LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

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-BF071015.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	2.156	4	6	14	rBV	118555	185025	29.58%	4.613%
2	2.270	14	16	23	rVB	251080	360701	57.67%	8.993%
3	5.356	284	286	298	rBB	45187	65795	10.52%	1.640%
4	5.767	320	322	330	rBB	135958	144795	23.15%	3.610%
5	6.156	354	356	360	rBB	12546	12202	1.95%	0.304%
6	6.785	409	411	420	rBB	60937	86205	13.78%	2.149%
7	6.910	420	422	425	rBV	346709	284204	45.44%	7.086%
8	7.127	440	441	444	rBB	48772	65869	10.53%	1.642%
9	7.287	453	455	458	rBB	234173	251183	40.16%	6.263%
10	7.699	489	491	493	rBV	250045	201787	32.26%	5.031%
11	8.419	552	554	557	rBB	119180	99701	15.94%	2.486%
12	9.459	643	645	646	rBV	22650	28645	4.58%	0.714%
13	9.493	646	648	650	rVB	581499	461827	73.83%	11.514%
14	9.893	681	683	684	rBV	13950	14552	2.33%	0.363%
15	10.122	701	703	706	rBV	6558	9154	1.46%	0.228%
16	10.179	706	708	710	rVB	149728	122190	19.53%	3.046%
17	10.545	739	740	743	rBV	90554	113876	18.21%	2.839%
18	10.888	768	770	772	rBB	12959	10957	1.75%	0.273%
19	10.968	775	777	780	rBB	306844	264207	42.24%	6.587%
20	11.665	837	838	841	rBB	111495	131730	21.06%	3.284%
21	12.168	881	882	885	rBV	16021	14309	2.29%	0.357%
22	12.648	922	924	925	rBV	5496	7293	1.17%	0.182%
23	13.288	978	980	983	rBV	739080	625509	100.00%	15.595%
24	14.202	1057	1060	1061	rVB2	8243	8965	1.43%	0.224%
25	14.237	1061	1063	1064	rBV	42577	43936	7.02%	1.095%
26	14.271	1064	1066	1073	rVB3	14390	25732	4.11%	0.642%
27	14.488	1082	1085	1088	rBV	186469	178190	28.49%	4.443%
28	16.214	1233	1236	1240	rBV	125071	192312	30.74%	4.795%

Sum of corrected areas: 4010851

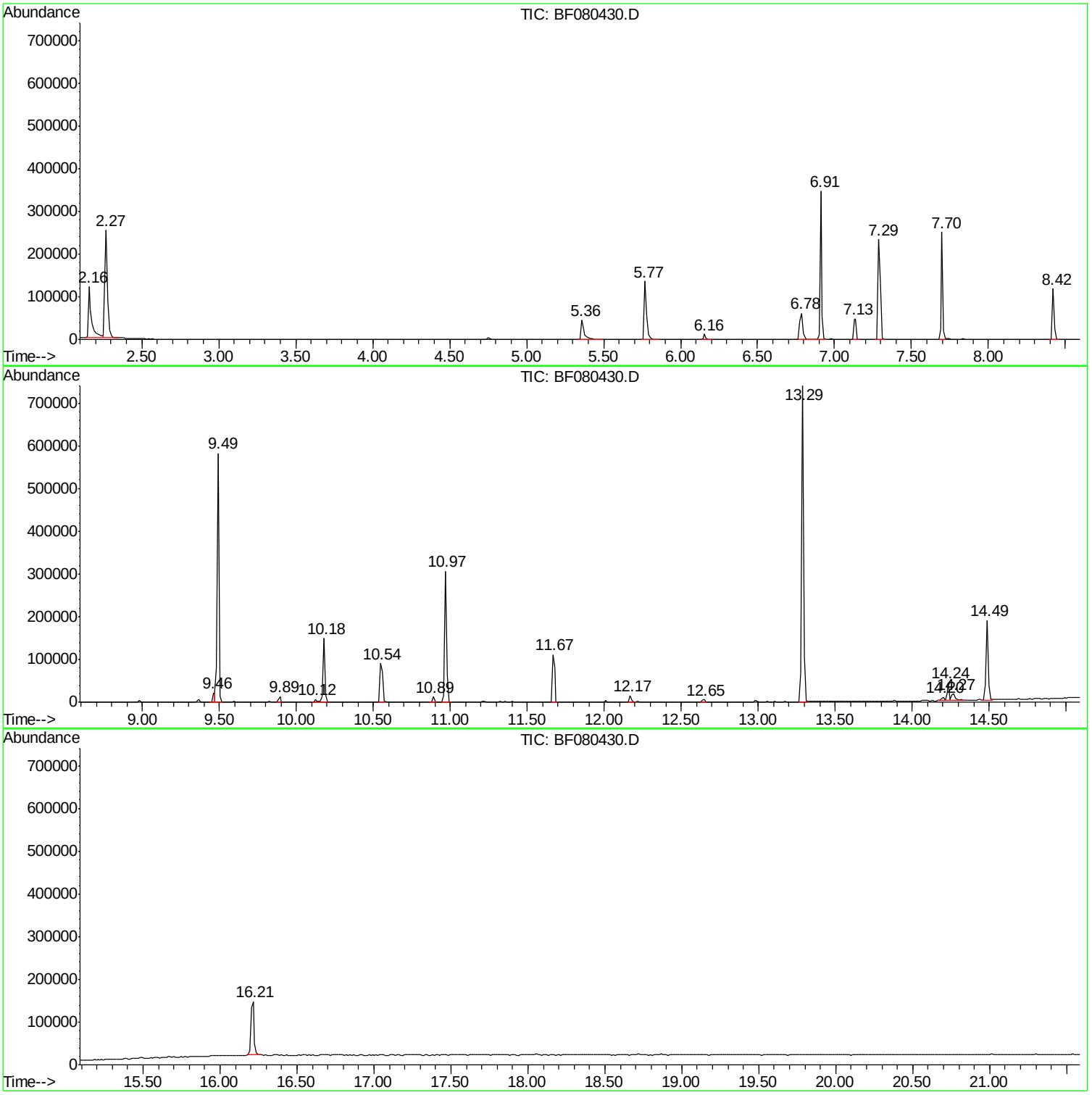
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

