

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072215\
 Data File : BF080570.D
 Acq On : 22 Jul 2015 23:10
 Operator : TP/UM
 Sample : G2973-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6D56

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-BF072215.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	4.464	206	208	213	rVB	38433	52606	3.74%	0.455%
2	5.116	262	265	268	rBV	796729	882578	62.73%	7.631%
3	5.539	299	302	304	rBV	1056561	1289488	91.65%	11.150%
4	5.962	337	339	341	rBV	63235	82874	5.89%	0.717%
5	6.567	389	392	394	rBV	1618985	1406958	100.00%	12.166%
6	6.716	403	405	407	rBV	1638160	1338064	95.10%	11.570%
7	6.956	424	426	428	rVB	408568	322484	22.92%	2.788%
8	7.116	437	440	442	rBV	1088459	1018246	72.37%	8.804%
9	7.516	473	475	477	rBV	1005873	771223	54.81%	6.669%
10	8.247	537	539	541	rBV	488874	393941	28.00%	3.406%
11	9.322	631	633	636	rVB	1526399	1265856	89.97%	10.945%
12	9.722	666	668	669	rBV	104945	128881	9.16%	1.114%
13	10.008	691	693	695	rBV	435116	376198	26.74%	3.253%
14	10.785	759	761	764	rBV2	471462	628530	44.67%	5.435%
15	10.911	771	772	776	rVB	11413	18252	1.30%	0.158%
16	11.493	821	823	825	rBV	427336	343121	24.39%	2.967%
17	13.117	963	965	968	rBV	984176	906243	64.41%	7.836%
18	14.134	1051	1054	1057	rBV3	8957	15709	1.12%	0.136%
19	14.294	1065	1068	1070	rBV	205099	203112	14.44%	1.756%
20	15.963	1211	1214	1217	rBV	98086	120729	8.58%	1.044%

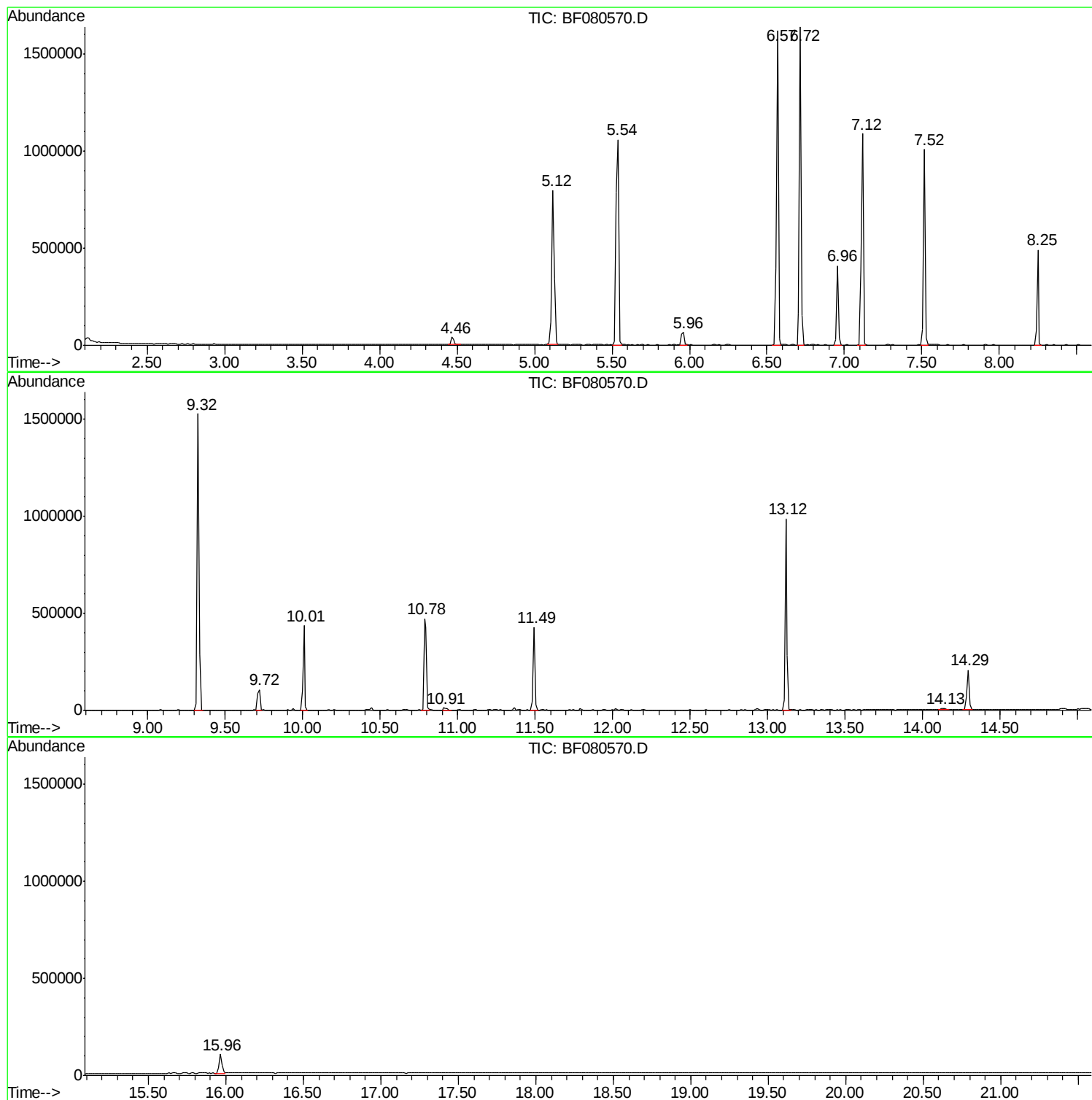
Sum of corrected areas: 11565093

