

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
 Data File : BF112911.D
 Acq On : 7 Mar 2019 5:16
 Operator : JU/SJ
 Sample : K1705-18
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-B004-022719

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-BF022719.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	5.346	549	554	557	rBV	4535603	4756115	95.76%	10.380%
2	6.369	723	728	746	rBV	4206756	4966507	100.00%	10.839%
3	6.504	746	751	754	rBV	5033126	4872391	98.10%	10.634%
4	6.734	786	790	793	rBV	1316559	1145748	23.07%	2.501%
5	6.887	812	816	820	rBV	3927140	3767216	75.85%	8.222%
6	7.292	880	885	888	rBV	3132504	3035254	61.11%	6.624%
7	8.010	1003	1007	1014	rBV	1340249	1309683	26.37%	2.858%
8	9.086	1186	1190	1202	rBV	4715117	4316043	86.90%	9.420%
9	9.481	1253	1257	1265	rBV	279357	257050	5.18%	0.561%
10	9.763	1301	1305	1318	rBV	1310315	1333161	26.84%	2.910%
11	10.545	1433	1438	1453	rBV	2779895	2770235	55.78%	6.046%
12	11.239	1552	1556	1558	rBV	1222496	1177798	23.71%	2.571%
13	11.257	1558	1559	1563	rVB	199708	158126	3.18%	0.345%
14	11.775	1643	1647	1657	rBV3	561659	636921	12.82%	1.390%
15	12.445	1757	1761	1764	rBV	267046	269742	5.43%	0.589%
16	12.498	1766	1770	1775	rVB7	35643	67801	1.37%	0.148%
17	12.557	1777	1780	1790	rVV2	240928	328527	6.61%	0.717%
18	12.669	1793	1799	1802	rBV	284128	310886	6.26%	0.679%
