LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

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-BF030717.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	2.470	48	51	62	rVB	67187	198390	3.15%	0.377%
2	4.184	197	201	218	rBV	502356	1214397	19.26%	2.306%
3	4.413	218	221	228	rVB	57817	123886	1.96%	0.235%
4	4.881	259	262	284	rBV	1248300	2710155	42.97%	5.147%
5	5.156	284	286	293	rVB	60664	95368	1.51%	0.181%
6	5.316	298	300	329	rBV	3938420	6306649	100.00%	11.978%
7	5.716	334	335	347	rVB	51204	122036	1.94%	0.232%
8	6.367	390	392	400	rBV	3345350	5528918	87.67%	10.501%
9	6.481	400	402	405	rVB	4956225	5133668	81.40%	9.750%
10	6.710	420	422	430	rVB	998792	1097700	17.41%	2.085%
11	6.859	433	435	438	rBV	4033589	4146912	65.75%	7.876%
12	7.282	470	472	487	rBV	3186830	3875130	61.45%	7.360%
13	8.002	532	535	547	rVB	1138306	1559213	24.72%	2.961%
14	9.076	626	629	632	rBV	4716884	5829958	92.44%	11.072%
15	9.750	686	688	691	rBV	1299824	1652230	26.20%	3.138%
16	10.550	756	758	761	rBV	2539941	3221293	51.08%	6.118%
17	11.248	816	819	824	rBV	1657643	1704465	27.03%	3.237%
18	12.653	940	942	944	rBV	210662	179734	2.85%	0.341%
19	12.836	955	958	960	rBV	4837815	5319151	84.34%	10.102%
20	13.351	1001	1003	1006	rBV2	88851	116601	1.85%	0.221%
21	13.888	1048	1050	1059	rVB	1048338	1476488	23.41%	2.804%
22	15.305	1171	1174	1185	rBV	614471	1040637	16.50%	1.976%

