

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121918\
 Data File : BF111606.D
 Acq On : 19 Dec 2018 22:39
 Operator : JU/SJ
 Sample : J6322-21
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-6-C-2-120718

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-BF121918.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	2.216	16	22	28	rVB	652460	877245	16.17%	1.731%
2	4.504	406	411	418	rBV	106295	123793	2.28%	0.244%
3	5.122	508	516	522	rBV	247712	309442	5.70%	0.611%
4	5.516	578	583	586	rBV	4638733	4892394	90.20%	9.654%
5	6.522	747	754	758	rBV	4937084	5424117	100.00%	10.704%
6	6.663	773	778	782	rBV	5166199	5109709	94.20%	10.083%
7	6.893	814	817	821	rVB	1446694	1178837	21.73%	2.326%
8	7.051	840	844	847	rBV	4521012	3882885	71.59%	7.662%
9	7.451	907	912	915	rBV	3578587	3227581	59.50%	6.369%
10	8.175	1031	1035	1038	rBV	1872402	1508278	27.81%	2.976%
11	9.251	1213	1218	1221	rBV	6167570	5234595	96.51%	10.330%
12	9.639	1280	1284	1287	rVB	365247	306246	5.65%	0.604%
13	9.928	1329	1333	1337	rBV2	2036699	1675197	30.88%	3.306%
14	10.710	1462	1466	1470	rBV	3645059	3509833	64.71%	6.926%
15	11.410	1581	1585	1587	rBV	1957640	1602865	29.55%	3.163%
16	11.433	1587	1589	1592	rVV	359054	271688	5.01%	0.536%
17	11.480	1592	1597	1600	rVB2	100660	102379	1.89%	0.202%
18	11.633	1618	1623	1627	rBV3	67053	69230	1.28%	0.137%
