

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104349.D
 Acq On : 7 Apr 2018 10:43
 Operator : JU/SJ
 Sample : J2255-04
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-JETB-E-U-B

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-BF040618.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	4.999	492	495	502	rVB	123107	121482	3.61%	0.563%
2	5.404	559	564	567	rBV	900966	855231	25.42%	3.964%
3	6.416	732	736	744	rVB	682347	534238	15.88%	2.476%
4	6.563	757	761	765	rBV	1840479	1673784	49.75%	7.757%
5	6.804	798	802	805	rBV	995827	869920	25.86%	4.032%
6	6.957	824	828	832	rVB	2575246	2345459	69.71%	10.870%
7	7.369	892	898	901	rBV	1901722	1858538	55.24%	8.613%
8	8.087	1016	1020	1023	rBV	1400616	1144295	34.01%	5.303%
9	9.163	1198	1203	1206	rBV	3663412	3364432	100.00%	15.592%
10	9.239	1213	1216	1218	rBV	57781	45382	1.35%	0.210%
11	9.557	1266	1270	1273	rBV	253654	225016	6.69%	1.043%
12	9.769	1303	1306	1309	rBV	146042	126035	3.75%	0.584%
13	9.839	1314	1318	1322	rVB2	1413398	1208188	35.91%	5.599%
14	10.092	1358	1361	1365	rBV2	35937	35383	1.05%	0.164%
