LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

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_G\METHODS\8270-BG070816.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	3.038	28	34	45	rBV	1401203	1961358	9.54%	2.506%
2	5.694	480	486	496	rVB	594245	960875	4.68%	1.228%
3	7.304	752	760	772	rBV	522750	1007684	4.90%	1.288%
4	7.680	817	824	834	rVB	915646	1581507	7.69%	2.021%
5	8.150	895	904	912	rBV	468138	858306	4.18%	1.097%
6	8.479	952	960	967	rVB	1416204	2506356	12.19%	3.203%
7	9.325	1096	1104	1111	rBV	1416037	2637420	12.83%	3.370%
8	10.976	1377	1385	1392	rBV	752626	1387727	6.75%	1.773%
9	13.414	1790	1800	1807	rBV	4040937	6666115	32.43%	8.518%
10	14.237	1934	1940	1946	rBV	435599	618347	3.01%	0.790%
11	14.795	2027	2035	2044	rBV2	1358668	2256408	10.98%	2.883%
12	16.287	2283	2289	2298	rVB	1798066	2780947	13.53%	3.554%
13	16.934	2393	2399	2406	rBV	2378011	3549747	17.27%	4.536%
14	17.551	2498	2504	2511	rBV2	1646244	2669581	12.99%	3.411%
15	17.697	2525	2529	2533	rBV2	264840	335745	1.63%	0.429%
16	18.449	2648	2657	2673	rBV	10472083	20552506	100.00%	26.263%
17	19.084	2762	2765	2770	rBV4	153612	226548	1.10%	0.289%
18	19.701	2864	2870	2883	rBV	5662497	7911978	38.50%	10.110%
19	19.795	2883	2886	2892	rVV	220613	414776	2.02%	0.530%
20	19.871	2894	2899	2910	rVV2	1042064	1671556	8.13%	2.136%
21	19.971	2913	2916	2923	rVB	266203	393265	1.91%	0.503%
22	20.153	2941	2947	2952	rBV	6484076	8989692	43.74%	11.488%
23	21.458	3165	3169	3175	rBV5	160348	304165	1.48%	0.389%
24	21.851	3229	3236	3244	rVB2	1798432	3068474	14.93%	3.921%
25	25.206	3797	3807	3820	rVB	1008551	2944098	14.32%	3.762%

Sum of corrected areas: 78255181

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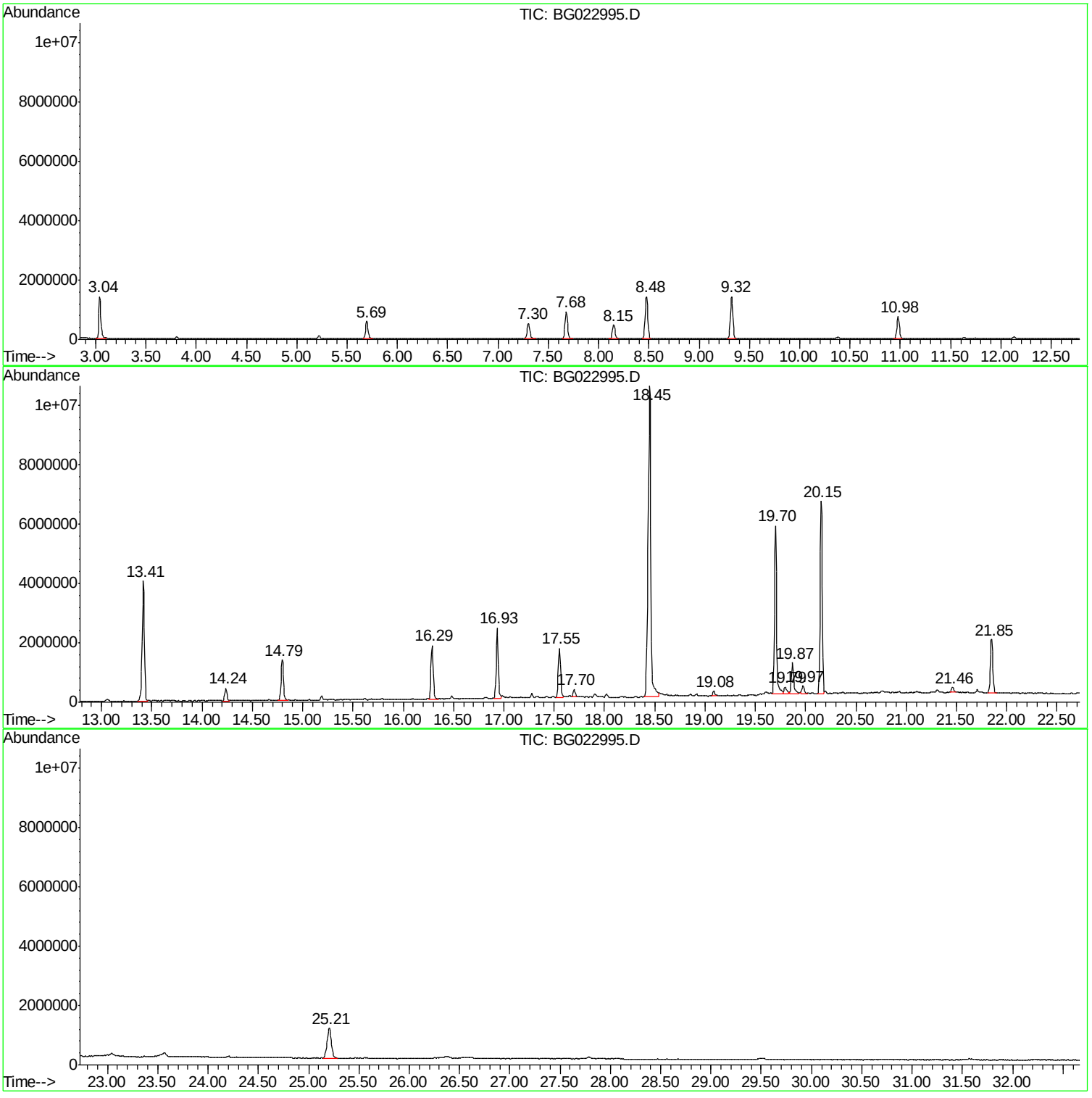
Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
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Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

