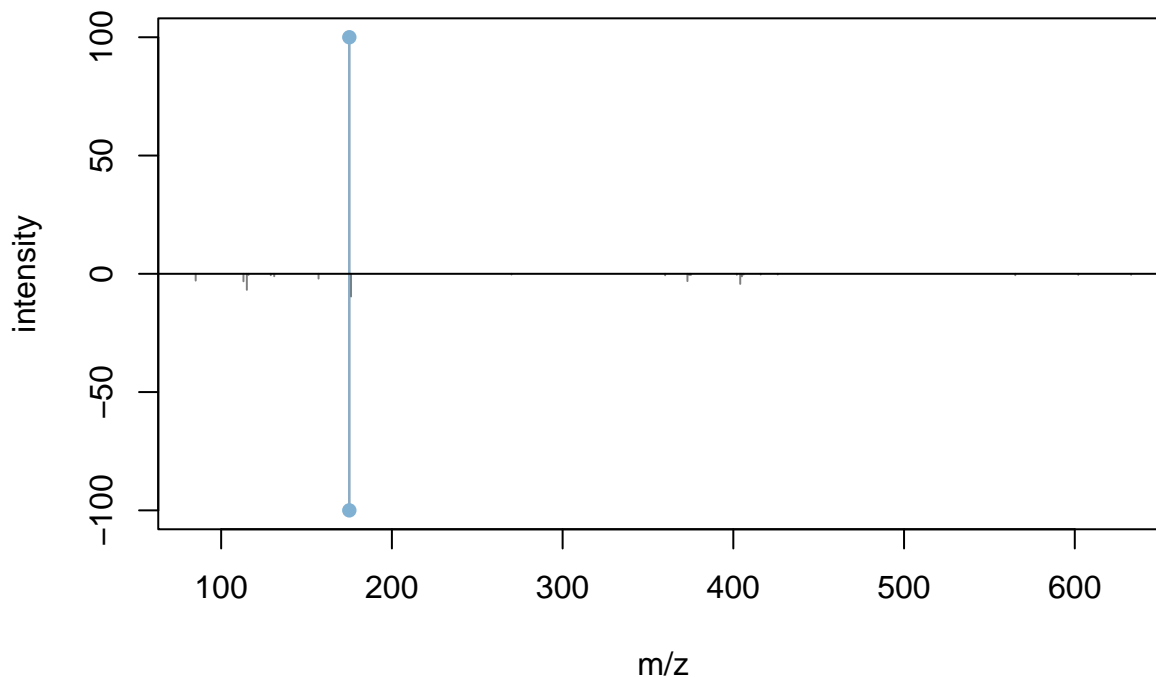
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H12O5/c1-4(2)7(12,6(10)11)3-5(8)9/h4,12H,3H2,1-2H3,(H,8,9)(H,10,11)
inchikey	BITYXLXUCSKTJS-UHFFFAOYSA-N	BITYXLXUCSKTJS-UHFFFAOYSA-N
smiles	O=C(O)CC(O)(C(=O)O)C(C)C	O=C(O)CC(O)(C(=O)O)C(C)C
formula	C7H12O5	C7H12O5

Retention time match

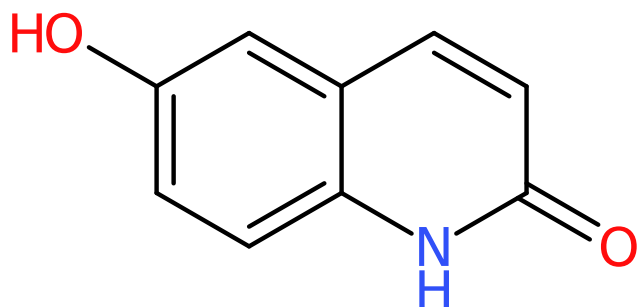
	DB	hit	error	rel. error	pcgroup
Retention time	3.14	2.84	-0.31	-9.8%	59

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
85.0654	2.9			✗	✗
113.0609	3.2		[M-H-H ₂ O-CO ₂]-	✗	✗
115.0399	6.8	[M] ⁺	[M-H-C ₂ H ₄ O ₂]-	✗	✗
116.0438	0.5	[M+1] ⁺		✗	✗
129.0564	0.6		[M-H-HCOOH]-	✗	✗
131.0721	1.0		[M-H-CO ₂]-	✗	✗
157.0487	2.0		[M-H-H ₂ O]-	✗	✗
175.0600	100.0	[M] ⁺	[M-H]-	175.0603	100.0
176.0668	9.6	[M+1] ⁺		✗	✗
270.0605	0.3			✗	✗
360.0472	0.6			✗	✗
373.1113	3.1	[M] ⁺	[2M-2H+Na]-	✗	✗
374.1147	0.5	[M+1] ⁺		✗	✗
375.0910	0.5		[2M-4H+Al ³⁺]-	✗	✗
402.0419	0.4			✗	✗
404.0409	4.3	[M] ⁺	[2M-4H+Fe ³⁺]-	✗	✗
405.0401	1.1	[M+1] ⁺		✗	✗
406.0422	0.3	[M+2] ⁺		✗	✗
416.0415	0.3			✗	✗
426.0296	0.3			✗	✗
565.1559	0.6		[3M-2H+K]-	✗	✗
602.0745	0.5			✗	✗
633.0126	0.4			✗	✗

2,6-dihydroxyquinoline



User identifiers

localidentifier	161
dataOrigin	14062019Q-072.mzML
CAS	19315-93-6
inchi	InChI=1S/C9H7NO2/c11-7-2-3-8-6(5-7)1-4-9(12)10-8/h1-5,11H,(H,10,12)

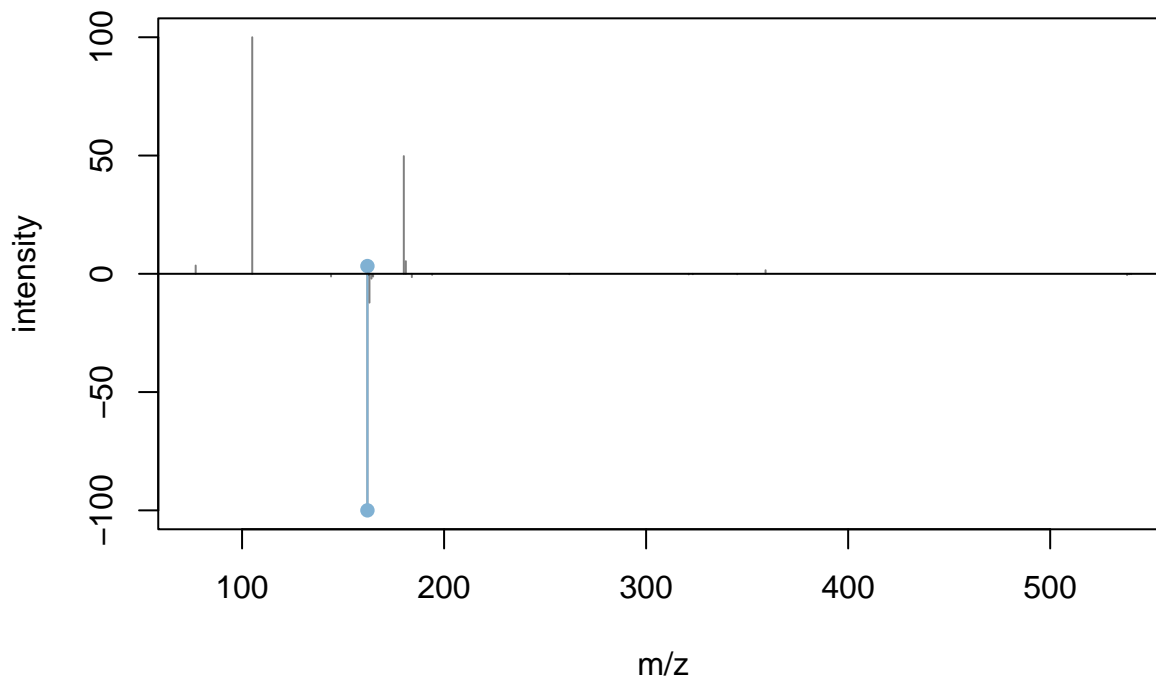
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H7NO2/c11-7-2-3-8-6(5-7)1-4-9(12)10-8/h1-5,11H,(H,10,12)
inchikey	AQLYZDRHNNHZZHIS-UHFFFAOYSA-N	AQLYZDRHNNHZZHIS-UHFFFAOYSA-N
smiles	O=C1C=CC=2C=C(O)C=CC2N1	O=C1C=CC=2C=C(O)C=CC2N1
formula	C9H7NO2	C9H7NO2

Retention time match

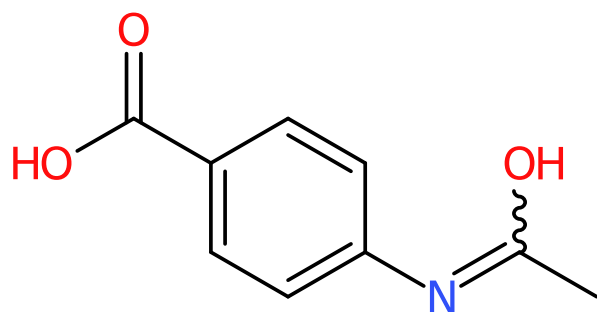
	DB	hit	error	rel. error	pcgroup
Retention time	2.93	3.06	0.13	4.4%	5

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
×	×			77.0385	3.5
×	×			105.0335	100.0
144.0466	1.1		[M+H-H ₂ O] ⁺	×	×
162.0562	100.0	[M] ⁺	[M+H] ⁺	162.0554	3.3
162.2374	0.6			×	×
162.5753	0.6			×	×
163.0606	12.2	[M+1] ⁺		×	×
164.0579	2.0	[M+2] ⁺		×	×
164.8690	1.2			×	×
×	×			180.0660	49.8
×	×			181.0693	5.3
184.0391	1.4		[M+Na] ⁺	×	×
194.0830	0.4			×	×
261.9847	0.2			×	×
321.0933	0.3			×	×
323.1069	0.2		[2M+H] ⁺	×	×
345.0828	0.2		[2M+Na] ⁺	×	×
×	×			359.1245	1.5
538.0668	0.6	[M] ⁺		×	×
539.0739	0.2	[M+1] ⁺		×	×
540.0679	0.2	[M+2] ⁺		×	×

4-Acetamidobenzoic acid



User identifiers

localidentifier	221
dataOrigin	20190701Q-145.mzML
CAS	556-08-1
inchi	InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)

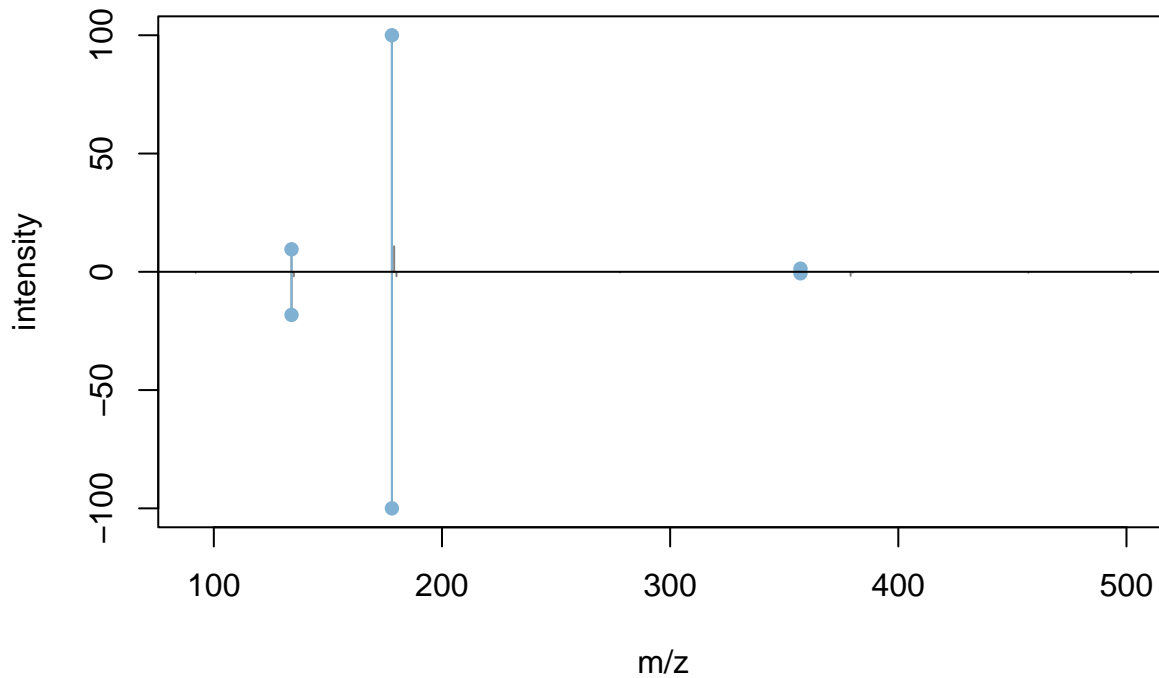
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
inchikey	QCXJEYYXVJIFCE-UHFFFAOYSA-N	QCXJEYYXVJIFCE-UHFFFAOYSA-N
smiles	O=C(O)C1=CC=C(N=C(O)C)C=C1	O=C(O)C1=CC=C(N=C(O)C)C=C1
formula	C9H9NO3	C9H9NO3

