

Formulæ RT AtI-T3 M Struct 1-Thio-b-D-gluName Class Benmet B-RT Diff [M]- [M-H] Desulfo [DS-H]- ITC [ITC-H]- Source CAS Observed PPM fit

Formulæ	RT	AtI-T3	M	Struct	1-Thio-b-D-gluName	Class	Benmet	B-RT	Diff	[M]- [M-H]	Desulfo [M-SO3]	[DS-H]-	ITC [M-Glu-SO3][G-SO3-H]- [C6H12O6-SC6H13O9S]-	Source	CAS	Observed PPM	fit
C8H15NO9S2	333.01882			51 Methyl	Glucosapparin B	Aliphatic-n	1	3.2		332.01155	252.05474	72.99862	71.99135		497-77-8		
C9H17NO9S2	347.03447			16 Ethyl	Glucosapparin B	Aliphatic-n	1	3.2		346.02720	267.07766	266.07039	87.01427	86.00700	363599-81-9		
C10H19NO9S2	5.325	359.03447		107 2-Propenyl	Singrin	Olefins	35	6.2	0.875	358.02720	279.07766	278.07039	99.01427	98.00700	B. carinata	3952-98-5	
C10H19NO9S2	361.05012			56 1-Methyl-2-propenyl	Glucosapparin B	Aliphatic-i	3	7.7		360.04285	281.09331	280.08604	101.02992	100.02265	18432-16-1		
C10H19NO9S2	8.604	361.05012		108 n-Propyl	Glucosapparin B	Aliphatic-n	2	8.2	-0.404	360.04285	281.09331	280.08604	101.02992	100.02265	B. carinata	119499-36-4	
C9H17NO10S2	363.02939			162 2-Hydroxyethyl	Glucosapparin E	Aliphatic alcohol-n	3	7.7		362.02212	283.07258	282.06531	103.00919	102.00192			
C11H19NO10S2	373.05012			118 3-Butenyl	Glucosapparin E	Olefins	36	9	-0.839	372.04285	293.09331	292.08604	113.02992	112.02265	l. tinctoria	19041-09-9	
C11H19NO9S2	373.05012			60 2-Methyl-2-propenyl	Glucosapparin D	Olefins	4	11.4	-0.767	372.04285	293.09331	292.08604	113.02992	112.02265	B. juncea	35635-42-3	
C11H21NO9S2	12.167	373.05012		13 n-Butyl	Dihydroquon B	Aliphatic-n	4	11.4		374.05880	293.10896	294.10169	115.04557	114.03830	l. tinctoria	M-01312	
C11H21NO9S2	14	373.05012		61 (1S)-Methylpro	Glucosapparin C	Aliphatic-i	5	10.6		374.05880	293.10896	294.10169	115.04557	114.03830		499-24-1	
C11H21NO9S2	373.05012			62 2-Methylpropyl	Glucosapparin C	Aliphatic-i	6	9.8		374.05880	293.10896	294.10169	115.04557	114.03830		M-01313	
C11H21NO9S2	373.05012			180 1,1-Dimethyl-ethyl	Glucosapparin C	Aliphatic-i	6	9.8		374.05880	293.10896	294.10169	115.04557	114.03830			
C10H19NO10S2	377.04504			42 3-Hydroxyprop	Glucosapparin E	Aliphatic alcohol-n	4	11.4		376.03777	297.08823	296.08096	117.02484	116.01757			
C10H19NO10S2	377.04504			42 3-Hydroxyprop	Glucosapparin E	Aliphatic alcohol-n	4	11.4		376.03777	297.08823	296.08096	117.02484	116.01757			
C10H19NO10S2	377.04504			57 (1R)-Methyl-2-	Glucosapparin E	Aliphatic alcohol-n	4	11.4		376.03777	297.08823	296.08096	117.02484	116.01757			
C12H23NO9S2	387.06577			52 3-Methyl-3-butyl	Glucosapparin D	Olefins	38	12.3		386.05880	307.10896	306.10169	127.04557	126.03830	l. tinctoria		
C12H23NO9S2	13.444	387.06577		100 1-Pentenyl	Glucosapparin D	Olefins	38	12.3		386.05880	307.10896	306.10169	127.04557	126.03830	l. tinctoria		
C12H23NO9S2	387.06577			101 4-Pentenyl	Glucosapparin D	Olefins	38	12.3		386.05880	307.10896	306.10169	127.04557	126.03830		19041-10-2	
C11H19NO10S2	4.971	389.04504		24 (2R)-2-Hydroxy	Propolin D	Olefins alcohol-n	37	6	1.029	388.03777	309.08823	308.08096	129.02484	128.01757	l. tinctoria	585-95-5	
C11H19NO10S2	6.193	389.04504		165 (2S)-2-Hydroxy	Epigallocatechin D	Olefins alcohol-n	39	6.6	0.407	388.03777	309.08823	308.08096	129.02484	128.01757	l. tinctoria	19237-18-4	
C12H23NO9S2	389.08142			53 1-Methylbutyl	Glucosapparin C	Aliphatic-i	39	6.6		388.03777	309.08823	308.08096	129.02484	128.01757			
C12H23NO9S2	389.08142			54 (2S)-Methylbut	Glucosapparin C	Aliphatic-i	39	6.6		388.03777	309.08823	308.08096	129.02484	128.01757			
C12H23NO9S2	389.08142			55 3-Methylbutyl	Glucosapparin C	Aliphatic-i	39	6.6		388.03777	309.08823	308.08096	129.02484	128.01757			
C12H23NO9S2	15.342	389.08142		102 n-Pentyl	Glucosapparin C	Aliphatic-n	7	14.4	-0.942	388.03777	309.08823	308.08096	129.02484	128.01757	Std mix	127929-24-2	
C11H21NO10S2	391.06068			17 (1R)-Ethyl-2-hy	Glucosapparin E	Aliphatic alcohol-n	37	6		390.05341	311.10387	310.09660	131.04048	130.03321			
C11H21NO10S2	391.06068			25 3-Hydroxybutyl	Glucosapparin E	Aliphatic alcohol-n	37	6		390.05341	311.10387	310.09660	131.04048	130.03321			
C11H21NO10S2	391.06068			28 4-Hydroxybutyl	Glucosapparin E	Aliphatic alcohol-n	37	6		390.05341	311.10387	310.09660	131.04048	130.03321			
C11H21NO10S2	391.06068			27 2-Hydroxybutyl	Glucosapparin E	Aliphatic alcohol-n	37	6		390.05341	311.10387	310.09660	131.04048	130.03321			
