

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
 Data File : BF111152.D
 Acq On : 6 Dec 2018 21:44
 Operator : JU/SJ
 Sample : J6219-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM-342-135-120418

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-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	5.022	488	499	507	rBV	670991	1002637	7.01%	0.834%
2	5.428	562	568	571	rBV	12307661	12826416	89.70%	10.670%
3	6.439	733	740	744	rBV	11957505	14074246	98.43%	11.709%
4	6.575	758	763	766	rBV	12871764	13229345	92.52%	11.006%
5	6.634	770	773	776	rBV	631547	473132	3.31%	0.394%
6	6.804	798	802	806	rBV	3766493	3037158	21.24%	2.527%
7	6.963	825	829	832	rBV	11512343	10178063	71.18%	8.467%
8	7.363	892	897	900	rBV	8340718	8928771	62.44%	7.428%
9	8.086	1016	1020	1023	rBV	4830362	3943845	27.58%	3.281%
10	9.169	1198	1204	1207	rBV	14066528	14299228	100.00%	11.896%
11	9.557	1266	1270	1273	rBV	1186852	1050537	7.35%	0.874%
12	9.839	1314	1318	1322	rVB2	4965384	4287241	29.98%	3.567%
13	10.627	1447	1452	1455	rBV	8986822	8120180	56.79%	6.755%
14	11.321	1566	1570	1572	rBV	4928303	4014649	28.08%	3.340%
