LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042621\
Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TT-059-RW8-IDWSO-202104-1

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-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.114	296	302	308	rVB2	21871	31766	2.03%	0.343%
2	5.596	375	384	393	rBV	306419	497963	31.86%	5.377%
3	7.212	651	659	669	rBV	321267	554542	35.48%	5.988%
4	8.040	793	800	807	rVB2	84809	138610	8.87%	1.497%
5	9.209	991	999	1007	rBV	220851	378926	24.24%	4.092%
6	10.860	1273	1280	1289	rVB	105114	183843	11.76%	1.985%
7	13.305	1689	1696	1702	rVB	548534	818650	52.37%	8.841%
8	13.563	1734	1740	1744	rBV3	16266	25192	1.61%	0.272%
9	14.127	1830	1836	1842	rBV3	13664	20949	1.34%	0.226%
10	14.685	1925	1931	1940	rVB	176333	258703	16.55%	2.794%
11	16.178	2175	2185	2197	rBV	398209	618832	39.59%	6.683%
12	16.853	2280	2300	2301	rBV	71456	257470	16.47%	2.780%
13	17.130	2331	2347	2369	rVB2	123037	666129	42.62%	7.194%
14	17.370	2369	2388	2396	rBV2	350510	1563106	100.00%	16.880%
15	17.435	2396	2399	2409	rVB	218870	323557	20.70%	3.494%
16	17.641	2424	2434	2438	rBV2	21088	60417	3.87%	0.652%
17	18.734	2611	2620	2632	rBV5	21215	64759	4.14%	0.699%
18	19.868	2805	2813	2822	rBV4	38526	93104	5.96%	1.005%
19	20.044	2837	2843	2849	rVB	1120839	1401258	89.65%	15.132%
20	20.737	2955	2961	2968	rVV4	39878	88282	5.65%	0.953%
21	21.342	3059	3064	3072	rBV3	57396	105478	6.75%	1.139%
22	21.430	3075	3079	3083	rVB3	12311	21812	1.40%	0.236%
23	21.601	3102	3108	3117	rVB4	46413	89463	5.72%	0.966%
24	21.718	3120	3128	3135	rVB2	229487	364815	23.34%	3.940%
25	22.600	3273	3278	3287	rVB5	26871	67076	4.29%	0.724%
26	23.781	3473	3479	3488	rVB5	27755	65769	4.21%	0.710%
27	24.027	3517	3521	3527	rVB6	17261	35654	2.28%	0.385%
28	25.003	3674	3687	3698	rVB2	136085	402189	25.73%	4.343%
29	25.185	3714	3718	3721	rBV5	9546	18501	1.18%	0.200%
30	26.154	3874	3883	3891	rBV10	13654	43329	2.77%	0.468%

Sum of corrected areas: 9260144

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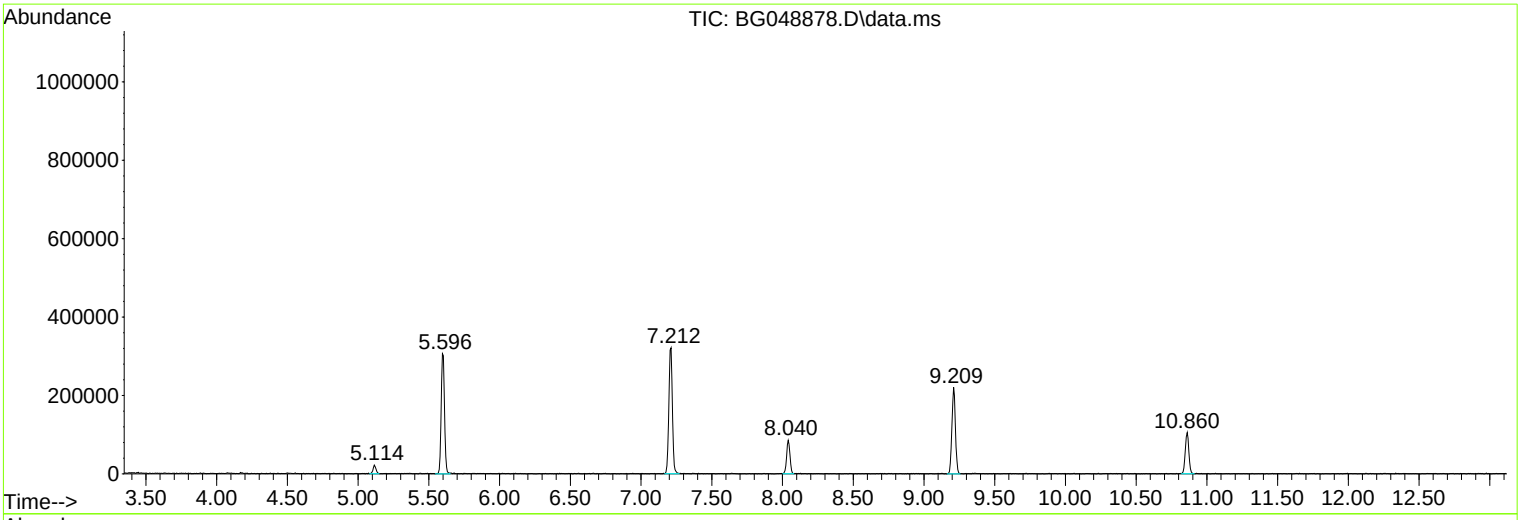
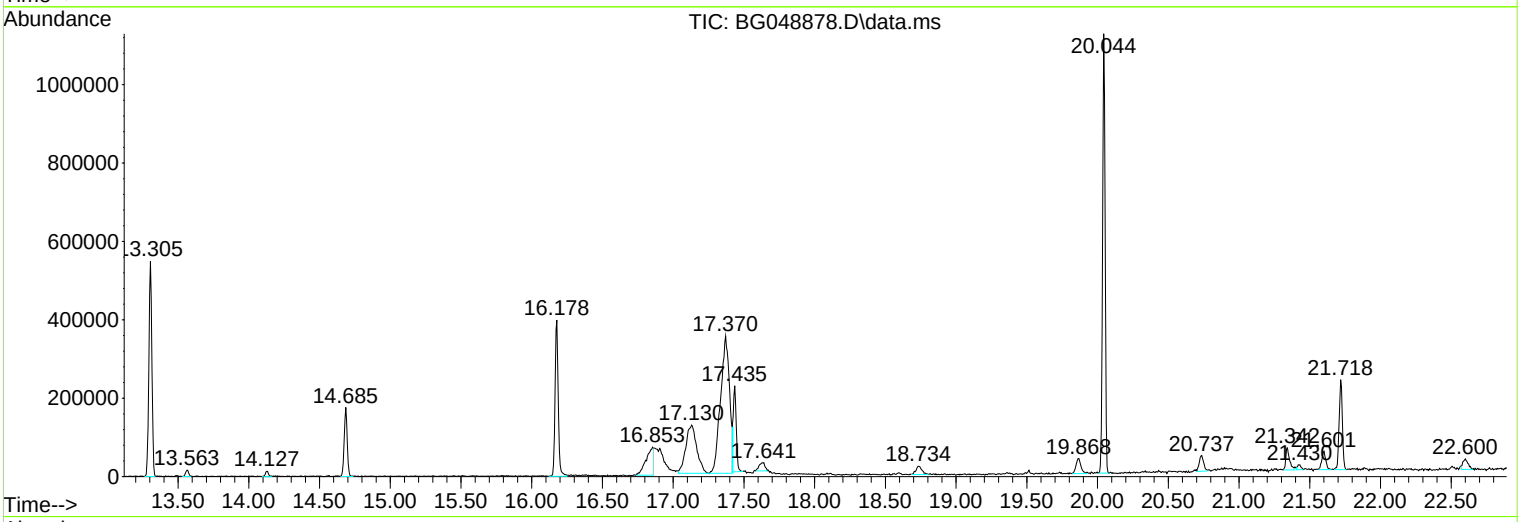
Misc :
ALS Vial : 5 Sample Multiplier: 1