19	12.816	1820	1824	1828	rBV	3735676	3530291	71.08%	7.705%
20	13.063	1864	1866	1869	rVB	64669	50253	1.01%	0.110%
21	13.098	1869	1872	1876	rBV	51255	50606	1.02%	0.110%
22	13.304	1902	1907	1912	rBV3	116182	126379	2.54%	0.276%
23	13.404	1921	1924	1926	rVB	61733	52157	1.05%	0.114%
24	13.498	1937	1940	1946	rVB	43231	69079	1.39%	0.151%
25	13.604	1955	1958	1962	rBV2	35680	52649	1.06%	0.115%
26	13.727	1972	1979	1987	rBV2	321347	474370	9.55%	1.035%
27	13.863	1997	2002	2005	rBV	1515207	1694974	34.13%	3.699%
28	13.886	2005	2006	2009	rVB	153978	76504	1.54%	0.167%
29	14.045	2030	2033	2036	rVB	154719	133277	2.68%	0.291%
30	14.345	2081	2084	2091	rBV3	235835	359696	7.24%	0.785%
31	14.639	2131	2134	2140	rVB	227330	235478	4.74%	0.514%
32	14.774	2154	2157	2162	rVB	141611	139979	2.82%	0.306%
33	14.868	2169	2173	2176	rBV	117495	184228	3.71%	0.402%
34	14.957	2185	2188	2191	rBV	386471	426167	8.58%	0.930%

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	14.986	2191	2193	2203	rVB3	153546	230021	4.63%	0.502%
36	15.145	2218	2220	2224	rVB	66713	64937	1.31%	0.142%
37	15.204	2227	2230	2235	rVB	81859	98664	1.99%	0.215%
38	15.262	2235	2240	2245	rBV	1028627	1279059	25.75%	2.792%
39	15.310	2245	2248	2253	rVB	220869	287903	5.80%	0.628%
40	15.715	2313	2317	2322	rBV	299486	398823	8.03%	0.870%
41	16.186	2392	2397	2408	rVB2	103179	201862	4.06%	0.441%
