

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
 Data File : BF117706.D
 Acq On : 7 Nov 2019 15:59
 Operator : JU
 Sample : K5710-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP- 31-S

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-BF110619.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	2.240	18	26	36	rVB	1379169	1801568	23.33%	2.405%
2	5.151	513	521	528	rBV	1265749	1616715	20.94%	2.158%
3	5.545	583	588	592	rBV	5990469	6400558	82.90%	8.545%
4	6.551	753	759	763	rBV	6483925	6854101	88.78%	9.151%
5	6.698	780	784	788	rBV	6690571	6860441	88.86%	9.159%
6	6.933	820	824	827	rBV	2478771	1899156	24.60%	2.536%
7	7.092	847	851	854	rVB	6313196	5351334	69.31%	7.145%
8	7.492	914	919	922	rBV	4488354	4266209	55.26%	5.696%
9	8.222	1038	1043	1046	rBV	2803367	2489766	32.25%	3.324%
10	9.298	1221	1226	1229	rBV	8398080	7720752	100.00%	10.308%
11	9.686	1288	1292	1296	rBV	1388737	1167856	15.13%	1.559%
12	9.980	1338	1342	1345	rBV	3459252	2875642	37.25%	3.839%
13	10.768	1471	1476	1479	rBV	5320785	4909759	63.59%	6.555%
14	11.468	1591	1595	1599	rBV	3231188	2939037	38.07%	3.924%
15	11.539	1601	1607	1609	rBV2	222127	195689	2.53%	0.261%
16	11.998	1679	1685	1698	rBV	982837	1158288	15.00%	1.546%
17	12.780	1814	1818	1827	rBV	305216	387709	5.02%	0.518%
18	13.062	1862	1866	1869	rBV	8049410	7516512	97.35%	10.035%
