

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
 Data File : BF088562.D
 Acq On : 1 Jul 2016 7:07
 Operator : UM/SJ
 Sample : H3701-02
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-COMP-B2A

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-BF063016.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	1.678	4	8	11	rVB	4846468	8774527	100.00%	18.802%
2	1.747	11	14	23	rVV	295578	750199	8.55%	1.608%
3	1.873	23	25	41	rVB	2501756	4446666	50.68%	9.528%
4	5.004	296	299	303	rBV	186861	263219	3.00%	0.564%
5	5.416	332	335	337	rBV	2742608	3058274	34.85%	6.553%
6	6.456	423	426	428	rVB	3069534	3679604	41.94%	7.885%
7	6.582	434	437	440	rBV	2480078	3517527	40.09%	7.537%
8	6.822	455	458	460	rBV	905130	959002	10.93%	2.055%
9	6.970	469	471	474	rVB	1901566	2737122	31.19%	5.865%
10	7.382	504	507	509	rBV	2187034	2187275	24.93%	4.687%
11	7.484	512	516	518	rVB	72529	113649	1.30%	0.244%
12	7.850	547	548	551	rVB	245881	203488	2.32%	0.436%
13	8.102	568	570	572	rBV	1528124	1270955	14.48%	2.723%
14	9.176	661	664	667	rBV	2644700	3665939	41.78%	7.855%
15	9.576	696	699	701	rVB	747542	782500	8.92%	1.677%
