

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
 Data File : BF109918.D
 Acq On : 17 Oct 2018 12:26
 Operator : JU/SJ
 Sample : J5516-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1011-S-DH-32

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-BF101518.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	33	39	47	rVB	801427	1044982	20.04%	1.769%
2	3.575	251	253	266	rBV2	53498	110286	2.11%	0.187%
3	5.216	527	532	539	rVB	114875	139085	2.67%	0.236%
4	5.598	592	597	600	rBV	4823091	4421534	84.78%	7.487%
5	6.592	761	766	769	rBV	4296498	4661820	89.38%	7.894%
6	6.745	787	792	795	rBV	5075383	4629285	88.76%	7.839%
7	6.981	828	832	835	rVB	1739913	1467343	28.13%	2.485%
8	7.134	854	858	862	rBV	4158821	3694132	70.83%	6.255%
9	7.539	922	927	930	rBV	3302057	2982624	57.19%	5.050%
10	8.263	1046	1050	1053	rBV	2375058	1955034	37.48%	3.310%
11	9.333	1226	1232	1236	rBV	5379040	5215599	100.00%	8.831%
12	9.439	1246	1250	1253	rVB	212050	181036	3.47%	0.307%
13	9.728	1295	1299	1302	rBV	526439	447300	8.58%	0.757%
14	10.022	1345	1349	1353	rBV2	2580531	2181494	41.83%	3.694%
15	10.810	1479	1483	1486	rBV	2790416	2361593	45.28%	3.999%
16	11.516	1598	1603	1606	rBV	2379260	2255916	43.25%	3.820%
17	12.022	1681	1689	1695	rBV	850661	1077817	20.67%	1.825%
18	12.727	1805	1809	1813	rBV	118944	138223	2.65%	0.234%
19	12.810	1817	1823	1837	rVV	955451	1339943	25.69%	2.269%
20	12.904	1837	1839	1843	rVV2	145588	147530	2.83%	0.250%
21	12.957	1846	1848	1850	rVV	156338	125977	2.42%	0.213%
22	12.980	1850	1852	1855	rVB	93730	69228	1.33%	0.117%
23	13.098	1868	1872	1875	rVB	5447745	4810757	92.24%	8.146%
