LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-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_M\METHODS\8270-BM051917.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	5.075	334	338	349	rBV	87319	132810	1.09%	0.253%
2	5.263	364	370	377	rBV	147095	225123	1.84%	0.429%
3	5.534	409	416	424	rBV	1390664	2036992	16.64%	3.882%
4	7.140	683	689	702	rBV	778808	1265586	10.34%	2.412%
5	7.498	743	750	763	rBV	2441774	3839387	31.37%	7.317%
6	7.957	820	828	840	rBV	540993	945427	7.72%	1.802%
7	8.275	871	882	895	rVB	2149933	3568191	29.16%	6.800%
8	9.034	1004	1011	1020	rBV3	64645	125668	1.03%	0.239%
9	9.145	1020	1030	1039	rBV	1627844	2717339	22.20%	5.178%
10	9.469	1077	1085	1092	rBV2	191652	327375	2.67%	0.624%
11	10.763	1299	1305	1313	rVB	659100	1103074	9.01%	2.102%
12	13.210	1708	1721	1729	rBV	4989646	6796084	55.53%	12.951%
13	14.045	1859	1863	1873	rBV	92290	149307	1.22%	0.285%
14	14.586	1949	1955	1962	rBV2	964169	1500060	12.26%	2.859%
15	16.080	2202	2209	2222	rBV	4103586	6061568	49.53%	11.551%
16	16.298	2242	2246	2259	rVB	131290	229243	1.87%	0.437%
17	16.615	2295	2300	2308	rBV2	158041	280551	2.29%	0.535%
18	17.333	2416	2422	2433	rVB	1410842	2022752	16.53%	3.855%
19	18.180	2562	2566	2574	rBV3	145254	228612	1.87%	0.436%
20	19.451	2779	2782	2791	rVB4	111414	158853	1.30%	0.303%
21	19.715	2823	2827	2830	rBV	138406	174266	1.42%	0.332%
22	19.933	2859	2864	2870	rBV	10197689	12238597	100.00%	23.323%
23	21.492	3124	3129	3136	rVB	2379398	3034236	24.79%	5.782%
24	23.856	3525	3531	3541	rVB	1630878	3314355	27.08%	6.316%

Sum of corrected areas: 52475456

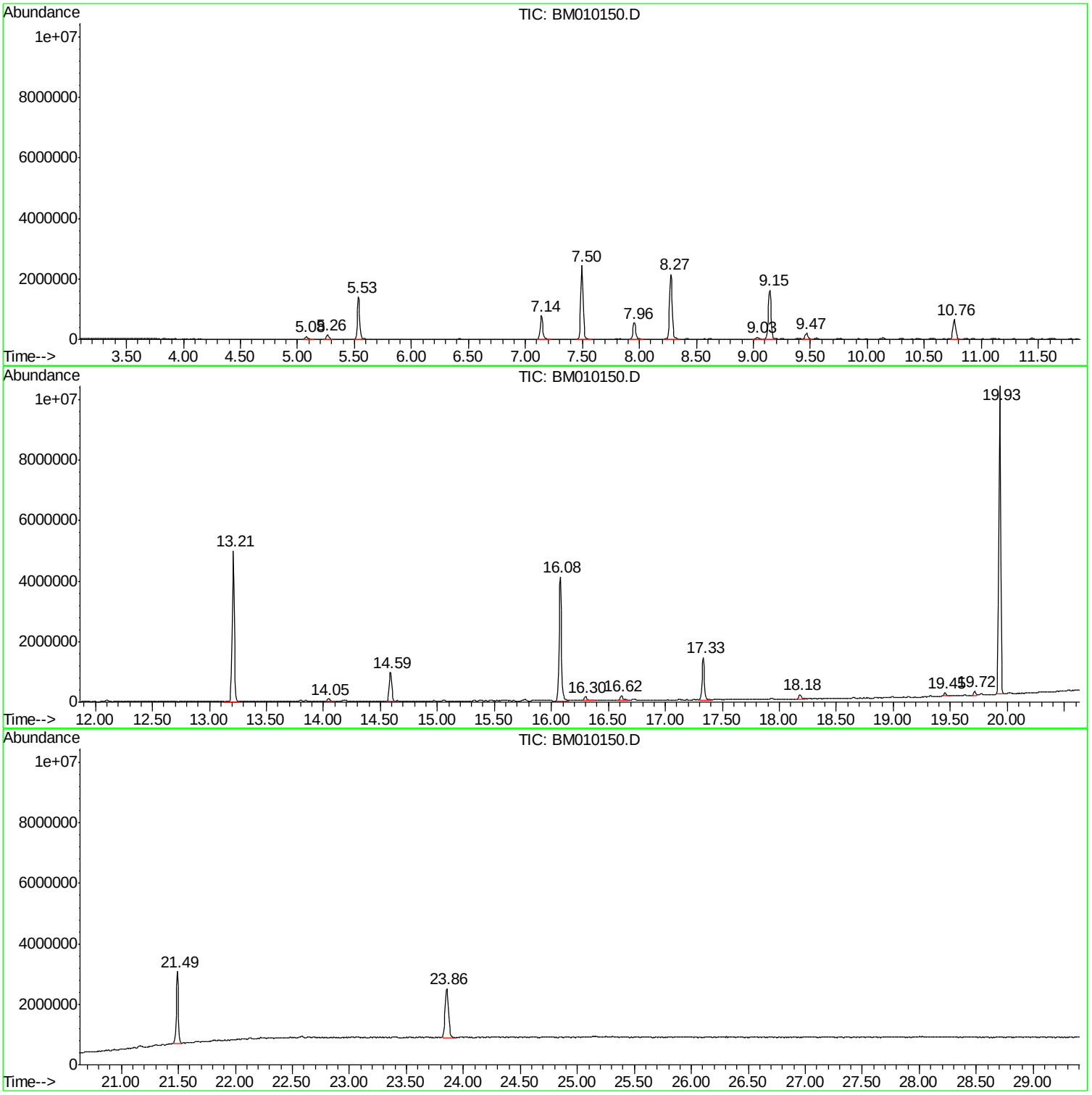
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.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_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