19	11.939	1671	1675	1685	rVB	718286	687422	12.67%	1.357%
20	12.451	1759	1762	1767	rBV2	89019	94300	1.74%	0.186%
21	12.616	1787	1790	1793	rBV	439090	396477	7.31%	0.782%
22	12.722	1804	1808	1815	rBV	364529	414845	7.65%	0.819%
23	12.845	1822	1829	1833	rBV	348284	377635	6.96%	0.745%
24	12.992	1850	1854	1858	rVB	4720430	4206722	77.56%	8.301%
25	13.786	1985	1989	1993	rBV2	39839	69754	1.29%	0.138%
26	13.886	2002	2006	2013	rBV2	260061	269047	4.96%	0.531%
27	14.039	2027	2032	2035	rBV	1592797	1627911	30.01%	3.212%
28	14.063	2035	2036	2041	rVB	165452	149924	2.76%	0.296%
29	14.521	2111	2114	2117	rBV	135171	122852	2.26%	0.242%
30	14.833	2164	2167	2171	rVB	89666	92897	1.71%	0.183%
31	14.910	2177	2180	2185	rVB	223800	220162	4.06%	0.434%
32	15.080	2205	2209	2212	rBV	127650	202942	3.74%	0.400%
33	15.174	2222	2225	2233	rBV2	150353	237475	4.38%	0.469%
34	15.386	2258	2261	2266	rVB	76623	95945	1.77%	0.189%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.445	2268	2271	2276	rVV	122302	172866	3.19%	0.341%
36	15.515	2278	2283	2287	rVV	1023625	1336461	24.64%	2.637%
37	15.563	2289	2291	2297	rVB	124611	142088	2.62%	0.280%
38	16.010	2362	2367	2372	rBV	295533	451169	8.32%	0.890%

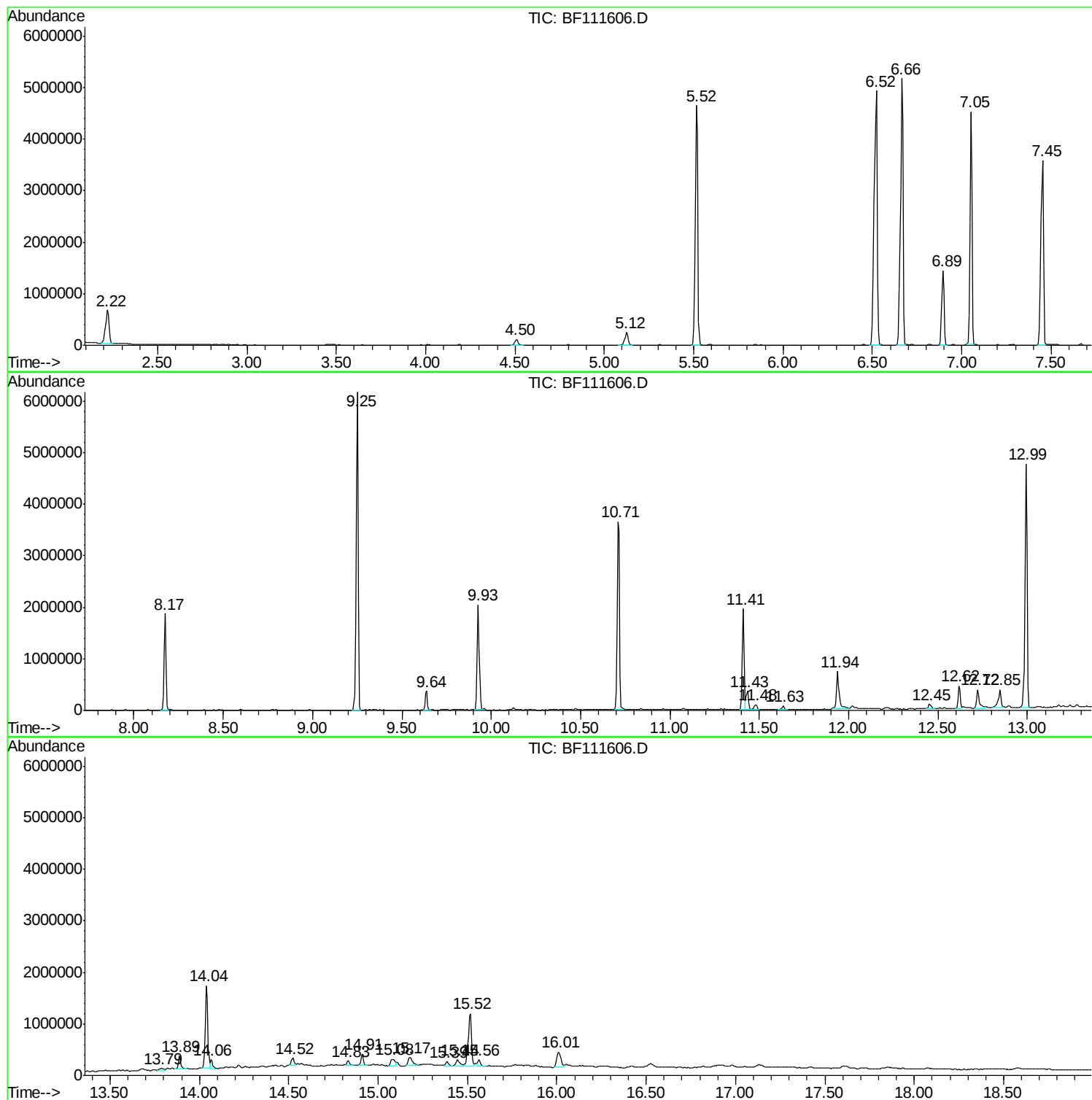
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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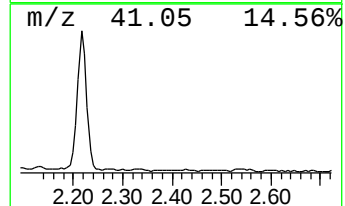
