

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
 Data File : BF109071.D
 Acq On : 18 Sep 2018 2:38
 Operator : JU/SJ
 Sample : J4936-09
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHASE-3

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-BF091418.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	4.266	324	328	338	rBV	107370	125688	3.73%	0.424%
2	4.913	433	438	448	rBV	697895	861742	25.60%	2.906%
3	5.337	504	510	513	rBV	2863010	2901173	86.19%	9.783%
4	6.360	678	684	687	rBV	3063410	3113494	92.50%	10.499%
5	6.490	701	706	709	rBV	3270327	3067649	91.13%	10.344%
6	6.719	742	745	749	rBV	1028106	833938	24.77%	2.812%
7	6.878	768	772	775	rBV	3026777	2519754	74.86%	8.497%
8	7.284	835	841	844	rBV	2069760	1974258	58.65%	6.657%
9	8.001	959	963	966	rBV	1269347	979944	29.11%	3.304%
10	9.078	1142	1146	1149	rBV	3820966	3366050	100.00%	11.351%
11	9.172	1159	1162	1166	rVB	110210	88067	2.62%	0.297%
12	9.472	1210	1213	1215	rBV	290286	250139	7.43%	0.843%
13	9.701	1248	1252	1255	rBV	144203	120381	3.58%	0.406%
14	9.748	1256	1260	1264	rBV	1057393	995792	29.58%	3.358%
15	10.195	1333	1336	1339	rVB	132126	101926	3.03%	0.344%
16	10.419	1367	1374	1377	rBV	46711	54815	1.63%	0.185%
17	10.536	1390	1394	1397	rBV	1911283	1745221	51.85%	5.885%
