

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080822.D
Acq On : 4 Aug 2015 2:09
Operator : TP
Sample : PB84720BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84720BL

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-BF080315.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	200	202	207	rVB	192850	242413	4.17%	0.500%
2	5.047	255	259	271	rBV	2834826	4324936	74.41%	8.915%
3	5.447	291	294	296	rBV	4767418	4905487	84.39%	10.111%
4	5.847	327	329	331	rBV	167272	138310	2.38%	0.285%
5	6.464	380	383	385	rBV	4781320	5141464	88.45%	10.598%
6	6.602	392	395	397	rBV	5103593	5118054	88.05%	10.549%
7	6.830	413	415	417	rVB	1408806	1163131	20.01%	2.397%
8	6.990	426	429	431	rVB	4081511	3978130	68.44%	8.200%
9	7.390	461	464	467	rBV	2686782	3151719	54.22%	6.496%
10	8.110	524	527	530	rBV	1432183	1384848	23.82%	2.854%
11	9.196	618	622	624	rBV	4253895	5812613	100.00%	11.981%
12	9.870	677	681	683	rBV	1041900	1524618	26.23%	3.143%
13	10.648	746	749	752	rBV2	2759370	3324396	57.19%	6.852%
14	11.345	808	810	812	rVB	1796698	1526135	26.26%	3.146%
15	12.934	946	949	951	rBV	5176105	4889732	84.12%	10.079%
16	13.974	1038	1040	1043	rBV	1251788	1104567	19.00%	2.277%
17	15.391	1161	1164	1167	rBV	579200	784735	13.50%	1.618%

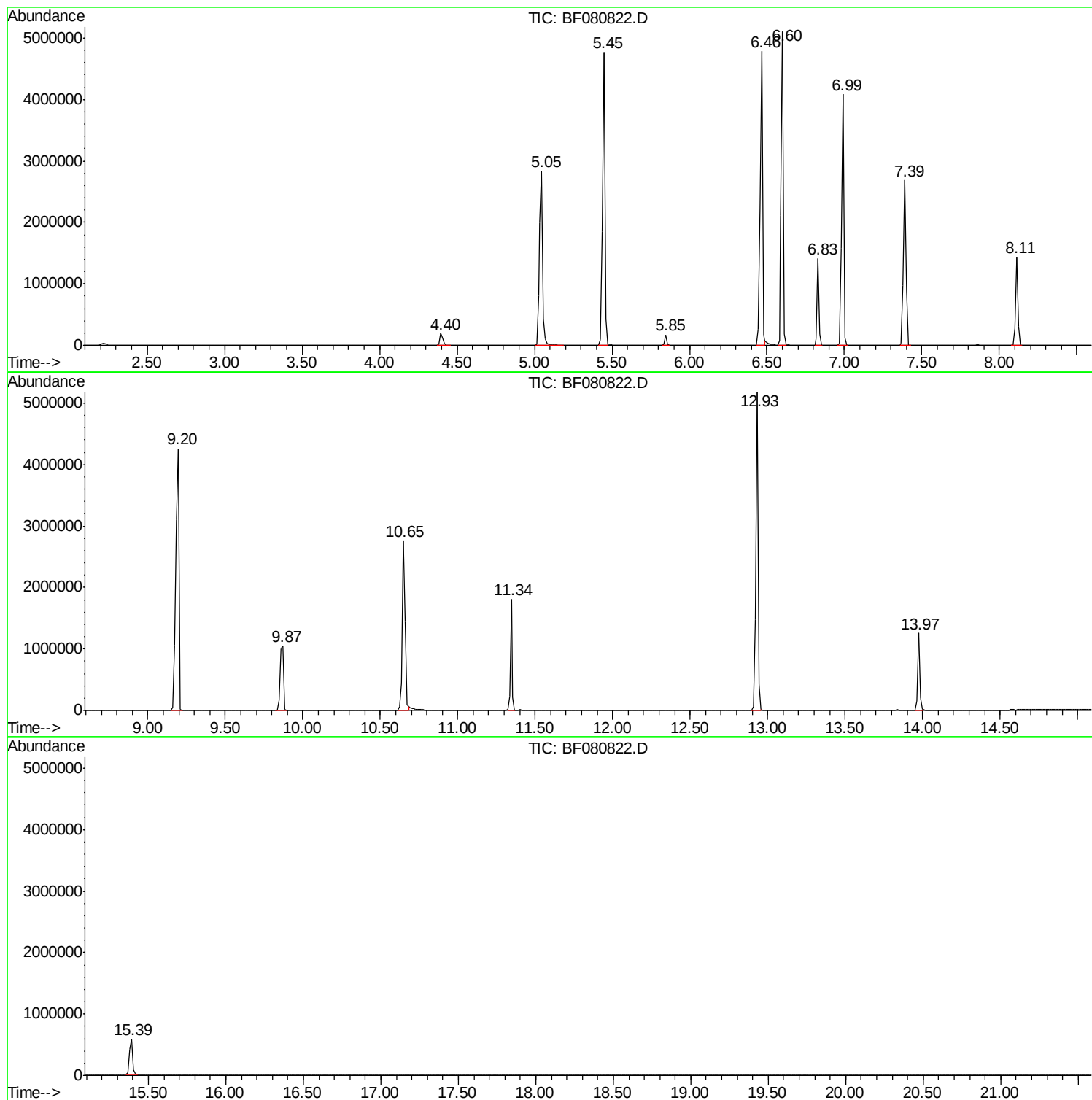
Sum of corrected areas: 48515288

