LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

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-BF032217.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	1.928	3	7	12	rBV	89618	104069	1.82%	0.223%
2	2.716	137	141	154	rBV	33299	65203	1.14%	0.140%
3	3.463	264	268	273	rBV	120031	128614	2.25%	0.276%
4	4.004	355	360	369	rBV	732032	1033070	18.10%	2.216%
5	4.398	421	427	430	rBV	4283862	4699973	82.36%	10.081%
6	5.463	602	608	613	rVB2	3739520	5342685	93.62%	11.460%
7	5.598	625	631	635	rBV	4064121	4971662	87.12%	10.664%
8	5.851	670	674	678	rBV	1166590	1001375	17.55%	2.148%
9	6.034	699	705	708	rBV	3734654	3885339	68.09%	8.334%
10	6.504	778	785	788	rBV	2717399	3257841	57.09%	6.988%
11	7.351	924	929	933	rBV	1409063	1387088	24.31%	2.975%
12	8.681	1148	1155	1158	rBV	4822646	5706484	100.00%	12.240%
13	9.175	1233	1239	1242	rBV	922177	891789	15.63%	1.913%
14	9.492	1286	1293	1297	rBV2	1500936	1566859	27.46%	3.361%
15	10.086	1389	1394	1398	rVB	63151	58459	1.02%	0.125%
16	10.469	1452	1459	1462	rBV	2661513	3248638	56.93%	6.968%
17	10.669	1485	1493	1496	rBV	87206	102731	1.80%	0.220%
18	11.227	1583	1588	1591	rBV	83616	81569	1.43%	0.175%
19	11.316	1598	1603	1607	rBV	1498997	1489843	26.11%	3.196%
20	11.751	1672	1677	1684	rVB	72592	77038	1.35%	0.165%
21	13.298	1933	1940	1944	rBV	3711271	4957092	86.87%	10.633%
22	14.457	2131	2137	2149	rBV	248833	415911	7.29%	0.892%
23	14.562	2150	2155	2160	rVV	1123644	1139509	19.97%	2.444%
24	14.621	2160	2165	2169	rVB	87312	100384	1.76%	0.215%
25	16.192	2426	2432	2444	rBV	738244	846433	14.83%	1.816%
26	17.162	2593	2597	2605	rVB3	34827	62181	1.09%	0.133%

