LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023028.D
Acq On : 12 Jul 2016 9:20
Operator : UM/SJ
Sample : H3936-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2(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-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	3.037	29	34	54	rVB	6248774	9459681	100.00%	15.762%
2	5.223	399	406	412	rBV2	109306	175248	1.85%	0.292%
3	5.699	479	487	501	rBV	2019727	3265801	34.52%	5.442%
4	7.309	753	761	773	rBV	2326097	4156033	43.93%	6.925%
5	7.685	816	825	837	rBV	2186990	3767356	39.83%	6.277%
6	8.155	899	905	913	rBV2	365618	626937	6.63%	1.045%
7	8.484	953	961	968	rBV	1388928	2501292	26.44%	4.168%
8	9.330	1096	1105	1115	rVB	1484312	2673301	28.26%	4.454%
9	10.987	1380	1387	1396	rBV	563160	1017141	10.75%	1.695%
10	13.419	1793	1801	1809	rBV	3758943	6083889	64.31%	10.137%
11	14.242	1935	1941	1948	rBV	708067	1030575	10.89%	1.717%
12	14.800	2030	2036	2044	rBV2	1047188	1737690	18.37%	2.895%
13	16.293	2282	2290	2299	rBV	3863438	5994564	63.37%	9.988%
14	16.486	2318	2323	2334	rVB2	147436	268171	2.83%	0.447%
15	17.556	2499	2505	2512	rBV2	1328451	2099168	22.19%	3.498%
16	18.425	2648	2653	2660	rBV3	198543	288447	3.05%	0.481%
17	19.606	2850	2854	2858	rBV	84105	107987	1.14%	0.180%
18	20.159	2942	2948	2955	rBV	6199573	8609018	91.01%	14.345%
19	21.469	3167	3171	3183	rVB3	168395	271784	2.87%	0.453%
20	21.868	3232	3239	3245	rBV	1402950	2436676	25.76%	4.060%
21	22.045	3264	3269	3274	rVB2	87749	132210	1.40%	0.220%
22	22.673	3372	3376	3380	rBV3	74176	115486	1.22%	0.192%
23	23.396	3495	3499	3504	rVB7	81635	130904	1.38%	0.218%
24	23.602	3526	3534	3541	rBV	241440	523193	5.53%	0.872%
25	24.248	3639	3644	3649	rVB7	88722	168589	1.78%	0.281%
26	25.253	3804	3815	3826	rBV	793800	2373792	25.09%	3.955%

