

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108457.D
 Acq On : 24 Aug 2018 8:39
 Operator : JU/SJ
 Sample : J4582-08
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082018-TIPC-E-U-M

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.384	3	8	17	rVB	2871005	4195393	84.62%	13.344%
2	5.237	490	493	503	rBV	81377	91494	1.85%	0.291%
3	5.625	555	559	569	rBV	1543931	1376389	27.76%	4.378%
4	6.613	723	727	731	rBV	1070973	941602	18.99%	2.995%
5	6.766	749	753	757	rBV	2679993	2496608	50.36%	7.941%
6	6.995	789	792	796	rBV	976108	892195	18.00%	2.838%
7	7.160	815	820	823	rBV	3411458	3341529	67.40%	10.628%
8	7.566	883	889	892	rBV	2757108	2872214	57.93%	9.135%
9	8.283	1006	1011	1014	rBV	1198834	1056541	21.31%	3.360%
10	9.360	1188	1194	1197	rBV	5348282	4957984	100.00%	15.769%
11	9.742	1256	1259	1265	rBV	147054	136707	2.76%	0.435%
12	10.013	1302	1305	1307	rBV	64959	54126	1.09%	0.172%
13	10.042	1307	1310	1322	rVB2	1297747	1152566	23.25%	3.666%
14	10.448	1371	1379	1383	rVB2	64900	59340	1.20%	0.189%
15	10.701	1419	1422	1425	rBV	226503	174860	3.53%	0.556%
16	10.836	1441	1445	1454	rBV	1779158	1592528	32.12%	5.065%
17	11.536	1560	1564	1568	rBV	1094254	978630	19.74%	3.113%
18	13.124	1829	1834	1837	rBV	3688209	3261846	65.79%	10.374%
19	14.142	1995	2007	2011	rBV8	32720	103035	2.08%	0.328%
20	14.189	2011	2015	2026	rVB	893597	835733	16.86%	2.658%
21	15.312	2202	2206	2214	rVB	52295	60536	1.22%	0.193%
22	15.742	2271	2279	2290	rVB	519886	737660	14.88%	2.346%
23	16.195	2351	2356	2363	rVB2	44005	71498	1.44%	0.227%