24	13.316	1906	1909	1912	rVB	108827	91360	1.75%	0.155%
25	13.568	1947	1952	1956	rBV	342701	444206	8.52%	0.752%
26	13.604	1956	1958	1962	rVV2	159690	177774	3.41%	0.301%
27	13.657	1962	1967	1969	rVV2	172777	196080	3.76%	0.332%
28	13.980	2018	2022	2029	rVB	451901	469324	9.00%	0.795%
29	14.157	2048	2052	2055	rBV	1852195	1615182	30.97%	2.735%
30	14.251	2065	2068	2073	rBV	90073	136708	2.62%	0.231%
31	14.304	2073	2077	2080	rVB	309272	305949	5.87%	0.518%
32	14.604	2124	2128	2136	rBV	609575	641055	12.29%	1.085%
33	14.927	2178	2183	2188	rBV	1112796	1236758	23.71%	2.094%
34	15.010	2194	2197	2203	rVB	61997	68795	1.32%	0.116%

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.286	2239	2244	2257	rVB	1512156	1870296	35.86%	3.167%
36	15.545	2283	2288	2296	rBV4	43367	93286	1.79%	0.158%
37	15.686	2306	2312	2322	rBV2	2092253	3482926	66.78%	5.897%
38	15.974	2359	2361	2366	rVB2	48528	54724	1.05%	0.093%
39	16.157	2385	2392	2398	rBV	938619	1514054	29.03%	2.564%
40	16.698	2478	2484	2492	rVB	403258	755576	14.49%	1.279%
41	17.339	2587	2593	2601	rVB	120565	257973	4.95%	0.437%
42	17.868	2678	2683	2693	rVB9	73088	187719	3.60%	0.318%

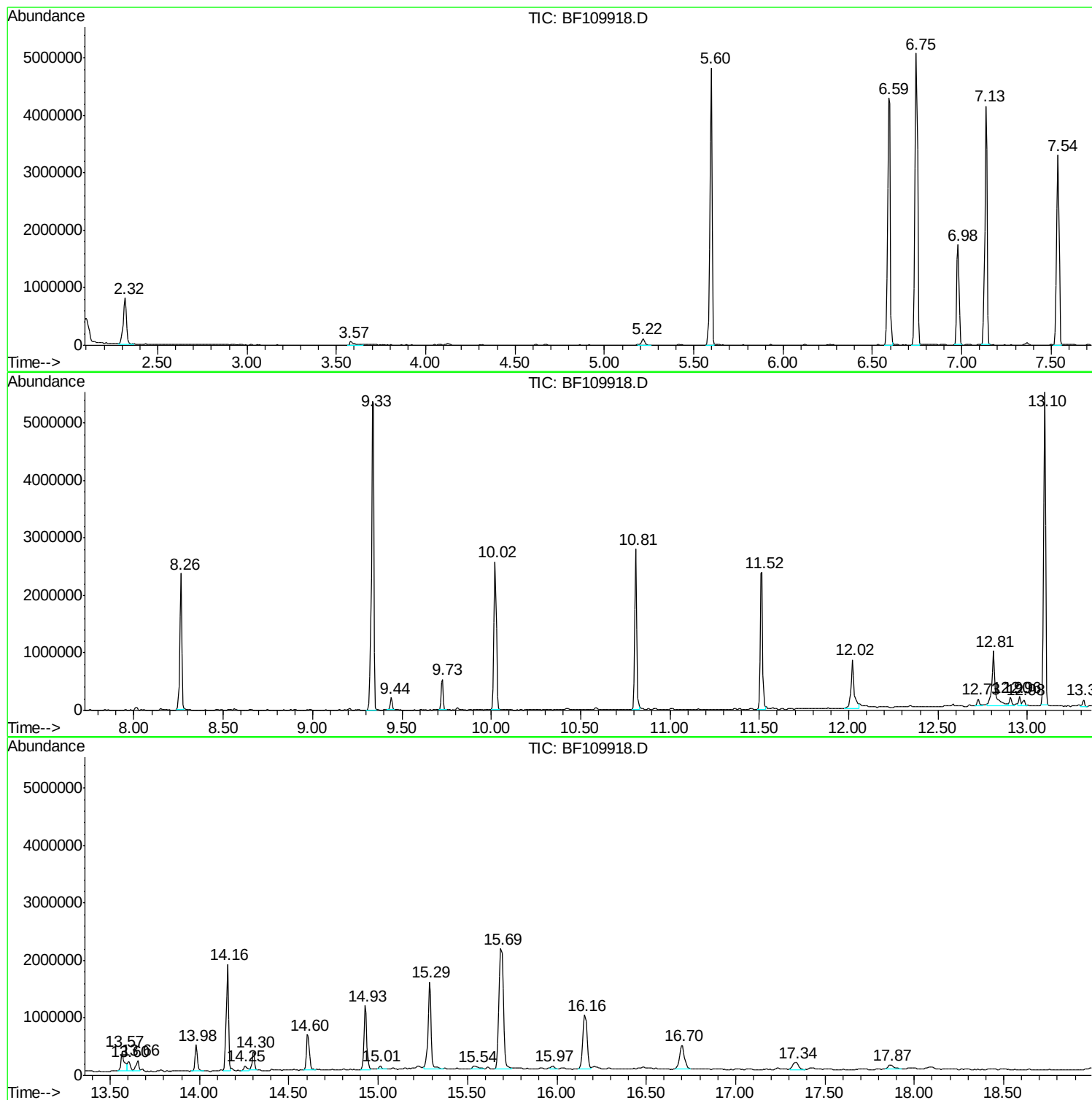
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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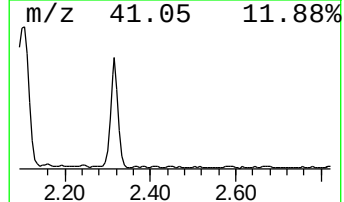
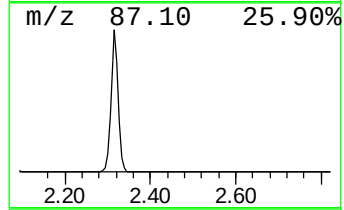
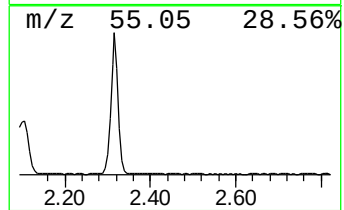
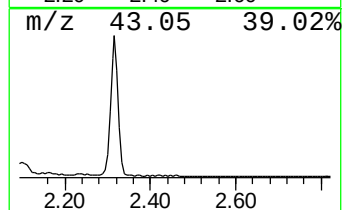
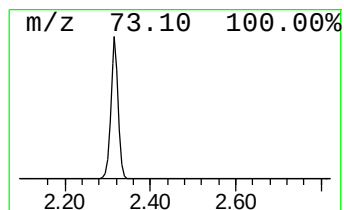
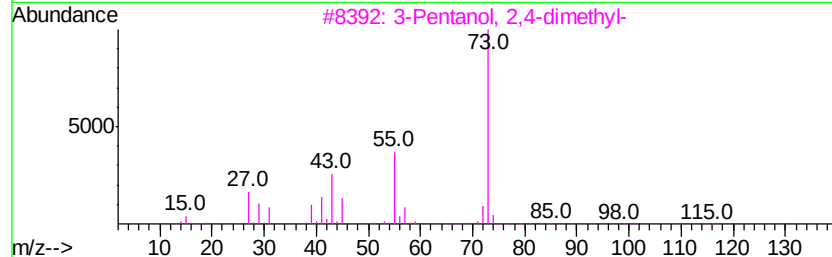
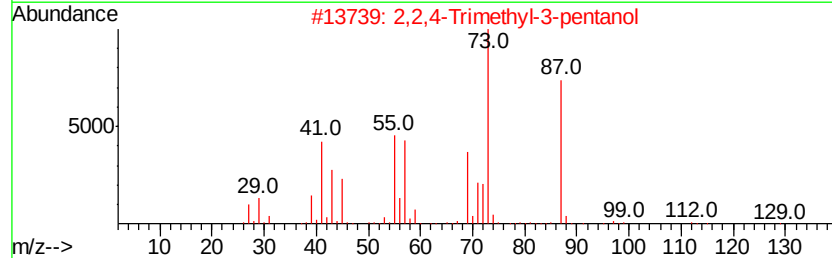
