LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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: BG055544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.353	4	11	25	rVB	493445	948078	22.72%	5.143%
2	3.646	57	61	69	rVB	96045	126070	3.02%	0.684%
3	4.087	131	136	147	rVB	201974	284211	6.81%	1.542%
4	4.716	236	243	255	rVB	827958	1245069	29.84%	6.754%
5	4.833	258	263	268	rBV2	38981	60179	1.44%	0.326%
6	5.297	337	342	344	rBV2	42741	66995	1.61%	0.363%
7	5.327	344	347	354	rVB	133458	188349	4.51%	1.022%
8	5.797	420	427	439	rVB	1006671	1628572	39.03%	8.834%
9	7.407	691	701	712	rBV	866855	1544994	37.03%	8.381%
10	8.270	838	848	855	rVB	179959	301643	7.23%	1.636%
11	8.835	938	944	950	rVB2	28292	46390	1.11%	0.252%
12	9.440	1036	1047	1058	rBV	609454	1077427	25.82%	5.844%
13	11.097	1322	1329	1336	rBV	223957	399585	9.58%	2.168%
14	13.517	1733	1741	1749	rBV	1606874	2434121	58.34%	13.204%
15	14.886	1966	1974	1981	rBV	297122	463561	11.11%	2.515%
16	16.367	2218	2226	2238	rBV	1239971	1905505	45.67%	10.336%
17	17.624	2434	2440	2448	rBV	448184	692222	16.59%	3.755%
18	18.488	2583	2587	2596	rBV4	42524	74203	1.78%	0.403%
19	19.751	2798	2802	2810	rBV4	36906	69211	1.66%	0.375%
20	20.215	2871	2881	2887	rBV	3061075	4172380	100.00%	22.633%
21	21.925	3165	3172	3179	rBV	392199	706331	16.93%	3.831%

