

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
 Data File : BF084568.D
 Acq On : 20 Jan 2016 16:54
 Operator : SJ/UM
 Sample : PB87882BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87882BL

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-BF123115.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	3.676	135	139	143	rVB	122969	189332	2.89%	0.332%
2	4.281	189	192	203	rBV	225712	298370	4.56%	0.524%
3	4.956	248	251	254	rBV	2446679	4294206	65.65%	7.539%
4	5.390	286	289	291	rBV	5236614	5620671	85.93%	9.867%
5	5.779	321	323	326	rBV	205280	231673	3.54%	0.407%
6	6.430	377	380	382	rBV	4399199	5737236	87.72%	10.072%
7	6.544	388	390	393	rBV	4308906	5141366	78.61%	9.026%
8	6.773	408	410	413	rBV	1213620	1311171	20.05%	2.302%
9	6.933	422	424	426	rBV	4601396	3994045	61.06%	7.012%
10	7.345	457	460	462	rBV	3355887	3257984	49.81%	5.720%
11	8.065	520	523	525	rBV	2063241	1867612	28.55%	3.279%
12	9.150	615	618	620	rBV	5593870	6540656	100.00%	11.483%
13	9.230	622	625	627	rBV	60983	68128	1.04%	0.120%
14	9.688	659	665	668	rBV2	44937	150643	2.30%	0.264%
15	9.768	668	672	674	rVV2	54138	130982	2.00%	0.230%
16	9.825	674	677	679	rVB	1891084	2103390	32.16%	3.693%
17	10.613	743	746	748	rBV	3998716	4098445	62.66%	7.195%
18	10.739	754	757	761	rVB	65190	112349	1.72%	0.197%
19	11.311	804	807	809	rBV	1661874	2107695	32.22%	3.700%
20	12.899	943	946	948	rBV	6437408	6386608	97.64%	11.212%
21	13.939	1035	1037	1040	rBV	1979626	1891802	28.92%	3.321%
