

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110917\
 Data File : BF100335.D
 Acq On : 9 Nov 2017 12:08
 Operator : SJ/JU
 Sample : I6354-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-S001-0001-02

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-BF110817.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	5.134	513	518	527	rBV	642157	798921	20.54%	2.266%
2	5.522	578	584	587	rBV	3708847	3771403	96.97%	10.697%
3	6.522	748	754	758	rBV	3292577	3822510	98.28%	10.842%
4	6.669	774	779	783	rBV	3696909	3801448	97.74%	10.782%
5	6.898	815	818	822	rBV	1200024	1086558	27.94%	3.082%
6	7.057	841	845	849	rBV	3279142	2982758	76.69%	8.460%
7	7.463	906	914	917	rBV	2528477	2430685	62.50%	6.894%
8	8.180	1032	1036	1040	rBV	1630031	1357437	34.90%	3.850%
9	8.733	1126	1130	1133	rVB	166692	126958	3.26%	0.360%
10	9.257	1214	1219	1222	rBV	4193791	3889335	100.00%	11.031%
11	9.521	1261	1264	1267	rBV	124630	96650	2.49%	0.274%
12	9.645	1282	1285	1288	rVB	132093	95450	2.45%	0.271%
13	9.939	1330	1335	1338	rBV	1382382	1293051	33.25%	3.668%
14	10.645	1452	1455	1460	rBV	402145	345774	8.89%	0.981%
15	10.721	1464	1468	1472	rBV	1987813	1859795	47.82%	5.275%
16	11.280	1560	1563	1565	rBV	53000	41006	1.05%	0.116%
17	11.421	1583	1587	1590	rBV	1317689	1086961	27.95%	3.083%
18	11.939	1672	1675	1680	rBV	506396	495744	12.75%	1.406%
19	12.115	1702	1705	1710	rVB	43862	41439	1.07%	0.118%
20	12.633	1790	1793	1794	rBV	64872	64860	1.67%	0.184%
21	12.727	1806	1809	1820	rBV	498325	502975	12.93%	1.427%
22	12.898	1836	1838	1841	rVB	48503	42684	1.10%	0.121%
23	13.010	1852	1857	1860	rBV	3004610	2729233	70.17%	7.741%
24	13.892	2004	2007	2014	rBV	241185	291621	7.50%	0.827%
25	14.039	2029	2032	2033	rBV	106432	100182	2.58%	0.284%
26	14.062	2033	2036	2039	rVB	1210232	1063671	27.35%	3.017%
27	14.821	2162	2165	2169	rBV2	197552	238812	6.14%	0.677%