42	17.192	2564	2568	2576	rVB10	50003	122108	2.46%	0.267%

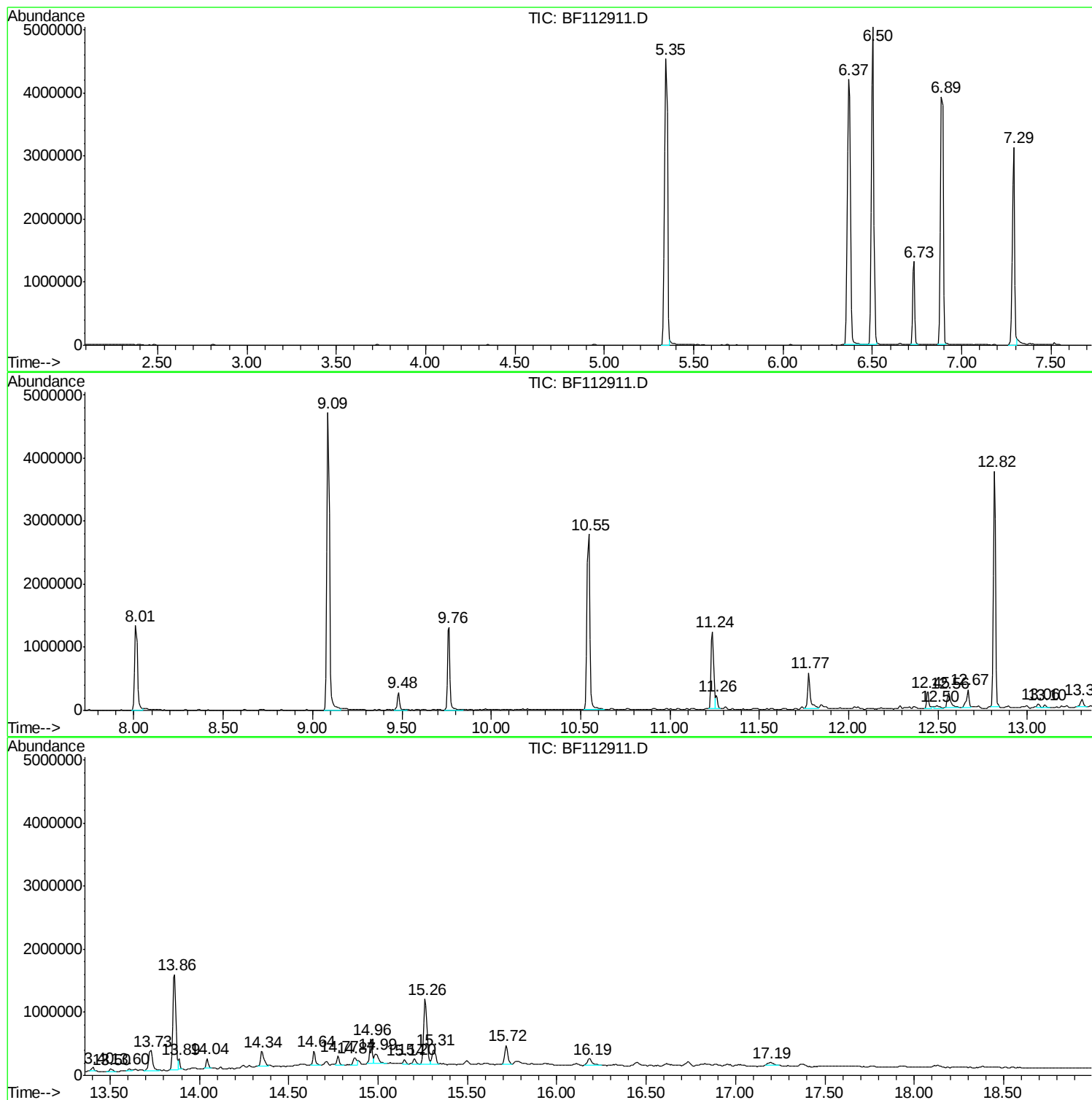
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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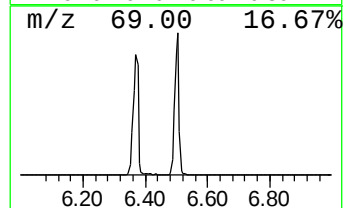
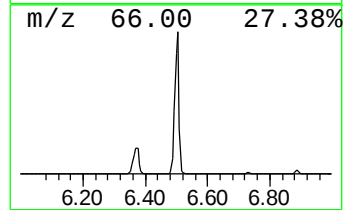
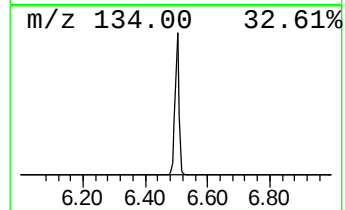
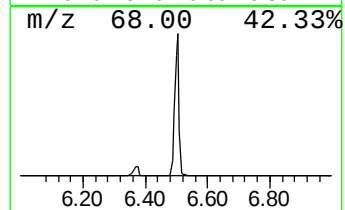
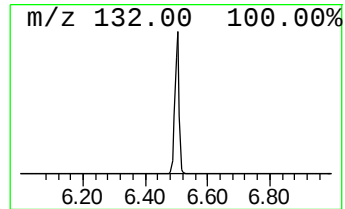
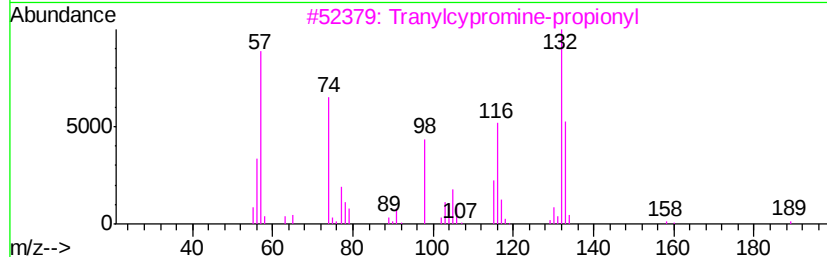
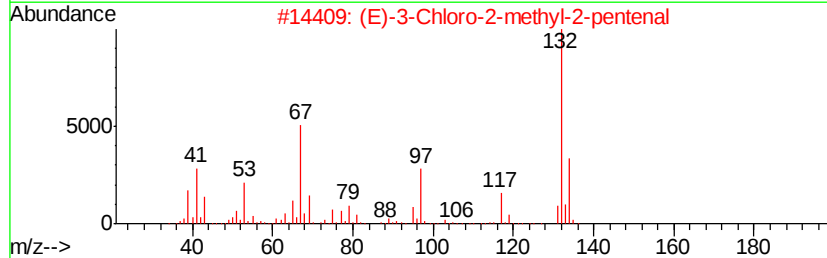
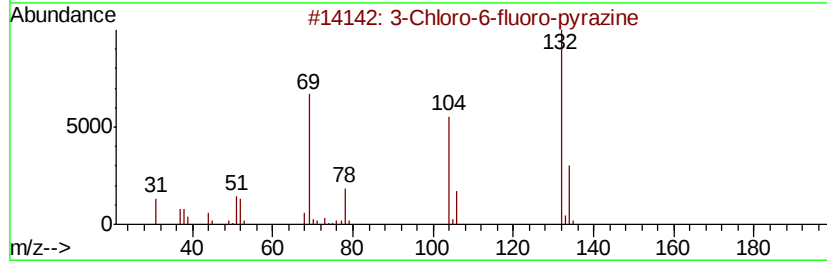
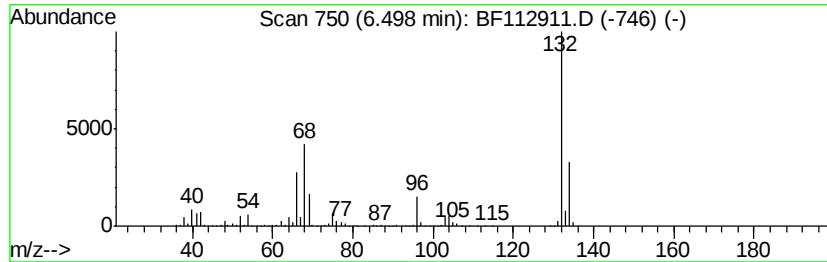
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	85.05 ng	4872390	1,4-Dichlorobenzene-d4	6.73

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	16
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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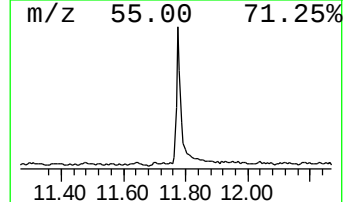
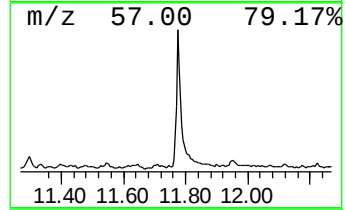
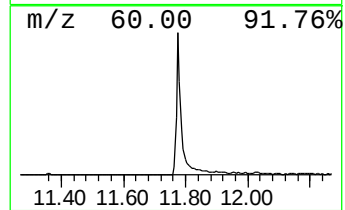
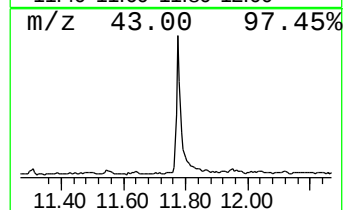
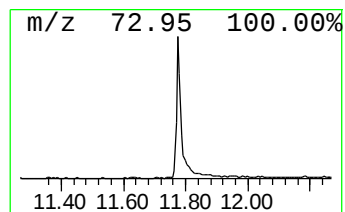
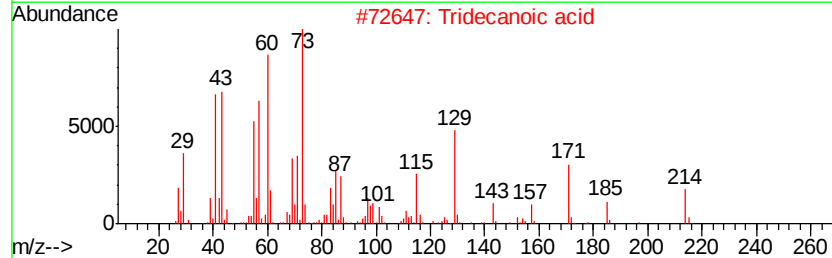
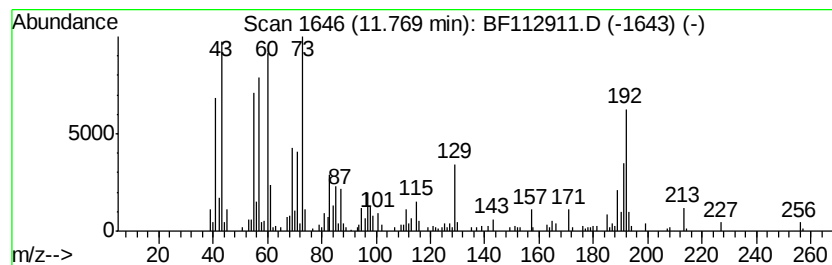
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	10.82 ng	636921	Phenanthrene-d10	11.24

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	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Nonanoic acid	158	C9H18O2	000112-05-0	43



