

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
 Data File : BF111123.D
 Acq On : 5 Dec 2018 22:39
 Operator : JU/SJ
 Sample : J6184-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-331

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	3.216	189	192	204	rBV	127993	276589	2.25%	0.273%
2	5.016	489	498	505	rBV	519540	700158	5.69%	0.691%
3	5.422	561	567	570	rBV	11256101	10953859	89.08%	10.808%
4	6.433	733	739	743	rBV2	11046678	12296550	100.00%	12.133%
5	6.575	758	763	766	rBV	11887990	11204090	91.12%	11.055%
6	6.804	799	802	806	rVB	3867898	3044989	24.76%	3.004%
7	6.963	825	829	832	rBV	9990734	8416062	68.44%	8.304%
8	7.363	892	897	900	rBV	7667539	7309149	59.44%	7.212%
9	8.086	1016	1020	1023	rBV	5006578	3884441	31.59%	3.833%
10	9.163	1199	1203	1207	rBV	12202833	11229617	91.32%	11.080%
11	9.557	1266	1270	1272	rBV	1380579	1171550	9.53%	1.156%
12	9.839	1314	1318	1322	rBV2	4645126	3934307	32.00%	3.882%
13	10.621	1447	1451	1455	rBV	6301509	5766718	46.90%	5.690%
14	11.321	1566	1570	1573	rBV	4002669	3317733	26.98%	3.274%
15	11.345	1573	1574	1577	rVB	267888	127858	1.04%	0.126%
16	11.857	1657	1661	1666	rBV2	1051772	1029958	8.38%	1.016%
17	12.527	1772	1775	1779	rBV	409851	379825	3.09%	0.375%
18	12.639	1790	1794	1800	rBV2	479397	538325	4.38%	0.531%
19	12.757	1808	1814	1818	rVB	385240	399190	3.25%	0.394%
20	12.910	1835	1840	1843	rBV	8434845	7596152	61.77%	7.495%
21	13.809	1990	1993	1999	rVB	722422	740768	6.02%	0.731%