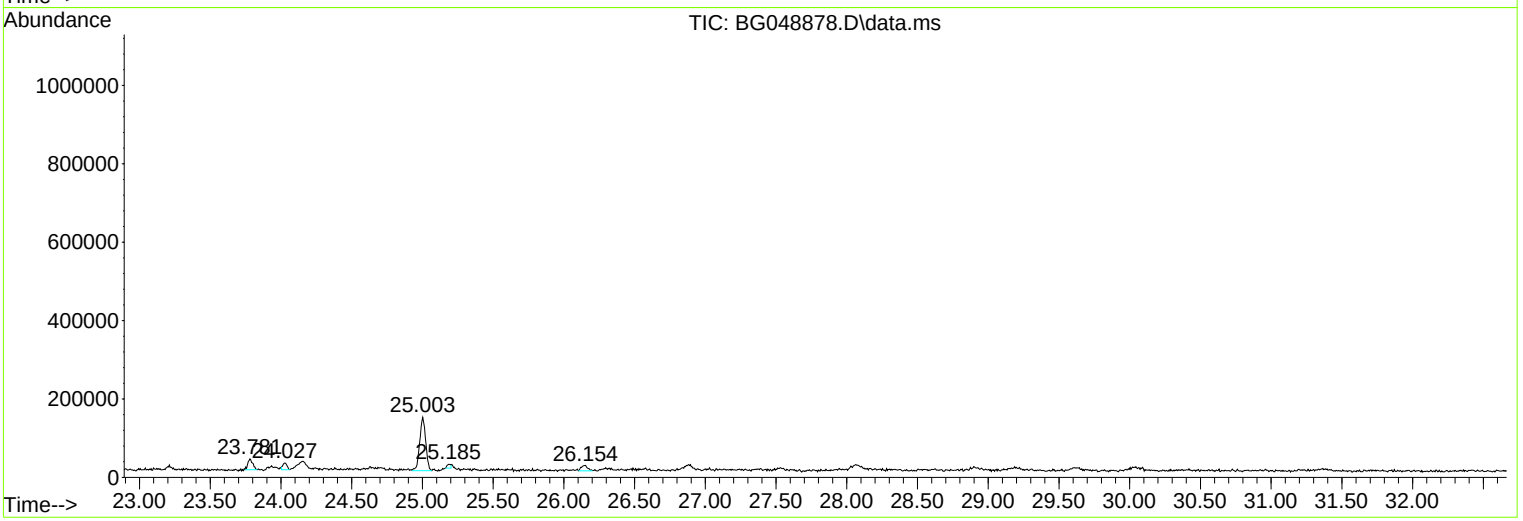
Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







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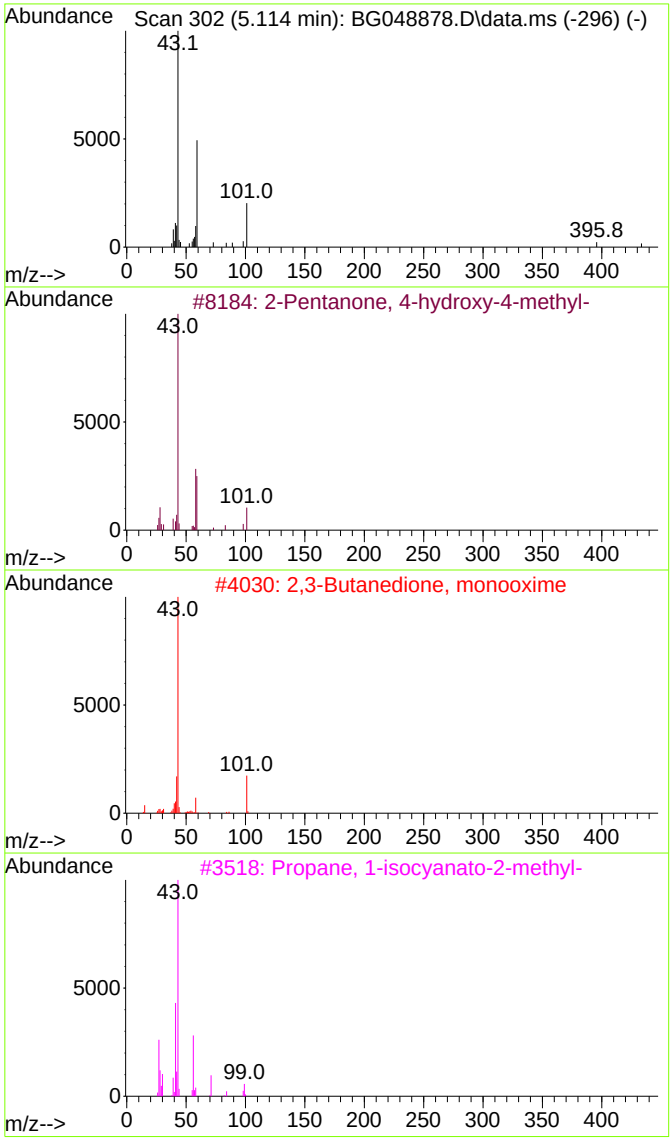
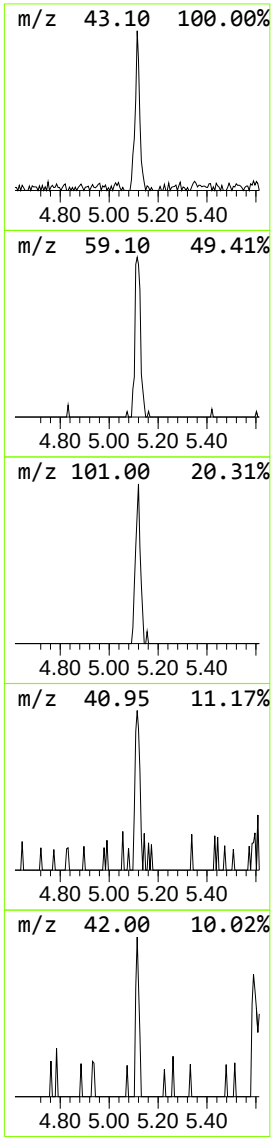
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.114	4.58 ng	31766	1,4-Dichlorobenzene-d4	8.046

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	10
4	Propylamine	59	C3H9N	000107-10-8	9
5	Butane	58	C4H10	000106-97-8	9





