

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
 Data File : BF106497.D
 Acq On : 15 Jun 2018 17:40
 Operator : JU/SJ
 Sample : J3464-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-41-COMP

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.207	483	488	496	rVB	220855	279419	10.52%	0.943%
2	5.613	553	557	564	rBV	2485498	2655094	100.00%	8.964%
3	6.607	722	726	739	rBV	2621693	2627468	98.96%	8.871%
4	6.748	745	750	753	rBV	2720180	2611586	98.36%	8.818%
5	6.966	783	787	790	rBV	1071235	828493	31.20%	2.797%
6	7.125	809	814	817	rBV	2272229	2115915	79.69%	7.144%
7	7.531	877	883	886	rBV	1821568	1800978	67.83%	6.081%
8	8.248	1001	1005	1008	rBV	1209281	1017255	38.31%	3.435%
9	9.319	1183	1187	1191	rBV	2682183	2597026	97.81%	8.768%
10	9.713	1250	1254	1257	rBV	385745	306297	11.54%	1.034%
11	9.919	1286	1289	1293	rBV	62479	48995	1.85%	0.165%
12	10.007	1300	1304	1308	rBV	1219512	1030065	38.80%	3.478%
13	10.419	1372	1374	1377	rVB	87976	62528	2.36%	0.211%
14	10.642	1406	1412	1414	rBV	22296	26660	1.00%	0.090%
15	10.801	1434	1439	1442	rBV	1627557	1531950	57.70%	5.172%
16	10.895	1452	1455	1464	rBV	75727	80702	3.04%	0.272%
17	11.342	1528	1531	1534	rBV	42016	31530	1.19%	0.106%
18	11.495	1554	1557	1561	rBV	1012641	885494	33.35%	2.990%
19	11.872	1618	1621	1624	rBV	858776	648536	24.43%	2.190%
20	12.566	1735	1739	1740	rBV	1770115	1635319	61.59%	5.521%
21	12.583	1740	1742	1749	rVV2	2354569	2219872	83.61%	7.495%
22	12.666	1753	1756	1760	rVB	367607	275424	10.37%	0.930%
23	13.083	1823	1827	1830	rBV	2407462	2116451	79.71%	7.146%
24	13.319	1864	1867	1870	rVB	35442	33144	1.25%	0.112%
25	13.395	1874	1880	1882	rBV	31193	29183	1.10%	0.099%
26	13.830	1949	1954	1959	rBV4	19003	28493	1.07%	0.096%
27	13.971	1974	1978	1986	rBV	195887	229833	8.66%	0.776%
28	14.154	2005	2009	2013	rBV	1033959	943220	35.52%	3.185%
