LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017023.D
Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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	2.916	34	39	47	rBV	233470	341787	7.01%	1.398%
2	2.993	47	52	61	rVB	499176	633611	12.99%	2.591%
3	4.908	372	378	385	rBV2	54279	82461	1.69%	0.337%
4	5.378	452	458	470	rBV	587039	853281	17.49%	3.489%
5	6.970	723	729	739	rBV	429409	673779	13.81%	2.755%
6	7.329	782	790	803	rBV	1102154	1749385	35.87%	7.154%
7	7.787	862	868	875	rBV	244334	379716	7.79%	1.553%
8	8.110	916	923	931	rBV	874350	1367289	28.03%	5.591%
9	8.950	1058	1066	1076	rBV	852859	1448025	29.69%	5.922%
10	10.578	1336	1343	1351	rBV	345032	590526	12.11%	2.415%
11	12.781	1712	1718	1725	rBV2	104182	161702	3.32%	0.661%
12	13.051	1754	1764	1775	rBV	2213502	3469194	71.13%	14.187%
13	14.426	1991	1998	2005	rBV3	546378	875341	17.95%	3.580%
14	15.249	2133	2138	2142	rVB	58938	80894	1.66%	0.331%
15	15.789	2225	2230	2238	rVB2	60999	115531	2.37%	0.472%
16	15.919	2245	2252	2262	rBV	2090798	3052116	62.58%	12.481%
17	17.170	2459	2465	2472	rBV2	756960	1058497	21.70%	4.329%
18	18.063	2612	2617	2627	rBV	159531	265696	5.45%	1.087%
19	19.344	2832	2835	2844	rBV	101510	154426	3.17%	0.632%
20	19.796	2906	2912	2918	rBV	4140453	4877430	100.00%	19.946%
21	21.054	3122	3126	3132	rBV6	62603	91853	1.88%	0.376%
22	21.342	3170	3175	3184	rBV	804019	1100433	22.56%	4.500%
23	23.639	3559	3566	3574	rVB	531335	1030423	21.13%	4.214%

Sum of corrected areas: 24453396

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
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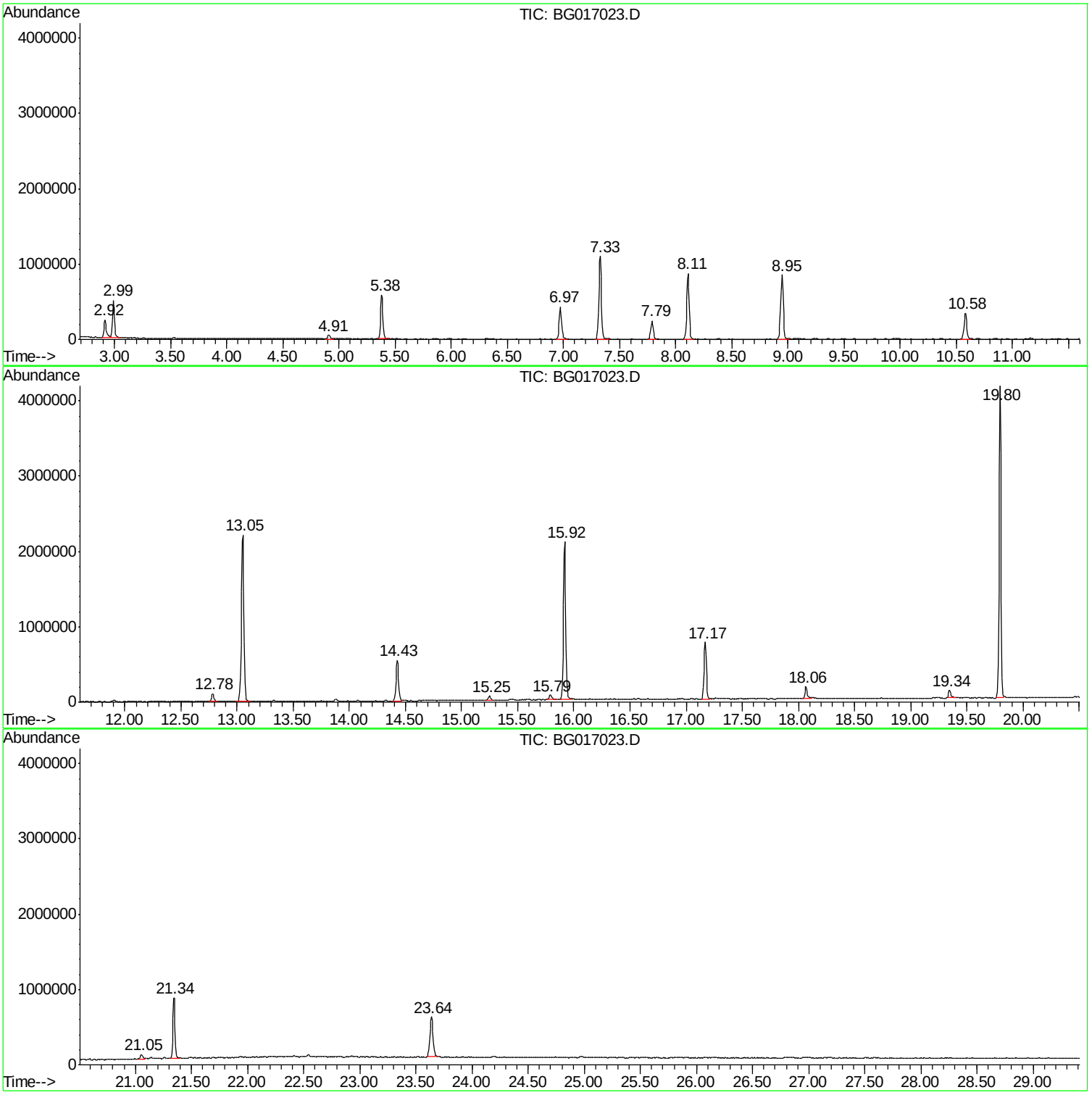
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-102

