LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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	3.039	29	34	43	rBV	4567906	7078921	85.48%	12.709%
2	5.225	400	406	414	rBV	367957	621913	7.51%	1.117%
3	5.701	477	487	500	rBV	1669714	2894496	34.95%	5.197%
4	7.305	752	760	769	rBV	1938172	3460589	41.79%	6.213%
5	7.681	817	824	834	rBV	1831740	3180801	38.41%	5.711%
6	8.151	897	904	911	rBV	369732	658999	7.96%	1.183%
7	8.480	951	960	969	rBV	1260863	2306169	27.85%	4.140%
8	9.326	1093	1104	1115	rBV	1227512	2270247	27.42%	4.076%
9	10.983	1378	1386	1394	rBV	537384	994637	12.01%	1.786%
10	13.416	1793	1800	1812	rBV	3387722	5326985	64.33%	9.564%
11	14.238	1932	1940	1947	rBV	635836	957384	11.56%	1.719%
12	14.796	2028	2035	2044	rBV2	1002851	1675719	20.24%	3.009%
13	16.289	2282	2289	2303	rBV	3436958	5405921	65.28%	9.706%
14	16.488	2317	2323	2330	rBV	448256	679466	8.21%	1.220%
15	17.276	2454	2457	2463	rBV2	86326	99455	1.20%	0.179%
16	17.558	2498	2505	2516	rBV2	1362412	2266554	27.37%	4.069%
17	18.421	2647	2652	2661	rBV2	386092	562700	6.80%	1.010%
18	19.691	2864	2868	2875	rVV6	106406	161235	1.95%	0.289%
19	20.161	2941	2948	2955	rBV	6293212	8280916	100.00%	14.867%
20	20.924	3074	3078	3085	rVB2	333832	452644	5.47%	0.813%
21	21.465	3167	3170	3178	rBV4	119659	226173	2.73%	0.406%
22	21.723	3209	3214	3221	rBV	260499	372465	4.50%	0.669%
23	21.864	3231	3238	3249	rBV2	1430499	2464655	29.76%	4.425%
24	23.069	3436	3443	3448	rBV	483445	854842	10.32%	1.535%
25	23.592	3529	3532	3540	rVB3	86875	187836	2.27%	0.337%
