LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022611.D
Acq On : 26 Jun 2016 15:24
Operator : UM/SJ
Sample : H3766-01
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2B

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-BG062516.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	3.055	32	37	57	rBV	9136084	15407961	100.00%	19.494%
2	5.240	403	409	415	rBV2	205018	319164	2.07%	0.404%
3	5.705	481	488	499	rBV	2980234	4868919	31.60%	6.160%
4	7.309	752	761	771	rBV	3186009	5597595	36.33%	7.082%
5	7.691	818	826	836	rVB	3090968	5236261	33.98%	6.625%
6	8.161	899	906	914	rBV	487635	867803	5.63%	1.098%
7	8.490	953	962	969	rBV	2084129	3695608	23.99%	4.676%
8	9.330	1097	1105	1113	rVB	1885590	3487428	22.63%	4.412%
9	10.987	1379	1387	1395	rBV	649142	1223990	7.94%	1.549%
10	13.419	1794	1801	1810	rVB	4341937	6900556	44.79%	8.730%
11	14.242	1934	1941	1947	rVB	550917	807216	5.24%	1.021%
12	14.800	2028	2036	2044	rVB2	1088573	1792735	11.64%	2.268%
13	16.286	2280	2289	2303	rBV	5081932	7905855	51.31%	10.002%
14	17.555	2499	2505	2511	rBV	1635587	2459691	15.96%	3.112%
15	18.431	2648	2654	2662	rBV2	389286	626930	4.07%	0.793%
16	19.694	2864	2869	2877	rBV2	348234	489345	3.18%	0.619%
17	20.158	2942	2948	2954	rBV	8197875	11031199	71.59%	13.956%
18	20.904	3071	3075	3078	rVB2	180989	201067	1.30%	0.254%
19	21.463	3166	3170	3181	rBV7	142757	331514	2.15%	0.419%
20	21.850	3229	3236	3242	rBV2	1743173	2947290	19.13%	3.729%
21	25.205	3798	3807	3821	rVB	970248	2843121	18.45%	3.597%

