LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053056.D
Acq On : 6 Apr 2022 15:50
Operator : CG/JU
Sample : N2269-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LP-2

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053056.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.690	386	392	401	rBV	363249	604515	19.21%	4.974%
2	7.288	654	664	671	rBV	312932	560796	17.82%	4.615%
3	8.128	800	807	813	rBV	122991	211285	6.71%	1.739%
4	9.285	996	1004	1013	rBV	439640	806522	25.63%	6.637%
5	9.849	1093	1100	1107	rVB2	39253	67035	2.13%	0.552%
6	10.243	1162	1167	1174	rVB5	25319	48381	1.54%	0.398%
7	10.484	1202	1208	1214	rBV2	21382	33895	1.08%	0.279%
8	10.936	1277	1285	1292	rBV	160241	296706	9.43%	2.441%
9	13.192	1664	1669	1675	rVB3	30908	47115	1.50%	0.388%
10	13.374	1692	1700	1707	rVB	1147066	1821424	57.87%	14.988%
11	14.748	1928	1934	1942	rVB	272482	432735	13.75%	3.561%
12	16.235	2179	2187	2195	rBV	1115106	1744928	55.44%	14.358%
13	17.492	2395	2401	2409	rVB	371650	563149	17.89%	4.634%
14	18.373	2546	2551	2559	rBV3	42711	77114	2.45%	0.635%
15	19.301	2704	2709	2712	rBV3	27270	33366	1.06%	0.275%
16	20.094	2838	2844	2850	rBV	2363898	3147345	100.00%	25.898%
17	21.398	3061	3066	3074	rBV2	102031	154710	4.92%	1.273%
18	21.645	3103	3108	3115	rVB7	46124	82638	2.63%	0.680%
19	21.774	3124	3130	3137	rVB	349483	579590	18.42%	4.769%
20	22.720	3286	3291	3297	rBV2	49919	97015	3.08%	0.798%
21	25.082	3683	3693	3704	rVB3	204379	616349	19.58%	5.072%
22	26.051	3850	3858	3865	rBV3	45057	126014	4.00%	1.037%

Sum of corrected areas: 12152627

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
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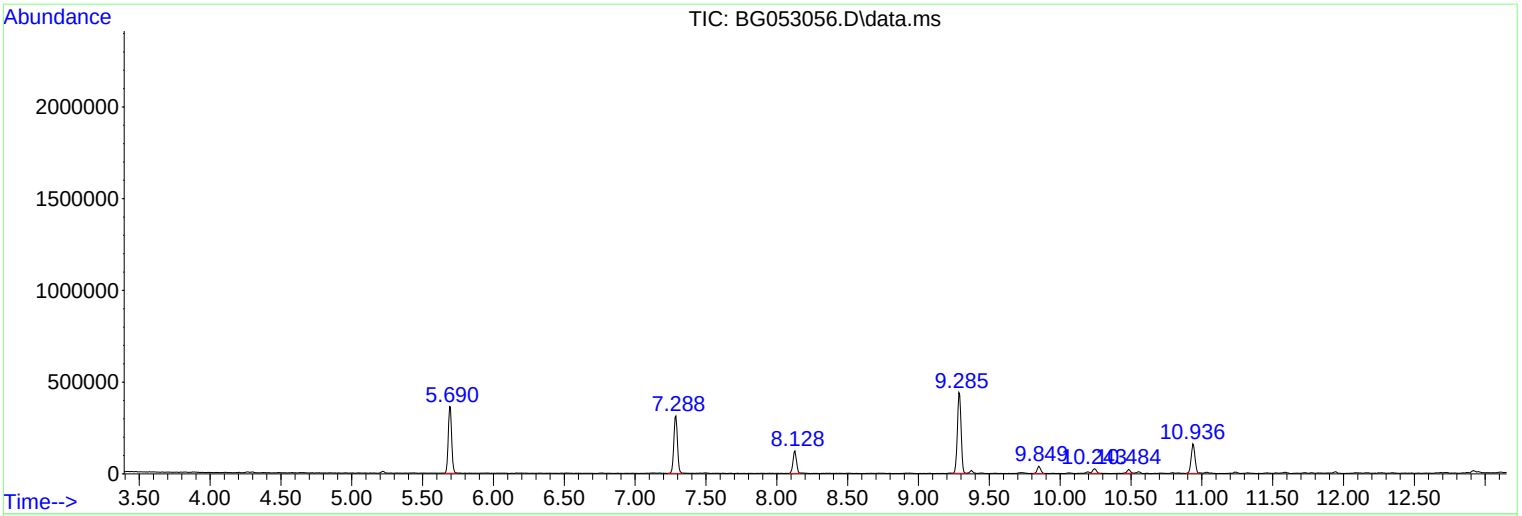
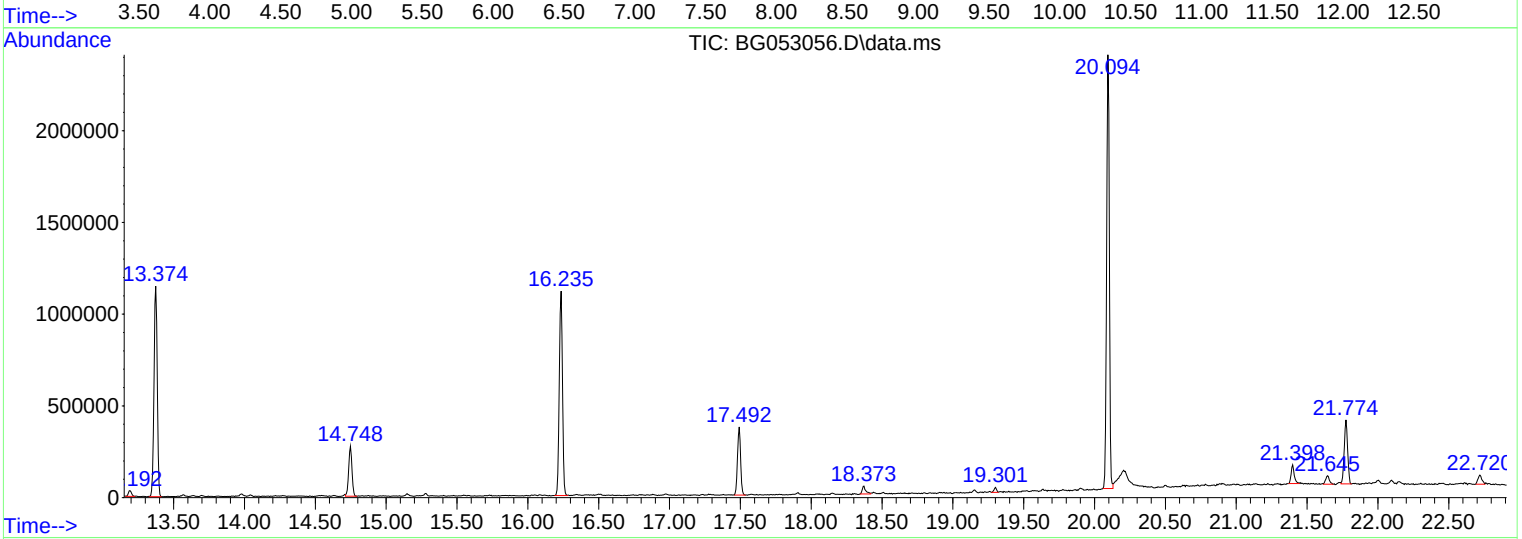
Misc :
ALS Vial : 6 Sample Multiplier: 1