15	11.345	1572	1574	1576	rVV	360372	280846	1.96%	0.234%
16	11.392	1576	1582	1585	rVB	190012	173005	1.21%	0.144%
17	11.857	1657	1661	1671	rBV	943028	1017543	7.12%	0.847%
18	12.639	1791	1794	1800	rBV	434303	427231	2.99%	0.355%
19	12.910	1835	1840	1843	rVB	11299137	10883428	76.11%	9.054%
20	13.810	1990	1993	2003	rBV	983492	1054170	7.37%	0.877%
21	13.951	2013	2017	2021	rBV	2758599	2664845	18.64%	2.217%
22	14.445	2098	2101	2112	rVB	253863	309481	2.16%	0.257%
23	15.074	2204	2208	2216	rBV	328778	435728	3.05%	0.362%
24	15.392	2257	2262	2266	rBV	2308063	2663604	18.63%	2.216%
25	15.445	2268	2271	2279	rVB	182803	262616	1.84%	0.218%
26	15.874	2340	2344	2348	rBV	189056	246508	1.72%	0.205%
27	15.921	2348	2352	2361	rVV3	175278	320310	2.24%	0.266%

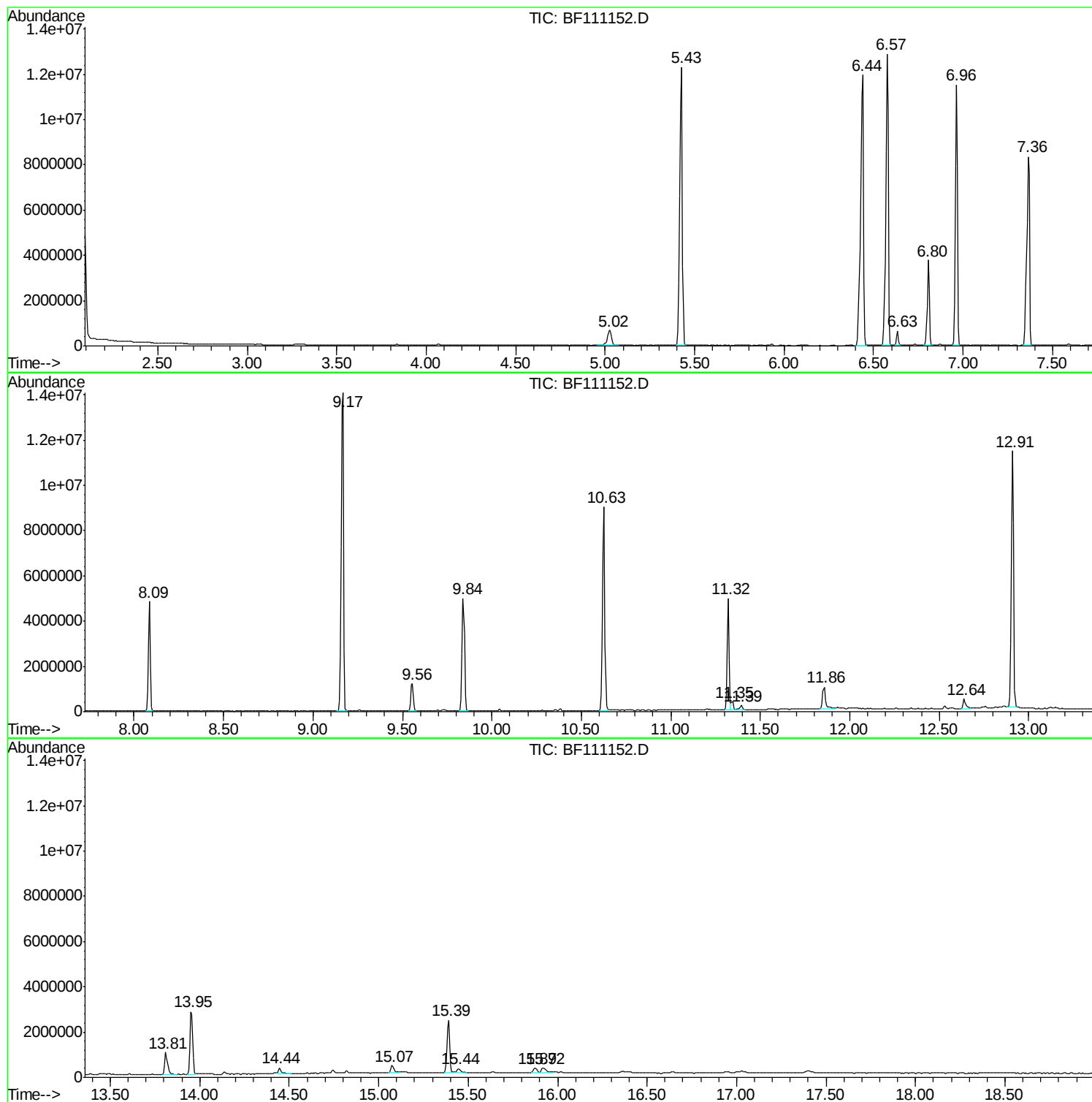
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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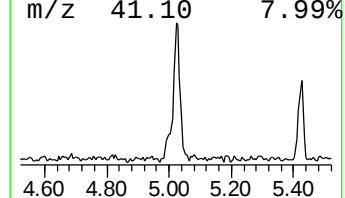
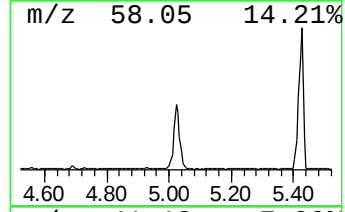
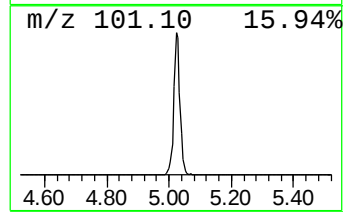
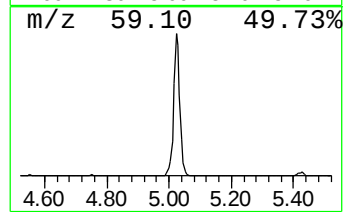
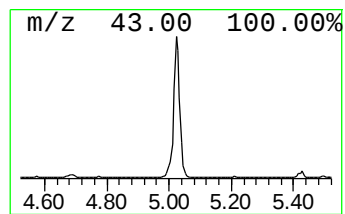
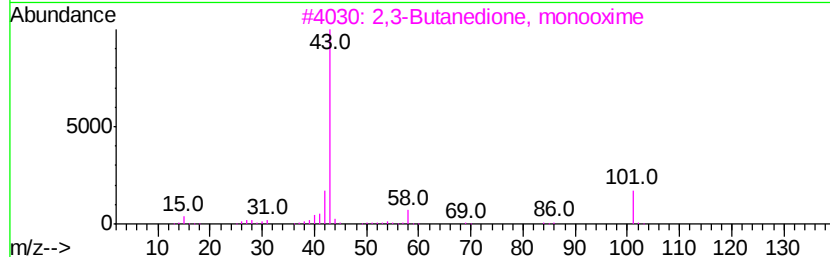
