

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111618\
 Data File : BF110820.D
 Acq On : 16 Nov 2018 16:52
 Operator : JU/SJ
 Sample : J5762-05 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-111518

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-BF110818.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	2.211	17	21	35	rVB	66158	106153	10.04%	0.973%
2	5.163	521	523	534	rBV	13413	22323	2.11%	0.205%
3	5.557	586	590	616	rBV	571370	675866	63.95%	6.194%
4	6.563	757	761	777	rBV	613889	713457	67.51%	6.538%
5	6.704	782	785	791	rBV	839939	739847	70.00%	6.780%
6	6.940	821	825	839	rVB	465950	426629	40.37%	3.910%
7	7.093	848	851	866	rBV	641953	560929	53.07%	5.141%
8	7.504	917	921	935	rBV	389341	458058	43.34%	4.198%
9	8.222	1039	1043	1057	rBV	557132	559300	52.92%	5.126%
10	9.292	1222	1225	1234	rBV	879463	792562	74.99%	7.263%
11	9.692	1286	1293	1299	rBV	27159	30527	2.89%	0.280%
12	9.981	1338	1342	1355	rVB2	658991	608952	57.62%	5.581%
13	10.386	1408	1411	1414	rVB	13275	10924	1.03%	0.100%
14	10.775	1473	1477	1489	rBV	356943	382287	36.17%	3.503%
15	10.863	1489	1492	1499	rVB	14762	16221	1.53%	0.149%
16	11.475	1593	1596	1608	rBV	552907	533829	50.51%	4.892%
17	11.839	1655	1658	1662	rBV	418068	350238	33.14%	3.210%
18	11.975	1677	1681	1686	rBV	14240	19052	1.80%	0.175%
