LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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	5.240	405	409	415	rBV	141497	223495	1.91%	0.371%
2	5.705	481	488	498	rVB	1283681	2034836	17.38%	3.378%
3	7.303	753	760	770	rVB	867234	1464511	12.51%	2.431%
4	7.690	819	826	835	rVB	2301728	3933845	33.61%	6.530%
5	8.166	899	907	913	rBV	546384	927616	7.92%	1.540%
6	8.490	952	962	973	rBV	1986744	3508530	29.97%	5.824%
7	9.336	1098	1106	1116	rVB	1858413	3334317	28.48%	5.535%
8	10.992	1378	1388	1397	rBV	720972	1347222	11.51%	2.236%
9	13.331	1781	1786	1794	rBV2	110824	206241	1.76%	0.342%
10	13.425	1794	1802	1809	rVB	4693374	7616949	65.07%	12.643%
11	14.065	1905	1911	1915	rBV3	80706	143883	1.23%	0.239%
12	14.800	2029	2036	2044	rVB2	1255501	2020581	17.26%	3.354%
13	16.286	2281	2289	2296	rBV	4725347	7536675	64.38%	12.510%
14	17.461	2483	2489	2498	rBV2	173665	250904	2.14%	0.416%
15	17.555	2498	2505	2511	rVV	1696052	2676797	22.87%	4.443%
16	18.161	2604	2608	2614	rBV	397690	564996	4.83%	0.938%
17	18.425	2649	2653	2658	rBV2	226575	320933	2.74%	0.533%
18	19.189	2777	2783	2792	rBV	2108055	2840983	24.27%	4.716%
19	19.688	2863	2868	2874	rBV6	175803	277699	2.37%	0.461%
20	20.158	2941	2948	2953	rBV	8531316	11706107	100.00%	19.431%
21	21.380	3153	3156	3159	rVB3	139989	155387	1.33%	0.258%
22	21.433	3160	3165	3169	rVB	416039	551142	4.71%	0.915%
23	21.844	3229	3235	3242	rVB2	1883052	3167973	27.06%	5.259%
24	22.555	3352	3356	3363	rVB5	202253	328568	2.81%	0.545%
25	25.205	3798	3807	3823	rVB2	996285	3103813	26.51%	5.152%

Sum of corrected areas: 60244003

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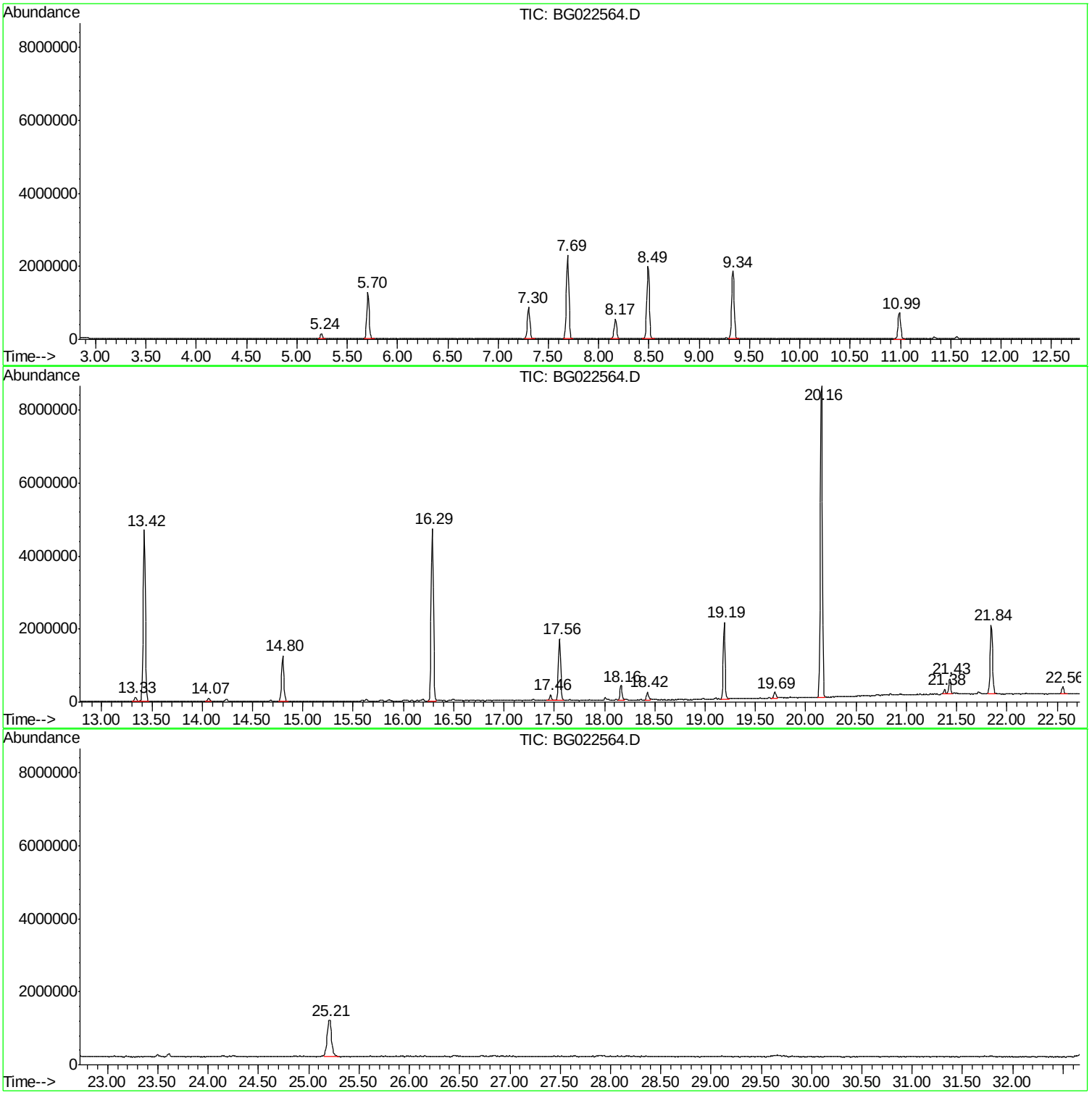
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TEPMW2-26