Sum of corrected areas: 60014933

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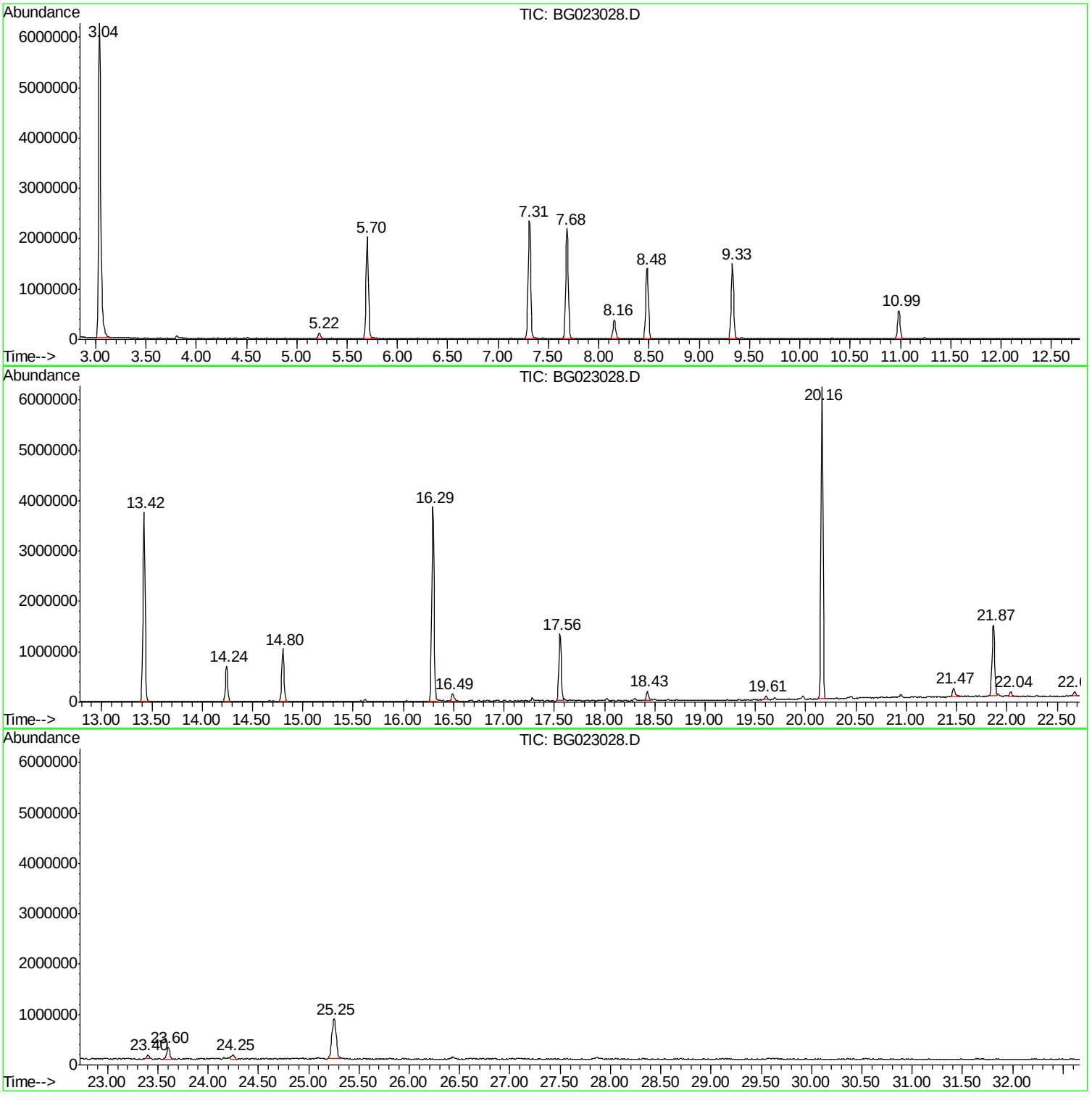
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-2(9-10)

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023028.D
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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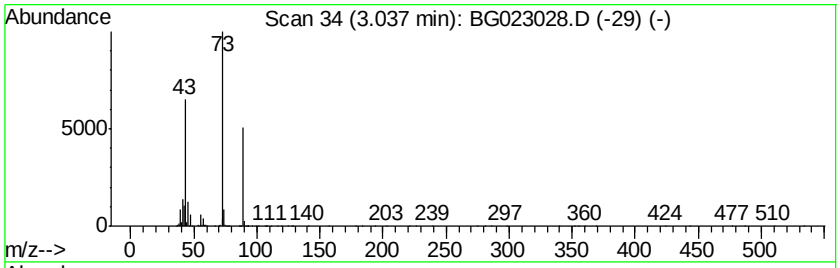
