LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020097.D
Acq On : 11 Dec 2015 6:04
Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

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-BG120215.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	3.138	45	51	60	rBV2	20346	40918	2.11%	0.476%
2	3.214	60	64	70	rVB2	17753	25279	1.30%	0.294%
3	5.183	393	399	406	rBV	40366	62041	3.19%	0.721%
4	5.653	473	479	488	rBV	186830	302725	15.58%	3.519%
5	7.257	742	752	761	rBV	133976	223978	11.53%	2.604%
6	7.639	808	817	826	rBV	351621	595930	30.67%	6.928%
7	8.109	889	897	907	rBV	75771	124696	6.42%	1.450%
8	8.432	945	952	962	rBV	303141	527634	27.16%	6.134%
9	9.278	1088	1096	1104	rBV	277595	483096	24.87%	5.616%
10	10.923	1369	1376	1384	rBV	105589	191359	9.85%	2.225%
11	13.361	1784	1791	1802	rBV	786260	1243623	64.01%	14.457%
12	14.178	1926	1930	1938	rVB	22007	32623	1.68%	0.379%
13	14.736	2019	2025	2033	rVB2	177906	286821	14.76%	3.334%
14	16.223	2269	2278	2289	rBV	662737	1029808	53.00%	11.971%
15	16.399	2302	2308	2317	rBV4	20668	46461	2.39%	0.540%
16	17.480	2485	2492	2499	rBV	244174	366080	18.84%	4.256%
17	18.350	2635	2640	2647	rBV2	39277	57879	2.98%	0.673%
18	19.619	2851	2856	2865	rBV2	50141	72723	3.74%	0.845%
19	20.083	2928	2935	2945	rBV	1535343	1942871	100.00%	22.586%
20	20.853	3063	3066	3070	rVB4	15927	19858	1.02%	0.231%
21	21.381	3151	3156	3167	rBV10	15303	33995	1.75%	0.395%
22	21.752	3213	3219	3226	rVB	285876	466794	24.03%	5.426%
23	25.036	3766	3778	3793	rBV2	144270	425100	21.88%	4.942%

