LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

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-BF090115.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	1.224	8	12	14	rBV	2389390	3667629	55.89%	16.611%
2	1.441	29	31	37	rBV	239269	686242	10.46%	3.108%
3	1.521	37	38	81	rVB	1736639	6562639	100.00%	29.723%
4	5.327	368	371	395	rBV	101075	312449	4.76%	1.415%
5	7.602	568	570	574	rBV	62766	156457	2.38%	0.709%
6	7.670	574	576	590	rVB	302769	700442	10.67%	3.172%
7	8.162	616	619	623	rBV	136058	244138	3.72%	1.106%
8	8.482	643	647	658	rVB	600779	1017445	15.50%	4.608%
9	9.465	729	733	746	rBV	491499	902109	13.75%	4.086%
10	11.053	869	872	879	rBV	193259	326388	4.97%	1.478%
11	11.545	911	915	923	rBV	39040	86199	1.31%	0.390%
12	12.014	951	956	965	rBV	707908	1388734	21.16%	6.290%
13	13.705	1100	1104	1107	rVV	890153	1501171	22.87%	6.799%
14	14.105	1135	1139	1144	rVB	39210	72521	1.11%	0.328%
15	14.219	1144	1149	1152	rBV	33335	82513	1.26%	0.374%
16	15.191	1230	1234	1239	rVB	186000	330843	5.04%	1.498%
17	15.385	1247	1251	1254	rVB	56340	102172	1.56%	0.463%
18	16.585	1348	1356	1360	rBV	35275	71598	1.09%	0.324%
19	17.088	1397	1400	1406	rBV	280919	553670	8.44%	2.508%
20	17.466	1430	1433	1441	rBV	32196	79147	1.21%	0.358%
21	18.700	1537	1541	1548	rVB	205875	451961	6.89%	2.047%
22	19.351	1594	1598	1605	rBV	93922	194565	2.96%	0.881%
23	20.472	1692	1696	1703	rBV	130586	319267	4.86%	1.446%
24	21.877	1816	1819	1826	rBV	234541	410412	6.25%	1.859%
25	22.072	1833	1836	1839	rBV	1199879	1401290	21.35%	6.347%
26	23.352	1946	1948	1950	rVB	188668	266013	4.05%	1.205%
27	24.781	2071	2073	2078	rVB	158619	191281	2.91%	0.866%

