

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
 Data File : BF110627.D
 Acq On : 9 Nov 2018 15:02
 Operator : JU/SJ
 Sample : J5813-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-H

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	2.252	23	28	36	rVB	239460	319783	17.72%	1.952%
2	5.187	523	527	539	rBV	36084	57374	3.18%	0.350%
3	5.569	587	592	604	rBV	1536199	1602810	88.82%	9.782%
4	6.569	758	762	779	rBV	1553534	1804532	100.00%	11.013%
5	6.716	783	787	790	rBV	1932688	1701727	94.30%	10.385%
6	6.945	822	826	832	rBV	567910	462921	25.65%	2.825%
7	7.104	848	853	866	rBV	1322627	1295621	71.80%	7.907%
8	7.510	917	922	936	rBV	1118859	1035273	57.37%	6.318%
9	8.228	1040	1044	1056	rBV	616579	561918	31.14%	3.429%
10	9.298	1222	1226	1236	rBV	1901167	1588357	88.02%	9.694%
11	9.692	1289	1293	1301	rBV	195161	171141	9.48%	1.044%
12	9.986	1339	1343	1355	rVB	581329	522957	28.98%	3.192%
13	10.775	1474	1477	1485	rBV	691784	710886	39.39%	4.338%
14	11.480	1593	1597	1599	rBV	537069	453630	25.14%	2.768%
15	11.504	1599	1601	1605	rVB	117009	99822	5.53%	0.609%
16	11.980	1680	1682	1686	rBV	23583	24713	1.37%	0.151%
17	12.698	1800	1804	1809	rBV	241957	198404	10.99%	1.211%
18	12.774	1814	1817	1822	rBV5	11202	18852	1.04%	0.115%
19	12.927	1837	1843	1849	rVB	161417	176759	9.80%	1.079%
20	13.063	1861	1866	1869	rBV	1492906	1226247	67.95%	7.484%
