

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
 Data File : BF084661.D
 Acq On : 30 Jan 2016 3:18
 Operator : SJ/IZ
 Sample : H1261-11
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SCARBOROUGH1516-00(0-4)

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-BF012916.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	2.453	29	32	38	rVB	120536	194610	2.99%	0.370%
2	4.213	183	186	191	rBV	941145	1362386	20.94%	2.592%
3	4.898	243	246	256	rVB	2075276	2956013	45.44%	5.625%
4	5.333	281	284	286	rBV	4555504	4532403	69.67%	8.624%
5	5.733	317	319	322	rBV	188917	184399	2.83%	0.351%
6	6.373	372	375	377	rBV	4202679	4018383	61.77%	7.646%
7	6.499	383	386	388	rBV	4794509	5135944	78.95%	9.772%
8	6.727	404	406	408	rBV	952250	1083582	16.66%	2.062%
9	6.876	417	419	422	rBV	3428761	3947784	60.68%	7.512%
10	7.287	452	455	458	rBV	2617759	3360500	51.66%	6.394%
11	8.007	516	518	522	rBV2	1677073	2606120	40.06%	4.959%
12	8.716	578	580	583	rVB	164733	192580	2.96%	0.366%
13	8.819	586	589	591	rVB	129598	109885	1.69%	0.209%
14	9.093	610	613	615	rBV	5770265	6505597	100.00%	12.379%
15	9.756	669	671	673	rBV	1634372	1592232	24.47%	3.030%
16	9.790	673	674	676	rVB	239598	173101	2.66%	0.329%
17	9.962	687	689	691	rBV	104623	86196	1.32%	0.164%
18	10.305	717	719	721	rVB	113404	94712	1.46%	0.180%
19	10.545	737	740	743	rBV	3354134	3657129	56.22%	6.959%
20	11.242	798	801	802	rBV	1583011	1681732	25.85%	3.200%
21	12.831	937	940	942	rBV	6135271	6319756	97.14%	12.025%