16	9.850	721	723	725	rBV	1343077	1222478	13.93%	2.620%
17	10.639	789	792	794	rBV	1785397	1812303	20.65%	3.883%
18	10.765	801	803	808	rBV	140250	168021	1.91%	0.360%
19	11.211	840	842	844	rBV	101749	95031	1.08%	0.204%
20	11.336	851	853	856	rVV	725751	1118165	12.74%	2.396%
21	11.576	870	874	877	rBV	93370	155233	1.77%	0.333%
22	11.874	897	900	901	rBV	126212	178392	2.03%	0.382%
23	12.536	956	958	960	rBV	248289	215284	2.45%	0.461%
24	12.651	966	968	970	rBV	91023	93695	1.07%	0.201%
25	12.765	974	978	980	rVV2	164687	246030	2.80%	0.527%
26	12.914	989	991	993	rBV	2262717	2225194	25.36%	4.768%
27	13.462	1037	1039	1041	rBV	97510	99176	1.13%	0.213%
28	13.828	1069	1071	1076	rVB	211795	241711	2.75%	0.518%
29	13.954	1079	1082	1088	rVV	928255	1131195	12.89%	2.424%
30	14.720	1147	1149	1150	rBV	205593	205533	2.34%	0.440%
31	14.960	1168	1170	1175	rVB	95845	206464	2.35%	0.442%
32	15.302	1198	1200	1202	rBV	70087	94161	1.07%	0.202%
33	15.360	1202	1205	1207	rBV	567771	749527	8.54%	1.606%

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ClientSampleId :
TEC-COMP-B2A

