

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051218\
 Data File : BF105340.D
 Acq On : 12 May 2018 16:29
 Operator : JU/SJ
 Sample : J2859-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-44791RT-RB-47188RT

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:\HPCHEM1\BNA_F\METHODS\8270-BF051018.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	4.998	491	495	503	rBV	146397	184795	5.07%	0.536%
2	5.404	559	564	588	rBV	3068324	3378715	92.78%	9.806%
3	6.422	733	737	756	rBV	2711786	3481491	95.60%	10.104%
4	6.557	756	760	769	rBV	3322936	3377952	92.76%	9.804%
5	6.787	796	799	807	rBV	958190	884725	24.29%	2.568%
6	6.845	807	809	821	rVB	59338	58387	1.60%	0.169%
7	6.945	821	826	842	rBV	2679658	2669616	73.31%	7.748%
8	7.351	890	895	906	rBV	2047870	2210839	60.71%	6.416%
9	8.069	1013	1017	1033	rBV	1426153	1283516	35.24%	3.725%
10	9.145	1195	1200	1210	rBV	3901819	3641764	100.00%	10.569%
11	9.257	1215	1219	1222	rVB2	66767	72167	1.98%	0.209%
12	9.539	1263	1267	1278	rBV	688146	646727	17.76%	1.877%
