LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098911.D
Acq On : 28 Sep 2017 16:26
Operator : SJ/JU
Sample : I5464-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092617-TIDO-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:\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	2.222	18	23	34	rVB	478841	641090	15.94%	2.477%
2	3.081	162	169	178	rVB	25023	42995	1.07%	0.166%
3	5.139	516	519	531	rVB	211580	213485	5.31%	0.825%
4	5.534	582	586	589	rBV	1548039	1324807	32.93%	5.118%
5	6.533	752	756	759	rBV	1095004	900546	22.39%	3.479%
6	6.557	759	760	766	rVB	129792	94101	2.34%	0.364%
7	6.686	777	782	785	rBV	2571418	2321388	57.71%	8.968%
8	6.916	817	821	825	rBV	1231711	957669	23.81%	3.700%
9	7.075	844	848	851	rVB	3411322	3053947	75.92%	11.798%
10	7.480	911	917	920	rBV	2386133	2442471	60.72%	9.436%
11	8.198	1035	1039	1042	rBV	1512636	1215456	30.22%	4.696%
12	8.345	1062	1064	1067	rBV	54327	45447	1.13%	0.176%
13	9.274	1216	1222	1225	rBV	4352554	4022559	100.00%	15.541%
14	9.663	1284	1288	1291	rBV	143030	114164	2.84%	0.441%
15	9.933	1331	1334	1335	rBV	117709	96124	2.39%	0.371%
16	9.957	1335	1338	1345	rVB	1241082	1134943	28.21%	4.385%
17	10.621	1447	1451	1454	rVB	1216429	902792	22.44%	3.488%
18	10.739	1468	1471	1475	rBV	1275222	1177635	29.28%	4.550%
19	10.845	1486	1489	1496	rVB	42779	43218	1.07%	0.167%
20	11.439	1586	1590	1594	rBV	1002627	898216	22.33%	3.470%