Retention time match

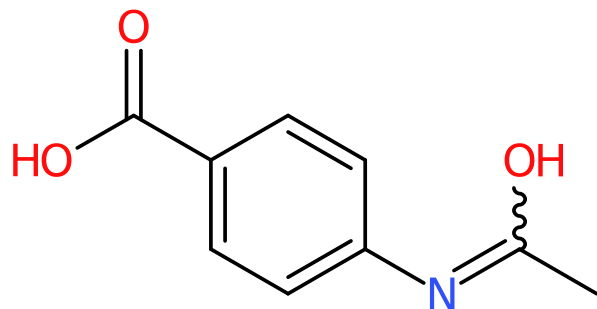
	DB	hit	error	rel. error	pcgroup
Retention time	3.27	3.06	-0.21	-6.5%	3

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
92.0487	0.4			✗	✗
134.0584	18.2	[M] ⁺	[M-H-CO ₂] ⁻	134.0606	9.5
135.0648	1.9	[M+1] ⁺		✗	✗
178.0511	100.0		[M-H] ⁻	178.0498	100.0
✗	✗			179.0545	10.8
180.0576	1.9			✗	✗
277.9763	0.2			✗	✗
357.1111	0.6		[2M-H] ⁻	357.1068	1.3
✗	✗			358.1121	0.3
379.0918	1.7	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
380.0912	0.3	[M+1] ⁺		✗	✗
457.0312	0.4			✗	✗
502.0325	0.5			✗	✗

4-Acetamidobenzoic acid



User identifiers

localidentifier	221
dataOrigin	20190701Q-038.mzML
CAS	556-08-1
inchi	InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)

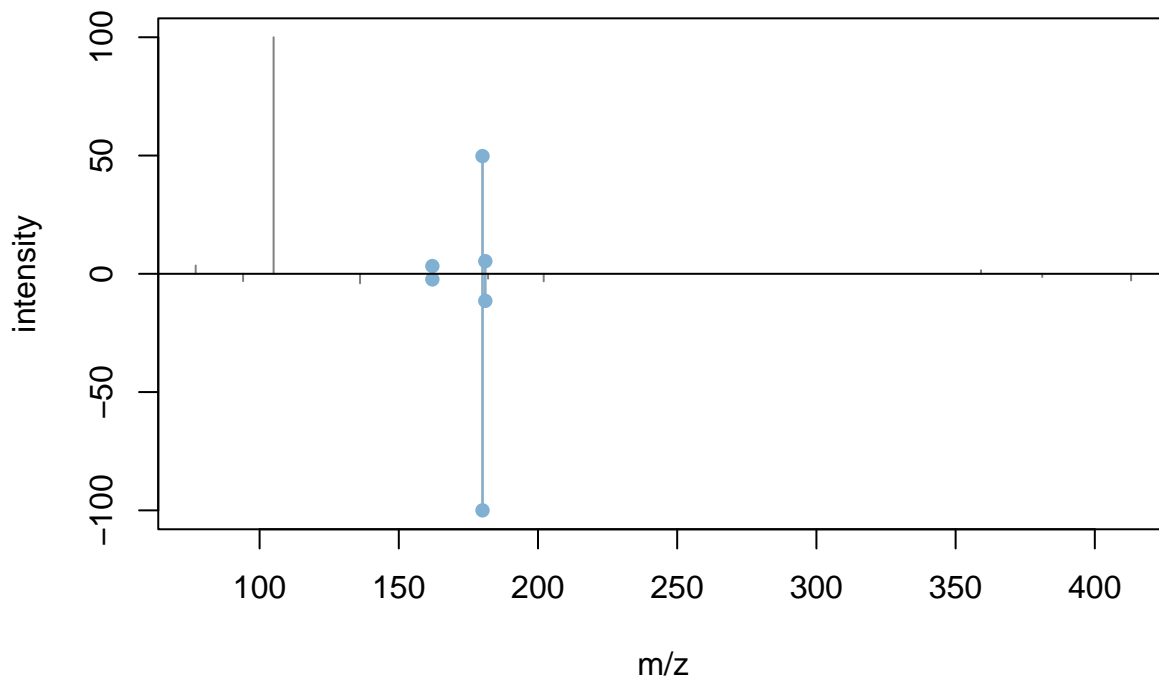
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
inchikey	QCXJEYYXVJIFCE-UHFFFAOYSA-N	QCXJEYYXVJIFCE-UHFFFAOYSA-N
smiles	O=C(O)C1=CC=C(N=C(O)C)C=C1	O=C(O)C1=CC=C(N=C(O)C)C=C1
formula	C9H9NO3	C9H9NO3

Retention time match

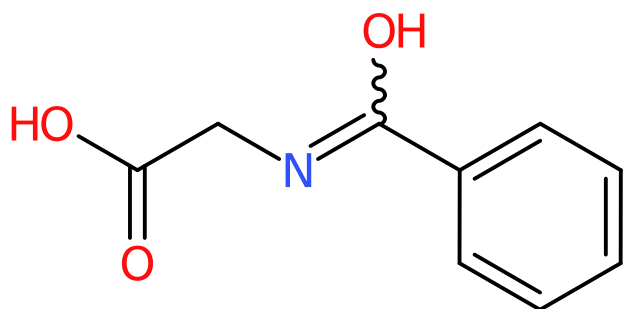
	DB	hit	error	rel. error	pcgroup
Retention time	3.27	3.06	-0.22	-6.6%	5

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
×	×			77.0385	3.5
94.0646	3.1			×	×
×	×			105.0335	100.0
136.0759	4.0		[M+H-CO ₂] ⁺	×	×
162.0544	2.4		[M+H-H ₂ O] ⁺	162.0554	3.3
180.0644	100.0	[M] ⁺	[M+H] ⁺	180.0660	49.8
181.0698	11.4	[M+1] ⁺		181.0693	5.3
182.0709	2.0	[M+2] ⁺		×	×
202.0471	3.2		[M+Na] ⁺	×	×
×	×			359.1245	1.5
381.1125	1.4		[2M+Na] ⁺	×	×
413.0452	2.8			×	×

Hippuric acid



User identifiers

localidentifier	339
dataOrigin	20190710Q-169.mzML
CAS	495-69-2
inchi	InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)

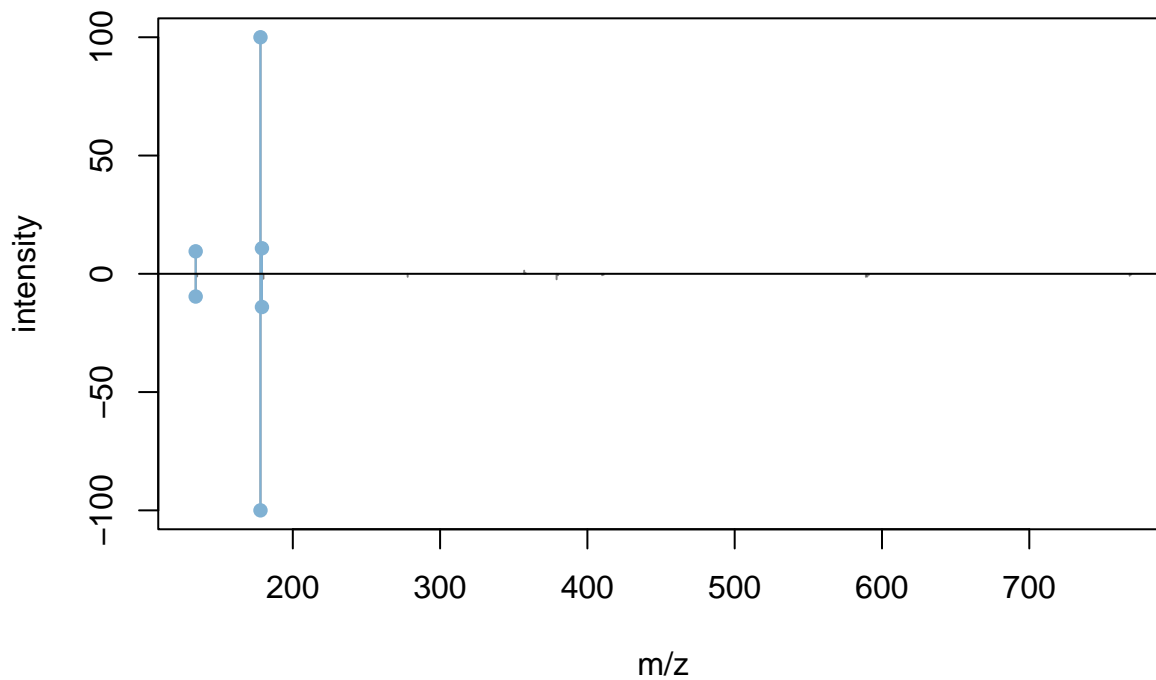
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)
inchikey	QIAFMBKCNZACKA-UHFFFAOYSA-N	QIAFMBKCNZACKA-UHFFFAOYSA-N
smiles	O=C(O)CN=C(O)C=1C=CC=CC1	O=C(O)CN=C(O)C=1C=CC=CC1
formula	C9H9NO3	C9H9NO3

Retention time match

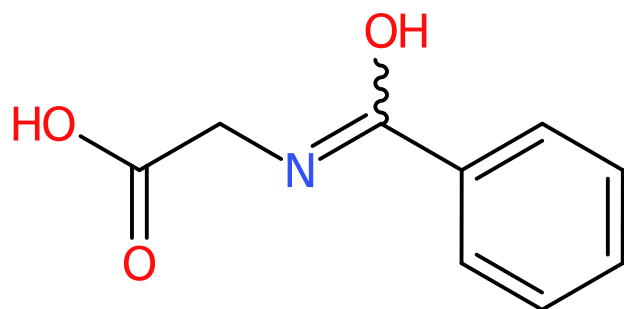
	DB	hit	error	rel. error	pcgroup
Retention time	3.08	3.06	-0.02	-0.5%	3

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
134.0593	9.6	[M] ⁺	[M-H-CO ₂] ⁻	134.0606	9.5
135.0639	1.1	[M+1] ⁺		✗	✗
178.0493	100.0	[M] ⁺	[M-H] ⁻	178.0498	100.0
179.0501	14.0	[M+1] ⁺		179.0545	10.8
180.0614	2.1	[M+2] ⁺		✗	✗
277.9776	1.3			✗	✗
✗	✗			357.1068	1.3
✗	✗			358.1121	0.3
379.0880	2.3	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
380.0925	0.6	[M+1] ⁺		✗	✗
410.0146	0.6		[2M-4H+Fe ³⁺] ⁻	✗	✗
411.0359	0.4		[2M-3H+Fe ²⁺] ⁻	✗	✗
589.0735	1.3		[3M-4H+Fe ³⁺] ⁻	✗	✗
590.0812	1.1	[M] ⁺	[3M-3H+Fe ²⁺] ⁻	✗	✗
591.0891	0.4	[M+1] ⁺		✗	✗
768.1321	0.8	[M] ⁺	[4M-4H+Fe ³⁺] ⁻	✗	✗
769.1422	0.3	[M+1] ⁺		✗	✗

Hippuric acid



User identifiers

localidentifier	339
dataOrigin	20190710Q-062.mzML
CAS	495-69-2
inchi	InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)

