

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
 Data File : BF087186.D
 Acq On : 19 May 2016 14:03
 Operator : UM/SJ
 Sample : PB90666BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90666BL

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	9	10	57	rVB	2711792	6629975	72.36%	12.436%
2	3.976	203	209	211	rBV	3787723	8310665	90.71%	15.589%
3	4.730	269	275	277	rBV	3857849	9162052	100.00%	17.186%
4	5.164	310	313	335	rBV	1657716	2409493	26.30%	4.520%
5	5.553	345	347	350	rBV	599401	676442	7.38%	1.269%
6	6.227	404	406	413	rBV	1967620	2333613	25.47%	4.377%
7	6.342	413	416	418	rBV	1750903	2346829	25.61%	4.402%
8	6.559	433	435	445	rVB	709834	935292	10.21%	1.754%
9	6.719	446	449	452	rBV	2849461	2601436	28.39%	4.880%
10	7.142	483	486	488	rBV	2313818	2365268	25.82%	4.437%
11	7.850	546	548	551	rBV	1177640	1185112	12.94%	2.223%
12	8.936	639	643	645	rBV	3315136	3900352	42.57%	7.316%
13	9.599	698	701	704	rBV	1435310	1360901	14.85%	2.553%
14	10.388	768	770	773	rBV	1794898	1749307	19.09%	3.281%
15	11.074	828	830	833	rBV	1254360	1348125	14.71%	2.529%
16	12.662	966	969	972	rBV	3760864	3707982	40.47%	6.955%
17	13.702	1058	1060	1063	rBV	1381885	1277689	13.95%	2.397%
18	15.051	1176	1178	1181	rBV	757409	1011131	11.04%	1.897%

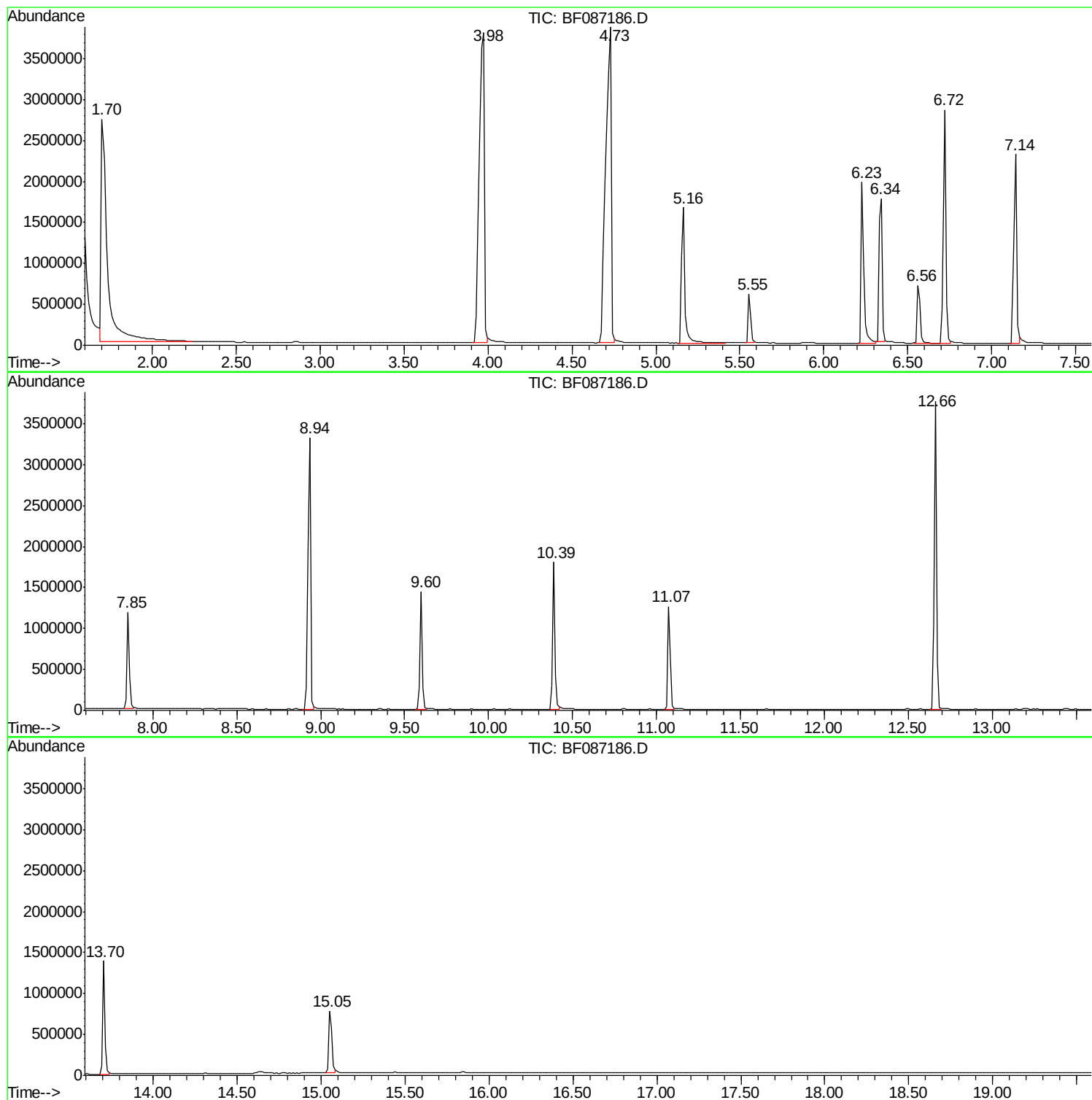
