LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107560.D
Acq On : 21 Jul 2018 8:03
Operator : JU/SJ
Sample : J4061-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-DBRI-E-D-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-BF072018.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	5.201	484	487	495	rVB	158886	174895	2.68%	0.368%
2	5.601	551	555	578	rBV	1926121	2698255	41.36%	5.673%
3	6.601	721	725	745	rBV	1227978	1973202	30.25%	4.149%
4	6.742	745	749	774	rVV	3746771	4499154	68.96%	9.460%
5	6.972	785	788	795	rBV	1457509	1621736	24.86%	3.410%
6	7.131	811	815	831	rBV	5483802	5691776	87.25%	11.967%
7	7.536	879	884	906	rBV	3754358	4707206	72.15%	9.897%
8	8.254	1002	1006	1024	rBV	1612265	1889062	28.96%	3.972%
9	9.330	1185	1189	1204	rBV	6554737	6459187	99.01%	13.581%
10	9.725	1252	1256	1268	rBV	440971	478367	7.33%	1.006%
11	10.019	1302	1306	1317	rVB	1447975	1532475	23.49%	3.222%
12	10.677	1415	1418	1425	rBV	367145	295927	4.54%	0.622%
13	10.807	1436	1440	1453	rBV	2570959	2748832	42.14%	5.780%
14	11.507	1556	1559	1576	rVB	1594323	1689212	25.89%	3.552%
15	12.013	1642	1645	1651	rBV2	55011	67860	1.04%	0.143%
16	13.095	1825	1829	1833	rBV	6052089	6523823	100.00%	13.717%
17	13.977	1975	1979	1986	rBV	123269	152309	2.33%	0.320%
18	14.160	2006	2010	2017	rBV	2218152	2091282	32.06%	4.397%
19	14.601	2082	2085	2090	rBV2	126811	125931	1.93%	0.265%
20	14.924	2136	2140	2147	rVB	118288	127834	1.96%	0.269%
21	15.283	2197	2201	2204	rVB	130832	141659	2.17%	0.298%
22	15.689	2265	2270	2278	rVB2	1116182	1636654	25.09%	3.441%
23	16.148	2344	2348	2354	rVB2	102586	154487	2.37%	0.325%
24	16.689	2437	2440	2445	rVB3	51728	79533	1.22%	0.167%