19	13.804	1982	1992	1998	rBV	27635	95205	1.23%	0.127%
20	13.957	2013	2018	2021	rBV2	923277	992230	12.85%	1.325%
21	14.115	2041	2045	2049	rBV	2453418	2229712	28.88%	2.977%
22	14.286	2070	2074	2079	rBV	174641	184404	2.39%	0.246%
23	14.592	2122	2126	2131	rBV	281251	274953	3.56%	0.367%
24	14.909	2176	2180	2185	rBV	279823	319060	4.13%	0.426%
25	14.992	2190	2194	2199	rVB	565899	561142	7.27%	0.749%
26	15.268	2237	2241	2248	rVB	291930	364193	4.72%	0.486%
27	15.627	2296	2302	2306	rBV	1835245	2308978	29.91%	3.083%
28	15.668	2306	2309	2323	rVB	227938	378458	4.90%	0.505%
29	16.133	2384	2388	2393	rBV	160136	265245	3.44%	0.354%
30	16.180	2393	2396	2407	rVB5	88279	194273	2.52%	0.259%
31	16.392	2428	2432	2440	rVB10	43163	99963	1.29%	0.133%
32	16.674	2476	2480	2492	rVB3	87634	222187	2.88%	0.297%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

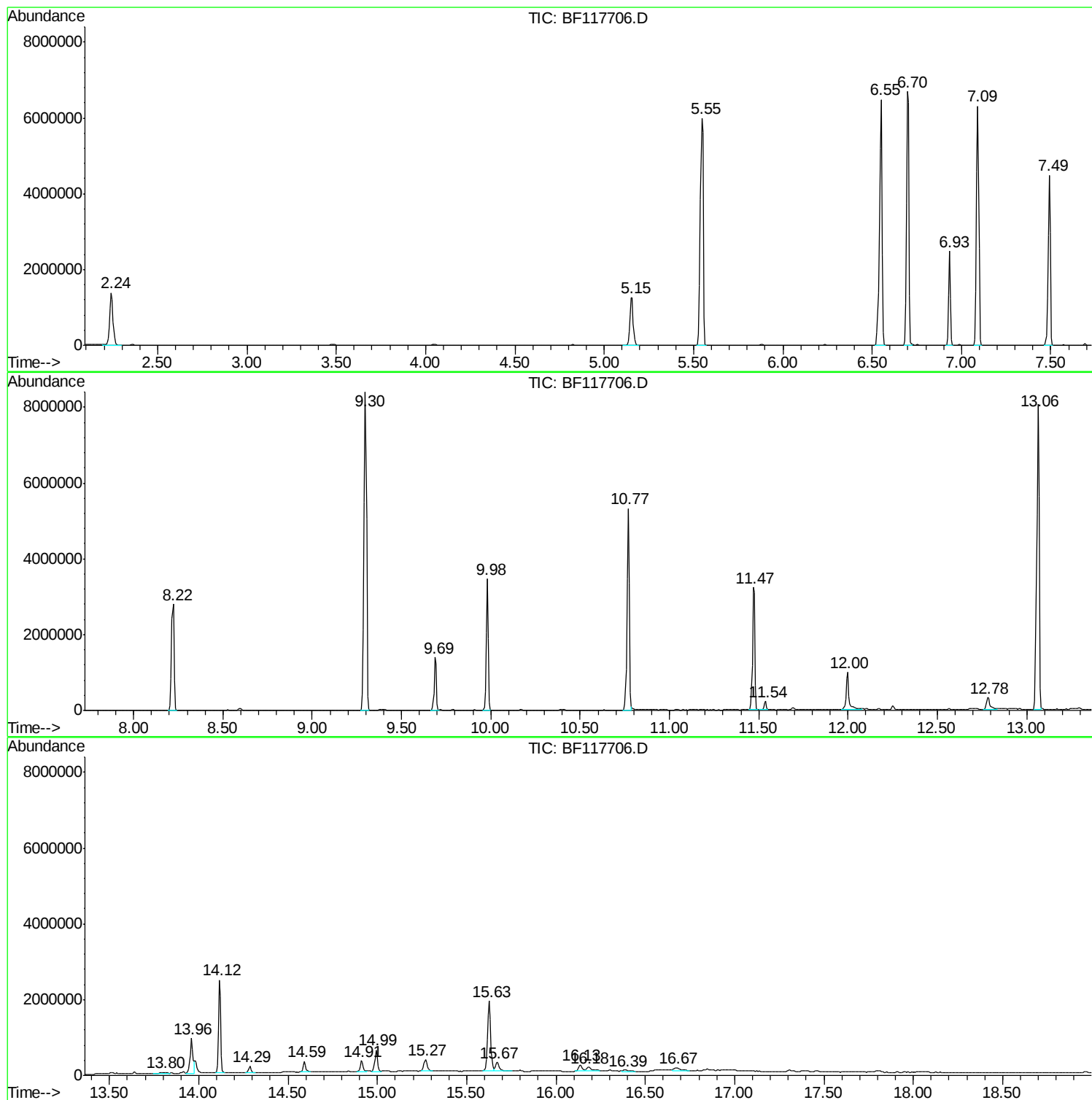
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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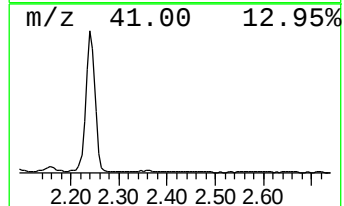
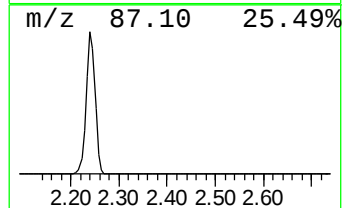
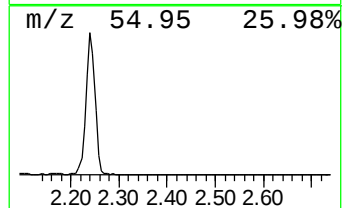
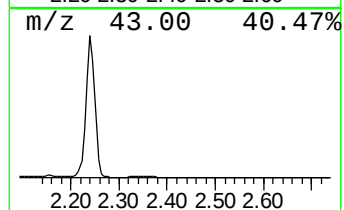
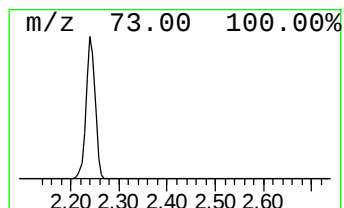
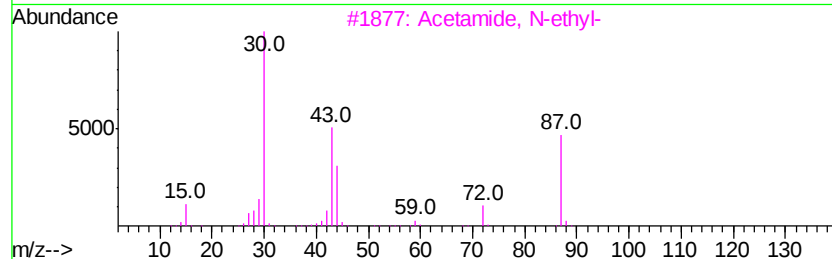
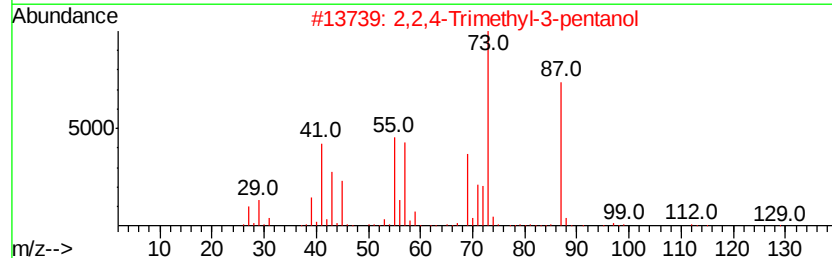
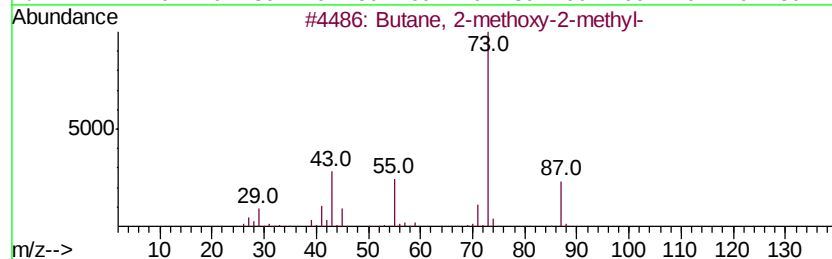
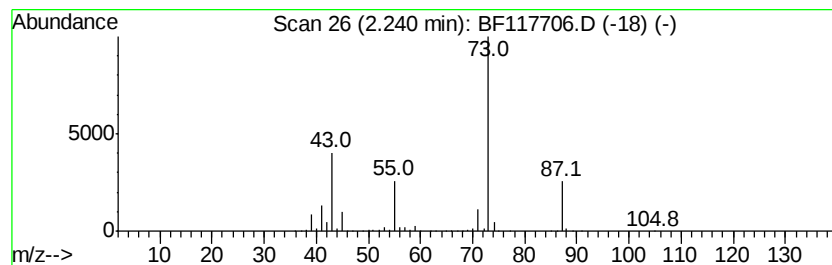
