

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121918\
 Data File : BF111617.D
 Acq On : 20 Dec 2018 3:42
 Operator : JU/SJ
 Sample : J6386-05
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS005-0006-01

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	2.199	16	19	27	rVB2	48253	73866	2.25%	0.221%
2	3.410	222	225	236	rBV	25332	59446	1.81%	0.178%
3	5.110	510	514	519	rVB	144592	168463	5.13%	0.505%
4	5.298	542	546	554	rVB	69127	70223	2.14%	0.210%
5	5.516	578	583	586	rBV	3299887	2939361	89.42%	8.806%
6	6.522	748	754	763	rBV	3078005	3287033	100.00%	9.848%
7	6.663	774	778	782	rBV	3235570	3099782	94.30%	9.287%
8	6.898	814	818	821	rVB	1373754	1118706	34.03%	3.352%
9	7.051	841	844	848	rVB	2728889	2434813	74.07%	7.295%
10	7.451	907	912	915	rBV	2291724	1867916	56.83%	5.596%
11	7.498	917	920	923	rVB	126571	97267	2.96%	0.291%
12	8.175	1032	1035	1039	rBV	1502223	1354453	41.21%	4.058%
13	9.251	1214	1218	1221	rBV	3892285	3058204	93.04%	9.162%
14	9.639	1281	1284	1288	rBV	361088	270559	8.23%	0.811%
15	9.933	1330	1334	1337	rBV	1635469	1442861	43.90%	4.323%
16	10.716	1462	1467	1470	rBV	2268810	1968418	59.88%	5.897%
17	11.357	1573	1576	1581	rBV4	37055	47738	1.45%	0.143%
18	11.416	1582	1586	1589	rVV	1576814	1356410	41.27%	4.064%
19	11.639	1620	1624	1627	rBV	53977	50668	1.54%	0.152%
20	11.939	1672	1675	1679	rBV	459138	426338	12.97%	1.277%