19	12.528	1772	1775	1777	rBV	1125002	1056885	100.00%	9.686%
20	12.551	1777	1779	1786	rVV2	1096453	920209	87.07%	8.433%
21	12.633	1790	1793	1796	rVB	191590	144157	13.64%	1.321%
22	12.698	1801	1804	1811	rVB	27388	27405	2.59%	0.251%
23	12.927	1841	1843	1848	rVB	22089	19266	1.82%	0.177%
24	13.057	1861	1865	1871	rVB	617539	526577	49.82%	4.826%
25	13.357	1914	1916	1920	rBV	10734	10885	1.03%	0.100%
26	13.933	2010	2014	2020	rBV	56260	74335	7.03%	0.681%
27	14.127	2043	2047	2056	rVB	473100	478840	45.31%	4.388%
28	14.551	2117	2119	2121	rBV2	16819	18881	1.79%	0.173%
29	14.869	2169	2173	2176	rBV	28012	29018	2.75%	0.266%
30	15.216	2227	2232	2237	rBV2	40790	61756	5.84%	0.566%
31	15.610	2296	2299	2302	rVB	25136	29218	2.76%	0.268%
32	15.657	2302	2307	2318	rVB	269290	396430	37.51%	3.633%
33	16.033	2366	2371	2372	rBV5	7782	10881	1.03%	0.100%
34	16.063	2372	2376	2382	rVV2	30871	54592	5.17%	0.500%

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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

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35	16.345	2420	2424	2427	rBV5	9066	16825	1.59%	0.154%
36	16.592	2462	2466	2471	rBV4	16971	28460	2.69%	0.261%

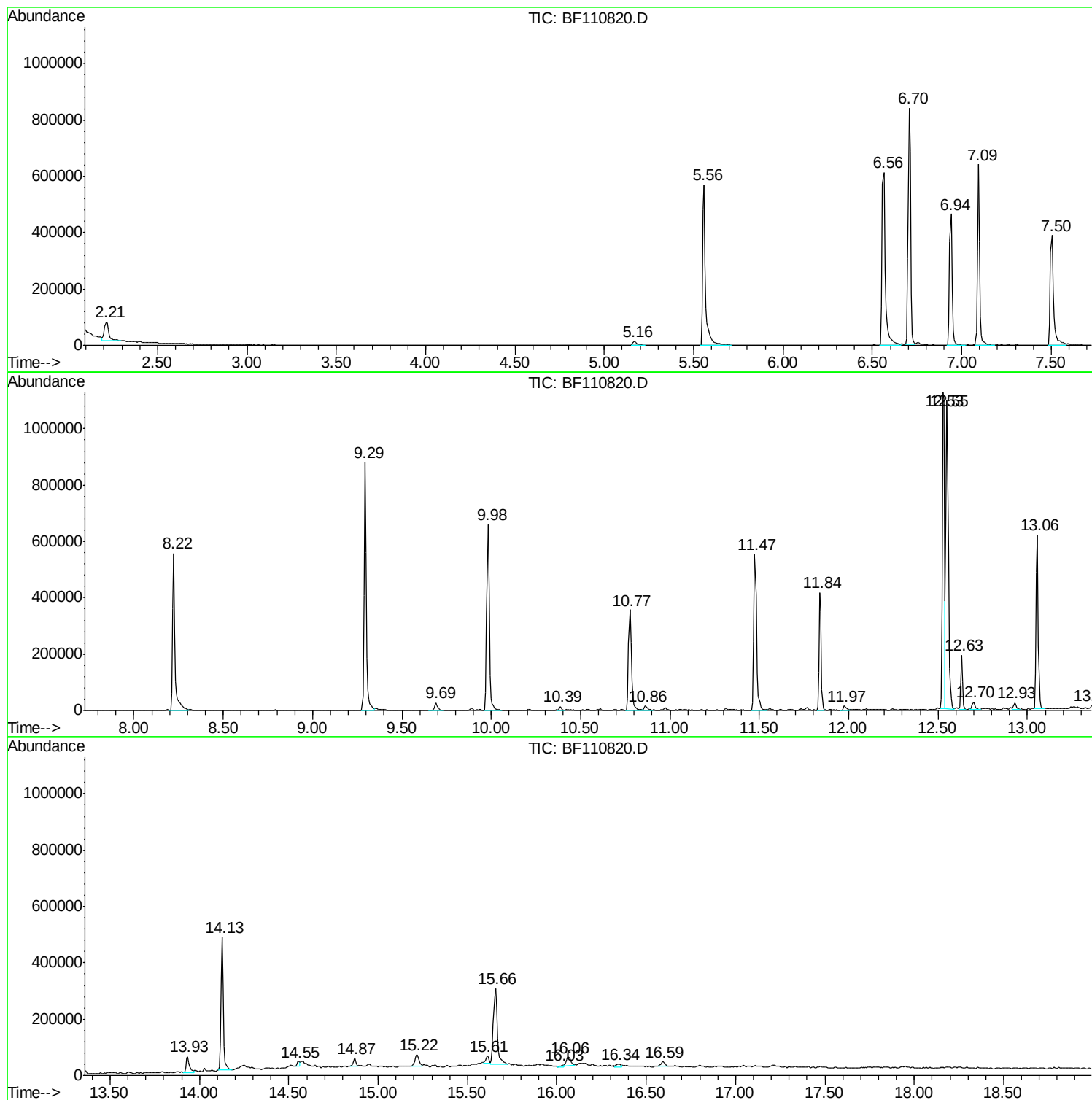