13	9.751	1297	1303	1307	rBV4	27241	55704	1.53%	0.162%
14	9.822	1311	1315	1319	rBV2	1496727	1337692	36.73%	3.882%
15	10.227	1381	1384	1390	rBV4	49107	81787	2.25%	0.237%
16	10.369	1405	1408	1412	rBV	48512	52157	1.43%	0.151%
17	10.616	1445	1450	1459	rBV	2305799	2541711	69.79%	7.377%
18	11.310	1564	1568	1571	rBV	1420106	1328675	36.48%	3.856%
19	11.333	1571	1572	1578	rVB	220884	154321	4.24%	0.448%
20	11.839	1654	1658	1662	rBV	321535	333694	9.16%	0.968%
21	12.351	1743	1745	1749	rVB3	87464	83309	2.29%	0.242%
22	12.521	1772	1774	1781	rVB	209131	188845	5.19%	0.548%
23	12.621	1788	1791	1794	rBV3	109955	101792	2.80%	0.295%
24	12.751	1810	1813	1816	rBV	133251	98838	2.71%	0.287%
25	12.904	1834	1839	1846	rVB	3019905	3077311	84.50%	8.931%
26	13.086	1867	1870	1874	rVB3	39745	38370	1.05%	0.111%
27	13.827	1992	1996	2001	rVB2	180122	204161	5.61%	0.593%
28	13.992	2018	2024	2027	rBV2	949350	1163402	31.95%	3.376%
29	14.521	2110	2114	2123	rBV3	85560	144686	3.97%	0.420%