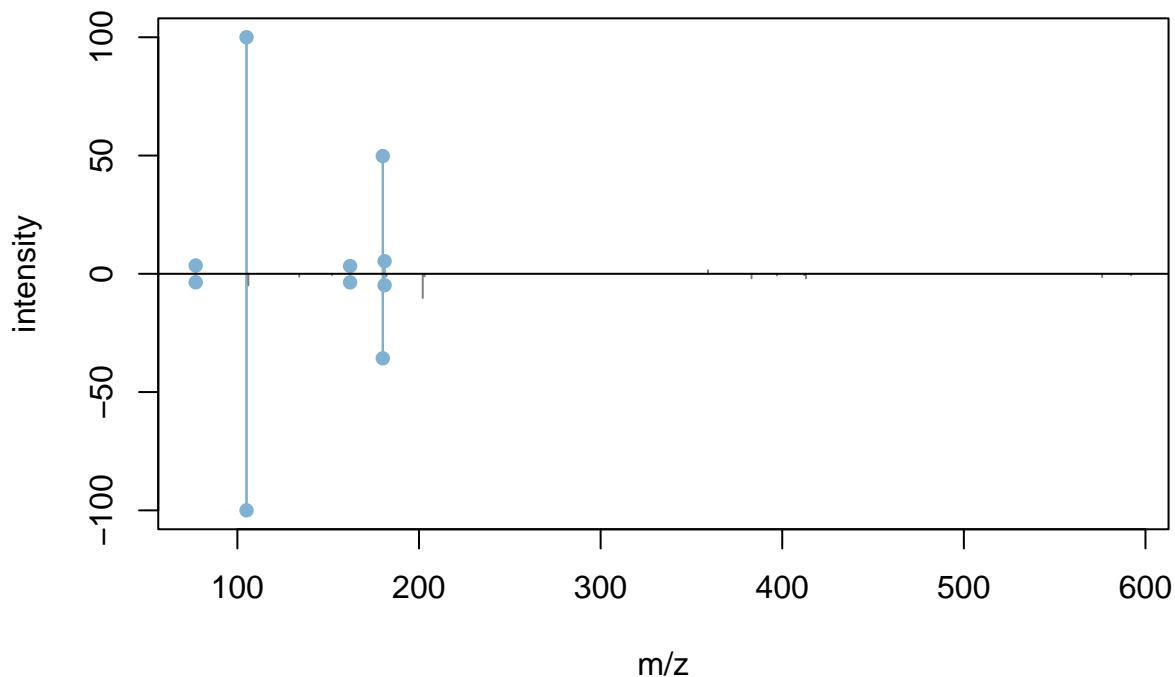
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)
inchikey	QIAFMBKCNZACKA-UHFFFAOYSA-N	QIAFMBKCNZACKA-UHFFFAOYSA-N
smiles	O=C(O)CN=C(O)C=1C=CC=CC1	O=C(O)CN=C(O)C=1C=CC=CC1
formula	C9H9NO3	C9H9NO3

Retention time match

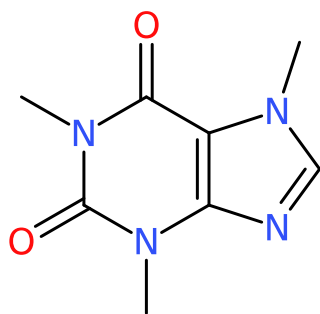
	DB	hit	error	rel. error	pcgroup
Retention time	3.08	3.06	-0.03	-0.8%	5

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
77.0367	3.6			77.0385	3.5
105.0328	100.0	[M] ⁺		105.0335	100.0
106.0295	4.9	[M+1] ⁺		✗	✗
134.0622	1.3		[M+H-HCOOH] ⁺	✗	✗
152.0760	0.5			✗	✗
162.0576	3.6		[M+H-H ₂ O] ⁺	162.0554	3.3
180.0631	35.7	[M] ⁺	[M+H] ⁺	180.0660	49.8
181.0681	4.8	[M+1] ⁺		181.0693	5.3
182.0702	0.9	[M+2] ⁺		✗	✗
202.0454	10.2	[M] ⁺	[M+Na] ⁺	✗	✗
203.0486	1.1	[M+1] ⁺		✗	✗
✗	✗			359.1245	1.5
383.0865	1.9		[2M-2H+Al ₃] ⁺	✗	✗
397.0743	0.7		[2M+K] ⁺	✗	✗
412.0400	0.6		[2M-2H+Fe ₃] ⁺	✗	✗
413.0404	1.9			✗	✗
576.1434	1.4		[3M+K] ⁺	✗	✗
592.0980	0.7			✗	✗

Caffeine



User identifiers

localidentifier	290
dataOrigin	20190710Q-009.mzML
CAS	58-08-2
inchi	InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3

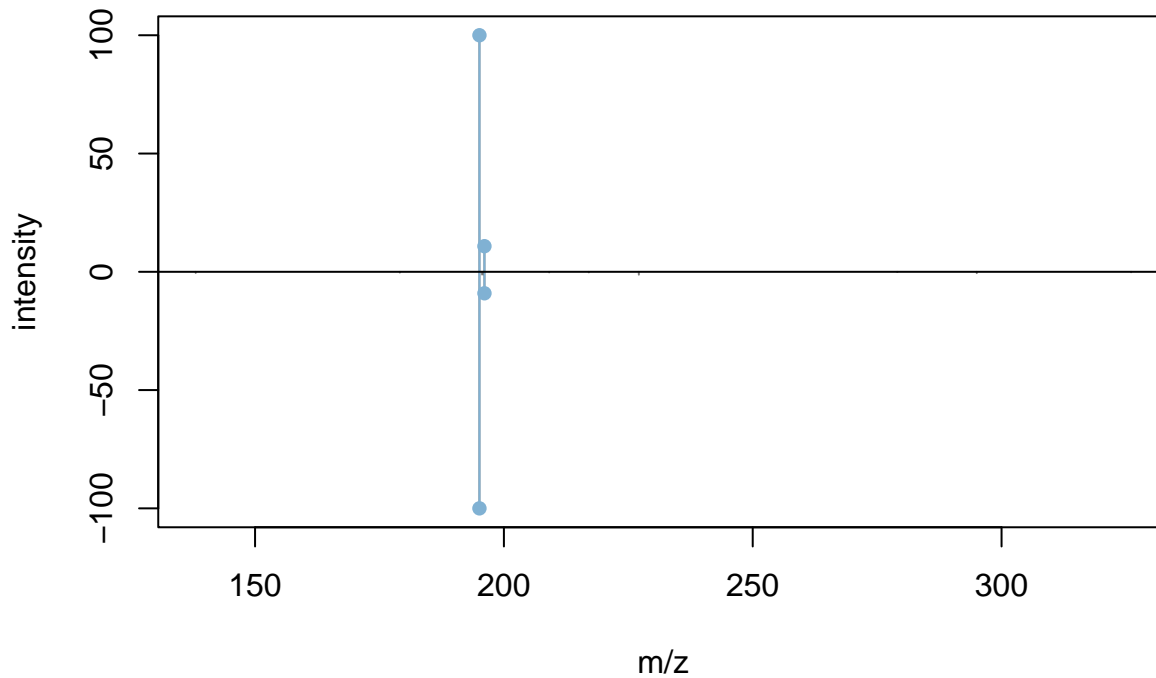
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
inchikey	RYYVLZVUVIJVGH-UHFFFAOYSA-N	RYYVLZVUVIJVGH-UHFFFAOYSA-N
smiles	O=C1C2=C(N=CN2C)N(C(=O)N1C)C	O=C1C2=C(N=CN2C)N(C(=O)N1C)C
formula	C8H10N4O2	C8H10N4O2

Retention time match

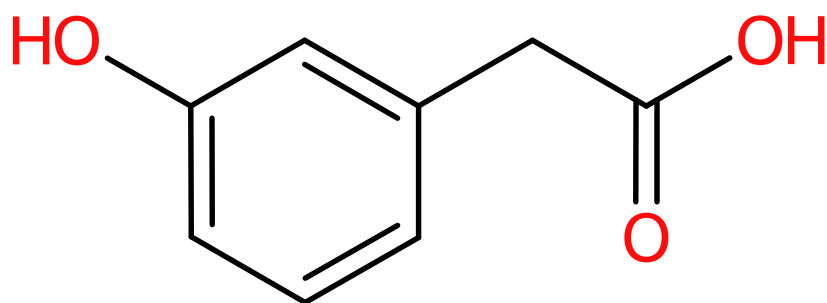
	DB	hit	error	rel. error	pcgroup
Retention time	3.23	3.09	-0.14	-4.3%	1

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
138.0652	0.5			✗	✗
179.0913	0.3		[M+H-O] ⁺	✗	✗
195.0873	100.0	[M] ⁺	[M+H] ⁺	195.0870	100.0
195.6173	1.2			✗	✗
195.9632	1.2			✗	✗
196.0938	9.1	[M+1] ⁺		196.0917	10.8
209.1013	0.2			✗	✗
217.0694	0.2		[M+Na] ⁺	✗	✗
227.1164	1.2			✗	✗
279.0473	0.1			✗	✗
295.0178	0.6			✗	✗
326.0401	0.2			✗	✗

3-Hydroxyphenylacetic acid



User identifiers

localidentifier	206
dataOrigin	20190701Q-128.mzML
CAS	621-37-4
inchi	InChI=1S/C8H8O3/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)

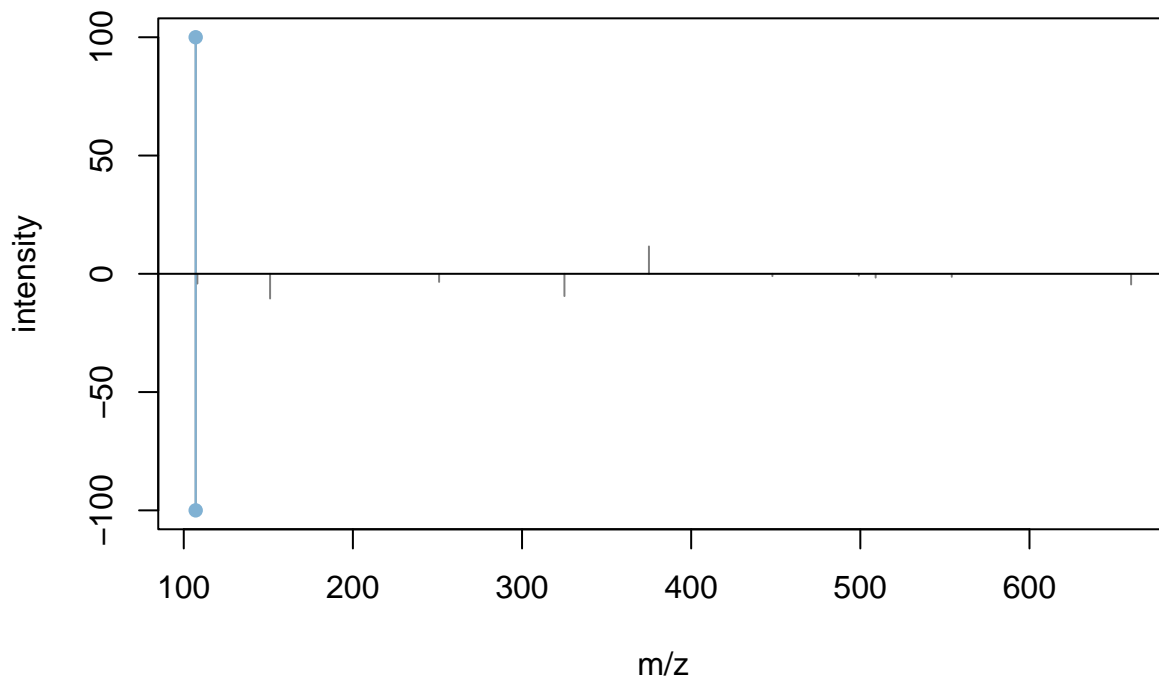
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H8O3/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)
inchikey	FVMDYYGIDFPZAX-UHFFFAOYSA-N	FVMDYYGIDFPZAX-UHFFFAOYSA-N
smiles	O=C(O)CC=1C=CC=C(O)C1	O=C(O)CC=1C=CC=C(O)C1
formula	C8H8O3	C8H8O3

Retention time match

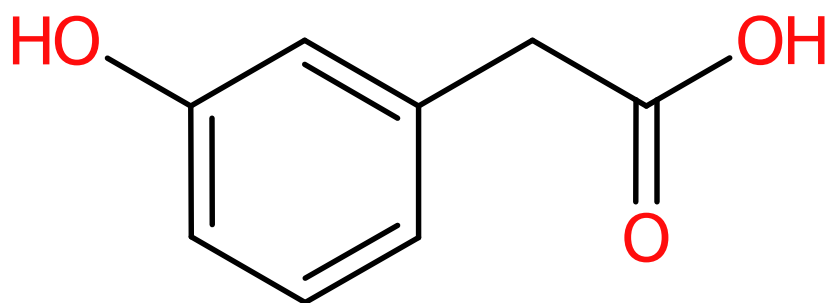
	DB	hit	error	rel. error	pcgroup
Retention time	3.24	3.40	0.16	5.0%	112

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
107.0509	100.0	[M] ⁺	[M-H-CO ₂] ⁻	107.0496	100.0
108.0545	4.1	[M+1] ⁺		✗	✗
151.0384	10.4		[M-H] ⁻	✗	✗
250.9680	3.4			✗	✗
325.0684	9.4		[2M-2H+Na] ⁻	✗	✗
✗	✗			375.0238	11.6
448.0103	1.0			✗	✗
499.0989	0.8			✗	✗
509.0488	1.6		[3M-3H+Fe ²⁺] ⁻	✗	✗
554.0505	1.3			✗	✗
660.0994	4.5		[4M-4H+Fe ³⁺] ⁻	✗	✗

3-Hydroxyphenylacetic acid



User identifiers

localidentifier	206
dataOrigin	20190701Q-128.mzML
CAS	621-37-4
inchi	InChI=1S/C8H8O3/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)

