LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.362	9	12	20	rVB	27185	41441	1.11%	0.201%
2	4.702	233	240	245	rBV	33015	50286	1.35%	0.243%
3	5.318	337	345	353	rBV	334981	517796	13.87%	2.506%
4	5.794	418	426	437	rBV	1105129	1760517	47.16%	8.519%
5	7.404	692	700	715	rVB	1102058	1924198	51.54%	9.311%
6	8.262	838	846	853	rBV	199692	340810	9.13%	1.649%
7	9.437	1036	1046	1055	rBV	657551	1182667	31.68%	5.723%
8	10.841	1278	1285	1293	rBV	58049	111615	2.99%	0.540%
9	11.094	1320	1328	1337	rBV	292720	529679	14.19%	2.563%
10	13.515	1730	1740	1747	rBV	1809689	2815351	75.41%	13.623%
11	14.884	1966	1973	1981	rVB	482645	785071	21.03%	3.799%
12	16.370	2218	2226	2236	rBV	1488885	2361243	63.25%	11.426%
13	17.628	2434	2440	2445	rBV	611303	941729	25.22%	4.557%
14	17.669	2445	2447	2455	rVB	44535	62791	1.68%	0.304%
15	18.485	2581	2586	2593	rBV	353738	538013	14.41%	2.603%
16	19.666	2783	2787	2793	rVB	135339	187267	5.02%	0.906%
17	19.749	2797	2801	2808	rBV	249047	342599	9.18%	1.658%
18	20.025	2845	2848	2854	rVB	105036	157468	4.22%	0.762%
19	20.219	2875	2881	2886	rBV	2745115	3733375	100.00%	18.065%
20	21.535	3102	3105	3118	rVB3	90038	198331	5.31%	0.960%
21	21.928	3165	3172	3178	rBV2	563659	1020928	27.35%	4.940%
22	25.360	3748	3756	3773	rVB2	338220	1062606	28.46%	5.142%

