

Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
 Data File : BF092809.D
 Acq On : 6 Feb 2017 21:27
 Operator : SJ/MA
 Sample : I1706-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-SCW-COMP-02

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	105	107	121	rBV4	30369	113660	2.16%	0.306%
2	4.773	233	235	244	rBV	36519	77705	1.48%	0.209%
3	5.116	260	265	268	rBV	2961017	5254515	100.00%	14.158%
4	5.516	298	300	303	rBV	1217884	1444109	27.48%	3.891%
5	6.453	379	382	386	rBV	87575	146845	2.79%	0.396%
6	6.556	388	391	393	rBV	2265216	3129301	59.55%	8.431%
7	6.682	399	402	404	rBV	2336531	2167106	41.24%	5.839%
8	6.910	420	422	424	rBV	1055759	864258	16.45%	2.329%
9	7.070	433	436	438	rBV	2785469	2756798	52.47%	7.428%
10	7.470	468	471	474	rBV	1551054	2199435	41.86%	5.926%
11	8.190	532	534	539	rBV2	903394	1422806	27.08%	3.834%
12	8.339	544	547	563	rVB	97936	212536	4.04%	0.573%
13	8.910	595	597	598	rBV	90074	94536	1.80%	0.255%
14	9.002	603	605	608	rVB	63604	66682	1.27%	0.180%
15	9.276	626	629	631	rBV	3116678	3727037	70.93%	10.042%
16	9.608	655	658	661	rBV	33918	54260	1.03%	0.146%
17	9.665	661	663	665	rVB	1063462	947761	18.04%	2.554%
18	9.813	673	676	677	rBV	56908	59210	1.13%	0.160%
19	9.870	677	681	683	rBV2	39755	73279	1.39%	0.197%
20	9.950	685	688	690	rBV	1515998	1326267	25.24%	3.573%
21	10.156	703	706	708	rVB	48333	52772	1.00%	0.142%
22	10.373	721	725	727	rBV2	48326	101437	1.93%	0.273%
23	10.499	734	736	738	rVB	89701	97174	1.85%	0.262%
24	10.739	754	757	759	rBV	1085852	1059755	20.17%	2.855%
25	10.853	764	767	770	rBV	106655	127003	2.42%	0.342%
26	11.299	803	806	807	rBV	139419	129376	2.46%	0.349%
27	11.436	815	818	819	rBV	1807556	1578048	30.03%	4.252%
28	11.505	822	824	826	rVB	50134	86122	1.64%	0.232%
29	11.665	835	838	842	rBV2	36076	61643	1.17%	0.166%
30	11.722	842	843	846	rVB	91455	101727	1.94%	0.274%
31	12.054	870	872	876	rVB2	48904	81506	1.55%	0.220%
