

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
 Data File : BF093202.D
 Acq On : 27 Feb 2017 12:10
 Operator : SJ/MA
 Sample : I1973-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-B1-B2-BASE-7

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	4.990	251	254	264	rVB	1208706	1682655	42.23%	4.344%
2	5.424	290	292	295	rBV	3204997	3353288	84.15%	8.657%
3	6.476	381	384	387	rBV	3449934	3894943	97.75%	10.055%
4	6.602	392	395	397	rBV	3194869	3837134	96.30%	9.906%
5	6.830	412	415	417	rBV	785235	953912	23.94%	2.463%
6	6.979	426	428	431	rBV	2312427	2695771	67.65%	6.959%
7	7.402	462	465	467	rBV	2527971	2610169	65.50%	6.738%
8	8.122	525	528	530	rBV	1412112	1359827	34.13%	3.510%
9	9.208	620	623	625	rBV	3678193	3984700	100.00%	10.287%
10	9.608	655	658	660	rBV	625623	784870	19.70%	2.026%
11	9.813	674	676	678	rBV	69661	62124	1.56%	0.160%
12	9.882	679	682	684	rVV	1622358	1438738	36.11%	3.714%
13	10.019	692	694	699	rBV	541336	552714	13.87%	1.427%
14	10.293	715	718	719	rBV	36158	57197	1.44%	0.148%