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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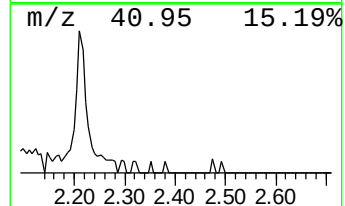
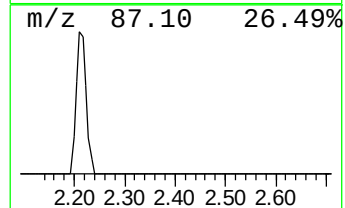
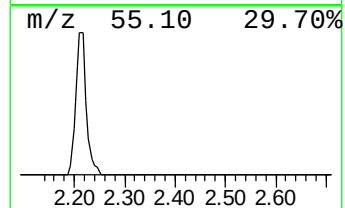
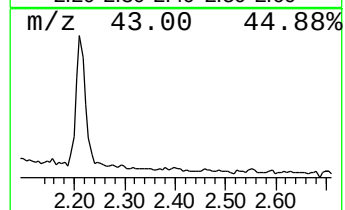
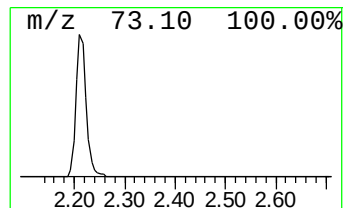
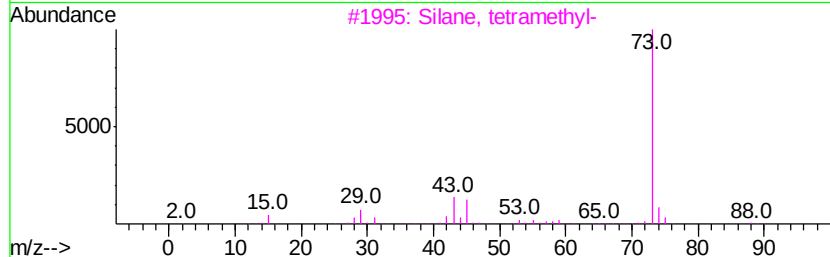
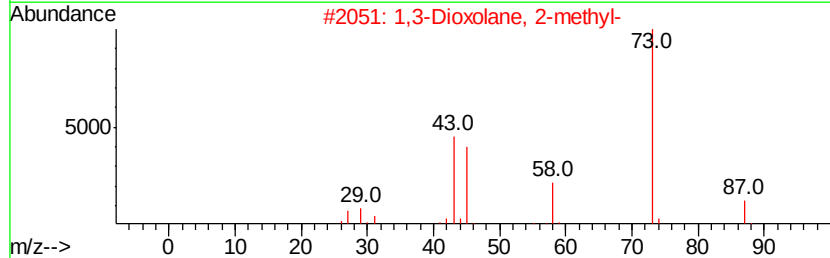
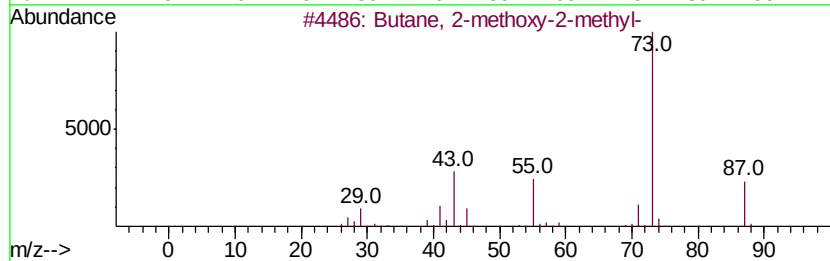
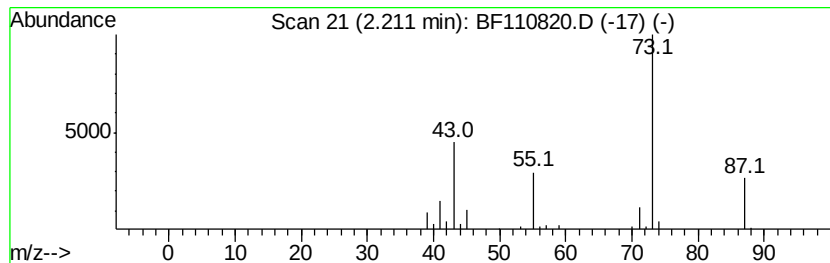
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	4.98 ng	106153	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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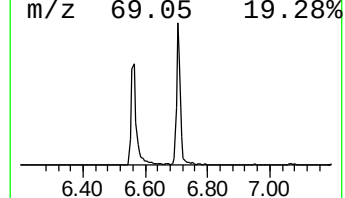
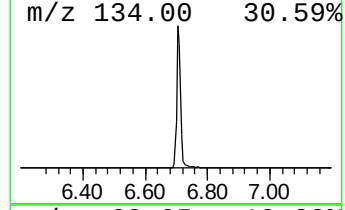
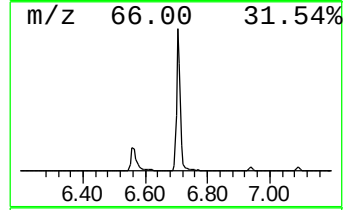
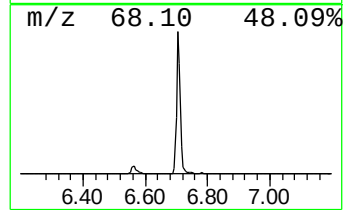
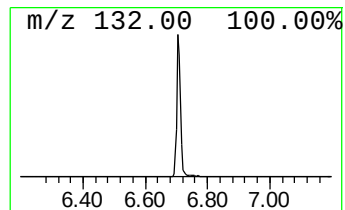
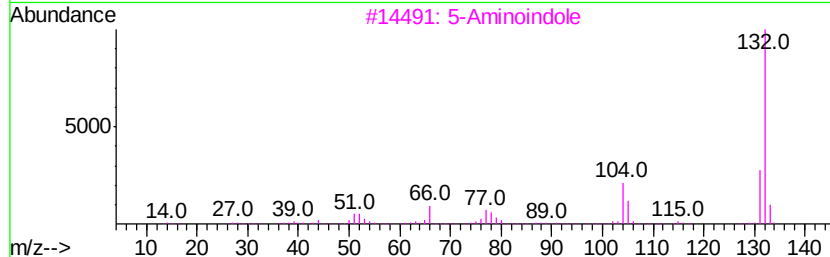
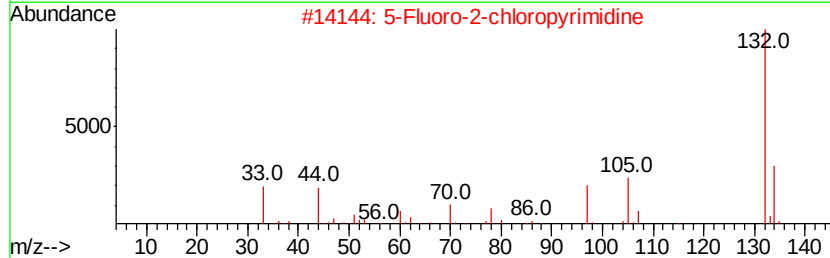
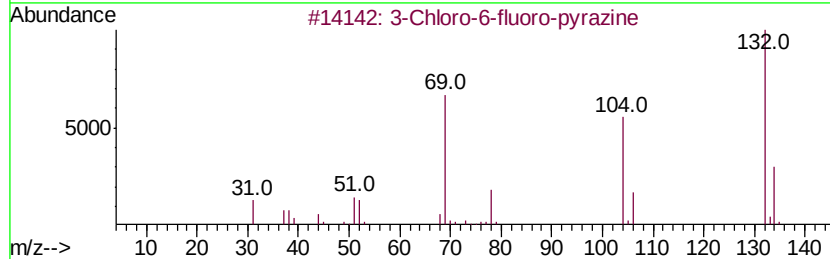
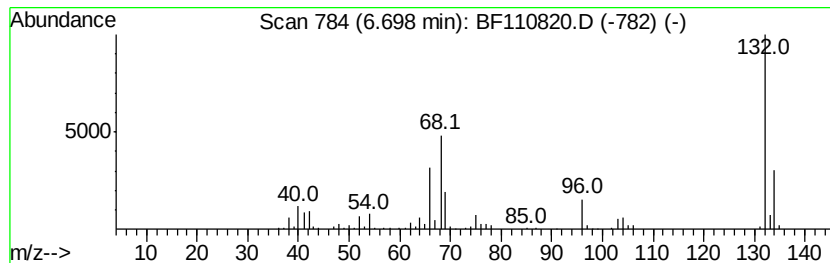
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	34.68 ng	739847	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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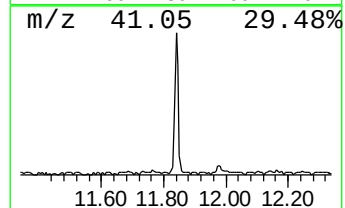
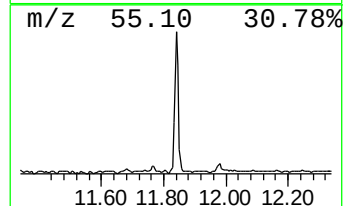
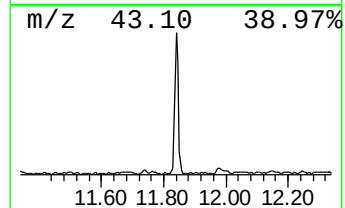
