

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
 Data File : BF088624.D
 Acq On : 2 Jul 2016 18:37
 Operator : UM/SJ
 Sample : H3847-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B4(0-11)C

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-BF063016.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	1.861	21	24	33	rVB	77808	138154	5.21%	0.603%
2	2.993	121	123	130	rBV	49627	90198	3.40%	0.393%
3	4.284	233	236	239	rVB	22809	30687	1.16%	0.134%
4	4.958	292	295	299	rBV	169141	213309	8.04%	0.930%
5	5.381	329	332	335	rBV	1867774	2348740	88.53%	10.243%
6	6.433	420	424	426	rVB	1793503	2653189	100.00%	11.571%
7	6.559	432	435	437	rBV	2513909	2358606	88.90%	10.286%
8	6.787	453	455	458	rBV	584706	721922	27.21%	3.148%
9	6.947	467	469	472	rVB	1960105	1842000	69.43%	8.033%
10	7.359	502	505	507	rBV	1771755	1739973	65.58%	7.588%
11	7.450	510	513	516	rBB	26354	28824	1.09%	0.126%
12	8.079	565	568	570	rBV	1179213	967640	36.47%	4.220%
13	9.153	660	662	665	rBV	2383741	2409632	90.82%	10.509%
14	9.553	694	697	699	rBV	589000	569412	21.46%	2.483%
15	9.828	719	721	723	rBV	1084231	935846	35.27%	4.081%
16	10.616	787	790	792	rBV	1130866	1320701	49.78%	5.760%
17	10.650	792	793	796	rVB	41040	39853	1.50%	0.174%
18	10.742	800	801	805	rVV	39734	43088	1.62%	0.188%
19	11.188	838	840	842	rBV	84398	82314	3.10%	0.359%
20	11.302	848	850	853	rBV	774769	755184	28.46%	3.294%
21	11.371	853	856	860	rVB2	25464	56438	2.13%	0.246%
22	11.542	869	871	876	rVB	24500	40363	1.52%	0.176%
23	11.611	876	877	880	rVB	49197	64036	2.41%	0.279%
24	11.839	895	897	899	rBV	26020	26556	1.00%	0.116%
25	12.514	954	956	958	rBV	58176	57924	2.18%	0.253%
26	12.731	972	975	978	rBV	34369	55649	2.10%	0.243%