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	18.97 ng	1801570	1,4-Dichlorobenzene-d4	6.93

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	39
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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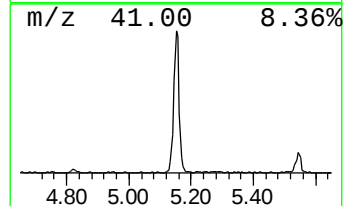
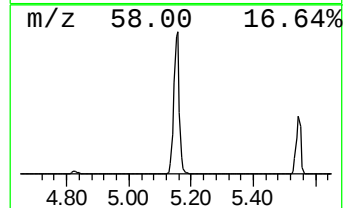
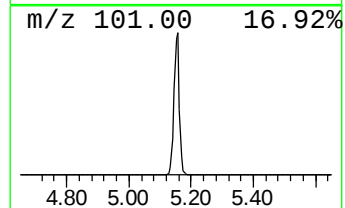
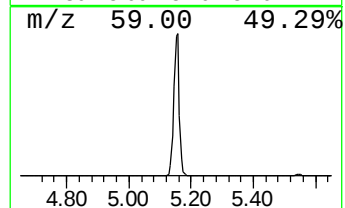
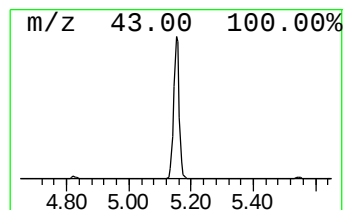
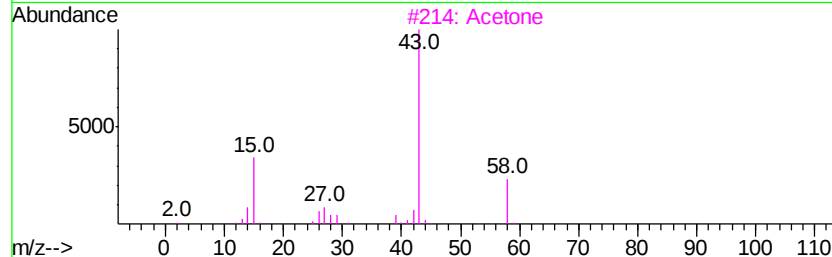
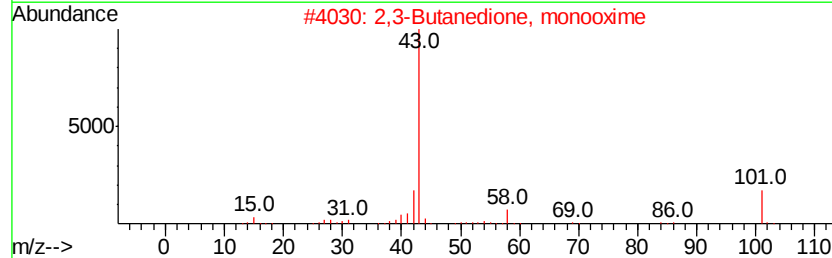
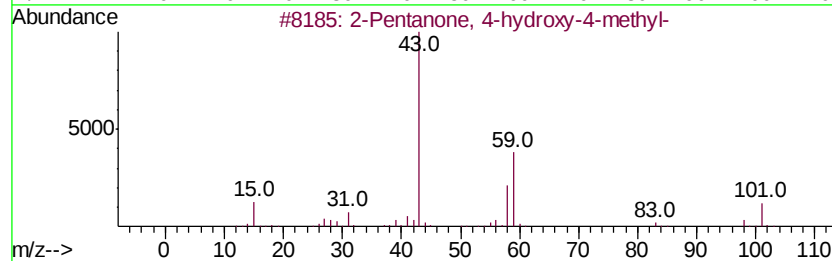
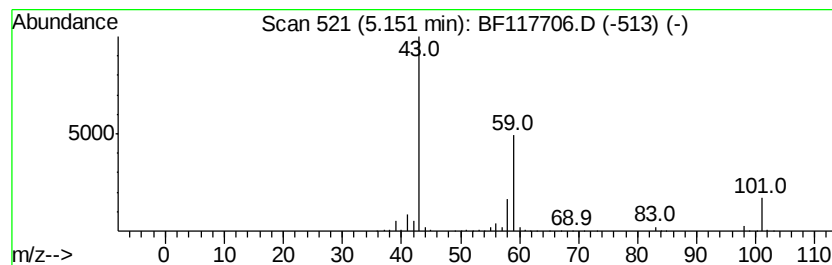
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	17.03 ng	1616720	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		Acetone	58	C3H6O	000067-64-1	12
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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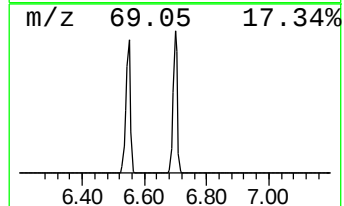
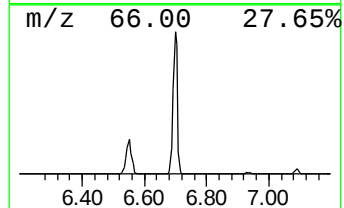
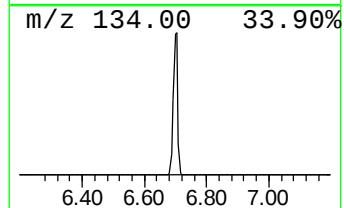
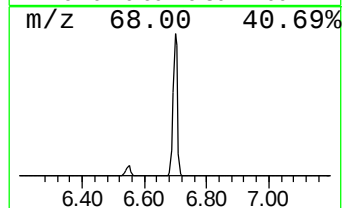
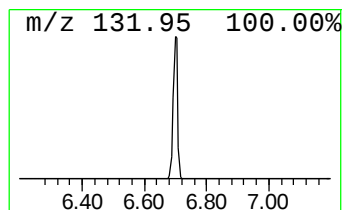
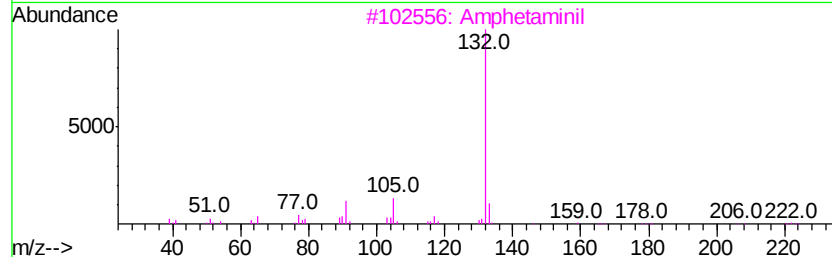
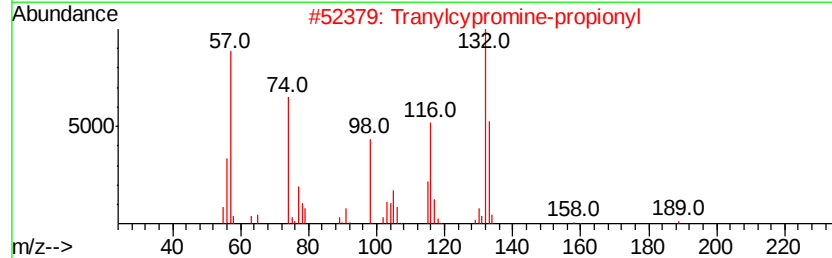
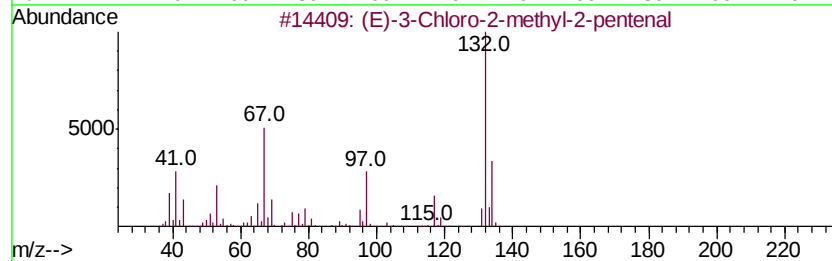
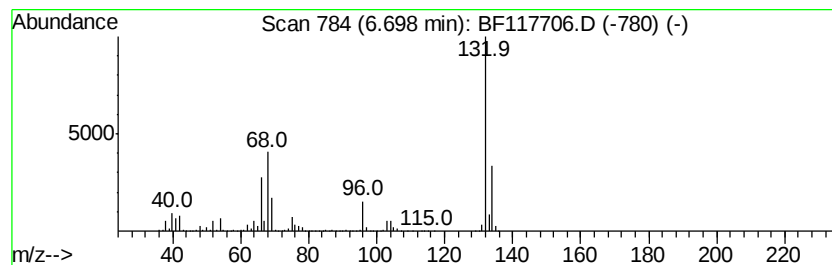
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	72.25 ng	6860440	1,4-Dichlorobenzene-d4	6.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
