

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
 Data File : BF093867.D
 Acq On : 23 Mar 2017 7:40
 Operator : SJ/MA
 Sample : I2349-01
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-212-207-COMP

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-BF032217.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	2.116	33	39	45	rVB	138349	163756	2.63%	0.313%
2	2.634	123	127	134	rBV	89399	103608	1.66%	0.198%
3	4.145	379	384	397	rVB	757027	1126812	18.11%	2.152%
4	4.522	441	448	451	rBV	4742754	5641408	90.66%	10.772%
5	4.910	509	514	521	rBV	72369	73761	1.19%	0.141%
6	5.581	619	628	632	rBV2	4084939	6222747	100.00%	11.882%
7	5.734	647	654	657	rBV	4760096	6024837	96.82%	11.504%
8	5.986	693	697	701	rBV	1410896	1242508	19.97%	2.372%
9	6.169	722	728	731	rBV	4337714	4609620	74.08%	8.802%
10	6.639	800	808	811	rBV	3021171	3991073	64.14%	7.621%
11	7.080	878	883	891	rVB	151441	162924	2.62%	0.311%
12	7.204	900	904	908	rVB	446345	438865	7.05%	0.838%
13	7.486	947	952	956	rBV	1550448	1672907	26.88%	3.194%
14	8.816	1171	1178	1182	rBV	5023251	6191477	99.50%	11.822%
15	9.304	1256	1261	1265	rBV	568624	502122	8.07%	0.959%
16	9.633	1308	1317	1321	rBV2	1706775	1768090	28.41%	3.376%
17	9.951	1368	1371	1376	rVB	58404	65273	1.05%	0.125%
18	10.221	1413	1417	1421	rVB	113609	103690	1.67%	0.198%
19	10.604	1475	1482	1486	rBV	2676178	3362658	54.04%	6.421%
20	10.804	1513	1516	1519	rBV	125891	144736	2.33%	0.276%
21	11.363	1607	1611	1614	rBV	119583	105383	1.69%	0.201%
22	11.457	1622	1627	1630	rBV	1639312	1542171	24.78%	2.945%
23	13.368	1948	1952	1957	rVB	109087	107836	1.73%	0.206%
24	13.439	1957	1964	1968	rBV	3662200	4355847	70.00%	8.317%
25	13.774	2017	2021	2025	rVB	72618	75828	1.22%	0.145%
26	14.145	2080	2084	2089	rBV	166577	153726	2.47%	0.294%
