

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
 Data File : BF104559.D
 Acq On : 17 Apr 2018 3:05
 Operator : JU/SJ
 Sample : J2360-04
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NAA-WS-004

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-BF040618.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	495	500	512	rVB	154521	213383	5.83%	0.663%
2	5.434	564	569	572	rBV	3284807	3331799	90.96%	10.350%
3	6.069	674	677	683	rBV	48135	65880	1.80%	0.205%
4	6.451	736	742	746	rBV	3100360	3425447	93.52%	10.641%
5	6.581	759	764	767	rBV	3336748	3404210	92.94%	10.575%
6	6.810	799	803	806	rBV	1296644	1000264	27.31%	3.107%
7	6.969	825	830	833	rBV	3067980	2733768	74.64%	8.493%
8	7.375	894	899	902	rBV	2185464	2185895	59.68%	6.791%
9	8.092	1017	1021	1025	rBV	1592872	1298139	35.44%	4.033%
10	9.169	1199	1204	1208	rBV	3659313	3662837	100.00%	11.379%
11	9.563	1267	1271	1274	rBV	496449	408719	11.16%	1.270%
12	9.775	1304	1307	1310	rBV	156326	114776	3.13%	0.357%
13	9.851	1316	1320	1328	rVB	1515734	1283115	35.03%	3.986%
14	10.275	1389	1392	1395	rVB	183617	138276	3.78%	0.430%