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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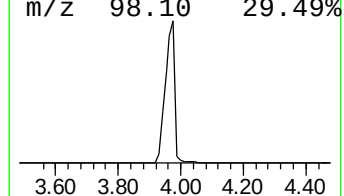
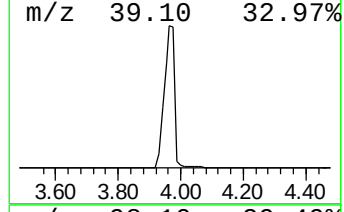
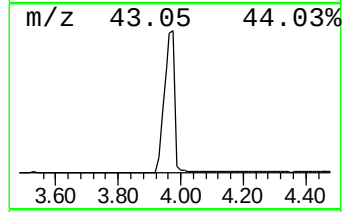
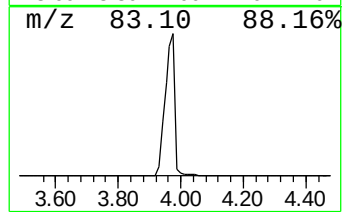
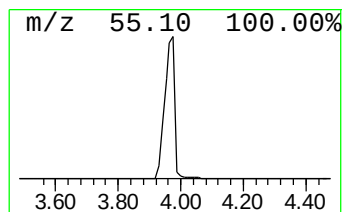
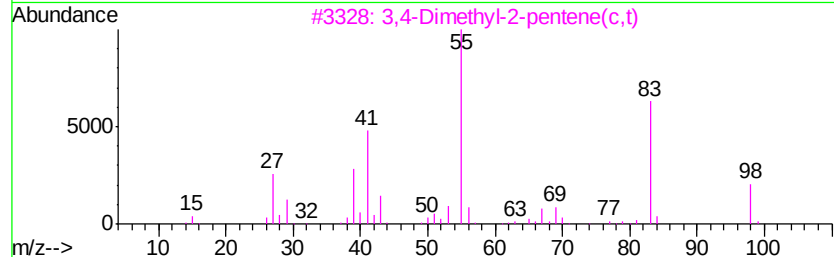
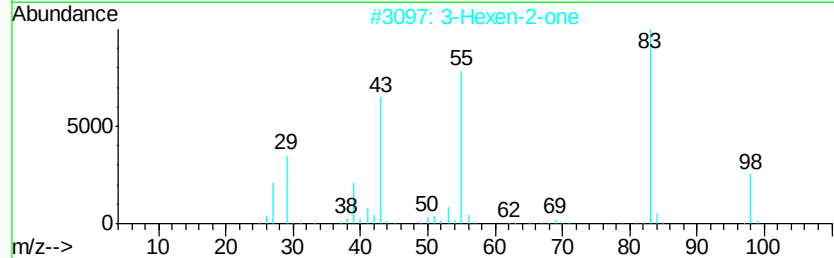
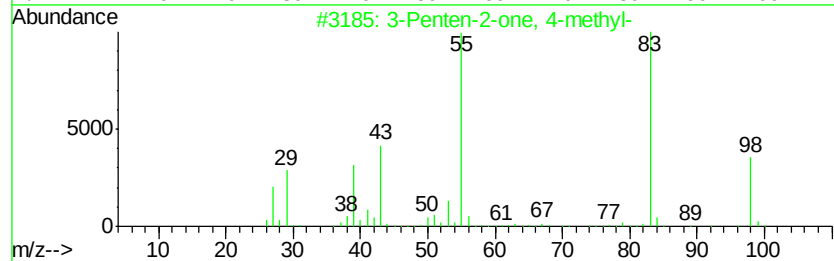
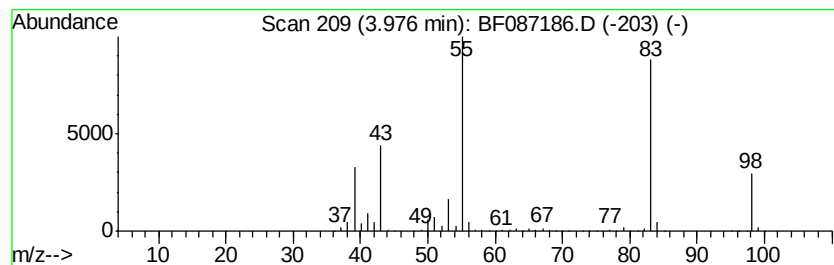
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	177.71 ng	8310670	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72



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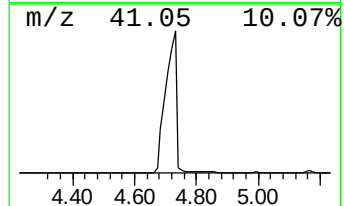
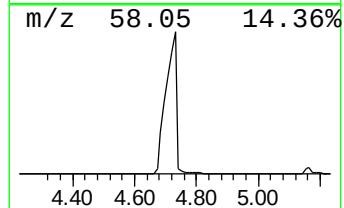