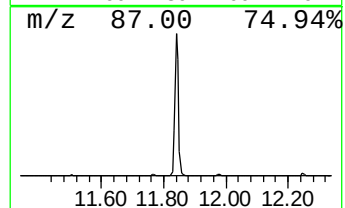
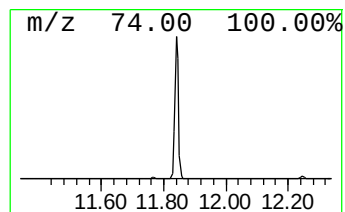
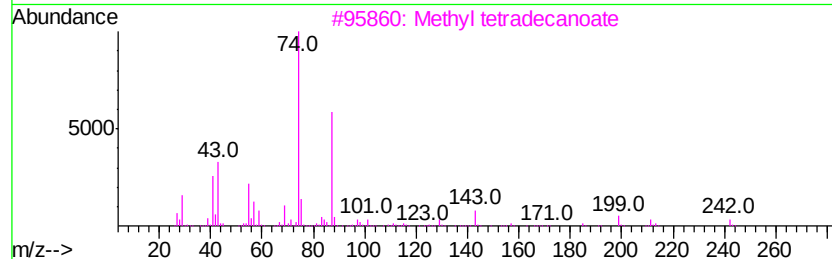
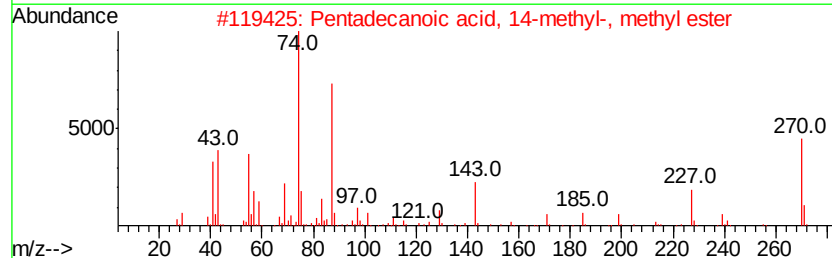
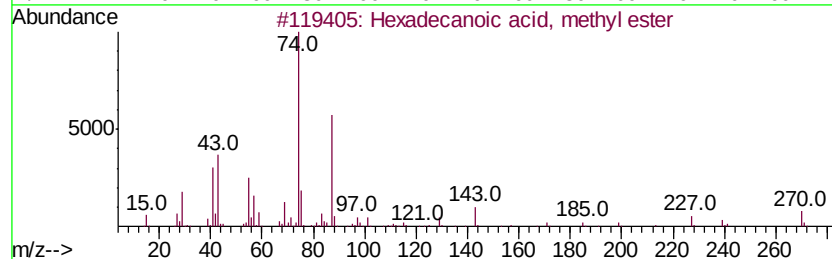
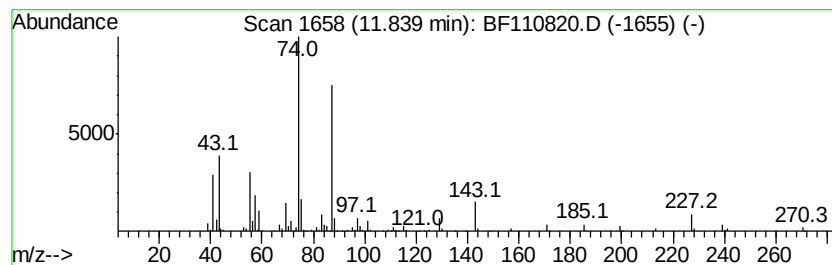
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.84	13.12 ng	350238	Phenanthrene-d10	11.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86



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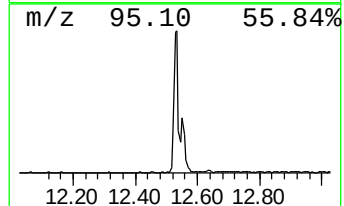
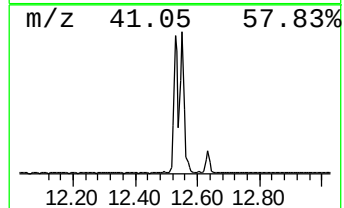
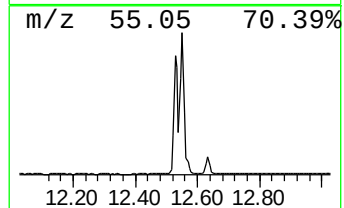
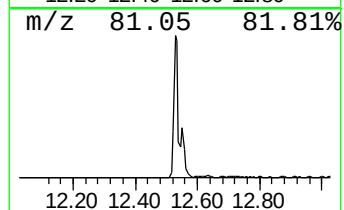
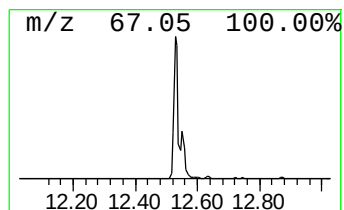
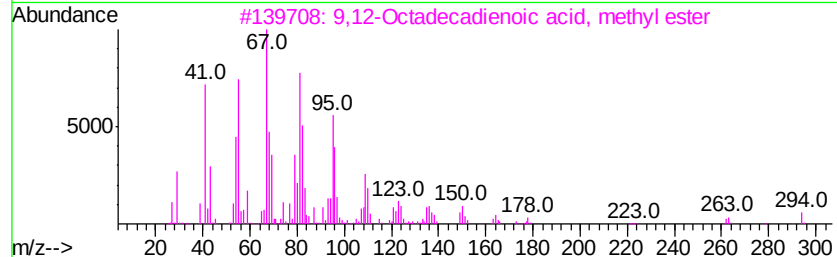
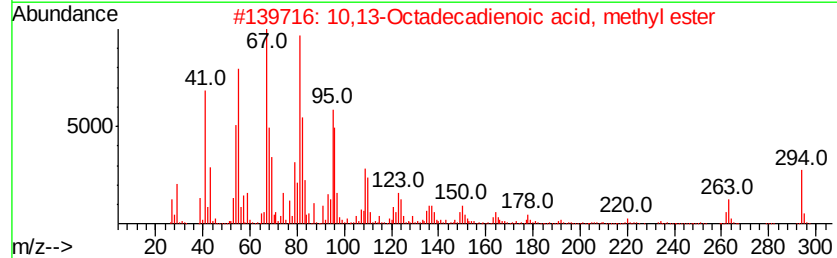
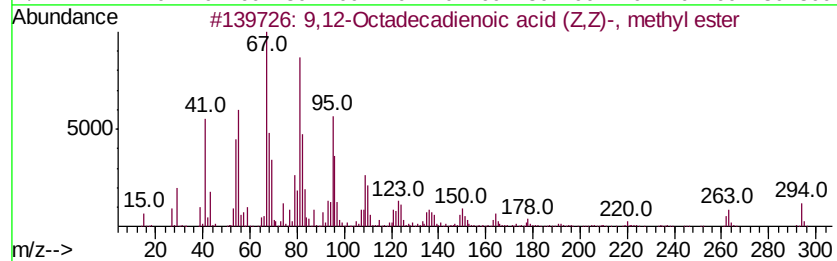
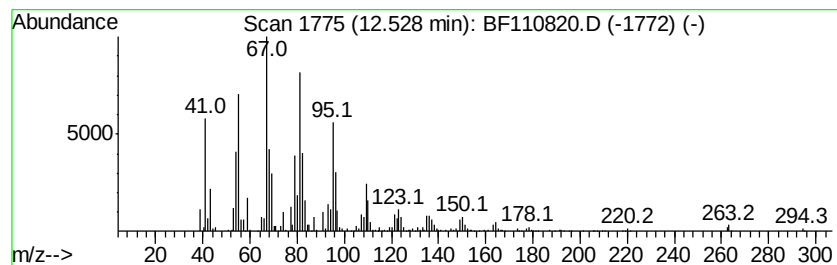
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	39.60 ng	1056890	Phenanthrene-d10	11.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3		9,12-Octadecadienoic acid, methv...	294	C19H34O2	002462-85-3	99
4		8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98



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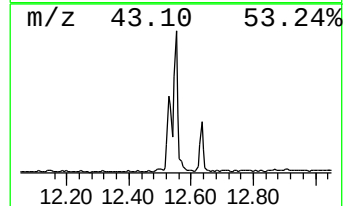
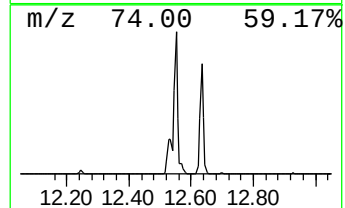
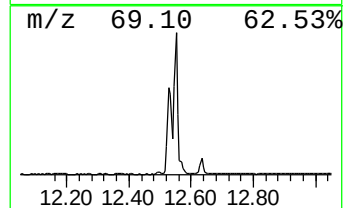