22	13.951	2013	2017	2020	rBV	3355710	3302772	26.86%	3.259%
23	13.980	2020	2022	2024	rVB	180912	138874	1.13%	0.137%
24	14.139	2046	2049	2052	rBV	163618	147788	1.20%	0.146%
25	14.445	2098	2101	2107	rBV	446490	489055	3.98%	0.483%
26	14.745	2149	2152	2156	rBV	203950	203177	1.65%	0.200%
27	14.821	2162	2165	2169	rVB2	232279	255488	2.08%	0.252%
28	15.074	2206	2208	2211	rBV	227822	239593	1.95%	0.236%
29	15.392	2257	2262	2266	rVV	1468459	1795763	14.60%	1.772%
30	15.451	2269	2272	2275	rVB	191139	230379	1.87%	0.227%
31	15.874	2341	2344	2348	rVB	178565	229042	1.86%	0.226%

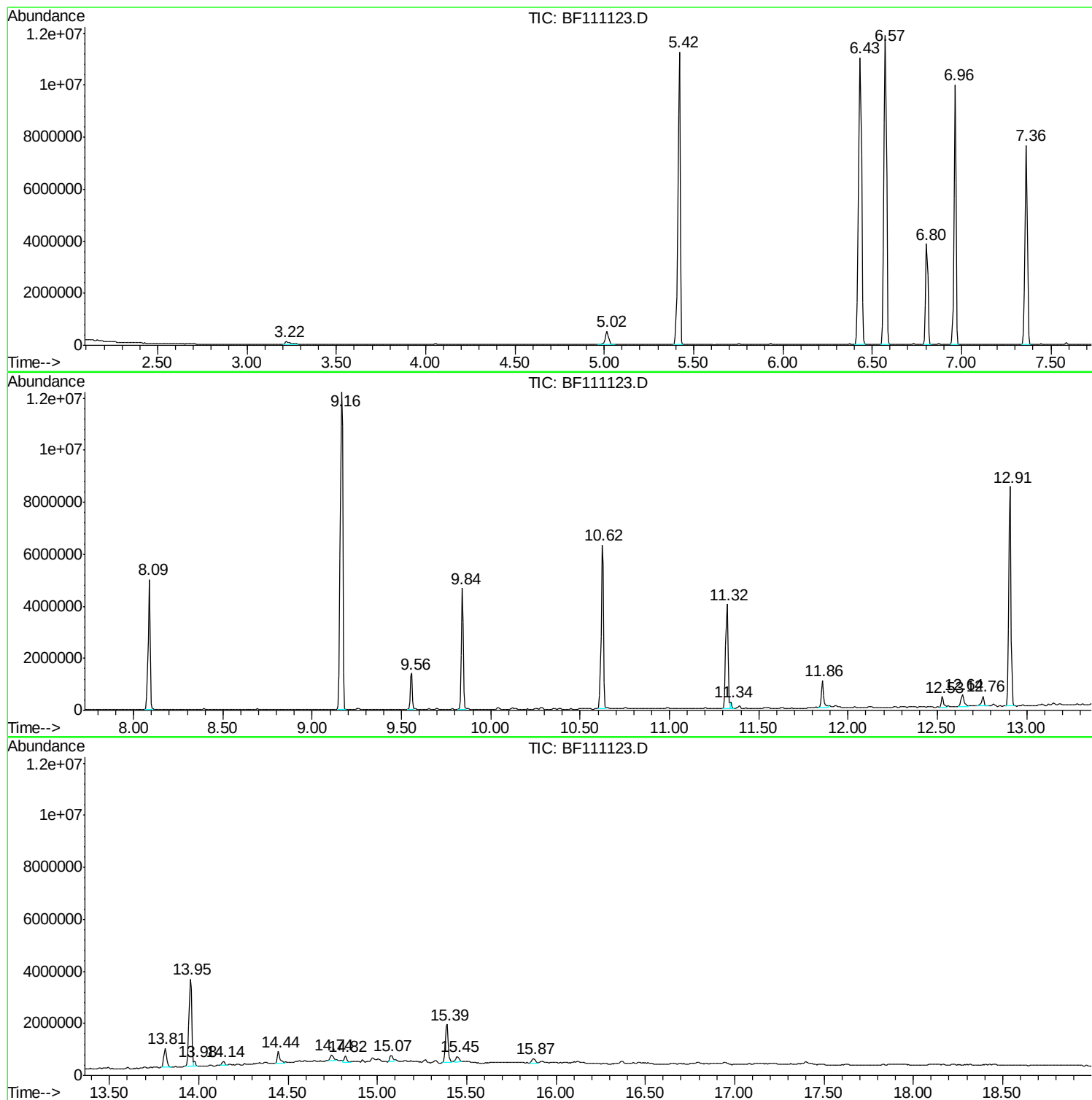
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BNA_F
ClientSampled :
RO-331

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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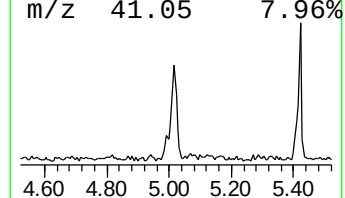
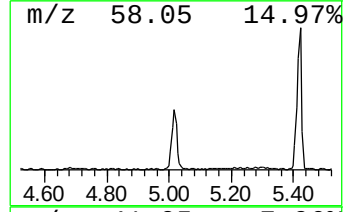
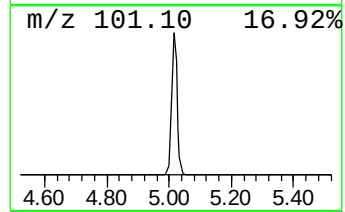
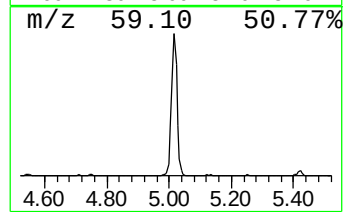
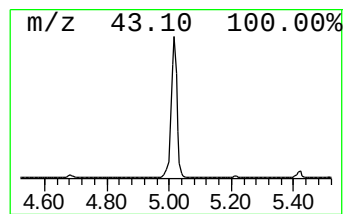
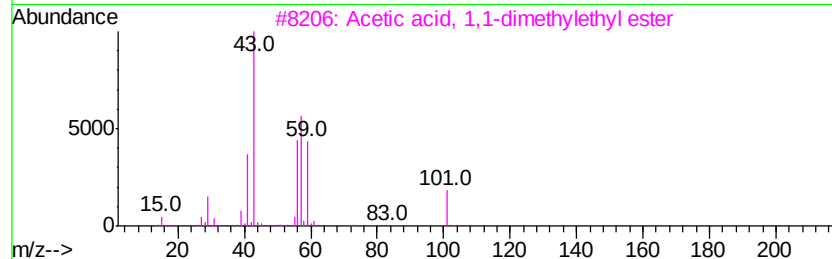
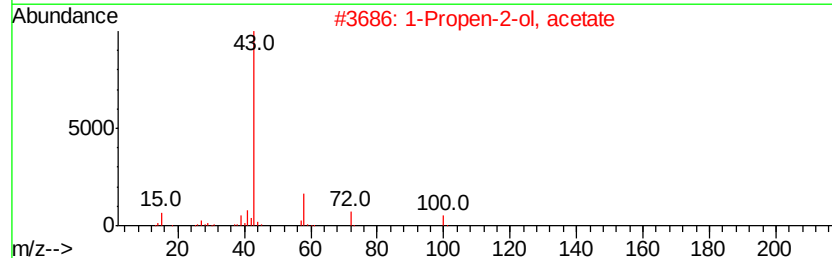
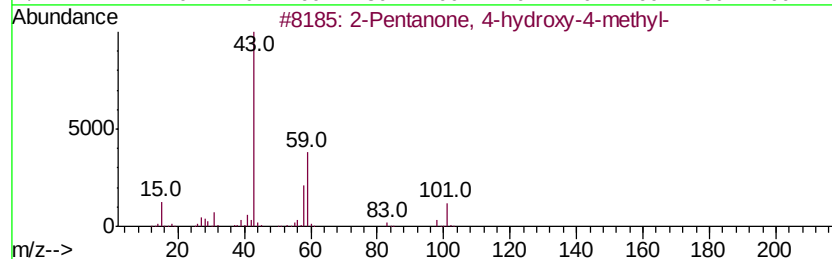
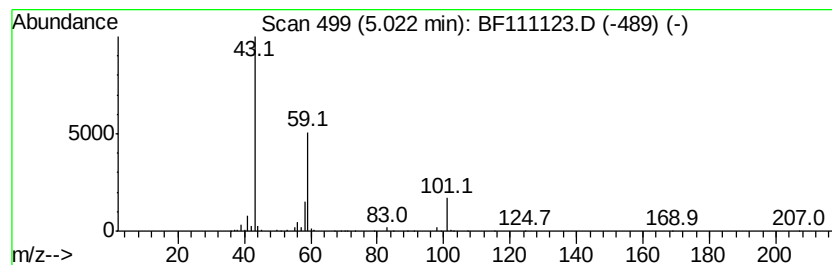
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.60 ng	700158	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			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			3,3-Dimethylbutylamine	101	C6H15N	015673-00-4	7
5			Acetone	58	C3H6O	000067-64-1	7