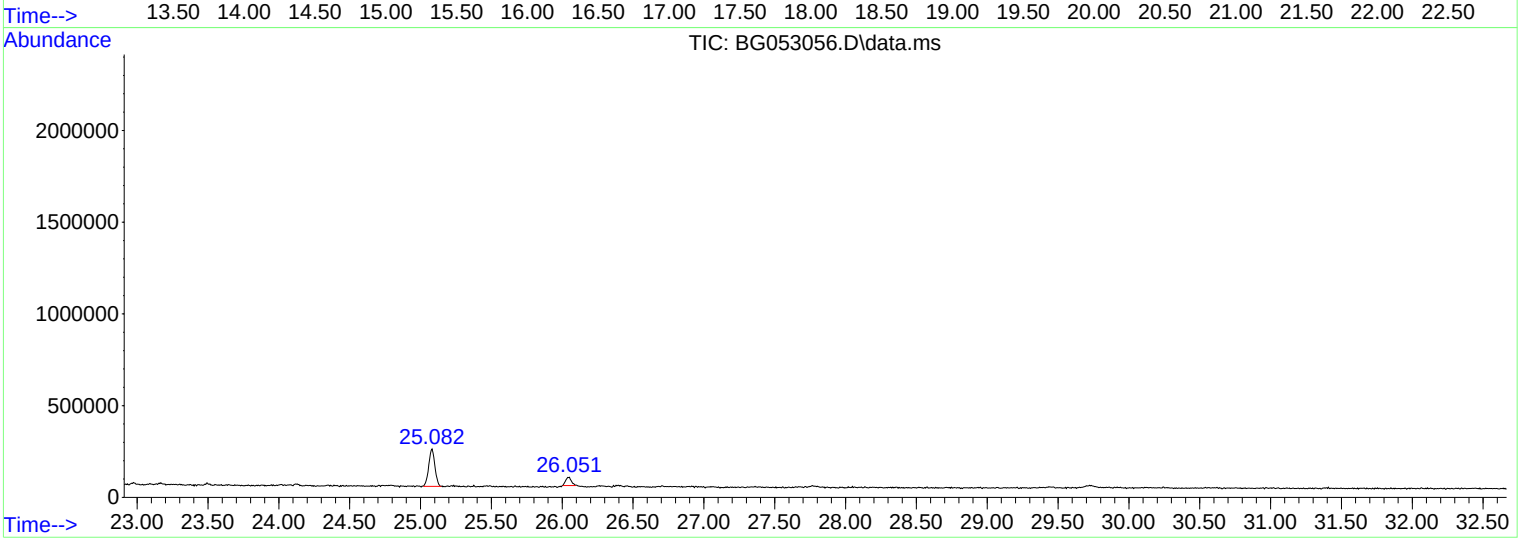
Instrument :
BNA_G
ClientSampleId :
LP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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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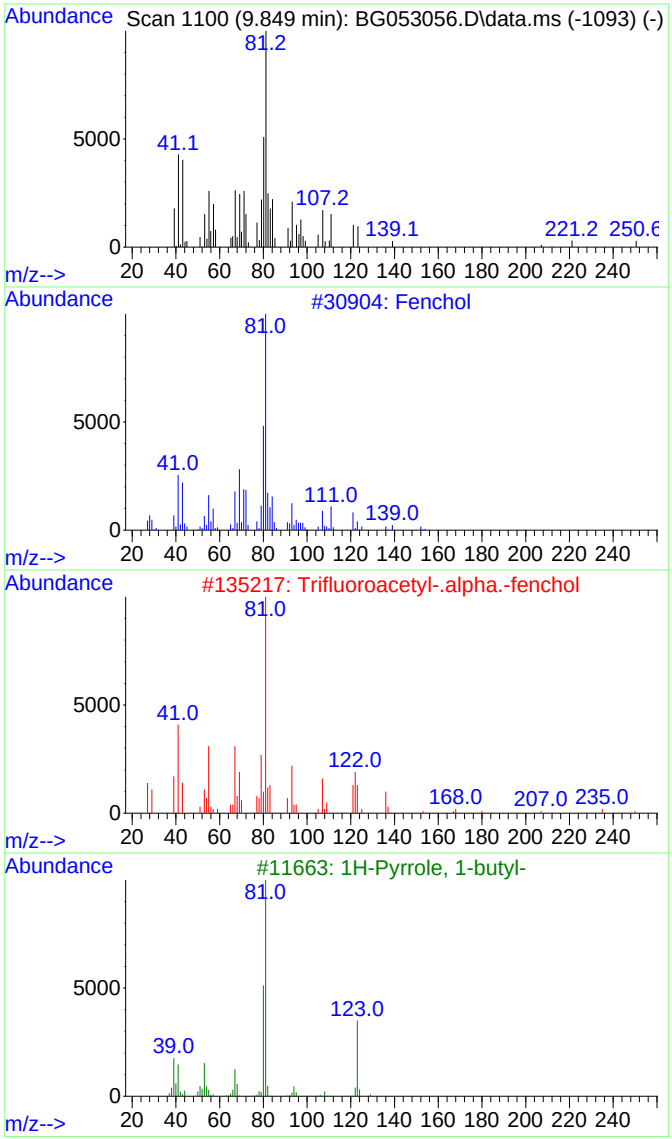
TIC Integration Parameters: LSCINT.P

