

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
 Data File : BF092869.D
 Acq On : 8 Feb 2017 22:35
 Operator : SJ/MA
 Sample : I1745-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-1

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	5.059	258	260	270	rBV	462976	497735	9.23%	1.485%
2	5.493	296	298	300	rBV	1870066	1786417	33.14%	5.332%
3	6.179	356	358	363	rVB	73589	72069	1.34%	0.215%
4	6.522	386	388	391	rBV	875499	1028891	19.09%	3.071%
5	6.659	398	400	403	rBV	2765045	3107889	57.65%	9.276%
6	6.899	418	421	423	rBV	621558	856758	15.89%	2.557%
7	7.047	432	434	437	rBV	2849827	3057940	56.73%	9.126%
8	7.459	467	470	473	rBV	2367455	2486310	46.12%	7.420%
9	8.179	531	533	535	rBV	1392189	1186422	22.01%	3.541%
10	9.253	624	627	630	rBV	3816704	4719288	87.55%	14.085%
11	9.928	684	686	689	rBV	1162647	1324901	24.58%	3.954%
12	10.728	752	756	758	rBV	2328023	2973429	55.16%	8.874%
13	11.414	814	816	819	rBV	1310966	1333329	24.73%	3.979%
14	12.819	936	939	941	rBV	182921	220653	4.09%	0.659%
15	13.014	952	956	958	rBV	3659469	5390604	100.00%	16.088%
16	13.494	994	998	1000	rBV	57629	68498	1.27%	0.204%
17	13.688	1013	1015	1017	rBV	203729	181099	3.36%	0.540%
18	14.054	1044	1047	1050	rBV	1573895	1438072	26.68%	4.292%
19	14.671	1096	1101	1111	rVB10	13491	63259	1.17%	0.189%
20	14.865	1115	1118	1120	rBV	395574	468978	8.70%	1.400%
21	15.505	1170	1174	1180	rVB	894045	1243725	23.07%	3.712%

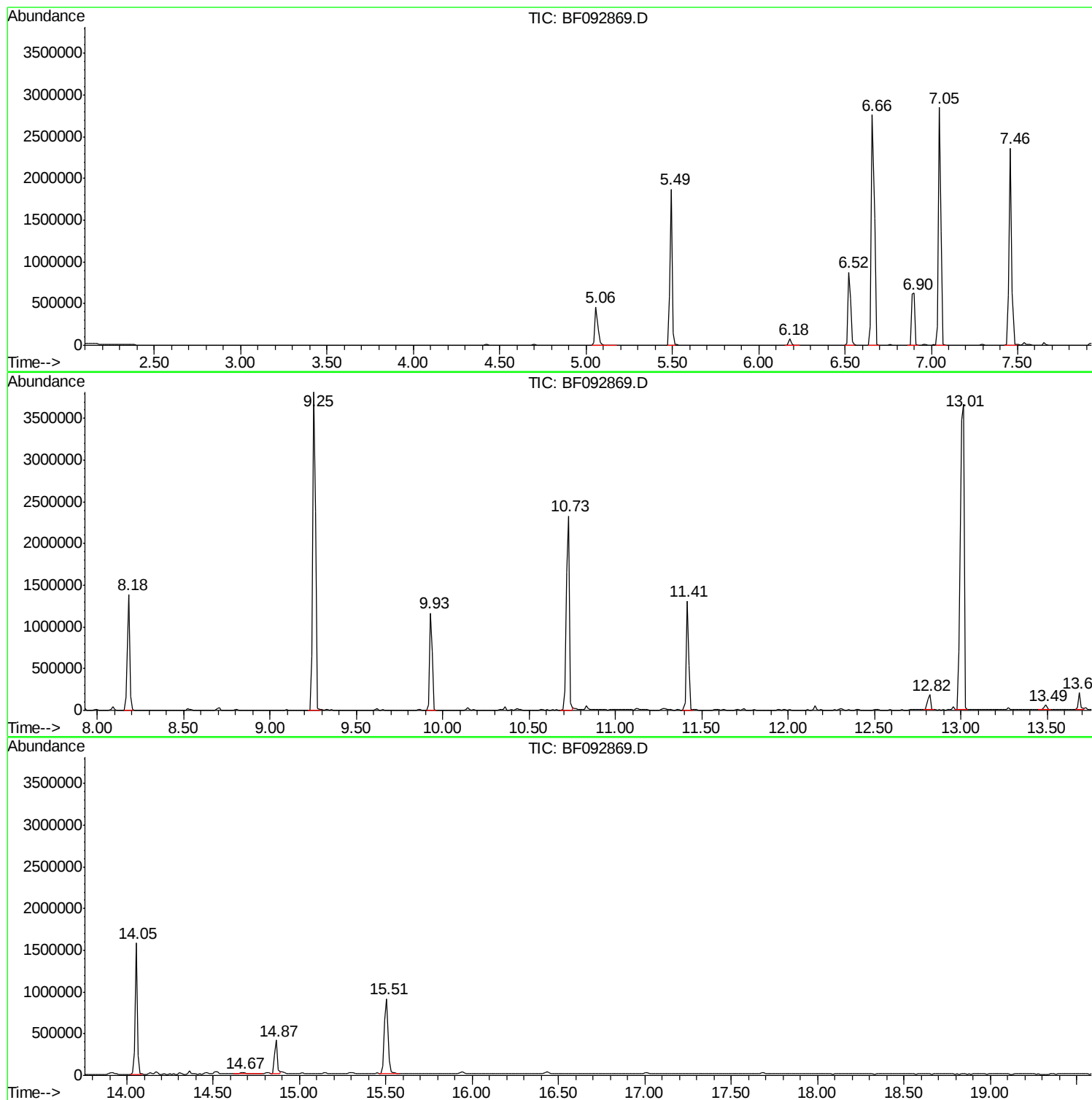
Sum of corrected areas: 33506266

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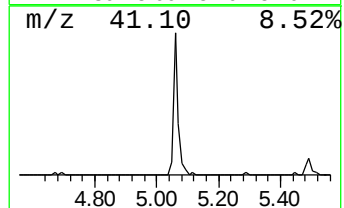
