

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108454.D
 Acq On : 24 Aug 2018 7:19
 Operator : JU/SJ
 Sample : J4582-05
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

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

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:\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	5.237	490	493	503	rVB	78586	90729	1.96%	0.359%
2	5.625	555	559	576	rBV	1279203	1254866	27.07%	4.965%
3	6.613	723	727	739	rBV	972700	865187	18.66%	3.423%
4	6.766	749	753	757	rBV	2505681	2275995	49.09%	9.006%
5	7.001	789	793	796	rBV	964496	861191	18.58%	3.408%
6	7.160	815	820	823	rBV	3191971	3093823	66.73%	12.242%
7	7.566	883	889	892	rBV	2655265	2641843	56.98%	10.453%
8	8.283	1006	1011	1024	rBV	1174820	1061586	22.90%	4.201%
9	9.360	1188	1194	1197	rBV	5033834	4636107	100.00%	18.345%
10	9.742	1256	1259	1265	rBV	99526	94489	2.04%	0.374%
11	10.042	1307	1310	1321	rVB2	1249723	1124745	24.26%	4.450%
12	10.701	1419	1422	1425	rBV	162328	124042	2.68%	0.491%
13	10.836	1441	1445	1457	rBV	1646525	1503600	32.43%	5.950%
14	10.936	1457	1462	1473	rVB2	66974	103127	2.22%	0.408%
15	11.536	1560	1564	1568	rBV	1027849	947351	20.43%	3.749%
16	13.124	1830	1834	1837	rBV	3530344	3055665	65.91%	12.091%
17	14.189	2011	2015	2023	rVB	840543	819597	17.68%	3.243%
18	15.748	2272	2280	2287	rBV	493123	718476	15.50%	2.843%

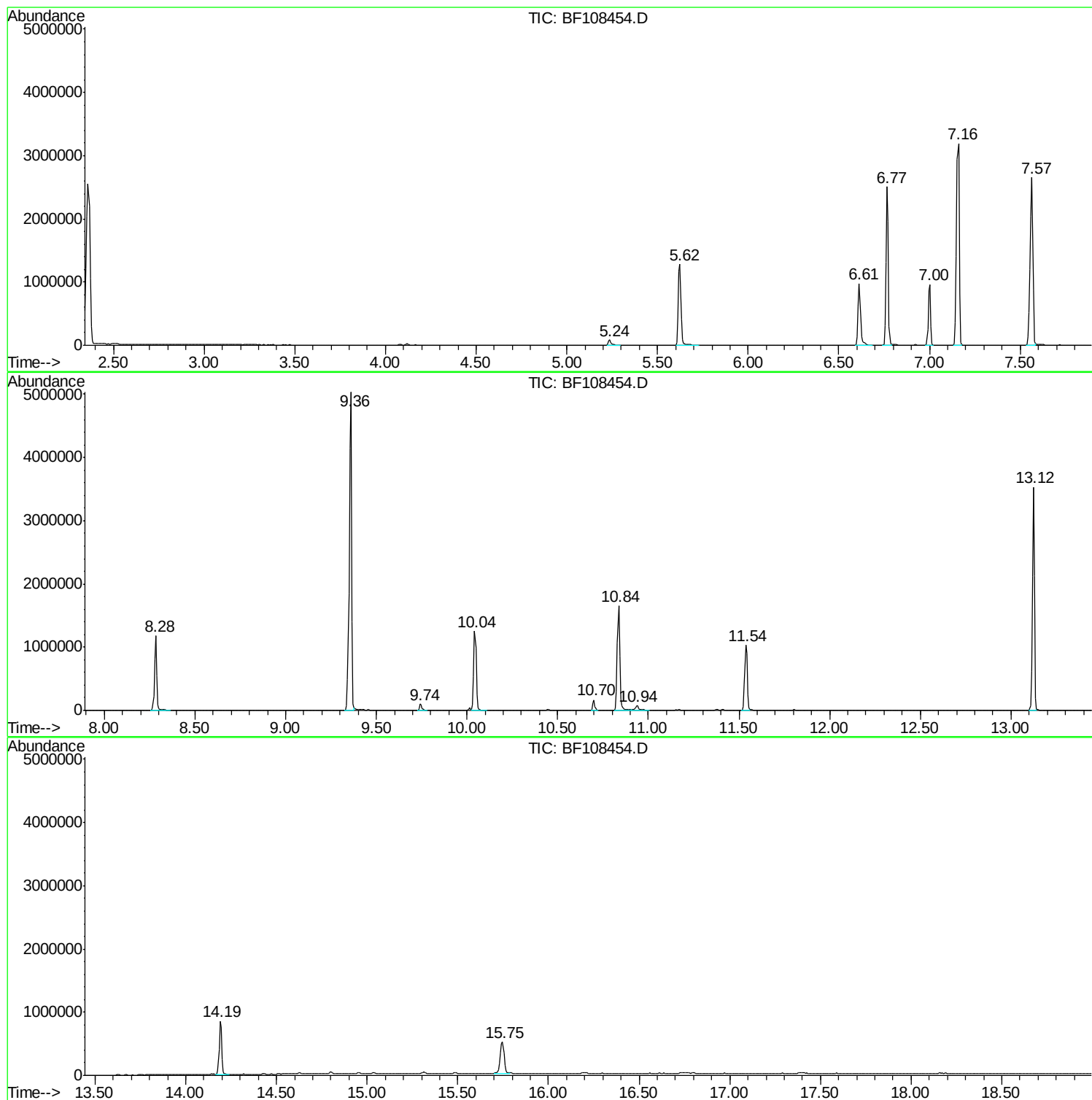
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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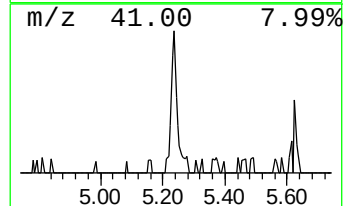