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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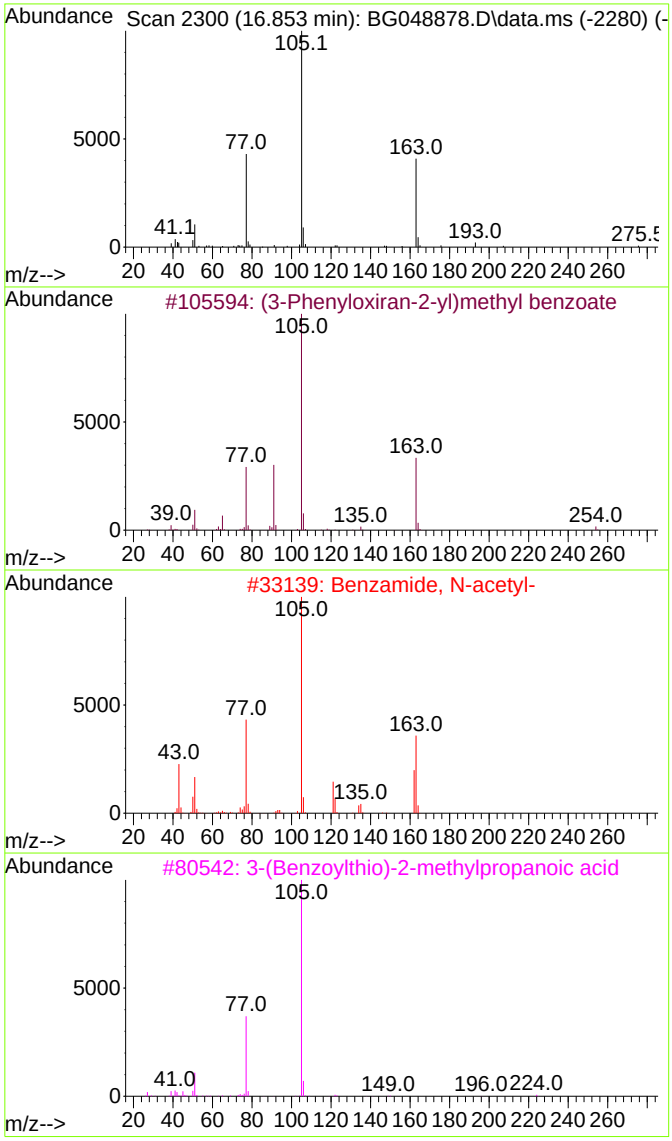
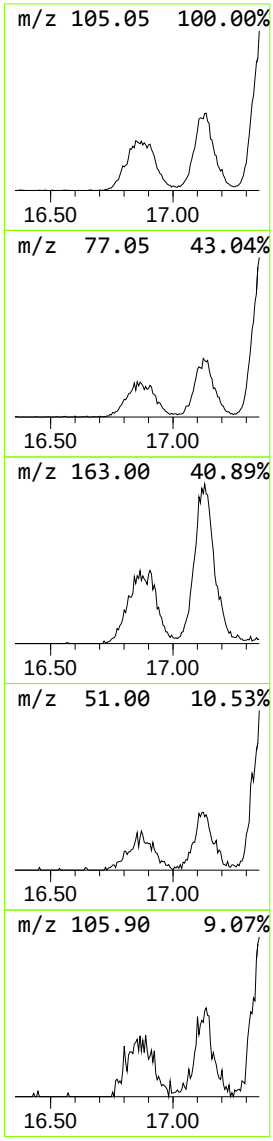
****
Peak Number 2 (3-Phenyloxiran-2-yl)methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.853	15.91 ng	257470	Phenanthrene-d10	17.435

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	59
2	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
3	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	47
4	Benzoic acid 5-methyl-2-phenyl-2...	278	C17H14N2O2	056159-67-2	47
5	1H-Pyrazole-4-carboxylic acid, 5...	275	C13H13N3O4	1000315-85-0	47





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Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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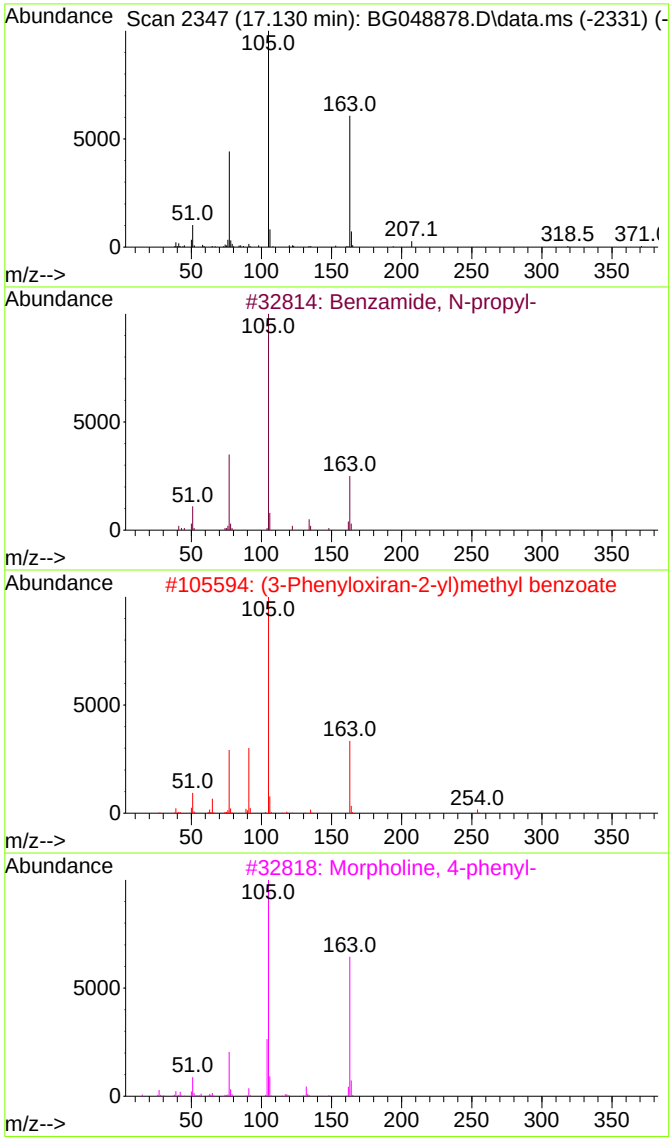
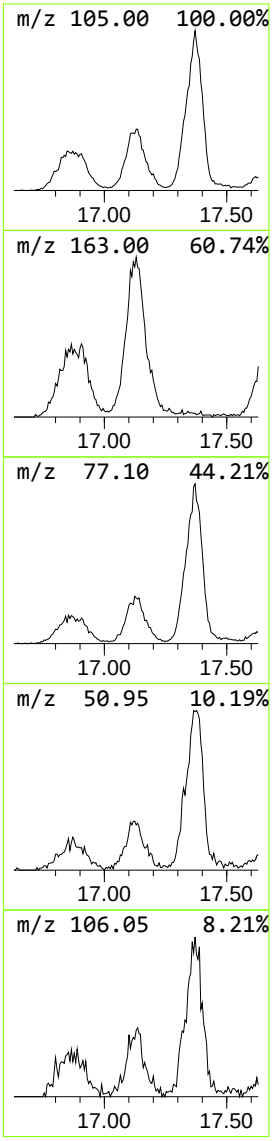
****

Peak Number 3 Benzamide, N-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.130	41.18 ng	666129	Phenanthrene-d10	17.435

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	59
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
4	1H-Benzimidazole, 2,3-dihydro-1,...	328	C21H16N2O2	1000262-54-9	47
5	1,3-Phenylenedibenzoate	318	C20H14O4	000094-01-9	47