28	15.545	2284	2288	2292	rBV	669396	798986	20.54%	2.266%

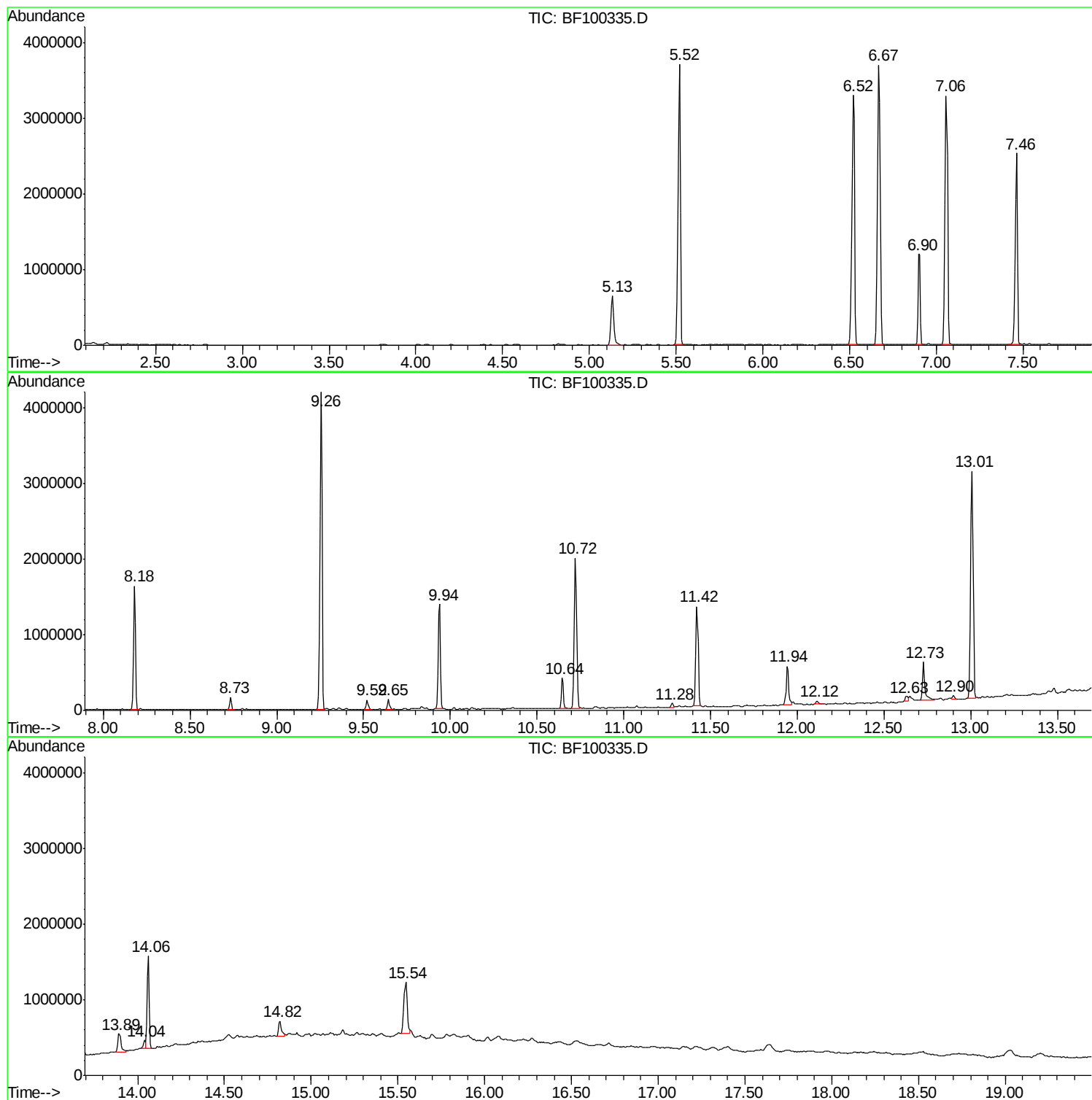
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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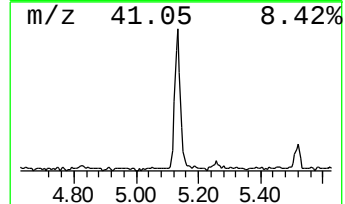
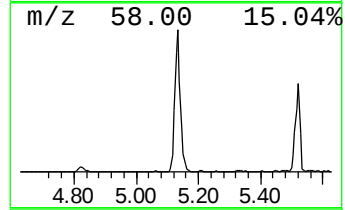
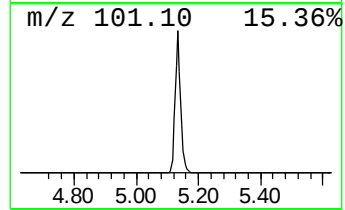
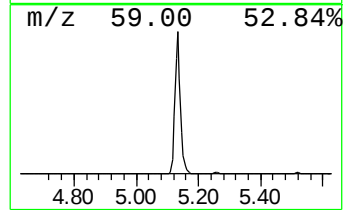
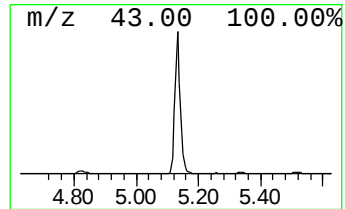
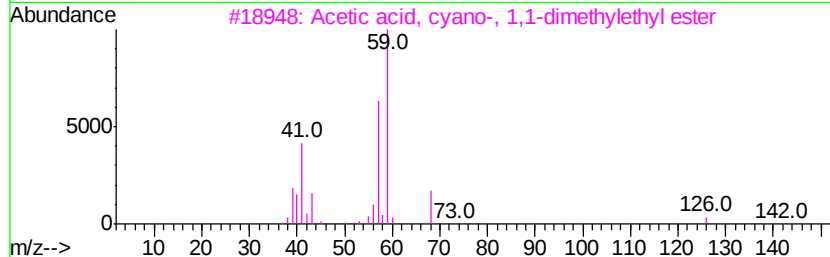
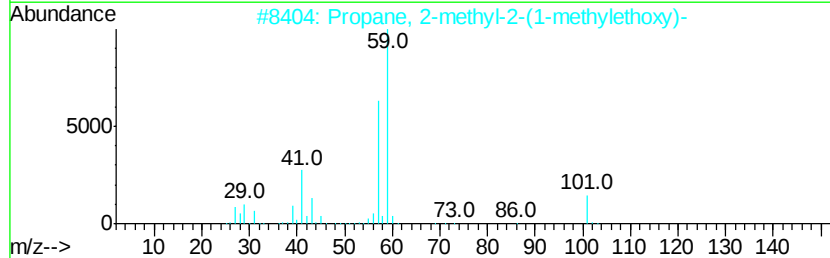
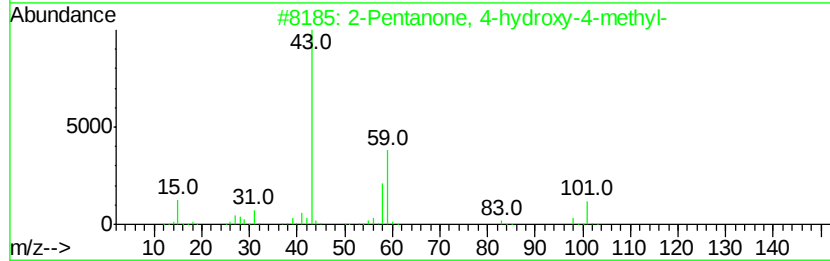
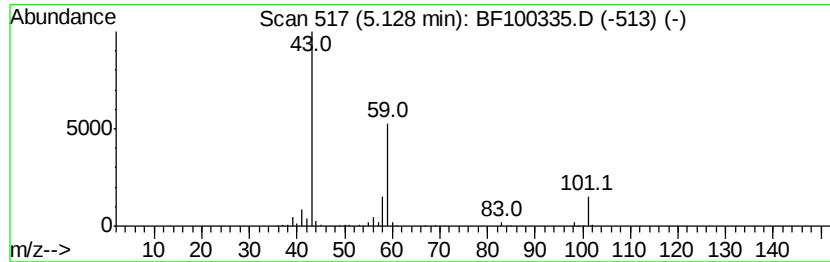
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	14.71 ng	798921	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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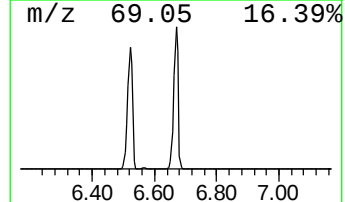
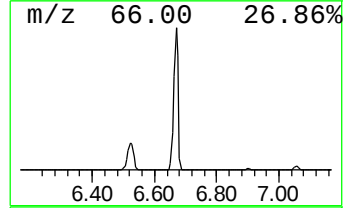
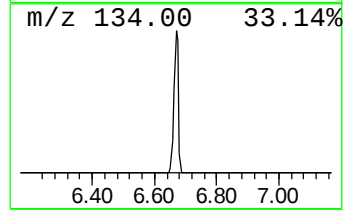
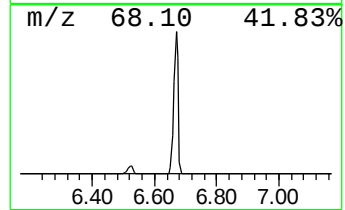
