

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012517\
 Data File : BF092497.D
 Acq On : 26 Jan 2017 00:42
 Operator : SJ/MA
 Sample : I1398-01
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PMW-1A-012017

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-BF012417.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	4.693	225	228	231	rVB	45453	64609	1.24%	0.162%
2	5.150	265	268	271	rBV	578373	709041	13.63%	1.781%
3	5.561	301	304	306	rVB	2342141	2714390	52.16%	6.818%
4	6.121	351	353	357	rBV	46733	62261	1.20%	0.156%
5	6.419	378	379	381	rVB	87236	69053	1.33%	0.173%
6	6.521	386	388	390	rVB	58537	57157	1.10%	0.144%
7	6.579	390	393	396	rVB	1821615	1594128	30.64%	4.004%
8	6.647	396	399	401	rBV	77870	71632	1.38%	0.180%
9	6.727	403	406	409	rBV	3478850	3783214	72.71%	9.503%
10	6.784	409	411	414	rVB	205375	237858	4.57%	0.597%
11	6.922	419	423	425	rBV3	25639	55916	1.07%	0.140%
12	6.967	425	427	429	rVV	1078808	1002318	19.26%	2.518%
13	7.024	431	432	435	rVV	74617	78308	1.50%	0.197%
14	7.127	438	441	443	rVV	3447722	3701280	71.13%	9.297%
15	7.219	447	449	450	rBV	86593	73599	1.41%	0.185%
16	7.287	453	455	460	rBV3	92690	144518	2.78%	0.363%
17	7.367	460	462	464	rBV	74315	82133	1.58%	0.206%
18	7.436	466	468	469	rVV	77377	70855	1.36%	0.178%
19	7.527	472	476	479	rVV	2227199	3525019	67.74%	8.855%
20	7.619	482	484	486	rVB2	62553	68227	1.31%	0.171%
21	7.653	486	487	492	rVB3	38229	63129	1.21%	0.159%
22	7.744	492	495	496	rBV2	97655	121441	2.33%	0.305%
23	7.767	496	497	500	rVB	130394	102623	1.97%	0.258%
24	7.927	507	511	514	rVB2	71538	148013	2.84%	0.372%
25	7.996	514	517	518	rBV2	119898	131895	2.53%	0.331%
26	8.259	537	540	542	rBV	1429909	1445400	27.78%	3.631%
27	8.533	560	564	568	rVV4	26732	52851	1.02%	0.133%
28	9.345	632	635	637	rBV	4536314	5189386	99.73%	13.035%
29	9.733	667	669	671	rBV	295306	241199	4.64%	0.606%
30	10.019	691	694	696	rBV	1654475	1473157	28.31%	3.700%