26	25.249	3803	3814	3825	rVB2	737430	2257609	27.26%	4.053%

Sum of corrected areas: 55699331

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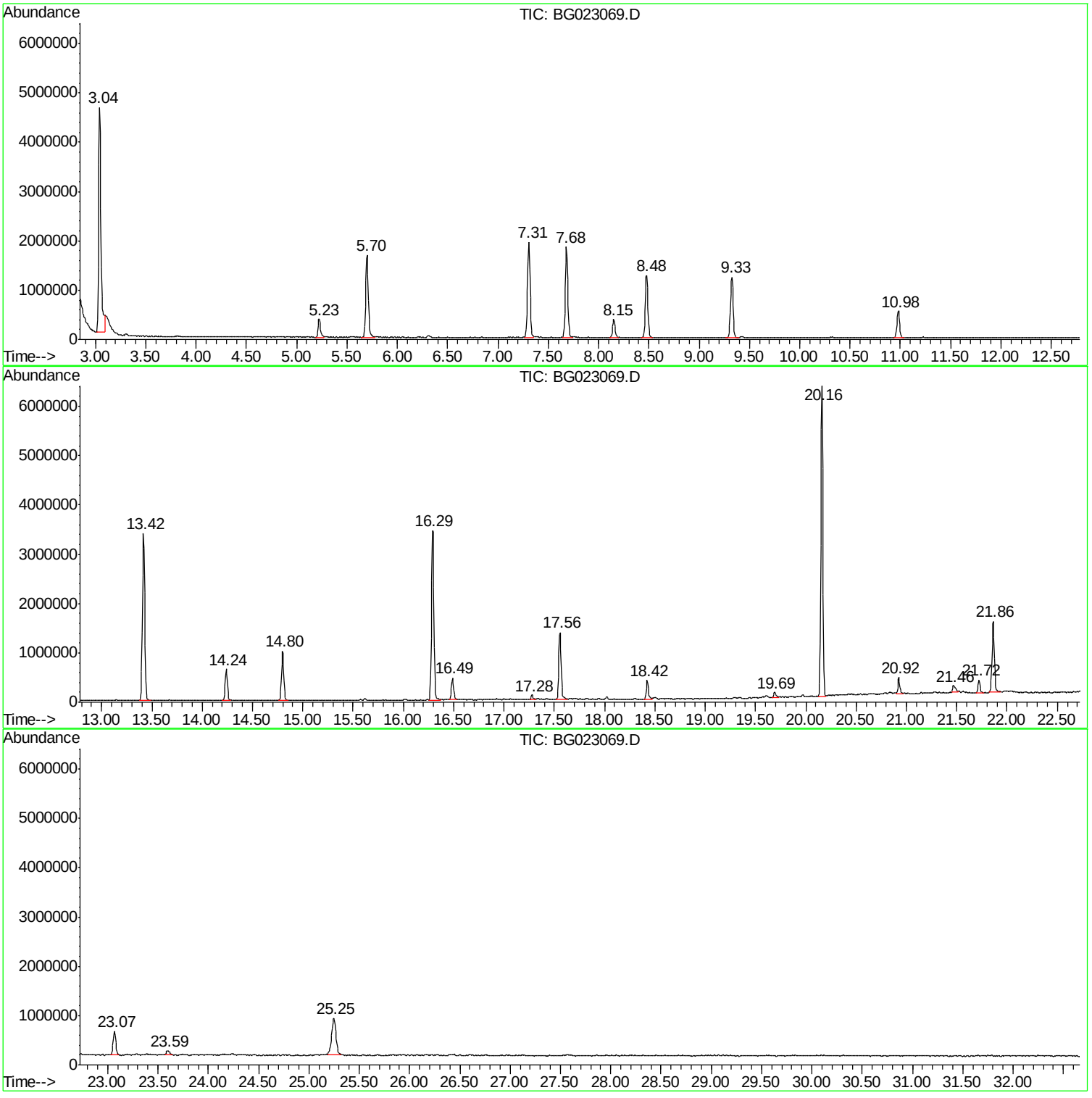
Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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\BG071316\
Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
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Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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

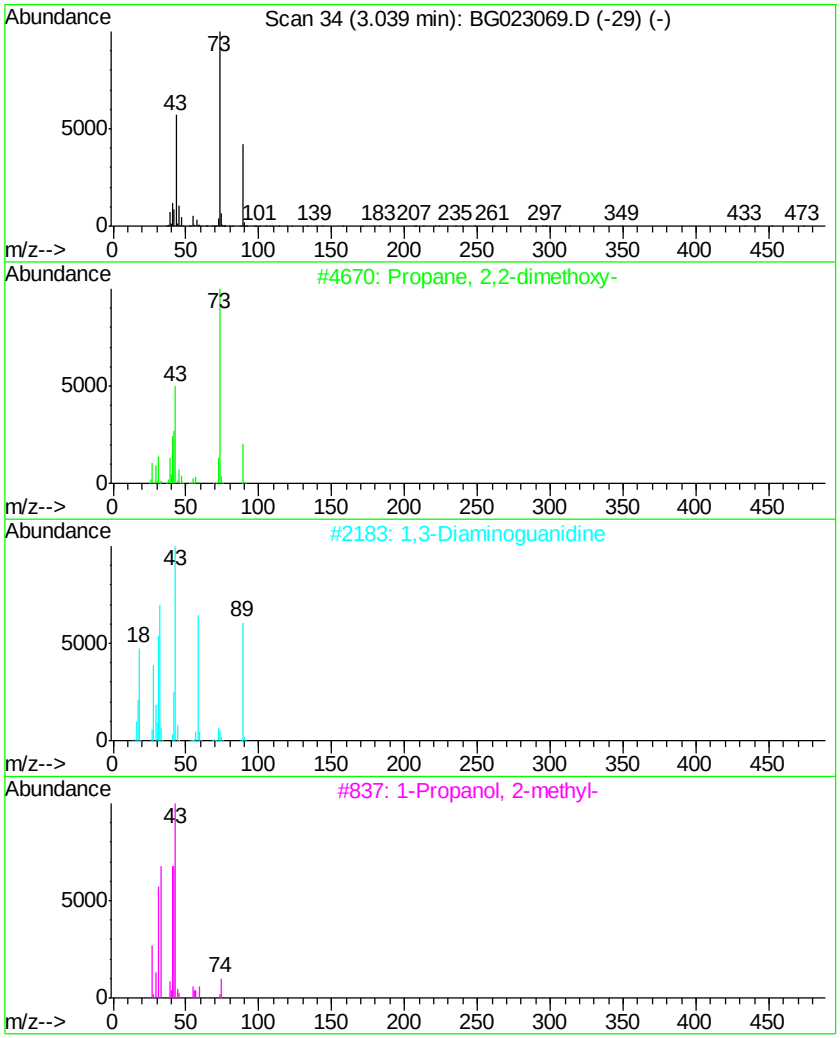
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

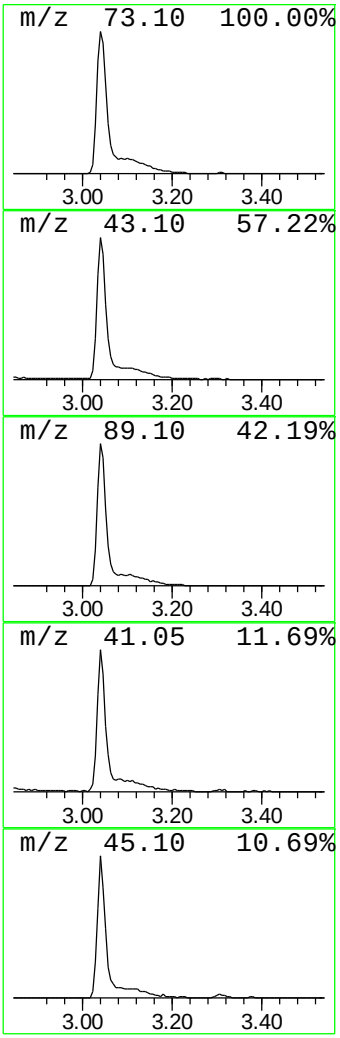