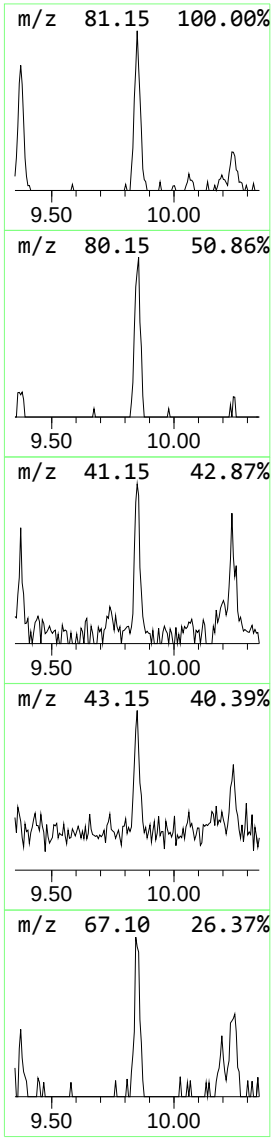
****

Peak Number 1 Fenchol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.849	4.52 ng	67035	Naphthalene-d8	10.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchol	154	C10H18O	001632-73-1	90
2	Trifluoroacetyl-.alpha.-fenchol	250	C12H17F3O2	031076-73-0	47
3	1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	47
4	Oct-3-enoic acid, 2-methyloct-5-...	264	C17H28O2	1000406-95-1	47
5	Bi-2-cyclohexen-1-yl	162	C12H18	001541-20-4	43





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Operator : CG/JU
Sample : N2269-03
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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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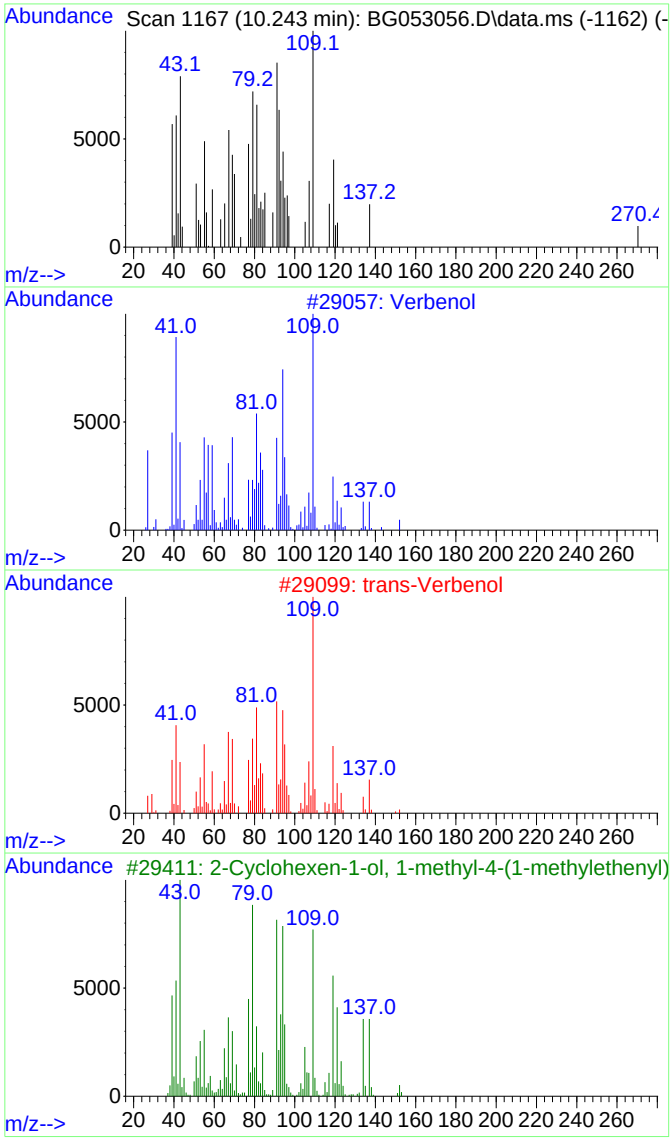
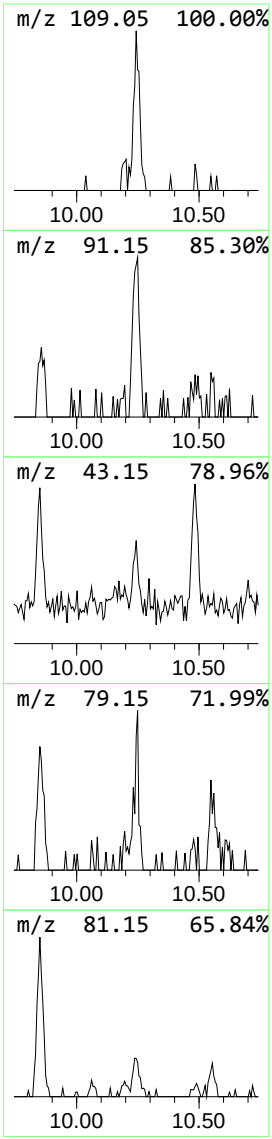
Peak Number 2 unknown11.243 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.243	3.26 ng	48381	Naphthalene-d8	10.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Verbenol	152	C10H16O	000473-67-6	47
2	trans-Verbenol	152	C10H16O	001820-09-3	38
3	2-Cyclohexen-1-ol, 1-methyl-4-(1...	152	C10H16O	007212-40-0	37
4	(3E,5E)-2,6-Dimethylocta-3,5,7-t...	152	C10H16O	206115-88-0	16
5	4-Bromo-7-methylenebicyclo[4.2.0...	198	C9H11Br	1000211-10-2	14





