

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
 Data File : BF081054.D
 Acq On : 18 Aug 2015 21:24
 Operator : UM/IZ
 Sample : PB85025BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB85025BL

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-BF081715.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	3.987	173	175	181	rBV	37665	63034	2.81%	0.364%
2	4.730	237	240	243	rBV	806005	1392605	62.17%	8.046%
3	5.187	276	280	282	rBV	1241800	1743940	77.85%	10.076%
4	5.599	314	316	319	rBV	62100	52093	2.33%	0.301%
5	6.250	370	373	375	rBV	1545667	1546353	69.03%	8.934%
6	6.364	381	383	386	rBV	1146863	1629233	72.73%	9.413%
7	6.604	401	404	406	rBV	448515	369781	16.51%	2.136%
8	6.765	415	418	420	rBV	1148643	1252780	55.93%	7.238%
9	7.176	451	454	456	rBV	1211418	1194756	53.34%	6.903%
10	7.885	514	516	519	rBV	337078	458071	20.45%	2.647%
11	8.970	608	611	613	rBV	2127726	1846411	82.43%	10.668%
12	9.633	667	669	672	rVB	623858	532366	23.77%	3.076%
13	10.422	735	738	740	rBV	1015446	1187697	53.02%	6.862%
14	11.108	795	798	800	rBV	599223	592934	26.47%	3.426%
15	12.537	921	923	924	rBB	43226	44359	1.98%	0.256%
16	12.697	934	937	939	rBV	1989289	2240069	100.00%	12.942%
17	13.234	982	984	986	rBB	46145	37466	1.67%	0.216%
18	13.725	1024	1027	1029	rBV	597634	618215	27.60%	3.572%
19	15.062	1142	1144	1147	rBV	365298	506378	22.61%	2.926%

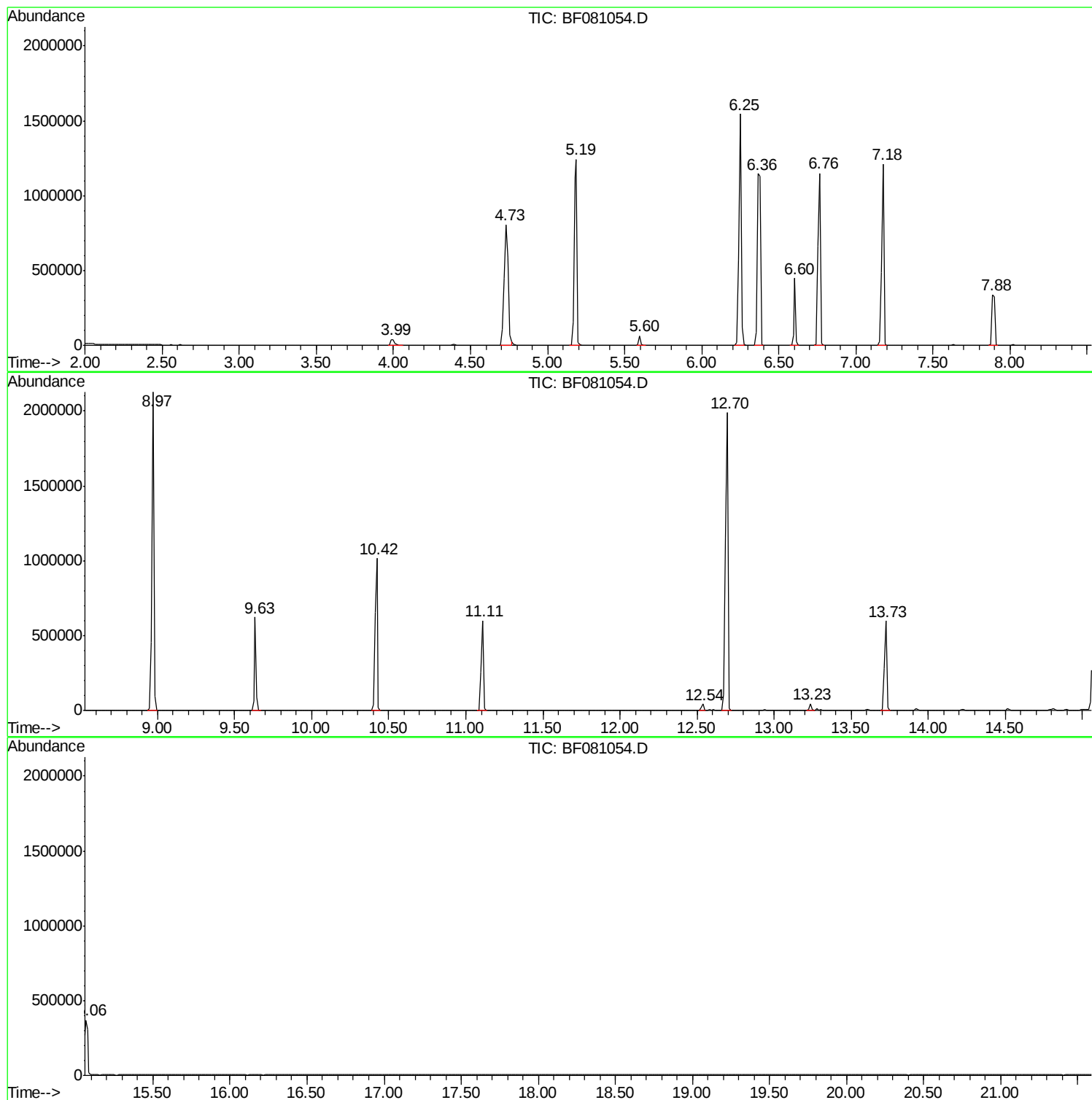
