LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023041.D
Acq On : 12 Jul 2016 18:04
Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

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-BG070816.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	2.897	6	10	23	rVB	180077	381458	2.17%	0.408%
2	3.038	29	34	54	rBV	5646390	8587843	48.75%	9.190%
3	3.184	54	59	75	rVB2	149967	316574	1.80%	0.339%
4	3.801	160	164	174	rBV	141954	247932	1.41%	0.265%
5	5.217	401	405	412	rBV2	118125	188547	1.07%	0.202%
6	5.699	478	487	500	rVB	1934731	3211789	18.23%	3.437%
7	7.309	753	761	770	rBV	2368847	4165531	23.65%	4.458%
8	7.679	816	824	834	rBV	2104975	3721799	21.13%	3.983%
9	8.149	897	904	915	rVB	346176	604577	3.43%	0.647%
10	8.478	951	960	971	rVB	1429467	2540689	14.42%	2.719%
11	9.324	1095	1104	1115	rBV	1433907	2625608	14.91%	2.810%
12	10.981	1379	1386	1395	rVB	569852	1006490	5.71%	1.077%
13	13.420	1791	1801	1811	rBV	3932918	6274385	35.62%	6.715%
14	14.242	1932	1941	1946	rBV	745986	1086127	6.17%	1.162%
15	14.800	2030	2036	2045	rVB2	1036733	1715295	9.74%	1.836%
16	16.293	2283	2290	2304	rBV	3854111	6099739	34.63%	6.528%
17	17.286	2455	2459	2463	rBV	152008	190300	1.08%	0.204%
18	17.562	2499	2506	2512	rBV	1289679	2105984	11.96%	2.254%
19	18.026	2581	2585	2592	rBV	150298	206027	1.17%	0.220%
20	18.425	2648	2653	2660	rBV2	208361	287924	1.63%	0.308%
21	20.165	2943	2949	2957	rBV	6282585	8575186	48.68%	9.177%
22	20.253	2959	2964	2969	rVV	187747	227552	1.29%	0.244%
23	21.487	3168	3174	3185	rBV5	196130	577062	3.28%	0.618%
24	21.704	3203	3211	3212	rBV	10066741	16154561	91.71%	17.288%
25	21.722	3212	3214	3225	rVB	11891464	17614624	100.00%	18.850%
26	21.868	3232	3239	3246	rVB2	1319018	2407376	13.67%	2.576%
27	25.253	3803	3815	3826	rBV2	756192	2323049	13.19%	2.486%

Sum of corrected areas: 93444028

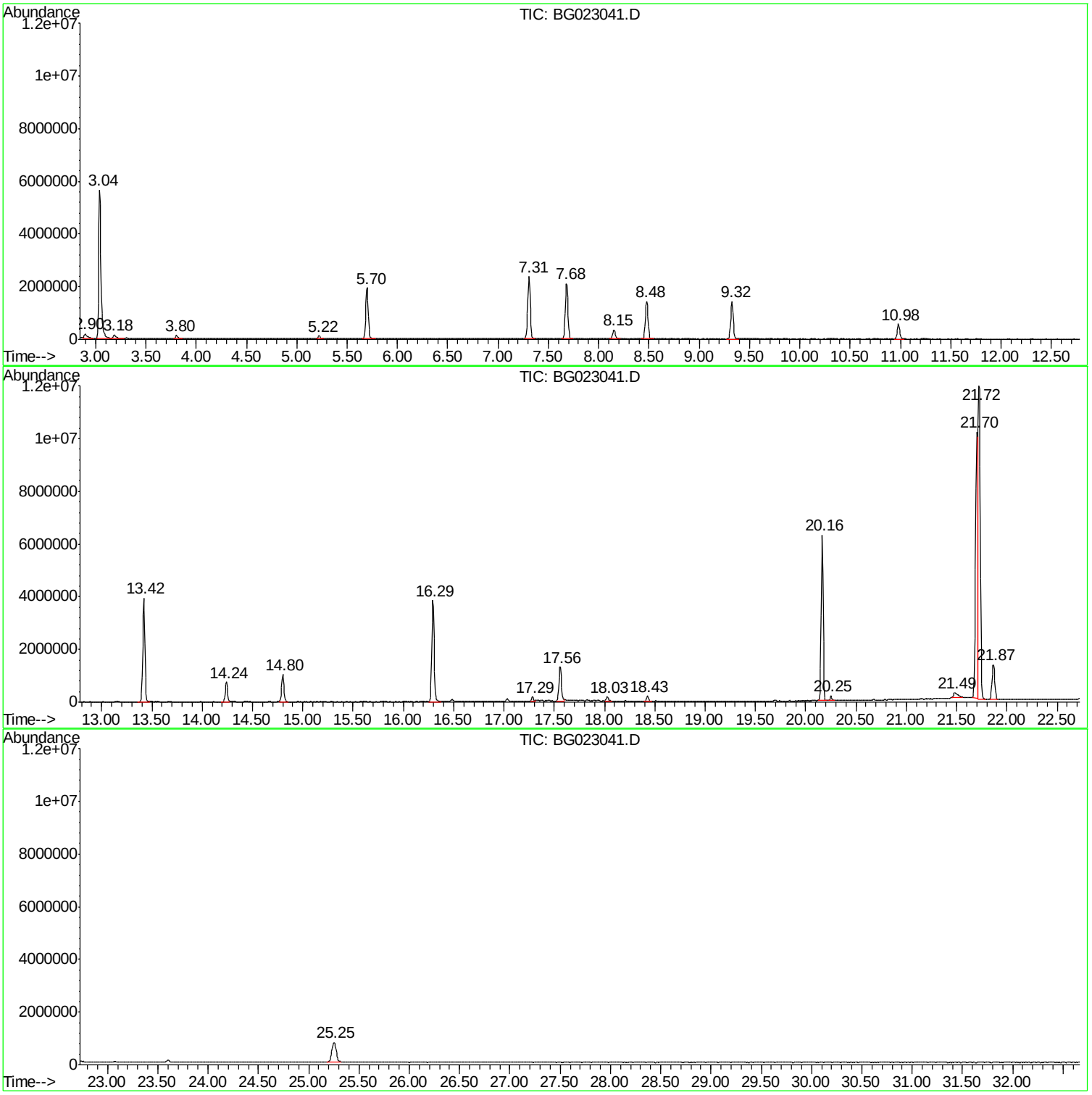
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023041.D
Acq On : 12 Jul 2016 18:04
Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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

