

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
 Data File : BF080744.D
 Acq On : 31 Jul 2015 20:23
 Operator : TP/UM
 Sample : PB84784BL
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84784BL

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-BF073015.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	4.419	202	204	209	rVB	180430	217823	5.09%	0.575%
2	5.059	257	260	263	rBV	2264034	3633350	84.89%	9.594%
3	5.459	292	295	298	rBV	2873022	3957385	92.46%	10.450%
4	5.870	328	331	333	rBV	142550	166178	3.88%	0.439%
5	6.476	381	384	387	rBV	3242139	3503354	81.85%	9.251%
6	6.613	394	396	399	rBV	2854770	3814892	89.13%	10.073%
7	6.853	414	417	419	rBV	972401	866267	20.24%	2.287%
8	7.002	428	430	433	rVB	2154985	2929197	68.44%	7.735%
9	7.413	463	466	468	rBV	2626276	2779571	64.94%	7.340%
10	8.133	526	529	531	rBV	1156967	1088215	25.43%	2.873%
11	9.208	620	623	626	rBV	3748077	4132817	96.56%	10.913%
12	9.882	679	682	685	rBV	1158217	1140196	26.64%	3.011%
13	10.671	748	751	753	rBV	2804710	2758583	64.45%	7.284%
14	11.368	809	812	814	rBV	1083589	1179005	27.55%	3.113%
15	12.957	948	951	953	rBV	3495292	4280000	100.00%	11.301%
16	13.985	1039	1041	1044	rBV	570756	806140	18.84%	2.129%
17	15.402	1162	1165	1168	rBV	409283	618184	14.44%	1.632%

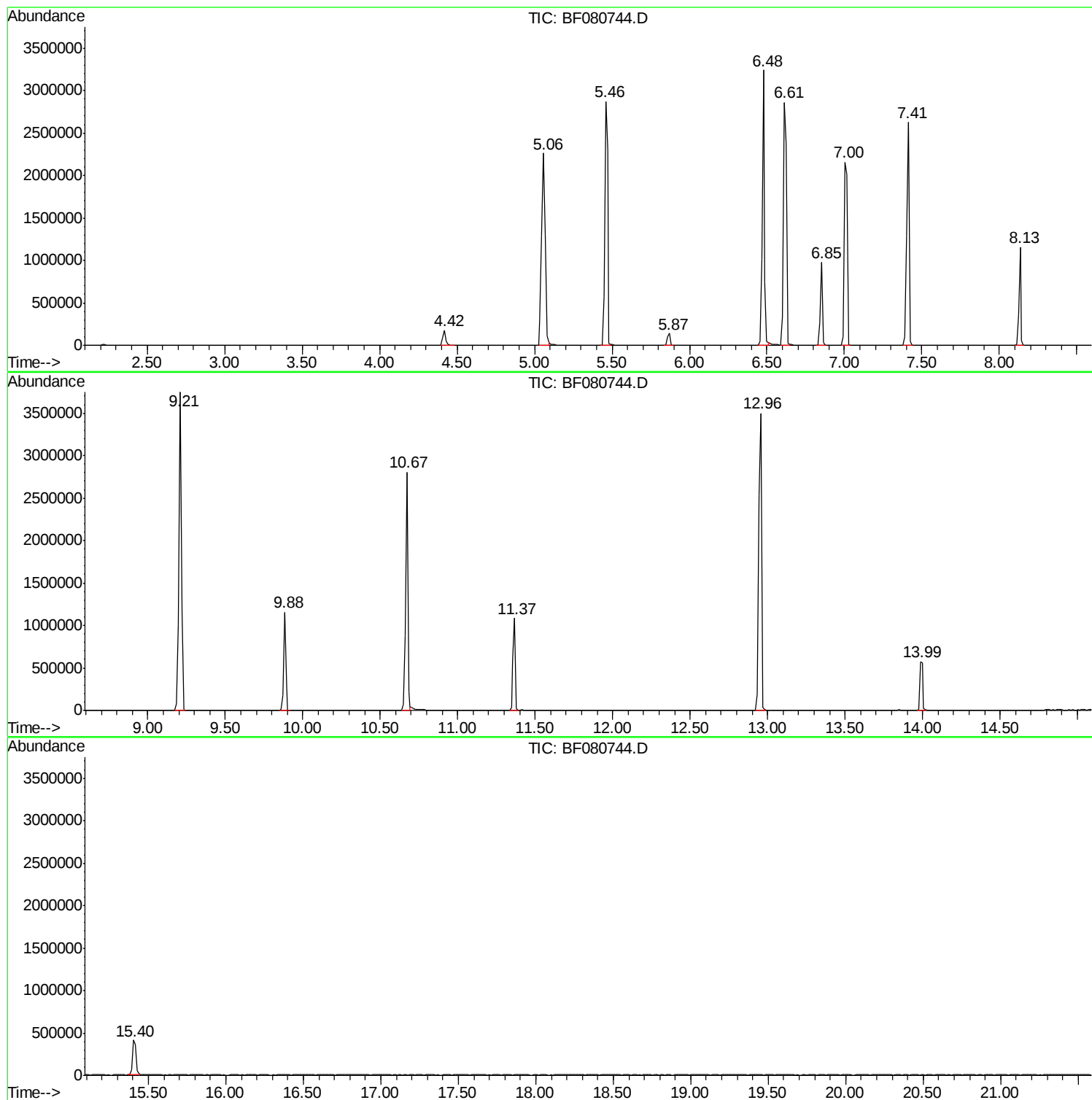