21	13.257	1892	1899	1904	rBV2	25762	41958	2.33%	0.256%
22	13.492	1935	1939	1942	rBV4	19129	26318	1.46%	0.161%
23	13.527	1942	1945	1950	rVB	120501	99064	5.49%	0.605%
24	13.880	2002	2005	2008	rBV	19449	20911	1.16%	0.128%
25	13.939	2012	2015	2020	rBV3	128370	166981	9.25%	1.019%
26	14.133	2043	2048	2050	rBV2	501323	525686	29.13%	3.208%
27	14.157	2050	2052	2059	rVB	83468	73980	4.10%	0.451%
28	14.563	2118	2121	2129	rBV6	35420	74653	4.14%	0.456%
29	14.874	2171	2174	2179	rVB	43754	47042	2.61%	0.287%
30	15.033	2197	2201	2205	rVB	247629	242543	13.44%	1.480%
31	15.204	2226	2230	2232	rBV	61394	90059	4.99%	0.550%
32	15.227	2232	2234	2237	rVV	98764	108743	6.03%	0.664%
33	15.262	2237	2240	2247	rVV4	95543	158795	8.80%	0.969%
34	15.592	2293	2296	2298	rBV	35348	40737	2.26%	0.249%

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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.621	2299	2301	2303	rVV	48196	50177	2.78%	0.306%
36	15.657	2303	2307	2312	rVB	224256	288728	16.00%	1.762%
37	15.839	2335	2338	2343	rVB5	22890	33521	1.86%	0.205%
38	16.080	2375	2379	2386	rVB	83646	124548	6.90%	0.760%
39	16.609	2465	2469	2473	rVB2	28806	44934	2.49%	0.274%
40	17.227	2570	2574	2583	rVB2	46419	92508	5.13%	0.565%

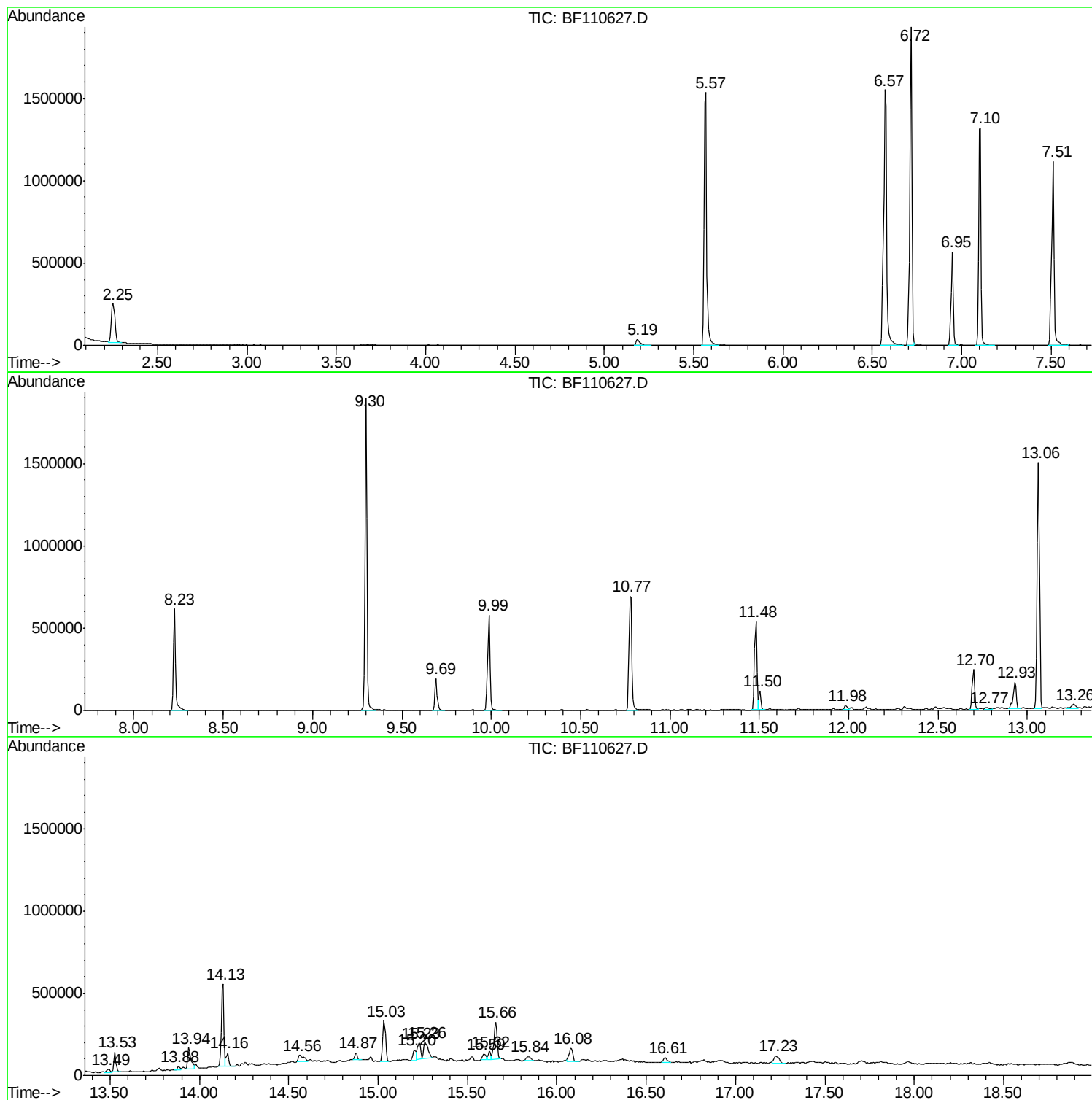
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Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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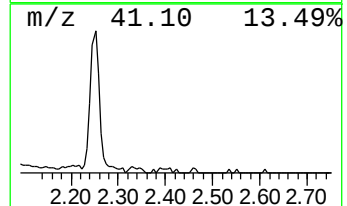
