

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052417\
 Data File : BF095387.D
 Acq On : 24 May 2017 14:10
 Operator : SJ/MA
 Sample : I3290-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3-TP-4

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-BF050217.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	5.125	538	542	552	rBV	59132	135823	5.84%	0.772%
2	5.719	640	643	688	rBV	641133	1741373	74.87%	9.892%
3	7.295	907	911	928	rBV	688095	1618144	69.58%	9.192%
4	7.419	928	932	951	rVB	1153759	2064522	88.77%	11.728%
5	7.754	985	989	1002	rBV	364864	463704	19.94%	2.634%
6	7.983	1024	1028	1044	rBV	1079489	1451567	62.41%	8.246%
7	8.654	1138	1142	1160	rBV	456205	956659	41.13%	5.435%
8	9.777	1329	1333	1354	rBV	324942	682434	29.34%	3.877%
9	11.542	1628	1633	1653	rBV	1419272	2325739	100.00%	13.212%
10	12.248	1749	1753	1771	rBV	163382	295590	12.71%	1.679%
11	12.607	1809	1814	1837	rBV2	493077	825194	35.48%	4.688%
12	13.436	1951	1955	1960	rVB	27338	30498	1.31%	0.173%
13	13.901	2030	2034	2047	rBV	584562	1069165	45.97%	6.074%
