

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
 Data File : BF111195.D
 Acq On : 7 Dec 2018 19:05
 Operator : JU/SJ
 Sample : J6214-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9(18-20)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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	3.216	189	192	213	rBV	193365	449941	3.42%	0.438%
2	5.016	489	498	510	rVB	546060	802174	6.11%	0.780%
3	5.422	561	567	570	rBV	10613529	10898095	82.96%	10.599%
4	6.434	733	739	744	rBV2	10640015	13137278	100.00%	12.777%
5	6.575	758	763	766	rBV	11345072	11121695	84.66%	10.817%
6	6.804	798	802	805	rBV	2695749	2110145	16.06%	2.052%
7	6.963	825	829	832	rVB	8560473	7219823	54.96%	7.022%
8	7.363	892	897	900	rBV	6842902	6527721	49.69%	6.349%
9	8.087	1016	1020	1023	rBV	3361336	2795476	21.28%	2.719%
10	9.163	1198	1203	1206	rBV	12221696	11398091	86.76%	11.086%
11	9.551	1266	1269	1273	rBV	1947216	1667676	12.69%	1.622%
12	9.839	1314	1318	1322	rVB	3822731	3094405	23.55%	3.010%
13	10.628	1447	1452	1455	rBV	6975616	6481091	49.33%	6.303%
14	11.322	1566	1570	1573	rBV	3799758	3117266	23.73%	3.032%
15	11.857	1656	1661	1670	rBV	2017637	1943794	14.80%	1.891%
16	12.527	1772	1775	1779	rBV	201464	238222	1.81%	0.232%
17	12.639	1790	1794	1807	rBV	1650487	1676375	12.76%	1.630%
18	12.757	1812	1814	1818	rVB	188999	163877	1.25%	0.159%