3	Amphetaminil	250	C17H18N2	017590-01-1	12	
4	5-Aminoindole	132	C8H8N2	005192-03-0	12	
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9	



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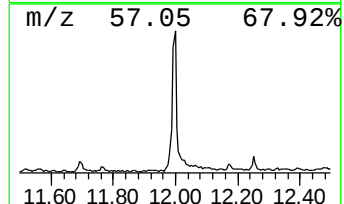
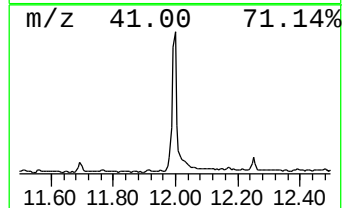
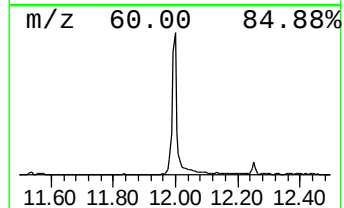
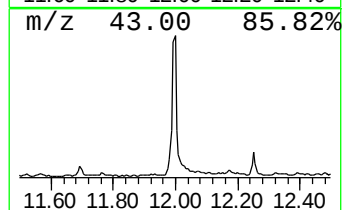
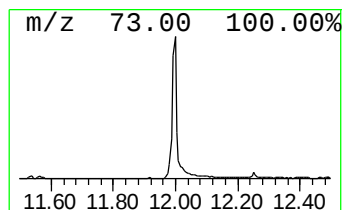
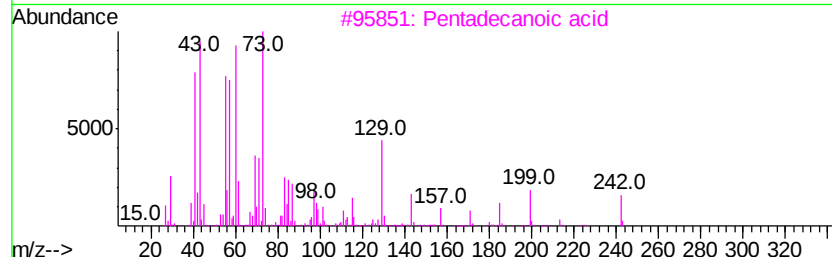
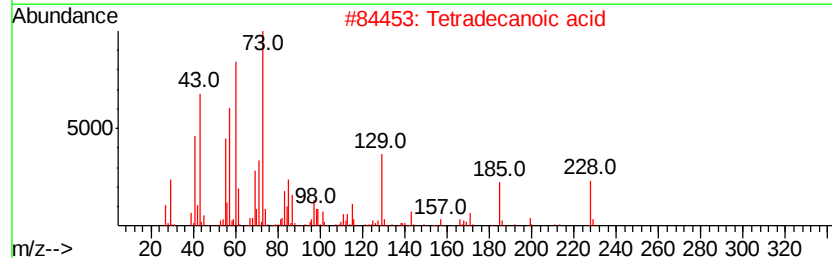
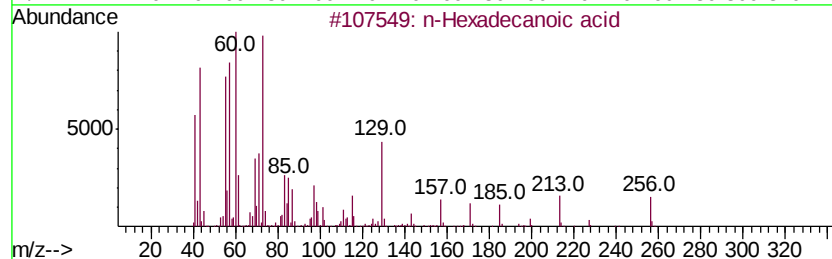
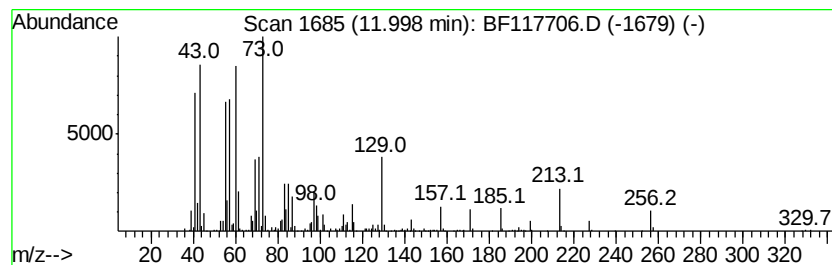
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	7.88 ng	1158290	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87



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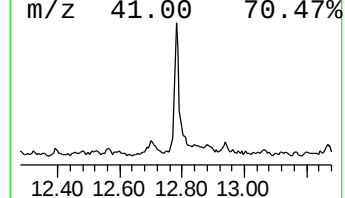
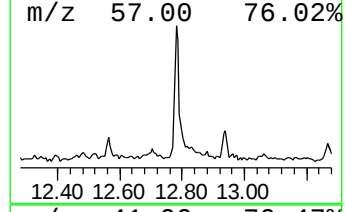
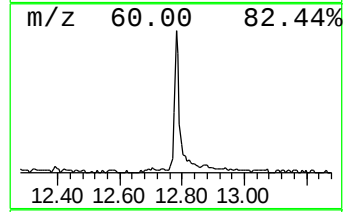
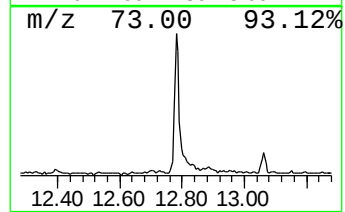
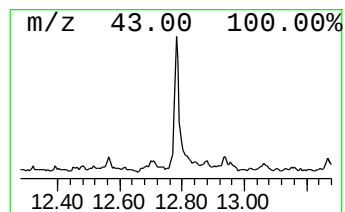
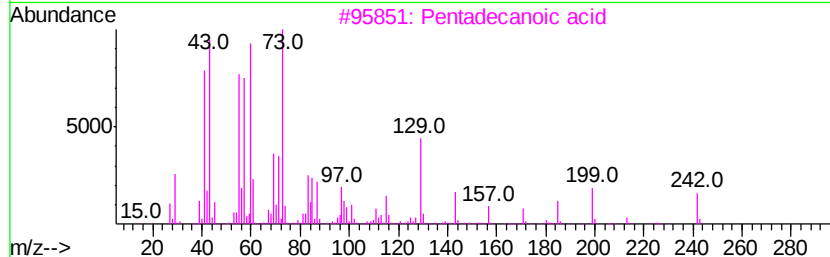
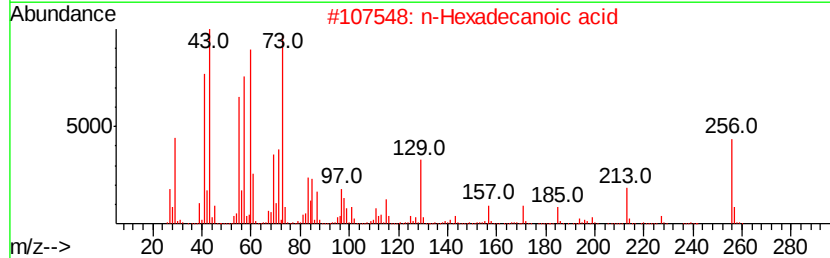
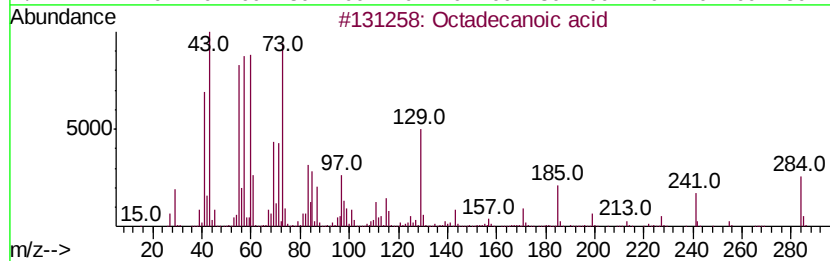
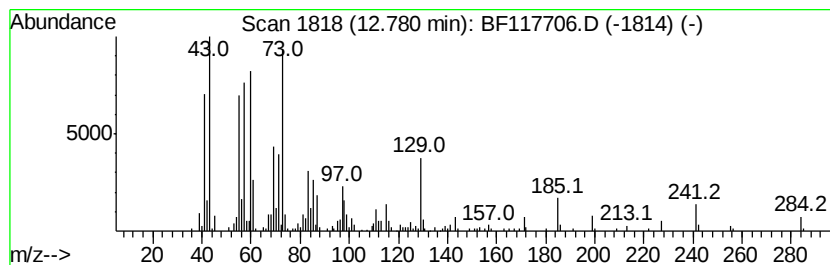
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Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.64 ng	387709	Phenanthrene-d10	11.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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Misc :