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Data File : BG053056.D
Acq On : 6 Apr 2022 15:50
Operator : CG/JU
Sample : N2269-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
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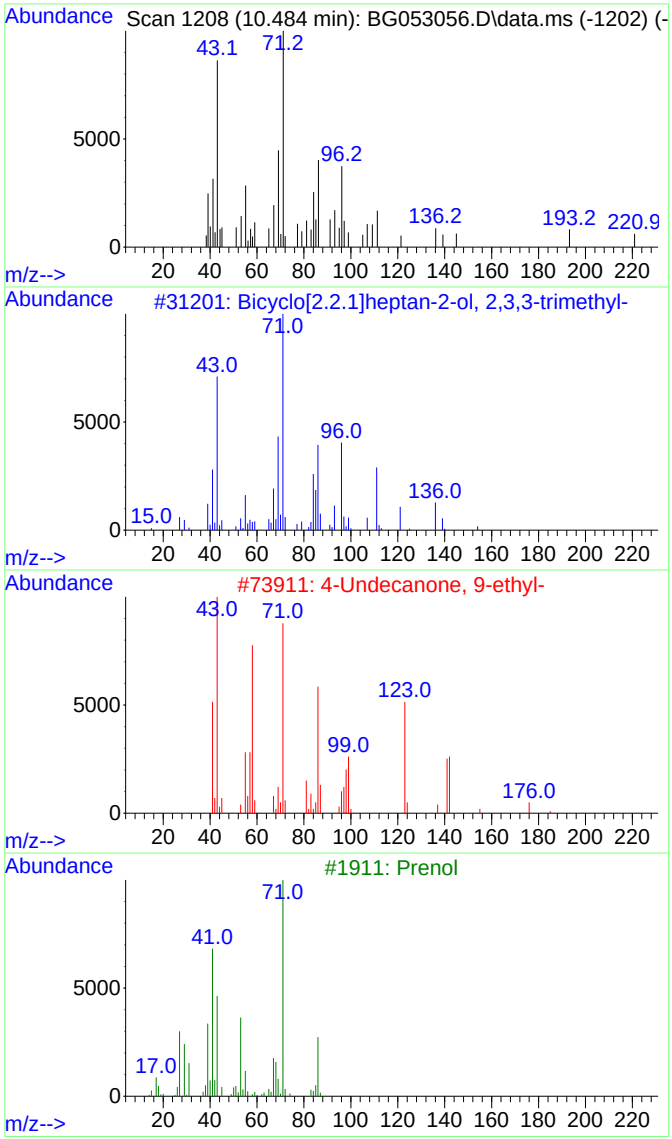
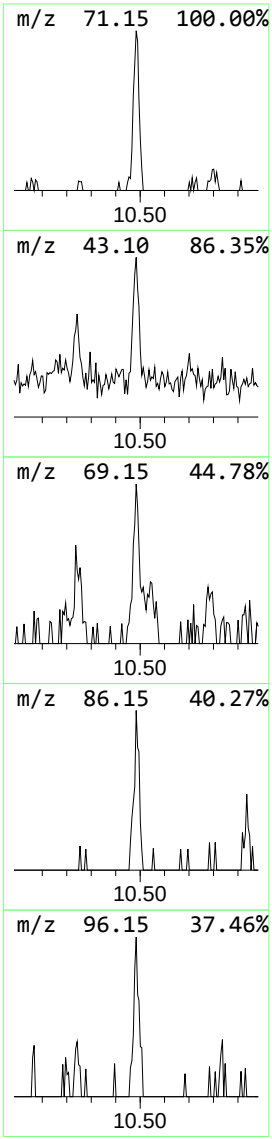
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.484	2.28 ng	33895	Naphthalene-d8	10.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	78
2	4-Undecanone, 9-ethyl-	198	C13H26O	054549-96-1	47
3	Prenol	86	C5H10O	000556-82-1	47
4	Acetic acid, (1,2-dimethyl-1-pro...	128	C7H12O2	003814-41-3	43
5	1-Propene, 1-methoxy-2-methyl-	86	C5H10O	017574-84-4	43





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Operator : CG/JU
Sample : N2269-03
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

