

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108456.D
 Acq On : 24 Aug 2018 8:13
 Operator : JU/SJ
 Sample : J4582-07
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082018-TIPC-E-D-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	2.372	3	6	18	rVB	2820963	3532937	74.46%	12.094%
2	5.237	490	493	502	rVB	74360	82502	1.74%	0.282%
3	5.625	555	559	570	rBV	1407882	1296552	27.33%	4.439%
4	6.613	723	727	741	rBV	1010275	917615	19.34%	3.141%
5	6.766	749	753	757	rBV	2501370	2369161	49.93%	8.110%
6	7.001	789	793	796	rBV	900755	823372	17.35%	2.819%
7	7.160	815	820	823	rBV	3226035	3201274	67.47%	10.959%
8	7.566	883	889	892	rBV	2721849	2737518	57.69%	9.371%
9	8.283	1006	1011	1025	rBV	1103970	1008445	21.25%	3.452%
10	9.360	1188	1194	1197	rBV	5120197	4744861	100.00%	16.243%
11	9.742	1256	1259	1268	rBV	180083	172545	3.64%	0.591%
12	10.042	1307	1310	1317	rVB2	1169335	1047988	22.09%	3.588%
13	10.701	1419	1422	1430	rVB	316665	246909	5.20%	0.845%
14	10.836	1441	1445	1454	rBV	1697233	1527231	32.19%	5.228%
15	11.536	1560	1564	1572	rBV	952213	896937	18.90%	3.071%
16	13.124	1829	1834	1837	rBV	3586482	3135320	66.08%	10.733%
17	14.189	2011	2015	2025	rVB	877905	777190	16.38%	2.661%
18	15.742	2272	2279	2287	rBV	485827	693024	14.61%	2.372%

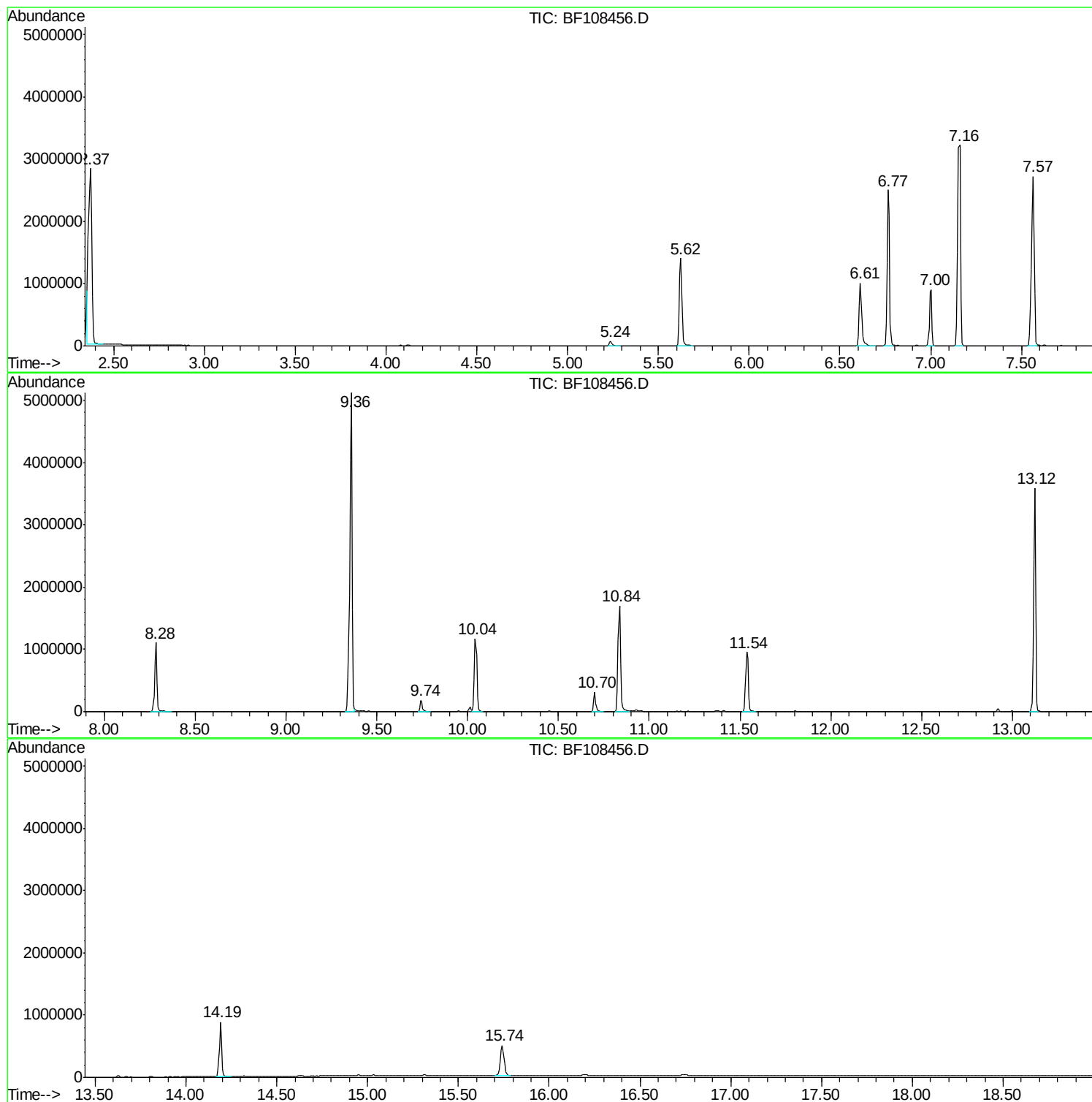
Sum of corrected areas: 29211381

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



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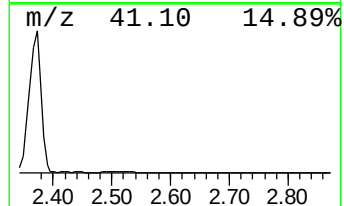
