

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098580.D
 Acq On : 15 Sep 2017 20:32
 Operator : SJ/JU
 Sample : I5229-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400S18

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-BF091117.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	2.987	152	153	167	rBV3	27116	80777	2.14%	0.238%
2	4.828	463	466	479	rBV	246910	386649	10.24%	1.140%
3	5.257	535	539	562	rBV	3749591	3726193	98.72%	10.989%
4	6.298	711	716	732	rBV	3273700	3774582	100.00%	11.132%
5	6.416	732	736	739	rBV	3944704	3726368	98.72%	10.990%
6	6.639	771	774	782	rBV	937626	834579	22.11%	2.461%
7	6.798	797	801	804	rBV	2967194	2567433	68.02%	7.572%
8	7.216	867	872	875	rBV	2365833	2314483	61.32%	6.826%
9	7.928	989	993	996	rBV	1263560	1095205	29.02%	3.230%
10	9.004	1171	1176	1179	rBV	3308321	2919300	77.34%	8.609%
11	9.404	1239	1244	1247	rBV	607107	503079	13.33%	1.484%
12	9.680	1284	1291	1294	rBV	1271023	1232244	32.65%	3.634%
13	10.116	1362	1365	1368	rVB	56657	48359	1.28%	0.143%
14	10.469	1418	1425	1436	rBV	2188993	2215190	58.69%	6.533%
15	10.586	1441	1445	1454	rVV	79538	83747	2.22%	0.247%
16	11.033	1518	1521	1524	rBV2	47494	39427	1.04%	0.116%
17	11.163	1539	1543	1546	rBV	1531912	1289302	34.16%	3.802%
18	12.380	1744	1750	1756	rVB3	24386	49818	1.32%	0.147%
19	12.651	1793	1796	1799	rVB	53941	49561	1.31%	0.146%
