

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
 Data File : BF085281.D
 Acq On : 9 Mar 2016 3:15
 Operator : UM/SJ
 Sample : H1703-06
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-40COMP(0.5-1.0)

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-BF030316.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	4.539	194	197	201	rBV	108440	130397	3.09%	0.307%
2	5.167	249	252	262	rVB	837617	1128282	26.75%	2.655%
3	5.567	284	287	290	rBV	3205951	3597696	85.28%	8.466%
4	6.584	373	376	378	rBV	3294522	3545425	84.04%	8.343%
5	6.733	386	389	391	rBV	2978141	4218641	100.00%	9.927%
6	6.962	407	409	411	rBV	1011629	942594	22.34%	2.218%
7	7.122	420	423	425	rBV	2724102	3260283	77.28%	7.672%
8	7.522	455	458	460	rBV	2590168	2546909	60.37%	5.993%
9	7.990	492	499	501	rVV2	193291	199565	4.73%	0.470%
10	8.242	519	521	524	rBV	1431728	1246243	29.54%	2.933%
11	9.316	613	615	618	rVB	2997344	3948354	93.59%	9.291%
12	9.716	648	650	651	rBV	455400	526460	12.48%	1.239%
13	9.933	666	669	671	rVB	106672	122175	2.90%	0.288%
14	10.002	673	675	677	rBV	1452841	1302924	30.88%	3.066%
15	10.162	686	689	690	rBV	32070	44588	1.06%	0.105%
16	10.425	710	712	714	rVB	187827	172545	4.09%	0.406%
17	10.642	729	731	735	rBV	54280	110991	2.63%	0.261%
18	10.791	741	744	746	rBV	2551931	2655641	62.95%	6.249%
19	10.905	752	754	758	rBV	146252	233548	5.54%	0.550%
20	11.099	768	771	772	rBV3	26001	47854	1.13%	0.113%
21	11.351	789	793	794	rBV	88805	96325	2.28%	0.227%
22	11.488	802	805	808	rBV	1177445	1537752	36.45%	3.619%
23	11.556	808	811	813	rVB	95862	102742	2.44%	0.242%
24	11.716	822	825	829	rBV2	23761	57648	1.37%	0.136%
25	11.979	846	848	849	rBV	44406	62224	1.47%	0.146%
26	12.002	849	850	853	rVV2	363198	546884	12.96%	1.287%