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Data File : BG048878.D
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Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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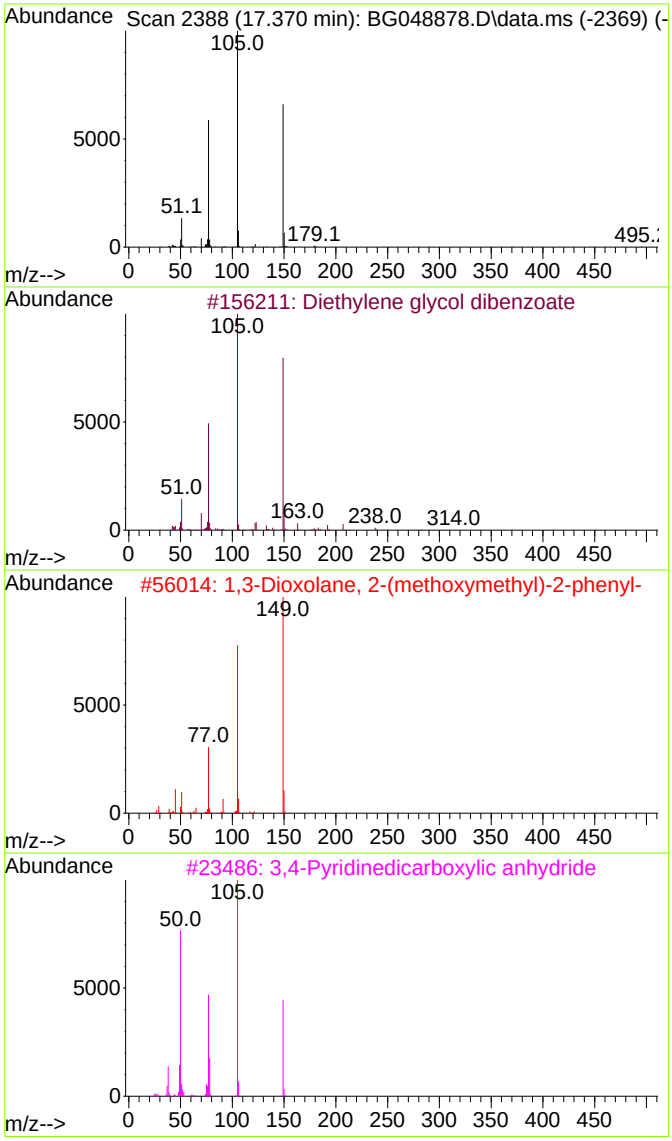
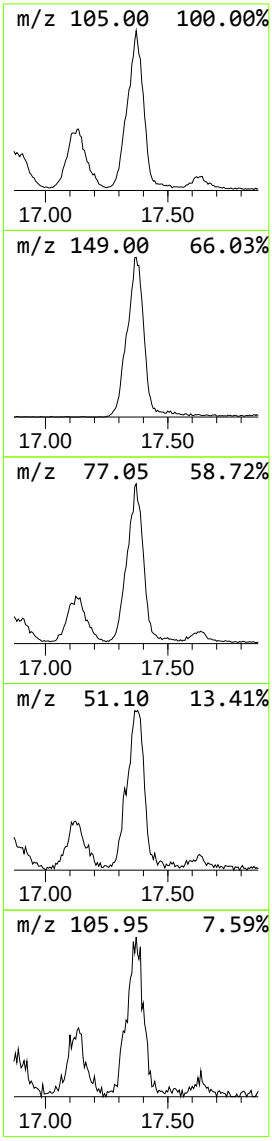
****

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.371	96.62 ng	1563110	Phenanthrene-d10	17.435

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3	3,4-Pyridinedicarboxylic anhydride	149	C7H3NO3	004664-08-8	64
4	1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





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Sample : M2163-01
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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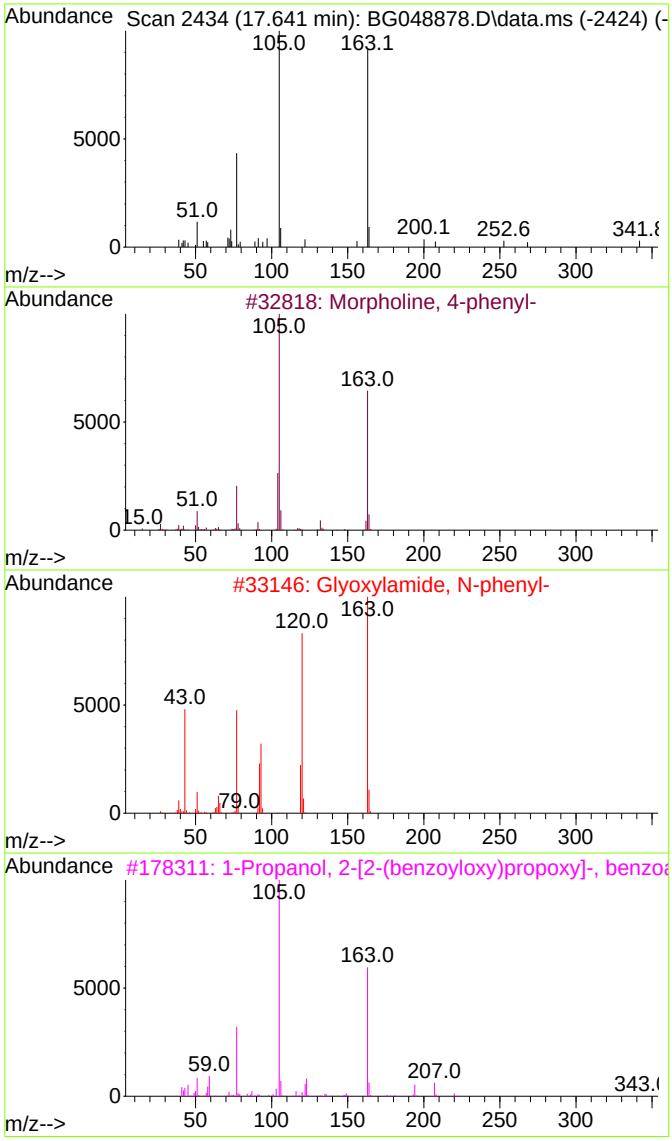
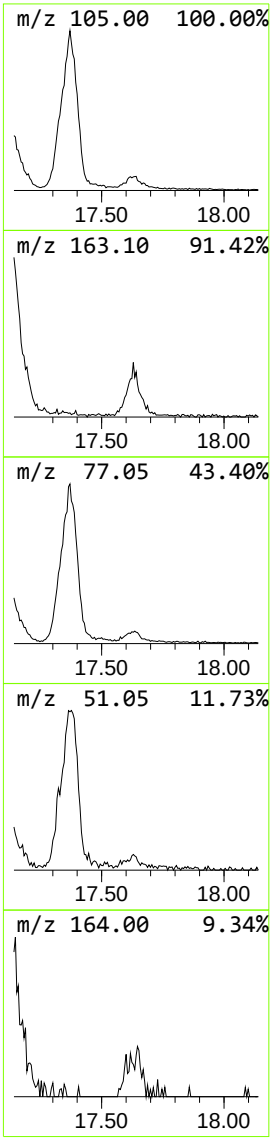
****

Peak Number 5 Morpholine, 4-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.641	3.73 ng	60417	Phenanthrene-d10	17.435

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	59
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	56
4	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	56
5	Benzonitrile, 2,3-dimethoxy-	163	C9H9NO2	005653-62-3	45