29	14.624	2086	2089	2097	rBV4	28882	42512	1.60%	0.144%
30	15.707	2267	2273	2278	rBV	662007	851221	32.06%	2.874%
31	16.171	2349	2352	2357	rBV4	18552	27456	1.03%	0.093%

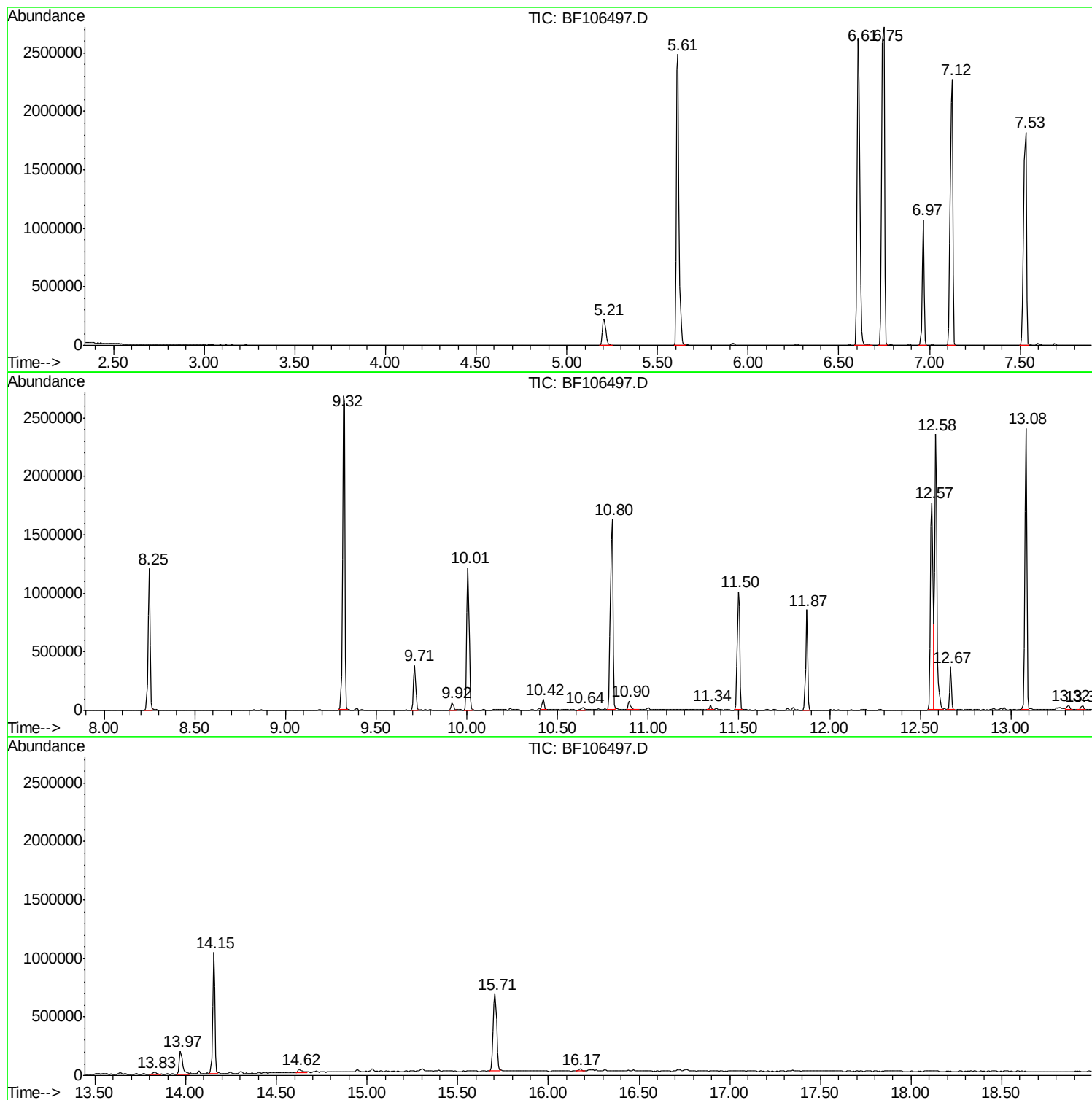
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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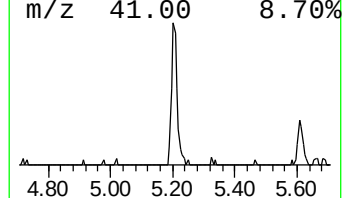
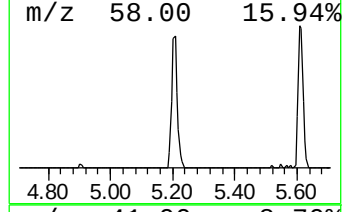
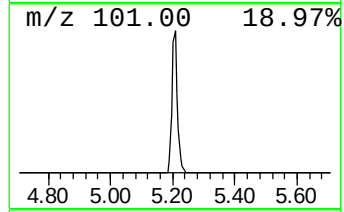
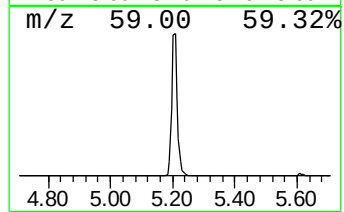
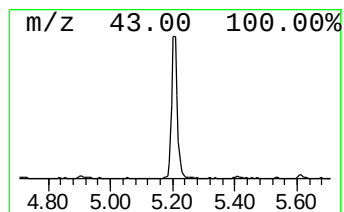
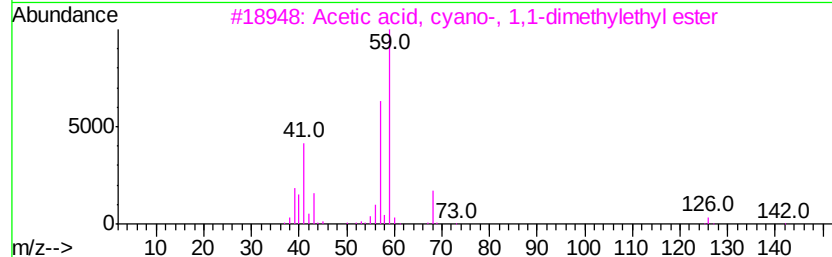
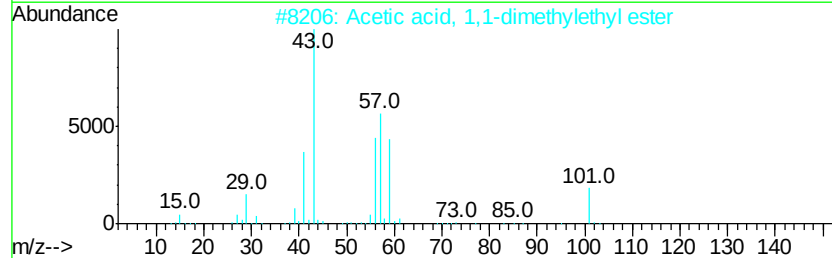
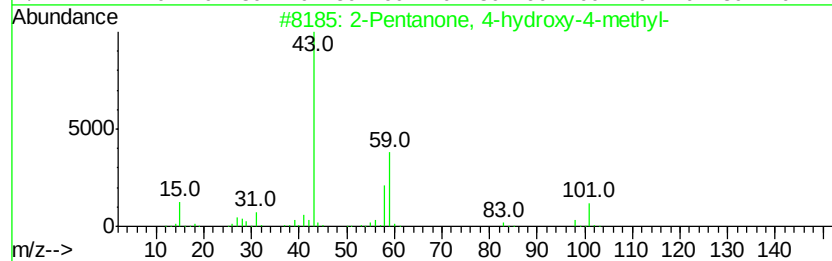
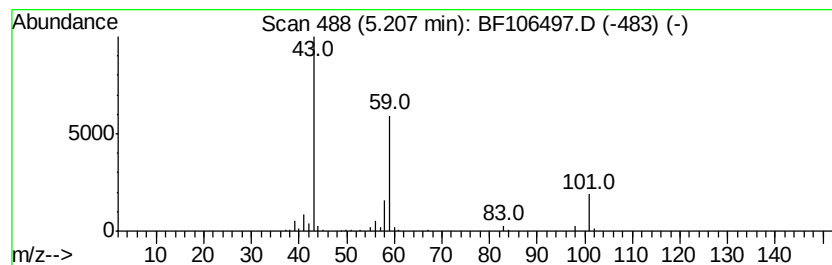
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.75 ng	279419	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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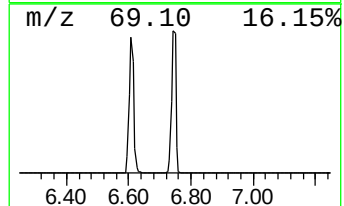
