

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112515\
Data File : BF083273.D
Acq On : 25 Nov 2015 14:57
Operator : UM/IZ
Sample : G4553-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
112115-A263-E-D-B

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-BF112115.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	3.976	172	174	187	rBV	64480	148733	2.45%	0.399%
2	4.696	235	237	248	rBV	550262	826637	13.64%	2.217%
3	5.176	277	279	294	rBV	1659330	1826610	30.15%	4.899%
4	5.576	312	314	322	rBV	65430	112988	1.86%	0.303%
5	6.250	371	373	380	rBV	1172074	1210027	19.97%	3.245%
6	6.353	380	382	385	rBV	2477155	3070630	50.68%	8.236%
7	6.582	400	402	405	rBV	879967	993640	16.40%	2.665%
8	6.742	414	416	419	rBV	4152942	3927441	64.82%	10.534%
9	7.165	450	453	455	rBV	2654209	3710848	61.24%	9.953%
10	7.873	513	515	518	rBV	1492386	1345082	22.20%	3.608%
11	8.959	607	610	612	rBV	6268647	6059254	100.00%	16.252%
12	9.622	666	668	671	rBV	1743877	1536945	25.37%	4.122%
13	10.411	734	737	739	rBV	2743174	2671461	44.09%	7.165%
14	11.096	795	797	800	rBV	1816774	1571594	25.94%	4.215%
15	11.656	844	846	851	rBV2	76355	127190	2.10%	0.341%
16	12.434	912	914	919	rBV	113029	138055	2.28%	0.370%
17	12.685	933	936	939	rBV	5206223	5358809	88.44%	14.373%
18	13.600	1012	1016	1019	rBV2	38884	80209	1.32%	0.215%
19	13.714	1024	1026	1029	rBV	1034767	1478837	24.41%	3.966%
20	15.074	1142	1145	1148	rBV	861536	1089153	17.98%	2.921%

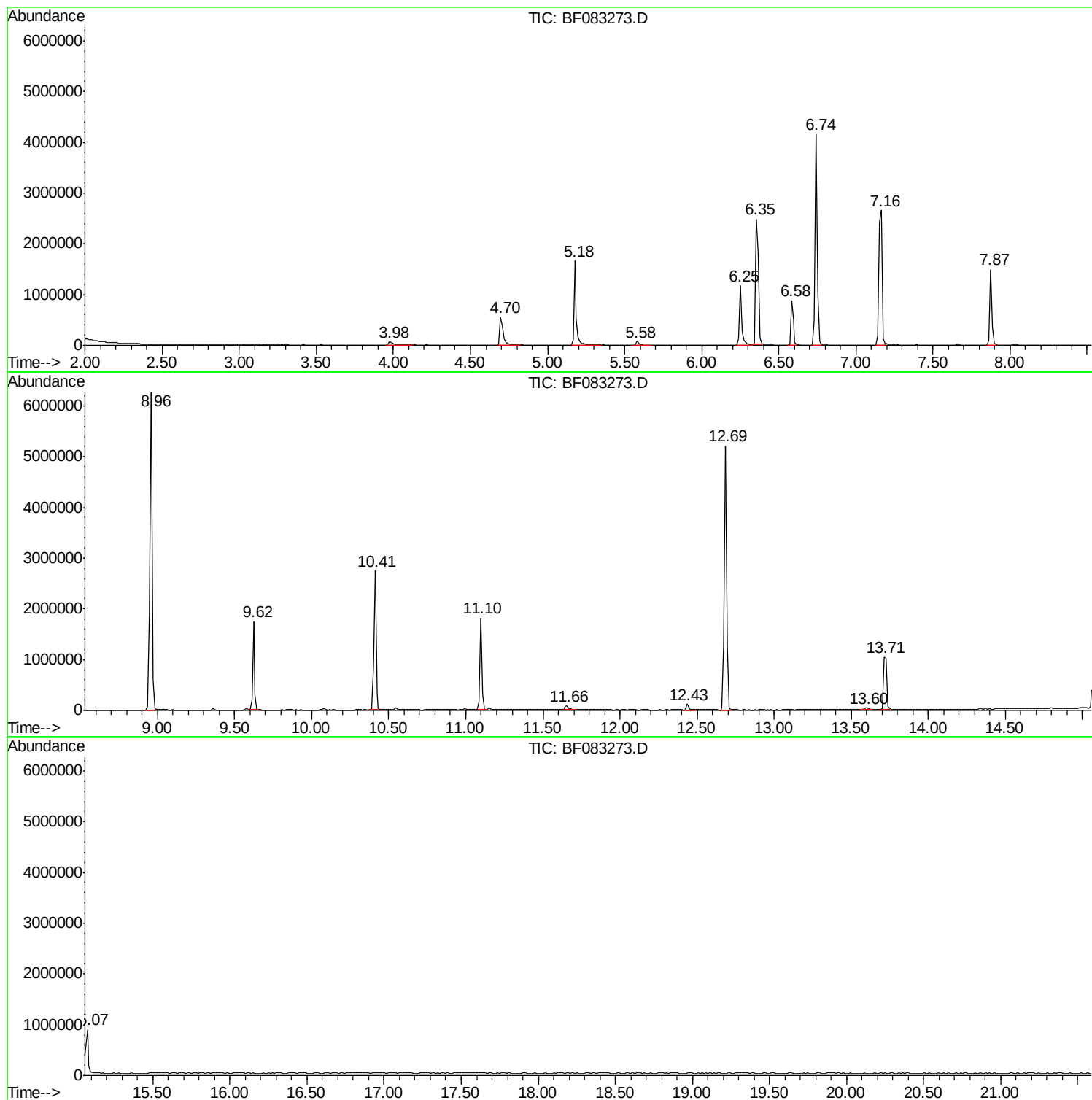