Sum of corrected areas: 47560658

LSC Report - Integrated Chromatogram

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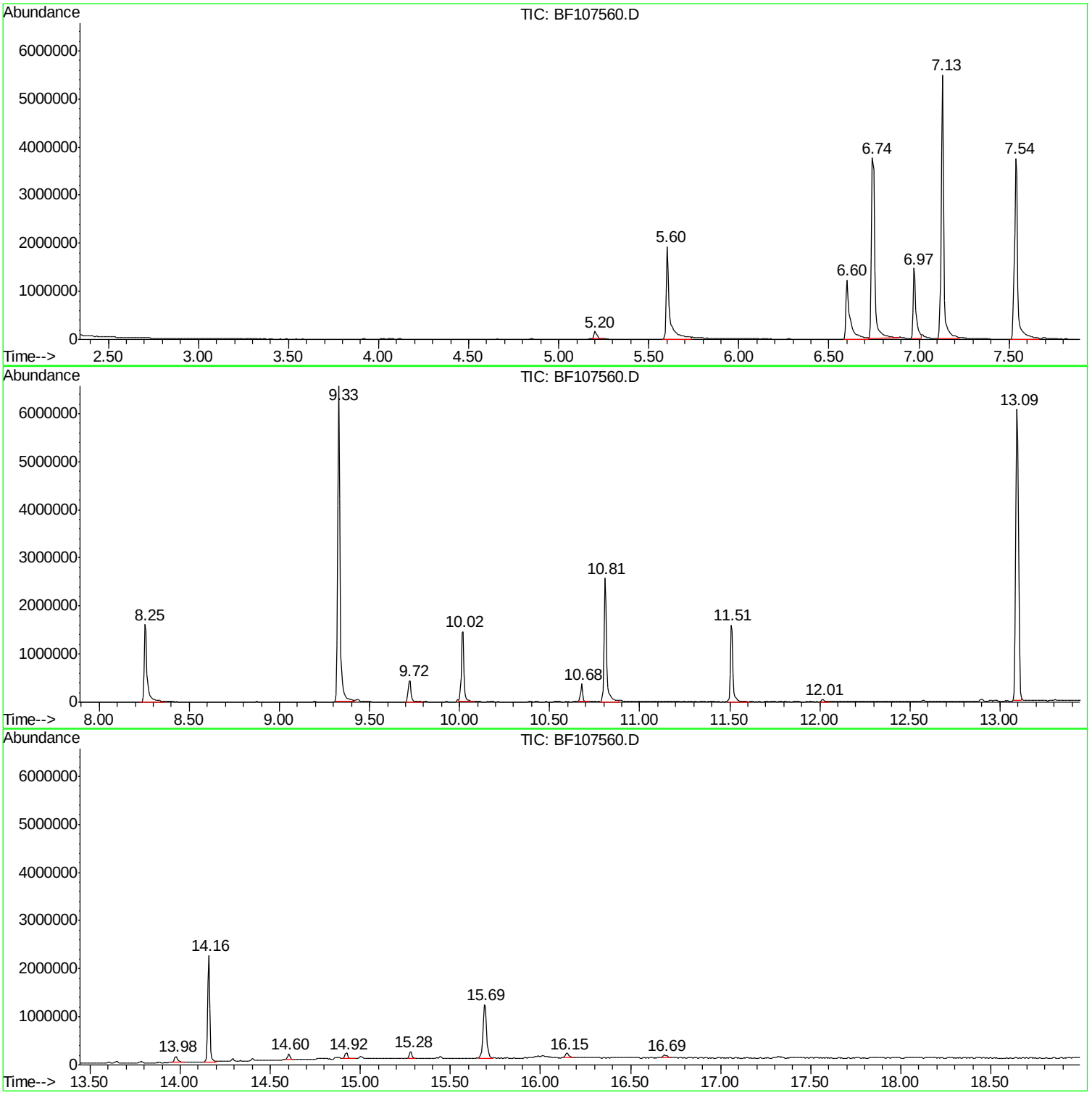
Sample : J4061-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107560.D
Acq On : 21 Jul 2018 8:03
Operator : JU/SJ
Sample : J4061-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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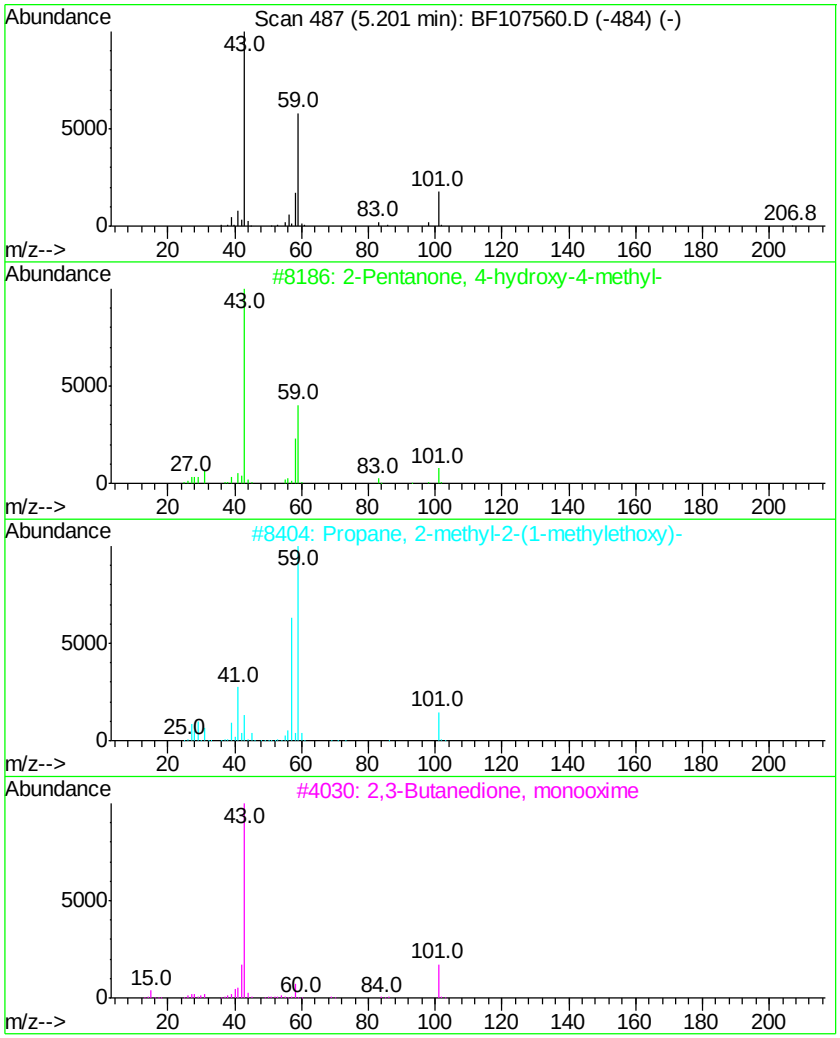
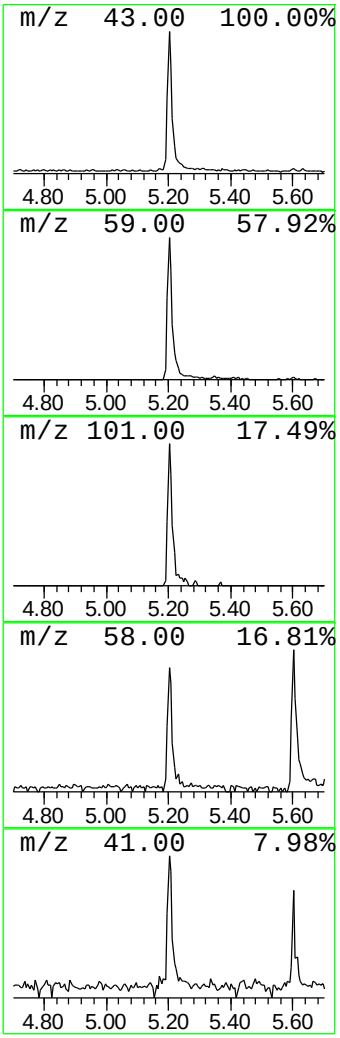