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.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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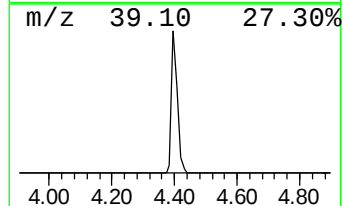
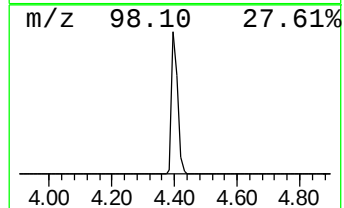
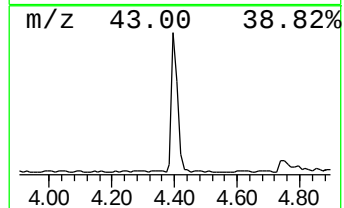
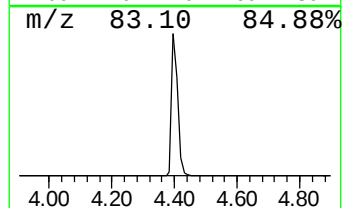
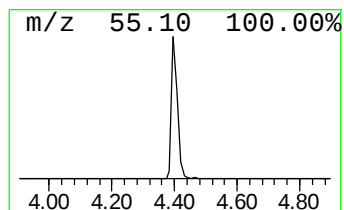
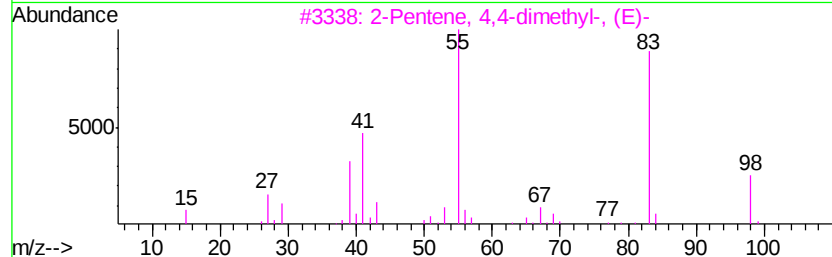
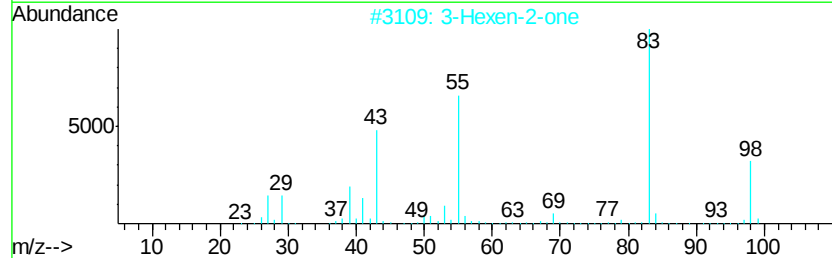
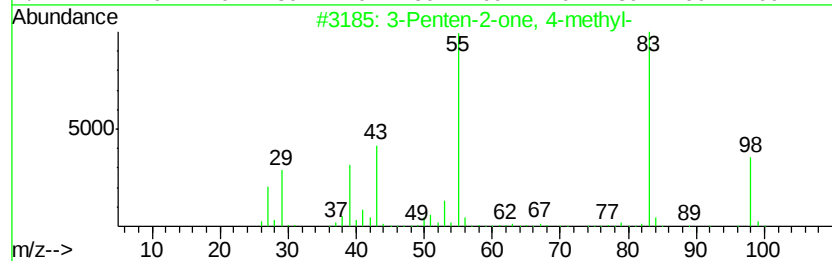
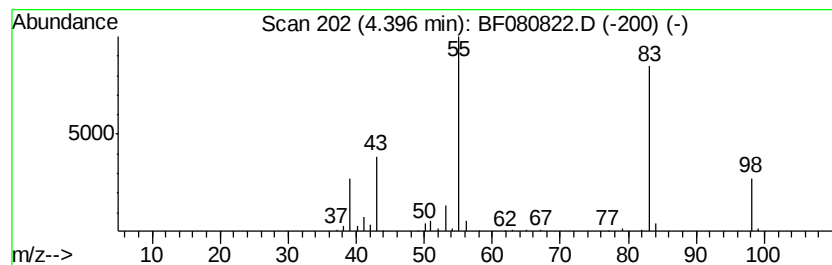
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	4.17 ng	242413	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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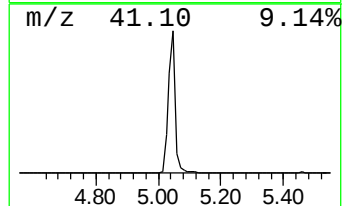