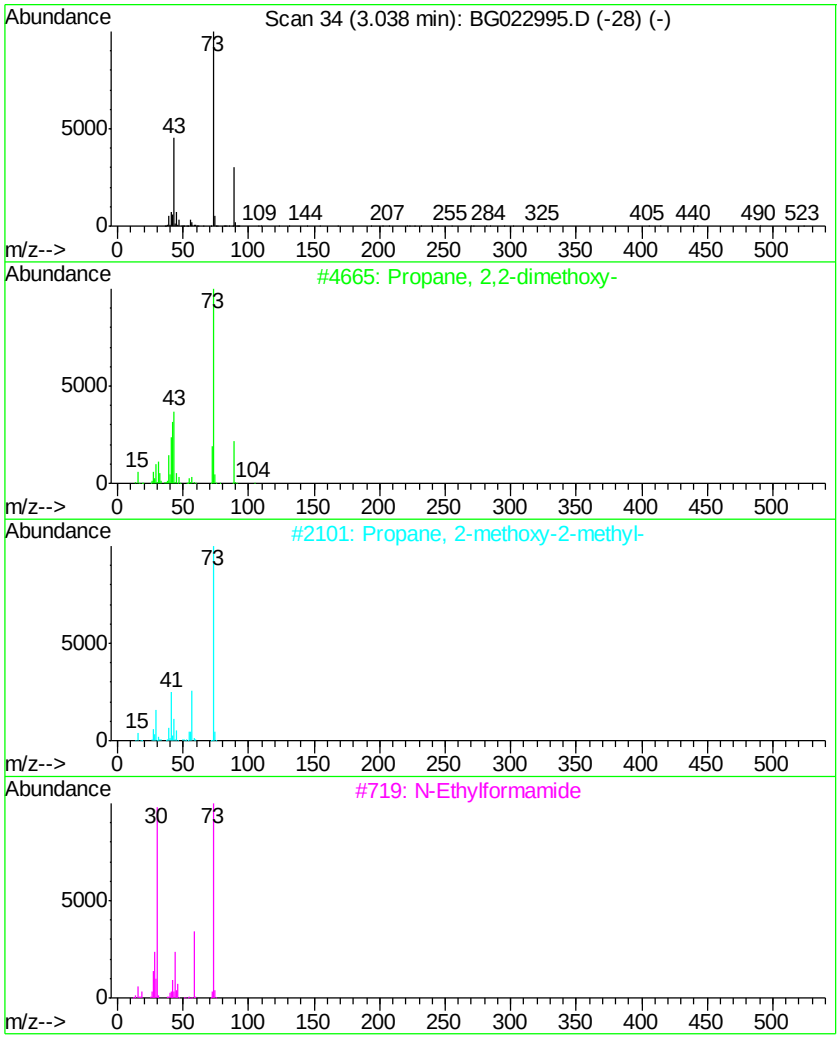
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

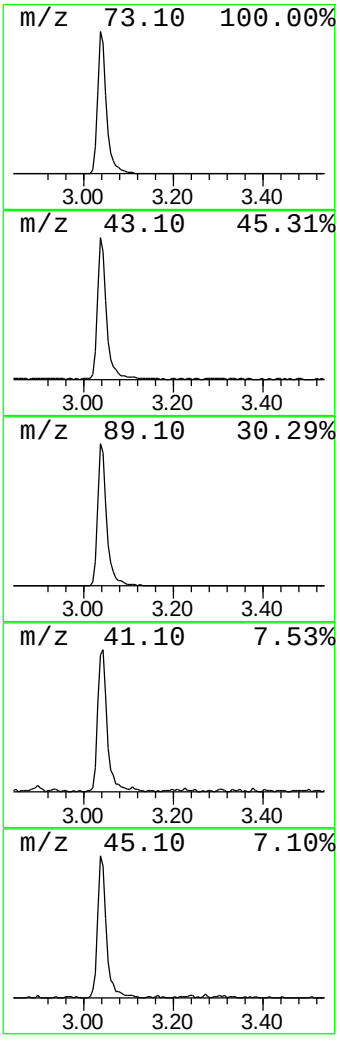
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	45.70 ng	1961360	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	7
4	1,3,5-Trioxane	90	C3H6O3	000110-88-3	4
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	4





