

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021518\
 Data File : BF103017.D
 Acq On : 15 Feb 2018 15:06
 Operator : SJ/JU
 Sample : J1539-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MAIN-ST-LINE-2-WW@4

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-BF020318.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	2.163	7	13	26	rVB	994008	1306102	25.89%	2.731%
2	5.122	513	516	525	rVB	122898	172313	3.42%	0.360%
3	5.504	575	581	584	rBV	4361310	5045750	100.00%	10.552%
4	6.510	746	752	764	rBV	4194987	5043478	99.95%	10.547%
5	6.651	770	776	779	rBV	4470246	4907020	97.25%	10.262%
6	6.875	810	814	818	rBV	1350727	1081605	21.44%	2.262%
7	7.034	836	841	844	rBV	4089184	3676415	72.86%	7.688%
8	7.439	905	910	913	rBV	2982937	3337249	66.14%	6.979%
9	8.157	1028	1032	1038	rBV	1671681	1420404	28.15%	2.970%
10	9.233	1210	1215	1218	rBV	4902796	4756766	94.27%	9.947%
11	9.304	1224	1227	1230	rBV	115975	87191	1.73%	0.182%
12	9.622	1277	1281	1289	rVB	392260	383884	7.61%	0.803%
13	9.833	1314	1317	1321	rVB	263800	198212	3.93%	0.415%
14	9.916	1326	1331	1335	rBV	1672319	1577187	31.26%	3.298%
15	10.157	1369	1372	1375	rBV2	49272	54322	1.08%	0.114%