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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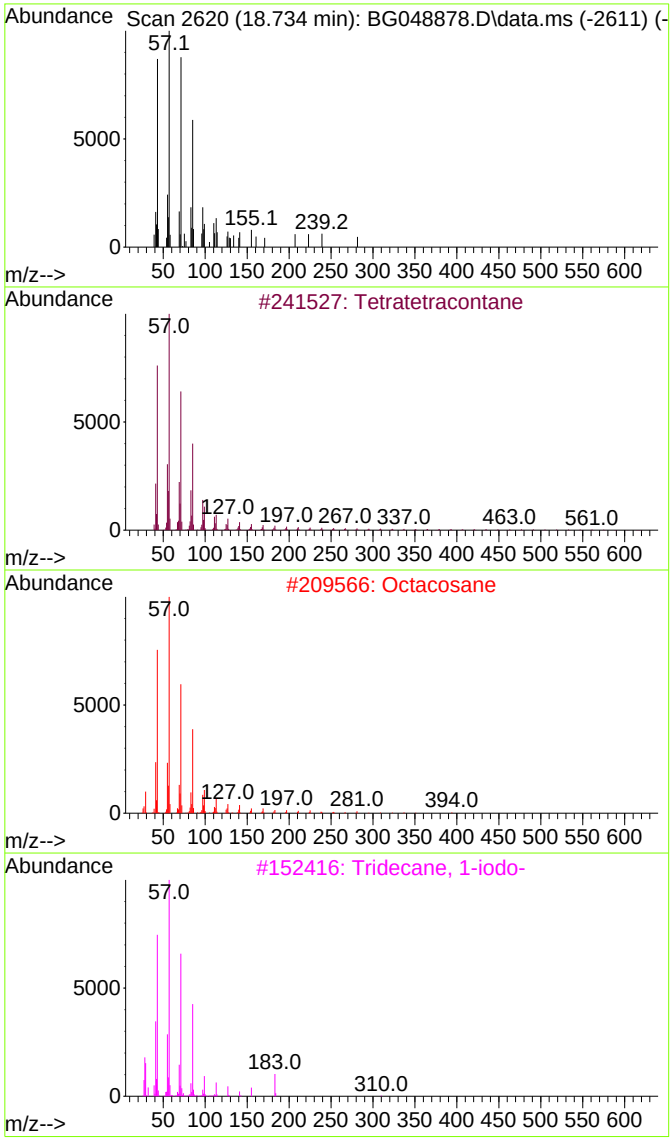
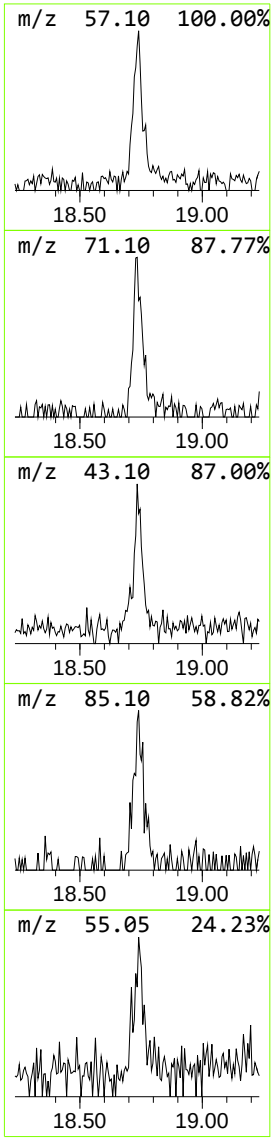
****

Peak Number 6 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.734	4.00 ng	64759	Phenanthrene-d10	17.435

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	80
2	Octacosane	394	C28H58	000630-02-4	72
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
4	Nonadecane	268	C19H40	000629-92-5	72
5	10-Methylnonadecane	282	C20H42	056862-62-5	64





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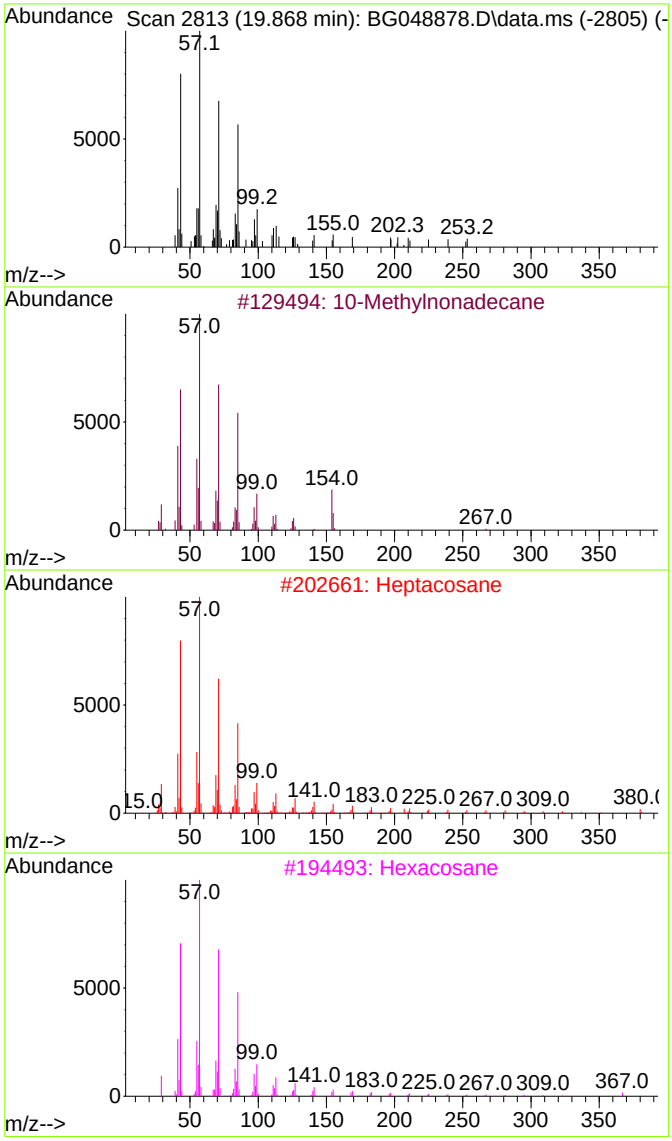
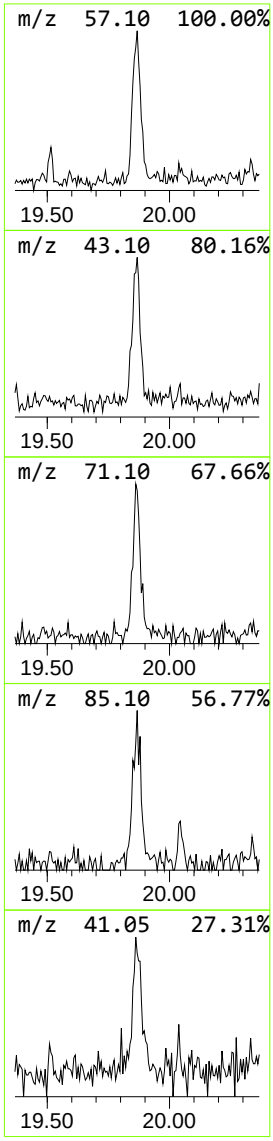
****

Peak Number 7 10-Methylnonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.868	5.10 ng	93104	Chrysene-d12	21.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86