C11H21NO10S2	391.06068			30 1-(Hydroxymethyl)	propyl E	Aliphatic alcohol-n	37	6		390.05341	311.10387	310.09660	131.04048	130.03321			
C10H19NO9S3	393.02219			86 2-(Methylthio)el	Glucosapparin A	Aliphatic alcohol-n	9	6.6		390.05341	311.10387	310.09660	131.04048	130.03321			
C13H17NO9S2	395.03447			103 Phenyl	Glucosapparin G	Aromatic phenyl	40	8		394.02720	315.07766	314.07039	135.01427	134.00700			
C12H21NO10S2	403.06068			19 5-Hexenyl	Glucosapparin D	Olefins	40	8		400.07415	321.12461	320.11734	141.06122	140.05395			
C12H21NO10S2	403.06068			38 (2S)-Hydroxy-4	Glucosapparin D	Olefins alcohol-n	40	8		402.05341	323.10387	322.09660	143.04048	142.03321			
C12H21NO10S2	403.06068			99 4-Oxyphenyl	Glucosapparin F	Olefins ketone-n	40	8		402.05341	323.10387	322.09660	143.04048	142.03321			
C12H21NO10S2	9.589	403.06068		164 (2R)-Hydroxy-4	Glucosapparin D	Olefins ketone-n	40	8		402.05341	323.10387	322.09660	143.04048	142.03321	Imp Gollim std		
C12H21NO10S2	16.734	403.06068		171 3-Oxyphenyl	Glucosapparin D	Aliphatic ketone-n	40	8		402.05341	323.10387	322.09660	143.04048	142.03321	Seed mix		
C12H23NO10S2	403.07633			29 (2R)-2-Hydroxy	Glucosapparin E	Aliphatic alcohol-n	8	20.7	0.870	402.08960	323.11952	322.11225	143.05613	142.04886			
C13H25NO9S2	403.09707			20 n-Hexyl	Glucosapparin B	Aliphatic-n	8	20.7		402.08960	323.11952	322.11225	143.05613	142.04886			
C13H25NO9S2	403.09707			58 3-Methylpentyl	(1-HX) C	Aliphatic-i	8	20.7		402.08960	323.11952	322.11225	143.05613	142.04886			
C13H25NO9S2	403.09707			59 4-Methylpentyl	(1-HX) C	Aliphatic-i	8	20.7		402.08960	323.11952	322.11225	143.05613	142.04886			
C13H25NO9S2	403.09707			116 Iso-Hexyl (e.g. 58/59)	C	Aliphatic-i	8	20.7		402.08960	323.11952	322.11225	143.05613	142.04886			
C12H23NO10S2	403.09707			151 2-Ethylbutyl	(1-HX) C	Aliphatic-i	8	20.7		402.08960	323.11952	322.11225	143.05613	142.04886			
C12H23NO10S2	403.09707			39 2-Hydroxyphenyl	Glucosapparin E	Aliphatic alcohol-n	40	8		404.08960	325.11952	324.11225	145.05613	144.04886			
C12H23NO10S2	403.09707			169 5-Hydroxyphenyl	Glucosapparin E	Aliphatic alcohol-n	40	8		404.08960	325.11952	324.11225	145.05613	144.04886			
C11H19NO9S3	406.97892			159 3-Butenylseleno	glucosinololate M	Seleno	11	10.8		405.97165	327.02211	326.01484	146.95872	145.95145			
C11H17NO9S3	10.517	407.03784		85 3-(Methylthio)el	Glucosapparin A	Alkyl-thio-alkyl	11	10.8		406.03057	327.02211	326.01484	146.95872	145.95145			
C10H19NO10S3	407.03784			185 4-Mercaptybutyl	Glucosapparin A	Alkyl-sulfinyl-alkyl	11	10.8		406.03057	327.02211	326.01484	146.95872	145.95145			
C14H19NO9S2	409.01711			124 2-(Methylsulfinyl)	propyl A	Alkyl-sulfinyl-alkyl	11	10.8		406.03057	327.02211	326.01484	146.95872	145.95145			
C14H19NO9S2	409.01711			11 Benzyl	Glucosapparin G	Aromatic benzyl	41	13.3	-0.632	408.04285	329.09331	328.08604	149.02992	148.02265			
C14H19NO9S2	415.09707			18 6-Heptenyl	Glucosapparin D	Olefins	41	13.3		416.10545	335.14026	334.13299	155.07687	154.06960			
C14H27NO9S2	417.11272			115 Iso-Heptyl	Glucosapparin D	Aliphatic-i	41	13.3		416.10545	335.14026	334.13299	155.07687	154.06960			
C14H27NO9S2	24.847	417.11272		167 n-Heptyl	Glucosapparin B	Aliphatic-n	13	14.2		418.10545	337.15591	336.14864	157.09252	156.08525	Seed mix		
C12H21NO10S3	418.03784			83 4-Methylthio-3-	dehydrocurc A	Alkyl-thio-alkenyl	13	14.2		418.10545	337.15591	336.14864	157.09252	156.08525	Seed mix		
C12H21NO11S2	418.05560			11 Methoxycarbon	Glucosapparin F	Ester	13	14.2		418.04833	339.09879	338.09152	159.03540	158.02813			
C13H25NO10S2	418.09198			170 6-Hydroxyhexyl	Glucosapparin E	Aliphatic alcohol-n	12	13.8		418.08471	339.13517	338.12790	159.07178	158.06451	seed mix		
C13H25NO9S3	13.681	421.05349		84 4-(Methylthio)el	Glucosapparin A	Alkyl-thio-alkyl	12	13.8	0.119	420.04622	341.09668	340.08941	161.03329	160.02602	D. muralis	21973-56-8	
C11H21NO10S3	4.178	423.03276		73 (R)-3-(Methylsul	Glucosapparin A	Alkyl-sulfinyl-alkyl	20	5.2	1.022	422.02549	343.07595	342.06868	163.01256	162.00529	Std mix	[M-01421]	
C15H21NO9S2	17.119	423.06577		105 2-Phenethyl	Glucosapparin G	Aromatic phenethyl	55	17.7	0.510	422.05850	343.10886	342.10169	163.04557	162.03830	B. vulgaris	499-30-9	
C14H19NO10S2	9.347	425.04504		21 2-Hydroxybenzyl	Glucosapparin G	Aromatic benzyl	42	10.4	1.053	424.03777	345.08823	344.08096	165.02484	164.01757	B. juncea	59204-84-7	
