

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
 Data File : BF080763.D
 Acq On : 1 Aug 2015 6:09
 Operator : TP/UM
 Sample : G3121-06
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB-7-28-15

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-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	4.396	199	202	205	rBV	375492	532476	11.85%	1.727%
2	5.036	255	258	267	rBV	834774	945150	21.03%	3.065%
3	5.447	291	294	296	rBV	1968984	1795556	39.95%	5.822%
4	5.710	315	317	320	rVB	72452	67140	1.49%	0.218%
5	5.859	328	330	333	rBV	132852	112606	2.51%	0.365%
6	6.465	381	383	386	rBV	789695	1011423	22.50%	3.280%
7	6.613	393	396	399	rBV	2936963	3041823	67.67%	9.864%
8	6.853	415	417	419	rBV	969220	877689	19.53%	2.846%
9	7.013	428	431	433	rVB	2327915	3088916	68.72%	10.016%
10	7.253	450	452	454	rBV	90349	78165	1.74%	0.253%
11	7.413	463	466	468	rBV	2718000	2758751	61.37%	8.946%
12	8.133	527	529	531	rVB	1219974	1082511	24.08%	3.510%
13	9.208	620	623	626	rBV	3824791	4495025	100.00%	14.576%
14	9.882	680	682	685	rBV	1177349	1101345	24.50%	3.571%
15	10.671	748	751	753	rBV	3048515	3027033	67.34%	9.816%
16	11.368	809	812	814	rBV	1005731	1100236	24.48%	3.568%
17	12.957	948	951	953	rBV	3219230	4419326	98.32%	14.331%
18	13.985	1039	1041	1044	rBV	562808	696343	15.49%	2.258%
19	15.403	1162	1165	1168	rBV	404812	606927	13.50%	1.968%

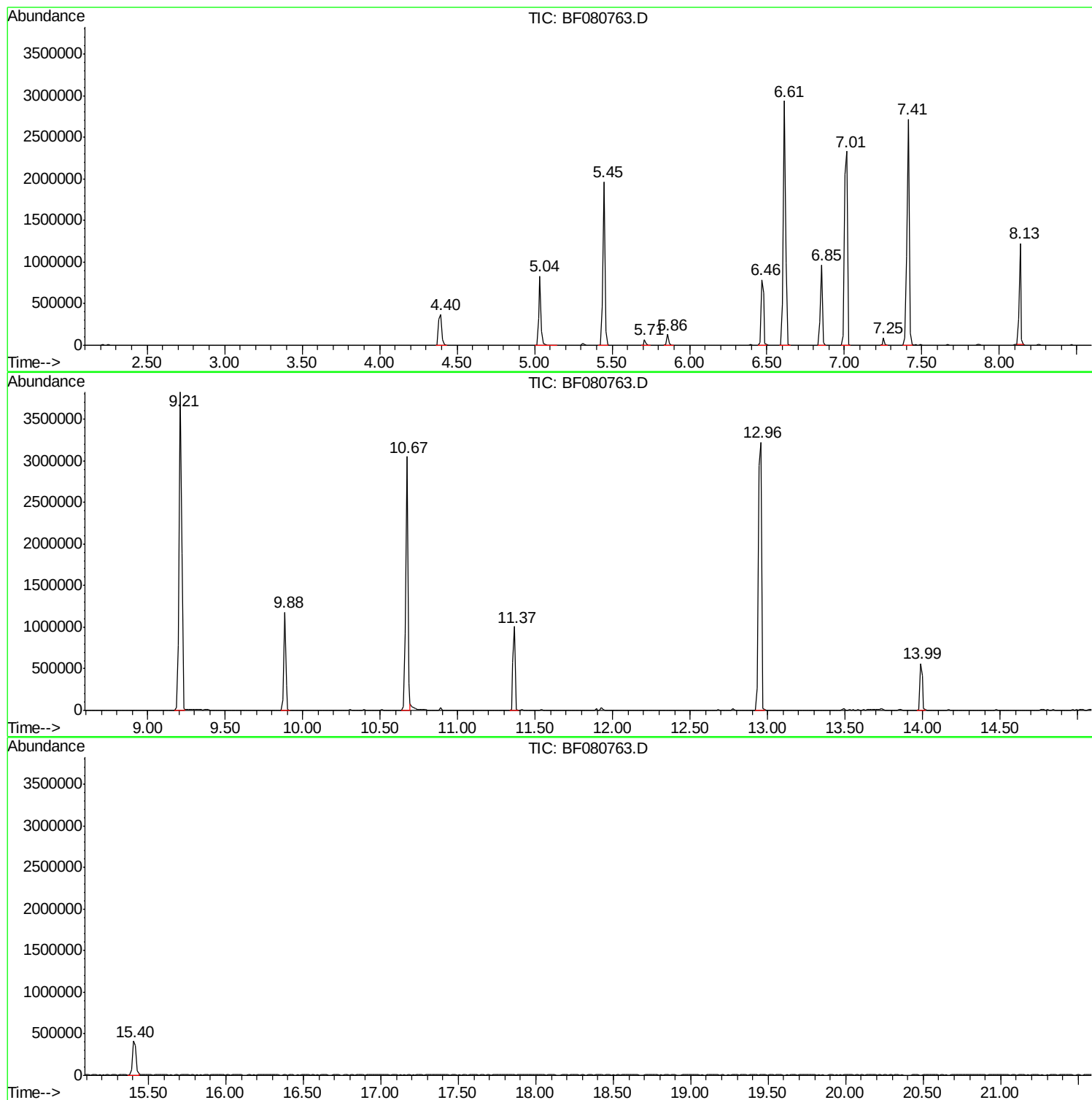
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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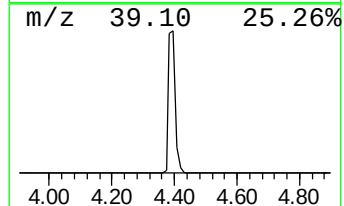