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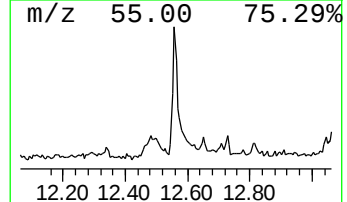
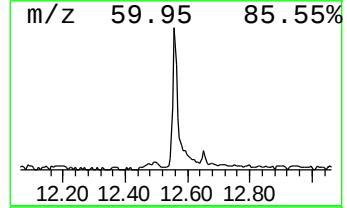
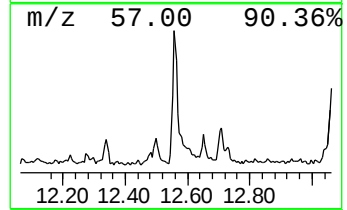
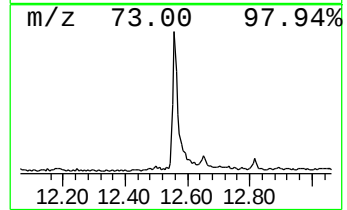
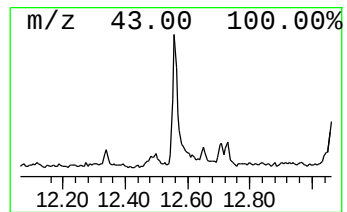
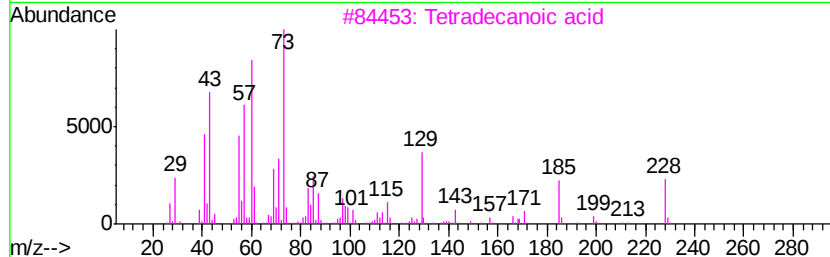
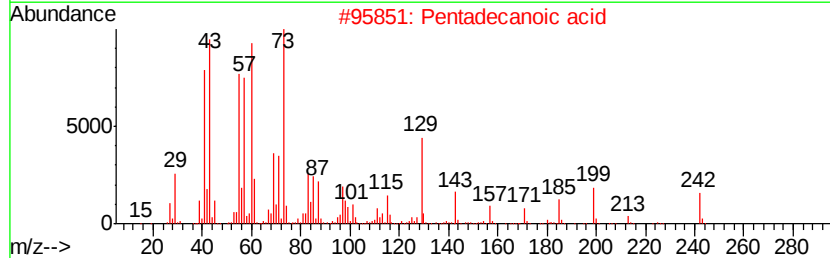
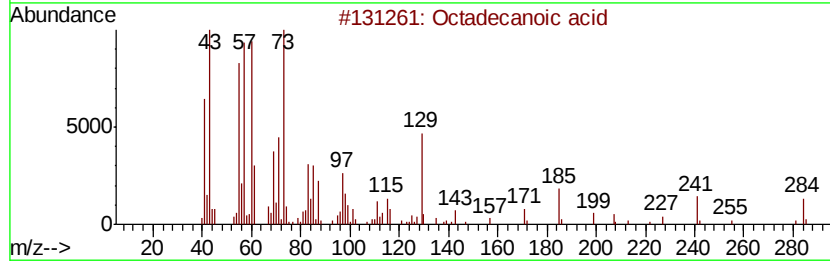
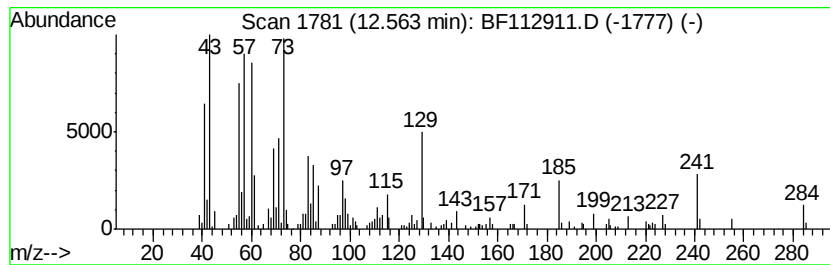
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.56	3.88 ng	328527	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25



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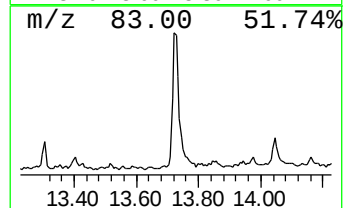
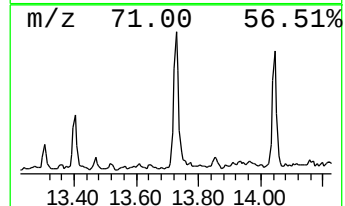
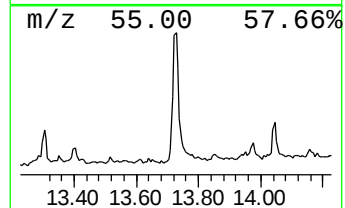
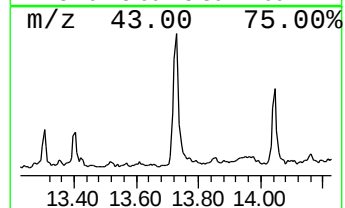
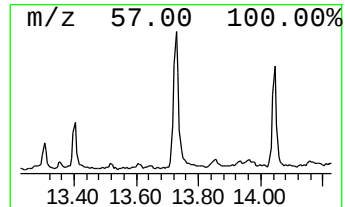
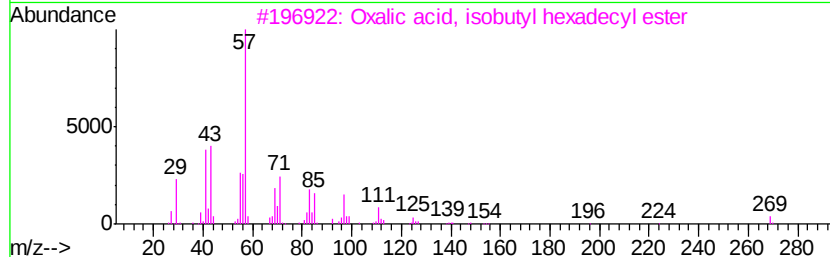
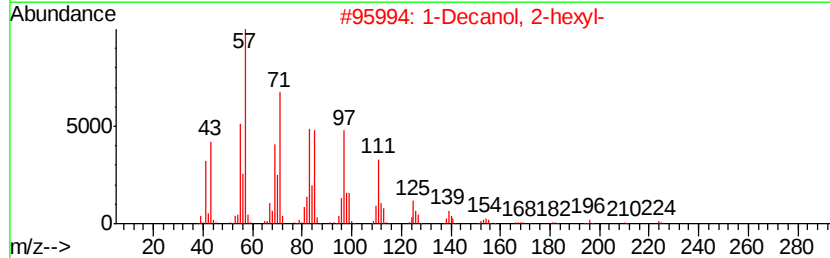
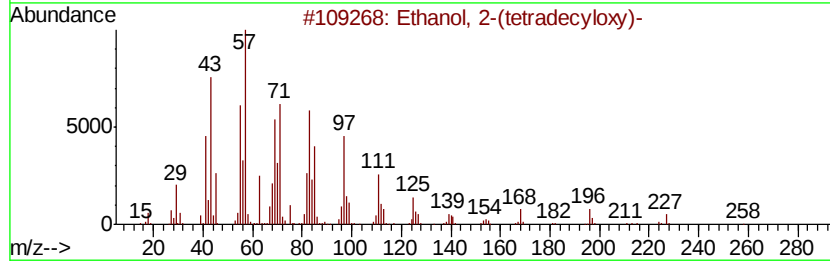
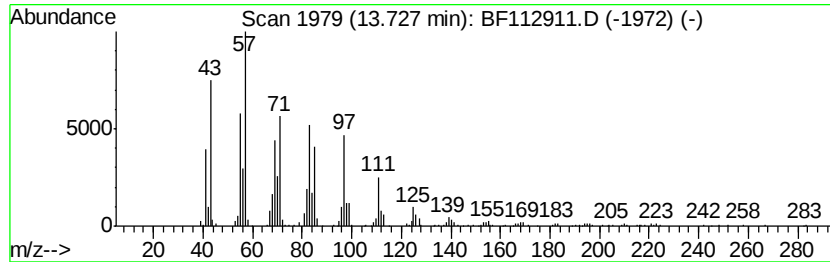
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.73	5.60 ng	474370	Chrysene-d12		13.86	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	90
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



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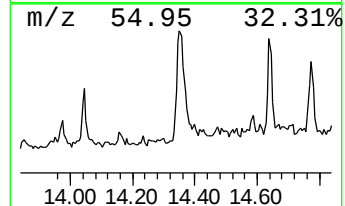