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\BG050815\
Data File : BG017023.D
Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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

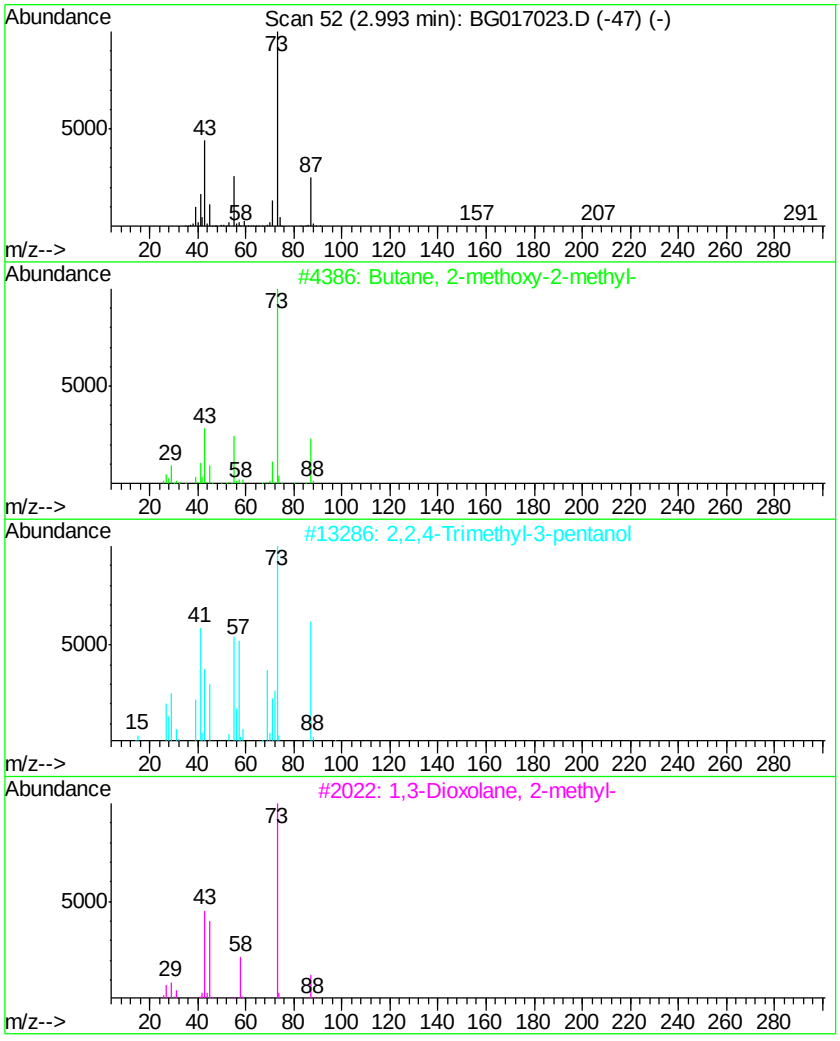
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