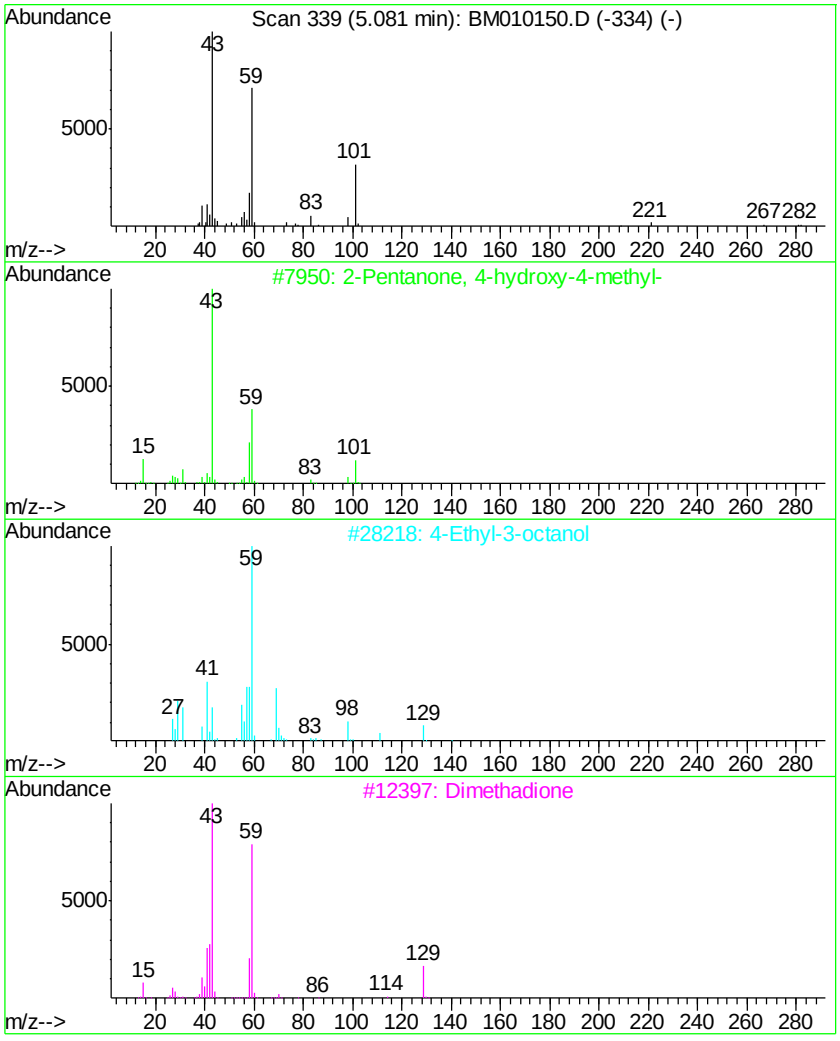
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

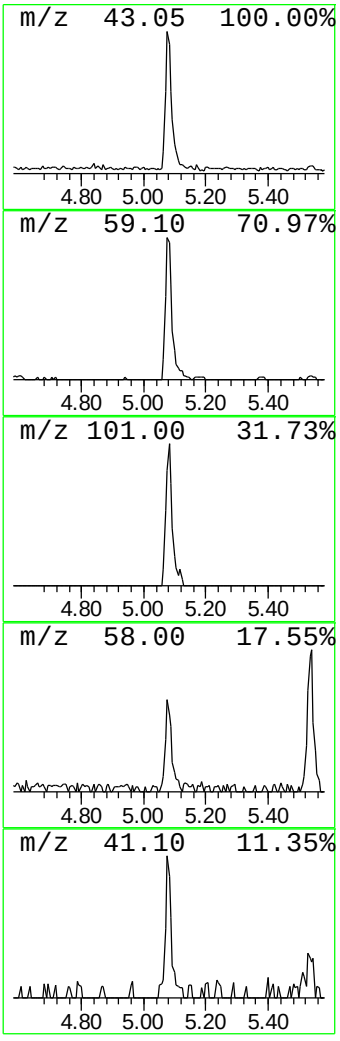
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.81 ng	132810	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	37
3	Dimethadione	129	C5H7NO3	000695-53-4	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	32
5	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	23