20	12.751	1808	1813	1816	rBV	3284349	3144842	83.32%	9.275%
21	13.215	1889	1892	1898	rVB4	35393	47295	1.25%	0.139%
22	13.645	1961	1965	1973	rBV	342464	404670	10.72%	1.193%
23	13.798	1987	1991	1998	rVB	1270741	1102920	29.22%	3.253%
24	14.274	2067	2072	2079	rBV2	121852	177523	4.70%	0.524%
25	14.545	2115	2118	2123	rBV	191901	192456	5.10%	0.568%
26	14.698	2141	2144	2147	rVB	52560	51119	1.35%	0.151%
27	14.868	2169	2173	2176	rBV	160834	164858	4.37%	0.486%
28	14.898	2176	2178	2183	rVB4	49004	52962	1.40%	0.156%
29	15.198	2224	2229	2237	rBV	695708	823512	21.82%	2.429%
30	15.398	2259	2263	2267	rVB3	43041	51939	1.38%	0.153%
31	15.604	2293	2298	2302	rBV2	82817	116575	3.09%	0.344%
32	15.656	2302	2307	2313	rVV3	51262	89919	2.38%	0.265%
33	16.309	2414	2418	2427	rVB4	40693	77578	2.06%	0.229%
34	17.021	2532	2539	2550	rBV7	79282	199482	5.28%	0.588%

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Sample : I5229-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400S18

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

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35	17.921	2690	2692	2701	rVB9	26415	62081	1.64%	0.183%
36	18.321	2753	2760	2772	rVB5	78556	212138	5.62%	0.626%

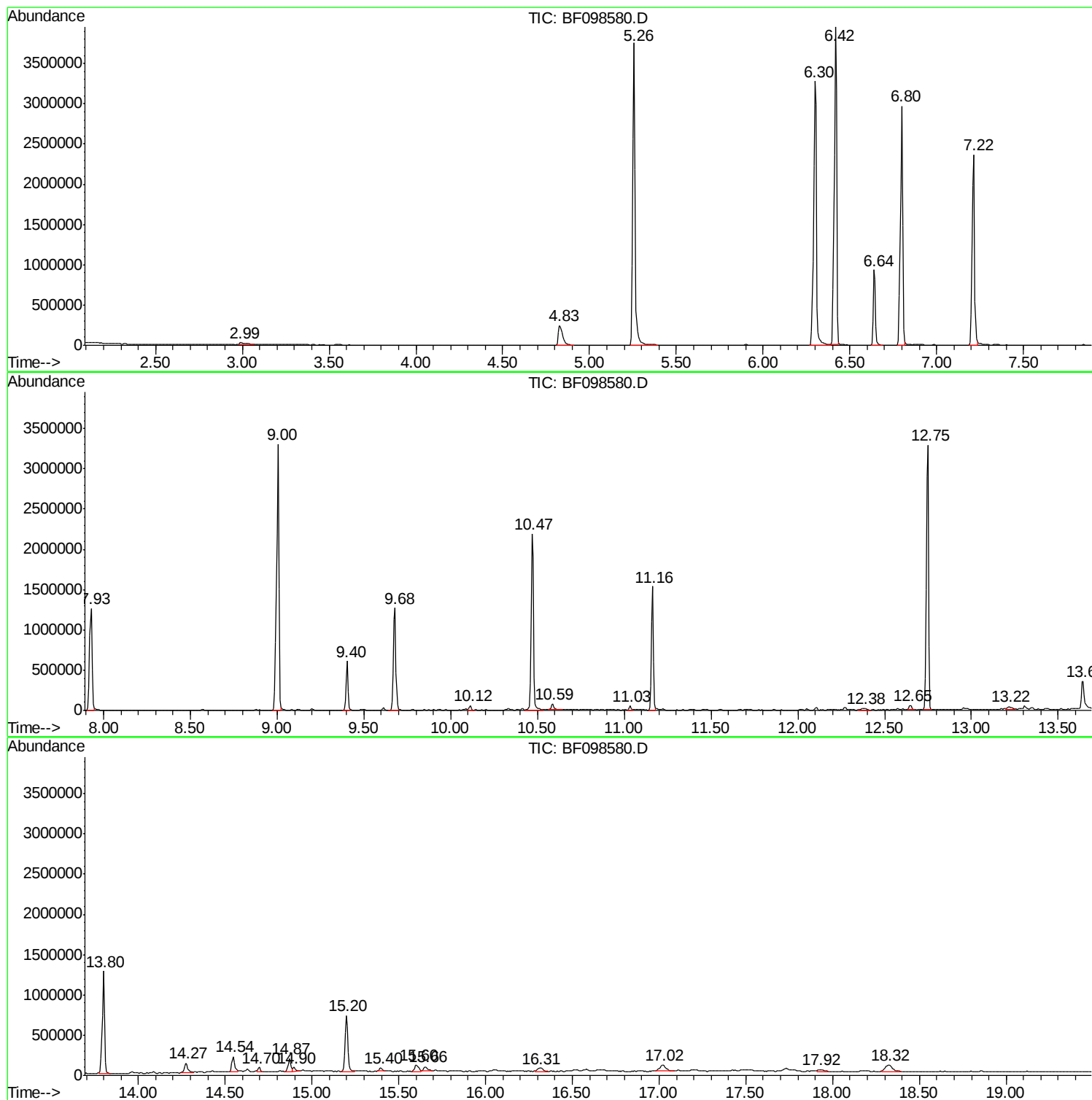
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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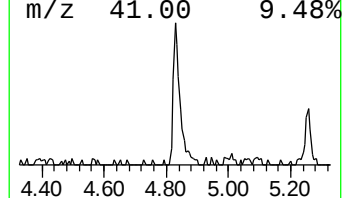