21	12.116	1700	1705	1712	rVB5	43791	60237	1.83%	0.180%
22	12.457	1760	1763	1767	rBV2	97858	97159	2.96%	0.291%
23	12.510	1767	1772	1775	rVV3	44862	57558	1.75%	0.172%
24	12.621	1788	1791	1794	rBV	155555	139517	4.24%	0.418%
25	12.663	1795	1798	1800	rVV	206677	181495	5.52%	0.544%
26	12.680	1800	1801	1805	rVB	70845	50364	1.53%	0.151%
27	12.721	1805	1808	1816	rBV3	134914	178224	5.42%	0.534%
28	12.851	1827	1830	1833	rBV	107328	103318	3.14%	0.310%
29	12.998	1851	1855	1858	rBV	2666796	2424762	73.77%	7.265%
30	13.233	1893	1895	1899	rBV3	52908	53794	1.64%	0.161%
31	13.468	1932	1935	1939	rVB	674056	552795	16.82%	1.656%
32	13.574	1951	1953	1960	rVB	62365	71619	2.18%	0.215%
33	13.892	2003	2007	2013	rBV3	444693	568671	17.30%	1.704%
34	14.045	2029	2033	2036	rBV	1452502	1436630	43.71%	4.304%

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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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35	14.068	2036	2037	2040	rVB	99726	82040	2.50%	0.246%
36	14.221	2060	2063	2066	rBV	97589	92788	2.82%	0.278%
37	14.527	2112	2115	2118	rBV	236472	237406	7.22%	0.711%
38	14.839	2165	2168	2172	rVB	153695	164263	5.00%	0.492%
39	15.086	2208	2210	2213	rBV	94910	108353	3.30%	0.325%
40	15.180	2223	2226	2234	rVB2	258950	459073	13.97%	1.375%
41	15.521	2280	2284	2288	rVB	745550	865554	26.33%	2.593%
42	16.015	2365	2368	2372	rVB2	170313	200087	6.09%	0.599%