18	10.666	1413	1416	1425	rVB	92226	110622	3.29%	0.373%
19	11.113	1489	1492	1495	rBV2	40803	36634	1.09%	0.124%
20	11.225	1508	1511	1515	rBV	1054225	941479	27.97%	3.175%
21	12.813	1776	1781	1784	rBV	3453837	3012913	89.51%	10.160%
22	13.719	1931	1935	1948	rBV2	142295	224112	6.66%	0.756%
23	13.854	1954	1958	1961	rBV	1000912	938564	27.88%	3.165%
24	14.036	1986	1989	1993	rBV	52674	50199	1.49%	0.169%
25	14.342	2038	2041	2046	rBV	72079	70983	2.11%	0.239%
26	14.636	2088	2091	2097	rVB	94561	96793	2.88%	0.326%
27	14.954	2142	2145	2150	rVB	94793	97651	2.90%	0.329%
28	15.254	2191	2196	2201	rBV	619052	722762	21.47%	2.437%
29	15.307	2202	2205	2212	rVB	90532	111747	3.32%	0.377%
30	15.713	2270	2274	2280	rBV	65716	87361	2.60%	0.295%
31	16.183	2349	2354	2358	rBV	34560	53595	1.59%	0.181%

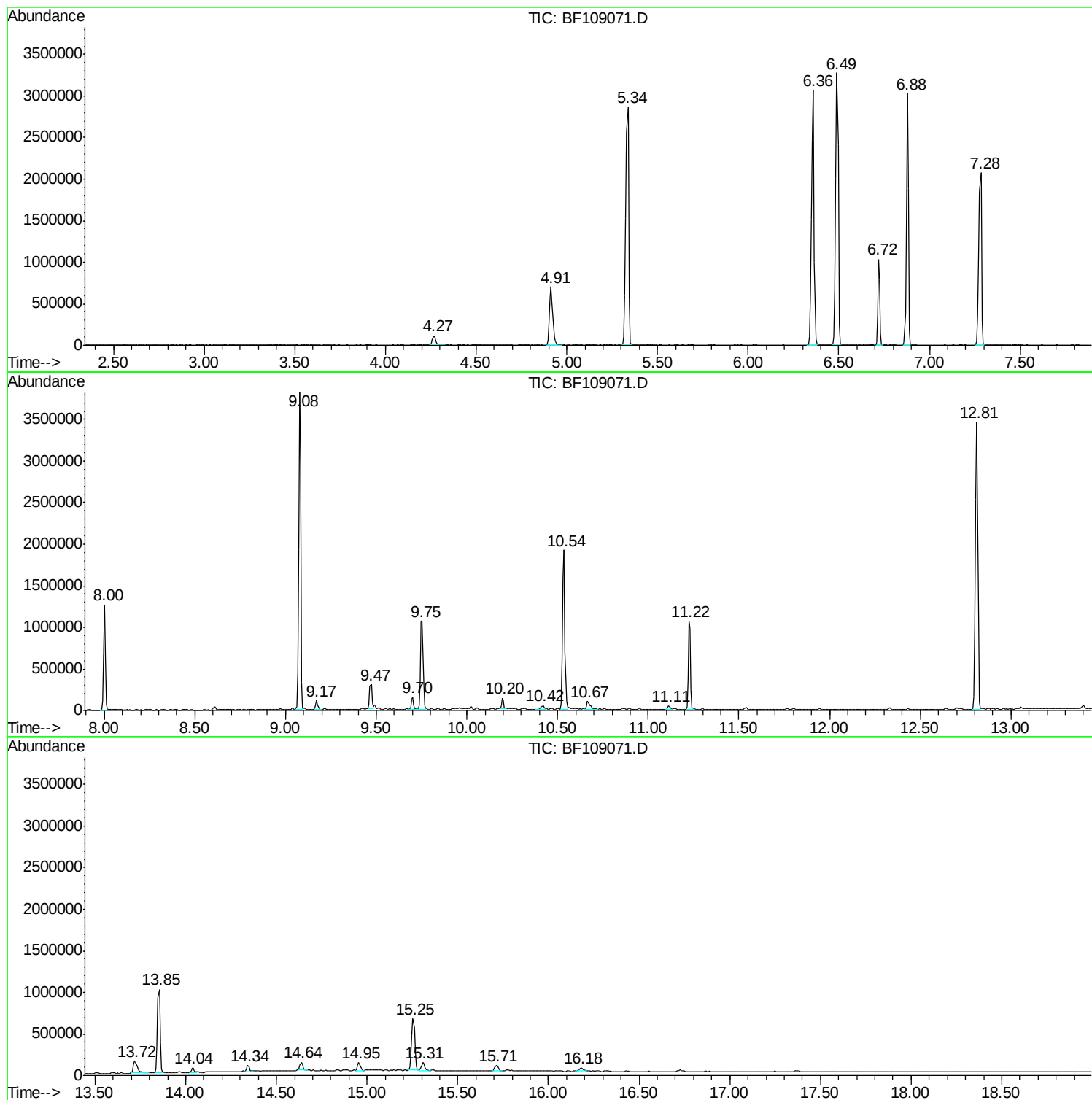
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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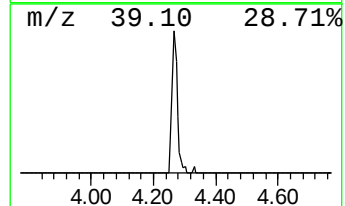
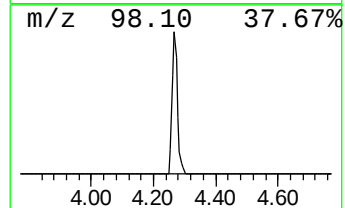
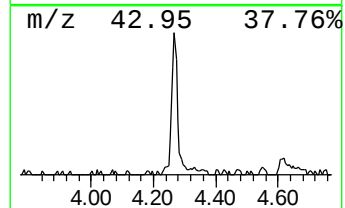
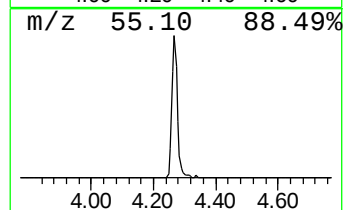
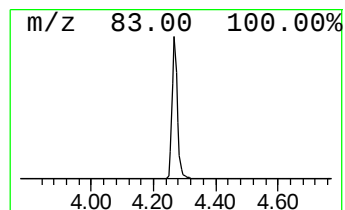
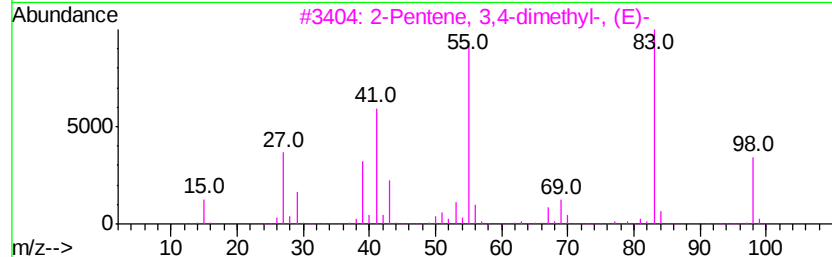
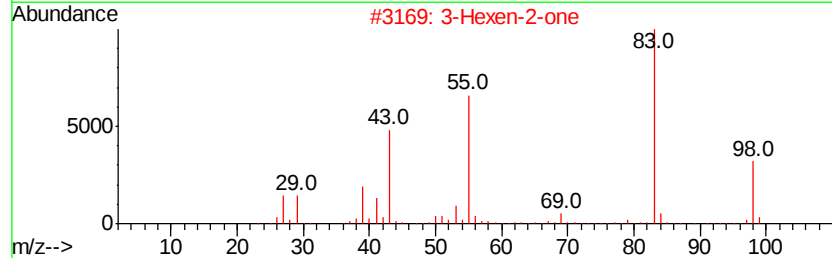
