LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055699.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.301	336	342	352	rVB	101770	155546	4.23%	0.776%
2	5.777	414	423	433	rBV	527688	867668	23.62%	4.329%
3	7.392	690	698	712	rVB	540248	928470	25.28%	4.633%
4	8.250	837	844	850	rBV	144554	251096	6.84%	1.253%
5	9.419	1035	1043	1054	rBV	334431	595120	16.20%	2.969%
6	11.076	1318	1325	1332	rBV	215794	384603	10.47%	1.919%
7	13.497	1728	1737	1744	rBV	950847	1468464	39.98%	7.327%
8	14.872	1964	1971	1977	rBV	358008	578689	15.75%	2.887%
9	15.847	2133	2137	2143	rBV	27287	42512	1.16%	0.212%
10	16.352	2216	2223	2230	rBV	784949	1181479	32.16%	5.895%
11	16.582	2258	2262	2267	rVB	55966	82326	2.24%	0.411%
12	16.676	2274	2278	2282	rBV	26904	44333	1.21%	0.221%
13	16.793	2294	2298	2301	rBV	52981	72280	1.97%	0.361%
14	16.840	2302	2306	2311	rVB2	76791	108210	2.95%	0.540%
15	16.940	2320	2323	2326	rVB	52194	65702	1.79%	0.328%
16	16.993	2326	2332	2339	rVB5	114008	252719	6.88%	1.261%
17	17.058	2339	2343	2347	rBV2	37902	57107	1.55%	0.285%
18	17.134	2352	2356	2361	rVB	55698	74602	2.03%	0.372%
19	17.610	2431	2437	2442	rBV	421004	671980	18.29%	3.353%
20	17.651	2442	2444	2450	rVB2	87195	138940	3.78%	0.693%
21	18.479	2579	2585	2592	rBV	921547	1438360	39.16%	7.177%
22	19.649	2781	2784	2791	rVB	235892	344999	9.39%	1.721%
23	19.748	2795	2801	2814	rBV	2118150	3673215	100.00%	18.328%
24	20.013	2843	2846	2853	rVB	245553	337961	9.20%	1.686%
25	20.201	2873	2878	2886	rBV	1400027	1841956	50.15%	9.190%
26	21.511	3098	3101	3109	rVB	207632	325053	8.85%	1.622%
27	21.770	3141	3145	3152	rVB	390005	559370	15.23%	2.791%
28	21.911	3165	3169	3175	rVB	353751	611364	16.64%	3.050%
29	25.330	3745	3751	3760	rVB	240919	662636	18.04%	3.306%
30	27.204	4062	4070	4082	rBV5	281993	1192785	32.47%	5.951%
31	29.490	4450	4459	4460	rBV2	454192	1032499	28.11%	5.152%

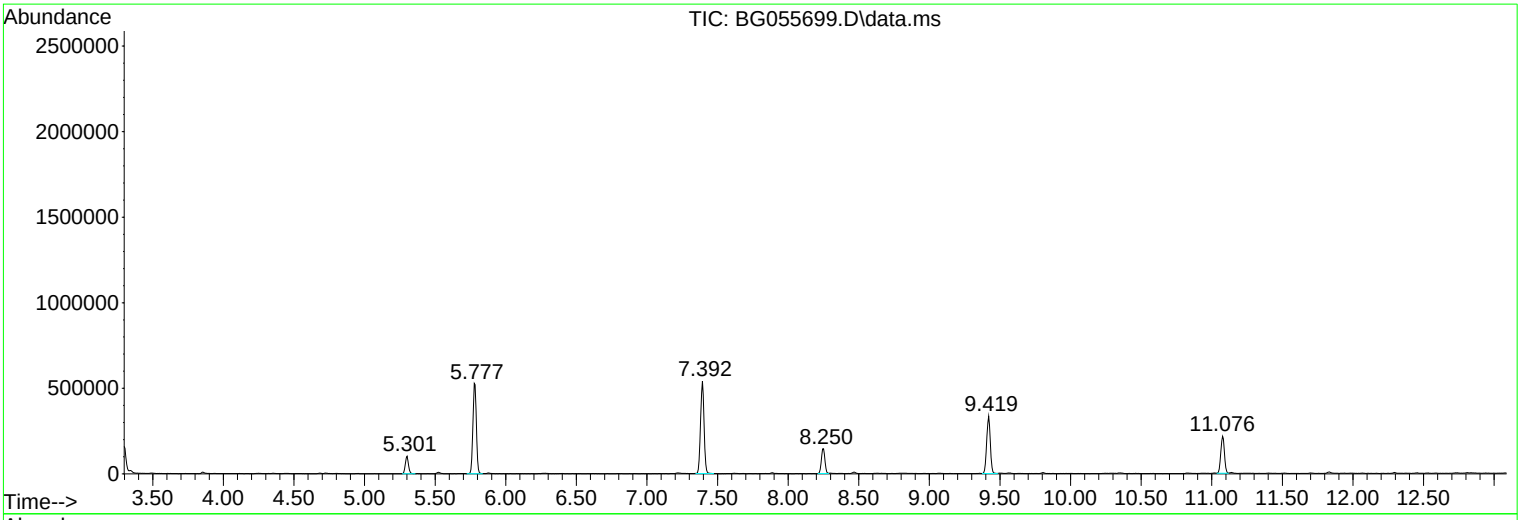
Sum of corrected areas: 20042044

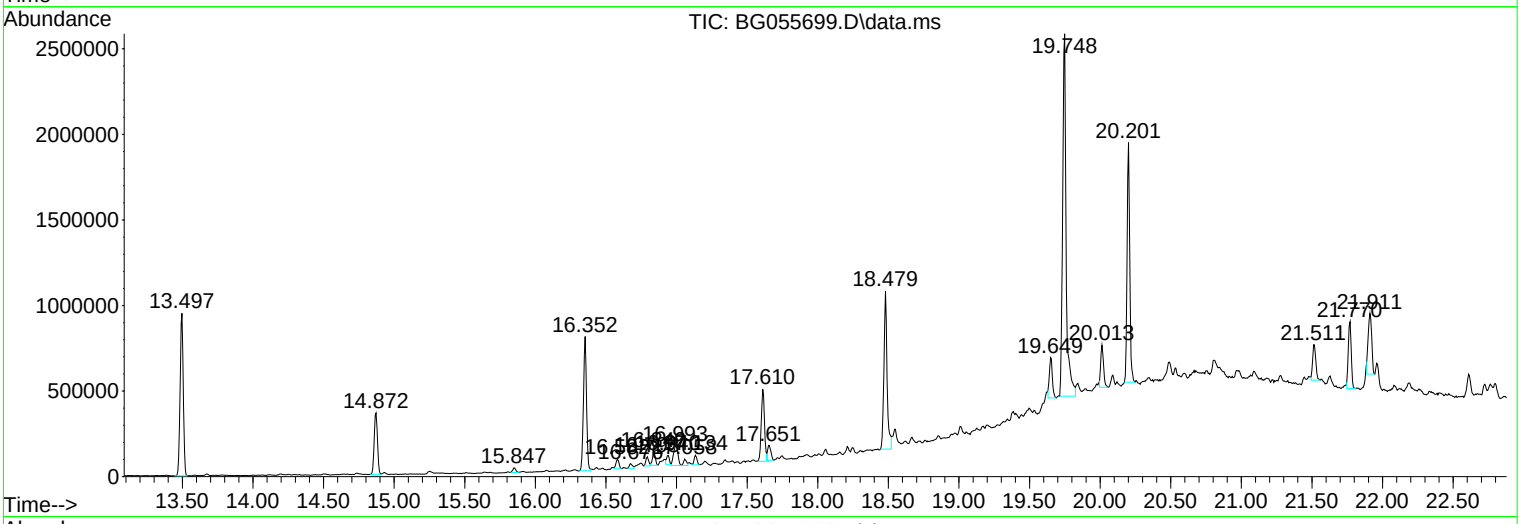
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

