

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112989.D
 Acq On : 12 Mar 2019 7:34
 Operator : JU/SJ
 Sample : K1817-07
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EXT-027-SW015-030719

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	3.698	264	274	279	rBV	4892040	8683409	100.00%	22.914%
2	5.334	548	552	563	rBV	2360253	2343105	26.98%	6.183%
3	6.369	723	728	746	rBV	2533914	2672848	30.78%	7.053%
4	6.498	746	750	753	rBV	3044534	2652247	30.54%	6.999%
5	6.728	786	789	793	rBV	984704	804607	9.27%	2.123%
6	6.886	812	816	819	rBV	2330885	1886502	21.73%	4.978%
7	7.286	880	884	897	rBV	1688964	1615443	18.60%	4.263%
8	8.010	1004	1007	1015	rBV	1081840	1062794	12.24%	2.804%
9	9.086	1186	1190	1204	rBV	2891786	2731694	31.46%	7.208%
10	9.480	1254	1257	1265	rVB	328343	305263	3.52%	0.806%
11	9.763	1301	1305	1315	rBV	1475970	1350742	15.56%	3.564%
12	10.416	1411	1416	1422	rBV	86502	93286	1.07%	0.246%
13	10.545	1434	1438	1453	rBV	2204051	2165119	24.93%	5.713%
14	11.239	1552	1556	1559	rBV	1488176	1353073	15.58%	3.570%
15	11.263	1559	1560	1566	rVB	197245	117697	1.36%	0.311%
16	11.774	1644	1647	1657	rBV3	389656	466024	5.37%	1.230%
17	12.445	1758	1761	1766	rBV	215374	201443	2.32%	0.532%
18	12.557	1777	1780	1792	rBV2	123737	189530	2.18%	0.500%
19	12.668	1793	1799	1803	rVV2	179695	212475	2.45%	0.561%
20	12.816	1820	1824	1832	rVB	2392280	2283115	26.29%	6.025%
21	13.727	1975	1979	1987	rVB2	212550	271460	3.13%	0.716%
22	13.862	1997	2002	2005	rBV	1151242	1205984	13.89%	3.182%
23	14.045	2029	2033	2036	rBV	108699	106252	1.22%	0.280%
24	14.345	2081	2084	2097	rBV2	147761	235724	2.71%	0.622%
25	14.639	2131	2134	2138	rBV	111291	116480	1.34%	0.307%
26	14.709	2143	2146	2153	rVV	146794	147242	1.70%	0.389%
27	14.774	2154	2157	2162	rVB	118605	119268	1.37%	0.315%
28	14.874	2170	2174	2181	rBV	77829	154636	1.78%	0.408%
29	14.957	2184	2188	2191	rVV	328275	377353	4.35%	0.996%
30	14.986	2191	2193	2204	rVB3	123652	213192	2.46%	0.563%
31	15.268	2236	2241	2245	rVV	621386	780052	8.98%	2.058%
32	15.309	2245	2248	2254	rVB2	122906	170860	1.97%	0.451%
33	15.715	2312	2317	2323	rBV	371805	536492	6.18%	1.416%
34	17.698	2650	2654	2669	rVB	45220	125042	1.44%	0.330%