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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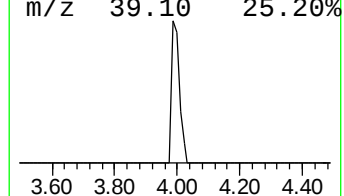
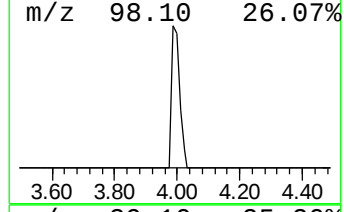
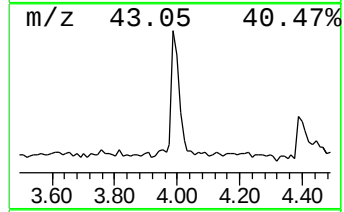
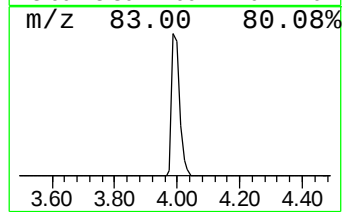
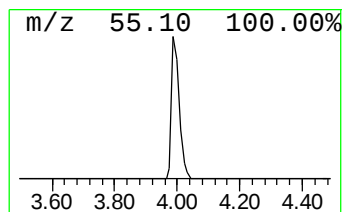
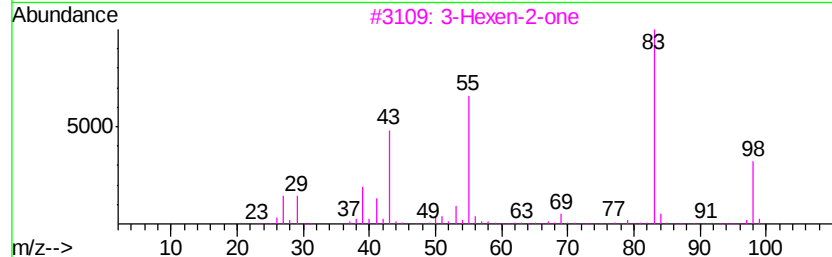
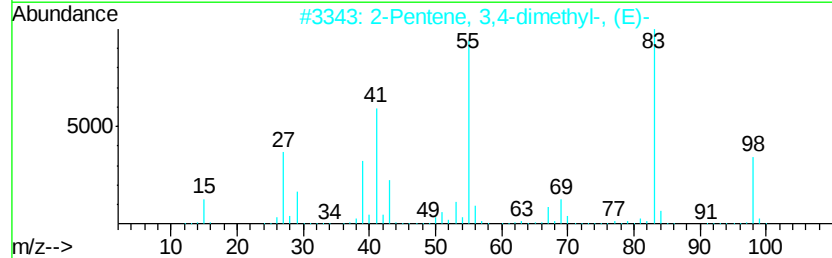
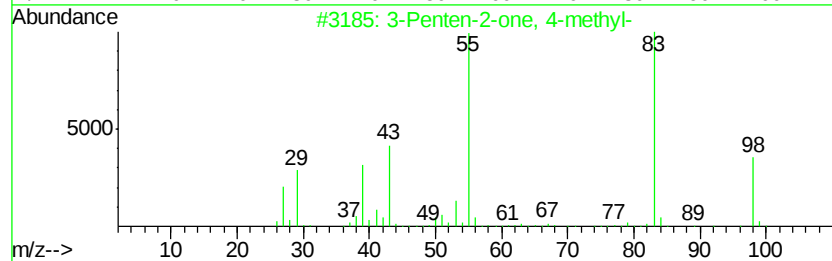
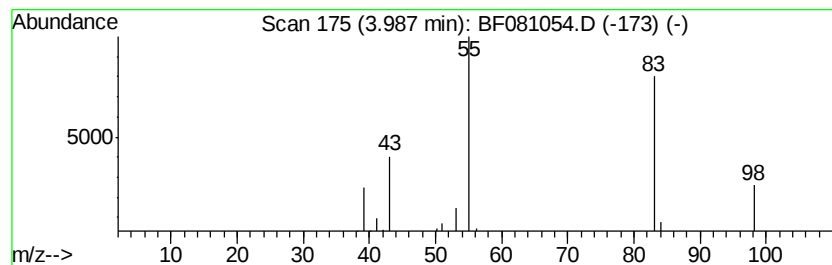
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	3.41 ng	63034	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3			3-Hexen-2-one	98	C6H10O	000763-93-9	86
4			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	80