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

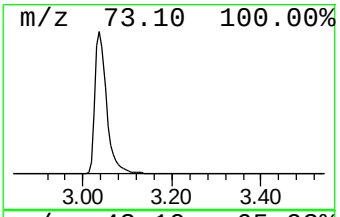
****

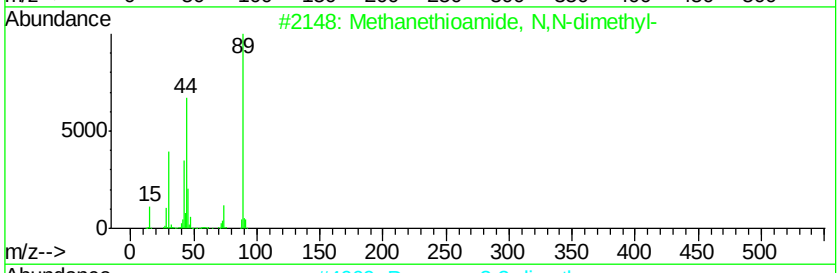
Peak Number 1 unknown3.04 Concentration Rank 1

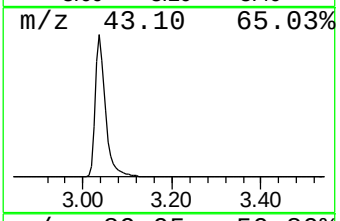
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	301.78 ng	9459680	1,4-Dichlorobenzene-d4	8.16

