

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
 Data File : BF095572.D
 Acq On : 31 May 2017 19:36
 Operator : SJ/MA
 Sample : I3329-10
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-9(2-6)

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-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	4.813	502	506	532	rBV2	83098	262113	7.73%	0.881%
2	5.466	613	617	652	rBV	1450150	2812335	82.98%	9.448%
3	7.107	891	896	909	rBV	1762555	2731855	80.61%	9.178%
4	7.213	909	914	928	rVB	2157232	3127999	92.30%	10.509%
5	7.554	967	972	984	rBV	392531	543886	16.05%	1.827%
6	7.789	1007	1012	1027	rVB	1652806	2230956	65.83%	7.495%
7	8.466	1122	1127	1146	rBV	1212764	1779058	52.50%	5.977%
8	8.830	1185	1189	1200	rBV2	19220	46973	1.39%	0.158%
9	9.583	1313	1317	1337	rBV	532032	781848	23.07%	2.627%
10	10.324	1440	1443	1463	rBV2	50461	163987	4.84%	0.551%
11	11.360	1613	1619	1633	rBV	2544992	3388986	100.00%	11.386%
12	12.054	1731	1737	1748	rBV	844060	1069627	31.56%	3.594%
13	12.407	1792	1797	1809	rBV2	744658	954607	28.17%	3.207%
14	13.254	1936	1941	1945	rBV	37148	43404	1.28%	0.146%
15	13.612	1990	2002	2006	rBV2	20380	39125	1.15%	0.131%
16	13.707	2013	2018	2033	rBV	1246461	1819333	53.68%	6.112%
17	14.024	2067	2072	2081	rBV	58665	107727	3.18%	0.362%
18	14.759	2193	2197	2201	rBV	33830	41003	1.21%	0.138%
19	14.812	2201	2206	2218	rVB	626626	900578	26.57%	3.026%
20	15.312	2285	2291	2304	rBV	206427	318176	9.39%	1.069%
21	15.800	2368	2374	2384	rBV	157606	220477	6.51%	0.741%