27	14.592	2156	2160	2170	rBV	132389	198322	3.19%	0.379%
28	14.704	2174	2179	2183	rBV	966234	1076131	17.29%	2.055%
29	16.345	2453	2458	2468	rBV	806307	940594	15.12%	1.796%
30	16.892	2547	2551	2555	rBV3	41783	65659	1.06%	0.125%
31	17.380	2629	2634	2645	rVB4	33813	64162	1.03%	0.123%
32	17.933	2723	2728	2739	rBV4	30356	74189	1.19%	0.142%

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Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-212-207-COMP

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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

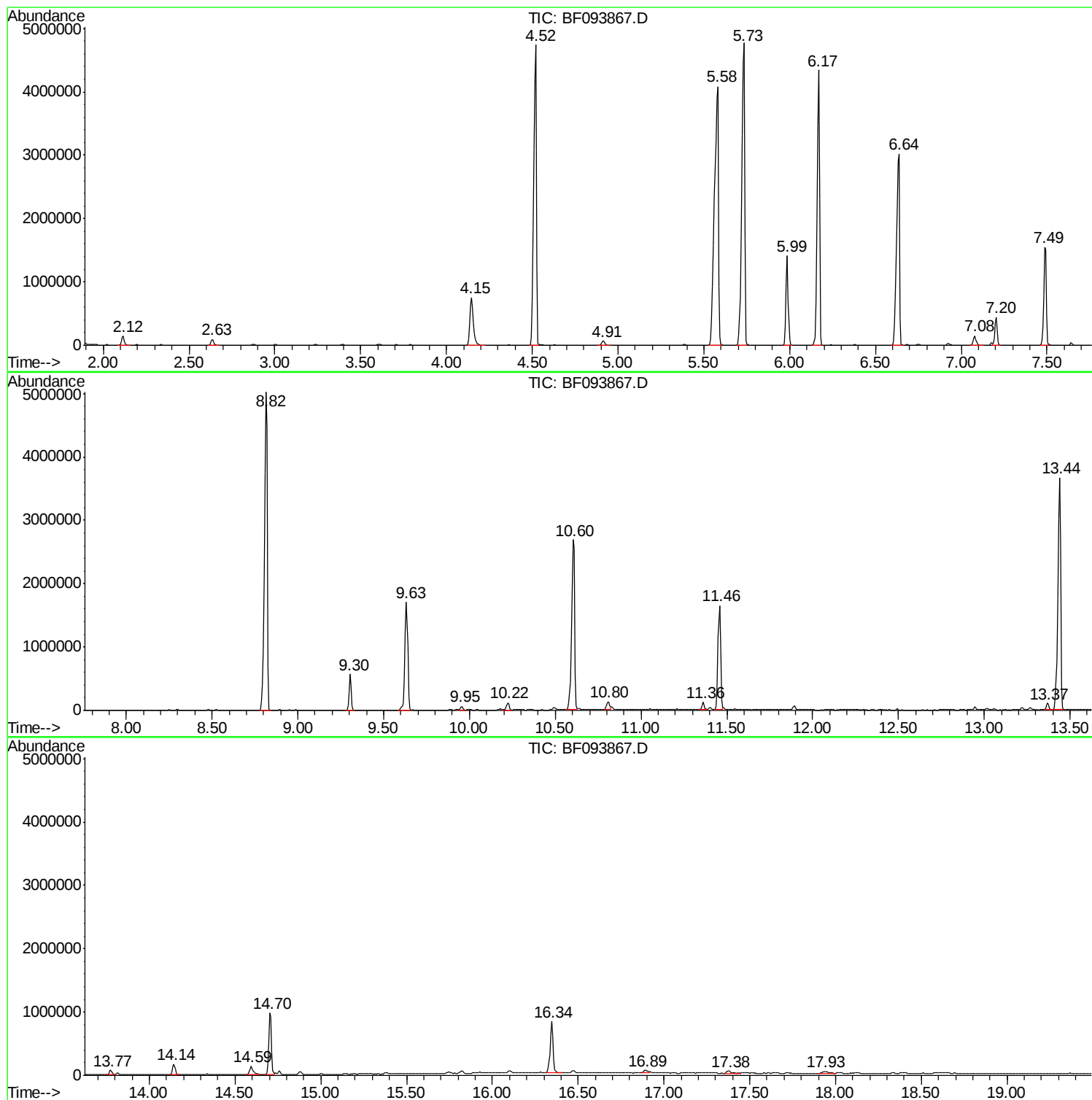
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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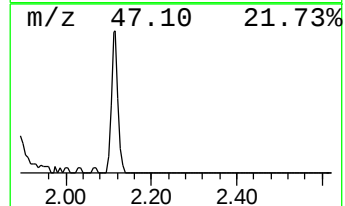
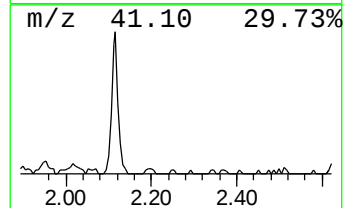
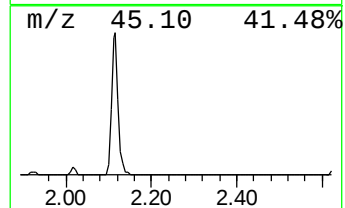
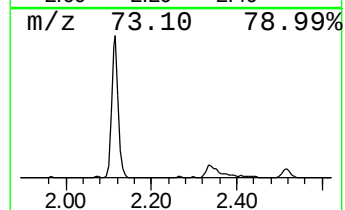
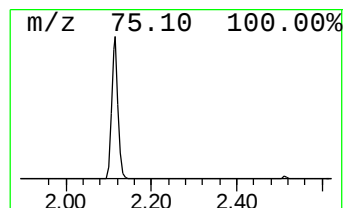