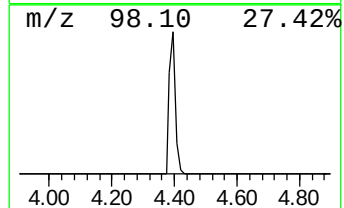
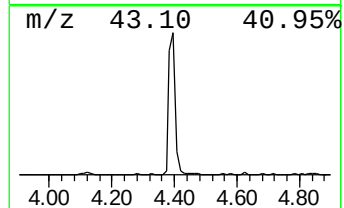
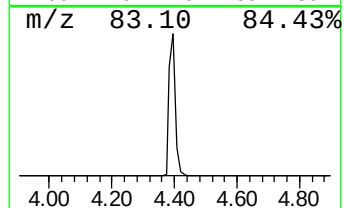
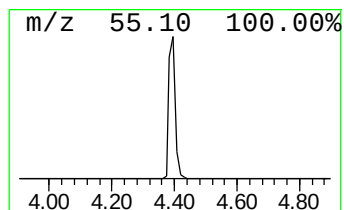
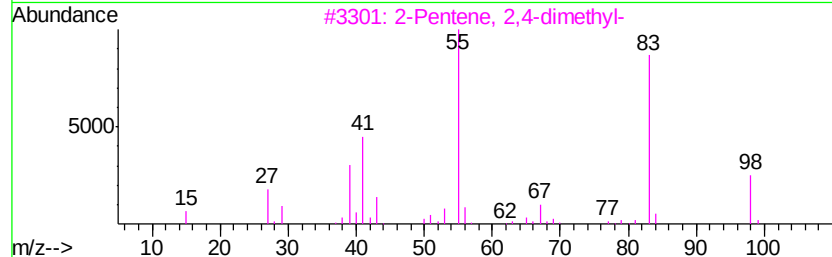
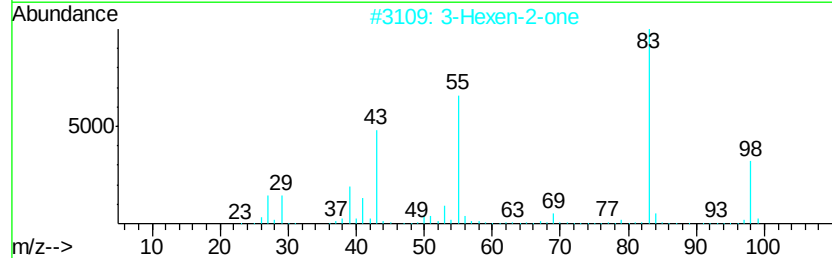
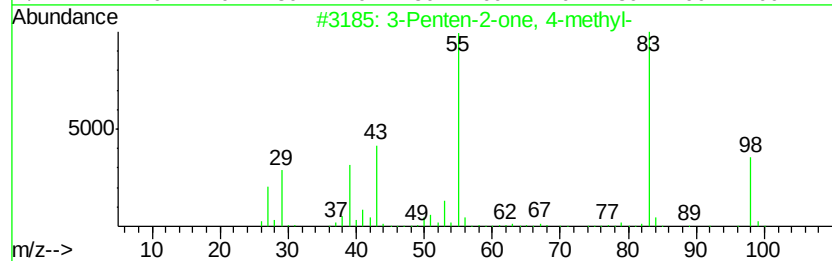
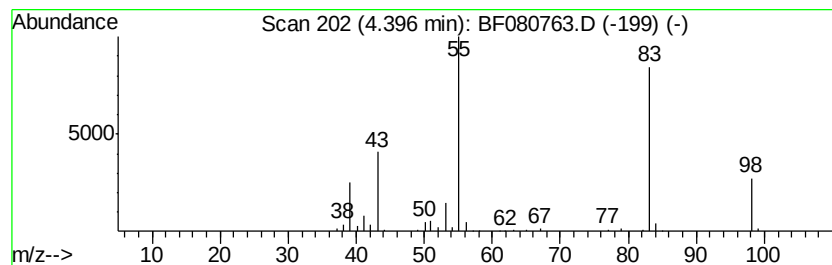
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.40	12.13 ng	532476	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	80
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
4		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72



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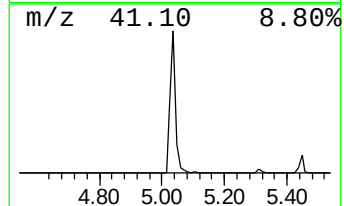