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\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

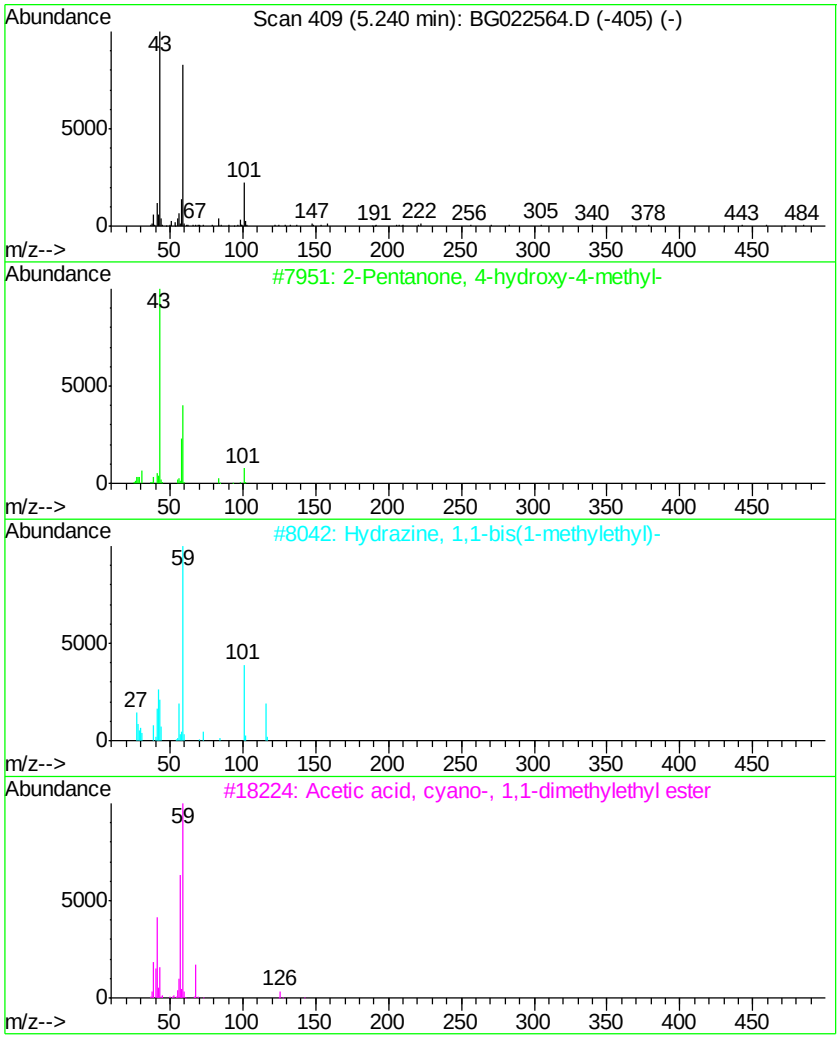
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

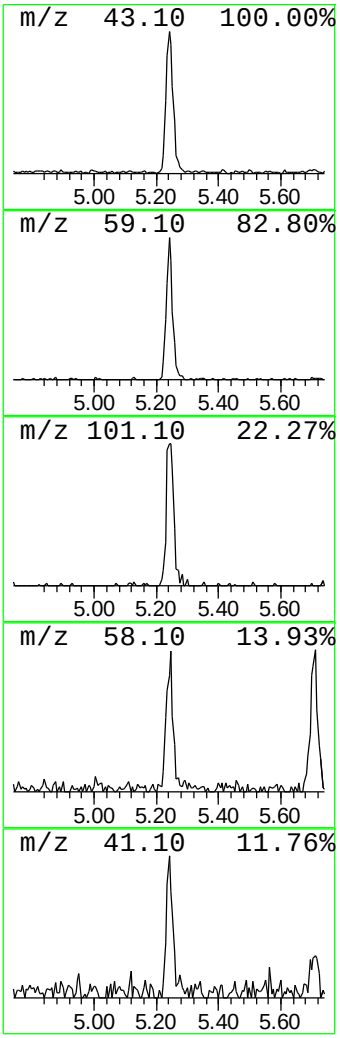
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	4.82 ng	223495	1,4-Dichlorobenzene-d4	8.17

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	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	33
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