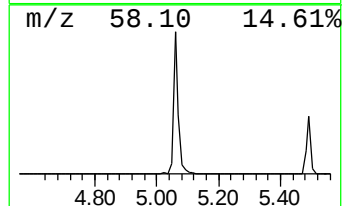
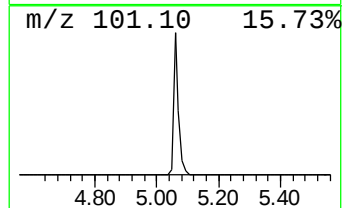
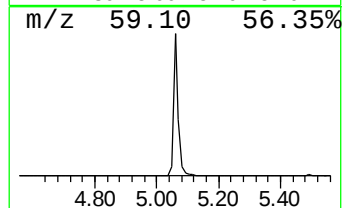
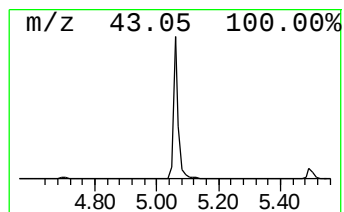
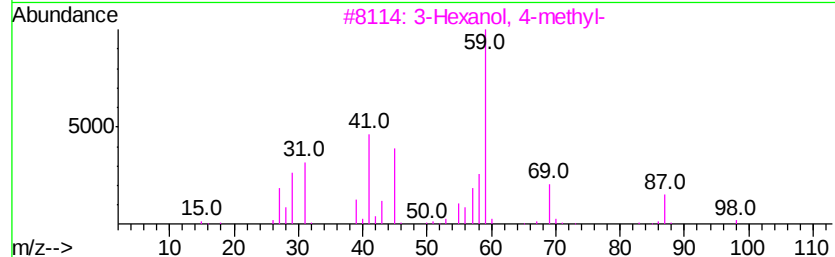
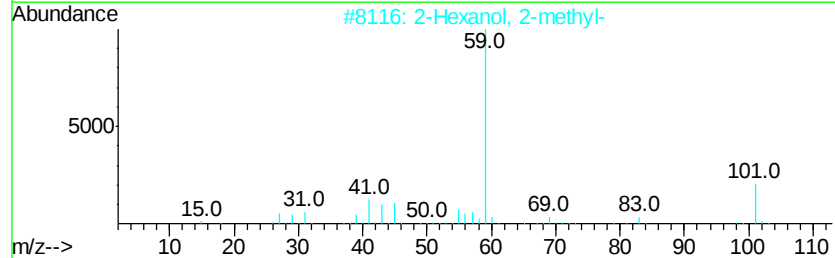
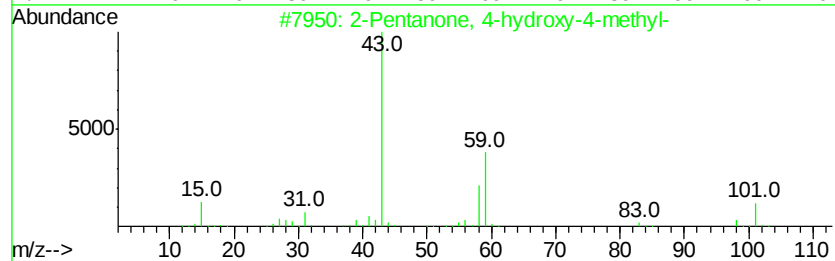
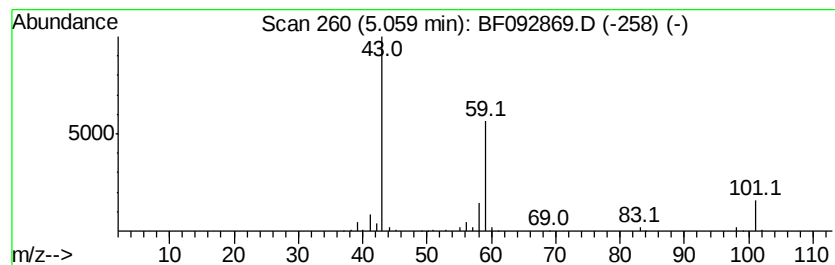
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	11.62 ng	497735	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		1,2-Butanediol, (./-.)-	90	C4H10O2	026171-83-5	9



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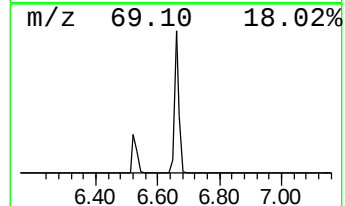
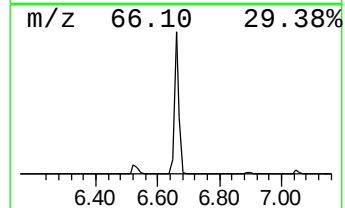
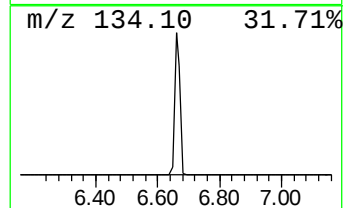
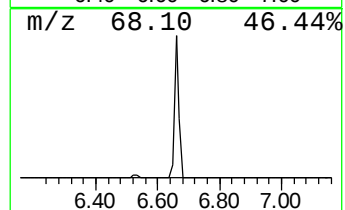
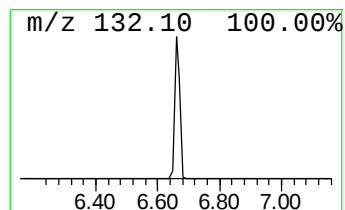
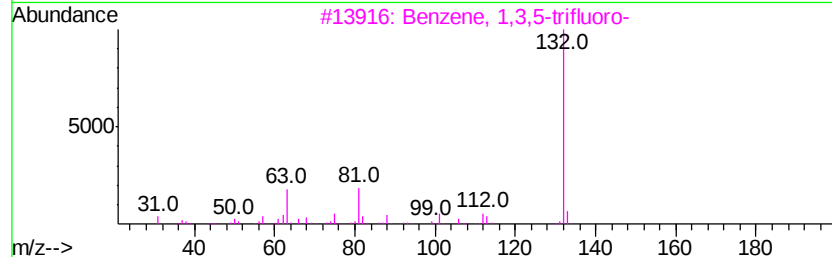