Sum of corrected areas: 79041248

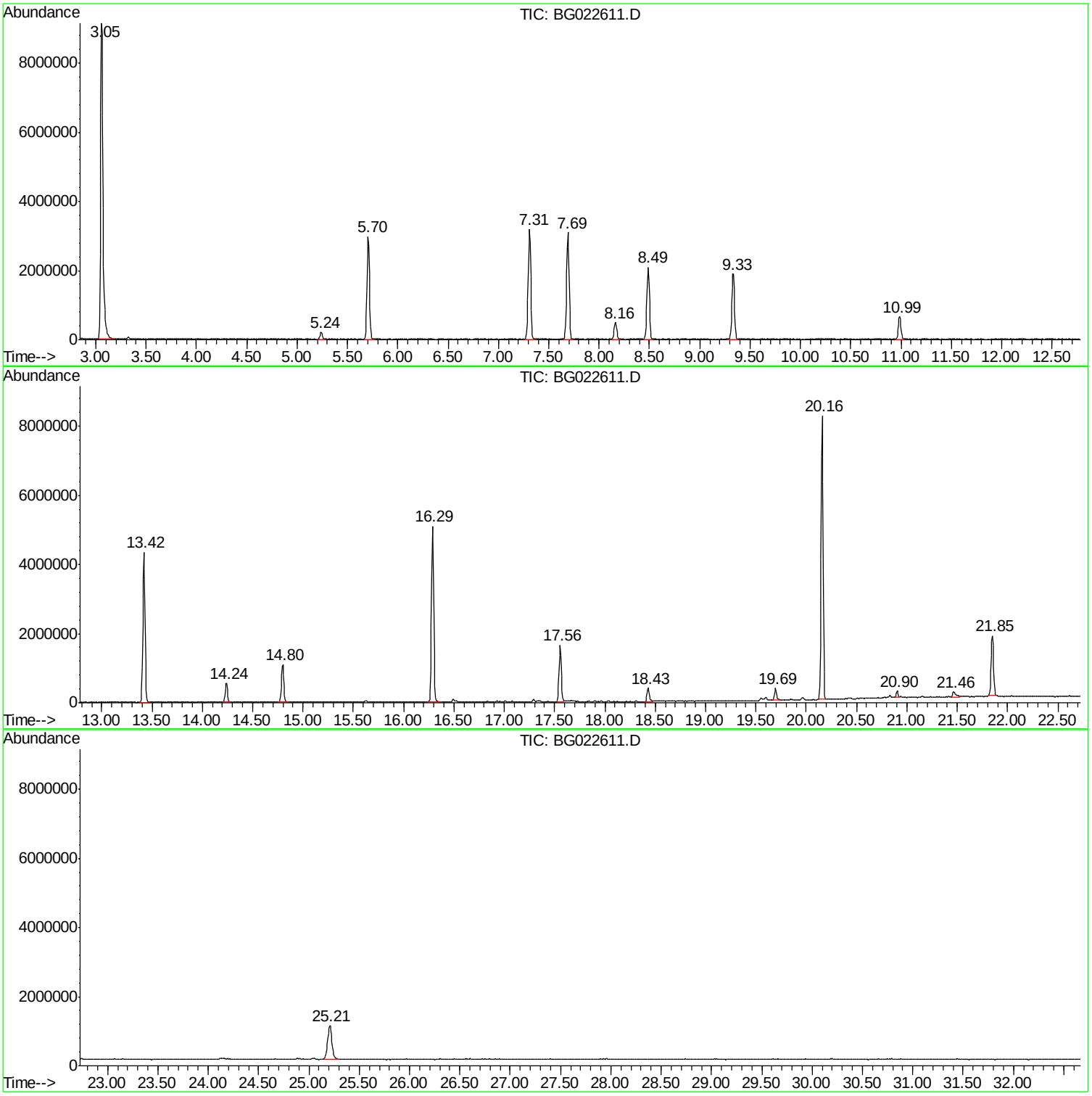
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022611.D
Acq On : 26 Jun 2016 15:24
Operator : UM/SJ
Sample : H3766-01
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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\BG062616\
Data File : BG022611.D
Acq On : 26 Jun 2016 15:24
Operator : UM/SJ
Sample : H3766-01
Misc :
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Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

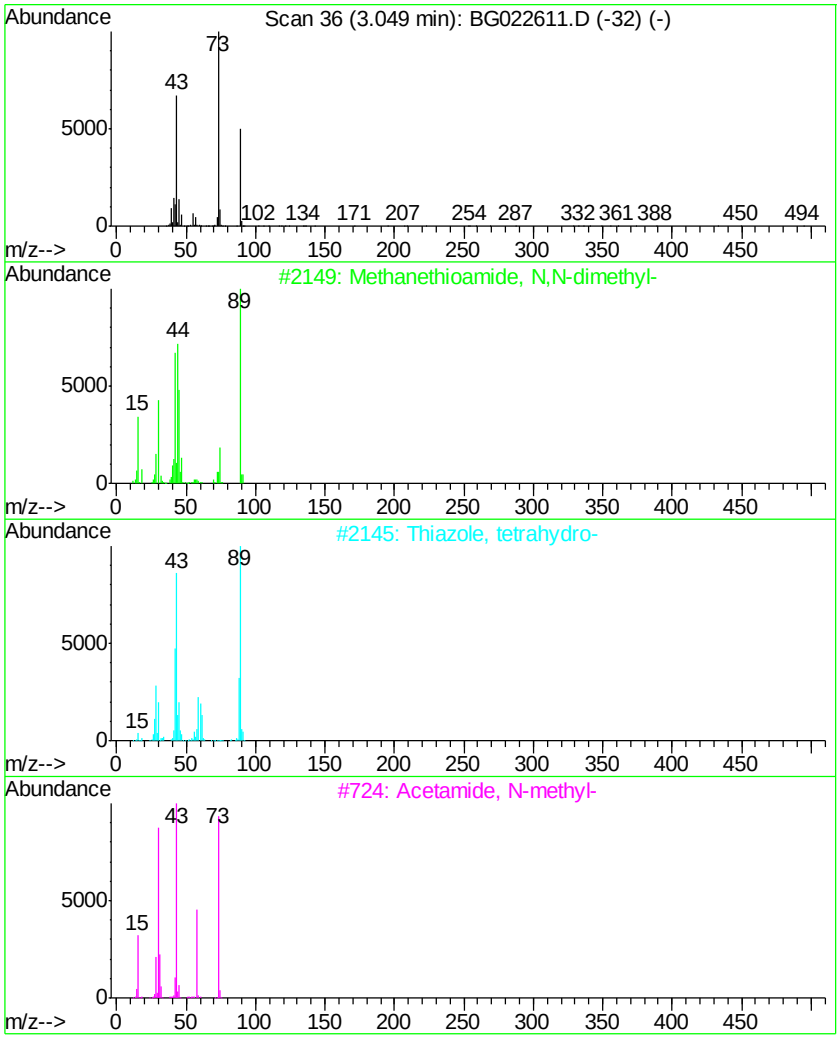
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

