

Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
 Data File : BF092810.D
 Acq On : 6 Feb 2017 21:54
 Operator : SJ/MA
 Sample : I1706-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-SCW-COMP-04

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	3.310	104	107	117	rBV	42009	145902	3.07%	0.418%
2	4.773	233	235	244	rBV	36230	60249	1.27%	0.173%
3	5.116	261	265	267	rBV	2939322	4751191	100.00%	13.607%
4	5.516	298	300	303	rBV	1382529	1696945	35.72%	4.860%
5	6.453	380	382	384	rBV	145279	192921	4.06%	0.553%
6	6.544	388	390	393	rVB	1975514	2881236	60.64%	8.252%
7	6.682	399	402	404	rBV	2393374	2317240	48.77%	6.636%
8	6.910	420	422	424	rBV	1047743	877510	18.47%	2.513%
9	7.070	433	436	438	rBV	2652483	2760154	58.09%	7.905%
10	7.470	468	471	474	rBV	1698437	2163627	45.54%	6.196%
11	8.190	532	534	537	rBV	949384	1131809	23.82%	3.241%
12	8.339	545	547	557	rBV	111939	240927	5.07%	0.690%
13	9.276	625	629	631	rBV	3094425	3969572	83.55%	11.368%
14	9.665	660	663	665	rBV	1282565	1116373	23.50%	3.197%
15	9.871	673	681	683	rBV2	42977	86334	1.82%	0.247%
16	9.951	685	688	690	rVB	1530360	1362788	28.68%	3.903%
17	10.739	754	757	759	rBV	1242859	1220349	25.69%	3.495%
18	10.853	765	767	770	rBV	75856	94020	1.98%	0.269%
19	11.299	804	806	807	rBV	94764	83394	1.76%	0.239%
20	11.436	815	818	820	rBV	1599129	1391806	29.29%	3.986%
21	11.722	841	843	846	rBV	72106	69754	1.47%	0.200%
22	13.025	954	957	959	rBV	3641284	3554313	74.81%	10.179%
23	13.917	1032	1035	1043	rBV	144693	245463	5.17%	0.703%
24	14.077	1046	1049	1051	rBV	1326737	1335695	28.11%	3.825%
25	15.528	1173	1176	1182	rBV	847564	1061670	22.35%	3.041%