Sum of corrected areas: 8602292

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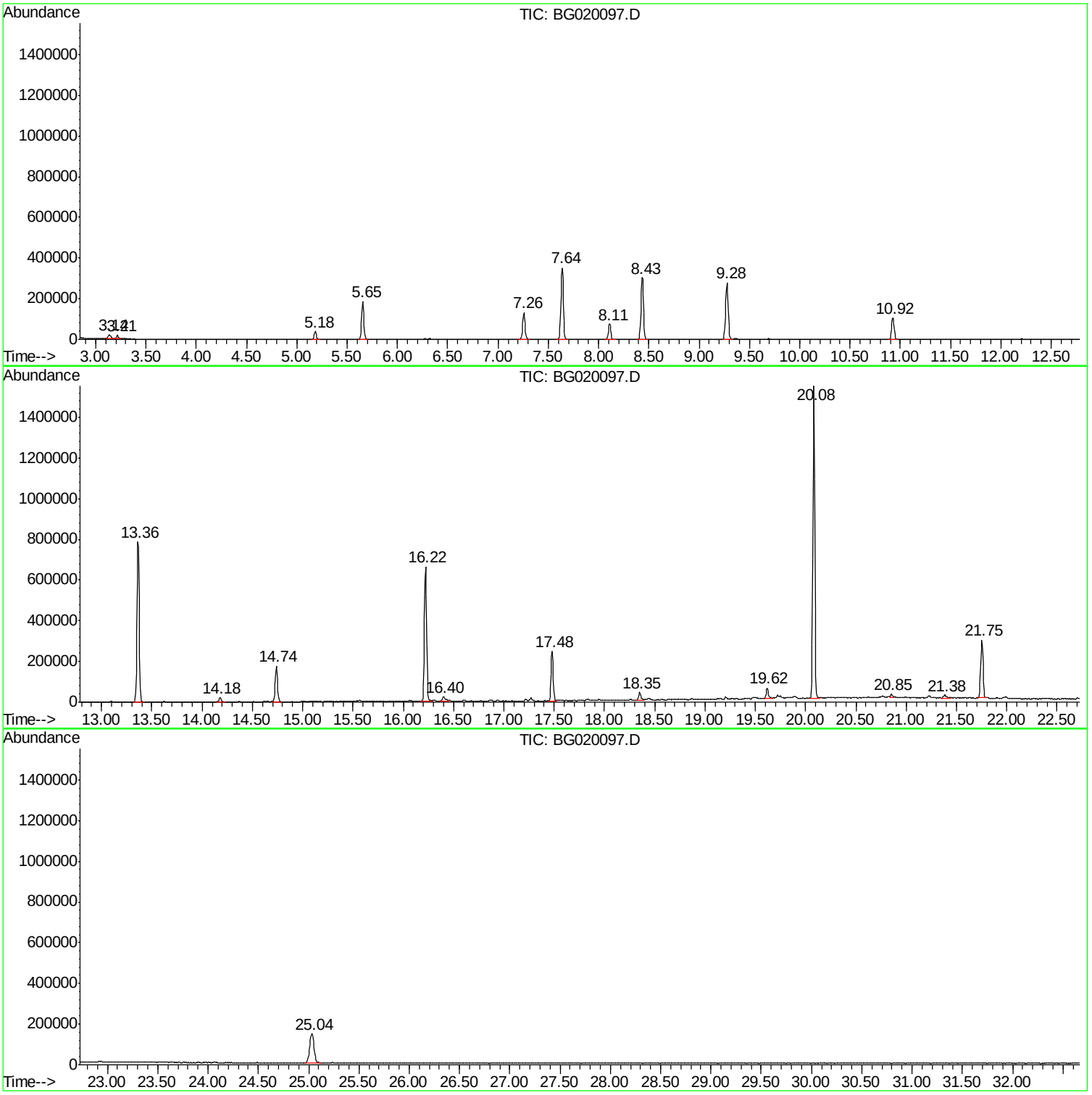
Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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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Acq On : 11 Dec 2015 6:04
Operator : UM/SJ
Sample : G4729-02
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

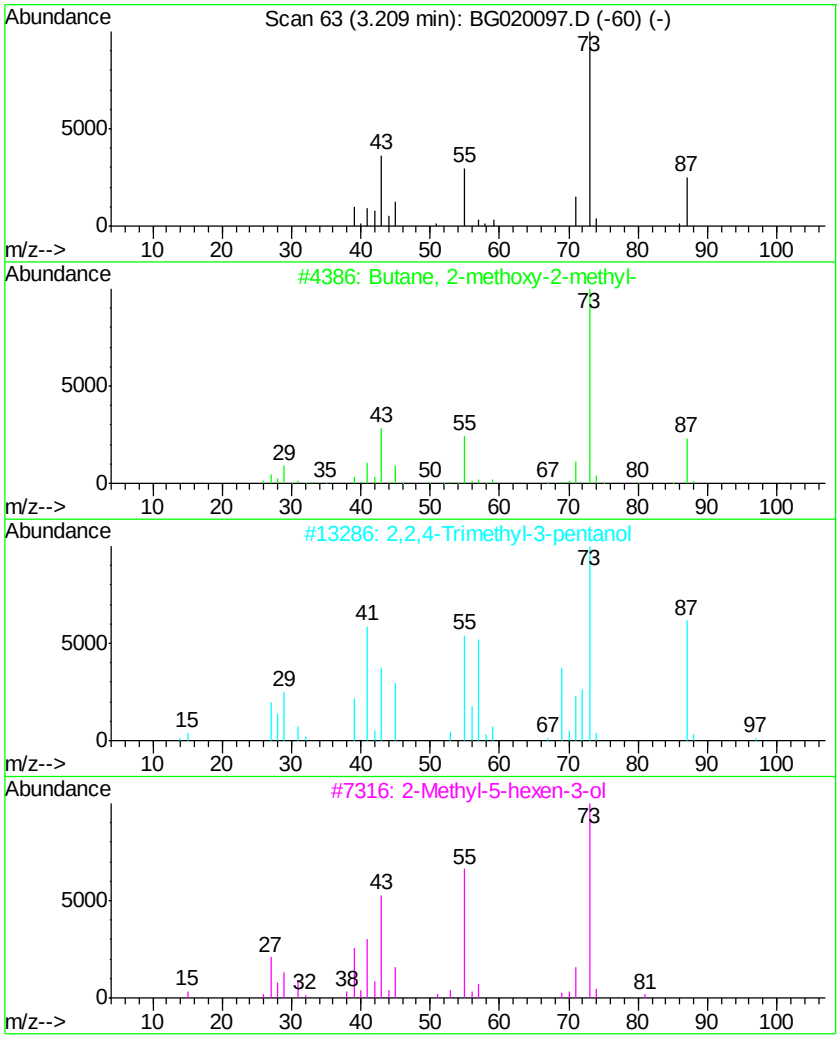
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