Sum of corrected areas: 46621839

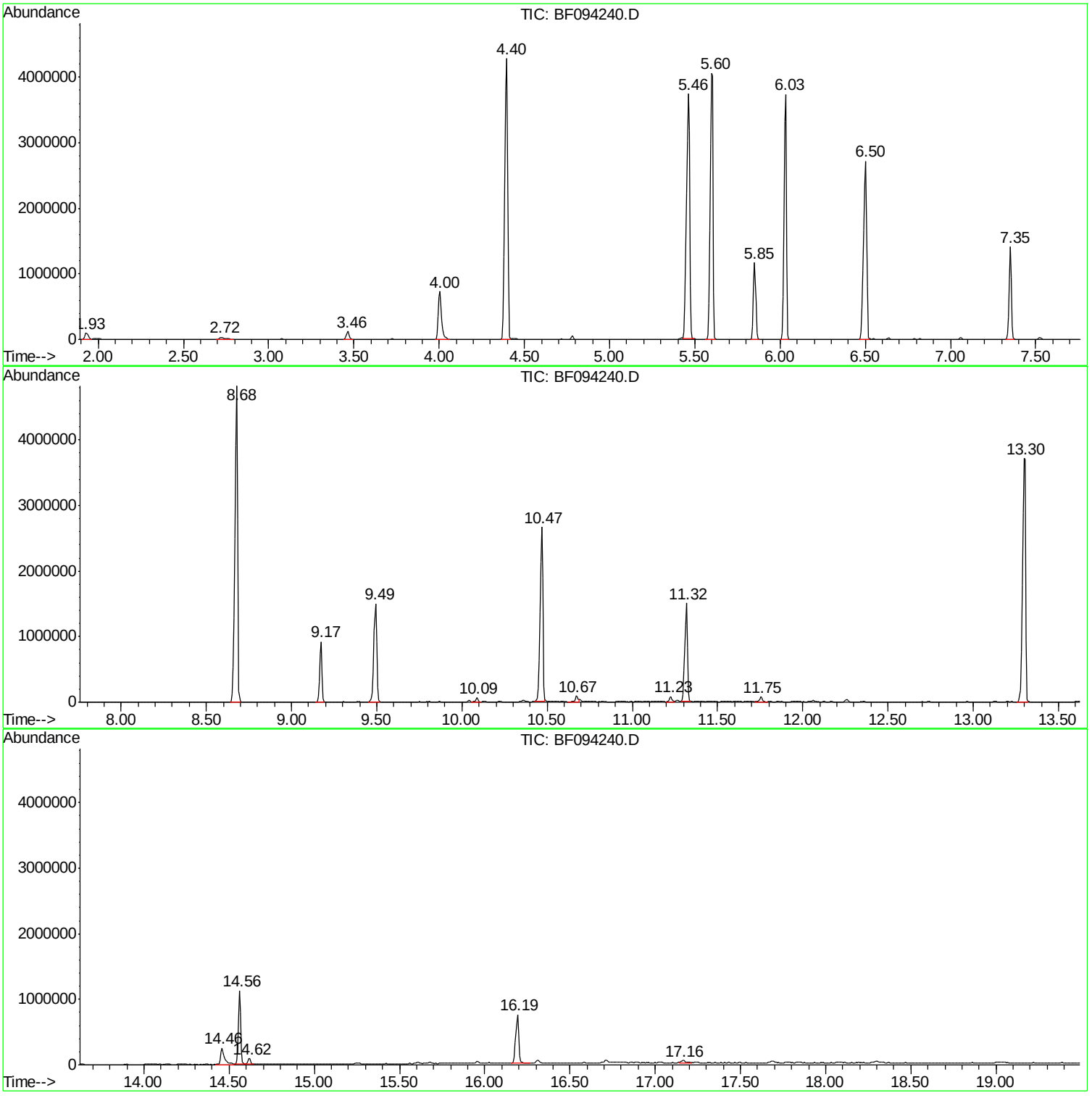
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

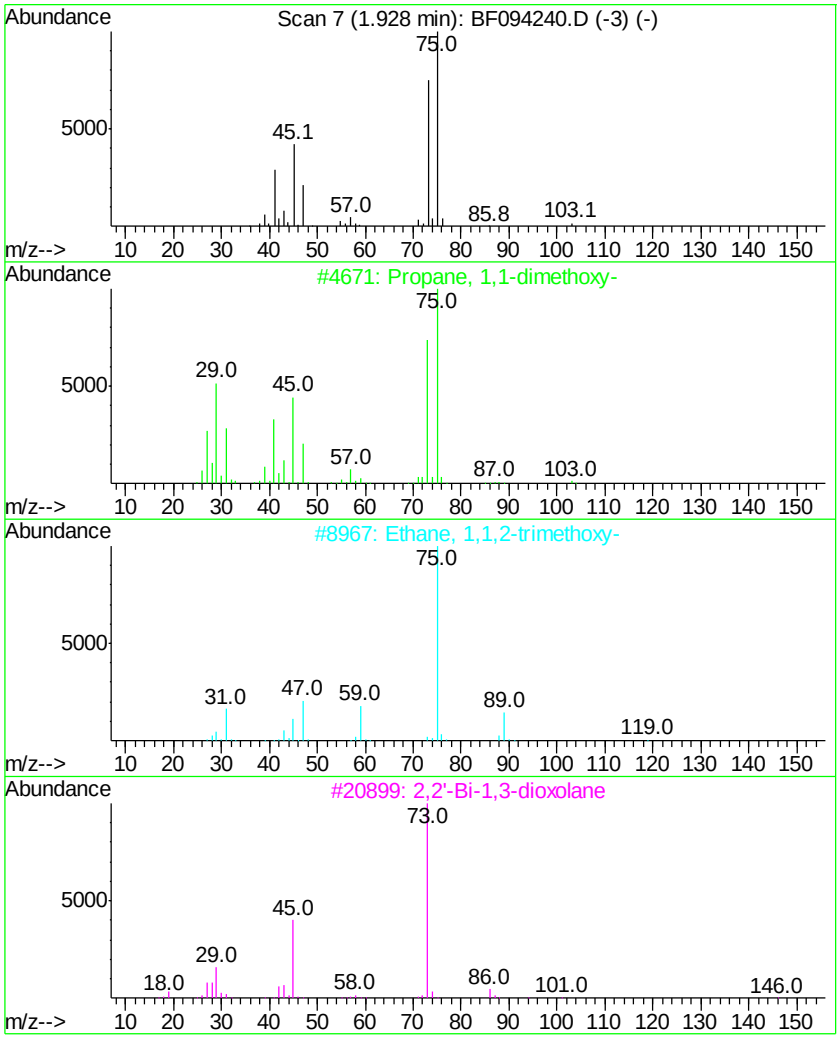
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