22	16.500	2489	2493	2503	rBV	288655	432333	12.76%	1.452%
23	16.636	2511	2516	2524	rVB3	19157	36573	1.08%	0.123%
24	16.895	2557	2560	2564	rBV2	51521	74469	2.20%	0.250%
25	17.000	2574	2578	2584	rBV	138878	163552	4.83%	0.549%
26	17.159	2599	2605	2609	rBV2	2187276	2654444	78.33%	8.918%
27	17.518	2661	2666	2668	rBV5	20195	35784	1.06%	0.120%
28	17.853	2716	2723	2726	rBV	525210	707184	20.87%	2.376%
29	17.883	2726	2728	2729	rVV	240105	236154	6.97%	0.793%
30	17.900	2729	2731	2739	rVV	268944	364392	10.75%	1.224%
31	17.965	2739	2742	2749	rVB	73269	106664	3.15%	0.358%
32	18.400	2812	2816	2826	rBV2	125020	197144	5.82%	0.662%
33	18.506	2829	2834	2842	rBV	545557	711183	20.99%	2.389%
34	18.730	2868	2872	2875	rBV2	91150	111848	3.30%	0.376%

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ClientSampleId :
B-9(2-6)

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

35	20.177	3114	3118	3129	rBV	410518	549578	16.22%	1.846%
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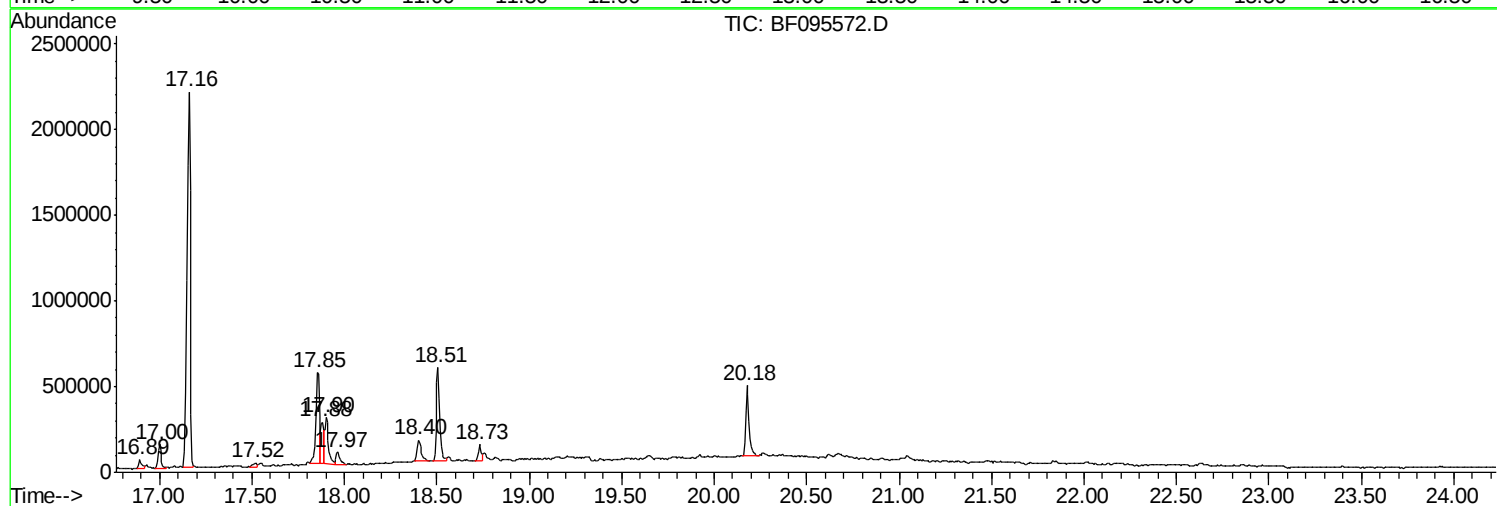
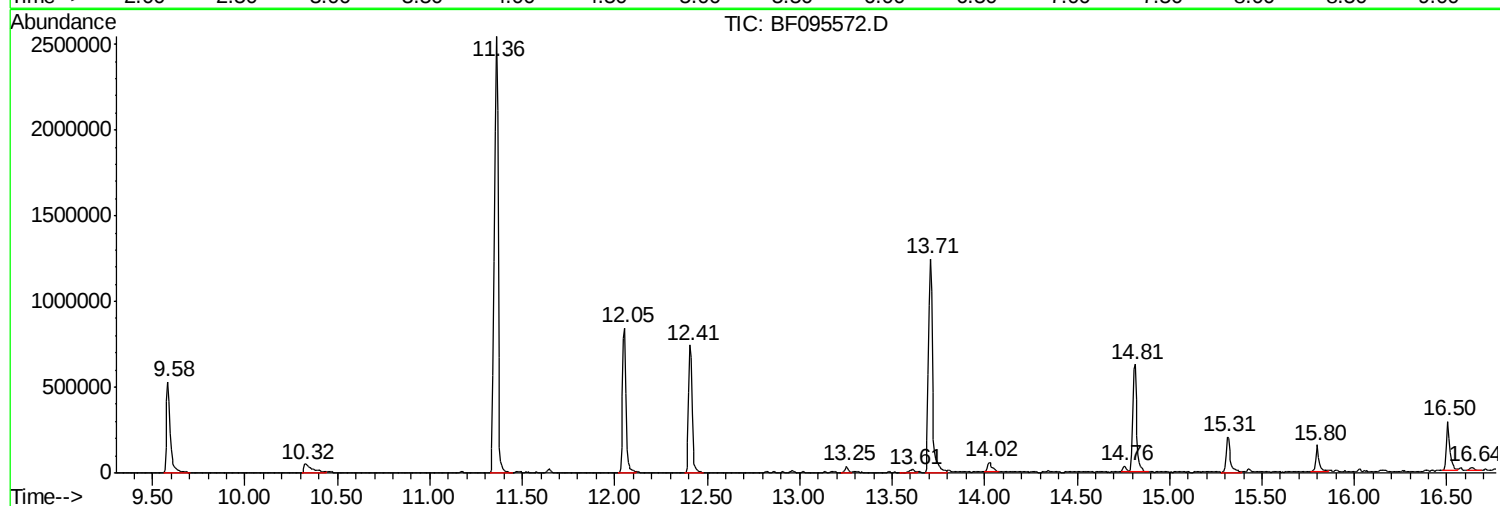
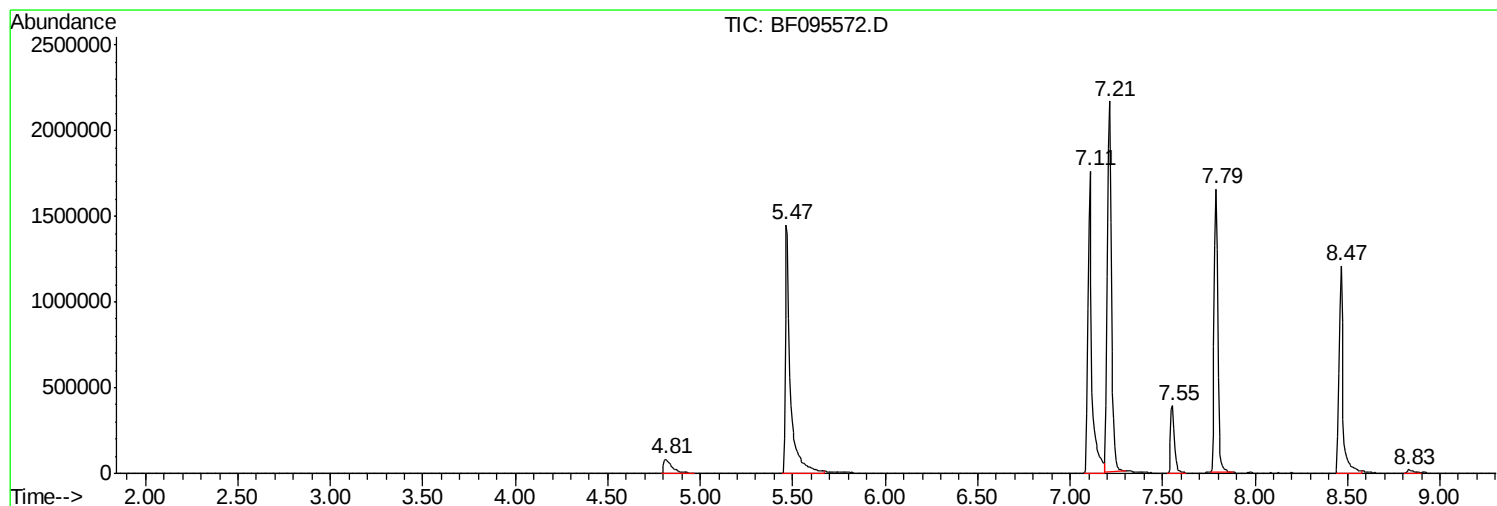
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Instrument :
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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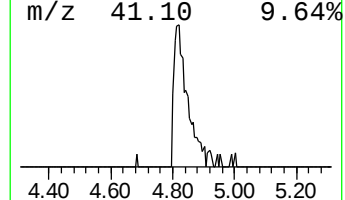
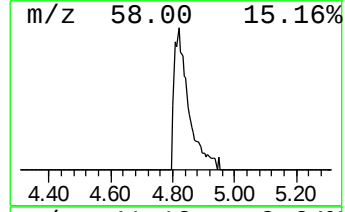
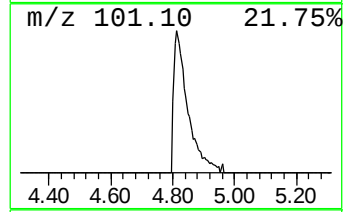
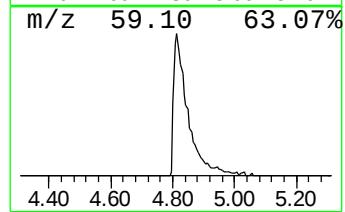