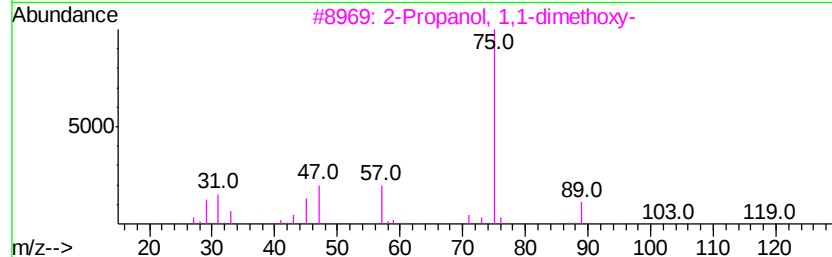
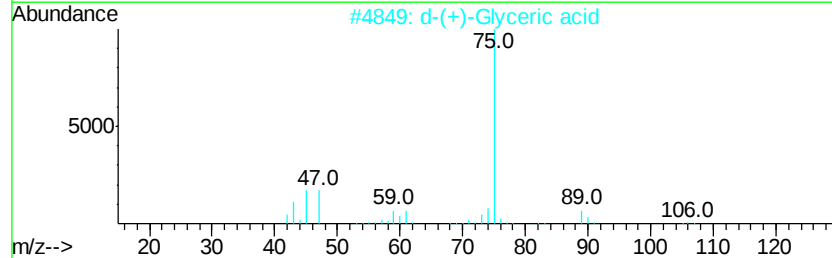
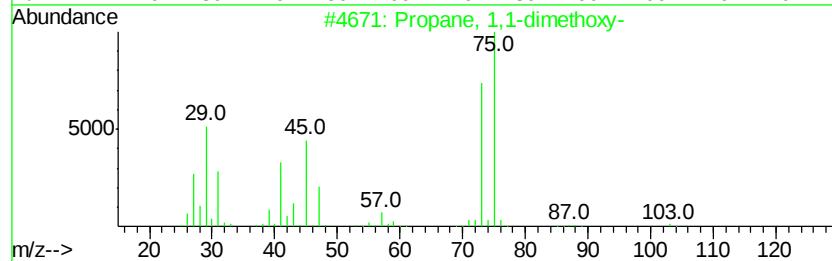
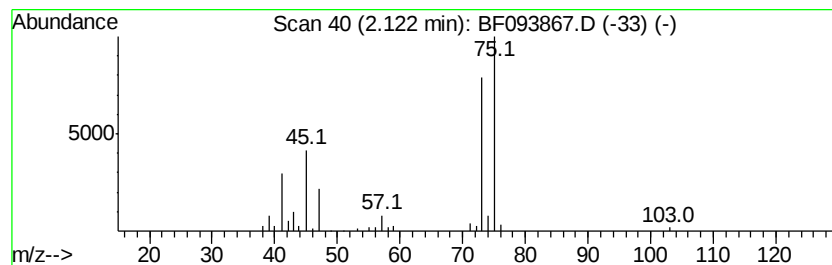
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.12	2.64 ng	163756	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		d-(+)-Glyceric acid	106	C3H6O4	1000211-40-8	36
3		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
4		Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
5		Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	33



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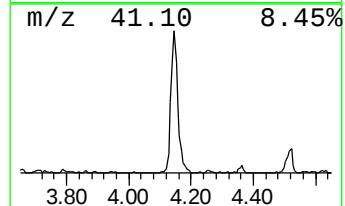
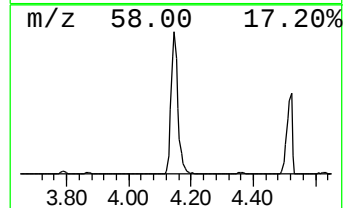
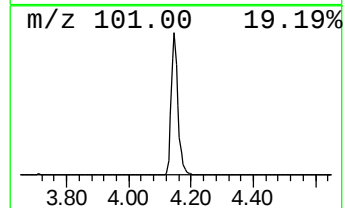
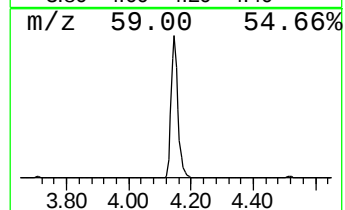
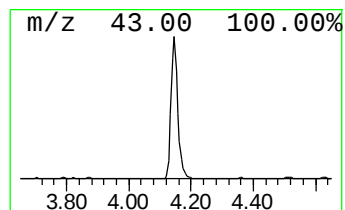
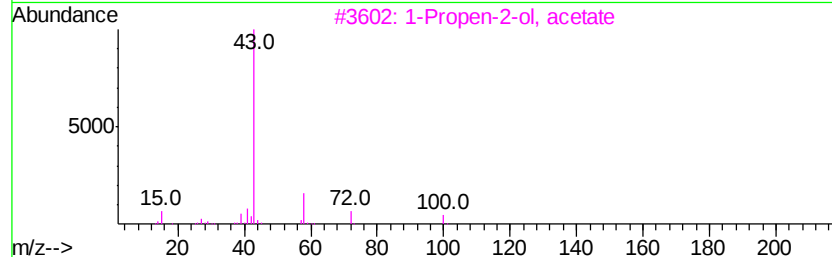
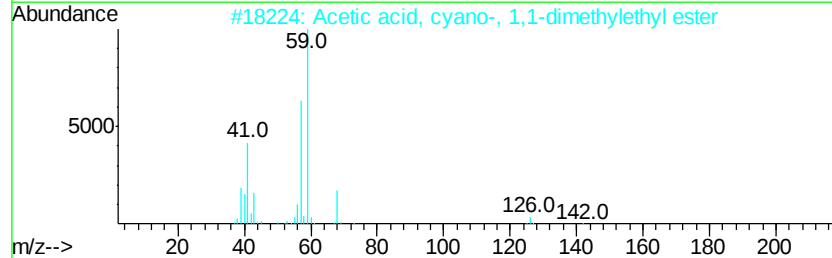
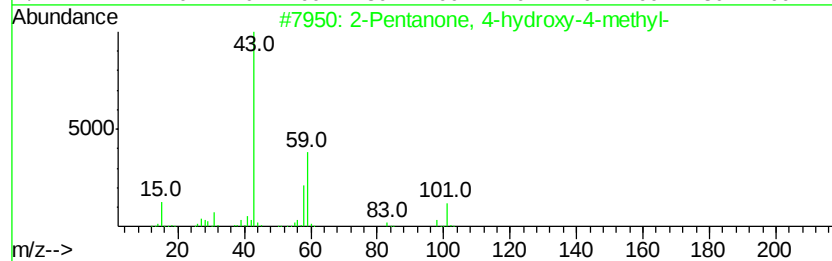
