

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
 Data File : BF109609.D
 Acq On : 5 Oct 2018 13:49
 Operator : JU/SJ
 Sample : J5150-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-0926-S-10B

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-BF092218.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	4.898	475	478	486	rBV	26822	37638	1.71%	0.162%
2	5.328	547	551	577	rBV	1413311	1597993	72.44%	6.875%
3	6.357	721	726	742	rBV	1475167	1810175	82.06%	7.788%
4	6.475	742	746	762	rVB	1812960	1765481	80.03%	7.596%
5	6.704	781	785	795	rBV	482044	538032	24.39%	2.315%
6	6.857	807	811	829	rBV	1532989	1386080	62.83%	5.964%
7	7.263	876	880	893	rBV	1086978	1130278	51.24%	4.863%
8	7.981	998	1002	1020	rBV	764540	733023	33.23%	3.154%
9	9.057	1181	1185	1199	rBV	2276285	2205999	100.00%	9.491%
10	9.451	1248	1252	1260	rBV	182132	157637	7.15%	0.678%
11	9.733	1296	1300	1311	rBV	816027	834840	37.84%	3.592%
12	10.516	1429	1433	1449	rBV	990707	991075	44.93%	4.264%
13	11.210	1547	1551	1554	rBV	830563	784291	35.55%	3.374%
14	11.757	1638	1644	1653	rBV	893353	1291720	58.55%	5.558%
15	12.069	1694	1697	1704	rVB2	34806	41404	1.88%	0.178%
16	12.416	1749	1756	1758	rBV	175994	193694	8.78%	0.833%
17	12.539	1770	1777	1789	rBV	951932	1344716	60.96%	5.786%
18	12.639	1790	1794	1798	rVB	127801	154074	6.98%	0.663%