32	12.134	876	879	881	rBV	63478	65230	1.24%	0.176%
33	12.648	922	924	926	rBV	195526	166835	3.18%	0.450%
34	12.876	939	944	946	rBV	226021	231003	4.40%	0.622%

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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

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35	13.025	954	957	959	rBV	3793947	3771197	71.77%	10.161%
36	13.917	1033	1035	1043	rVB	151043	221897	4.22%	0.598%
37	14.077	1046	1049	1051	rBV	1477514	1454039	27.67%	3.918%
38	14.545	1087	1090	1094	rBV3	22414	62770	1.19%	0.169%
39	15.105	1137	1139	1143	rBV	31997	65881	1.25%	0.178%
40	15.174	1143	1145	1147	rBV	49281	54575	1.04%	0.147%
41	15.528	1173	1176	1182	rBV	845902	1165555	22.18%	3.140%
42	15.974	1212	1215	1219	rBV	57508	88773	1.69%	0.239%
43	16.465	1255	1258	1266	rBV2	46800	91880	1.75%	0.248%
44	17.048	1305	1309	1313	rVB	26583	60302	1.15%	0.162%

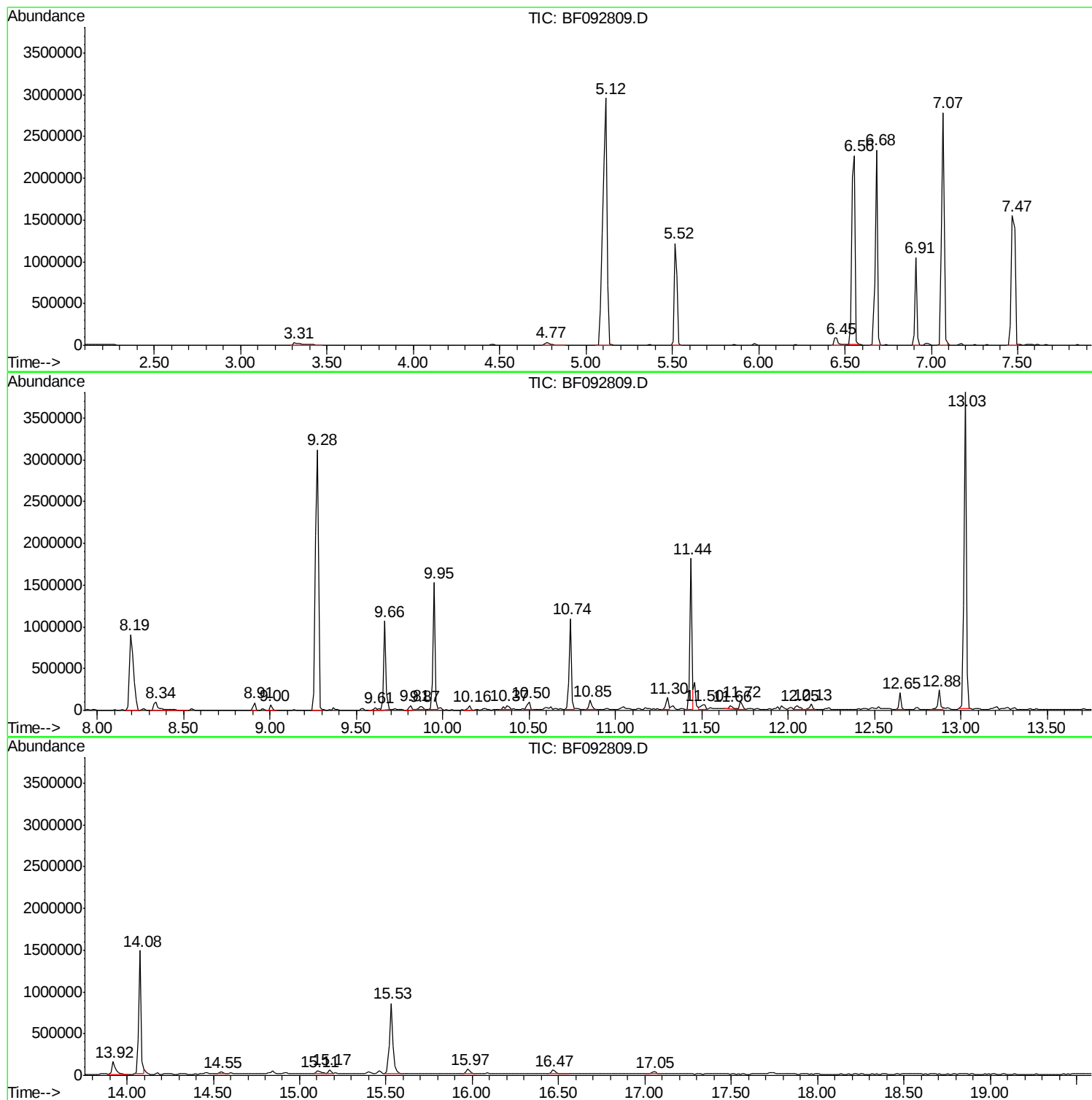