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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

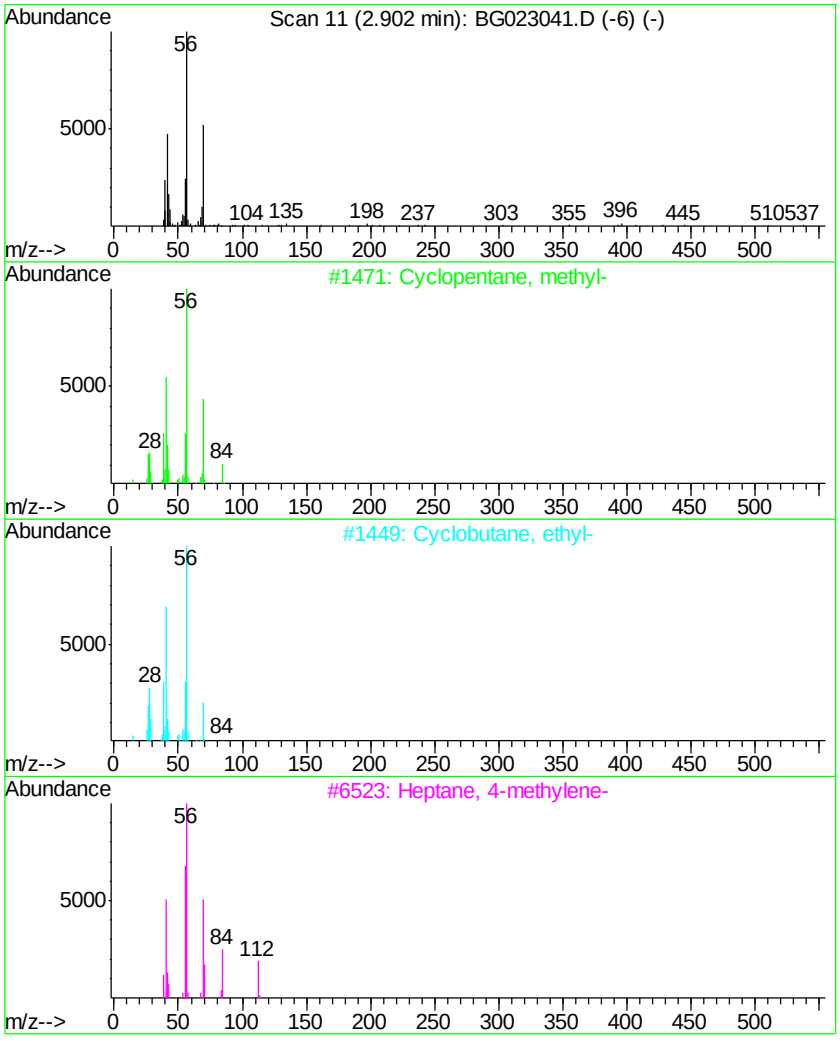
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

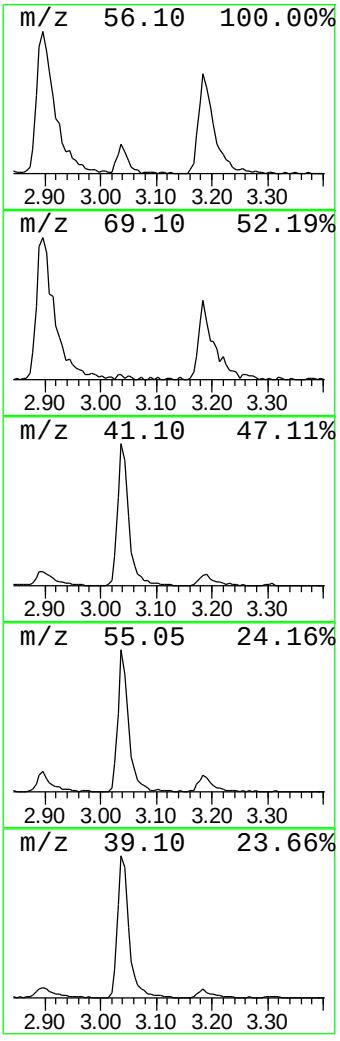
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	12.62 ng	381458	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
3	Heptane, 4-methylene-	112	C8H16	015918-08-8	39
4	2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	38
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	38





