LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.205	15	20	30	rVB	295541	376144	7.04%	1.109%
2	5.134	514	518	527	rVB	304457	317776	5.94%	0.937%
3	5.528	581	585	588	rBV	2005509	1704415	31.88%	5.023%
4	6.528	751	755	758	rBV	1330243	1096196	20.50%	3.231%
5	6.681	776	781	784	rBV	3170582	2895303	54.15%	8.533%
6	6.910	817	820	824	rBV	1070323	962879	18.01%	2.838%
7	7.075	843	848	851	rBV	3592623	3626437	67.83%	10.688%
8	7.481	911	917	920	rBV	2842413	3063561	57.30%	9.029%
9	8.192	1034	1038	1042	rBV	1439551	1320684	24.70%	3.892%
10	9.275	1216	1222	1225	rBV	5121862	5346434	100.00%	15.757%
11	9.928	1331	1333	1334	rBV	166532	128023	2.39%	0.377%
12	9.951	1334	1337	1341	rVB2	1715772	1417393	26.51%	4.177%
13	10.363	1402	1407	1411	rVB	55296	54677	1.02%	0.161%
14	10.622	1446	1451	1454	rBV	2277298	1809707	33.85%	5.334%
15	10.739	1466	1471	1474	rBV	2136960	2032683	38.02%	5.991%
16	11.439	1586	1590	1593	rBV	1602650	1342617	25.11%	3.957%
17	13.027	1854	1860	1863	rBV	4086673	4351678	81.39%	12.825%
18	13.904	2006	2009	2018	rVB	53226	55865	1.04%	0.165%
19	14.074	2034	2038	2042	rBV	1181422	1038610	19.43%	3.061%
20	15.568	2286	2292	2298	rBV	798557	989772	18.51%	2.917%

