

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093611.D
 Acq On : 13 Mar 2017 17:02
 Operator : SJ/MA
 Sample : I2174-21
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-69

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-BF030717.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	2.401	43	45	56	rVB	75388	177330	3.94%	0.450%
2	3.121	106	108	114	rBV	28423	83946	1.87%	0.213%
3	4.150	195	198	200	rBV	65912	91509	2.03%	0.232%
4	4.196	200	202	217	rVB	71765	219286	4.87%	0.557%
5	4.401	217	220	223	rBV	43657	89588	1.99%	0.228%
6	4.859	258	260	276	rBV	833574	1581989	35.16%	4.019%
7	5.316	298	300	320	rBV	2694762	4491309	99.81%	11.409%
8	5.716	333	335	347	rVB	44348	83734	1.86%	0.213%
9	6.367	390	392	400	rBV	3176803	4142313	92.05%	10.523%
10	6.482	400	402	405	rVB	4367091	4235682	94.13%	10.760%
11	6.710	420	422	430	rVB	913616	969117	21.54%	2.462%
12	6.859	433	435	438	rBV	3161746	3218002	71.51%	8.175%
13	7.282	470	472	486	rBV	2694870	3003507	66.75%	7.630%
14	8.002	532	535	545	rBV	1149793	1282362	28.50%	3.258%
15	9.076	627	629	632	rBV	3514759	4499880	100.00%	11.431%
16	9.762	686	689	691	rBV	1092993	1359243	30.21%	3.453%
17	10.550	756	758	761	rBV	2066770	2493658	55.42%	6.335%
18	11.248	817	819	824	rBV	1473738	1386706	30.82%	3.523%
19	12.836	955	958	960	rBV	4186222	4211371	93.59%	10.698%
20	13.899	1049	1051	1060	rBV	726501	1008555	22.41%	2.562%