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

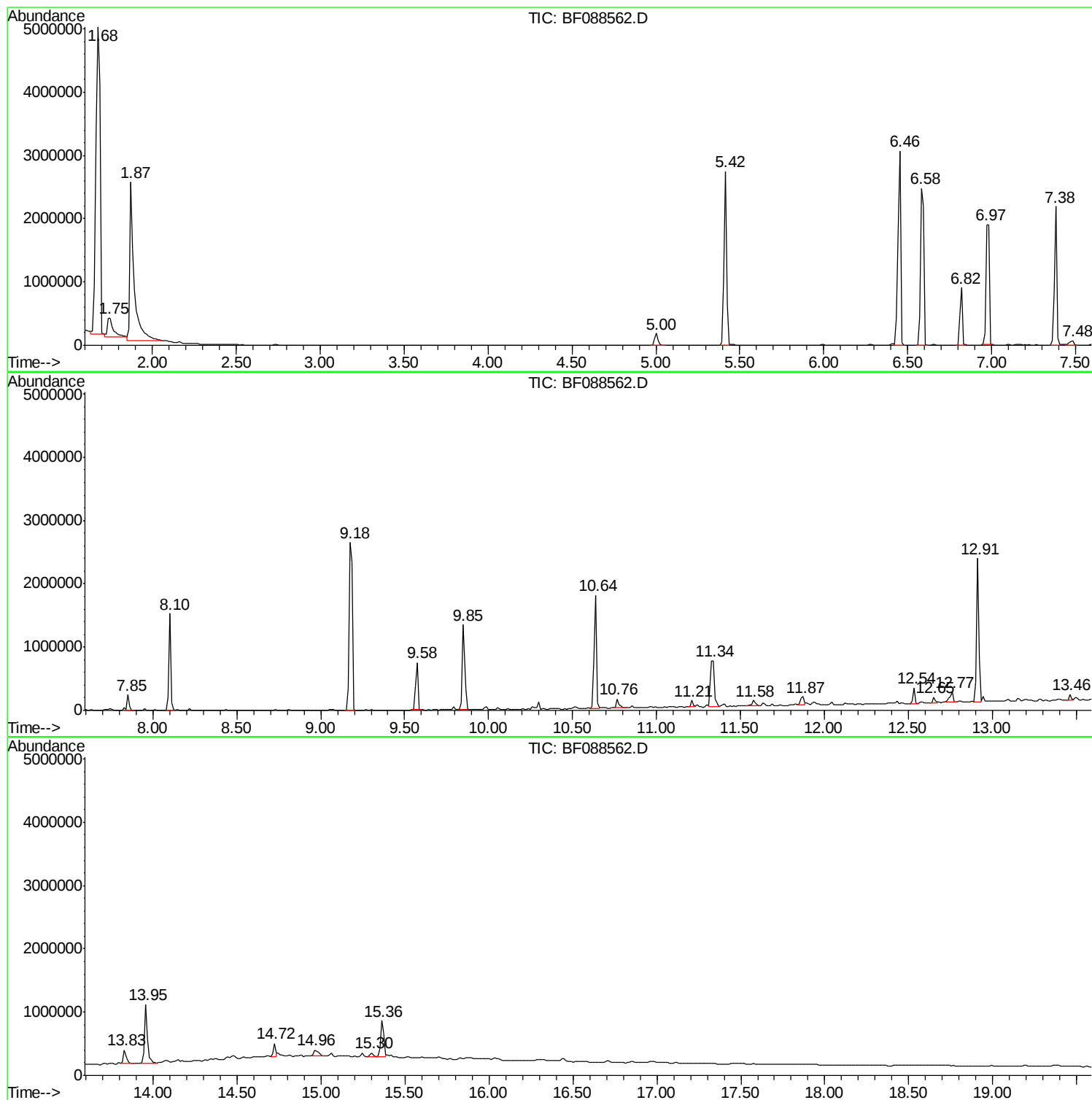
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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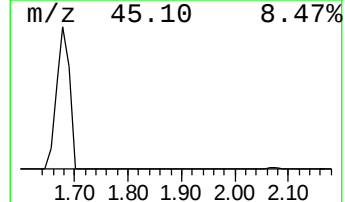
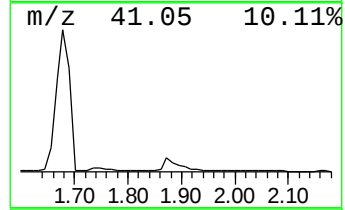
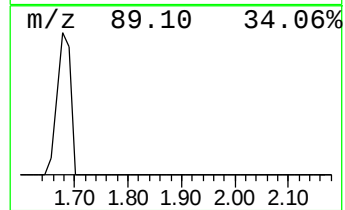
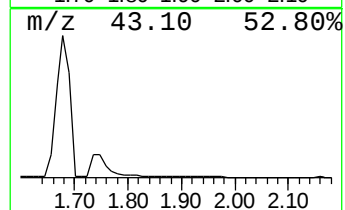
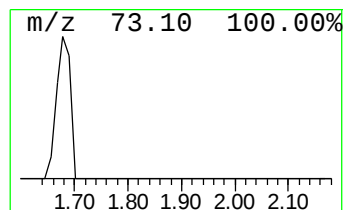
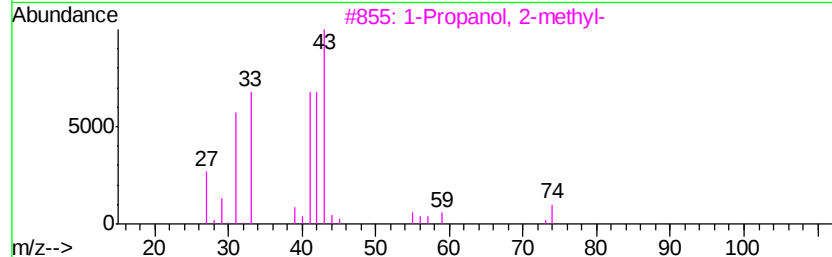
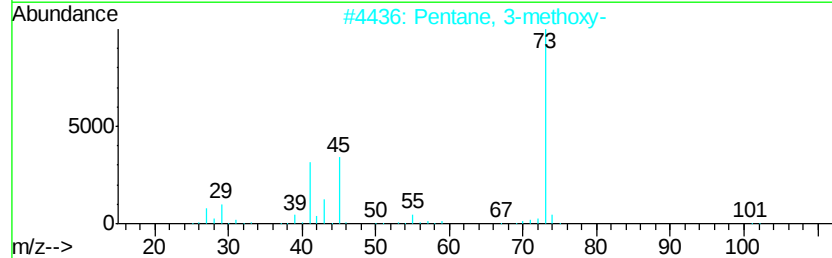
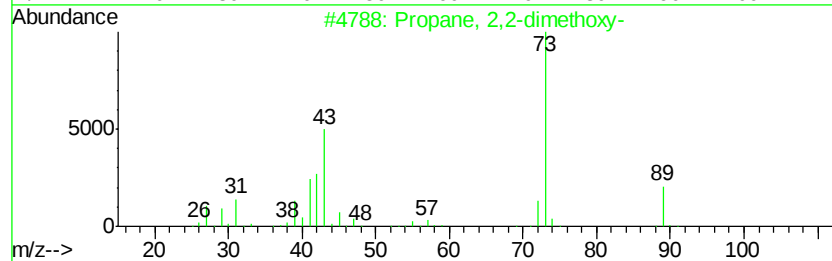
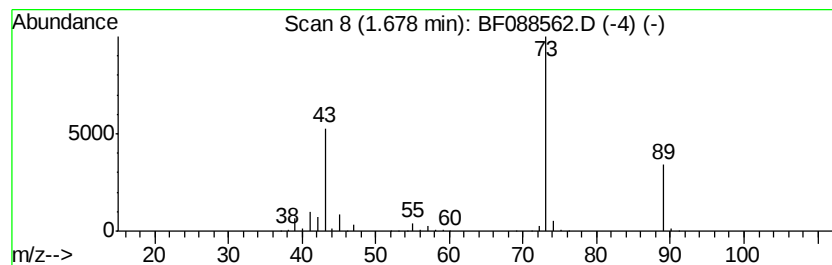
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	182.99 ng	8774530	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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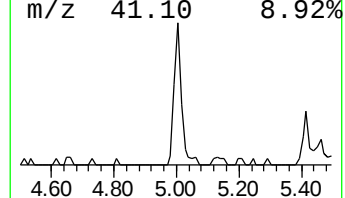
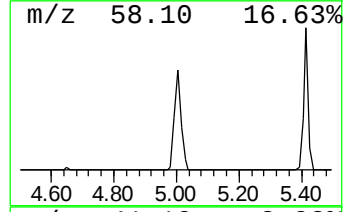
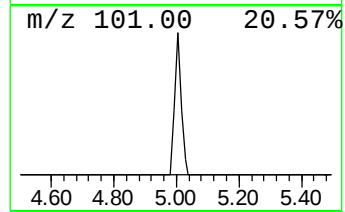
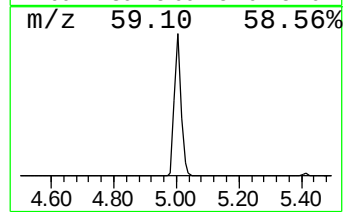
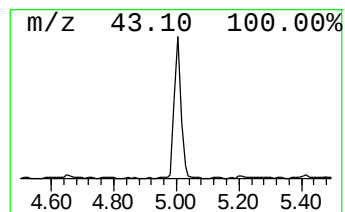
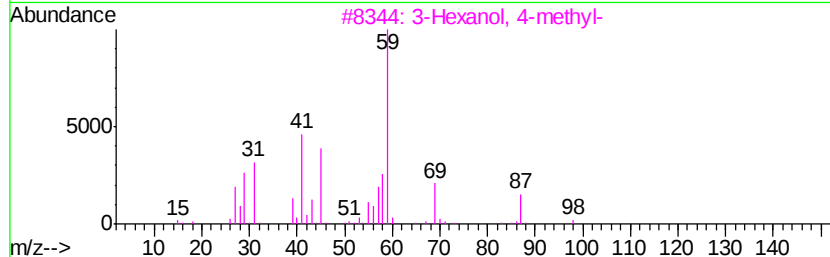
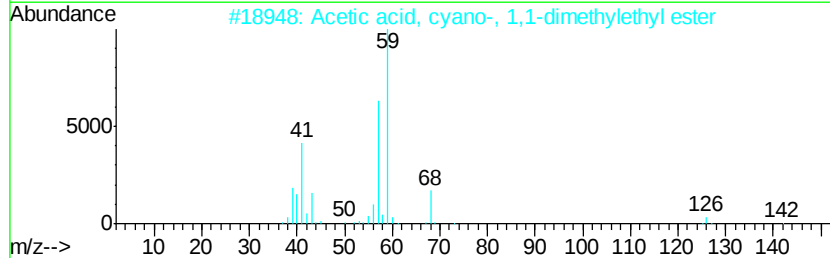
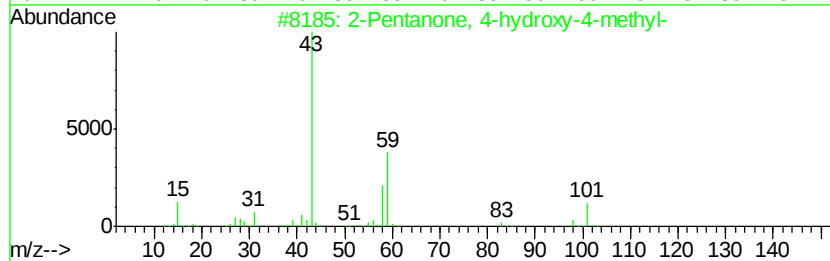
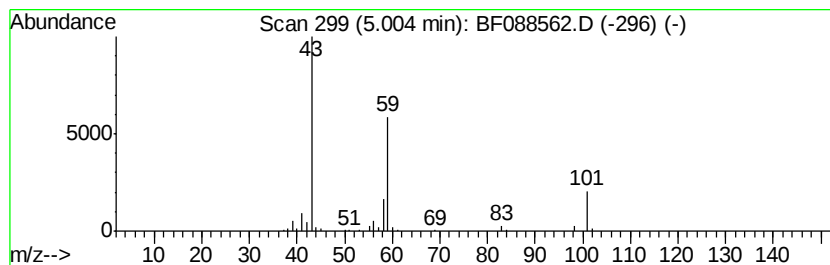
