LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059866.D
Acq On : 24 Nov 2023 20:23
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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: BG059866.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.350	328	334	339	rBV3	74099	116119	2.48%	0.669%
2	5.814	405	413	422	rBV	656681	1062951	22.73%	6.123%
3	7.442	681	690	700	rVB	629212	1065801	22.79%	6.139%
4	8.317	832	839	845	rBV3	113474	199172	4.26%	1.147%
5	9.516	1036	1043	1052	rVB	462118	831706	17.79%	4.791%
6	11.161	1316	1323	1333	rBV	158144	295635	6.32%	1.703%
7	13.570	1727	1733	1741	rVB	1593550	2387447	51.06%	13.753%
8	14.951	1960	1968	1973	rBV	342789	544948	11.65%	3.139%
9	16.437	2210	2221	2229	rBV	1777914	2640097	56.46%	15.208%
10	17.700	2430	2436	2442	rBV	474151	739285	15.81%	4.259%
11	18.511	2568	2574	2580	rBV	205370	262086	5.60%	1.510%
12	19.769	2784	2788	2793	rVB7	66688	80062	1.71%	0.461%
13	20.274	2869	2874	2880	rBV	3683965	4676068	100.00%	26.936%
14	20.926	2980	2985	2989	rBV2	136413	171213	3.66%	0.986%
15	20.979	2989	2994	2998	rVV	508239	595664	12.74%	3.431%
16	21.555	3089	3092	3099	rVB5	90180	139474	2.98%	0.803%
17	22.019	3163	3171	3178	rBV2	372173	666984	14.26%	3.842%
18	22.518	3254	3256	3262	rVB7	32647	50959	1.09%	0.294%
19	23.411	3404	3408	3413	rBV8	40368	72879	1.56%	0.420%
20	24.475	3586	3589	3596	rVB8	40296	79506	1.70%	0.458%
21	25.380	3739	3743	3750	rVB10	44604	99836	2.14%	0.575%
22	25.585	3769	3778	3789	rVB3	194558	582112	12.45%	3.353%

Sum of corrected areas: 17360004

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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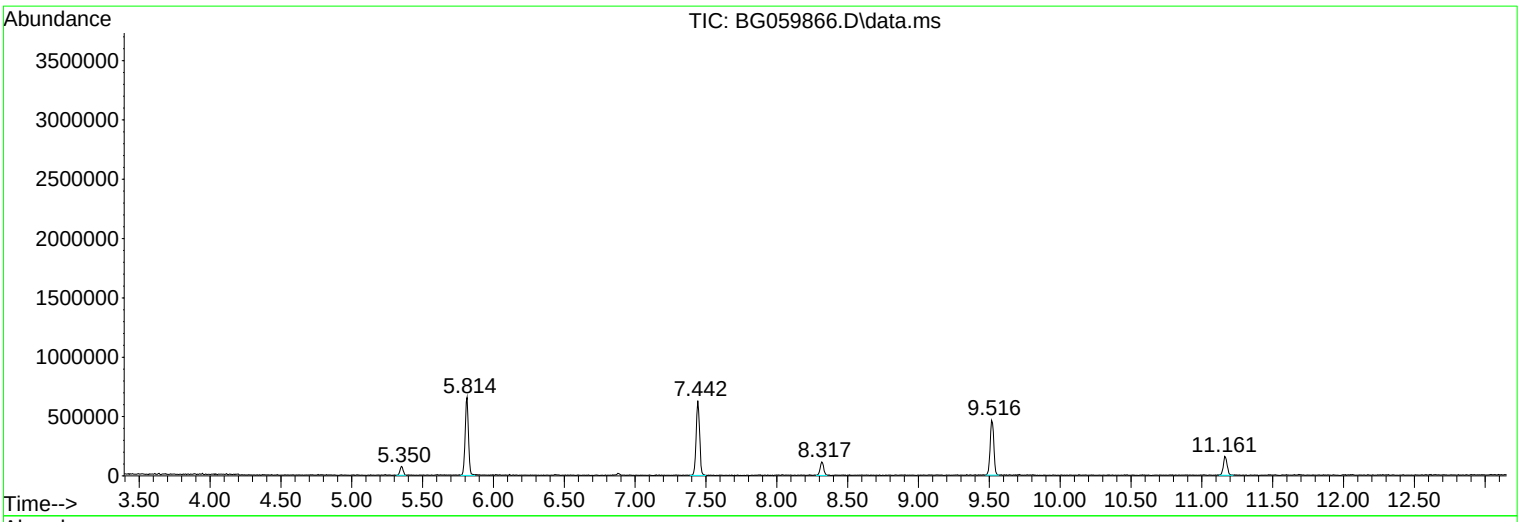
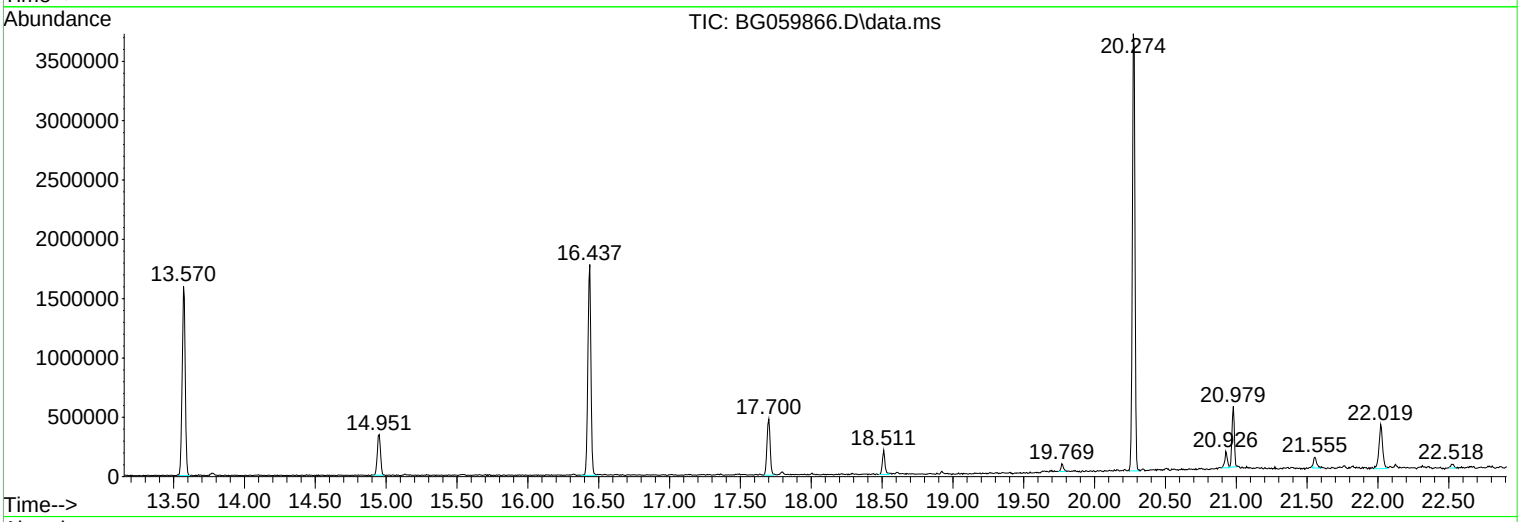
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