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Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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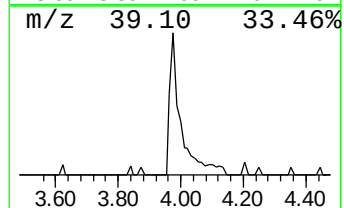
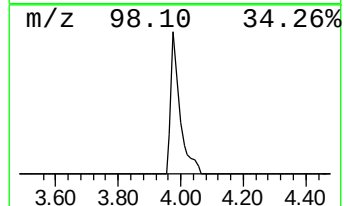
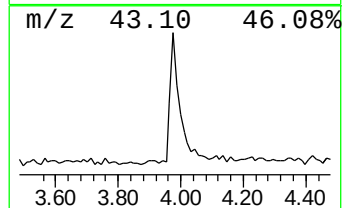
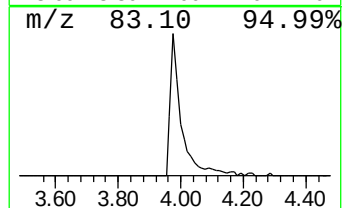
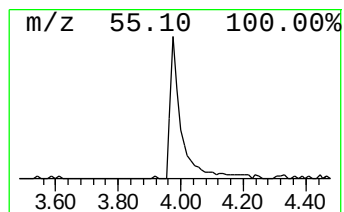
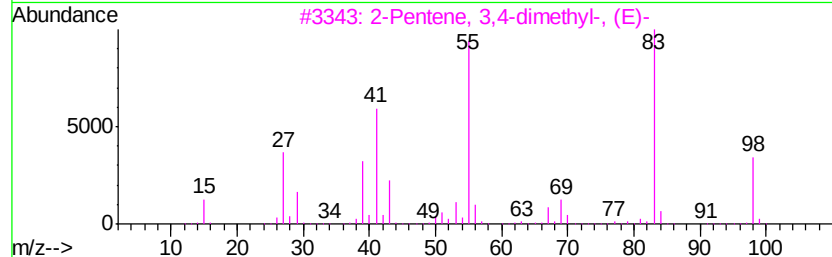
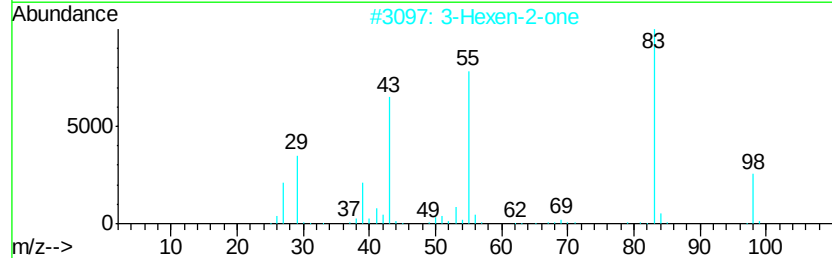
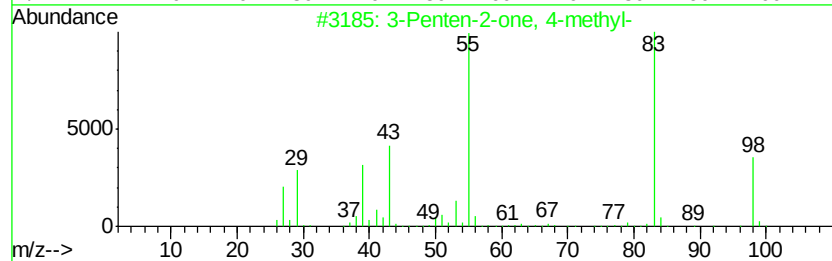
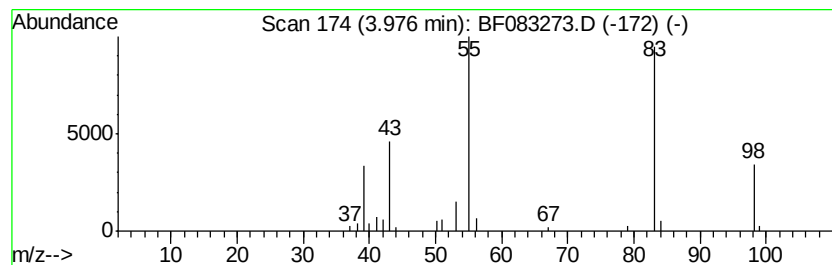
Quant Method : Z:\HPCHEM1\BNA F\Methods\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.98	2.99 ng	148733	1,4-Dichlorobenzene-d4	6.58

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	87
