LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.206	299	309	318	rBV	1428822	2609898	100.00%	25.642%
2	5.659	380	386	395	rBV	41520	72961	2.80%	0.717%
3	7.239	645	655	662	rBV	164271	293618	11.25%	2.885%
4	7.380	671	679	685	rBV	24252	45116	1.73%	0.443%
5	8.091	793	800	807	rBV	103894	188264	7.21%	1.850%
6	9.249	988	997	1004	rBV	294044	548375	21.01%	5.388%
7	9.613	1050	1059	1068	rBV	70082	141707	5.43%	1.392%
8	10.900	1268	1278	1291	rBV	140349	283088	10.85%	2.781%
9	11.070	1298	1307	1313	rVB4	19745	42053	1.61%	0.413%
10	11.328	1339	1351	1359	rBV4	7431	27432	1.05%	0.270%
11	12.186	1490	1497	1502	rBV4	16484	31883	1.22%	0.313%
12	13.261	1677	1680	1686	rVB	19984	29535	1.13%	0.290%
13	13.344	1686	1694	1702	rVB	735906	1200104	45.98%	11.791%
14	13.749	1754	1763	1774	rVB	26216	63344	2.43%	0.622%
15	14.202	1836	1840	1844	rVV2	19904	28220	1.08%	0.277%
16	14.613	1906	1910	1915	rBV2	25467	44528	1.71%	0.437%
17	14.713	1920	1927	1935	rVB	215990	373280	14.30%	3.667%
18	15.970	2137	2141	2148	rVB2	19194	28686	1.10%	0.282%
19	16.199	2175	2180	2187	rVB9	19234	41958	1.61%	0.412%
20	16.422	2213	2218	2230	rVB3	63009	147688	5.66%	1.451%
21	17.198	2346	2350	2359	rBV5	46009	103952	3.98%	1.021%
22	17.269	2359	2362	2370	rVB3	17995	33678	1.29%	0.331%
23	17.457	2387	2394	2399	rBV	263577	428242	16.41%	4.207%
24	19.078	2667	2670	2675	rVB4	22761	28447	1.09%	0.279%
25	19.507	2739	2743	2749	rVB	47981	69447	2.66%	0.682%
26	19.566	2749	2753	2758	rBV3	27030	41130	1.58%	0.404%
27	19.866	2801	2804	2813	rVB	46394	81201	3.11%	0.798%
28	20.065	2832	2838	2844	rBV	1129146	1540186	59.01%	15.132%
29	20.500	2909	2912	2919	rVB3	23575	44870	1.72%	0.441%
30	21.375	3057	3061	3069	rVB4	62192	106089	4.06%	1.042%
31	21.628	3099	3104	3111	rVB	332438	478125	18.32%	4.698%
32	21.734	3115	3122	3127	rBV	268398	489603	18.76%	4.810%
33	24.102	3522	3525	3533	rVB2	22574	48666	1.86%	0.478%
34	25.001	3669	3678	3689	rBV2	148626	442850	16.97%	4.351%

Sum of corrected areas: 10178224

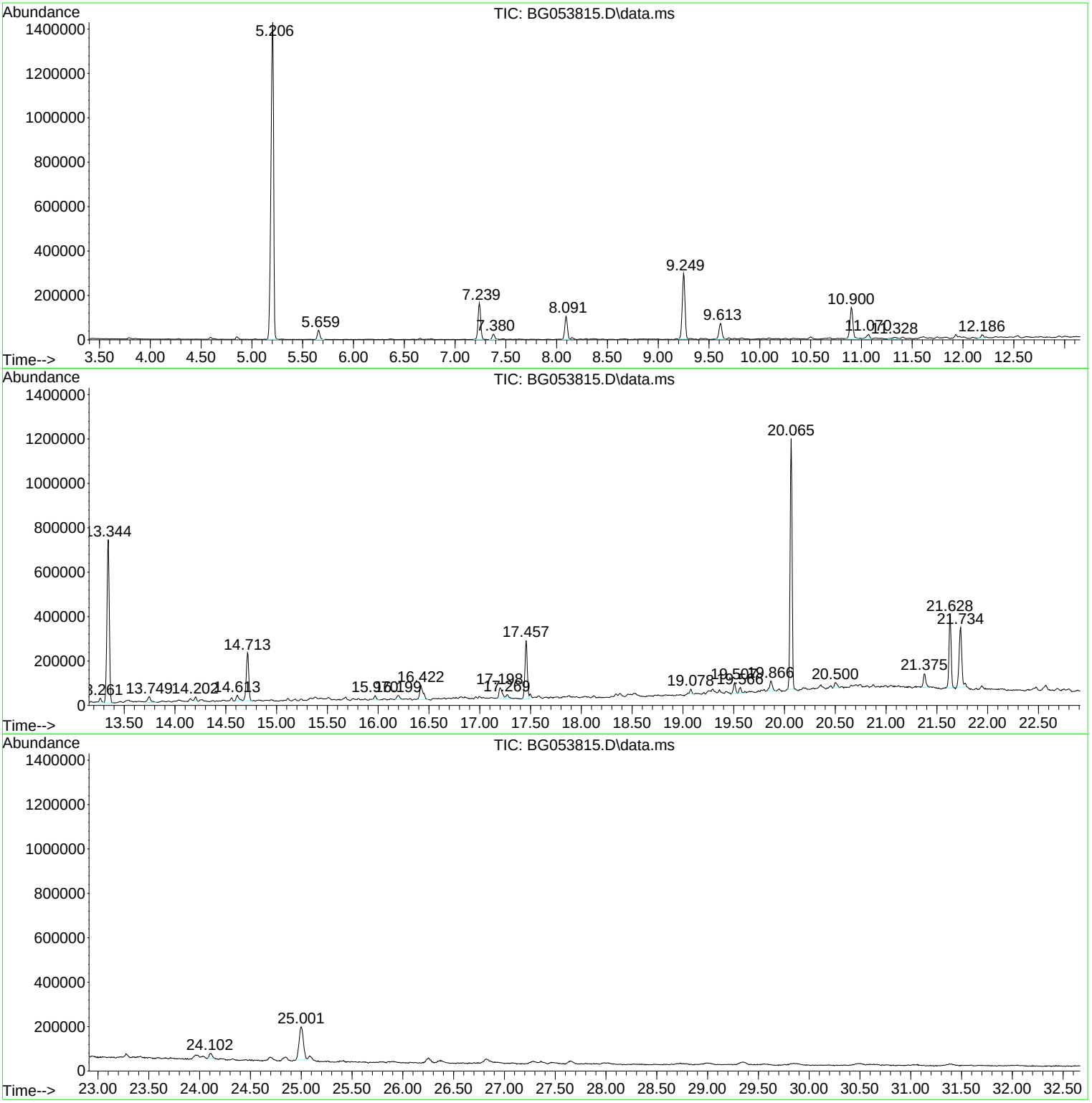
Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
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ClientSampleId :
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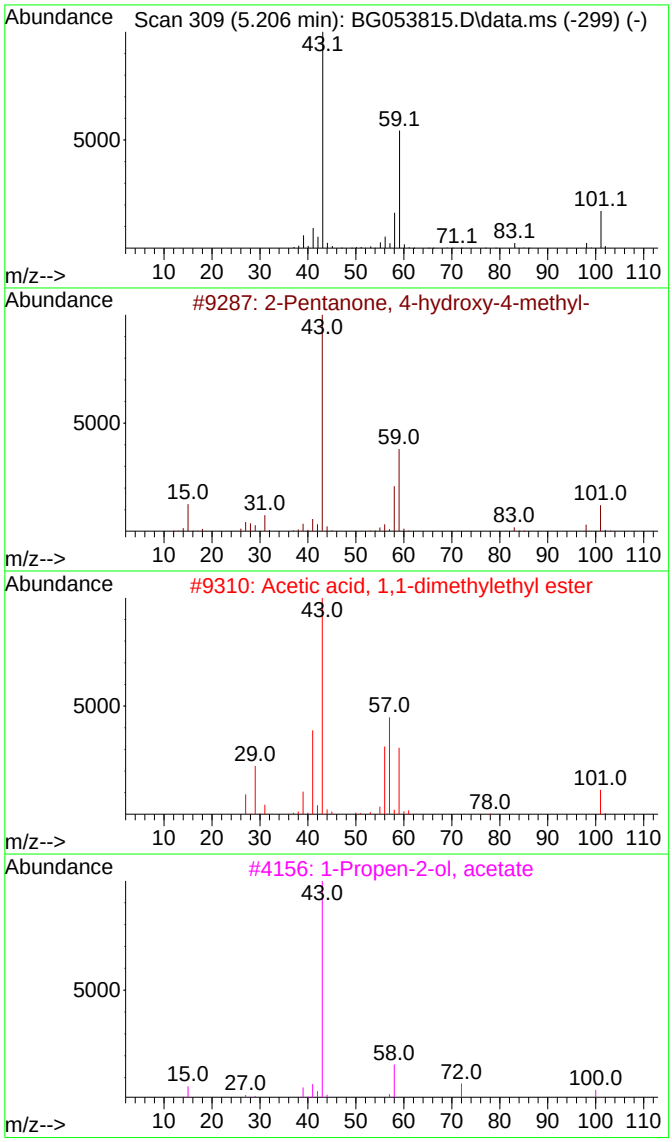
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