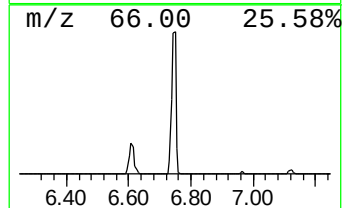
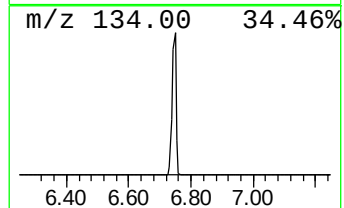
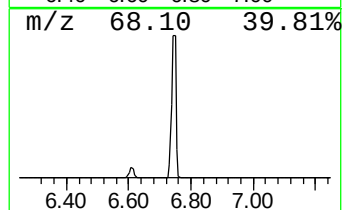
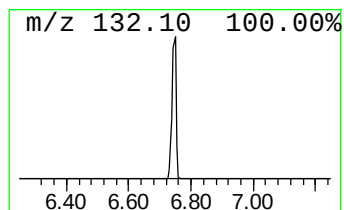
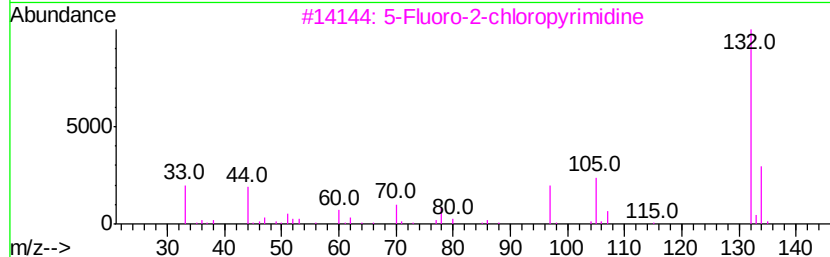
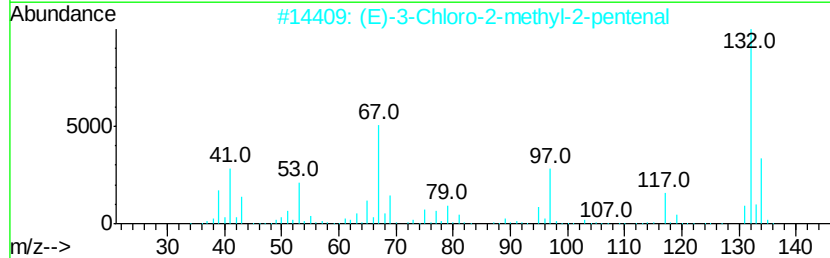
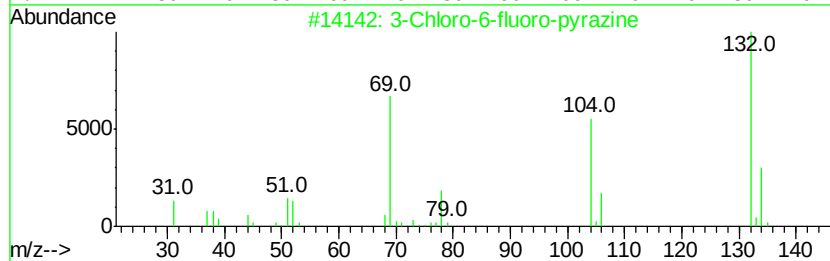
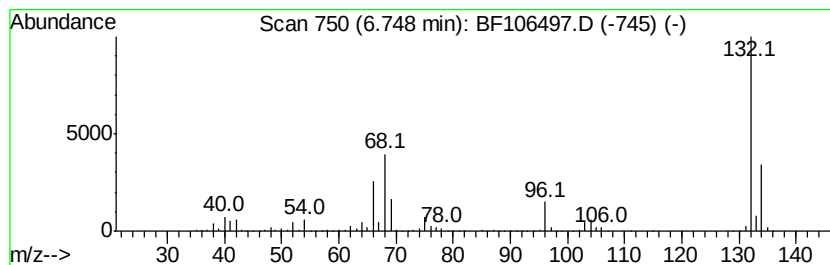
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	63.04 ng	2611590	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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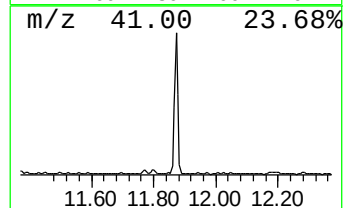
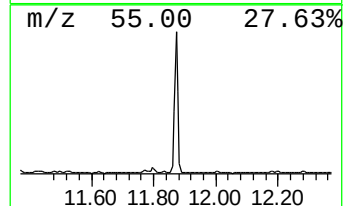
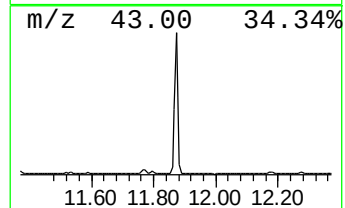
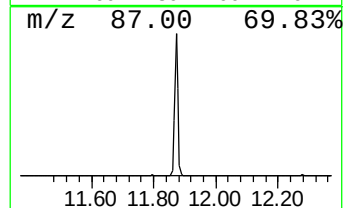
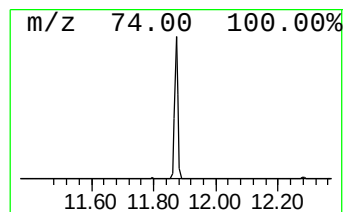
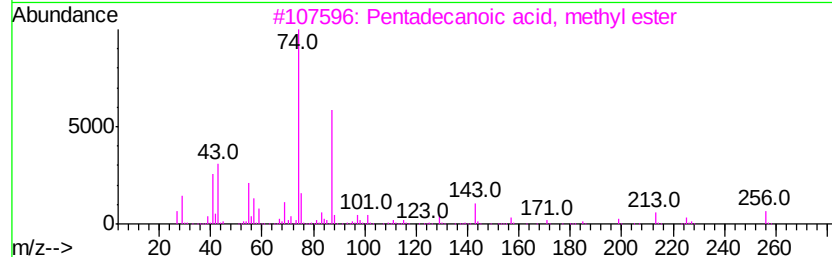
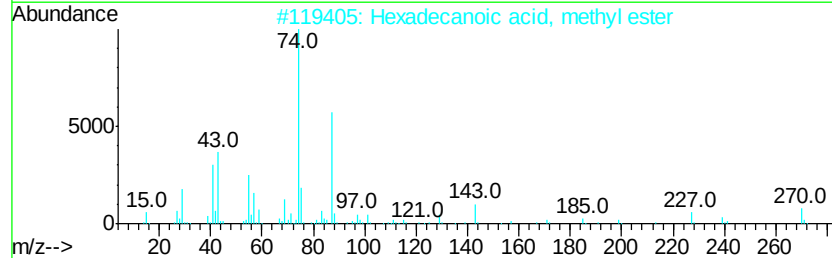
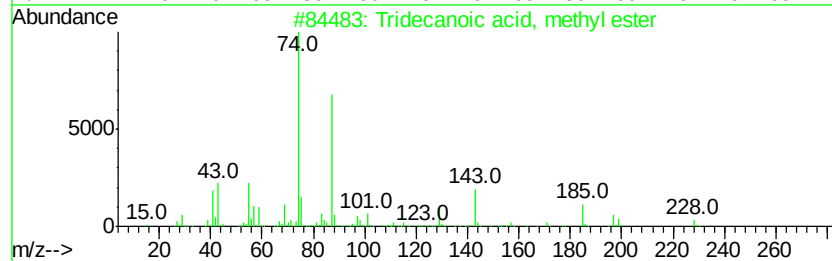
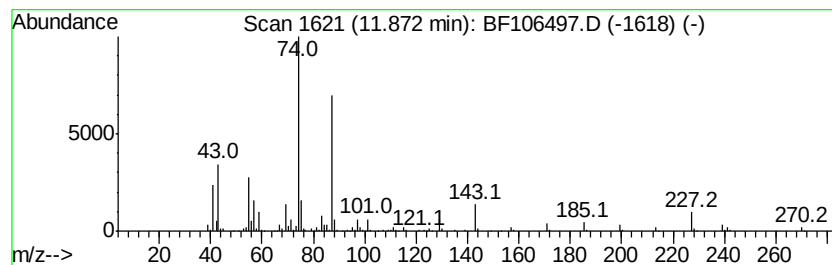
