

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
 Data File : BF114156.D
 Acq On : 11 May 2019 14:54
 Operator : JU/SJ
 Sample : K2763-09
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS006-0206-01

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-BF051019.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	2.140	3	9	40	rVB	1871318	2941362	34.08%	3.562%
2	5.087	507	510	519	rVB	76119	99843	1.16%	0.121%
3	5.481	572	577	580	rBV	7821163	8041301	93.17%	9.739%
4	6.492	743	749	752	rBV	8066531	8630716	100.00%	10.453%
5	6.628	767	772	775	rBV	8198381	8244471	95.52%	9.985%
6	6.851	806	810	819	rVB	2215056	1836263	21.28%	2.224%
7	7.010	832	837	840	rBV	7026448	6287154	72.85%	7.614%
8	7.410	900	905	908	rBV	5742672	5731394	66.41%	6.941%
9	8.128	1023	1027	1031	rBV	2598454	2243108	25.99%	2.717%
10	8.816	1141	1144	1151	rBV	94384	103602	1.20%	0.125%
11	9.204	1205	1210	1213	rBV	8737549	8291983	96.08%	10.043%
12	9.592	1273	1276	1280	rBV	1146149	873969	10.13%	1.058%
13	9.880	1321	1325	1329	rBV	2875042	2675711	31.00%	3.241%
14	10.674	1455	1460	1463	rBV	5644468	5641876	65.37%	6.833%
15	11.369	1573	1578	1581	rBV	3038979	2849282	33.01%	3.451%
16	11.892	1664	1667	1671	rBV	1048475	982139	11.38%	1.189%
17	12.598	1785	1787	1793	rVV	149539	155983	1.81%	0.189%
18	12.674	1797	1800	1811	rVV2	349156	425966	4.94%	0.516%
19	12.951	1842	1847	1850	rBV	7124095	6661982	77.19%	8.068%
20	13.474	1933	1936	1939	rBV	136943	121010	1.40%	0.147%