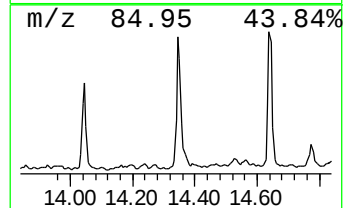
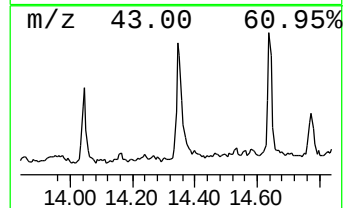
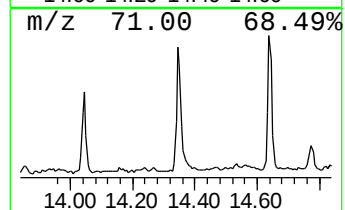
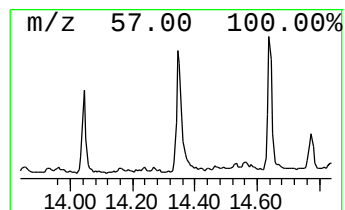
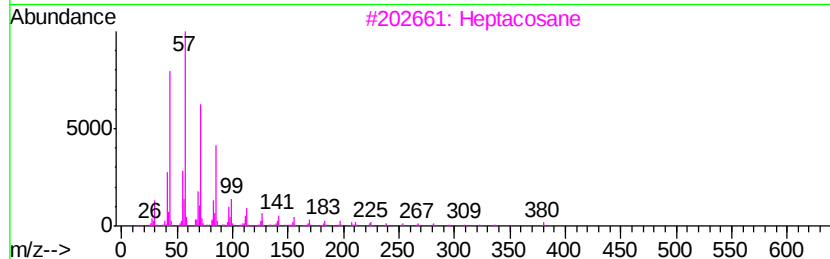
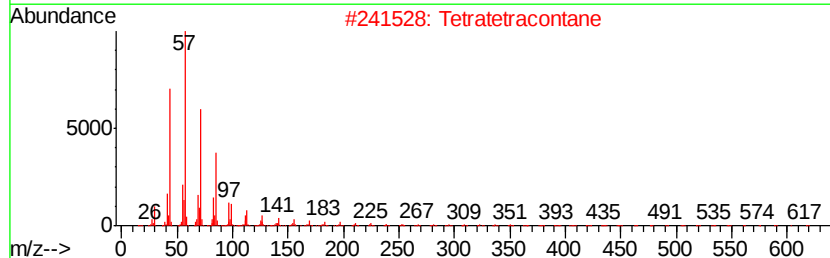
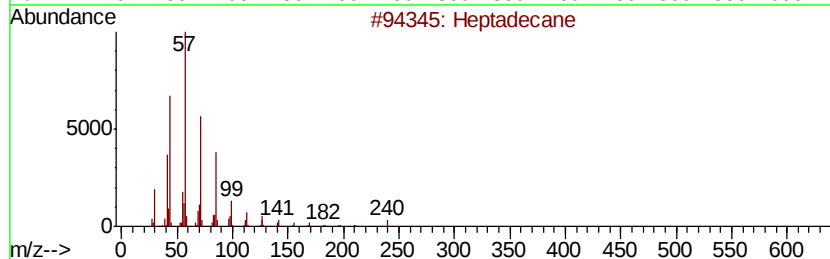
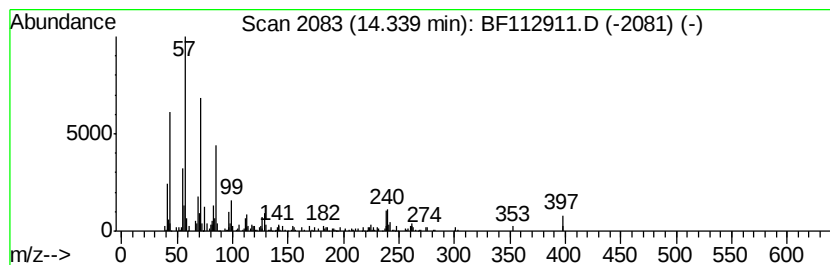
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.24 ng	359696	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Tetratetracontane		619	C44H90	007098-22-8	87
3	Heptacosane		380	C27H56	000593-49-7	83
4	Hexatriacontane		507	C36H74	000630-06-8	83
5	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112911.D
Acq On : 7 Mar 2019 5:16
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B004-022719

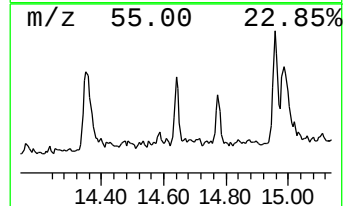
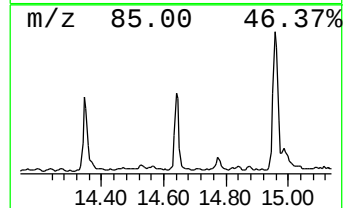
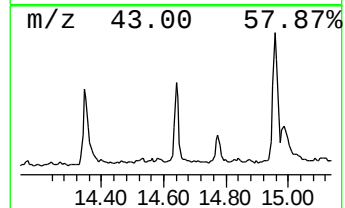
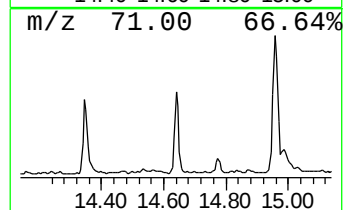
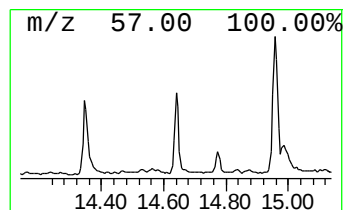
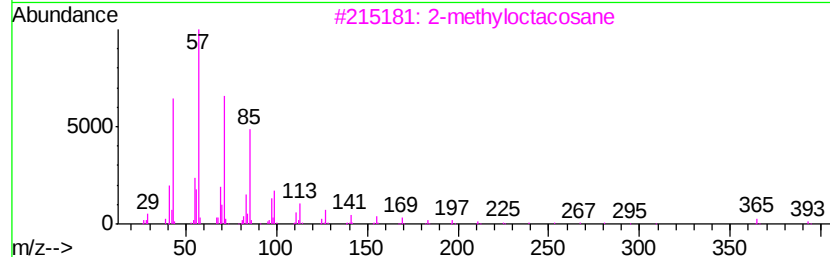
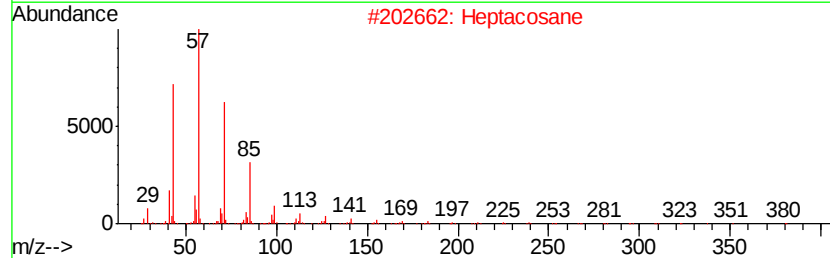
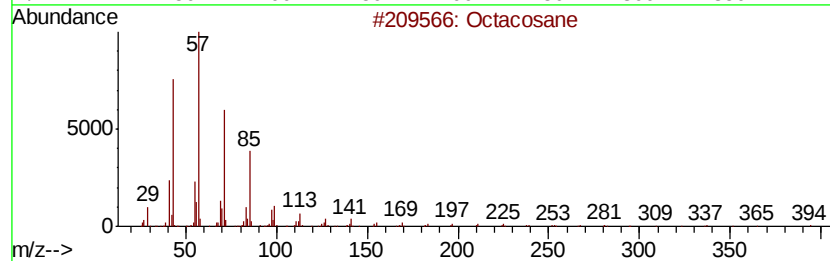
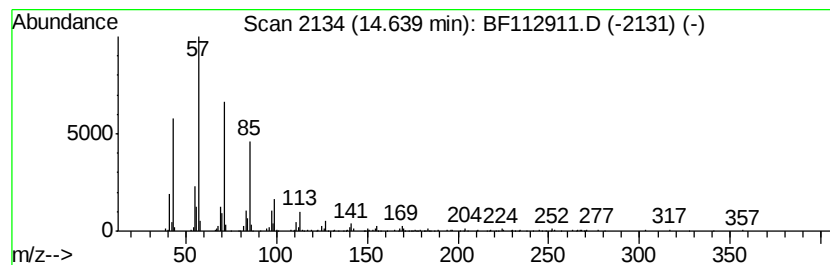
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.68 ng	235478	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heneicosane	296	C21H44	000629-94-7	83
5		Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Sample : K1705-18
