LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059844.D
Acq On : 23 Nov 2023 9:15
Operator : MA/JU
Sample : 05449-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-SED-01

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.363	331	336	342	rBV2	34871	53867	2.08%	0.419%
2	5.827	408	415	422	rBV	490560	789082	30.52%	6.143%
3	7.454	685	692	701	rBV	600073	1024359	39.62%	7.974%
4	7.619	714	720	727	rBV4	14284	27953	1.08%	0.218%
5	8.330	834	841	847	rBV2	149922	258611	10.00%	2.013%
6	9.076	963	968	978	rVB3	20130	43471	1.68%	0.338%
7	9.528	1038	1045	1055	rVB	392228	702666	27.18%	5.470%
8	11.180	1320	1326	1334	rVB	171609	303145	11.72%	2.360%
9	12.660	1572	1578	1583	rBV3	15578	30189	1.17%	0.235%
10	13.583	1728	1735	1744	rVB	1407645	2035152	78.71%	15.843%
11	13.788	1764	1770	1780	rVB2	254433	403494	15.61%	3.141%
12	14.963	1964	1970	1976	rVB	316948	504941	19.53%	3.931%
13	15.228	2012	2015	2023	rBV3	26080	43559	1.68%	0.339%
14	15.662	2084	2089	2094	rBV8	16851	27844	1.08%	0.217%
15	16.444	2215	2222	2229	rBV2	1221872	1885610	72.93%	14.679%
16	17.713	2432	2438	2445	rBV	381979	582016	22.51%	4.531%
17	18.524	2572	2576	2581	rBV4	98928	129876	5.02%	1.011%
18	18.618	2588	2592	2597	rBV7	25989	45942	1.78%	0.358%
19	19.464	2733	2736	2744	rVB10	34899	52089	2.01%	0.405%
20	19.652	2764	2768	2771	rBV5	25115	46771	1.81%	0.364%
21	19.752	2781	2785	2787	rVV5	27908	39112	1.51%	0.304%
22	19.781	2787	2790	2797	rVV9	39616	72697	2.81%	0.566%
23	20.104	2842	2845	2850	rBV6	34219	56849	2.20%	0.443%
24	20.286	2871	2876	2882	rVB	2025497	2585601	100.00%	20.128%
25	22.037	3168	3174	3180	rVB	295048	541458	20.94%	4.215%
26	25.621	3775	3784	3794	rBV2	163328	525642	20.33%	4.092%