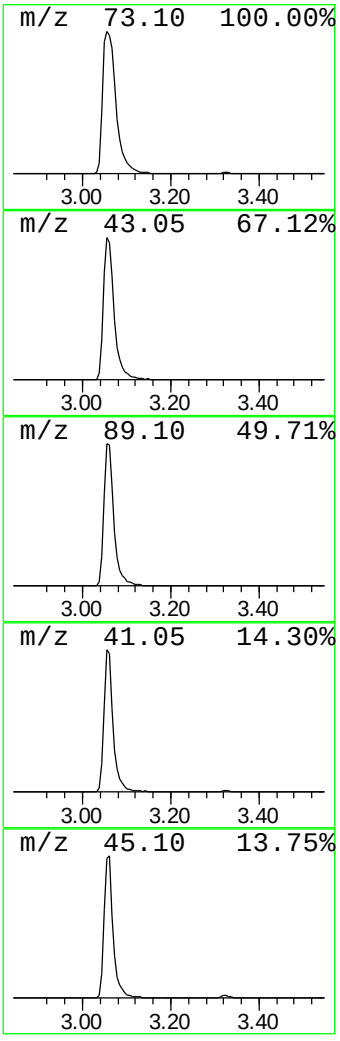
****

Peak Number 1 unknown3.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	355.10 ng	15408000	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	32
2	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	28
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
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Operator : UM/SJ
Sample : H3766-01
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

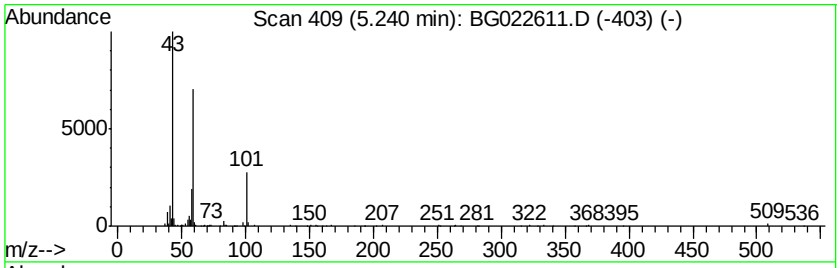
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

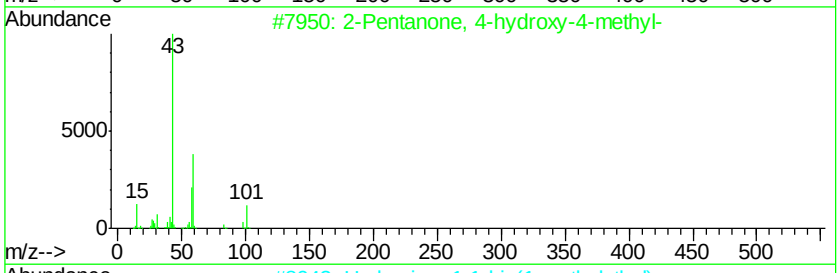
****

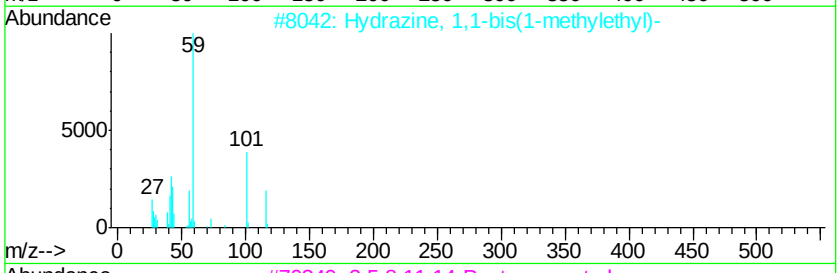
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