22	15.345	1157	1160	1163	rBV	1043705	1427147	21.82%	2.505%

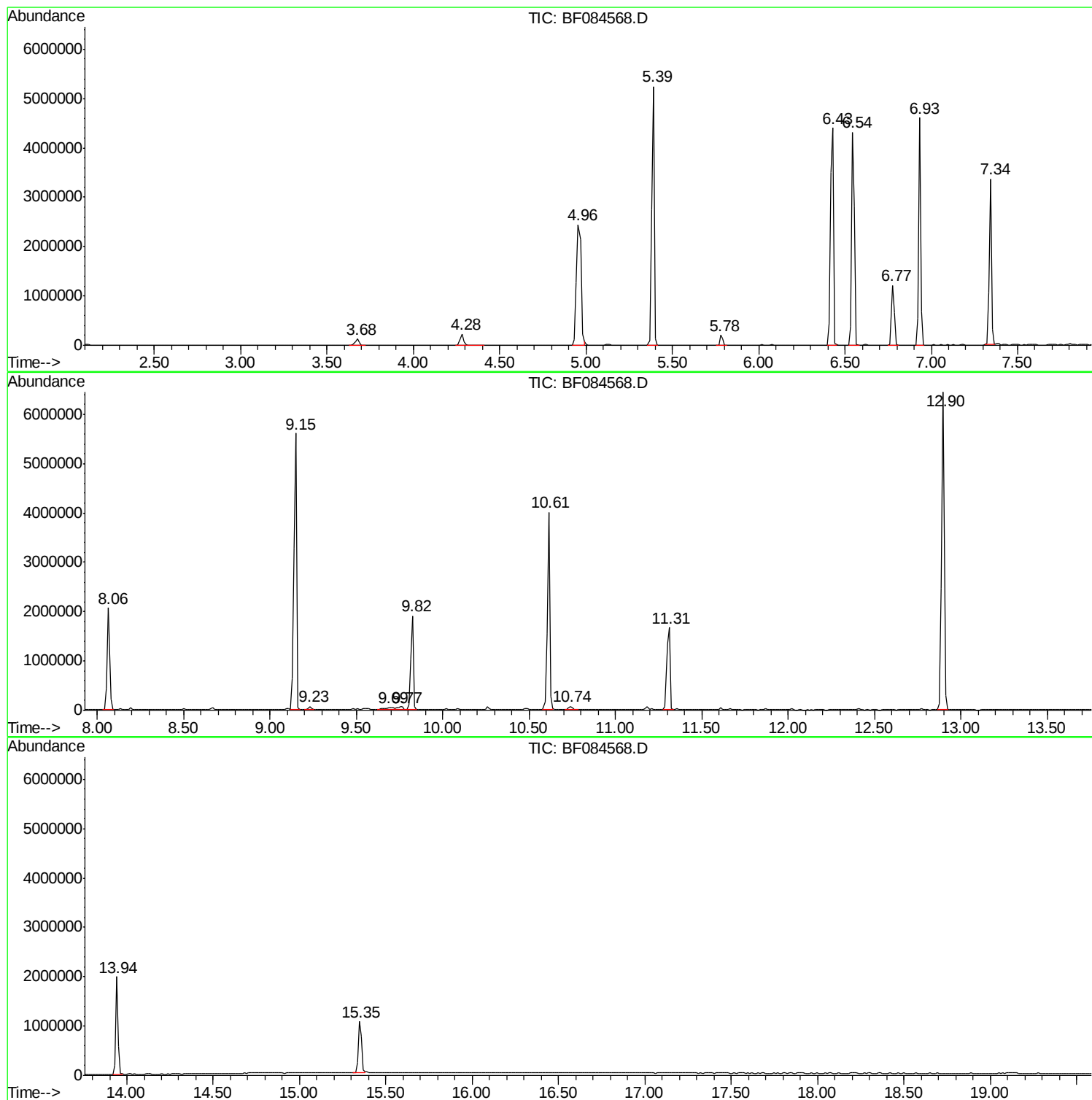
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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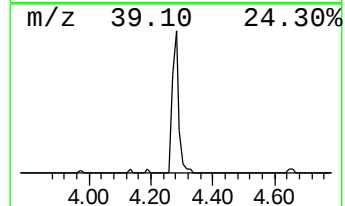
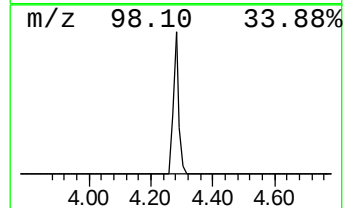
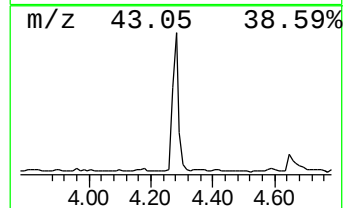
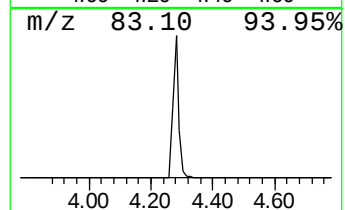
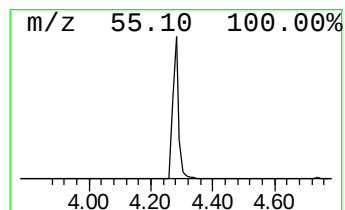
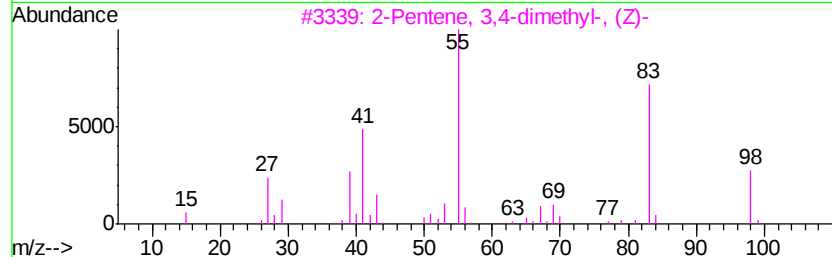
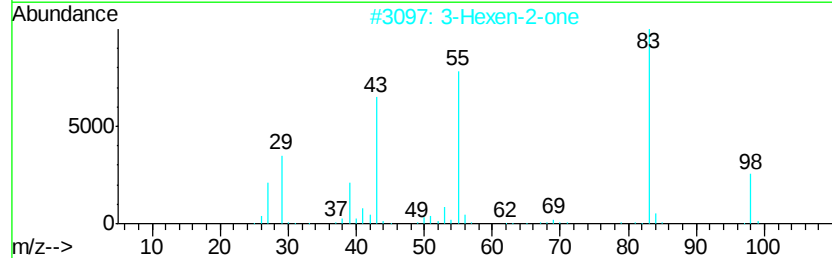
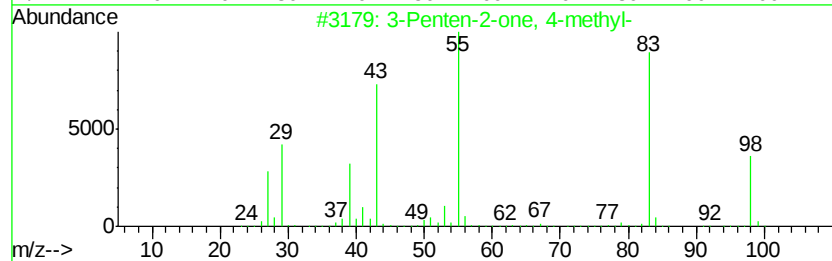
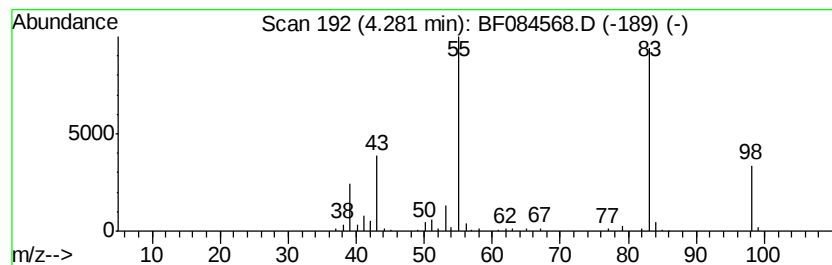
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	4.55 ng	298370	1,4-Dichlorobenzene-d4	6.77

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	91