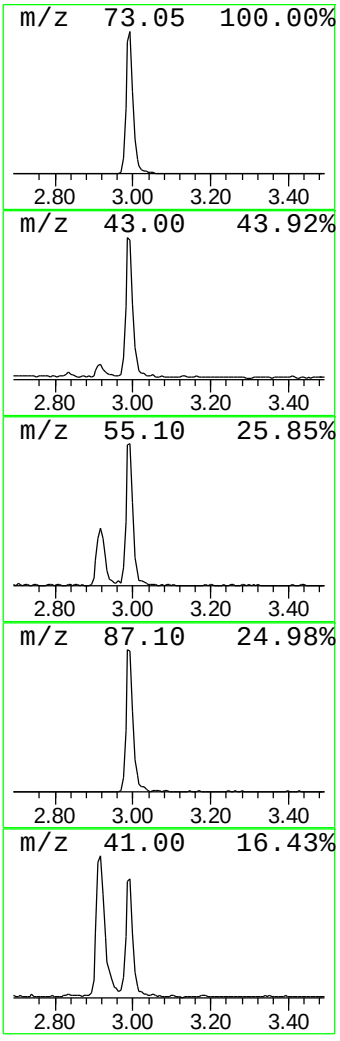
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	33.37 ng	633611	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BG017023.D
Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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

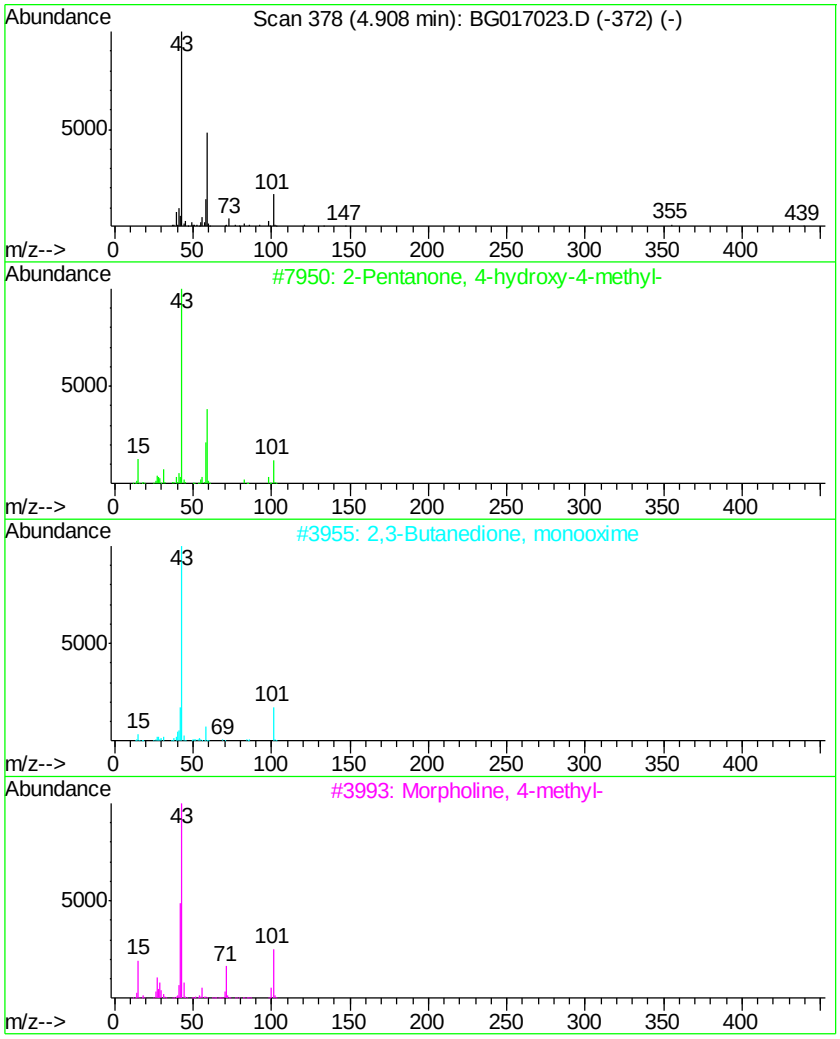
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