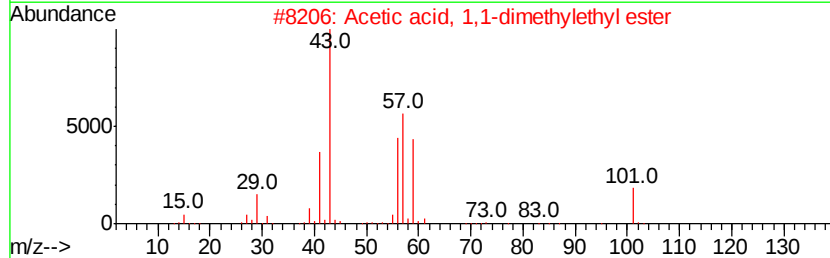
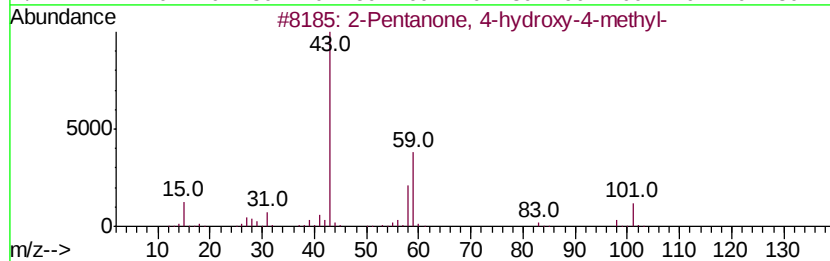
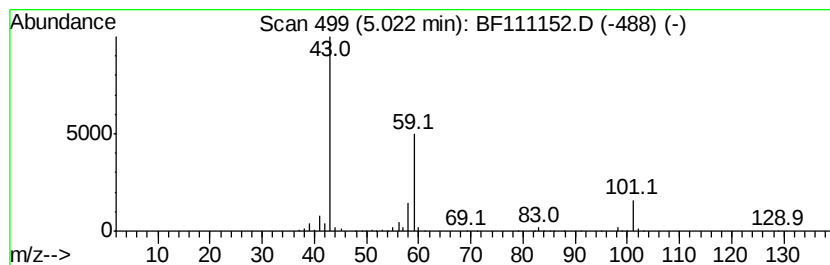
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	6.60 ng	1002640	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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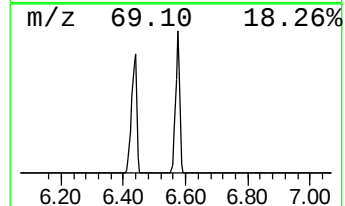
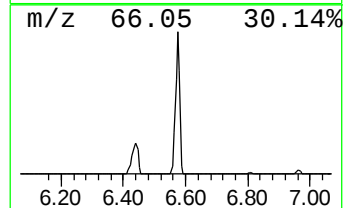
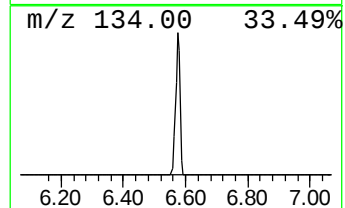
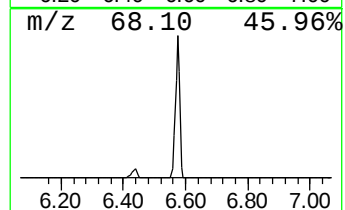
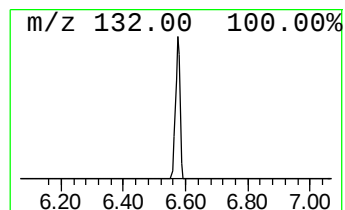
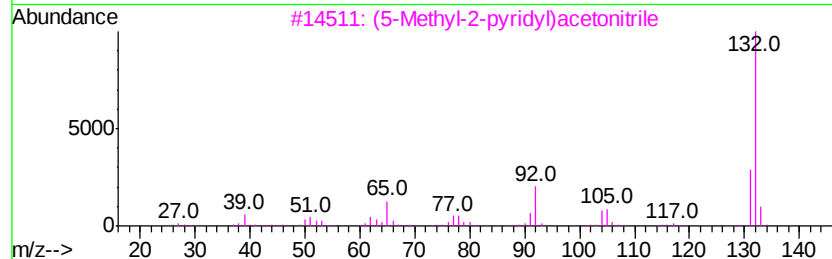
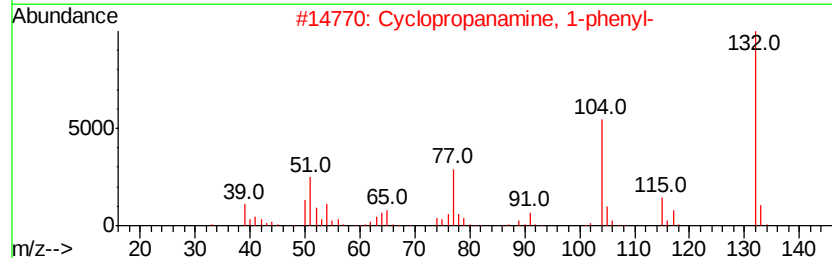
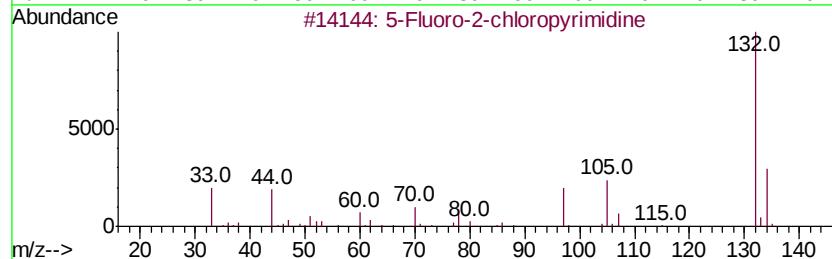
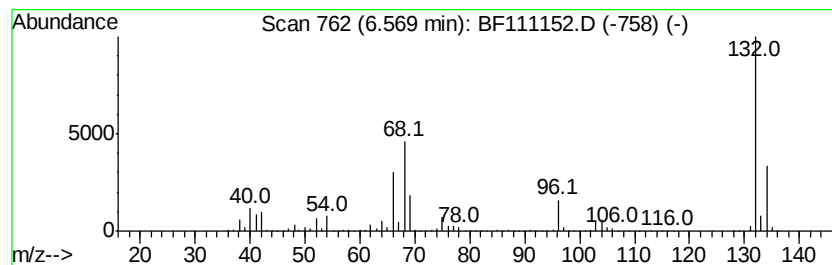
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	87.12 ng	13229300	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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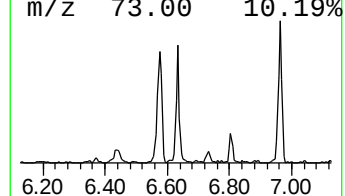
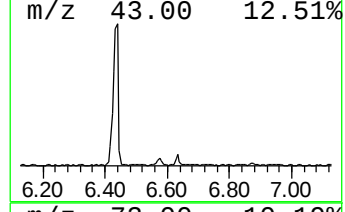
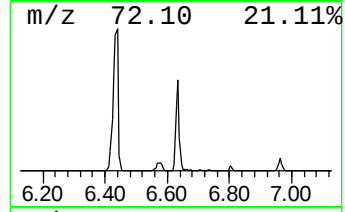
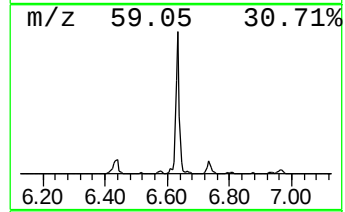
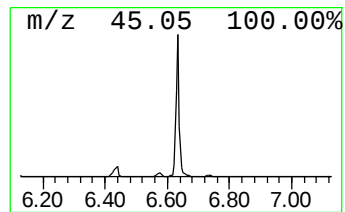
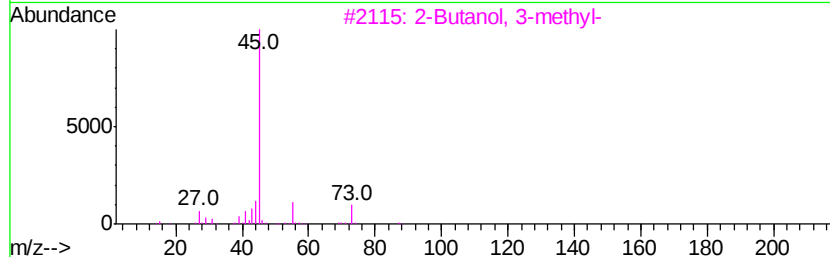
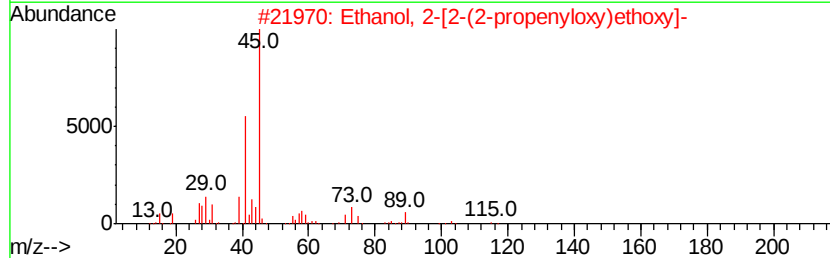