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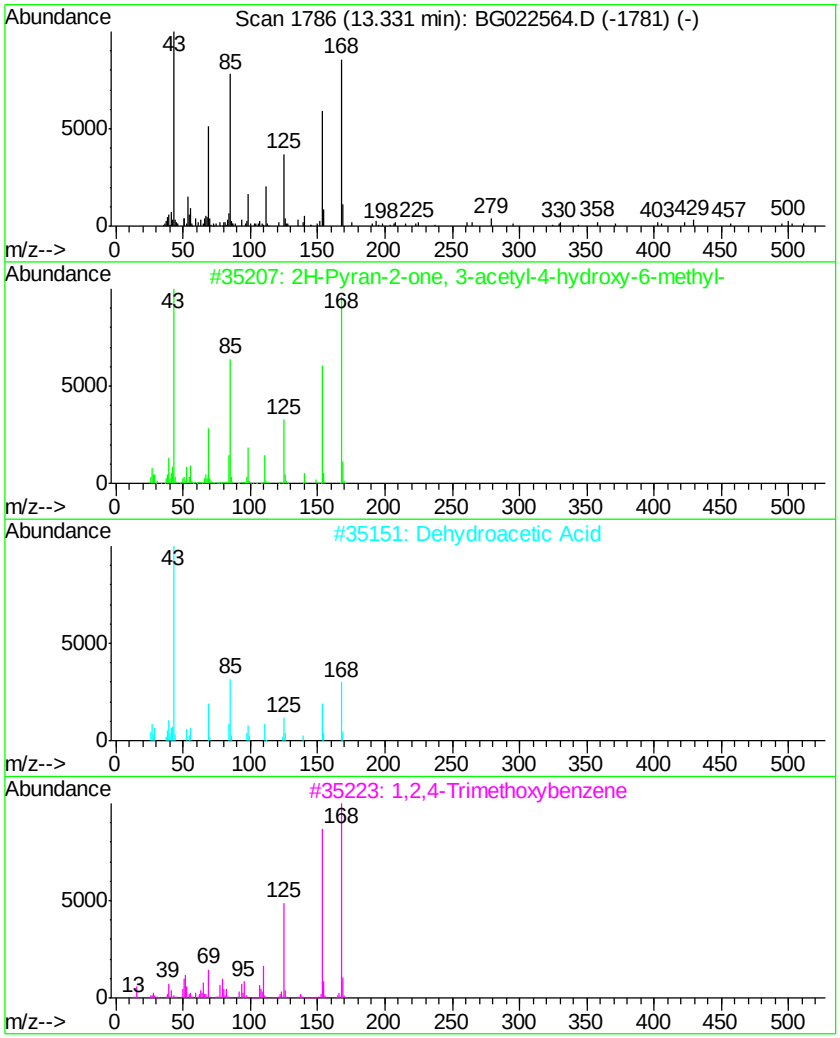
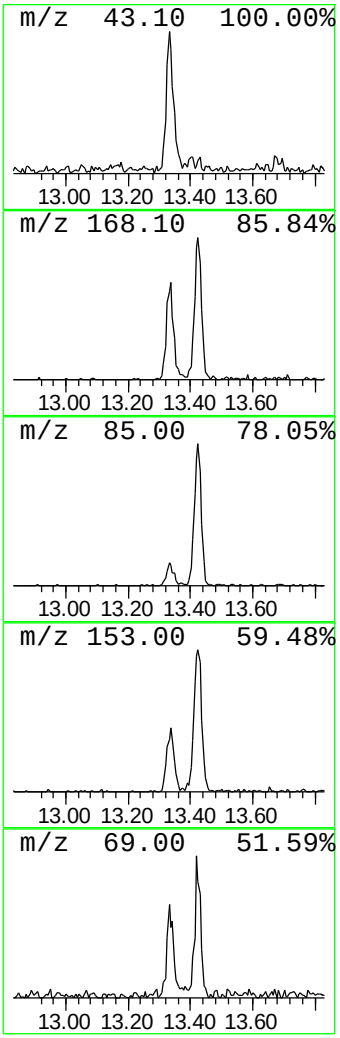
Peak Number 4 2H-Pyran-2-one, 3-acetyl-4-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	2.04 ng	206241	Acenaphthene-d10	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, 3-acetyl-4-hydro...	168	C8H8O4	000771-03-9	93
2	Dehydroacetic Acid	168	C8H8O4	000520-45-6	91
3	1,2,4-Trimethoxybenzene	168	C9H12O3	000135-77-3	46
4	Benzoic acid, 4-hydroxy-3-methoxy-	168	C8H8O4	000121-34-6	43
5	1,2,3-Trimethoxybenzene	168	C9H12O3	000634-36-6	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