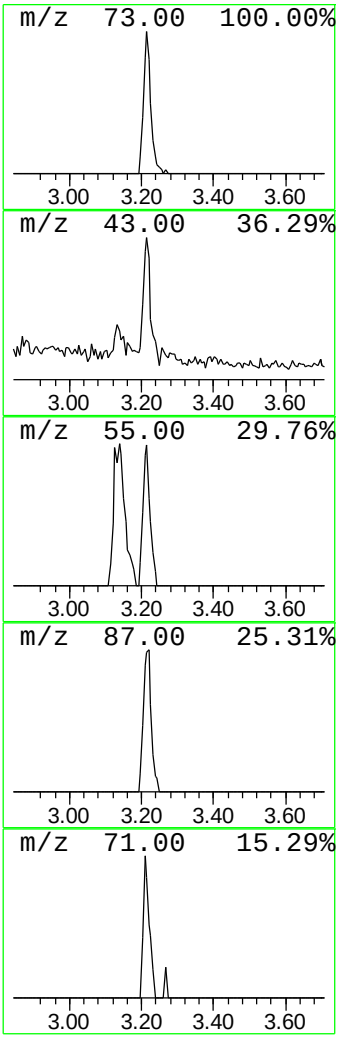
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	4.05 ng	25279	1,4-Dichlorobenzene-d4	8.11

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	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020097.D
Acq On : 11 Dec 2015 6:04
Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

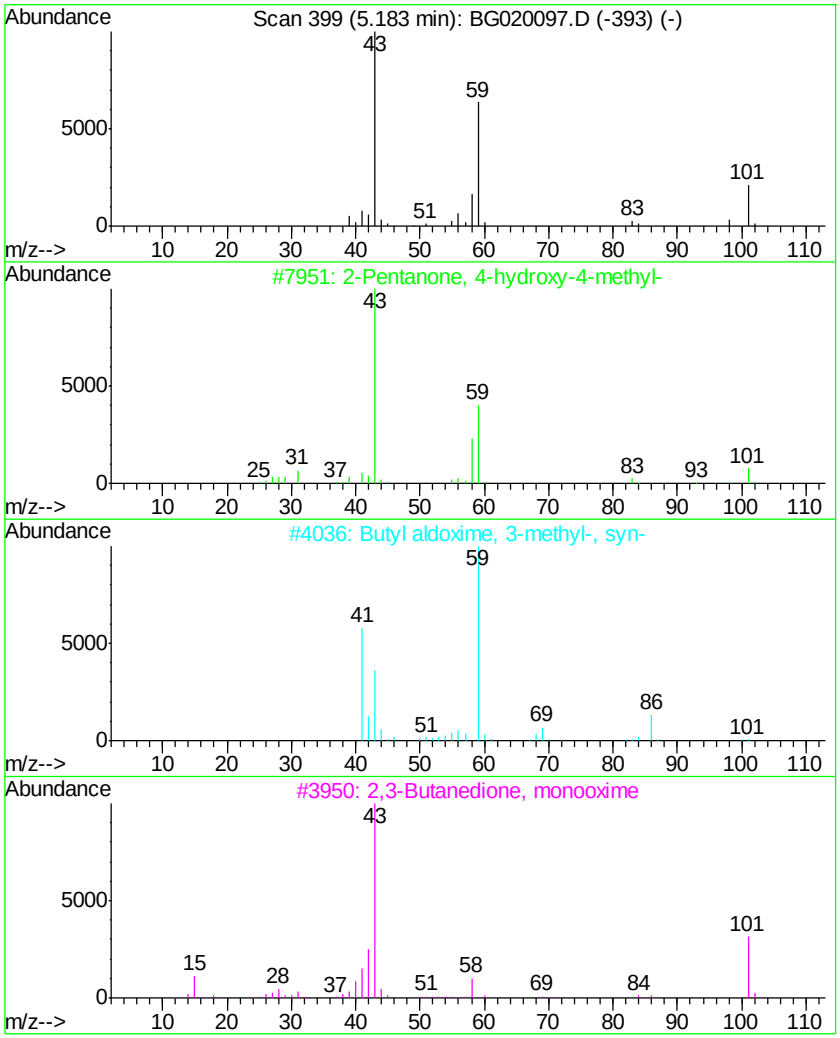
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

