

Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
 Data File : BF093480.D
 Acq On : 9 Mar 2017 16:17
 Operator : SJ/MA
 Sample : I2133-04
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HY-SB411

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:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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	1.944	3	5	12	rVB	103762	145106	2.54%	0.311%
2	4.916	262	265	277	rBV	877217	1465563	25.67%	3.137%
3	5.361	302	304	321	rBV	4088249	5708472	100.00%	12.218%
4	5.761	336	339	347	rVB	55252	77770	1.36%	0.166%
5	6.413	394	396	399	rBV	3754968	5041613	88.32%	10.791%
6	6.539	404	407	409	rVV	4065742	5183335	90.80%	11.094%
7	6.756	425	426	429	rBV	757651	1040940	18.24%	2.228%
8	6.916	438	440	443	rBV	3928599	3735302	65.43%	7.995%
9	7.339	475	477	479	rBV	3463715	3377735	59.17%	7.230%
10	7.464	485	488	498	rVB4	59252	145373	2.55%	0.311%
11	7.842	519	521	531	rBV2	23738	60669	1.06%	0.130%
12	8.047	537	539	542	rBV	936125	1331413	23.32%	2.850%
13	9.007	620	623	627	rBV	30645	63655	1.12%	0.136%
14	9.133	631	634	636	rBV	4251111	5161646	90.42%	11.048%
15	9.522	666	668	671	rBV	352742	493402	8.64%	1.056%
16	9.808	690	693	695	rBV	1079401	1321150	23.14%	2.828%
17	10.208	726	728	732	rBV2	52049	95408	1.67%	0.204%
18	10.448	747	749	752	rBV	46530	57679	1.01%	0.123%
19	10.596	759	762	768	rBV	2310670	2416217	42.33%	5.172%
20	10.711	770	772	776	rVB	90471	136410	2.39%	0.292%
21	11.145	808	810	812	rBV2	39577	61613	1.08%	0.132%
22	11.282	820	822	825	rBV	792829	1138624	19.95%	2.437%
23	11.533	841	844	846	rBV	44914	97911	1.72%	0.210%
24	11.819	867	869	875	rBV5	68080	125798	2.20%	0.269%
25	11.979	882	883	889	rVB2	64640	105269	1.84%	0.225%
26	12.059	889	890	895	rVV3	58978	107527	1.88%	0.230%
27	12.128	895	896	903	rVB2	80857	116339	2.04%	0.249%
28	12.368	913	917	923	rVB4	46182	94937	1.66%	0.203%
29	12.688	943	945	947	rBV	193464	169737	2.97%	0.363%
30	12.871	958	961	964	rBV	3464992	3331315	58.36%	7.130%
31	13.099	979	981	985	rVB	45161	68415	1.20%	0.146%
32	13.396	1005	1007	1009	rBV	97771	100812	1.77%	0.216%
33	13.785	1037	1041	1048	rBV	204621	466011	8.16%	0.997%
34	13.934	1052	1054	1056	rVV	795301	1037450	18.17%	2.221%

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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.425	1095	1097	1100	rBV2	47129	79366	1.39%	0.170%
36	15.351	1175	1178	1184	rBV	507675	824135	14.44%	1.764%
37	16.185	1249	1251	1259	rVB2	26113	72680	1.27%	0.156%
38	16.723	1294	1298	1301	rBV3	20945	63121	1.11%	0.135%
39	17.054	1322	1327	1334	rVB	676172	1394036	24.42%	2.984%
40	17.214	1337	1341	1346	rBV8	32715	121990	2.14%	0.261%
41	19.043	1498	1501	1507	rVB7	24428	85102	1.49%	0.182%