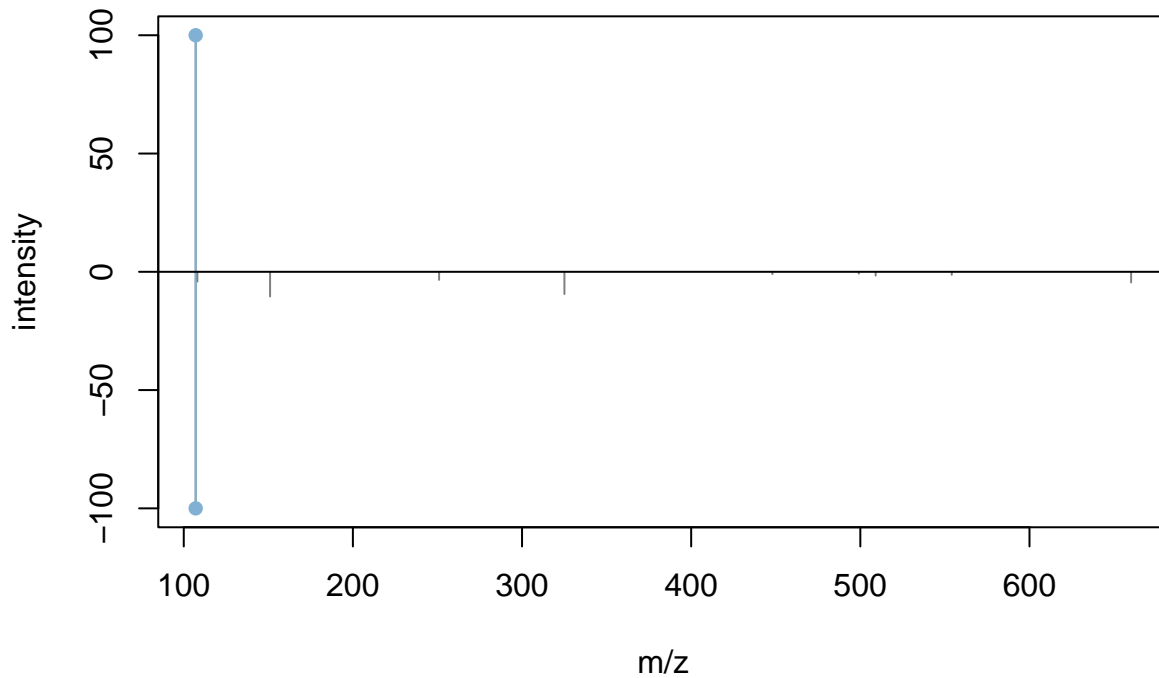
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H8O3/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)
inchikey	FVMDYYGIDFPZAX-UHFFFAOYSA-N	FVMDYYGIDFPZAX-UHFFFAOYSA-N
smiles	O=C(O)CC=1C=CC=C(O)C1	O=C(O)CC=1C=CC=C(O)C1
formula	C8H8O3	C8H8O3

Retention time match

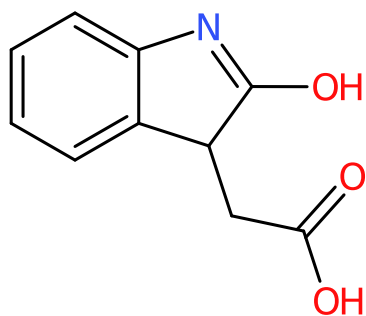
	DB	hit	error	rel. error	pcgroup
Retention time	3.24	3.25	0.00	0.1%	169

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
107.0509	100.0	[M] ⁺	[M-H-CO ₂] ⁻	107.0498	100.0
108.0545	4.1	[M+1] ⁺		✗	✗
151.0384	10.4		[M-H] ⁻	✗	✗
250.9680	3.4			✗	✗
325.0684	9.4		[2M-2H+Na] ⁻	✗	✗
448.0103	1.0			✗	✗
499.0989	0.8			✗	✗
509.0488	1.6		[3M-3H+Fe ²⁺] ⁻	✗	✗
554.0505	1.3			✗	✗
660.0994	4.5		[4M-4H+Fe ³⁺] ⁻	✗	✗

2-oxo-2,3-dihydro-1H-indol-3-yl-acetic acid



User identifiers

localidentifier	3
dataOrigin	12062019Q-025.mzML
CAS	2971-31-5
inchi	InChI=1S/C10H9NO3/c12-9(13)5-7-6-3-1-2-4-8(6)11-10(7)14/h1-4,7H,5H2,(H,11,14)(H,12,13)

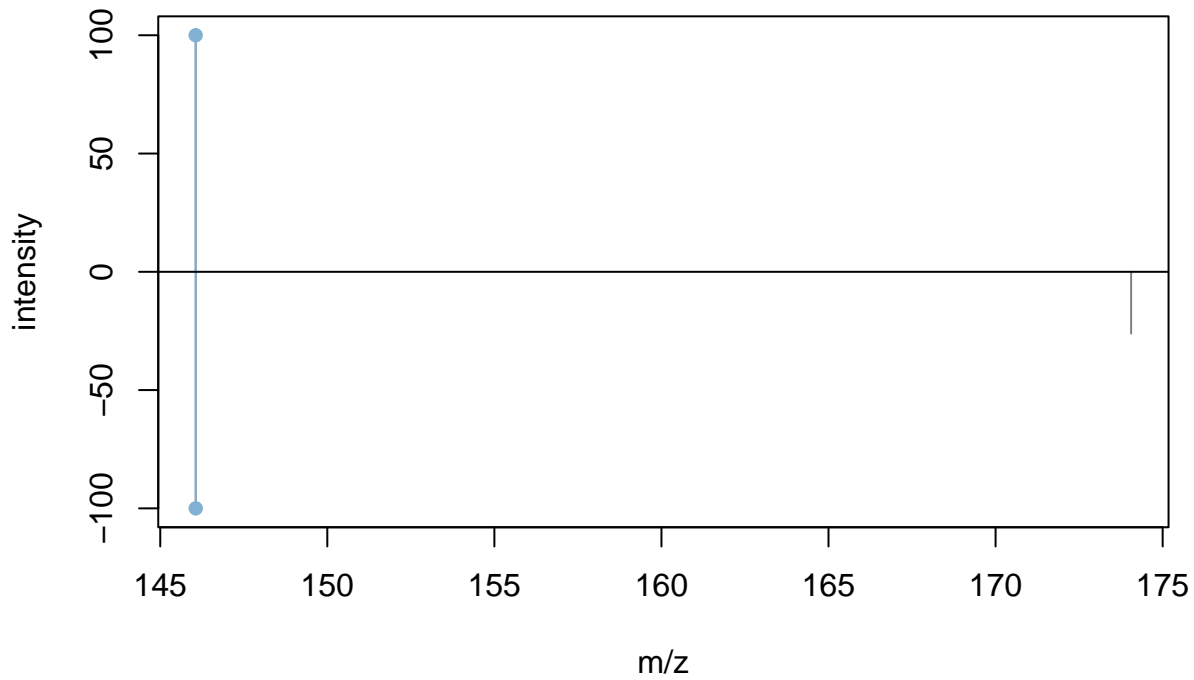
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C10H9NO3/c12-9(13)5-7-6-3-1-2-4-8(6)11-10(7)14/h1-4,7H,5H2,(H,11,14)(H,12,13)
inchikey	ILGMGHZPXRDCS-UHFFFAOYSA-N	ILGMGHZPXRDCS-UHFFFAOYSA-N
smiles	O=C(O)CC1C(O)=NC=2C=CC=CC21	O=C(O)CC1C(O)=NC=2C=CC=CC21
formula	C10H9NO3	C10H9NO3

Retention time match

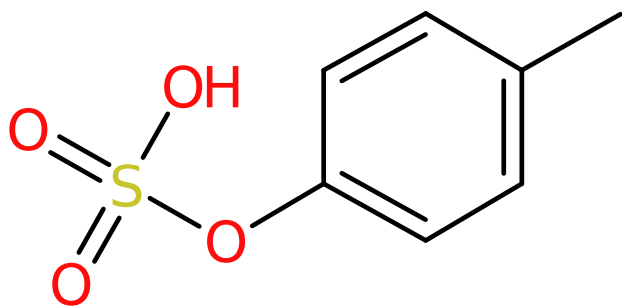
	DB	hit	error	rel. error	pcgroup
Retention time	3.36	3.39	0.03	0.9%	186

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
146.0620	100.0		[M+H-HCOOH] ⁺	146.0601	100.0
174.0567	26.1		[M+H-H ₂ O] ⁺	✗	✗

p-Cresol sulfate



User identifiers

localidentifier	705
dataOrigin	20190725Q-149.mzML
CAS	3233-58-7
inchi	InChI=1S/C7H8O4S/c1-6-2-4-7(5-3-6)11-12(8,9)10/h2-5H,1H3,(H,8,9,10)

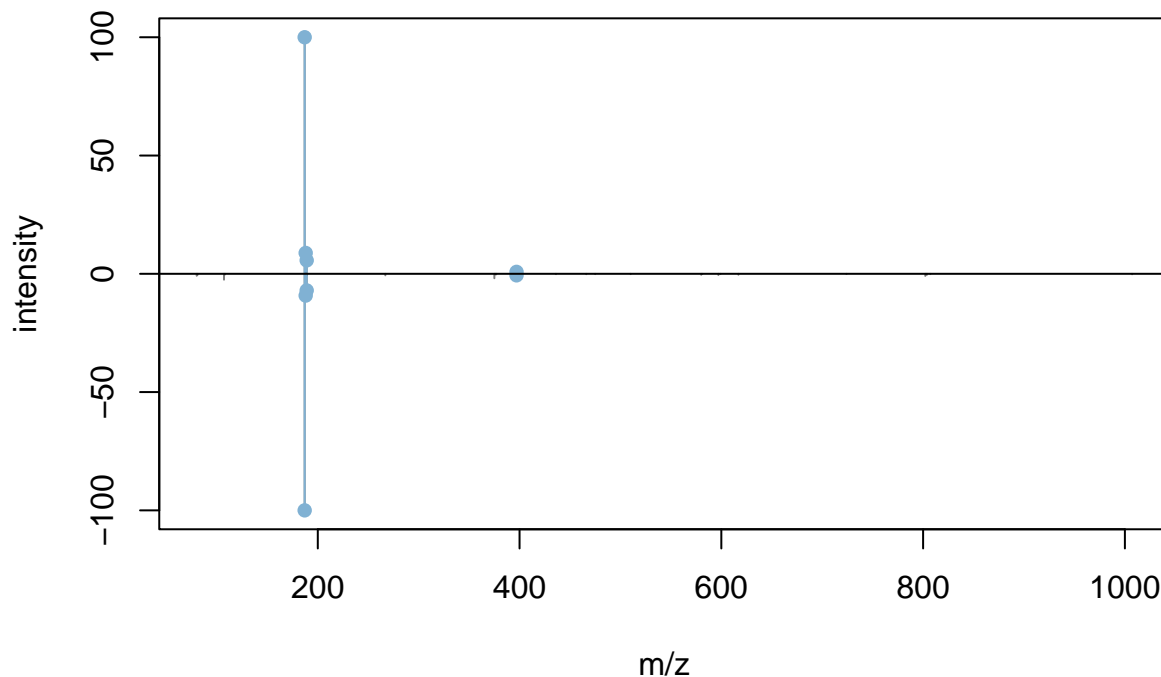
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C7H8O4S/c1-6-2-4-7(5-3-6)11-12(8,9)10/h2-5H,1H3,(H,8,9,10)
inchikey	WGNAKZGUSRVWRH-UHFFFAOYSA-N	WGNAKZGUSRVWRH-UHFFFAOYSA-N
smiles	O=S(=O)(O)OC1=CC=C(C=C1)C	O=S(=O)(O)OC1=CC=C(C=C1)C
formula	C7H8O4S	C7H8O4S

Retention time match

	DB	hit	error	rel. error	pcgroup
Retention time	3.25	3.41	0.16	5.0%	1

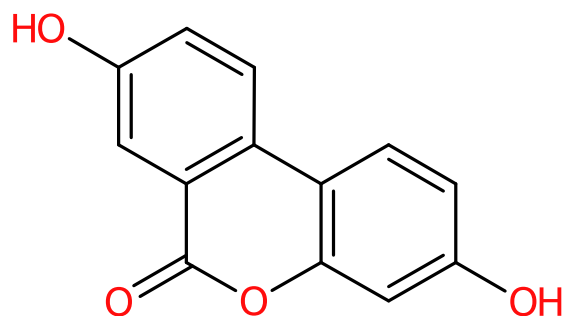
Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
79.9563	0.8			✗	✗
80.9652	0.4			✗	✗
107.0489	2.5	[M] ⁺	[M-H-SO ₃] ⁻	✗	✗
108.0526	0.3	[M+1] ⁺		✗	✗
187.0036	100.0	[M] ⁺	[M-H] ⁻	187.0052	100.0
188.0113	9.2	[M+1] ⁺		188.0106	8.8
188.1816	0.4			✗	✗
188.3324	0.4			✗	✗
188.3665	0.8			✗	✗
188.6462	0.4			✗	✗
189.0045	7.0	[M+2] ⁺		189.0053	5.7
189.3549	0.4			✗	✗
266.9635	0.7			✗	✗
375.0208	1.9	[M] ⁺	[2M-H] ⁻	✗	✗
376.0139	0.3	[M+1] ⁺		✗	✗
377.0137	0.2	[M+2] ⁺		✗	✗
392.0468	1.2	[M] ⁺		✗	✗
393.0529	0.2	[M+1] ⁺		✗	✗
396.9936	0.6		[2M-2H+Na] ⁻	397.0039	0.8
436.0630	0.2			✗	✗
466.0894	0.2			✗	✗
474.9427	0.1			✗	✗
510.1009	0.1			✗	✗
580.0594	0.4	[M] ⁺		✗	✗
581.0621	0.1	[M+1] ⁺		✗	✗
597.0922	0.5			✗	✗
599.0762	0.1			✗	✗
616.9500	0.4		[3M-3H+Fe ²⁺] ⁻	✗	✗
724.0201	0.1			✗	✗
802.1315	0.9	[M] ⁺		✗	✗