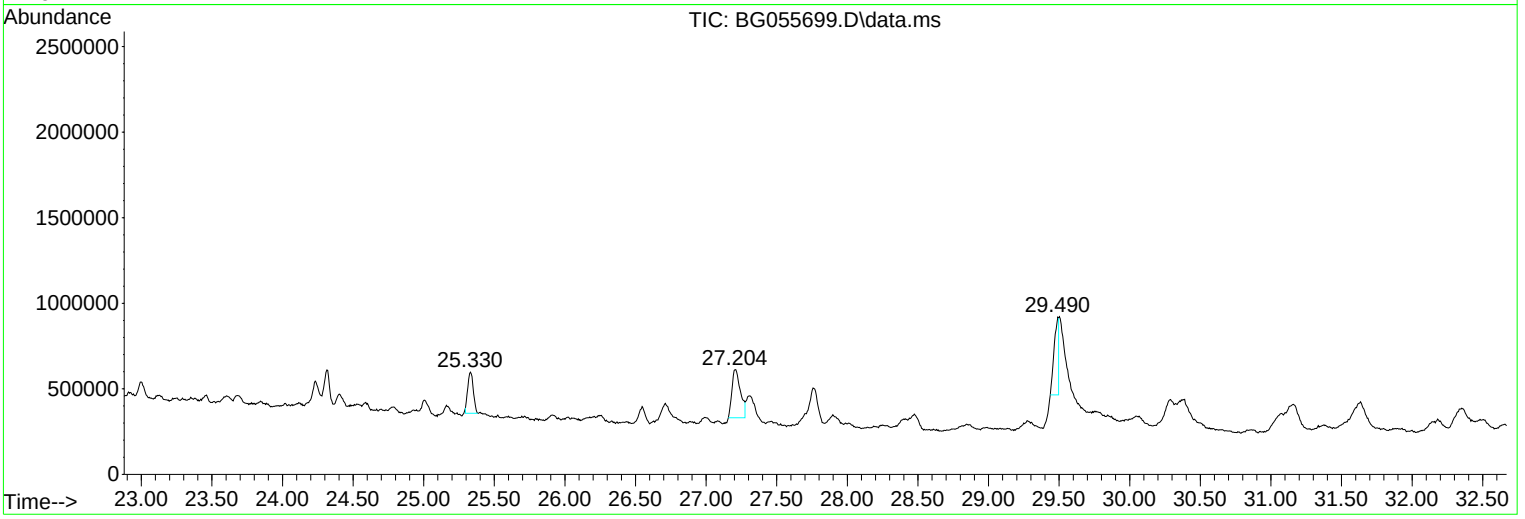
Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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Data File : BG055699.D
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TIC Library : C:\Database\NIST20.L
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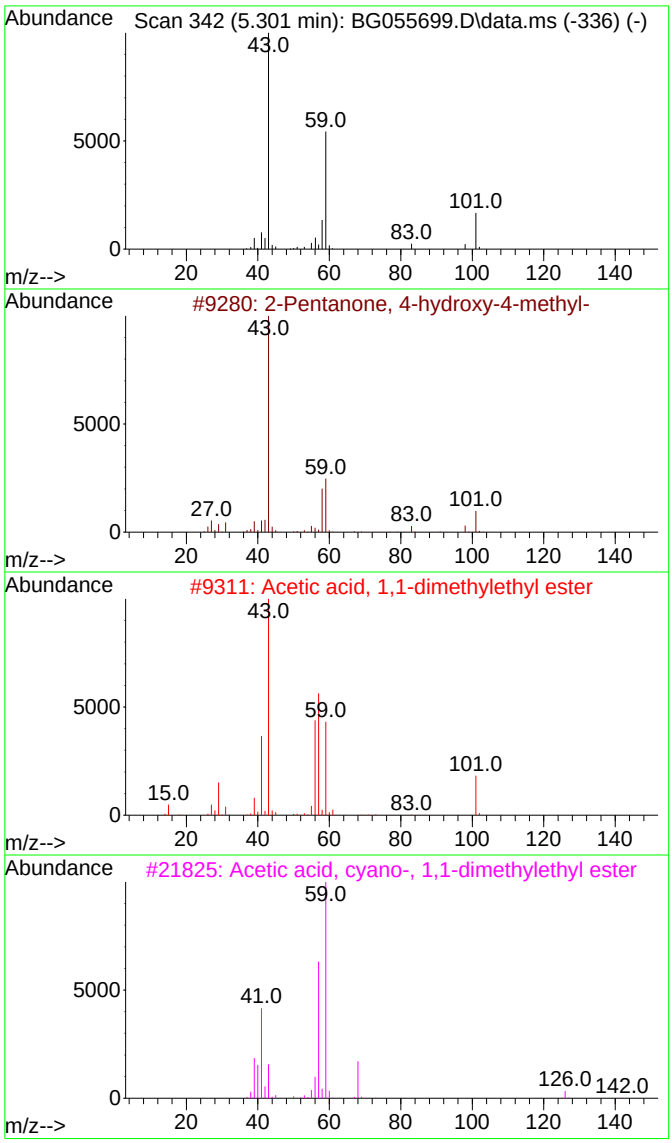
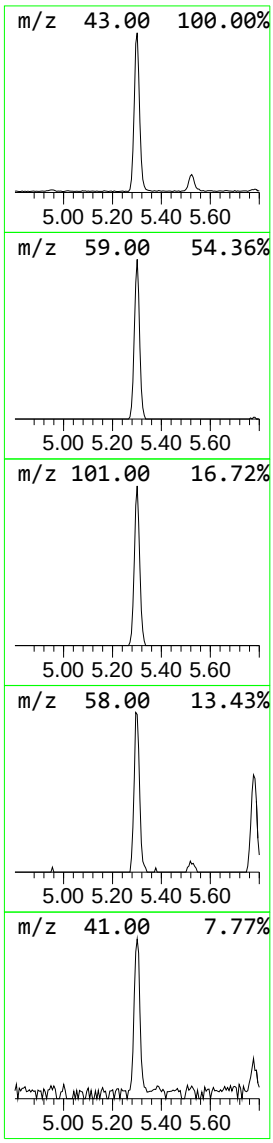
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.301	12.39 ng	155546	1,4-Dichlorobenzene-d4	8.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