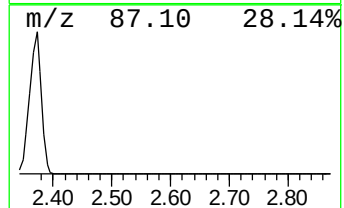
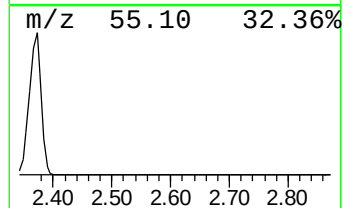
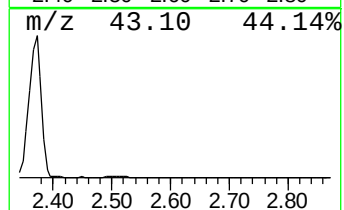
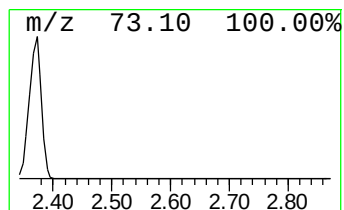
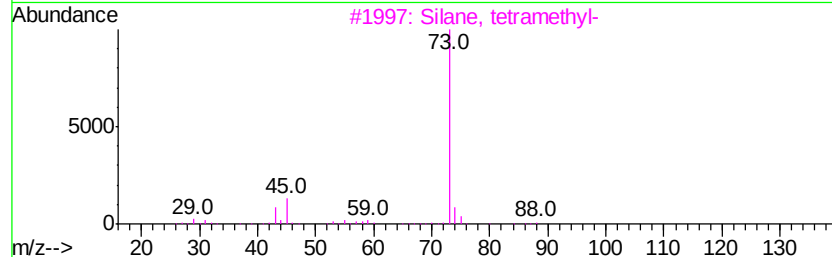
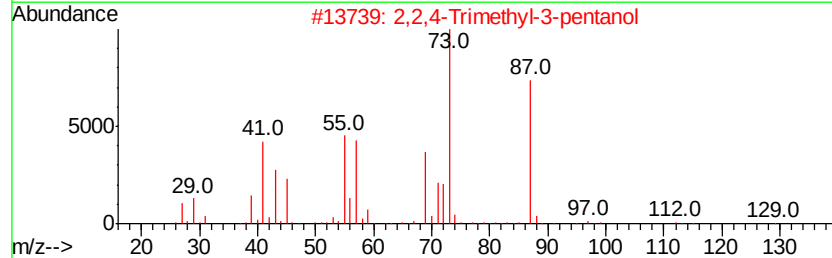
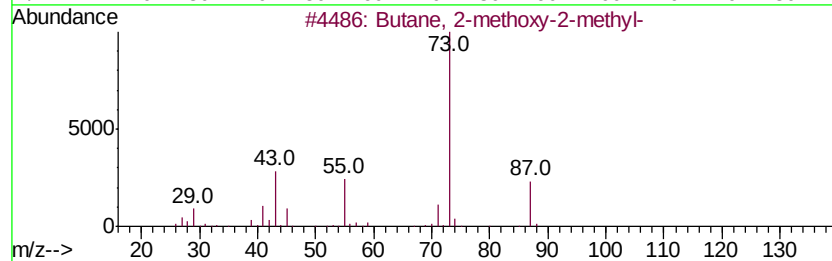
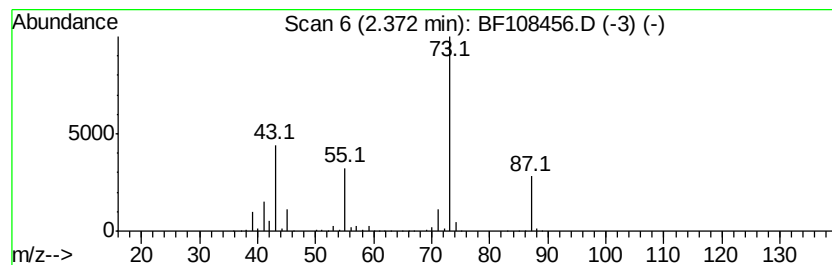
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	85.82 ng	3532940	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	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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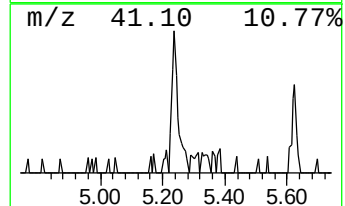
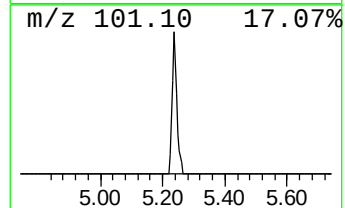
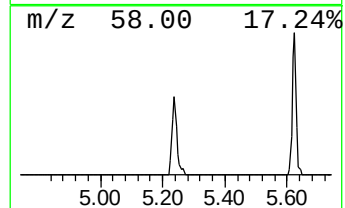
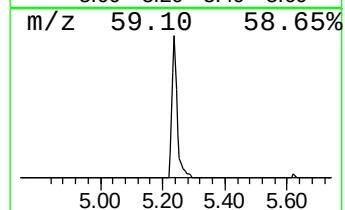
