

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
 Data File : BF087313.D
 Acq On : 23 May 2016 22:16
 Operator : UM/SJ
 Sample : PB90662BL
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90662BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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	1.678	7	8	44	rVB	2598014	5323774	42.71%	8.091%
2	3.976	203	209	212	rBV	4058299	12069197	96.82%	18.342%
3	4.947	285	294	297	rBV2	3233397	12465401	100.00%	18.944%
4	5.542	344	346	375	rBV	1975055	3032163	24.32%	4.608%
5	6.113	393	396	409	rBV	564796	896711	7.19%	1.363%
6	7.142	484	486	494	rBV	2046919	2932749	23.53%	4.457%
7	7.256	494	496	503	rVB	1892891	3053620	24.50%	4.641%
8	7.610	525	527	539	rVB	717584	968240	7.77%	1.471%
9	7.850	545	548	558	rBV	2090375	3373304	27.06%	5.126%
10	8.525	604	607	609	rBV	1780178	2740925	21.99%	4.165%
11	9.645	702	705	725	rBV	700453	1251458	10.04%	1.902%
12	11.416	856	860	863	rBV	3019888	4895349	39.27%	7.440%
13	12.468	949	952	969	rBV	1034673	1401393	11.24%	2.130%
14	13.760	1063	1065	1090	rBV	1415101	2182123	17.51%	3.316%
15	14.880	1160	1163	1173	rBV	865479	1479876	11.87%	2.249%
16	17.211	1364	1367	1370	rBV	3368001	5236829	42.01%	7.958%
17	18.549	1482	1484	1499	rBV	882072	1392744	11.17%	2.117%
18	20.217	1628	1630	1637	rBV	814350	1105863	8.87%	1.681%

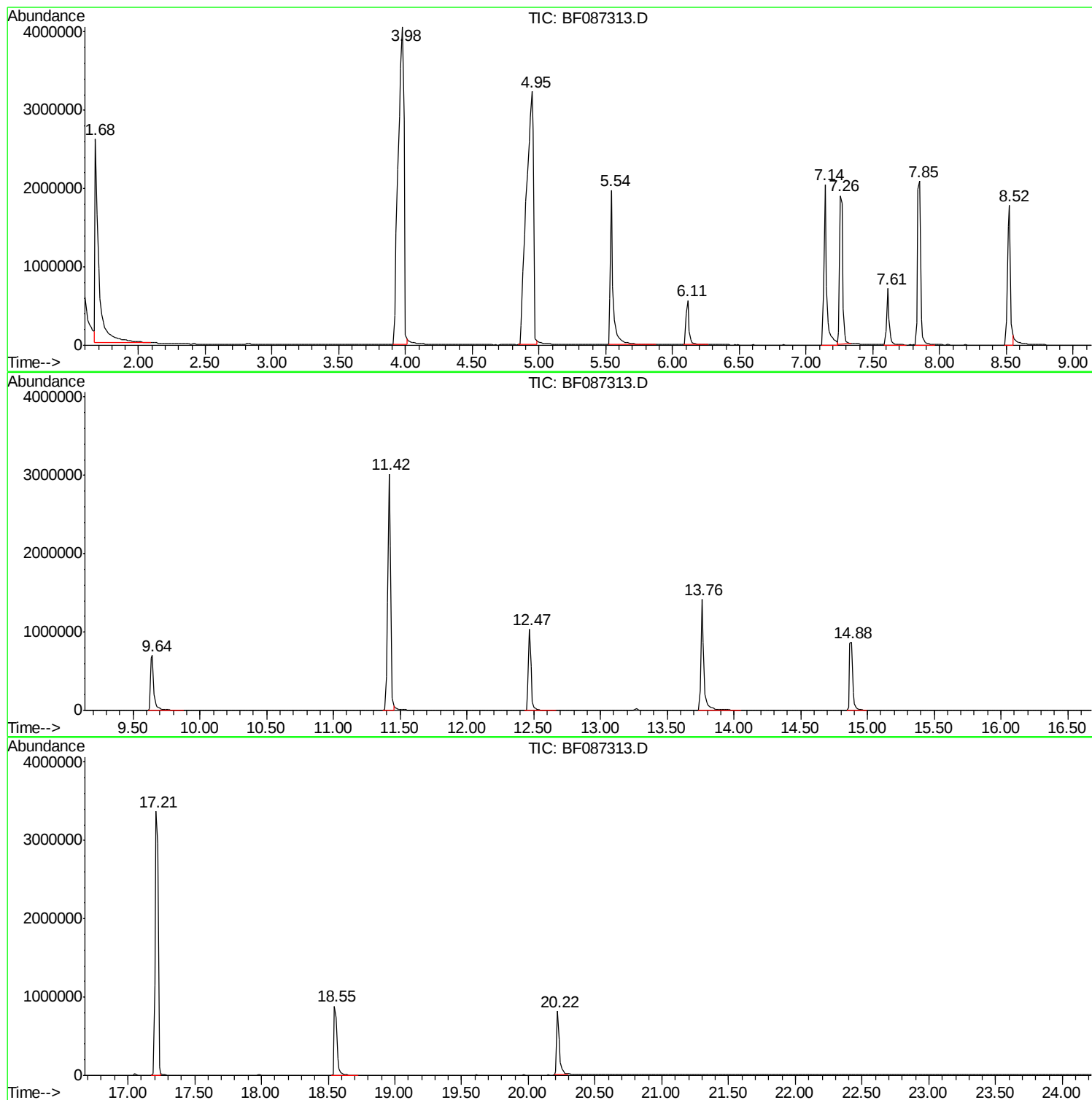