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.16 ng	174895	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Acetone	58	C3H6O	000067-64-1	9
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107560.D
Acq On : 21 Jul 2018 8:03
Operator : JU/SJ
Sample : J4061-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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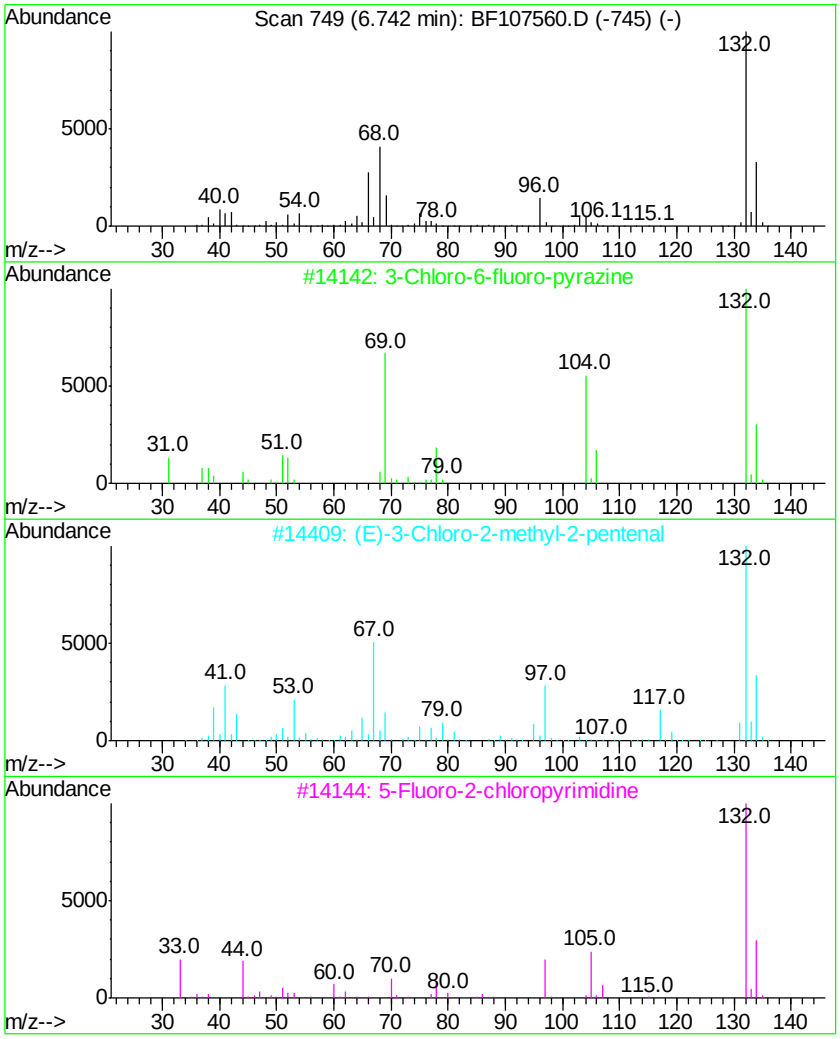
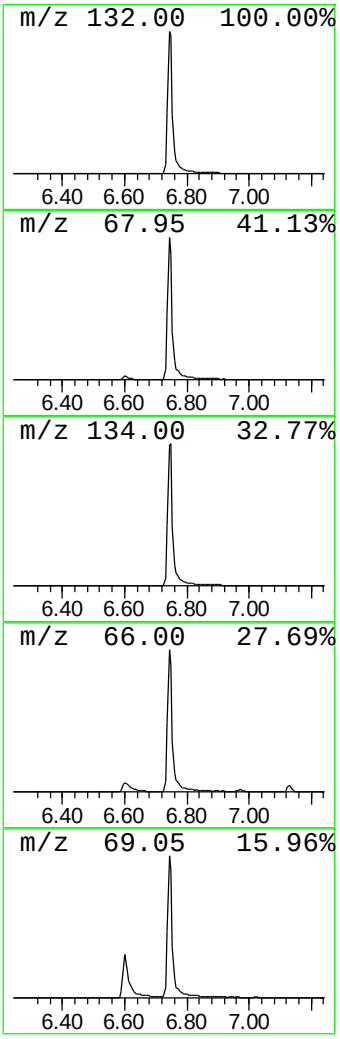