14	14.206	2082	2086	2092	rBV	23361	33119	1.42%	0.188%
15	14.942	2205	2211	2216	rBV3	15497	23759	1.02%	0.135%
16	15.012	2219	2223	2236	rBV	321675	581654	25.01%	3.304%
17	15.671	2330	2335	2340	rBV	29441	39378	1.69%	0.224%
18	15.971	2381	2386	2394	rBV3	49526	91004	3.91%	0.517%
19	17.324	2611	2616	2628	rBV	1413902	1823785	78.42%	10.361%
20	18.571	2824	2828	2832	rBV4	29437	54815	2.36%	0.311%
21	18.689	2844	2848	2859	rBV	268704	534614	22.99%	3.037%
22	19.541	2989	2993	2995	rBV5	20758	31115	1.34%	0.177%
23	19.688	3014	3018	3027	rVB	174236	277982	11.95%	1.579%
24	20.036	3075	3077	3079	rBV2	22192	24996	1.07%	0.142%
25	20.365	3129	3133	3138	rBV	202992	313768	13.49%	1.782%
26	20.806	3204	3208	3210	rBV3	28137	43527	1.87%	0.247%
27	23.823	3717	3721	3728	rVB9	28744	69249	2.98%	0.393%

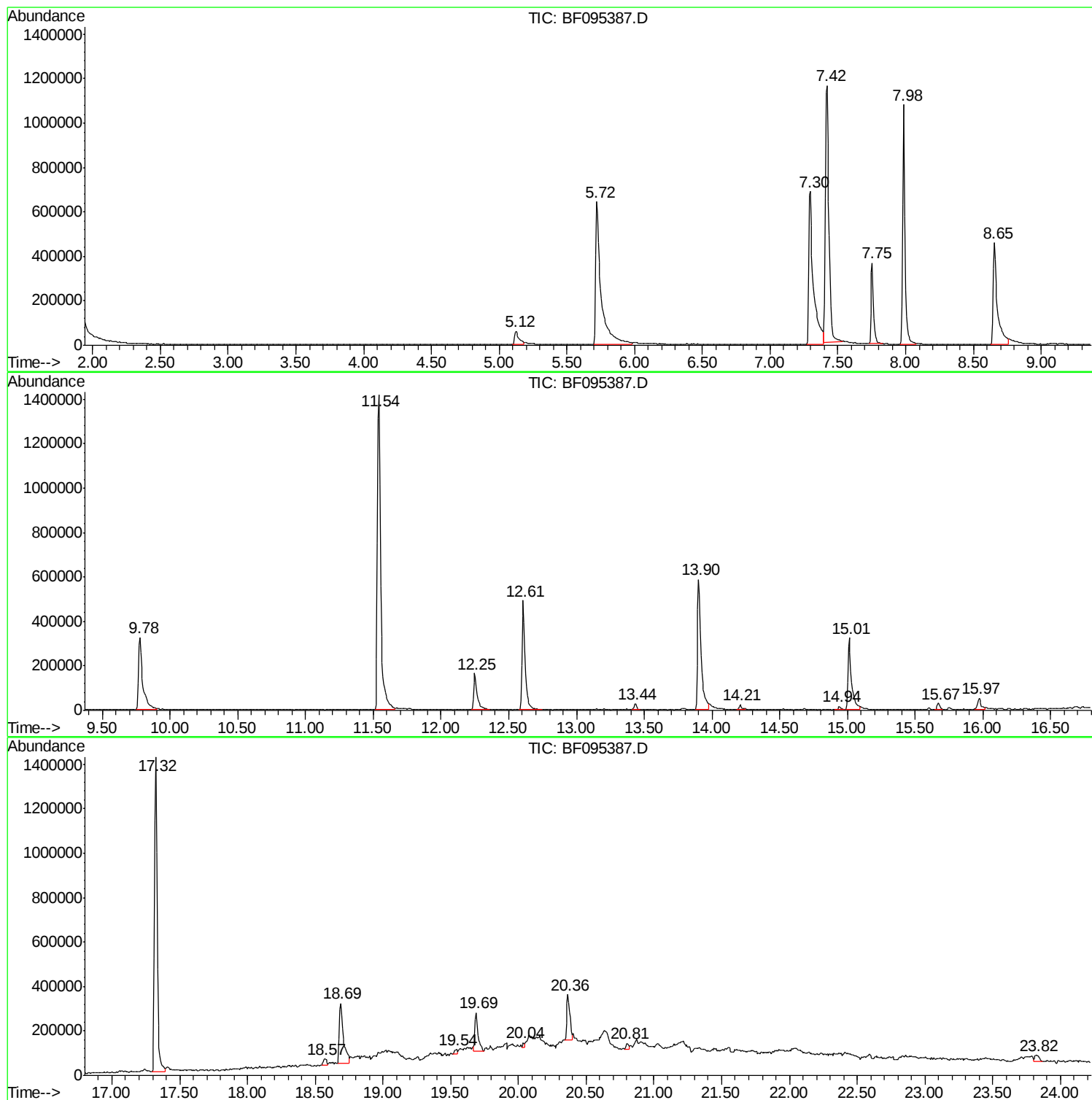
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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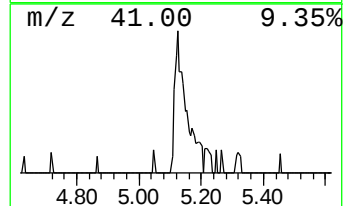
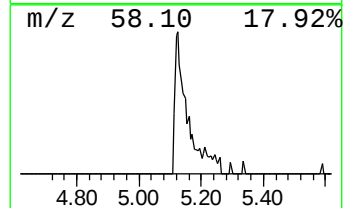