27	12.094	856	858	863	rVV	96196	160876	3.81%	0.379%
28	12.185	863	866	868	rVV2	24188	44246	1.05%	0.104%
29	12.276	870	874	878	rVV3	39544	100854	2.39%	0.237%
30	12.699	908	911	913	rBV	389779	545376	12.93%	1.283%
31	12.791	917	919	923	rBV	282715	312579	7.41%	0.736%
32	12.928	928	931	933	rVV	314868	486614	11.53%	1.145%
33	13.065	941	943	946	rVB	2461710	2450754	58.09%	5.767%
34	13.248	955	959	961	rBV	62885	82602	1.96%	0.194%

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35	13.351	966	968	970	rBV	38392	44331	1.05%	0.104%
36	13.637	990	993	998	rBV5	27280	77176	1.83%	0.182%
37	13.865	1010	1013	1015	rBV	38940	77908	1.85%	0.183%
38	13.957	1019	1021	1027	rVV	519644	735354	17.43%	1.730%
39	14.117	1031	1035	1042	rBV2	941408	1362816	32.30%	3.207%
40	14.220	1042	1044	1048	rVV	33677	49382	1.17%	0.116%
41	14.288	1048	1050	1053	rVV3	21989	46647	1.11%	0.110%
42	14.597	1074	1077	1079	rBV3	73736	130497	3.09%	0.307%
43	14.745	1088	1090	1093	rBV	747894	713045	16.90%	1.678%
44	14.871	1099	1101	1105	rBV	175056	214588	5.09%	0.505%
45	14.974	1107	1110	1113	rVV3	32813	51588	1.22%	0.121%
46	15.157	1123	1126	1130	rBV	166437	331088	7.85%	0.779%
47	15.225	1130	1132	1134	rVV	39264	56912	1.35%	0.134%
48	15.454	1150	1152	1155	rVB	92184	131705	3.12%	0.310%
49	15.523	1155	1158	1161	rVB	124107	180976	4.29%	0.426%
50	15.580	1161	1163	1165	rBV	502929	779517	18.48%	1.834%
51	16.048	1202	1204	1207	rBV	30139	50803	1.20%	0.120%
52	16.105	1207	1209	1216	rVB3	50196	147857	3.50%	0.348%
53	16.471	1239	1241	1246	rVB5	40128	91882	2.18%	0.216%
54	16.597	1249	1252	1255	rVB	40058	74774	1.77%	0.176%
55	17.043	1288	1291	1297	rVB2	66473	137872	3.27%	0.324%
56	17.226	1304	1307	1309	rBV3	26455	60634	1.44%	0.143%
