LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

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-BG050515.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	2.805	16	20	30	rBV2	65592	118506	3.15%	0.651%
2	2.887	30	34	45	rVB	111502	150692	4.00%	0.827%
3	4.826	359	364	369	rBV	47887	64180	1.71%	0.352%
4	5.314	440	447	454	rBV	960995	1339993	35.60%	7.356%
5	6.918	712	720	727	rBV	1014760	1540634	40.93%	8.457%
6	7.259	770	778	785	rBV	992095	1499348	39.84%	8.231%
7	7.717	847	856	862	rBV	154932	236207	6.28%	1.297%
8	8.034	902	910	917	rBV	667752	1086713	28.87%	5.966%
9	8.875	1045	1053	1062	rVB	568641	941771	25.02%	5.170%
10	10.508	1324	1331	1337	rBV	191441	307750	8.18%	1.689%
11	12.987	1744	1753	1760	rBV	1525627	2131324	56.63%	11.700%
12	13.822	1890	1895	1903	rVB2	66437	97280	2.58%	0.534%
13	14.368	1982	1988	1995	rBV2	287193	440557	11.71%	2.418%
14	15.861	2235	2242	2253	rBV	1593835	2220470	59.00%	12.189%
15	17.112	2449	2455	2463	rVB2	440679	602532	16.01%	3.308%
16	18.011	2603	2608	2614	rBV2	58402	85597	2.27%	0.470%
17	19.744	2898	2903	2912	rVB	2986943	3763713	100.00%	20.661%
18	20.390	3007	3013	3016	rBV6	32118	47283	1.26%	0.260%
19	20.426	3016	3019	3027	rVB9	27367	44208	1.17%	0.243%
20	21.007	3113	3118	3127	rBV2	105031	159753	4.24%	0.877%
21	21.295	3161	3167	3173	rBV	539678	693043	18.41%	3.804%
22	23.563	3546	3553	3559	rVB	346208	644955	17.14%	3.540%

Sum of corrected areas: 18216509

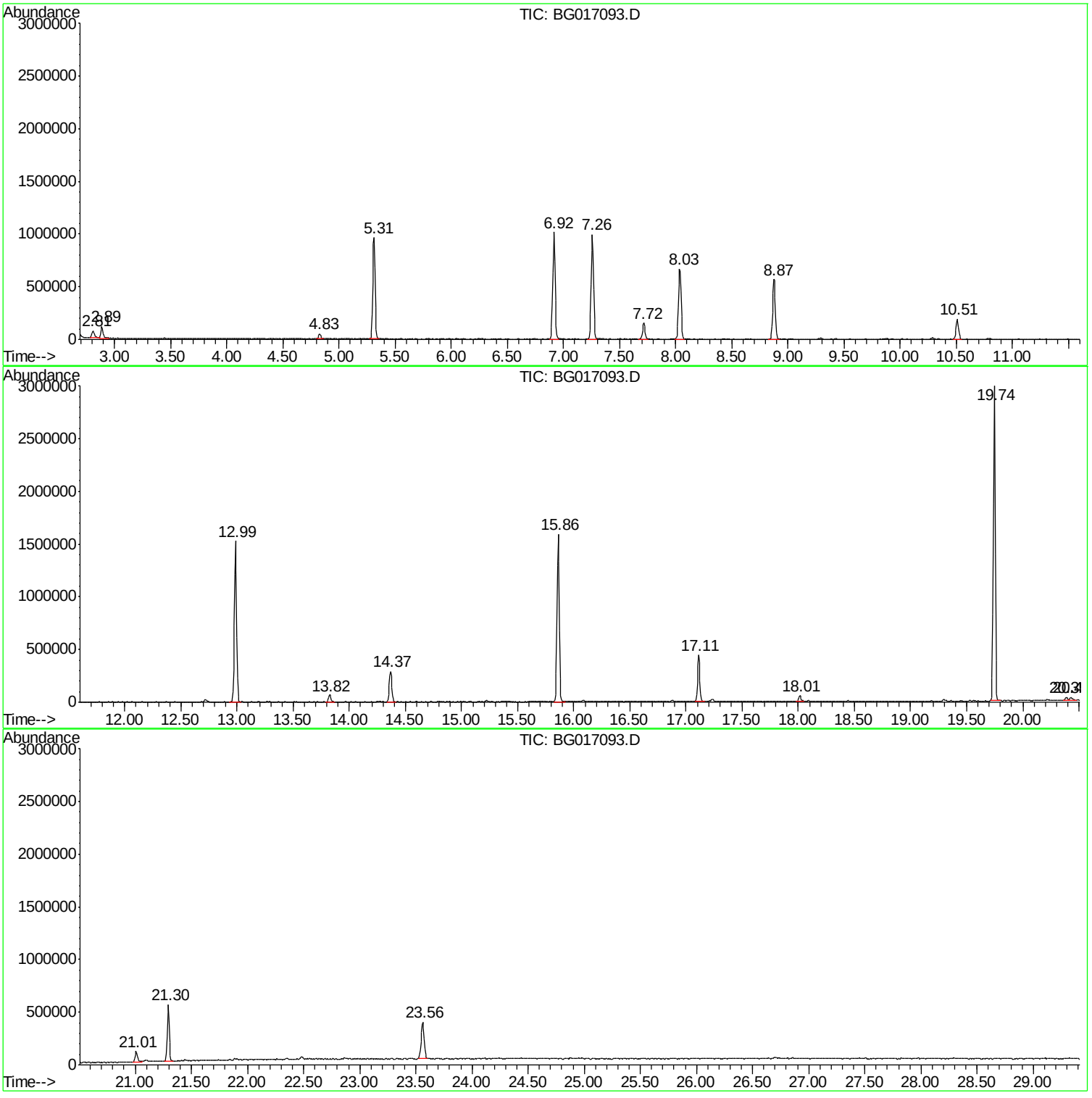
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