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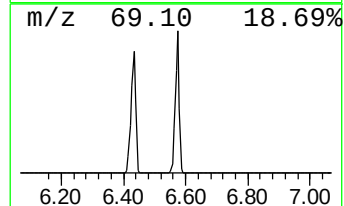
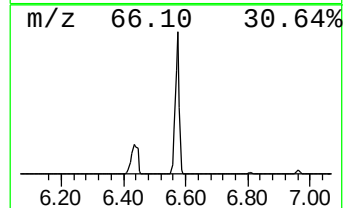
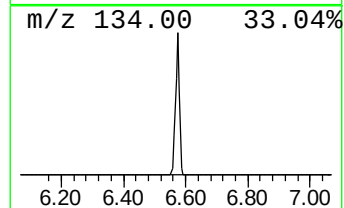
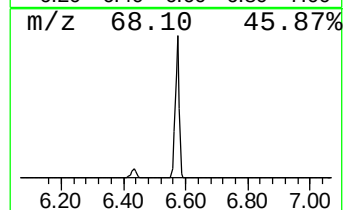
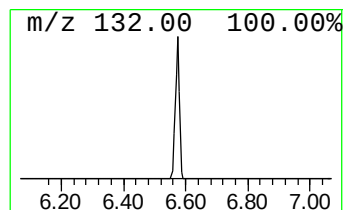
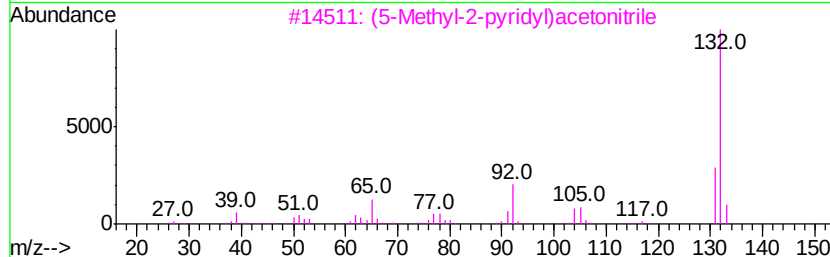
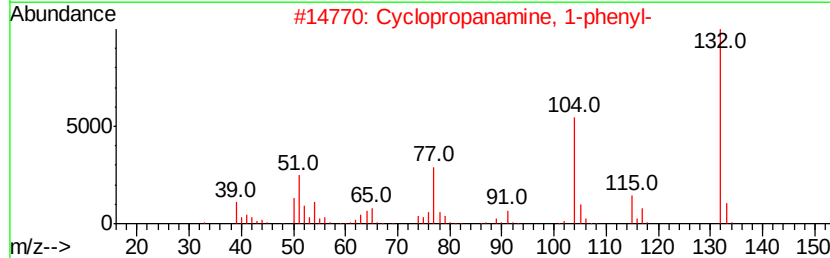
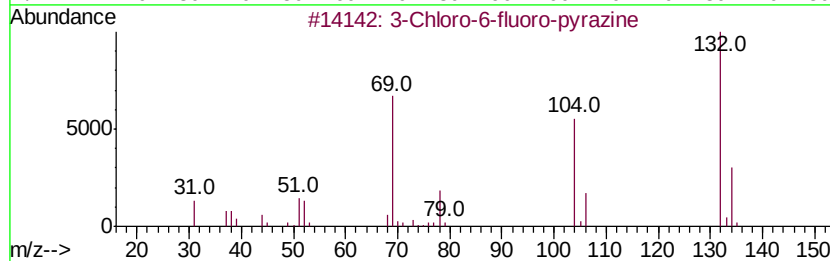
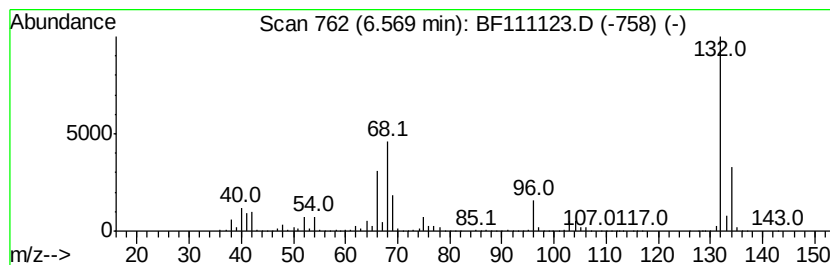
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	73.59 ng	11204100	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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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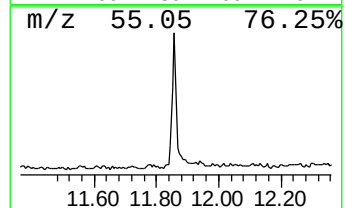
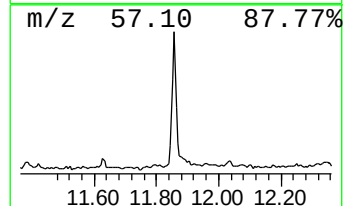
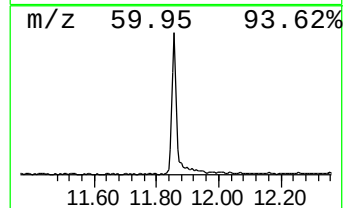
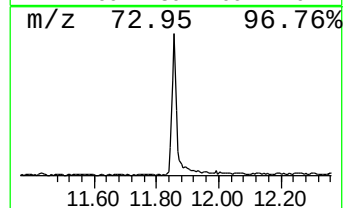
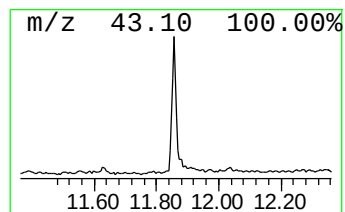
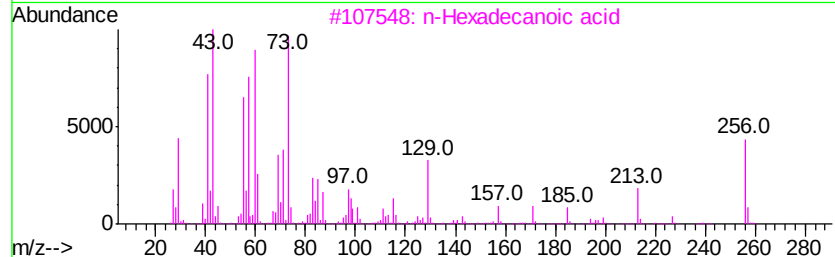
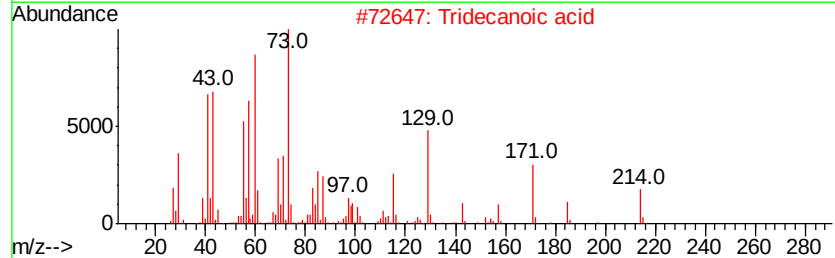
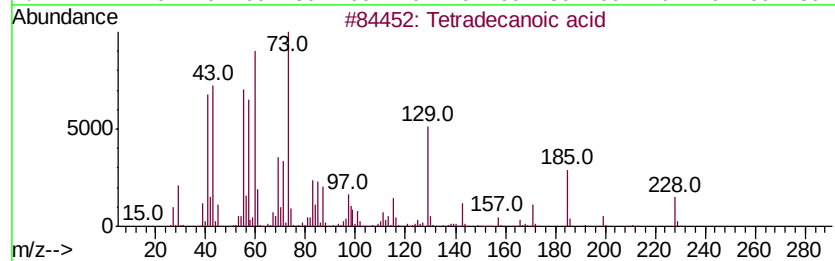
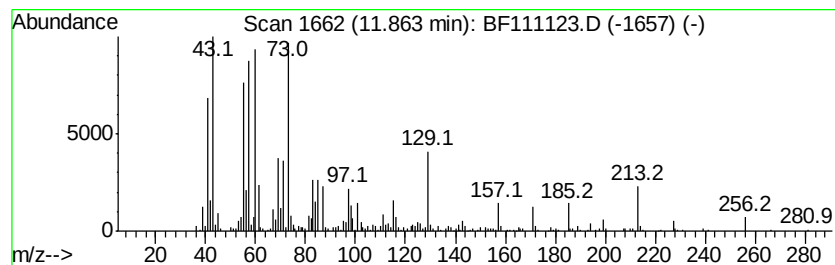
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Peak Number 4 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	6.21 ng	1029960	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90



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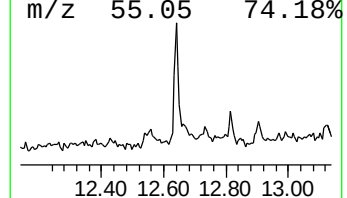
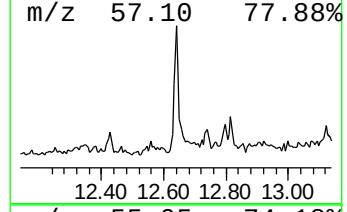
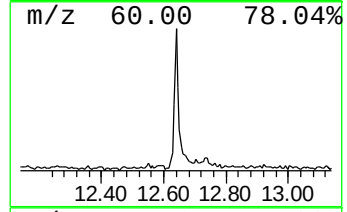
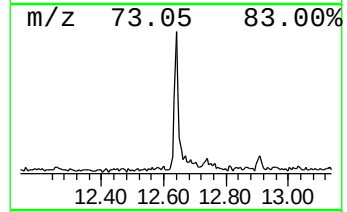