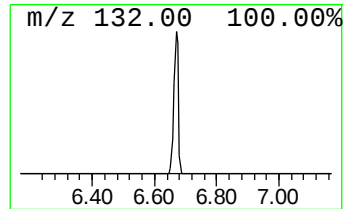
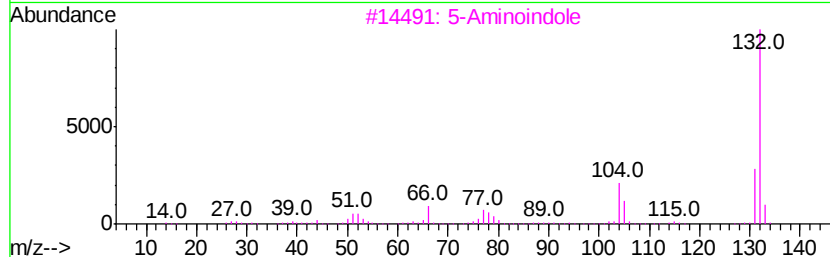
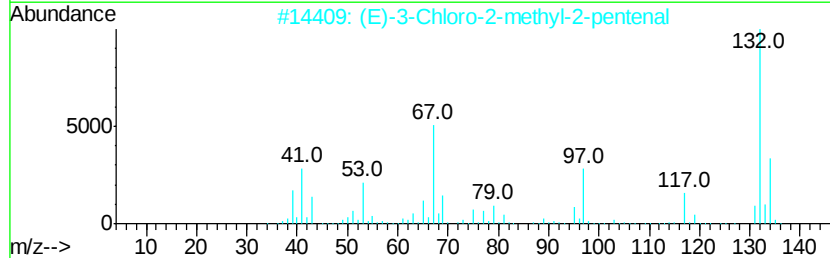
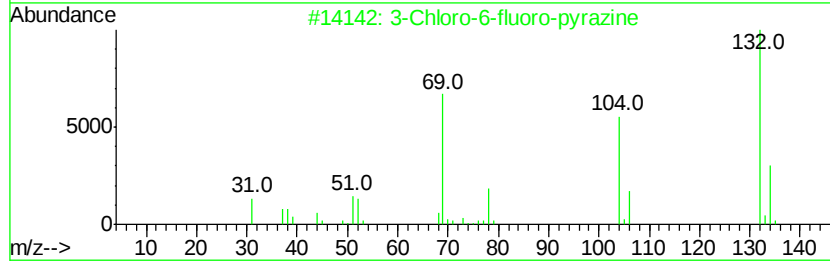
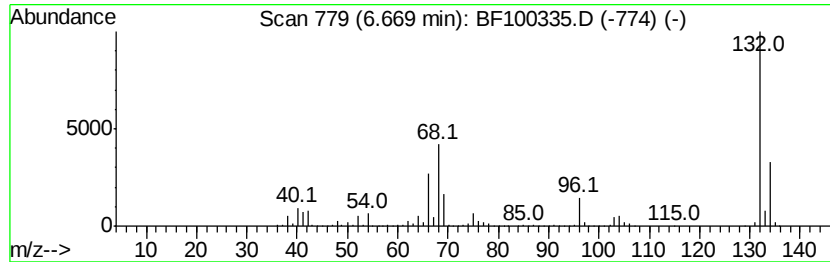
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	69.97 ng	3801450	1,4-Dichlorobenzene-d4	6.90

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-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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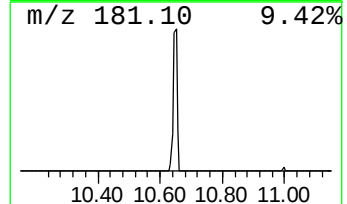
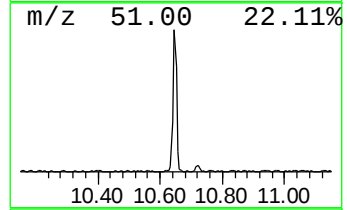
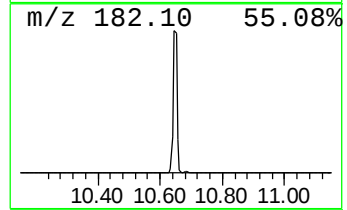
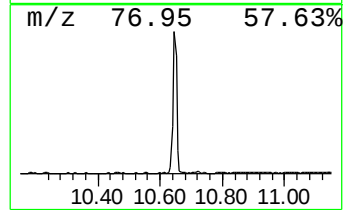
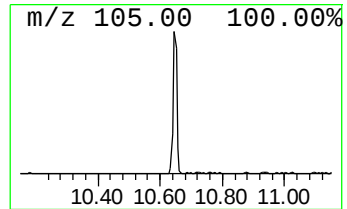
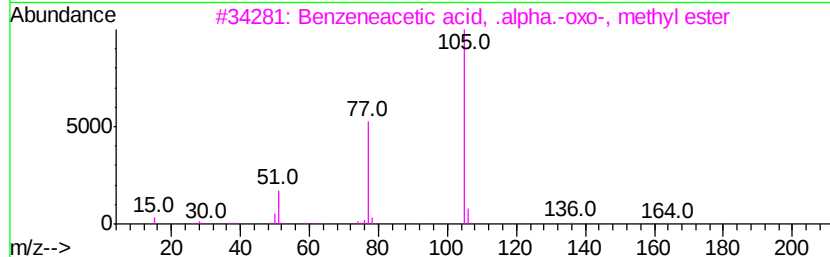
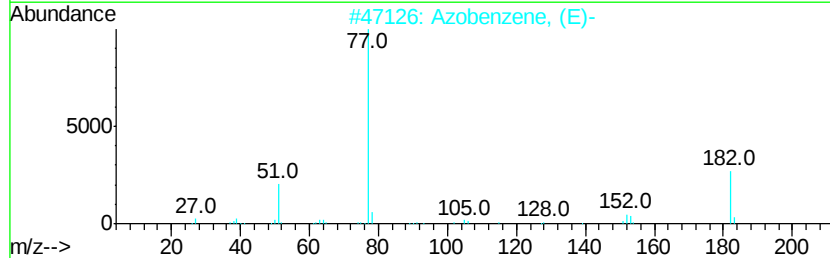
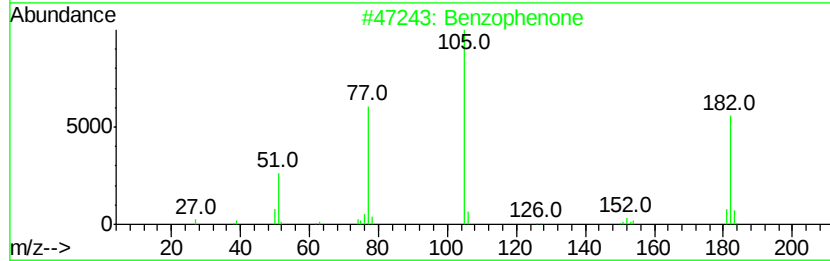
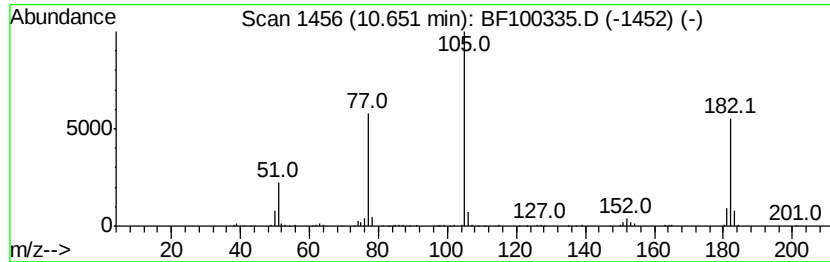
