LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.653	378	385	398	rBV	181454	313109	9.19%	2.092%
2	7.251	650	657	670	rBV	113724	210834	6.19%	1.409%
3	8.085	792	799	807	rBV	83446	147397	4.33%	0.985%
4	8.790	904	919	936	rBV2	152949	673886	19.79%	4.503%
5	9.248	990	997	1008	rVB	301779	559383	16.42%	3.738%
6	9.618	1027	1060	1081	rBV2	476294	3405943	100.00%	22.758%
7	10.311	1165	1178	1190	rBV2	147336	593517	17.43%	3.966%
8	10.899	1269	1278	1285	rBV	105200	197180	5.79%	1.317%
9	11.128	1312	1317	1331	rBV5	11390	43717	1.28%	0.292%
10	11.380	1354	1360	1373	rVB6	14854	48728	1.43%	0.326%
11	11.815	1416	1434	1447	rBV3	417335	1758122	51.62%	11.747%
12	11.944	1453	1456	1479	rVB	97936	218142	6.40%	1.458%
13	13.336	1686	1693	1700	rBV	892443	1367626	40.15%	9.138%
14	14.711	1918	1927	1934	rBV	197647	313130	9.19%	2.092%
15	14.999	1971	1976	1986	rBV2	33342	68679	2.02%	0.459%
16	15.422	2043	2048	2058	rBV	44042	104436	3.07%	0.698%
17	15.951	2129	2138	2143	rBV2	18603	36659	1.08%	0.245%
18	16.197	2174	2180	2188	rBV	756938	1186139	34.83%	7.925%
19	16.426	2212	2219	2227	rBV	81590	139769	4.10%	0.934%
20	17.249	2355	2359	2365	rVB2	100763	148264	4.35%	0.991%
21	17.454	2389	2394	2401	rBV	255716	417834	12.27%	2.792%
22	17.860	2459	2463	2467	rBV4	59763	96358	2.83%	0.644%
23	20.063	2832	2838	2843	rVB	1449960	1942445	57.03%	12.979%
24	21.737	3117	3123	3130	rVB	284046	467579	13.73%	3.124%
25	25.015	3671	3681	3692	rVB2	165628	507363	14.90%	3.390%

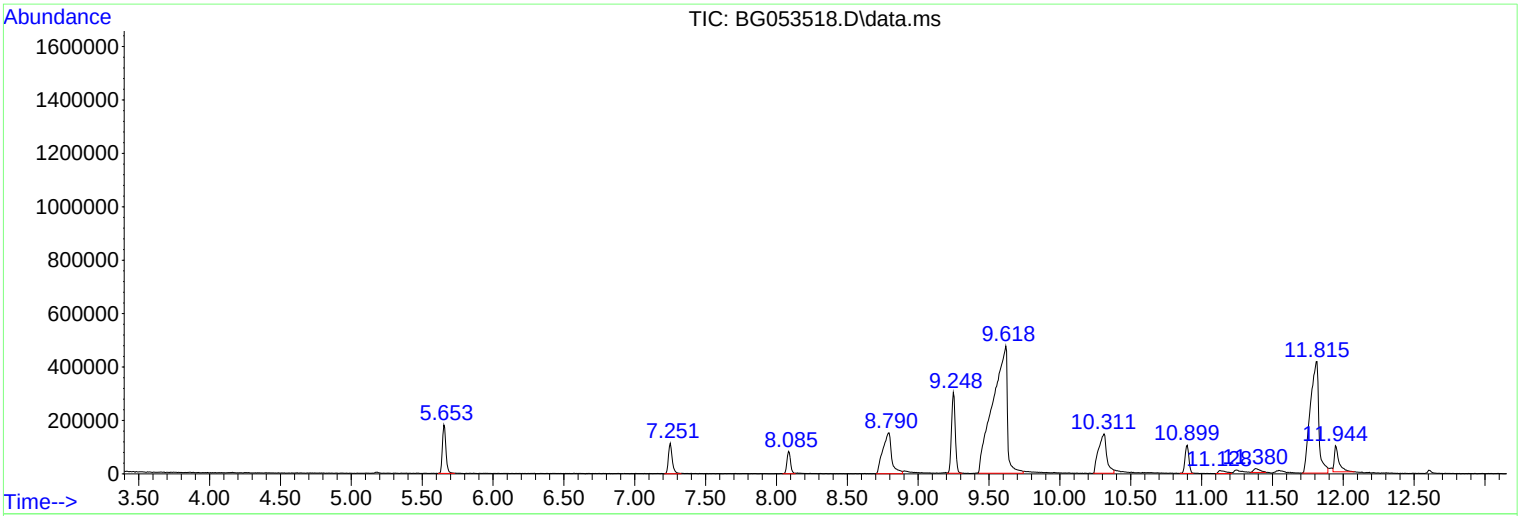
Sum of corrected areas: 14966239

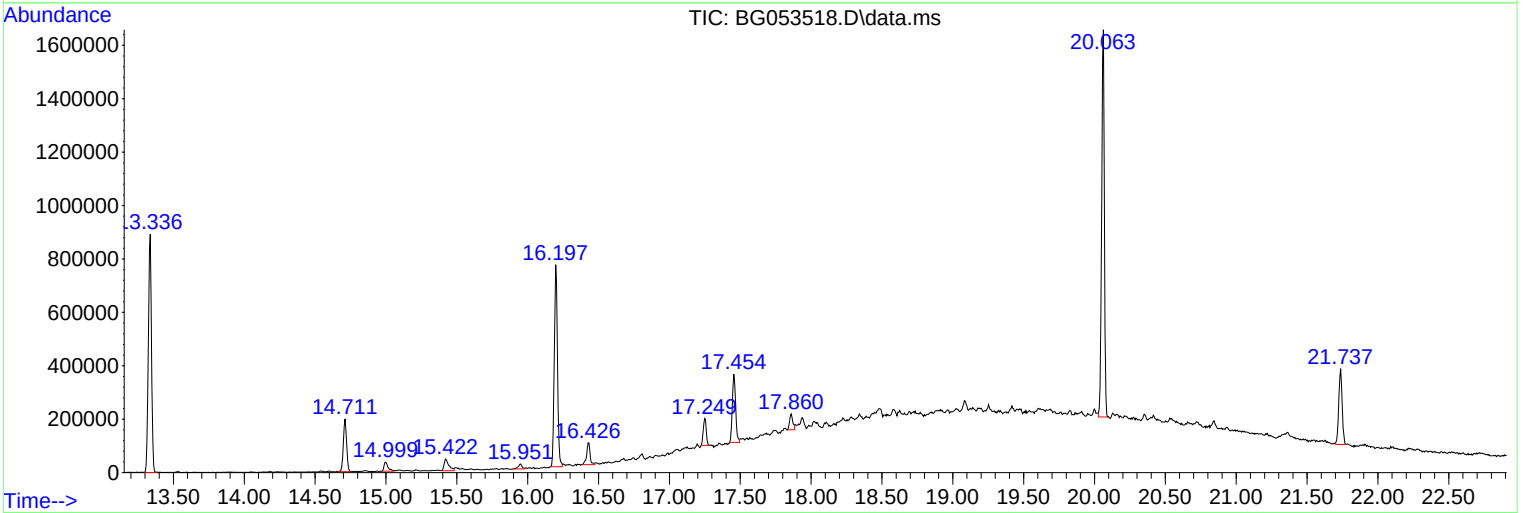
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