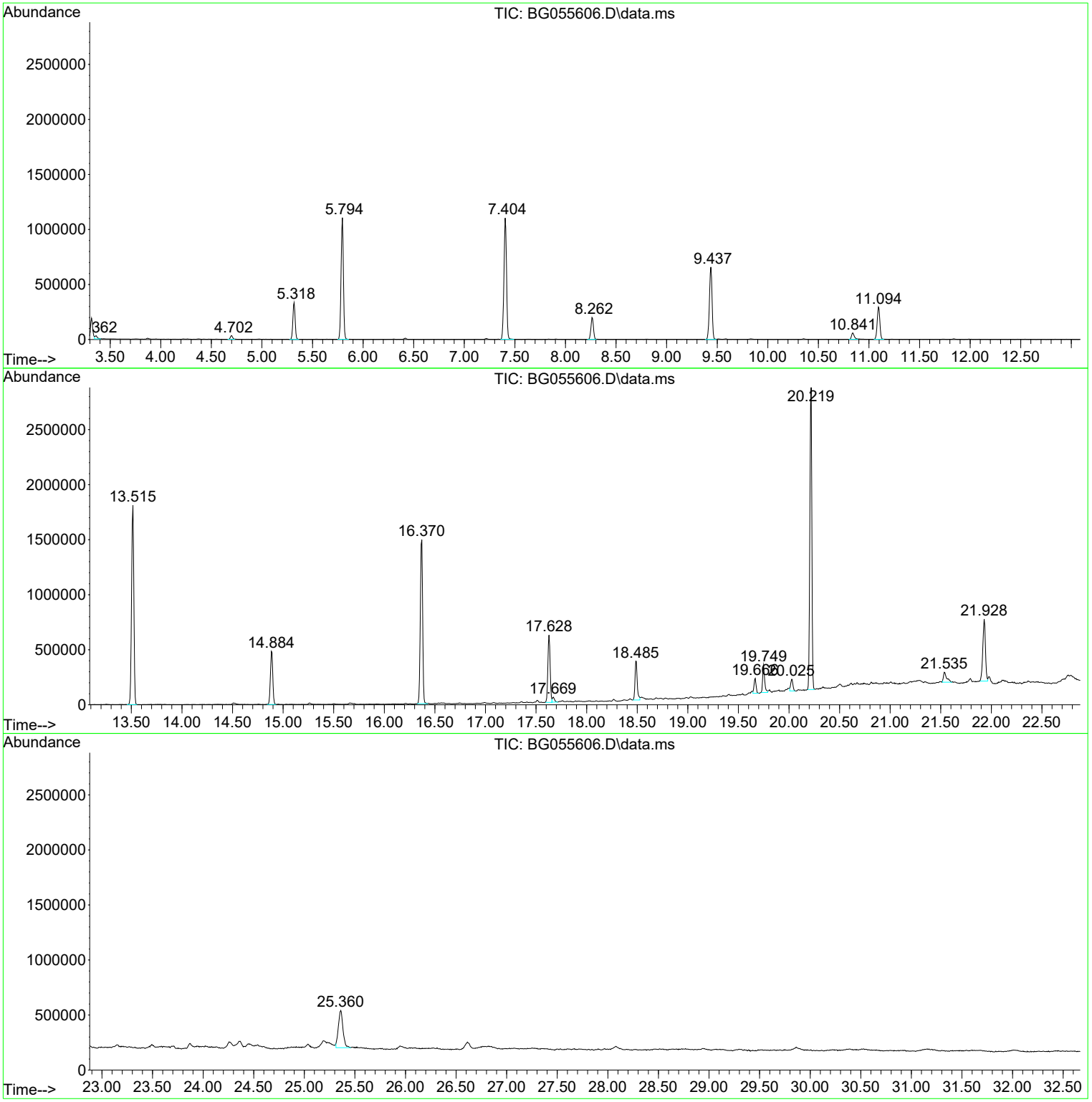
Sum of corrected areas: 20665781

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

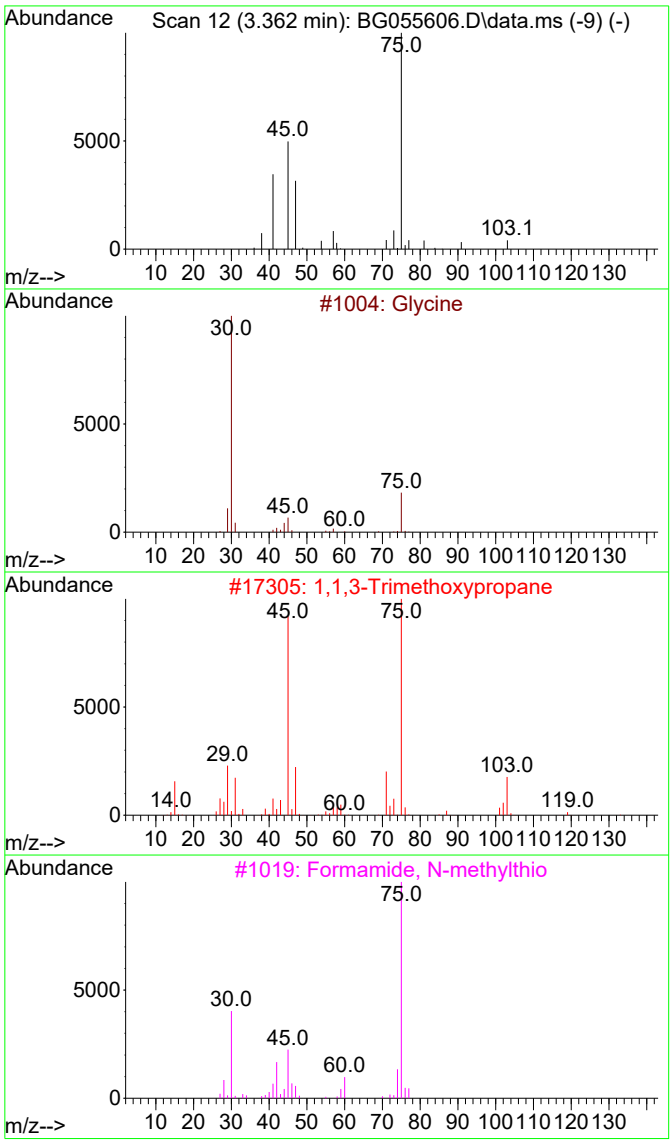
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