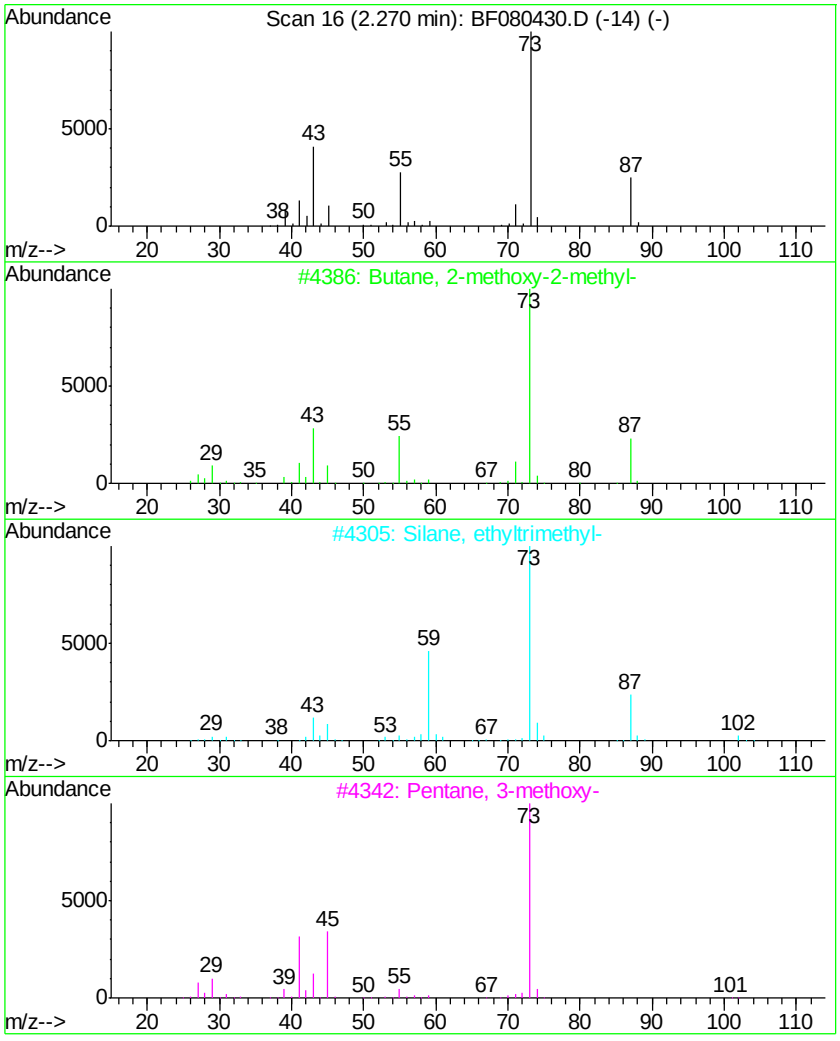
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

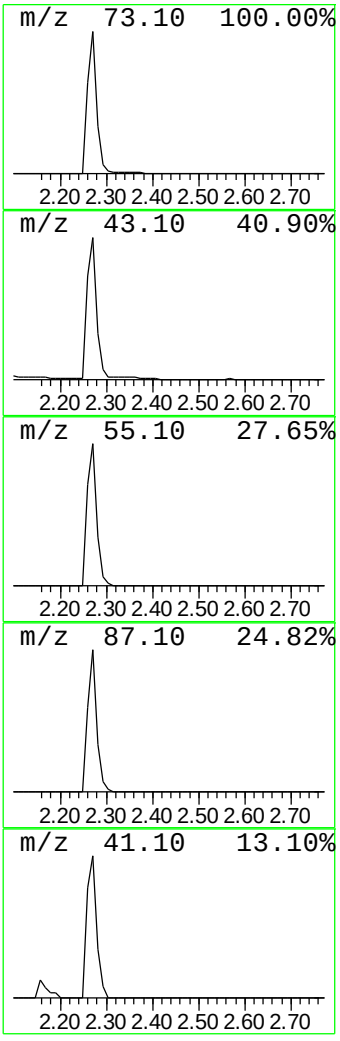
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	109.52 ng	360701	1,4-Dichlorobenzene-d4	7.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