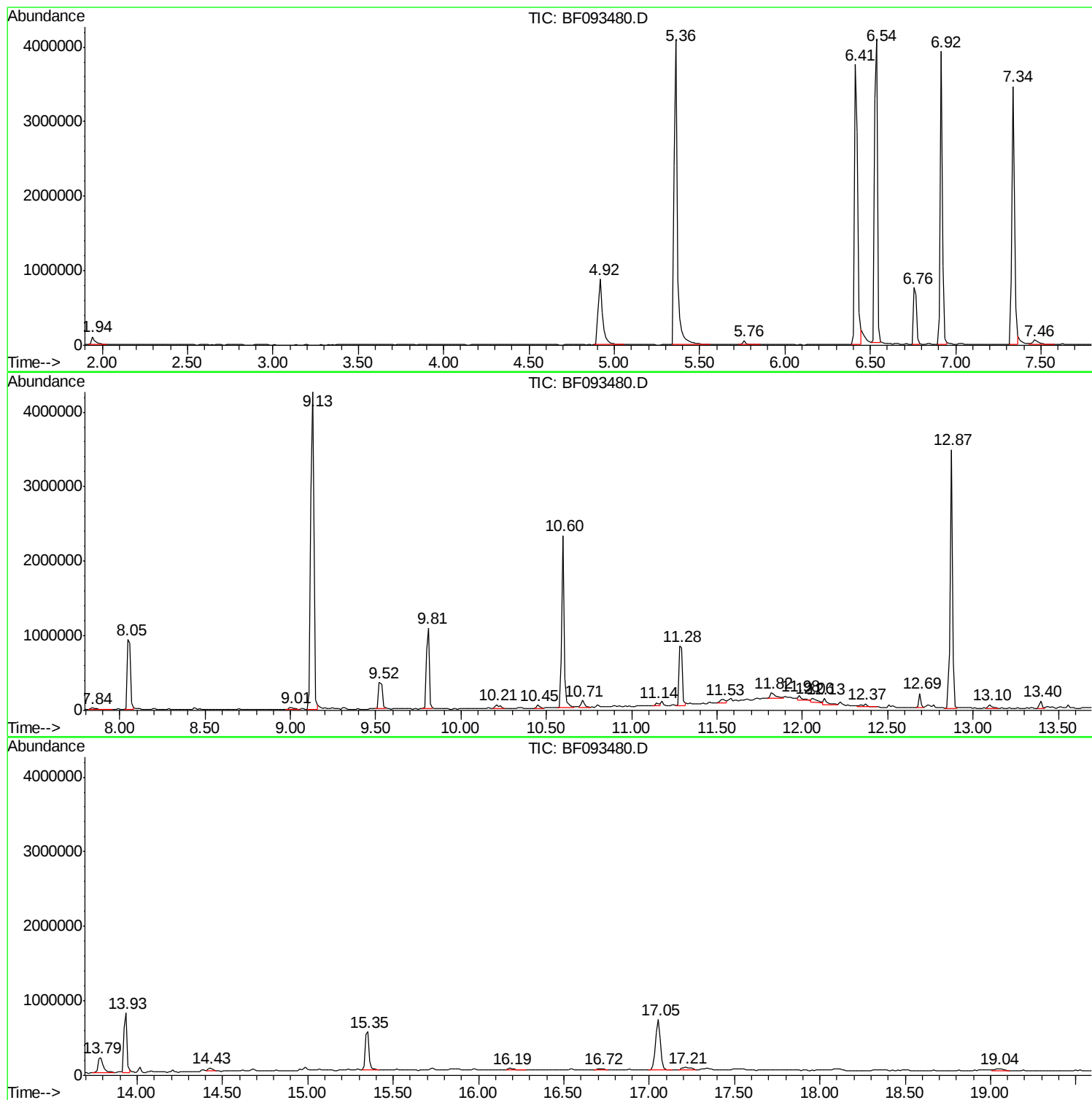
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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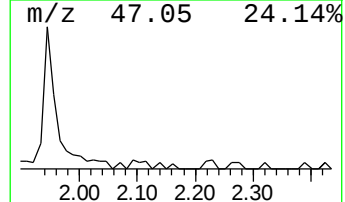
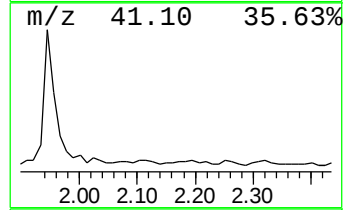
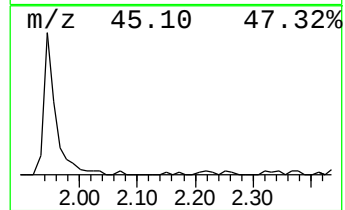
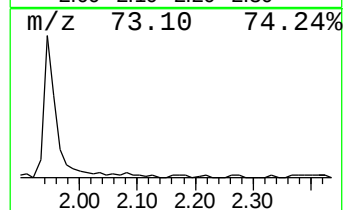
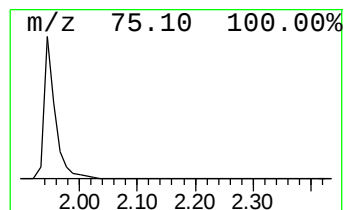
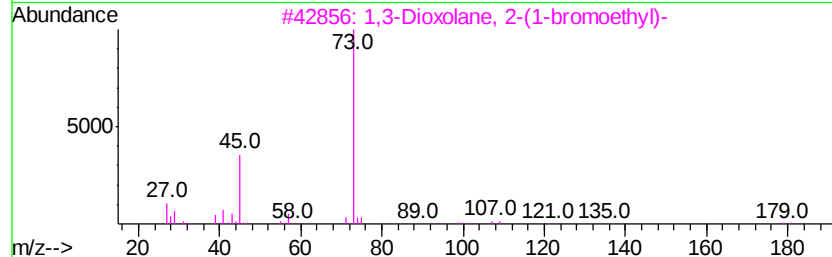
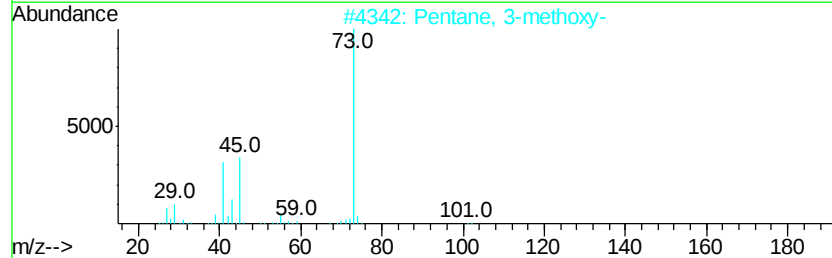
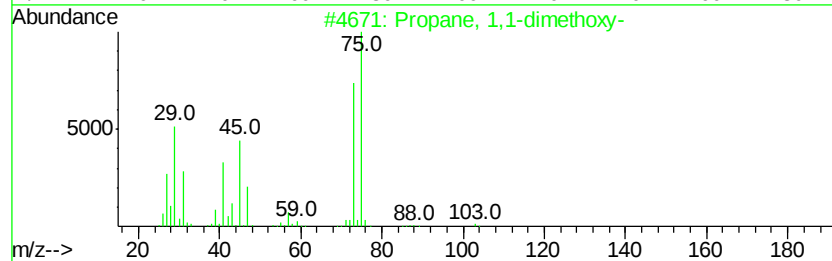
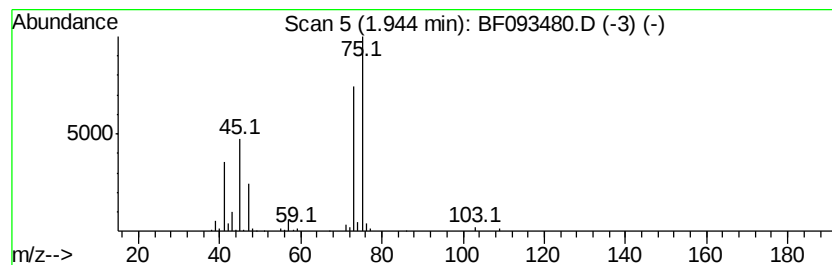
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.94	2.79 ng	145106	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
4		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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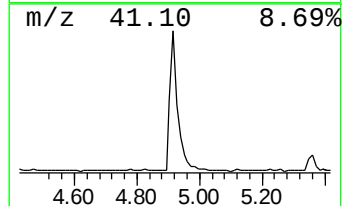
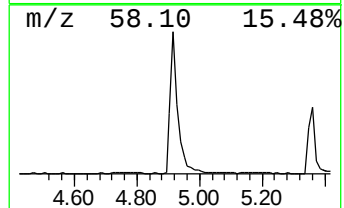
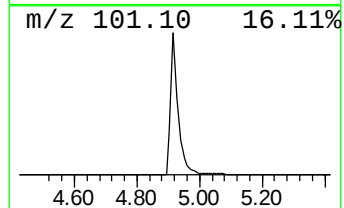
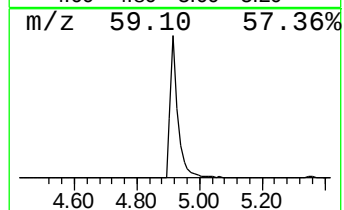
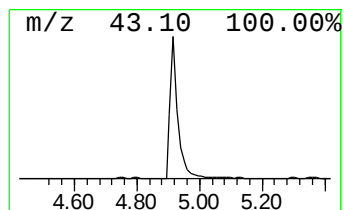
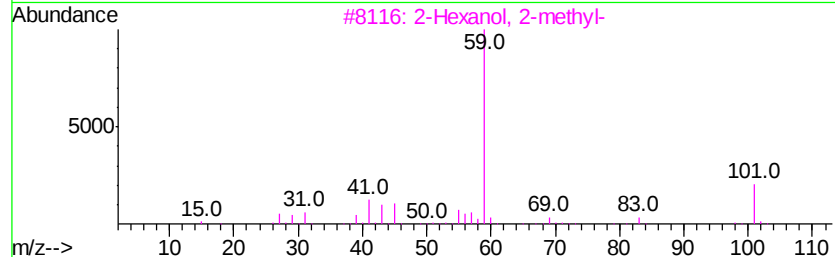
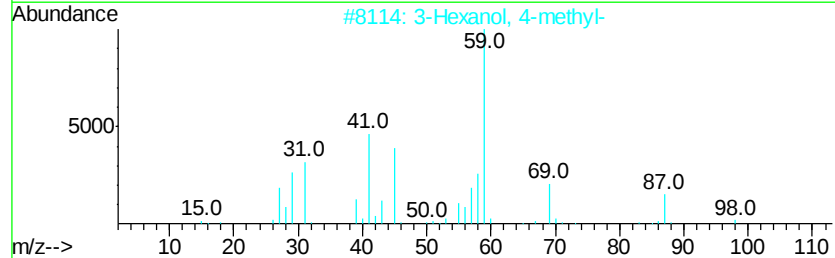
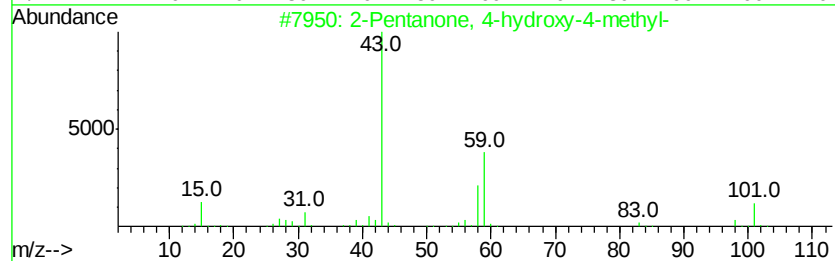
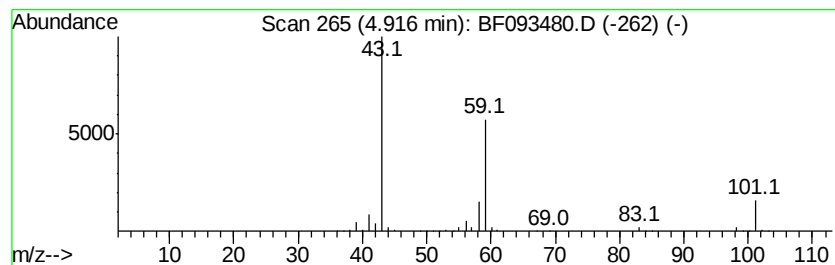
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	28.16 ng	1465560	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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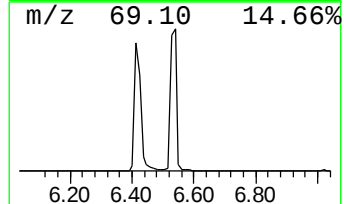