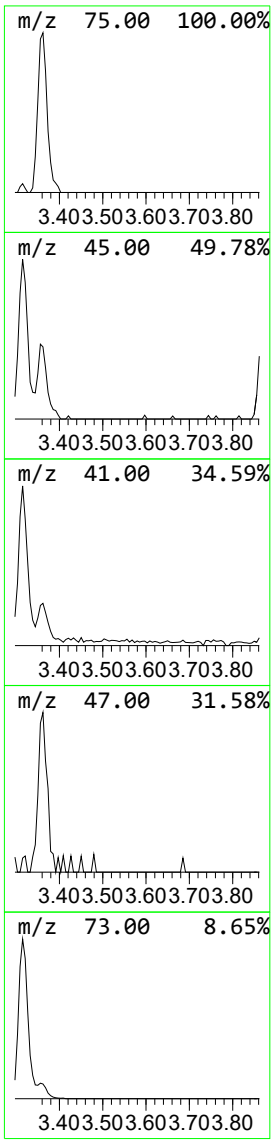
****

Peak Number 1 unknown3.362 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.362	2.43 ng	41441	1,4-Dichlorobenzene-d4	8.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycine	75	C2H5NO2	000056-40-6	4
2	1,1,3-Trimethoxypropane	134	C6H14O3	014315-97-0	4
3	Formamide, N-methylthio	75	C2H5NS	018952-41-5	3
4	Ethanethioamide	75	C2H5NS	000062-55-5	3
5	N-Formylglycine	103	C3H5NO3	002491-15-8	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

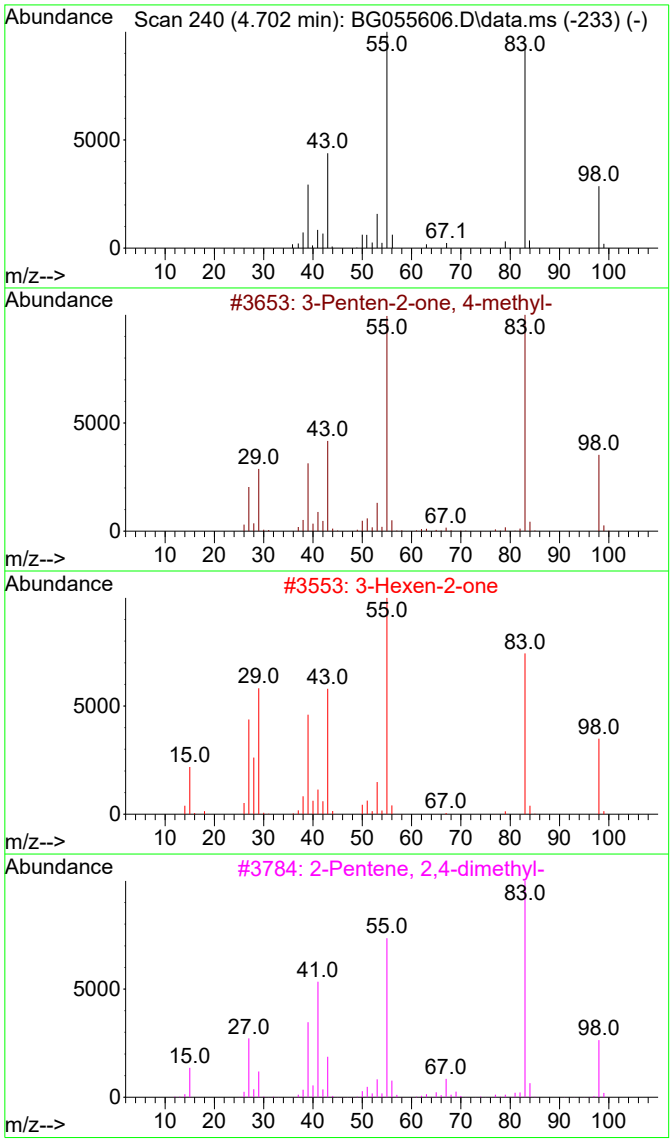
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