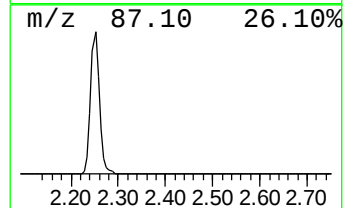
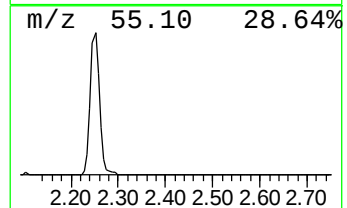
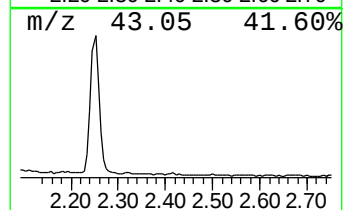
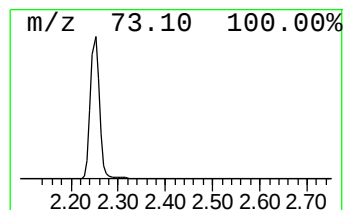
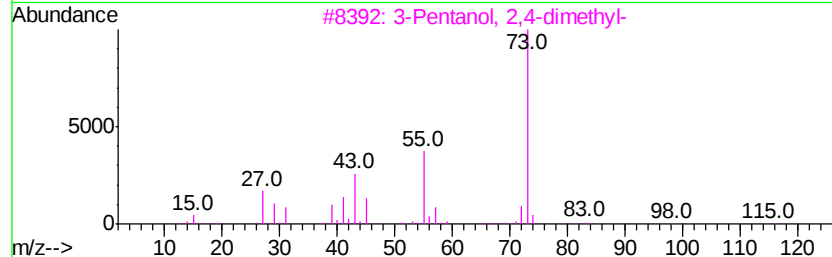
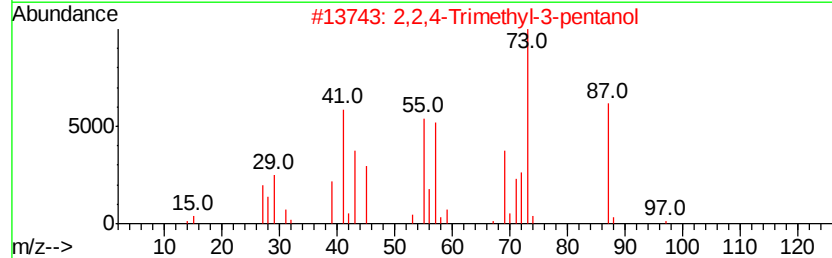
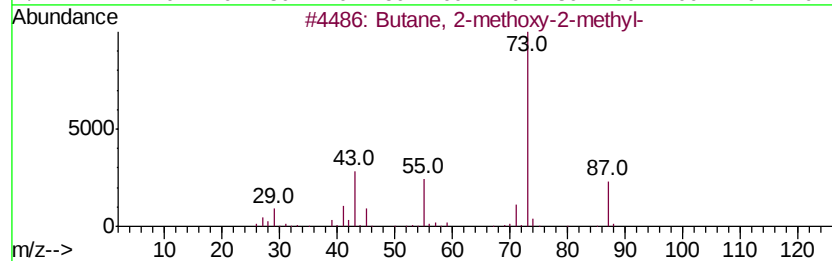
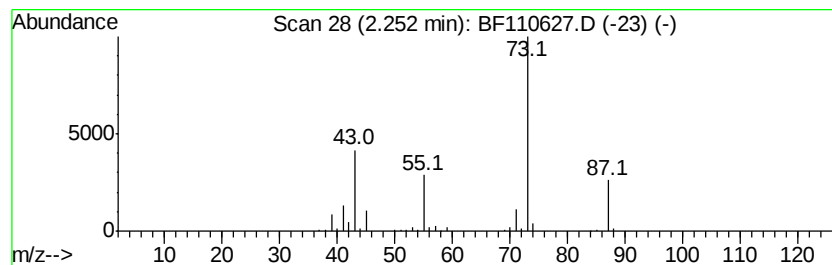
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	13.82 ng	319783	1,4-Dichlorobenzene-d4	6.95

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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



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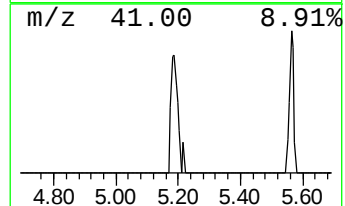
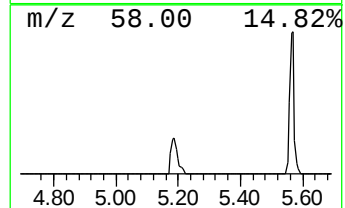
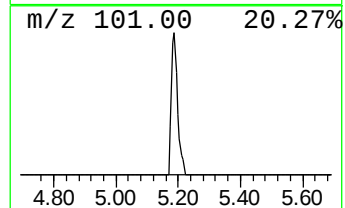
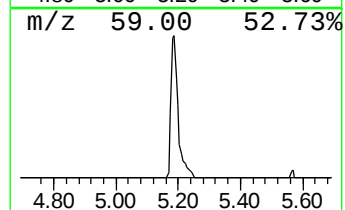
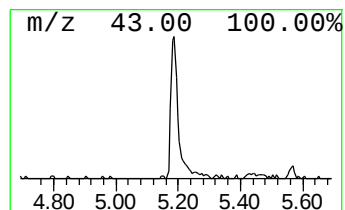
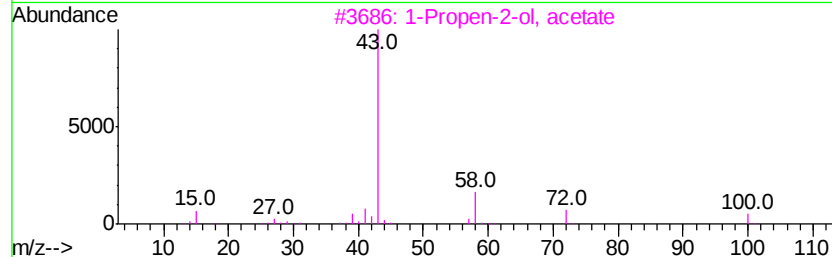
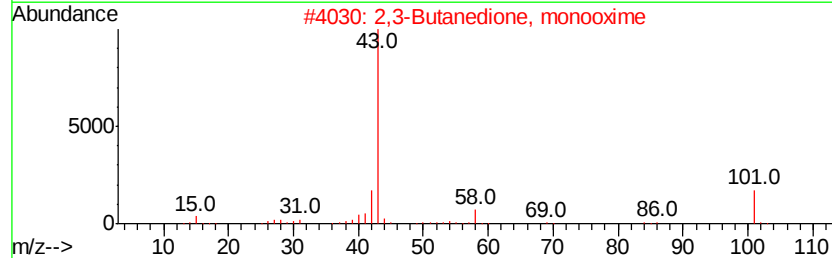
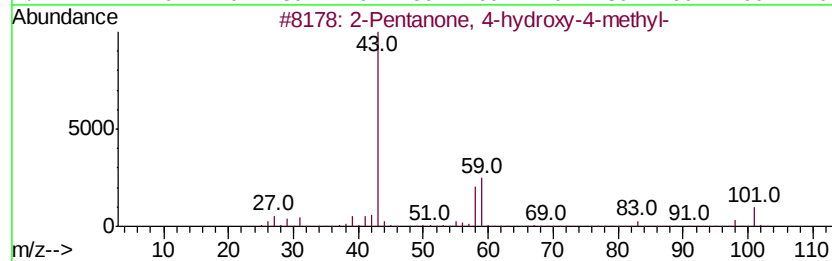
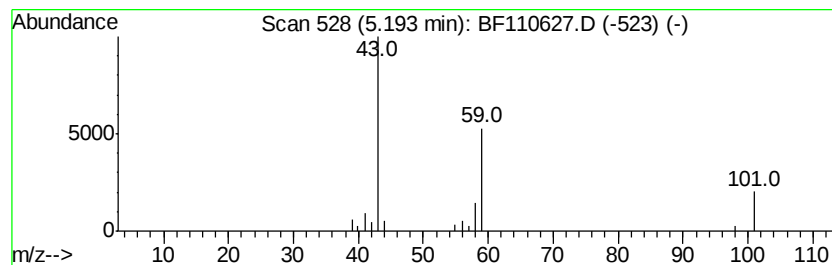
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.48 ng	57374	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		Butane	58	C4H10	000106-97-8	7
5		Propylamine	59	C3H9N	000107-10-8	7



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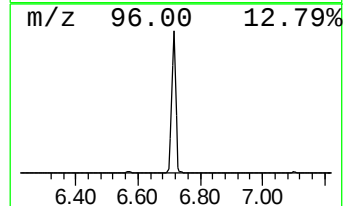
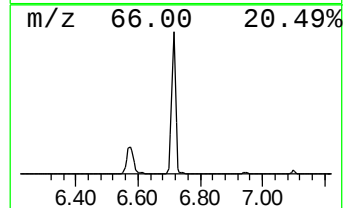