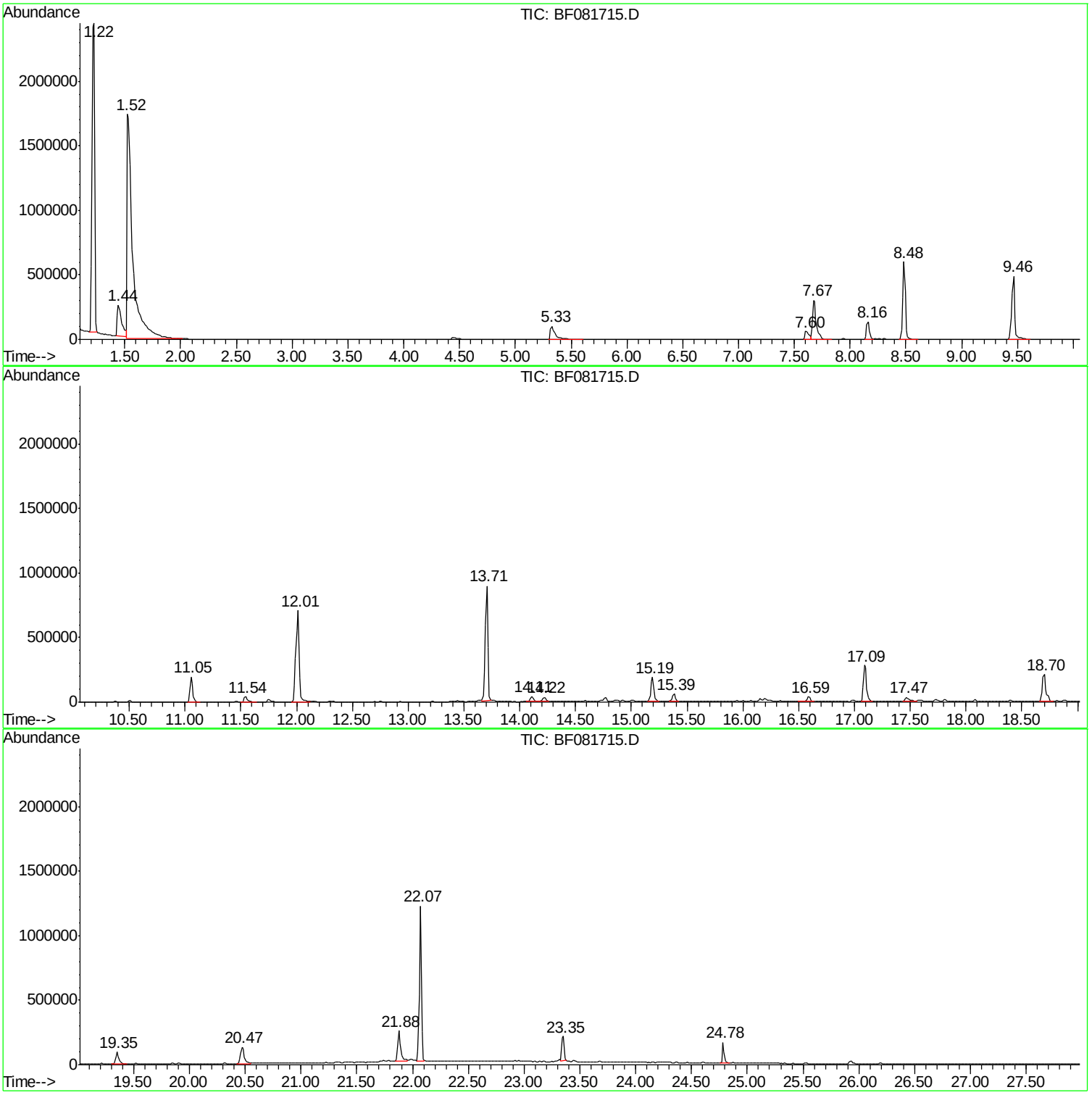
Sum of corrected areas: 22079295

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

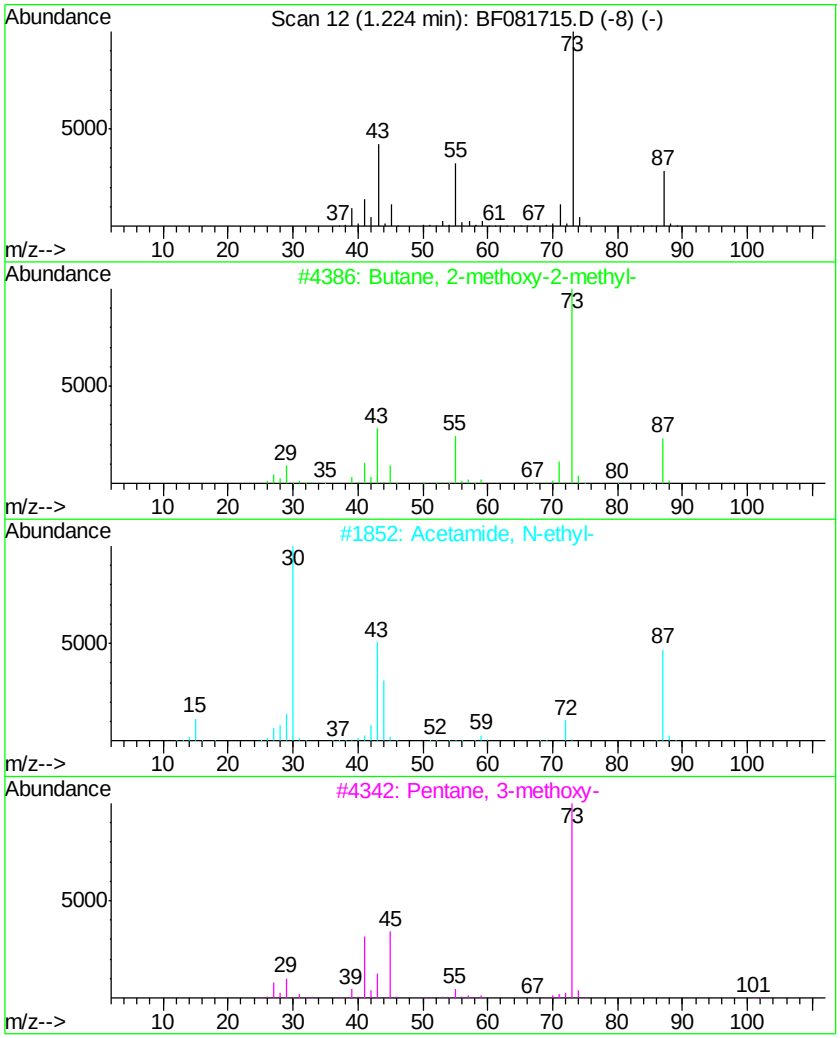
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

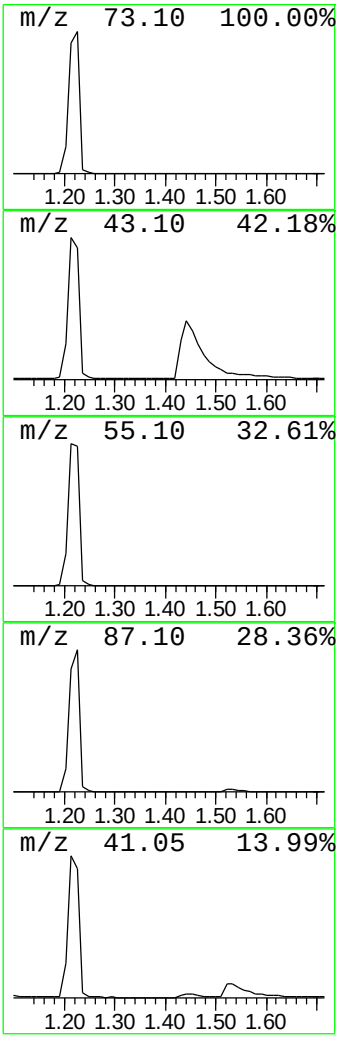
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.22	300.46 ng	3667630	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

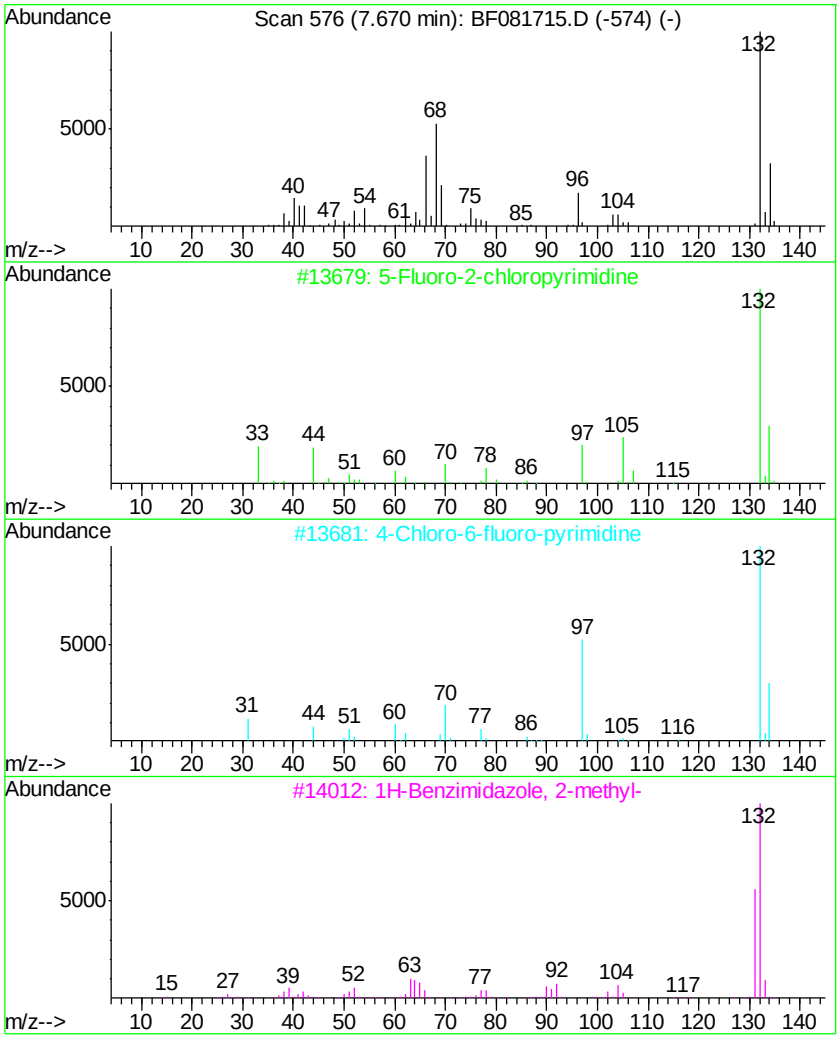
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

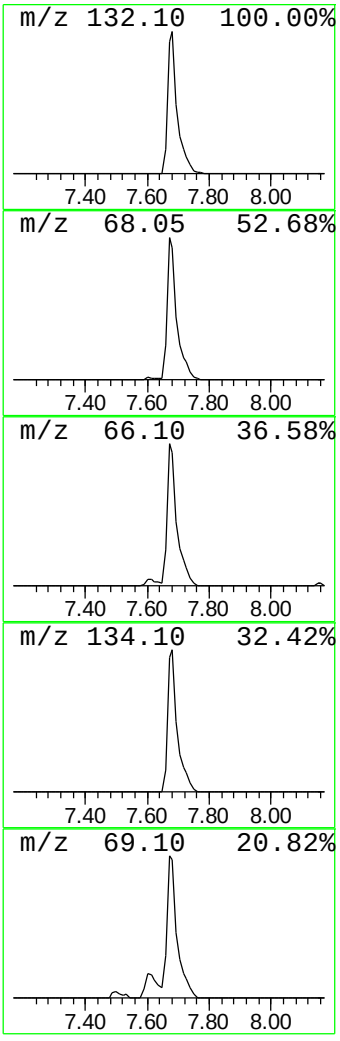
****

Peak Number 4 unknown7.67 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	57.38 ng	700442	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