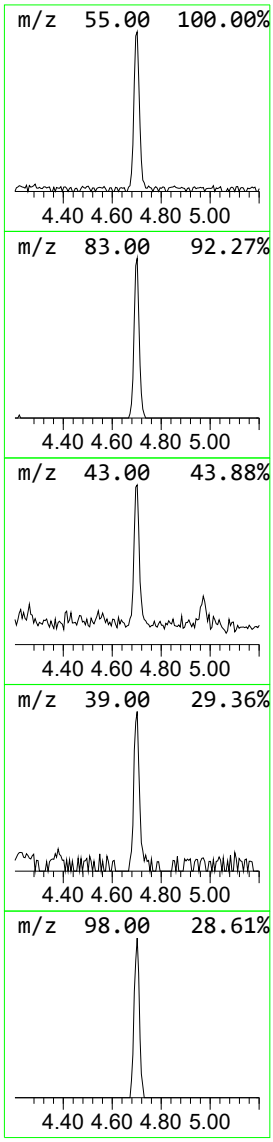
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.702	2.95 ng	50286	1,4-Dichlorobenzene-d4	8.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

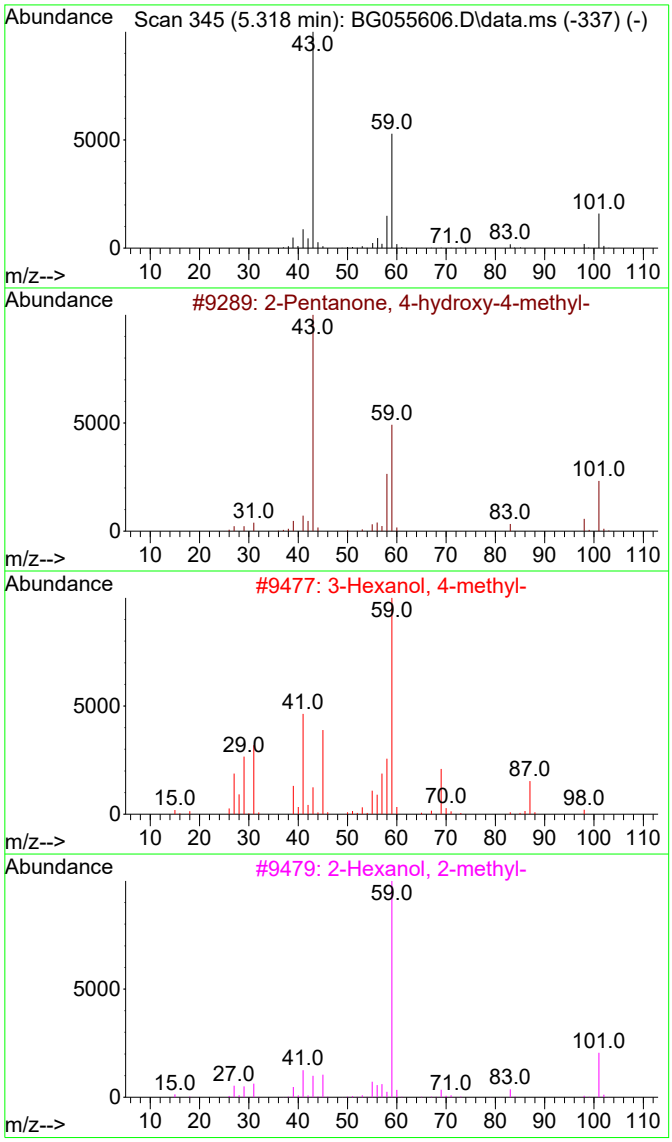
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