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	214.84 ng	7078920	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	56
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9





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Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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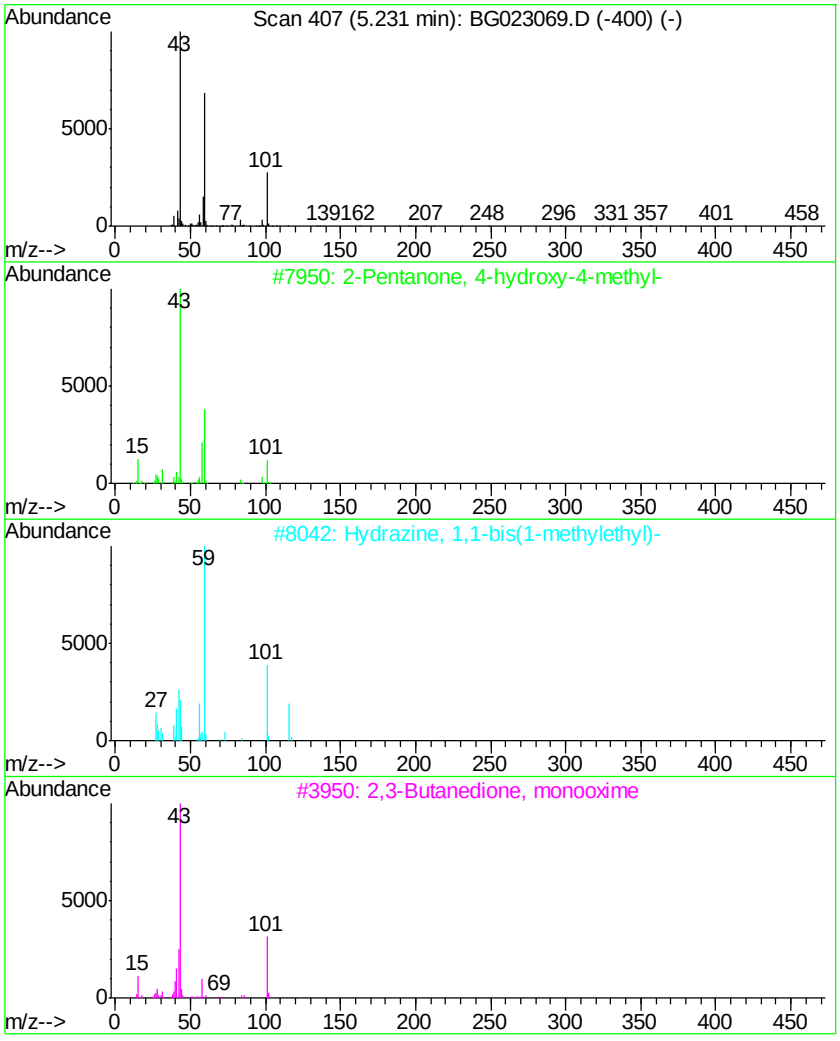
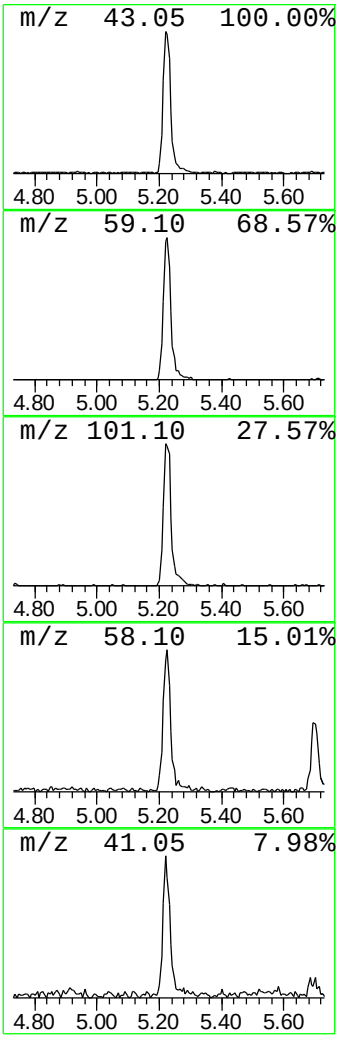
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	18.87 ng	621913	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	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	25
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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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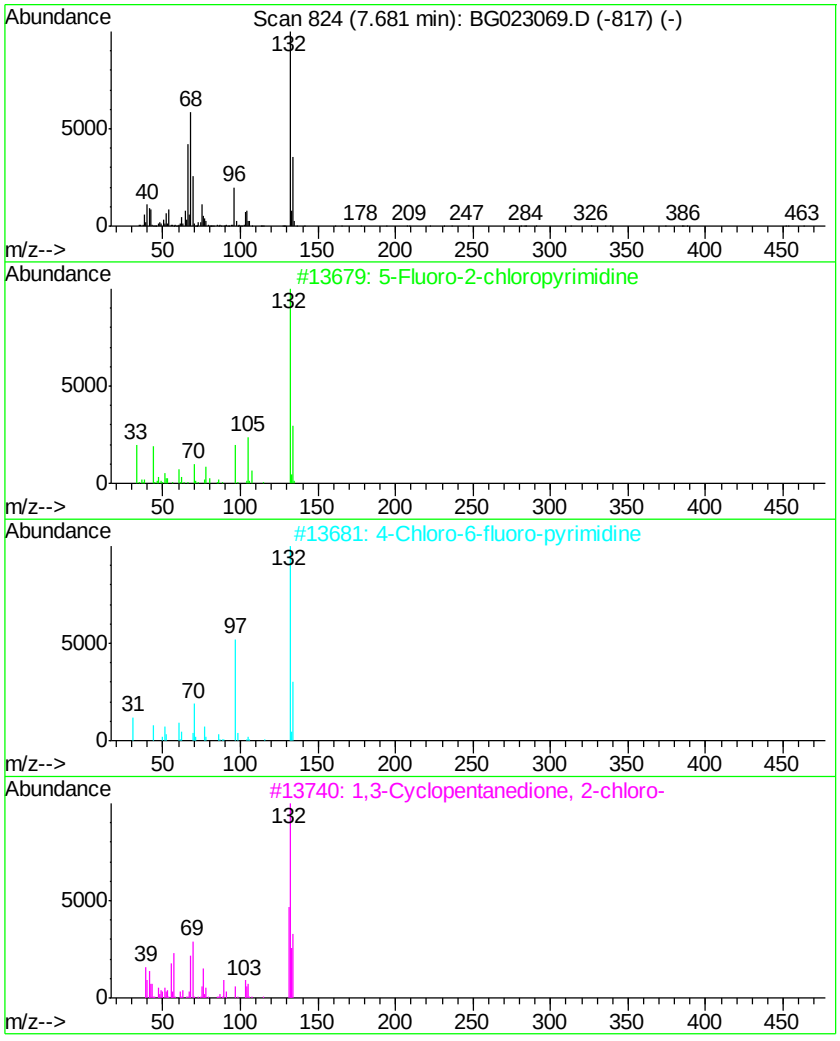
