

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101917\
 Data File : BF099667.D
 Acq On : 19 Oct 2017 19:59
 Operator : SJ/JU
 Sample : I5924-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BACKFILL-COMP-1RE

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-BF092317.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	5.040	499	502	519	rBV	192685	266443	14.46%	1.682%
2	5.451	568	572	595	rBV	1600678	1567246	85.05%	9.895%
3	6.463	740	744	757	rBV	1603403	1592020	86.39%	10.051%
4	6.592	762	766	770	rVV	1891084	1644792	89.25%	10.384%
5	6.645	772	775	782	rVB	36536	30425	1.65%	0.192%
6	6.822	801	805	810	rBV	588476	515189	27.96%	3.253%
7	6.975	827	831	835	rBV	1580267	1310302	71.10%	8.273%
8	7.386	897	901	904	rBV	1116666	983762	53.38%	6.211%
9	8.069	1014	1017	1019	rBV	58817	52203	2.83%	0.330%
10	8.098	1019	1022	1026	rVB	766499	680301	36.92%	4.295%
11	8.680	1115	1121	1124	rBV2	93426	74647	4.05%	0.471%
12	9.175	1200	1205	1208	rBV	2122195	1842829	100.00%	11.635%
13	9.245	1214	1217	1220	rBV	104361	78510	4.26%	0.496%
14	9.569	1266	1272	1279	rVB2	60015	71605	3.89%	0.452%