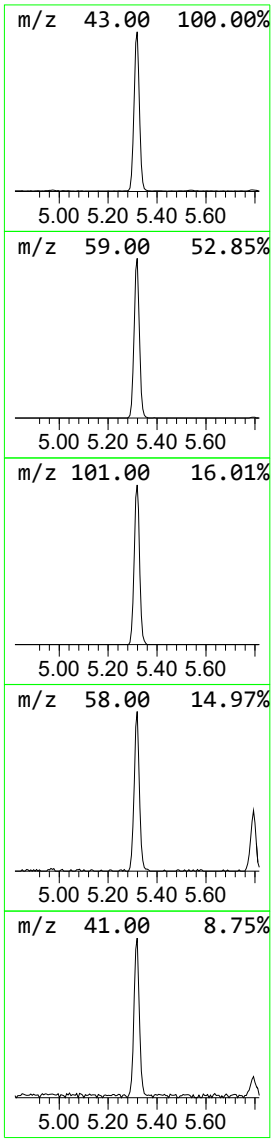
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.318	30.39 ng	517796	1,4-Dichlorobenzene-d4	8.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

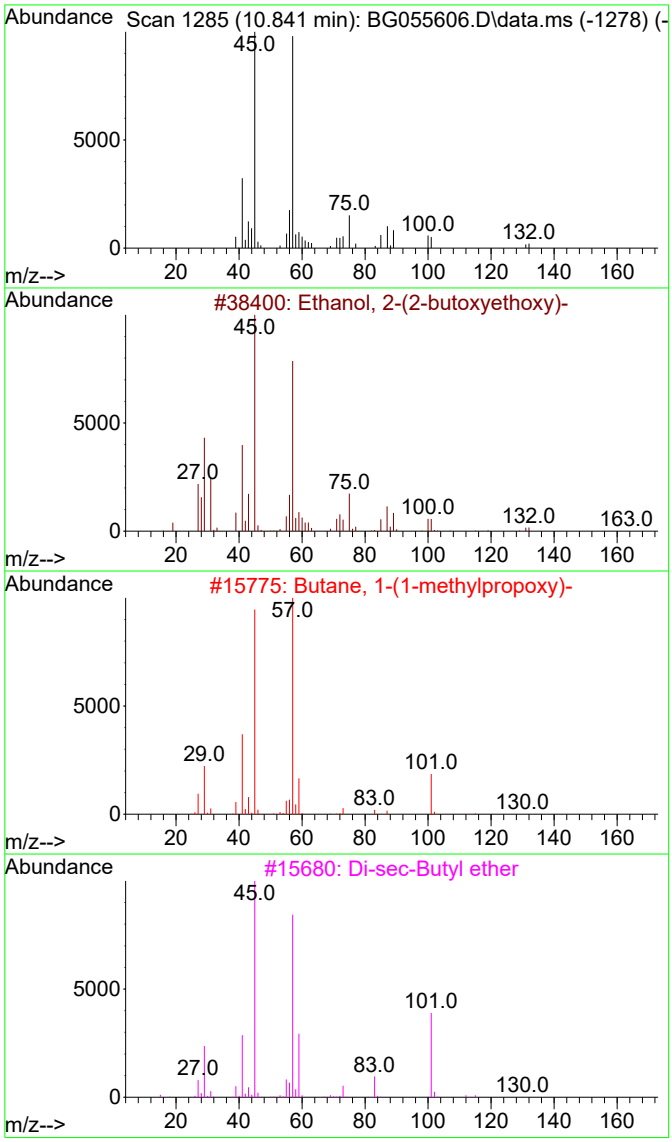
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

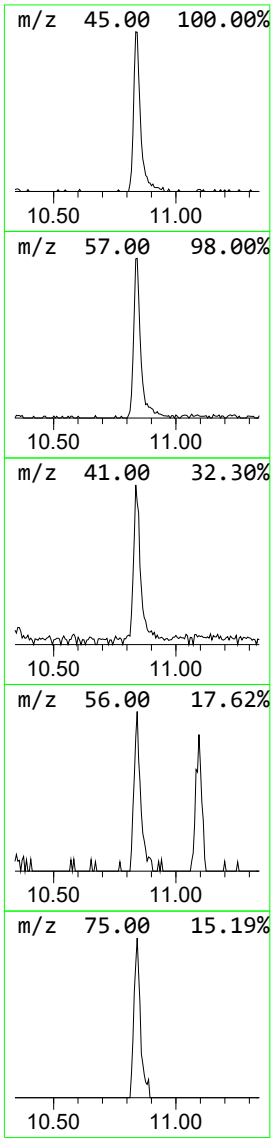
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.841	4.21 ng	111615	Naphthalene-d8	11.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

