LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058660.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.581	80	84	91	rVB	62366	79554	2.20%	0.531%
2	4.909	305	310	321	rVB	109161	158076	4.37%	1.055%
3	5.385	385	391	401	rBV	344821	540258	14.92%	3.607%
4	6.983	657	663	682	rVB	183296	315135	8.70%	2.104%
5	7.811	798	804	811	rBV	164122	279131	7.71%	1.863%
6	8.975	994	1002	1016	rBV	495671	926054	25.58%	6.182%
7	10.614	1274	1281	1292	rVB	224915	406901	11.24%	2.716%
8	11.137	1363	1370	1376	rBV	193047	323790	8.94%	2.162%
9	11.202	1376	1381	1397	rVB	230630	426155	11.77%	2.845%
10	12.494	1594	1601	1614	rBV	29069	50922	1.41%	0.340%
11	13.082	1694	1701	1715	rBV	1342055	2148457	59.34%	14.343%
12	13.352	1740	1747	1763	rBV	460485	773329	21.36%	5.163%
13	14.463	1928	1936	1945	rBV	372915	605714	16.73%	4.044%
14	15.949	2183	2189	2215	rBV	886411	1655868	45.74%	11.054%
15	17.206	2396	2403	2419	rBV	508925	802381	22.16%	5.357%
16	17.488	2438	2451	2476	rVB8	23940	107207	2.96%	0.716%
17	19.827	2842	2849	2862	rBV	2658787	3620565	100.00%	24.170%
18	21.448	3118	3125	3144	rBV	474078	860147	23.76%	5.742%
19	24.521	3637	3648	3672	rBV	247632	899772	24.85%	6.007%