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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	18.480	2782	2787	2796	rBV6	60406	145676	1.68%	0.384%
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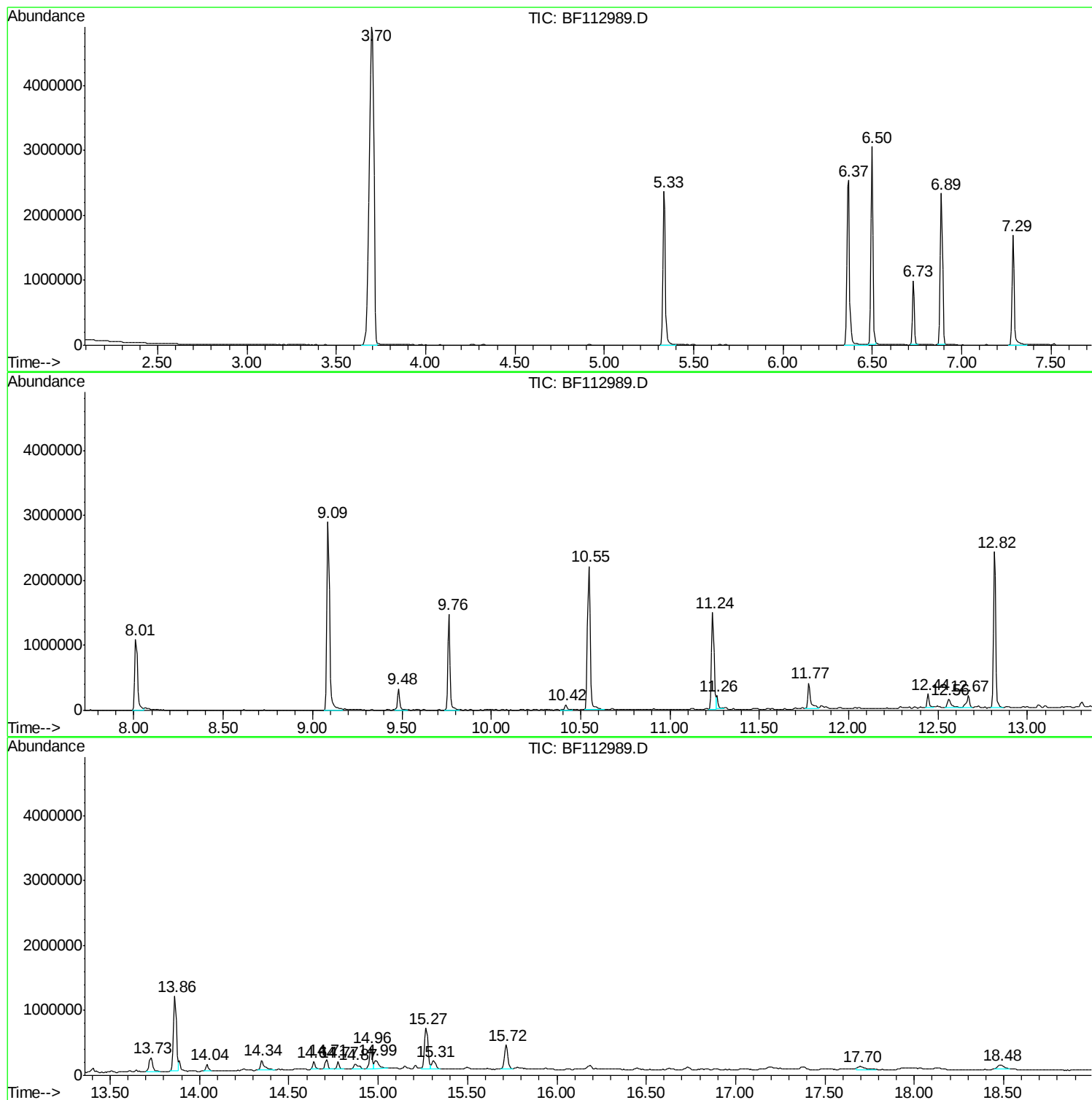
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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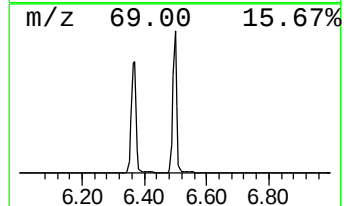
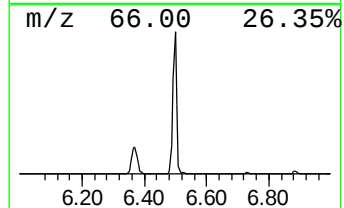
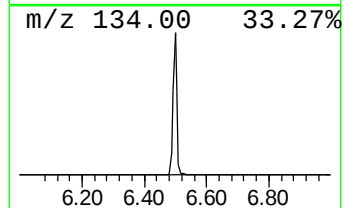
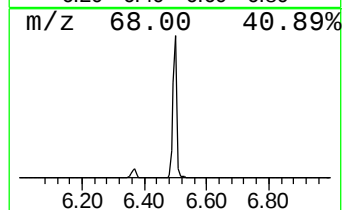
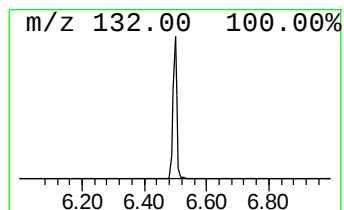
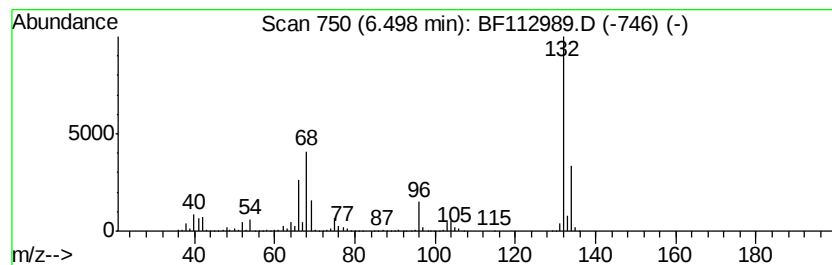
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	65.93 ng	2652250	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	12
3		Tranvlcyproline-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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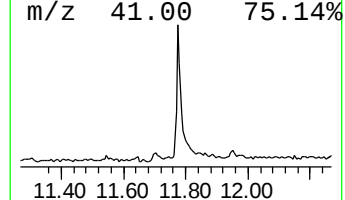
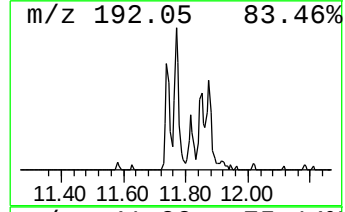
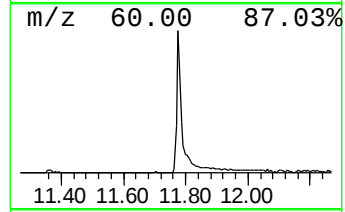
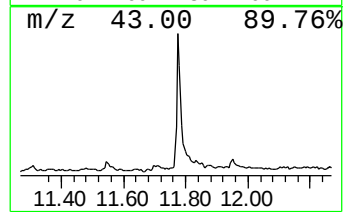
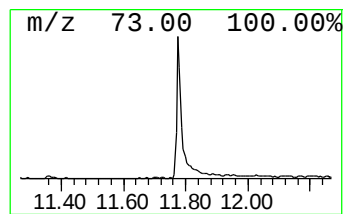
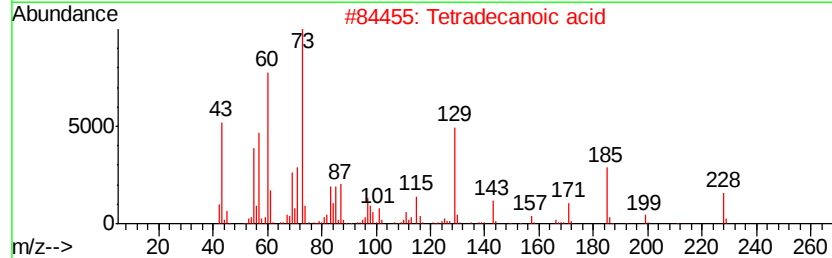
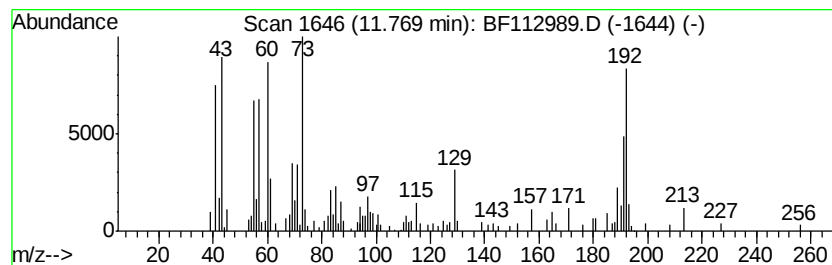
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	6.89 ng	466024	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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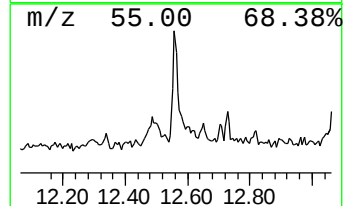
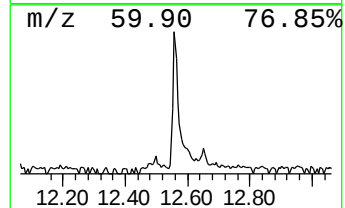
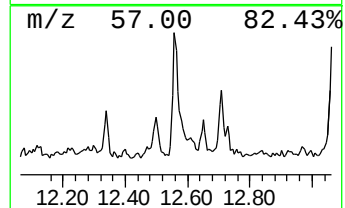
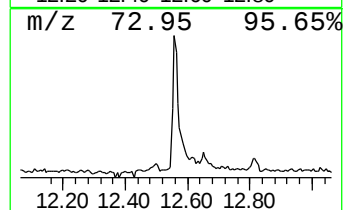
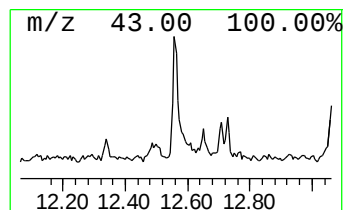
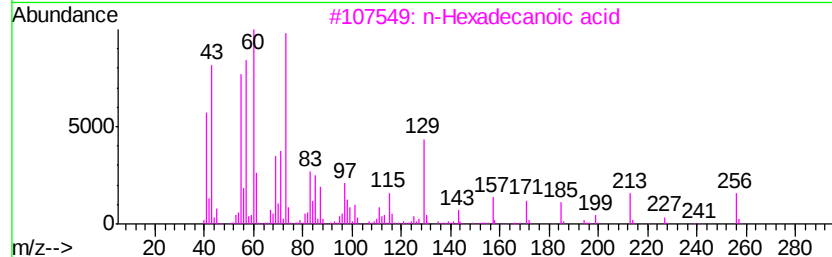
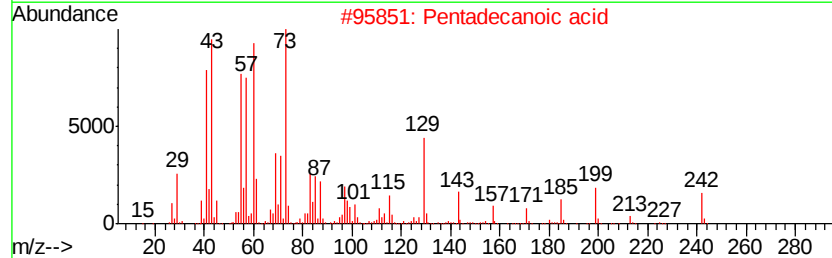
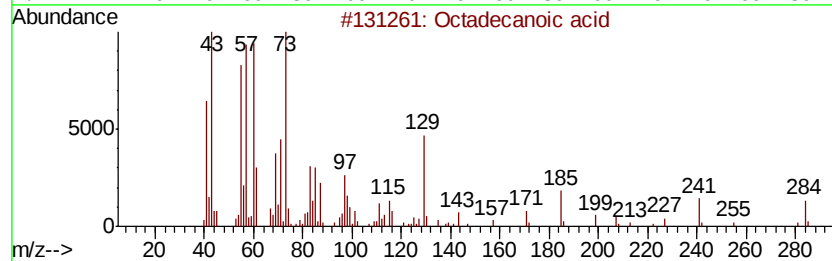
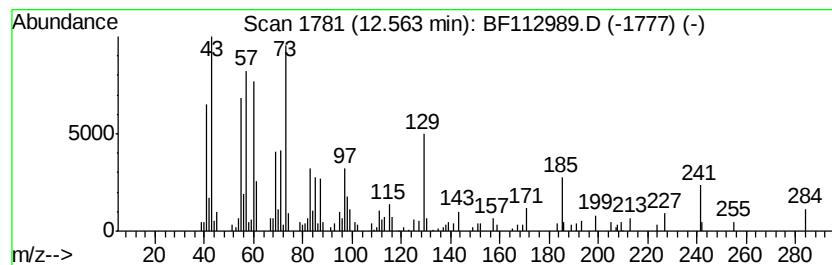
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.56	3.14 ng	189530	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80



