

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
 Data File : BF094712.D
 Acq On : 30 Apr 2017 14:11
 Operator : SJ/MA
 Sample : PB98552BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98552BL

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-BF041717.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	3.384	241	246	260	rBV	1547466	1582245	47.20%	5.966%
2	3.943	333	341	344	rBV	2103483	3064299	91.40%	11.554%
3	4.325	403	406	422	rBV	1675674	1788510	53.35%	6.744%
4	4.701	467	470	478	rBV	240688	227003	6.77%	0.856%
5	5.390	583	587	605	rBV	1798045	1748174	52.14%	6.592%
6	5.519	605	609	618	rVB	2079377	1877926	56.01%	7.081%
7	5.766	647	651	657	rBV	712205	613377	18.30%	2.313%
8	5.942	677	681	685	rBV	2309116	2122535	63.31%	8.003%
9	6.419	757	762	765	rBV	1536432	1634005	48.74%	6.161%
10	7.254	901	904	913	rBV	853381	835283	24.91%	3.149%
11	8.578	1125	1129	1133	rBV	3061992	3227366	96.27%	12.169%
12	9.389	1263	1267	1281	rBV2	945238	954652	28.48%	3.600%
13	10.366	1429	1433	1445	rBV	963671	990750	29.55%	3.736%
14	11.213	1573	1577	1587	rBV	999526	992769	29.61%	3.743%
15	13.195	1908	1914	1918	rBV	2916147	3352548	100.00%	12.641%
16	14.465	2125	2130	2137	rBV	844666	885437	26.41%	3.339%
17	16.095	2402	2407	2417	rBV	503974	624311	18.62%	2.354%

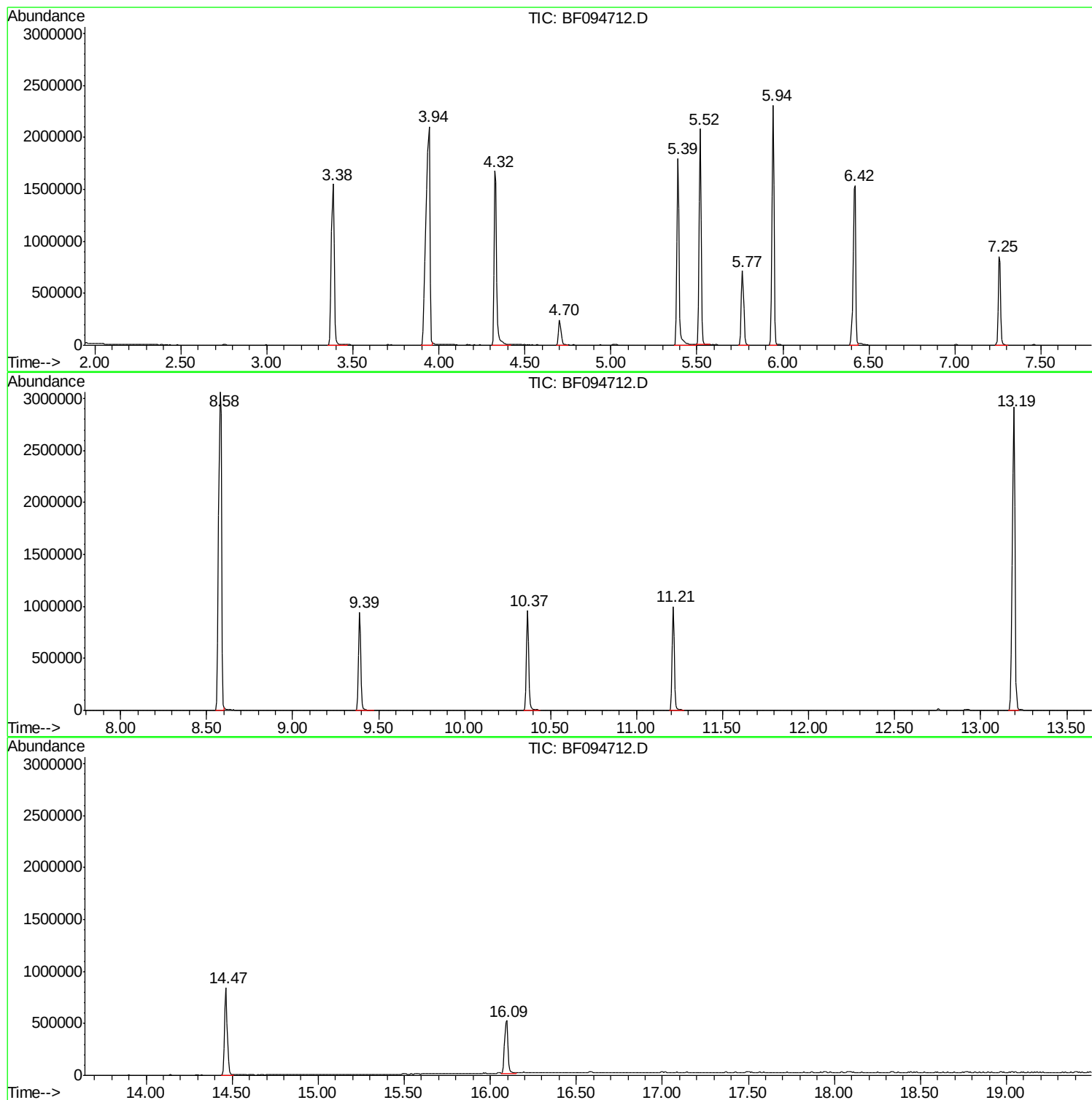
Sum of corrected areas: 26521190