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

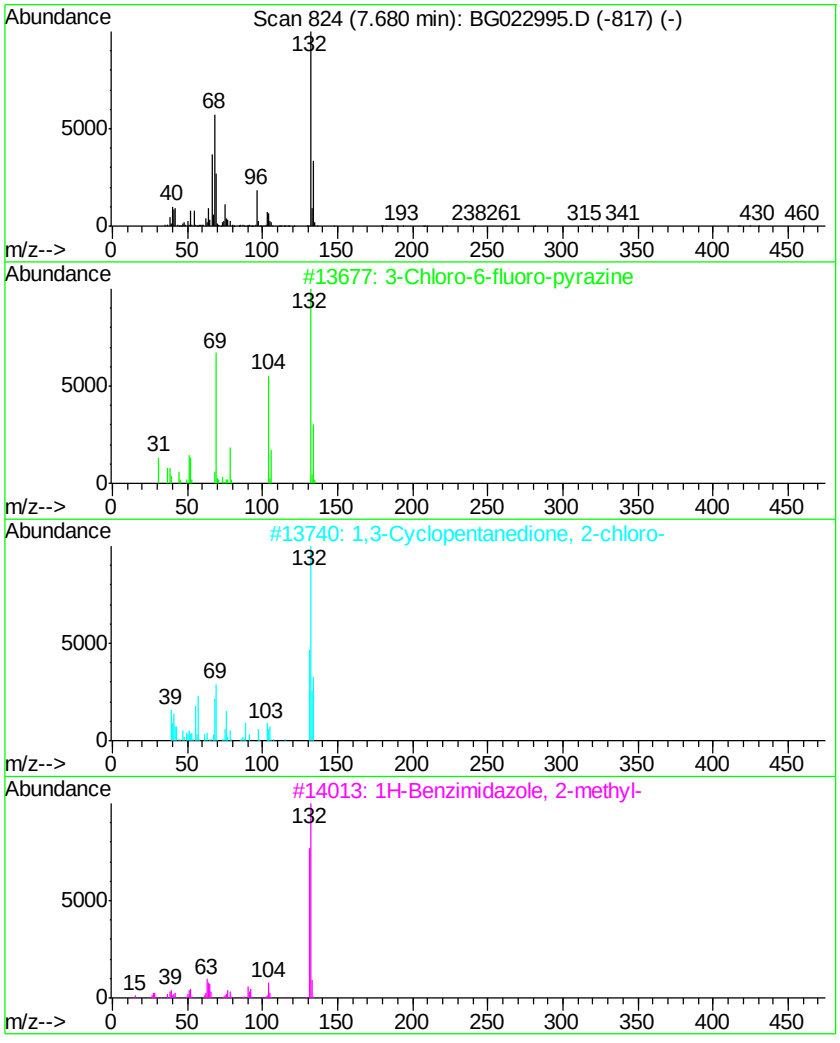
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