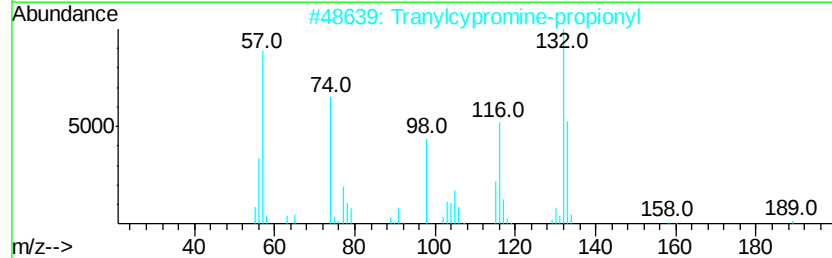
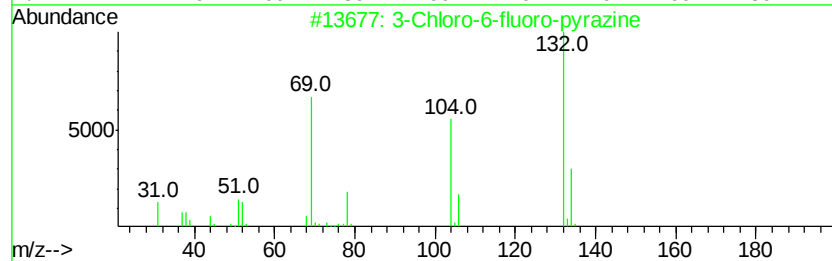
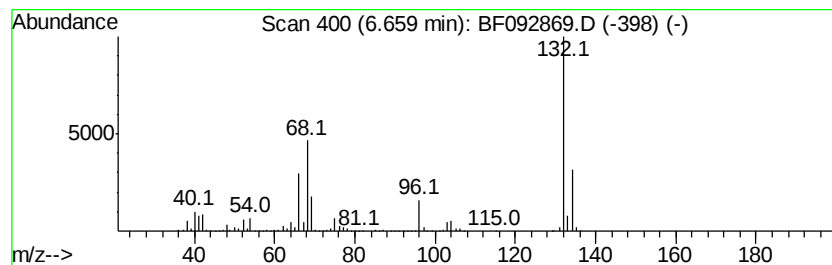
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	72.55 ng	3107890	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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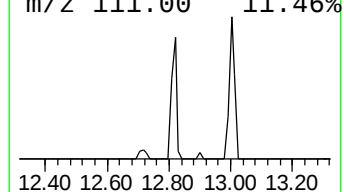
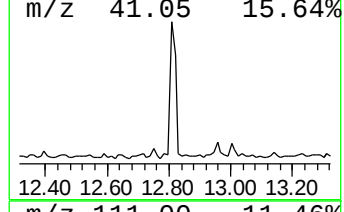
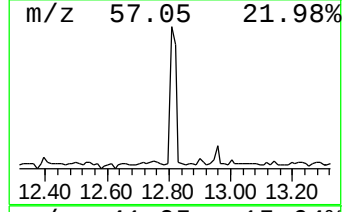
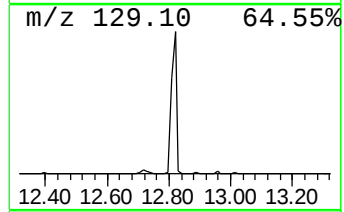
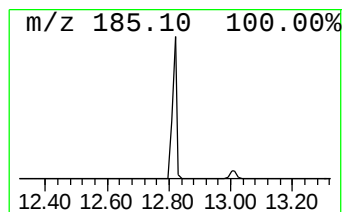
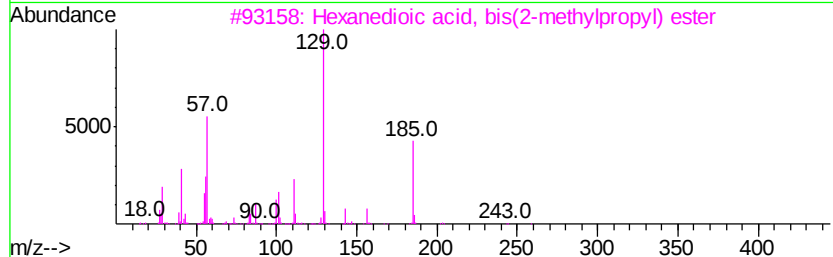
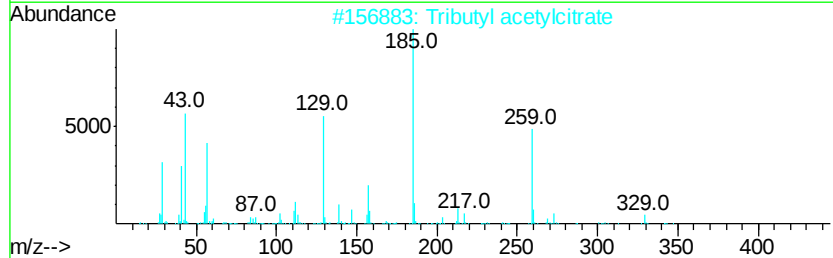
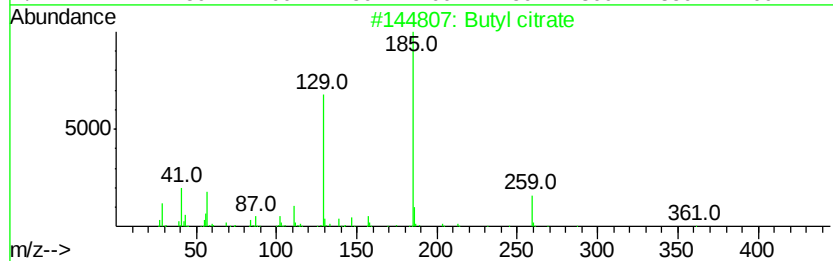
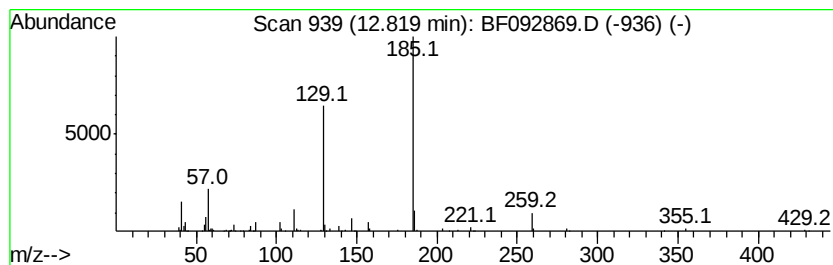