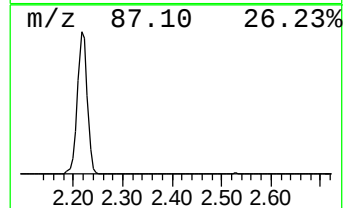
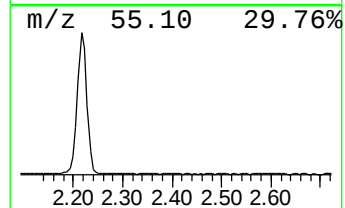
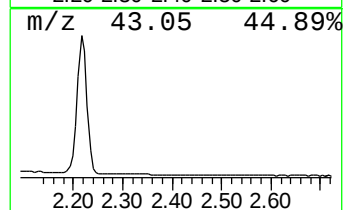
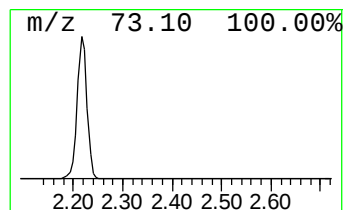
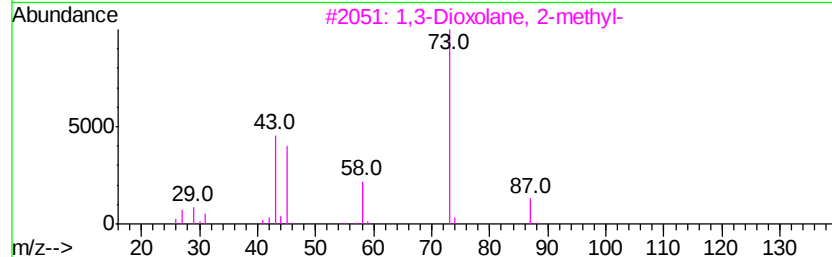
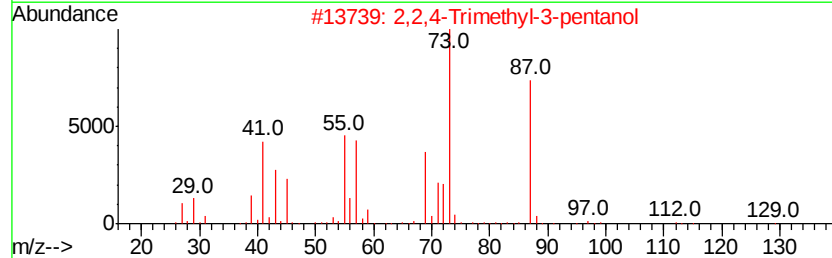
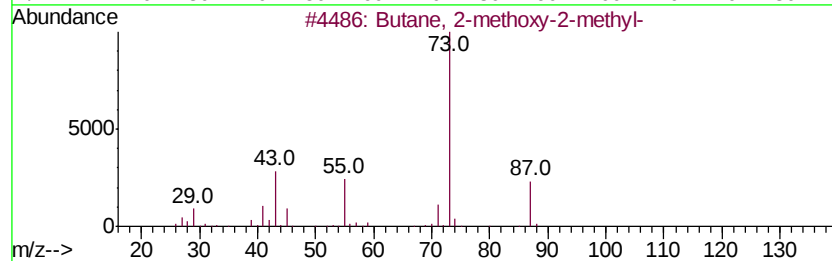
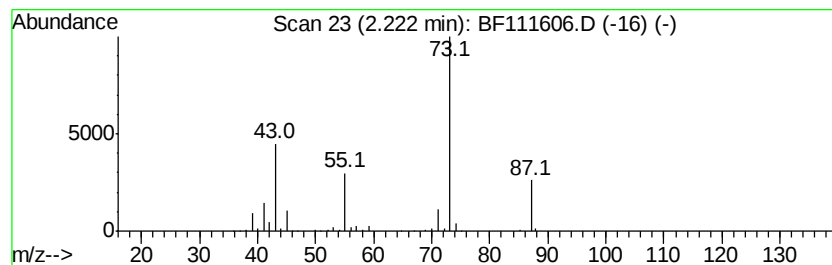
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	14.88 ng	877245	1,4-Dichlorobenzene-d4	6.89

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	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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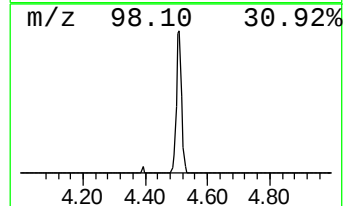
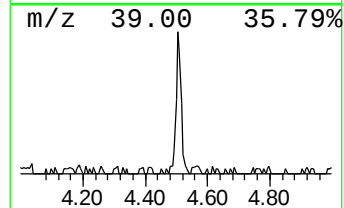
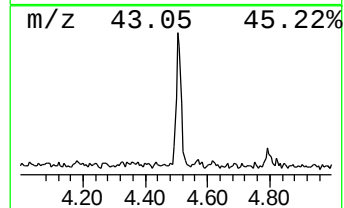
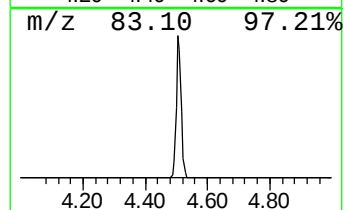
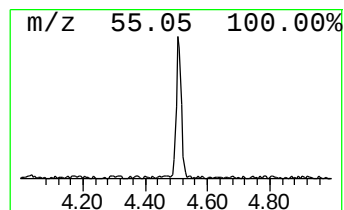
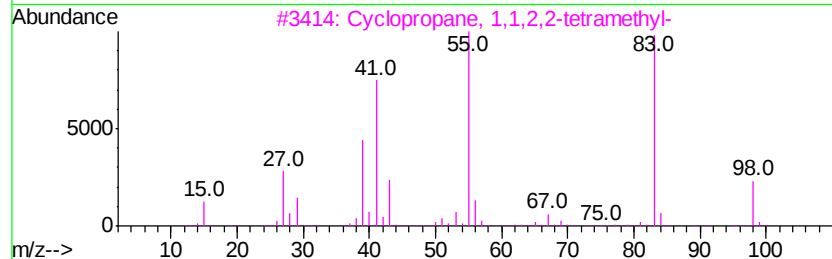
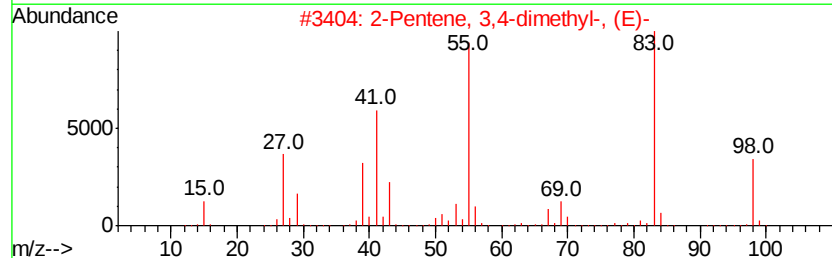
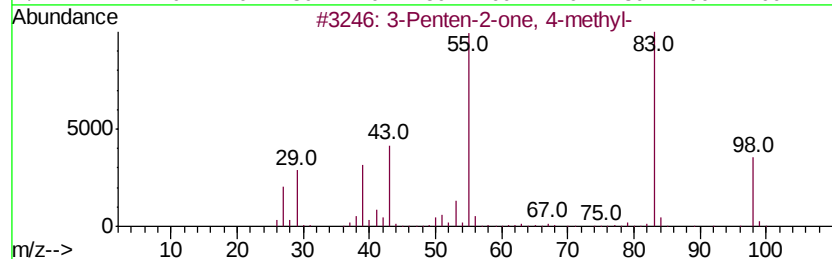
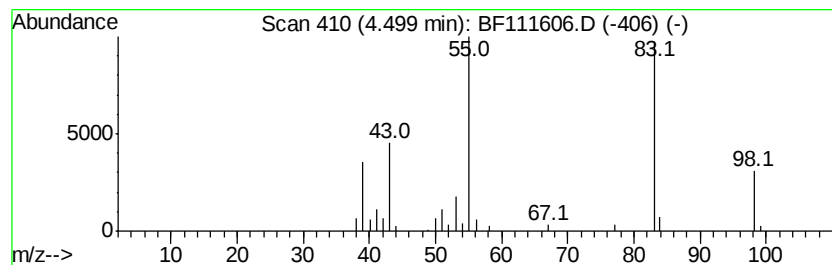
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	2.10 ng	123793	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3			Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	80
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80



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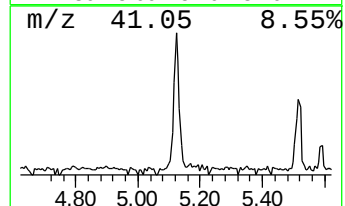
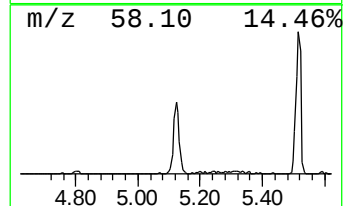