15	9.774	1301	1307	1310	rBV	102544	83880	4.55%	0.530%
16	9.851	1316	1320	1324	rBV	744353	691282	37.51%	4.364%
17	10.274	1384	1392	1395	rBV	93949	88923	4.83%	0.561%
18	10.645	1451	1455	1464	rBV	901447	779570	42.30%	4.922%
19	10.745	1469	1472	1481	rVB	99218	103532	5.62%	0.654%
20	11.192	1544	1548	1551	rBV	88981	66813	3.63%	0.422%
21	11.339	1570	1573	1577	rBV	630196	540980	29.36%	3.415%
22	11.616	1617	1620	1624	rVB	80936	60796	3.30%	0.384%
23	12.021	1686	1689	1693	rBV	69389	52394	2.84%	0.331%
24	12.410	1753	1755	1759	rVB	58145	45212	2.45%	0.285%
25	12.780	1816	1818	1821	rBV	49707	38255	2.08%	0.242%
26	12.921	1838	1842	1845	rBV	1297865	1090296	59.16%	6.884%
27	13.139	1872	1879	1881	rBV	45826	46525	2.52%	0.294%
28	13.480	1933	1937	1940	rBV2	36727	38123	2.07%	0.241%
29	13.804	1988	1992	1996	rBV	145336	157665	8.56%	0.995%
30	13.839	1996	1998	2003	rVB	26552	27753	1.51%	0.175%
31	13.980	2019	2022	2026	rBV	475846	447612	24.29%	2.826%
32	14.121	2043	2046	2049	rVB	29593	23625	1.28%	0.149%
33	14.427	2095	2098	2110	rBV3	32382	57087	3.10%	0.360%
34	14.727	2145	2149	2153	rBV4	27696	37383	2.03%	0.236%