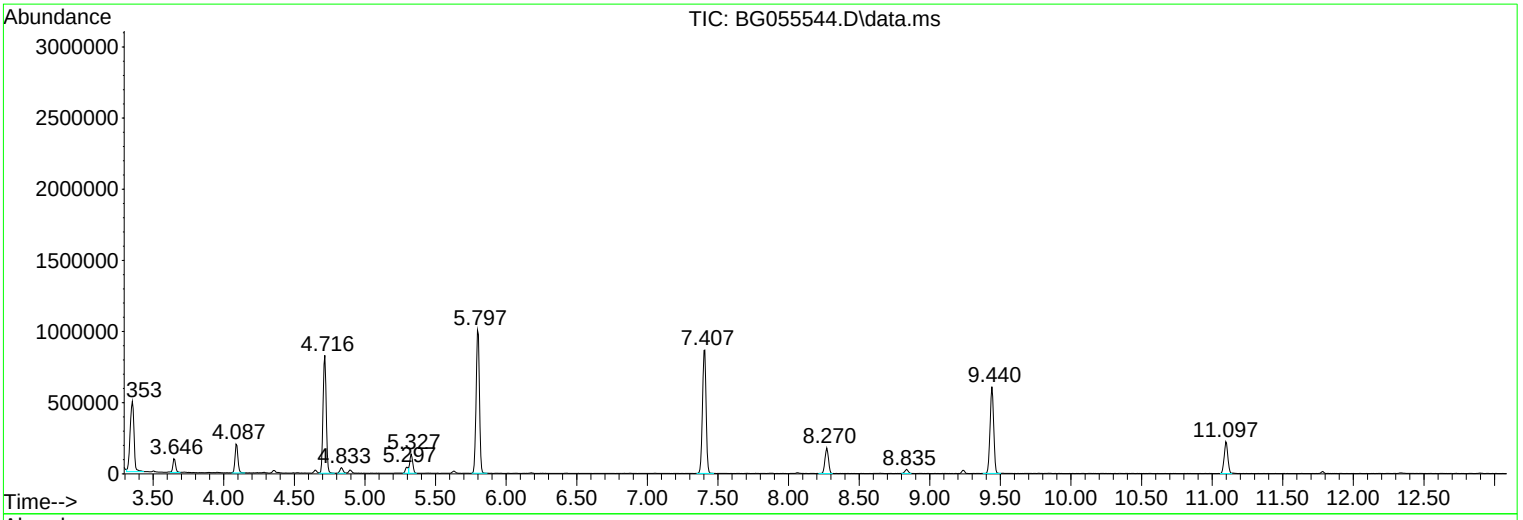
Sum of corrected areas: 18435096

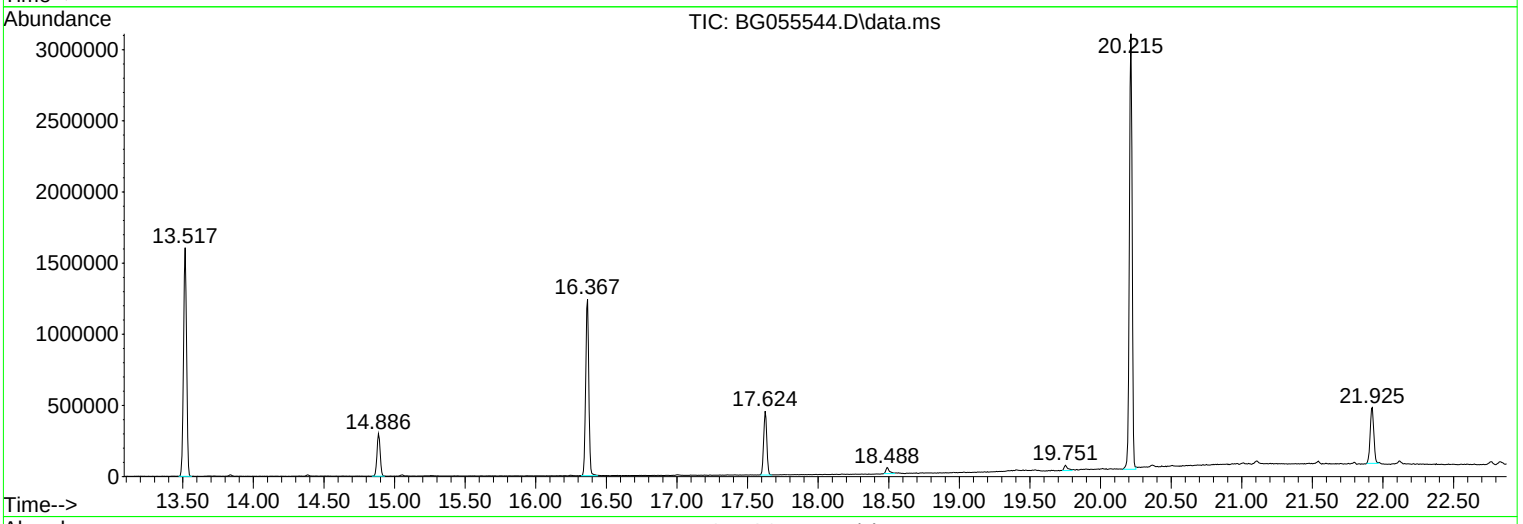
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

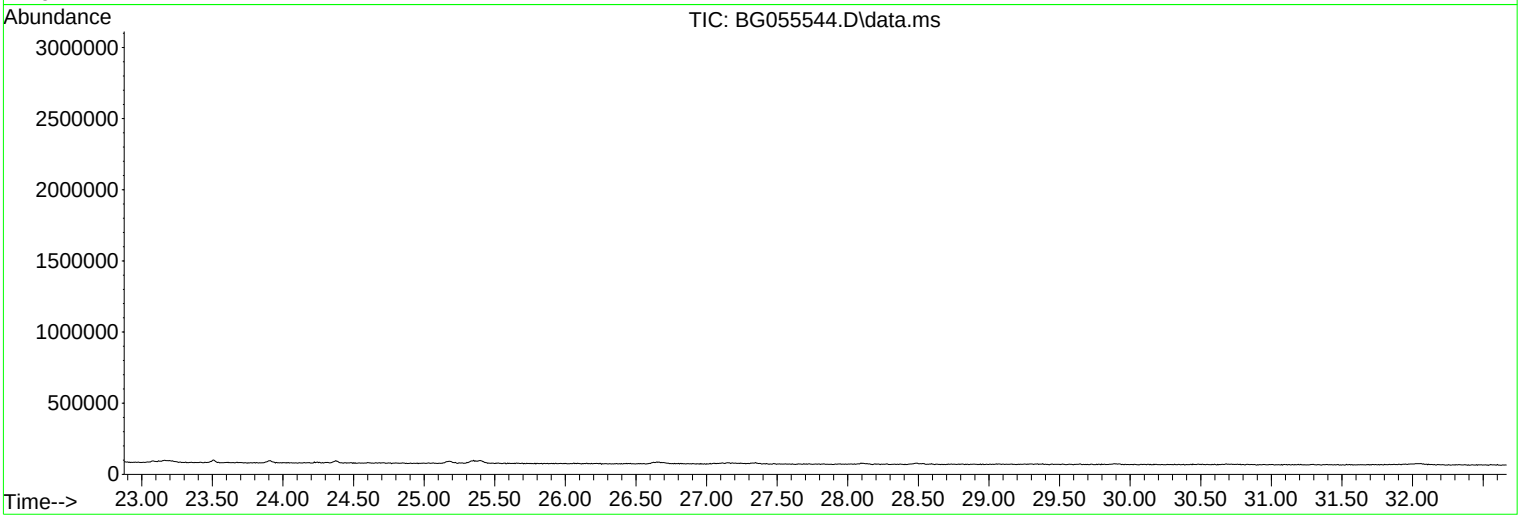
Instrument :
BNA_G
ClientSampleId :
TP-4

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\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