30	15.104	2209	2213	2216	rBV	59791	91391	2.51%	0.265%
31	15.198	2226	2229	2238	rVB2	86485	121090	3.33%	0.351%
32	15.404	2261	2264	2269	rBV	33823	50397	1.38%	0.146%
33	15.468	2271	2275	2281	rVB	49490	70069	1.92%	0.203%
34	15.533	2281	2286	2292	rBV	771629	1029380	28.27%	2.988%

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Instrument :
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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.009	2363	2367	2372	rBV	75212	113849	3.13%	0.330%
36	17.556	2625	2630	2639	rVB	48257	102800	2.82%	0.298%

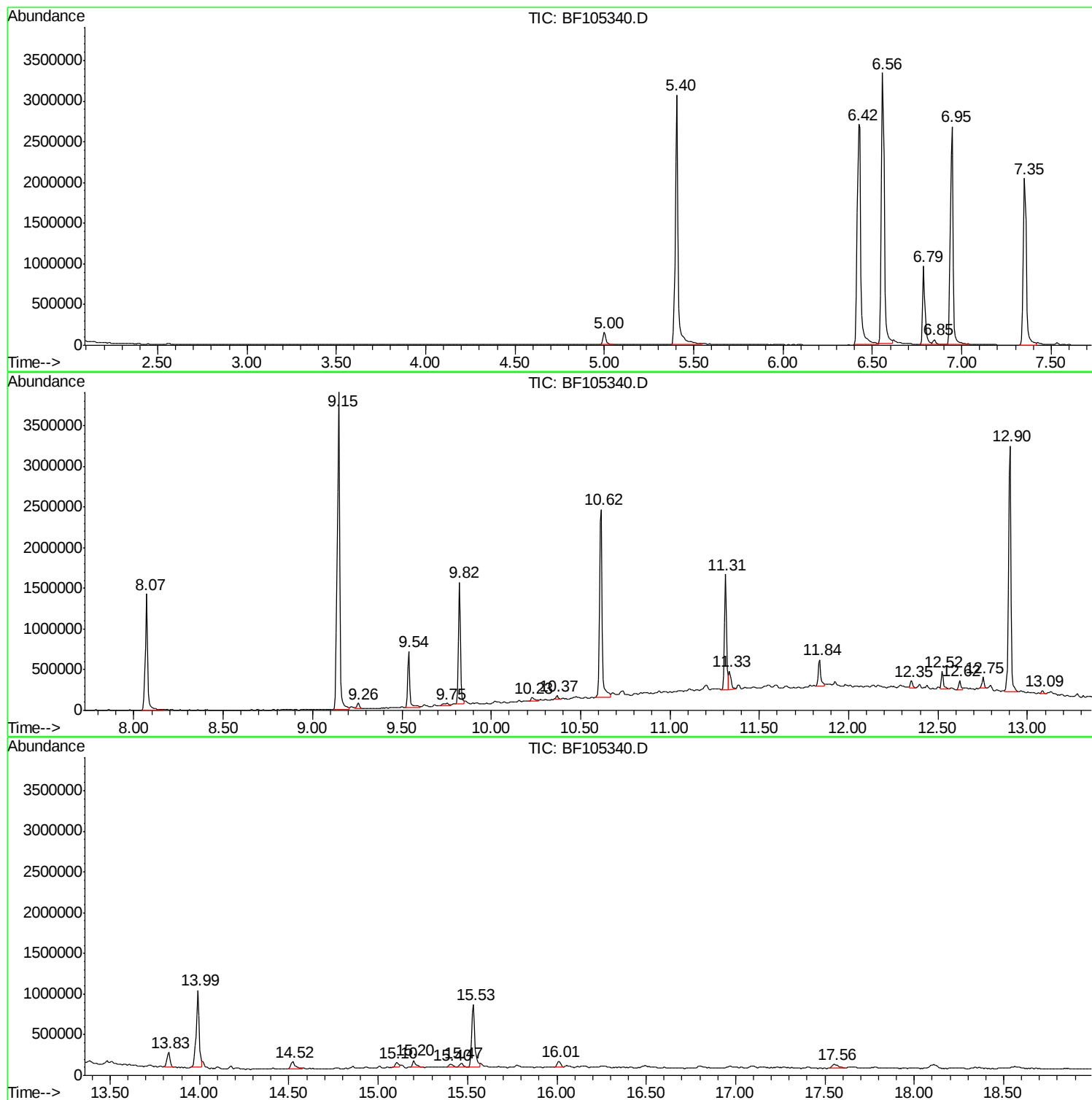
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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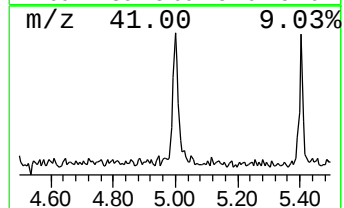
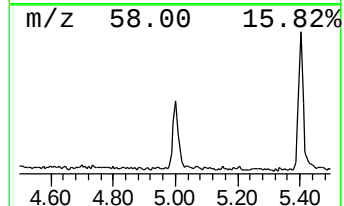
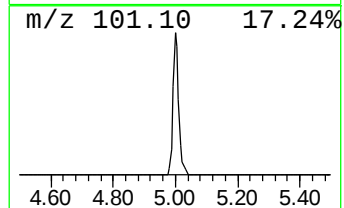
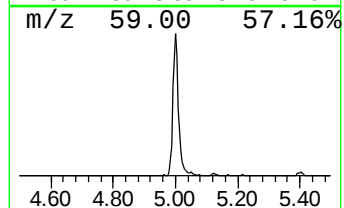
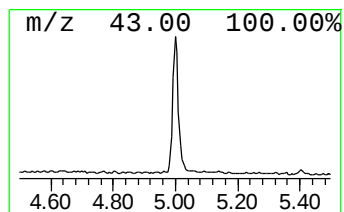
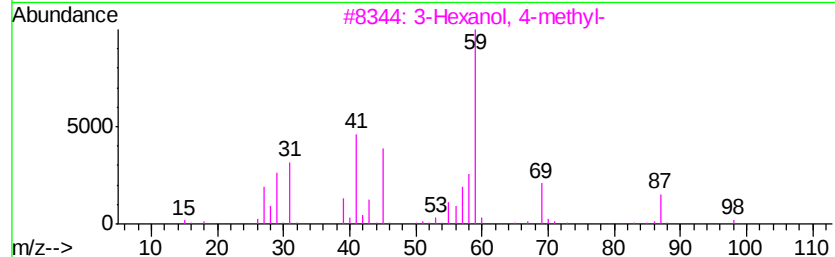
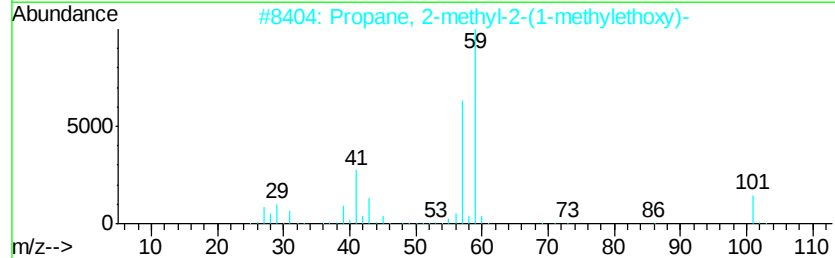