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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-BF092317.M
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35	15.056	2201	2205	2208	rBV	24423	27809	1.51%	0.176%
36	15.445	2264	2271	2281	rVB2	420630	538905	29.24%	3.402%
37	15.845	2336	2339	2344	rBV2	21020	26747	1.45%	0.169%
38	15.909	2346	2350	2356	rVB8	12886	27823	1.51%	0.176%
39	16.339	2419	2423	2427	rBV5	17669	29776	1.62%	0.188%

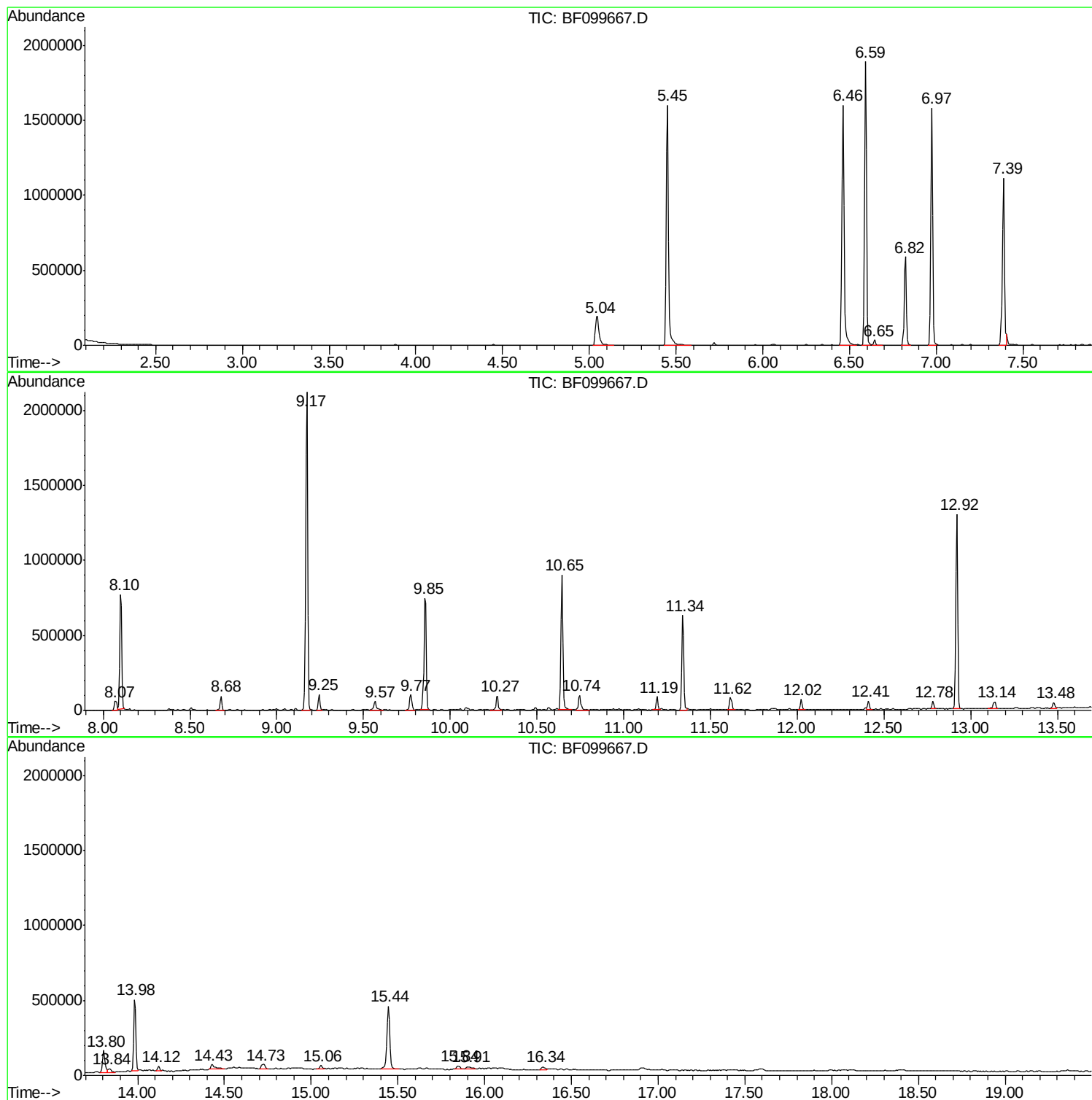
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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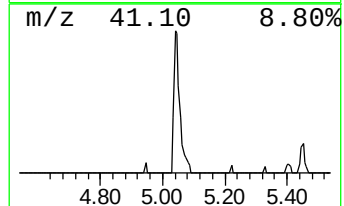
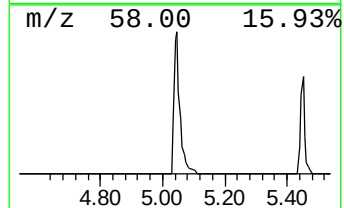
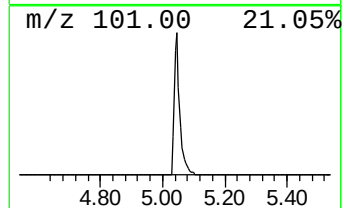
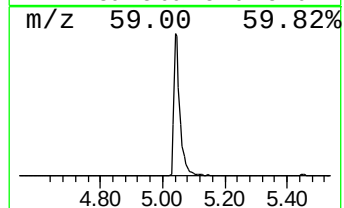
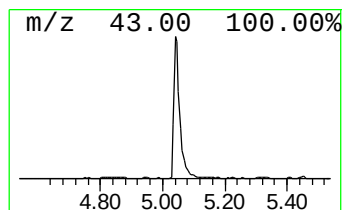
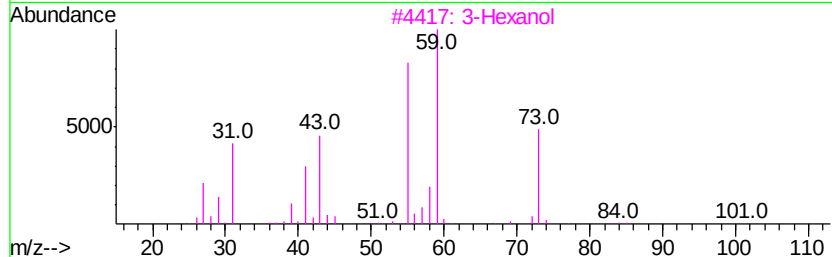
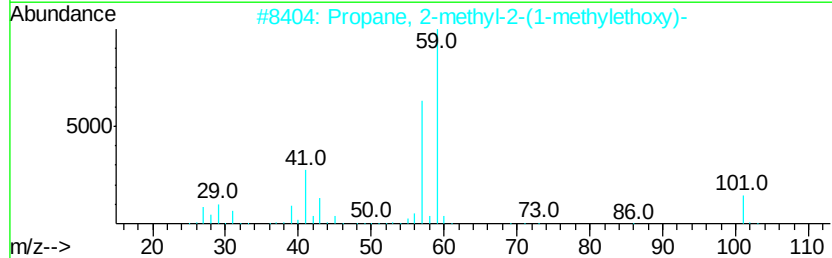
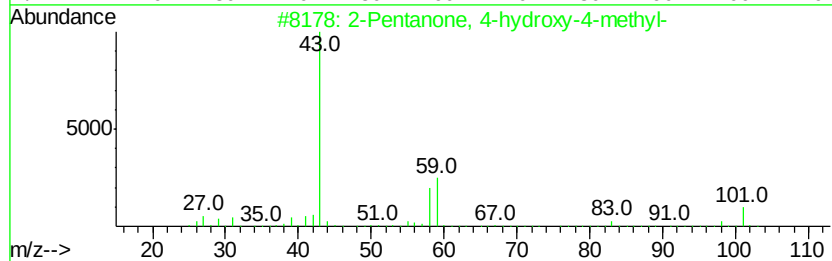
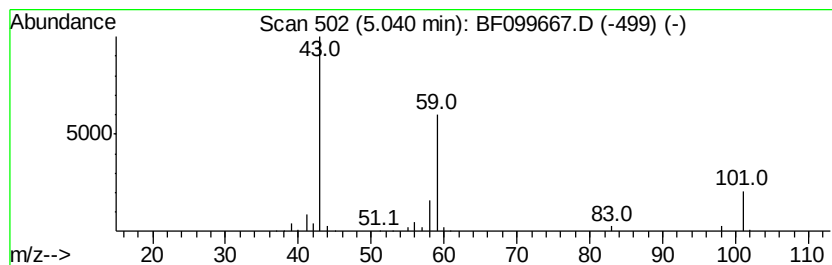
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	10.34 ng	266443	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	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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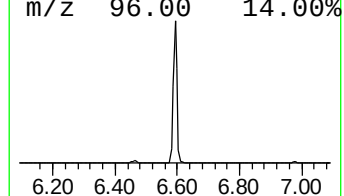