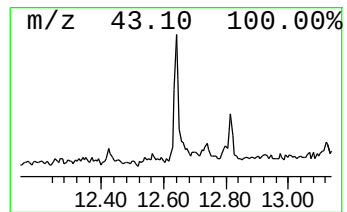
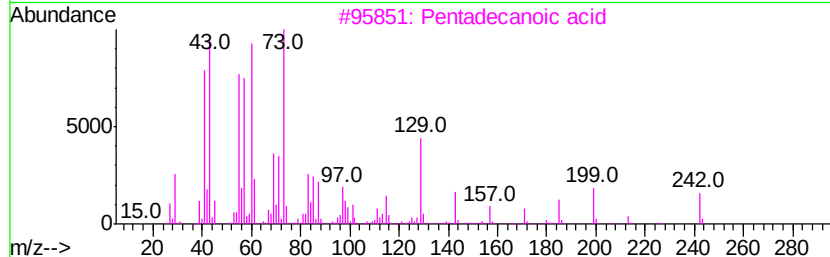
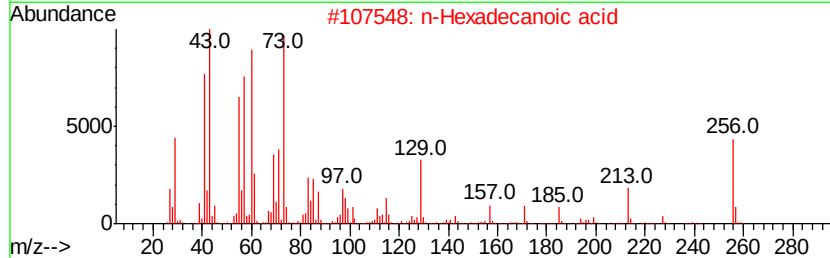
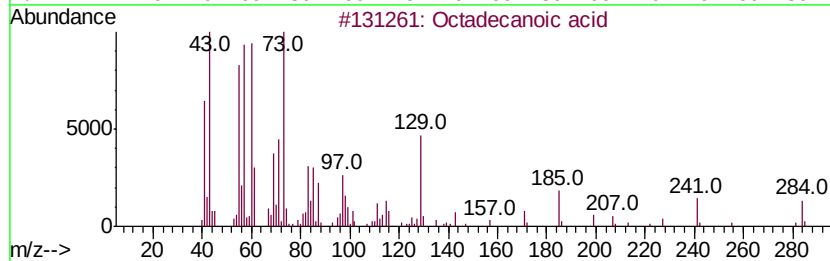
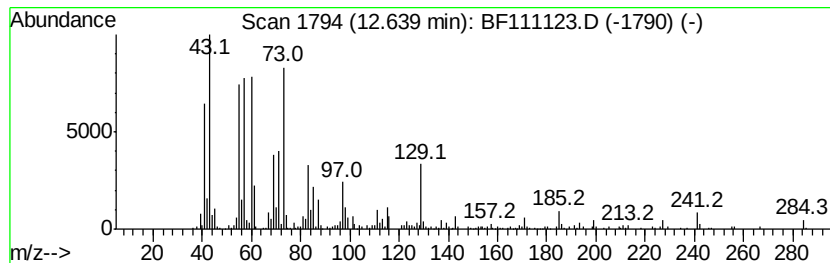
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.64	3.26 ng	538325	Chrysene-d12		13.96
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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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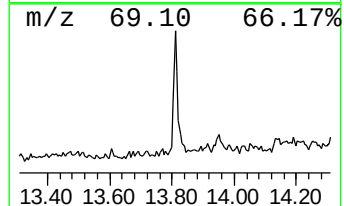
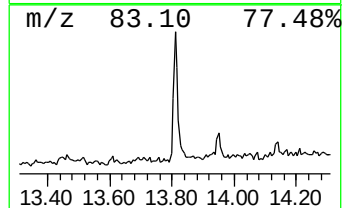
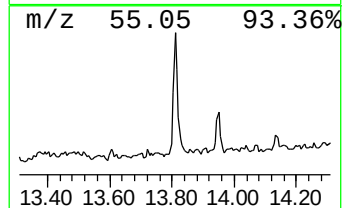
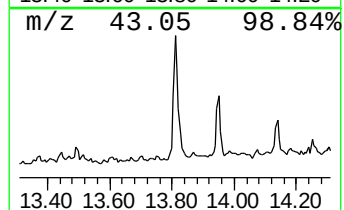
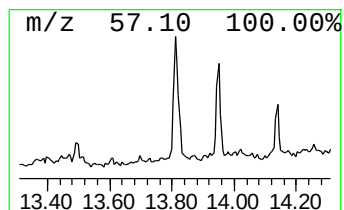
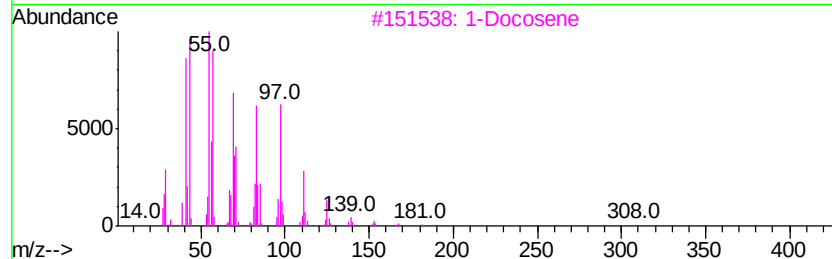
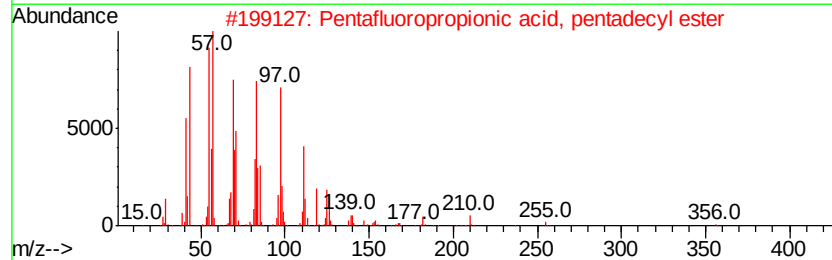
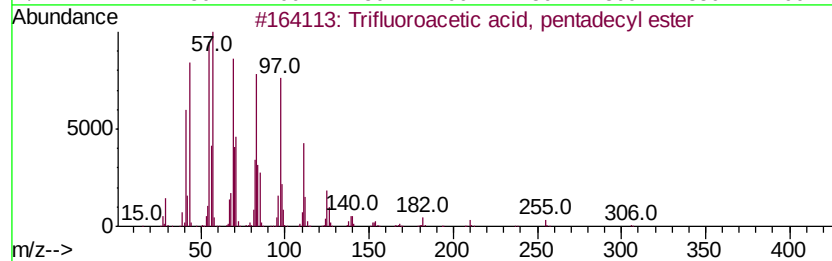
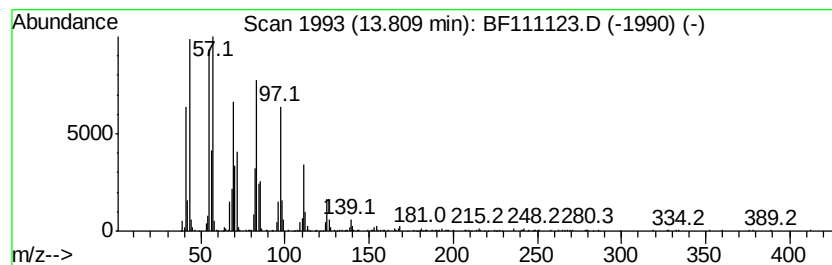
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.49 ng	740768	Chrysene-d12	13.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			1-Docosene	308	C22H44	001599-67-3	94
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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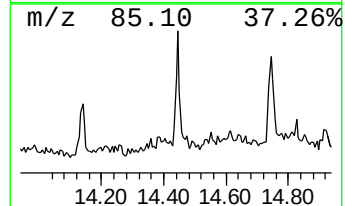
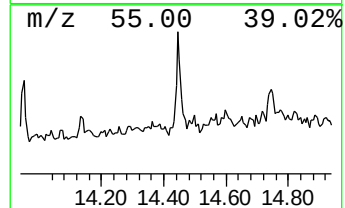
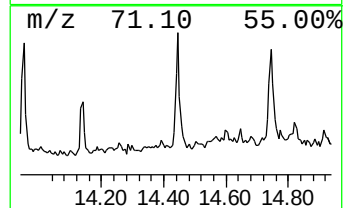
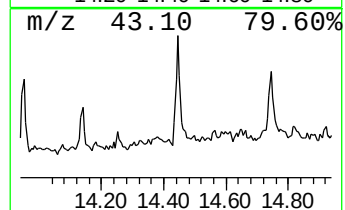
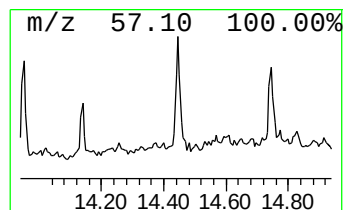
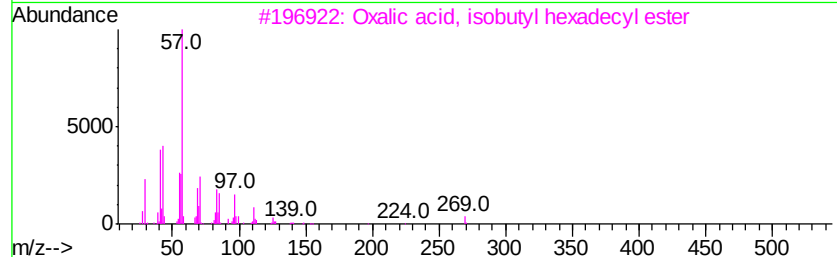
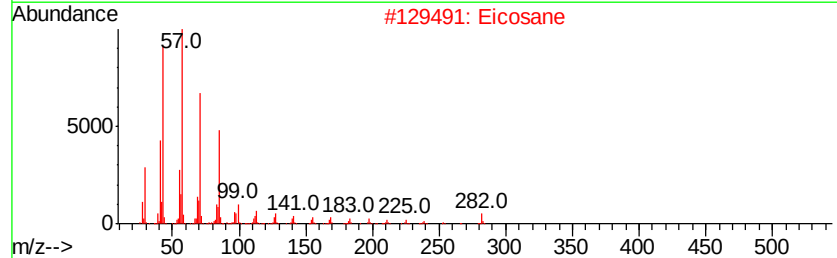
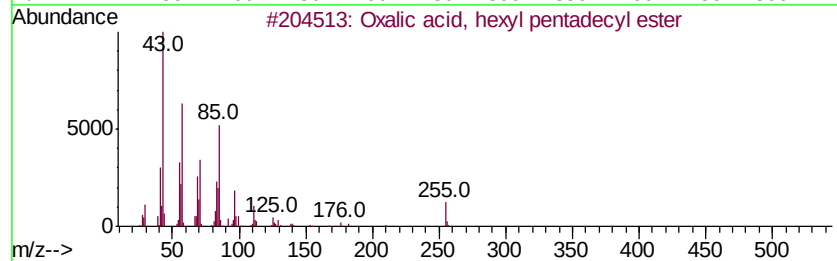