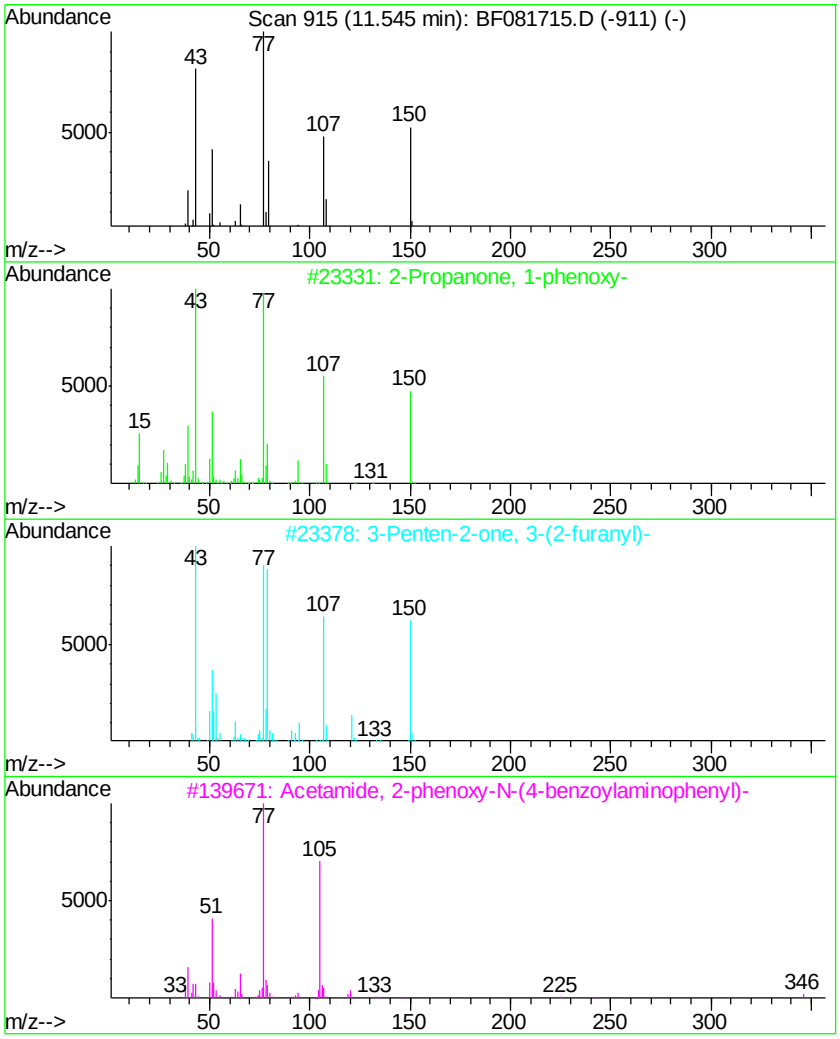
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

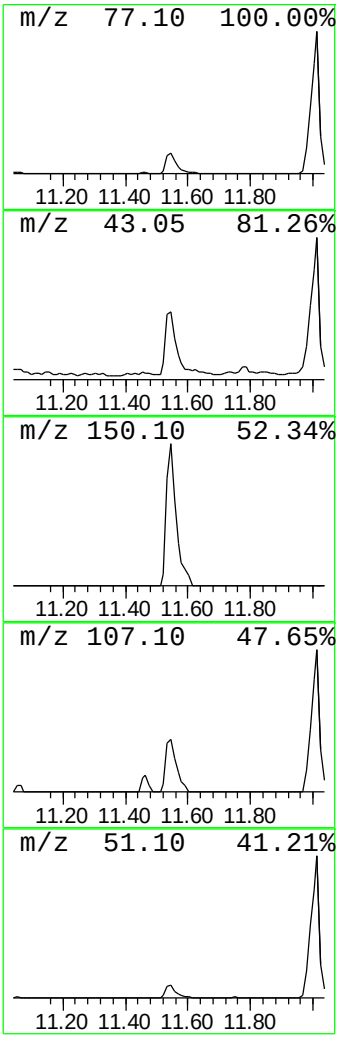
****

Peak Number 6 2-Propanone, 1-phenoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	5.28 ng	86199	Naphthalene-d8	11.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-phenoxy-	150	C9H10O2	000621-87-4	87
2	3-Penten-2-one, 3-(2-furanyl)-	150	C9H10O2	056335-77-4	50
3	Acetamide, 2-phenoxy-N-(4-benzoy...	346	C21H18N2O3	312755-44-5	43
4	2-Adamantanone	150	C10H14O	000700-58-3	22
5	Tricyclo[2.2.1.0(1,4)]heptan-2-o...	153	C7H7NO3	056666-50-3	20





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

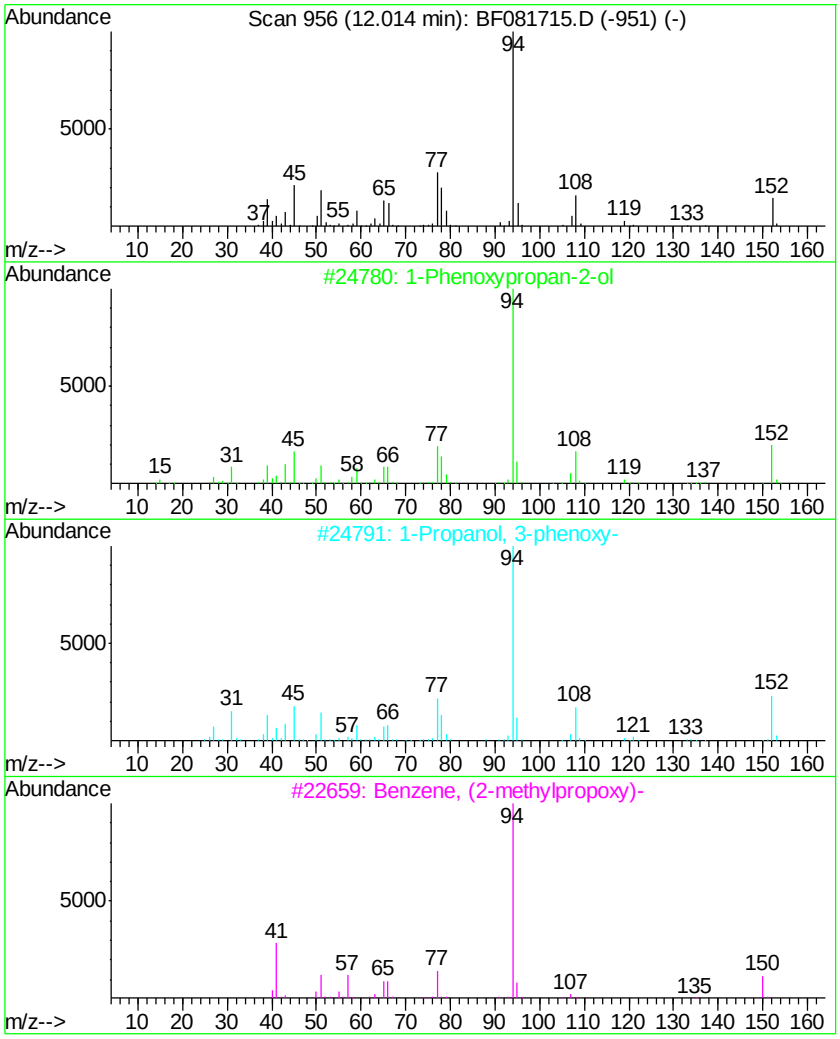
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