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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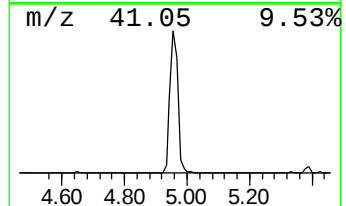
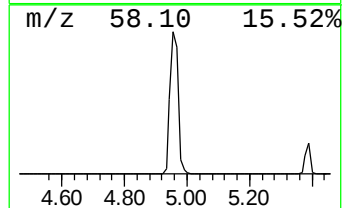
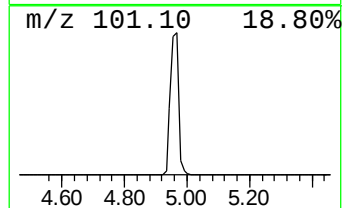
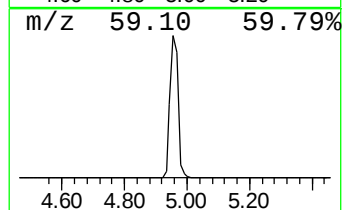
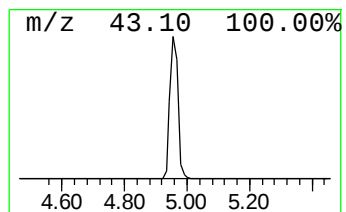
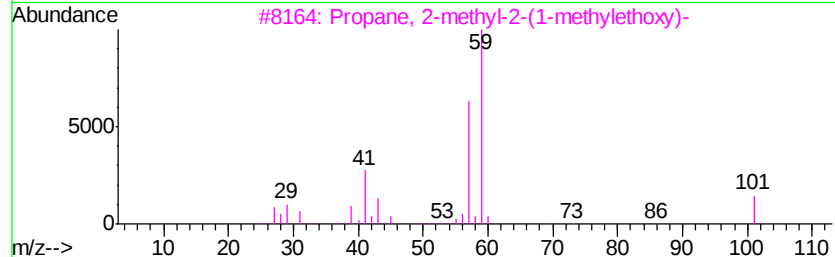
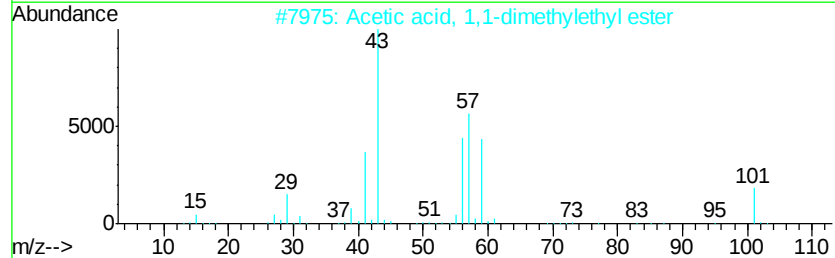
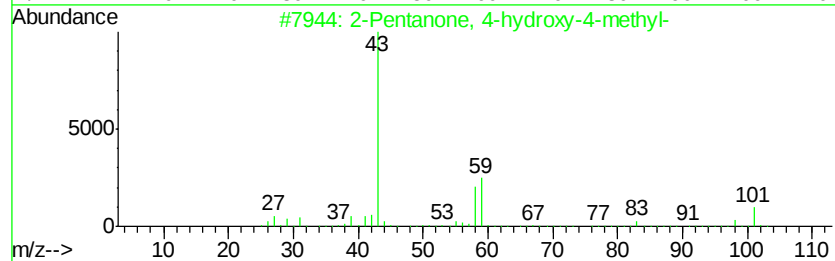
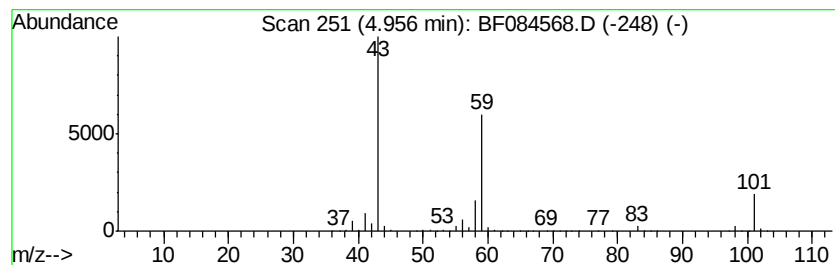
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	65.50 ng	4294210	1,4-Dichlorobenzene-d4	6.77

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	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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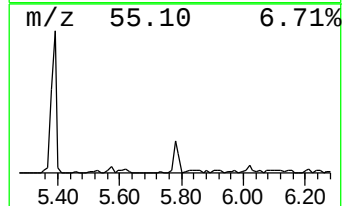