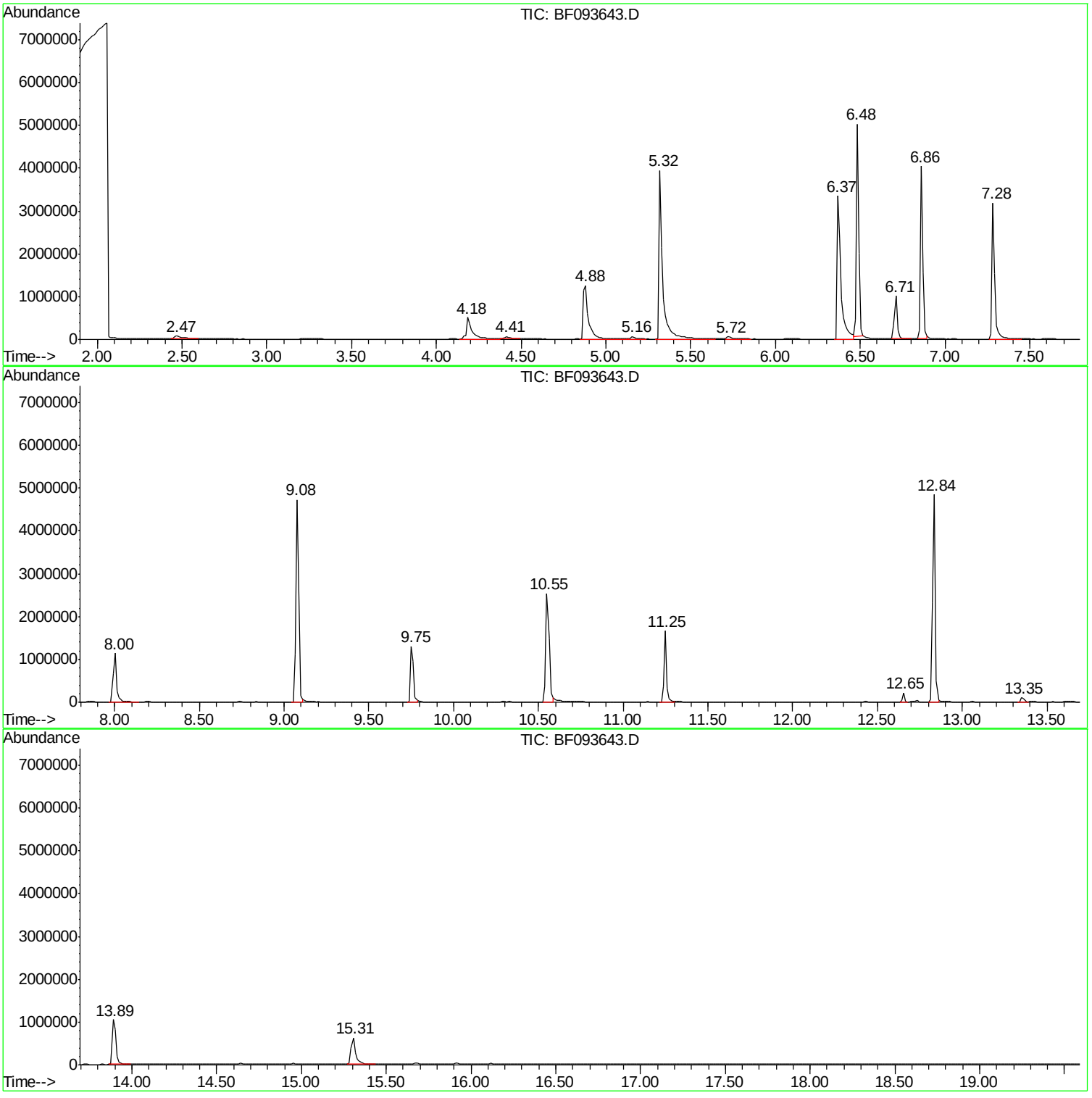
Sum of corrected areas: 52652979

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

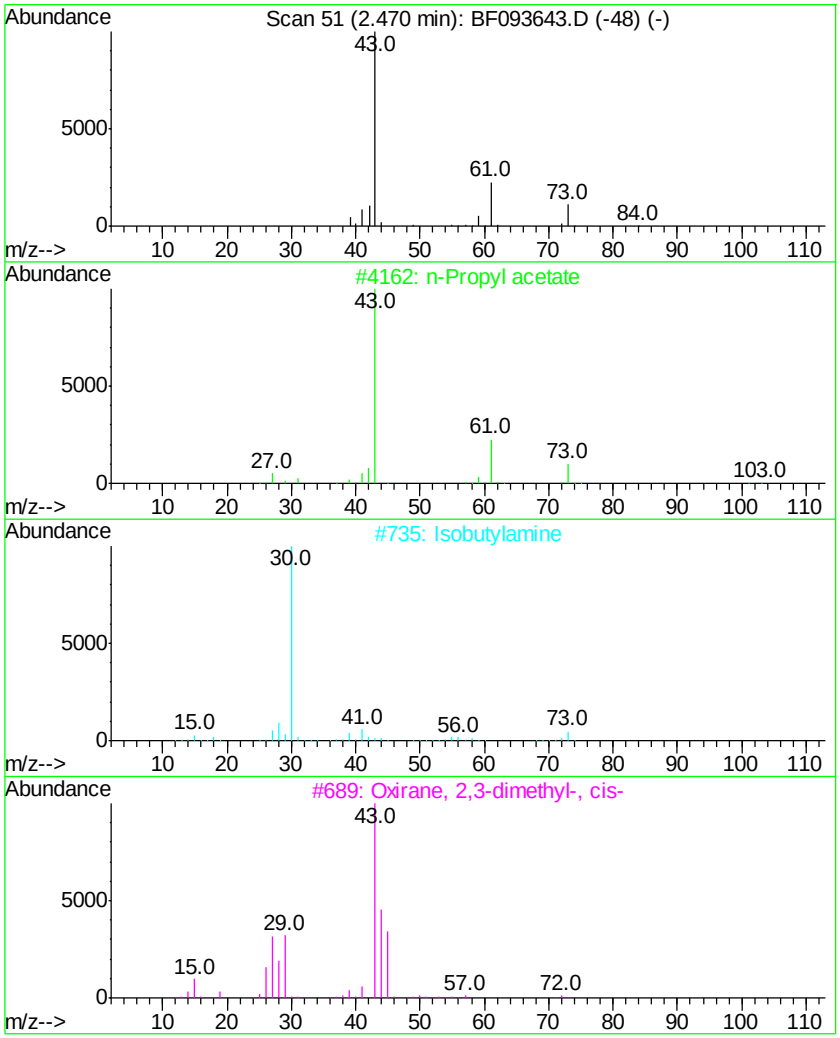
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