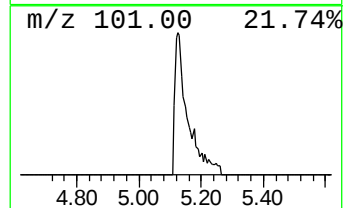
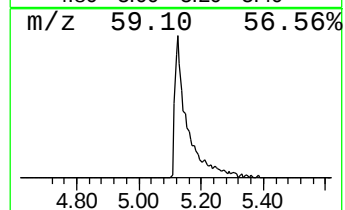
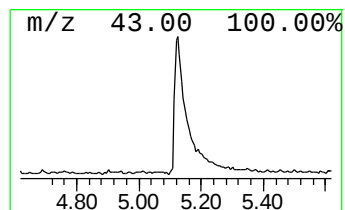
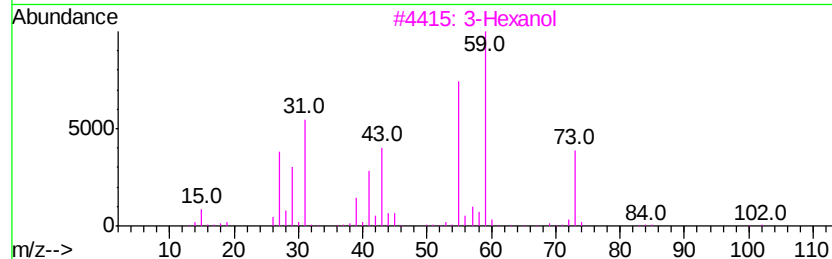
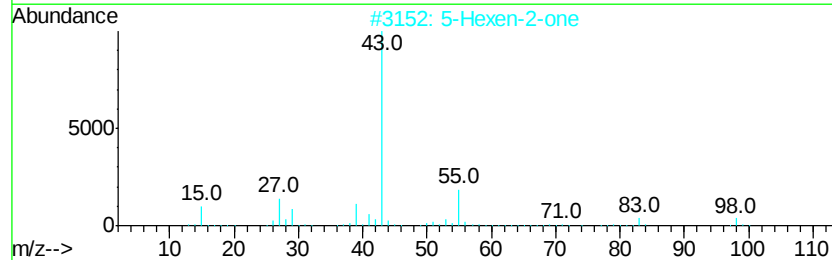
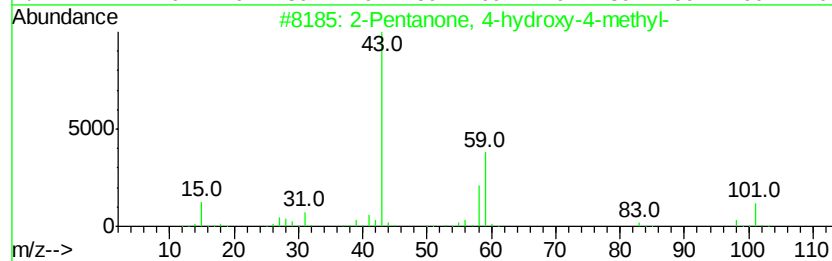
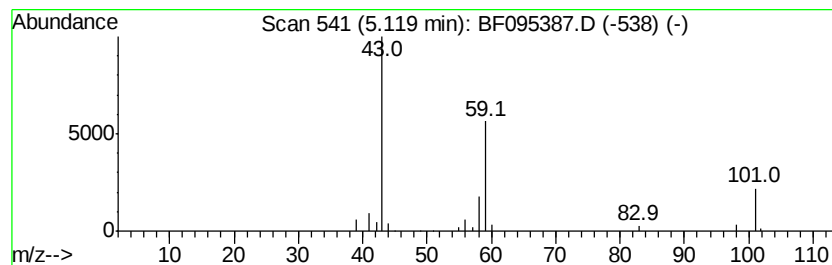
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	5.86 ng	135823	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	50
2	5-Hexen-2-one	98	C6H10O		000109-49-9	9
3	3-Hexanol	102	C6H14O		000623-37-0	9
4	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3		1000306-64-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O		000625-23-0	9



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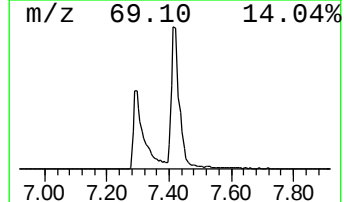
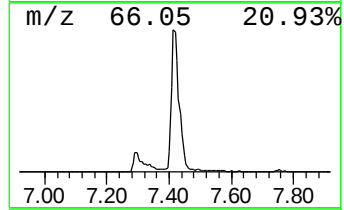
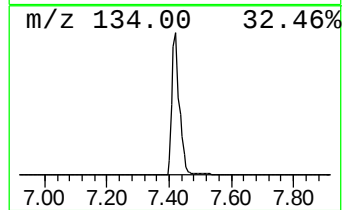
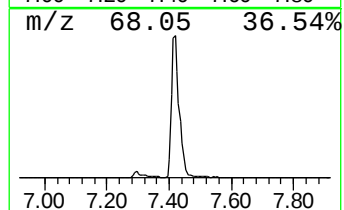
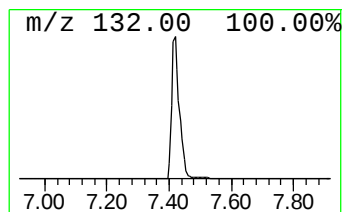
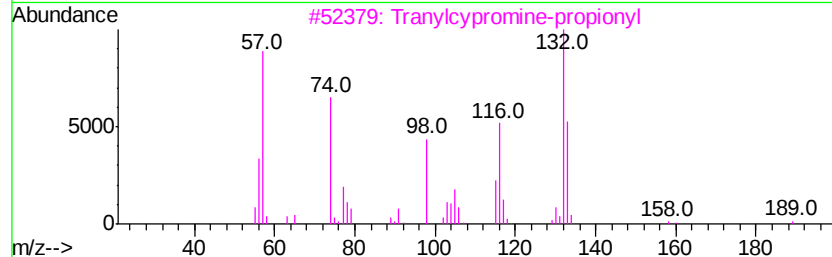
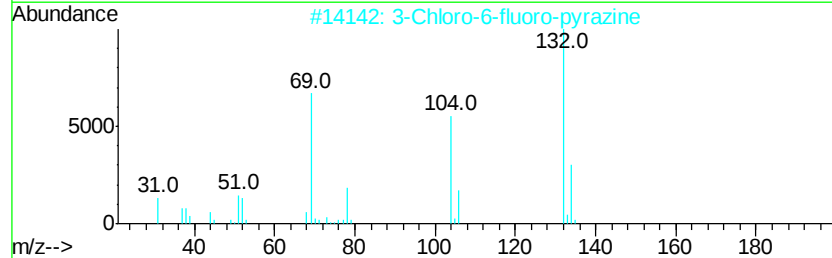
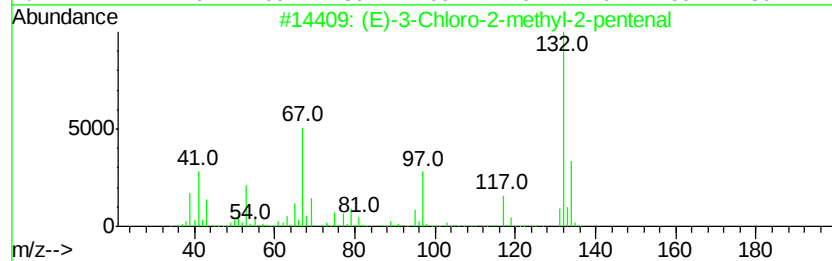