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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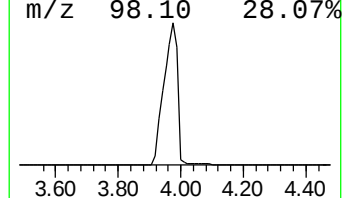
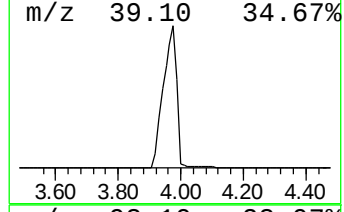
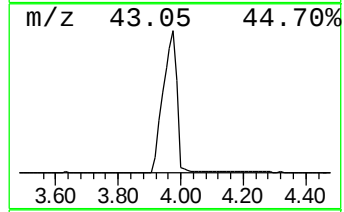
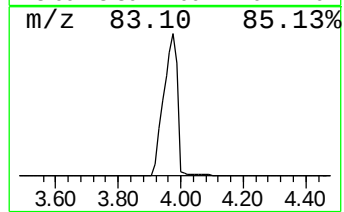
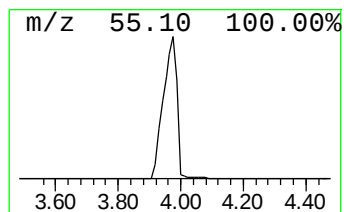
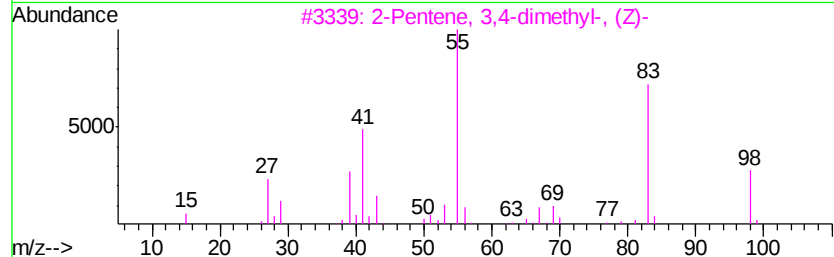
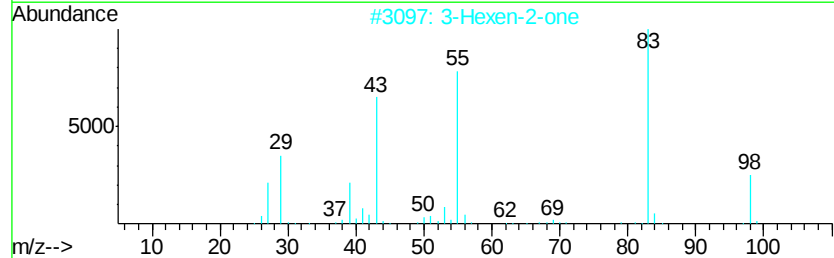
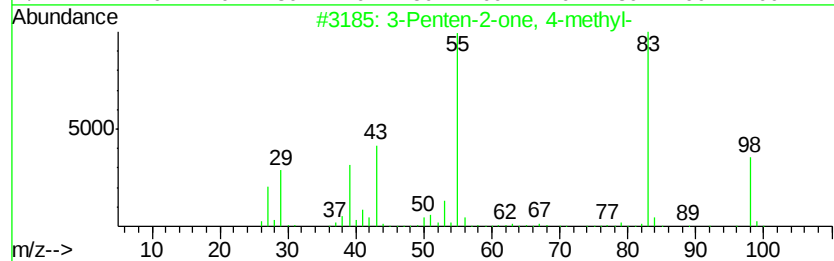
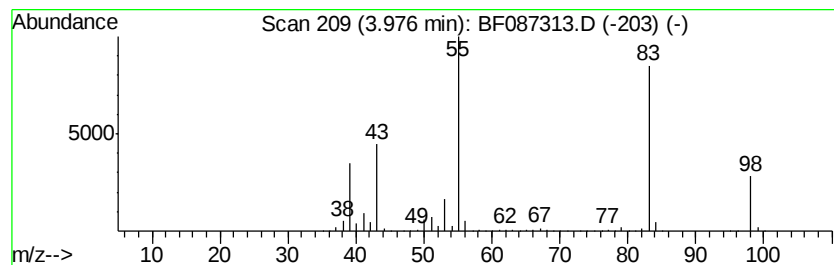
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	249.30 ng	12069200	1,4-Dichlorobenzene-d4	7.61

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			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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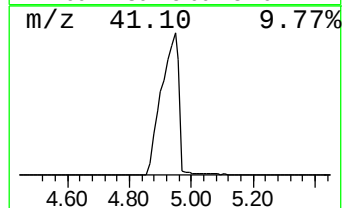