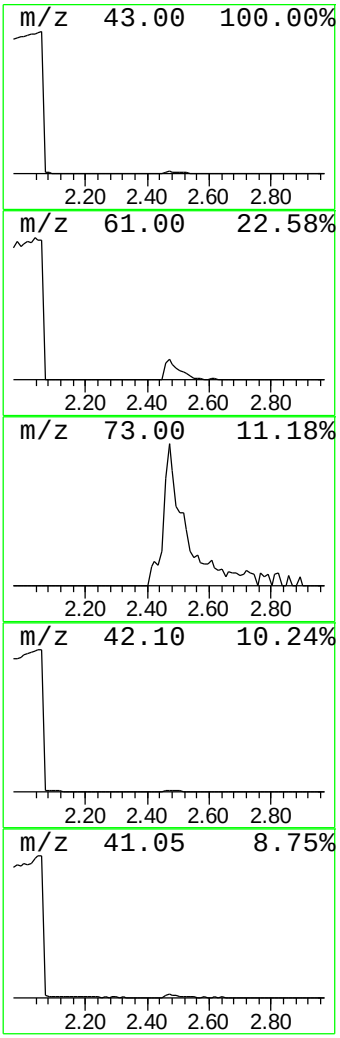
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.47	3.61 ng	198390	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isobutylamine	73	C4H11N	000078-81-9	7
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	1-Butanamine	73	C4H11N	000109-73-9	5
5	Pentane	72	C5H12	000109-66-0	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

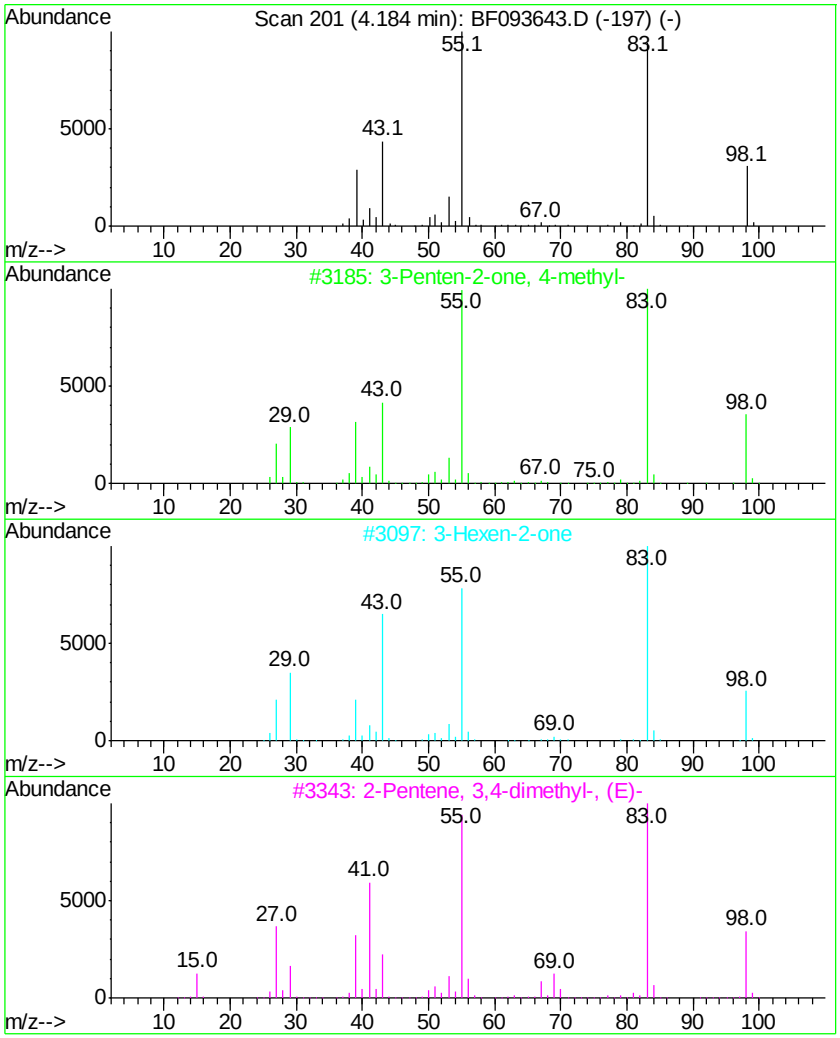
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

