

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011017\
 Data File : BF092192.D
 Acq On : 10 Jan 2017 19:54
 Operator : UM/SJ
 Sample : I1078-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROLL-OFF-0-2-COMP

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-BF122116.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	4.767	249	252	263	rVB	1518659	2303025	33.58%	3.710%
2	5.236	290	293	307	rBV	4277040	4750448	69.27%	7.652%
3	6.299	383	386	389	rBV	4248841	5535310	80.72%	8.916%
4	6.402	393	395	398	rVV	4684889	5035783	73.43%	8.111%
5	6.630	412	415	417	rBV	1412387	1541757	22.48%	2.483%
6	6.779	426	428	431	rBV	3590719	4573665	66.69%	7.367%
7	7.202	461	465	467	rBV	3819017	4305465	62.78%	6.935%
8	7.910	525	527	530	rBV	1752104	2114334	30.83%	3.406%
9	8.996	619	622	625	rBV	5843712	6533179	95.27%	10.523%
10	9.396	654	657	659	rBV	624121	574881	8.38%	0.926%
11	9.613	672	676	678	rBV	169285	198583	2.90%	0.320%
12	9.671	678	681	683	rVB	2485735	2551507	37.21%	4.110%
13	9.842	693	696	698	rBV2	33626	72622	1.06%	0.117%
14	10.116	712	720	721	rBV	289459	376384	5.49%	0.606%