803.1211	0.4	[M+1] ⁺			×	×
804.1218	0.3	[M+2] ⁺			×	×
807.0763	0.1				×	×
1007.1730	0.2				×	×

Urolithin A



User identifiers

localidentifier	434
dataOrigin	20190715Q-168.mzML
CAS	1143-70-0
inchi	InChI=1S/C13H8O4/c14-7-1-3-9-10-4-2-8(15)6-12(10)17-13(16)11(9)5-7/h1-6,14-15H

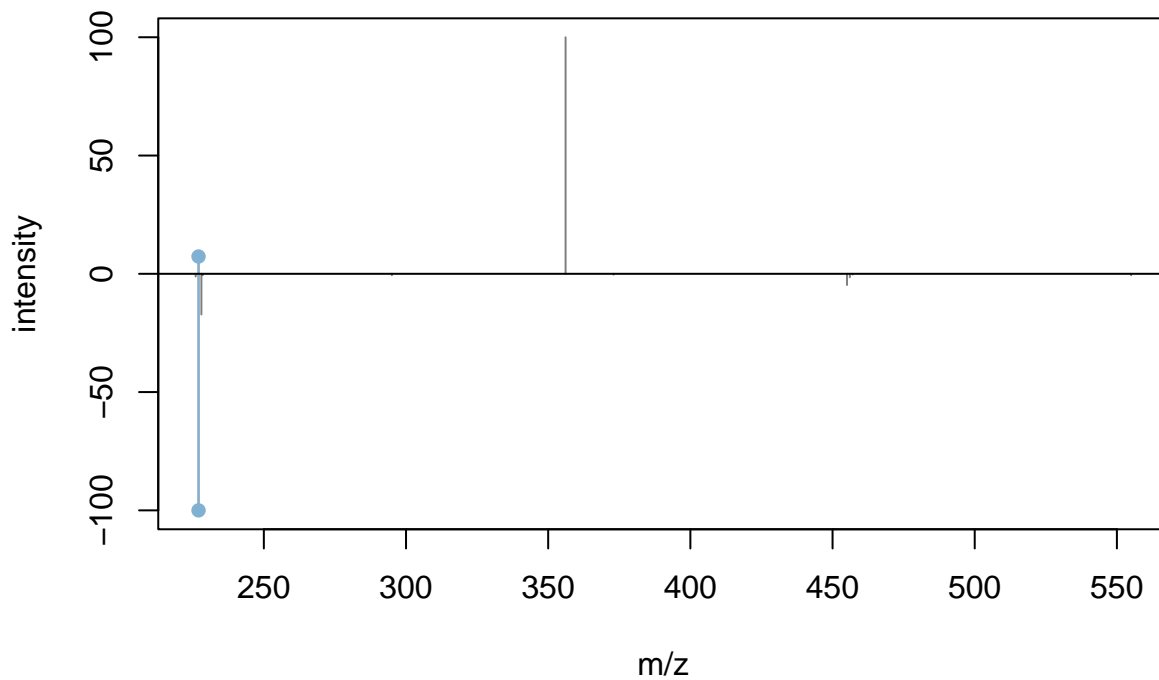
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C13H8O4/c14-7-1-3-9-10-4-2-8(15)6-12(10)17-13(16)11(9)5-7/h1-6,14-15H
inchikey	RIUPLDUFZCXCHM-UHFFFAOYSA-N	RIUPLDUFZCXCHM-UHFFFAOYSA-N
smiles	O=C1OC=2C=C(O)C=CC2C3=CC=C(O)C=C13	O=C1OC=2C=C(O)C=CC2C3=CC=C(O)C=C13
formula	C13H8O4	C13H8O4

Retention time match

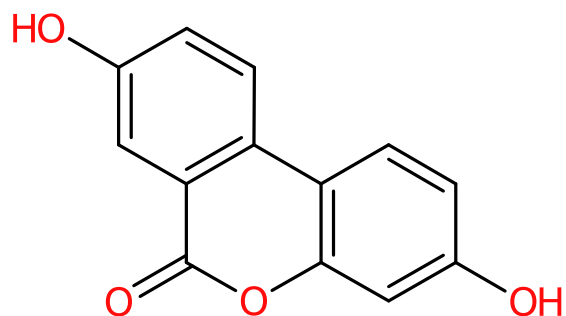
	DB	hit	error	rel. error	pcgroup
Retention time	3.75	3.89	0.14	3.7%	46

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
226.0271	1.2			✗	✗
227.0321	100.0	[M] ⁺	[M-H] ⁻	227.0386	7.3
228.0380	17.2	[M+1] ⁺		✗	✗
228.5040	0.6			✗	✗
295.0237	0.6		[M-H+HCOONa] ⁻	✗	✗
✗	✗			356.1173	100.0
372.9676	0.4			✗	✗
455.0767	4.7	[M] ⁺	[2M-H] ⁻	✗	✗
456.0825	1.5	[M+1] ⁺		✗	✗
457.0808	0.3	[M+2] ⁺		✗	✗
555.0029	0.6			✗	✗

Urolithin A



User identifiers

localidentifier	434
dataOrigin	20190715Q-061.mzML
CAS	1143-70-0
inchi	InChI=1S/C13H8O4/c14-7-1-3-9-10-4-2-8(15)6-12(10)17-13(16)11(9)5-7/h1-6,14-15H

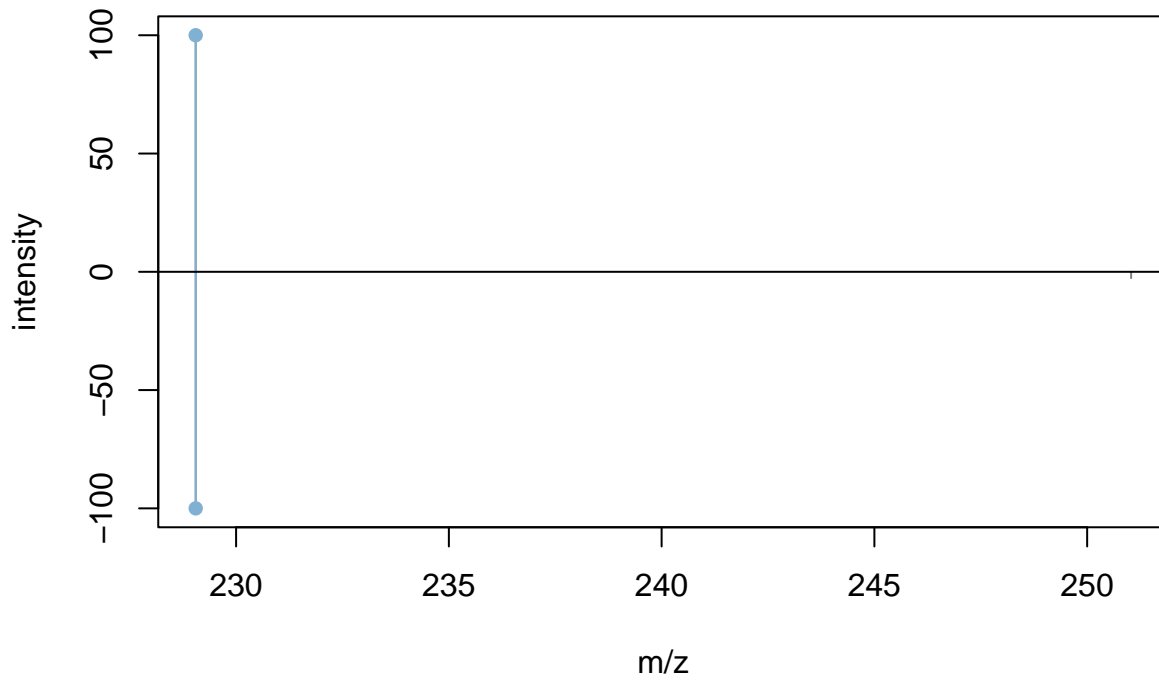
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C13H8O4/c14-7-1-3-9-10-4-2-8(15)6-12(10)17-13(16)11(9)5-7/h1-6,14-15H
inchikey	RIUPLDUFZCXCHM-UHFFFAOYSA-N	RIUPLDUFZCXCHM-UHFFFAOYSA-N
smiles	O=C1OC=2C=C(O)C=CC2C3=CC=C(O)C=C13	O=C1OC=2C=C(O)C=CC2C3=CC=C(O)C=C13
formula	C13H8O4	C13H8O4

Retention time match

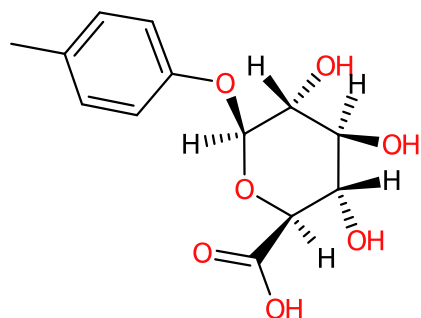
	DB	hit	error	rel. error	pcgroup
Retention time	3.74	3.42	-0.32	-8.7%	157

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
229.0506	100.0		[M+H] ⁺	229.0499	100.0
251.0336	2.7		[M+Na] ⁺	×	×

P-cresol glucuronide



User identifiers

localidentifier	805
dataOrigin	20191206Q-073.mzML
CAS	17680-99-8
inchi	InChI=1S/C13H16O7/c1-6-2-4-7(5-3-6)19-13-10(16)8(14)9(15)11(20-13)12(17)18/h2-5,8-11,13-16H,1H3,(H,17,18)/t8-,9-,10+,11-,13+/m0/s1

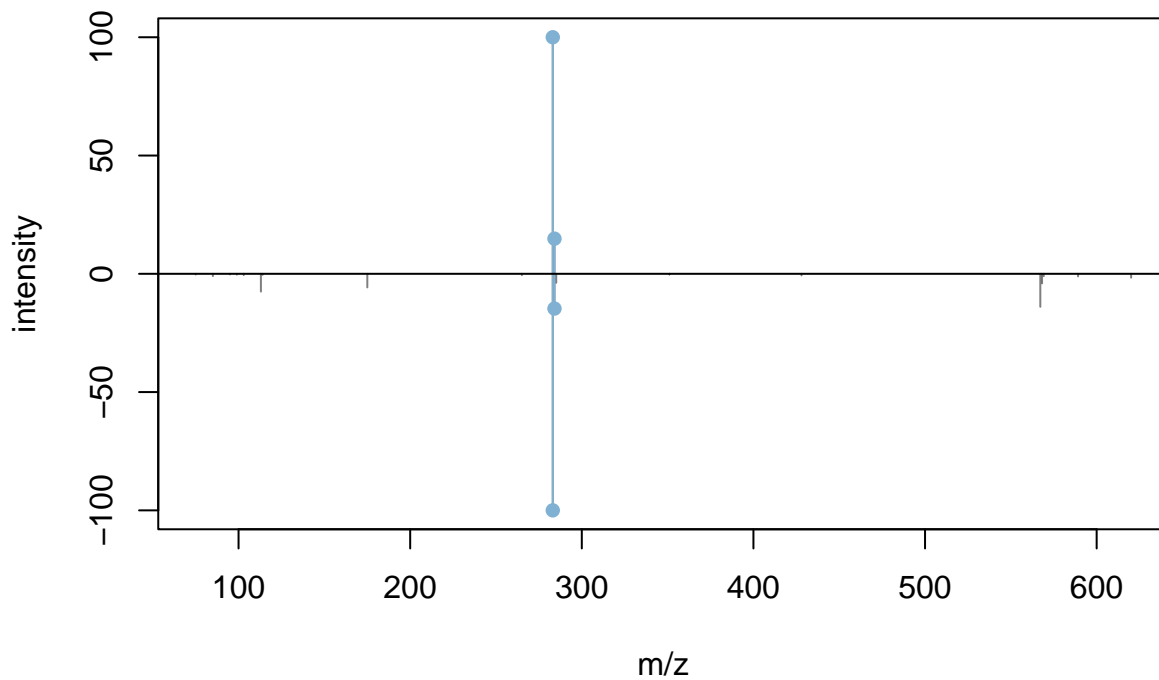
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C13H16O7/c1-6-2-4-7(5-3-6)19-13-10(16)8(14)9(15)11(20-13)12(17)18/h2-5,8-11,13-16H,1H3,(H,17,18)/t8-,9-,10+,11-,13+/m0/s1
inchikey	JPAUCQAJHLSMQW-XPORZQOISA-N	JPAUCQAJHLSMQW-XPORZQOISA-N
smiles	[H]C1(OC2=CC=C(C=C2)C)OC([H])(C(=O)O)C([H])(OC(=O)C)OC([H])(C(=O)O)C([H])(O)C1O	[H]C1(OC2=CC=C(C=C2)C)OC([H])(C(=O)O)C([H])(OC(=O)C)OC([H])(C(=O)O)C([H])(O)C1O
formula	C13H16O7	C13H16O7

