LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
Acq On : 6 May 2015 13:15
Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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-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	2.787	13	17	36	rBV	5628400	7707258	100.00%	19.432%
2	2.923	36	40	50	rVB2	155423	291738	3.79%	0.736%
3	3.005	50	54	59	rBV	218263	265688	3.45%	0.670%
4	4.920	375	380	387	rBV	358825	518989	6.73%	1.309%
5	5.384	451	459	471	rBV	1696065	2460873	31.93%	6.205%
6	6.971	720	729	737	rBV	1775406	2855500	37.05%	7.199%
7	7.335	783	791	799	rVB	1722620	2661044	34.53%	6.709%
8	7.799	864	870	877	rBV	304913	482971	6.27%	1.218%
9	8.122	917	925	931	rBV	1139919	1806193	23.43%	4.554%
10	8.957	1060	1067	1075	rVB	1036101	1717428	22.28%	4.330%
11	10.590	1337	1345	1354	rBV	427566	730042	9.47%	1.841%
12	13.064	1759	1766	1774	rVB	2400719	3442359	44.66%	8.679%
13	13.892	1902	1907	1917	rBV	126145	191079	2.48%	0.482%
14	14.438	1991	2000	2008	rBV2	670218	1021777	13.26%	2.576%
15	15.925	2246	2253	2265	rBV	2298198	3104870	40.29%	7.828%
16	17.182	2460	2467	2474	rBV	885599	1219359	15.82%	3.074%
17	18.081	2615	2620	2630	rBV2	165566	258917	3.36%	0.653%
18	19.362	2834	2838	2843	rBV3	88240	115590	1.50%	0.291%
19	19.621	2870	2882	2890	rBV3	43926	111905	1.45%	0.282%
20	19.815	2909	2915	2920	rBV	3844945	4975994	64.56%	12.546%
21	21.078	3125	3130	3140	rBV	483445	603136	7.83%	1.521%
22	21.360	3172	3178	3187	rBV	1056341	1336861	17.35%	3.371%
23	22.182	3313	3318	3324	rBV	88192	126111	1.64%	0.318%
24	22.970	3448	3452	3456	rBV3	54347	88971	1.15%	0.224%
