

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118243.D
 Acq On : 17 Dec 2019 23:08
 Operator : JU
 Sample : K6324-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-12

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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	2.128	3	7	16	rVB	311220	394817	12.75%	1.569%
2	5.069	503	507	518	rVB	357984	440252	14.22%	1.750%
3	5.481	572	577	580	rBV	2592909	2337741	75.52%	9.292%
4	6.492	744	749	752	rBV	2543379	2516631	81.30%	10.003%
5	6.634	768	773	776	rBV	2985825	2751518	88.89%	10.937%
6	6.857	808	811	818	rBV	802743	689201	22.26%	2.739%
7	7.016	834	838	841	rBV	2603590	2161858	69.84%	8.593%
8	7.428	903	908	920	rBV	1508042	1584154	51.18%	6.297%
9	8.145	1026	1030	1043	rBV	978914	876276	28.31%	3.483%
10	9.228	1209	1214	1217	rBV	3635603	3095541	100.00%	12.304%
11	9.622	1277	1281	1291	rBV	129780	133749	4.32%	0.532%
12	9.910	1326	1330	1339	rBV	1008391	938973	30.33%	3.732%
13	10.698	1461	1464	1478	rBV	1639221	1645619	53.16%	6.541%
14	11.404	1580	1584	1593	rBV	787258	798646	25.80%	3.175%