26	15.974	1212	1215	1218	rBV	29072	47988	1.01%	0.137%
27	16.465	1255	1258	1264	rBV2	23990	58351	1.23%	0.167%

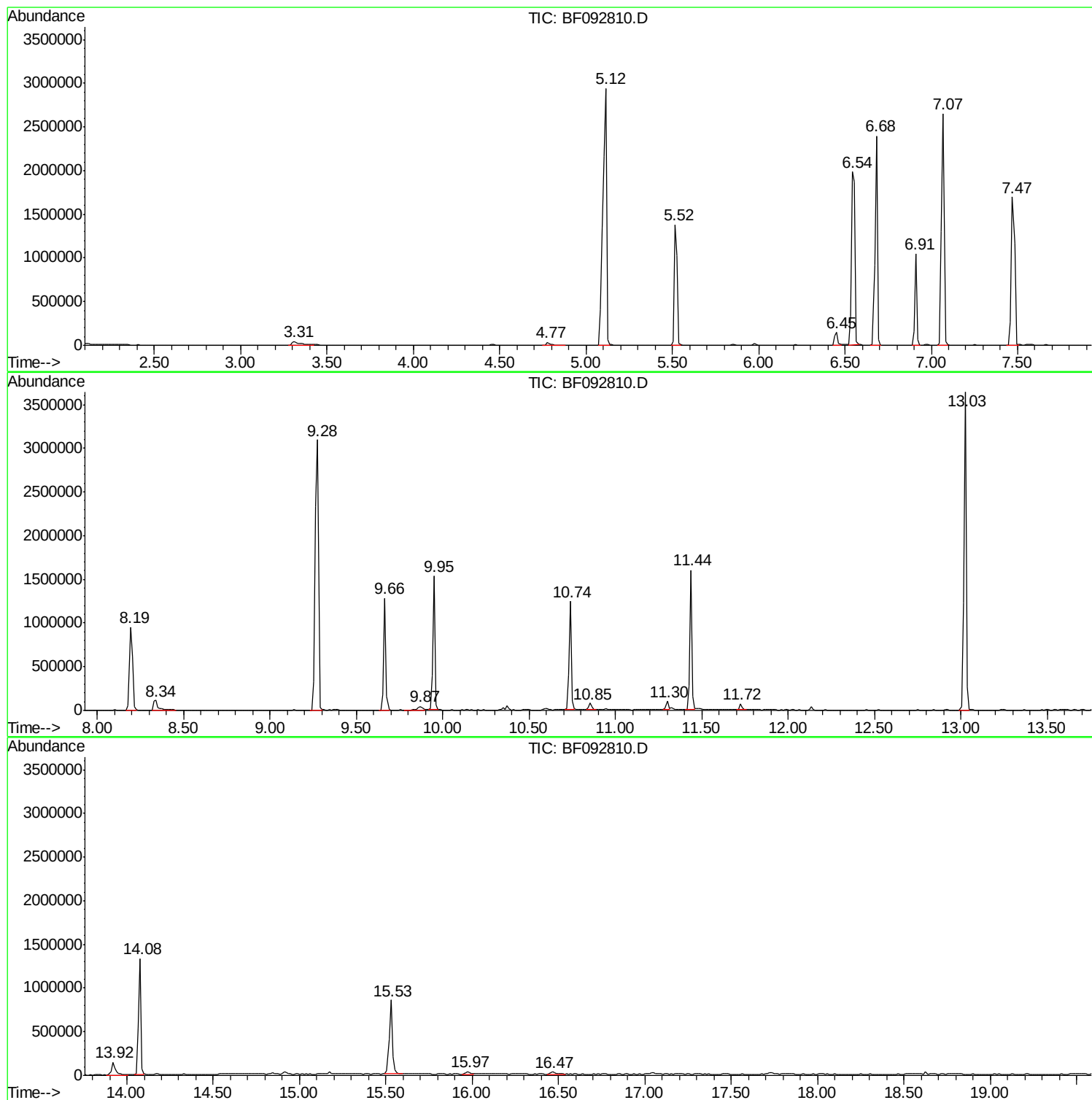
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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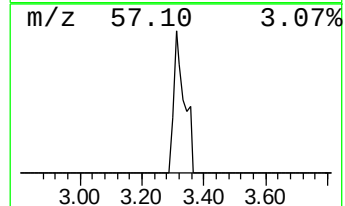
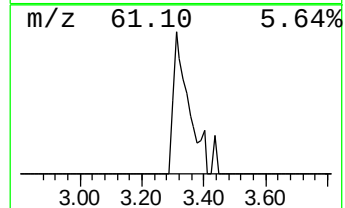
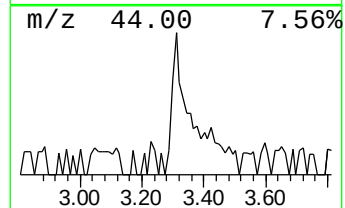
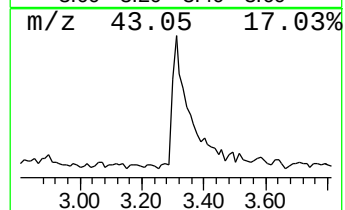
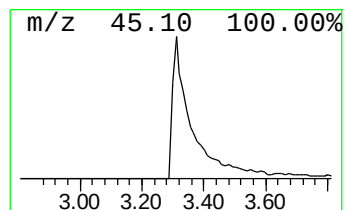
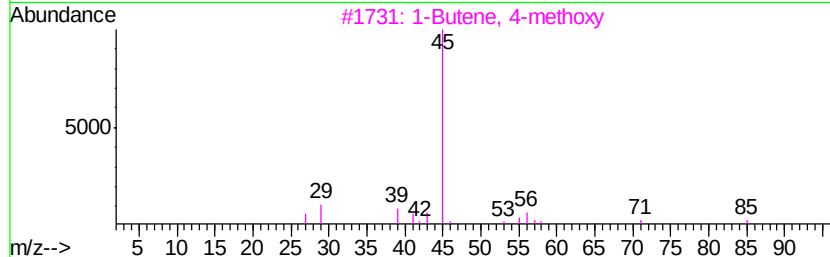
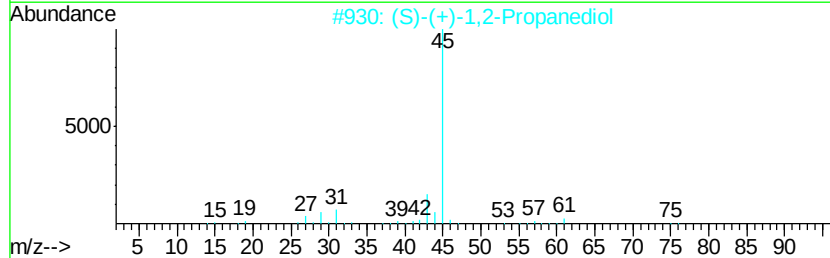
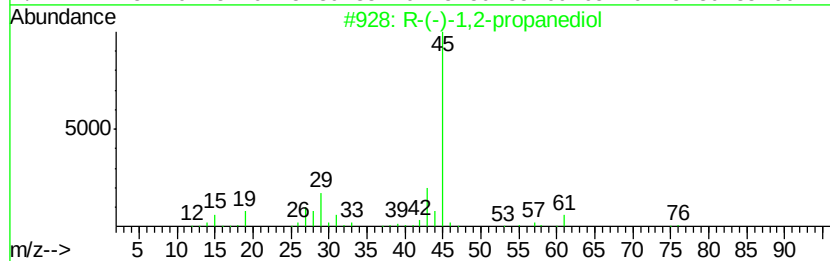
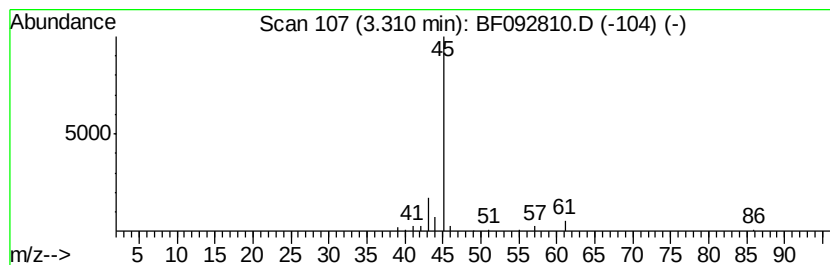
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.31 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	3.33 ng	145902	1,4-Dichlorobenzene-d4	6.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		2-Pentanol	88	C5H12O	006032-29-7	9