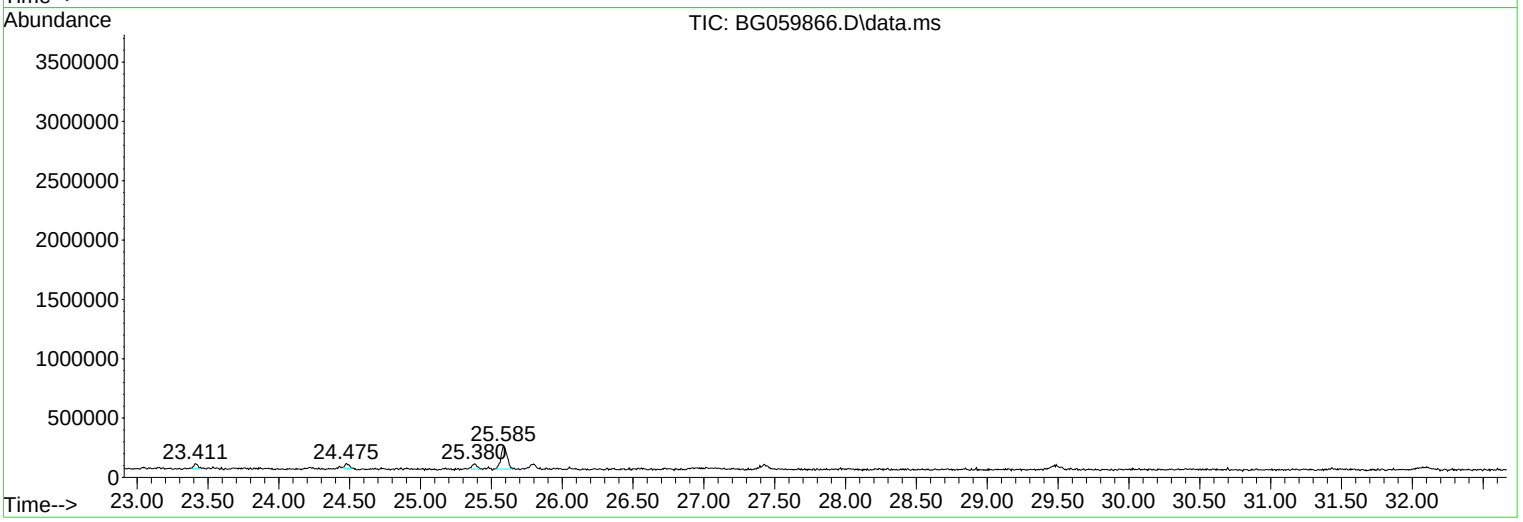
Instrument :
BNA_G
ClientSampleId :
TP-12