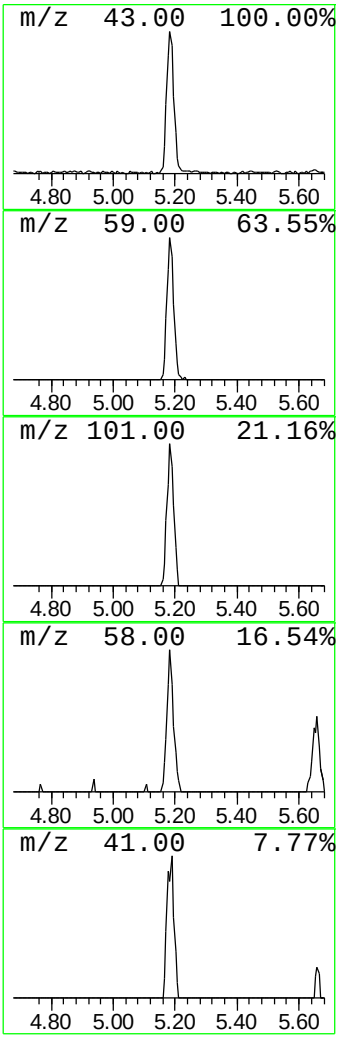
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	9.95 ng	62041	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Acetone	58	C3H6O	000067-64-1	9