22	13.871	1028	1031	1033	rBV	1542904	1642525	25.25%	3.125%
23	15.254	1149	1152	1155	rBV	974130	1117830	17.18%	2.127%

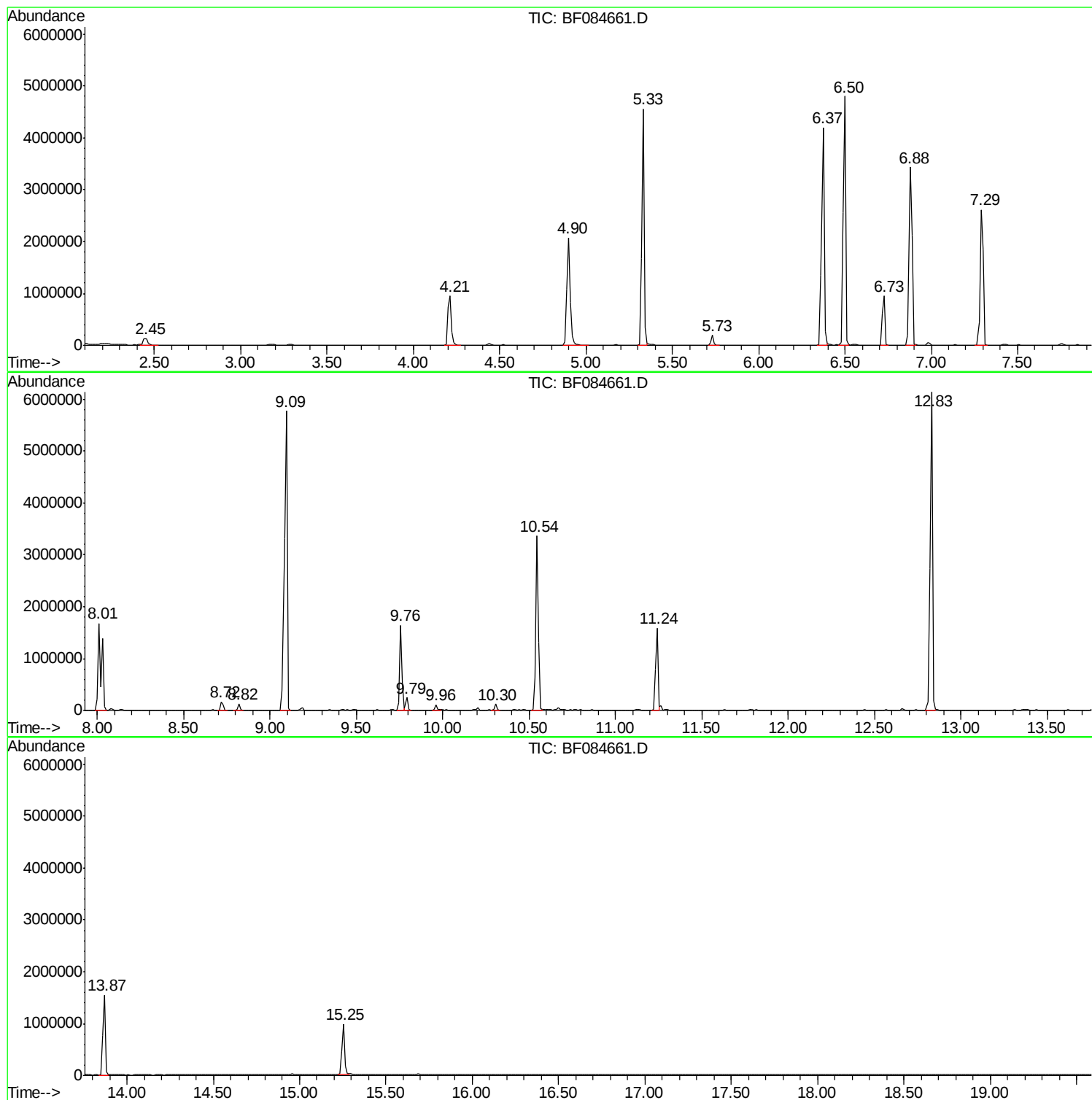
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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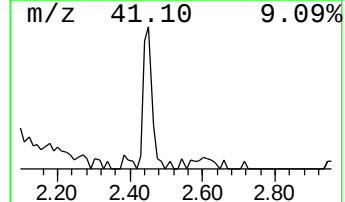
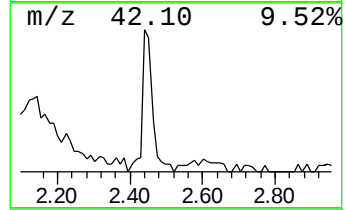
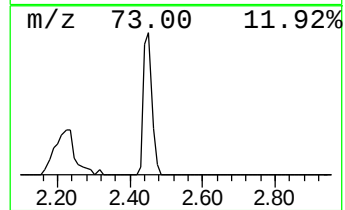
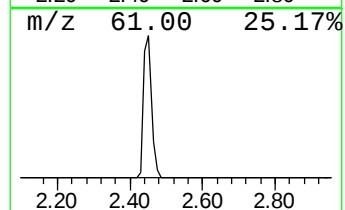
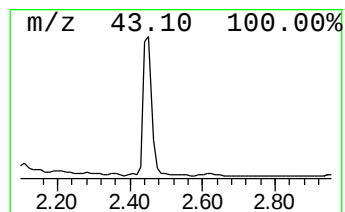
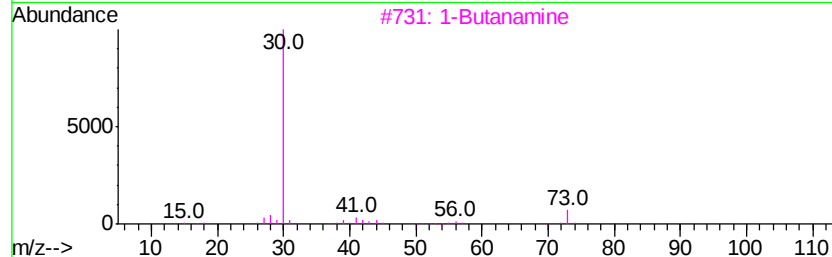
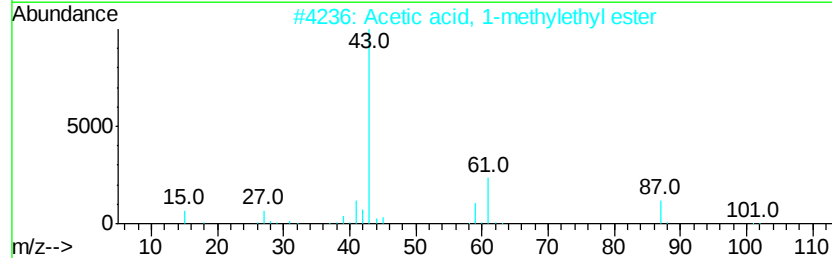
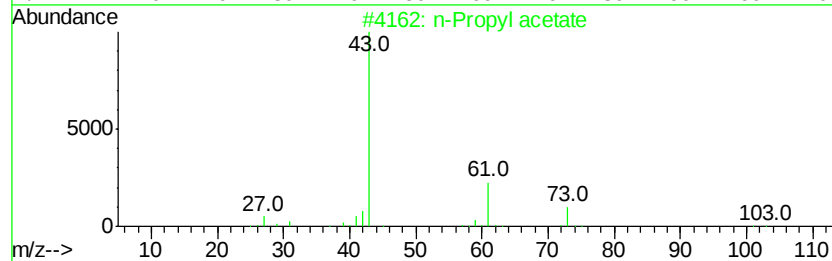
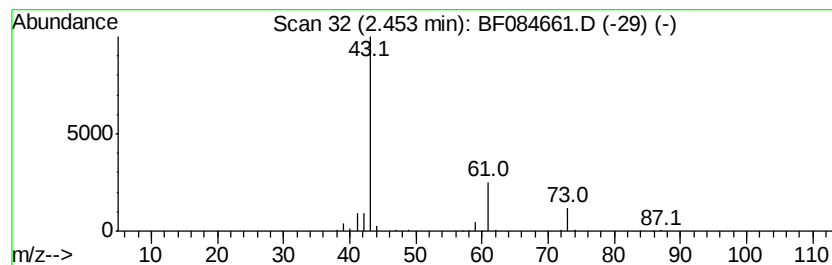