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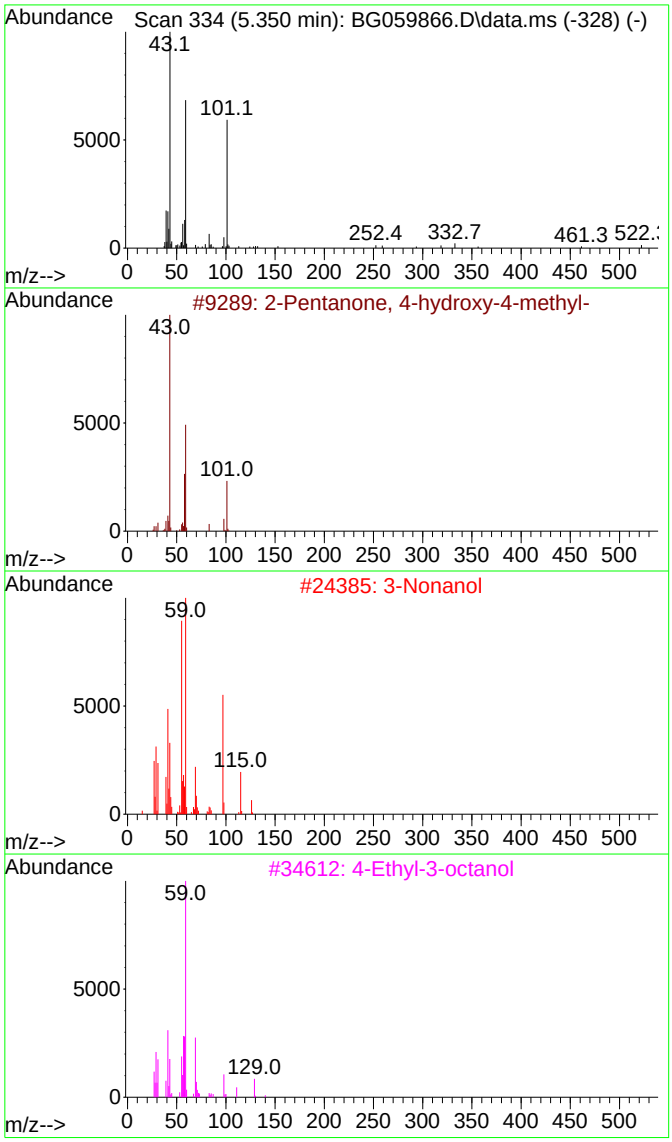
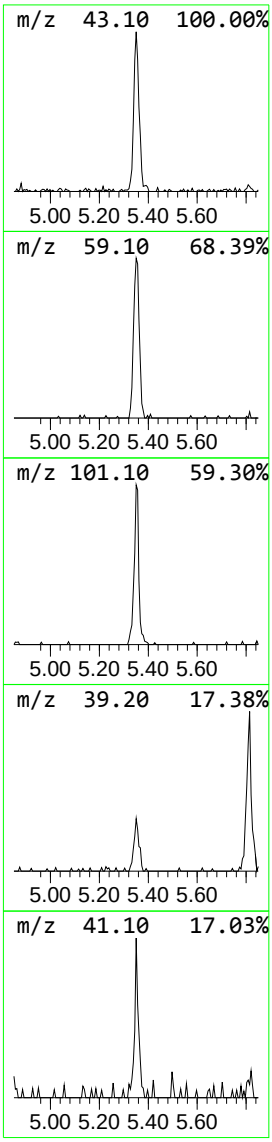
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.350	11.66 ng	116119	1,4-Dichlorobenzene-d4	8.323

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Nonanol	144	C9H20O	000624-51-1	25
3	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	23
4	5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	23
5	Succinic acid, 3-heptyl isobutyl...	272	C15H28O4	1000349-48-5	17





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Data File : BG059866.D
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Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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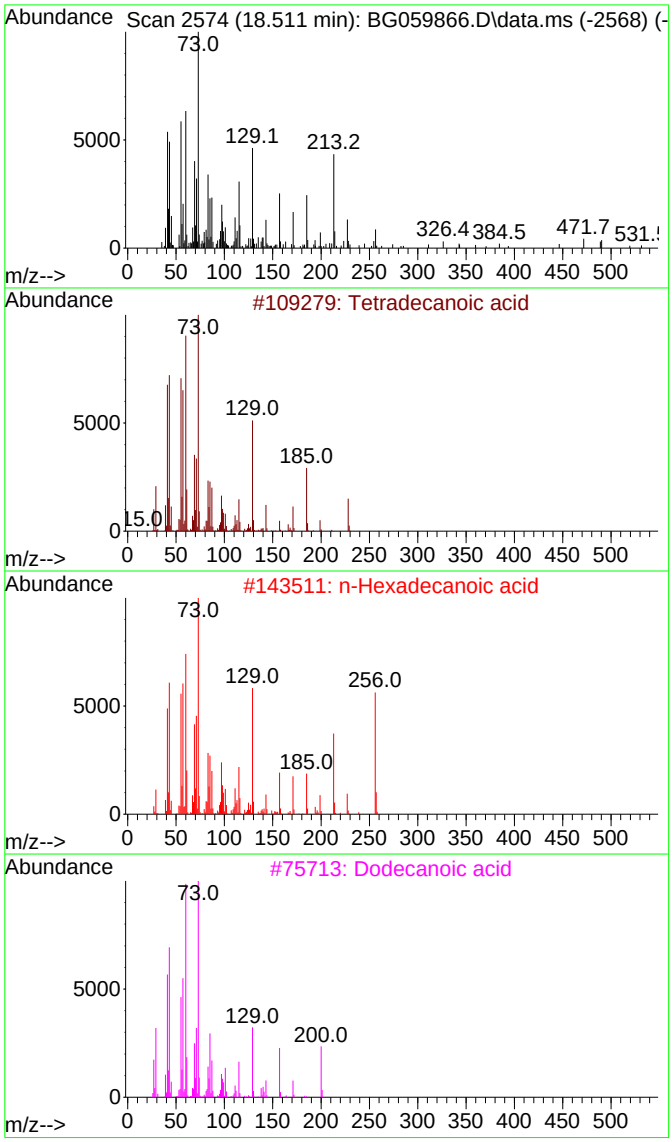
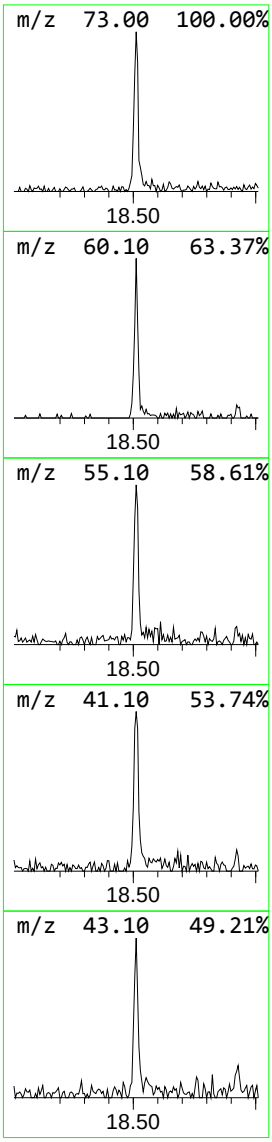
****

Peak Number 2 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	7.09 ng	262086	Phenanthrene-d10	17.700

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3	Dodecanoic acid	200	C12H24O2	000143-07-7	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	35
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	22