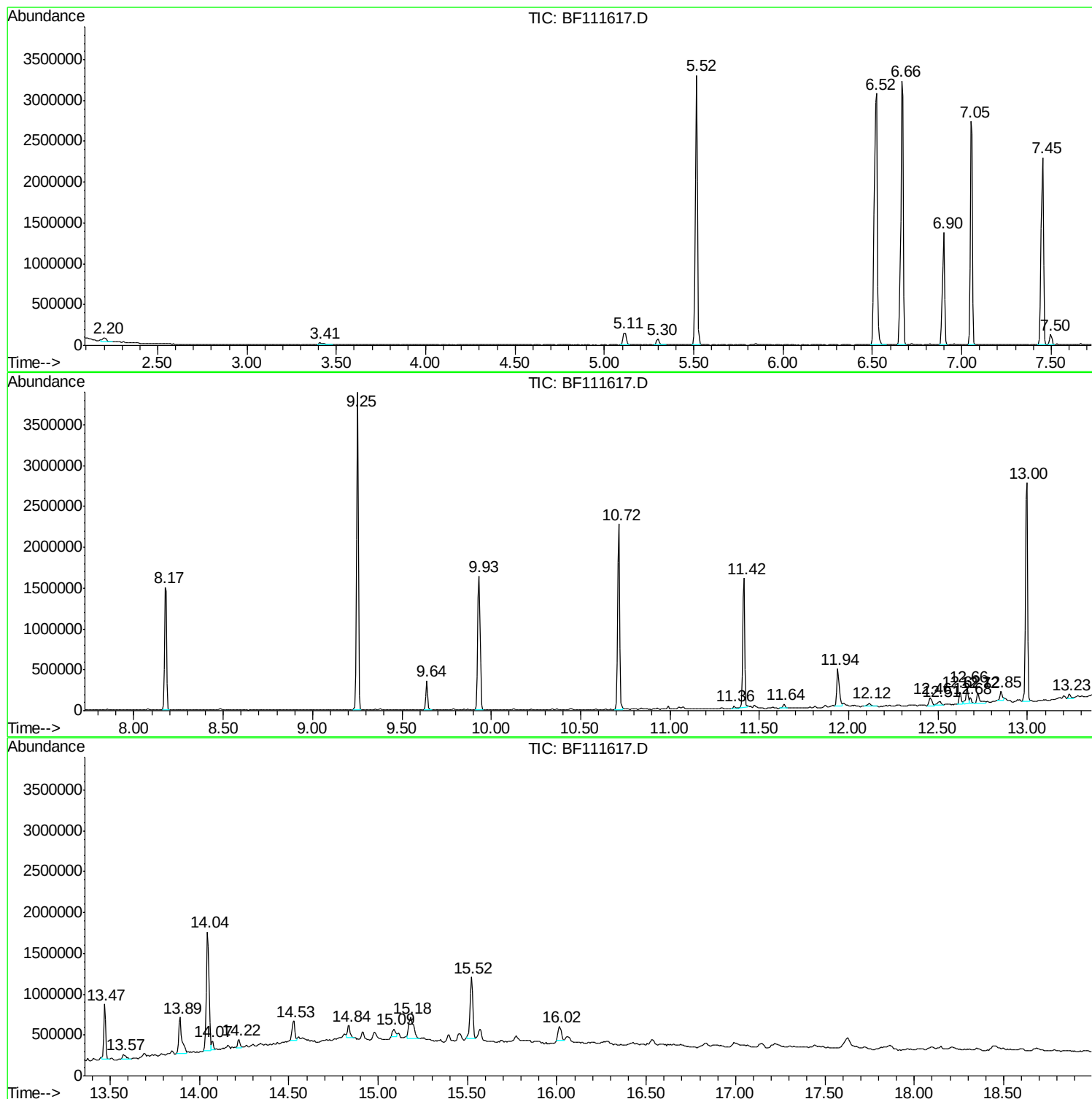
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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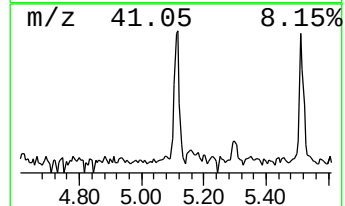
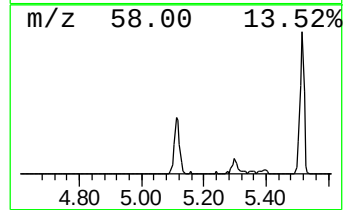
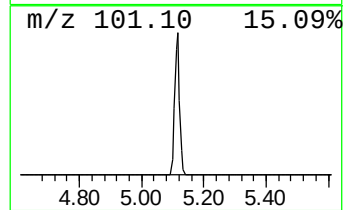
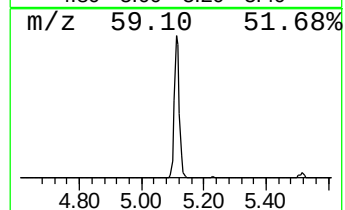
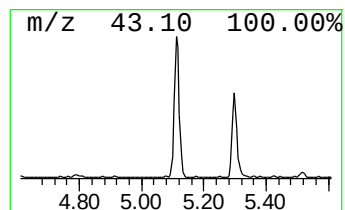
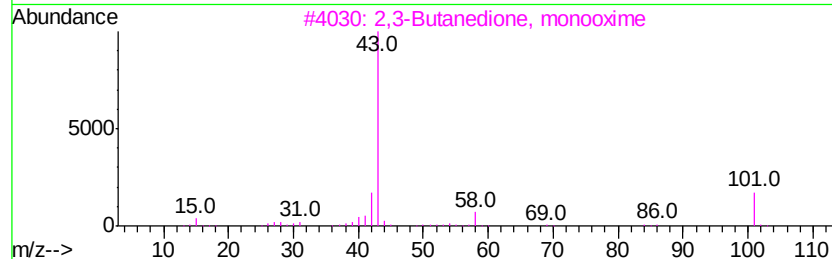
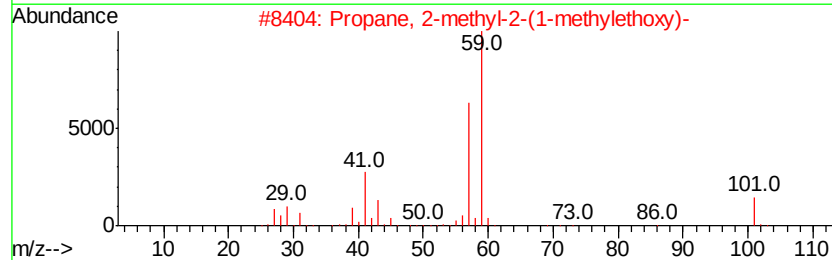
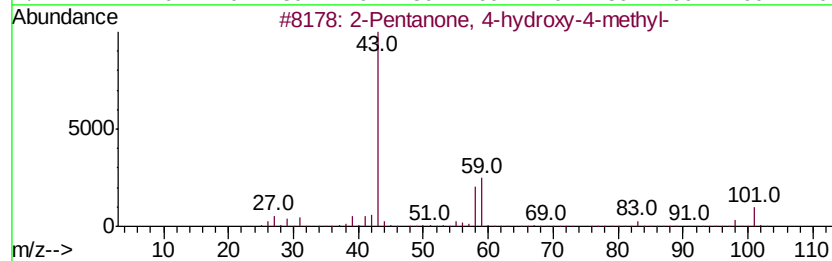
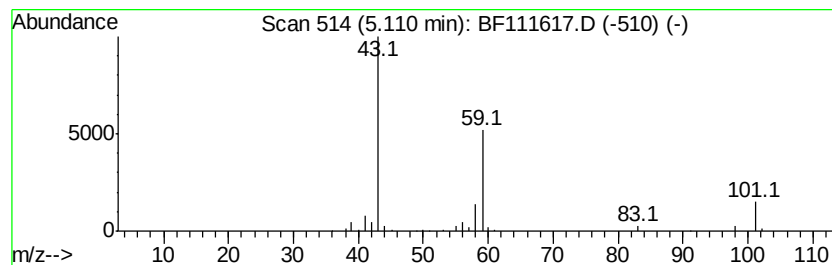
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.01 ng	168463	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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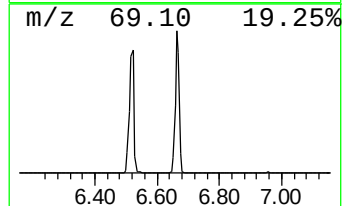
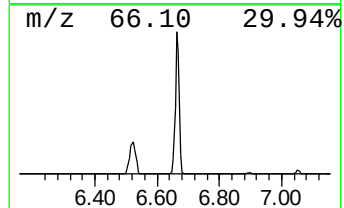
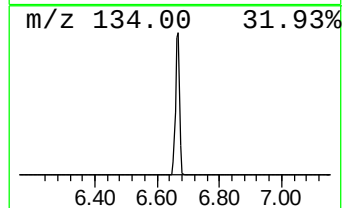
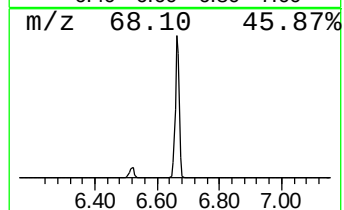
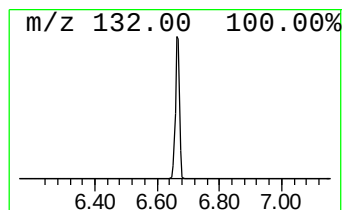
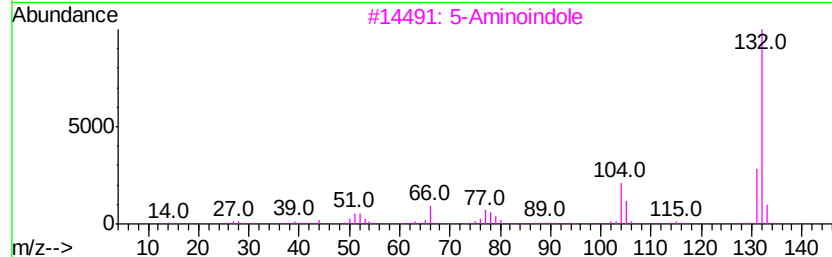
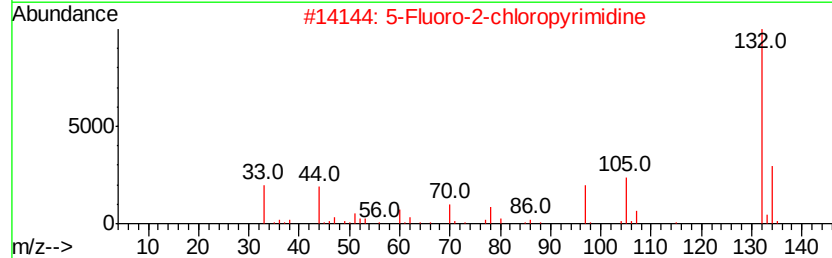
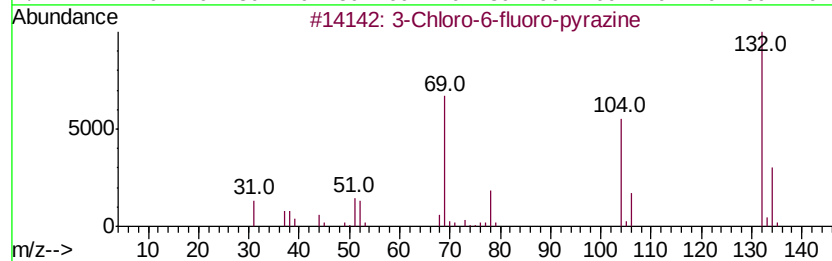
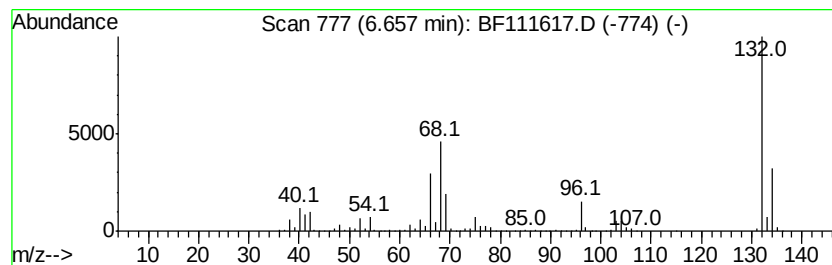
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	55.42 ng	3099780	1,4-Dichlorobenzene-d4	6.90

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	12		
3	5-Aminoindole	132	C8H8N2	005192-03-0	12		
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9		
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9		