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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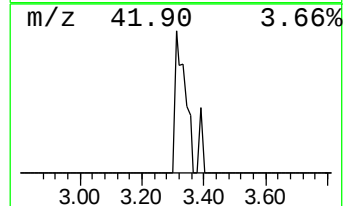
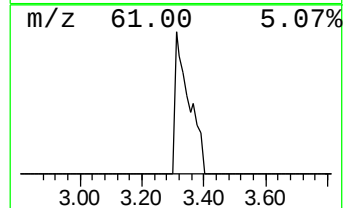
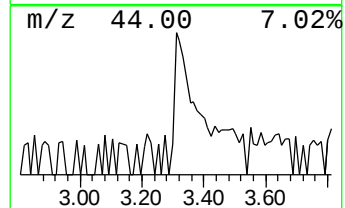
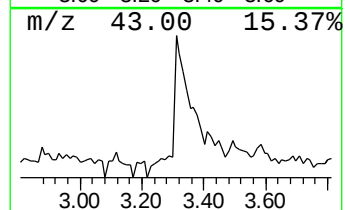
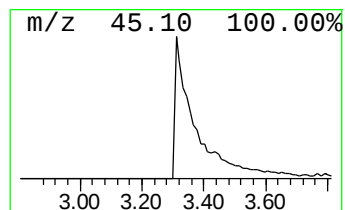
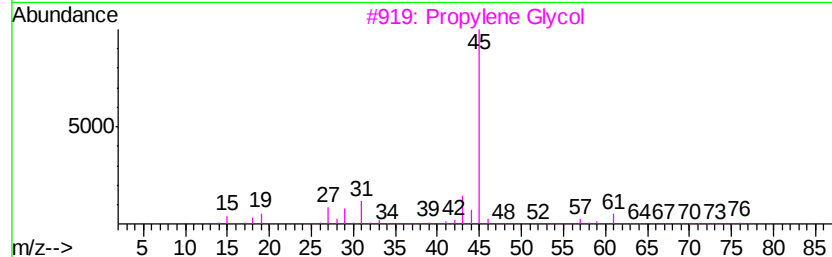
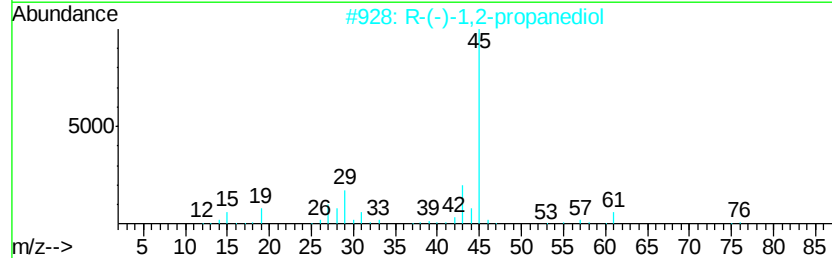
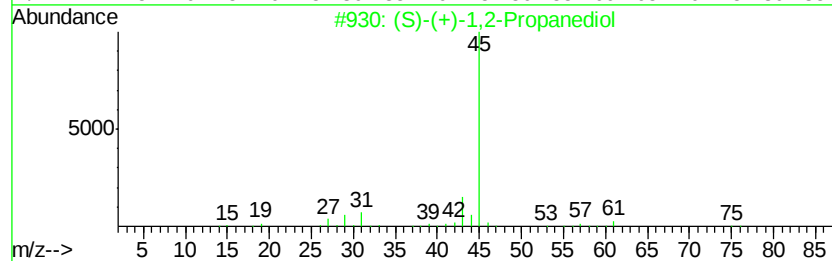
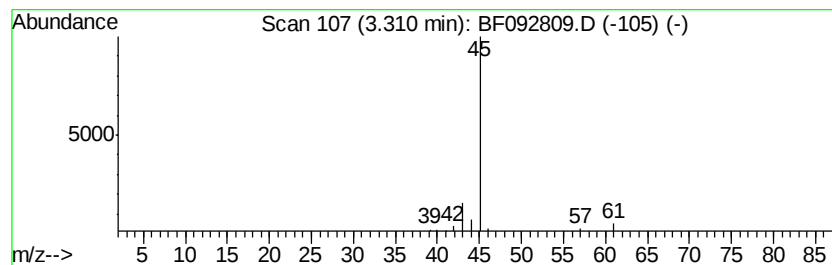
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	2.63 ng	113660	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3			Propylene Glycol	76	C3H8O2	000057-55-6	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Formamide	45	CH3NO	000075-12-7	7



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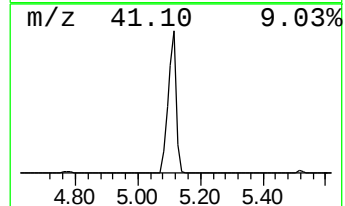
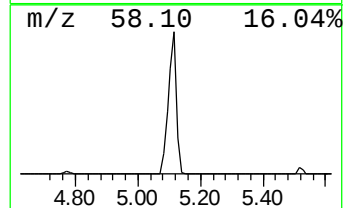
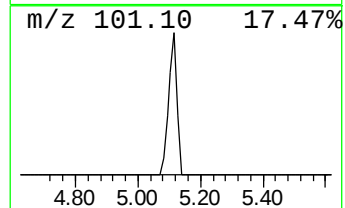
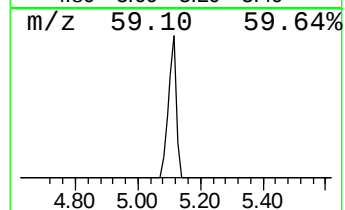
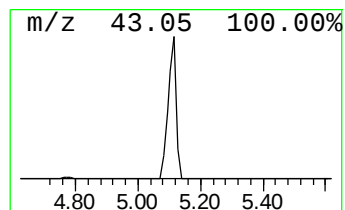