Retention time match

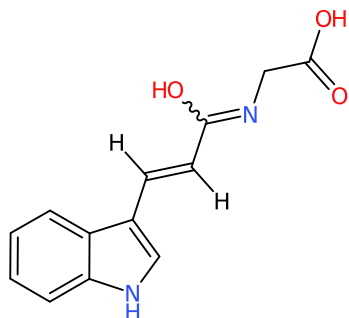
	DB	hit	error	rel. error	pcgroup
Retention time	3.37	3.43	0.06	1.7%	76

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
75.0097	0.3			✗	✗
85.0312	1.0			✗	✗
95.0116	0.3			✗	✗
99.0084	0.4			✗	✗
103.0053	0.6			✗	✗
113.0231	7.5	[M] ⁺		✗	✗
114.0276	0.4	[M+1] ⁺		✗	✗
175.0251	5.8			✗	✗
265.0757	0.6		[M-H-H ₂ O] ⁻	✗	✗
283.0826	100.0	[M] ⁺	[M-H] ⁻	283.0821	100.0
284.0858	14.7	[M+1] ⁺		284.0873	14.9
285.0939	3.8	[M+2] ⁺		✗	✗
351.0571	0.3			✗	✗
351.0718	0.2		[M-H+HCOONa] ⁻	✗	✗
428.0112	0.7			✗	✗
567.1713	14.0	[M] ⁺	[2M-H] ⁻	✗	✗
568.1753	4.1	[M+1] ⁺		✗	✗
569.1789	1.0	[M+2] ⁺		✗	✗
589.1636	1.1		[2M-2H+Na] ⁻	✗	✗
620.0829	1.6		[2M-4H+Fe ³⁺] ⁻	✗	✗

Indol-3-acrolylglycine



User identifiers

localidentifier	349
dataOrigin	20190710Q-179.mzML
CAS	3475-68-1
inchi	InChI=1S/C13H12N2O3/c16-12(15-8-13(17)18)6-5-9-7-14-11-4-2-1-3-10(9)11/h1-7,14H,8H2,(H,15,16)(H,17,18)/b6-5+

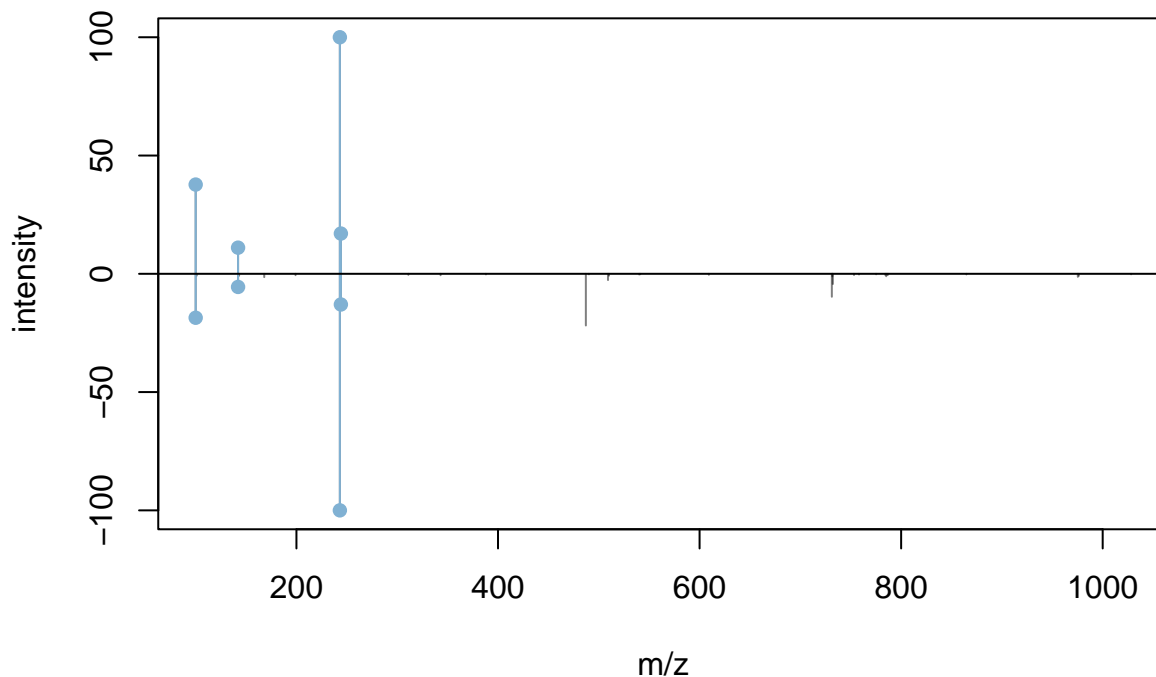
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C13H12N2O3/c16-12(15-8-13(17)18)6-5-9-7-14-11-4-2-1-3-10(9)11/h1-7,14H,8H2,(H,15,16)(H,17,18)/b6-5+
inchikey	DUIFVCFSAWHIOD-AATRIKPKSA-N	DUIFVCFSAWHIOD-AATRIKPKSA-N
smiles	[H]C(C(O)=NCC(=O)O)=C([H])C1=CNC=2C=CC=CC2	[H]C(C(O)=NCC(=O)O)=C([H])C1=CNC=2C=CC=CC2
formula	C13H12N2O3	C13H12N2O3

Retention time match

	DB	hit	error	rel. error	pcgroup
Retention time	3.54	3.54	0.00	0.0%	109

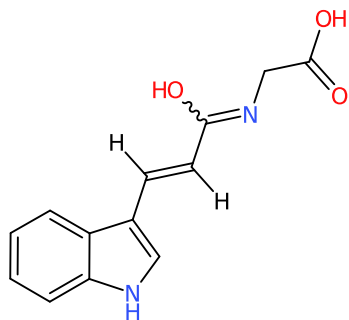
Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
100.0020	18.6	[M] ⁺		100.0036	37.7
101.0065	0.8	[M+1] ⁺		✗	✗
142.0652	5.6	[M] ⁺		142.0663	11.1
143.0680	0.8	[M+1] ⁺		✗	✗
168.0443	1.4			✗	✗
199.0881	0.6		[M-H-CO ₂] ⁻	✗	✗
243.0761	100.0	[M] ⁺	[M-H] ⁻	243.0762	100.0
244.0815	13.0	[M+1] ⁺		244.0813	17.0
311.0655	0.5		[M-H+HCOONa] ⁻	✗	✗
343.0052	0.6			✗	✗
387.9963	0.3			✗	✗
487.1664	21.9		[2M-H] ⁻	✗	✗
490.1897	0.2			✗	✗
509.1443	2.7	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
510.1491	0.8	[M+1] ⁺		✗	✗
540.0809	0.3		[2M-4H+Fe ³⁺] ⁻	✗	✗
541.0777	0.2		[2M-3H+Fe ²⁺] ⁻	✗	✗
609.2052	0.4			✗	✗
731.2407	9.7	[M] ²⁺	[3M-H] ⁻	✗	✗
731.7459	1.1	[M+1] ²⁺		✗	✗
732.2465	4.3	[M+2] ²⁺		✗	✗
753.2350	0.5		[3M-2H+Na] ⁻	✗	✗
758.1932	0.3			✗	✗
775.2071	0.2			✗	✗
784.1712	0.4		[3M-4H+Fe ³⁺] ⁻	✗	✗
785.1716	1.0	[M] ⁺	[3M-3H+Fe ²⁺] ⁻	✗	✗
786.1578	0.5	[M+1] ⁺		✗	✗
787.1732	0.3	[M+2] ⁺		✗	✗
864.7888	0.3			✗	✗
975.3262	1.3	[M] ⁺	[4M-H] ⁻	✗	✗

976.3332	0.9	[M+1] ⁺		×	×
1028.2206	0.2		[4M-4H+Fe3] ⁺	×	×

Indol-3-acrolylglycine



User identifiers

localidentifier	349
dataOrigin	20190710Q-179.mzML
CAS	3475-68-1
inchi	InChI=1S/C13H12N2O3/c16-12(15-8-13(17)18)6-5-9-7-14-11-4-2-1-3-10(9)11/h1-7,14H,8H2,(H,15,16)(H,17,18)/b6-5+

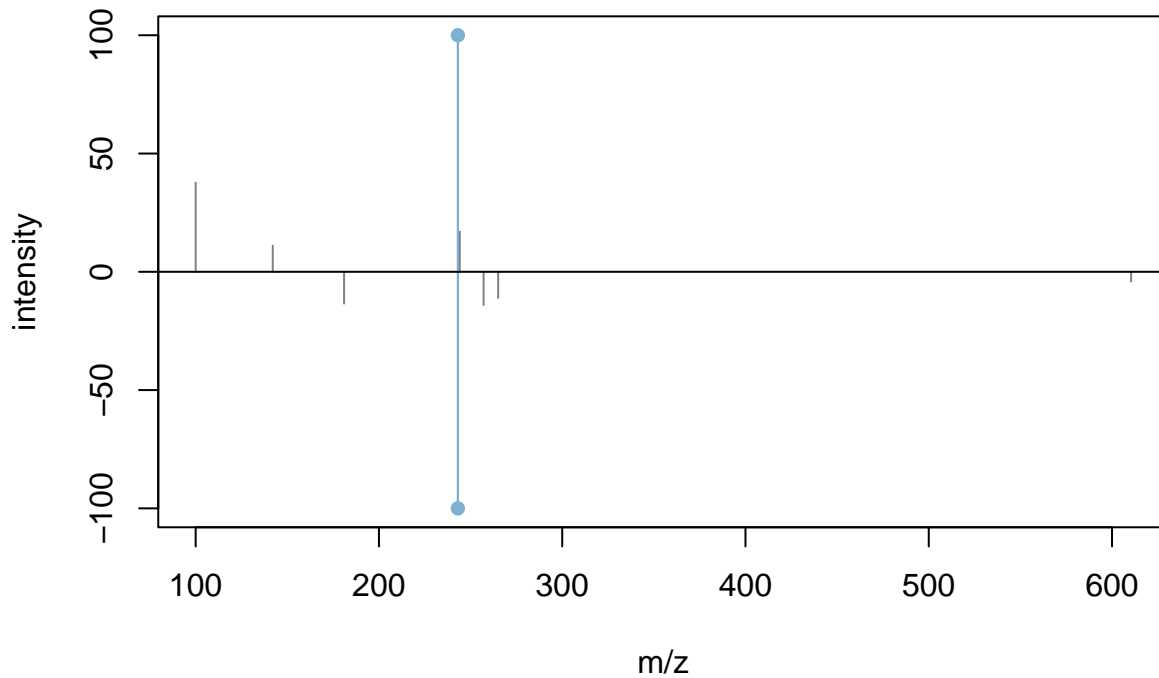
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C13H12N2O3/c16-12(15-8-13(17)18)6-5-9-7-14-11-4-2-1-3-10(9)11/h1-7,14H,8H2,(H,15,16)(H,17,18)/b6-5+
inchikey	DUIFVCFSAWHIOD-AATRIKPKSA-N	DUIFVCFSAWHIOD-AATRIKPKSA-N
smiles	[H]C(C(O)=NCC(=O)O)=C([H])C1=CNC=2C=CC=CC2	[H]C(C(O)=NCC(=O)O)=C([H])C1=CNC=2C=CC=CC2
formula	C13H12N2O3	C13H12N2O3