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072215.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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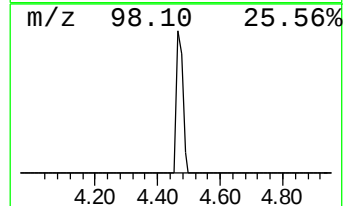
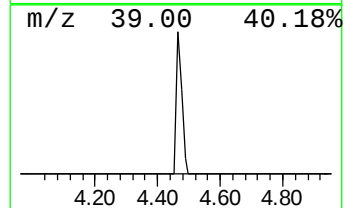
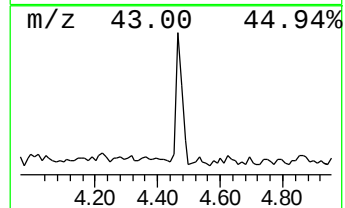
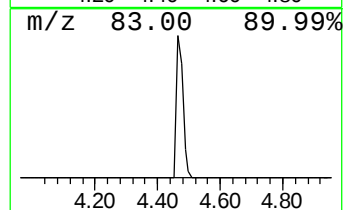
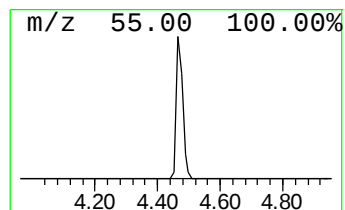
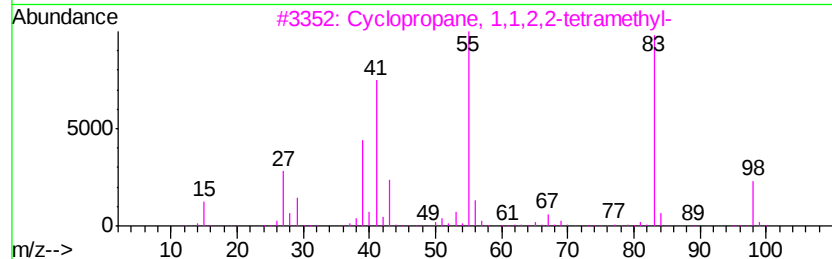
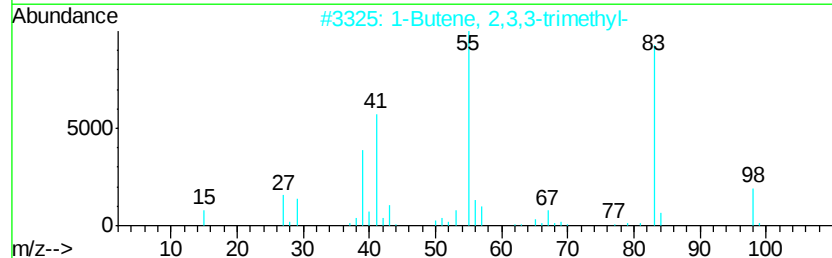
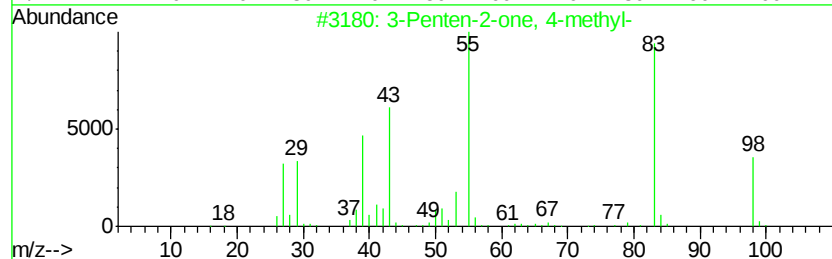
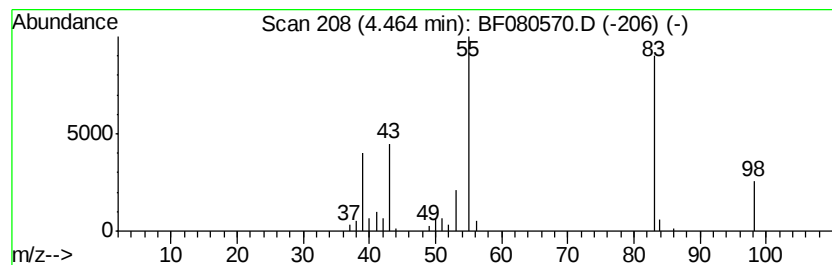
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	3.26 ng	52606	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	80
3			Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	80
4			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	59
5			3-Hexen-2-one	98	C6H10O	000763-93-9	58



