

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
 Data File : BF092892.D
 Acq On : 10 Feb 2017 19:28
 Operator : SJ/MA
 Sample : I1777-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38-SB-02-5-7

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-BF013017.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	5.082	258	262	270	rBV	1122904	1769017	38.32%	4.203%
2	5.504	296	299	301	rBV	3193470	4257403	92.23%	10.116%
3	6.533	386	389	392	rBV	3532422	4004419	86.75%	9.515%
4	6.659	398	400	403	rBV	3018256	4144920	89.79%	9.849%
5	6.887	418	420	423	rBV	843436	972448	21.07%	2.311%
6	7.047	432	434	437	rBV	2985395	2982408	64.61%	7.086%
7	7.459	467	470	473	rBV	2432757	2525804	54.72%	6.002%
8	8.179	530	533	535	rBV	1530542	1360193	29.47%	3.232%
9	9.265	624	628	630	rBV	3243723	4616284	100.00%	10.969%
10	9.653	660	662	664	rBV	293964	264318	5.73%	0.628%
11	9.859	674	680	684	rBV	141727	295029	6.39%	0.701%
12	9.939	684	687	689	rVB	1462303	1627450	35.25%	3.867%
13	10.339	716	722	723	rBV2	20666	60561	1.31%	0.144%
14	10.362	723	724	726	rVB	137035	120516	2.61%	0.286%
15	10.579	740	743	747	rBV	43143	76502	1.66%	0.182%
16	10.728	753	756	758	rBV	2501502	2709768	58.70%	6.439%
17	10.842	764	766	769	rBV	129320	201725	4.37%	0.479%
18	11.288	802	805	806	rBV	107509	118562	2.57%	0.282%
19	11.425	814	817	819	rBV	1371596	1650410	35.75%	3.922%
20	12.465	900	908	910	rBV	27170	49457	1.07%	0.118%
21	13.014	952	956	958	rBV	3042590	4358970	94.43%	10.357%
22	13.482	991	997	1002	rBV2	46769	99684	2.16%	0.237%
23	13.894	1031	1033	1041	rBV	203300	283019	6.13%	0.672%
24	14.054	1045	1047	1050	rVB	1466521	1421962	30.80%	3.379%
25	14.522	1080	1088	1091	rBV	48916	110525	2.39%	0.263%
26	14.808	1110	1113	1117	rBV2	263666	348824	7.56%	0.829%
