

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108455.D
 Acq On : 24 Aug 2018 7:46
 Operator : JU/SJ
 Sample : J4582-06
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

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

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	2.378	3	7	24	rVB	2881731	3967630	86.18%	13.772%
2	5.236	490	493	500	rBV	89125	94378	2.05%	0.328%
3	5.625	555	559	573	rBV	1468096	1321318	28.70%	4.586%
4	6.613	723	727	731	rBV	1038497	901333	19.58%	3.129%
5	6.766	749	753	757	rBV	2512066	2320853	50.41%	8.056%
6	7.001	789	793	796	rBV	906431	824612	17.91%	2.862%
7	7.160	815	820	823	rBV	3244801	3126120	67.90%	10.851%
8	7.566	883	889	892	rBV	2574351	2649813	57.56%	9.198%
9	8.283	1006	1011	1024	rBV	1156676	1010602	21.95%	3.508%
10	9.360	1188	1194	1197	rBV	5110600	4603882	100.00%	15.980%
11	9.742	1256	1259	1269	rVB	131937	133407	2.90%	0.463%
12	10.042	1307	1310	1318	rVB2	1112665	1035567	22.49%	3.595%
13	10.701	1419	1422	1425	rBV	164807	124660	2.71%	0.433%
14	10.836	1441	1445	1458	rBV	1576192	1428658	31.03%	4.959%
15	11.536	1561	1564	1568	rBV	920071	873532	18.97%	3.032%
16	13.124	1830	1834	1837	rBV	3432043	2992171	64.99%	10.386%
17	14.189	2011	2015	2024	rVB	812745	744962	16.18%	2.586%
18	15.742	2272	2279	2288	rVB	460855	656037	14.25%	2.277%

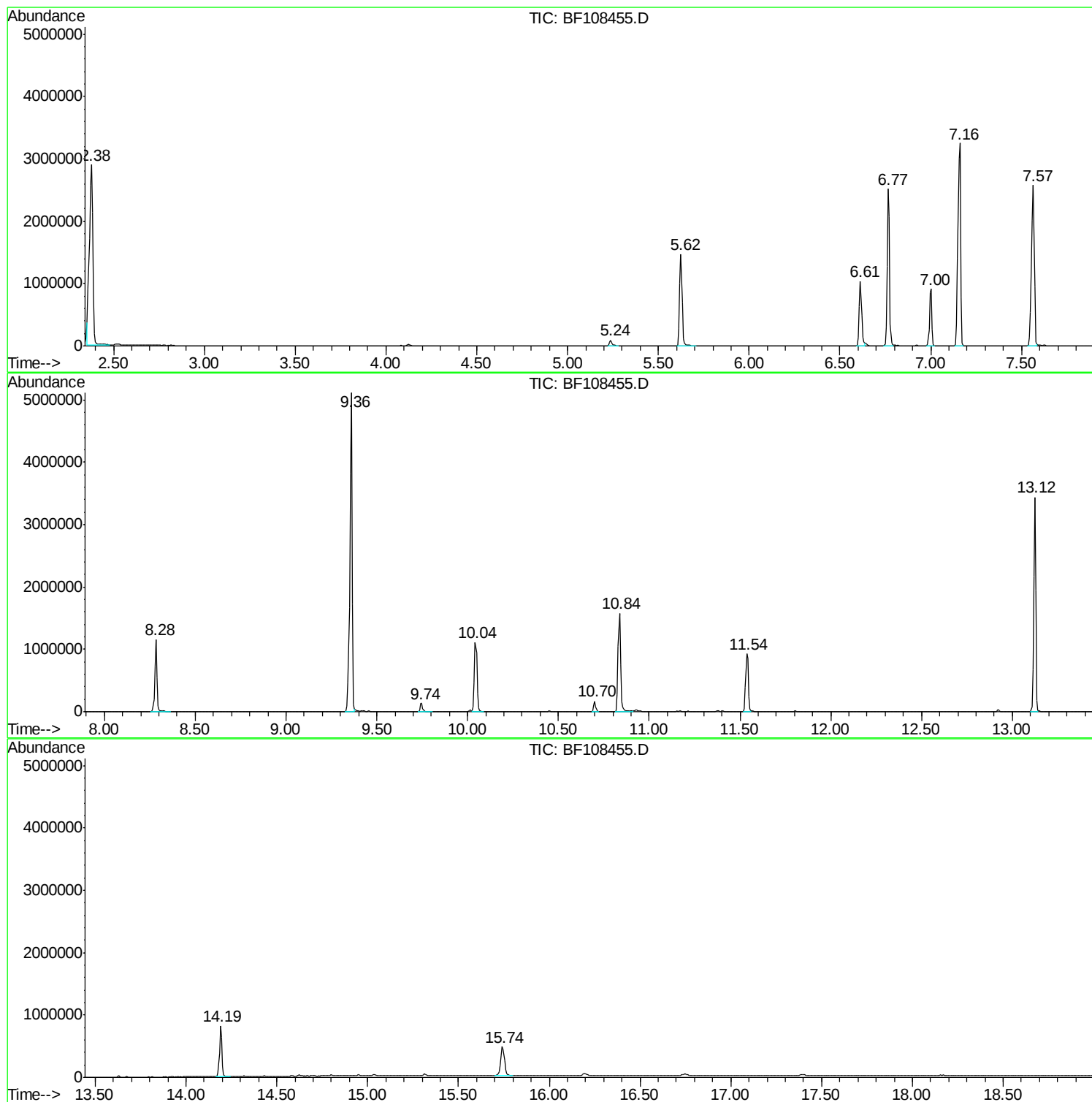
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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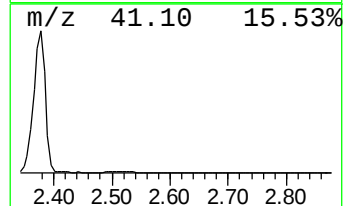
