

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062518\
 Data File : BF106810.D
 Acq On : 26 Jun 2018 9:03
 Operator : JU/SJ
 Sample : J3689-08
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 062118-TIPC-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-BF061918.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	5.190	482	485	495	rBB	30011	31650	2.36%	0.390%
2	5.601	551	555	565	rBV	432381	407457	30.42%	5.020%
3	6.595	721	724	736	rBB	327237	286162	21.36%	3.526%
4	6.737	744	748	751	rBV	773511	695404	51.92%	8.568%
5	6.960	782	786	789	rBV	322735	261448	19.52%	3.221%
6	7.119	808	813	816	rBV	1062652	980389	73.20%	12.079%
7	7.525	877	882	885	rBV	759618	780448	58.27%	9.616%
8	8.242	1000	1004	1019	rBV	347900	304291	22.72%	3.749%
9	9.319	1182	1187	1190	rBV	1430760	1339402	100.00%	16.503%
10	9.707	1248	1253	1259	rBB	23760	23510	1.76%	0.290%
11	9.907	1284	1287	1292	rBV	32942	25893	1.93%	0.319%
12	10.001	1300	1303	1310	rVB	355887	299063	22.33%	3.685%
13	10.407	1370	1372	1375	rVB	20779	16498	1.23%	0.203%
14	10.660	1412	1415	1418	rBV	72384	53230	3.97%	0.656%
15	10.795	1434	1438	1445	rBV	534516	481617	35.96%	5.934%
16	10.883	1449	1453	1456	rBV	16166	14124	1.05%	0.174%
17	11.495	1553	1557	1564	rBV	331090	288420	21.53%	3.554%
18	13.077	1822	1826	1829	rBV	1322308	1261938	94.22%	15.548%
19	13.960	1973	1976	1981	rVB2	13950	16719	1.25%	0.206%
20	14.148	2004	2008	2013	rBV	319434	288308	21.53%	3.552%
21	14.401	2043	2051	2053	rBV5	8332	17148	1.28%	0.211%
22	14.548	2066	2076	2082	rBV7	8636	31270	2.33%	0.385%
23	14.807	2113	2120	2123	rBV	8663	15935	1.19%	0.196%
24	15.695	2266	2271	2277	rVB2	142667	195861	14.62%	2.413%