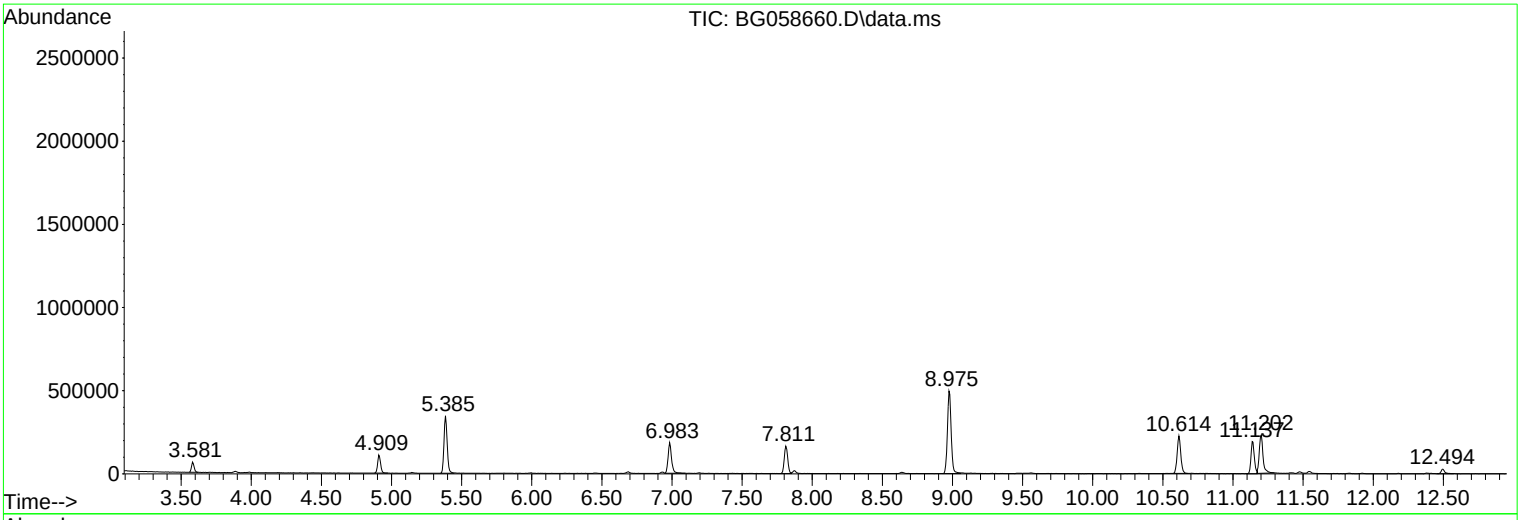
Sum of corrected areas: 14979416

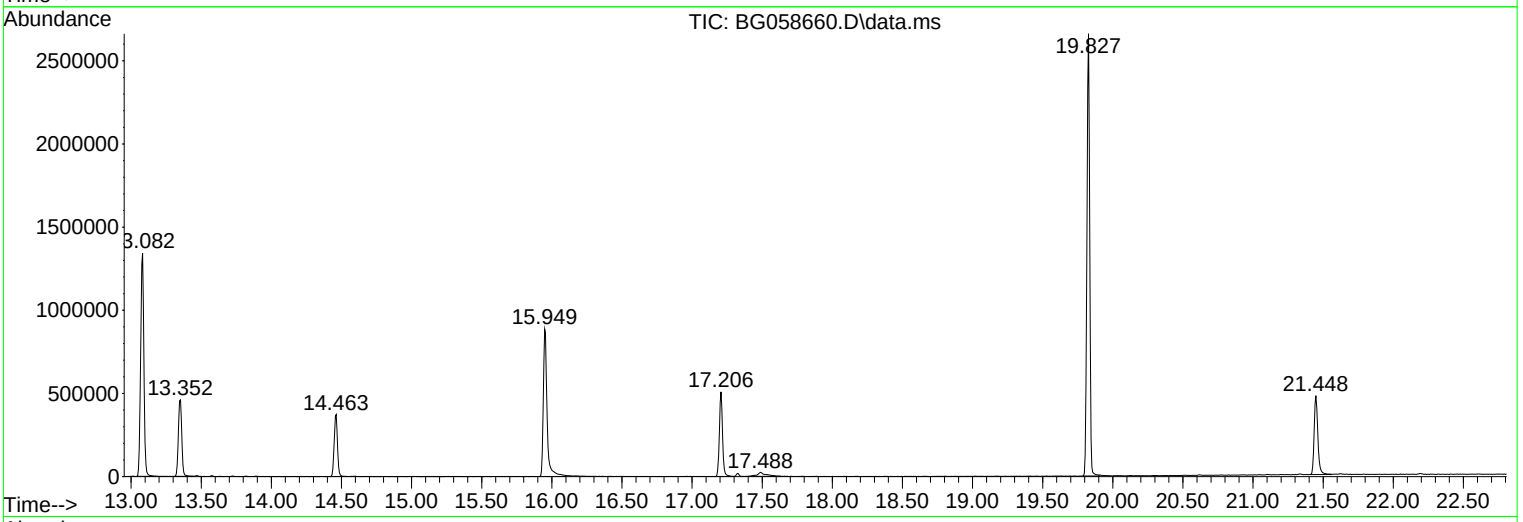
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

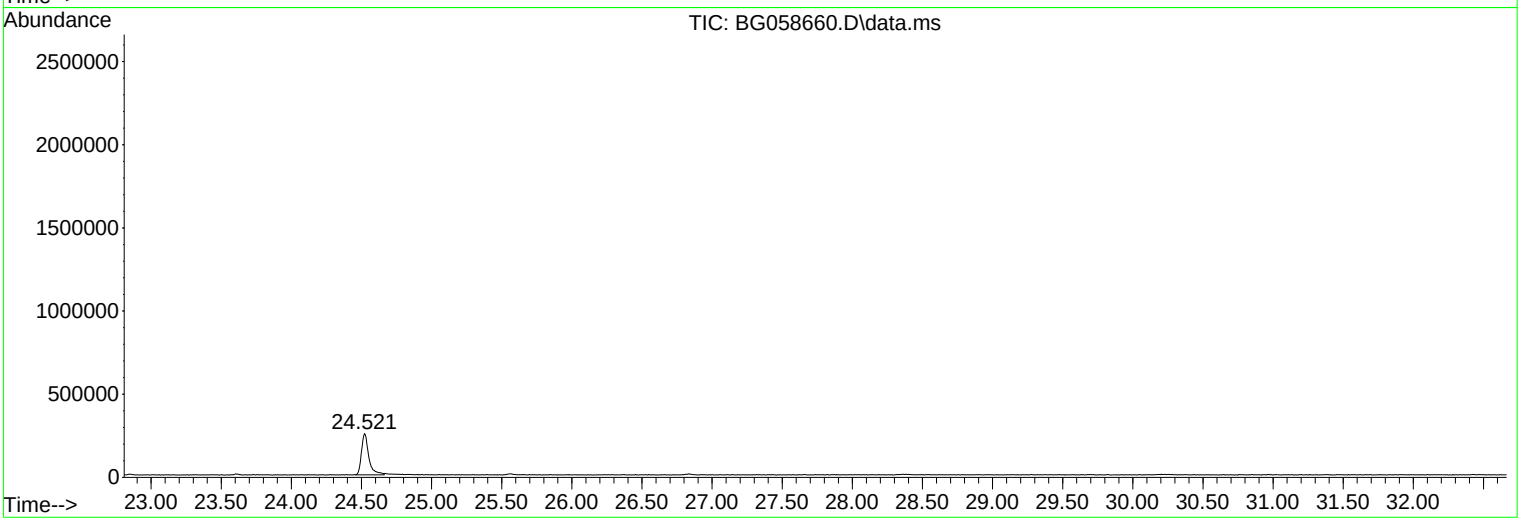
Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