21	13.792	1986	1990	1995	rBV4	125740	151158	1.75%	0.183%
22	13.839	1995	1998	2009	rVV	1148062	1376553	15.95%	1.667%
23	14.004	2020	2026	2029	rBV	2106529	1893530	21.94%	2.293%
24	14.168	2050	2054	2062	rBV2	186623	223568	2.59%	0.271%
25	14.480	2103	2107	2113	rBV2	322542	416143	4.82%	0.504%
26	14.715	2144	2147	2152	rVB	108612	116426	1.35%	0.141%
27	14.762	2152	2155	2156	rBV	137754	134461	1.56%	0.163%
28	14.786	2156	2159	2166	rVB	277738	318373	3.69%	0.386%
29	14.927	2179	2183	2188	rBV	200470	197263	2.29%	0.239%
30	15.121	2211	2216	2218	rBV	494202	549916	6.37%	0.666%
31	15.145	2218	2220	2227	rVB2	199499	279388	3.24%	0.338%
32	15.362	2252	2257	2261	rBV4	53454	100612	1.17%	0.122%
33	15.474	2271	2276	2279	rBV	1498468	2005832	23.24%	2.429%
34	15.698	2310	2314	2320	rVB2	101902	145987	1.69%	0.177%

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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	15.933	2349	2354	2358	rBV	466620	665230	7.71%	0.806%
36	15.986	2358	2363	2370	rVV2	127051	254243	2.95%	0.308%
37	16.433	2434	2439	2445	rBV	209054	352981	4.09%	0.428%
38	16.721	2484	2488	2495	rVB4	82506	141619	1.64%	0.172%
39	17.027	2535	2540	2548	rVB2	97017	192093	2.23%	0.233%
40	17.274	2578	2582	2590	rVB7	104138	213974	2.48%	0.259%

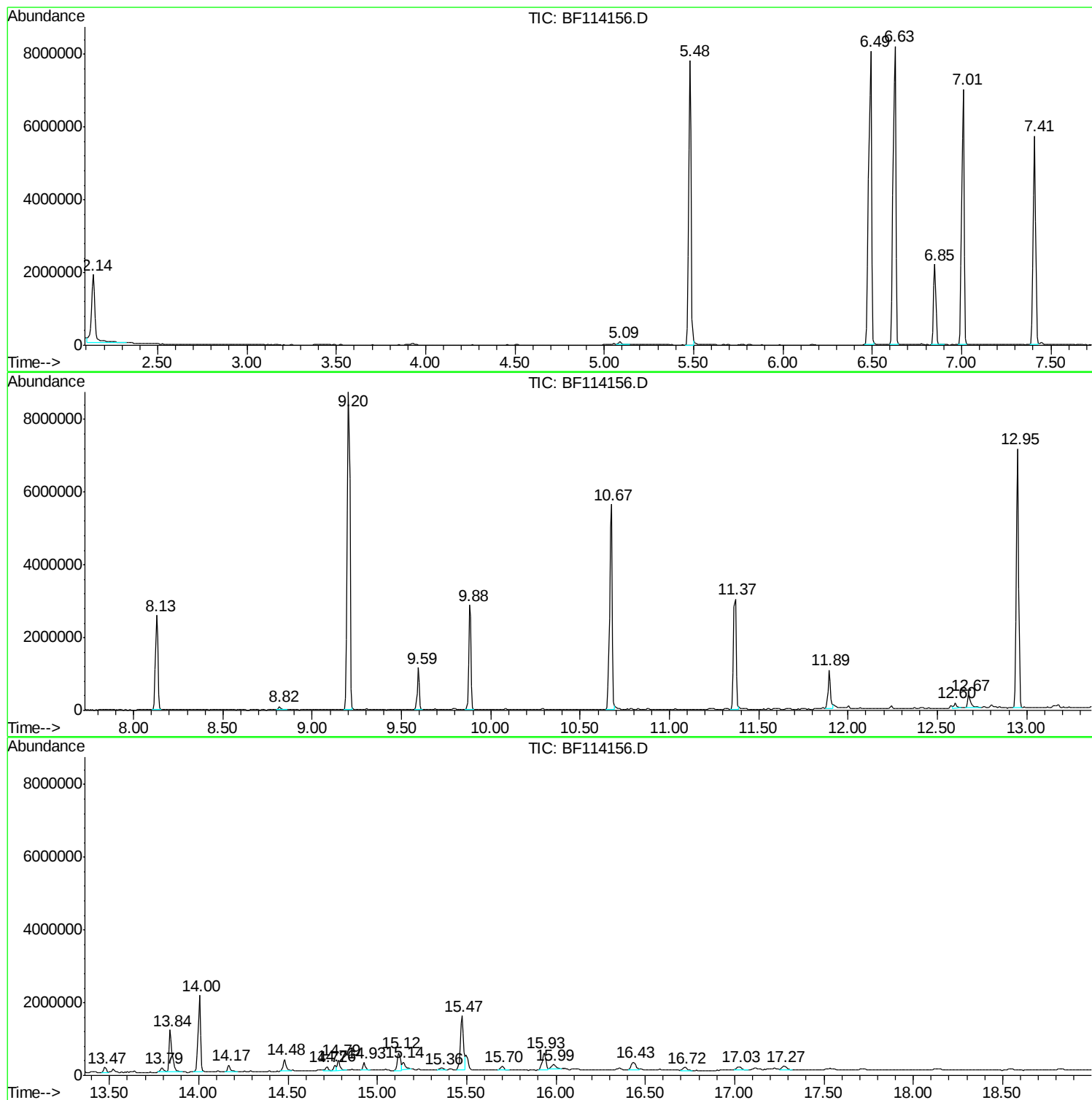
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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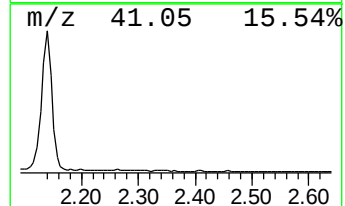
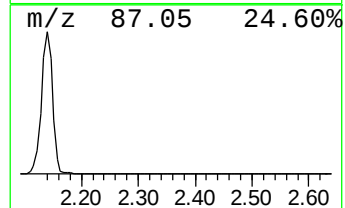