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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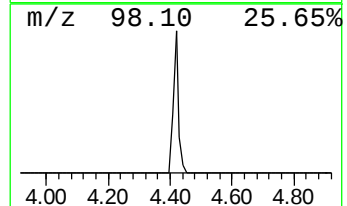
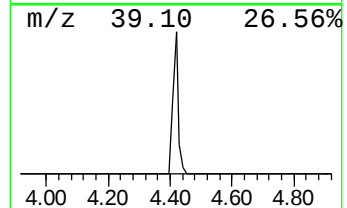
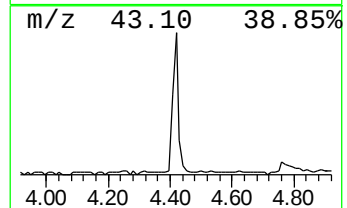
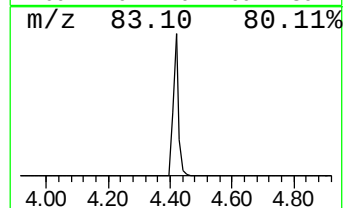
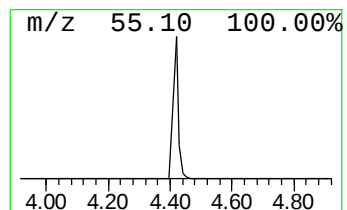
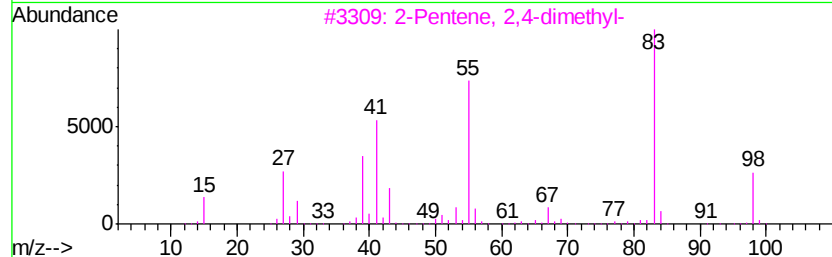
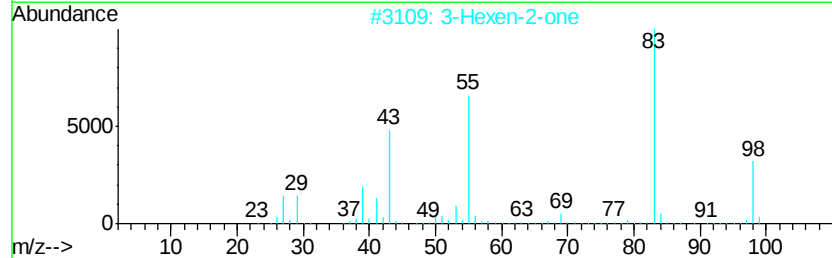
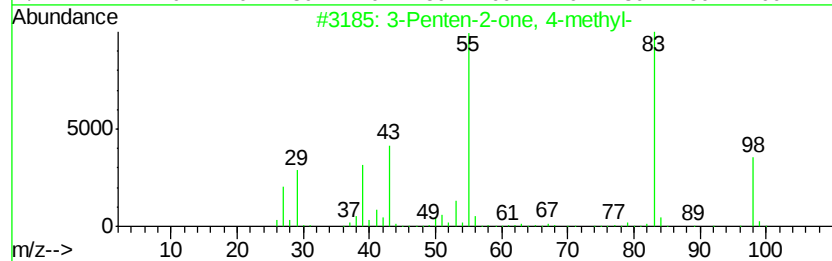
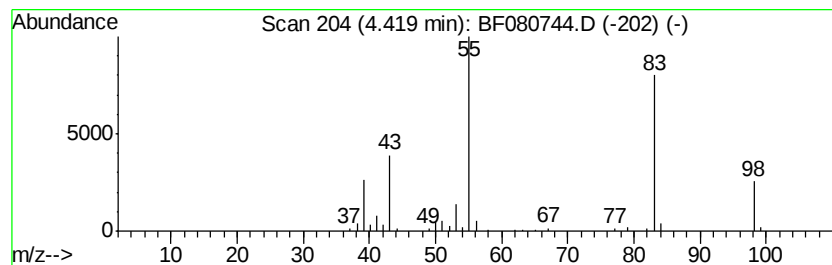
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.42	5.03 ng	217823	1,4-Dichlorobenzene-d4	6.85

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	87
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72