31	10.442	729	731	734	rVB2	65480	90160	1.73%	0.226%
32	10.808	760	763	766	rBV	2571783	2945426	56.61%	7.399%
33	10.922	772	773	778	rVB	40383	63261	1.22%	0.159%
34	11.505	821	824	826	rBV	1695232	1478952	28.42%	3.715%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.031	868	870	873 rBV	74845	104462	2.01%	0.262%
36	13.105	960	964	966 rBV	4272257	5203471	100.00%	13.071%
37	13.997	1039	1042	1047 rBV	86111	110619	2.13%	0.278%
38	14.145	1052	1055	1058 rBV	1516716	1457297	28.01%	3.661%
39	15.620	1181	1184	1187 rBV	868940	1221429	23.47%	3.068%

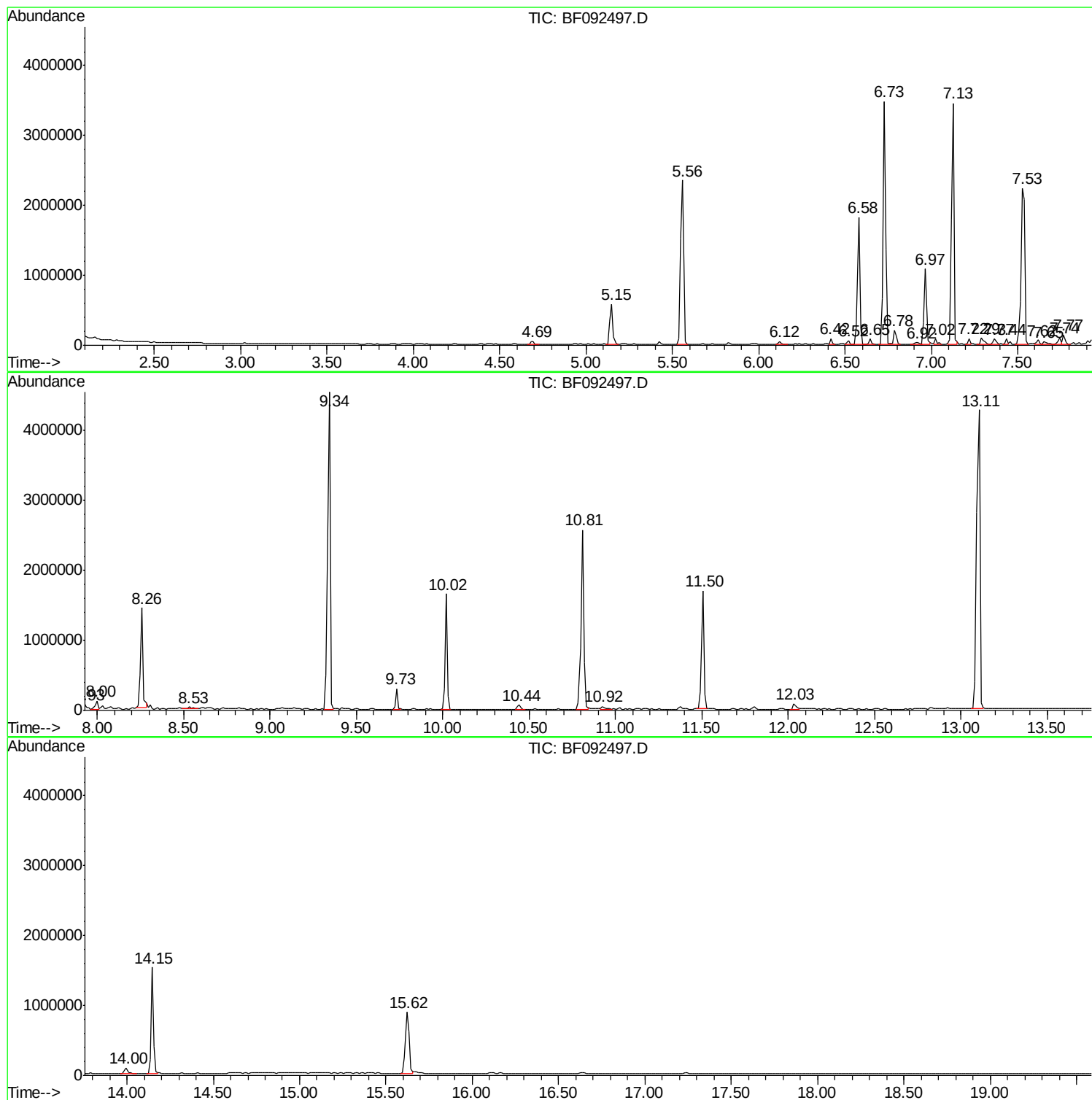
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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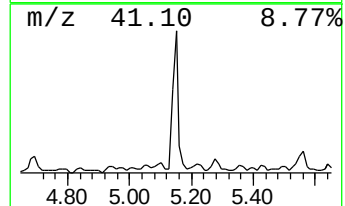
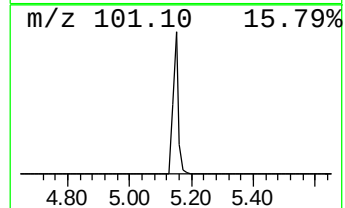
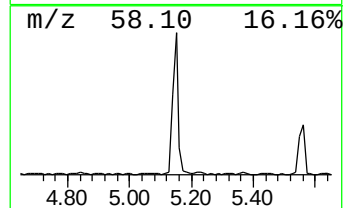
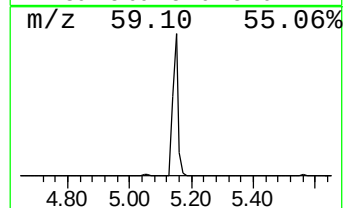
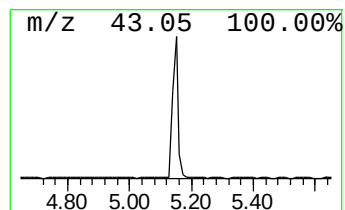