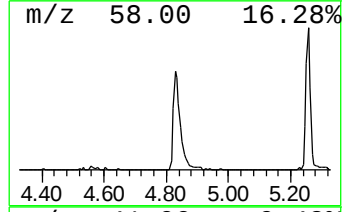
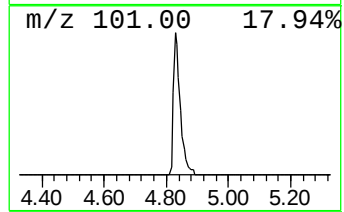
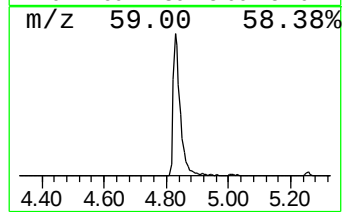
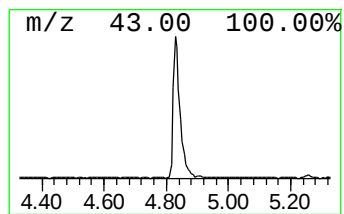
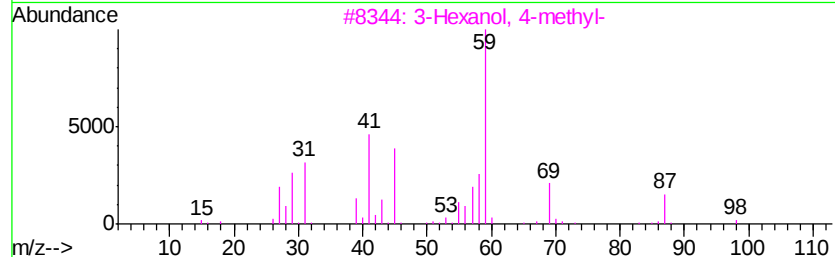
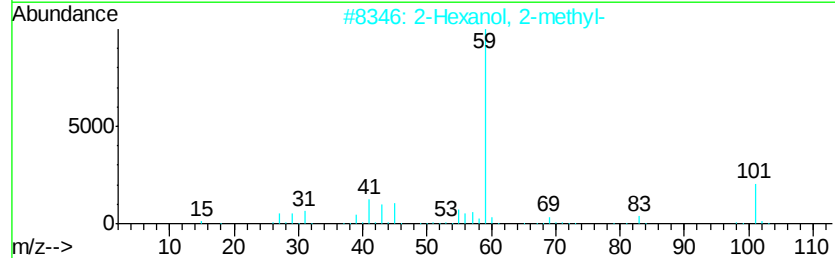
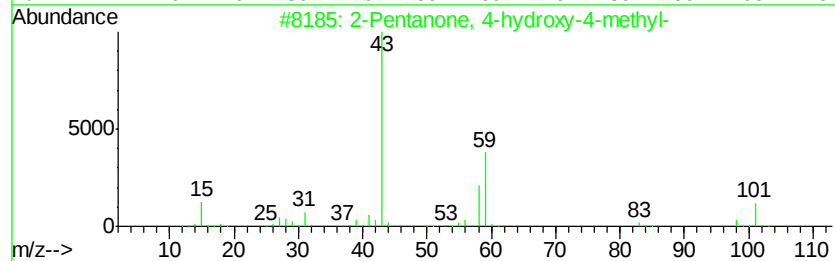
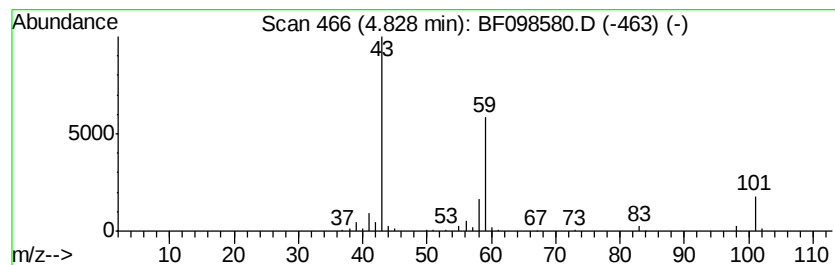
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	9.27 ng	386649	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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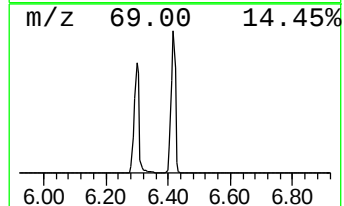
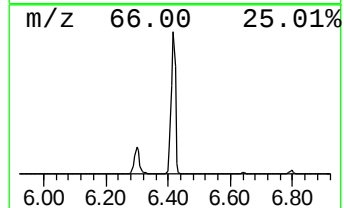
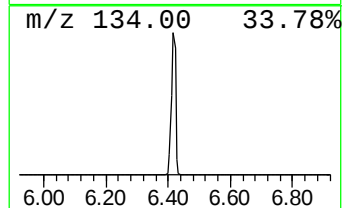
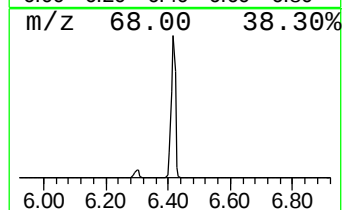
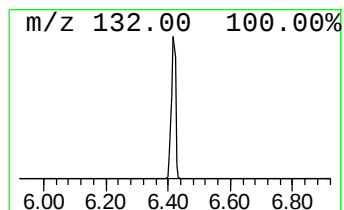
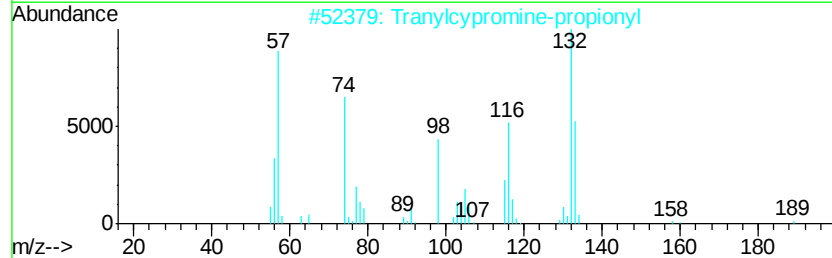
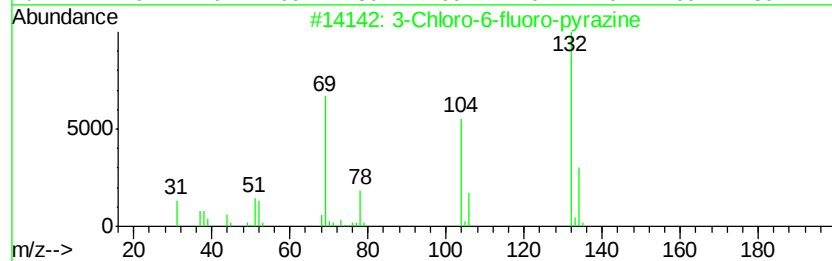
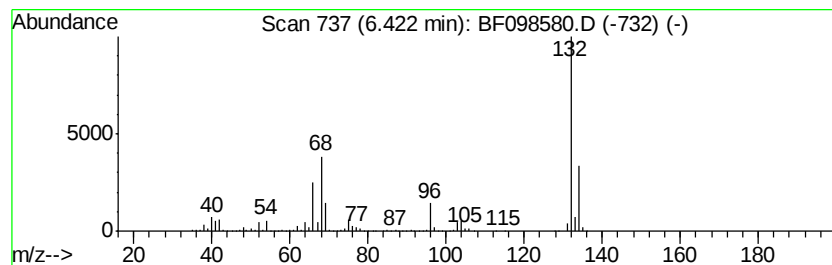
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	89.30 ng	3726370	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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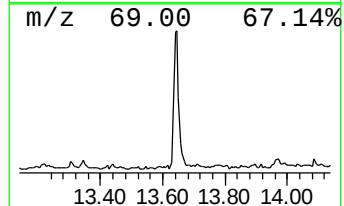
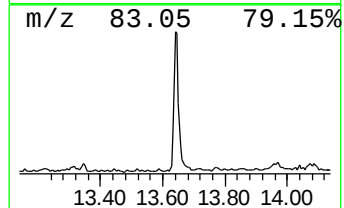
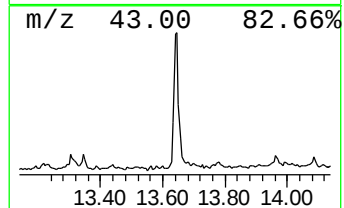
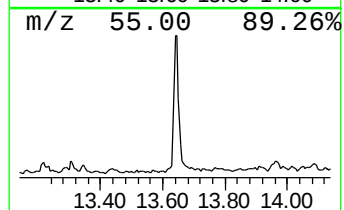
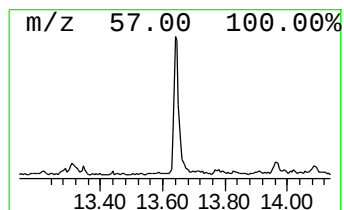
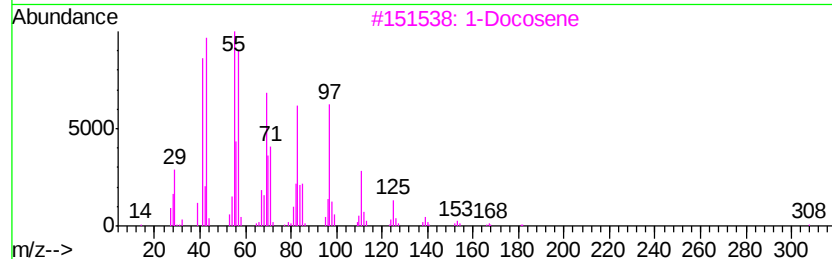
