

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
 Data File : BF081684.D
 Acq On : 17 Sep 2015 18:16
 Operator : UM/IZ
 Sample : G3664-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GP-1(6-9)

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-BF090115.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	1.235	10	13	16	rVB	792673	833476	28.98%	6.155%
2	1.315	18	20	28	rVB	17640	33183	1.15%	0.245%
3	1.441	30	31	37	rBV	101879	264228	9.19%	1.951%
4	1.533	37	39	75	rVB	758868	2875564	100.00%	21.235%
5	4.447	290	294	313	rBV	212647	547816	19.05%	4.045%
6	5.327	368	371	389	rBV	458711	930329	32.35%	6.870%
7	7.590	566	569	574	rBV	540770	960049	33.39%	7.090%
8	7.682	574	577	589	rVB	584425	1017734	35.39%	7.515%
9	8.173	617	620	626	rVB	193283	313466	10.90%	2.315%
10	8.493	645	648	656	rBB	393716	657527	22.87%	4.856%
11	9.465	730	733	749	rBV	344019	618370	21.50%	4.566%
12	11.065	870	873	885	rBV	224167	399986	13.91%	2.954%
13	13.705	1100	1104	1108	rBV	483627	807539	28.08%	5.963%
14	14.768	1194	1197	1206	rBB	104774	166286	5.78%	1.228%
15	15.191	1231	1234	1240	rBV	228240	422656	14.70%	3.121%
16	17.100	1397	1401	1409	rBV	297282	583668	20.30%	4.310%
17	17.740	1454	1457	1463	rBV	12689	28993	1.01%	0.214%
18	18.700	1537	1541	1544	rBV	270291	437119	15.20%	3.228%
19	20.460	1692	1695	1703	rBV	24166	58693	2.04%	0.433%
20	21.386	1774	1776	1779	rVB	33308	40723	1.42%	0.301%
21	21.740	1804	1807	1811	rVB	33774	53366	1.86%	0.394%
22	22.072	1833	1836	1838	rBV	581508	725838	25.24%	5.360%