15	10.316	719	720	721	rVB	96114	66368	1.67%	0.171%
16	10.533	737	739	742	rBV	32971	44742	1.12%	0.116%
17	10.671	749	751	754	rBV2	1503782	2022168	50.75%	5.220%
18	10.785	760	761	766	rVB	127820	150327	3.77%	0.388%
19	11.231	798	800	802	rBV	113906	113328	2.84%	0.293%
20	11.368	810	812	814	rBV	1648355	1513637	37.99%	3.908%
21	11.448	816	819	820	rVB2	25269	45009	1.13%	0.116%
22	11.654	836	837	840	rBV	80807	99672	2.50%	0.257%
23	11.894	857	858	862	rBV3	30040	41571	1.04%	0.107%
24	11.974	864	865	869	rVB2	32291	55197	1.39%	0.142%
25	12.065	871	873	875	rVB	72496	66355	1.67%	0.171%
26	12.454	905	907	909	rBV	46952	43815	1.10%	0.113%
27	12.579	916	918	920	rVB	255278	229697	5.76%	0.593%
28	12.808	933	938	940	rBV	215274	277871	6.97%	0.717%
29	12.957	948	951	953	rVB	2454069	3191025	80.08%	8.238%
30	13.128	963	966	968	rBV	25030	57052	1.43%	0.147%
31	13.642	1007	1011	1013	rVB2	27405	42338	1.06%	0.109%
32	13.745	1017	1020	1022	rBV2	20584	45946	1.15%	0.119%
33	13.848	1026	1029	1033	rVB3	169526	317870	7.98%	0.821%