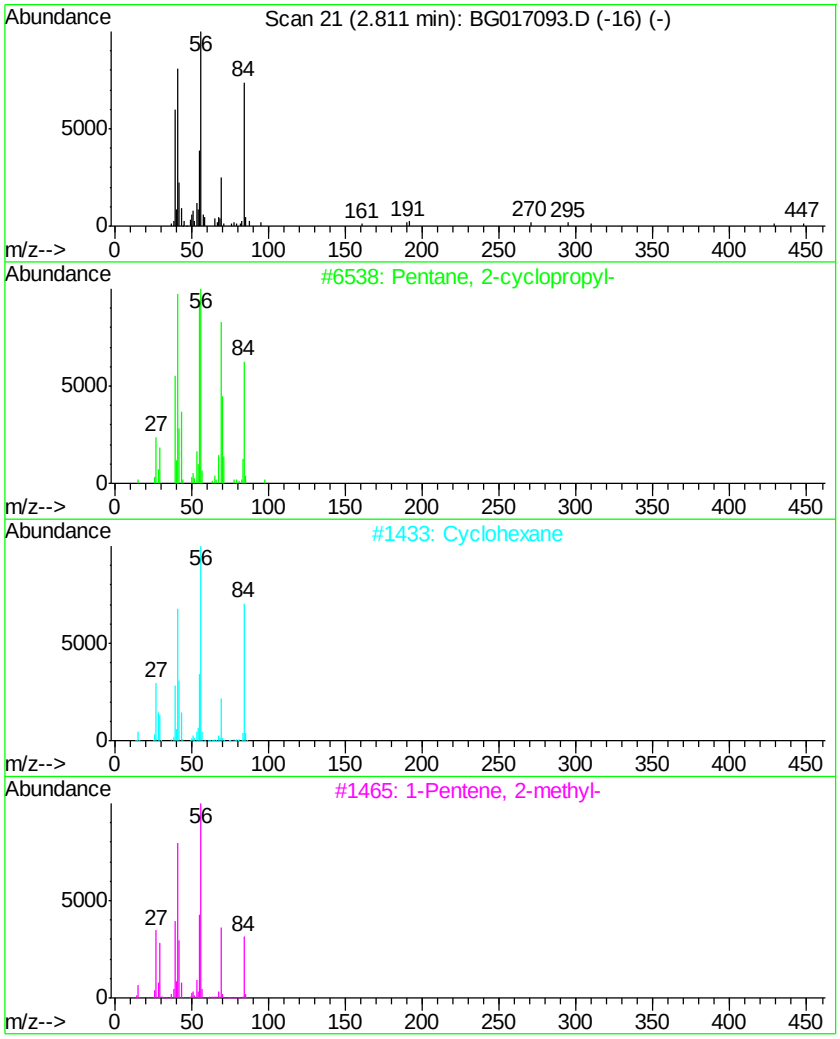
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