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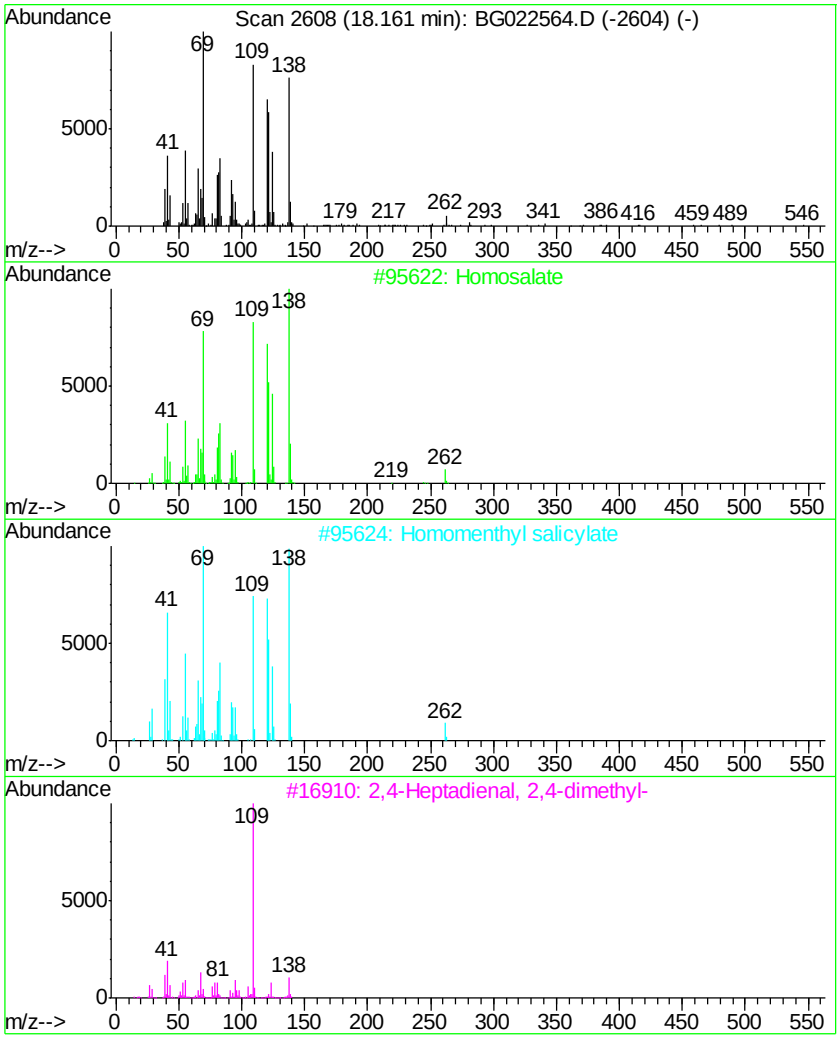
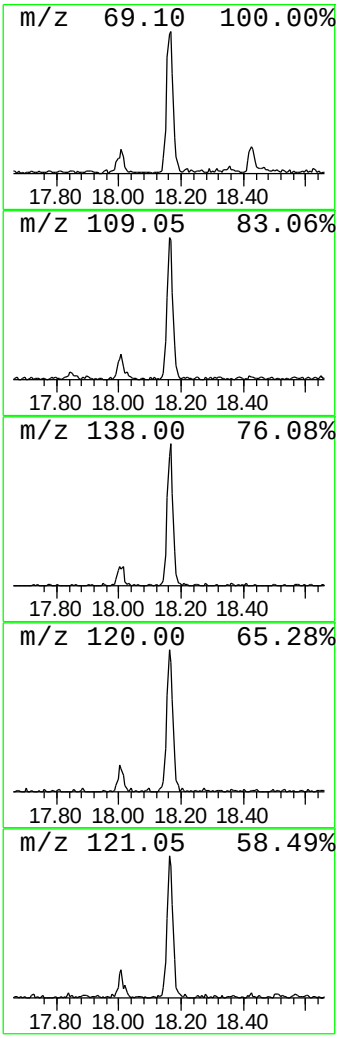
Peak Number 5 Homosalate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	4.22 ng	564996	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Homosalate	262	C16H22O3	000118-56-9	64
2	Homomenthyl salicylate	262	C16H22O3	052253-93-7	60
3	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	41
4	3-Amino-4,6-dimethylpyridone-2(1H)	138	C7H10N2O	143708-29-6	38
5	3-Heptyne, 2,2-dimethyl-	124	C9H16	029022-29-5	30