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.45	3.59 ng	194610	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	33
3		1-Butanamine	73	C4H11N	000109-73-9	5
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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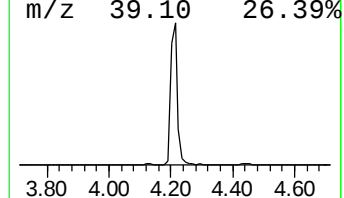
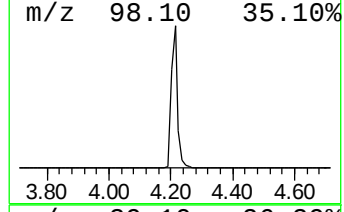
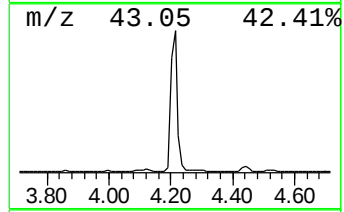
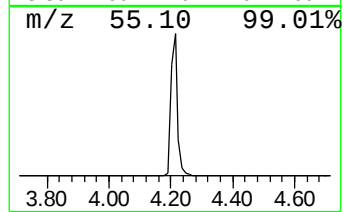
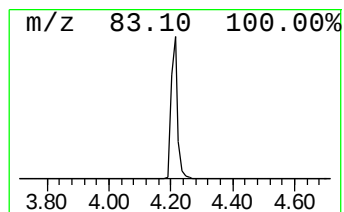
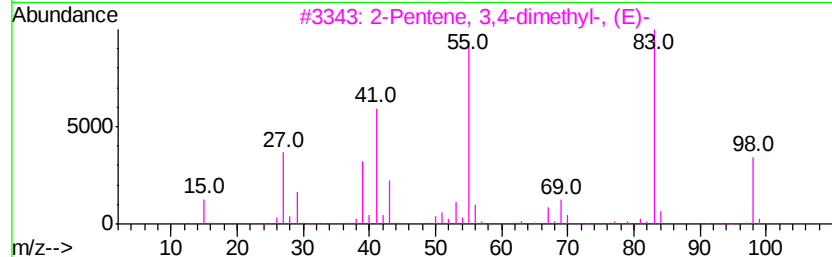
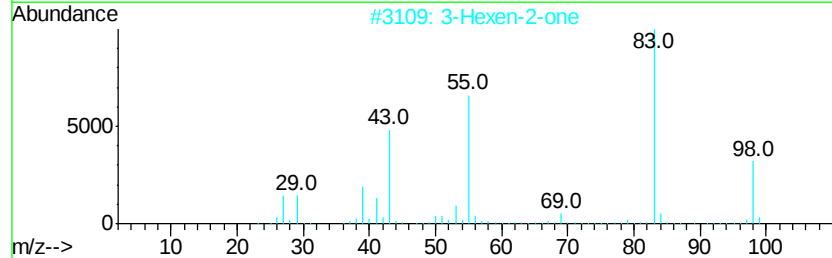
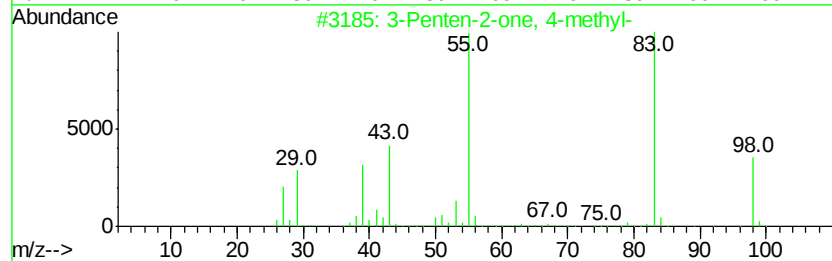
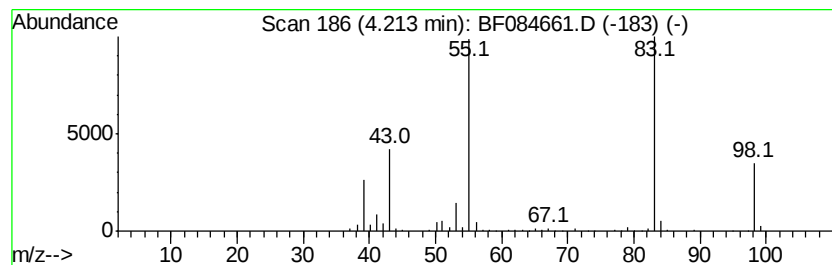
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 Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	25.15 ng	1362390	1,4-Dichlorobenzene-d4	6.73