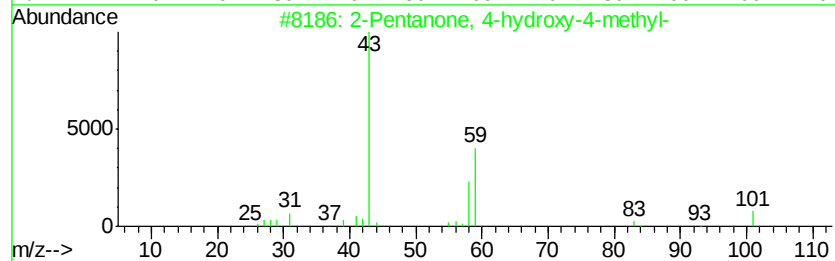
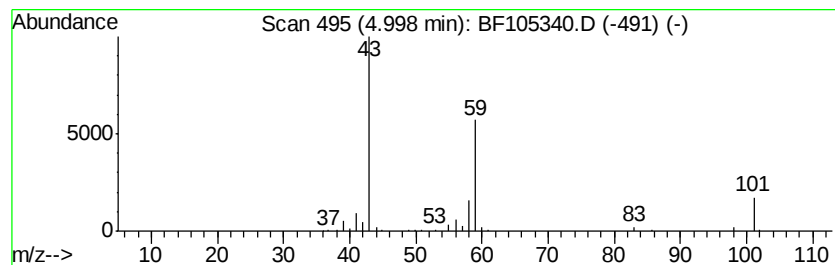
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.18 ng	184795	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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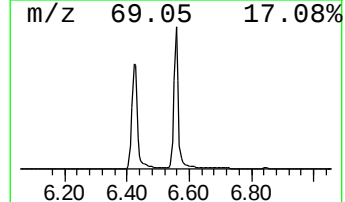
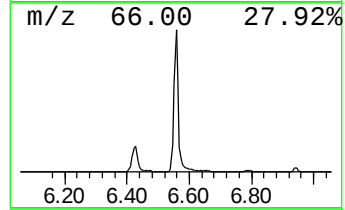
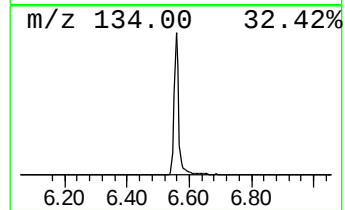
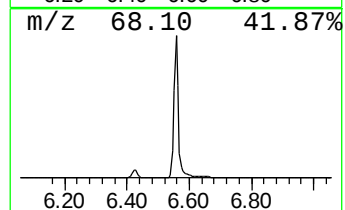
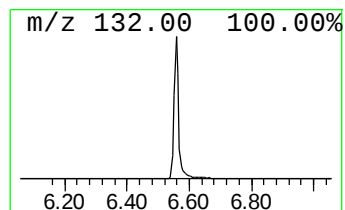
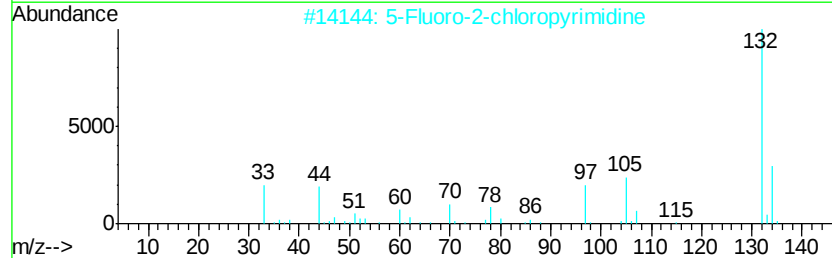
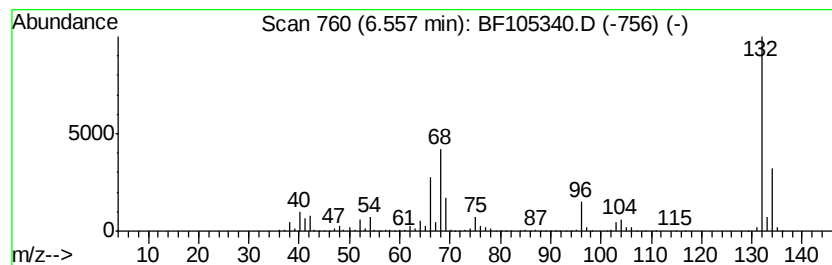
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	76.36 ng	3377950	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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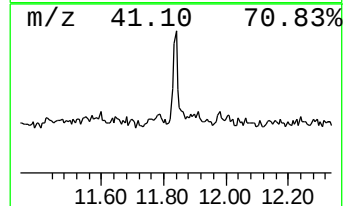
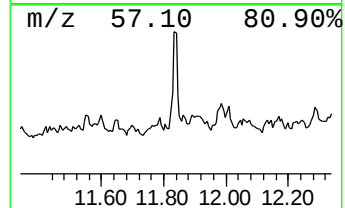
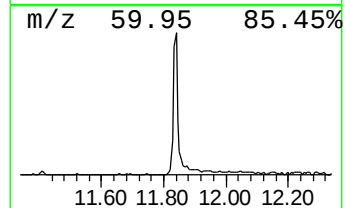
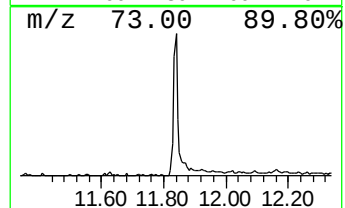
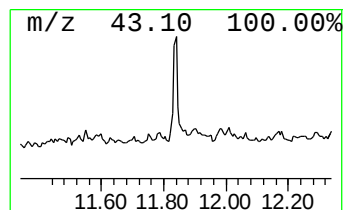
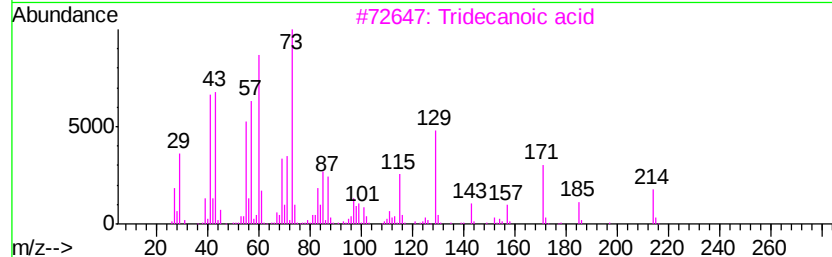
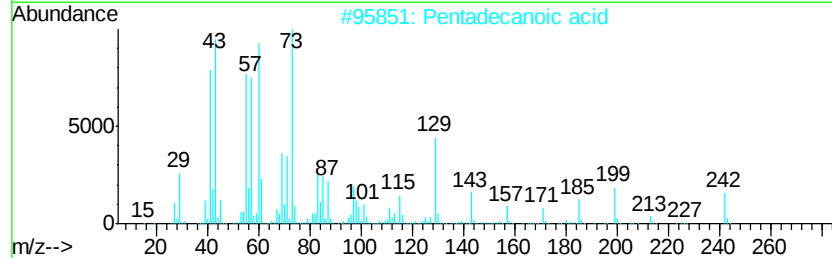
