LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

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-BG022916.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	3.061	32	38	57	rVV	1263974	1872202	100.00%	25.887%
2	3.208	57	63	72	rVB	10993	22640	1.21%	0.313%
3	5.235	402	408	418	rVB	58534	94561	5.05%	1.308%
4	5.705	481	488	496	rBV	256492	428737	22.90%	5.928%
5	7.298	749	759	768	rBV	291905	508497	27.16%	7.031%
6	7.679	816	824	831	rBV	286525	485115	25.91%	6.708%
7	8.149	897	904	910	rVB	57605	96700	5.17%	1.337%
8	8.473	952	959	967	rVB	181646	313195	16.73%	4.331%
9	9.313	1094	1102	1110	rBV	188079	331235	17.69%	4.580%
10	10.958	1375	1382	1389	rBV	85873	149841	8.00%	2.072%
11	13.385	1788	1795	1802	rVB	365886	558032	29.81%	7.716%
12	14.195	1928	1933	1940	rBV	65448	97411	5.20%	1.347%
13	14.754	2023	2028	2037	rVB2	114719	190860	10.19%	2.639%
14	15.576	2164	2168	2173	rVB	16296	20711	1.11%	0.286%
15	16.234	2271	2280	2287	rBV	318629	474526	25.35%	6.561%
16	16.434	2310	2314	2323	rBV2	15541	26872	1.44%	0.372%
17	17.491	2488	2494	2499	rBV	146081	218610	11.68%	3.023%
18	18.355	2636	2641	2647	rBV	50395	71825	3.84%	0.993%
19	19.530	2837	2841	2847	rVB	20554	31758	1.70%	0.439%
20	19.618	2852	2856	2863	rVV5	15447	26225	1.40%	0.363%
21	19.889	2898	2902	2907	rBV2	21969	30715	1.64%	0.425%
22	20.083	2929	2935	2941	rBV	516057	657363	35.11%	9.090%
23	20.752	3045	3049	3055	rBV2	19842	34446	1.84%	0.476%
24	21.375	3151	3155	3159	rBV2	26129	37347	1.99%	0.516%
25	21.751	3213	3219	3225	rBV	144070	249920	13.35%	3.456%
26	25.030	3771	3777	3792	rVB2	64721	202742	10.83%	2.803%

Sum of corrected areas: 7232086

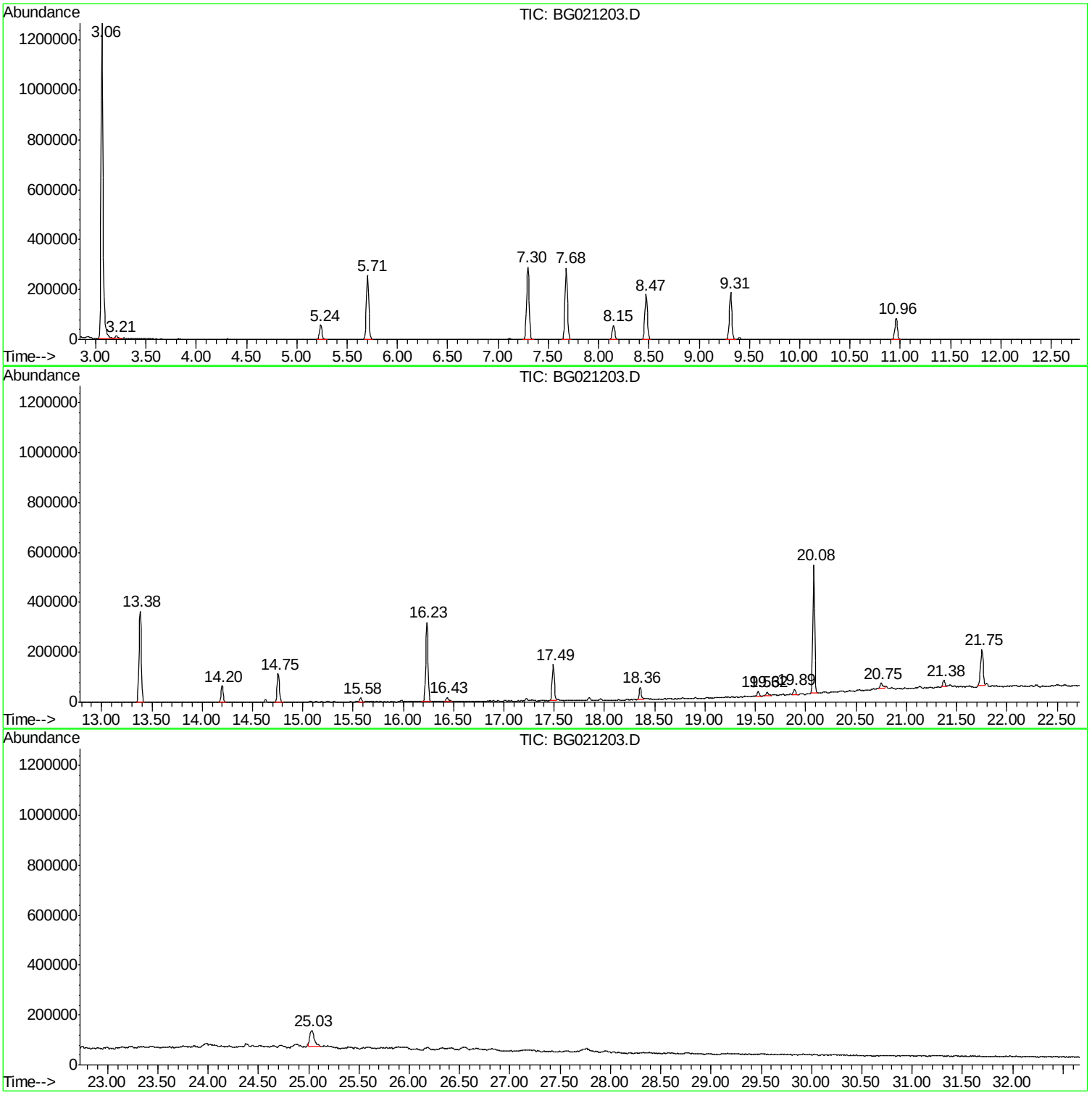
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.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 G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