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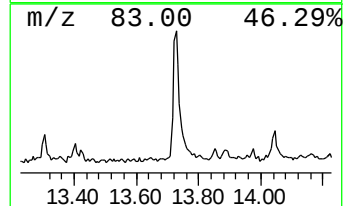
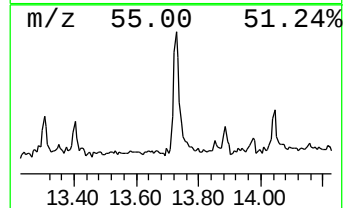
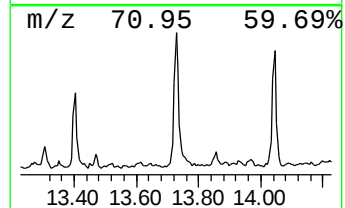
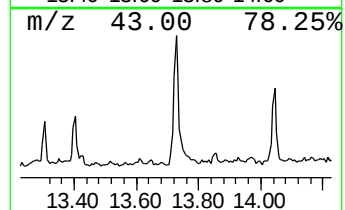
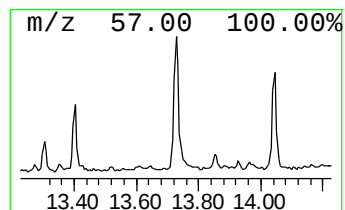
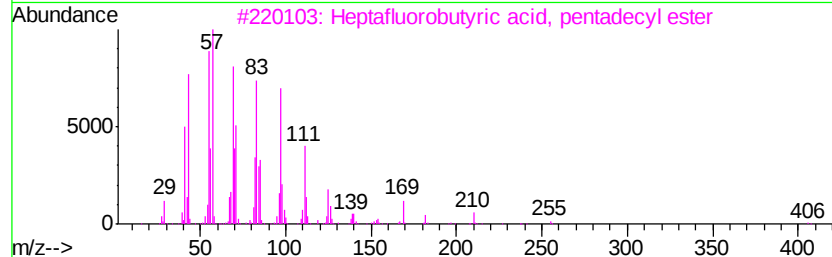
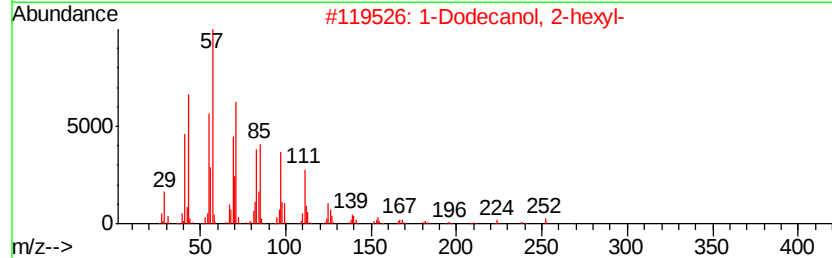
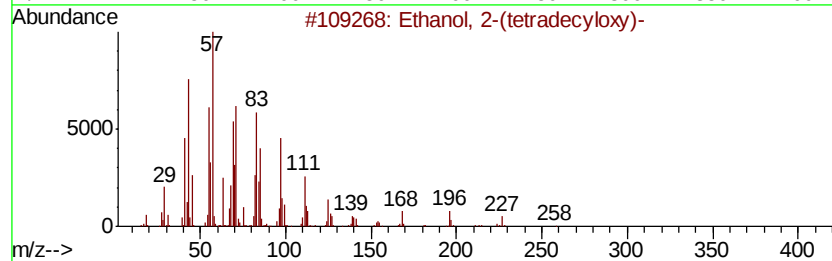
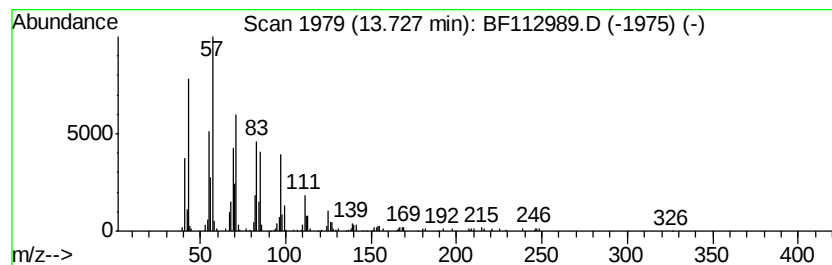
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.73	4.50 ng	271460	Chrysene-d12	13.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	74
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	70
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	70



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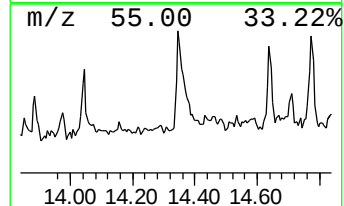
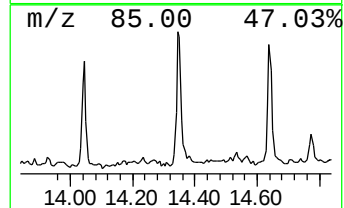
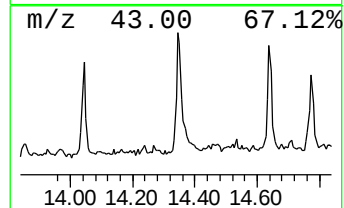
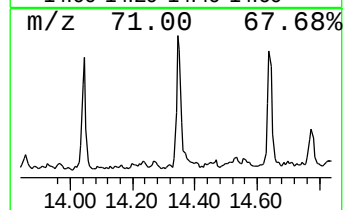
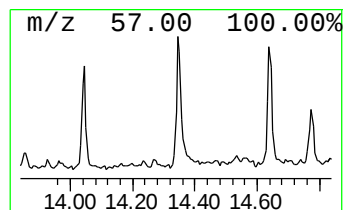
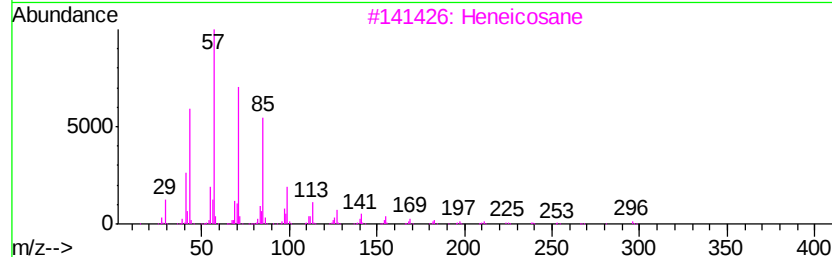
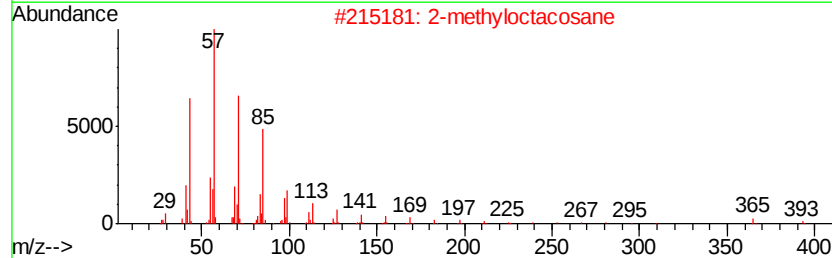
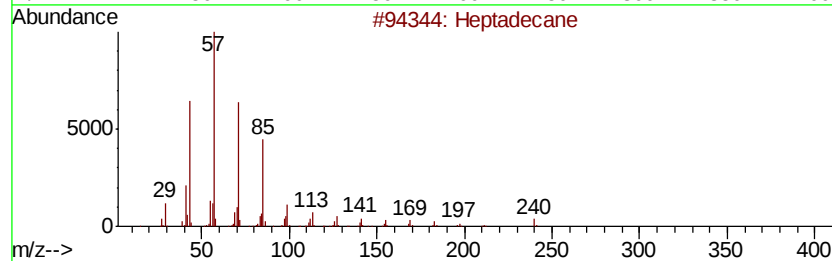
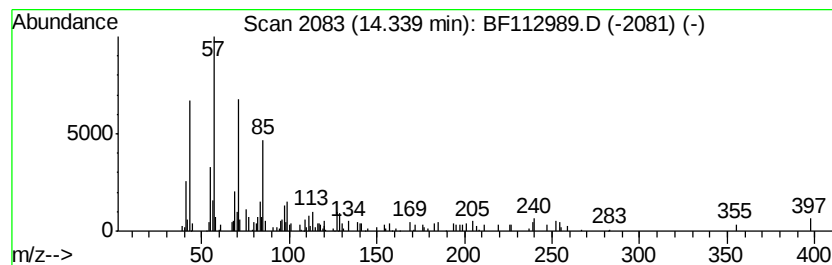
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.91 ng	235724	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	93
2		2-methyloctacosane	408	C29H60	1000376-72-8	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Hexacosane	366	C26H54	000630-01-3	90