19	12.910	1835	1840	1843	rBV	10973291	10295278	78.37%	10.013%
20	13.816	1990	1994	2001	rBV2	647706	797884	6.07%	0.776%
21	13.957	2011	2018	2021	rBV	2707900	2646176	20.14%	2.574%
22	14.139	2045	2049	2054	rBV	275747	261194	1.99%	0.254%
23	14.445	2098	2101	2106	rBV2	321914	329350	2.51%	0.320%
24	14.745	2149	2152	2156	rVB	259908	247603	1.88%	0.241%
25	15.080	2205	2209	2212	rBV	230011	254732	1.94%	0.248%
26	15.398	2257	2263	2268	rBV	1926160	2326028	17.71%	2.262%
27	15.451	2268	2272	2278	rVB	223826	269541	2.05%	0.262%
28	15.874	2340	2344	2349	rBV	167419	239206	1.82%	0.233%
29	15.927	2350	2353	2363	rVB9	67184	156777	1.19%	0.152%
30	16.368	2424	2428	2435	rVB3	93698	151663	1.15%	0.148%

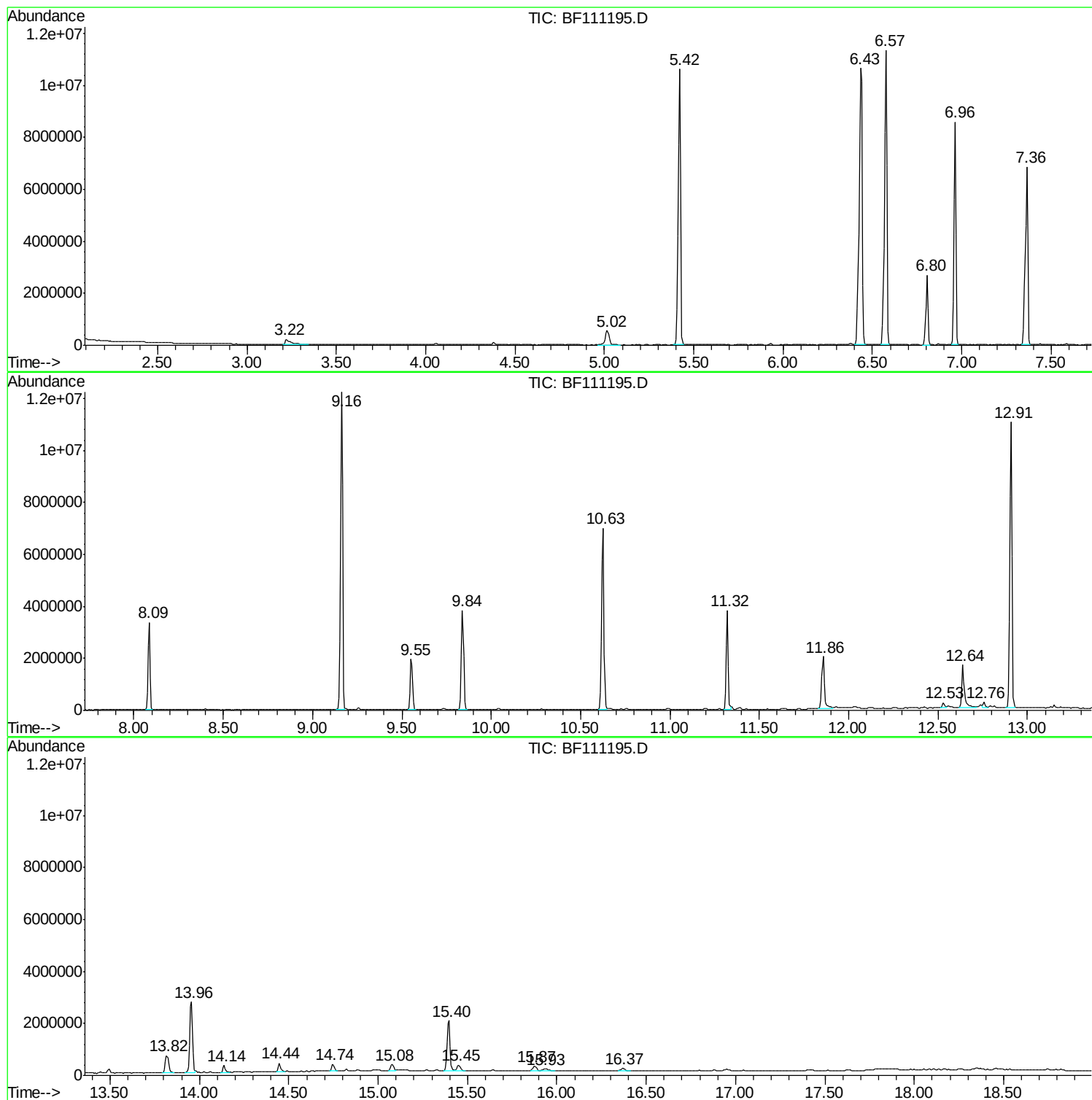
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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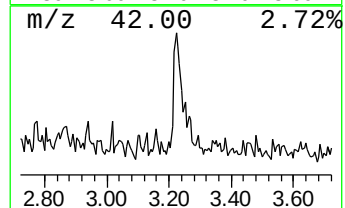
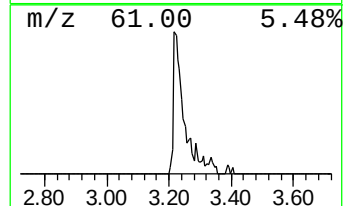
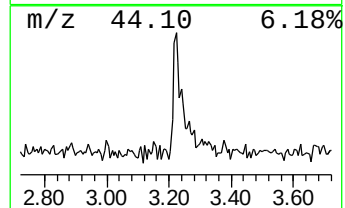
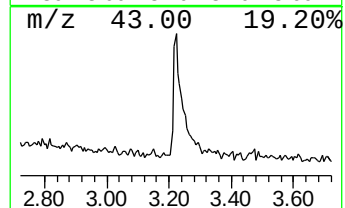
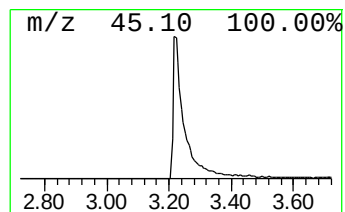
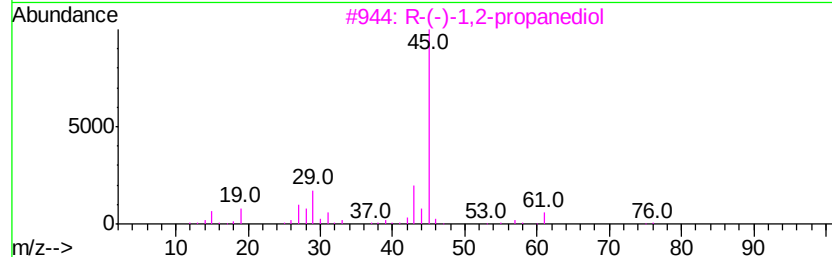
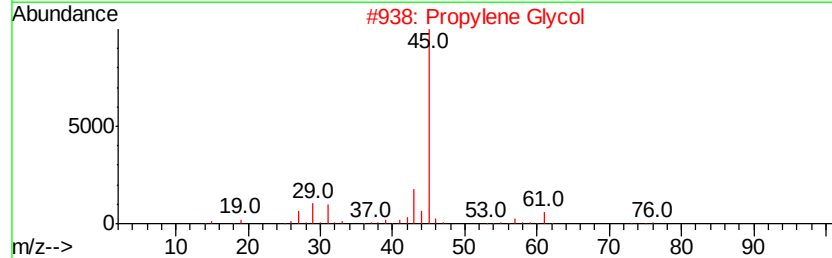
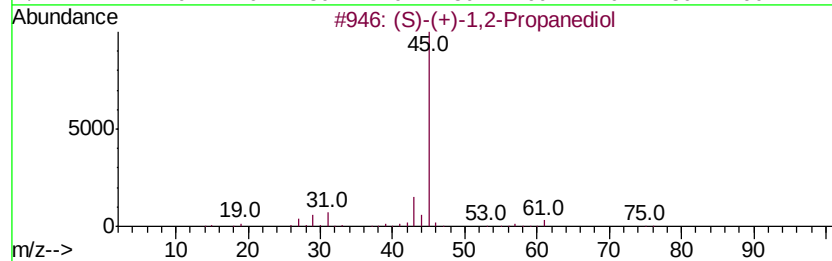
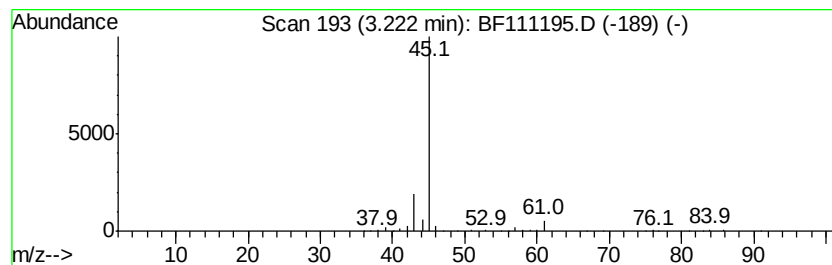
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	4.26 ng	449941	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2	Propylene Glycol	76	C3H8O2	000057-55-6	32