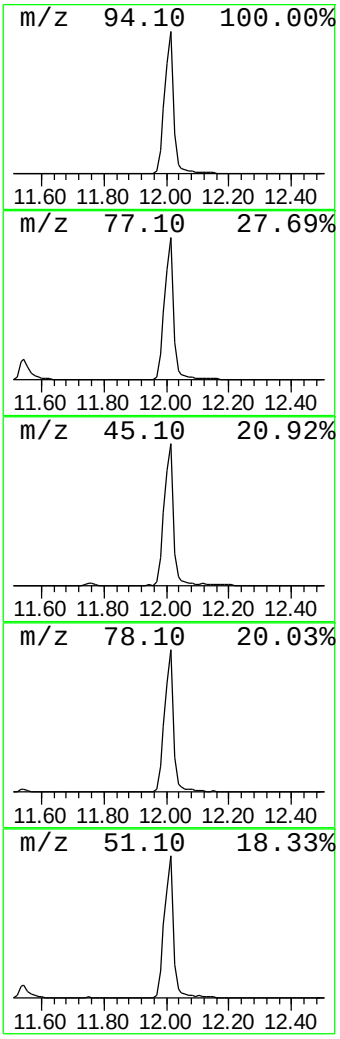
****

Peak Number 7 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	85.10 ng	1388730	Naphthalene-d8	11.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	47
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

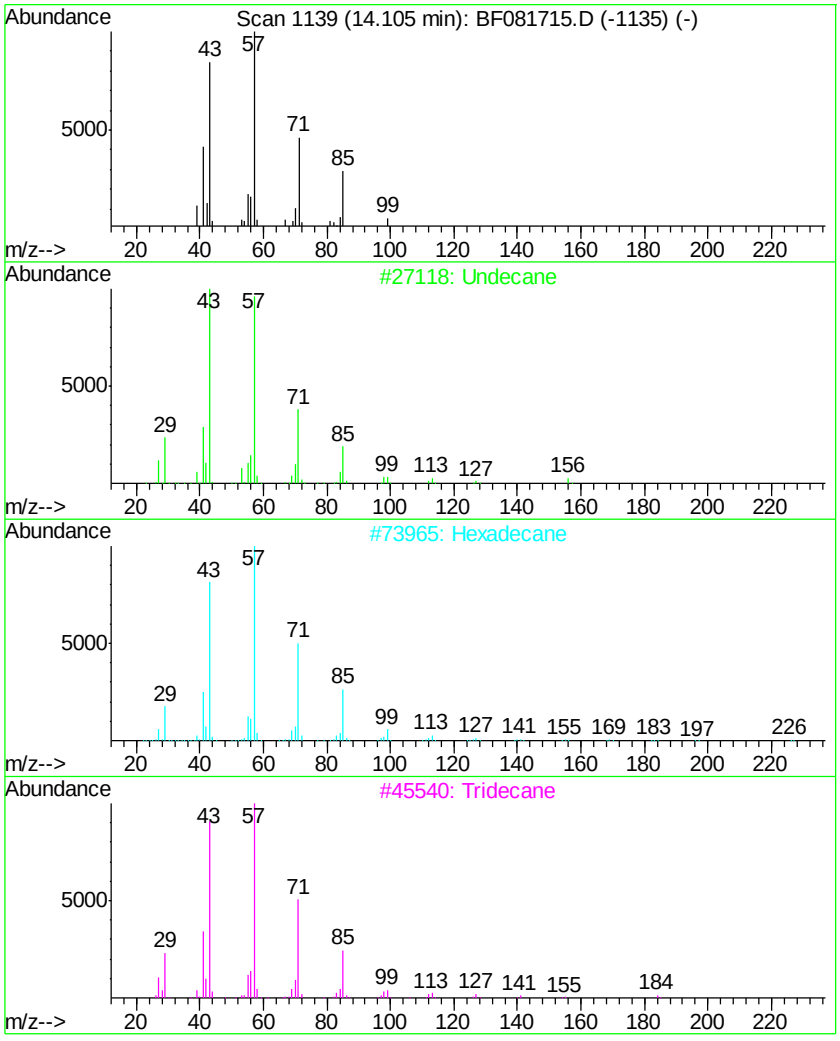
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

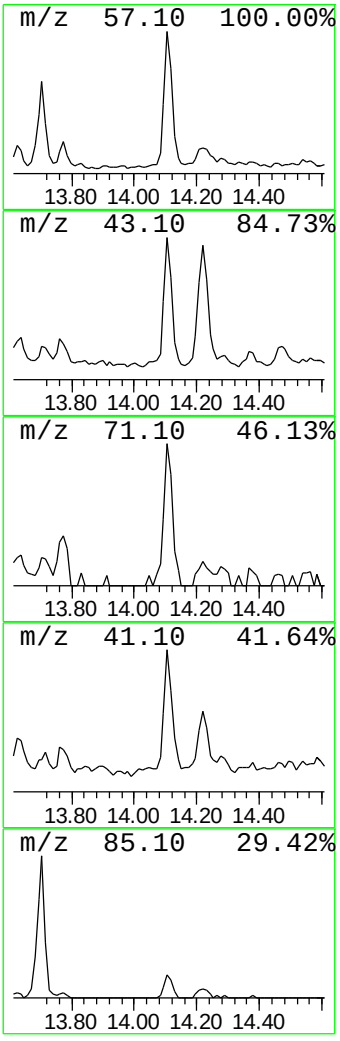
****

Peak Number 8 Undecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	4.38 ng	72521	Acenaphthene-d10	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	83
2	Hexadecane	226	C16H34	000544-76-3	83
3	Tridecane	184	C13H28	000629-50-5	78
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	59
5	Decane	142	C10H22	000124-18-5	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

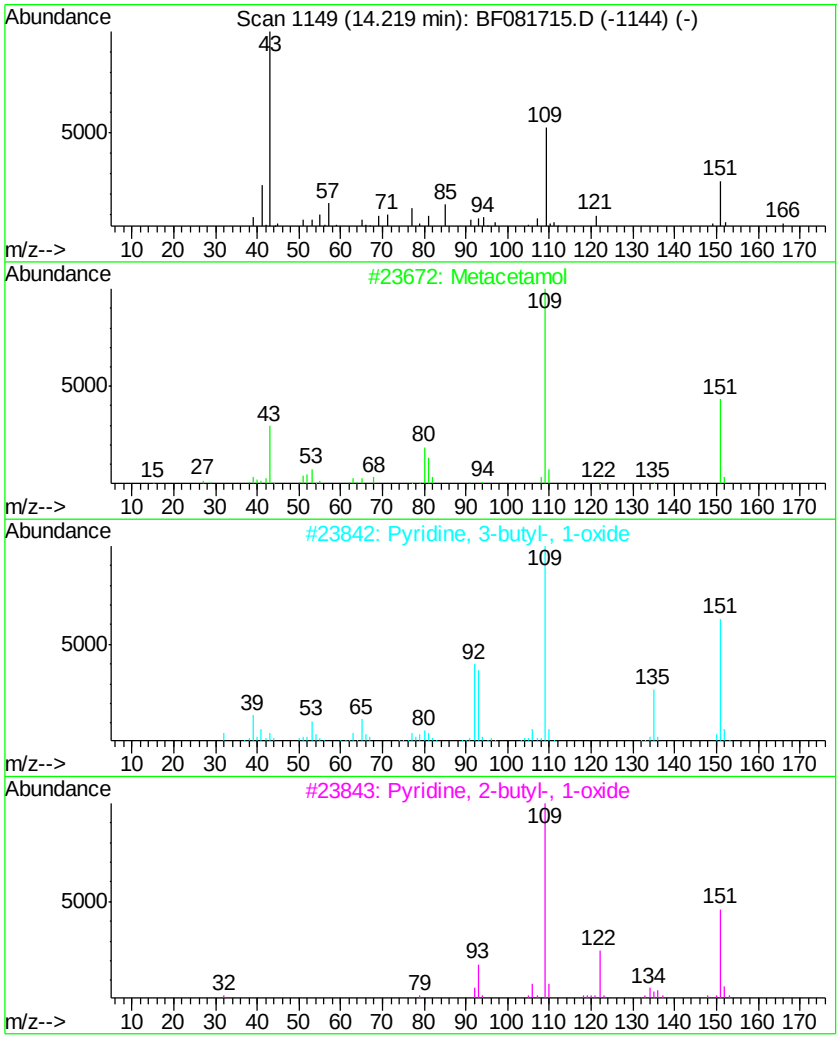
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