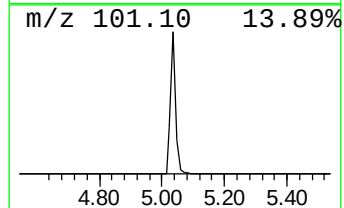
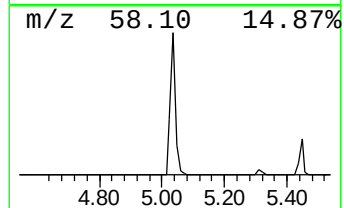
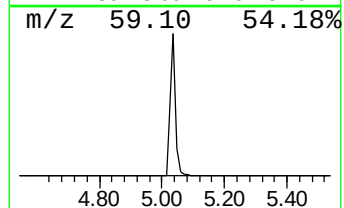
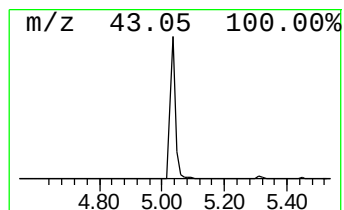
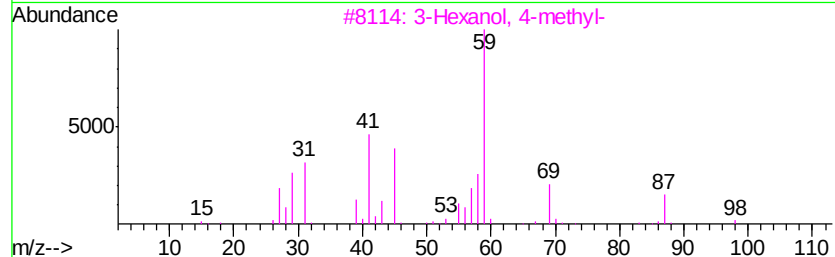
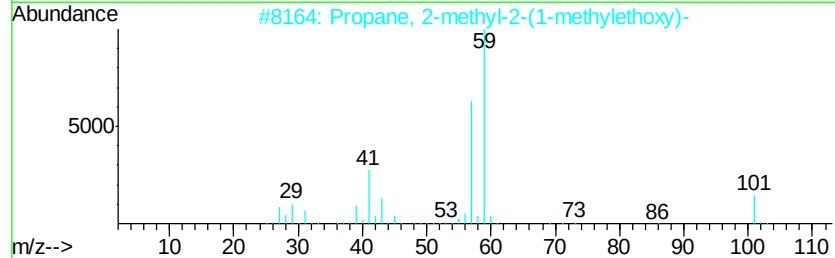
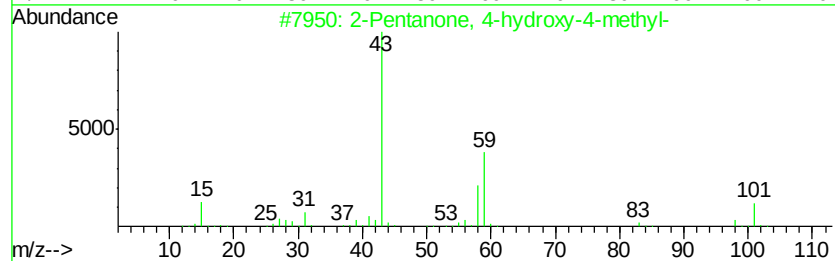
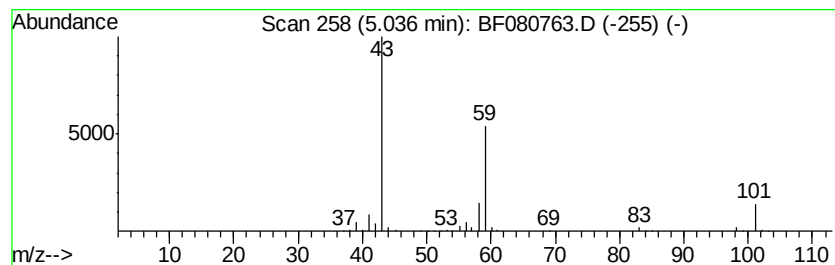
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	21.54 ng	945150	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	50
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	32



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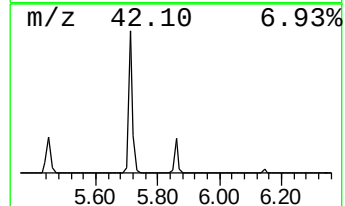
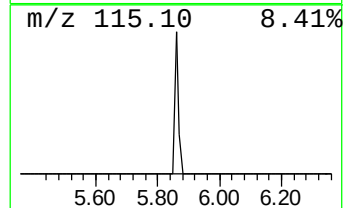
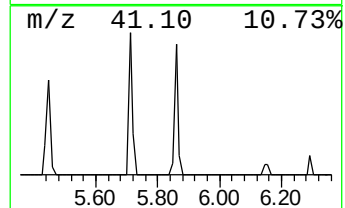
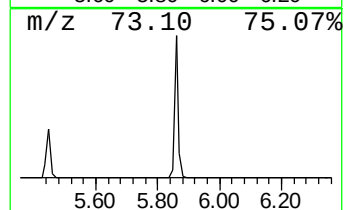