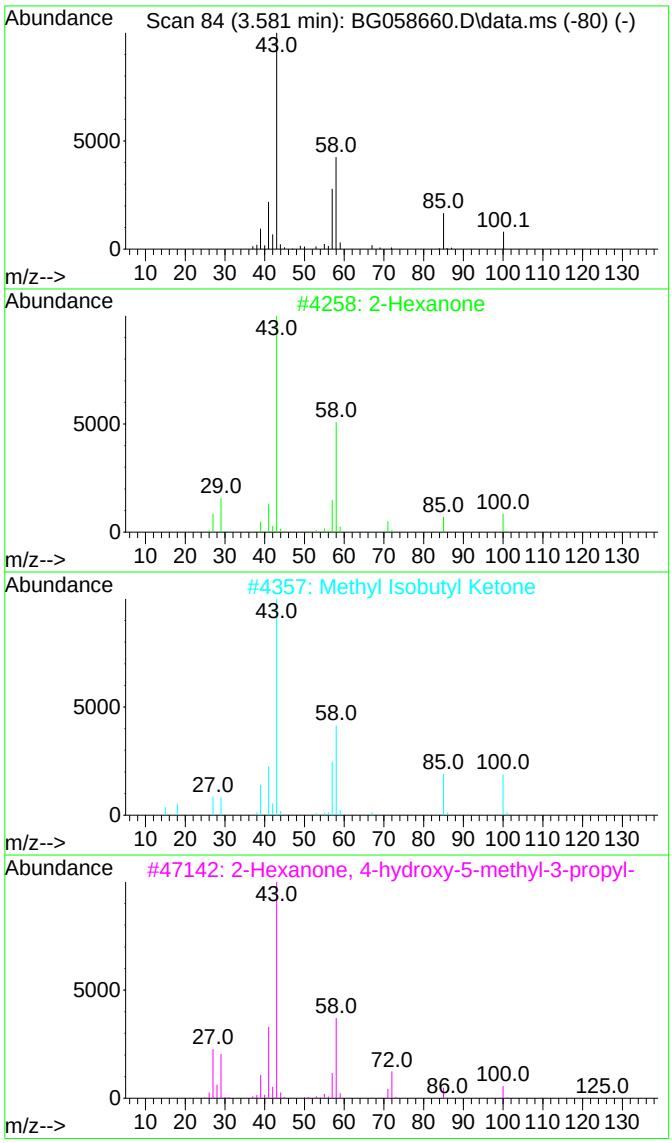
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

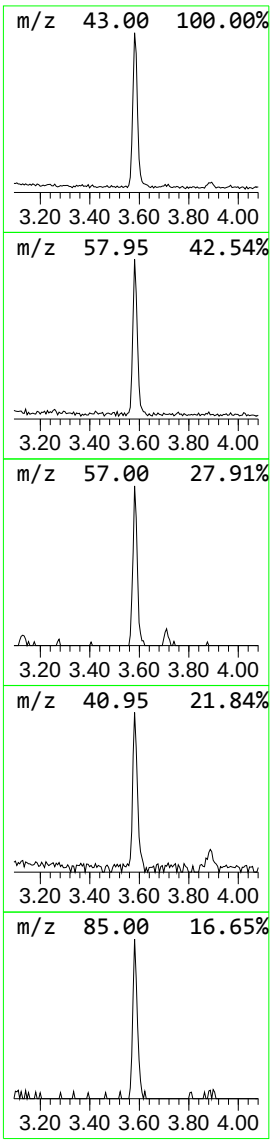
****

Peak Number 1 2-Hexanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	5.70 ng	79554	1,4-Dichlorobenzene-d4	7.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone	100	C6H12O	000591-78-6	78
2	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	78
3	2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	64
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	37
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