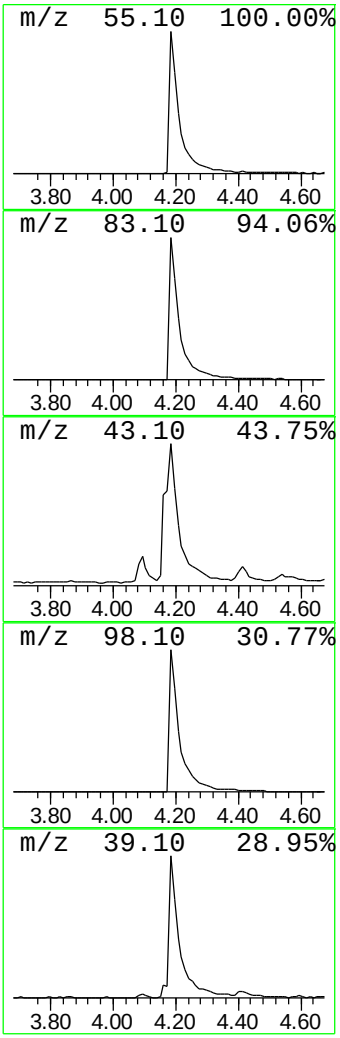
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	22.13 ng	1214400	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

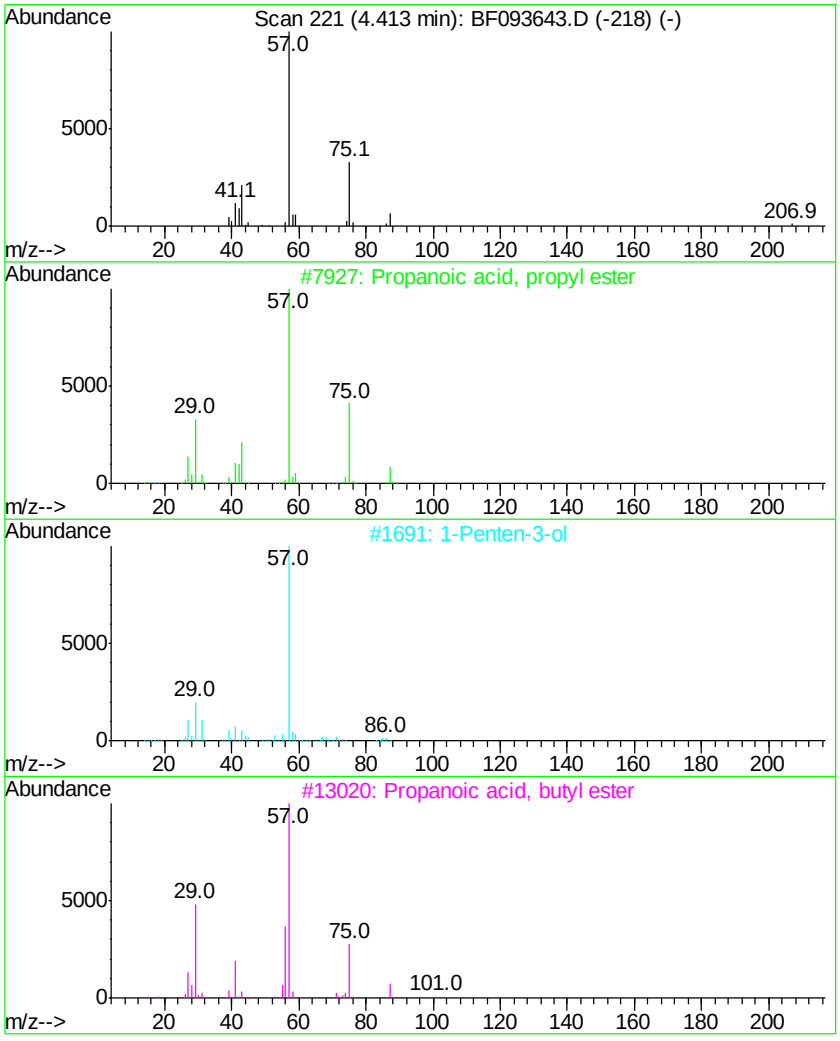
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

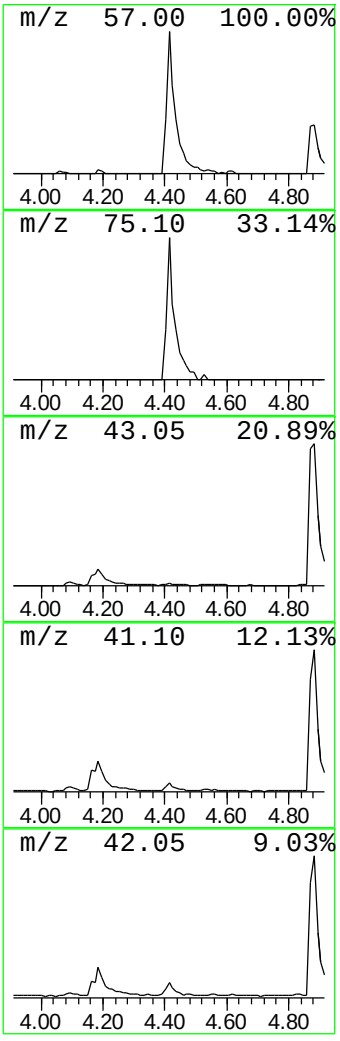
****

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.26 ng	123886	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	1-Penten-3-ol	86	C5H10O	000616-25-1	9
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
4	Propionic acid, 4-hydroxy-3-hexy...	174	C9H18O3	1000151-16-9	9
5	Azetidine	57	C3H7N	000503-29-7	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