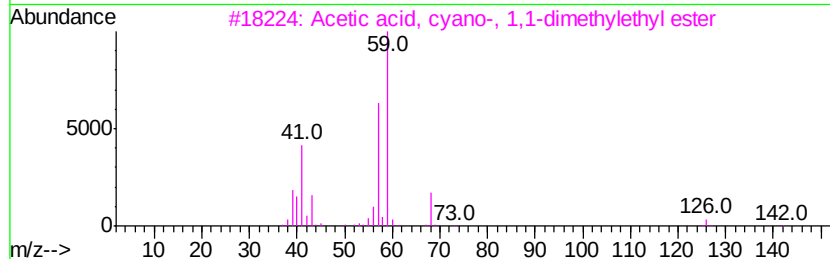
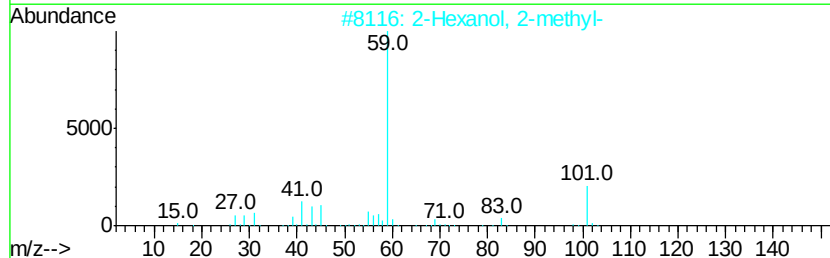
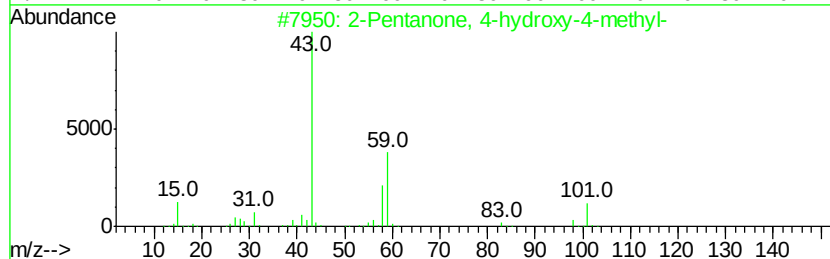
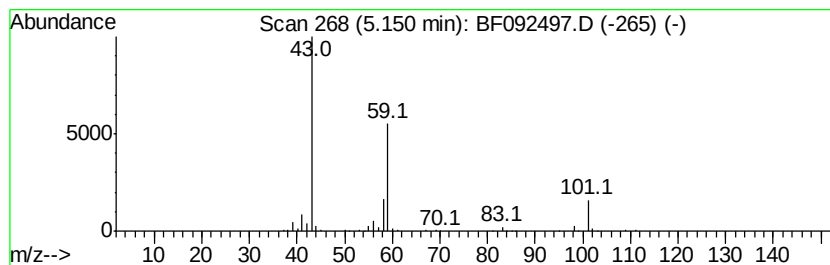
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.15	14.15 ng	709041	1,4-Dichlorobenzene-d4	6.97

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	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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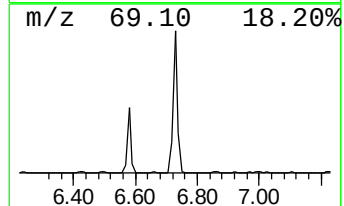
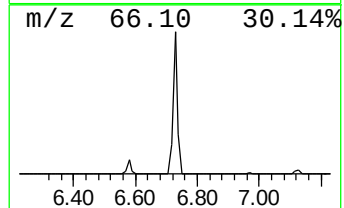
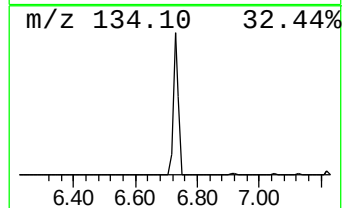
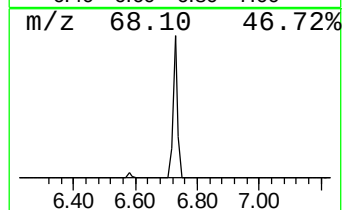
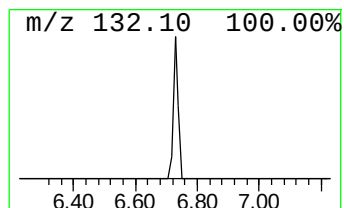
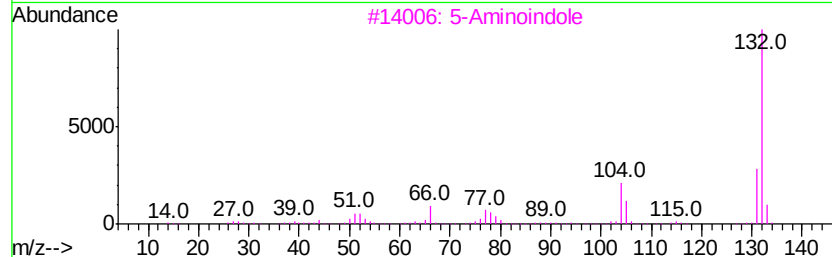
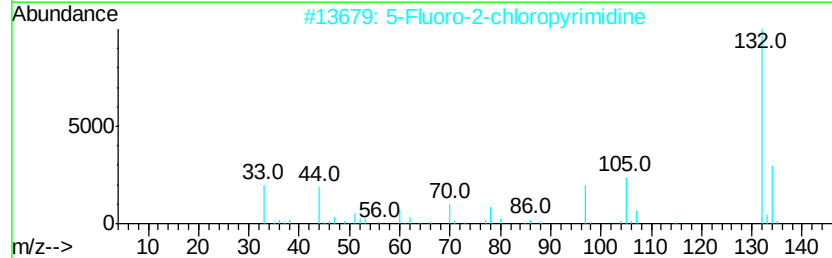
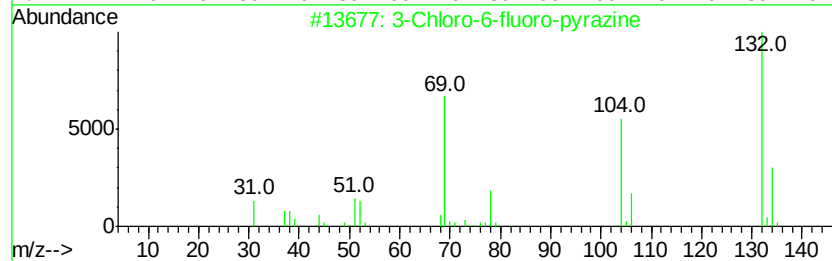
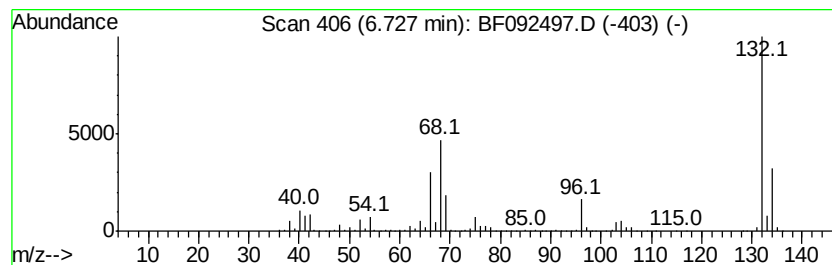
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	75.49 ng	3783210	1,4-Dichlorobenzene-d4	6.97

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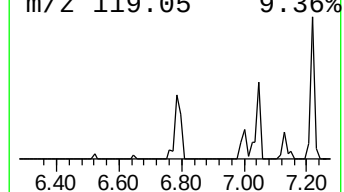