15	10.498	1425	1430	1432	rBV	43611	54068	1.48%	0.168%
16	10.639	1451	1454	1465	rVB	1700140	1693447	46.23%	5.261%
17	10.751	1470	1473	1482	rVB	135679	147767	4.03%	0.459%
18	11.198	1546	1549	1551	rBV	66074	48220	1.32%	0.150%
19	11.339	1569	1573	1577	rBV	1224530	1023552	27.94%	3.180%
20	12.745	1808	1812	1815	rBV	545701	431401	11.78%	1.340%
21	12.821	1822	1825	1829	rVB	87783	71977	1.97%	0.224%
22	12.927	1839	1843	1847	rBV	2600046	2574571	70.29%	7.998%
23	13.451	1928	1932	1935	rBV	414114	328058	8.96%	1.019%
24	13.498	1935	1940	1942	rBV2	47924	43447	1.19%	0.135%
25	13.721	1971	1978	1985	rBV2	21480	45419	1.24%	0.141%
26	13.821	1991	1995	2004	rBV	146608	164041	4.48%	0.510%
27	13.986	2019	2023	2032	rVB	1006960	915120	24.98%	2.843%
28	14.145	2046	2050	2054	rBV	85507	73705	2.01%	0.229%
29	14.451	2098	2102	2107	rBV	84660	85000	2.32%	0.264%
30	14.757	2151	2154	2158	rVB	95781	87250	2.38%	0.271%
31	15.092	2207	2211	2218	rBV	82149	92657	2.53%	0.288%
32	15.451	2266	2272	2284	rBV	543360	792539	21.64%	2.462%
33	15.904	2344	2349	2354	rBV	52164	76005	2.08%	0.236%