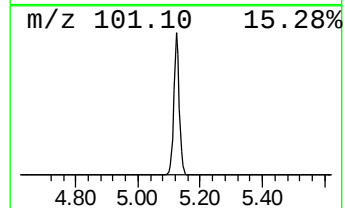
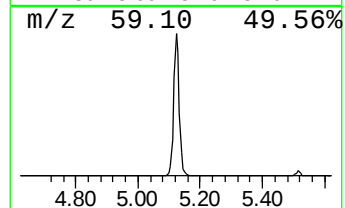
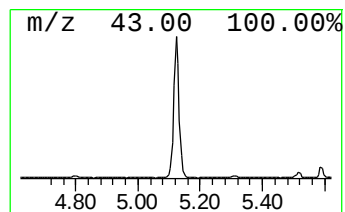
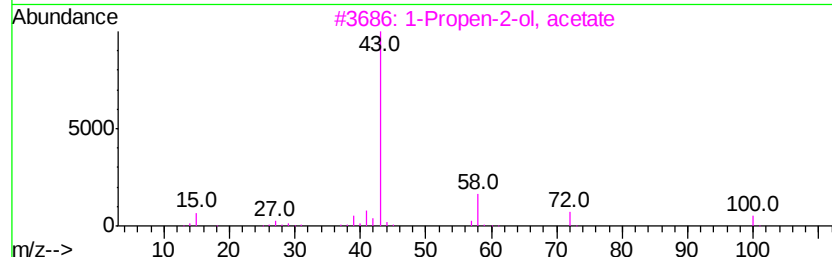
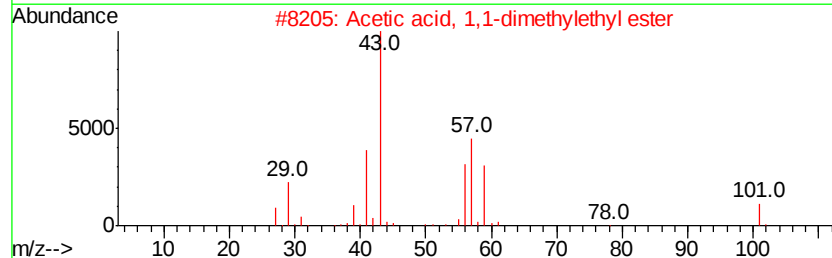
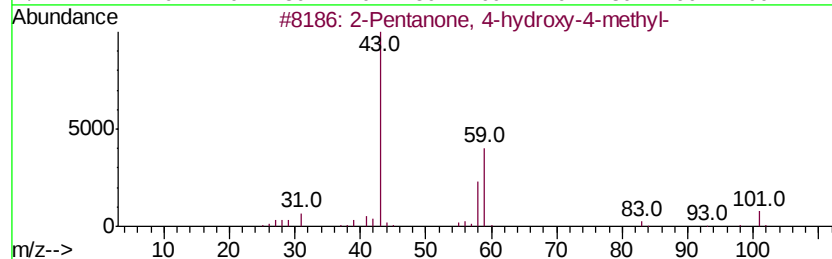
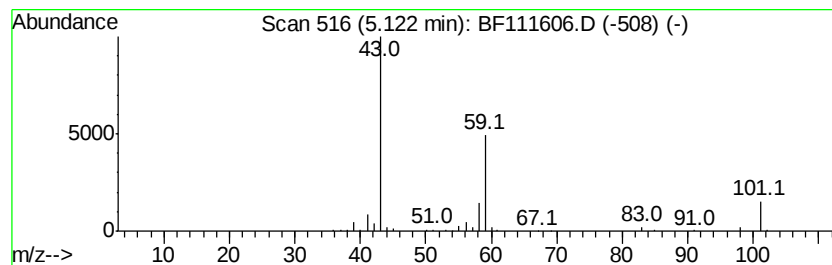
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.25 ng	309442	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Allyl acetate	100	C5H8O2	000591-87-7	9



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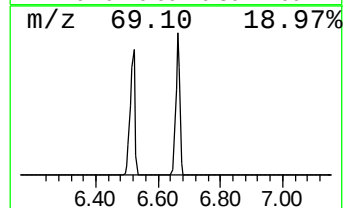
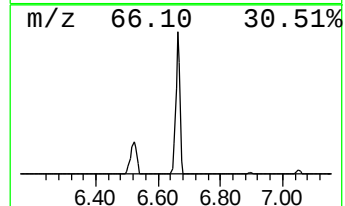
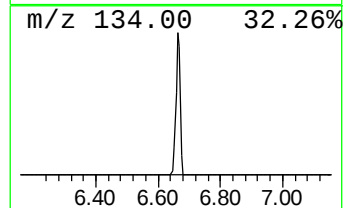
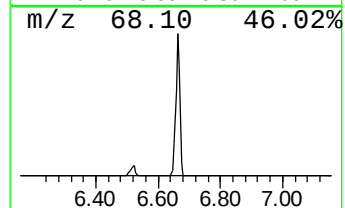
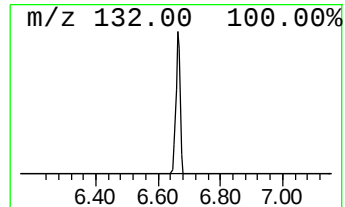
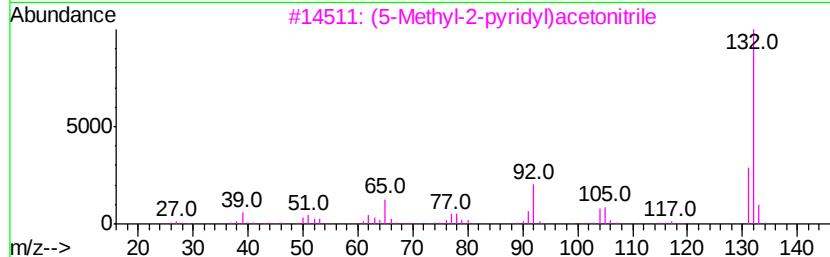
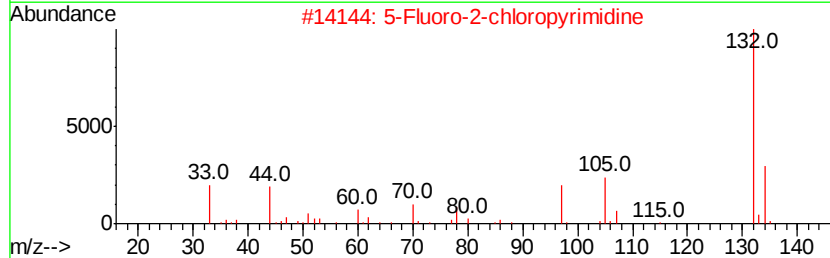
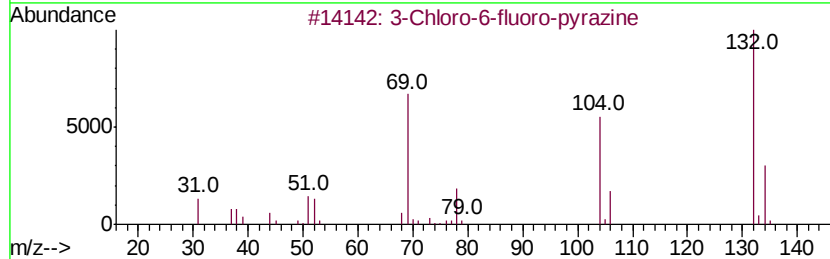
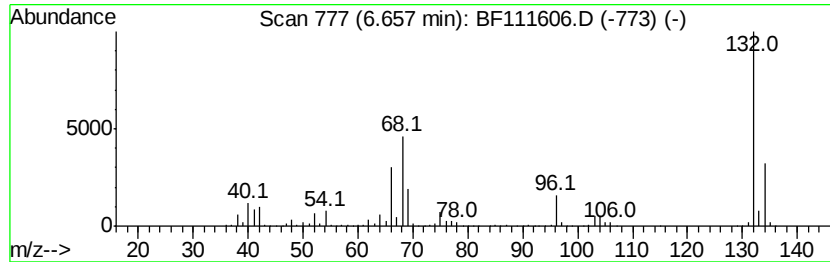
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	86.69 ng	5109710	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	(5-Methyl-2-pyridyl)acetonitrile			132	C8H8N2	1000241-93-9	10
4	1,3,5-Trifluorobenzene			132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9



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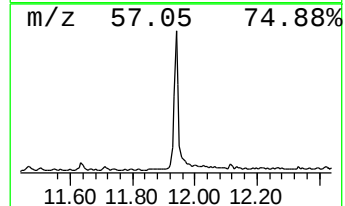
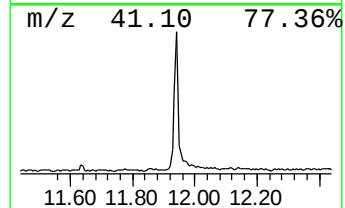
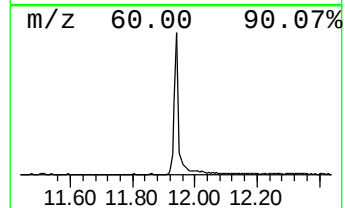