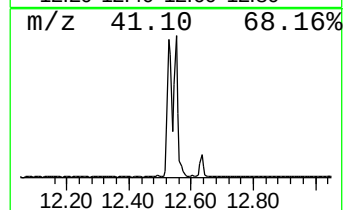
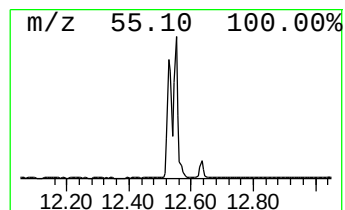
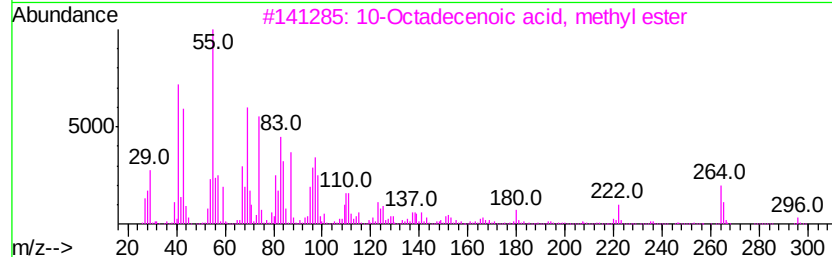
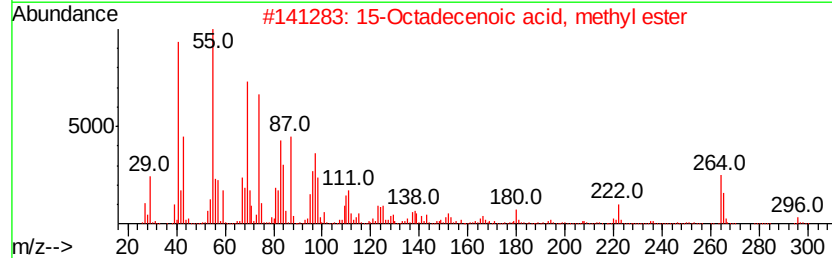
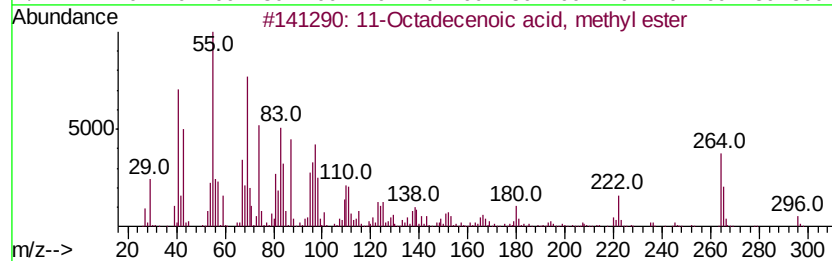
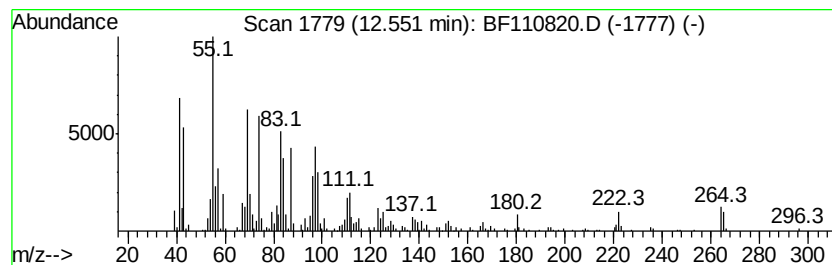
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TIC Integration Parameters: LSCINT.P

Peak Number 6 11-Octadecenoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	34.48 ng	920209	Phenanthrene-d10	11.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	96
2		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
3		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
4		11-Octadecenoic acid, methyl ester	296	C19H36O2	001937-63-9	94
5		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111618\
Data File : BF110820.D
Acq On : 16 Nov 2018 16:52
Operator : JU/SJ
Sample : J5762-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

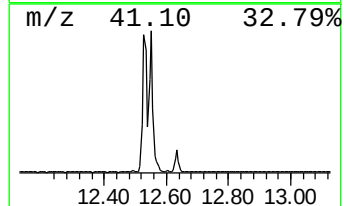
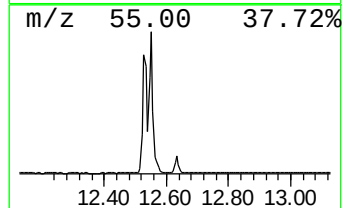
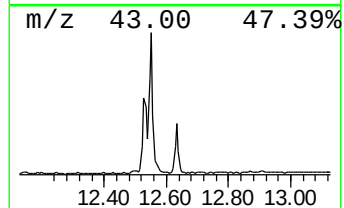
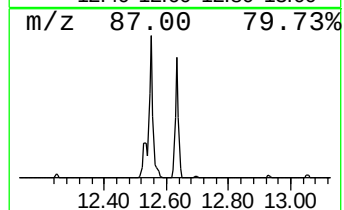
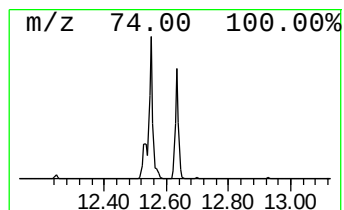
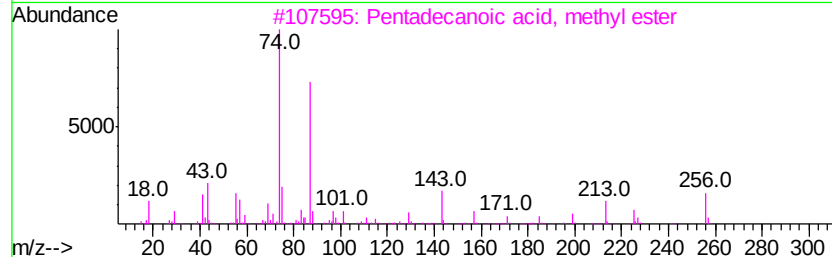
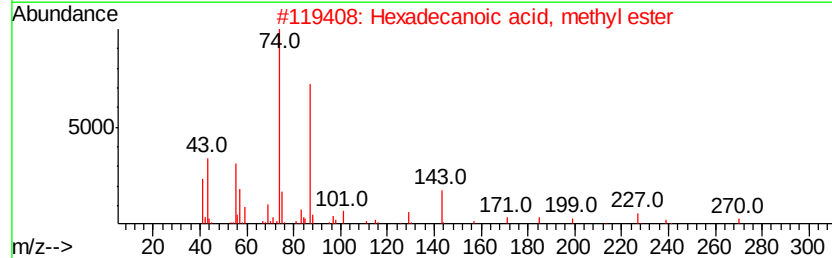
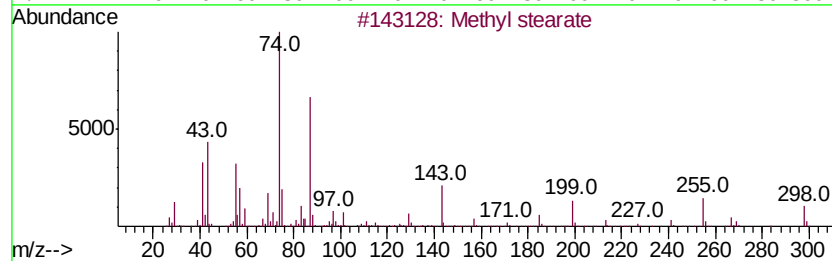
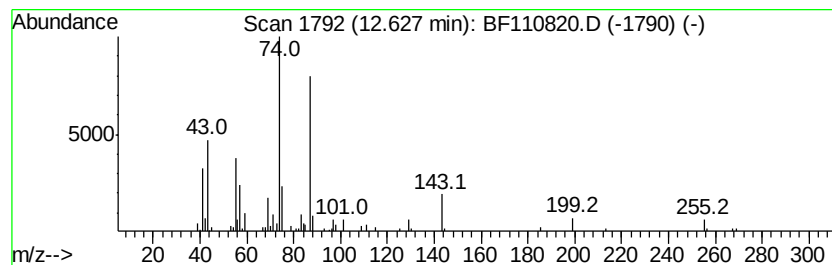