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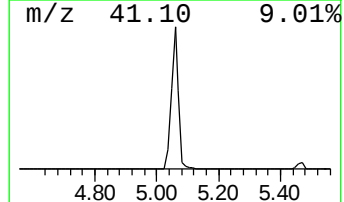
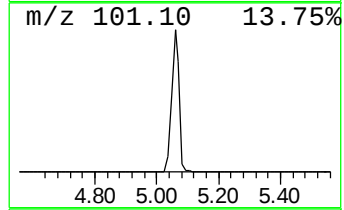
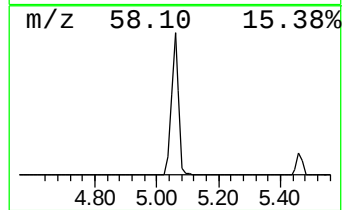
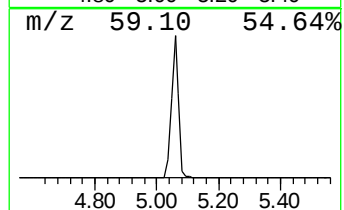
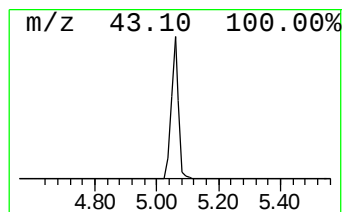
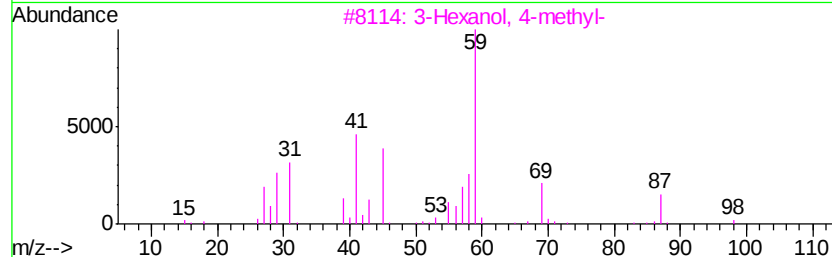
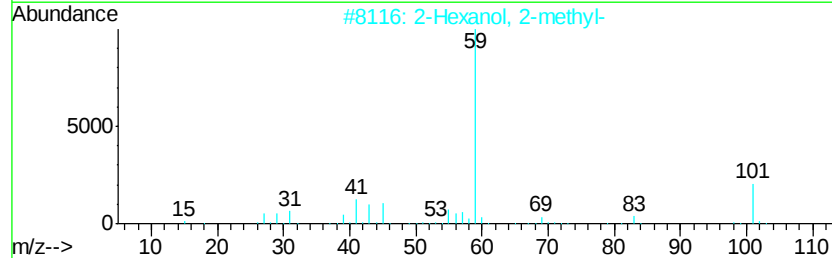
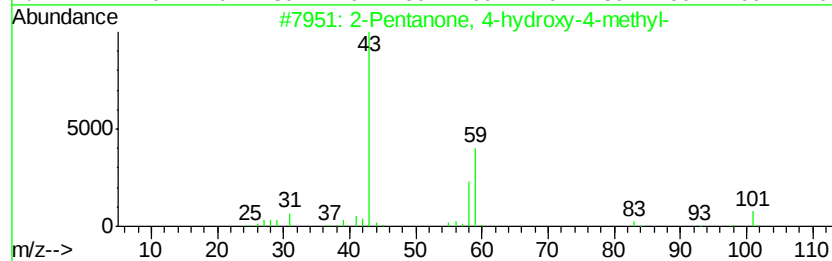
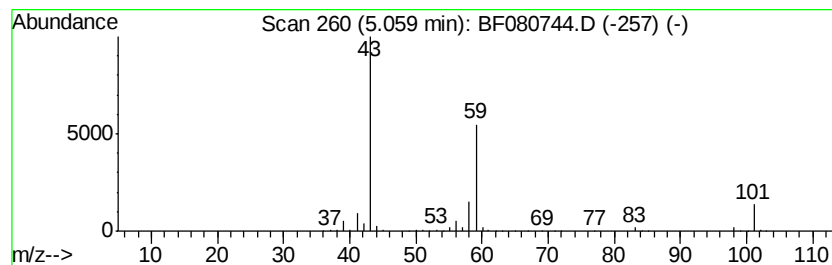
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	83.89 ng	3633350	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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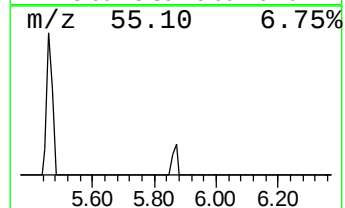