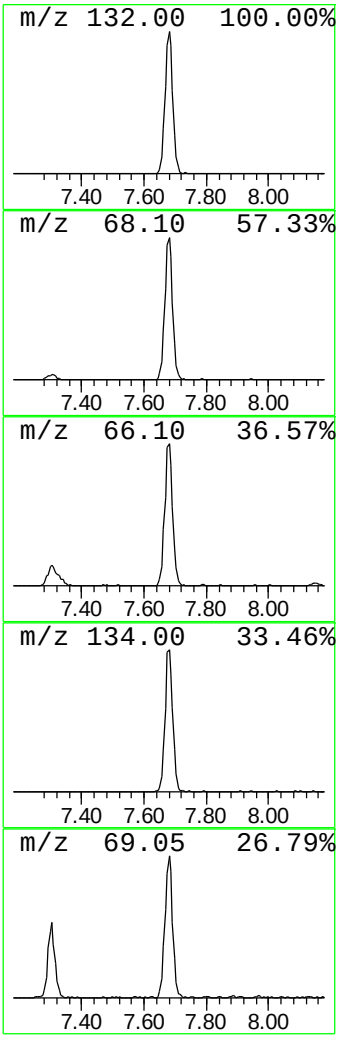
****

Peak Number 2 unknown7.68 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	36.85 ng	1581510	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
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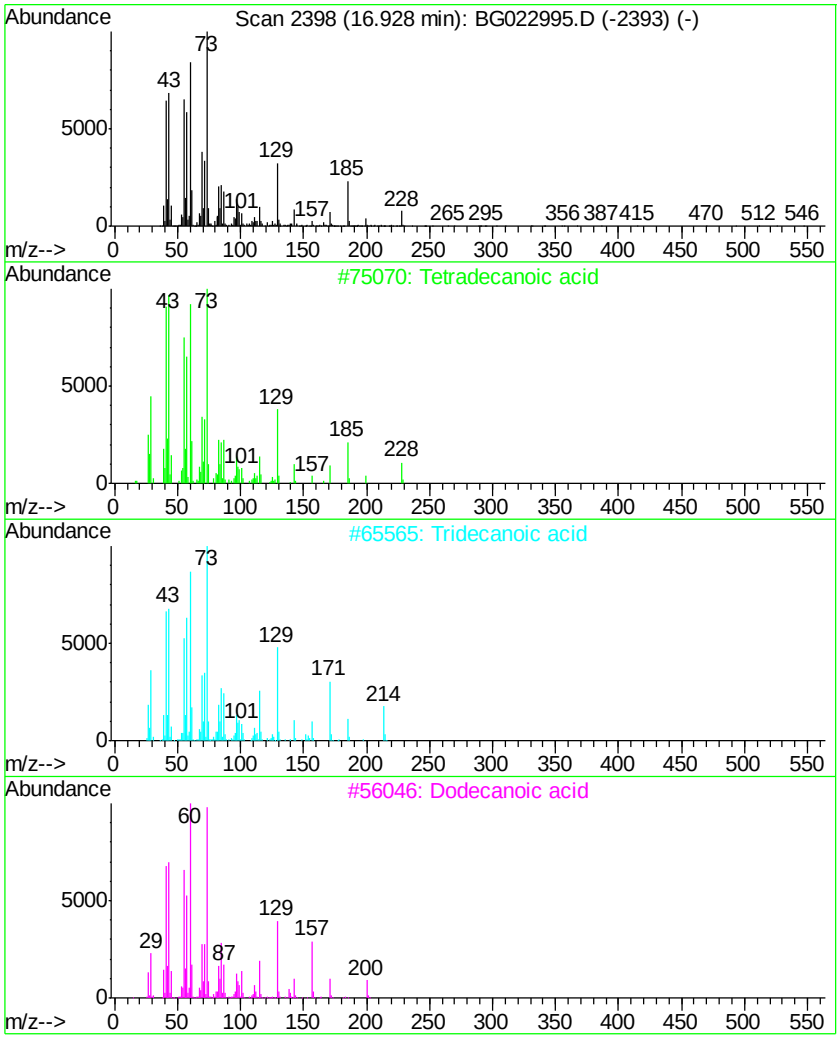
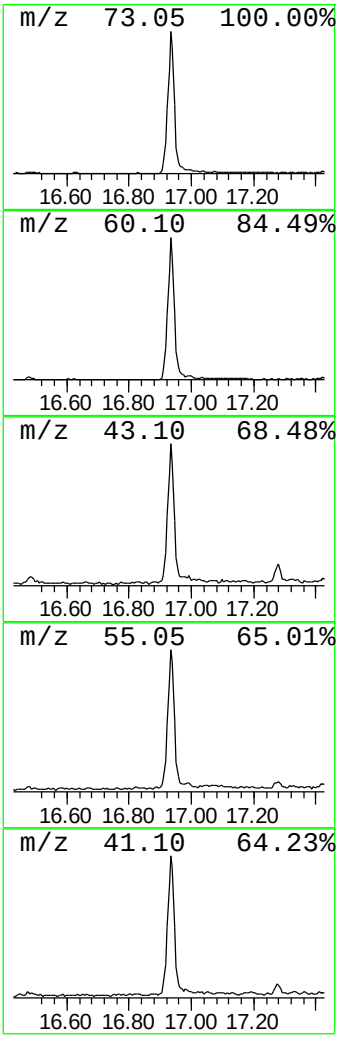
****

Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	26.59 ng	3549750	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

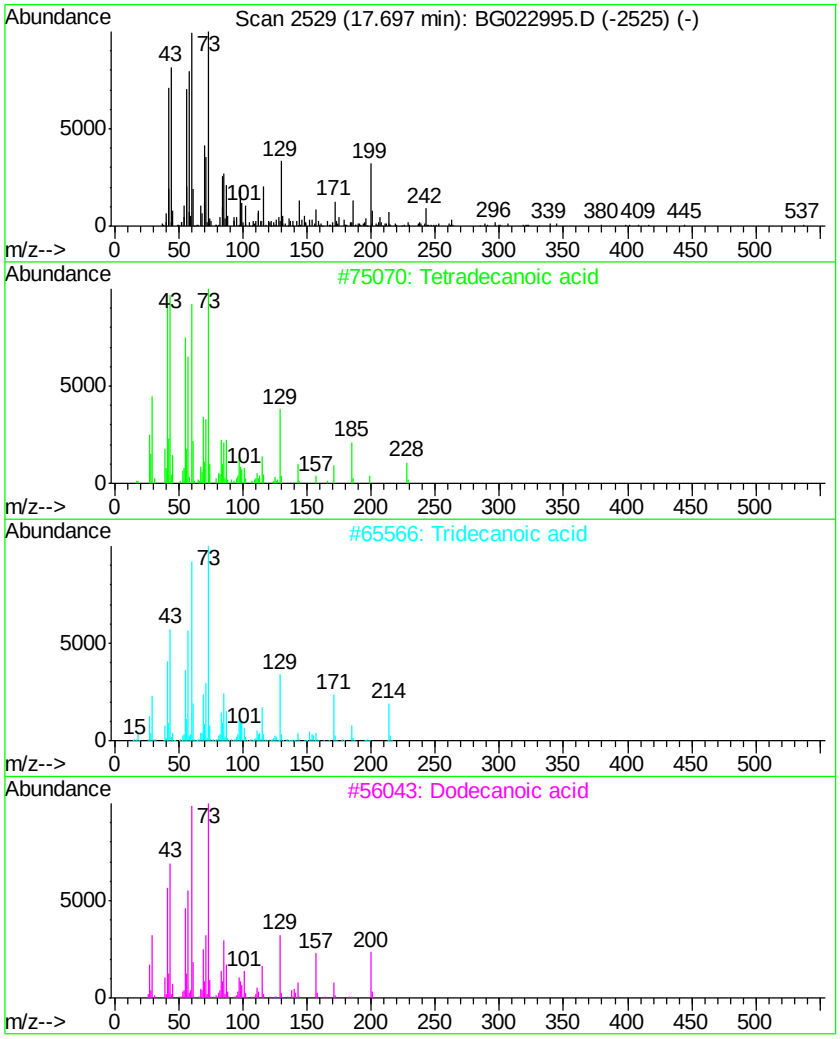
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