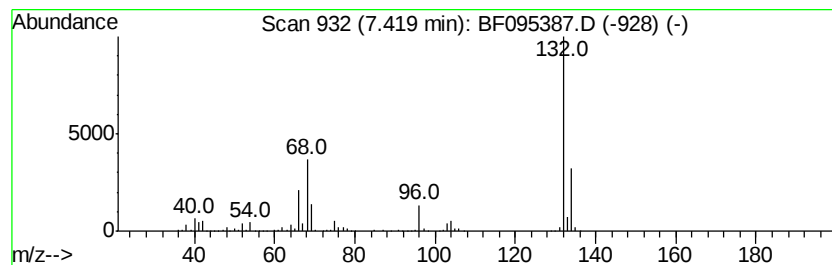
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	89.04 ng	2064520	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25	
3	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12	
4	5-Aminoindole	132	C8H8N2	005192-03-0	12	
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9	



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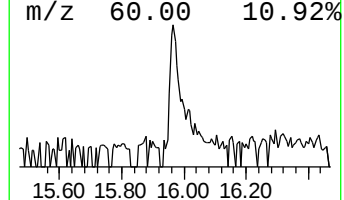
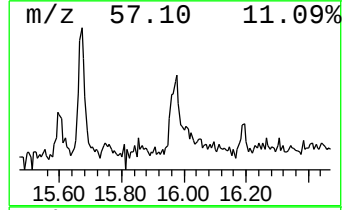
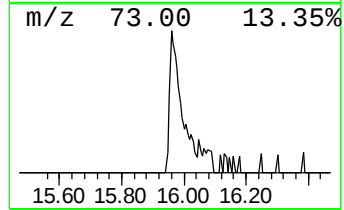
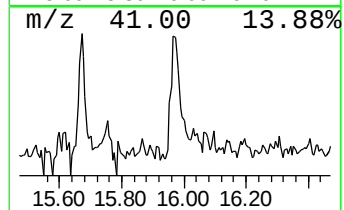
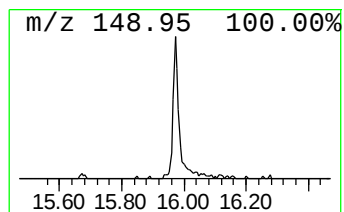
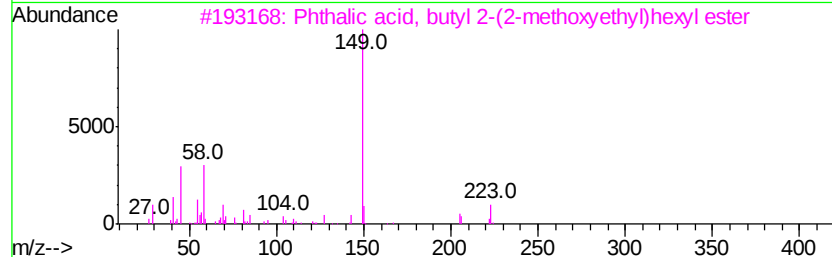
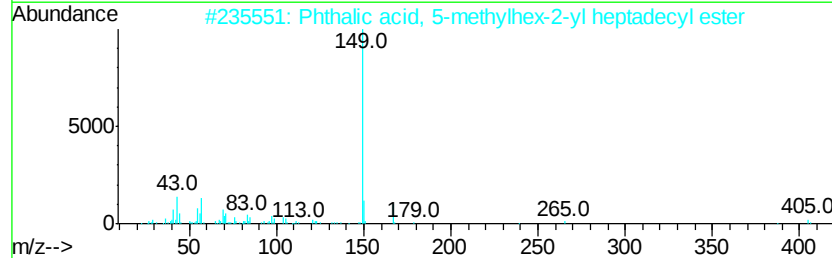
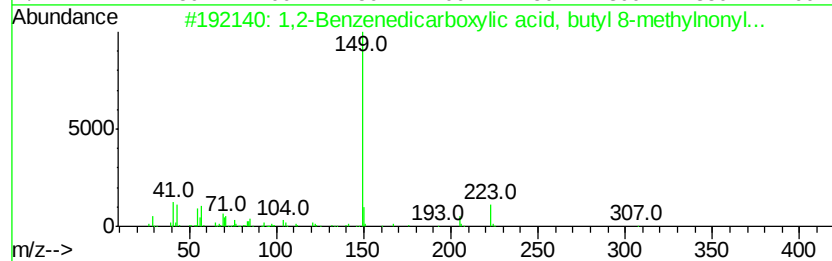
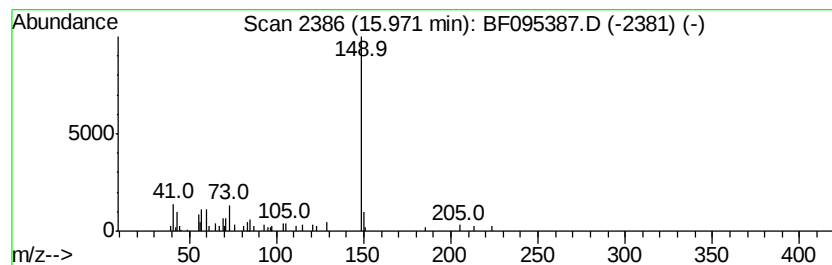
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Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.13 ng	91004	Phenanthrene-d10	15.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	64
2		Phthalic acid, 5-methylhex-2-yl ...	502	C32H54O4	1000371-07-7	64