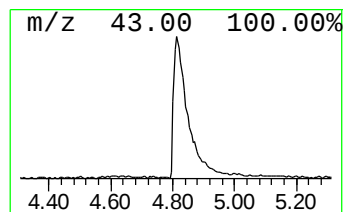
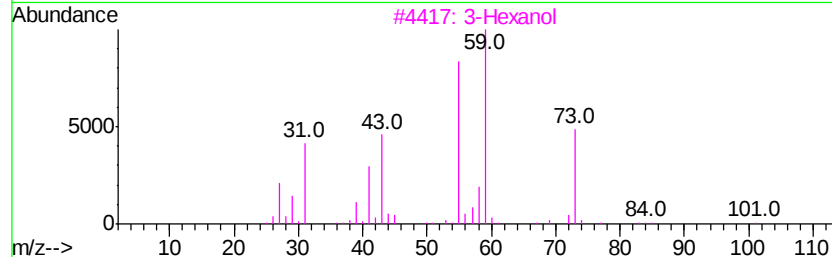
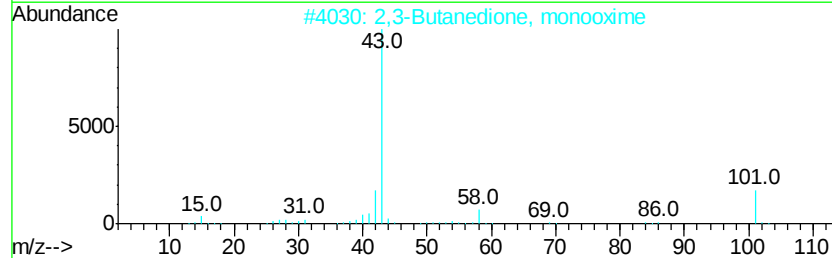
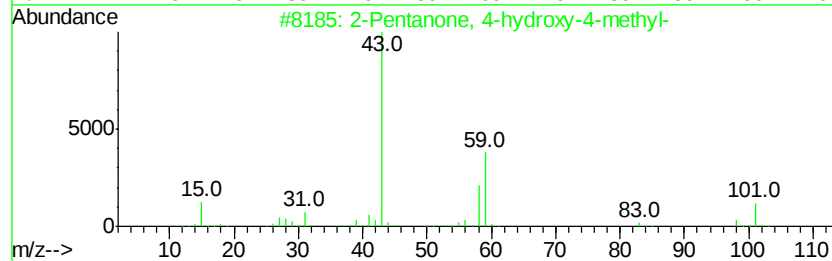
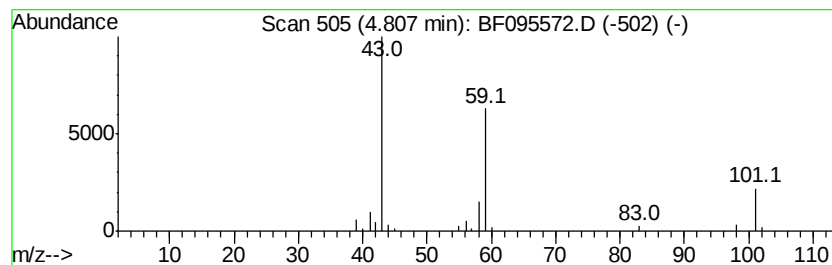
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	9.64 ng	262113	1,4-Dichlorobenzene-d4	7.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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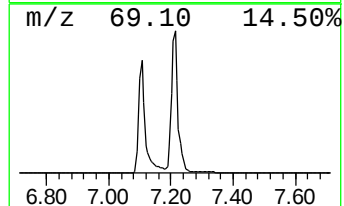
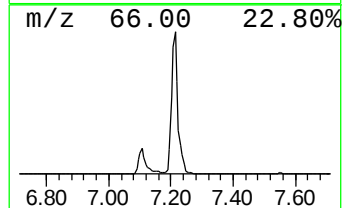
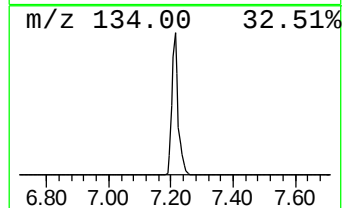
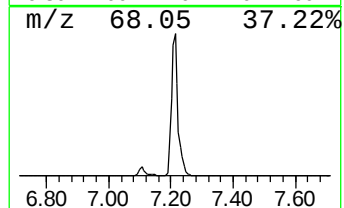
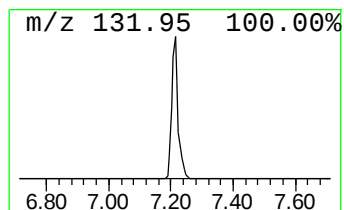
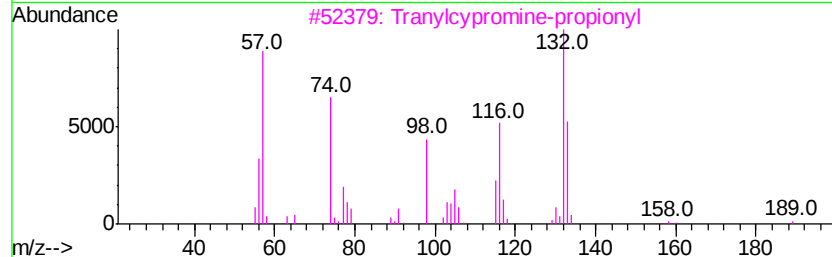
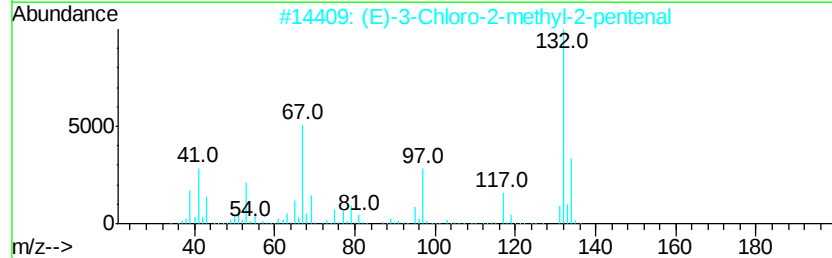
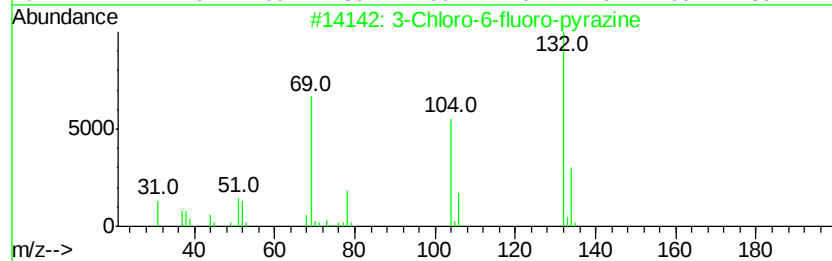
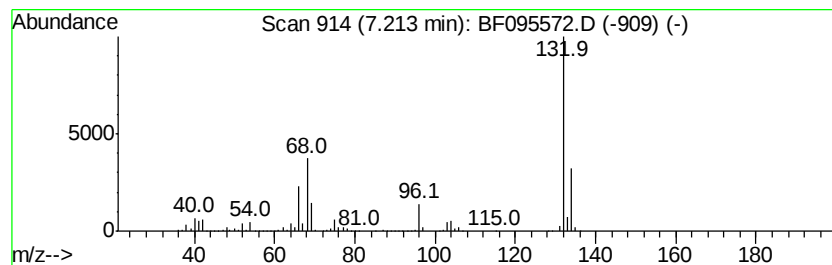
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	115.02 ng	3128000	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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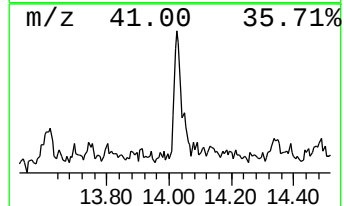
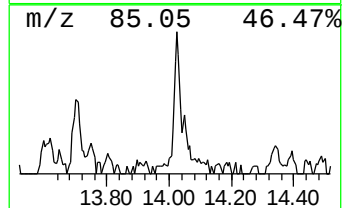
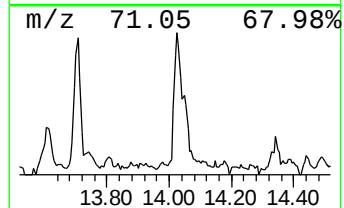
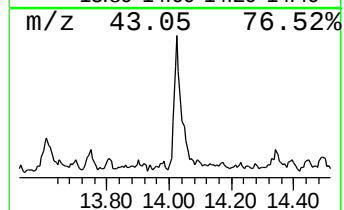
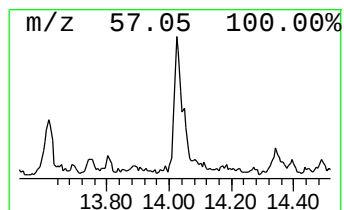
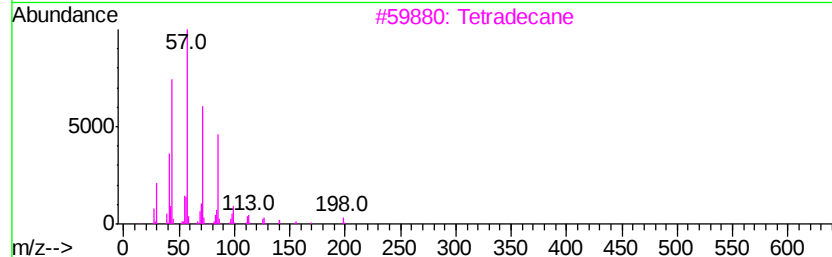
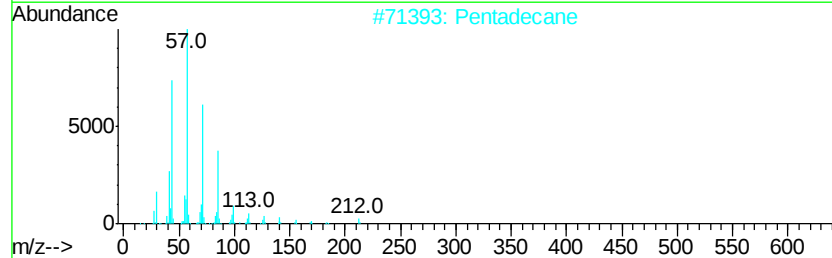
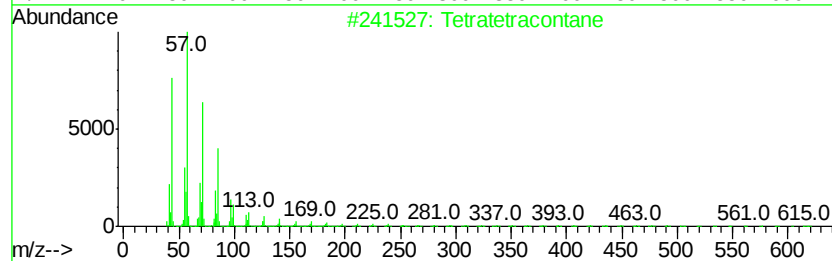
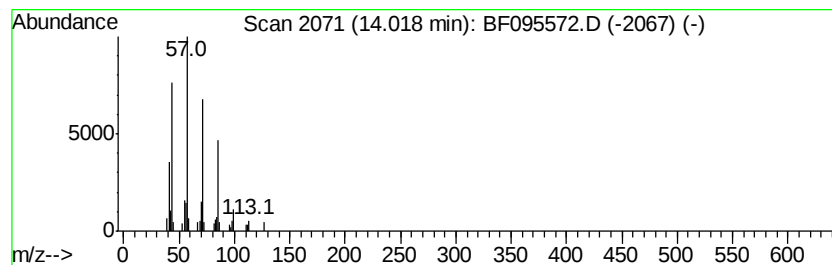
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetratetracontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	2.39 ng	107727	Phenanthrene-d10	14.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	86