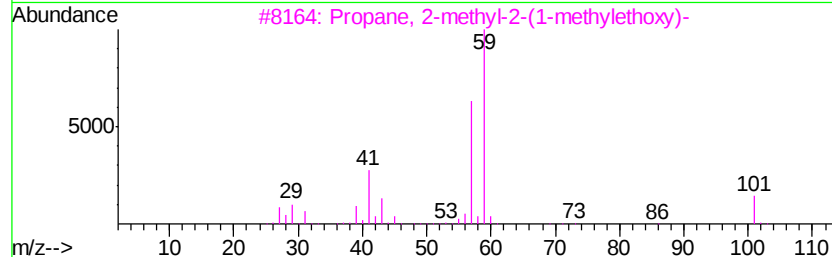
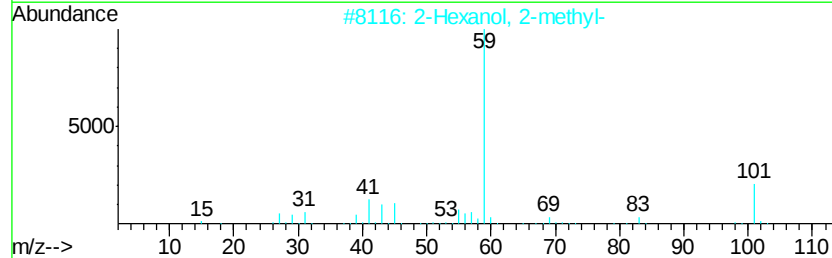
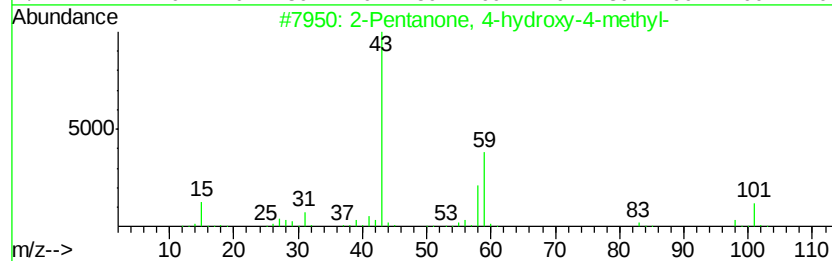
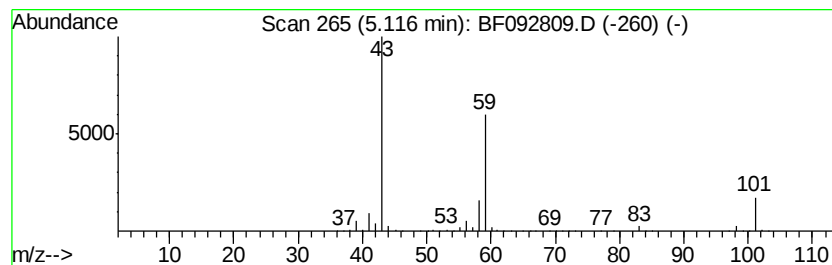
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.12	121.60 ng	5254520	1,4-Dichlorobenzene-d4	6.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32



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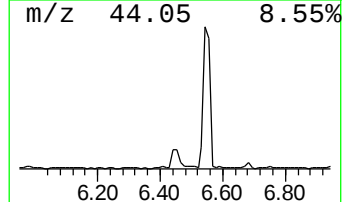
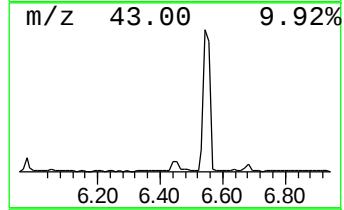
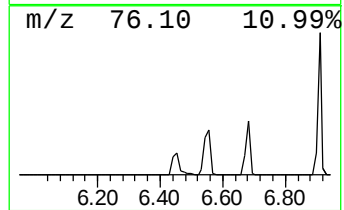
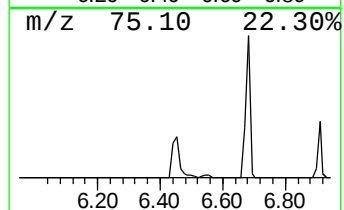
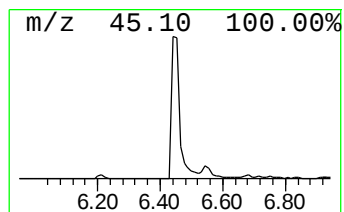
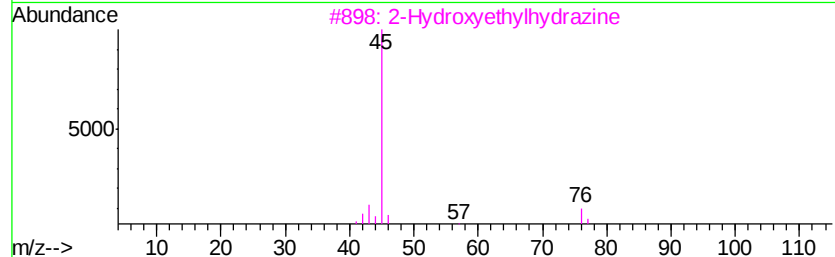
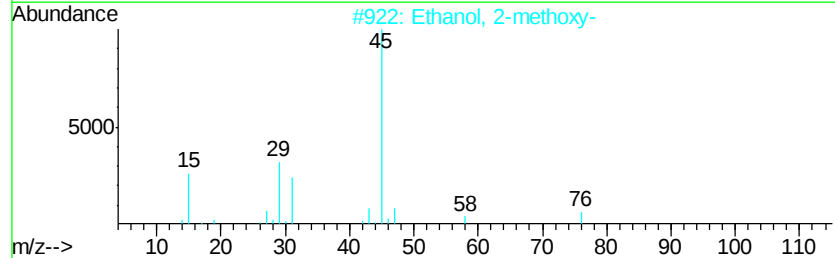
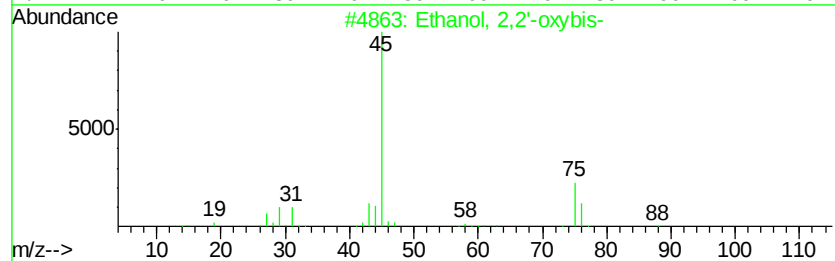
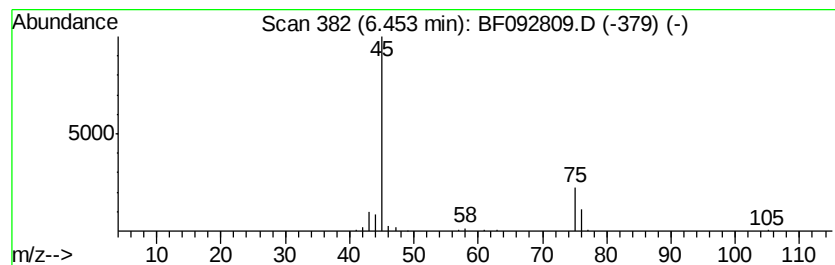
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.45	3.40 ng	146845	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	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
