

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093621.D
 Acq On : 13 Mar 2017 21:34
 Operator : SJ/MA
 Sample : I2230-06
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-3-CHAR

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	2.458	48	50	64	rVB	59556	170638	2.94%	0.354%
2	4.173	197	200	202	rBV	52941	89026	1.53%	0.185%
3	4.207	202	203	218	rVV2	87156	264492	4.56%	0.548%
4	4.413	218	221	228	rVB	41175	93665	1.61%	0.194%
5	4.870	259	261	284	rBV	1113978	2208354	38.07%	4.577%
6	5.316	298	300	328	rBV	4145670	5800559	100.00%	12.022%
7	5.716	333	335	343	rVB	74709	122371	2.11%	0.254%
8	6.367	390	392	400	rBV	3712226	5094105	87.82%	10.558%
9	6.482	400	402	405	rVB	4961477	5015521	86.47%	10.395%
10	6.710	419	422	427	rBV	949888	1082350	18.66%	2.243%
11	6.859	433	435	438	rBV	3878722	3927642	67.71%	8.141%
12	7.282	470	472	486	rBV	3174976	3699759	63.78%	7.668%
13	8.002	533	535	547	rBV	1222106	1419032	24.46%	2.941%
14	9.076	626	629	632	rBV	3992978	5768580	99.45%	11.956%
15	9.762	686	689	691	rBV	1094305	1525688	26.30%	3.162%
16	10.551	756	758	761	rBV2	2321189	3125062	53.88%	6.477%
17	11.248	817	819	825	rBV	1684352	1600150	27.59%	3.317%
18	12.837	955	958	961	rBV	4531379	4971132	85.70%	10.303%
19	13.900	1049	1051	1059	rBV	923263	1314404	22.66%	2.724%
20	15.305	1171	1174	1183	rBV	649395	955570	16.47%	1.981%

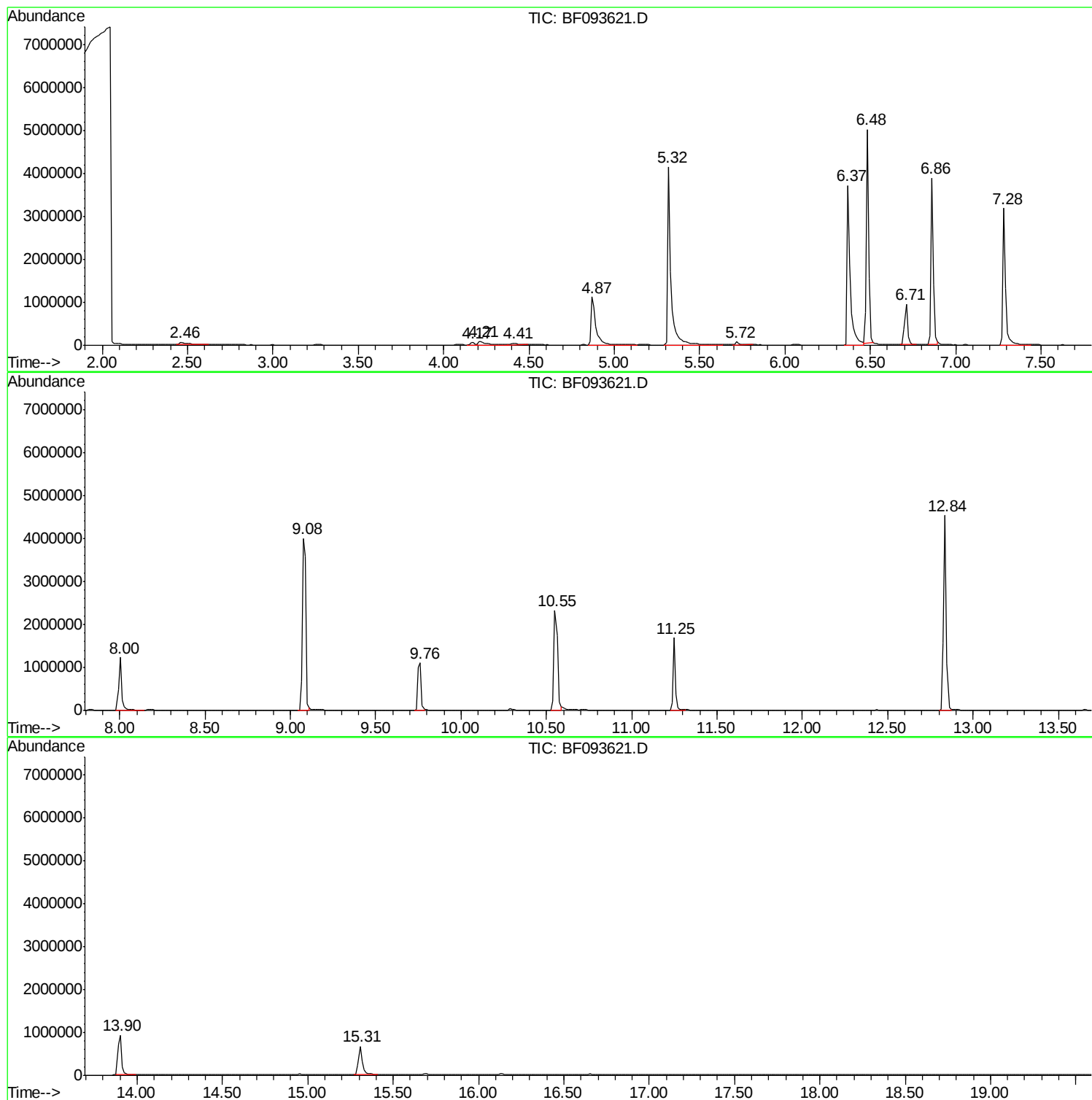
Sum of corrected areas: 48248100