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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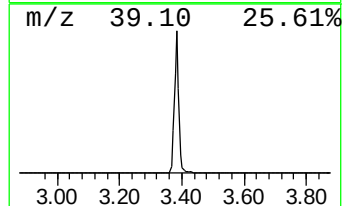
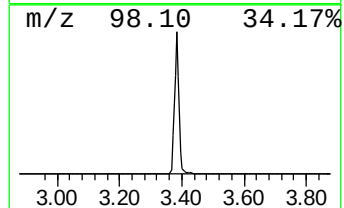
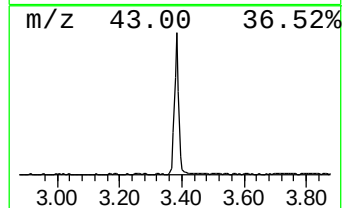
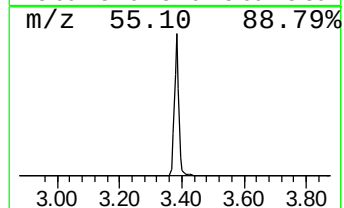
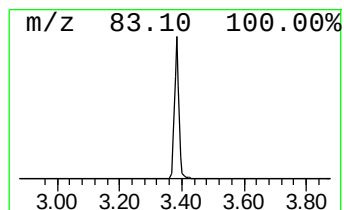
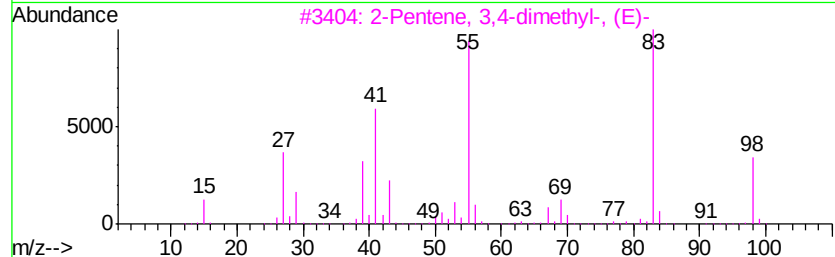
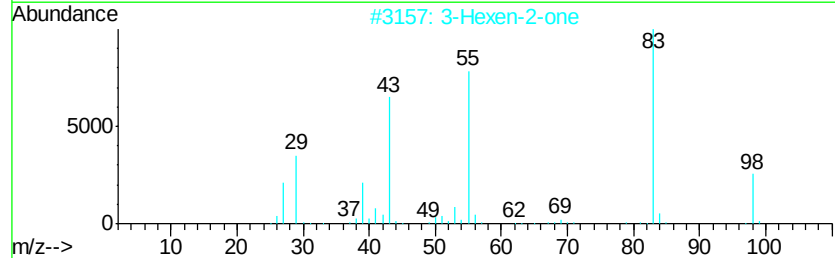
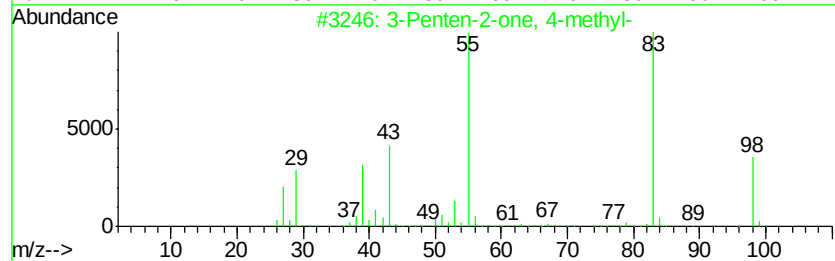
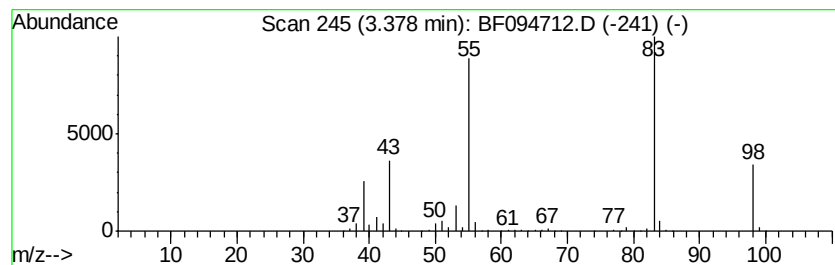
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
3.38	51.59 ng	1582250	1,4-Dichlorobenzene-d4	5.77

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		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
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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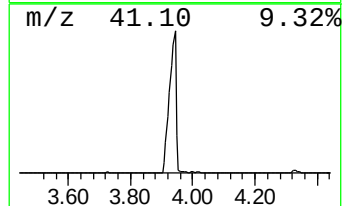