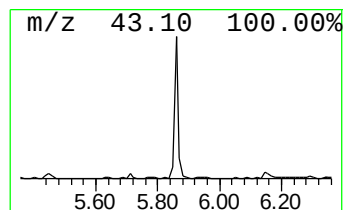
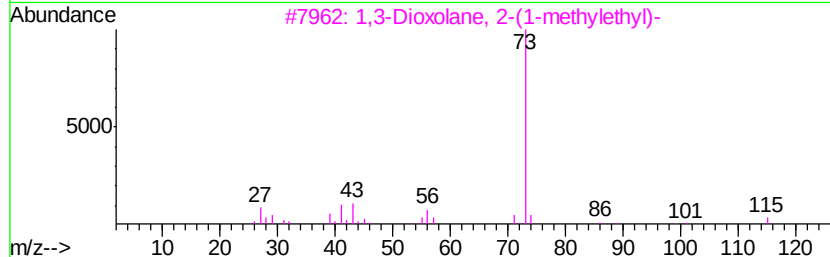
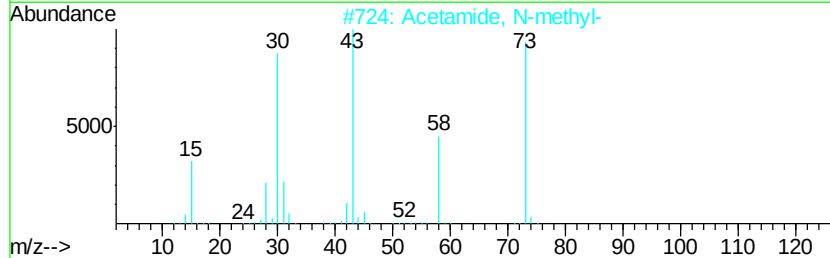
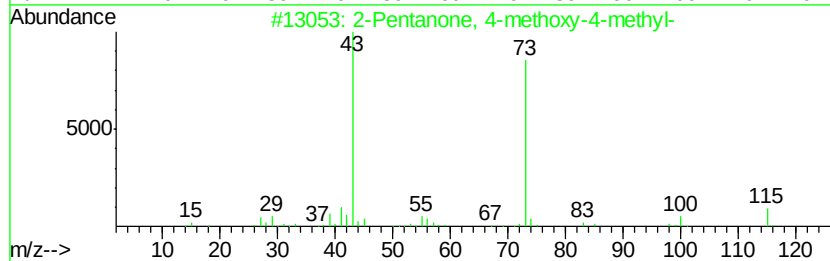
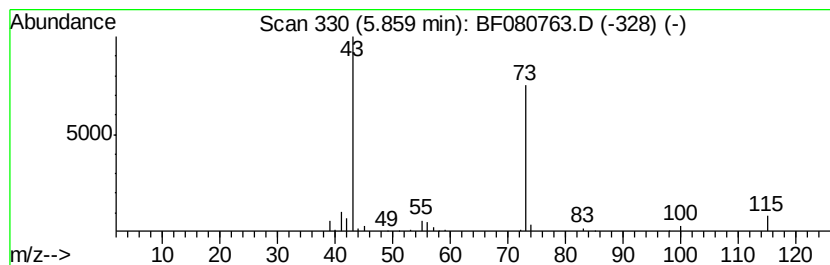
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Peak Number 3 unknown5.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.57 ng	112606	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	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32	
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	23	
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23	
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9	



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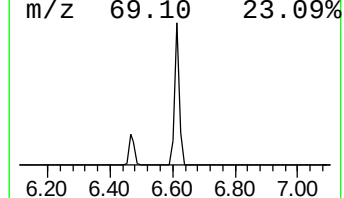