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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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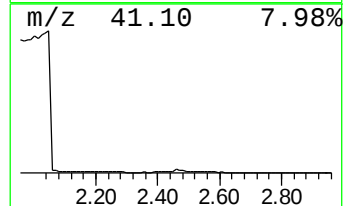
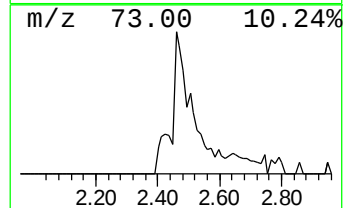
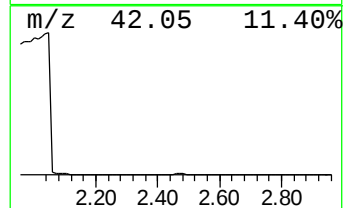
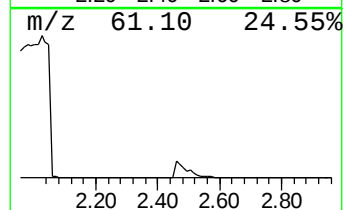
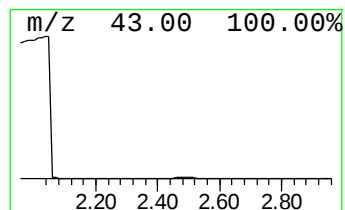
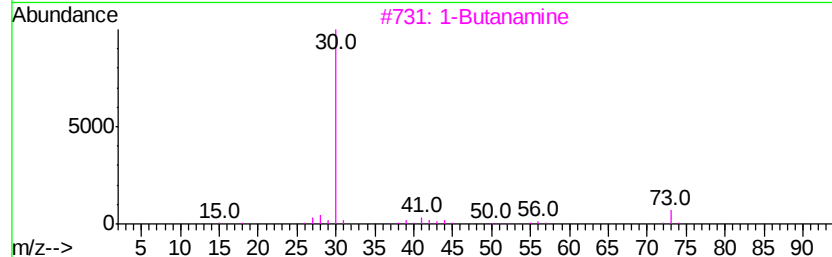
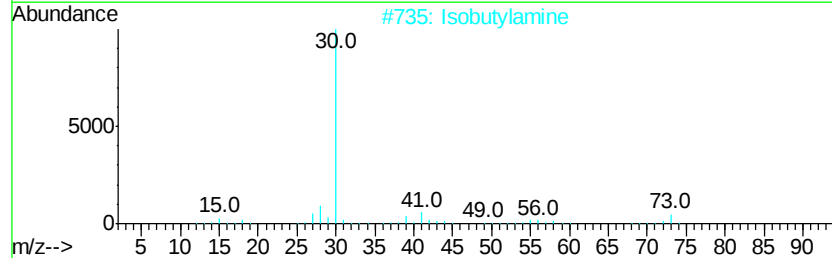
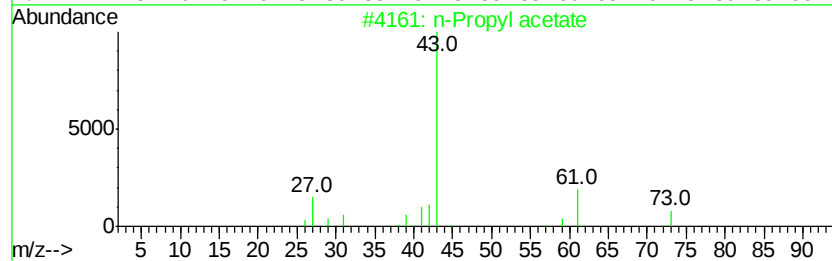
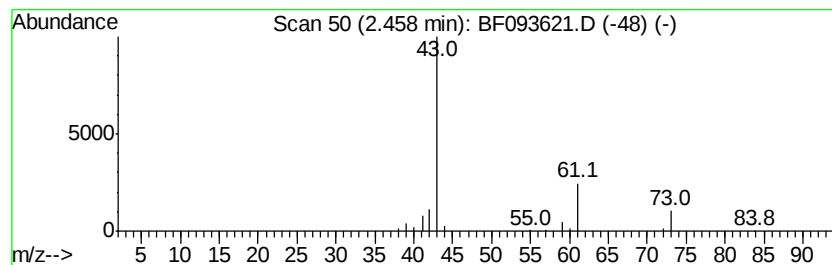
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	3.15 ng	170638	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Isobutylamine	73	C4H11N	000078-81-9	7
