

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051215\
 Data File : BF079161.D
 Acq On : 12 May 2015 16:53
 Operator : TP/IZ
 Sample : G2155-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-42D

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-BF043015.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	1.427	19	21	24	rVB	477801	501545	11.42%	2.495%
2	1.564	30	33	45	rVB2	146383	338427	7.70%	1.683%
3	1.724	45	47	56	rVV2	284393	634033	14.43%	3.154%
4	1.850	56	58	91	rVB	2361359	4393393	100.00%	21.852%
5	5.084	339	341	346	rVB	29610	52200	1.19%	0.260%
6	5.587	382	385	387	rBV	727434	995418	22.66%	4.951%
7	6.845	493	495	498	rBV	1213263	1052936	23.97%	5.237%
8	6.993	505	508	511	rBV	1222958	1096460	24.96%	5.454%
9	7.279	531	533	536	rBV	416216	384756	8.76%	1.914%
10	7.462	547	549	552	rVB	586119	791017	18.00%	3.934%
11	7.976	591	594	596	rBV	537060	647945	14.75%	3.223%
12	8.856	669	671	675	rBV	627532	570619	12.99%	2.838%
13	10.205	786	789	791	rBV	1305885	1195882	27.22%	5.948%
14	10.708	831	833	835	rBV	52505	46462	1.06%	0.231%
15	11.028	859	861	864	rBV	545931	627061	14.27%	3.119%
16	12.011	944	947	950	rBV	895595	856627	19.50%	4.261%
17	12.880	1020	1023	1024	rBV	629906	664776	15.13%	3.306%
18	12.902	1024	1025	1027	rVB	209607	194358	4.42%	0.967%
19	12.971	1027	1031	1033	rBV	58974	62632	1.43%	0.312%
20	14.388	1152	1155	1157	rBV	174698	218440	4.97%	1.086%
21	14.663	1176	1179	1181	rBV	232384	265702	6.05%	1.322%
22	14.868	1195	1197	1200	rBV	936600	1231893	28.04%	6.127%
23	16.080	1300	1303	1307	rVV3	96660	197017	4.48%	0.980%
24	16.206	1308	1314	1316	rVV	740630	1124061	25.59%	5.591%
25	16.240	1316	1317	1322	rVB	138104	182265	4.15%	0.907%
26	17.417	1418	1420	1424	rVV	34738	53559	1.22%	0.266%
27	17.543	1428	1431	1437	rVV	91223	244040	5.55%	1.214%