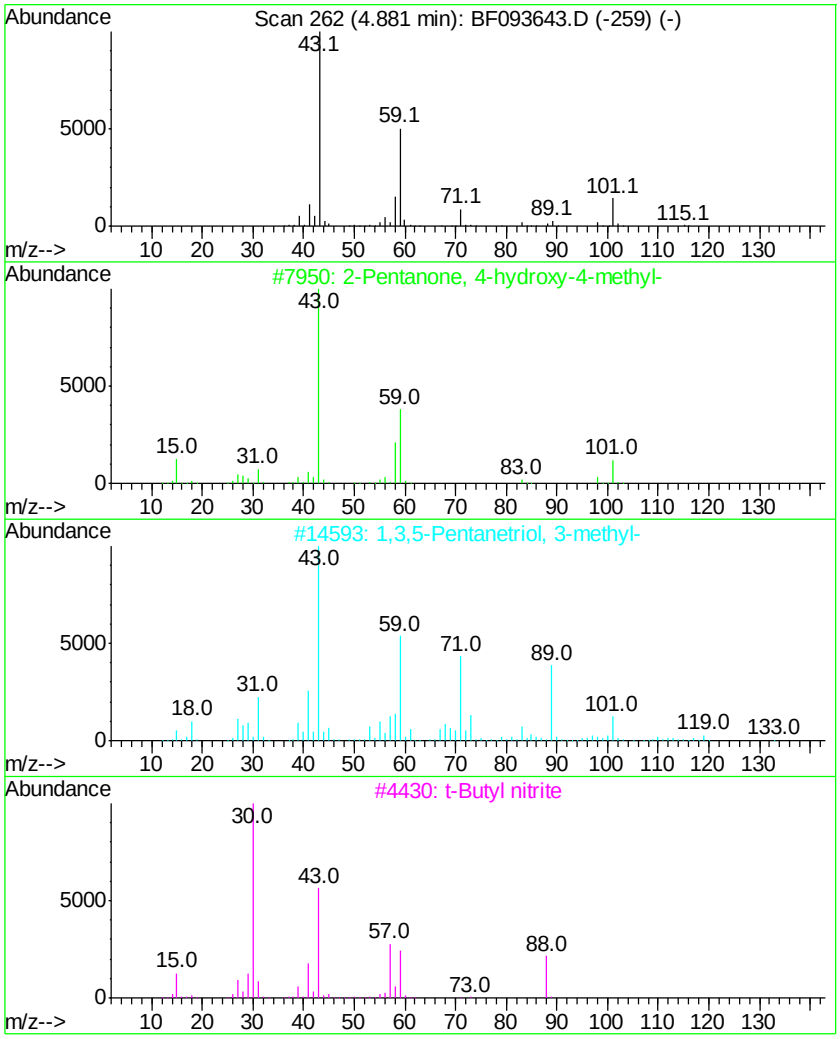
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

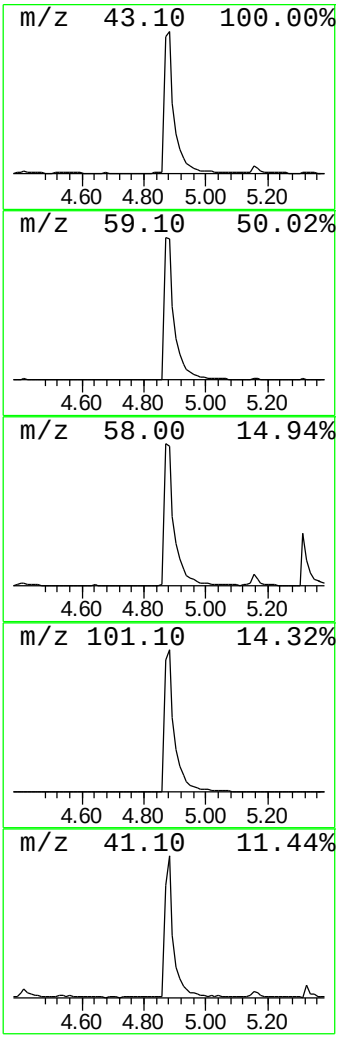
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	49.38 ng	2710160	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	40
3	t-Butyl nitrite	103	C4H9NO2	000540-80-7	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