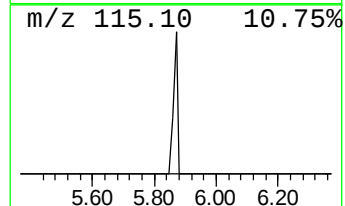
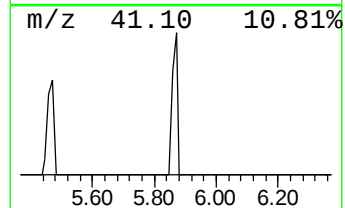
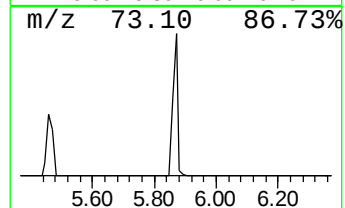
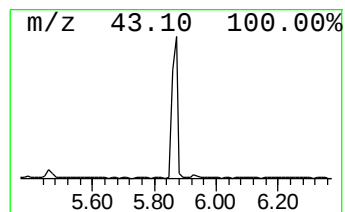
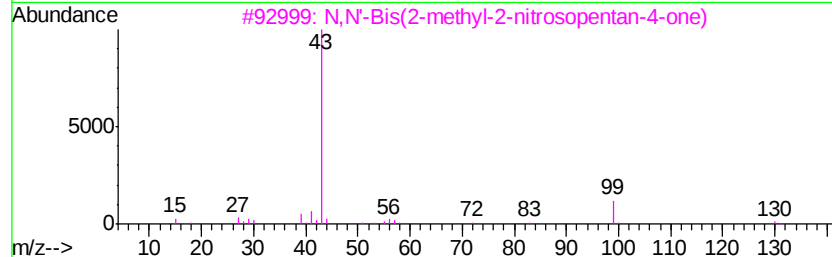
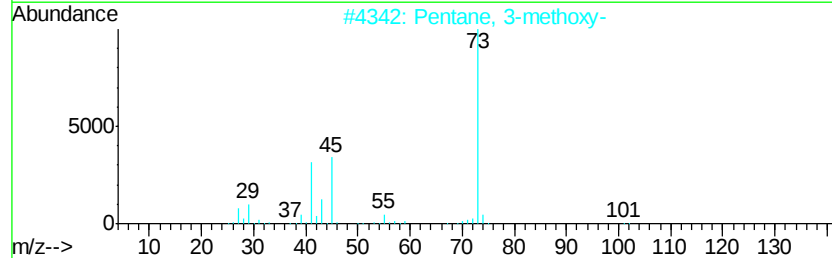
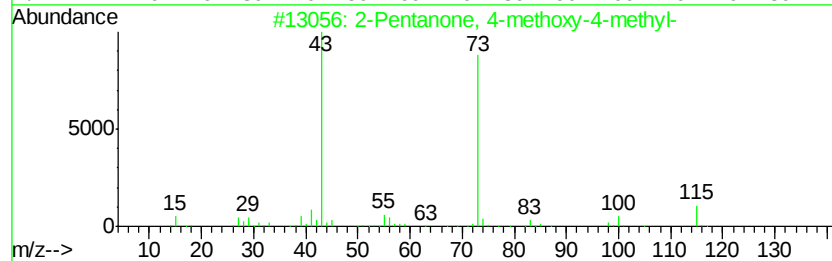
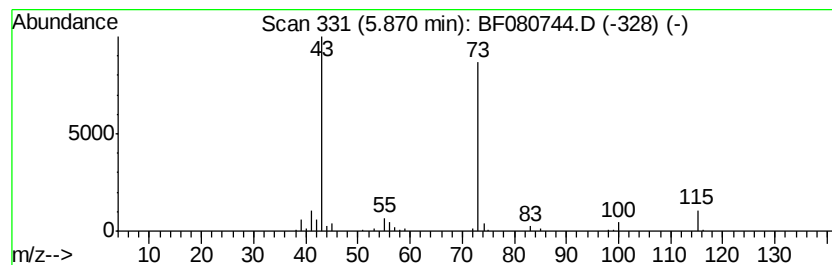
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Peak Number 3 unknown5.87 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	3.84 ng	166178	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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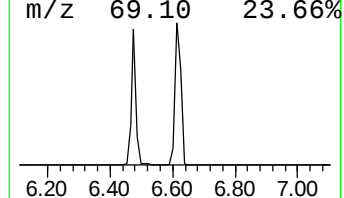
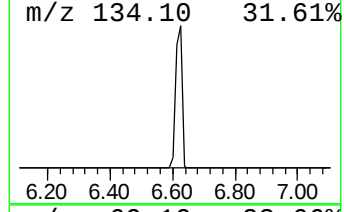