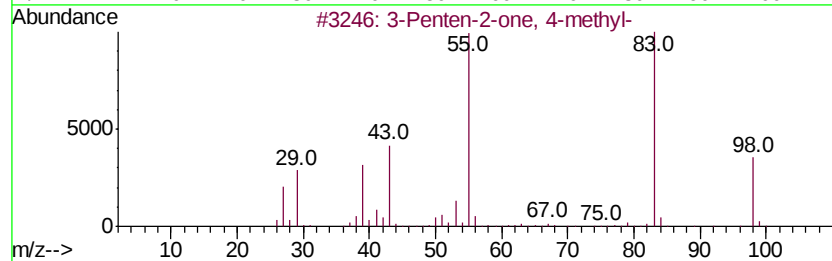
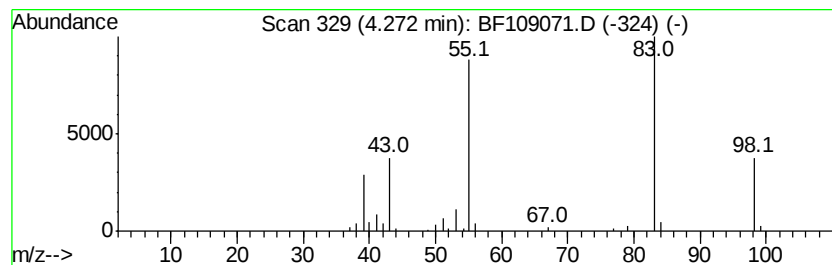
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	3.01 ng	125688	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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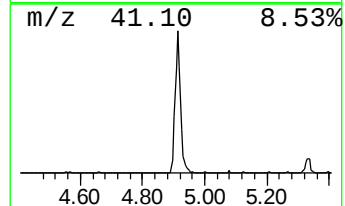
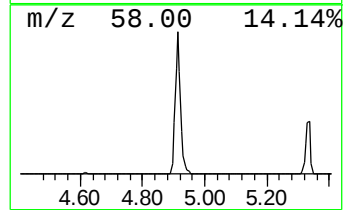
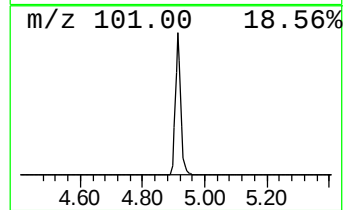
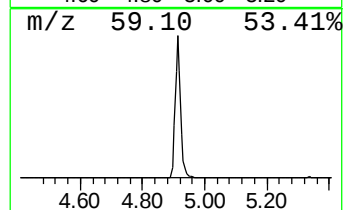
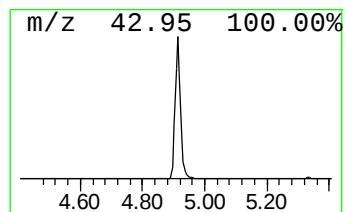
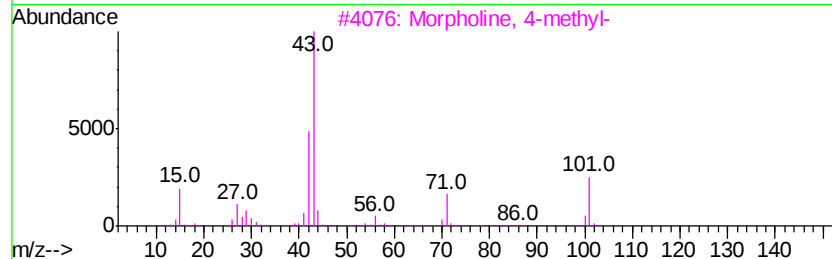
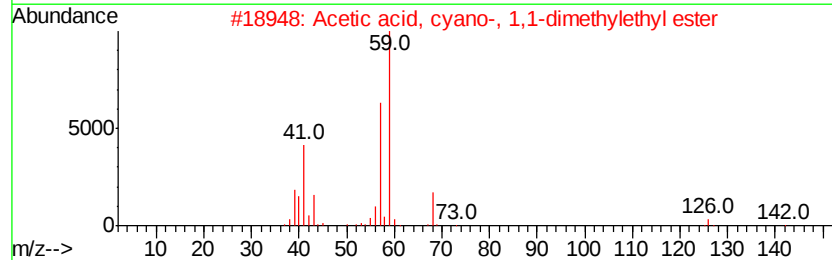
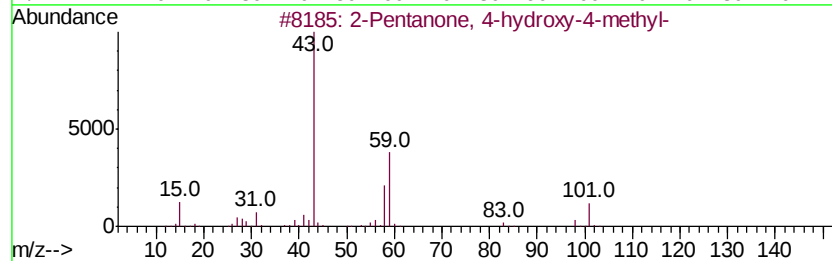
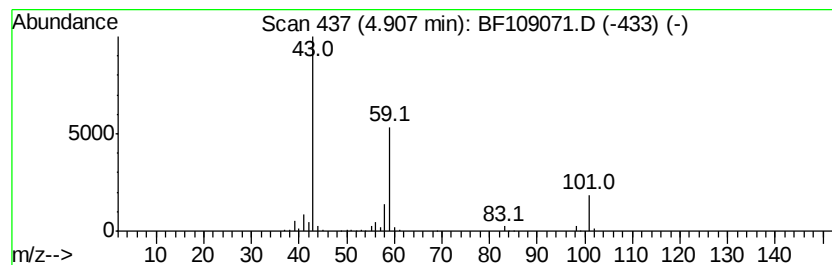
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	20.67 ng	861742	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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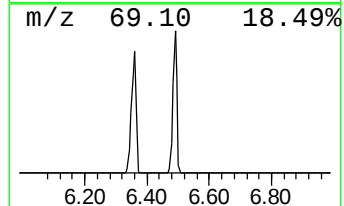
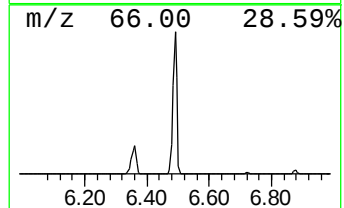
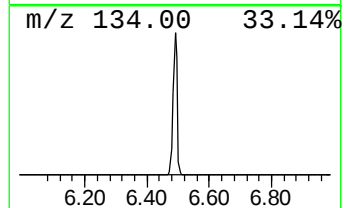
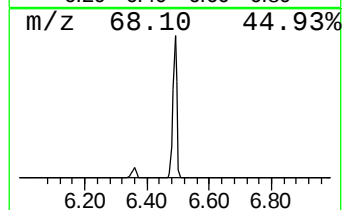
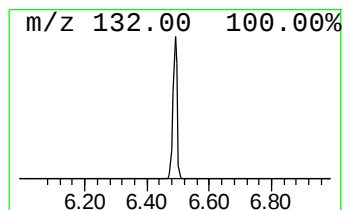
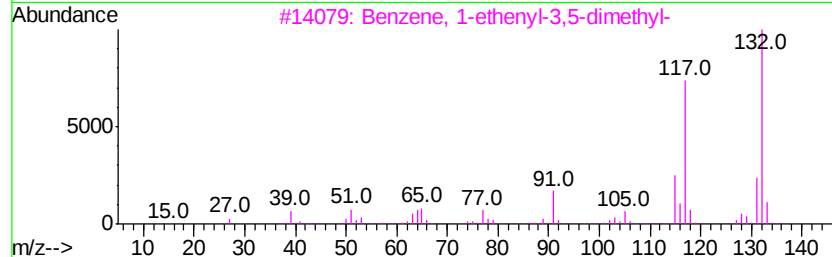
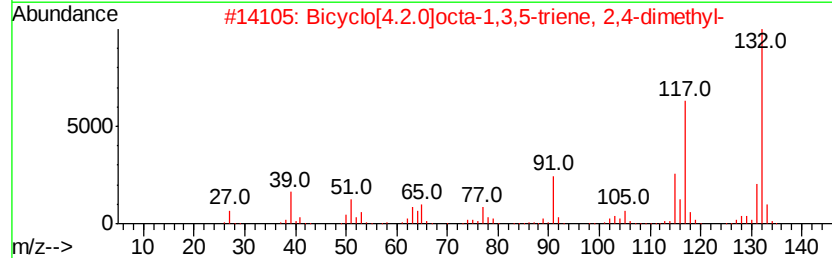
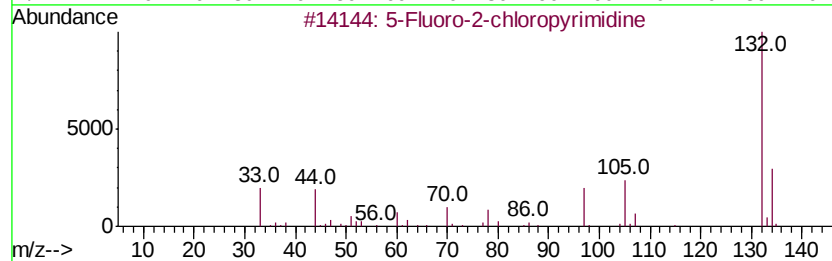
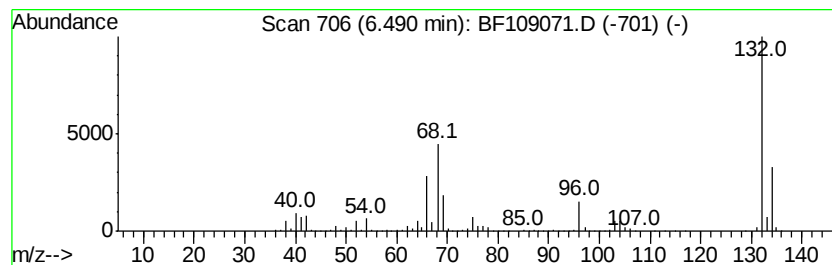