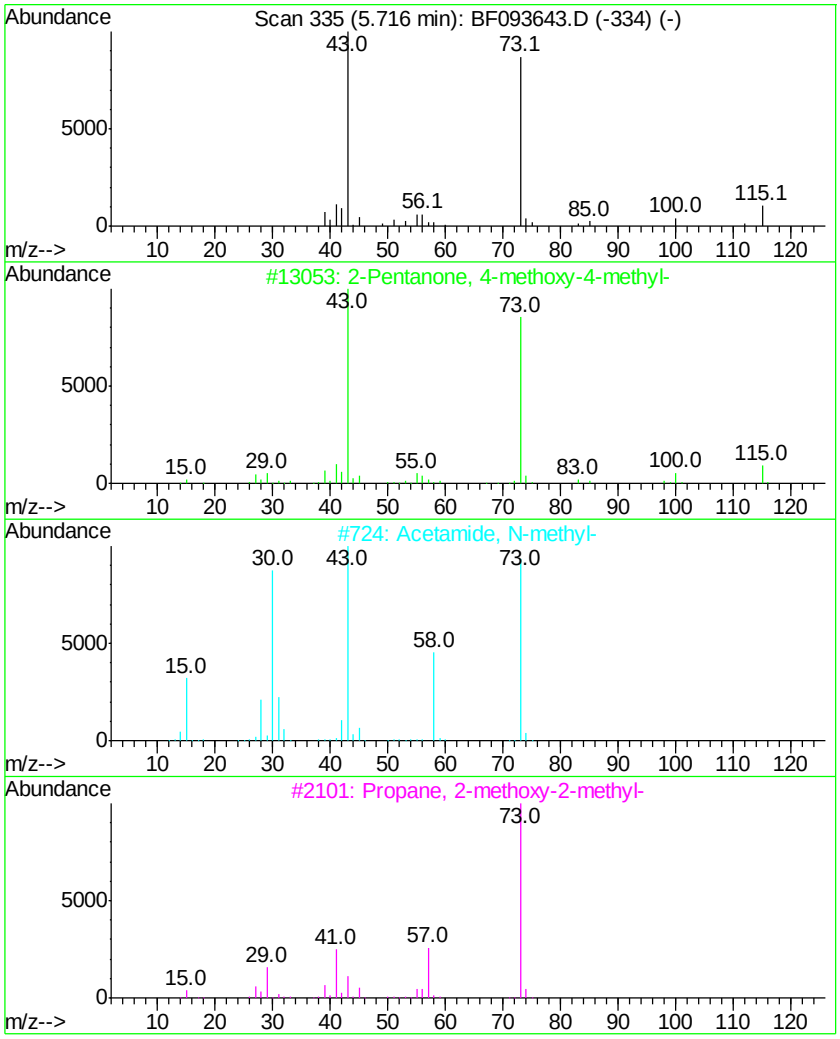
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

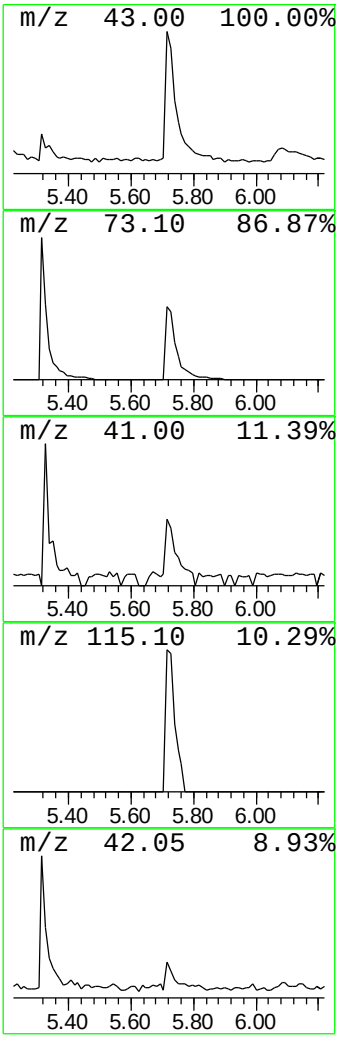
****

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.22 ng	122036	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