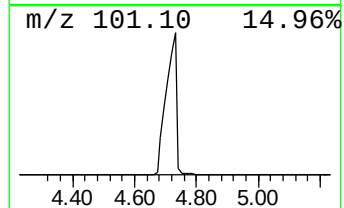
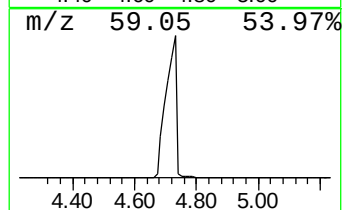
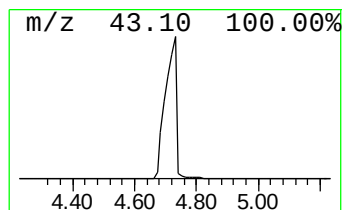
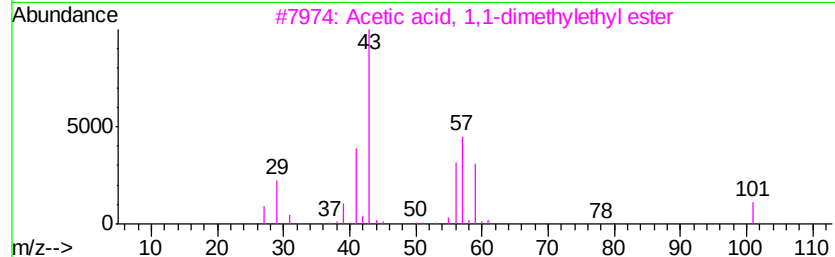
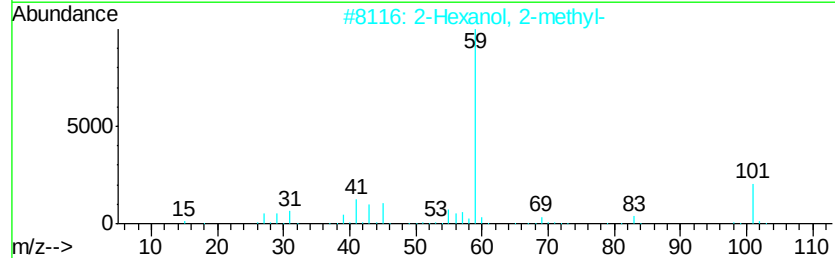
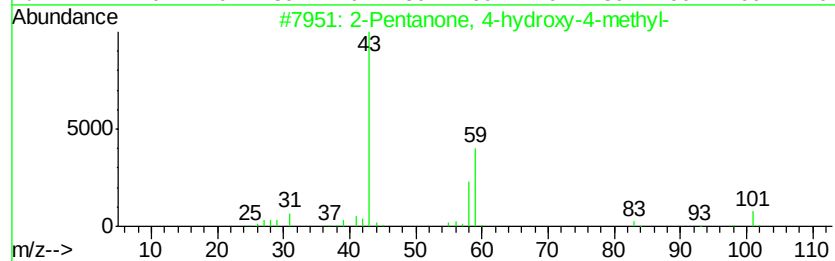
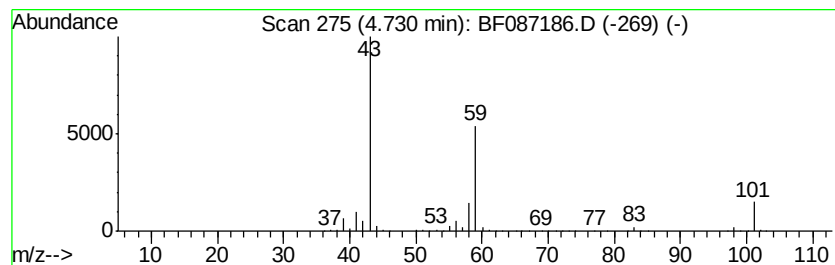
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	195.92 ng	9162050	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	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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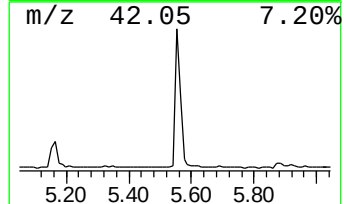
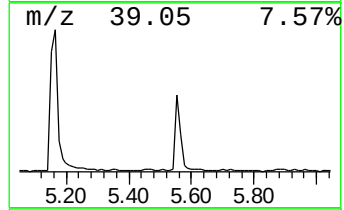
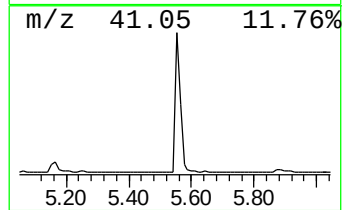
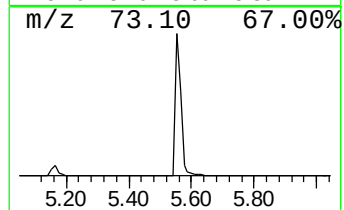