15	11.922	1669	1672	1686	rBV	122574	151297	4.89%	0.601%
16	12.992	1850	1854	1857	rBV	3020095	2545755	82.24%	10.119%
17	13.886	2002	2006	2019	rBV	225768	344786	11.14%	1.370%
18	14.057	2031	2035	2044	rVB	751919	753893	24.35%	2.997%
19	14.210	2057	2061	2064	rBV	39523	44254	1.43%	0.176%
20	14.515	2109	2113	2123	rBV2	54027	90782	2.93%	0.361%
21	14.821	2160	2165	2169	rBV	60067	72119	2.33%	0.287%
22	15.168	2220	2224	2229	rVB2	59693	68909	2.23%	0.274%
23	15.545	2283	2288	2295	rBV	466671	655423	21.17%	2.605%
24	15.998	2362	2365	2371	rVB2	41369	65915	2.13%	0.262%

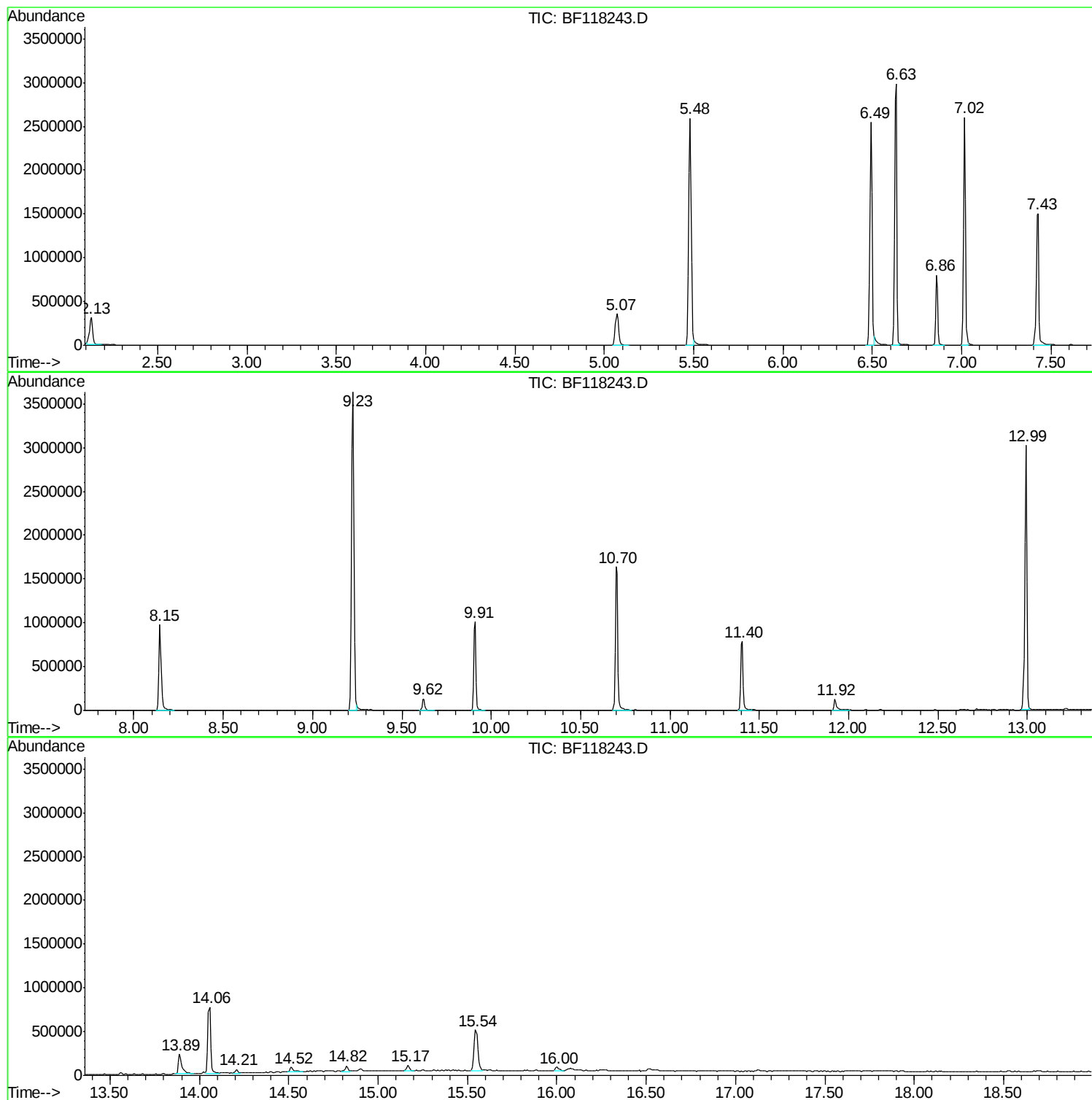
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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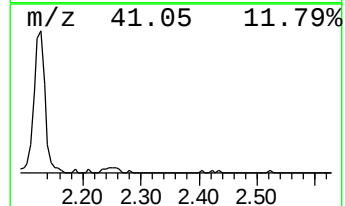
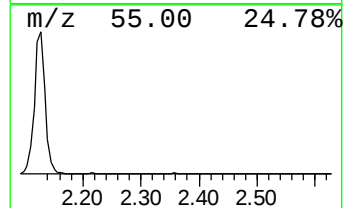
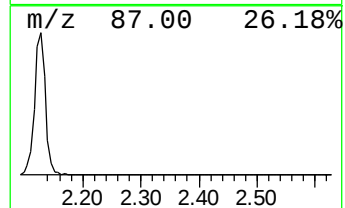
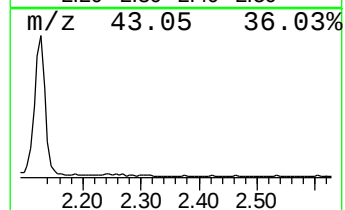
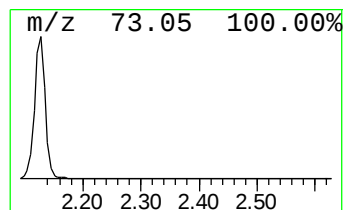
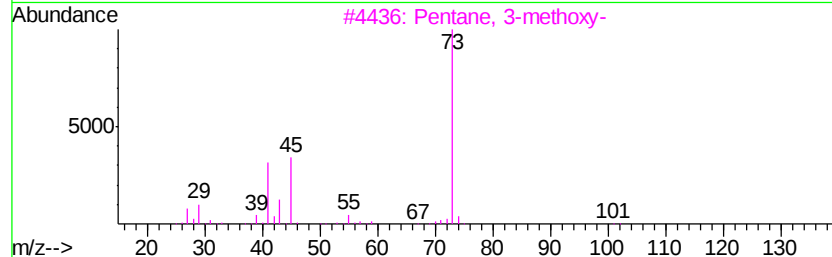
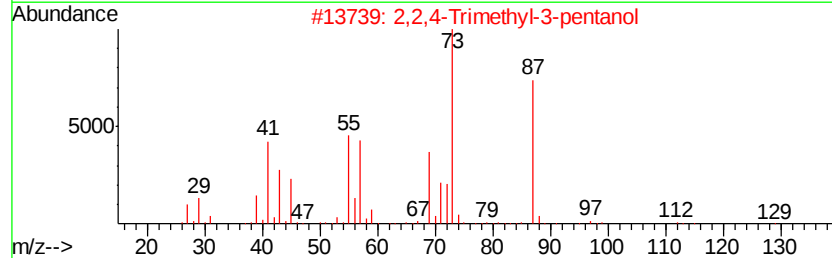
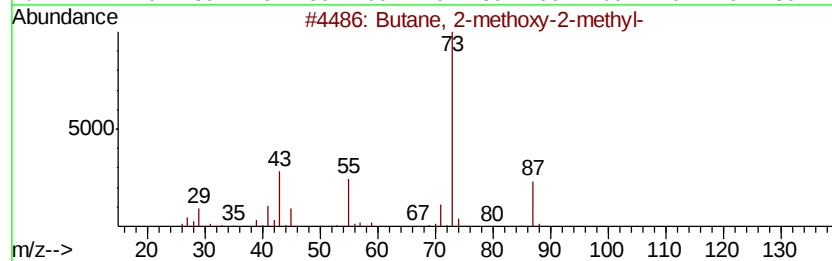
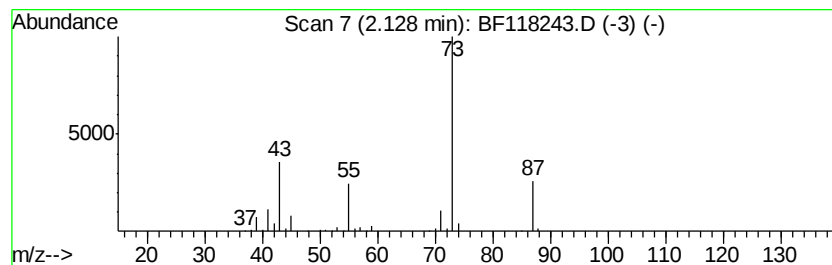