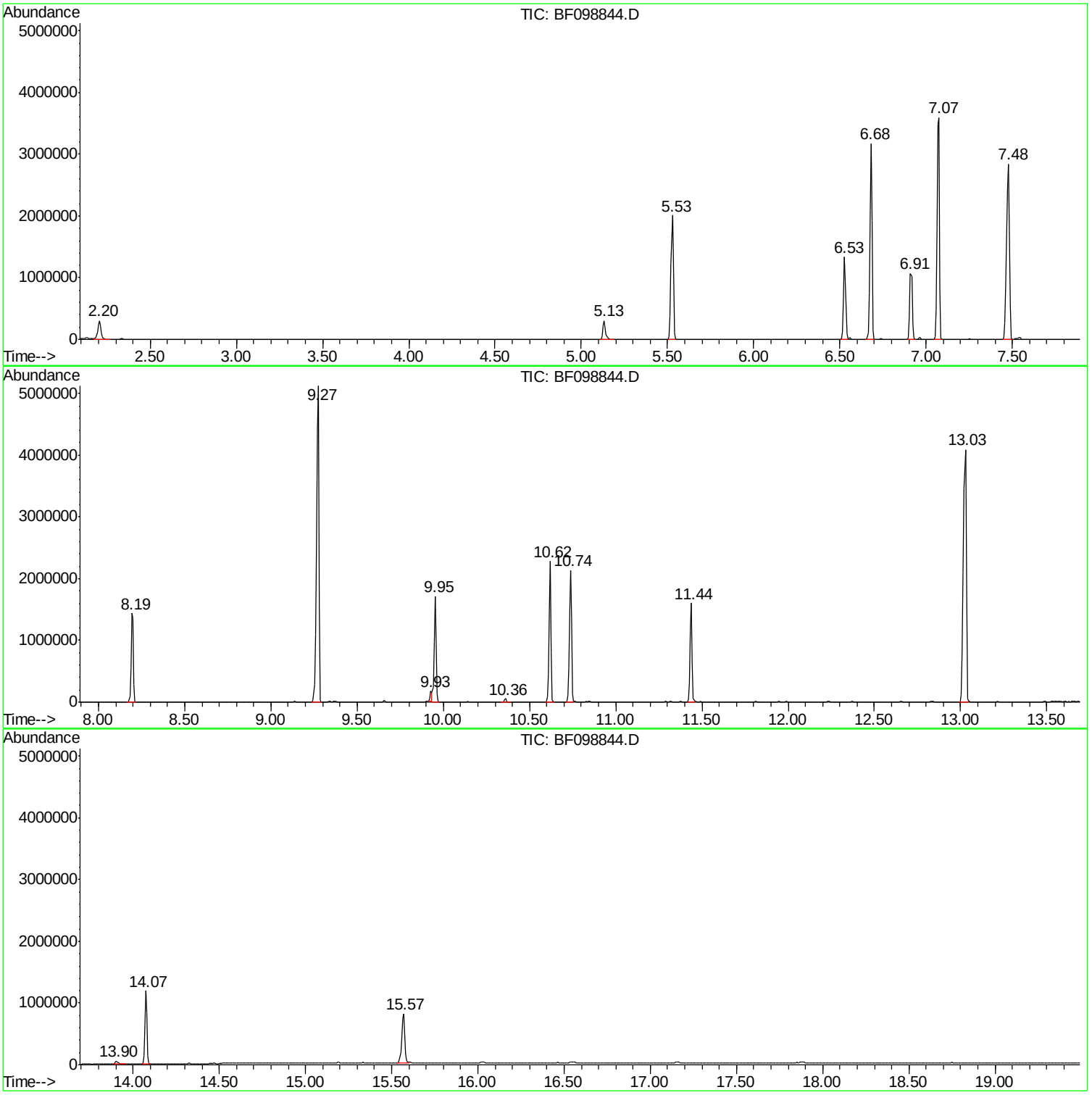
Sum of corrected areas: 33930854

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

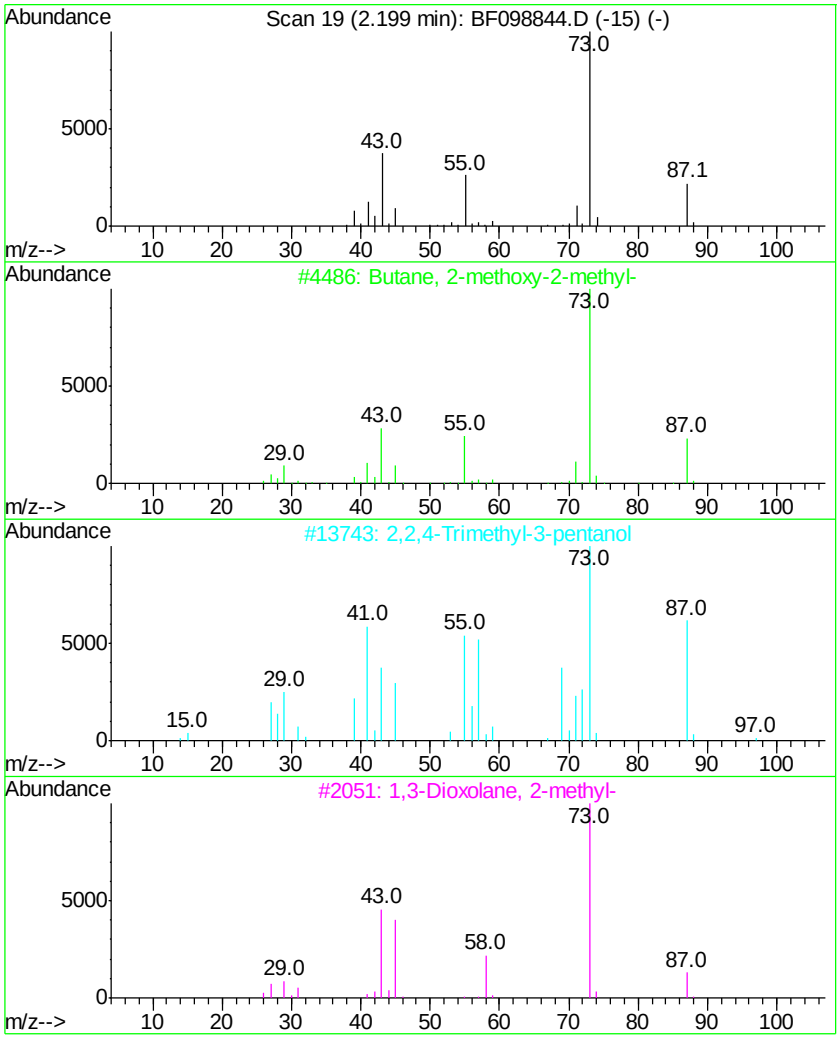
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