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Peak Number 4 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	14.65 ng	648536	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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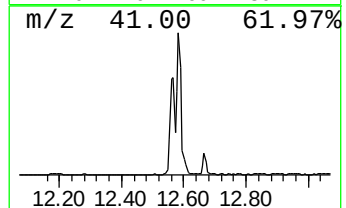
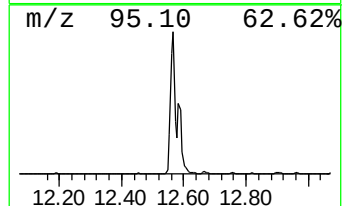
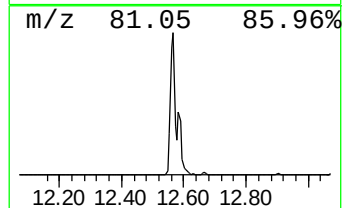
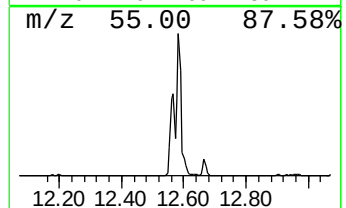
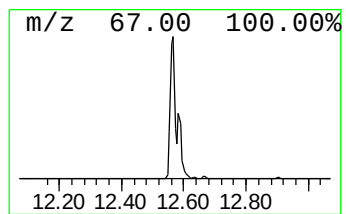
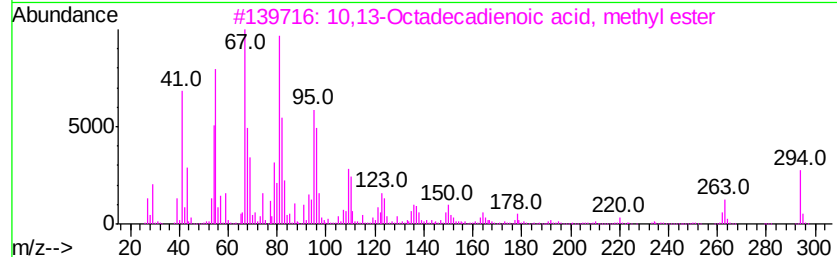
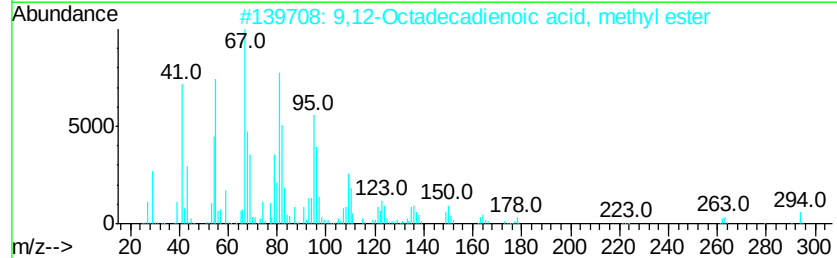
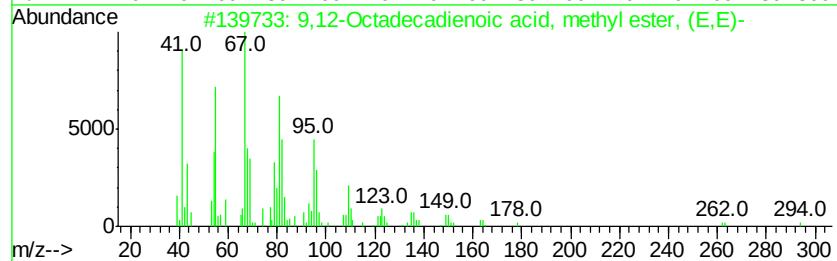
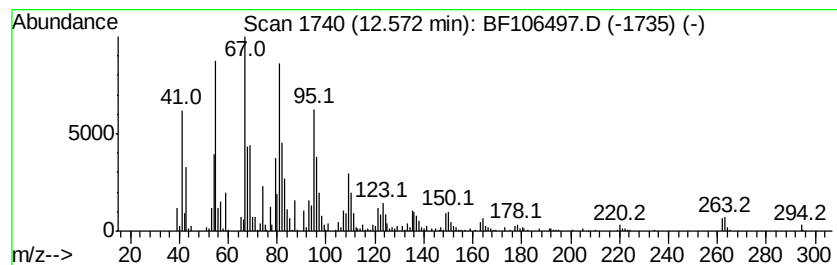
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Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	36.94 ng	1635320	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98



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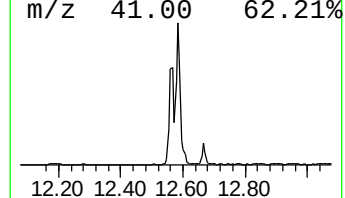
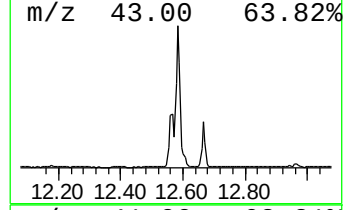
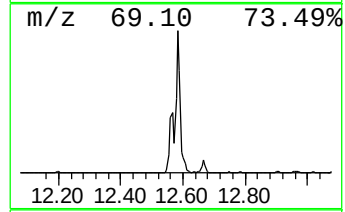