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	11.46 ng	394817	1,4-Dichlorobenzene-d4	6.86

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		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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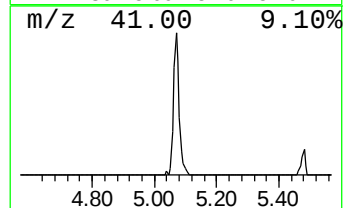
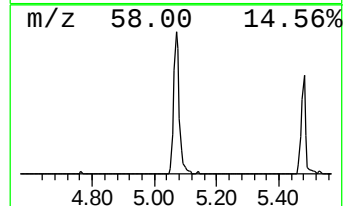
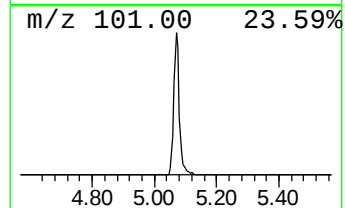
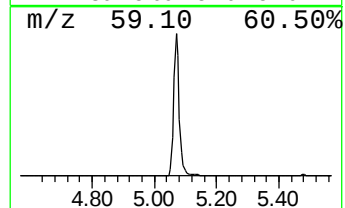
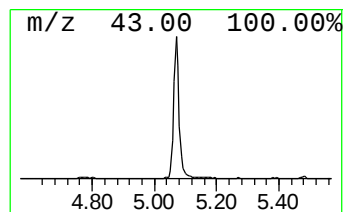
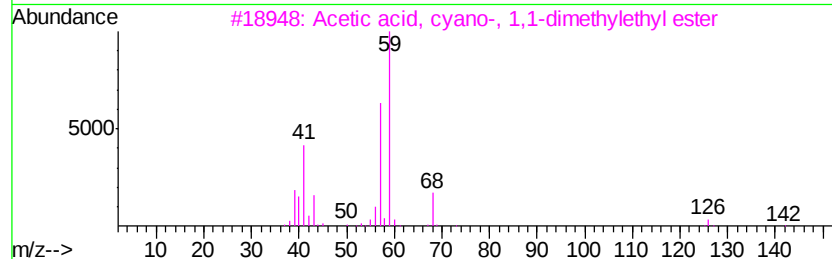
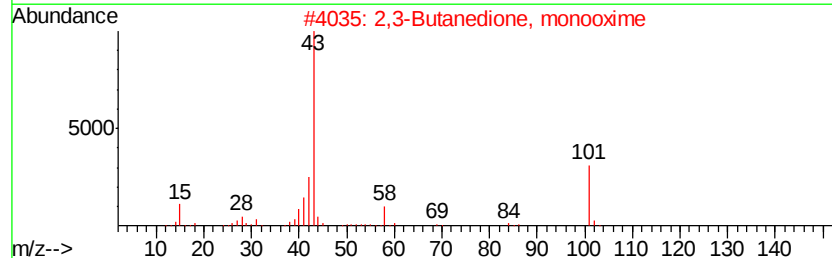
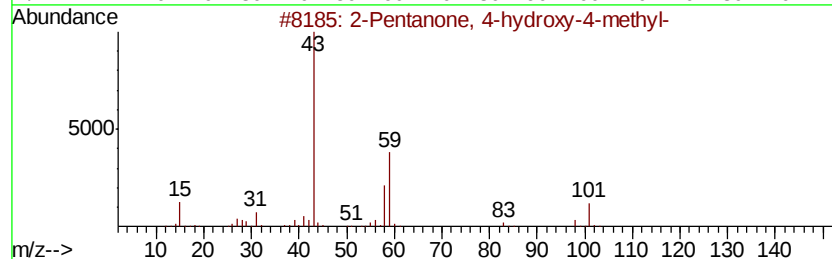
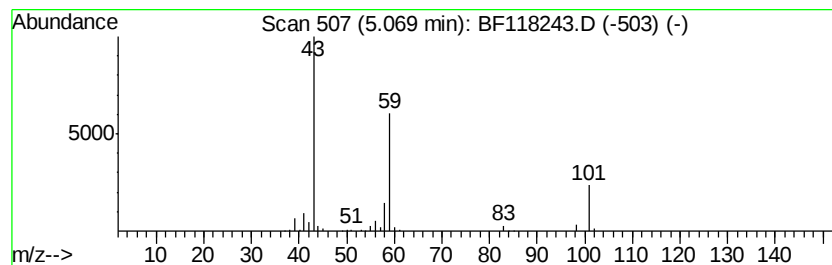
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.78 ng	440252	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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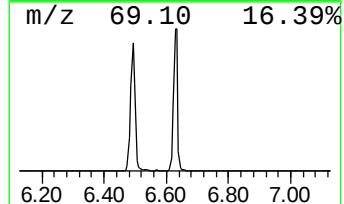
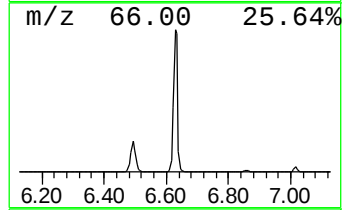
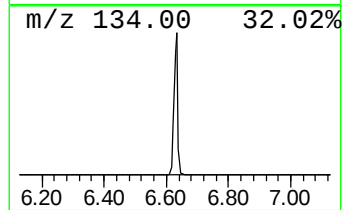
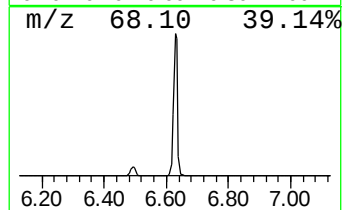
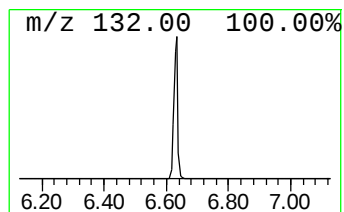
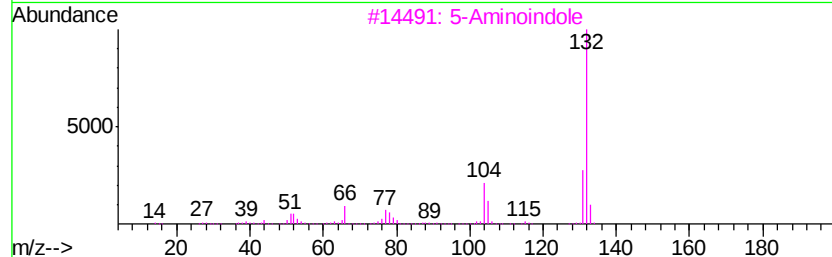
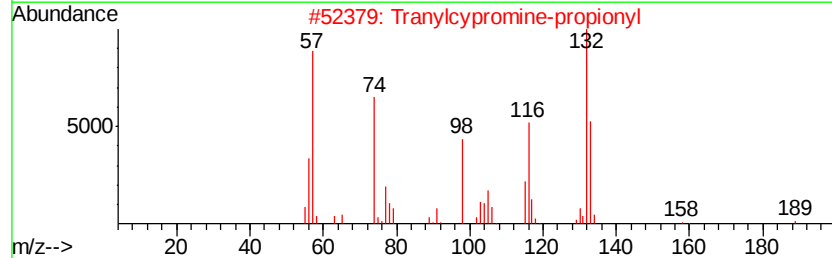
