

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
 Data File : BF087229.D
 Acq On : 20 May 2016 17:30
 Operator : UM/SJ
 Sample : PB90711BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90711BL

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-BF051716.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	1.701	8	10	43	rVB	862872	1536450	31.03%	3.599%
2	3.930	203	205	215	rBV	83242	187509	3.79%	0.439%
3	4.673	267	270	286	rBV	1239220	2393970	48.34%	5.608%
4	5.141	309	311	333	rBV	3167668	3872033	78.19%	9.071%
5	5.541	345	346	358	rVB	140308	200698	4.05%	0.470%
6	6.227	403	406	408	rBV	3929081	4337149	87.58%	10.160%
7	6.330	412	415	417	rBV	4174001	4314842	87.13%	10.108%
8	6.559	432	435	444	rVB	665077	989023	19.97%	2.317%
9	6.707	446	448	451	rBV	3220692	2972691	60.03%	6.964%
10	7.130	483	485	497	rBV	2544503	2654925	53.61%	6.219%
11	7.839	545	547	550	rBV	1253174	1328525	26.83%	3.112%
12	8.925	639	642	644	rBV	4826646	4952207	100.00%	11.601%
13	9.588	697	700	702	rBV	1797409	1599355	32.30%	3.747%
14	10.376	766	769	772	rBV	2683354	2899404	58.55%	6.792%
15	11.062	827	829	832	rBV	1562842	1529007	30.88%	3.582%
16	12.651	965	968	970	rBV	4457410	4502959	90.93%	10.548%
17	13.691	1056	1059	1062	rBV	1421225	1338250	27.02%	3.135%
18	14.582	1131	1137	1146	rBV3	20345	89508	1.81%	0.210%
19	15.039	1175	1177	1188	rBV	824769	989688	19.98%	2.318%

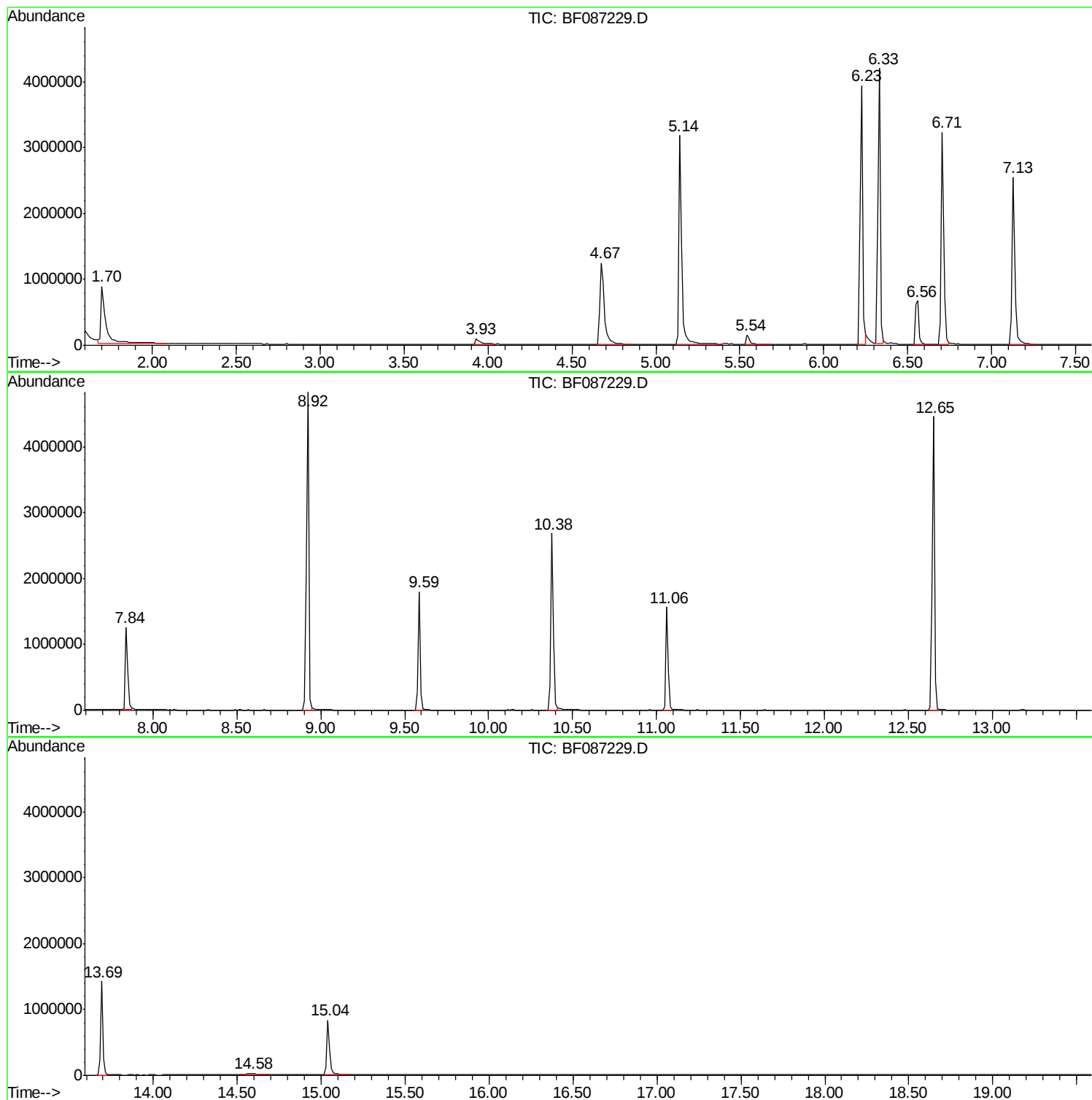