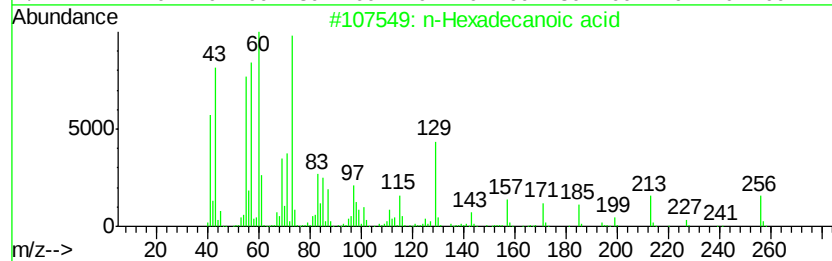
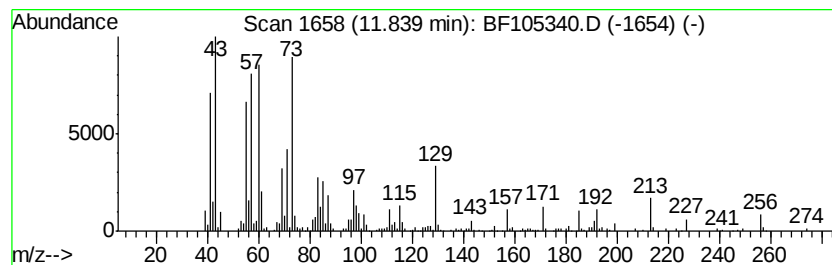
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	5.02 ng	333694	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Isopropyl palmitate	298	C19H38O2	000142-91-6	72
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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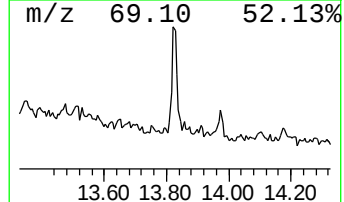
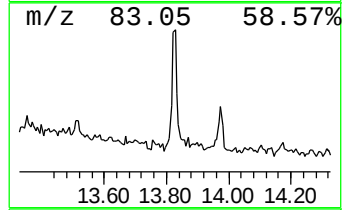
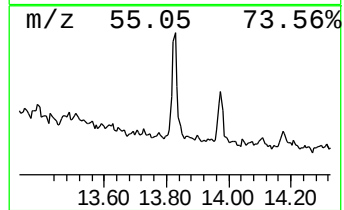
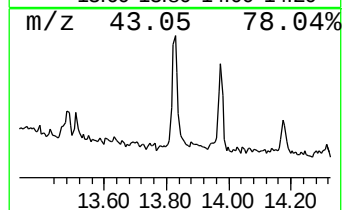
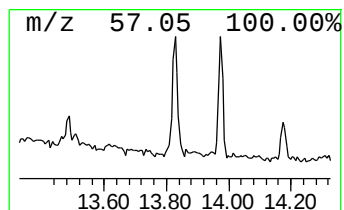
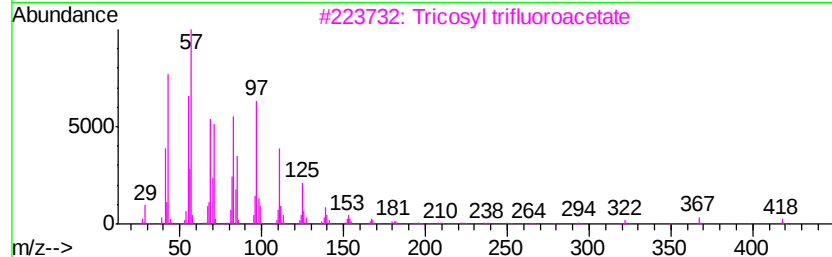
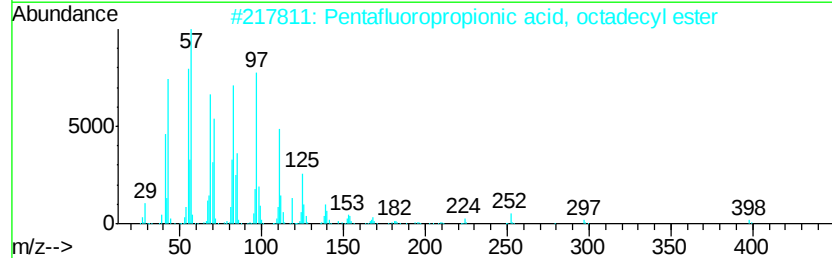
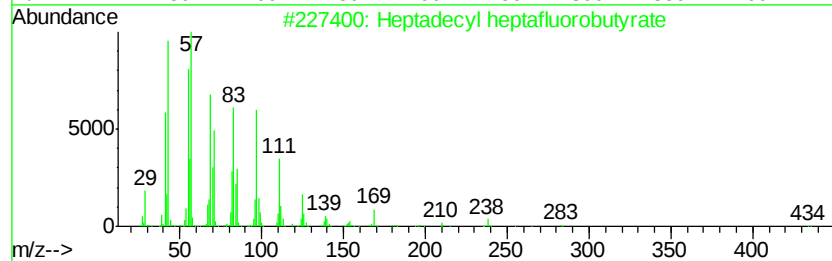
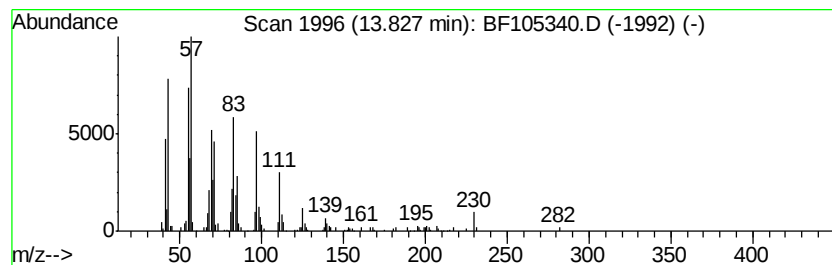
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.51 ng	204161	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



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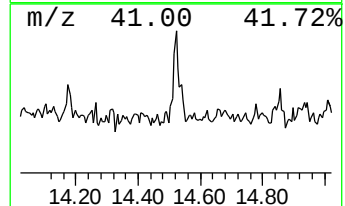
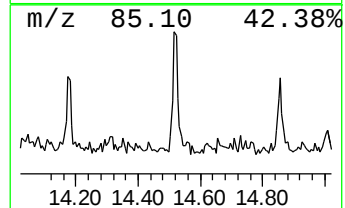