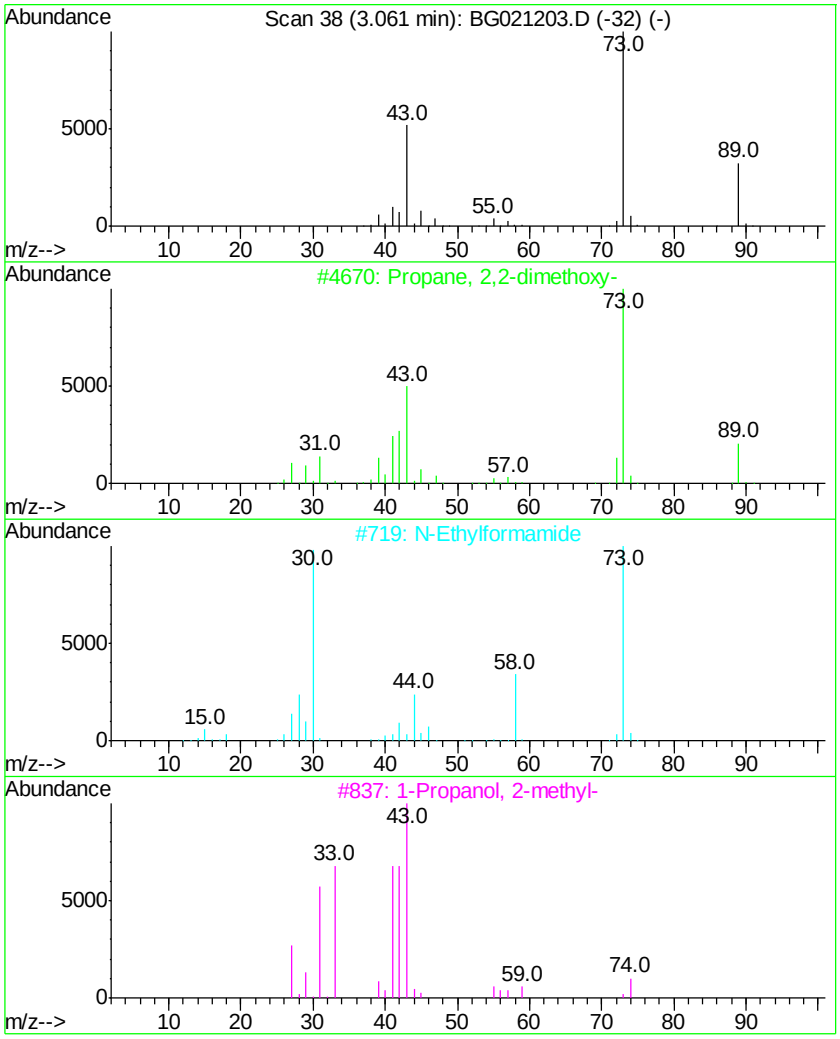
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

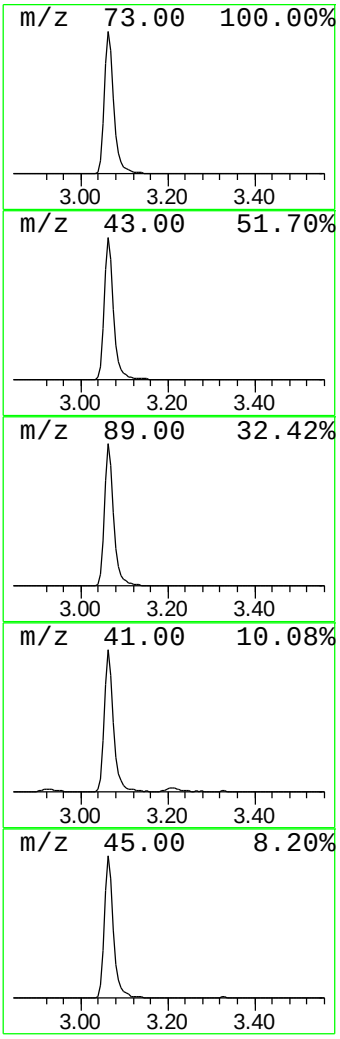
****

Peak Number 1 unknown3.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	387.22 ng	1872200	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	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