27	12.891	987	989	991	rBV	1755299	1572484	59.27%	6.858%
28	13.794	1065	1068	1075	rBV2	95026	137712	5.19%	0.601%
29	13.931	1077	1080	1082	rBV	798488	741700	27.96%	3.235%
30	14.788	1153	1155	1157	rVB	37498	37556	1.42%	0.164%
31	14.937	1165	1168	1172	rBV	33431	76504	2.88%	0.334%
32	15.268	1195	1197	1199	rBV	25191	29714	1.12%	0.130%
33	15.325	1199	1202	1205	rBV	507685	657312	24.77%	2.867%
34	15.828	1244	1246	1251	rVB5	11675	29853	1.13%	0.130%

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ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
S4-B4(0-11)C

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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35	15.988	1258	1260	1267	rVB6	11793	28773	1.08%	0.125%
36	19.108	1531	1533	1539	rVB5	9905	27444	1.03%	0.120%

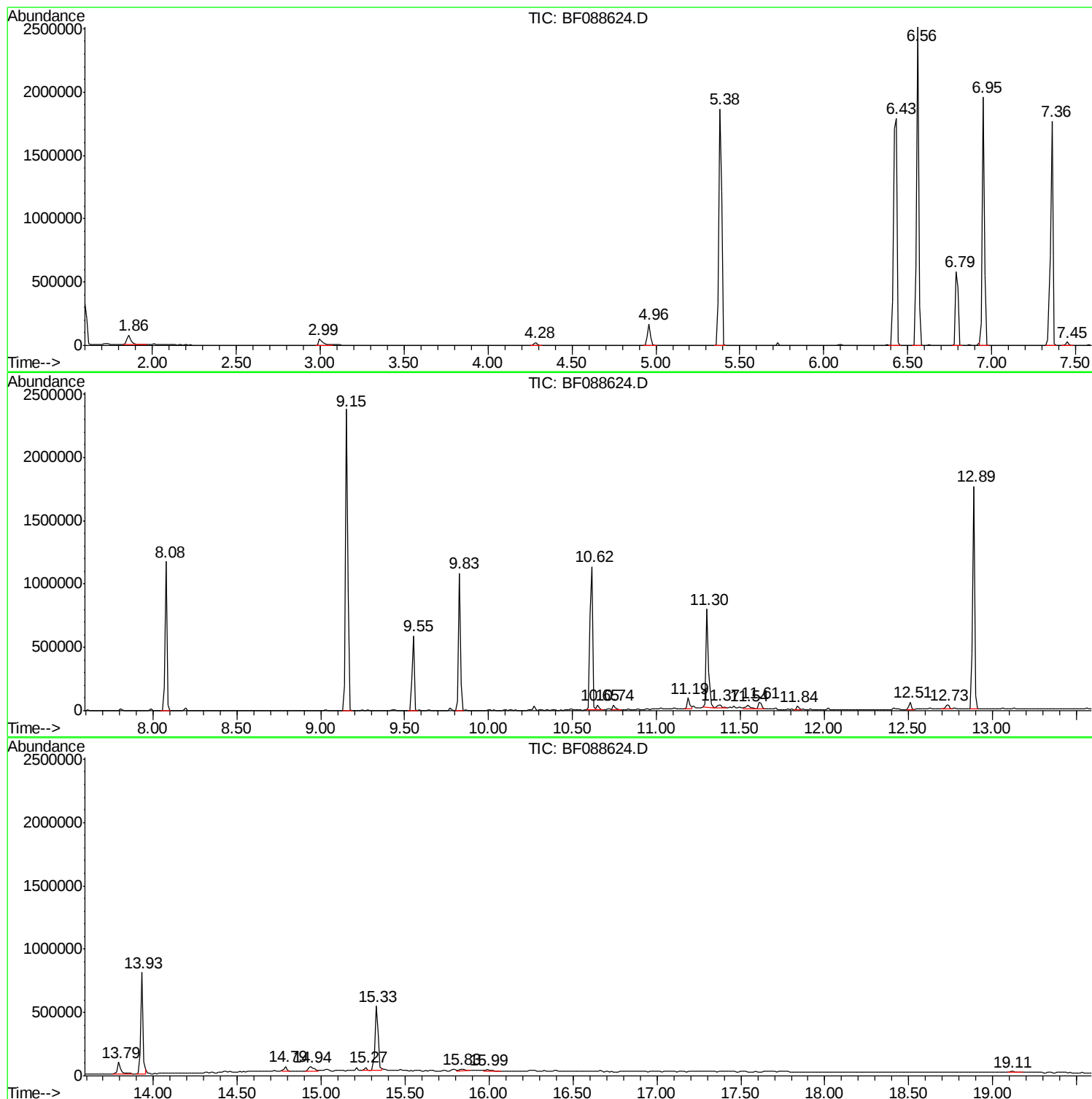