Instrument :
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ClientSampleId :
BU-03-111518

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.63	5.40 ng	144157	Phenanthrene-d10	11.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111618\
Data File : BF110820.D
Acq On : 16 Nov 2018 16:52
Operator : JU/SJ
Sample : J5762-05 2X
Misc :
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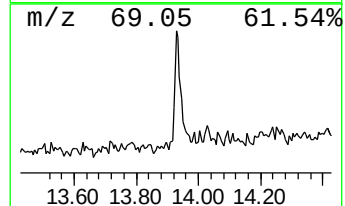
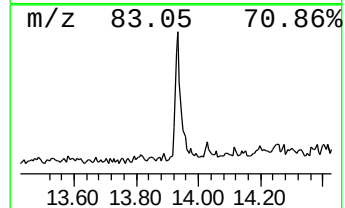
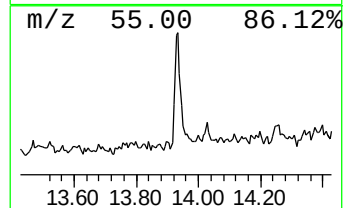
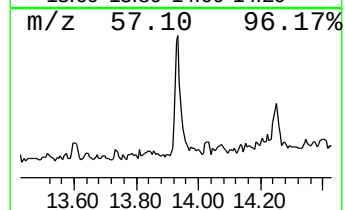
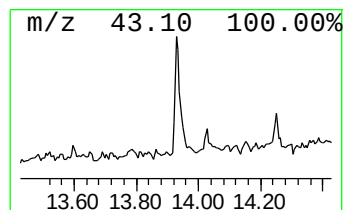
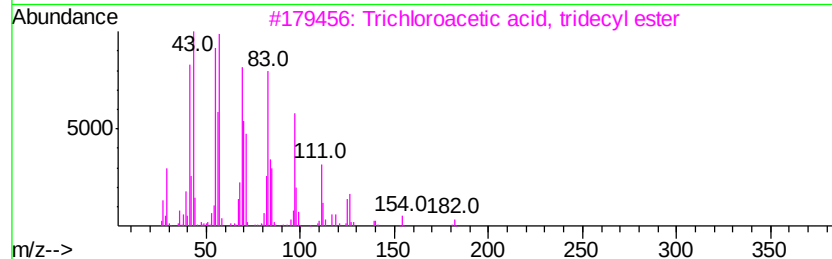
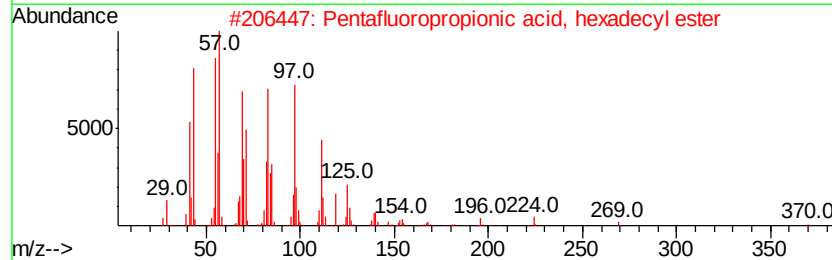
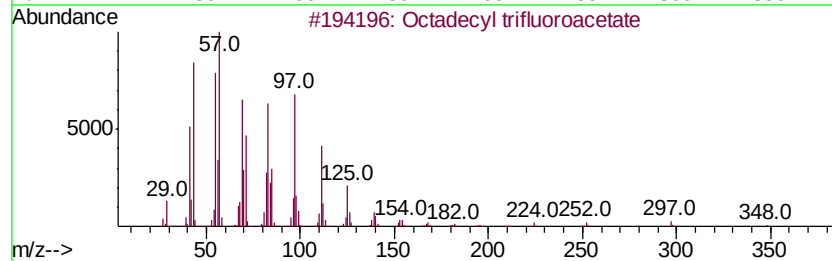
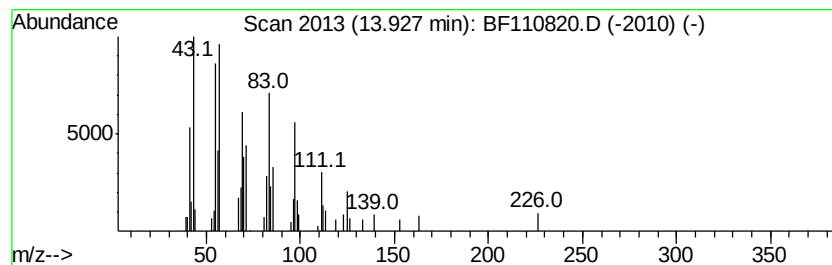
Instrument :
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ClientSampleId :
BU-03-111518

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.93	3.10 ng	74335	Chrysene-d12	14.13		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
2		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	90
3		Trichloroacetic acid, tridecyl ester	344	C15H27Cl3O2	074339-51-8	87
4		Trichloroacetic acid, tetradecyl ester	358	C16H29Cl3O2	074339-52-9	87