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Data File : BG020097.D
Acq On : 11 Dec 2015 6:04
Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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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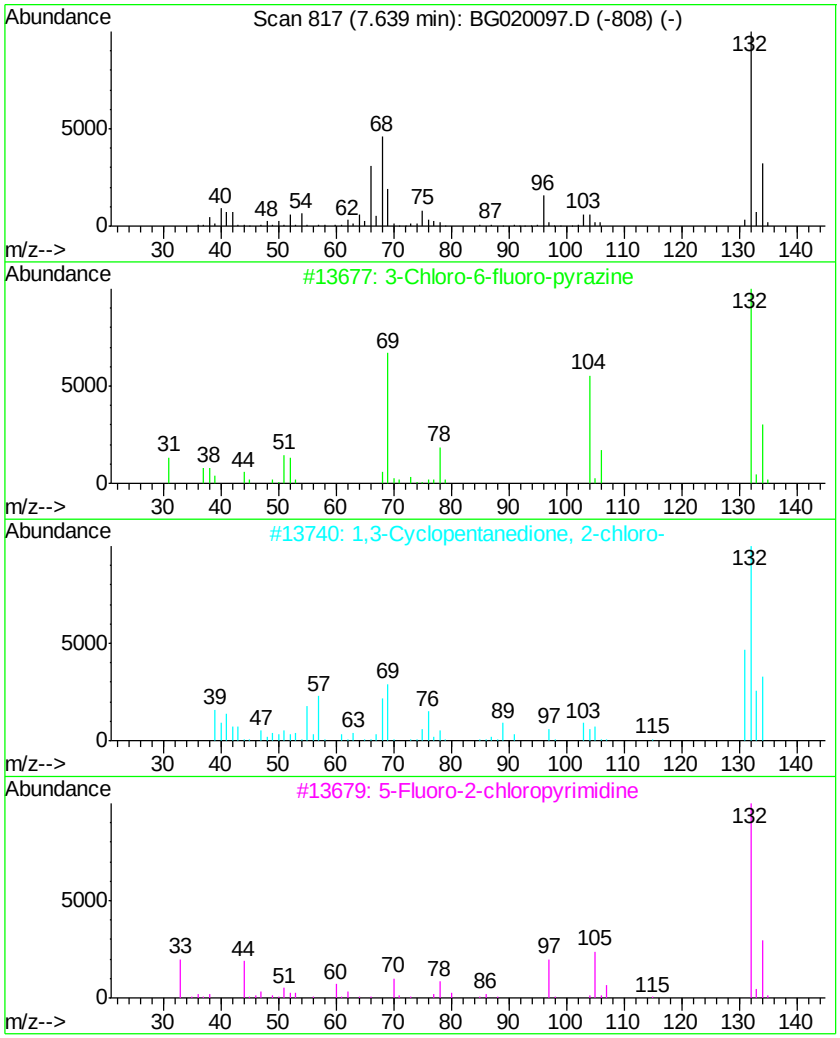
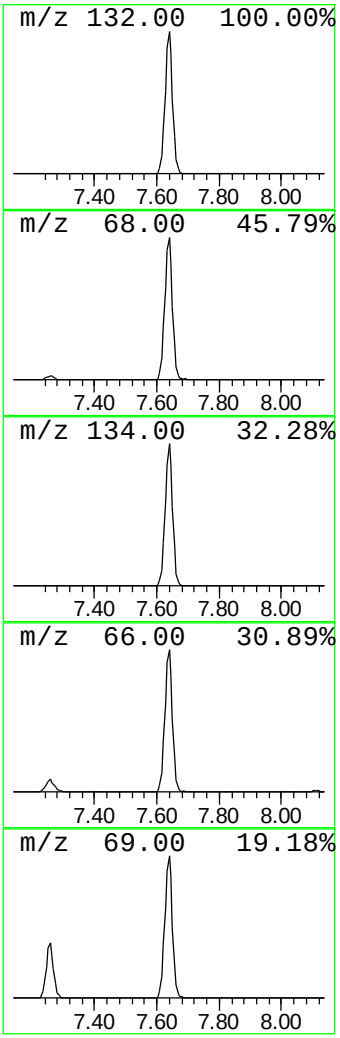
Peak Number 4 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	95.58 ng	595930	1,4-Dichlorobenzene-d4	8.11