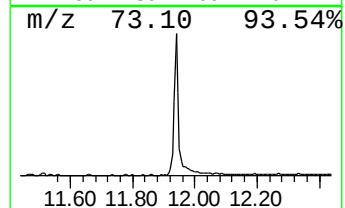
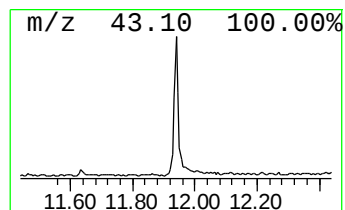
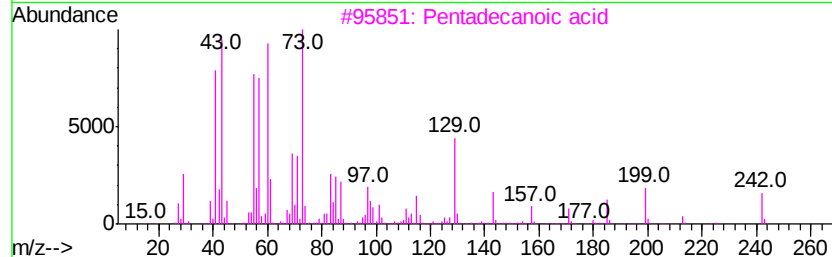
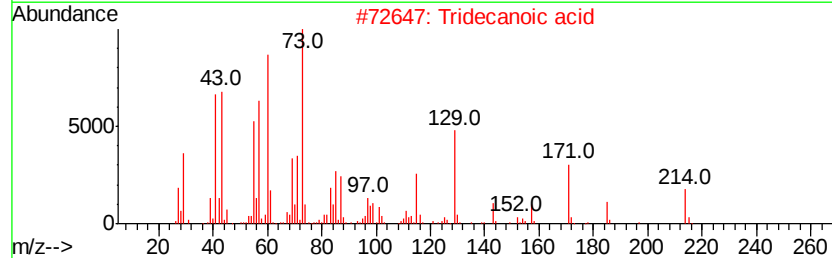
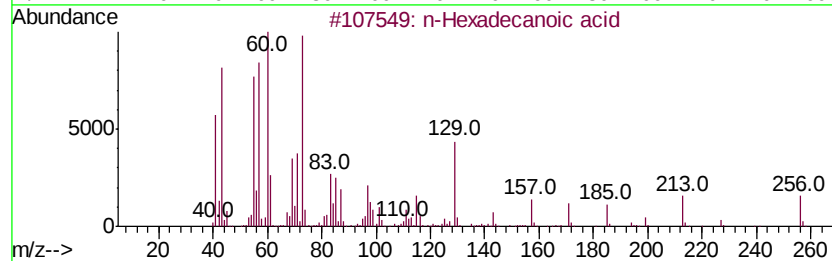
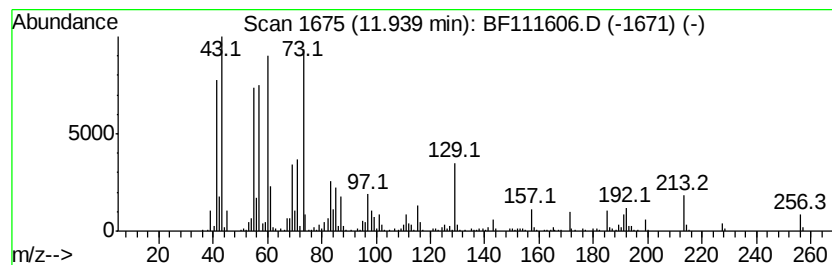
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	8.58 ng	687422	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
Data File : BF111606.D
Acq On : 19 Dec 2018 22:39
Operator : JU/SJ
Sample : J6322-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

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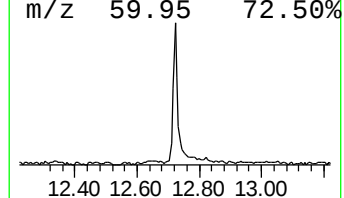
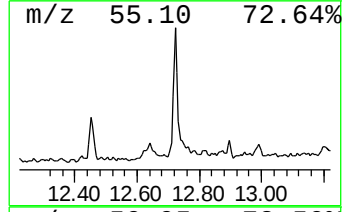
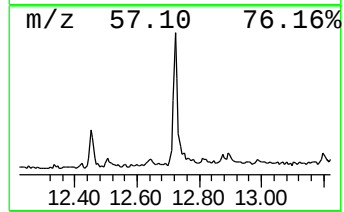
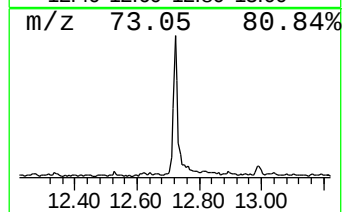
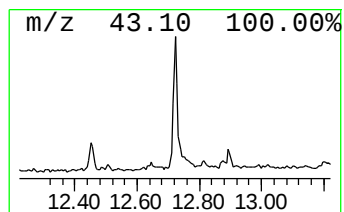
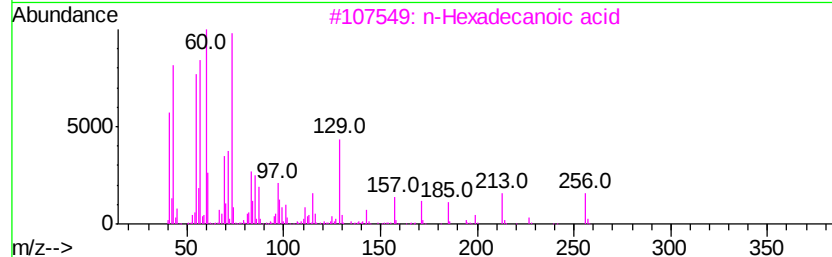
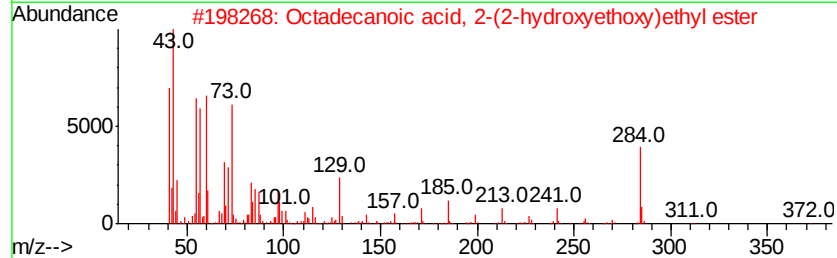
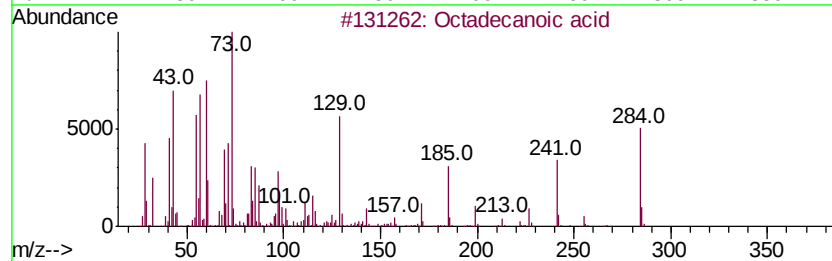
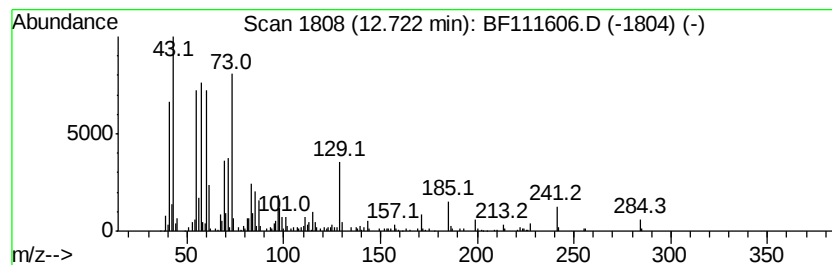
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	5.18 ng	414845	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		Tridecanoic acid	214	C13H26O2	000638-53-9	81



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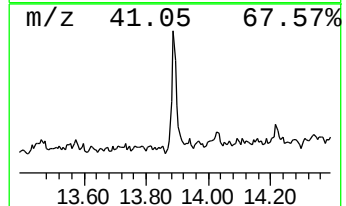
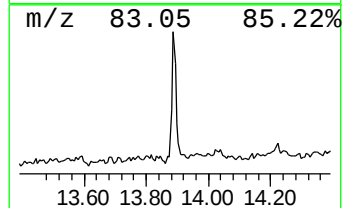
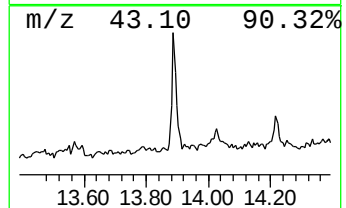
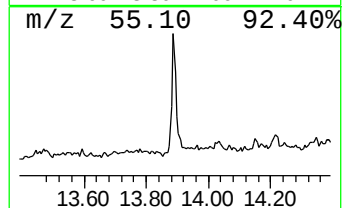
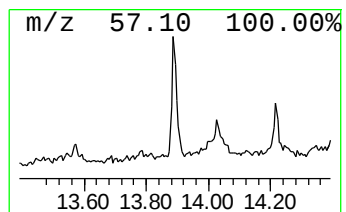
