

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
 Data File : BF089159.D
 Acq On : 21 Jul 2016 4:50
 Operator : UM/SJ
 Sample : PB91543BL
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91543BL

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-BF072016.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	1.724	10	12	37	rVB	876147	1296483	41.95%	6.709%
2	4.044	210	215	228	rBV	1088081	2147129	69.48%	11.111%
3	4.787	273	280	282	rBV	1164957	3090249	100.00%	15.992%
4	5.199	314	316	344	rVB	750789	1010334	32.69%	5.228%
5	5.599	349	351	353	rBV	231211	244985	7.93%	1.268%
6	6.262	406	409	416	rBV	696556	1052237	34.05%	5.445%
7	6.365	416	418	437	rVV	786525	1104278	35.73%	5.715%
8	6.593	437	438	450	rVV	220230	352389	11.40%	1.824%
9	6.753	450	452	472	rVB	1216208	1231465	39.85%	6.373%
10	7.165	486	488	491	rBV	632345	959198	31.04%	4.964%
11	7.885	548	551	563	rBV	422984	475854	15.40%	2.463%
12	8.959	642	645	648	rBV	1488082	1841020	59.58%	9.527%
13	9.622	701	703	706	rBV	367251	517464	16.75%	2.678%
14	10.411	770	772	784	rBB	657378	746718	24.16%	3.864%
15	11.096	830	832	835	rBV	508669	571552	18.50%	2.958%
16	12.685	968	971	974	rBV	1815339	1844482	59.69%	9.545%
17	13.714	1059	1061	1064	rBV	439037	482311	15.61%	2.496%
18	15.063	1176	1179	1182	rBV	314934	355677	11.51%	1.841%

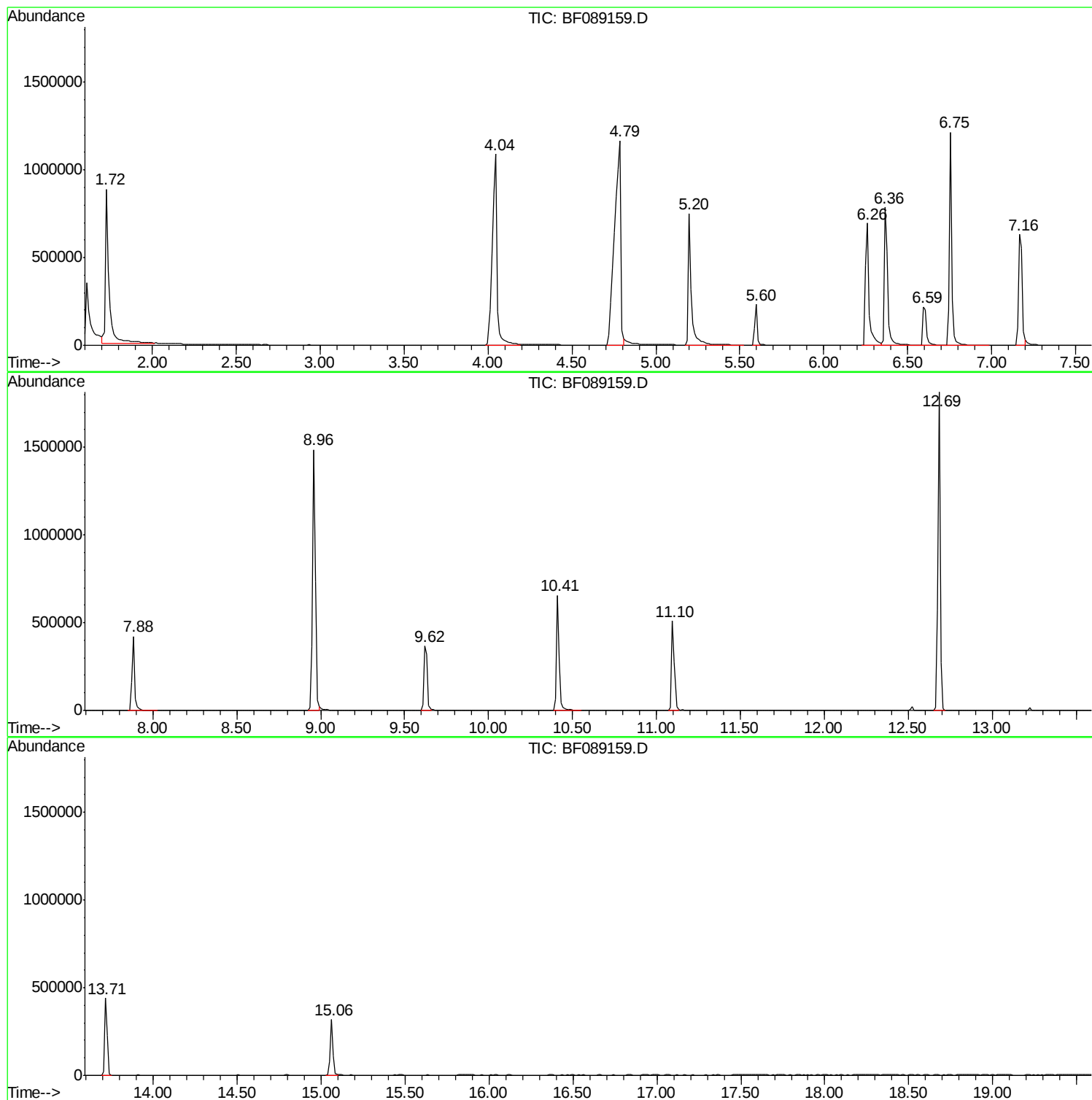
Sum of corrected areas: 19323825