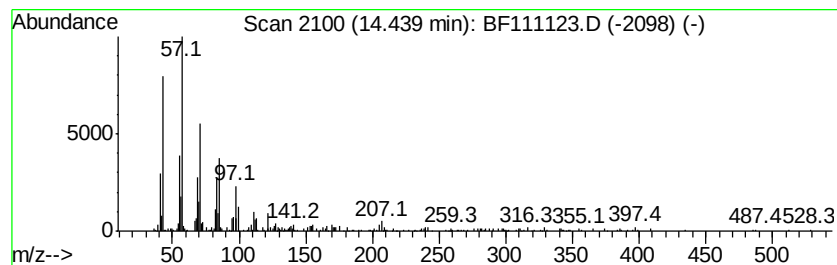
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxalic acid, hexyl pentadec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.96 ng	489055	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, hexyl pentadecyl ester	384	C23H44O4	1000309-24-9	72
2		Eicosane	282	C20H42	000112-95-8	60
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	58
4		Tetracosane	338	C24H50	000646-31-1	55
5		Oxalic acid, heptadecyl hexyl ester	412	C25H48O4	1000309-25-1	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111123.D
Acq On : 5 Dec 2018 22:39
Operator : JU/SJ
Sample : J6184-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-331

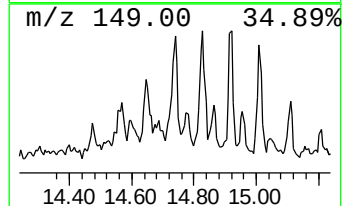
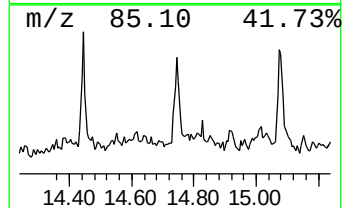
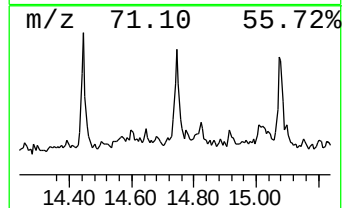
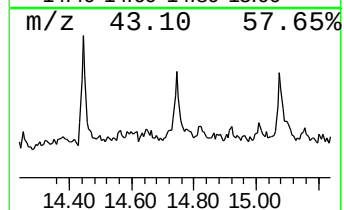
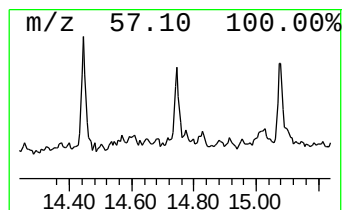
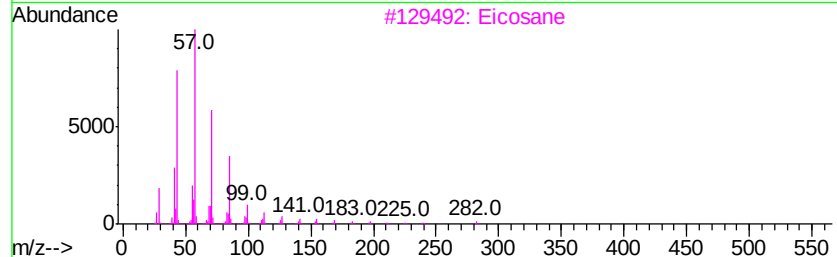
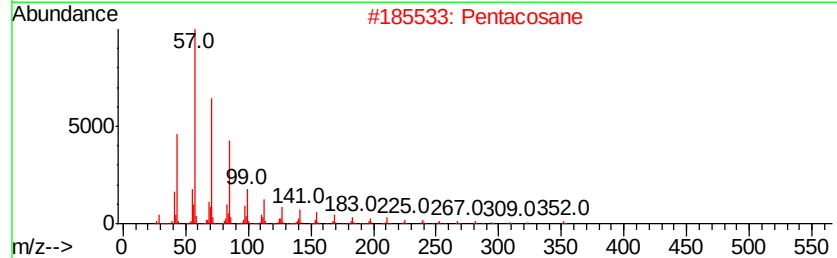
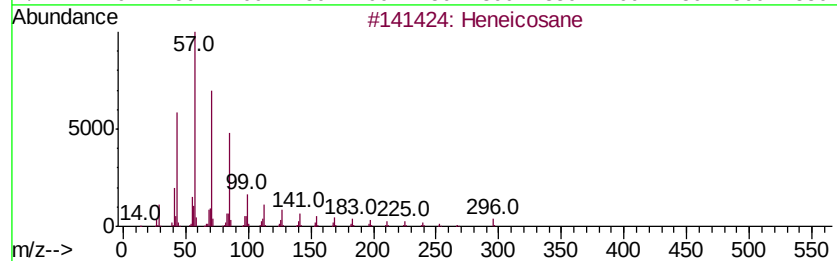
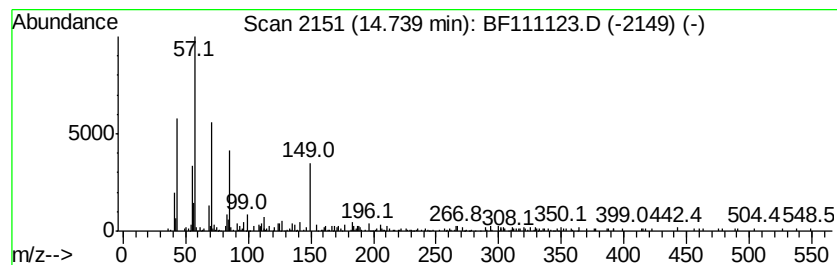
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.26 ng	203177	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Pentacosane	352	C25H52	000629-99-2	90
3		Eicosane	282	C20H42	000112-95-8	81
4		Triacontane	422	C30H62	000638-68-6	81
5		Hexadecane	226	C16H34	000544-76-3	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
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Sample : J6184-01
Misc :