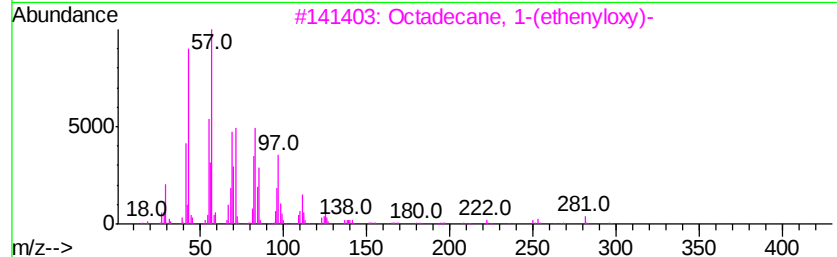
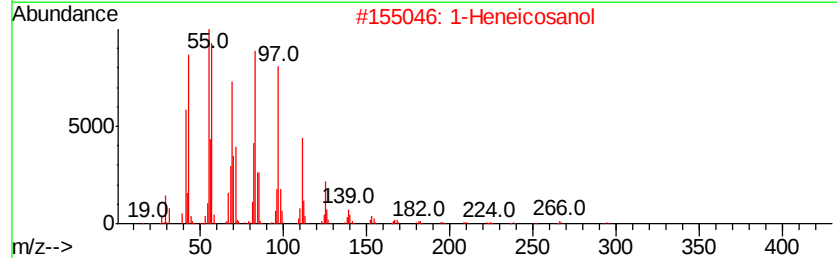
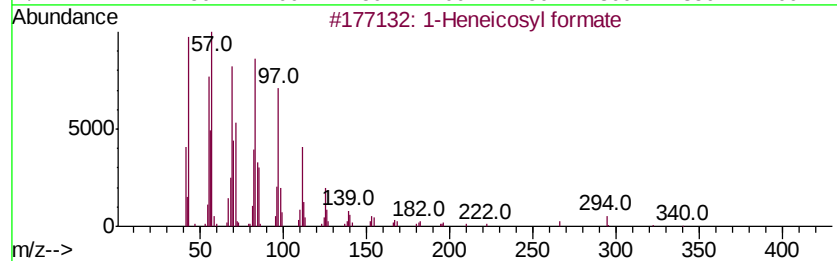
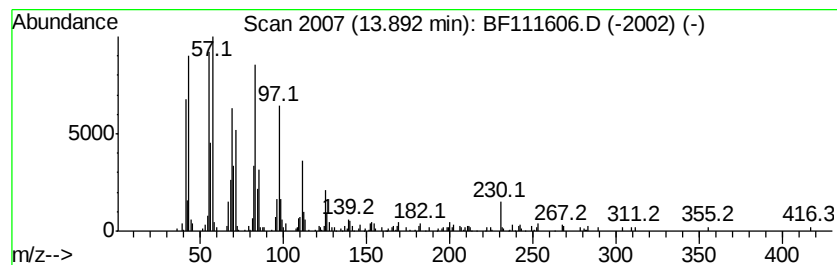
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.89	3.31 ng	269047	Chrysene-d12		14.04
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Octadecane, 1-(ethenvloxy)-	296	C20H40O	000930-02-9	91
4	Octacosanol	410	C28H58O	000557-61-9	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87



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Sample : J6322-21
Misc :
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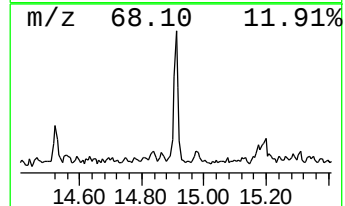
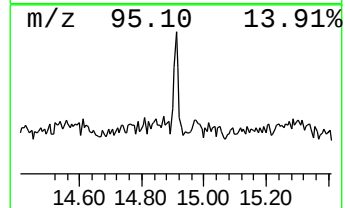
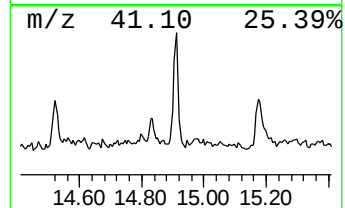
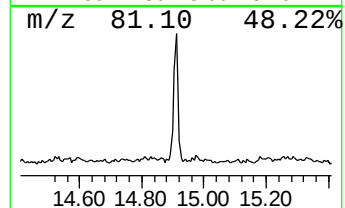
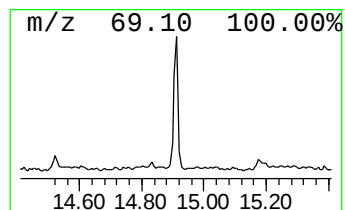
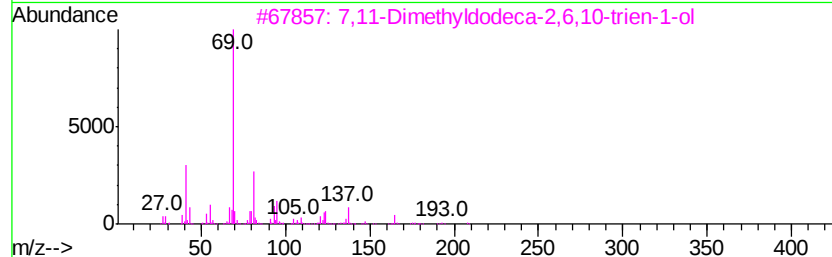
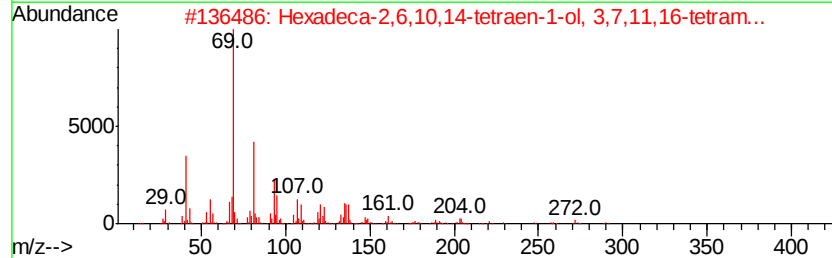
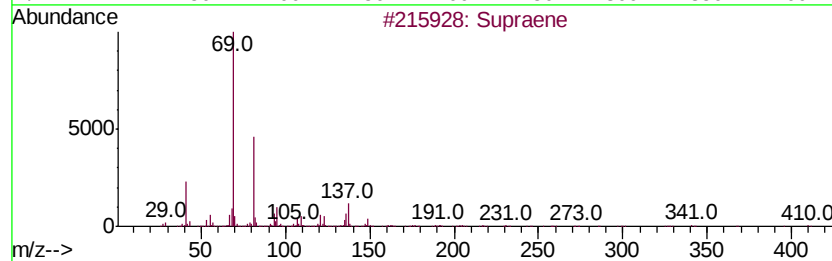
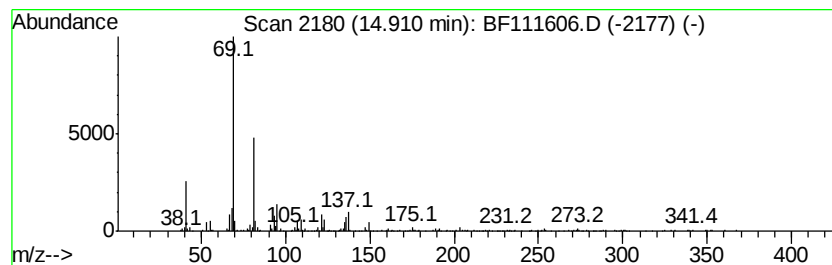
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	3.29 ng	220162	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	83
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4		Squalene	410	C30H50	000111-02-4	80
5		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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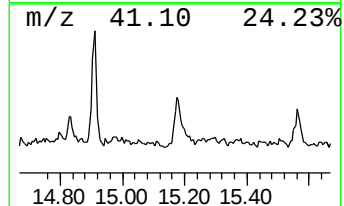