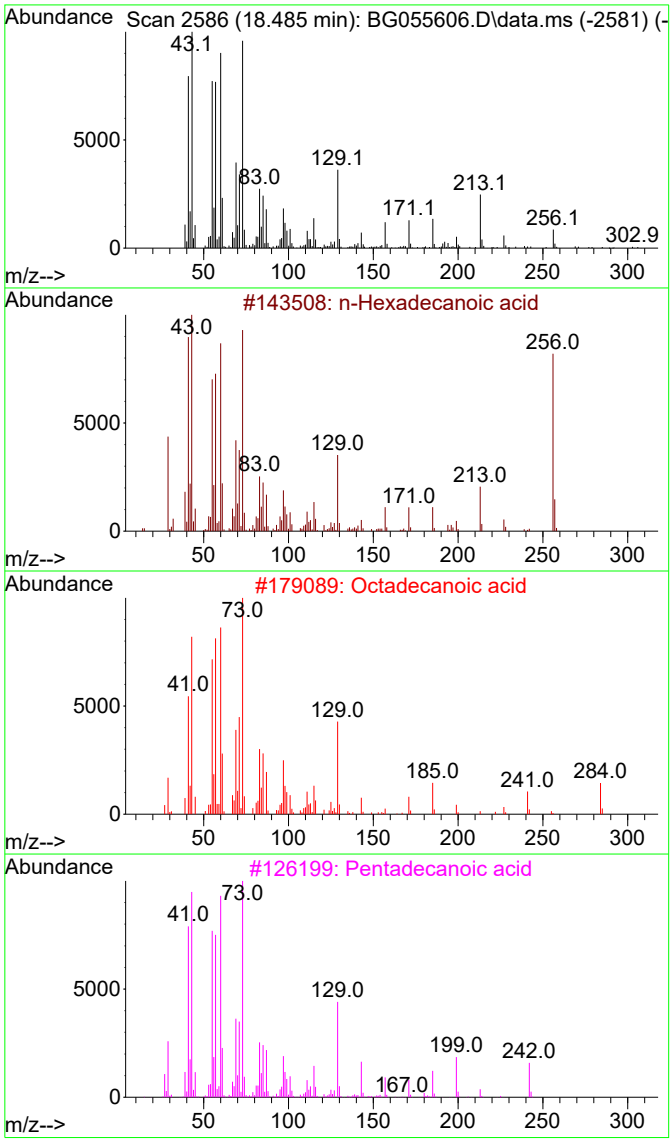
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

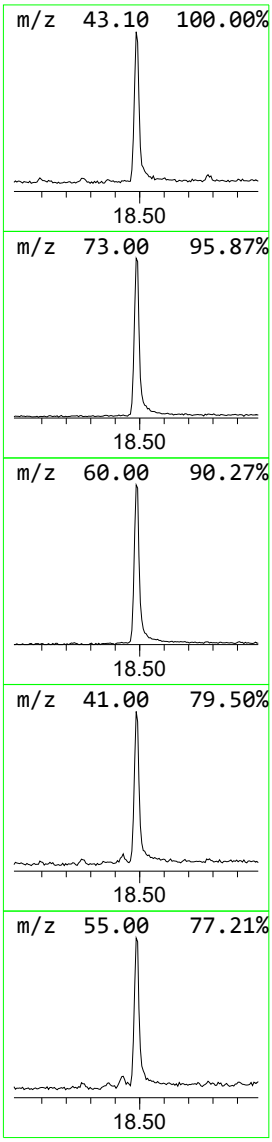
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.485	11.43 ng	538013	Phenanthrene-d10	17.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