34	16.404	2429	2434	2439	rBV3	44299	76283	2.08%	0.237%

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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NAA-WS-004

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	16.992	2530	2534	2539	rVB5	20440	38140	1.04%	0.118%
36	17.480	2613	2617	2626	rVB5	25518	60745	1.66%	0.189%

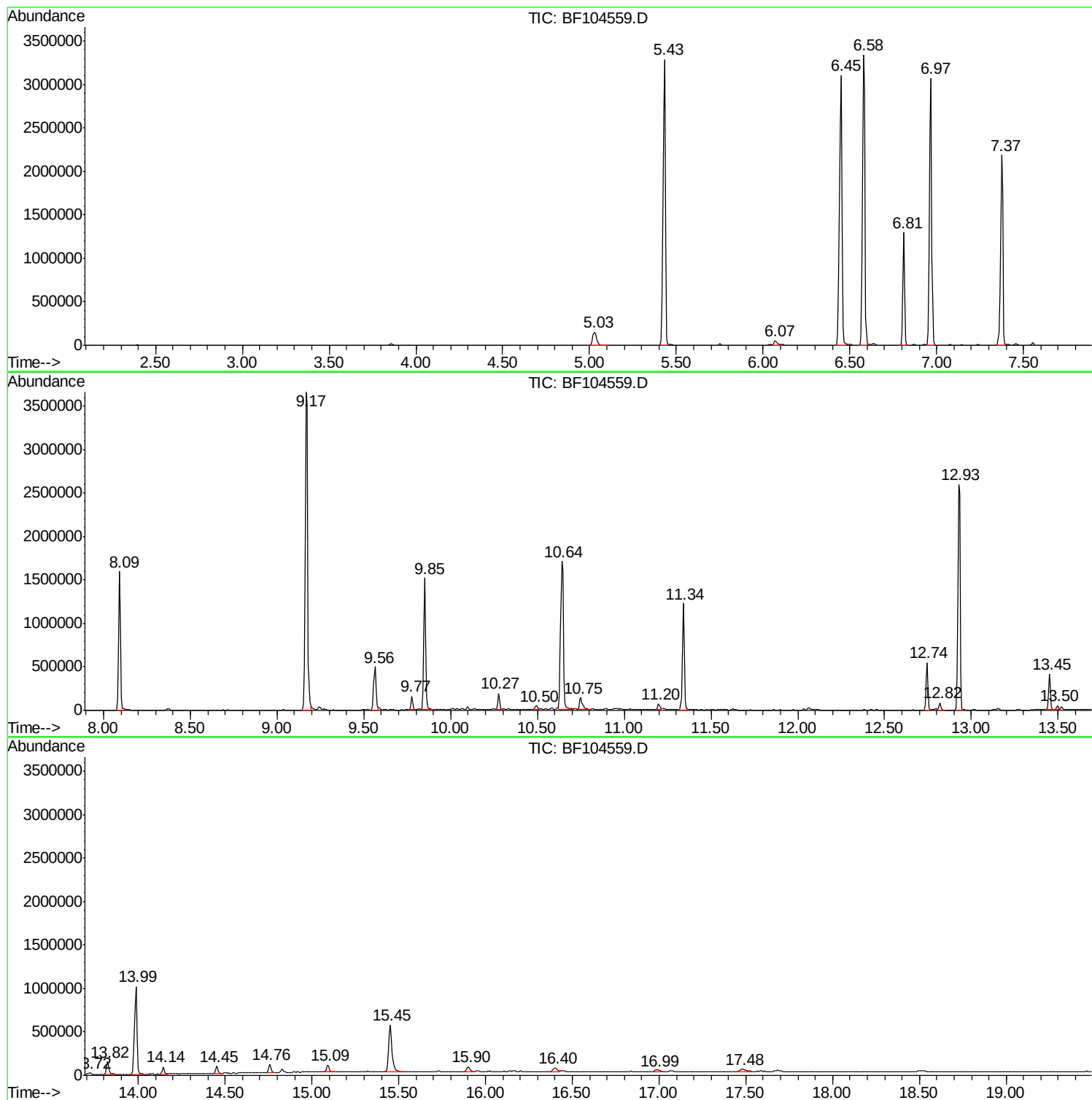
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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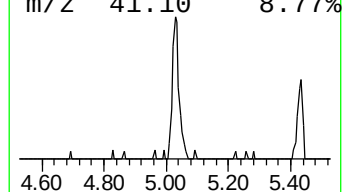
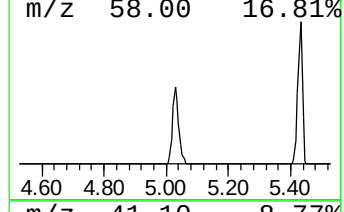
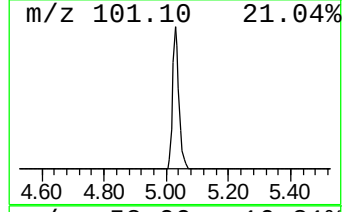
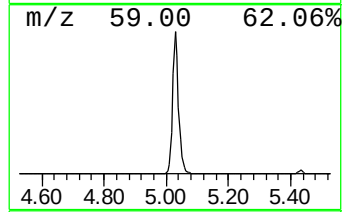
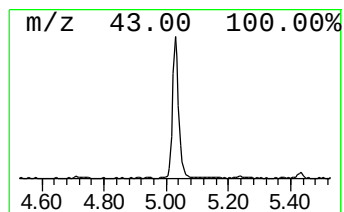
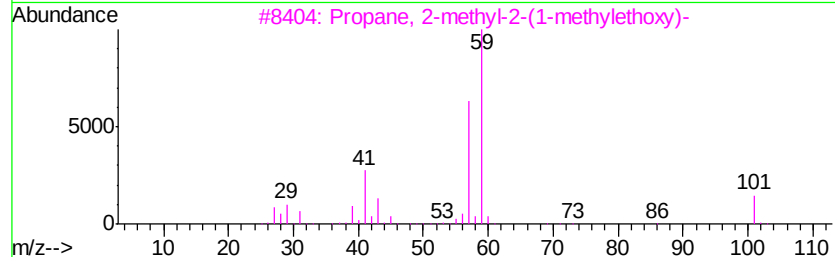
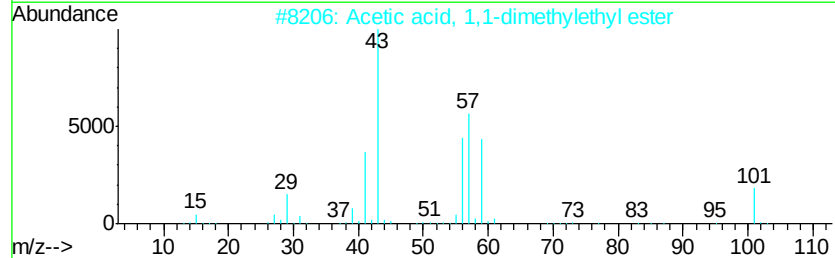
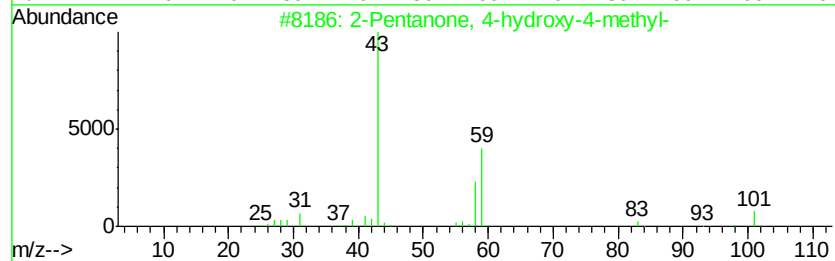
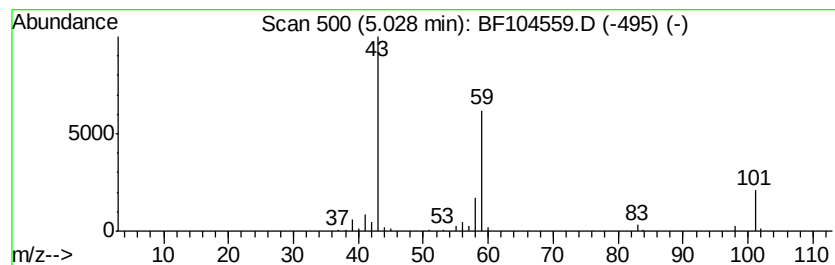
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	4.27 ng	213383	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28	
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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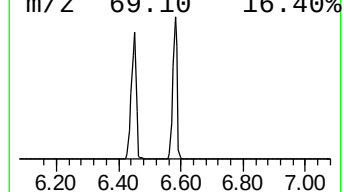