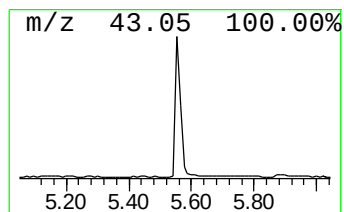
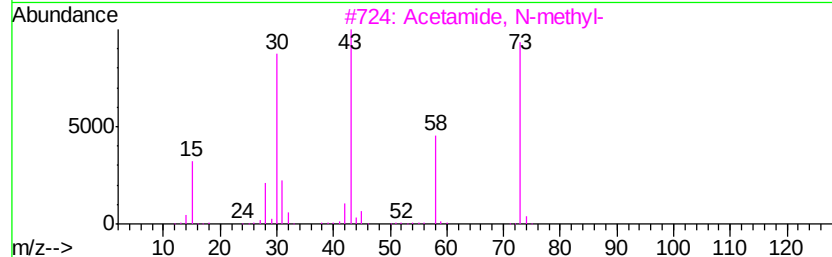
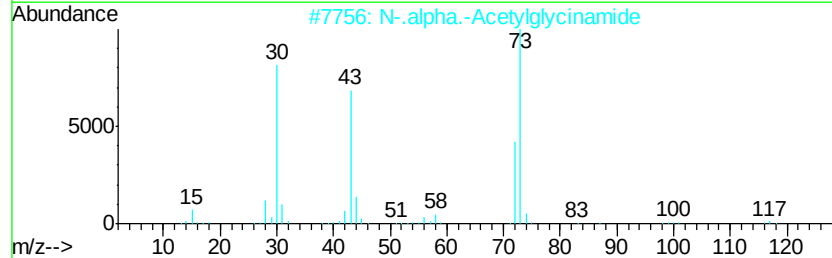
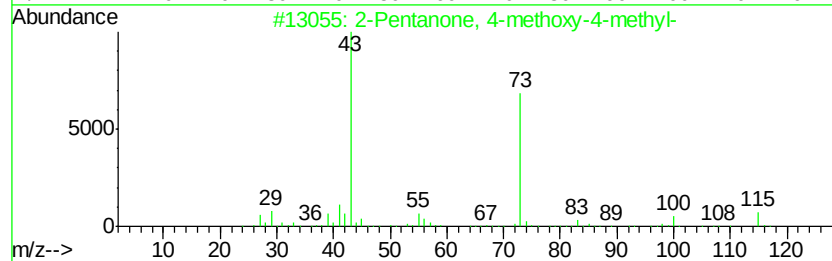
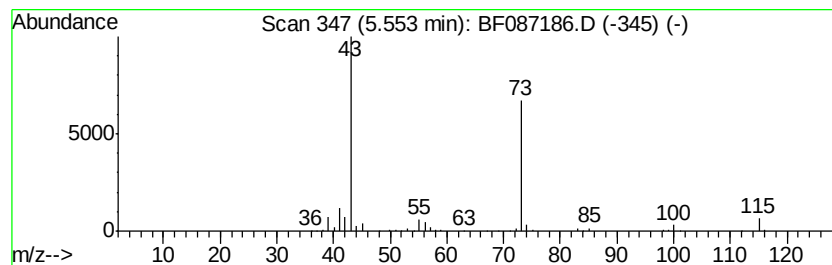
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	14.46 ng	676442	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	74
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		2-Heptanone	114	C7H14O	000110-43-0	25
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	23



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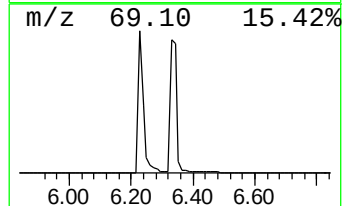
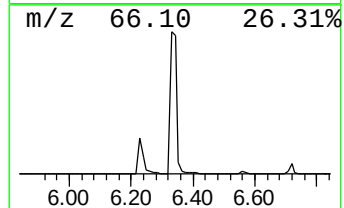
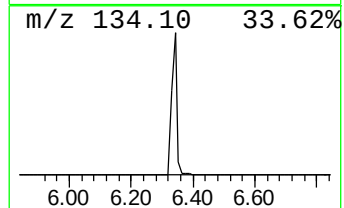