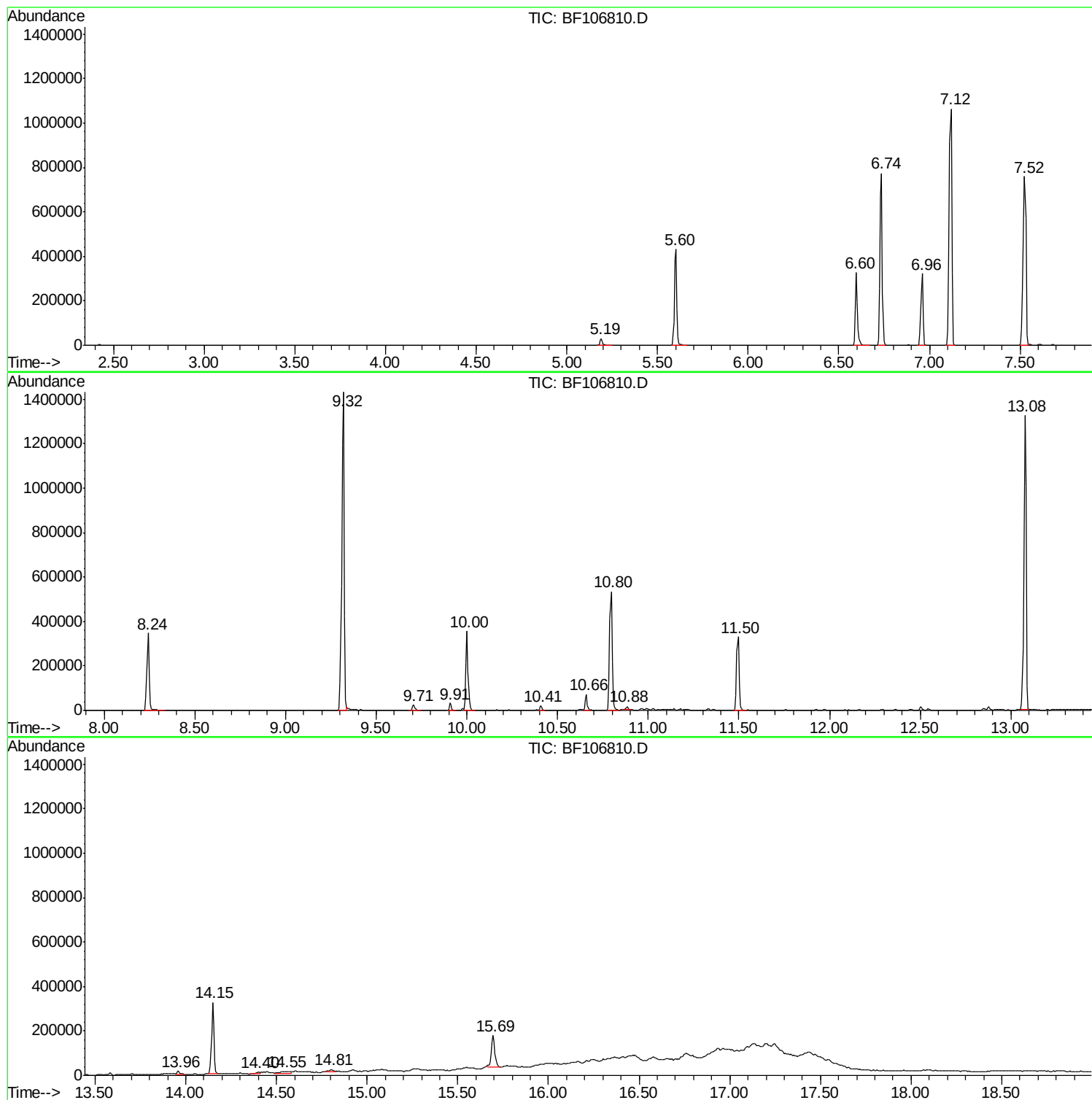
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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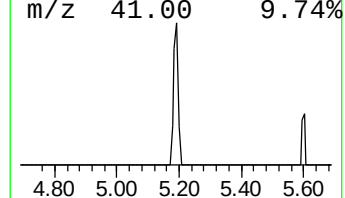
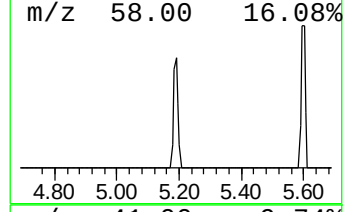
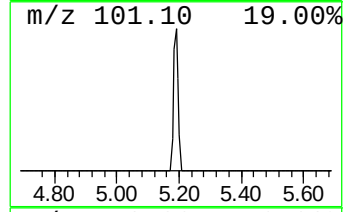
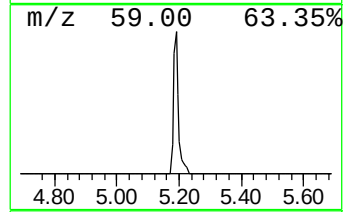
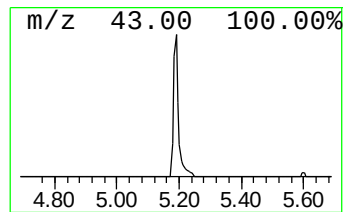
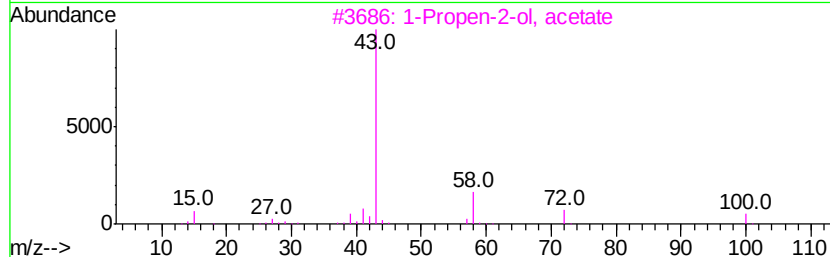
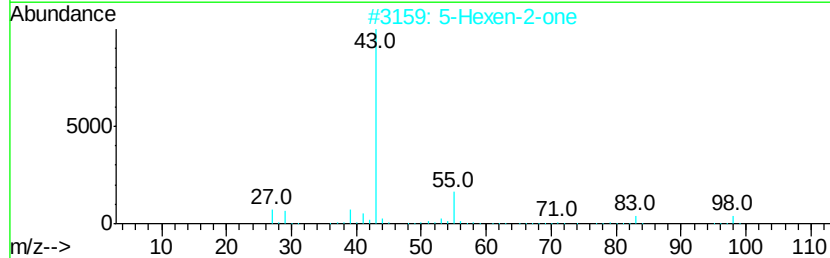
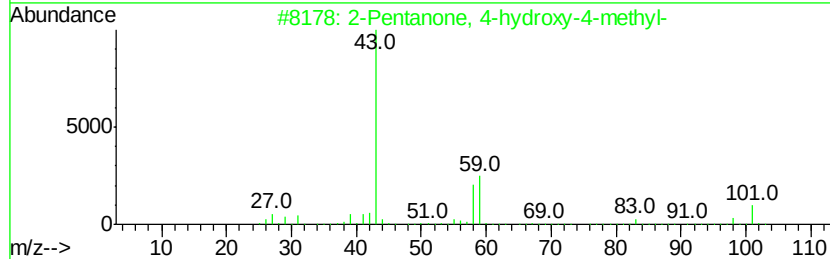
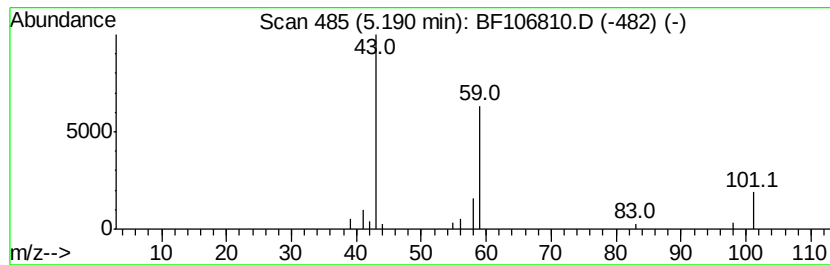
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.42 ng	31650	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	38
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7



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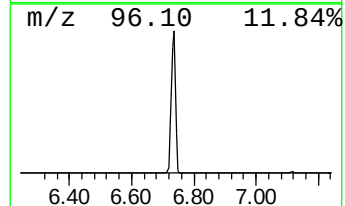
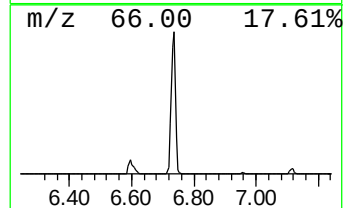