25	23.017	3456	3460	3469	rVB3	55949	102735	1.33%	0.259%
26	23.563	3549	3553	3561	rVB3	51973	93440	1.21%	0.236%
27	23.663	3563	3570	3579	rVB2	632050	1251208	16.23%	3.155%
28	24.345	3681	3686	3695	rVB9	56718	120504	1.56%	0.304%

Sum of corrected areas: 39662540

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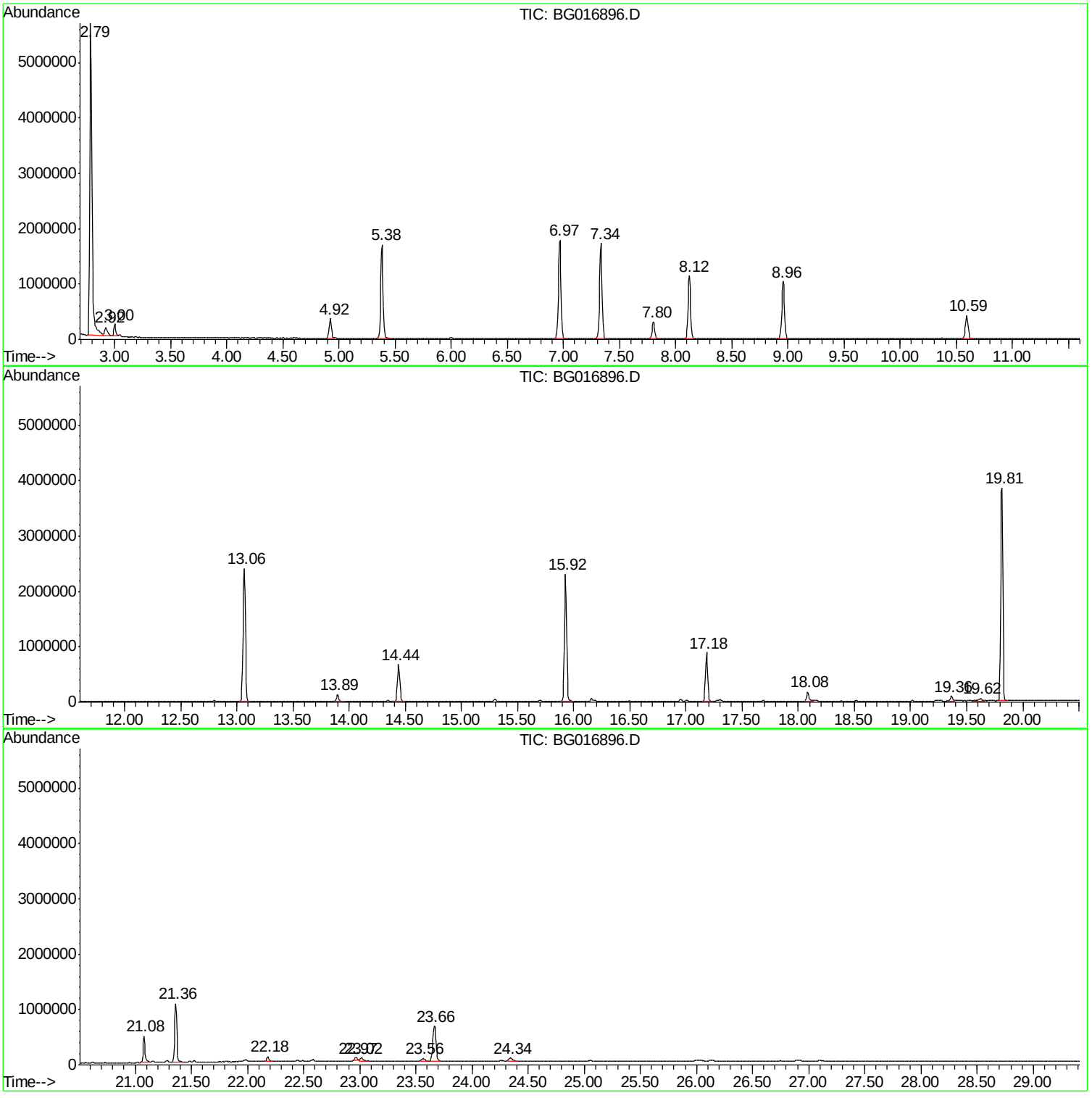
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8-D5.5

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
Acq On : 6 May 2015 13:15
Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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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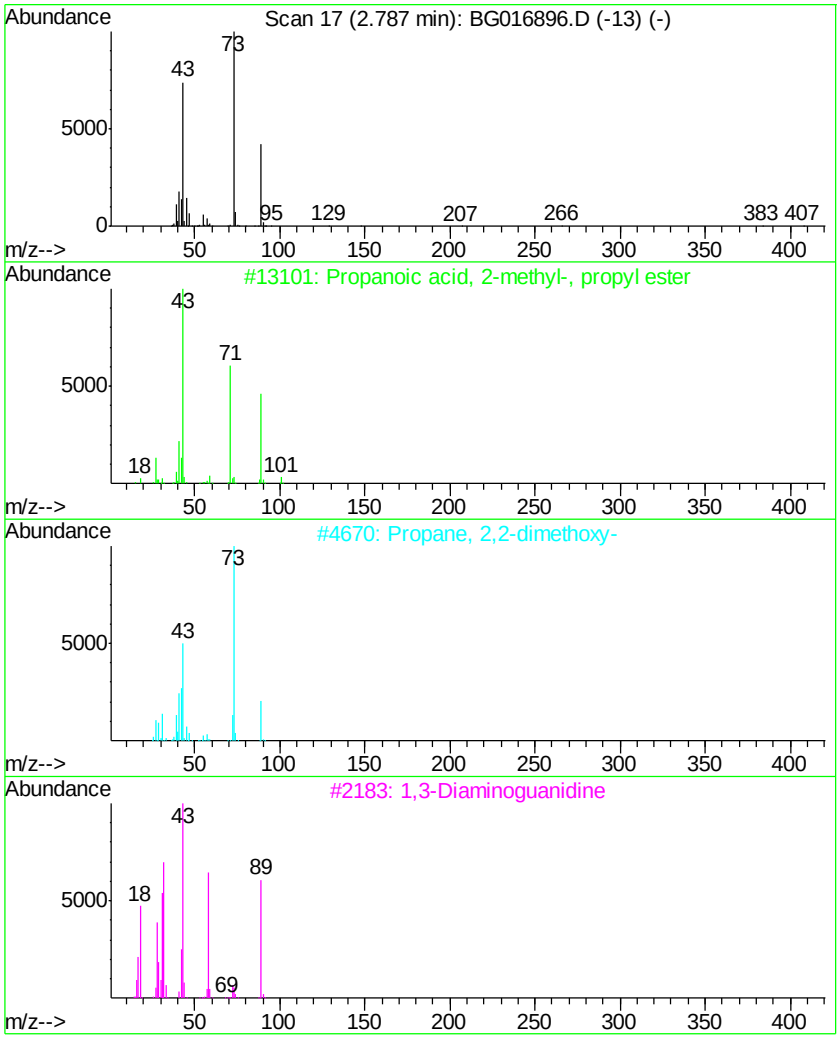
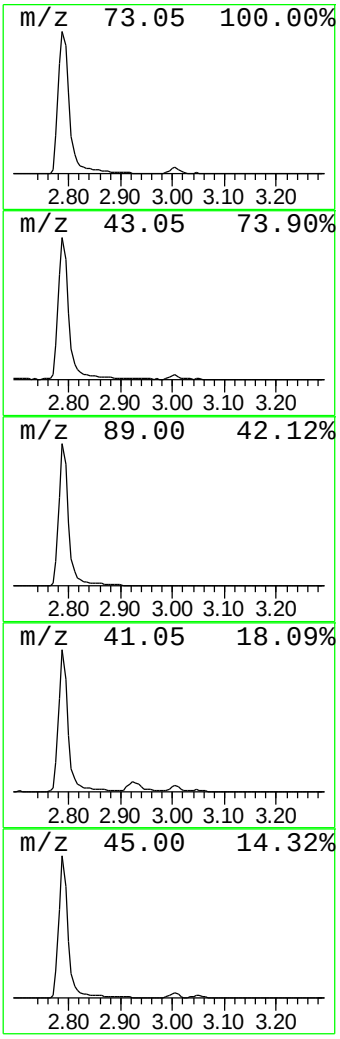