2		Pentadecane	212	C15H32	000629-62-9	86
3		Tetradecane	198	C14H30	000629-59-4	86
4		Octacosane	394	C28H58	000630-02-4	86
5		Heptadecane	240	C17H36	000629-78-7	86



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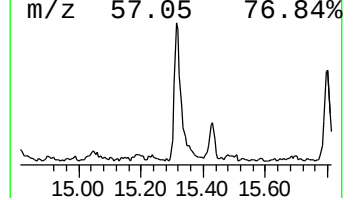
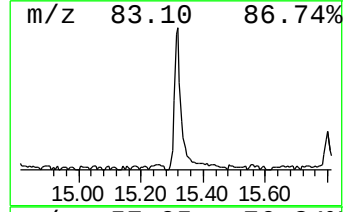
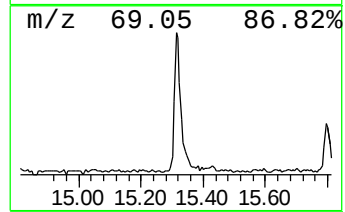
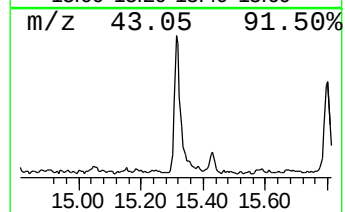
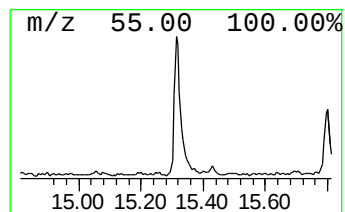
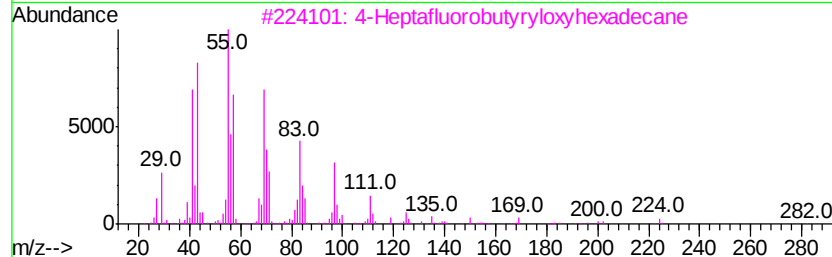
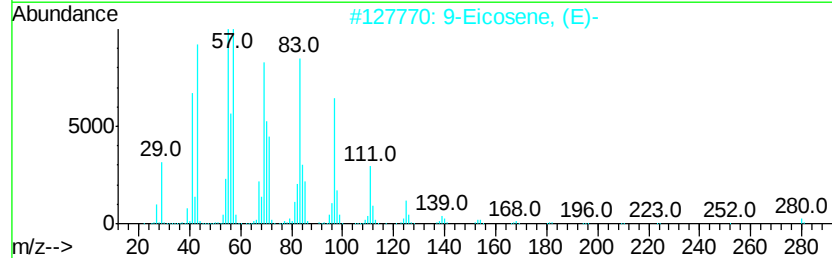
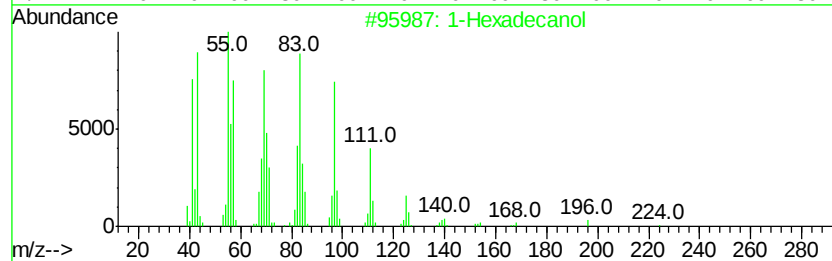
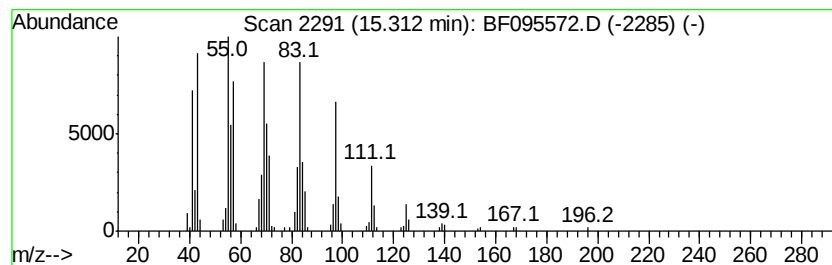
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.31	7.07 ng	318176	Phenanthrene-d10	14.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	4-Heptafluorobutylrvloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
4	Cyclotetradecane	196	C14H28	000295-17-0	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91



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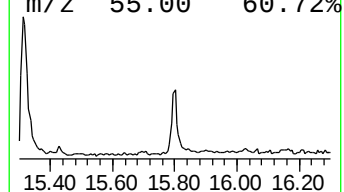
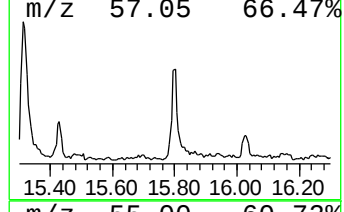
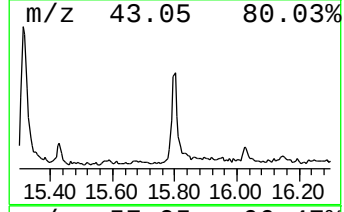
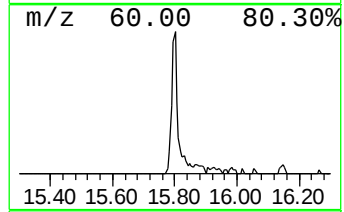
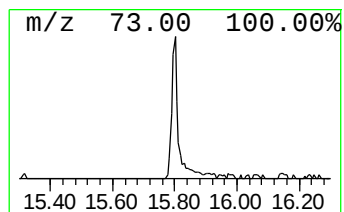
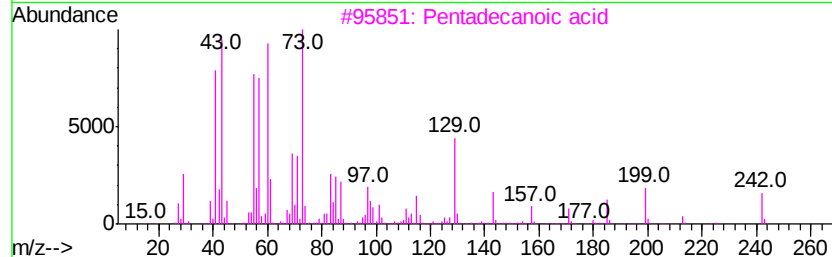
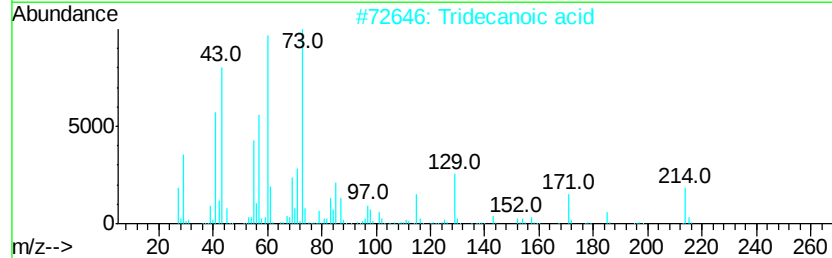
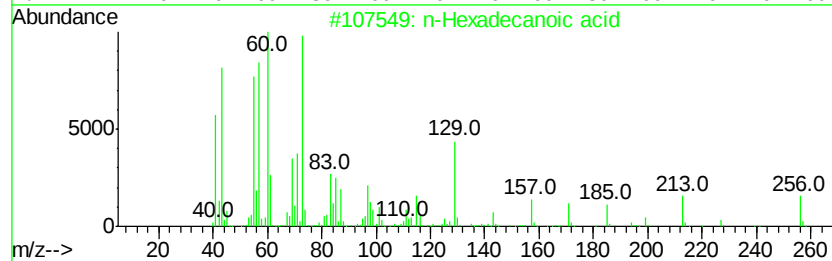
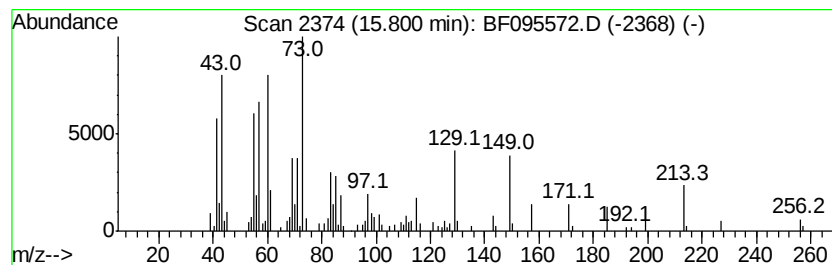