19	12.792	1816	1820	1828	rVB	1942768	1742656	79.00%	7.498%
20	13.027	1858	1860	1864	rVB2	31932	29196	1.32%	0.126%
21	13.368	1915	1918	1922	rVB	45512	40542	1.84%	0.174%
22	13.486	1934	1938	1939	rBV3	33563	45710	2.07%	0.197%
23	13.533	1939	1946	1947	rVV3	39731	89546	4.06%	0.385%
24	13.692	1969	1973	1981	rVB2	140779	190700	8.64%	0.820%
25	13.833	1993	1997	2001	rBV	637937	746410	33.84%	3.211%
26	13.863	2001	2002	2011	rVB	87705	62273	2.82%	0.268%
27	14.010	2024	2027	2032	rBV	71893	70734	3.21%	0.304%
28	14.315	2075	2079	2083	rBV	149178	143884	6.52%	0.619%
29	14.610	2125	2129	2137	rBV	244880	262942	11.92%	1.131%
30	14.674	2137	2140	2148	rVB	101537	109010	4.94%	0.469%
31	14.845	2165	2169	2178	rVB	96336	197053	8.93%	0.848%
32	14.921	2178	2182	2190	rBV	347045	385971	17.50%	1.661%
33	15.121	2213	2216	2220	rBV	34072	52803	2.39%	0.227%
34	15.180	2223	2226	2230	rVV	82241	153449	6.96%	0.660%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.239	2231	2236	2239	rVV	601316	876395	39.73%	3.771%
36	15.274	2239	2242	2251	rVB	355113	490438	22.23%	2.110%
37	15.668	2304	2309	2315	rBV	213648	322159	14.60%	1.386%
38	16.127	2383	2387	2395	rVB	103631	162484	7.37%	0.699%
39	16.668	2474	2479	2484	rVB	39254	69507	3.15%	0.299%

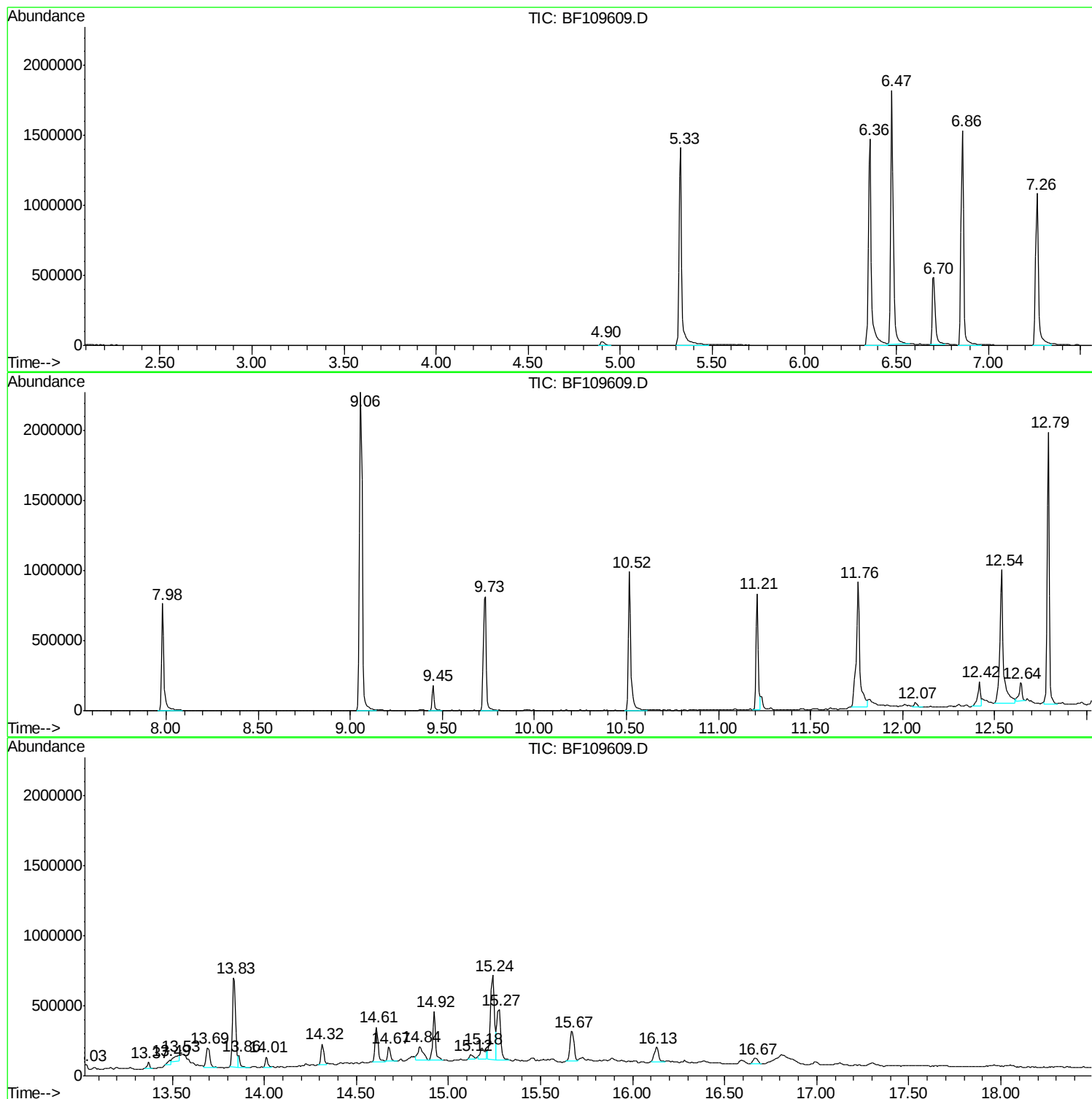
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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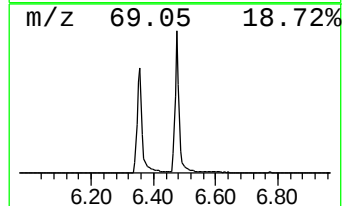