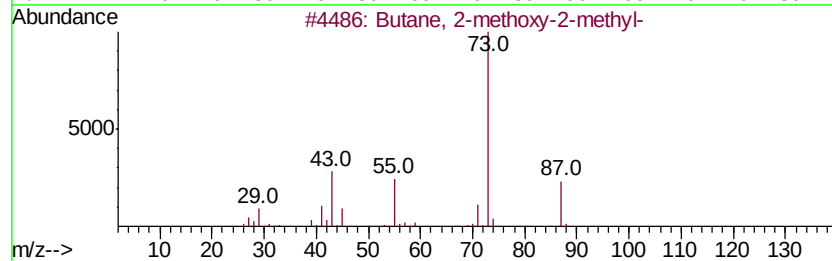
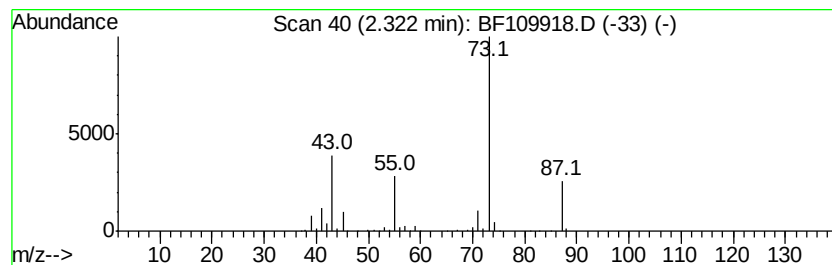
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	14.24 ng	1044980	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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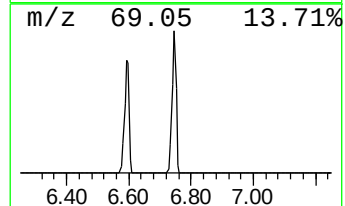
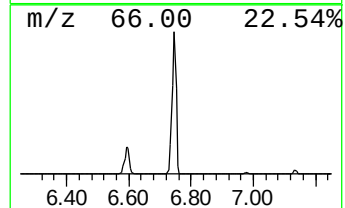
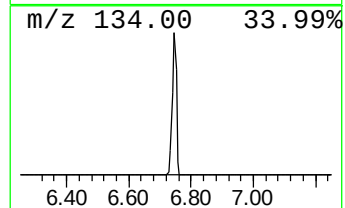
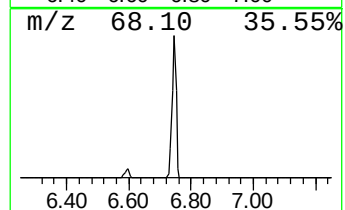
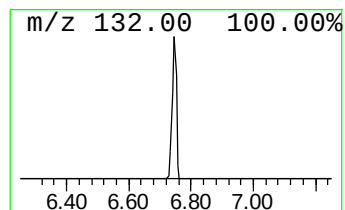
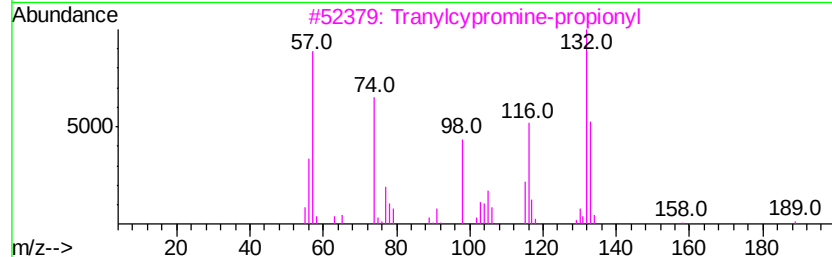
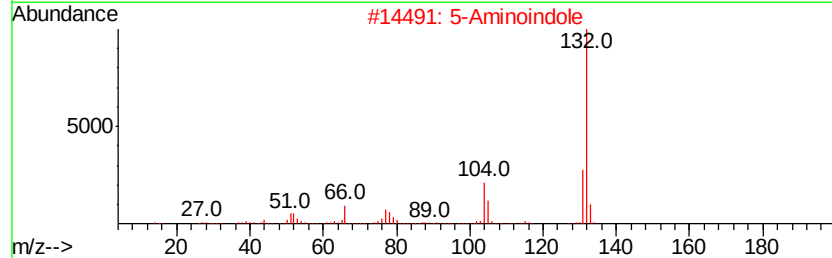
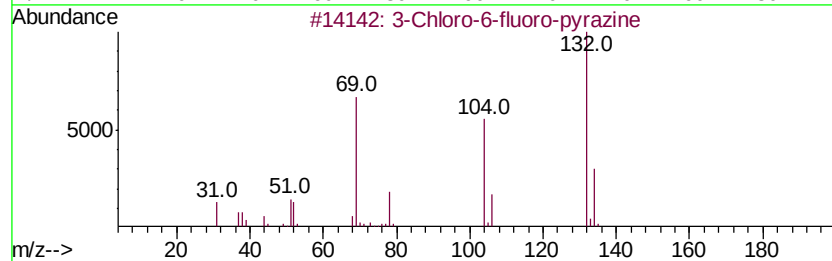
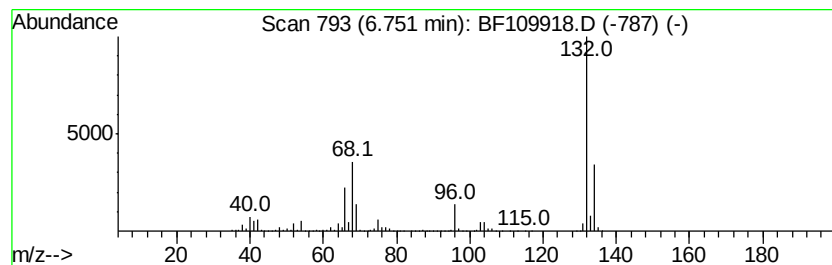
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	63.10 ng	4629290	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5	Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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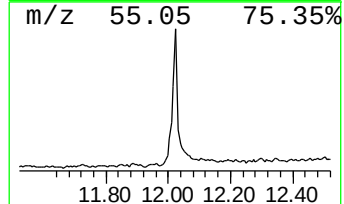
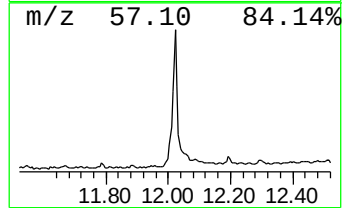
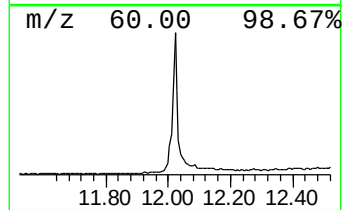
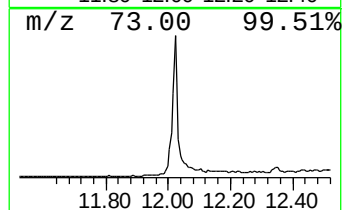
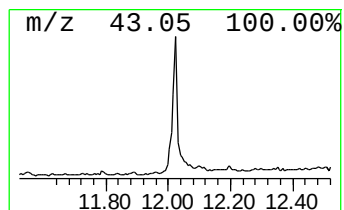
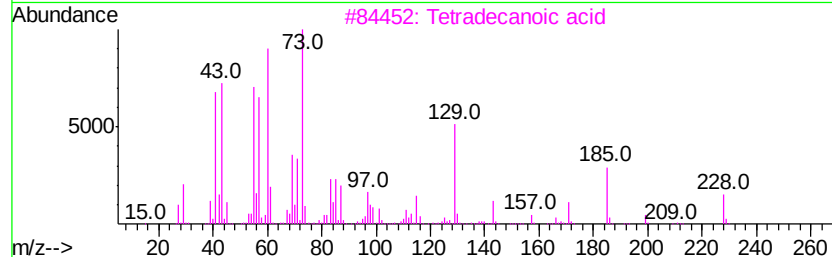
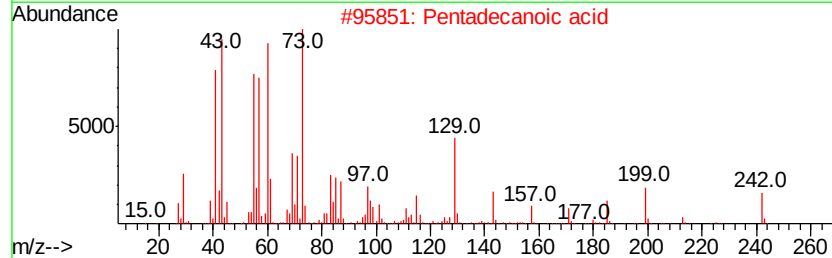
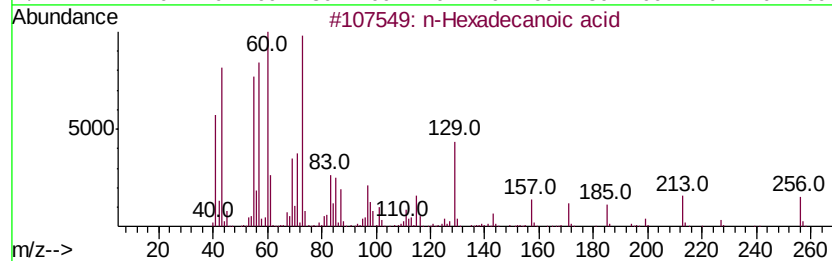
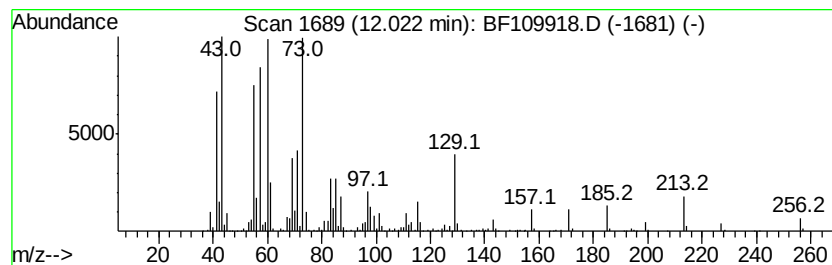
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	9.56 ng	1077820	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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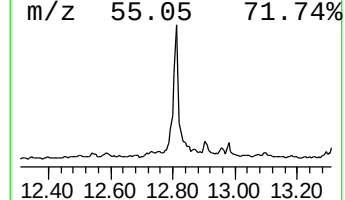
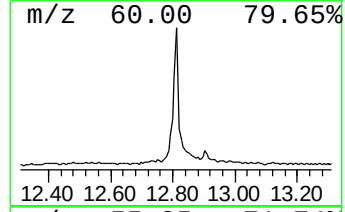
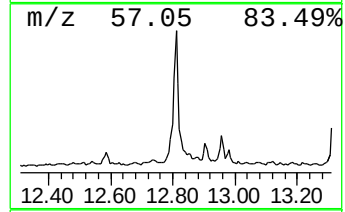
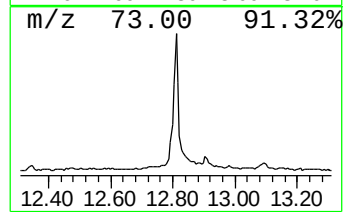
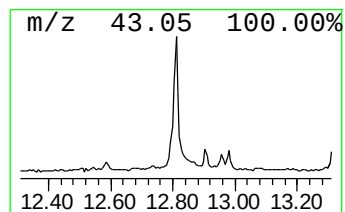