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	87
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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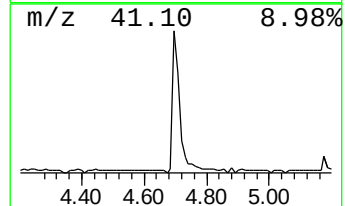
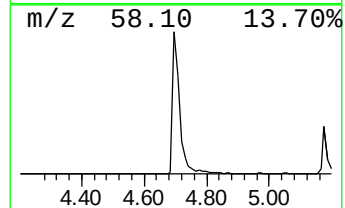
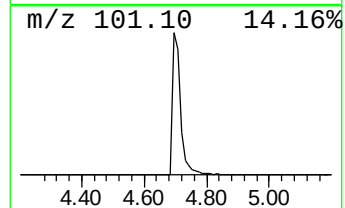
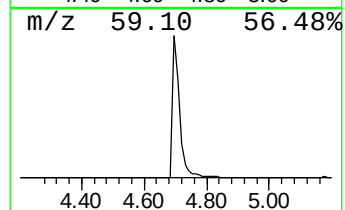
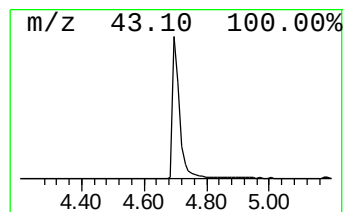
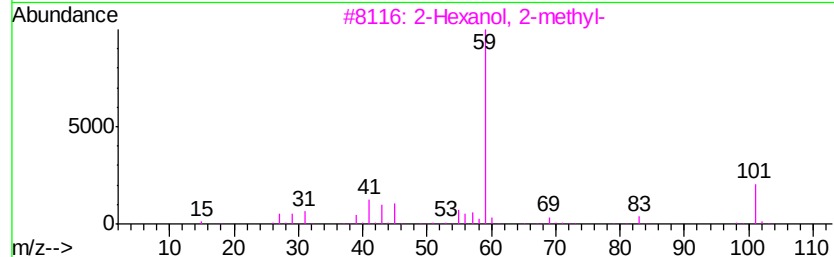
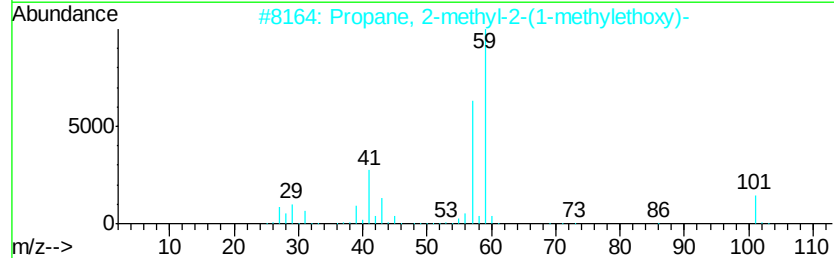
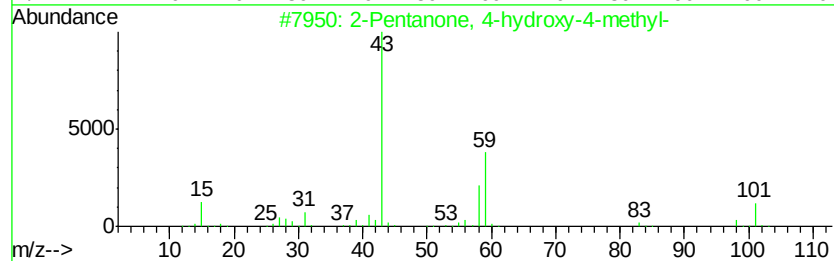
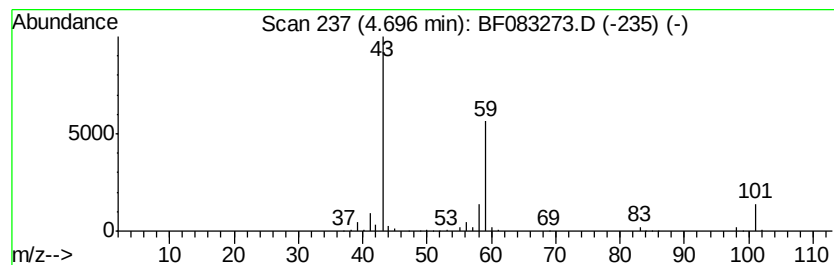
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	16.64 ng	826637	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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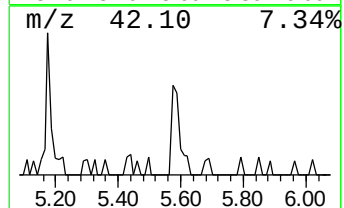