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.80	4.90 ng	220477	Phenanthrene-d10	14.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
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Acq On : 31 May 2017 19:36
Operator : SJ/MA
Sample : I3329-10
Misc :
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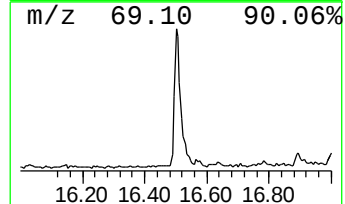
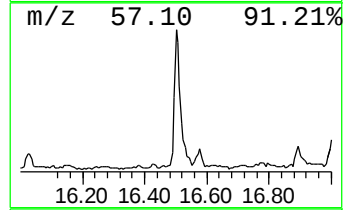
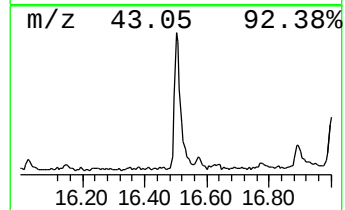
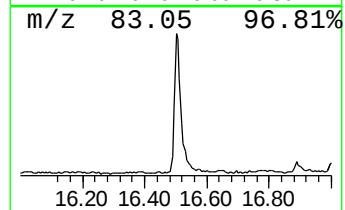
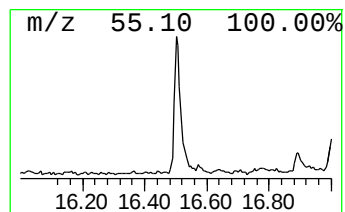
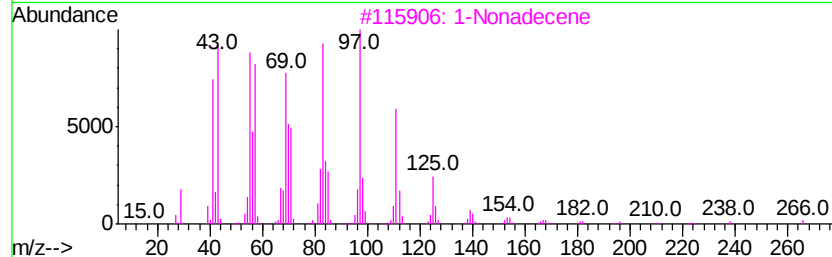
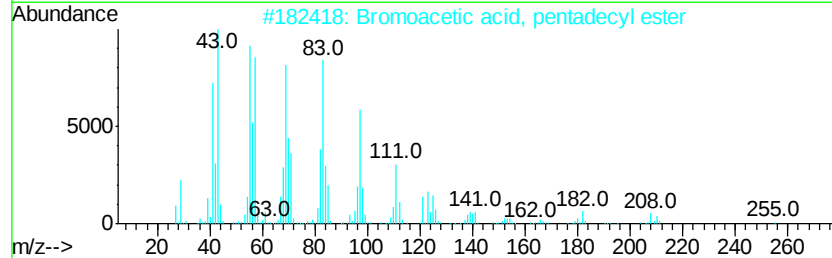
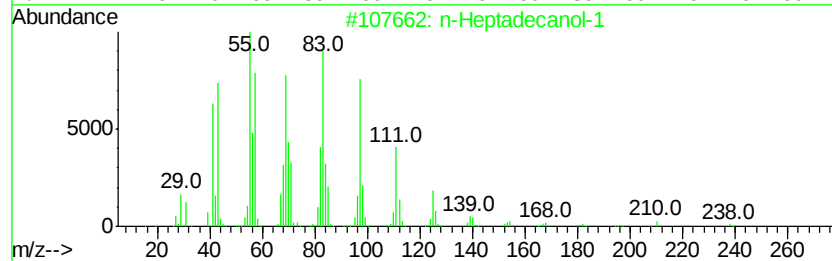
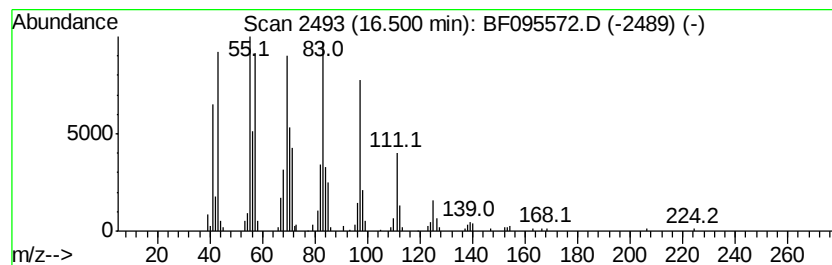
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B-9(2-6)

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 7 n-Heptadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.50	9.60 ng	432333	Phenanthrene-d10	14.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	1-Hexadecanol	242	C16H34O	036653-82-4	93
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095572.D
Acq On : 31 May 2017 19:36
Operator : SJ/MA
Sample : I3329-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-9(2-6)

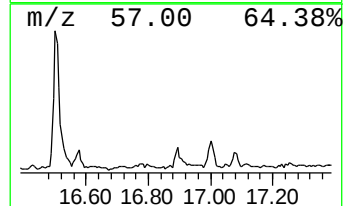
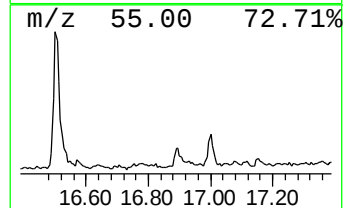
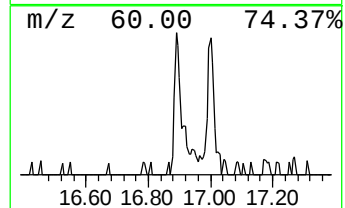
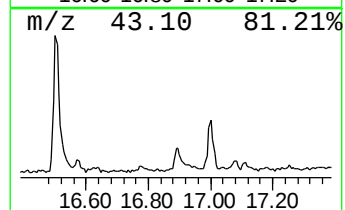
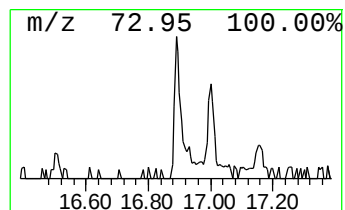
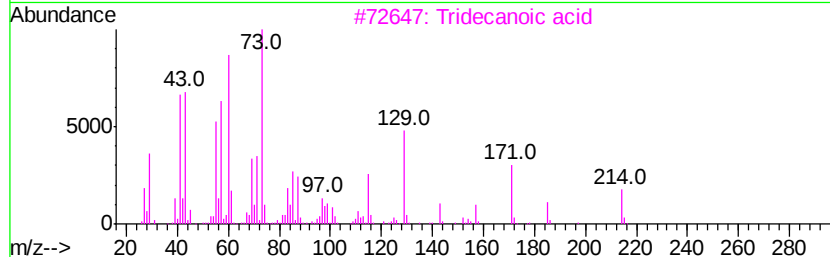
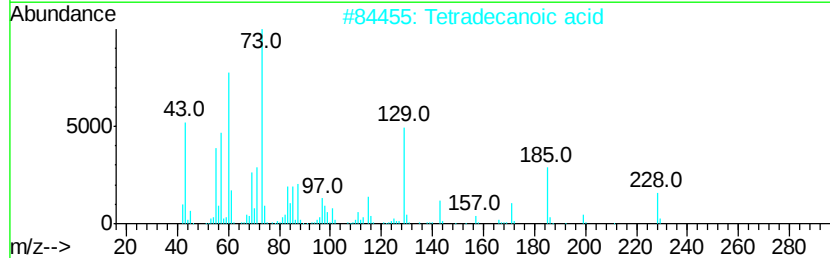
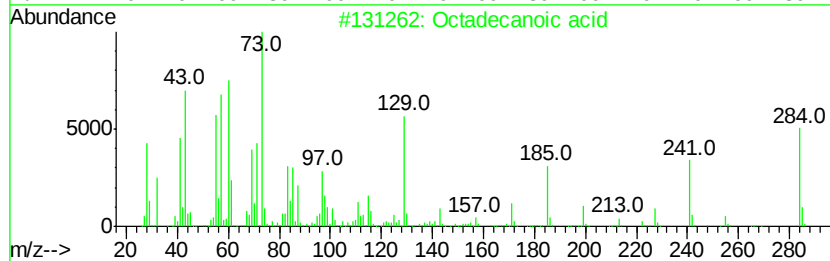