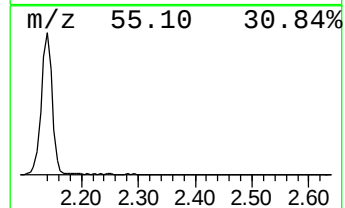
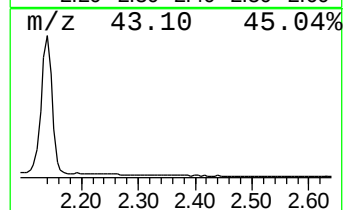
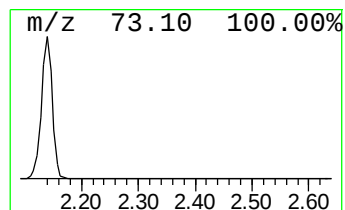
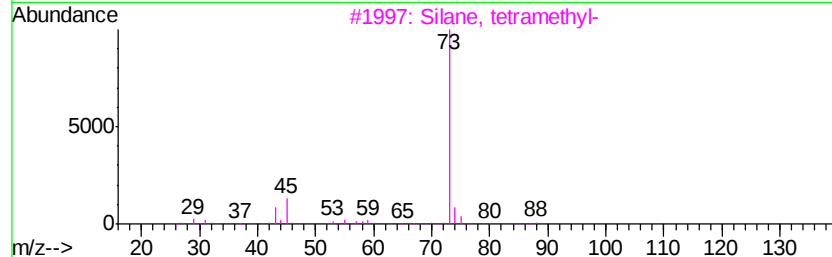
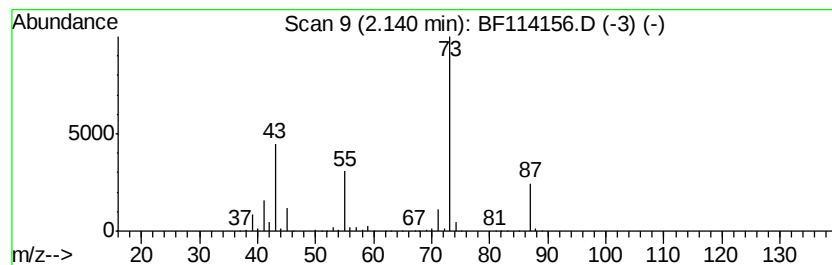
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	32.04 ng	2941360	1,4-Dichlorobenzene-d4	6.85

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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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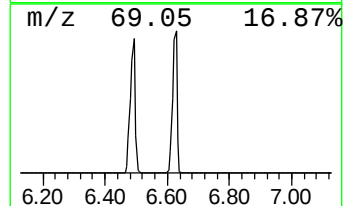
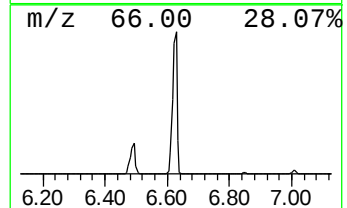
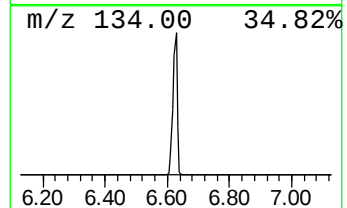
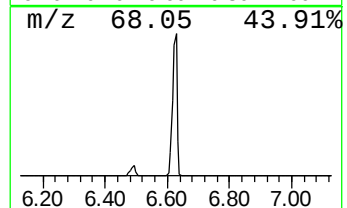
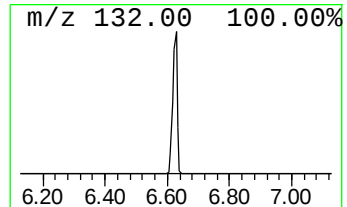
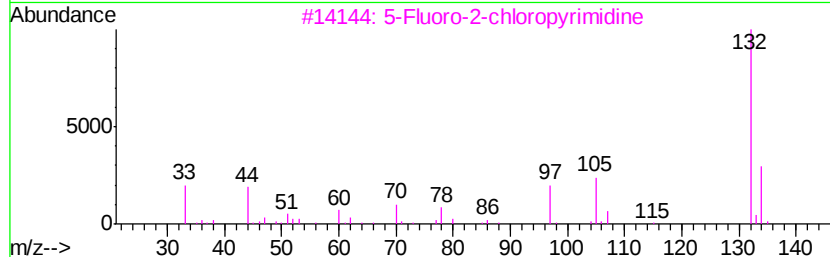
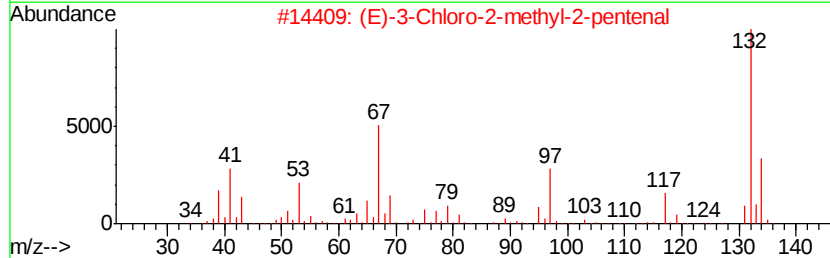
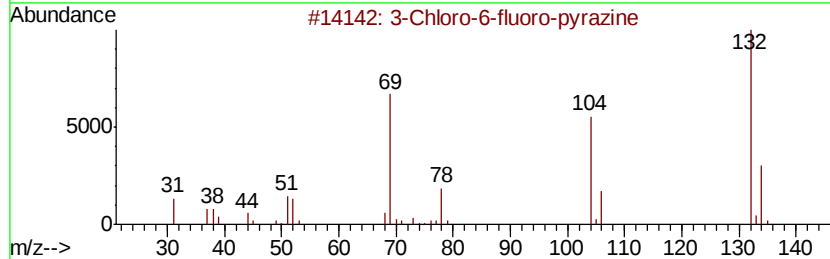
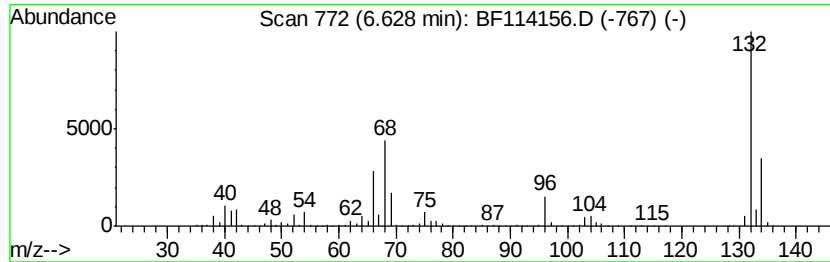
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.63	89.80 ng	8244470	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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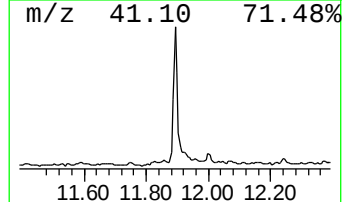
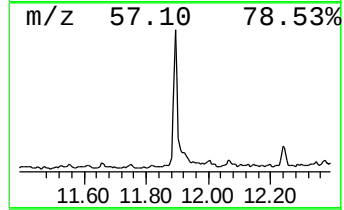
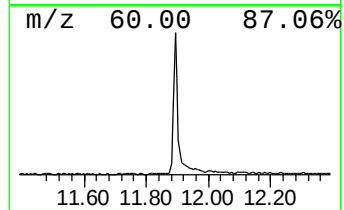
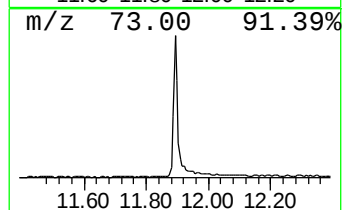
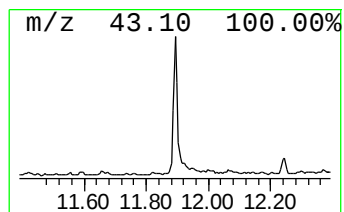
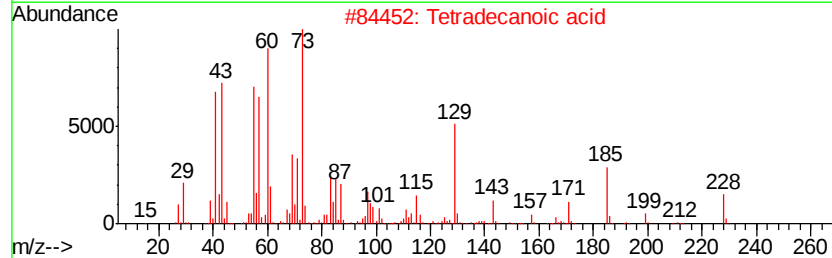
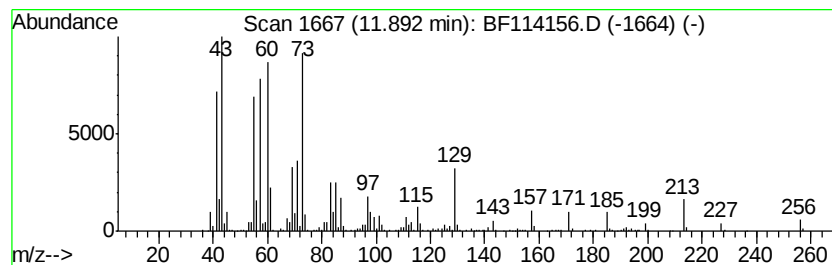
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	6.89 ng	982139	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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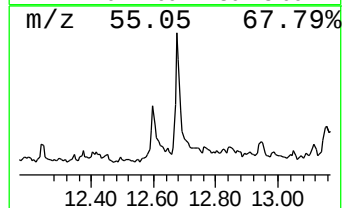