5		Carbonic acid, hexadecyl 2,2,2-trifluoroethyl ester	416	C19H35Cl3O3	1000314-56-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111618\
Data File : BF110820.D
Acq On : 16 Nov 2018 16:52
Operator : JU/SJ
Sample : J5762-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-111518

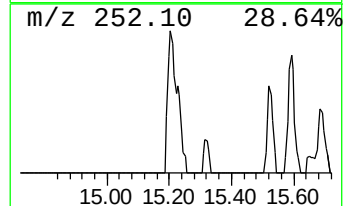
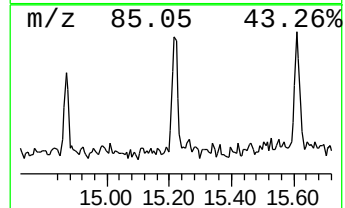
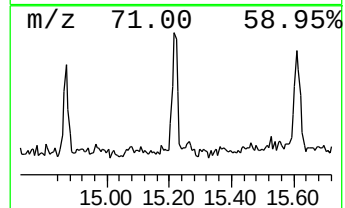
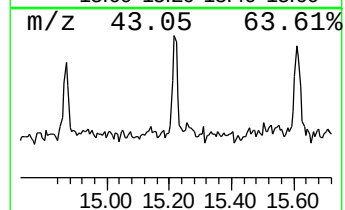
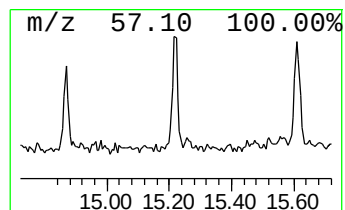
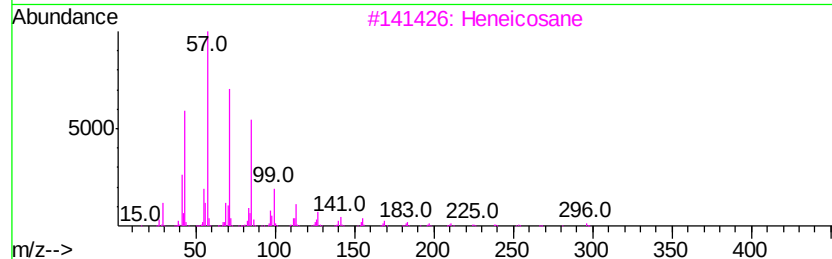
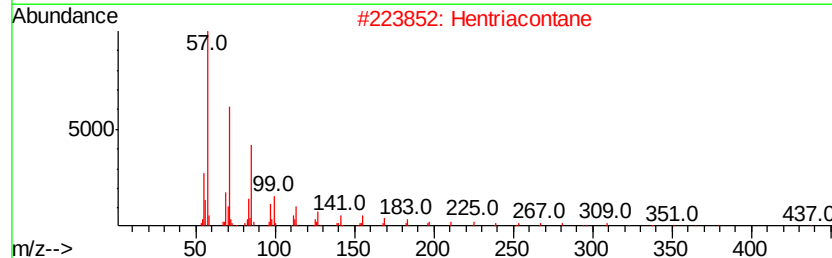
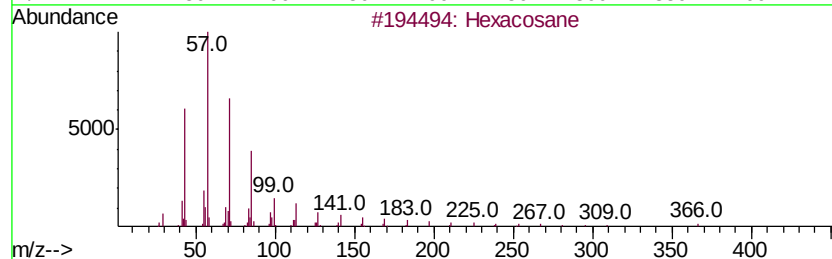
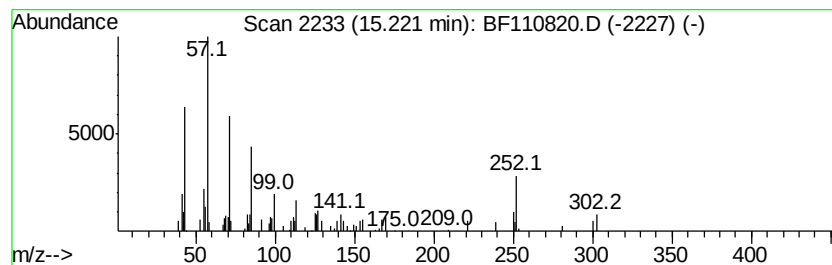
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	3.12 ng	61756	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	70
2		Hentriacontane	437	C31H64	000630-04-6	68
3		Heneicosane	296	C21H44	000629-94-7	68
4		Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	64
5		triacontane	422	C30H62	000638-68-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111618\
Data File : BF110820.D
Acq On : 16 Nov 2018 16:52
Operator : JU/SJ
Sample : J5762-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-111518

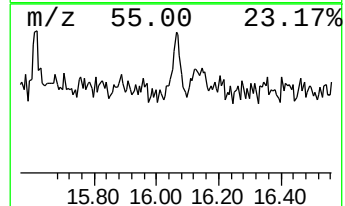
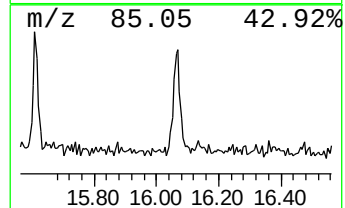
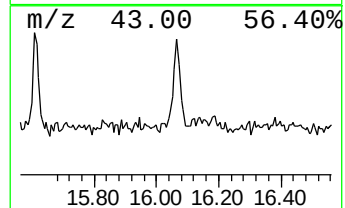