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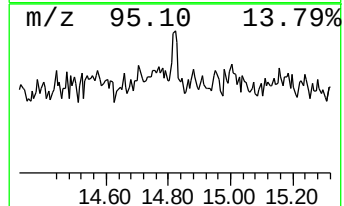
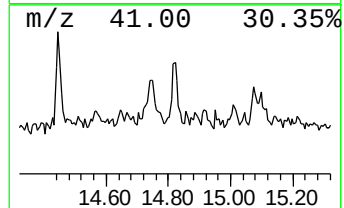
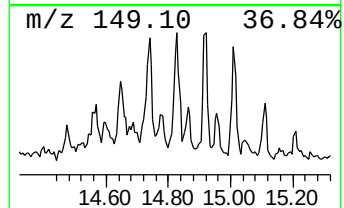
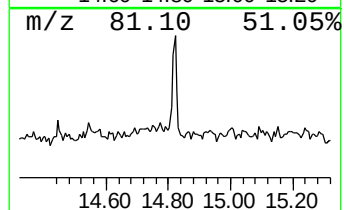
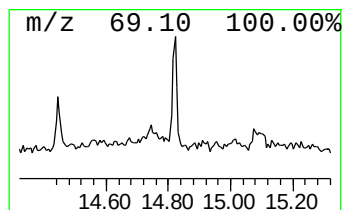
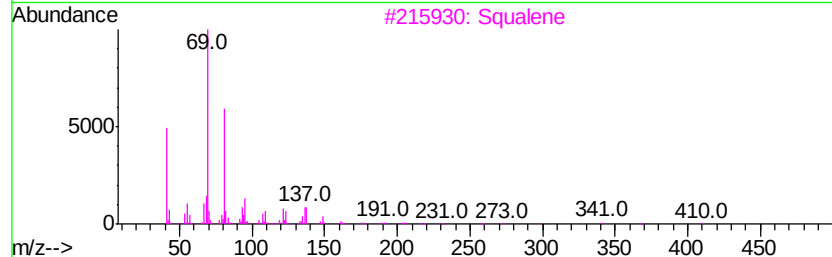
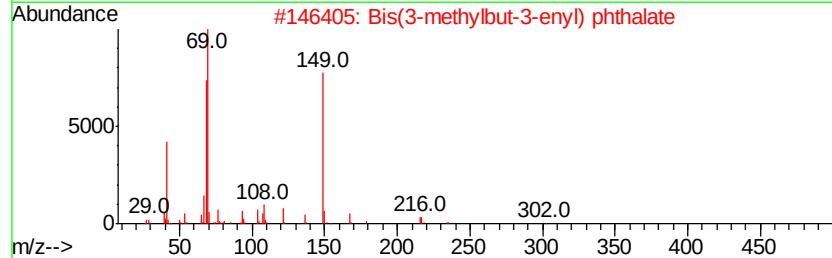
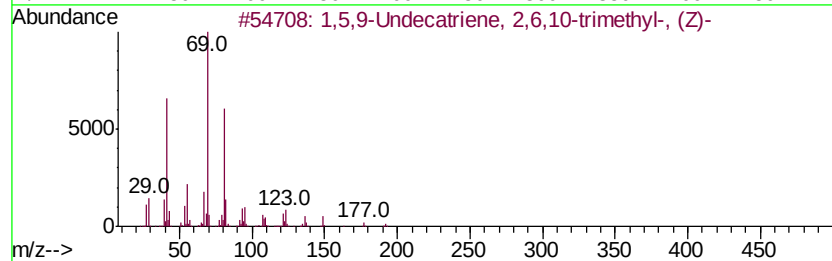
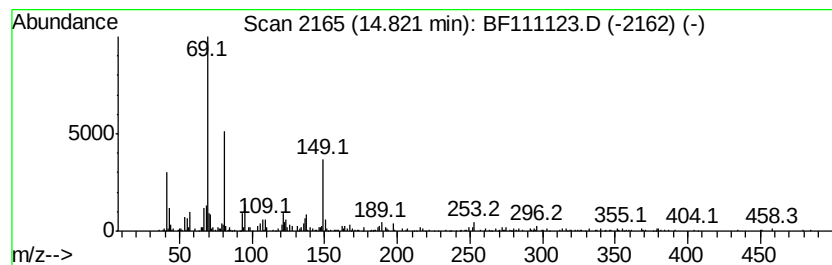
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.82	2.85 ng	255488	Perylene-d12	15.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	89
2	Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	64
3	Squalene	410	C30H50	000111-02-4	64
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	Supraene	410	C30H50	007683-64-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111123.D
Acq On : 5 Dec 2018 22:39
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Sample : J6184-01
Misc :
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ClientSampleId :
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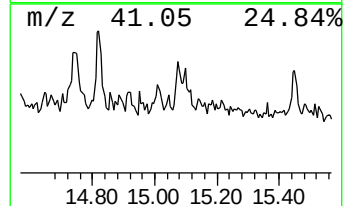
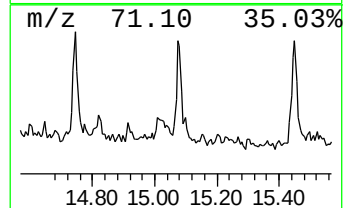
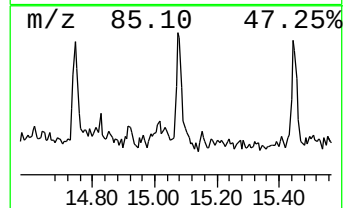
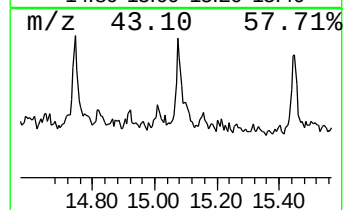
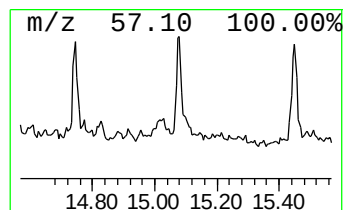
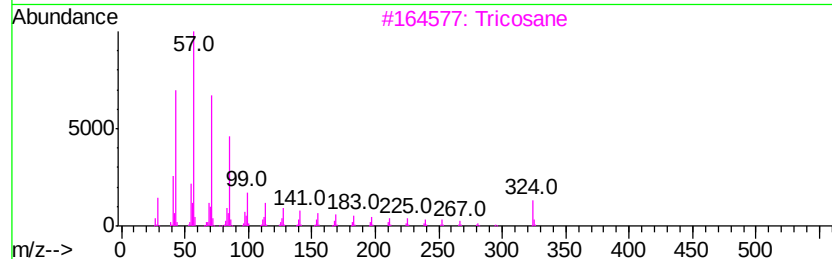
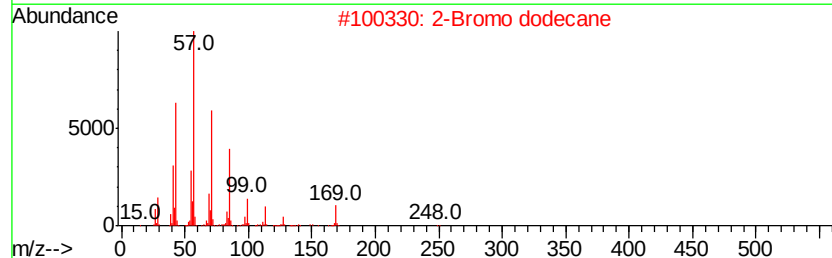
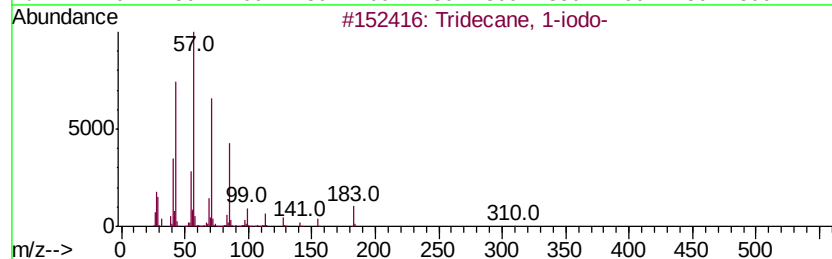
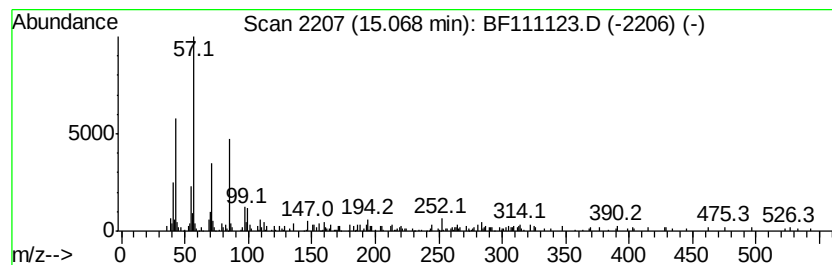