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Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	5.35 ng	345774	Acenaphthene-d10	9.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Azobenzene, (E)-	182 C12H10N2	017082-12-1 50
3		Benzeneacetic acid, .alpha.-oxo-...	164 C9H8O3	015206-55-0 49
4		1,2-Propanedione, 1-phenyl-	148 C9H8O2	000579-07-7 47
5		Benzenepropanenitrile, .beta.-oxo-	145 C9H7NO	000614-16-4 47



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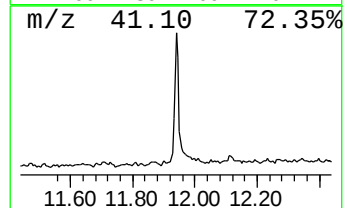
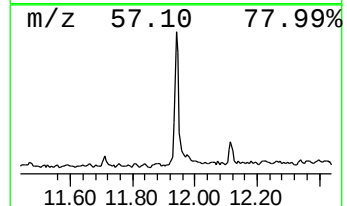
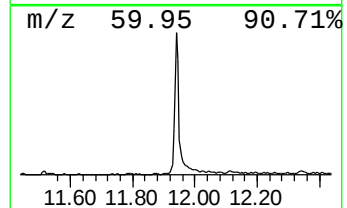
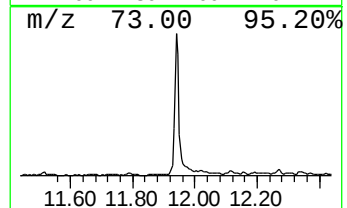
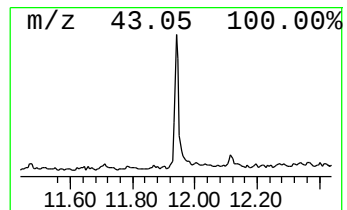
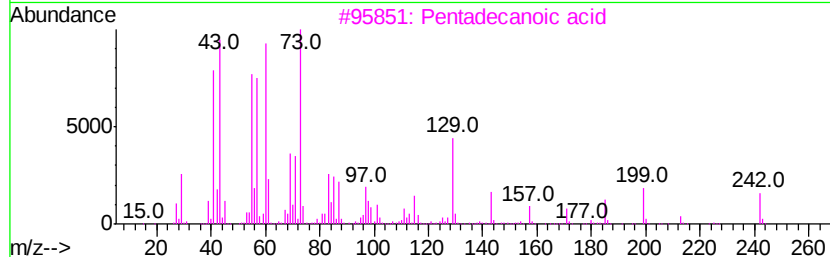
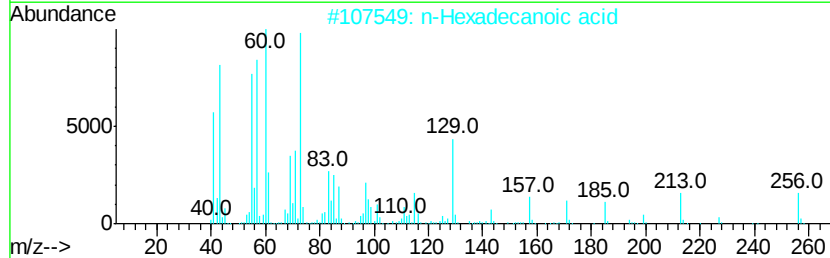
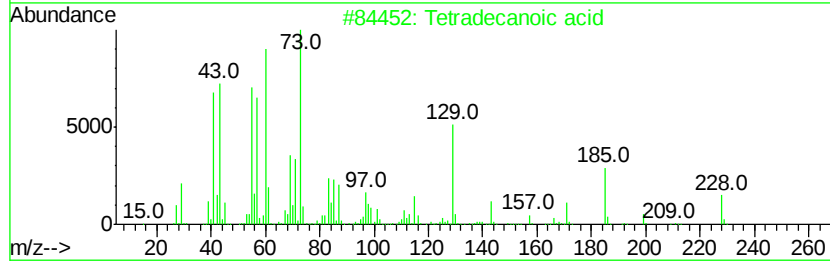
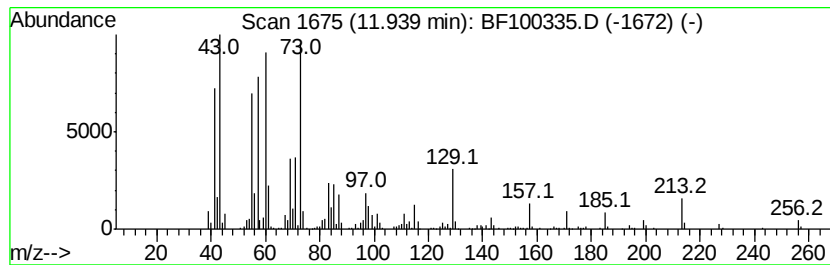
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	9.12 ng	495744	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	74



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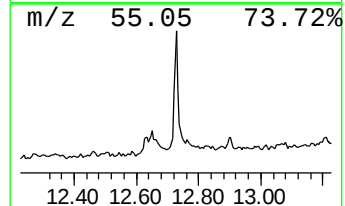