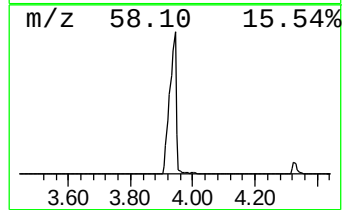
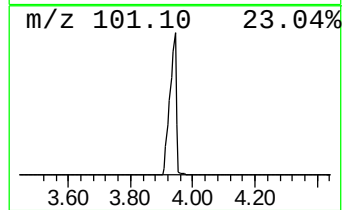
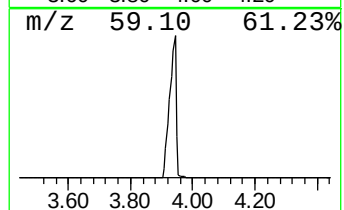
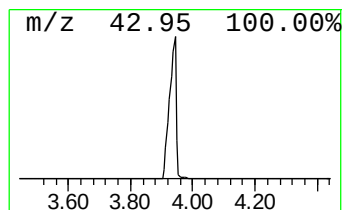
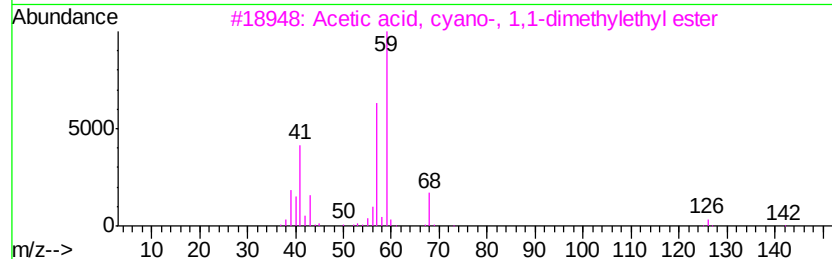
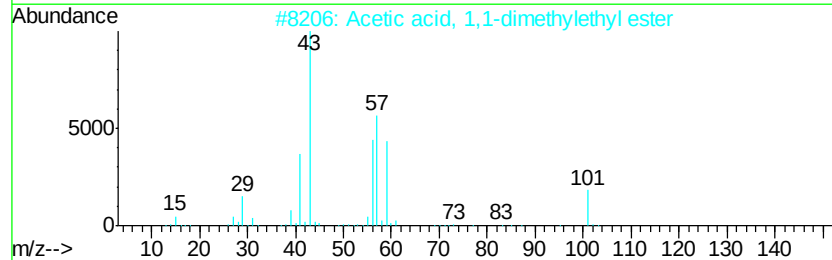
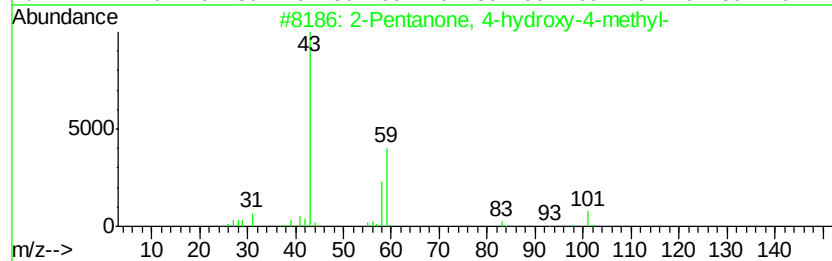
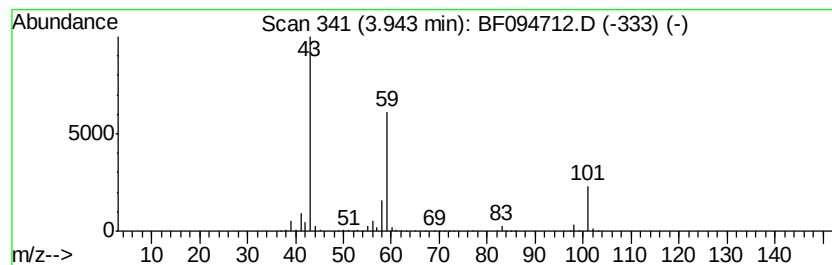
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	99.92 ng	3064300	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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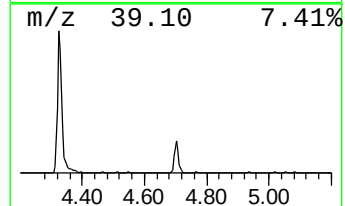
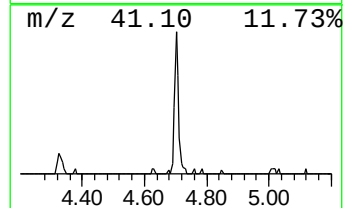
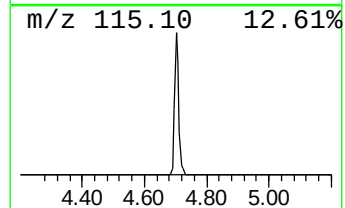