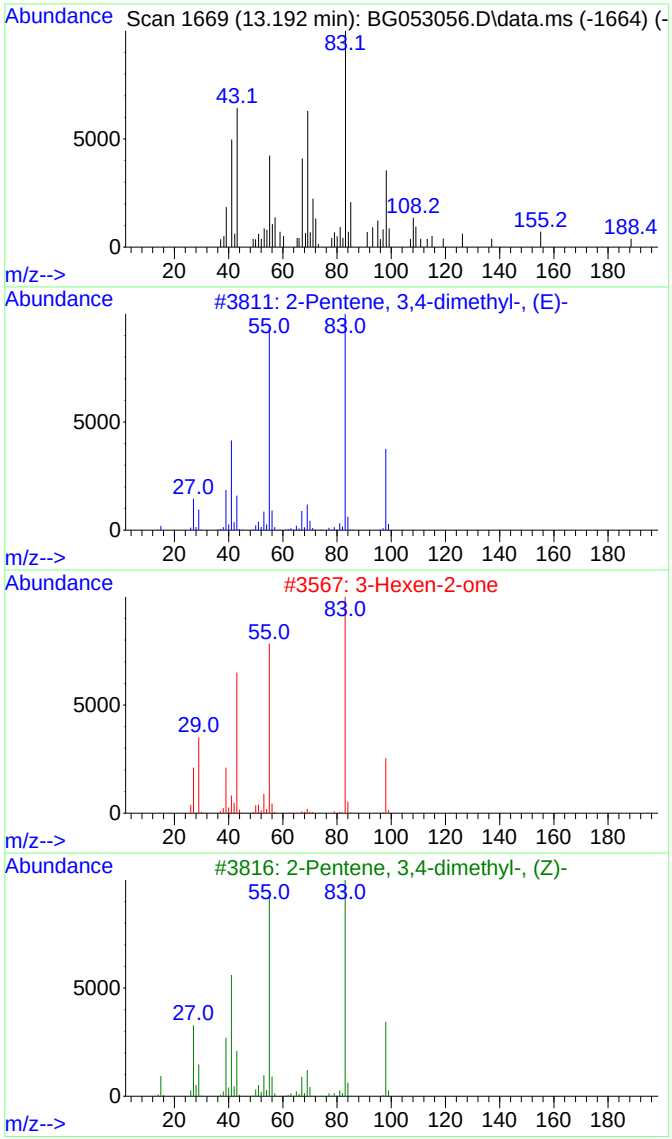
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

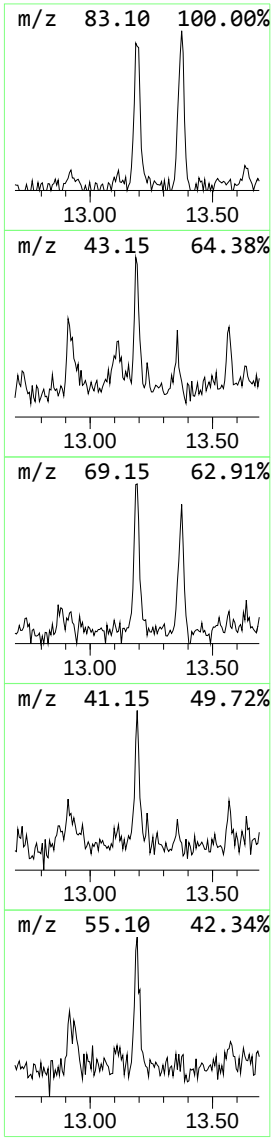
****

Peak Number 4 unknown13.192 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	2.18 ng	47115	Acenaphthene-d10	14.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	38
2	3-Hexen-2-one	98	C6H10O	000763-93-9	38
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	38
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	38
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	38





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Operator : CG/JU
Sample : N2269-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

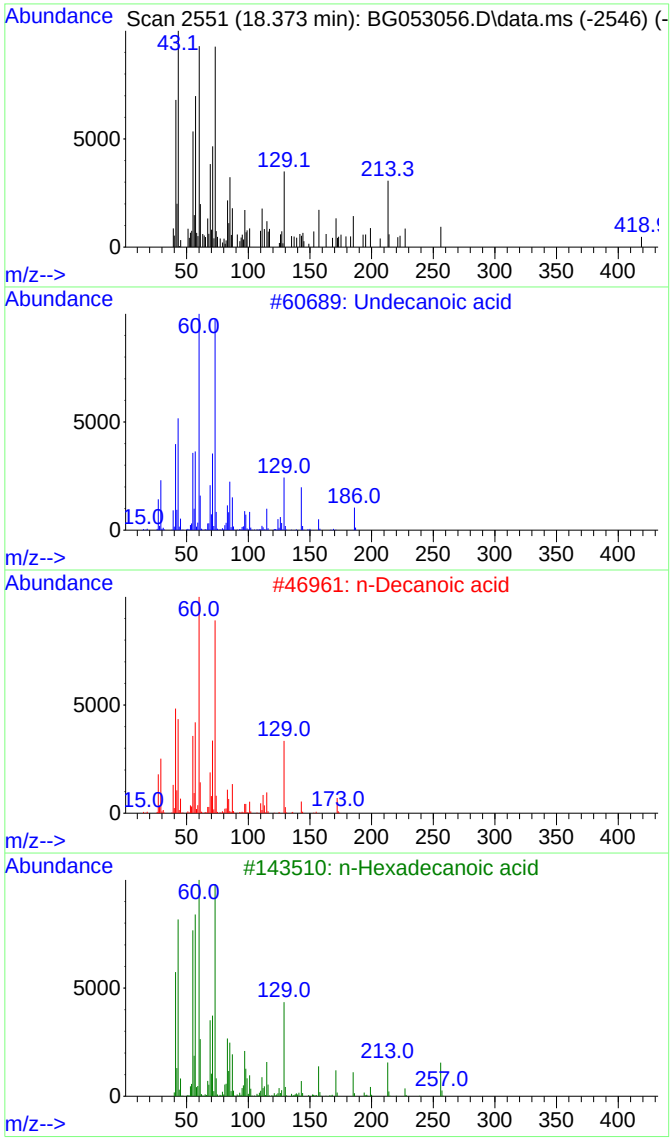
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