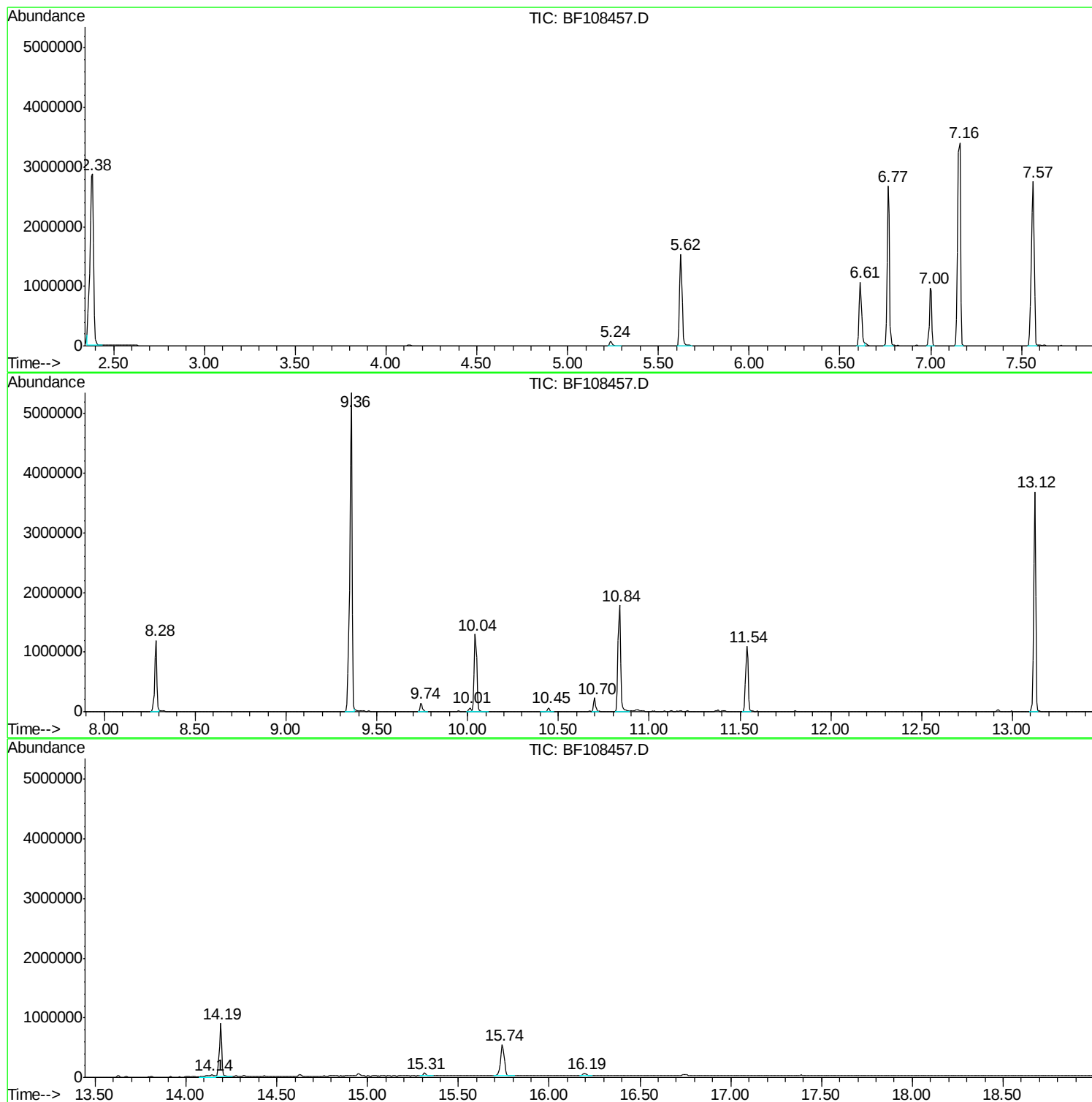
Sum of corrected areas: 31441014

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



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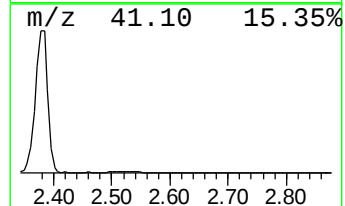
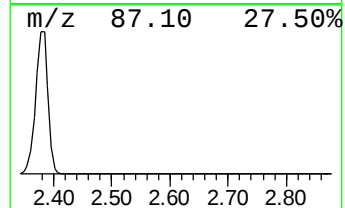
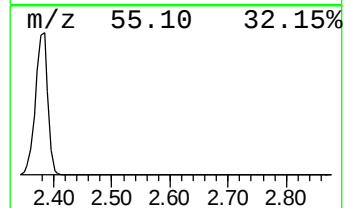
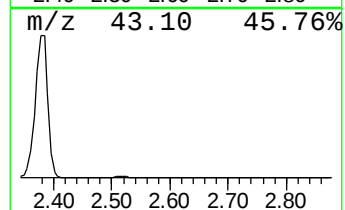
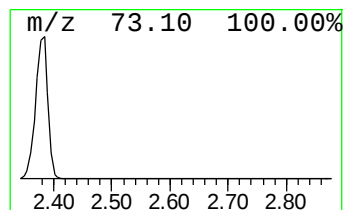
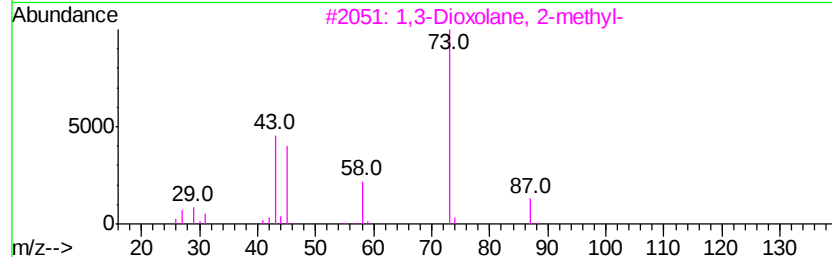
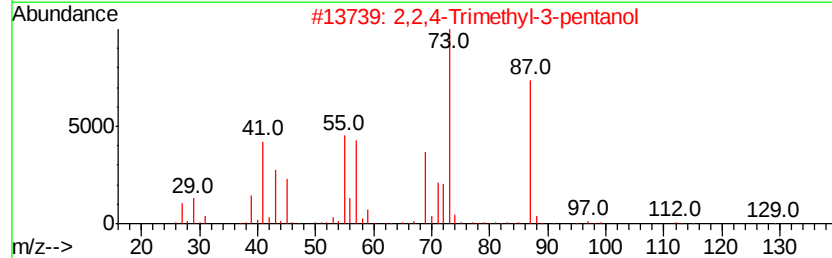
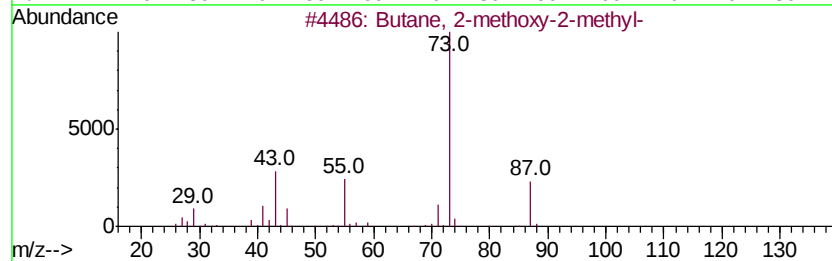
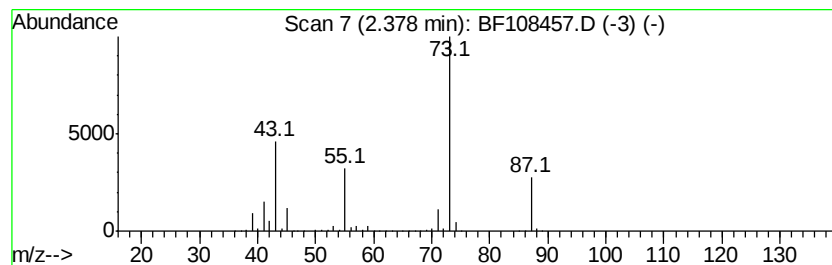
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	94.05 ng	4195390	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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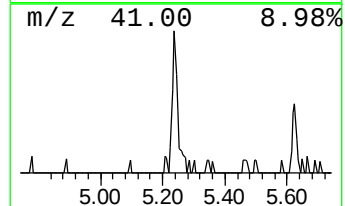