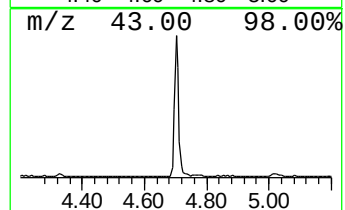
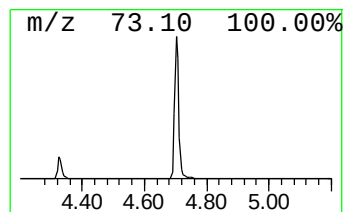
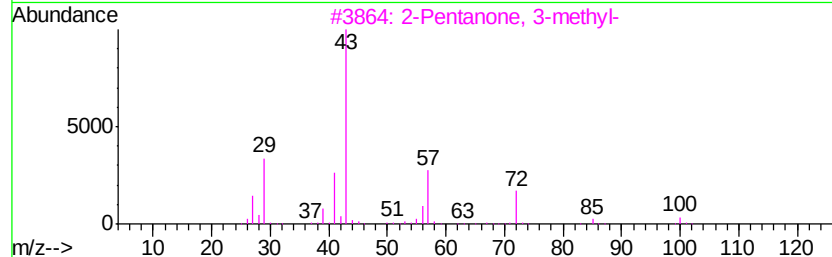
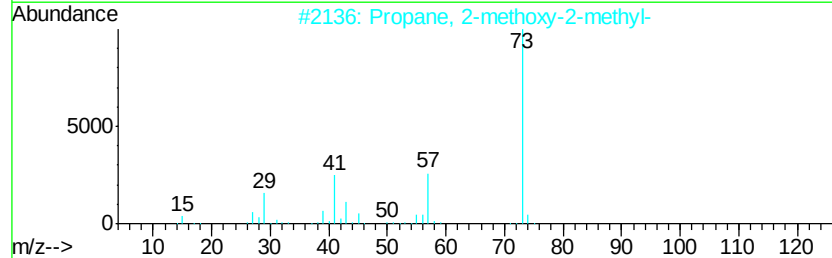
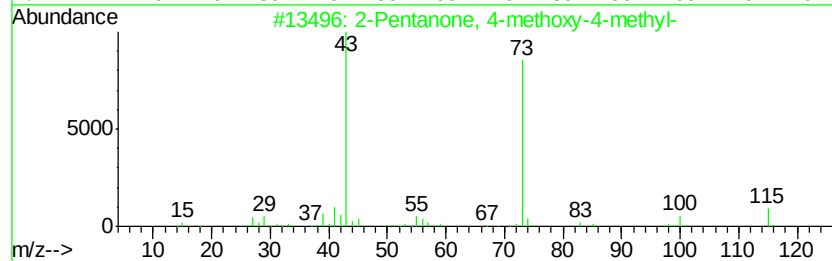
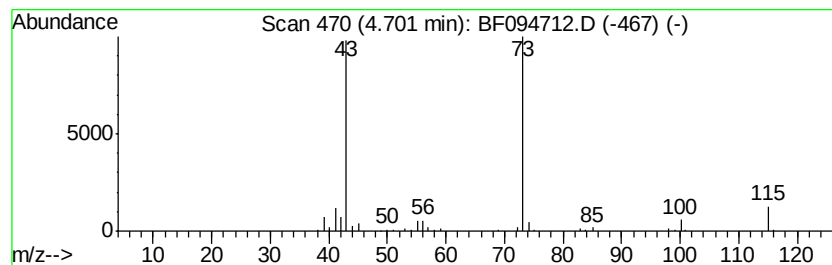
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	7.40 ng	227003	1,4-Dichlorobenzene-d4	5.77

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	12
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9



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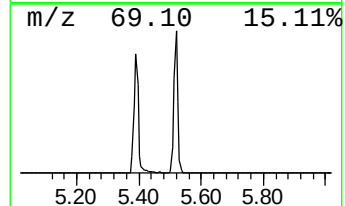
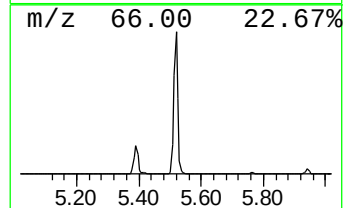
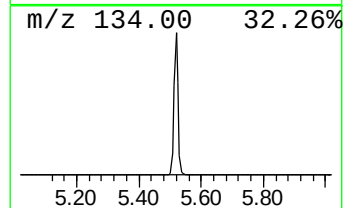
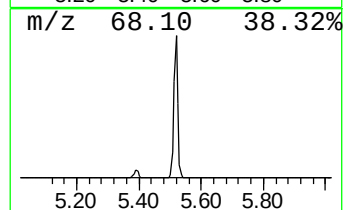
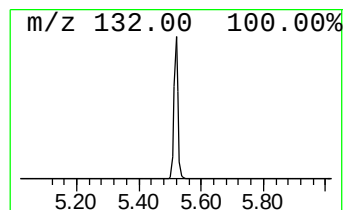