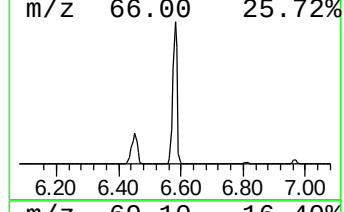
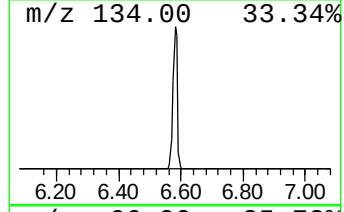
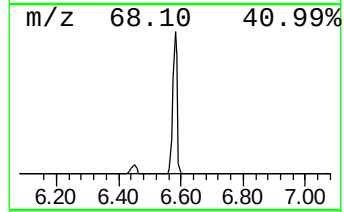
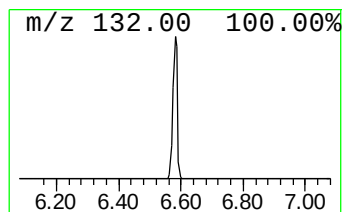
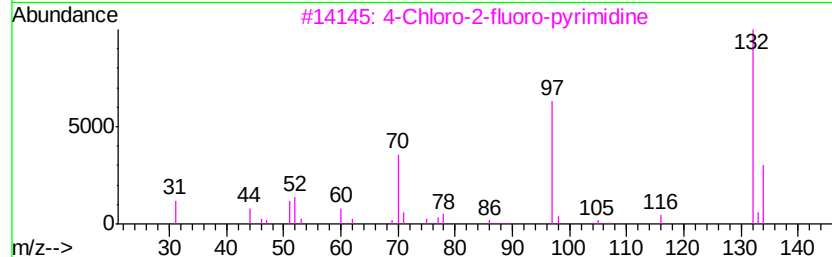
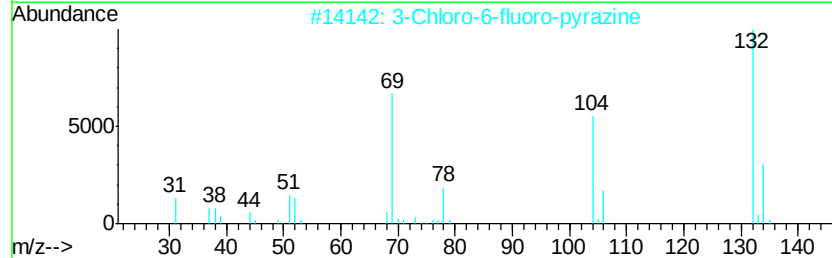
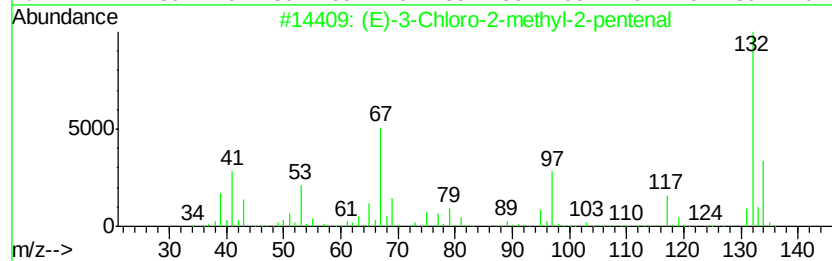
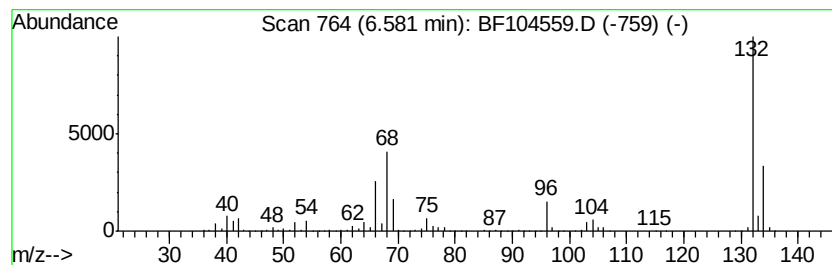
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	68.07 ng	3404210	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



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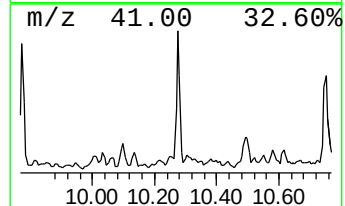
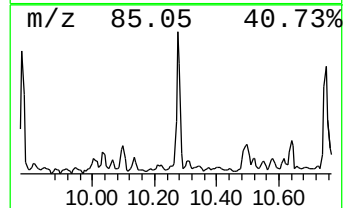
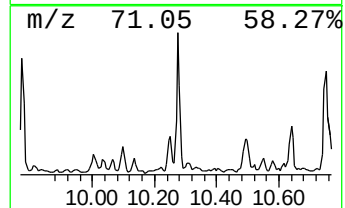
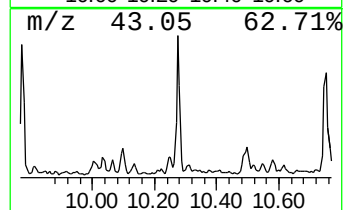
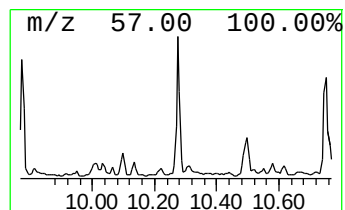
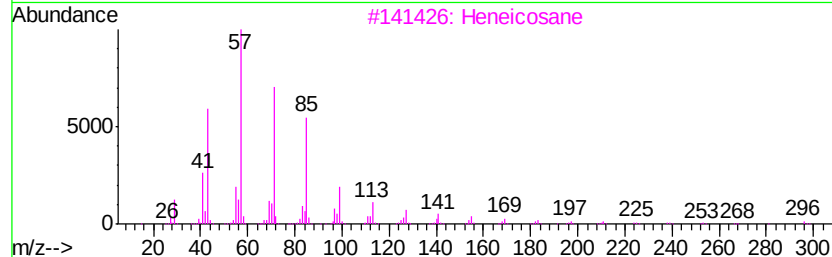
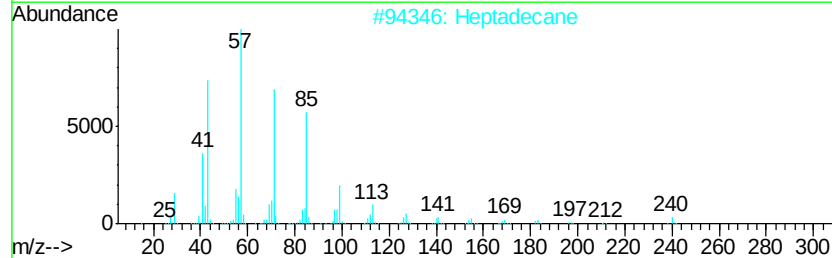
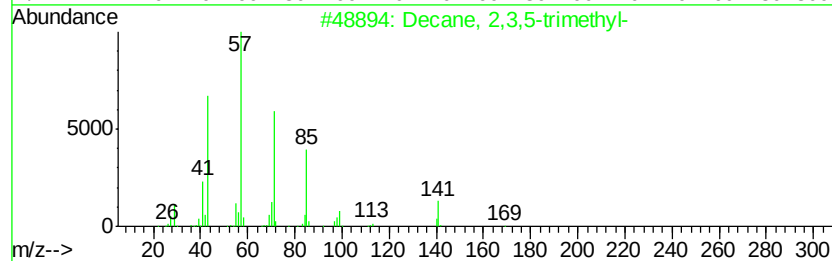
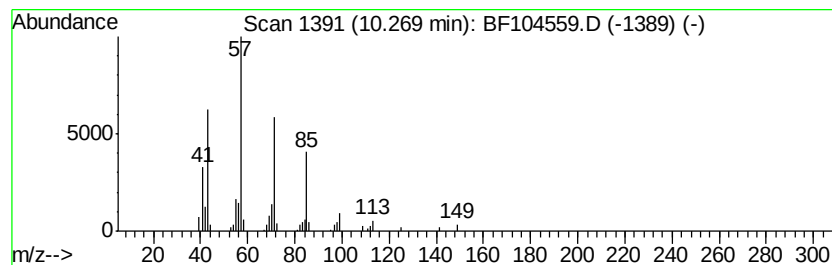
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane, 2,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.16 ng	138276	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2		Heptadecane	240	C17H36	000629-78-7	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5		Hexadecane	226	C16H34	000544-76-3	76