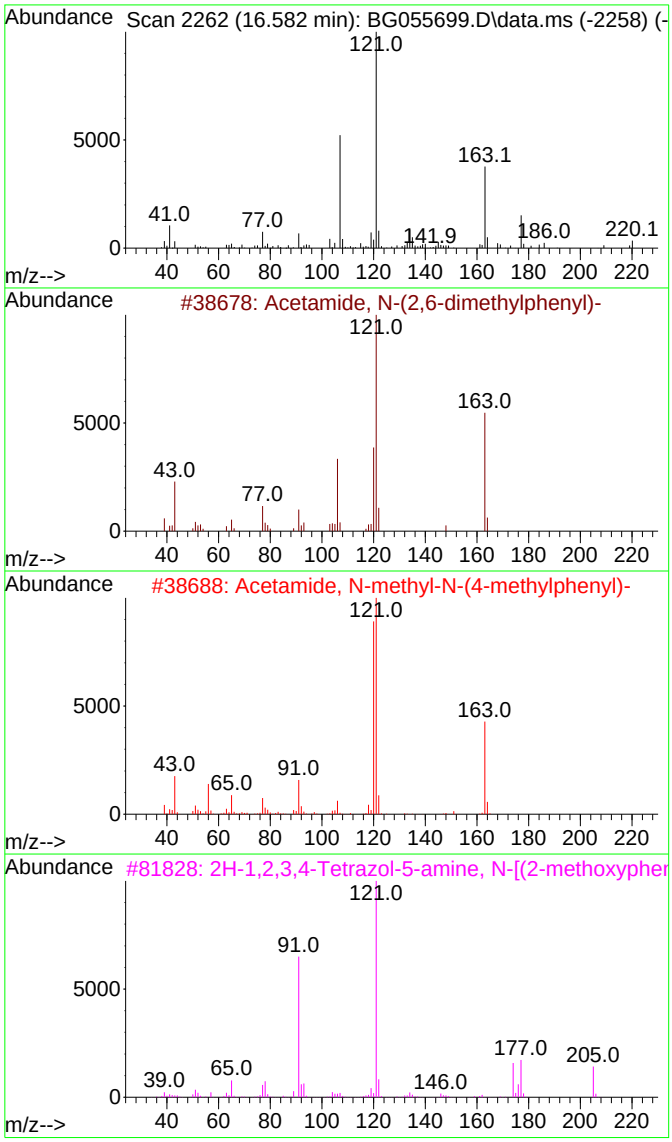
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

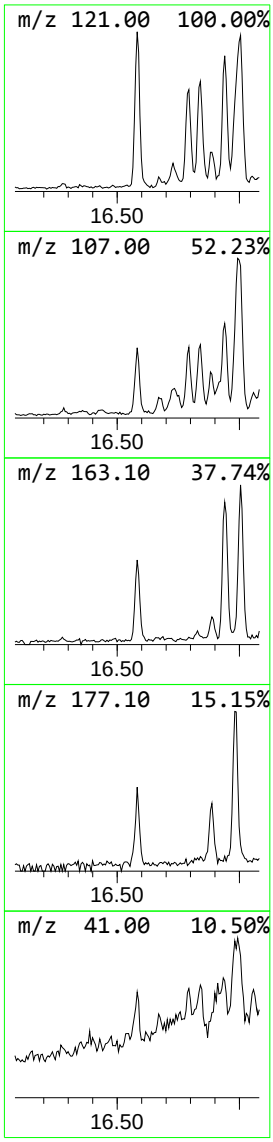
****

Peak Number 2 unknown16.582 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.582	2.45 ng	82326	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	49
2	Acetamide, N-methyl-N-(4-methylp...	163	C10H13NO	000612-03-3	47
3	2H-1,2,3,4-Tetrazol-5-amine, N-[...	205	C9H11N5O	1000337-56-1	43
4	4-sec-Butylphenol, O-(n-propylox...	236	C14H20O3	1000487-26-7	43
5	1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	40





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Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

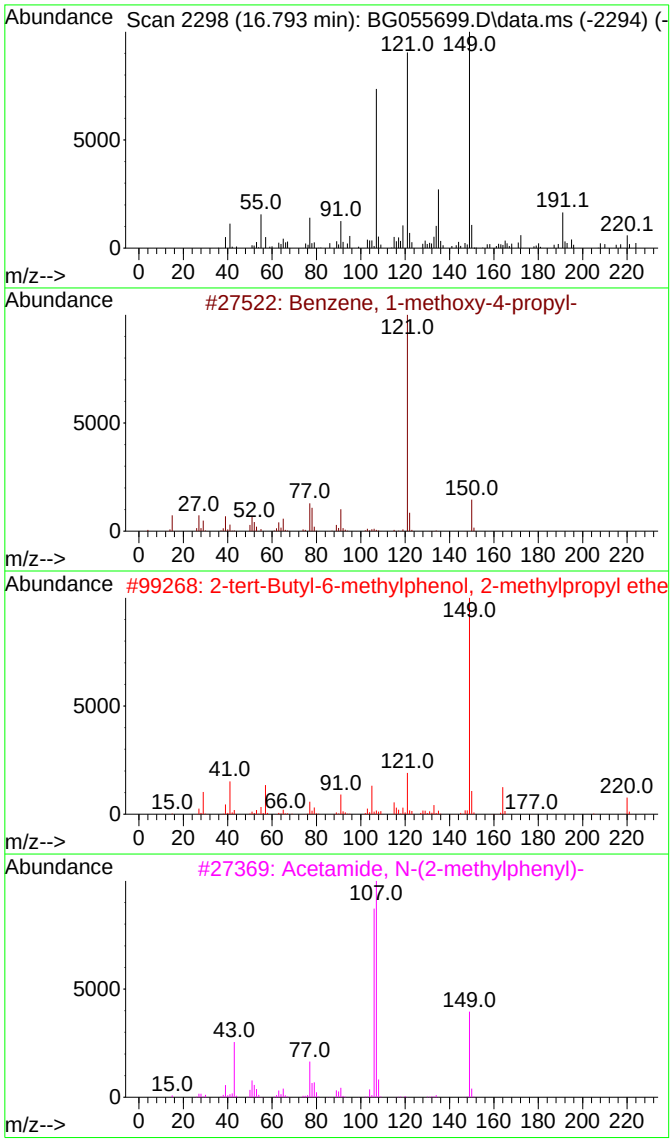
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