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

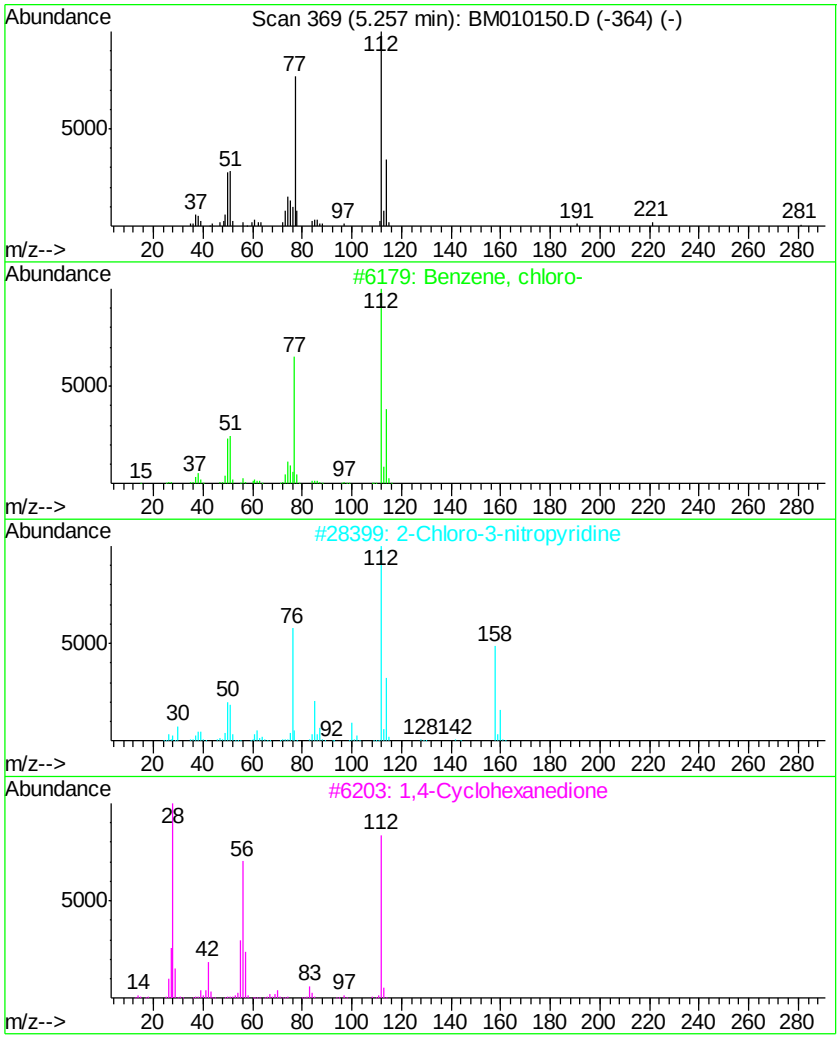
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

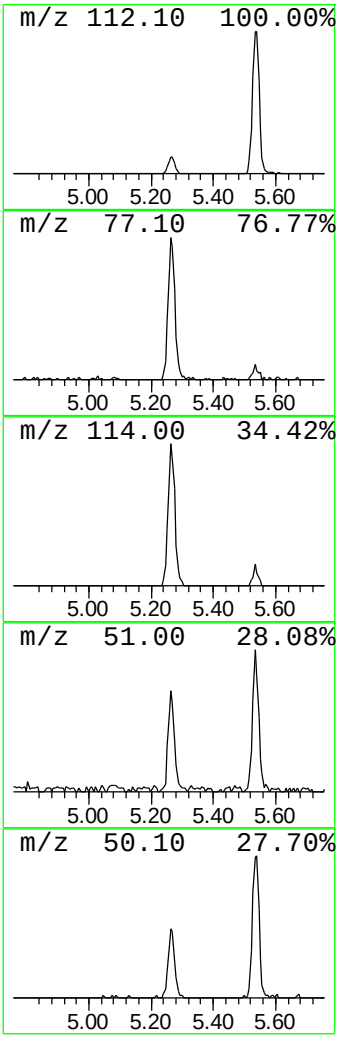
****

Peak Number 2 Benzene, chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	4.76 ng	225123	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	95
2	2-Chloro-3-nitropyridine	158	C5H3ClN2O2	005470-18-8	42
3	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	27
4	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	27
5	2-Benzoylamino-1-cyclohexylamino...	322	C21H26N2O	1000216-06-9	25