27	15.151	1140	1143	1146	rBV	52864	55793	1.21%	0.133%
28	15.505	1171	1174	1183	rBV	954316	1293196	28.01%	3.073%
29	15.940	1209	1212	1215	rBV	49685	82993	1.80%	0.197%
30	16.431	1252	1255	1261	rBV2	44970	94620	2.05%	0.225%
31	17.003	1301	1305	1310	rBV	27986	67812	1.47%	0.161%
32	17.689	1360	1365	1370	rVB3	21091	61285	1.33%	0.146%

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ALS Vial : 12 Sample Multiplier: 1

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

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

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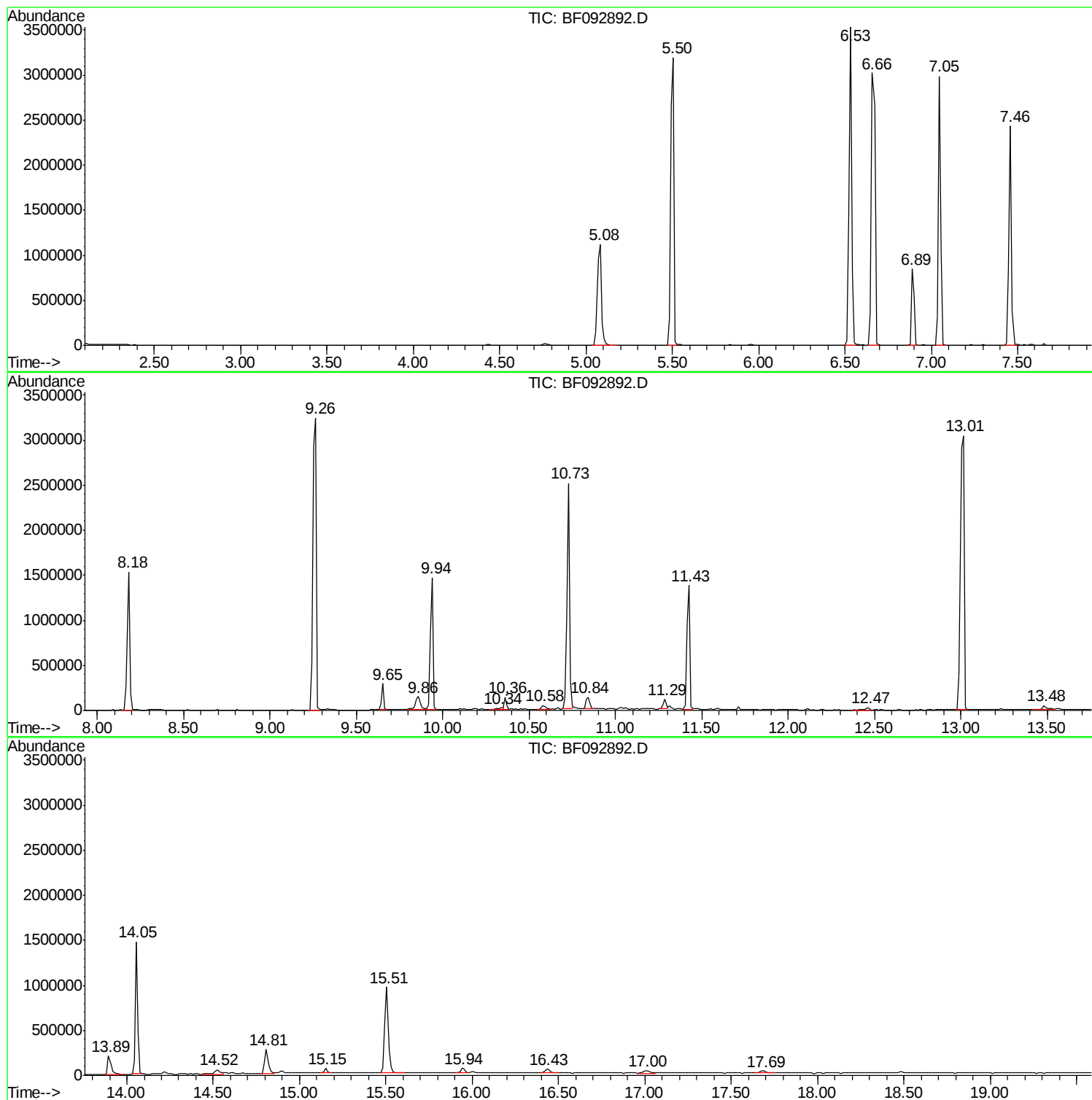
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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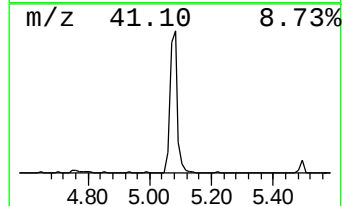
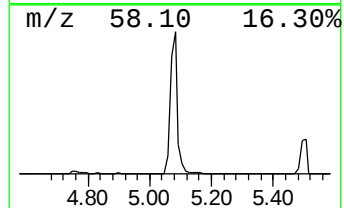
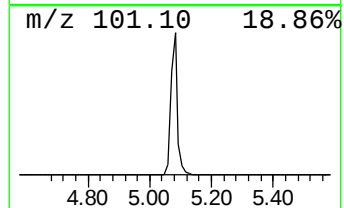
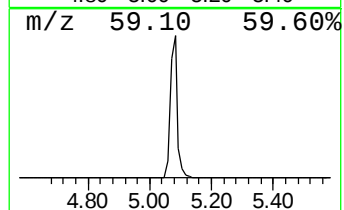