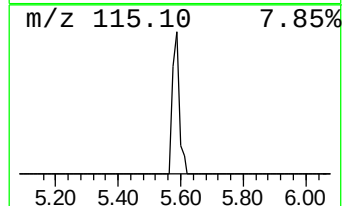
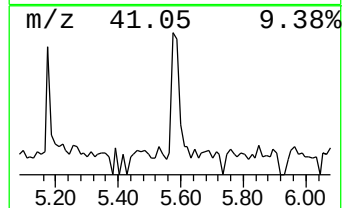
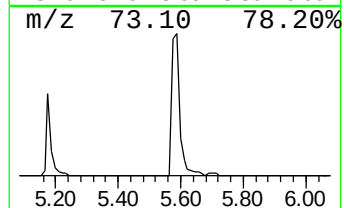
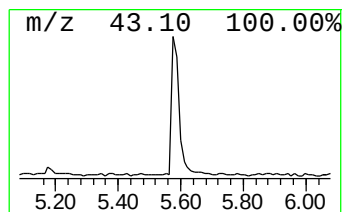
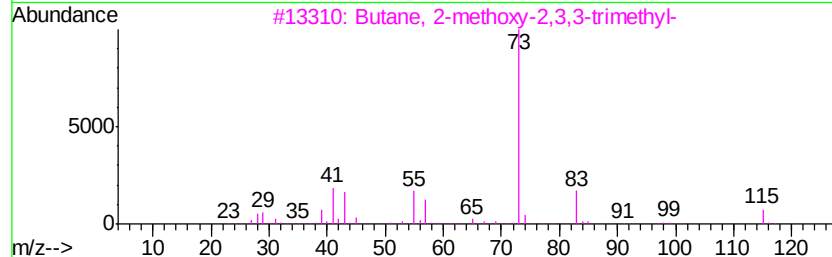
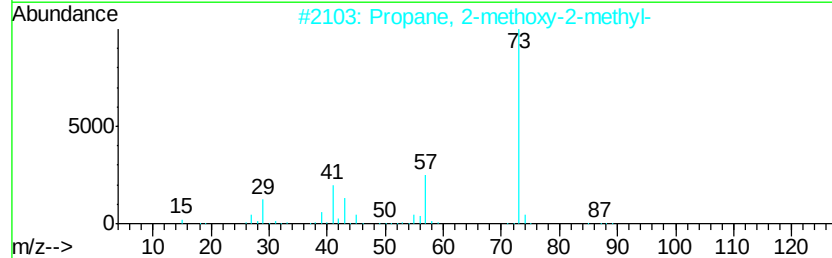
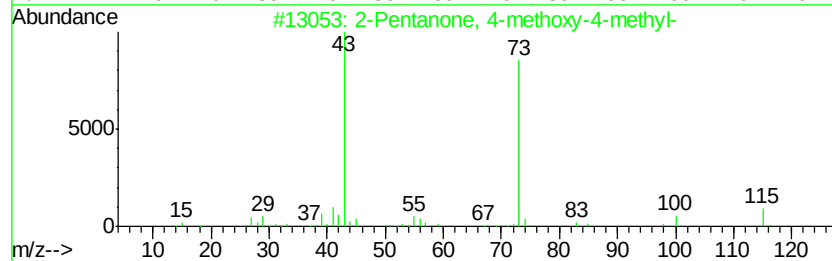
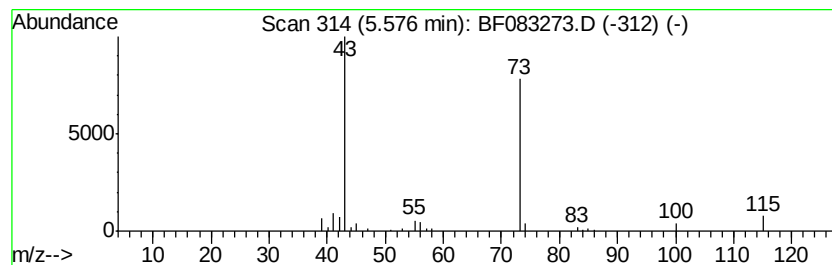
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.58	2.27 ng	112988	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	23
3		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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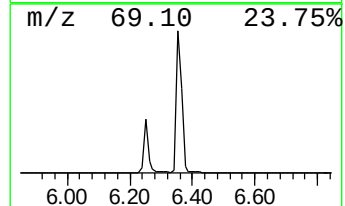
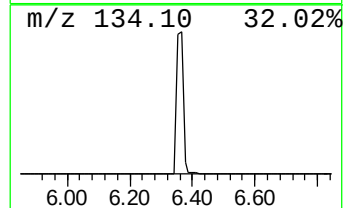
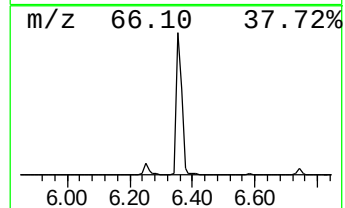