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5		Pentane	72	C5H12	000109-66-0	4



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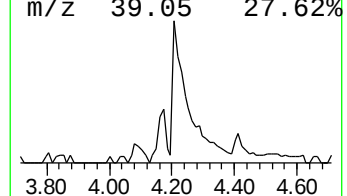
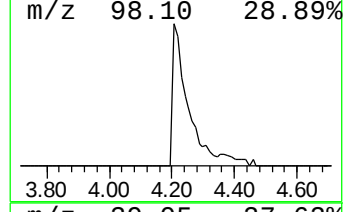
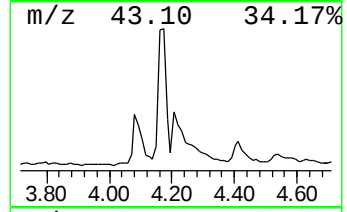
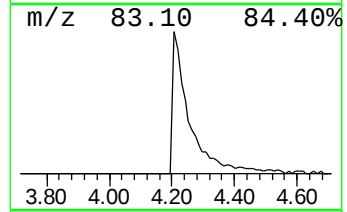
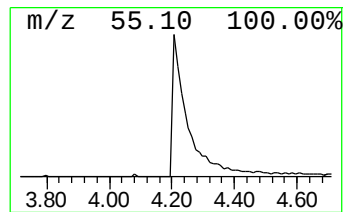
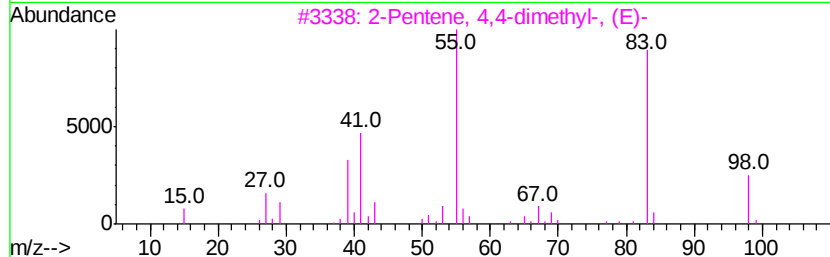
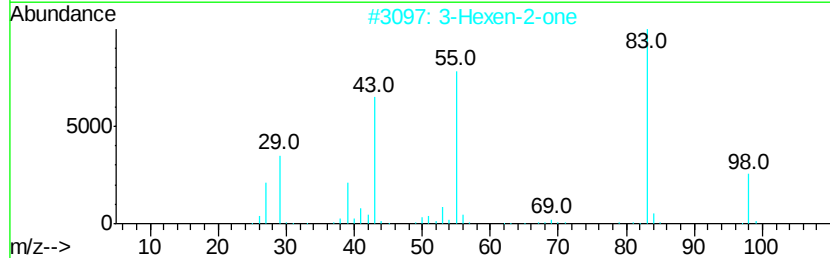
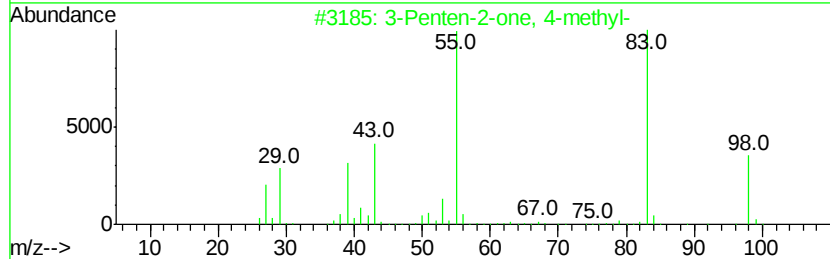
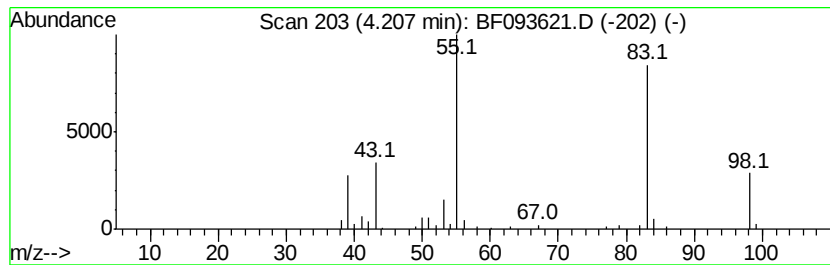
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	4.89 ng	264492	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	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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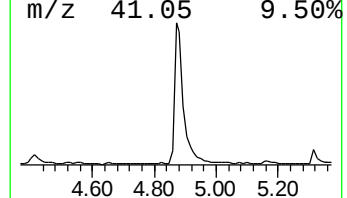