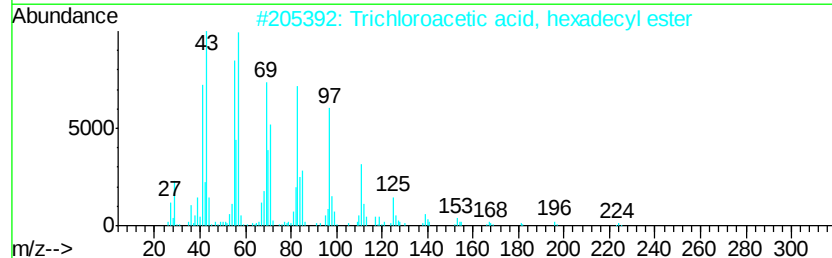
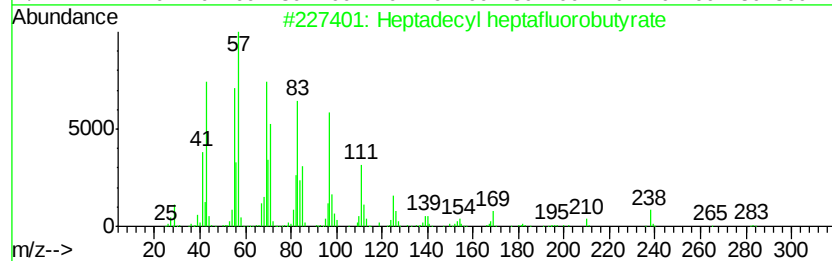
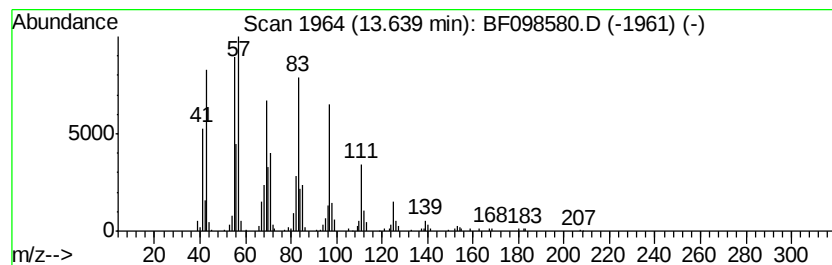
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	7.34 ng	404670	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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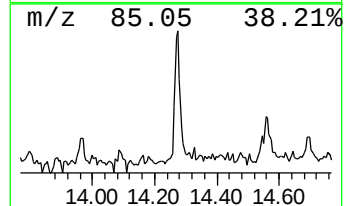
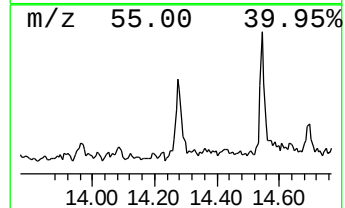
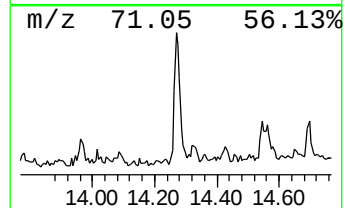
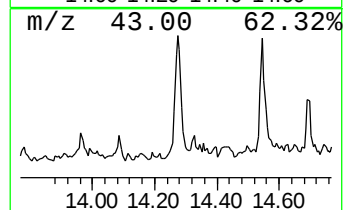
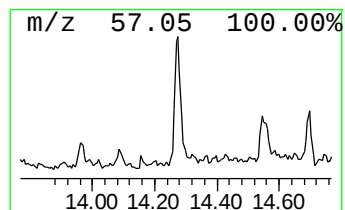
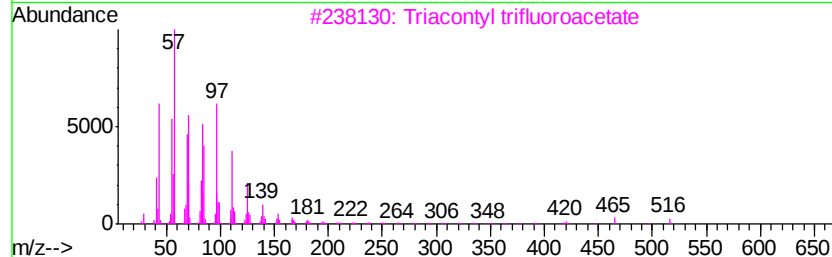
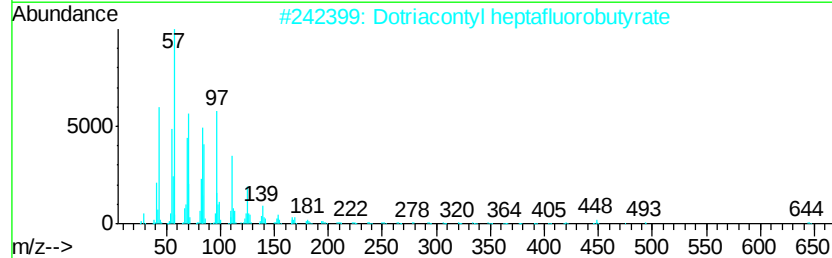
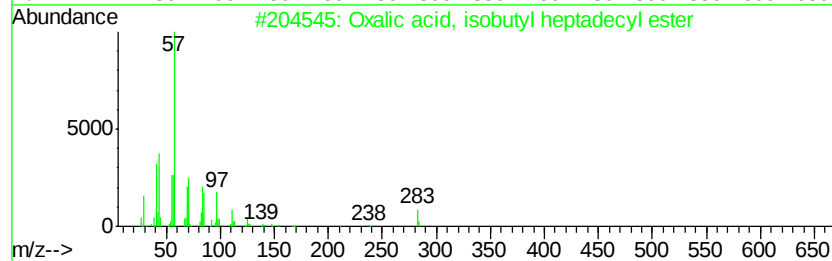
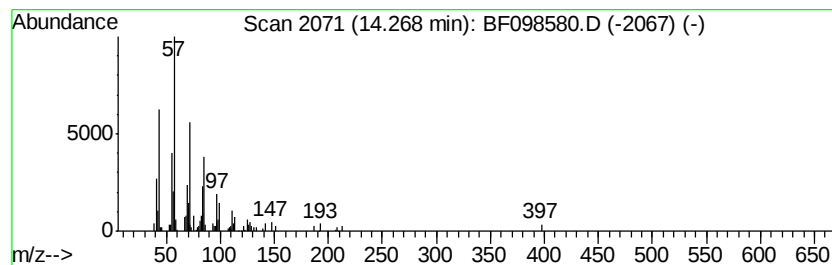
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oxalic acid, isobutyl hepta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	3.22 ng	177523	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
2		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
3		Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
4		Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91



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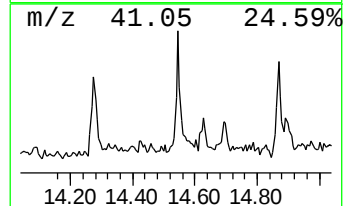
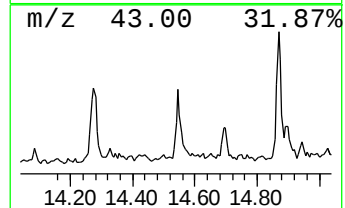
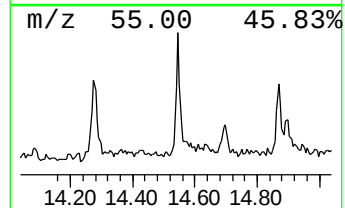
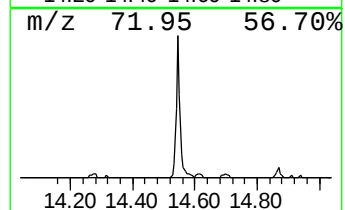
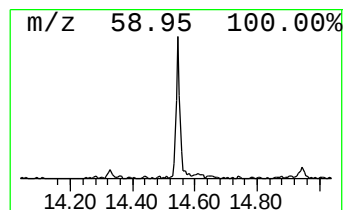
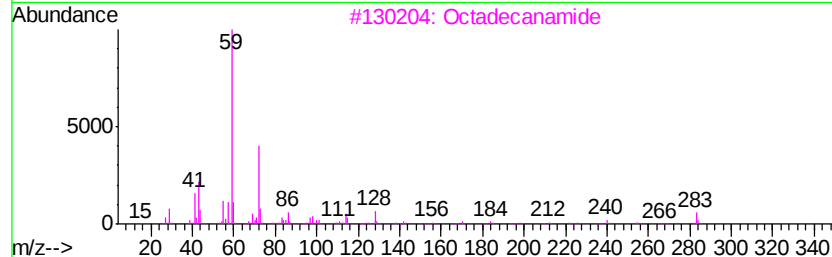