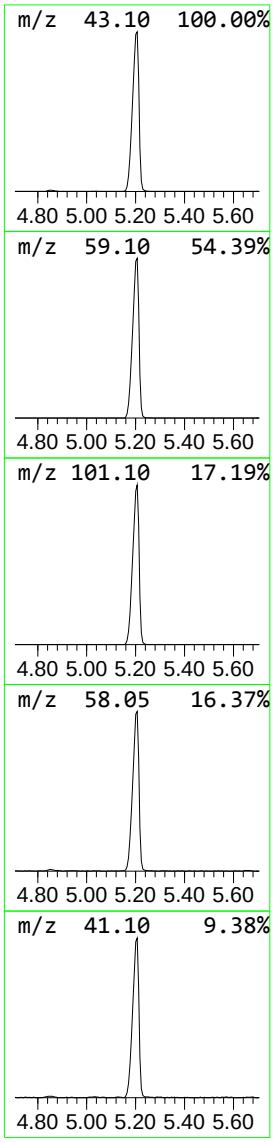
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.206	277.26 ng	2609900	1,4-Dichlorobenzene-d4	8.091

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetone	58	C3H6O	000067-64-1	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





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Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

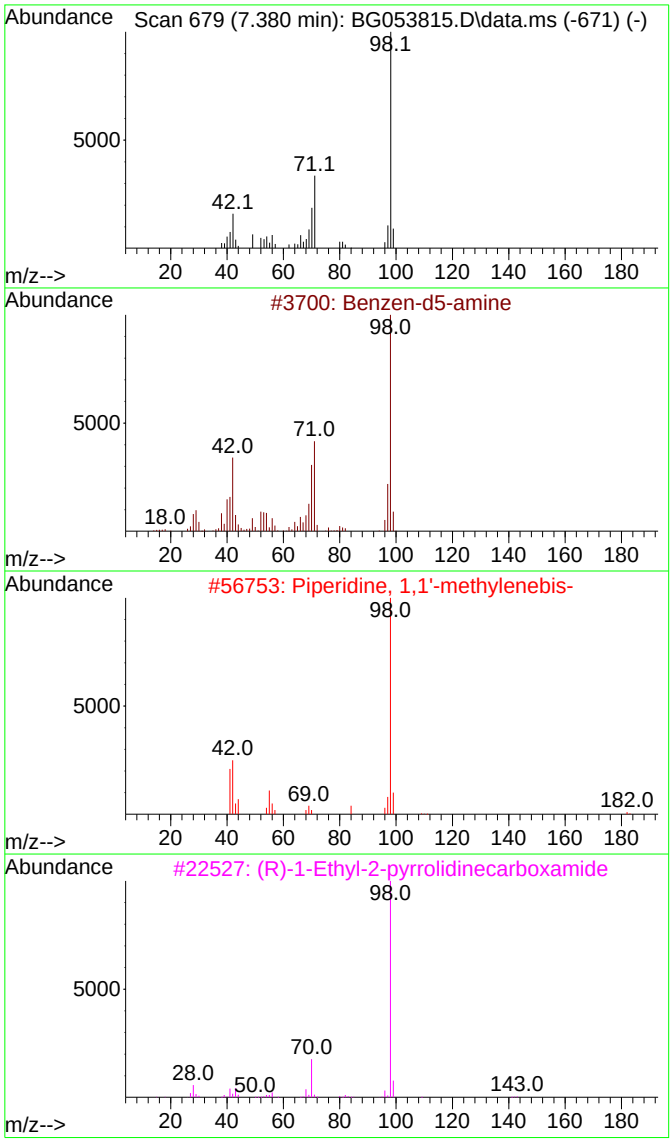
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