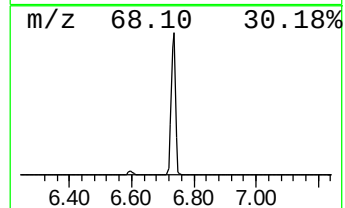
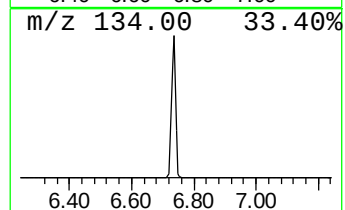
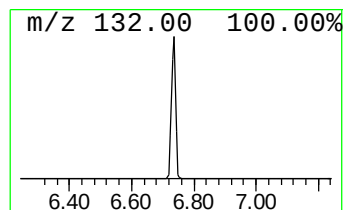
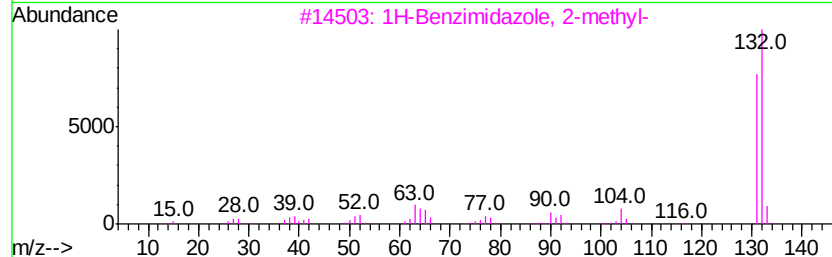
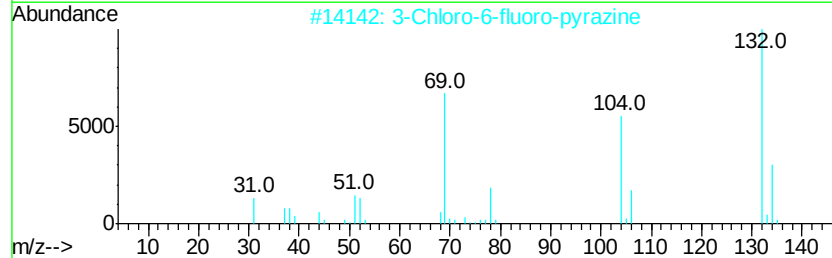
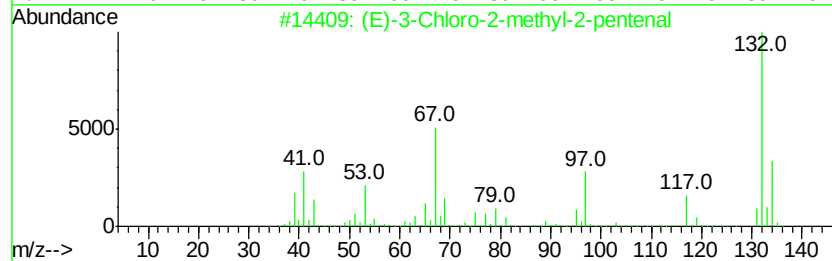
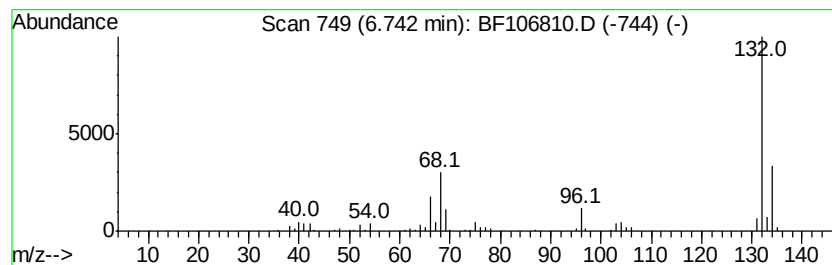
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Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	53.20 ng	695404	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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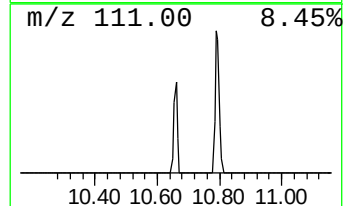
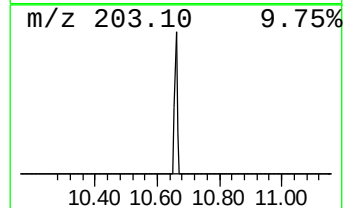
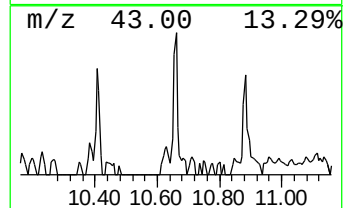
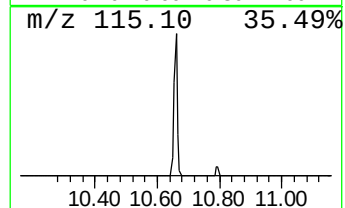
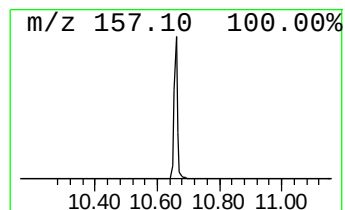
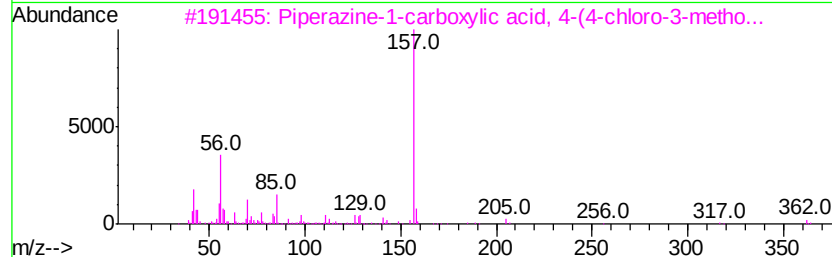
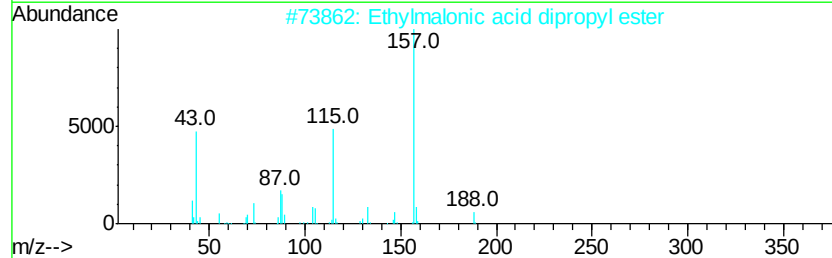
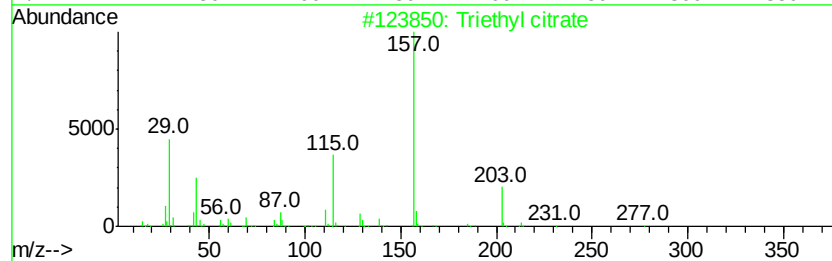