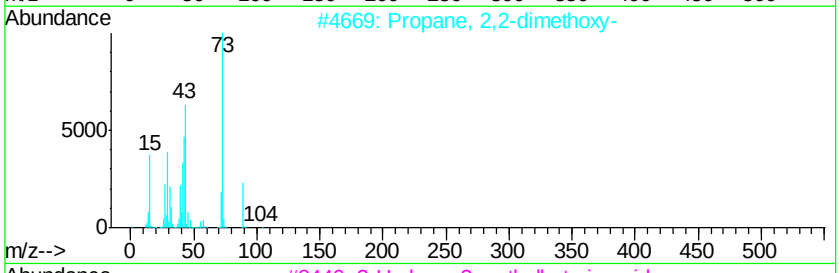
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9
5	N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	9

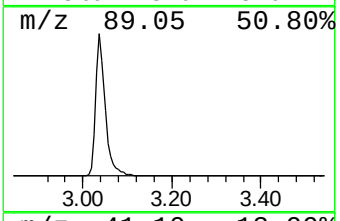


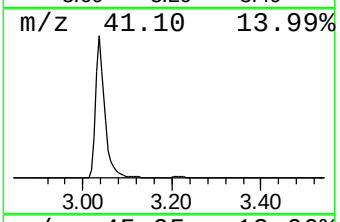


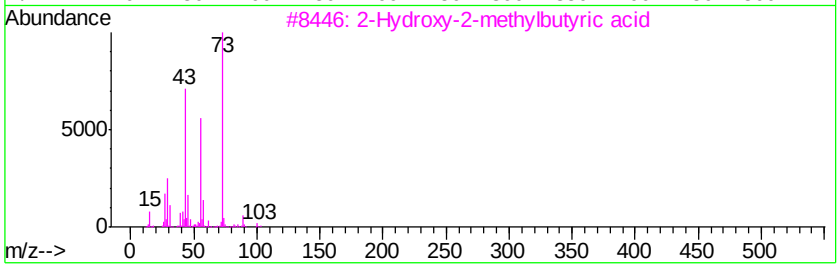


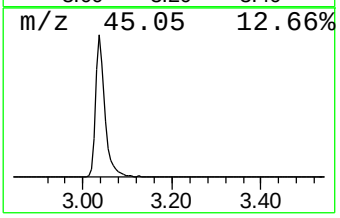












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023028.D
Acq On : 12 Jul 2016 9:20
Operator : UM/SJ
Sample : H3936-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2(9-10)

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

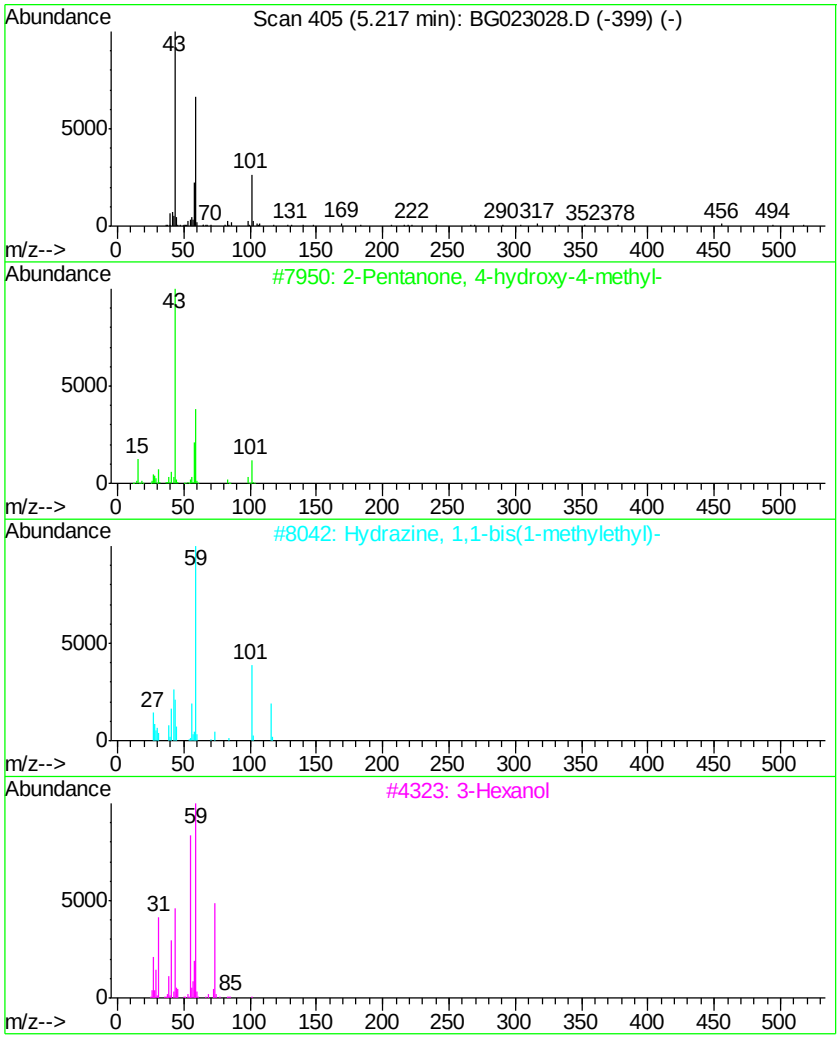
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