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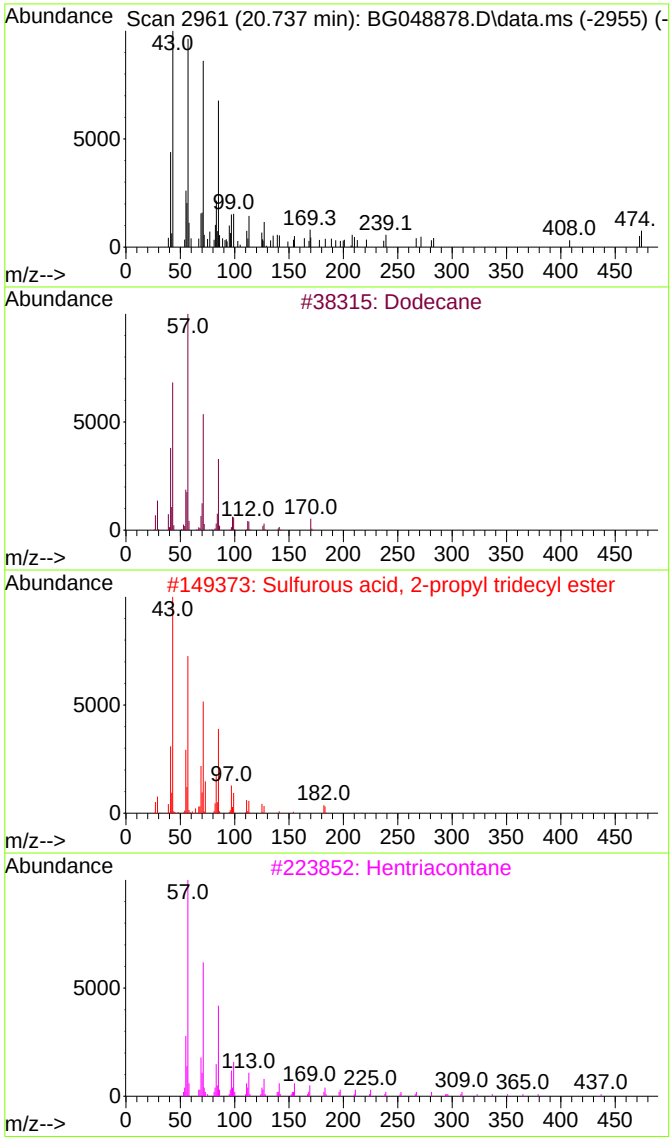
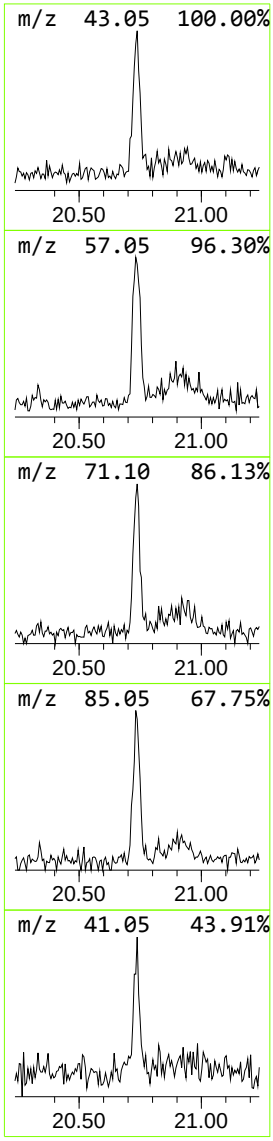
****

Peak Number 8 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.737	4.84 ng	88282	Chrysene-d12	21.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	81
2	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	74
3	Hentriacontane	437	C31H64	000630-04-6	74
4	2-methyloctacosane	408	C29H60	1000376-72-8	72
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	72





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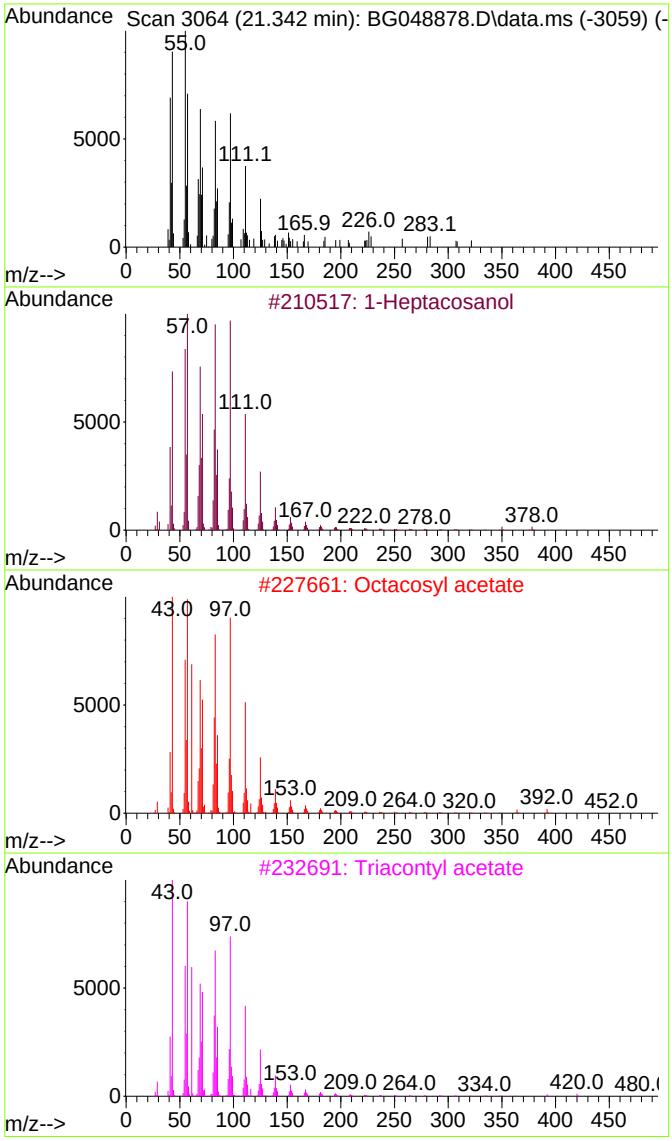
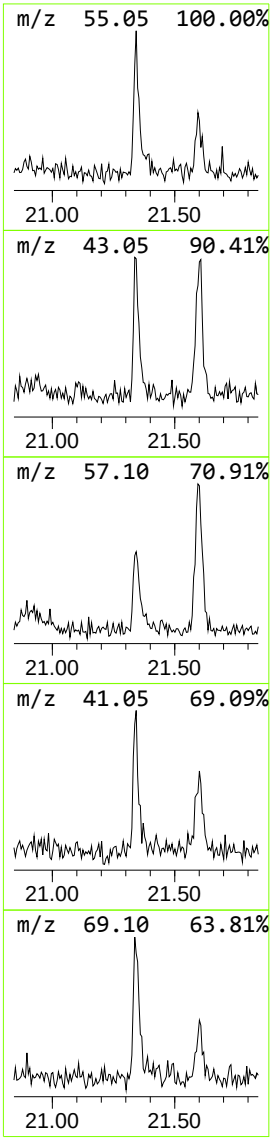
Peak Number 9 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.342	5.78 ng	105478	Chrysene-d12	21.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Octacosyl acetate	452	C30H60O2	018206-97-8	90
3	Triacontyl acetate	480	C32H64O2	041755-58-2	87
4	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	83
5	Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042621\
Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