21	11.651	1623	1626	1635	rBV	44565	48832	1.21%	0.189%
22	13.027	1855	1860	1863	rBV	2945209	2730826	67.89%	10.550%
23	14.080	2035	2039	2043	rBV	890664	799115	19.87%	3.087%
24	15.574	2288	2293	2300	rVB	488781	662458	16.47%	2.559%

Sum of corrected areas: 25884284

LSC Report - Integrated Chromatogram

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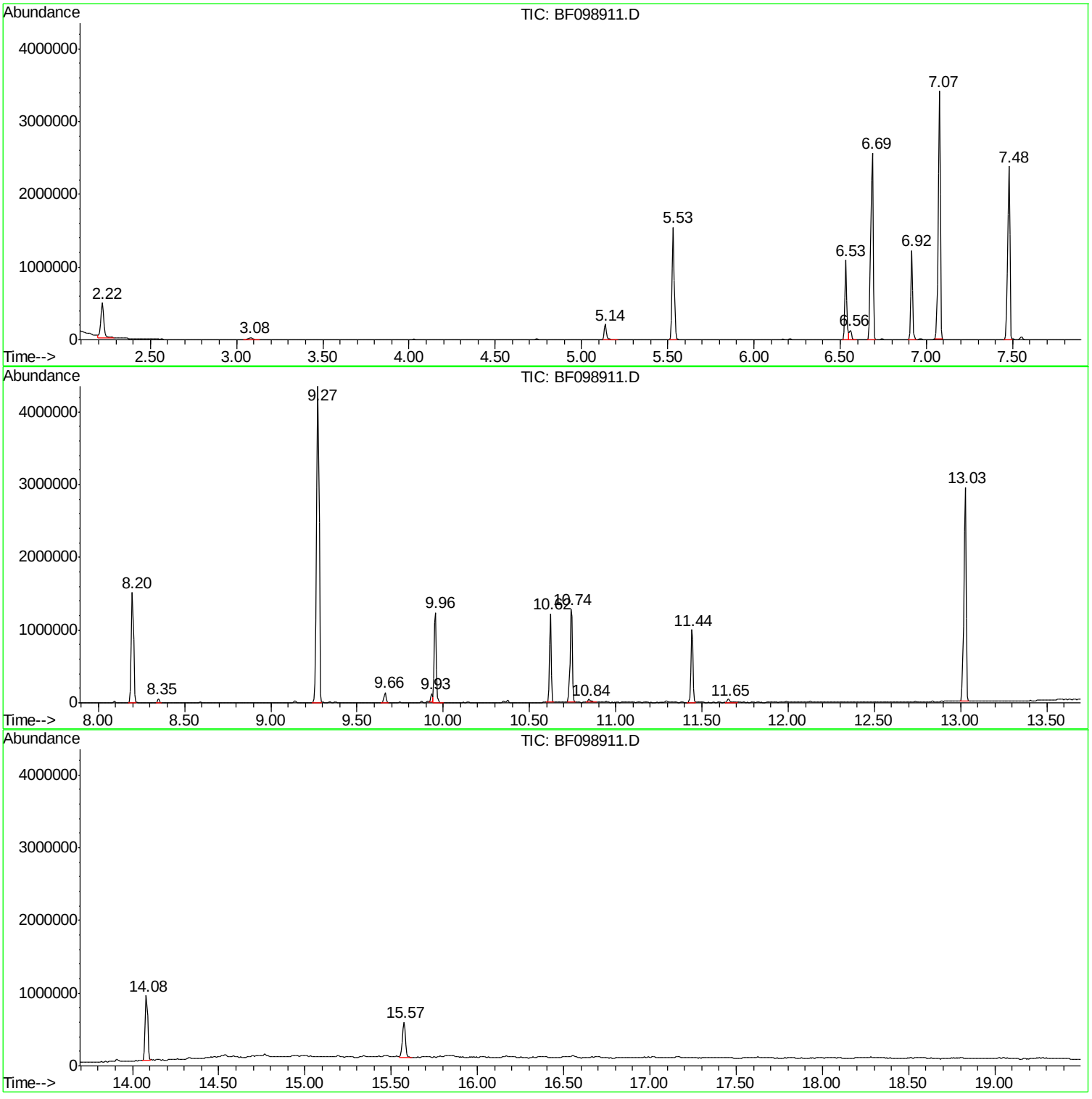
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092617-TIDO-E-D-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\BF092817\
Data File : BF098911.D
Acq On : 28 Sep 2017 16:26
Operator : SJ/JU
Sample : I5464-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092617-TIDO-E-D-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