Library Search Compound Report

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Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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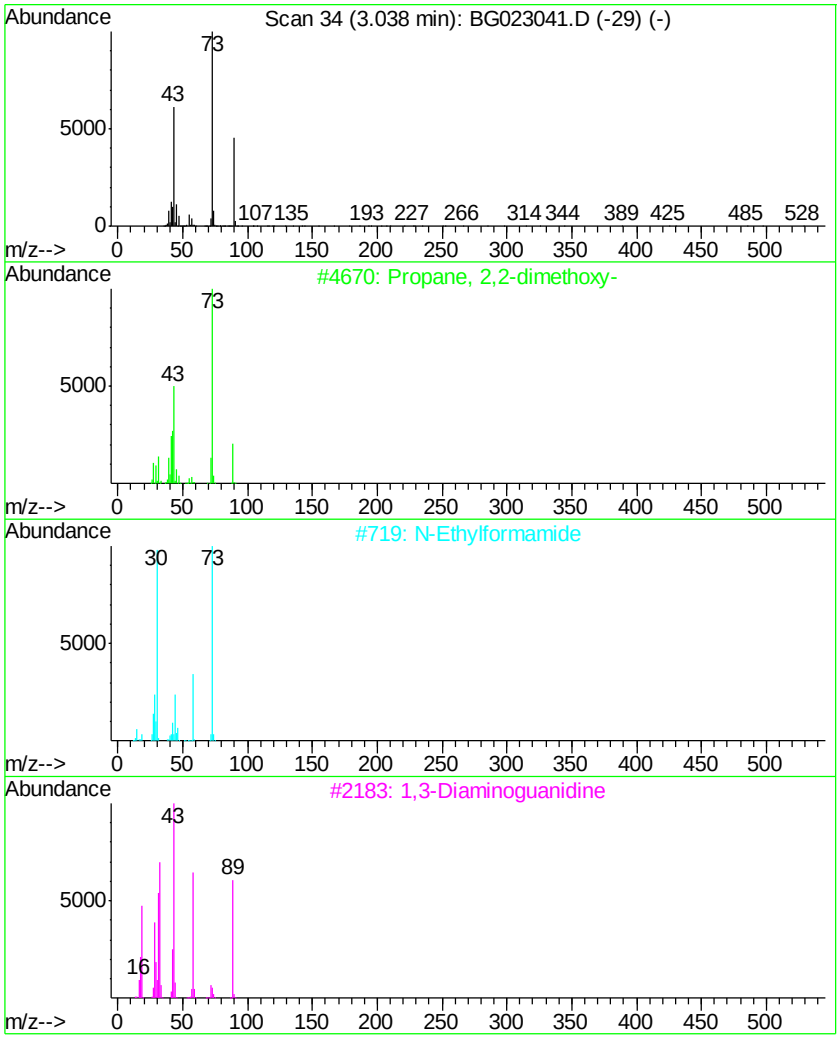
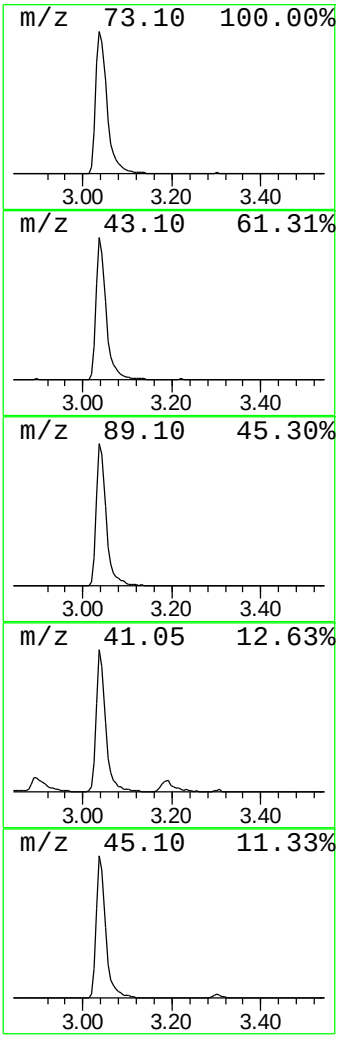
Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	284.09 ng	8587840	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	40
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023041.D
Acq On : 12 Jul 2016 18:04
Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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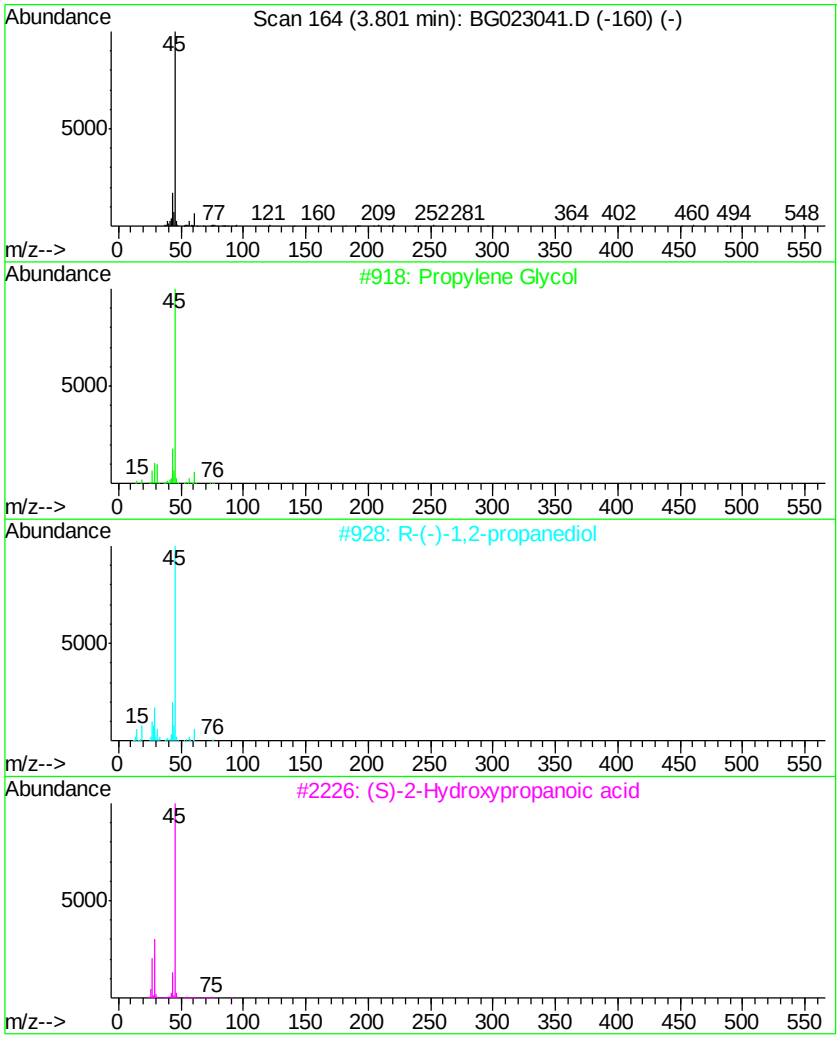
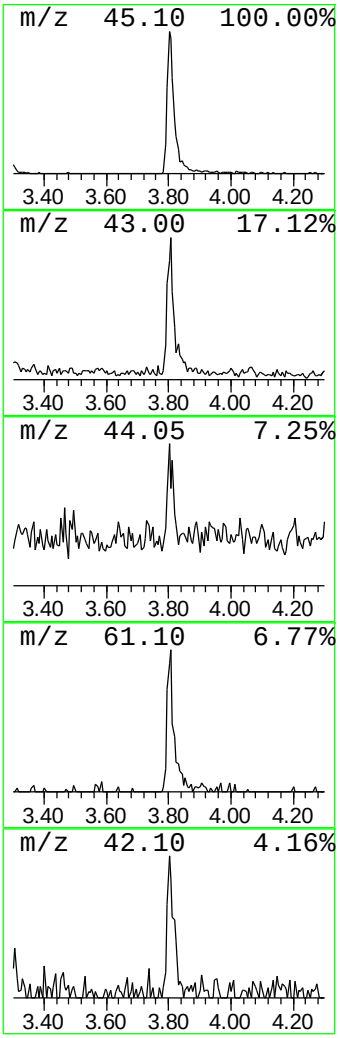