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9



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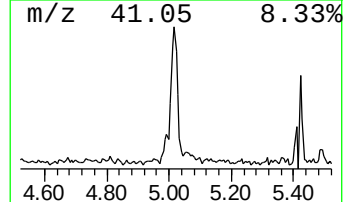
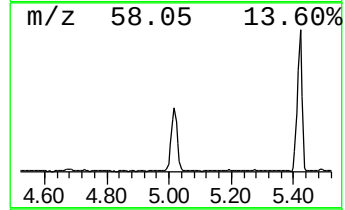
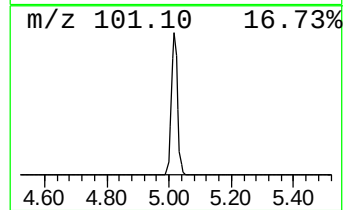
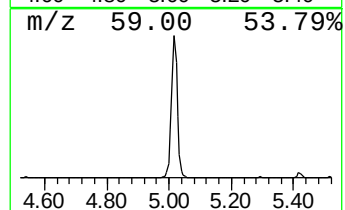
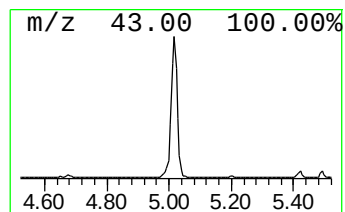
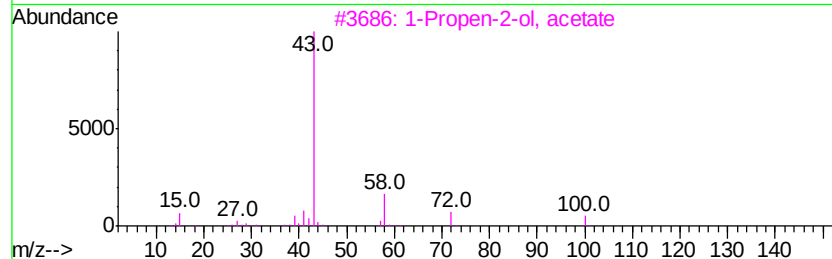
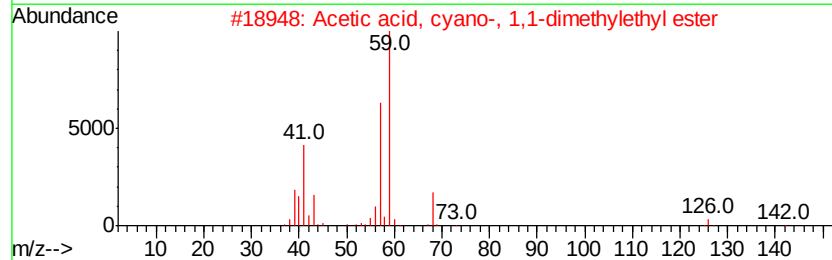
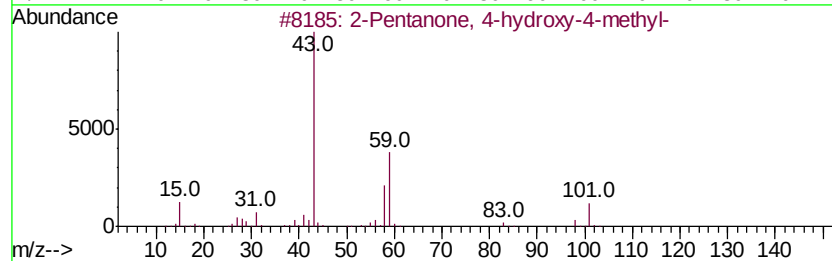
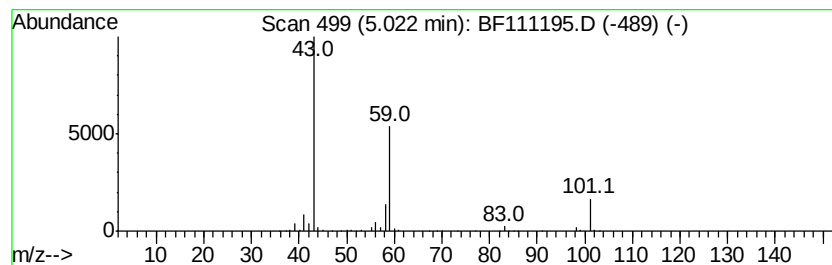
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	7.60 ng	802174	1,4-Dichlorobenzene-d4	6.80	
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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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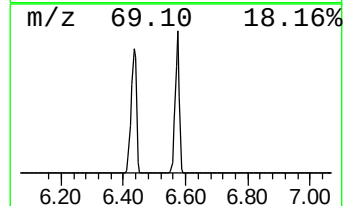
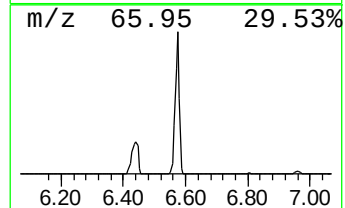
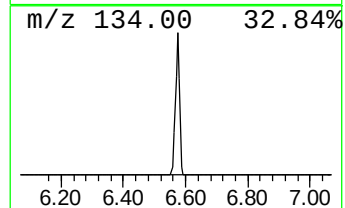
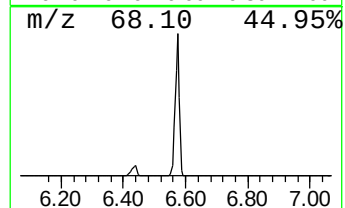
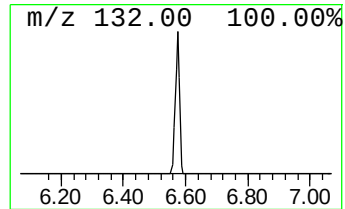
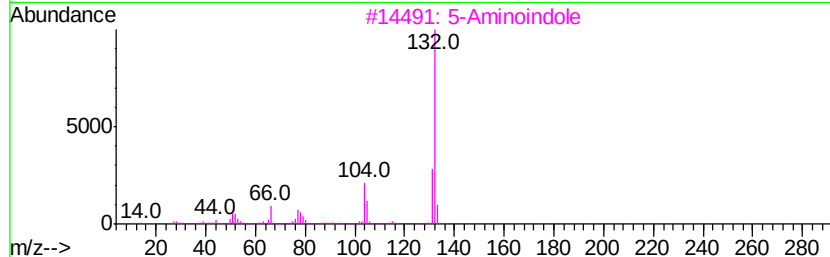
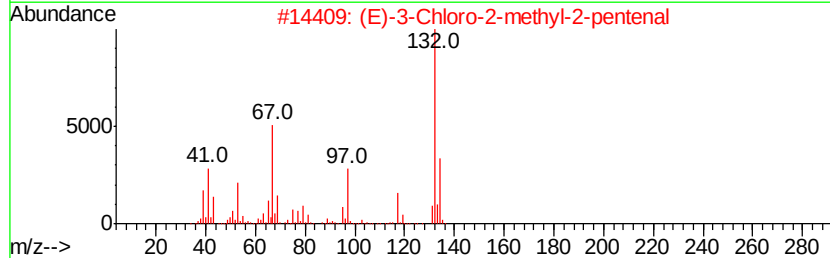
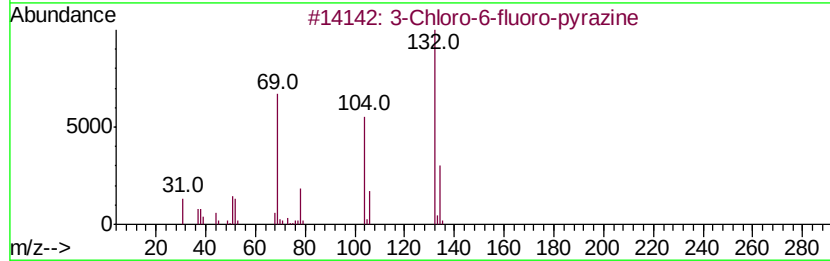
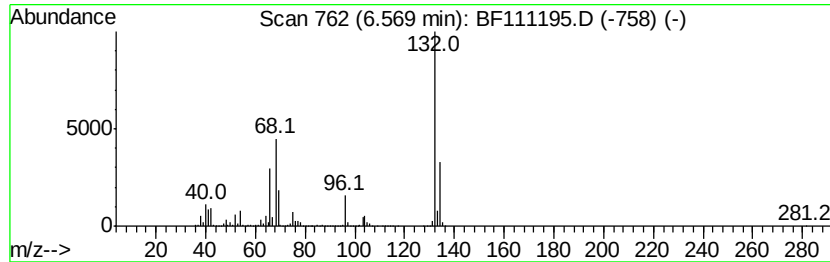
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Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	105.41 ng	11121700	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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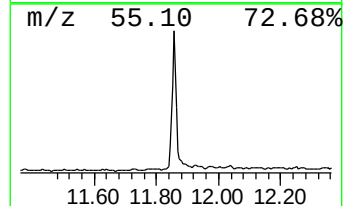