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	73.57 ng	3067650	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		Xenon	132	Xe	007440-63-3	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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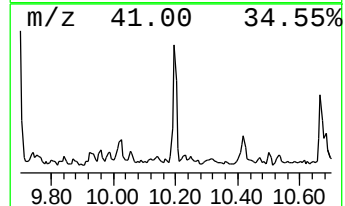
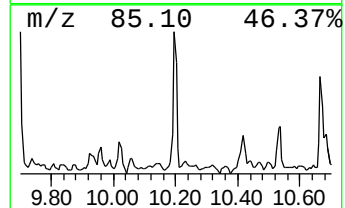
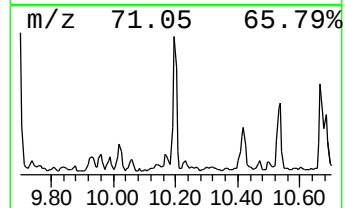
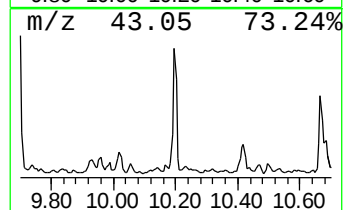
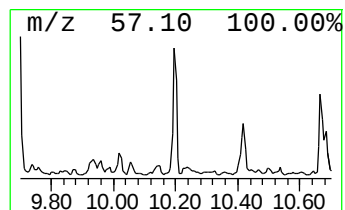
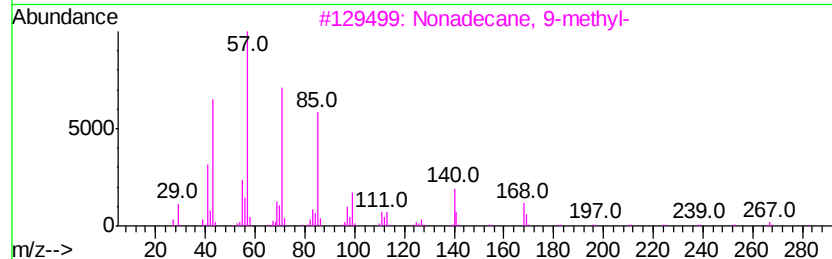
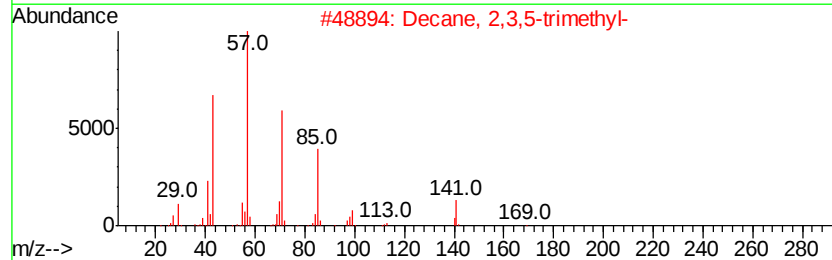
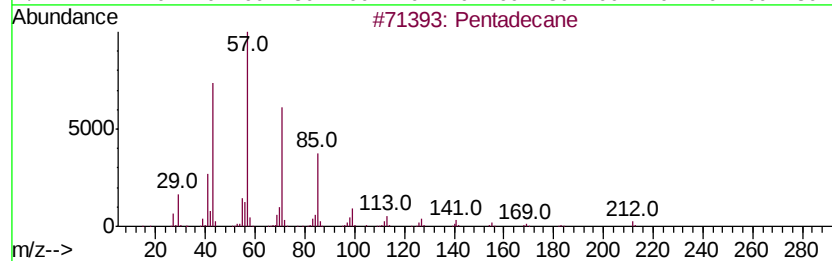
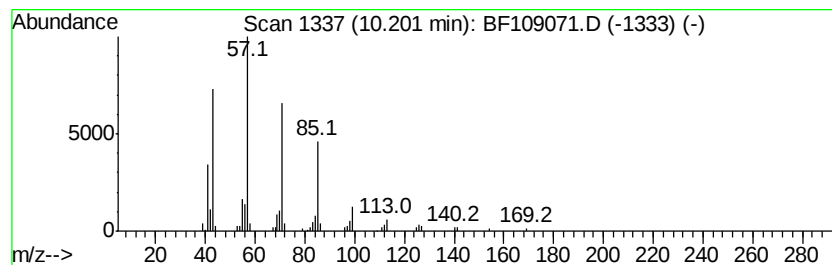
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Peak Number 5 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	2.05 ng	101926	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	90
3	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	86
4	Heptacosane		380	C27H56	000593-49-7	83
5	Tetradecane		198	C14H30	000629-59-4	78



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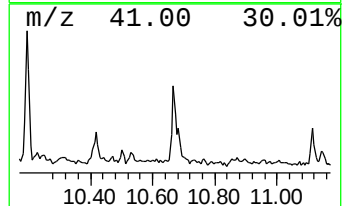
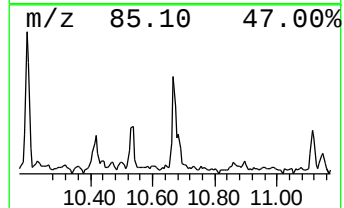
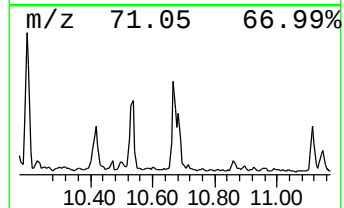
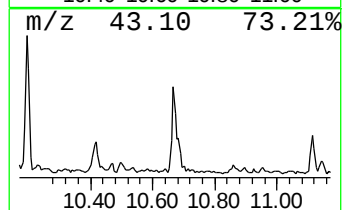
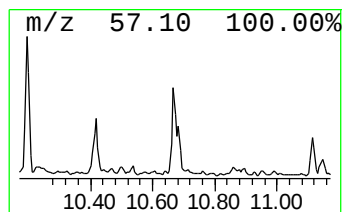
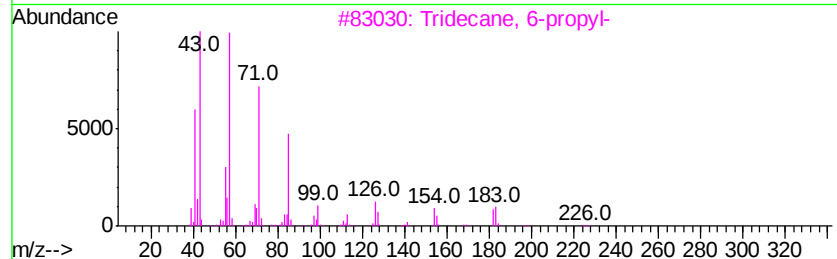