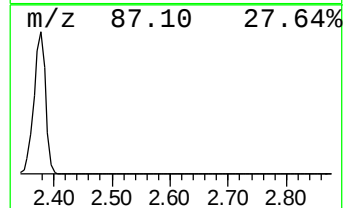
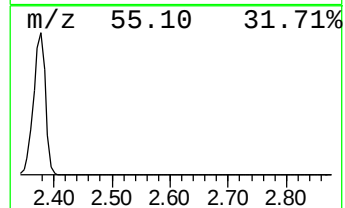
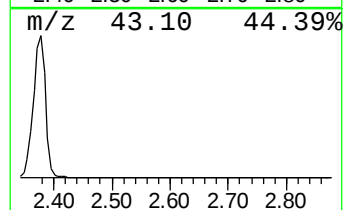
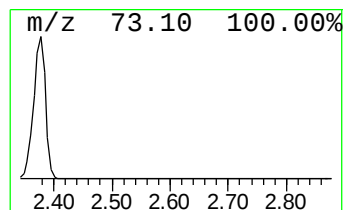
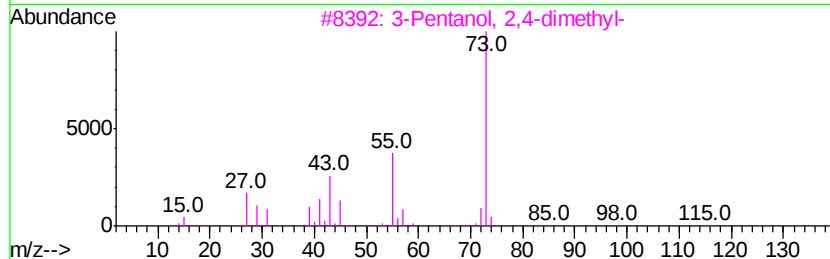
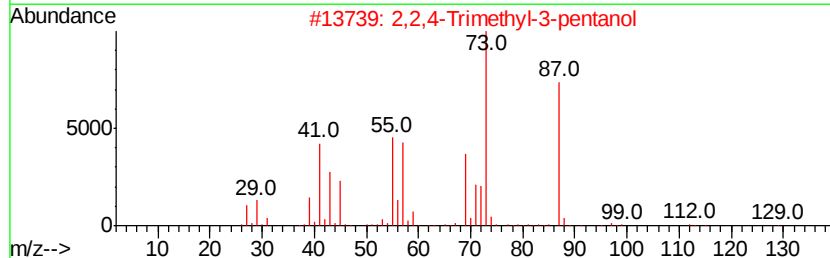
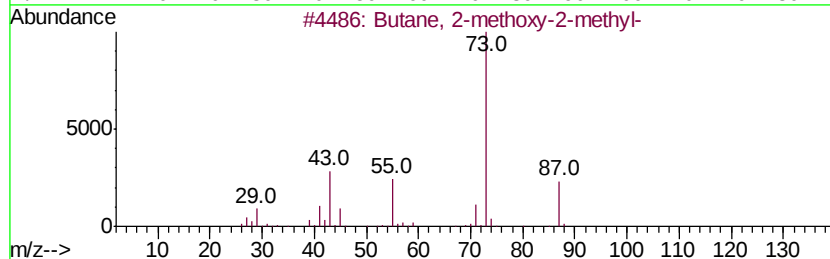
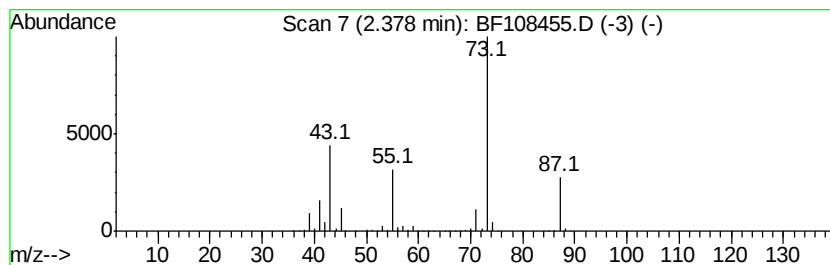
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	96.23 ng	3967630	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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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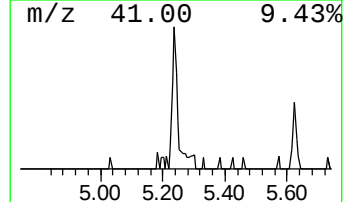
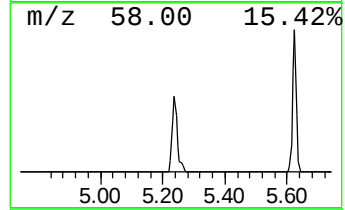
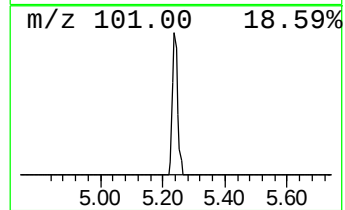