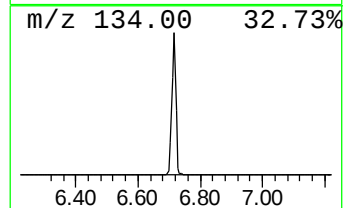
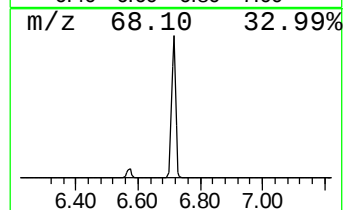
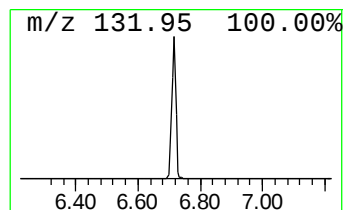
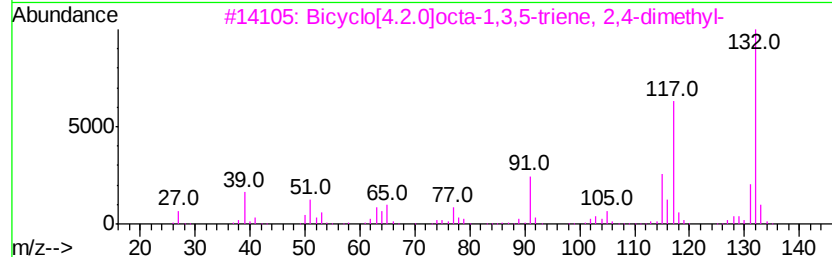
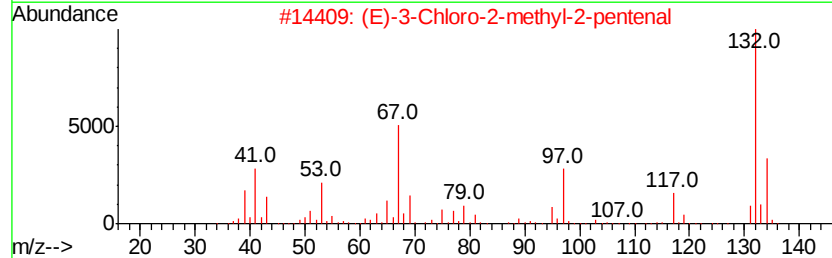
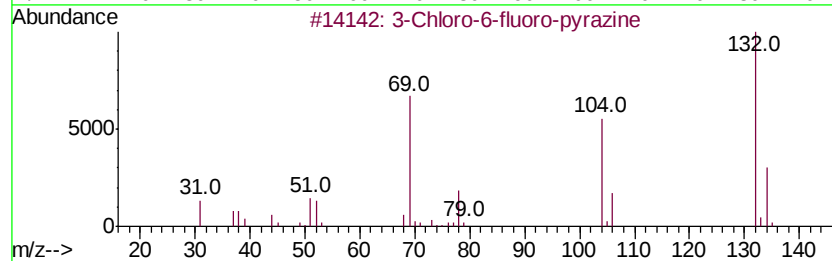
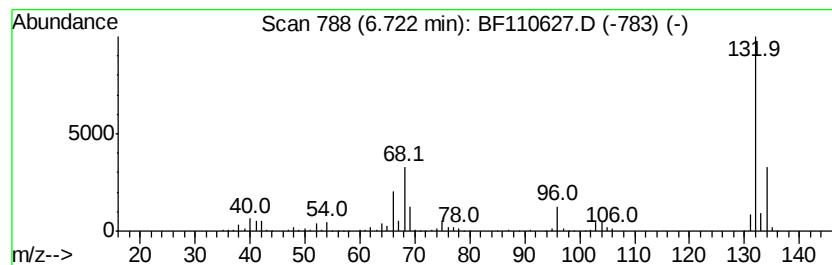
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	73.52 ng	1701730	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		Xenon	132	Xe	007440-63-3	9



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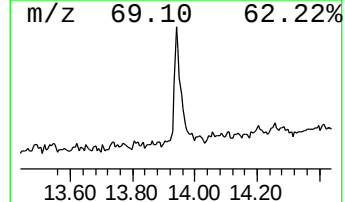
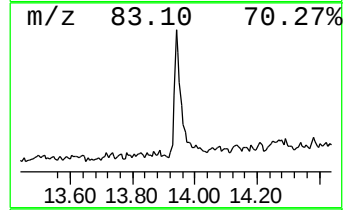
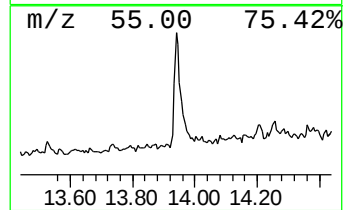
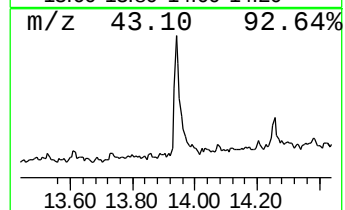
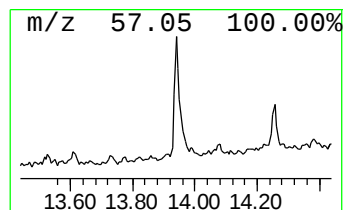
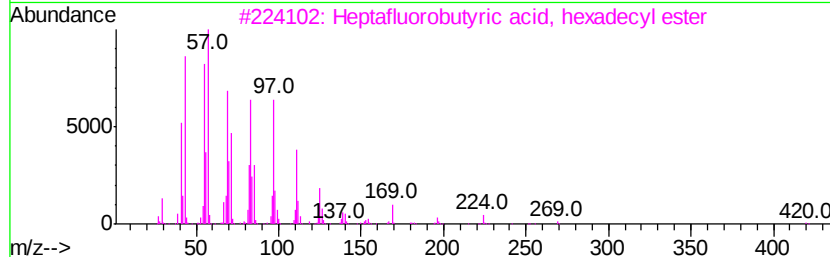
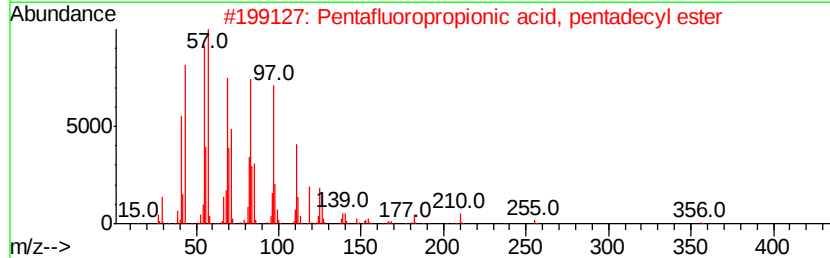
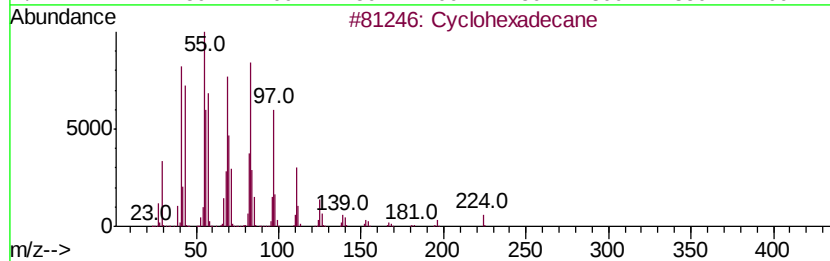
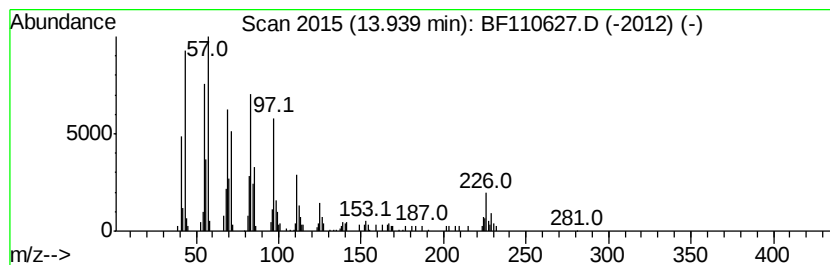
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	6.35 ng	166981	Chrysene-d12	14.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 98
2		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 92
3		Heptafluorobutyric acid, hexadec...	438 C20H33F7O2	006385-15-5 91
4		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 90
5		Carbonic acid, isobutyl octadecy...	370 C23H46O3	1000314-61-5 87



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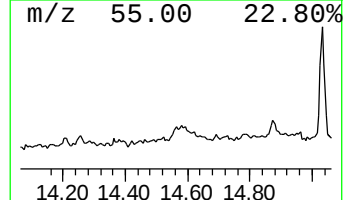