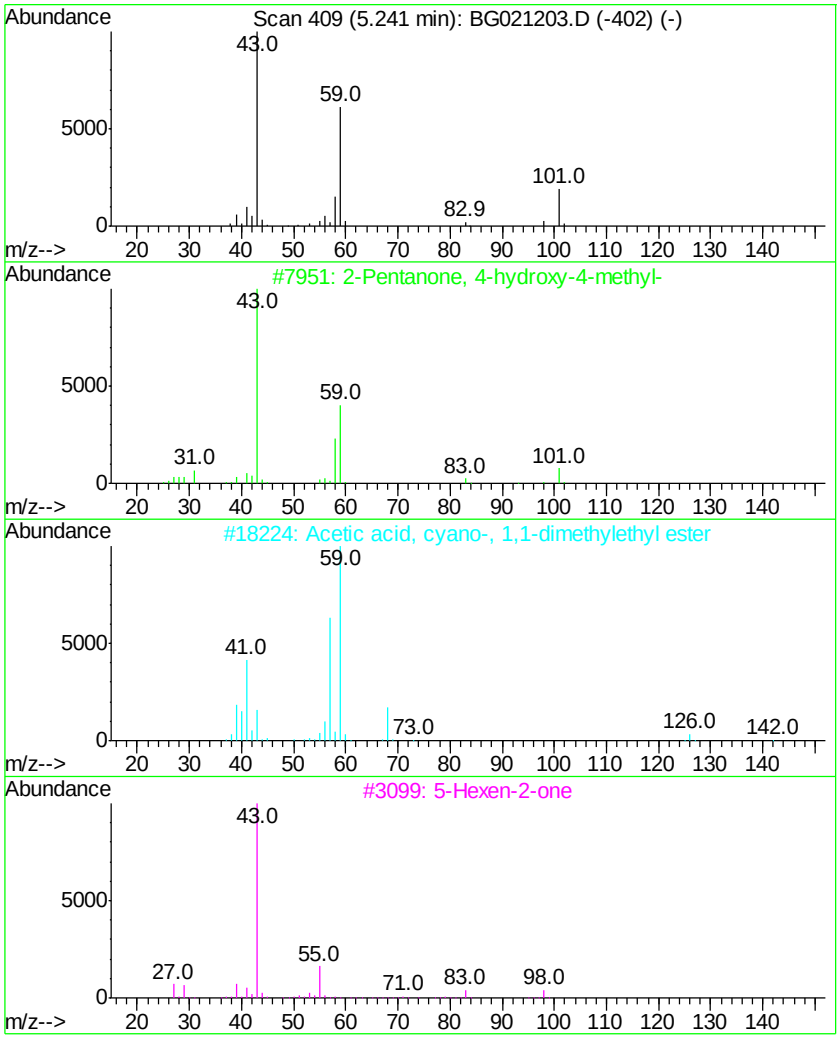
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