23	23.340	1943	1947	1950	rBV	285987	507027	17.63%	3.744%
24	24.449	2041	2044	2049	rVV	21437	38089	1.32%	0.281%
25	24.781	2071	2073	2076	rVV	200837	220105	7.65%	1.625%

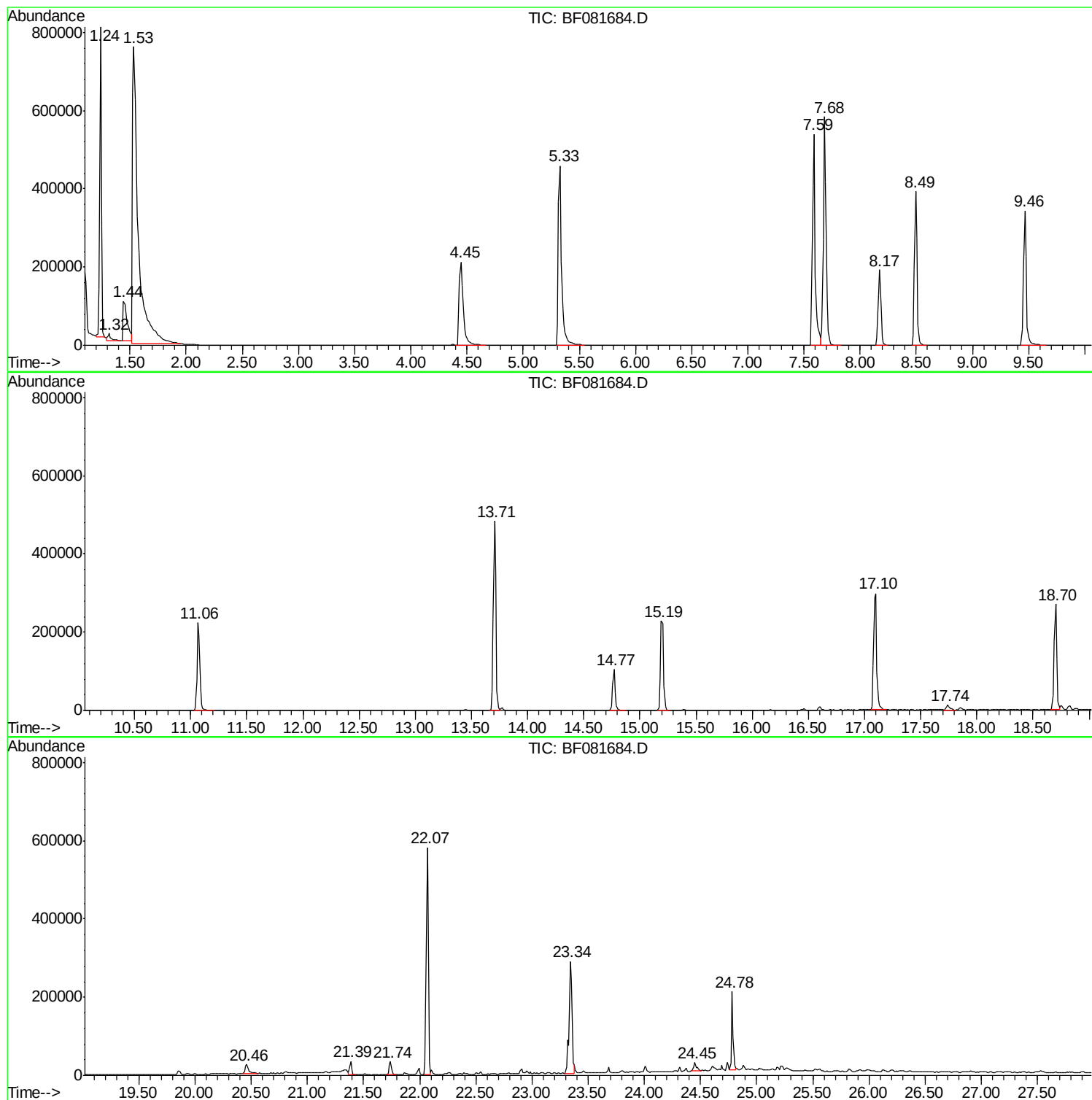
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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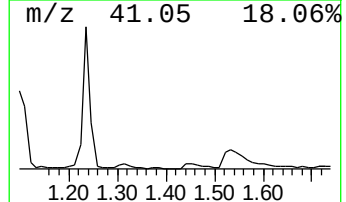
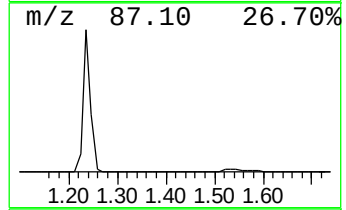
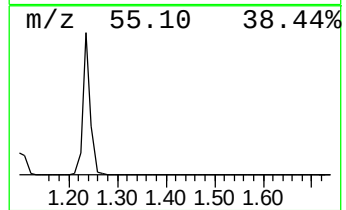
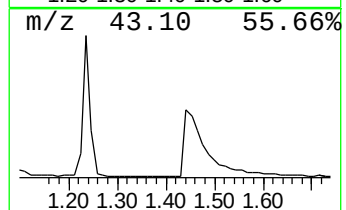
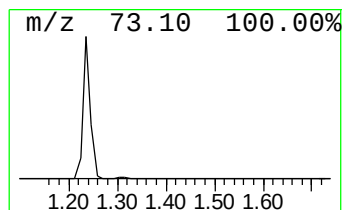
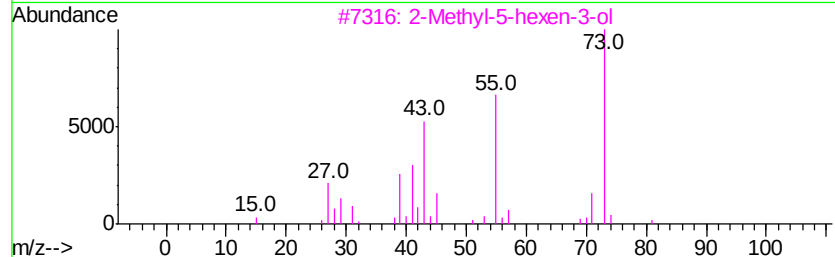
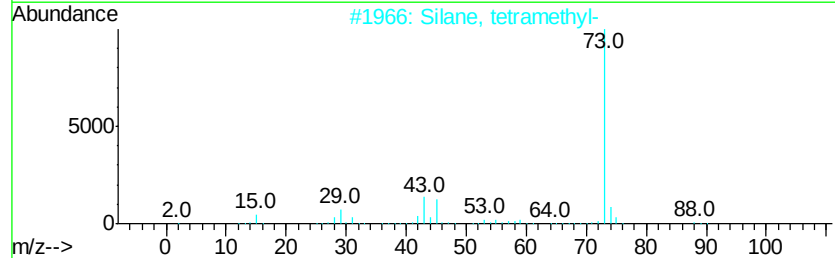
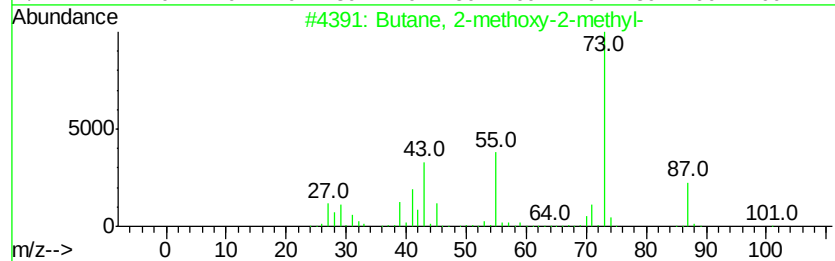
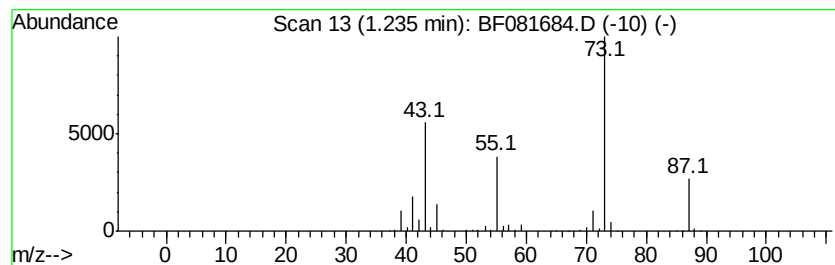