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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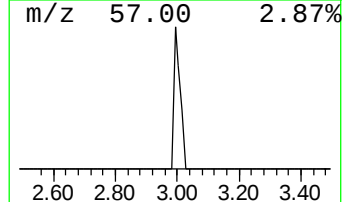
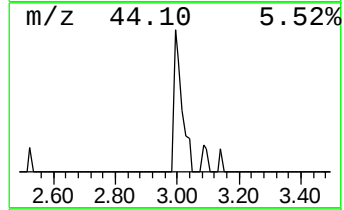
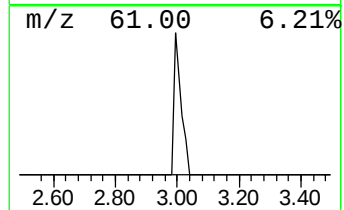
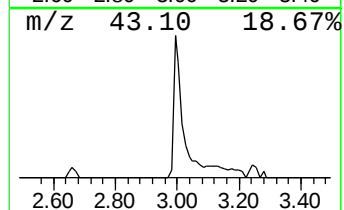
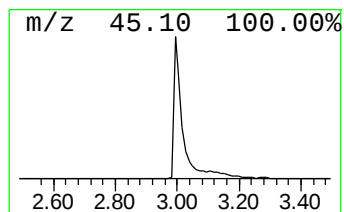
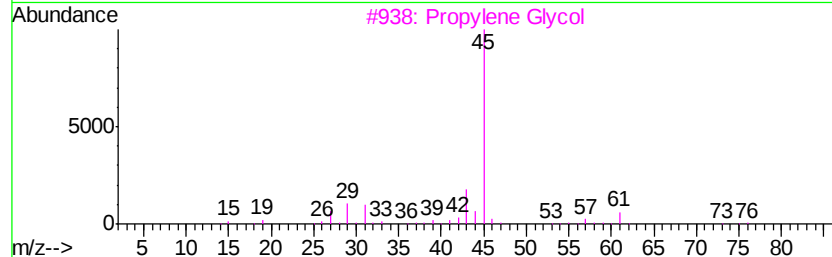
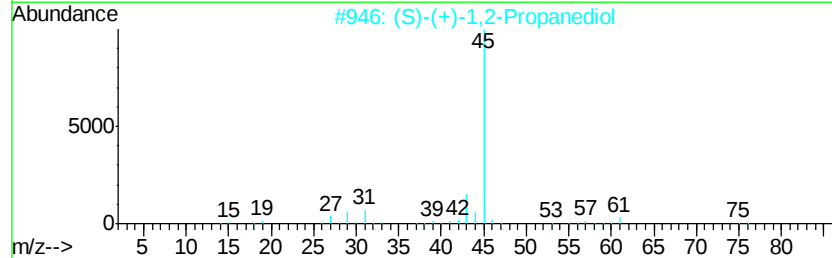
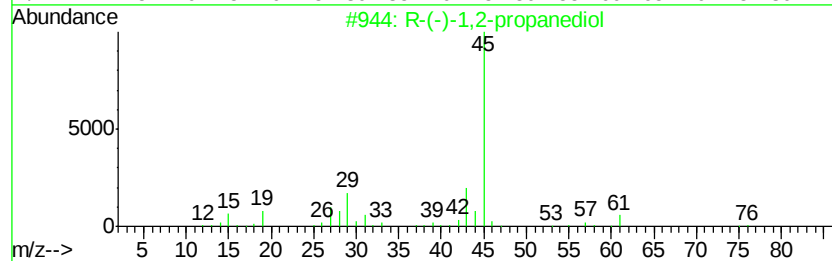
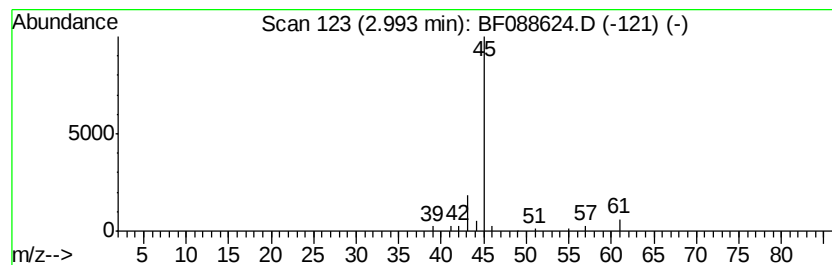
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	2.50 ng	90198	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5		Formamide	45	CH3NO	000075-12-7	7



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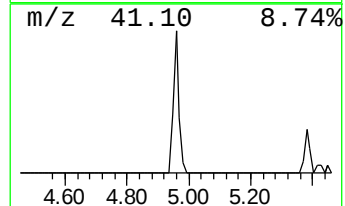
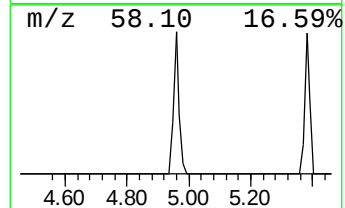
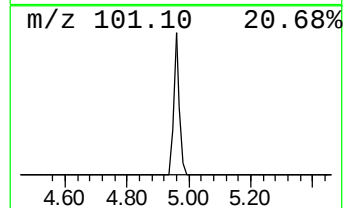