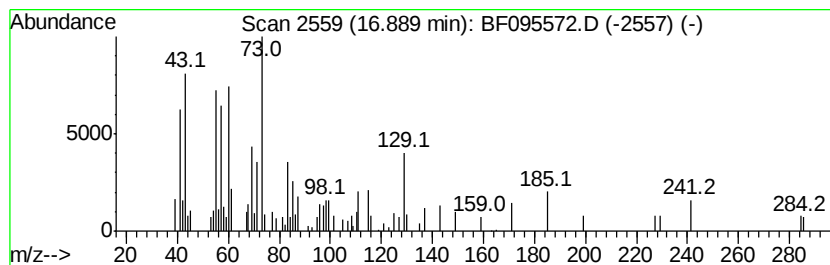
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.09 ng	74469	Chrysene-d12	18.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3		Tridecanoic acid	214	C13H26O2	000638-53-9	49
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095572.D
Acq On : 31 May 2017 19:36
Operator : SJ/MA
Sample : I3329-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
B-9(2-6)

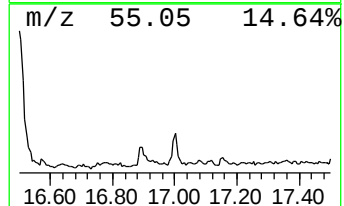
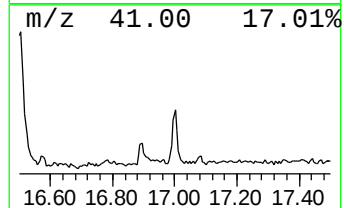
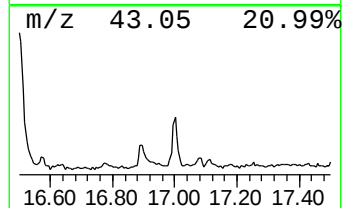
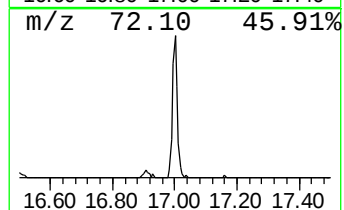
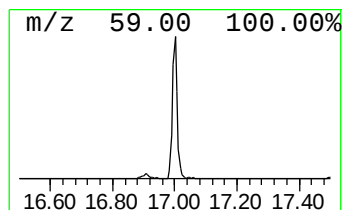
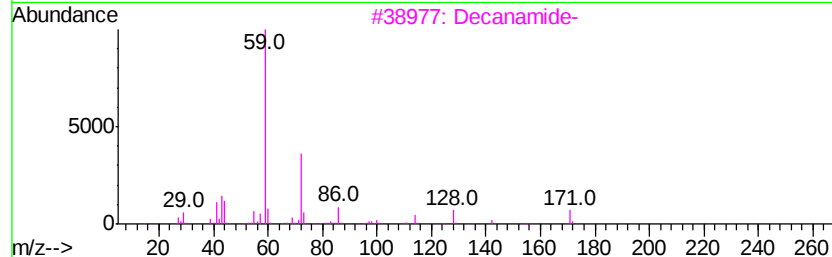
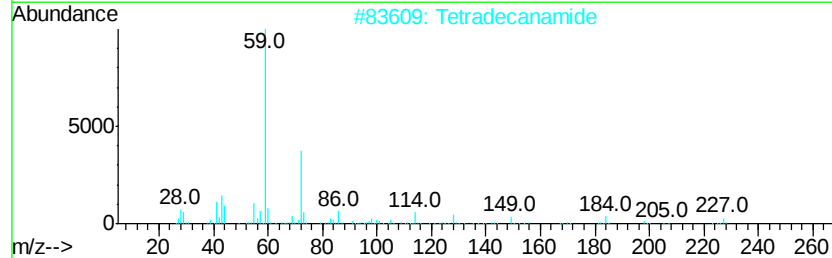
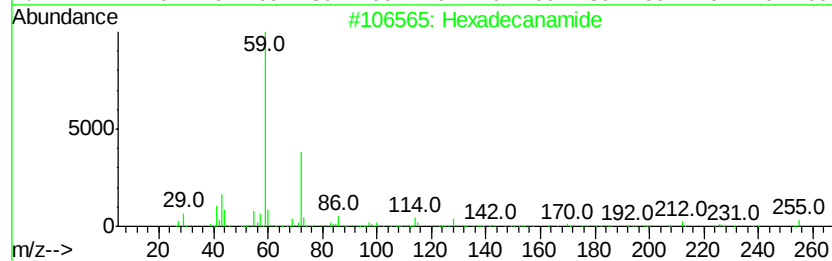
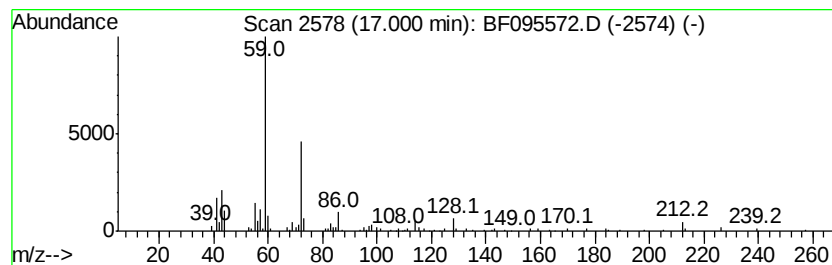
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	4.60 ng	163552	Chrysene-d12	18.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide		255	C16H33NO	000629-54-9	91
2	Tetradecanamide		227	C14H29NO	000638-58-4	86
3	Decanamide-		171	C10H21NO	002319-29-1	78
4	Octanamide		143	C8H17NO	000629-01-6	72
5	Dodecanamide		199	C12H25NO	001120-16-7	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095572.D
Acq On : 31 May 2017 19:36
Operator : SJ/MA
Sample : I3329-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-9(2-6)

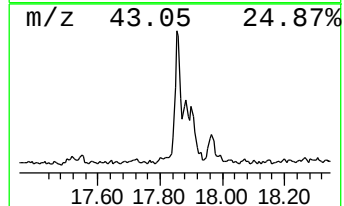
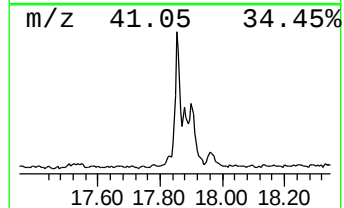
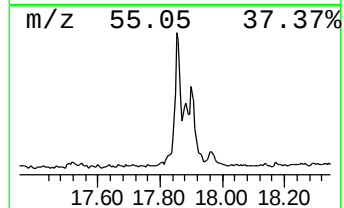
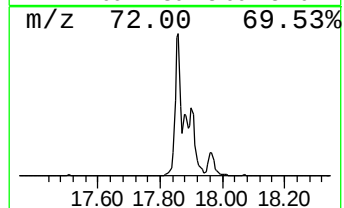