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.49 ng	263219	1,4-Dichlorobenzene-d4	6.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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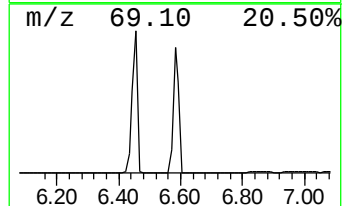
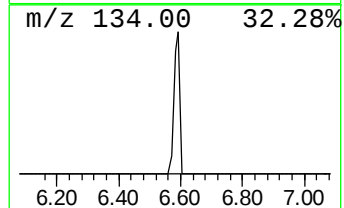
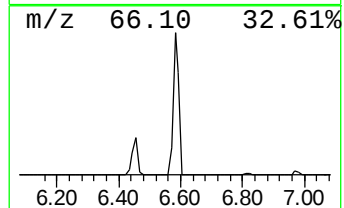
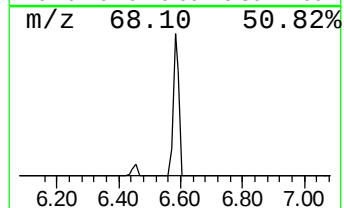
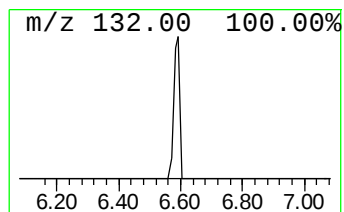
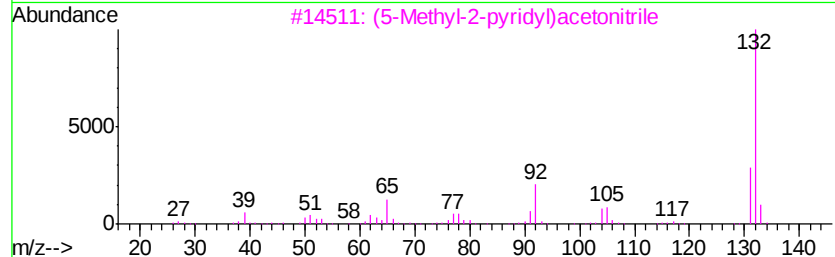
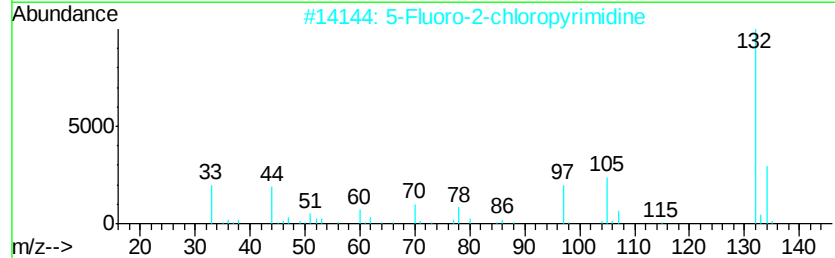
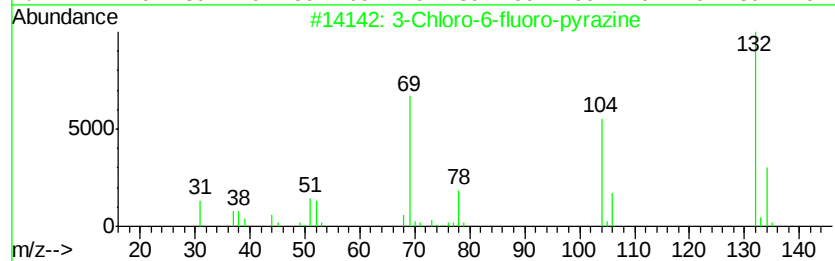
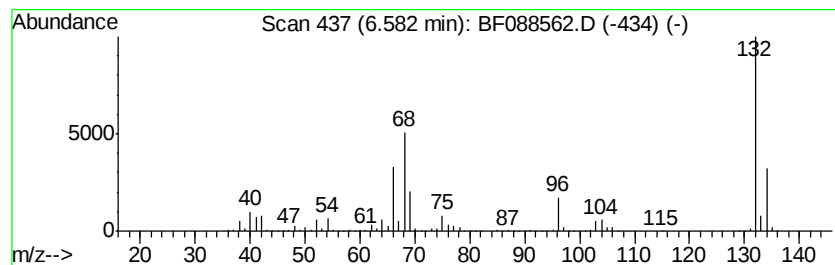
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	73.36 ng	3517530	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10	
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10	
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10	



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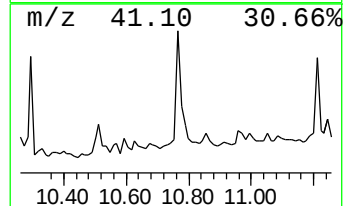
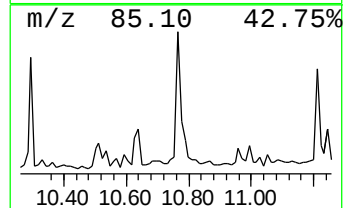
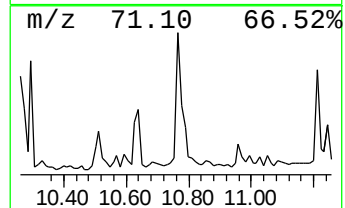
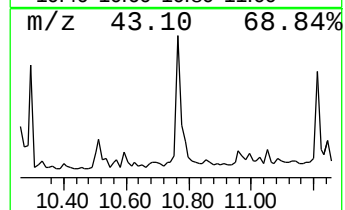
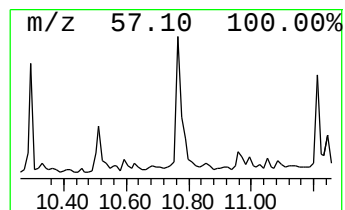