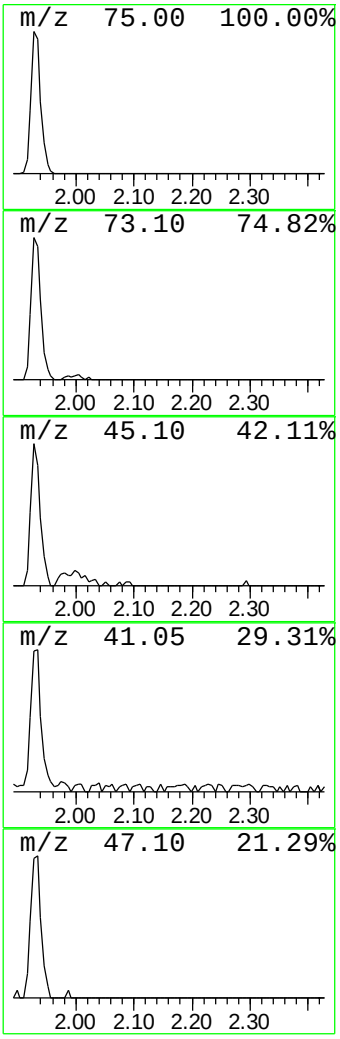
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.93	2.08 ng	104069	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
3	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

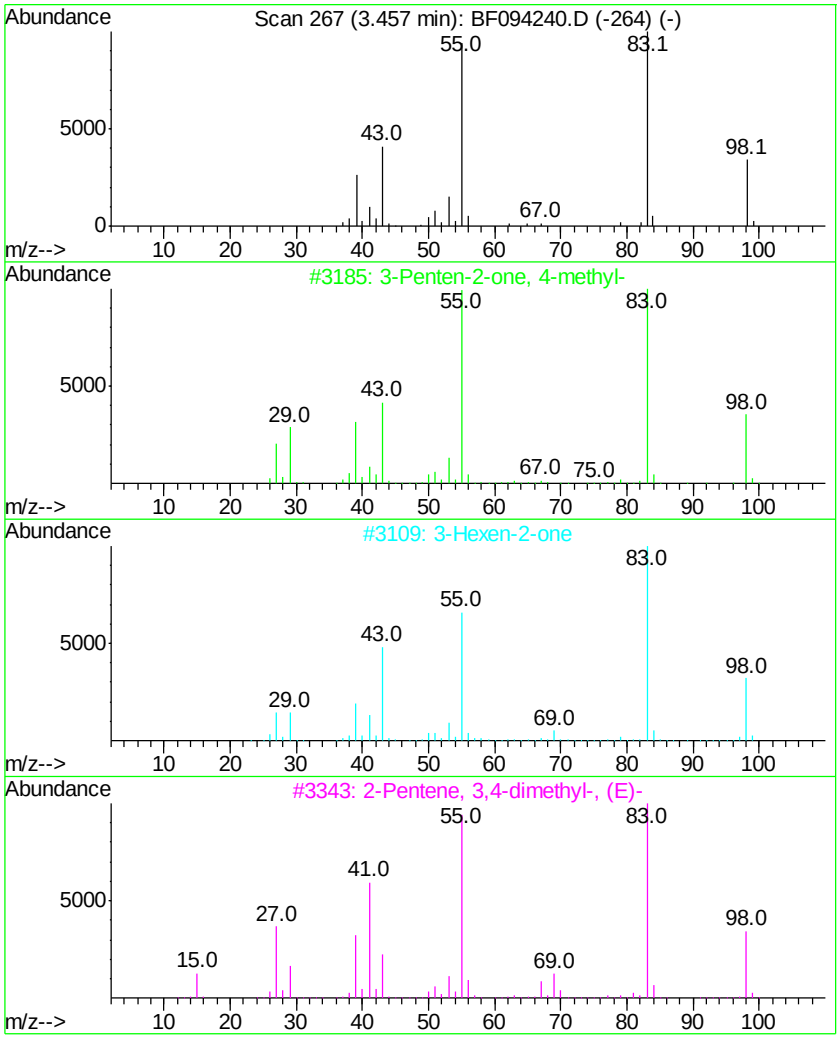
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