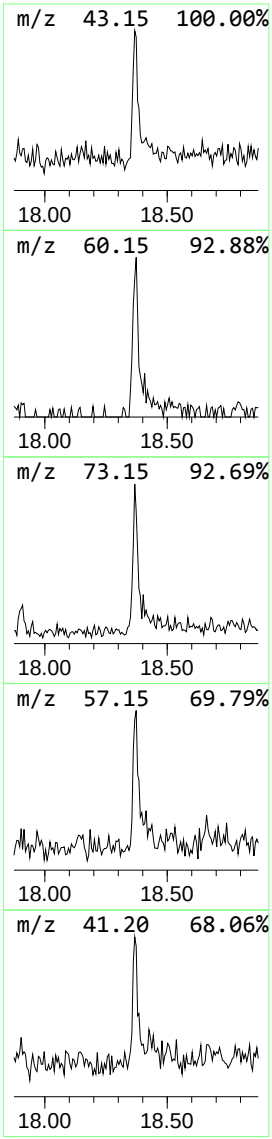
****

Peak Number 5 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	2.74 ng	77114	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	70
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
4	Tridecanoic acid	214	C13H26O2	000638-53-9	30
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25





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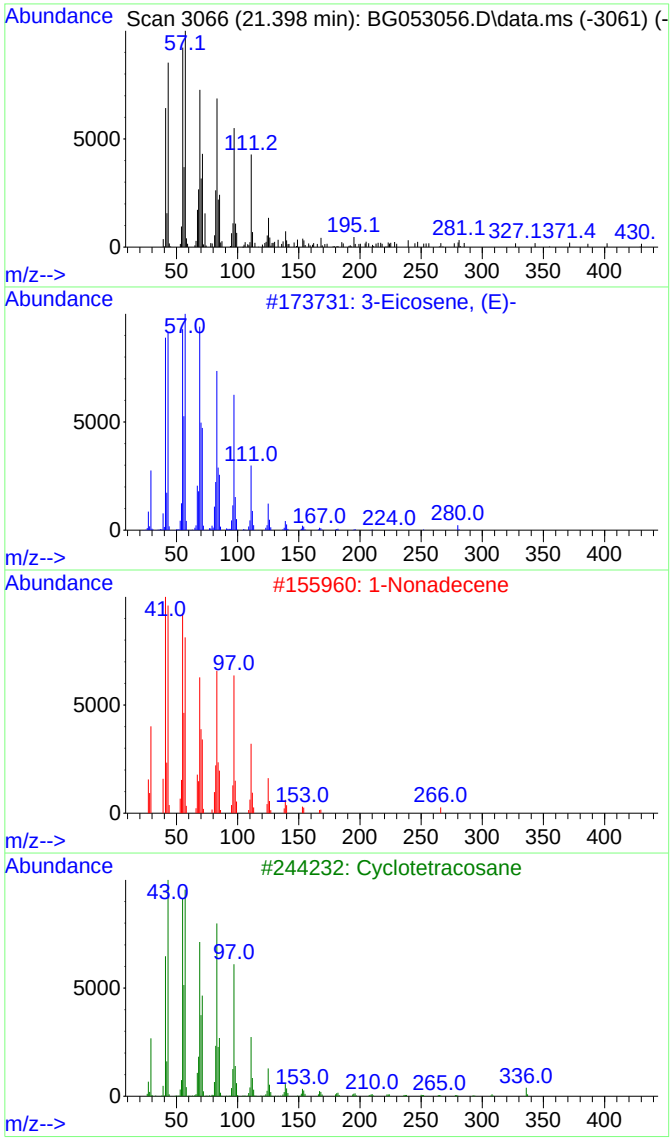
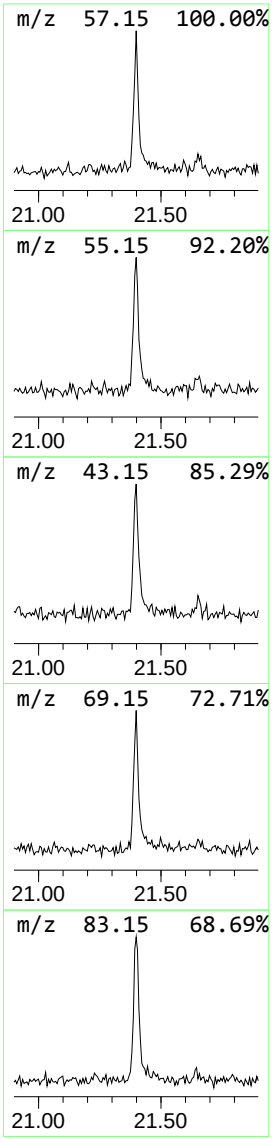
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	5.34 ng	154710	Chrysene-d12	21.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	1-Nonadecene	266	C19H38	018435-45-5	96
3	Cyclotetracosane	336	C24H48	000297-03-0	93
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	92
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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TIC Library : C:\Database\NIST20.L
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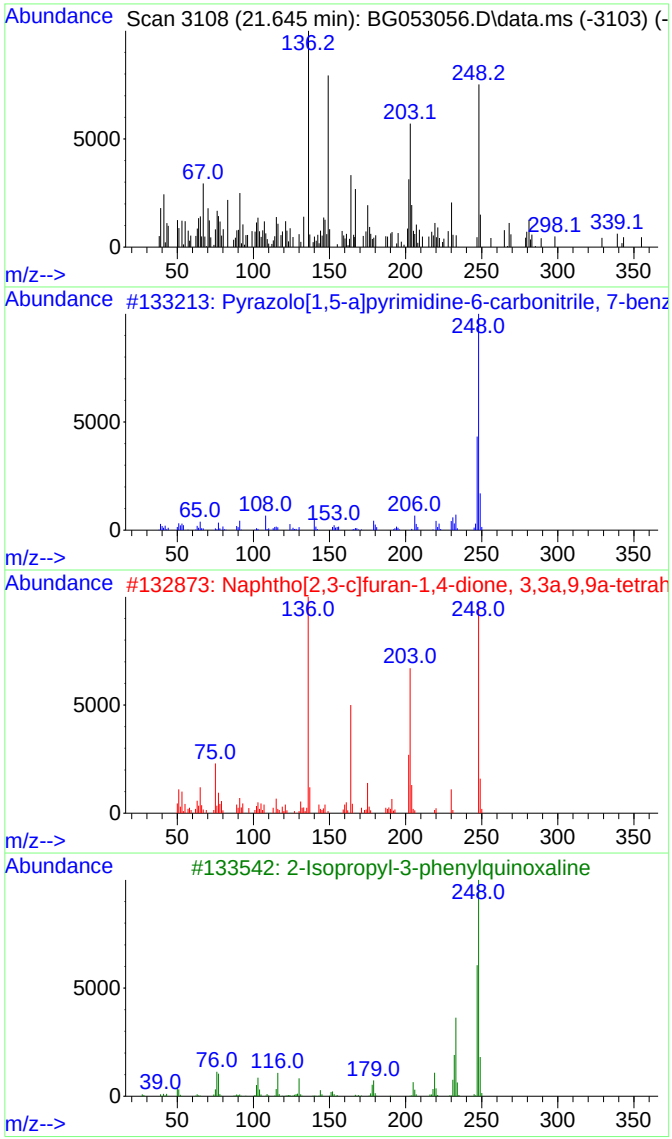
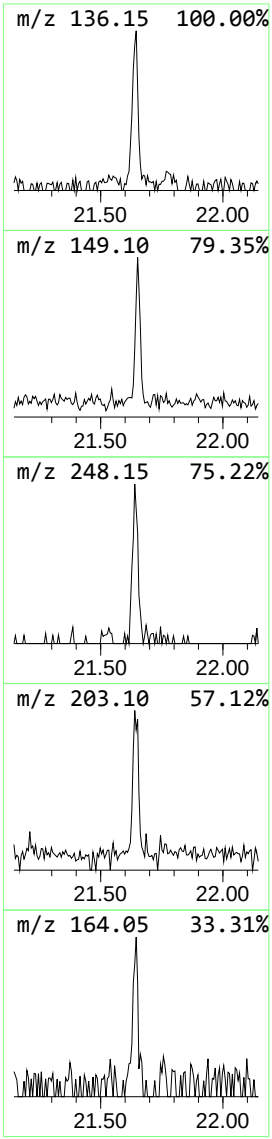
Peak Number 7 unknown21.645 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.645	2.85 ng	82638	Chrysene-d12	21.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[1,5-a]pyrimidine-6-carb...	248	C15H12N4	250646-38-9	44
2	Naphtho[2,3-c]furan-1,4-dione, 3...	248	C13H12O5	027828-86-0	43
3	2-Isopropyl-3-phenylquinoxaline	248	C17H16N2	010130-27-5	25
4	[4-(Difluoromethoxy)-3-methoxyph...	203	C9H11F2NO2	847744-28-9	25
5	2-Methyl-1H-phenanthro[3,4-d)imi...	248	C16H12N2O	098033-26-2	20