16	10.310	1395	1398	1400	rBV	53634	53544	1.06%	0.112%
17	10.333	1400	1402	1405	rVB	266346	204140	4.05%	0.427%
18	10.551	1435	1439	1442	rBV	67443	85609	1.70%	0.179%
19	10.704	1461	1465	1469	rBV	2758781	3042413	60.30%	6.362%
20	10.804	1480	1482	1492	rVB	205301	236153	4.68%	0.494%
21	10.957	1505	1508	1512	rVB	74487	74183	1.47%	0.155%
22	11.045	1520	1523	1528	rVB2	37707	50925	1.01%	0.106%
23	11.257	1555	1559	1561	rBV	97378	88866	1.76%	0.186%
24	11.280	1561	1563	1570	rVB	45377	57009	1.13%	0.119%
25	11.404	1580	1584	1587	rBV	1706082	1572271	31.16%	3.288%
26	11.427	1587	1588	1593	rVB2	68738	58691	1.16%	0.123%
27	11.921	1668	1672	1679	rBV3	117135	138969	2.75%	0.291%
28	12.086	1696	1700	1705	rBV	54857	54001	1.07%	0.113%
29	12.616	1787	1790	1794	rBV	68470	60435	1.20%	0.126%
30	12.992	1848	1854	1857	rBV	4011143	4473901	88.67%	9.356%
31	13.457	1928	1933	1938	rVB3	50387	68583	1.36%	0.143%
32	13.533	1943	1946	1950	rBV2	50404	64564	1.28%	0.135%
33	13.868	1999	2003	2012	rBV	981791	993678	19.69%	2.078%
34	14.045	2028	2033	2036	rBV	1534733	1451853	28.77%	3.036%

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Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-2-WW@4