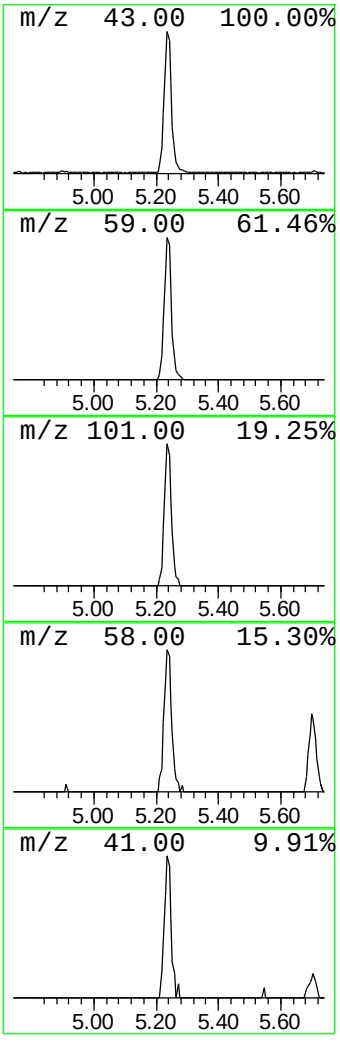
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	19.56 ng	94561	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.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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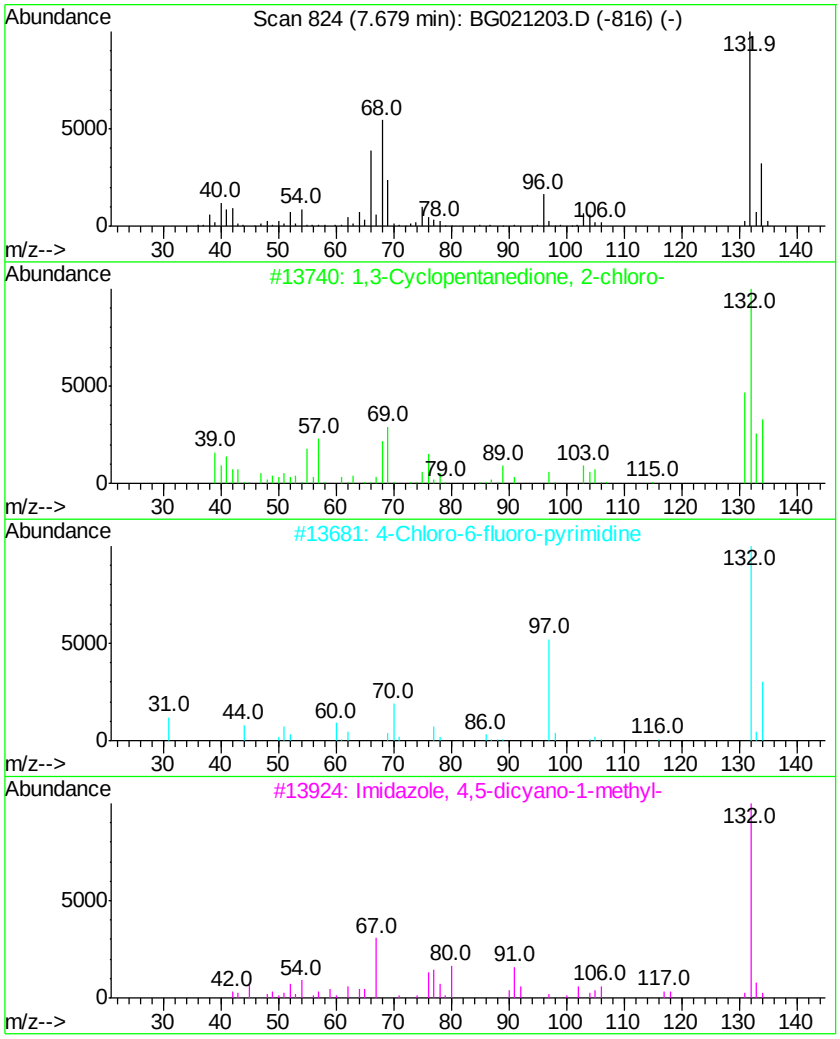
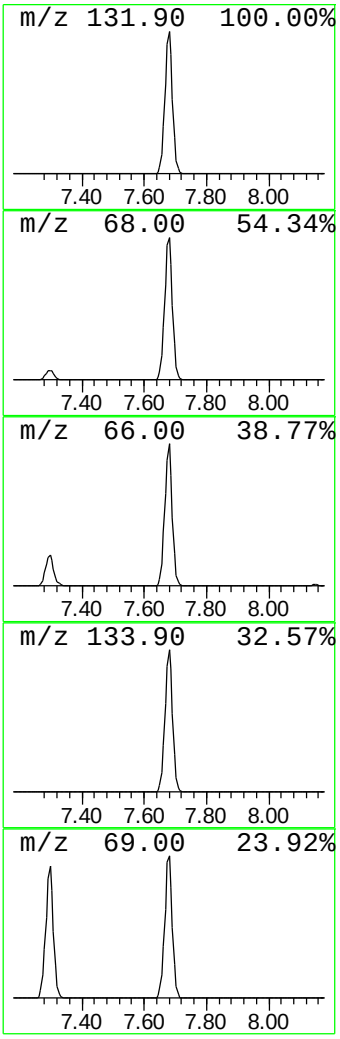
Peak Number 4 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	100.33 ng	485115	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.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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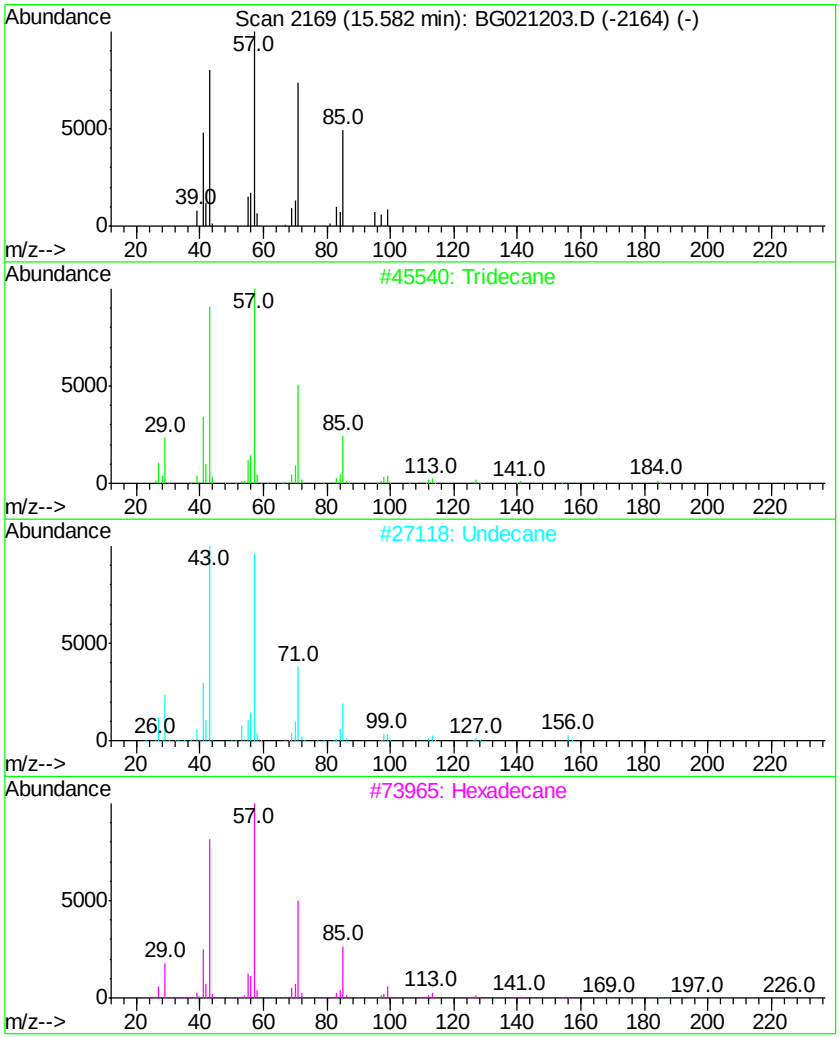
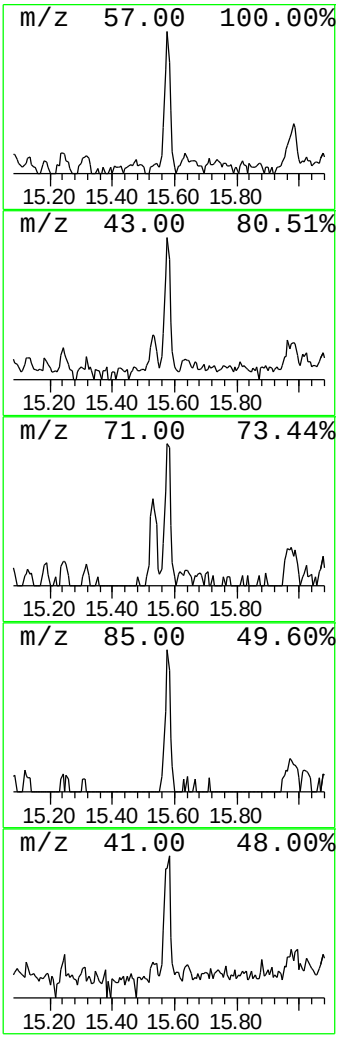
Peak Number 6 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.17 ng	20711	Acenaphthene-d10	14.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	78
2	Undecane	156	C11H24	001120-21-4	72
3	Hexadecane	226	C16H34	000544-76-3	72
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.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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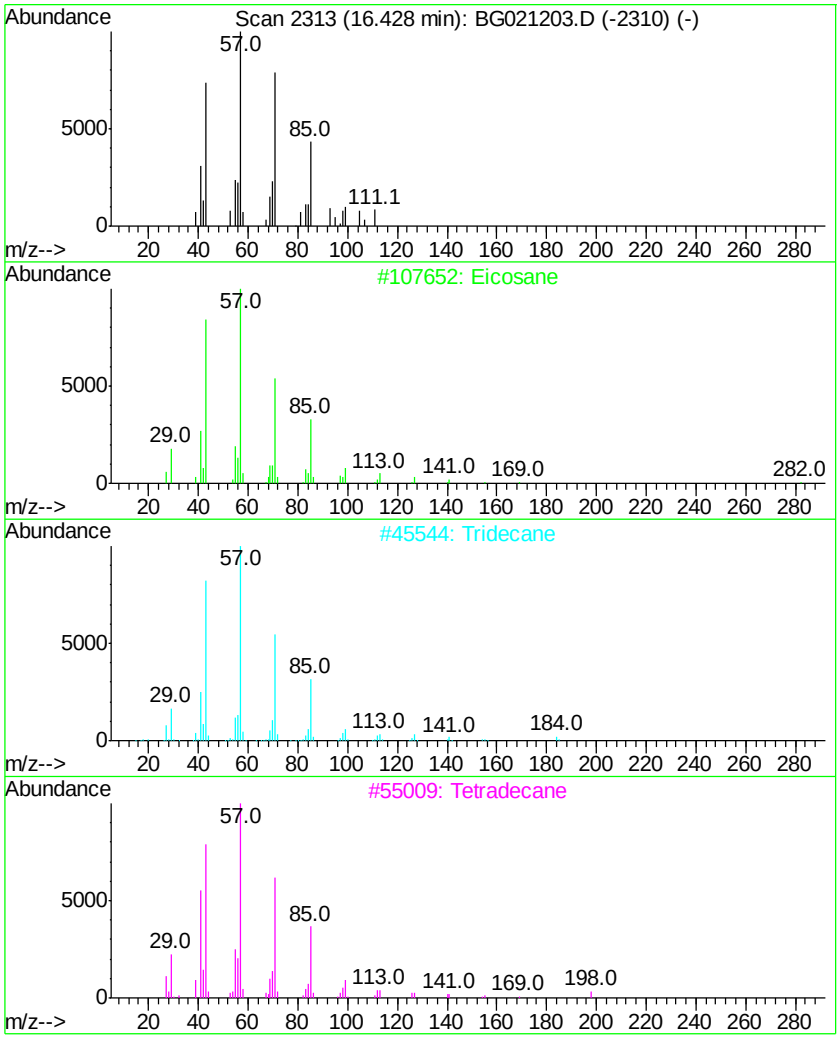
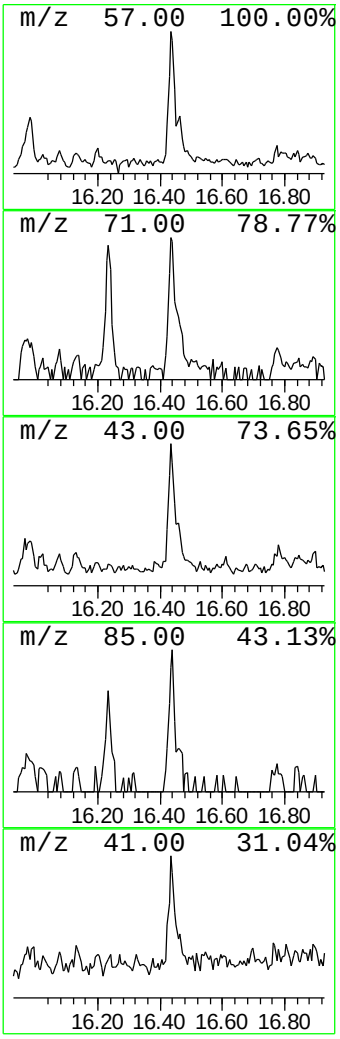
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.46 ng	26872	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Tridecane	184	C13H28	000629-50-5	78
3	Tetradecane	198	C14H30	000629-59-4	78
4	Hexadecane	226	C16H34	000544-76-3	78
5	Pentadecane	212	C15H32	000629-62-9	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
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Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