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Data File : BG059866.D
Acq On : 24 Nov 2023 20:23
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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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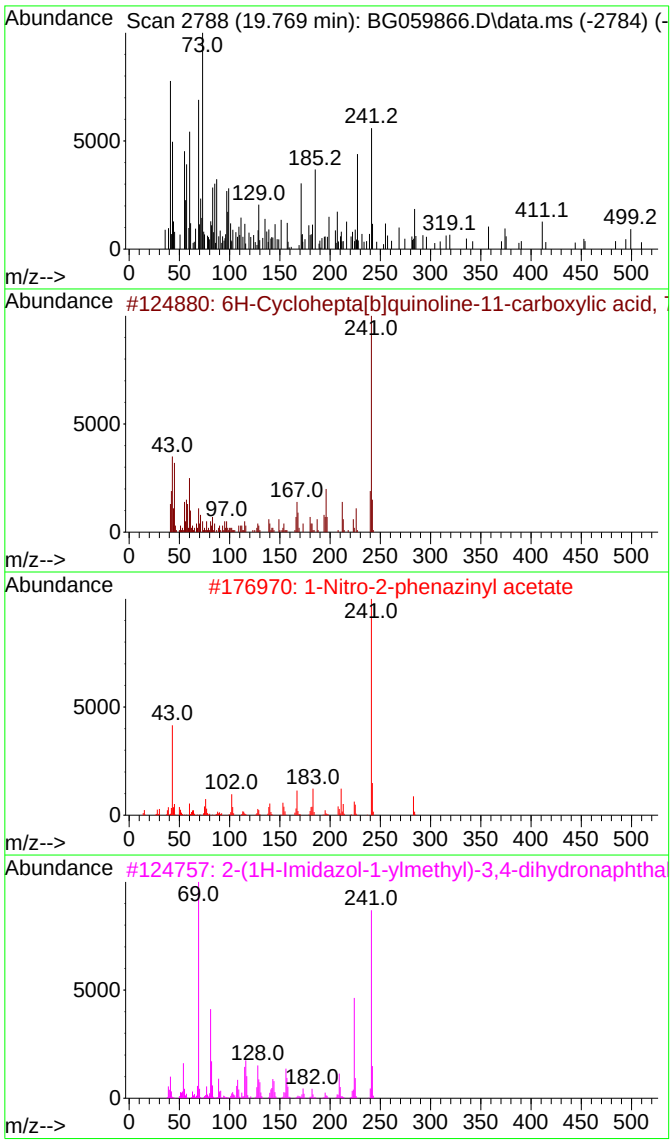
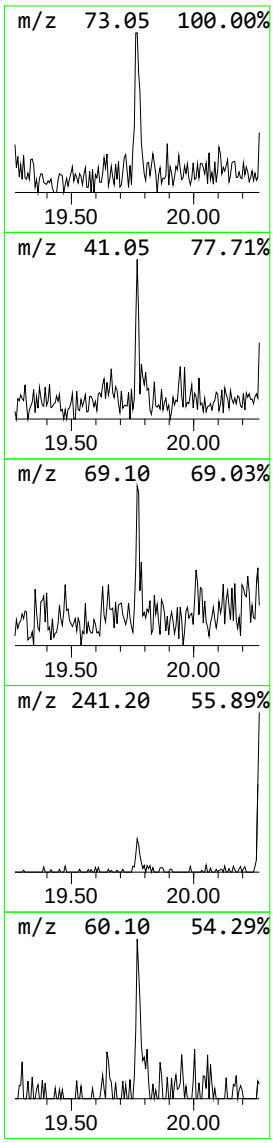
Peak Number 3 unknown19.769 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.769	2.17 ng	80062	Phenanthrene-d10	17.700

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclohepta[b]quinoline-11-car...	241	C15H15NO2	007101-63-5	14
2	1-Nitro-2-phenazinyl acetate	283	C14H9N3O4	1000240-03-2	11
3	2-(1H-Imidazol-1-ylmethyl)-3,4-d...	241	C14H15N3O	1000266-23-6	11
4	Mefenamic Acid	241	C15H15NO2	000061-68-7	11
5	1,3-benzoxathiol-2-one, 5-hydrox...	241	C9H7NO5S	1000396-51-3	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059866.D
Acq On : 24 Nov 2023 20:23
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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

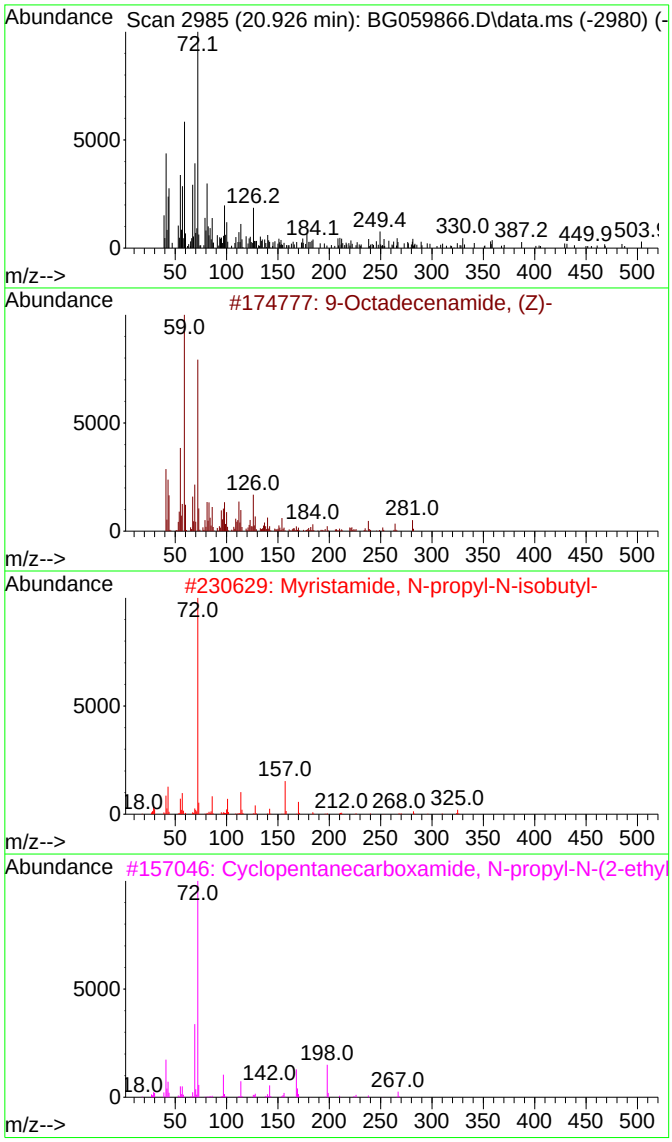
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