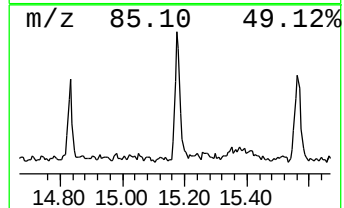
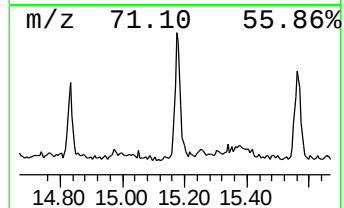
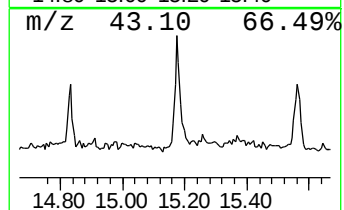
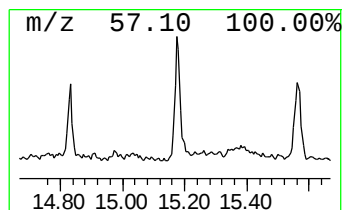
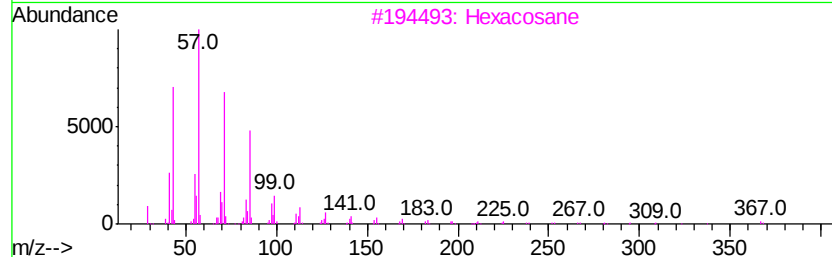
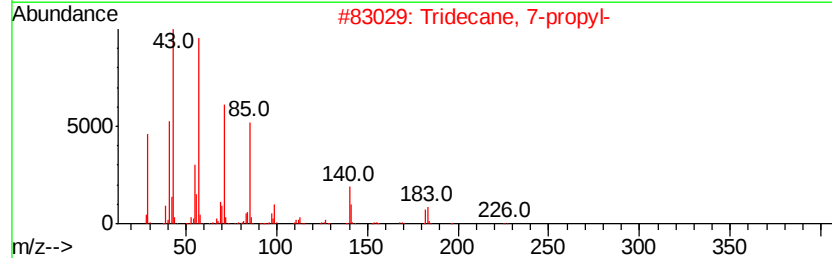
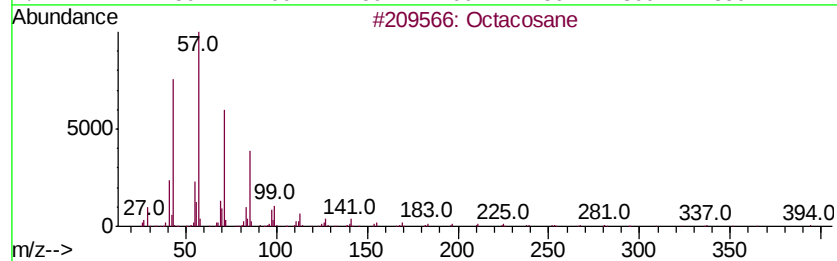
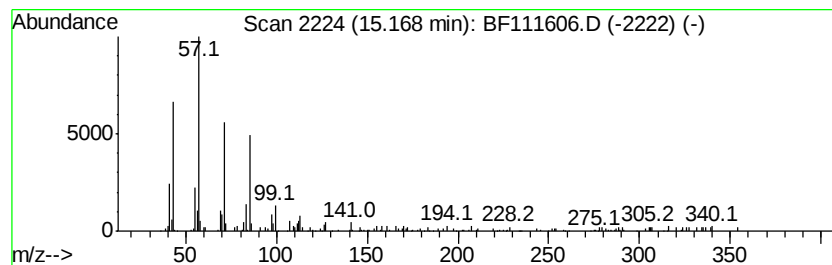
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.55 ng	237475	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Tridecane, 7-propyl-	226	C16H34	055045-09-5	87
3			Hexacosane	366	C26H54	000630-01-3	83
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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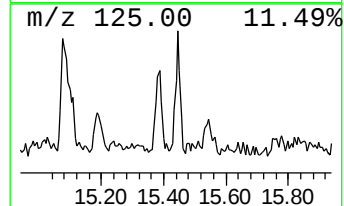
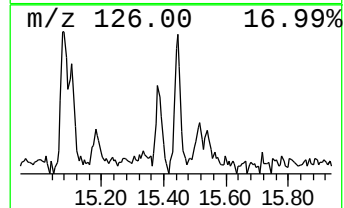
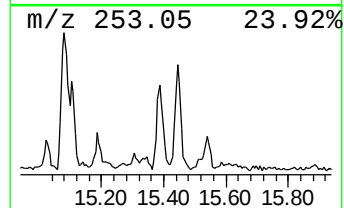
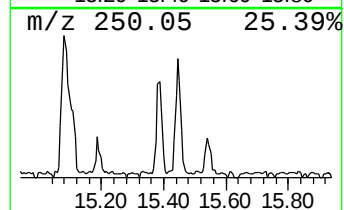
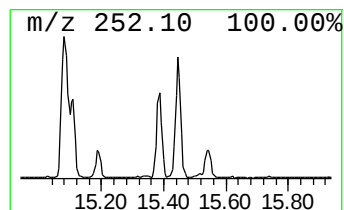
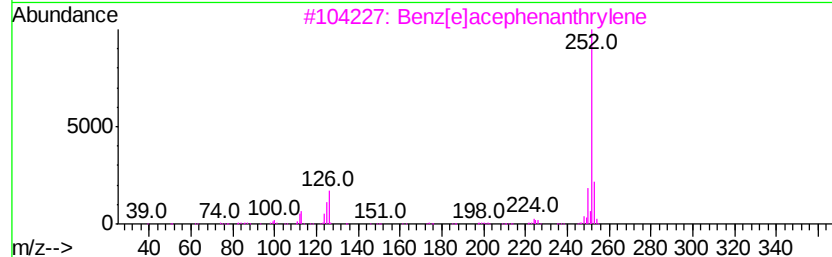
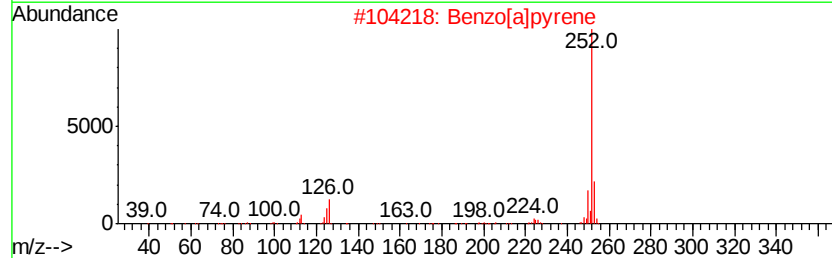
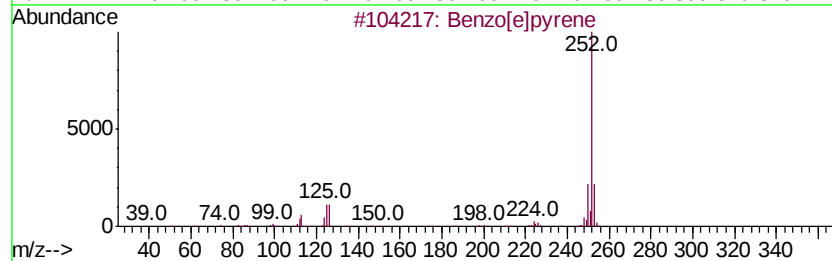
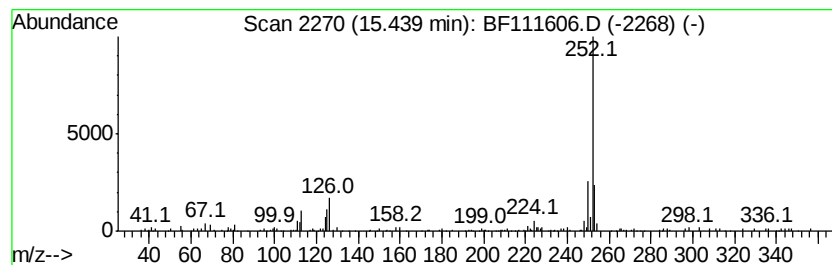
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.59 ng	172866	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzo[e]pyrene	252 C20H12	000192-97-2 96
2		Benzo[a]pyrene	252 C20H12	000050-32-8 96
3		Benzo[e]acephenanthrylene	252 C20H12	000205-99-2 94
4		Benzo[k]fluoranthene	252 C20H12	000207-08-9 90