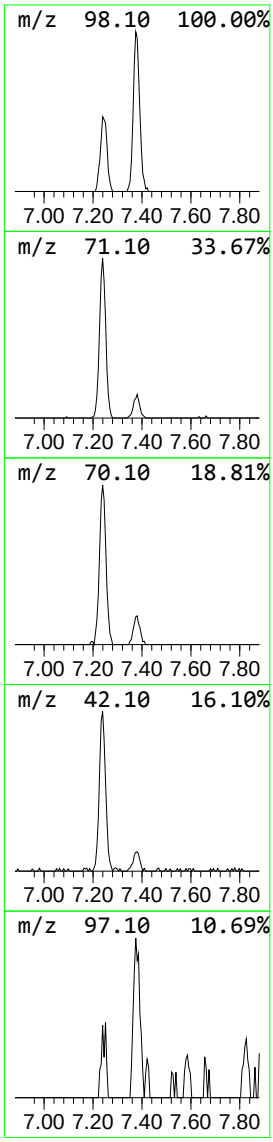
****

Peak Number 2 Benzen-d5-amine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.380	4.79 ng	45116	1,4-Dichlorobenzene-d4	8.091

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	72
2	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	59
3	(R)-1-Ethyl-2-pyrrolidinecarboxa...	142	C7H14N2O	1000237-69-9	53
4	Ethyl 1-methylpipecolinate	171	C9H17NO2	030727-18-5	53
5	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	53





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Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

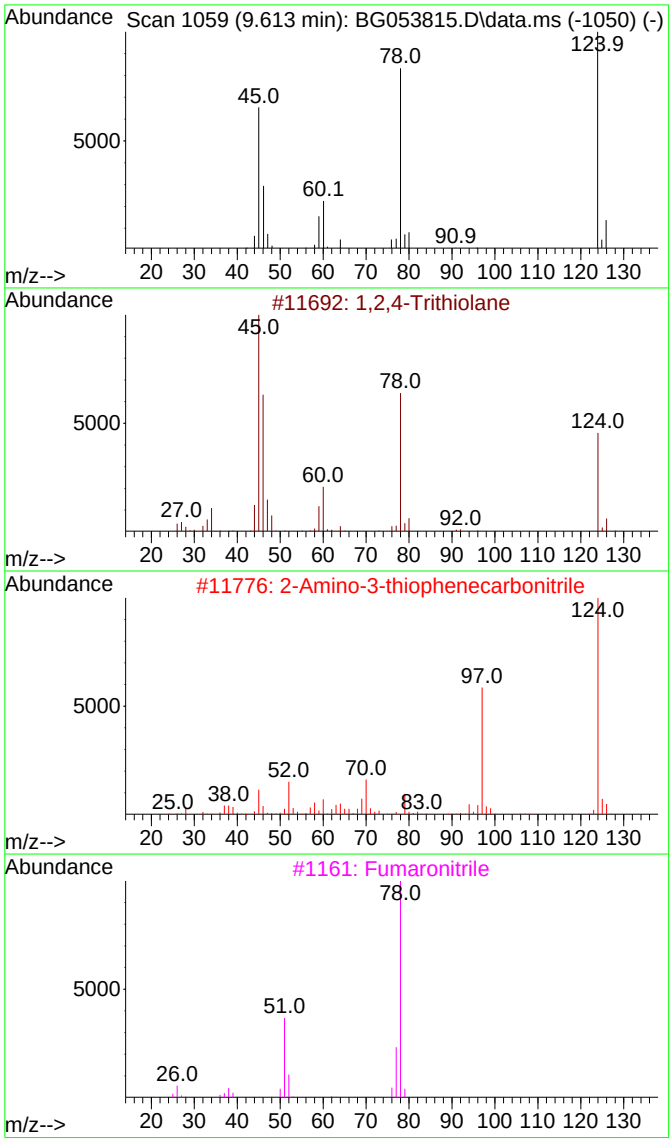
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

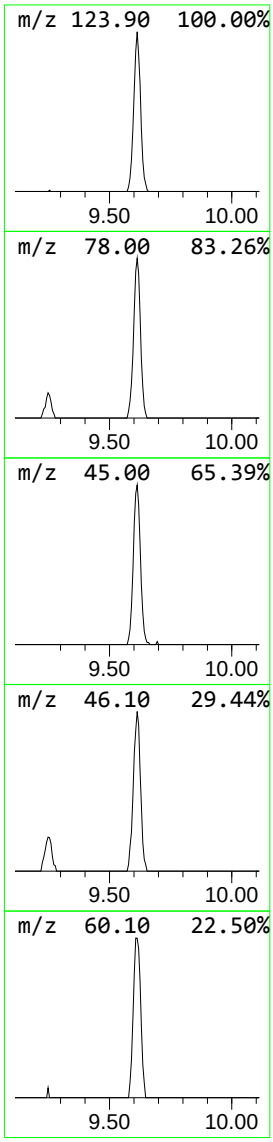
****

Peak Number 3 unknown9.613 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.613	10.01 ng	141707	Naphthalene-d8	10.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	36
2	2-Amino-3-thiophenecarbonitrile	124	C5H4N2S	004651-82-5	9
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	9
5	Benzene	78	C6H6	000071-43-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