Peak Number 4 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.80	8.20 ng	247932	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	80
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	25
3	(S)-2-Hydroxypropanoic acid	90	C3H6O3	000079-33-4	9
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023041.D
Acq On : 12 Jul 2016 18:04
Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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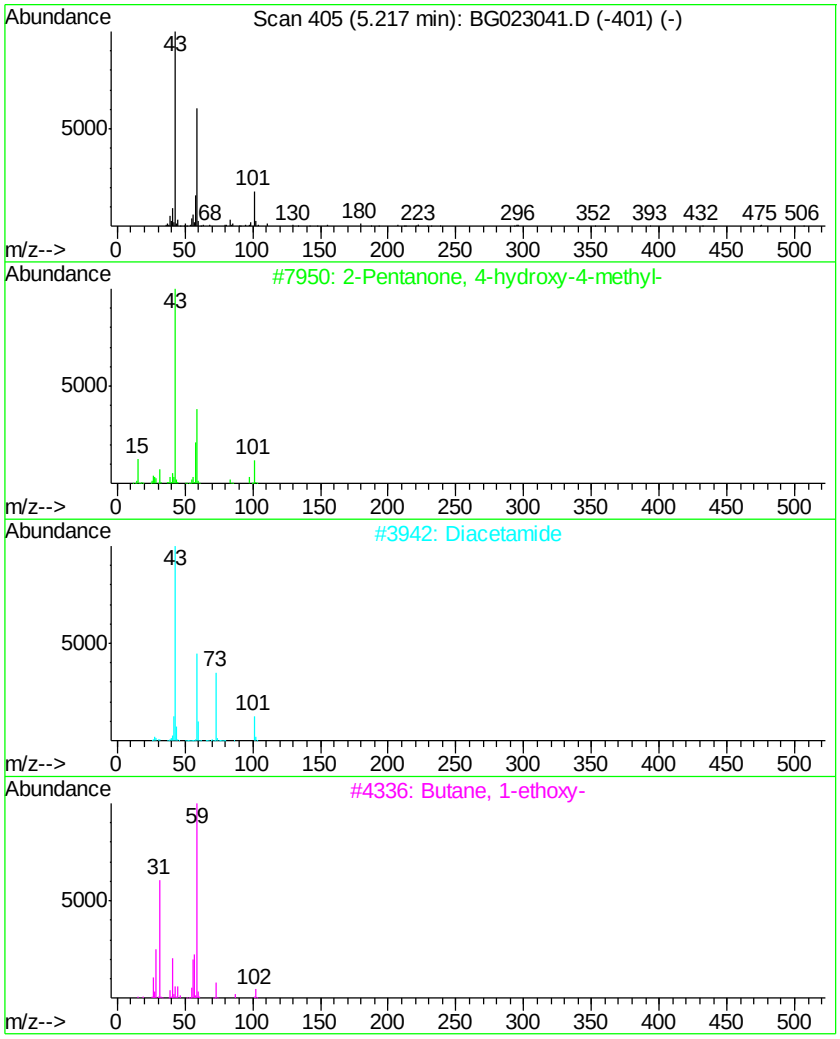
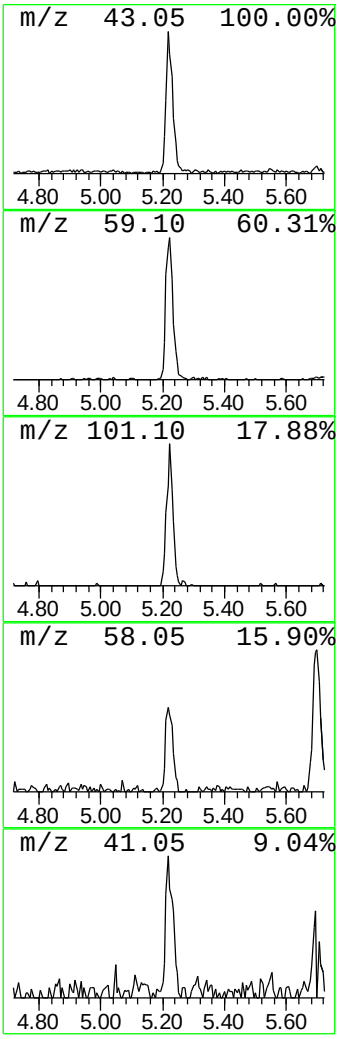
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	6.24 ng	188547	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	42
2	Diacetamide	101	C4H7NO2	000625-77-4	36
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	27
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	25