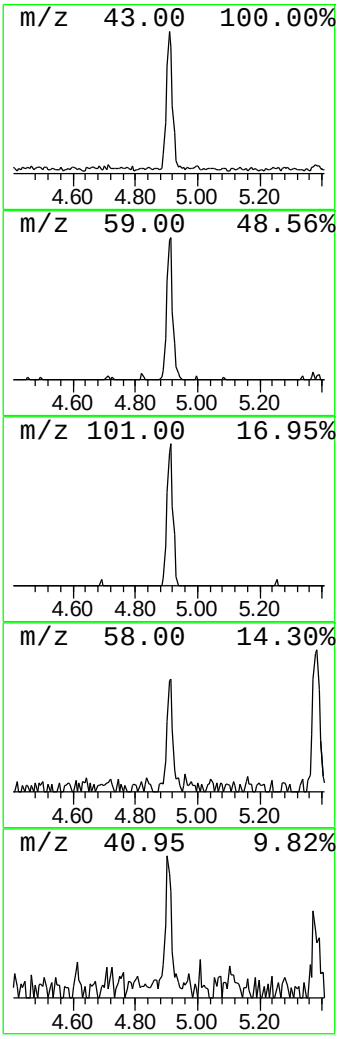
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.34 ng	82461	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	30
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017023.D
Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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

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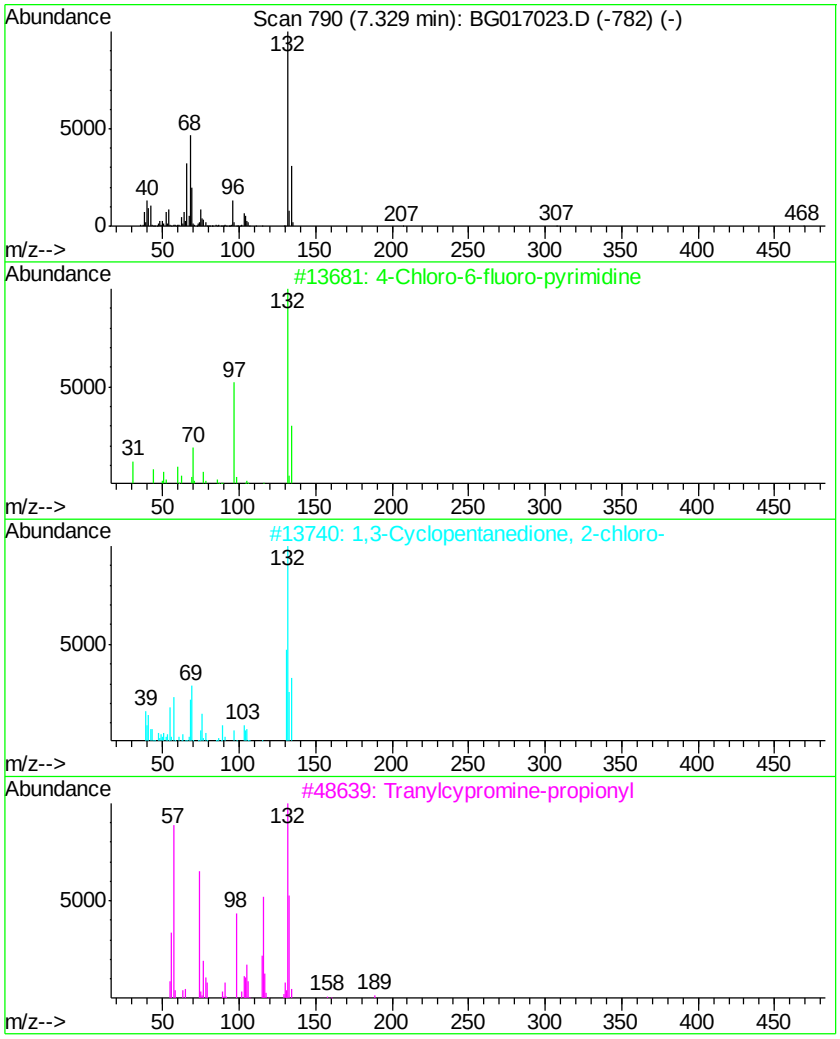
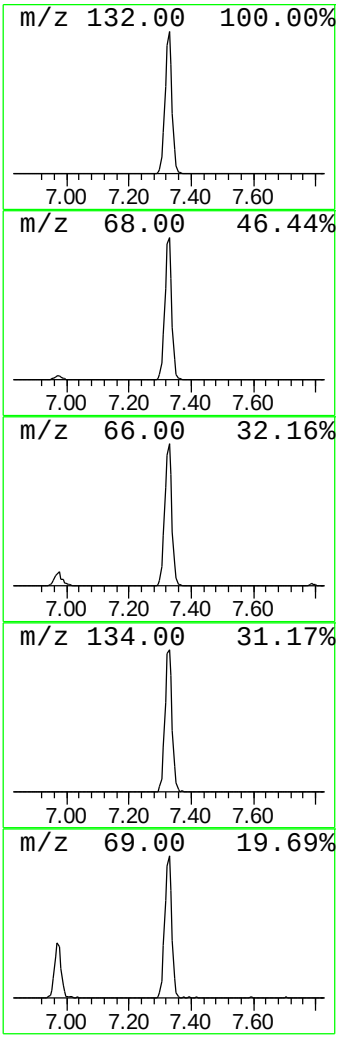
Peak Number 4 unknown7.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	92.14 ng	1749390	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Data File : BG017023.D
Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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