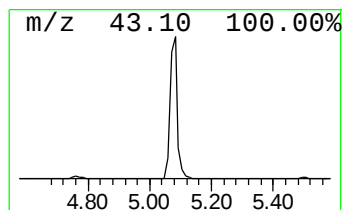
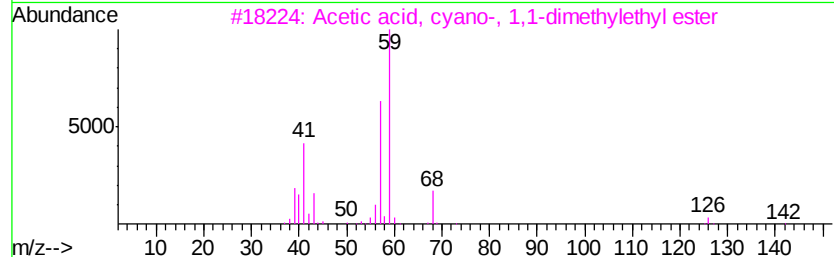
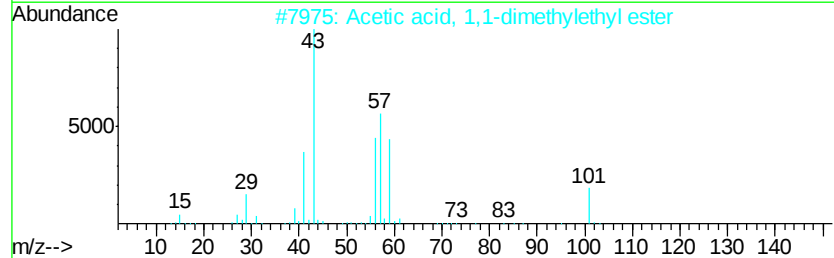
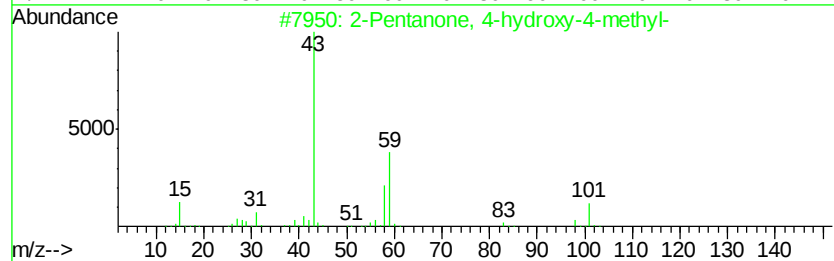
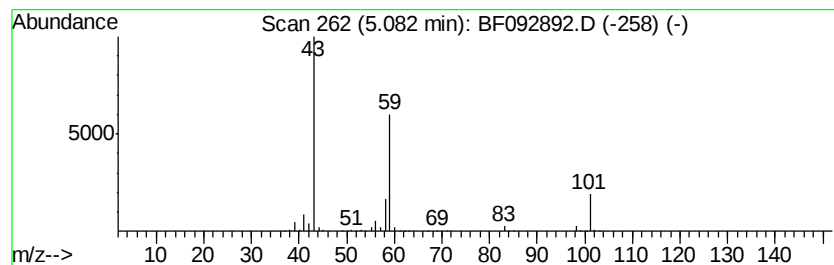
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	36.38 ng	1769020	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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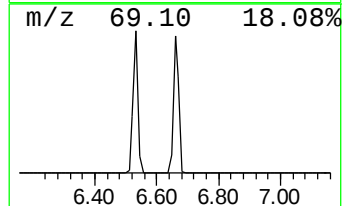
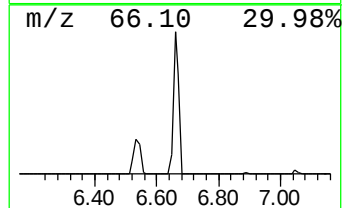
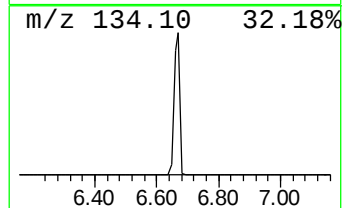
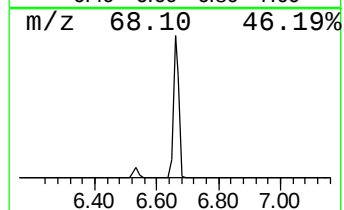
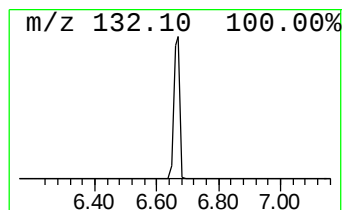
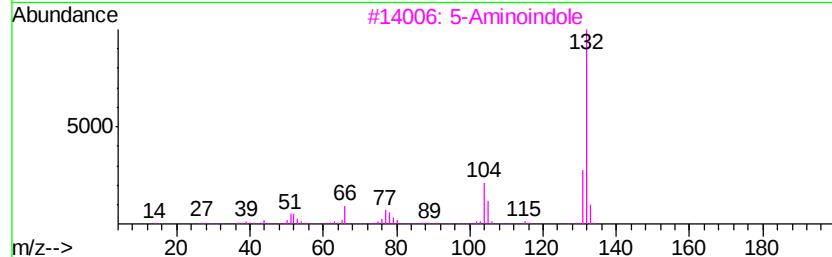
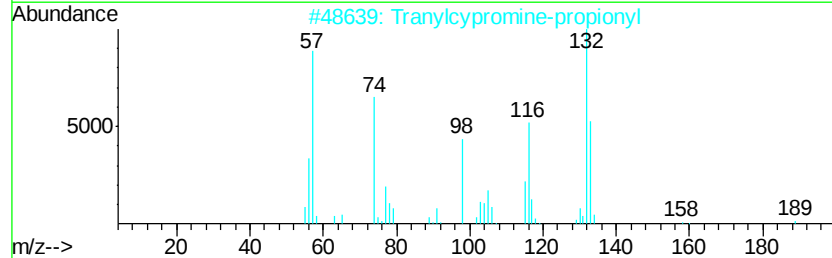
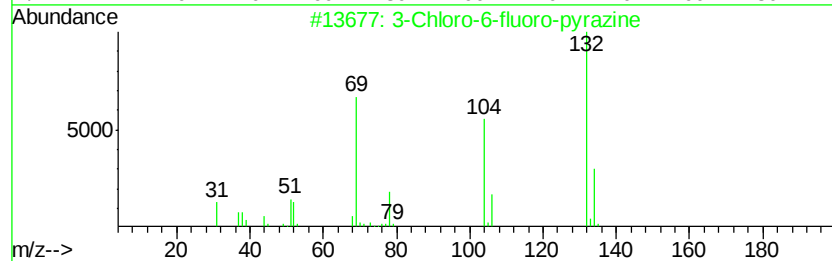
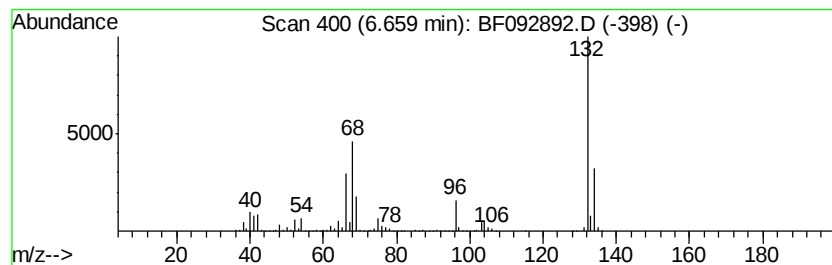
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	85.25 ng	4144920	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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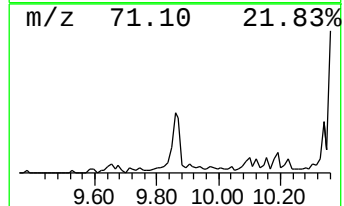