Misc :
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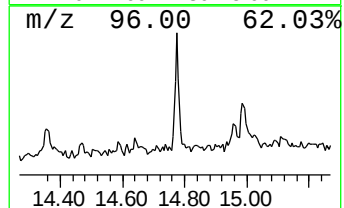
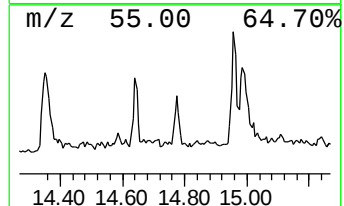
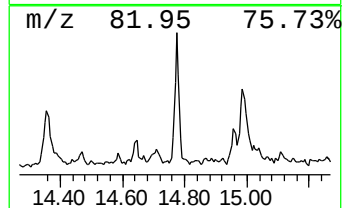
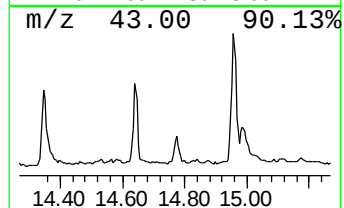
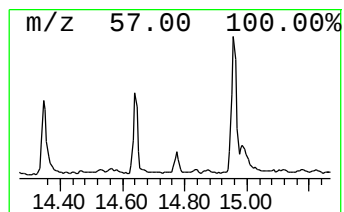
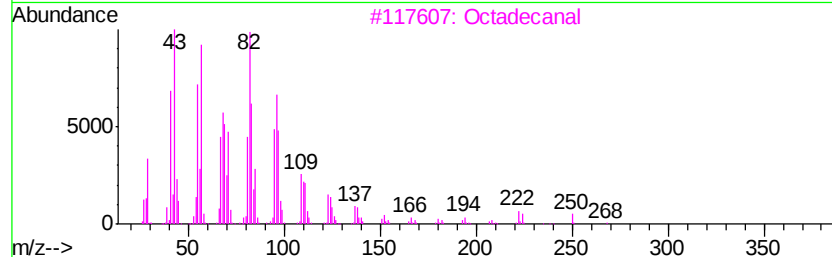
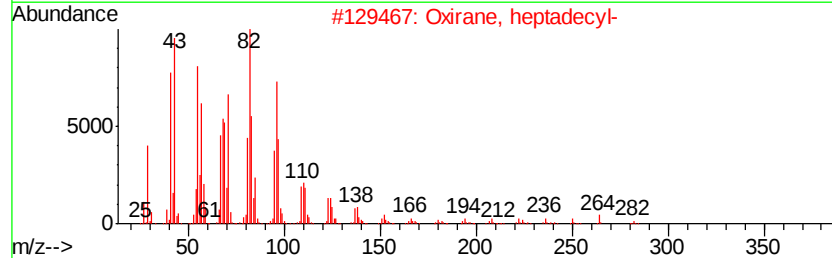
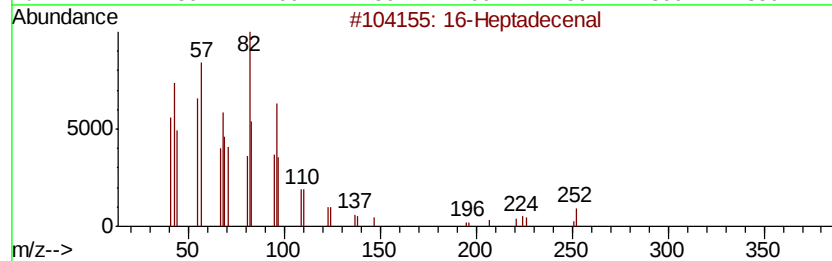
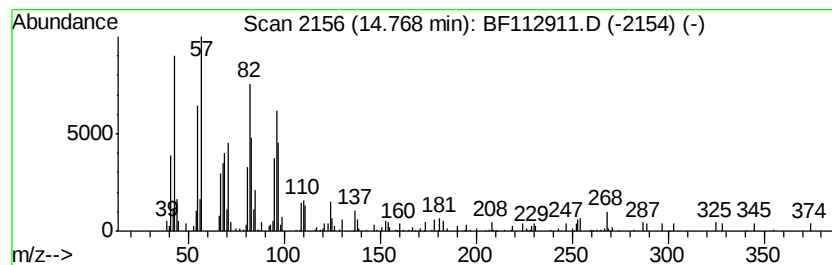
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 16-Heptadecenal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.19 ng	139979	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	16-Heptadecenal	252 C17H32O	1000144-57-9	96
2	Oxirane, heptadecyl-	282 C19H38O	067860-04-2	94
3	Octadecanal	268 C18H36O	000638-66-4	91
4	1,19-Eicosadiene	278 C20H38	014811-95-1	89
5	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112911.D
Acq On : 7 Mar 2019 5:16
Operator : JU/SJ
Sample : K1705-18
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Instrument :
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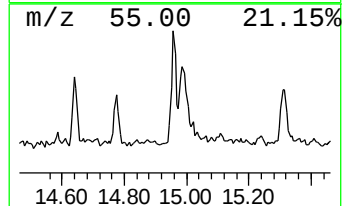
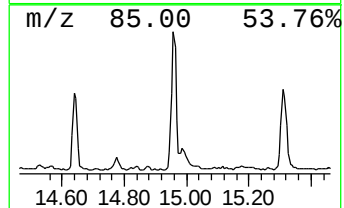
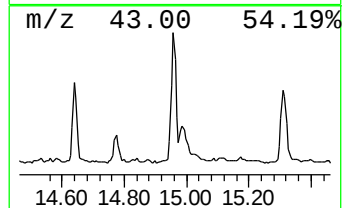
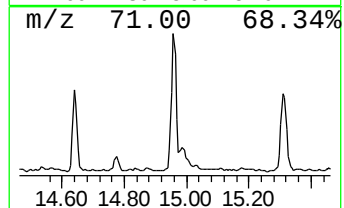
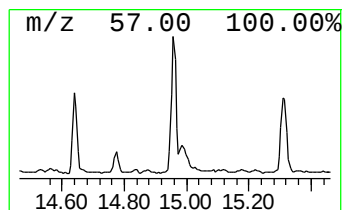
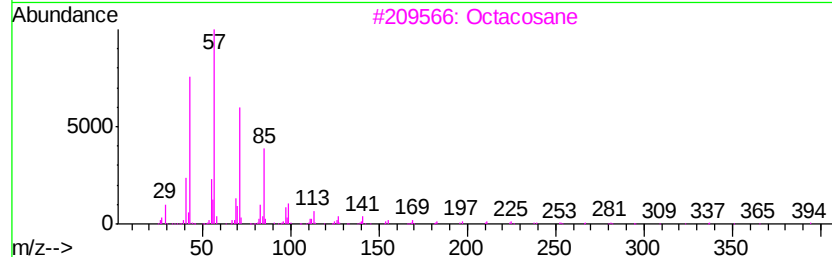