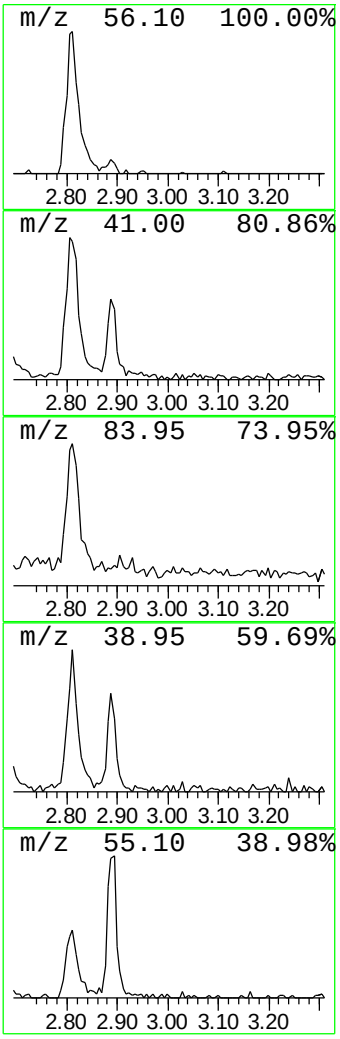
****

Peak Number 1 Pentane, 2-cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	10.03 ng	118506	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	72
2	Cyclohexane	84	C6H12	000110-82-7	62
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
4	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	47
5	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

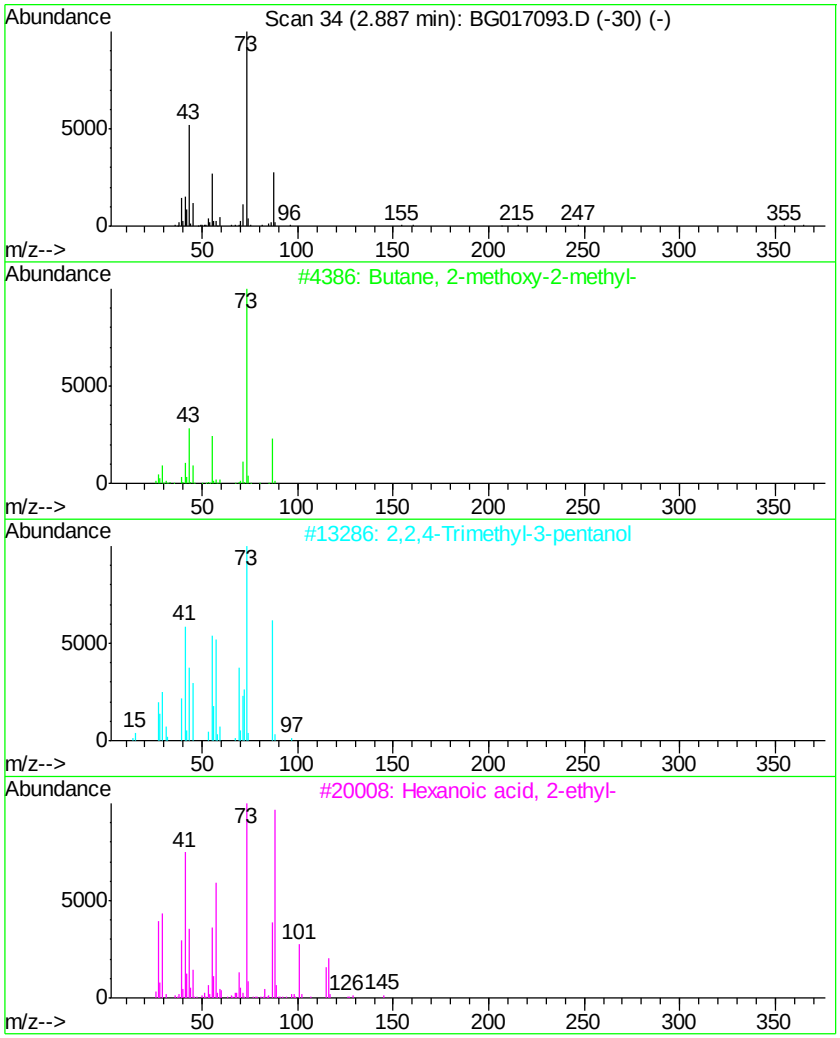
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