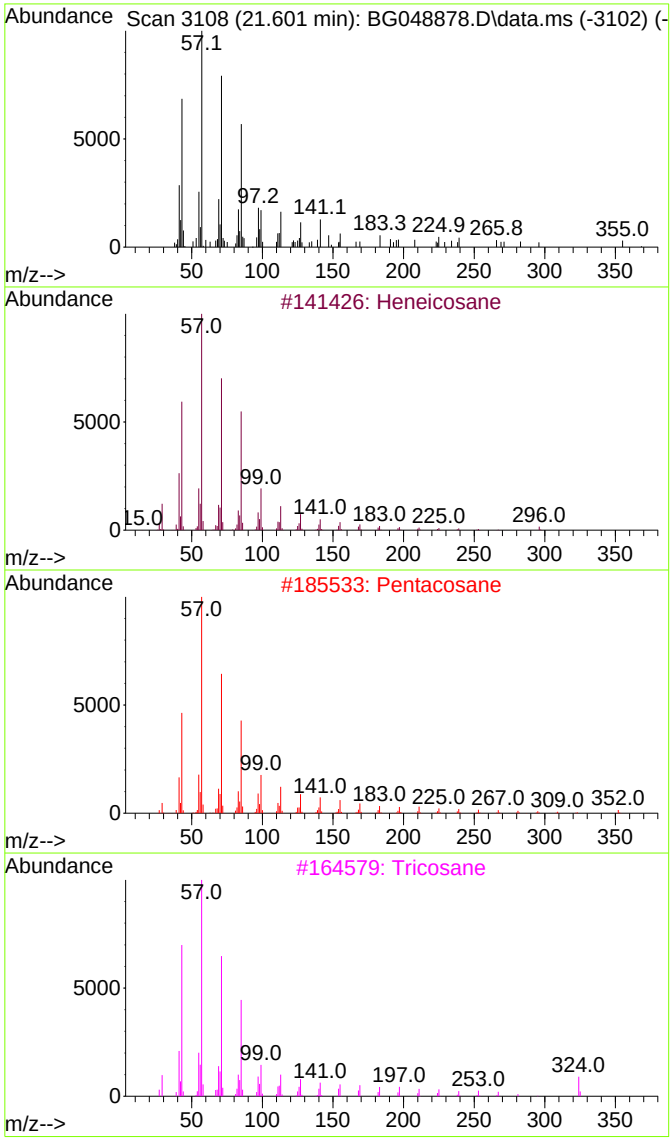
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

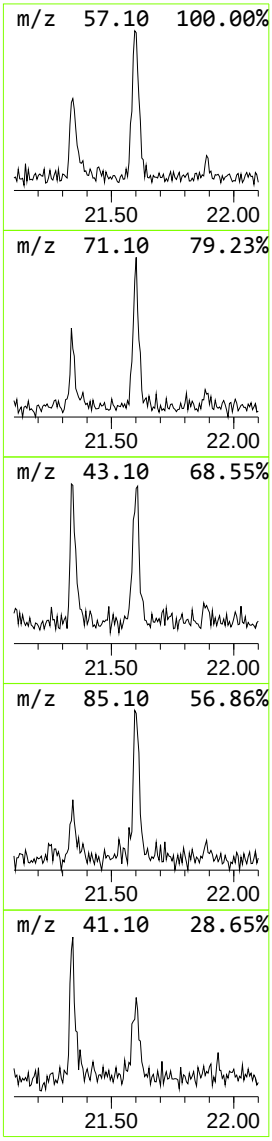
****

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.601	4.90 ng	89463	Chrysene-d12	21.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Pentacosane	352	C25H52	000629-99-2	91
3	Tricosane	324	C23H48	000638-67-5	91
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042621\
Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

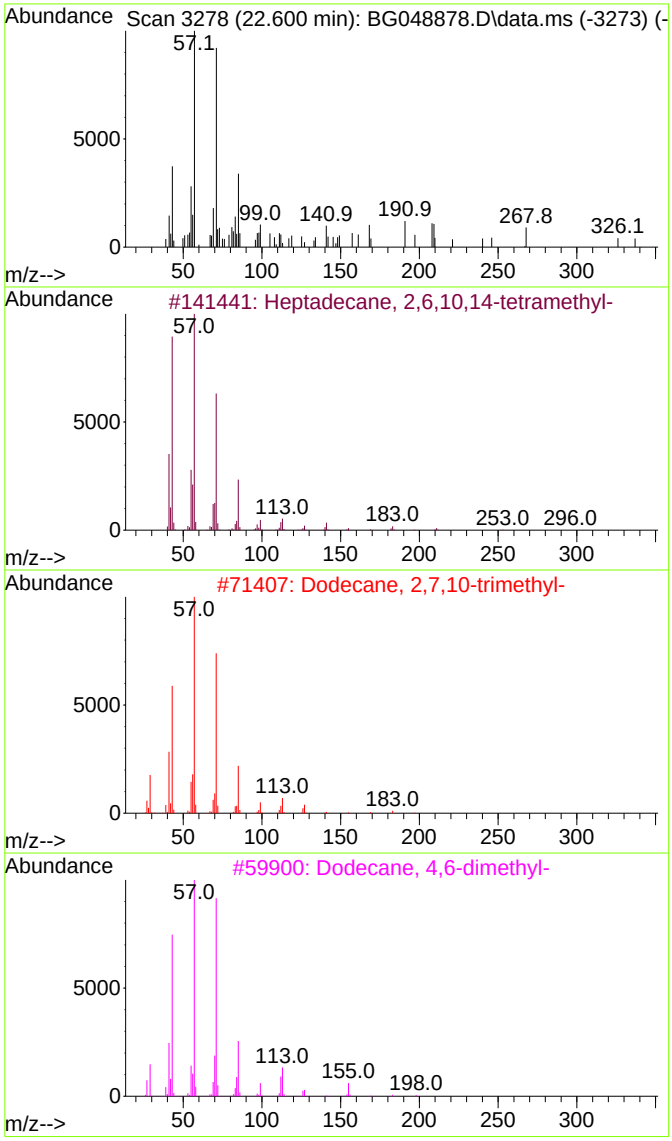
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

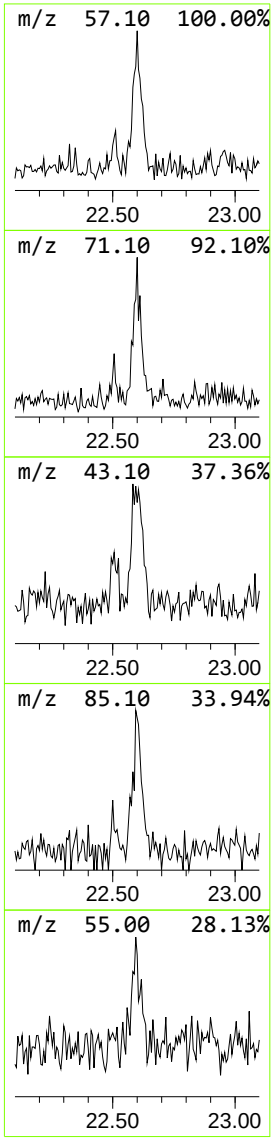
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptadecane, 2,6,10,14-tetr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.600	3.68 ng	67076	Chrysene-d12	21.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	50
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	50
3	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	50
4	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	50
5	Heptadecane	240	C17H36	000629-78-7	46