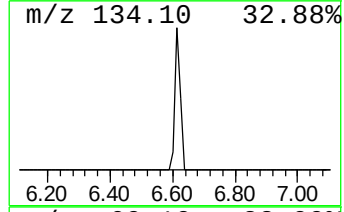
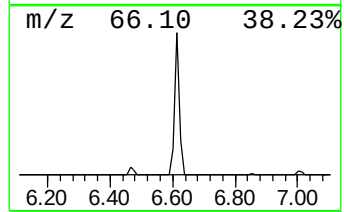
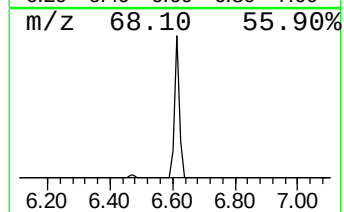
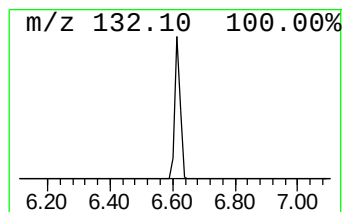
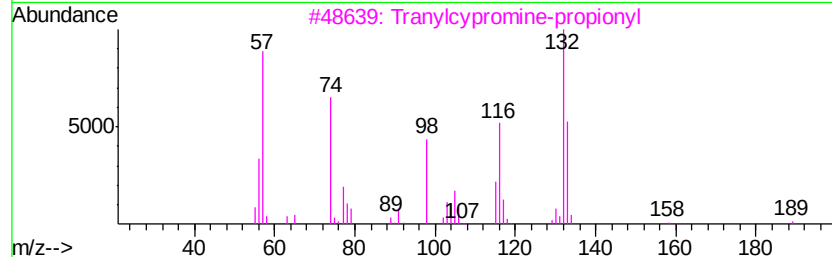
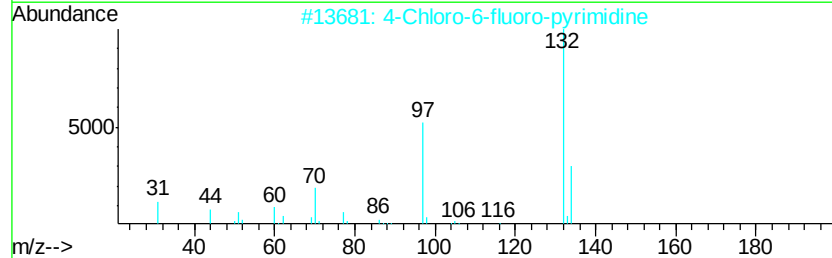
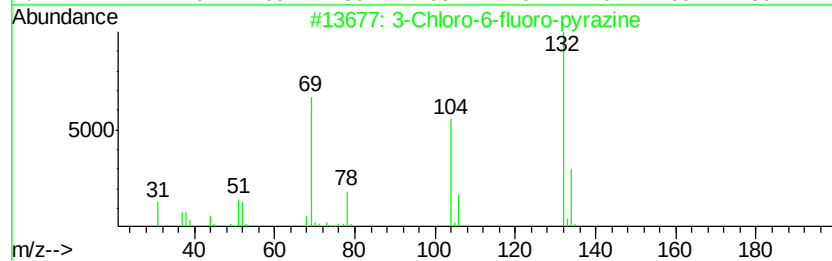
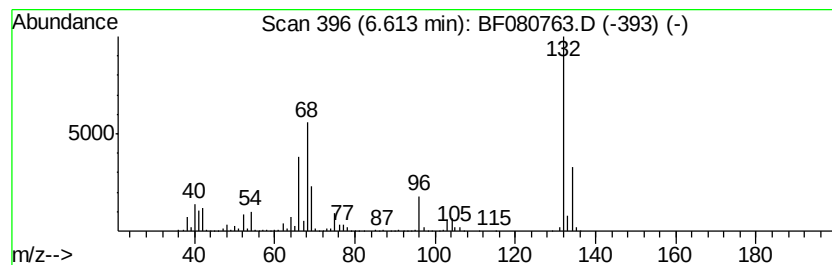
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Peak Number 4 unknown6.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	69.31 ng	3041820	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.40	12.1	ng	532476	1	6.85	877689	20.0
2-Pentanone, 4-hy...	5.04	21.5	ng	945150	1	6.85	877689	20.0
unknown5.86	5.86	2.6	ng	112606	1	6.85	877689	20.0
unknown6.61	6.61	69.3	ng	3041820	1	6.85	877689	20.0