3		Phthalic acid, butyl 2-(2-methox...	364	C21H32O5	1000314-92-8	59
4		Phthalic acid, 2,7-dimethyloct-7...	356	C22H28O4	1000315-49-7	59
5		Phthalic acid, pent-4-enyl tetra...	430	C27H42O4	1000360-47-3	59



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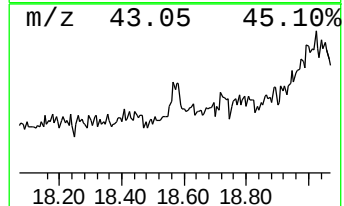
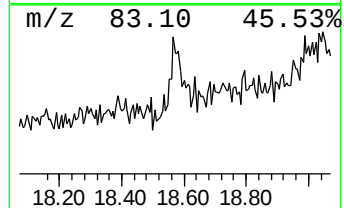
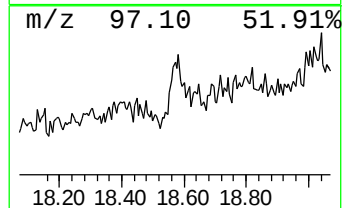
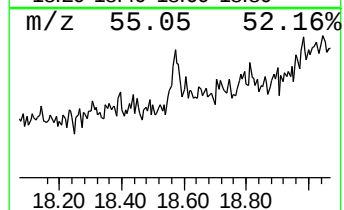
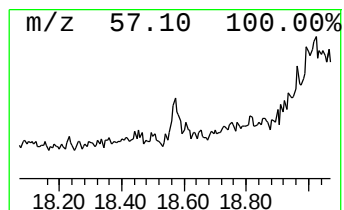
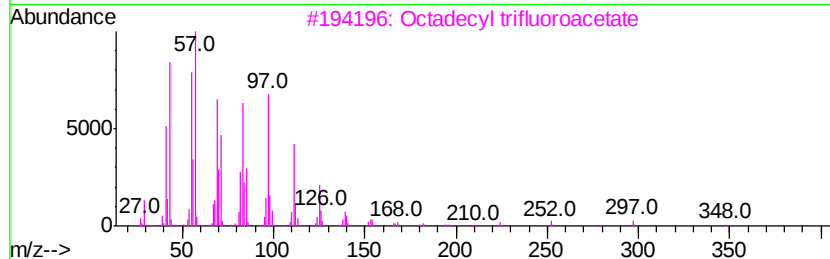
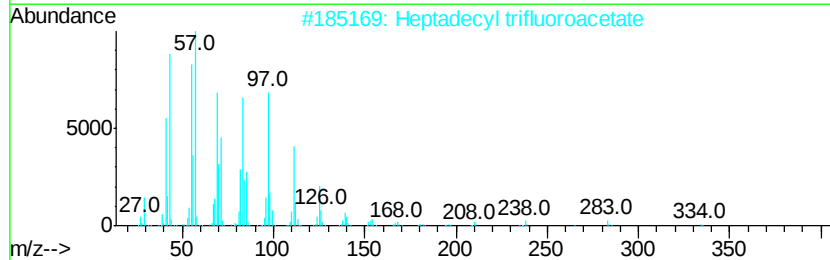
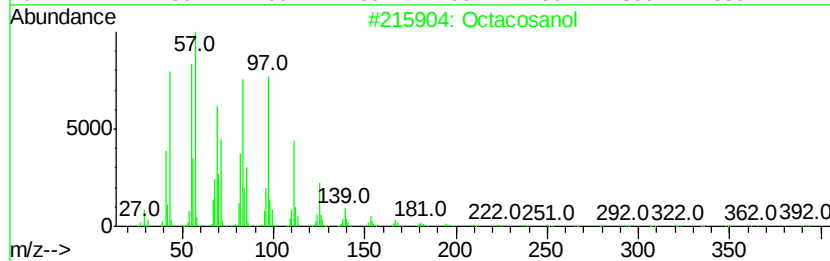
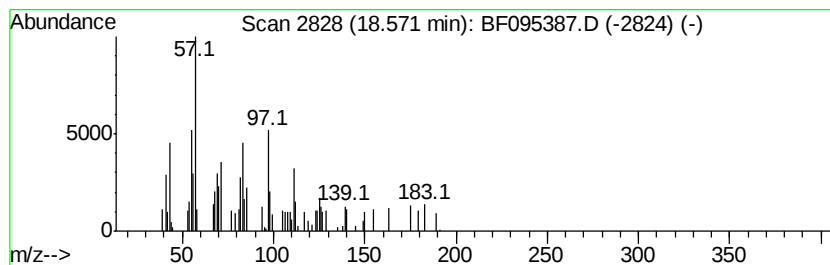
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Peak Number 5 Octacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.57	2.05 ng	54815	Chrysene-d12	18.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	64
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	58
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	58
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	52