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

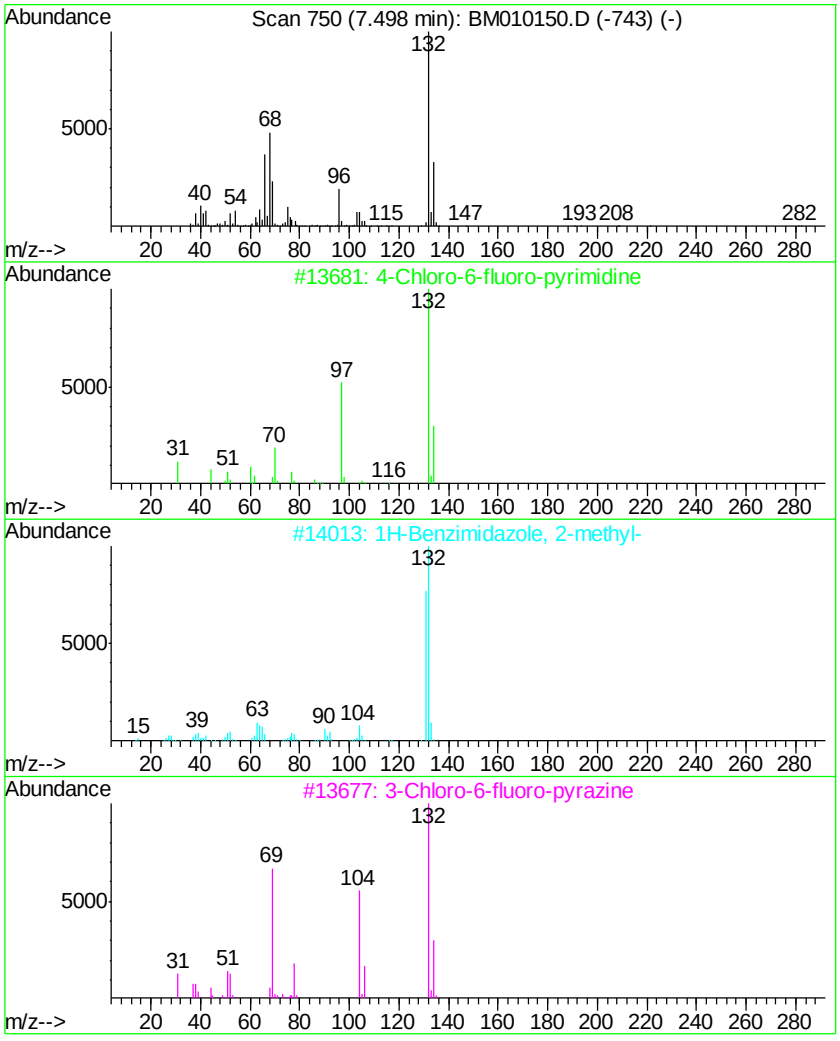
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

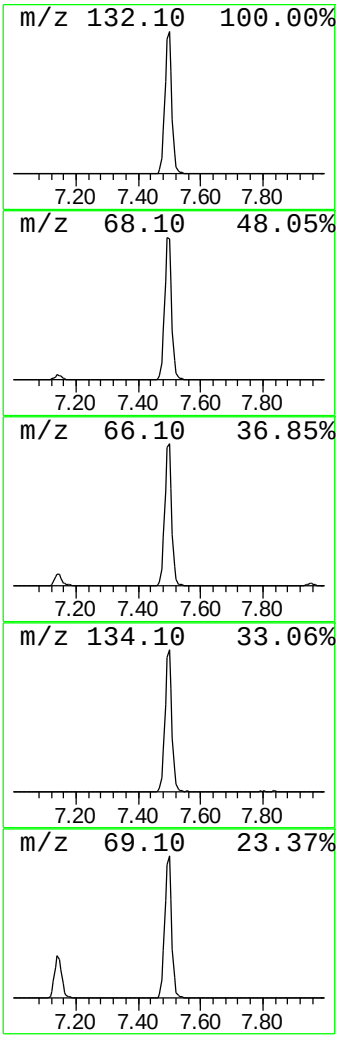
****

Peak Number 3 4-Chloro-6-fluoro-pyrimidine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	81.22 ng	3839390	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

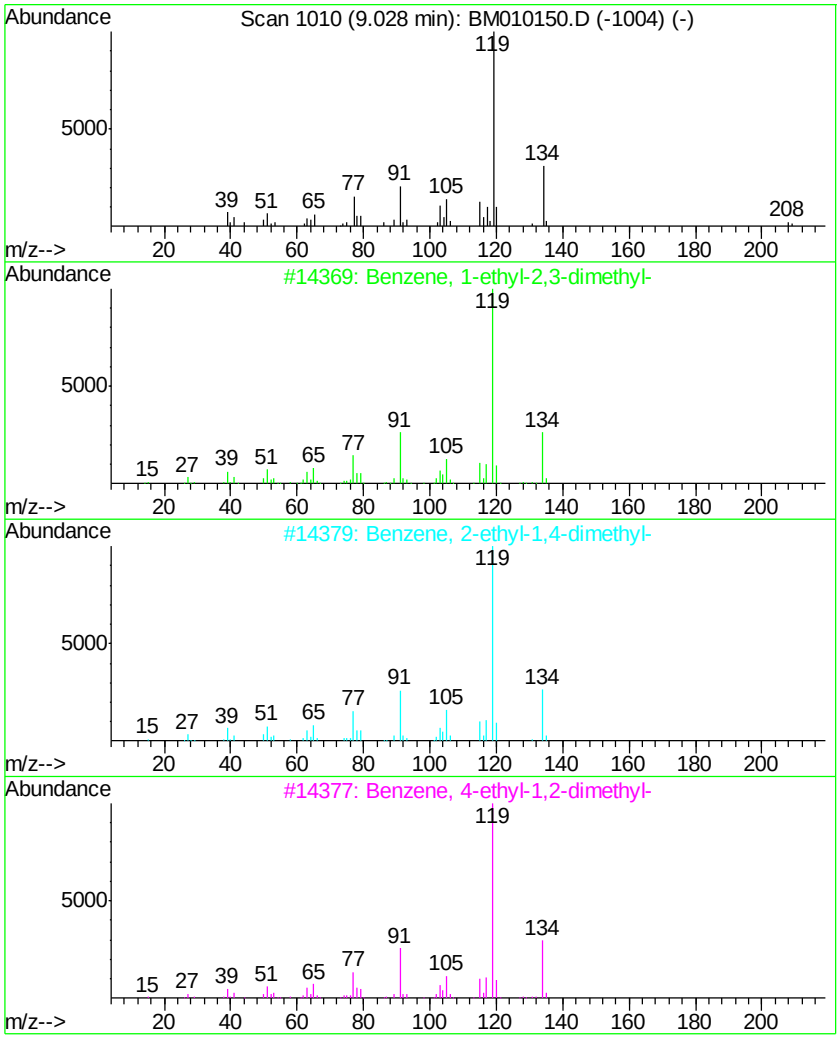
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