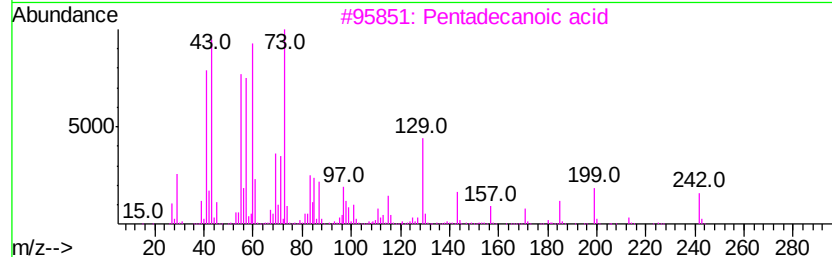
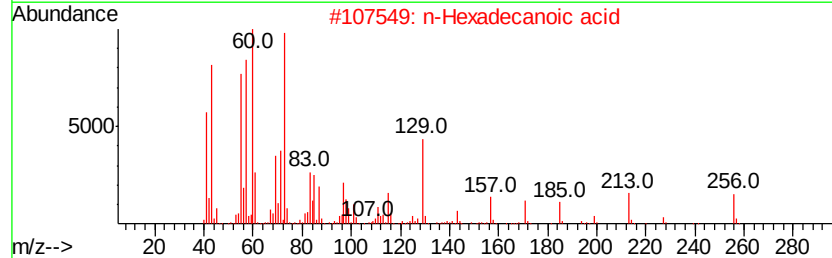
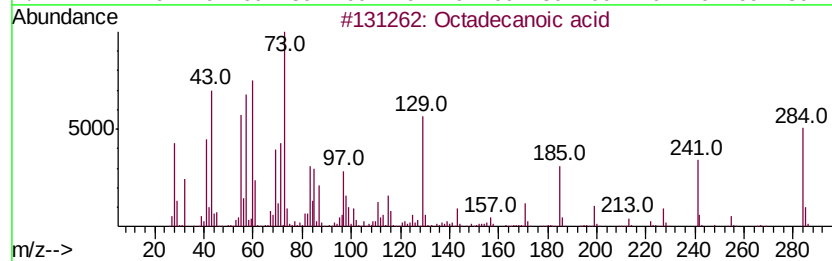
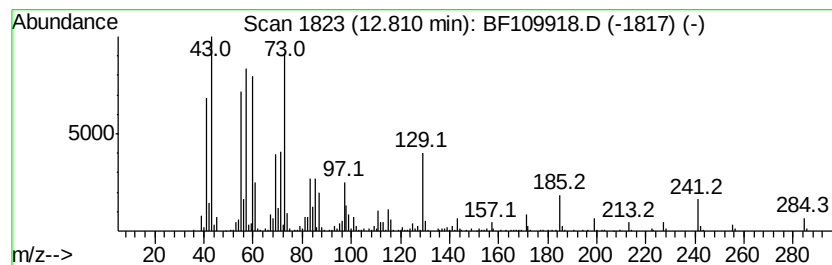
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	11.88 ng	1339940	Phenanthrene-d10	11.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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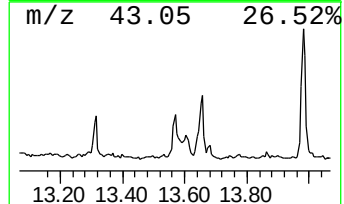
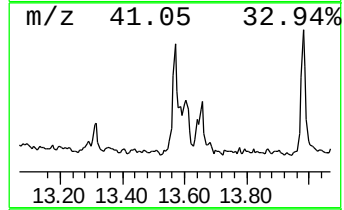
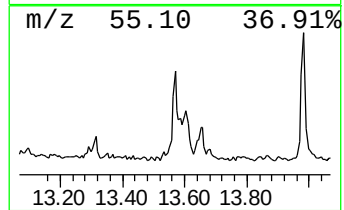
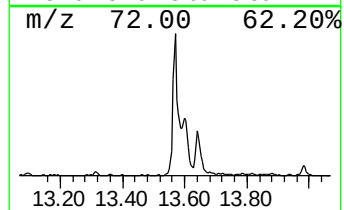
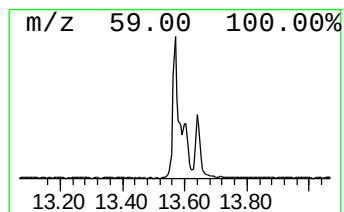
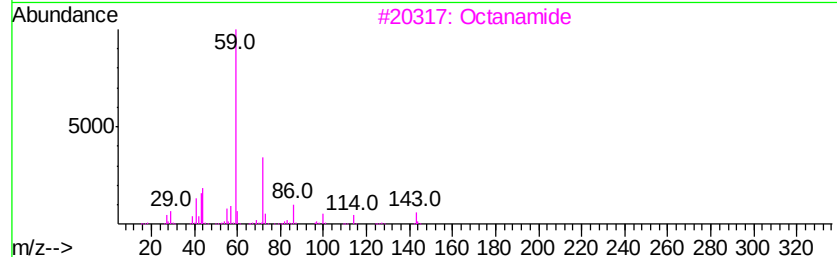
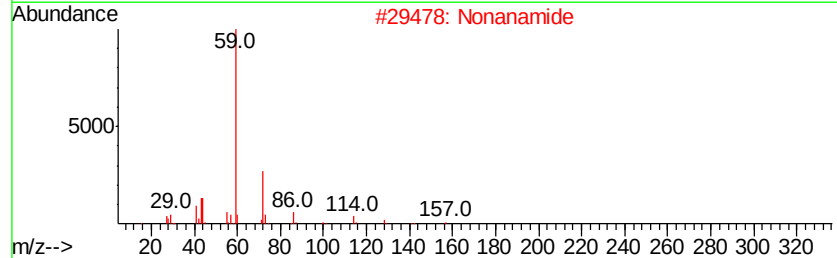
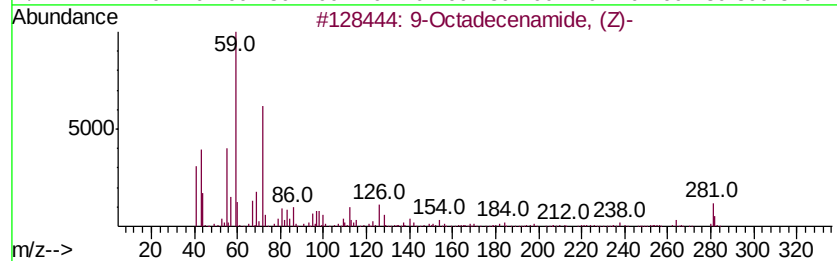
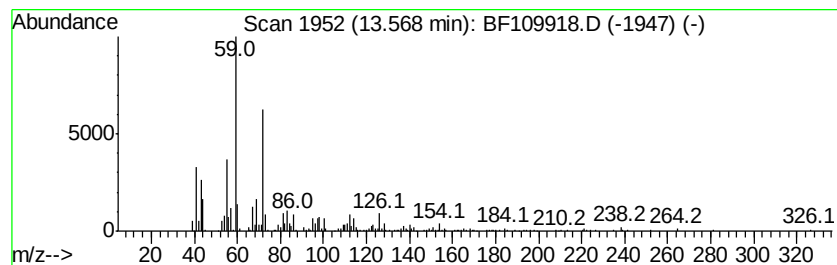
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ClientSampleId :
SSSI-1011-S-DH-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.57	5.50 ng	444206	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Nonanamide	157	C9H19NO	001120-07-6	59
3	Octanamide	143	C8H17NO	000629-01-6	56
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43



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Operator : JU/SJ
Sample : J5516-02
Misc :
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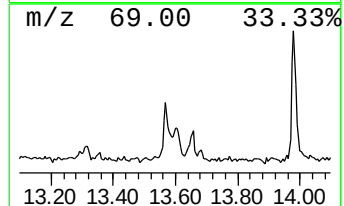
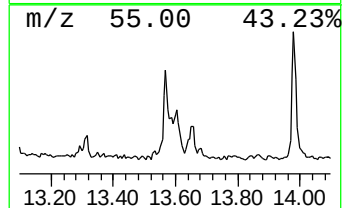
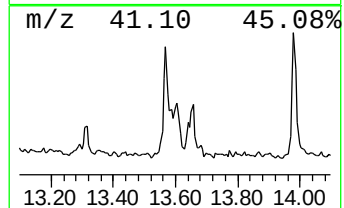
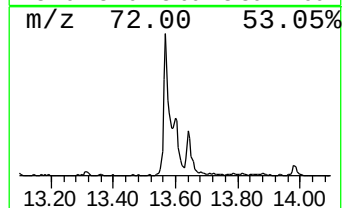
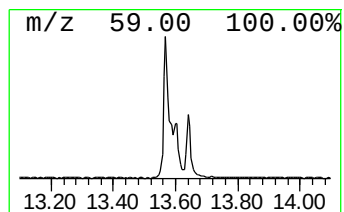
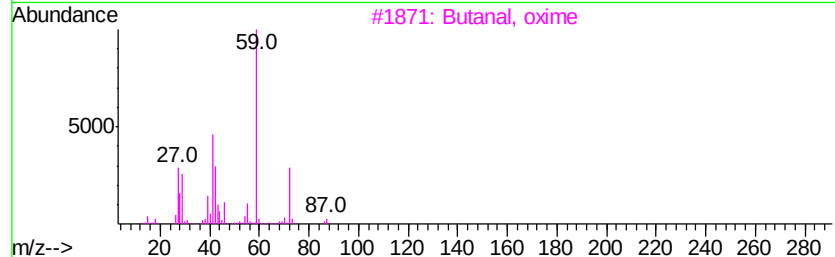
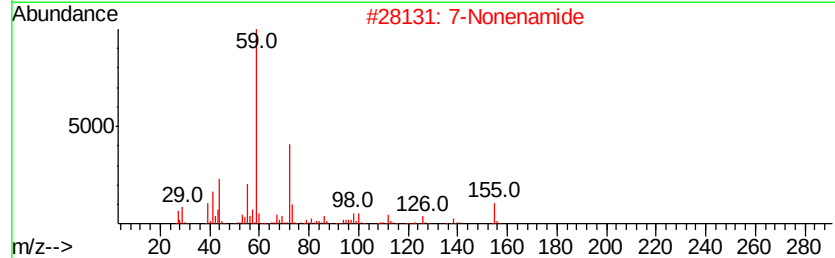
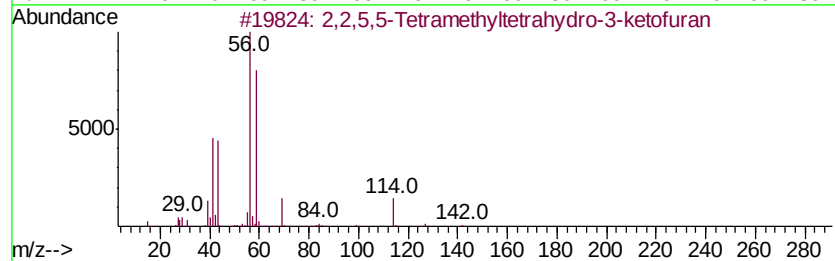
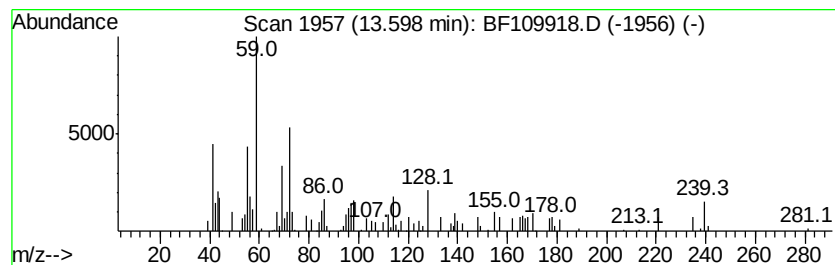