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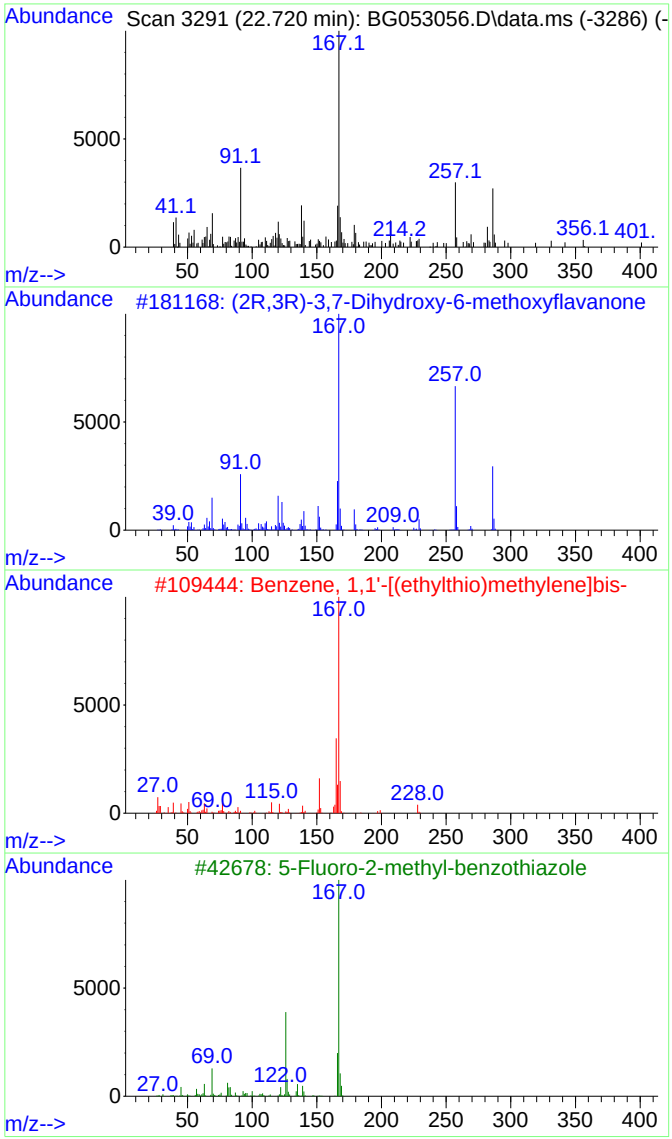
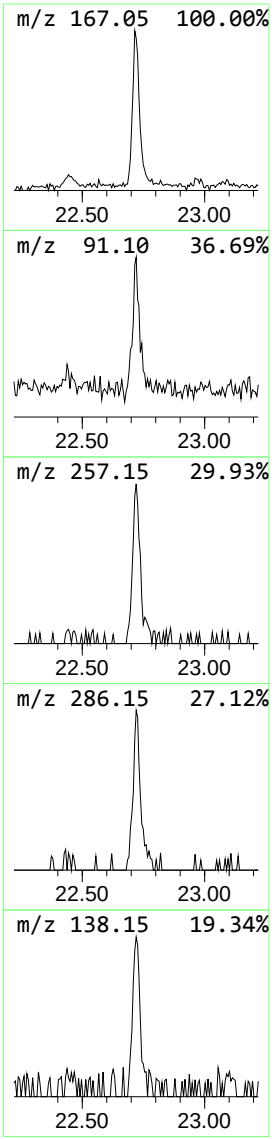
****
Peak Number 8 (2R,3R)-3,7-Dihydroxy-6-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.720	3.35 ng	97015	Chrysene-d12	21.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2R,3R)-3,7-Dihydroxy-6-methoxyf...	286	C16H14O5	034050-66-3	58
2	Benzene, 1,1'-[(ethylthio)methyl...	228	C15H16S	038793-64-5	50
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	50
4	Carbazole	167	C12H9N	000086-74-8	49
5	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	45