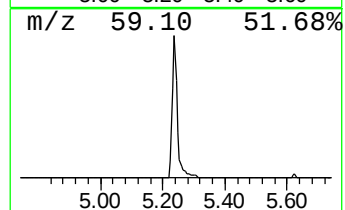
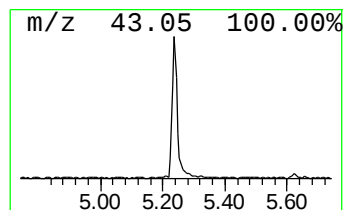
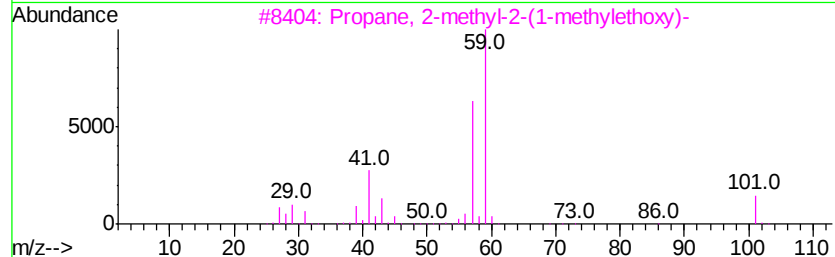
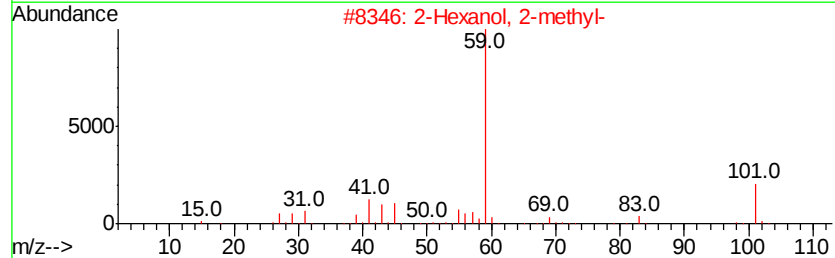
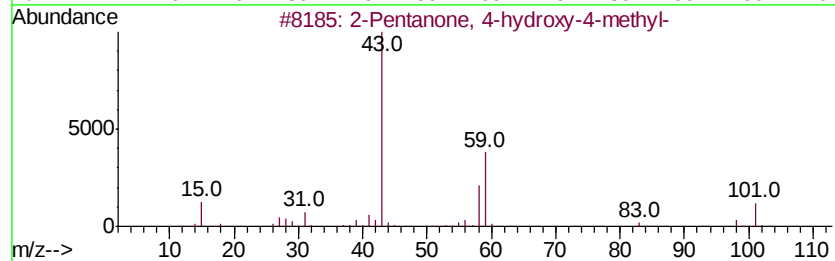
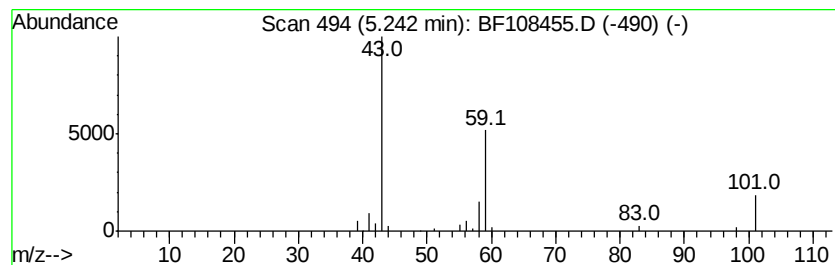
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.29 ng	94378	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	53
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	36
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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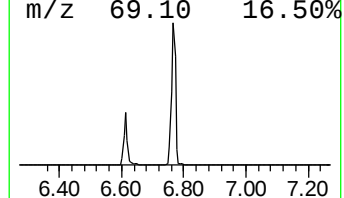
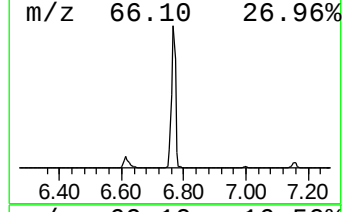
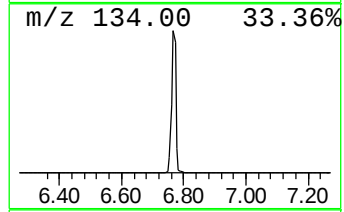
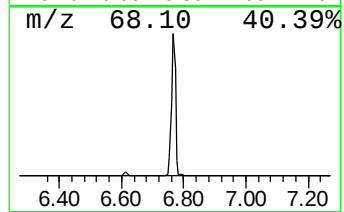
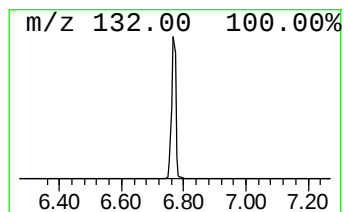