34	13.997	1038	1042	1044	rBV	1044297	1387540	34.82%	3.582%

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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-BF013017.M
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35	14.157	1054	1056	1060	rBV3	28613	62169	1.56%	0.160%
36	14.465	1081	1083	1086	rBV4	31562	59499	1.49%	0.154%
37	14.831	1113	1115	1117	rVB	45989	43763	1.10%	0.113%
38	15.025	1129	1132	1135	rBV	79413	165010	4.14%	0.426%
39	15.082	1135	1137	1139	rVB2	35558	45271	1.14%	0.117%
40	15.311	1155	1157	1160	rVB	47531	58871	1.48%	0.152%
41	15.368	1160	1162	1165	rVB	64277	77643	1.95%	0.200%
42	15.425	1165	1167	1170	rBV	607957	875071	21.96%	2.259%
43	16.831	1287	1290	1292	rBV	38812	82579	2.07%	0.213%
44	17.254	1324	1327	1332	rBV	22179	55029	1.38%	0.142%
45	17.357	1333	1336	1342	rVB5	32820	86776	2.18%	0.224%
46	18.317	1416	1420	1425	rBV8	13304	45283	1.14%	0.117%

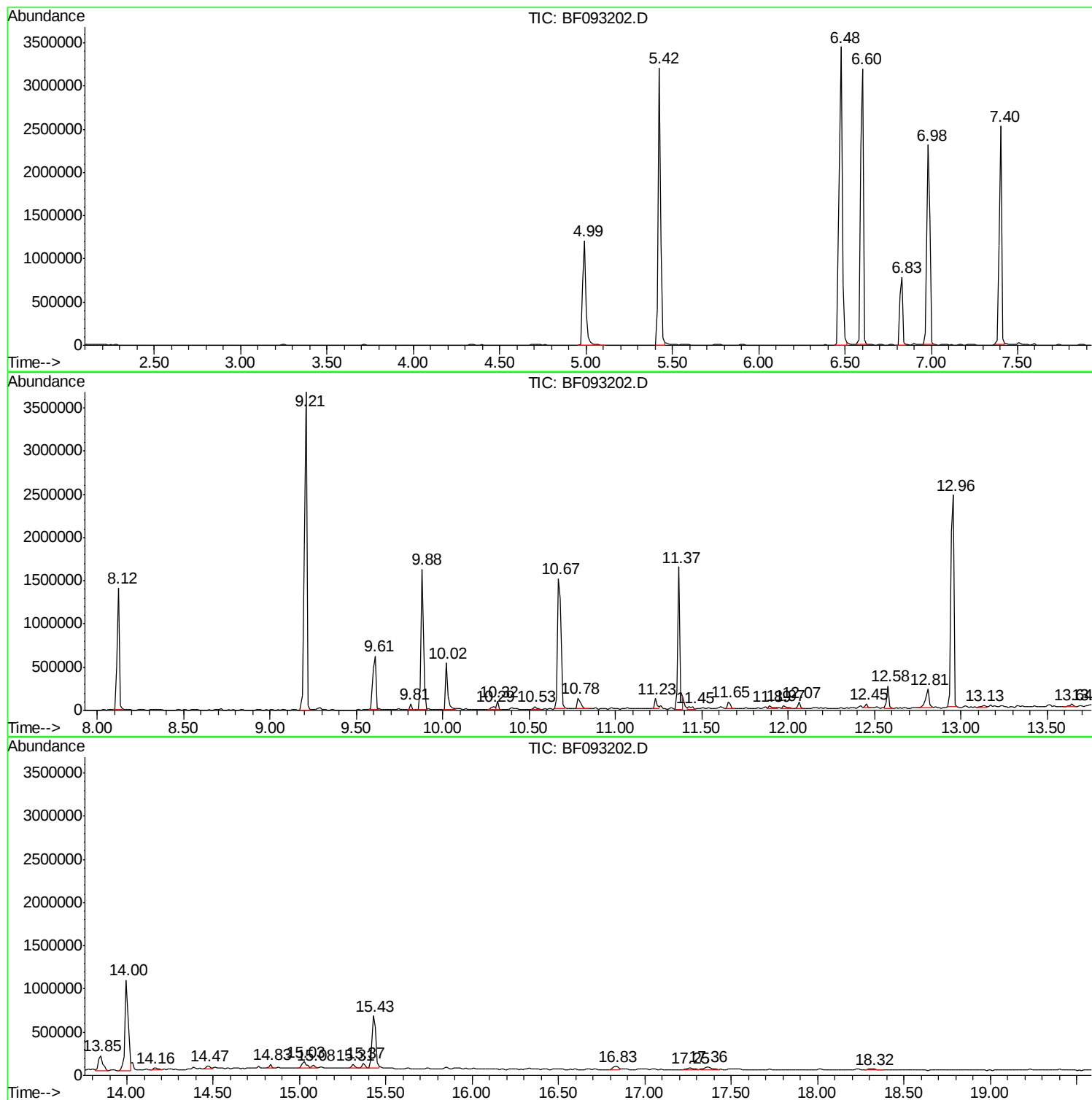