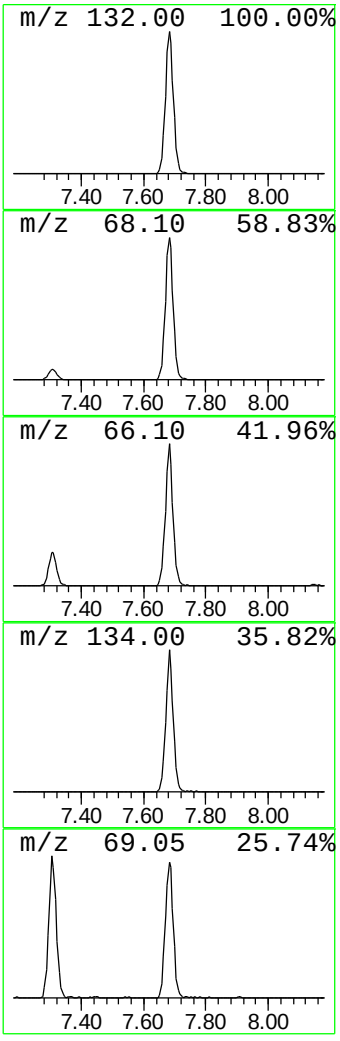
Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	96.53 ng	3180800	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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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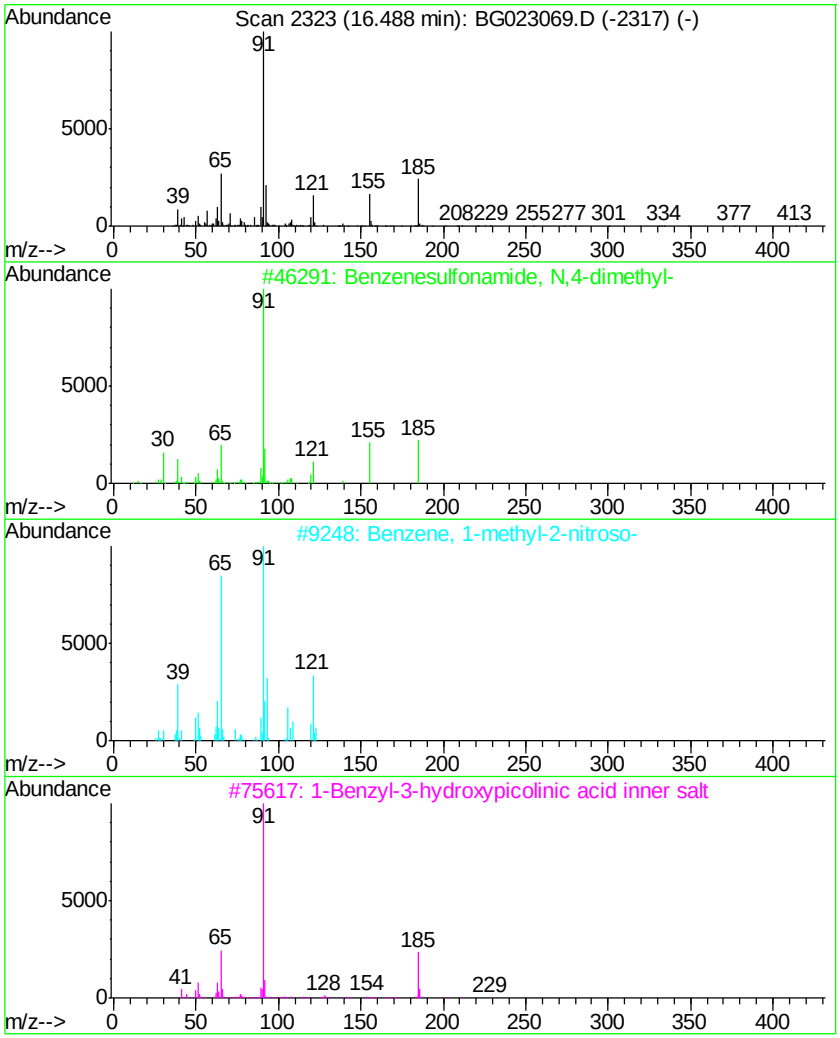
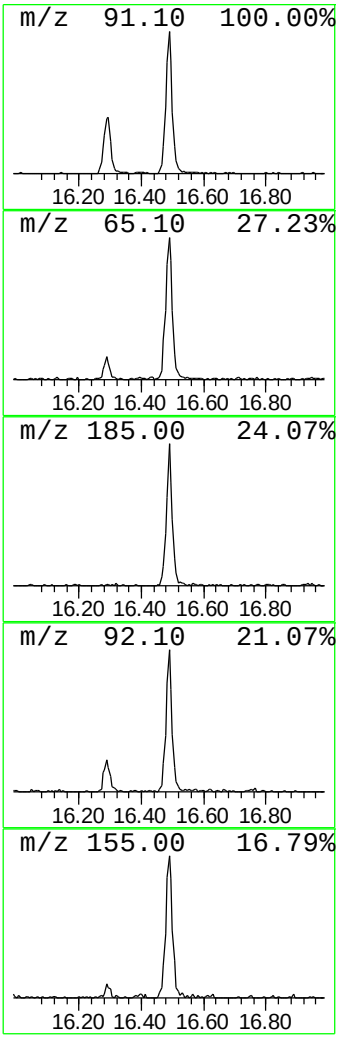
Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	6.00 ng	679466	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	81
2	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	62
3	1-Benzyl-3-hydroxypicolinic acid...	229	C13H11NO3	1000212-09-1	50
4	Benzeneethanamine	121	C8H11N	000064-04-0	47
5	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023069.D
Acq On : 13 Jul 2016 14:30