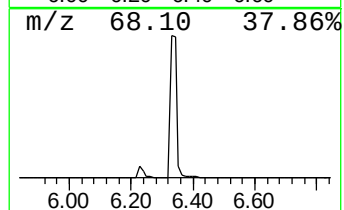
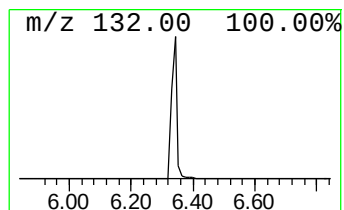
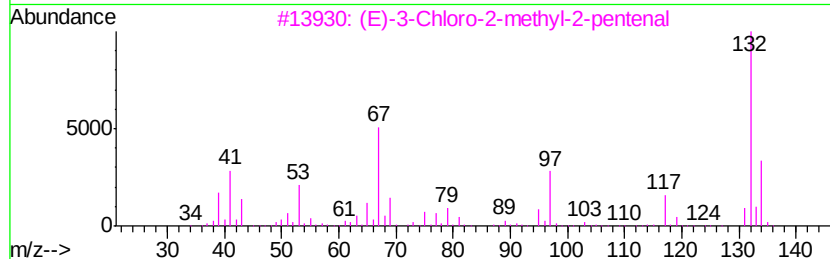
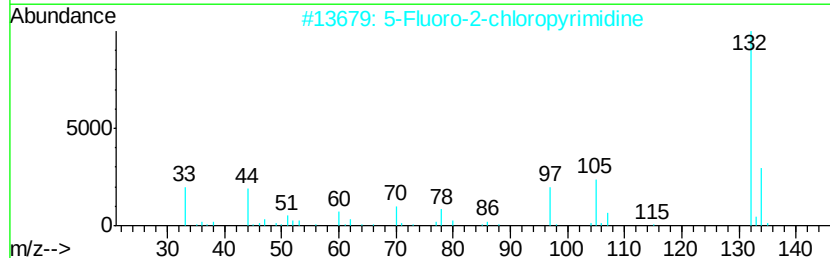
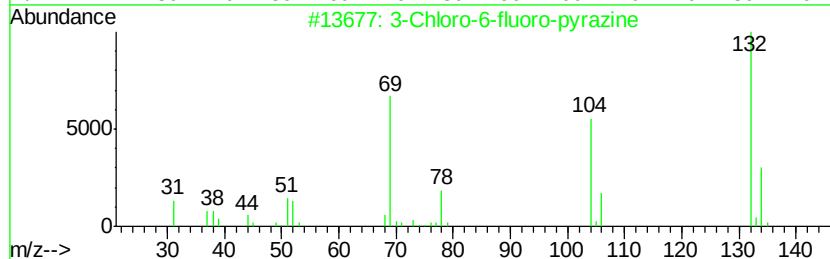
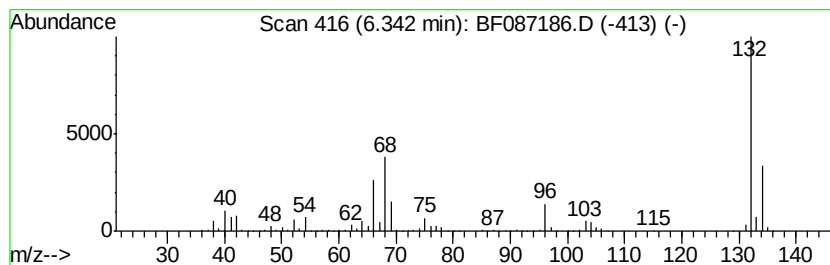
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Peak Number 5 unknown6.34 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	50.18 ng	2346830	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.98	177.7	ng	8310670	1	6.56	935292	20.0
2-Pentanone, 4-hy...	4.73	195.9	ng	9162050	1	6.56	935292	20.0
2-Pentanone, 4-me...	5.55	14.5	ng	676442	1	6.56	935292	20.0
unknown6.34	6.34	50.2	ng	2346830	1	6.56	935292	20.0