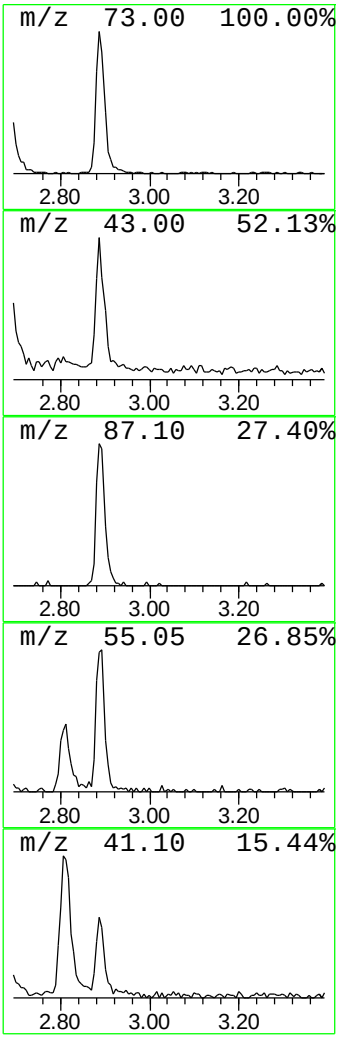
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	12.76 ng	150692	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	36
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
5	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

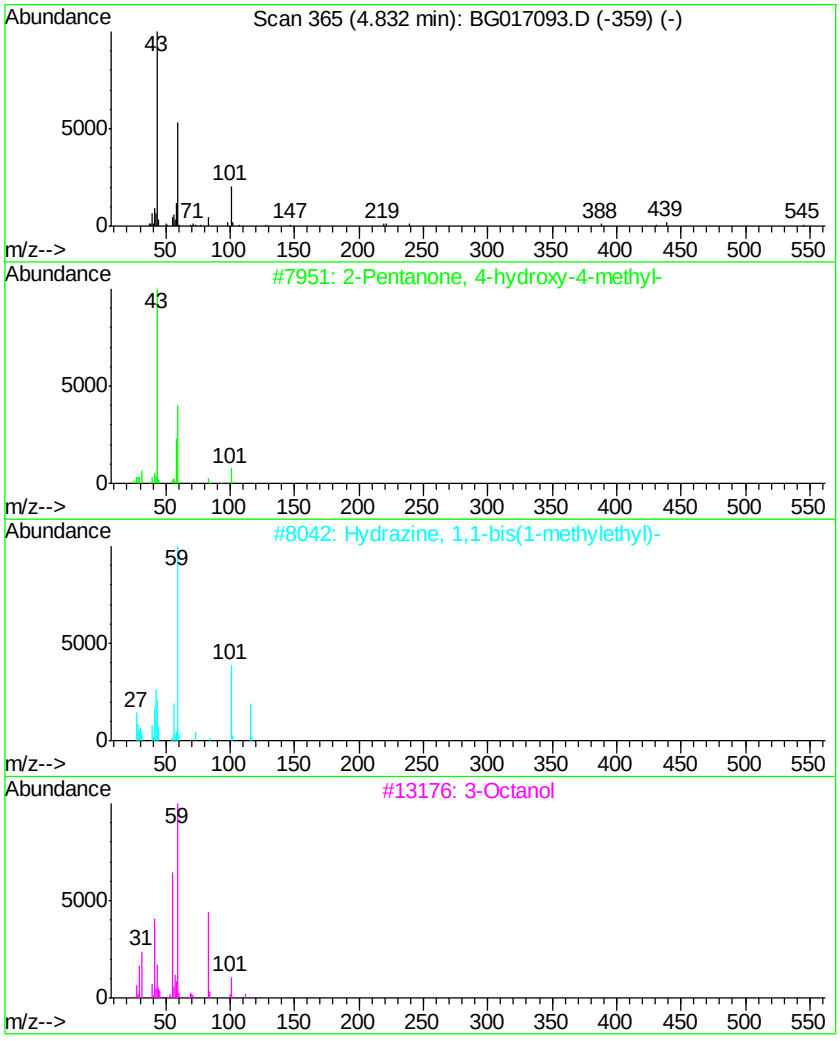
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