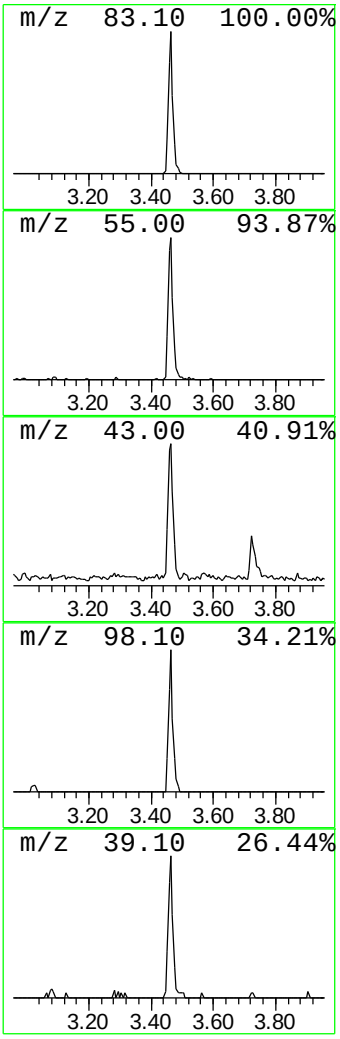
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	2.57 ng	128614	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	83
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