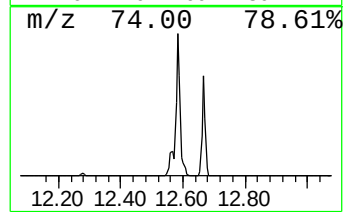
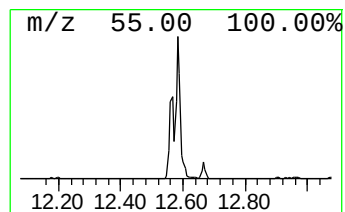
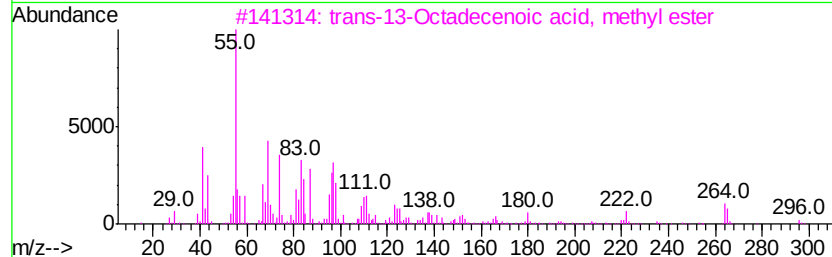
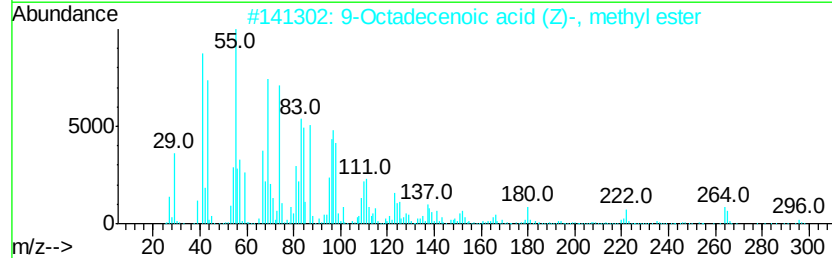
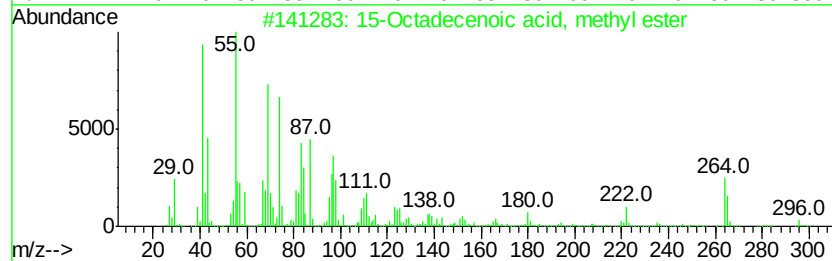
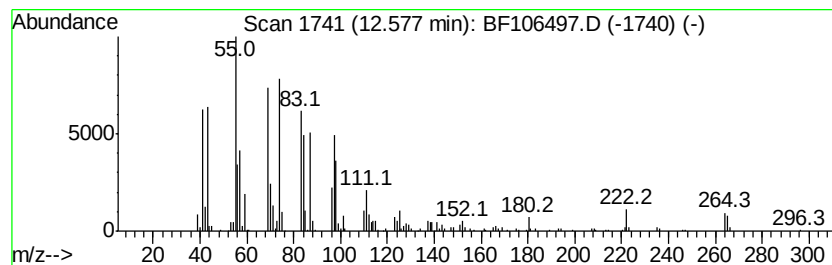
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Peak Number 6 15-Octadecenoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	50.14 ng	2219870	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	94
2		9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	94
3		trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	91
4		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
5		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



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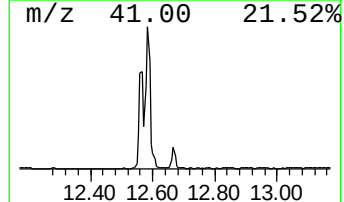
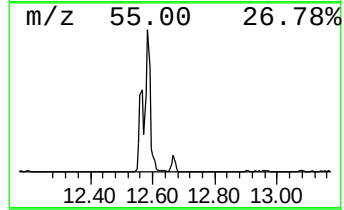
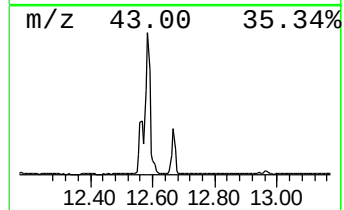
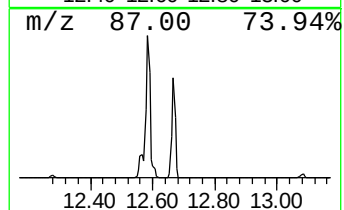