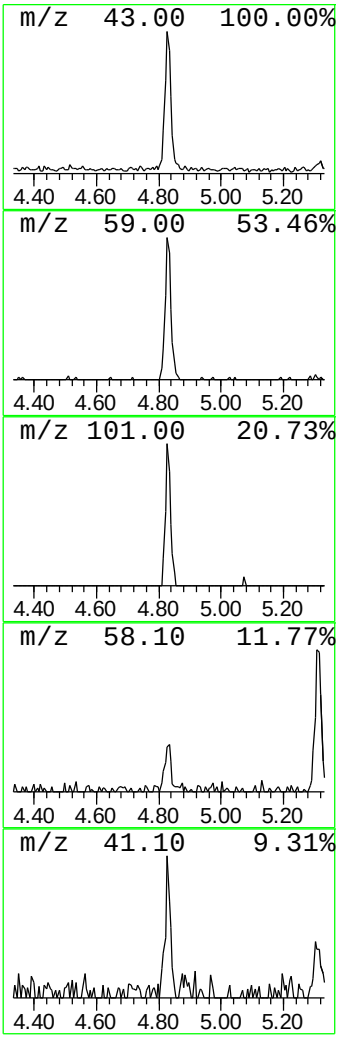
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	5.43 ng	64180	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	3-Octanol	130	C8H18O	000589-98-0	23
4	2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	12
5	5-Hydroxypentanehydroxylamine, N...	245	C11H19NO5	104556-13-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

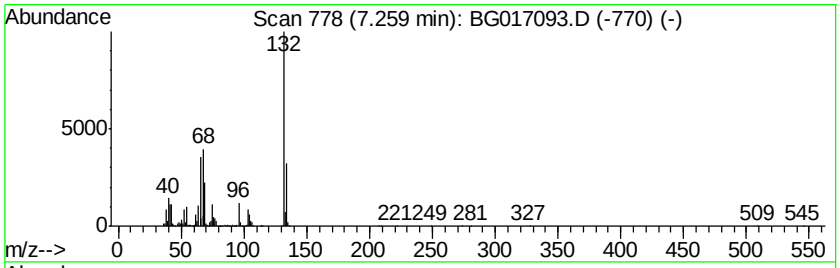
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

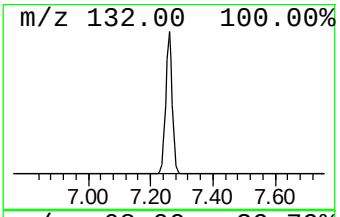
****

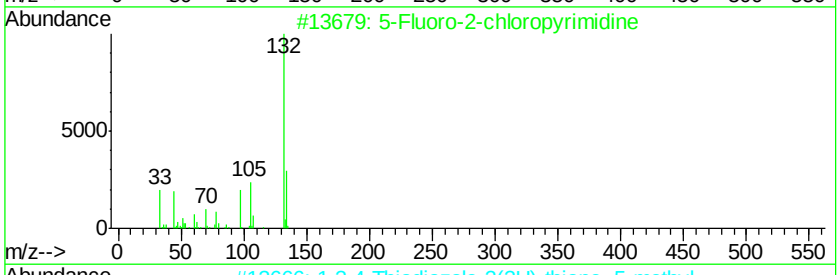
Peak Number 4 unknown7.26 Concentration Rank 1