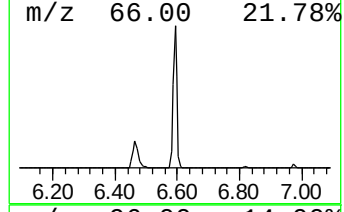
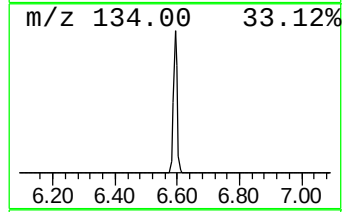
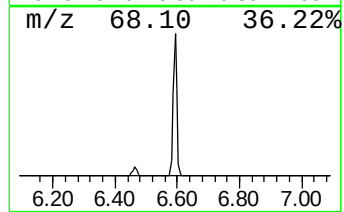
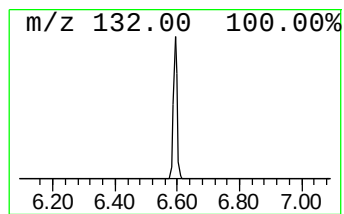
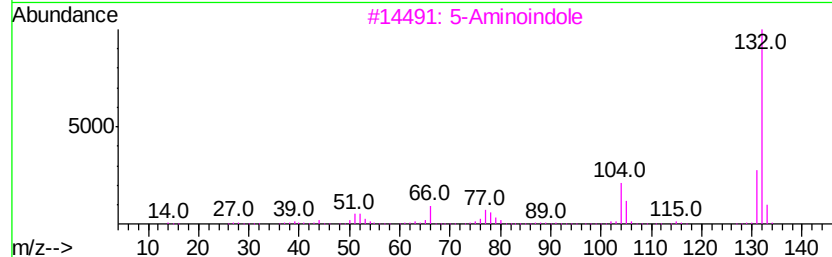
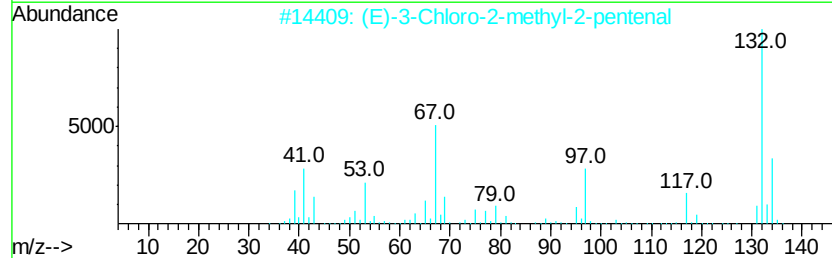
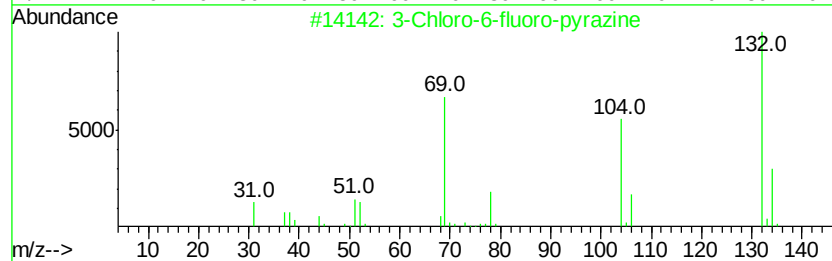
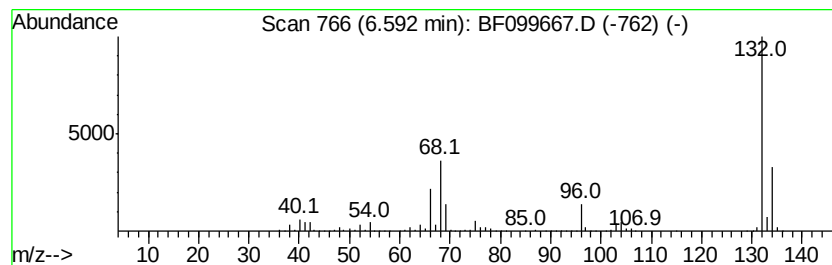
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	63.85 ng	1644790	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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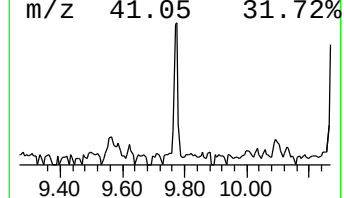
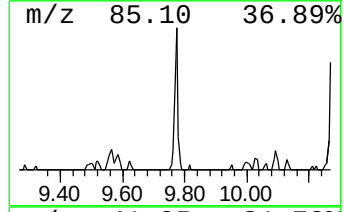
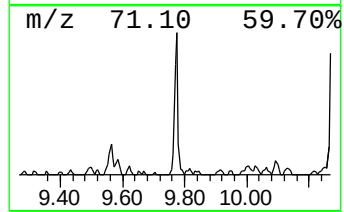
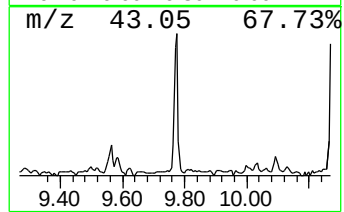
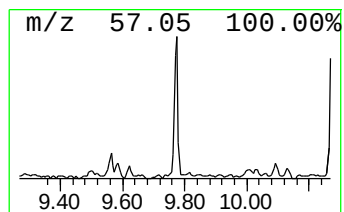
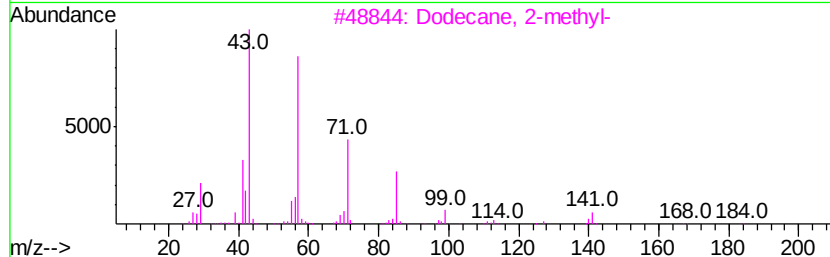
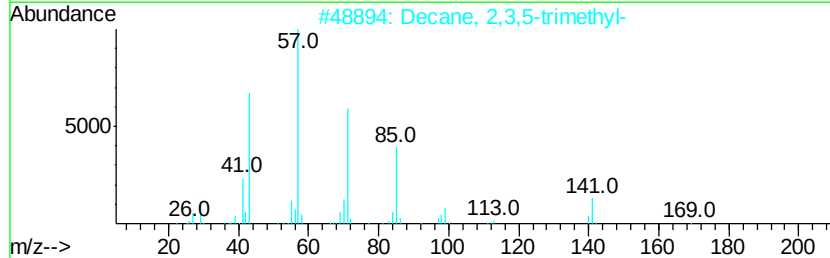
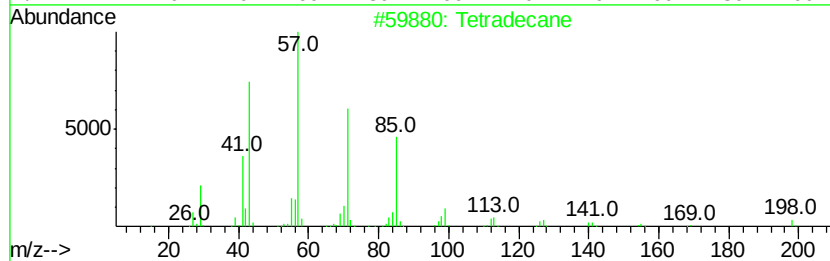
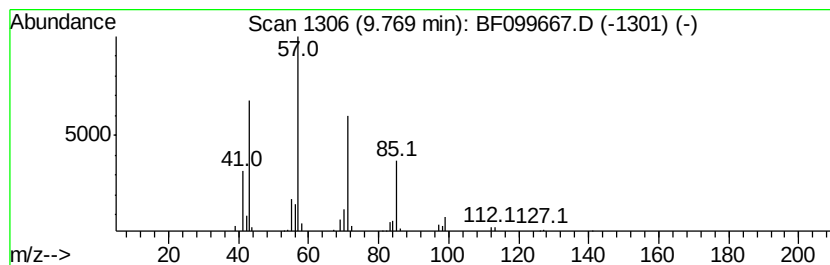
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.77	2.43 ng	83880	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	91