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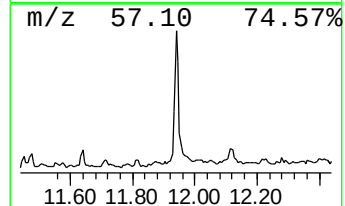
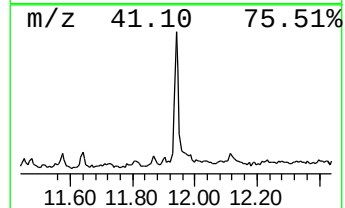
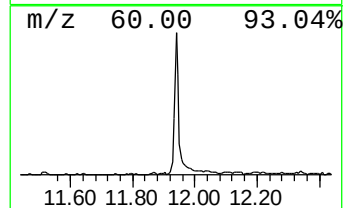
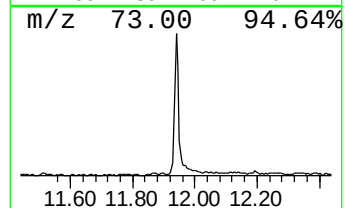
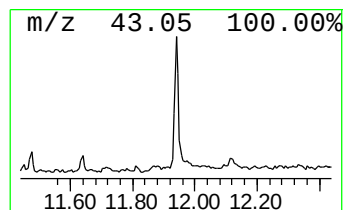
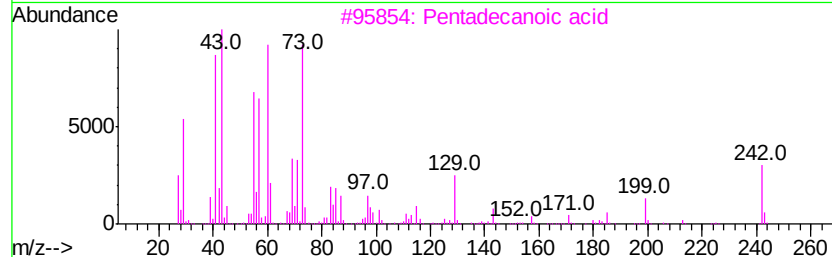
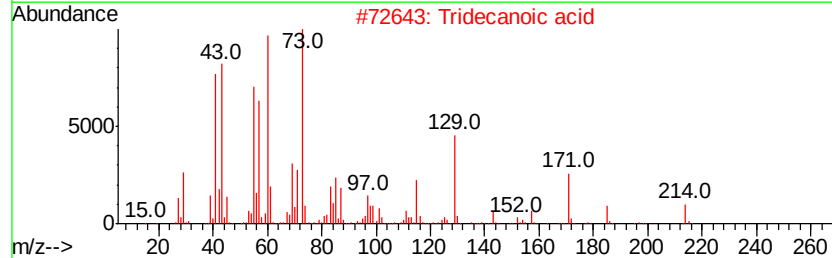
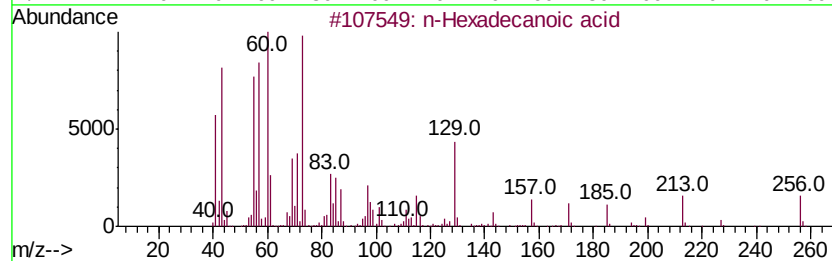
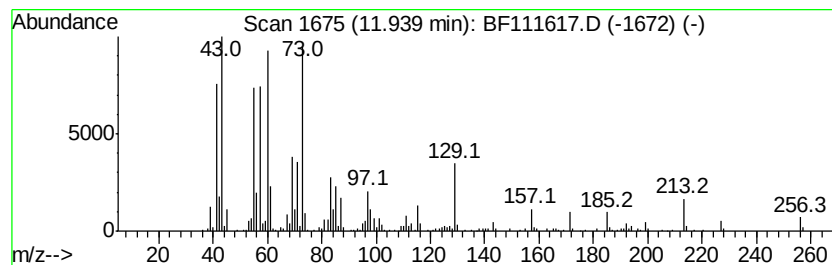
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.94	6.29 ng	426338	Phenanthrene-d10		11.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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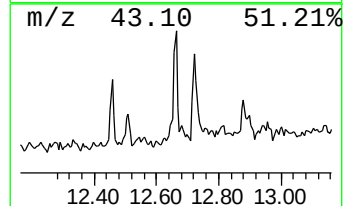
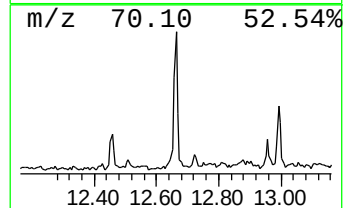
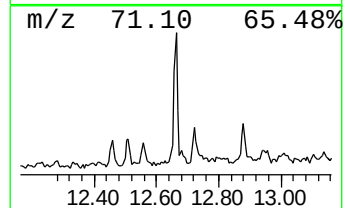
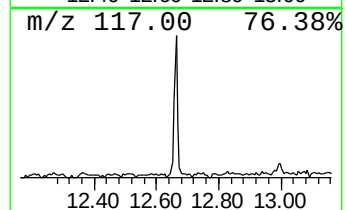
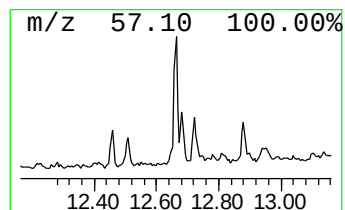
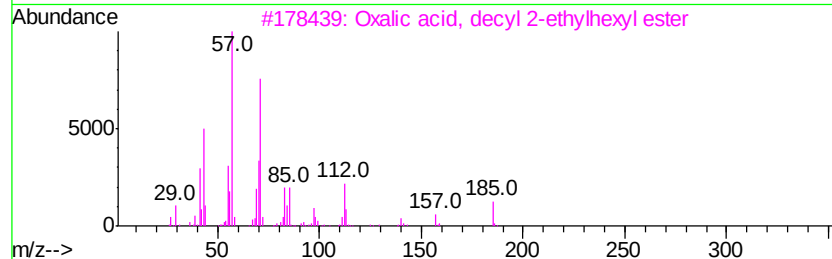
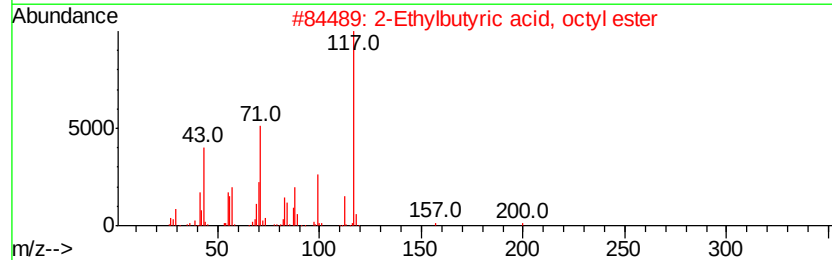
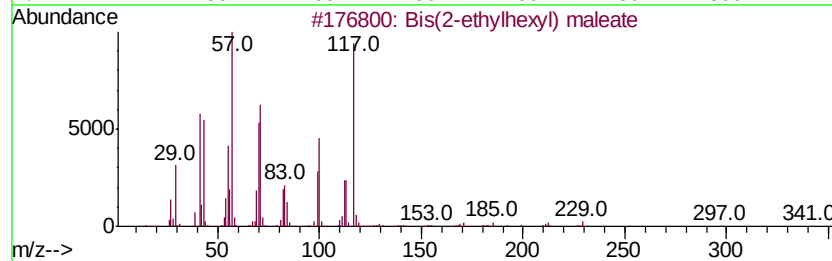
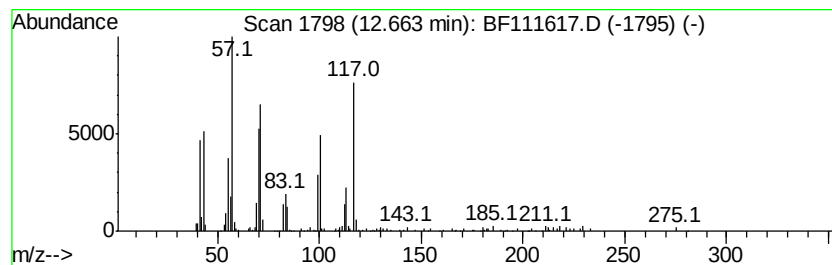
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.66	2.68 ng	181495	Phenanthrene-d10	11.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	90
2		2-Ethylbutyric acid, octyl ester	228	C14H28O2	1000340-24-3	47
3		Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	27
4		Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	27
5		Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	27