27	25.821	3814	3818	3819	rBV4	30093	33841	1.31%	0.263%

Sum of corrected areas: 12845837

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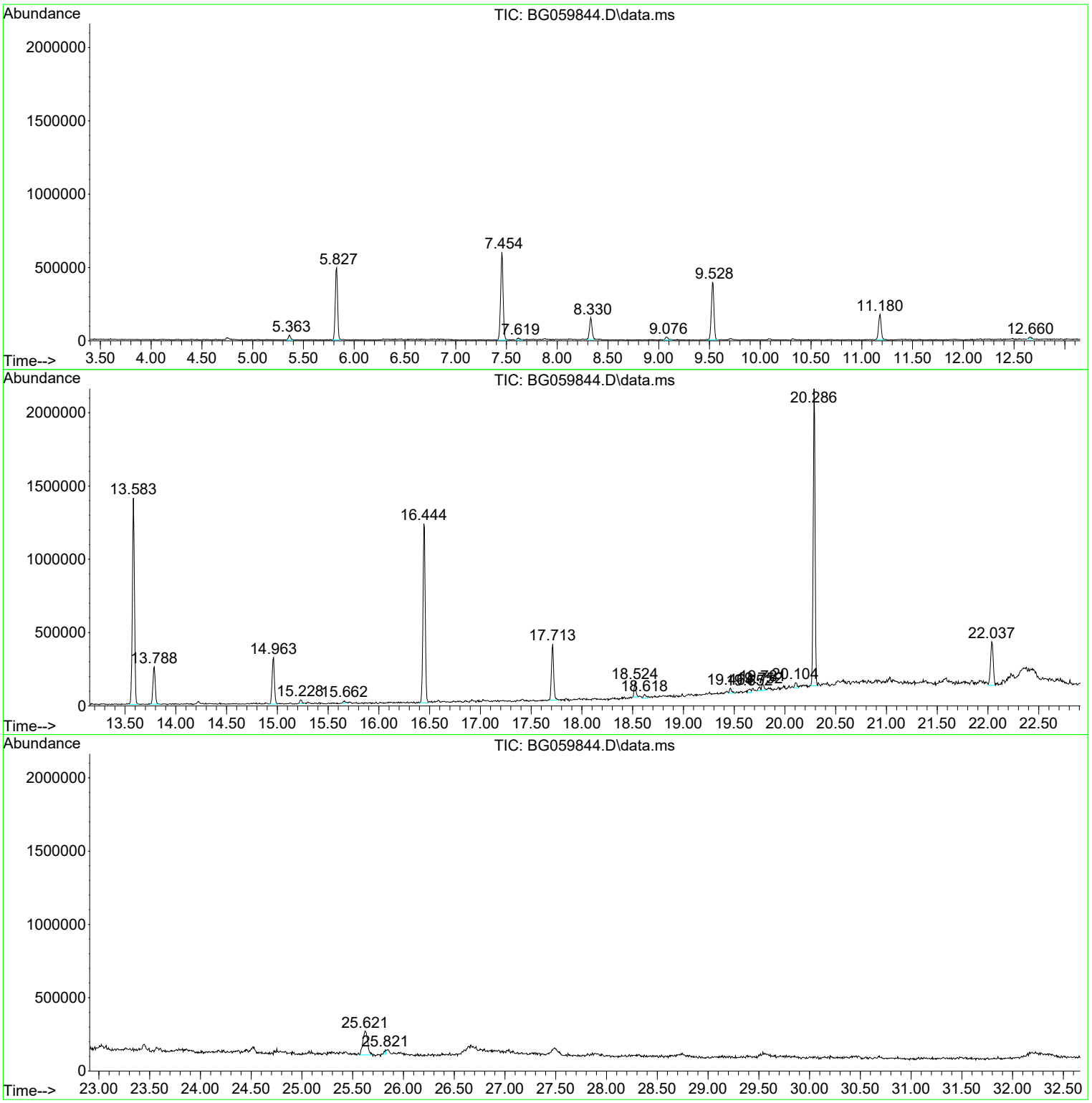
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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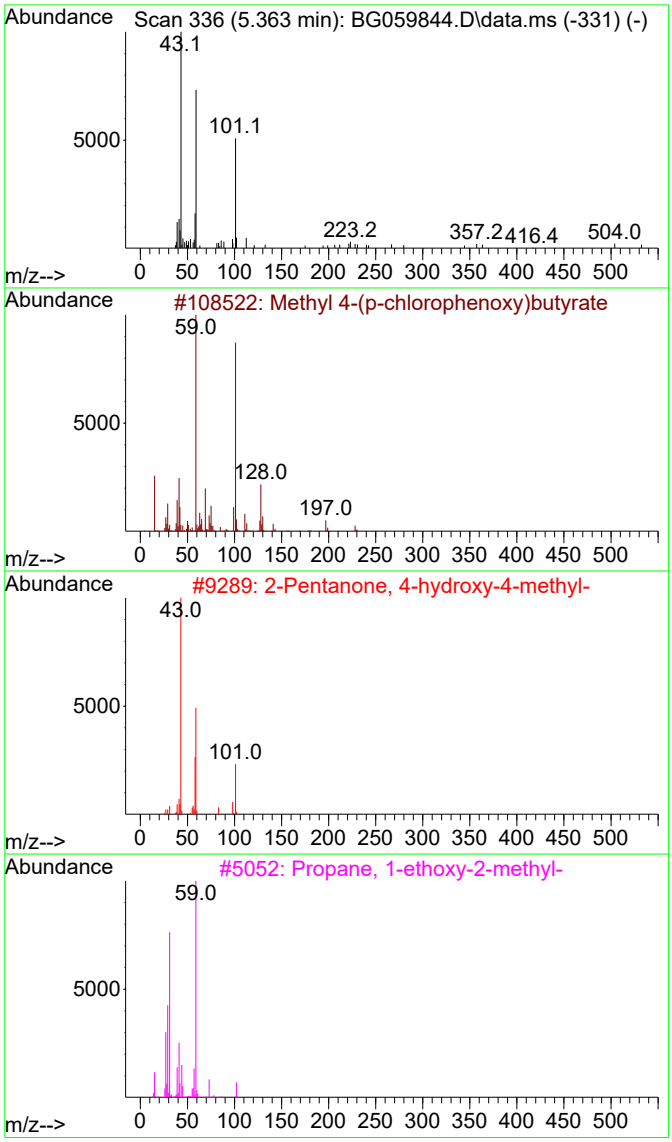
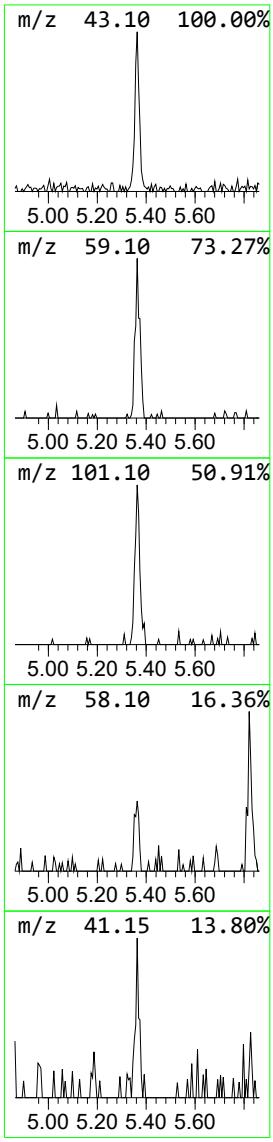
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Methyl 4-(p-chlorophenoxy)b... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.363	4.17 ng	53867	1,4-Dichlorobenzene-d4	8.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 4-(p-chlorophenoxy)butyrate	228	C11H13ClO3	209052-80-2	72
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	3-Hexanol	102	C6H14O	000623-37-0	25
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	18