57	17.477	1326	1329	1338	rVB	63188	161248	3.82%	0.379%
58	17.648	1340	1344	1348	rBV5	45712	145028	3.44%	0.341%
59	18.666	1431	1433	1439	rVB6	23522	72616	1.72%	0.171%

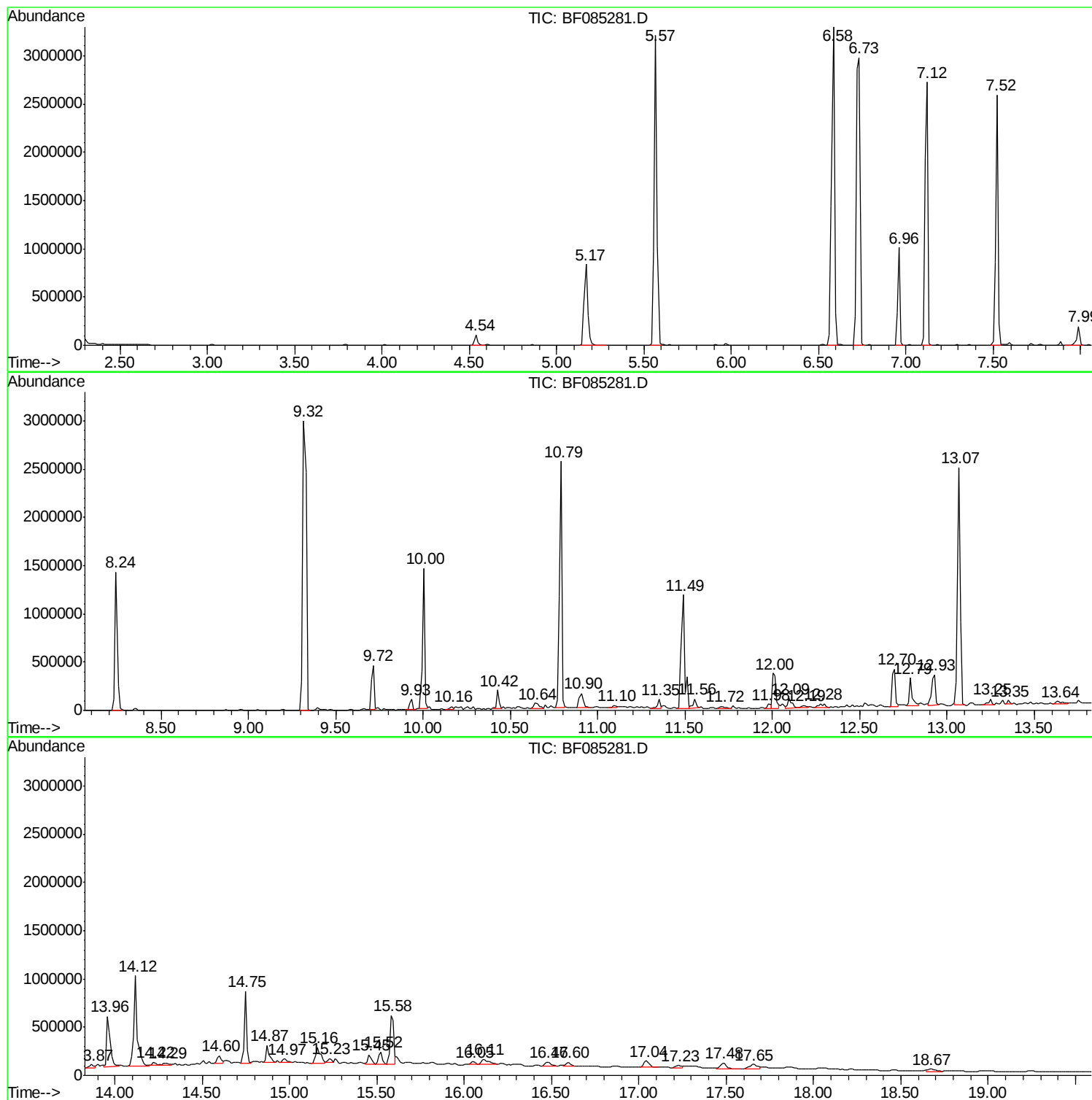
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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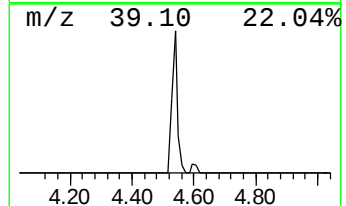
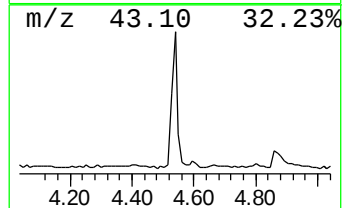
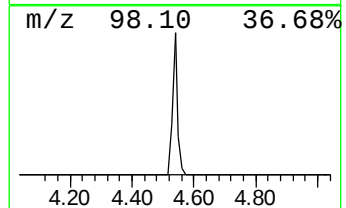
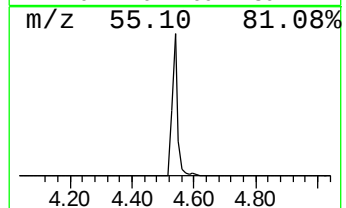
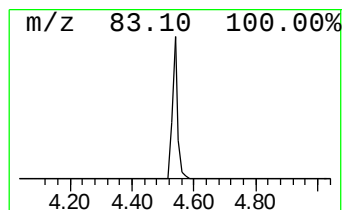
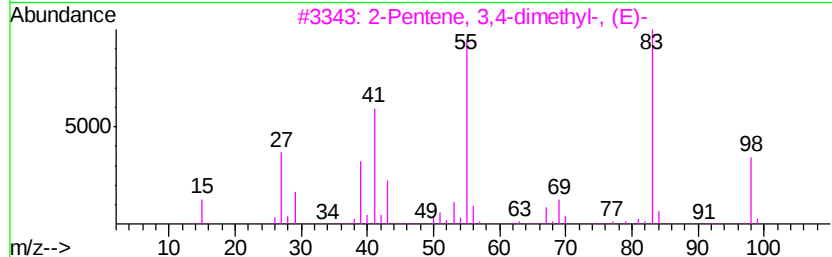
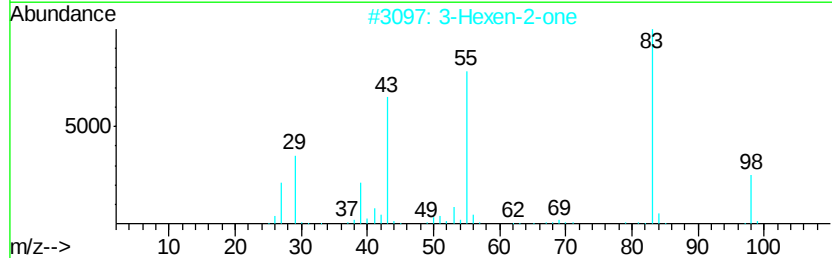
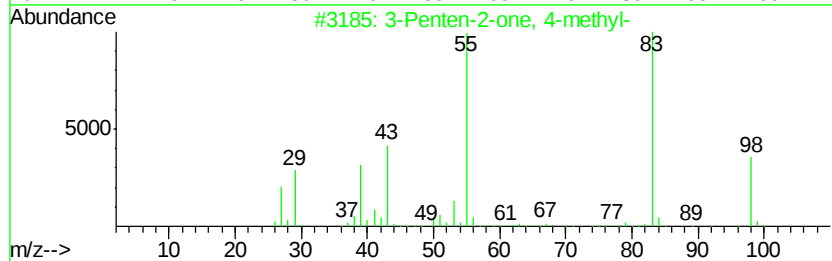
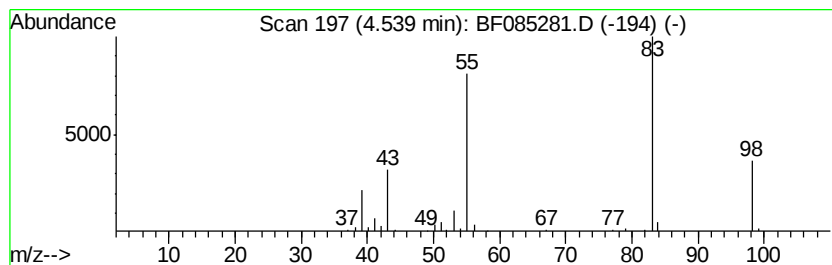
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	2.77 ng	130397	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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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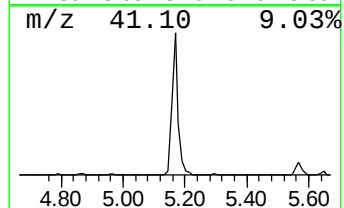
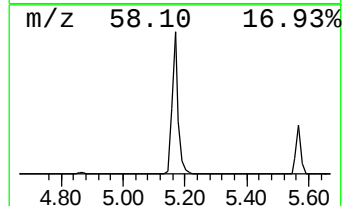
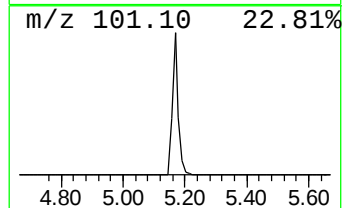
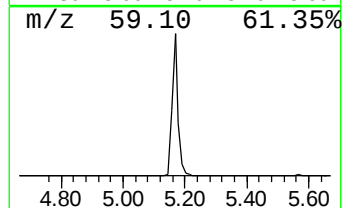
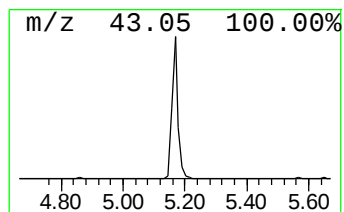
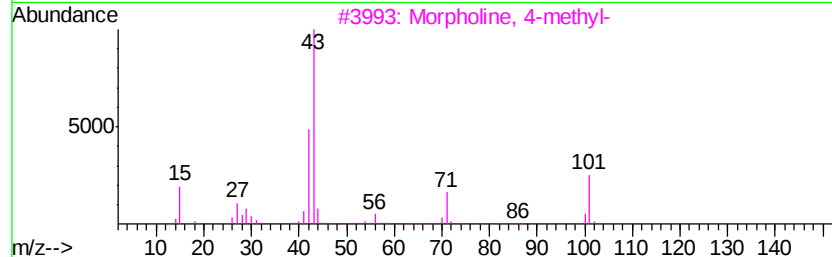
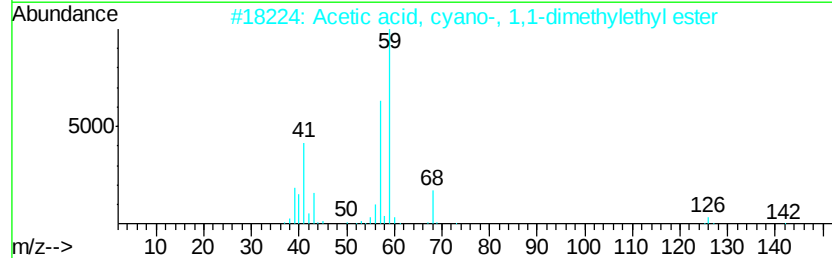
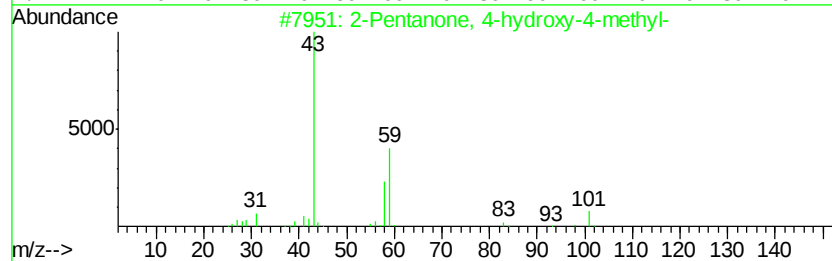
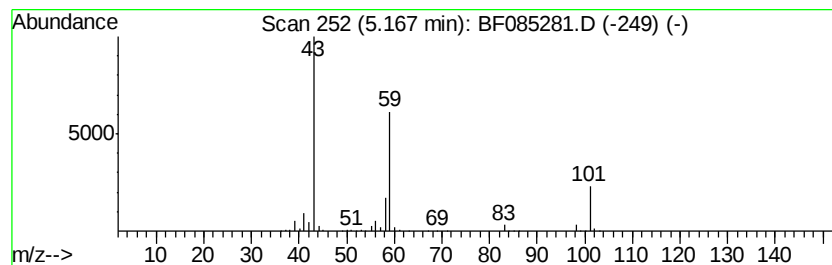
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	23.94 ng	1128280	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	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		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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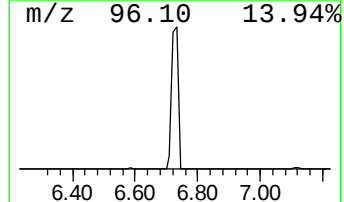
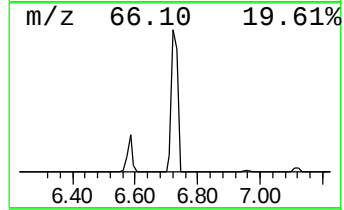
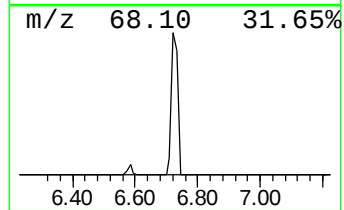