C14H19NO10S2	425.04504			2													

C14H25NO10S2	431.09198	97.5-Oxheptyl	Aliphatic ketone-n	430.08471	351.13517	350.12790	171.07178	170.06451	20016-82-4
C14H25NO10S2	431.09198	172.6-Oxheptyl	Aliphatic ketone-n	430.08471	351.13517	350.12790	171.07178	170.06451	
C15H29NO9S2	431.12837	183.1-n-Octyl (Un-natural)	Aliphatic-n	430.12110	351.17156	350.16429	171.10817	170.10390	
C17H21NO10S3	8.379	63(R)-4-Methylsulfinylglucosaminic	Alkyl-thio-alkenyl	434.02549	355.07595	354.06868	175.01256	174.00529	28463-24-3
C17H21NO10S3	17.158	94.5-(Methylthio)glucobacteriofuran	Alkyl-thio-alkyl	434.06187	354.12233	354.10506	175.04894	174.04167	29611-01-6
C17H21NO10S3	5	64(R)-4-(Methylsulfinyl)glucosaminic	Alkyl-sulfinyl-alkyl	436.04114	357.09160	356.08433	177.02821	176.02094	21414-41-5
C16H23NO9S2	18.303	3.3-Phenylpropylglucosaminic	Aromatic phenethyl	436.07415	356.12461	355.11734	177.06122	176.05395	Seed mix
C11H21NO11S3	433.02767	82.3-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	438.02040	359.07086	358.06359	179.00747	178.00020	[M-01421]
C15H21NO10S2	438.06668	40.2(S)-2-Hydroxyglucosaminic	Aromatic phenethyl	438.05341	359.10387	358.09660	179.04048	178.03321	21087-78-5
C15H21NO10S2	438.06668	44.2-Methoxybenzyl	Aromatic benzyl	438.05341	359.10387	358.09660	179.04048	178.03321	
C16H21NO10S2	438.06668	45.3-Methoxybenzyl	Aromatic benzyl	438.05341	359.10387	358.09660	179.04048	178.03321	
C16H21NO10S2	438.06668	46.4-Methoxybenzyl	Aromatic benzyl	438.05341	359.10387	358.09660	179.04048	178.03321	499-27-4
C15H21NO10S2	438.06668	47.1-Methoxybenzyl	Aromatic benzyl	438.05341	359.10387	358.09660	179.04048	178.03321	14449-25-8
C15H21NO10S2	13.188	122.2(R)-2-Hydroxyglucosaminic	G	438.05341	359.10387	358.09660	179.04048	178.03321	
C15H21NO10S2	438.06668	139.2-(4-Hydroxyphenyl)ethyl	Aromatic phenethyl	438.05341	359.10387	358.09660	179.04048	178.03321	
C14H19NO11S2	10.182	14.3-(4-dihydroxy)glucosaminic	Aromatic benzyl	440.03268	361.08314	360.07587	181.01975	180.01248	31297-84-0
C16H29NO9S2	443.12837	178.8-Nonenyl	Olefins	442.12110	363.17156	362.16429	183.10817	182.10090	
C15H21NO10S2	15.6	95.5-Oxocetyl	Aliphatic ketone-n	444.10036	365.15082	364.14355	185.08743	184.08016	Seed mix
C16H31NO9S2	32.034	184.1-n-Nonyl (Un-natural)	Aliphatic-n	444.13675	365.18721	364.17994	185.12382	184.11655	Seed mix
C16H20NO20S2	14.765	43.3-Indol-3-ylmethylglucobrossidol	Indole	447.05375	368.10421	367.09694	188.04082	187.03355	S. alba
C14H27NO9S3	448.08479	88.6-(Methylthio)glucosaminic	Alkyl-thio-alkyl	448.07752	368.12798	367.12071	189.06459	188.05732	74542-17-9
C12H21NO11S3	451.02767	79.4-Methylsulfonyl-3-butenyl	Alkyl-thio-alkenyl	450.02040	371.07086	370.06359	191.00747	190.00020	
C13H25NO10S3	451.06406	37.3-Hydroxy-5-(methylthio)pentyl	Alkyl-thio-alkyl	450.05679	371.10725	370.09998	191.04386	190.03659	499-37-6
C13H25NO10S3	10.82	72.1(R)-5-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	450.05679	371.10725	370.09998	191.04386	190.03659	
C17H25NO9S2	451.09707	104.4-Phenylbutyl	Aromatic phenethyl	450.05980	371.14026	370.13299	191.07687	190.06360	
C15H19NO11S2	453.03995	8-Benzoyloxymethyl	Benzoates	452.03268	373.08314	372.07587	193.01975	192.01248	
C12H23NO11S3	453.04332	76.4-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	452.03605	373.08651	372.07924	193.02312	192.01585	22149-26-4
C16H23NO10S2	453.07633	140.2-(4-Methoxyphenyl)ethyl	Aromatic phenethyl	452.06906	373.11952	372.11225	193.05613	192.04866	
C15H21NO11S2	455.05560	132.2(S)-2-Hydroxyglucosaminic	Aromatic phenethyl	454.04833	375.09879	374.09152	195.03540	194.02813	
C15H21NO11S2	455.05560	133.2(R)-2-Hydroxyglucosaminic	Aromatic phenethyl	454.04833	375.09879	374.09152	195.03540	194.02813	
C15H21NO11S2	12.797	176.4-Hydroxy-3-m-Glucosaminic	Aromatic benzyl	456.13675	377.18721	376.17994	197.12382	196.11655	Seed mix
C17H31NO9S2	457.14402	179.9-Decenyl	Olefins	462.05679	383.10725	382.09998	203.04386	202.03659	Seed mix
C14H25NO10S3	23.719	91.6-Methylthio-3-oxohexyl	Thio-oxo-alkyl	462.05679	383.10725	382.09998	203.04386	202.03659	
C15H29NO9S3	463.10044	87.7-(Methylthio)glucosaminic	Alkyl-thio-alkyl	462.09317	383.14363	382.13636	203.08024	202.07297	80667-87-0
C16H20NO20S2	10.263	28.4-Hydroxy-indol-5-Hydroxygluc	Indole	463.04866	384.09912	383.09185	204.03573	203.02846	83327-20-2