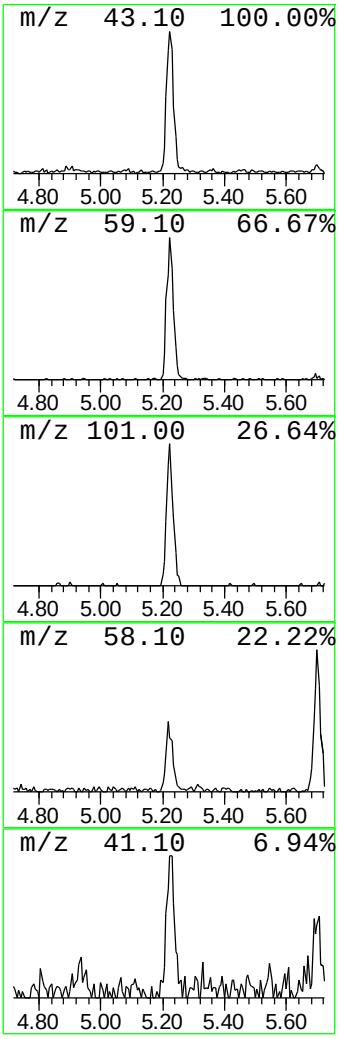
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.59 ng	175248	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	28





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
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Sample : H3936-02
Misc :
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Instrument : BNA_G
ClientSampleId : SB-2(9-10)

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

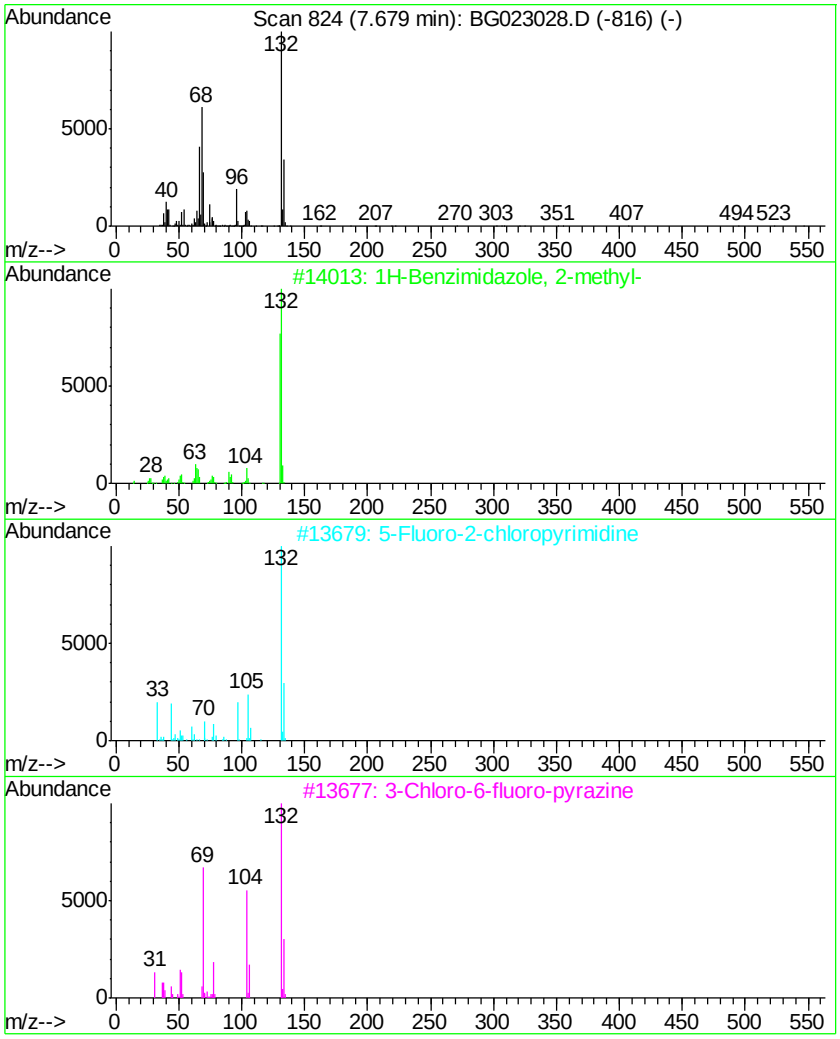
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