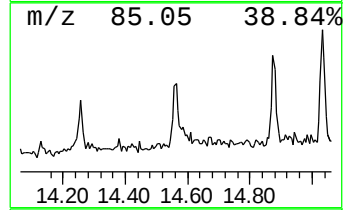
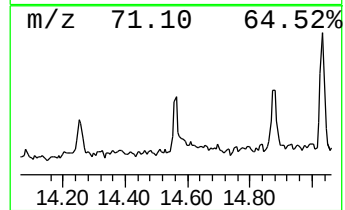
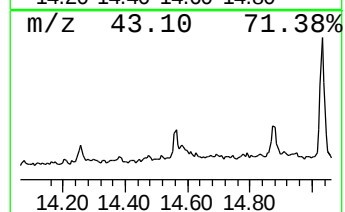
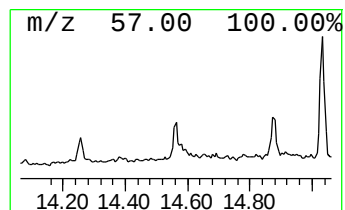
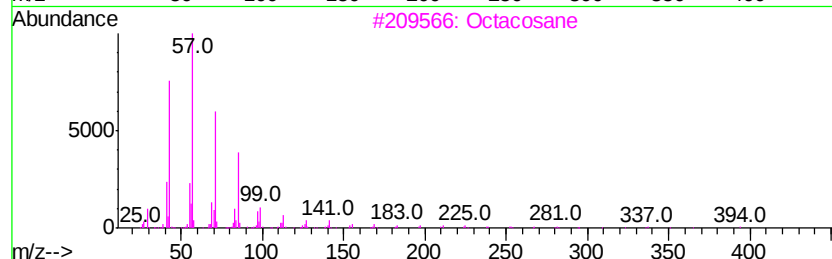
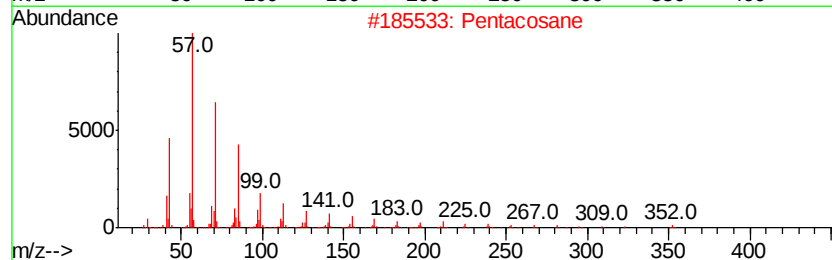
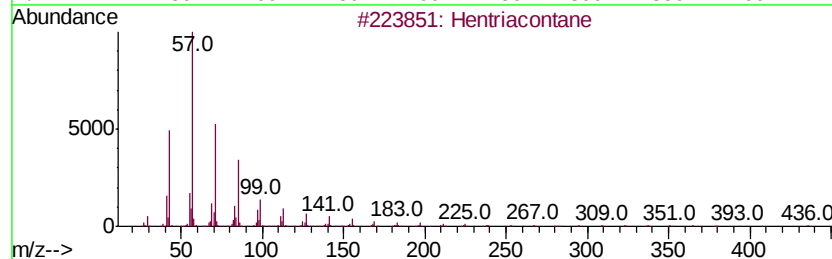
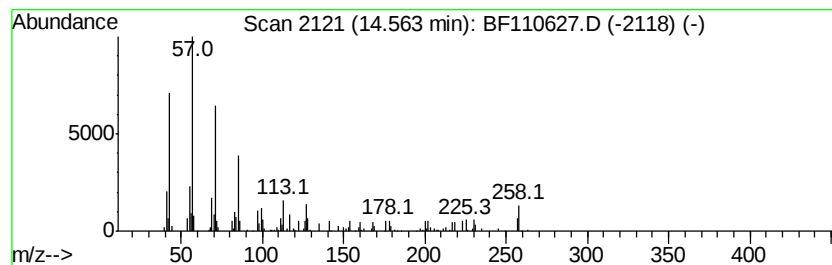
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.84 ng	74653	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	80
2	Pentacosane		352	C25H52	000629-99-2	80
3	Octacosane		394	C28H58	000630-02-4	74
4	Hexatriacontane		507	C36H74	000630-06-8	72
5	Tetratetracontane		619	C44H90	007098-22-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110627.D
Acq On : 9 Nov 2018 15:02
Operator : JU/SJ
Sample : J5813-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-H

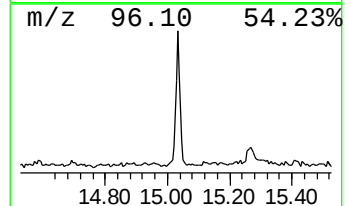
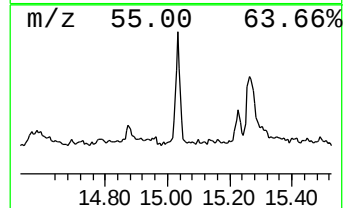
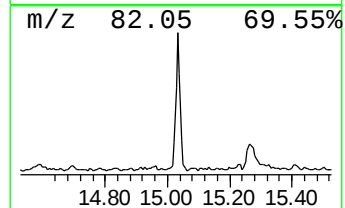
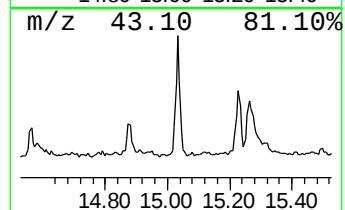
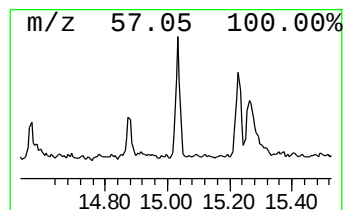
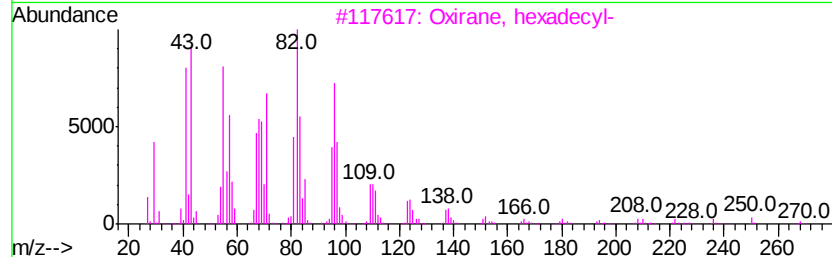
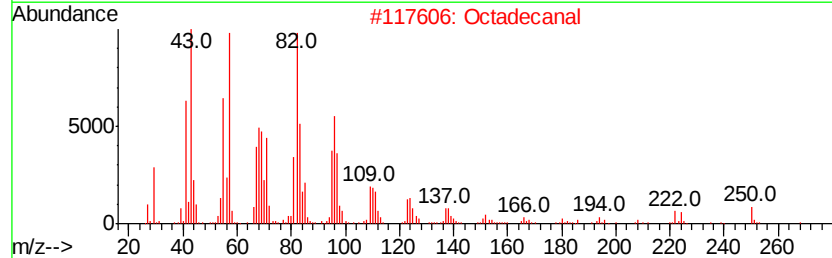
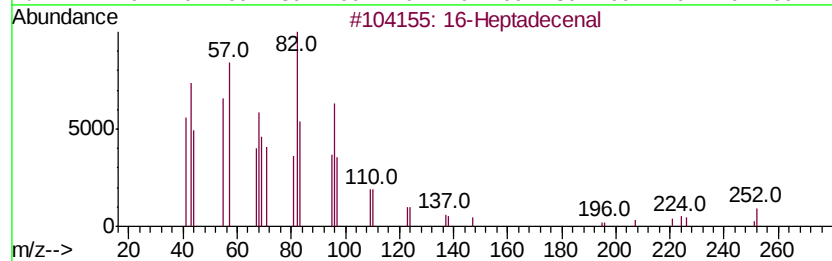
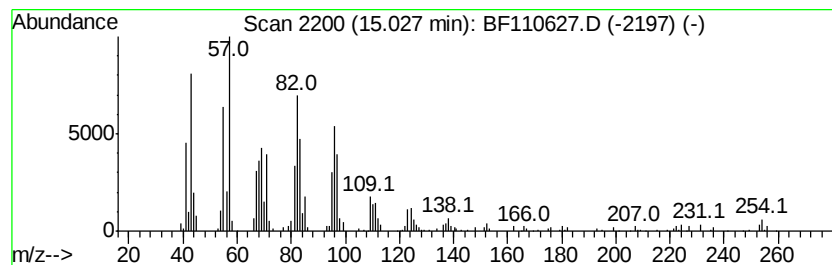
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 16-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	16.80 ng	242543	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		16-Heptadecenal	252	C17H32O	1000144-57-9	93