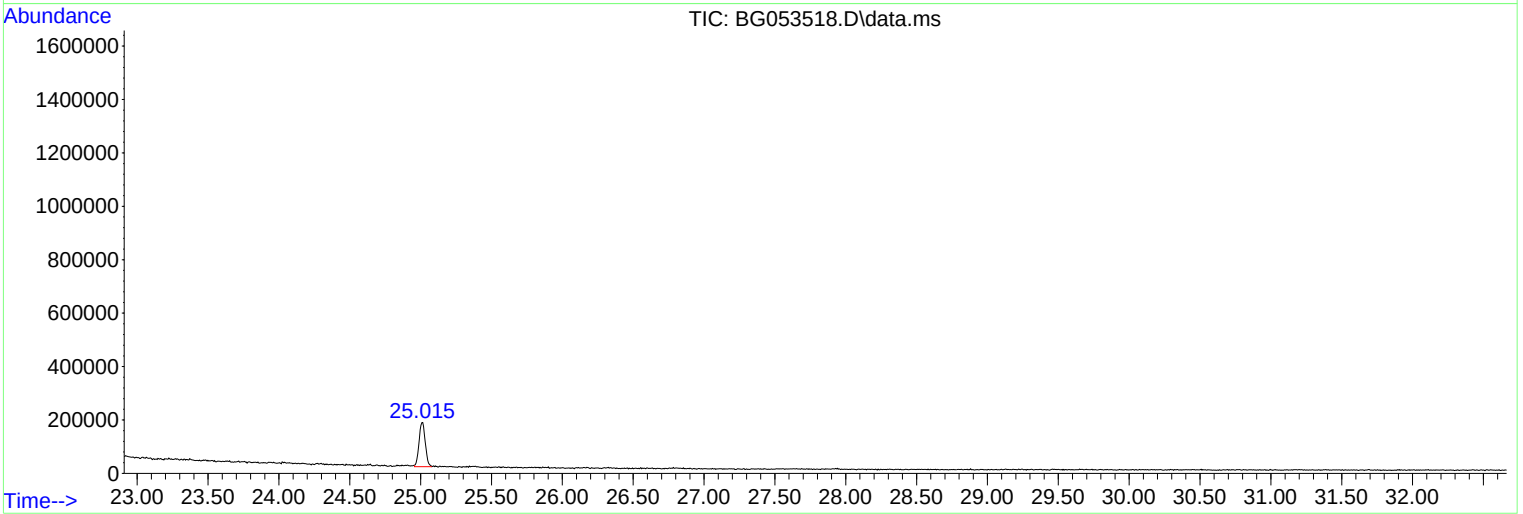
Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

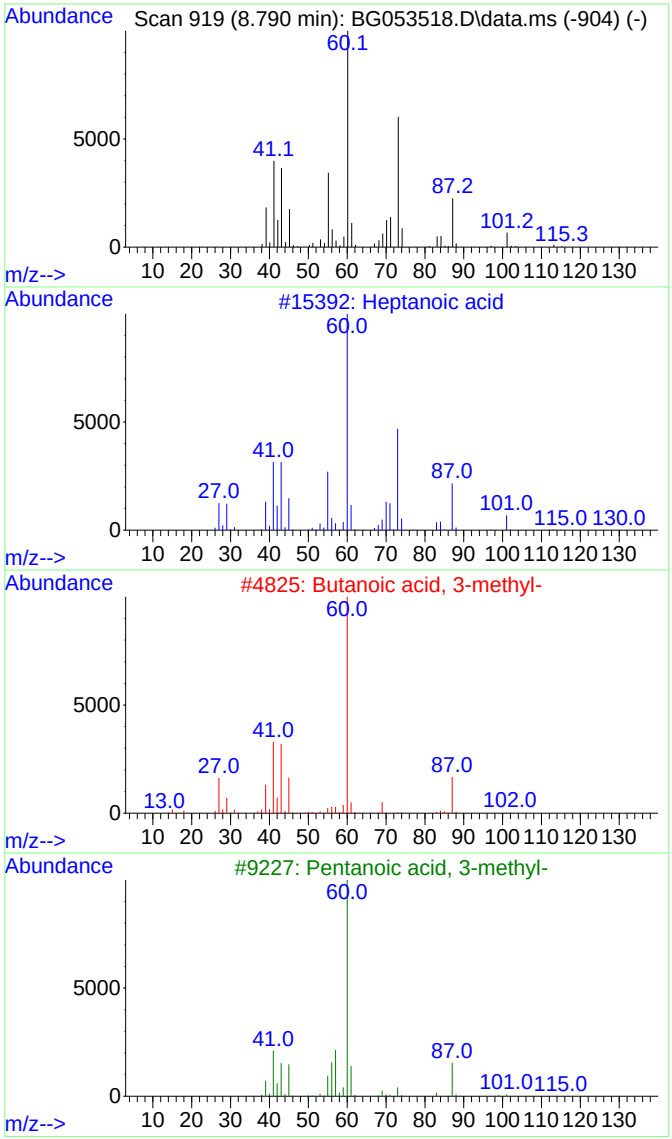
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