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Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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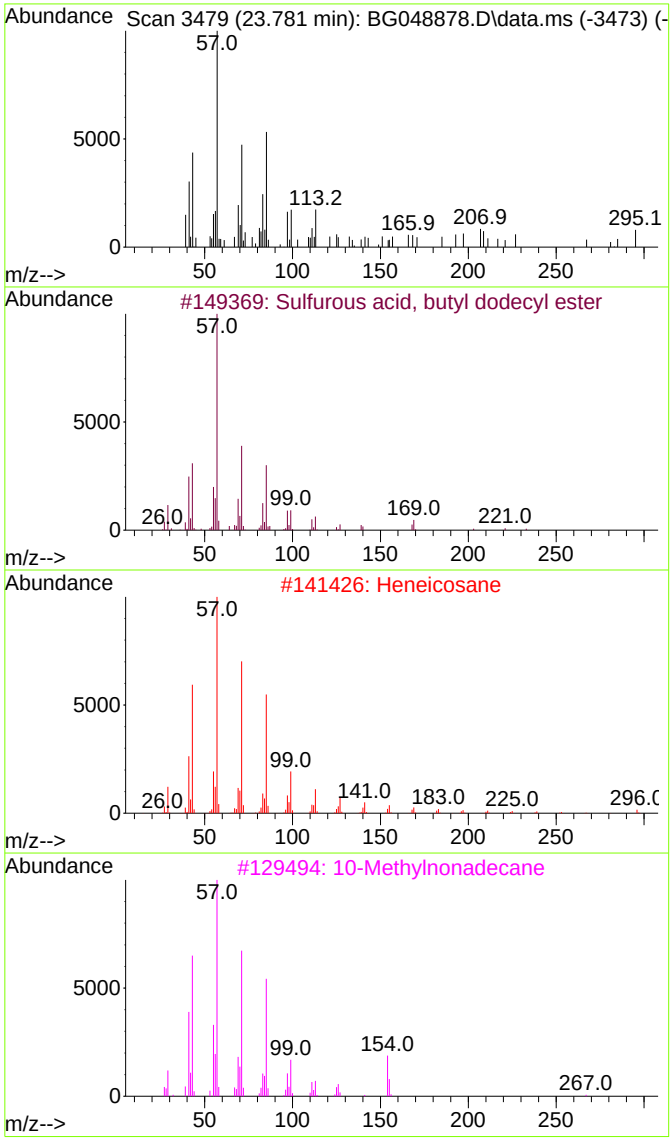
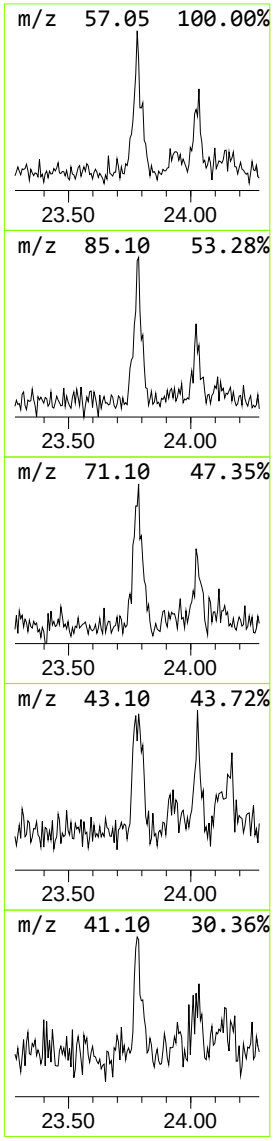
Peak Number 12 Sulfurous acid, butyl dodec... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.781	3.27 ng	65769	Perylene-d12	25.003

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2	Heneicosane	296	C21H44	000629-94-7	64
3	10-Methylnonadecane	282	C20H42	056862-62-5	64
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	64





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Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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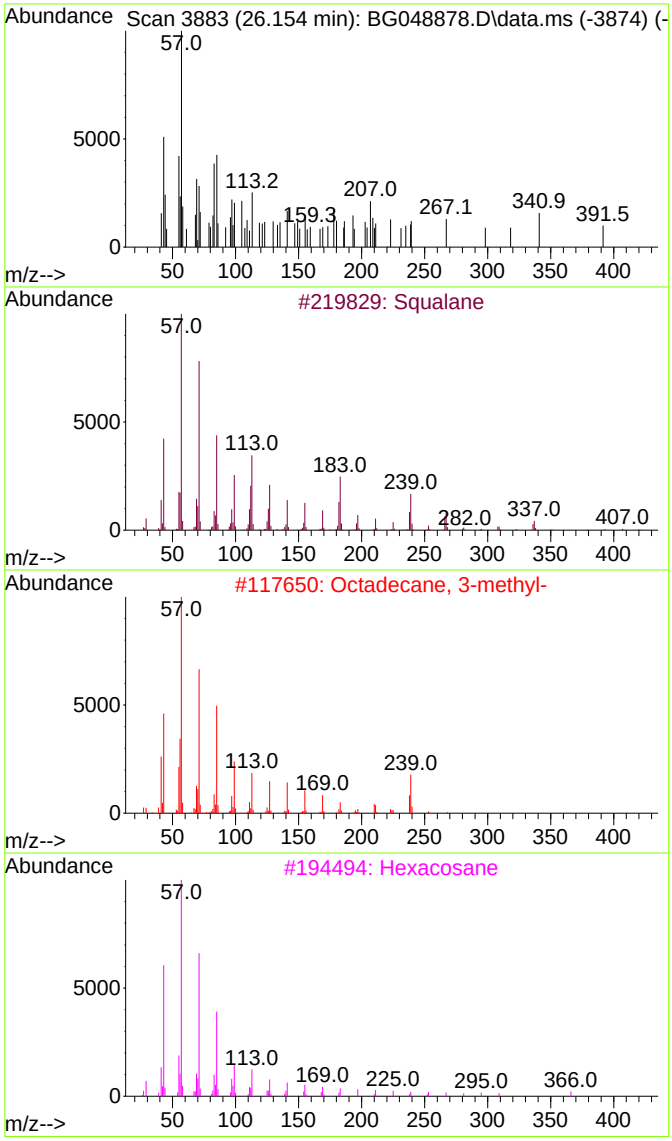
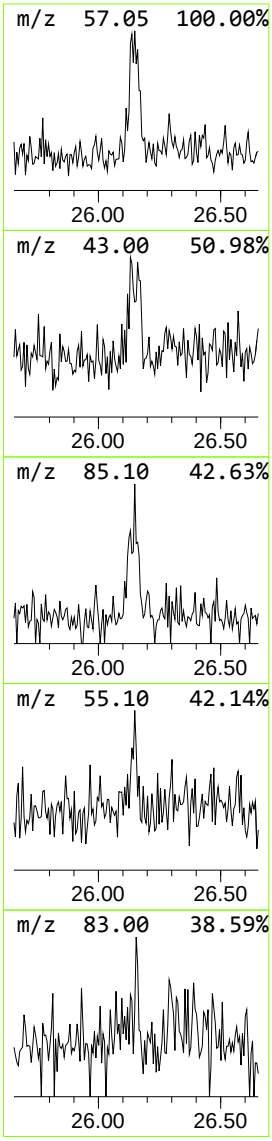
Peak Number 13 unknown26.15 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.154	2.15 ng	43329	Perylene-d12	25.003

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalane	422	C30H62	000111-01-3	32
2	Octadecane, 3-methyl-	268	C19H40	006561-44-0	25
3	Hexacosane	366	C26H54	000630-01-3	22
4	Tetratetracontane	619	C44H90	007098-22-8	22
5	Docosane, 1,22-dibromo-	466	C22H44Br2	034540-49-3	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042621\
Data File : BG048878.D
Acq On : 26 Apr 2021 14:52
Operator : CG/JU
Sample : M2163-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TT-059-RW8-IDWSO-202104-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.114	4.6	ng	31766	1	8.046	138610	20.0
(3-Phenyloxiran...	16.853	15.9	ng	257470	4	17.435	323557	20.0
Benzamide, N-pr...	17.130	41.2	ng	666129	4	17.435	323557	20.0
Diethylene glyc...	17.371	96.6	ng	1563110	4	17.435	323557	20.0
Morpholine, 4-p...	17.641	3.7	ng	60417	4	17.435	323557	20.0
Tetratetracontane	18.734	4.0	ng	64759	4	17.435	323557	20.0
10-Methylnonade...	19.868	5.1	ng	93104	5	21.718	364815	20.0
Dodecane	20.737	4.8	ng	88282	5	21.718	364815	20.0
1-Heptacosanol	21.342	5.8	ng	105478	5	21.718	364815	20.0
Heneicosane	21.601	4.9	ng	89463	5	21.718	364815	20.0
Heptadecane, 2,...	22.600	3.7	ng	67076	5	21.718	364815	20.0
Sulfurous acid,...	23.781	3.3	ng	65769	6	25.003	402189	20.0
unknown26.15	26.154	2.1	ng	43329	6	25.003	402189	20.0