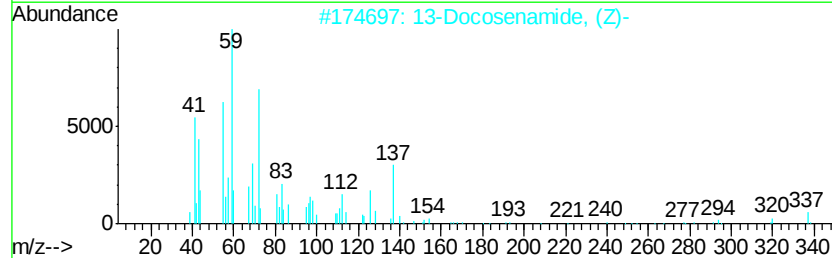
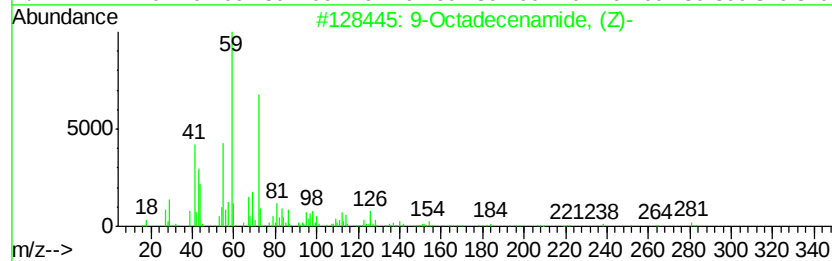
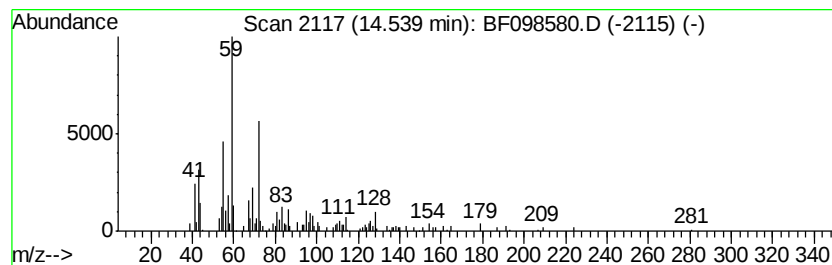
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	4.67 ng	192456	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
3		Octadecanamide	283	C18H37NO	000124-26-5	72
4		Tetradecanamide	227	C14H29NO	000638-58-4	59
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53



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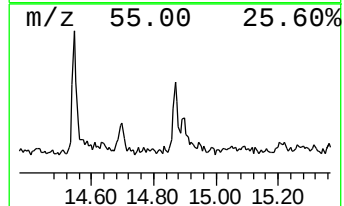
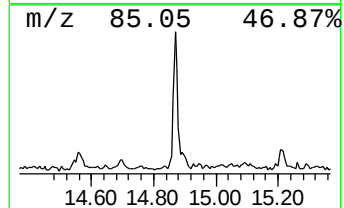
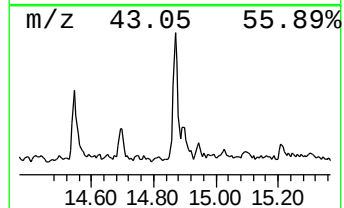
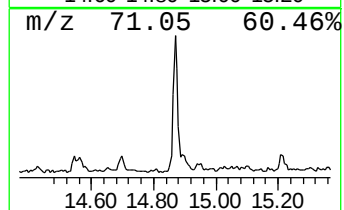
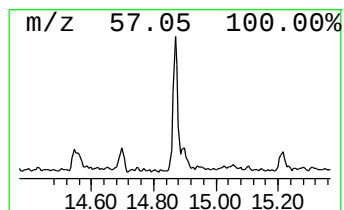
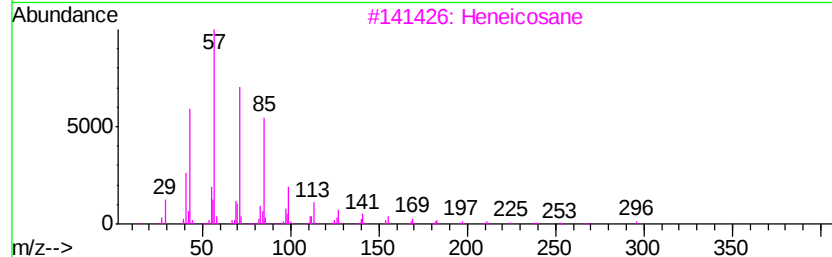
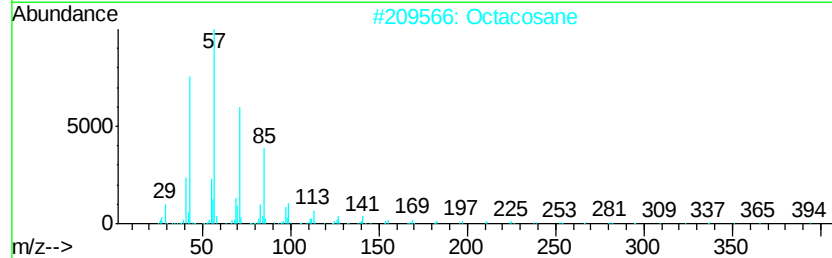
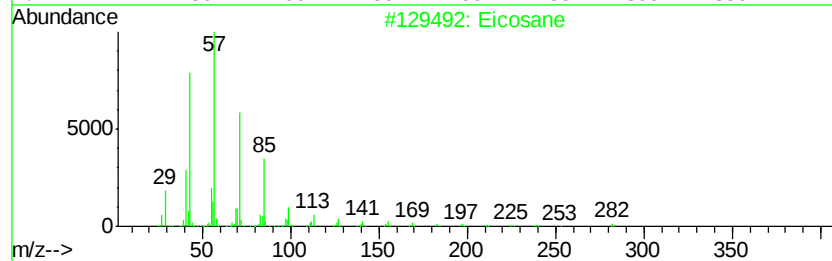
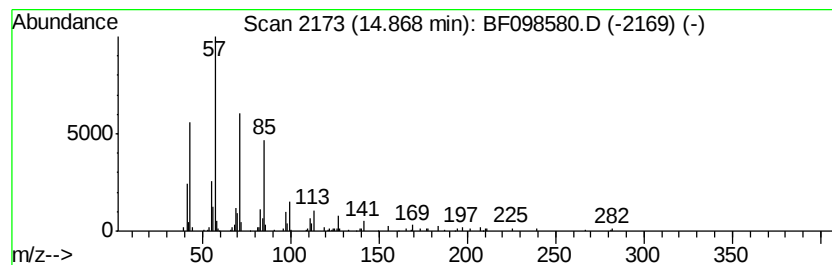
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.00 ng	164858	Perylene-d12	15.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Octacosane		394	C28H58	000630-02-4	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098580.D
Acq On : 15 Sep 2017 20:32
Operator : SJ/JU
Sample : I5229-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400S18

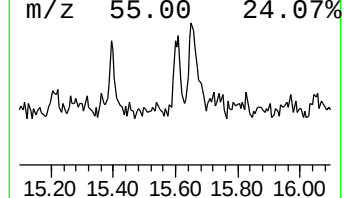
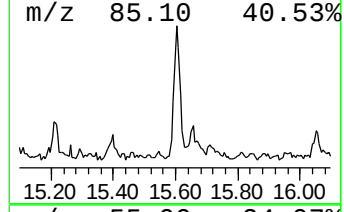
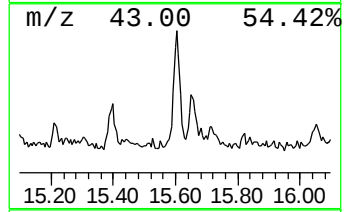
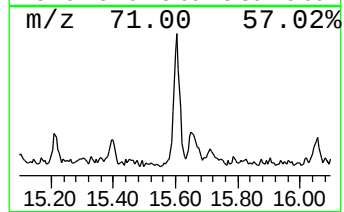