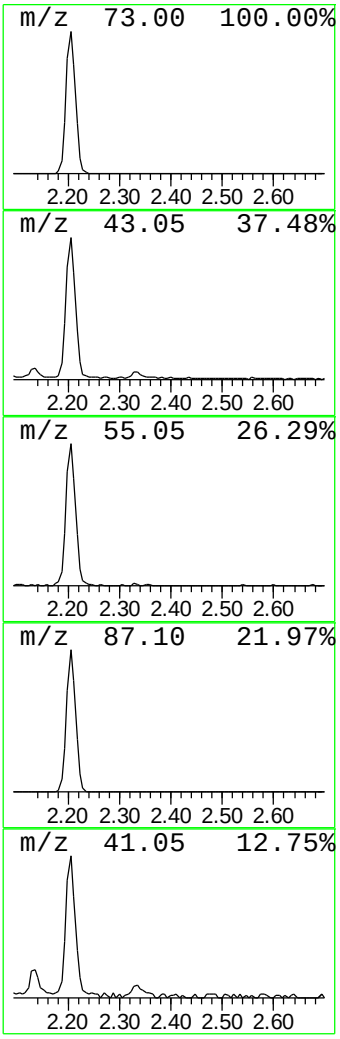
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	7.81 ng	376144	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

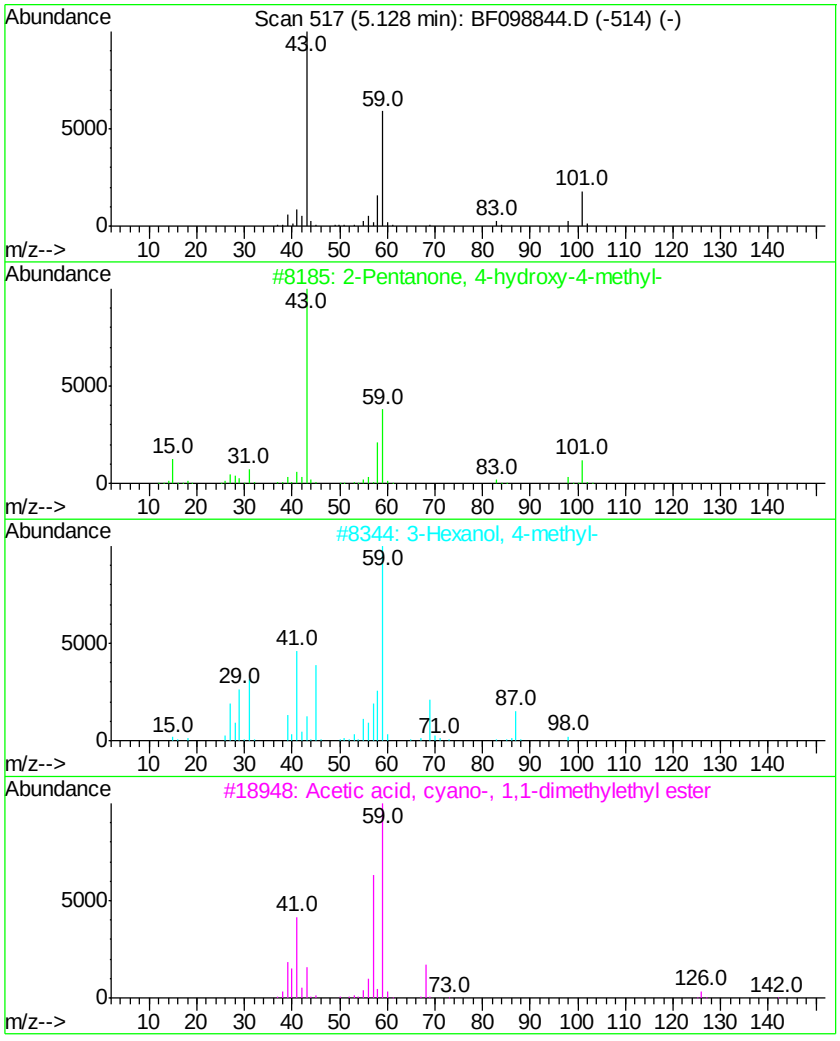
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

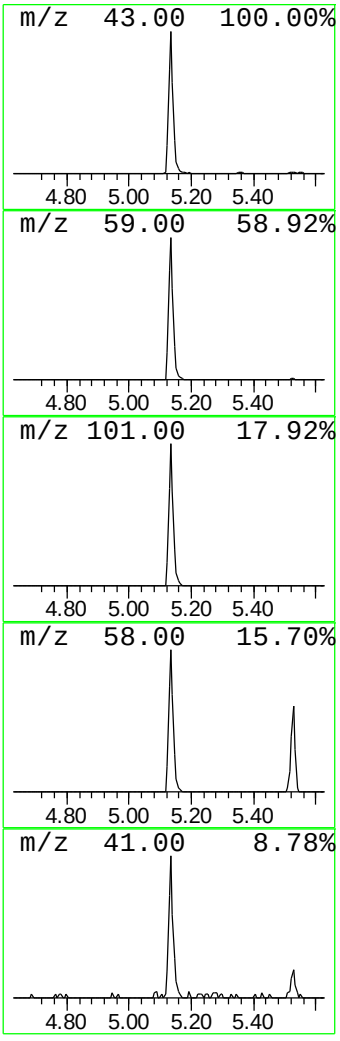
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.60 ng	317776	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