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

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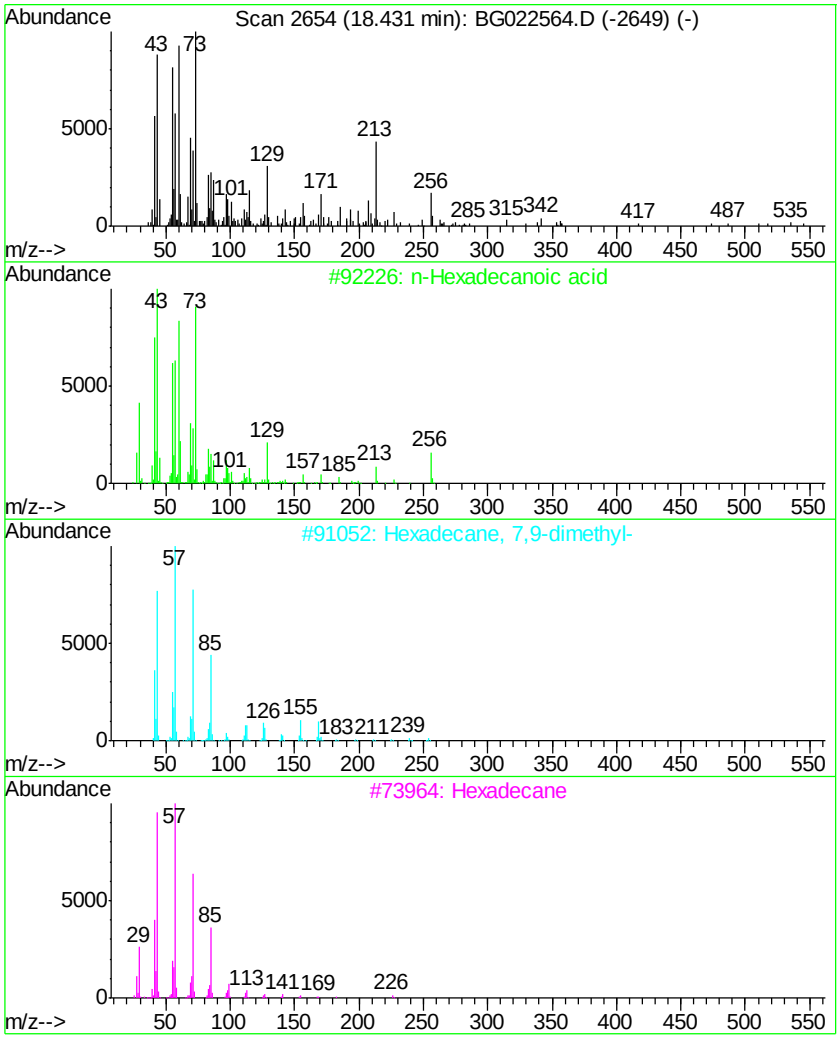
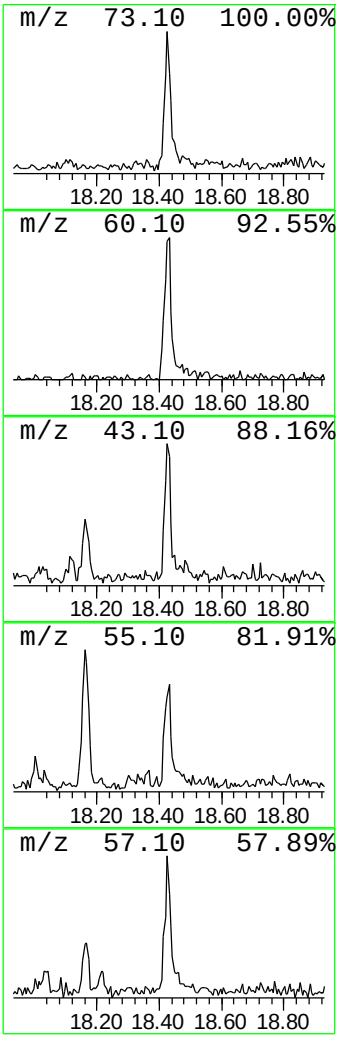
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.40 ng	320933	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	35
3	Hexadecane	226	C16H34	000544-76-3	35
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	35





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

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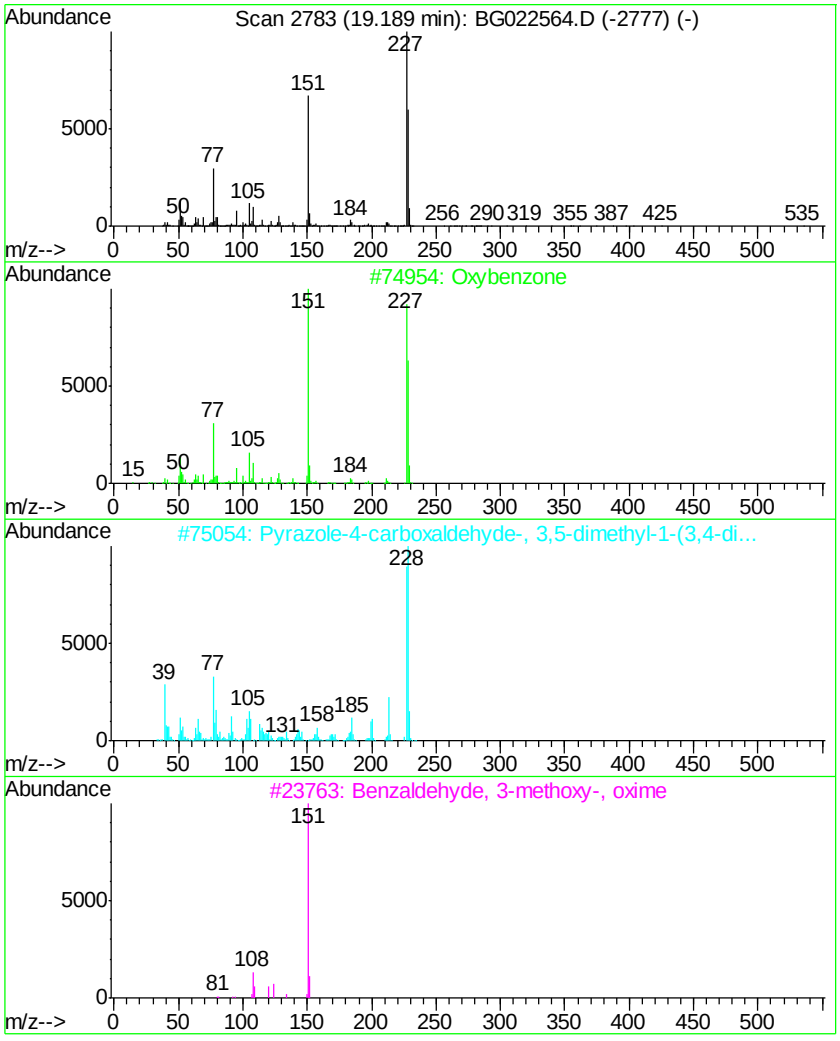
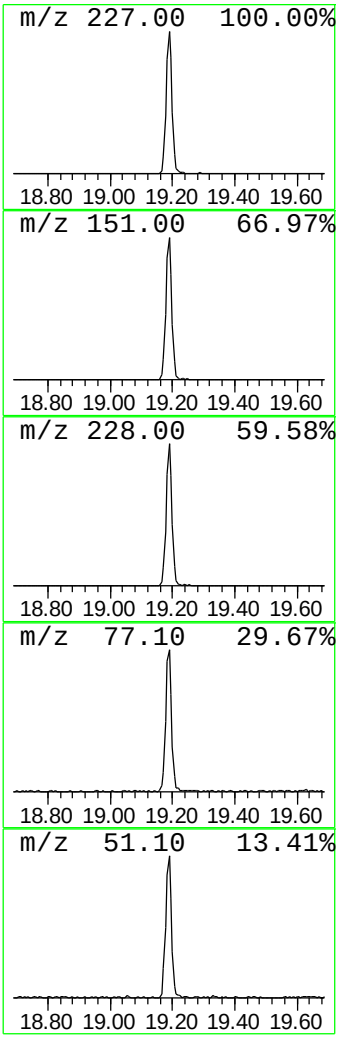
Peak Number 7 Oxybenzone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	21.23 ng	2840980	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybenzone	228	C14H12O3	000131-57-7	97
2	Pyrazole-4-carboxaldehyde-, 3,5-...	228	C14H16N2O	1000272-54-8	35
3	Benzaldehyde, 3-methoxy-, oxime	151	C8H9NO2	038489-80-4	14
4	2-Hydrazino-7-phenoxytropone	228	C13H12N2O2	000724-81-2	14
5	1,4-Dimethylphenoxathin	228	C14H12OS	016314-44-6	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