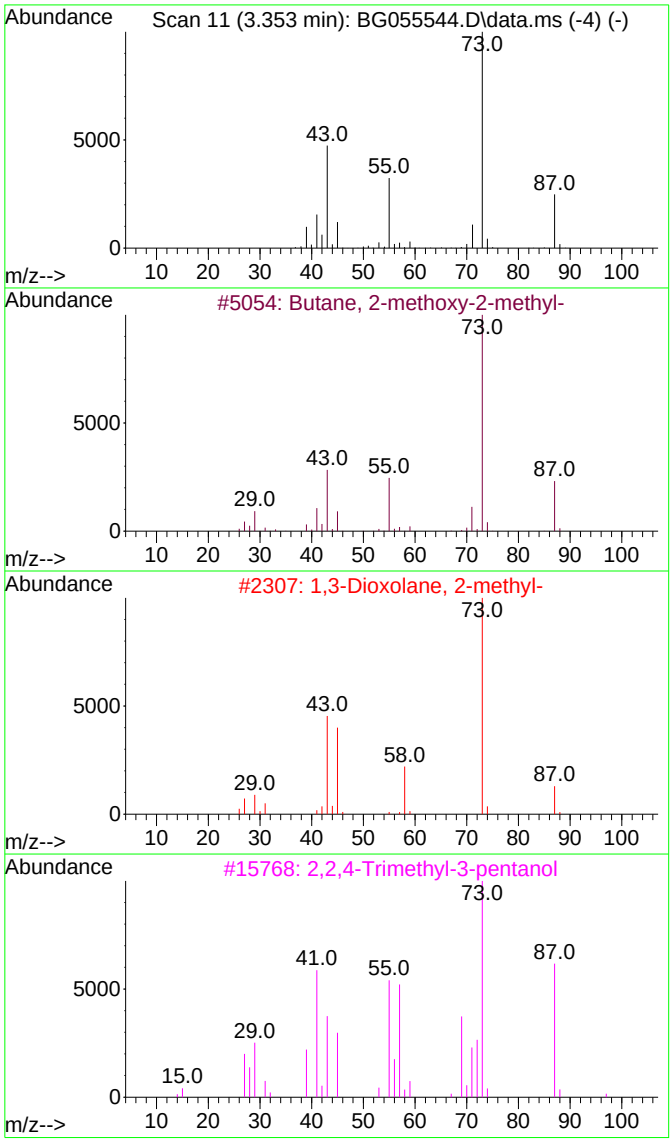
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

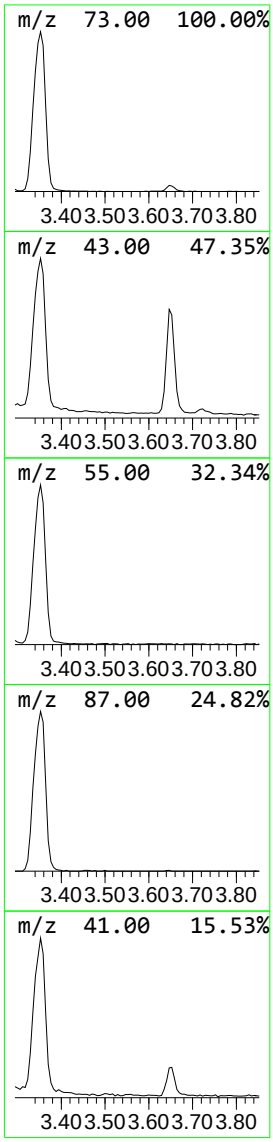
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.353	62.86 ng	948078	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

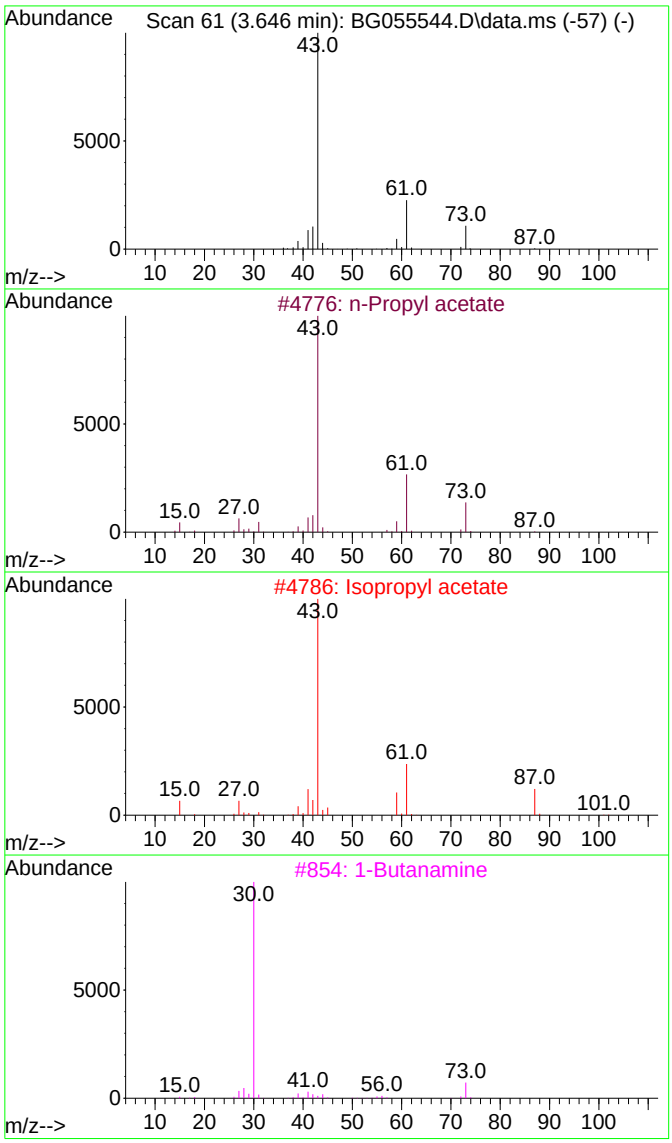
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