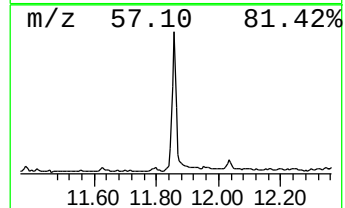
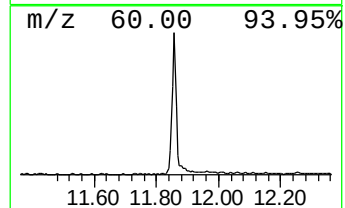
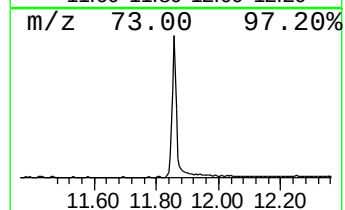
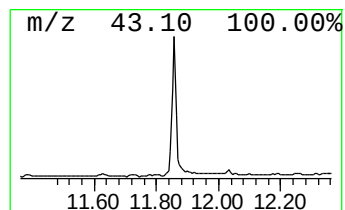
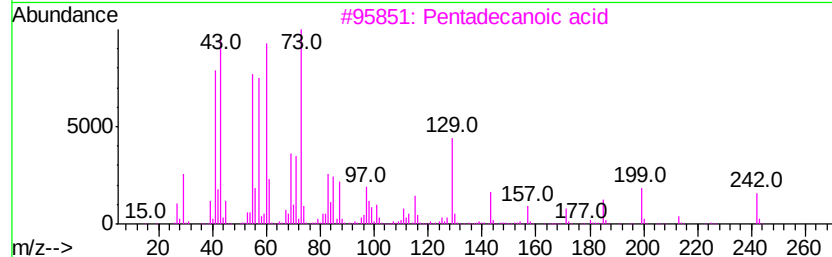
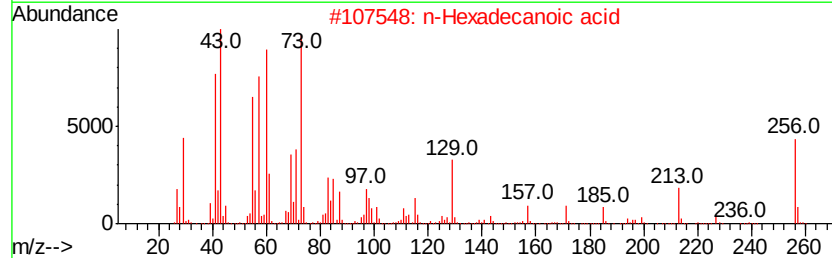
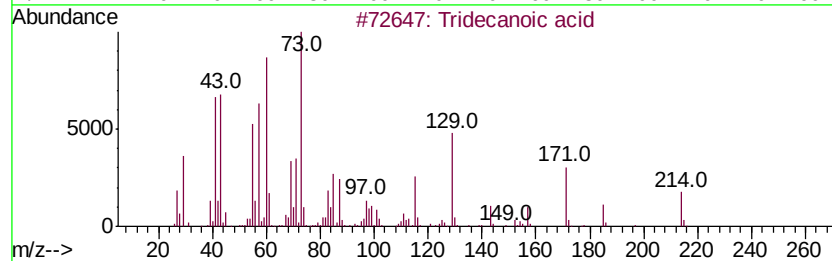
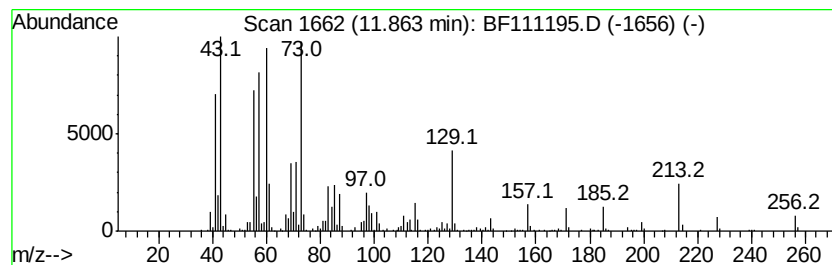
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Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	12.47 ng	1943790	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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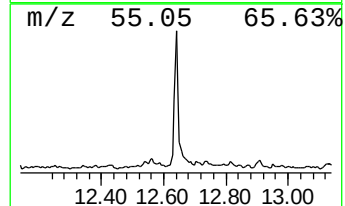
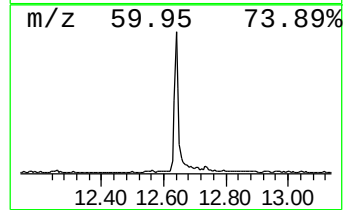
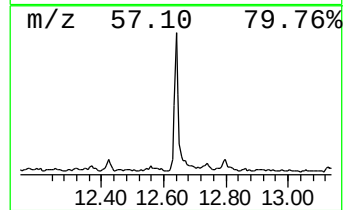
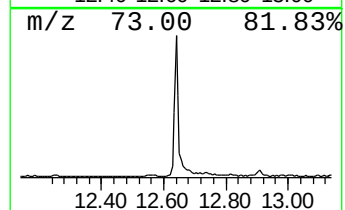
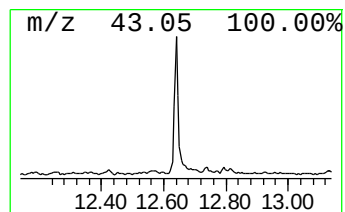
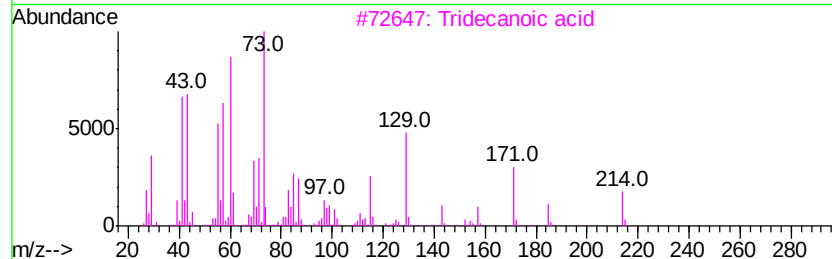
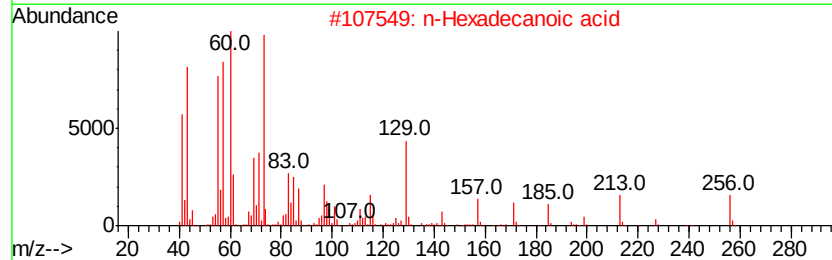
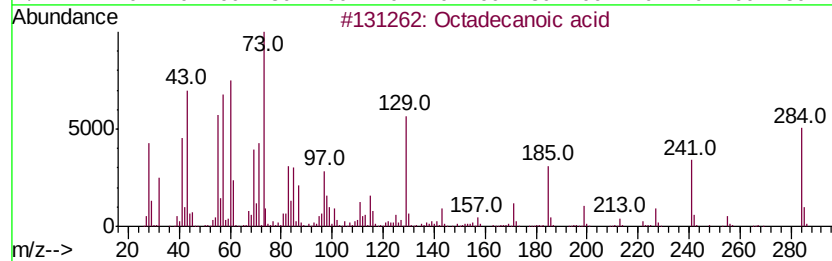
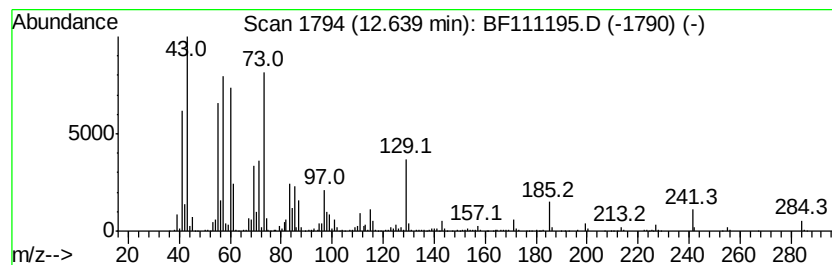
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	10.76 ng	1676380	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	74
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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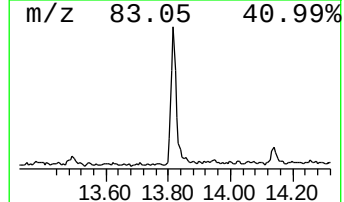
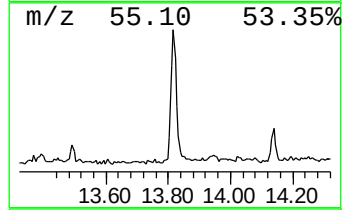
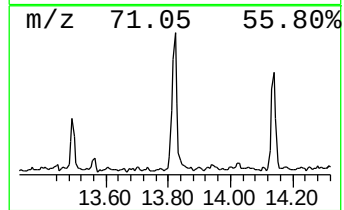