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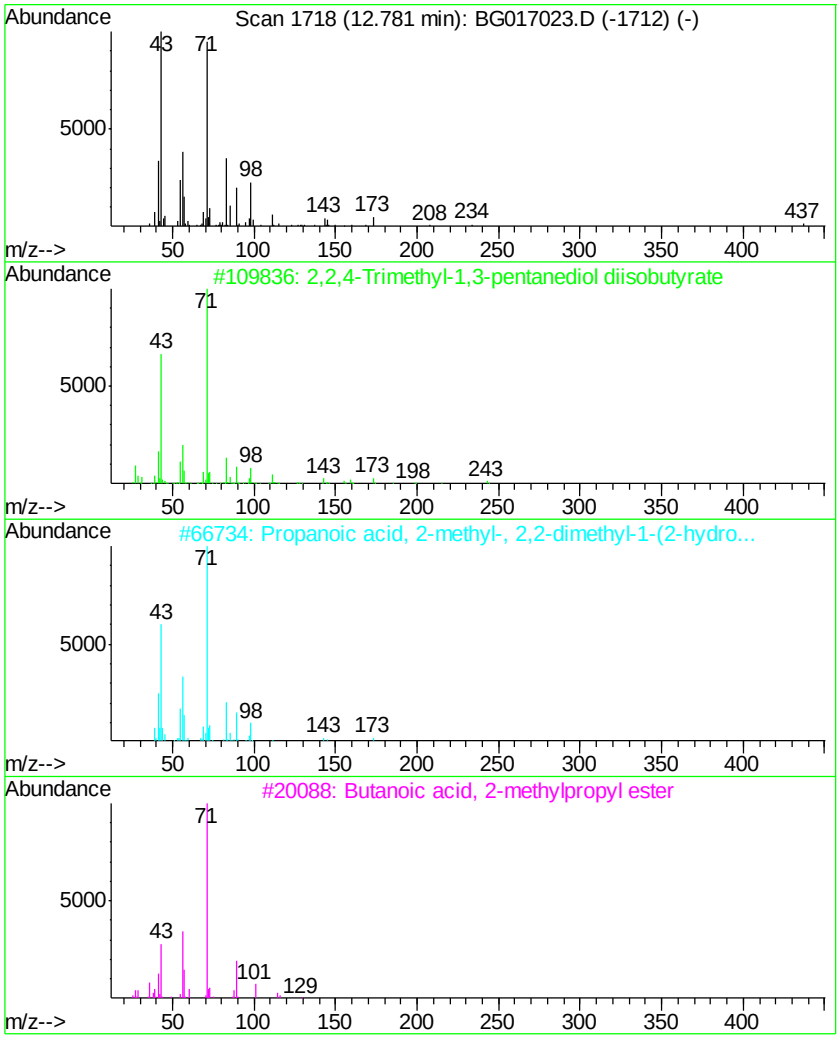
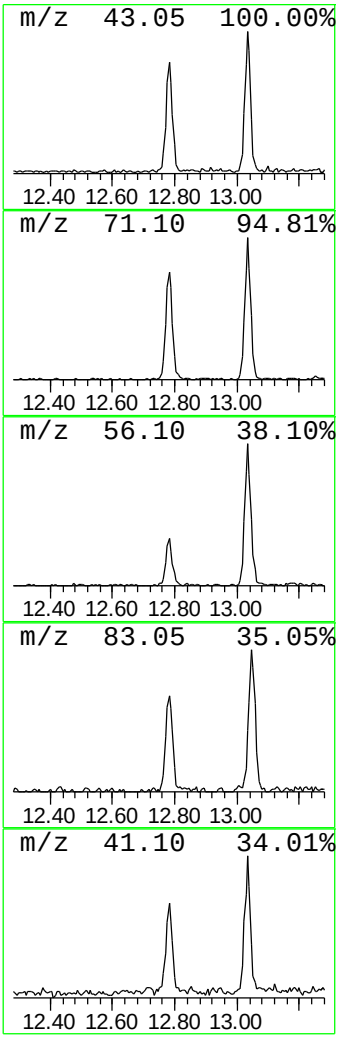
Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	3.69 ng	161702	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
2	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	50
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	42
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	38