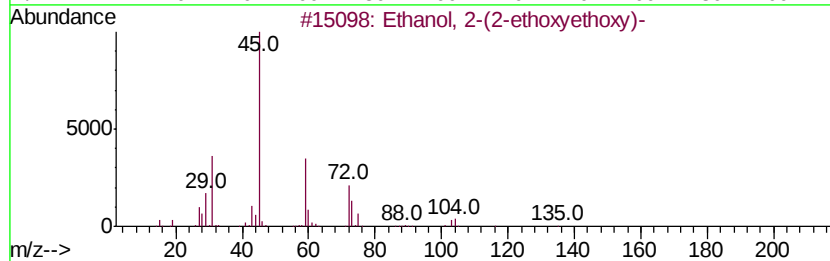
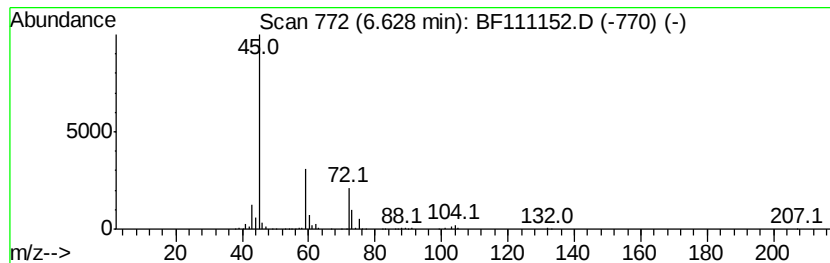
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.63	3.12 ng	473132	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	45
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	40
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
5	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9



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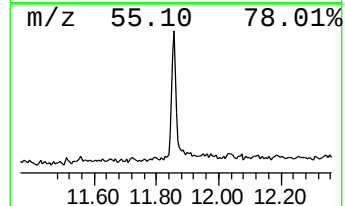
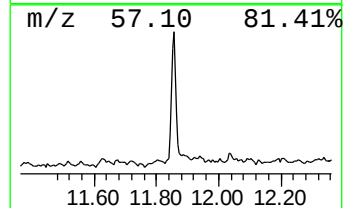
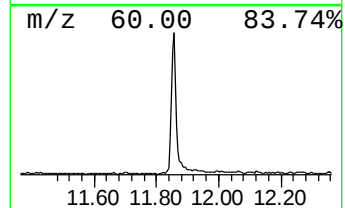
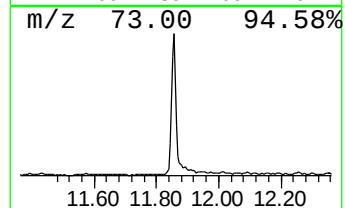
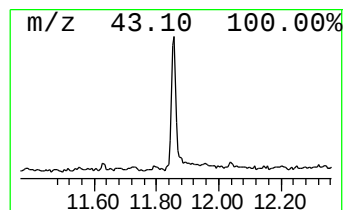
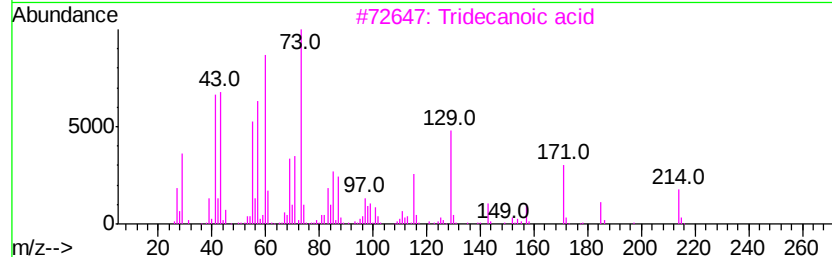
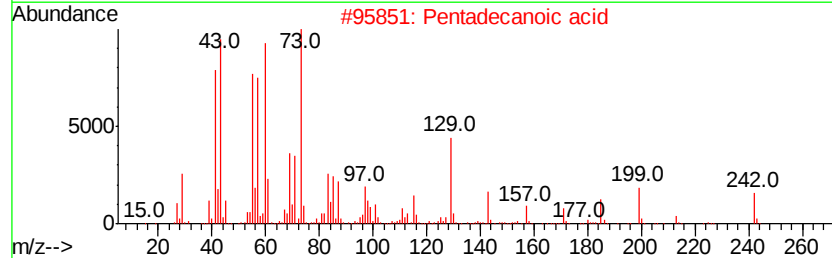
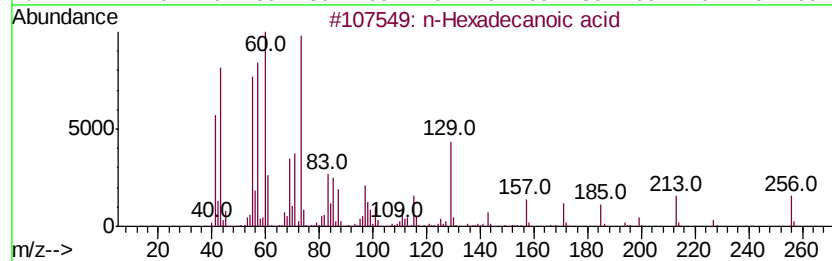
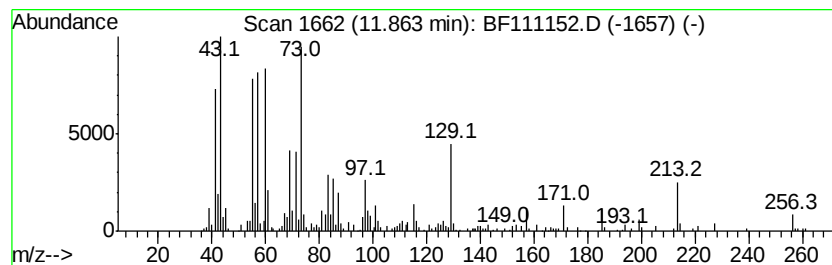
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	5.07 ng	1017540	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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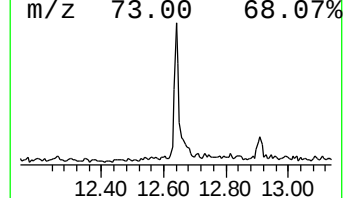
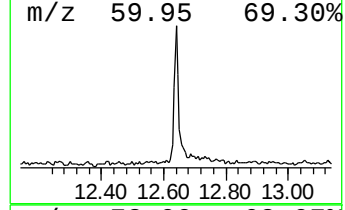
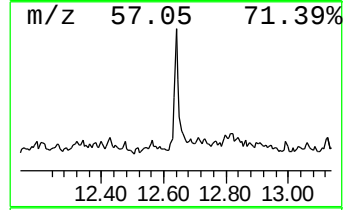