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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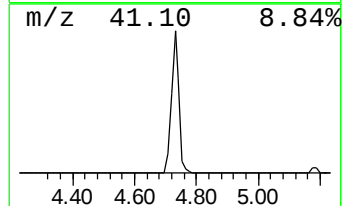
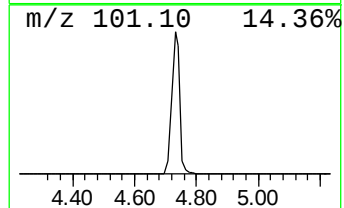
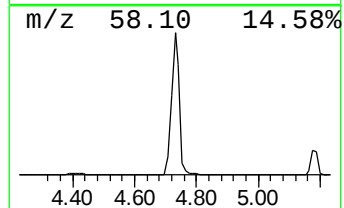
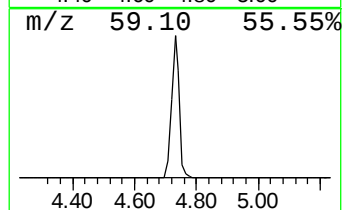
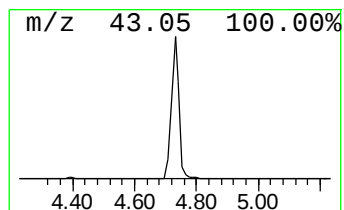
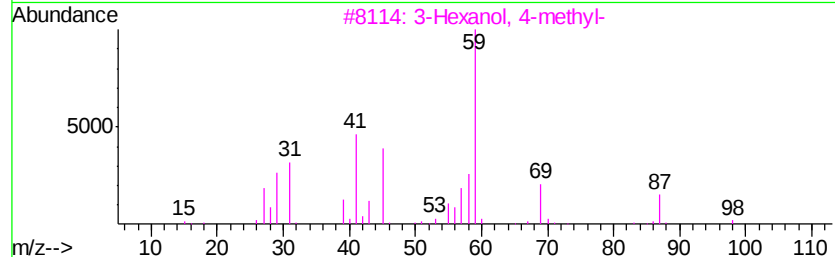
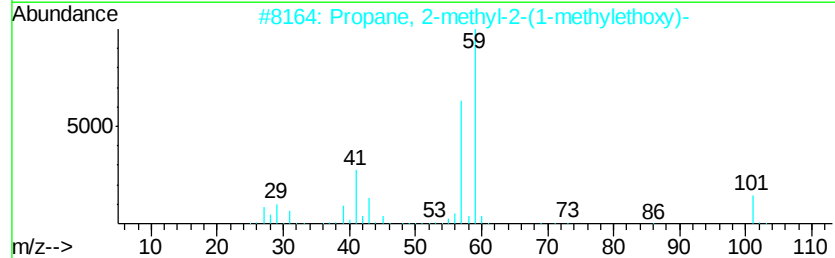
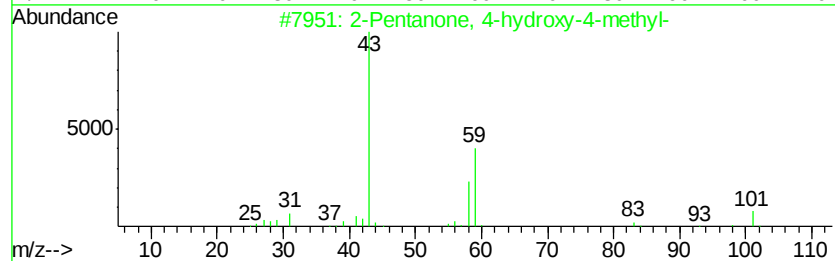
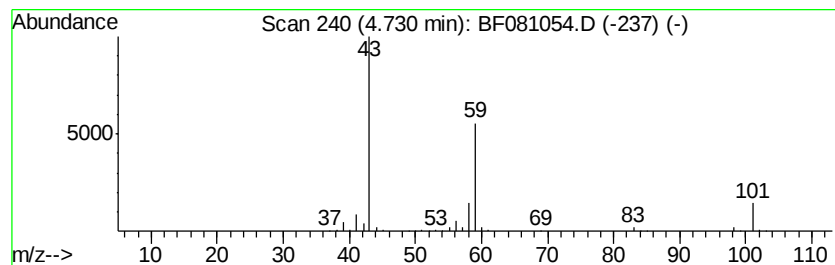
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	75.32 ng	1392610	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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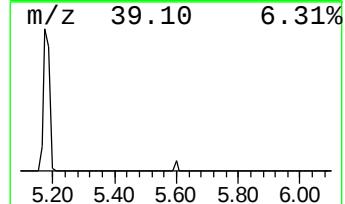