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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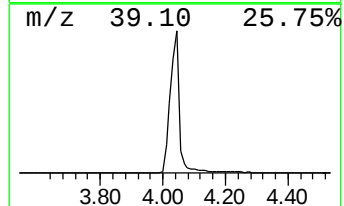
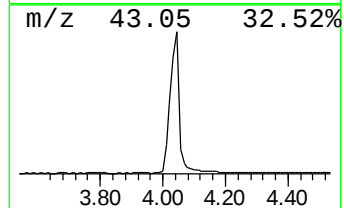
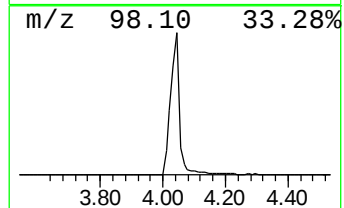
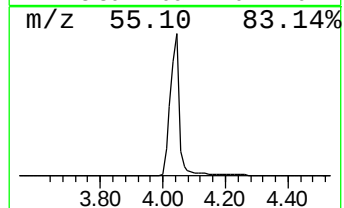
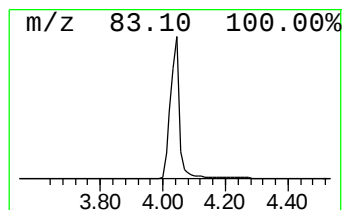
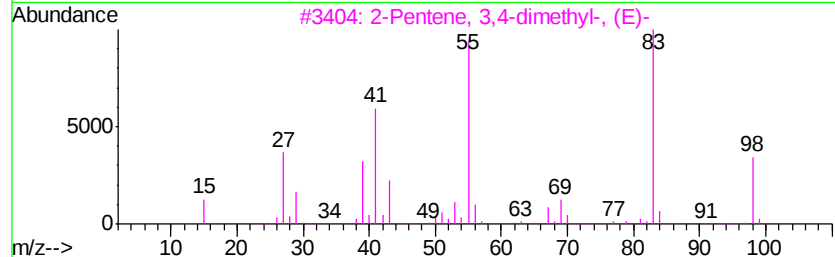
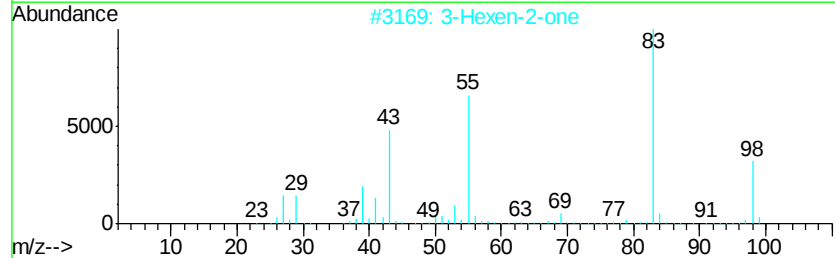
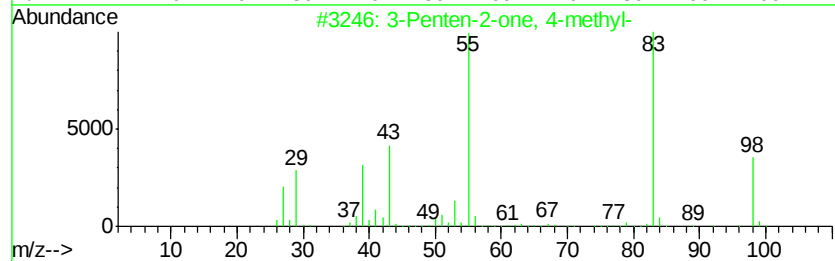
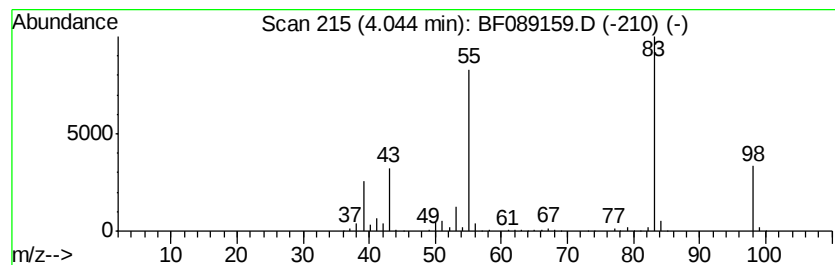
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
4.04	121.86 ng	2147130	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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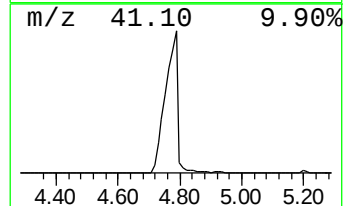