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.504	2107	2111	2115	rBV	84950	105941	2.10%	0.222%
36	14.786	2155	2159	2164	rBV	415088	439503	8.71%	0.919%
37	15.521	2279	2284	2293	rVB2	959718	1223741	24.25%	2.559%
38	16.021	2365	2369	2377	rVV2	96915	172326	3.42%	0.360%

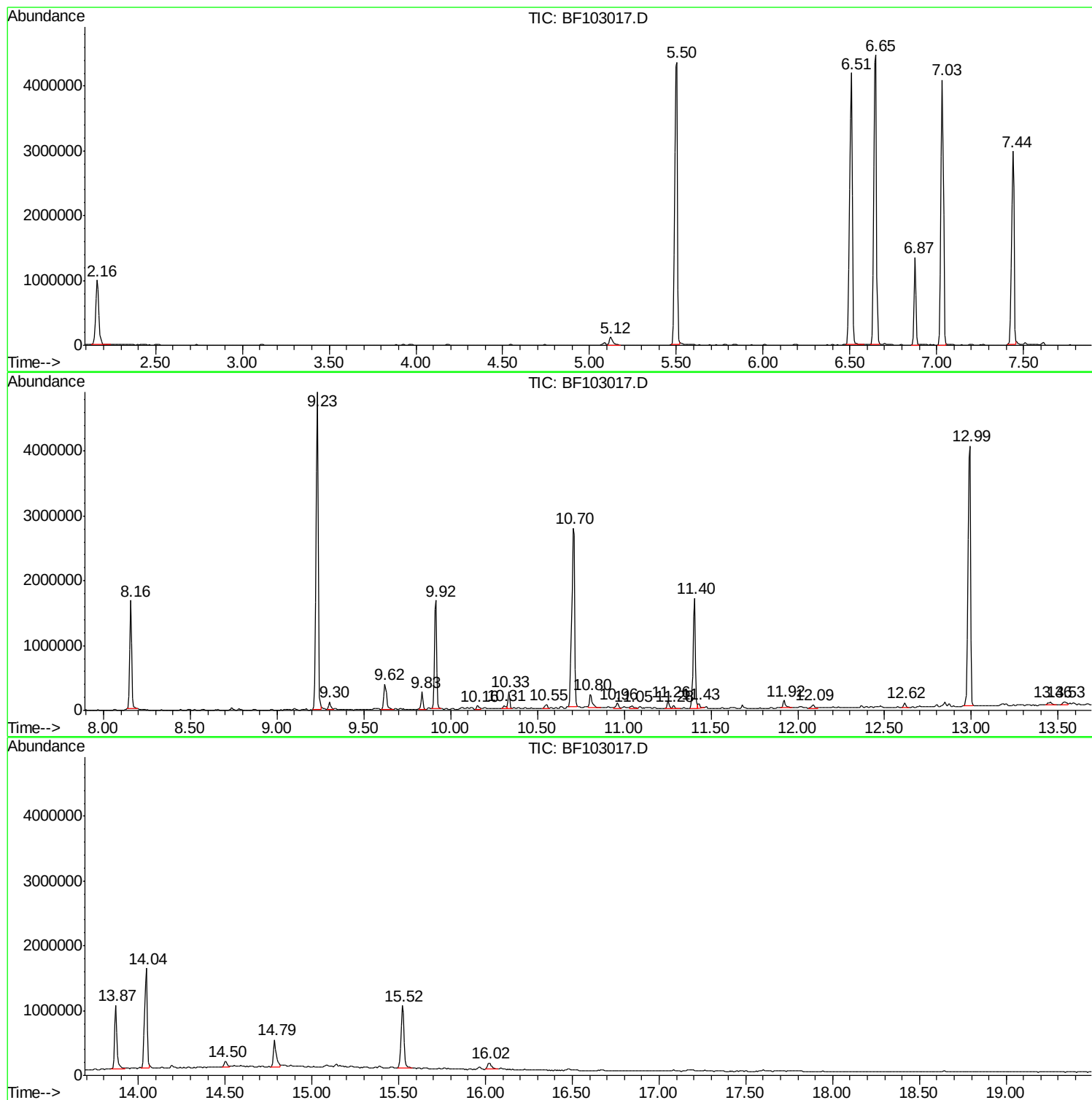
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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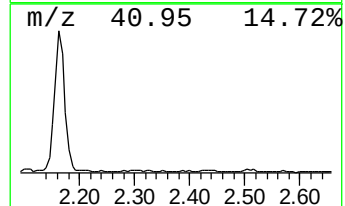
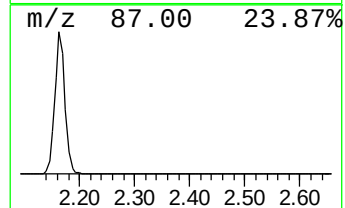
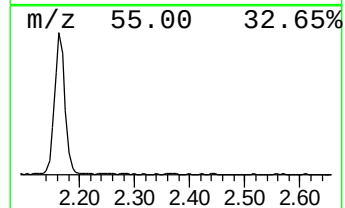
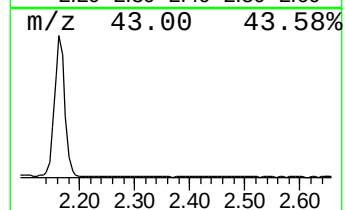
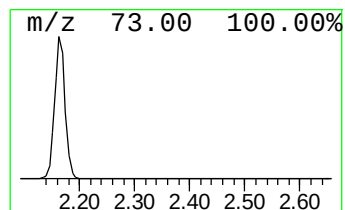
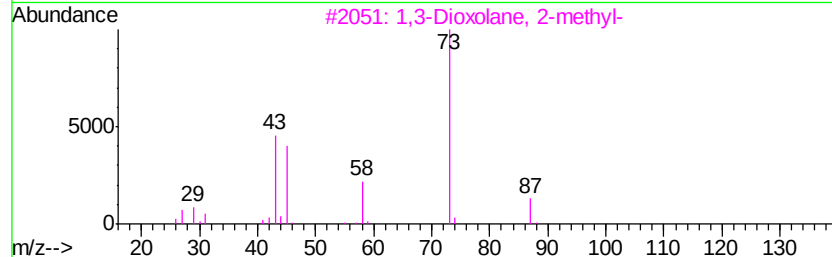
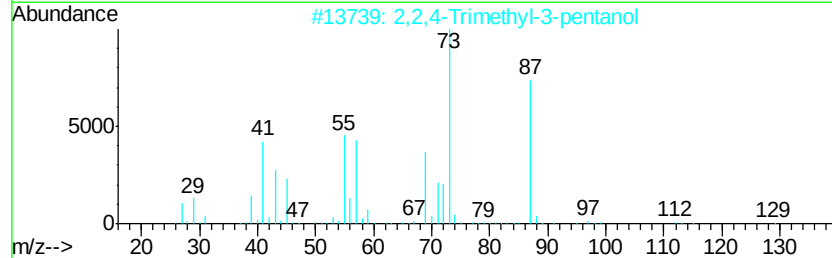
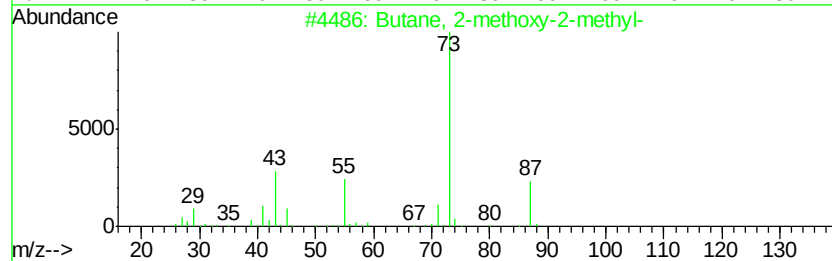
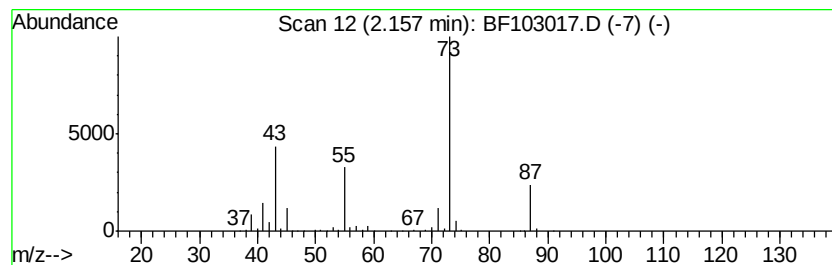
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	24.15 ng	1306100	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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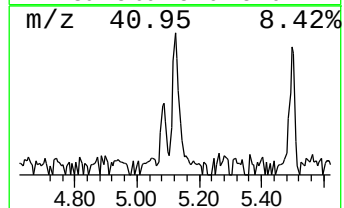
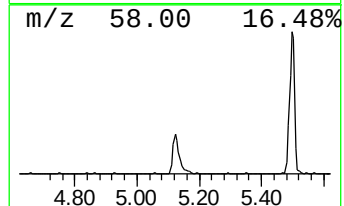
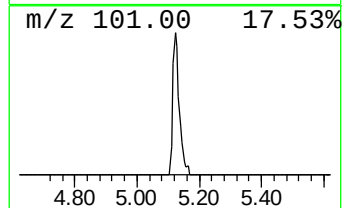
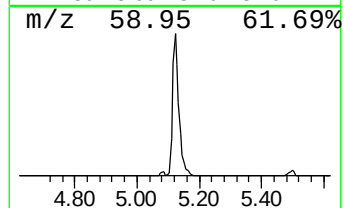