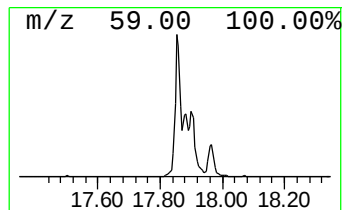
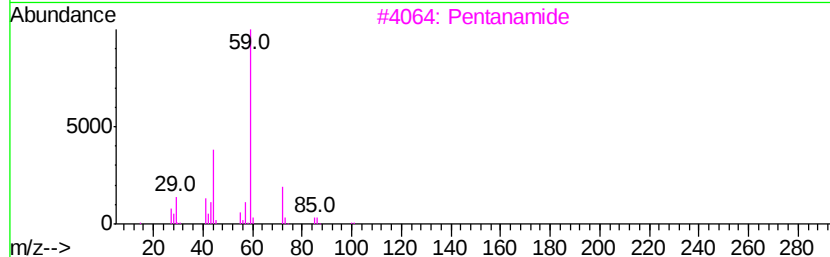
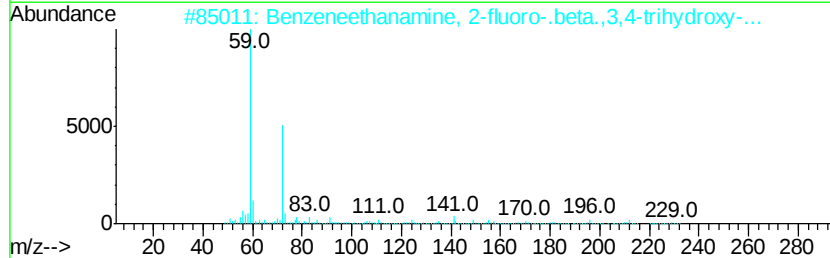
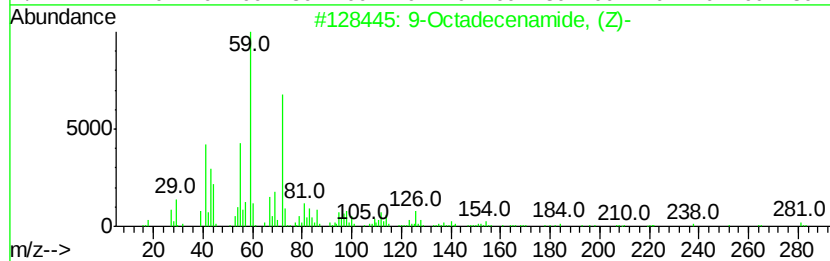
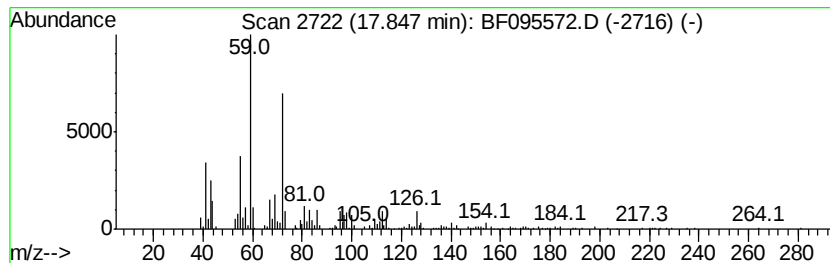
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzeneethanamine, 2-fluoro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	19.89 ng	707184	Chrysene-d12	18.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	80
3		Pentanamide	101	C5H11NO	000626-97-1	64
4		Hexadecanamide	255	C16H33NO	000629-54-9	64
5		Dodecanamide	199	C12H25NO	001120-16-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
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Acq On : 31 May 2017 19:36
Operator : SJ/MA
Sample : I3329-10
Misc :
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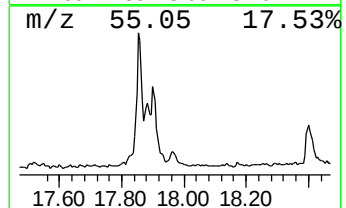
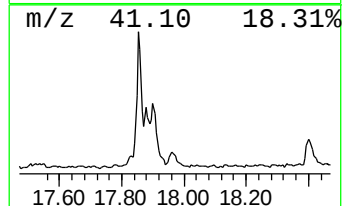
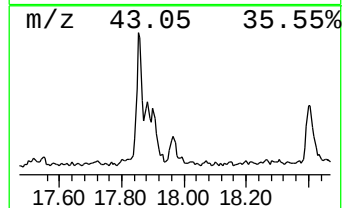
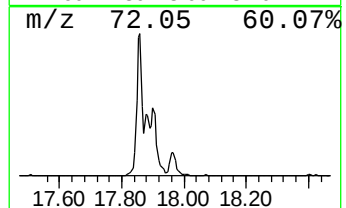
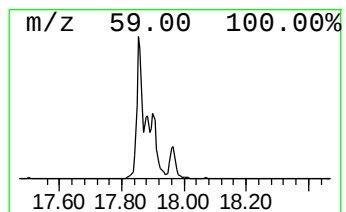
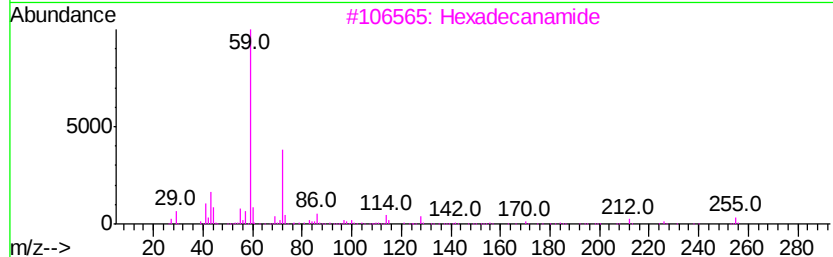
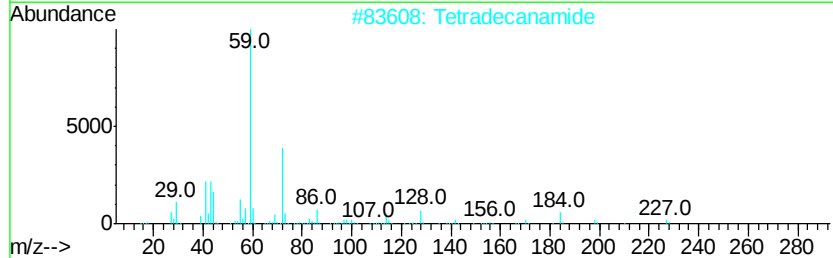
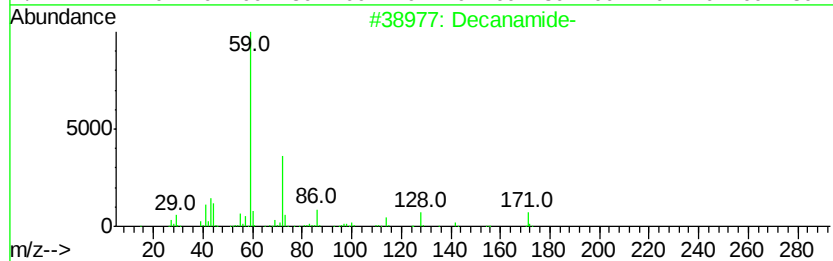
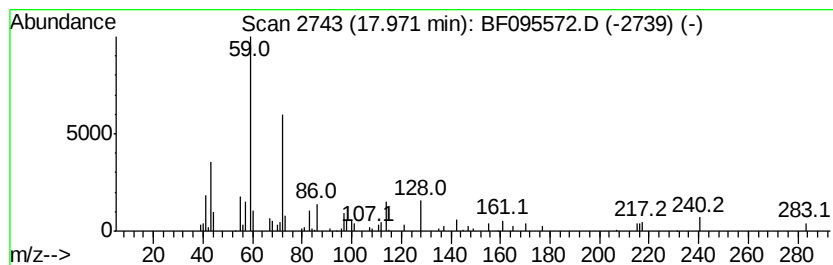
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Decanamide- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.97	3.00 ng	106664	Chrysene-d12	18.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanamide-	171	C10H21NO	002319-29-1	90
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Dodecanamide	199	C12H25NO	001120-16-7	78