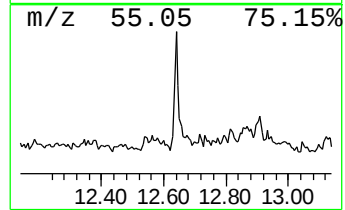
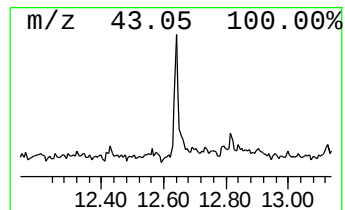
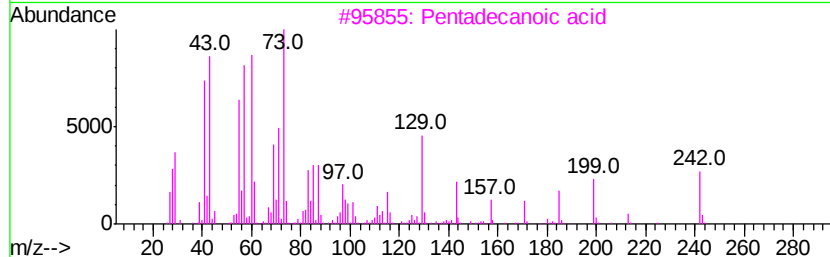
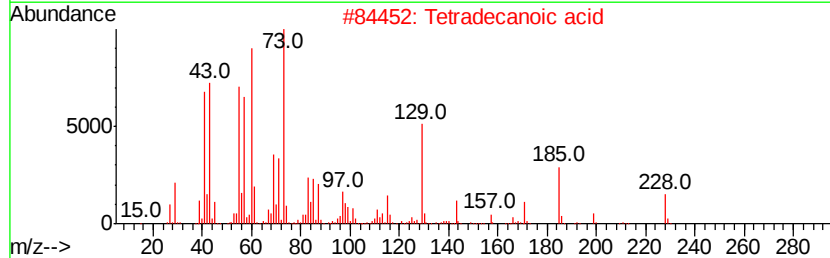
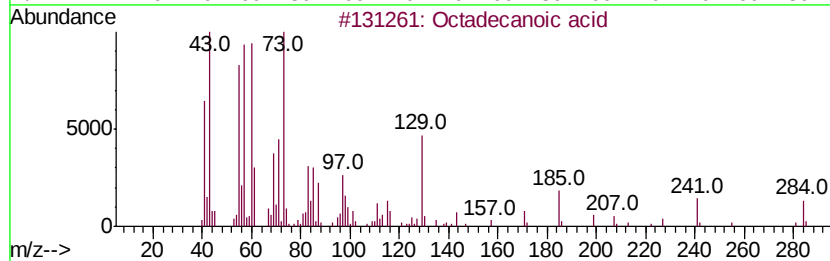
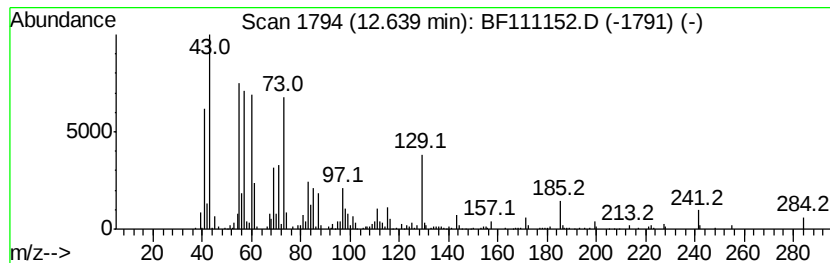
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Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.64	3.21 ng	427231	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58



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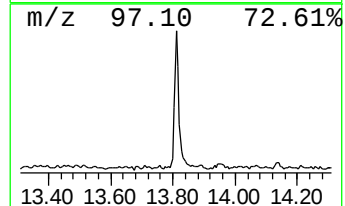
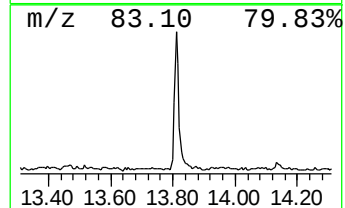
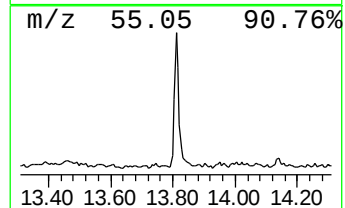
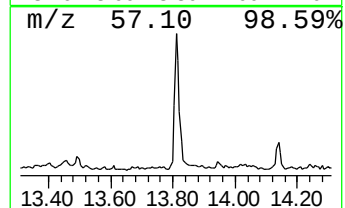
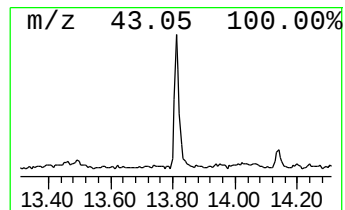
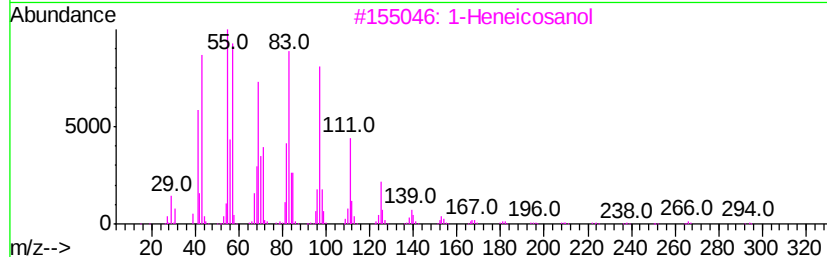
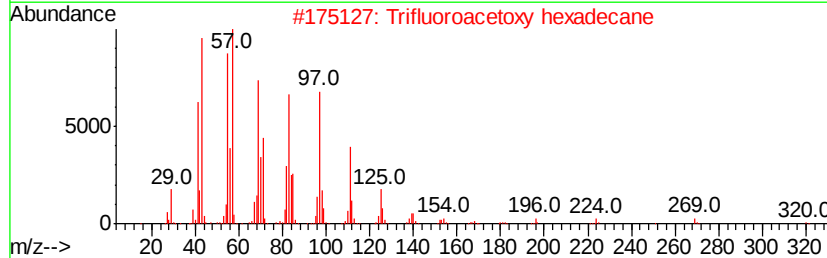
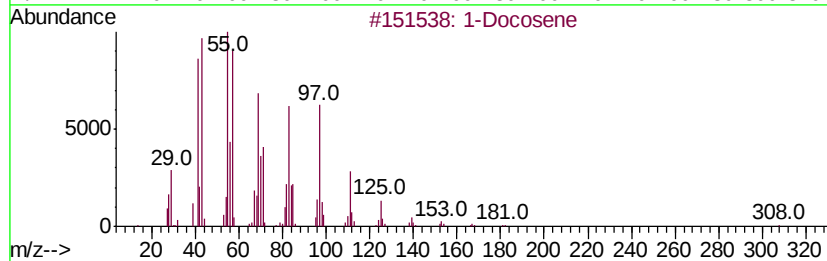
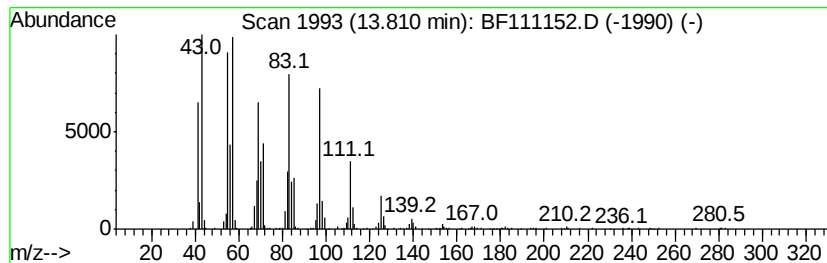
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	7.91 ng	1054170	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		2-Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
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Acq On : 6 Dec 2018 21:44
Operator : JU/SJ