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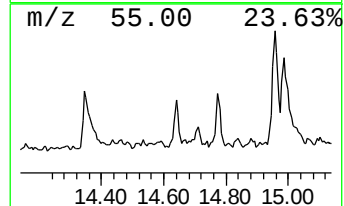
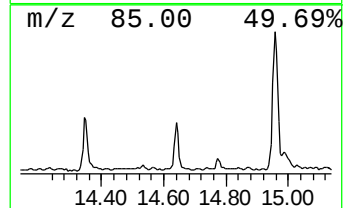
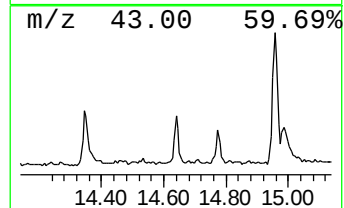
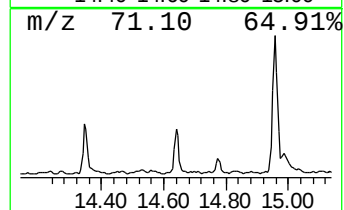
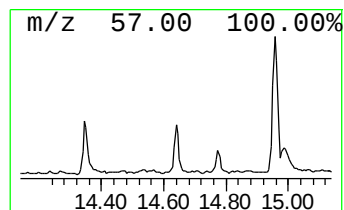
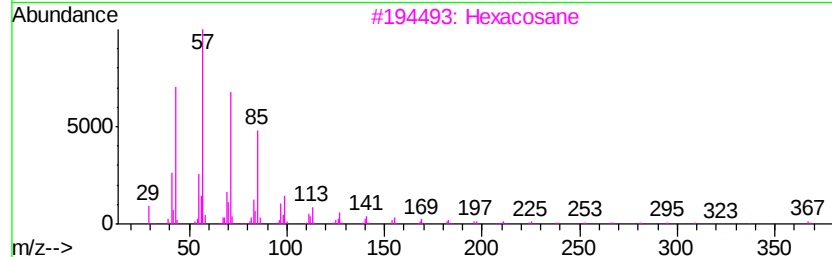
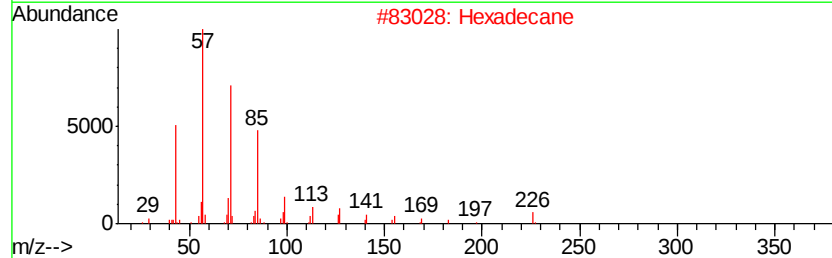
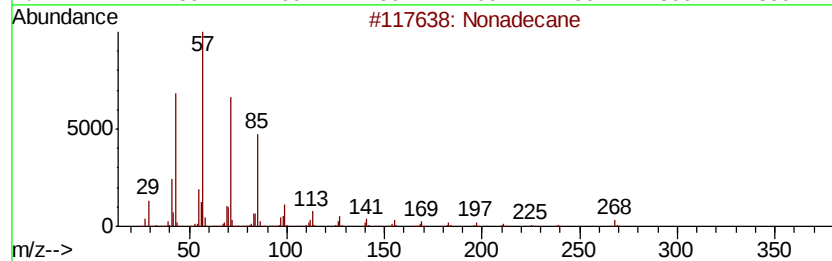
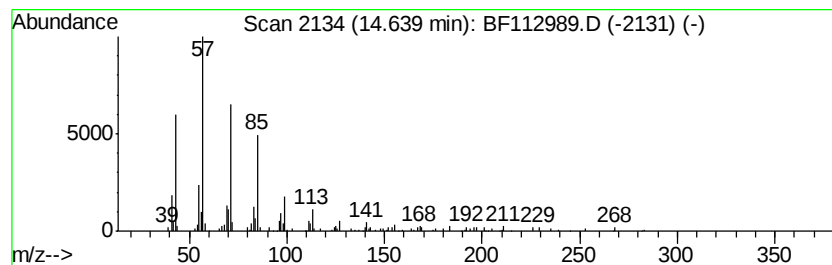
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.99 ng	116480	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	94
2		Hexadecane	226	C16H34	000544-76-3	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112989.D
Acq On : 12 Mar 2019 7:34
Operator : JU/SJ
Sample : K1817-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EXT-027-SW015-030719

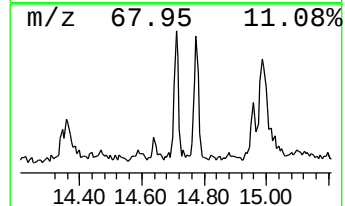
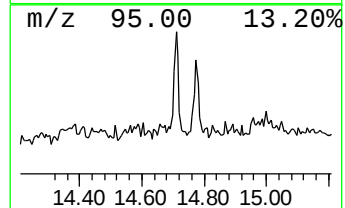
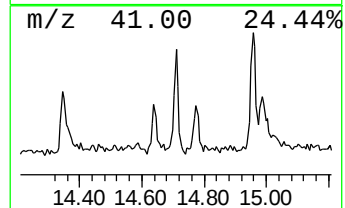
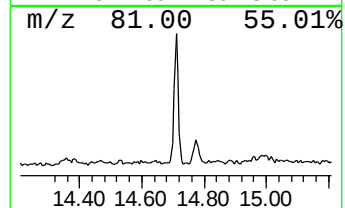
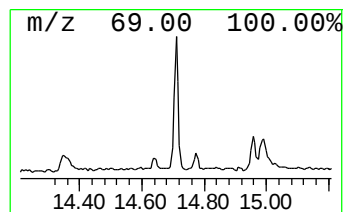
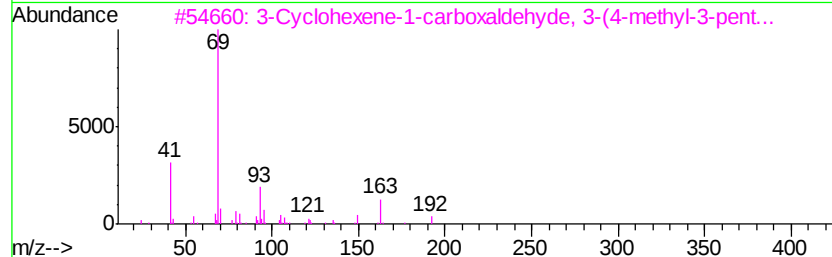
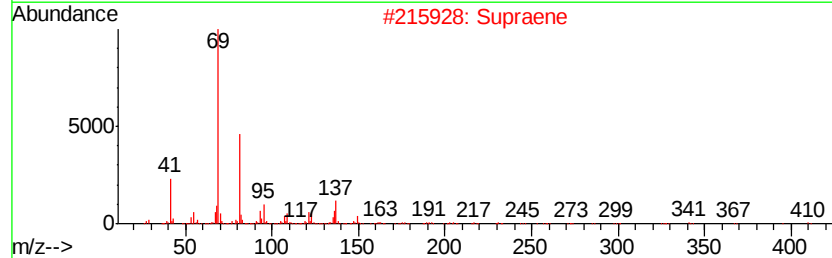
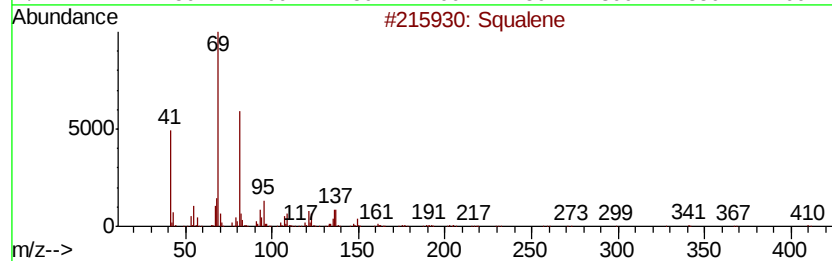
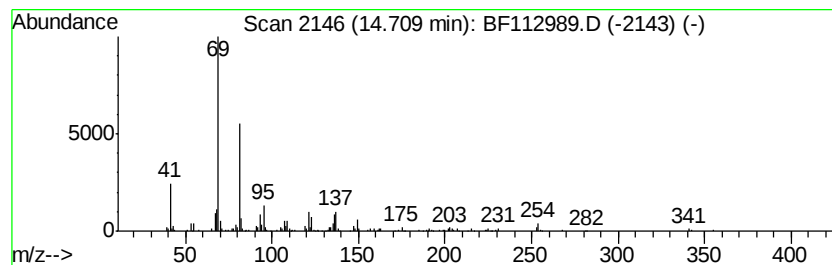
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.78 ng	147242	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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ClientSampleId :
EXT-027-SW015-030719