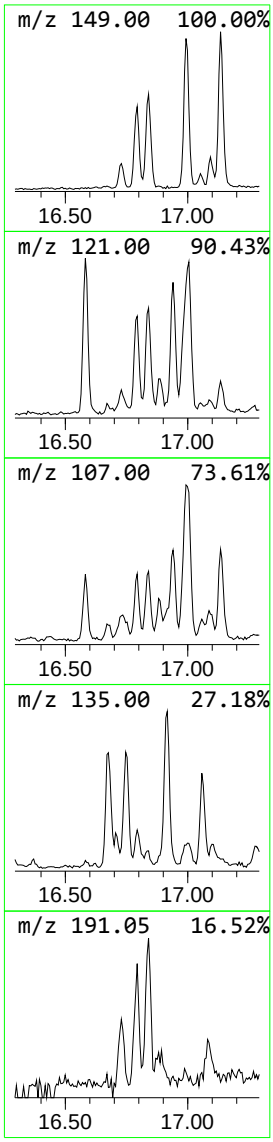
****

Peak Number 3 unknown16.793 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.793	2.15 ng	72280	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	35
2	2-tert-Butyl-6-methylphenol, 2-m...	220	C15H24O	1000395-19-4	25
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	25
4	Ethanol, 2-(3,3-dimethylbicyclo[...	166	C11H18O	002226-05-3	25
5	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

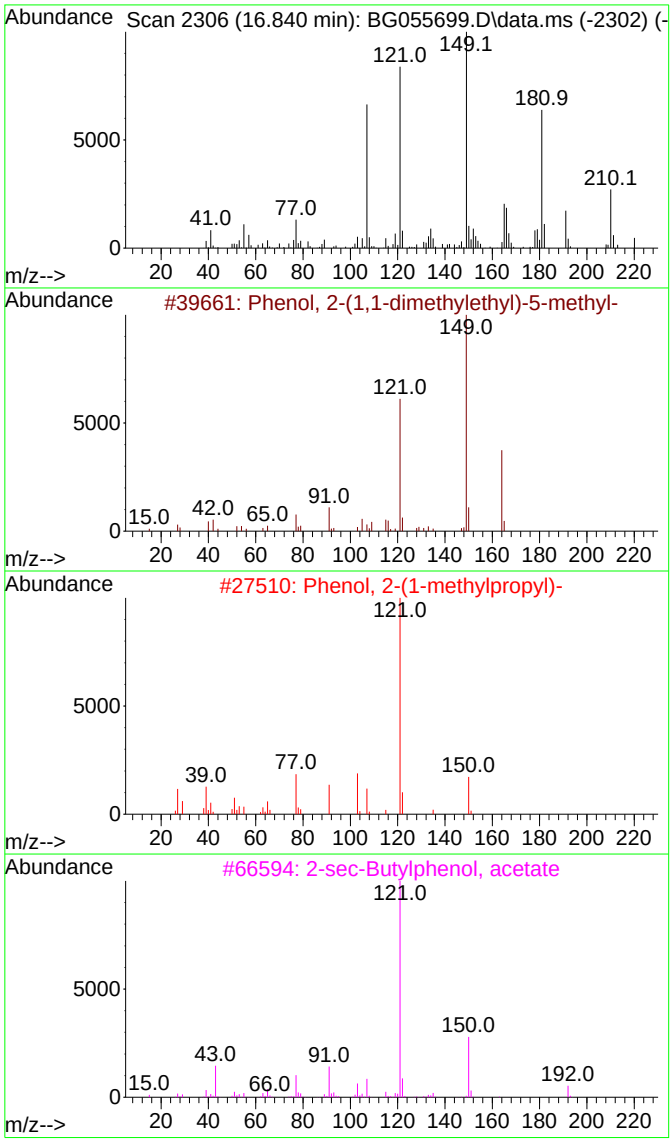
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

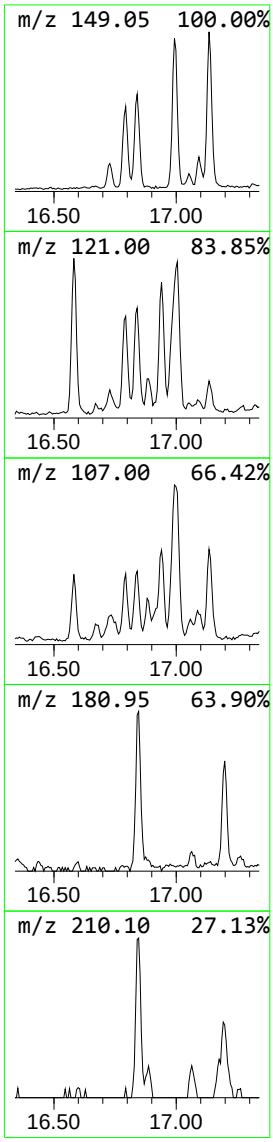
****

Peak Number 4 unknown16.840 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.840	3.22 ng	108210	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	38
2	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	18
3	2-sec-Butylphenol, acetate	192	C12H16O2	003056-61-9	18
4	1,1'-Biphenyl, 2,2'-diethyl-	210	C16H18	013049-35-9	18
5	3-Mercaptoindole, S-acetyl-	191	C10H9NOS	1081542-19-9	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