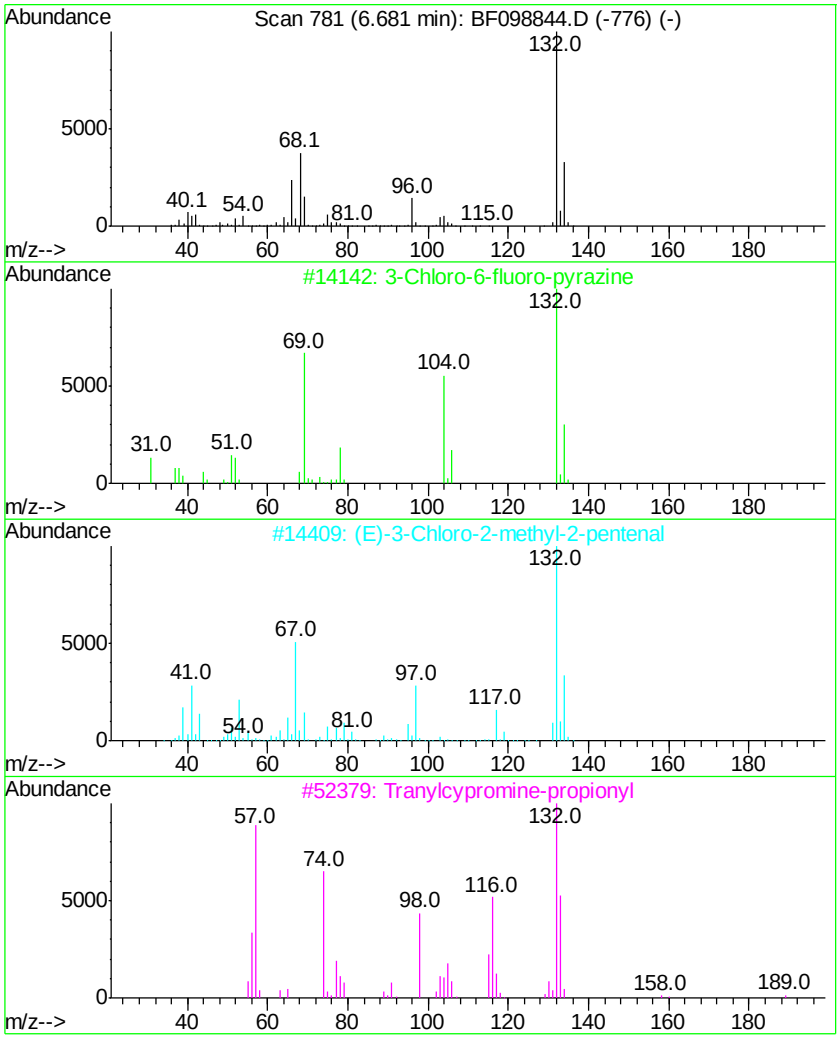
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

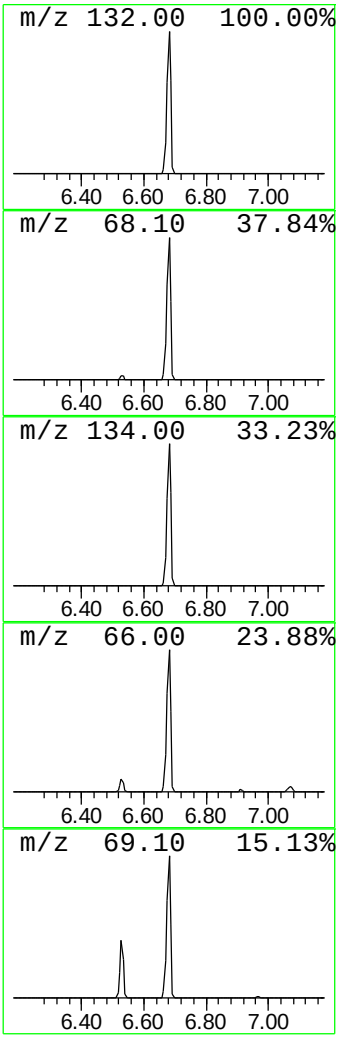
****

Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	60.14 ng	2895300	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