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	50



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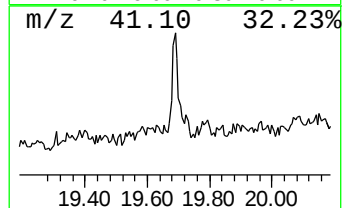
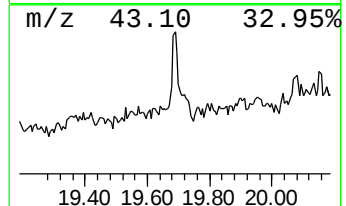
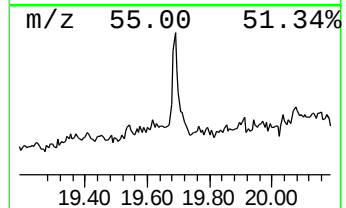
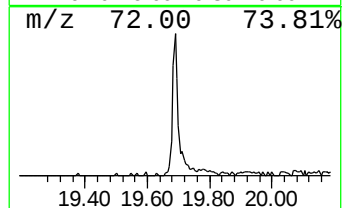
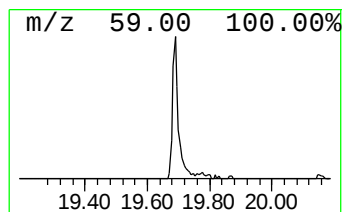
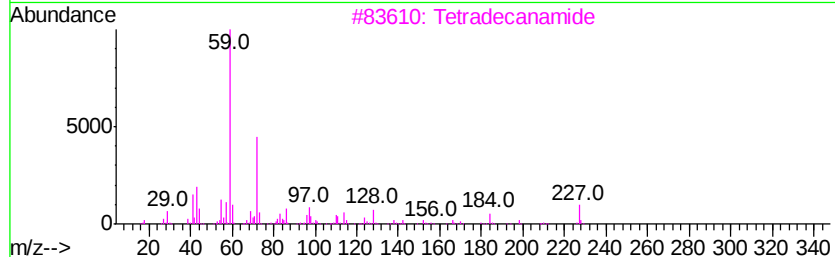
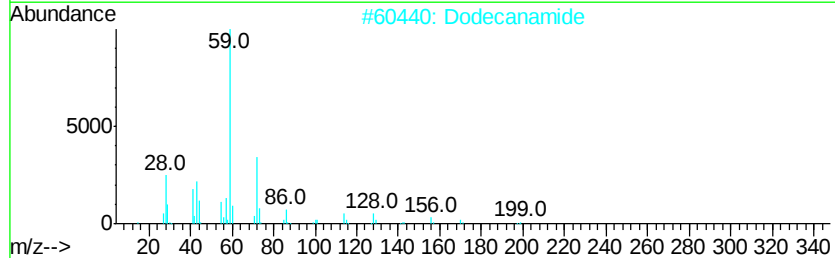
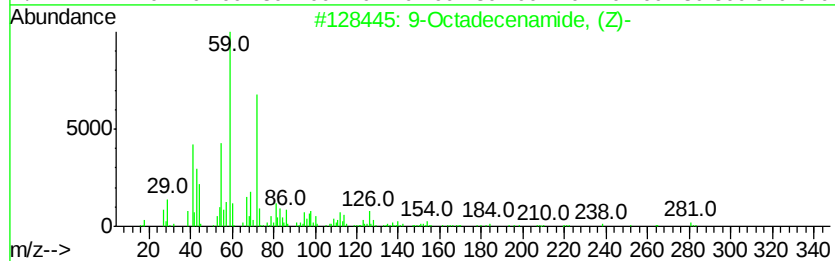
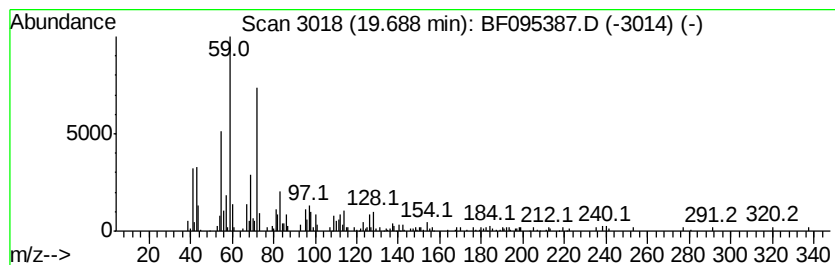
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	17.72 ng	277982	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Dodecanamide	199	C12H25NO	001120-16-7	50
3		Tetradecanamide	227	C14H29NO	000638-58-4	27
4		Acetic acid, cyanohydroxvimino-,...	128	C4H4N2O3	061295-92-9	27
5		2,7-Dioxatricyclo[4.4.0.0(3,8)]d...	155	C8H13NO2	040076-28-6	27



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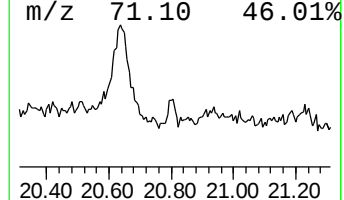
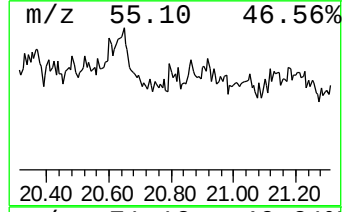
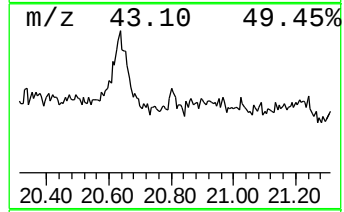
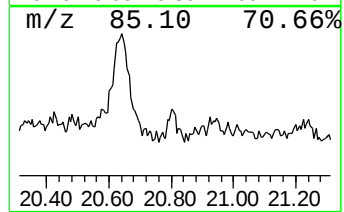