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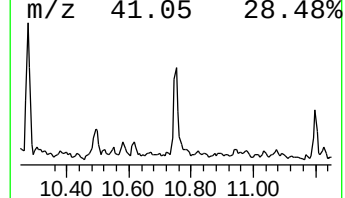
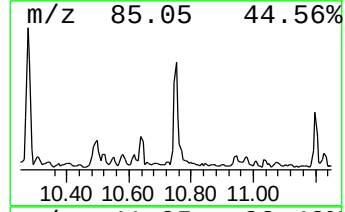
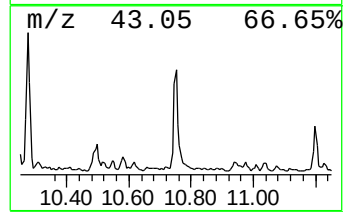
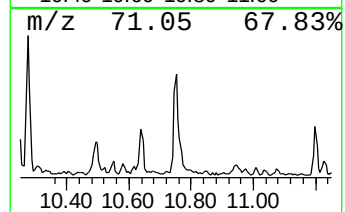
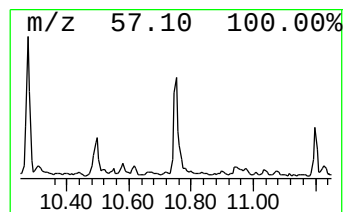
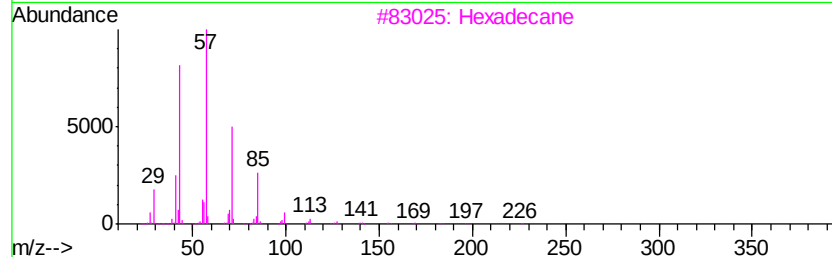
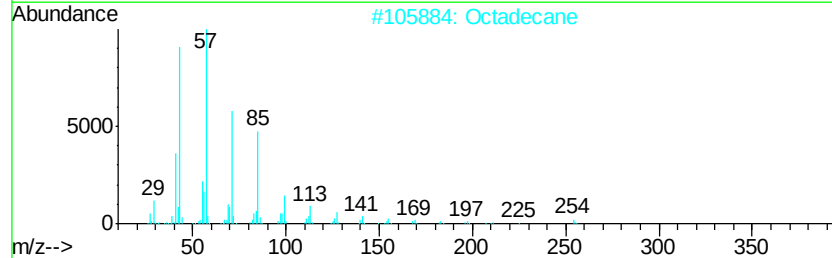
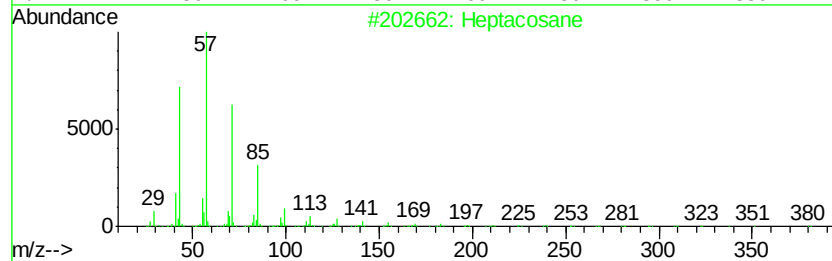
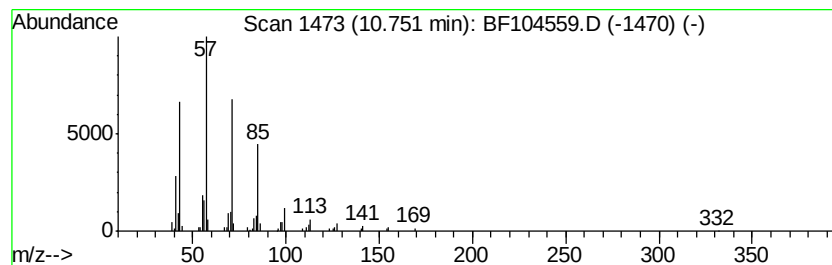
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.89 ng	147767	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Pentadecane		212	C15H32	000629-62-9	87
5	Heptadecane		240	C17H36	000629-78-7	87



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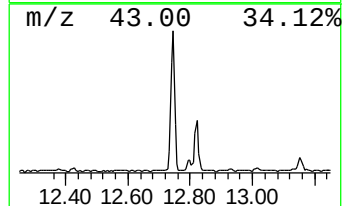
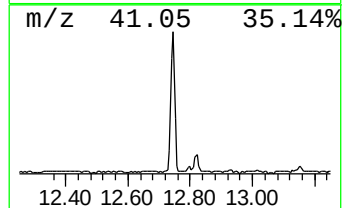
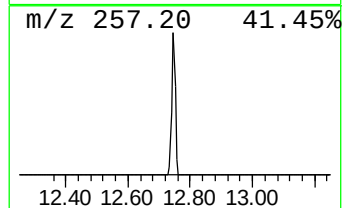
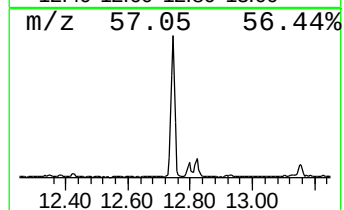
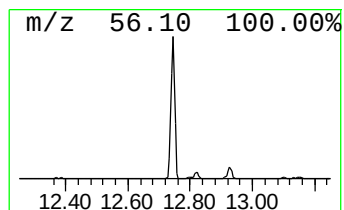
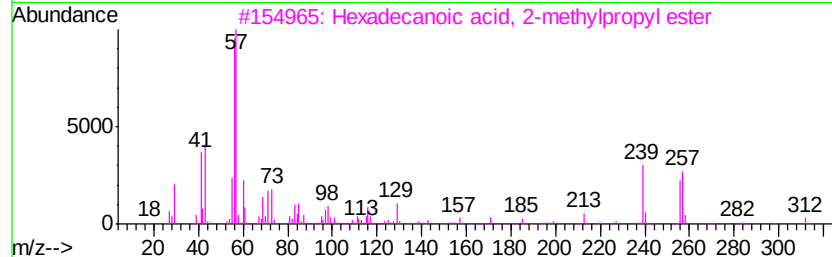
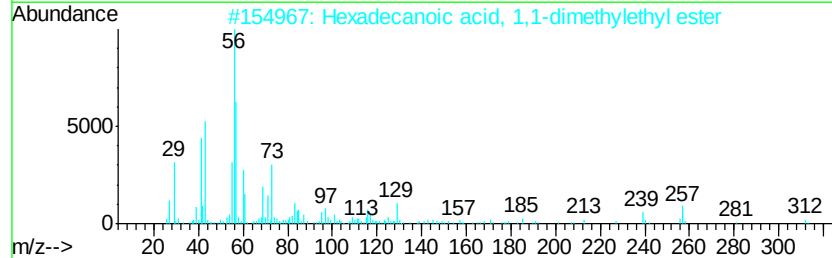