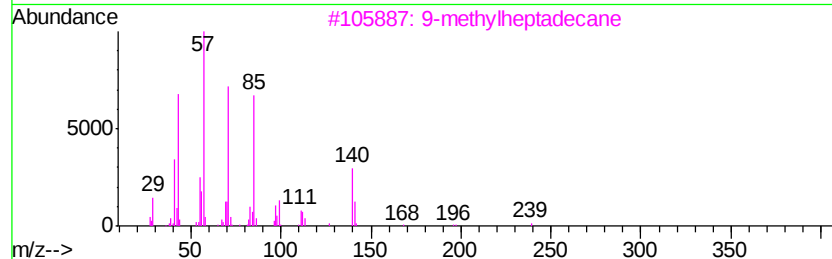
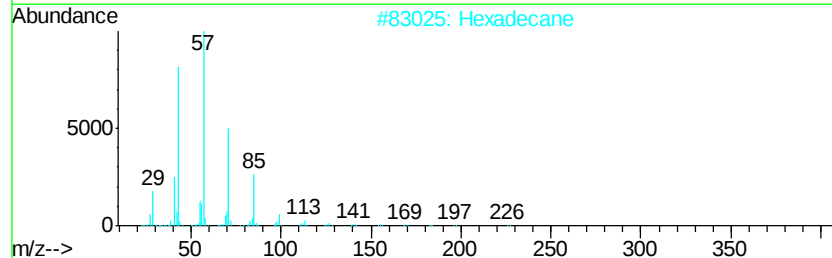
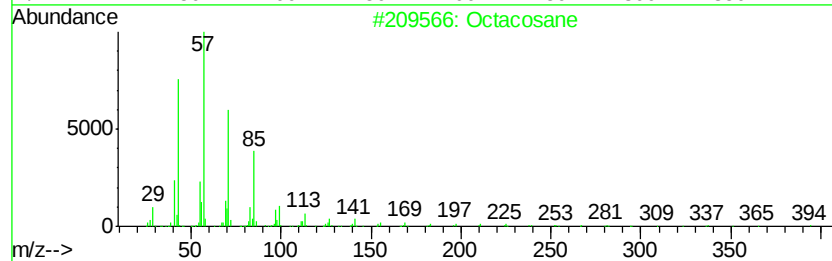
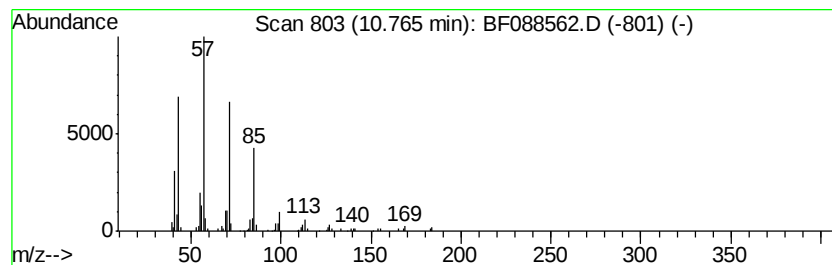
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	3.01 ng	168021	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		9-methylheptadecane	254	C18H38	026741-18-4	90
4		Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
5		Heptadecane	240	C17H36	000629-78-7	90



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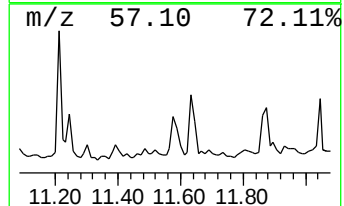
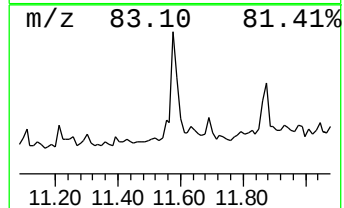
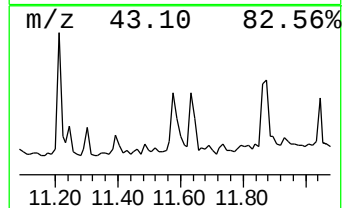
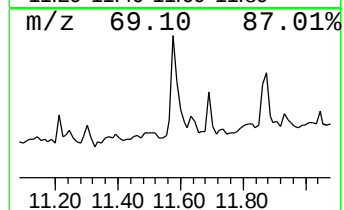
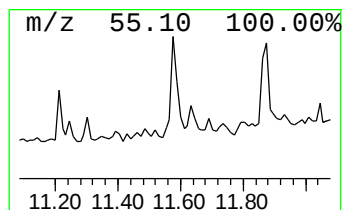
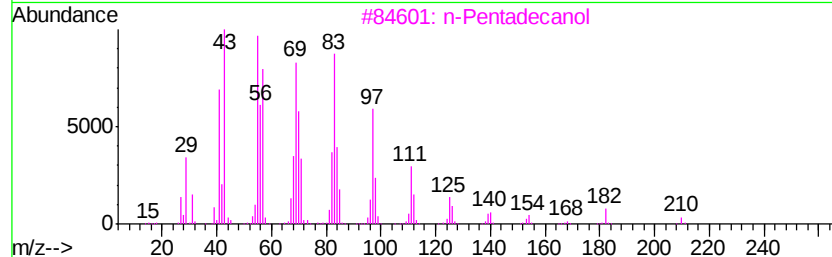
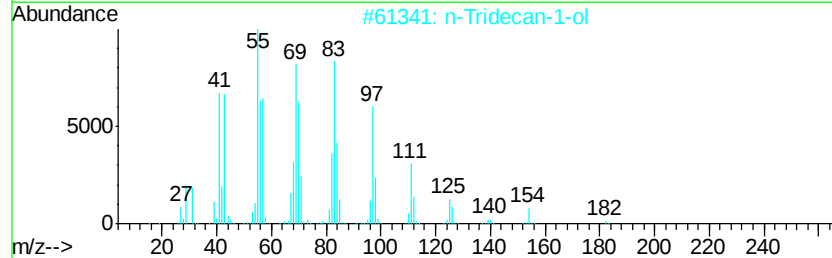
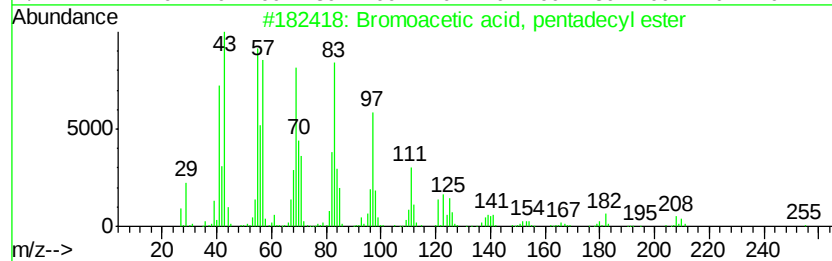
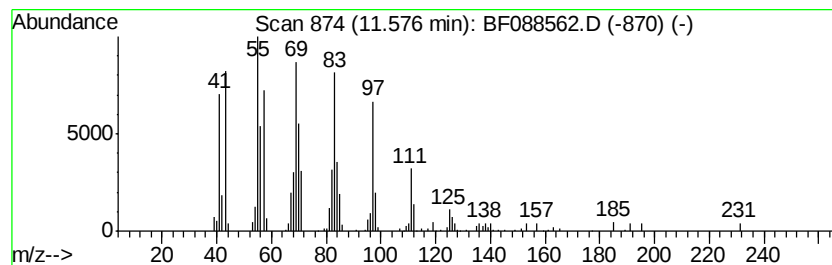
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Bromoacetic acid, pentadecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	2.78 ng	155233	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
2		n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