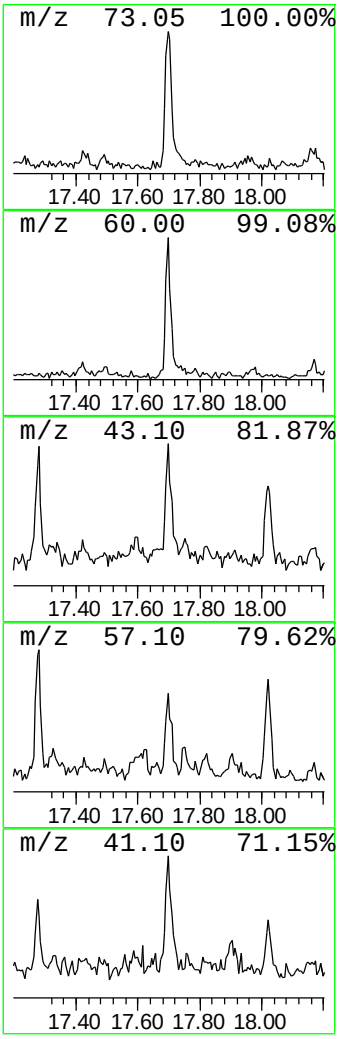
****

Peak Number 5 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	2.52 ng	335745	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

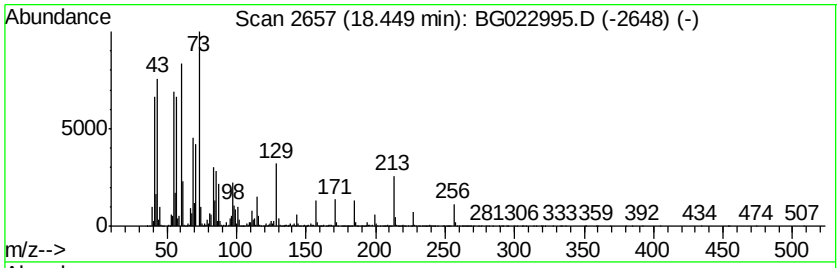
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

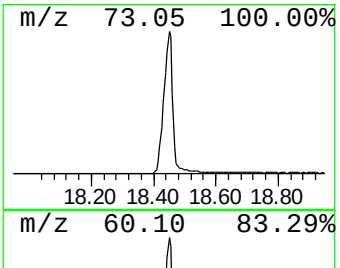
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.45	153.98 ng	20552500	Phenanthrene-d10	17.55

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

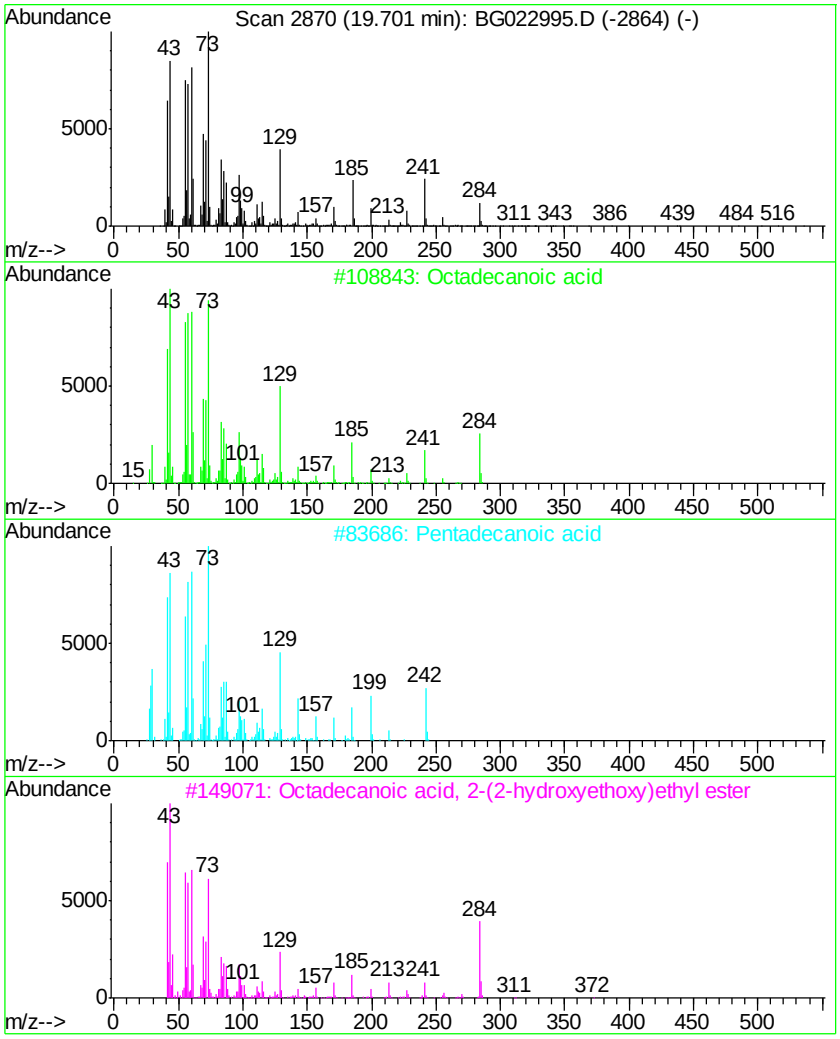
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