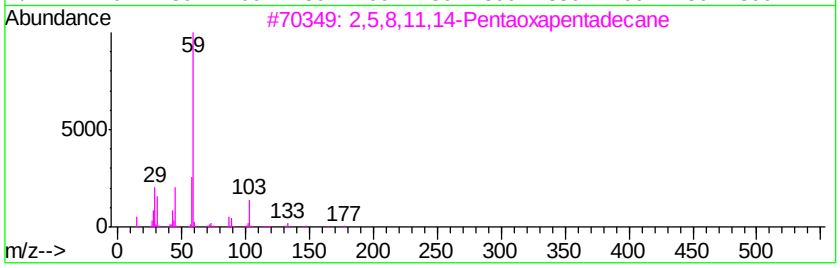
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	7.36 ng	319164	1,4-Dichlorobenzene-d4	8.16

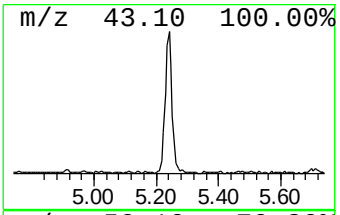
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
3	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	23
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23

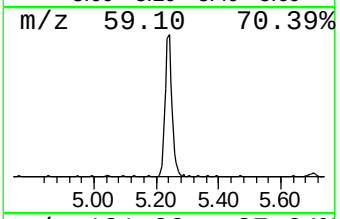


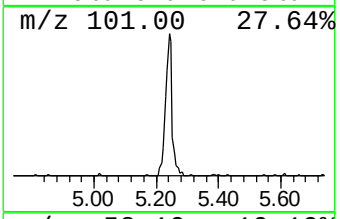


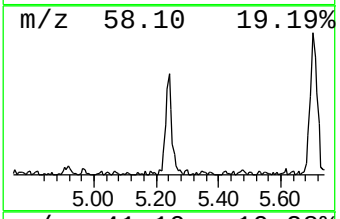


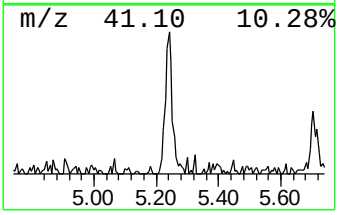












Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022611.D
Acq On : 26 Jun 2016 15:24
Operator : UM/SJ
Sample : H3766-01
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

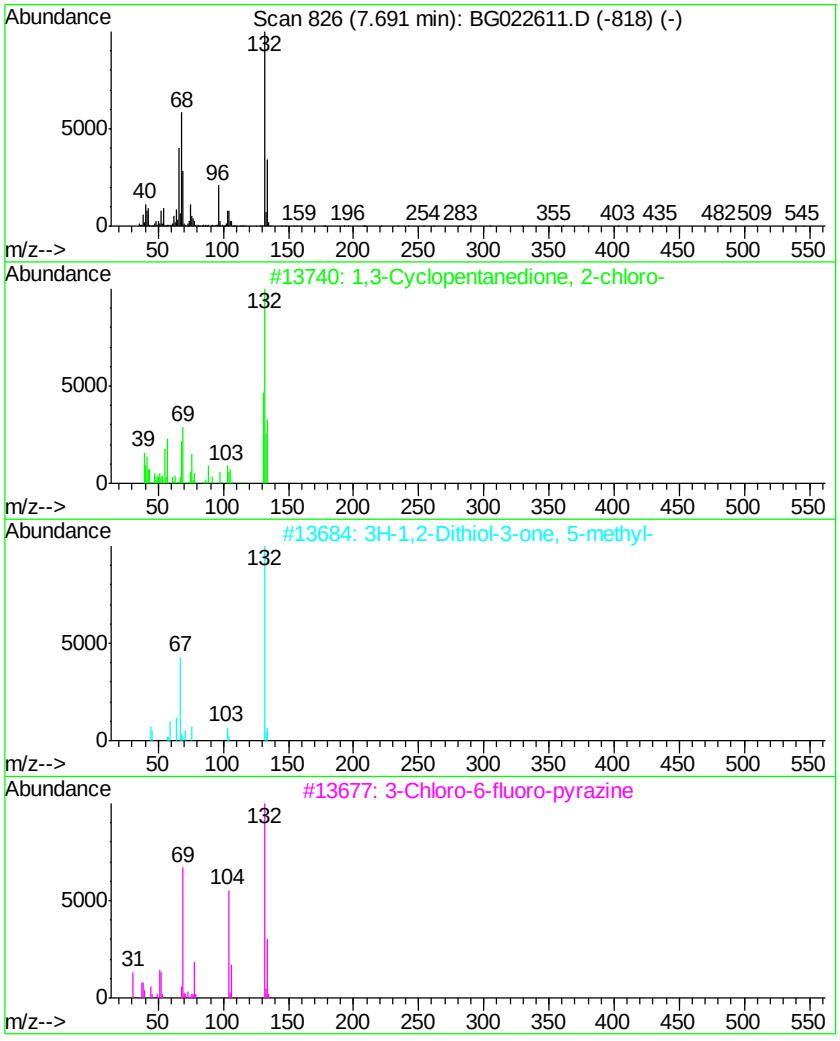
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