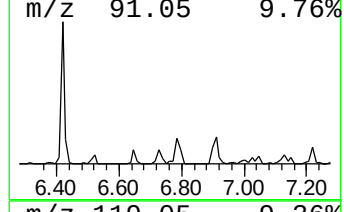
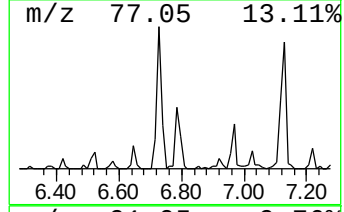
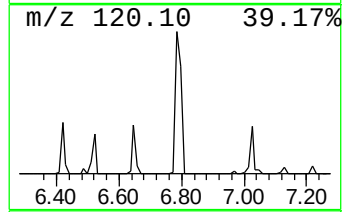
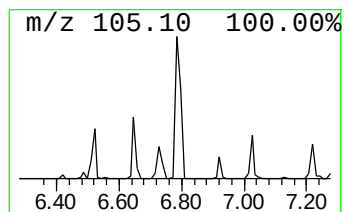
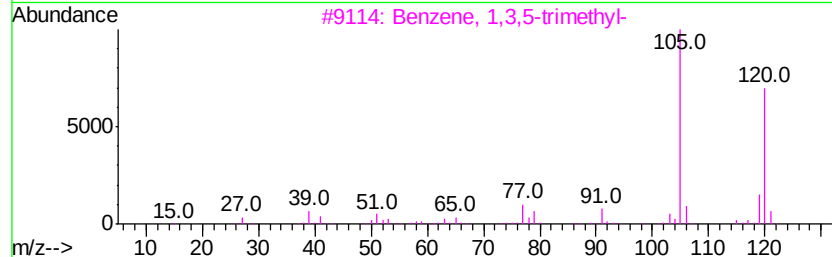
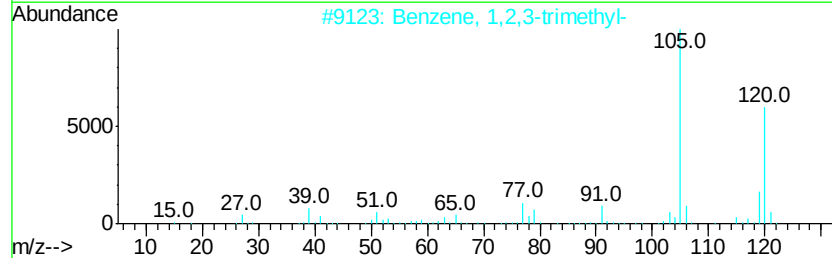
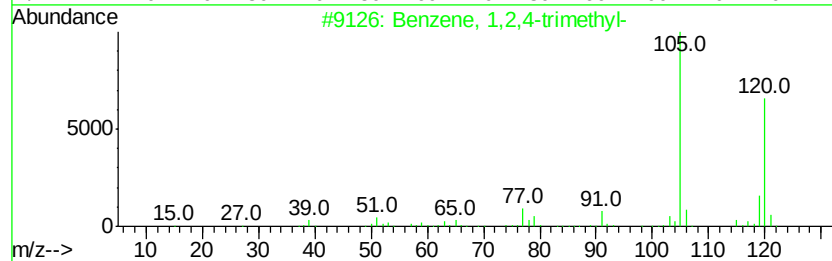
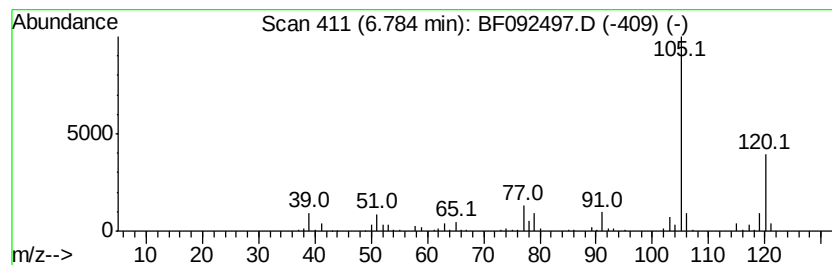
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	4.75 ng	237858	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3		Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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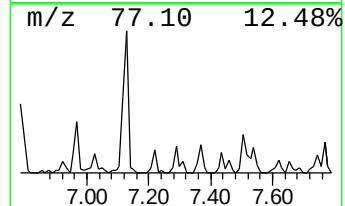
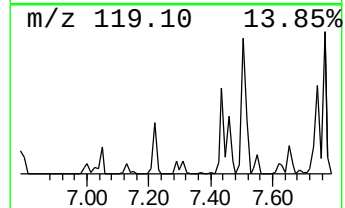
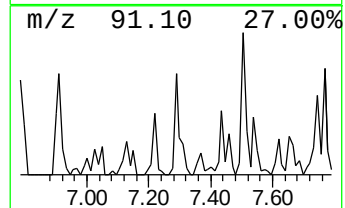
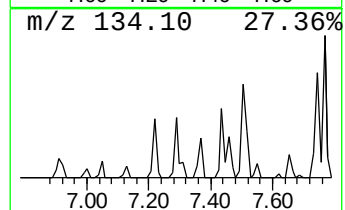
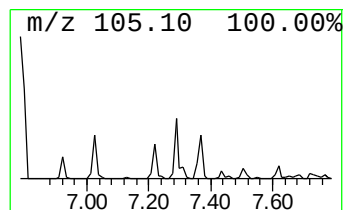
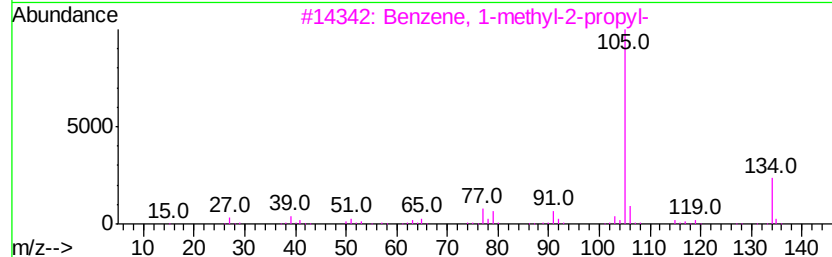
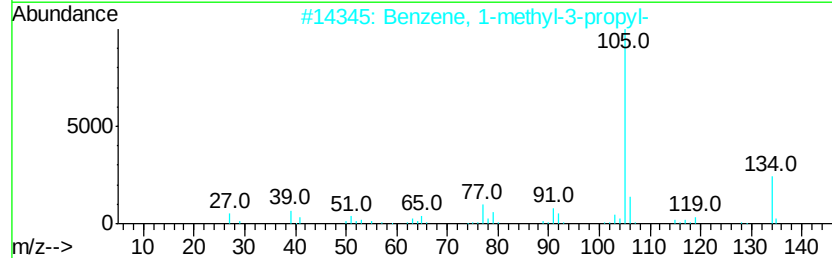
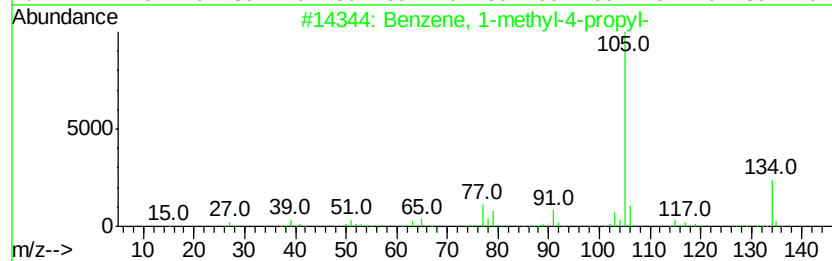