Sample : J6219-01
Misc :
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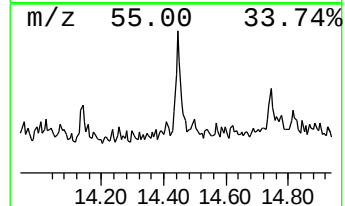
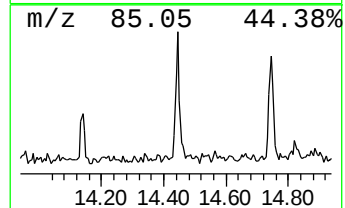
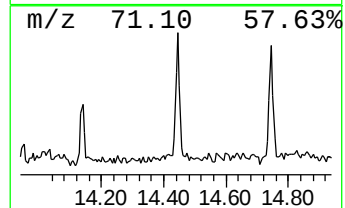
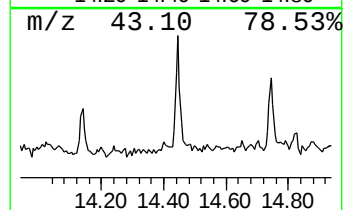
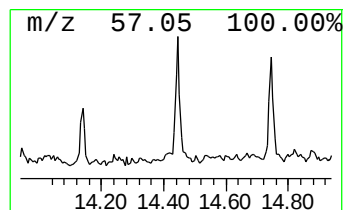
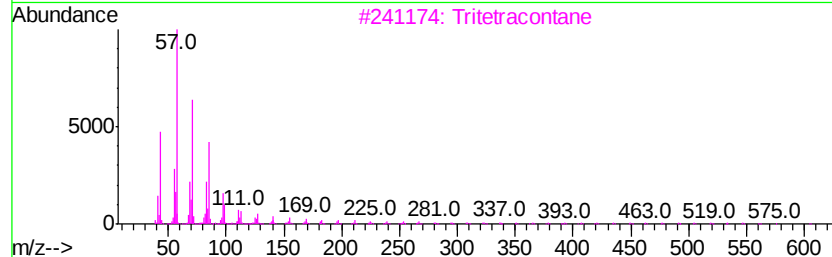
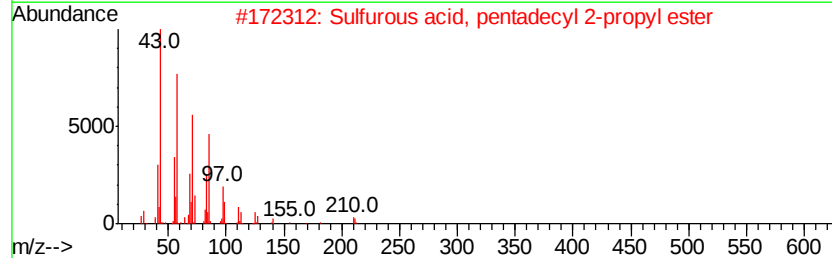
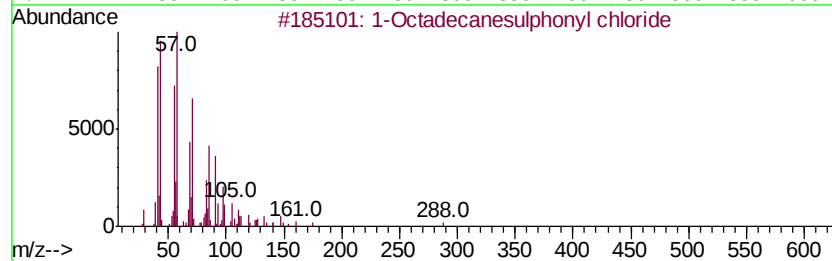
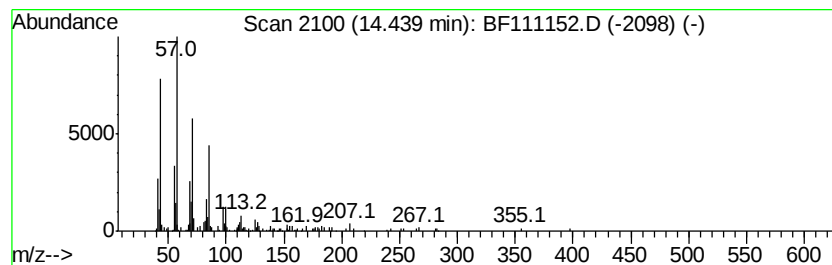
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ClientSampleId :
NM-342-135-120418

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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 1-Octadecanesulphonyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.44	2.32 ng	309481	Chrysene-d12		13.96	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
3		Tritetracontane	605	C43H88	007098-21-7	72
4		1-Chloroeicosane	316	C20H41Cl	042217-02-7	64
5		Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111152.D
Acq On : 6 Dec 2018 21:44
Operator : JU/SJ
Sample : J6219-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM-342-135-120418