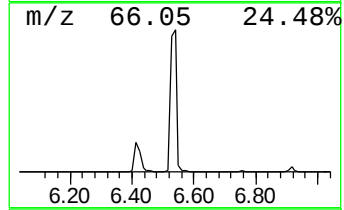
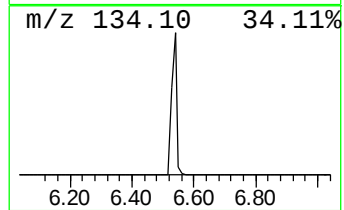
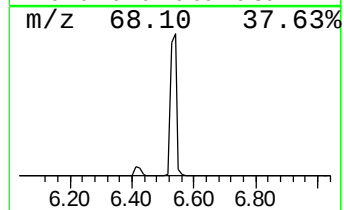
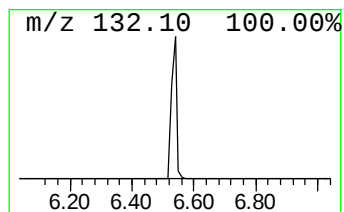
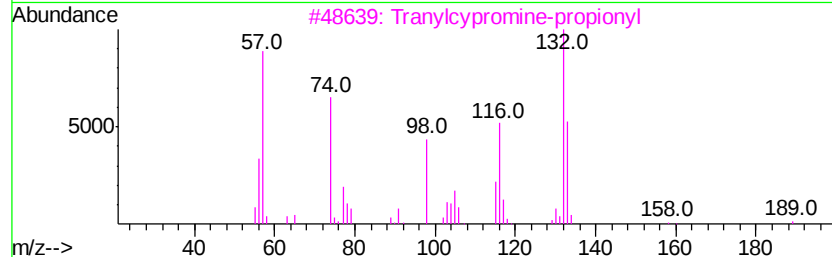
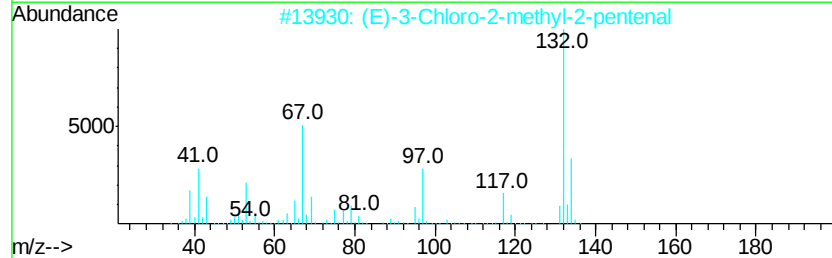
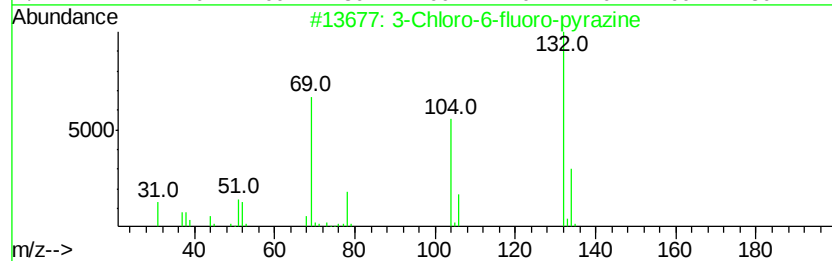
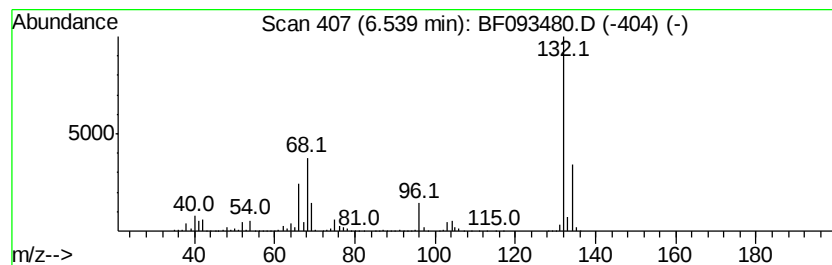
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	99.59 ng	5183340	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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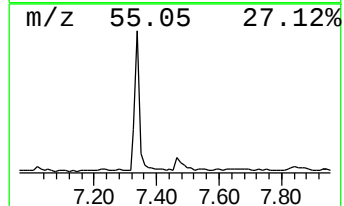
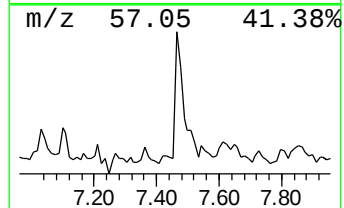
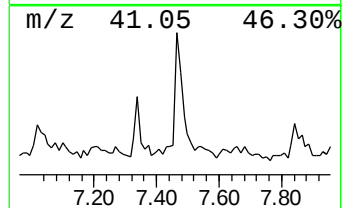
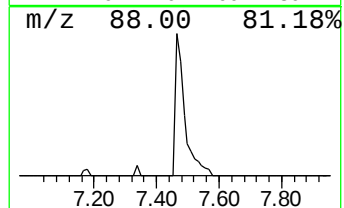
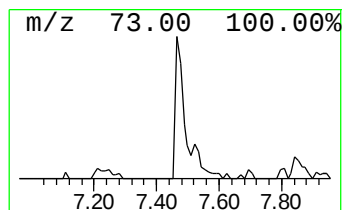
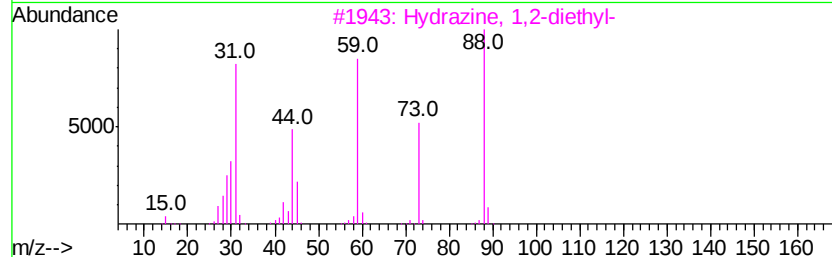
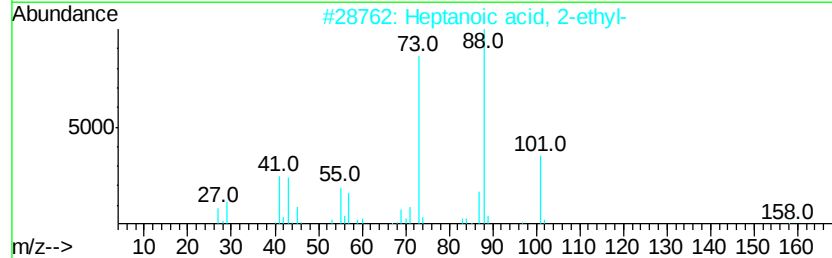
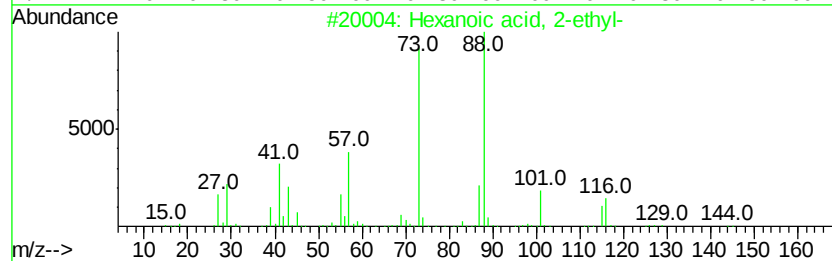
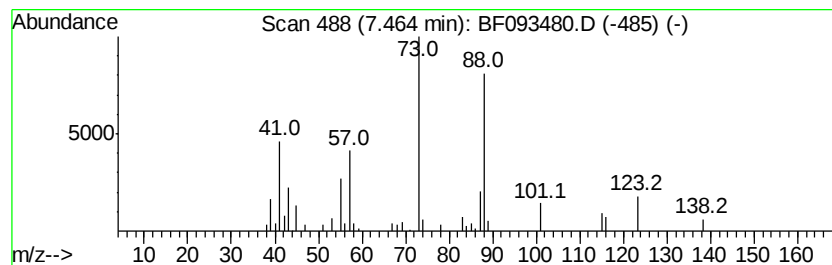
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.18 ng	145373	Naphthalene-d8	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	50
3		Hvdrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	47
4		Methyl 4-O-acetyl-2,3-di-O-methy...	248	C11H20O6	072945-56-3	33
5		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	33