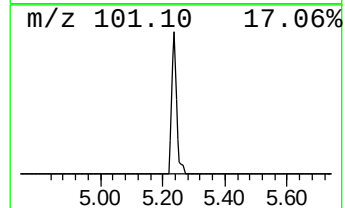
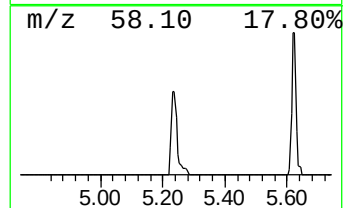
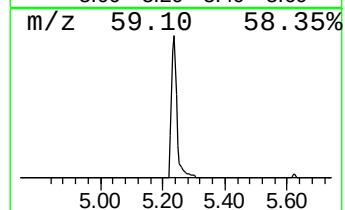
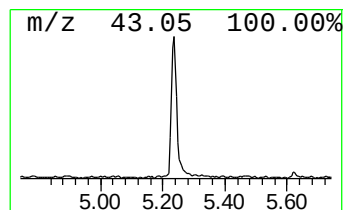
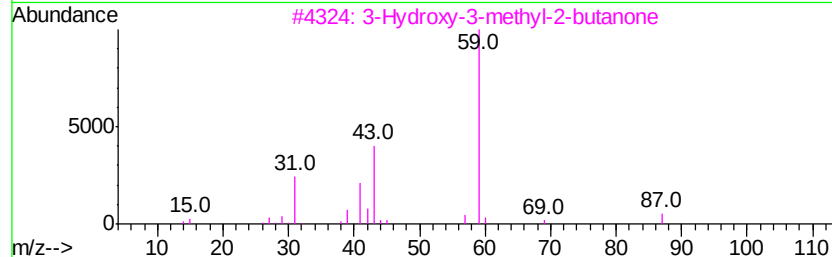
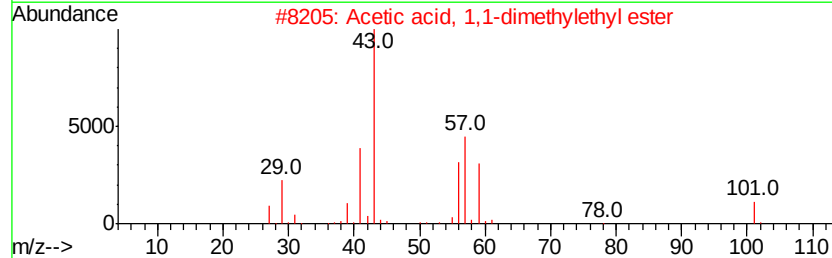
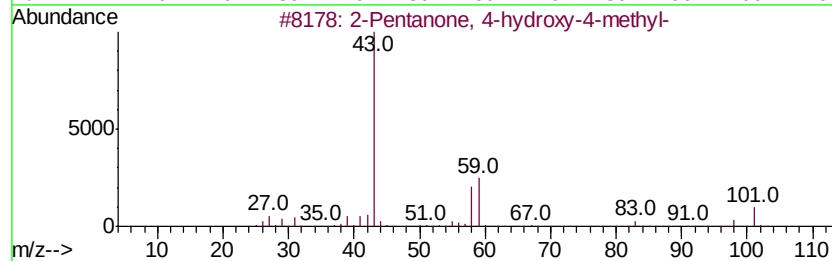
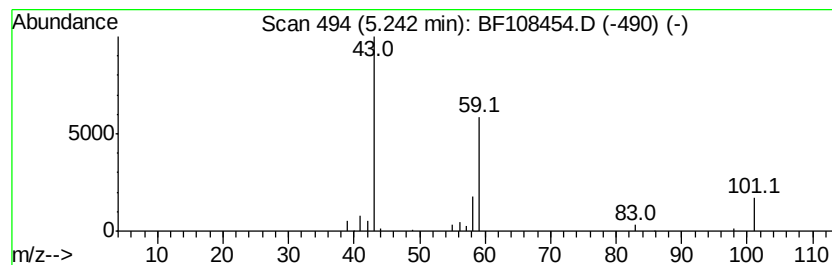
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.11 ng	90729	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	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5		Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9



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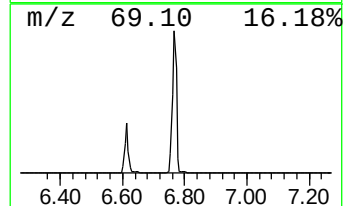
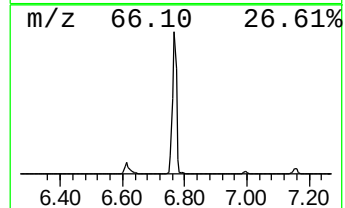
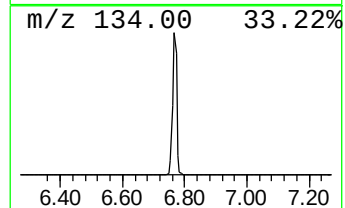