Retention time match

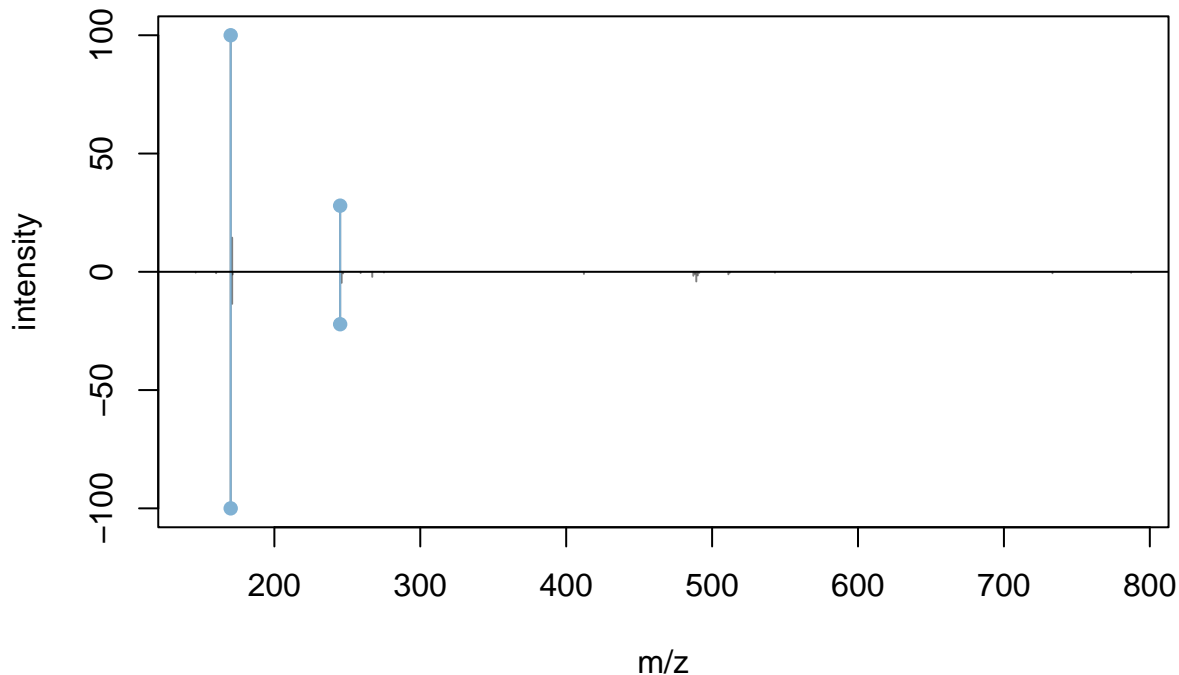
	DB	hit	error	rel. error	pcgroup
Retention time	3.64	3.54	-0.10	-2.7%	109

Spectral match



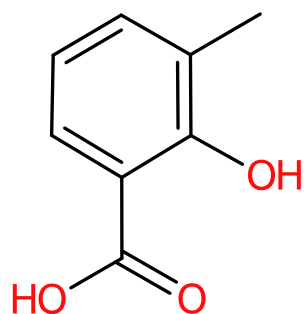
DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
×	×			100.0036	37.7
×	×			142.0663	11.1
180.9855	13.4			×	×
243.0750	100.0		[M-H]-	243.0762	100.0
×	×			244.0813	17.0
257.0955	14.0			×	×
265.0584	11.0		[M-2H+Na]-	×	×
610.4196	4.1			×	×

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
146.0596	0.3			✗	✗
160.0725	0.6			✗	✗
170.0605	100.0	[M] ⁺		170.0595	100.0
171.0563	13.5	[M+1] ⁺		✗	✗
✗	✗			171.0647	14.4
171.3677	1.1			✗	✗
245.0888	22.2	[M] ⁺	[M+H] ⁺	245.0922	28.0
246.0964	4.6	[M+1] ⁺		✗	✗
247.0930	0.7	[M+2] ⁺		✗	✗
259.1069	0.5			✗	✗
267.0743	2.1		[M+Na] ⁺	✗	✗
275.1013	0.3			✗	✗
412.1353	0.9			✗	✗
487.1654	1.7			✗	✗
488.1790	0.9			✗	✗
489.1739	4.1	[M] ⁺	[2M+H] ⁺	✗	✗
490.1791	1.5	[M+1] ⁺		✗	✗
491.1832	0.5	[M+2] ⁺		✗	✗
511.1555	1.0	[M] ⁺	[2M+Na] ⁺	✗	✗
512.1566	0.4	[M+1] ⁺		✗	✗
543.0908	0.4			✗	✗
733.2747	0.6		[3M+H] ⁺	✗	✗
787.1863	0.4			✗	✗

3-Methylsalicylic acid



User identifiers

localidentifier	208
dataOrigin	20190701Q-130.mzML
CAS	83-40-9
inchi	InChI=1S/C8H8O3/c1-5-3-2-4-6(7(5)9)8(10)11/h2-4,9H,1H3,(H,10,11)

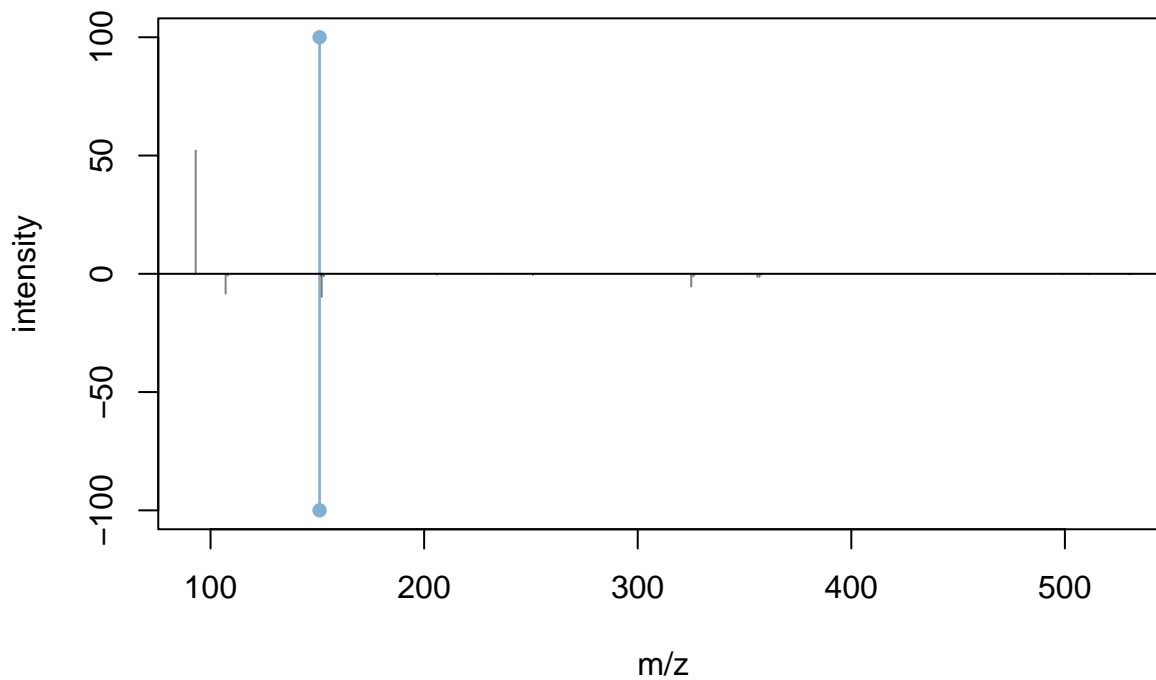
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H8O3/c1-5-3-2-4-6(7(5)9)8(10)11/h2-4,9H,1H3,(H,10,11)
inchikey	WHSXTWFYRGOBGO-UHFFFAOYSA-N	WHSXTWFYRGOBGO-UHFFFAOYSA-N
smiles	O=C(O)C1=CC=CC(=C1O)C	O=C(O)C1=CC=CC(=C1O)C
formula	C8H8O3	C8H8O3

Retention time match

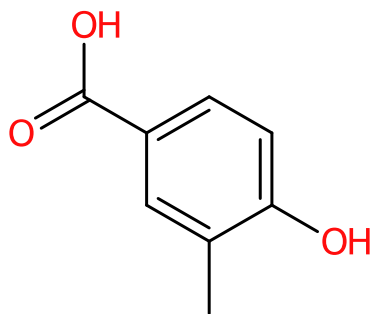
	DB	hit	error	rel. error	pcgroup
Retention time	3.99	3.58	-0.40	-10.1%	147

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
×	×			93.0343	52.1
107.0477	8.4	[M] ⁺	[M-H-CO ₂] ⁻	×	×
108.0544	0.8	[M+1] ⁺		×	×
151.0395	100.0	[M] ⁺	[M-H] ⁻	151.0394	100.0
151.5649	0.4			×	×
151.6601	0.9			×	×
151.8909	0.4			×	×
152.0442	9.8	[M+1] ⁺		×	×
153.0405	1.1	[M+2] ⁺		×	×
205.9709	0.3			×	×
233.9654	0.1			×	×
250.9676	0.5			×	×
325.0675	5.4	[M] ⁺	[2M-2H+Na] ⁻	×	×
326.0737	1.1	[M+1] ⁺		×	×
327.0539	0.3	[M+2] ⁺		×	×
352.0023	0.1			×	×
356.0000	1.3		[2M-4H+Fe ³⁺] ⁻	×	×
357.0016	1.3	[M] ⁺	[2M-3H+Fe ²⁺] ⁻	×	×
358.0085	0.3	[M+1] ⁺		×	×
499.0960	0.2			×	×
509.0612	0.1		[3M-3H+Fe ²⁺] ⁻	×	×
511.0536	0.2			×	×
530.0336	0.3			×	×
531.0163	0.1			×	×

4-Hydroxy-3-methylbenzoic acid



User identifiers

localidentifier	231
dataOrigin	20190701Q-155.mzML
CAS	499-76-3
inchi	InChI=1S/C8H8O3/c1-5-4-6(8(10)11)2-3-7(5)9/h2-4,9H,1H3,(H,10,11)

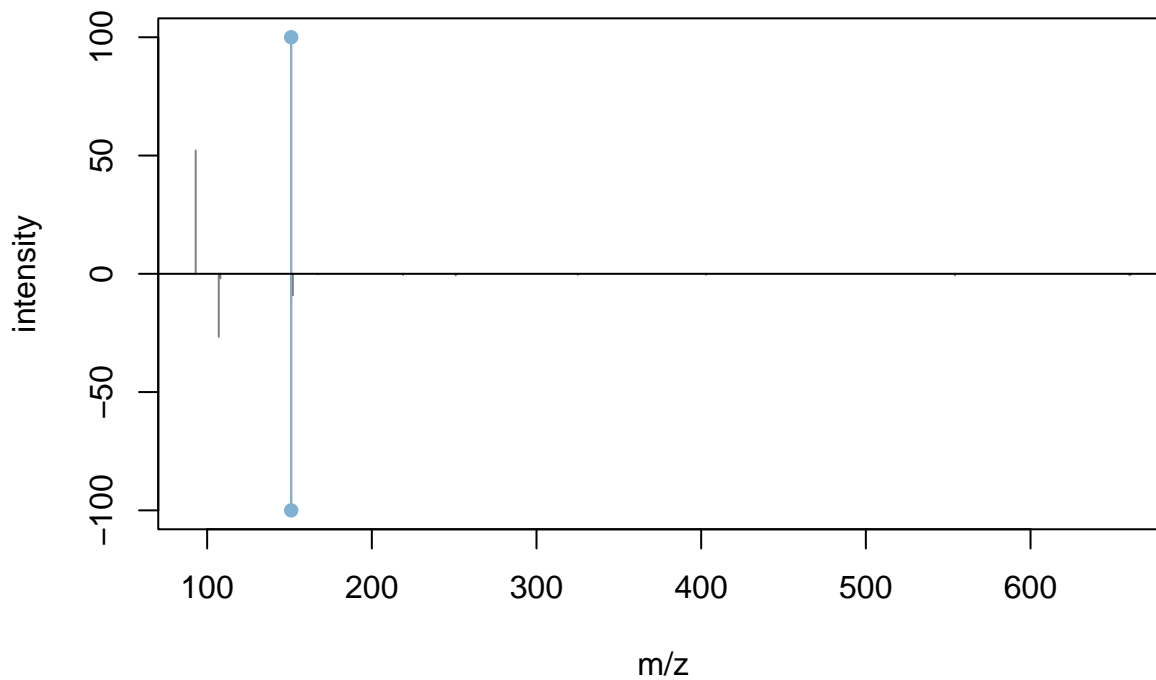
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C8H8O3/c1-5-4-6(8(10)11)2-3-7(5)9/h2-4,9H,1H3,(H,10,11)
inchikey	LTFH NKUKQYVHDX-UHFFFAOYSA-N	LTFH NKUKQYVHDX-UHFFFAOYSA-N
smiles	O=C(O)C1=CC=C(O)C(=C1)C	O=C(O)C1=CC=C(O)C(=C1)C
formula	C8H8O3	C8H8O3