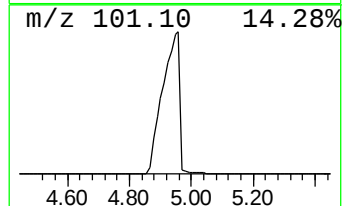
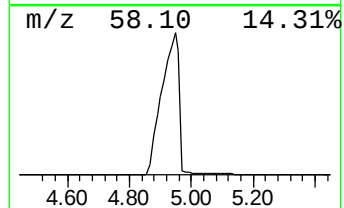
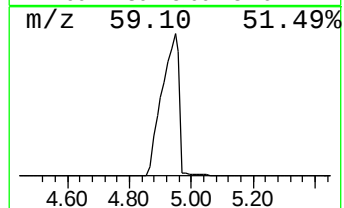
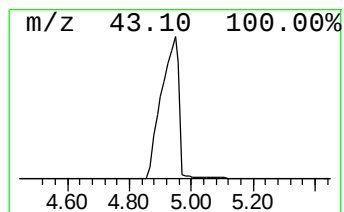
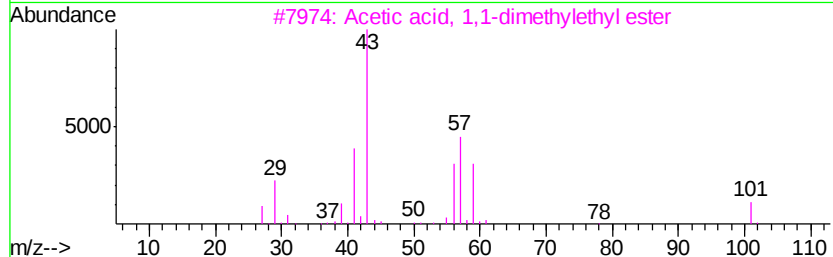
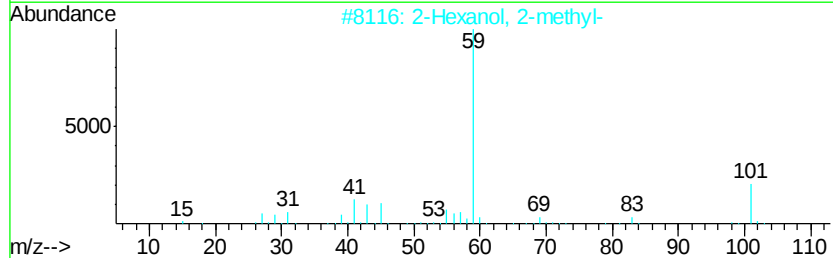
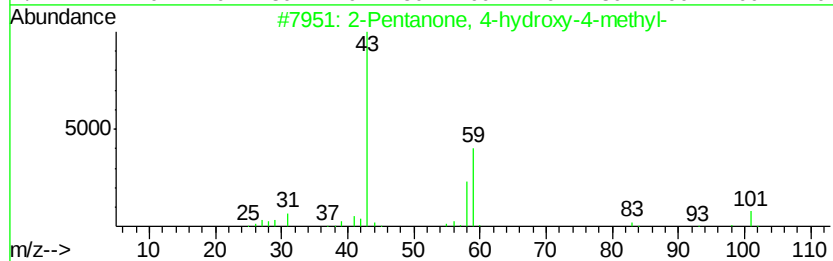
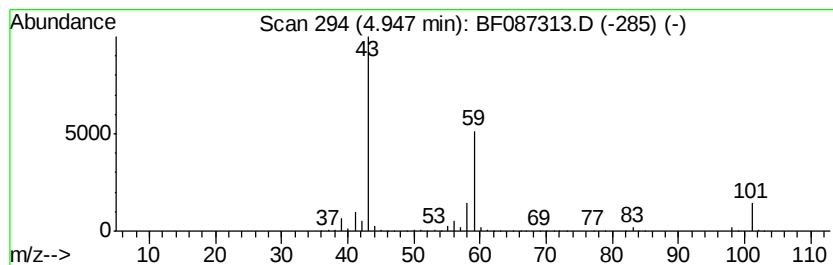
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	257.49 ng	12465400	1,4-Dichlorobenzene-d4	7.61

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	28
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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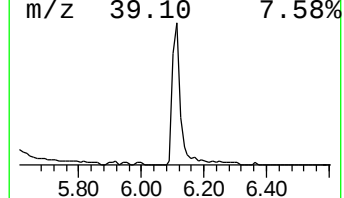