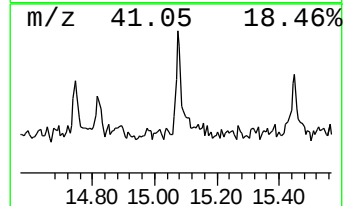
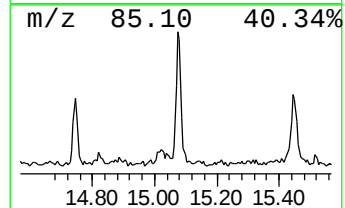
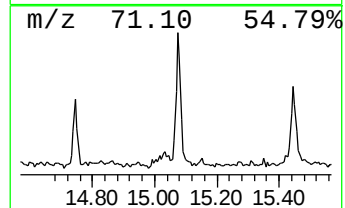
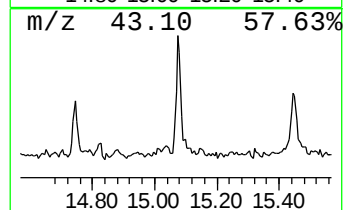
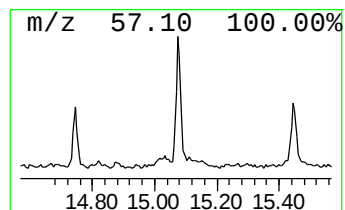
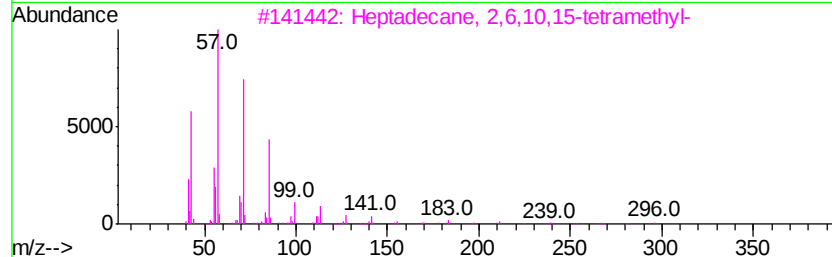
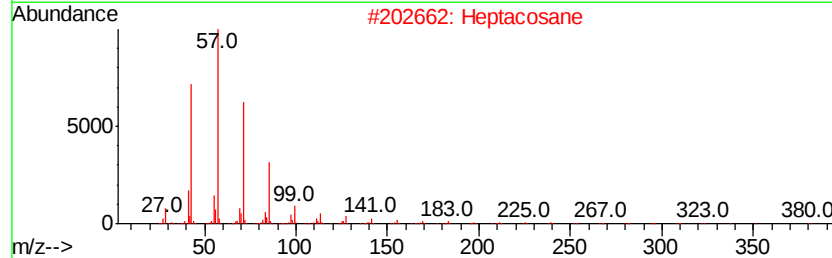
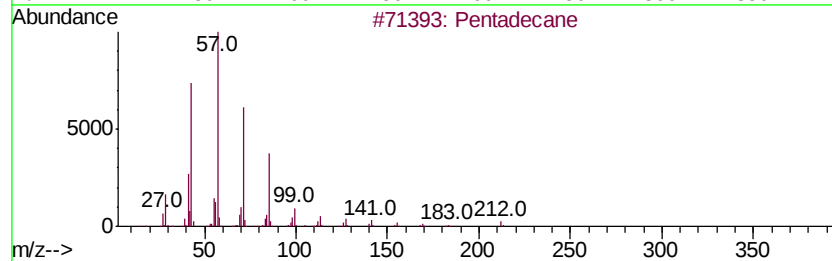
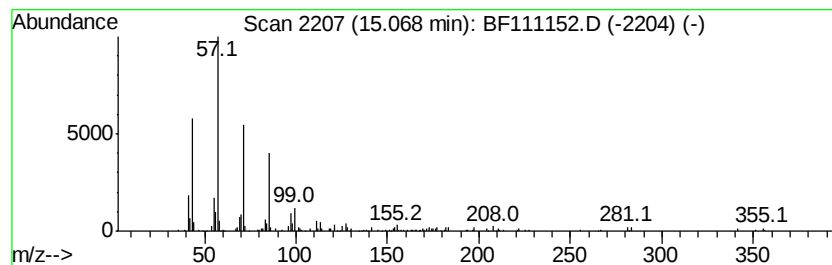
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	3.27 ng	435728	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	93
2	Heptacosane		380	C27H56	000593-49-7	91
3	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	90
4	Hexatriacontane		507	C36H74	000630-06-8	90
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120618\
Data File : BF111152.D
Acq On : 6 Dec 2018 21:44
Operator : JU/SJ
Sample : J6219-01
Misc :
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ClientSampleId :
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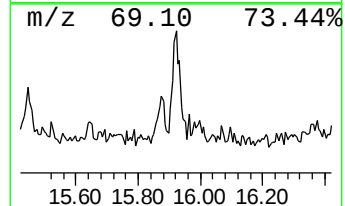
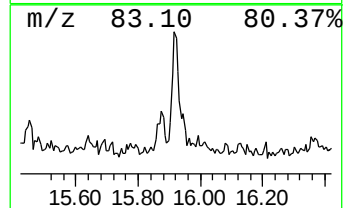
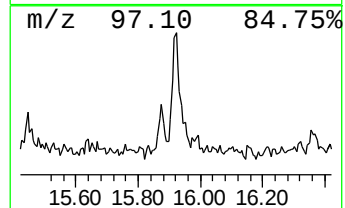
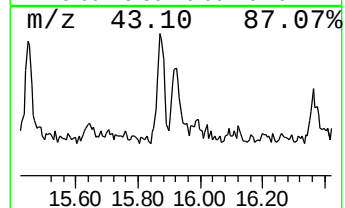
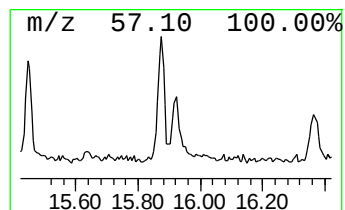
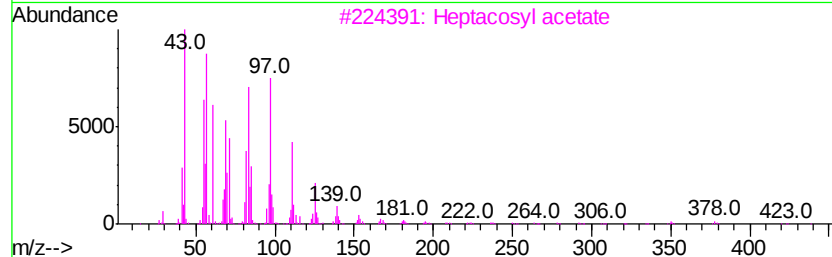