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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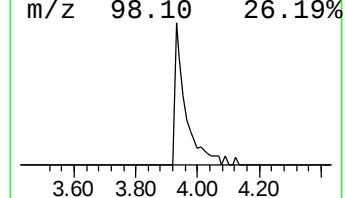
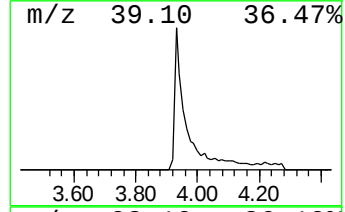
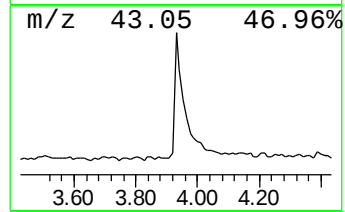
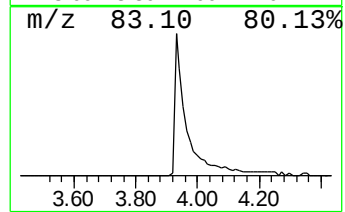
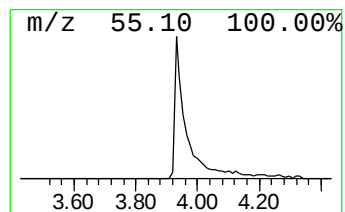
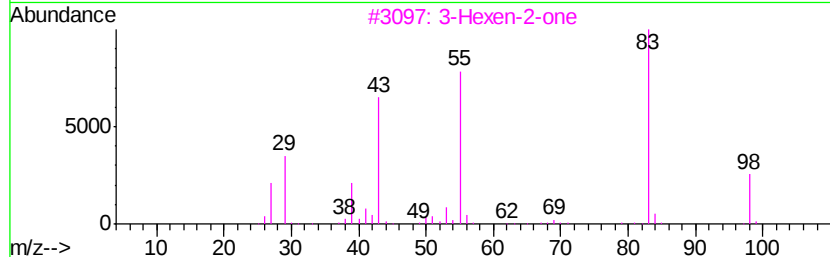
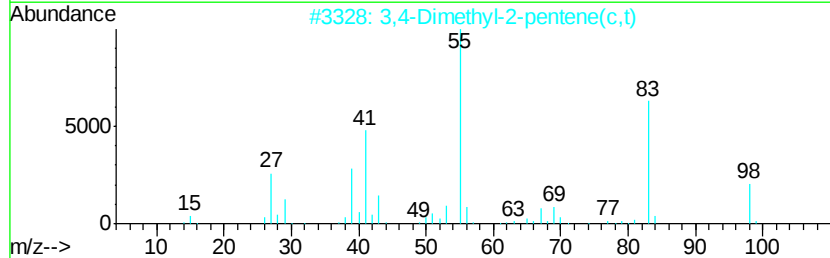
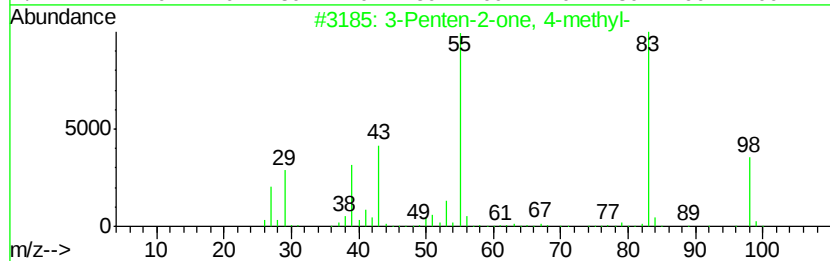
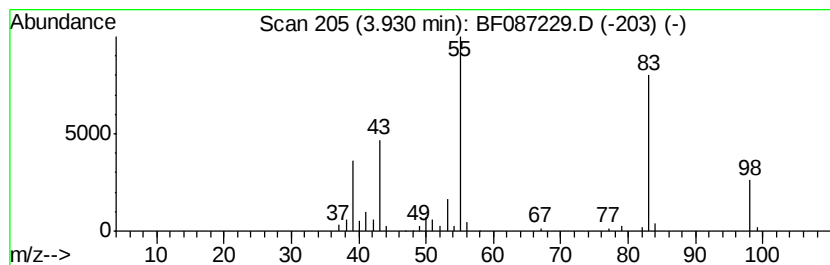
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	3.79 ng	187509	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3			3-Hexen-2-one	98	C6H10O	000763-93-9	80
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64