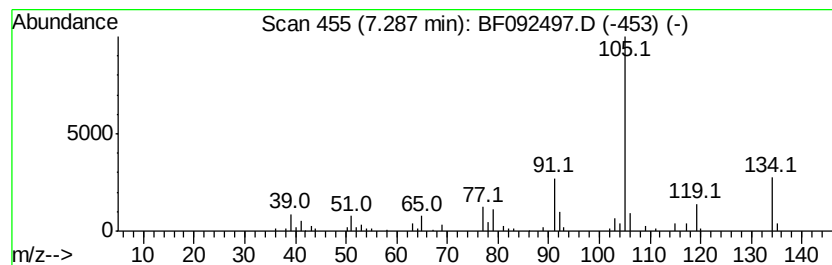
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1-methyl-4-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	2.88 ng	144518	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	87
2		Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	87
3		Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	72
4		Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	64
5		2-Tolylloxirane	134	C9H10O	002783-26-8	58



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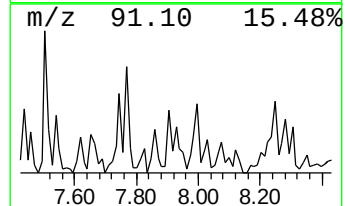
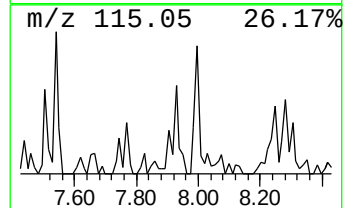
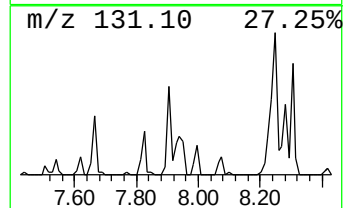
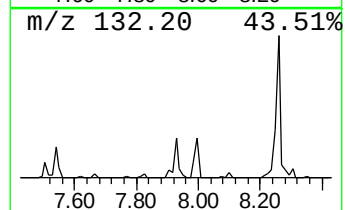
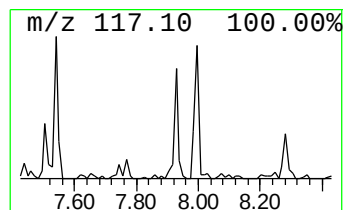
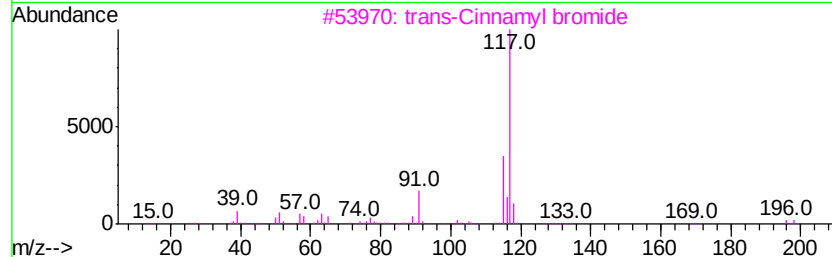
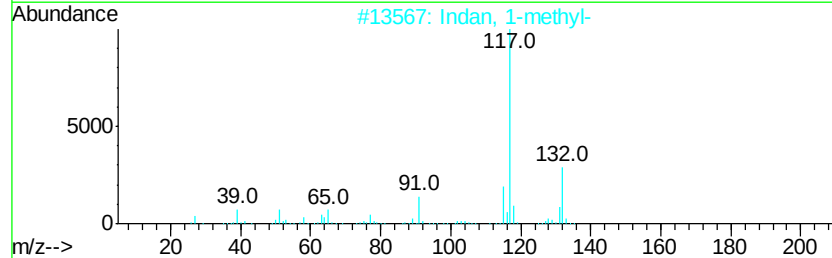
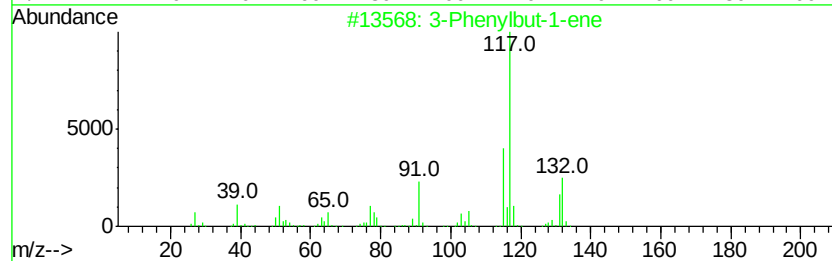
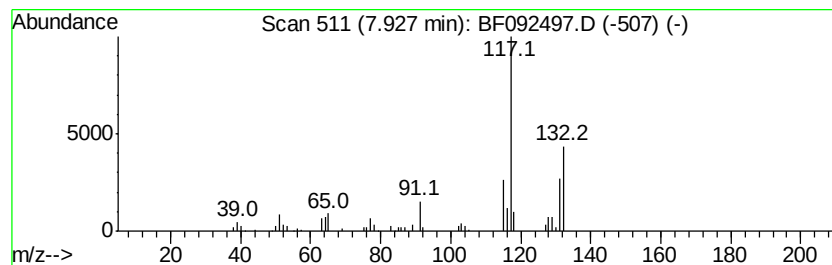
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TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Phenylbut-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	2.05 ng	148013	Naphthalene-d8	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
2		Indan, 1-methyl-	132	C10H12	000767-58-8	83
3		trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47
4		Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	47
5		5H-1-Pyridine	117	C8H7N	000270-91-7	43



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Sample : I1398-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PMW-1A-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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
2-Pentanone, 4-hy...	5.15	14.2	ng	709041	1	6.97	1002320	20.0
unknown6.73	6.73	75.5	ng	3783210	1	6.97	1002320	20.0
Benzene, 1,2,4-tr...	6.78	4.8	ng	237858	1	6.97	1002320	20.0
Benzene, 1-methyl...	7.29	2.9	ng	144518	1	6.97	1002320	20.0
3-Phenylbut-1-ene	7.93	2.0	ng	148013	2	8.26	1445400	20.0