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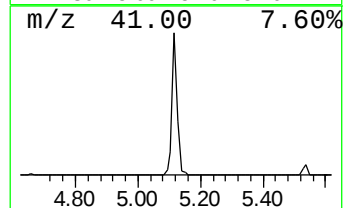
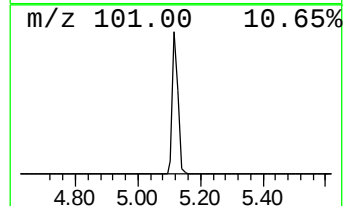
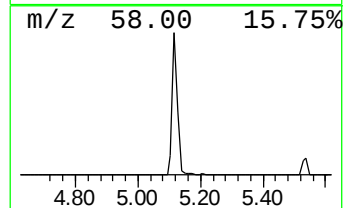
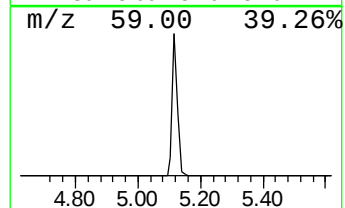
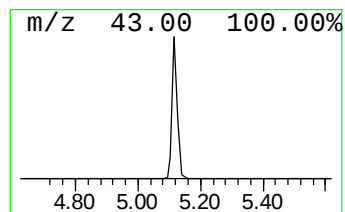
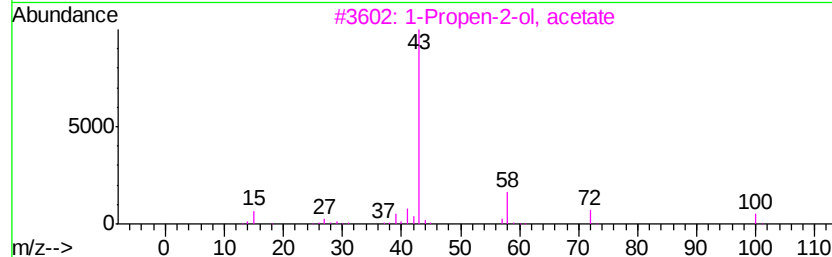
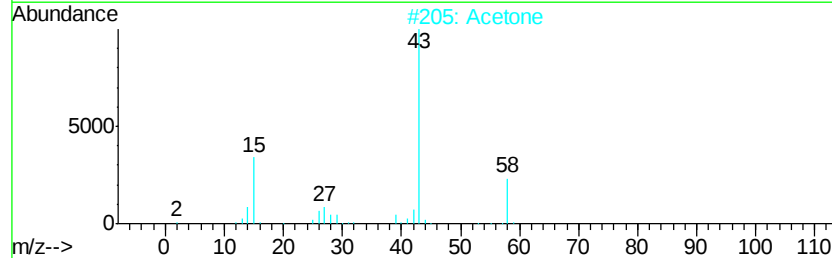
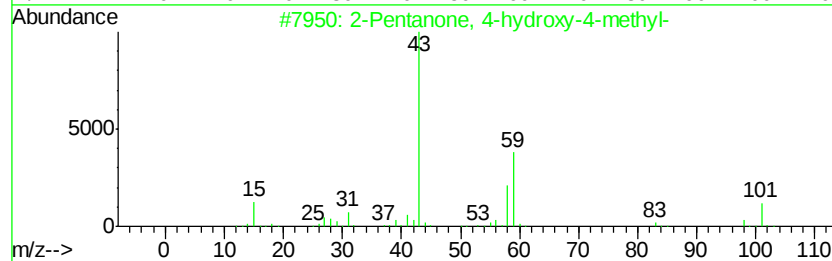
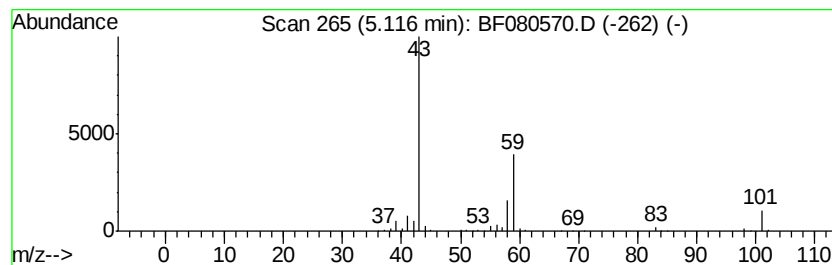
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	54.74 ng	882578	1,4-Dichlorobenzene-d4	6.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	83
2	Acetone	58	C3H6O		000067-64-1	12
3	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10
4	Diacetamide	101	C4H7NO2		000625-77-4	9
5	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3		005185-97-7	9