C16H20NO20S2	464.05593	149.5-Hydroxy-indol-5-Hydroxygluc	Indole	463.04866	384.09912	383.09185	204.03573	203.02846	B. juncea
C14H27NO10S3	465.07970	36.3-Hydroxy-6-(methylthio)hexyl	Alkyl-thio-alkyl	464.07243	385.12289	384.11562	205.05950	204.05223	
C16H21NO11S2	467.05660	67.1(R)-6-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	466.04833	387.09879	386.09152	207.03540	206.02813	
C13H25NO11S3	467.05660	6.2-(Benzoyloxy)ethyl	Benzoates	466.05170	387.10216	386.09489	207.03877	206.03150	
C13H25NO11S3	467.05660	33.1(R)-3-Hydroxyglucosaminic	Alkyl-thio-alkyl	466.05170	387.10216	386.09489	207.03877	206.03150	
C16H23NO11S2	468.07125	81.5-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	468.06398	389.11444	388.10717	209.05105	208.04378	88162-43-0
C16H23NO11S2	468.07125	15.3-(4-Dimethoxy)glucosaminic	Aromatic benzyl	468.06398	389.11444	388.10717	209.05105	208.04378	
C16H23NO11S2	468.07125	134.3-Hydroxy-4-methoxy-2-phenyl	Aromatic phenethyl	468.06398	389.11444	388.10717	209.05105	208.04378	
C16H23NO11S2	468.07125	174.2(R)-2-Hydroxy-2-(4-methoxy)gluc	Aromatic phenethyl	468.06398	389.11444	388.10717	209.05105	208.04378	
C15H27NO10S3	26.052	90.7-(Methylthio-3-oxohexyl)	Thio-oxo-alkyl	476.07243	397.12289	396.11562	217.05950	216.05223	Seed mix
C16H31NO9S3	477.11609	92.8-(Methylthio)glucosaminic	Alkyl-thio-alkyl	476.10882	397.12289	396.11562	217.05950	216.05223	
C17H22NO10S2	18.225	47.7-Methoxy-indol-5-methoxygluc	Indole	477.06431	398.11477	397.10750	218.05138	217.04411	80667-88-1
C17H22NO10S2	20.551	48.4-Methoxy-indol-5-methoxygluc	Indole	477.06431	398.11477	397.10750	218.05138	217.04411	5187-84-8
C17H22NO10S2	478.07158	150.5-Methoxy-indol-5-methoxygluc	Indole	477.06431	398.11477	397.10750	218.05138	217.04411	83327-21-3
C15H29NO10S3	479.05535	66.7(R)-7-(Methylsulfonyl)glucosaminic	Alkyl-sulfonyl-alkyl	478.08808	399.13854	398.13127	219.07515	218.06788	112572-51-7
C17H23NO11S2	481.07125	9.1(R)-2-Benzoylglucosaminic	Benzoates	480.06398	401.11444	400.10717	221.05105	220.04378	
C17H23NO11S2	481.07125	10.3-(Benzoyloxy)glucosaminic	Benzoates	480.06398	401.11444	400.10717	221.05105	220.04378	75331-11-2
C14H27NO11S3	481.07462	32.3-Hydroxy-6-(methylsulfonyl)hexyl	Alkyl-thio-alkyl	480.06735	401.11781	400.11054	221.05442	220.04715	
C14H27NO11S3	481.07462	78.6-(Methylsulfonyl)hexyl	Alkyl-sulfonyl-alkyl	480.06735	401.11781	400.11054	221.05442	220.04715	74542-18-0
C18H29NO10S2	481.10776	49.2-dimethyl-2-(4-methoxy)phenyl	Aromatic phenethyl	480.10049	401.15095	400.14368	221.08756	220.08029	
C13H25NO12S3	483.05589	35.3-Hydroxy-5-(methylsulfonyl)ethyl	Aromatic phenethyl	482.04662	403.09708	402.08981	223.03369	222.02642	
C16H29NO10S3	30.41	93.8-Methylthio-3-oxohexyl	Thio-oxo-alkyl	482.06808	411.13854	410.13127	231.07515	230.06788	Seed mix
C17H33NO9S3	491.13174	89.9-(Methylthio)glucosaminic	Alkyl-thio-alkyl	490.12447	411.17493	410.16766	231.11154	230.10427	M-01406
C16H31NO10S3	493.07462	70.7-Methylsulfonyl(R)-3-oxohexyl	Thio-oxo-alkyl	492.06735	413.11781	412.11054	233.05442	232.04715	M-01403
C14H31NO11S3	493.11100	121.4-(Cystein-S-yl)glucosaminic	Alkyl-sulfonyl-alkyl	493.10373	414.16419	412.14692	233.09080	232.04715	[M01405]
C14H29NO11S3	20.18	49.4-Benzoyloxybutyl	Cystein-thio-alkyl	493.06260	414.11306	413.10579	234.04967	233.04240	D. muralis
C18H25NO11S2	495.08690	5.4-(Benzoyloxy)butyl	Benzoates	494.07963	415.13009	414.12282	235.06670	234.05943	
C15H25NO11S2	495.08690	7.1(R)-2-Benzoylglucosaminic	Benzoates	494.07963	415.13009	414.12282	235.06670	234.05943	80667-89-2
C16H29NO11S3	495.09027	166.7-(Methylsulfonyl)heptyl	Alkyl-sulfonyl-alkyl	494.09630	415.13346	414.12619	235.07007	234.06280	
C14H27NO12S3	497.06953	34.3-Hydroxy-6-(methylsulfonyl)hexyl	Alkyl-thio-alkyl	496.06226	417.11250	416.10545	237.04933	236.04206	
C17H25NO12S2	499.08181	114.3-(4,5-Tri-methoxy)glucosaminic	Aromatic benzyl	498.07454	419.12500	418.11773	239.01611	238.05434	32214-77-0
C18H35NO9S3	505.14739	85.10-(Methylthio)decyl	Alkyl-thio-alkyl	504.14012	425.19058	424.18331	245.12719	244.11992	
C18H29NO11S2	506.06650	2.1-N-Acetyl-indol-1-Acetyl-glucos	Indole	505.05923	426.10969	425.10242	246.04630	245.03903	103951-50-4
C19H29NO11S2	507.08690	123.2(S)-Benzoyloxy-3-butenyl	Benzoates	506.07963	427.13009	426.12682	247.06670	246.05943	356534-71-9



C16H29NO9S3	475.10044	205 8-Methylthio-7-oxoethyl	A	Methyl-thio-alkene	474.09317	395.14363	394.13636	215.08024	214.07297