21	15.305	1171	1174	1184	rBV	469465	736598	16.37%	1.871%

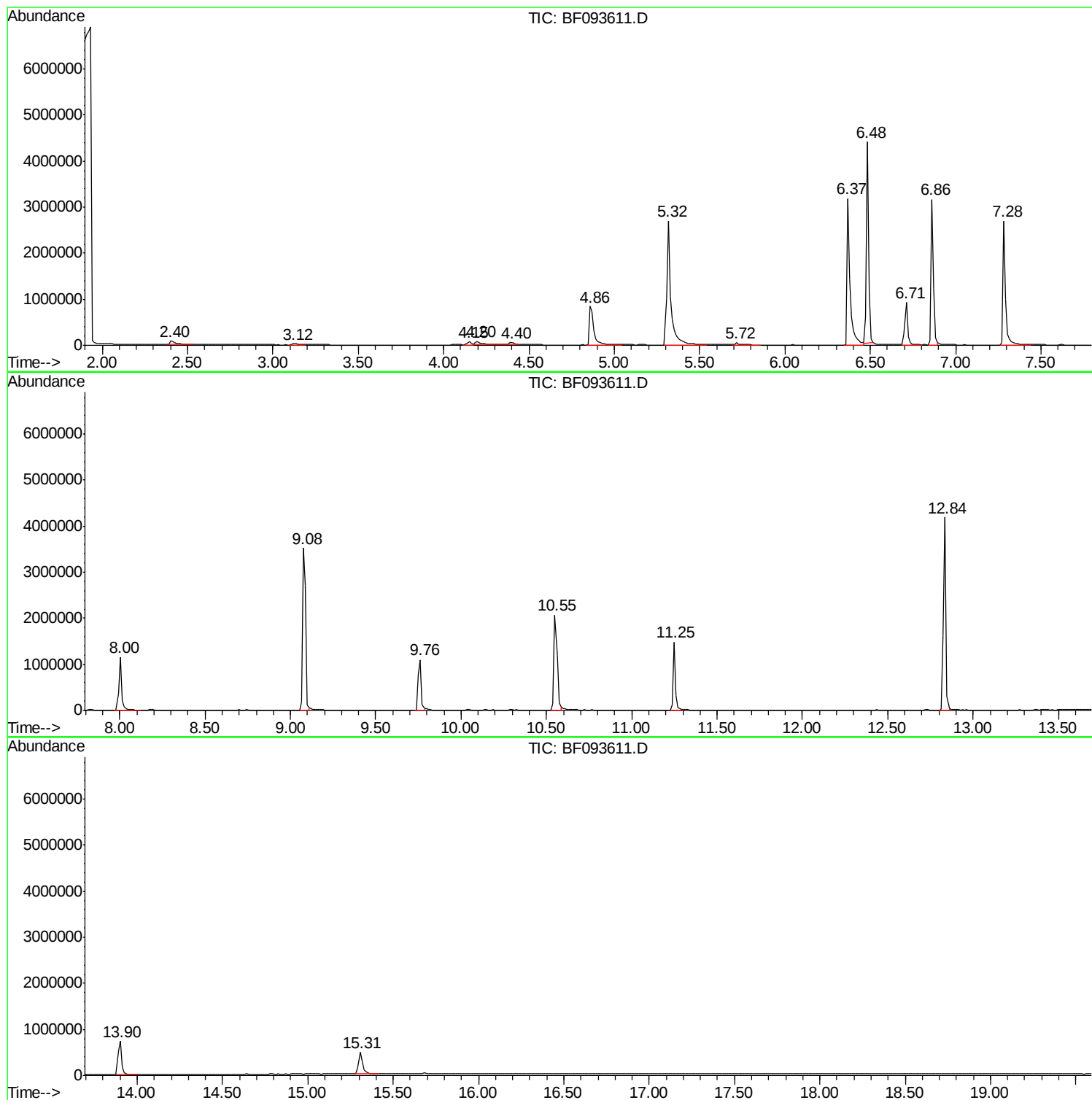
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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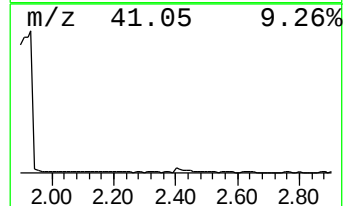
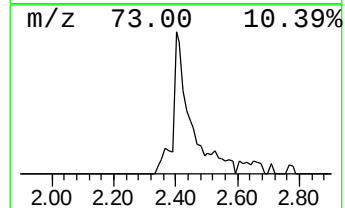
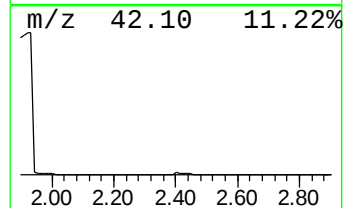
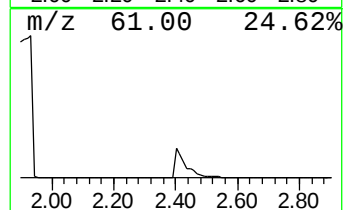
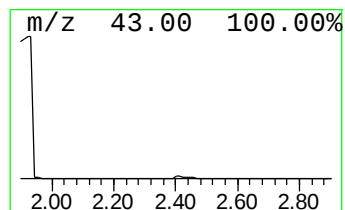
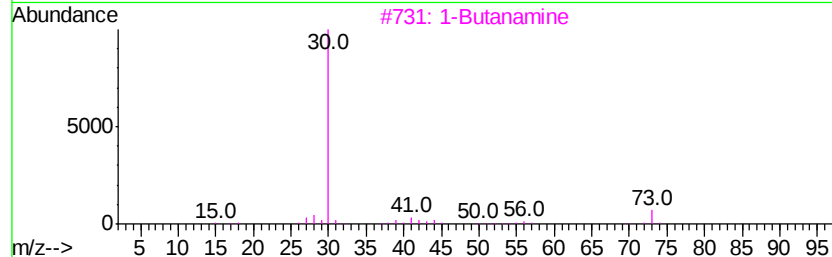
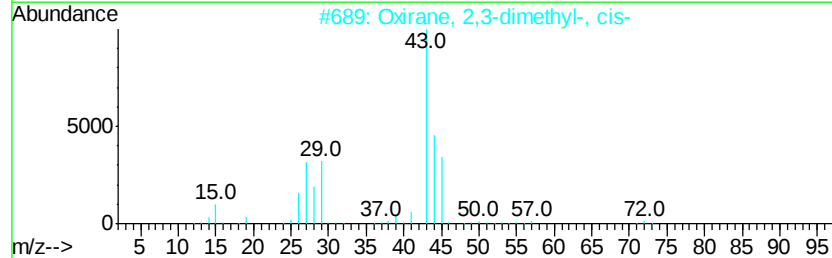
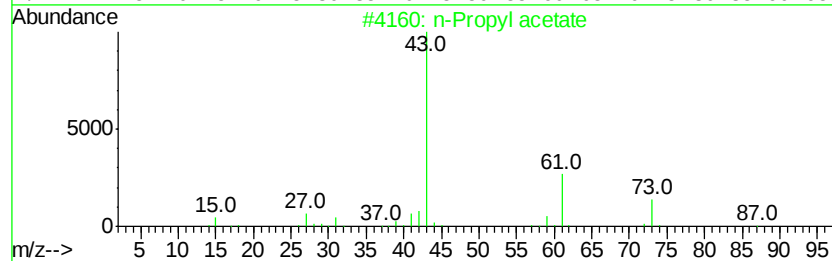
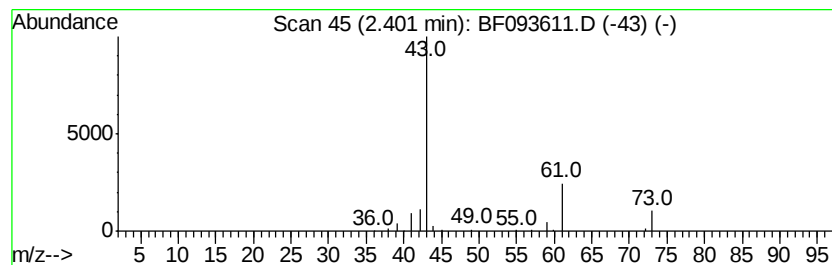
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	3.66 ng	177330	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	9