Peak Number 1 unknown2.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	319.16 ng	7707260	1,4-Dichlorobenzene-d4	7.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	47
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	33
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	32
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
Acq On : 6 May 2015 13:15
Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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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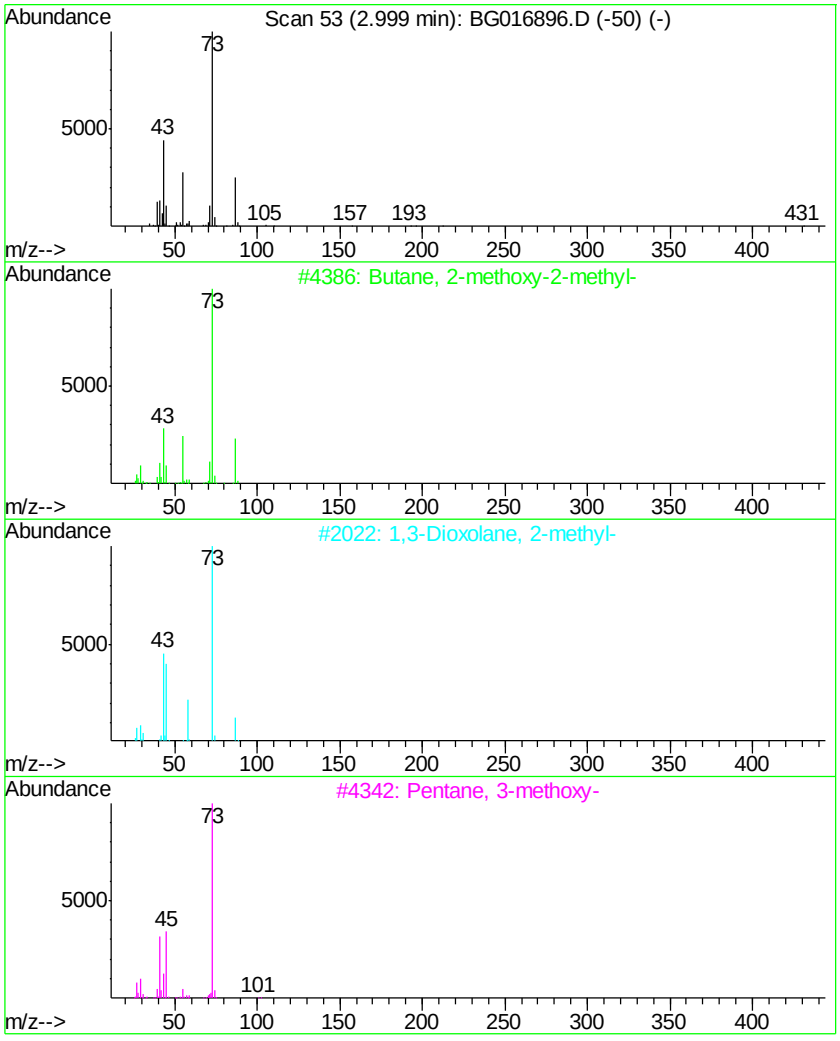
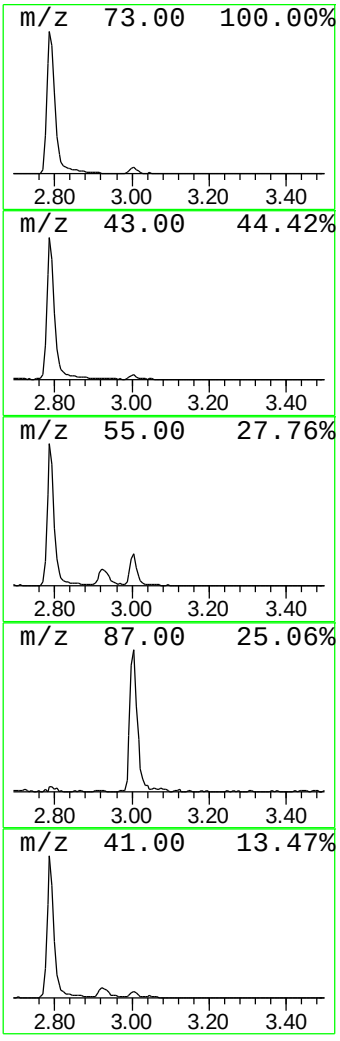
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	11.00 ng	265688	1,4-Dichlorobenzene-d4	7.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
Acq On : 6 May 2015 13:15
Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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

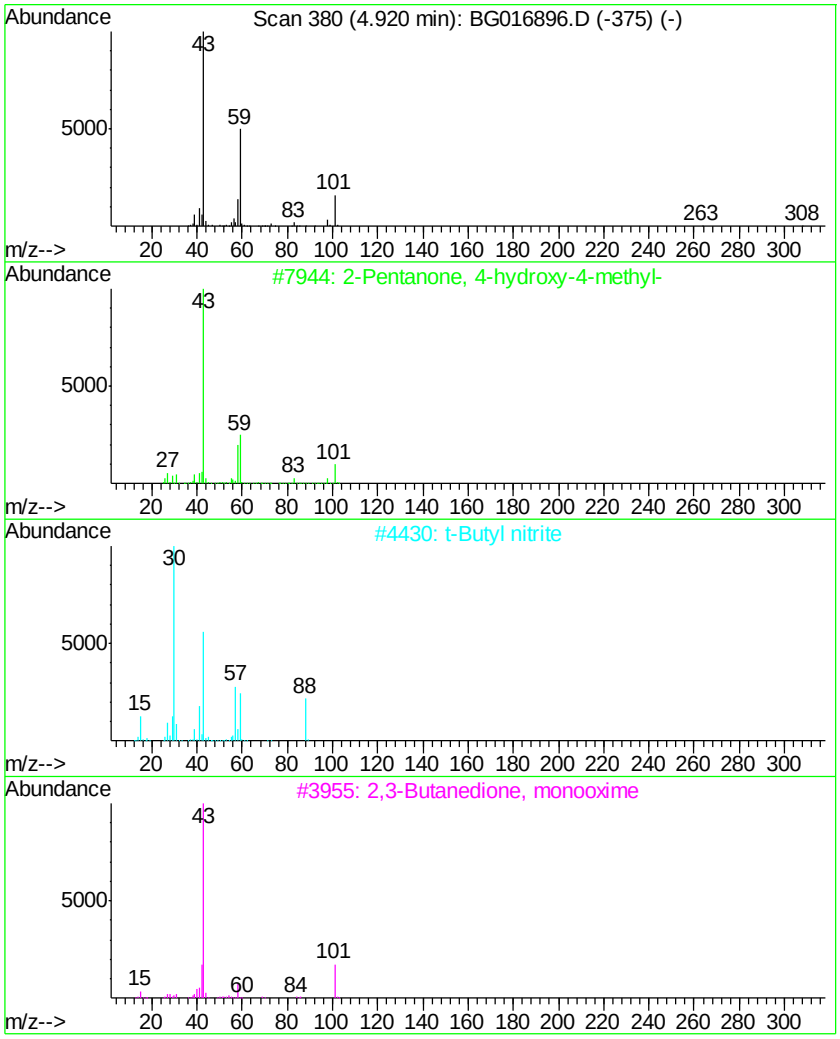
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

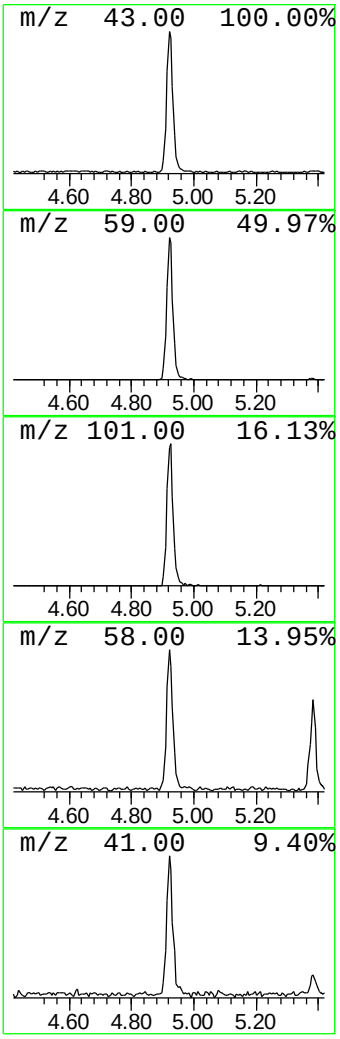
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	21.49 ng	518989	1,4-Dichlorobenzene-d4	7.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
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Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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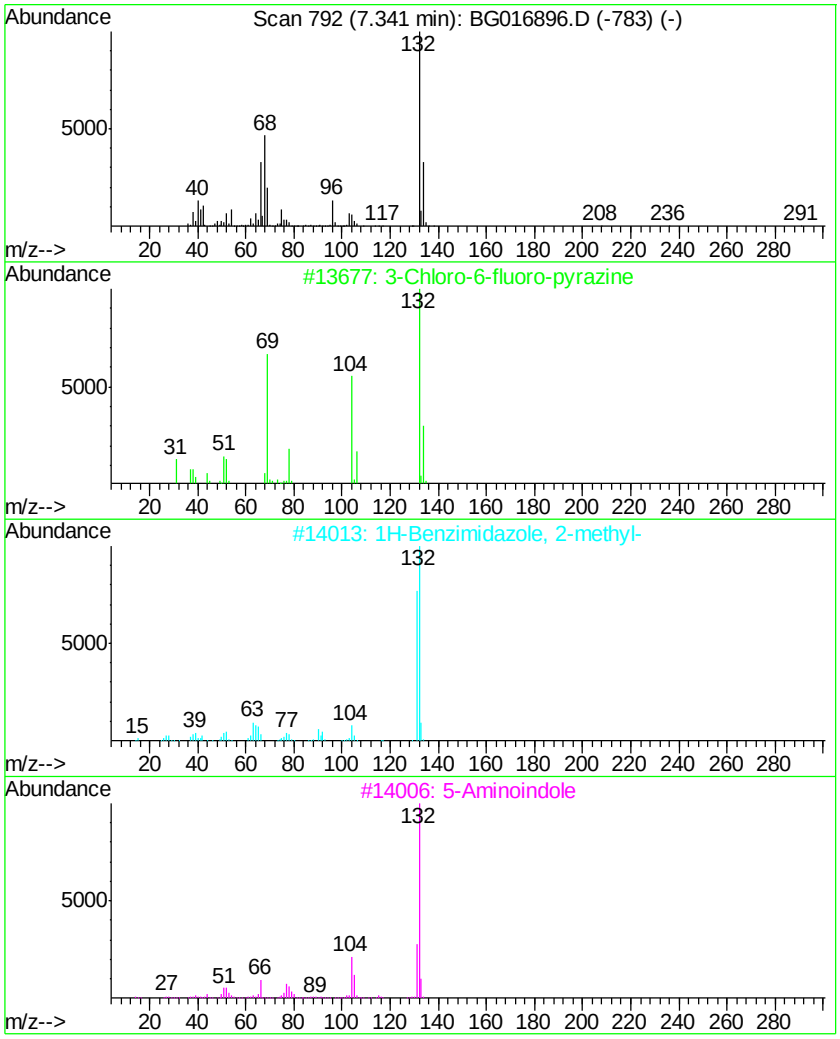
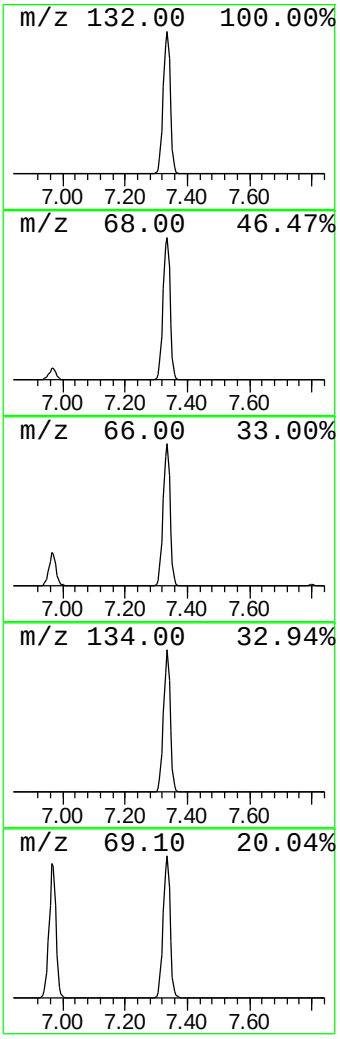
Peak Number 5 unknown7.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	110.20 ng	2661040	1,4-Dichlorobenzene-d4	7.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050615\