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.60 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.60	2.20 ng	177774	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,5,5-Tetramethyltetrahydro-3-...	142	C8H14O2	005455-94-7	43
2	7-Nonenamide	155	C9H17NO	090949-53-4	35
3	Butanal, oxime	87	C4H9NO	000110-69-0	27
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	27
5	trans-2-Aminocyclohexanol	115	C6H13NO	006982-39-4	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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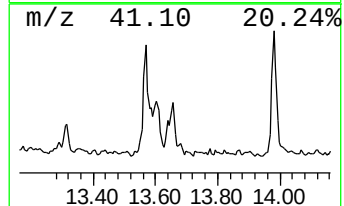
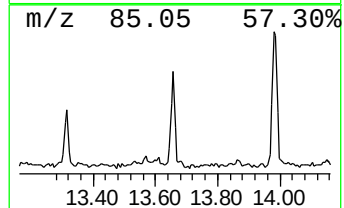
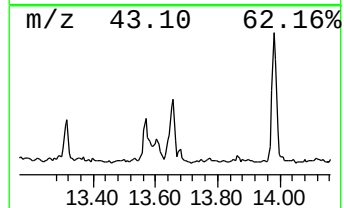
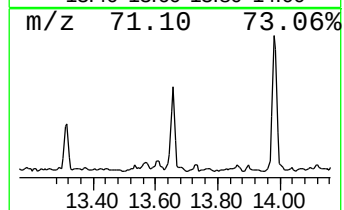
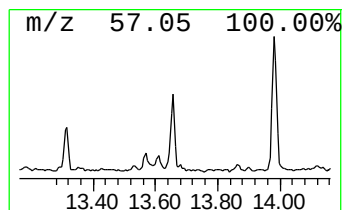
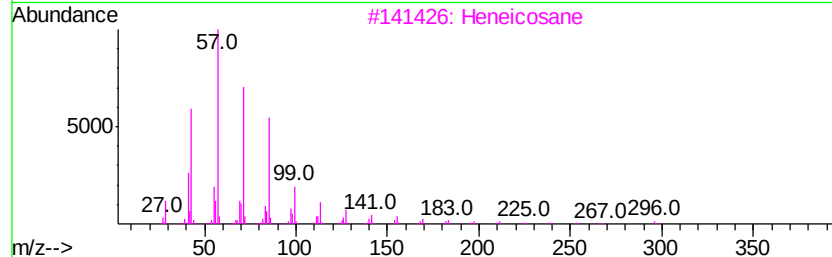
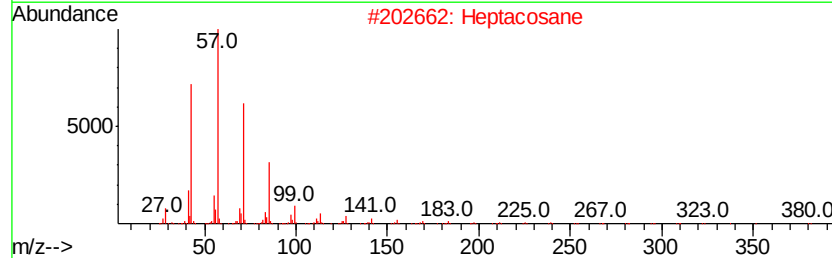
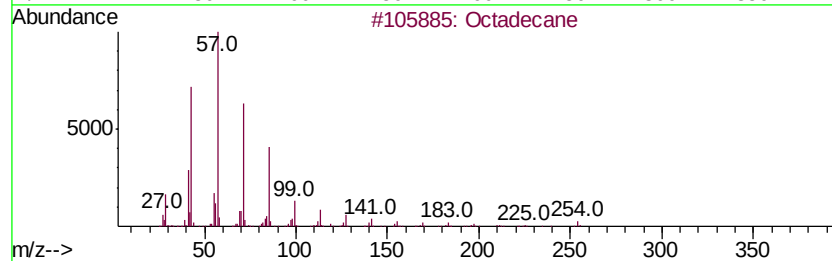
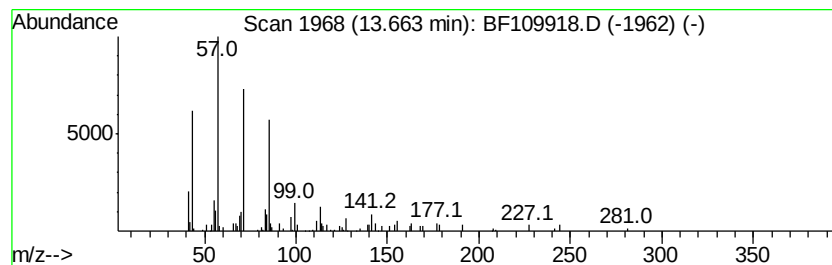
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.43 ng	196080	Chrysene-d12	14.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Heptacosane	380 C27H56	000593-49-7	91
3	Heneicosane	296 C21H44	000629-94-7	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	90
5	Nonadecane	268 C19H40	000629-92-5	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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Acq On : 17 Oct 2018 12:26
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Sample : J5516-02
Misc :
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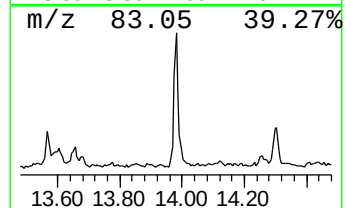
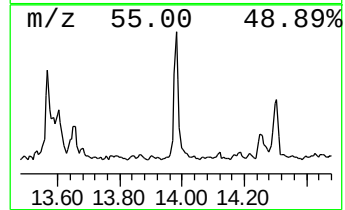
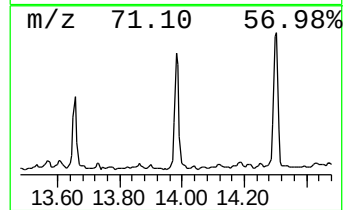