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.24	53.18 ng	833476	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	10



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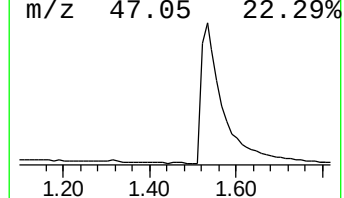
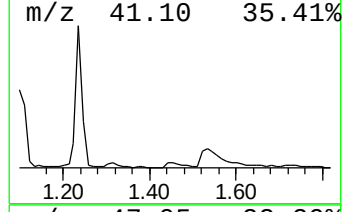
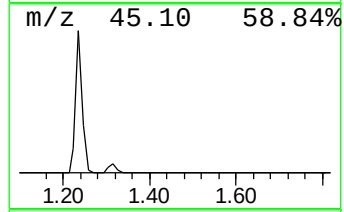
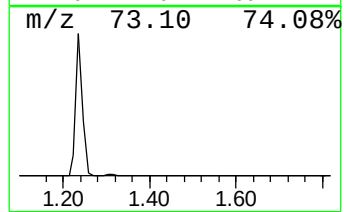
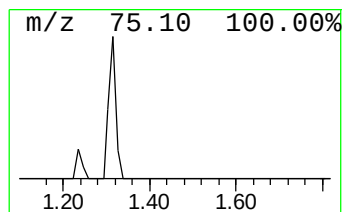
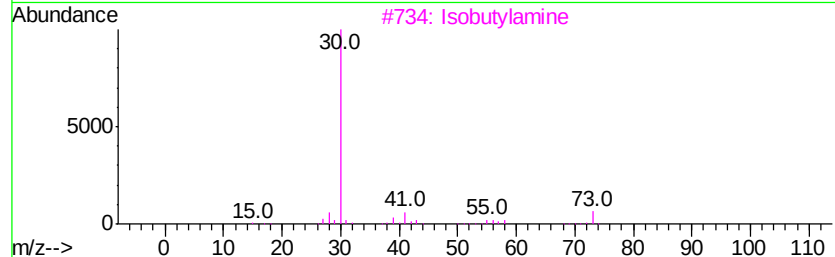
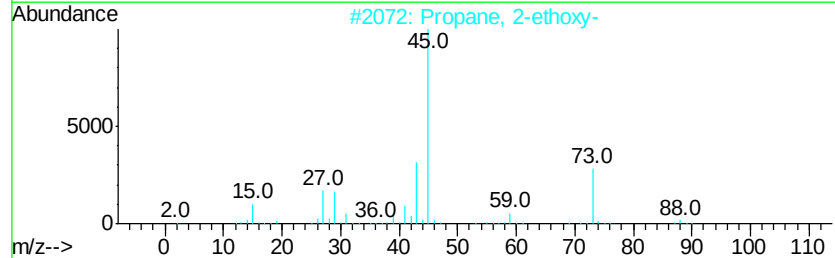
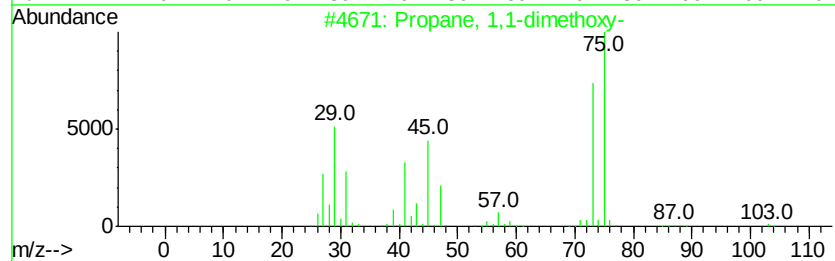
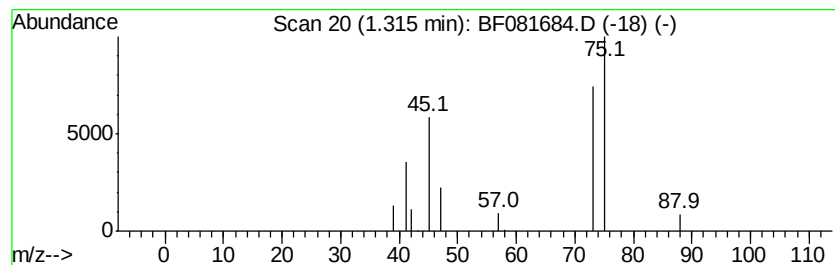
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	2.12 ng	33183	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	7
3			Isobutylamine	73	C4H11N	000078-81-9	4
4			Formamide, N-methylthio	75	C2H5NS	018952-41-5	4