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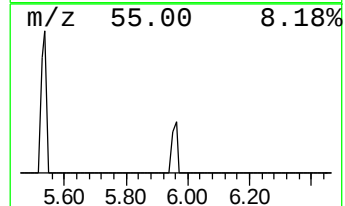
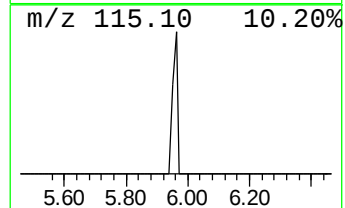
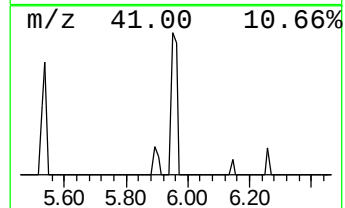
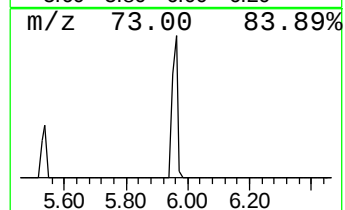
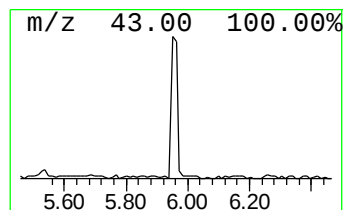
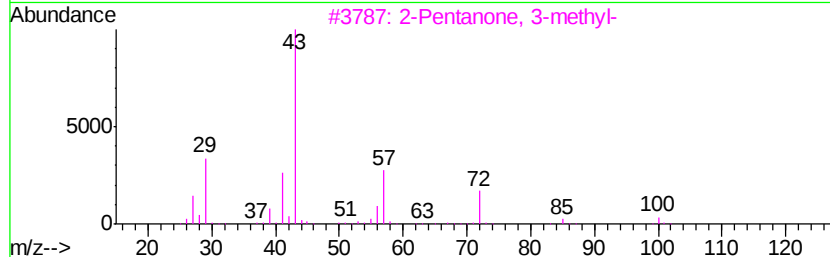
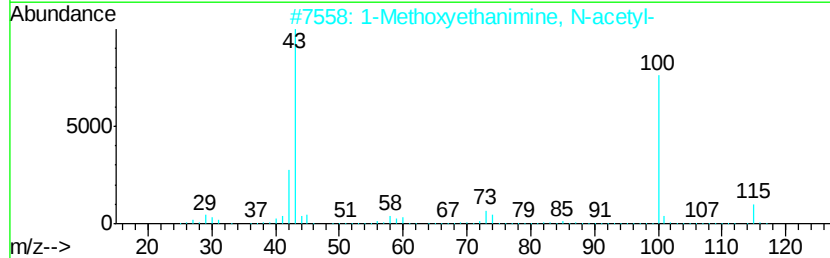
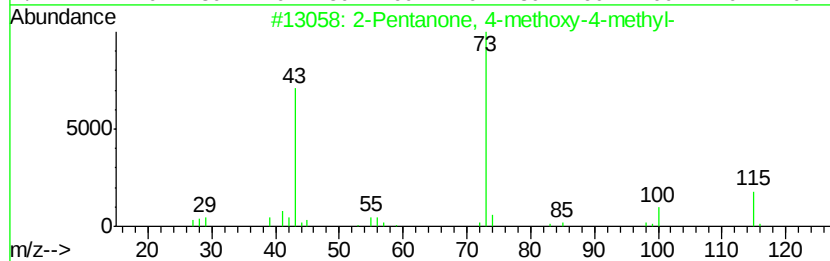
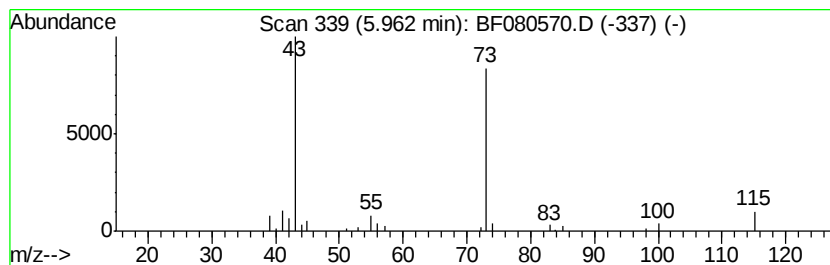
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Peak Number 3 unknown5.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	5.14 ng	82874	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
3			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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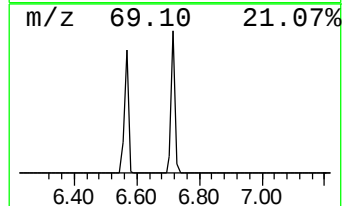