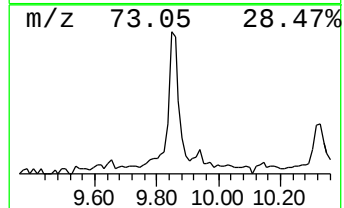
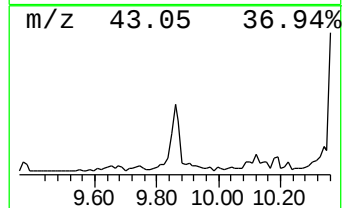
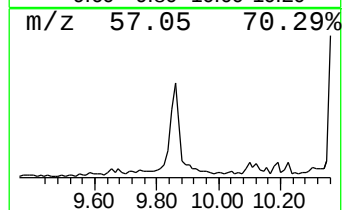
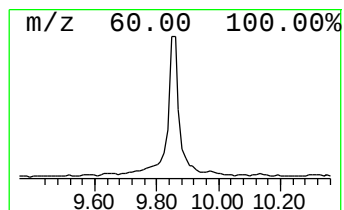
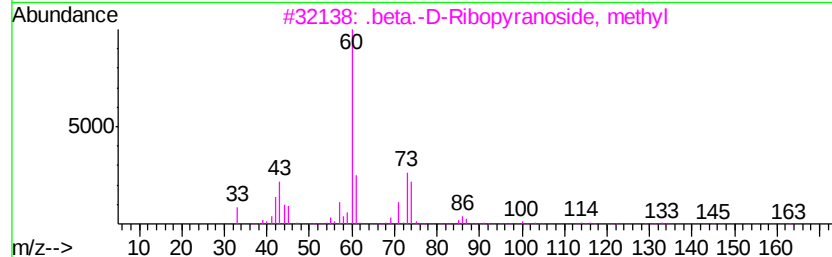
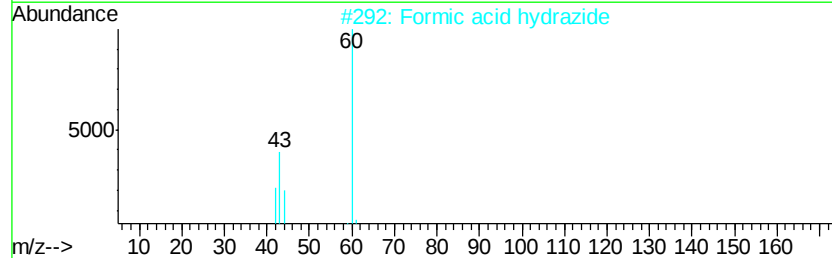
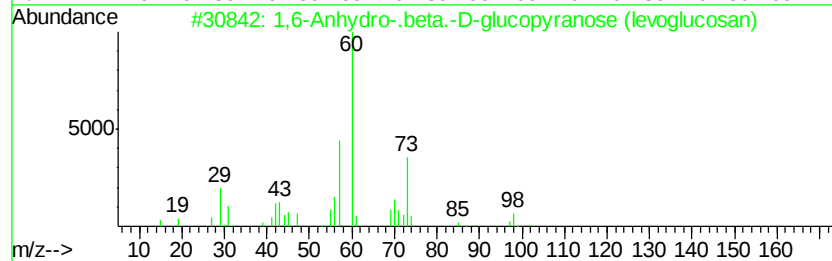
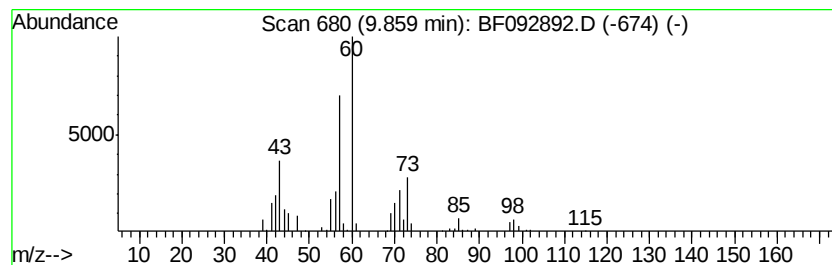
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	3.63 ng	295029	Acenaphthene-d10	9.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	59
2		Formic acid hydrazide	60	CH4N2O	000624-84-0	43
3		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	40
4		3,4-Altrosan	162	C6H10O5	1000129-76-4	37
5		Pentanoic acid	102	C5H10O2	000109-52-4	37



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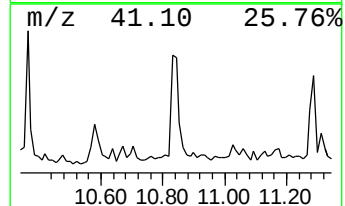