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



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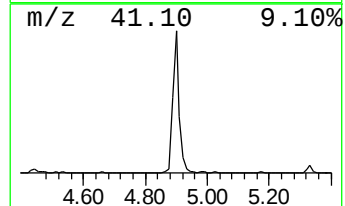
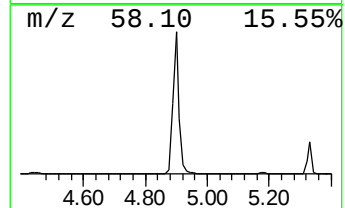
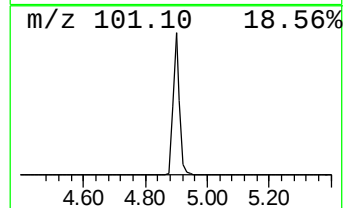
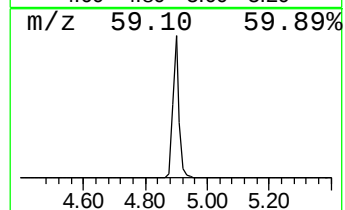
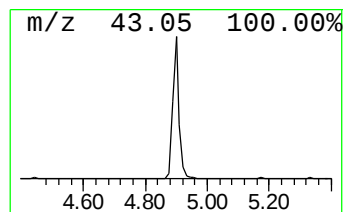
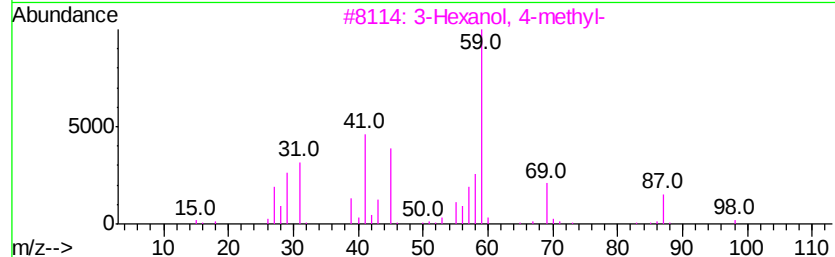
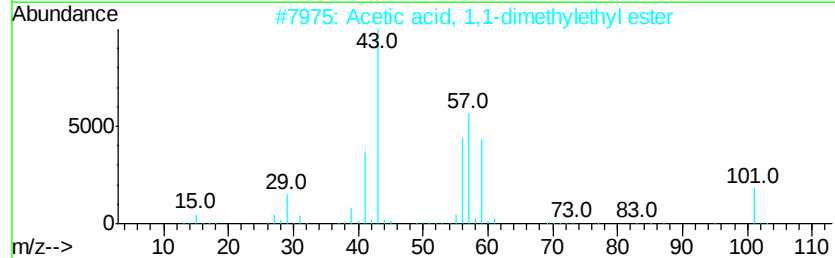
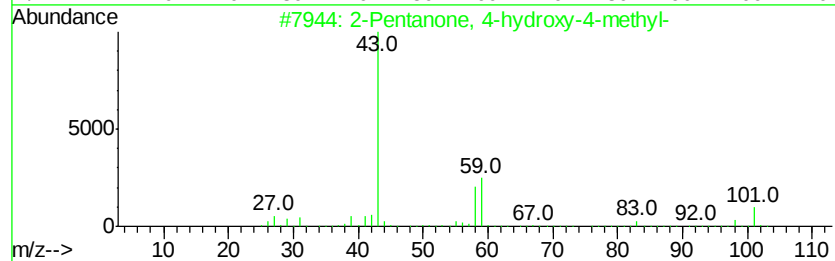
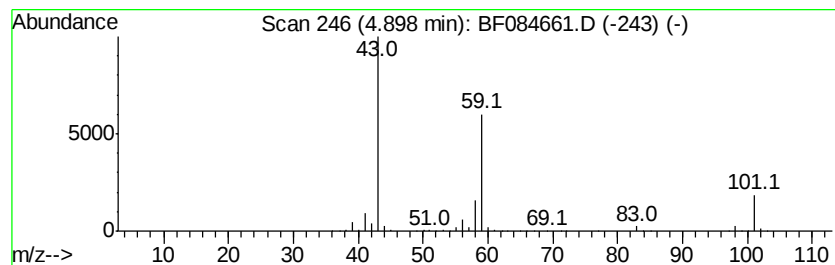
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	54.56 ng	2956010	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



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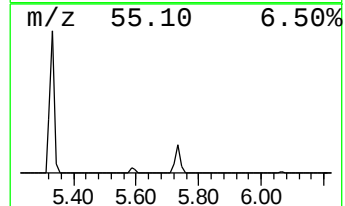