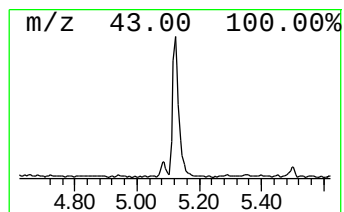
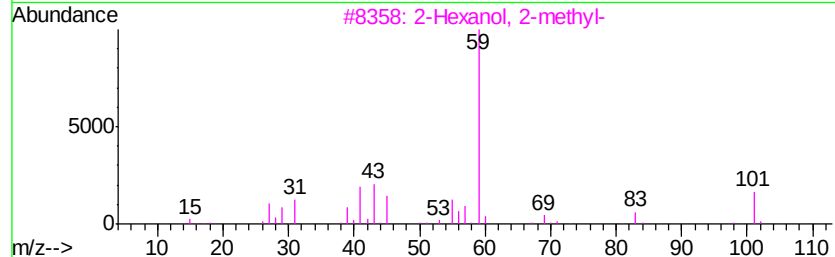
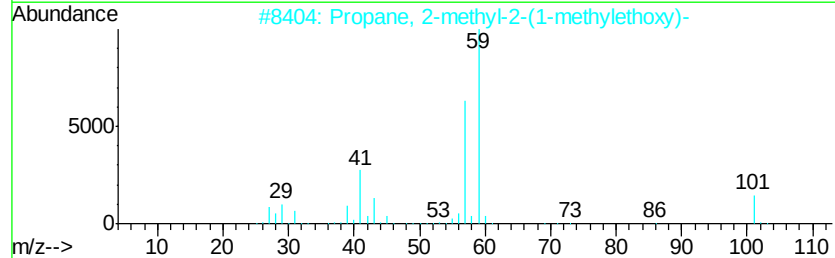
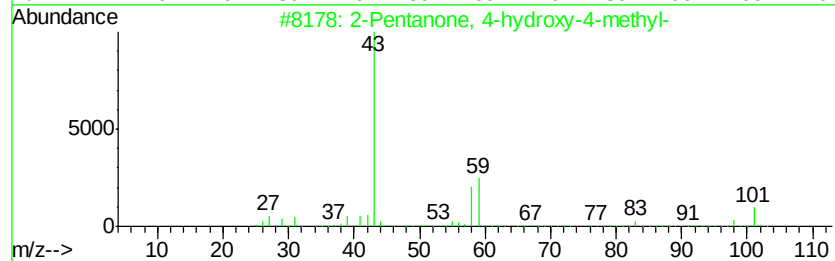
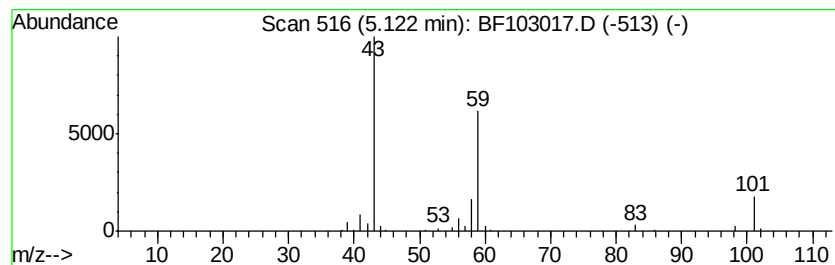
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.19 ng	172313	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		Guanidine	59	CH5N3	000113-00-8	9



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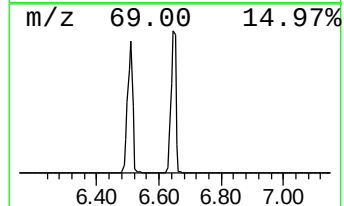
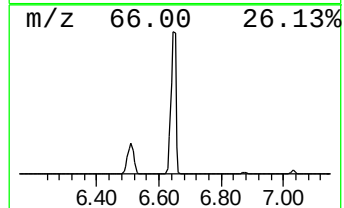
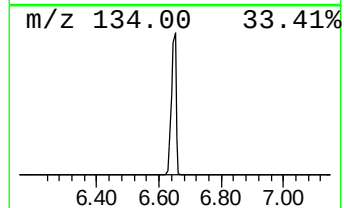
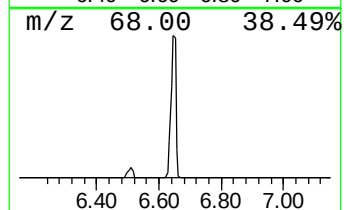
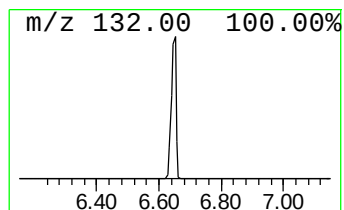
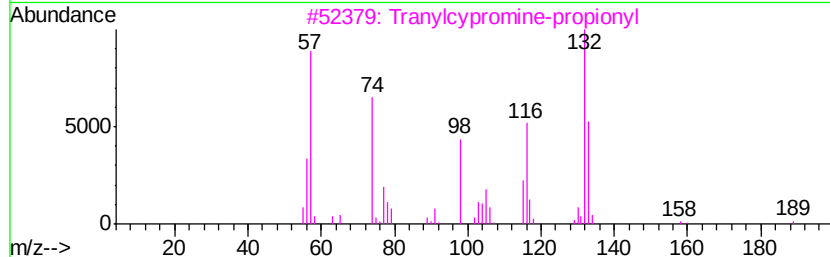
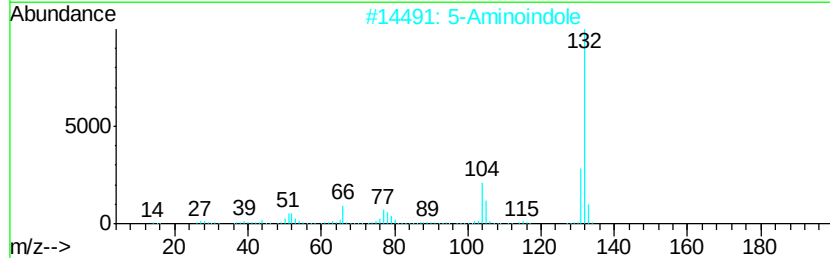
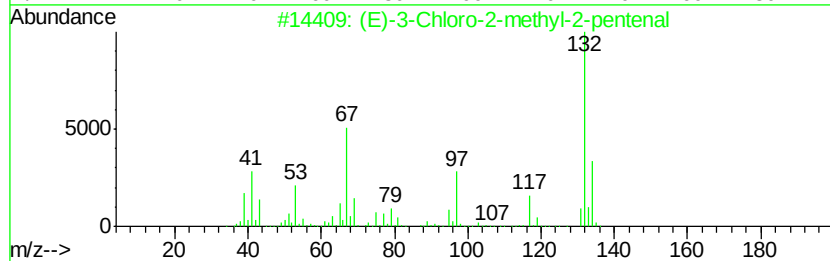
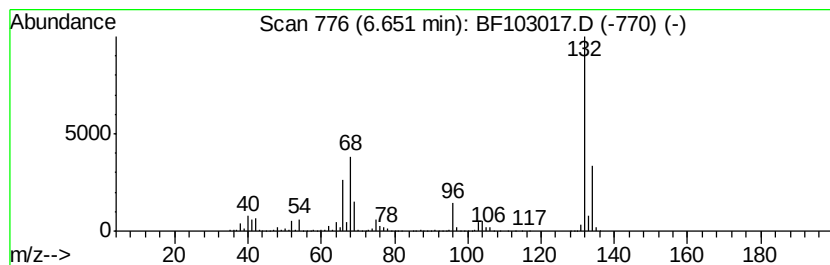
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	90.74 ng	4907020	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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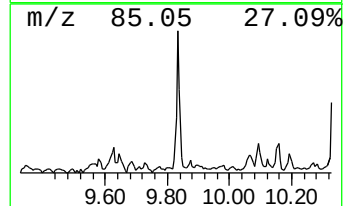
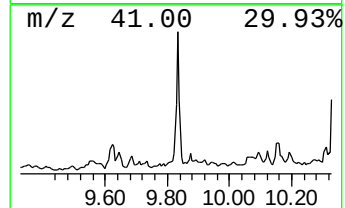
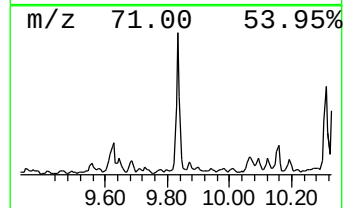
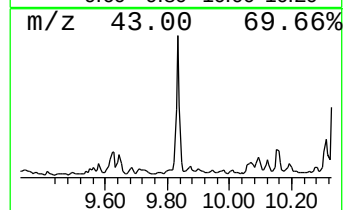