2		Octadecanal	268	C18H36O	000638-66-4	91
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90
5		Pentadecanal-	226	C15H30O	002765-11-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Operator : JU/SJ
Sample : J5813-08
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ClientSampleId :
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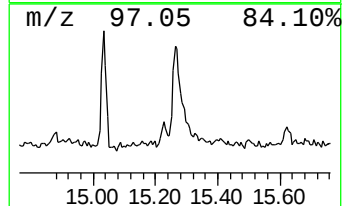
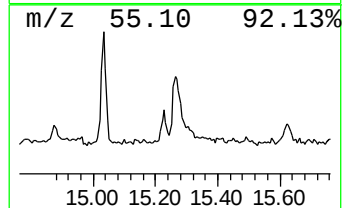
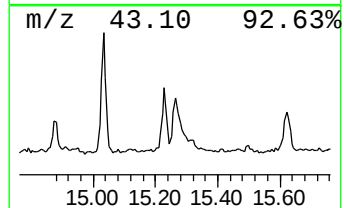
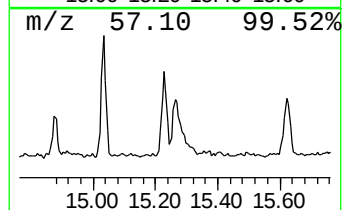
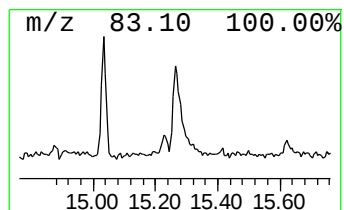
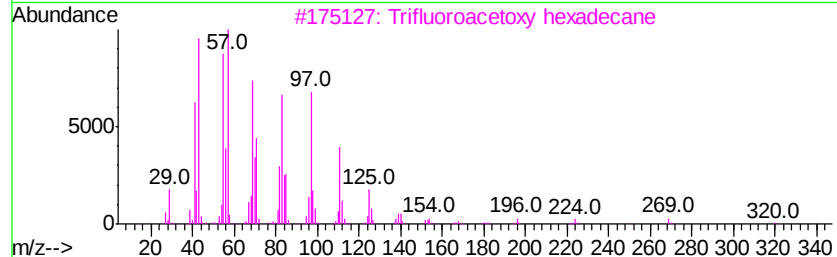
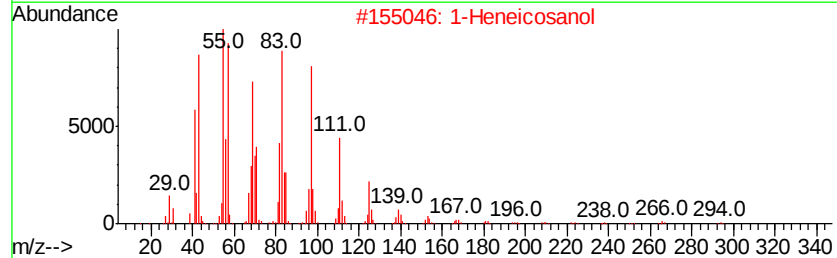
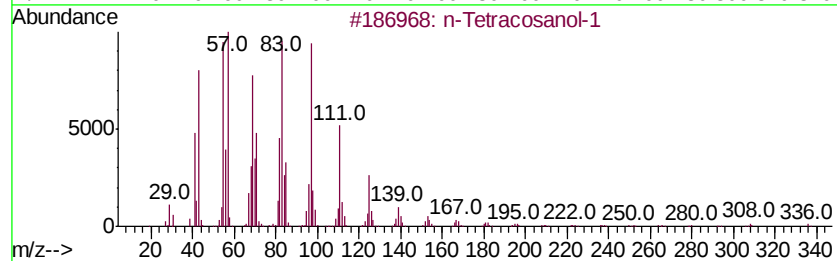
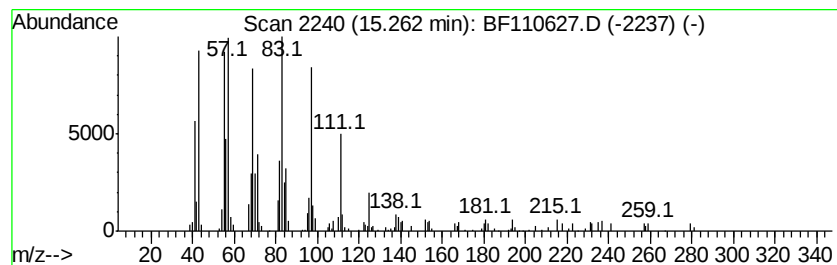
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	11.00 ng	158795	Perylene-d12	15.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	91
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Acq On : 9 Nov 2018 15:02
Operator : JU/SJ
Sample : J5813-08
Misc :
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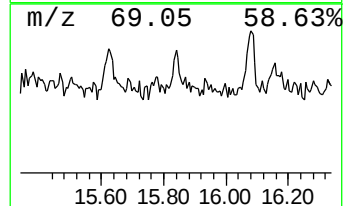
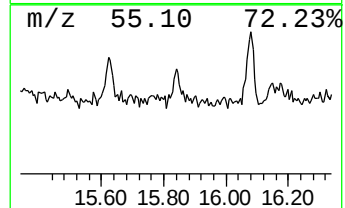
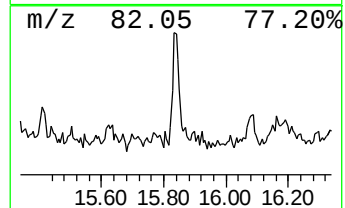
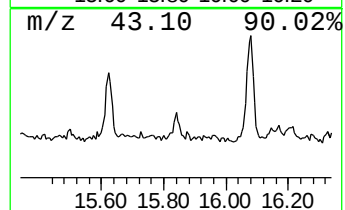
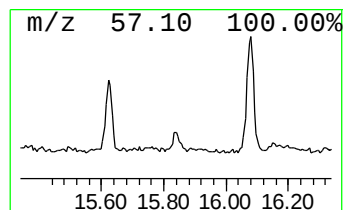
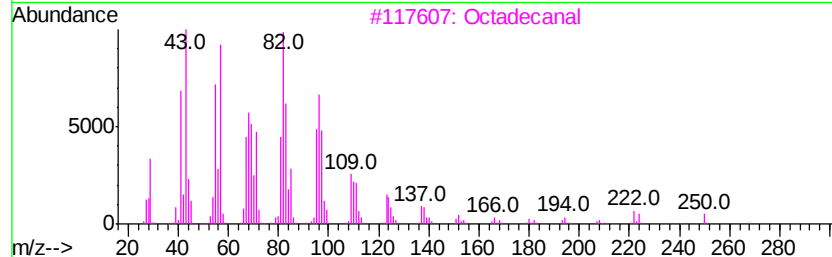
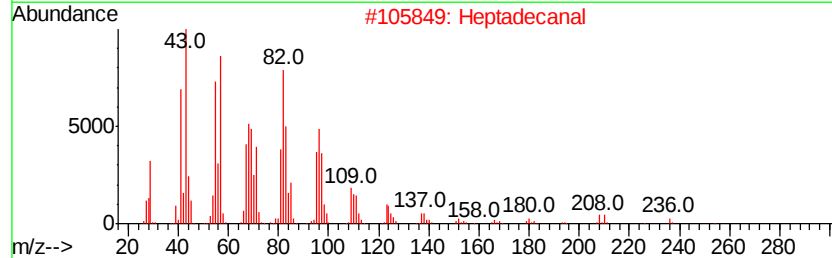
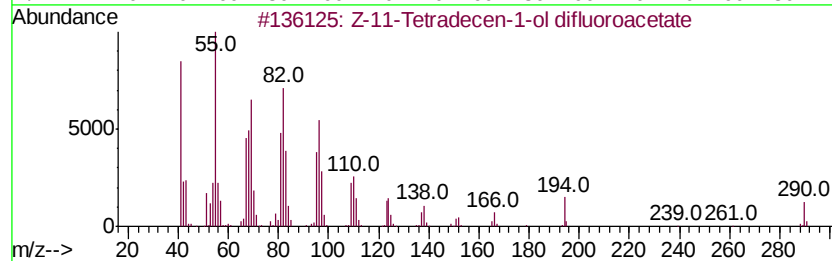