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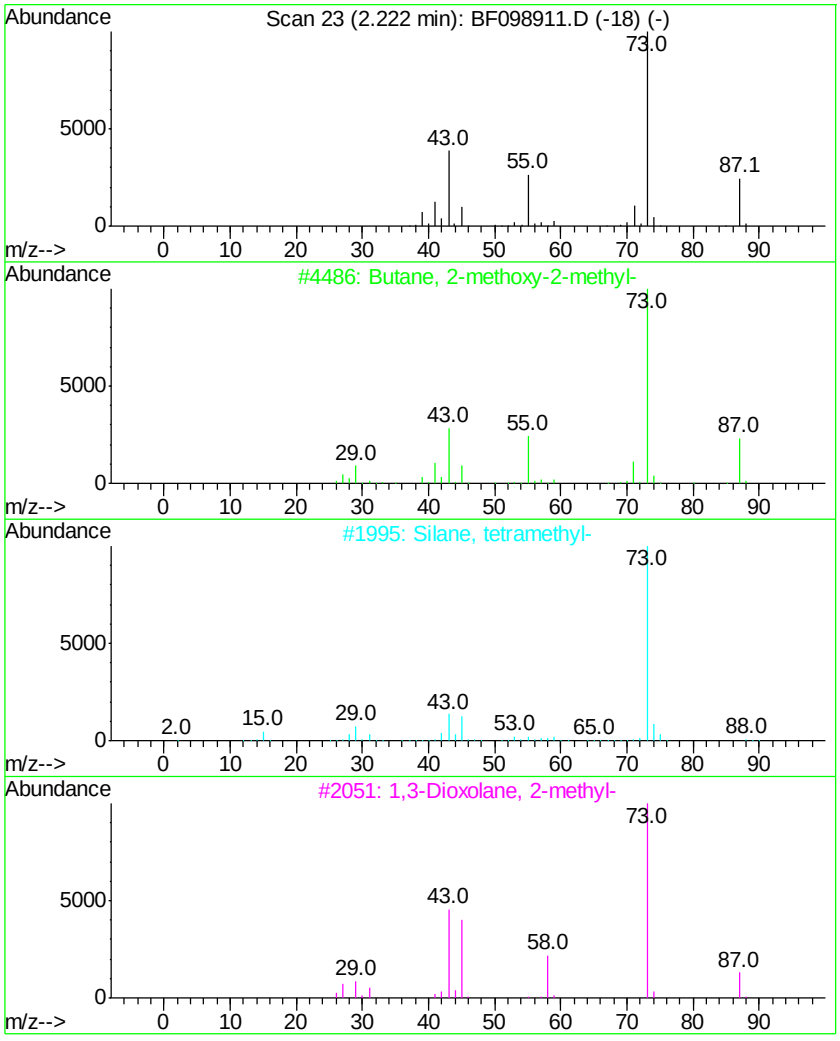
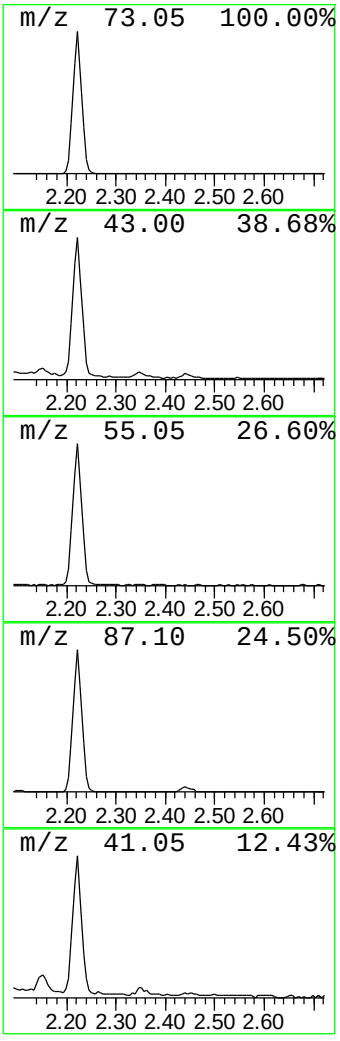
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	13.39 ng	641090	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument : BNA_F
ClientSampleId : 092617-TIDO-E-D-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

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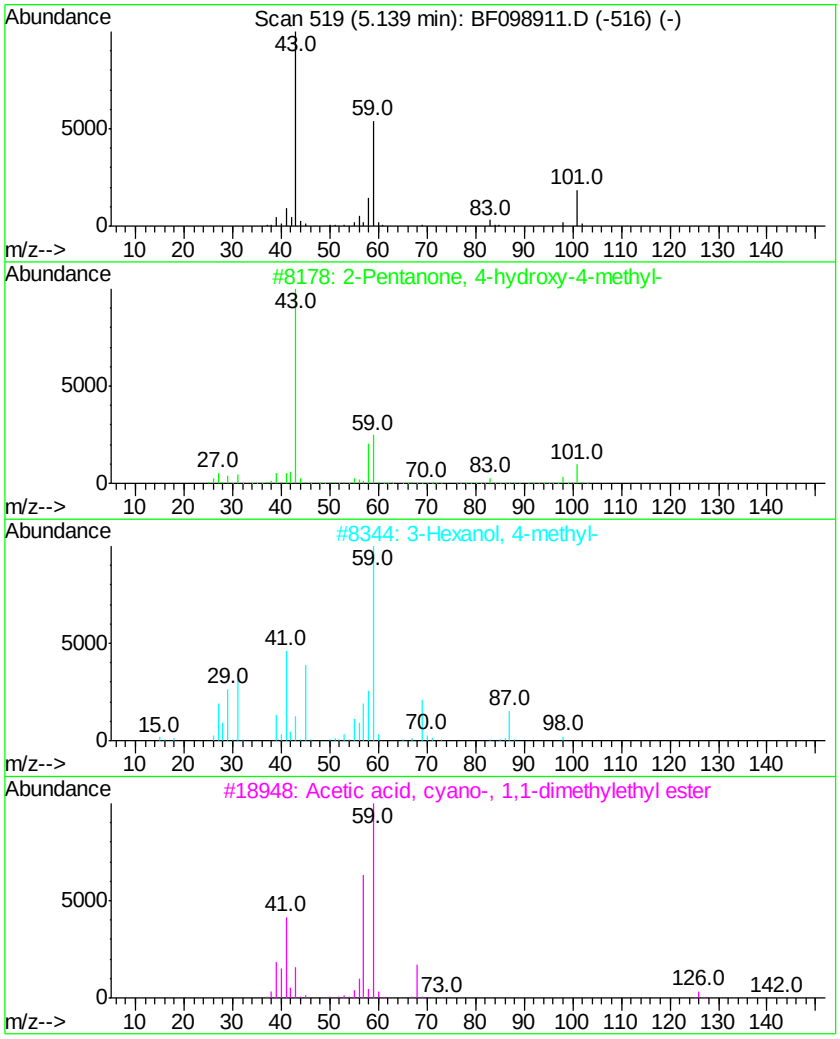
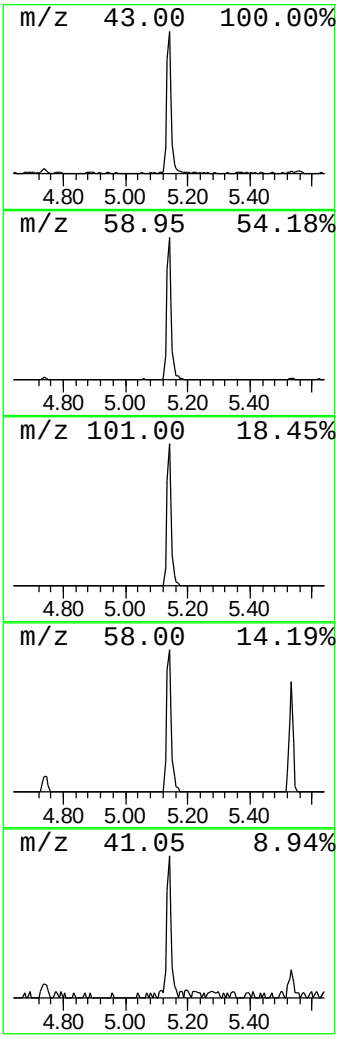
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	4.46 ng	213485	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	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098911.D