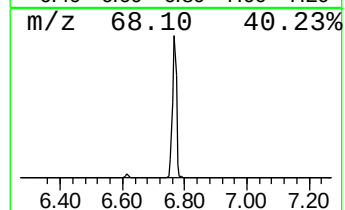
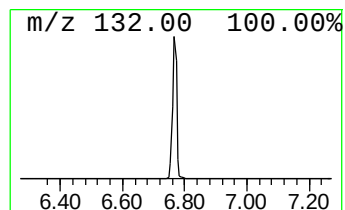
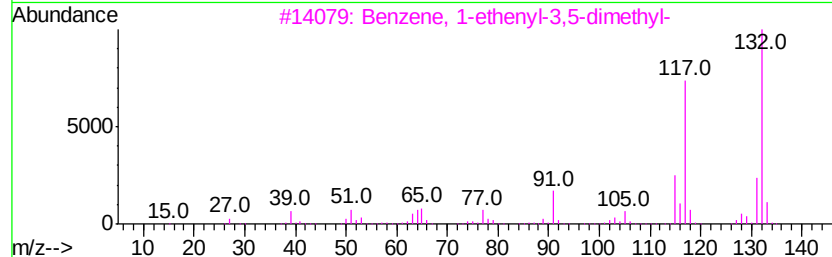
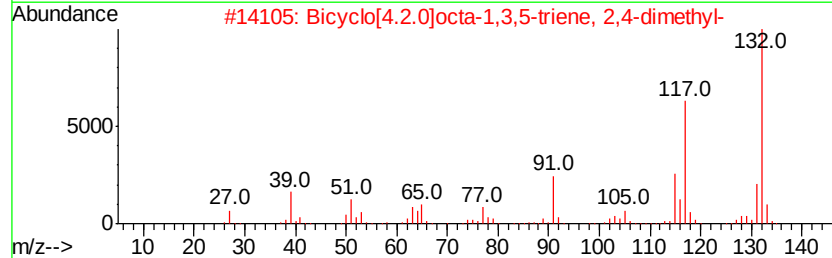
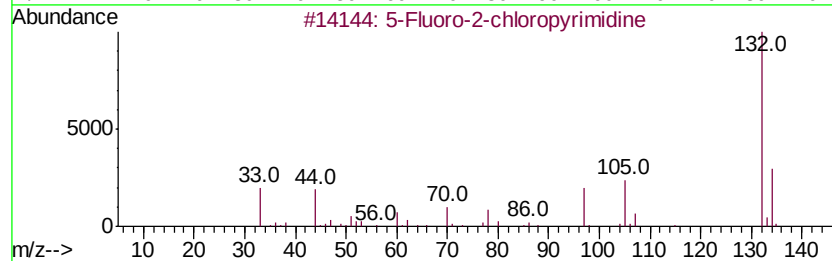
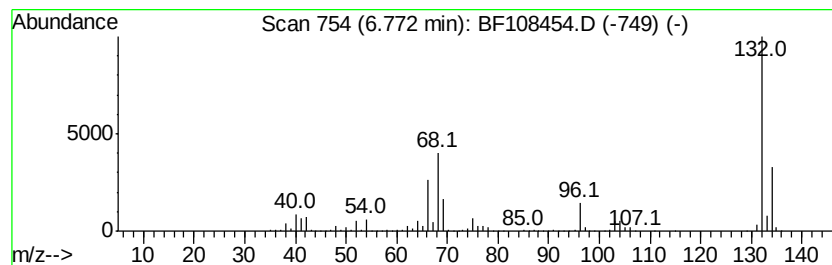
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Peak Number 2 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	52.86 ng	2276000	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		Xenon	132	Xe	007440-63-3	9
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9



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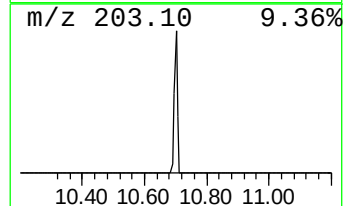
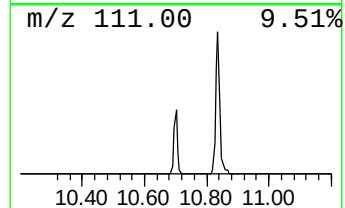
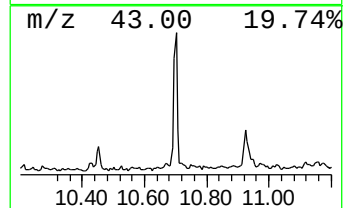
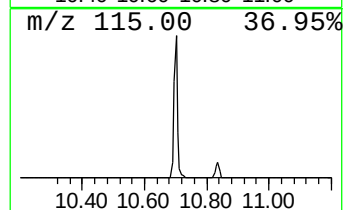
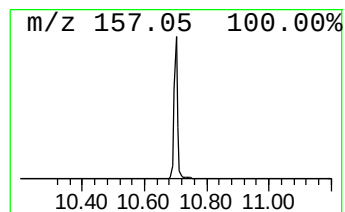