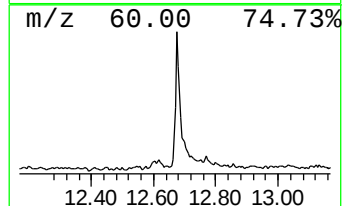
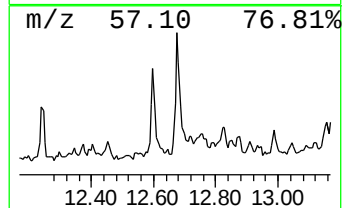
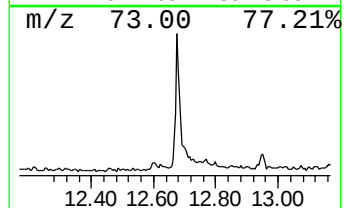
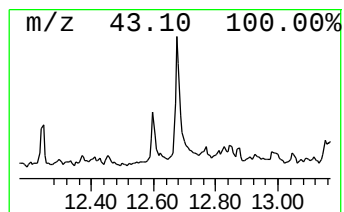
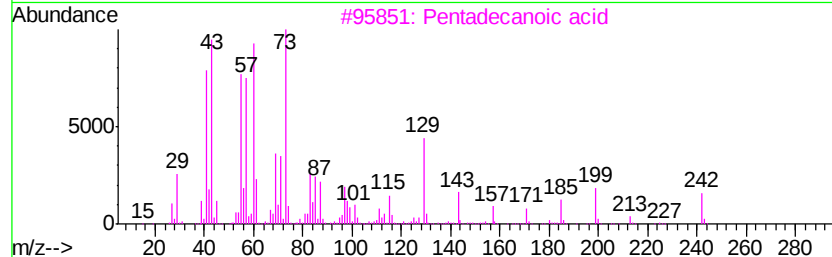
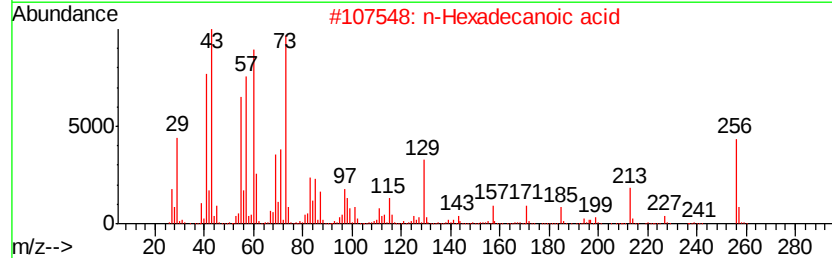
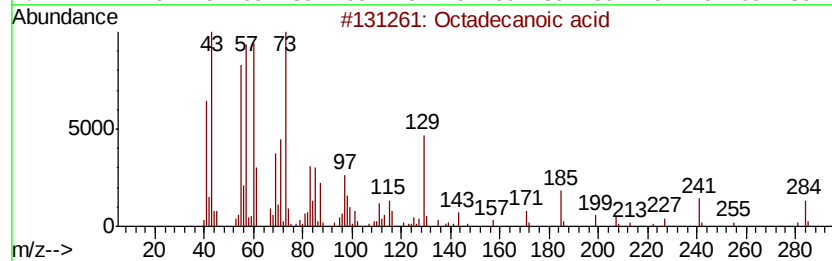
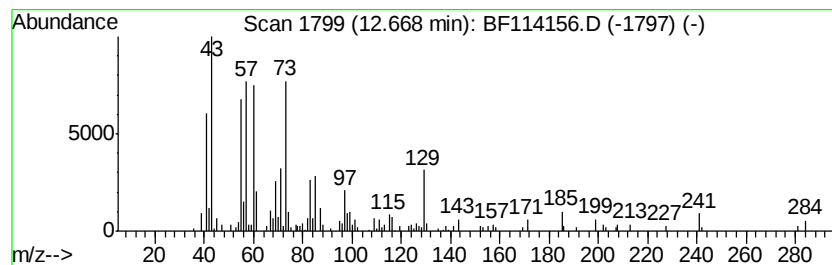
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.67	2.99 ng	425966	Phenanthrene-d10		11.37
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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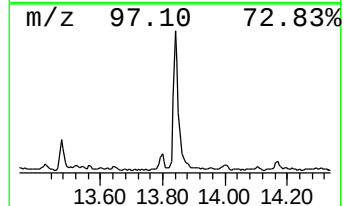
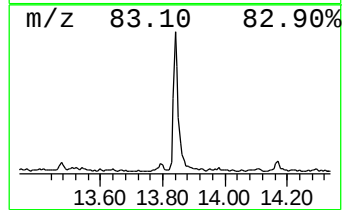
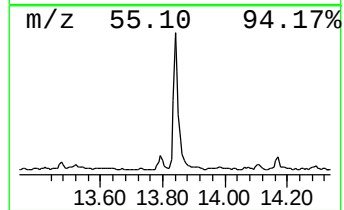
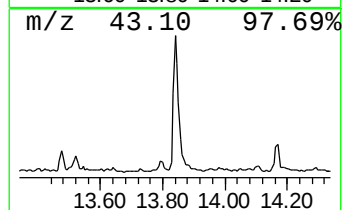
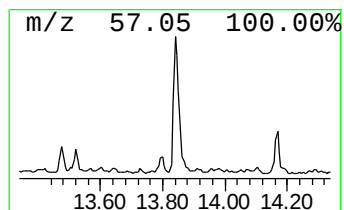
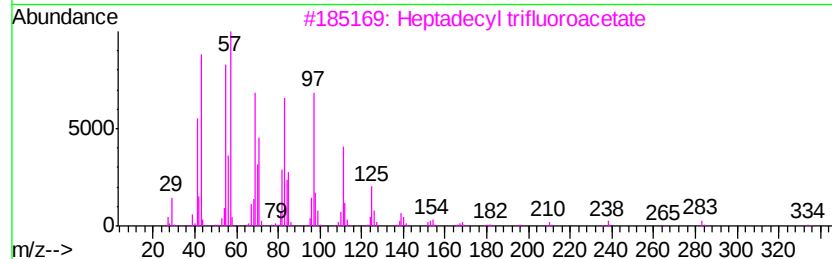
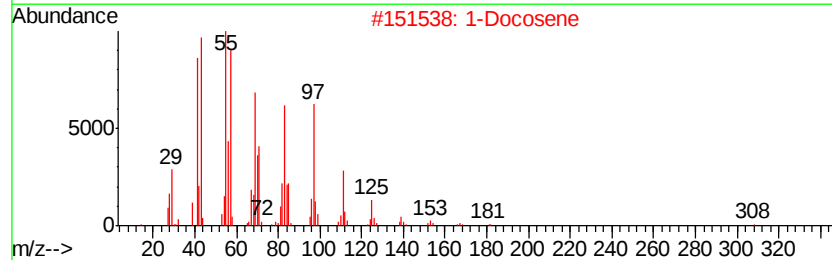
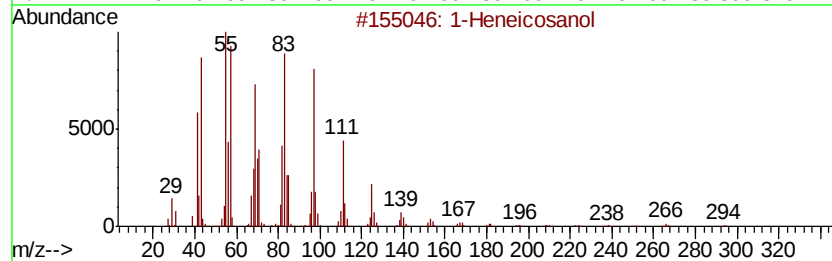
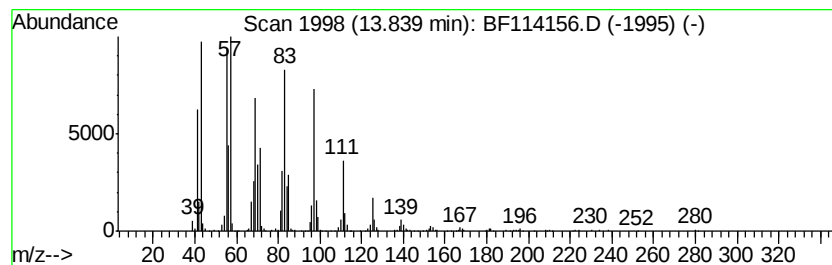
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	14.54 ng	1376550	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		1-Docosene	308	C22H44	001599-67-3	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



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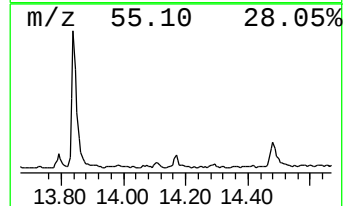
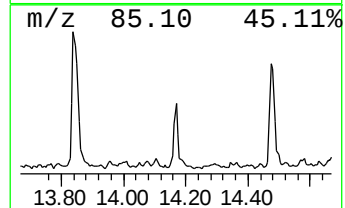
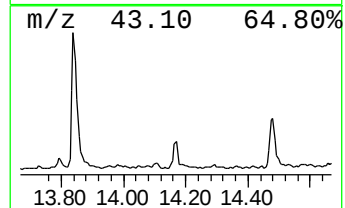
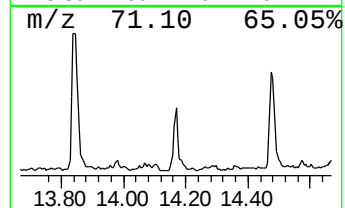
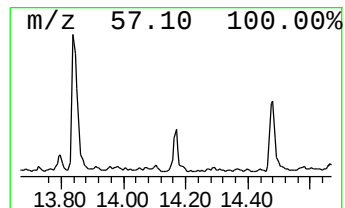