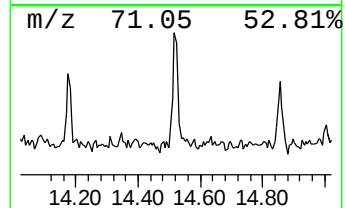
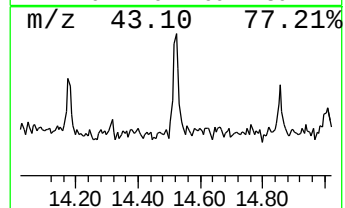
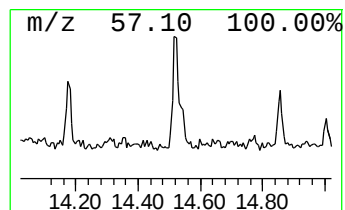
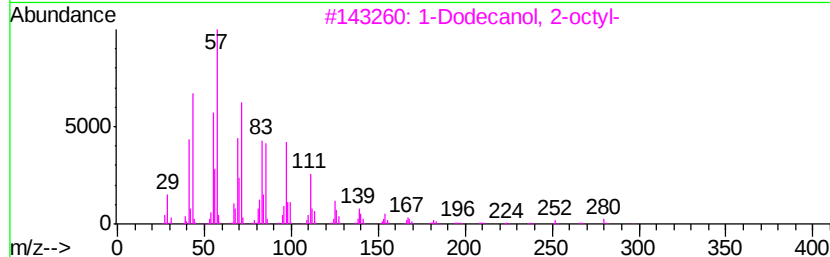
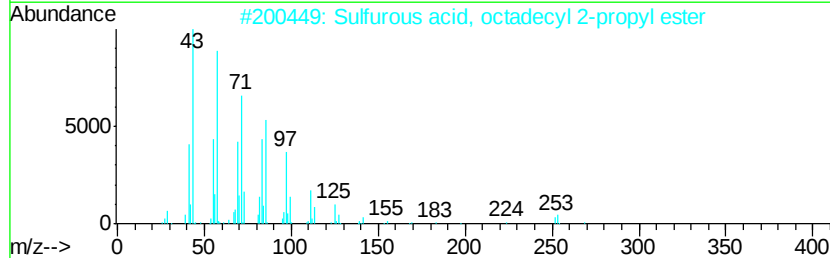
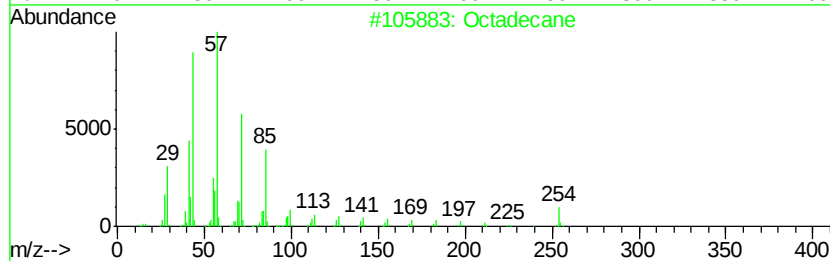
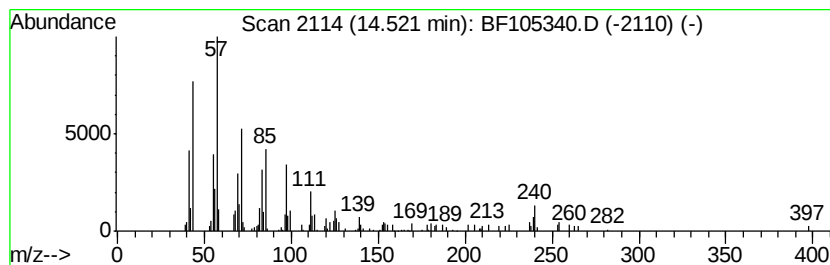
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.49 ng	144686	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	83
2	Sulfurous acid, octadecyl 2-prop...		376	C21H44O3S	1000309-12-7	81
3	1-Dodecanol, 2-octyl-		298	C20H42O	005333-42-6	76
4	Hexatriacontyl pentafluoropropio...		669	C39H73F5O2	1000351-89-0	68
5	Dotriacontyl heptafluorobutyrate		662	C36H65F7O2	1000351-84-2	64



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Misc :
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ClientSampleID :
RB-44791RT-RB-47188RT

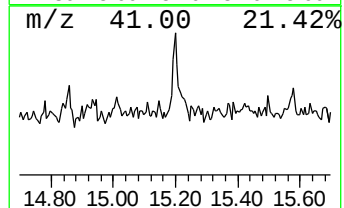
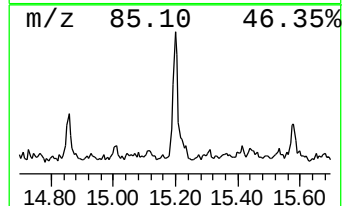
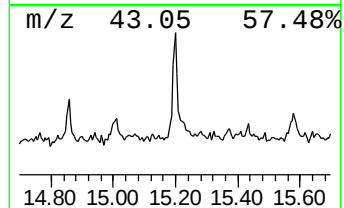
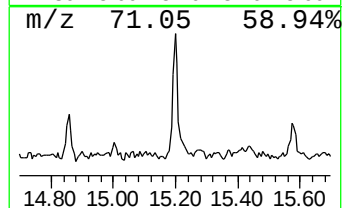