Data File : BG016896.D
Acq On : 6 May 2015 13:15
Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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

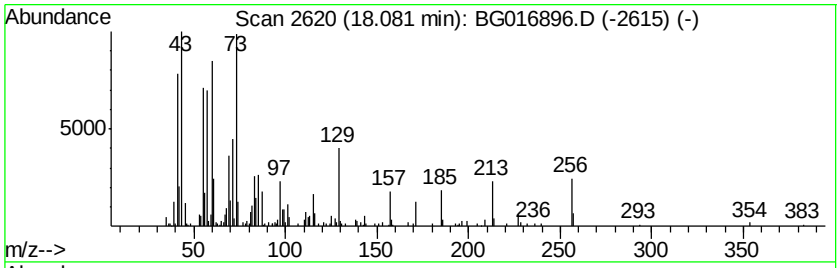
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

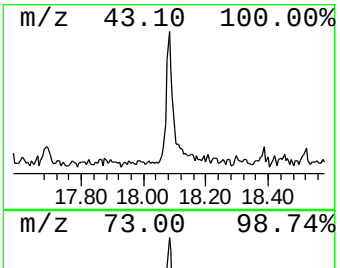
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	4.25 ng	258917	Phenanthrene-d10	17.18

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	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	11
5	Eicosane	282	C20H42	000112-95-8	11





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Operator : TP/IZ
Sample : G2035-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8-D5.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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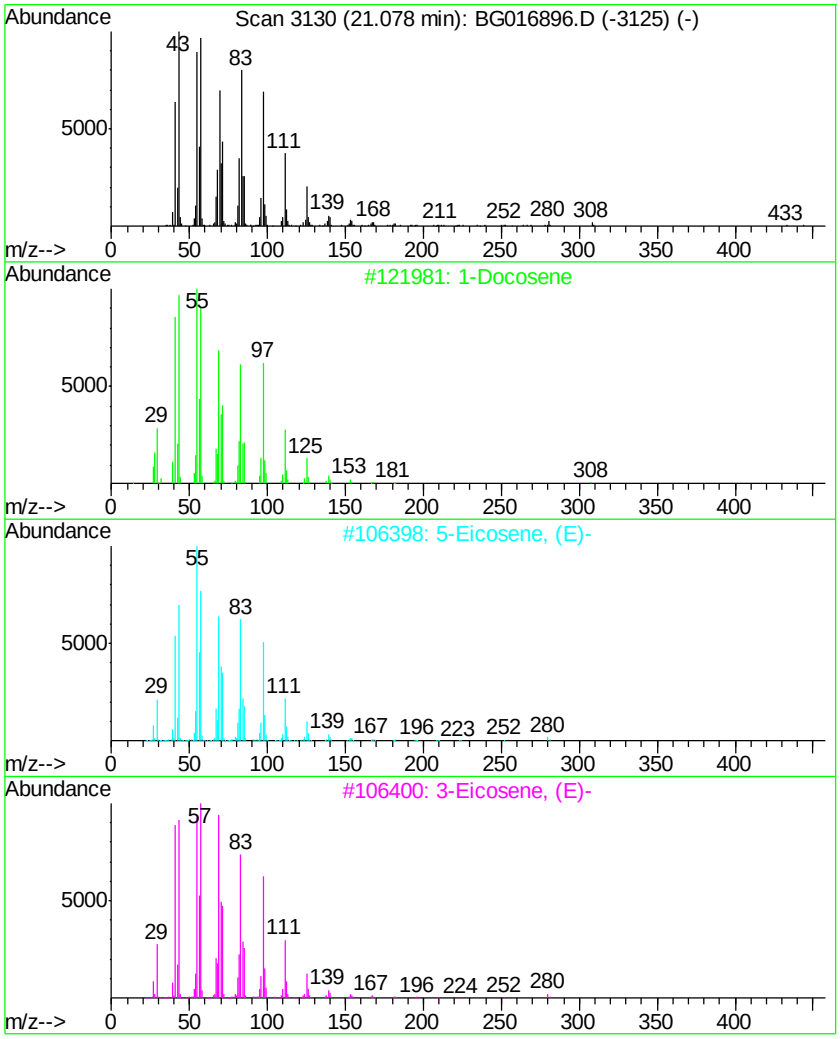