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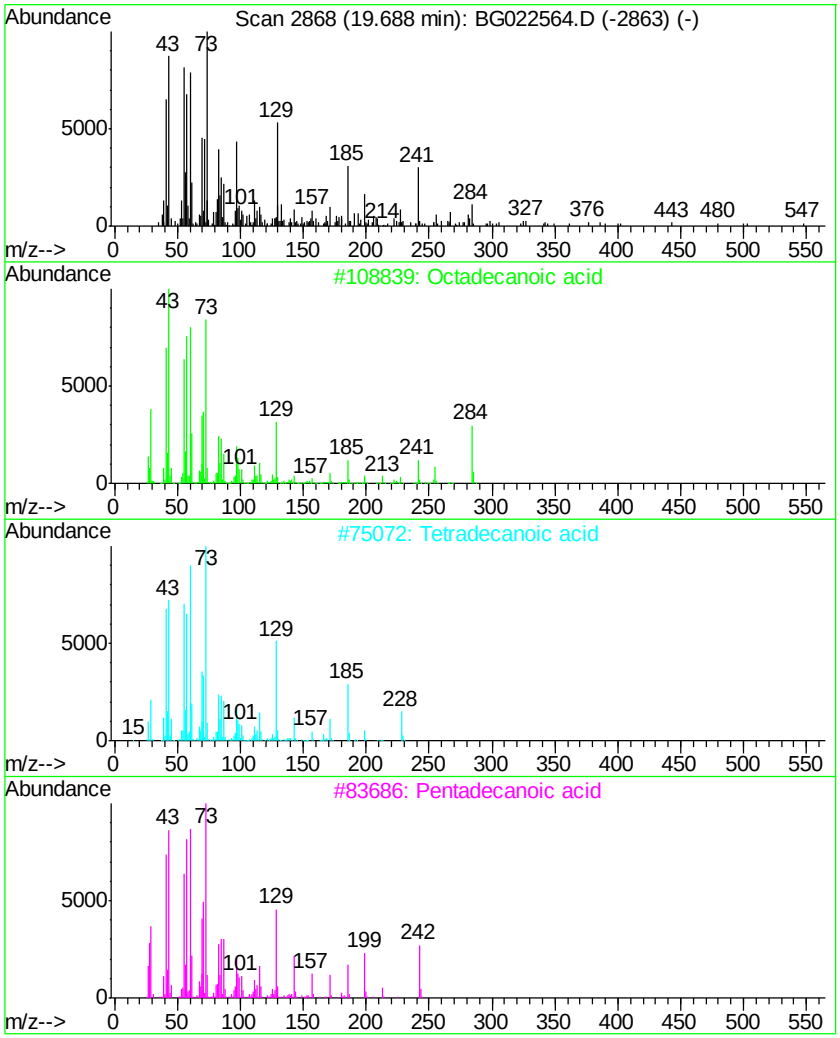
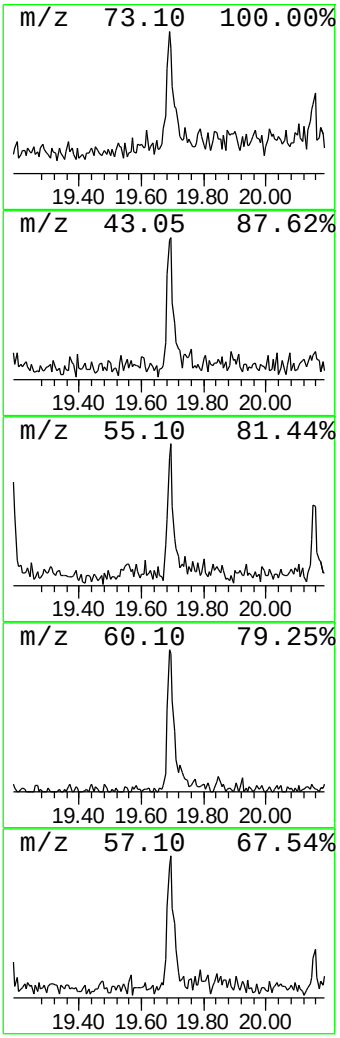
Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	2.07 ng	277699	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