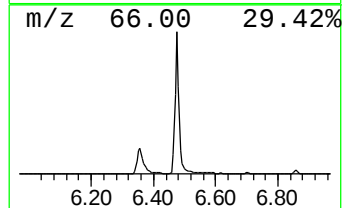
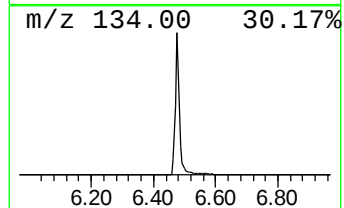
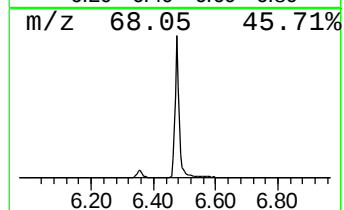
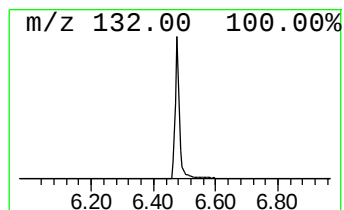
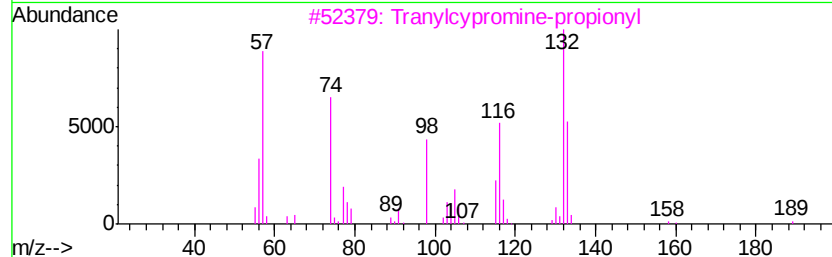
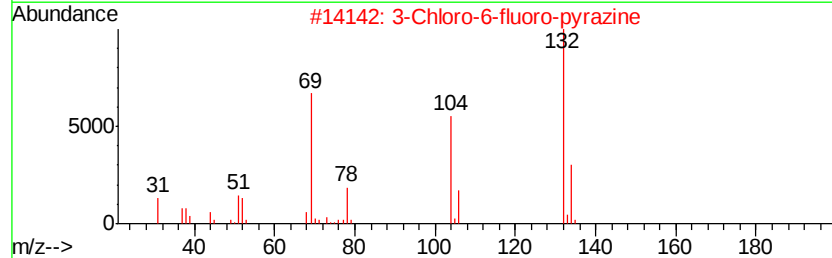
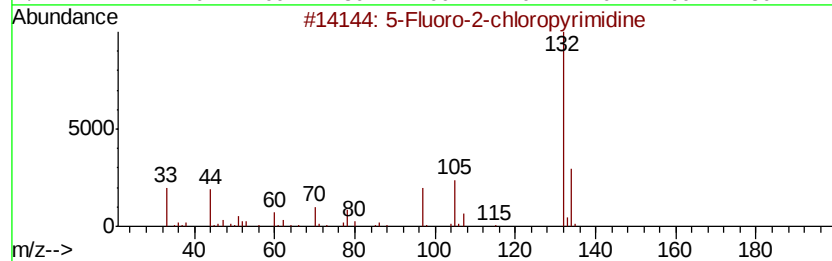
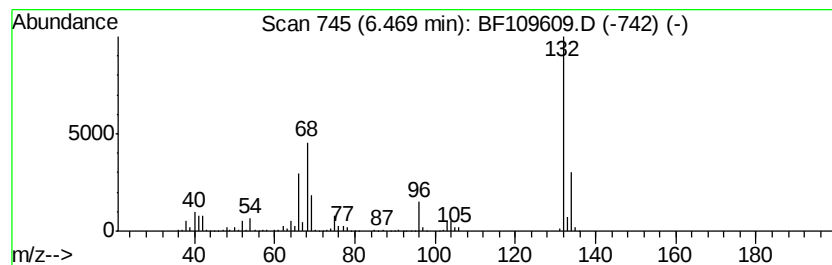
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	65.63 ng	1765480	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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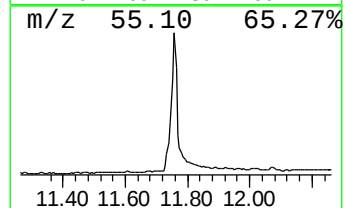
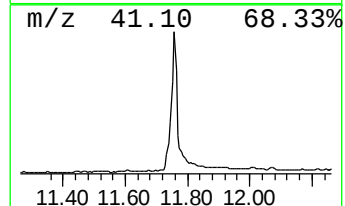
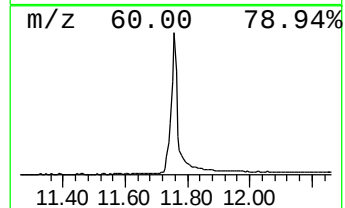
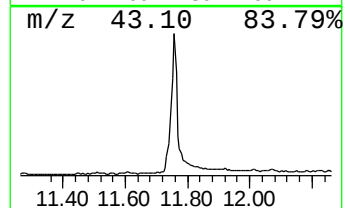
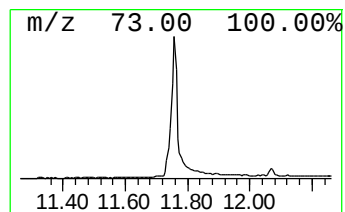
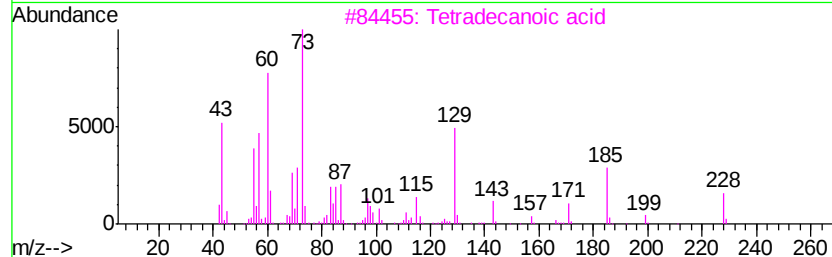
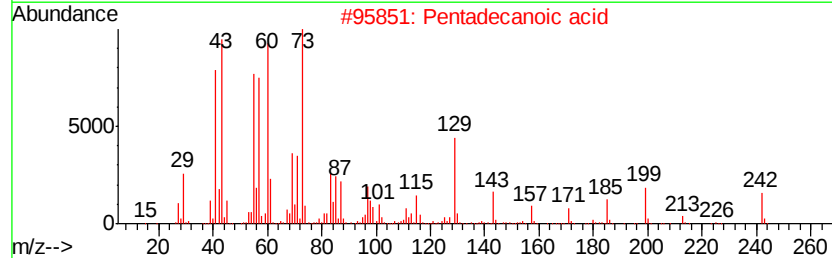
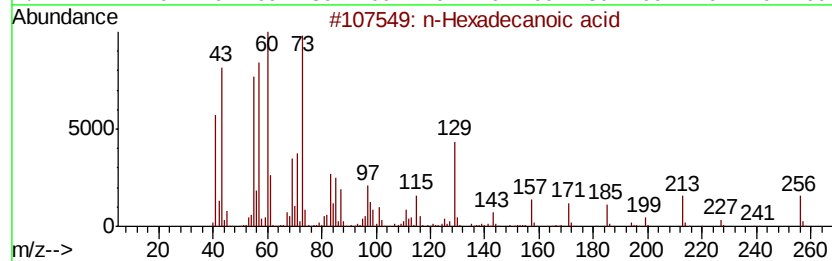
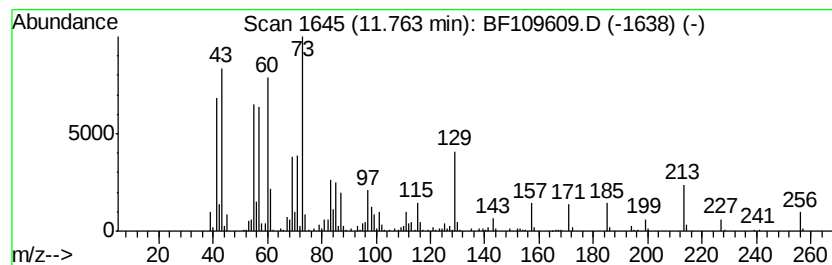
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	32.94 ng	1291720	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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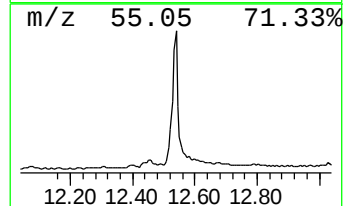
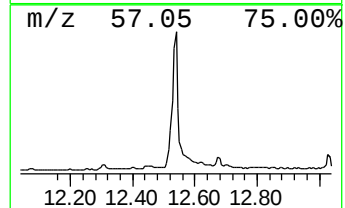
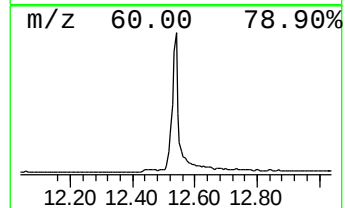
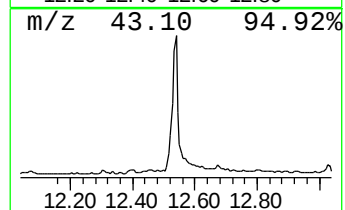
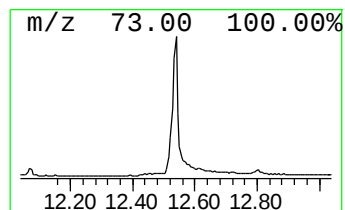
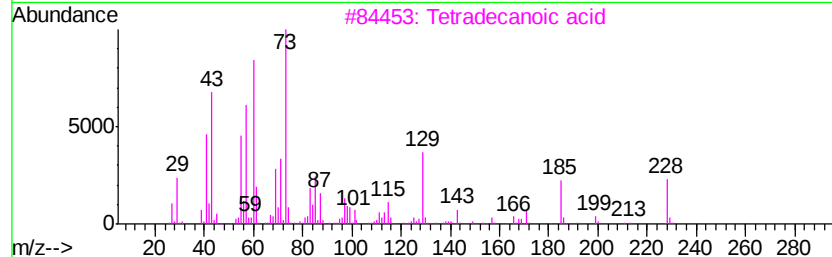