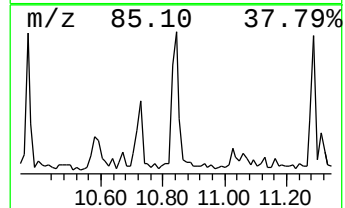
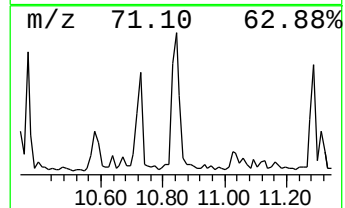
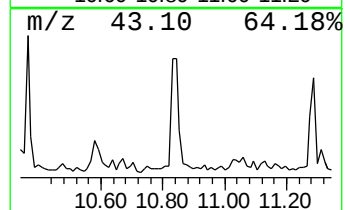
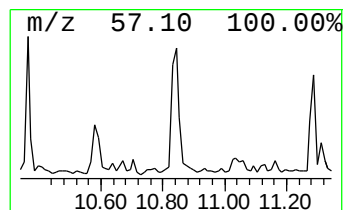
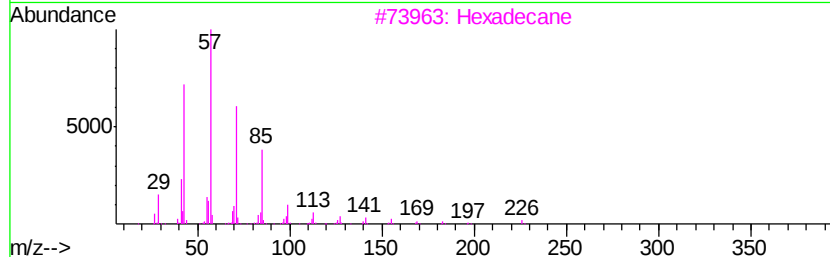
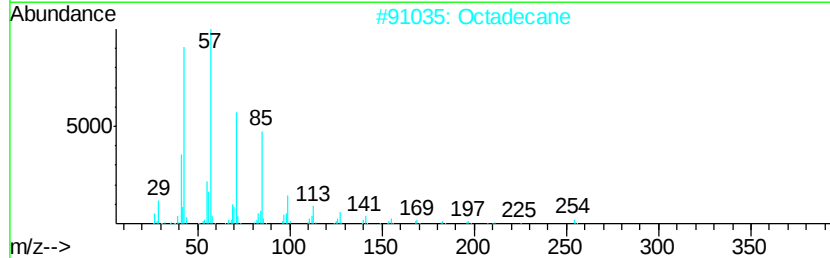
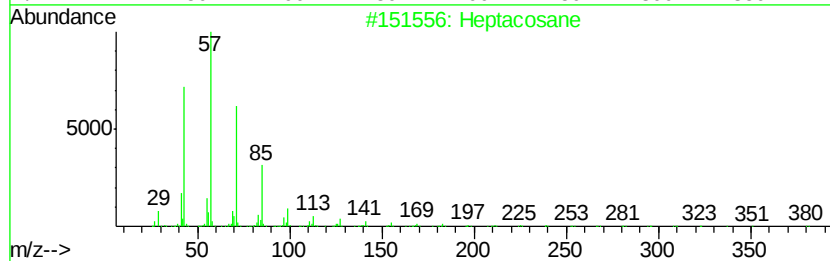
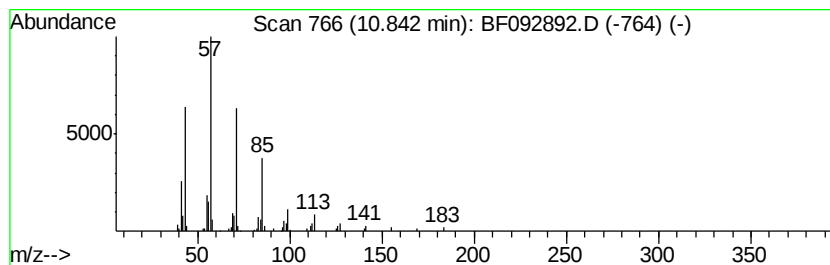
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.44 ng	201725	Phenanthrene-d10	11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Hexadecane		226	C16H34	000544-76-3	91
4	Tetradecane		198	C14H30	000629-59-4	91
5	Heptadecane		240	C17H36	000629-78-7	91



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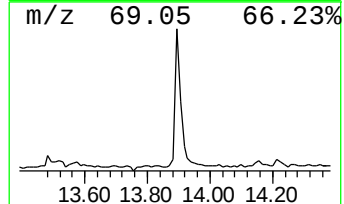
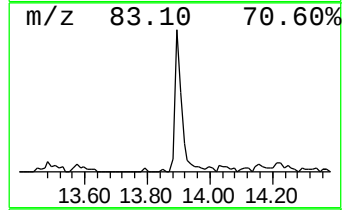
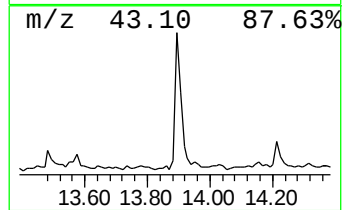
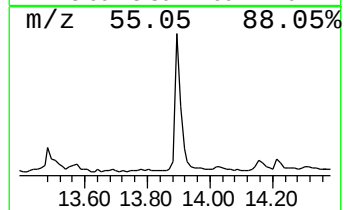
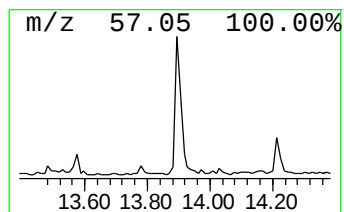
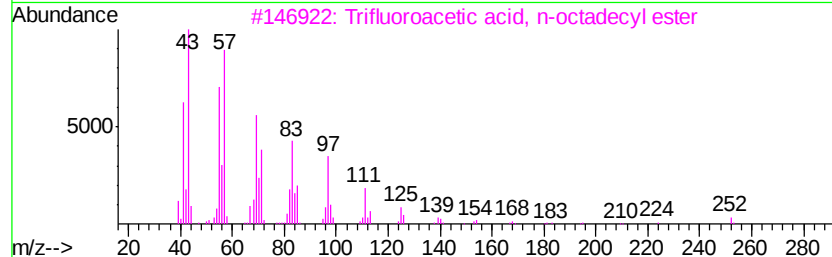