Acq On : 28 Sep 2017 16:26
Operator : SJ/JU
Sample : I5464-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092617-TIDO-E-D-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

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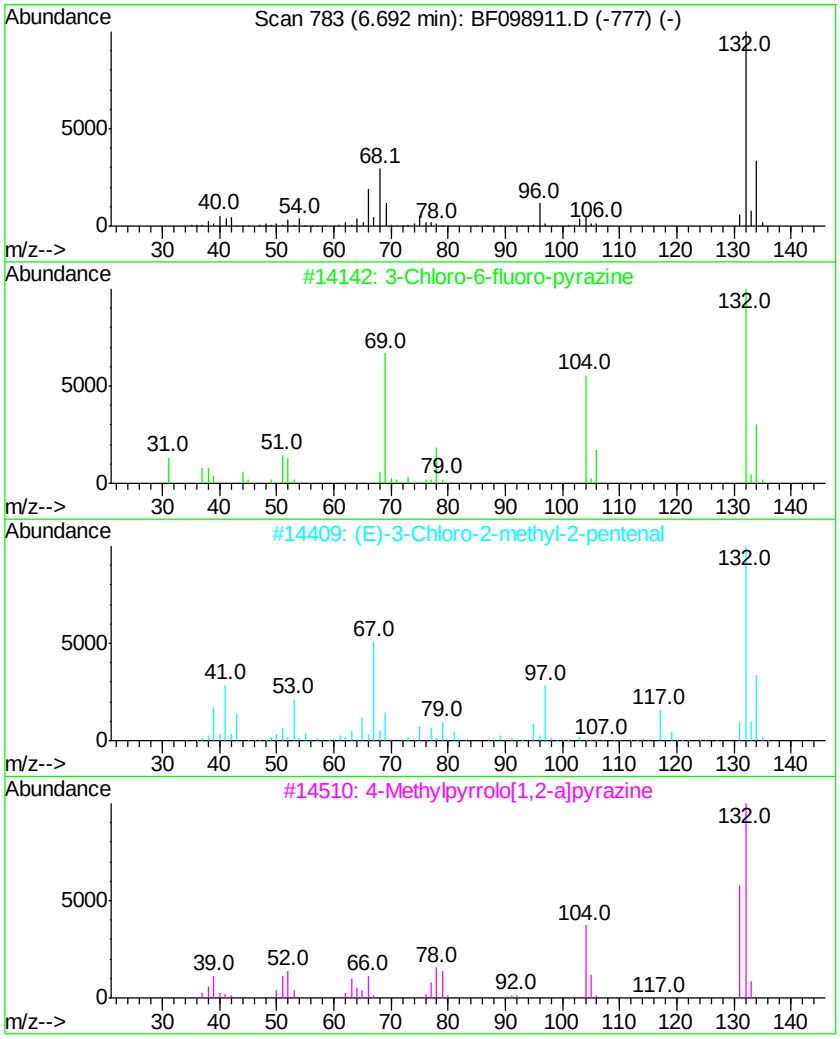
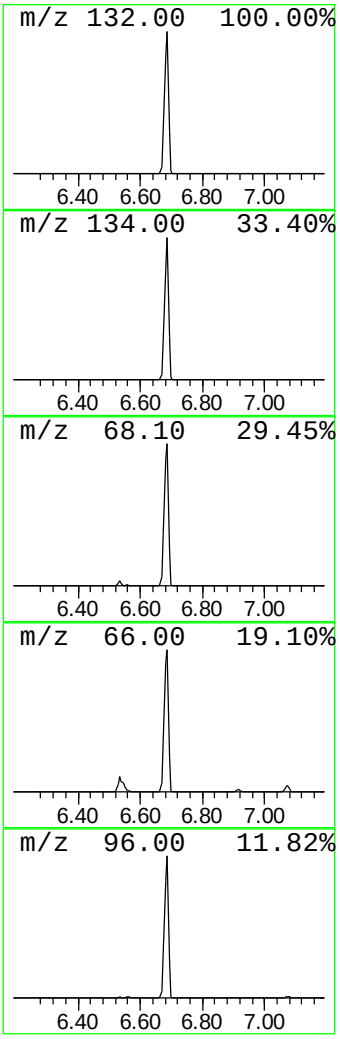
Peak Number 3 unknown6.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	48.48 ng	2321390	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	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I5464-01
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092617-TIDO-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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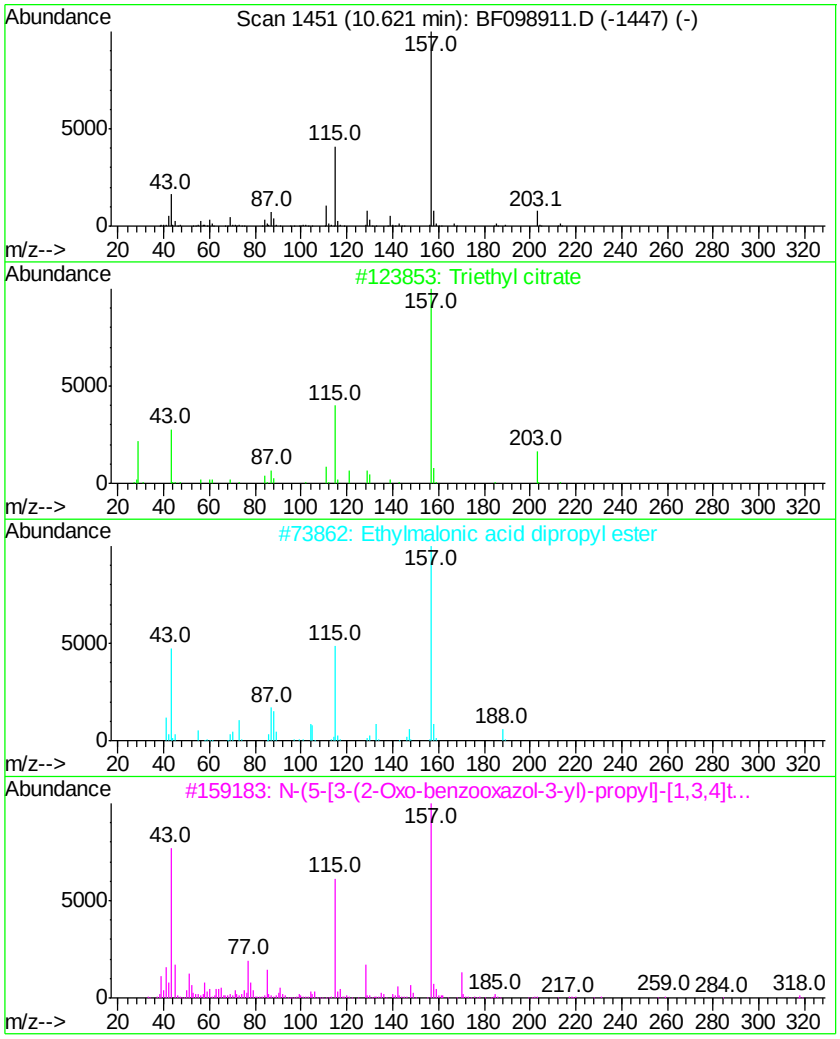