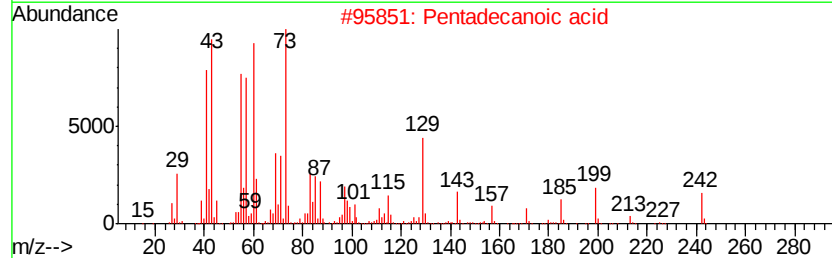
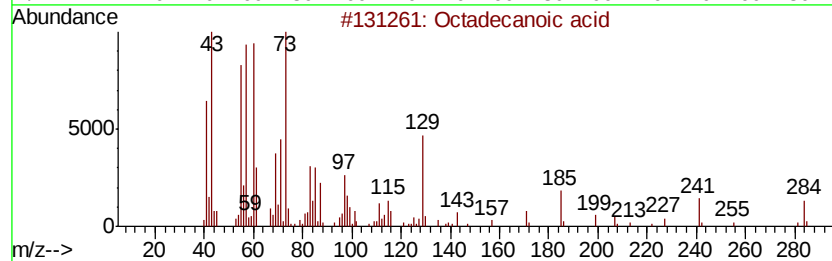
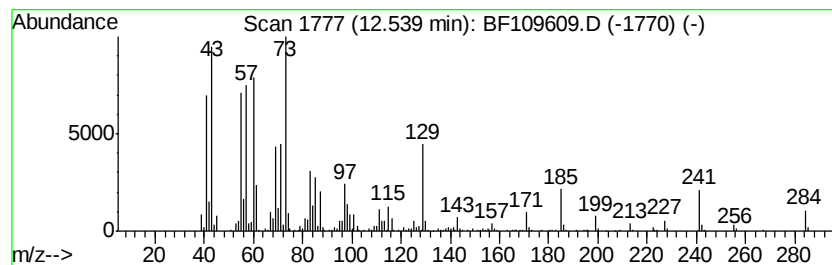
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	36.03 ng	1344720	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



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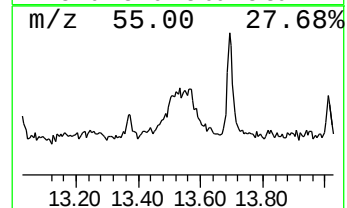
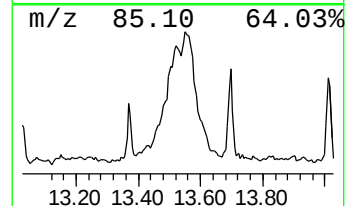
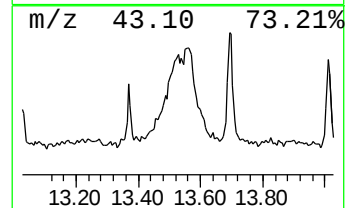
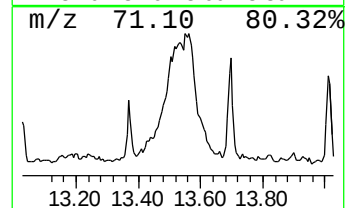
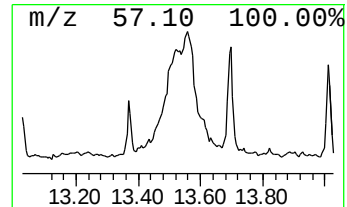
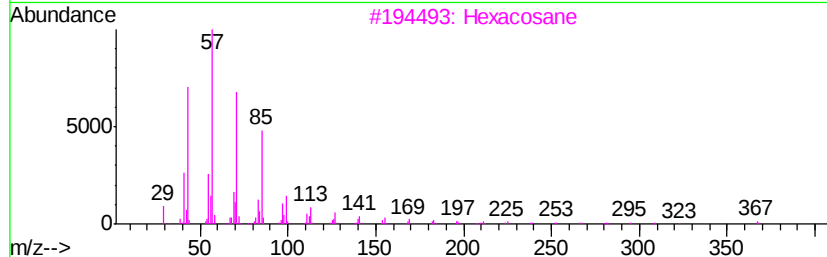
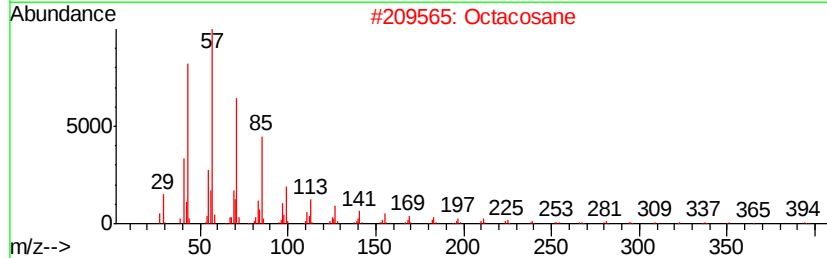
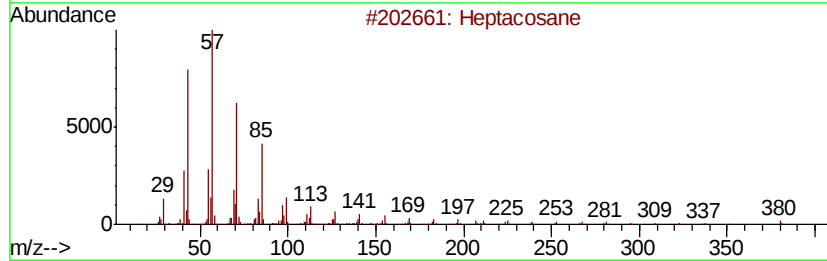
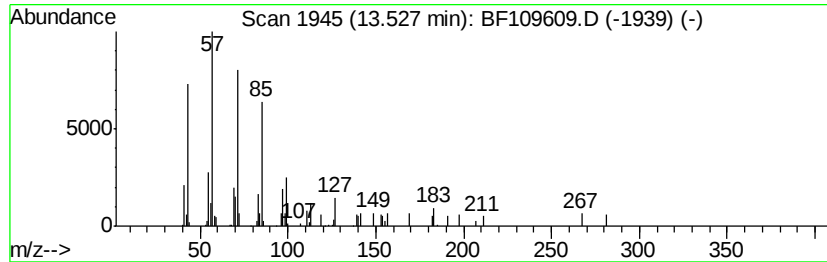
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Peak Number 5 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.40 ng	89546	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Octacosane		394	C28H58	000630-02-4	86
3	Hexacosane		366	C26H54	000630-01-3	80
4	Tetratriacontane		479	C34H70	014167-59-0	80
5	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	80



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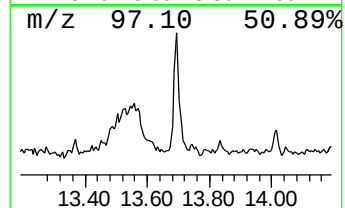
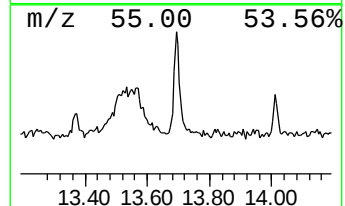
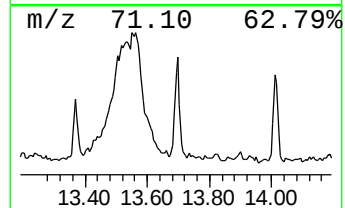
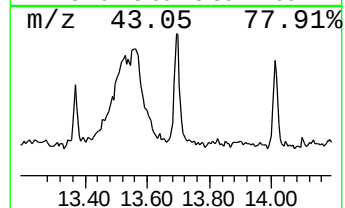
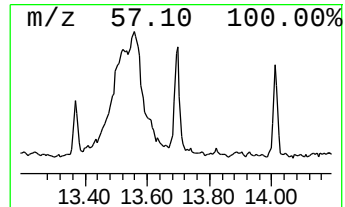