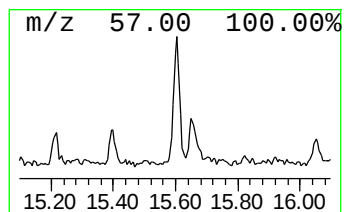
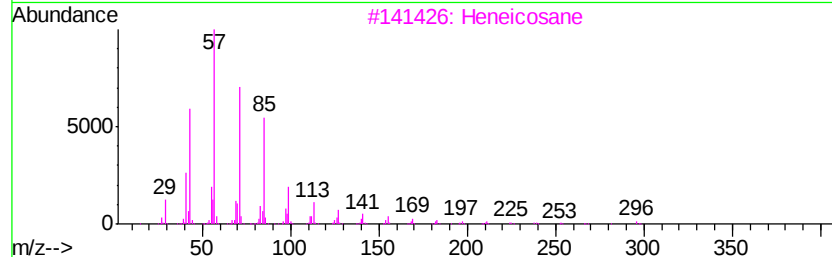
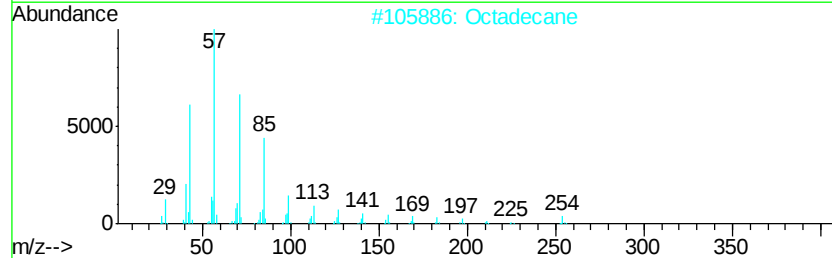
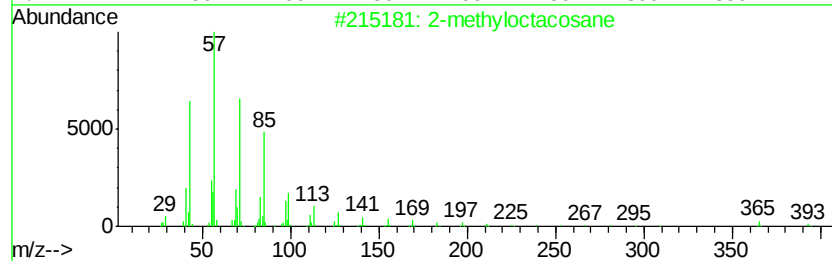
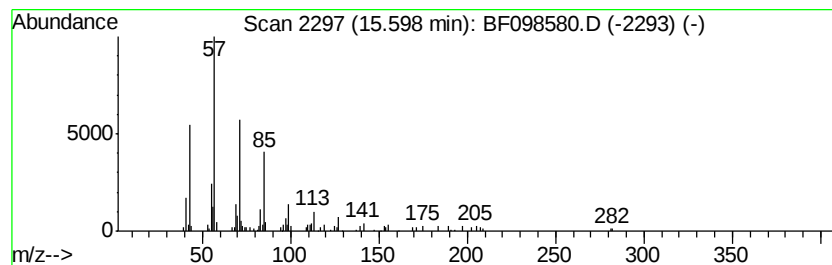
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.83 ng	116575	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Octadecane	254	C18H38	000593-45-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Operator : SJ/JU
Sample : I5229-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

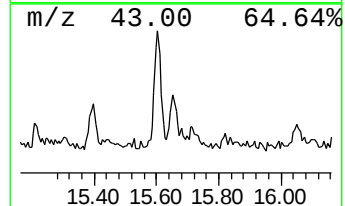
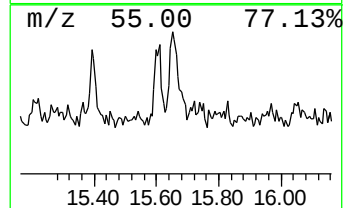
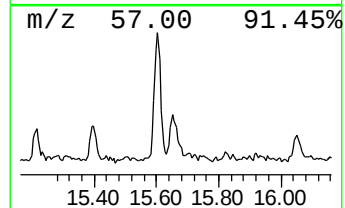
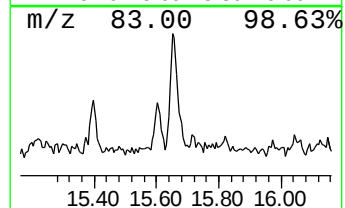
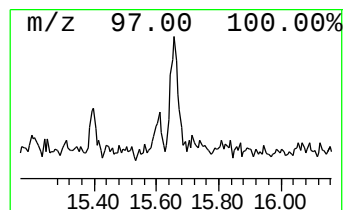
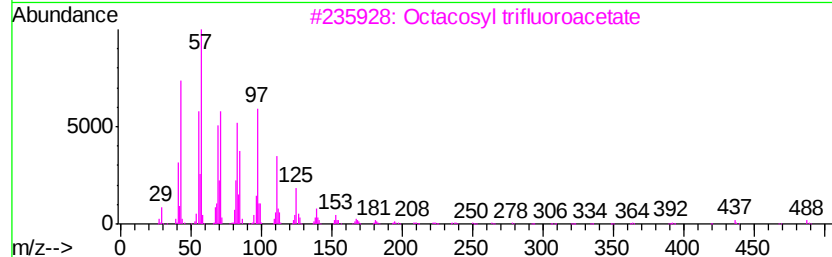
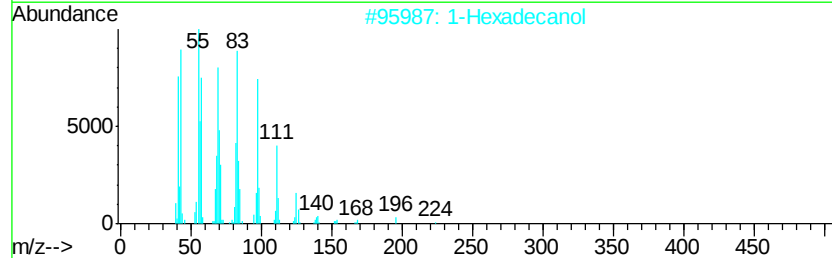
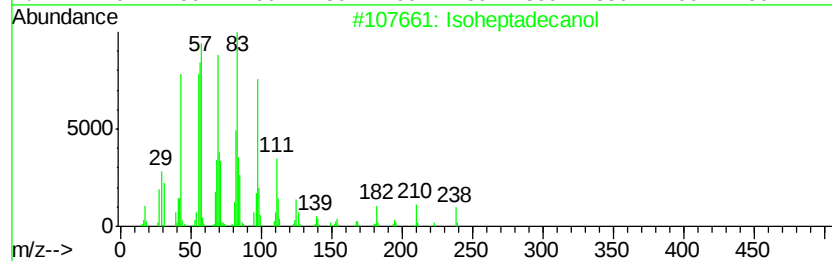
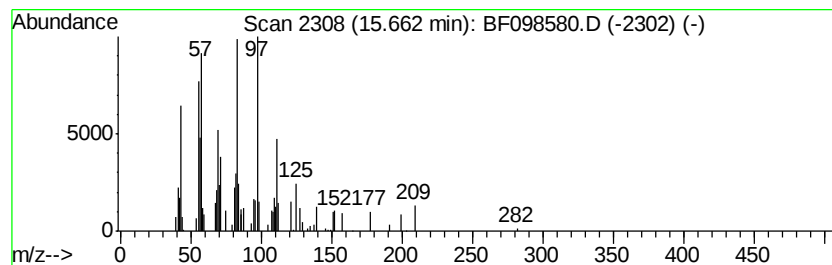
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Isoheptadecanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.18 ng	89919	Perylene-d12	15.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Isoheptadecanol	256 C17H36O	057289-07-3 83
2		1-Hexadecanol	242 C16H34O	036653-82-4 80
3		Octacosyl trifluoroacetate	506 C30H57F3O2	1000351-74-9 49
4		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	959218-78-1 49