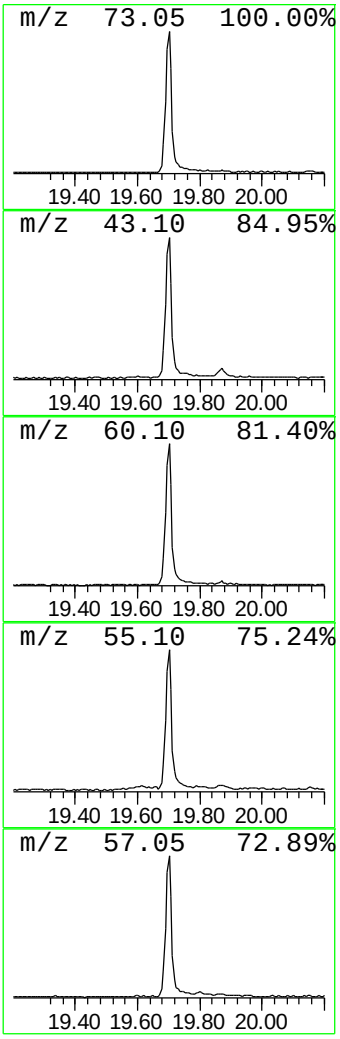
****

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	51.57 ng	7911980	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

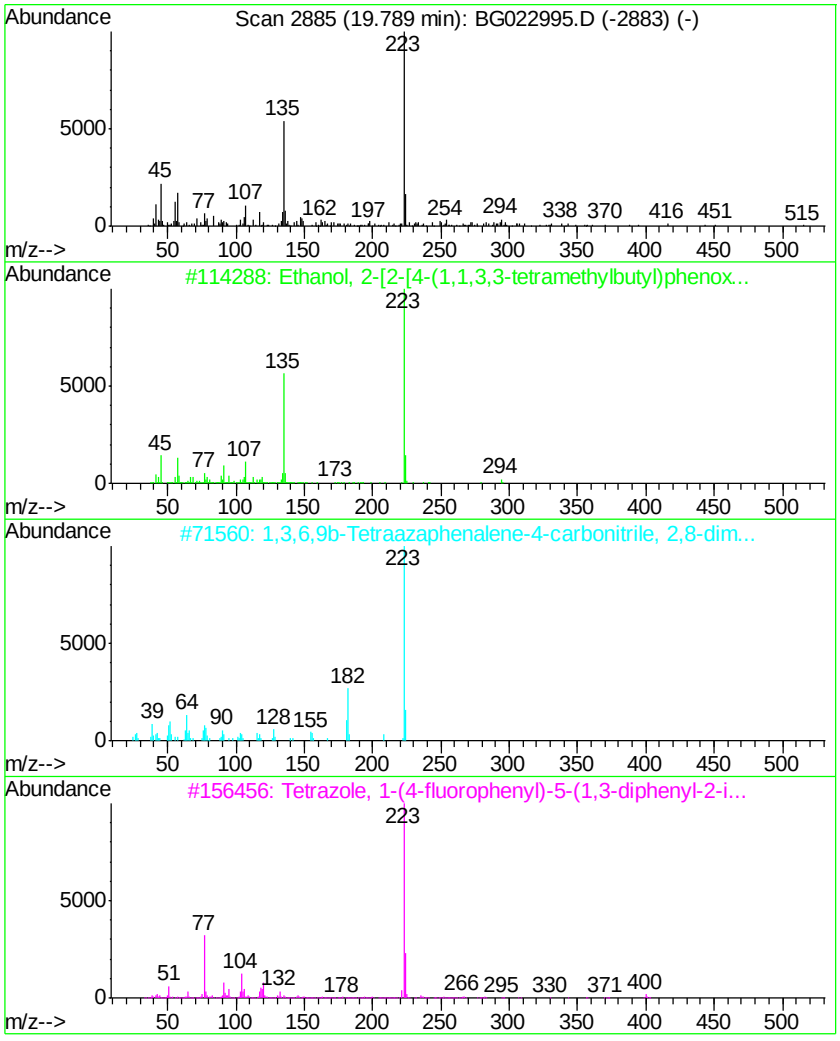
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

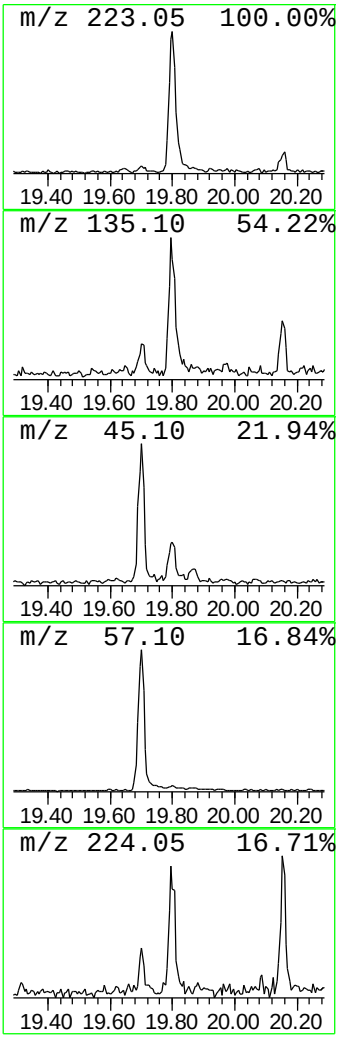
****

Peak Number 8 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	2.70 ng	414776	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	87
2	1,3,6,9b-Tetraazaphenalene-4-car...	223	C12H9N5	038439-32-6	32
3	Tetrazole, 1-(4-fluorophenyl)-5-...	400	C23H21FN6	125038-07-5	32
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	10
5	p-Methoxybenzenepentanoic acid, ...	222	C12H14O4	004609-10-3	10