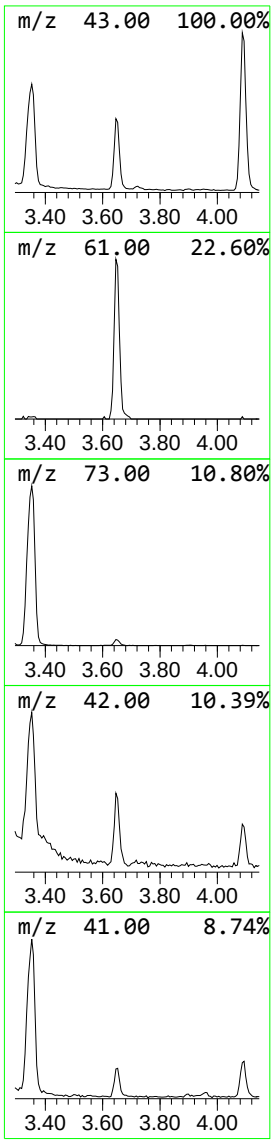
****

Peak Number 2 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.646	8.36 ng	126070	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	38
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

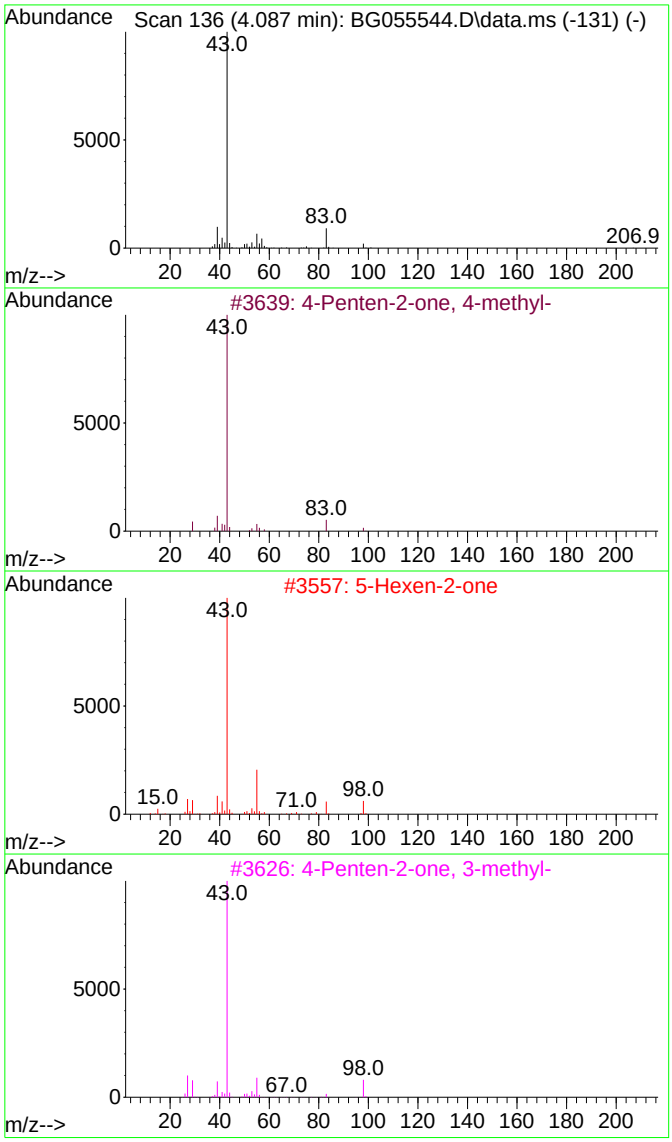
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

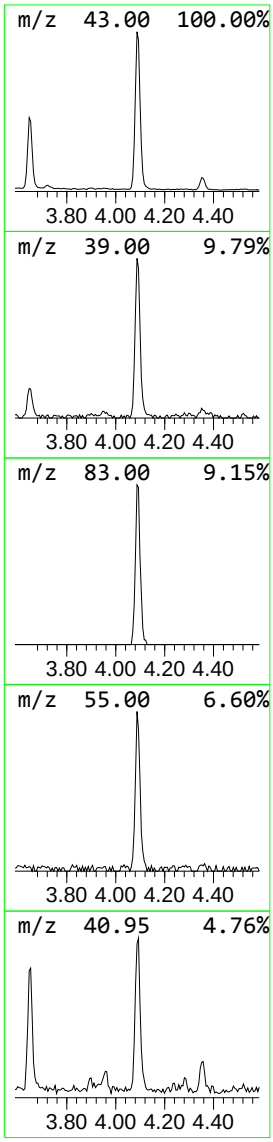
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.087	18.84 ng	284211	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	52
2	5-Hexen-2-one	98	C6H10O	000109-49-9	25
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10
5	3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

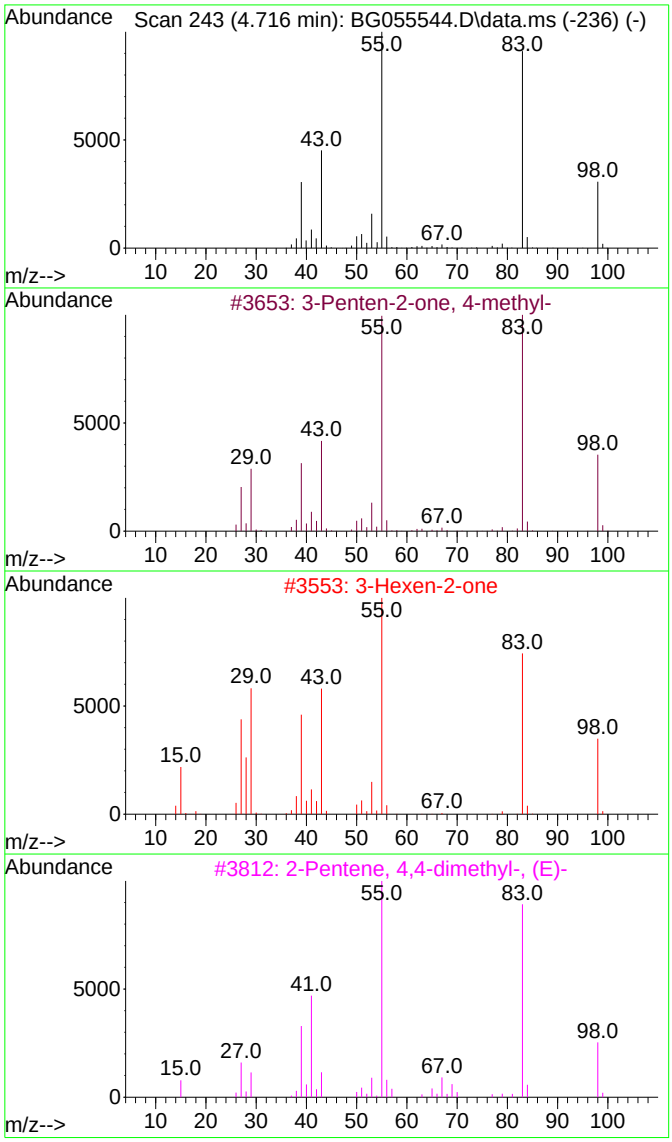
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