5		Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0 49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098580.D
Acq On : 15 Sep 2017 20:32
Operator : SJ/JU
Sample : I5229-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400S18

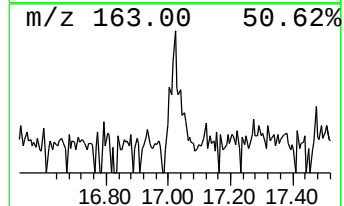
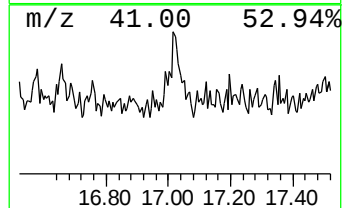
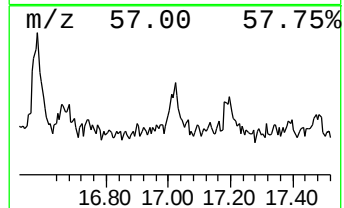
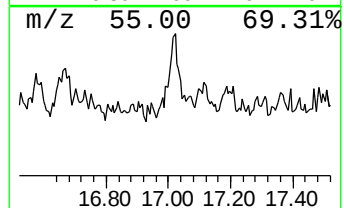
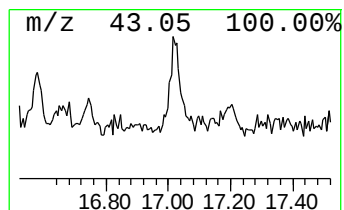
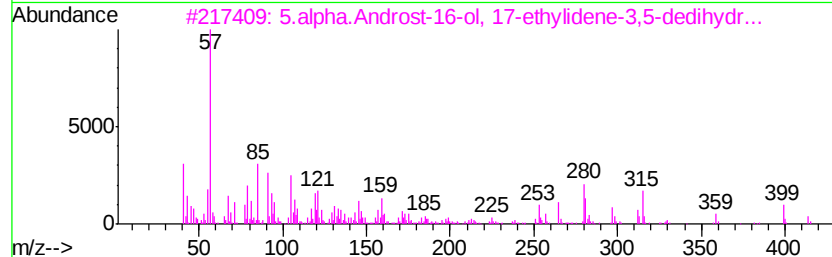
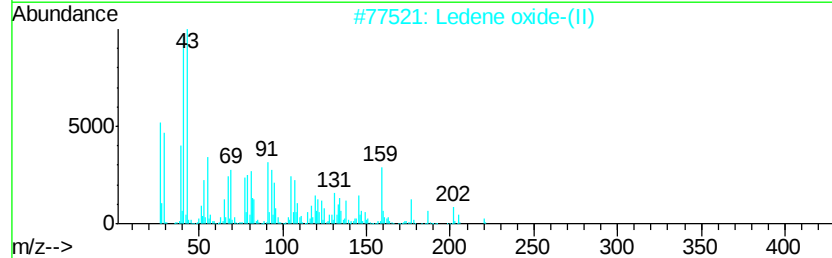
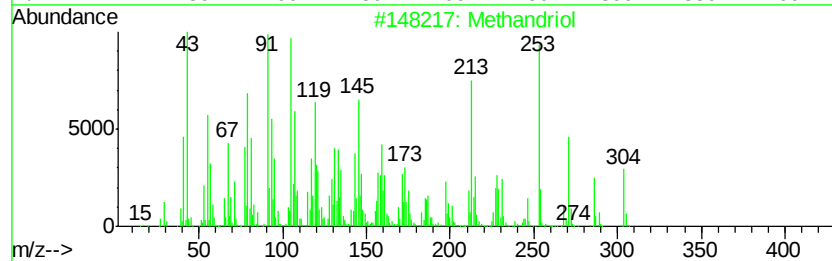
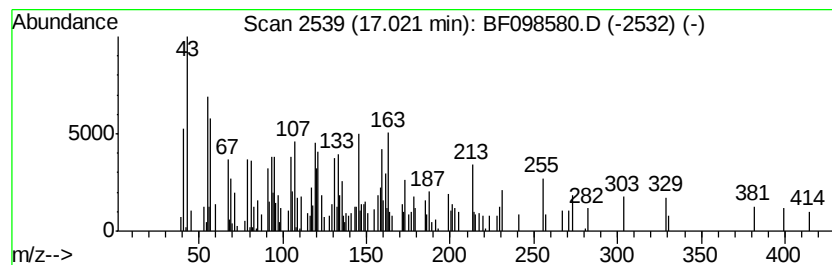
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	4.84 ng	199482	Perylene-d12	15.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methandriol	304	C20H32O2	000521-10-8	46
2			Ledene oxide-(II)	220	C15H24O	1000159-36-7	38
3			5.alpha.Androst-16-ol, 17-ethyliden...	414	C27H42O3	1000124-58-6	27
4			Ethanethiol, 2-(triethoxysilyl)-	224	C8H20O3SSi	018236-15-2	25
5			1,3,3-Trimethyl-2-(2-methyl-cycl...	178	C13H22	285129-06-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098580.D
Acq On : 15 Sep 2017 20:32
Operator : SJ/JU
Sample : I5229-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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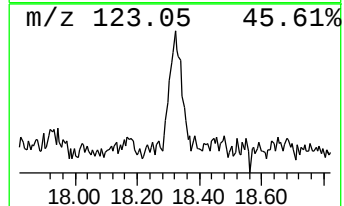
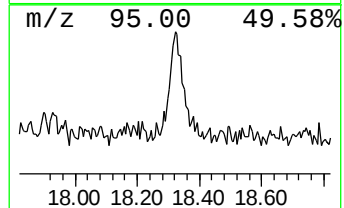
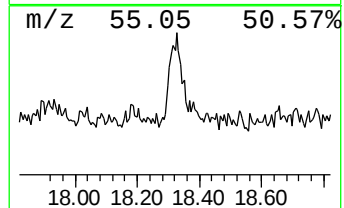