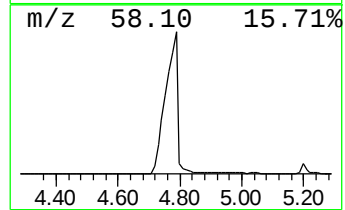
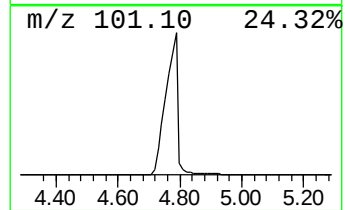
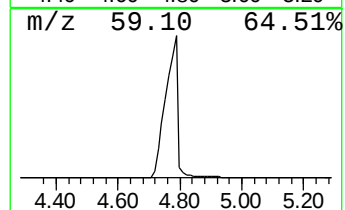
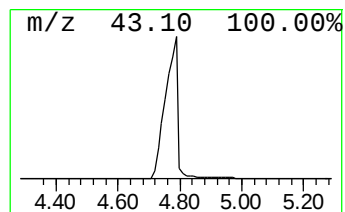
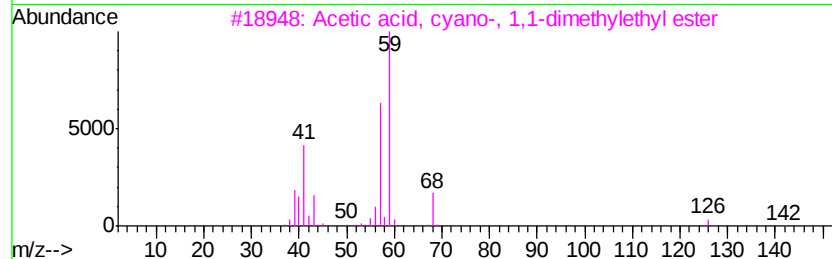
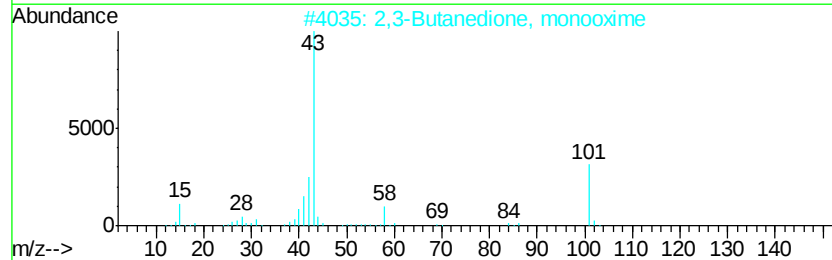
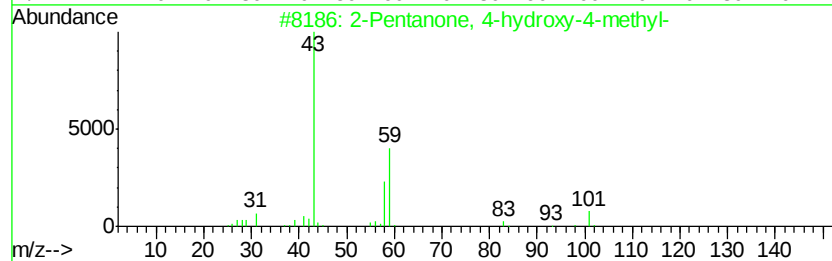
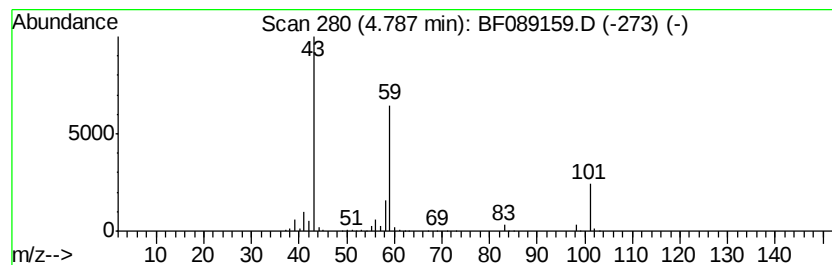
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	175.39 ng	3090250	1,4-Dichlorobenzene-d4	6.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
4	Acetone	58	C3H6O	000067-64-1	10	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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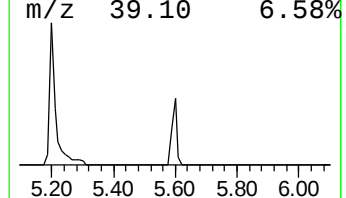
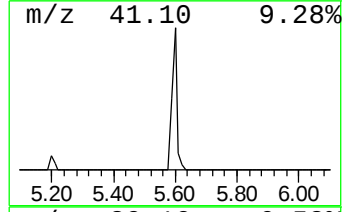