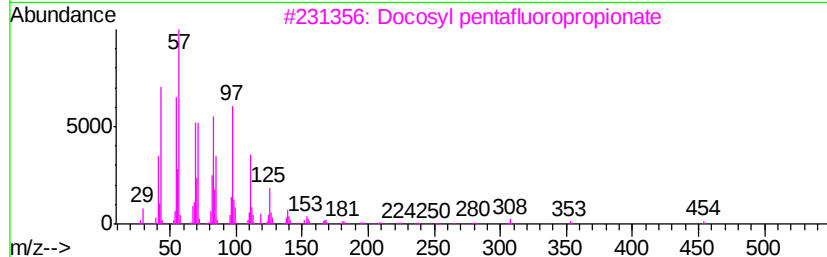
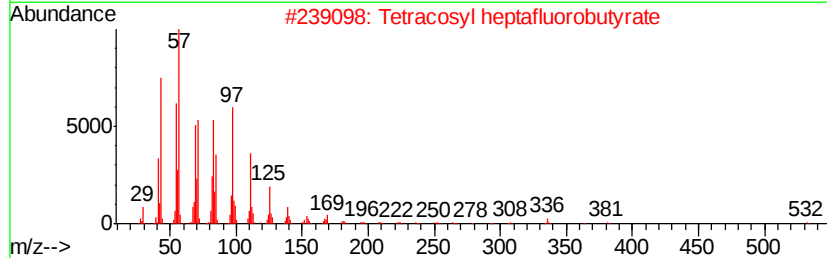
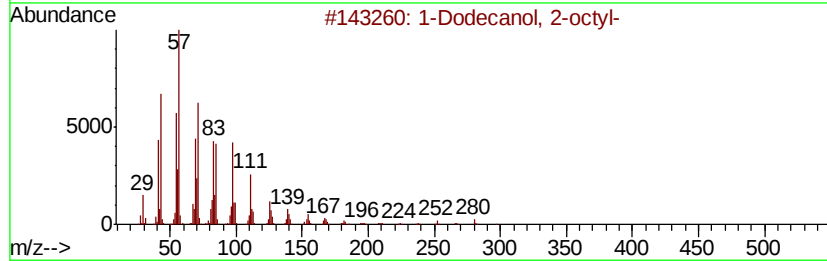
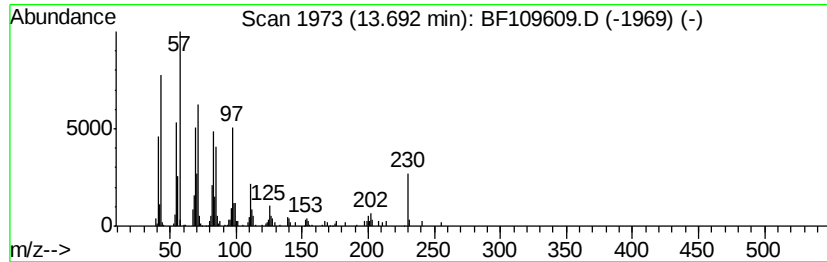
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	5.11 ng	190700	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	81
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	81
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
Sample : J5150-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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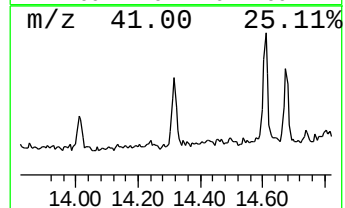
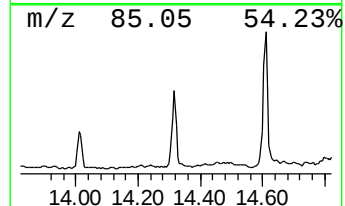
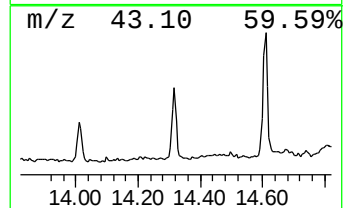
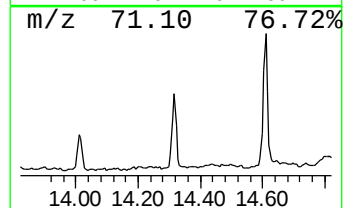
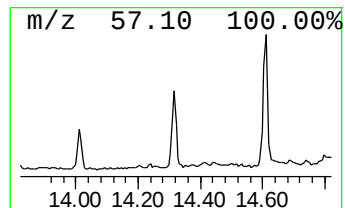
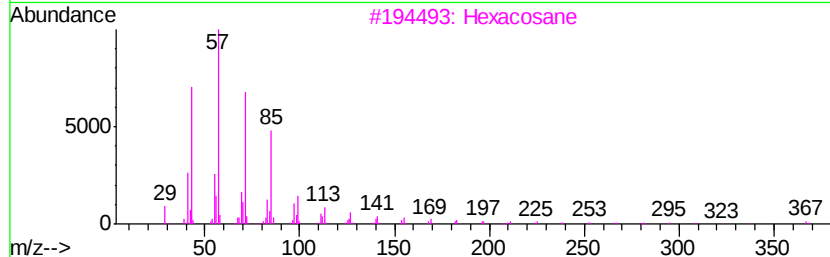
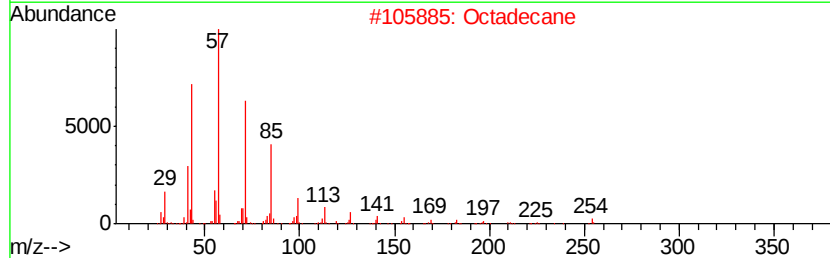
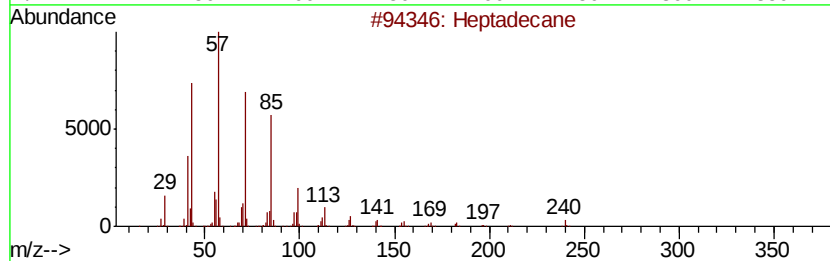
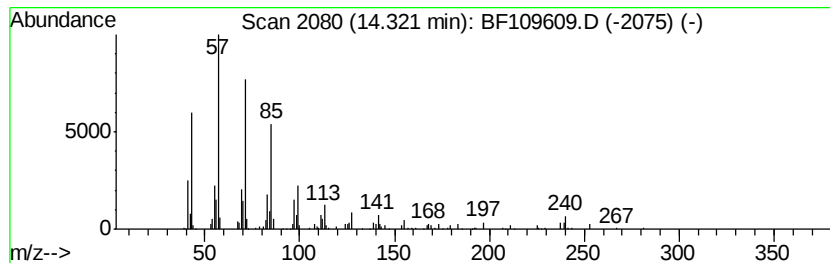
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	3.86 ng	143884	Chrysene-d12	13.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	98
2			Octadecane	254	C18H38	000593-45-3	96
3			Hexacosane	366	C26H54	000630-01-3	93
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
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ClientSampleId :
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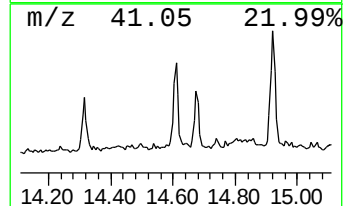