28	17.874	1458	1460	1464	rBV	56280	103094	2.35%	0.513%
29	17.943	1464	1466	1469	rBV	104648	121866	2.77%	0.606%
30	18.011	1469	1472	1475	rBV	625240	789617	17.97%	3.927%
31	19.474	1597	1600	1605	rVB2	49233	122249	2.78%	0.608%
32	19.634	1612	1614	1619	rBV3	21116	61822	1.41%	0.307%
33	19.909	1635	1638	1647	rVB	55426	158502	3.61%	0.788%
34	21.143	1742	1746	1754	rVB3	34472	124832	2.84%	0.621%

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-42D

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-BF043015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

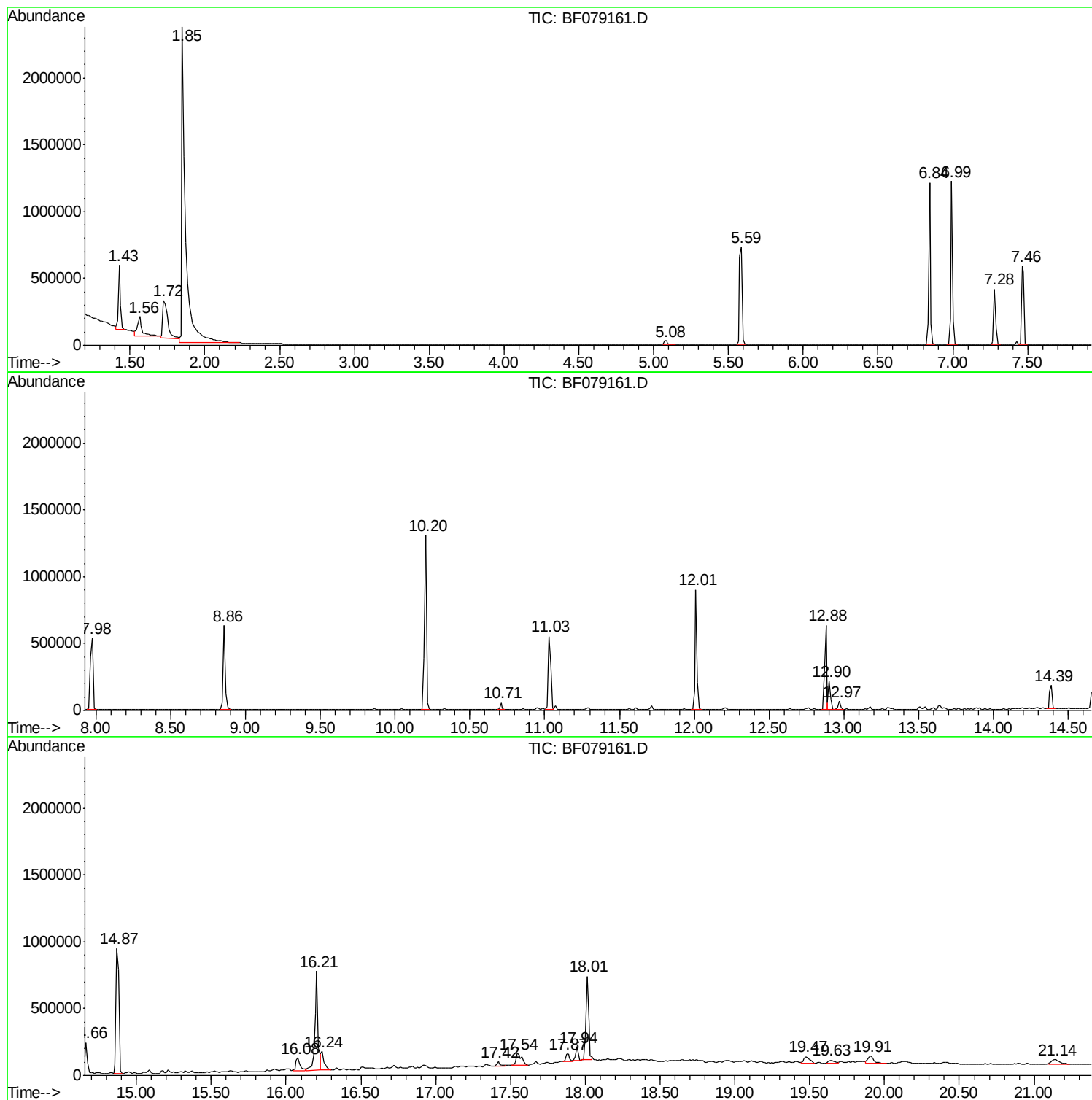
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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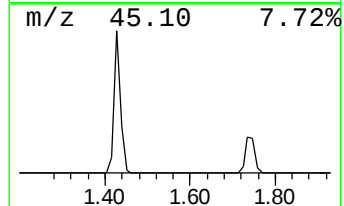
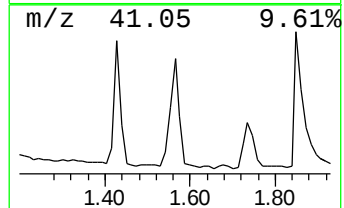
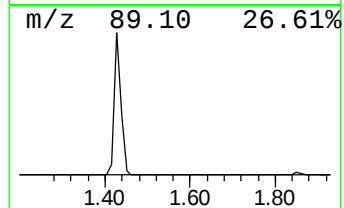
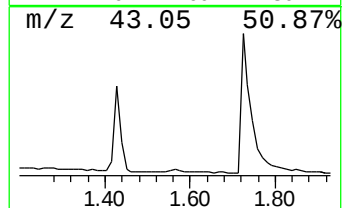