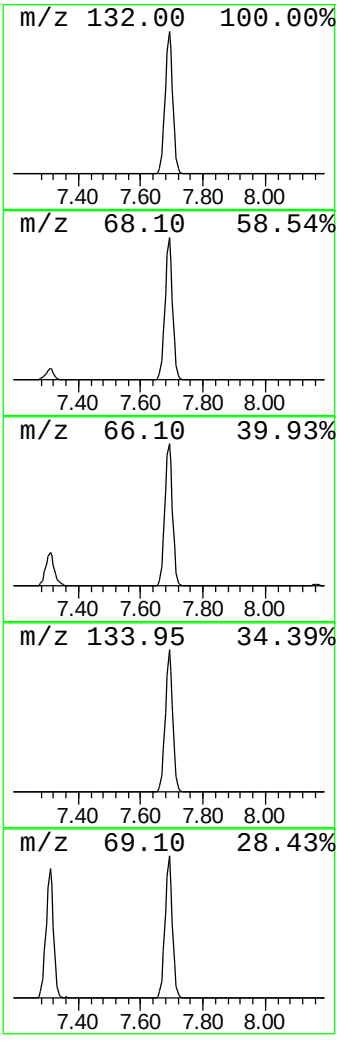
****

Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	120.68 ng	5236260	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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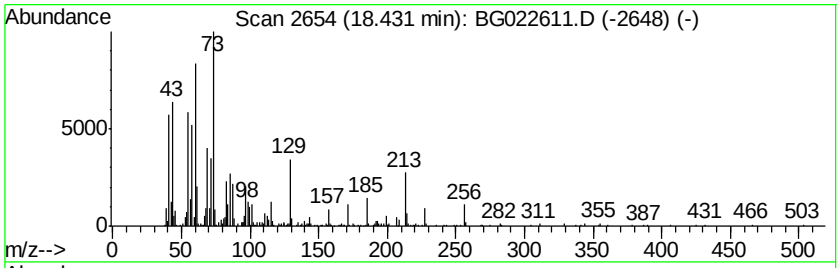
TIC Integration Parameters: LSCINT.P