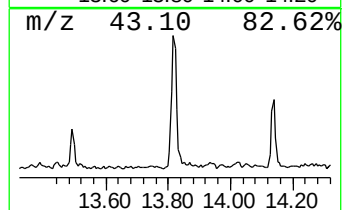
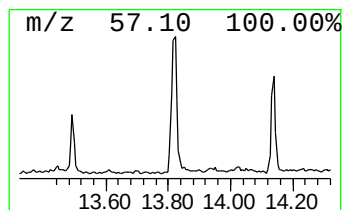
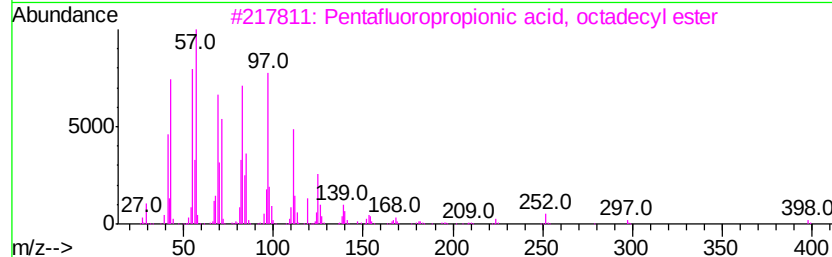
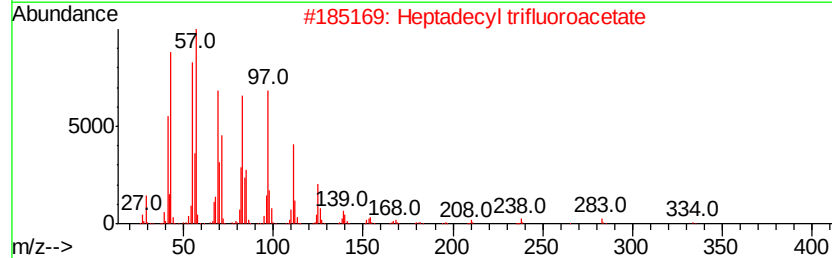
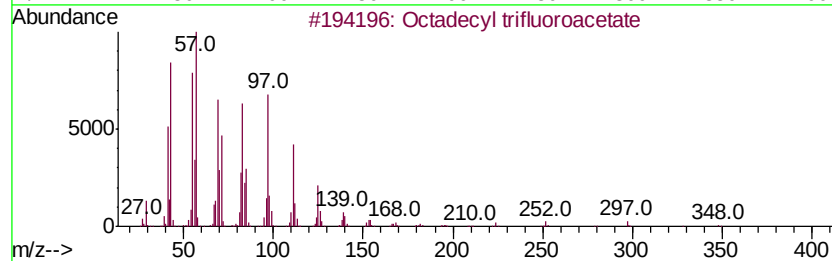
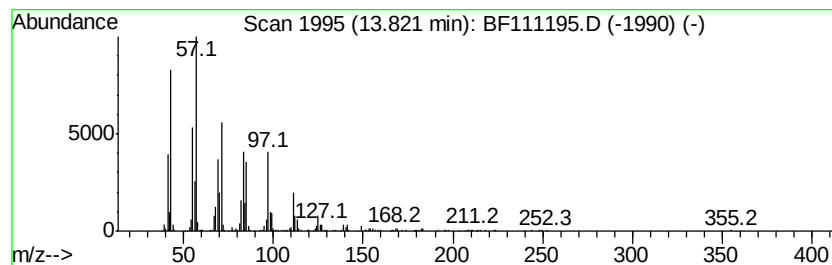
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ClientSampleId :
SB-9(18-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	6.03 ng	797884	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
Operator : JU/SJ
Sample : J6214-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(18-20)

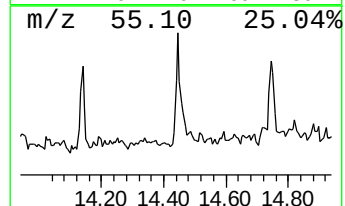
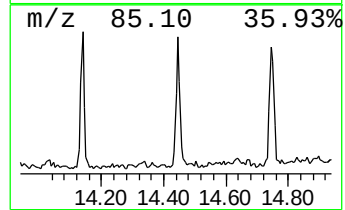
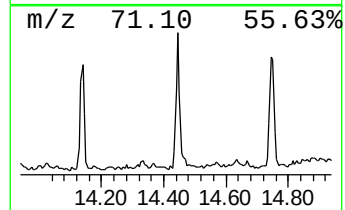
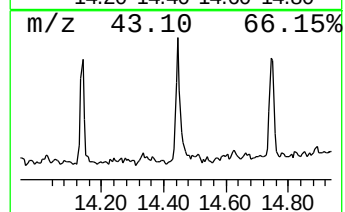
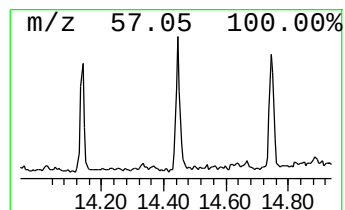
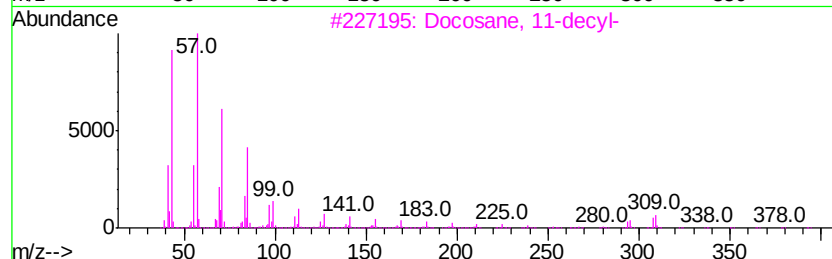
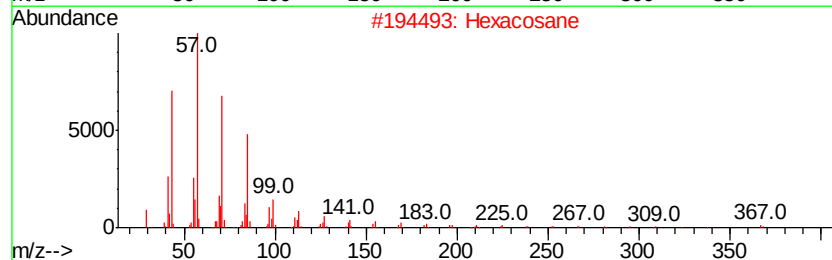
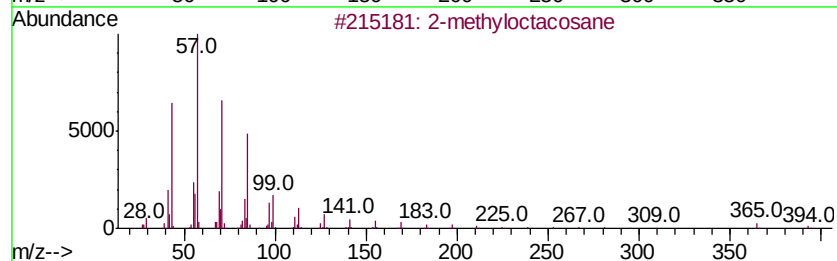
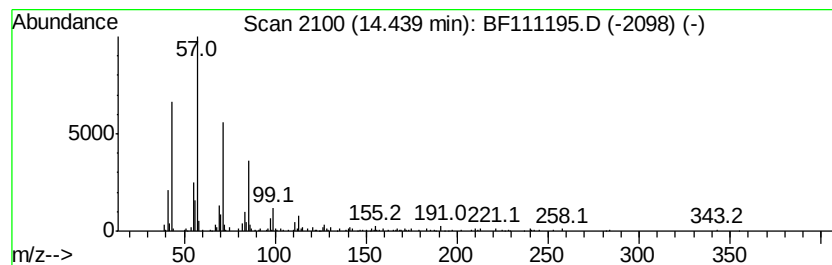
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.49 ng	329350	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Docosane, 11-decyl-	451	C32H66	055401-55-3	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
Operator : JU/SJ
Sample : J6214-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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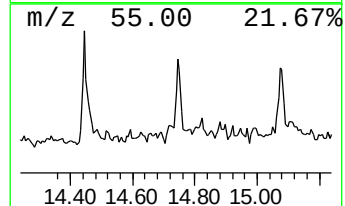