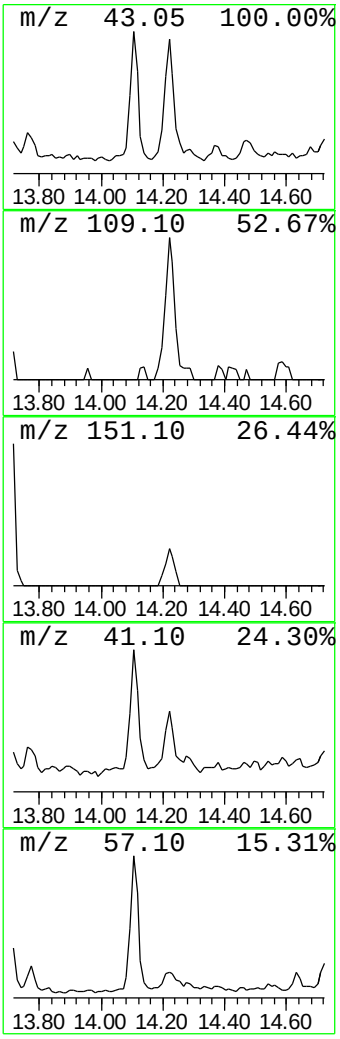
****

Peak Number 9 unknown14.22 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	4.99 ng	82513	Acenaphthene-d10	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	47
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	47
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	38
4	Acetaminophen	151	C8H9NO2	000103-90-2	38
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

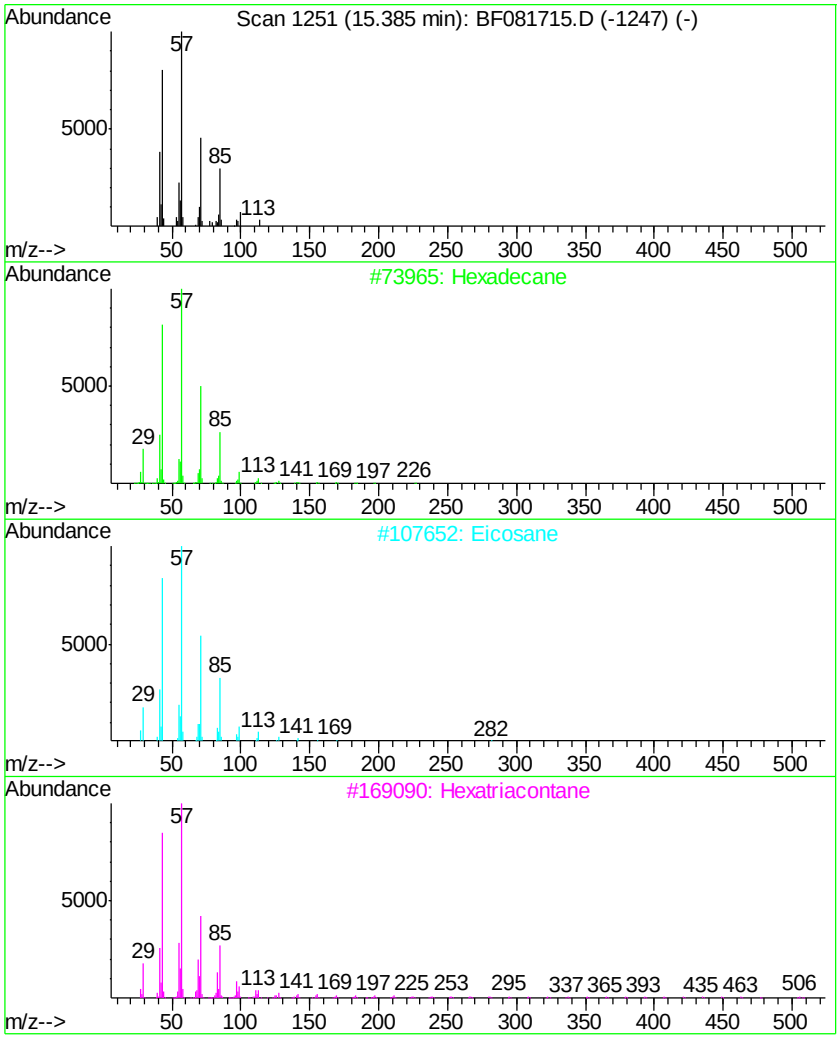
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

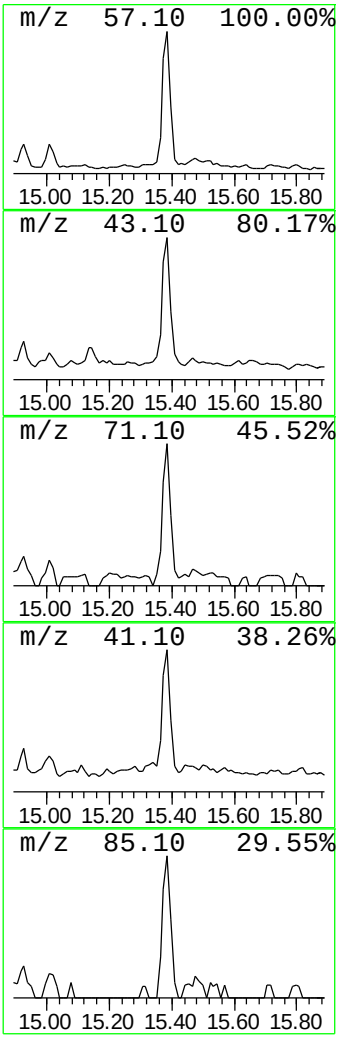
****

Peak Number 10 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	6.18 ng	102172	Acenaphthene-d10	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	83
3	Hexatriacontane	507	C36H74	000630-06-8	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Pentadecane	212	C15H32	000629-62-9	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