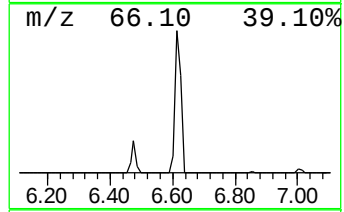
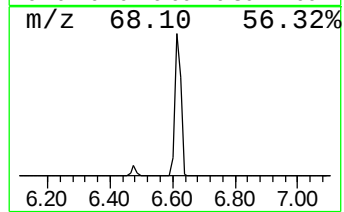
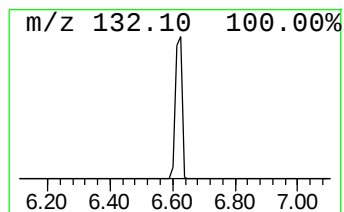
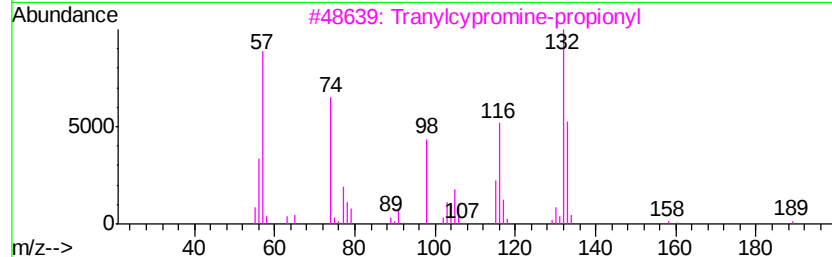
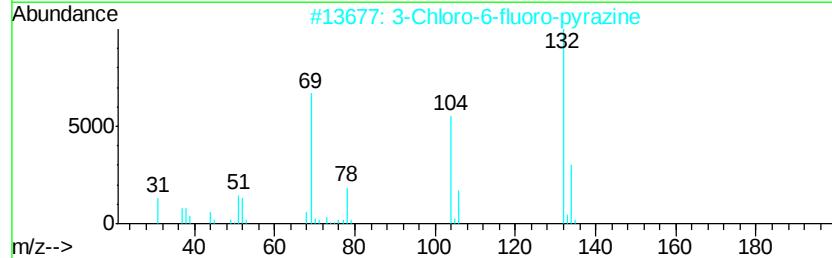
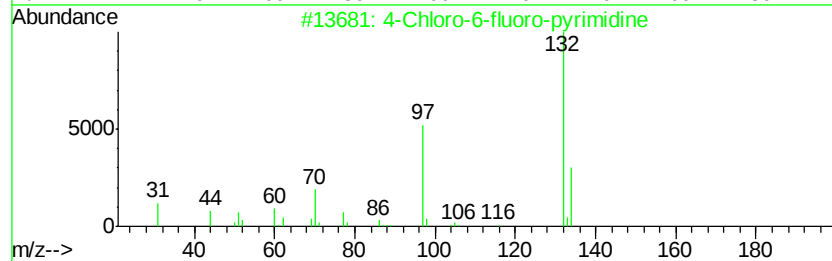
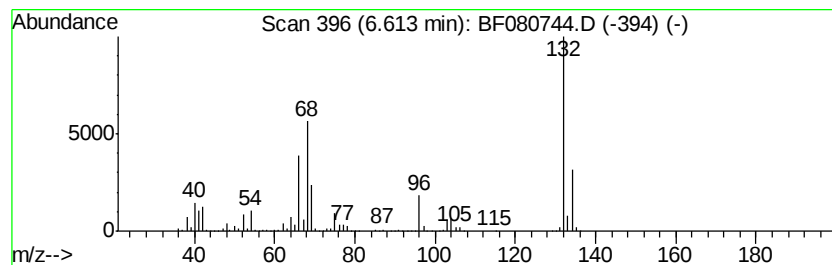
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Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	88.08 ng	3814890	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.42	5.0	ng	217823	1	6.85	866267	20.0
2-Pentanone, 4-hy...	5.06	83.9	ng	3633350	1	6.85	866267	20.0
unknown5.87	5.87	3.8	ng	166178	1	6.85	866267	20.0
unknown6.61	6.61	88.1	ng	3814890	1	6.85	866267	20.0