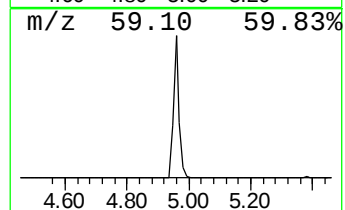
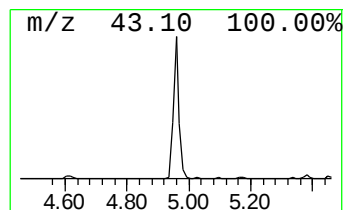
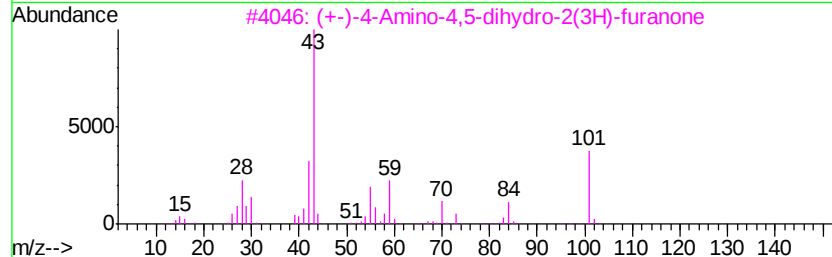
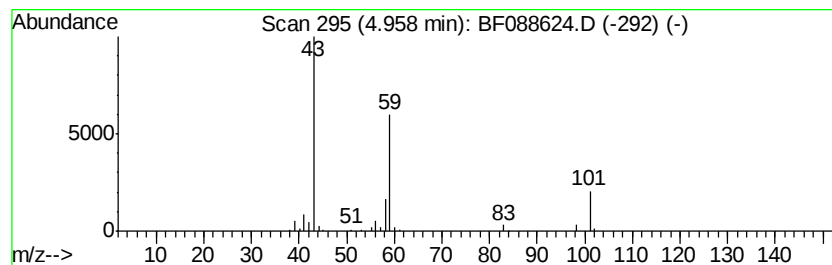
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	5.91 ng	213309	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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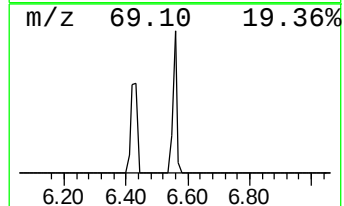
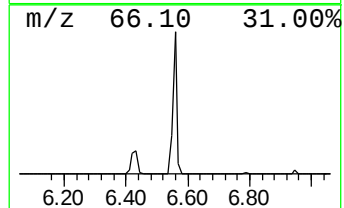
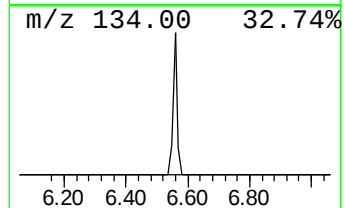
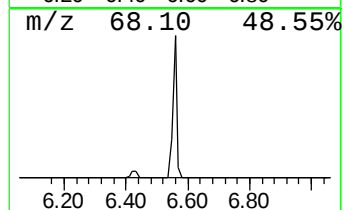
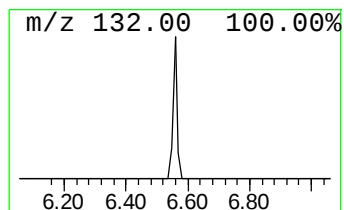
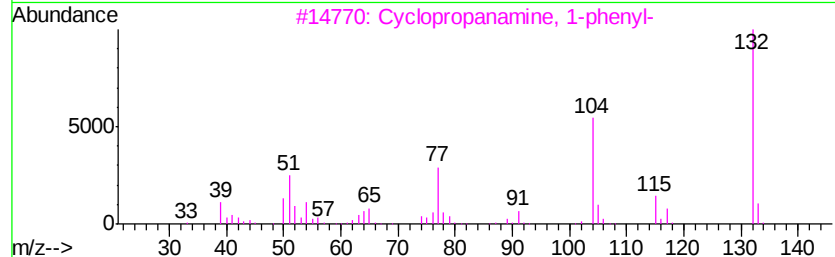
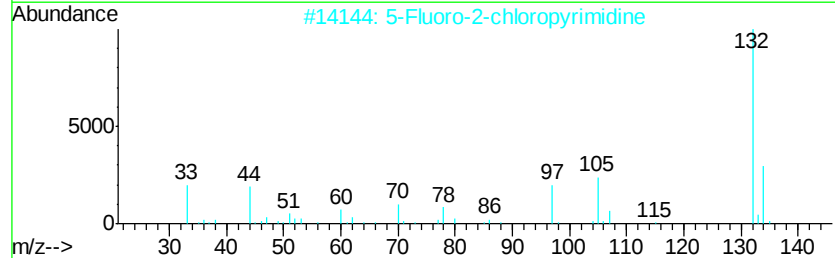
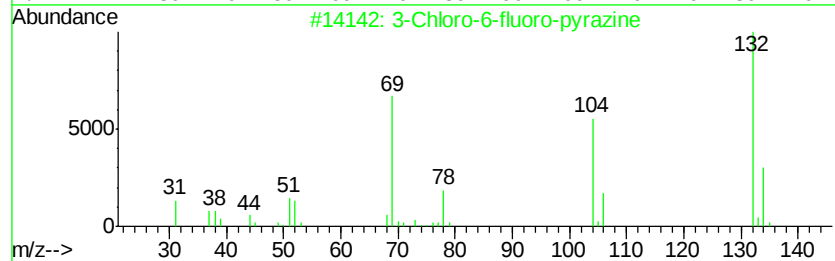
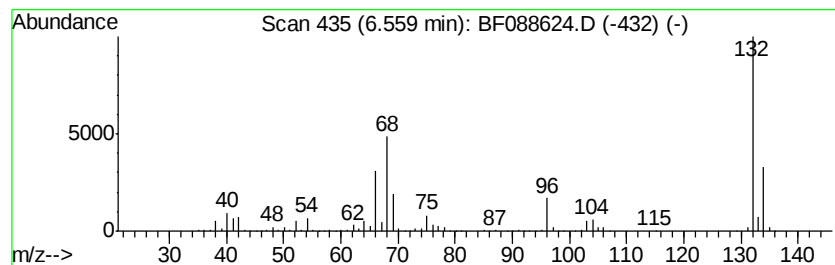
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	65.34 ng	2358610	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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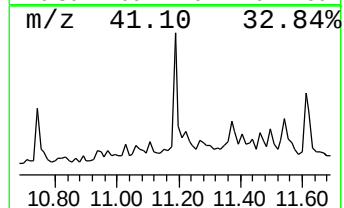