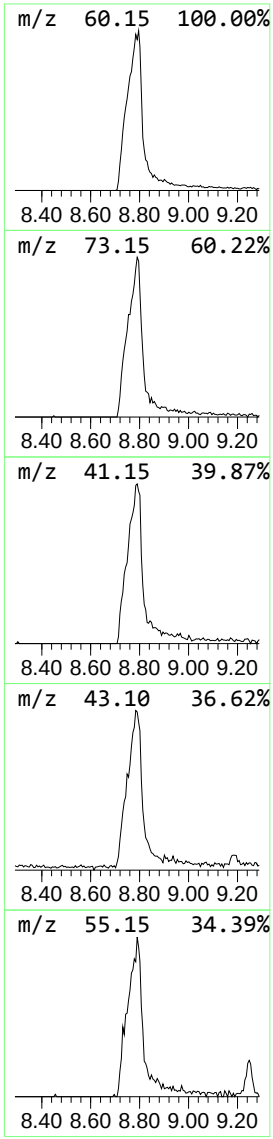
****

Peak Number 1 Heptanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.790	91.44 ng	673886	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	91
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
3	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	59
4	Pentanoic acid	102	C5H10O2	000109-52-4	58
5	Hexanoic acid	116	C6H12O2	000142-62-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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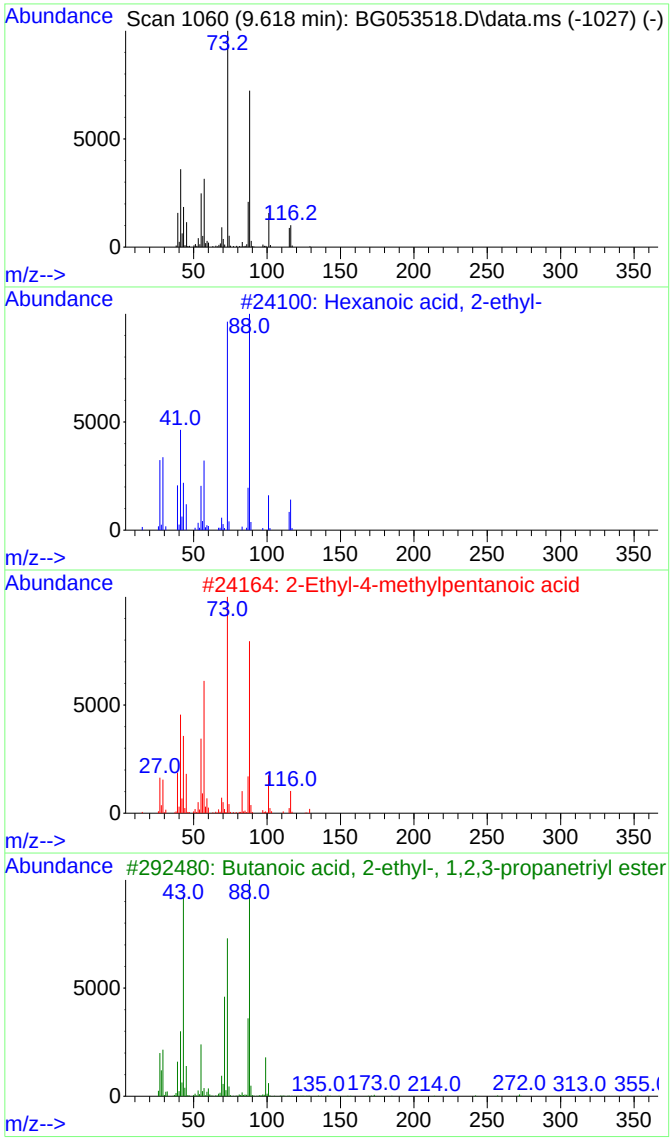
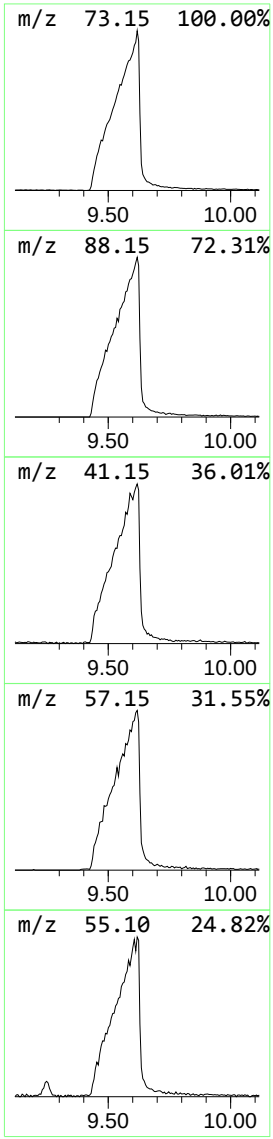
Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.618	345.46 ng	3405940	Naphthalene-d8	10.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	37
5	1,4-Dioxane	88	C4H8O2	000123-91-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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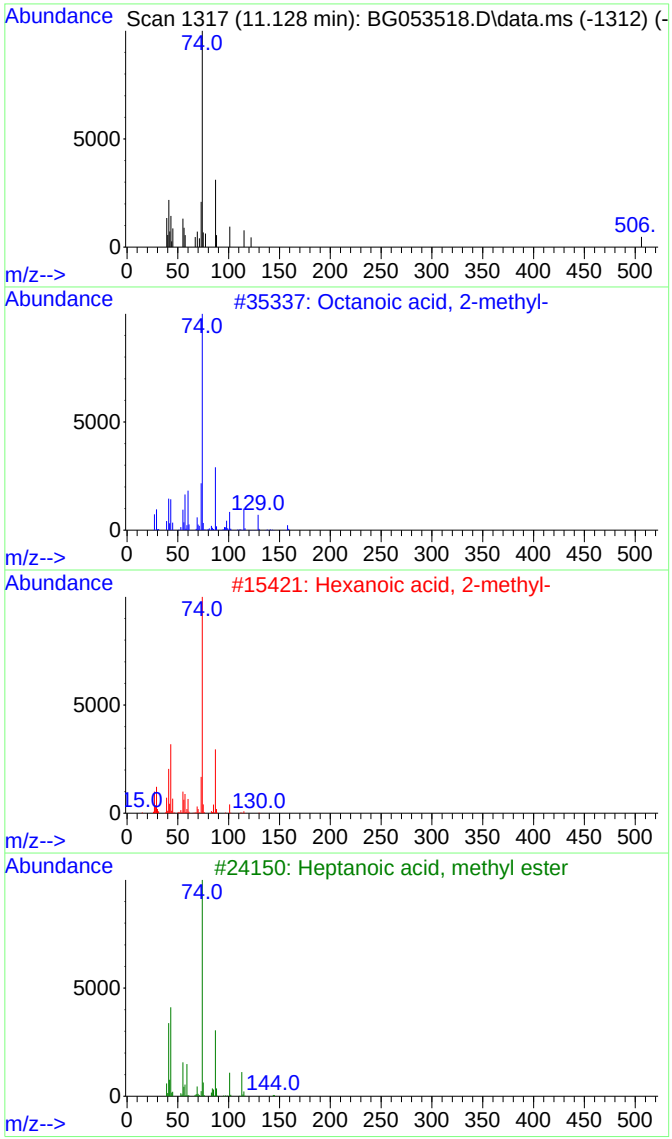
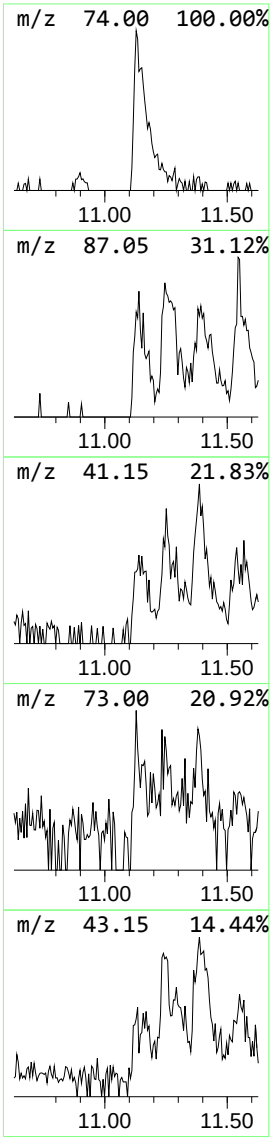
Peak Number 3 Octanoic acid, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.128	4.43 ng	43717	Naphthalene-d8	10.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	72
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3	Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	59