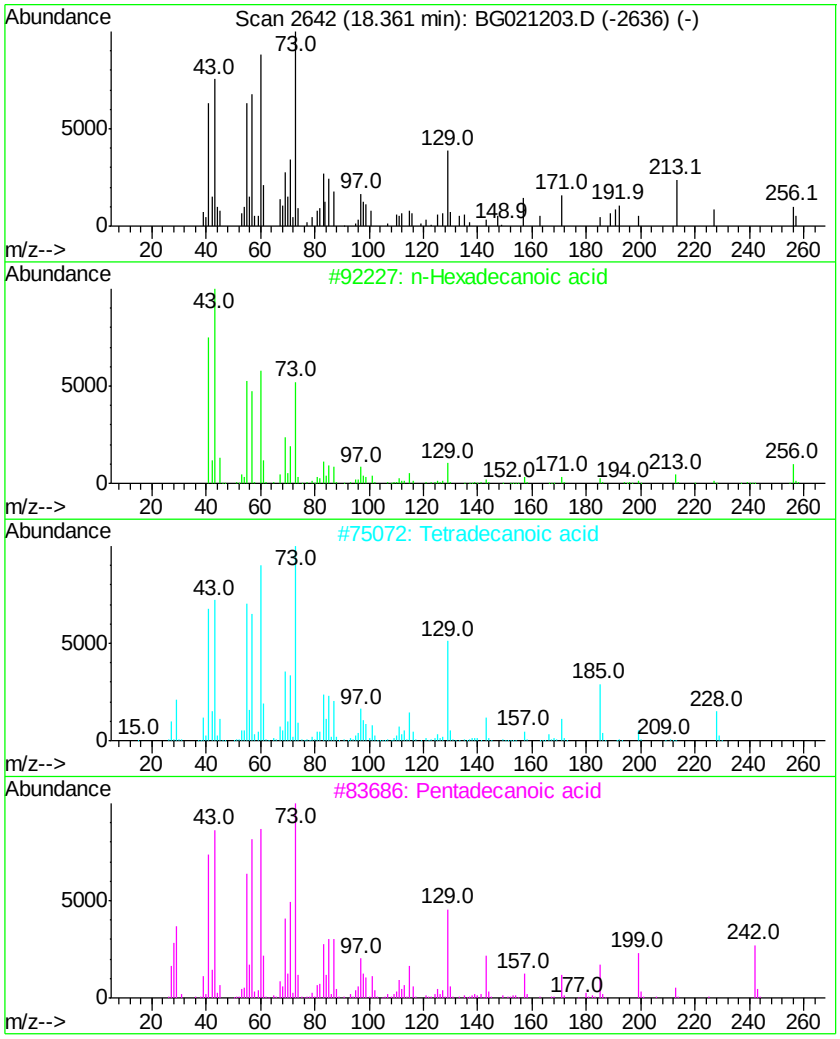
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