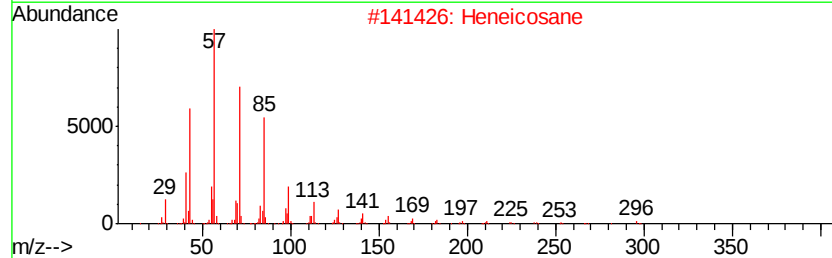
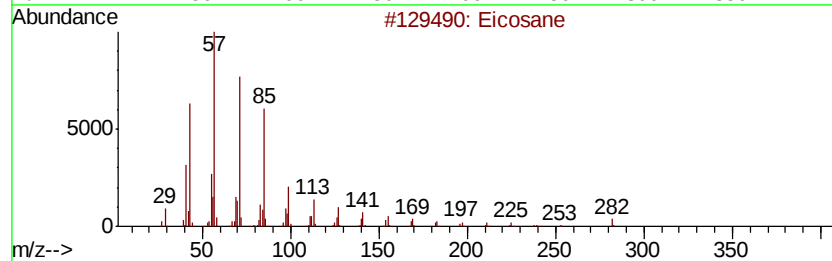
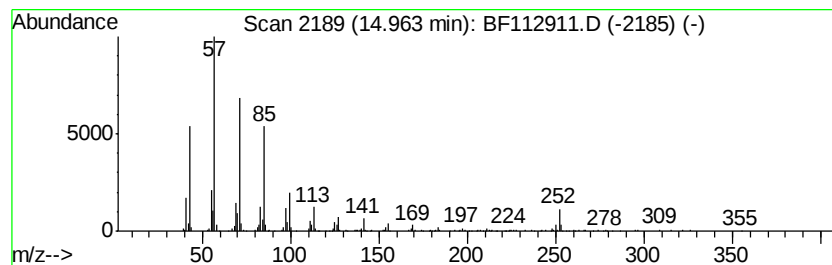
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.66 ng	426167	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112911.D
Acq On : 7 Mar 2019 5:16
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

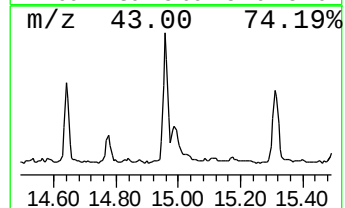
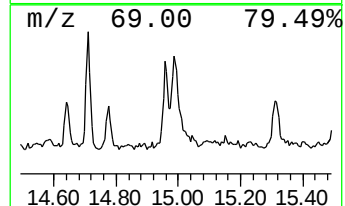
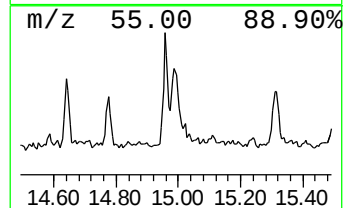
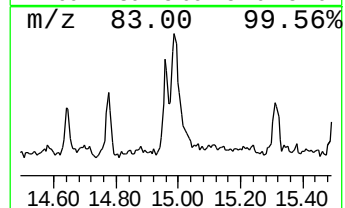
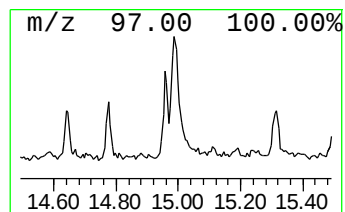
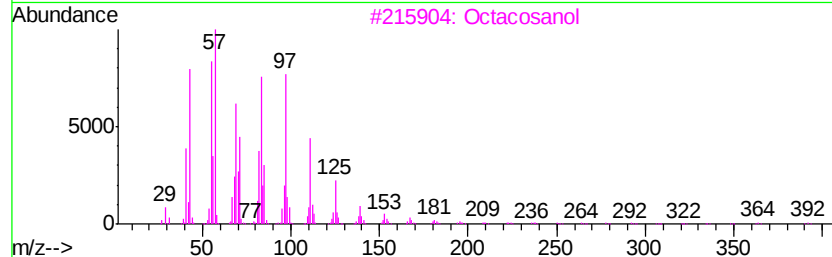
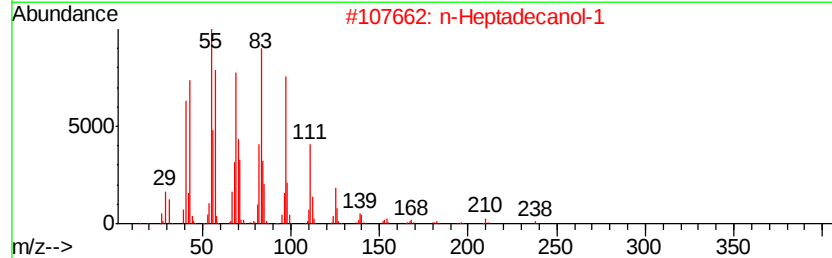
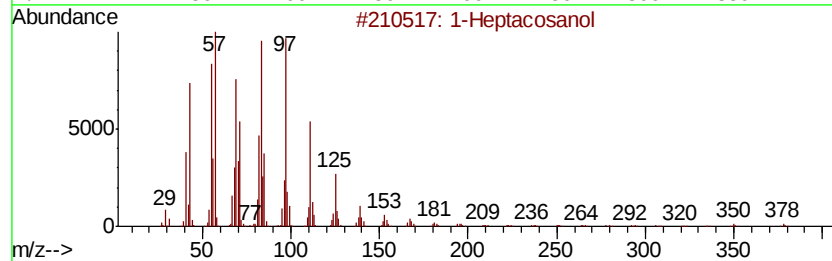
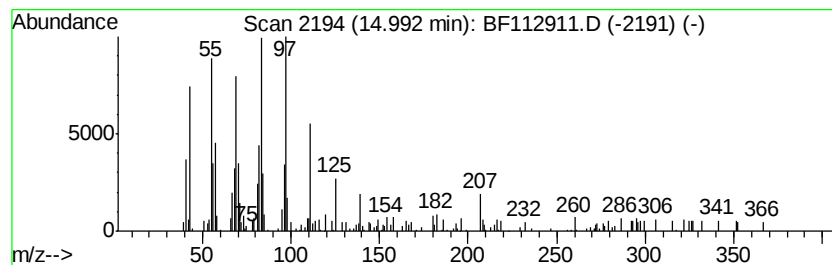
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.60 ng	230021	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	91
2	n-Heptadecanol-1	256 C17H36O	001454-85-9	90
3	Octacosanol	410 C28H58O	000557-61-9	68
4	Heptacosyl acetate	438 C29H58O2	1000351-78-2	68
5	1-Octadecanol	270 C18H38O	000112-92-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112911.D
Acq On : 7 Mar 2019 5:16
Operator : JU/SJ
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Misc :
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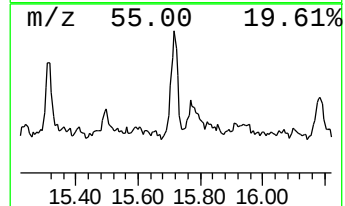
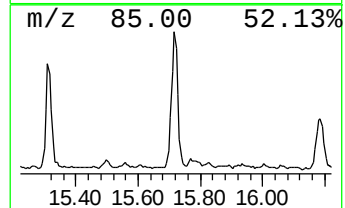
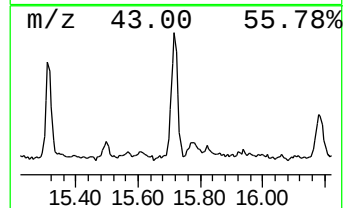