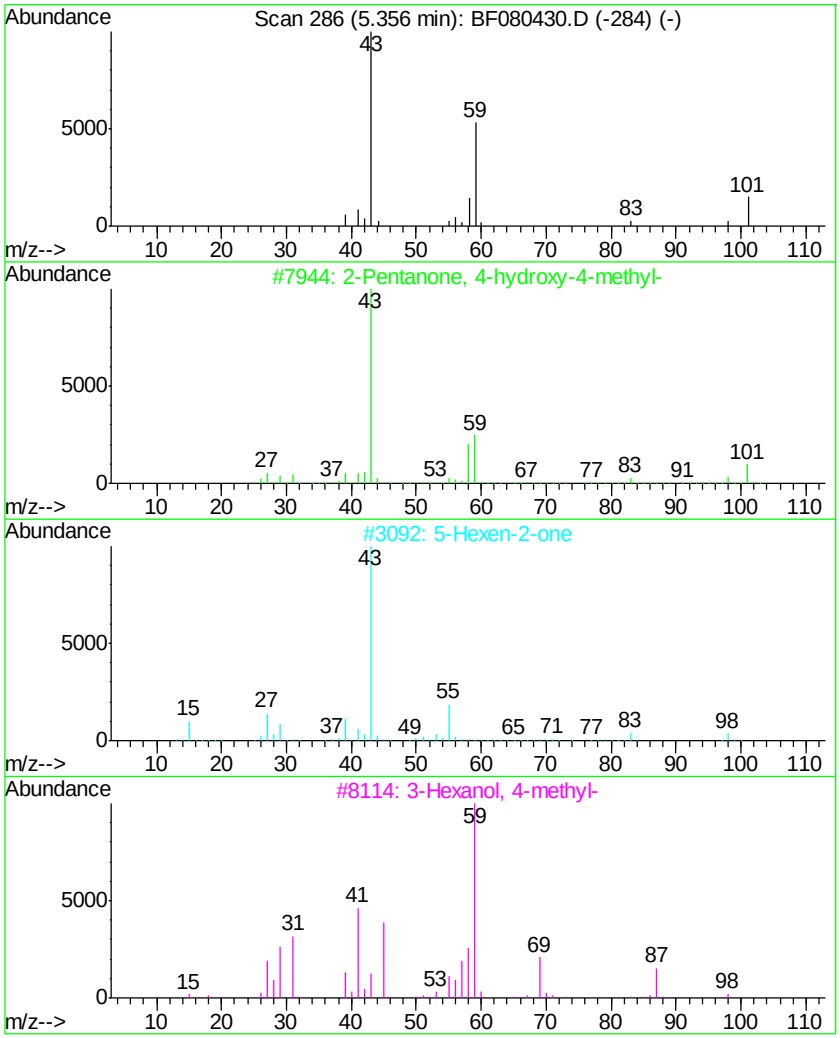
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