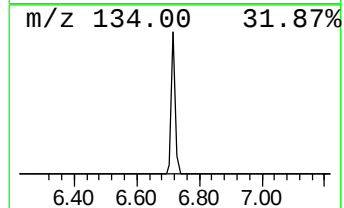
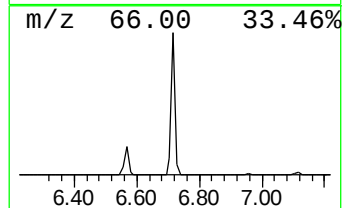
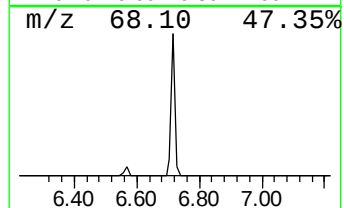
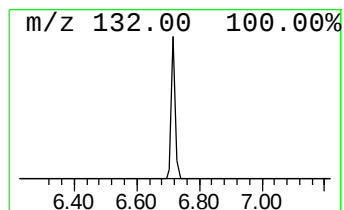
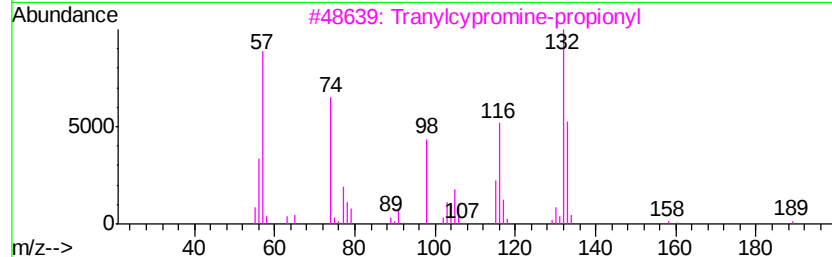
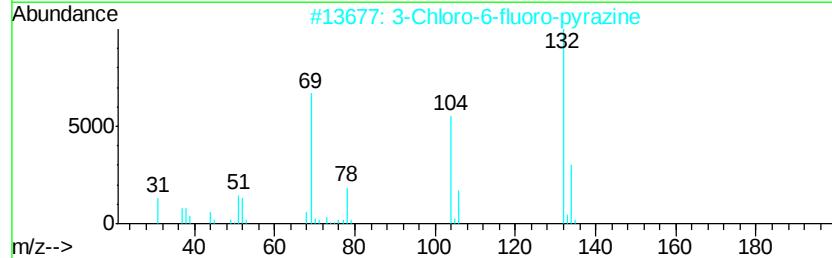
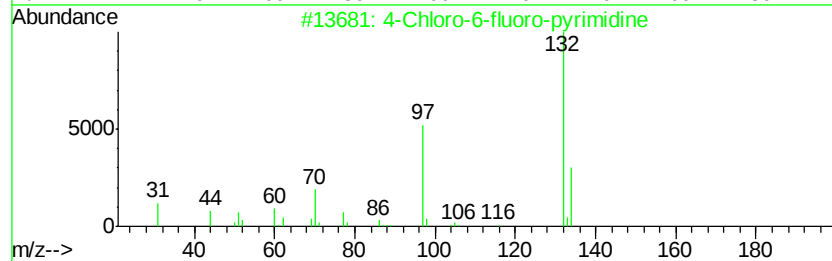
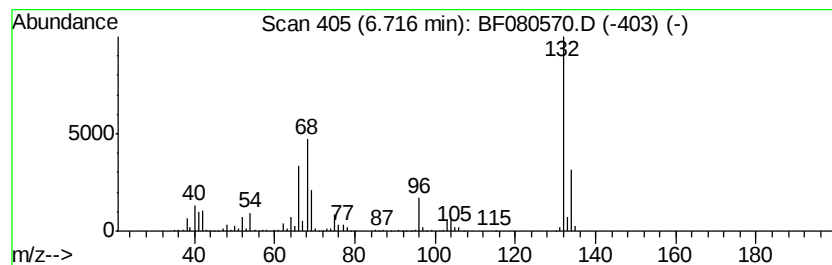
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Peak Number 4 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	82.98 ng	1338060	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.46	3.3	ng	52606	1	6.96	322484	20.0
2-Pentanone, 4-hy...	5.12	54.7	ng	882578	1	6.96	322484	20.0
unknown5.96	5.96	5.1	ng	82874	1	6.96	322484	20.0
unknown6.72	6.72	83.0	ng	1338060	1	6.96	322484	20.0