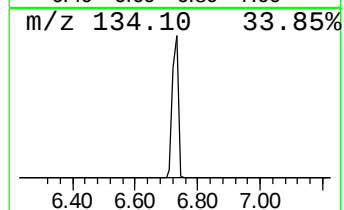
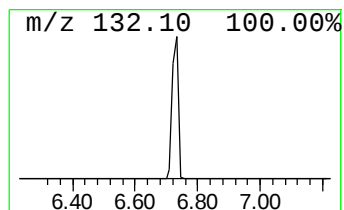
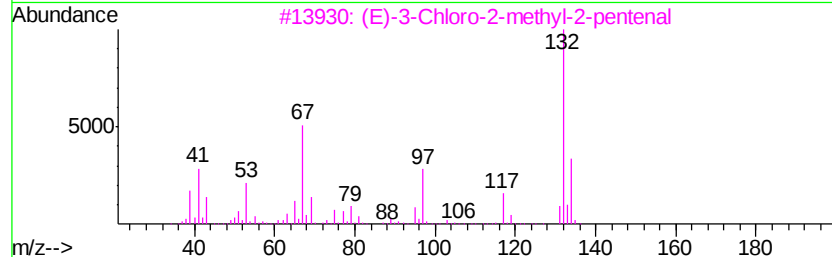
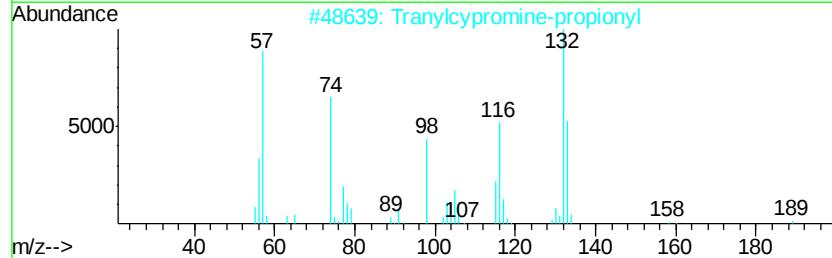
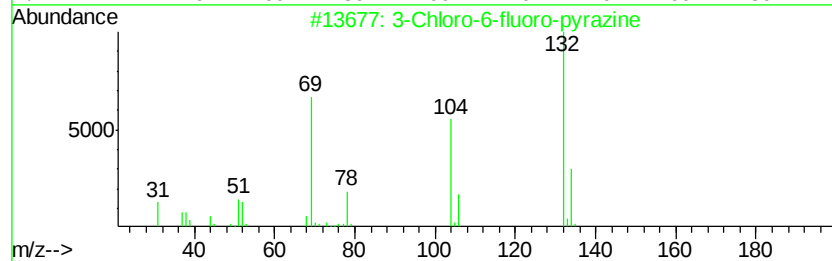
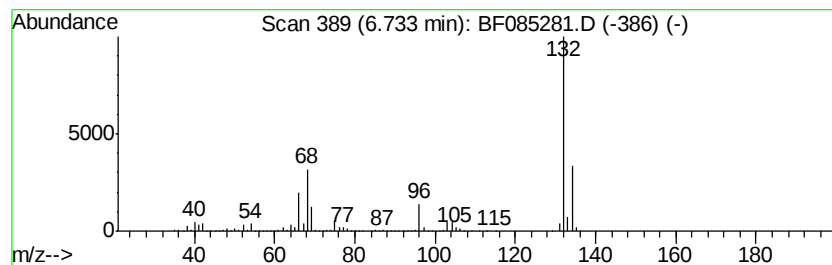
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	89.51 ng	4218640	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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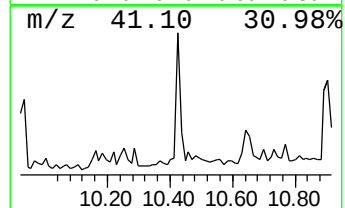
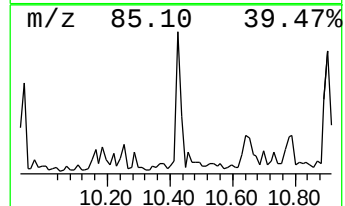
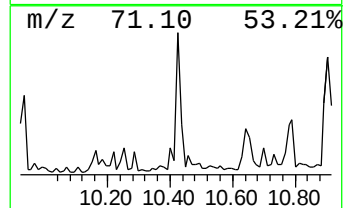
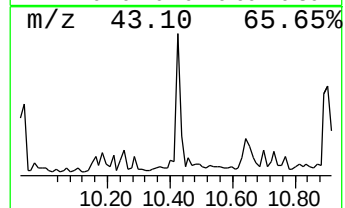
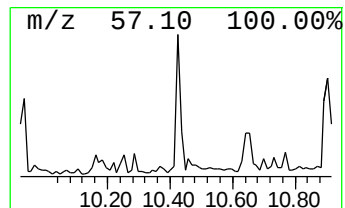
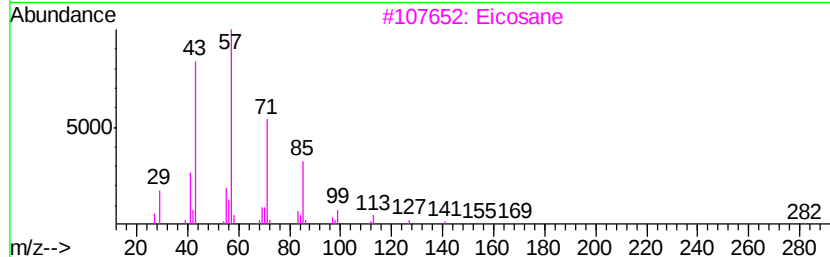
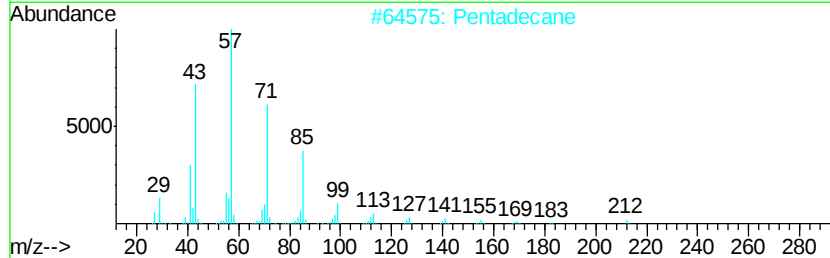
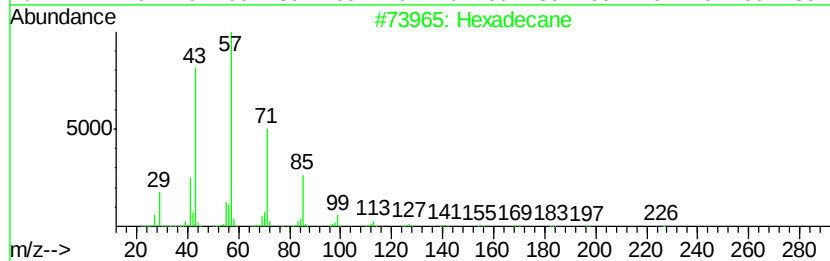
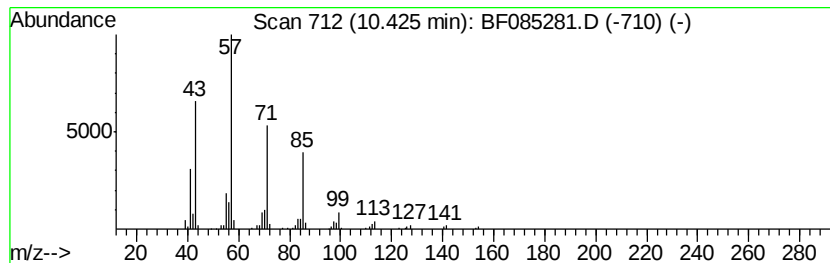
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.65 ng	172545	Acenaphthene-d10	10.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	90
2	Pentadecane	212 C15H32	000629-62-9	90
3	Eicosane	282 C20H42	000112-95-8	83
4	Nonane, 5-butyl-	184 C13H28	017312-63-9	80
5	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	78



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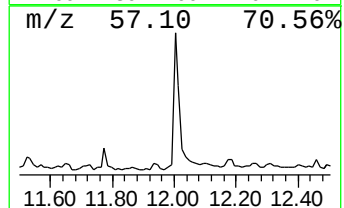
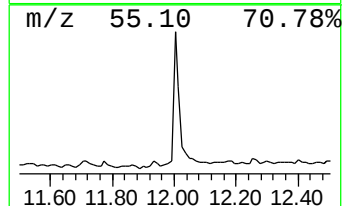
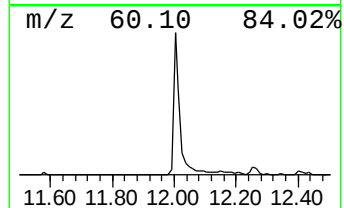
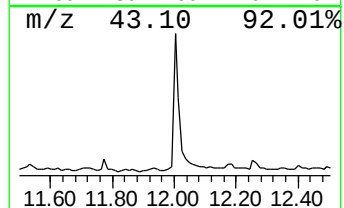
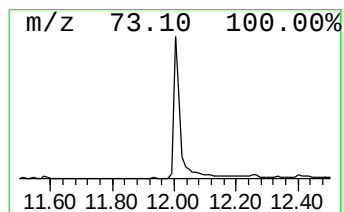
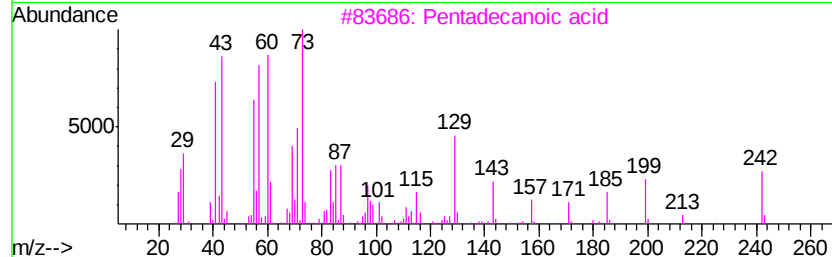
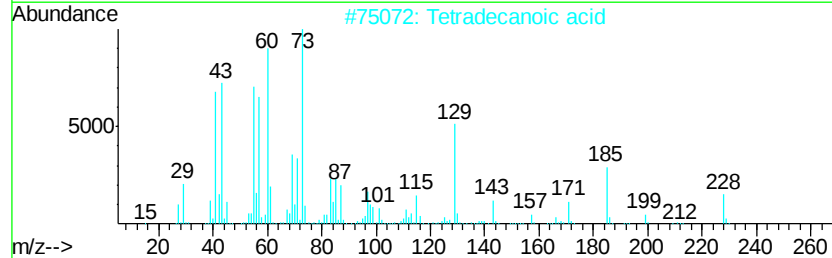
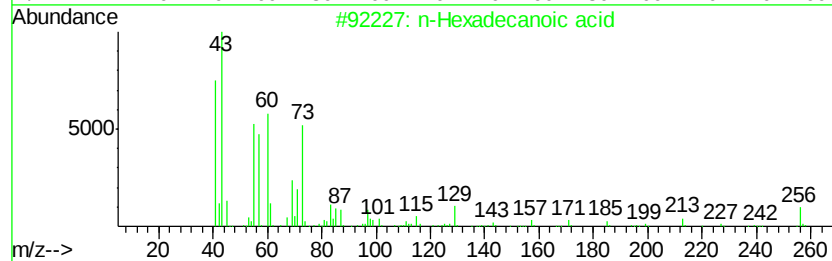
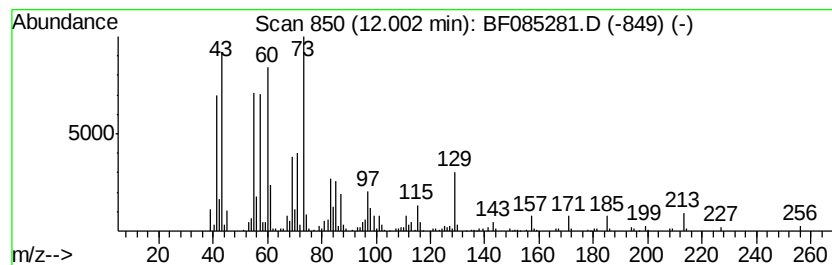
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	7.11 ng	546884	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Amyl Nitrite	117	C5H11NO2	000110-46-3	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-40COMP(0.5-1.0)