Retention time match

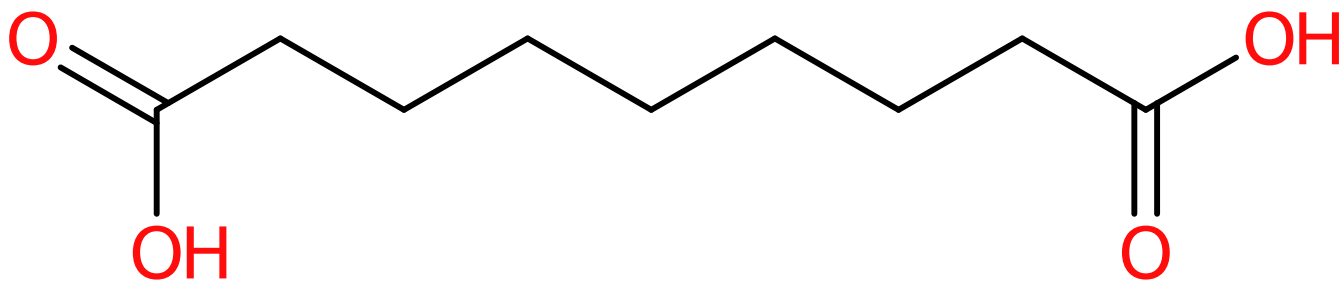
	DB	hit	error	rel. error	pcgroup
Retention time	3.48	3.58	0.11	3.1%	147

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
×	×			93.0343	52.1
107.0498	26.6	[M] ⁺	[M-H-CO ₂] ⁻	×	×
108.0535	1.9	[M+1] ⁺		×	×
151.0394	100.0	[M] ⁺	[M-H] ⁻	151.0394	100.0
152.0418	9.1	[M+1] ⁺		×	×
167.0351	0.2			×	×
219.0266	0.5		[M-H+HCOONa] ⁻	×	×
250.9679	0.7			×	×
325.0652	0.4		[2M-2H+Na] ⁻	×	×
403.0168	0.4			×	×
554.0532	0.7			×	×
660.0972	0.7	[M] ⁺	[4M-4H+Fe ³⁺] ⁻	×	×
661.1022	0.3	[M+1] ⁺		×	×

Azelaic acid



User identifiers

localidentifier	283
dataOrigin	20190701Q-211.mzML
CAS	123-99-9
inchi	InChI=1S/C9H16O4/c10-8(11)6-4-2-1-3-5-7-9(12)13/h1-7H2,(H,10,11)(H,12,13)

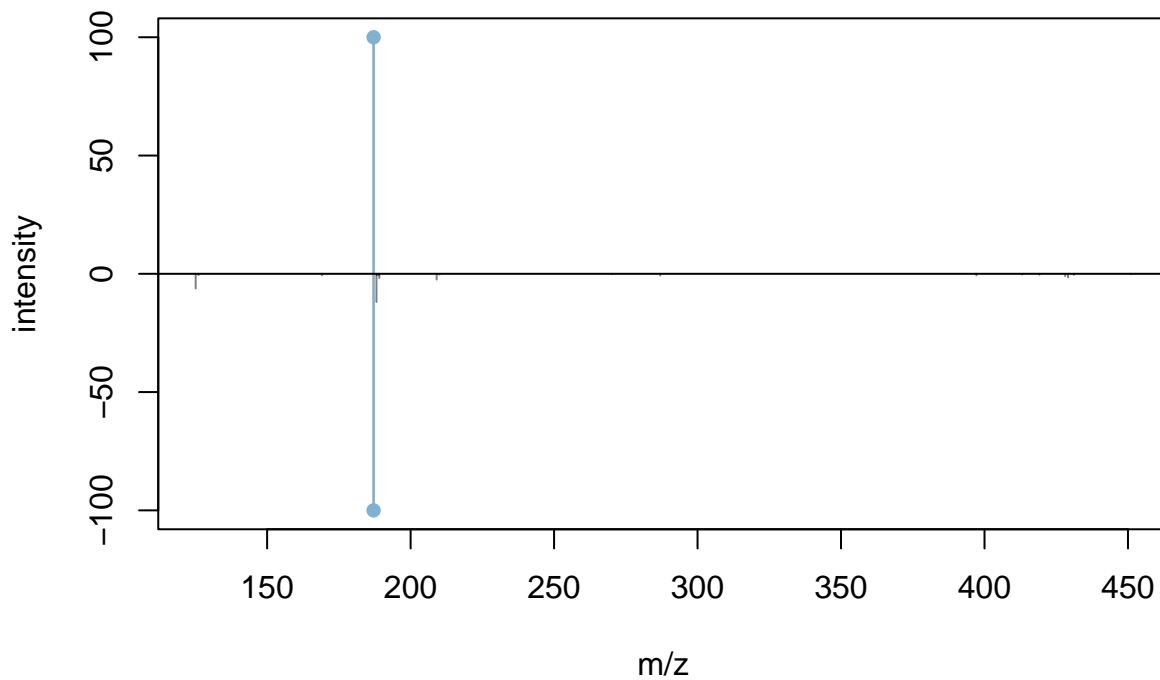
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C9H16O4/c10-8(11)6-4-2-1-3-5-7-9(12)13/h1-7H2,(H,10,11)(H,12,13)
inchikey	BDJRBEXGNYIS-UHFFFAOYSA-N	BDJRBEXGNYIS-UHFFFAOYSA-N
smiles	O=C(O)CCCCCCC(=O)O	O=C(O)CCCCCCC(=O)O
formula	C9H16O4	C9H16O4

Retention time match

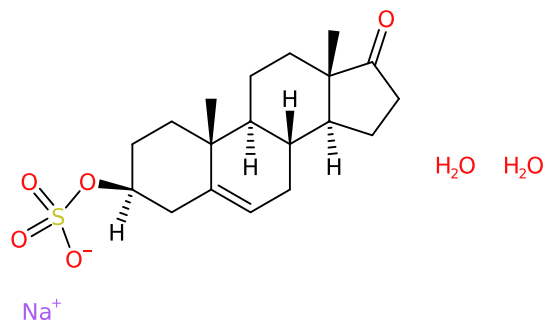
	DB	hit	error	rel. error	pcgroup
Retention time	3.69	3.61	-0.08	-2.1%	35

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
125.0965	6.2	[M] ⁺	[M-H-H ₂ O-CO ₂] ⁻	✗	✗
126.0981	0.6	[M+1] ⁺		✗	✗
169.0832	0.7		[M-H-H ₂ O] ⁻	✗	✗
187.0954	100.0	[M] ⁺	[M-H] ⁻	187.0960	100.0
188.1019	11.9	[M+1] ⁺		✗	✗
188.2381	0.6			✗	✗
188.9322	0.6			✗	✗
189.0942	1.8	[M+2] ⁺		✗	✗
209.0807	2.4	[M] ⁺	[M-2H+Na] ⁻	✗	✗
210.0831	0.3	[M+1] ⁺		✗	✗
270.0200	0.2			✗	✗
287.0228	0.7			✗	✗
397.1858	0.7		[2M-2H+Na] ⁻	✗	✗
413.1491	0.3		[2M-2H+K] ⁻	✗	✗
419.1659	0.4			✗	✗
428.1176	1.0		[2M-4H+Fe ³⁺] ⁻	✗	✗
429.1230	1.5		[2M-3H+Fe ²⁺] ⁻	✗	✗
431.1158	0.5			✗	✗
451.1007	0.2			✗	✗

Dehydroisoandrosterone 3-sulfate



User identifiers

localidentifier	48
dataOrigin	12062019Q-179.mzML
CAS	78590-17-7
inchi	InChI=1S/C19H28O5S.Na.2H2O/c1-18-9-7-13(24-25(21,22)23)11-12(18)3-4-14-15-5-6-17(20)19(15,2)10-8-16(14)18;;;/h3,13-16H,4-11H2,1-2H3,(H,21,22,23);;2*1H2/q;+1;;/p-1/t13-,14-,15-,16-,18-,19-;;;/m0.../s1

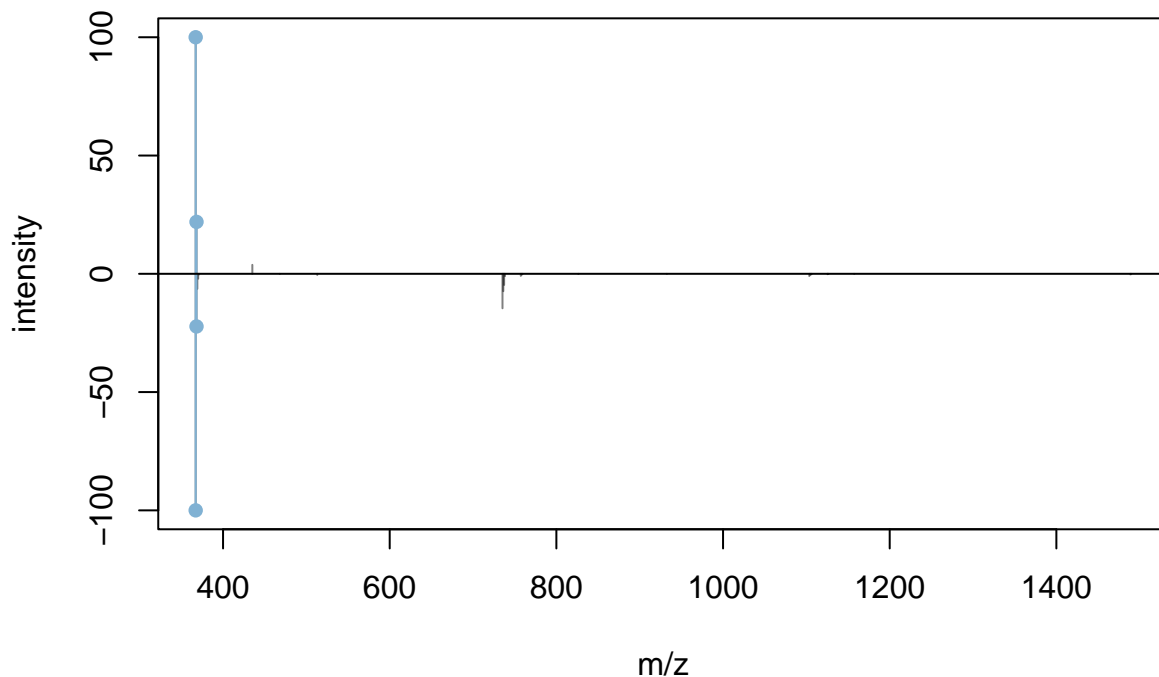
Computed identifiers

	Input as-is	Standardized structure
charge	0	0
inchi		InChI=1S/C19H28O5S/c1-18-9-7-13(24-25(21,22)23)11-12(18)3-4-14-15-5-6-17(20)19(15,2)10-8-16(14)18/h3,13-16H,4-11H2,1-2H3,(H,21,22,23)/p-1/t13-,14-,15-,16-,18-,19-/m0/s1
inchikey	NLNMKDUYGPNWAO-OXNWJOIVSA-M	CZWCKYRVOZZJNM-USOAJAOKSA-M
smiles	[Na+].[H]C1(OS(=O)(=O)[O-])CC2=C[C@@]3([H])C4([H])CCC(=O)C4(C)CCC3([H])C2(C)C	[H]C1(OS(=O)(=O)[O-])CC2=C[C@@]3([H])C4([H])CCC(=O)C4(C)CCC3([H])C2(C)C
formula	C19H31NaO7S	[C19H27O5S]-

Retention time match

	DB	hit	error	rel. error	pcgroup
Retention time	4.19	4.13	-0.06	-1.5%	10

Spectral match



DB m/z	DB int	isotope	adduct	pcgroup m/z	pcgroup int
367.1580	100.0	[M] ⁺	[M-H] ⁻	367.1589	100.0
367.9667	0.6			✗	✗
368.1631	22.3	[M+1] ⁺		368.1631	21.9
369.1554	6.4	[M+2] ⁺		✗	✗
370.1504	2.1	[M+3] ⁺		✗	✗
371.2979	0.3			✗	✗
✗	✗			435.1471	3.8
468.0899	0.1			✗	✗
513.0878	0.5			✗	✗
735.3284	14.6	[M] ⁺	[2M-H] ⁻	✗	✗
736.3260	7.4	[M+1] ⁺		✗	✗
737.3320	4.7	[M+2] ⁺		✗	✗
738.3053	1.0	[M+3] ⁺		✗	✗
757.3104	0.9	[M] ⁺	[2M-2H+Na] ⁻	✗	✗
758.3079	0.4	[M+1] ⁺		✗	✗
759.3219	0.2	[M+2] ⁺		✗	✗
826.3828	0.1			✗	✗
932.5865	0.1			✗	✗
1103.4935	1.0	[M] ⁺	[3M-H] ⁻	✗	✗
1104.4976	0.5	[M+1] ⁺		✗	✗
1105.4868	0.3	[M+2] ⁺		✗	✗
1106.5020	0.1	[M+3] ⁺		✗	✗
1125.4624	0.2	[M] ⁺	[3M-2H+Na] ⁻	✗	✗
1125.4774	0.1		[3M-2H+Na] ⁻	✗	✗
1126.4902	0.1	[M+1] ⁺		✗	✗
1157.4021	0.1		[3M-3H+Fe2+] ⁻	✗	✗
1488.6935	0.3	[M] ⁺		✗	✗
1489.7124	0.2	[M+1] ⁺		✗	✗