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Acq On : 10 May 2015 13:09
Operator : TP/IZ
Sample : G2104-07
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-102

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
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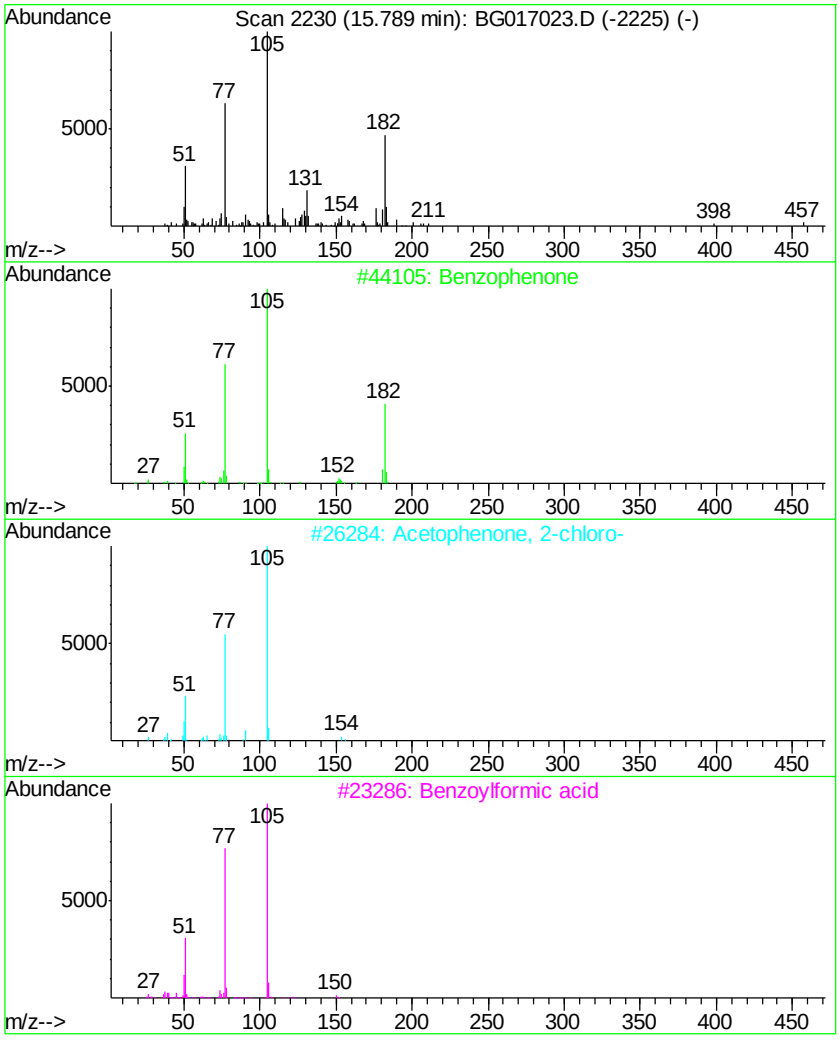
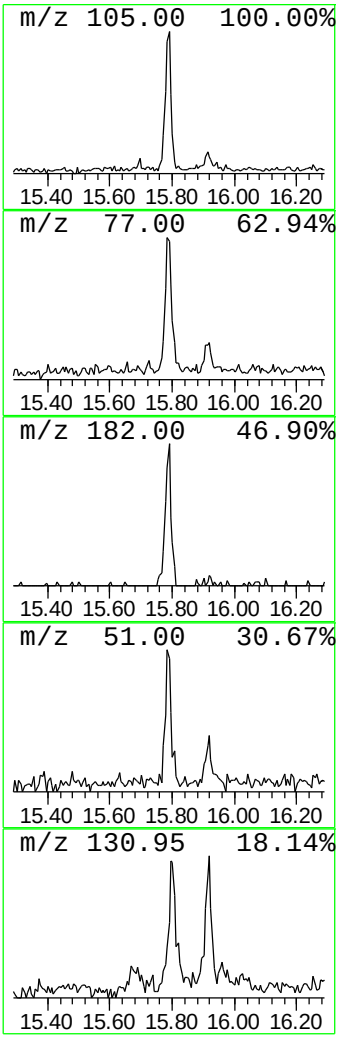
****

Peak Number 7 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.64 ng	115531	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	93
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	50
3	Benzoylformic acid	150	C8H6O3	000611-73-4	43
4	Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	43
5	Benzeneacetonitrile, .alpha.-oxo-	131	C8H5NO	000613-90-1	43