4	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	45
5	Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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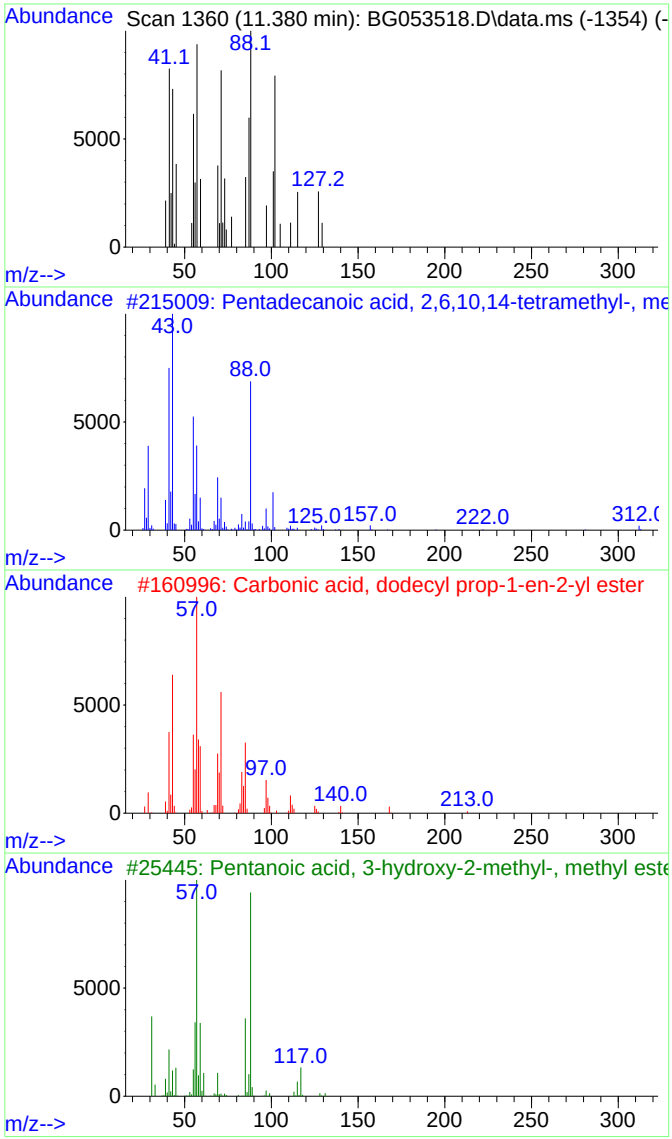
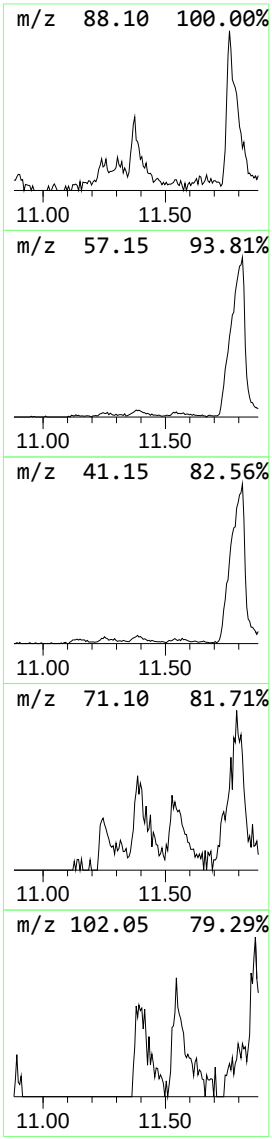
Peak Number 4 unknown11.380 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	4.94 ng	48728	Naphthalene-d8	10.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 2,6,10,14-te...	312	C20H40O2	001001-80-5	25
2	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	22
3	Pentanoic acid, 3-hydroxy-2-meth...	146	C7H14O3	060665-94-3	14
4	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	14
5	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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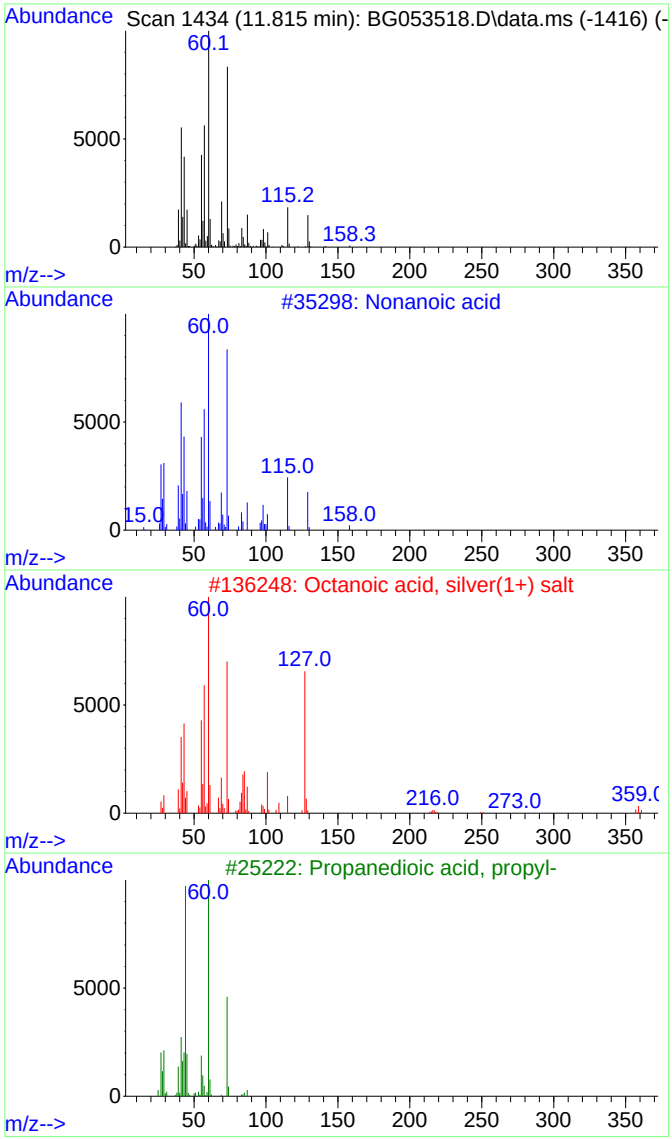
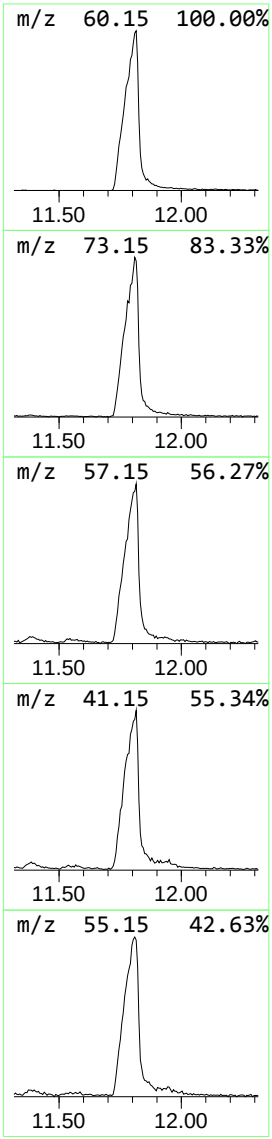
Peak Number 5 Nonanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.815	178.33 ng	1758120	Naphthalene-d8	10.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	90
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	59
4	Hexanoic acid	116	C6H12O2	000142-62-1	52
5	Butanoic acid	88	C4H8O2	000107-92-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