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Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

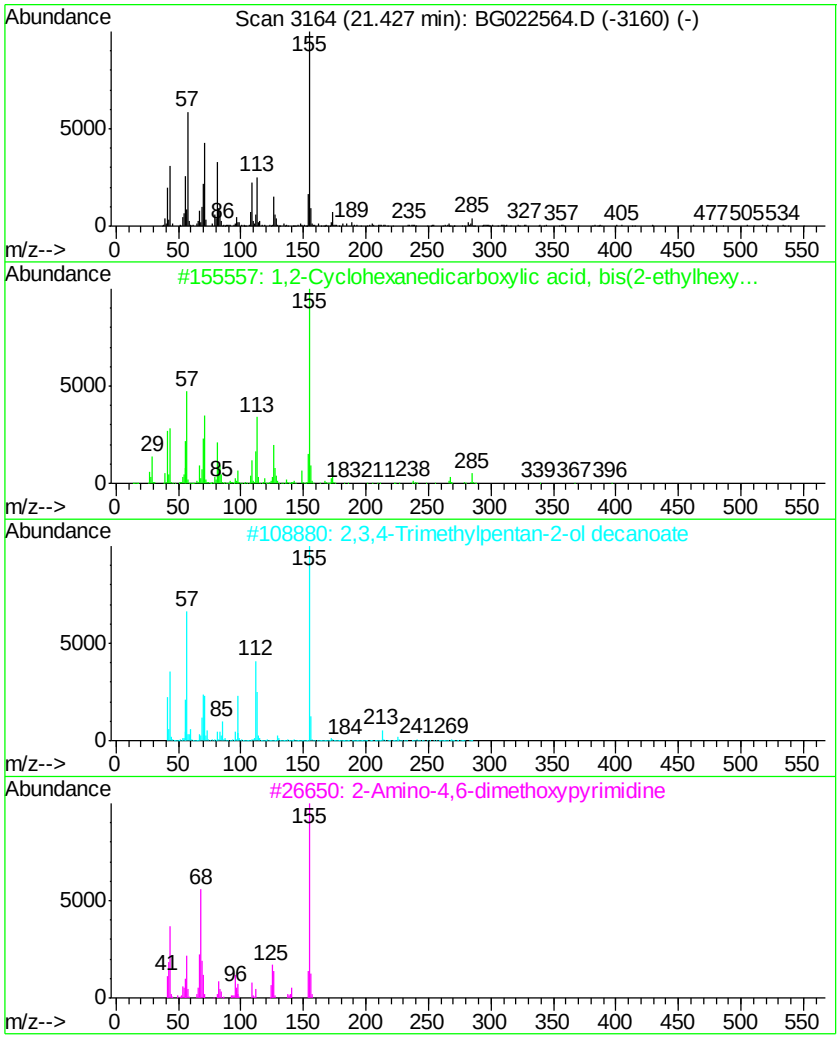
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

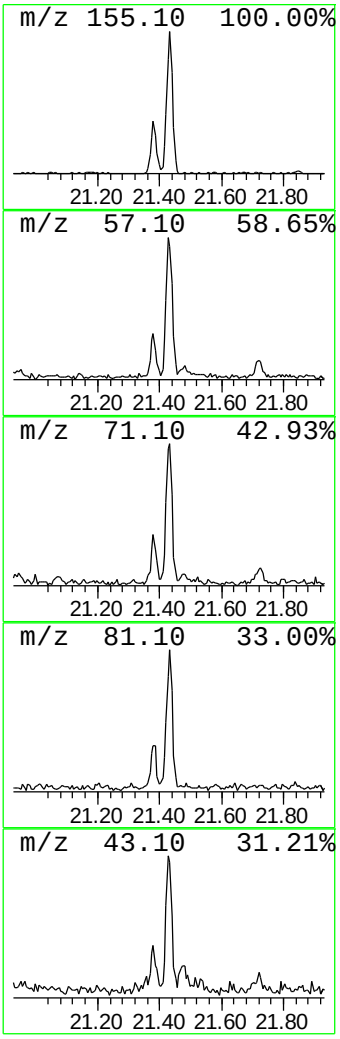
****

Peak Number 9 unknown21.43 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	3.48 ng	551142	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	49
2	2,3,4-Trimethylpentan-2-ol decan...	284	C18H36O2	1000130-74-2	40
3	2-Amino-4,6-dimethoxypyrimidine	155	C6H9N3O2	036315-01-2	40
4	2-Naphthalenebutanoic acid, .gam...	228	C14H12O3	001590-22-3	37
5	4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	37





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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