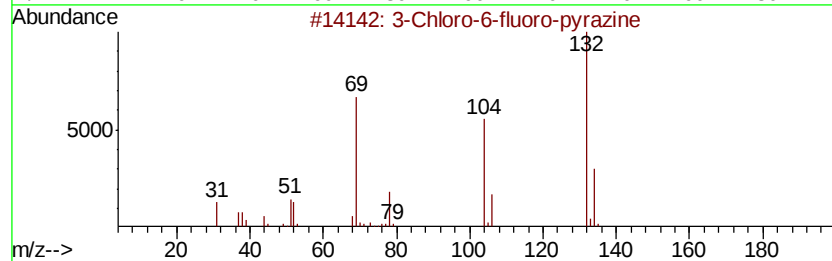
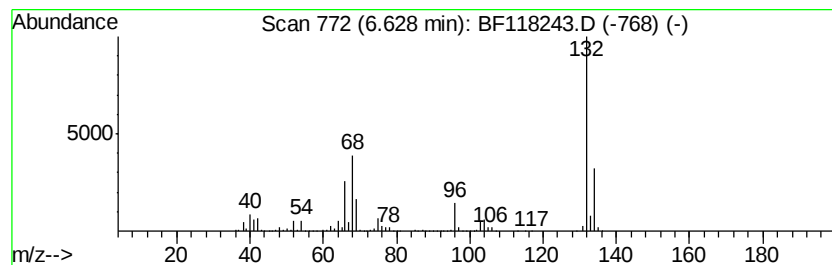
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	79.85 ng	2751520	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	16
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	9



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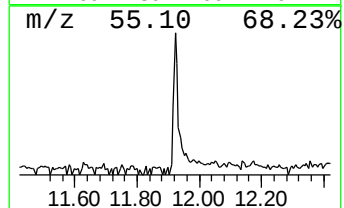
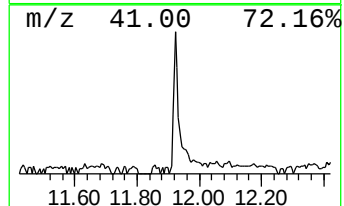
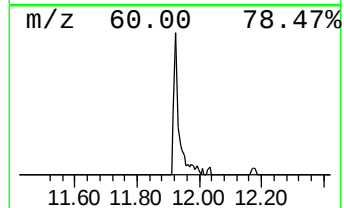
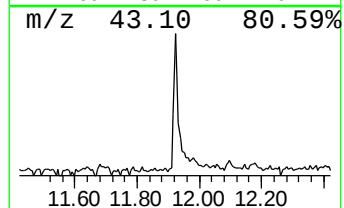
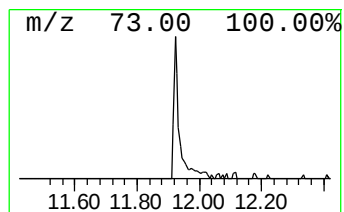
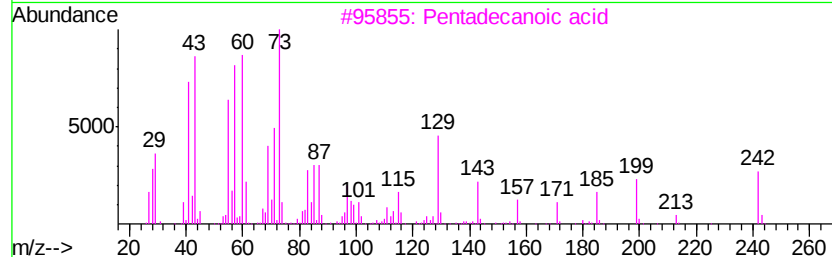
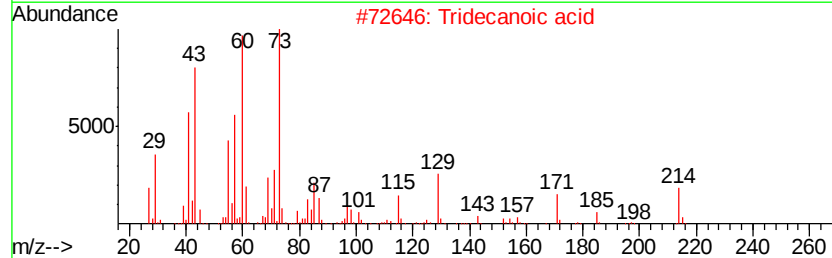
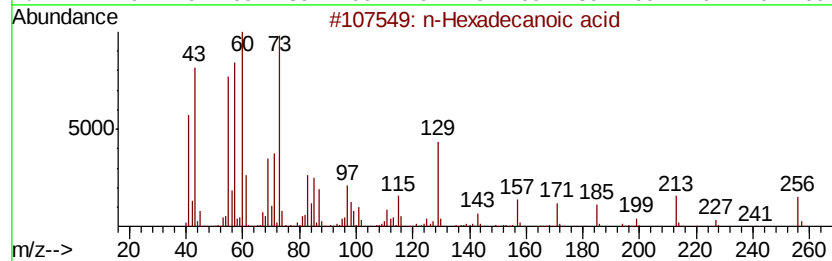
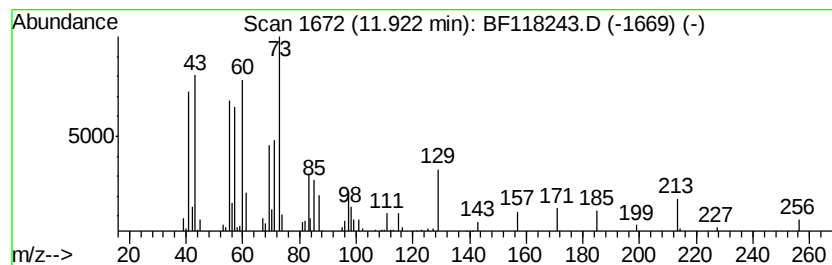
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	3.79 ng	151297	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Oxalic acid, allvl octadecyl ester	382	C23H42O4	1000309-24-5	35
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	20



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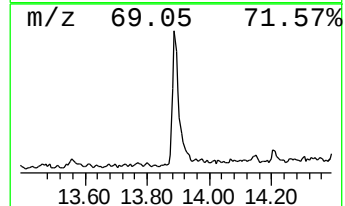
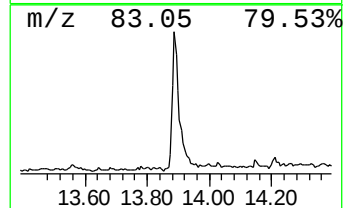