5			2-Butanone, 3-hydroxy-	88	C4H8O2	000513-86-0	4



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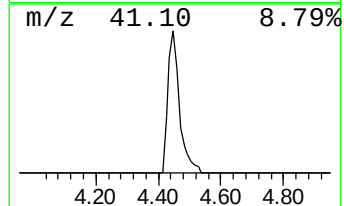
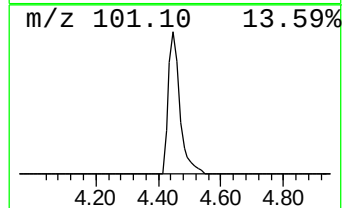
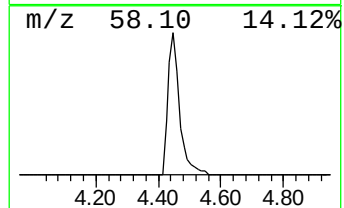
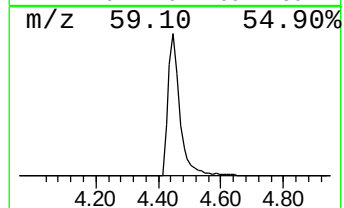
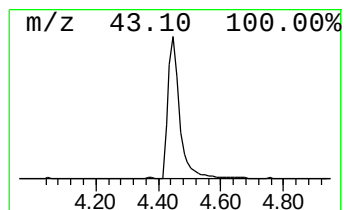
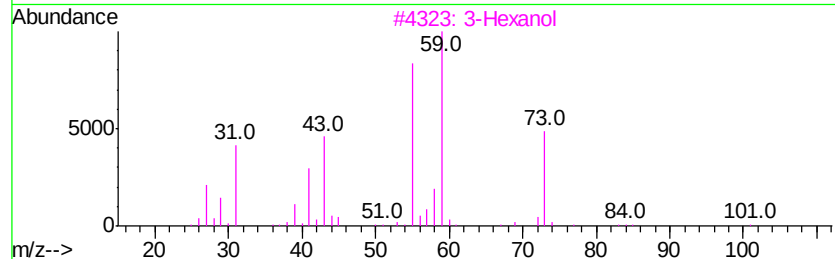
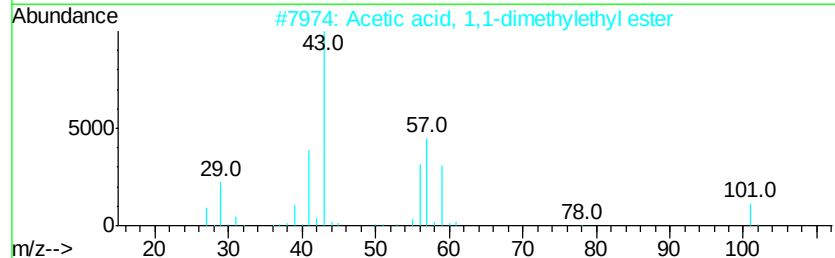
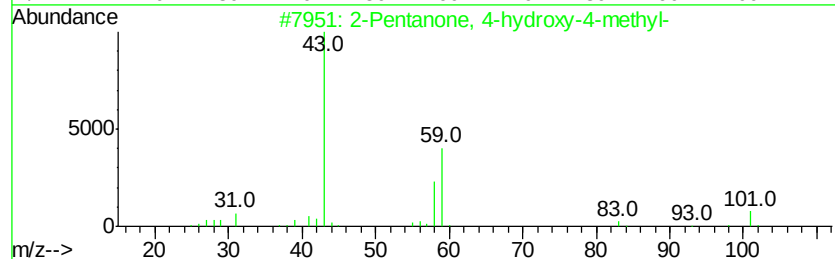
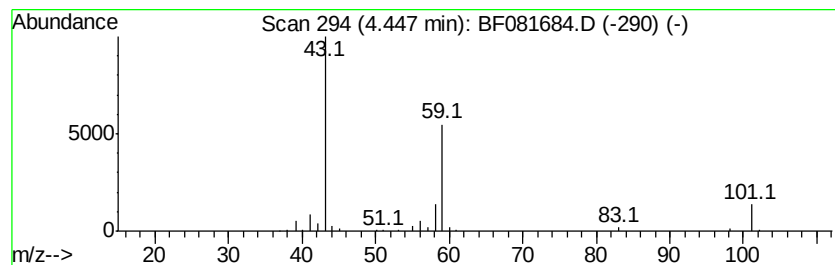
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	34.95 ng	547816	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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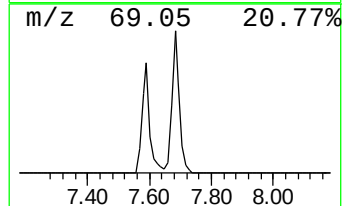
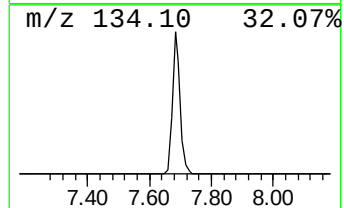