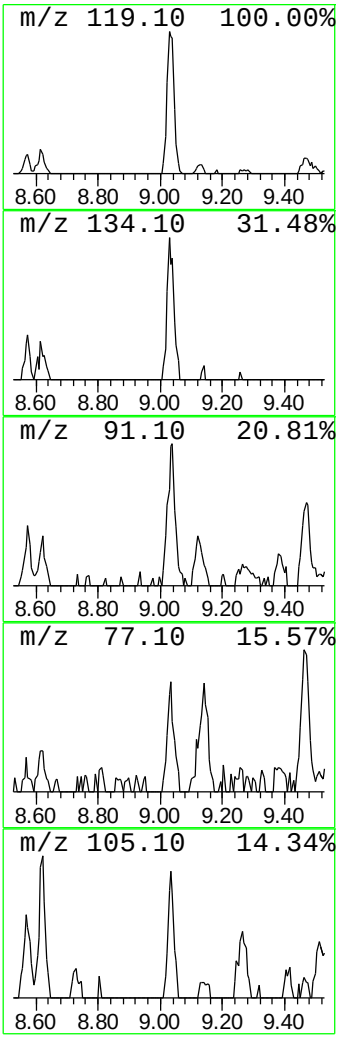
****

Peak Number 5 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	2.66 ng	125668	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90
4	Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	90
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

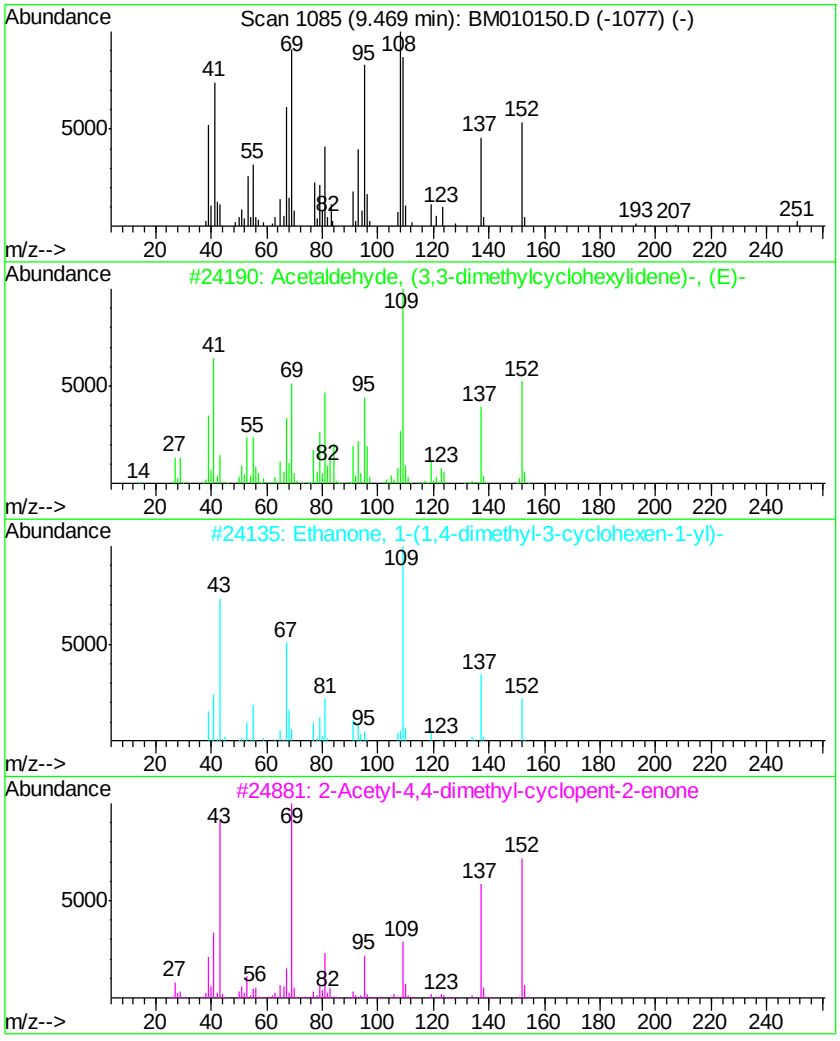
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