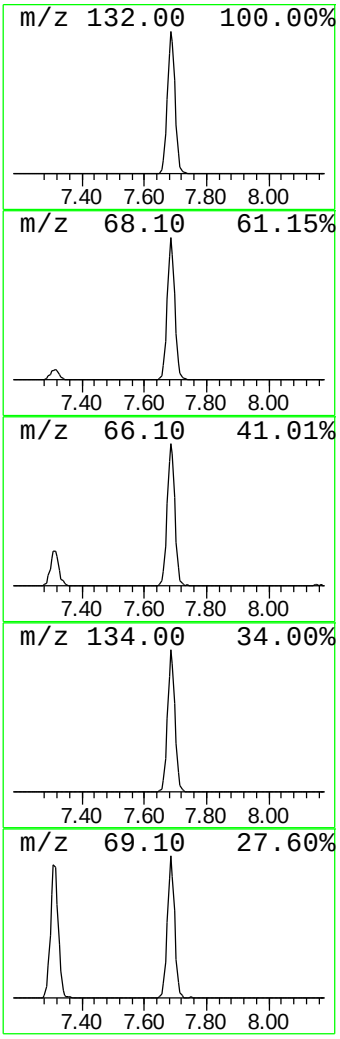
****

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	120.18 ng	3767360	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10





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Sample : H3936-02
Misc :
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Instrument : BNA_G
ClientSampleId : SB-2(9-10)

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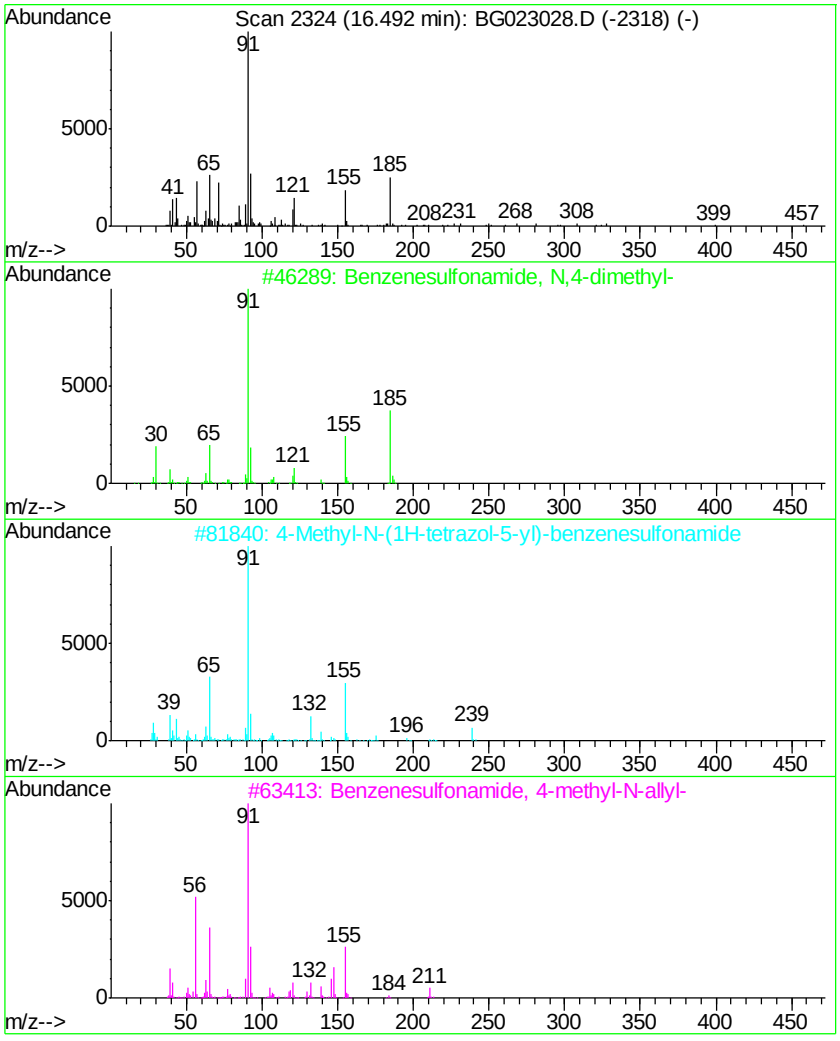
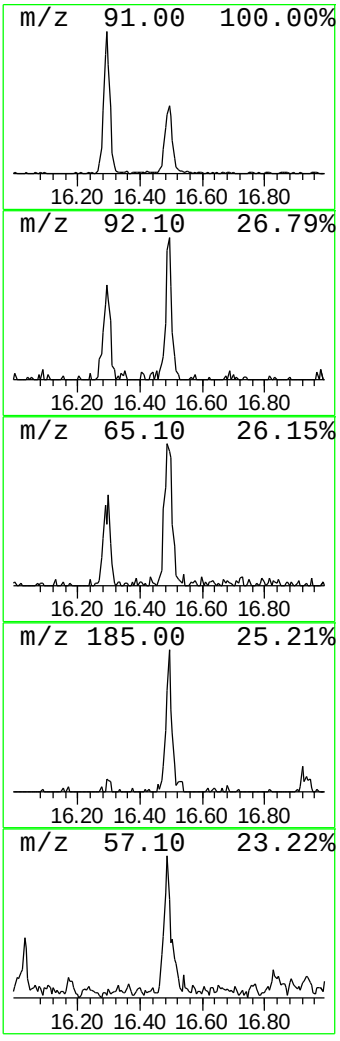
****