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Peak Number 4 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	3.07 ng	220653	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl citrate	360	C18H32O7	000077-94-1	83
2		Tributyl acetylcitrate	402	C20H34O8	000077-90-7	78
3		Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
4		Hexanedioic acid, dibutyl ester	258	C14H26O4	000105-99-7	50
5		3-Hydroxydiphenylamine	185	C12H11NO	000101-18-8	43



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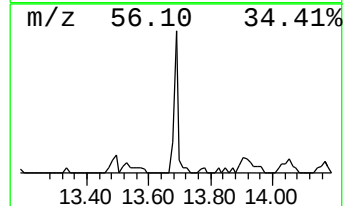
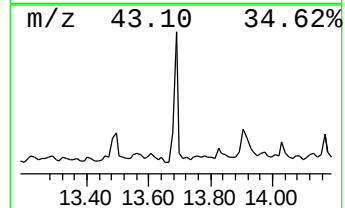
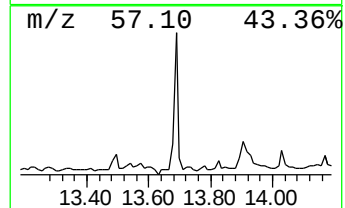
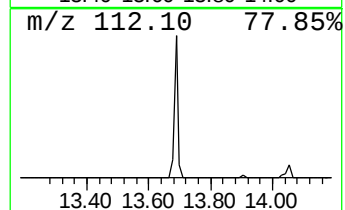
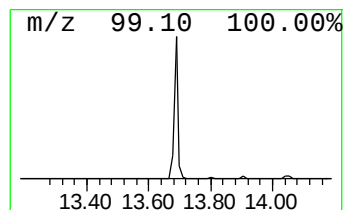
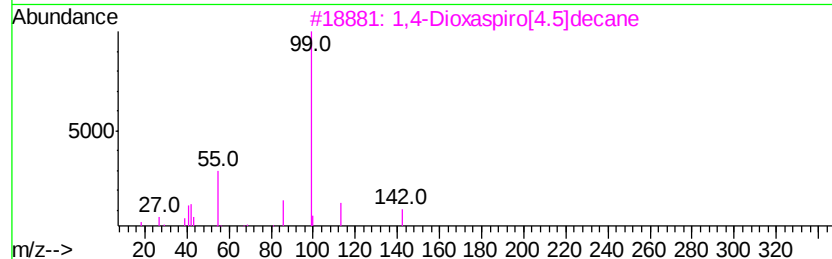
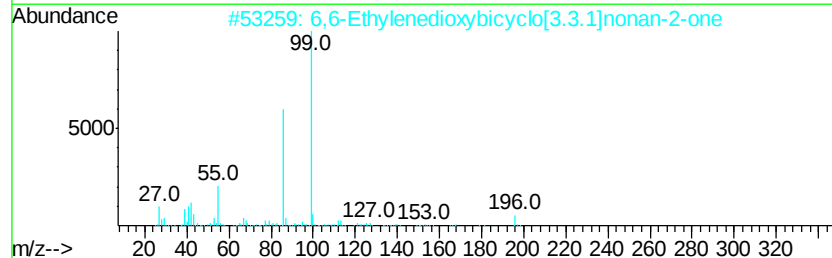
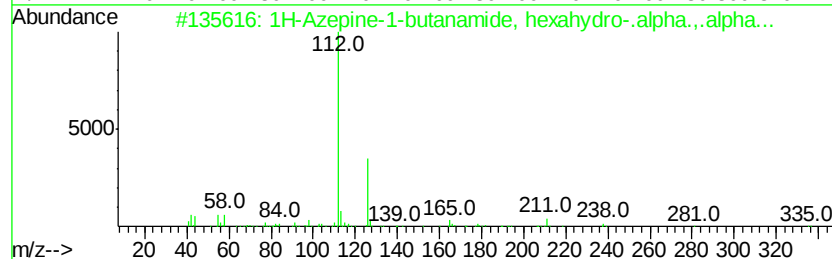
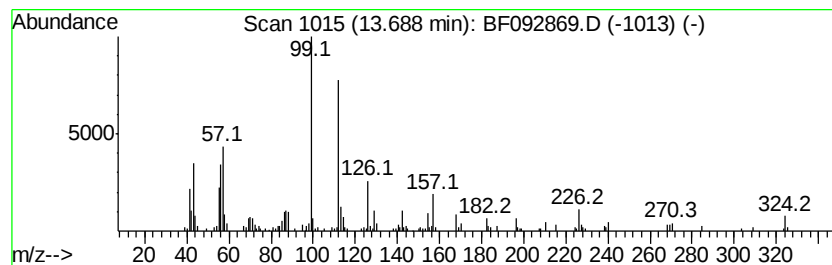