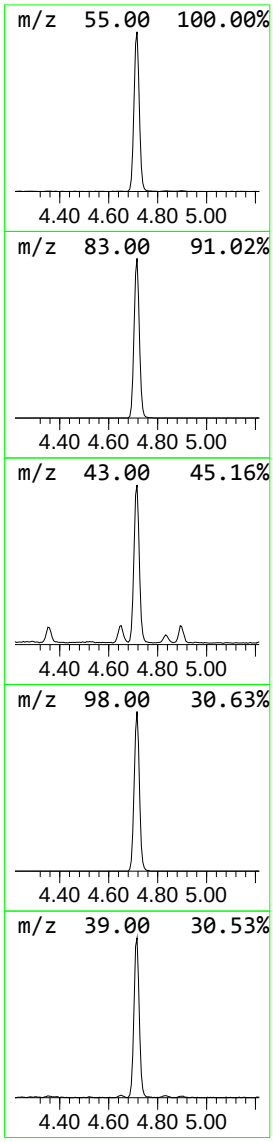
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.716	82.55 ng	1245070	1,4-Dichlorobenzene-d4	8.270

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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

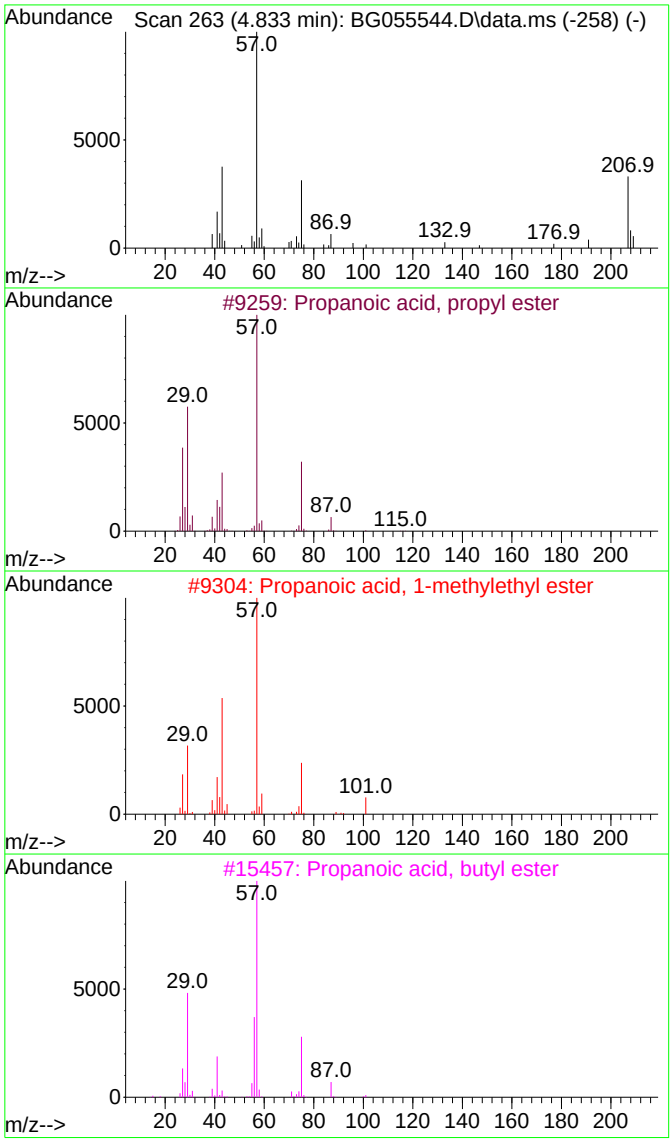
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

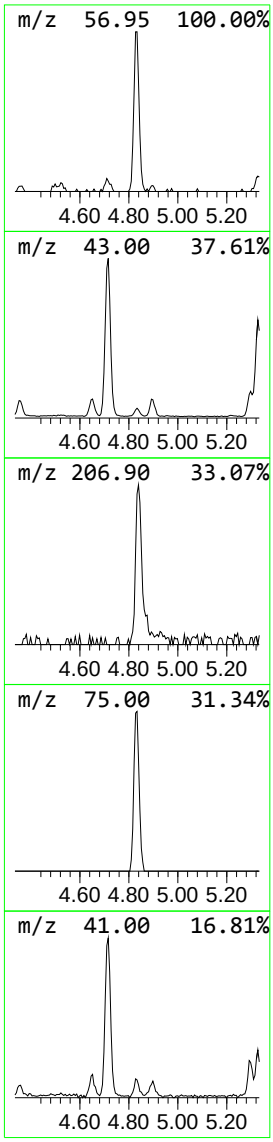
****

Peak Number 5 unknown4.833 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.833	3.99 ng	60179	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	43
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	32
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	10
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