ALS Vial : 3 Sample Multiplier: 1

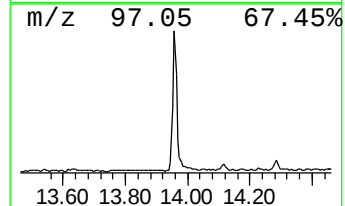
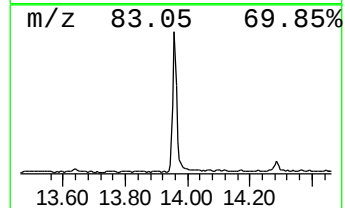
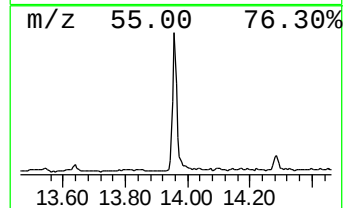
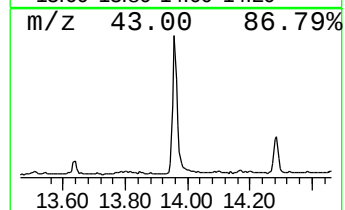
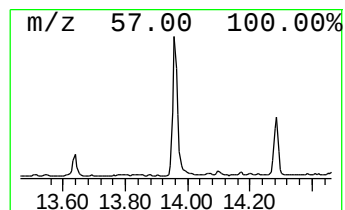
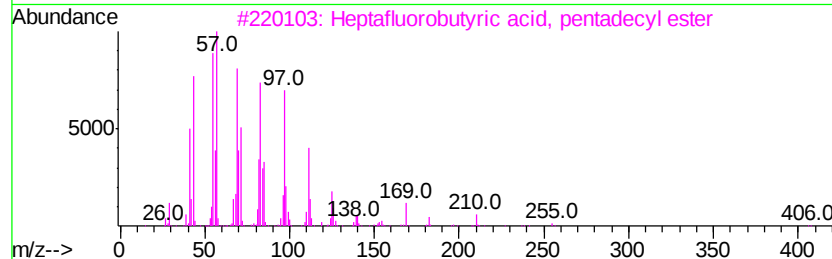
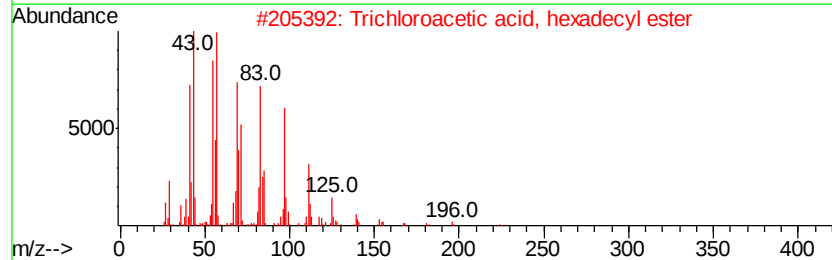
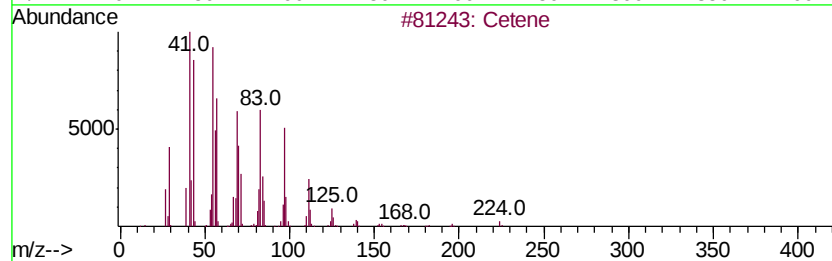
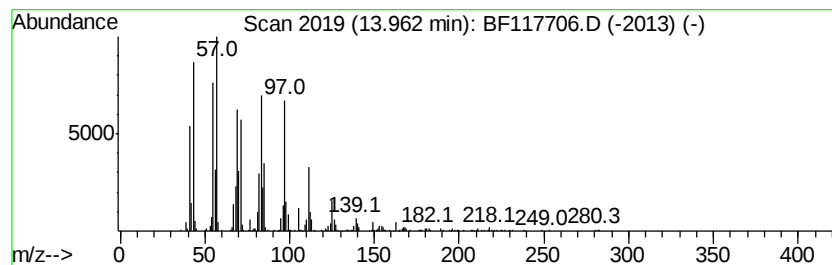
Instrument :
BNA_F
ClientSampleId :
TP- 31-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cetene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	8.90 ng	992230	Chrysene-d12	14.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cetene		224 C16H32	000629-73-2 94
2	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 94
3	Heptafluorobutyric acid, pentade...		424 C19H31F7O2	959261-23-5 94
4	1-Heneicosanol		312 C21H44O	015594-90-8 93
5	Cyclopentadecane		210 C15H30	000295-48-7 93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117706.D
Acq On : 7 Nov 2019 15:59
Operator : JU
Sample : K5710-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

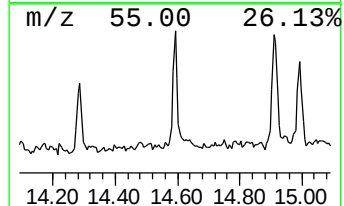
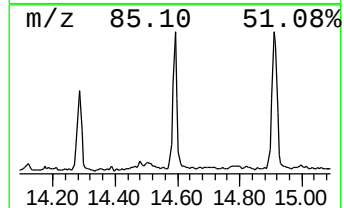
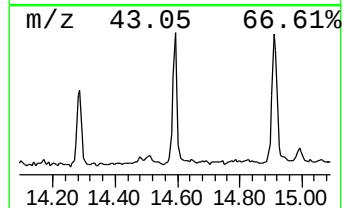
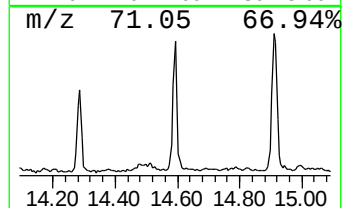