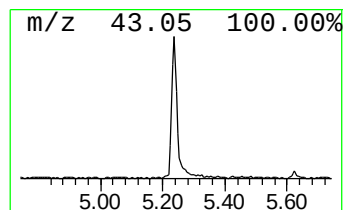
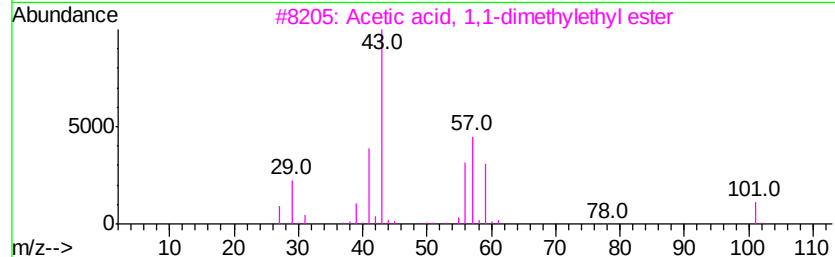
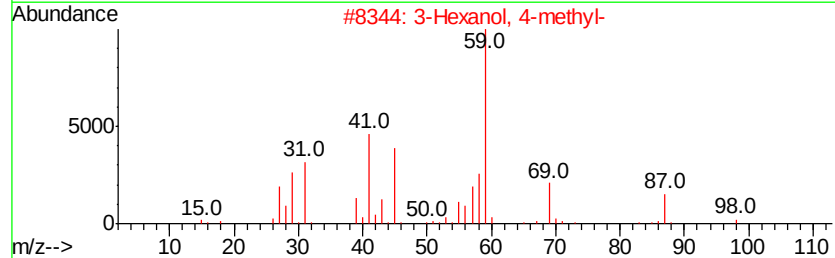
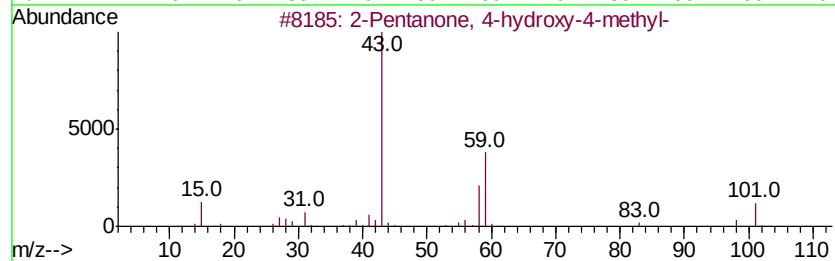
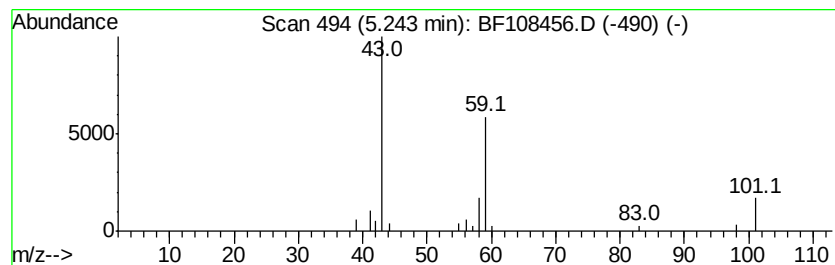
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.00 ng	82502	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	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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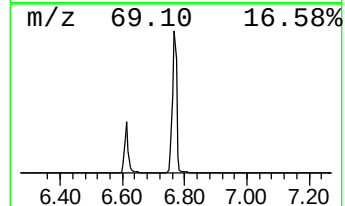
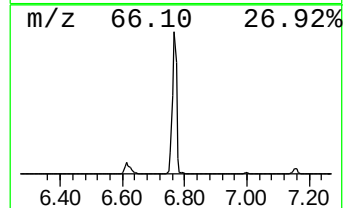
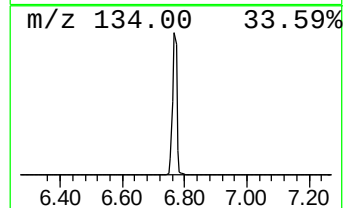
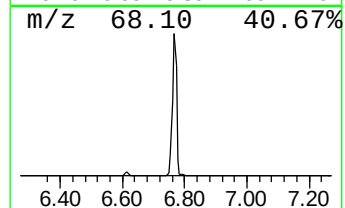
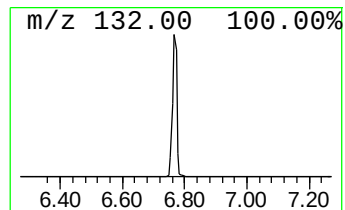
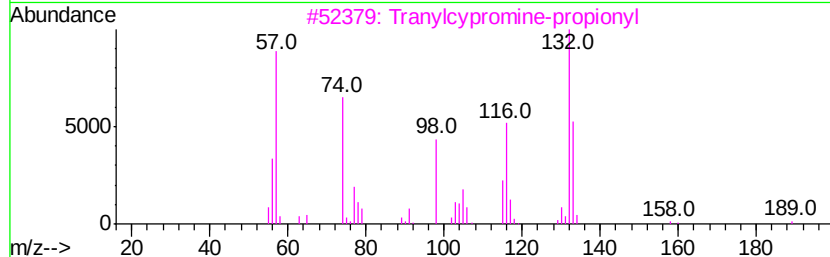
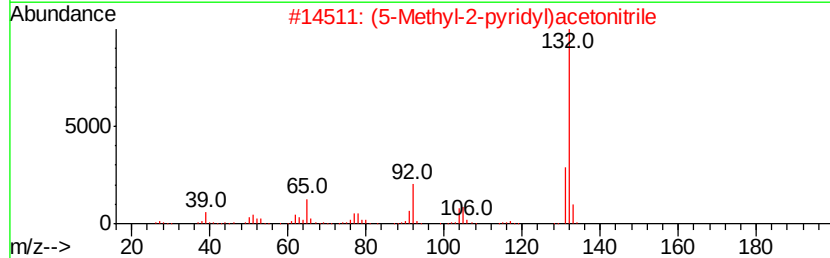