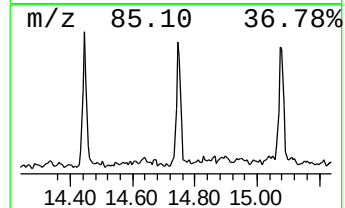
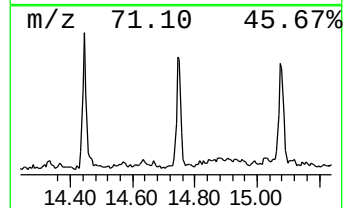
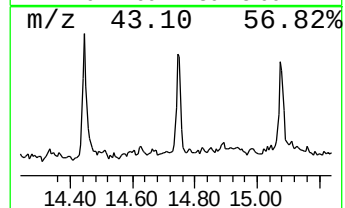
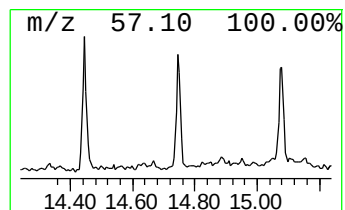
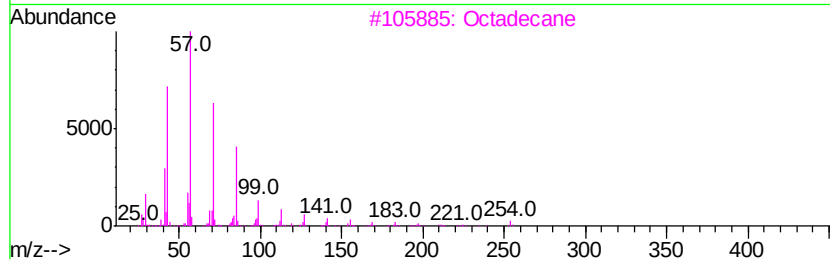
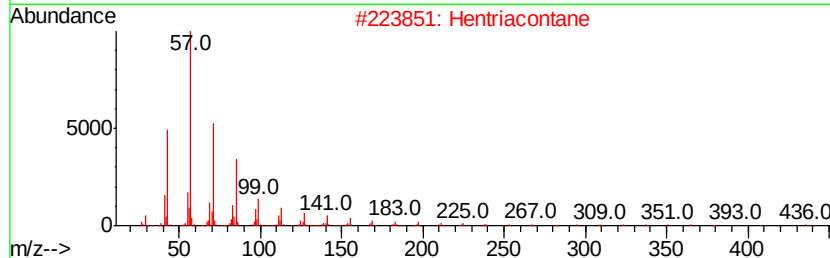
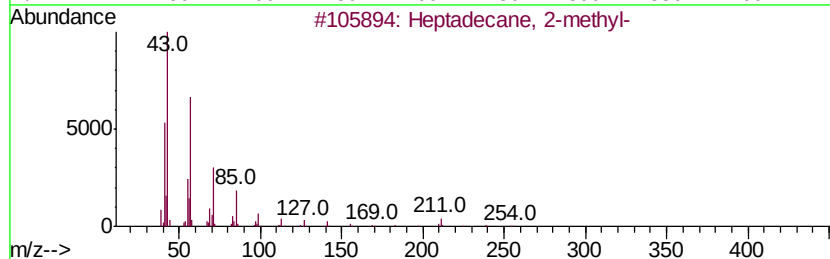
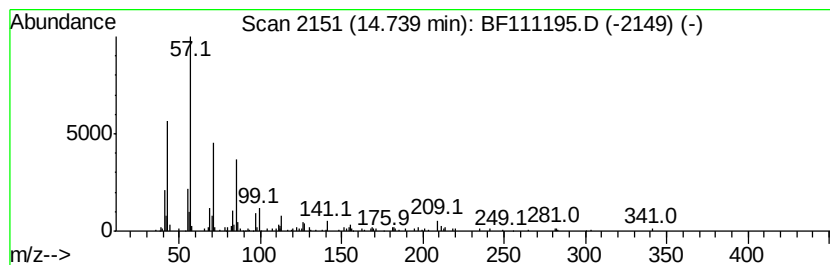
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.13 ng	247603	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Octadecane	254	C18H38	000593-45-3	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
Operator : JU/SJ
Sample : J6214-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

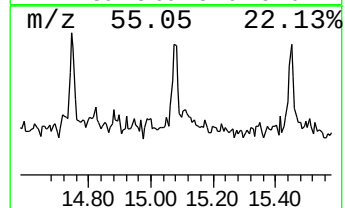
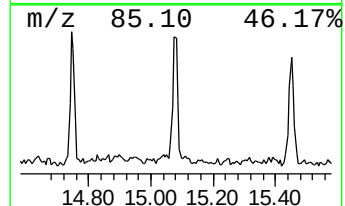
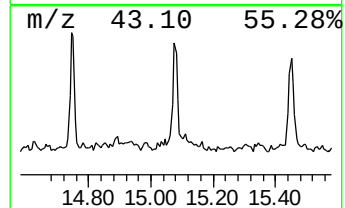
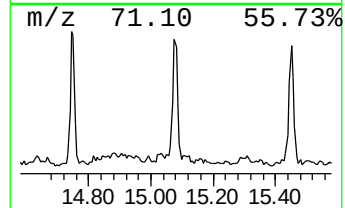
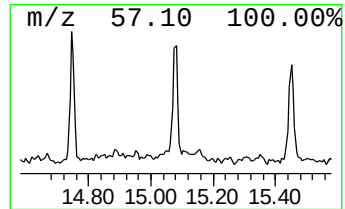
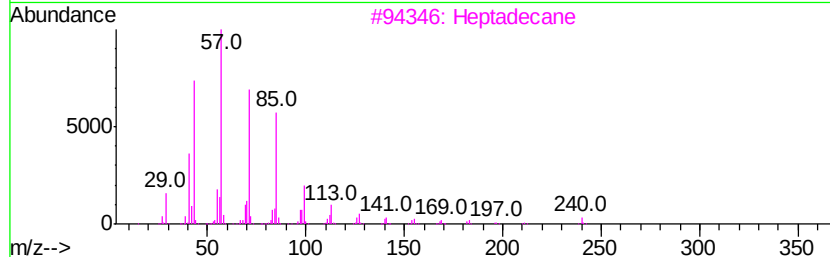
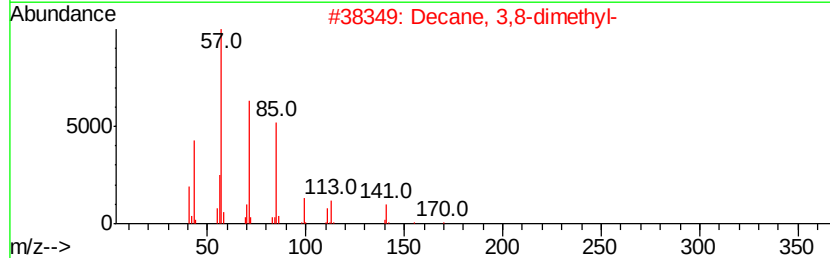
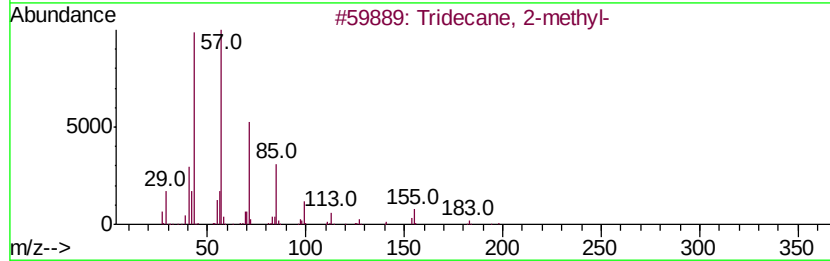
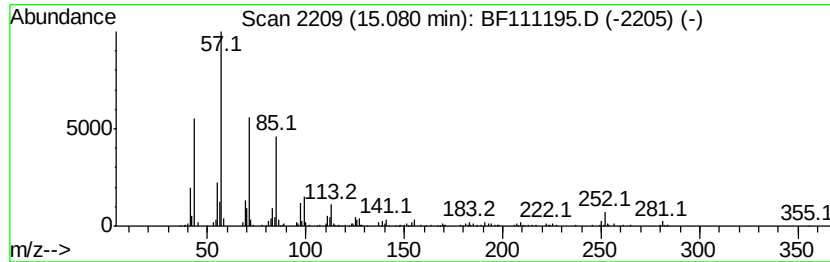
Instrument :
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ClientSampleId :
SB-9(18-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.19 ng	254732	Perylene-d12	15.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tridecane, 2-methyl-	198 C14H30	001560-96-9 83
2		Decane, 3,8-dimethyl-	170 C12H26	017312-55-9 80
3		Heptadecane	240 C17H36	000629-78-7 72