15	10.269	1384	1391	1394	rBV	173323	159676	4.75%	0.740%
16	10.492	1423	1429	1431	rBV	47495	62302	1.85%	0.289%
17	10.628	1447	1452	1455	rBV	1332064	1155228	34.34%	5.354%
18	10.745	1469	1472	1480	rVB	153159	145928	4.34%	0.676%
19	11.192	1546	1548	1551	rBV2	55281	43081	1.28%	0.200%
20	11.328	1567	1571	1574	rBV	1094926	921455	27.39%	4.270%
21	11.851	1657	1660	1670	rBV4	60113	60821	1.81%	0.282%
22	12.027	1687	1690	1695	rVB2	46607	39881	1.19%	0.185%
23	12.739	1807	1811	1814	rBV	200538	150622	4.48%	0.698%
24	12.916	1837	1841	1845	rBV	2455519	2361430	70.19%	10.944%
25	13.445	1927	1931	1934	rBV	124721	101532	3.02%	0.471%
26	13.810	1990	1993	2003	rBV	136099	147019	4.37%	0.681%
27	13.969	2016	2020	2023	rBV	909434	818451	24.33%	3.793%
28	15.086	2206	2210	2216	rBV	36652	43605	1.30%	0.202%
29	15.427	2262	2268	2272	rBV	619005	753342	22.39%	3.491%
30	15.463	2272	2274	2284	rVB	37133	44751	1.33%	0.207%
31	15.892	2343	2347	2352	rBV2	28691	42236	1.26%	0.196%
32	16.398	2425	2433	2445	rVB3	28885	57582	1.71%	0.267%
33	17.445	2604	2611	2620	rVB7	28318	61032	1.81%	0.283%