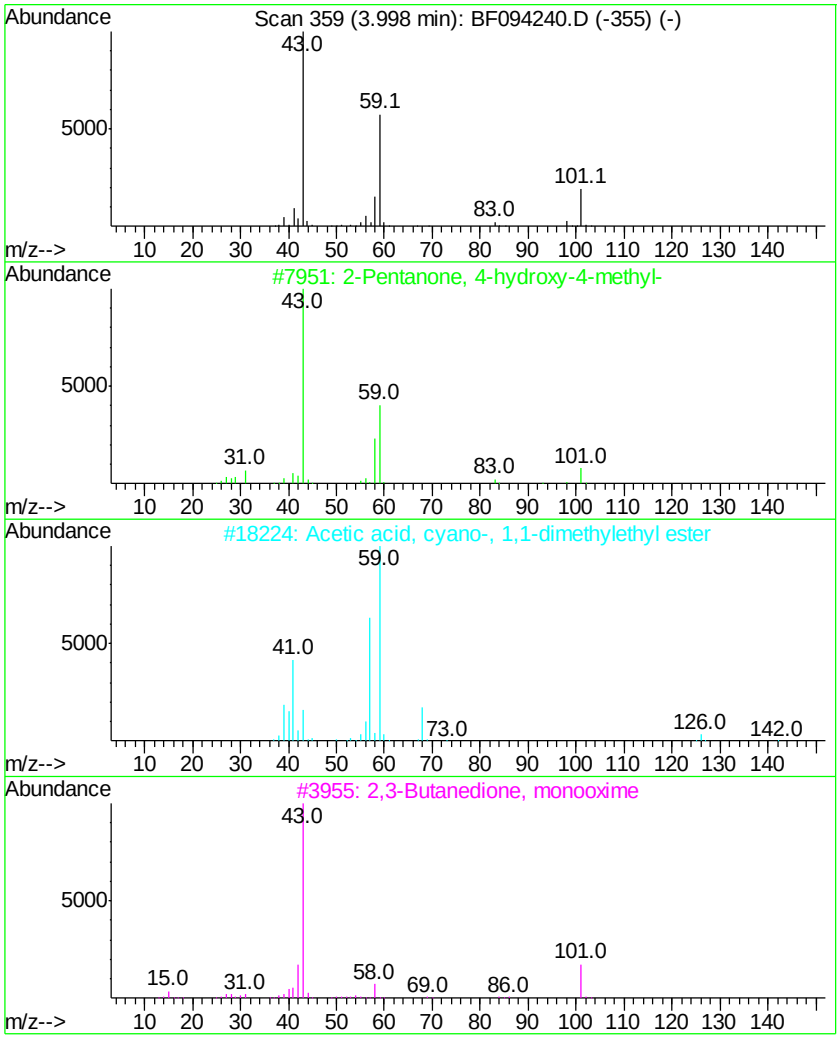
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

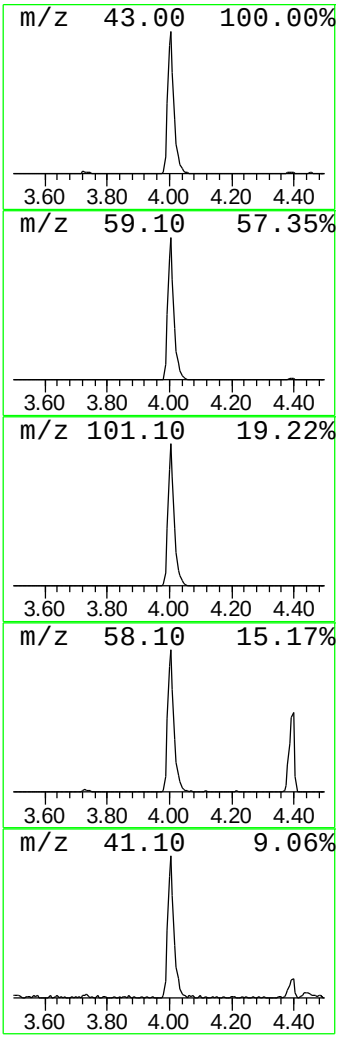
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	20.63 ng	1033070	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