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	55.49 ng	4499150	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
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Acq On : 21 Jul 2018 8:03
Operator : JU/SJ
Sample : J4061-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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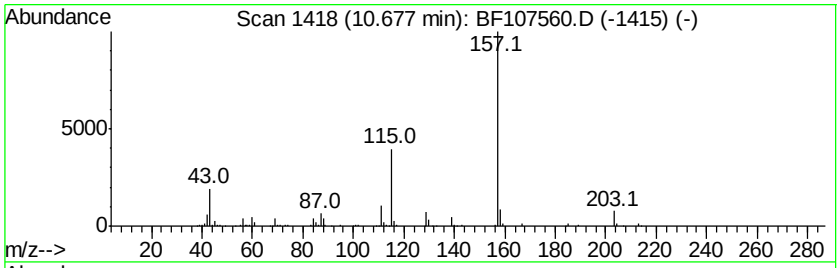
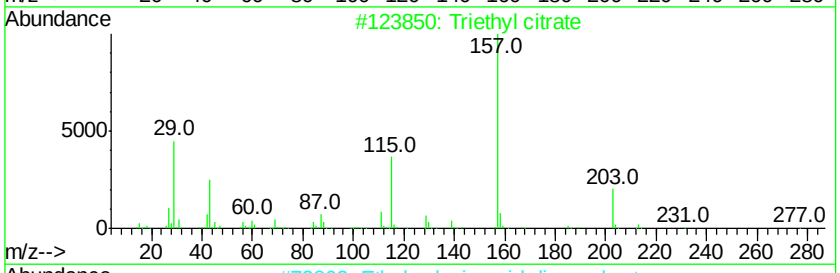
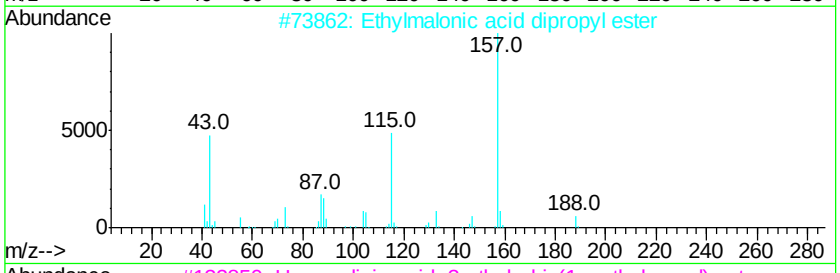
Peak Number 4 Triethyl citrate Concentration Rank 3