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Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-U-B

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

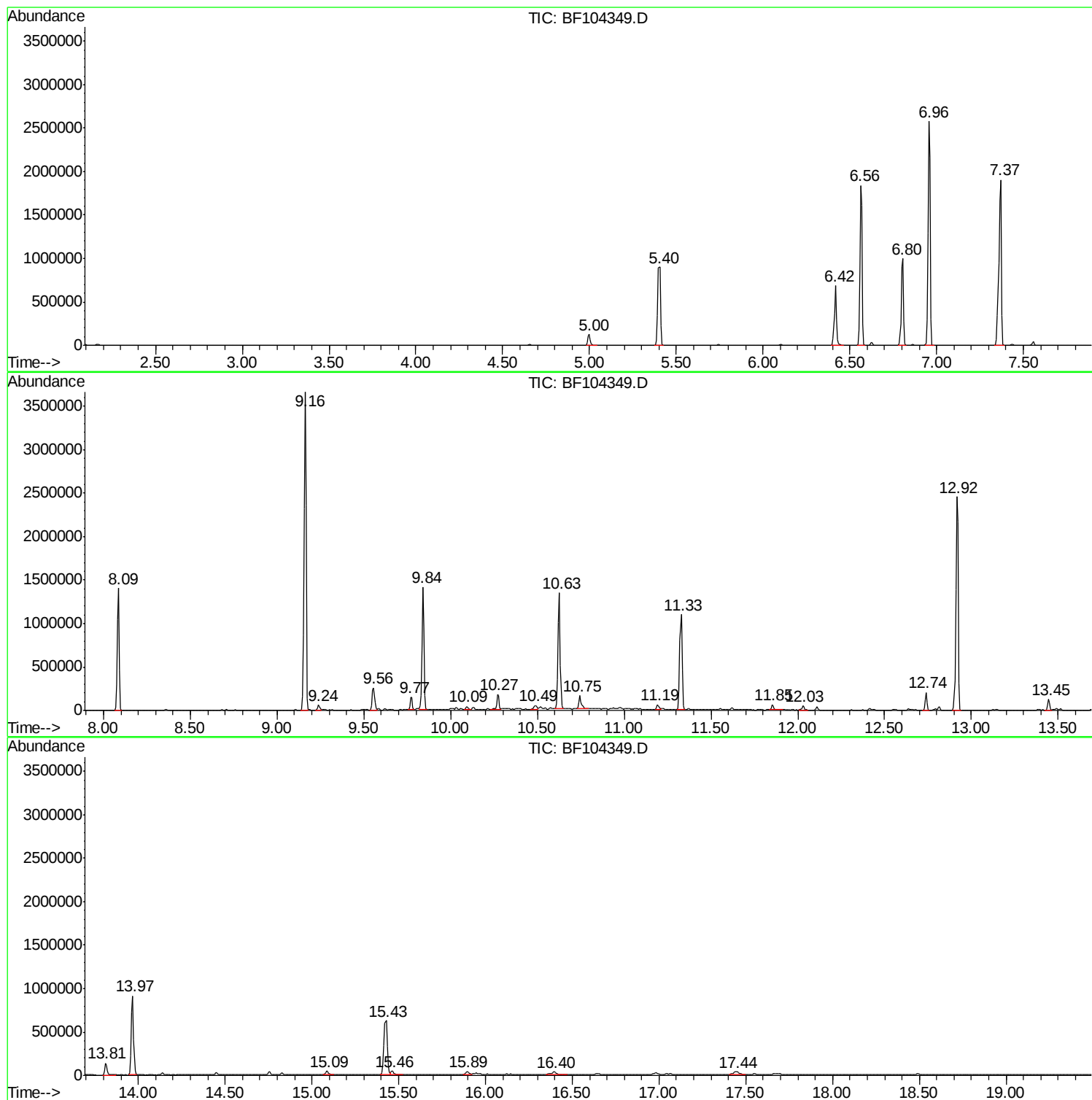
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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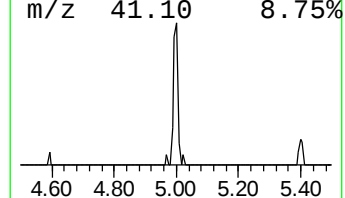
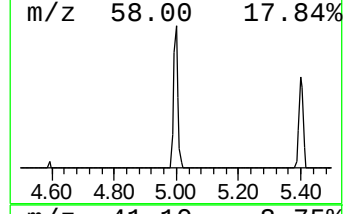
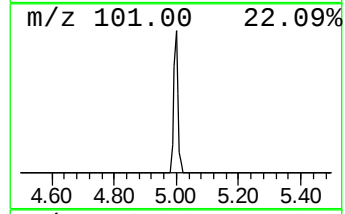
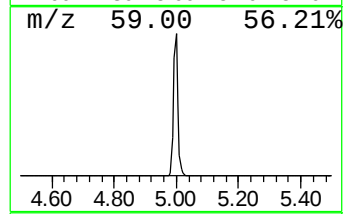
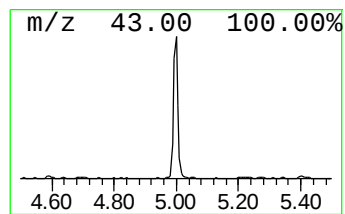
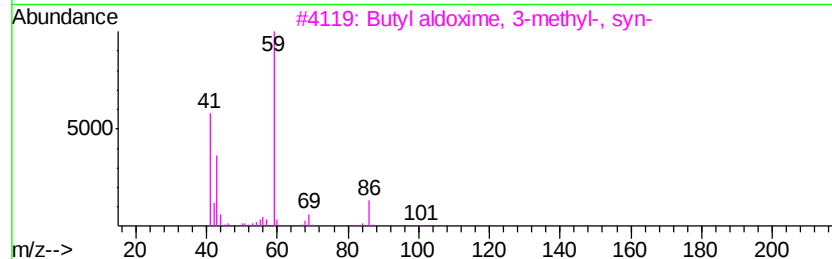
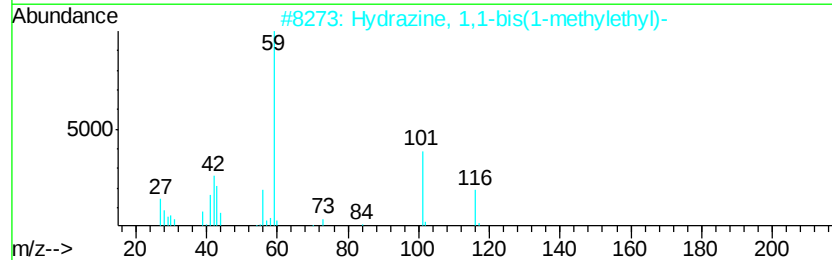
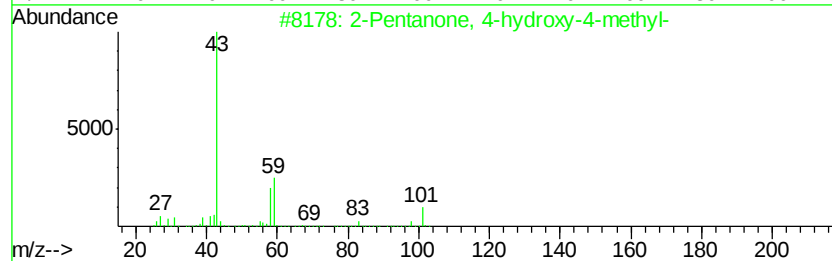
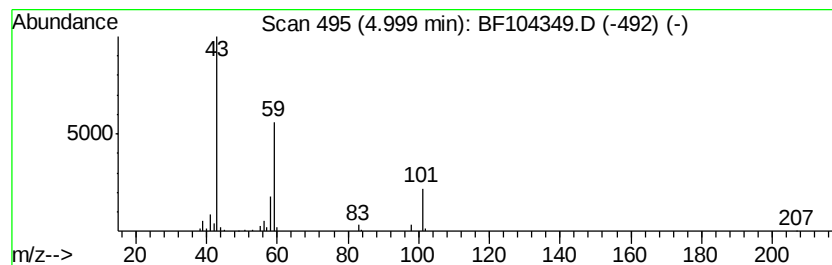
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.79 ng	121482	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
4	Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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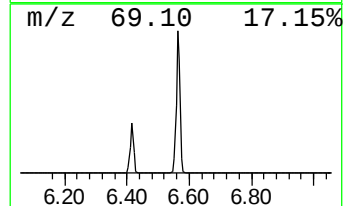
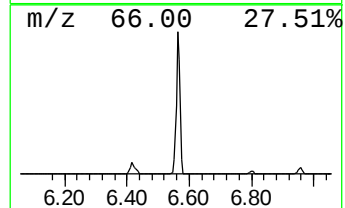
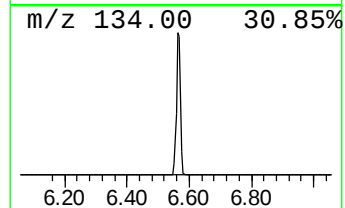
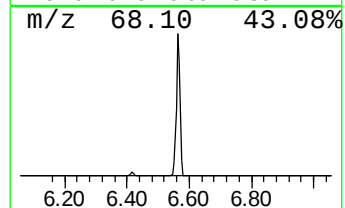