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.67 ng	239593	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	76
3		Tricosane	324	C23H48	000638-67-5	68
4		Eicosane	282	C20H42	000112-95-8	64
5		Octadecane	254	C18H38	000593-45-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
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Operator : JU/SJ
Sample : J6184-01
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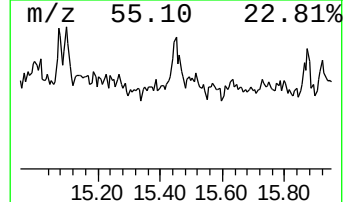
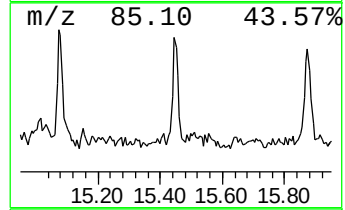
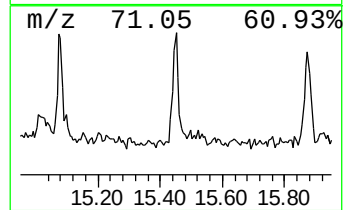
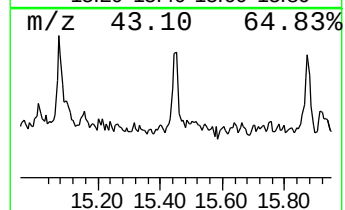
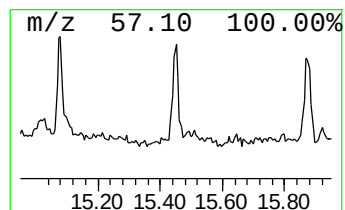
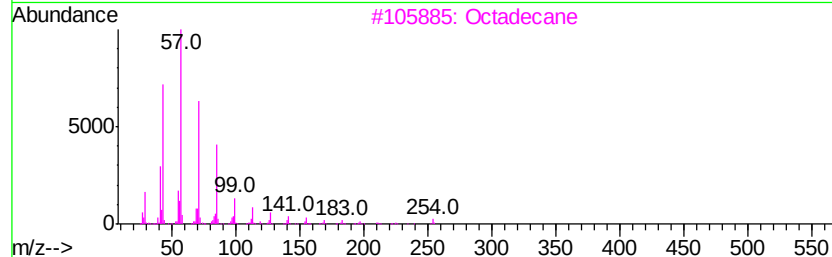
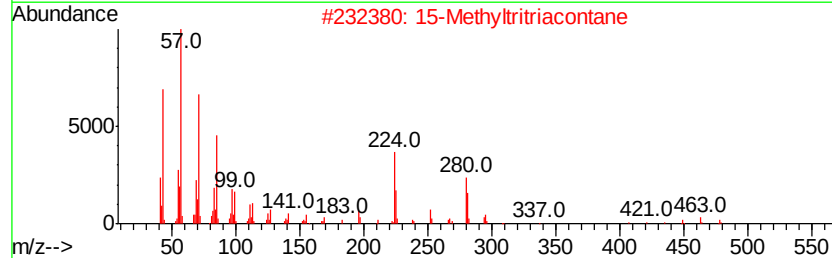
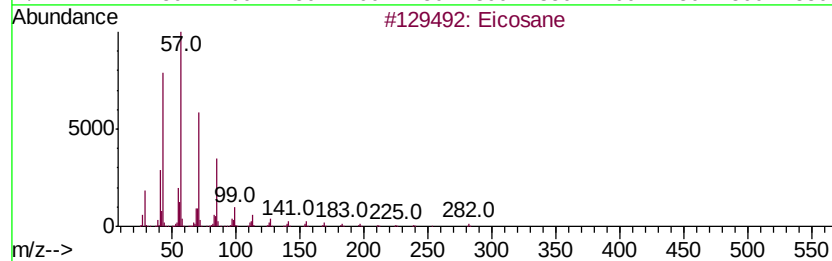
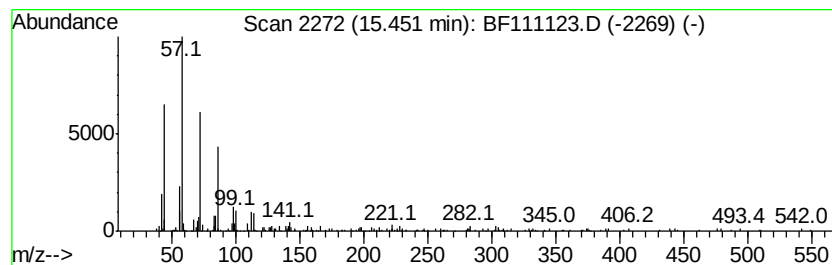
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.57 ng	230379	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 81
2	15-Methyltritriacontane		479 C34H70	1000131-20-3 81
3	Octadecane		254 C18H38	000593-45-3 72
4	Tetracosane		338 C24H50	000646-31-1 72
5	Tetratetracontane		619 C44H90	007098-22-8 64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111123.D
Acq On : 5 Dec 2018 22:39
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ALS Vial : 20 Sample Multiplier: 1

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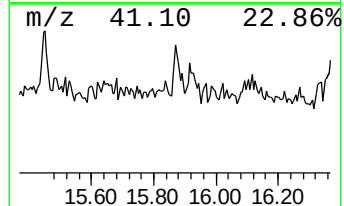
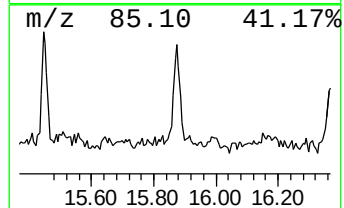
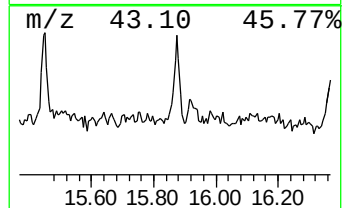