2		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4		Heneicosane	296	C21H44	000629-94-7	80
5		Tridecane	184	C13H28	000629-50-5	72



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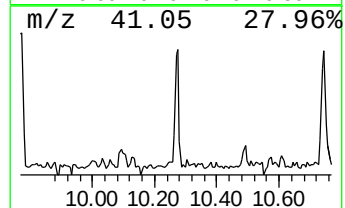
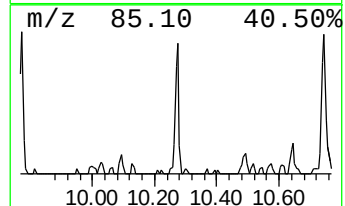
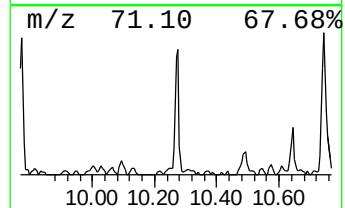
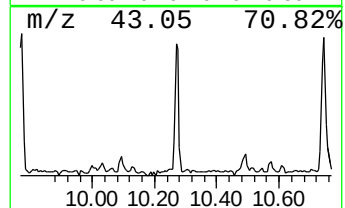
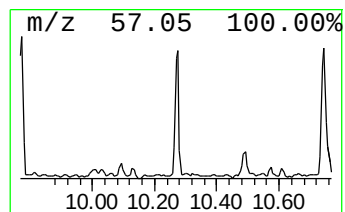
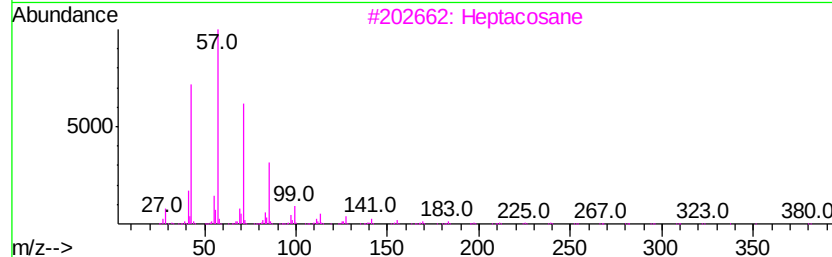
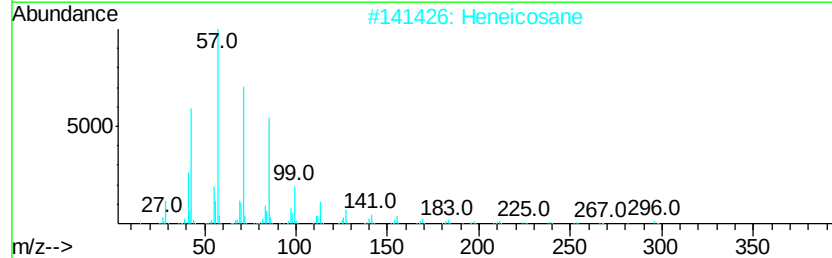
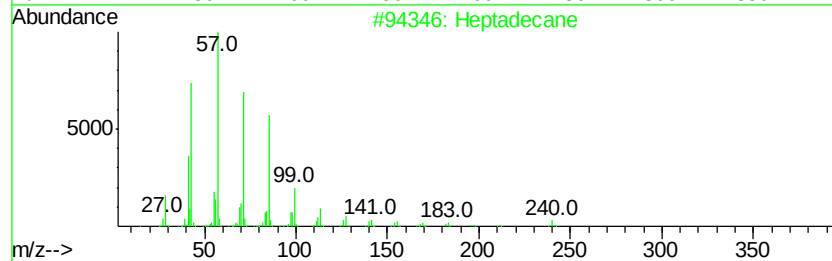
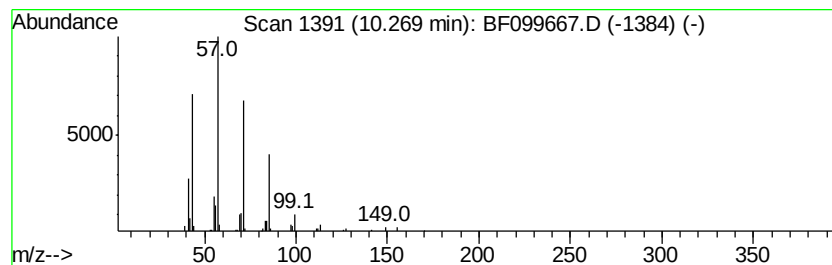
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.57 ng	88923	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	91
2	Heneicosane	296 C21H44	000629-94-7	90
3	Heptacosane	380 C27H56	000593-49-7	90
4	Hexadecane	226 C16H34	000544-76-3	90
5	Tetradecane	198 C14H30	000629-59-4	86



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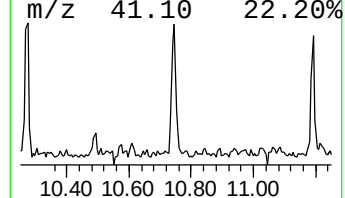
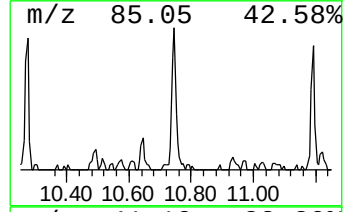
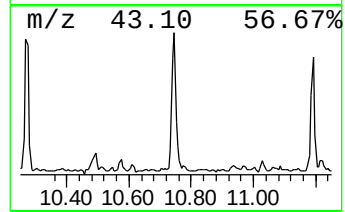
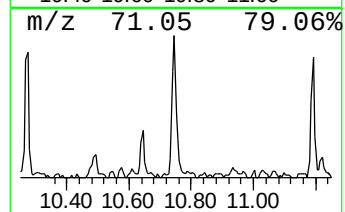
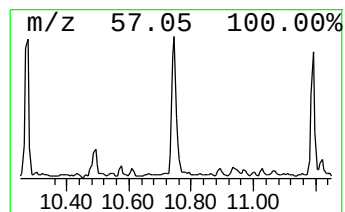