5	Acetic acid, bromo-, methyl ester	152	C3H5BrO2	000096-32-2	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
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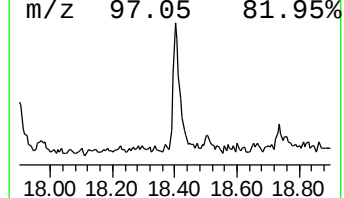
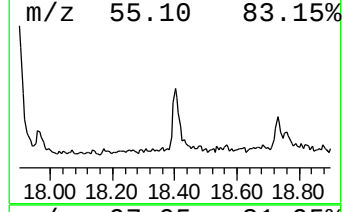
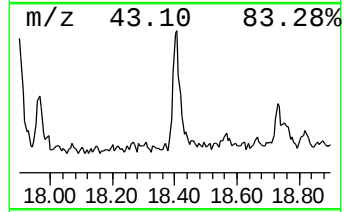
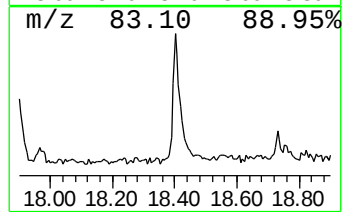
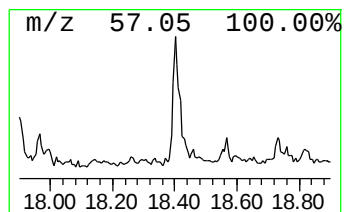
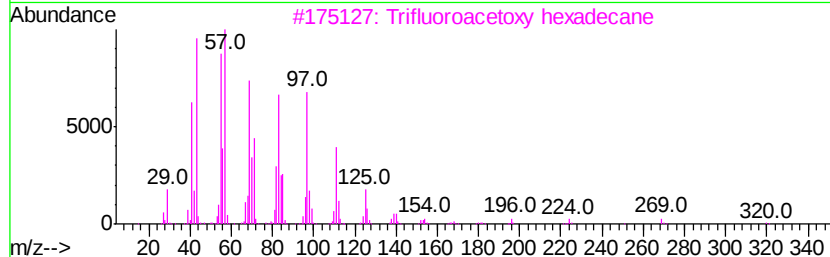
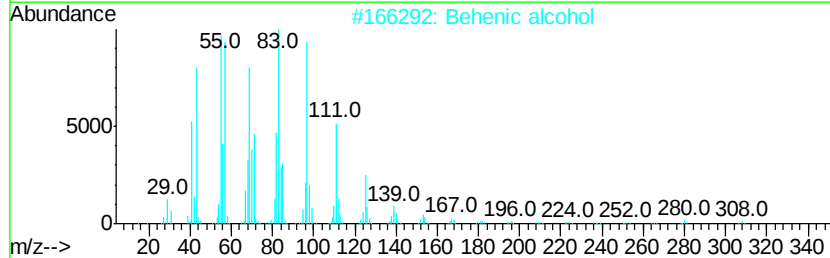
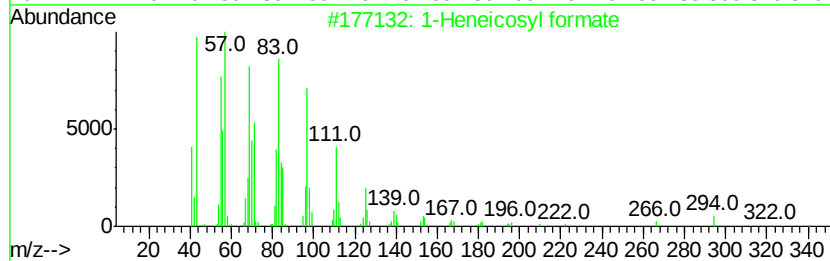
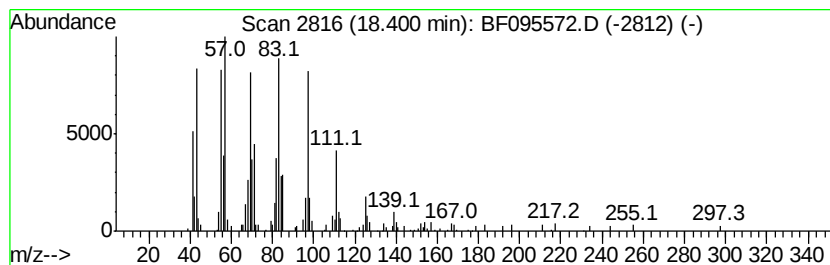
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Heneicosyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.40	5.54 ng	197144	Chrysene-d12	18.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
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 ALS Vial : 12 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.21	7.21	115.0	ng	3128000	1	7.55	543886	20.0
Tetratetracontane	14.02	2.4	ng	107727	4	14.81	900578	20.0
1-Hexadecanol	15.31	7.1	ng	318176	4	14.81	900578	20.0
n-Hexadecanoic acid	15.80	4.9	ng	220477	4	14.81	900578	20.0
n-Heptadecanol-1	16.50	9.6	ng	432333	4	14.81	900578	20.0
Octadecanoic acid	16.89	2.1	ng	74469	5	18.51	711183	20.0
Hexadecanamide	17.00	4.6	ng	163552	5	18.51	711183	20.0
Benzeneethanamine...	17.85	19.9	ng	707184	5	18.51	711183	20.0
Decanamide-	17.97	3.0	ng	106664	5	18.51	711183	20.0
1-Heneicosyl formate	18.40	5.5	ng	197144	5	18.51	711183	20.0