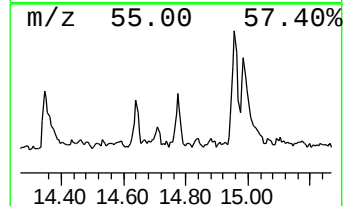
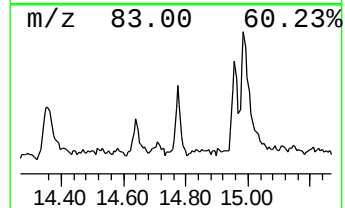
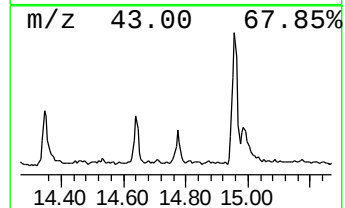
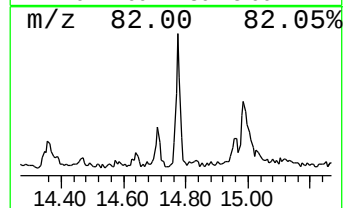
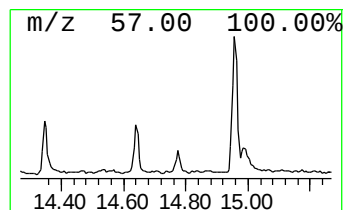
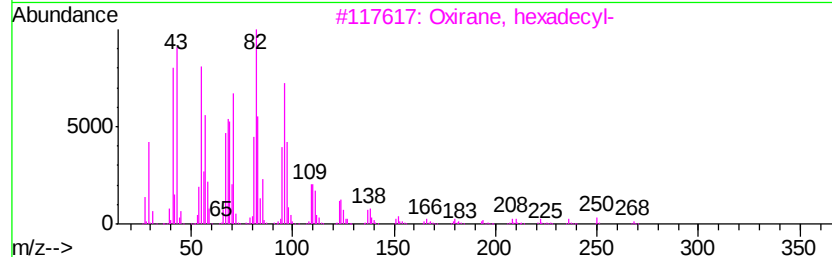
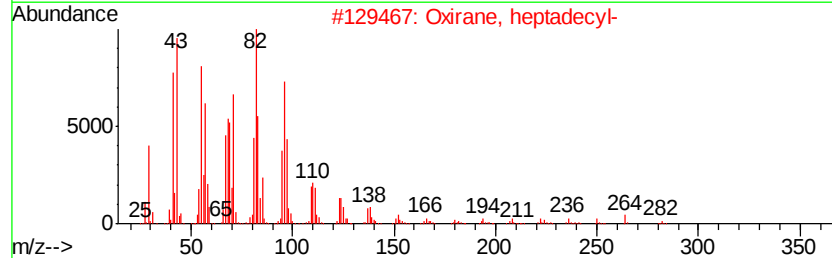
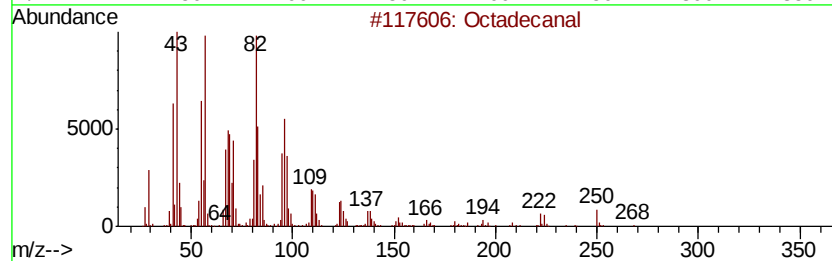
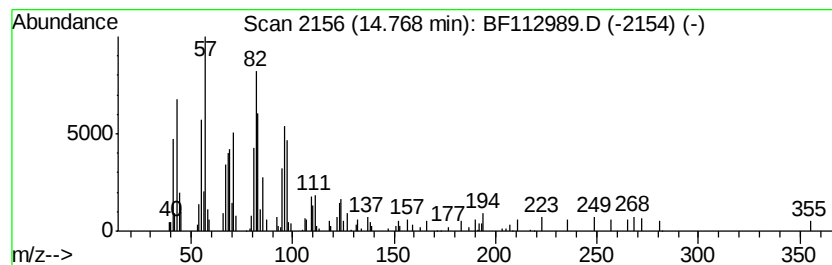
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.06 ng	119268	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	90
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4		13-Octadecenal	266	C18H34O	056554-90-6	83
5		14-Heptadecenal	252	C17H32O	1000144-58-0	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112989.D
Acq On : 12 Mar 2019 7:34
Operator : JU/SJ
Sample : K1817-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

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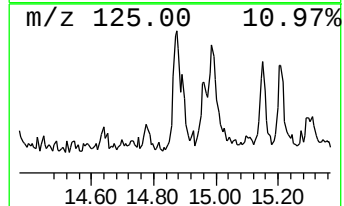
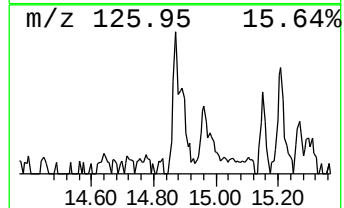
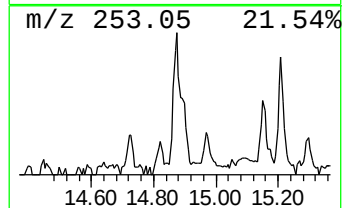
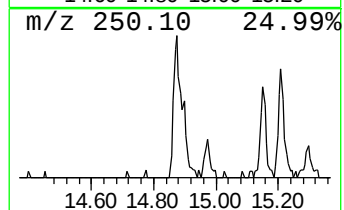
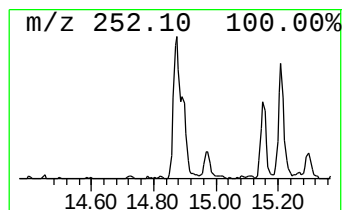
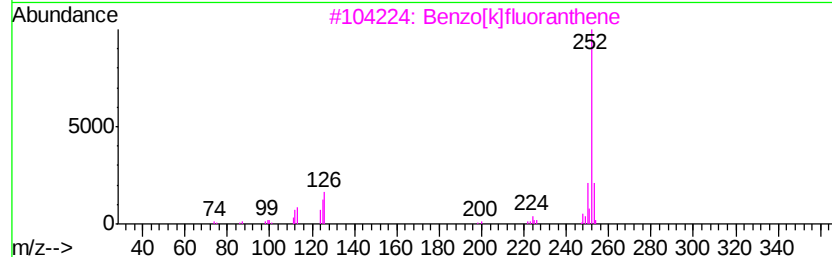
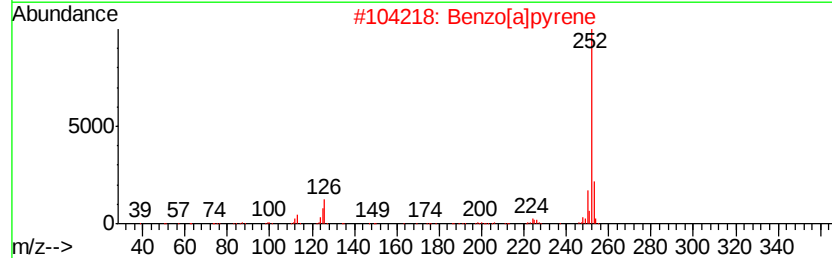
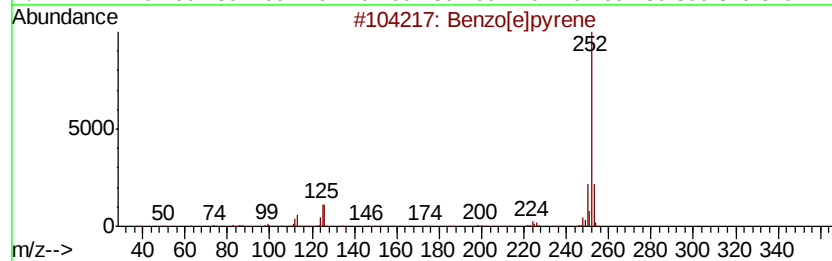
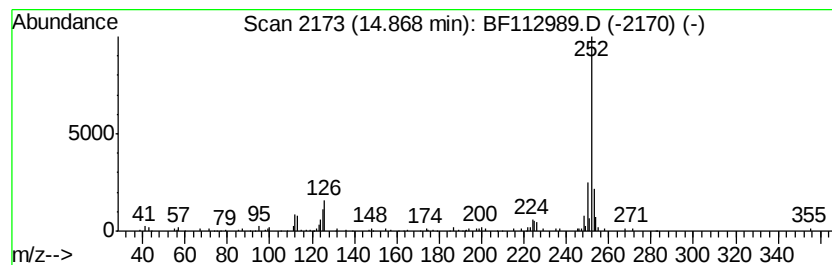
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.96 ng	154636	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[a]pyrene	252	C20H12	000050-32-8	94
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5		Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112989.D
Acq On : 12 Mar 2019 7:34
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EXT-027-SW015-030719