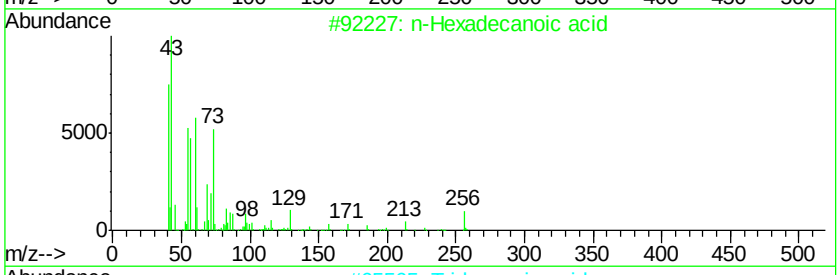
****

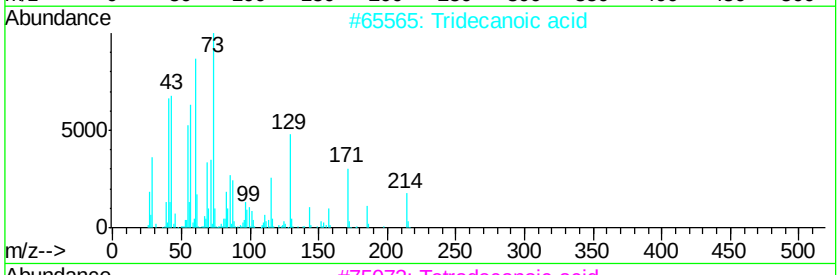
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

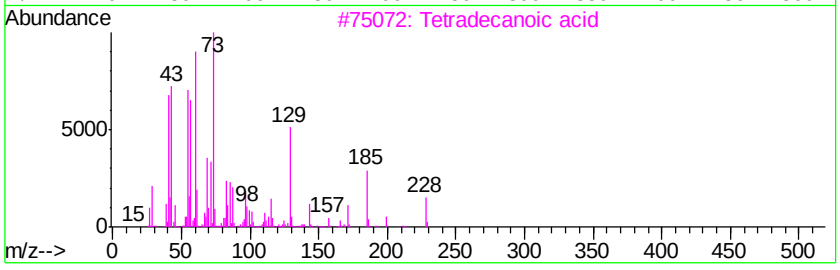
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	5.10 ng	626930	Phenanthrene-d10	17.56

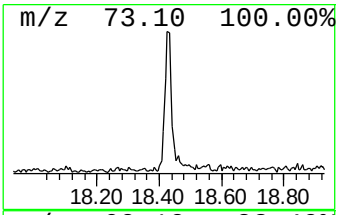
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59

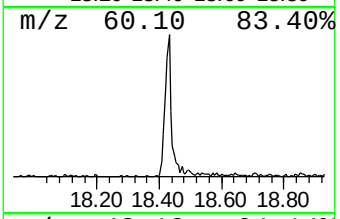


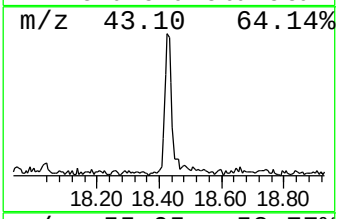


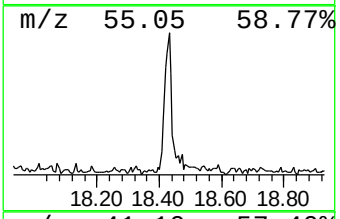


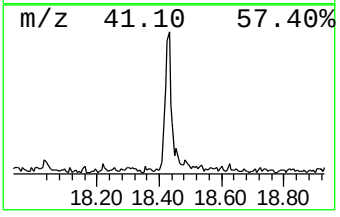












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Misc :
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Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