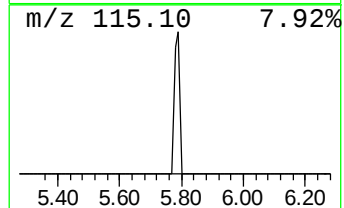
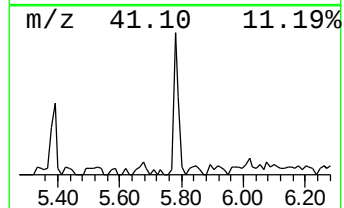
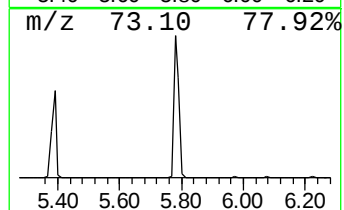
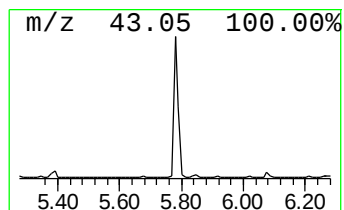
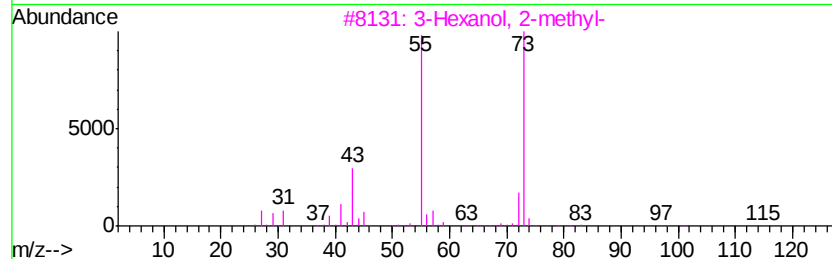
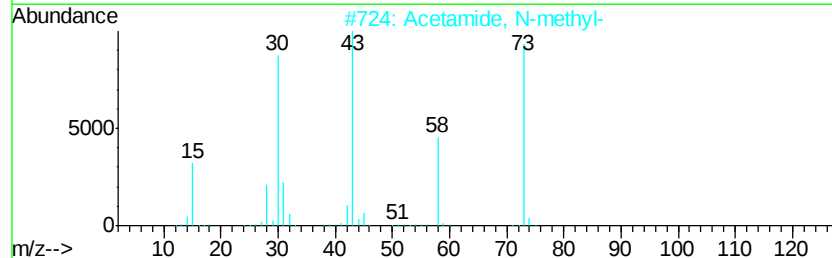
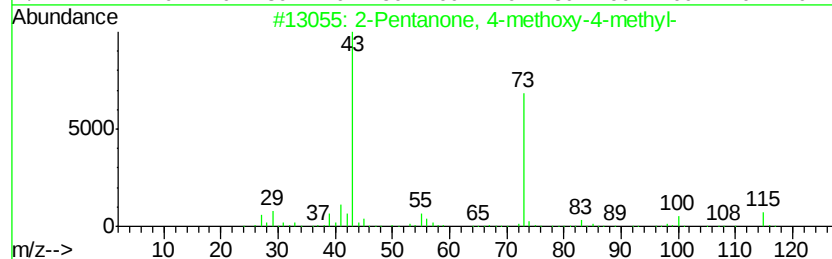
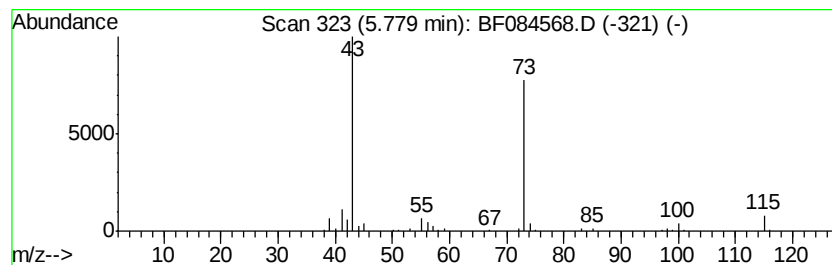
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	3.53 ng	231673	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
4		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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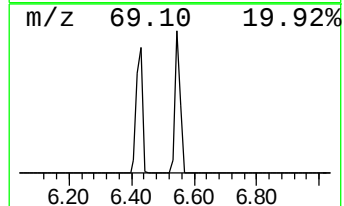
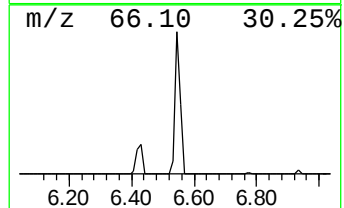
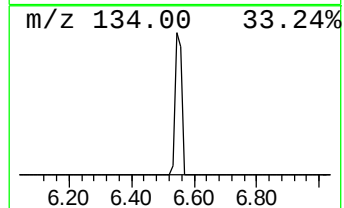