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	2.52 ng	181099	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Azepine-1-butanamide, hexahyd...	336	C22H28N2O	003691-21-2	35
2		6,6-Ethylenedioxybicyclo[3.3.1]n...	196	C11H16O3	029927-56-8	30
3		1,4-Dioxaspiro[4.5]decane	142	C8H14O2	000177-10-6	30
4		1,4-Dioxaspiro[4.6]undec-7-ene	154	C9H14O2	007140-60-5	27
5		Piperidine, 1-(1-methylpentyl)-	169	C11H23N	021901-99-5	25



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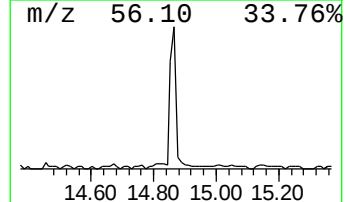
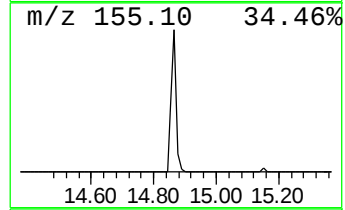
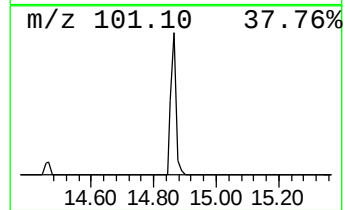
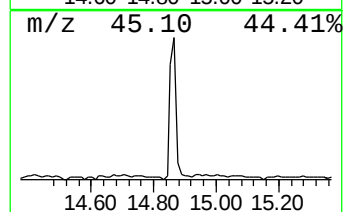
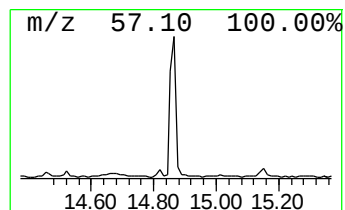
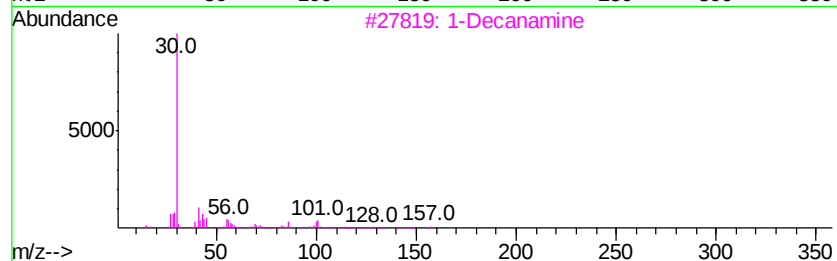
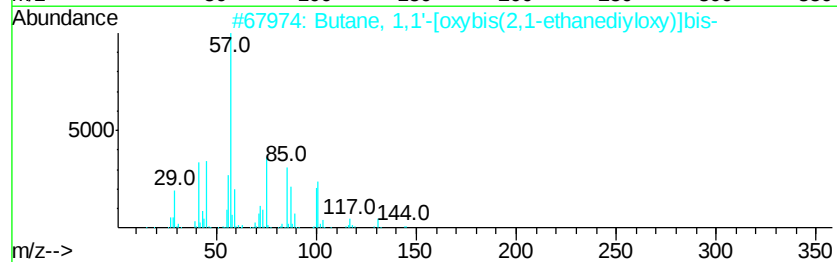