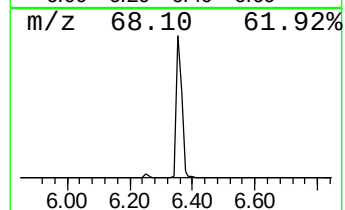
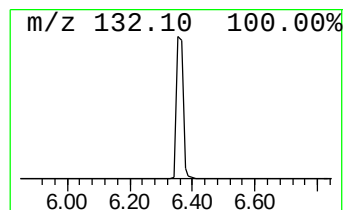
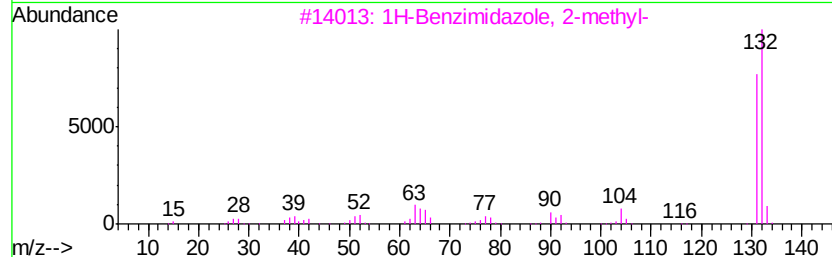
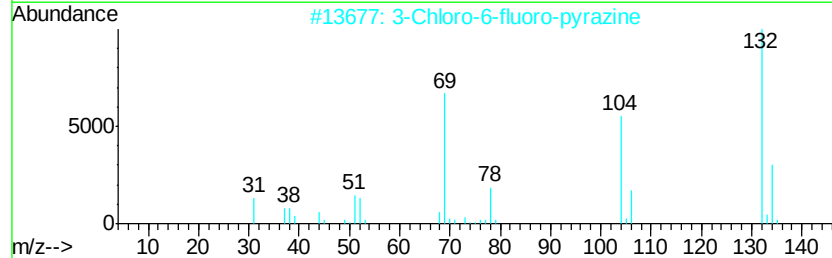
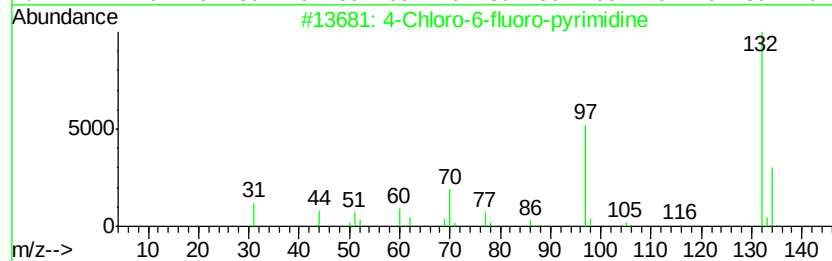
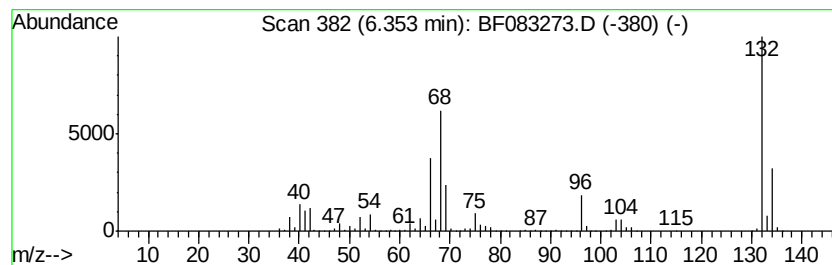
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Peak Number 4 unknown6.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	61.81 ng	3070630	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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...	3.98	3.0	ng	148733	1	6.58	993640	20.0
2-Pentanone, 4-hy...	4.70	16.6	ng	826637	1	6.58	993640	20.0
2-Pentanone, 4-me...	5.58	2.3	ng	112988	1	6.58	993640	20.0
unknown6.35	6.35	61.8	ng	3070630	1	6.58	993640	20.0