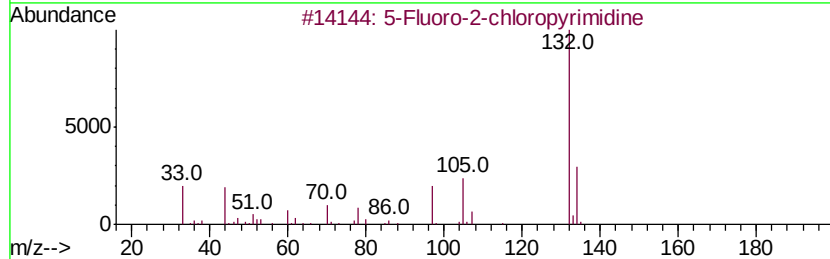
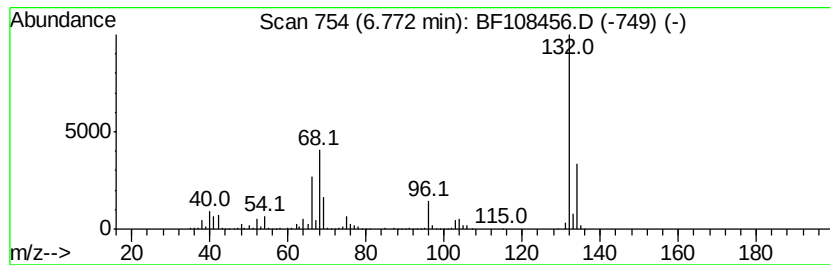
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Peak Number 3 unknown6.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	57.55 ng	2369160	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		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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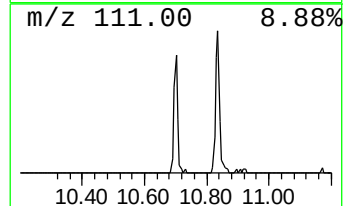
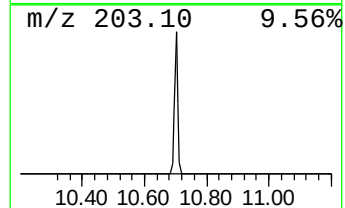
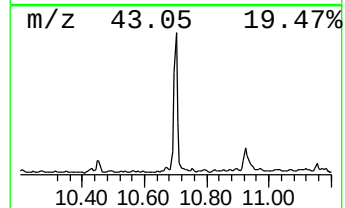
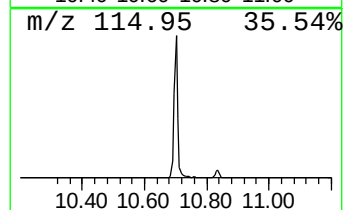
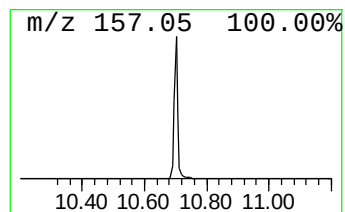
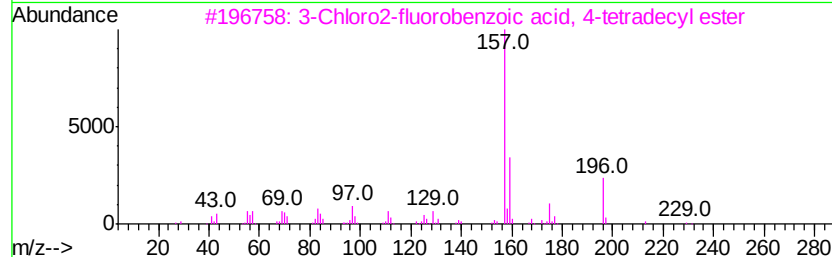
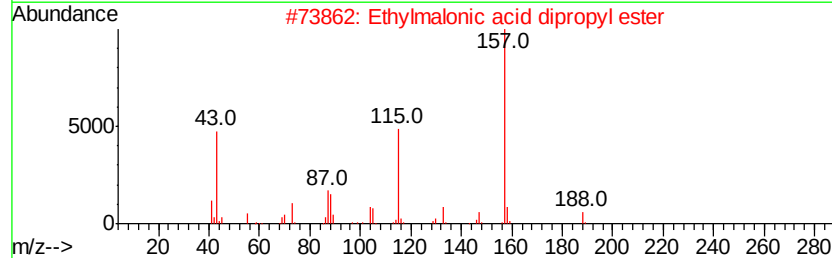
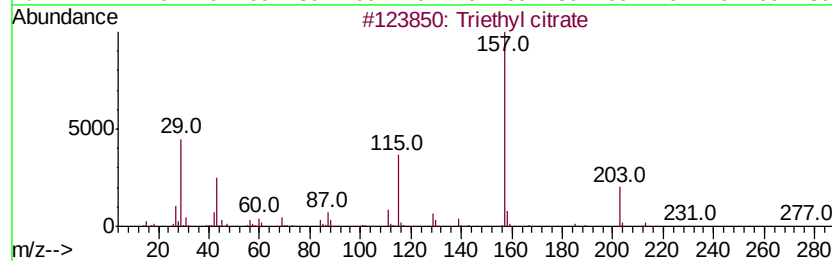