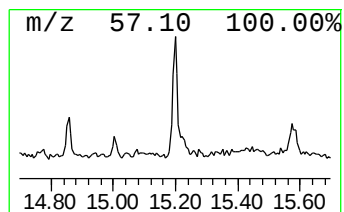
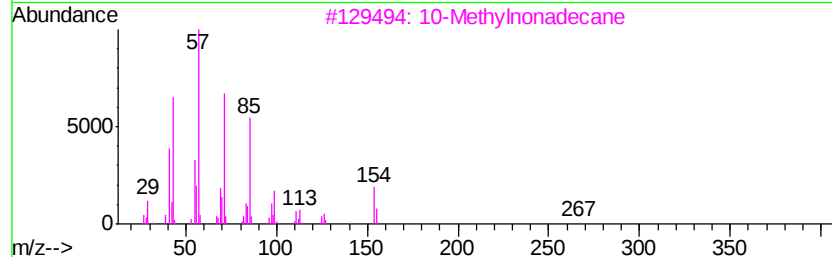
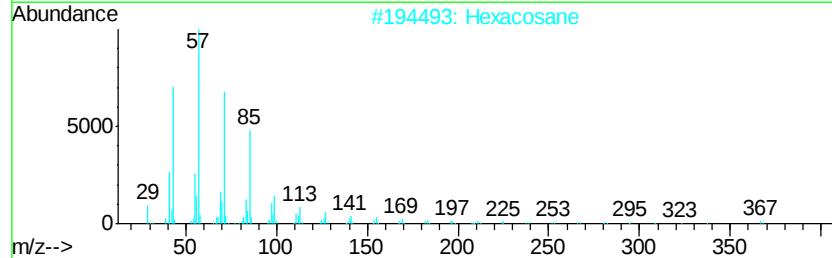
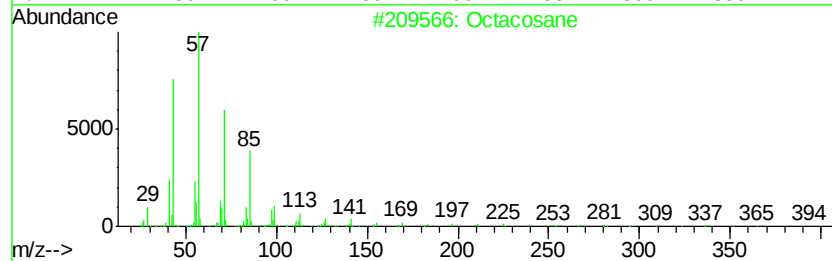
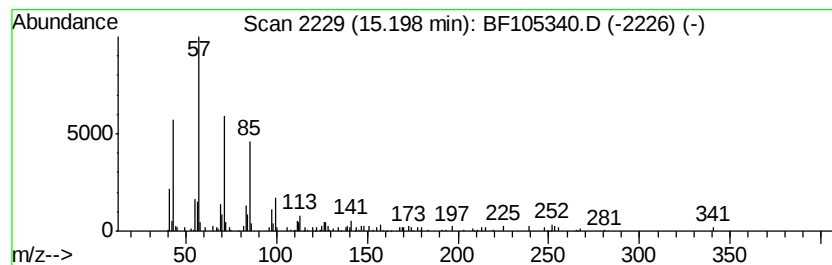
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	2.35 ng	121090	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		10-Methylnonadecane	282	C20H42	056862-62-5	80
4		Eicosane	282	C20H42	000112-95-8	80
5		Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051218\
Data File : BF105340.D
Acq On : 12 May 2018 16:29
Operator : JU/SJ
Sample : J2859-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44791RT-RB-47188RT

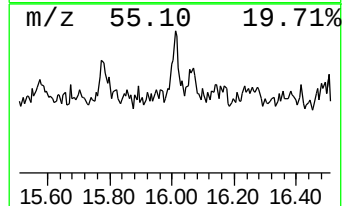
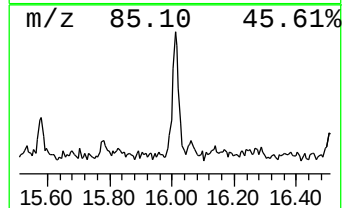
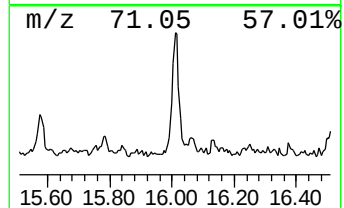
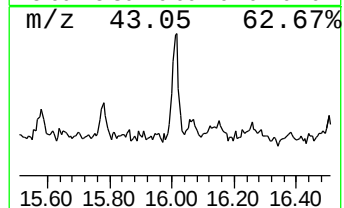
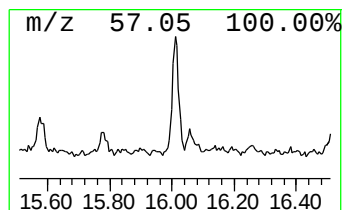
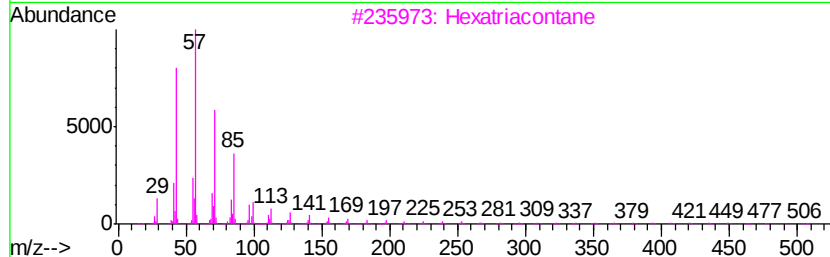
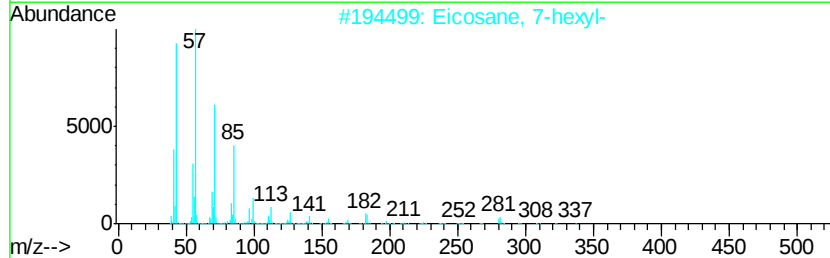
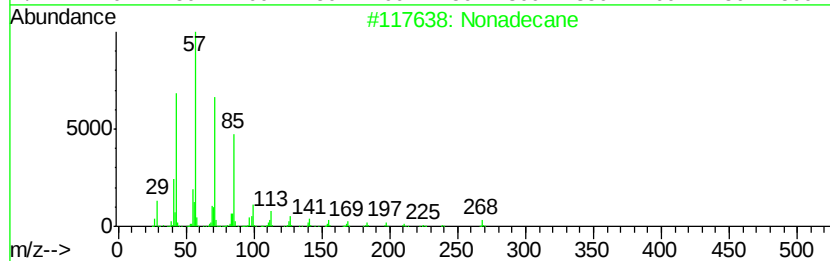