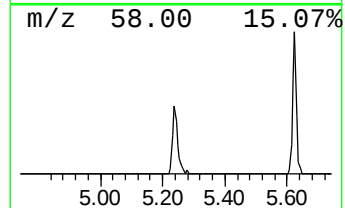
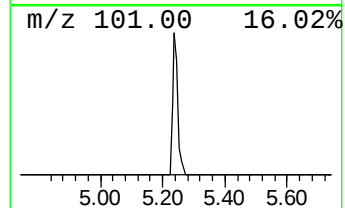
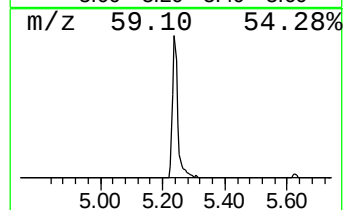
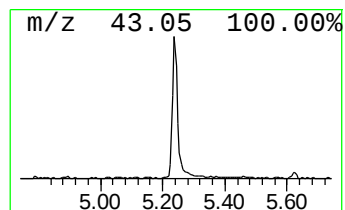
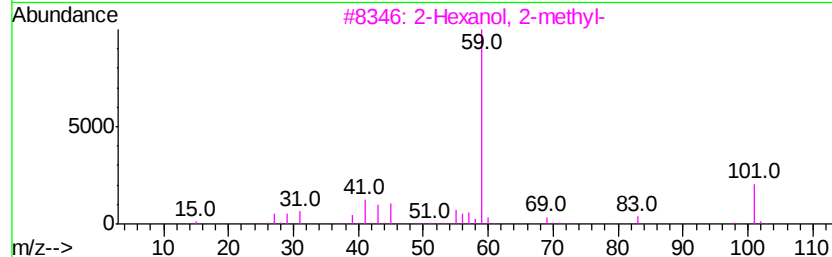
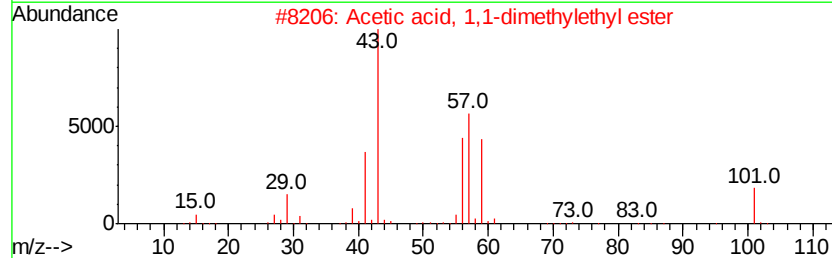
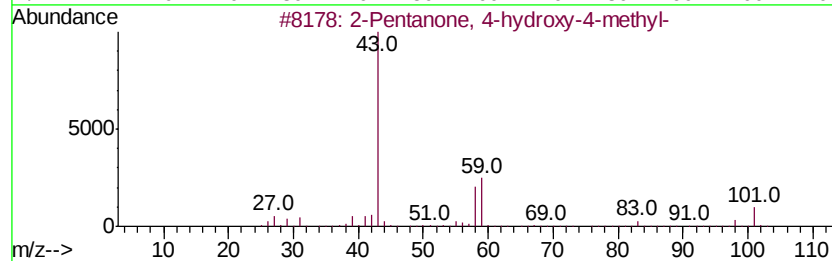
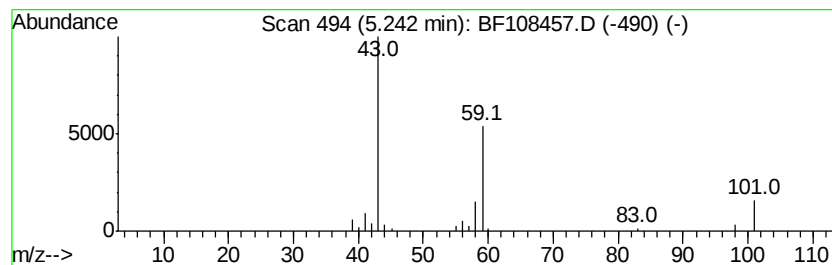
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.05 ng	91494	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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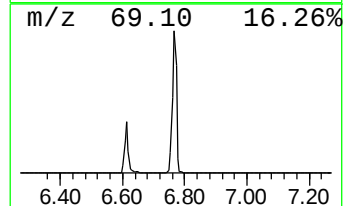
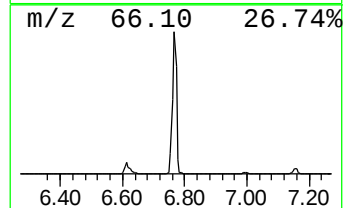
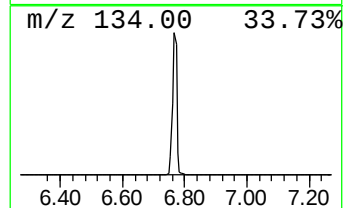
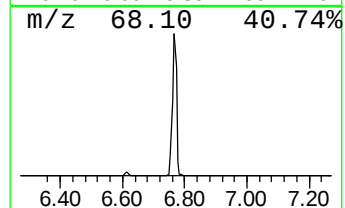
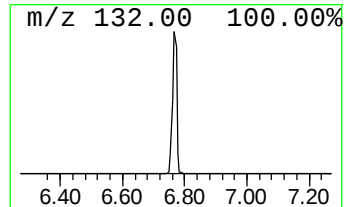