Peak Number 5 unknown16.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.56 ng	268171	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	49
2	4-Methyl-N-(1H-tetrazol-5-yl)-be...	239	C8H9N5O2S	006455-80-7	38
3	Benzenesulfonamide, 4-methyl-N-a...	211	C10H13NO2S	050487-71-3	38
4	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	35
5	1,3-O-Methylene-tris(p-toluenesu...	626	C27H30O11S3	1000126-23-5	35





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ClientSampleId : SB-2(9-10)

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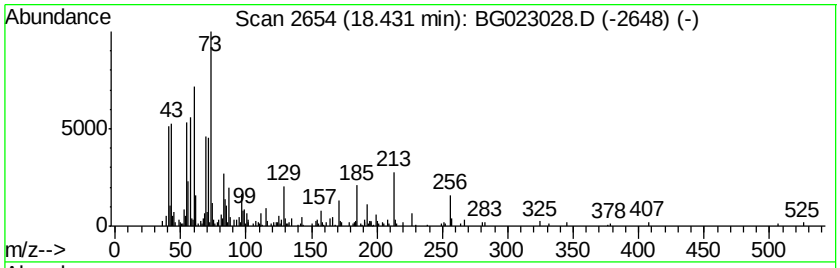
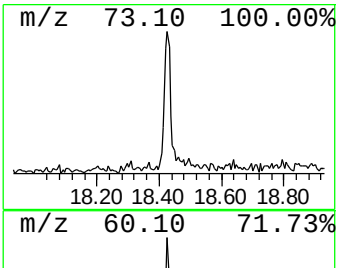
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.75 ng	288447	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Dodecanoic acid	200	C12H24O2	000143-07-7	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Sample : H3936-02
Misc :
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Instrument : BNA_G
ClientSampleId : SB-2(9-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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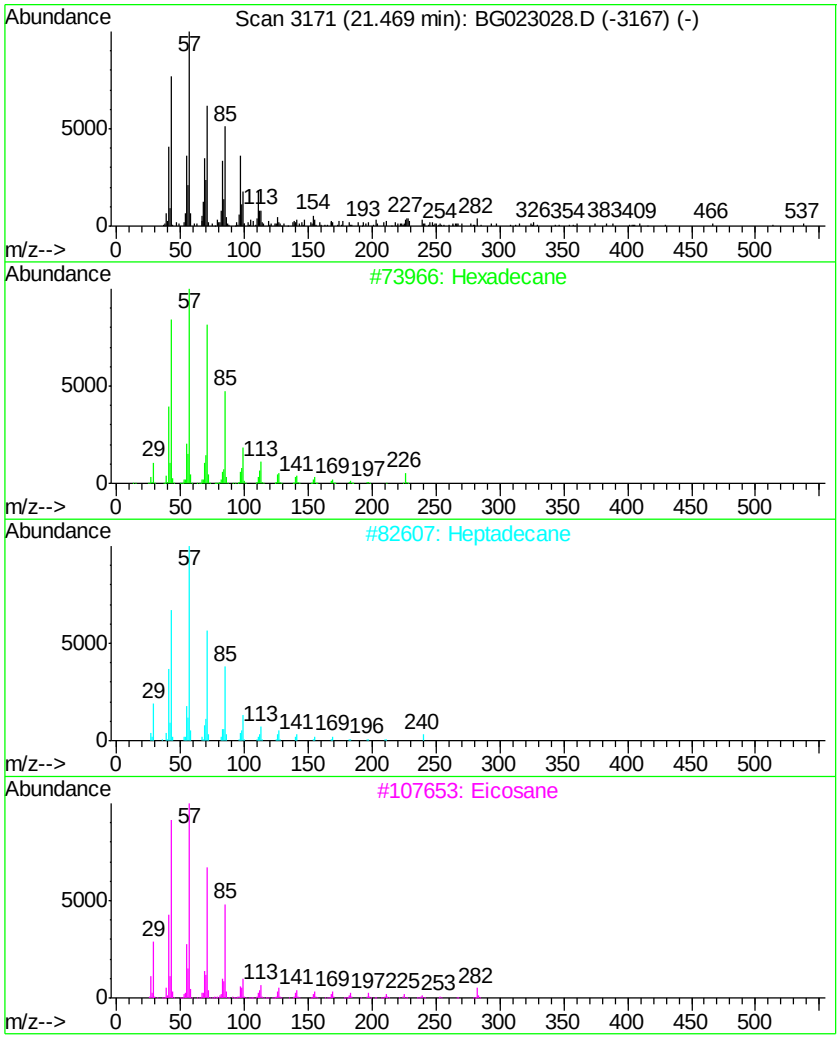
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

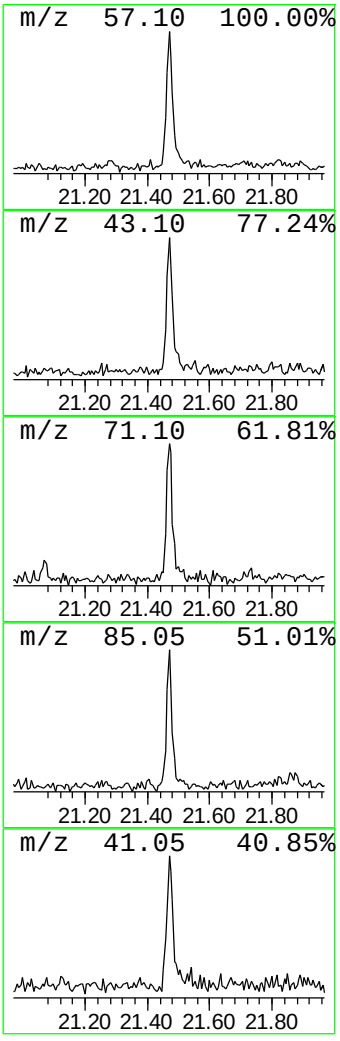
****

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	2.23 ng	271784	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	64
2	Heptadecane	240	C17H36	000629-78-7	64
3	Eicosane	282	C20H42	000112-95-8	62
4	Tridecane	184	C13H28	000629-50-5	60
5	Octadecane	254	C18H38	000593-45-3	60