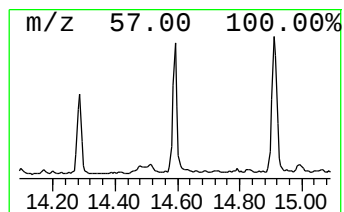
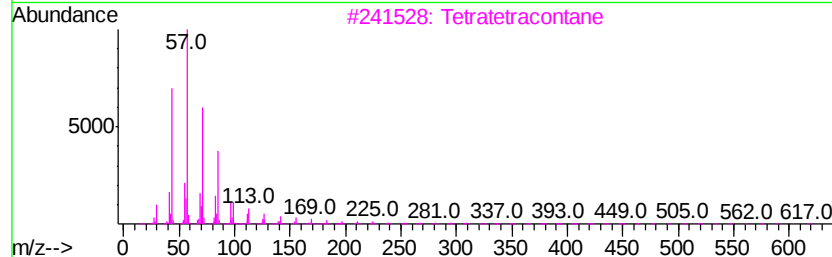
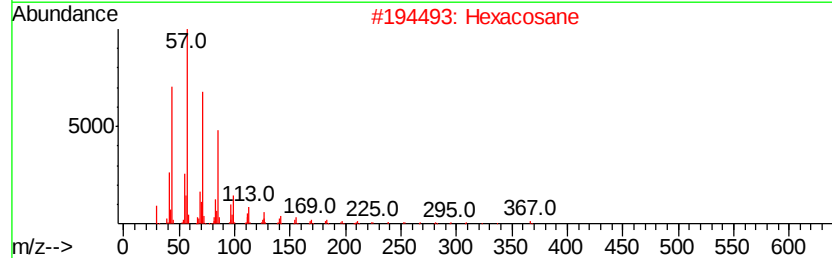
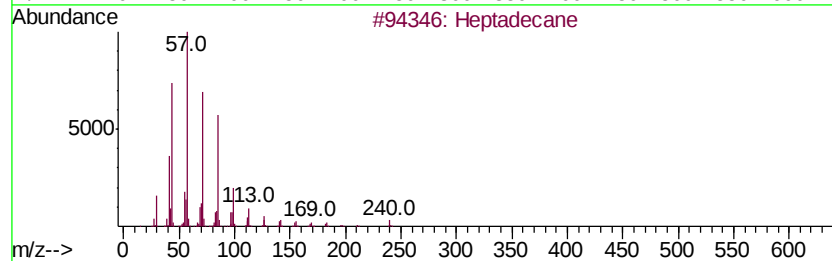
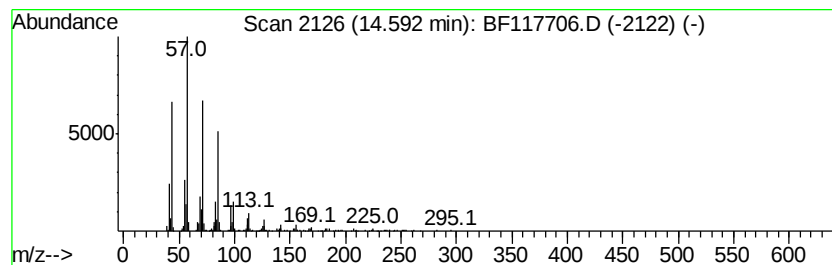
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.47 ng	274953	Chrysene-d12	14.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	95
2	Hexacosane	366 C26H54	000630-01-3	91
3	Tetratetracontane	619 C44H90	007098-22-8	91
4	Hexatriacontane	507 C36H74	000630-06-8	91
5	Sulfurous acid, butyl dodecyl ester	306 C16H34O3S	1000309-17-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
 Data File : BF117706.D
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 Misc :
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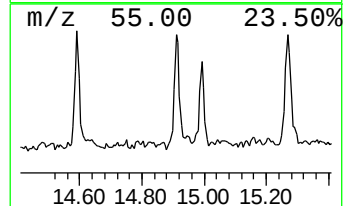
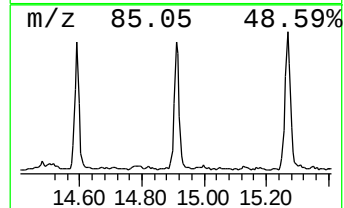
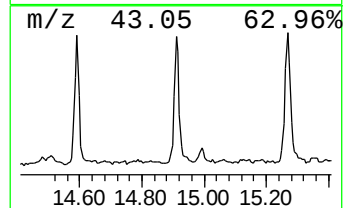
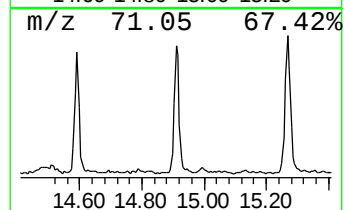
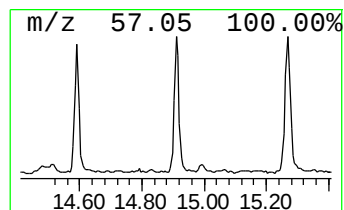
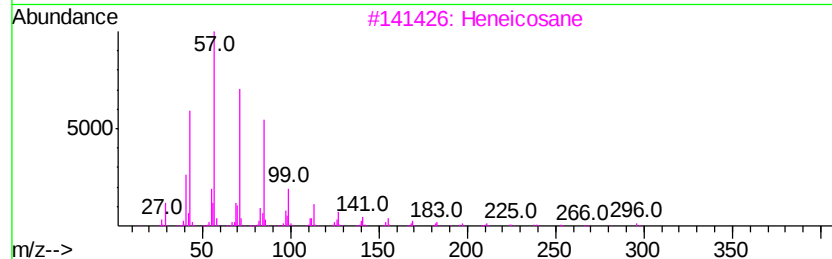
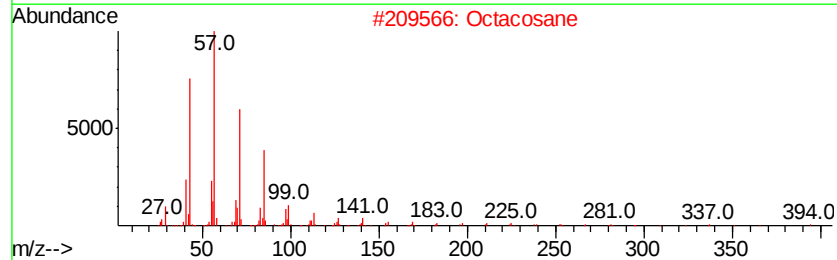
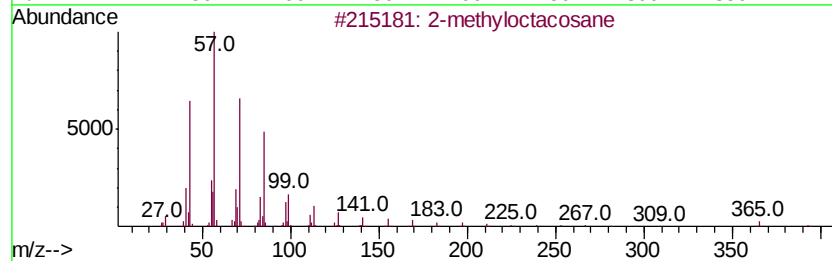
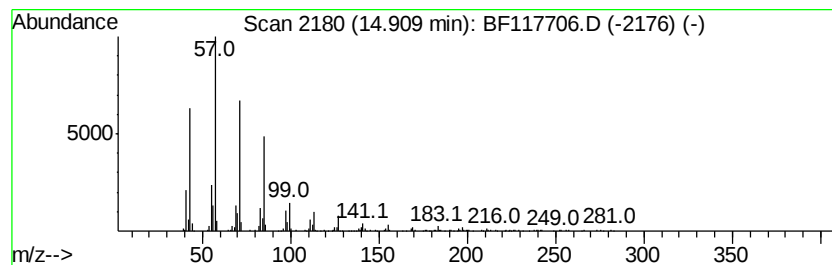
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.91	2.76 ng	319060	Perylene-d12		15.63	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117706.D
Acq On : 7 Nov 2019 15:59
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Sample : K5710-03
Misc :