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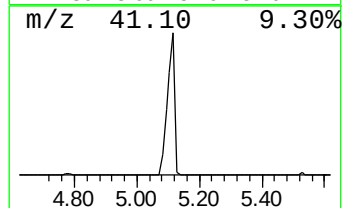
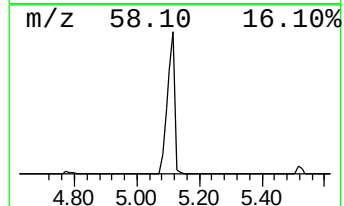
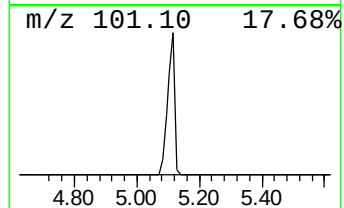
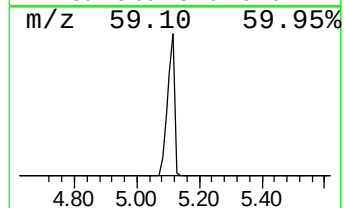
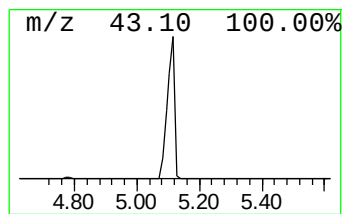
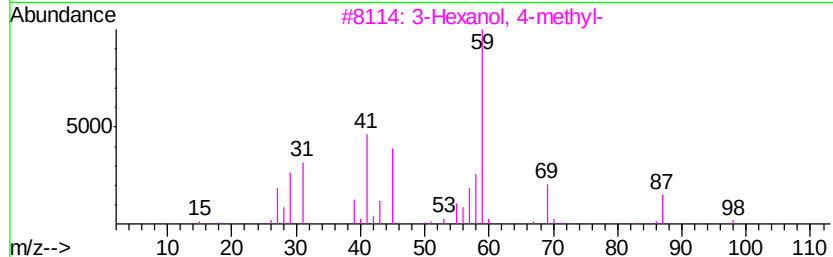
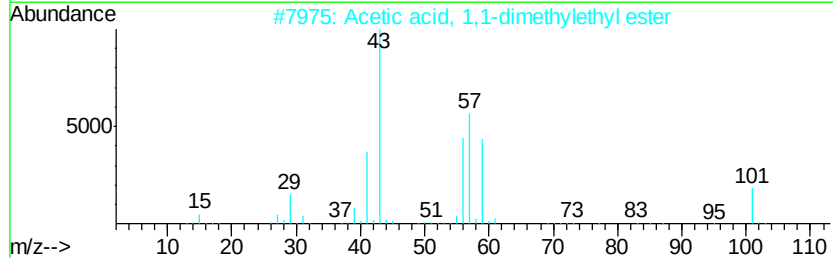
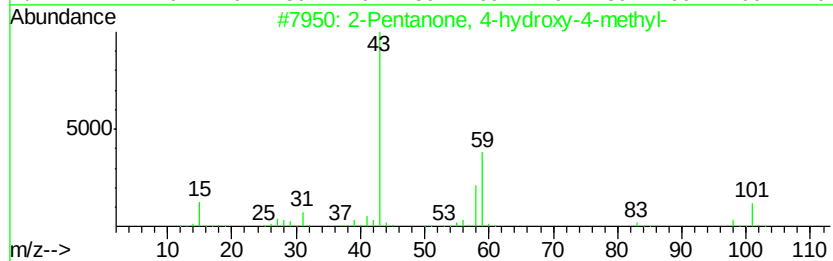
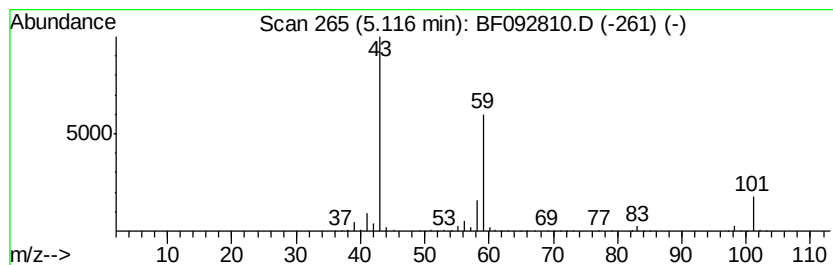
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	108.29 ng	4751190	1,4-Dichlorobenzene-d4	6.91

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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	9



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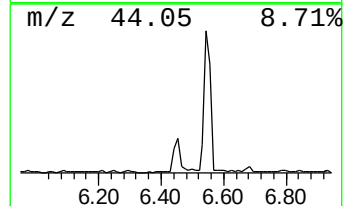
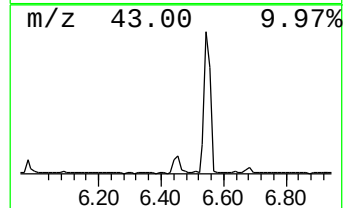