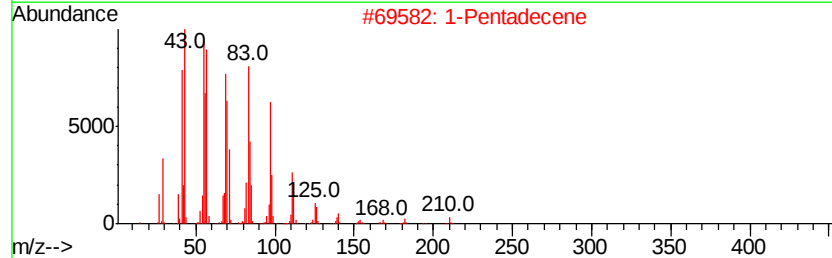
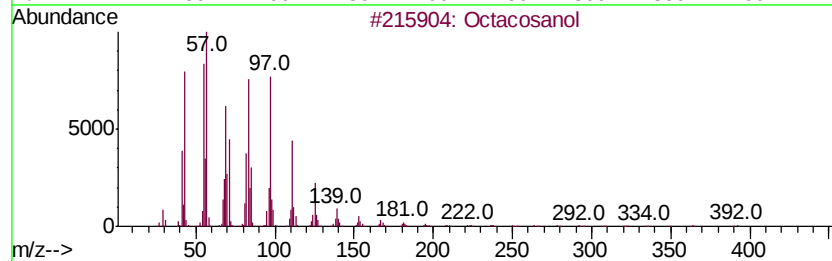
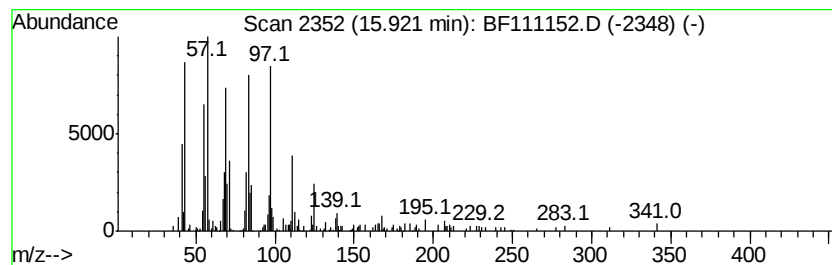
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	2.41 ng	320310	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	89
2		1-Pentadecene	210	C15H30	013360-61-7	74
3		Heptacosyl acetate	438	C29H58O2	1000351-78-2	68
4		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	62
5		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120618\
Data File : BF111152.D
Acq On : 6 Dec 2018 21:44
Operator : JU/SJ
Sample : J6219-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	6.6 ng		1002640	1	6.80	3037160	20.0
unknown6.57	6.57	87.1 ng		13229300	1	6.80	3037160	20.0
Ethanol, 2-(2-eth...	6.63	3.1 ng		473132	1	6.80	3037160	20.0
n-Hexadecanoic acid	11.86	5.1 ng		1017540	4	11.32	4014650	20.0
Octadecanoic acid	12.64	3.2 ng		427231	5	13.96	2664850	20.0
1-Docosene	13.81	7.9 ng		1054170	5	13.96	2664850	20.0
1-Octadecanesulph...	14.44	2.3 ng		309481	5	13.96	2664850	20.0
Pentadecane	15.07	3.3 ng		435728	6	15.39	2663600	20.0
Octacosanol	15.92	2.4 ng		320310	6	15.39	2663600	20.0