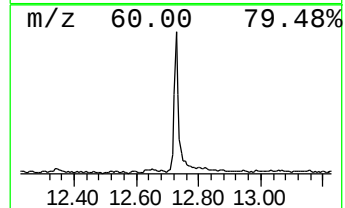
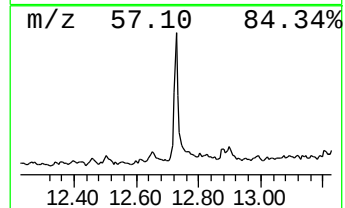
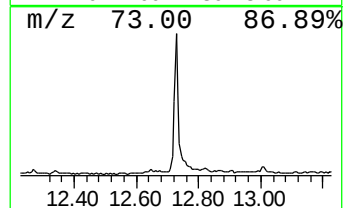
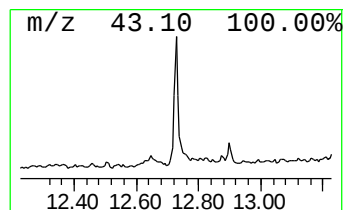
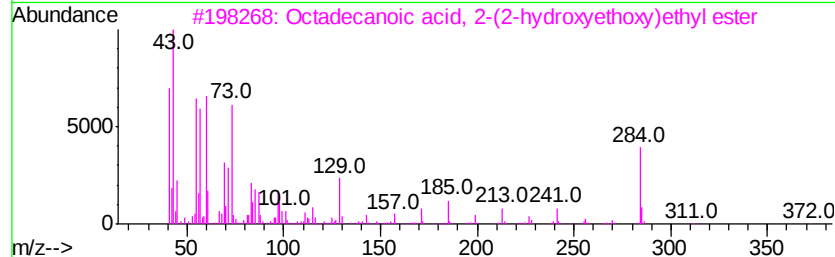
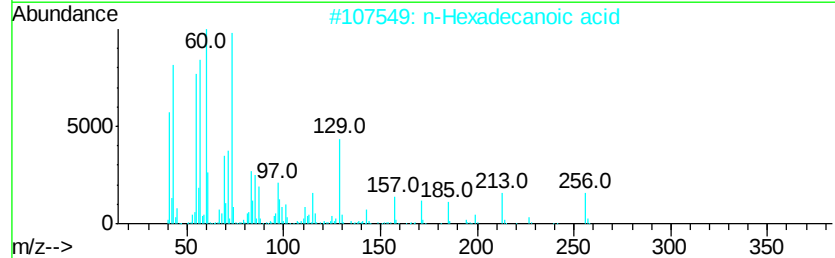
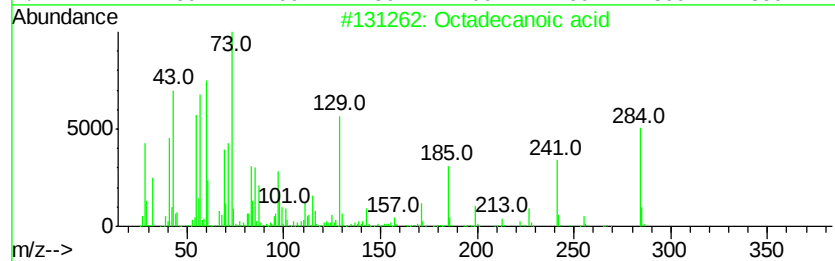
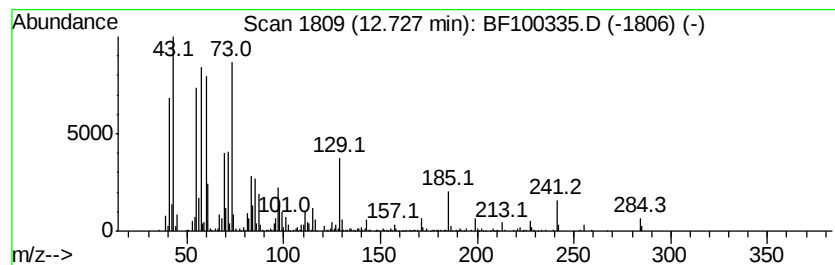
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	9.25 ng	502975	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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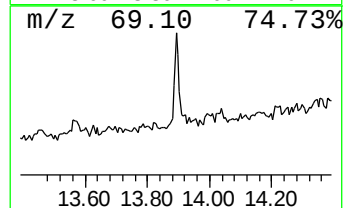
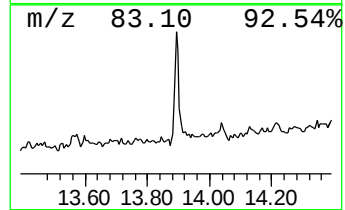
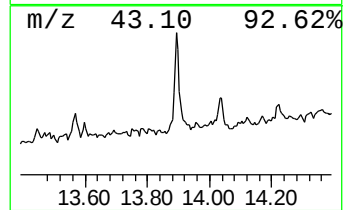
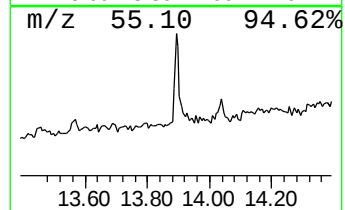
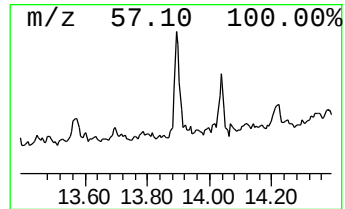
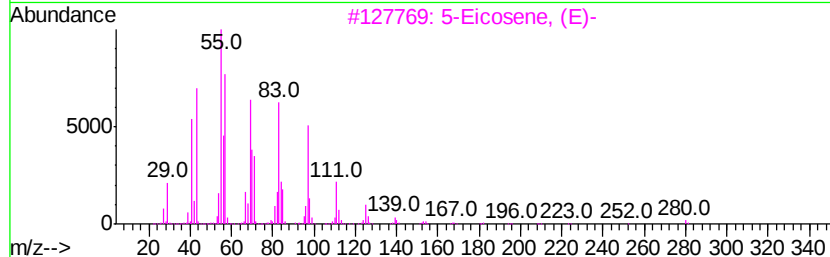
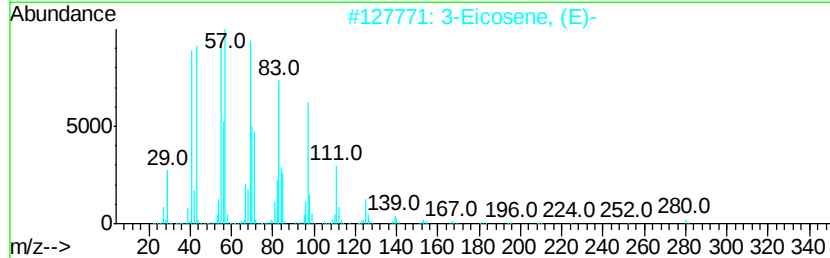
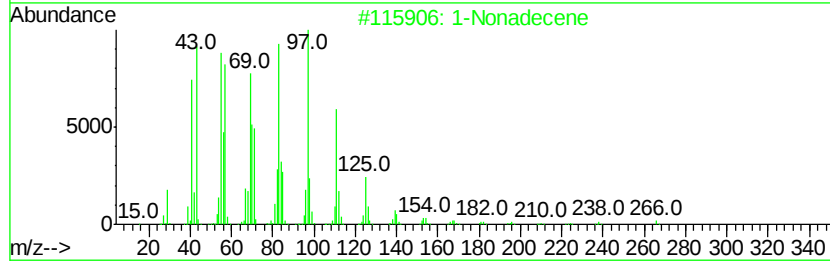
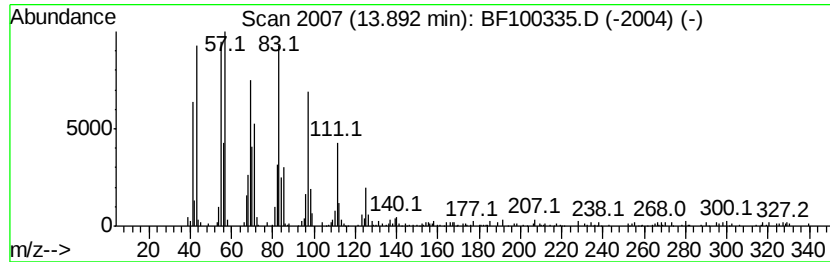