Operator : UM/SJ
Sample : H3946-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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

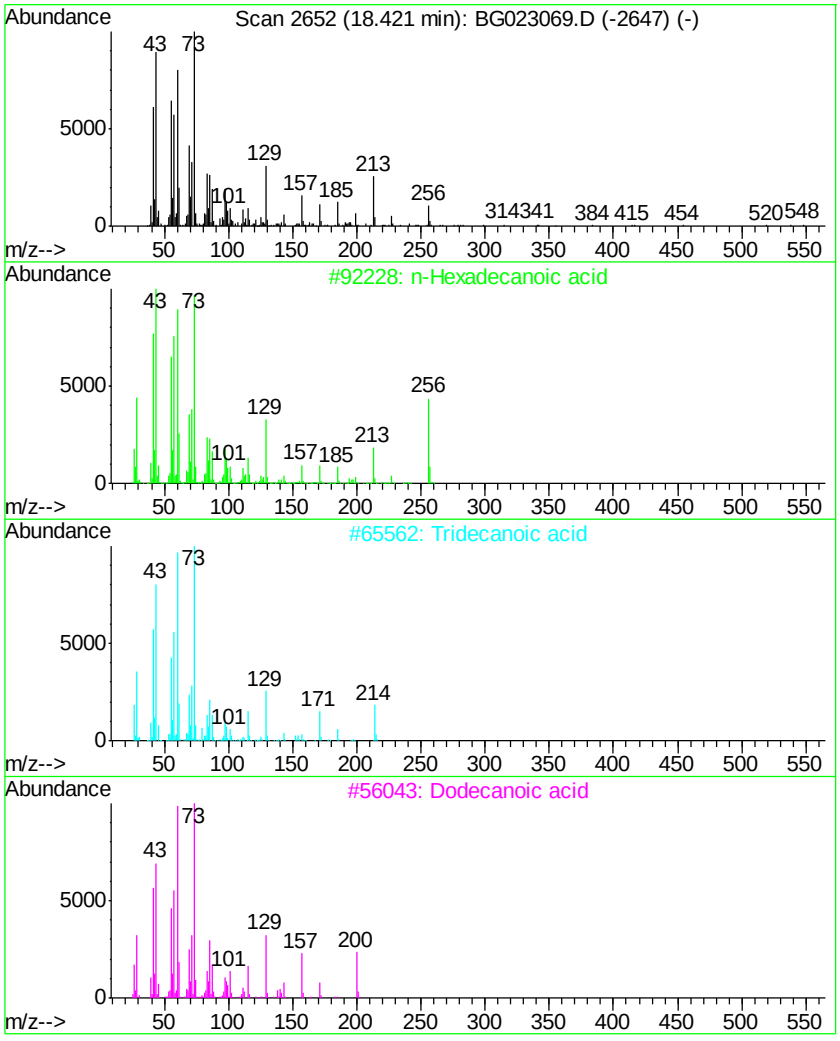
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

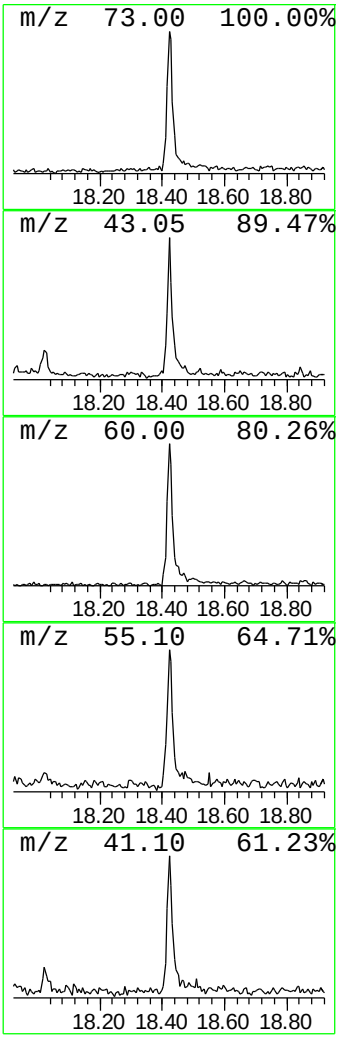
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.97 ng	562700	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Dodecanoic acid	200	C12H24O2	000143-07-7	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Instrument : BNA_G
ClientSampleId : M8-B1(6-12)C

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

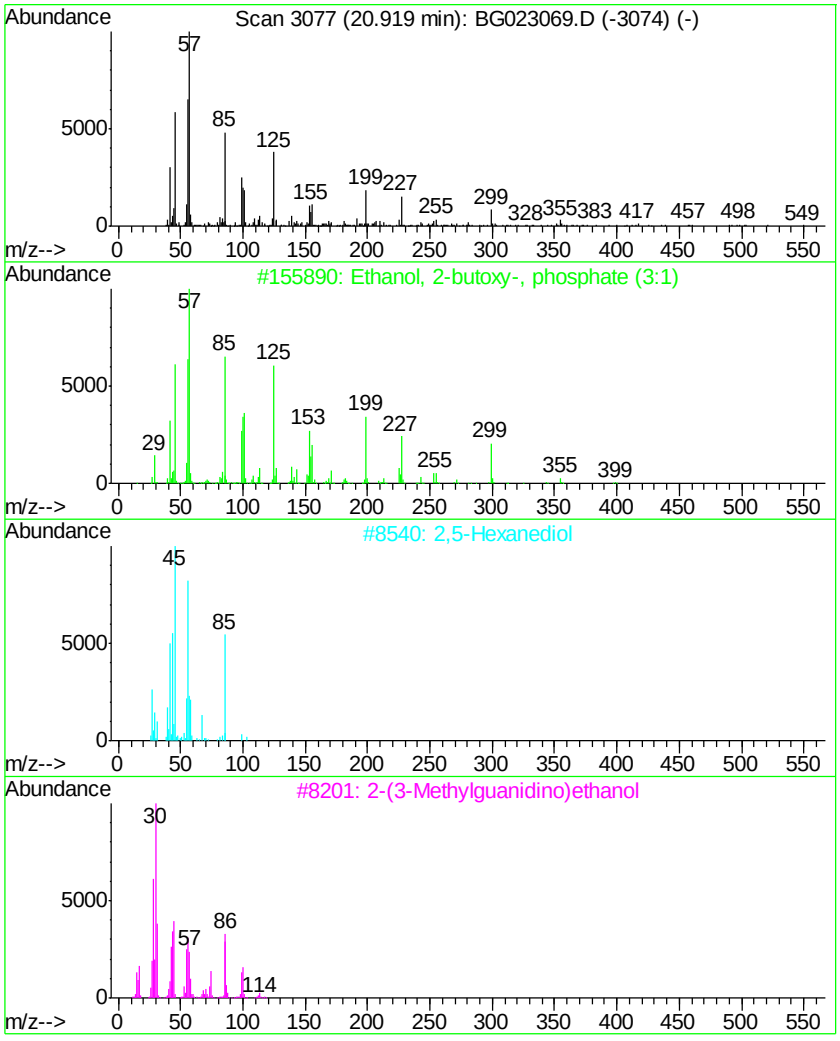
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

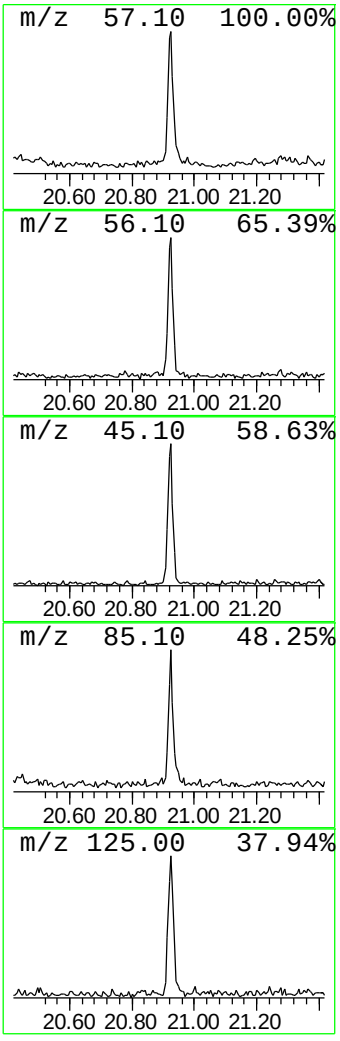