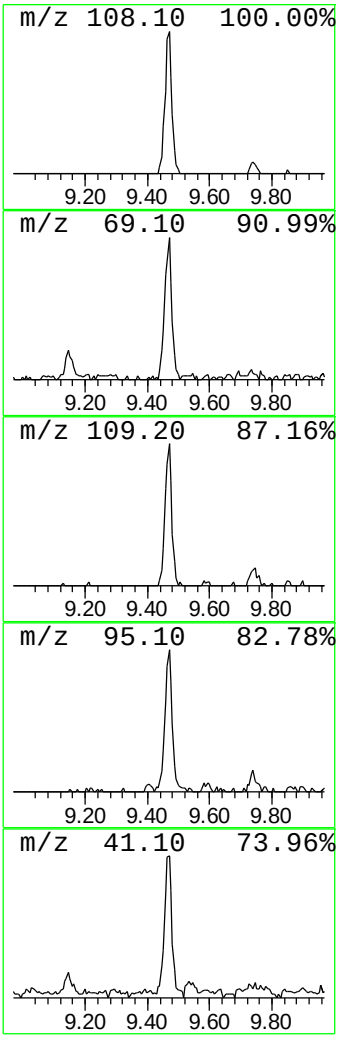
****

Peak Number 6 Acetaldehyde, (3,3-dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	5.94 ng	327375	Naphthalene-d8	10.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	60
2	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	38
3	2-Acetyl-4,4-dimethyl-cyclopent-...	152	C9H12O2	081979-96-6	30
4	3-t-Butyl-6-methyl-2H-pyran	152	C10H16O	1000188-12-8	22
5	3-Cyclopentene-1-acetaldehyde, 2...	152	C10H16O	004501-58-0	22





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

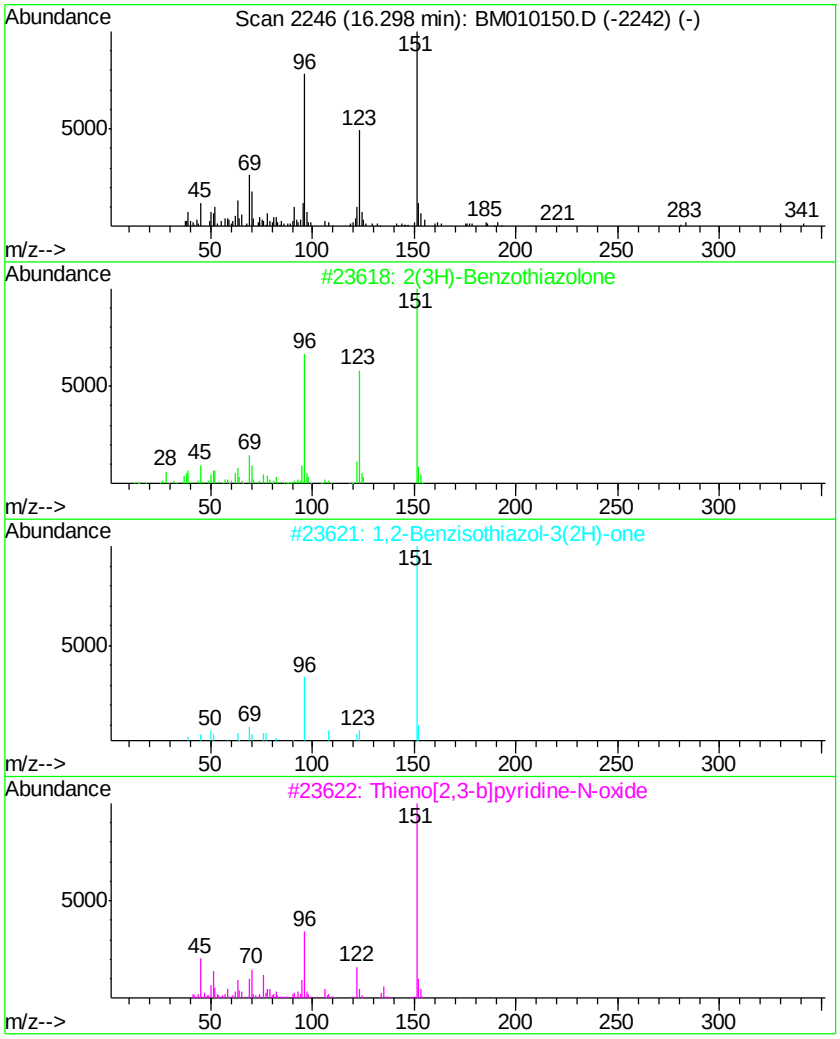
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

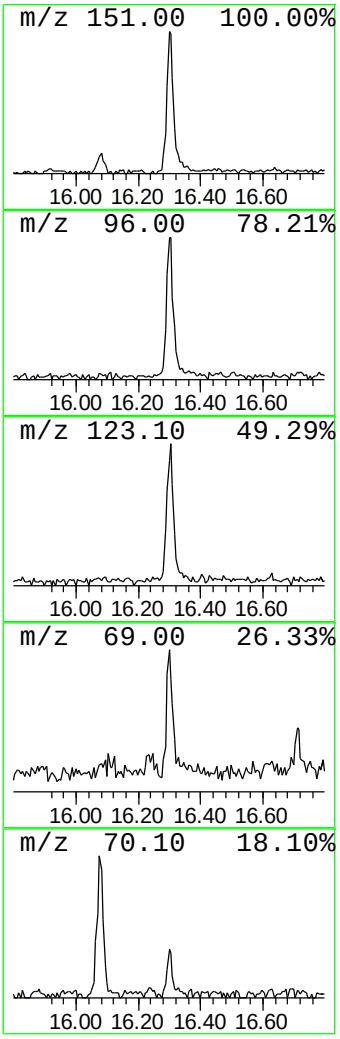
****

Peak Number 7 2(3H)-Benzothiazolone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	2.27 ng	229243	Phenanthrene-d10	17.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	68
3	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	45
4	Silane, (3,3-dimethylbut-2-yloxy...	208	C12H20OSi	1000163-31-6	43
5	Quinuclidine-3-carbonitrile, 3-a...	194	C10H14N2O2	099169-94-5	38