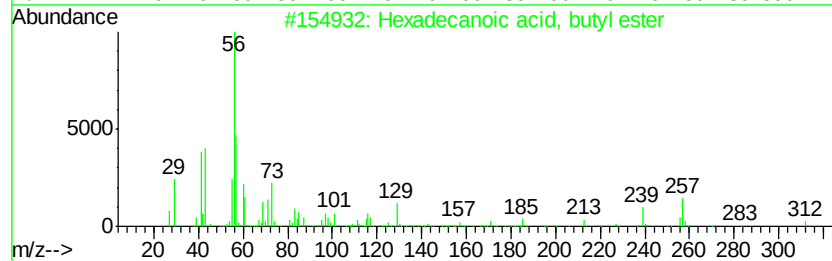
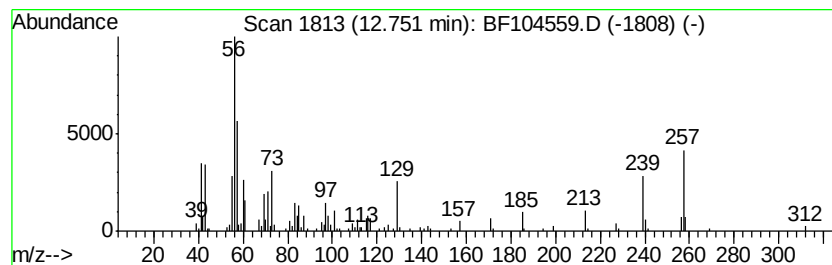
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	9.43 ng	431401	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	76
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	64
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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ClientSampleId :
NAA-WS-004

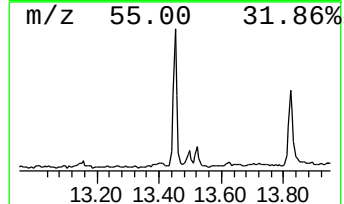
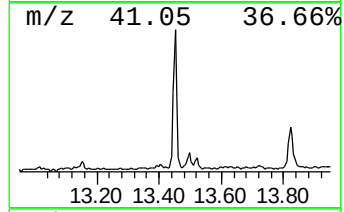
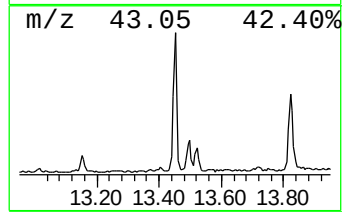
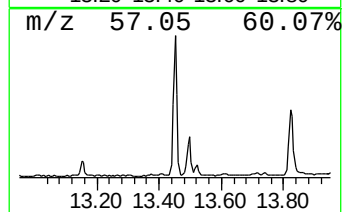
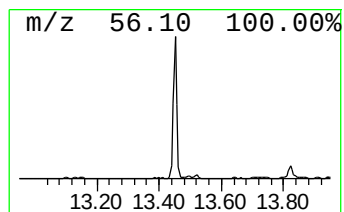
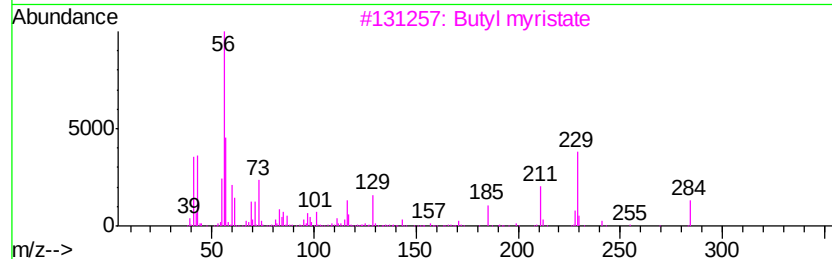
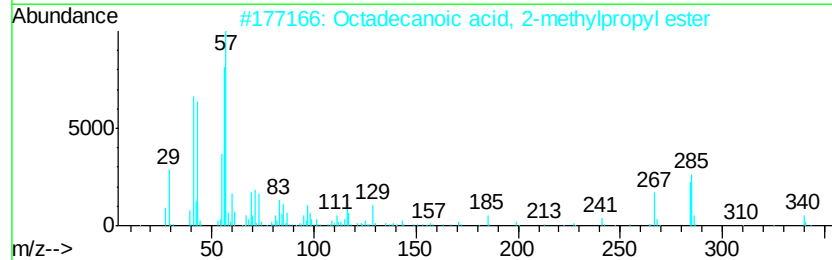
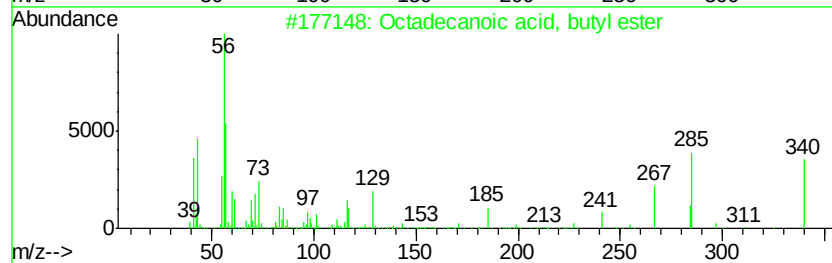
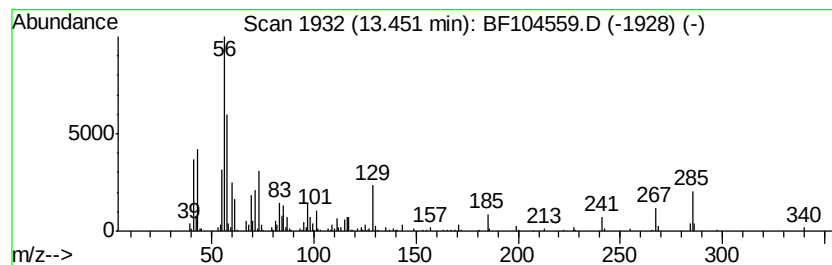
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	7.17 ng	328058	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	43
3		Butyl myristate	284	C18H36O2	000110-36-1	42
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		Cyclohexanamine	99	C6H13N	000108-91-8	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104559.D