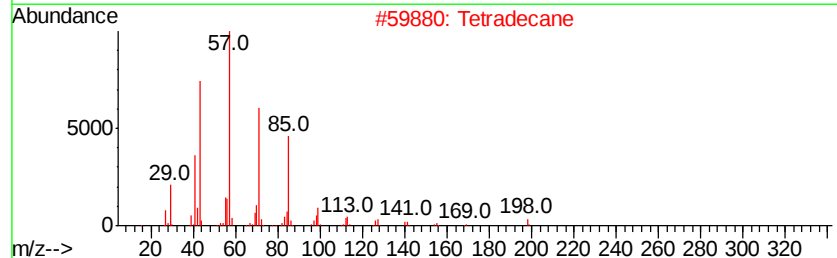
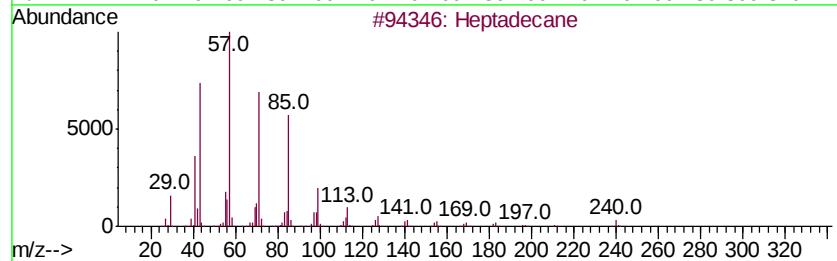
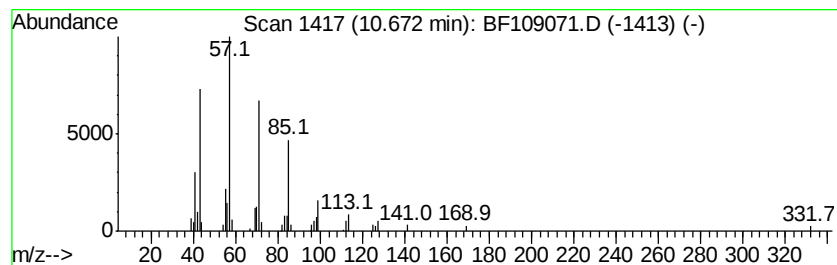
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Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.35 ng	110622	Phenanthrene-d10	11.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Tetradecane		198	C14H30	000629-59-4	87
3	Tridecane, 6-propyl-		226	C16H34	055045-10-8	86
4	Heneicosane		296	C21H44	000629-94-7	86
5	Hexadecane		226	C16H34	000544-76-3	86



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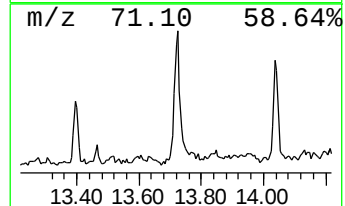
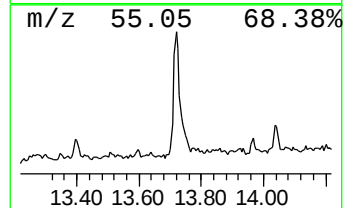
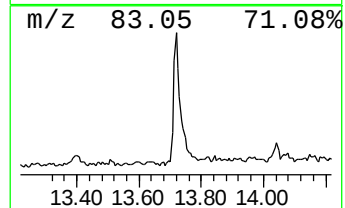
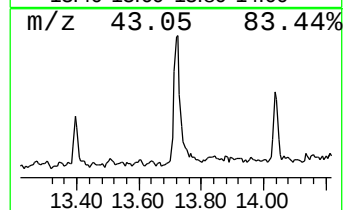
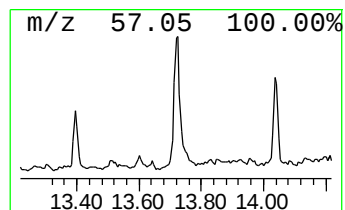
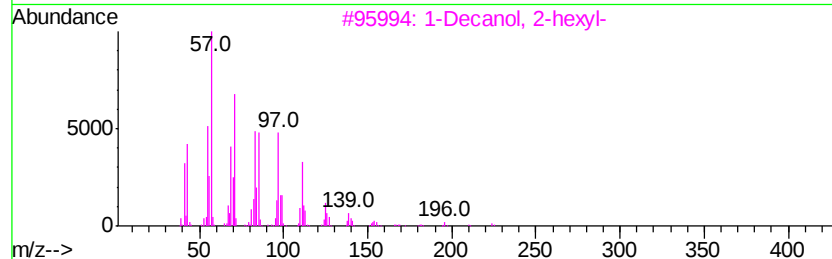
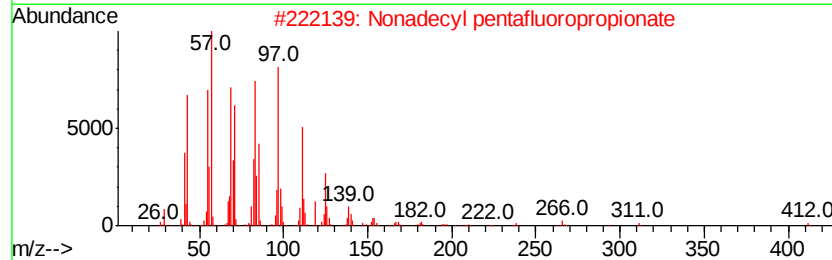
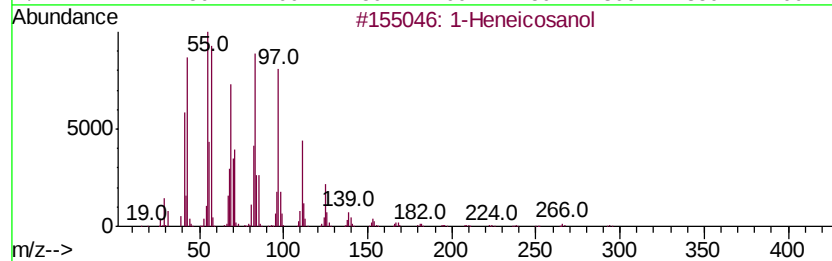
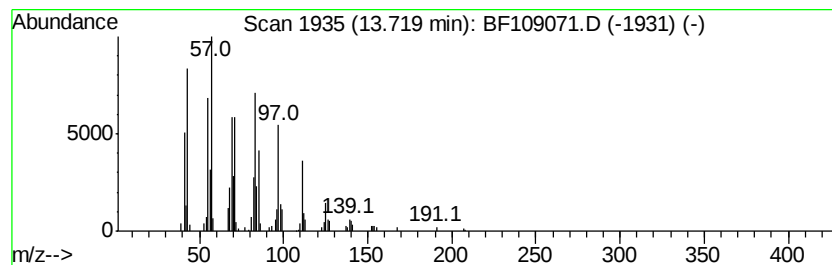
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.78 ng	224112	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	83
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109071.D
Acq On : 18 Sep 2018 2:38
Operator : JU/SJ
Sample : J4936-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHASE-3