3	2-Hydroxyethylhydrazine	76	C2H8N2O	000109-84-2	9
4	Ethanol, 2-(2-hydroxyethoxy)-, 1...	151	C4H9NO5	020633-16-3	9
5	2-Propanol, 1,3-dimethoxy-	120	C5H12O3	000623-69-8	9



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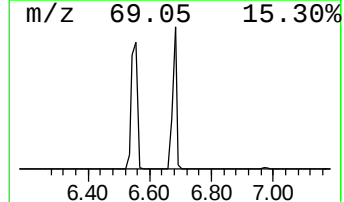
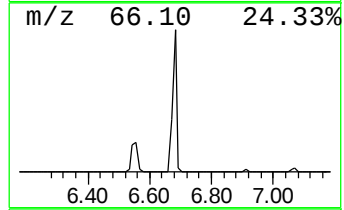
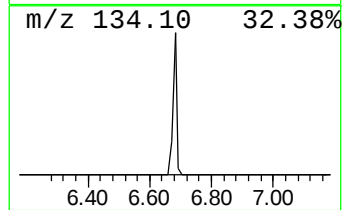
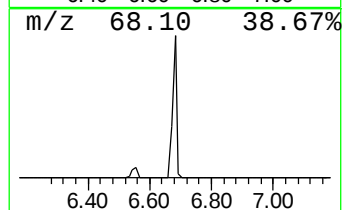
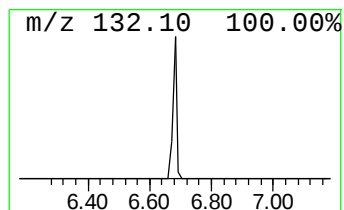
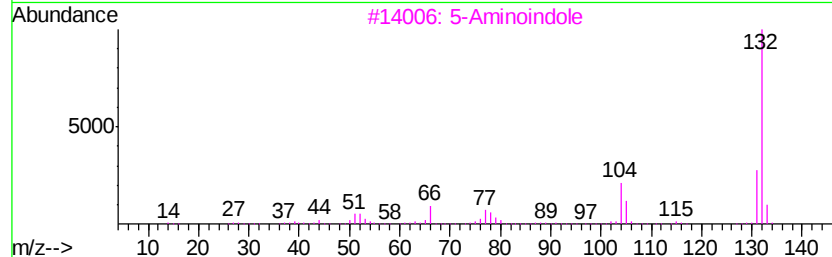
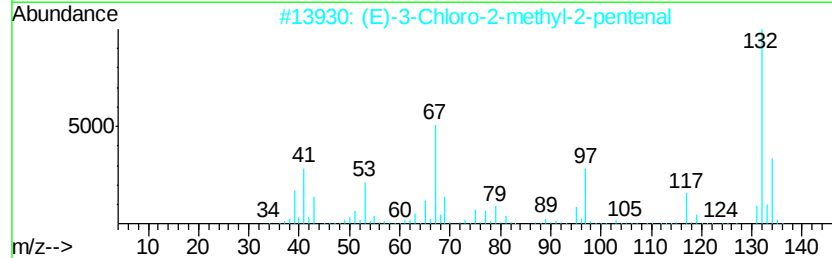
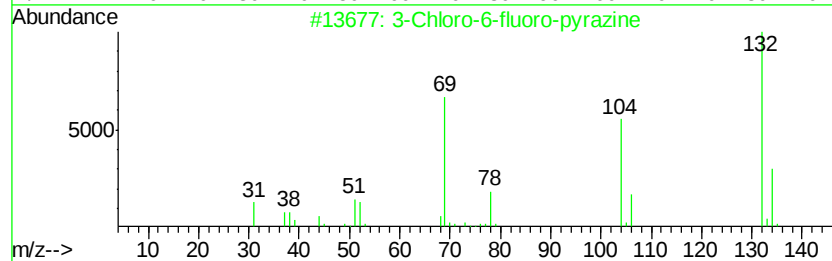
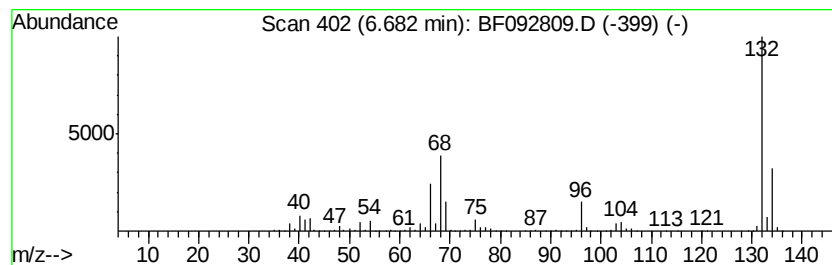
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	50.15 ng	2167110	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
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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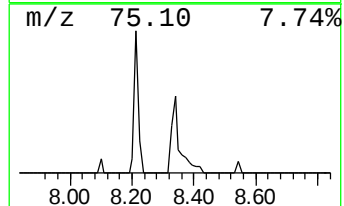
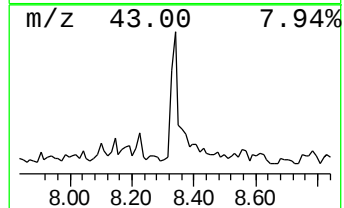
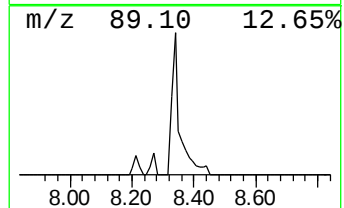