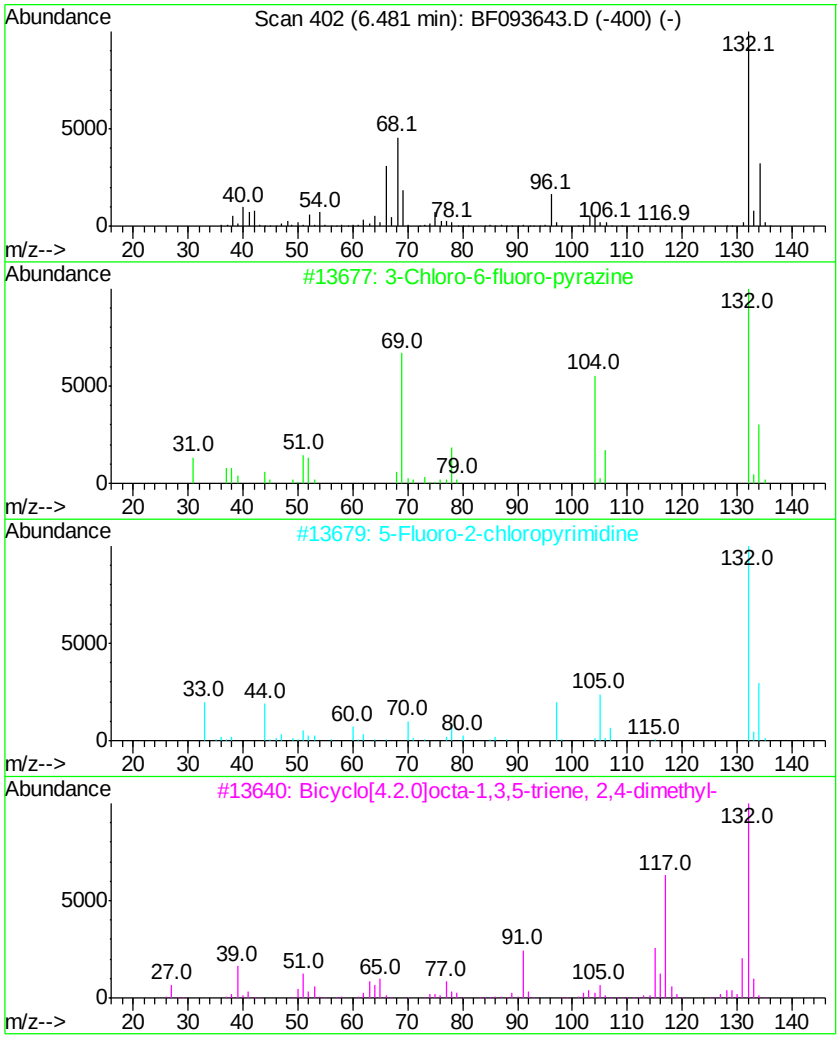
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

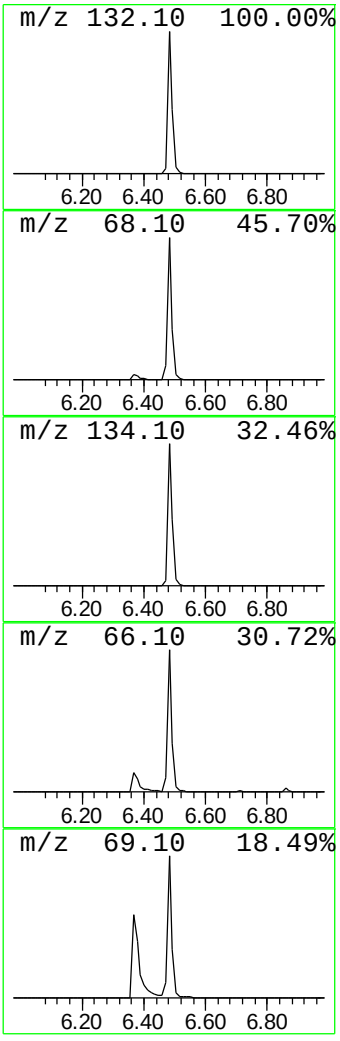
****

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	93.54 ng	5133670	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