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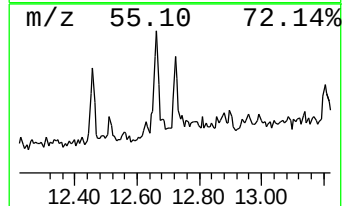
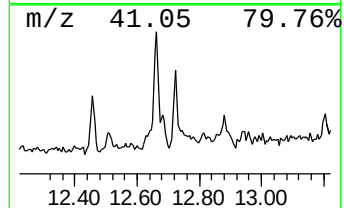
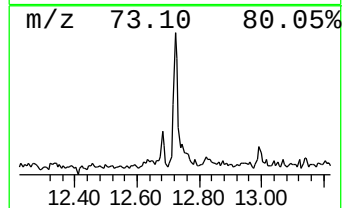
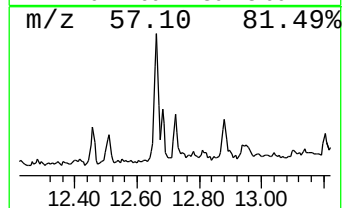
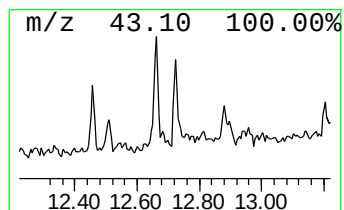
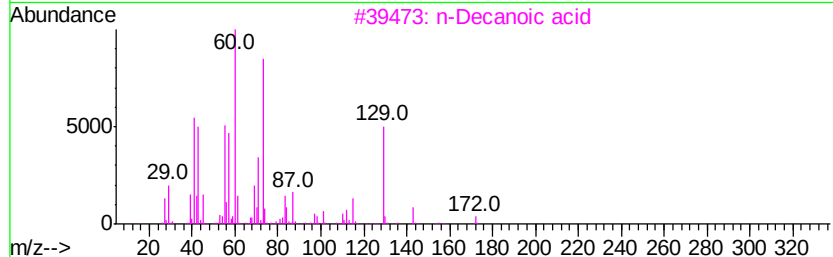
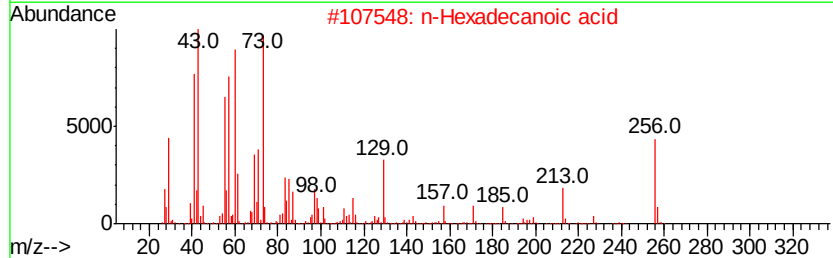
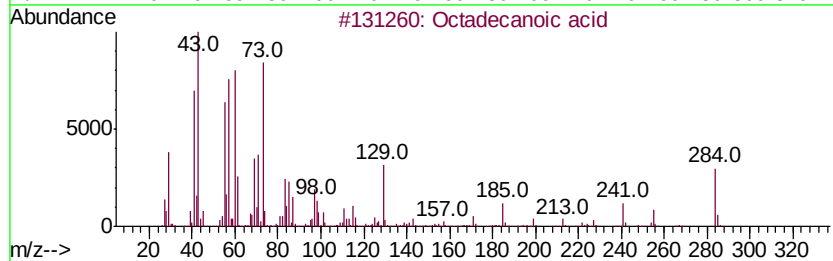
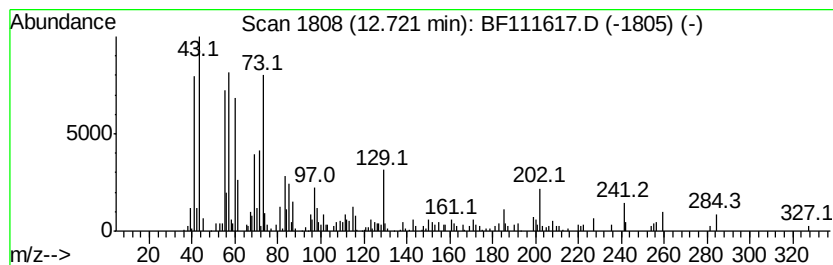
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.72	2.63 ng	178224	Phenanthrene-d10		11.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
Data File : BF111617.D
Acq On : 20 Dec 2018 3:42
Operator : JU/SJ
Sample : J6386-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

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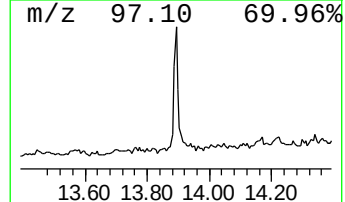
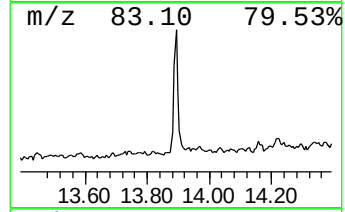
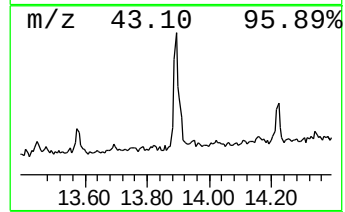
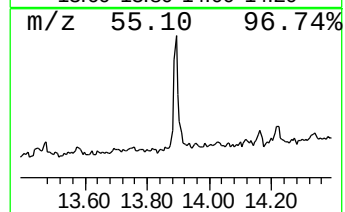
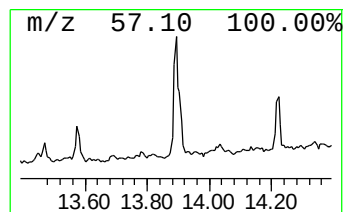
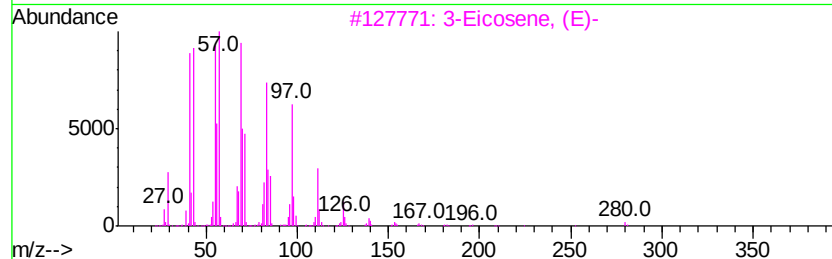
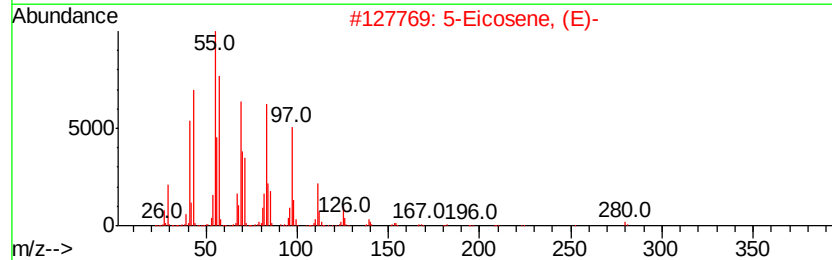
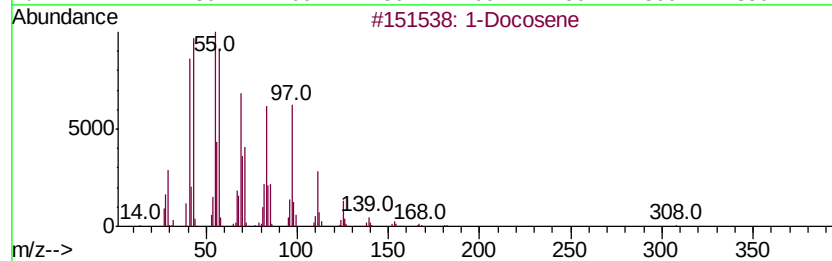
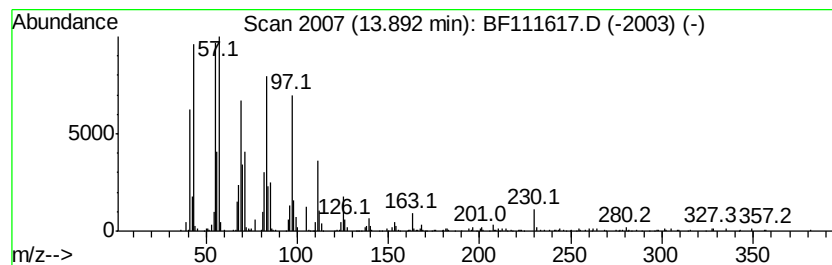
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.92 ng	568671	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	99
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	98
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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Sample : J6386-05