15	10.334	736	739	742	rBV	173828	230840	3.37%	0.372%
16	10.459	747	750	753	rBV2	3155684	4179199	60.94%	6.731%
17	10.585	758	761	765	rVV2	492399	704018	10.27%	1.134%
18	10.779	776	778	780	rBV2	50446	79048	1.15%	0.127%
19	11.031	798	800	801	rBV	388248	340956	4.97%	0.549%
20	11.065	801	803	806	rVB	133840	167730	2.45%	0.270%
21	11.145	808	810	813	rVV	2234351	2413561	35.20%	3.888%
22	11.454	835	837	840	rBV	169032	197091	2.87%	0.317%
23	11.705	856	859	862	rBV	606415	883148	12.88%	1.422%
24	11.865	869	873	875	rBV2	126661	159895	2.33%	0.258%
25	12.254	905	907	909	rVB	90380	87689	1.28%	0.141%
26	12.482	924	927	933	rBV	261901	327131	4.77%	0.527%
27	12.619	938	939	943	rVB	43089	72616	1.06%	0.117%
28	12.745	946	950	952	rBV	5373054	6857592	100.00%	11.046%
29	12.974	967	970	972	rBV2	44935	96845	1.41%	0.156%
30	13.637	1026	1028	1032	rBV	439553	684391	9.98%	1.102%
31	13.785	1038	1041	1043	rBV	2094397	2248765	32.79%	3.622%
32	14.277	1082	1084	1087	rBV	111315	190582	2.78%	0.307%
33	15.157	1158	1161	1163	rBV	1219528	1448552	21.12%	2.333%
34	17.729	1385	1386	1389	rBV2	94992	247886	3.61%	0.399%