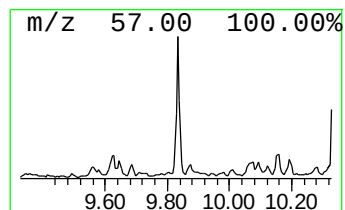
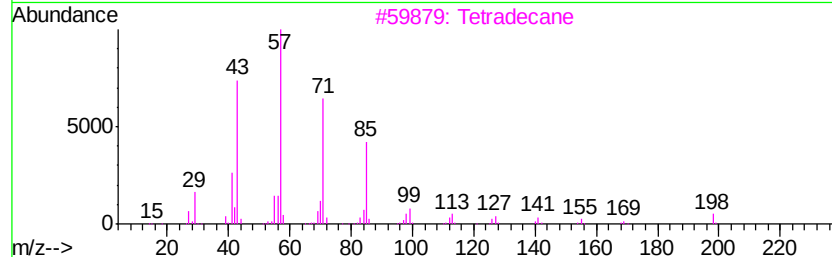
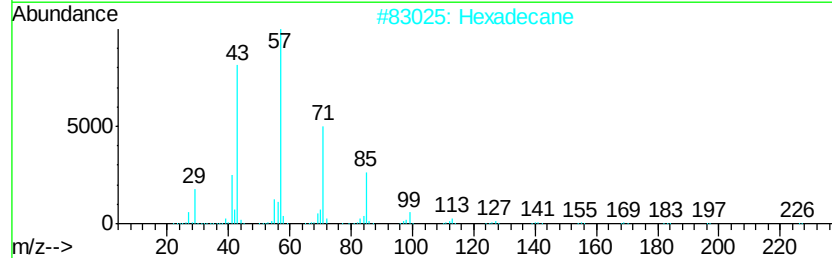
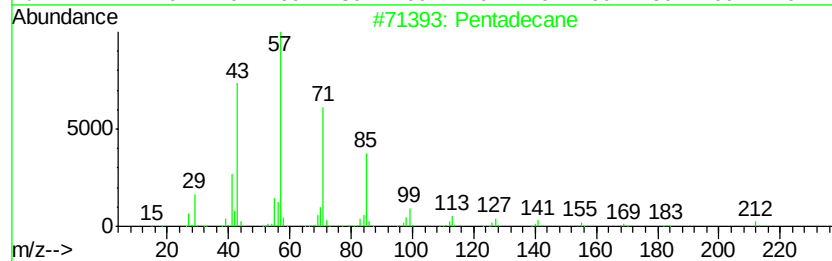
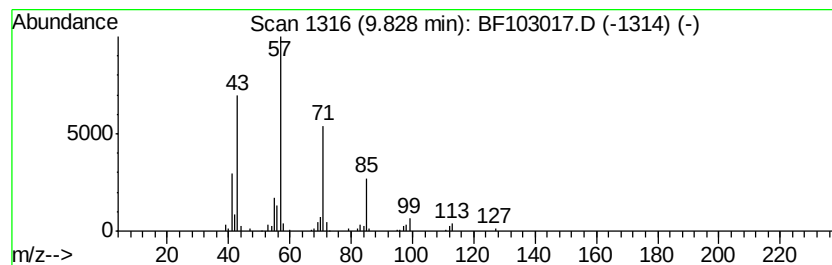
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.51 ng	198212	Acenaphthene-d10	9.92
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	Tetradecane	198 C14H30	000629-59-4	90
4	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	86
5	Tridecane, 6-methyl-	198 C14H30	013287-21-3	78



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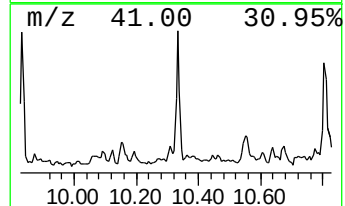
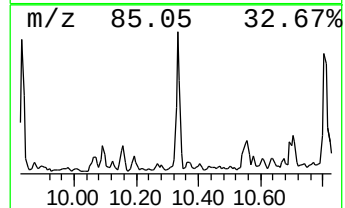
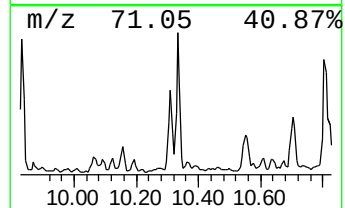
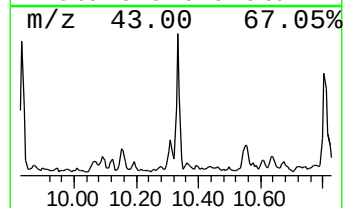
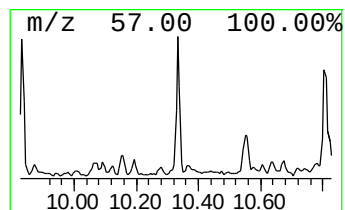
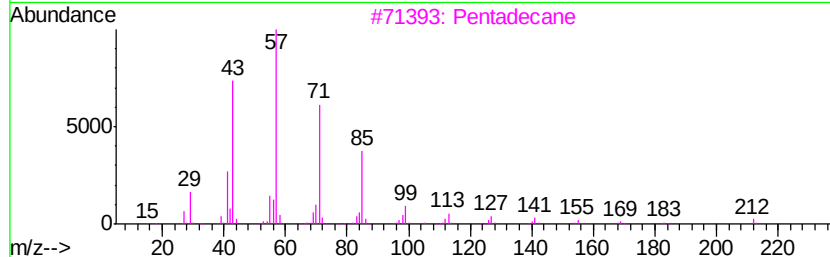
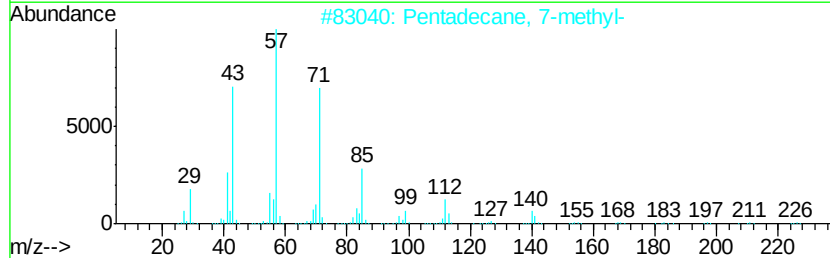
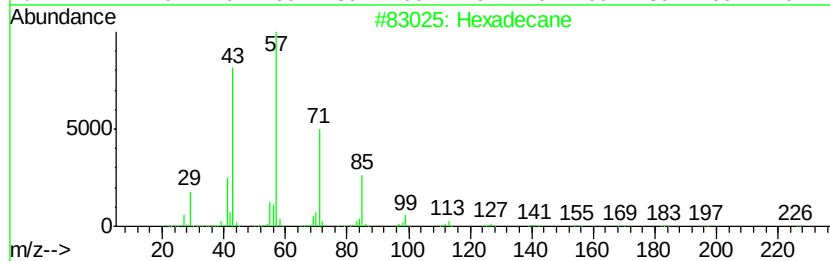
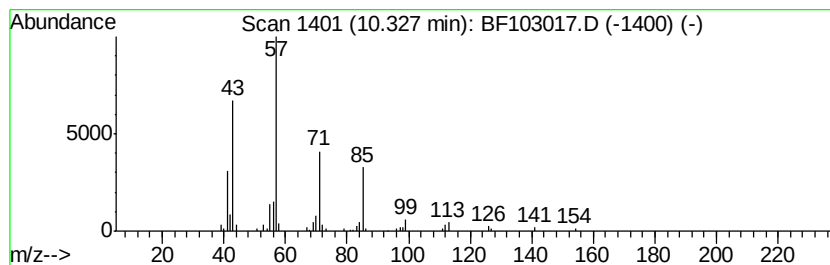
Instrument :
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Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.59 ng	204140	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	96
2	Pentadecane, 7-methyl-	226 C16H34	006165-40-8	91