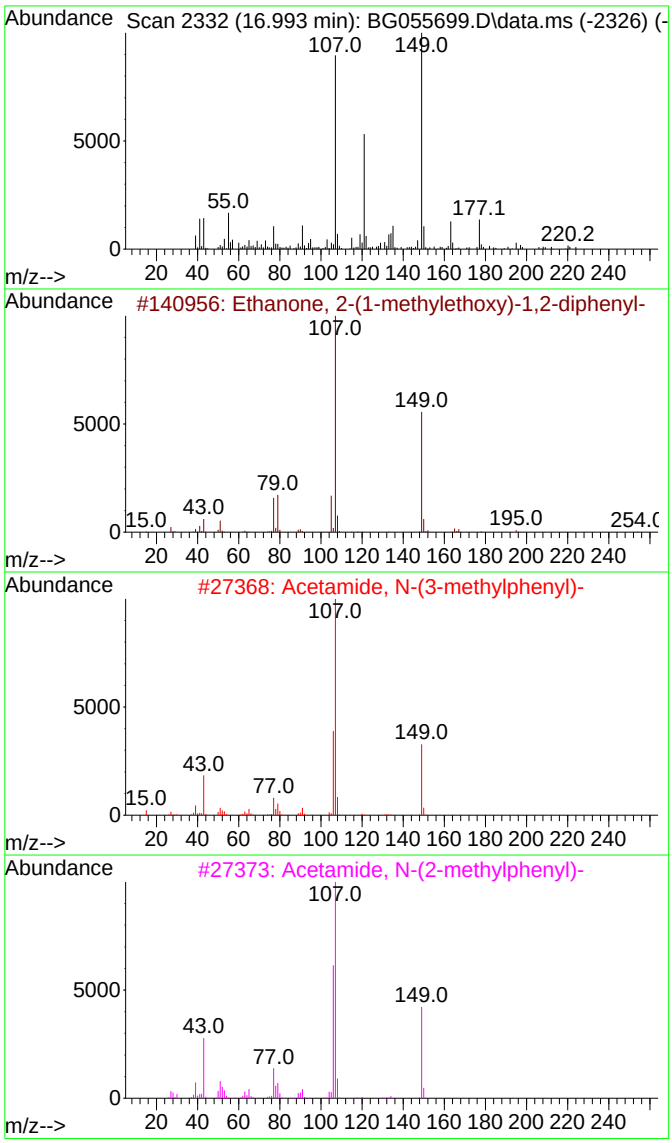
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

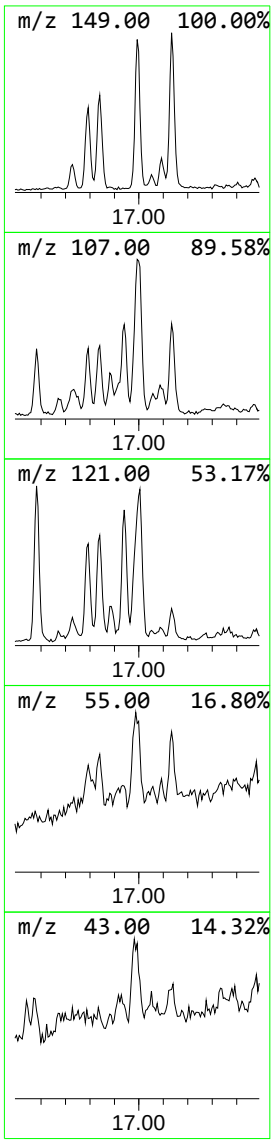
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanone, 2-(1-methylethoxy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.993	7.52 ng	252719	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 2-(1-methylethoxy)-1,2...	254	C17H18O2	006652-28-4	59
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	47
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	47
4	Ethanol, 2-(3,3-dimethylbicyclo[...	166	C11H18O	002226-05-3	42
5	3-Methyl-1-adamantaneacetic acid	208	C13H20O2	014202-13-2	38





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Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

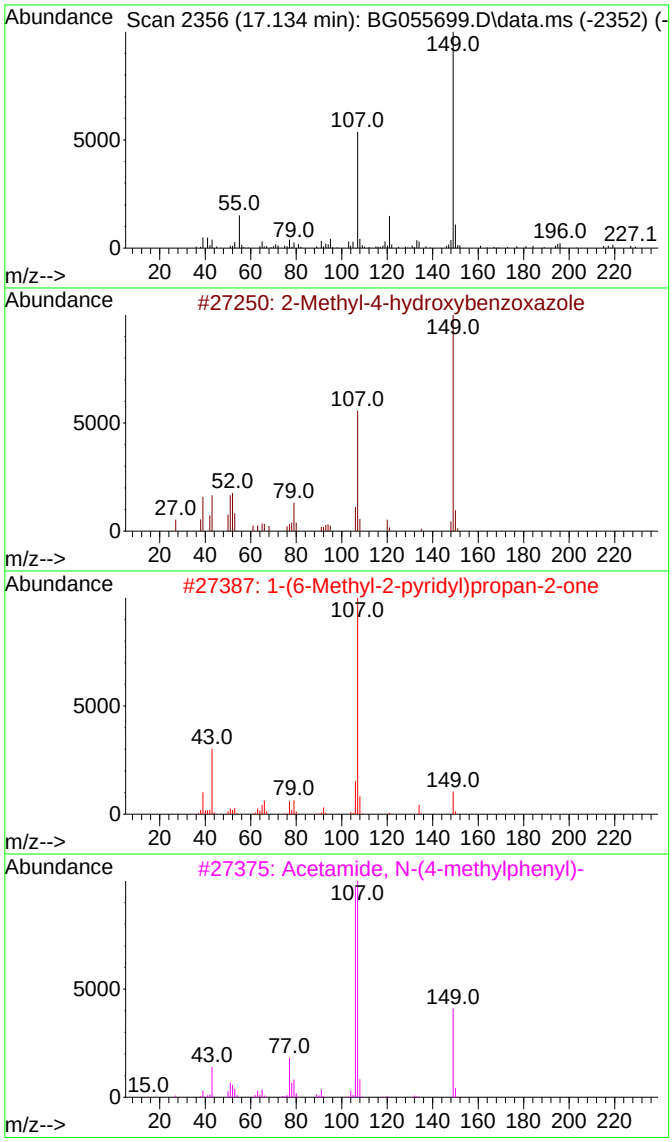
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

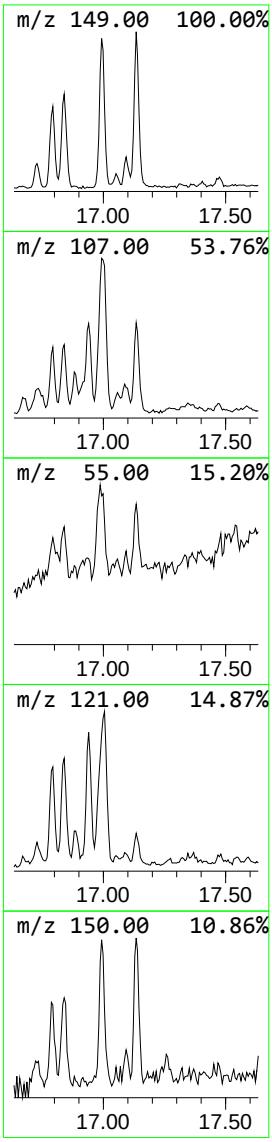
****

Peak Number 6 2-Methyl-4-hydroxybenzoxazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.134	2.22 ng	74602	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	72
2	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	64
3	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	58
4	2-t-Butyl-5-[hydroxy-(2,4,6-trim...	306	C18H26O4	092572-63-9	50
5	Benzene, 1-(1,1-dimethylethyl)-4...	164	C11H16O	005396-38-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