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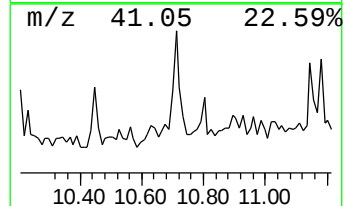
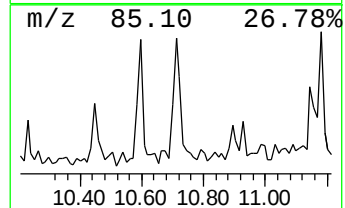
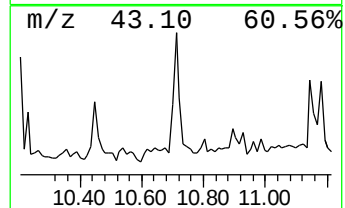
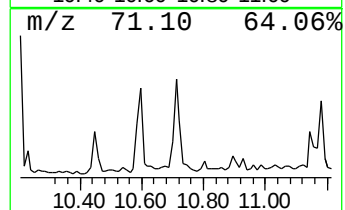
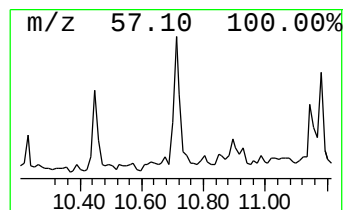
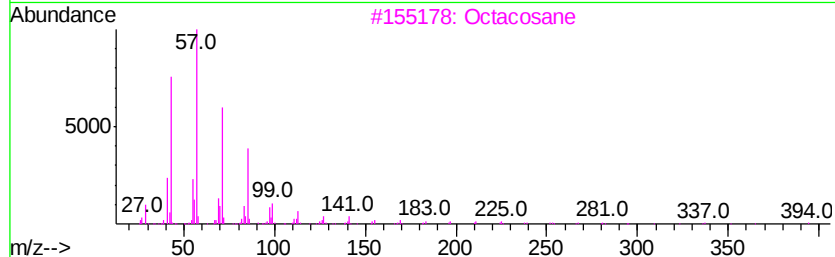
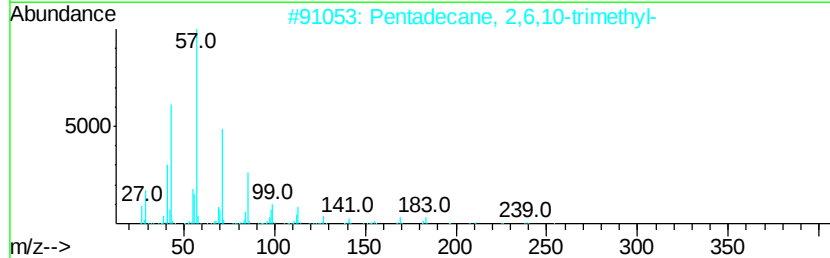
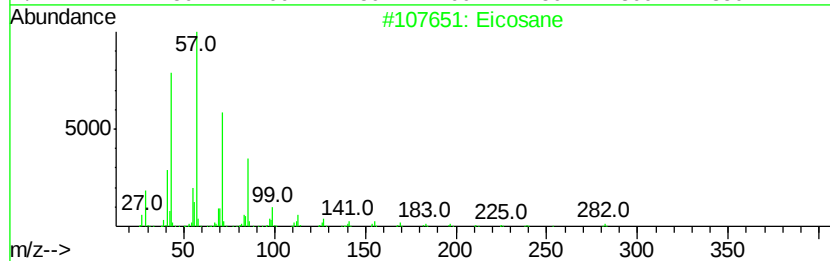
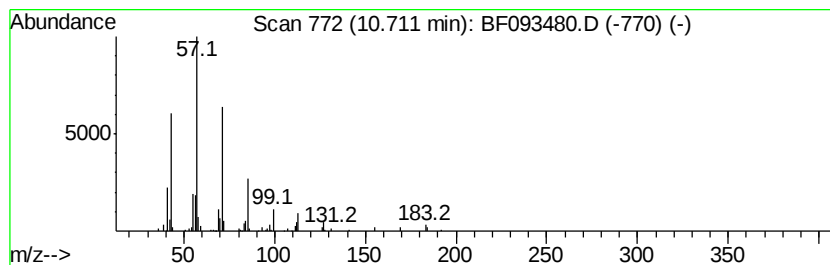
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	2.40 ng	136410	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	86
2	Pentadecane, 2,6,10-trimethyl-		254	C18H38	003892-00-0	86
3	Octacosane		394	C28H58	000630-02-4	86
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	80
5	Tridecane, 4-methyl-		198	C14H30	026730-12-1	78