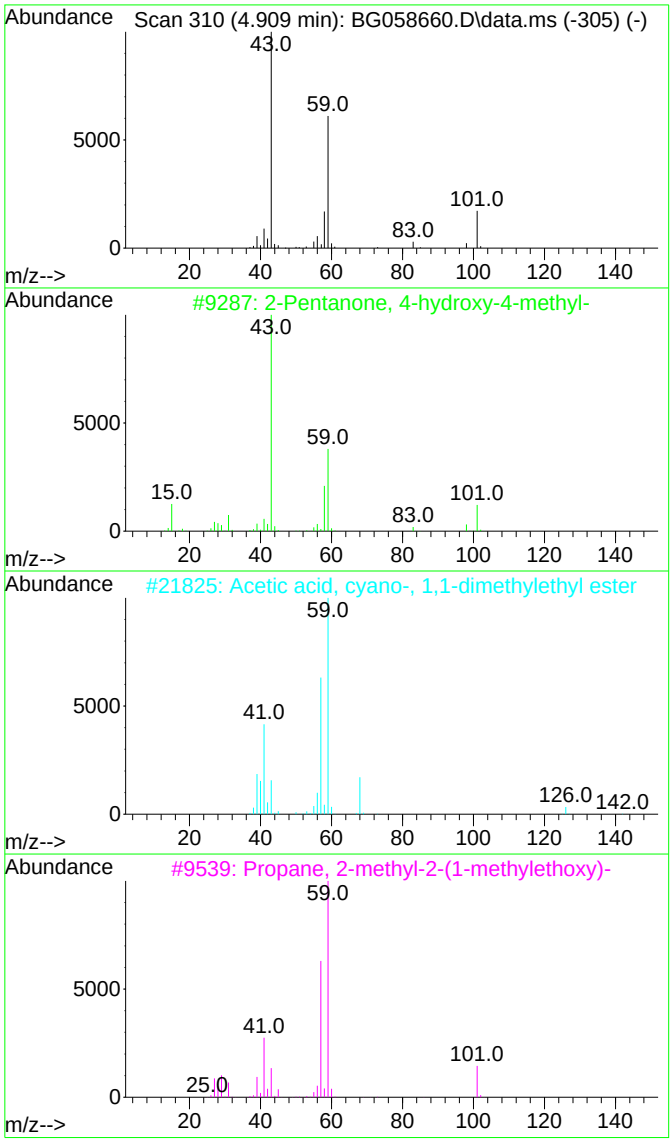
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

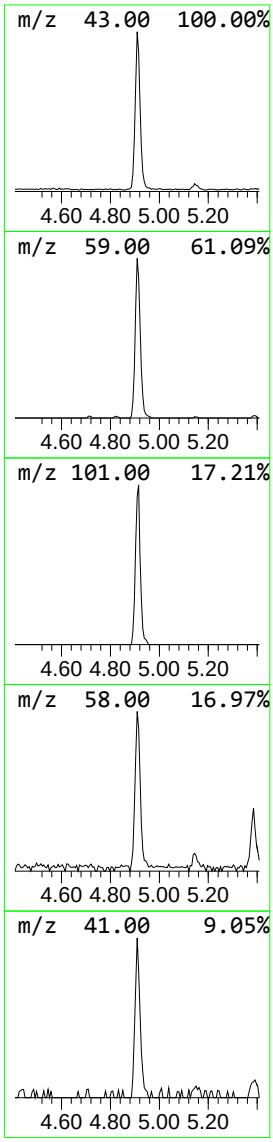
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.909	11.33 ng	158076	1,4-Dichlorobenzene-d4	7.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Octanol	130	C8H18O	000589-98-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