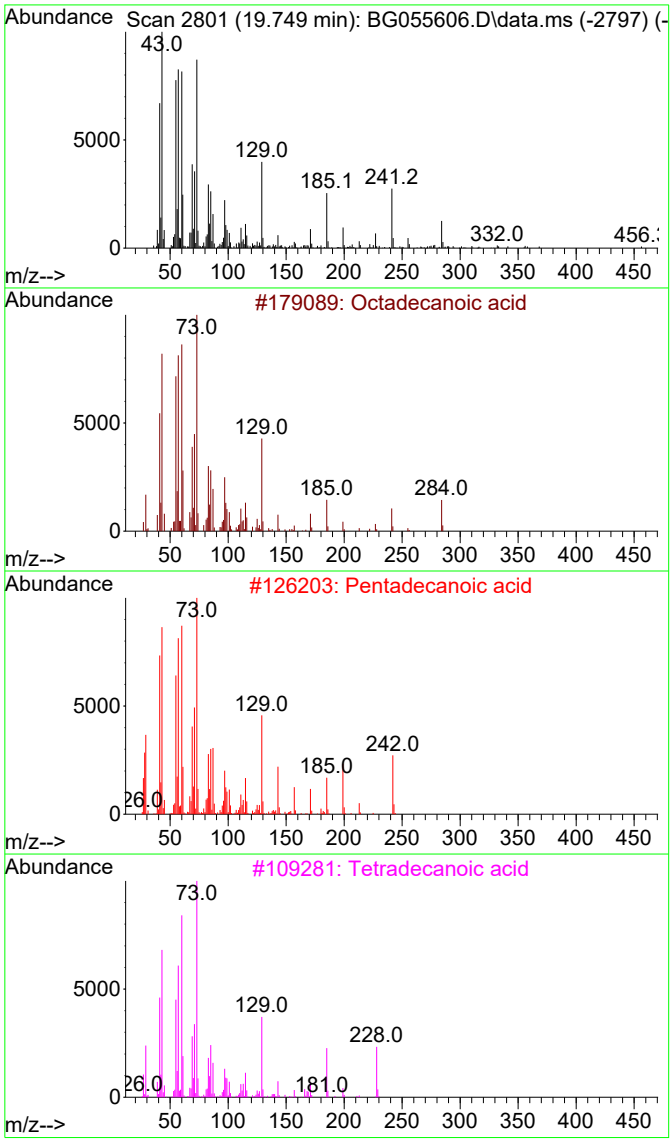
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

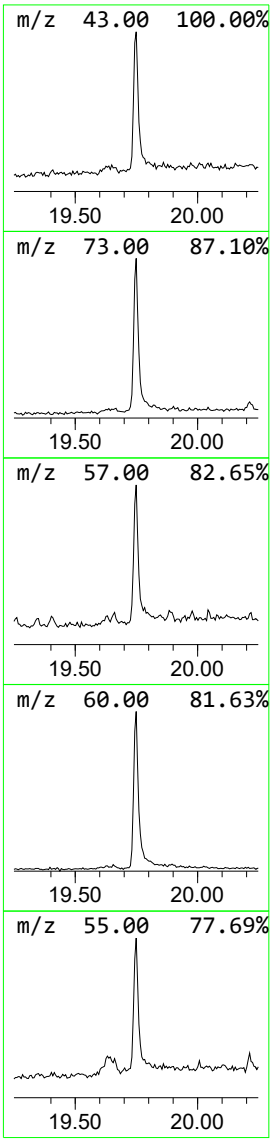
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.749	7.28 ng	342599	Phenanthrene-d10	17.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