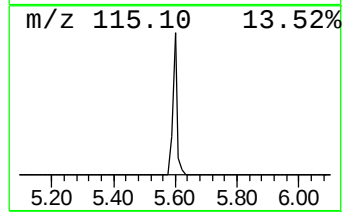
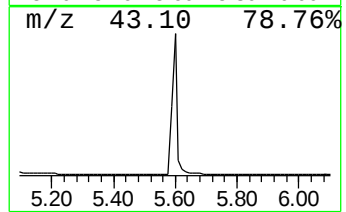
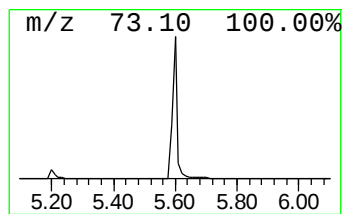
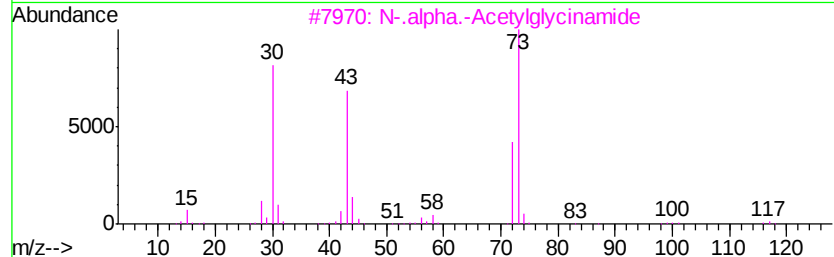
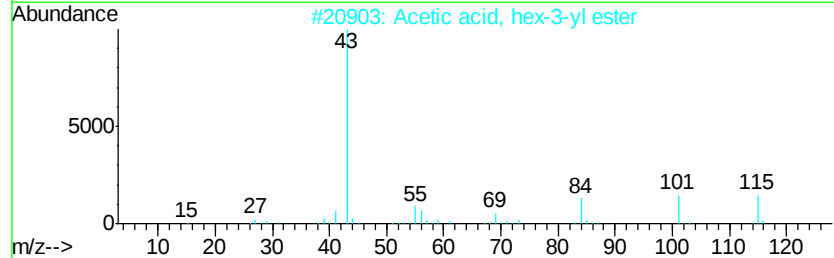
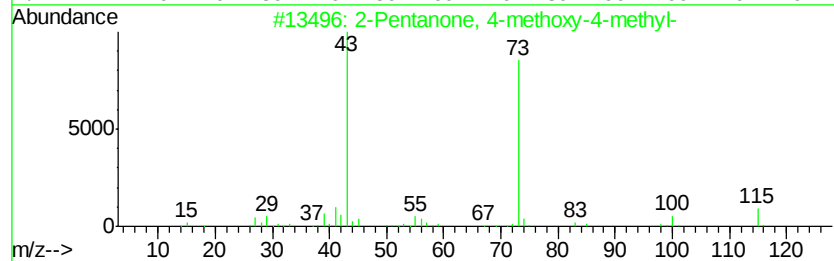
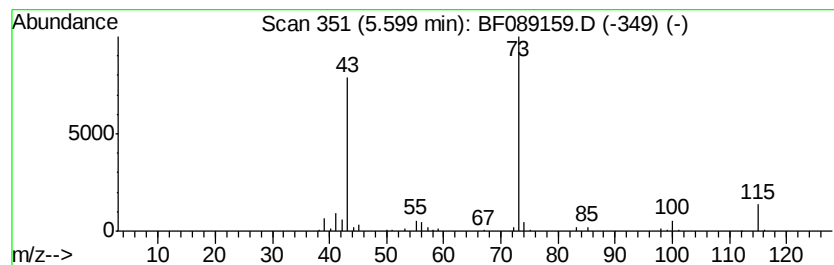
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	13.90 ng	244985	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetic acid, hex-3-yl ester	144	C8H16O2	1000367-94-5	37
3		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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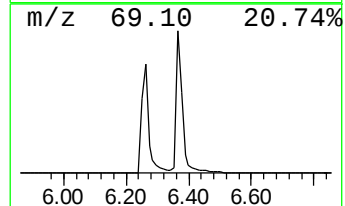
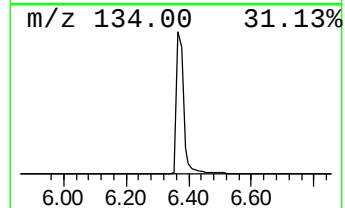
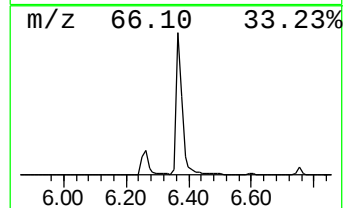