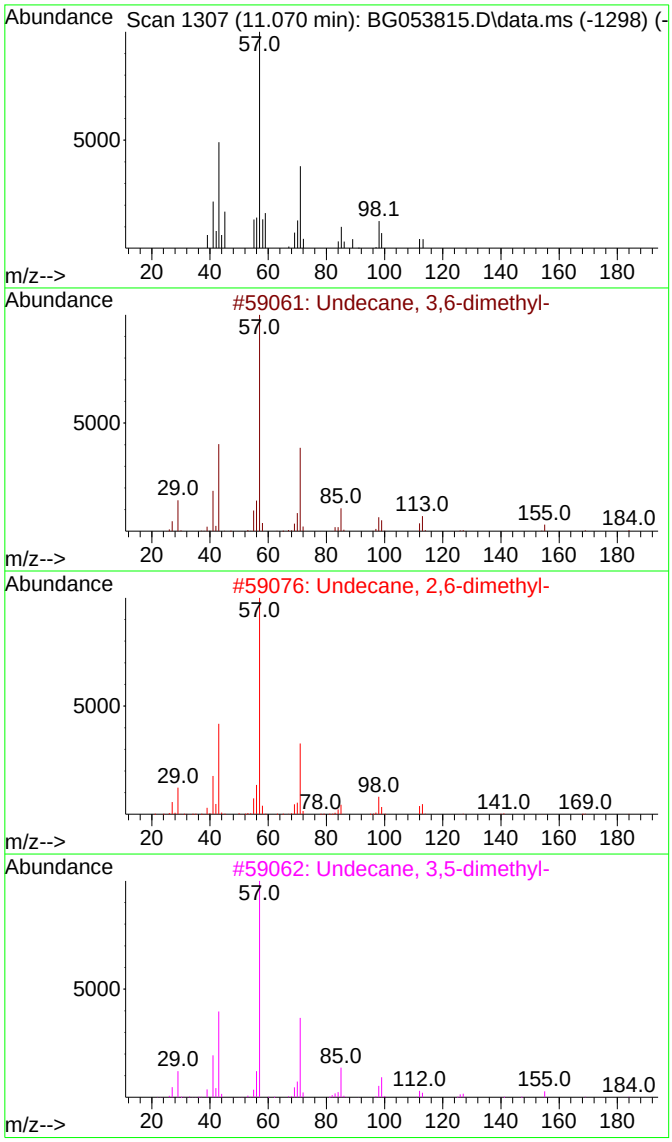
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

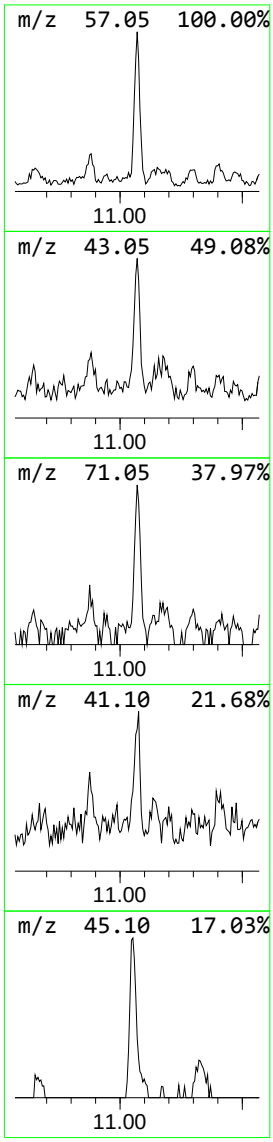
****

Peak Number 4 Undecane, 3,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.070	2.97 ng	42053	Naphthalene-d8	10.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	59
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	53
3	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	53
4	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	47
5	Dodecane, 6-methyl-	184	C13H28	006044-71-9	43





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Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

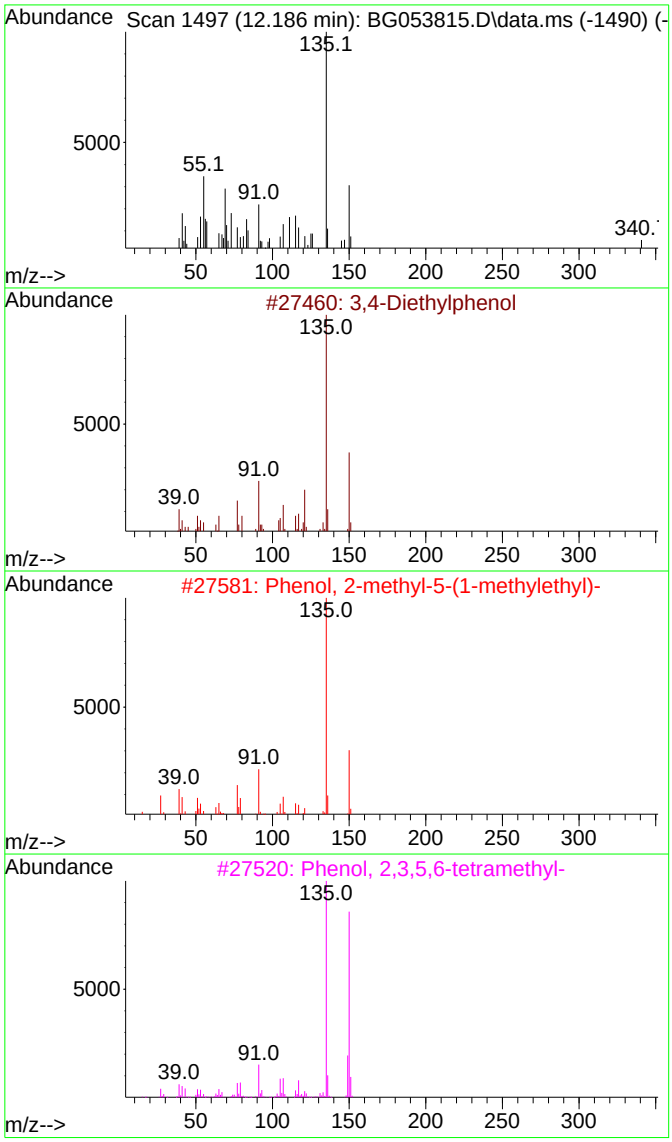
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

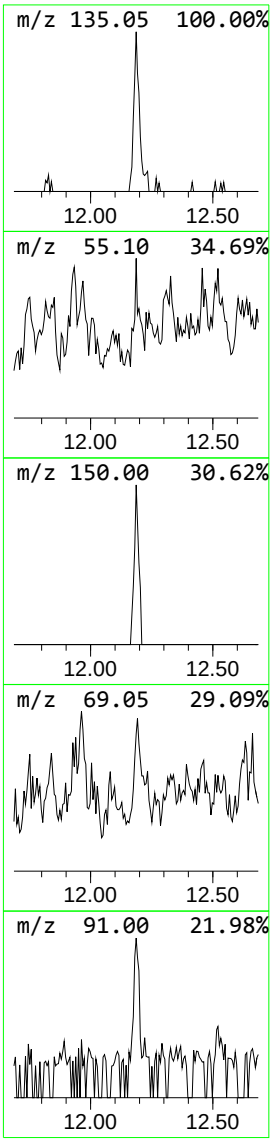
****

Peak Number 5 3,4-Diethylphenol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	2.25 ng	31883	Naphthalene-d8	10.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Diethylphenol	150	C10H14O	000875-85-4	72
2	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	72
3	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	64
4	Phenol, 3-methyl-5-(1-methylethy...	207	C12H17NO2	002631-37-0	59
5	Thymol	150	C10H14O	000089-83-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
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Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