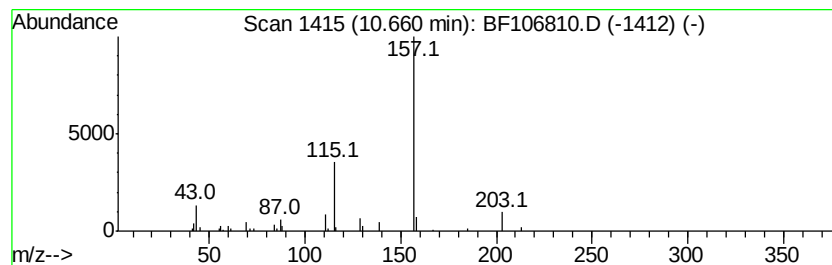
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.56 ng	53230	Acenaphthene-d10	10.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 50
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 38
3		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-79-9 33
4		Piperazine-1-carboxylic acid, 4-...	396 C14H18Cl2N2O5S	1000303-80-3 33
5		Adipic acid, ethyl pent-4-en-2-y...	242 C13H22O4	1000354-11-7 28



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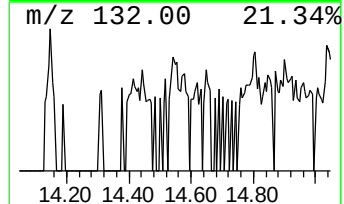
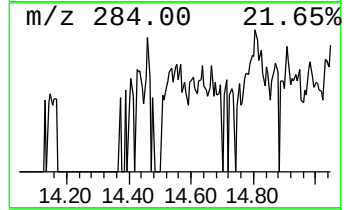
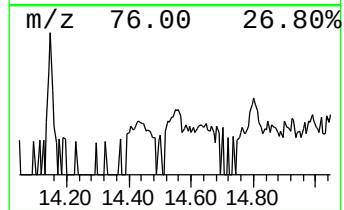
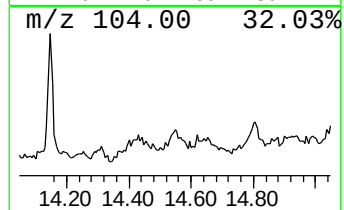
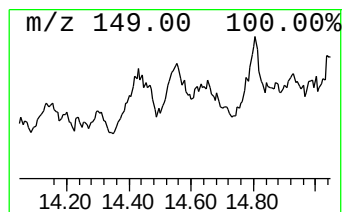
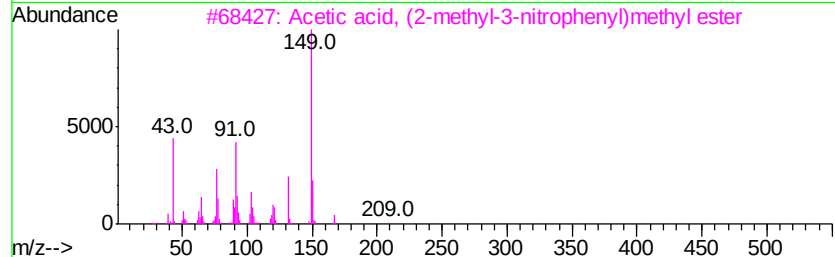
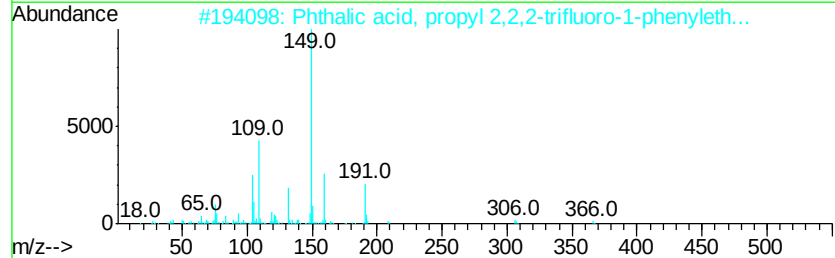