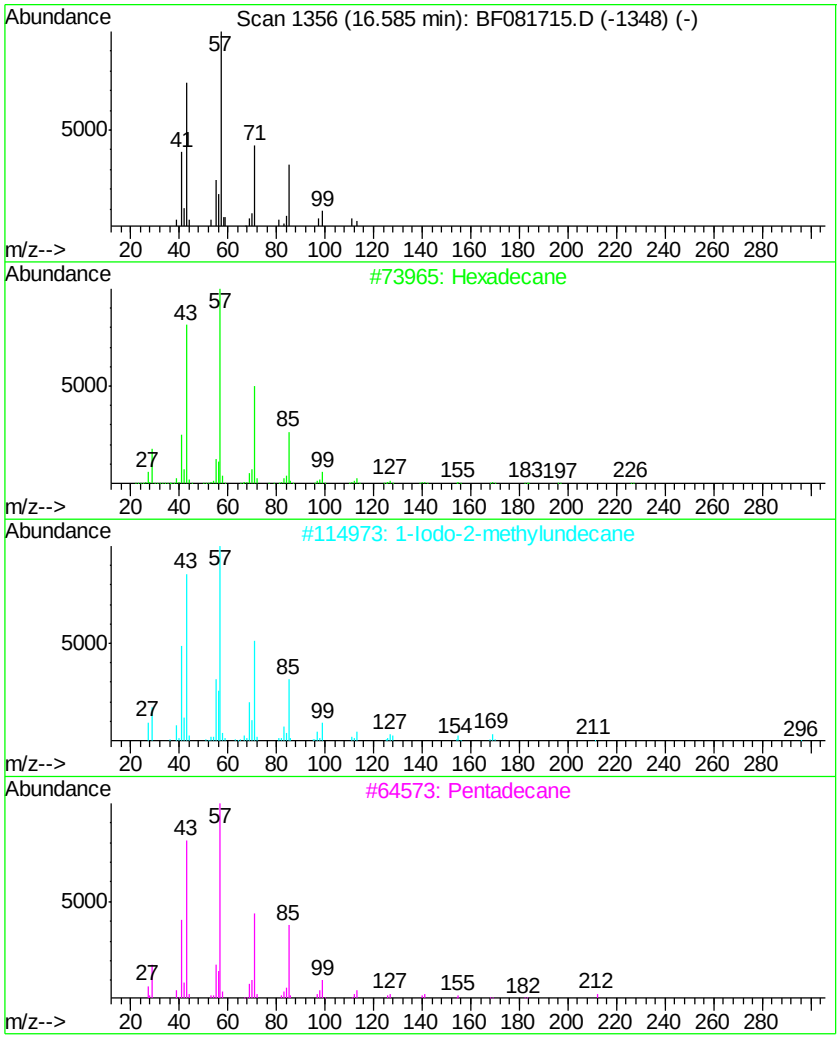
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

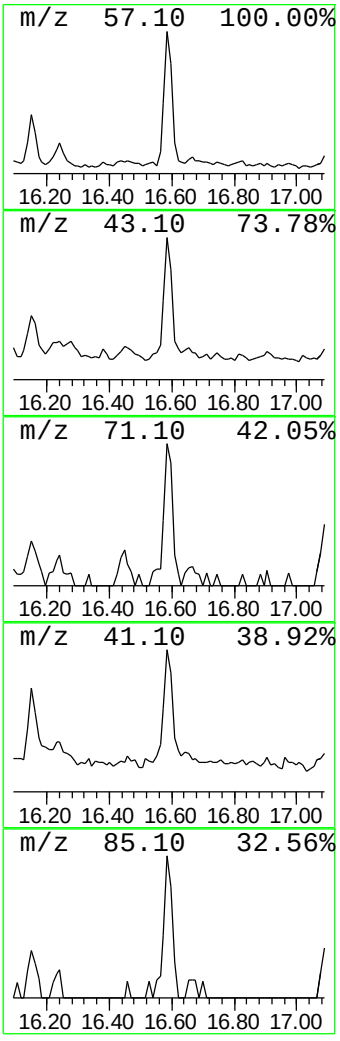
****

Peak Number 11 1-Iodo-2-methylundecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	4.33 ng	71598	Acenaphthene-d10	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	78
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78
3	Pentadecane	212	C15H32	000629-62-9	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Tetradecane	198	C14H30	000629-59-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

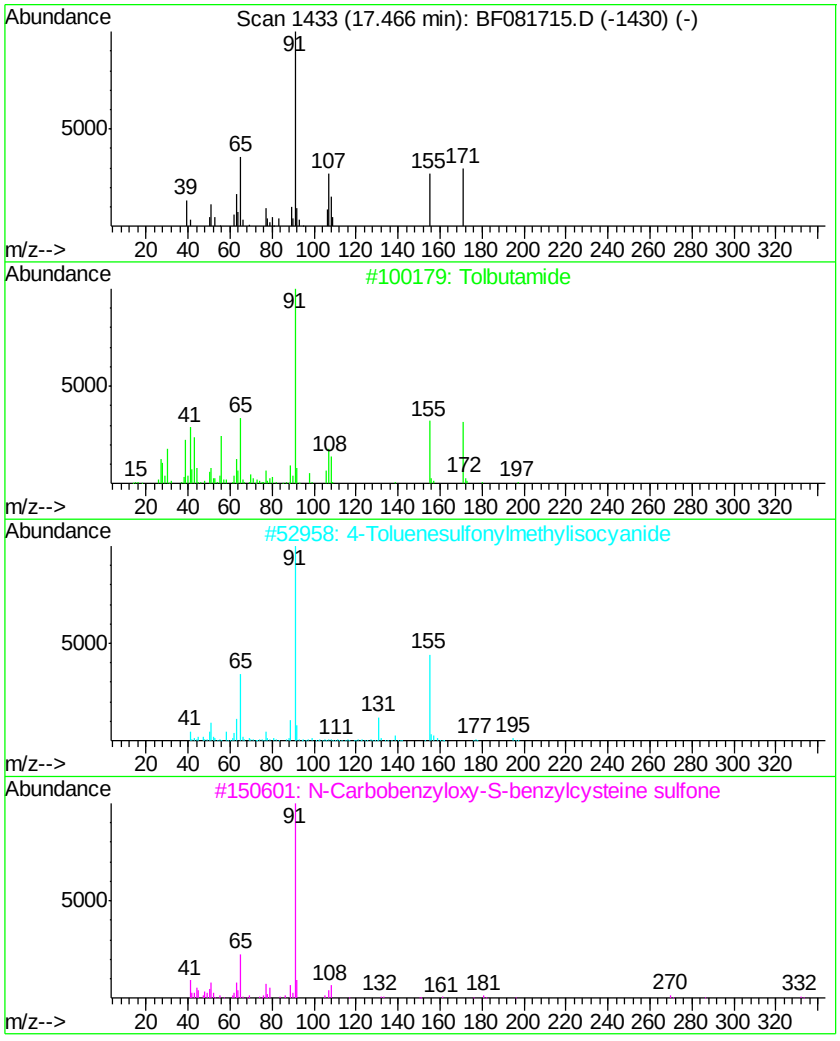
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

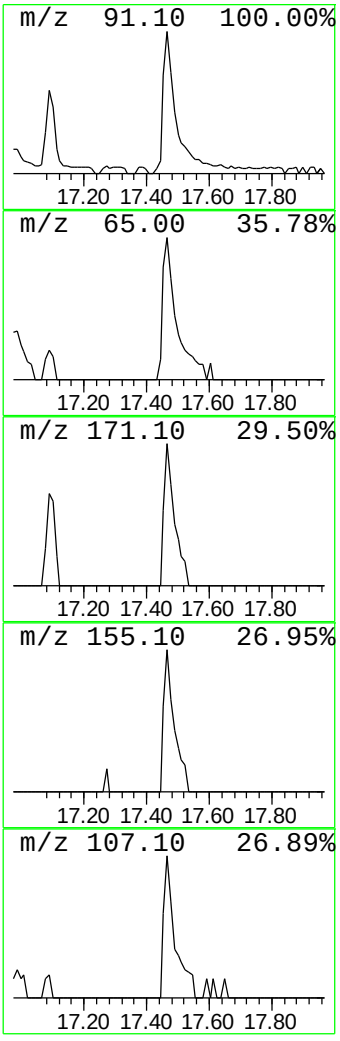
****

Peak Number 12 Tolbutamide Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	3.50 ng	79147	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tolbutamide	270	C12H18N2O3S	000064-77-7	86
2	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	43
3	N-Carbobenzyloxy-S-benzylcystein...	377	C18H19NO6S	101730-77-2	38
4	1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	38
5	S-Benzylcysteine	211	C10H13NO2S	1000131-22-4	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