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Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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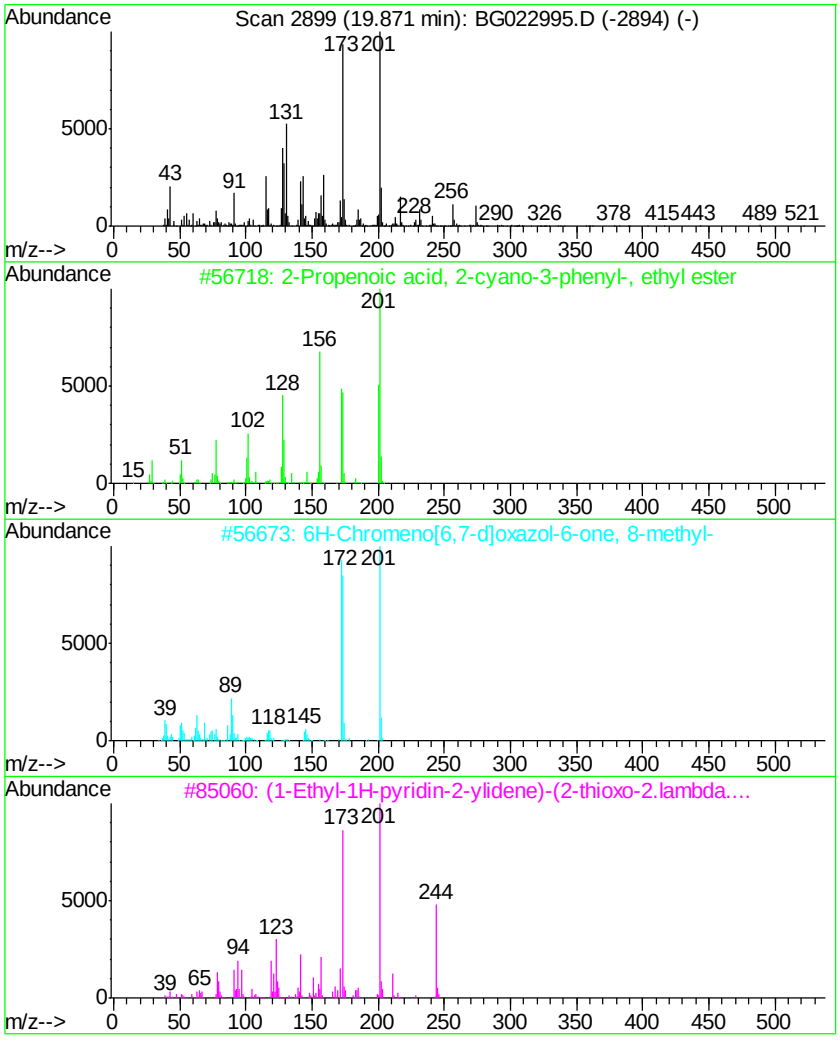
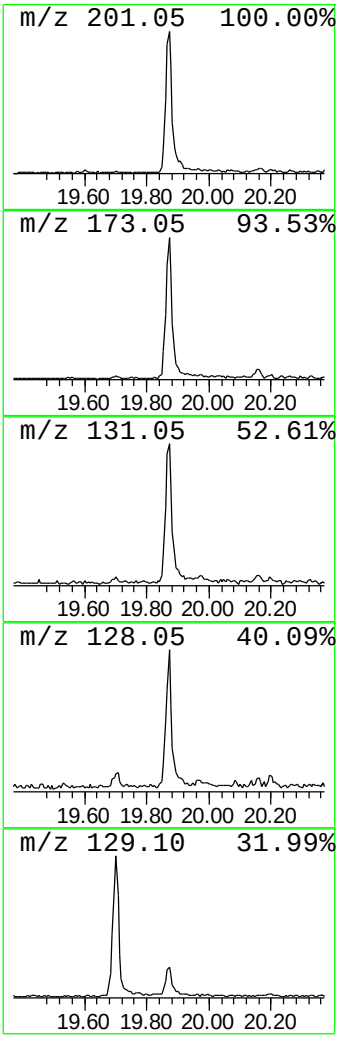
Peak Number 9 unknown19.87 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	10.90 ng	1671560	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-cyano-3-phen...	201	C12H11NO2	002025-40-3	43
2	6H-Chromeno[6,7-d]oxazol-6-one, ...	201	C11H7NO3	1000272-31-8	35
3	(1-Ethyl-1H-pyridin-2-ylidene)-(...	244	C9H13N2O2PS	1000296-45-1	32
4	Imidazo(2,1-a)phthalazine, 5-met...	201	C11H11N3O	057100-17-1	27
5	1H-Indene, 2,3-dihydro-1,1,2,3,3...	188	C14H20	001203-17-4	27





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Sample : H3840-03
Misc :
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Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