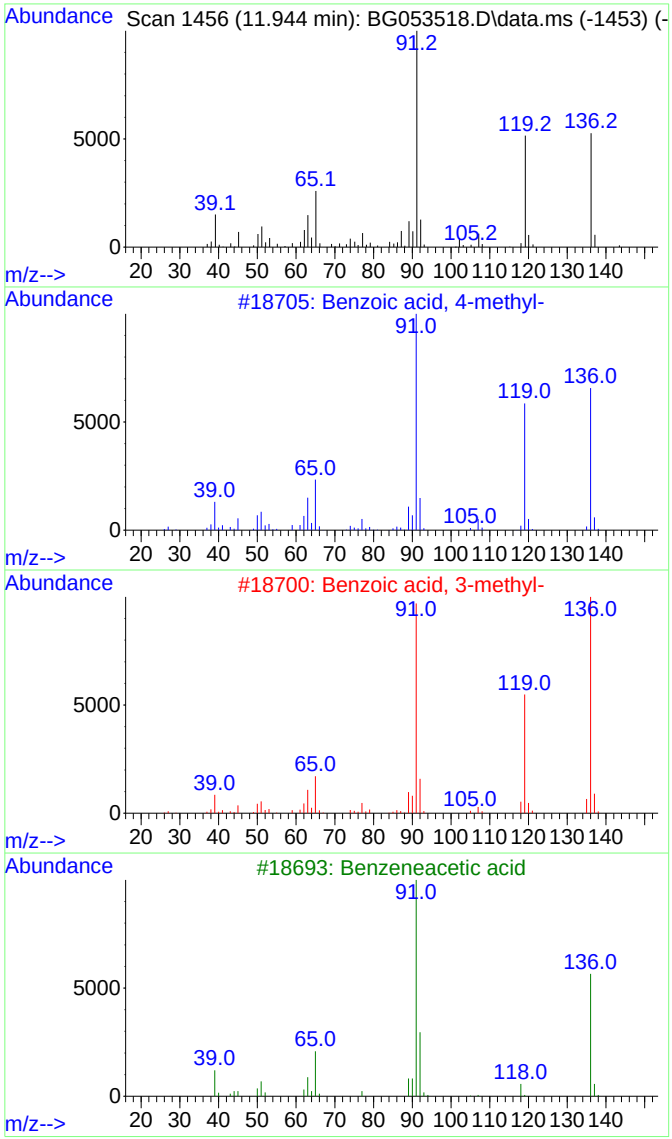
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

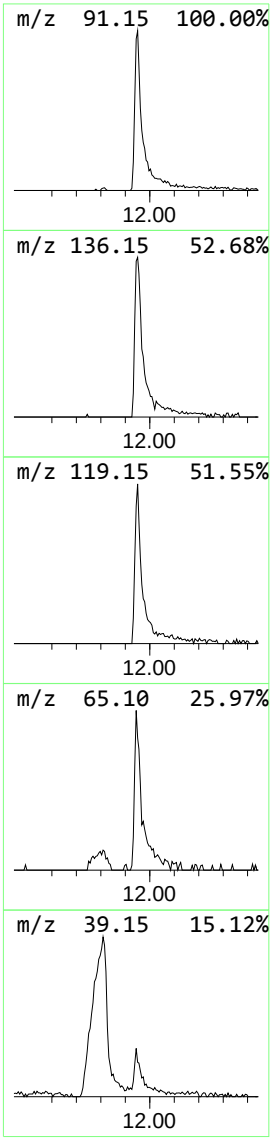
****

Peak Number 6 Benzoic acid, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	22.13 ng	218142	Naphthalene-d8	10.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	87
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	60
4	4-Methylbenzoyl isothiocyanate	177	C9H7NOS	016794-68-6	52
5	m-Toluamide	135	C8H9NO	000618-47-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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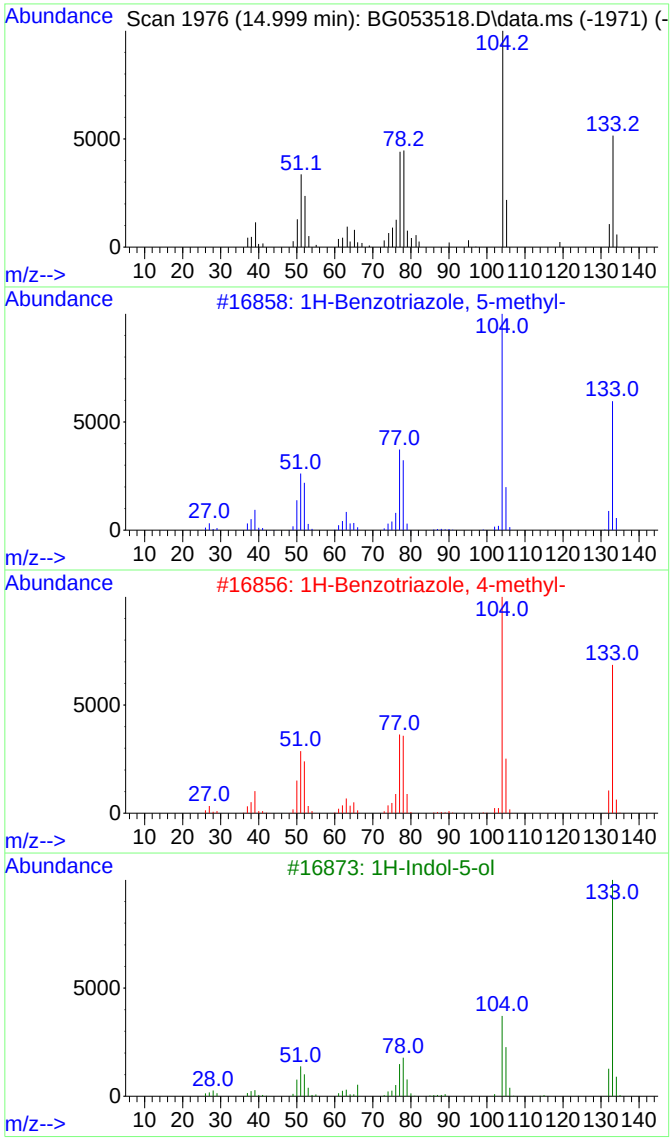
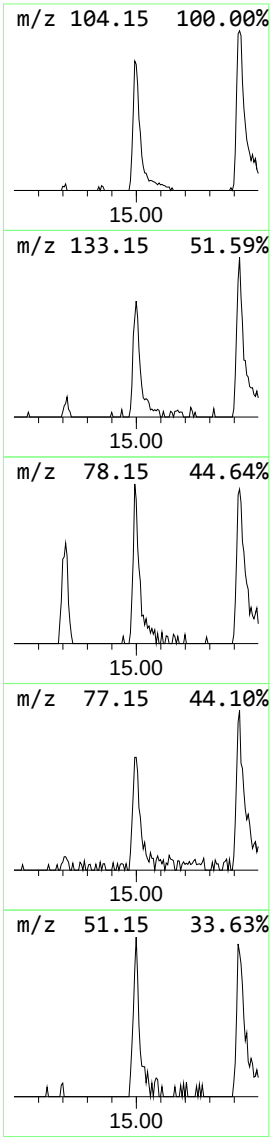
Peak Number 7 1H-Benzotriazole, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.999	4.39 ng	68679	Acenaphthene-d10	14.711