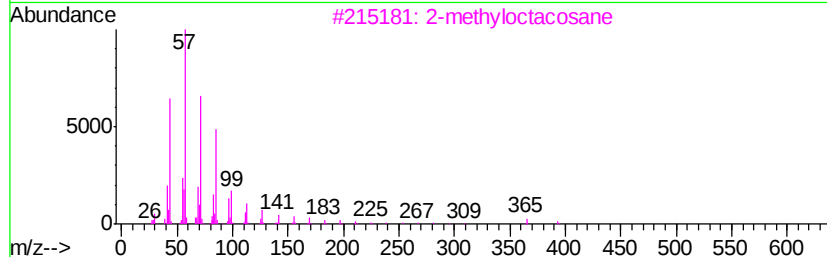
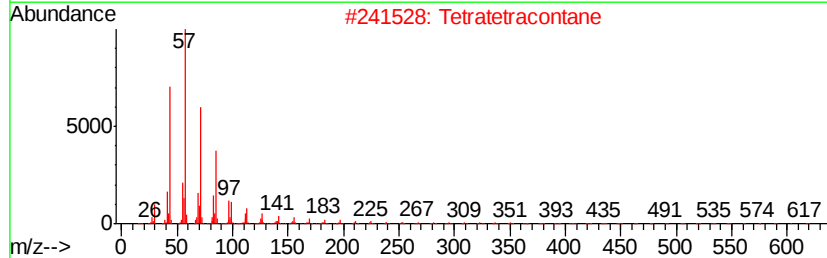
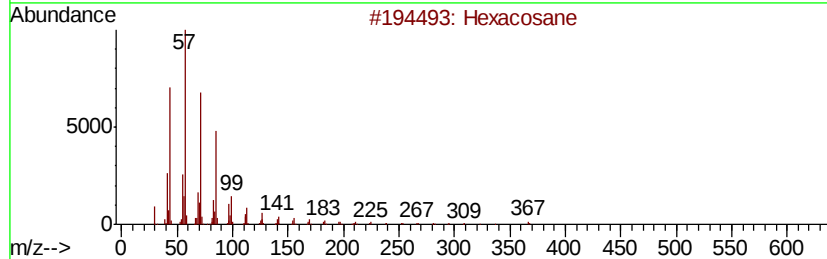
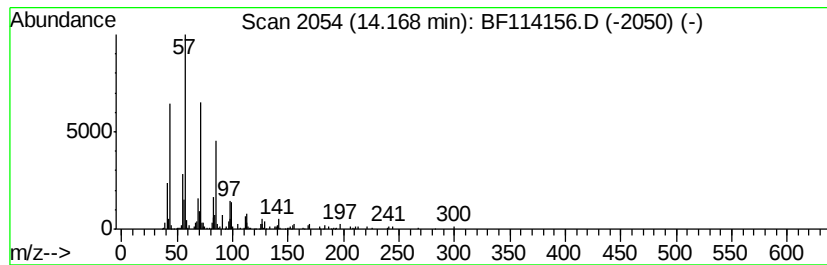
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	2.36 ng	223568	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Tetratetracontane	619	C44H90	007098-22-8	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Hexatriacontane	507	C36H74	000630-06-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114156.D
Acq On : 11 May 2019 14:54
Operator : JU/SJ
Sample : K2763-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

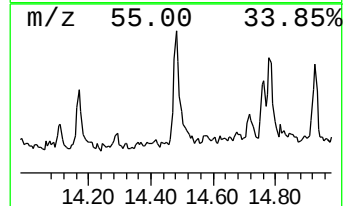
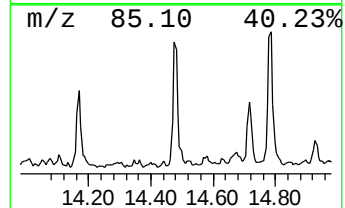
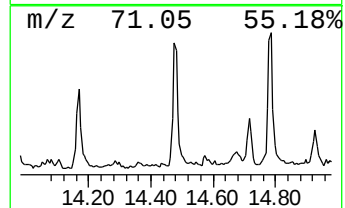
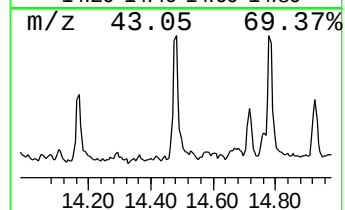
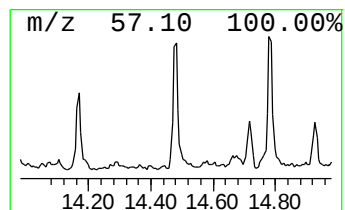
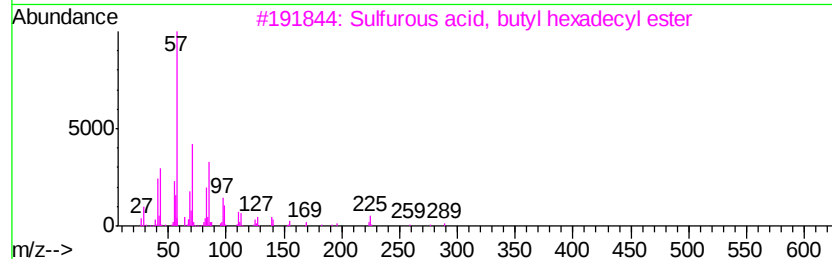
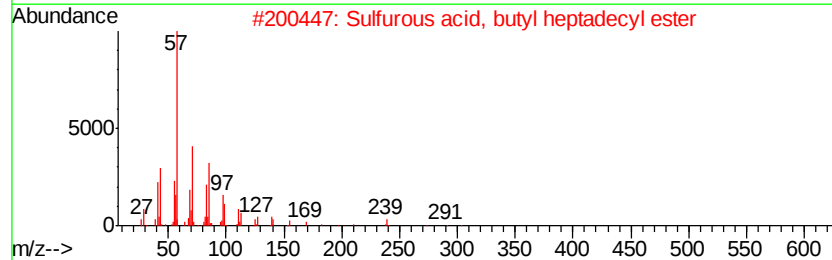
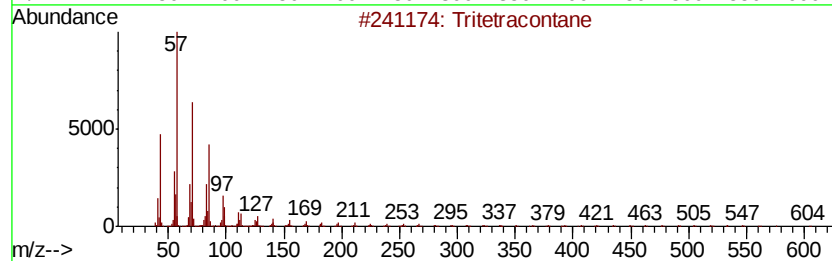
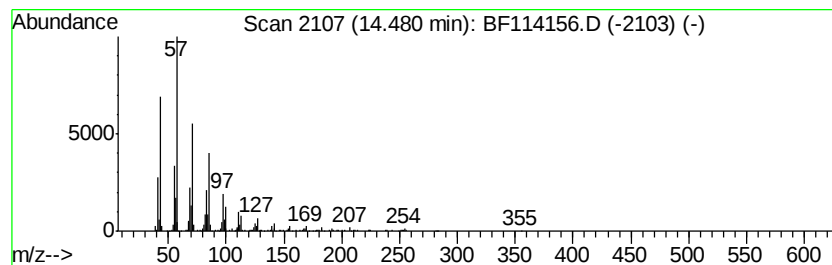
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	4.40 ng	416143	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tritetracontane	605 C43H88	007098-21-7 91
2		Sulfurous acid, butyl heptadecyl...	376 C21H44O3S	1000309-18-4 91
3		Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3 91
4		Sulfurous acid, butyl tetradecyl...	334 C18H38O3S	1000309-18-1 87
5		Tetratetracontane	619 C44H90	007098-22-8 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
 Data File : BF114156.D