Library Search Compound Report

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Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
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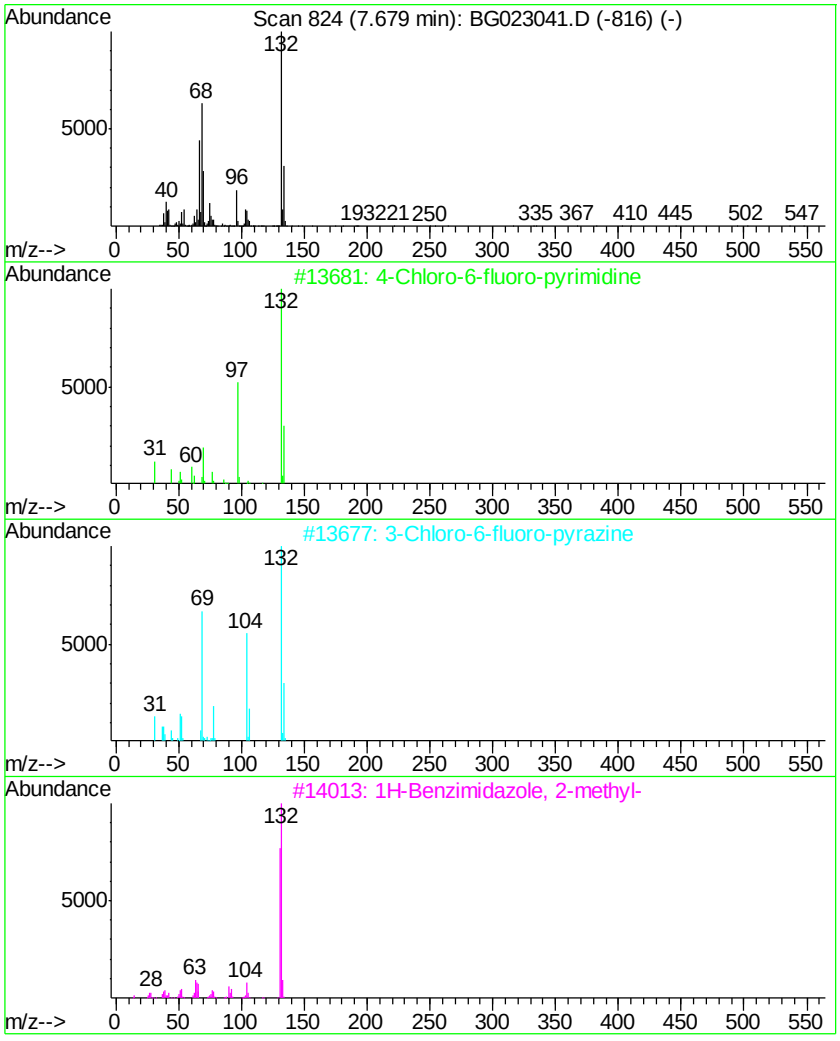
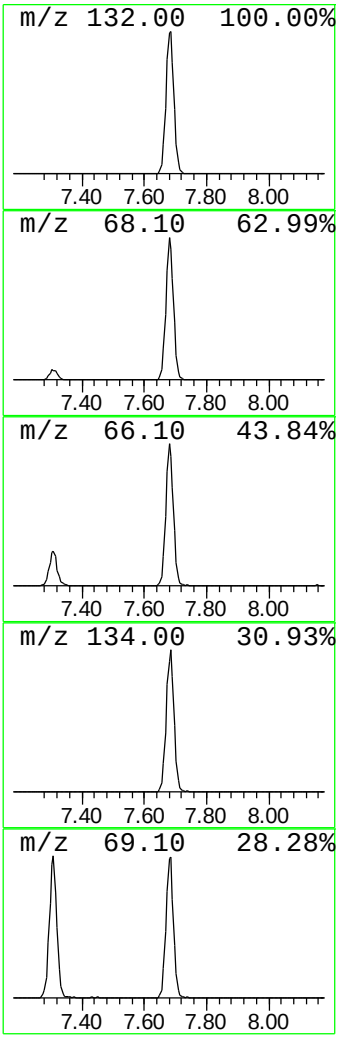
Peak Number 6 unknown7.68 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	123.12 ng	3721800	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	5-Aminoindole	132	C8H8N2	005192-03-0	14
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
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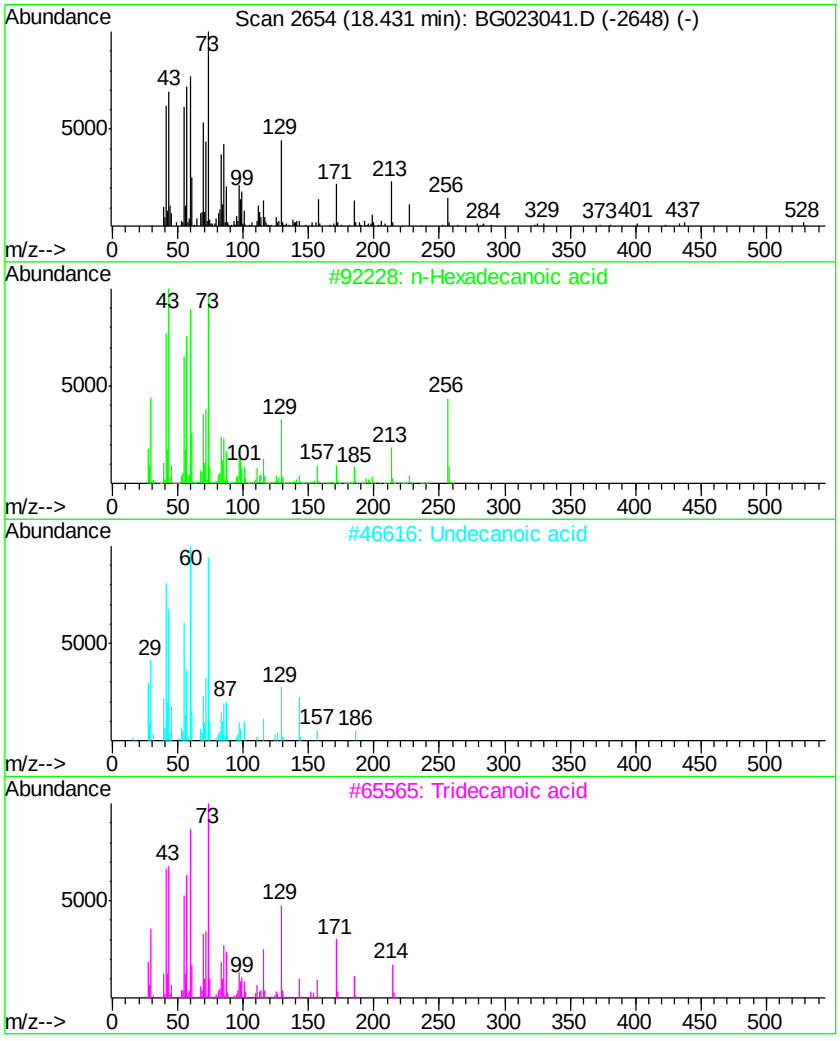
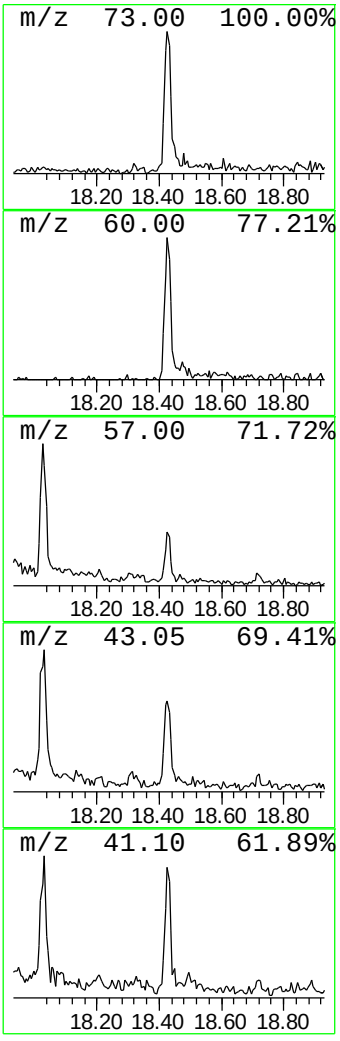
Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.73 ng	287924	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	53