C17H31NO9S3	488.11609	206 9-Methylthio-8-nonenyl	A	Methyl-thio-alkene	488.10882	409.15928	408.15201	229.09589	228.08862
C18H33NO9S3	503.13174	207 10-Methylthio-9-decenyl	A	Methyl-thio-alkene	502.12447	423.17493	422.16766	243.11154	242.10427
C19H35NO9S3	517.14739	208 11-Methylthio-10-undecenyl	A	Methyl-thio-alkene	516.14012	437.19058	436.18331	257.12719	256.11992
C20H37NO9S3	531.16304	209 12-Methylthio-11-dodecenyl	A	Methyl-thio-alkene	530.15577	451.20623	450.19896	271.14284	270.13557
C10H19NO10S3	408.01711	210 2-Methylthio-hydroxyethyl	A	Methyl-thio-hydroxyalkyl	408.00984	329.06030	328.05303	148.99691	147.98964
C11H21NO10S3	423.03276	211 3-Methylthio-hydroxypropyl	A	Methyl-thio-hydroxyalkyl	422.02549	343.07585	342.06868	163.01256	162.00529
C12H23NO10S3	437.04841	212 4-Methylthio-hydroxybutyl	A	Methyl-thio-hydroxyalkyl	436.04114	357.09160	356.08433	177.02821	176.02094
C13H25NO10S3	451.06406	37 5-Methylthio-hydroxypentyl	A	Methyl-thio-hydroxyalkyl	450.05679	371.10725	370.09998	191.04386	190.03659
C14H27NO10S3	465.07970	36 6-Methylthio-hydroxyhexyl	A	Methyl-thio-hydroxyalkyl	464.07243	385.12289	384.11562	205.05950	204.05223
C15H29NO10S3	479.09535	213 7-Methylthio-hydroxyheptyl	A	Methyl-thio-hydroxyalkyl	478.08808	399.13854	398.13127	219.07515	218.06788
C16H31NO10S3	493.11100	214 8-Methylthio-hydroxyoctyl	A	Methyl-thio-hydroxyalkyl	492.10373	413.15419	412.14692	233.09080	232.08353
C17H33NO10S3	507.12665	215 9-Methylthio-hydroxynonyl	A	Methyl-thio-hydroxyalkyl	506.11938	427.16984	426.16257	247.10645	246.09918
C18H35NO10S3	521.14230	216 10-Methylthio-hydroxydeyl	A	Methyl-thio-hydroxyalkyl	520.13503	441.18549	440.17822	261.12210	260.11483
C19H37NO10S3	535.15795	217 11-Methylthio-hydroxyundecyl	A	Methyl-thio-hydroxyalkyl	534.15068	455.20114	454.19387	275.13775	274.13048
C10H17NO10S3	407.00146	218 2-Methylthio-oxoethyl	A	Methyl-thio-oxo-alkyl	405.98419	327.04465	326.03738	146.98126	145.97399
C11H19NO10S3	421.01711	219 3-Methylthio-oxopropyl	A	Methyl-thio-oxo-alkyl	420.00984	341.06030	340.05303	160.99691	159.98964
C12H21NO10S3	435.03276	220 4-Methylthio-oxobutyl	A	Methyl-thio-oxo-alkyl	434.02549	355.07595	354.06868	175.01256	174.00529
C13H23NO10S3	449.04841	221 5-Methylthio-oxopentyl	A	Methyl-thio-oxo-alkyl	448.04114	369.09160	368.08433	189.02821	188.02094
C14H25NO10S3	463.06406	91 6-Methylthio-oxohexyl	A	Methyl-thio-oxo-alkyl	462.05679	383.10725	382.09998	203.04386	202.03659
C15H27NO10S3	477.07970	90 7-Methylthio-oxoheptyl	A	Methyl-thio-oxo-alkyl	476.07243	397.12289	396.11562	217.05950	216.05223
C16H29NO10S3	491.09535	93 8-Methylthio-oxooctyl	A	Methyl-thio-oxo-alkyl	490.08808	411.13854	410.13127	231.07515	230.06788
C17H31NO10S3	505.11100	223 9-Methylthio-oxononyl	A	Methyl-thio-oxo-alkyl	504.10373	425.15419	424.14692	245.09080	244.08353
C18H33NO10S3	507.12665	224 10-Methylthio-oxodecyl	A	Methyl-thio-oxo-alkyl	506.11938	427.16984	426.16257	247.10645	246.09918
C12H21NO11S3	435.03276	63 4-Methylsulfinyl-Glucoaphenir	A	Methyl-sulfinyl-alkene	434.02549	355.07595	354.06868	175.01256	174.00529
C13H23NO11S3	449.04841	228 5-Methylsulfinyl-4-pentyl	A	Methyl-sulfinyl-alkene	448.04114	369.09160	368.08433	189.02821	188.02094
C14H25NO11S3	463.06406	227 6-Methylsulfinyl-5-hexyl	A	Methyl-sulfinyl-alkene	462.05679	383.10725	382.09998	203.04386	202.03659
C15H27NO11S3	477.07970	229 7-Methylsulfinyl-6-heptyl	A	Methyl-sulfinyl-alkene	476.07243	397.12289	396.11562	217.05950	216.05223
C16H29NO11S3	491.09535	229 8-Methylsulfinyl-8-nonyl	A	Methyl-sulfinyl-alkene	490.08808	411.13854	410.13127	231.07515	230.06788
C17H31NO11S3	505.11100	230 9-Methylsulfinyl-9-decyl	A	Methyl-sulfinyl-alkene	504.10373	425.15419	424.14692	245.09080	244.08353
C18H33NO11S3	519.12665	232 11-Methylsulfinyl-10-undecyl	A	Methyl-sulfinyl-alkene	517.11568	438.16202	437.15475	258.09863	257.09136
C19H35NO11S3	533.14230	232 11-Methylsulfinyl-11-dodecyl	A	Methyl-sulfinyl-alkene	530.11938	451.16984	450.16257	271.10645	270.09918
C20H37NO11S3	547.15795	233 12-Methylsulfinyl-11-dodecyl	A	Methyl-sulfinyl-alkene	543.12721	464.17677	463.17040	284.11428	283.10701
C11H19NO11S3	425.01202	234 2-Hydroxy-2-(methylsulfinyl)ethyl	A	Methyl-sulfinyl-hydroxy-alkyl	424.00475	345.05521	344.04794	164.99182	163.98455
C12H21NO11S3	439.02767	235 3-Hydroxy-3-(methylsulfinyl)propyl	A	Methyl-sulfinyl-hydroxy-alkyl	438.02040	359.07086	358.06359	179.00747	178.00020