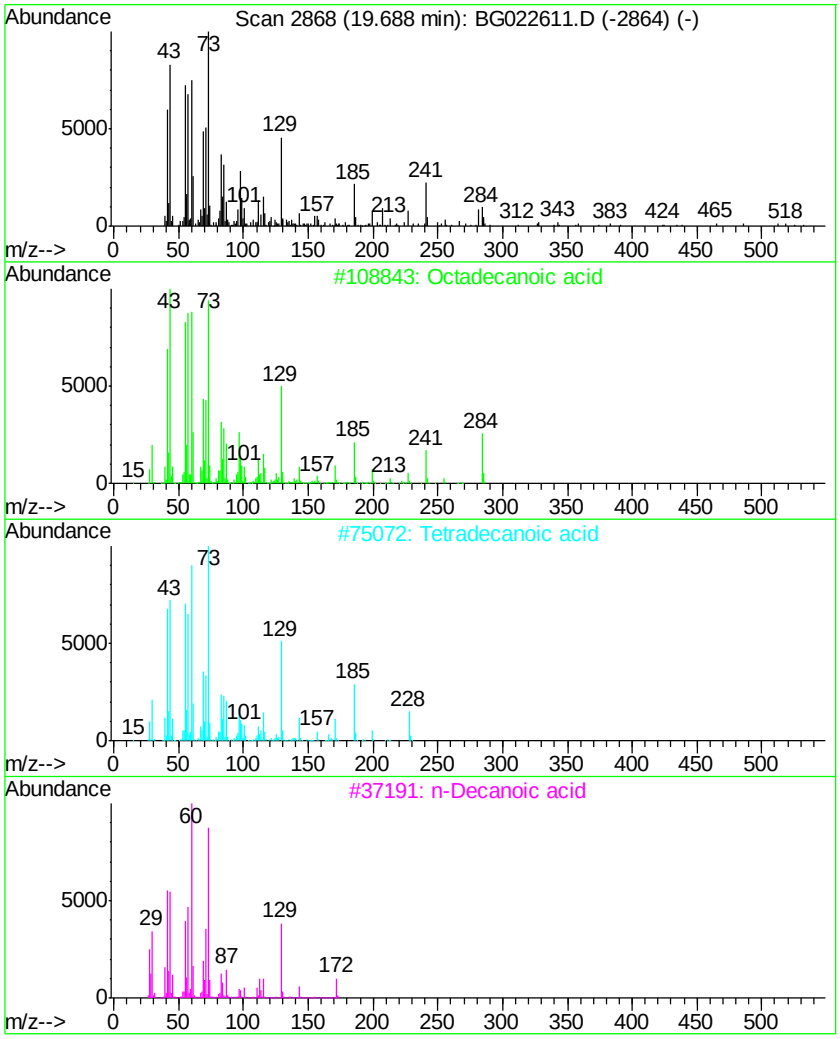
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

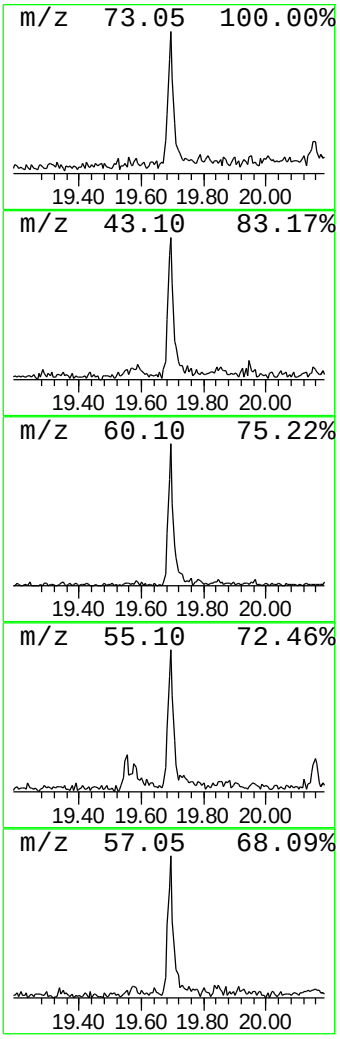
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.98 ng	489345	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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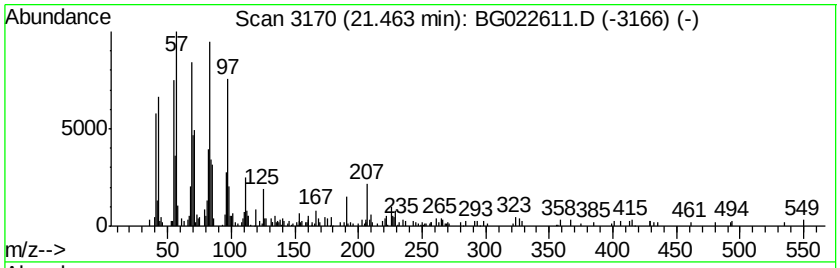
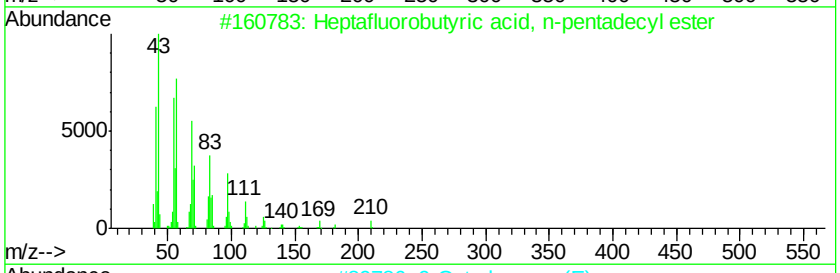
****