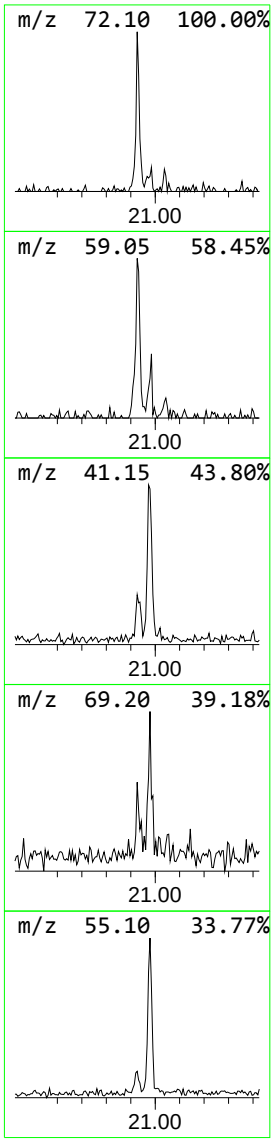
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.926	5.13 ng	171213	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	Myristamide, N-propyl-N-isobutyl-	325	C21H43NO	1000438-47-3	46
3	Cyclopentanecarboxamide, N-propy...	267	C17H33NO	1000437-86-5	46
4	Valeramide, 2-methyl-N-(2-pentyl...	213	C13H27NO	1010490-11-8	46
5	Palmitoleamide	253	C16H31NO	106010-22-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059866.D
Acq On : 24 Nov 2023 20:23
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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

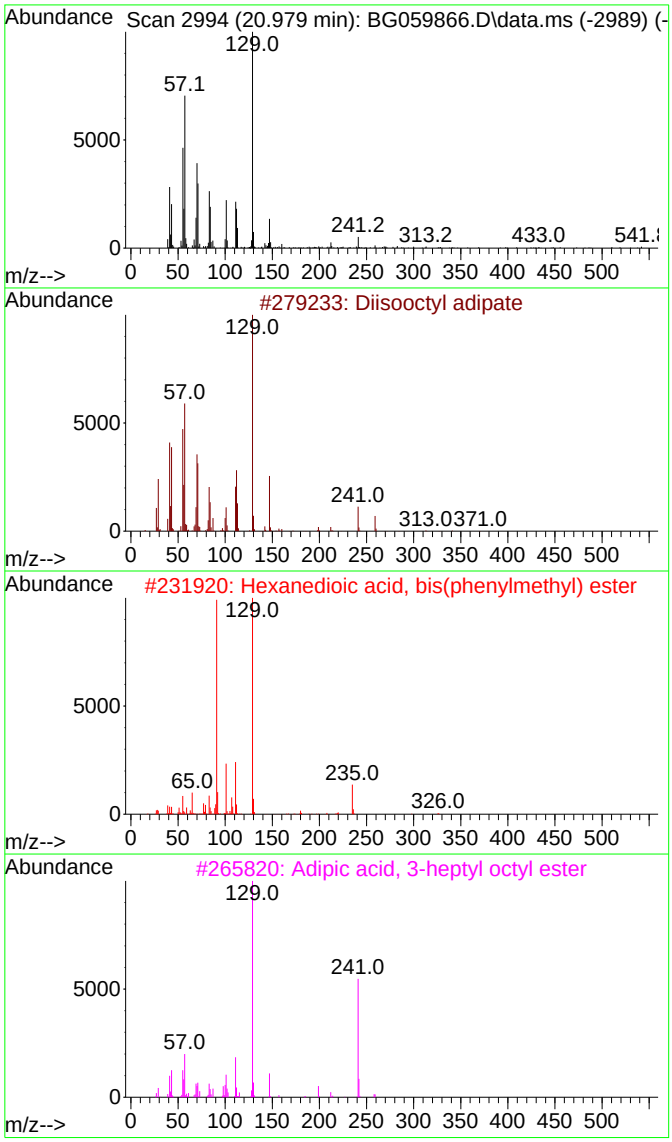
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

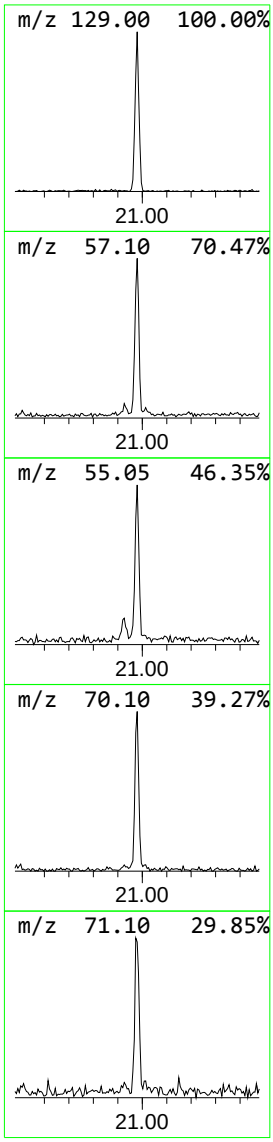
****

Peak Number 5 Diisooctyl adipate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.979	17.86 ng	595664	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	64
2	Hexanedioic acid, bis(phenylmeth...	326	C20H22O4	002451-84-5	47
3	Adipic acid, 3-heptyl octyl ester	356	C21H40O4	1000353-65-3	47
4	Adipic acid, cycloheptyl octyl e...	354	C21H38O4	1000324-72-1	47
5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	47