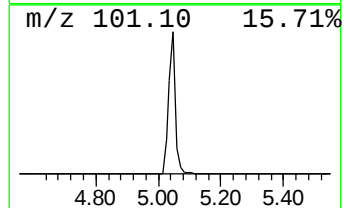
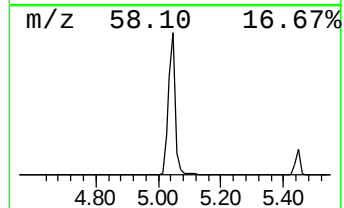
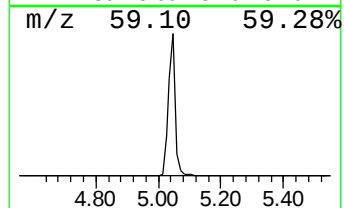
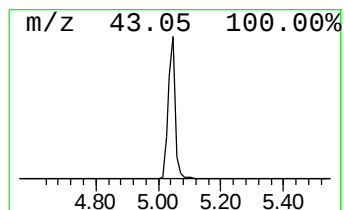
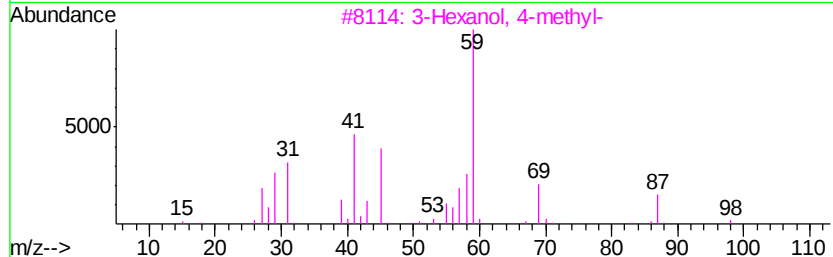
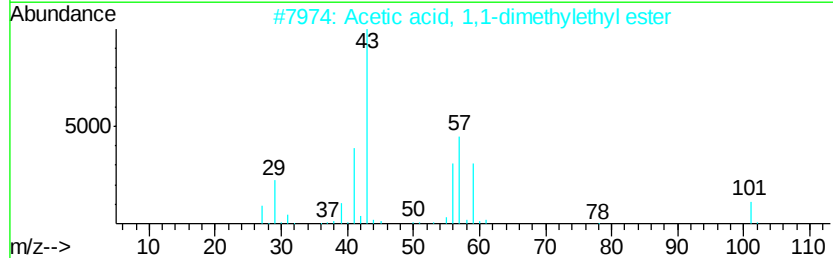
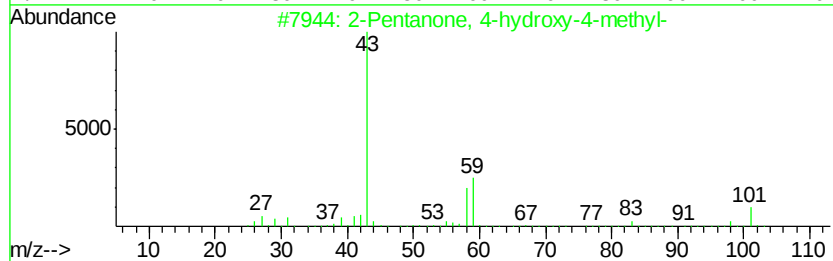
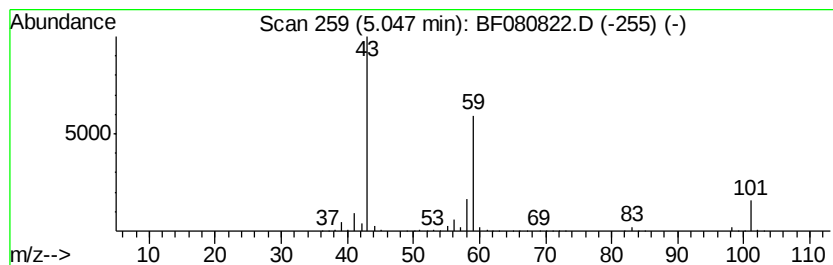
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	74.37 ng	4324940	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
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	25



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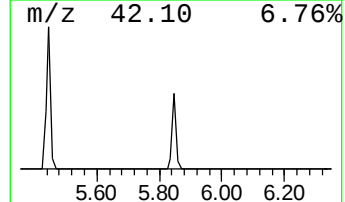
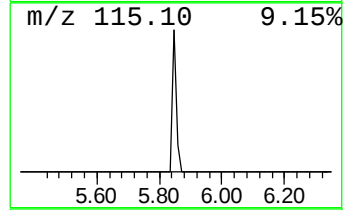
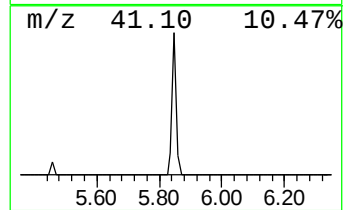