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Operator : MA/JU
Sample : 05449-01
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

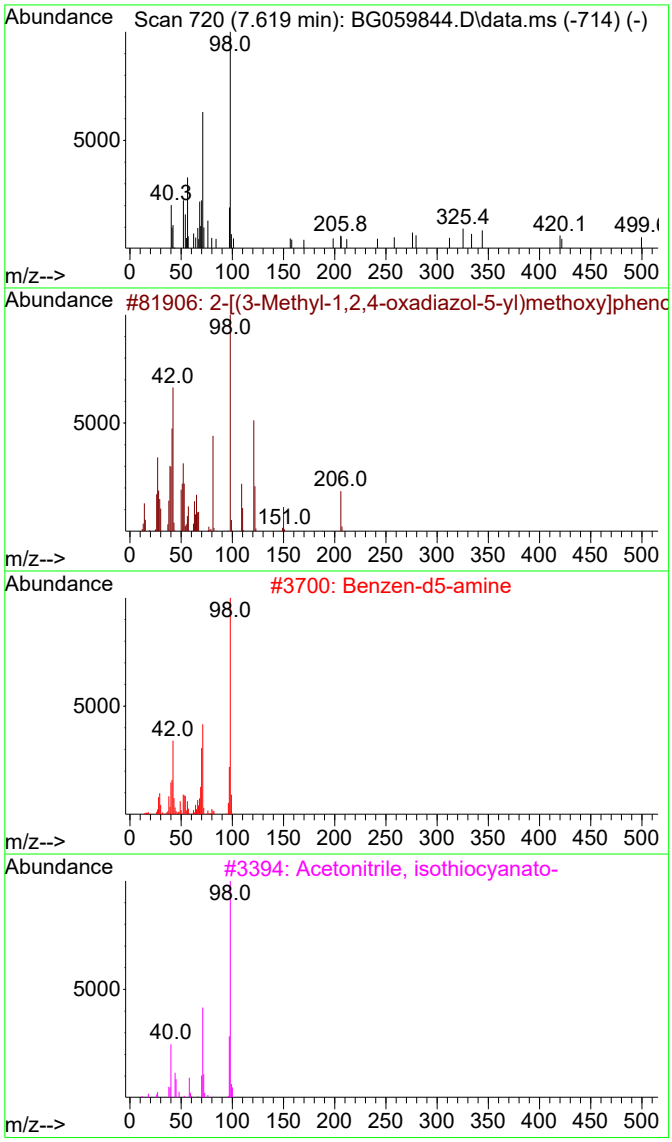
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

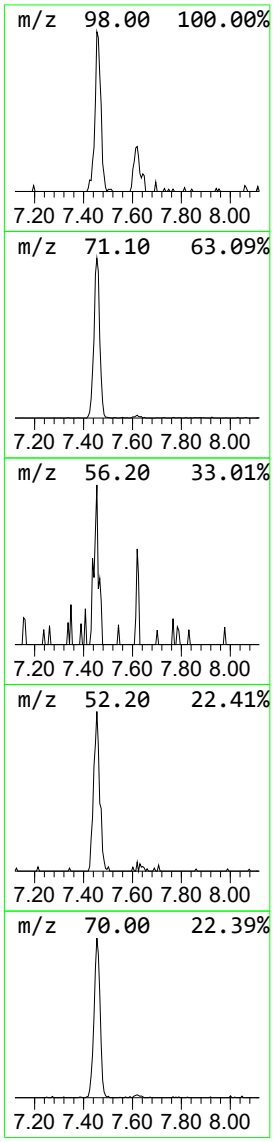
****

Peak Number 2 unknown7.619 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.619	2.16 ng	27953	1,4-Dichlorobenzene-d4	8.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[(3-Methyl-1,2,4-oxadiazol-5-y...	206	C10H10N2O3	1000444-76-2	38
2	Benzen-d5-amine	98	C6H2D5N	004165-61-1	38
3	Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	35
4	3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	25
5	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059844.D
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Operator : MA/JU