5		Perylene	252 C20H12	000198-55-0 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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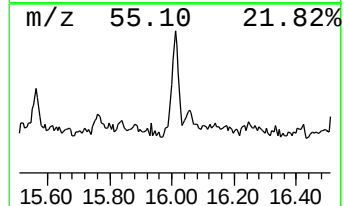
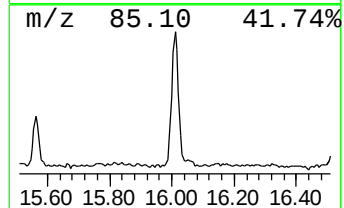
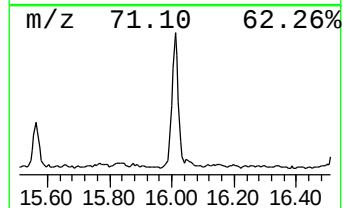
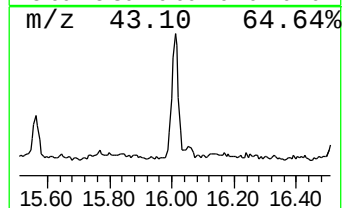
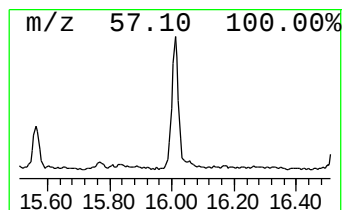
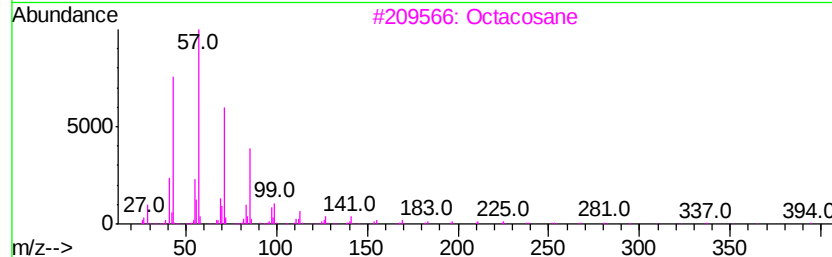
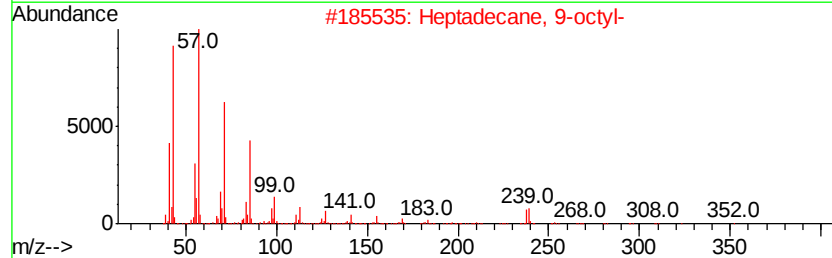
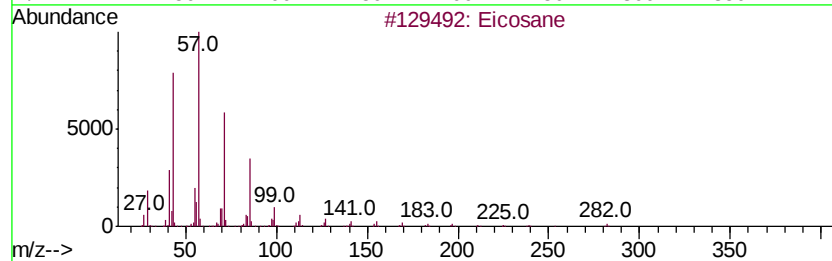
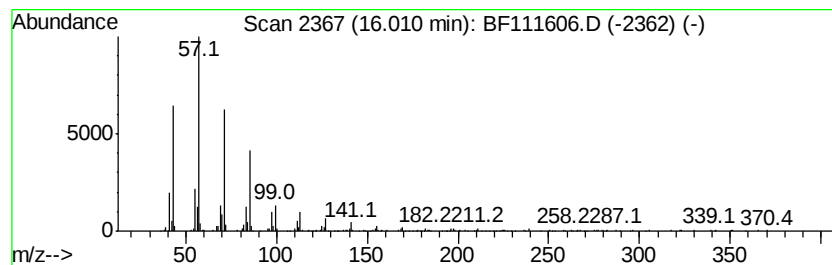
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	6.75 ng	451169	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SUP-6-C-2-120718

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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
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3-Penten-2-one, 4...	4.50	2.1	ng	123793	1	6.89	1178840	20.0
2-Pentanone, 4-hy...	5.12	5.3	ng	309442	1	6.89	1178840	20.0
unknown6.66	6.66	86.7	ng	5109710	1	6.89	1178840	20.0
n-Hexadecanoic acid	11.94	8.6	ng	687422	4	11.41	1602870	20.0
Octadecanoic acid	12.72	5.2	ng	414845	4	11.41	1602870	20.0
1-Heneicosyl formate	13.89	3.3	ng	269047	5	14.04	1627910	20.0
Supraene	14.91	3.3	ng	220162	6	15.52	1336460	20.0
Octacosane	15.17	3.5	ng	237475	6	15.52	1336460	20.0
Benzo[e]pyrene	15.44	2.6	ng	172866	6	15.52	1336460	20.0
Eicosane	16.01	6.8	ng	451169	6	15.52	1336460	20.0