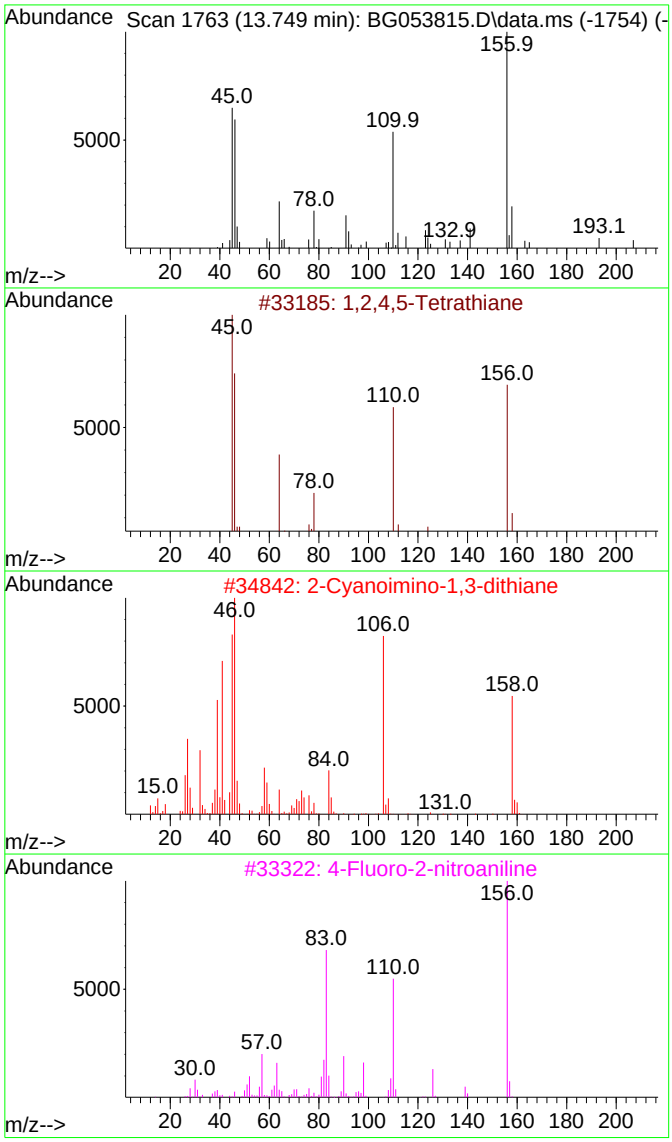
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

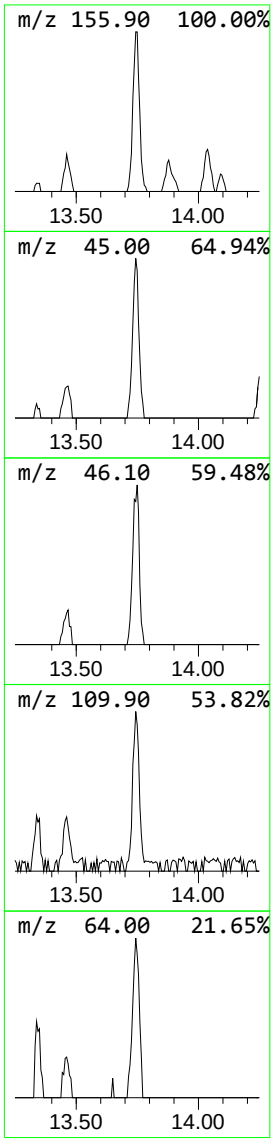
****

Peak Number 6 1,2,4,5-Tetrathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.749	3.39 ng	63344	Acenaphthene-d10	14.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	87
2	2-Cyanoimino-1,3-dithiane	158	C5H6N2S2	010191-73-8	30
3	4-Fluoro-2-nitroaniline	156	C6H5FN2O2	000364-78-3	25
4	Omethoate	213	C5H12NO4PS	001113-02-6	23
5	4,5-Diamino-6-methyl-2-thiopyrim...	156	C5H8N4S	006305-99-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

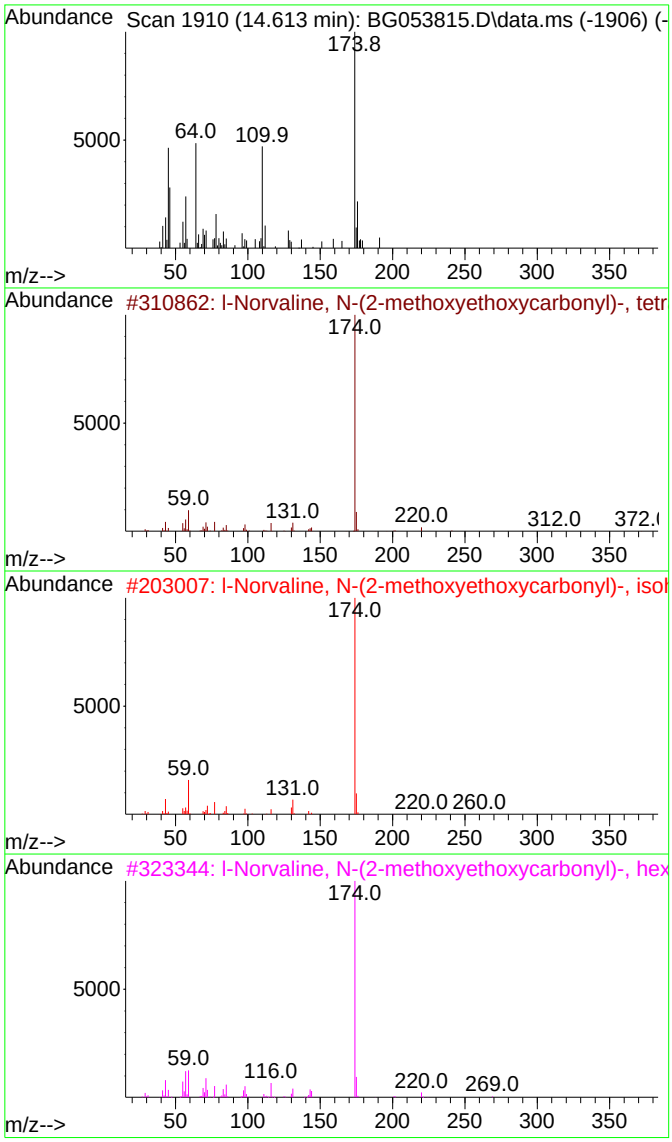
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