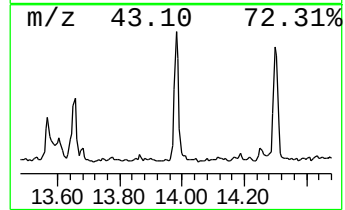
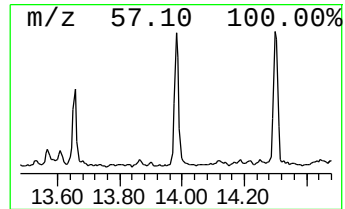
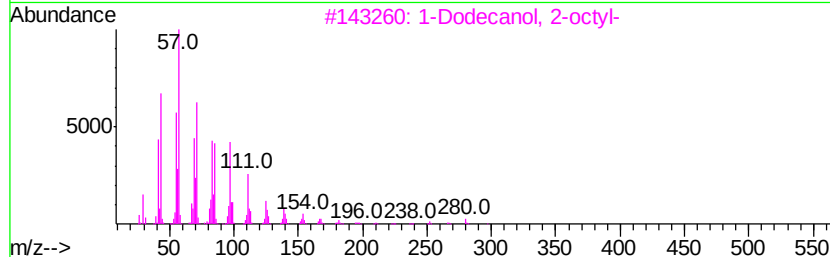
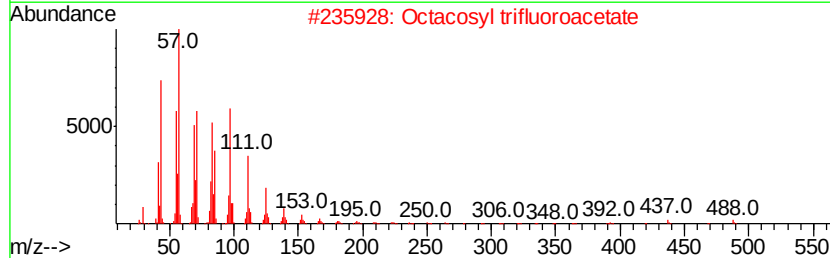
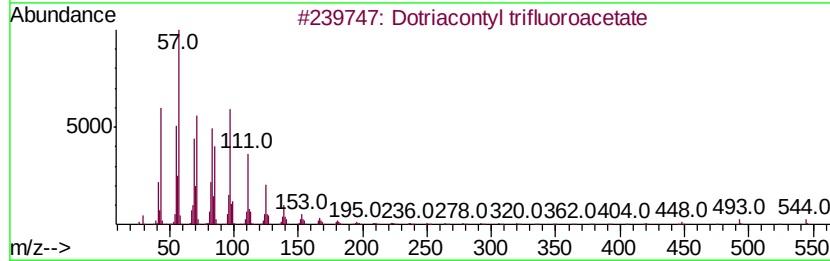
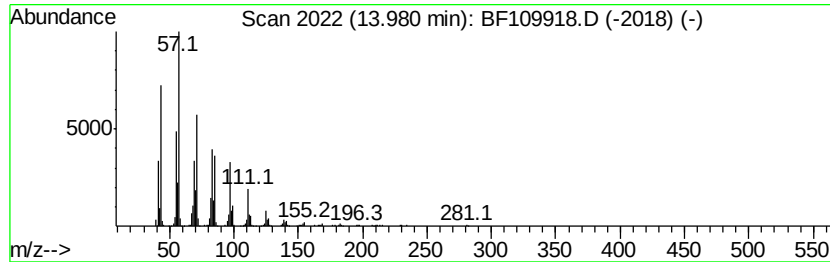
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dotriacontyl trifluoroacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.98	5.81 ng	469324	Chrysene-d12		14.16	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	91
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
5		Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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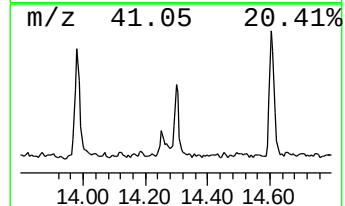
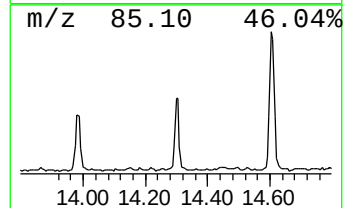
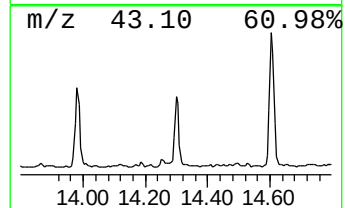
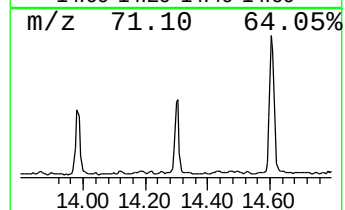
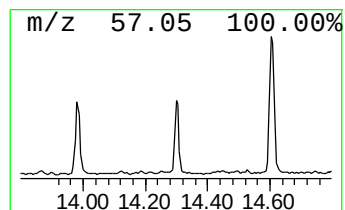
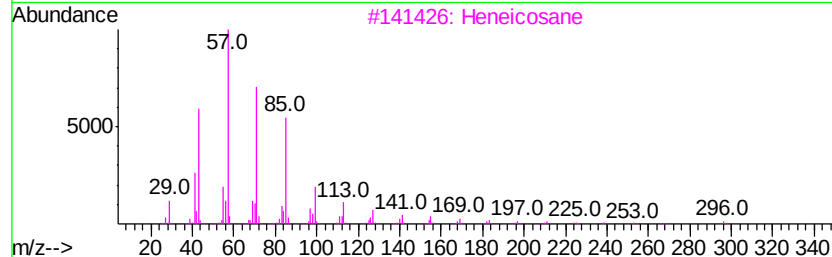
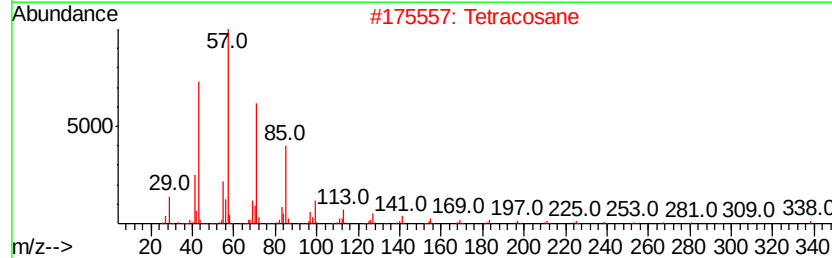
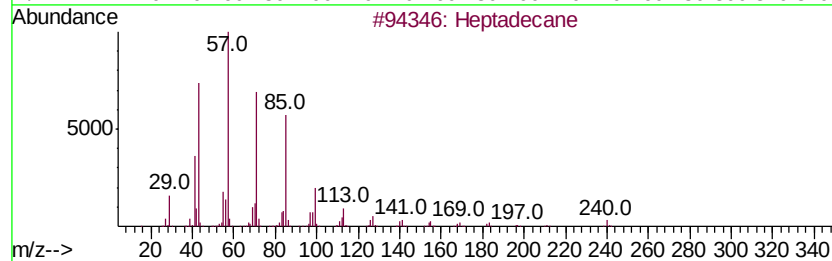
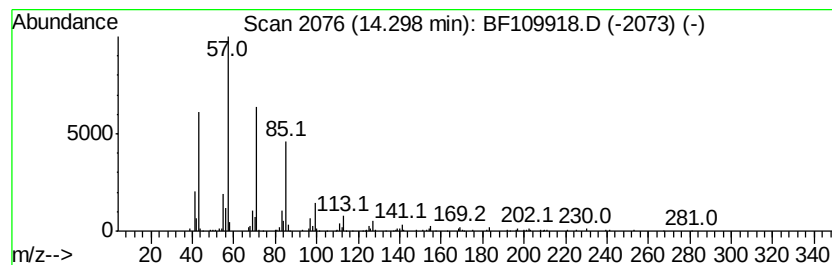
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	3.79 ng	305949	Chrysene-d12	14.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	93
2	Tetracosane	338 C24H50	000646-31-1	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Triacontane	422 C30H62	000638-68-6	91
5	Docosane	310 C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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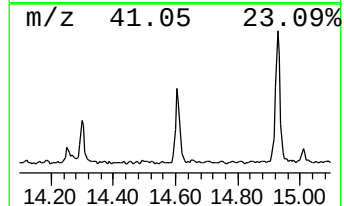
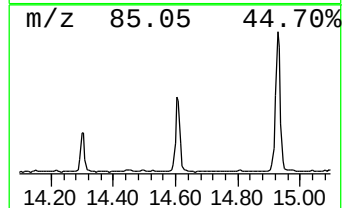
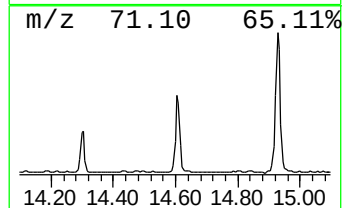
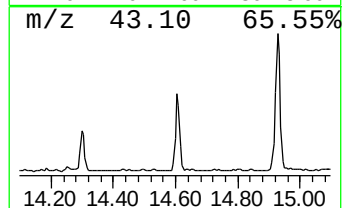