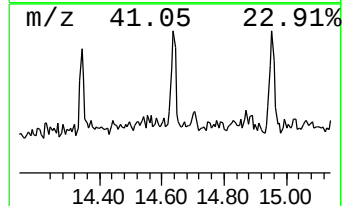
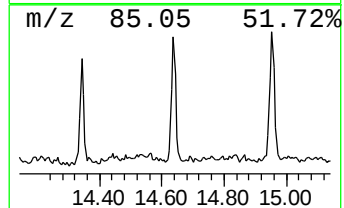
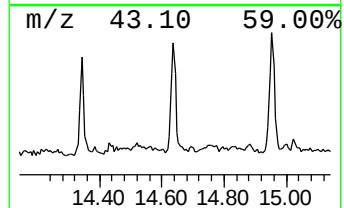
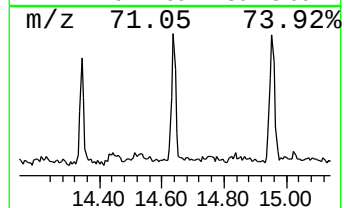
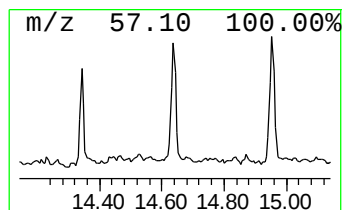
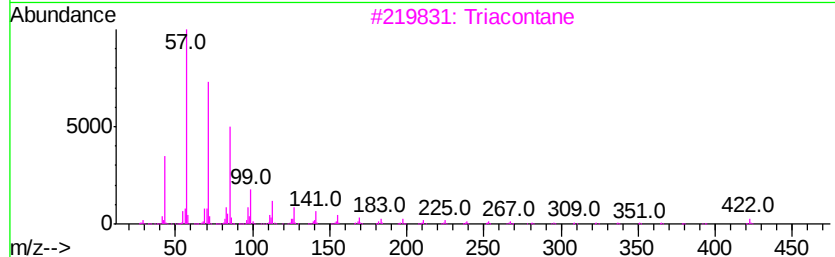
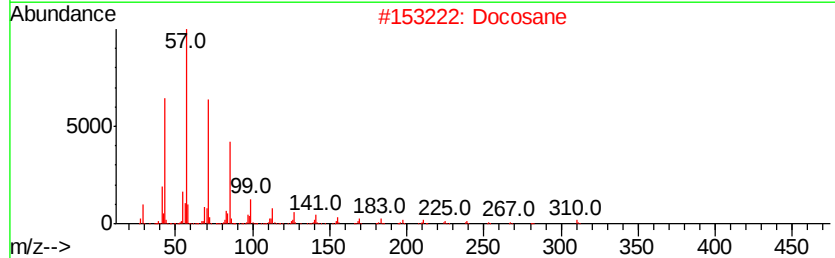
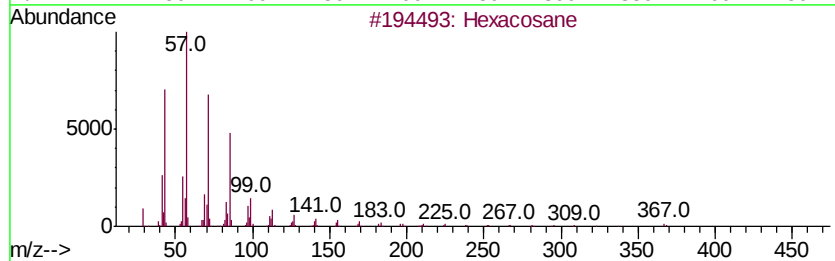
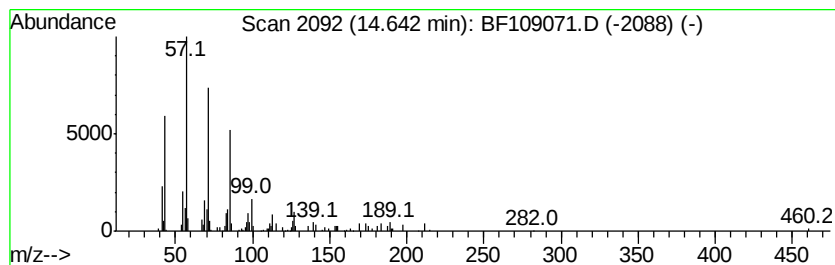
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.68 ng	96793	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Docosane	310	C22H46	000629-97-0	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109071.D
Acq On : 18 Sep 2018 2:38
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Sample : J4936-09
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Instrument :
BNA_F
ClientSampleId :
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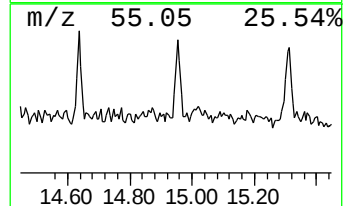
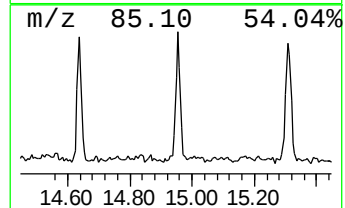
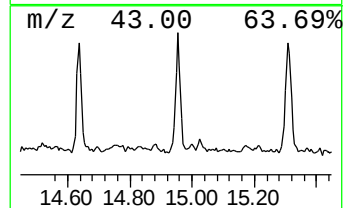
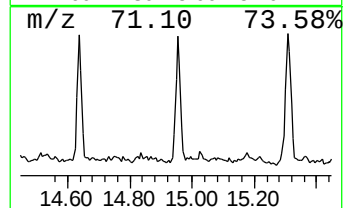
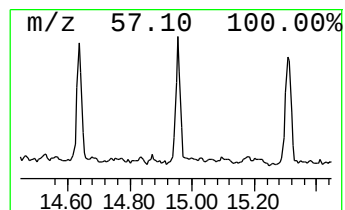
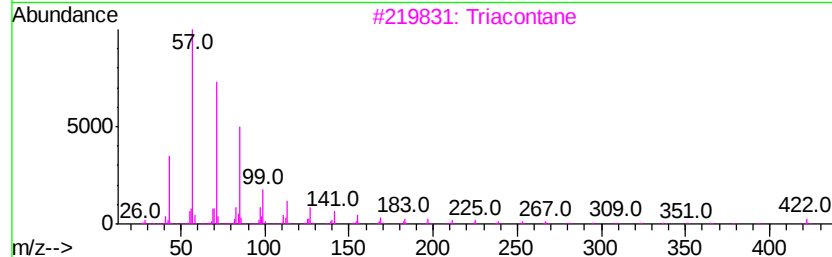
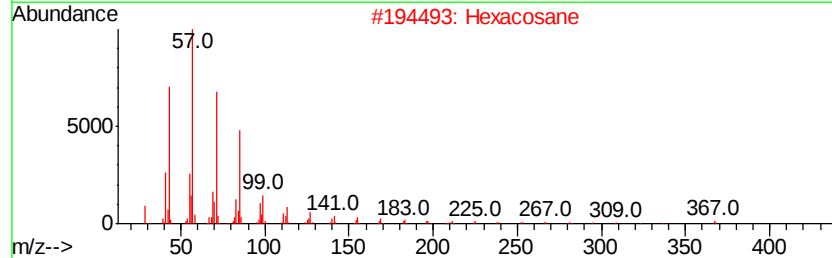
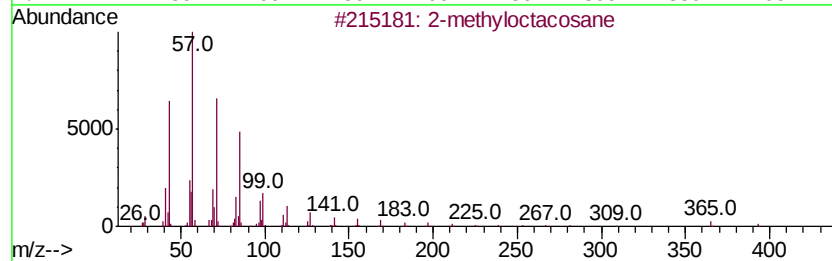
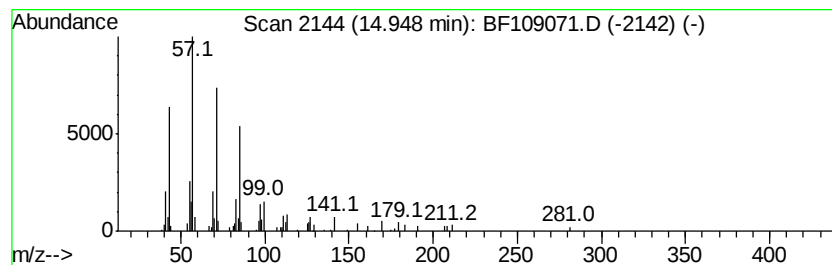