Data Path : Z:\HPCHEM1\BNA_F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HY-SB411

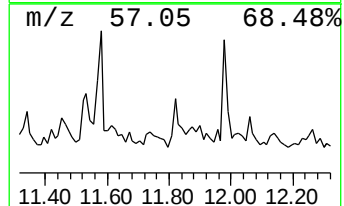
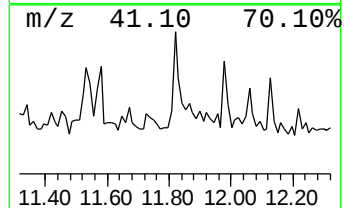
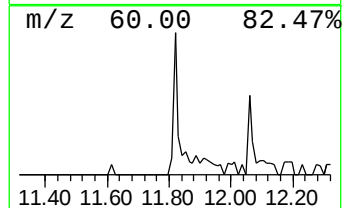
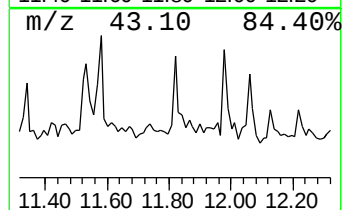
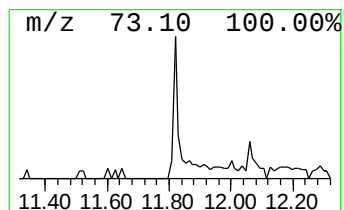
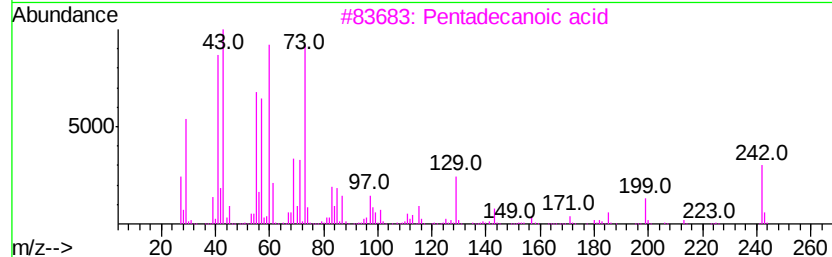
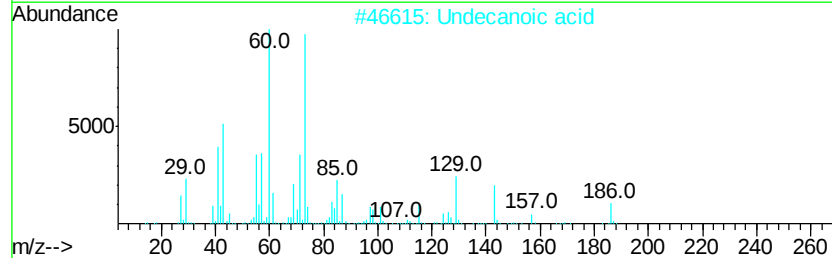
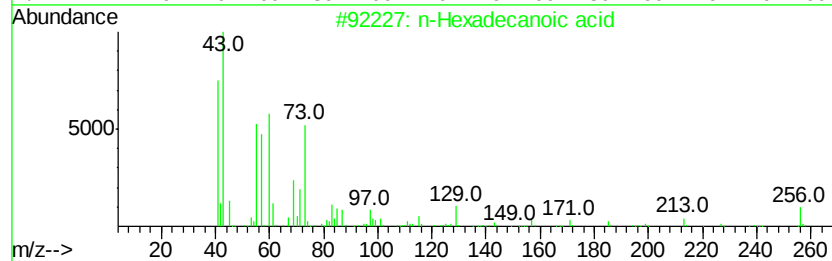
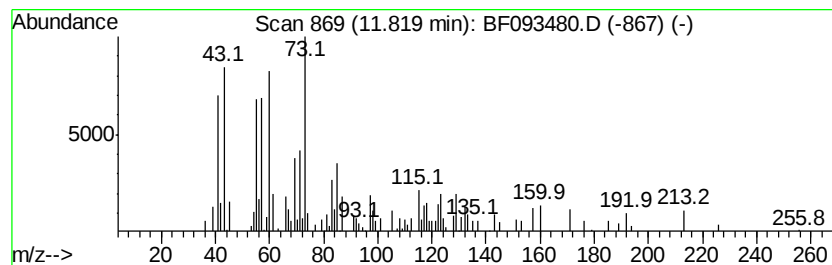
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.21 ng	125798	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2		Undecanoic acid	186	C11H22O2	000112-37-8	59
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HY-SB411

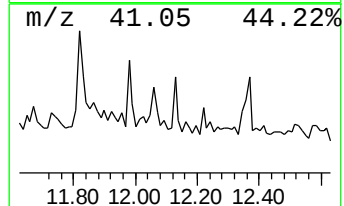
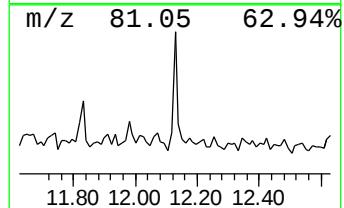
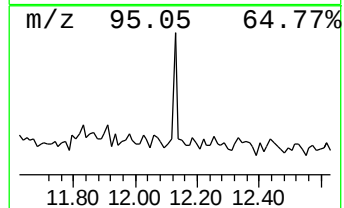
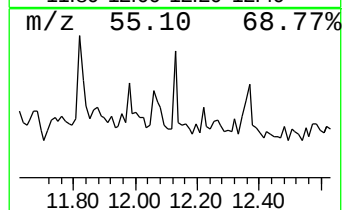
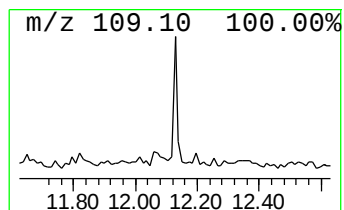
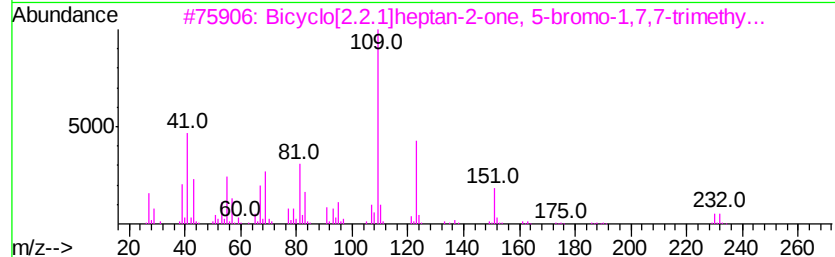
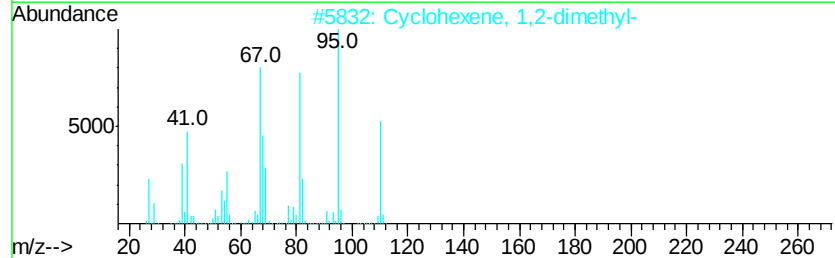
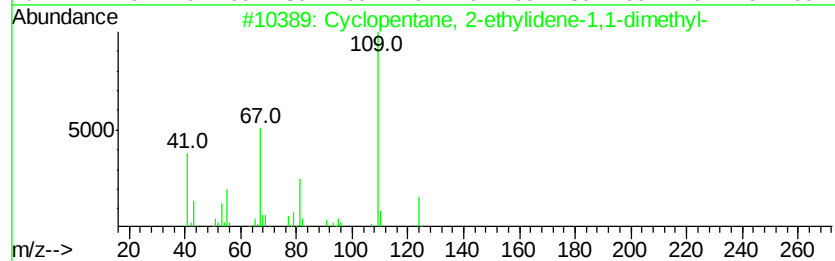
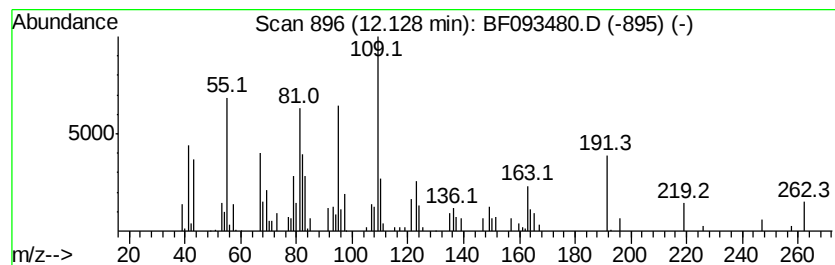
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown12.13 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	2.04 ng	116339	Phenanthrene-d10	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	27
2		Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	25
3		Bicyclo[2.2.1]heptan-2-one, 5-br...	230	C10H15BrO	010293-00-2	22
4		Cyclopropane, tetramethylmethylen-	110	C8H14	054376-39-5	18
5		cis-Bicyclo[2.2.1]heptane, 2,3-d...	124	C9H16	1000262-02-5	18