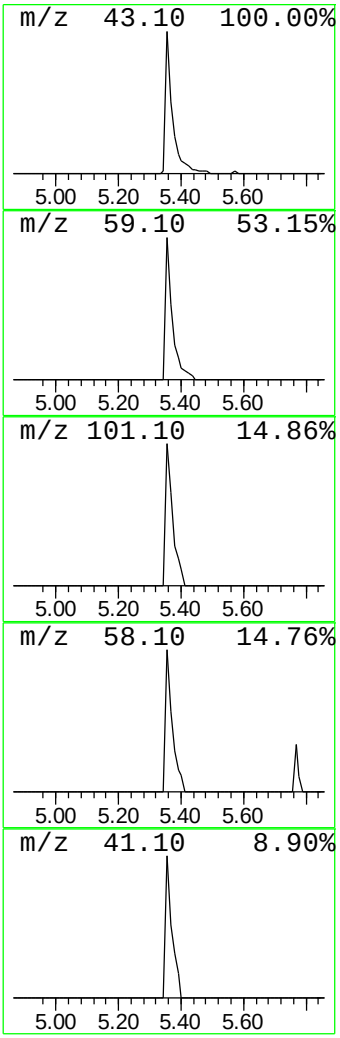
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.36	19.98 ng	65795	1,4-Dichlorobenzene-d4	7.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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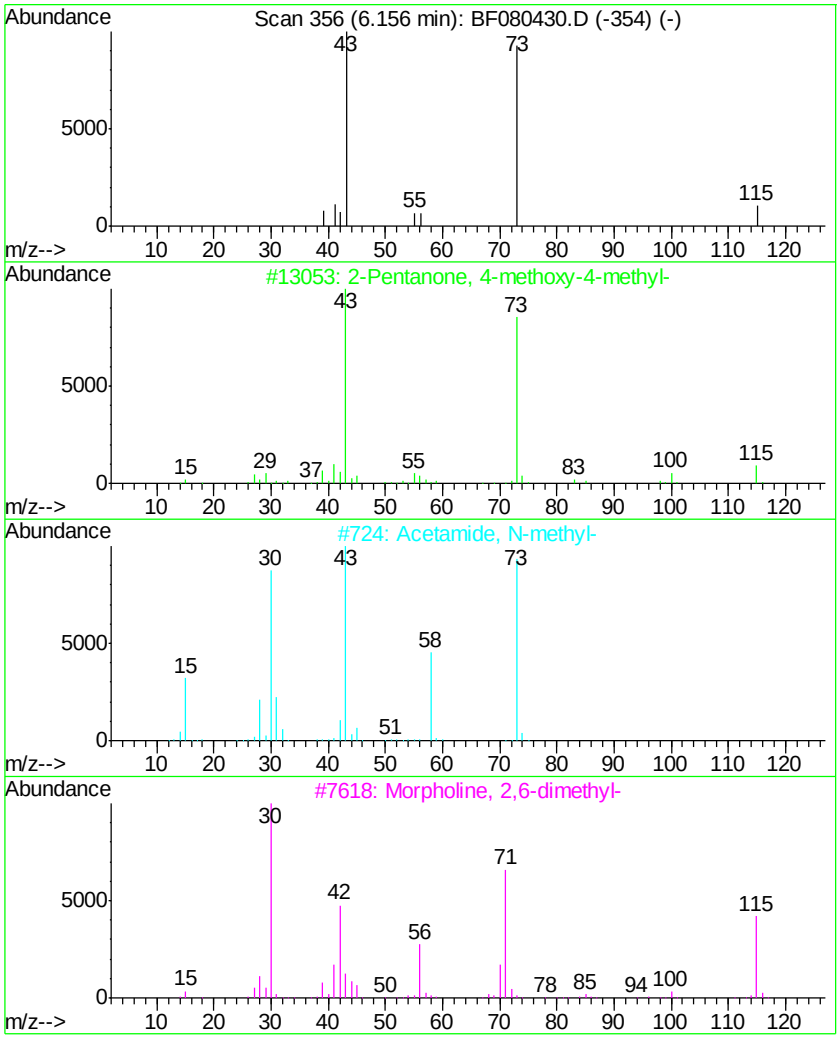
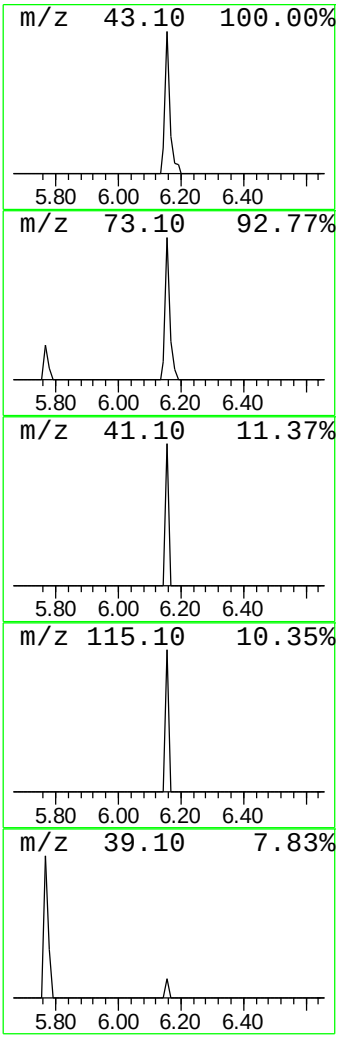
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	3.70 ng	12202	1,4-Dichlorobenzene-d4	7.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
3	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	4
4	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
5	N-Ethylformamide	73	C3H7NO	000627-45-2	3





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

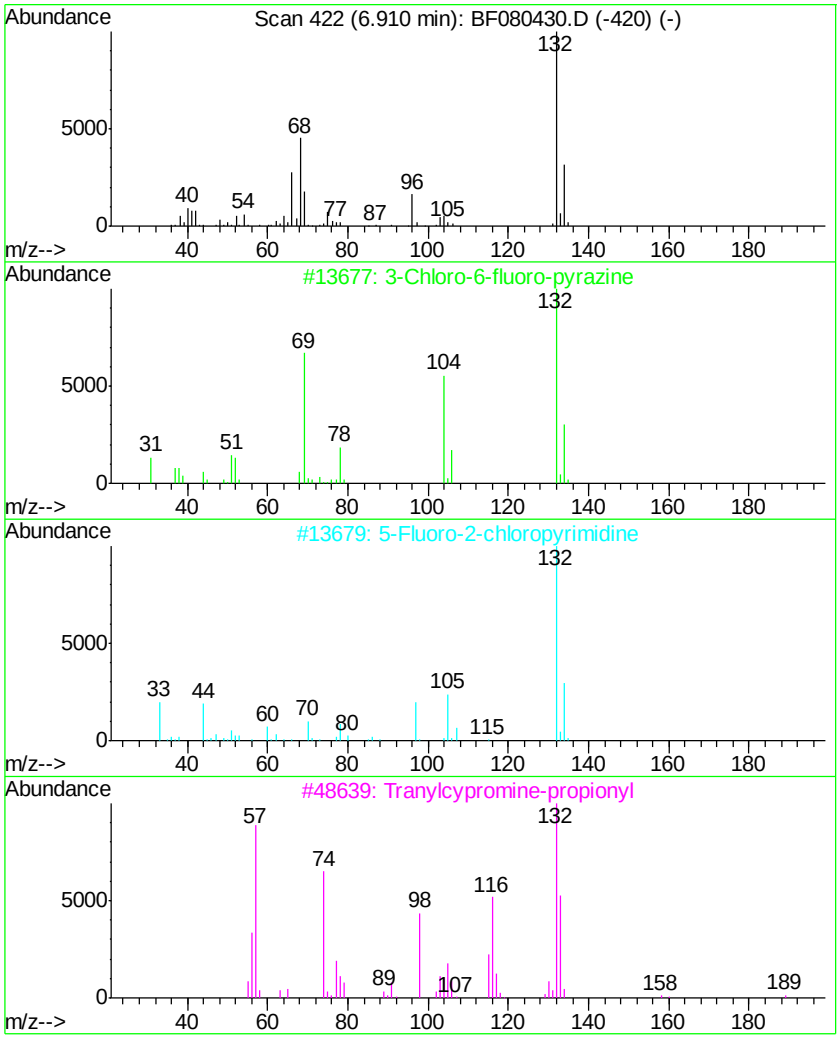
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