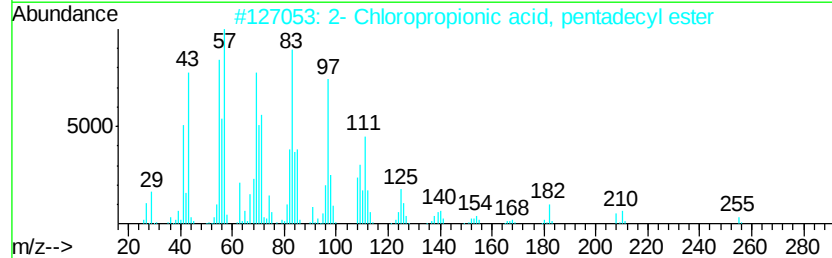
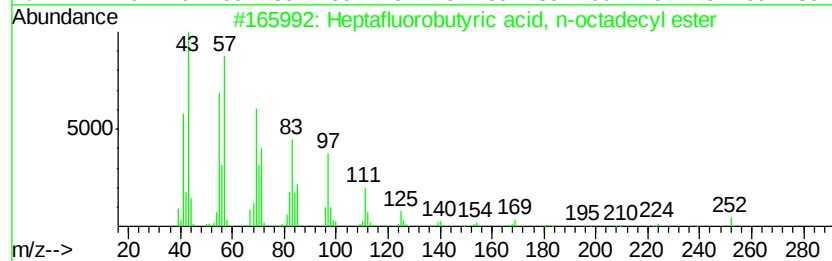
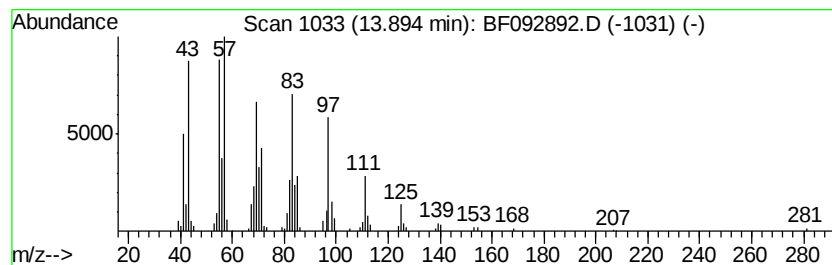
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.98 ng	283019	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
2		2-Chloropropionic acid, pentadecyl ester	318	C18H35ClO2	1000292-44-1	91
3		Trifluoroacetic acid, n-octadecyl ester	366	C20H37F3O2	079392-43-1	91
4		Pentafluoropropionic acid, hepta-decyl ester	402	C20H35F5O2	1000283-04-2	91
5		1-Docosene	308	C22H44	001599-67-3	90



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ClientSampleId :
38-SB-02-5-7

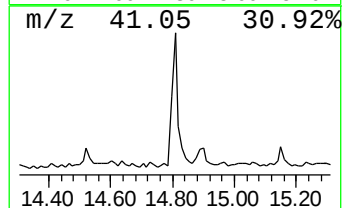
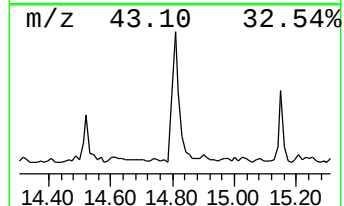
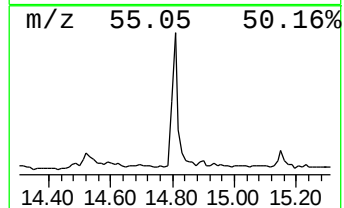
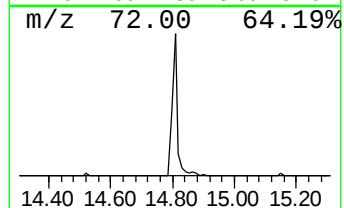
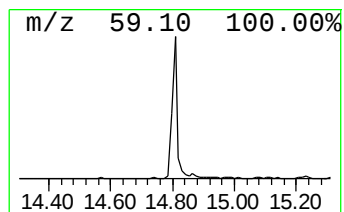
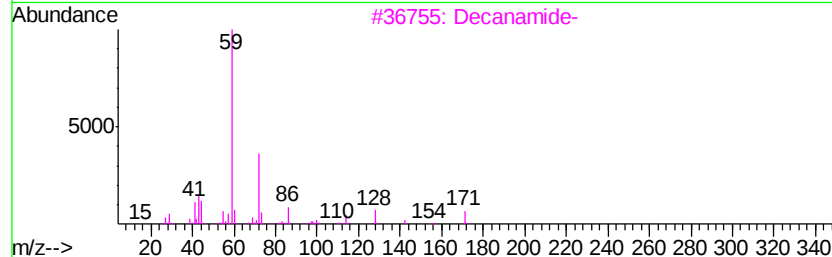
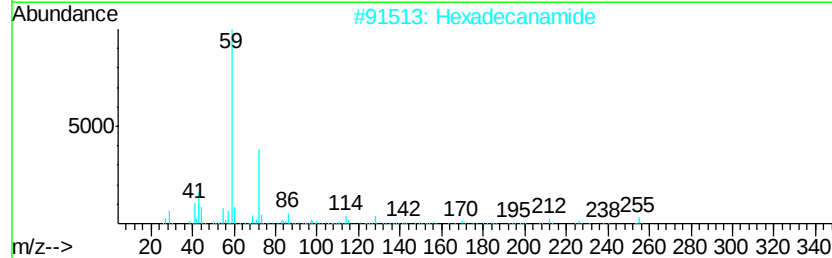