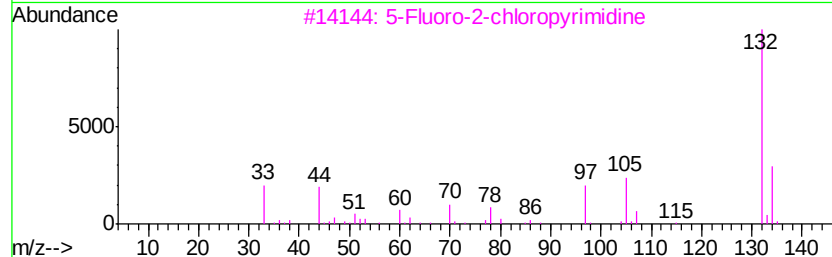
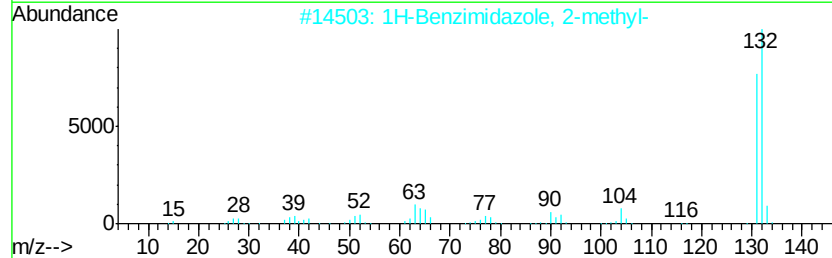
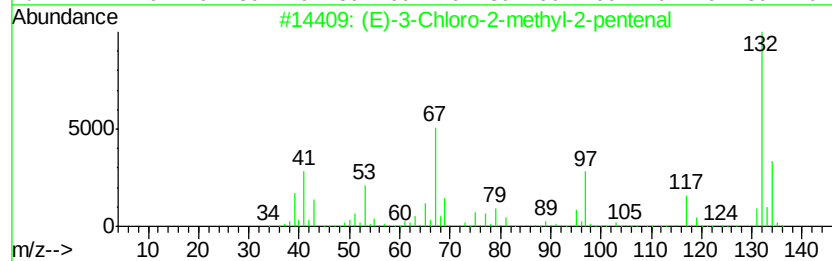
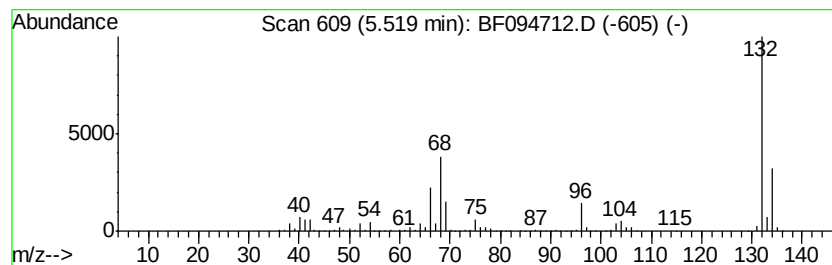
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Peak Number 4 unknown5.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	61.23 ng	1877930	1,4-Dichlorobenzene-d4	5.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27	
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9	
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.38	51.6	ng	1582250	1	5.77	613377	20.0
2-Pentanone, 4-hy...	3.94	99.9	ng	3064300	1	5.77	613377	20.0
2-Pentanone, 4-me...	4.70	7.4	ng	227003	1	5.77	613377	20.0
unknown5.52	5.52	61.2	ng	1877930	1	5.77	613377	20.0