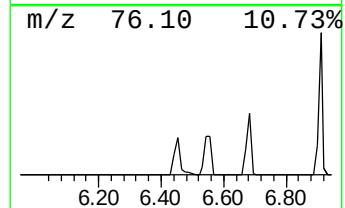
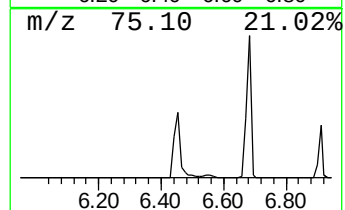
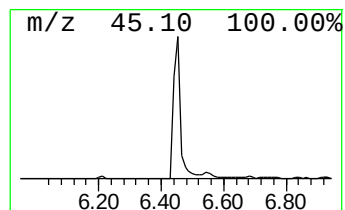
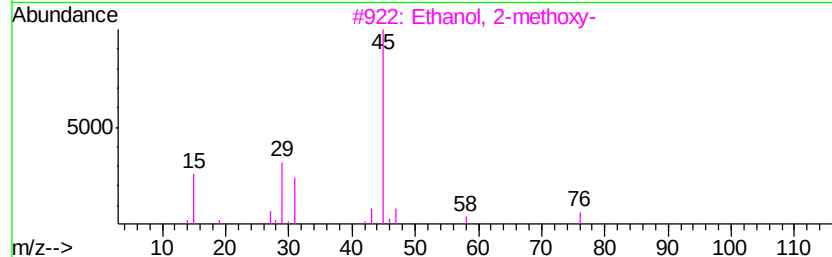
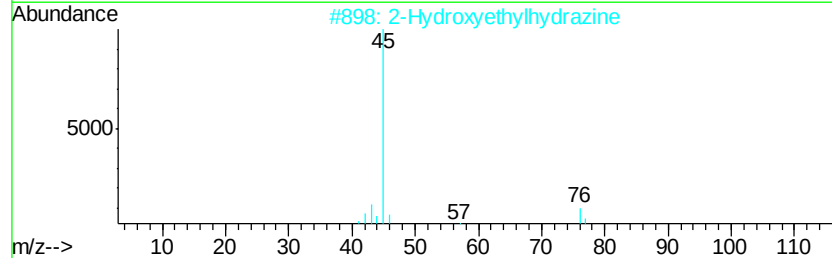
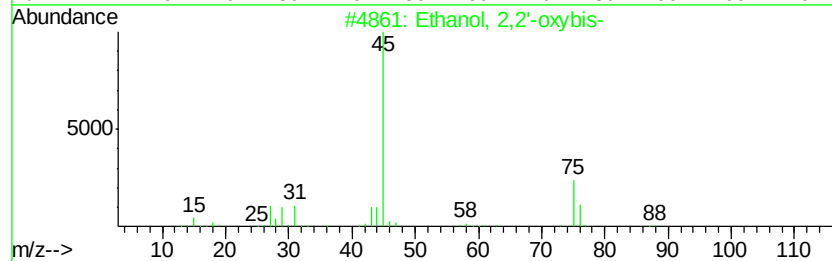
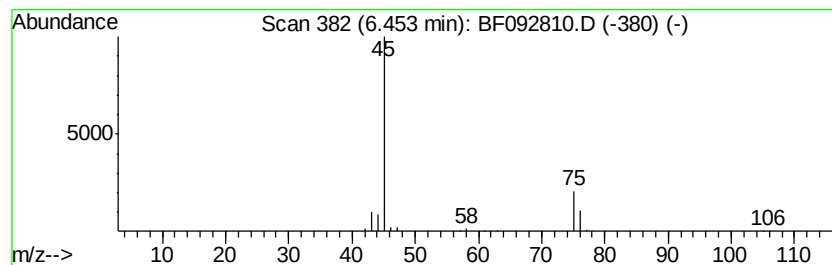
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.45	4.40 ng	192921	1,4-Dichlorobenzene-d4	6.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	83
2	2-Hydroxyethylhydrazine	76	C2H8N2O	000109-84-2	9
3	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
4	1,2-Propanediol, 3-methoxy-	106	C4H10O3	000623-39-2	9
5	2-Propanol, 1,3-dimethoxy-	120	C5H12O3	000623-69-8	9



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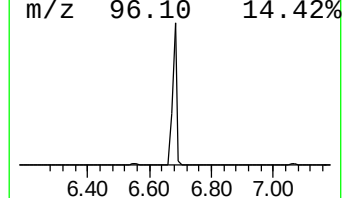
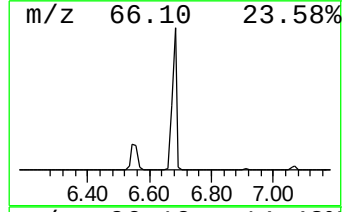