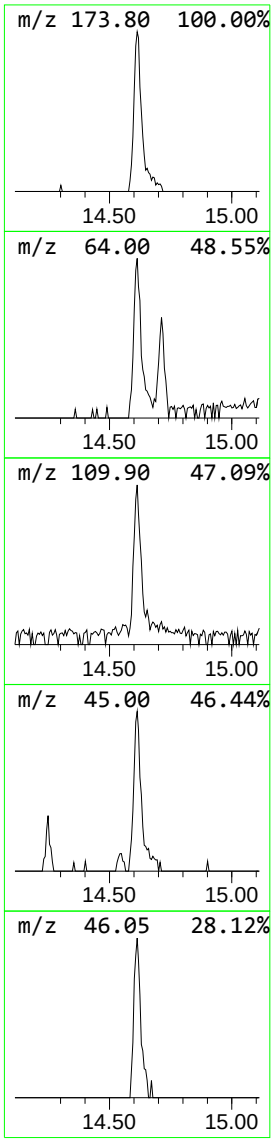
****

Peak Number 7 unknown14.613 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.613	2.39 ng	44528	Acenaphthene-d10	14.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-Norvaline, N-(2-methoxyethoxyc...	415	C23H45NO5	1000328-64-5	10
2	l-Norvaline, N-(2-methoxyethoxyc...	303	C15H29NO5	1000328-63-8	10
3	l-Norvaline, N-(2-methoxyethoxyc...	443	C25H49NO5	1000328-64-7	10
4	2-(4-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-17-2	9
5	3H-Pyrazol-3-one, 2,4-dihydro-5-...	174	C10H10N2O	000089-25-8	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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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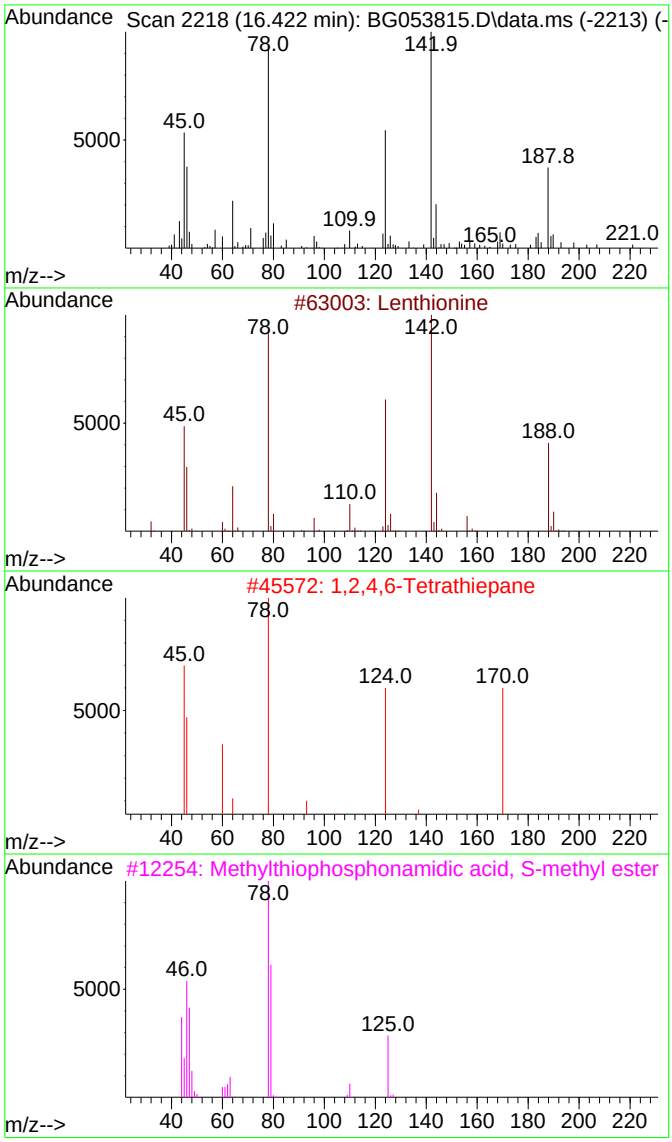
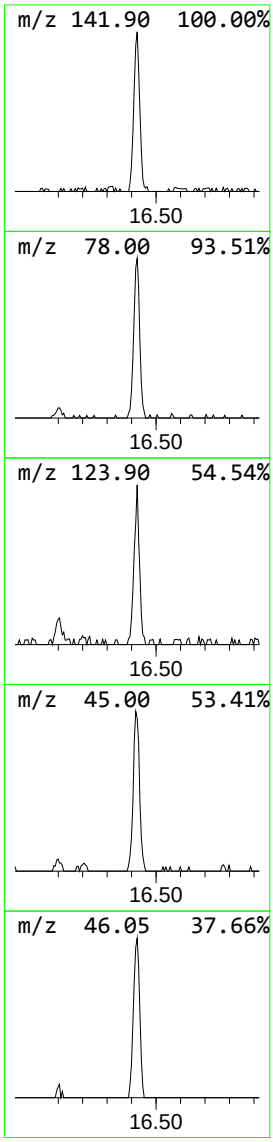
Peak Number 8 Lenthionine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.422	6.90 ng	147688	Phenanthrene-d10	17.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	94
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	36
3	Methylthiophosphonamidic acid, S...	125	C2H8NOPS	1000306-03-2	25
4	Hexathiepane	206	CH2S6	017233-71-5	12
5	Fumaronitrile	78	C4H2N2	000764-42-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