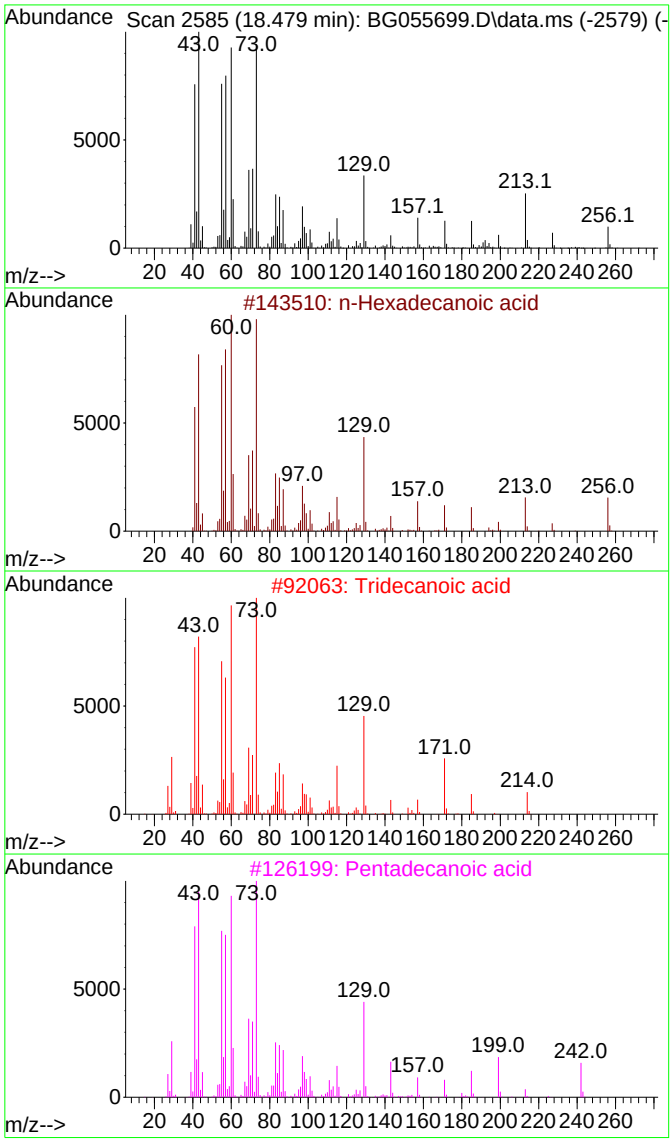
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

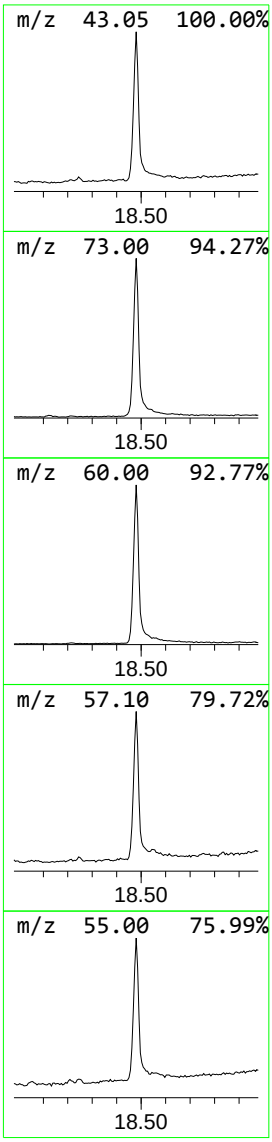
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.479	42.81 ng	1438360	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

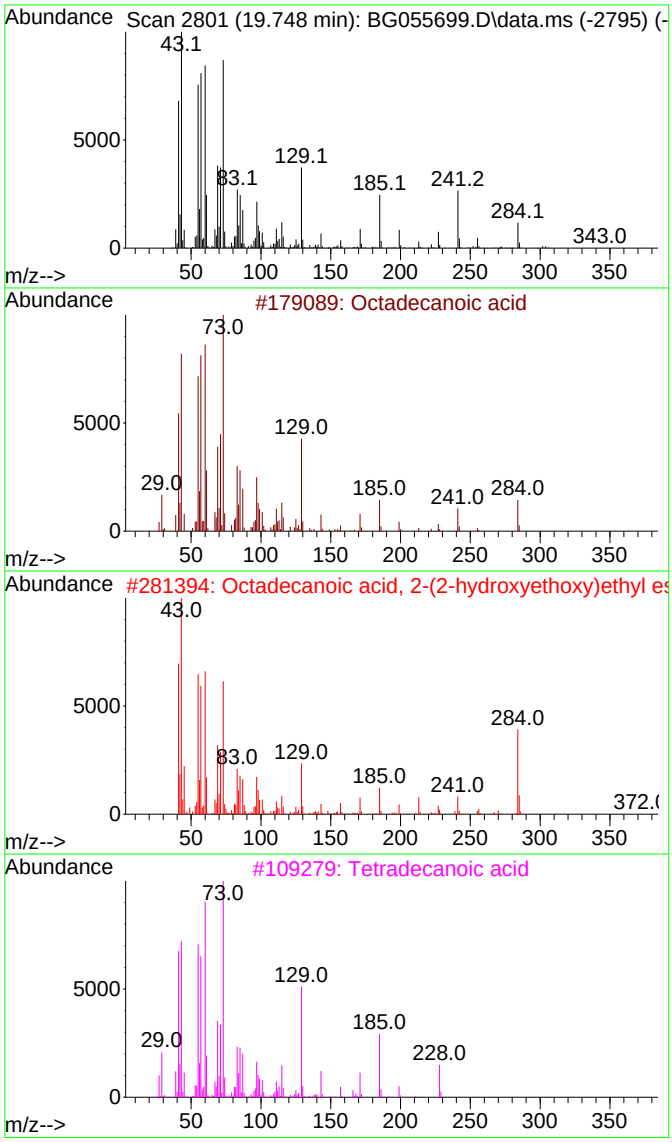
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