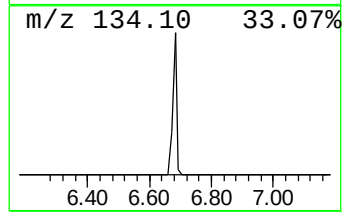
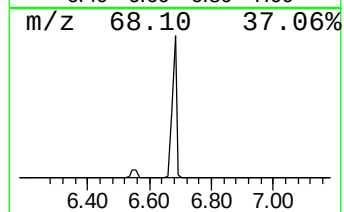
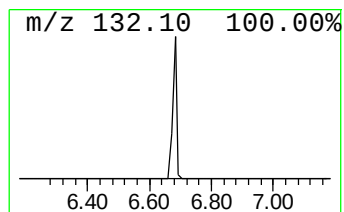
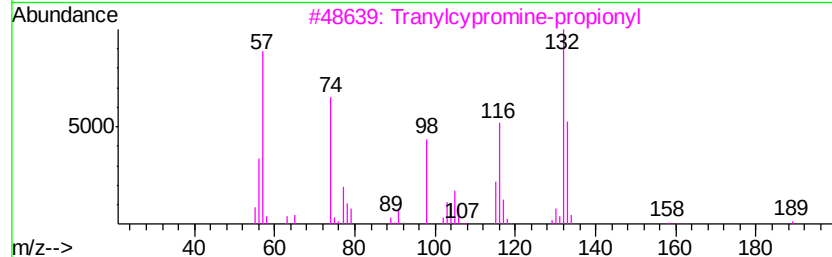
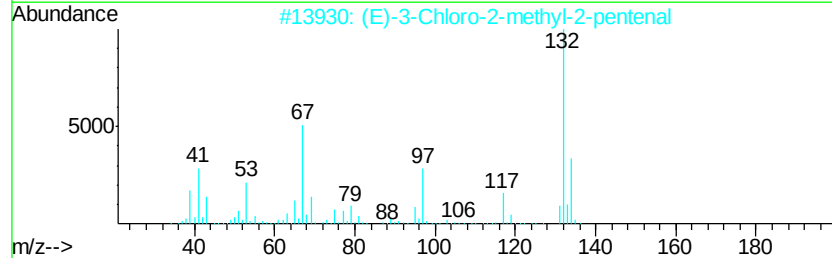
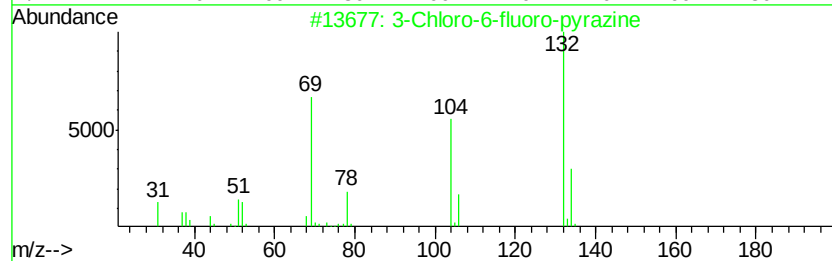
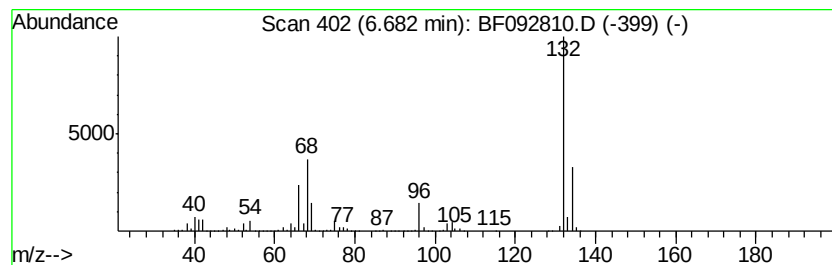
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	52.81 ng	2317240	1,4-Dichlorobenzene-d4	6.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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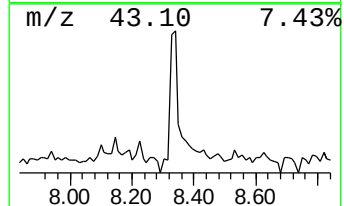
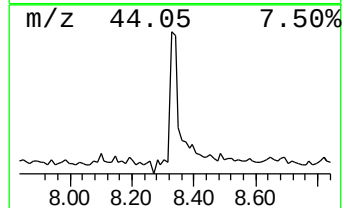
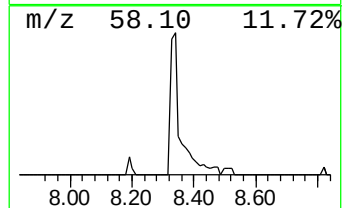
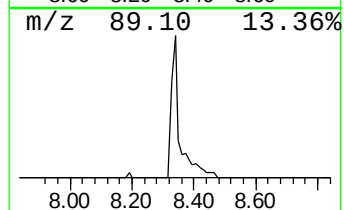
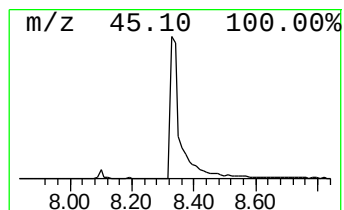
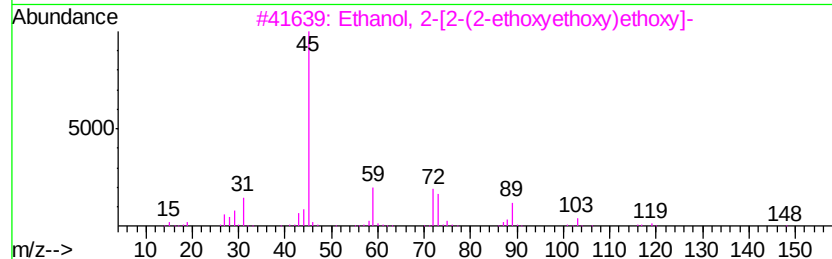
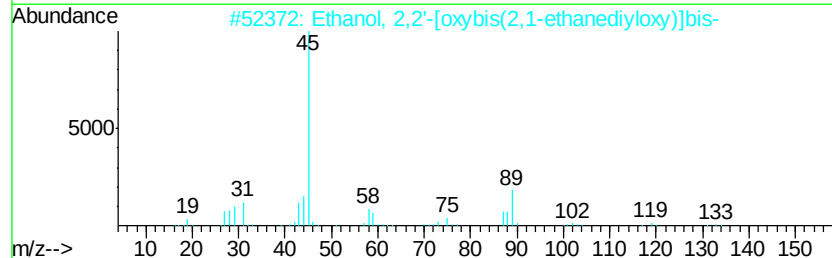
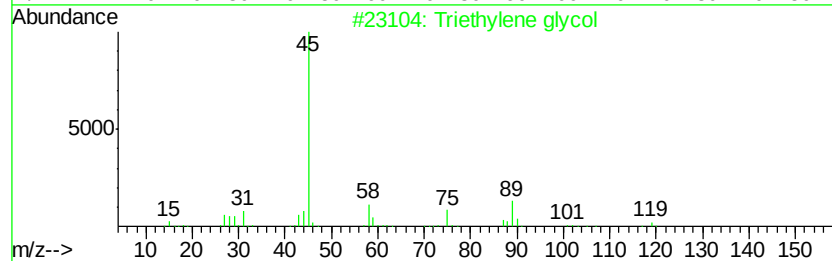