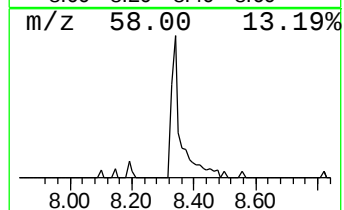
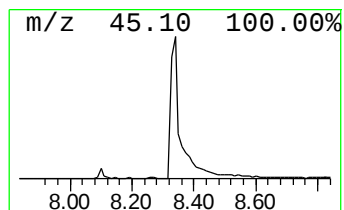
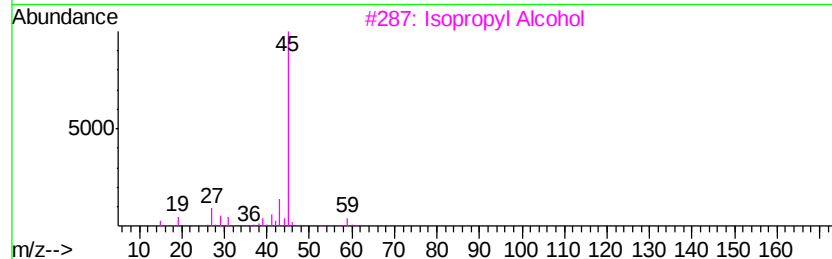
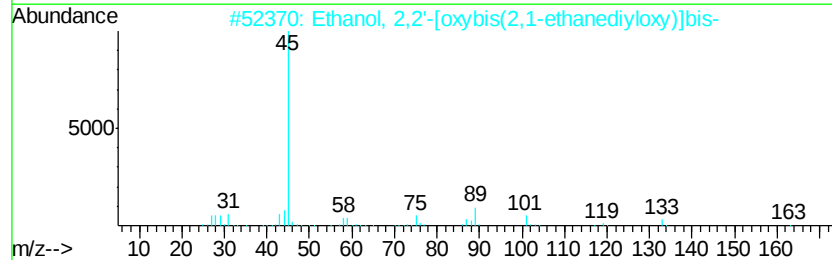
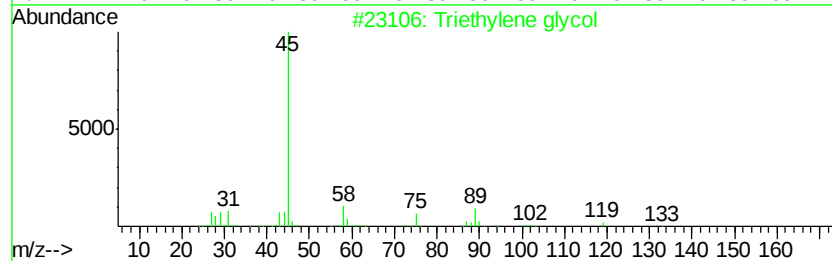
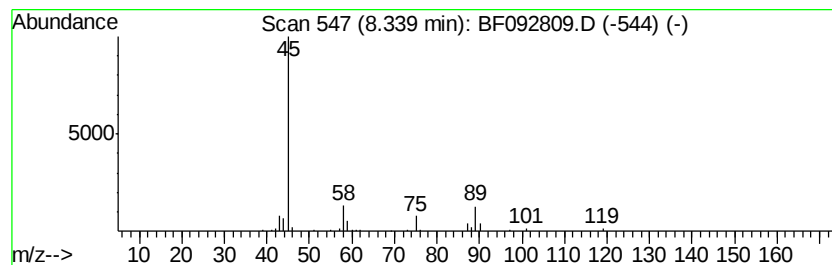
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	2.99 ng	212536	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		Isopropyl Alcohol	60	C3H8O	000067-63-0	42
4		Pentaethylene glycol	238	C10H22O6	004792-15-8	38
5		Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	25



Data Path : Z:\HPCHEM1\BNA F\Data\BF020617\
Data File : BF092809.D
Acq On : 6 Feb 2017 21:27
Operator : SJ/MA
Sample : I1706-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SCW-COMP-02

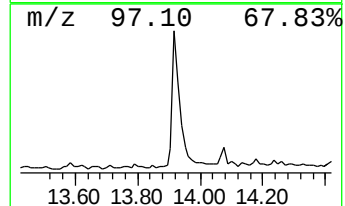
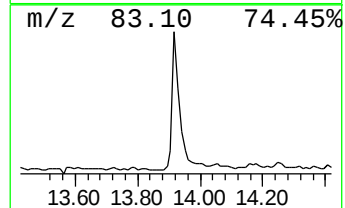
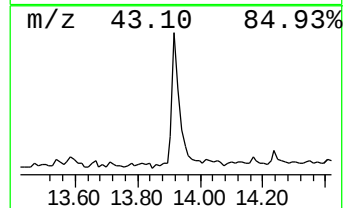
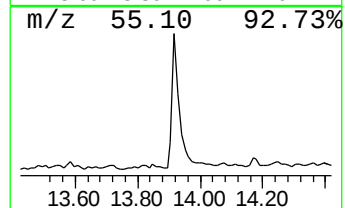
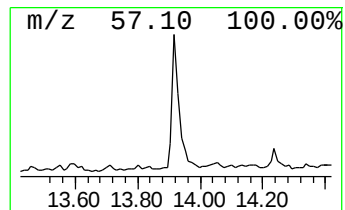
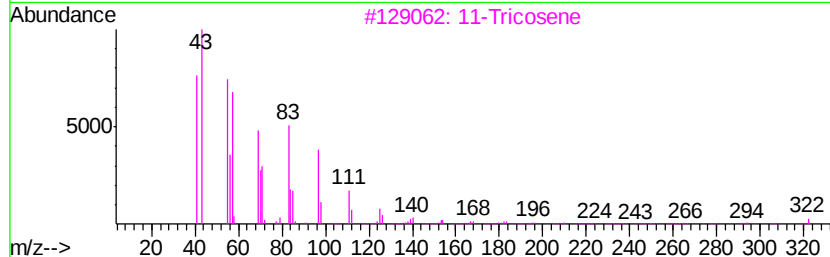