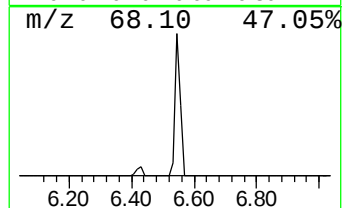
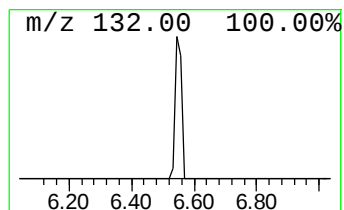
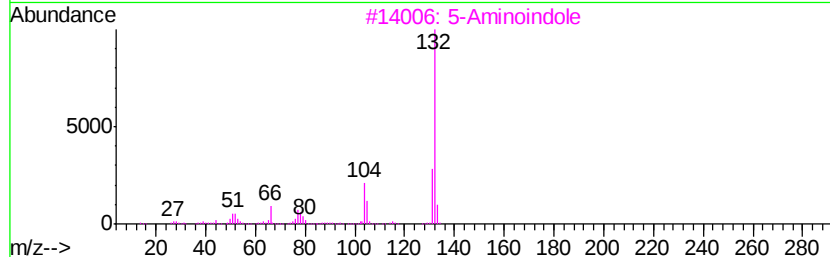
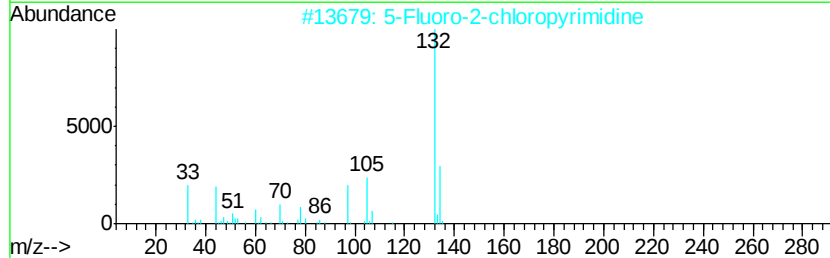
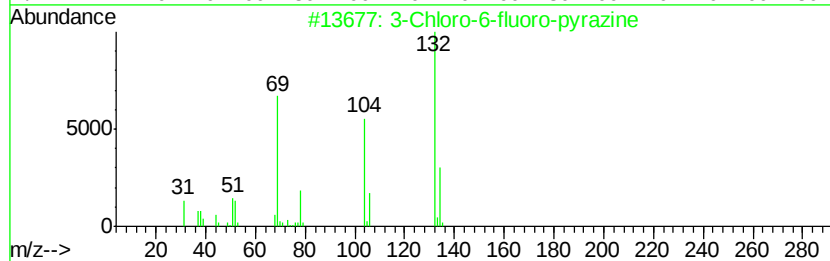
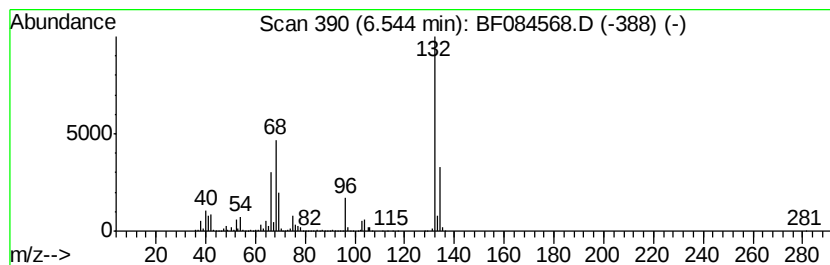
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Peak Number 5 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	78.42 ng	5141370	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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...	4.28	4.5	ng	298370	1	6.77	1311170	20.0
2-Pentanone, 4-hy...	4.96	65.5	ng	4294210	1	6.77	1311170	20.0
2-Pentanone, 4-me...	5.78	3.5	ng	231673	1	6.77	1311170	20.0
unknown6.54	6.54	78.4	ng	5141370	1	6.77	1311170	20.0