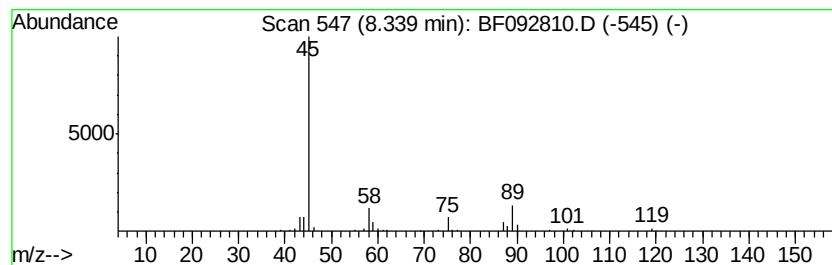
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	4.26 ng	240927	Naphthalene-d8	8.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triethylene glycol	150	C6H14O4	000112-27-6	83
2		Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	72
3		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4		Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	38
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	37



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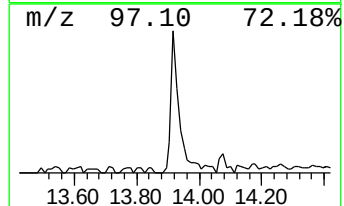
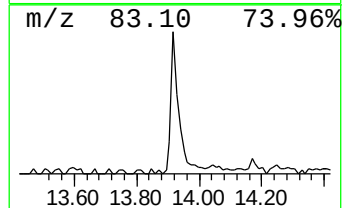
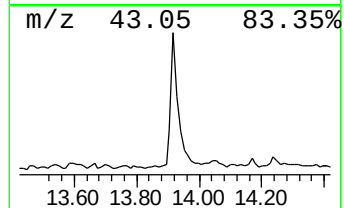
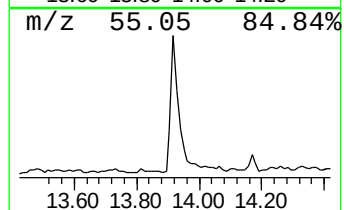
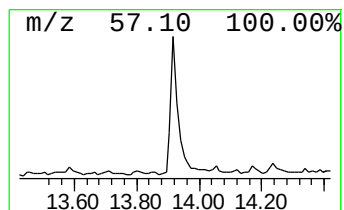
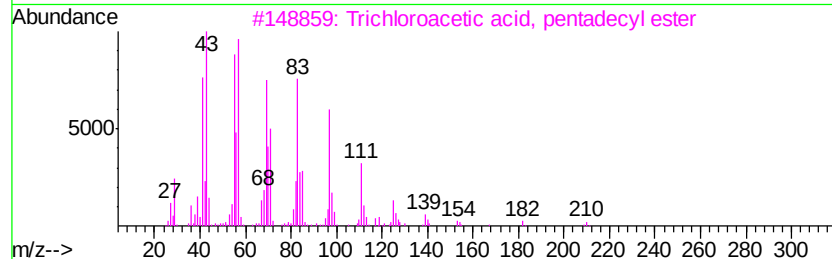
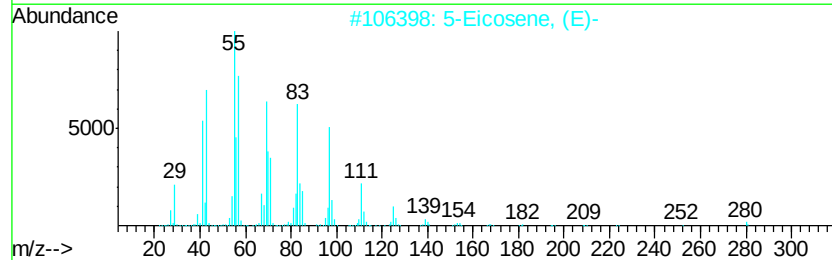
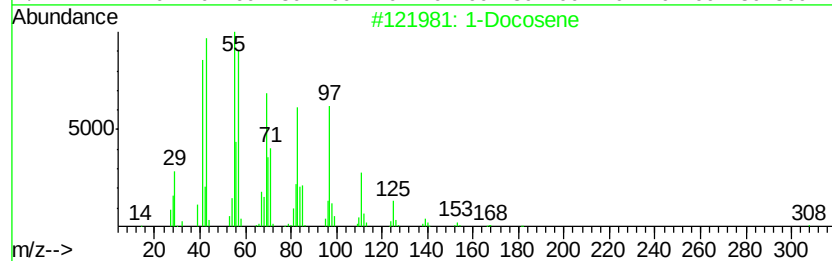