 Acq On : 11 May 2019 14:54
 Operator : JU/SJ
 Sample : K2763-09
 Misc :
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Instrument :
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 ClientSampleId :
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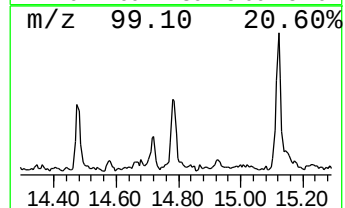
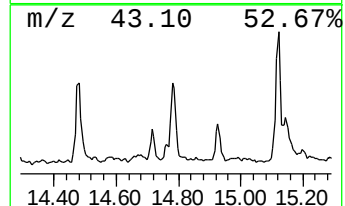
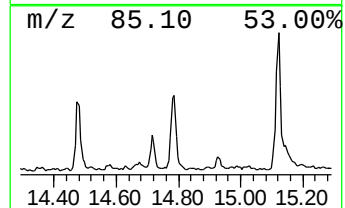
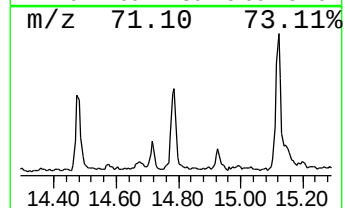
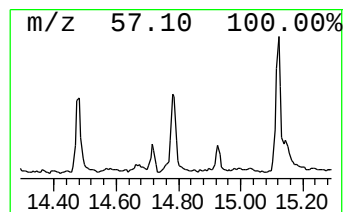
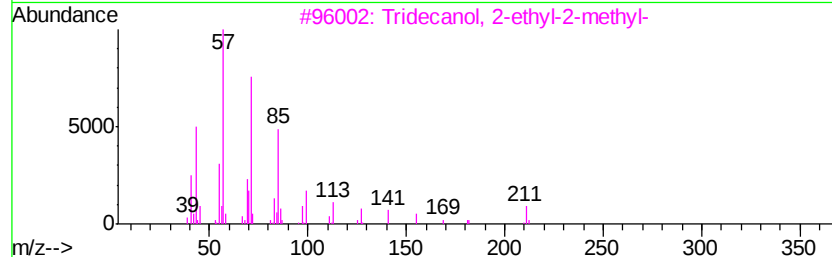
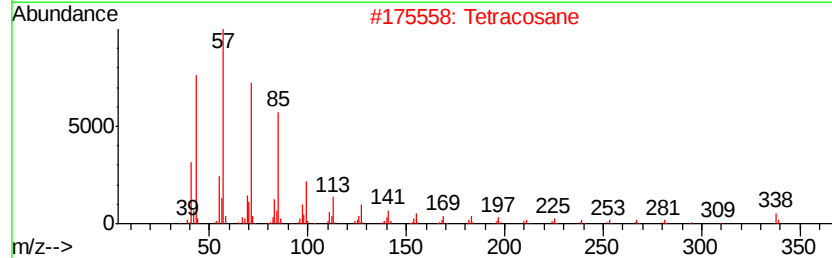
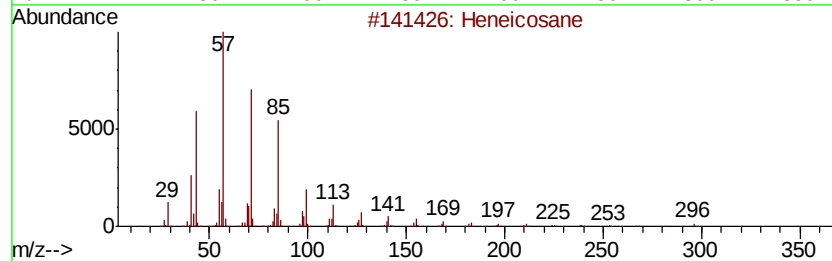
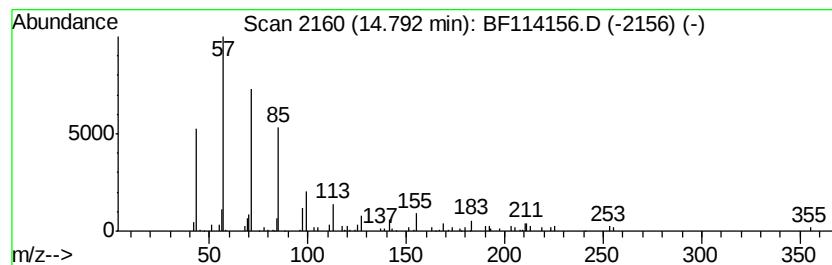
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.17 ng	318373	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Tetracosane		338	C24H50	000646-31-1	90
3	Tridecanol, 2-ethyl-2-methyl-		242	C16H34O	1000115-66-1	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114156.D
Acq On : 11 May 2019 14:54
Operator : JU/SJ
Sample : K2763-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

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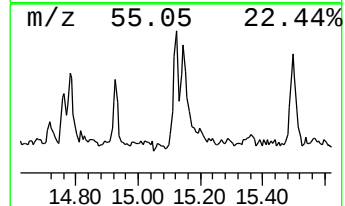
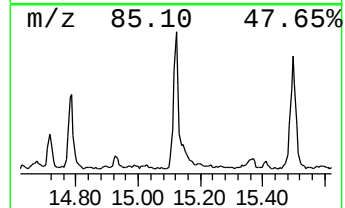
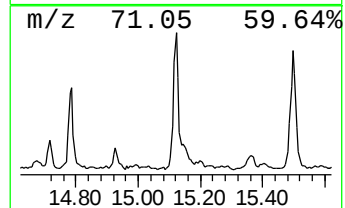
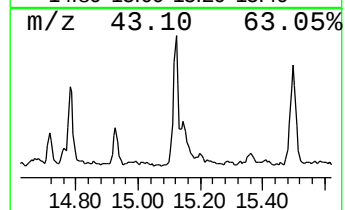
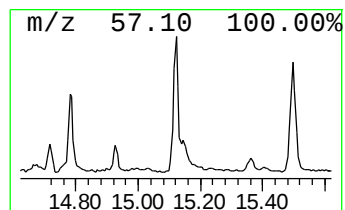
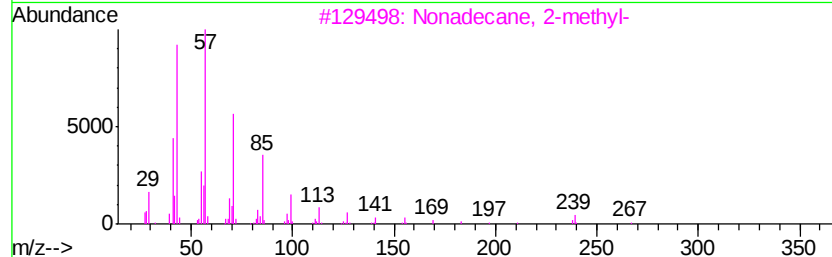
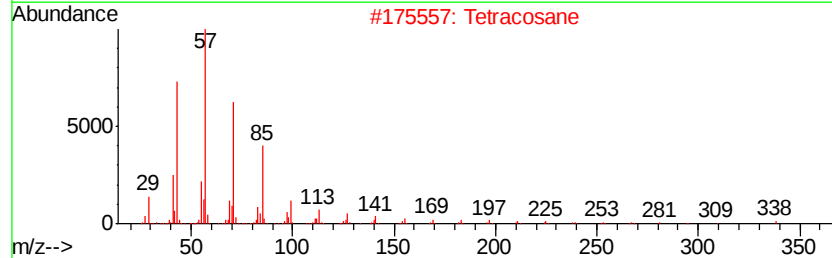
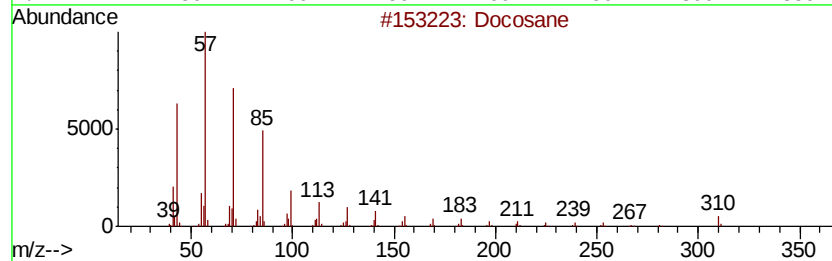
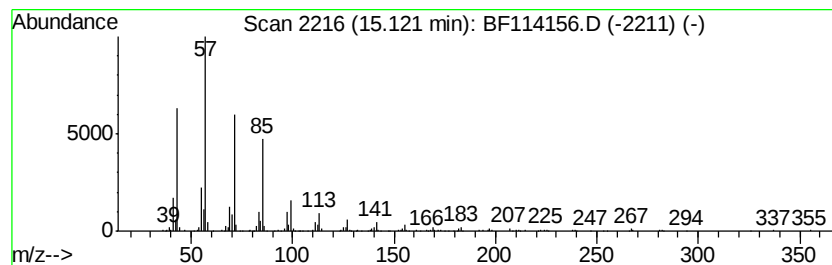