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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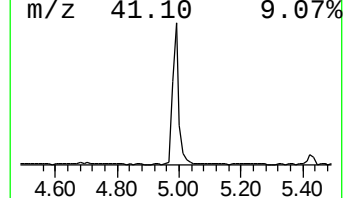
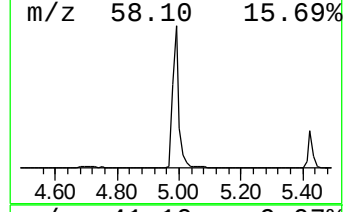
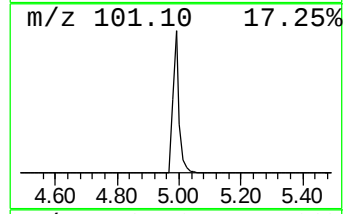
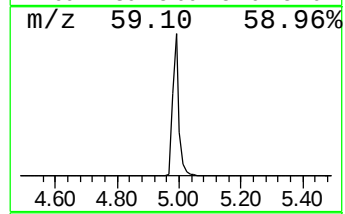
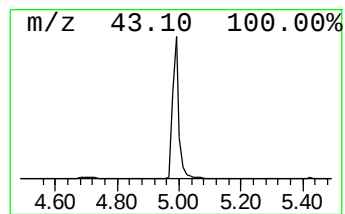
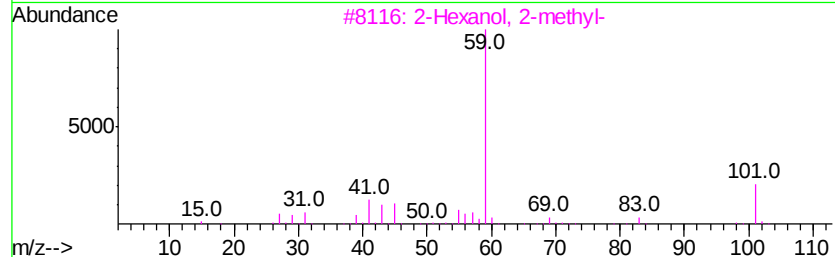
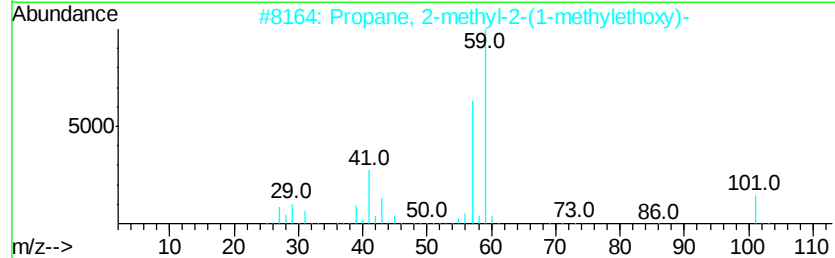
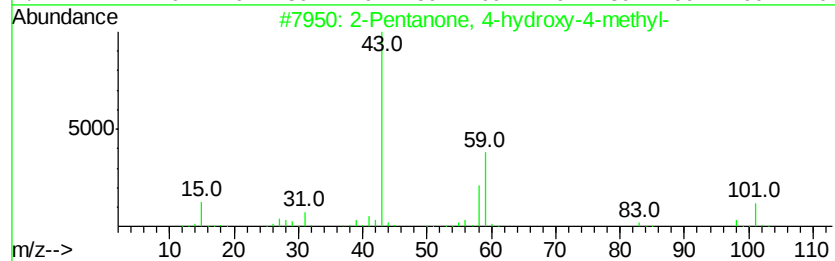
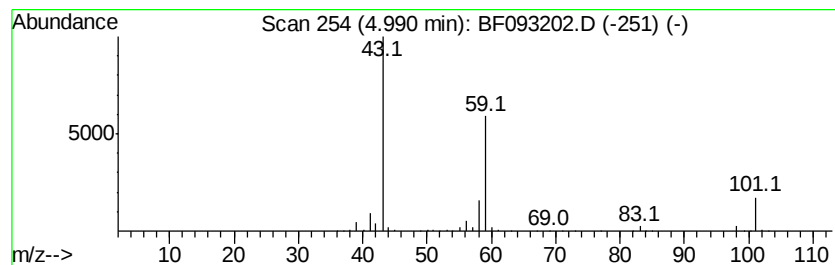
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	35.28 ng	1682660	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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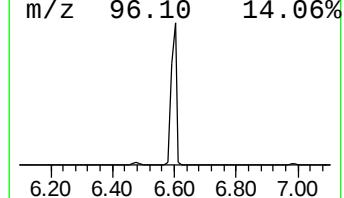
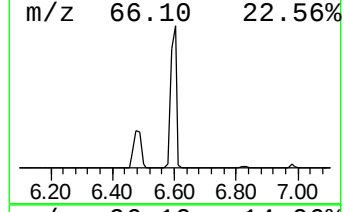
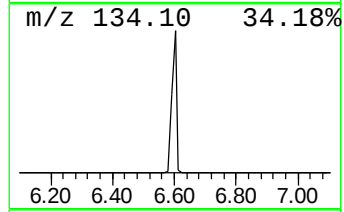
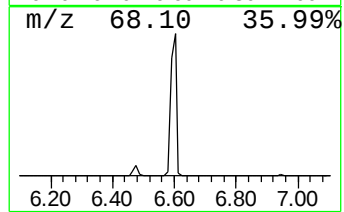
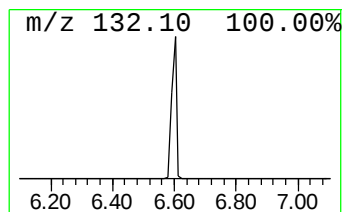
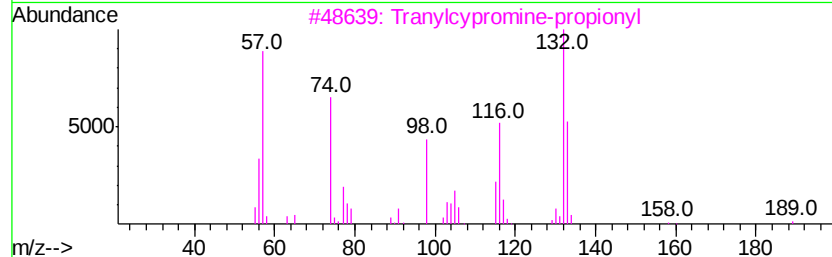
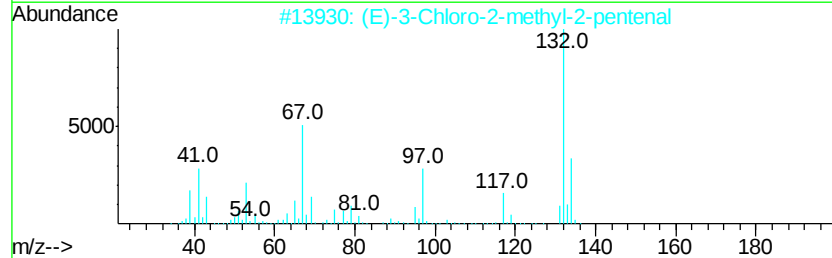
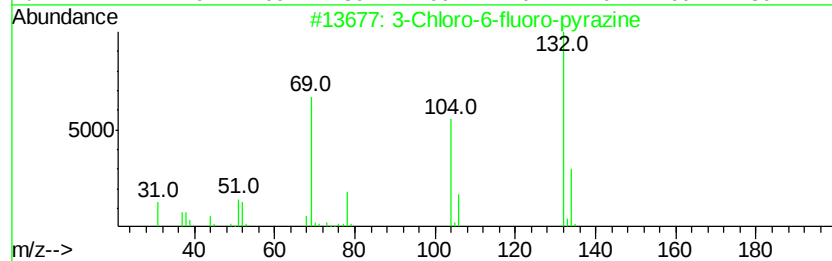
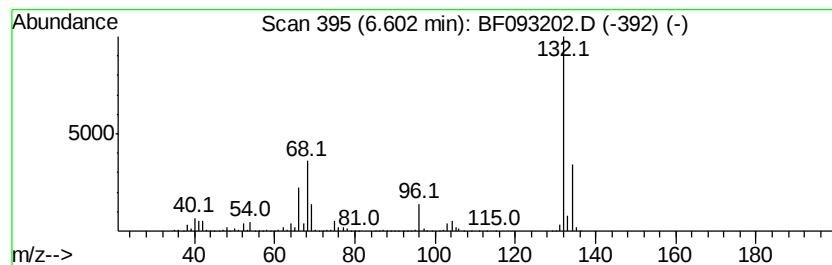