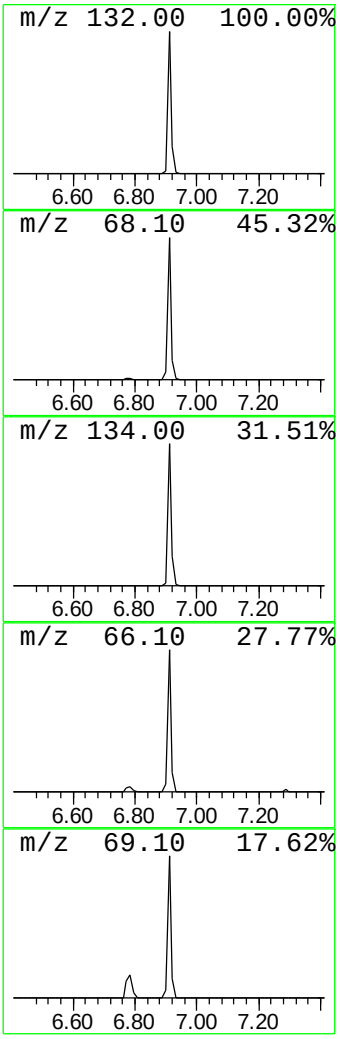
****

Peak Number 5 unknown6.91 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	86.29 ng	284204	1,4-Dichlorobenzene-d4	7.14

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

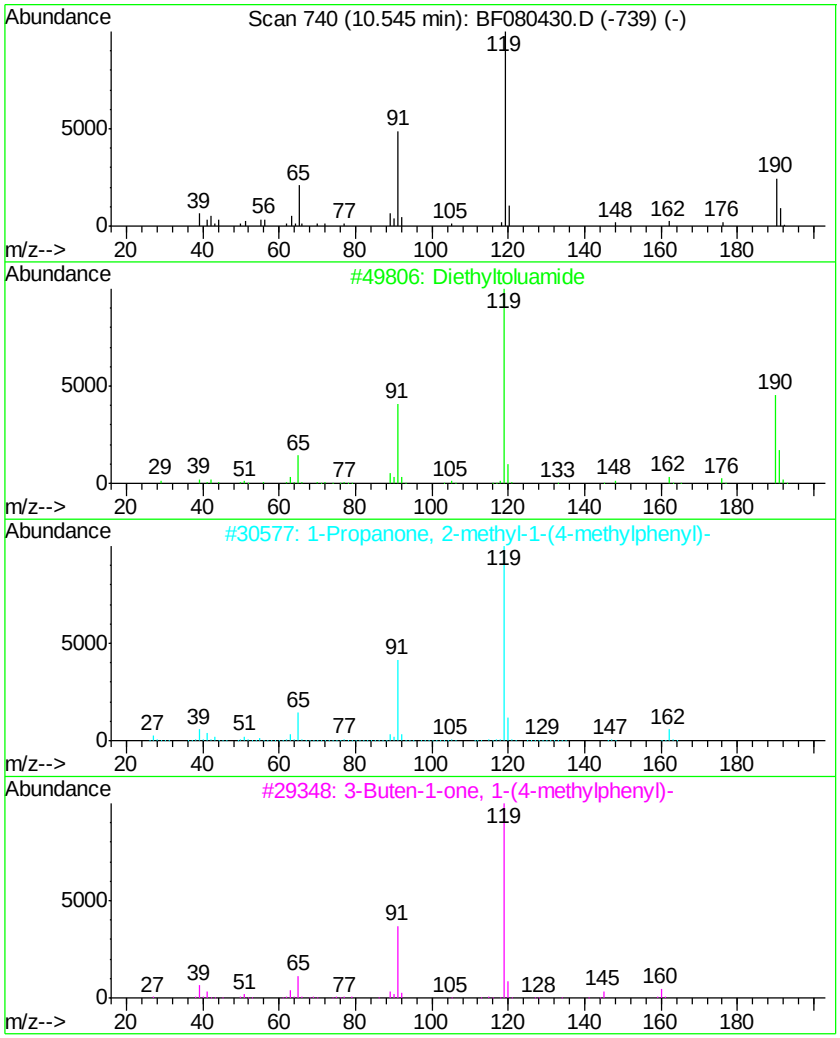
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