3	Pentadecane	212 C15H32	000629-62-9	90
4	Tetradecane	198 C14H30	000629-59-4	90
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	86



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Acq On : 15 Feb 2018 15:06
Operator : SJ/JU
Sample : J1539-03
Misc :
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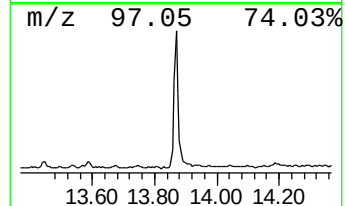
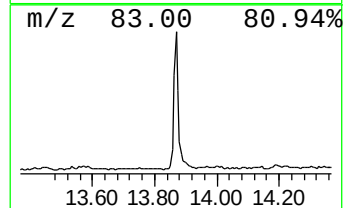
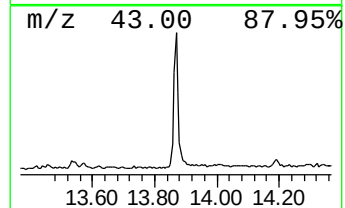
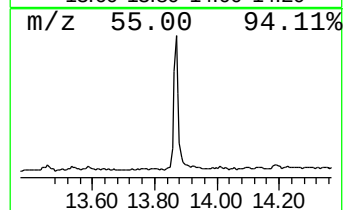
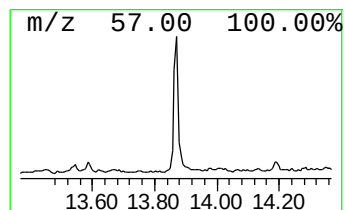
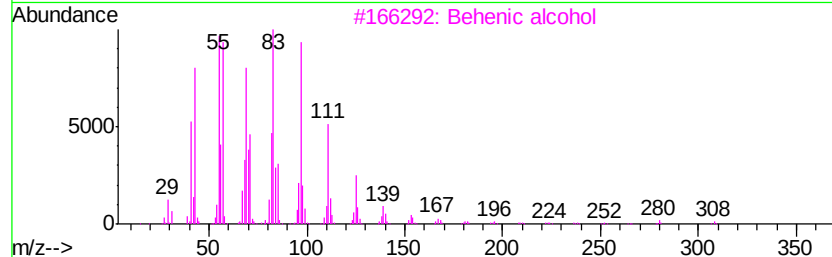
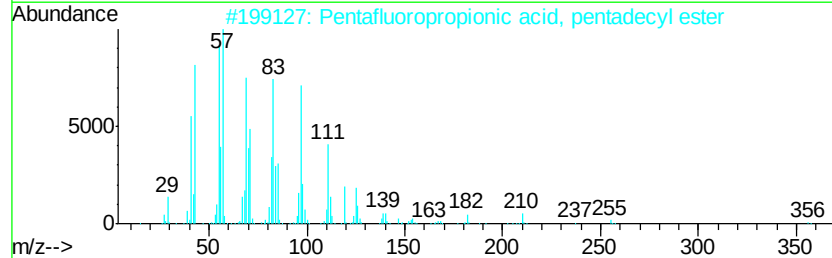
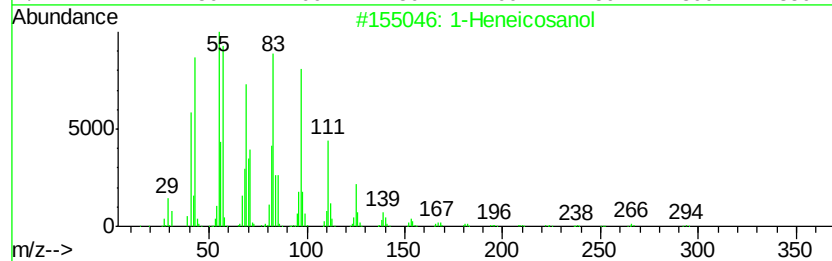
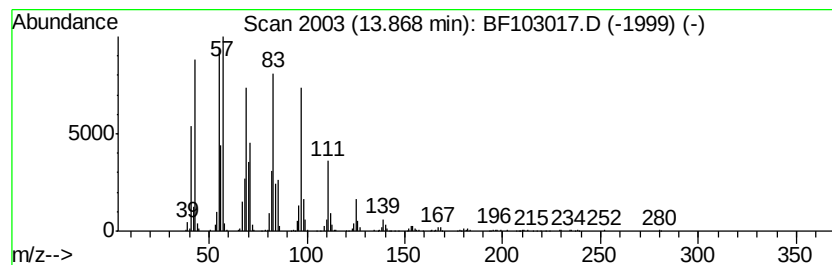
Instrument :
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ClientSampleId :
MAIN-ST-LINE-2-WW@4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	13.69 ng	993678	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1	91
3	Behenic alcohol	326 C22H46O	000661-19-8	91
4	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	91
5	n-Tetracosanol-1	354 C24H50O	000506-51-4	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103017.D
Acq On : 15 Feb 2018 15:06