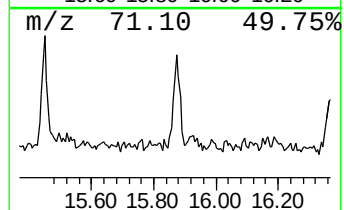
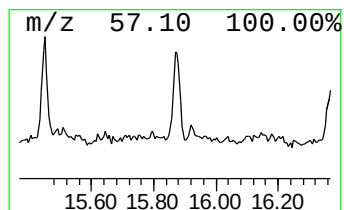
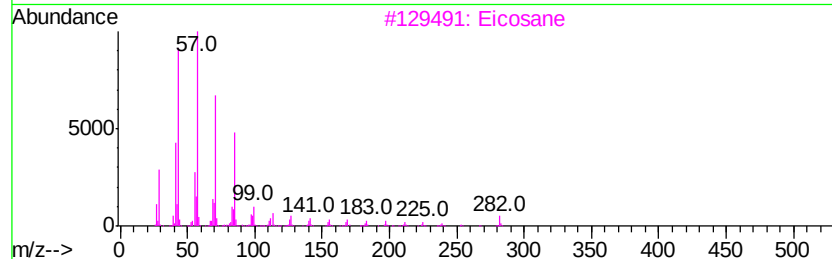
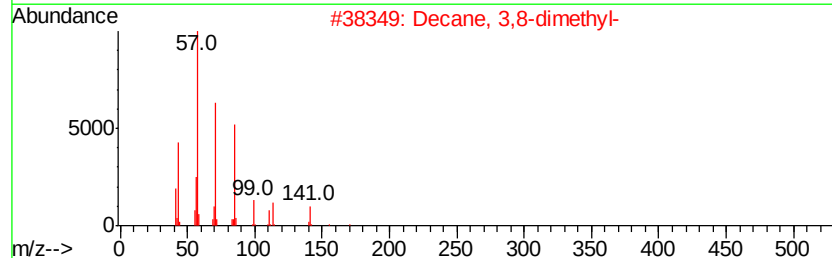
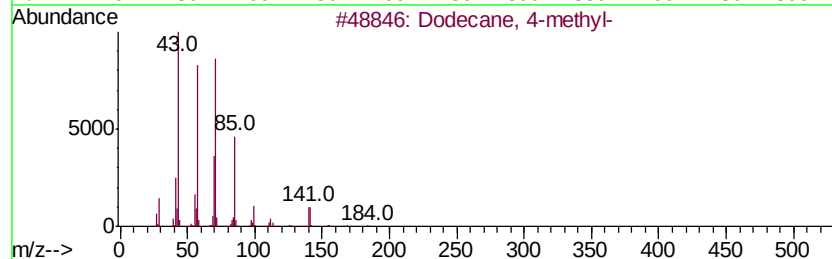
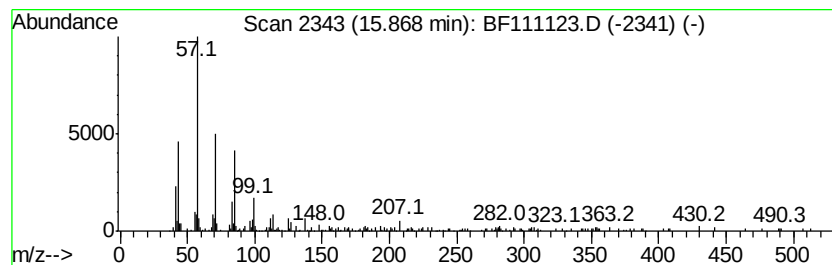
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Dodecane, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.55 ng	229042	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 4-methyl-	184	C13H28	006117-97-1	70
2		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	68
3		Eicosane	282	C20H42	000112-95-8	68
4		Octacosane	394	C28H58	000630-02-4	64
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120518\
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Operator : JU/SJ
Sample : J6184-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
2-Pentanone, 4-hy...	5.02	4.6 ng		700158	1	6.80	3044990	20.0
unknown6.57	6.57	73.6 ng		11204100	1	6.80	3044990	20.0
Tetradecanoic acid	11.86	6.2 ng		1029960	4	11.32	3317730	20.0
Octadecanoic acid	12.64	3.3 ng		538325	5	13.96	3302770	20.0
Trifluoroacetic a...	13.81	4.5 ng		740768	5	13.96	3302770	20.0
Oxalic acid, hexy...	14.44	3.0 ng		489055	5	13.96	3302770	20.0
Heneicosane	14.74	2.3 ng		203177	6	15.39	1795760	20.0
1,5,9-Undecatrien...	14.82	2.9 ng		255488	6	15.39	1795760	20.0
Tridecane, 1-iodo-	15.07	2.7 ng		239593	6	15.39	1795760	20.0
Eicosane	15.45	2.6 ng		230379	6	15.39	1795760	20.0
Dodecane, 4-methyl-	15.87	2.5 ng		229042	6	15.39	1795760	20.0