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	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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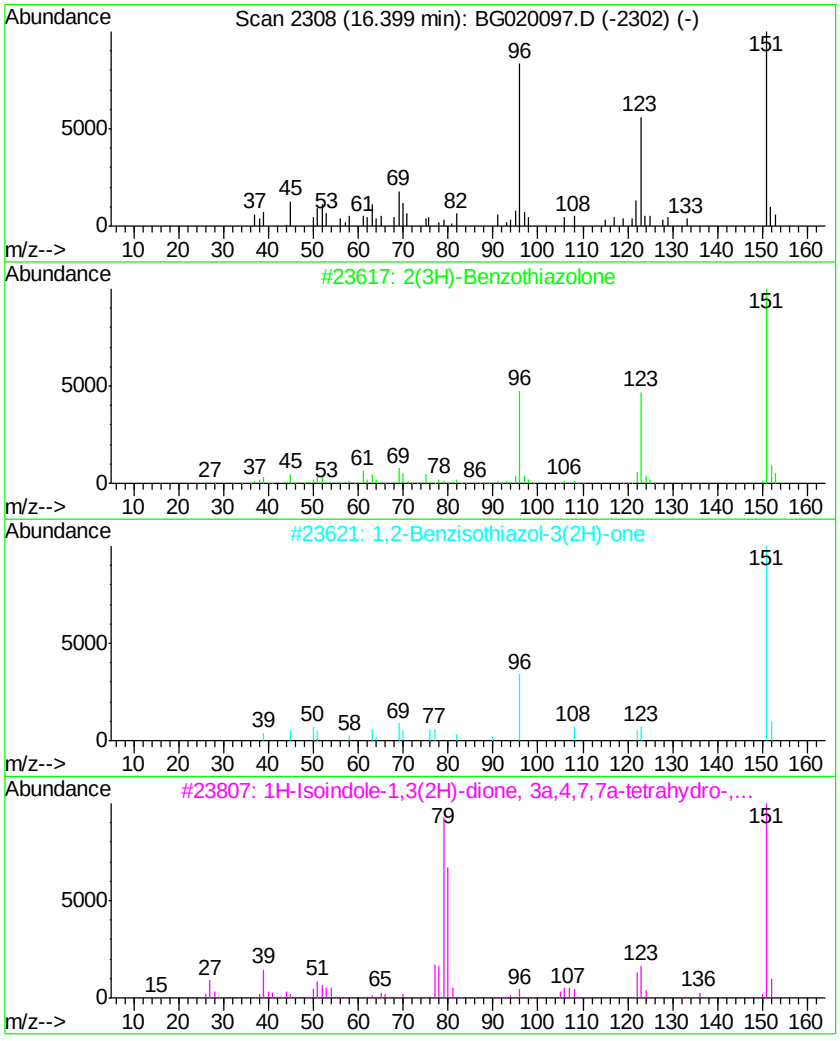
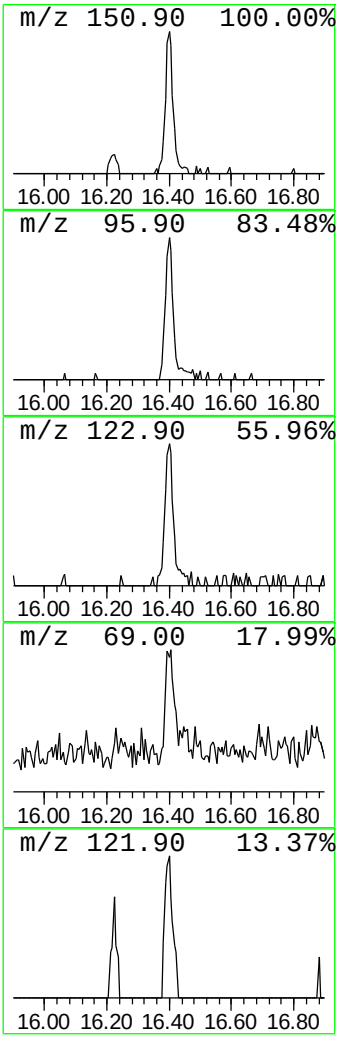
Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.54 ng	46461	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	90
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3	1H-Isoindole-1,3(2H)-dione, 3a,4...	151	C8H9NO2	001469-48-3	35
4	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	35
5	4-Methoxyformanilide	151	C8H9NO2	023896-88-0	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020097.D
Acq On : 11 Dec 2015 6:04
Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