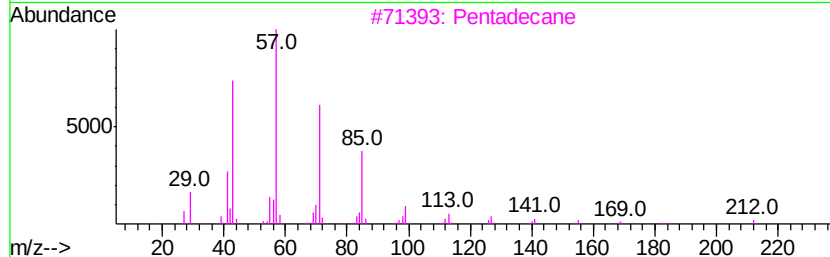
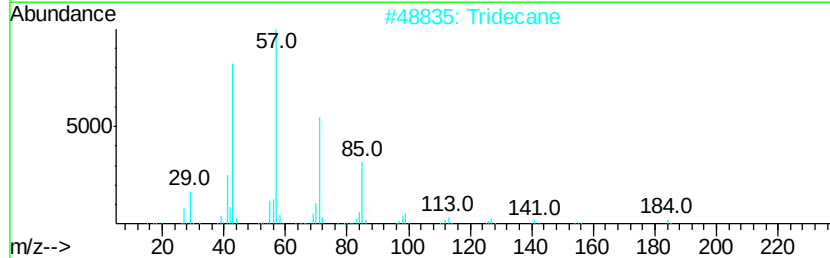
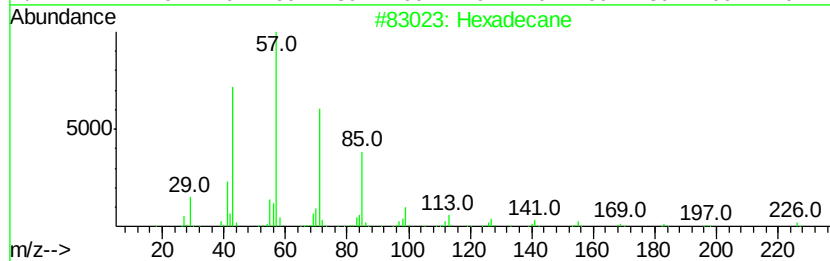
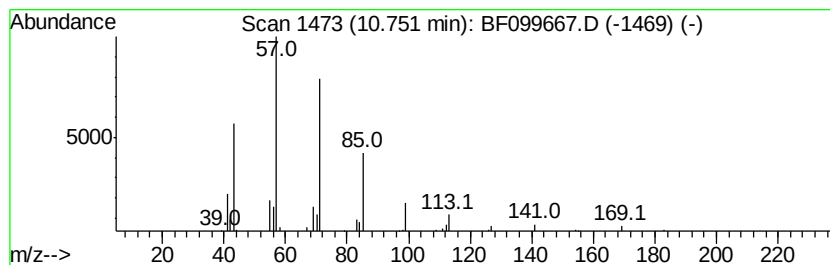
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.75	3.83 ng	103532	Phenanthrene-d10	11.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Pentadecane	212	C15H32	000629-62-9	87
4	Eicosane	282	C20H42	000112-95-8	72
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64



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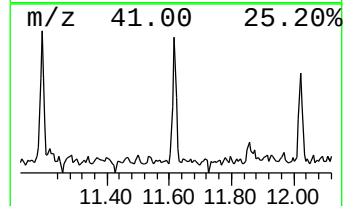
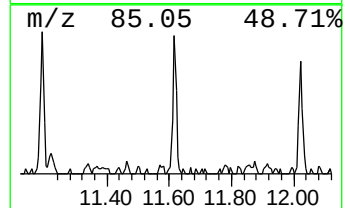
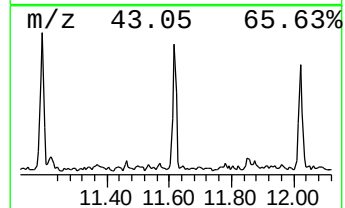
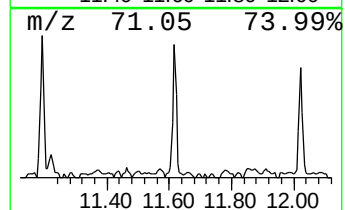
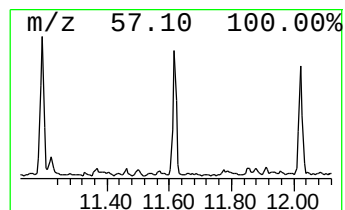
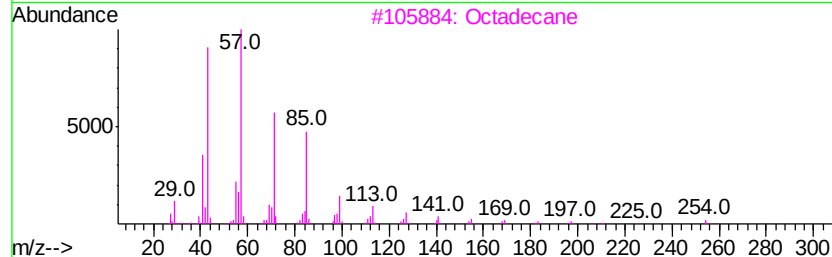
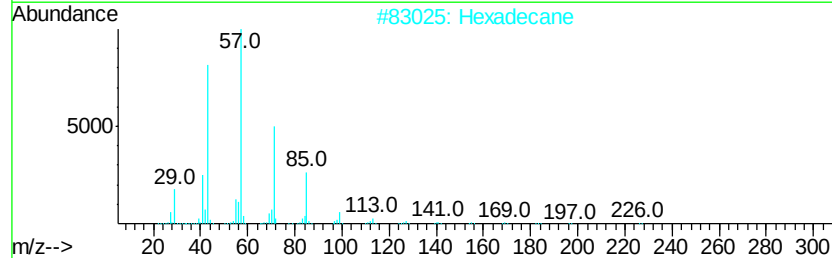
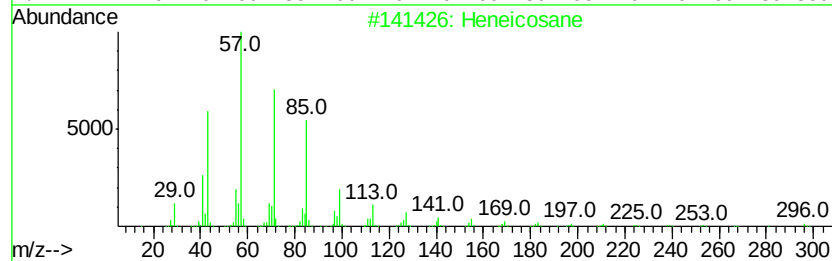
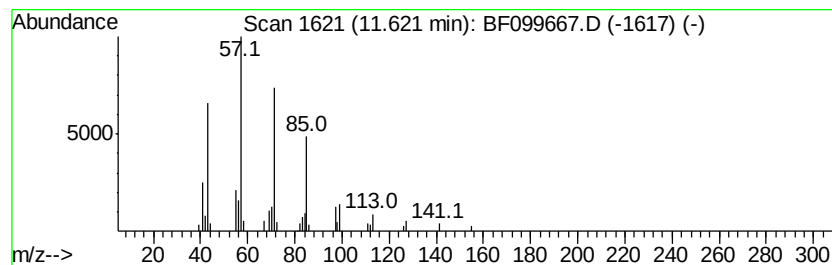
Instrument :
BNA_F
ClientSampleId :
BACKFILL-COMP-1RE

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.62	2.25 ng	60796	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
Data File : BF099667.D
Acq On : 19 Oct 2017 19:59