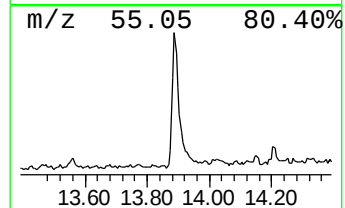
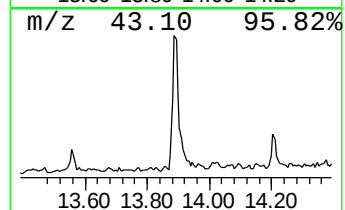
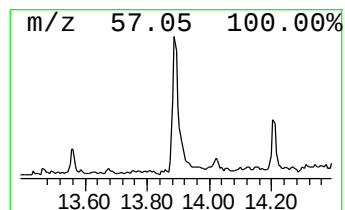
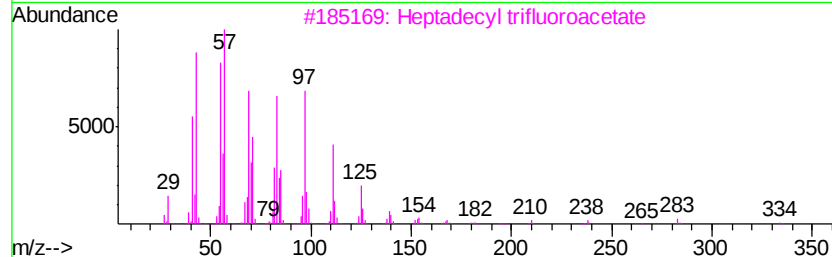
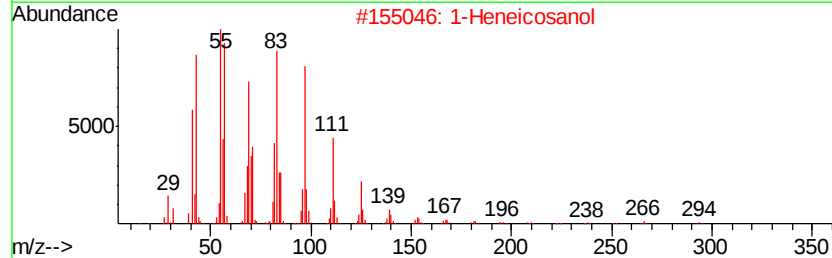
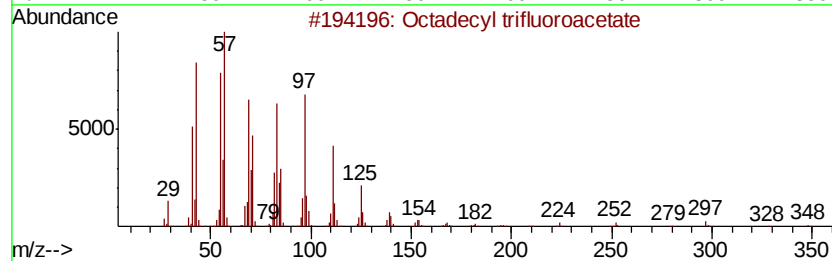
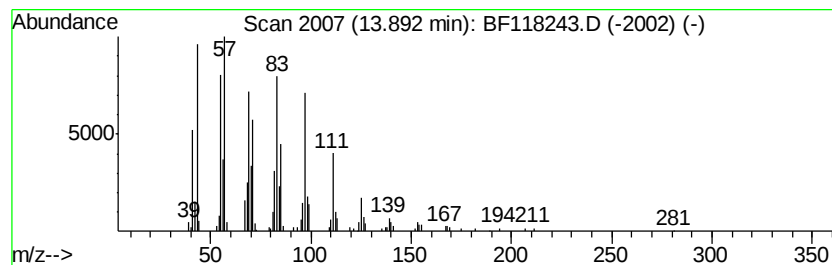
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	9.15 ng	344786	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	87



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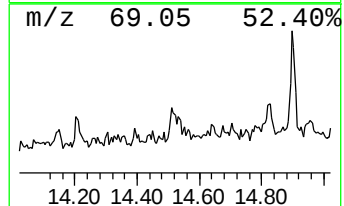
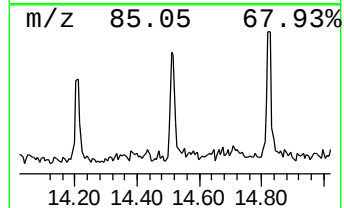
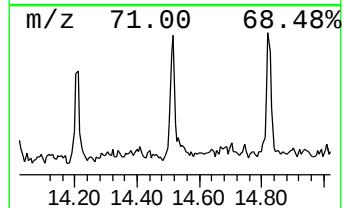
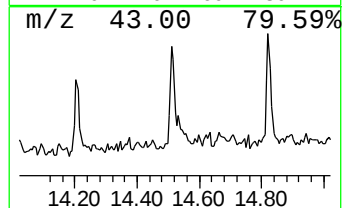
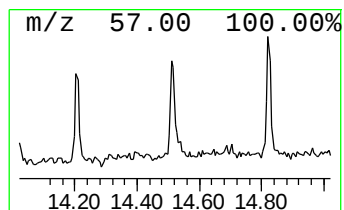
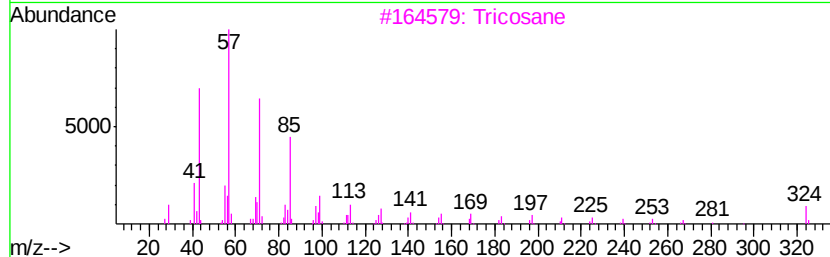
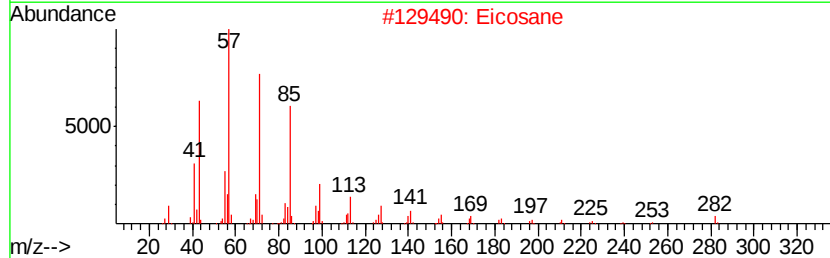
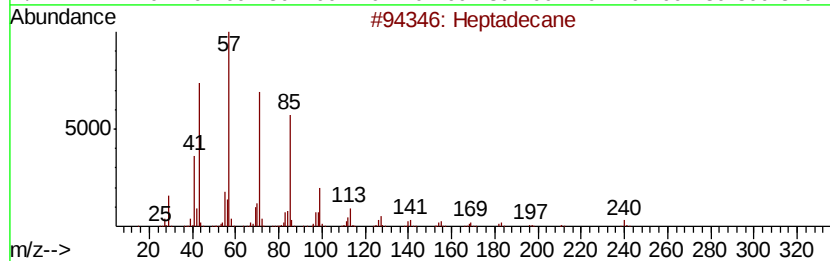
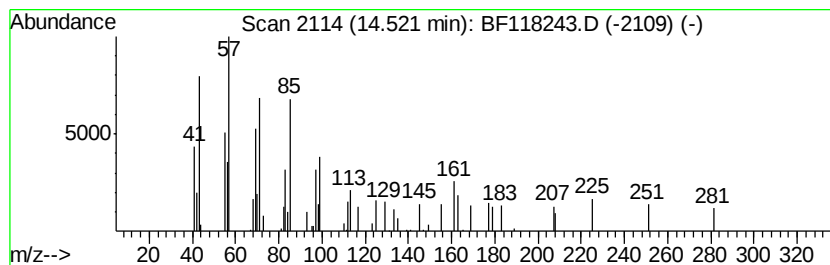
Instrument :
BNA_F
ClientSampleId :
EP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.41 ng	90782	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	83
2	Eicosane	282 C20H42	000112-95-8	80
3	Tricosane	324 C23H48	000638-67-5	80