3		n-Pentadecanol	228	C15H32O	000629-76-5	91
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5		3-Hexadecene, (Z)-	224	C16H32	034303-81-6	91



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TEC-COMP-B2A

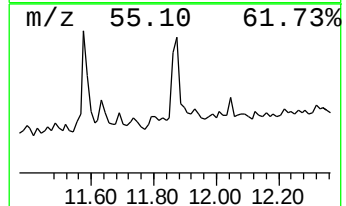
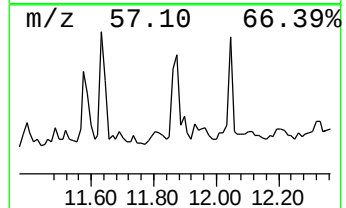
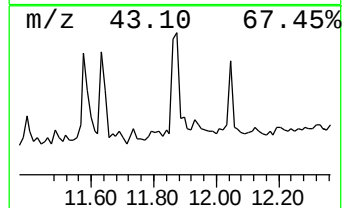
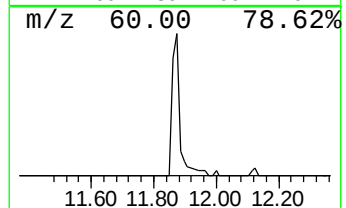
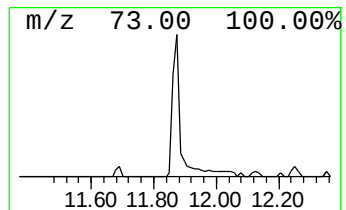
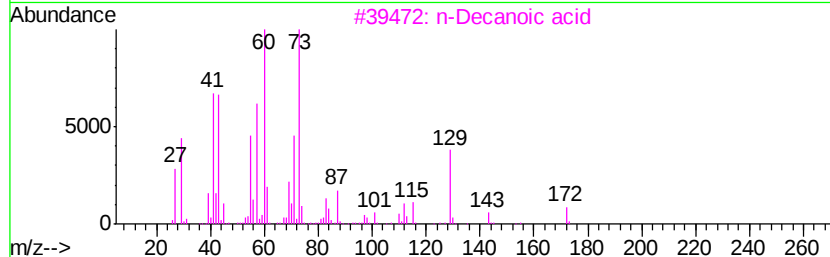
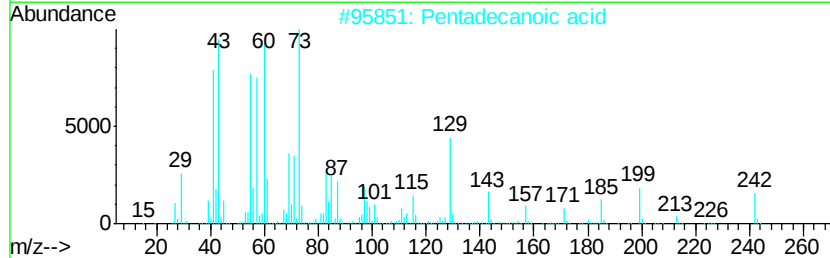
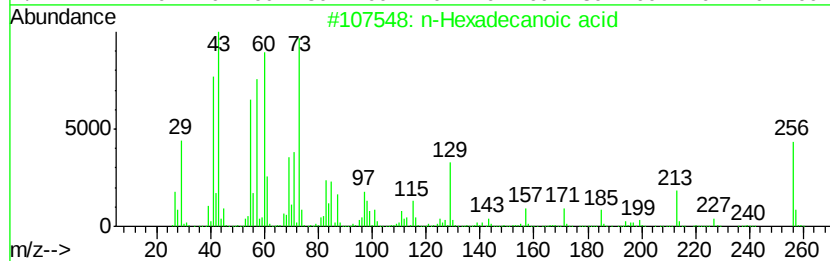
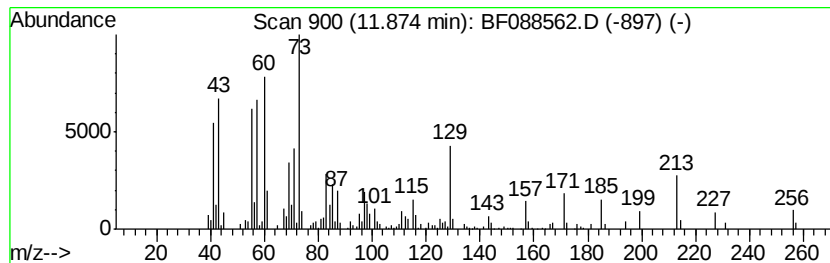
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.19 ng	178392	Phenanthrene-d10	11.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Decanoic acid	172	C10H20O2	000334-48-5	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
Data File : BF088562.D
Acq On : 1 Jul 2016 7:07
Operator : UM/SJ
Sample : H3701-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP-B2A

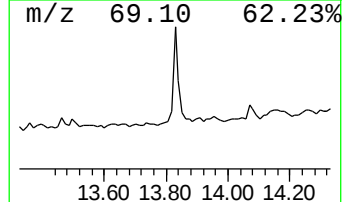
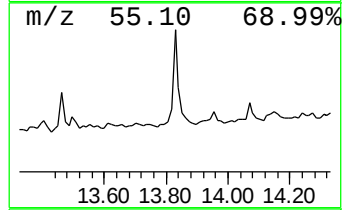
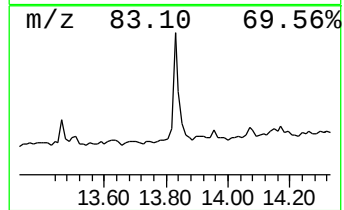