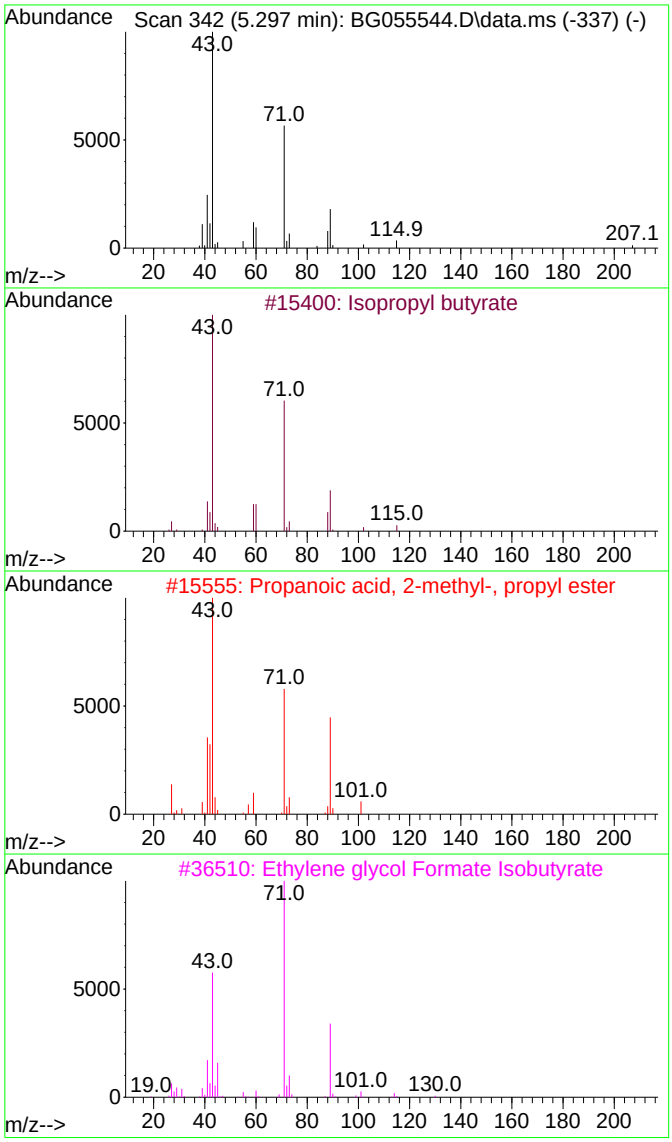
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

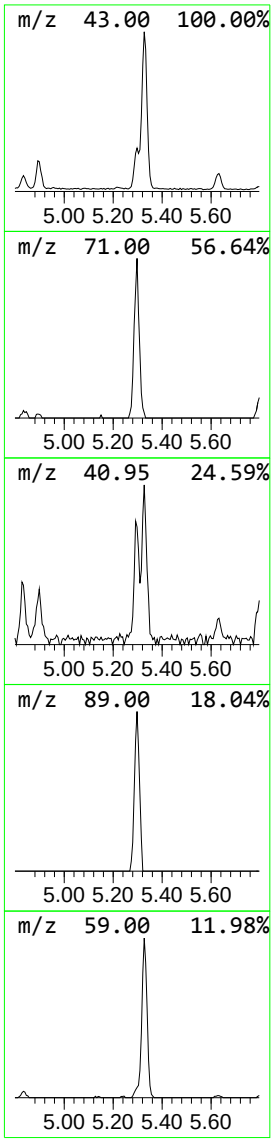
****

Peak Number 6 Isopropyl butyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.297	4.44 ng	66995	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
3	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	59
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
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Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

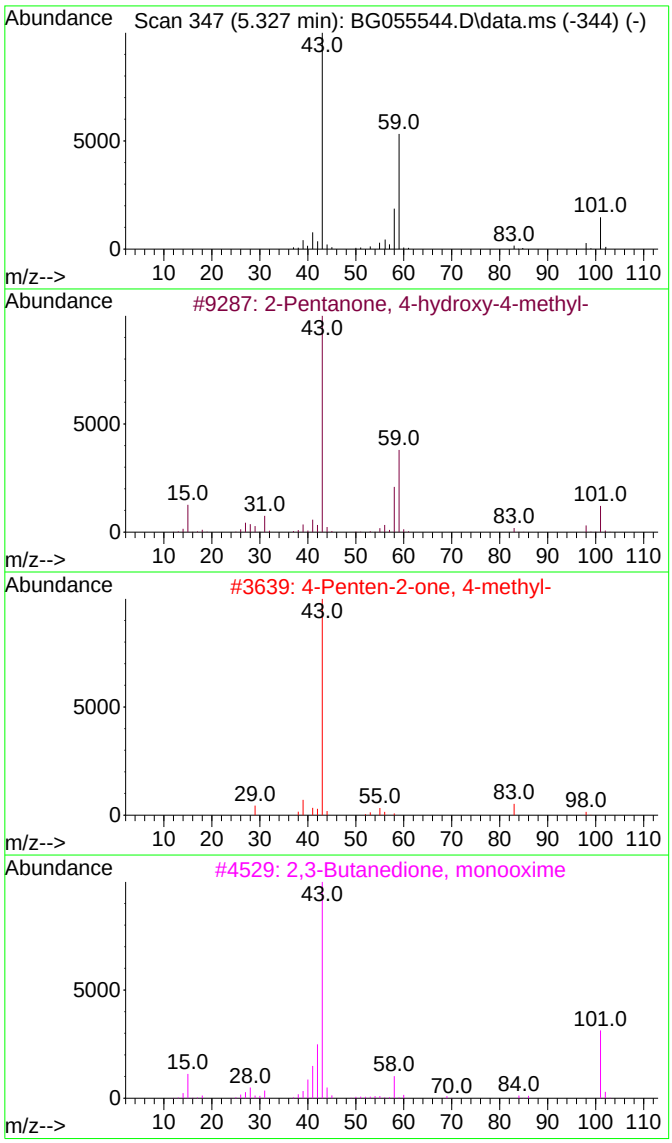
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