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ALS Vial : 20 Sample Multiplier: 1

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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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

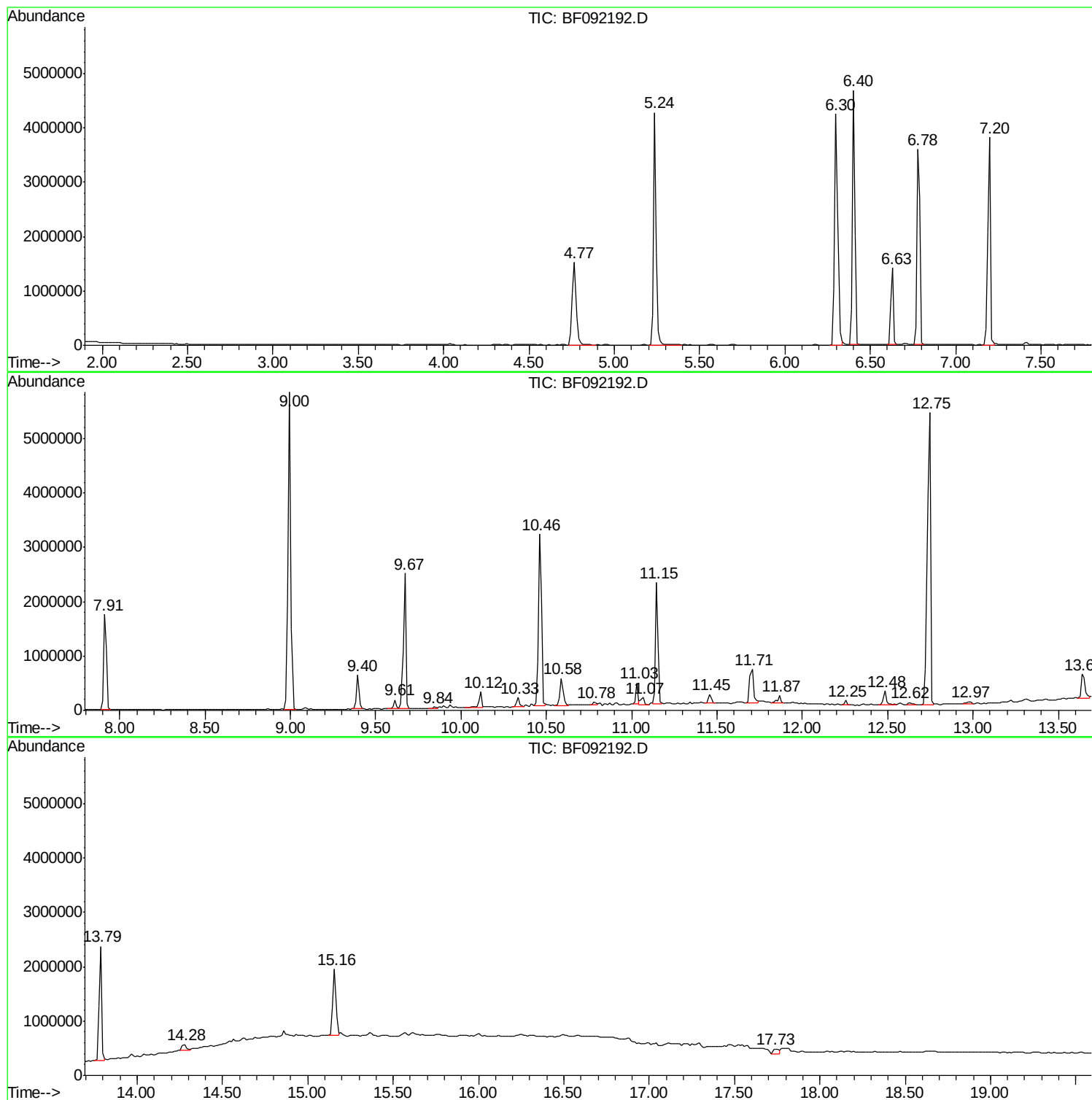
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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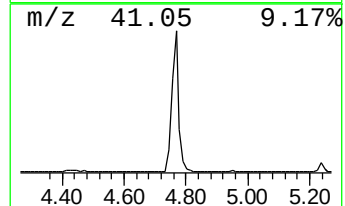
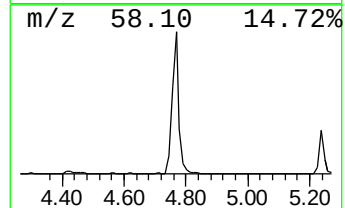
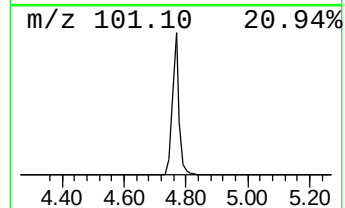
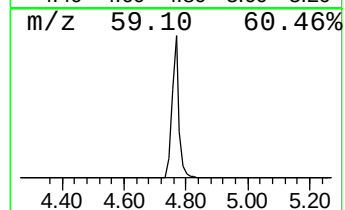
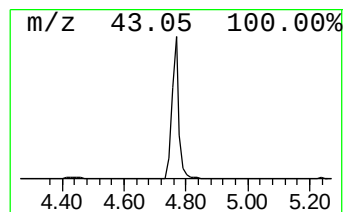
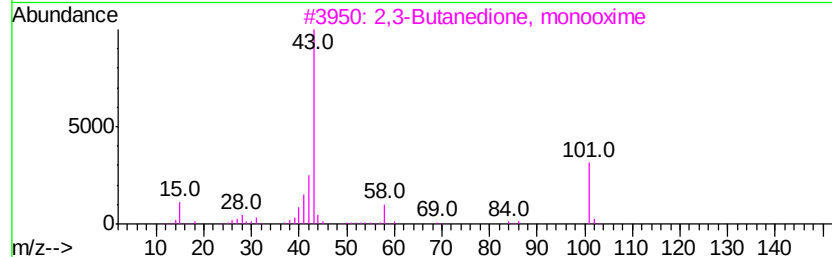
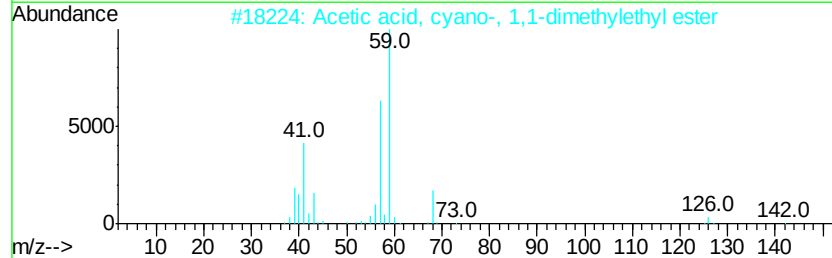
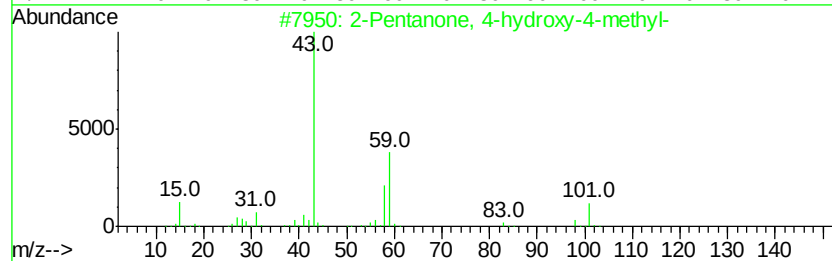
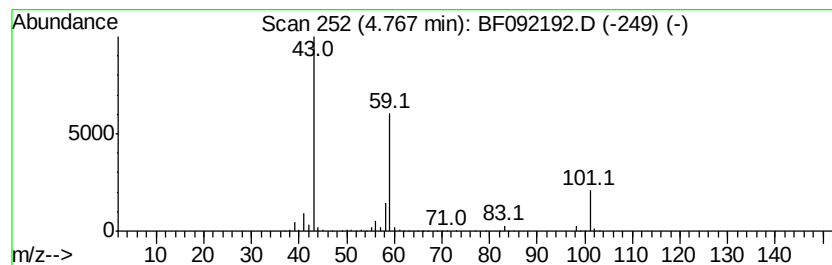
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	29.88 ng	2303030	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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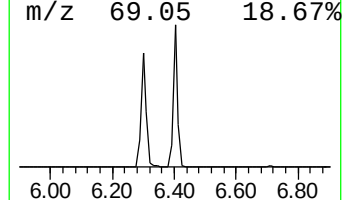
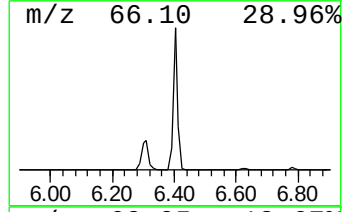
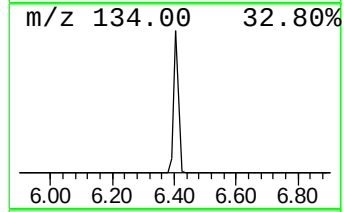