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

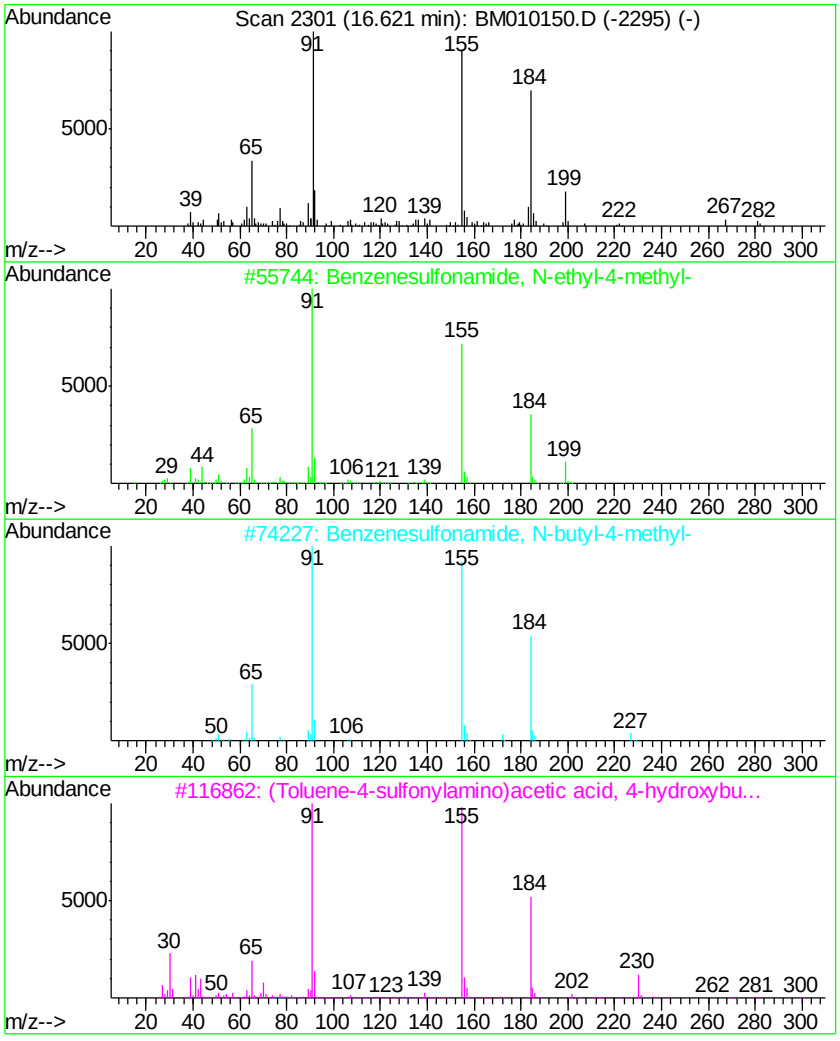
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

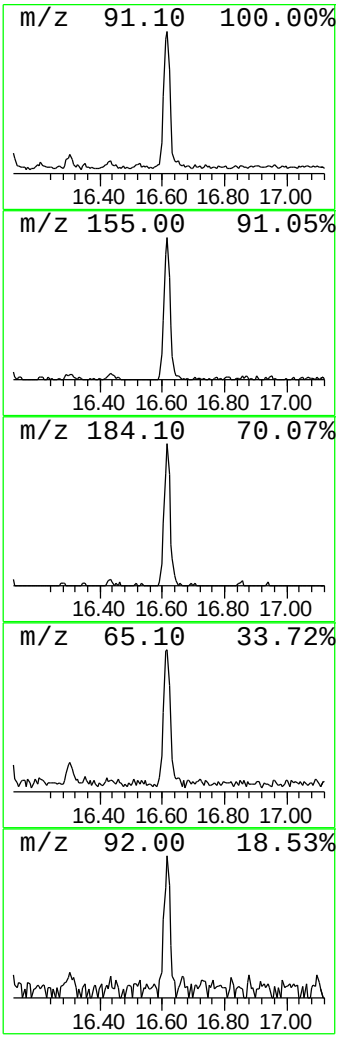
****

Peak Number 8 Benzenesulfonamide, N-ethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	2.77 ng	280551	Phenanthrene-d10	17.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	95
2	Benzenesulfonamide, N-butyl-4-me...	227	C11H17NO2S	001907-65-9	86
3	(Toluene-4-sulfonylamino)acetic ...	299	C13H17NO5S	1000191-28-9	80
4	Glycine, N-[(4-methylphenyl)sulf...	229	C9H11NO4S	001080-44-0	72
5	Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	58