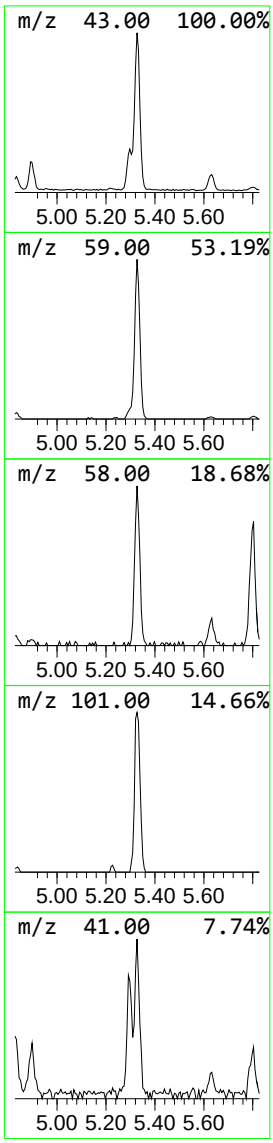
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.327	12.49 ng	188349	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
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Acq On : 10 Nov 2022 18:11
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Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

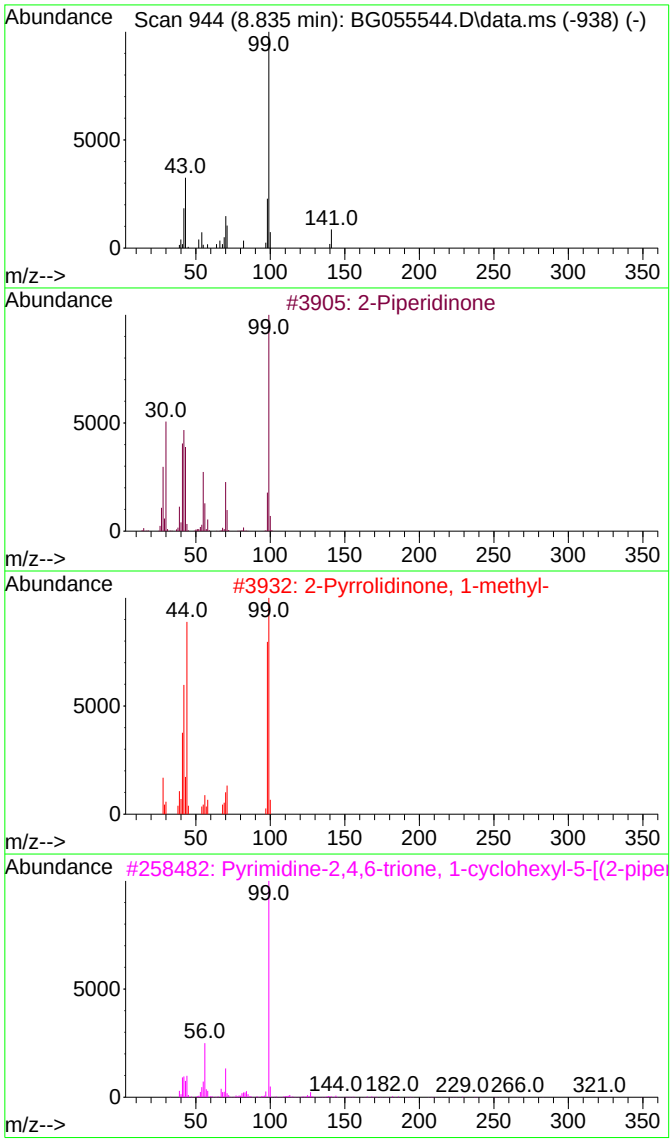
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