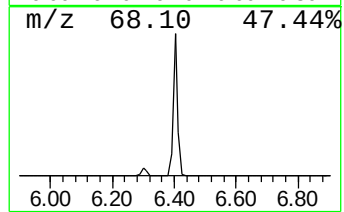
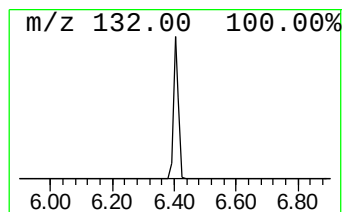
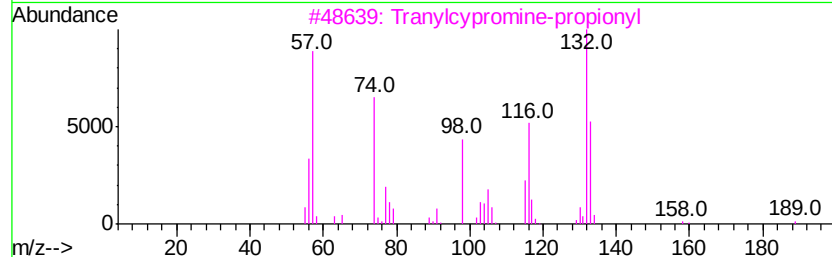
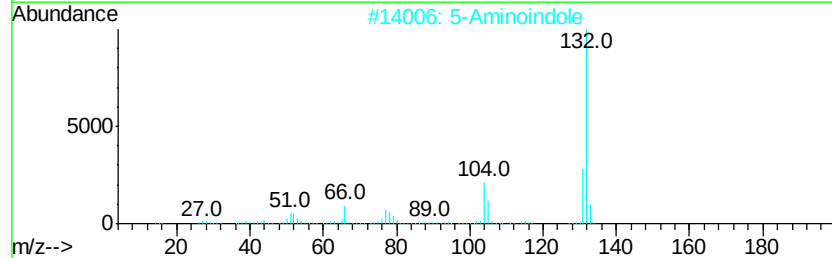
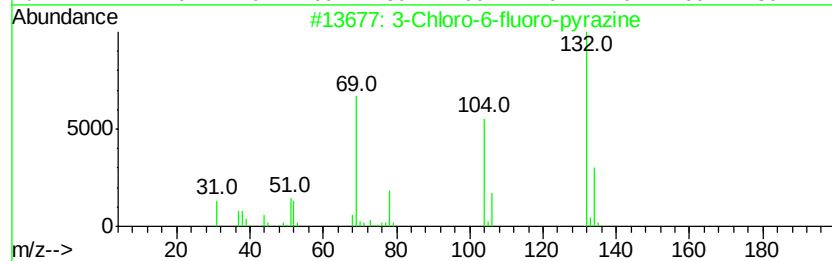
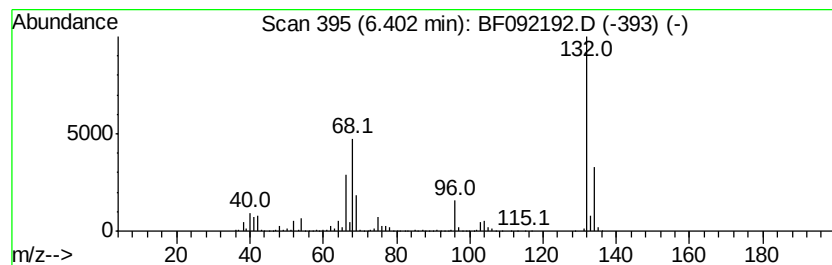
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	65.33 ng	5035780	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9



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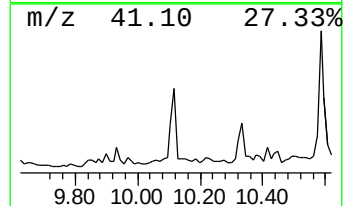
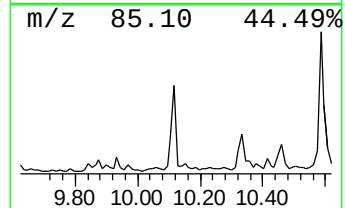
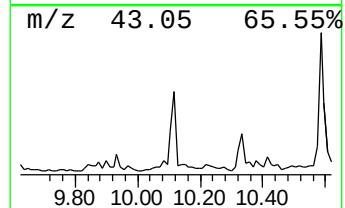
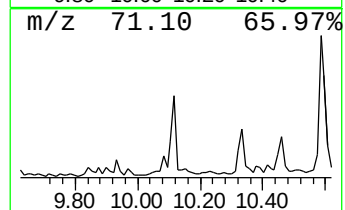
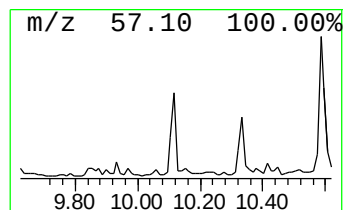
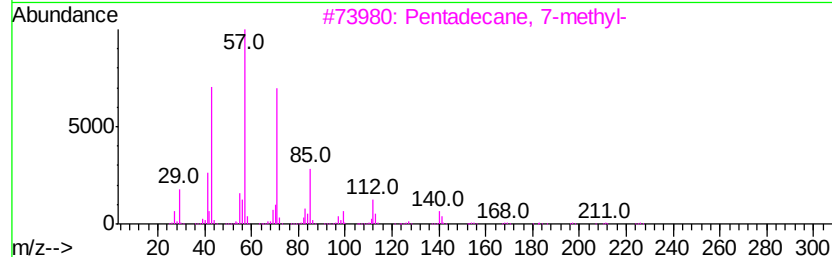
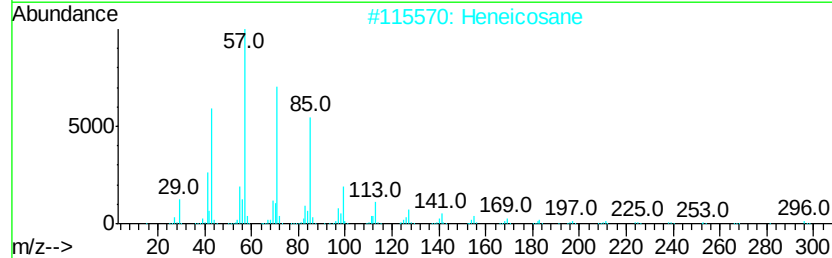
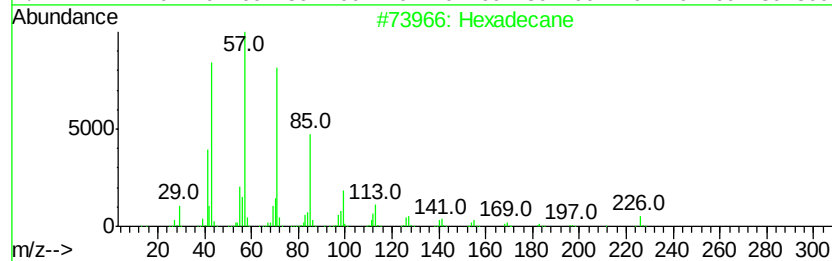
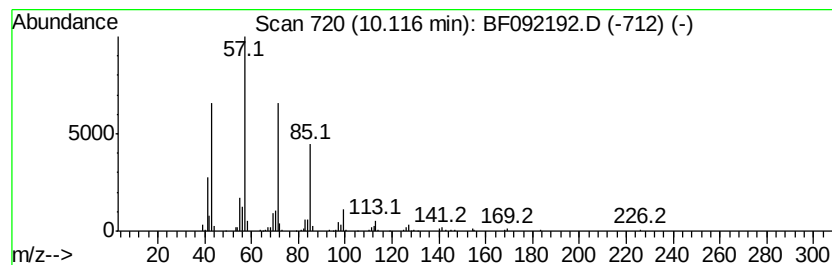
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	2.95 ng	376384	Acenaphthene-d10	9.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	93
2	Heneicosane	296 C21H44	000629-94-7	90
3	Pentadecane, 7-methyl-	226 C16H34	006165-40-8	87
4	Eicosane	282 C20H42	000112-95-8	83