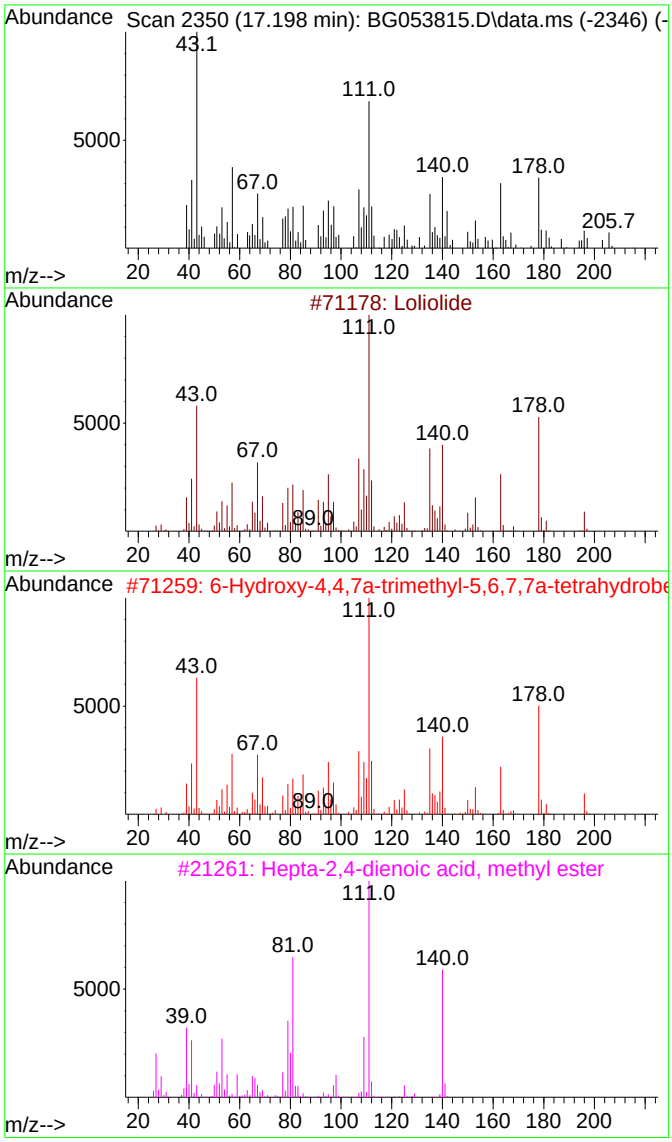
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

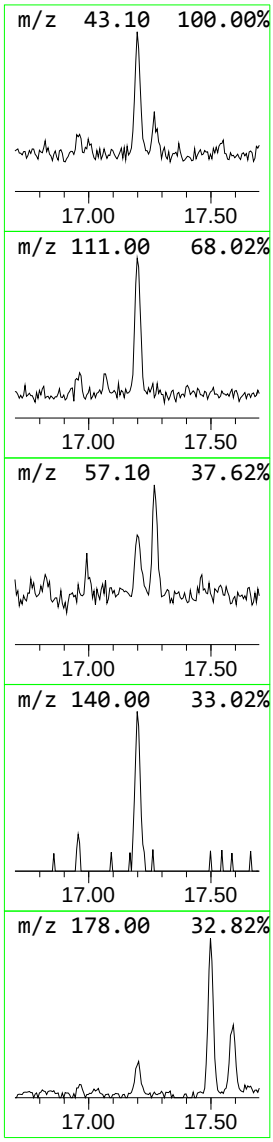
****

Peak Number 9 Loliolide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	4.85 ng	103952	Phenanthrene-d10	17.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Loliolide	196	C11H16O3	005989-02-6	89
2	6-Hydroxy-4,4,7a-trimethyl-5,6,7...	196	C11H16O3	073410-02-3	60
3	Hepta-2,4-dienoic acid, methyl e...	140	C8H12O2	056424-97-6	38
4	2-Propenal, 2-methyl-, diethylhy...	140	C8H16N2	075268-11-0	22
5	Boroxin, ethyldimethyl-	140	C4H11B3O3	1000162-60-8	22





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Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

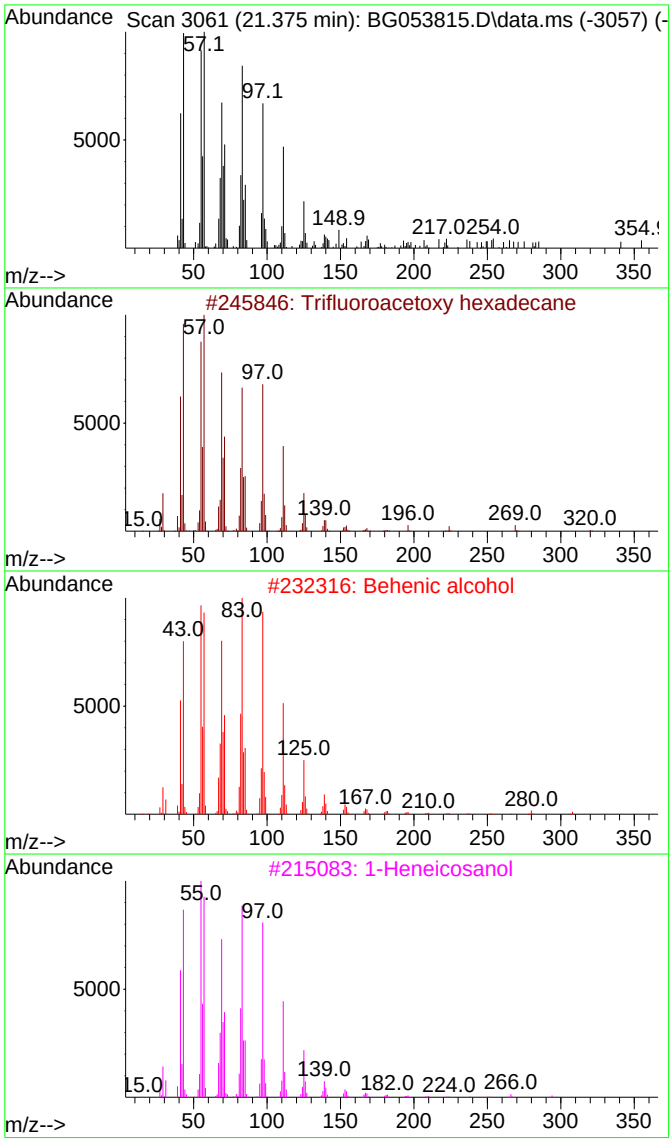
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