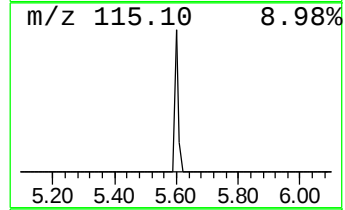
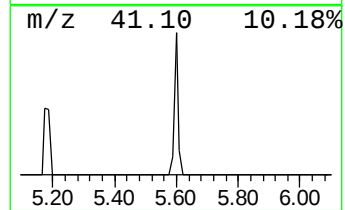
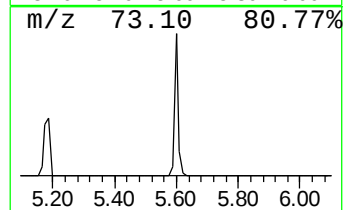
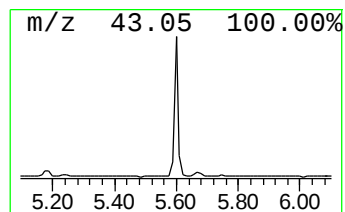
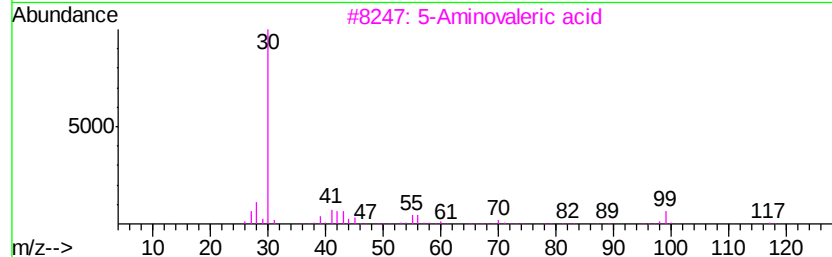
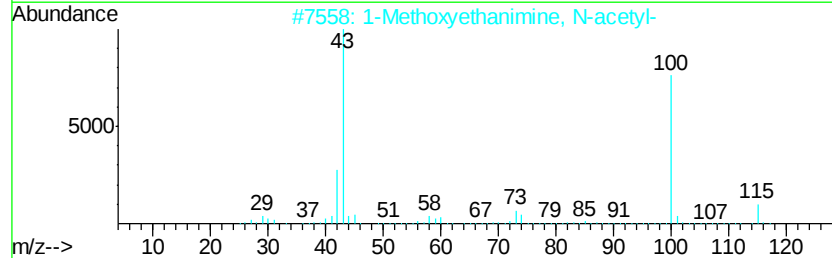
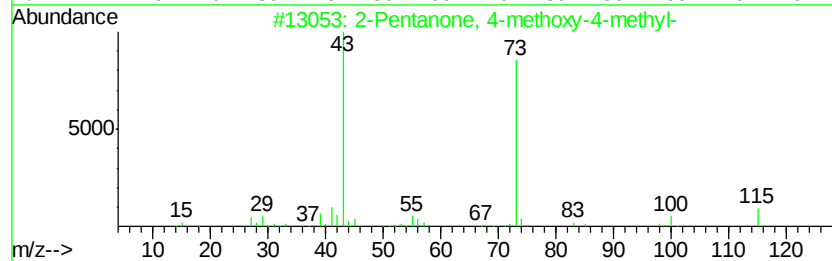
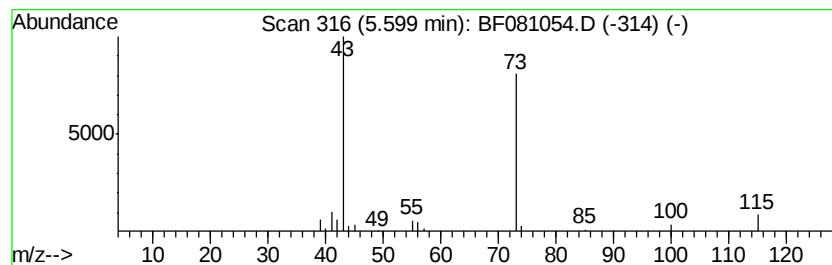
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	2.82 ng	52093	1,4-Dichlorobenzene-d4	6.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	23
3		5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Octane, 4-methyl-	128	C9H20	002216-34-4	9



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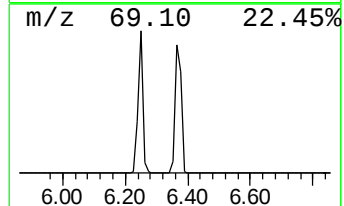
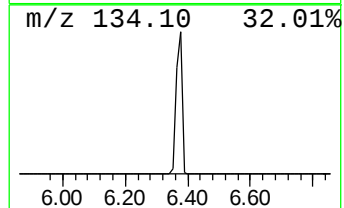