Sample : 05449-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-SED-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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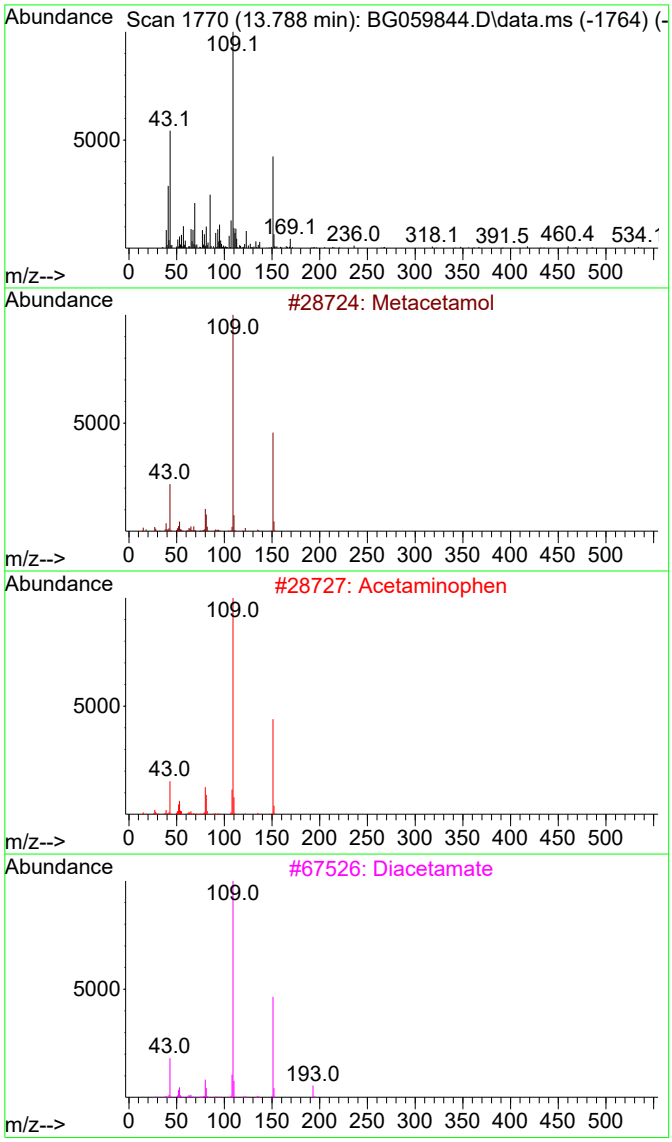
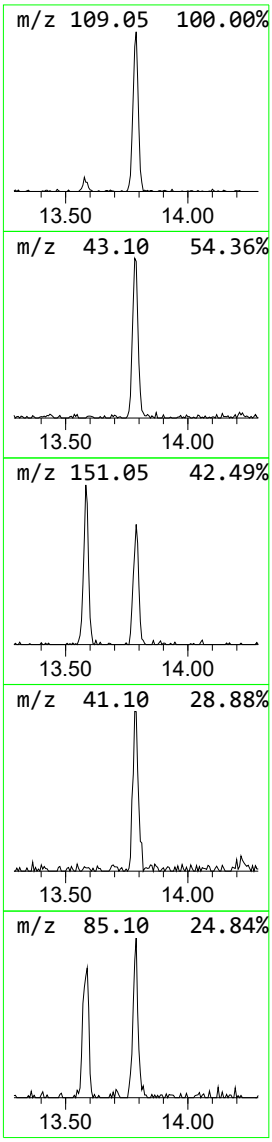
Peak Number 3 Metacetamol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	15.98 ng	403494	Acenaphthene-d10	14.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	58
2	Acetaminophen	151	C8H9NO2	000103-90-2	58
3	Diacetamate	193	C10H11NO3	002623-33-8	53
4	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	53
5	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
Data File : BG059844.D
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Operator : MA/JU
Sample : 05449-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-SED-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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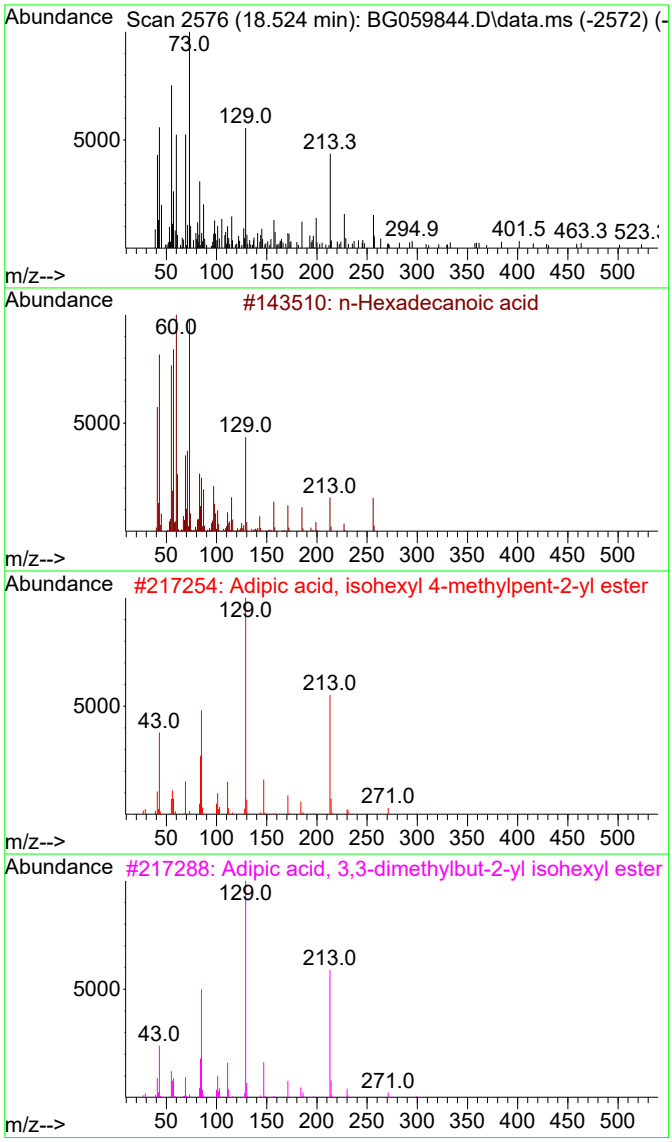