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	93
3	1H-Indol-5-ol	133	C8H7NO	001953-54-4	91
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	80
5	1H-Indol-4-ol	133	C8H7NO	002380-94-1	49





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Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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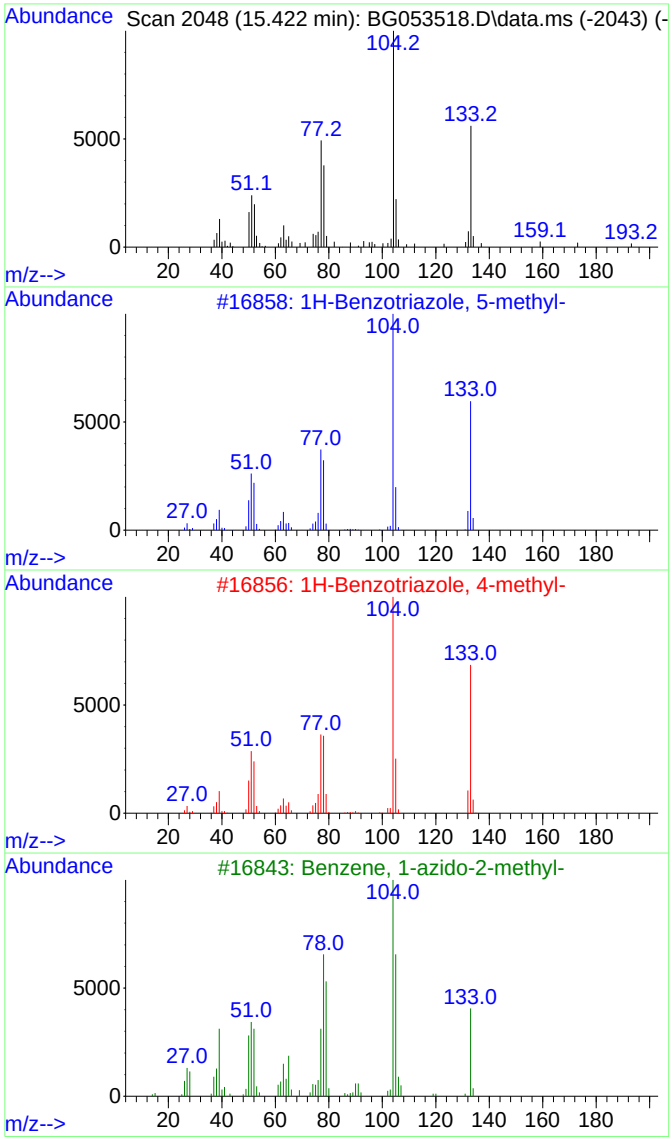
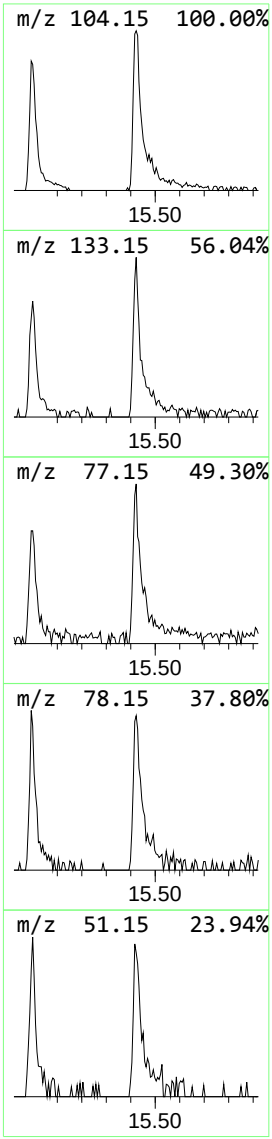
Peak Number 8 1H-Benzotriazole, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.422	6.67 ng	104436	Acenaphthene-d10	14.711

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	94
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	90
3	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	74
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	74
5	1H-Indol-5-ol	133	C8H7NO	001953-54-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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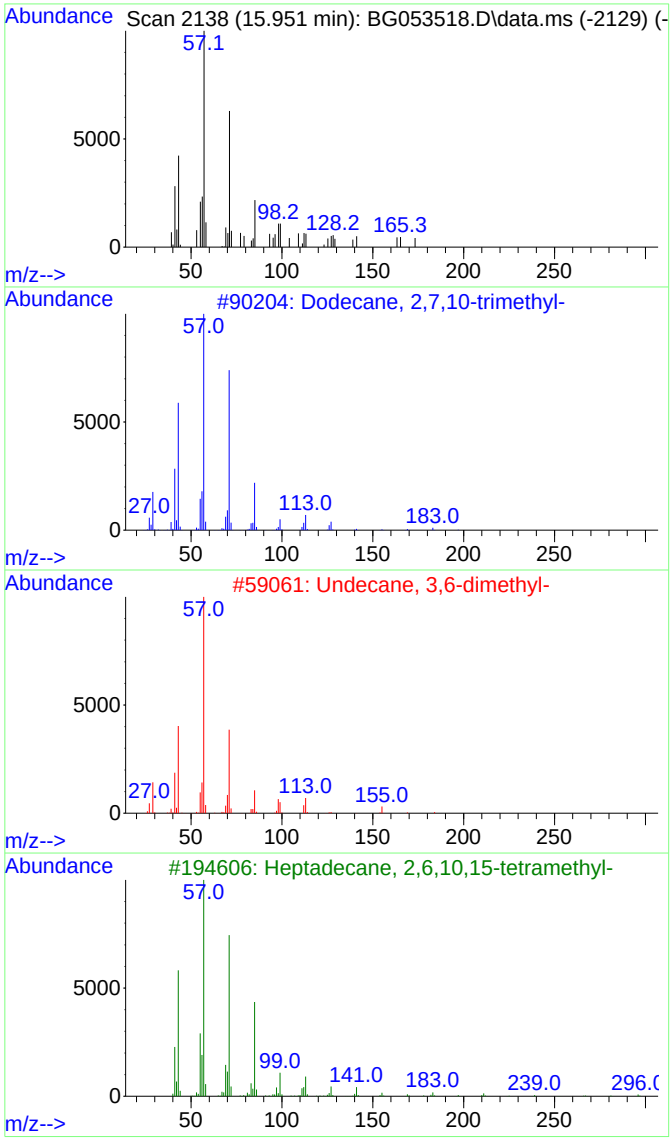
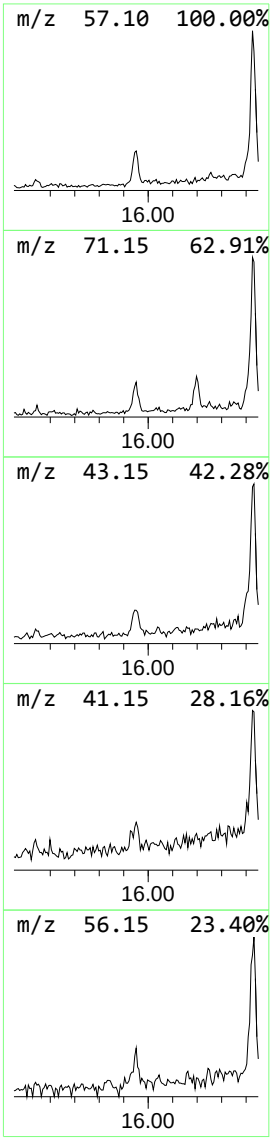
Peak Number 9 Dodecane, 2,7,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.34 ng	36659	Acenaphthene-d10	14.711