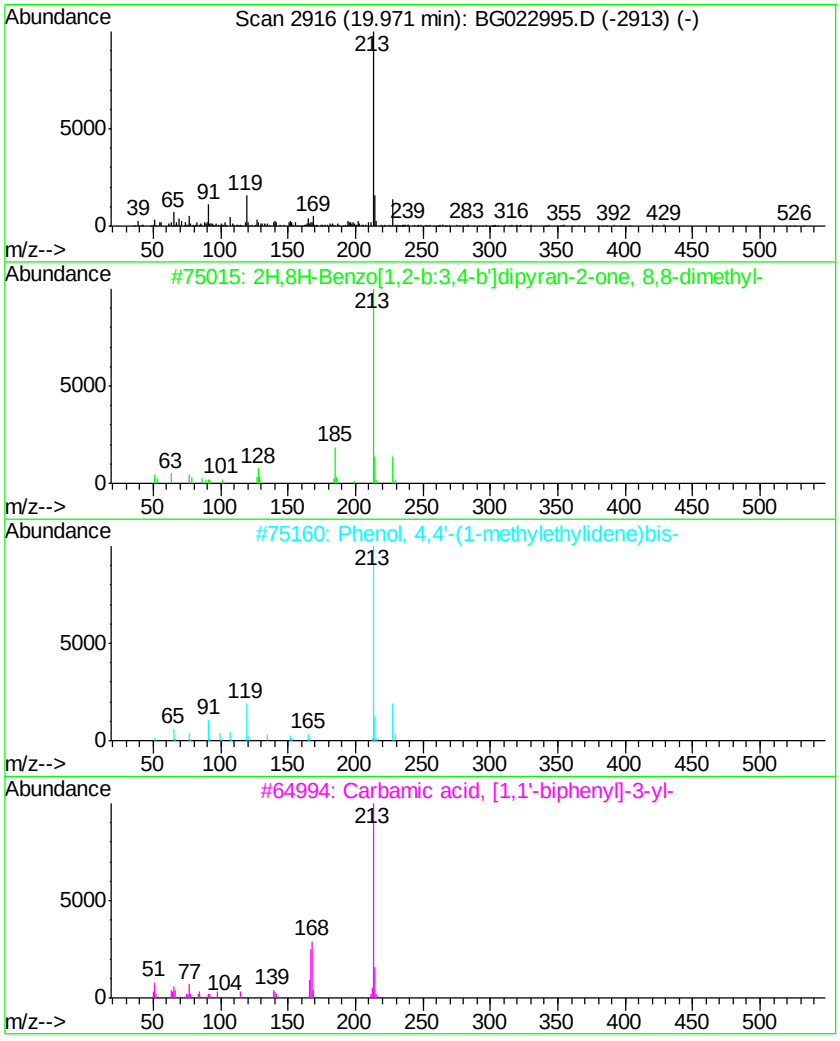
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

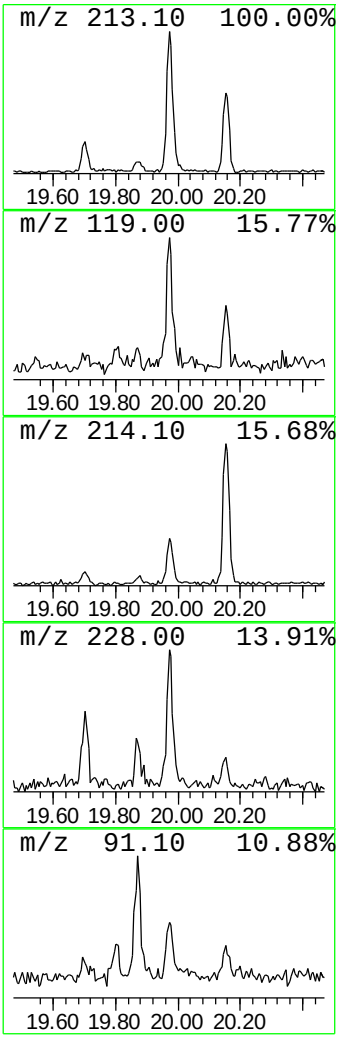
****

Peak Number 10 2H,8H-Benzo[1,2-b:3,4-b']di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.97	2.56 ng	393265	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	72
2	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	70
3	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	58
4	.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	53
5	Stannane, chlorotriethyl-	242	C6H15ClSn	000994-31-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022995.D
Acq On : 10 Jul 2016 11:28
Operator : UM/SJ
Sample : H3840-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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, 2,2-dime...	3.04	45.7	ng	1961360	1	8.15	858306	20.0
unknown7.68	7.68	36.9	ng	1581510	1	8.15	858306	20.0
Tetradecanoic acid	16.93	26.6	ng	3549750	4	17.55	2669580	20.0
Tridecanoic acid	17.70	2.5	ng	335745	4	17.55	2669580	20.0
n-Hexadecanoic acid	18.45	154.0	ng	20552500	4	17.55	2669580	20.0
Octadecanoic acid	19.70	51.6	ng	7911980	5	21.85	3068470	20.0
Ethanol, 2-[2-[4-...	19.79	2.7	ng	414776	5	21.85	3068470	20.0
unknown19.87	19.87	10.9	ng	1671560	5	21.85	3068470	20.0
2H,8H-Benzo[1,2-b...	19.97	2.6	ng	393265	5	21.85	3068470	20.0