Misc :
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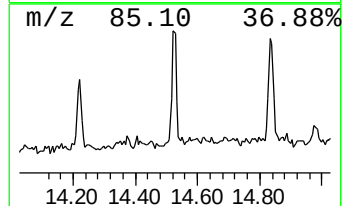
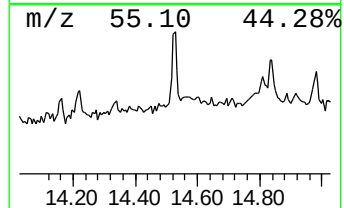
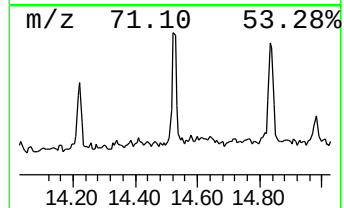
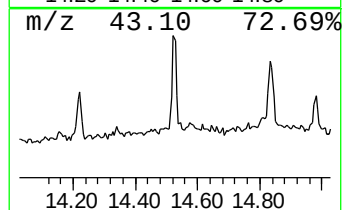
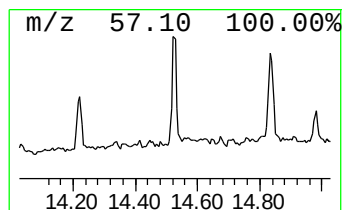
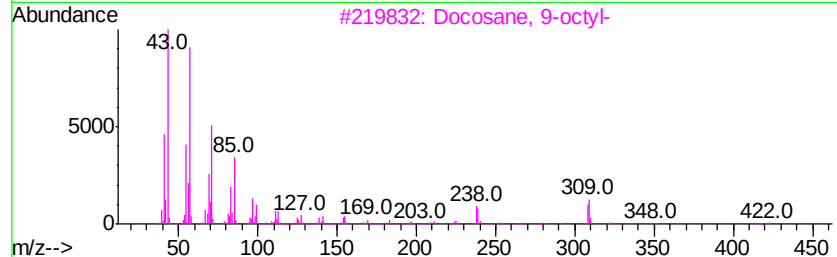
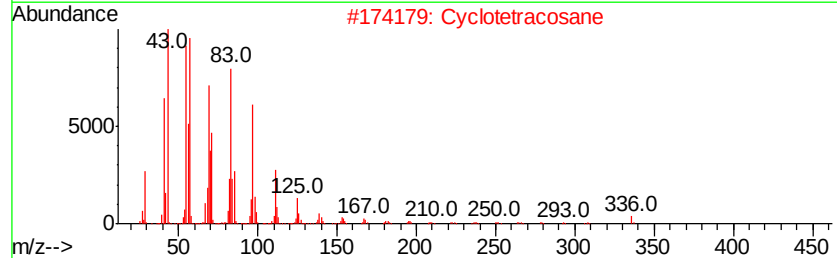
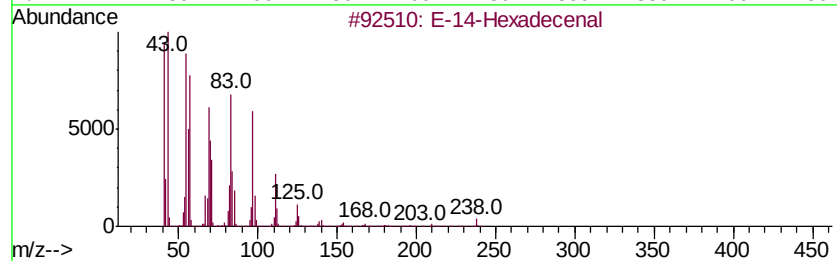
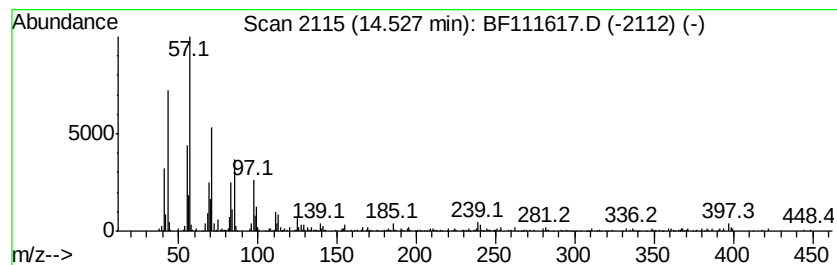
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-14-Hexadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	3.31 ng	237406	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-14-Hexadecenal	238 C16H30O	330207-53-9	94
2	Cyclotetracosane	336 C24H48	000297-03-0	94
3	Docosane, 9-octyl-	422 C30H62	055319-83-0	90
4	Heptadecane	240 C17H36	000629-78-7	86
5	9-Eicosene, (E)-	280 C20H40	074685-29-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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Sample : J6386-05
Misc :
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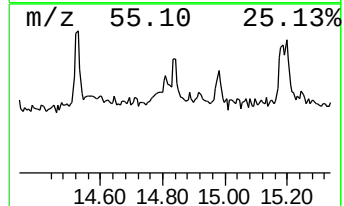
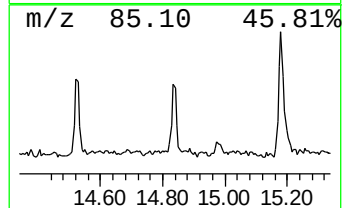
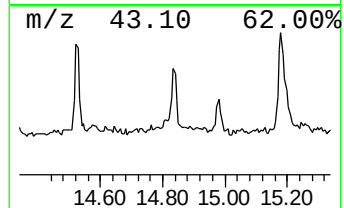
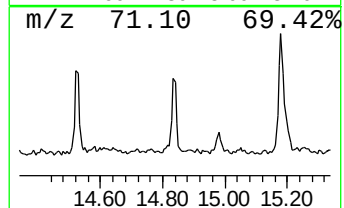
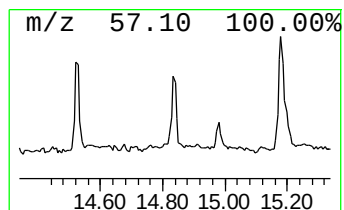
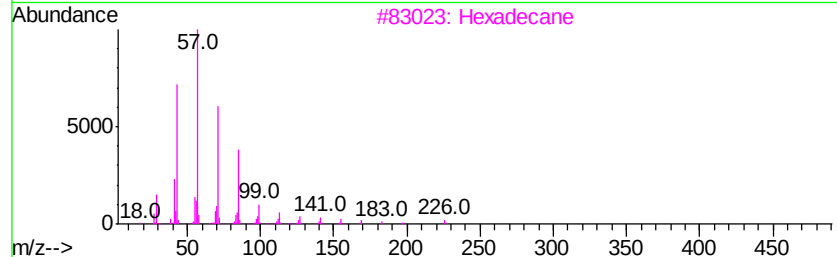
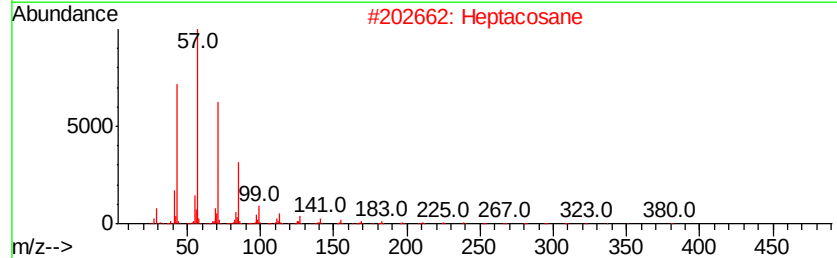
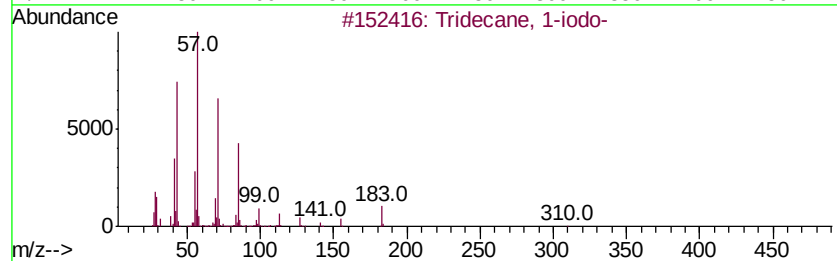