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	53
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	50
4	Dodecane	170	C12H26	000112-40-3	50
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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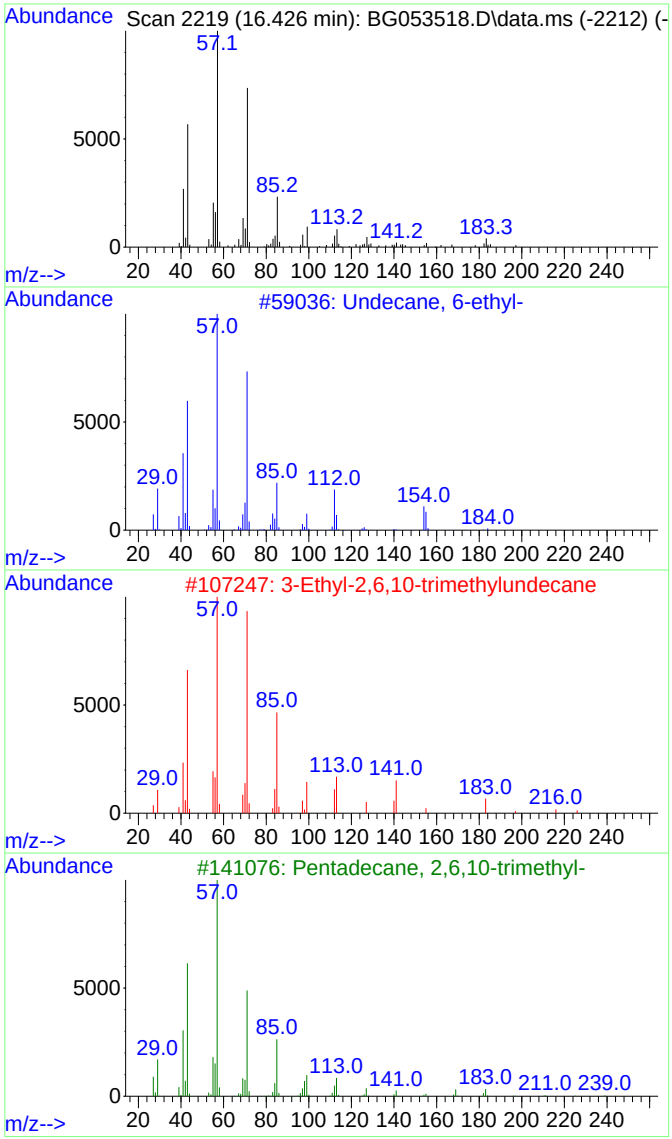
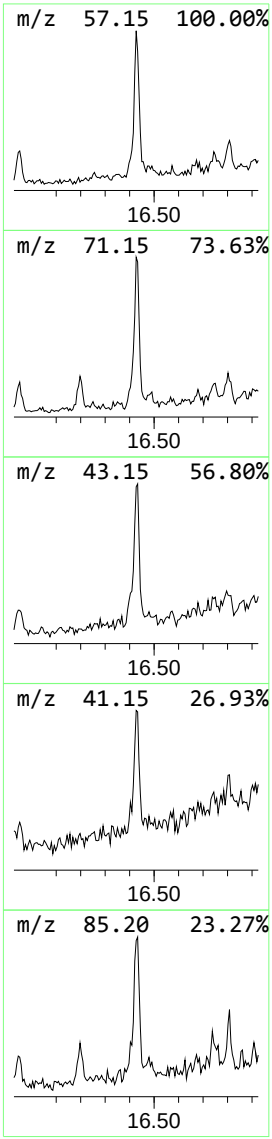
Peak Number 10 Undecane, 6-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.426	6.69 ng	139769	Phenanthrene-d10	17.454