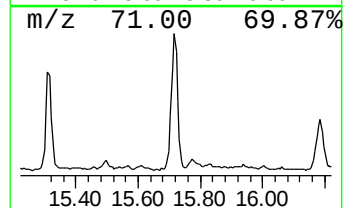
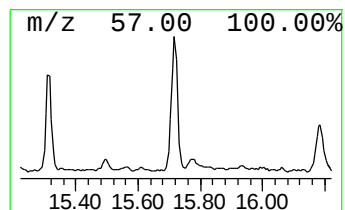
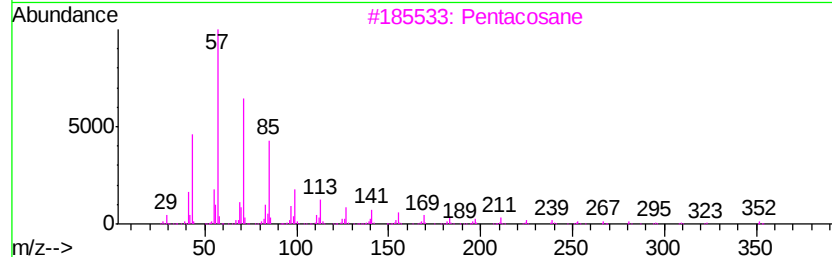
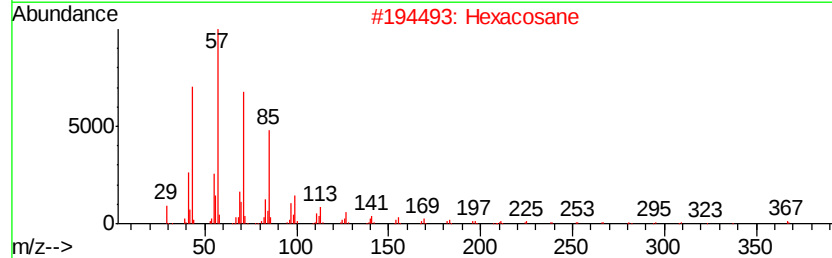
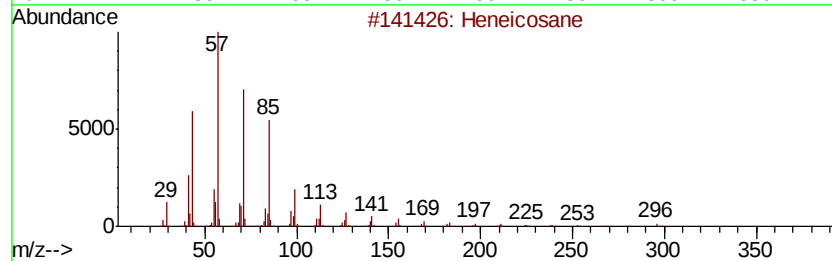
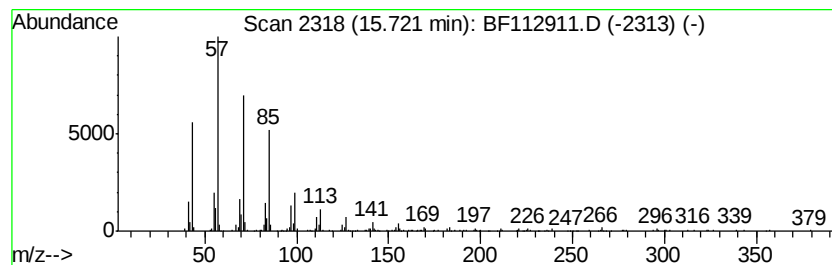
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	6.24 ng	398823	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Pentacosane	352	C25H52	000629-99-2	90
4		triacontane	422	C30H62	000638-68-6	90
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
 Data File : BF112911.D
 Acq On : 7 Mar 2019 5:16
 Operator : JU/SJ
 Sample : K1705-18
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Instrument :
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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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n-Hexadecanoic acid	11.77	10.8	ng	636921	4	11.24	1177800	20.0
Octadecanoic acid	12.56	3.9	ng	328527	5	13.86	1694970	20.0
Ethanol, 2-(tetra...	13.73	5.6	ng	474370	5	13.86	1694970	20.0
Heptadecane	14.34	4.2	ng	359696	5	13.86	1694970	20.0
Octacosane	14.64	3.7	ng	235478	6	15.26	1279060	20.0
16-Heptadecenal	14.77	2.2	ng	139979	6	15.26	1279060	20.0
Eicosane	14.96	6.7	ng	426167	6	15.26	1279060	20.0
1-Heptacosanol	14.99	3.6	ng	230021	6	15.26	1279060	20.0
Heneicosane	15.72	6.2	ng	398823	6	15.26	1279060	20.0