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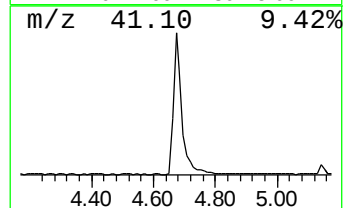
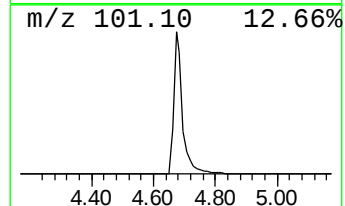
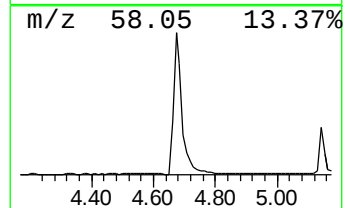
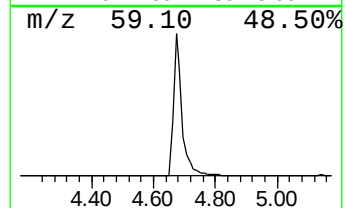
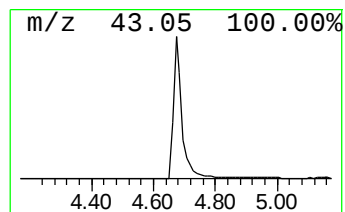
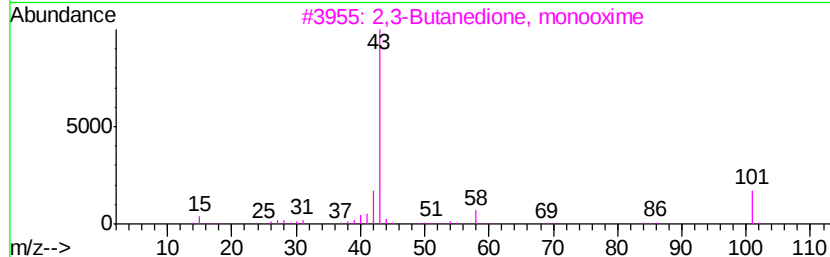
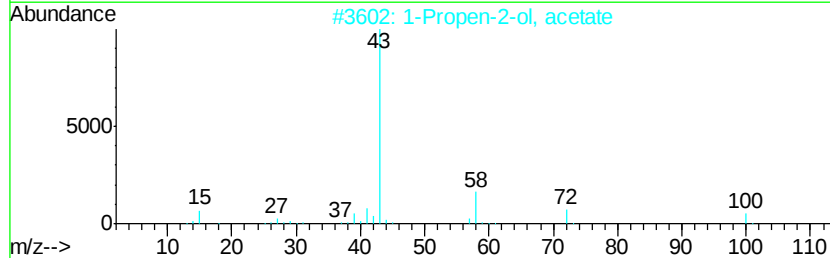
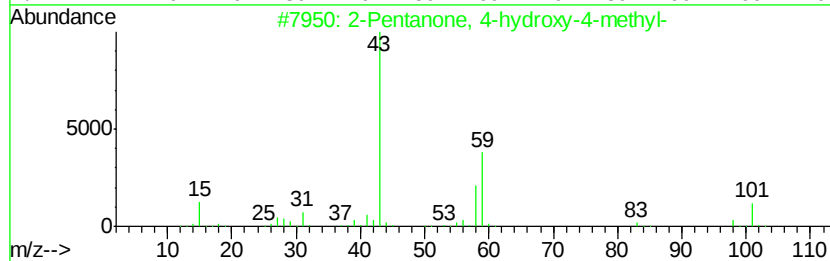
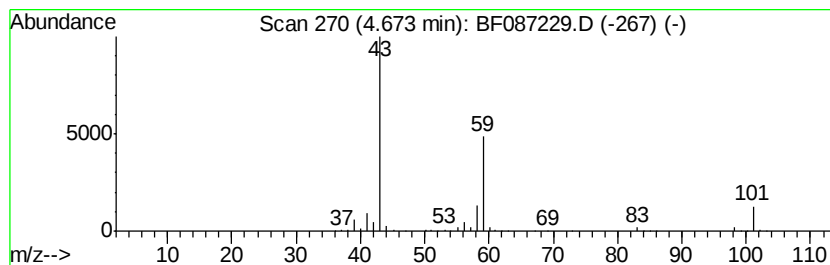
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	48.41 ng	2393970	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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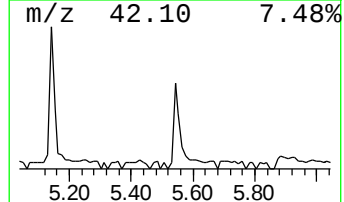
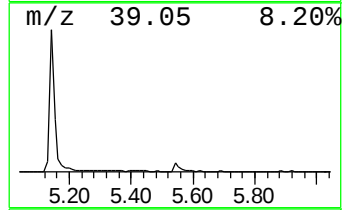
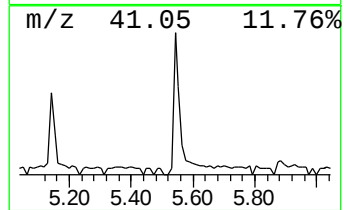
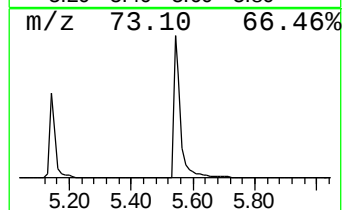