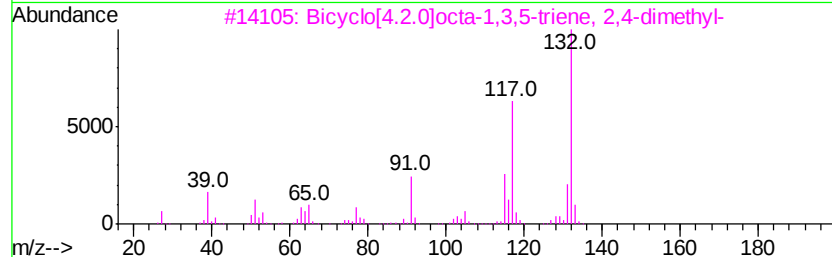
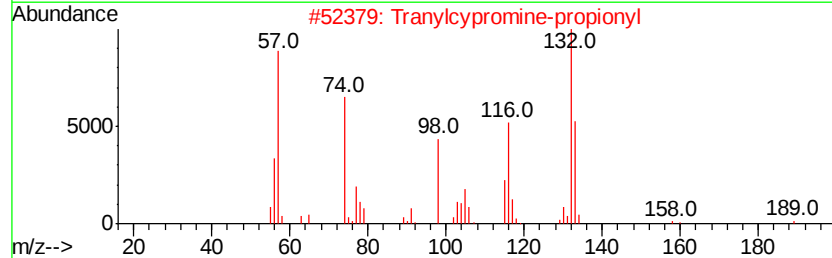
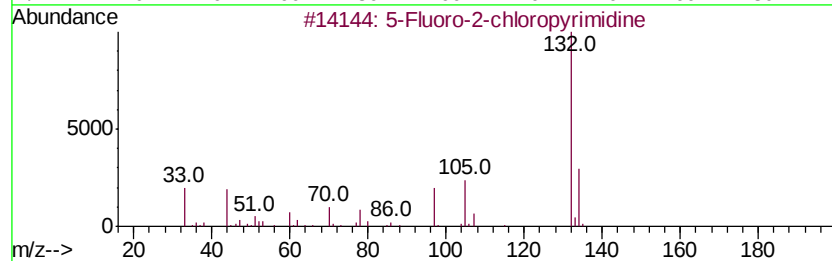
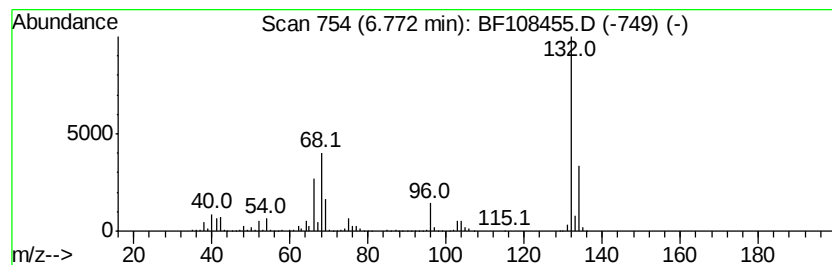
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Peak Number 3 unknown6.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	56.29 ng	2320850	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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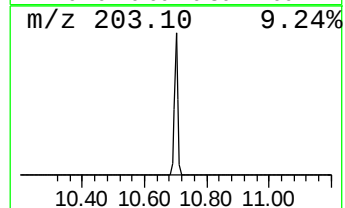
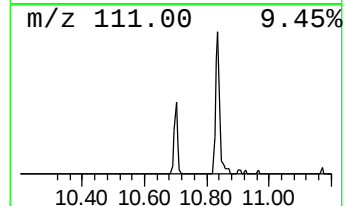
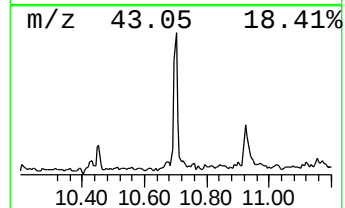
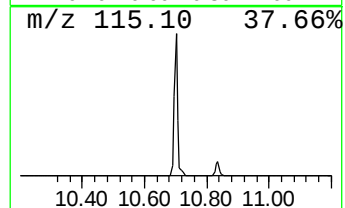
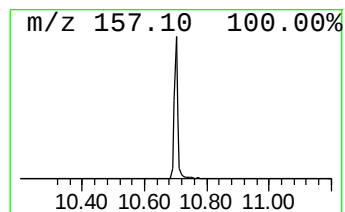
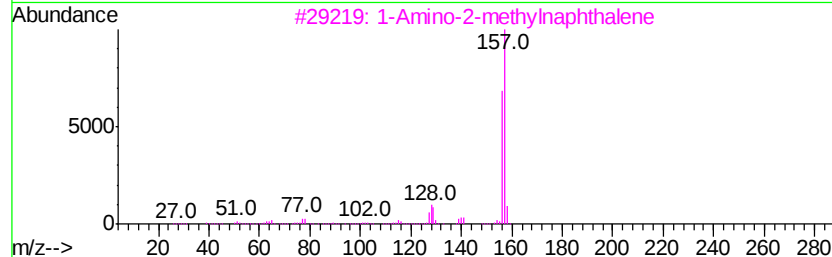
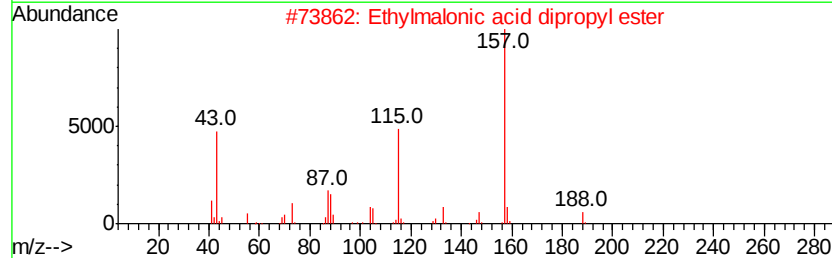