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

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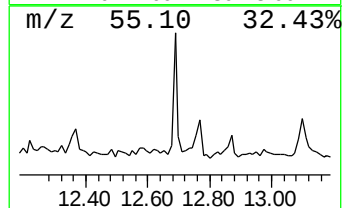
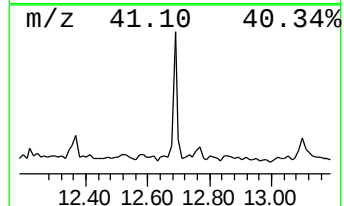
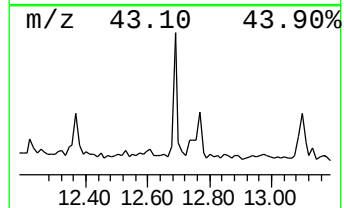
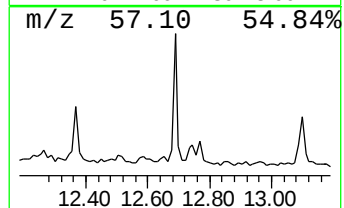
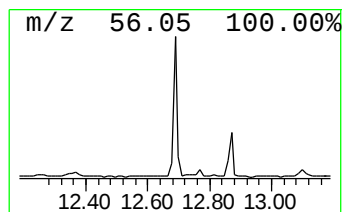
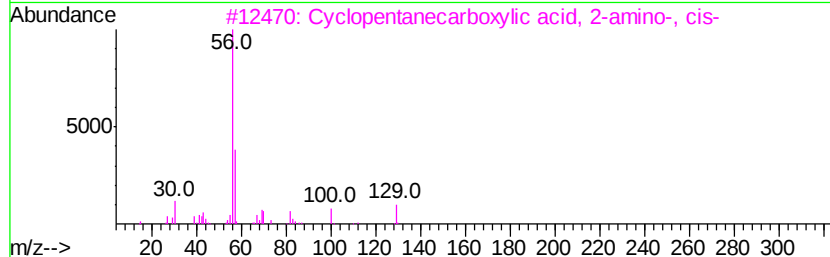
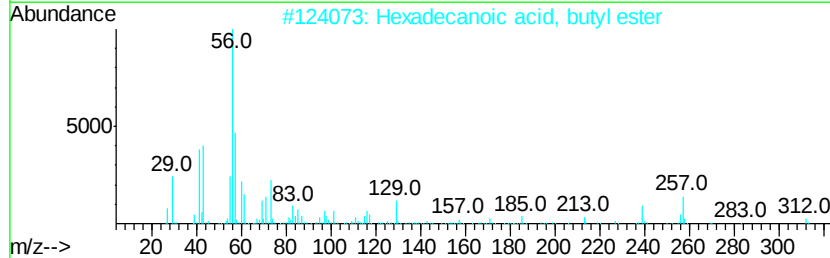
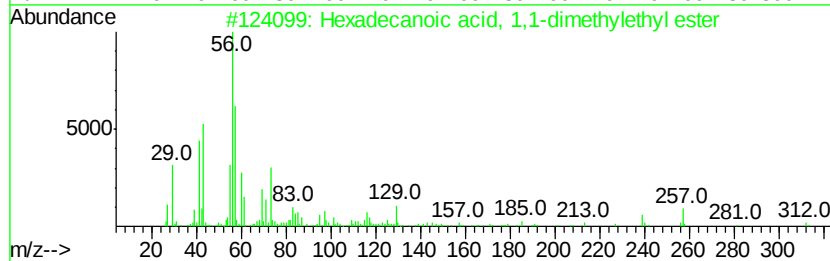
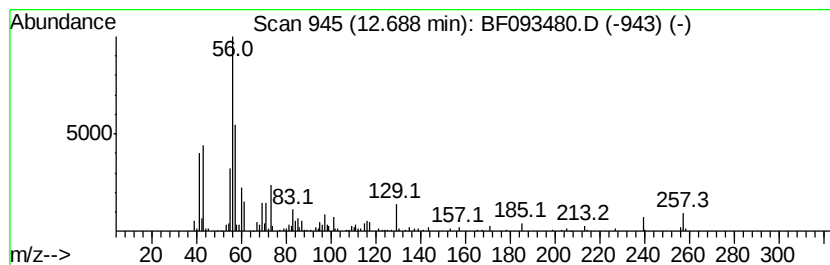
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	3.27 ng	169737	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	49
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HY-SB411

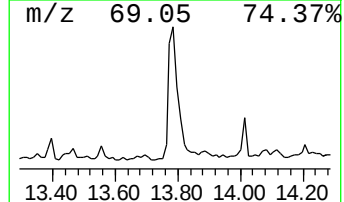
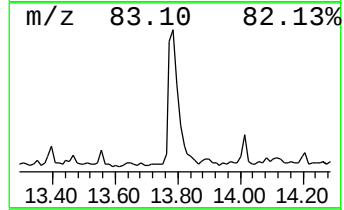
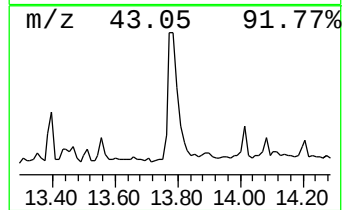
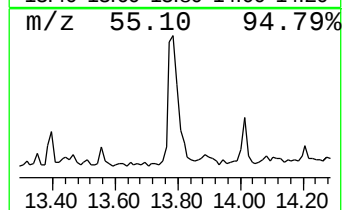
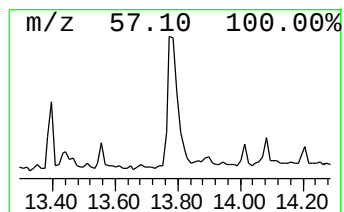
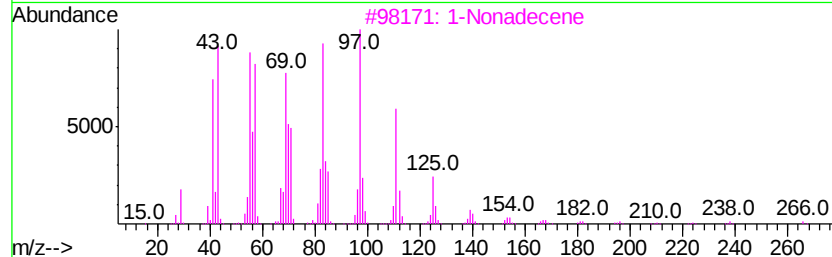
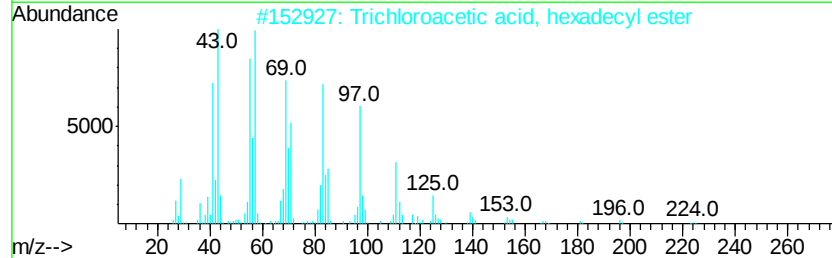
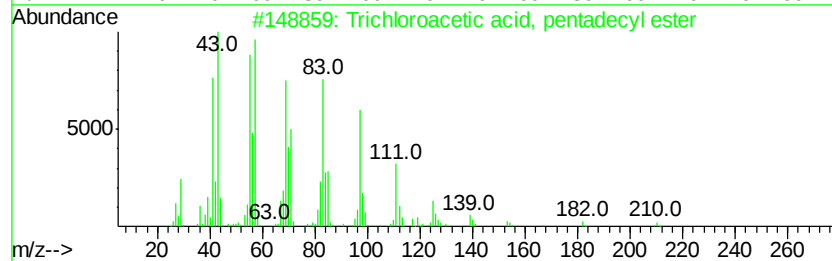
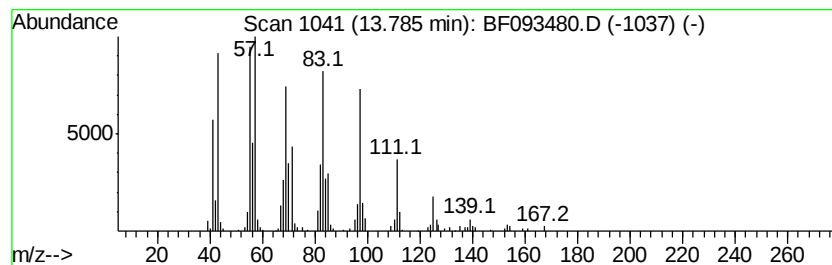
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	8.98 ng	466011	Chrysene-d12	13.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			1-Nonadecene	266	C19H38	018435-45-5	90
4			11-Tricosene	322	C23H46	052078-56-5	90
5			1-Docosene	308	C22H44	001599-67-3	89