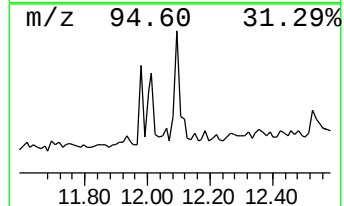
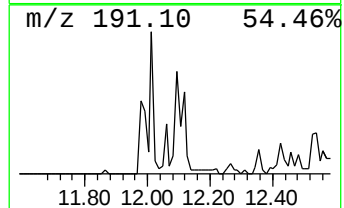
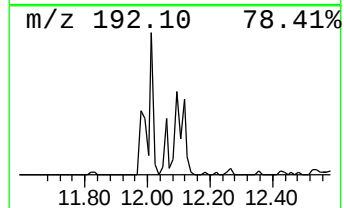
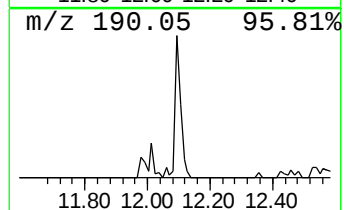
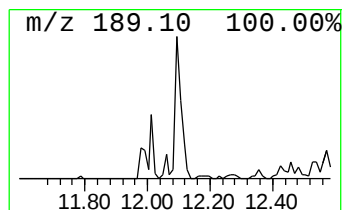
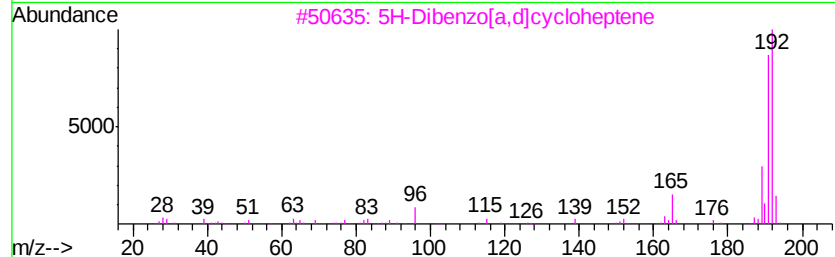
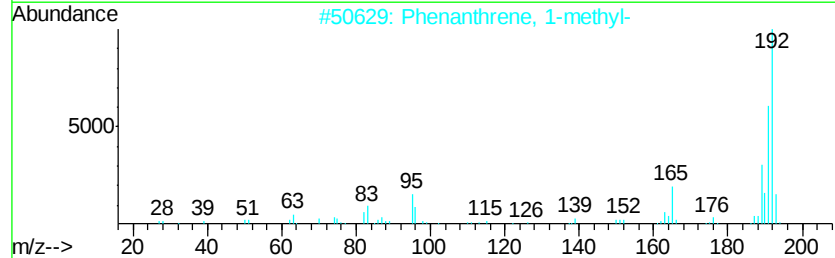
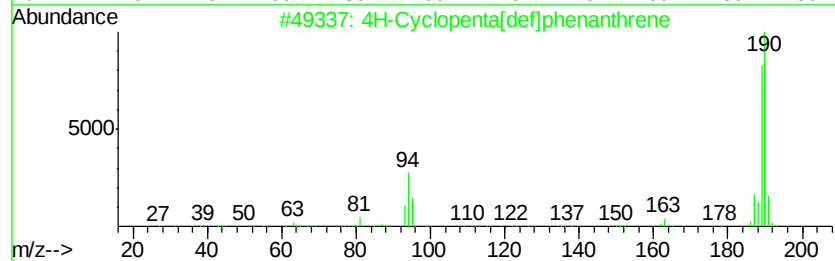
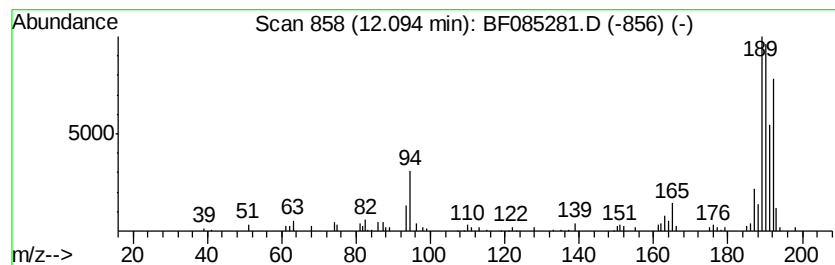
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	2.09 ng	160876	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
3		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
4		1H-Cyclopropa[1]phenanthrene, 1a, ...	192	C15H12	000949-41-7	38
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
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Instrument :
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ClientSampleId :
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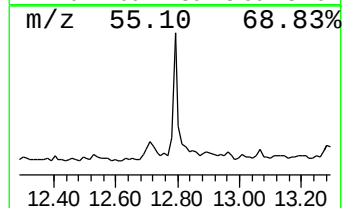
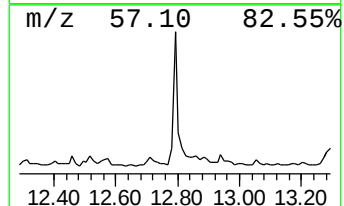
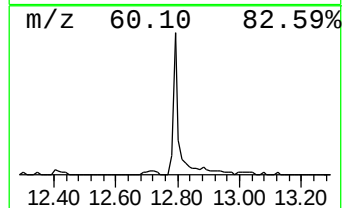
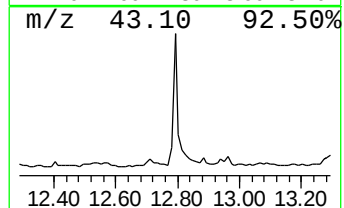
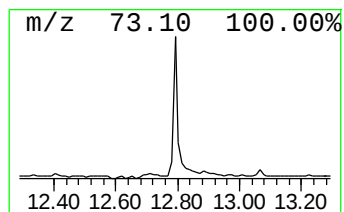
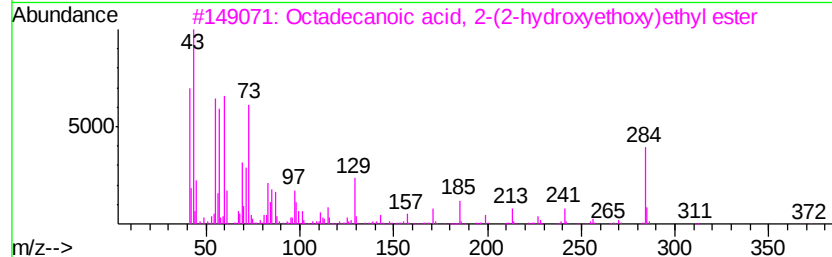
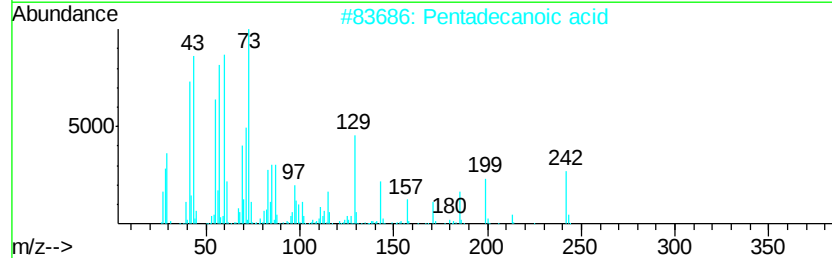
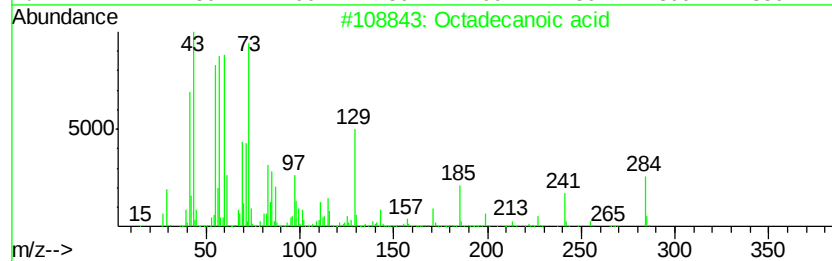
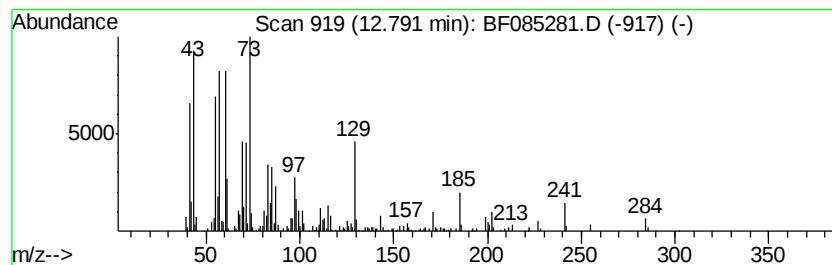
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.07 ng	312579	Phenanthrene-d10	11.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

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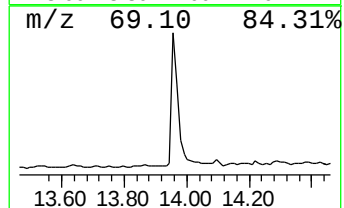
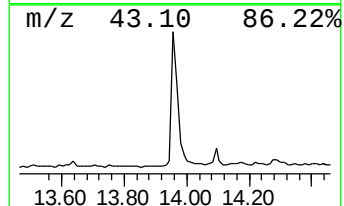
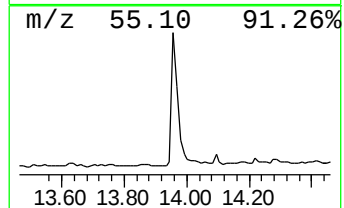
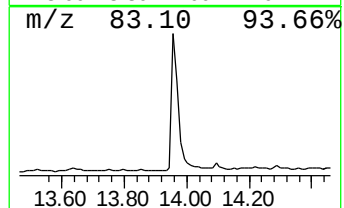
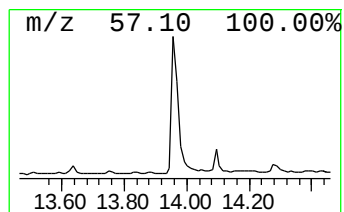
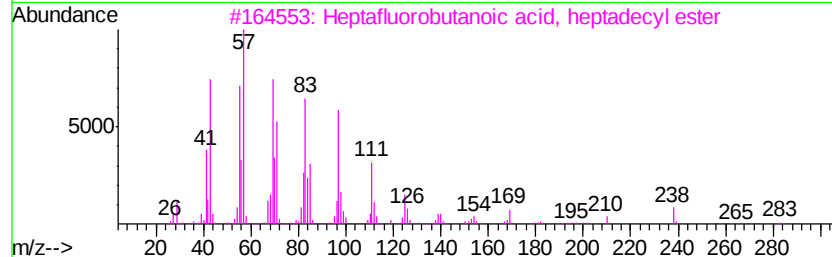