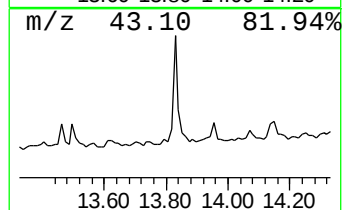
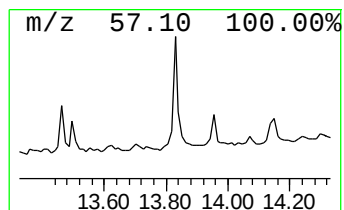
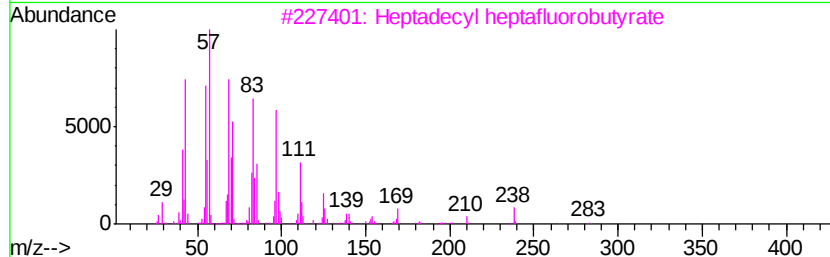
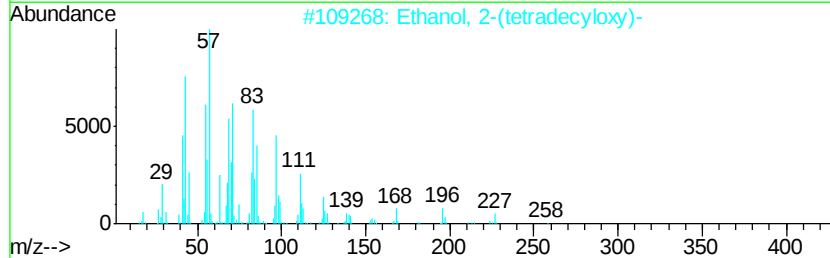
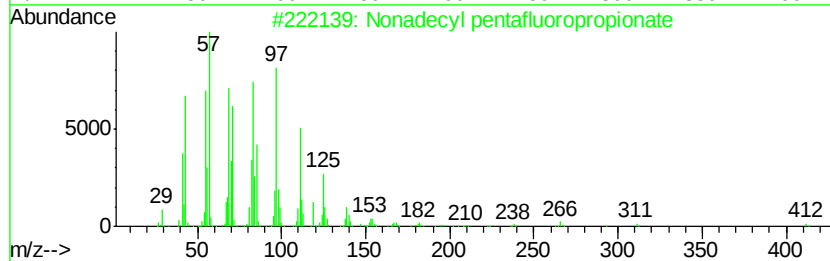
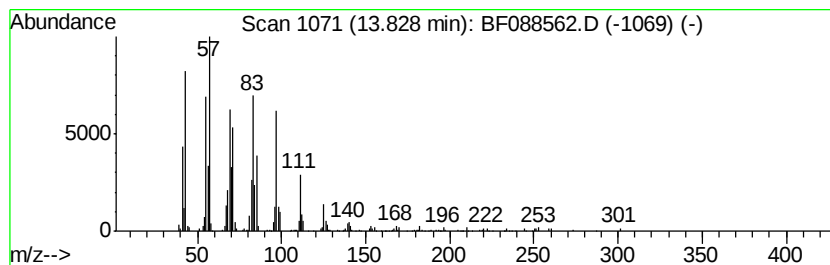
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecyl pentafluoropropio... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.27 ng	241711	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	87
4		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	81
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF063016\
Data File : BF088562.D
Acq On : 1 Jul 2016 7:07
Operator : UM/SJ
Sample : H3701-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP-B2A

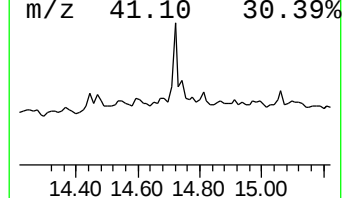
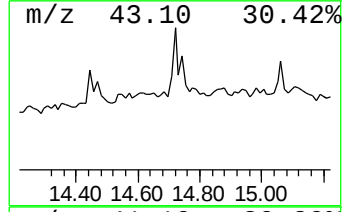
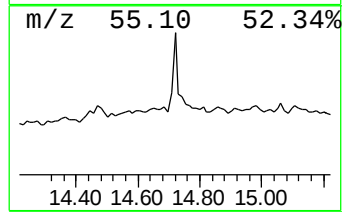
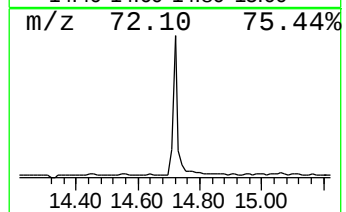
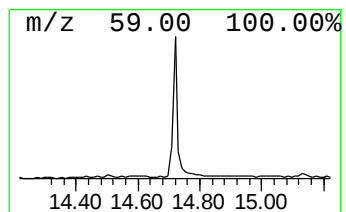
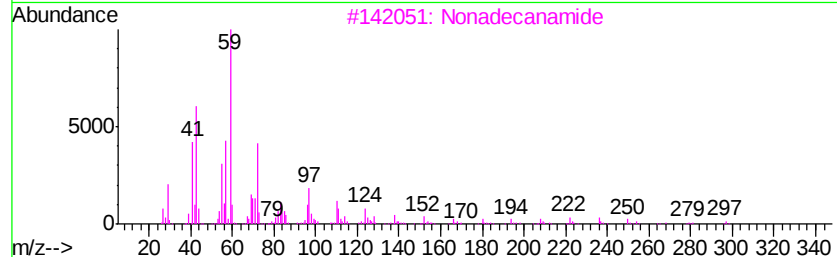
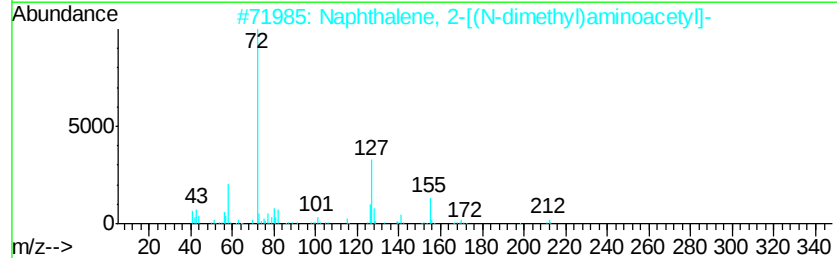
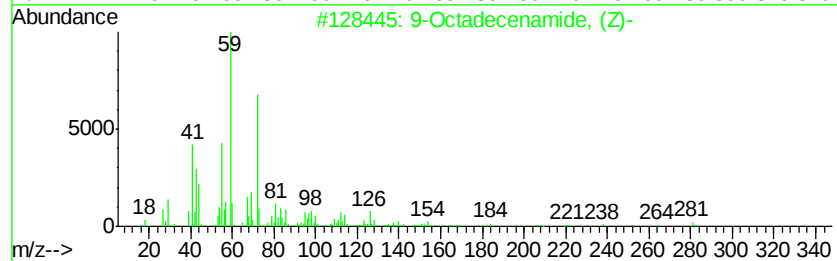
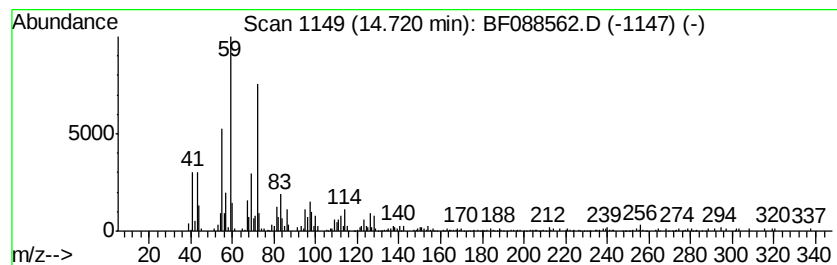