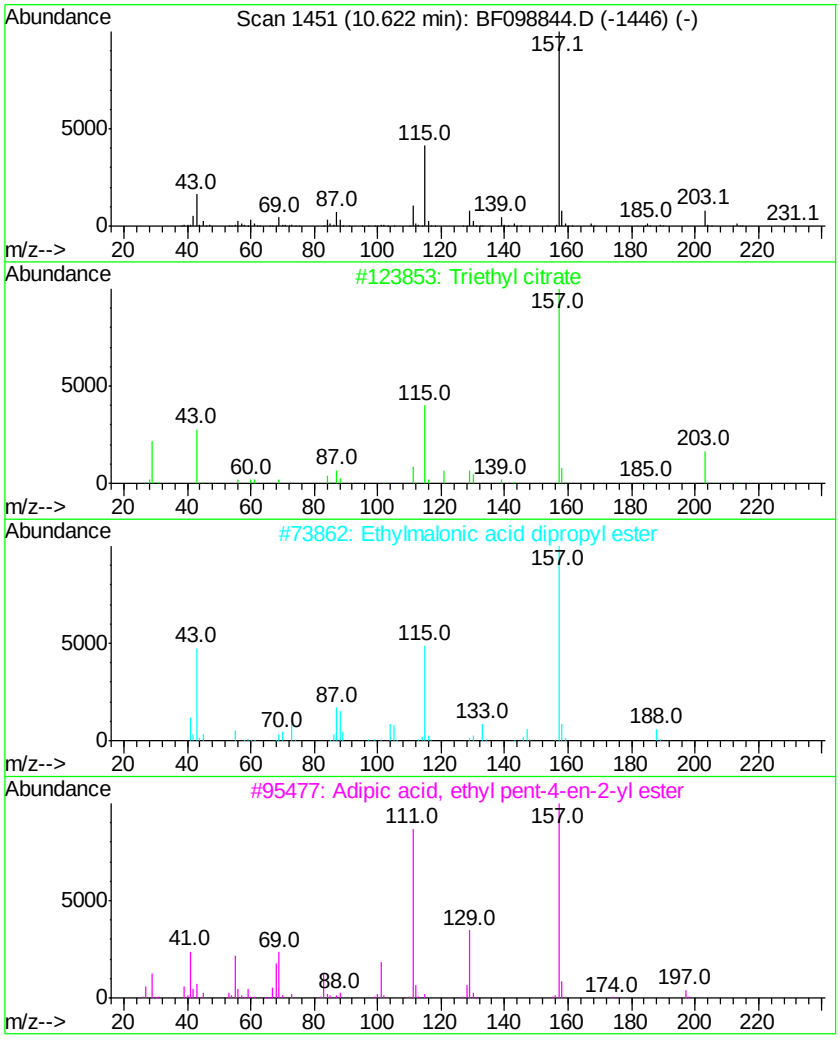
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

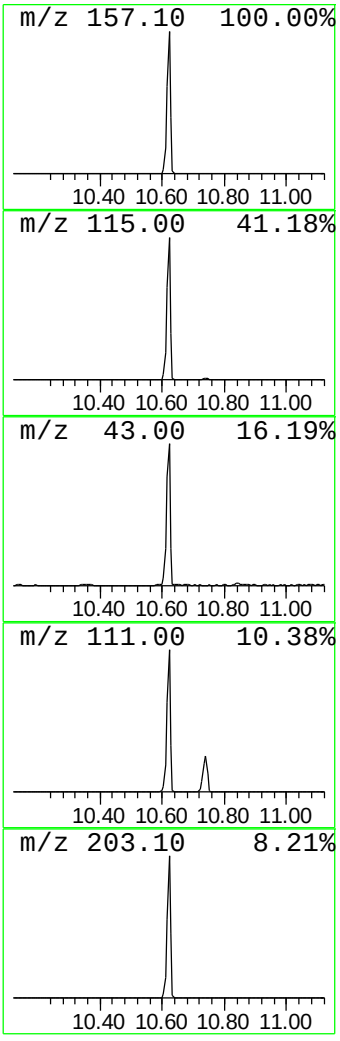
****

Peak Number 5 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	25.54 ng	1809710	Acenaphthene-d10	9.95

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	53
3	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	38
4	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	38
5	N-(5-[3-(2-Oxo-benzooxazol-3-yl)...	318	C14H14N4O3S	1000300-11-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098844.D
Acq On : 26 Sep 2017 20:47
Operator : SJ/JU
Sample : I5426-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092517-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	7.8	ng	376144	1	6.92	962879	20.0
2-Pentanone, 4-hy...	5.13	6.6	ng	317776	1	6.92	962879	20.0
unknown6.68	6.68	60.1	ng	2895300	1	6.92	962879	20.0
Triethyl citrate	10.62	25.5	ng	1809710	3	9.95	1417390	20.0