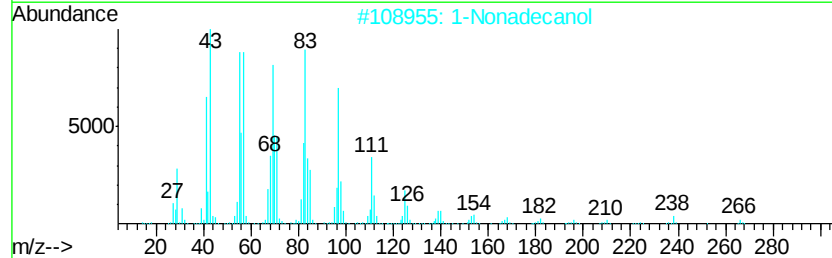
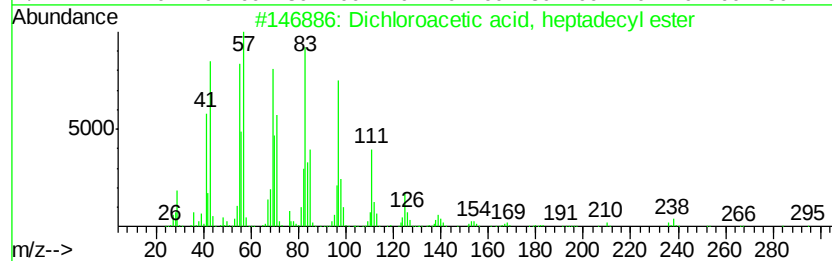
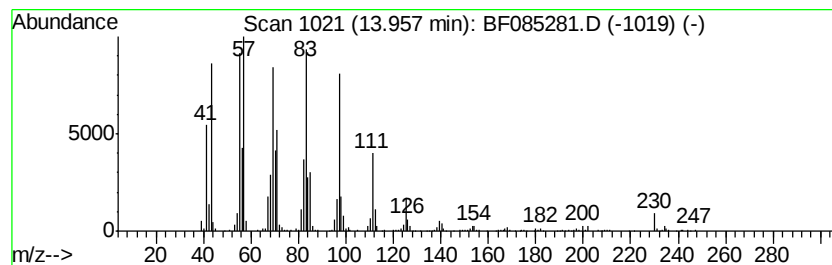
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	10.79 ng	735354	Chrysene-d12	14.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		1-Nonadecanol	284	C19H40O	001454-84-8	94
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
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Operator : UM/SJ
Sample : H1703-06
Misc :
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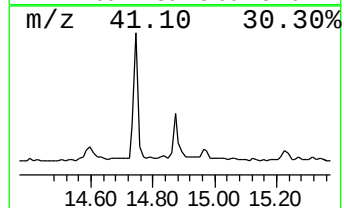
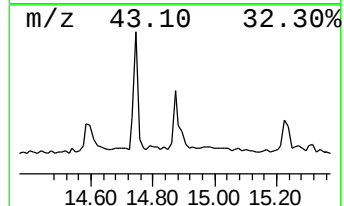
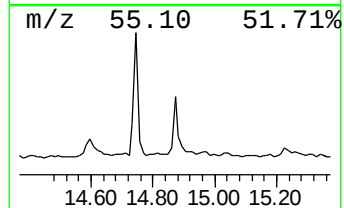
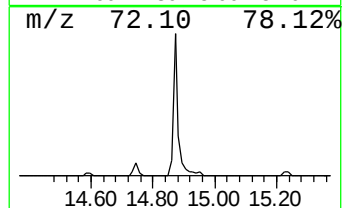
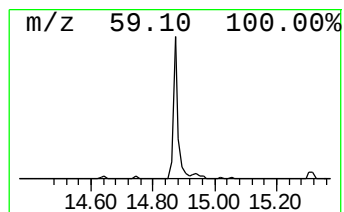
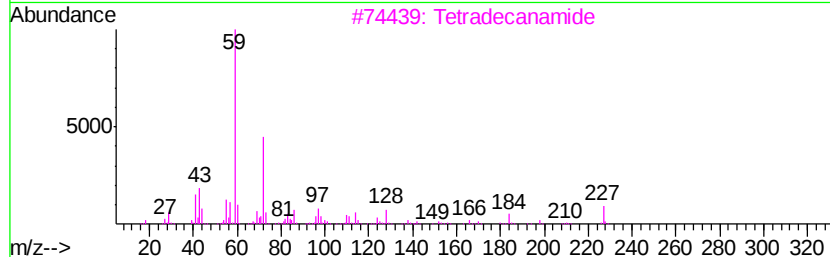
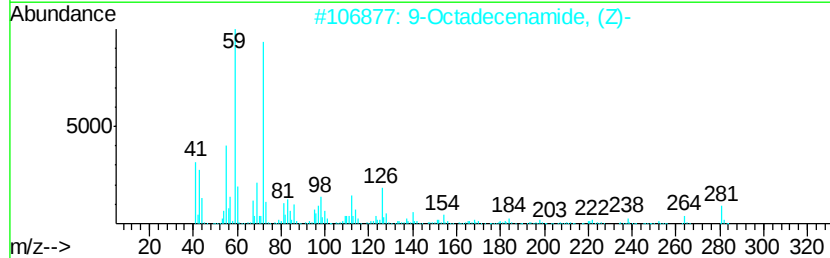
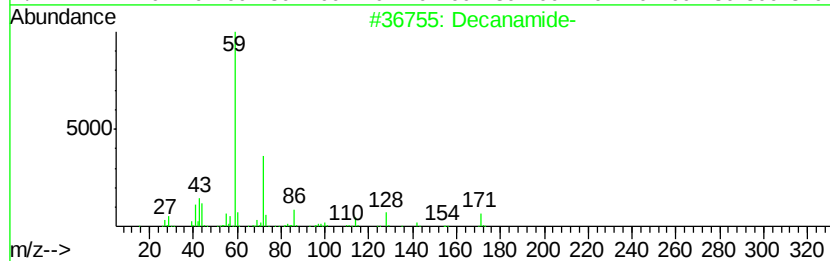
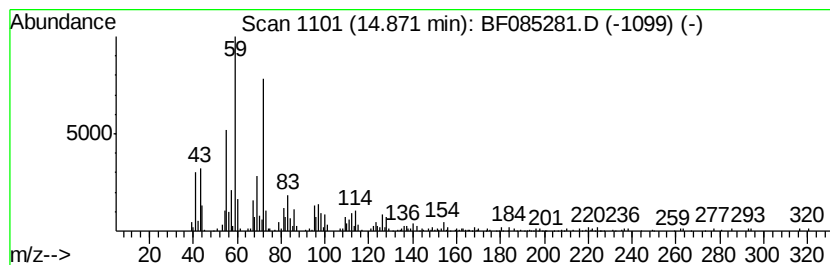
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Decanamide- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.87	5.51 ng	214588	Perylene-d12	15.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanamide-	171	C10H21NO	002319-29-1	64
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	47
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	N-Isopropylidene-hexadecano-hydr...	310	C19H38N2O	093612-49-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
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Instrument :
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ClientSampleId :
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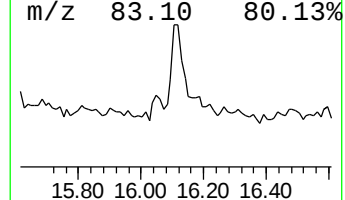
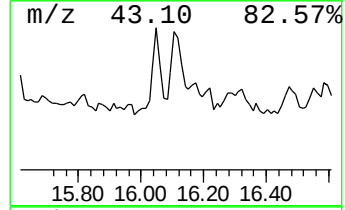
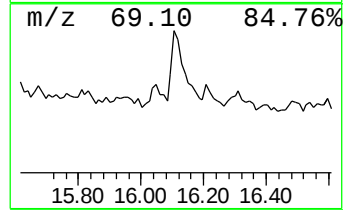
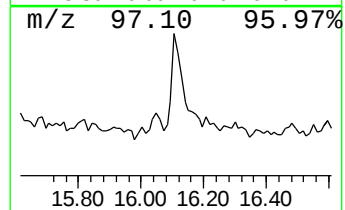