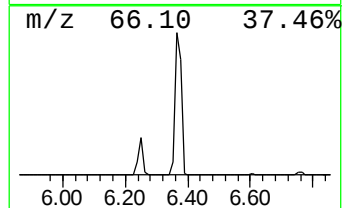
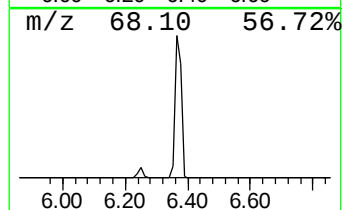
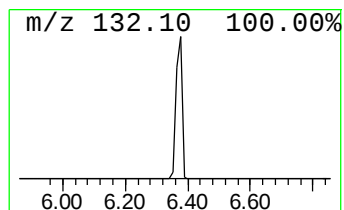
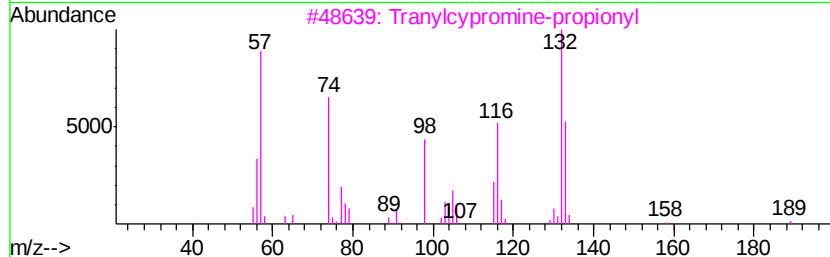
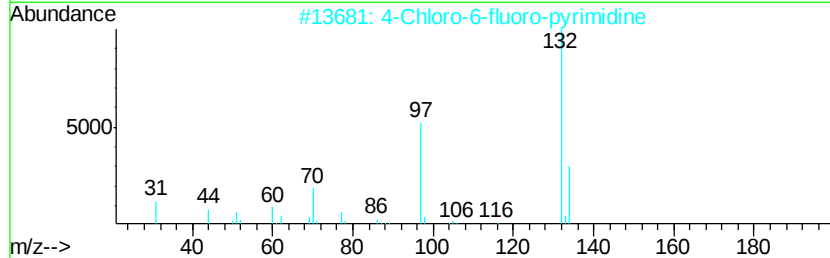
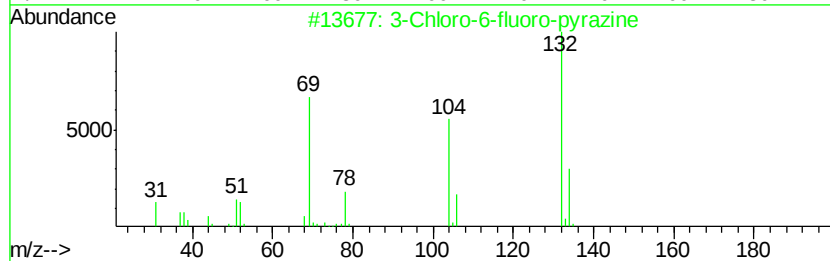
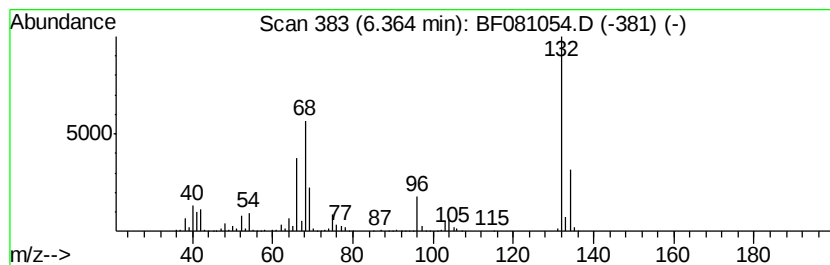
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Peak Number 4 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	88.12 ng	1629230	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.99	3.4	ng	63034	1	6.60	369781	20.0
2-Pentanone, 4-hy...	4.73	75.3	ng	1392610	1	6.60	369781	20.0
2-Pentanone, 4-me...	5.60	2.8	ng	52093	1	6.60	369781	20.0
unknown6.36	6.36	88.1	ng	1629230	1	6.60	369781	20.0