C13H23NO11S3	453.04332	236 3-Hydroxy-4-(methylsulfinyl)butyl	A	Methyl-sulfinyl-hydroxy-alkyl	452.03605	373.08651	372.07924	193.02312	192.01585
C14H25NO11S3	467.05897	33 3-Hydroxy-5-(methylsulfinyl)pentyl	A	Methyl-sulfinyl-hydroxy-alkyl	466.05170	387.10216	386.09489	207.03877	206.03150
C15H27NO11S3	481.07462	32 3-Hydroxy-6-(methylsulfinyl)hexyl	A	Methyl-sulfinyl-hydroxy-alkyl	480.06735	401.11781	400.11054	221.05442	220.04715
C16H29NO11S3	495.09027	237 3-Hydroxy-7-(methylsulfinyl)heptyl	A	Methyl-sulfinyl-hydroxy-alkyl	494.09300	415.13348	414.12619	235.07007	234.06280
C17H31NO11S3	509.10592	238 3-Hydroxy-8-(methylsulfinyl)octyl	A	Methyl-sulfinyl-hydroxy-alkyl	508.09865	429.14911	428.14184	249.08572	248.07845
C18H33NO11S3	523.12157	239 3-Hydroxy-9-(methylsulfinyl)nonyl	A	Methyl-sulfinyl-hydroxy-alkyl	522.11430	443.16476	442.15749	263.10137	262.09410
C19H35NO11S3	537.13722	240 3-Hydroxy-10-(methylsulfinyl)decyl	A	Methyl-sulfinyl-hydroxy-alkyl	536.12965	457.18041	456.17314	277.11702	276.10975
C10H17NO11S3	422.99637	241 3-Hydroxy-11-(methylsulfinyl)undecyl	A	Methyl-sulfinyl-hydroxy-alkyl	421.98910	343.03956	342.03229	162.97617	161.96890
C11H19NO11S3	437.01202	243 3-Methylsulfinyl-3-oxopropyl	A	Methyl-sulfinyl-oxo-alkyl	436.00475	357.05521	356.04794	176.99182	175.98455
C12H21NO11S3	451.02767	244 4-Methylsulfinyl-3-oxobutyl	A	Methyl-sulfinyl-oxo-alkyl	450.02040	371.07086	370.06359	191.00747	190.00020
C13H23NO11S3	465.04332	245 5-Methylsulfinyl-3-oxopentyl	A	Methyl-sulfinyl-oxo-alkyl	464.03605	385.08651	384.07924	205.02312	204.01585
C14H25NO11S3	479.05897	246 6-Methylsulfinyl-3-oxohexyl	A	Methyl-sulfinyl-oxo-alkyl	478.05170	399.10216	398.09489	219.03877	218.03150
C15H27NO11S3	493.07462	70 7-Methylsulfinyl-3-oxohexyl	A	Methyl-sulfinyl-oxo-alkyl	492.06735	413.11781	412.11054	233.05442	232.04715
C16H29NO11S3	507.09027	71 8-Methylsulfinyl-3-oxooctyl	A	Methyl-sulfinyl-oxo-alkyl	506.08300	427.13348	426.12619	247.07007	246.06280
C17H31NO11S3	521.10592	247 9-Methylthio-3-oxononyl	A	Methyl-sulfinyl-oxo-alkyl	520.09865	441.14911	440.14184	261.08572	260.07845
C18H33NO11S3	535.12157	248 10-Methylthio-3-oxodecyl	A	Methyl-sulfinyl-oxo-alkyl	534.11430	455.16476	454.15749	275.10137	274.09410
C19H35NO11S3	549.13722	249 11-Methylthio-3-oxododecyl	A	Methyl-sulfinyl-oxo-alkyl	548.12995	469.18041	468.17314	289.11702	288.10975
C11H19NO11S3	437.01202	250 3-Methylsulfonyl-2-propenyl	A	Methyl-sulfonyl-alkene	436.00475	357.05521	356.04794	176.99182	175.98455
C12H21NO11S3	451.02767	75 4-Methylsulfonyl-3-butenyl	A	Methyl-sulfonyl-alkene	450.02040	371.07086	370.06359	191.00747	190.00020
C13H23NO11S3	465.04332	251 5-Methylsulfonyl-4-pentenyl	A	Methyl-sulfonyl-alkene	464.03605	385.08651	384.07924	205.02312	204.01585
C14H25NO11S3	479.05897	252 6-Methylsulfonyl-5-hexenyl	A	Methyl-sulfonyl-alkene	478.05170	399.10216	398.09489	219.03877	218.03150
C15H27NO11S3	493.07462	253 7-Methylsulfonyl-6-heptenyl	A	Methyl-sulfonyl-alkene	492.06735	413.11781	412.11054	233.05442	232.04715
C16H29NO11S3	507.09027	254 8-Methylsulfonyl-7-octenyl	A	Methyl-sulfonyl-alkene	506.08300	427.13348	426.12619	247.07007	246.06280
C17H31NO11S3	521.10592	255 9-Methylsulfonyl-8-nonenyl	A	Methyl-sulfonyl-alkene	520.09865	441.14911	440.14184	261.08572	260.07845
C18H33NO11S3	535.12157	256 10-Methylsulfonyl-9-decenyl	A	Methyl-sulfonyl-alkene	534.11430	455.16476	454.15749	275.10137	274.09410
C19H35NO11S3	549.13722	257 11-Methylsulfonyl-10-undecenyl	A	Methyl-sulfonyl-alkene	548.12995	469.18041	468.17314	289.11702	288.10975
C20H37NO11S3	563.15287	258 12-Methylsulfonyl-11-dodecyl	A	Methyl-sulfonyl-alkene	562.14560	483.19606	482.18879	303.13267	302.12540
C10H19NO12S3	441.00694	259 2-Methylsulfonyl-hydroxyethyl	A	Methyl-sulfonyl-hydroxy-alkyl	439.99967	361.05013	360.04286	180.98674	179.97947
C11H21NO12S3	455.02259	260 3-Methylsulfonyl-hydroxypropyl	A	Methyl-sulfonyl-hydroxy-alkyl	454.01532	375.06578	374.05851	195.00239	193.99512
C12H23NO12S3	469.03824	261 4-Methylsulfonyl-hydroxybutyl	A	Methyl-sulfonyl-hydroxy-alkyl	468.03097	389.08143	388.07416	209.01804	208.01077
C13H25NO12S3	483.05369	35 5-Methylsulfonyl-hydroxy-pentyl	A	Methyl-sulfonyl-hydroxy-alkyl	482.04662	403.09708	402.08981	223.03369	222.02642