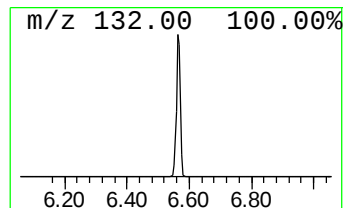
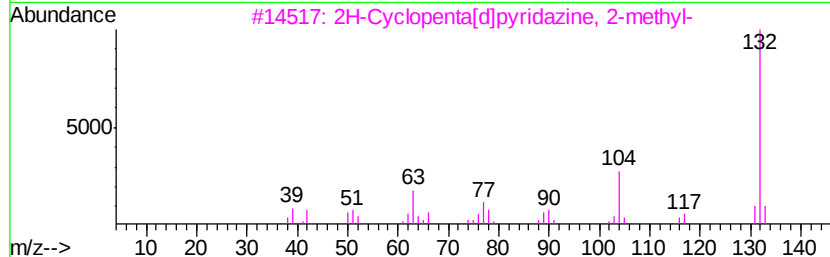
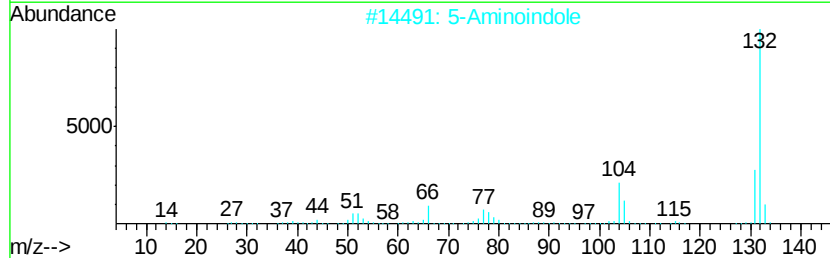
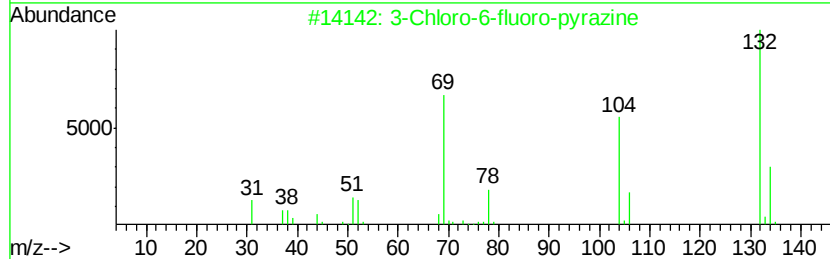
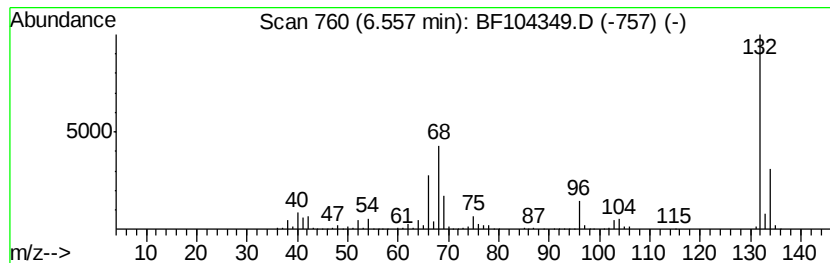
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	38.48 ng	1673780	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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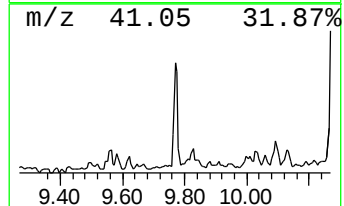
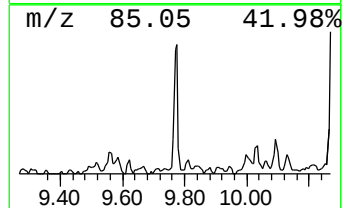
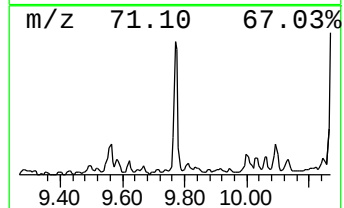
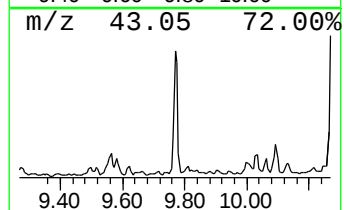
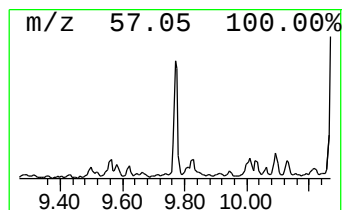
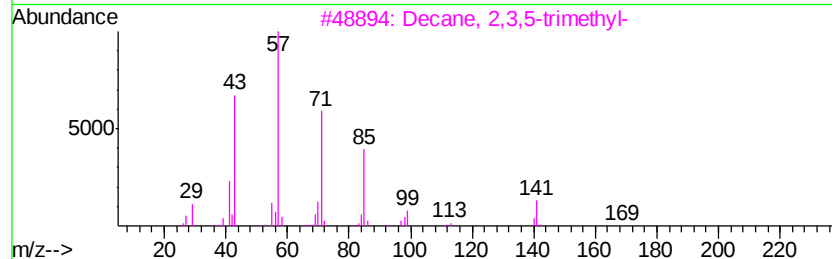
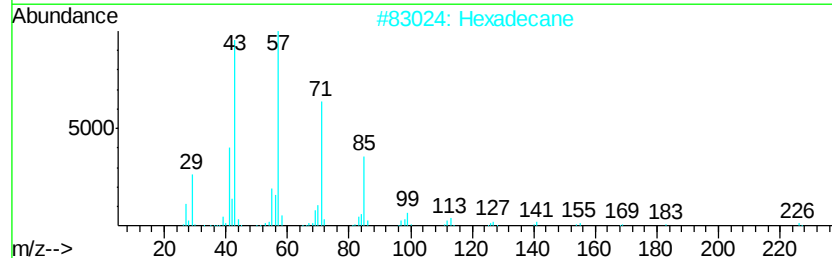
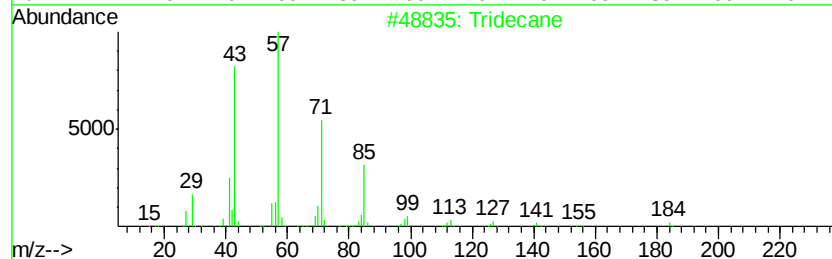
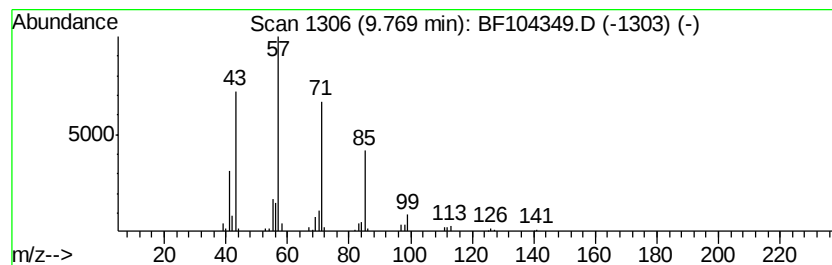
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.77	2.09 ng	126035	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	83
2		Hexadecane	226	C16H34	000544-76-3	83
3		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
5		Nonane, 5-butyl-	184	C13H28	017312-63-9	72



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Misc :