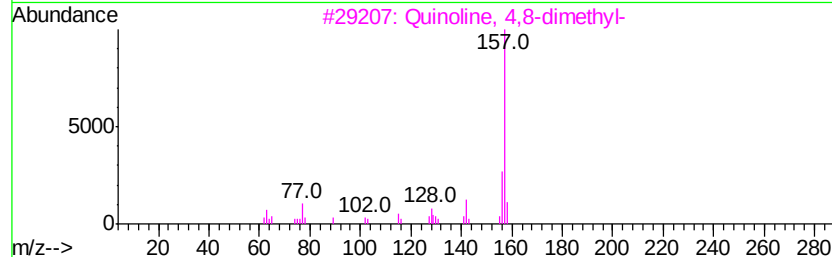
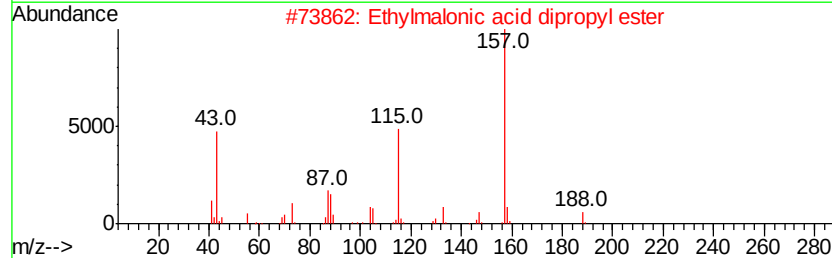
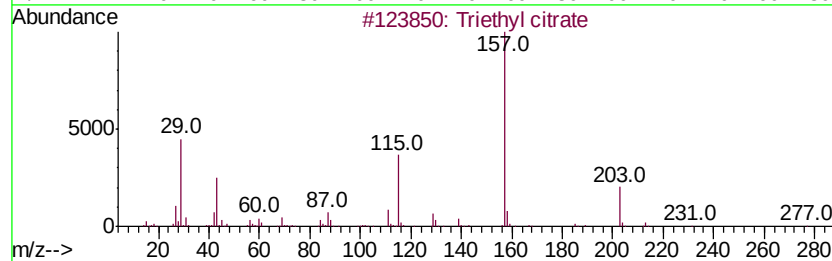
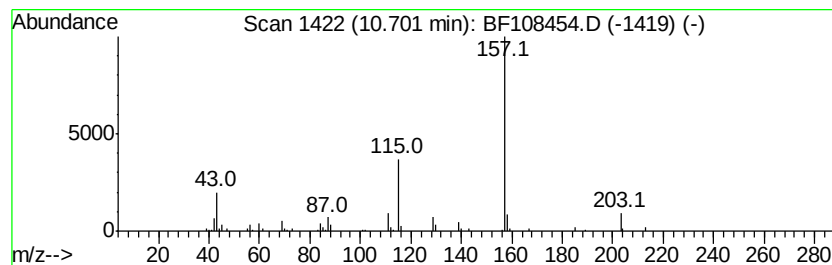
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.70	2.21 ng	124042	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	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	38
4	3-Chloro2-fluorobenzoic acid, 4-...	384	C22H34ClF02	1000338-65-1	36
5	Piperazine-1-carboxylic acid, 4-...	396	C14H18Cl2N2O5S	1000303-80-3	36



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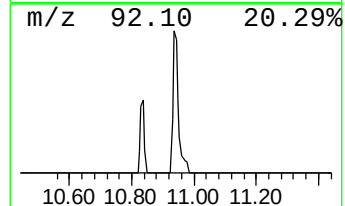
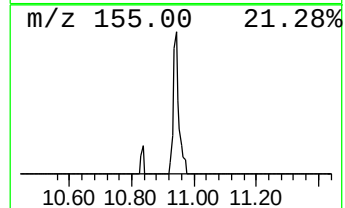
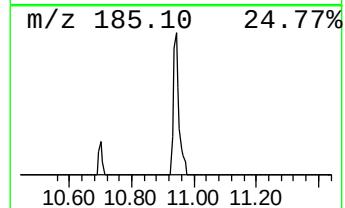
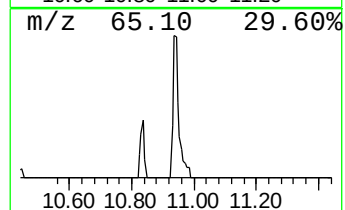
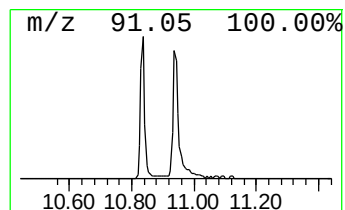