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HY-SB411

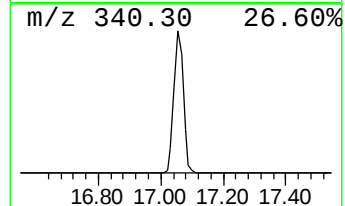
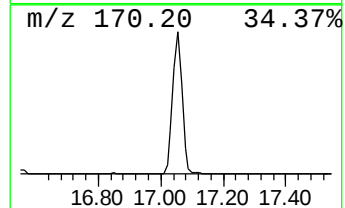
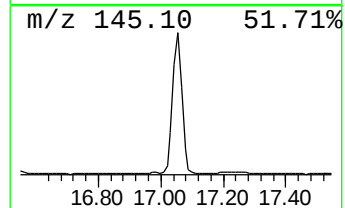
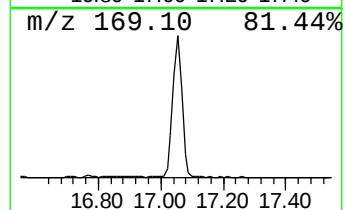
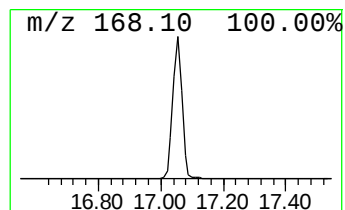
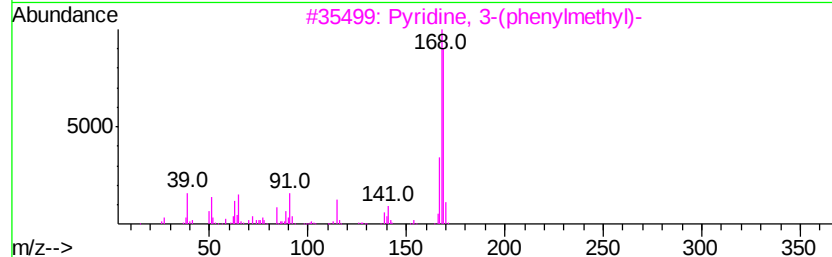
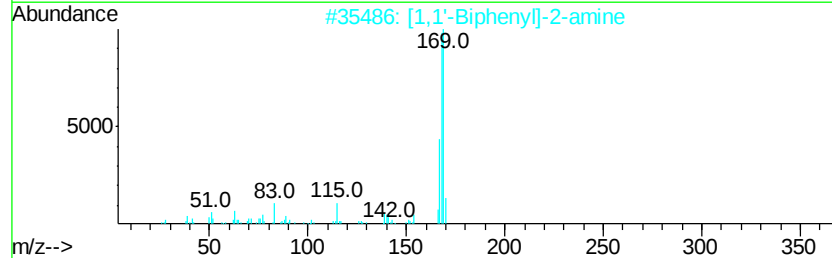
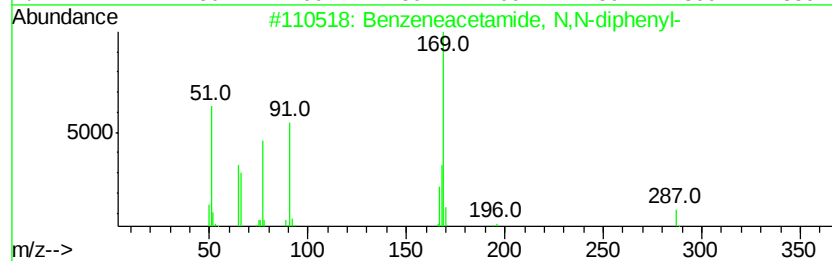
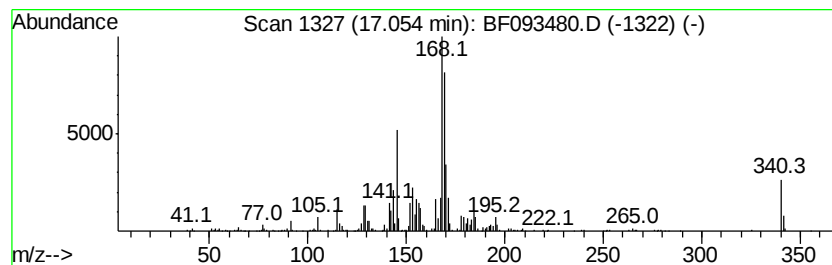
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown17.05 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	33.83 ng	1394040	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetamide, N,N-diphenyl-	287	C20H17NO	033675-70-6	47
2		[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	43
3		Pyridine, 3-(phenylmethyl)-	169	C12H11N	000620-95-1	37
4		Nickel,bis(1,2,3-eta.)-2-methyl...	168	C8H14Ni	012261-14-2	35
5		3-Phenyl-3-(2-pyridyl)-N,N-dimet...	240	C16H20N2	000086-21-5	22



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

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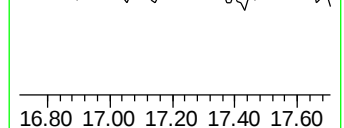
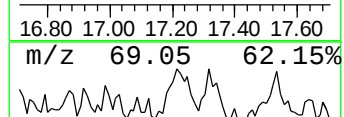
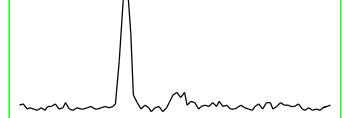
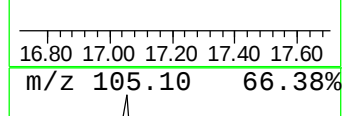
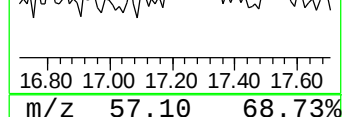
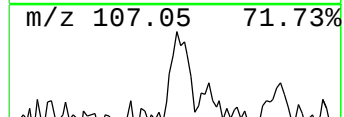
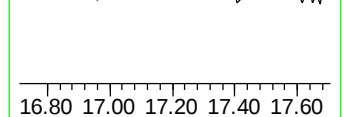
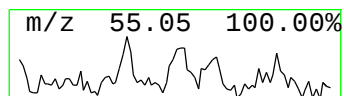
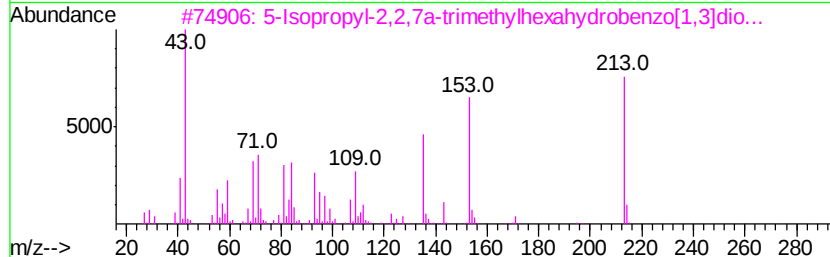
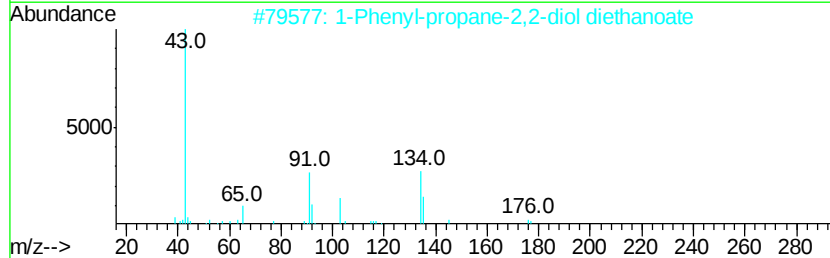
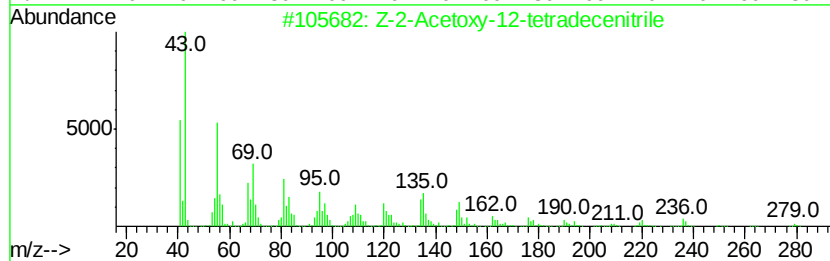
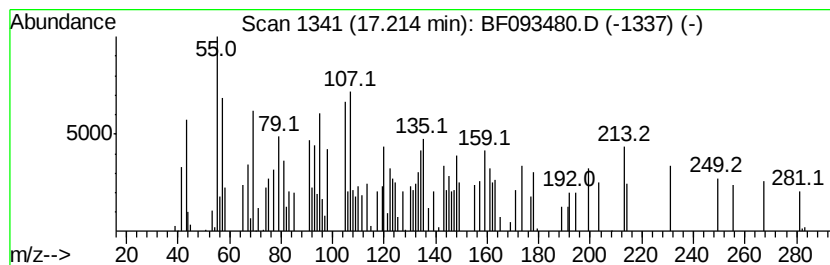
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown17.21 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	2.96 ng	121990	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-2-Acetoxy-12-tetradecenitrile	279	C17H29NO2	1000130-78-6	9
2		1-Phenyl-propane-2,2-diol dietha...	236	C13H16O4	064847-83-2	9
3		5-Isopropyl-2,2,7a-trimethylhexa...	228	C13H24O3	075316-52-8	9
4		Dodecane, 1,12-dibromo-	326	C12H24Br2	003344-70-5	9
5		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	9