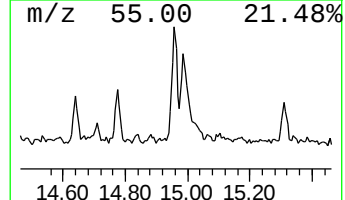
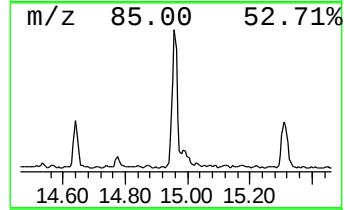
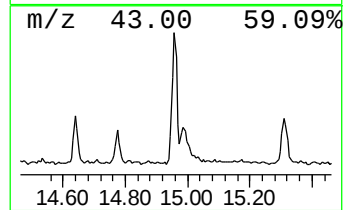
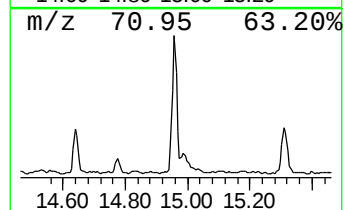
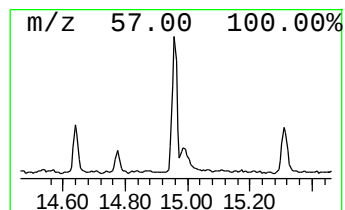
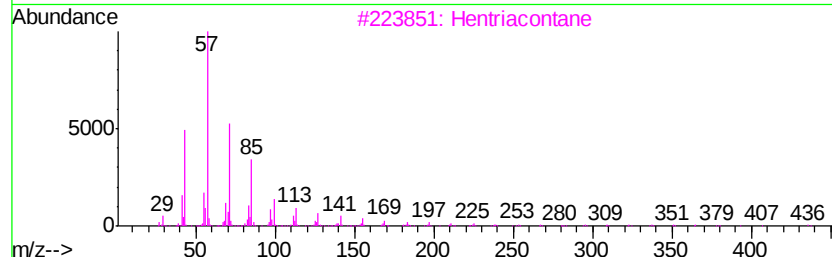
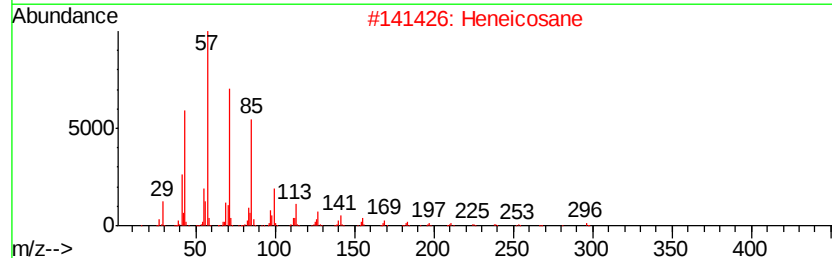
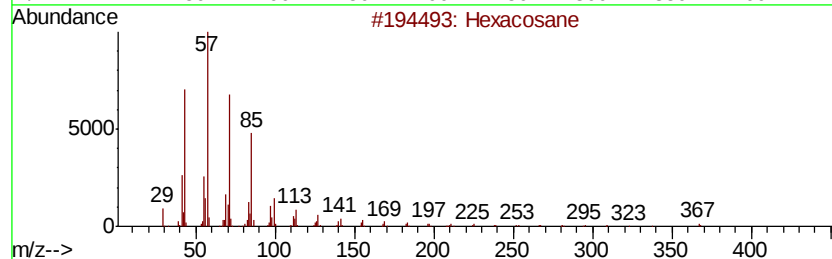
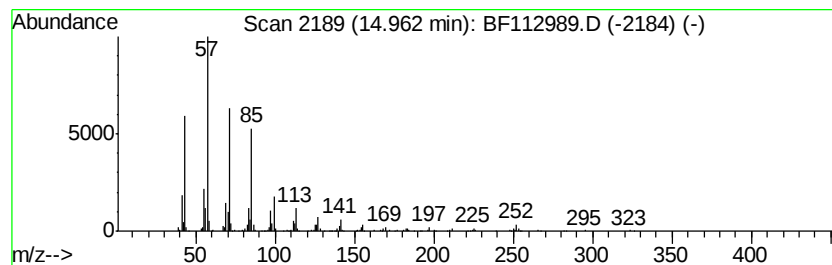
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	9.68 ng	377353	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Eicosane	282	C20H42	000112-95-8	91