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	5.48 ng	549916	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4		Pentadecane	212	C15H32	000629-62-9	83
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114156.D
Acq On : 11 May 2019 14:54
Operator : JU/SJ
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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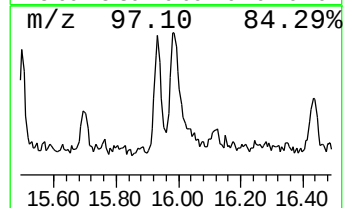
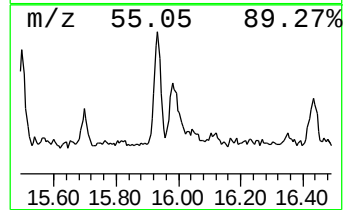
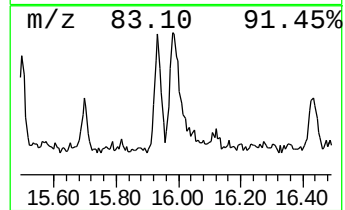
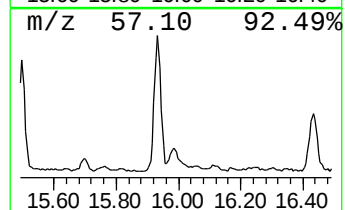
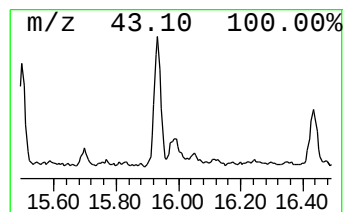
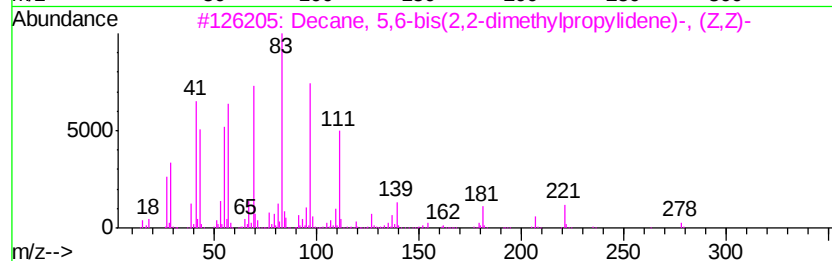
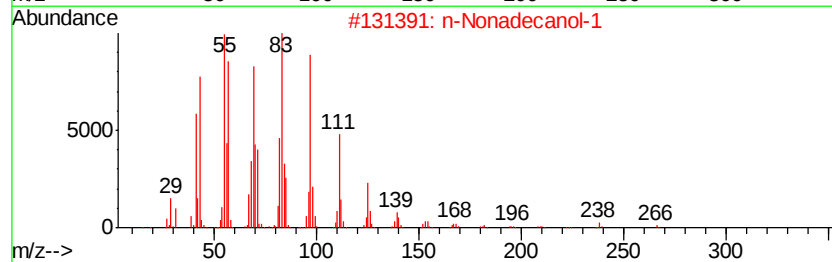
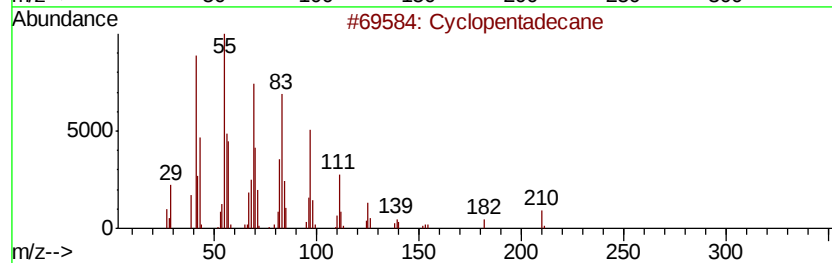
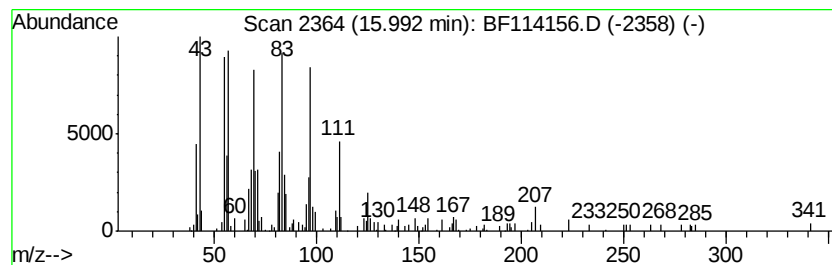
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cyclopentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.54 ng	254243	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	93
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3		Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	76
4		1-Octadecanol	270	C18H38O	000112-92-5	76
5		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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Sample : K2763-09
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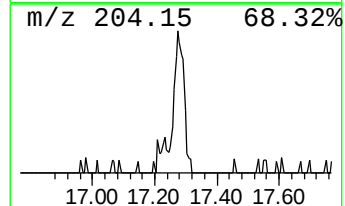
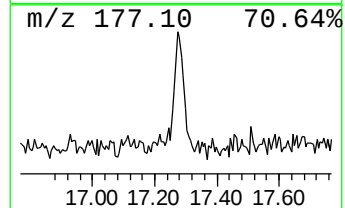
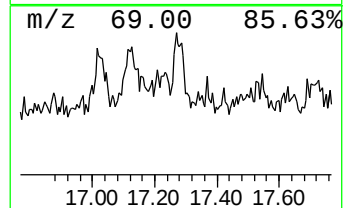
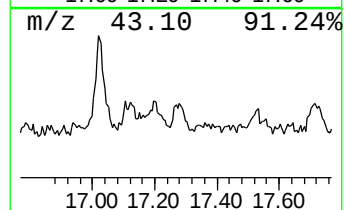
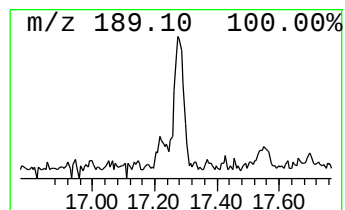