Operator : SJ/JU
Sample : I5924-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-COMP-1RE

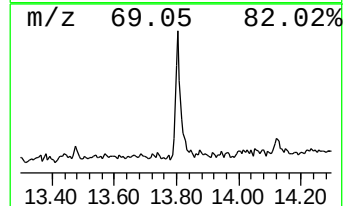
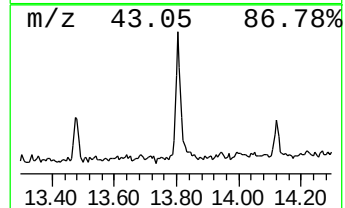
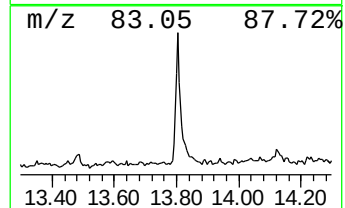
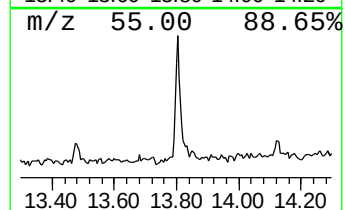
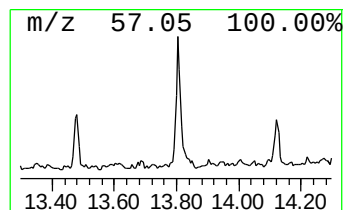
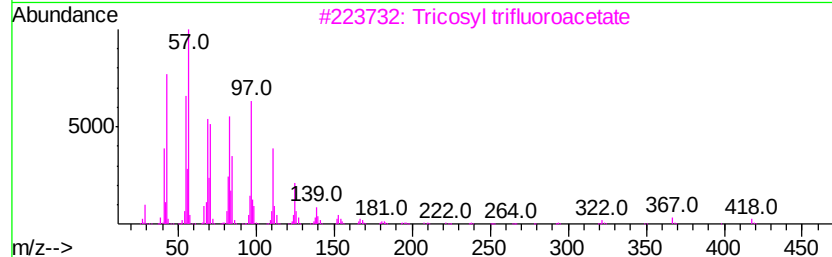
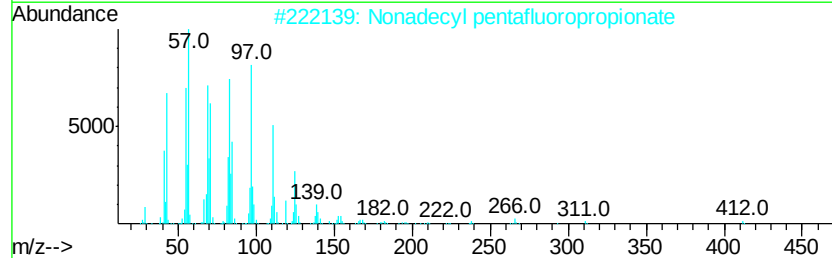
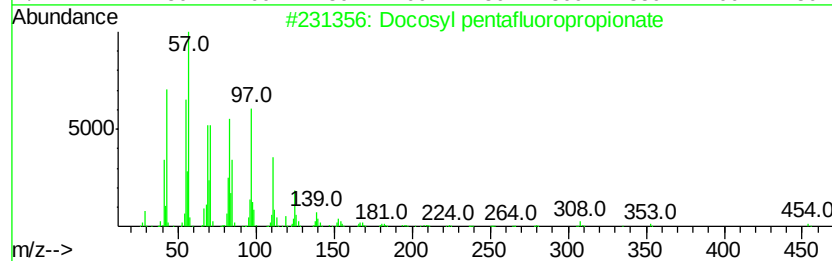
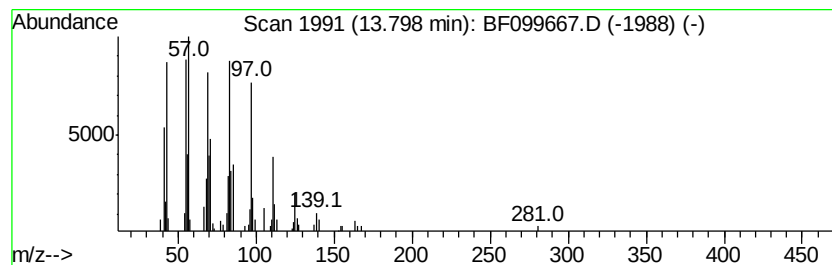
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosyl pentafluoropropionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	7.04 ng	157665	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4		Tetracosyl heptafluorobutyrte	550	C28H49F7O2	1000351-83-7	90
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
Data File : BF099667.D
Acq On : 19 Oct 2017 19:59
Operator : SJ/JU
Sample : I5924-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-COMP-1RE

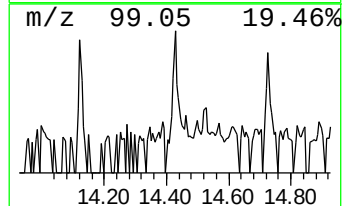
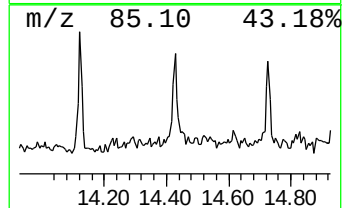
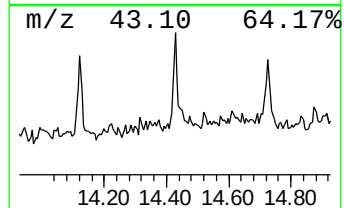
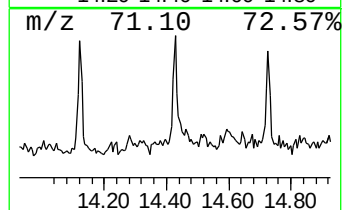