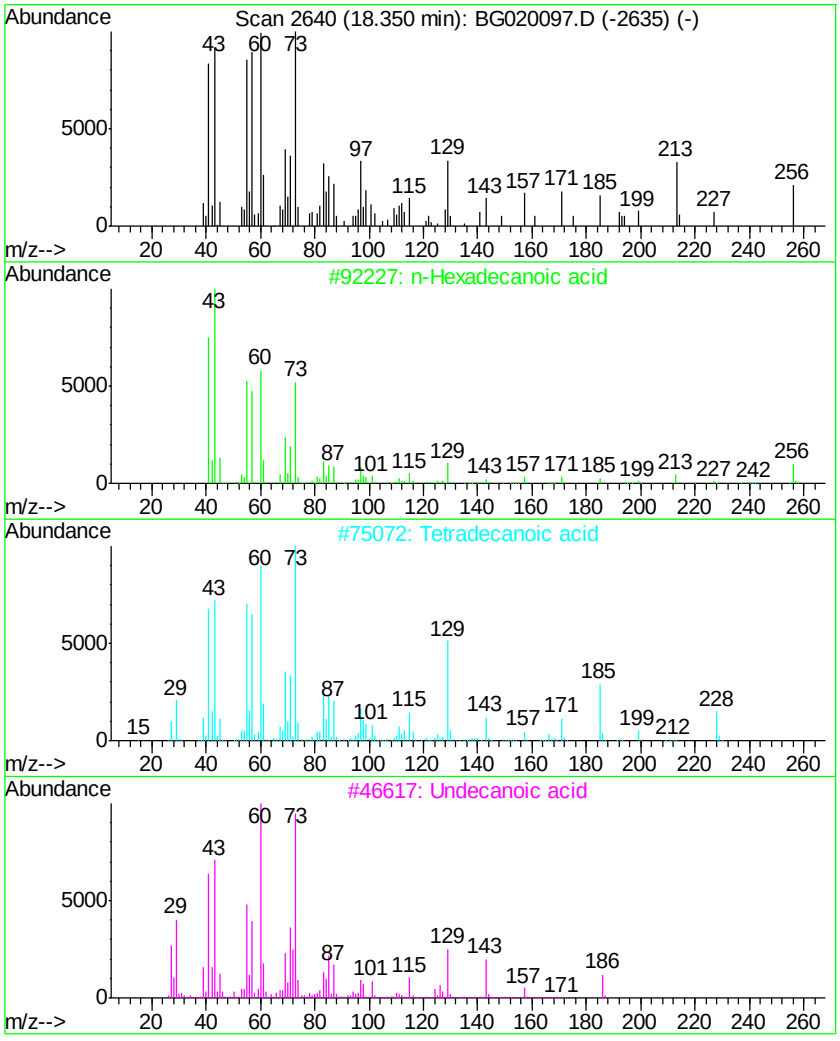
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

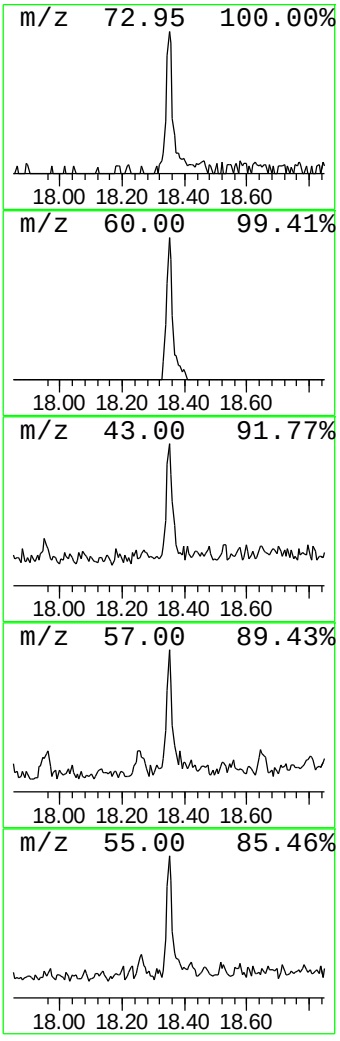
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	3.16 ng	57879	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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Operator : UM/SJ
Sample : G4729-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