ALS Vial : 43 Sample Multiplier: 1

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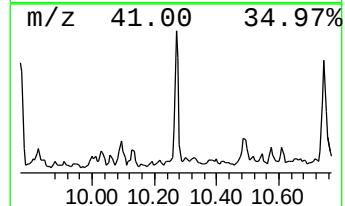
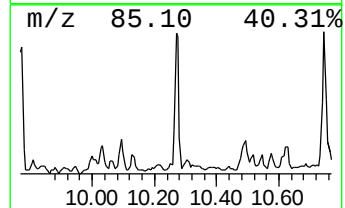
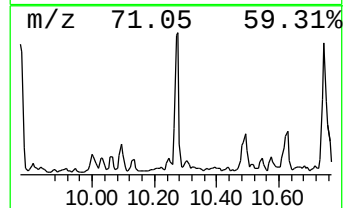
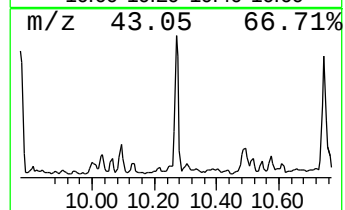
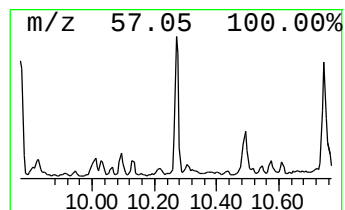
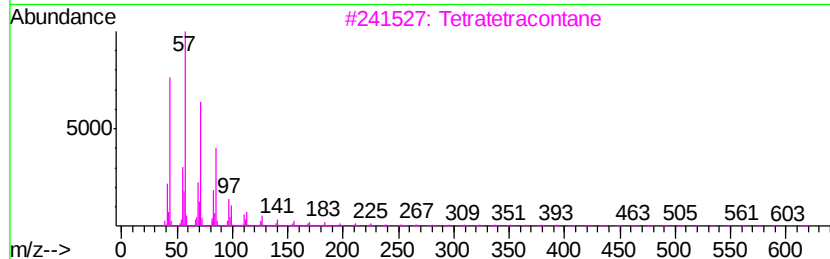
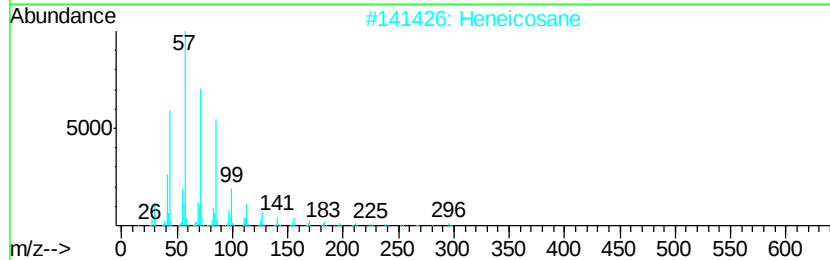
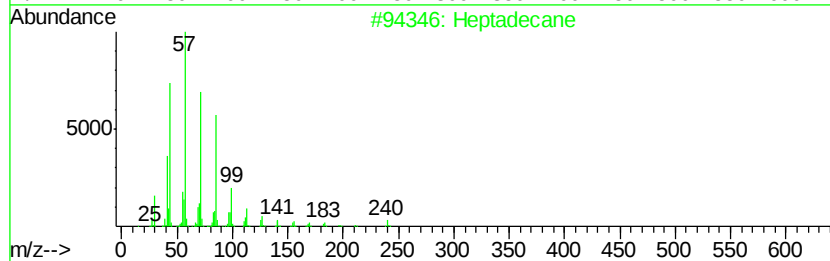
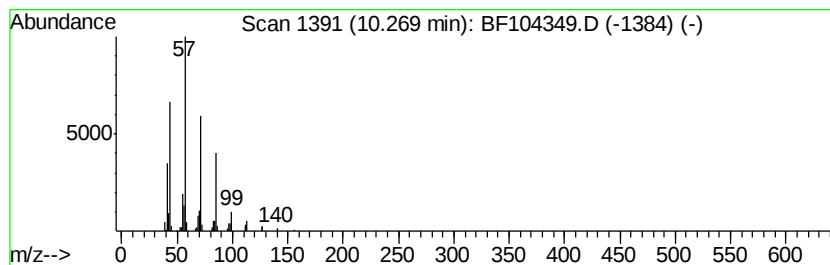
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.64 ng	159676	Acenaphthene-d10	9.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Heneicosane		296	C21H44	000629-94-7	83
3	Tetratetracontane		619	C44H90	007098-22-8	83
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	83
5	Tetradecane		198	C14H30	000629-59-4	80



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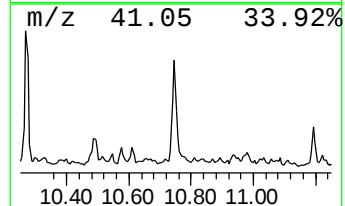
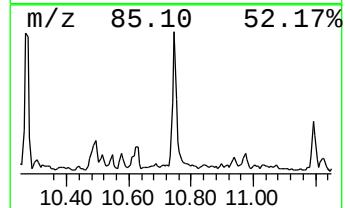
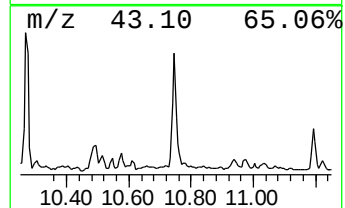
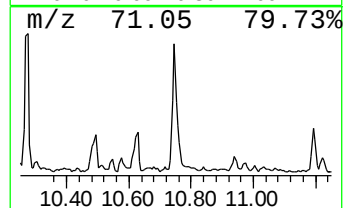
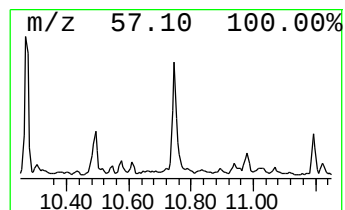