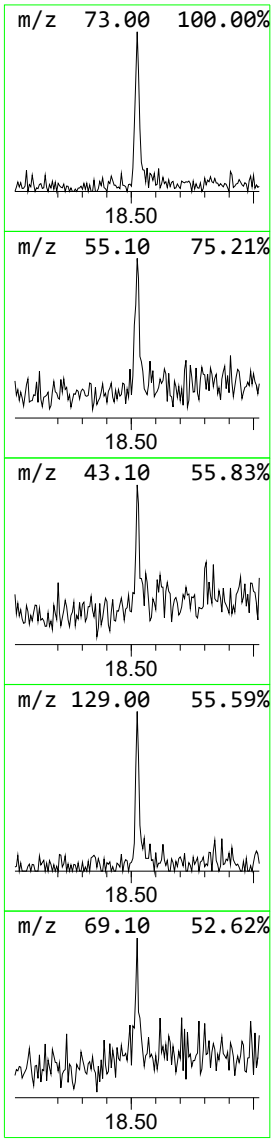
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.524	4.46 ng	129876	Phenanthrene-d10	17.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Adipic acid, isohexyl 4-methylpe...	314	C18H34O4	1000353-50-4	35
3	Adipic acid, 3,3-dimethylbut-2-y...	314	C18H34O4	1000353-67-0	35
4	Piperidine, 1-(1-oxo-3-phenyl-2-...	213	C14H15NO	014143-92-1	35
5	Adipic acid, 2-hexyl isohexyl ester	314	C18H34O4	1000353-71-2	35





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Acq On : 23 Nov 2023 9:15
Operator : MA/JU
Sample : 05449-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-SED-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

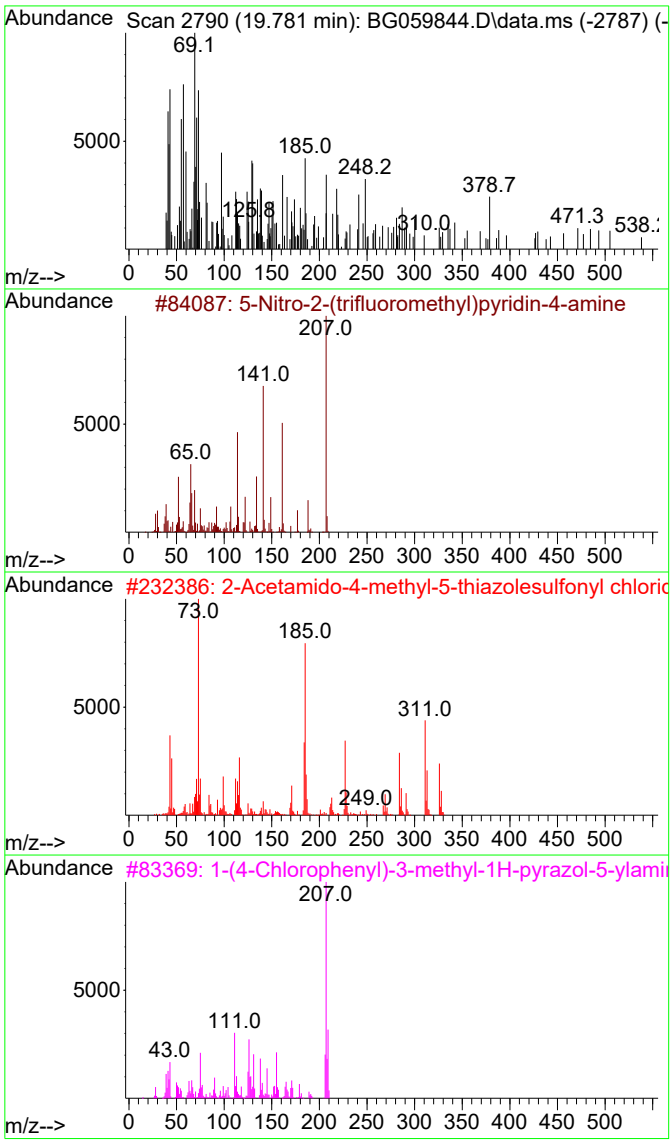