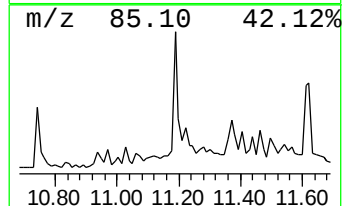
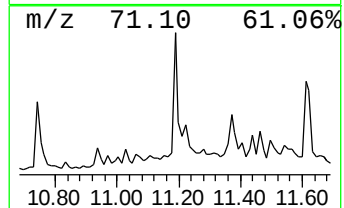
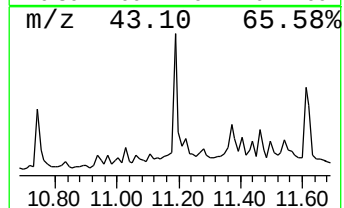
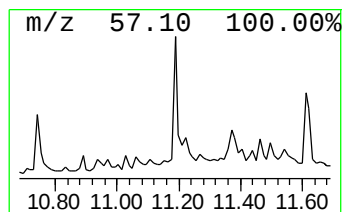
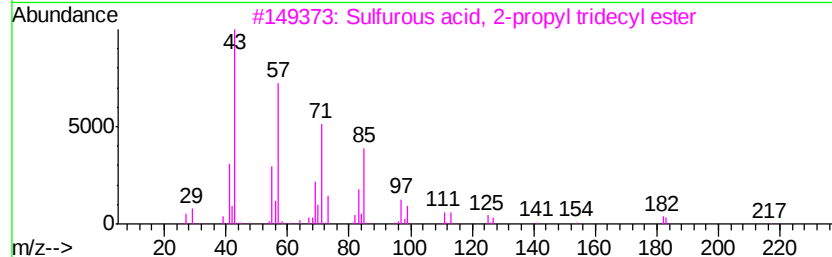
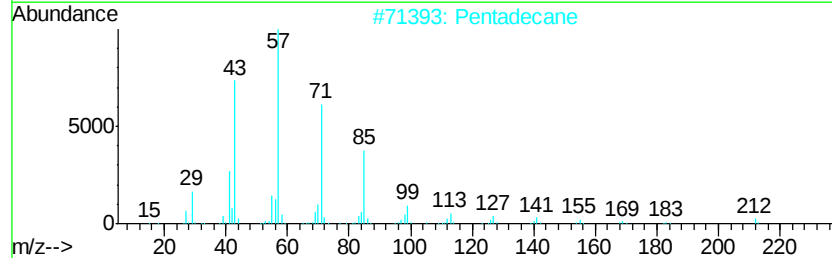
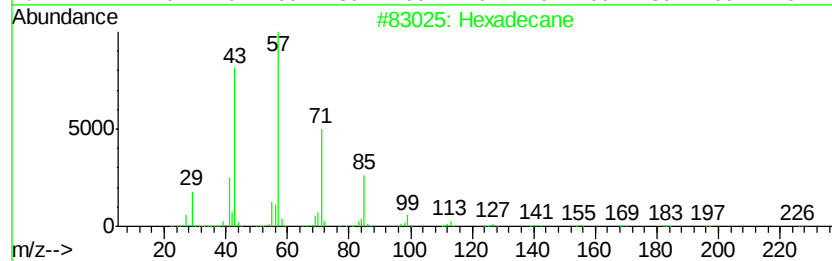
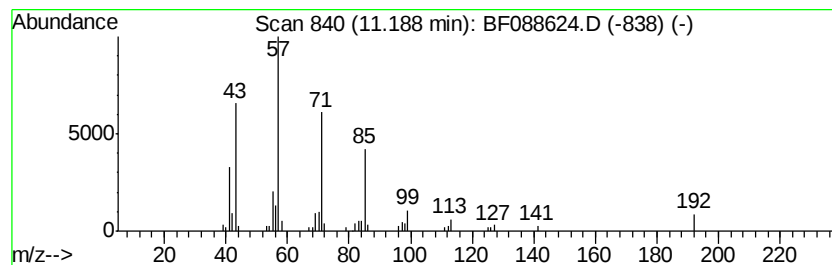
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.18 ng	82314	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Pentadecane		212	C15H32	000629-62-9	86
3	Sulfurous acid, 2-propyl tridecy...		306	C16H34O3S	1000309-12-4	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Tetradecane		198	C14H30	000629-59-4	86



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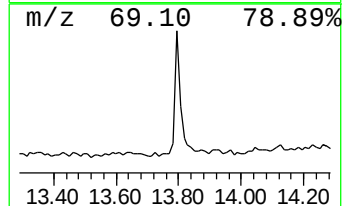