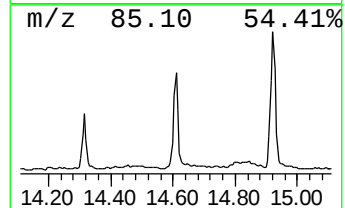
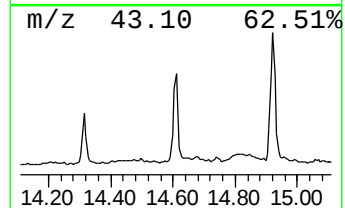
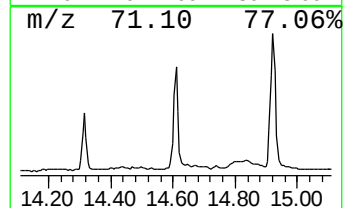
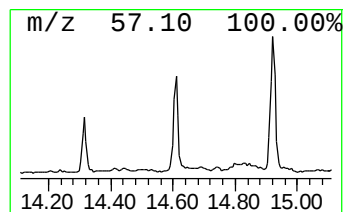
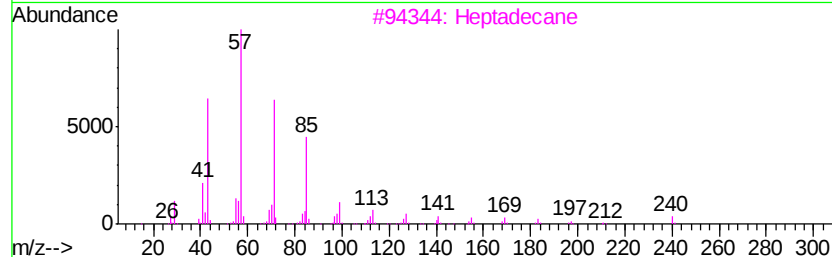
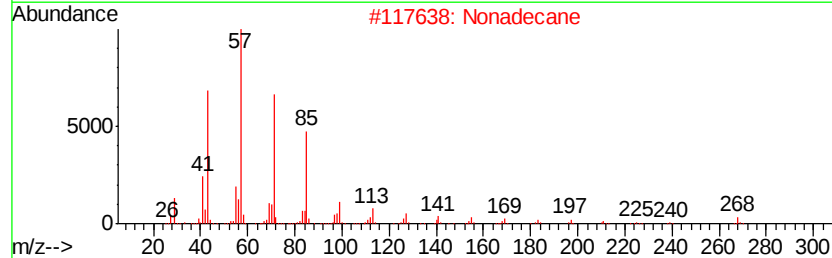
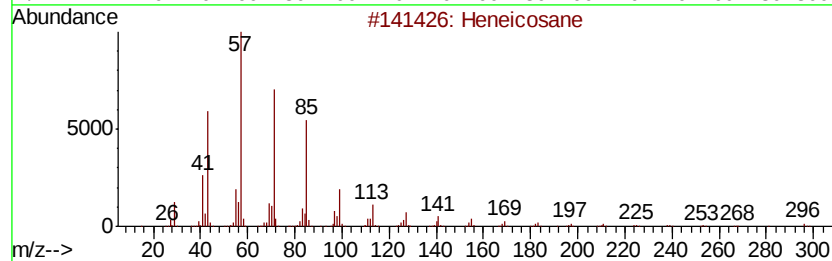
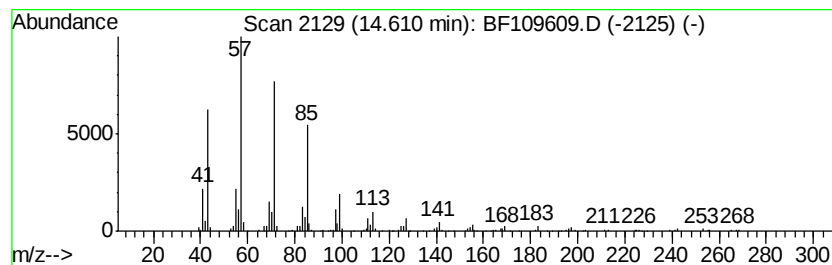
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	6.00 ng	262942	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Nonadecane	268	C19H40	000629-92-5	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
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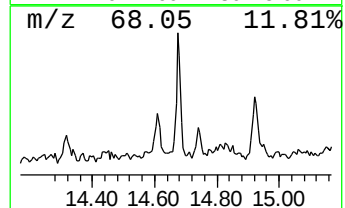
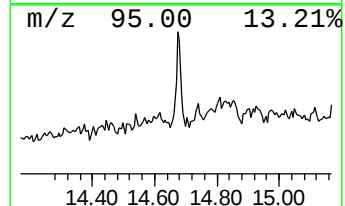
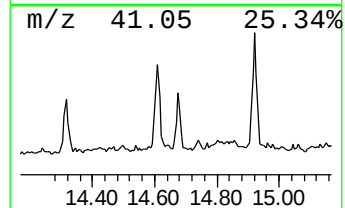
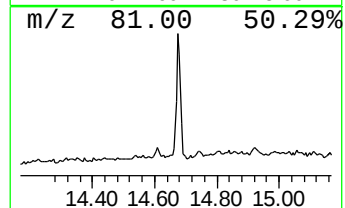
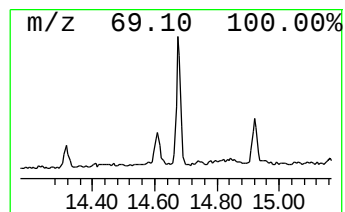
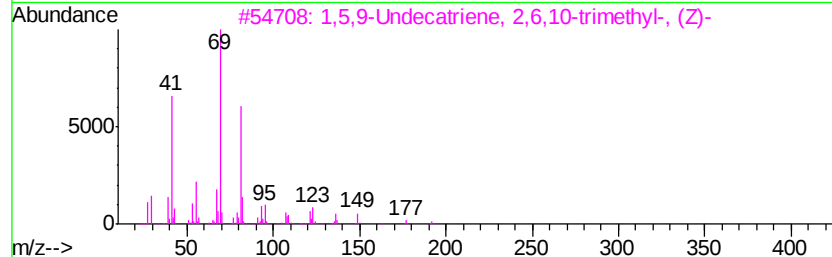
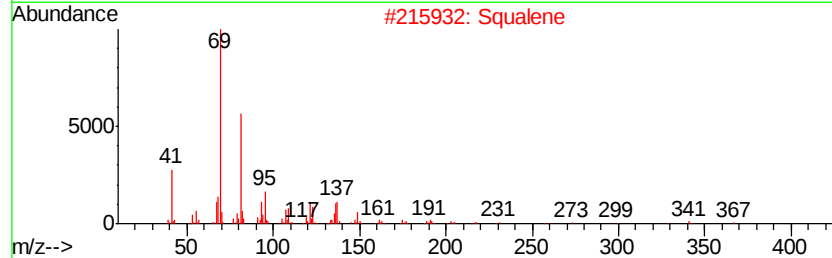
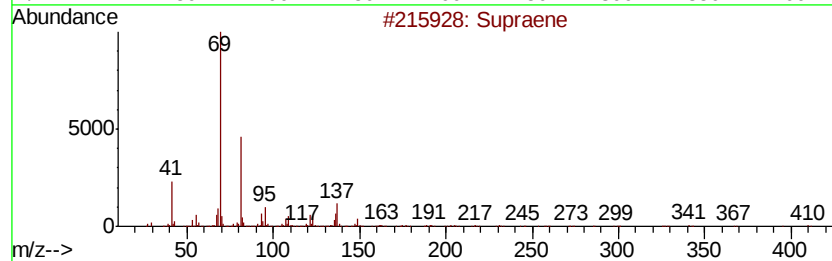
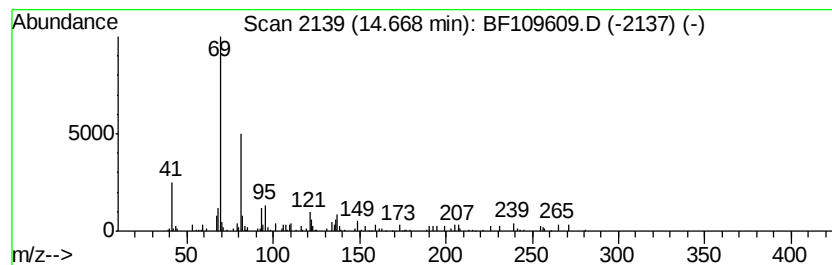
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.49 ng	109010	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	87
2	Squalene		410	C30H50	000111-02-4	83
3	1,5,9-Undecatriene, 2,6,10-trime...		192	C14H24	062951-96-6	81
4	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72
5	Trideca-1,3,7,11-tetraene-1,1-di...		268	C18H24N2	1000159-88-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