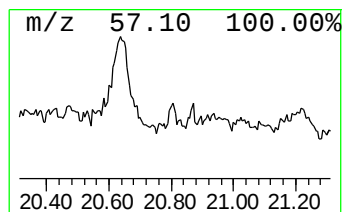
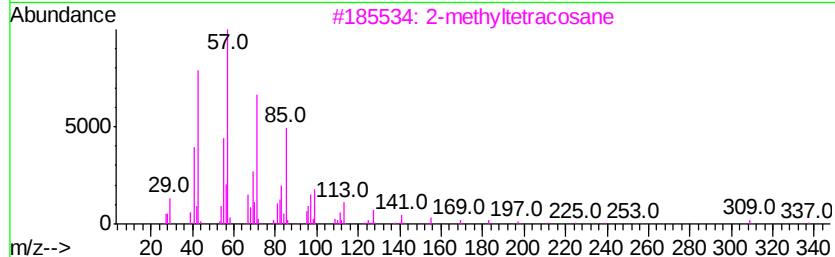
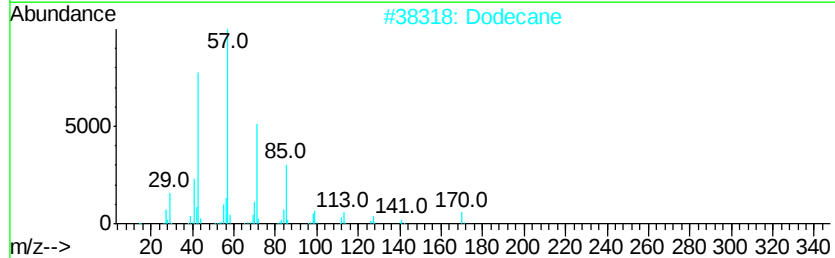
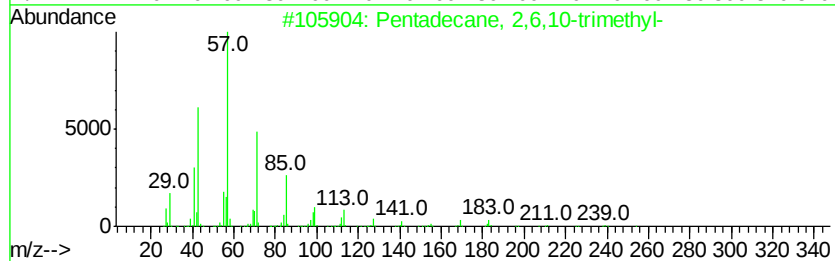
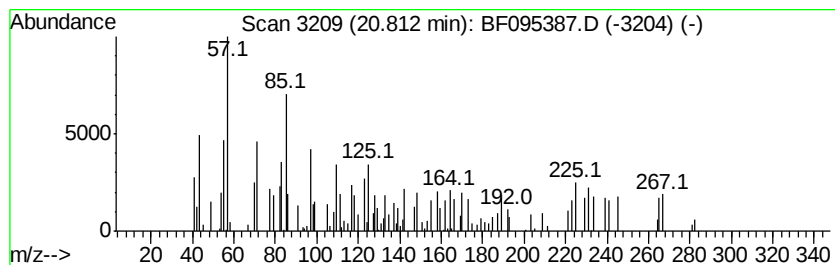
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	2.77 ng	43527	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	27
2		Dodecane	170	C12H26	000112-40-3	25
3		2-methyltetracosane	352	C25H52	1000376-72-6	25
4		DL-3-Aminoisobutyric acid, N-dim...	172	C8H16N2O2	1000375-50-3	22
5		Tetrapentacontane	759	C54H110	005856-66-6	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052417\
Data File : BF095387.D
Acq On : 24 May 2017 14:10
Operator : SJ/MA
Sample : I3290-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4

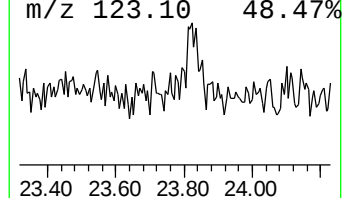
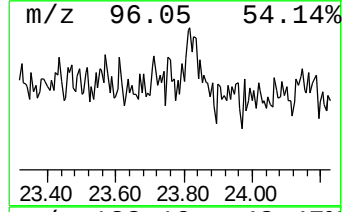
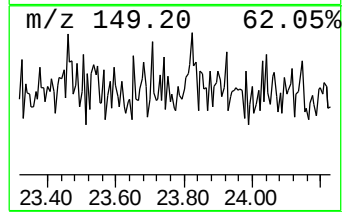
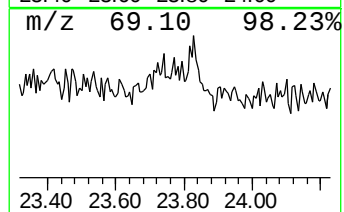
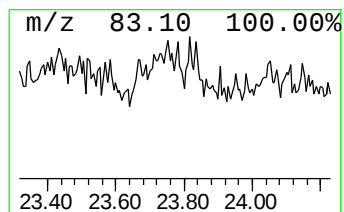
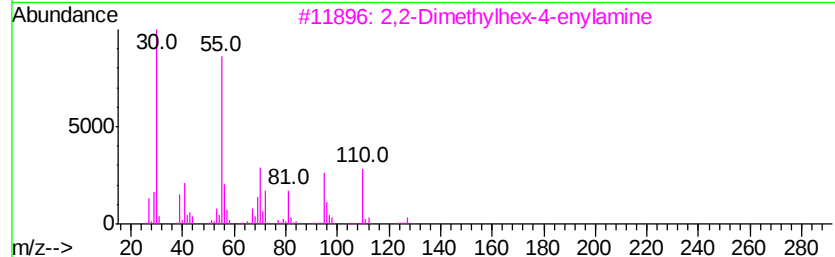
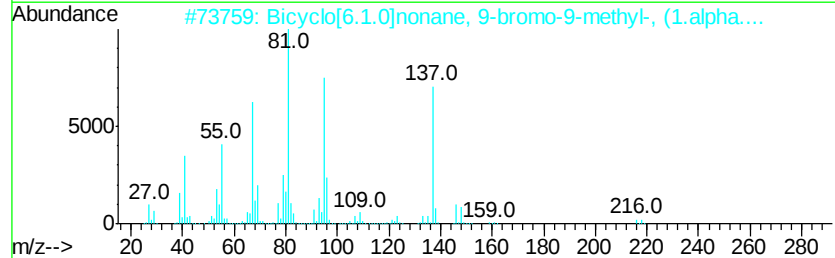