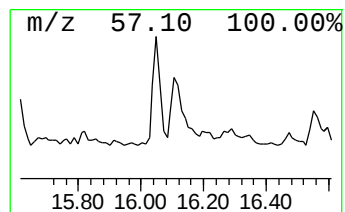
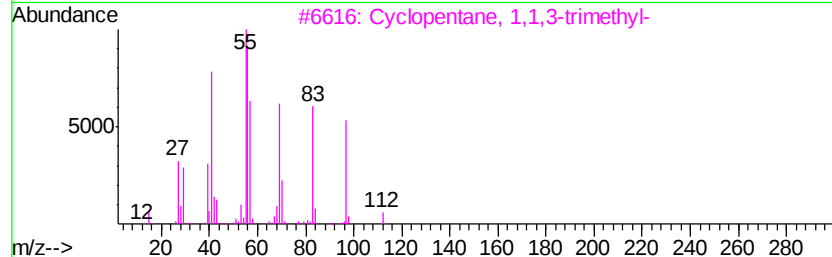
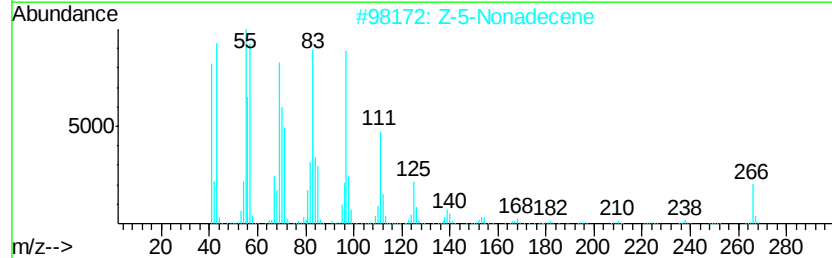
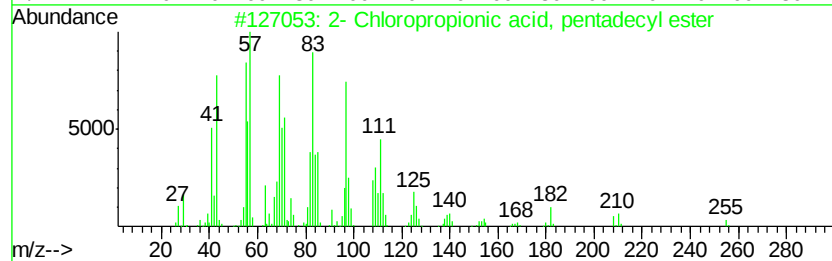
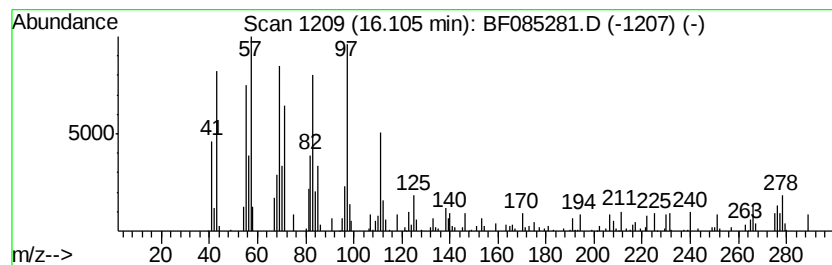
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2- Chloropropionic acid, pe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	3.79 ng	147857	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	74
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	70
3			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	58
4			Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
5			2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
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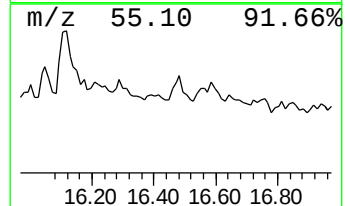
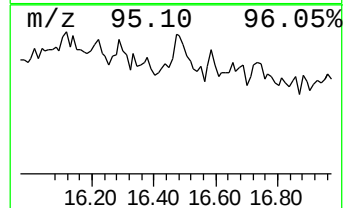
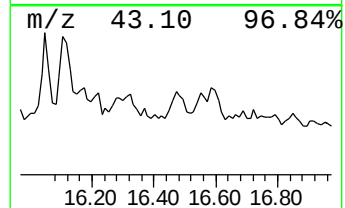
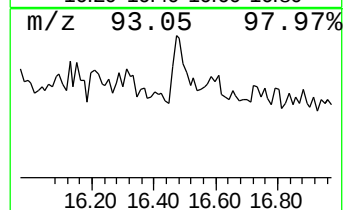
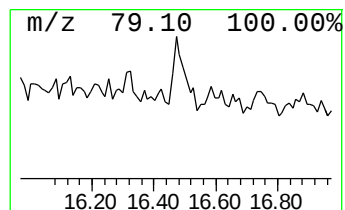
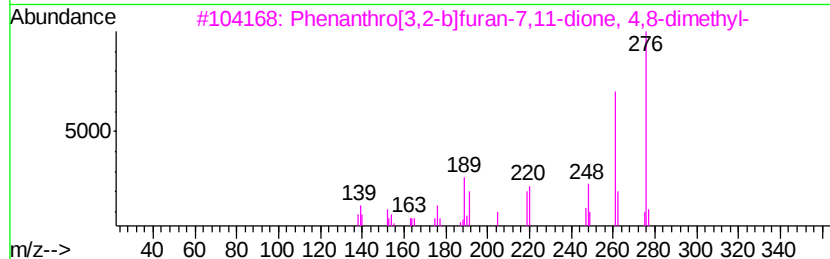
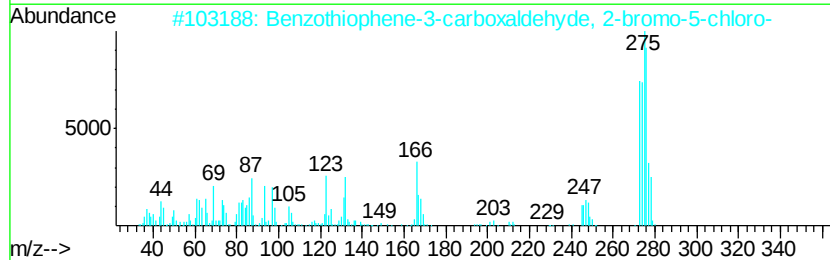
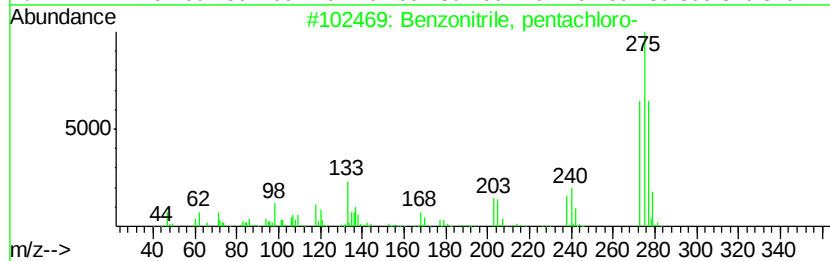
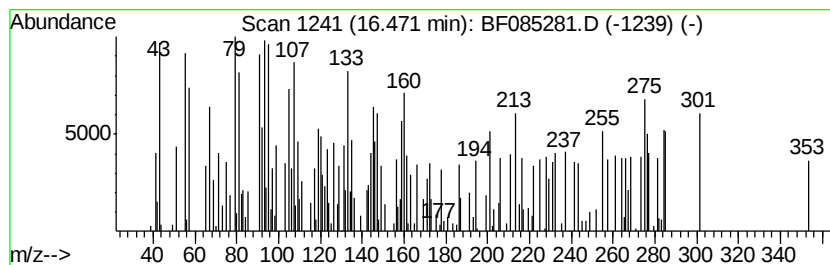
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown16.47 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.36 ng	91882	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzonitrile, pentachloro-	273	C7Cl5N	020925-85-3	20
2		Benzo[thiophene]-3-carboxaldehyde, ...	274	C9H4BrClOS	1000266-56-5	14
3		Phenanthro[3,2-b]furan-7,11-dion...	276	C18H12O3	020958-17-2	11
4		1H-Pyrrolo[2,3-b]pyridine, 3,3'-...	276	C17H16N4	023709-49-1	11
5		2'-Cyanospiro(1,2,3,4,6,7,12,12b...	277	C18H19N3	116839-62-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-40COMP(0.5-1.0)

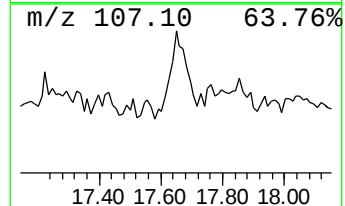
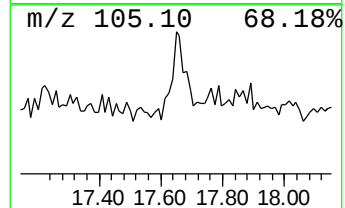