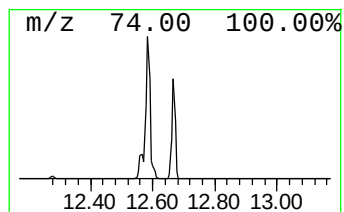
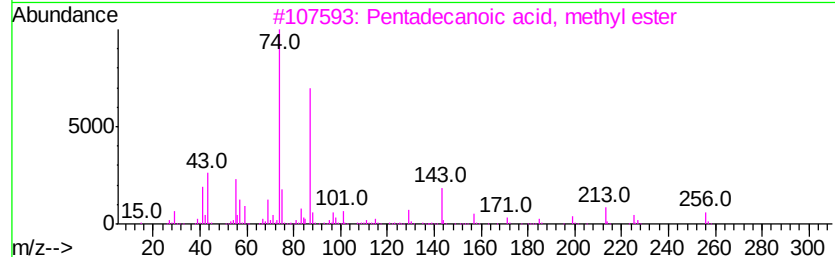
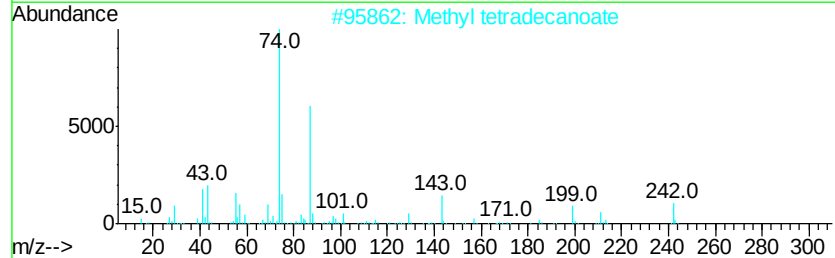
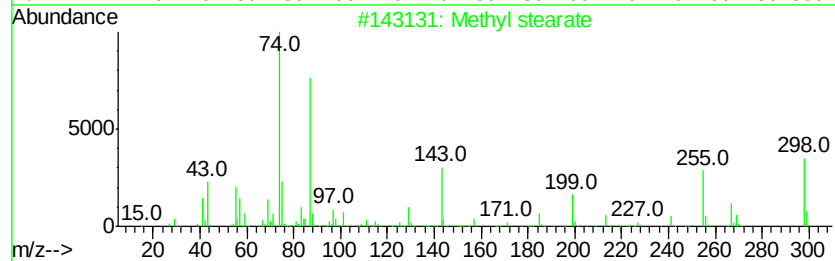
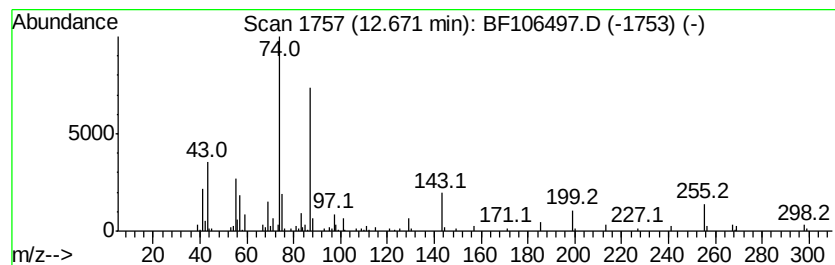
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	6.22 ng	275424	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl stearate	298	C19H38O2	000112-61-8	97
2		Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	94
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
5		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106497.D
Acq On : 15 Jun 2018 17:40
Operator : JU/SJ
Sample : J3464-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

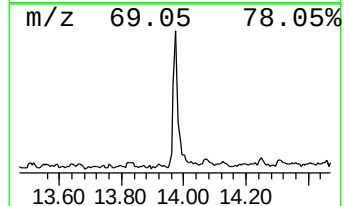
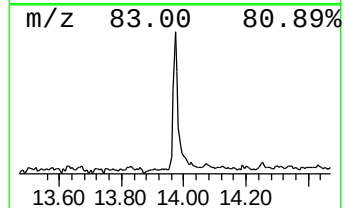
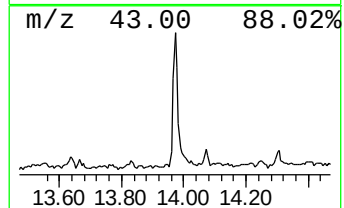
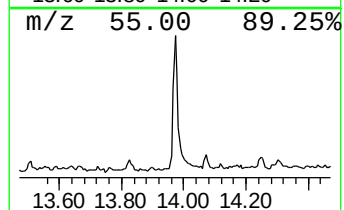
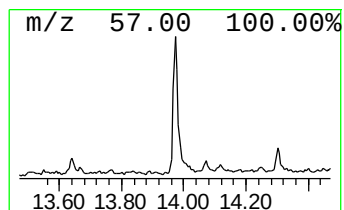
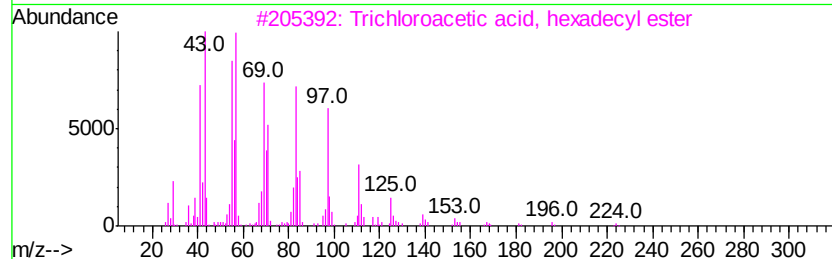