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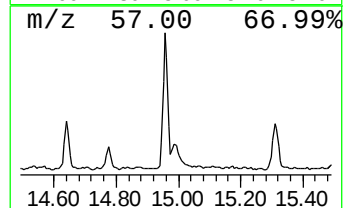
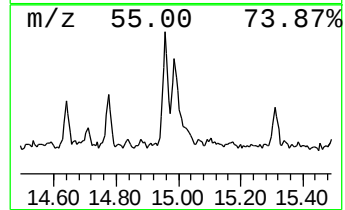
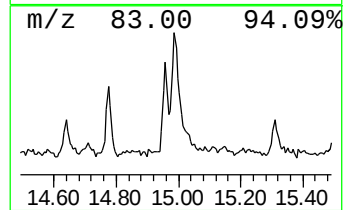
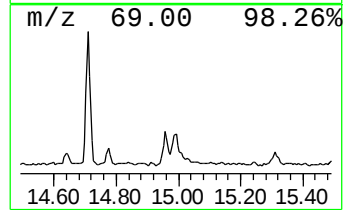
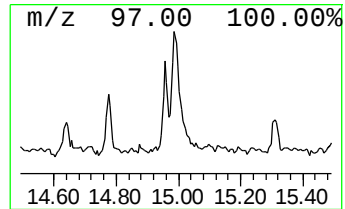
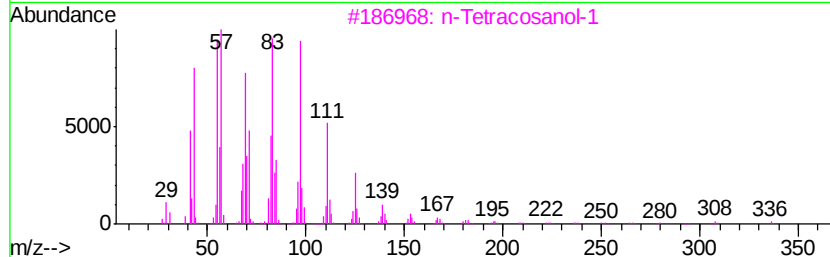
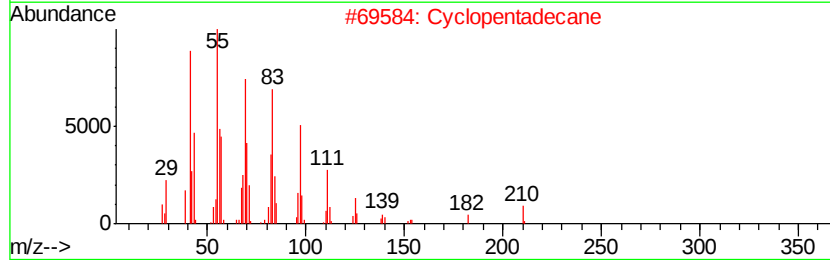
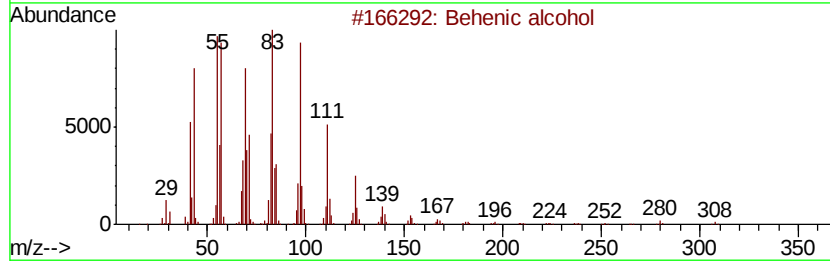
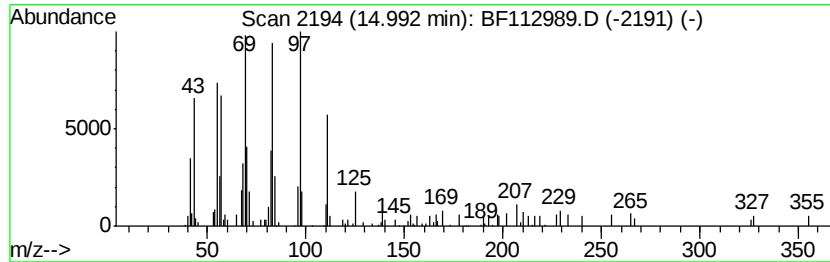
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	5.47 ng	213192	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		Cyclopentadecane	210 C15H30	000295-48-7 90
3		n-Tetracosanol-1	354 C24H50O	000506-51-4 90
4		n-Nonadecanol-1	284 C19H40O	001454-84-8 81
5		1-Heneicosanol	312 C21H44O	015594-90-8 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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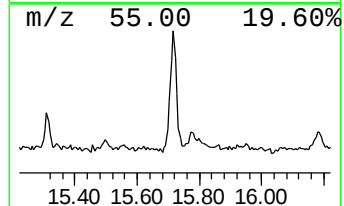
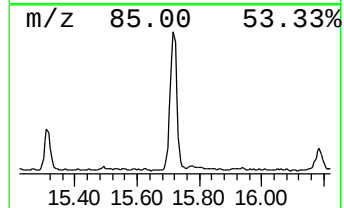
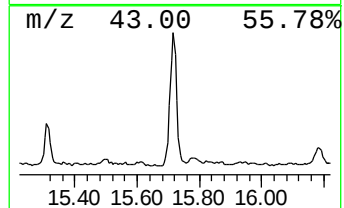
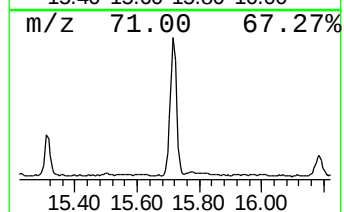
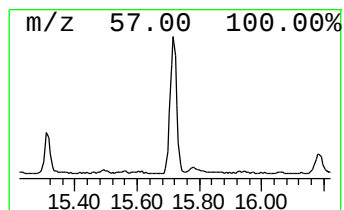
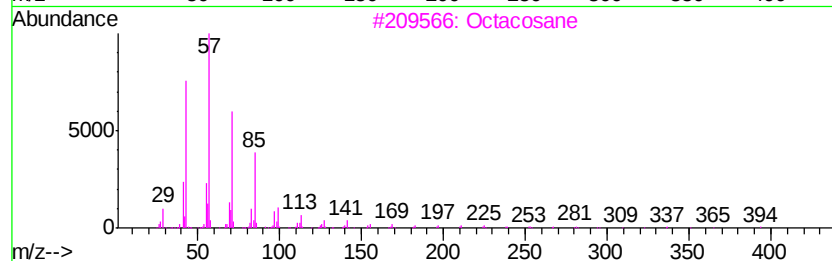
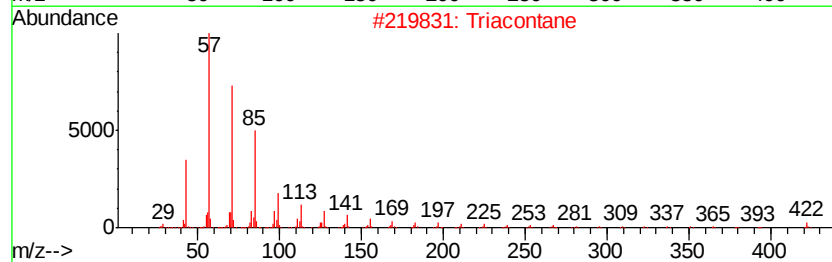
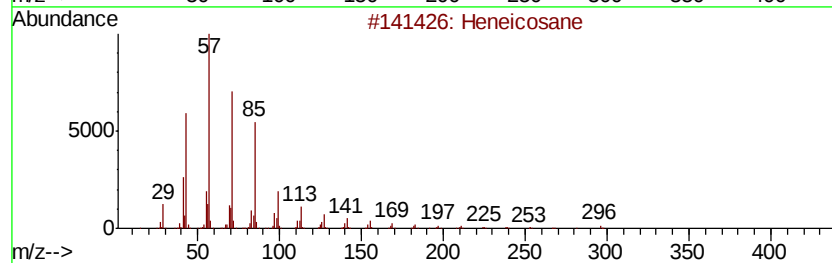
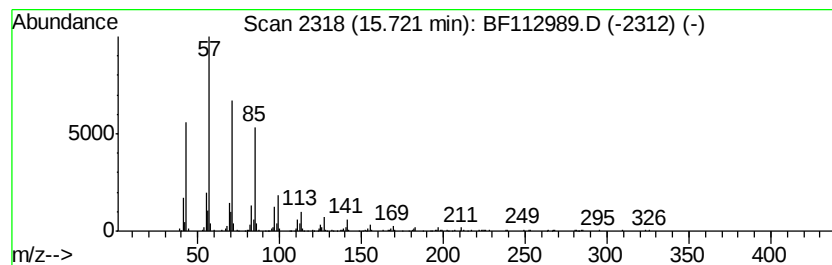
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	13.76 ng	536492	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5		Hentriacontane	437	C31H64	000630-04-6	87



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Misc :
ALS Vial : 35 Sample Multiplier: 1

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ClientSampleId :
EXT-027-SW015-030719

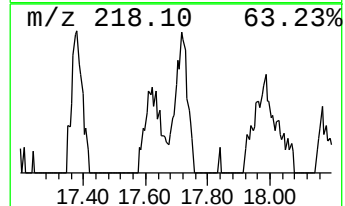
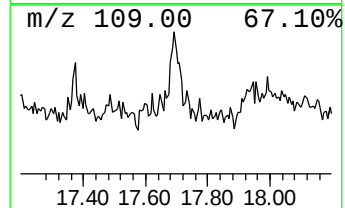
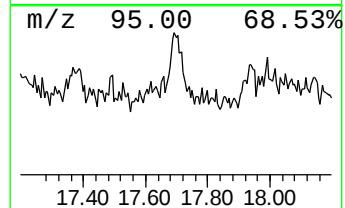
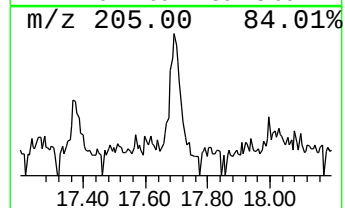
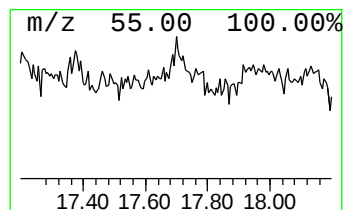
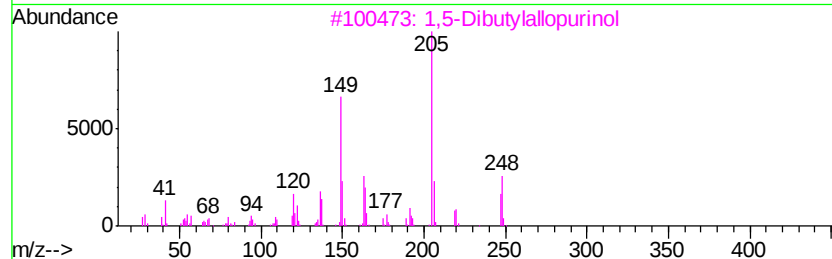
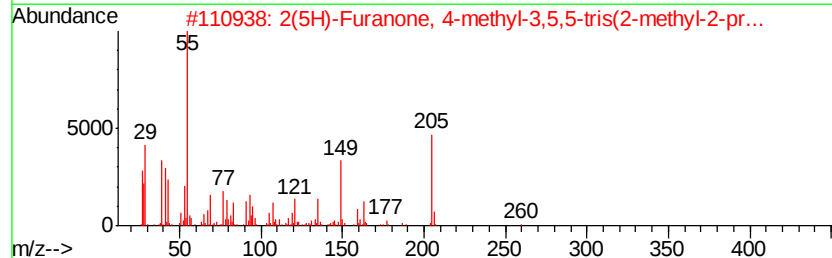
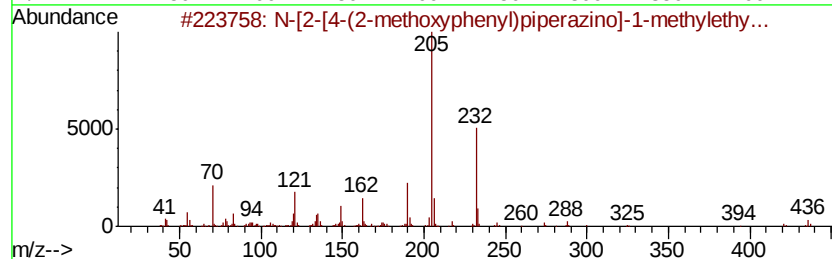
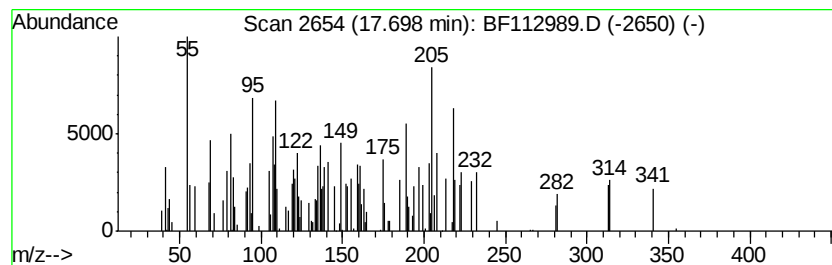
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.70 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	3.21 ng	125042	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-[2-[4-(2-methoxyphenyl)piperaz...	436	C26H36N4O2	302900-97-6	14
2		2(5H)-Furanone, 4-methyl-3,5,5-t...	260	C17H24O2	089902-28-3	12
3		1,5-Dibutylallopurinol	248	C13H20N4O	1000100-00-0	12
4		Cyclopentanecarboxylic acid, 4-m...	292	C20H20O2	1000152-26-8	12
5		1-Hydroxy-2,2,5,5-tetramethyl-4-...	236	C13H17FN2O	087703-52-4	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112989.D
Acq On : 12 Mar 2019 7:34
Operator : JU/SJ
Sample : K1817-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-027-SW015-030719