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ClientSampleId : MW-102

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

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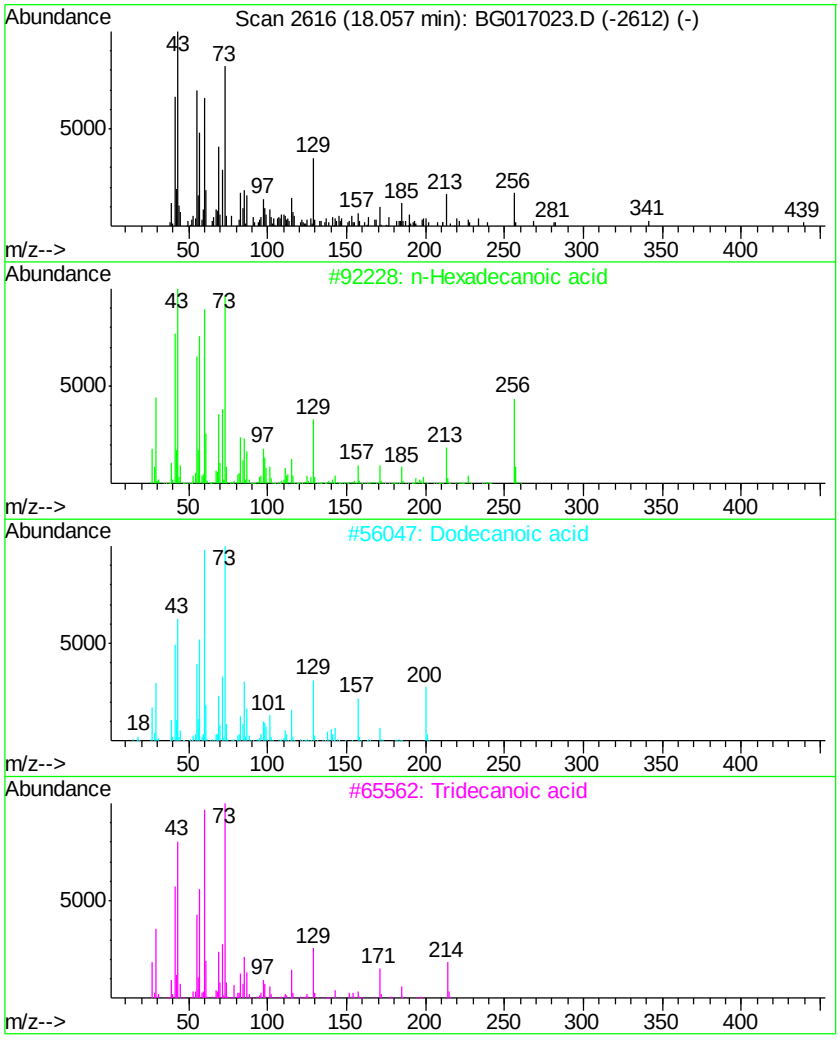
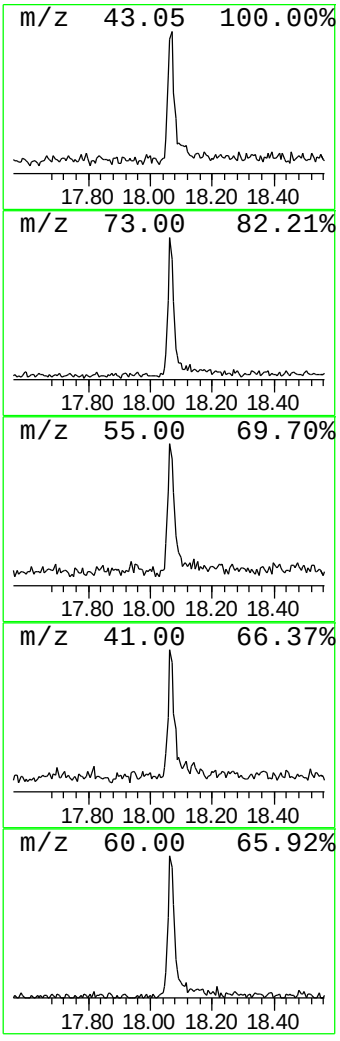
Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	5.02 ng	265696	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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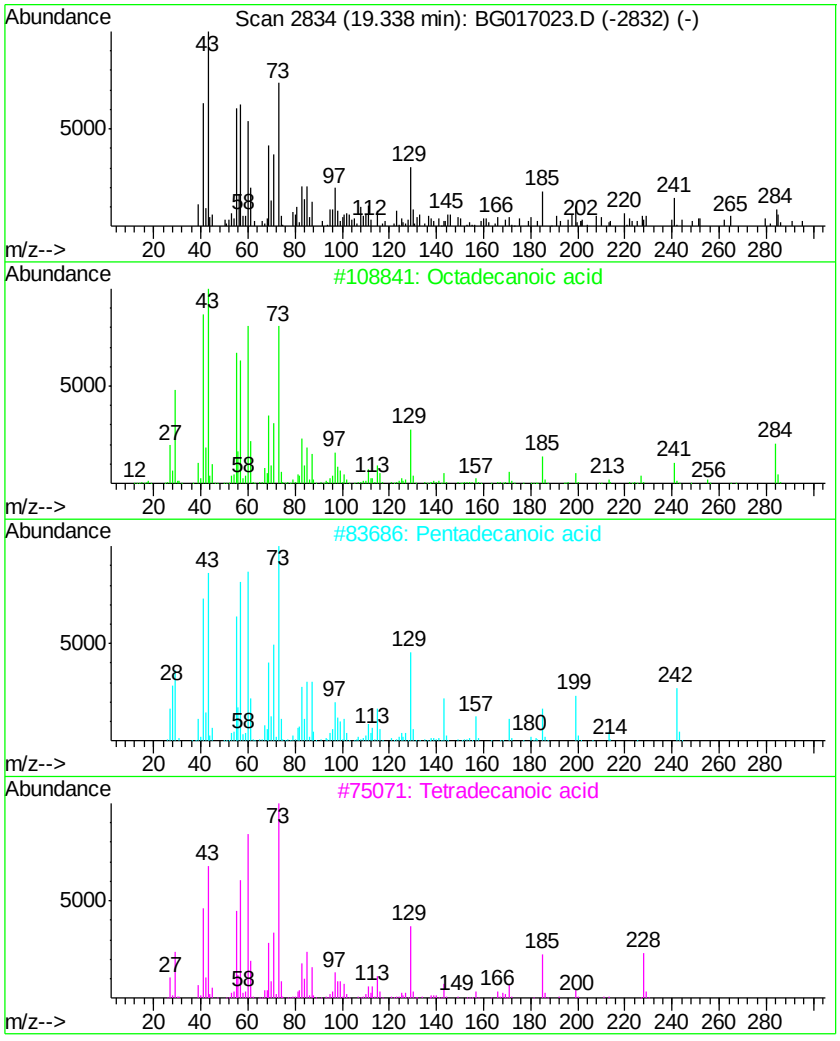
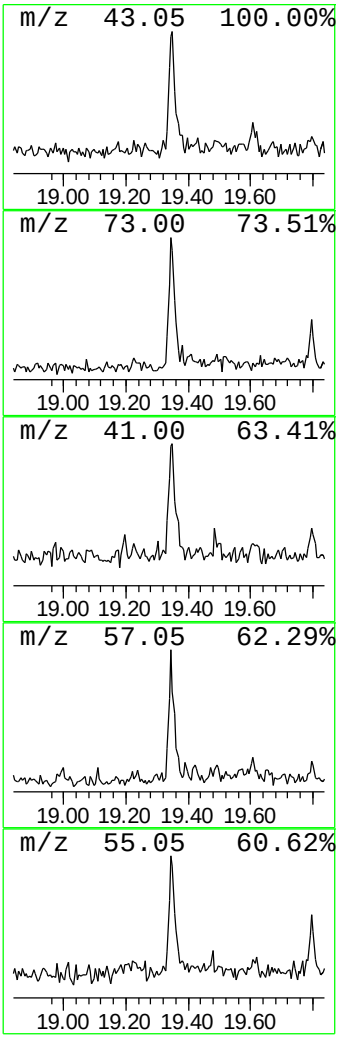
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.81 ng	154426	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
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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
Butane, 2-methoxy...	2.99	33.4	ng	633611	1	7.79	379716	20.0
2-Pentanone, 4-hy...	4.91	4.3	ng	82461	1	7.79	379716	20.0
unknown7.33	7.33	92.1	ng	1749390	1	7.79	379716	20.0
2,2,4-Trimethyl-1...	12.78	3.7	ng	161702	3	14.43	875341	20.0
Benzophenone	15.79	2.6	ng	115531	3	14.43	875341	20.0
n-Hexadecanoic acid	18.06	5.0	ng	265696	4	17.17	1058500	20.0
Octadecanoic acid	19.34	2.8	ng	154426	5	21.34	1100430	20.0