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

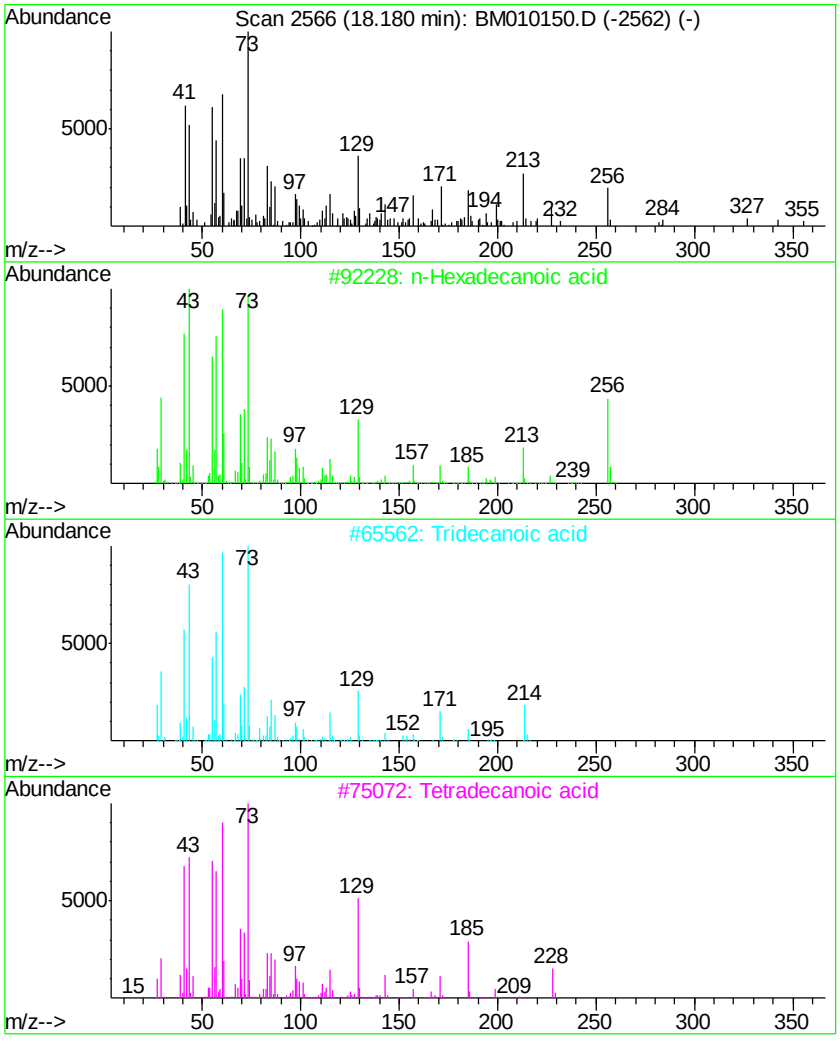
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

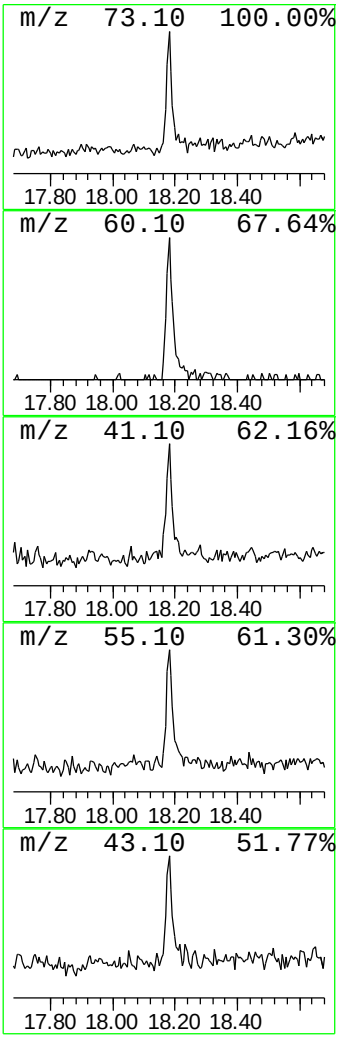
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.18	2.26 ng	228612	Phenanthrene-d10	17.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052317\
Data File : BM010150.D
Acq On : 23 May 2017 20:05
Operator : SJ/MA
Sample : I3282-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PZ-15

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.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
2-Pentanone, 4-hy...	5.08	2.8	ng	132810	1	7.96	945427	20.0
Benzene, chloro-	5.26	4.8	ng	225123	1	7.96	945427	20.0
4-Chloro-6-fluoro...	7.50	81.2	ng	3839390	1	7.96	945427	20.0
Benzene, 1-ethyl-...	9.03	2.7	ng	125668	1	7.96	945427	20.0
Acetaldehyde, (3,...	9.47	5.9	ng	327375	2	10.76	1103070	20.0
2(3H)-Benzothiazo...	16.30	2.3	ng	229243	4	17.33	2022750	20.0
Benzenesulfonamid...	16.62	2.8	ng	280551	4	17.33	2022750	20.0
n-Hexadecanoic acid	18.18	2.3	ng	228612	4	17.33	2022750	20.0