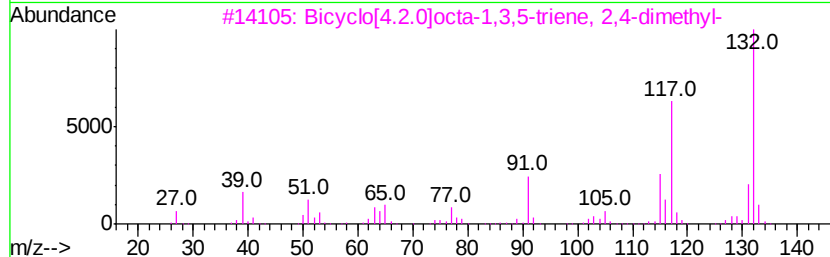
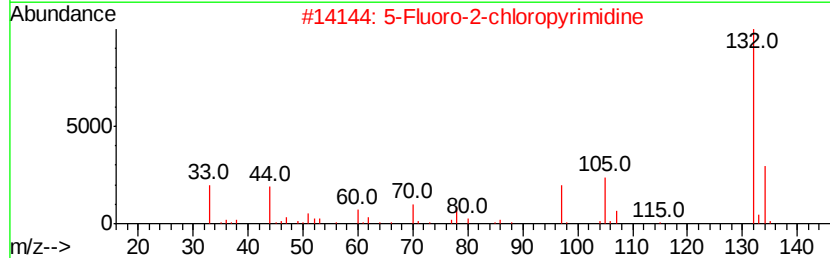
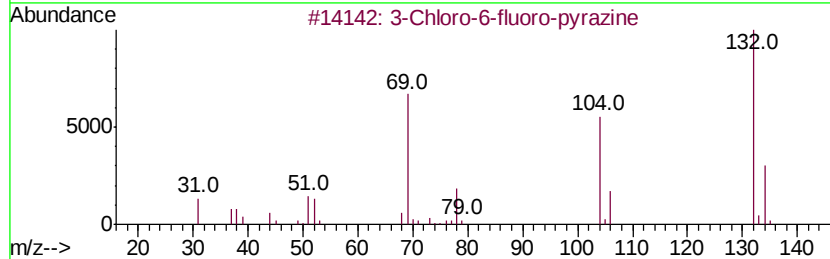
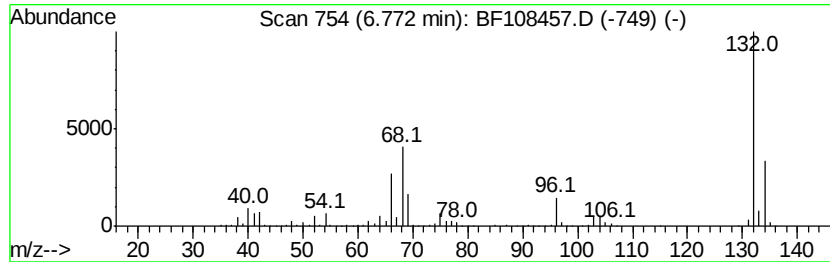
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Peak Number 3 unknown6.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	55.97 ng	2496610	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9	



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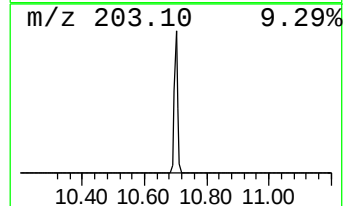
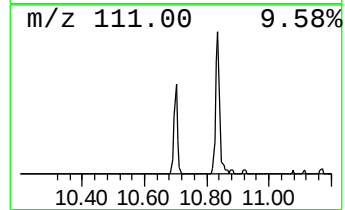
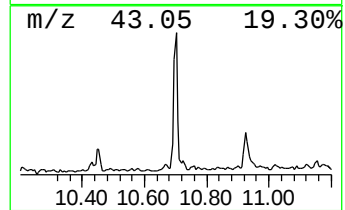
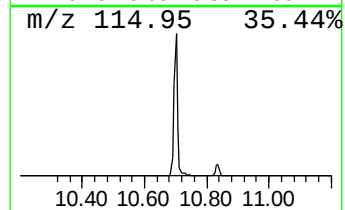
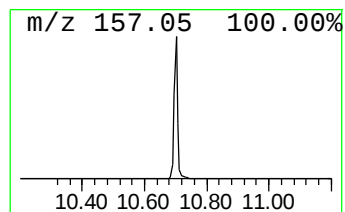
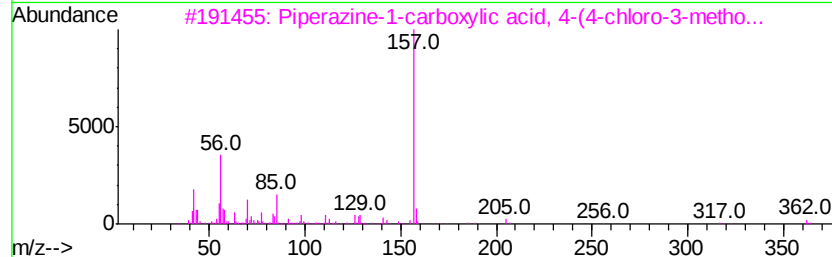
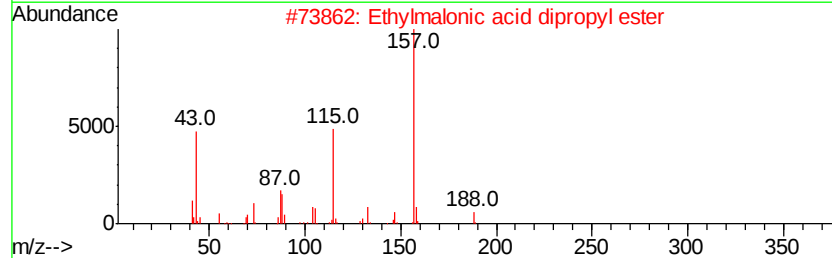
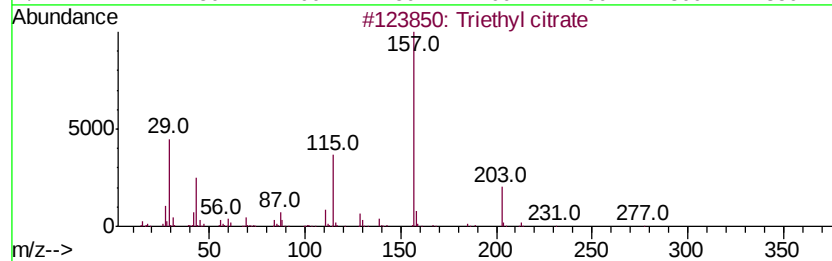