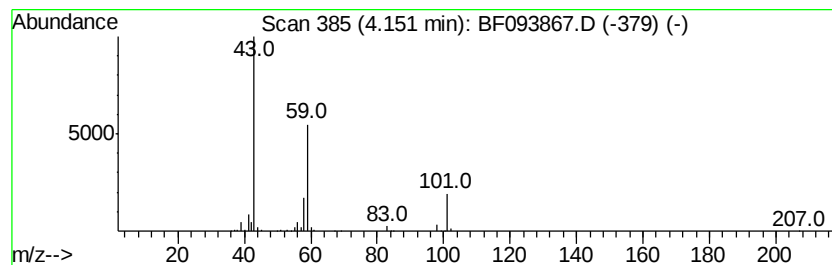
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	18.14 ng	1126810	1,4-Dichlorobenzene-d4	5.99

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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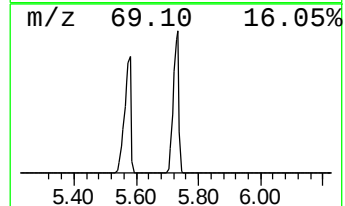
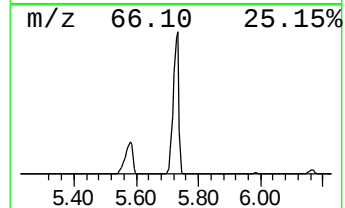
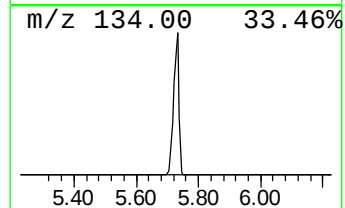
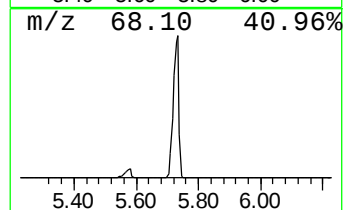
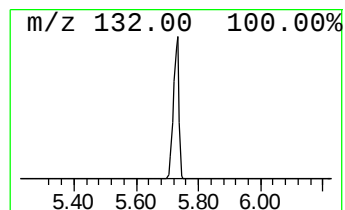
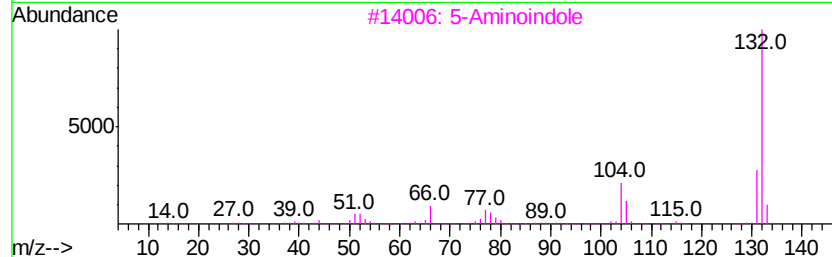
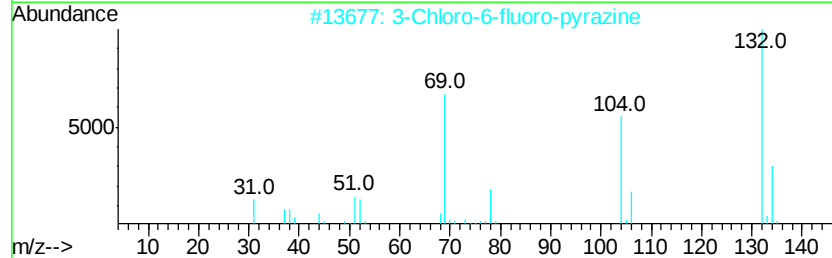
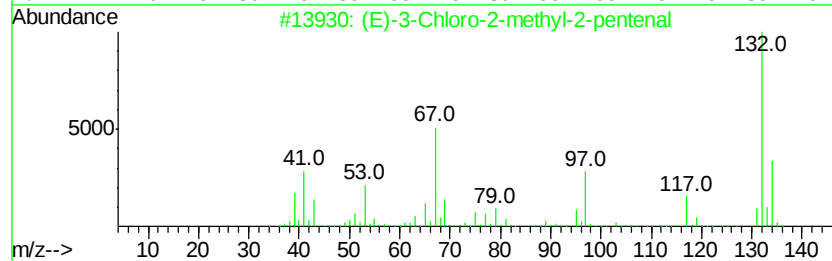
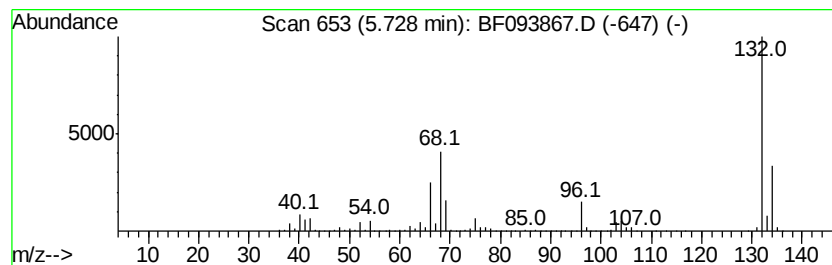
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	96.98 ng	6024840	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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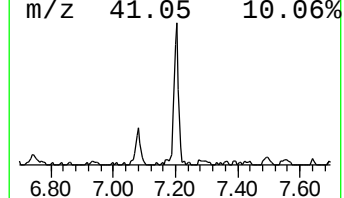
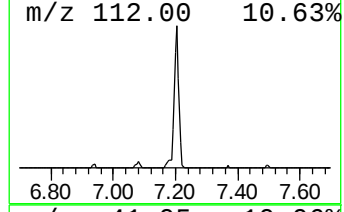