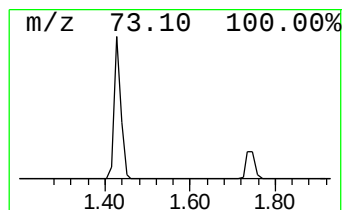
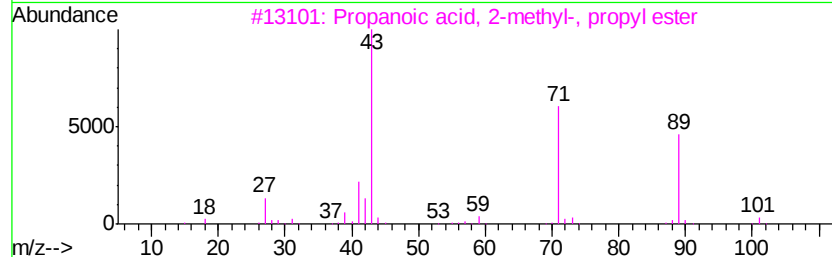
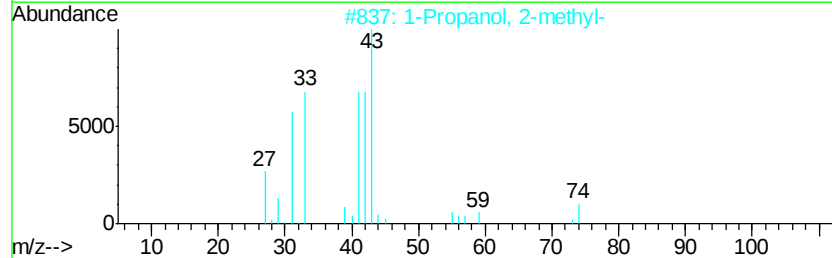
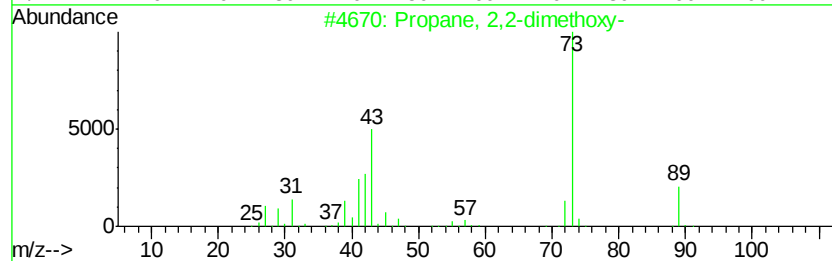
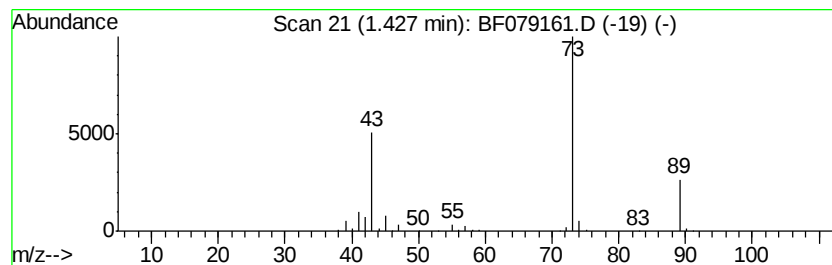
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.43	26.07 ng	501545	1,4-Dichlorobenzene-d4	7.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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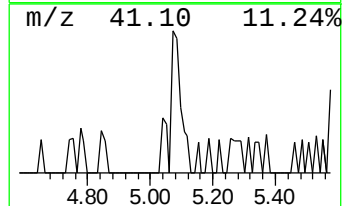
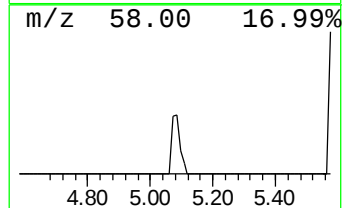
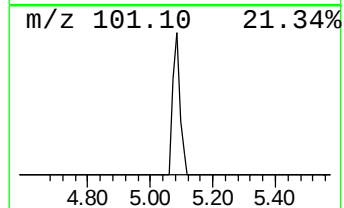
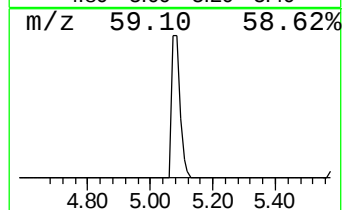
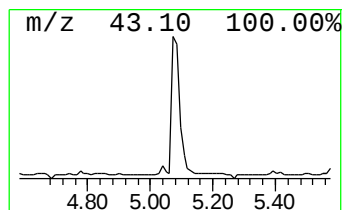
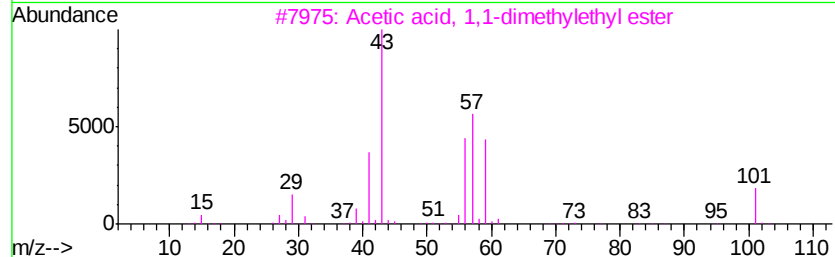
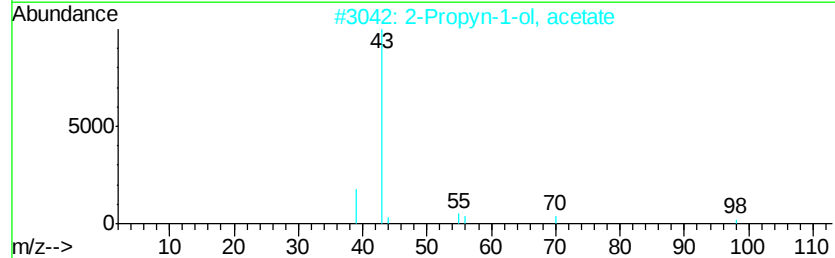
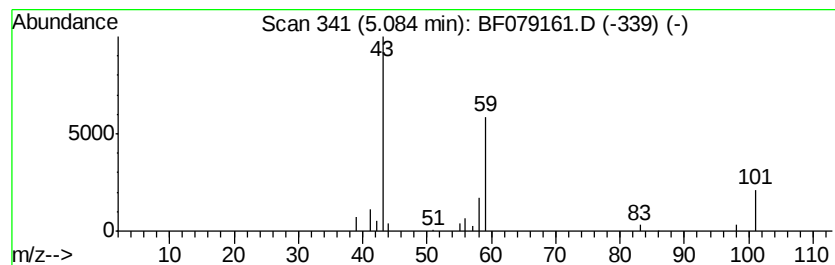
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.71 ng	52200	1,4-Dichlorobenzene-d4	7.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