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ClientSampleId :
TP- 31-S

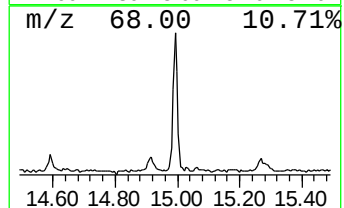
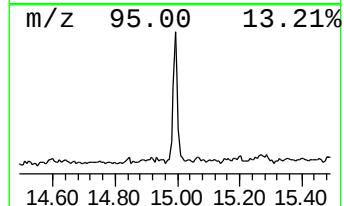
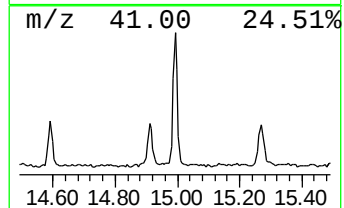
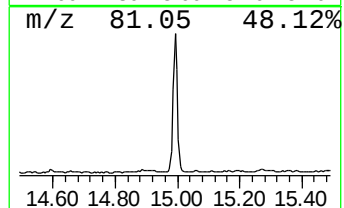
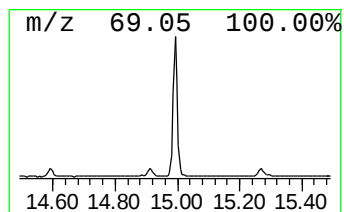
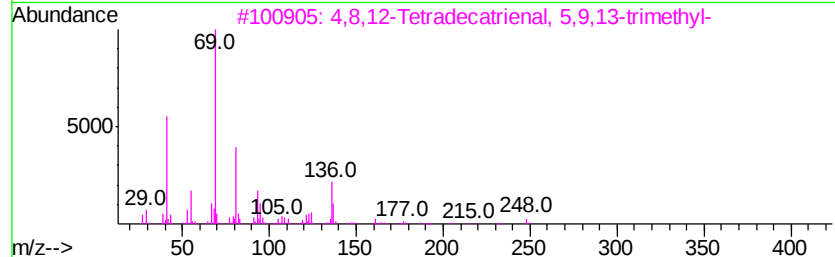
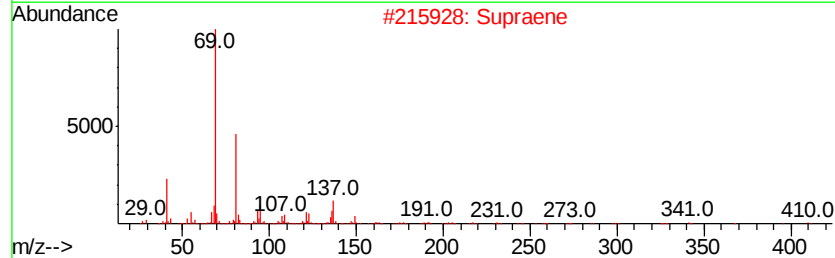
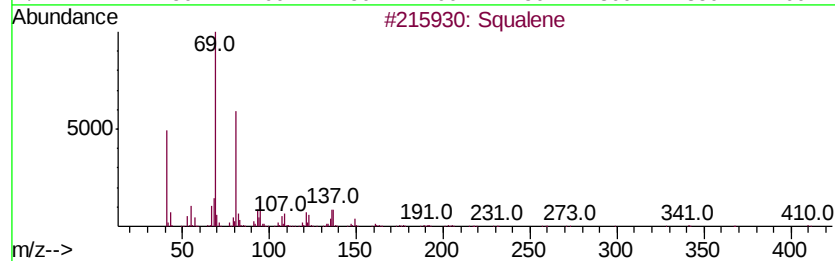
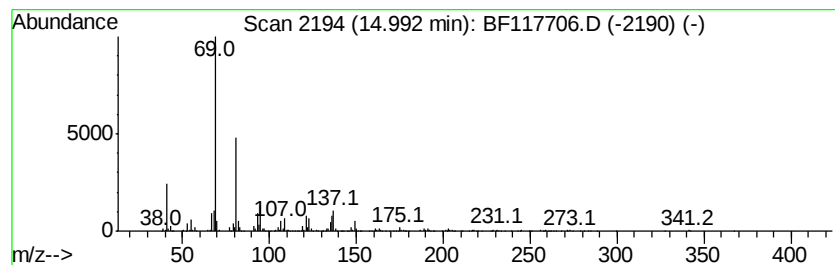
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	4.86 ng	561142	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
 Data File : BF117706.D
 Acq On : 7 Nov 2019 15:59
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 TP- 31-S

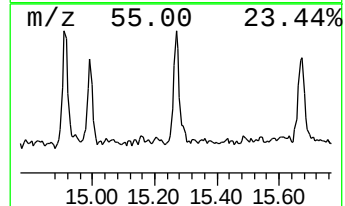
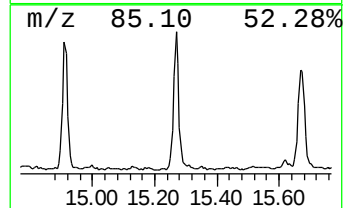
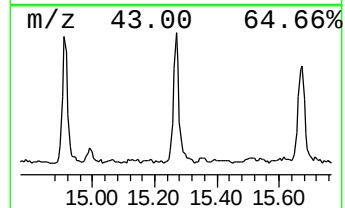
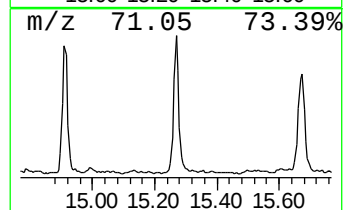
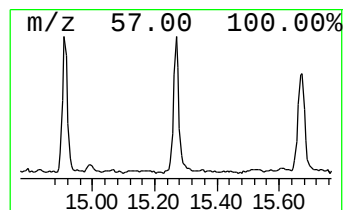
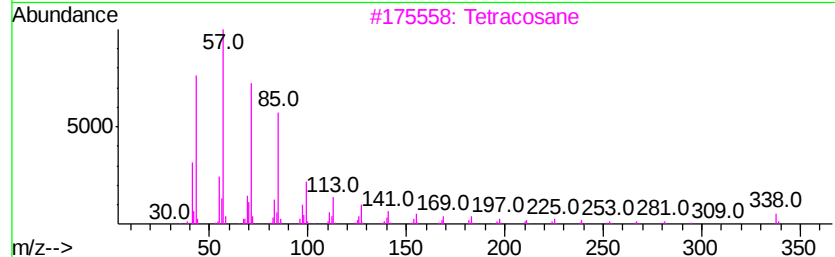
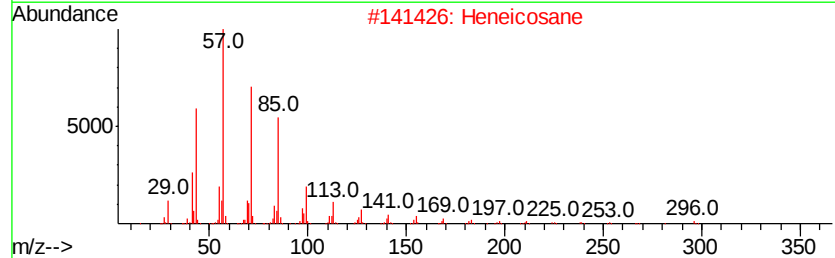
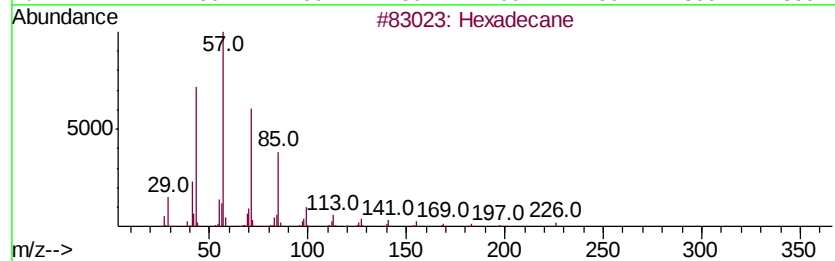
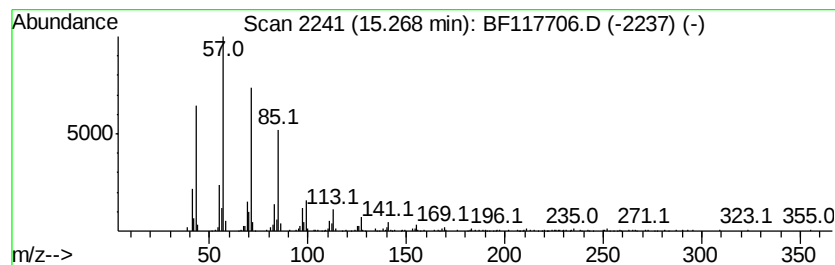
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.15 ng	364193	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117706.D
Acq On : 7 Nov 2019 15:59
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Misc :
ALS Vial : 3 Sample Multiplier: 1

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ClientSampleId :