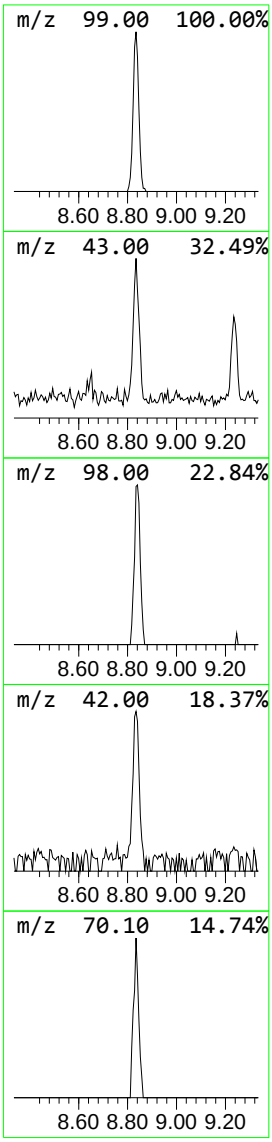
****

Peak Number 8 2-Piperidinone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.08 ng	46390	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone	99	C5H9NO	000675-20-7	78
2	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	53
3	Pyrimidine-2,4,6-trione, 1-cyclo...	349	C17H27N5O3	1000304-66-3	42
4	Benzo[1,2,5]thiadiazole, 4-bromo...	376	C11H13BrN4O2S2	1000296-37-8	42
5	5-Aminopentanamide	116	C5H12N2O	013023-70-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
Sample : N5491-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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

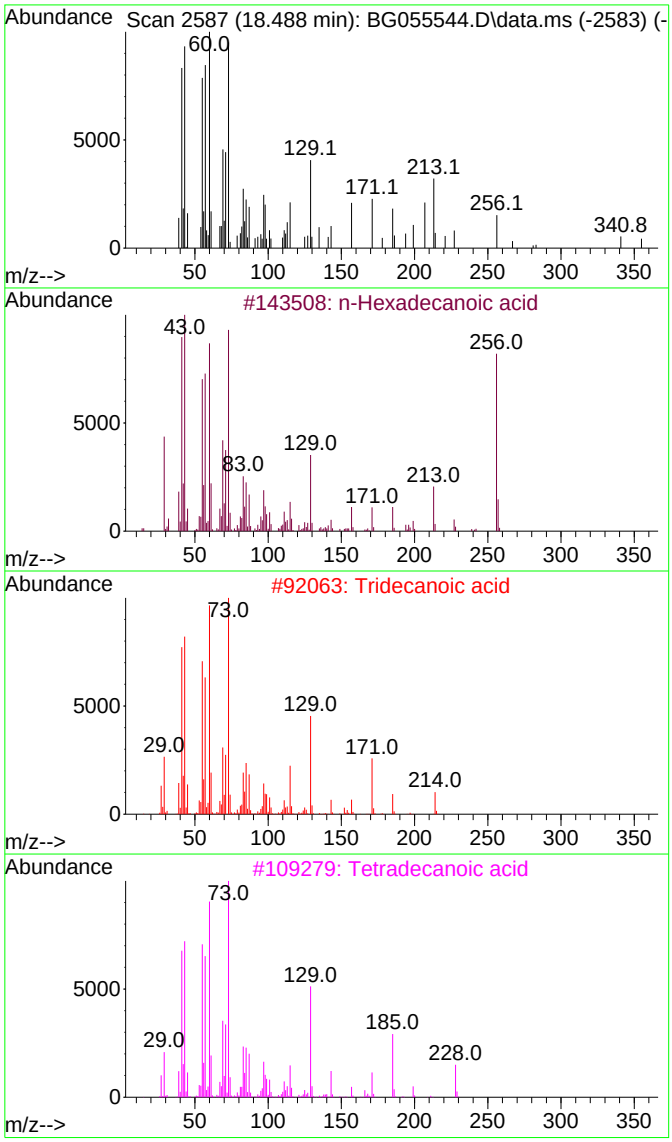
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

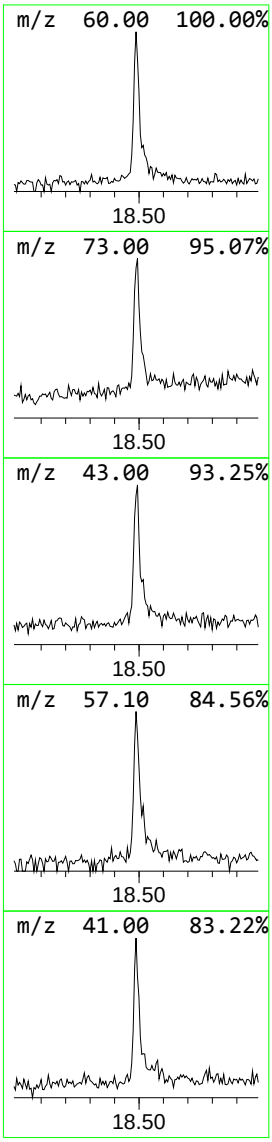
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	2.14 ng	74203	Phenanthrene-d10	17.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055544.D
Acq On : 10 Nov 2022 18:11
Operator : CG/JU
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Misc :
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Instrument :
BNA_G
ClientSampleId :
TP-4

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
Butane, 2-metho...	3.353	62.9	ng	948078	1	8.270	301643	20.0
n-Propyl acetate	3.646	8.4	ng	126070	1	8.270	301643	20.0
4-Penten-2-one,...	4.087	18.8	ng	284211	1	8.270	301643	20.0
3-Penten-2-one,...	4.716	82.5	ng	1245070	1	8.270	301643	20.0
unknown4.833	4.833	4.0	ng	60179	1	8.270	301643	20.0
Isopropyl butyrate	5.297	4.4	ng	66995	1	8.270	301643	20.0
2-Pentanone, 4-...	5.327	12.5	ng	188349	1	8.270	301643	20.0
2-Piperidinone	8.835	3.1	ng	46390	1	8.270	301643	20.0
n-Hexadecanoic ...	18.488	2.1	ng	74203	4	17.624	692222	20.0