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Isobutylamine	73	C4H11N	000078-81-9	5
5		Pentane	72	C5H12	000109-66-0	4



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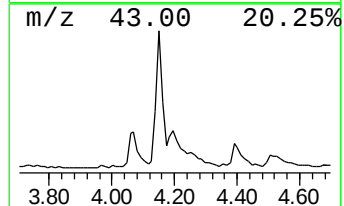
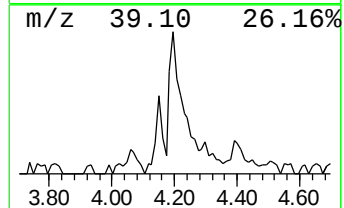
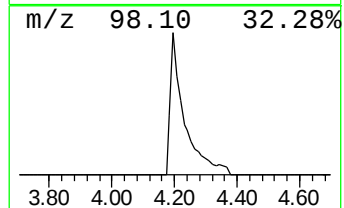
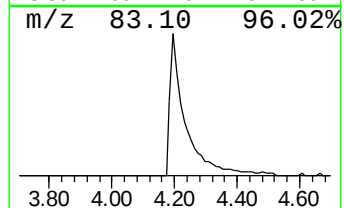
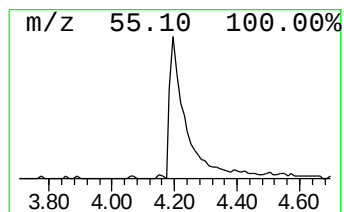
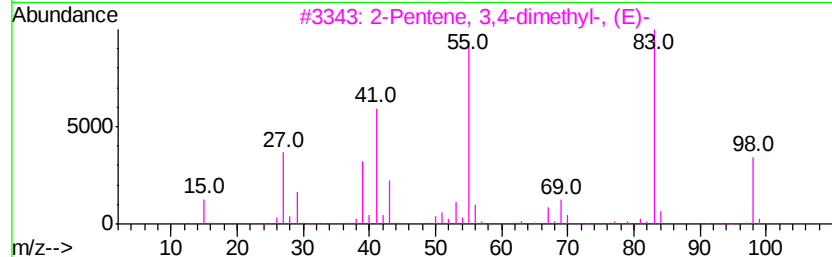
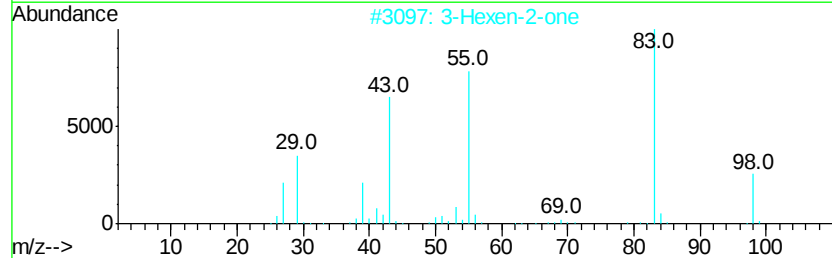
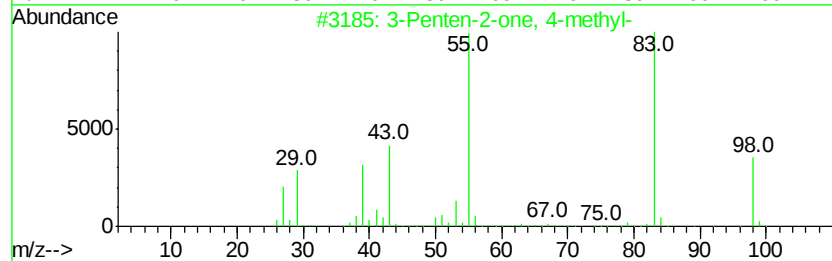
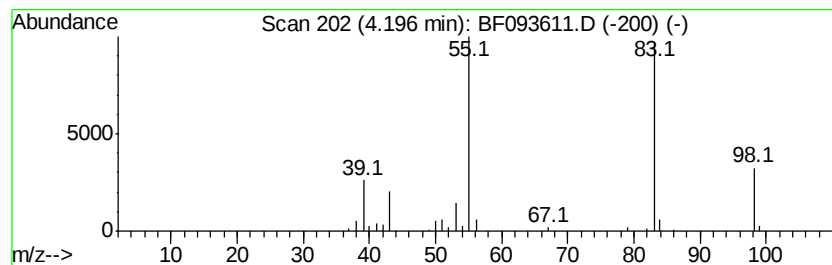