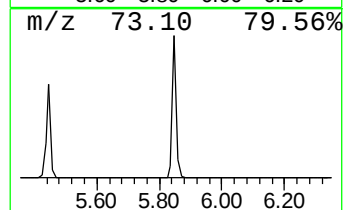
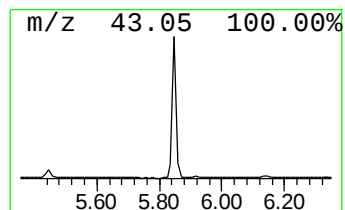
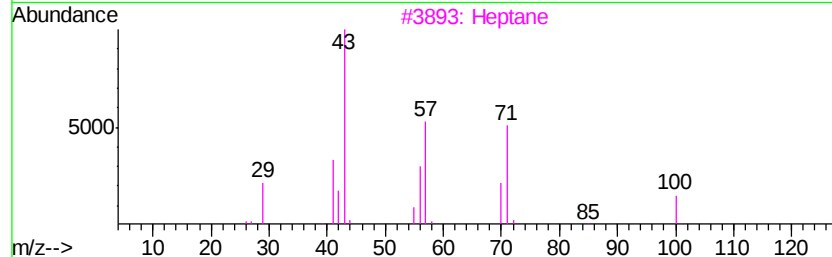
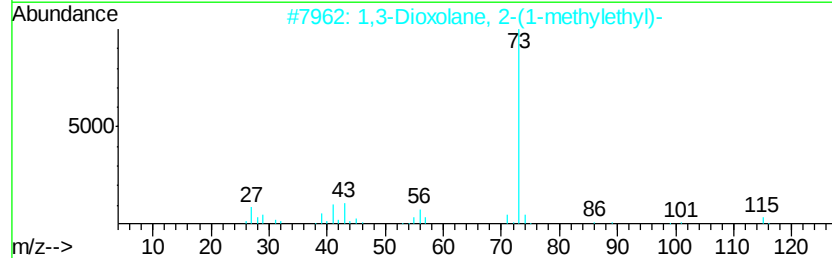
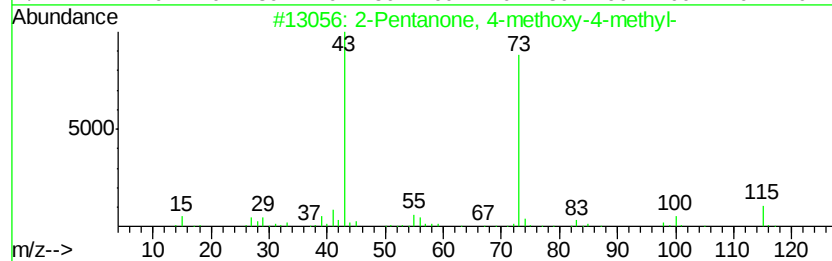
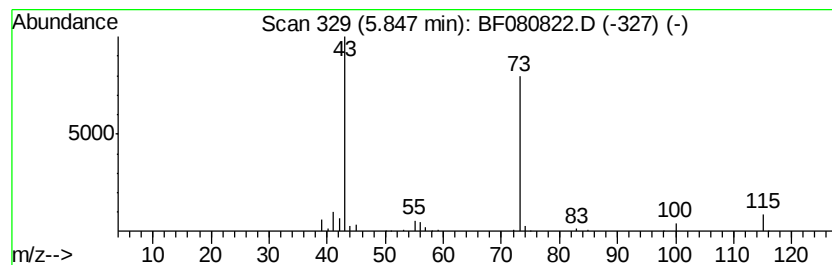
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.85	2.38 ng	138310	1,4-Dichlorobenzene-d4	6.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
3		Heptane	100	C7H16	000142-82-5	9
4		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	9
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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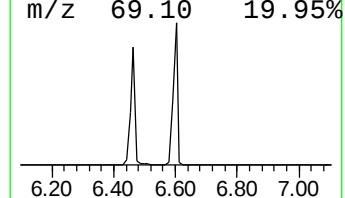
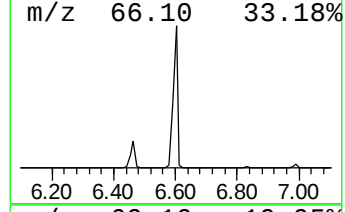