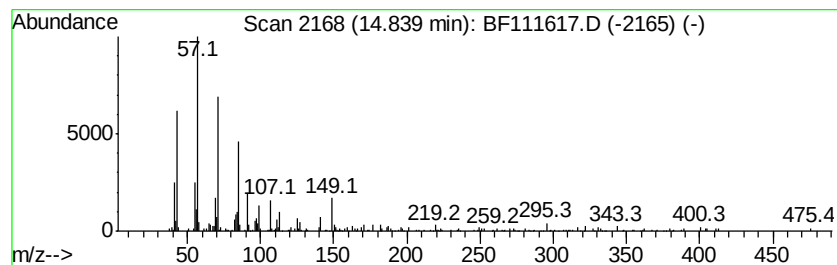
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.84	3.80 ng	164263	Perylene-d12	15.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	89
2	Heptacosane	380	C27H56	000593-49-7	64
3	Hexadecane	226	C16H34	000544-76-3	64
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5	Hexacosane	366	C26H54	000630-01-3	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121918\
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Sample : J6386-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

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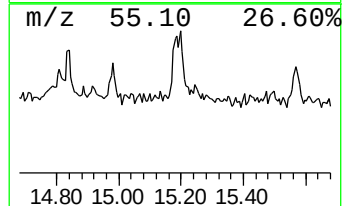
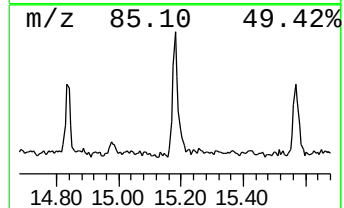
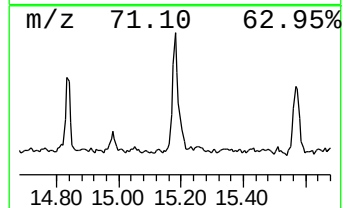
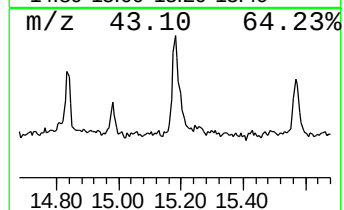
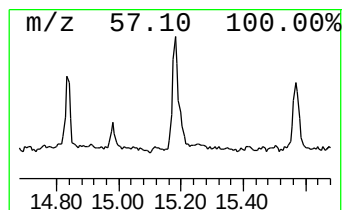
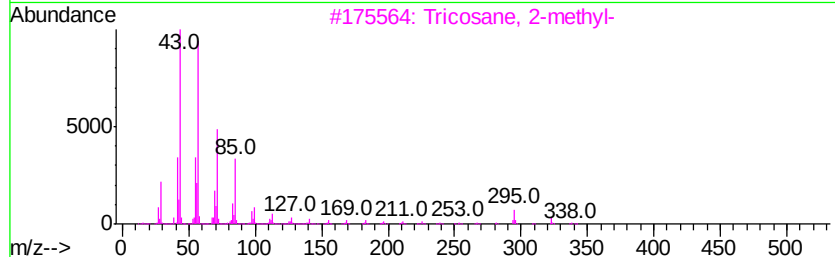
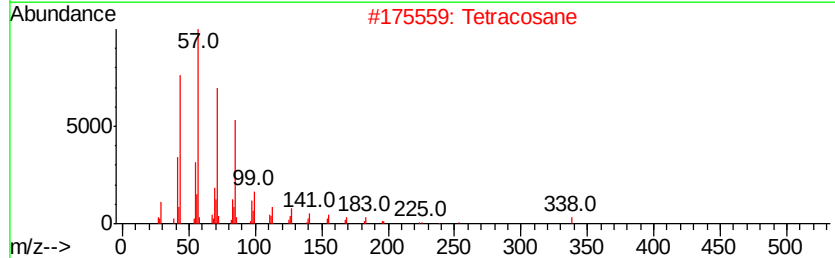
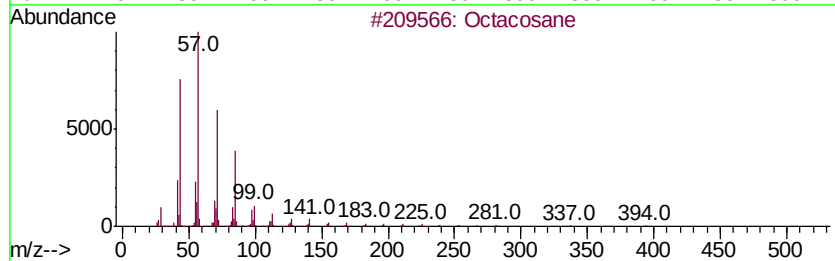
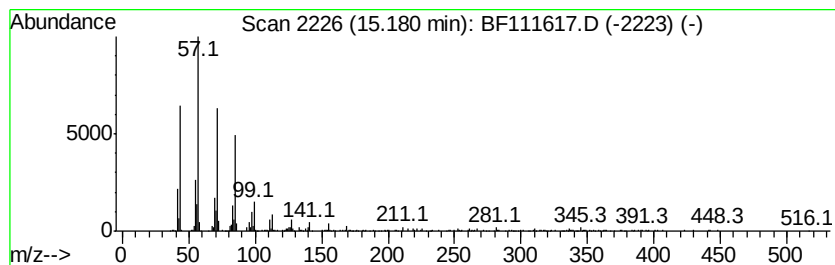
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	10.61 ng	459073	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	94
2		Tetracosane	338	C24H50	000646-31-1	93
3		Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
4		Eicosane	282	C20H42	000112-95-8	93
5		Docosane	310	C22H46	000629-97-0	93



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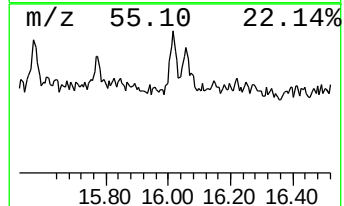