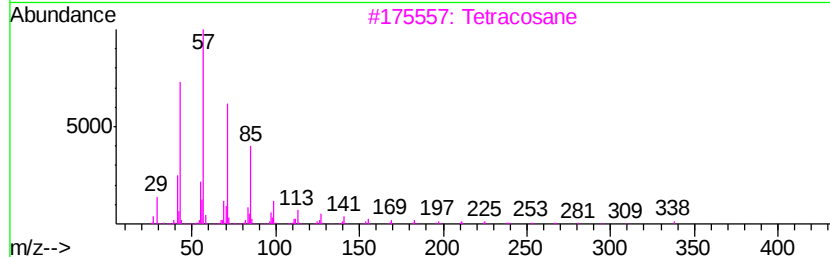
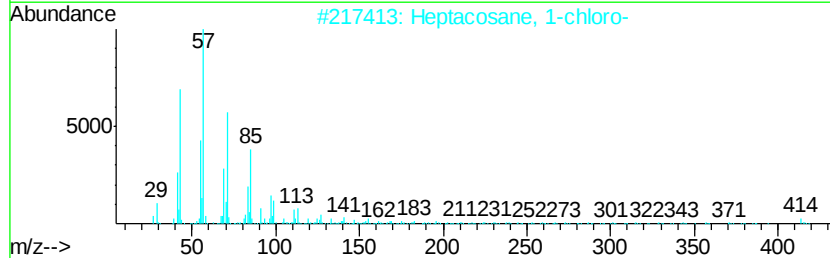
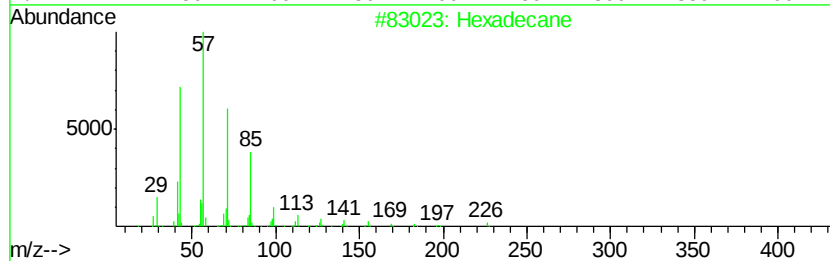
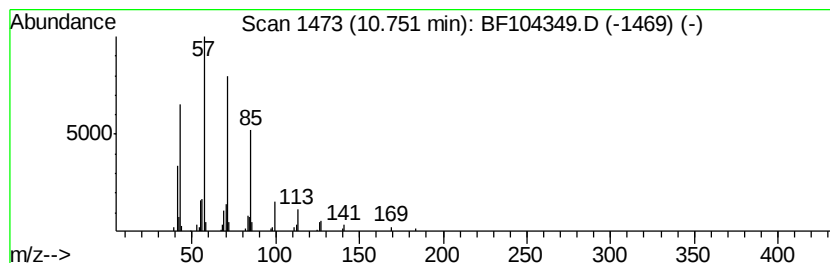
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.75	3.17 ng	145928	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



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ClientSampleId :
040418-JETB-E-U-B

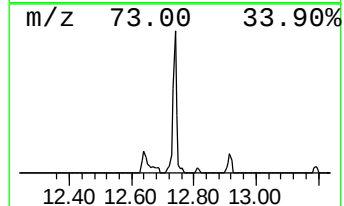
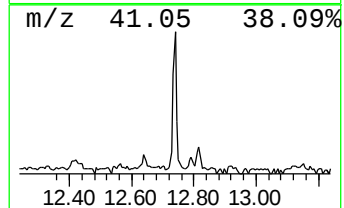
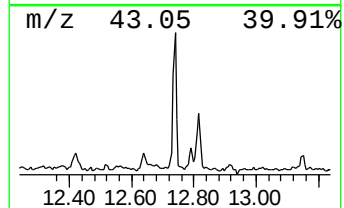
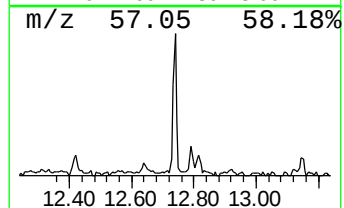
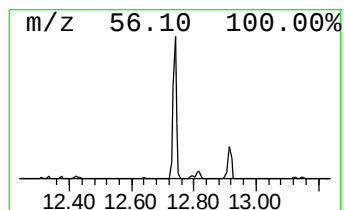
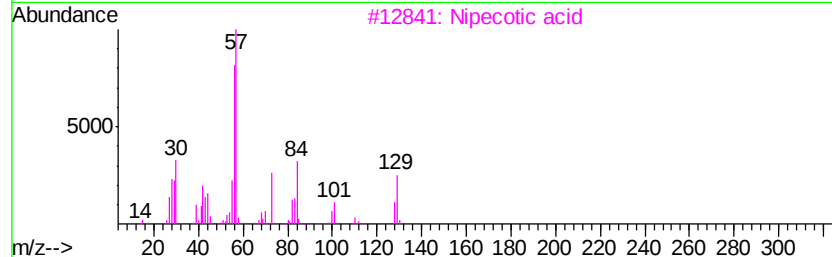
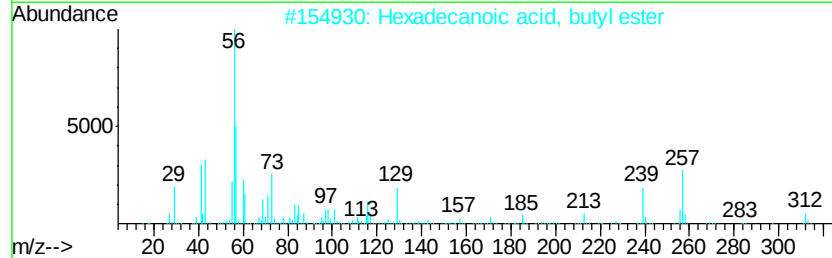
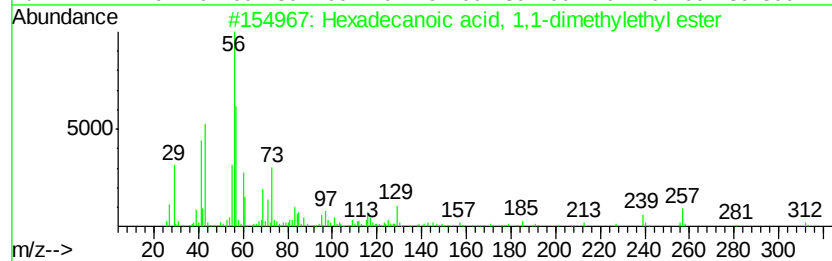
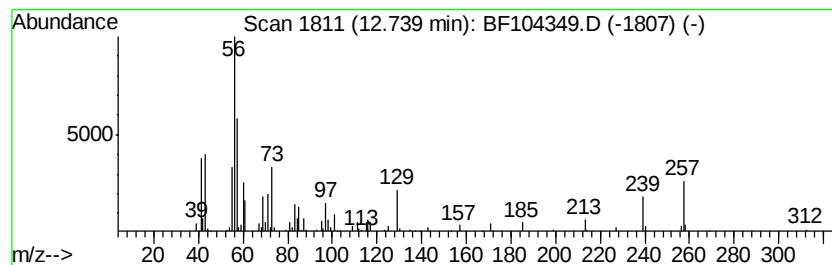
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.68 ng	150622	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3			Nipecotic acid	129	C6H11NO2	000498-95-3	50
4			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
5			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
Data File : BF104349.D
Acq On : 7 Apr 2018 10:43