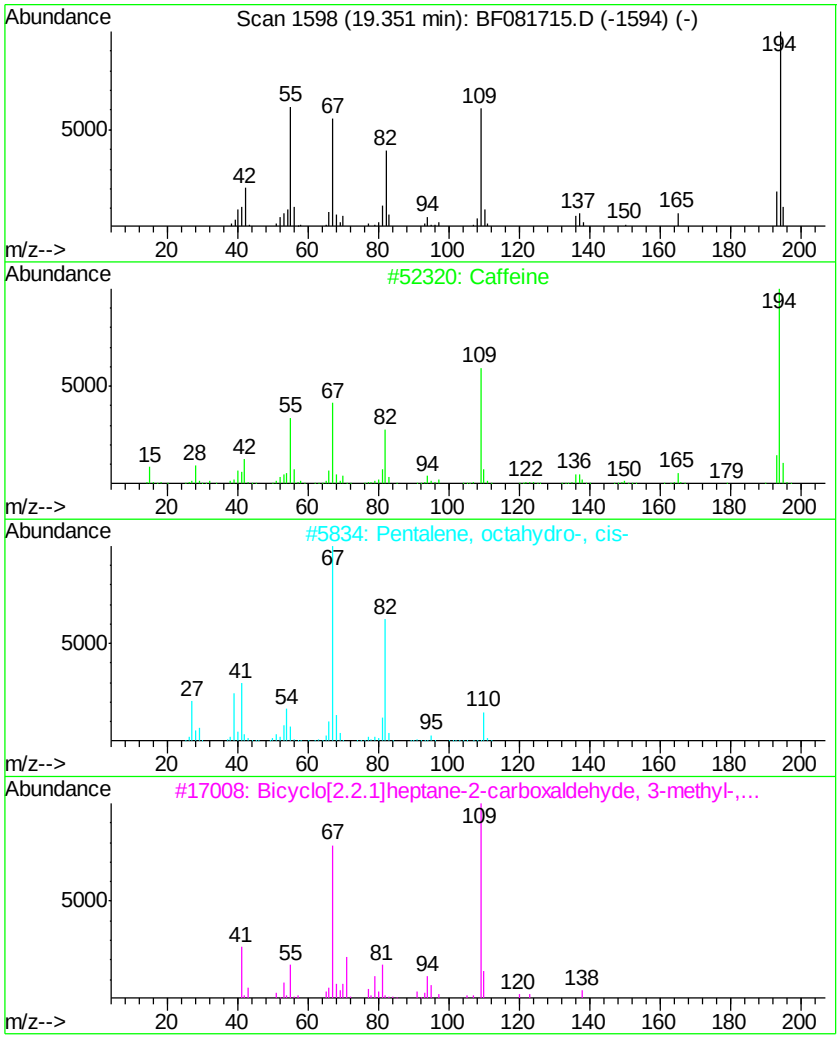
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

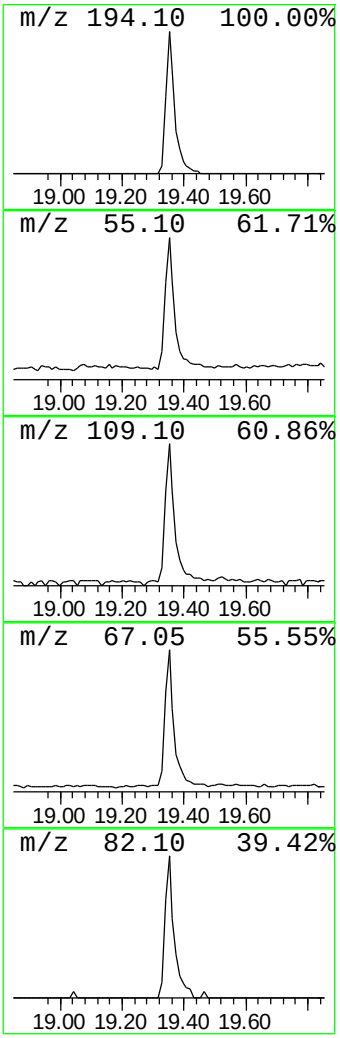
****

Peak Number 13 Caffeine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	8.61 ng	194565	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	98
2	Pentalene, octahydro-, cis-	110	C8H14	001755-05-1	38
3	Bicyclo[2.2.1]heptane-2-carboxal...	138	C9H14O	015780-36-6	25
4	5-Methyl-1,10-phenanthroline	194	C13H10N2	003002-78-6	25
5	1H-Benzimidazole, 2-phenyl-	194	C13H10N2	000716-79-0	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

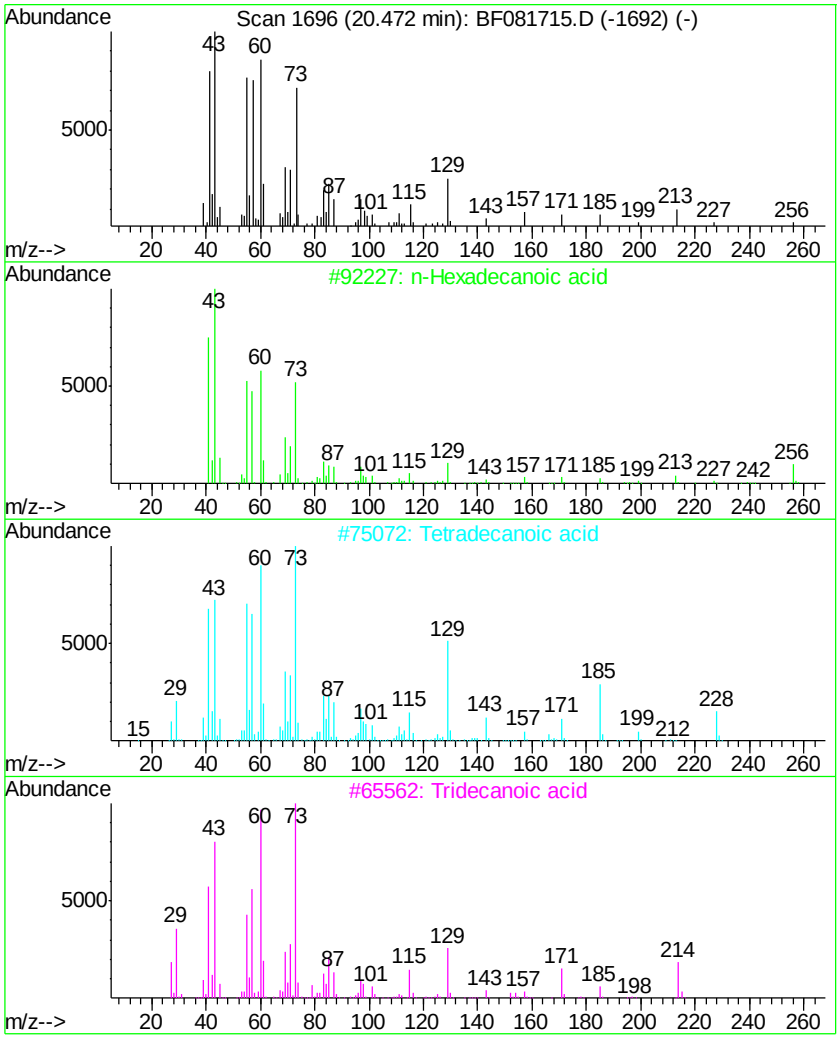
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