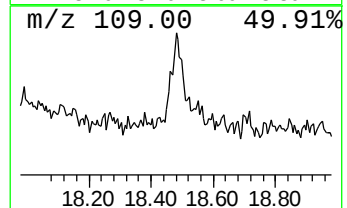
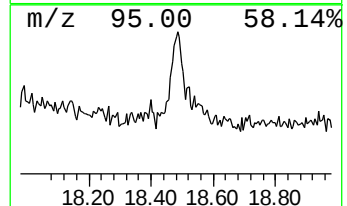
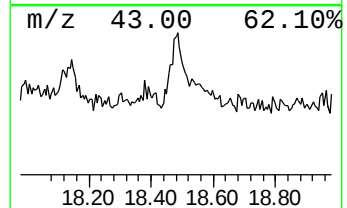
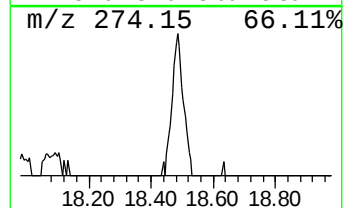
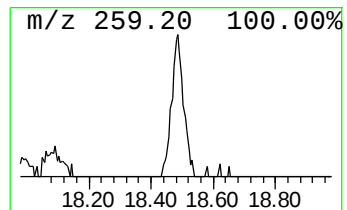
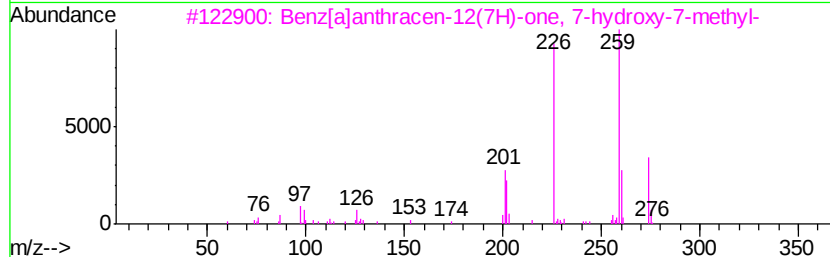
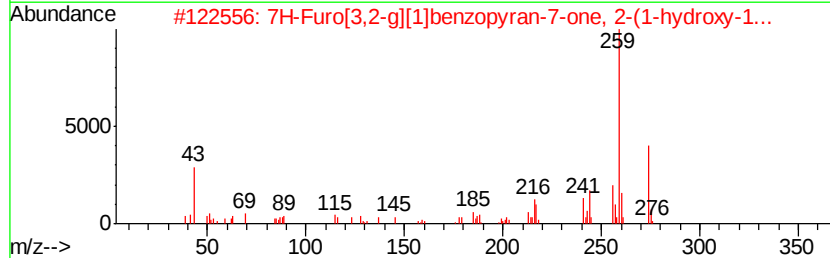
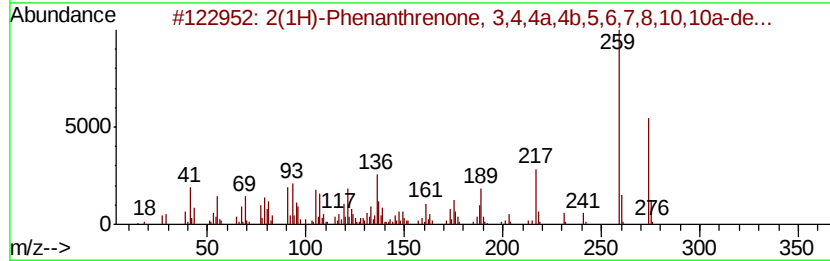
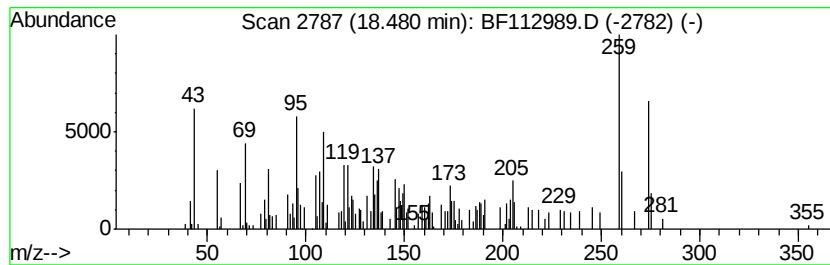
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown18.48 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	3.74 ng	145676	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H300	007715-44-8	46
2		7H-Furo[3,2-q][1]benzopyran-7-on...	274	C15H1405	054087-32-0	38
3		Benz[alanthracen-12(7H)-one, 7-h...	274	C19H1402	017513-43-8	38
4		1,3-DIETHYL-2-HYDROXYBENZOTHAZO...	274	C14H14N202S	1000227-15-3	38
5		D-Homoandrostande, (5.alpha.,13.a...	274	C20H34	054482-31-4	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112989.D
 Acq On : 12 Mar 2019 7:34
 Operator : JU/SJ
 Sample : K1817-07
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EXT-027-SW015-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	65.9	ng	2652250	1	6.73	804607	20.0
n-Hexadecanoic acid	11.77	6.9	ng	466024	4	11.24	1353070	20.0
Octadecanoic acid	12.56	3.1	ng	189530	5	13.86	1205980	20.0
Ethanol, 2-(tetra...	13.73	4.5	ng	271460	5	13.86	1205980	20.0
Heptadecane	14.34	3.9	ng	235724	5	13.86	1205980	20.0
Nonadecane	14.64	3.0	ng	116480	6	15.27	780052	20.0
Squalene	14.71	3.8	ng	147242	6	15.27	780052	20.0
Octadecanal	14.77	3.1	ng	119268	6	15.27	780052	20.0
Benzo[e]pyrene	14.87	4.0	ng	154636	6	15.27	780052	20.0
Hexacosane	14.96	9.7	ng	377353	6	15.27	780052	20.0
Behenic alcohol	14.99	5.5	ng	213192	6	15.27	780052	20.0
unknown15.72	15.72	13.8	ng	536492	6	15.27	780052	20.0
unknown17.70	17.70	3.2	ng	125042	6	15.27	780052	20.0
unknown18.48	18.48	3.7	ng	145676	6	15.27	780052	20.0