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	80.45 ng	3837130	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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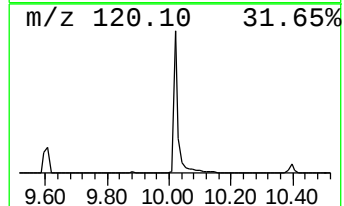
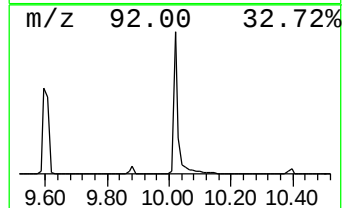
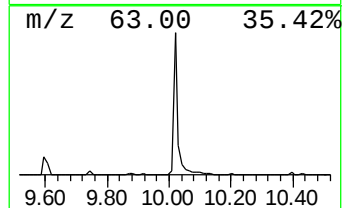
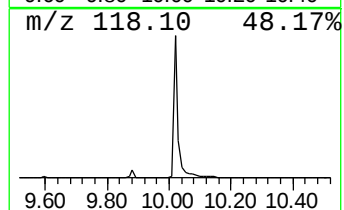
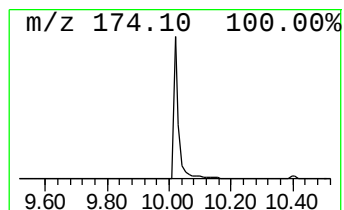
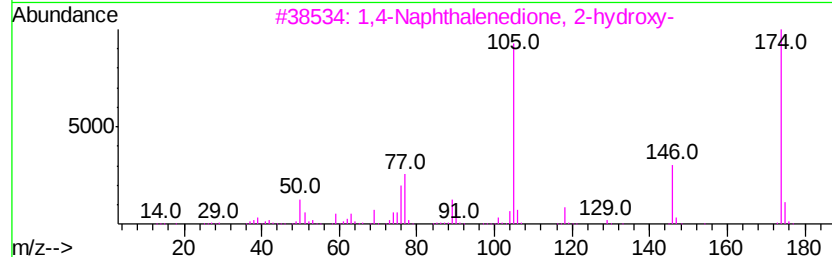
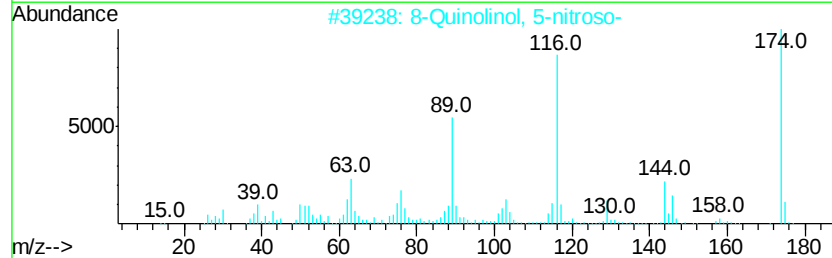
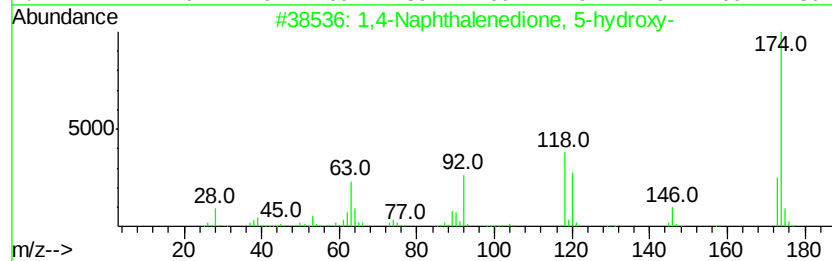
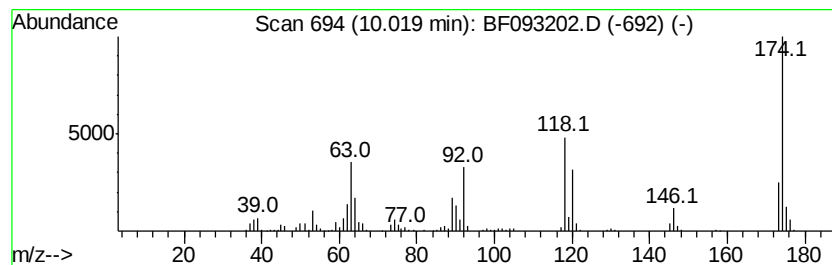
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,4-Naphthalenedione, 5-hyd... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	7.68 ng	552714	Acenaphthene-d10	9.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Naphthalenedione, 5-hydroxy-	174	C10H6O3	000481-39-0	96
2			8-Quinolinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43
3			1,4-Naphthalenedione, 2-hydroxy-	174	C10H6O3	000083-72-7	35
4			Benzaldehyde, 2,6-difluoro-3,4-d...	174	C7H4F2O3	152434-98-5	27