****

Peak Number 7 Ethanol, 2-butoxy-, phospha... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	3.67 ng	452644	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	83
2	2,5-Hexanediol	118	C6H14O2	002935-44-6	38
3	2-(3-Methylguanidino)ethanol	117	C4H11N3O	1000242-22-5	35
4	2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	27
5	2-Iodomethyl-5-methyltetrahydrof...	226	C6H11IO	019056-49-6	22





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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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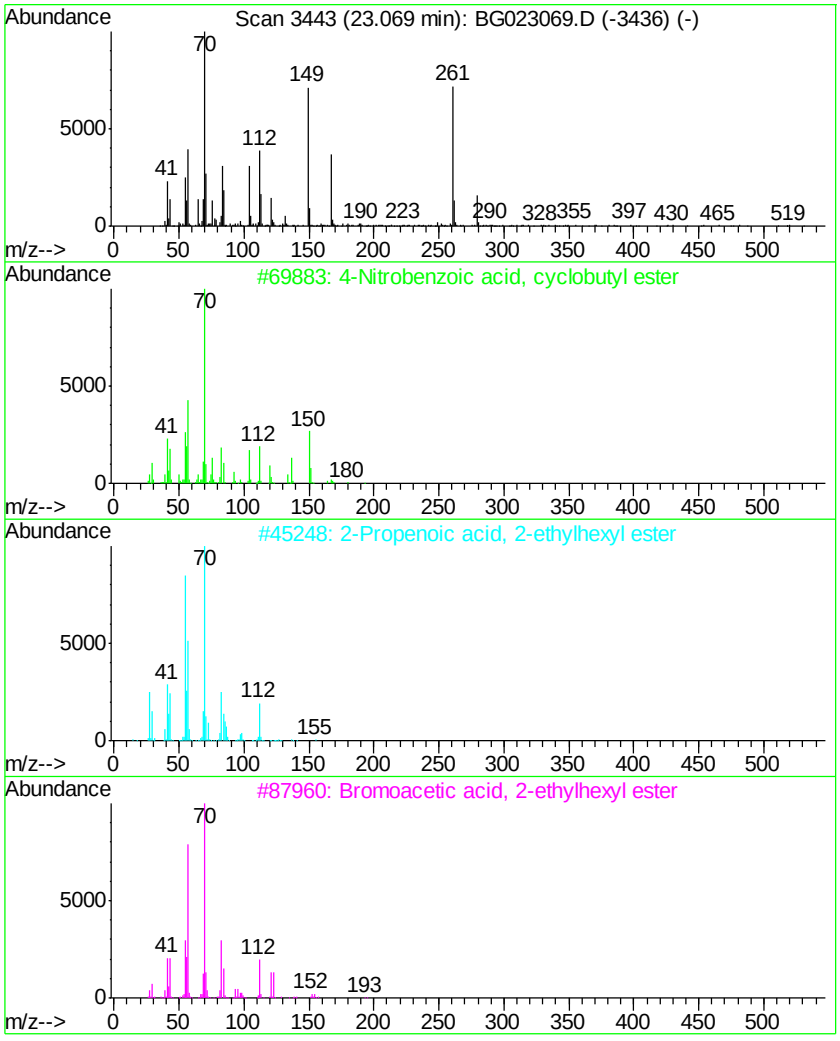
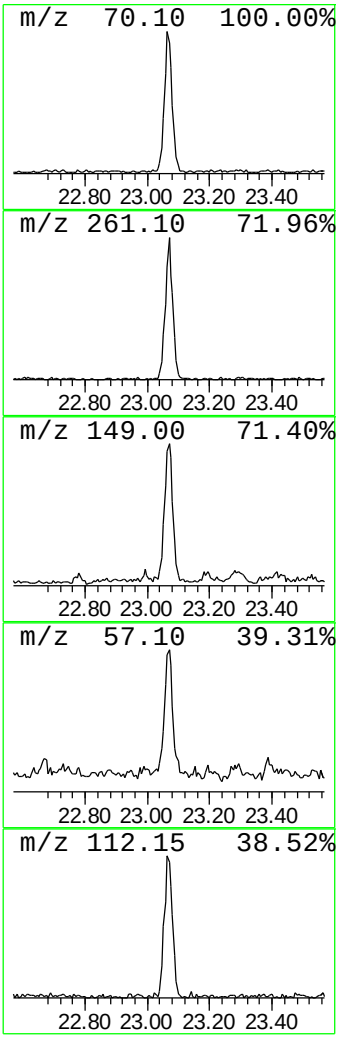
Peak Number 8 unknown23.07 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.07	6.94 ng	854842	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	35
2	2-Propenoic acid, 2-ethylhexyl e...	184	C11H20O2	000103-11-7	35
3	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	22
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22
5	2-Ethylhexyl methacrylate	198	C12H22O2	000688-84-6	17





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	3.04	214.8	ng	7078920	1	8.15	658999	20.0
2-Pentanone, 4-hy...	5.23	18.9	ng	621913	1	8.15	658999	20.0
unknown7.68	7.68	96.5	ng	3180800	1	8.15	658999	20.0
Benzenesulfonamid...	16.49	6.0	ng	679466	4	17.56	2266550	20.0
n-Hexadecanoic acid	18.42	5.0	ng	562700	4	17.56	2266550	20.0
Ethanol, 2-butoxy...	20.92	3.7	ng	452644	5	21.86	2464660	20.0
unknown23.07	23.07	6.9	ng	854842	5	21.86	2464660	20.0