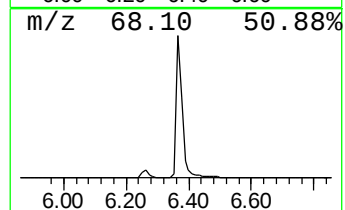
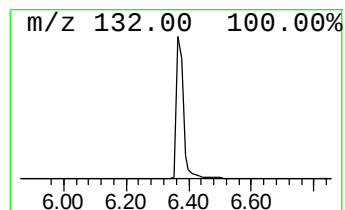
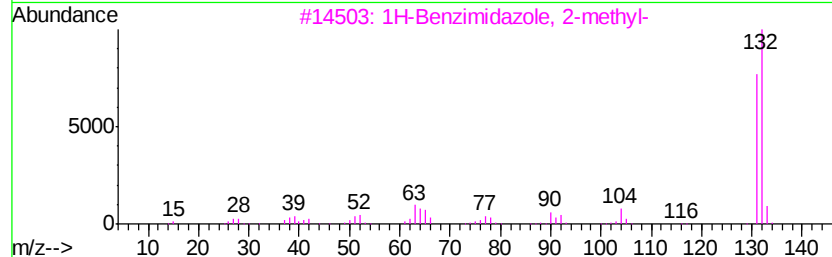
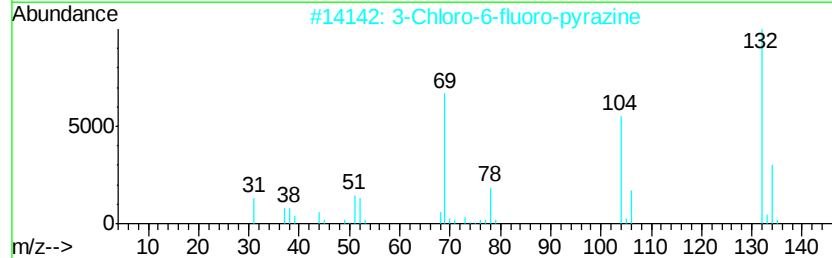
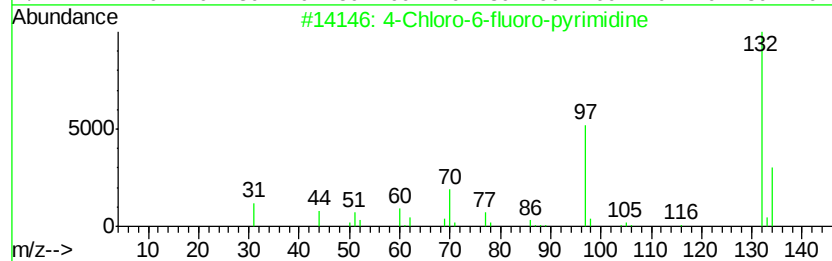
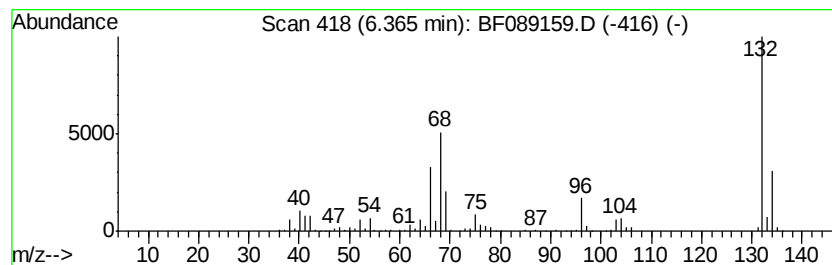
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Peak Number 5 unknown6.36 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	62.67 ng	1104280	1,4-Dichlorobenzene-d4	6.60

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...	4.04	121.9	ng	2147130	1	6.60	352389	20.0
2-Pentanone, 4-hy...	4.79	175.4	ng	3090250	1	6.60	352389	20.0
2-Pentanone, 4-me...	5.60	13.9	ng	244985	1	6.60	352389	20.0
unknown6.36	6.36	62.7	ng	1104280	1	6.60	352389	20.0