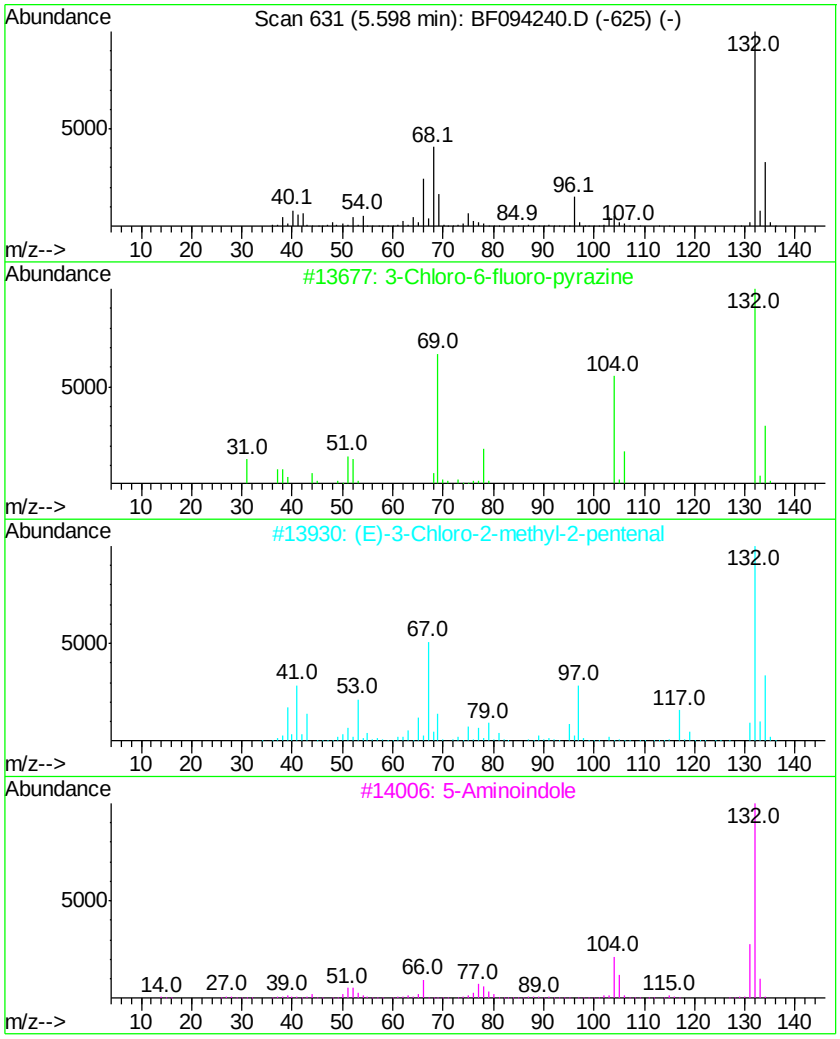
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

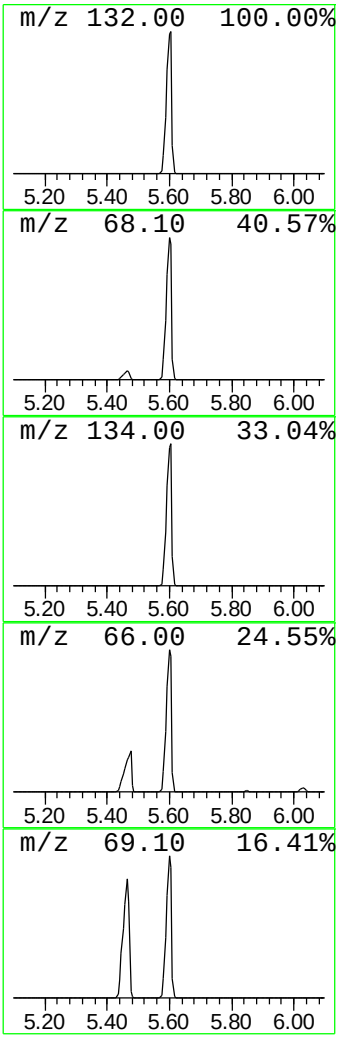
****

Peak Number 4 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	99.30 ng	4971660	1,4-Dichlorobenzene-d4	5.85

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-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