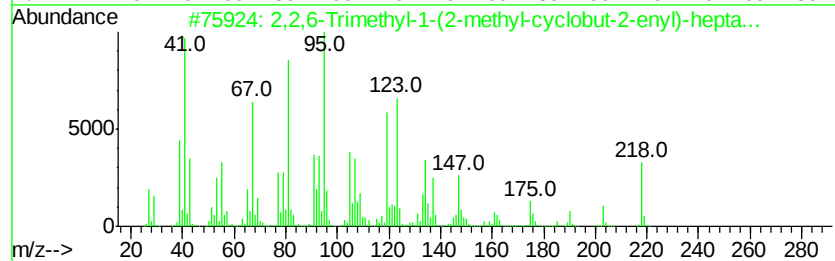
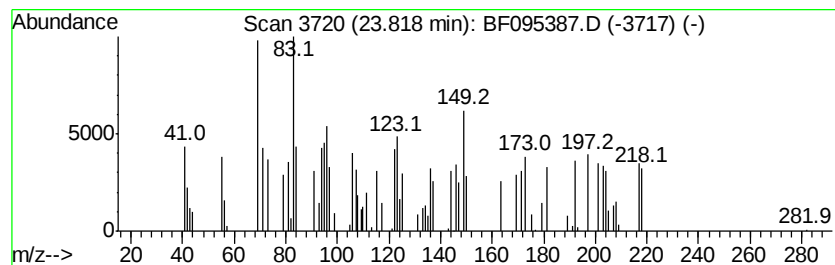
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown23.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	4.41 ng	69249	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	35
2		Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	22
3		2,2-Dimethylhex-4-enylamine	127	C8H17N	133885-74-2	22
4		1-Cycloheptene-1-acetic acid, .a...	182	C11H18O2	016642-56-1	22
5		Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052417\
Data File : BF095387.D
Acq On : 24 May 2017 14:10
Operator : SJ/MA
Sample : I3290-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.12	5.9	ng	135823	1	7.75	463704	20.0
unknown7.42	7.42	89.0	ng	2064520	1	7.75	463704	20.0
1,2-Benzenedicarb...	15.97	3.1	ng	91004	4	15.01	581654	20.0
Octacosanol	18.57	2.0	ng	54815	5	18.69	534614	20.0
9-Octadecenamide, ...	19.69	17.7	ng	277982	6	20.36	313768	20.0
unknown20.81	20.81	2.8	ng	43527	6	20.36	313768	20.0
unknown23.82	23.82	4.4	ng	69249	6	20.36	313768	20.0