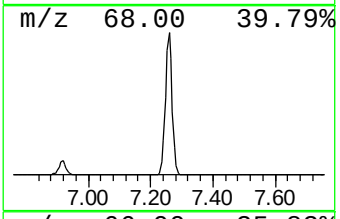
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	126.95 ng	1499350	1,4-Dichlorobenzene-d4	7.72

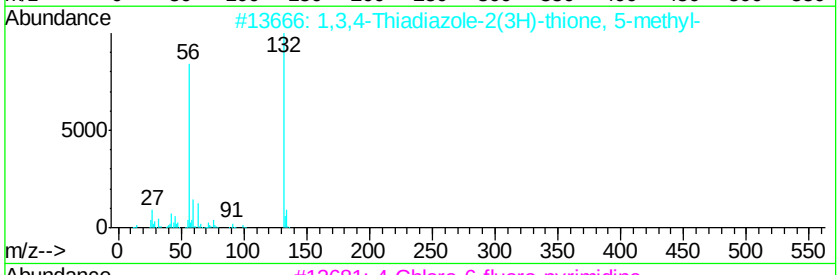
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	20

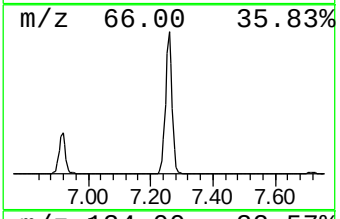


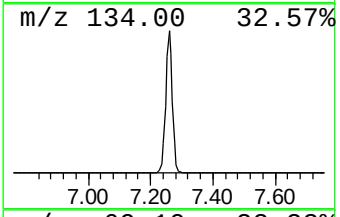


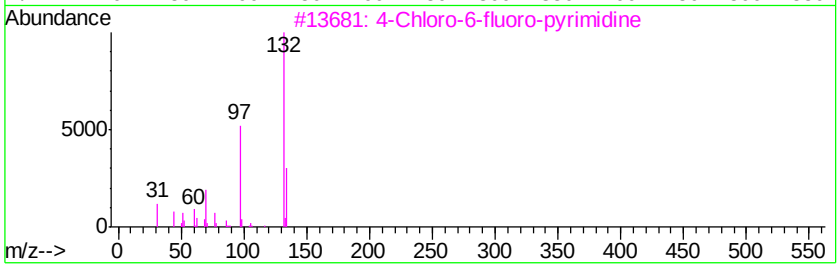


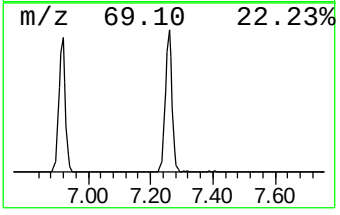












Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

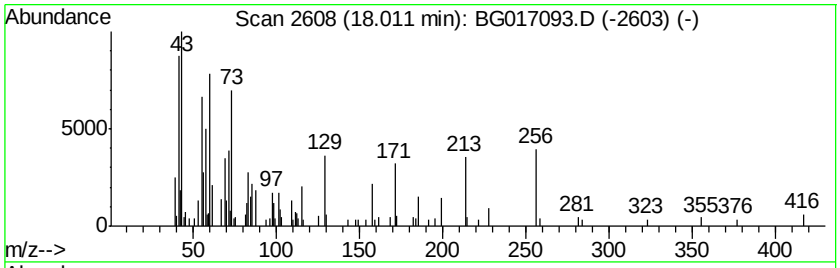
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