Operator : JU/SJ
Sample : J2255-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

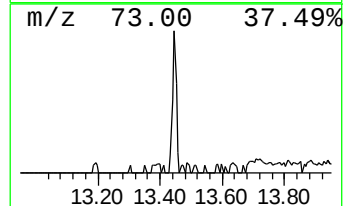
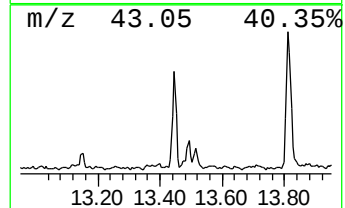
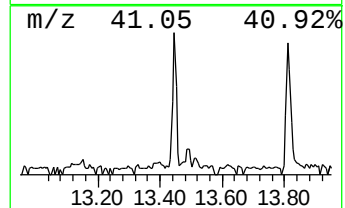
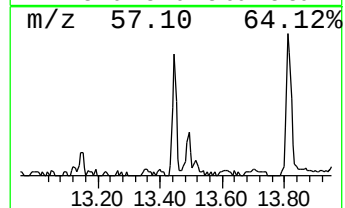
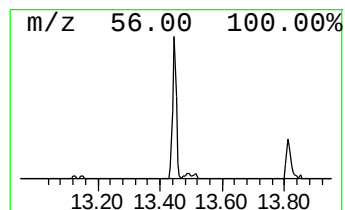
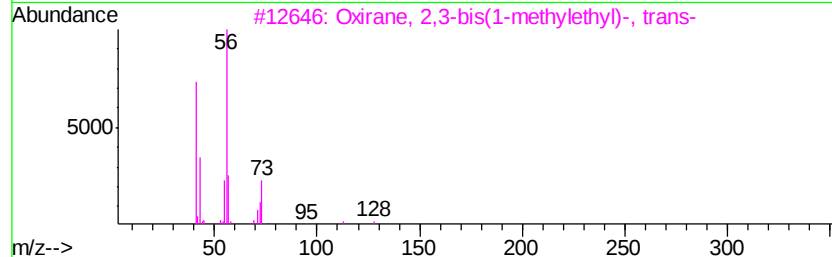
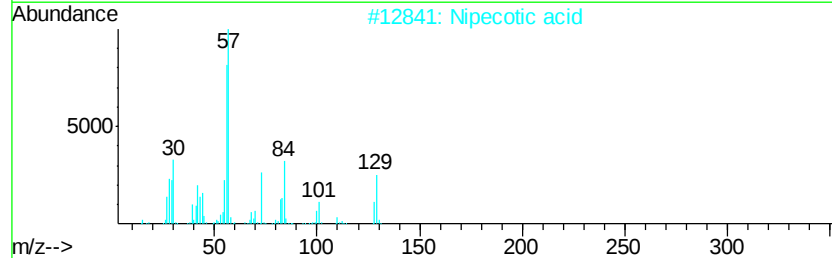
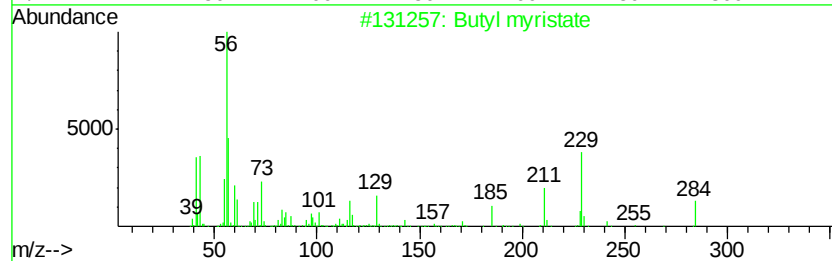
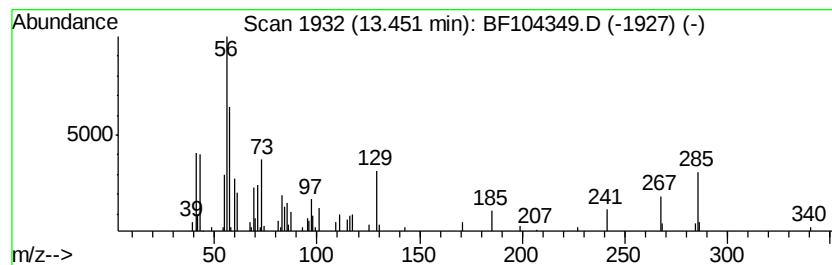
Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.48 ng	101532	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl myristate	284 C18H36O2	000110-36-1	80
2	Nipecotic acid	129 C6H11NO2	000498-95-3	50
3	Oxirane, 2,3-bis(1-methylethyl)-...	128 C8H16O	054644-32-5	32
4	1-Heptene, 2-methyl-	112 C8H16	015870-10-7	30
5	Cyclohexanol, 4-amino-, trans-	115 C6H13NO	027489-62-9	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040618\
Data File : BF104349.D
Acq On : 7 Apr 2018 10:43
Operator : JU/SJ
Sample : J2255-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-U-B

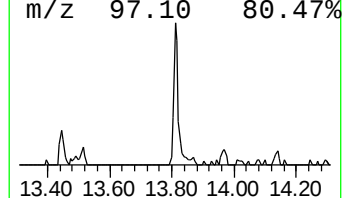