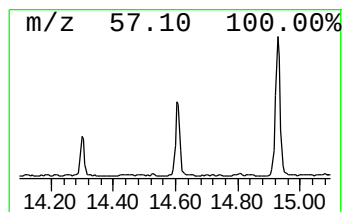
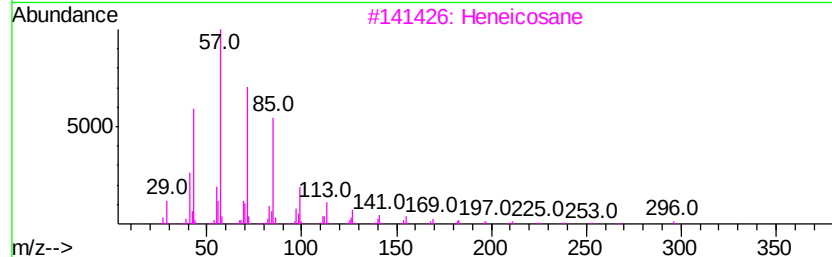
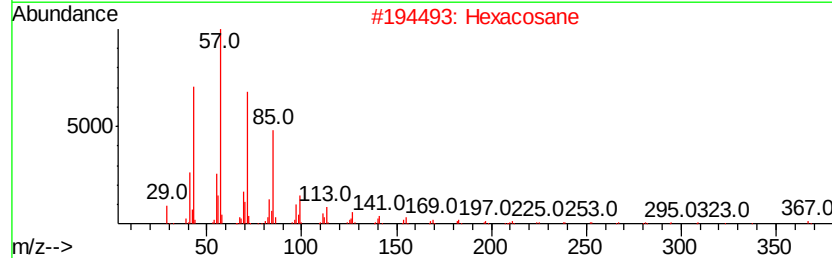
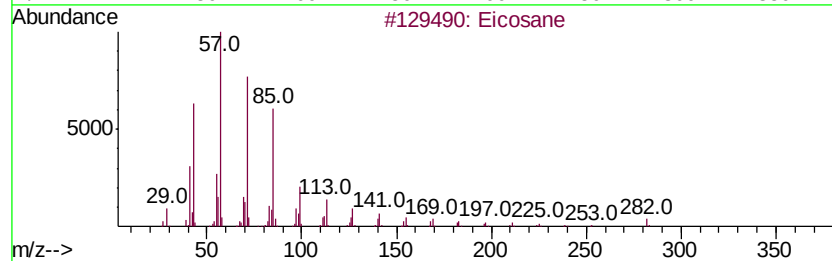
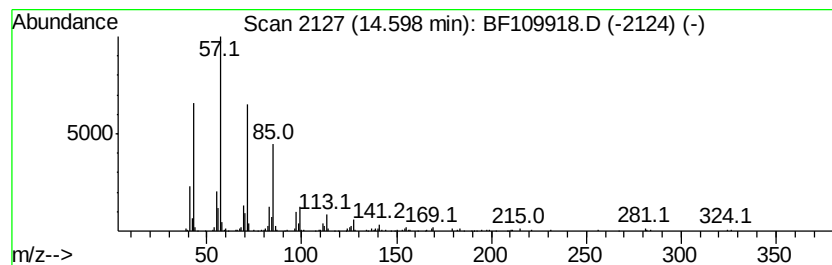
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	7.94 ng	641055	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octadecane	254	C18H38	000593-45-3	87
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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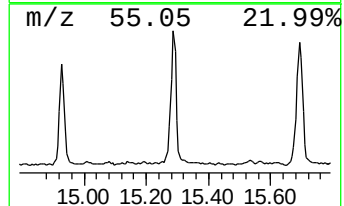
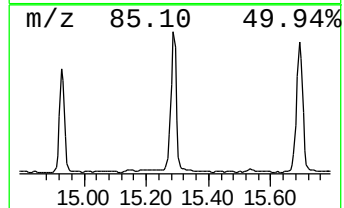
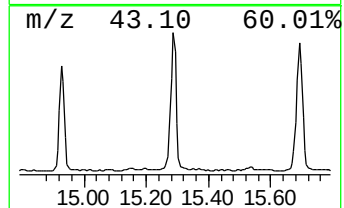
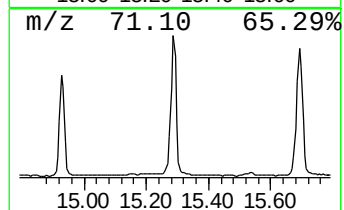
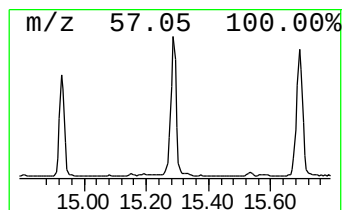
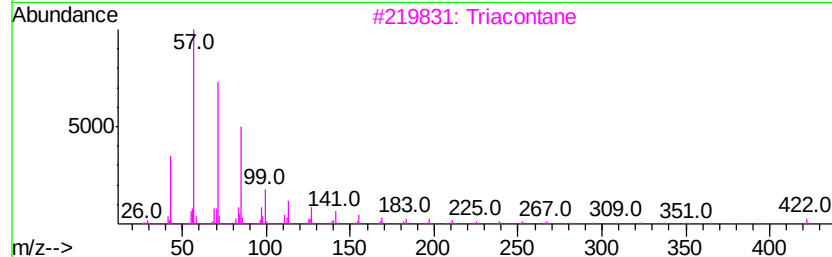
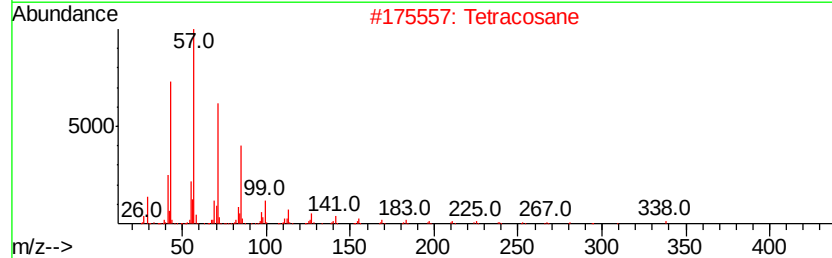
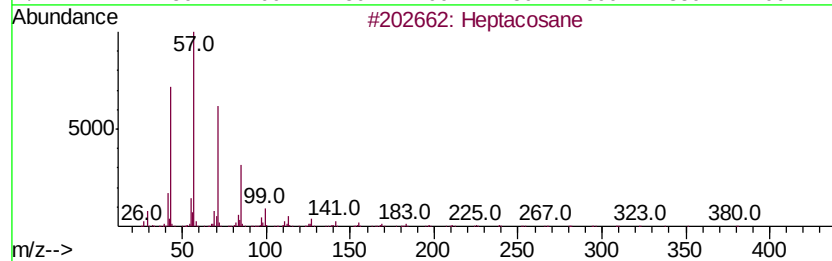
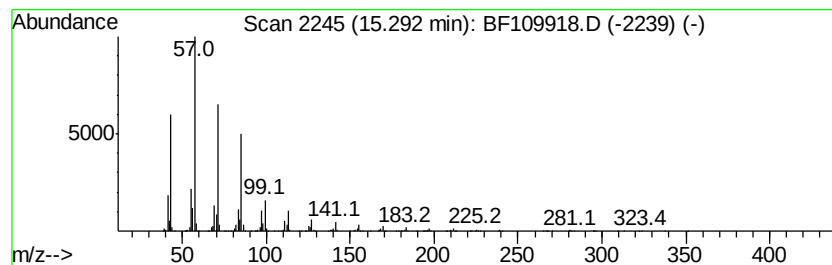
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	10.74 ng	1870300	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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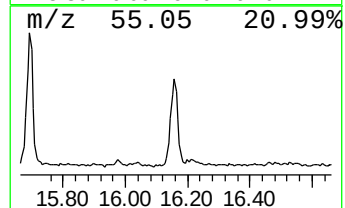
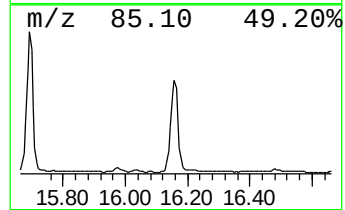
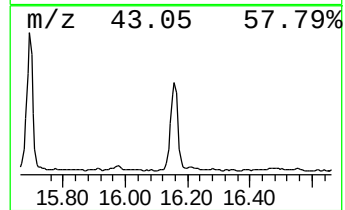
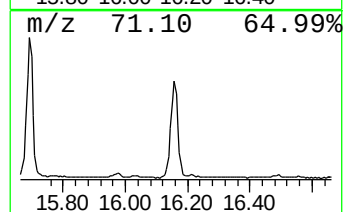
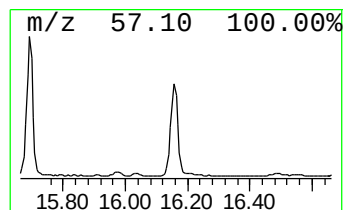
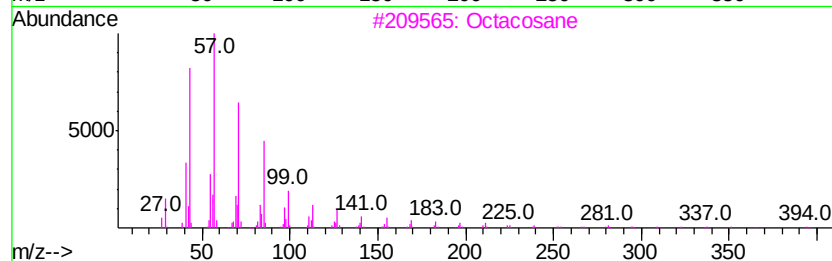
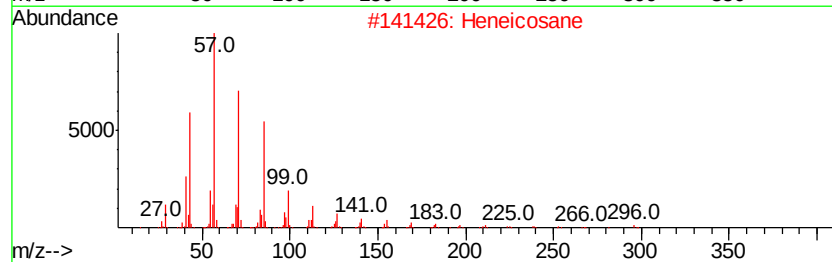
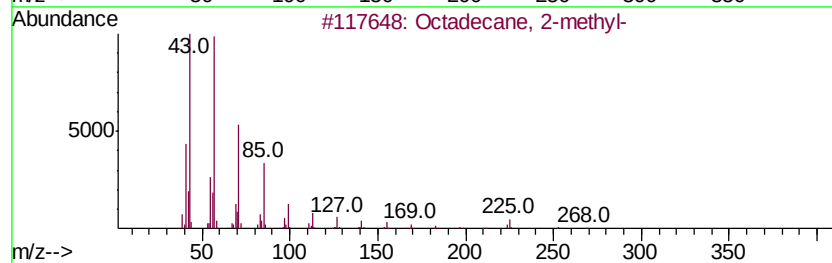
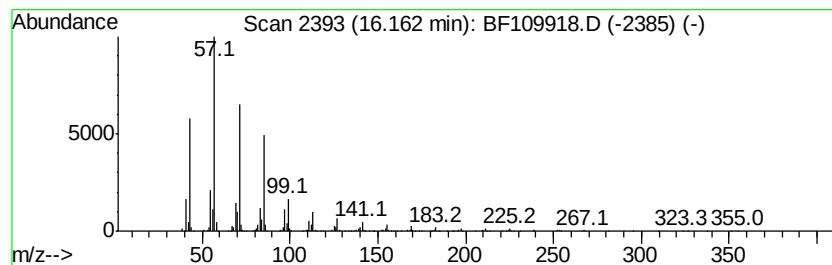
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Octadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	8.69 ng	1514050	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109918.D
Acq On : 17 Oct 2018 12:26