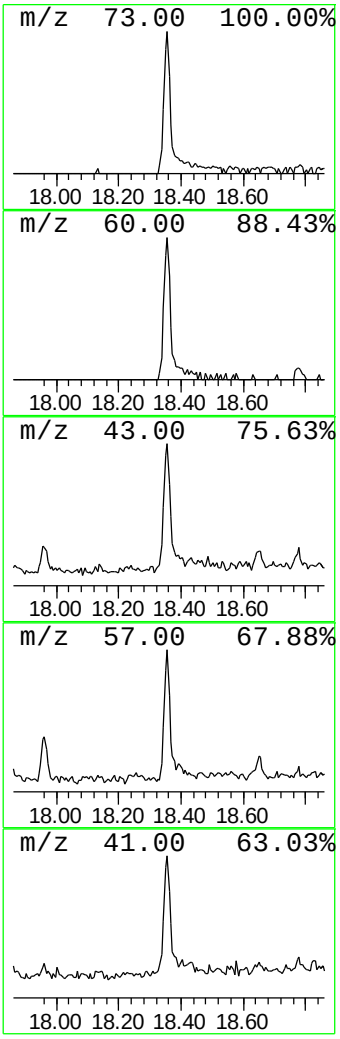
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	6.57 ng	71825	Phenanthrene-d10	17.49

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	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Data File : BG021203.D
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Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

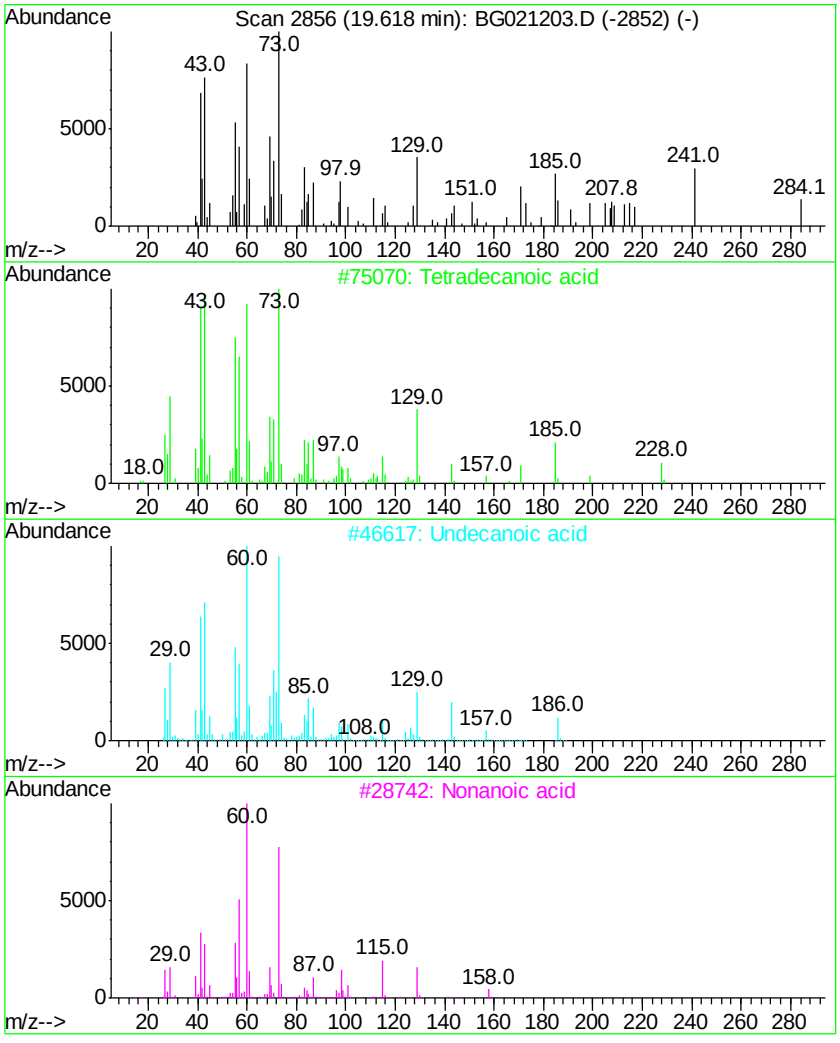
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