Operator : SJ/JU
Sample : J1539-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-2-WW@4

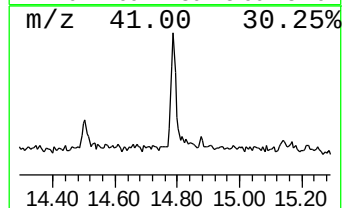
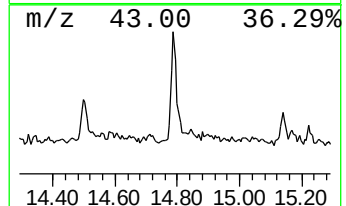
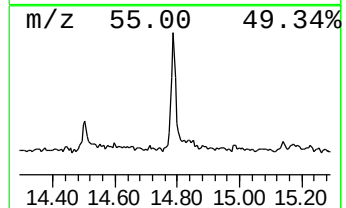
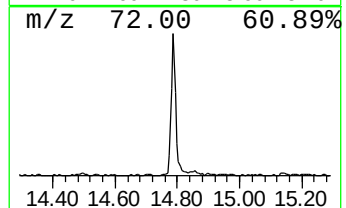
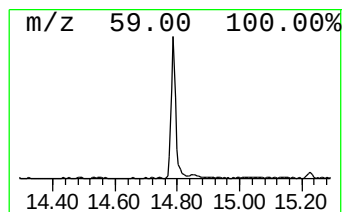
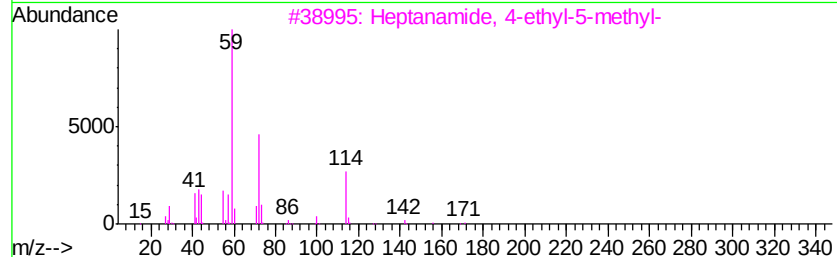
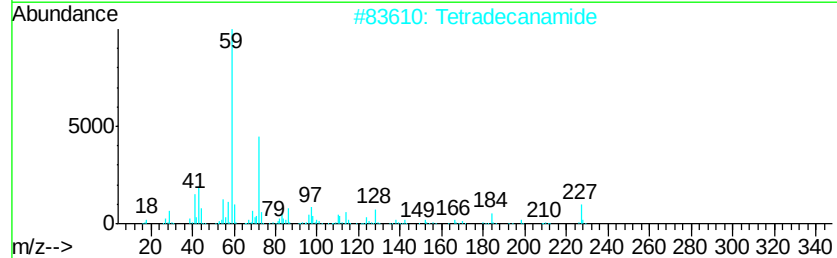
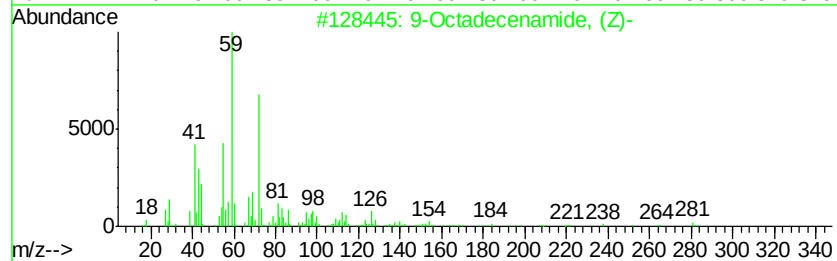
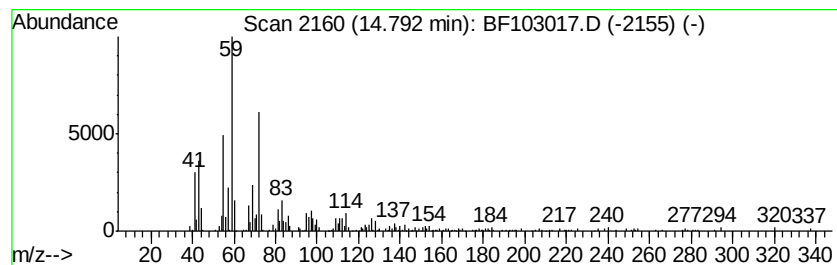
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	7.18 ng	439503	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Nonanamide	157	C9H19NO	001120-07-6	58



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021518\
 Data File : BF103017.D
 Acq On : 15 Feb 2018 15:06
 Operator : SJ/JU
 Sample : J1539-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MAIN-ST-LINE-2-WW@4

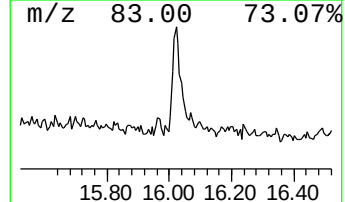
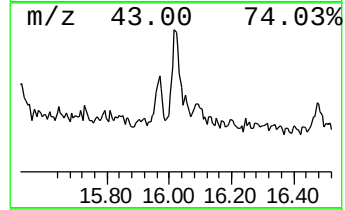
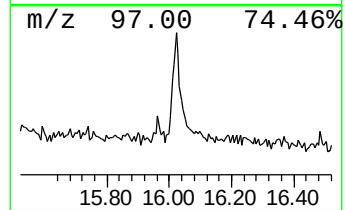
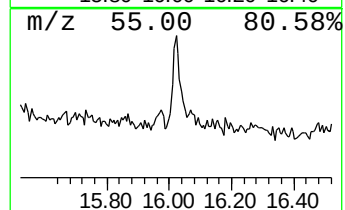
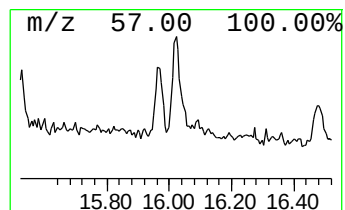
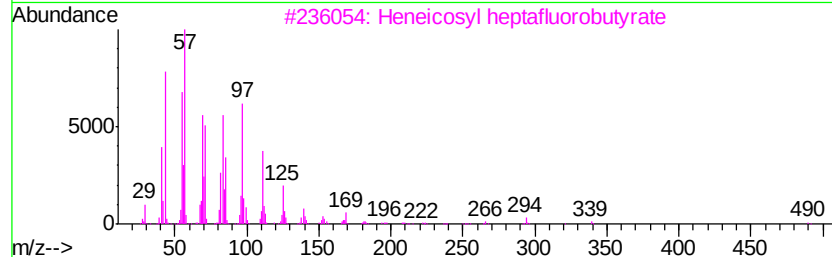
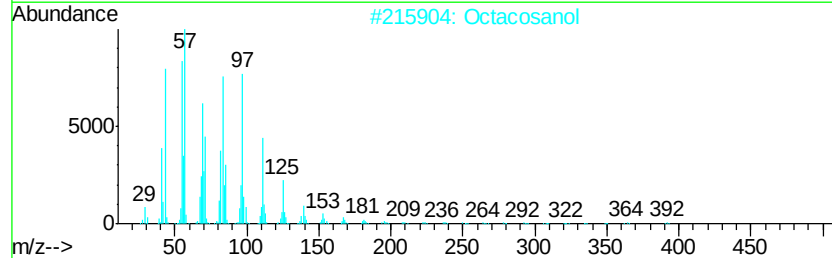
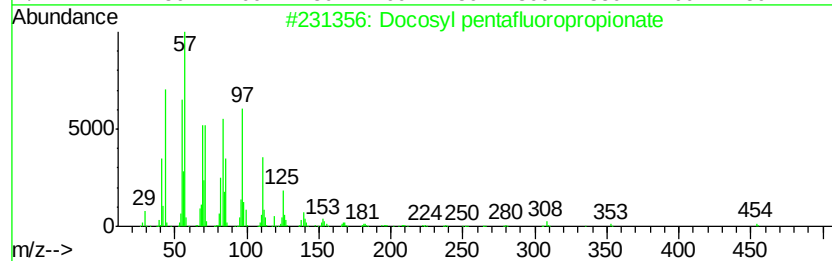