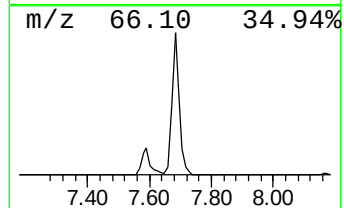
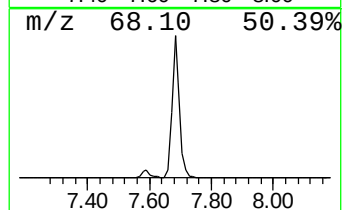
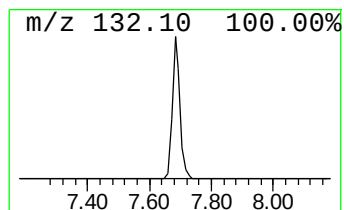
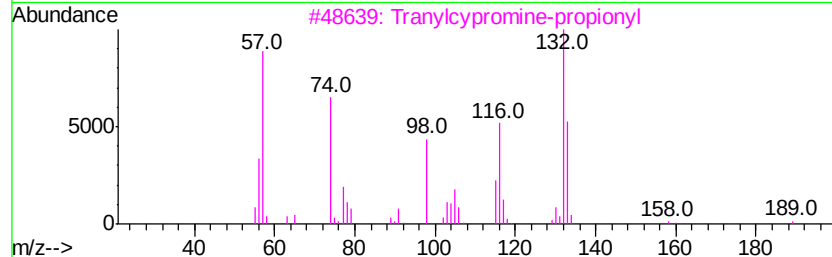
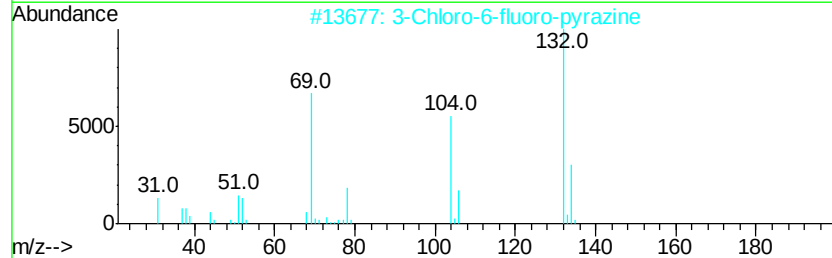
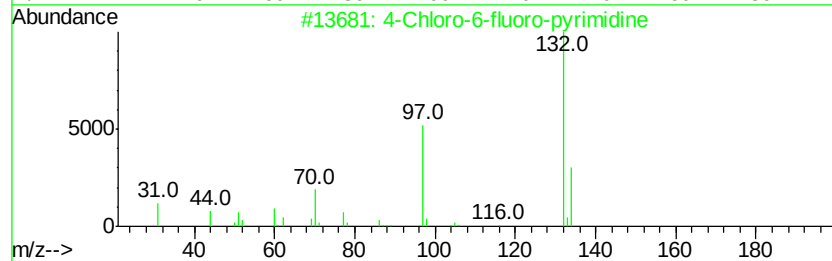
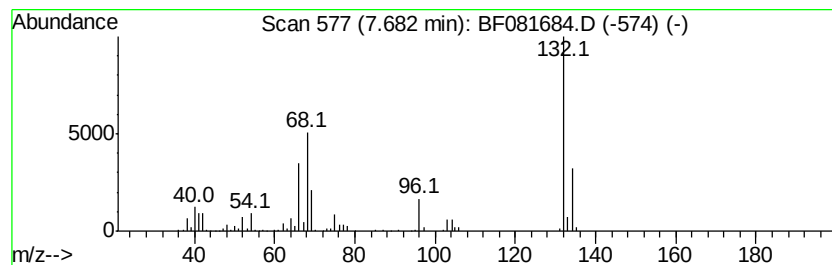
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	64.93 ng	1017730	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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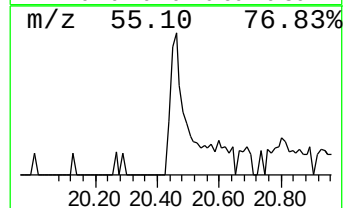
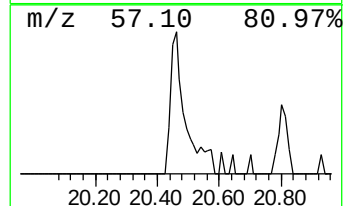
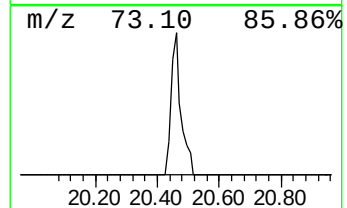
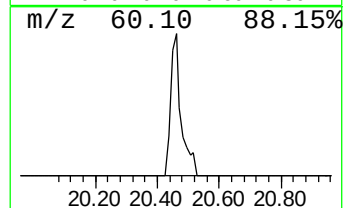
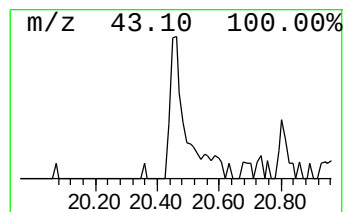
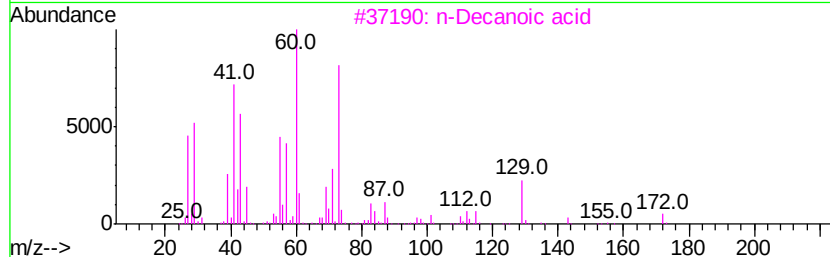