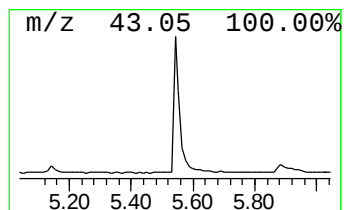
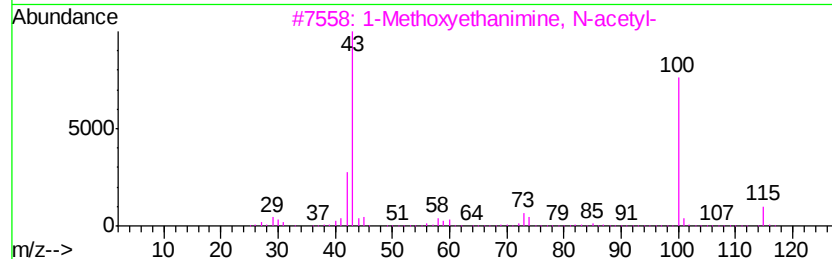
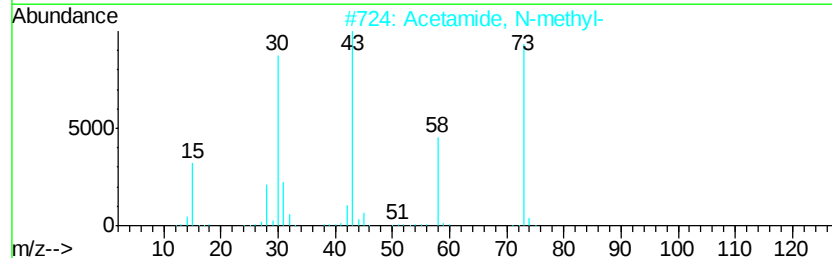
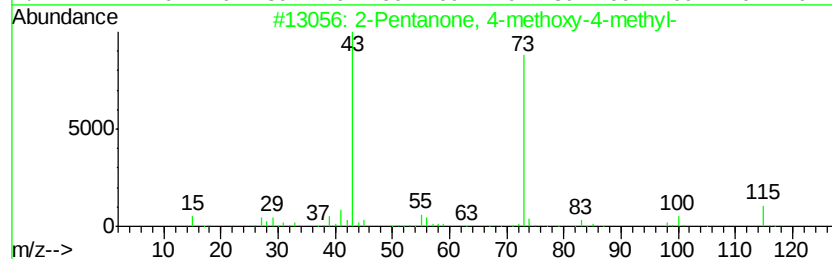
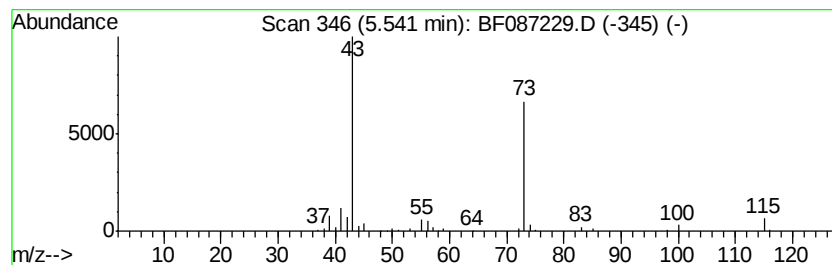
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	4.06 ng	200698	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	23
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
5		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	12



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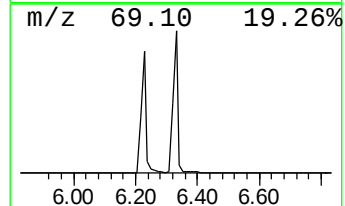
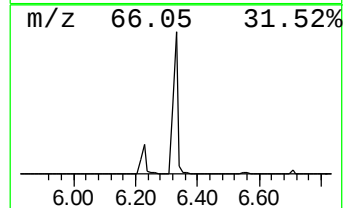
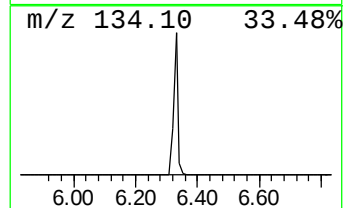
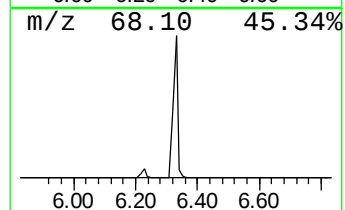
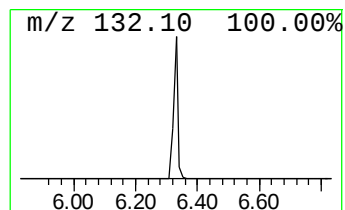