4	Hexacosane	366 C26H54	000630-01-3	80
5	Hexadecane	226 C16H34	000544-76-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
 Data File : BF118243.D
 Acq On : 17 Dec 2019 23:08
 Operator : JU
 Sample : K6324-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-12

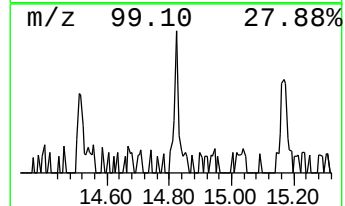
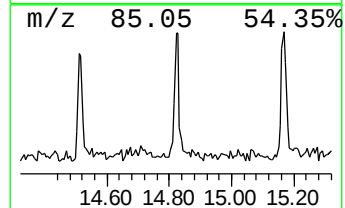
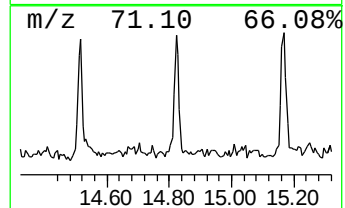
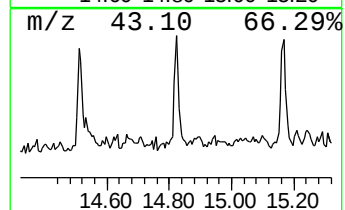
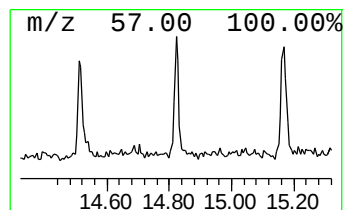
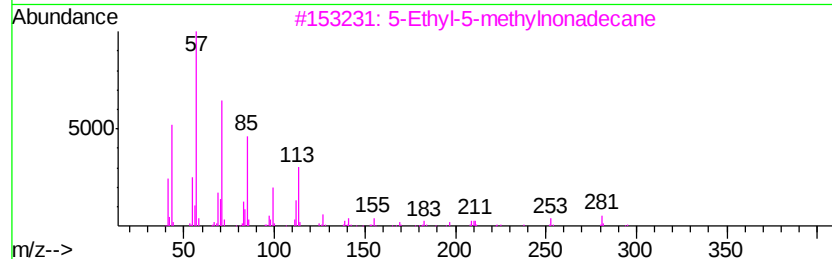
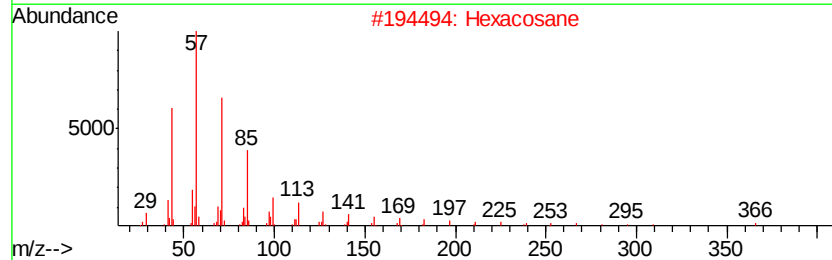
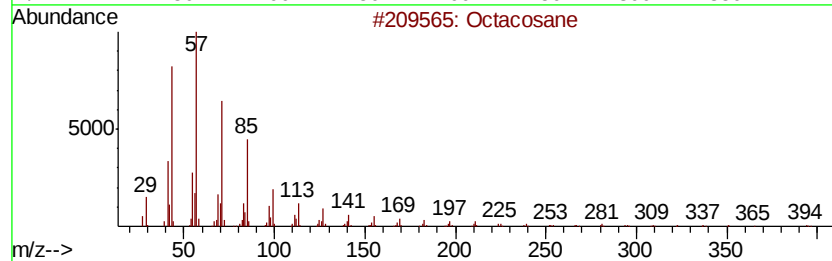
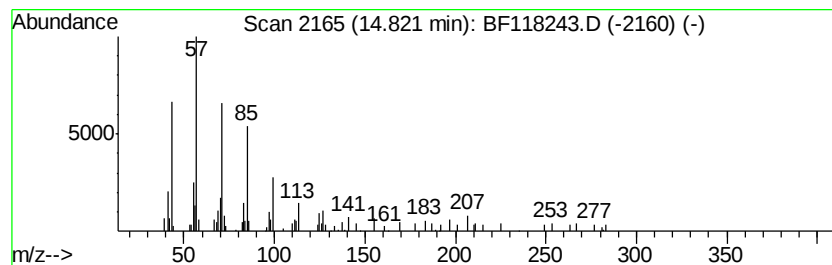
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.20 ng	72119	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Hexacosane		366	C26H54	000630-01-3	81
3	5-Ethyl-5-methylnonadecane		310	C22H46	1000360-42-7	74
4	Hentriacontane		437	C31H64	000630-04-6	74
5	Eicosane		282	C20H42	000112-95-8	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118243.D
Acq On : 17 Dec 2019 23:08
Operator : JU