5			Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	27



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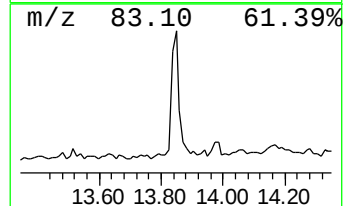
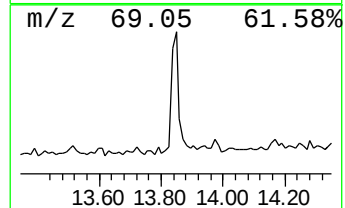
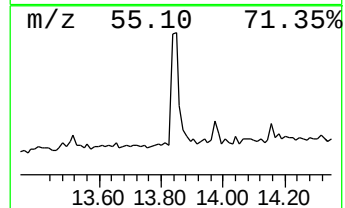
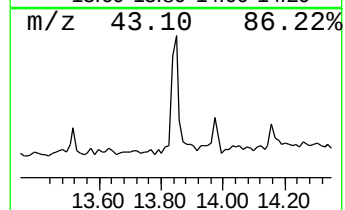
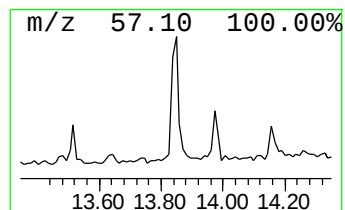
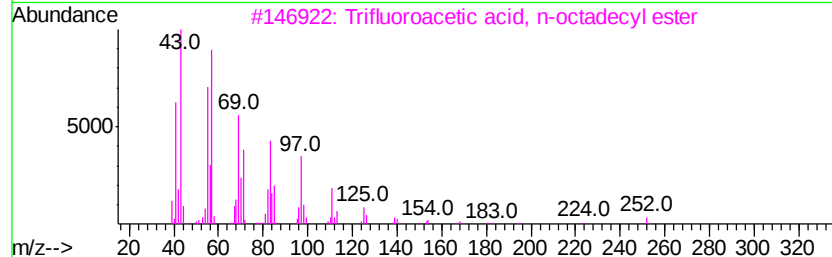
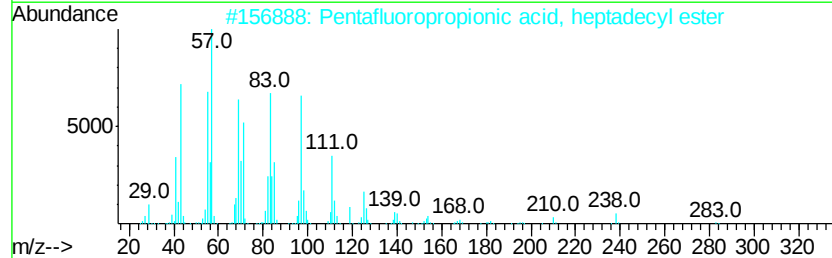
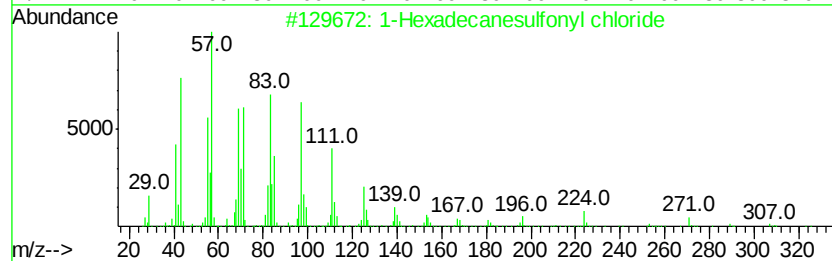
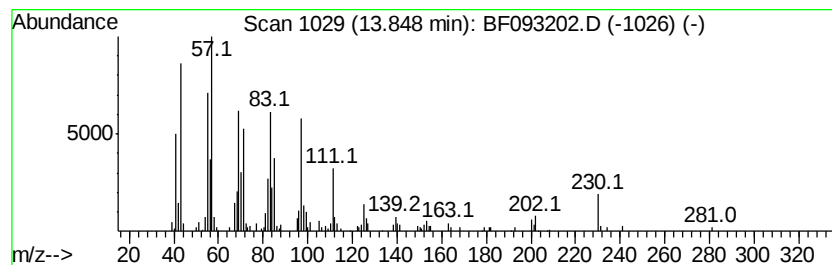
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.58 ng	317870	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	87
4		17-Pentatriacontene	491	C35H70	006971-40-0	83
5		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	81



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	35.3	ng	1682660	1	6.83	953912	20.0
unknown6.60	6.60	80.5	ng	3837130	1	6.83	953912	20.0
1,4-Naphthalenedi...	10.02	7.7	ng	552714	3	9.88	1438740	20.0
1-Hexadecanesulfo...	13.85	4.6	ng	317870	5	14.00	1387540	20.0