4	2-Methyl-2,3-pentanediol	118	C6H14O2	007795-80-4	9		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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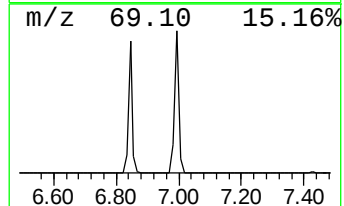
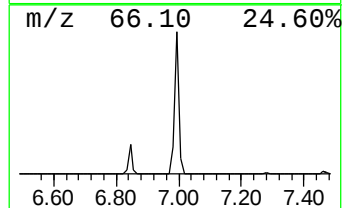
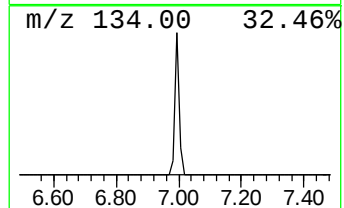
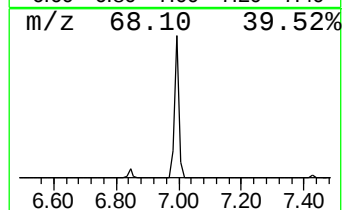
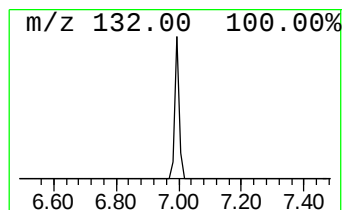
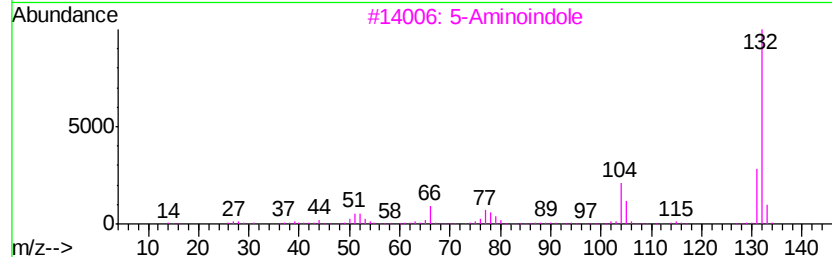
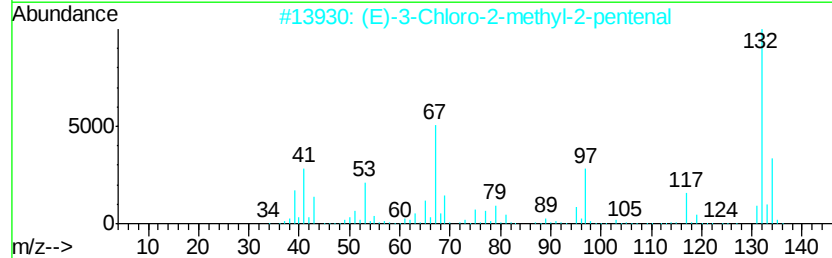
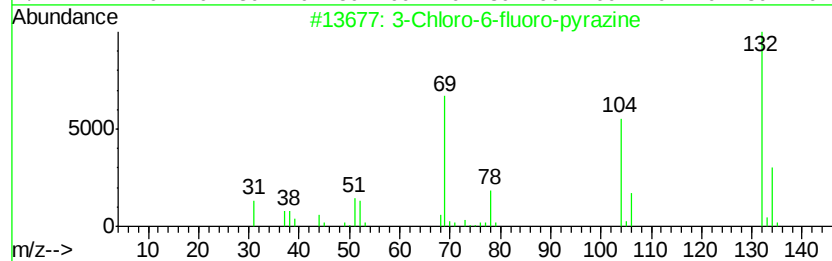
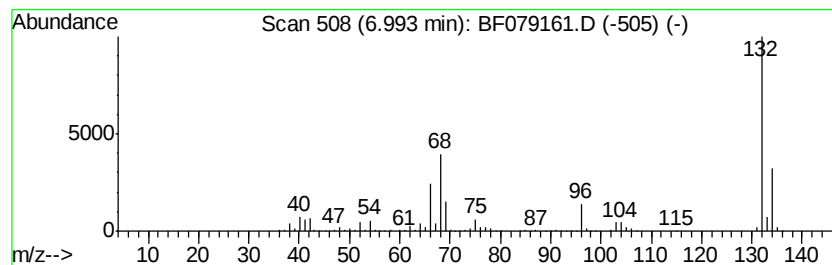
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.99 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	57.00 ng	1096460	1,4-Dichlorobenzene-d4	7.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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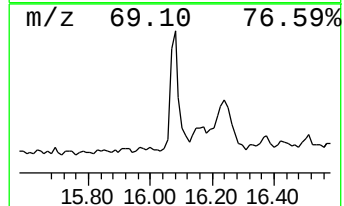
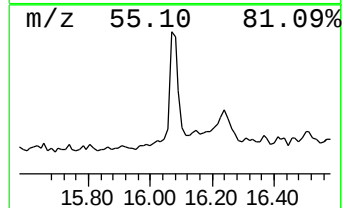