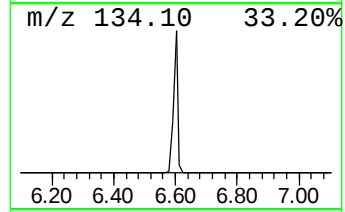
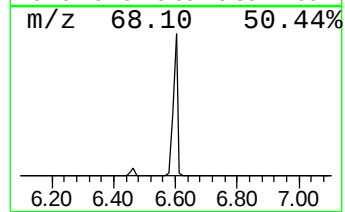
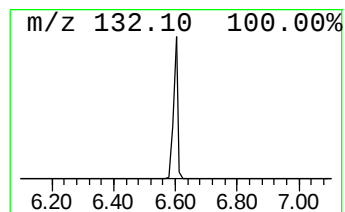
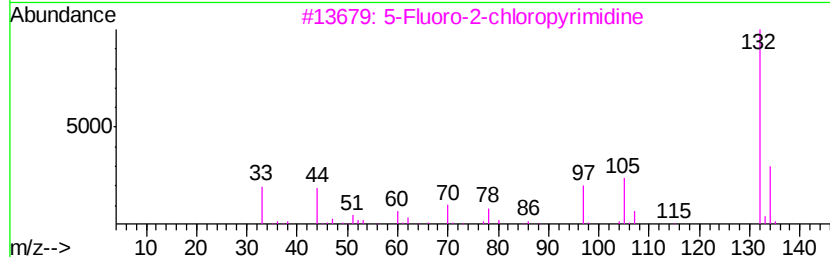
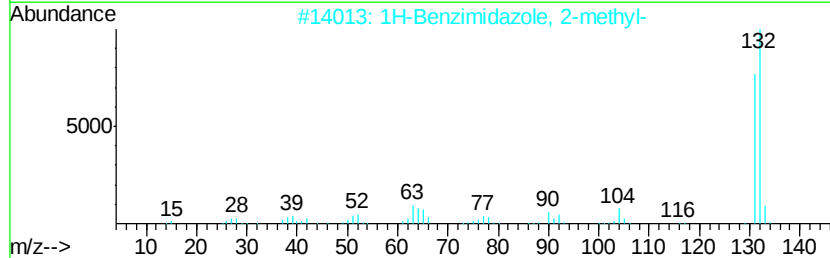
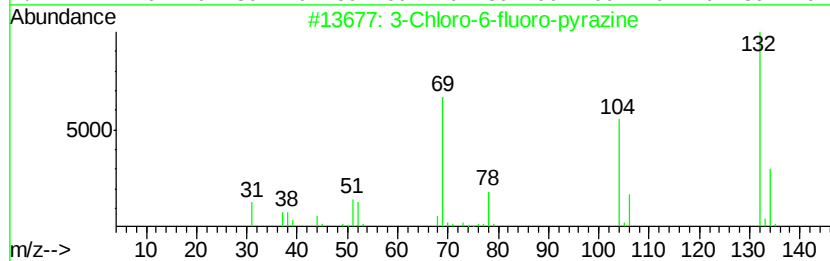
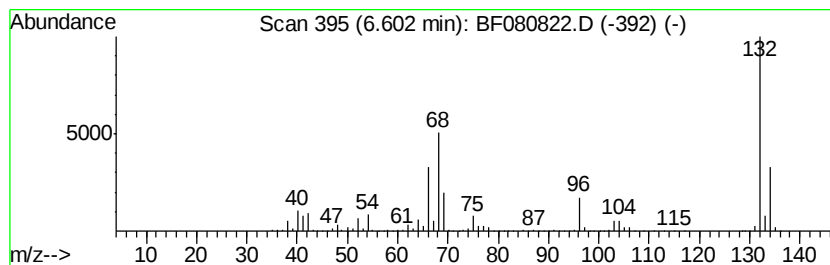
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Peak Number 4 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	88.00 ng	5118050	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.40	4.2	ng	242413	1	6.83	1163130	20.0
2-Pentanone, 4-hy...	5.05	74.4	ng	4324940	1	6.83	1163130	20.0
2-Pentanone, 4-me...	5.85	2.4	ng	138310	1	6.83	1163130	20.0
unknown6.60	6.60	88.0	ng	5118050	1	6.83	1163130	20.0