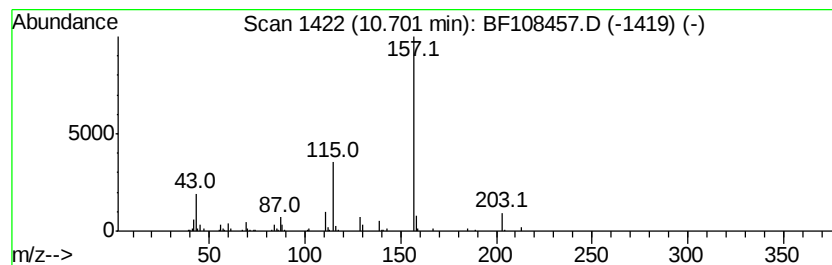
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Peak Number 5 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	3.03 ng	174860	Acenaphthene-d10	10.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 87
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 59
3		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-79-9 42
4		Quinoline, 4,8-dimethyl-	157 C11H11N	013362-80-6 38
5		Piperazine-1-carboxylic acid, 4-...	396 C14H18Cl2N2O5S	1000303-80-3 36



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.38	94.0	ng	4195390	1	7.00	892195	20.0
2-Pentanone, 4-hy...	5.24	2.0	ng	91494	1	7.00	892195	20.0
unknown6.77	6.77	56.0	ng	2496610	1	7.00	892195	20.0
Triethyl citrate	10.70	3.0	ng	174860	3	10.04	1152570	20.0