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	5.48 ng	205533	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2			Naphthalene, 2-[(N-dimethyl)amin...	213	C14H15NO	1000128-37-5	38
3			Nonadecanamide	297	C19H39NO	058185-32-3	38
4			6-Chlorohexanoic acid, 2-ethoxye...	222	C10H19ClO3	1000331-04-6	35
5			Octadecanamide	283	C18H37NO	000124-26-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
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Acq On : 1 Jul 2016 7:07
Operator : UM/SJ
Sample : H3701-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP-B2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 2,2-dime...	1.68	183.0	ng	8774530	1	6.82	959002	20.0
2-Pentanone, 4-hy...	5.00	5.5	ng	263219	1	6.82	959002	20.0
unknown6.58	6.58	73.4	ng	3517530	1	6.82	959002	20.0
Octacosane	10.76	3.0	ng	168021	4	11.34	1118170	20.0
Bromoacetic acid,...	11.58	2.8	ng	155233	4	11.34	1118170	20.0
n-Hexadecanoic acid	11.87	3.2	ng	178392	4	11.34	1118170	20.0
Nonadecyl pentafl...	13.83	4.3	ng	241711	5	13.95	1131200	20.0
9-Octadecenamide,...	14.72	5.5	ng	205533	6	15.36	749527	20.0