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.70 ng	97651	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91	
2	Hexacosane	366	C26H54	000630-01-3	91	
3	Triacotane	422	C30H62	000638-68-6	91	
4	Heneicosane	296	C21H44	000629-94-7	91	
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109071.D
Acq On : 18 Sep 2018 2:38
Operator : JU/SJ
Sample : J4936-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

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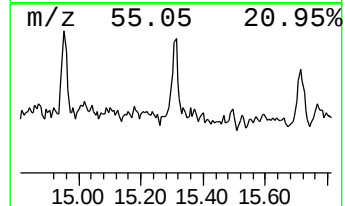
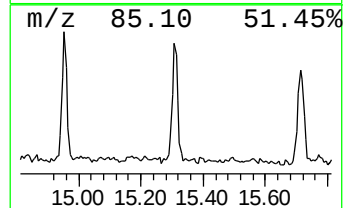
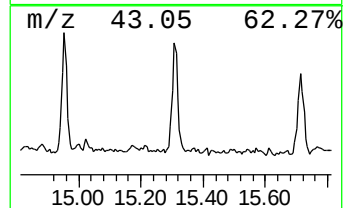
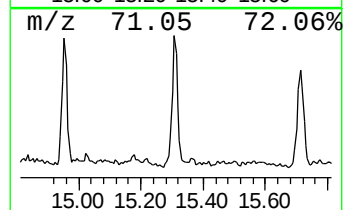
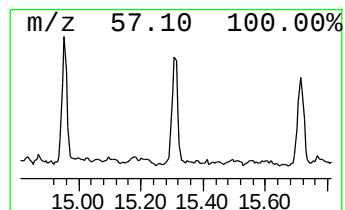
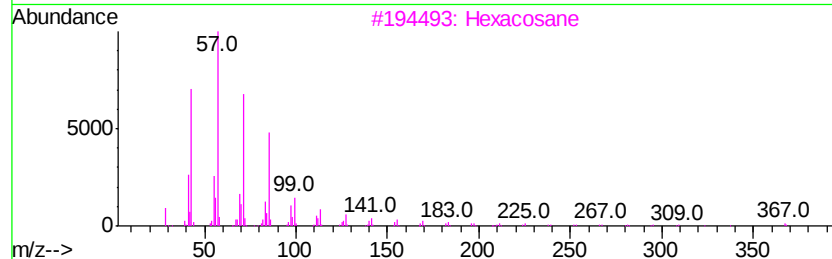
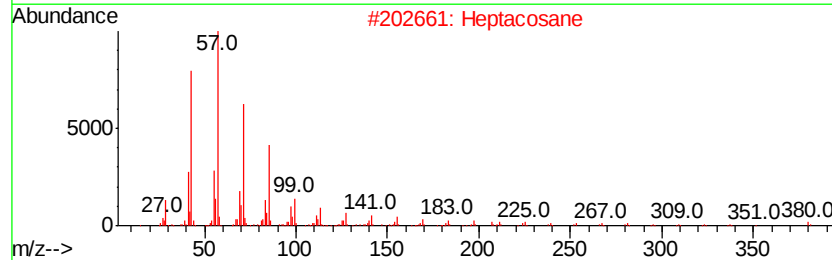
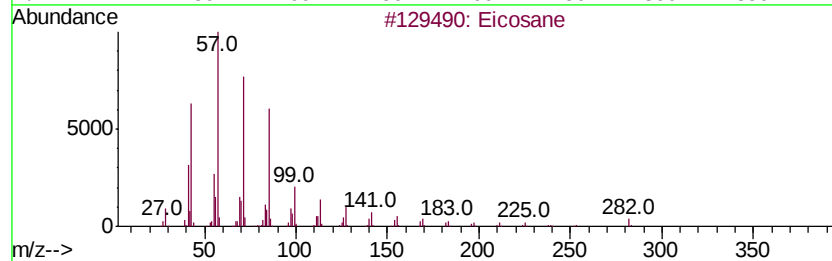
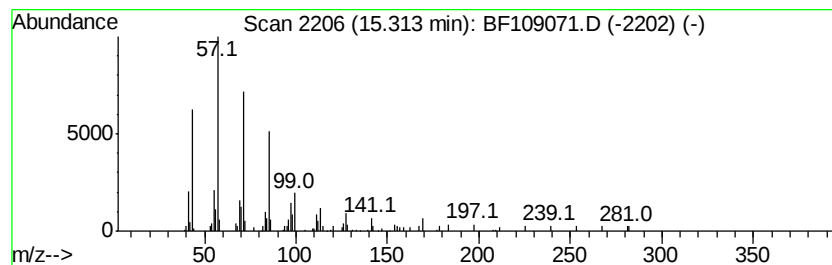
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.09 ng	111747	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
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Acq On : 18 Sep 2018 2:38
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Sample : J4936-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

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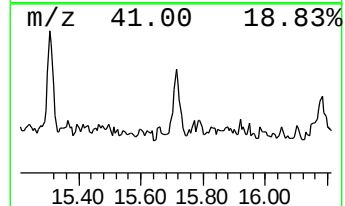