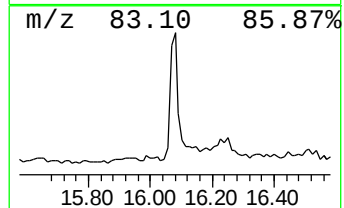
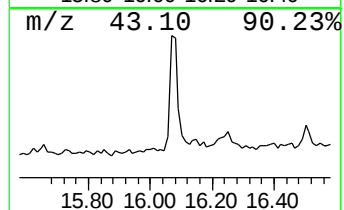
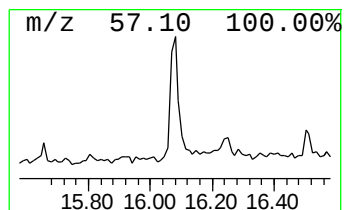
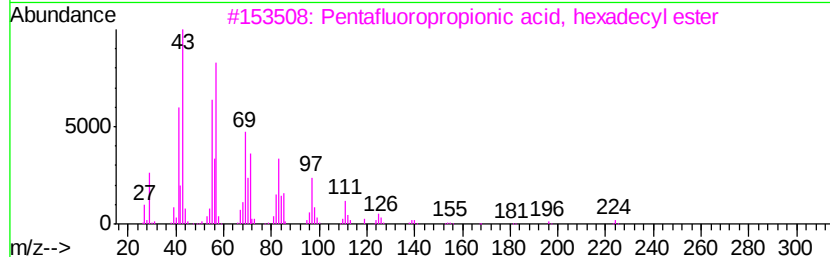
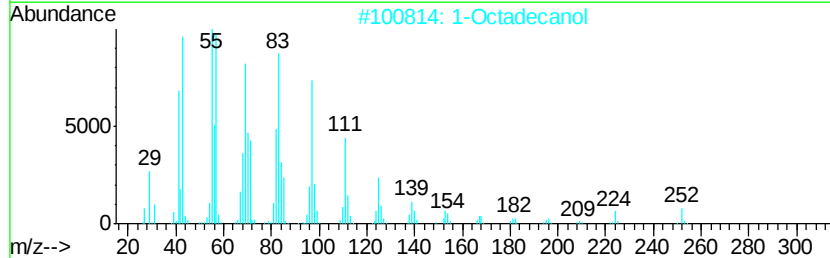
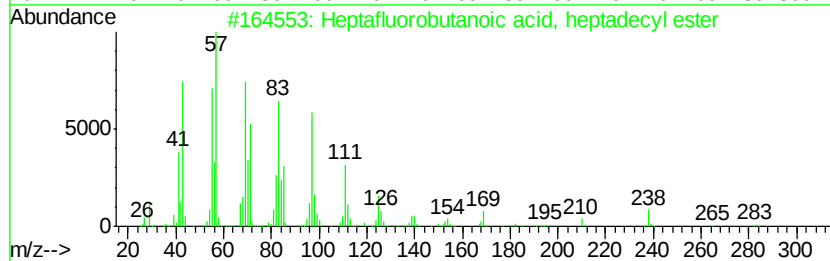
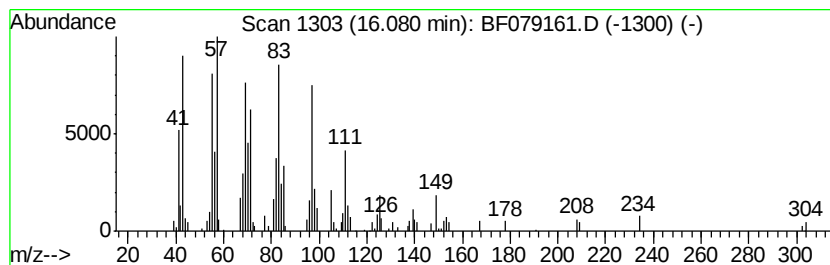
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutanoic acid, h... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.51 ng	197017	Chrysene-d12	16.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		1-Octadecanol	270	C18H38O	000112-92-5	93
3		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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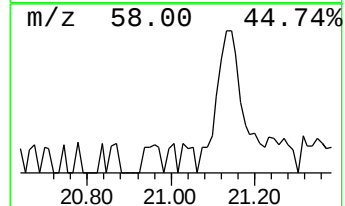
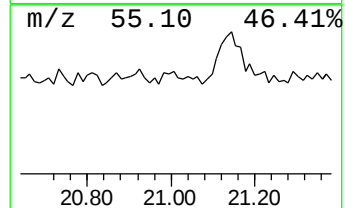
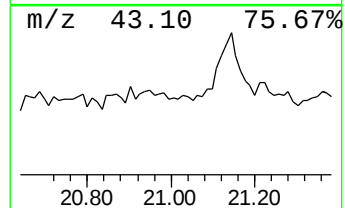
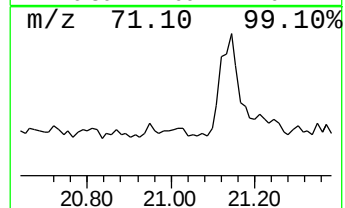
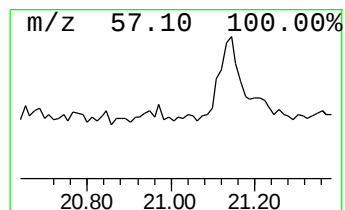