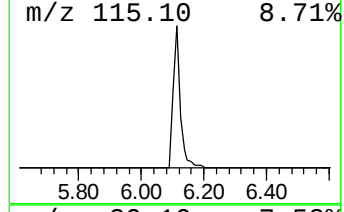
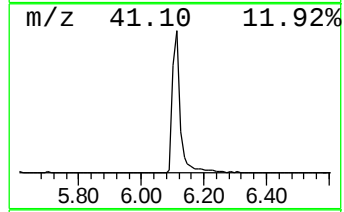
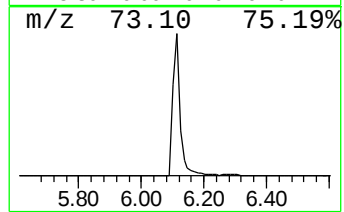
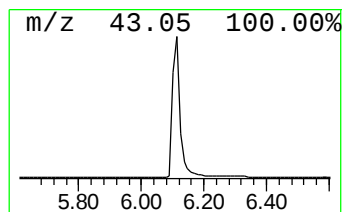
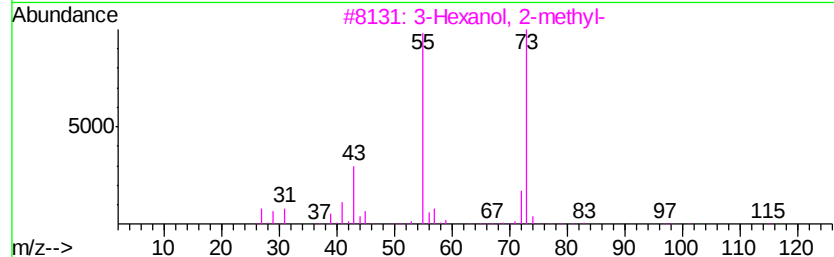
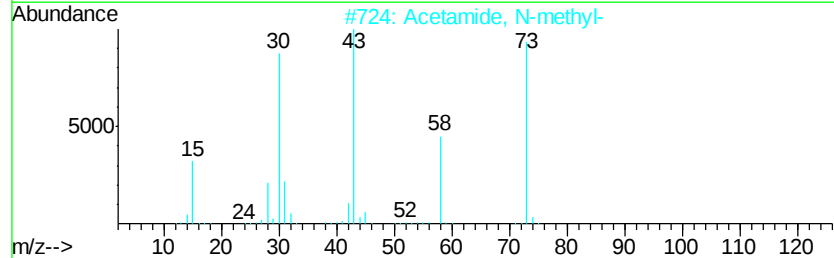
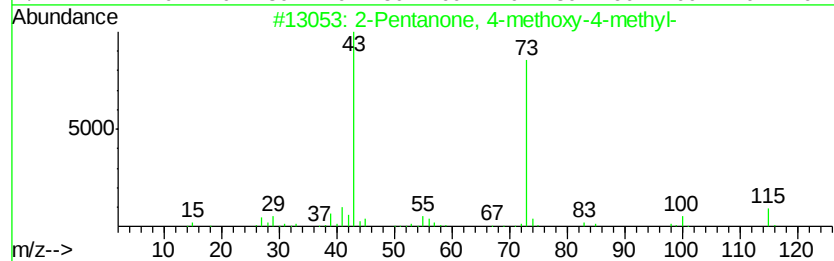
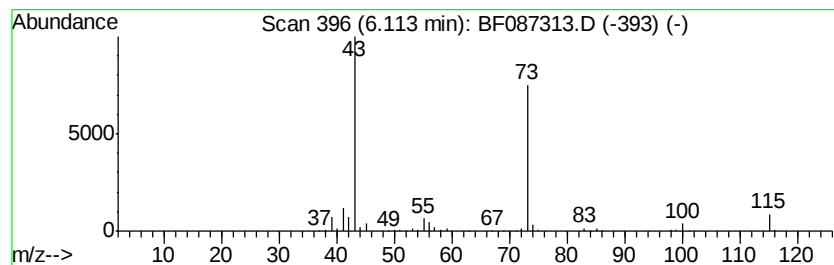
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.11	18.52 ng	896711	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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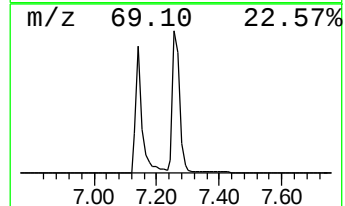
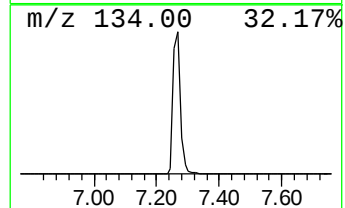
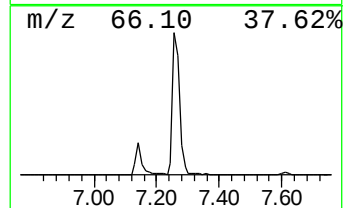