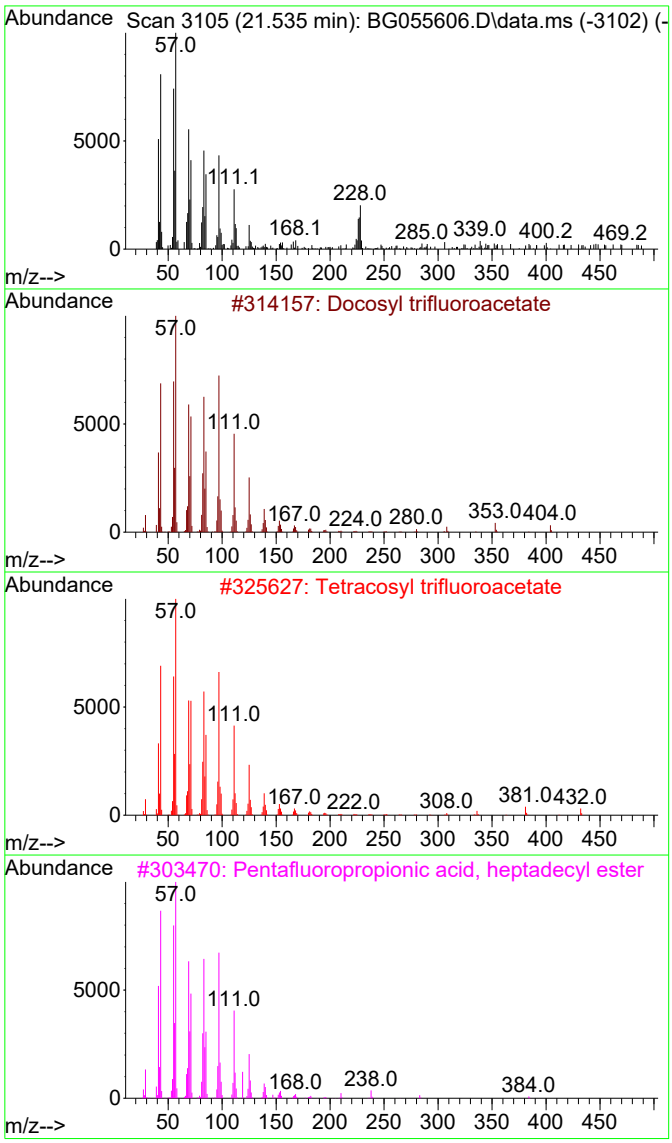
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

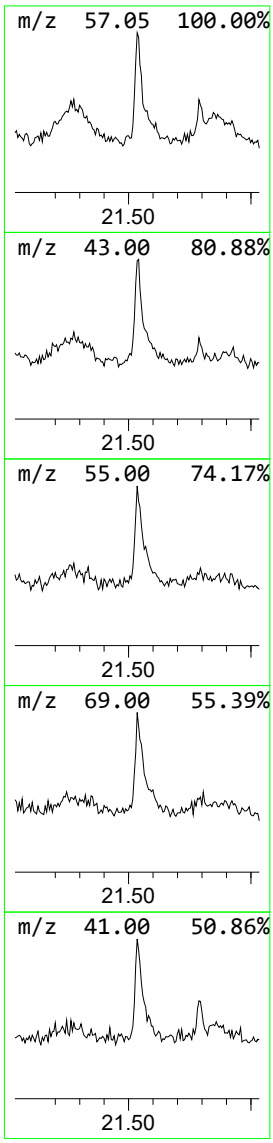
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Docosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.535	3.89 ng	198331	Chrysene-d12	21.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	74
2	Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	74
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	74
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	74
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055606.D
Acq On : 14 Nov 2022 16:00
Operator : CG/JU
Sample : N5537-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
unknown3.362	3.362	2.4	ng	41441	1	8.262	340810	20.0
3-Penten-2-one,...	4.702	3.0	ng	50286	1	8.262	340810	20.0
2-Pentanone, 4-...	5.318	30.4	ng	517796	1	8.262	340810	20.0
Ethanol, 2-(2-b...	10.841	4.2	ng	111615	2	11.094	529679	20.0
n-Hexadecanoic ...	18.485	11.4	ng	538013	4	17.628	941729	20.0
Octadecanoic acid	19.749	7.3	ng	342599	4	17.628	941729	20.0
Docosyl trifluo...	21.535	3.9	ng	198331	5	21.928	1020930	20.0