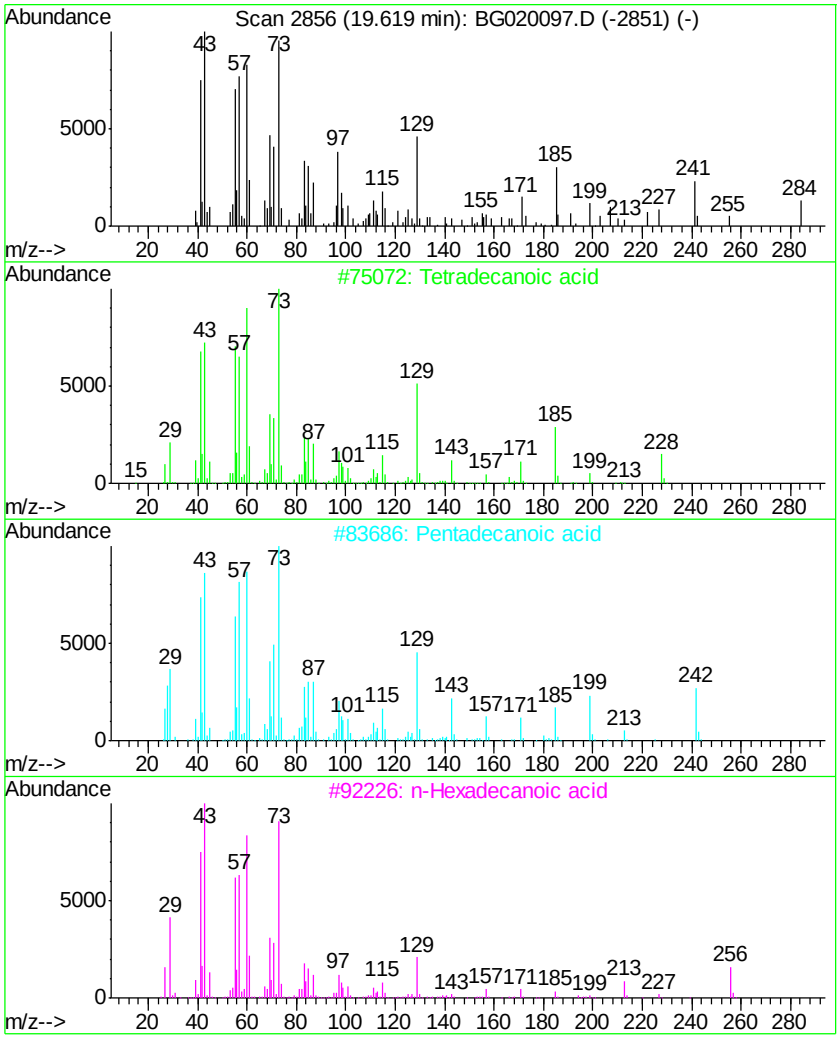
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

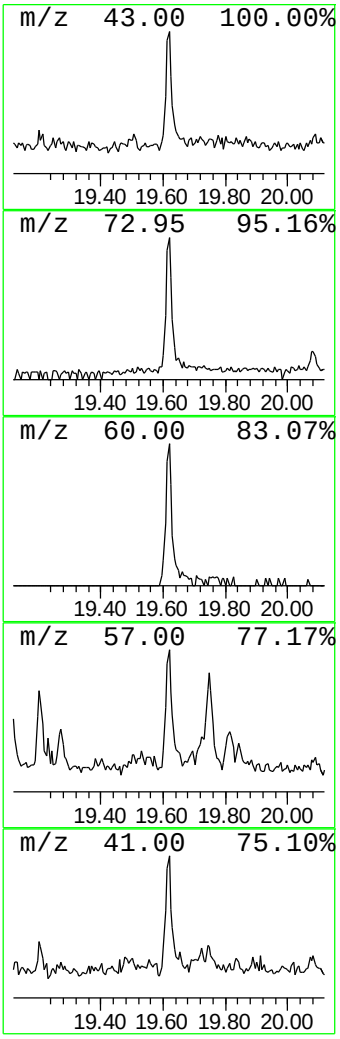
****

Peak Number 8 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	3.12 ng	72723	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
Sample : G4729-02
Misc :
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Instrument : BNA_G
ClientSampleId : W-30

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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...	3.21	4.0	ng	25279	1	8.11	124696	20.0
2-Pentanone, 4-hy...	5.18	9.9	ng	62041	1	8.11	124696	20.0
unknown7.64	7.64	95.6	ng	595930	1	8.11	124696	20.0
2(3H)-Benzothiazo...	16.40	2.5	ng	46461	4	17.48	366080	20.0
n-Hexadecanoic acid	18.35	3.2	ng	57879	4	17.48	366080	20.0
Tetradecanoic acid	19.62	3.1	ng	72723	5	21.75	466794	20.0