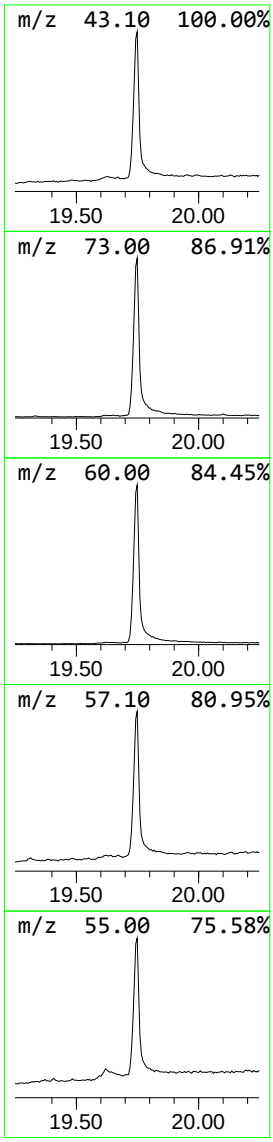
****

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.749	109.33 ng	3673220	Phenanthrene-d10	17.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





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Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

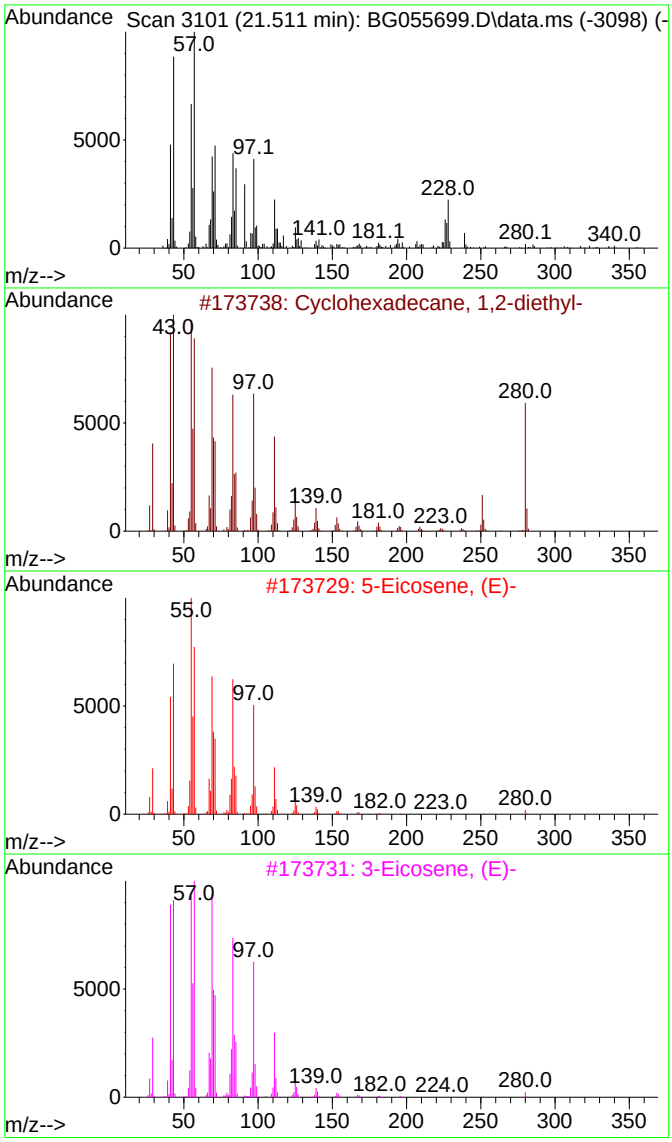
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

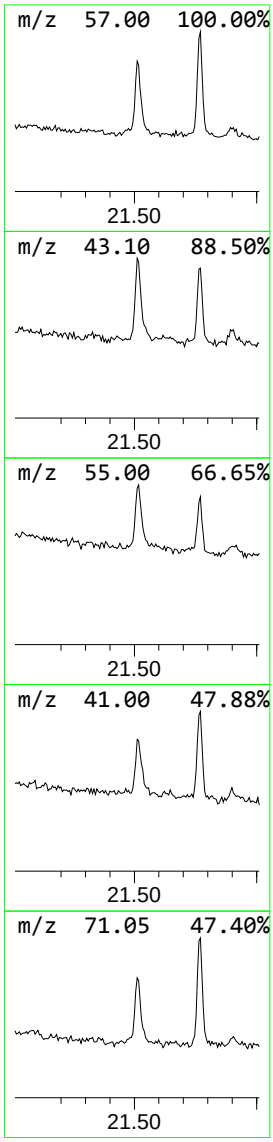
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexadecane, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.511	10.63 ng	325053	Chrysene-d12	21.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
4	Cyclohexadecane	224	C16H32	000295-65-8	83
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81





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Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

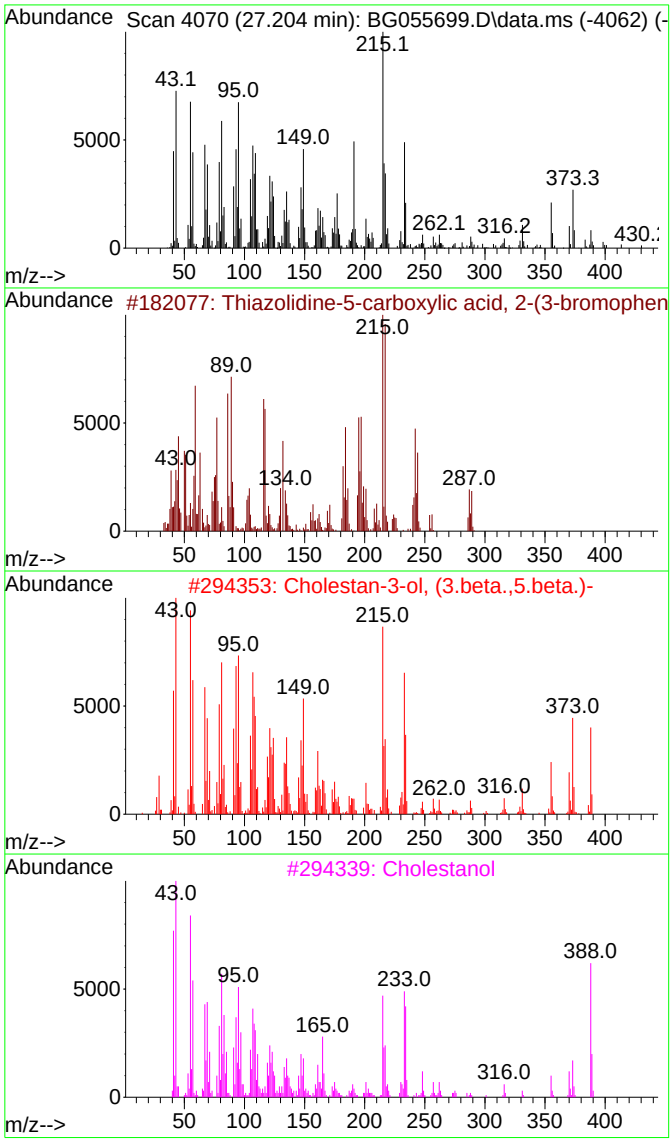
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