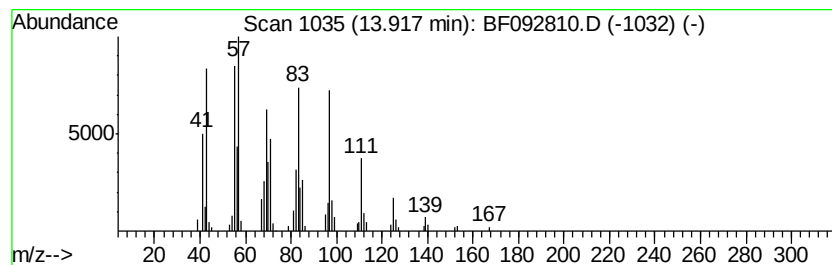
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.68 ng	245463	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		11-Tricosene	322	C23H46	052078-56-5	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF020617\
Data File : BF092810.D
Acq On : 6 Feb 2017 21:54
Operator : SJ/MA
Sample : I1706-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SCW-COMP-04

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
unknown3.31	3.31	3.3	ng	145902	1	6.91	877510	20.0
2-Pentanone, 4-hy...	5.12	108.3	ng	4751190	1	6.91	877510	20.0
Ethanol, 2,2'-oxy...	6.45	4.4	ng	192921	1	6.91	877510	20.0
unknown6.68	6.68	52.8	ng	2317240	1	6.91	877510	20.0
Triethylene glycol	8.34	4.3	ng	240927	2	8.19	1131810	20.0
1-Docosene	13.92	3.7	ng	245463	5	14.08	1335700	20.0