5	Dodecane, 2-methyl-6-propyl-	226 C16H34	055045-08-4	80



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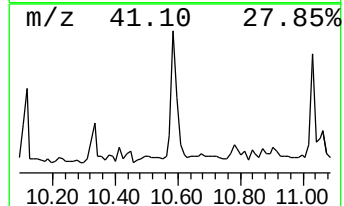
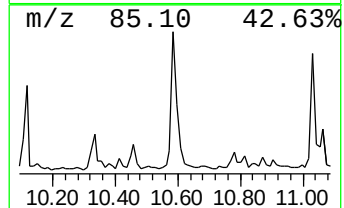
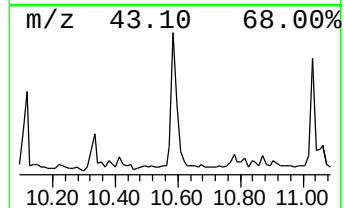
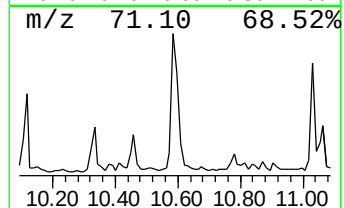
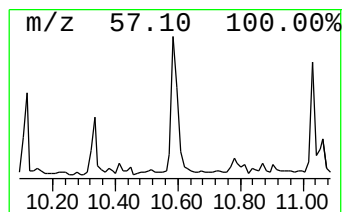
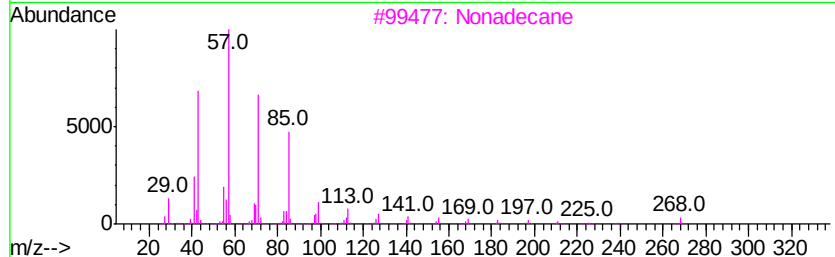
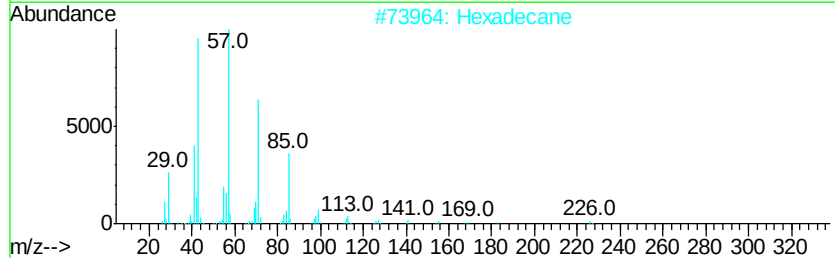
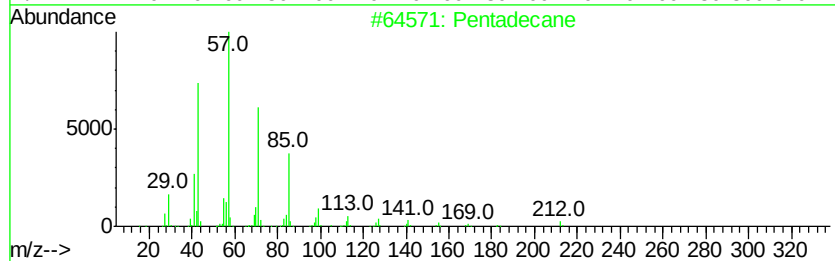
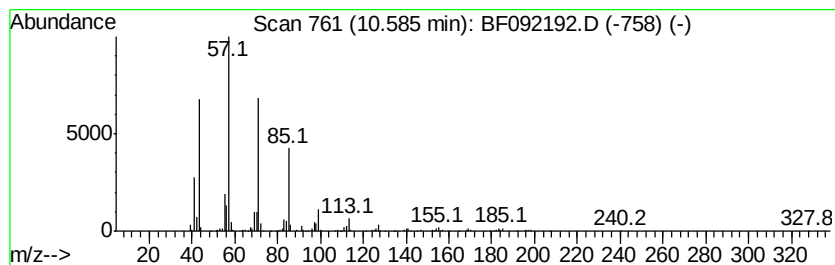
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	5.83 ng	704018	Phenanthrene-d10	11.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	91
2	Hexadecane	226 C16H34	000544-76-3	90
3	Nonadecane	268 C19H40	000629-92-5	90
4	Heneicosane	296 C21H44	000629-94-7	90
5	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	86



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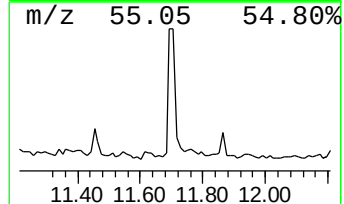
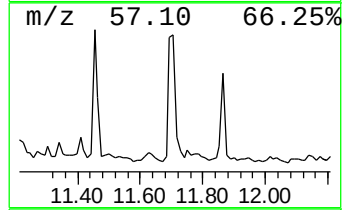
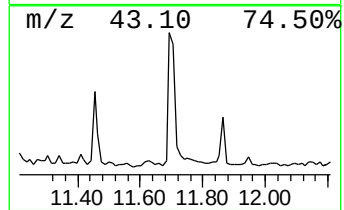
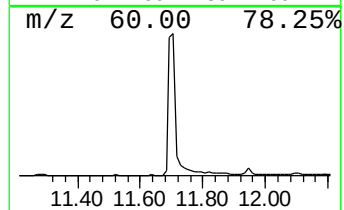
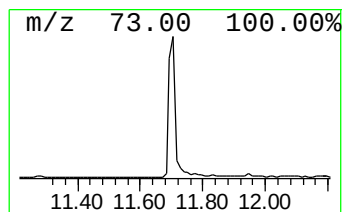
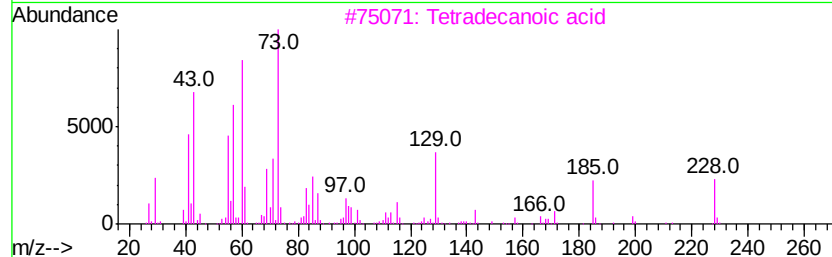