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	4.53 ng	219286	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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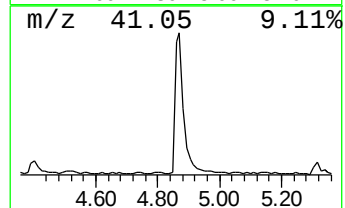
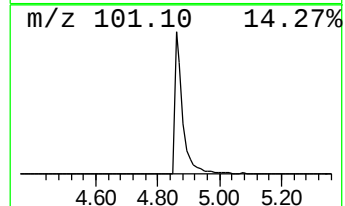
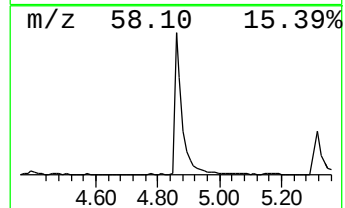
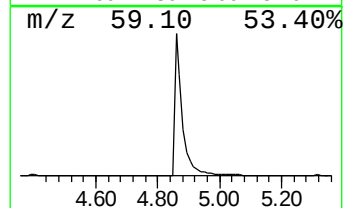
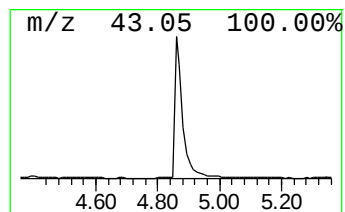
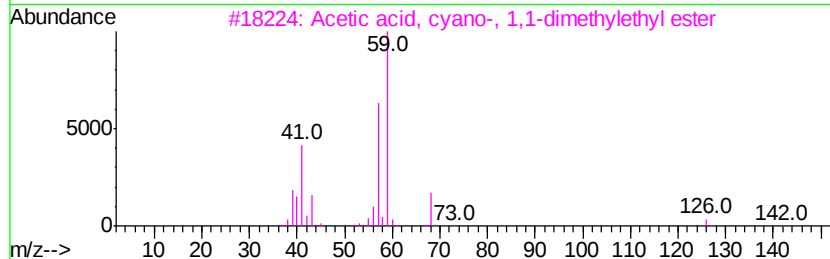
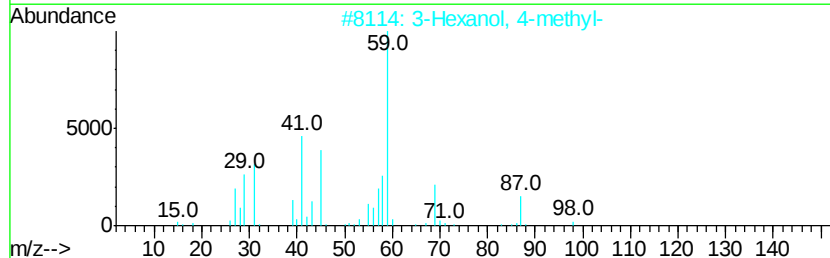
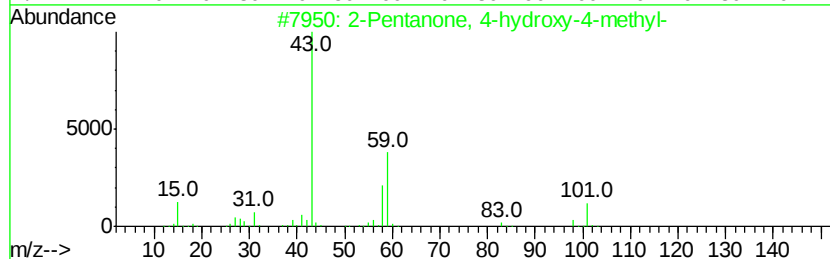
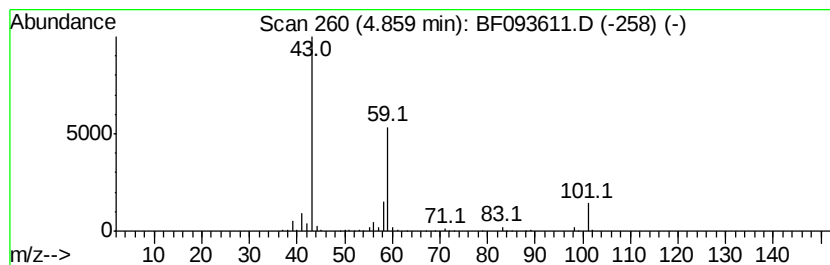
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	32.65 ng	1581990	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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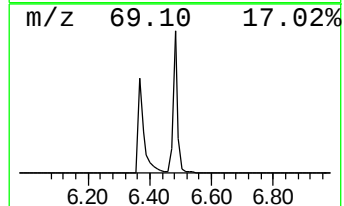