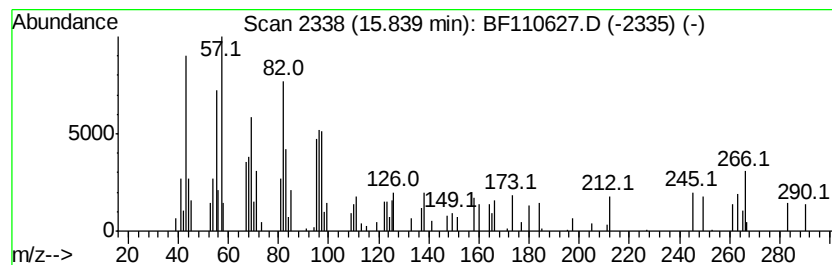
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Z-11-Tetradecen-1-ol difluo... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.32 ng	33521	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-11-Tetradecen-1-ol difluoroace...	290	C16H28F2O2	1000130-82-7	52
2		Heptadecanal	254	C17H34O	1000376-70-0	49
3		Octadecanal	268	C18H36O	000638-66-4	46
4		Hexadecanal	240	C16H32O	000629-80-1	43
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Sample : J5813-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TS-H

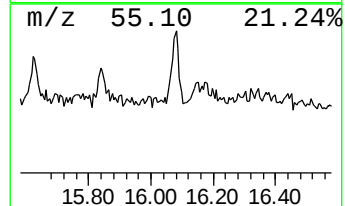
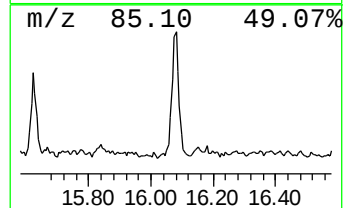
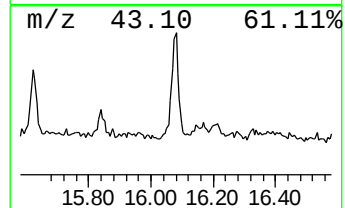
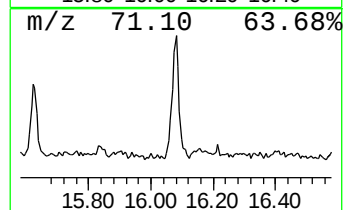
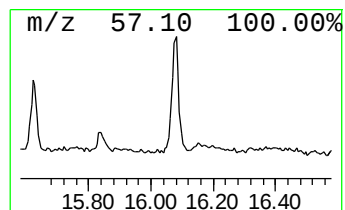
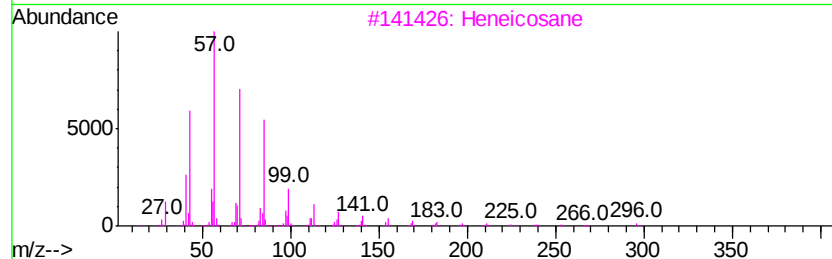
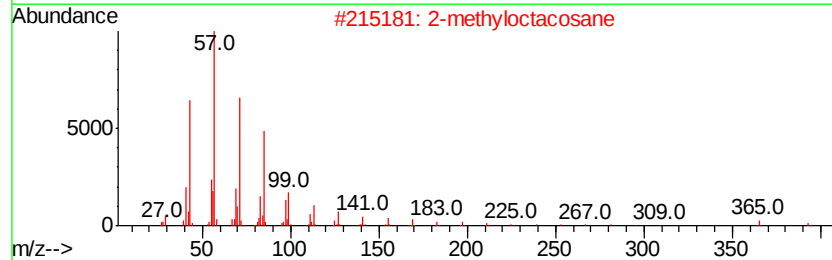
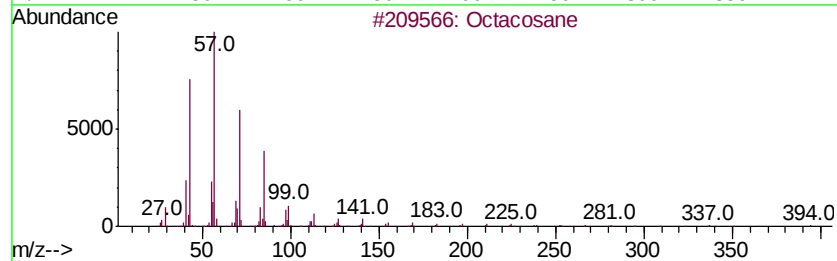
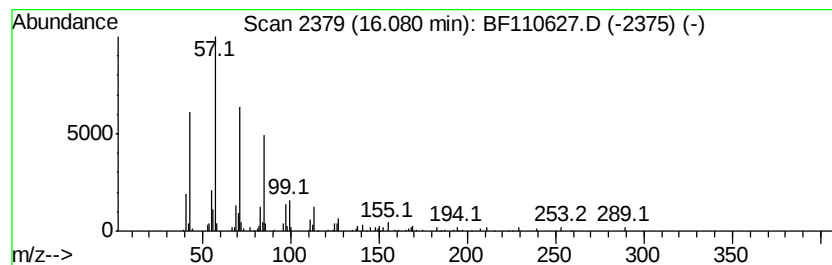
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	8.63 ng	124548	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	90
3			Heneicosane	296	C21H44	000629-94-7	86
4			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Acq On : 9 Nov 2018 15:02
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Sample : J5813-08
Misc :
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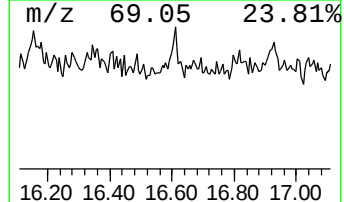