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
2	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	50
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	46
4	Eicosane	282	C20H42	000112-95-8	46
5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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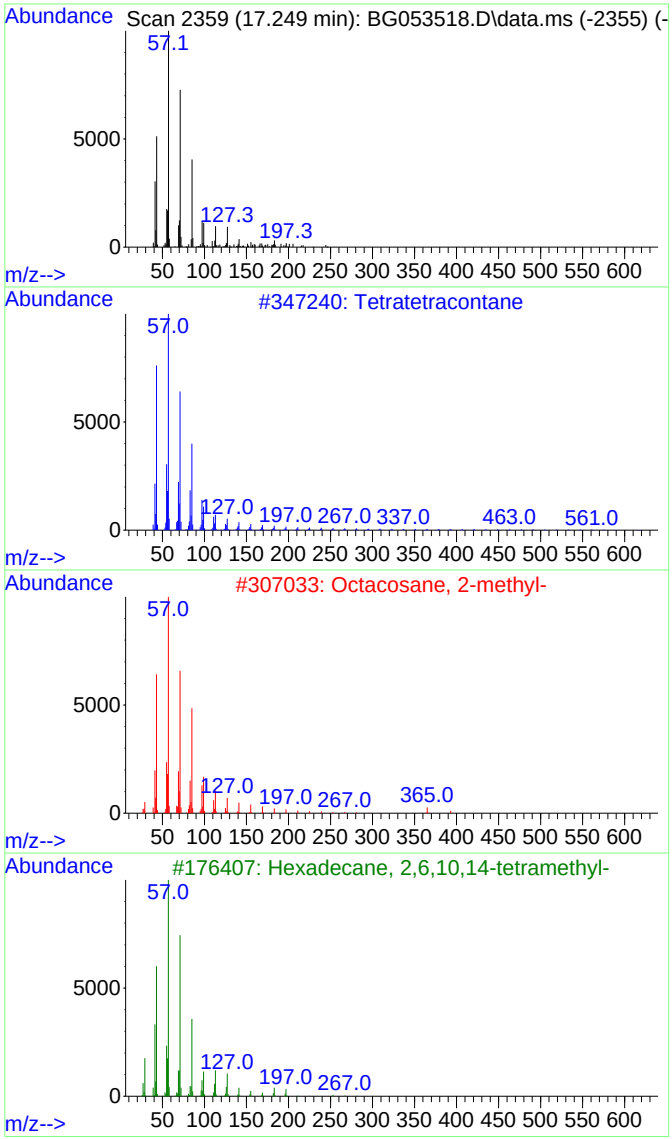
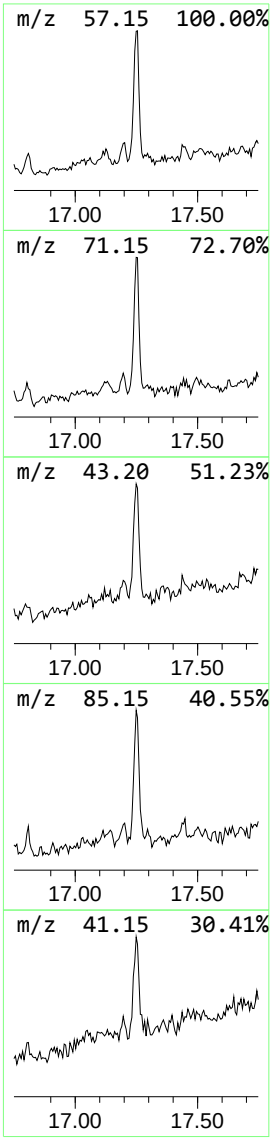
Peak Number 11 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.249	7.10 ng	148264	Phenanthrene-d10	17.454

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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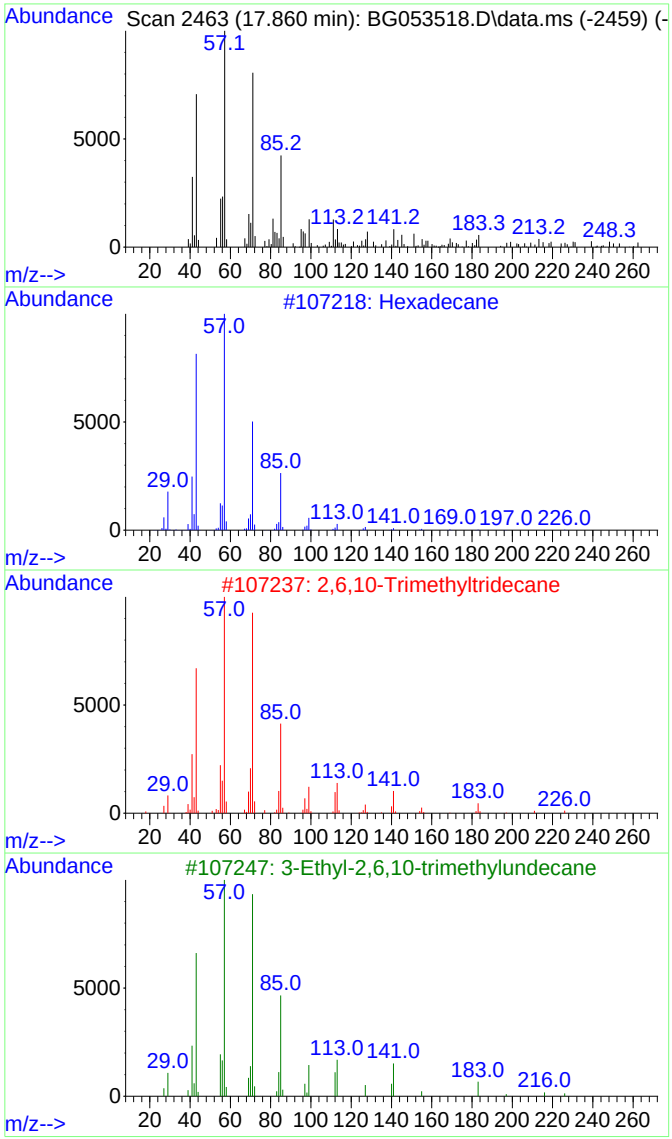
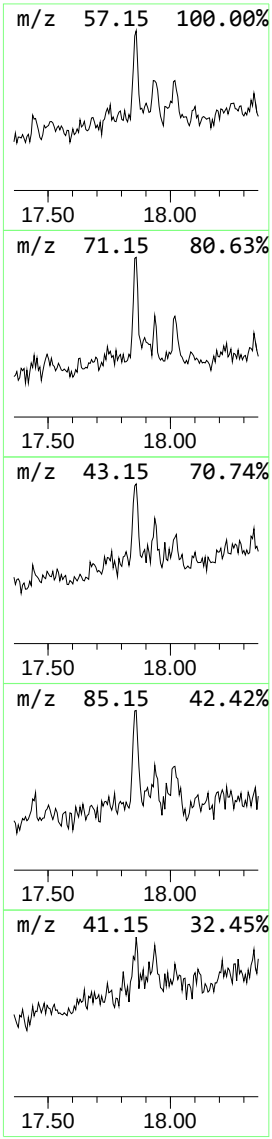
Peak Number 12 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.860	4.61 ng	96358	Phenanthrene-d10	17.454

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	87
3	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	83
4	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	83
5	Octane, 2-methyl-	128	C9H20	003221-61-2	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051022\
Data File : BG053518.D
Acq On : 10 May 2022 21:31
Operator : CG/JU
Sample : N2763-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4-20220509-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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
Heptanoic acid	8.790	91.4	ng	673886	1	8.085	147397	20.0
Hexanoic acid, ...	9.618	345.5	ng	3405940	2	10.899	197180	20.0
Octanoic acid, ...	11.128	4.4	ng	43717	2	10.899	197180	20.0
unknown11.380	11.380	4.9	ng	48728	2	10.899	197180	20.0
Nonanoic acid	11.815	178.3	ng	1758120	2	10.899	197180	20.0
Benzoic acid, 4...	11.944	22.1	ng	218142	2	10.899	197180	20.0
1H-Benzotriazol...	14.999	4.4	ng	68679	3	14.711	313130	20.0
1H-Benzotriazol...	15.422	6.7	ng	104436	3	14.711	313130	20.0
Dodecane, 2,7,1...	15.951	2.3	ng	36659	3	14.711	313130	20.0
Undecane, 6-ethyl-	16.426	6.7	ng	139769	4	17.454	417834	20.0
Tetratetracontane	17.249	7.1	ng	148264	4	17.454	417834	20.0
Hexadecane	17.860	4.6	ng	96358	4	17.454	417834	20.0