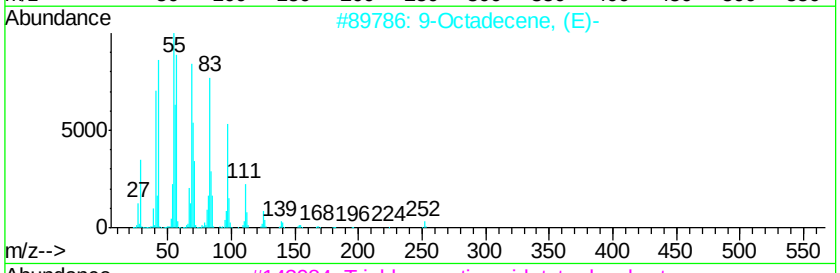
Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 7

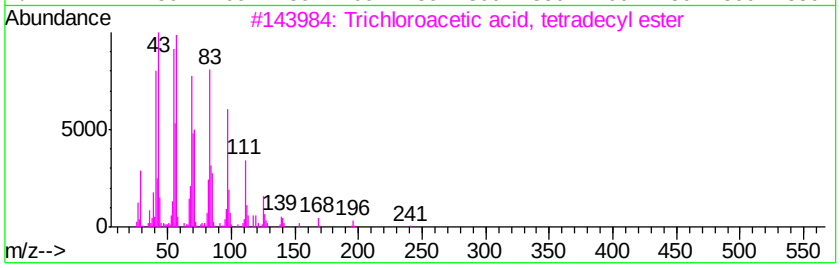
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	2.25 ng	331514	Chrysene-d12	21.85

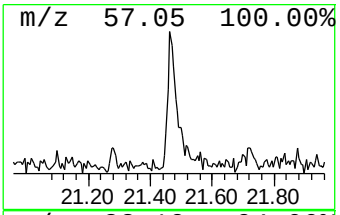
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	87
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	86
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83
4	11-Tricosene	322	C23H46	052078-56-5	80
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	80

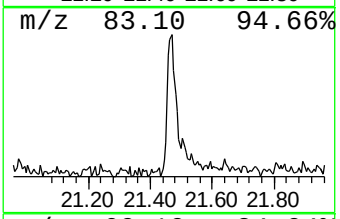


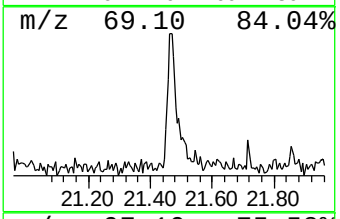


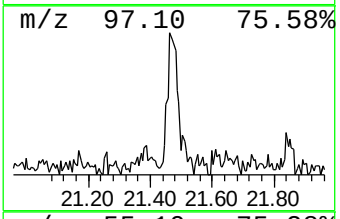


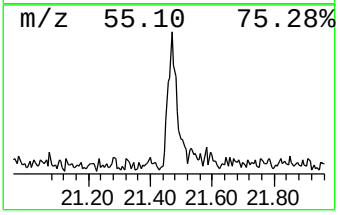












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022611.D
Acq On : 26 Jun 2016 15:24
Operator : UM/SJ
Sample : H3766-01
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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
unknown3.05	3.05	355.1	ng	15408000	1	8.16	867803	20.0
2-Pentanone, 4-hy...	5.24	7.4	ng	319164	1	8.16	867803	20.0
unknown7.69	7.69	120.7	ng	5236260	1	8.16	867803	20.0
n-Hexadecanoic acid	18.43	5.1	ng	626930	4	17.56	2459690	20.0
Octadecanoic acid	19.69	4.0	ng	489345	4	17.56	2459690	20.0
Heptafluorobutyri...	21.46	2.3	ng	331514	5	21.85	2947290	20.0