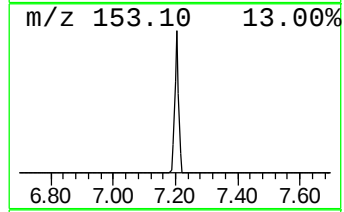
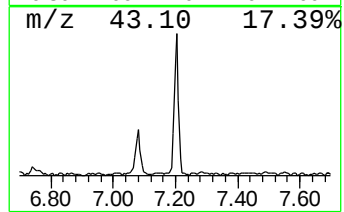
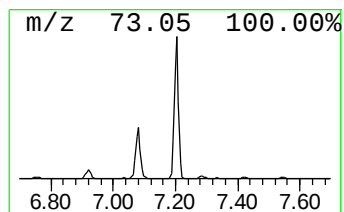
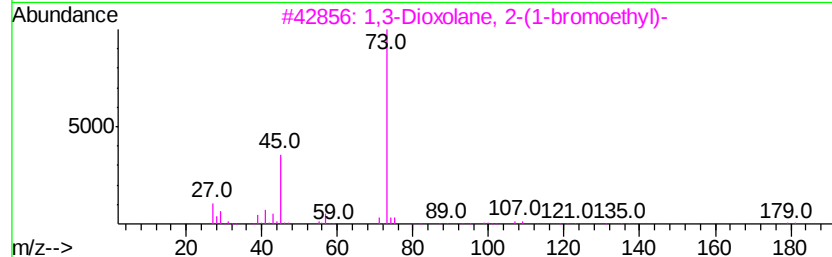
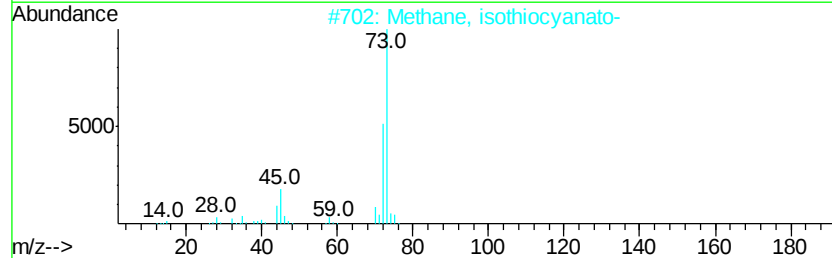
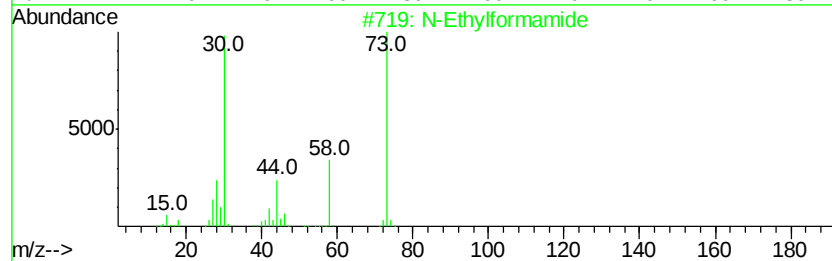
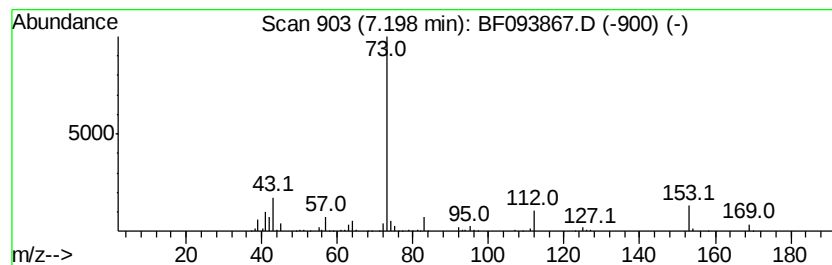
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.20 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	5.25 ng	438865	Napthalene-d8	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Ethylformamide	73	C3H7NO	000627-45-2	12
2		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4		1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	9
5		3(2H)-Isoquinolinone, octahydro-...	153	C9H15NO	076097-42-2	7



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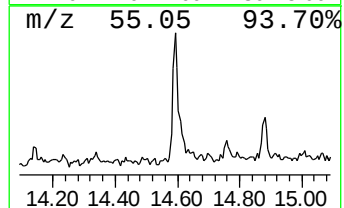
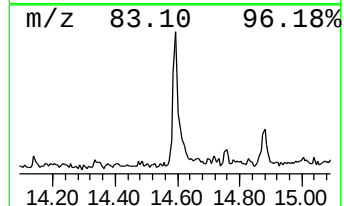
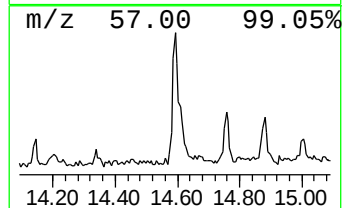