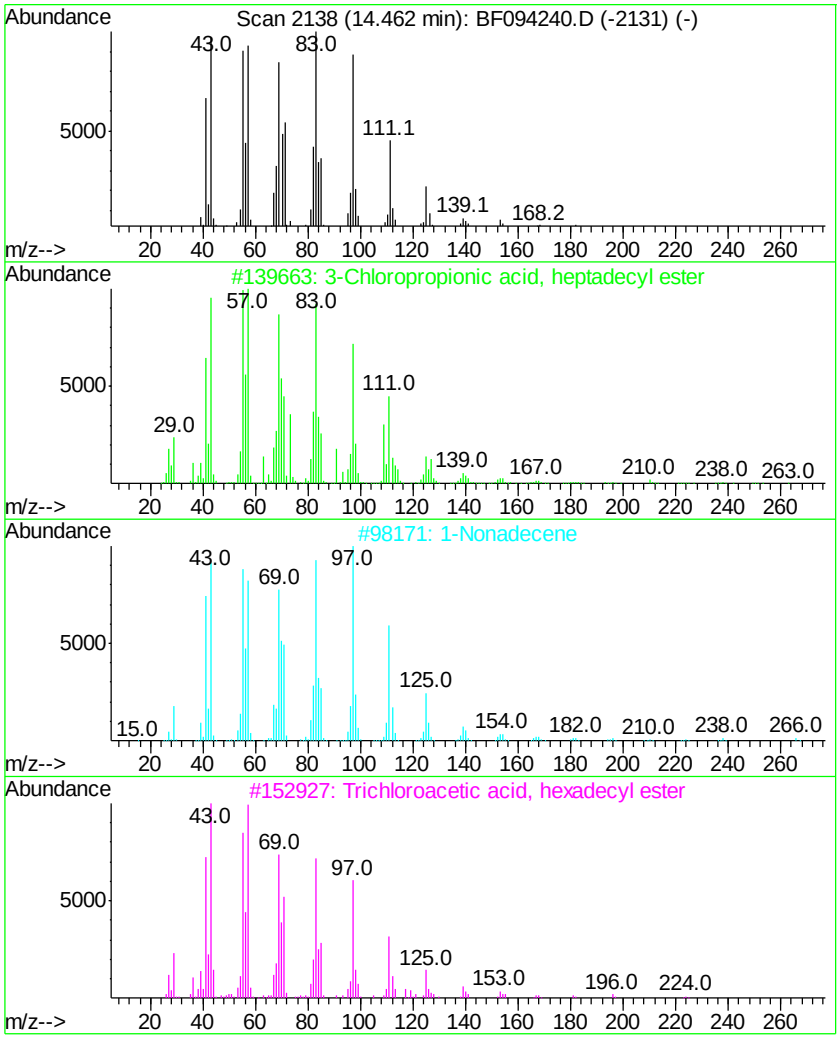
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

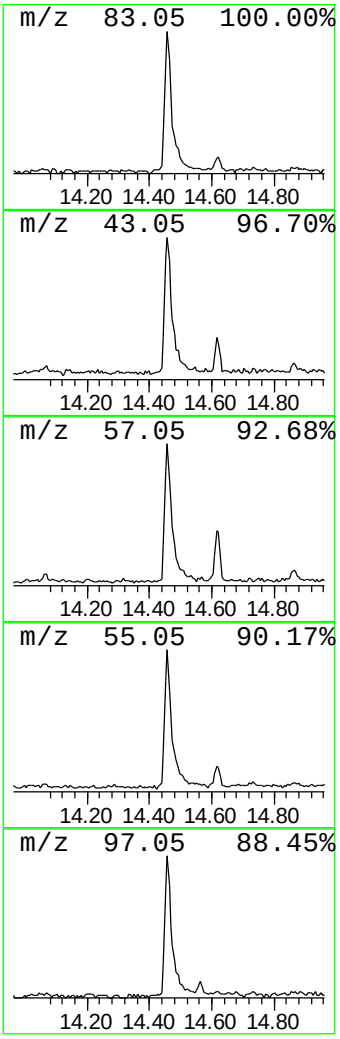
****

Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	7.30 ng	415911	Chrysene-d12	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	1-Docosene	308	C22H44	001599-67-3	76
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094240.D
Acq On : 6 Apr 2017 20:46
Operator : SJ/MA
Sample : I2534-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-B-01(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.93	2.1	ng	104069	1	5.85	1001380	20.0
3-Penten-2-one, 4...	3.46	2.6	ng	128614	1	5.85	1001380	20.0
2-Pentanone, 4-hy...	4.00	20.6	ng	1033070	1	5.85	1001380	20.0
unknown5.60	5.60	99.3	ng	4971660	1	5.85	1001380	20.0
3-Chloropropionic...	14.46	7.3	ng	415911	5	14.56	1139510	20.0