Instrument :
BNA_F
ClientSampleId :
P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	5.48 ng	291621	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene		266 C19H38	018435-45-5 98
2	3-Eicosene, (E)-		280 C20H40	074685-33-9 98
3	5-Eicosene, (E)-		280 C20H40	074685-30-6 95
4	1-Heneicosanol		312 C21H44O	015594-90-8 94
5	9-Eicosene, (E)-		280 C20H40	074685-29-3 93



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100335.D
Acq On : 9 Nov 2017 12:08
Operator : SJ/JU
Sample : I6354-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

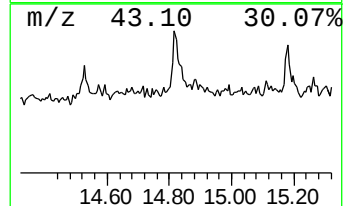
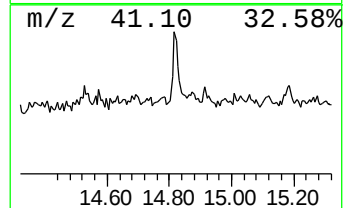
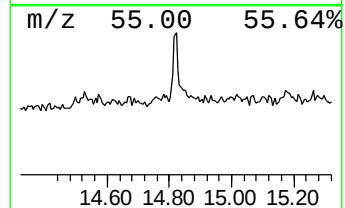
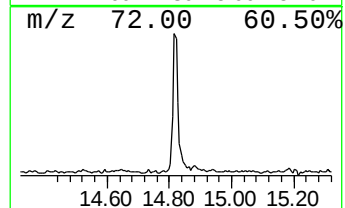
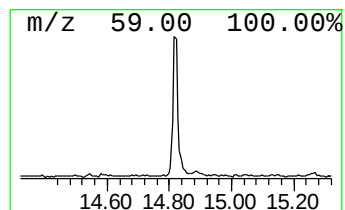
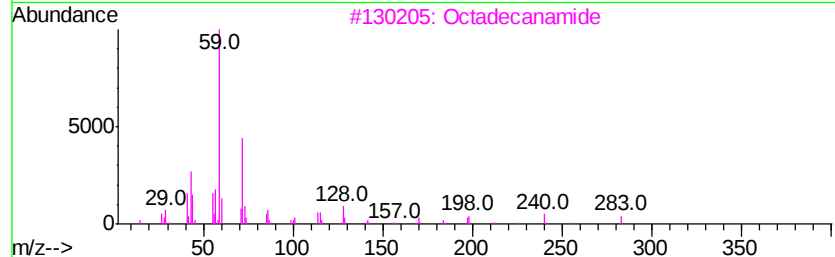
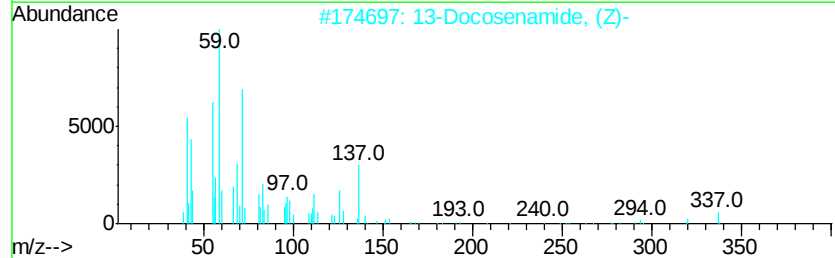
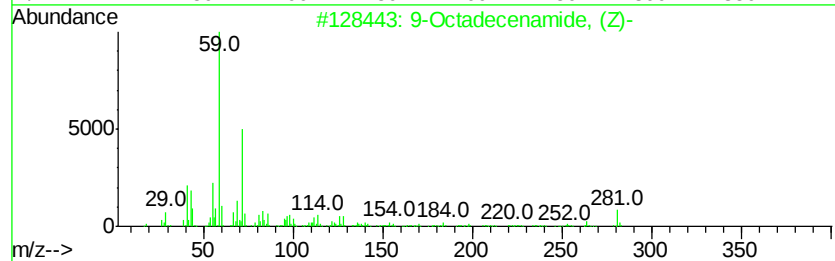
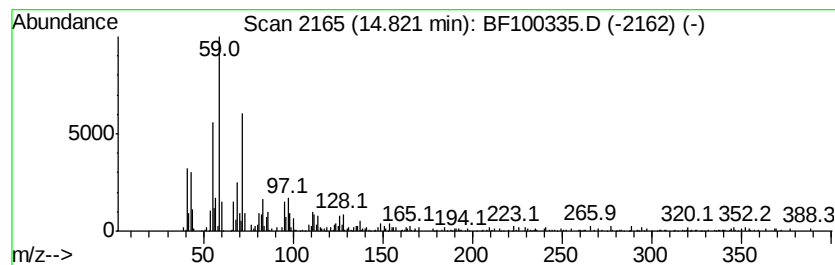
Instrument :
BNA_F
ClientSampleId :
P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	5.98 ng	238812	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0 83
2		13-Docosenamide, (Z)-	337 C22H43NO	000112-84-5 81
3		Octadecanamide	283 C18H37NO	000124-26-5 59
4		Hexadecanamide	255 C16H33NO	000629-54-9 53
5		d-Glucosamine	179 C6H13NO5	000090-77-7 53



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110917\
Data File : BF100335.D
Acq On : 9 Nov 2017 12:08
Operator : SJ/JU
Sample : I6354-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.13	14.7	ng	798921	1	6.90	1086560	20.0
unknown6.67	6.67	70.0	ng	3801450	1	6.90	1086560	20.0
Benzophenone	10.65	5.3	ng	345774	3	9.94	1293050	20.0
Tetradecanoic acid	11.94	9.1	ng	495744	4	11.42	1086960	20.0
Octadecanoic acid	12.73	9.3	ng	502975	4	11.42	1086960	20.0
1-Nonadecene	13.89	5.5	ng	291621	5	14.06	1063670	20.0
9-Octadecenamide, ...	14.82	6.0	ng	238812	6	15.54	798986	20.0