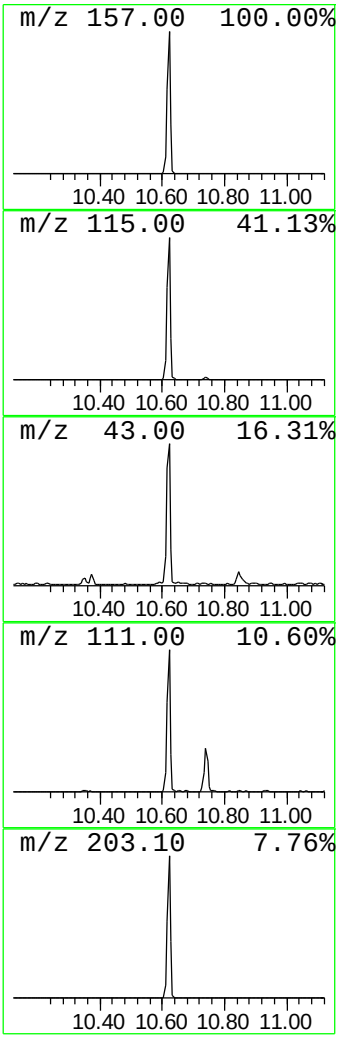
Peak Number 5 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	15.91 ng	902792	Acenaphthene-d10	9.96

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	50
3	N-(5-[3-(2-Oxo-benzooxazol-3-yl)...	318	C14H14N4O3S	1000300-11-5	38
4	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	38
5	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	13.4	ng	641090	1	6.92	957669	20.0
2-Pentanone, 4-hy...	5.14	4.5	ng	213485	1	6.92	957669	20.0
unknown6.69	6.69	48.5	ng	2321390	1	6.92	957669	20.0
Triethyl citrate	10.62	15.9	ng	902792	3	9.96	1134940	20.0