C14H27NO12S3	497.06953	34 6-Methylsulfonyl-hydroxy-hexyl	A	Methyl-sulfonyl-hydroxy-alkyl	496.06226	417.11272	416.10545	237.04933	236.04206

C15H29NO12S3	511.08518	262	7-Methylsulfonylhydroxy-heptA	Methyl-sulfonylhydroxy-alkyl	510.07791	431.12837	430.12110	251.06498	250.05771		
C16H31NO12S3	528.10083	263	8-Methylsulfonylhydroxy-octyl	Methyl-sulfonylhydroxy-alkyl	524.09356	445.14402	444.13675	265.08063	264.07336		
C17H33NO12S3	539.11648	264	9-Methylsulfonylhydroxy-nonyl	Methyl-sulfonylhydroxy-alkyl	538.10921	459.15987	458.15240	279.09628	278.08901		
C18H35NO12S3	553.13213	265	10-Methylsulfonylhydroxy-decyl	Methyl-sulfonylhydroxy-alkyl	552.12486	473.17532	472.16805	293.11193	292.10466		
C19H37NO12S3	567.14778	266	11-Methylsulfonylhydroxy-undecyl	Methyl-sulfonylhydroxy-alkyl	566.14051	487.19097	486.18370	307.12758	306.12031		
C10H17NO12S3	438.99129	267	2-Methylsulfonyl-oxo-ethyl	Methyl-sulfonyl-oxo-alkyl	437.98402	359.03448	358.02721	178.97109	177.96382		
C11H19NO12S3	453.00694	268	3-Methylsulfonyl-oxo-propyl	Methyl-sulfonyl-oxo-alkyl	451.99967	373.05013	372.04286	192.98674	191.97947		
C12H21NO12S3	467.02259	269	4-Methylsulfonyl-oxo-butyl	Methyl-sulfonyl-oxo-alkyl	466.01532	387.06578	386.05851	207.00239	205.99512		
C13H23NO12S3	481.03824	270	5-Methylsulfonyl-oxo-pentyl	Methyl-sulfonyl-oxo-alkyl	480.03097	401.08143	400.07416	221.01804	220.01077		
C14H25NO12S3	495.05389	271	6-Methylsulfonyl-oxo-hexyl	Methyl-sulfonyl-oxo-alkyl	494.04662	415.09708	414.08981	235.03369	234.02642		
C15H27NO12S3	509.06953	272	7-Methylsulfonyl-oxo-heptyl	Methyl-sulfonyl-oxo-alkyl	508.06226	429.11272	428.10545	249.04933	248.04206		
C16H29NO12S3	523.08518	273	8-Methylsulfonyl-oxo-octyl	Methyl-sulfonyl-oxo-alkyl	522.07791	443.12837	442.12110	263.06498	262.05771		
C17H31NO12S3	537.10083	274	9-Methylsulfonyl-oxo-nonyl	Methyl-sulfonyl-oxo-alkyl	536.09356	457.14402	456.13675	277.08063	276.07336		
C18H33NO12S3	551.11648	275	10-Methylsulfonyl-oxo-decyl	Methyl-sulfonyl-oxo-alkyl	550.10921	471.15967	470.15240	291.09628	290.08901		
C19H35NO12S3	565.13213	276	11-Methylsulfonyl-oxo-undecyl	Methyl-sulfonyl-oxo-alkyl	564.12486	485.17532	484.16805	305.11193	304.10466		
C14H23NO9S3	445.05349	277	Butenyl-thio-propene	Butenyl-thio-alkene	444.04622	365.09668	364.08941	185.03329	184.02602		
C15H25NO9S3	459.06914	278	Butenyl-thio-butene	Butenyl-thio-alkene	458.06187	379.11233	378.10506	199.04894	198.04167		
C16H27NO9S3	473.08479	279	Butenyl-thio-pentene	Butenyl-thio-alkene	472.07752	393.12798	392.12071	213.06459	212.05732		
C17H29NO9S3	487.10044	280	Butenyl-thio-hexene	Butenyl-thio-alkene	486.09317	407.14363	406.13636	227.08024	226.07297		
C18H31NO9S3	501.11609	281	Butenyl-thio-heptene	Butenyl-thio-alkene	500.10982	421.15928	420.15201	241.09589	240.08862		
C19H33NO9S3	515.13174	282	Butenyl-thio-octene	Butenyl-thio-alkene	514.12447	435.17493	434.16766	255.11154	254.10427		
C20H35NO9S3	529.14739	283	Butenyl-thio-nonene	Butenyl-thio-alkene	528.14012	449.19058	448.18331	269.12719	268.11992		
C21H37NO9S3	543.16304	284	Butenyl-thio-decene	Butenyl-thio-alkene	542.15577	463.20623	462.19896	283.14284	282.13557		
C22H39NO9S3	557.17868	182	Butenyl-thio-undecene	Butenyl-thio-alkene	556.17141	477.22187	476.21460	297.15848	296.15121		
C23H41NO9S3	571.19433	285	Butenyl-thio-dodecene	Butenyl-thio-alkene	570.18706	491.23752	490.23025	311.17413	310.16686		
C17H23NO11S3	513.04332	286	Benzyl-sulfonyl-propenyl	Benzyl-sulfonyl-alkene	512.03605	433.09651	432.07924	253.02312	252.01585		
C18H25NO11S3	527.05897	287	Benzyl-sulfonyl-butenyl	Benzyl-sulfonyl-alkene	526.05170	447.10218	446.09489	267.03877	266.03150		
C19H27NO11S3	541.07462	181	Benzyl-sulfonyl-pentenyl	Benzyl-sulfonyl-alkene	540.06735	461.11781	460.11054	281.05442	280.04715		
C20H29NO11S3	555.09027	288	Benzyl-sulfonyl-hexenyl	Benzyl-sulfonyl-alkene	554.08300	475.13346	474.12619	295.07007	294.06280		
C21H31NO11S3	569.10592	289	Benzyl-sulfonyl-heptenyl	Benzyl-sulfonyl-alkene	568.09655	489.14911	488.14184	309.08572	308.07845		
C22H33NO11S3	583.12157	290	Benzyl-sulfonyl-octenyl	Benzyl-sulfonyl-alkene	582.11430	503.16476	502.15749	323.10137	322.09410		
C23H35NO11S3	597.13722	291	Benzyl-sulfonyl-nonenyl	Benzyl-sulfonyl-alkene	594.1430	515.18476	514.15749	335.10137	334.09410		
C24H37NO11S3	609.15287	292	Benzyl-sulfonyl-decenyl	Benzyl-sulfonyl-alkene	608.12995	529.18041	528.17314	349.11702	348.10975		