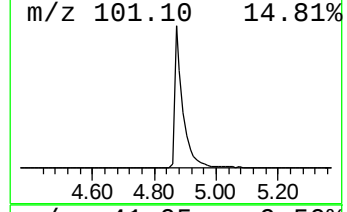
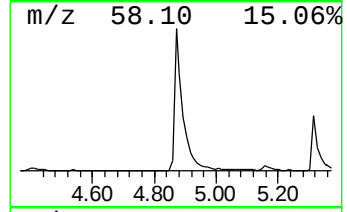
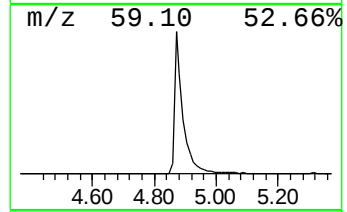
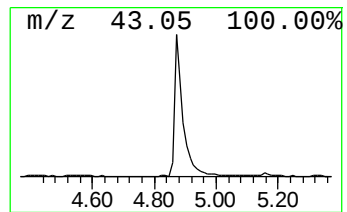
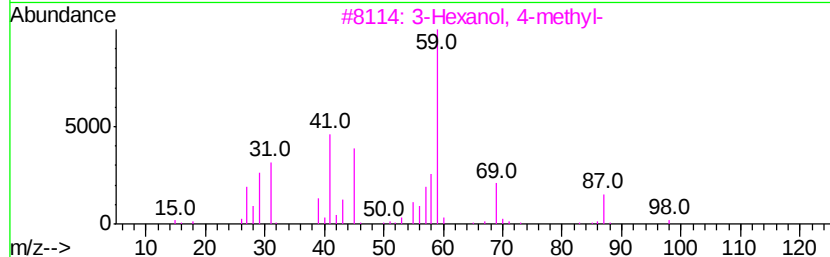
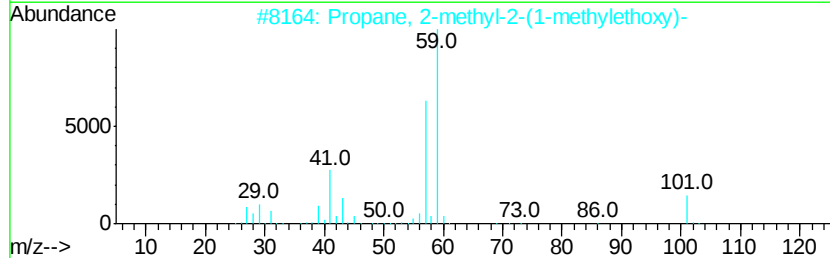
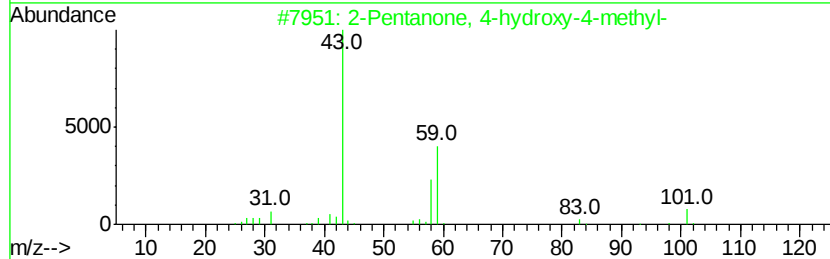
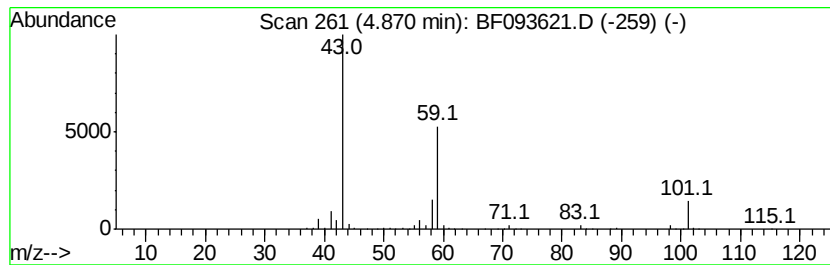
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	40.81 ng	2208350	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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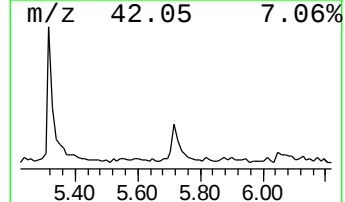
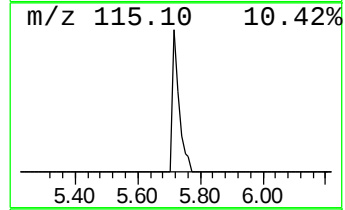