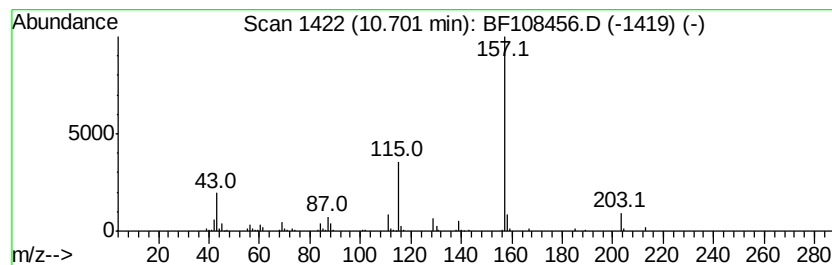
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Peak Number 5 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.70	4.71 ng	246909	Acenaphthene-d10		10.04	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethyl citrate	276	C12H20O7	000077-93-0	86
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3		3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClF02	1000338-64-7	42
4		Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
5		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.37	85.8	ng	3532940	1	7.00	823372	20.0
2-Pentanone, 4-hy...	5.24	2.0	ng	82502	1	7.00	823372	20.0
unknown6.77	6.77	57.5	ng	2369160	1	7.00	823372	20.0
Triethyl citrate	10.70	4.7	ng	246909	3	10.04	1047990	20.0