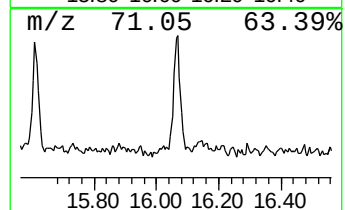
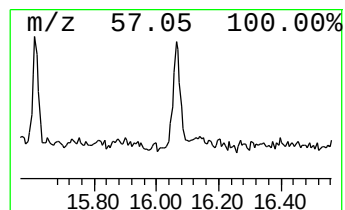
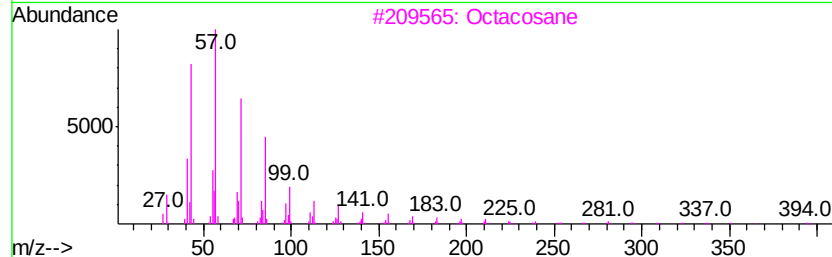
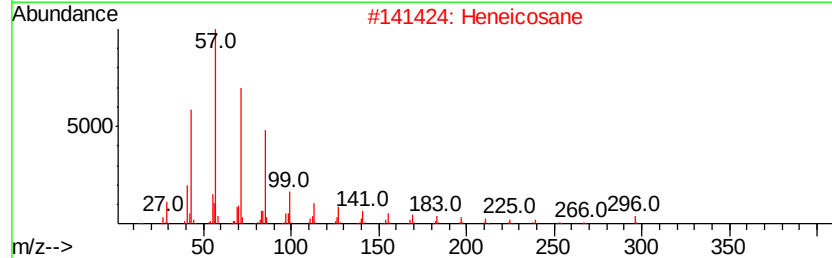
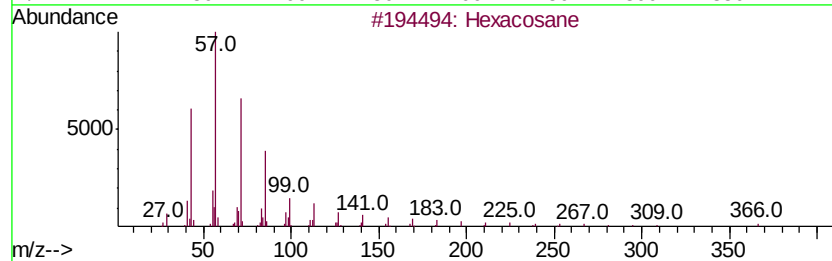
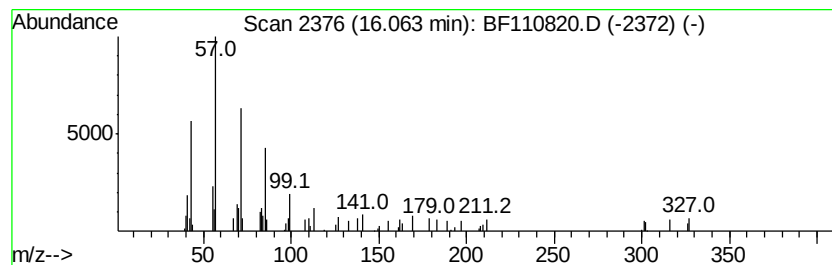
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.75 ng	54592	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	74
2		Heneicosane	296	C21H44	000629-94-7	74
3		Octacosane	394	C28H58	000630-02-4	72
4		Pentacosane	352	C25H52	000629-99-2	72
5		Hentriacontane	437	C31H64	000630-04-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111618\
Data File : BF110820.D
Acq On : 16 Nov 2018 16:52
Operator : JU/SJ
Sample : J5762-05 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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...	2.21	5.0	ng	106153	1	6.94	426629	20.0
unknown6.70	6.70	34.7	ng	739847	1	6.94	426629	20.0
Hexadecanoic acid...	11.84	13.1	ng	350238	4	11.47	533829	20.0
9,12-Octadecadien...	12.53	39.6	ng	1056890	4	11.47	533829	20.0
11-Octadecenoic a...	12.55	34.5	ng	920209	4	11.47	533829	20.0
Methyl stearate	12.63	5.4	ng	144157	4	11.47	533829	20.0
Octadecyl trifluo...	13.93	3.1	ng	74335	5	14.13	478840	20.0
Hentriacontane	15.22	3.1	ng	61756	6	15.66	396430	20.0
Hexacosane	16.06	2.8	ng	54592	6	15.66	396430	20.0