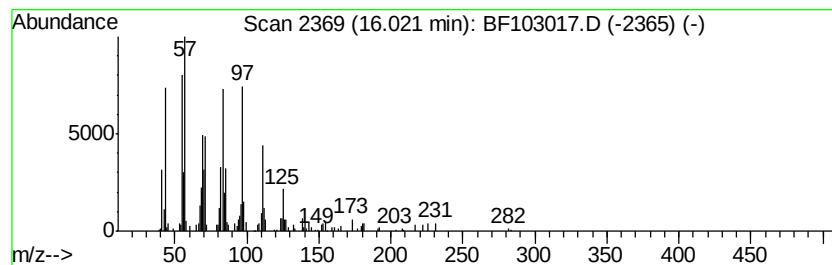
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Docosyl pentafluoropropionate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.82 ng	172326	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
2		Octacosanol	410	C28H58O	000557-61-9	94
3		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	94
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
5		Octacosyl acetate	452	C30H60O2	018206-97-8	94



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103017.D
Acq On : 15 Feb 2018 15:06
Operator : SJ/JU
Sample : J1539-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MAIN-ST-LINE-2-WW@4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.16	24.1	ng	1306100	1	6.87	1081610	20.0
2-Pentanone, 4-hy...	5.12	3.2	ng	172313	1	6.87	1081610	20.0
unknown6.65	6.65	90.7	ng	4907020	1	6.87	1081610	20.0
Pentadecane	9.83	2.5	ng	198212	3	9.92	1577190	20.0
Hexadecane	10.33	2.6	ng	204140	3	9.92	1577190	20.0
1-Heneicosanol	13.87	13.7	ng	993678	5	14.04	1451850	20.0
9-Octadecenamide, ...	14.79	7.2	ng	439503	6	15.52	1223740	20.0
Docosyl pentafluo...	16.02	2.8	ng	172326	6	15.52	1223740	20.0