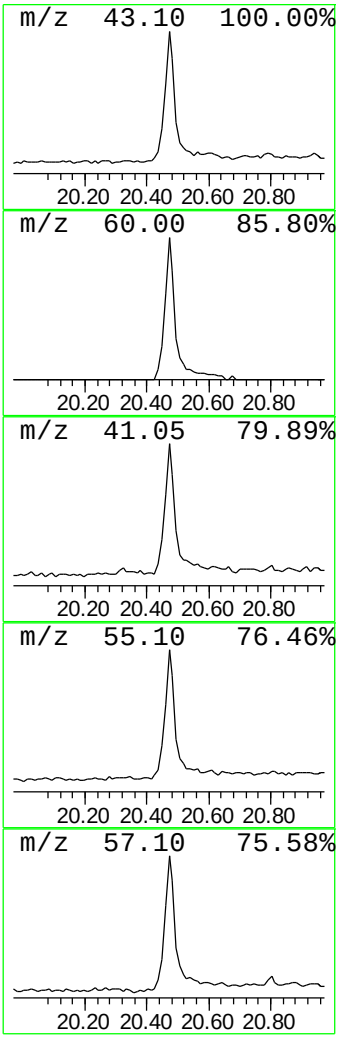
****

Peak Number 14 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	14.13 ng	319267	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

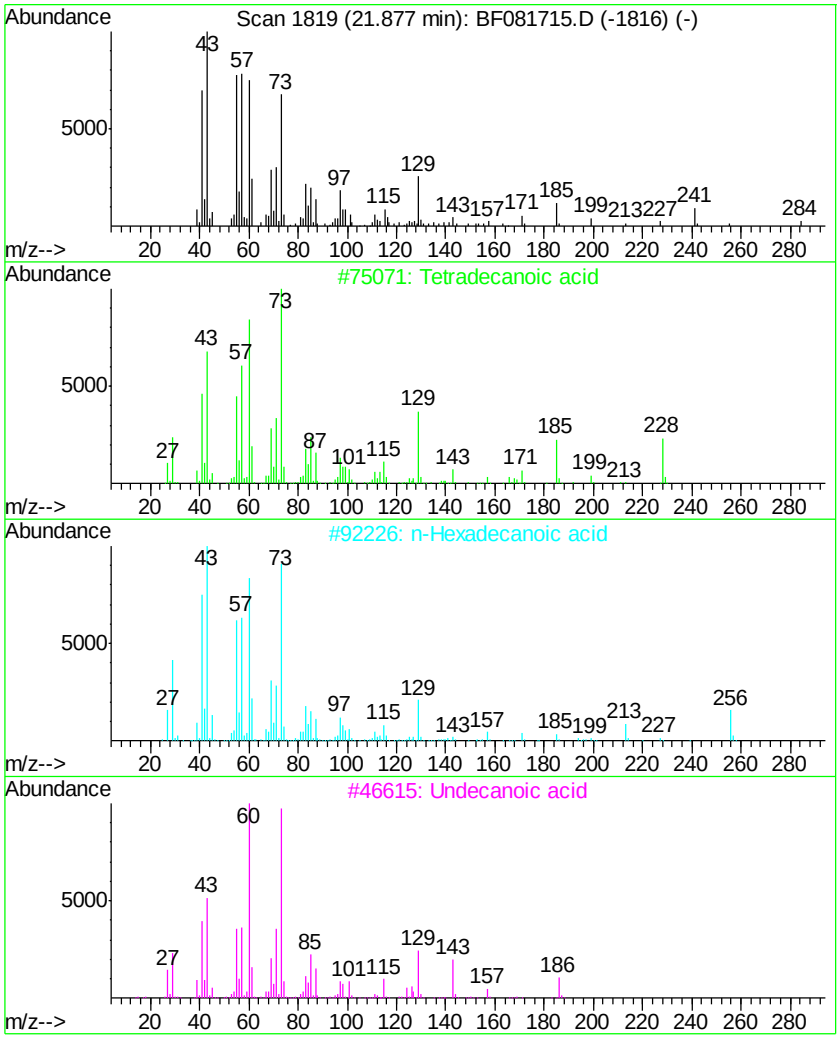
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

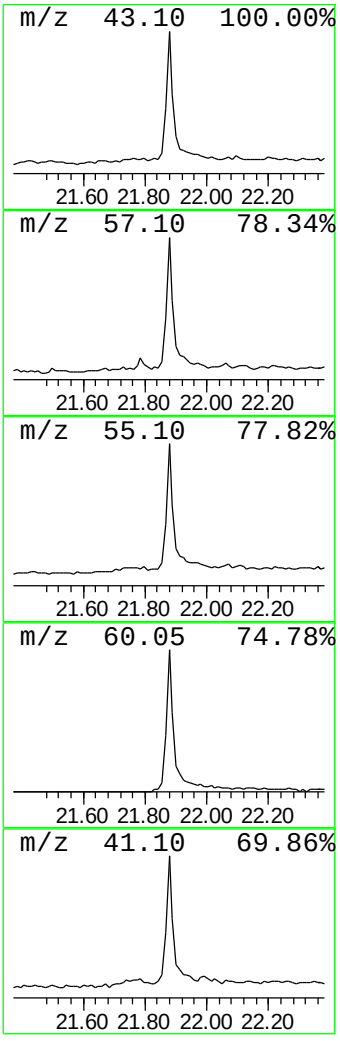
****

Peak Number 15 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	30.86 ng	410412	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	58
4	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	50
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092115\
Data File : BF081715.D
Acq On : 21 Sep 2015 15:22
Operator : UM/IZ
Sample : G3676-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
Butane, 2-methoxy...	1.22	300.5	ng	3667630	1	8.16	244138	20.0
unknown7.67	7.67	57.4	ng	700442	1	8.16	244138	20.0
2-Propanone, 1-ph...	11.54	5.3	ng	86199	2	11.05	326388	20.0
1-Phenoxypropan-2-ol	12.01	85.1	ng	1388730	2	11.05	326388	20.0
Undecane	14.11	4.4	ng	72521	3	15.19	330843	20.0
unknown14.22	14.22	5.0	ng	82513	3	15.19	330843	20.0
Hexadecane	15.39	6.2	ng	102172	3	15.19	330843	20.0
1-Iodo-2-methylun...	16.59	4.3	ng	71598	3	15.19	330843	20.0
Tolbutamide	17.47	3.5	ng	79147	4	18.70	451961	20.0
Caffeine	19.35	8.6	ng	194565	4	18.70	451961	20.0
n-Hexadecanoic acid	20.47	14.1	ng	319267	4	18.70	451961	20.0
Tetradecanoic acid	21.88	30.9	ng	410412	5	23.35	266013	20.0