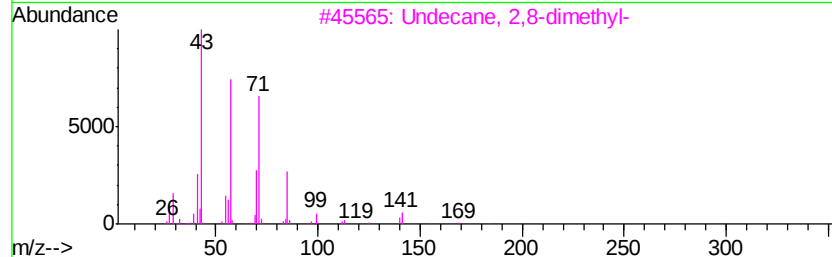
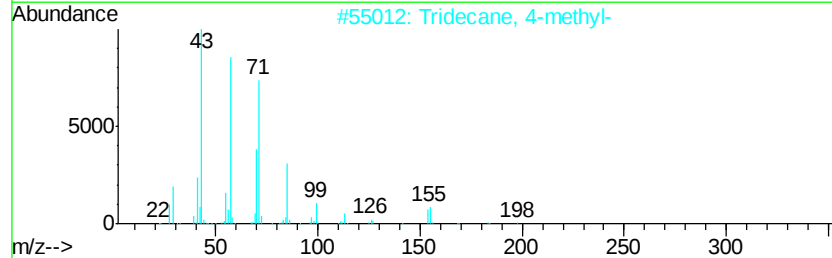
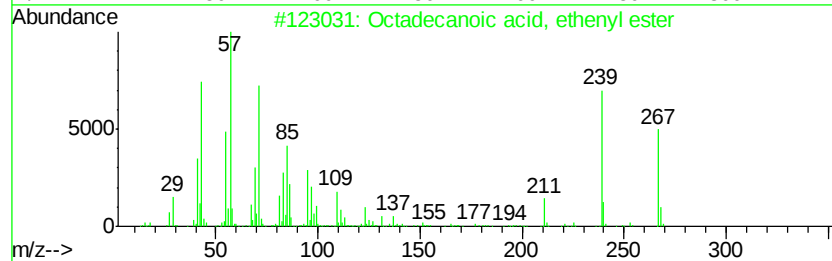
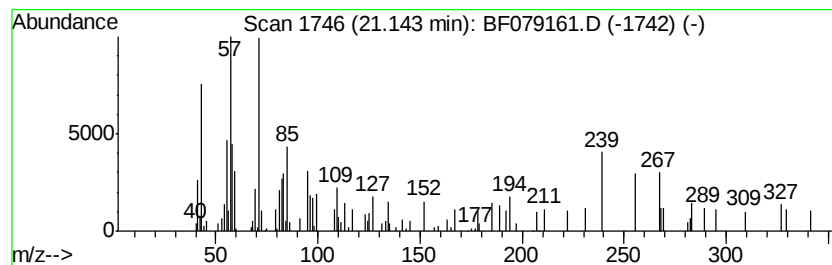
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown21.14 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.14	3.16 ng	124832	Perylene-d12	18.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	43
2		Tridecane, 4-methyl-	198	C14H30	026730-12-1	38
3		Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	38
4		Hexadecane, 3-methyl-	240	C17H36	006418-43-5	38
5		Nonane, 1-iodo-	254	C9H19I	004282-42-2	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.43	1.43	26.1	ng	501545	1	7.28	384756	20.0
2-Pentanone, 4-hy...	5.08	2.7	ng	52200	1	7.28	384756	20.0
unknown6.99	6.99	57.0	ng	1096460	1	7.28	384756	20.0
Heptafluorobutano...	16.08	3.5	ng	197017	5	16.21	1124060	20.0
unknown21.14	21.14	3.2	ng	124832	6	18.01	789617	20.0