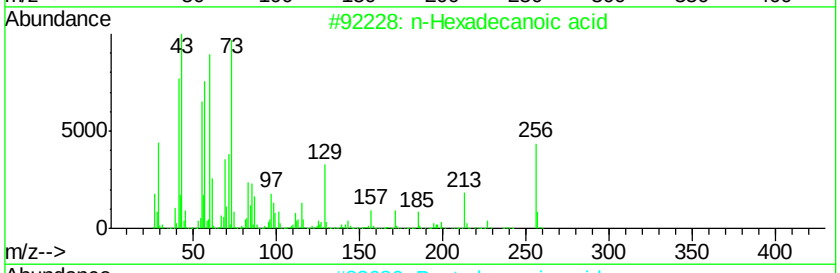
****

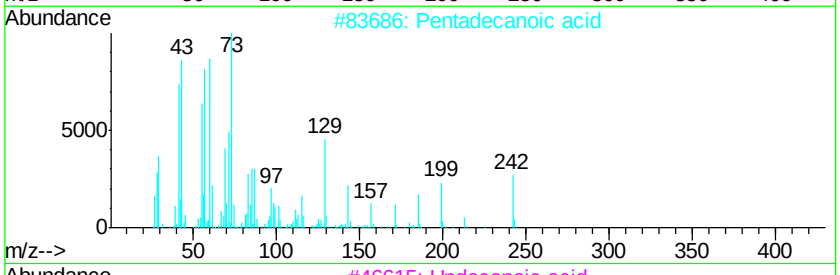
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

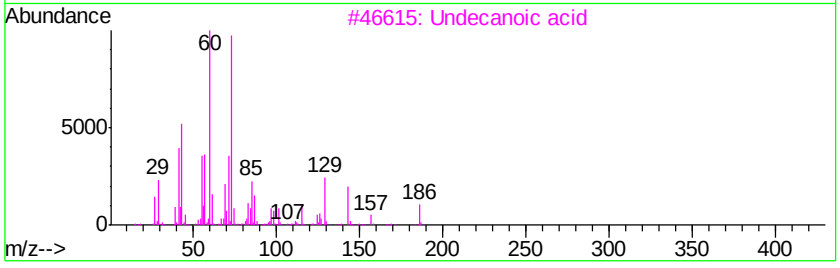
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	2.84 ng	85597	Phenanthrene-d10	17.11

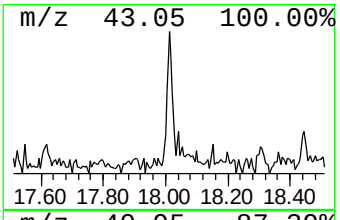
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Undecanoic acid	186	C11H22O2	000112-37-8	47
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
5	n-Decanoic acid	172	C10H20O2	000334-48-5	45

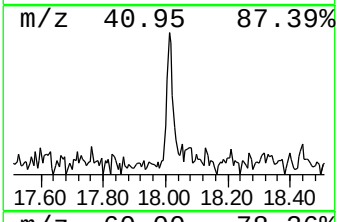


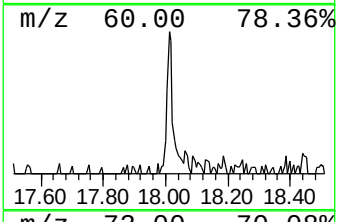


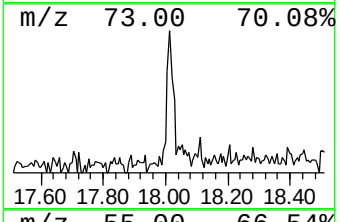


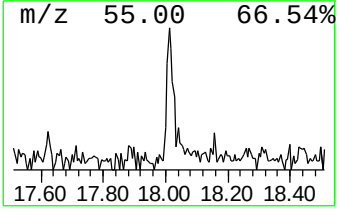












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Instrument : BNA_G
ClientSampleId : KBY-SB-4(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