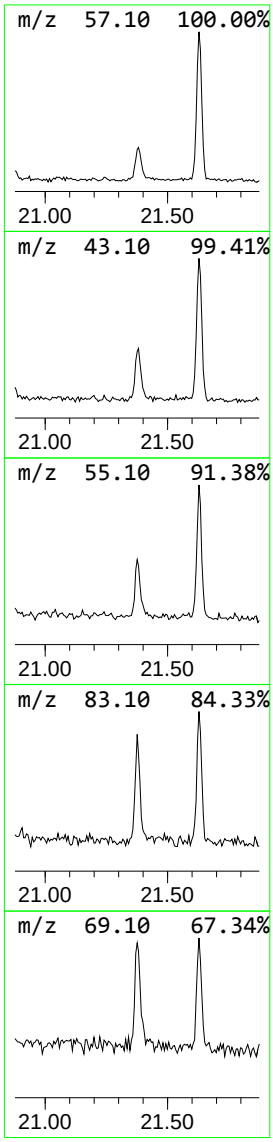
****

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.375	4.33 ng	106089	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

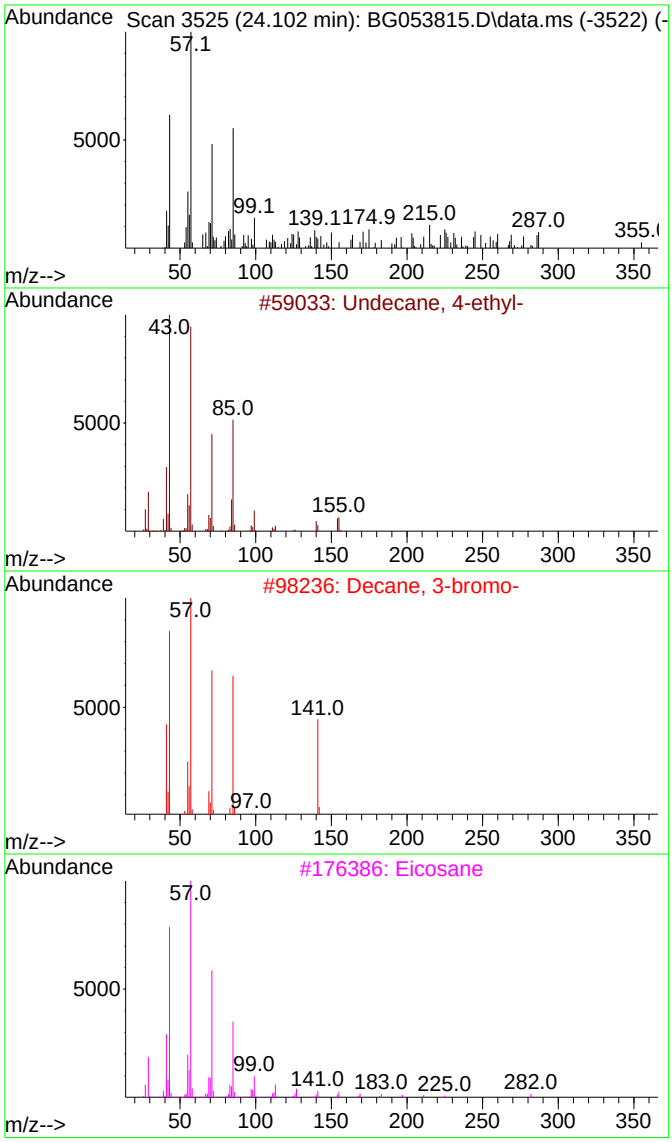
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

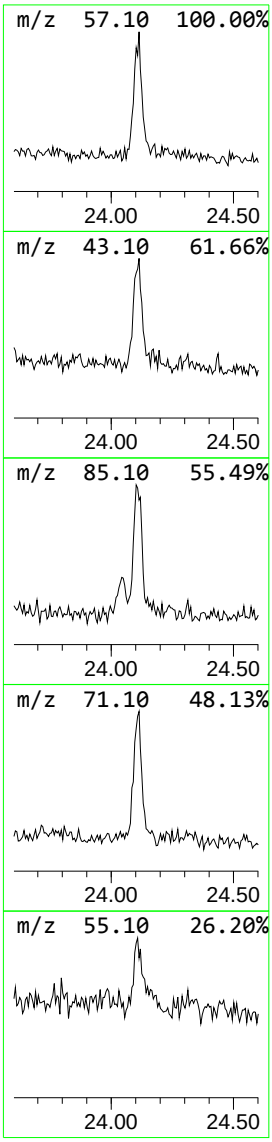
****

Peak Number 11 Undecane, 4-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.102	2.20 ng	48666	Perylene-d12	25.001

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4-ethyl-	184	C13H28	017312-59-3	50
2	Decane, 3-bromo-	220	C10H21Br	030571-71-2	50
3	Eicosane	282	C20H42	000112-95-8	45
4	Hexadecane	226	C16H34	000544-76-3	45
5	Nonadecane	268	C19H40	000629-92-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053815.D
Acq On : 3 Jun 2022 16:18
Operator : CG/JU
Sample : N3170-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20220424-AMENDED-COMPOSITE-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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-...	5.206	277.3	ng	2609900	1	8.091	188264	20.0
Benzen-d5-amine	7.380	4.8	ng	45116	1	8.091	188264	20.0
unknown9.613	9.613	10.0	ng	141707	2	10.900	283088	20.0
Undecane, 3,6-d...	11.070	3.0	ng	42053	2	10.900	283088	20.0
3,4-Diethylphenol	12.186	2.3	ng	31883	2	10.900	283088	20.0
1,2,4,5-Tetrath...	13.749	3.4	ng	63344	3	14.713	373280	20.0
unknown14.613	14.613	2.4	ng	44528	3	14.713	373280	20.0
Lenthionine	16.422	6.9	ng	147688	4	17.457	428242	20.0
Loliolide	17.198	4.8	ng	103952	4	17.457	428242	20.0
Trifluoroacetox...	21.375	4.3	ng	106089	5	21.734	489603	20.0
Undecane, 4-ethyl-	24.102	2.2	ng	48666	6	25.001	442850	20.0