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

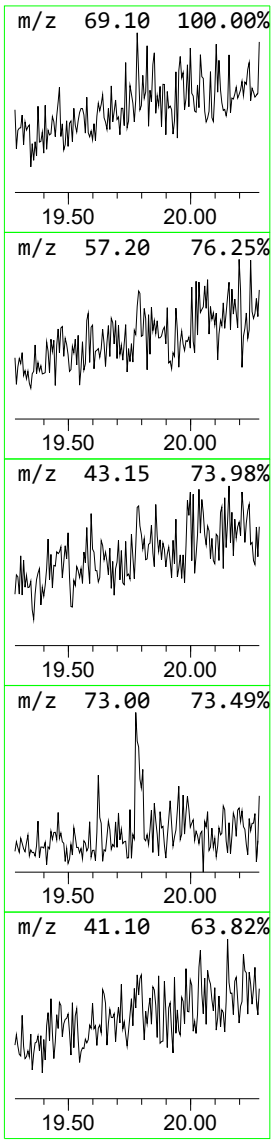
****

Peak Number 5 unknown19.781 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.781	2.50 ng	72697	Phenanthrene-d10	17.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nitro-2-(trifluoromethyl)pyrid...	207	C6H4F3N3O2	438564-36-4	11
2	2-Acetamido-4-methyl-5-thiazoles...	326	C9H15ClN2O3S2Si	1000496-27-2	10
3	1-(4-Chlorophenyl)-3-methyl-1H-p...	207	C10H10ClN3	040401-39-6	10
4	8-Chloro-1-ethyl-4-oxo-1,4-dihyd...	251	C12H10ClNO3	051395-55-2	10
5	N-Cyclohexyl-7H-purin-6-amine, TMS	289	C14H23N5Si	1000501-31-1	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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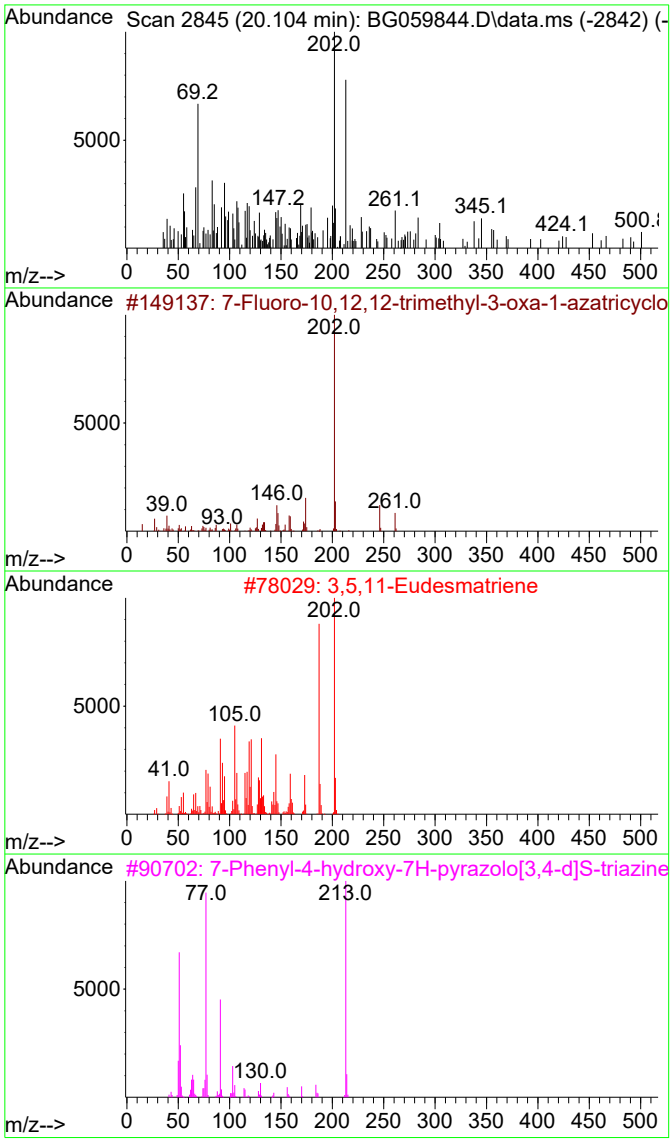
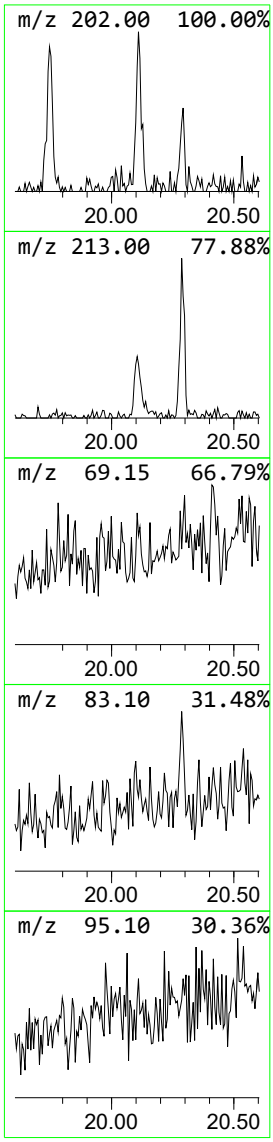
Peak Number 6 unknown20.104 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.104	2.10 ng	56849	Chrysene-d12	22.037

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Fluoro-10,12,12-trimethyl-3-ox...	261	C14H12FNO3	1000445-00-7	42
2	3,5,11-Eudesmatriene	202	C15H22	193615-07-5	38
3	7-Phenyl-4-hydroxy-7H-pyrazolo[3...	213	C10H7N5O	114163-48-3	30
4	4-{5H,6H,7H,8H-Imidazo[1,5-a]pyr...	213	C13H15N3	1010409-68-6	30
5	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	30





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Methyl 4-(p-chl...	5.363	4.2	ng	53867	1	8.330	258611	20.0
unknown7.619	7.619	2.2	ng	27953	1	8.330	258611	20.0
Metacetamol	13.788	16.0	ng	403494	3	14.963	504941	20.0
n-Hexadecanoic ...	18.524	4.5	ng	129876	4	17.713	582016	20.0
unknown19.781	19.781	2.5	ng	72697	4	17.713	582016	20.0
unknown20.104	20.104	2.1	ng	56849	5	22.037	541458	20.0