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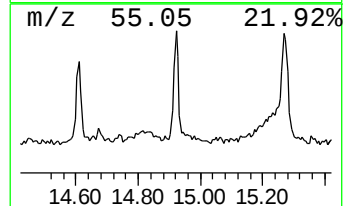
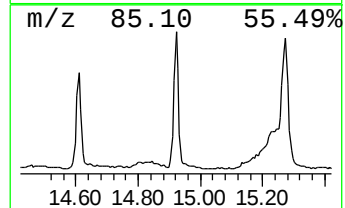
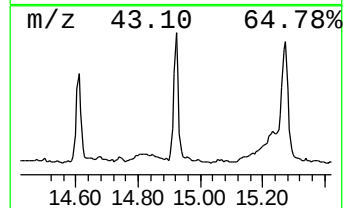
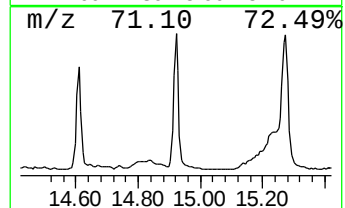
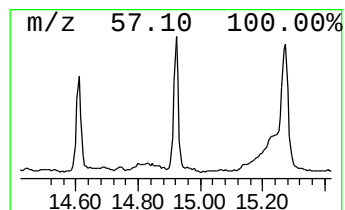
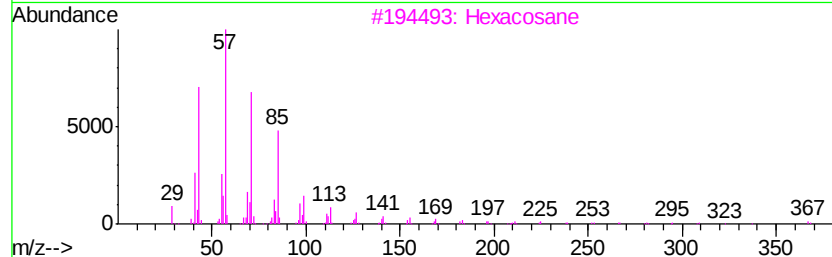
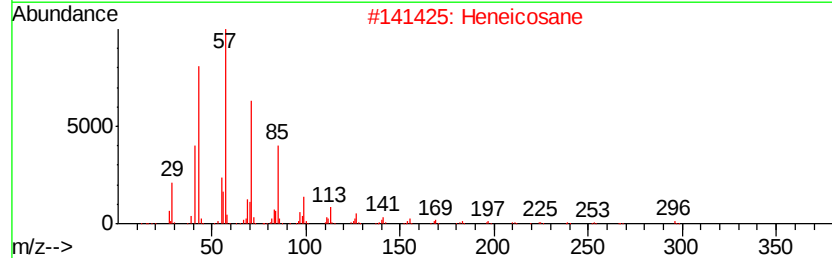
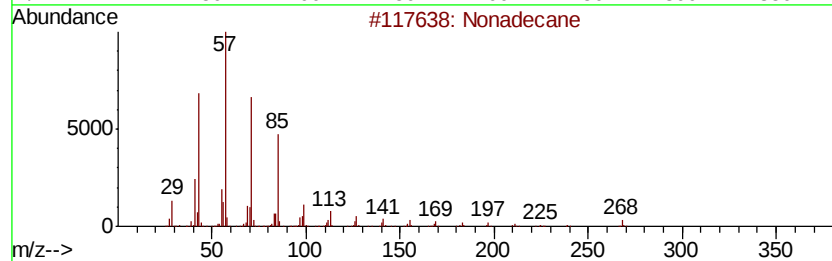
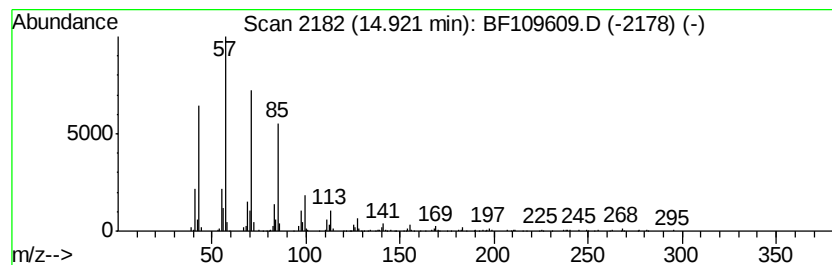
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	8.81 ng	385971	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
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Instrument :
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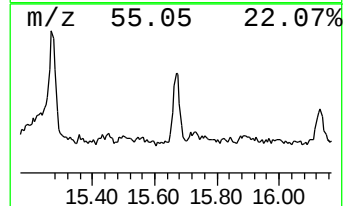
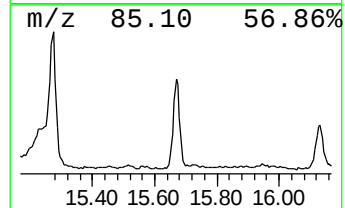
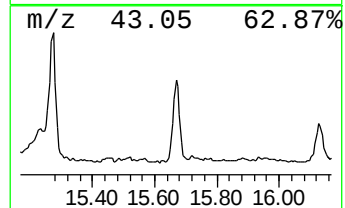
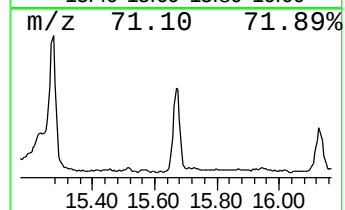
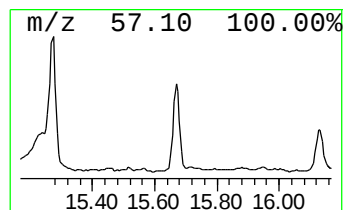
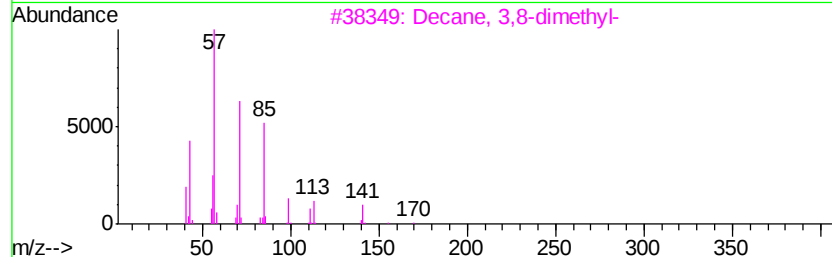
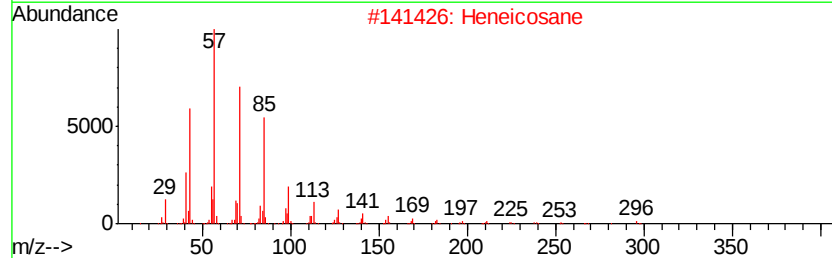
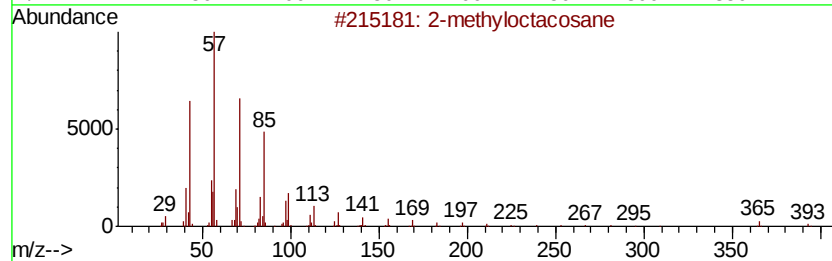
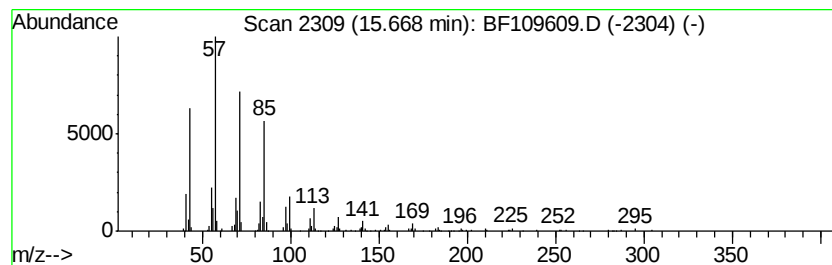
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	7.35 ng	322159	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109609.D
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Operator : JU/SJ
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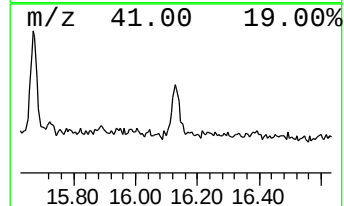