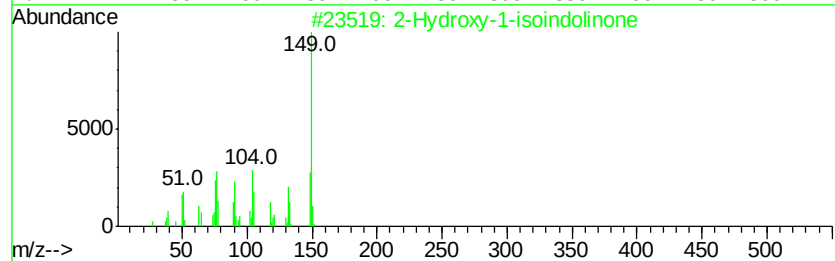
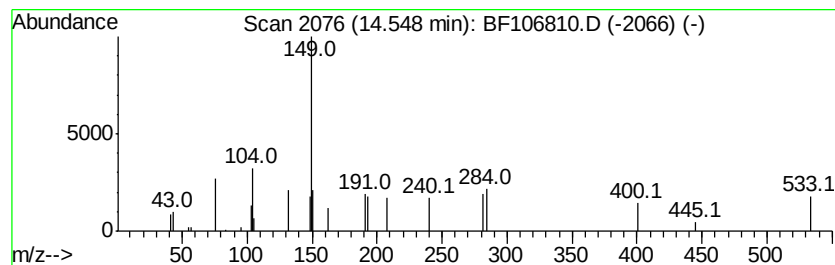
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Peak Number 5 unknown14.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.17 ng	31270	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-1-isoindolinone	149	C8H7NO2	1000289-12-0	27
2		Phthalic acid, propyl 2,2,2-trif...	366	C19H17F3O4	1000377-70-0	23
3		Acetic acid, (2-methyl-3-nitroph...	209	C10H11NO4	1000367-94-9	17
4		Phthalic acid, 3-fluorobenzyl he...	512	C32H45FO4	1000377-90-1	17
5		Phthalic acid, di-(1-hexen-5-yl)...	330	C20H26O4	1000160-80-2	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	2.4	ng	31650	1	6.96	261448	20.0
unknown6.74	6.74	53.2	ng	695404	1	6.96	261448	20.0
Triethyl citrate	10.66	3.6	ng	53230	3	10.00	299063	20.0
unknown14.55	14.55	2.2	ng	31270	5	14.15	288308	20.0