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Instrument :
BNA_G
ClientSampleId :
TP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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TIC Library : C:\Database\NIST20.L
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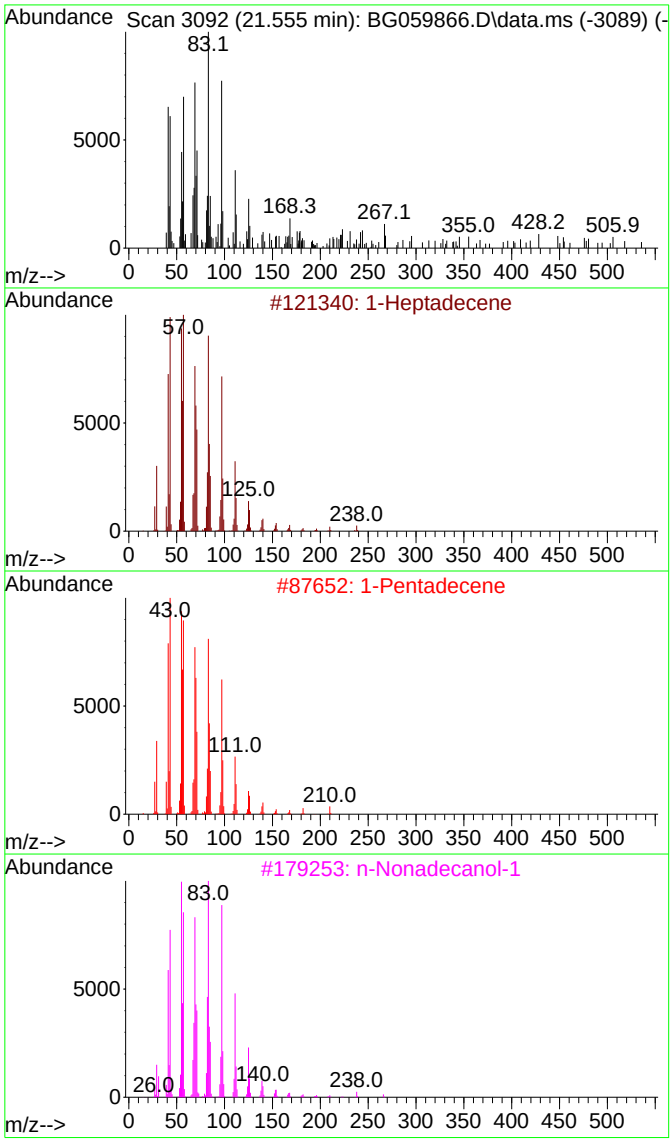
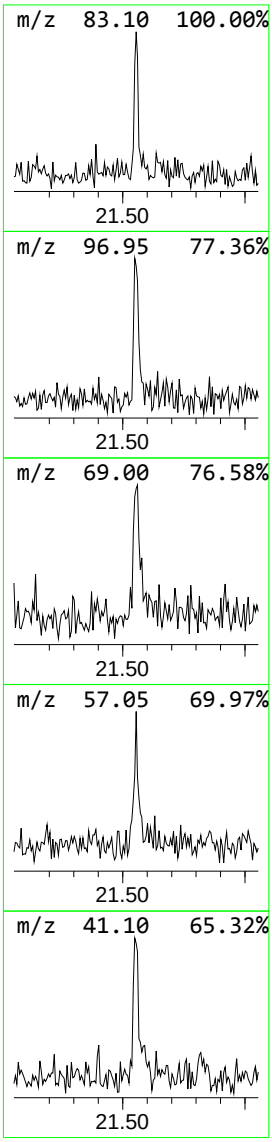
****

Peak Number 6 1-Heptadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	4.18 ng	139474	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	90
2	1-Pentadecene	210	C15H30	013360-61-7	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	86
4	1-Octadecanol	270	C18H38O	000112-92-5	86
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	78