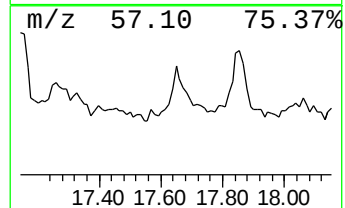
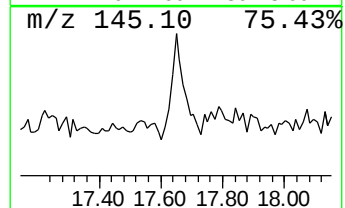
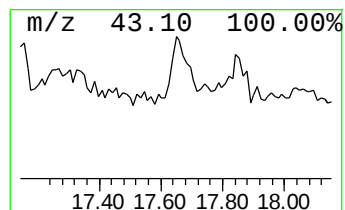
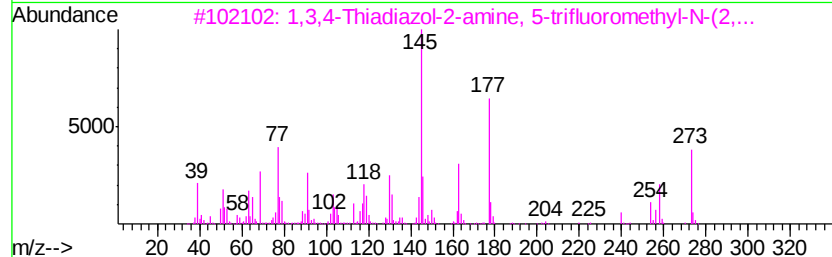
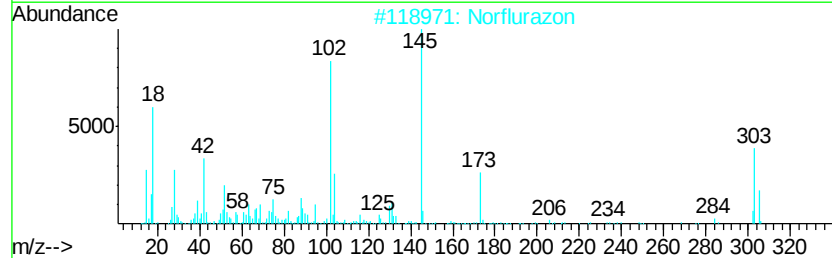
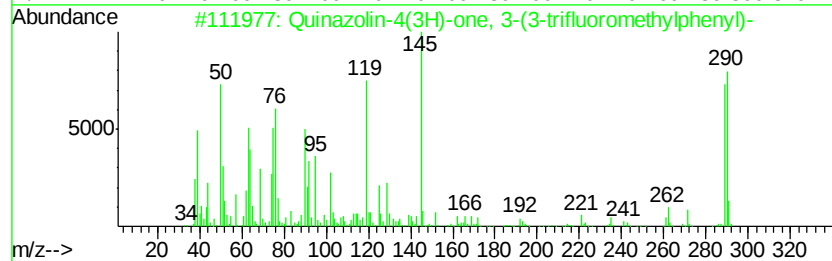
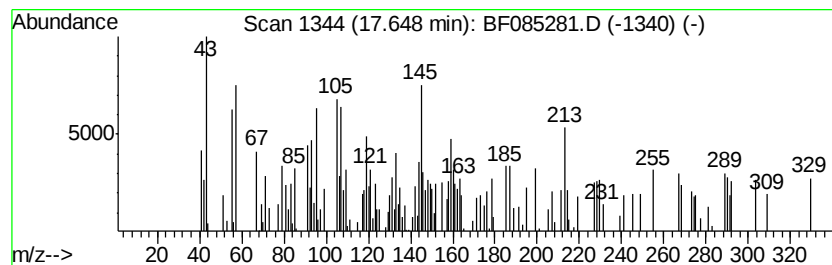
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.65 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	3.72 ng	145028	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinazolin-4(3H)-one, 3-(3-trifl...	290	C15H9F3N2O	024122-28-9	35
2			Norflurazon	303	C12H9ClF3N3O	027314-13-2	22
3			1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	284488-18-2	22
4			Triethylpropoxysilane	174	C9H22OSi	017841-44-0	18
5			2(1H)-Quinolinone, 1-propyl-	187	C12H13NO	000944-70-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085281.D
Acq On : 9 Mar 2016 3:15
Operator : UM/SJ
Sample : H1703-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-40COMP(0.5-1.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
3-Penten-2-one, 4...	4.54	2.8	ng	130397	1	6.96	942594	20.0
2-Pentanone, 4-hy...	5.17	23.9	ng	1128280	1	6.96	942594	20.0
unknown6.73	6.73	89.5	ng	4218640	1	6.96	942594	20.0
Hexadecane	10.42	2.6	ng	172545	3	10.00	1302920	20.0
n-Hexadecanoic acid	12.00	7.1	ng	546884	4	11.49	1537750	20.0
4H-Cyclopenta[def...	12.09	2.1	ng	160876	4	11.49	1537750	20.0
Octadecanoic acid	12.79	4.1	ng	312579	4	11.49	1537750	20.0
Dichloroacetic ac...	13.96	10.8	ng	735354	5	14.12	1362820	20.0
Decanamide-	14.87	5.5	ng	214588	6	15.59	779517	20.0
2-Chloropropioni...	16.11	3.8	ng	147857	6	15.59	779517	20.0
unknown16.47	16.47	2.4	ng	91882	6	15.59	779517	20.0
unknown17.65	17.65	3.7	ng	145028	6	15.59	779517	20.0