4		Heptadecane, 2-methyl-	254 C18H38	001560-89-0 70
5		Sulfurous acid, 2-ethylhexyl iso...	278 C14H30O3S	1000309-19-0 64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
Operator : JU/SJ
Sample : J6214-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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SB-9(18-20)

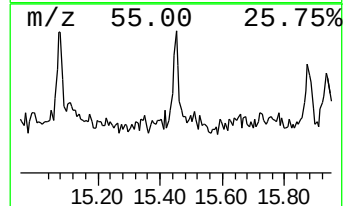
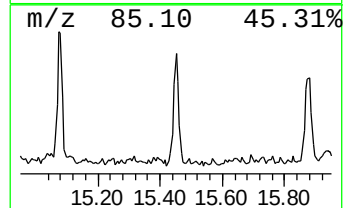
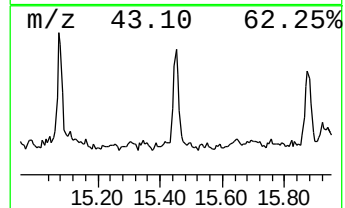
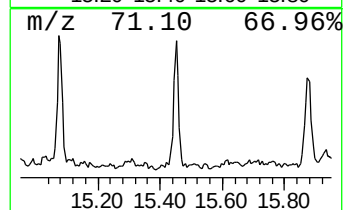
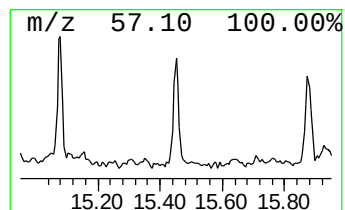
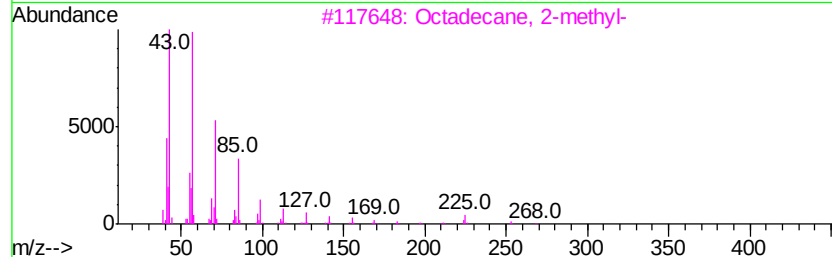
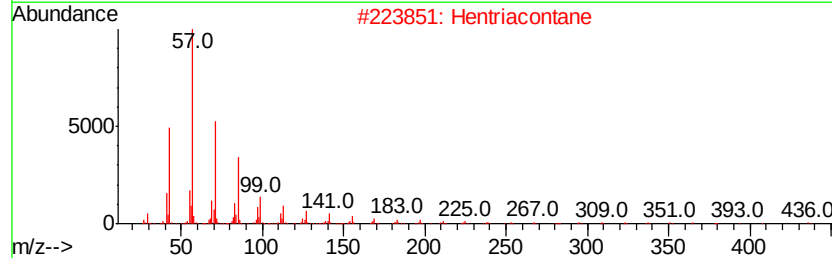
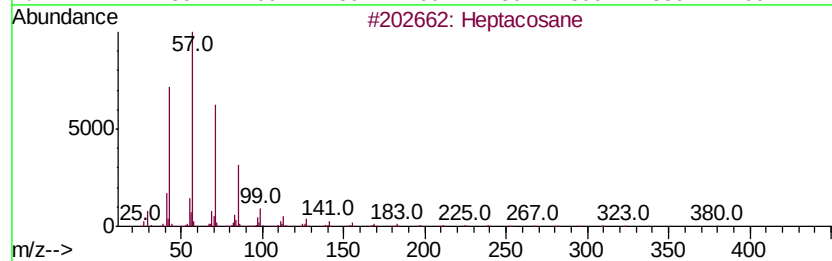
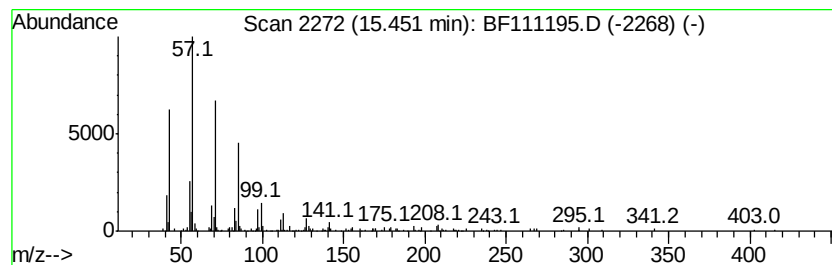
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.32 ng	269541	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	86
2	Hentriacontane		437	C31H64	000630-04-6	86
3	Octadecane, 2-methyl-		268	C19H40	001560-88-9	78
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72
5	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
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ALS Vial : 19 Sample Multiplier: 1

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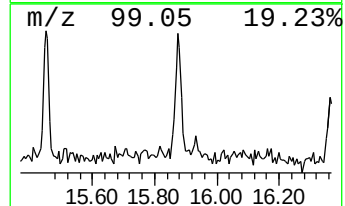
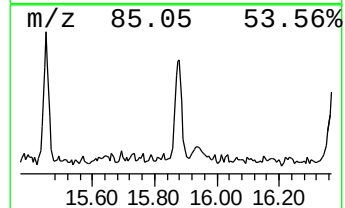
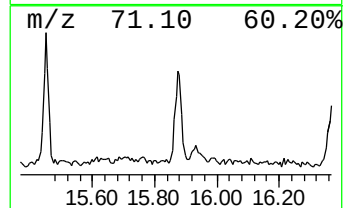
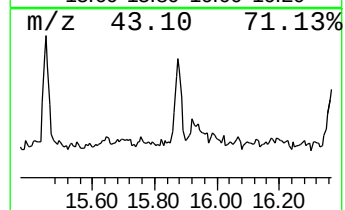