Sample : K6324-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

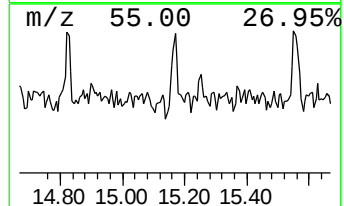
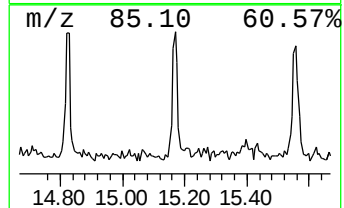
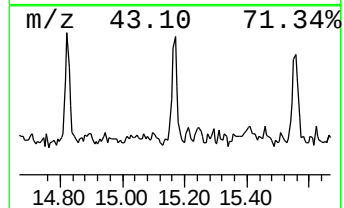
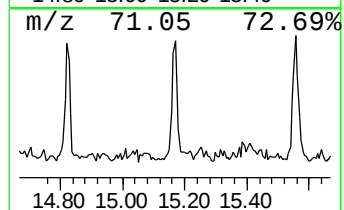
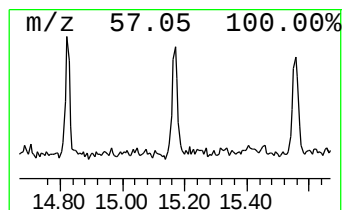
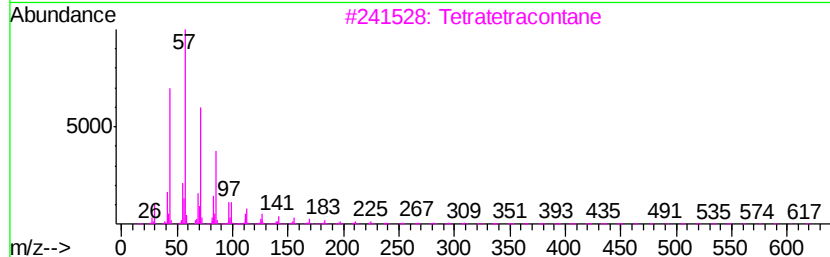
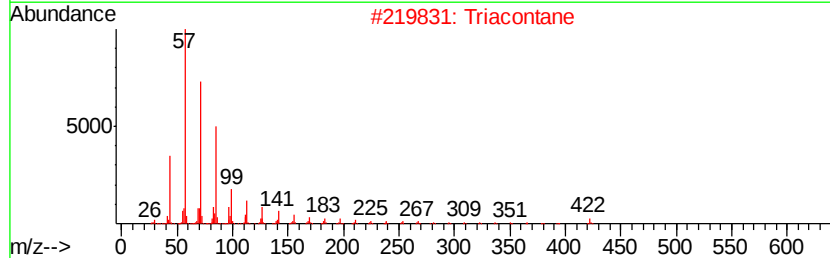
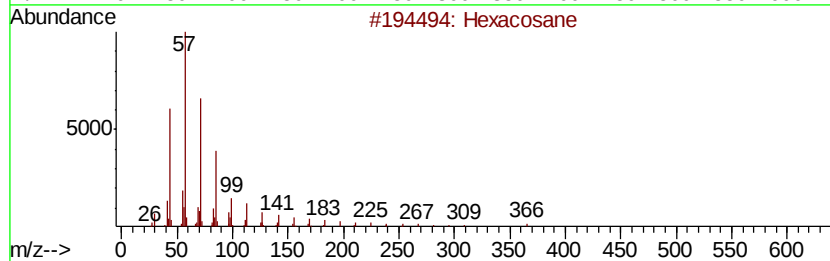
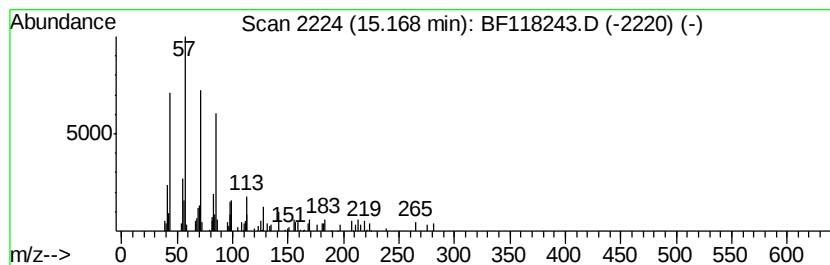
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.10 ng	68909	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Triacontane	422	C30H62	000638-68-6	87
3		Tetratetracontane	619	C44H90	007098-22-8	86
4		Octacosane	394	C28H58	000630-02-4	86
5		Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118243.D
Acq On : 17 Dec 2019 23:08
Operator : JU
Sample : K6324-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

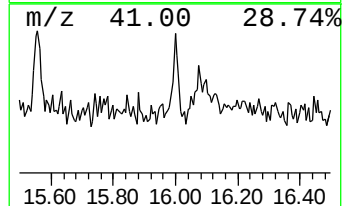
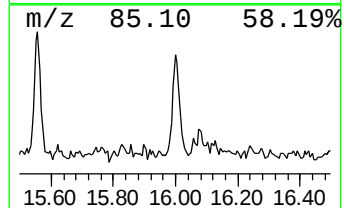
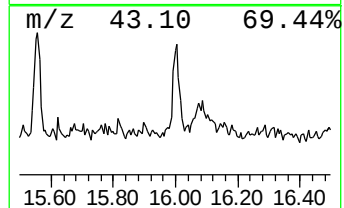
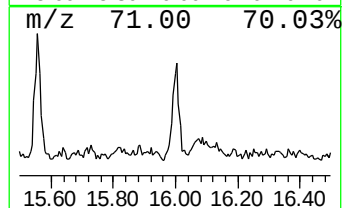
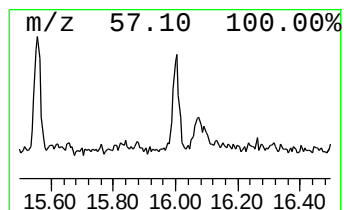
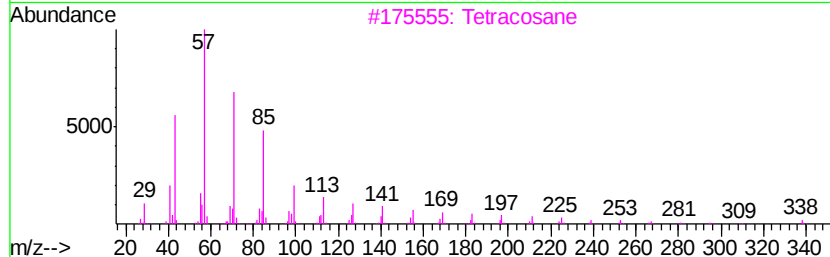