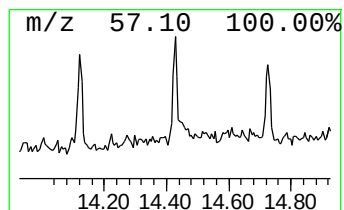
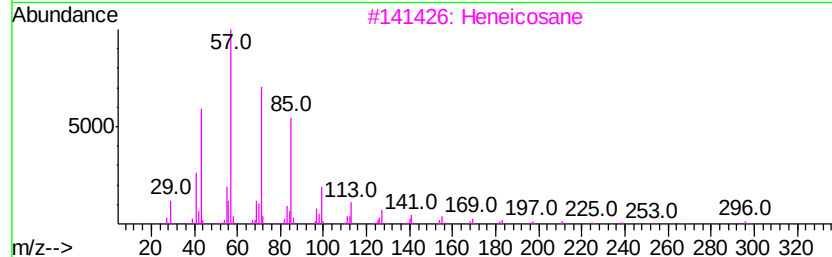
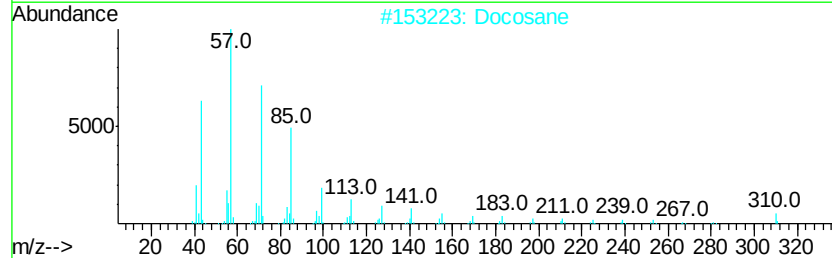
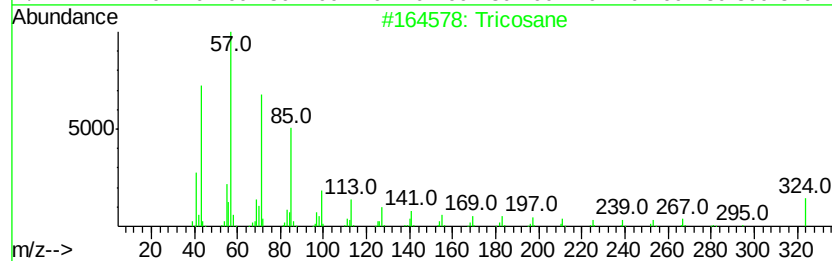
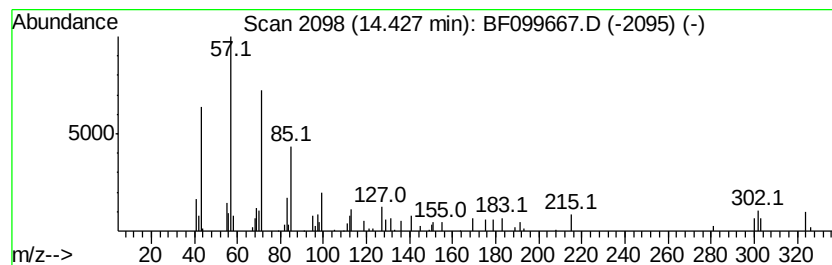
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.55 ng	57087	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	95
2		Docosane	310	C22H46	000629-97-0	74
3		Heneicosane	296	C21H44	000629-94-7	74
4		Octacosane	394	C28H58	000630-02-4	72
5		Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101917\
Data File : BF099667.D
Acq On : 19 Oct 2017 19:59
Operator : SJ/JU
Sample : I5924-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BACKFILL-COMP-1RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.04	10.3	ng	266443	1	6.82	515189	20.0
unknown6.59	6.59	63.9	ng	1644790	1	6.82	515189	20.0
Tetradecane	9.77	2.4	ng	83880	3	9.85	691282	20.0
Heptadecane	10.27	2.6	ng	88923	3	9.85	691282	20.0
Hexadecane	10.75	3.8	ng	103532	4	11.34	540980	20.0
Heneicosane	11.62	2.3	ng	60796	4	11.34	540980	20.0
Docosyl pentaflu...	13.80	7.0	ng	157665	5	13.98	447612	20.0
Tricosane	14.43	2.5	ng	57087	5	13.98	447612	20.0