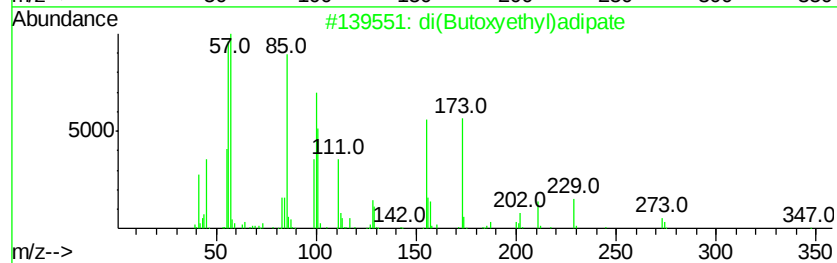
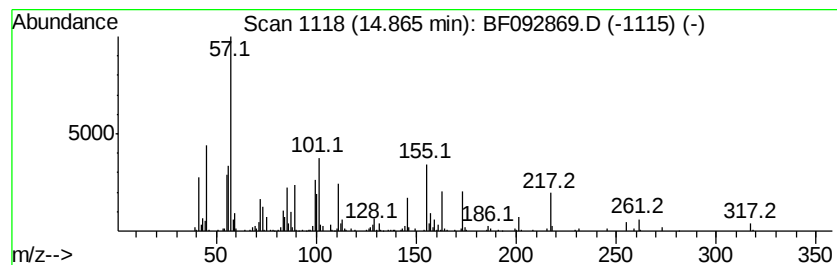
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.87 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	7.54 ng	468978	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	16
2		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	10
3		1-Decanamine	157	C10H23N	002016-57-1	10
4		N-Allyl-2,2,N-trimethylpropionamide	155	C9H17NO	1000187-48-8	9
5		1,4-Bis-(vinylloxy)-butane	142	C8H14O2	003891-33-6	9



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	11.6	ng	497735	1	6.90	856758	20.0
unknown6.66	6.66	72.5	ng	3107890	1	6.90	856758	20.0
Butyl citrate	12.82	3.1	ng	220653	5	14.05	1438070	20.0
unknown13.69	13.69	2.5	ng	181099	5	14.05	1438070	20.0
unknown14.87	14.87	7.5	ng	468978	6	15.51	1243730	20.0