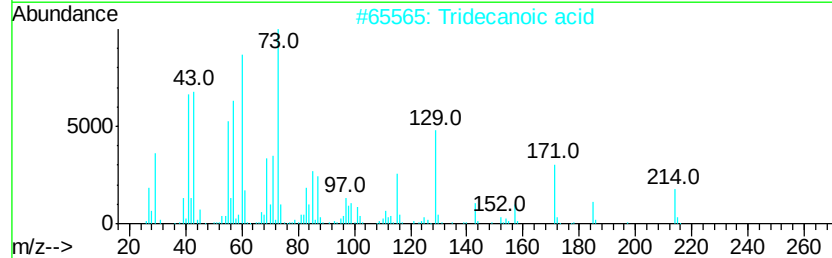
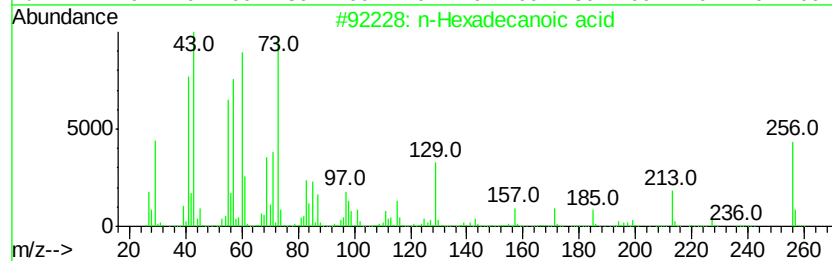
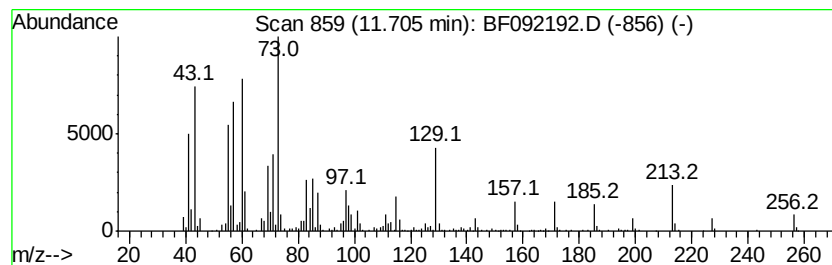
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	7.32 ng	883148	Phenanthrene-d10	11.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	80



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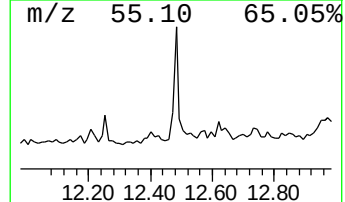
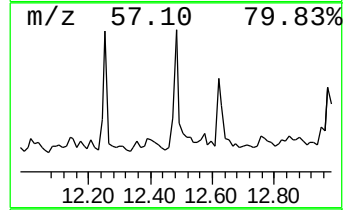
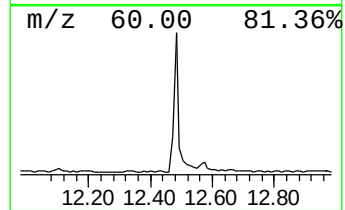
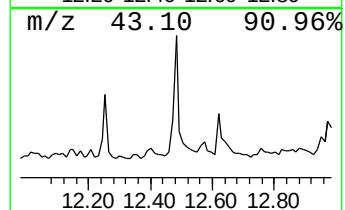
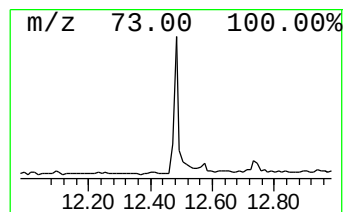
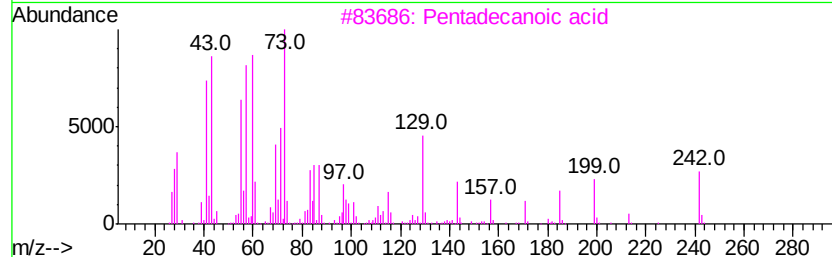
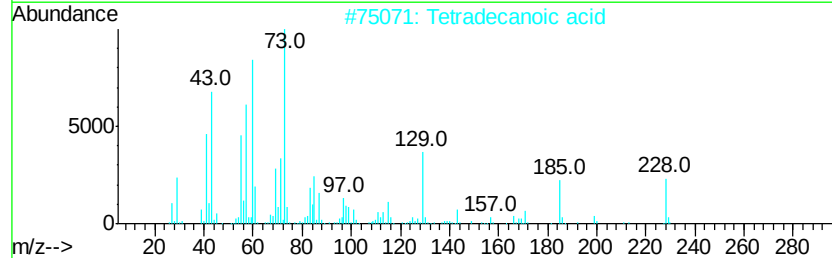
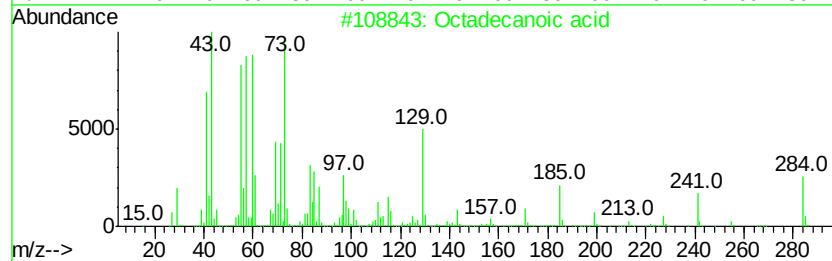
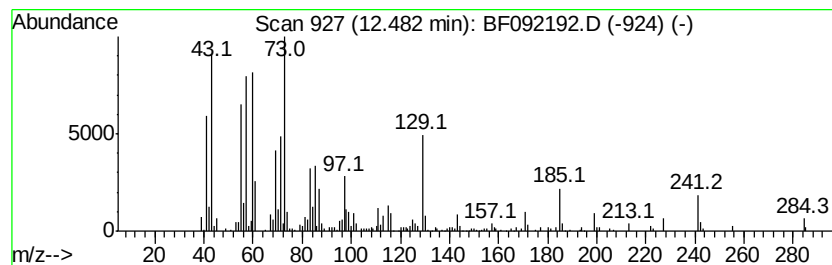
Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-0-2-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.48	2.91 ng	327131	Chrysene-d12		13.79
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011017\
Data File : BF092192.D
Acq On : 10 Jan 2017 19:54
Operator : UM/SJ
Sample : I1078-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

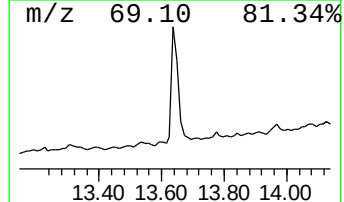