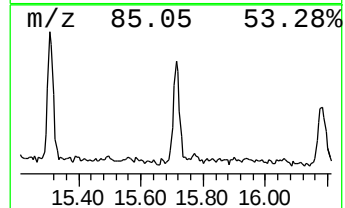
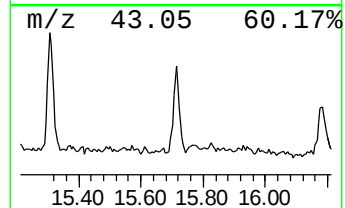
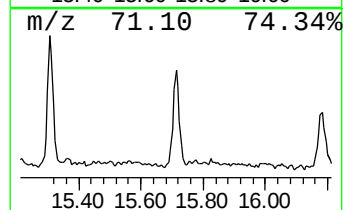
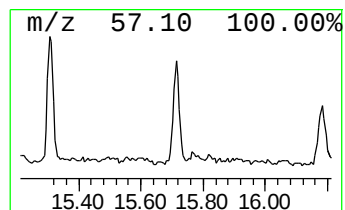
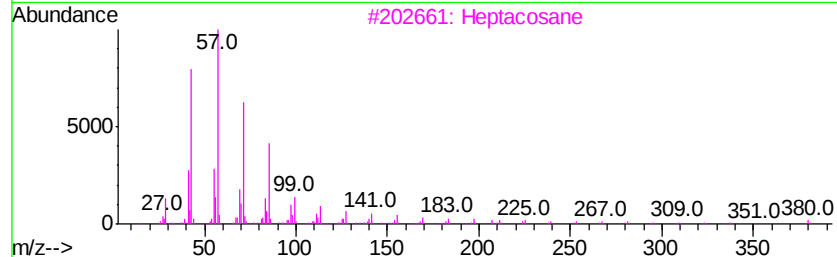
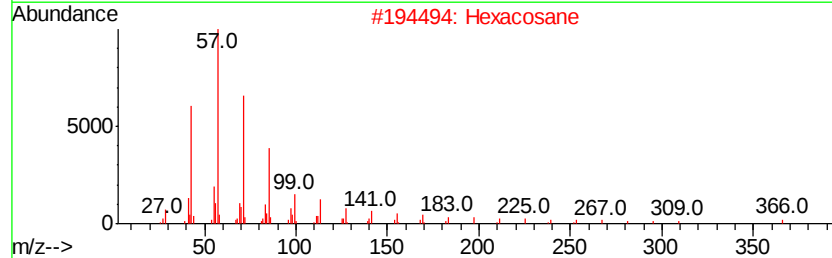
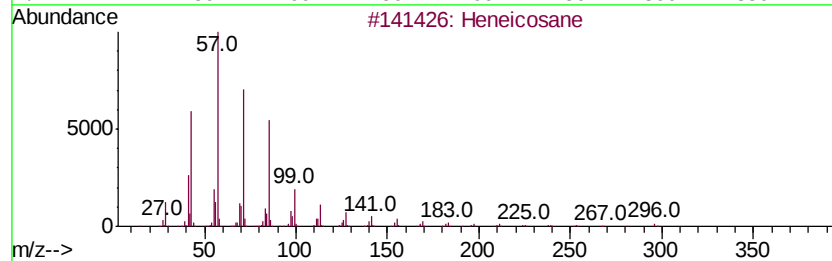
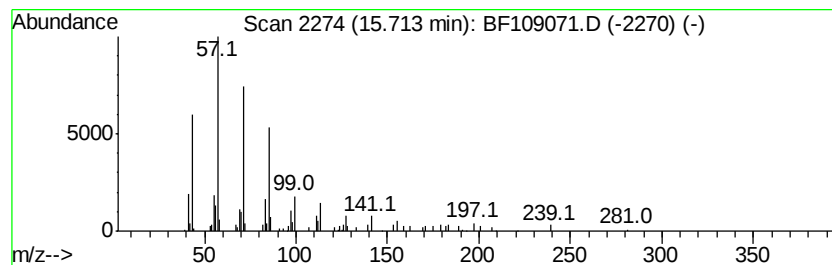
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.42 ng	87361	Perylene-d12	15.25

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		Triacontane	422	C30H62	000638-68-6	90
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
 Data File : BF109071.D
 Acq On : 18 Sep 2018 2:38
 Operator : JU/SJ
 Sample : J4936-09
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
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2-Pentanone, 4-hy...	4.91	20.7	ng	861742	1	6.72	833938	20.0
unknown6.49	6.49	73.6	ng	3067650	1	6.72	833938	20.0
Pentadecane	10.20	2.0	ng	101926	3	9.75	995792	20.0
Heptadecane	10.67	2.4	ng	110622	4	11.22	941479	20.0
1-Heneicosanol	13.72	4.8	ng	224112	5	13.85	938564	20.0
Hexacosane	14.64	2.7	ng	96793	6	15.25	722762	20.0
2-methyloctacosane	14.95	2.7	ng	97651	6	15.25	722762	20.0
Eicosane	15.31	3.1	ng	111747	6	15.25	722762	20.0
Heneicosane	15.71	2.4	ng	87361	6	15.25	722762	20.0