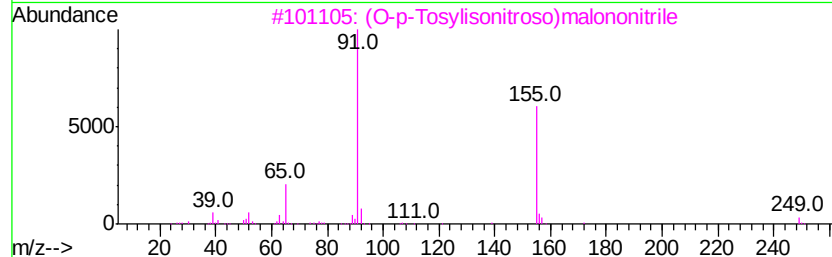
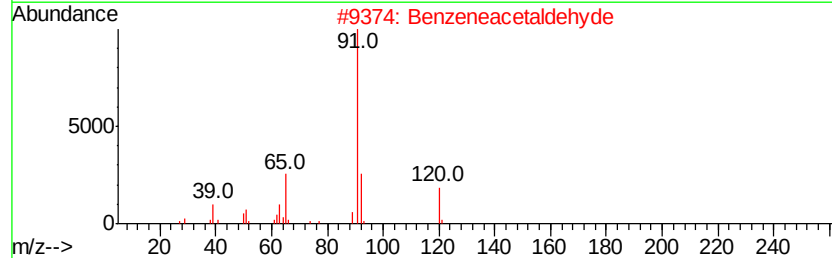
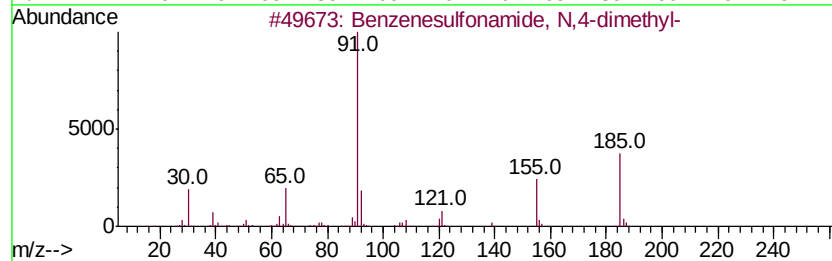
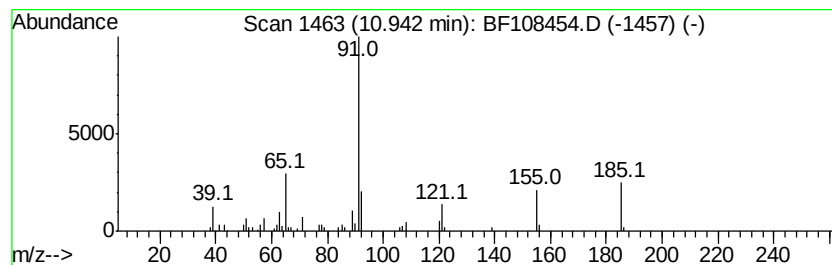
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Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	2.18 ng	103127	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	87
2		Benzeneacetaldehyde	120	C8H8O	000122-78-1	49
3		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43
4		3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	43
5		p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	2.1	ng	90729	1	7.00	861191	20.0
unknown6.77	6.77	52.9	ng	2276000	1	7.00	861191	20.0
Triethyl citrate	10.70	2.2	ng	124042	3	10.04	1124750	20.0
Benzenesulfonamid...	10.94	2.2	ng	103127	4	11.54	947351	20.0