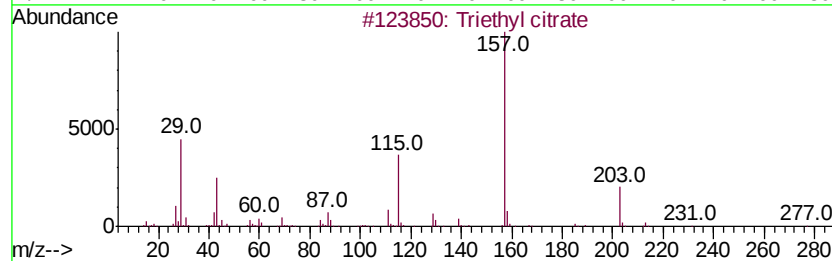
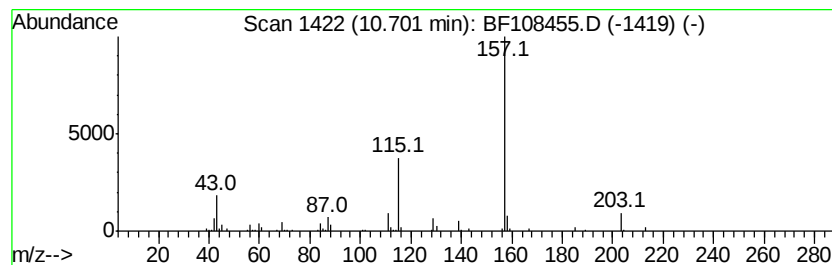
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Peak Number 5 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.41 ng	124660	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	45
3		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38
4		3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClF02	1000338-64-4	36
5		3-Chloro2-fluorobenzoic acid, 6-...	342	C19H28ClF02	1000338-64-1	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.38	96.2	ng	3967630	1	7.00	824612	20.0
2-Pentanone, 4-hy...	5.24	2.3	ng	94378	1	7.00	824612	20.0
unknown6.77	6.77	56.3	ng	2320850	1	7.00	824612	20.0
Triethyl citrate	10.70	2.4	ng	124660	3	10.04	1035570	20.0