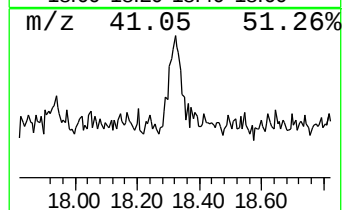
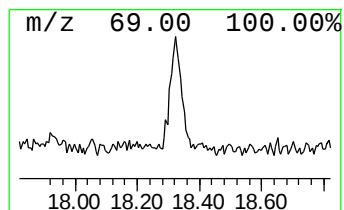
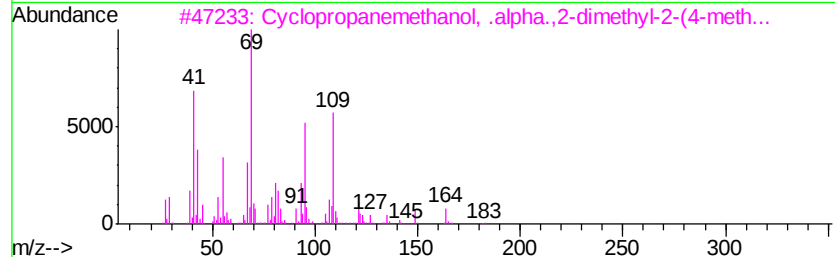
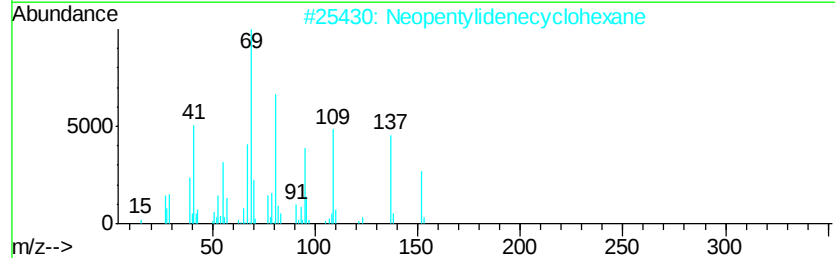
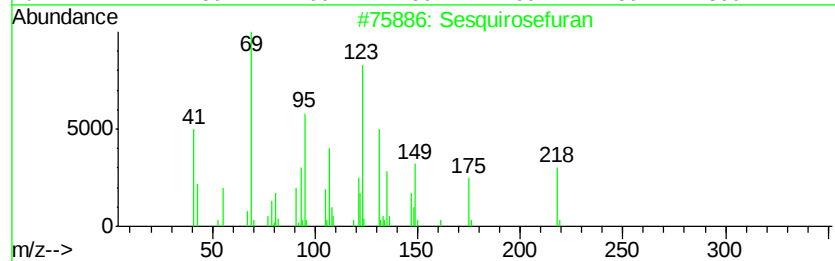
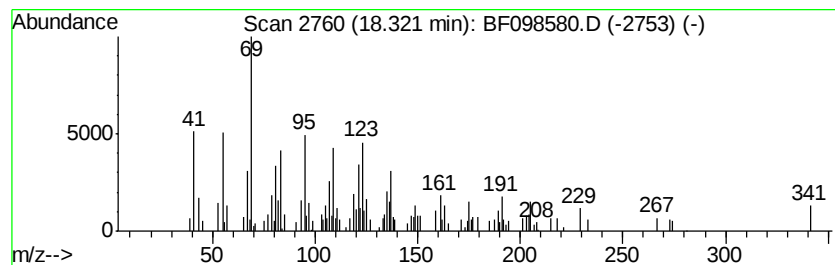
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	5.15 ng	212138	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sesquirosefuran	218	C15H22O	039007-93-7	43
2		Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
3		Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	43
4		1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	43
5		2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098580.D
 Acq On : 15 Sep 2017 20:32
 Operator : SJ/JU
 Sample : I5229-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.83	9.3	ng	386649	1	6.64	834579	20.0
unknown6.42	6.42	89.3	ng	3726370	1	6.64	834579	20.0
Heptadecyl heptaf...	13.64	7.3	ng	404670	5	13.80	1102920	20.0
Oxalic acid, isob...	14.27	3.2	ng	177523	5	13.80	1102920	20.0
9-Octadecenamide,...	14.54	4.7	ng	192456	6	15.20	823512	20.0
Eicosane	14.87	4.0	ng	164858	6	15.20	823512	20.0
2-methyloctacosane	15.60	2.8	ng	116575	6	15.20	823512	20.0
Isoheptadecanol	15.66	2.2	ng	89919	6	15.20	823512	20.0
unknown17.02	17.02	4.8	ng	199482	6	15.20	823512	20.0
unknown18.32	18.32	5.2	ng	212138	6	15.20	823512	20.0