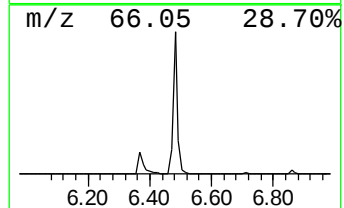
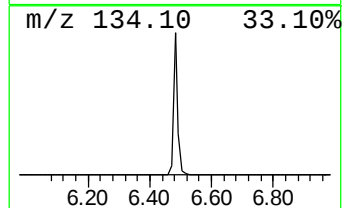
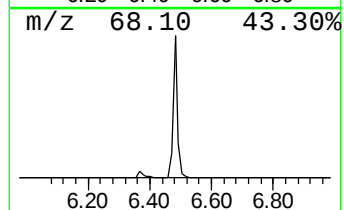
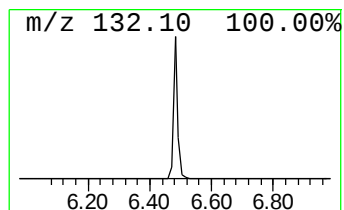
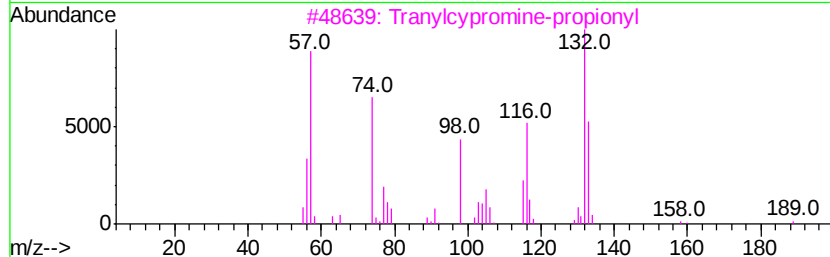
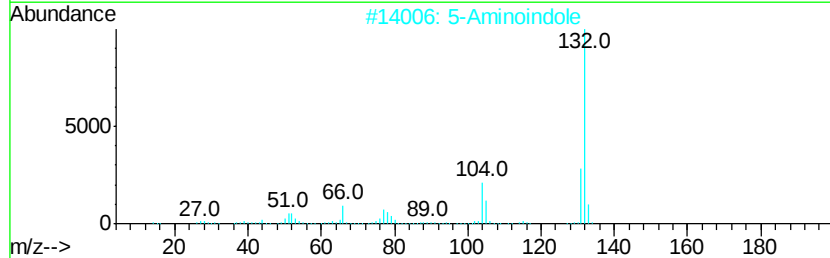
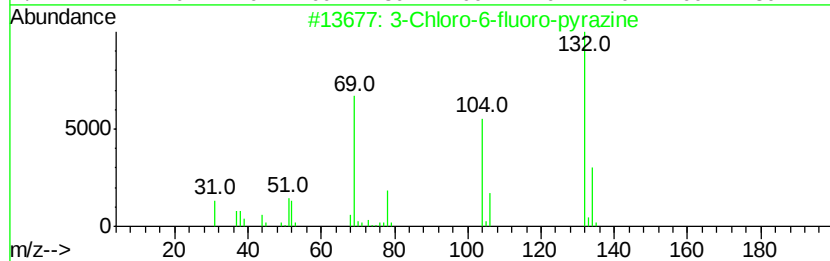
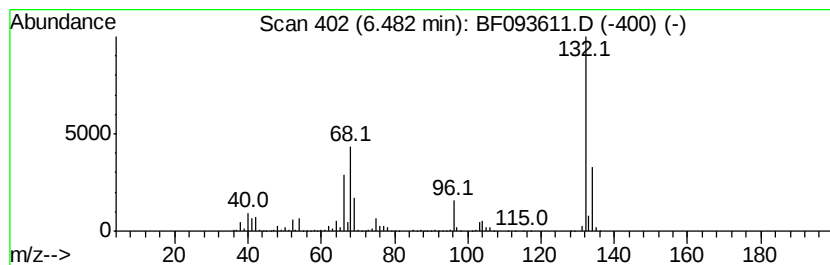
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	87.41 ng	4235680	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.40	3.7	ng	177330	1	6.71	969117	20.0
3-Penten-2-one, 4...	4.20	4.5	ng	219286	1	6.71	969117	20.0
2-Pentanone, 4-hy...	4.86	32.6	ng	1581990	1	6.71	969117	20.0
unknown6.48	6.48	87.4	ng	4235680	1	6.71	969117	20.0