Acq On : 17 Apr 2018 3:05
Operator : JU/SJ
Sample : J2360-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NAA-WS-004

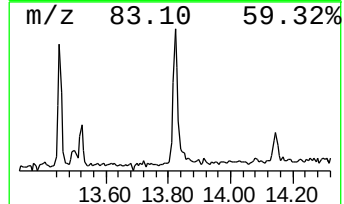
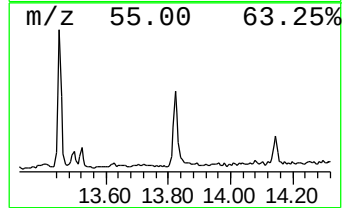
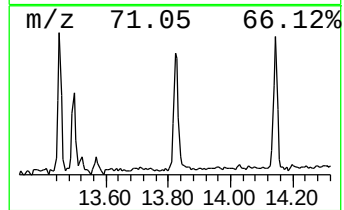
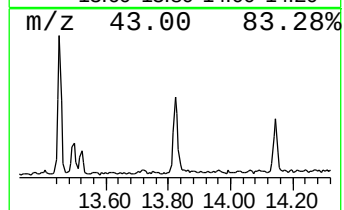
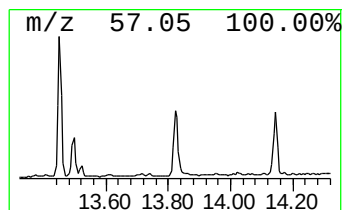
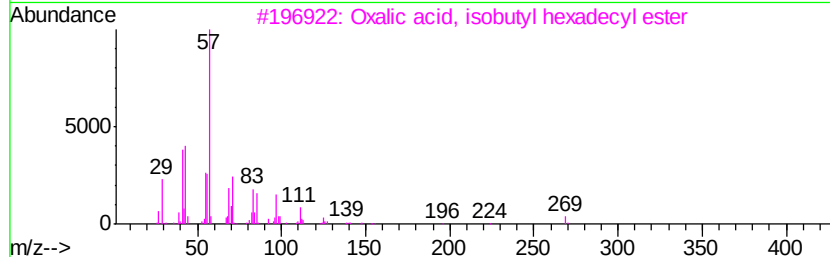
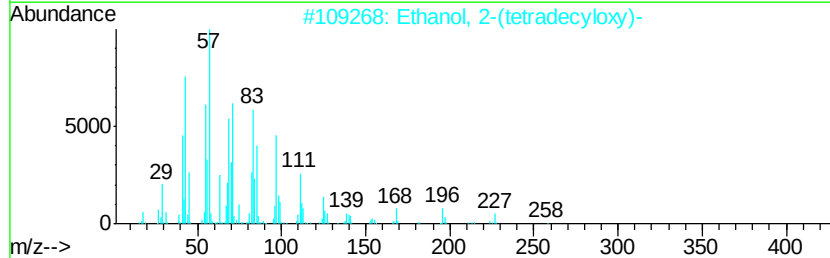
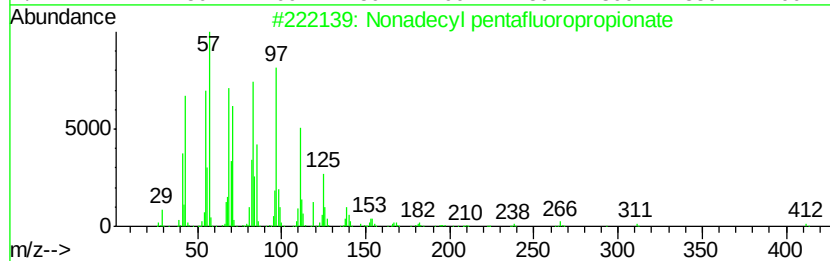
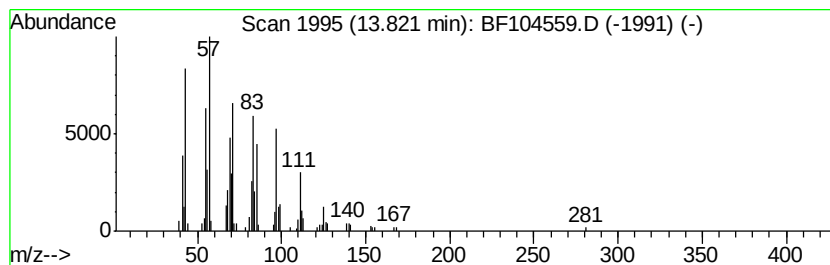
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecyl pentafluoropropio... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.59 ng	164041	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	81
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104559.D
Acq On : 17 Apr 2018 3:05
Operator : JU/SJ
Sample : J2360-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NAA-WS-004

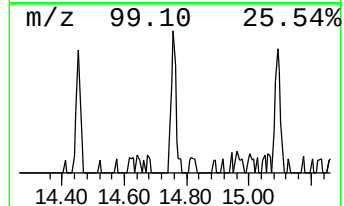
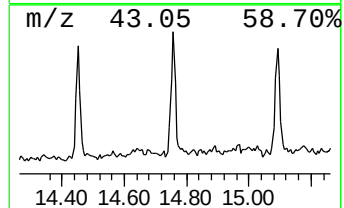
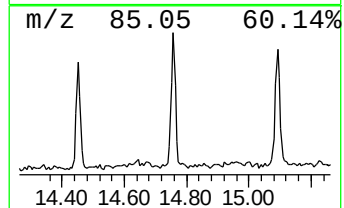
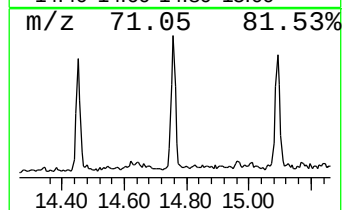