TP- 31-S

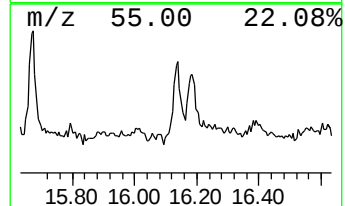
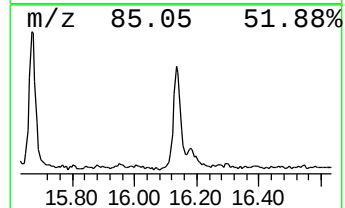
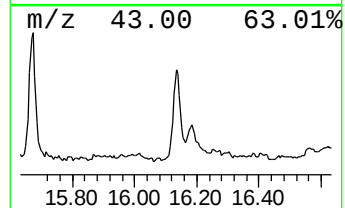
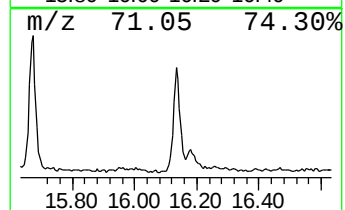
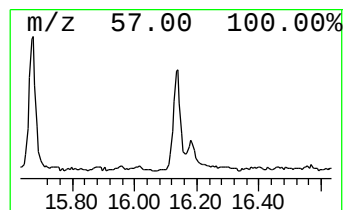
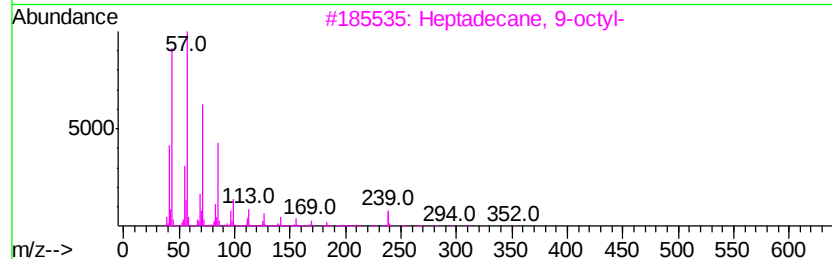
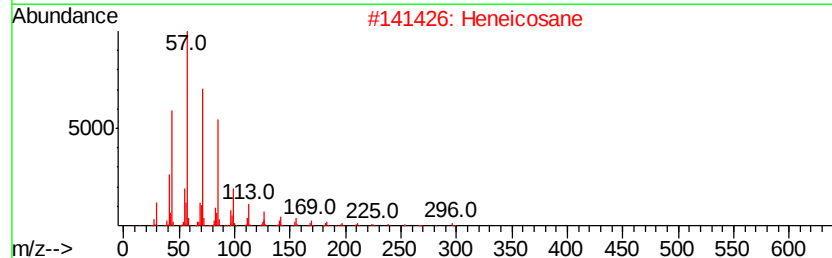
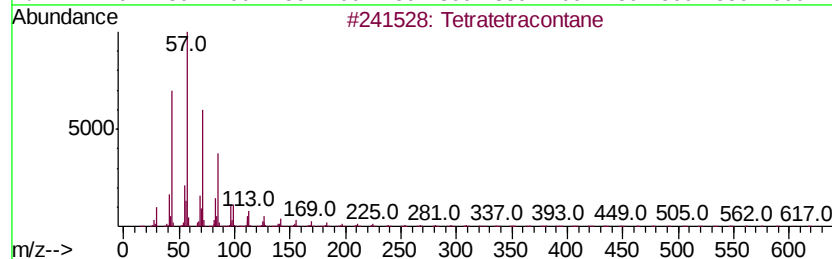
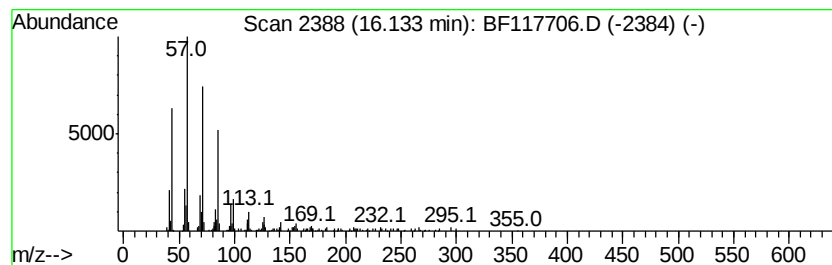
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.30 ng	265245	Perylene-d12	15.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110719\
 Data File : BF117706.D
 Acq On : 7 Nov 2019 15:59
 Operator : JU
 Sample : K5710-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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...	2.24	19.0	ng	1801570	1	6.93	1899160	20.0
2-Pentanone, 4-hy...	5.15	17.0	ng	1616720	1	6.93	1899160	20.0
unknown6.70	6.70	72.3	ng	6860440	1	6.93	1899160	20.0
n-Hexadecanoic acid	12.00	7.9	ng	1158290	4	11.47	2939040	20.0
Octadecanoic acid	12.78	2.6	ng	387709	4	11.47	2939040	20.0
Cetene	13.96	8.9	ng	992230	5	14.12	2229710	20.0
Heptadecane	14.59	2.5	ng	274953	5	14.12	2229710	20.0
2-methyloctacosane	14.91	2.8	ng	319060	6	15.63	2308980	20.0
Squalene	14.99	4.9	ng	561142	6	15.63	2308980	20.0
Hexadecane	15.27	3.1	ng	364193	6	15.63	2308980	20.0
Tetratetracontane	16.13	2.3	ng	265245	6	15.63	2308980	20.0