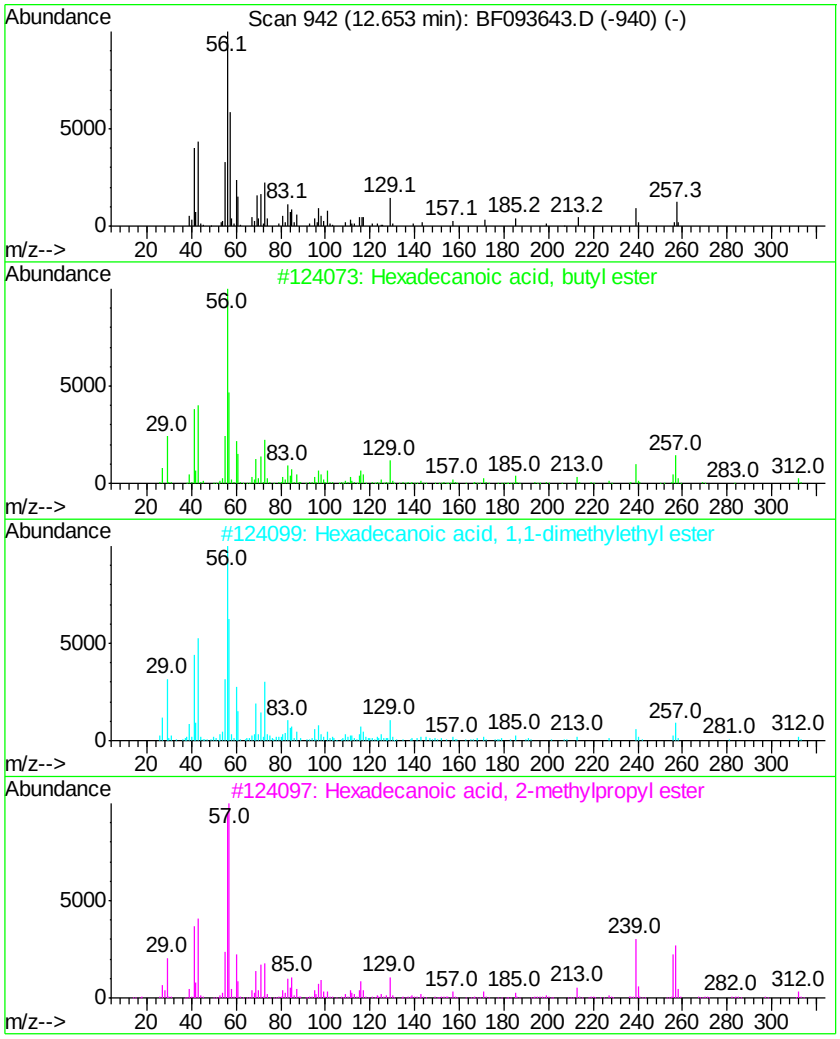
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

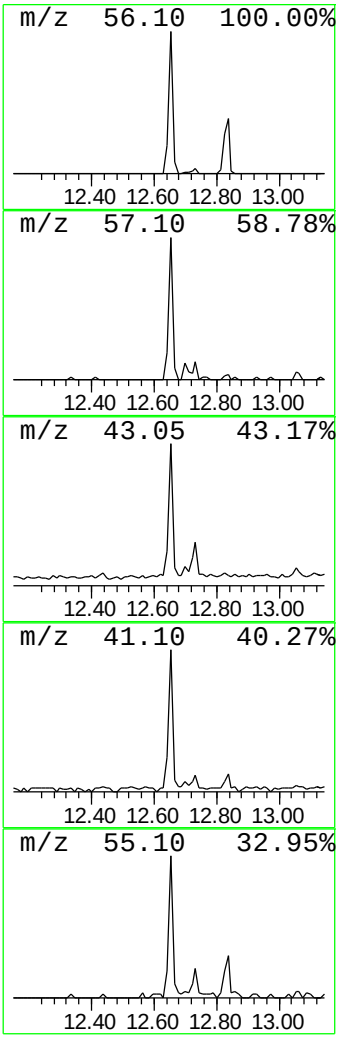
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.43 ng	179734	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093643.D
Acq On : 14 Mar 2017 8:02
Operator : SJ/MA
Sample : I2201-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-119

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
n-Propyl acetate	2.47	3.6	ng	198390	1	6.71	1097700	20.0
3-Penten-2-one, 4...	4.18	22.1	ng	1214400	1	6.71	1097700	20.0
Propanoic acid, p...	4.41	2.3	ng	123886	1	6.71	1097700	20.0
2-Pentanone, 4-hy...	4.88	49.4	ng	2710160	1	6.71	1097700	20.0
2-Pentanone, 4-me...	5.72	2.2	ng	122036	1	6.71	1097700	20.0
unknown6.48	6.48	93.5	ng	5133670	1	6.71	1097700	20.0
Hexadecanoic acid...	12.65	2.4	ng	179734	5	13.89	1476490	20.0