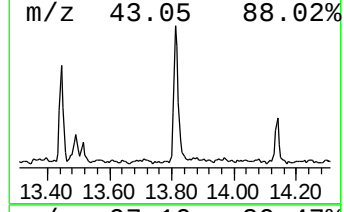
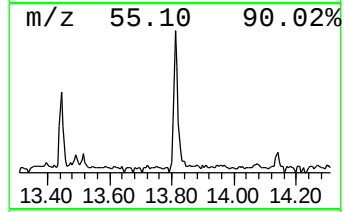
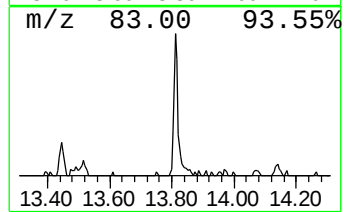
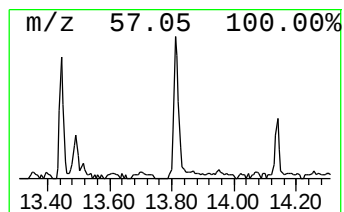
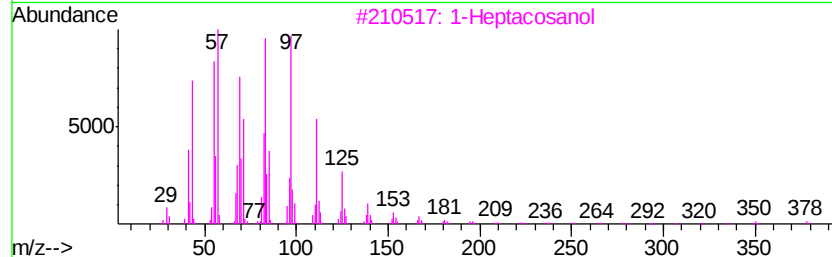
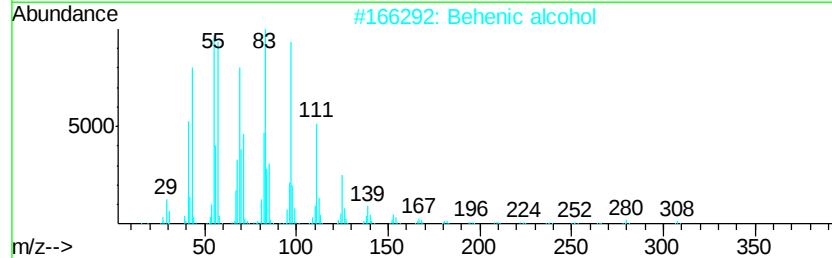
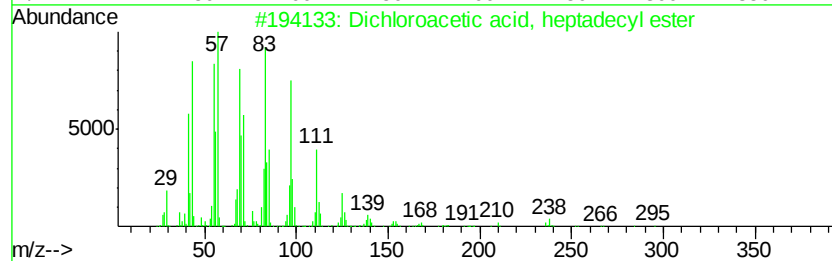
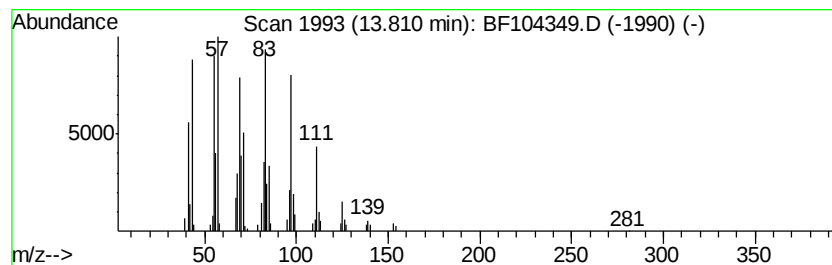
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.59 ng	147019	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
Data File : BF104349.D
Acq On : 7 Apr 2018 10:43
Operator : JU/SJ
Sample : J2255-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040418-JETB-E-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.00	2.8	ng	121482	1	6.80	869920	20.0
unknown6.56	6.56	38.5	ng	1673780	1	6.80	869920	20.0
Tridecane	9.77	2.1	ng	126035	3	9.84	1208190	20.0
Heptadecane	10.27	2.6	ng	159676	3	9.84	1208190	20.0
Hexadecane	10.75	3.2	ng	145928	4	11.33	921455	20.0
Hexadecanoic acid...	12.74	3.7	ng	150622	5	13.97	818451	20.0
Butyl myristate	13.45	2.5	ng	101532	5	13.97	818451	20.0
Dichloroacetic ac...	13.81	3.6	ng	147019	5	13.97	818451	20.0