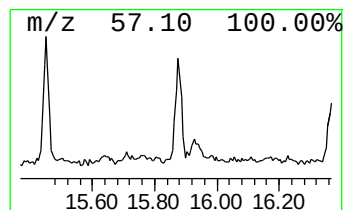
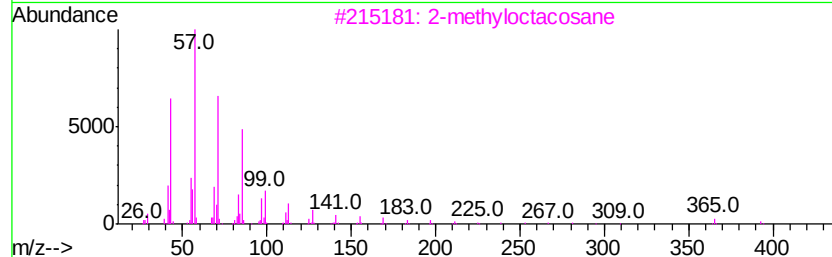
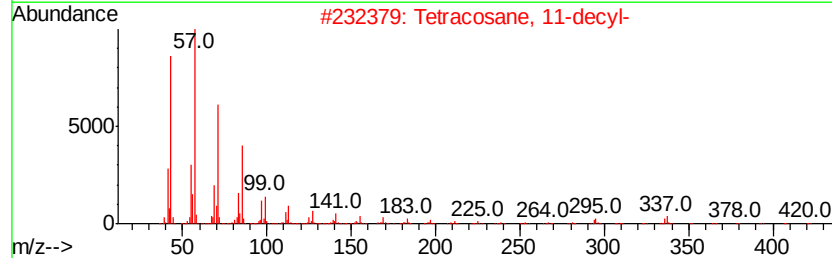
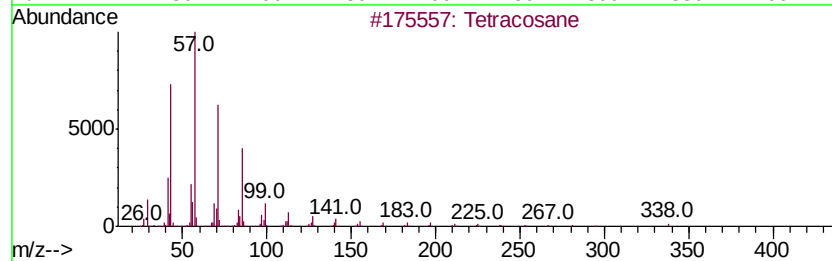
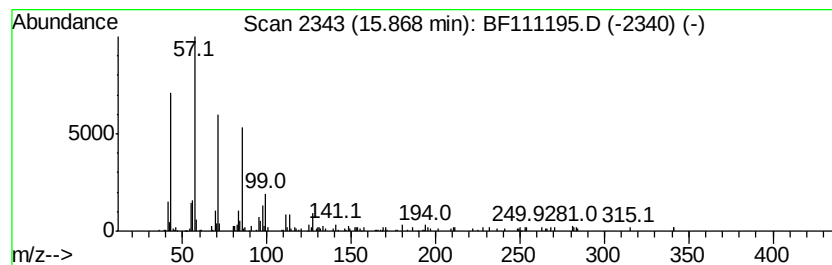
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.06 ng	239206	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
3			2-methyloctacosane	408	C29H60	1000376-72-8	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120718\
Data File : BF111195.D
Acq On : 7 Dec 2018 19:05
Operator : JU/SJ
Sample : J6214-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-9(18-20)

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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
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2-Pentanone, 4-hy...	5.02	7.6	ng	802174	1	6.80	2110150	20.0
unknown6.57	6.57	105.4	ng	11121700	1	6.80	2110150	20.0
Tridecanoic acid	11.86	12.5	ng	1943790	4	11.32	3117270	20.0
Octadecanoic acid	12.64	10.8	ng	1676380	4	11.32	3117270	20.0
Octadecyl trifluo...	13.82	6.0	ng	797884	5	13.96	2646180	20.0
2-methyloctacosane	14.44	2.5	ng	329350	5	13.96	2646180	20.0
Heptadecane, 2-me...	14.74	2.1	ng	247603	6	15.40	2326030	20.0
Tridecane, 2-methyl-	15.08	2.2	ng	254732	6	15.40	2326030	20.0
Heptacosane	15.45	2.3	ng	269541	6	15.40	2326030	20.0
Tetracosane	15.87	2.1	ng	239206	6	15.40	2326030	20.0