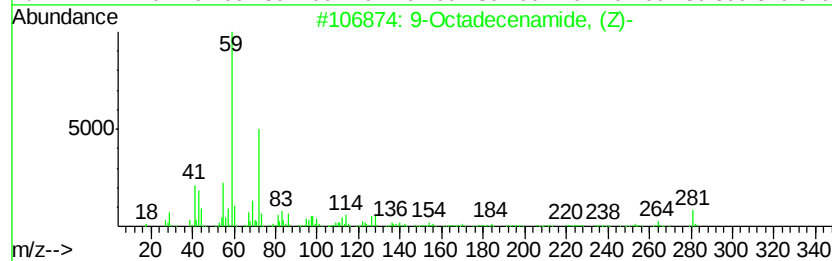
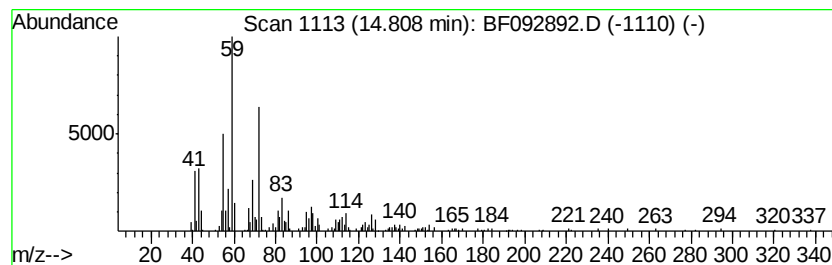
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.39 ng	348824	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		Decanamide-	171	C10H21NO	002319-29-1	53
4		Octadecanamide	283	C18H37NO	000124-26-5	53
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092892.D
Acq On : 10 Feb 2017 19:28
Operator : SJ/MA
Sample : I1777-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-02-5-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
2-Pentanone, 4-hy...	5.08	36.4	ng	1769020	1	6.89	972448	20.0
unknown6.66	6.66	85.3	ng	4144920	1	6.89	972448	20.0
1,6-Anhydro-.beta...	9.86	3.6	ng	295029	3	9.94	1627450	20.0
Heptacosane	10.84	2.4	ng	201725	4	11.43	1650410	20.0
Heptafluorobutyri...	13.89	4.0	ng	283019	5	14.05	1421960	20.0
9-Octadecenamide,...	14.81	5.4	ng	348824	6	15.51	1293200	20.0