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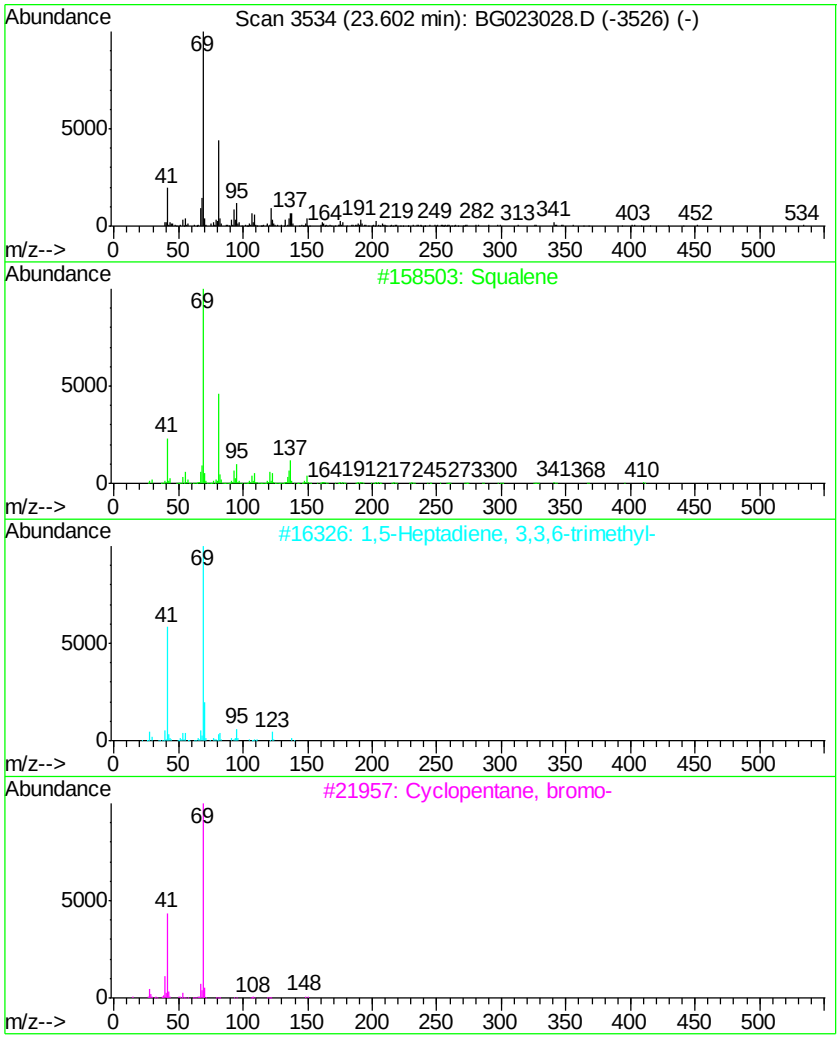
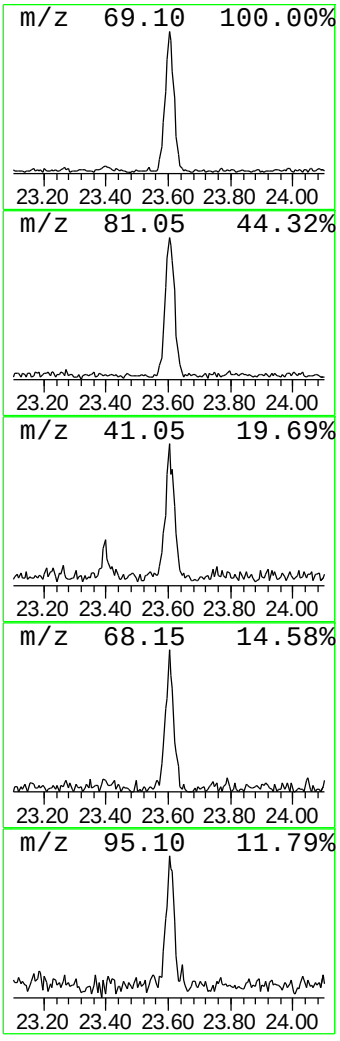
****

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.60	4.41 ng	523193	Perylene-d12	25.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	72
2	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	58
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	56
5	3,5-Dinitrobenzoic acid, 3,7,11-...	416	C22H28N2O6	054605-44-6	56





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.04	3.04	301.8	ng	9459680	1	8.16	626937	20.0
2-Pentanone, 4-hy...	5.22	5.6	ng	175248	1	8.16	626937	20.0
unknown7.68	7.68	120.2	ng	3767360	1	8.16	626937	20.0
unknown16.49	16.49	2.6	ng	268171	4	17.56	2099170	20.0
n-Hexadecanoic acid	18.43	2.8	ng	288447	4	17.56	2099170	20.0
Hexadecane	21.47	2.2	ng	271784	5	21.87	2436680	20.0
Squalene	23.60	4.4	ng	523193	6	25.25	2373790	20.0