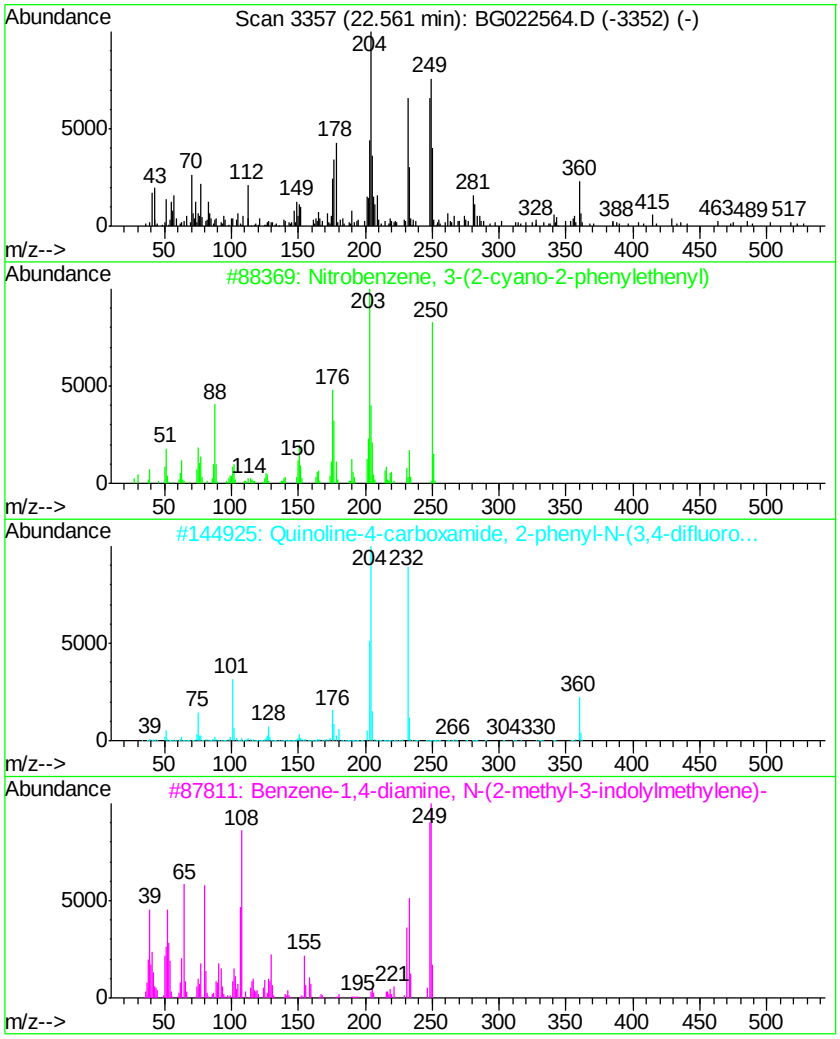
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

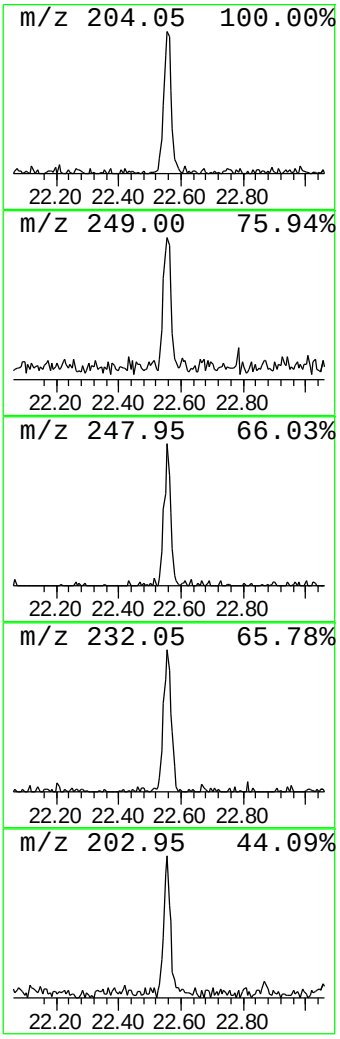
****

Peak Number 10 unknown22.56 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.56	2.07 ng	328568	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nitrobenzene, 3-(2-cyano-2-pheny...	250	C15H10N2O2	006720-37-2	45
2	Quinoline-4-carboxamide, 2-pheny...	360	C22H14F2N2O	303133-50-8	38
3	Benzene-1,4-diamine, N-(2-methyl...	249	C16H15N3	1000269-06-5	25
4	4-Pyrazolemethanamine, 1,3-diphe...	249	C16H15N3	1000273-77-9	22
5	1,4-Naphthoquinone, 6-acetyl-2,5...	248	C12H8O6	013379-24-3	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062516\
Data File : BG022564.D
Acq On : 25 Jun 2016 8:07
Operator : UM/SJ
Sample : H3633-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEPMW2-26

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
2-Pentanone, 4-hy...	5.24	4.8	ng	223495	1	8.17	927616	20.0
2H-Pyran-2-one, 3...	13.33	2.0	ng	206241	3	14.80	2020580	20.0
Homosalate	18.16	4.2	ng	564996	4	17.56	2676800	20.0
n-Hexadecanoic acid	18.43	2.4	ng	320933	4	17.56	2676800	20.0
Oxybenzone	19.19	21.2	ng	2840980	4	17.56	2676800	20.0
Octadecanoic acid	19.69	2.1	ng	277699	4	17.56	2676800	20.0
unknown21.43	21.43	3.5	ng	551142	5	21.84	3167970	20.0
unknown22.56	22.56	2.1	ng	328568	5	21.84	3167970	20.0