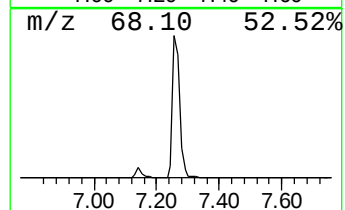
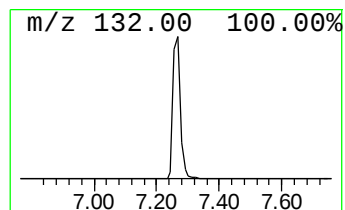
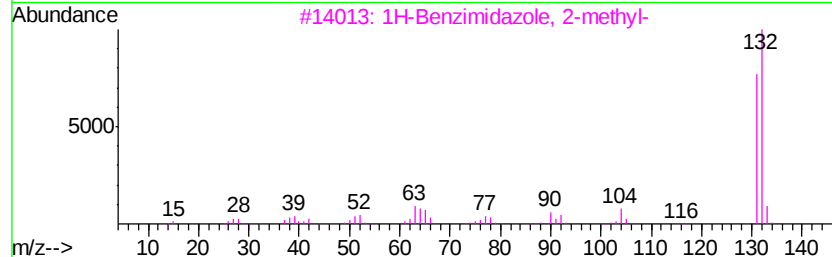
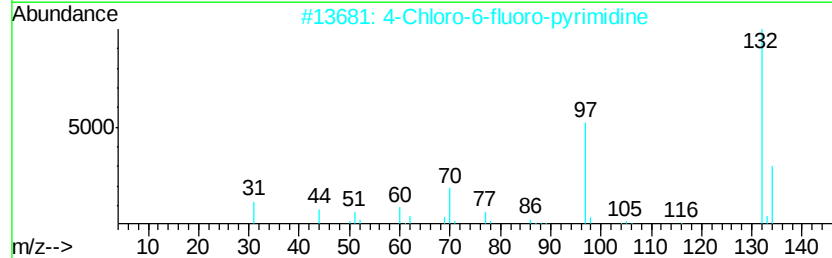
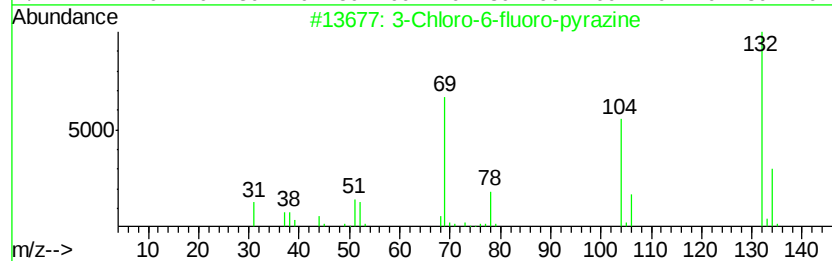
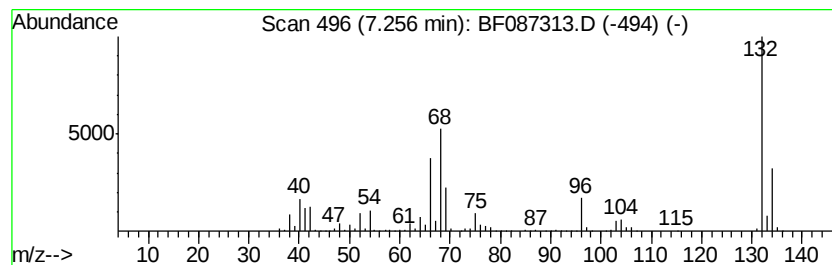
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Peak Number 5 unknown7.26 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	63.08 ng	3053620	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.98	249.3	ng	12069200	1	7.61	968240	20.0
2-Pentanone, 4-hy...	4.95	257.5	ng	12465400	1	7.61	968240	20.0
2-Pentanone, 4-me...	6.11	18.5	ng	896711	1	7.61	968240	20.0
unknown7.26	7.26	63.1	ng	3053620	1	7.61	968240	20.0