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Operator : MA/JU
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Instrument :
BNA_G
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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
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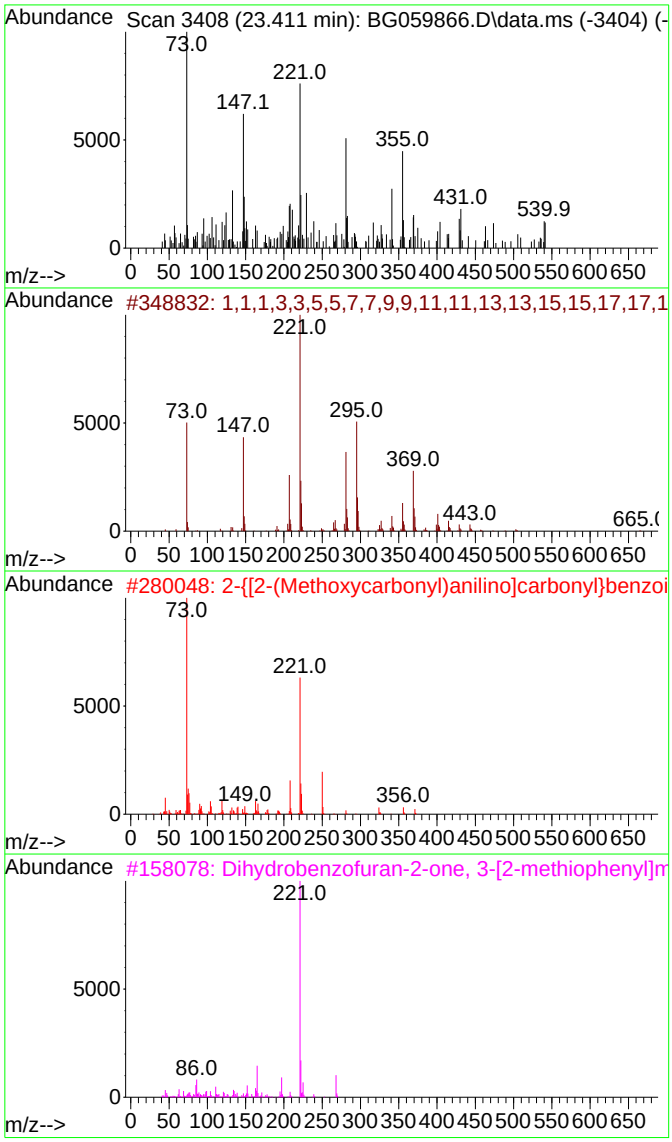
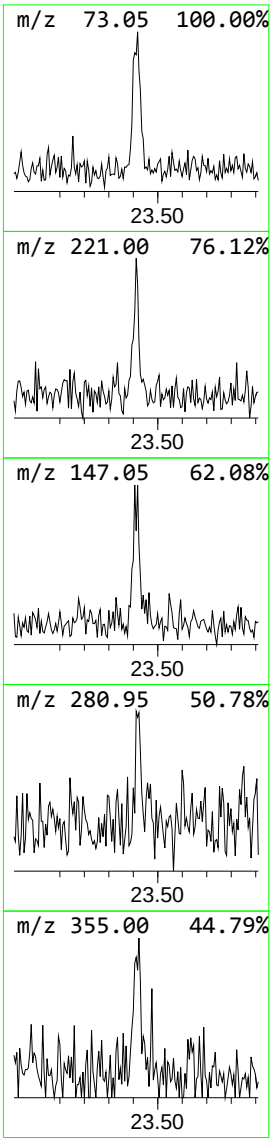
Peak Number 7 unknown23.411 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.411	2.19 ng	72879	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	38
2	2-{[2-(Methoxycarbonyl)anilino]c...	371	C19H21NO5Si	1000475-02-2	30
3	Dihydrobenzofuran-2-one, 3-[2-me...	268	C16H12O2S	1000132-67-5	27
4	Boric acid, 3TMS derivative	278	C9H27BO3Si3	004325-85-3	27
5	4-(m-Nitrophenyl)-2-thiazolamine	221	C9H7N3O2S	057493-24-0	27





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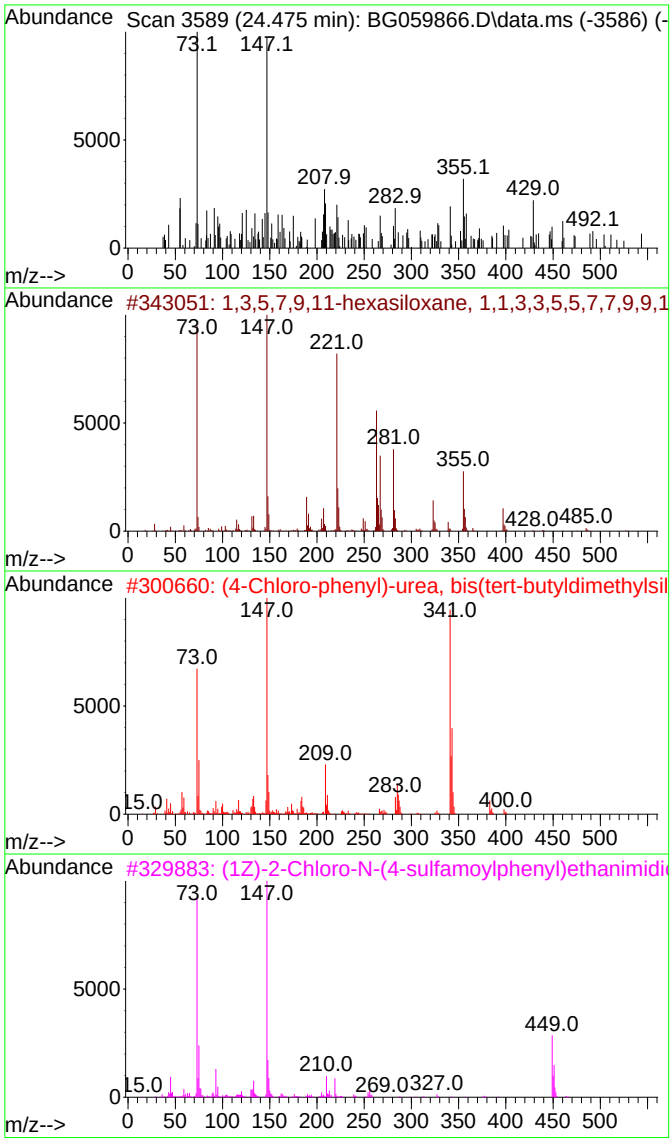
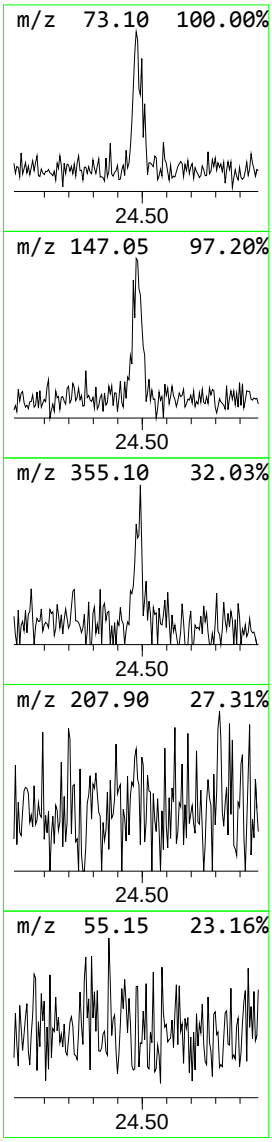
Peak Number 8 unknown24.475 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.475	2.73 ng	79506	Perylene-d12	25.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7,9,11-hexasiloxane, 1,1,3...	542	C20H54O5Si6	1000458-50-7	38
2	(4-Chloro-phenyl)-urea, bis(tert...	398	C19H35ClN2OSi2	1000385-82-2	37
3	(1Z)-2-Chloro-N-(4-sulfamoylphen...	464	C17H33ClN2O3SSi3	1000477-47-5	35
4	4-(3-Aminophenoxy)phthalic acid,...	489	C23H35NO5Si3	1000468-77-9	35
5	2-[(4-Chlorophenyl)acetyl]benzoi...	418	C21H27ClO3Si2	1000468-21-5	35