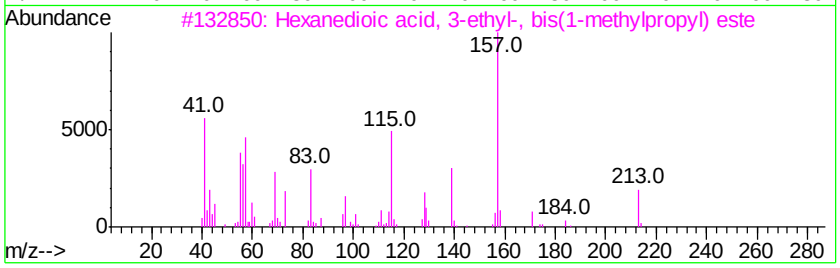
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.86 ng	295927	Acenaphthene-d10	10.01

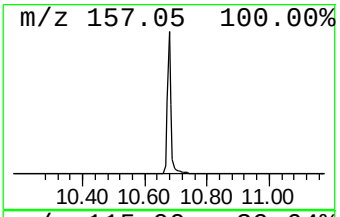
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	40
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	38
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	38

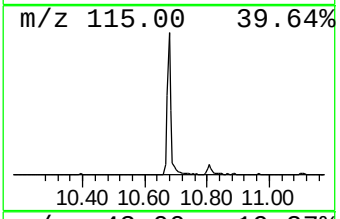


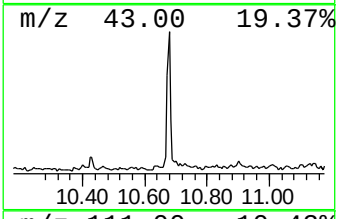


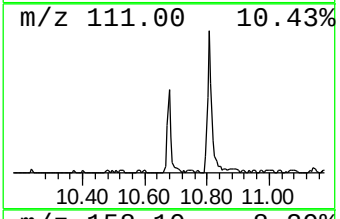


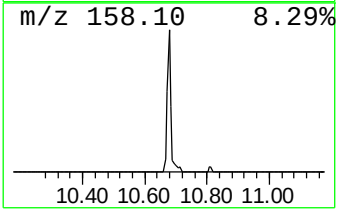












Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	2.2	ng	174895	1	6.97	1621740	20.0
unknown6.74	6.74	55.5	ng	4499150	1	6.97	1621740	20.0
Triethyl citrate	10.68	3.9	ng	295927	3	10.01	1532480	20.0