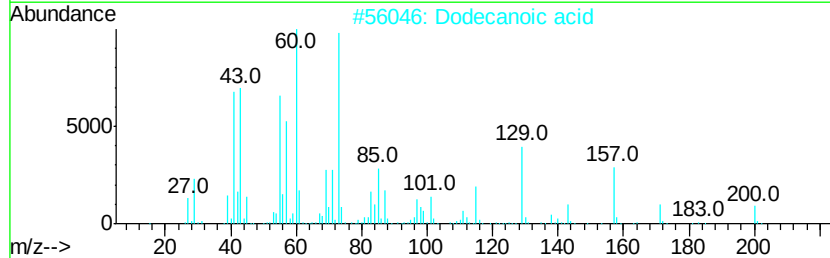
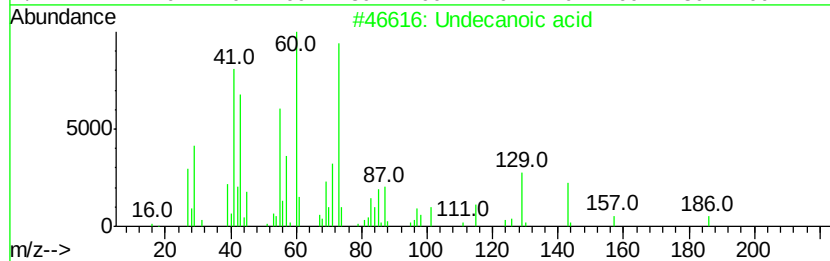
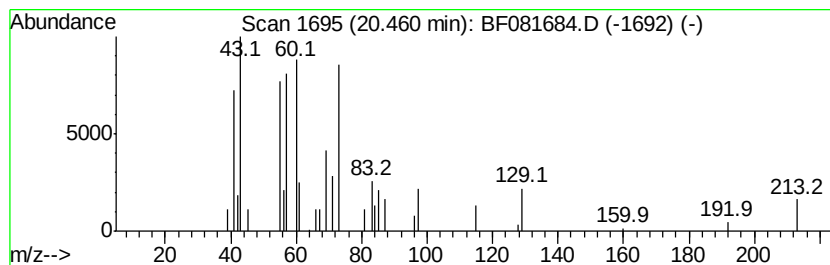
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	2.69 ng	58693	Phenanthrene-d10	18.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	64
2		Dodecanoic acid	200	C12H24O2	000143-07-7	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
5		n-Octanoic acid isopropyl ester	186	C11H22O2	005458-59-3	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.24	53.2	ng	833476	1	8.17	313466	20.0
Propane, 1,1-dime...	1.32	2.1	ng	33183	1	8.17	313466	20.0
2-Pentanone, 4-hy...	4.45	35.0	ng	547816	1	8.17	313466	20.0
unknown7.68	7.68	64.9	ng	1017730	1	8.17	313466	20.0
Undecanoic acid	20.46	2.7	ng	58693	4	18.70	437119	20.0