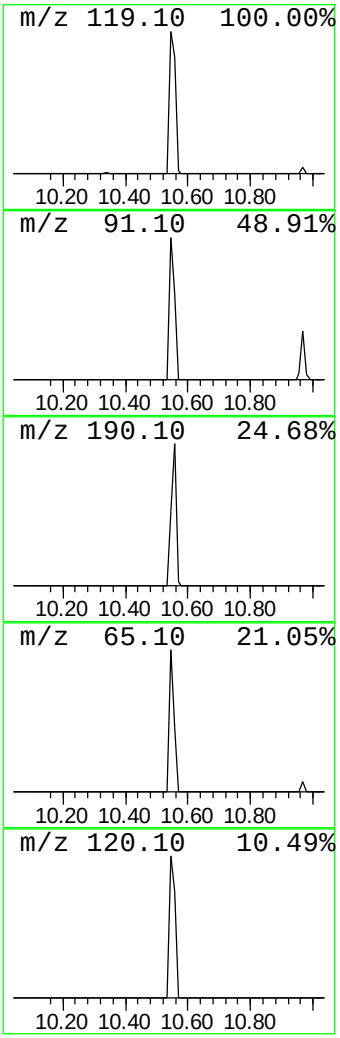
****

Peak Number 7 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	18.64 ng	113876	Acenaphthene-d10	10.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	95
2	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	74
3	3-Buten-1-one, 1-(4-methylphenyl)-	160	C11H12O	130649-66-0	64
4	N-(m-Toluoyl)glycine	193	C10H11NO3	027115-49-7	64
5	Benzoic acid, 4-methyl-, methyl ...	150	C9H10O2	000099-75-2	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

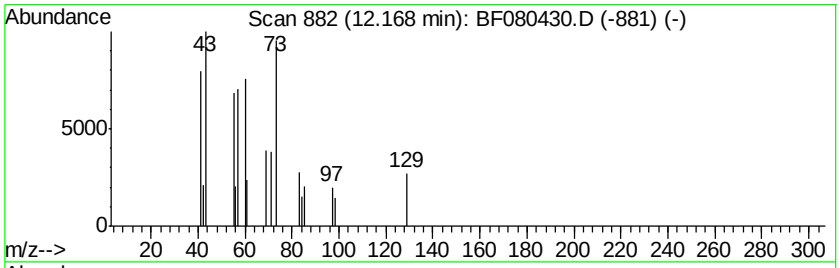
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

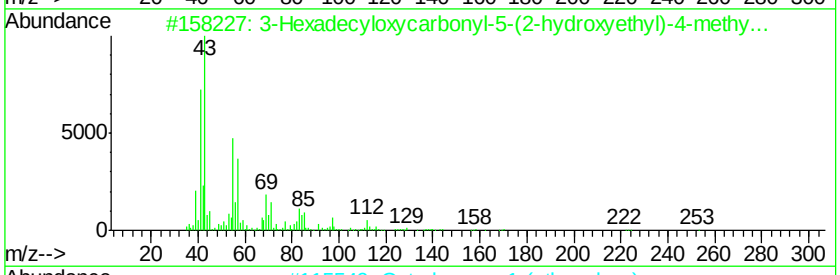
****

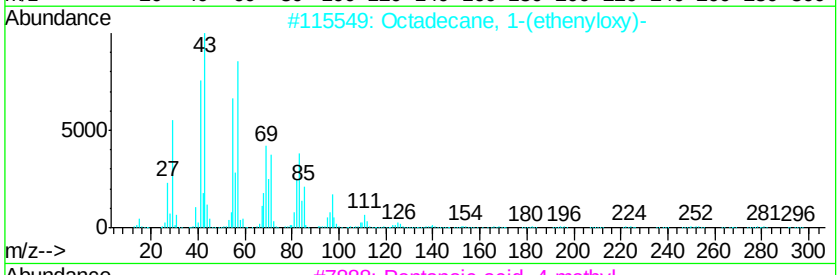
Peak Number 8 unknown12.17 Concentration Rank 10

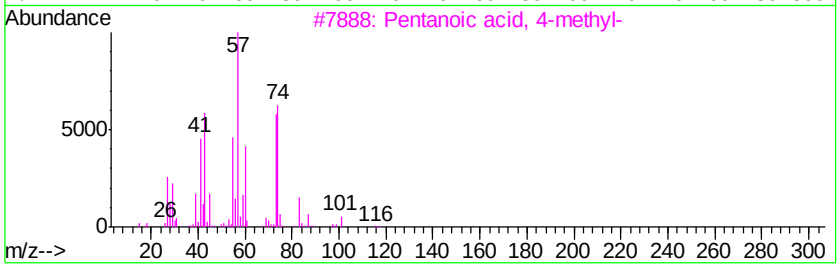
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	2.17 ng	14309	Phenanthrene-d10	11.66

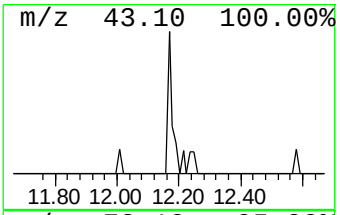
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexadecyloxycarbonyl-5-(2-hydr...	409	C24H45N2O3	1000222-82-8	30
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	27
3	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	25
4	Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	16
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	16