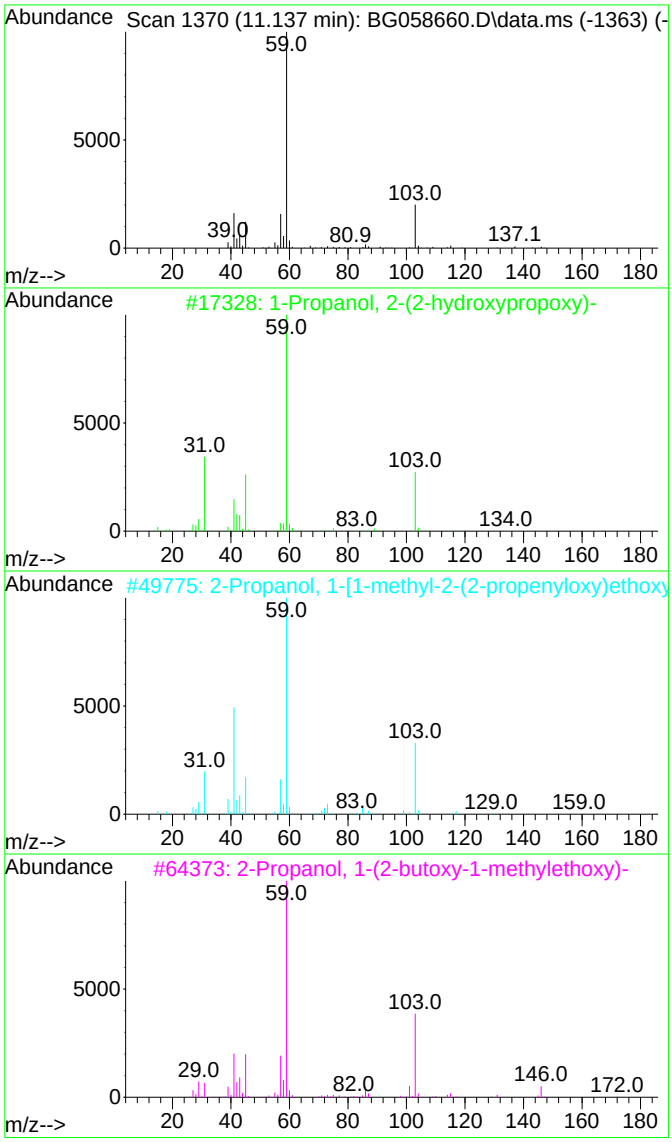
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

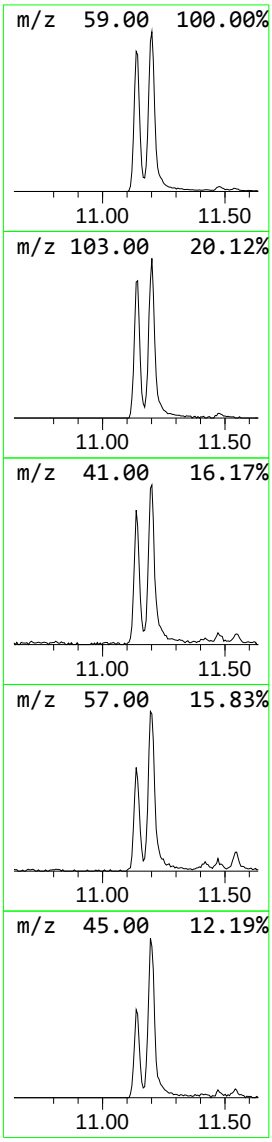
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.137	15.91 ng	323790	Naphthalene-d8	10.614

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	64
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

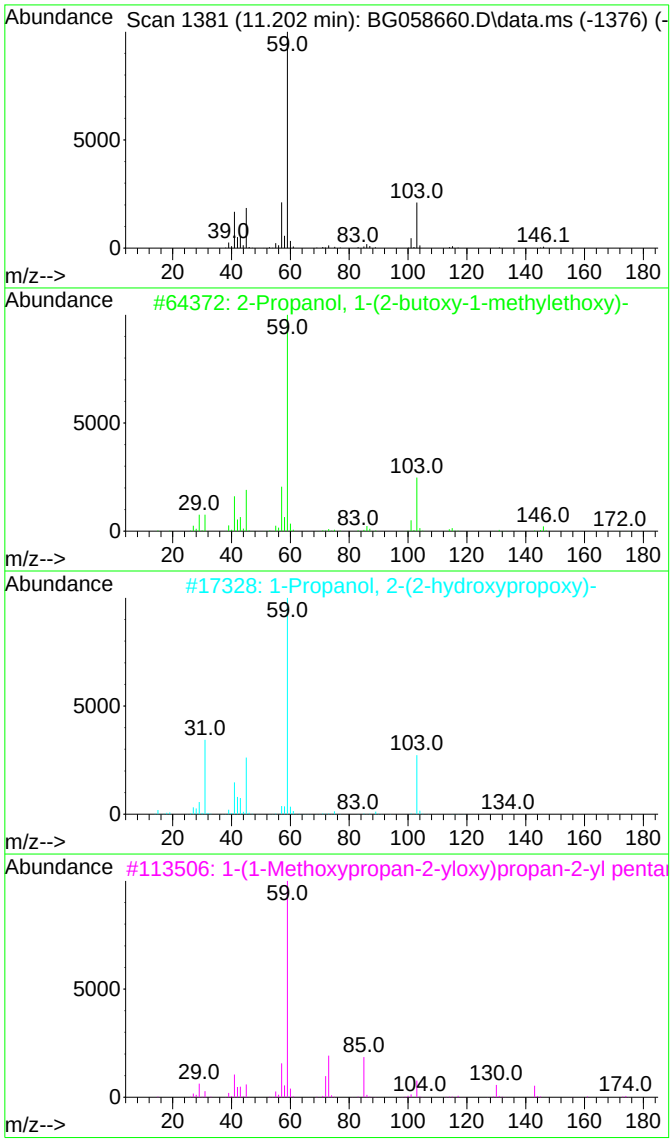
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