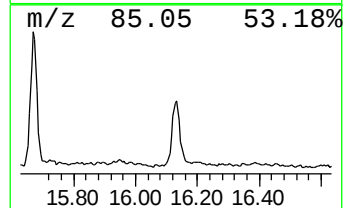
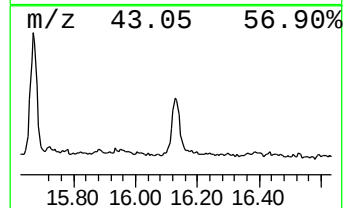
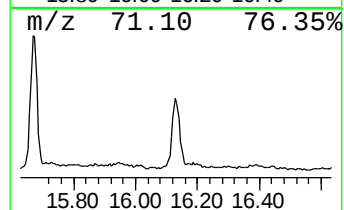
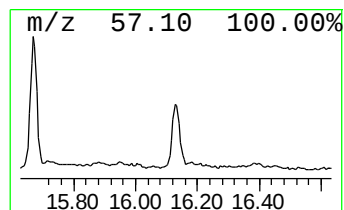
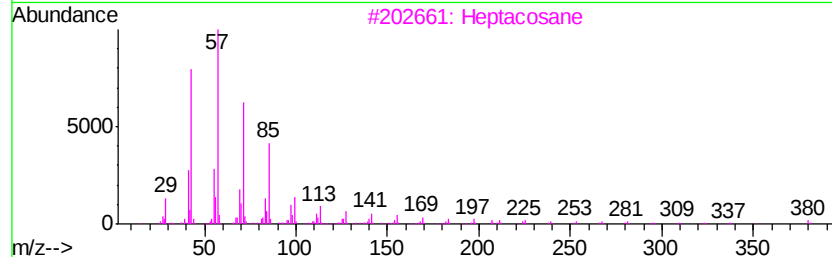
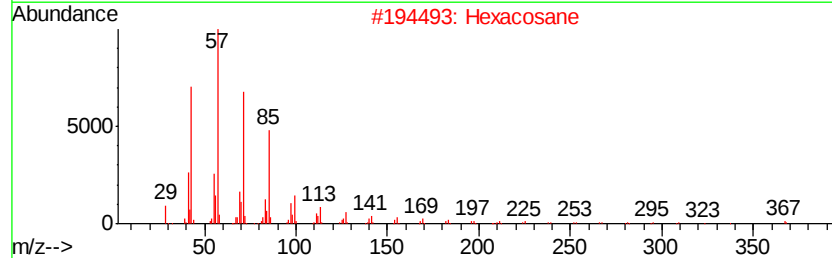
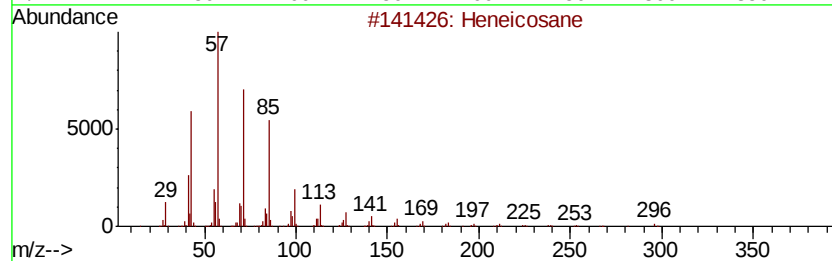
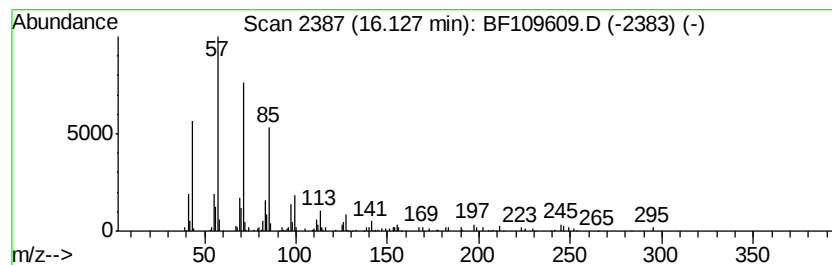
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.71 ng	162484	Perylene-d12	15.24

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		Heptacosane	380	C27H56	000593-49-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100518\
Data File : BF109609.D
Acq On : 5 Oct 2018 13:49
Operator : JU/SJ
Sample : J5150-01
Misc :
ALS Vial : 4 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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n-Hexadecanoic acid	11.76	32.9	ng	1291720	4	11.21	784291	20.0
Octadecanoic acid	12.54	36.0	ng	1344720	5	13.84	746410	20.0
Heptacosane	13.53	2.4	ng	89546	5	13.84	746410	20.0
1-Dodecanol, 2-oc...	13.69	5.1	ng	190700	5	13.84	746410	20.0
Heptadecane	14.32	3.9	ng	143884	5	13.84	746410	20.0
Heneicosane	14.61	6.0	ng	262942	6	15.24	876395	20.0
Supraene	14.67	2.5	ng	109010	6	15.24	876395	20.0
Nonadecane	14.92	8.8	ng	385971	6	15.24	876395	20.0
2-methyloctacosane	15.67	7.3	ng	322159	6	15.24	876395	20.0
Octacosane	16.13	3.7	ng	162484	6	15.24	876395	20.0