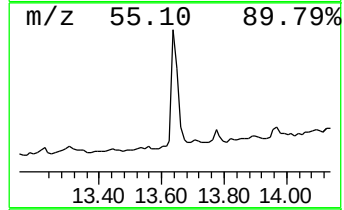
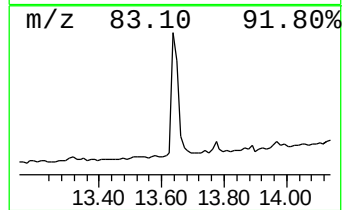
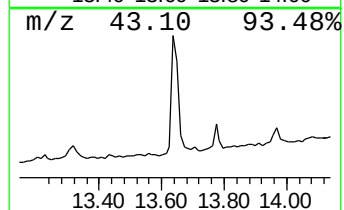
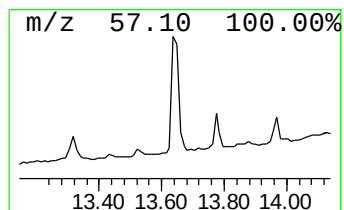
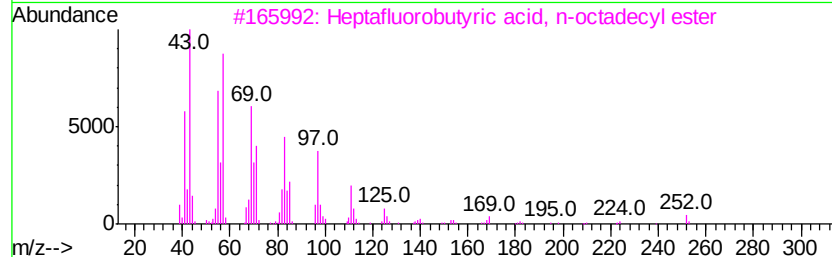
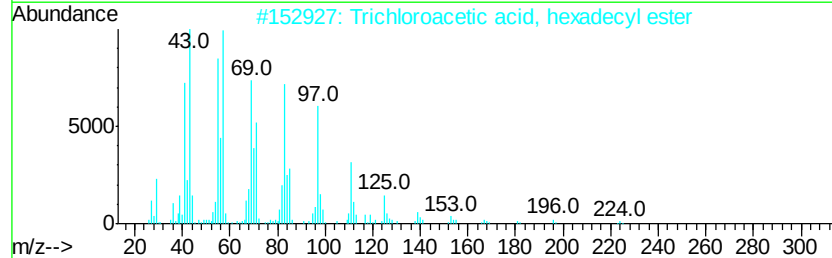
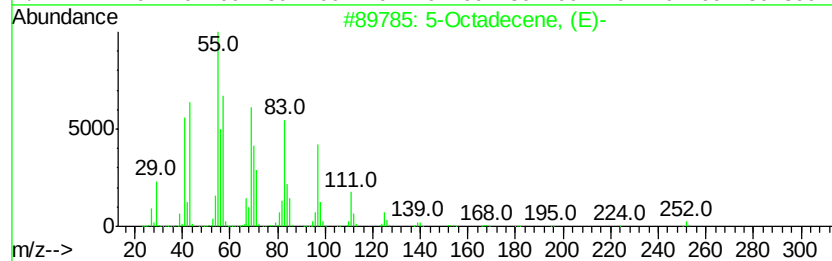
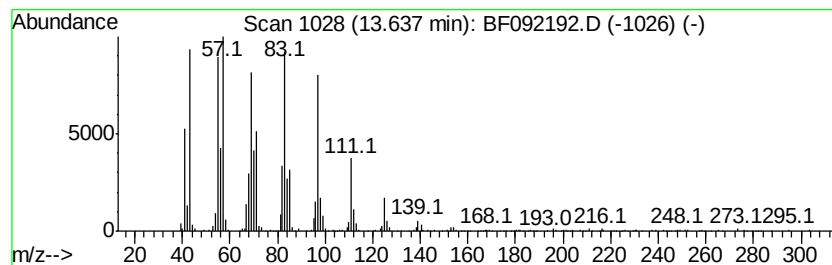
Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-0-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.64	6.09 ng	684391	Chrysene-d12	13.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011017\
Data File : BF092192.D
Acq On : 10 Jan 2017 19:54
Operator : UM/SJ
Sample : I1078-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-0-2-COMP

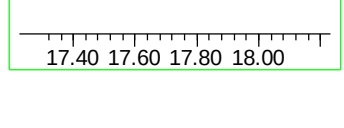
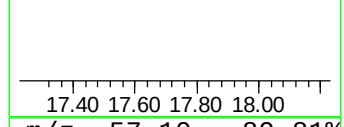
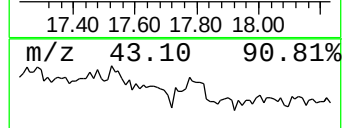
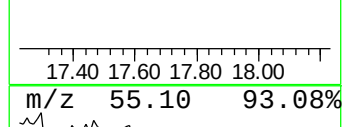
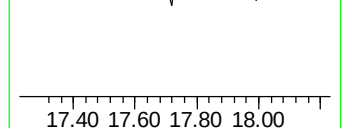
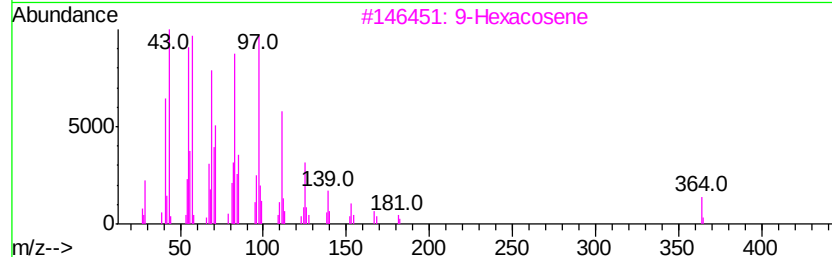
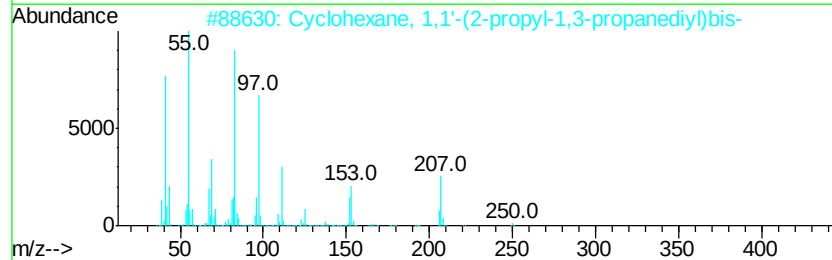
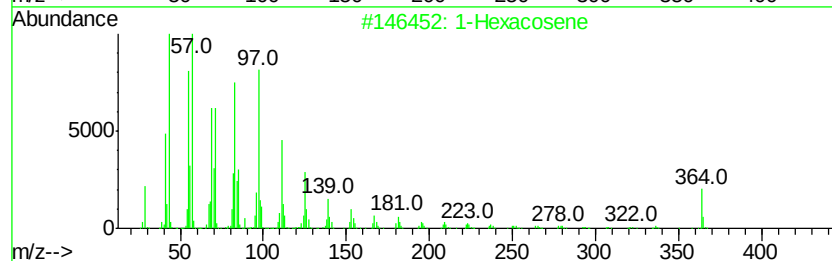
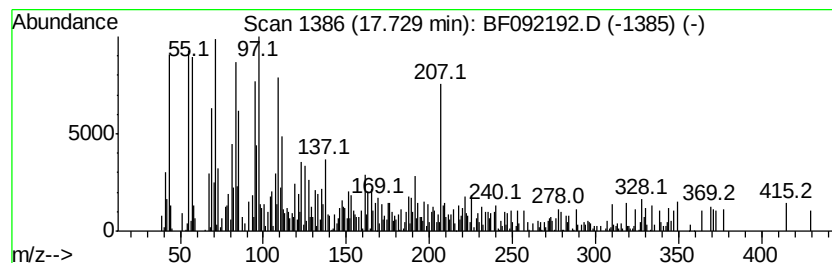
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown17.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	3.42 ng	247886	Perylene-d12	15.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	46
2			Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	45
3			9-Hexacosene	364	C26H52	071502-22-2	38
4			E,E,Z-1,3,12-Nonadecatriene-5,14...	294	C19H34O2	1000131-11-4	30
5			2H-1,2,3-Triazole-4-carboxylic a...	207	C9H6FN3O2	051306-44-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011017\
Data File : BF092192.D
Acq On : 10 Jan 2017 19:54
Operator : UM/SJ
Sample : I1078-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-0-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.77	29.9	ng	2303030	1	6.63	1541760	20.0
unknown6.40	6.40	65.3	ng	5035780	1	6.63	1541760	20.0
Hexadecane	10.12	3.0	ng	376384	3	9.67	2551510	20.0
Pentadecane	10.59	5.8	ng	704018	4	11.15	2413560	20.0
n-Hexadecanoic acid	11.71	7.3	ng	883148	4	11.15	2413560	20.0
Octadecanoic acid	12.48	2.9	ng	327131	5	13.79	2248770	20.0
5-Octadecene, (E)-	13.64	6.1	ng	684391	5	13.79	2248770	20.0
unknown17.73	17.73	3.4	ng	247886	6	15.16	1448550	20.0