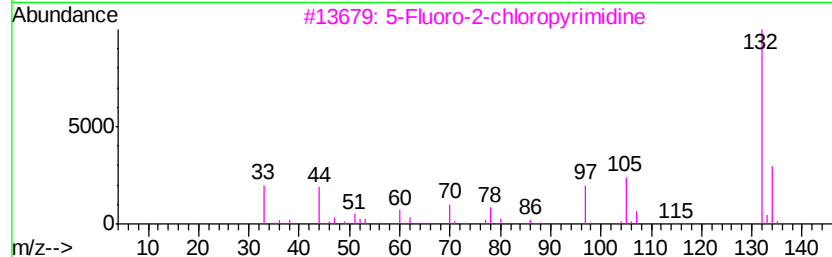
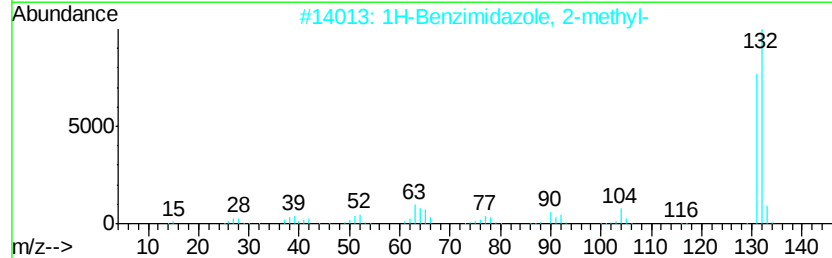
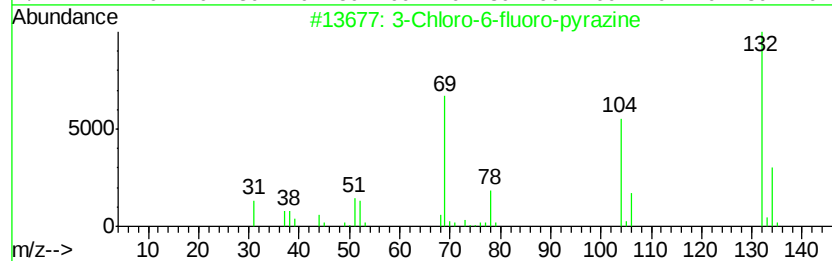
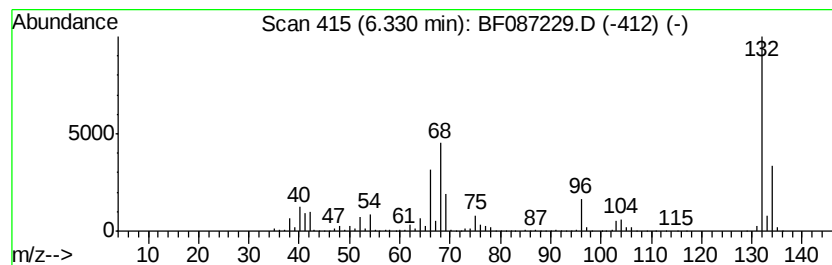
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Peak Number 5 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	87.25 ng	4314840	1,4-Dichlorobenzene-d4	6.56

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	22
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	12
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...	3.93	3.8	ng	187509	1	6.56	989023	20.0
2-Pentanone, 4-hy...	4.67	48.4	ng	2393970	1	6.56	989023	20.0
2-Pentanone, 4-me...	5.54	4.1	ng	200698	1	6.56	989023	20.0
unknown6.33	6.33	87.3	ng	4314840	1	6.56	989023	20.0