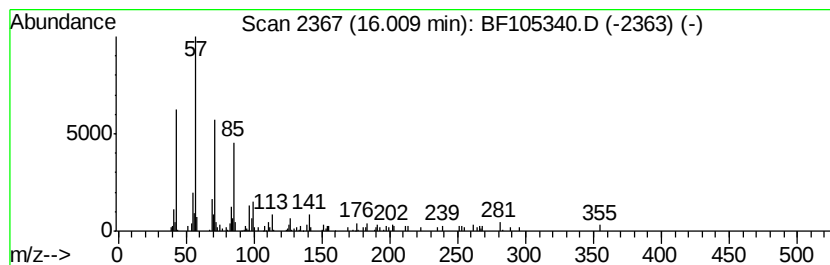
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	2.21 ng	113849	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	94
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
3		Hexatriacontane	507	C36H74	000630-06-8	83
4		Heptacosane	380	C27H56	000593-49-7	83
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051218\
Data File : BF105340.D
Acq On : 12 May 2018 16:29
Operator : JU/SJ
Sample : J2859-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-44791RT-RB-47188RT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051018.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...	5.00	4.2	ng	184795	1	6.79	884725	20.0
unknown6.56	6.56	76.4	ng	3377950	1	6.79	884725	20.0
n-Hexadecanoic acid	11.84	5.0	ng	333694	4	11.31	1328680	20.0
Heptadecyl heptaf...	13.83	3.5	ng	204161	5	13.99	1163400	20.0
Octadecane	14.52	2.5	ng	144686	5	13.99	1163400	20.0
Octacosane	15.20	2.4	ng	121090	6	15.53	1029380	20.0
Nonadecane	16.01	2.2	ng	113849	6	15.53	1029380	20.0