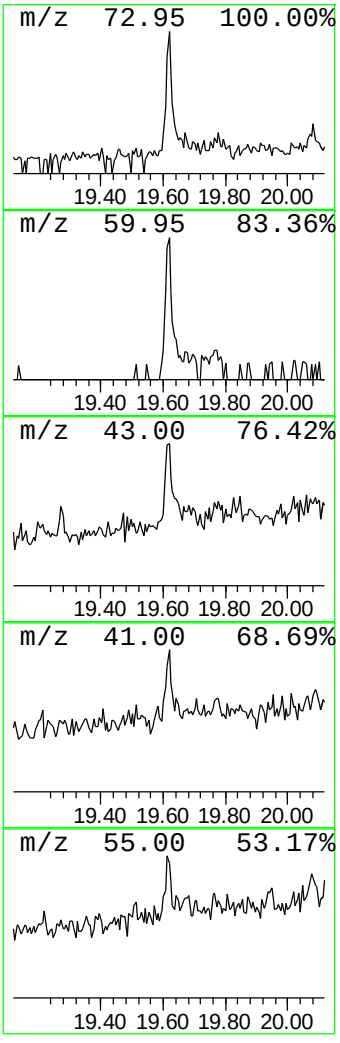
****

Peak Number 9 unknown19.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.40 ng	26225	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
2	Undecanoic acid	186	C11H22O2	000112-37-8	43
3	Nonanoic acid	158	C9H18O2	000112-05-0	43
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
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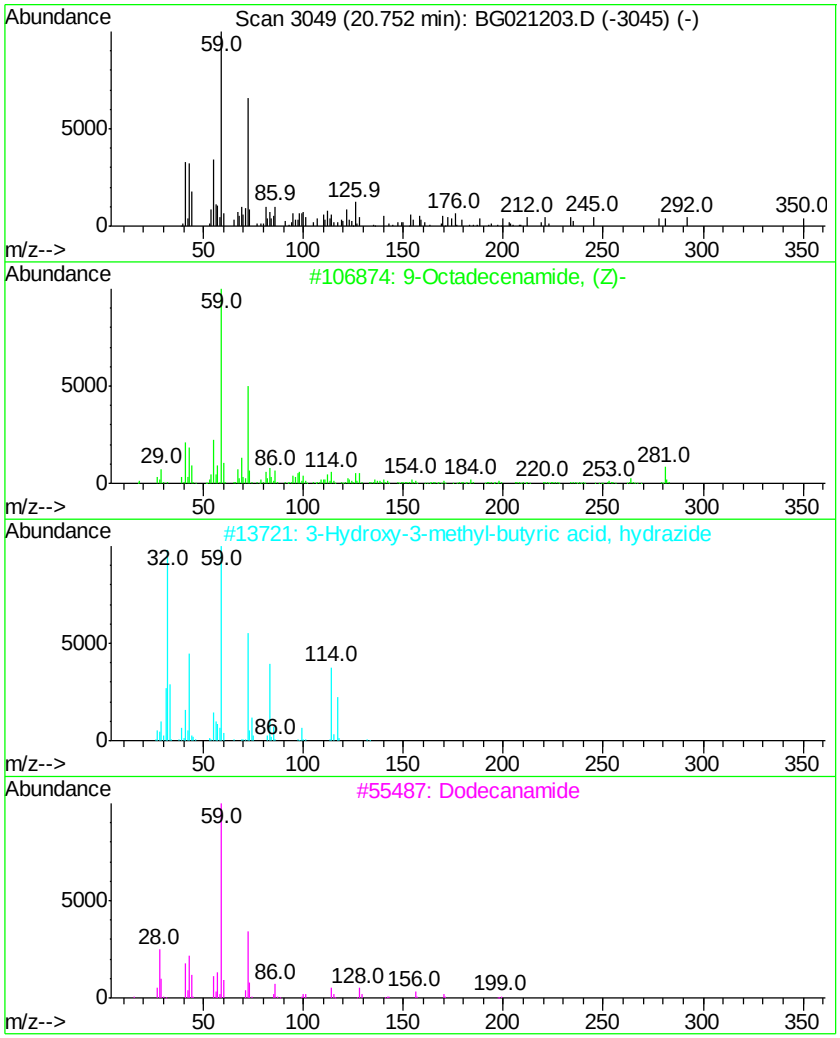
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

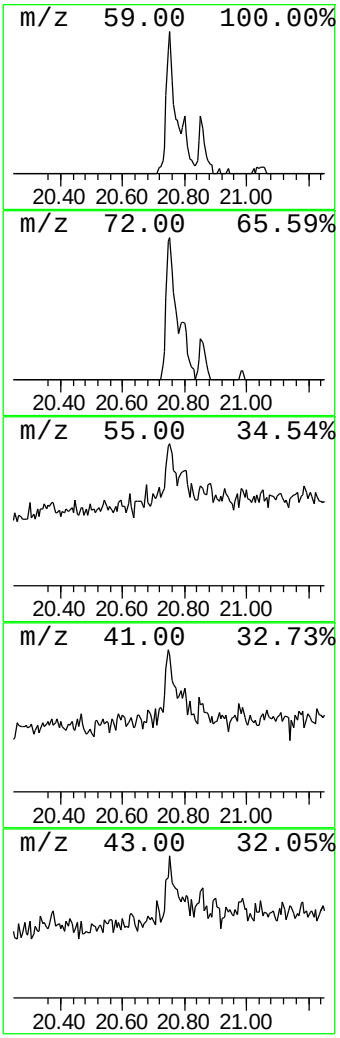
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	2.76 ng	34446	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	59
3	Dodecanamide	199	C12H25NO	001120-16-7	47
4	Octanamide	143	C8H17NO	000629-01-6	47
5	Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	38