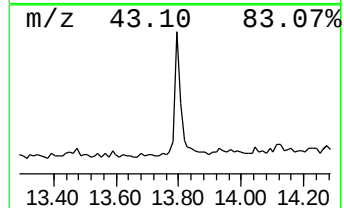
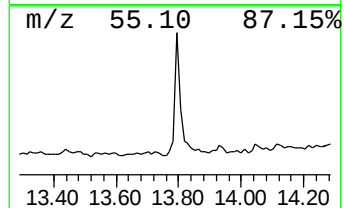
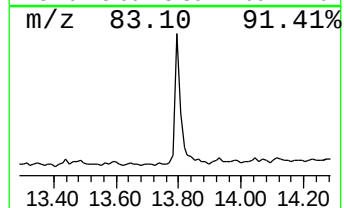
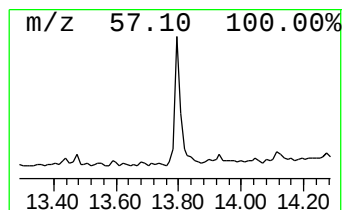
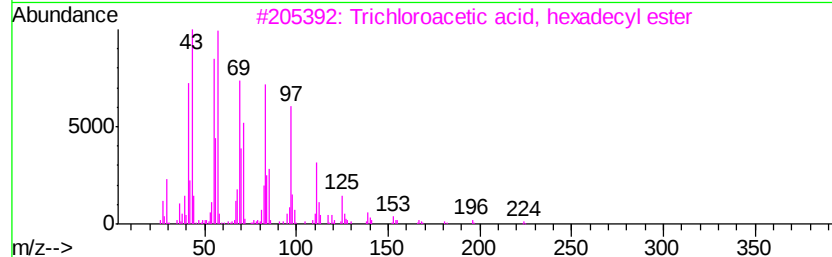
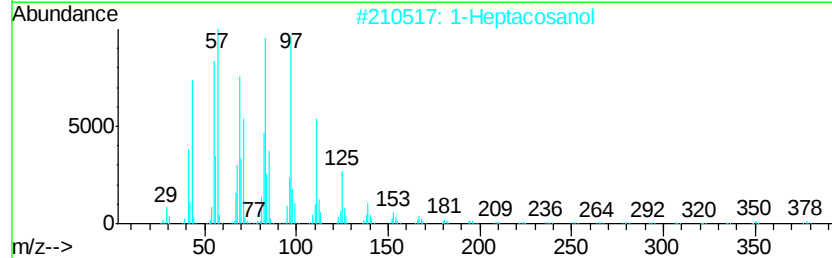
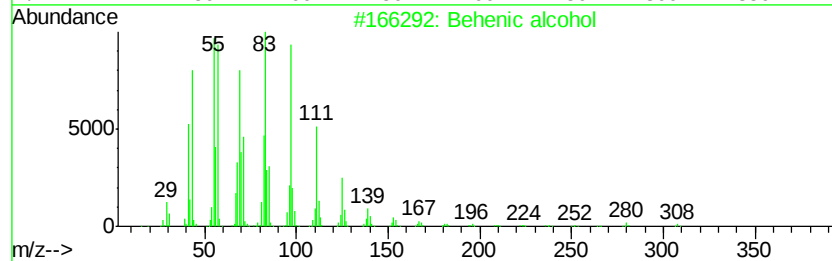
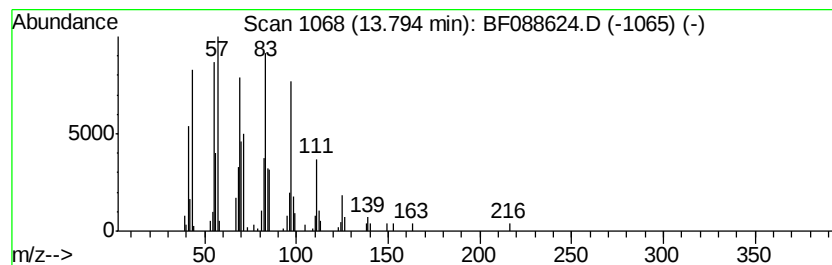
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.71 ng	137712	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	94
2		1-Heptacosanol	396	C27H56O	002004-39-9	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
R-(-)-1,2-propane...	2.99	2.5	ng	90198	1	6.80	721922	20.0
2-Pentanone, 4-hy...	4.96	5.9	ng	213309	1	6.80	721922	20.0
unknown6.56	6.56	65.3	ng	2358610	1	6.80	721922	20.0
Hexadecane	11.19	2.2	ng	82314	4	11.30	755184	20.0
Behenic alcohol	13.79	3.7	ng	137712	5	13.93	741700	20.0