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Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

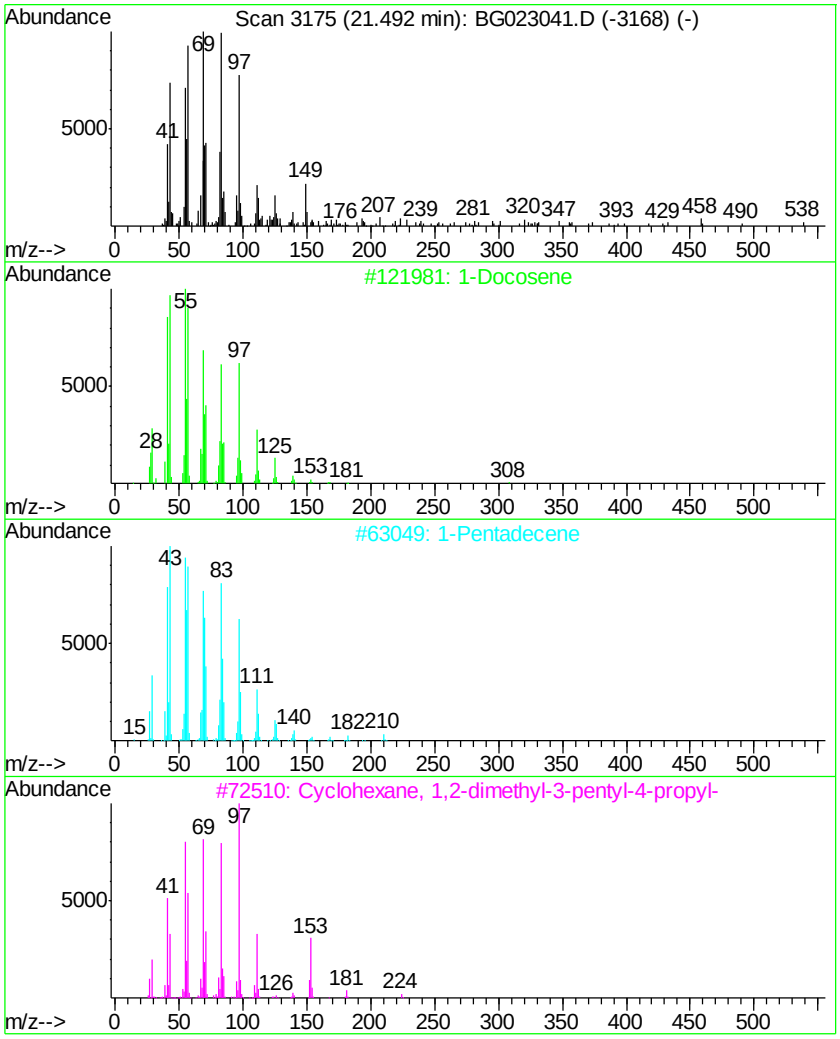
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