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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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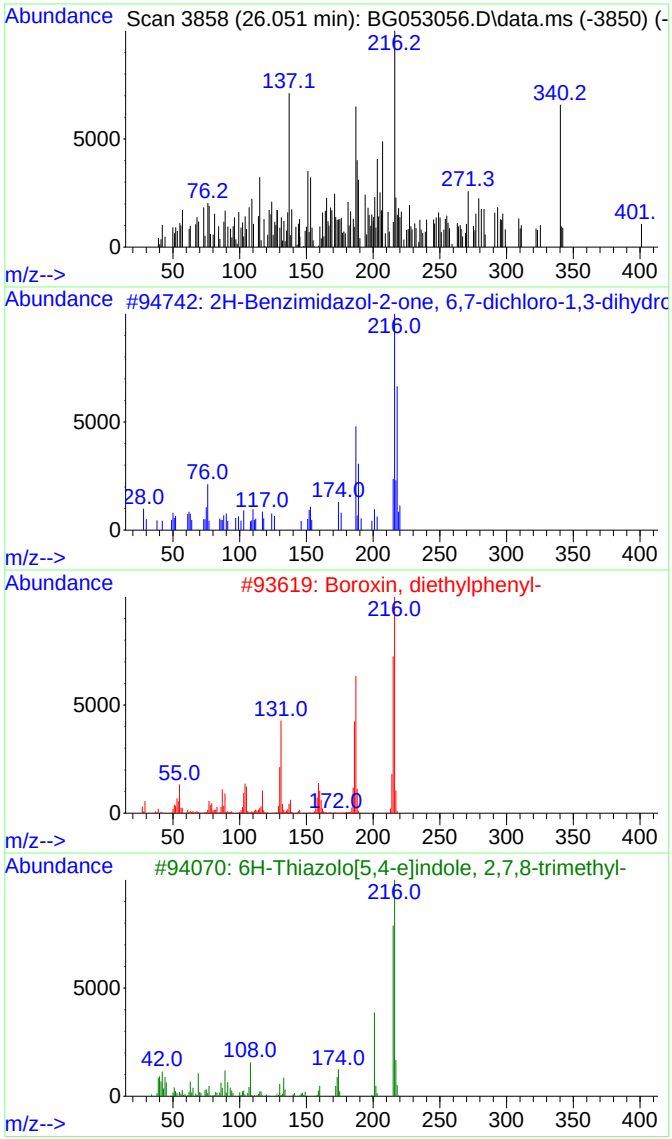
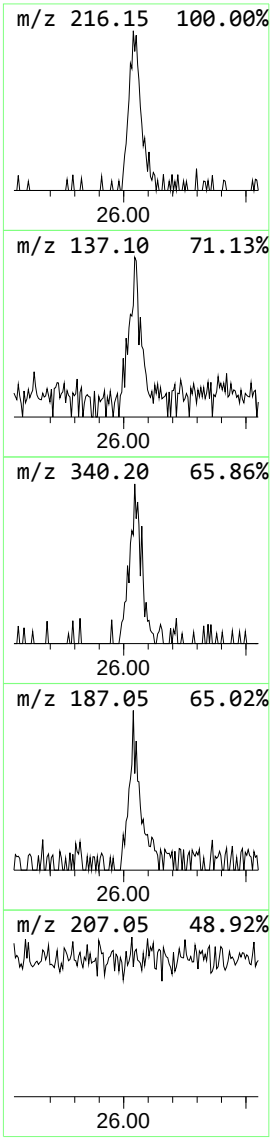
Peak Number 9 unknown26.051 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.051	4.09 ng	126014	Perylene-d12	25.082

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Benzimidazol-2-one, 6,7-dichl...	216	C8H6Cl2N2O	077572-79-3	38
2	Boroxin, diethylphenyl-	216	C10H15B3O3	1000151-81-1	25
3	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	25
4	Thianthrene	216	C12H8S2	000092-85-3	25
5	Dibenzothiophene sulfone	216	C12H8O2S	001016-05-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053056.D
Acq On : 6 Apr 2022 15:50
Operator : CG/JU
Sample : N2269-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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
Fenchol	9.849	4.5	ng	67035	2	10.936	296706	20.0
unknown11.243	10.243	3.3	ng	48381	2	10.936	296706	20.0
Bicyclo[2.2.1]h...	10.484	2.3	ng	33895	2	10.936	296706	20.0
unknown13.192	13.192	2.2	ng	47115	3	14.749	432735	20.0
Undecanoic acid	18.373	2.7	ng	77114	4	17.492	563149	20.0
3-Eicosene, (E)-	21.398	5.3	ng	154710	5	21.774	579590	20.0
unknown21.645	21.645	2.9	ng	82638	5	21.774	579590	20.0
(2R,3R)-3,7-Dih...	22.720	3.4	ng	97015	5	21.774	579590	20.0
unknown26.051	26.051	4.1	ng	126014	6	25.082	616349	20.0