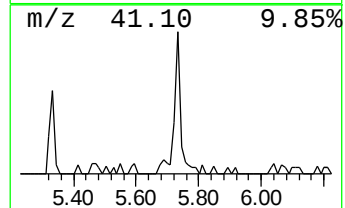
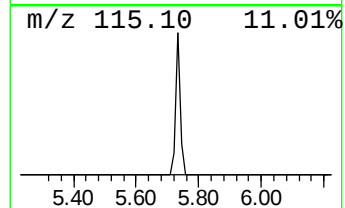
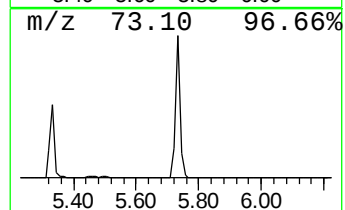
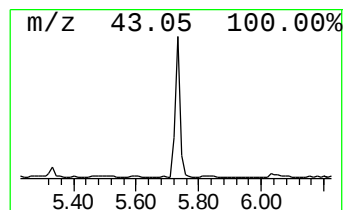
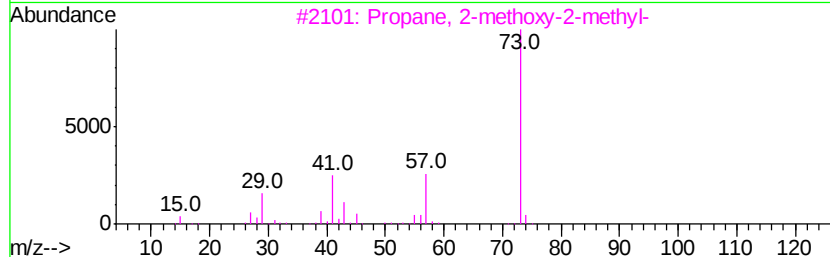
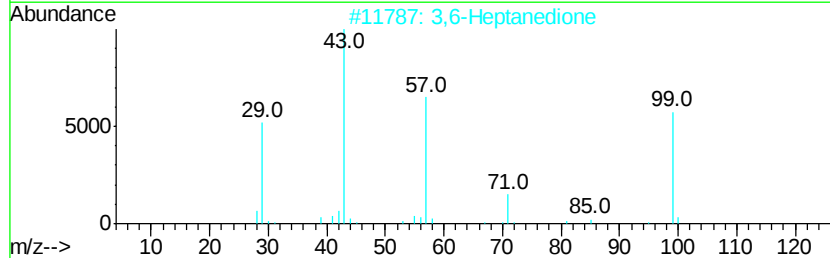
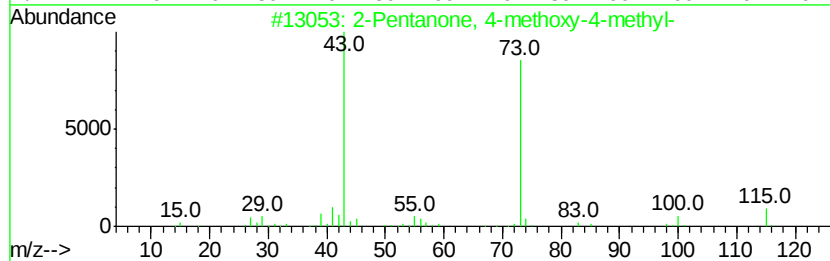
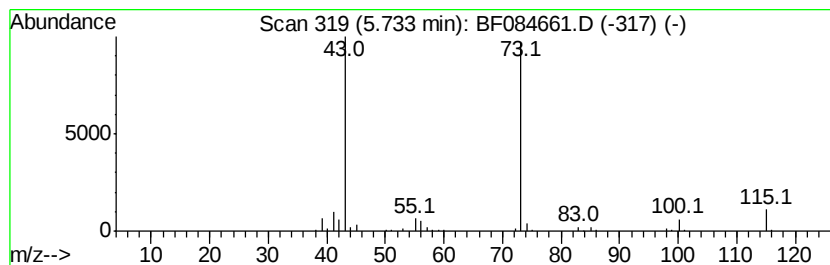
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	3.40 ng	184399	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		3,6-Heptanedione	128	C7H12O2	001703-51-1	23
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10



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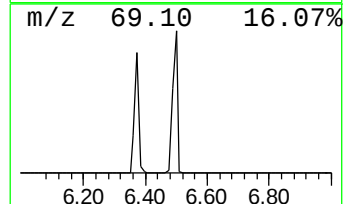
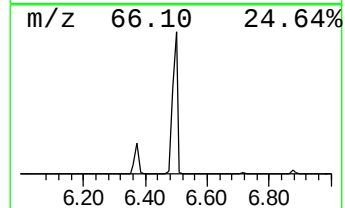
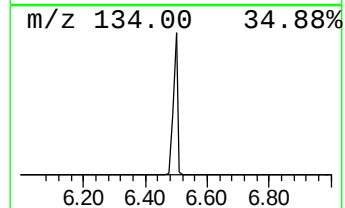