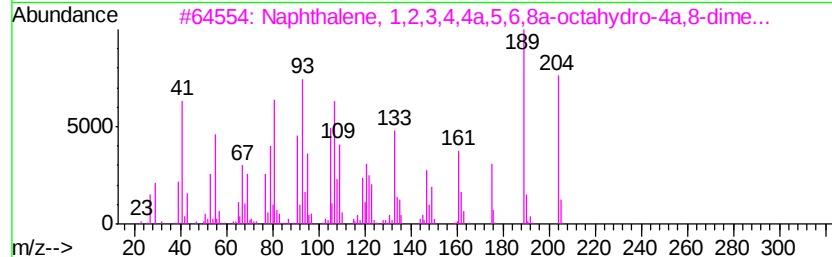
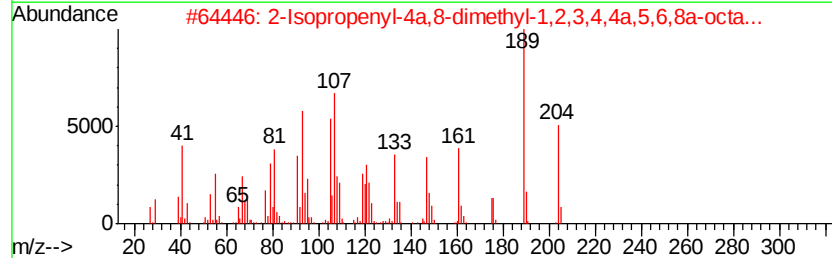
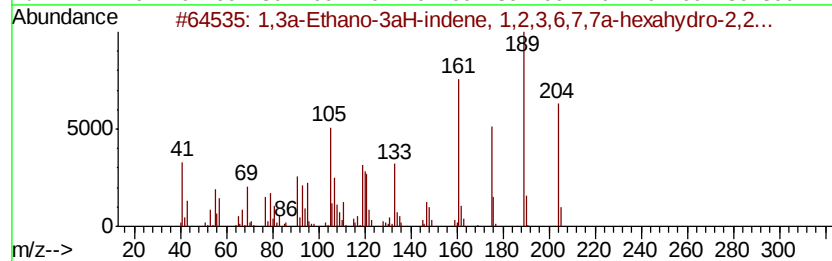
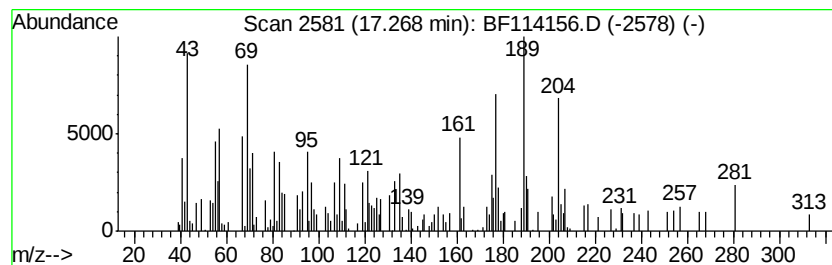
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1,3a-Ethano-3aH-indene, 1,2... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	2.13 ng	213974	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0 83
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0 78
3	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2 76
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3 52
5	2H-1,3-Oxazine, 2-[(2,6-dimethyl...	204	C12H16N2O	054708-09-7 46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
Data File : BF114156.D
Acq On : 11 May 2019 14:54
Operator : JU/SJ
Sample : K2763-09
Misc :
ALS Vial : 9 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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unknown6.63	6.63	89.8	ng	8244470	1	6.85	1836260	20.0
n-Hexadecanoic acid	11.89	6.9	ng	982139	4	11.37	2849280	20.0
Octadecanoic acid	12.67	3.0	ng	425966	4	11.37	2849280	20.0
1-Heneicosanol	13.84	14.5	ng	1376550	5	14.00	1893530	20.0
Hexacosane	14.17	2.4	ng	223568	5	14.00	1893530	20.0
Tritetracontane	14.48	4.4	ng	416143	5	14.00	1893530	20.0
Heneicosane	14.79	3.2	ng	318373	6	15.47	2005830	20.0
Docosane	15.12	5.5	ng	549916	6	15.47	2005830	20.0
Cyclopentadecane	15.99	2.5	ng	254243	6	15.47	2005830	20.0
1,3a-Ethano-3aH-i...	17.27	2.1	ng	213974	6	15.47	2005830	20.0