Data Path : Z:\HPCHEM1\BNA F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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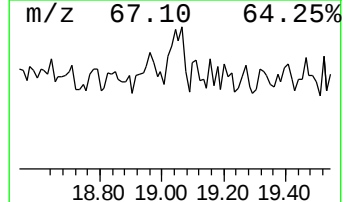
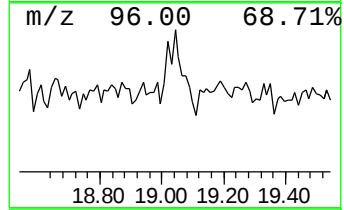
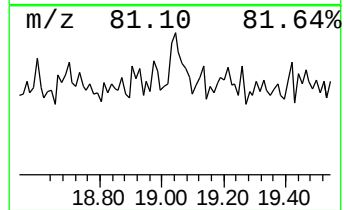
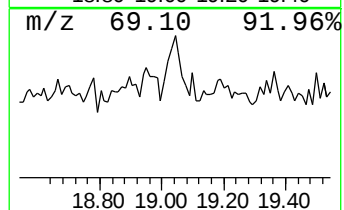
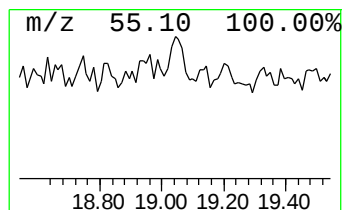
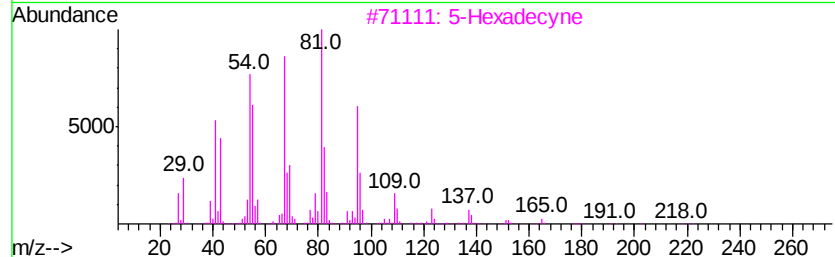
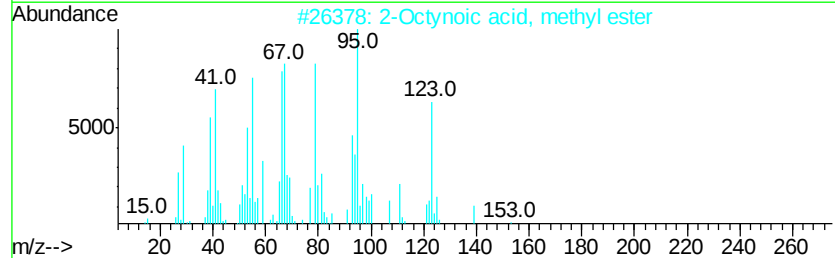
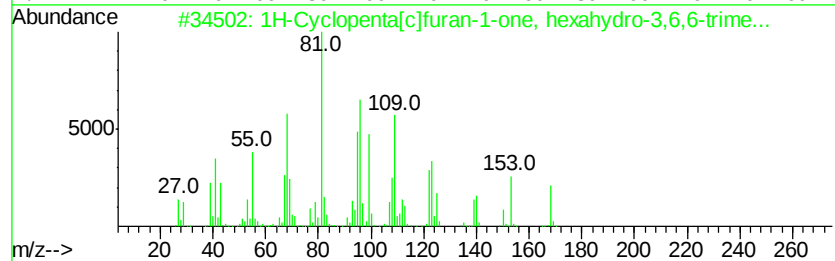
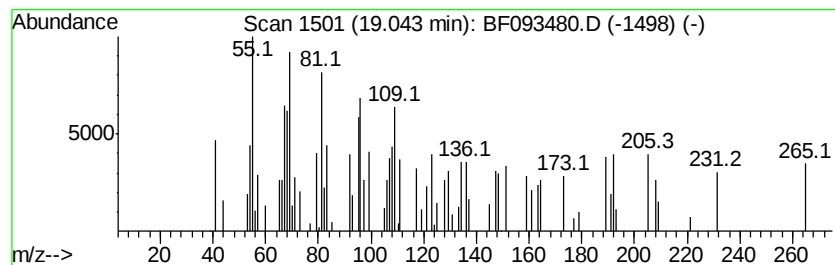
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown19.04 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	2.07 ng	85102	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Cyclopenta[c]furan-1-one, hex...	168	C10H16O2	077384-13-5	38
2		2-Octynoic acid, methyl ester	154	C9H14O2	000111-12-6	14
3		5-Hexadecyne	222	C16H30	071899-37-1	14
4		Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	14
5		4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	12



Data Path : Z:\HPCHEM1\BNA_F\Data\BF030817\
Data File : BF093480.D
Acq On : 9 Mar 2017 16:17
Operator : SJ/MA
Sample : I2133-04
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HY-SB411

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.94	2.8 ng		145106	1	6.77	1040940	20.0
2-Pentanone, 4-hy...	4.92	28.2 ng		1465560	1	6.77	1040940	20.0
unknown6.54	6.54	99.6 ng		5183340	1	6.77	1040940	20.0
Hexanoic acid, 2-...	7.46	2.2 ng		145373	2	8.06	1331410	20.0
Eicosane	10.71	2.4 ng		136410	4	11.29	1138620	20.0
n-Hexadecanoic acid	11.82	2.2 ng		125798	4	11.29	1138620	20.0
unknown12.13	12.13	2.0 ng		116339	4	11.29	1138620	20.0
Hexadecanoic acid...	12.69	3.3 ng		169737	5	13.93	1037450	20.0
Trichloroacetic a...	13.79	9.0 ng		466011	5	13.93	1037450	20.0
unknown17.05	17.05	33.8 ng		1394040	6	15.35	824135	20.0
unknown17.21	17.21	3.0 ng		121990	6	15.35	824135	20.0
unknown19.04	19.04	2.1 ng		85102	6	15.35	824135	20.0