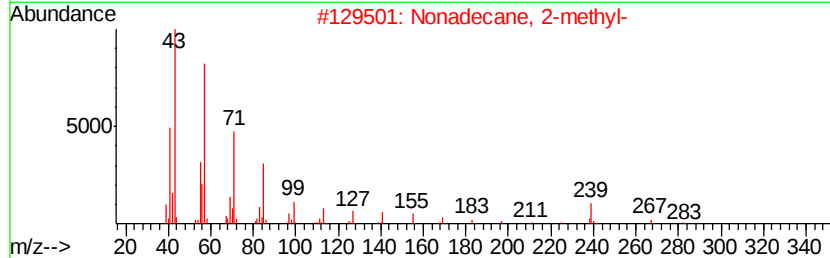
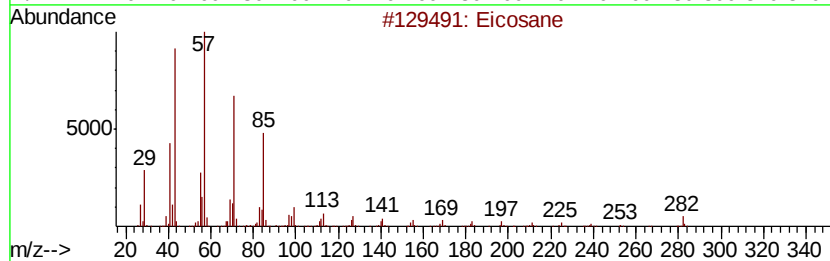
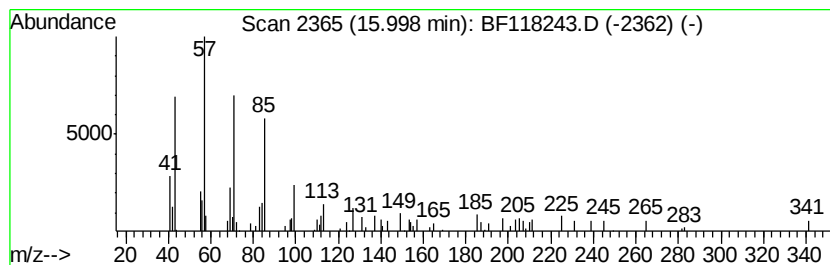
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.01 ng	65915	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	86
2		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	72
3		Tetracosane	338	C24H50	000646-31-1	64
4		Tetratriacontane	479	C34H70	014167-59-0	64
5		5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
Data File : BF118243.D
Acq On : 17 Dec 2019 23:08
Operator : JU
Sample : K6324-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	2.13	11.5	ng	394817	1	6.86	689201	20.0
2-Pentanone, 4-hy...	5.07	12.8	ng	440252	1	6.86	689201	20.0
unknown6.63	6.63	79.8	ng	2751520	1	6.86	689201	20.0
n-Hexadecanoic acid	11.92	3.8	ng	151297	4	11.40	798646	20.0
Octadecyl trifluo...	13.89	9.2	ng	344786	5	14.06	753893	20.0
Heptadecane	14.52	2.4	ng	90782	5	14.06	753893	20.0
Octacosane	14.82	2.2	ng	72119	6	15.54	655423	20.0
Hexacosane	15.17	2.1	ng	68909	6	15.54	655423	20.0
Eicosane	16.00	2.0	ng	65915	6	15.54	655423	20.0