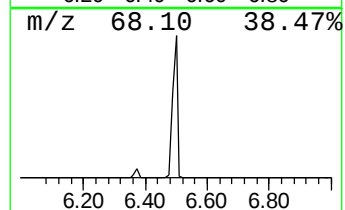
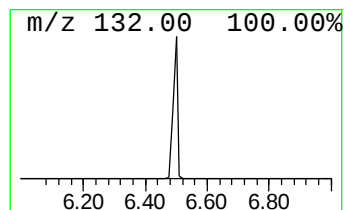
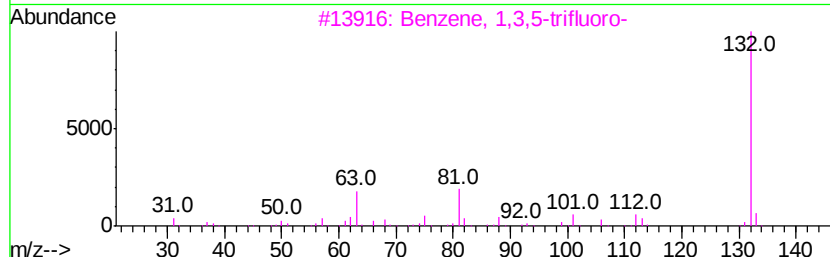
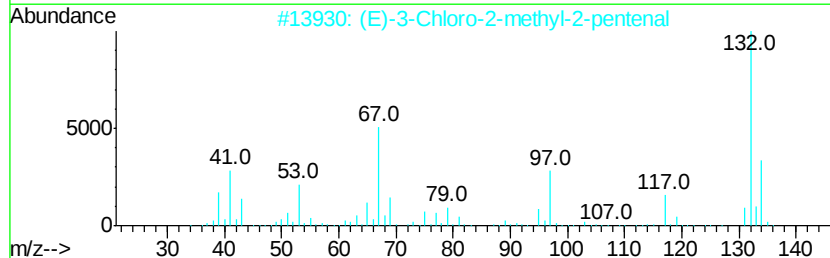
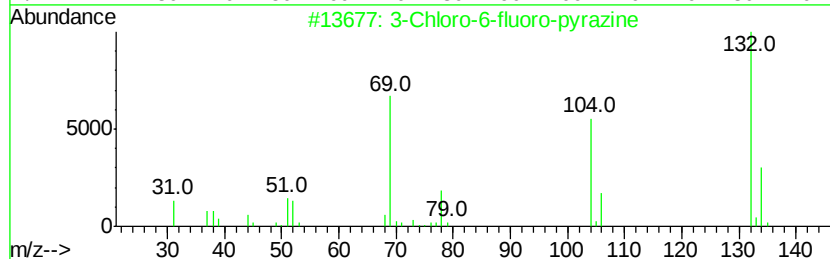
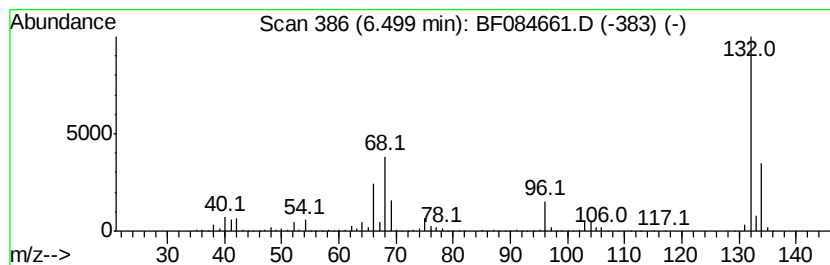
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Peak Number 5 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	94.80 ng	5135940	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.45	3.6	ng	194610	1	6.73	1083580	20.0
3-Penten-2-one, 4...	4.21	25.1	ng	1362390	1	6.73	1083580	20.0
2-Pentanone, 4-hy...	4.90	54.6	ng	2956010	1	6.73	1083580	20.0
2-Pentanone, 4-me...	5.73	3.4	ng	184399	1	6.73	1083580	20.0
unknown6.50	6.50	94.8	ng	5135940	1	6.73	1083580	20.0