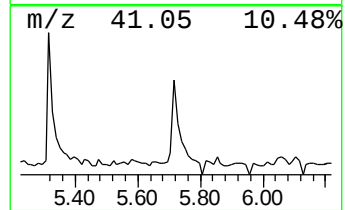
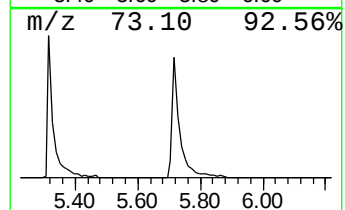
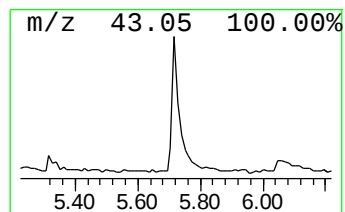
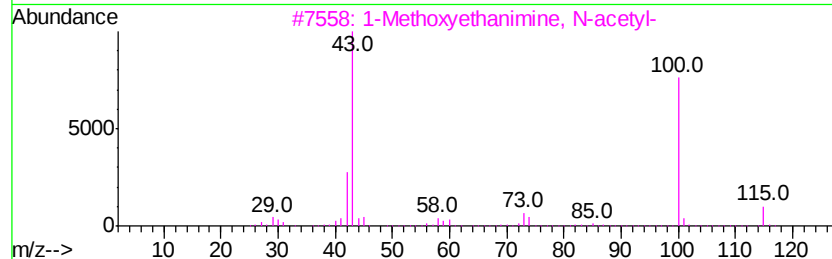
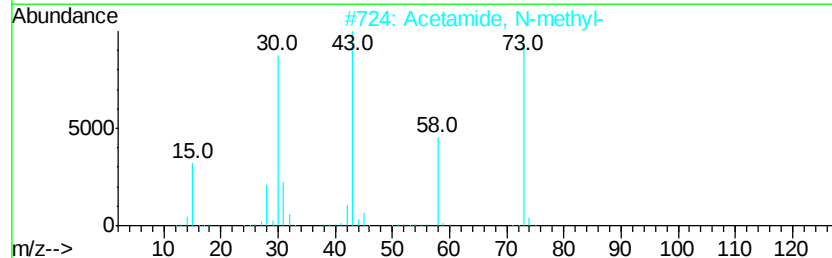
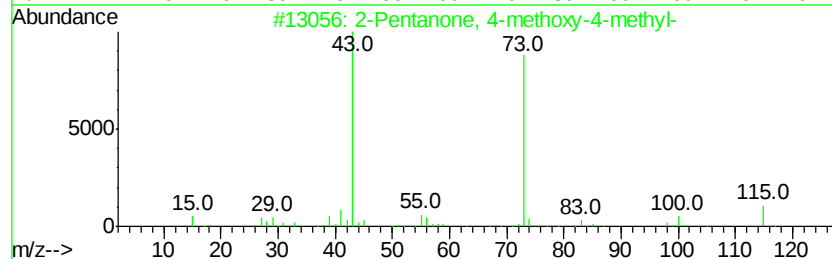
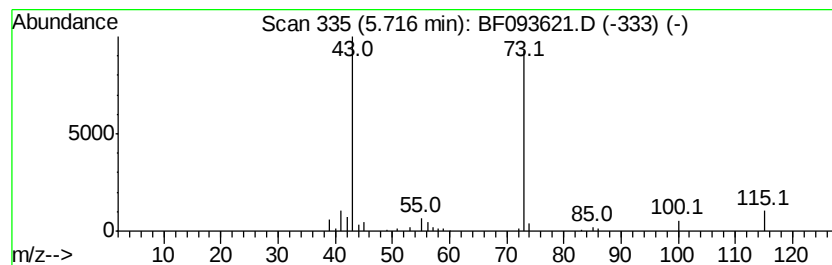
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.26 ng	122371	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
4		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	17
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12



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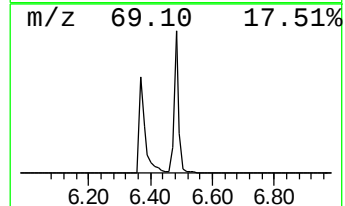
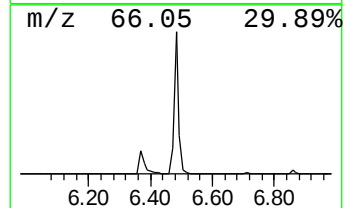
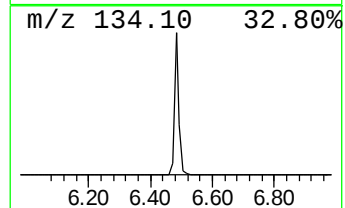