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Misc :
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Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

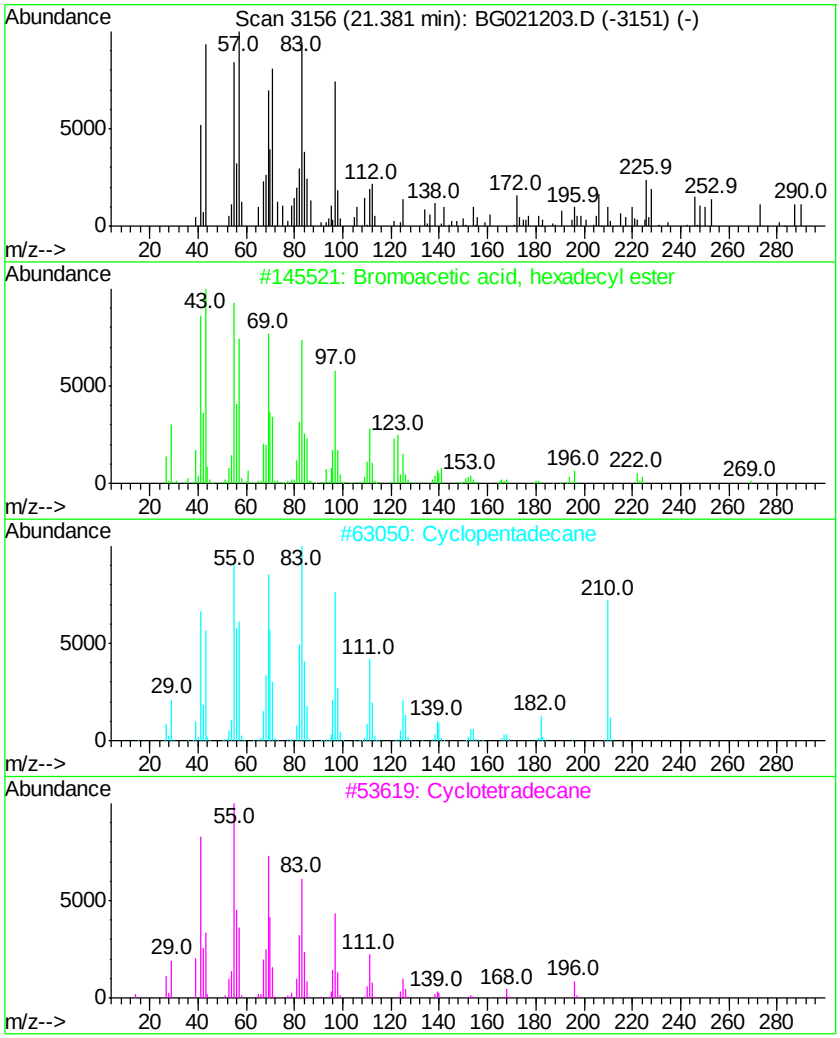
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

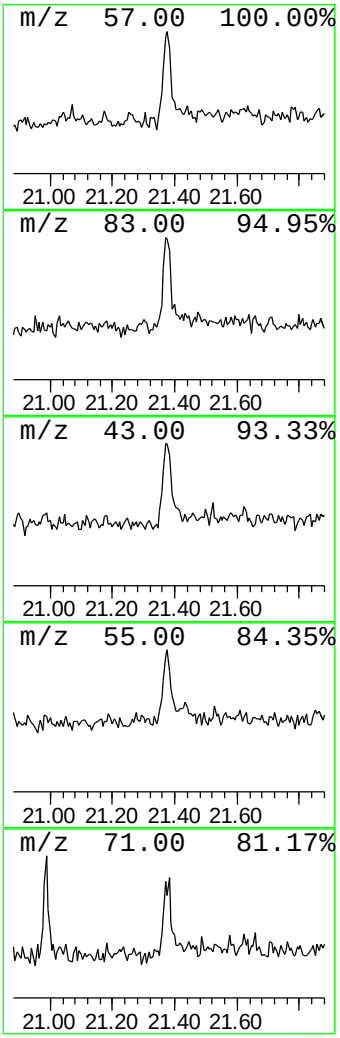
****

Peak Number 11 Bromoacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	2.99 ng	37347	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2	Cyclopentadecane	210	C15H30	000295-48-7	83
3	Cyclotetradecane	196	C14H28	000295-17-0	83
4	11-Tricosene	322	C23H46	052078-56-5	81
5	1-Pentadecene	210	C15H30	013360-61-7	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030116\
Data File : BG021203.D
Acq On : 2 Mar 2016 3:41
Operator : UM/SJ
Sample : H1579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-11

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022916.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
unknown3.06	3.06	387.2	ng	1872200	1	8.15	96700	20.0
2-Pentanone, 4-hy...	5.24	19.6	ng	94561	1	8.15	96700	20.0
unknown7.68	7.68	100.3	ng	485115	1	8.15	96700	20.0
Tridecane	15.58	2.2	ng	20711	3	14.75	190860	20.0
Eicosane	16.43	2.5	ng	26872	4	17.49	218610	20.0
n-Hexadecanoic acid	18.36	6.6	ng	71825	4	17.49	218610	20.0
unknown19.62	19.62	2.4	ng	26225	4	17.49	218610	20.0
9-Octadecenamide,...	20.75	2.8	ng	34446	5	21.75	249920	20.0
Bromoacetic acid,...	21.38	3.0	ng	37347	5	21.75	249920	20.0