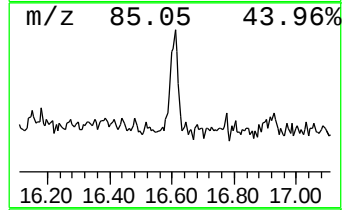
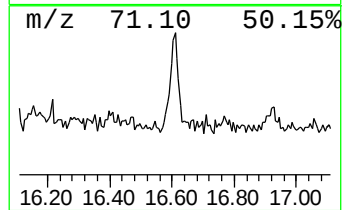
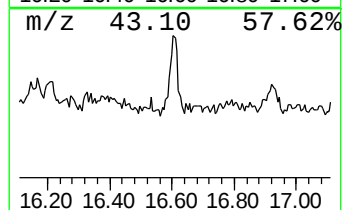
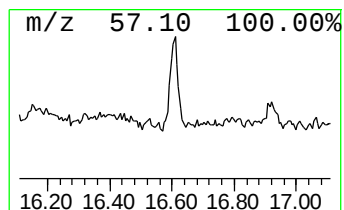
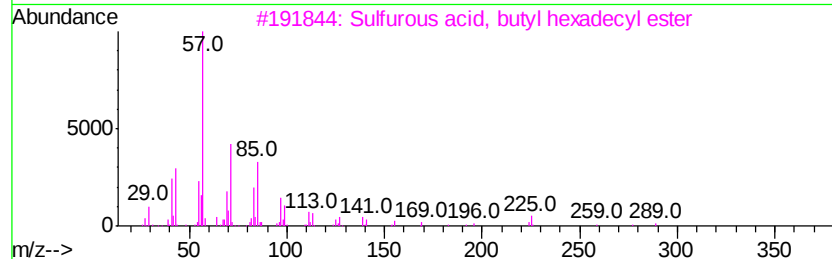
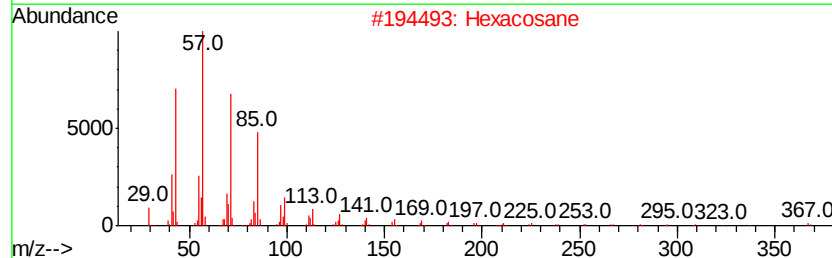
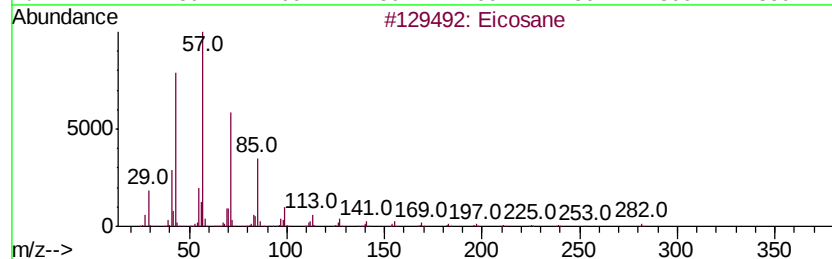
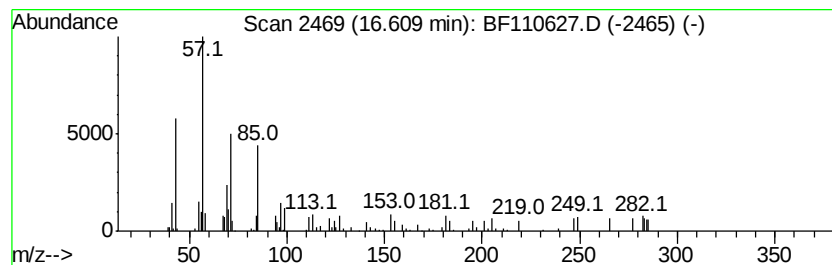
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	3.11 ng	44934	Perylene-d12	15.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hexacosane	366	C26H54	000630-01-3	64
3			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	64
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	64
5			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
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Misc :
ALS Vial : 14 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
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2-Pentanone, 4-hy...	5.19	2.5	ng	57374	1	6.95	462921	20.0
unknown6.72	6.72	73.5	ng	1701730	1	6.95	462921	20.0
Cyclohexadecane	13.94	6.3	ng	166981	5	14.13	525686	20.0
Hentriacontane	14.56	2.8	ng	74653	5	14.13	525686	20.0
16-Heptadecenal	15.03	16.8	ng	242543	6	15.66	288728	20.0
n-Tetracosanol-1	15.26	11.0	ng	158795	6	15.66	288728	20.0
Z-11-Tetradecen-1...	15.84	2.3	ng	33521	6	15.66	288728	20.0
Octacosane	16.08	8.6	ng	124548	6	15.66	288728	20.0
Eicosane	16.61	3.1	ng	44934	6	15.66	288728	20.0