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

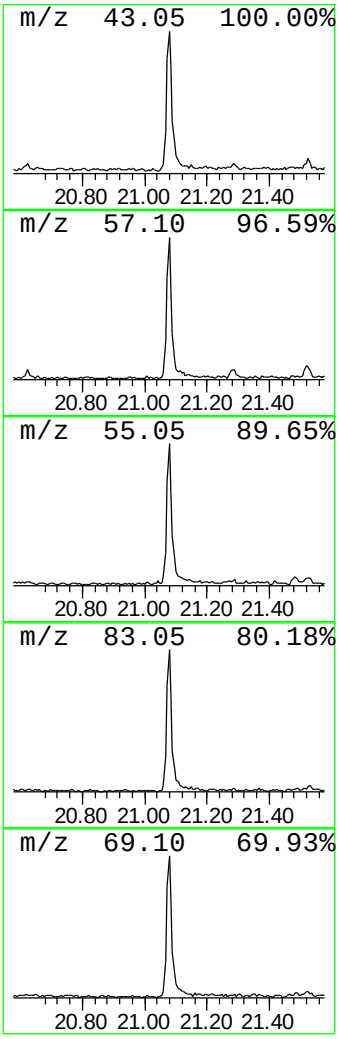
****

Peak Number 8 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	9.02 ng	603136	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : TP-8-D5.5

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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
unknown2.79	2.79	319.2	ng	7707260	1	7.80	482971	20.0
Butane, 2-methoxy...	3.00	11.0	ng	265688	1	7.80	482971	20.0
2-Pentanone, 4-hy...	4.92	21.5	ng	518989	1	7.80	482971	20.0
unknown7.34	7.34	110.2	ng	2661040	1	7.80	482971	20.0
n-Hexadecanoic acid	18.08	4.3	ng	258917	4	17.18	1219360	20.0
1-Docosene	21.08	9.0	ng	603136	5	21.36	1336860	20.0