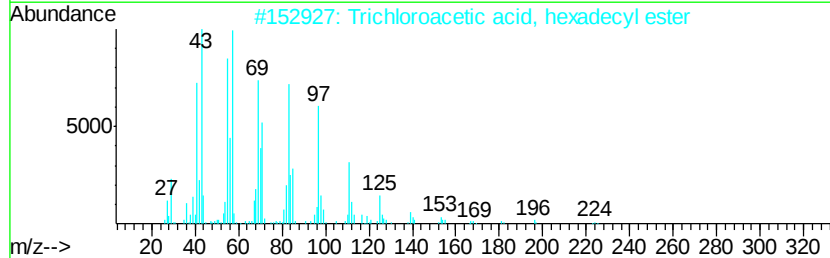
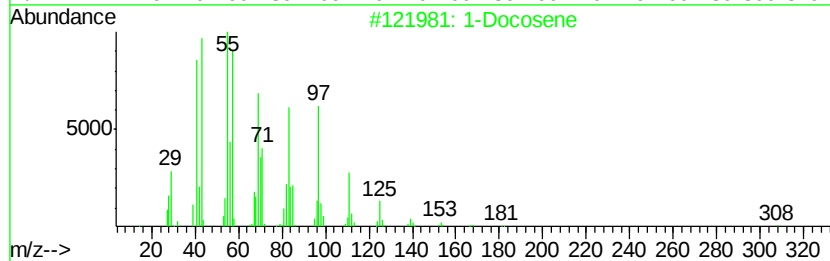
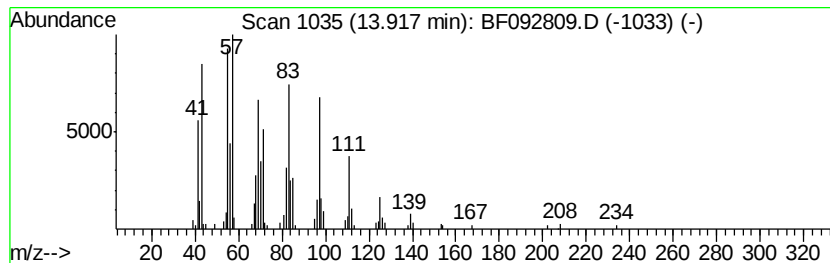
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.05 ng	221897	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		11-Tricosene	322	C23H46	052078-56-5	91
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	87



Data Path : Z:\HPCHEM1\BNA_F\Data\BF020617\
Data File : BF092809.D
Acq On : 6 Feb 2017 21:27
Operator : SJ/MA
Sample : I1706-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SCW-COMP-02

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
(S)-(+)-1,2-Propa...	3.31	2.6	ng	113660	1	6.91	864258	20.0
2-Pentanone, 4-hy...	5.12	121.6	ng	5254520	1	6.91	864258	20.0
Ethanol, 2,2'-oxy...	6.45	3.4	ng	146845	1	6.91	864258	20.0
unknown6.68	6.68	50.1	ng	2167110	1	6.91	864258	20.0
Triethylene glycol	8.34	3.0	ng	212536	2	8.19	1422810	20.0
1-Docosene	13.92	3.0	ng	221897	5	14.08	1454040	20.0