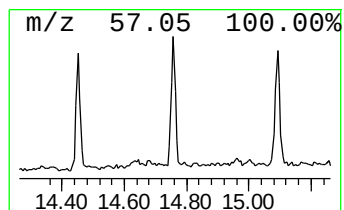
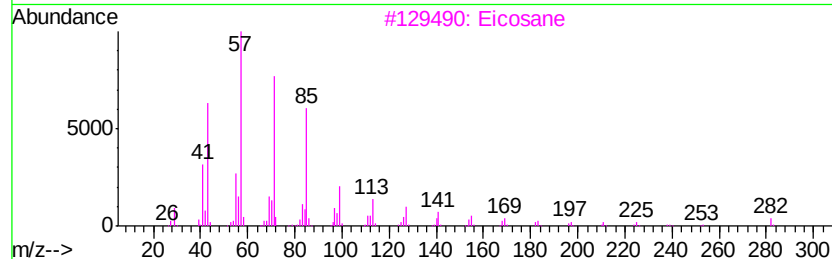
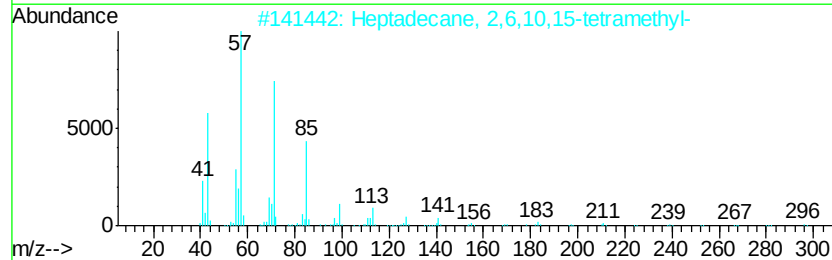
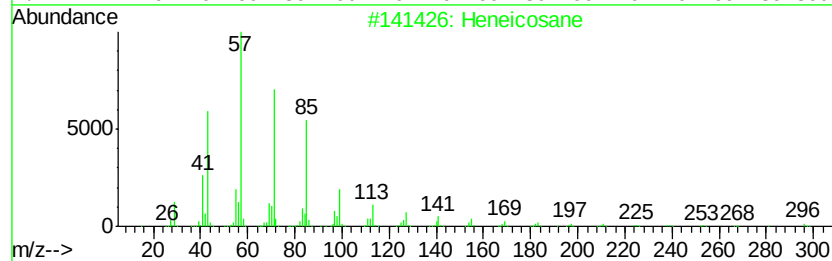
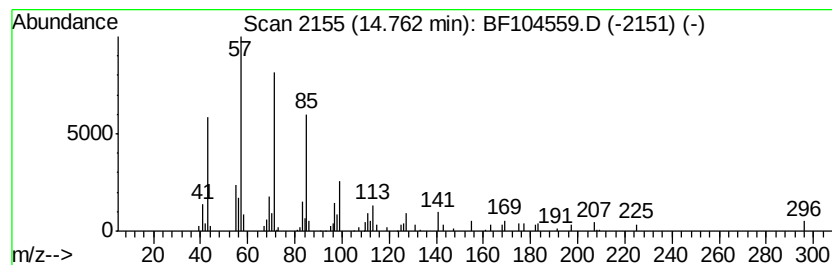
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.20 ng	87250	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	95
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	93
3	Eicosane		282	C20H42	000112-95-8	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104559.D
Acq On : 17 Apr 2018 3:05
Operator : JU/SJ
Sample : J2360-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NAA-WS-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	4.3	ng	213383	1	6.81	1000260	20.0
unknown6.58	6.58	68.1	ng	3404210	1	6.81	1000260	20.0
Decane, 2,3,5-tri...	10.27	2.2	ng	138276	3	9.85	1283120	20.0
Heptacosane	10.75	2.9	ng	147767	4	11.34	1023550	20.0
Hexadecanoic acid...	12.75	9.4	ng	431401	5	13.99	915120	20.0
Octadecanoic acid...	13.45	7.2	ng	328058	5	13.99	915120	20.0
Nonadecyl pentafl...	13.82	3.6	ng	164041	5	13.99	915120	20.0
Heneicosane	14.76	2.2	ng	87250	6	15.45	792539	20.0