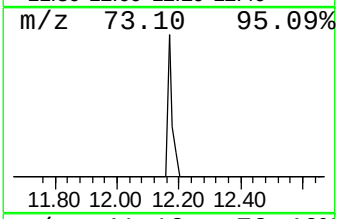


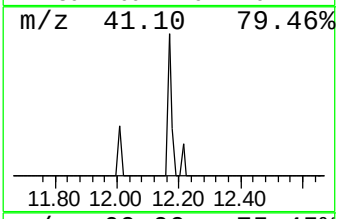


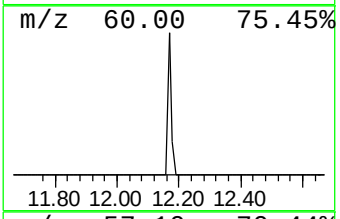


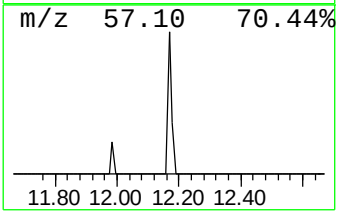












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

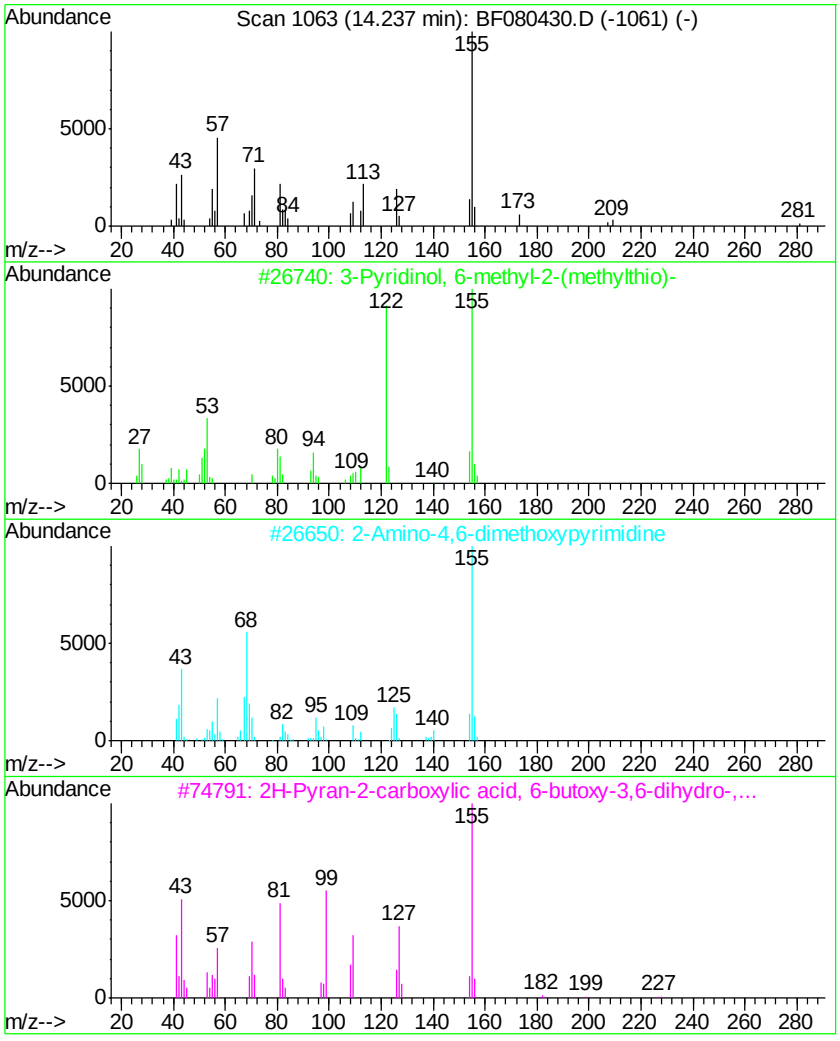
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

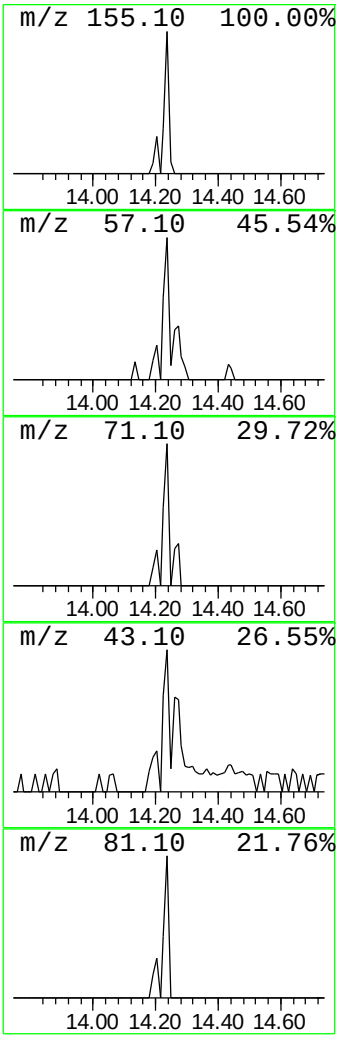
****

Peak Number 9 unknown14.24 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	4.93 ng	43936	Chrysene-d12	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridinol, 6-methyl-2-(methylt...	155	C7H9NOS	023003-25-0	47
2	2-Amino-4,6-dimethoxypyrimidine	155	C6H9N3O2	036315-01-2	47
3	2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	40
4	4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	38
5	Benzaldehyde, 4-chloro-, oxime, ...	155	C7H6ClNO	003717-23-5	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