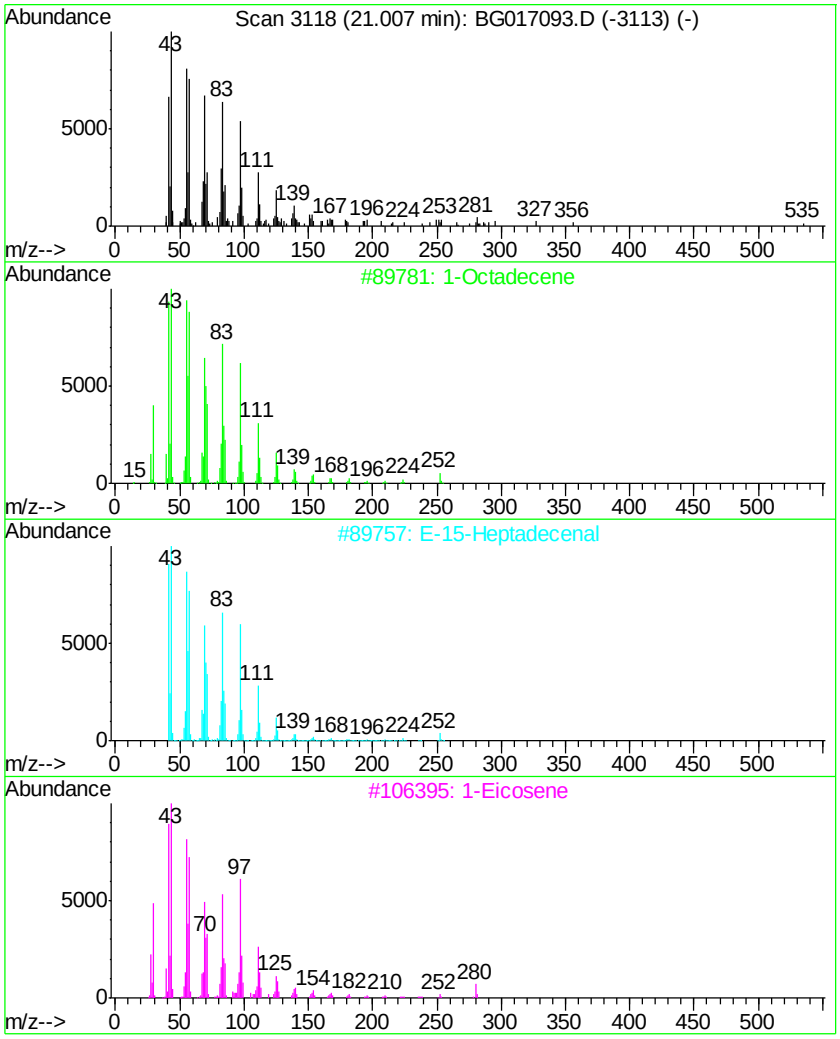
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

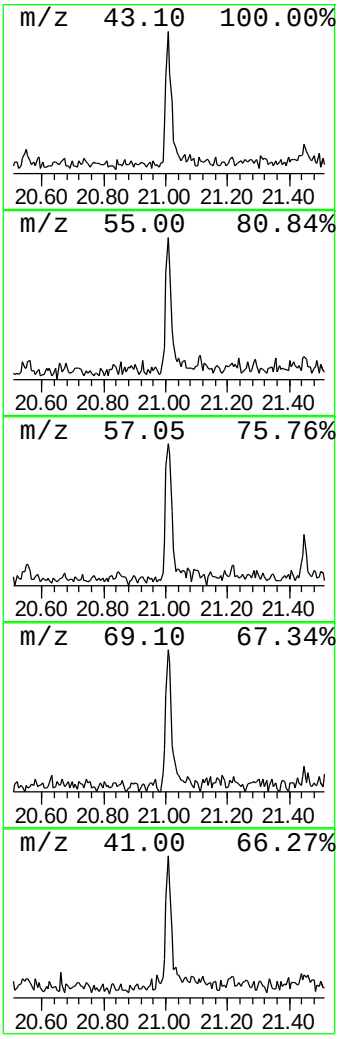
****

Peak Number 7 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.01	4.61 ng	159753	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
3	1-Eicosene	280	C20H40	003452-07-1	83
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
5	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051215\
Data File : BG017093.D
Acq On : 12 May 2015 21:11
Operator : TP/IZ
Sample : G2196-06
Misc :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2-cyclop...	2.81	10.0	ng	118506	1	7.72	236207	20.0
Butane, 2-methoxy...	2.89	12.8	ng	150692	1	7.72	236207	20.0
2-Pentanone, 4-hy...	4.83	5.4	ng	64180	1	7.72	236207	20.0
unknown7.26	7.26	127.0	ng	1499350	1	7.72	236207	20.0
n-Hexadecanoic acid	18.01	2.8	ng	85597	4	17.11	602532	20.0
1-Octadecene	21.01	4.6	ng	159753	5	21.30	693043	20.0