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
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
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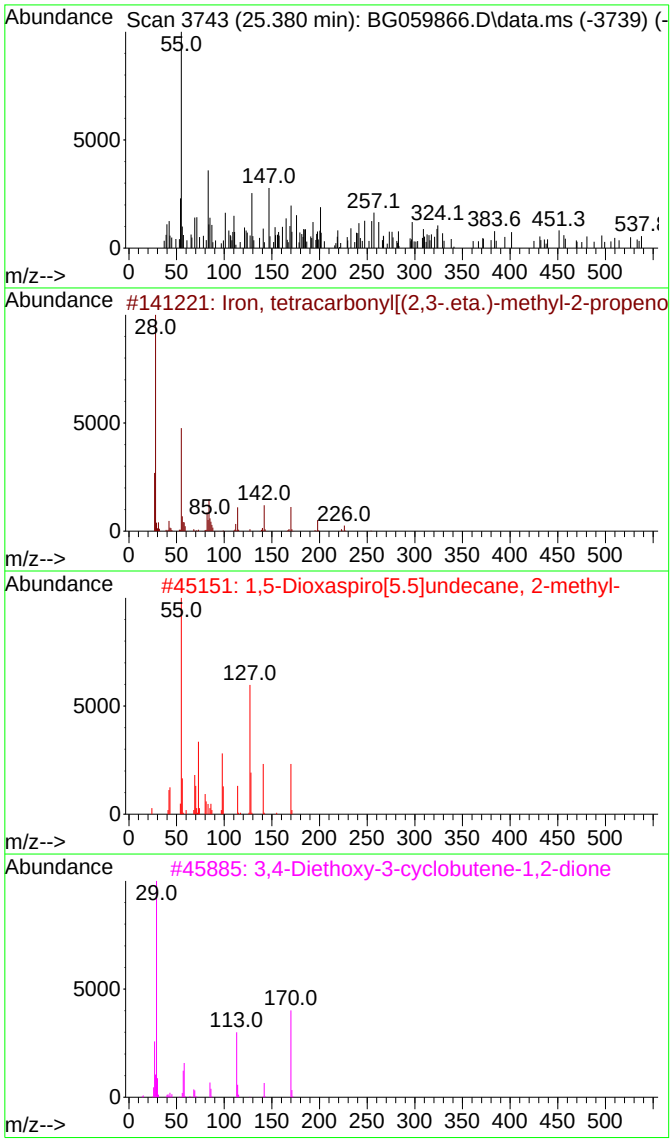
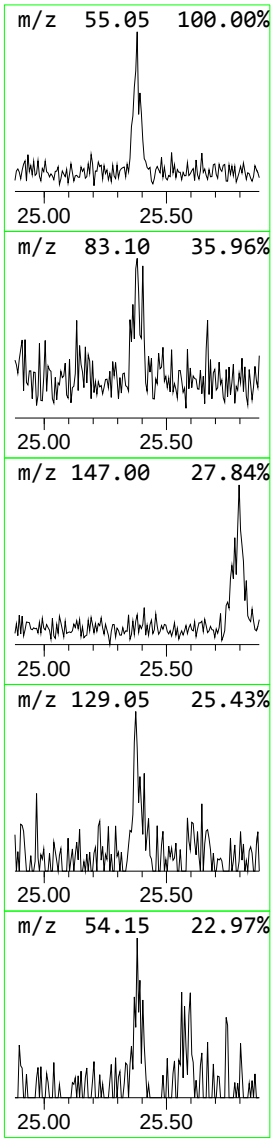
Peak Number 9 unknown25.380 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.380	3.43 ng	99836	Perylene-d12	25.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Iron, tetracarbonyl[(2,3-.eta.)-...	254	C8H6FeO6	012287-67-1	10
2	1,5-Dioxaspiro[5.5]undecane, 2-m...	170	C10H18O2	006413-26-9	9
3	3,4-Diethoxy-3-cyclobutene-1,2-d...	170	C8H10O4	005231-87-8	5
4	5-(2-Cyclopentylethyl)-1,3,4-thi...	225	C11H19N3S	1000511-74-1	4
5	1(4H)-Naphthalenone, 2-[(4-cyclo...	446	C30H42N2O	1000255-69-0	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059866.D
Acq On : 24 Nov 2023 20:23
Operator : MA/JU
Sample : 05469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.350	11.7	ng	116119	1	8.323	199172	20.0
Tetradecanoic acid	18.511	7.1	ng	262086	4	17.700	739285	20.0
unknown19.769	19.769	2.2	ng	80062	4	17.700	739285	20.0
9-Octadecenamid...	20.926	5.1	ng	171213	5	22.019	666984	20.0
Diisooctyl adipate	20.979	17.9	ng	595664	5	22.019	666984	20.0
1-Heptadecene	21.555	4.2	ng	139474	5	22.019	666984	20.0
unknown23.411	23.411	2.2	ng	72879	5	22.019	666984	20.0
unknown24.475	24.475	2.7	ng	79506	6	25.585	582112	20.0
unknown25.380	25.380	3.4	ng	99836	6	25.585	582112	20.0