Operator : JU/SJ
Sample : J5516-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1011-S-DH-32

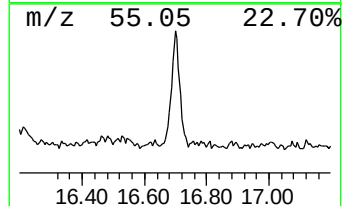
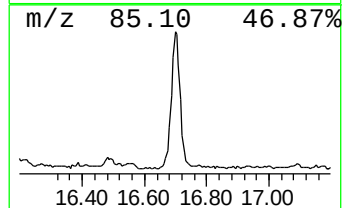
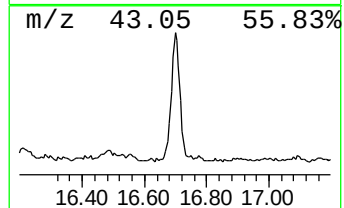
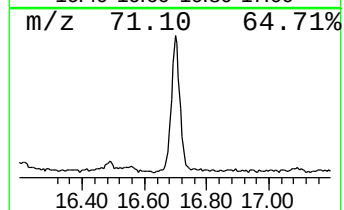
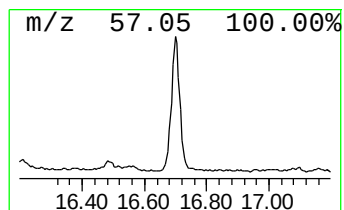
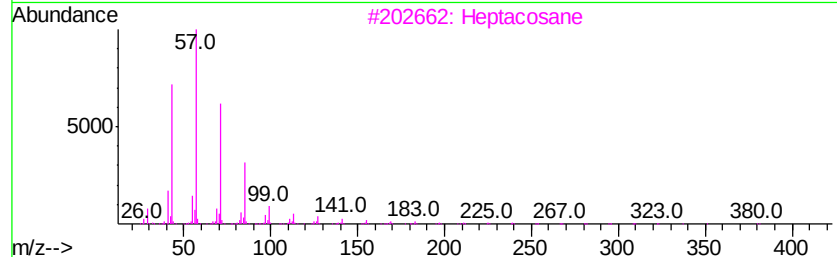
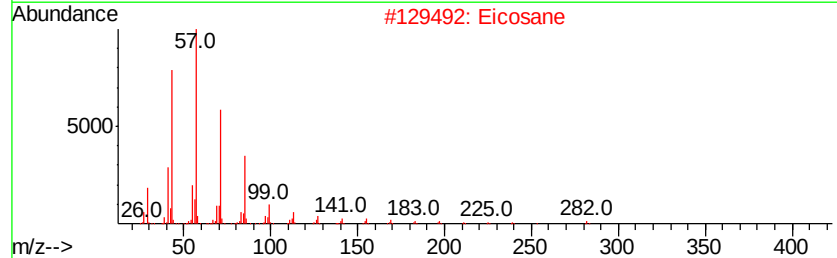
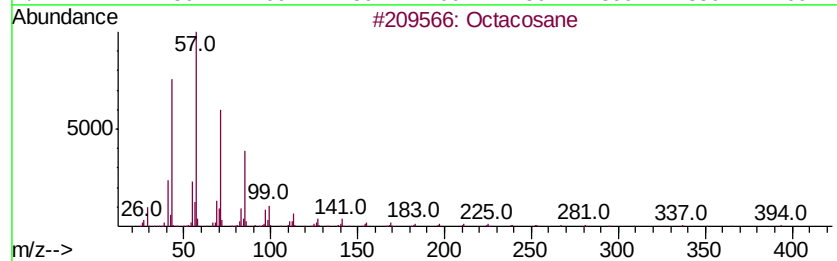
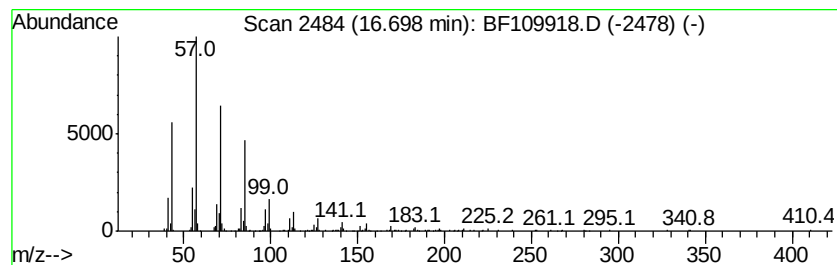
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	4.34 ng	755576	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
 Data File : BF109918.D
 Acq On : 17 Oct 2018 12:26
 Operator : JU/SJ
 Sample : J5516-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1011-S-DH-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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
Butane, 2-methoxy...	2.32	14.2	ng	1044980	1	6.98	1467340	20.0
unknown6.75	6.75	63.1	ng	4629290	1	6.98	1467340	20.0
n-Hexadecanoic acid	12.02	9.6	ng	1077820	4	11.52	2255920	20.0
Octadecanoic acid	12.81	11.9	ng	1339940	4	11.52	2255920	20.0
9-Octadecenamide,...	13.57	5.5	ng	444206	5	14.16	1615180	20.0
unknown13.60	13.60	2.2	ng	177774	5	14.16	1615180	20.0
Octadecane	13.66	2.4	ng	196080	5	14.16	1615180	20.0
Dotriacontyl trif...	13.98	5.8	ng	469324	5	14.16	1615180	20.0
Heptadecane	14.30	3.8	ng	305949	5	14.16	1615180	20.0
Eicosane	14.60	7.9	ng	641055	5	14.16	1615180	20.0
Heptacosane	15.29	10.7	ng	1870300	6	15.69	3482930	20.0
Octadecane, 2-met...	16.16	8.7	ng	1514050	6	15.69	3482930	20.0
Octacosane	16.70	4.3	ng	755576	6	15.69	3482930	20.0