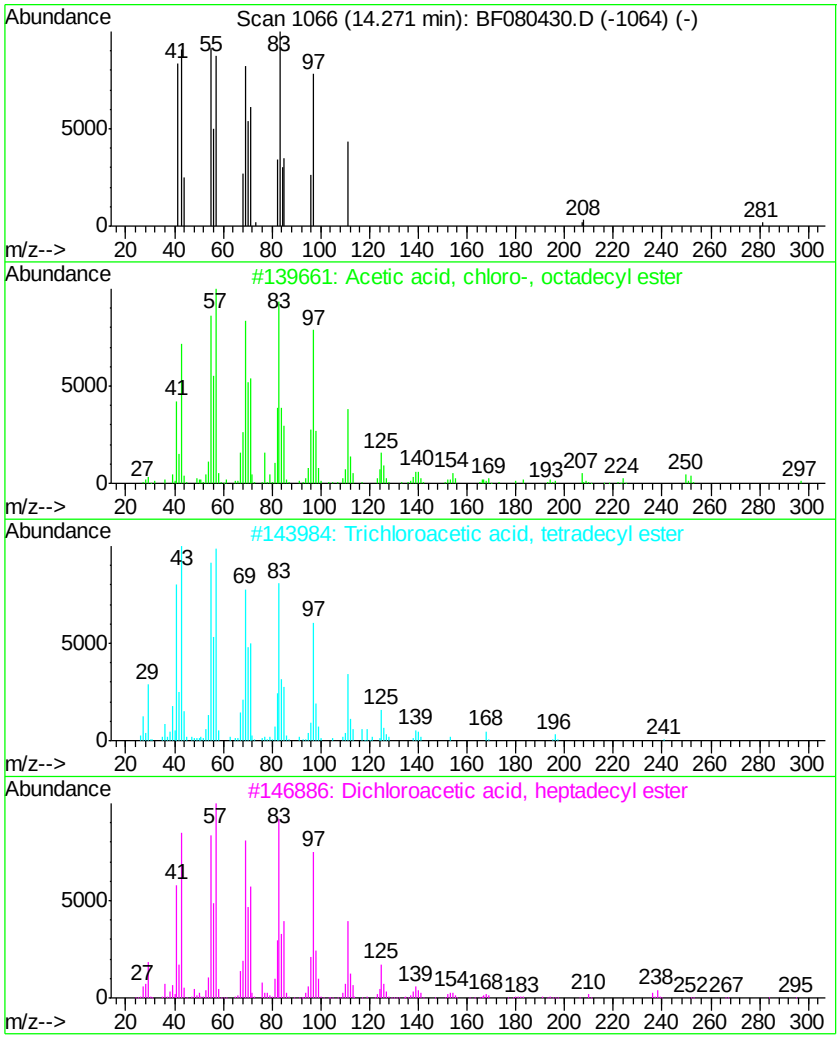
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

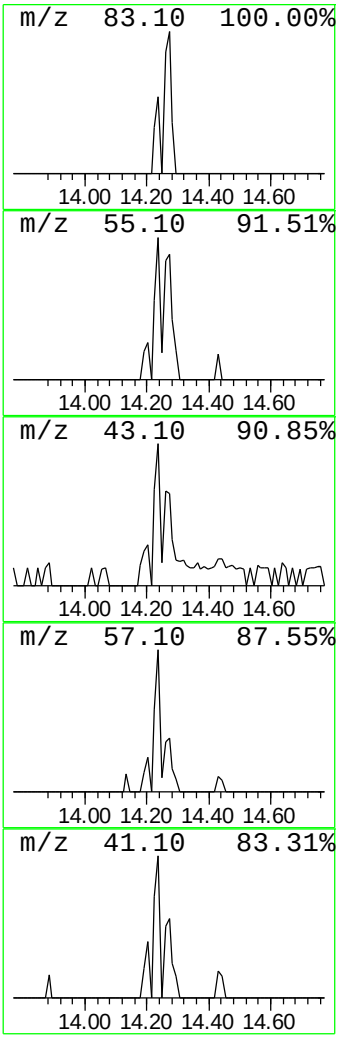
****

Peak Number 10 Acetic acid, chloro-, octad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	2.89 ng	25732	Chrysene-d12	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080430.D
Acq On : 13 Jul 2015 17:07
Operator : TP/UM
Sample : G2945-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-RMW-2-26D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.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...	2.27	109.5	ng	360701	1	7.14	65869	20.0
2-Pentanone, 4-hy...	5.36	20.0	ng	65795	1	7.14	65869	20.0
2-Pentanone, 4-me...	6.16	3.7	ng	12202	1	7.14	65869	20.0
unknown6.91	6.91	86.3	ng	284204	1	7.14	65869	20.0
Diethyltoluamide	10.54	18.6	ng	113876	3	10.18	122190	20.0
unknown12.17	12.17	2.2	ng	14309	4	11.66	131730	20.0
unknown14.24	14.24	4.9	ng	43936	5	14.49	178190	20.0
Acetic acid, chlo...	14.27	2.9	ng	25732	5	14.49	178190	20.0