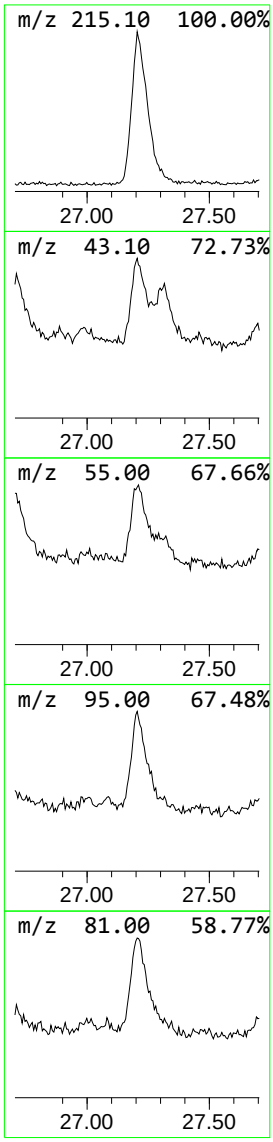
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Thiazolidine-5-carboxylic a... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.204	36.00 ng	1192790	Perylene-d12	25.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazolidine-5-carboxylic acid, ...	287	C10H10BrNO2S	1000267-68-3	90
2	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	55
3	Cholestanol	388	C27H48O	000080-97-7	38
4	2-((1S,3R)-3-hydroxycyclohexyl)-...	332	C22H36O2	132296-11-8	38
5	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

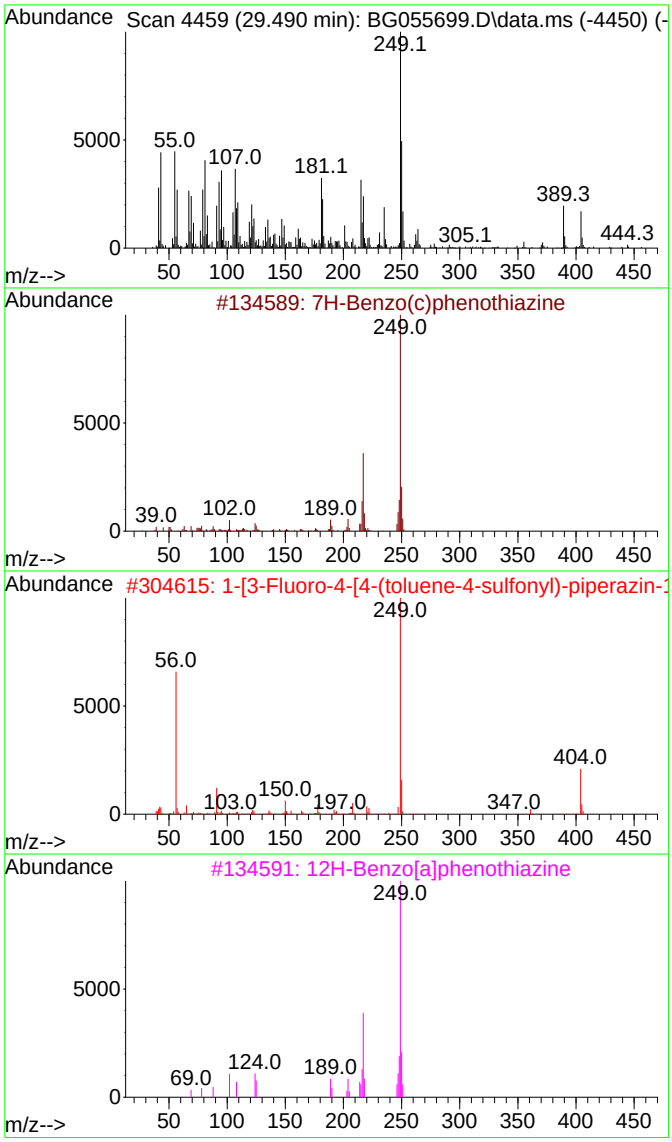
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

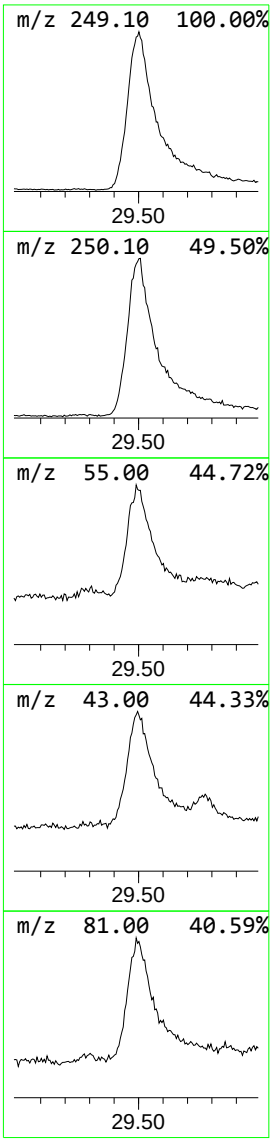
****

Peak Number 11 unknown29.490 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.490	31.16 ng	1032500	Perylene-d12	25.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	47
2	1-[3-Fluoro-4-[4-(toluene-4-sulf...	404	C21H25FN2O3S	333751-65-8	46
3	12H-Benzo[a]phenothiazine	249	C16H11NS	000225-83-2	43
4	2-Cyclopropyl-4-methyl-5-pyrimid...	250	C12H18N2O2Si	1000477-09-5	41
5	2,4-Diamino-6-(4-methylphenyl)py...	249	C14H11N5	1000460-13-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055699.D
Acq On : 18 Nov 2022 20:57
Operator : CG/JU
Sample : N5528-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.301	12.4	ng	155546	1	8.250	251096	20.0
unknown16.582	16.582	2.5	ng	82326	4	17.610	671980	20.0
unknown16.793	16.793	2.1	ng	72280	4	17.610	671980	20.0
unknown16.840	16.840	3.2	ng	108210	4	17.610	671980	20.0
Ethanone, 2-(1-...	16.993	7.5	ng	252719	4	17.610	671980	20.0
2-Methyl-4-hydr...	17.134	2.2	ng	74602	4	17.610	671980	20.0
n-Hexadecanoic ...	18.479	42.8	ng	1438360	4	17.610	671980	20.0
Octadecanoic acid	19.749	109.3	ng	3673220	4	17.610	671980	20.0
Cyclohexadecane...	21.511	10.6	ng	325053	5	21.911	611364	20.0
Thiazolidine-5-...	27.204	36.0	ng	1192790	6	25.330	662636	20.0
unknown29.490	29.490	31.2	ng	1032500	6	25.330	662636	20.0