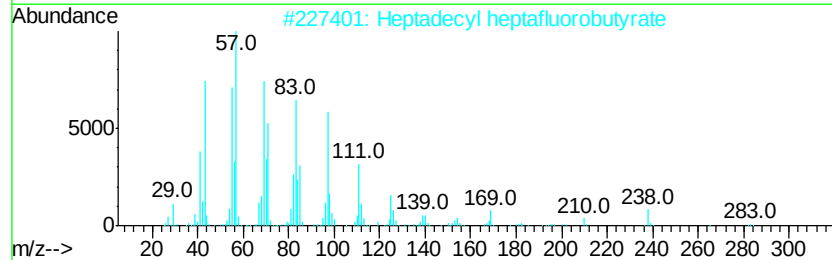
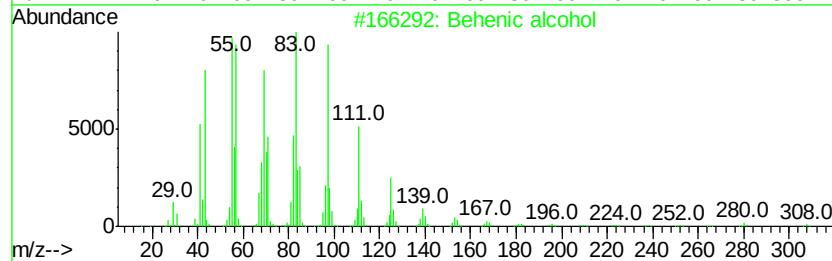
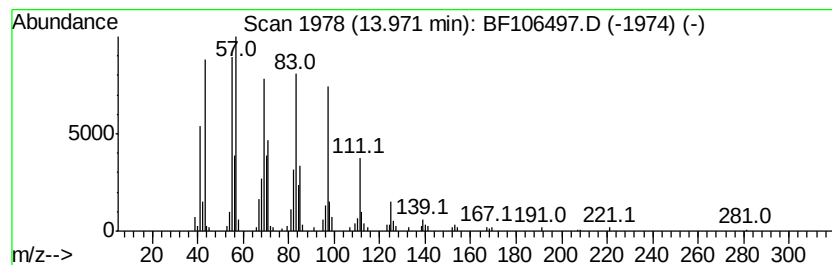
Instrument :
BNA_F
ClientSampleId :
SB-41-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.97	4.87 ng	229833	Chrysene-d12		14.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061518\
Data File : BF106497.D
Acq On : 15 Jun 2018 17:40
Operator : JU/SJ
Sample : J3464-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-41-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	6.8	ng	279419	1	6.97	828493	20.0
unknown6.75	6.75	63.0	ng	2611590	1	6.97	828493	20.0
Tridecanoic acid,...	11.87	14.7	ng	648536	4	11.50	885494	20.0
9,12-Octadecadien...	12.57	36.9	ng	1635320	4	11.50	885494	20.0
15-Octadecenoic a...	12.58	50.1	ng	2219870	4	11.50	885494	20.0
Methyl stearate	12.67	6.2	ng	275424	4	11.50	885494	20.0
Behenic alcohol	13.97	4.9	ng	229833	5	14.15	943220	20.0