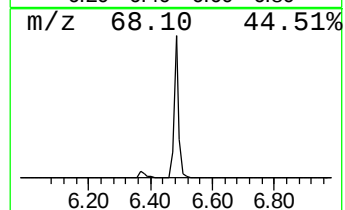
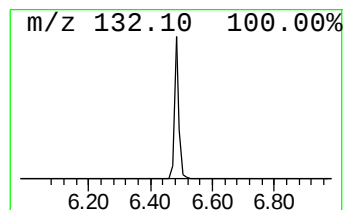
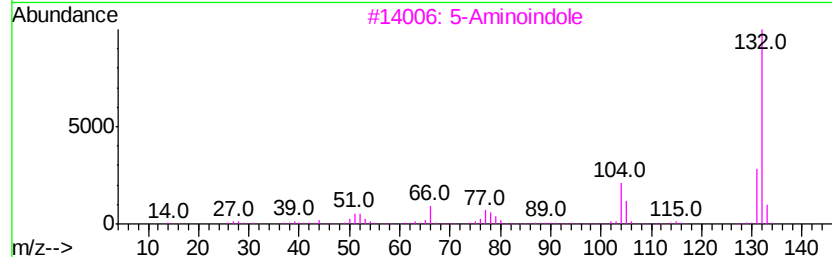
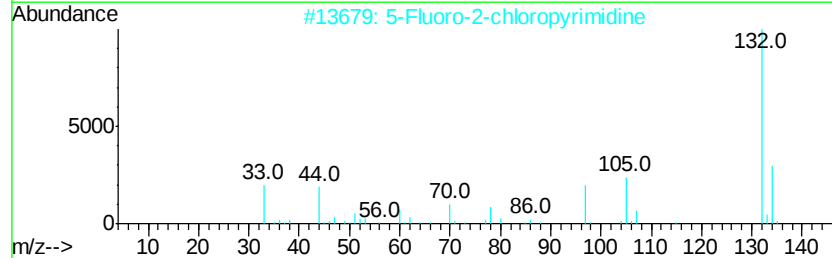
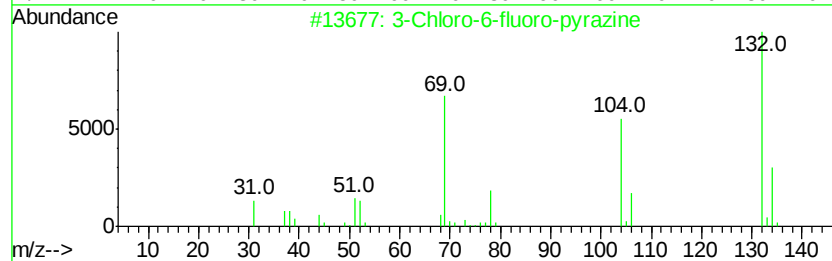
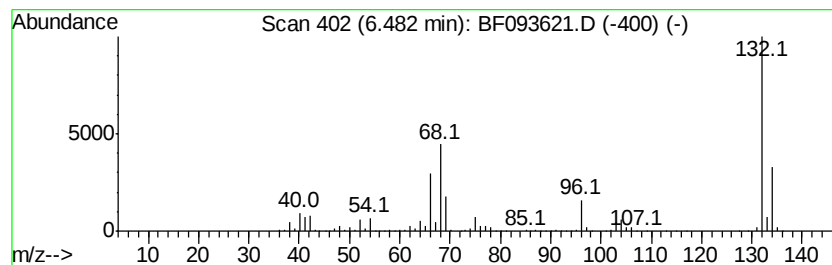
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Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	92.68 ng	5015520	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.46	3.1	ng	170638	1	6.71	1082350	20.0
3-Penten-2-one, 4...	4.21	4.9	ng	264492	1	6.71	1082350	20.0
2-Pentanone, 4-hy...	4.87	40.8	ng	2208350	1	6.71	1082350	20.0
2-Pentanone, 4-me...	5.72	2.3	ng	122371	1	6.71	1082350	20.0
unknown6.48	6.48	92.7	ng	5015520	1	6.71	1082350	20.0