C25H39NO11S3	623.16851	293	Benzyl-sulfonyl-undecenyl	Benzyl-sulfonyl-alkene	624.16124	543.21170	542.20443	365.14831	364.14104		
C26H41NO11S3	637.18416	294	Benzyl-sulfonyl-dodecenyl	Benzyl-sulfonyl-alkene	636.17699	557.22735	556.22008	379.16396	378.15669		
C14H25NO14S2	558.01579	295	(glucosyl-disulfanyl)Methyl	Glucosyl-disulfanyl-alkyl	558.00852	479.03898	478.05171	298.99559	297.98832		
C15H27NO14S2	573.03144	296	(glucosyl-disulfanyl)Ethyl	Glucosyl-disulfanyl-alkyl	572.02417	493.07463	492.06736	313.01124	312.00397		
C16H29NO14S2	587.04709	297	(glucosyl-disulfanyl)Propyl	Glucosyl-disulfanyl-alkyl	586.03982	507.09028	506.08301	327.02689	326.01962		
C17H31NO14S2	601.06273	135	(glucosyl-disulfanyl)Butyl	Glucosyl-disulfanyl-alkyl	600.05946	521.10592	520.09865	341.04253	340.03526		
C18H33NO14S2	615.07838	298	(glucosyl-disulfanyl)Pentyl	Glucosyl-disulfanyl-alkyl	614.07111	535.12157	534.11430	355.05818	354.05091		
C19H35NO14S2	629.09403	299	(glucosyl-disulfanyl)Hexyl	Glucosyl-disulfanyl-alkyl	628.08676	549.13722	548.12995	369.07383	368.06656		
C20H37NO14S2	643.10968	300	(glucosyl-disulfanyl)Heptyl	Glucosyl-disulfanyl-alkyl	642.10241	563.15287	562.14560	383.08948	382.08221		
C21H39NO14S2	657.12533	301	(glucosyl-disulfanyl)Octyl	Glucosyl-disulfanyl-alkyl	656.11806	577.16852	576.16125	397.10513	396.09786		
C22H41NO14S2	671.14098	302	(glucosyl-disulfanyl)Nonyl	Glucosyl-disulfanyl-alkyl	670.13371	591.18417	590.17690	411.12078	410.11351		
C23H43NO14S2	685.15663	303	(glucosyl-disulfanyl)Decyl	Glucosyl-disulfanyl-alkyl	684.14936	605.19982	604.19255	425.13643	424.12916		
C16H28NO18S6	727.96614	304	Dimeric 4-mercaptomethyl	Dimer-mercapto	726.95887	648.00933	647.00206	467.94594	466.93867		
C18H32NO18S6	755.99744	305	Dimeric 4-mercaptoethyl	Dimer-mercapto	754.99017	676.04063	675.03336	495.97724	494.96997		
C20H36NO18S6	784.02874	306	Dimeric 4-mercaptoPropyl	Dimer-mercapto	783.02147	704.07193	703.06466	524.00854	523.00127		
C22H40NO18S6	812.06003	136	4-MercaptoButyl dimer	Dimer-mercapto	811.05276	732.10322	731.09595	552.03983	551.03256		
C24H44NO18S6	840.09133	307	Dimeric 4-mercaptoPentyl	Dimer-mercapto	839.08406	760.13452	759.12725	580.07113	579.06386	std mix	
C26H48NO18S6	868.12263	308	Dimeric 4-mercaptoHexyl	Dimer-mercapto	867.11536	788.16582	787.15855	608.10243	607.09516		
C28H52NO18S6	896.15393	309	Dimeric 4-mercaptoHeptyl	Dimer-mercapto	895.14686	816.19712	815.18985	636.13373	635.12646		
C30H56NO18S6	924.18523	310	Dimeric 4-mercaptoOctyl	Dimer-mercapto	923.17796	844.22842	843.22115	664.16503	663.15776		
C32H60NO18S6	952.21653	311	Dimeric 4-mercaptoNonyl	Dimer-mercapto	951.20926	872.25972	871.25245	692.19633	691.18906		
C33H62NO18S6	980.24782	312	Dimeric 4-mercaptoDecyl	Dimer-mercapto	979.24055	900.29101	899.28374	720.22762	719.22035		
C11H20N2O11S3	455.02292	313	(Cystein-S-yl)methyl	Cysteinyl-alkyl	451.01565	372.06611	371.05884	192.00272	190.99545		
C12H22N2O11S3	469.03857	314	(Cystein-S-yl)ethyl	Cysteinyl-alkyl	465.03130	386.08176	385.07449	206.01837	205.01110		
C13H24N2O11S3	483.05422	315	(Cystein-S-yl)propyl	Cysteinyl-alkyl	479.04695	400.09741	399.09014	220.03402	219.02675		
C14H26N2O11S3	497.06987	121	(Cystein-S-yl)butyl	Cysteinyl-alkyl	493.06260	414.11306	413.10579	234.04967	233.04240		
C15H28N2O11S3	508.0855	316	(Cystein-S-yl)pentyl	Cysteinyl-alkyl	507.07823	428.12869	427.12142	248.06530	247.05803		
C16H30N2O11S3	522.10117	317	(Cystein-S-yl)hexyl	Cysteinyl-alkyl	521.09390	442.14436	441.13709	262.08097	261.07370		
C17H32N2O11S3	536.11682	318	(Cystein-S-yl)heptyl	Cysteinyl-alkyl	535.10955	456.16001	455.15274	276.09662	275.08935		
C18H34N2O11S3	550.13247	319	(Cystein-S-yl)octyl	Cysteinyl-alkyl	549.12520	470.17566	469.16839	290.11227	289.10500		
C19H36N2O11S3	564.14811	320	(Cystein-S-yl)nonyl	Cysteinyl-alkyl	563.14084	484.19130	483.18403	304.12791	303.12064		
C20H38N2O11S3	578.16376	321	(Cystein-S-yl)decyl	Cysteinyl-alkyl	577.15649	498.20695	497.19968	318.14356	317.13629		
C9H16N2O11S2	392.01955	322	2-(glycinyl)methyl CH(NH2)OC	Glycine-alkyl	391.01228	312.06274	311.05547	131.99935	130.99208		
C10H18N2O11S2	409.03562	323	2-(glycinyl)ethyl CH2CH(NH2)K	Glycine-alkyl	405.02793	326.07839	325.07112	146.01500	145.00773		
C11H20N2O11S2	426.05085	324	2-(glycinyl)propyl CH2CH2CH(NH2)K	Glycine-alkyl	419.04358	340.09404	339.08677	160.03065	159.02338		