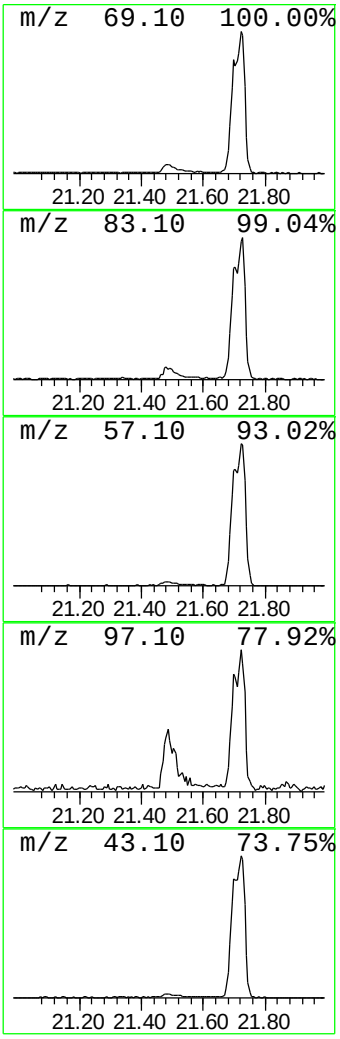
****

Peak Number 9 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	4.79 ng	577062	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Pentadecene	210	C15H30	013360-61-7	91
3	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	72
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	68
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	64





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TIC Library : C:\DATABASE\NIST02.L
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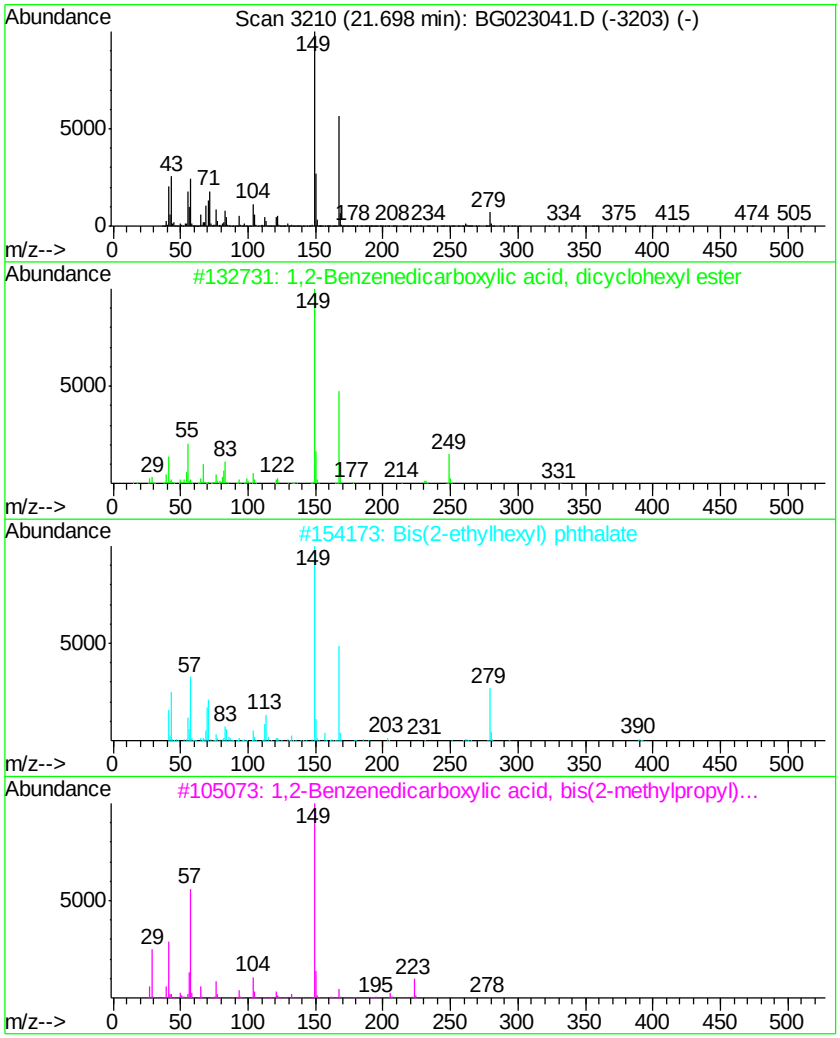
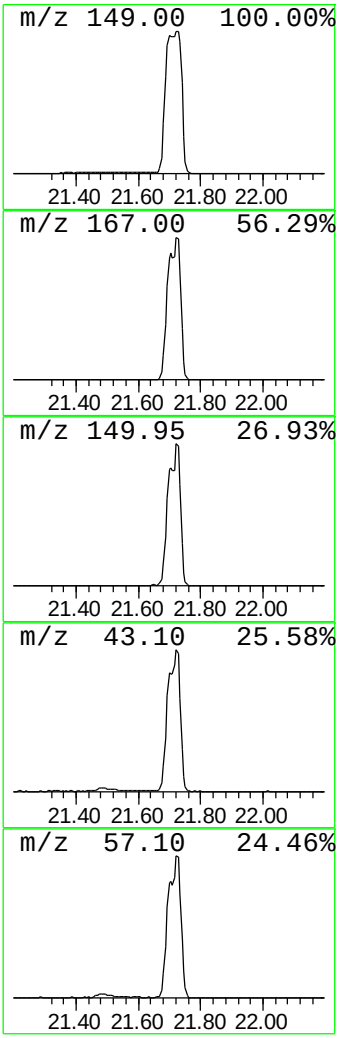
Peak Number 10 1,2-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	134.21 ng	16154600	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	330	C20H26O4	000084-61-7	56
2	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	56
3	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	50
4	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	50
5	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	49