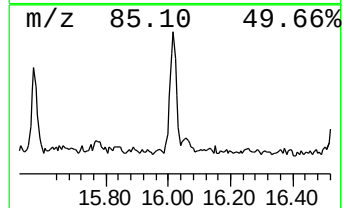
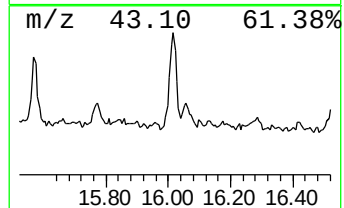
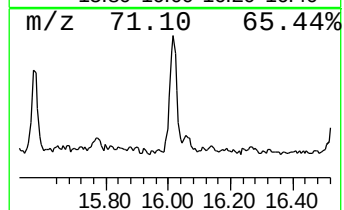
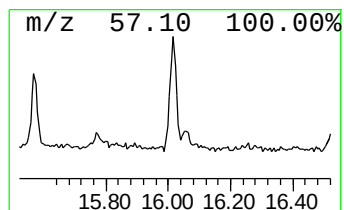
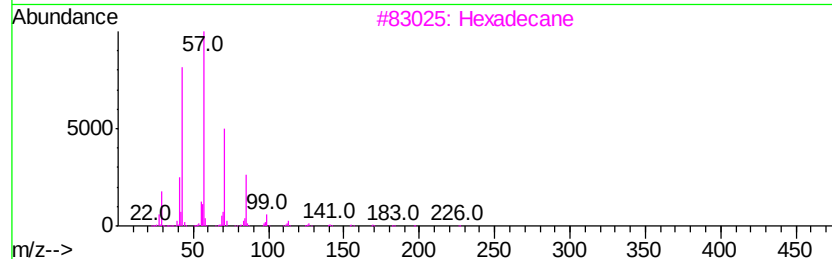
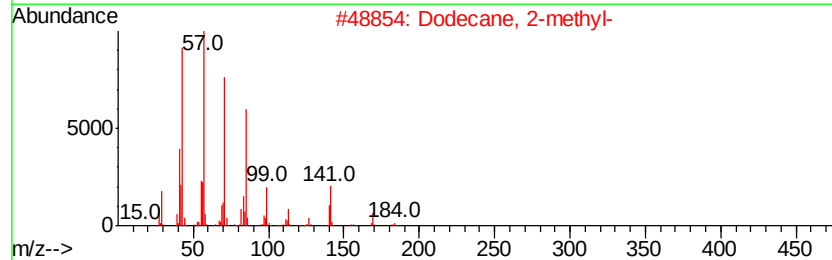
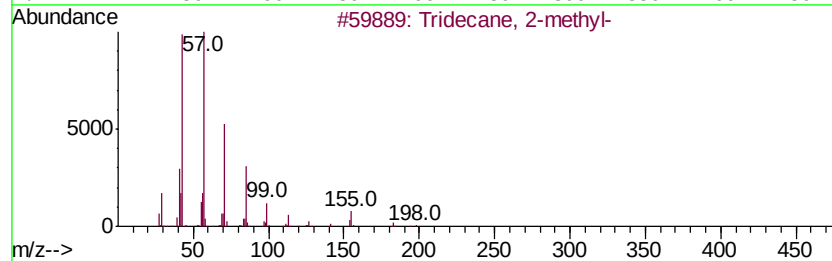
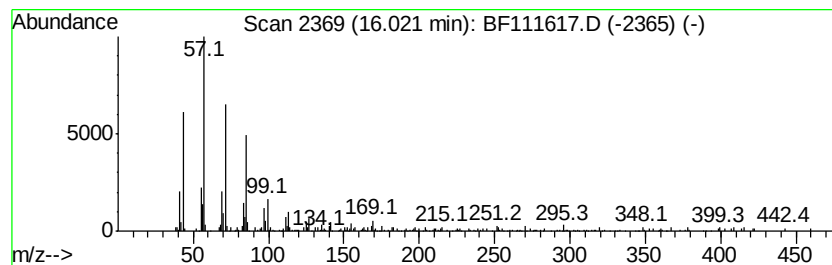
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.02	4.62 ng	200087	Perylene-d12	15.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	81
3	Hexadecane	226	C16H34	000544-76-3	80
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
5	Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	80



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ALS Vial : 21 Sample Multiplier: 1

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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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unknown6.66	6.66	55.4	ng	3099780	1	6.90	1118710	20.0
n-Hexadecanoic acid	11.94	6.3	ng	426338	4	11.42	1356410	20.0
Bis(2-ethylhexyl)...	12.66	2.7	ng	181495	4	11.42	1356410	20.0
Octadecanoic acid	12.72	2.6	ng	178224	4	11.42	1356410	20.0
1-Docosene	13.89	7.9	ng	568671	5	14.04	1436630	20.0
E-14-Hexadecenal	14.53	3.3	ng	237406	5	14.04	1436630	20.0
Tridecane, 1-iodo-	14.84	3.8	ng	164263	6	15.52	865554	20.0
Octacosane	15.18	10.6	ng	459073	6	15.52	865554	20.0
Tridecane, 2-methyl-	16.02	4.6	ng	200087	6	15.52	865554	20.0