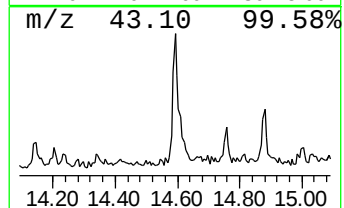
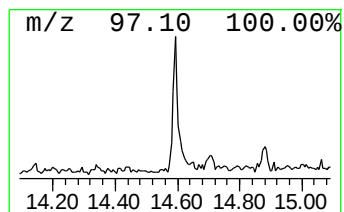
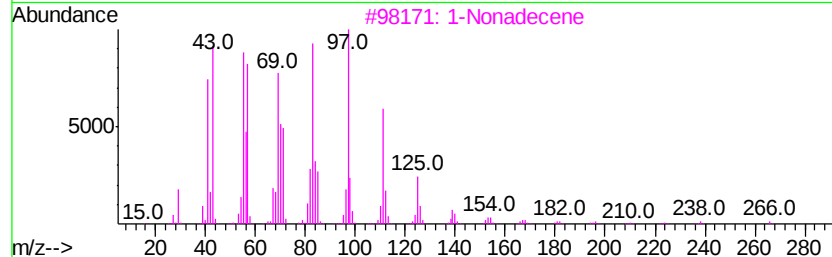
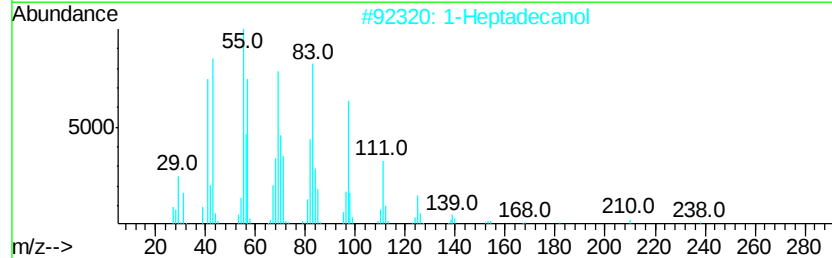
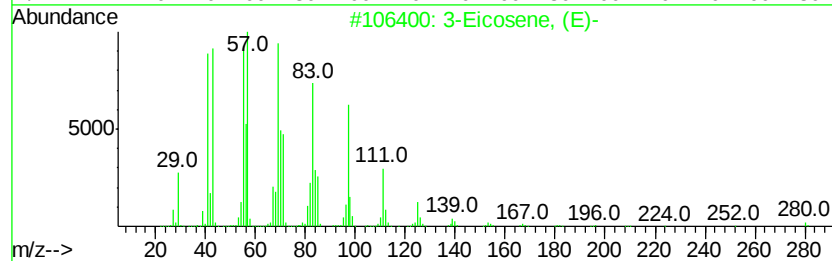
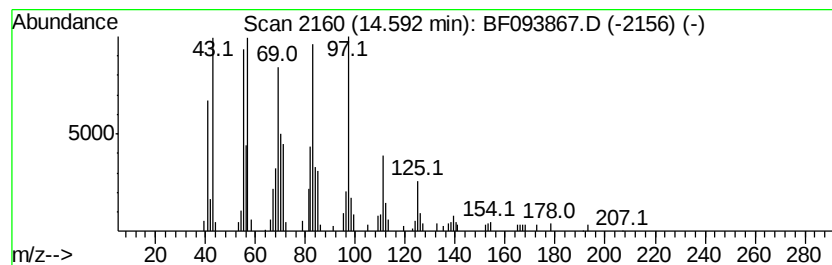
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	3.69 ng	198322	Chrysene-d12	14.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
2	1-Heptadecanol	256	C17H36O	001454-85-9	87
3	1-Nonadecene	266	C19H38	018435-45-5	83
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
5	1-Tetracosanol	354	C24H50O	000506-51-4	80



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	2.12	2.6	ng	163756	1	5.99	1242510	20.0
2-Pentanone, 4-hy...	4.15	18.1	ng	1126810	1	5.99	1242510	20.0
unknown5.73	5.73	97.0	ng	6024840	1	5.99	1242510	20.0
unknown7.20	7.20	5.3	ng	438865	2	7.49	1672910	20.0
3-Eicosene, (E)-	14.59	3.7	ng	198322	5	14.70	1076130	20.0