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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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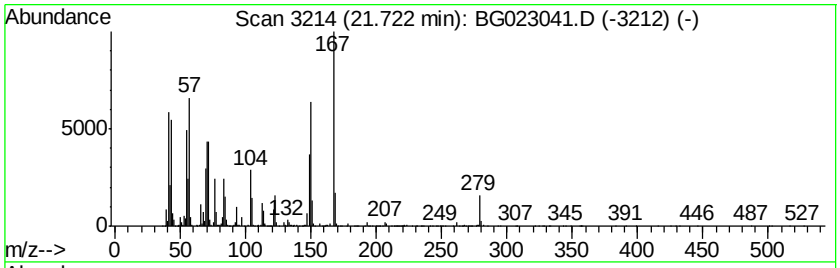
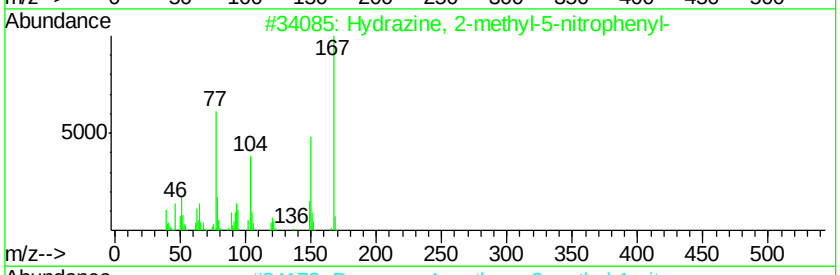
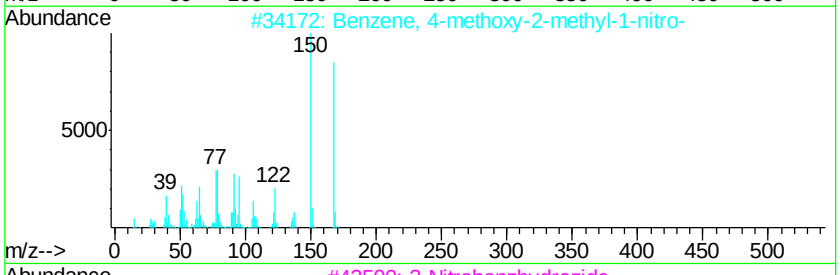
Peak Number 11 unknown21.72 Concentration Rank 2

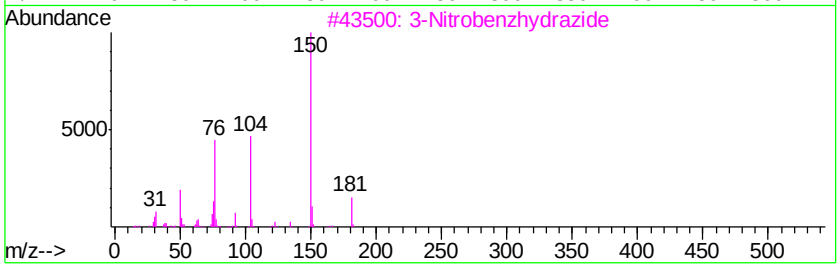
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	146.34 ng	17614600	Chrysene-d12	21.86

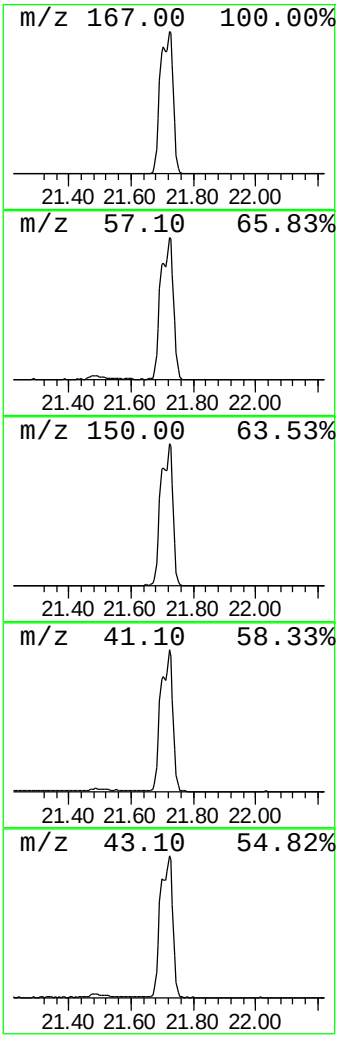
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 2-methyl-5-nitrophenyl-	167	C7H9N3O2	005089-08-7	32
2	Benzene, 4-methoxy-2-methyl-1-ni...	167	C8H9NO3	005367-32-8	25
3	3-Nitrobenzhydrazide	181	C7H7N3O3	000618-94-0	14
4	Benzoic acid, 4-nitro-, ethyl ester	195	C9H9NO4	000099-77-4	12
5	Benzoic acid, 4-nitro-, methyl e...	181	C8H7NO4	000619-50-1	10











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071216\
Data File : BG023041.D
Acq On : 12 Jul 2016 18:04
Operator : UM/SJ
Sample : H3937-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LOCATION-2A-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
Cyclopentane, met...	2.90	12.6	ng	381458	1	8.15	604577	20.0
unknown3.04	3.04	284.1	ng	8587840	1	8.15	604577	20.0
Propylene Glycol	3.80	8.2	ng	247932	1	8.15	604577	20.0
2-Pentanone, 4-hy...	5.22	6.2	ng	188547	1	8.15	604577	20.0
unknown7.68	7.68	123.1	ng	3721800	1	8.15	604577	20.0
n-Hexadecanoic acid	18.43	2.7	ng	287924	4	17.56	2105980	20.0
1-Docosene	21.49	4.8	ng	577062	5	21.86	2407380	20.0
1,2-Benzenedicarb...	21.70	134.2	ng	16154600	5	21.86	2407380	20.0
unknown21.72	21.72	146.3	ng	17614600	5	21.86	2407380	20.0