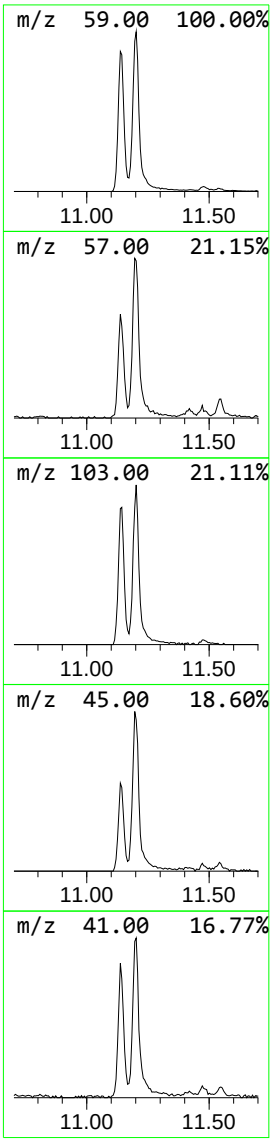
****

Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.202	20.95 ng	426155	Naphthalene-d8	10.614

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	64
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

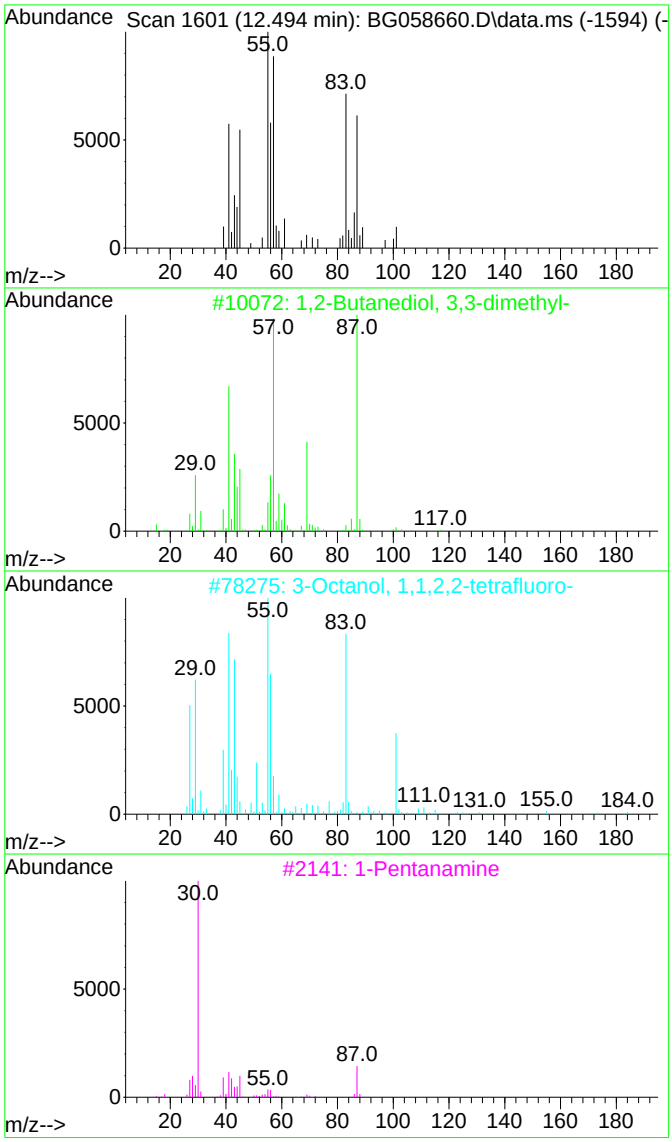
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

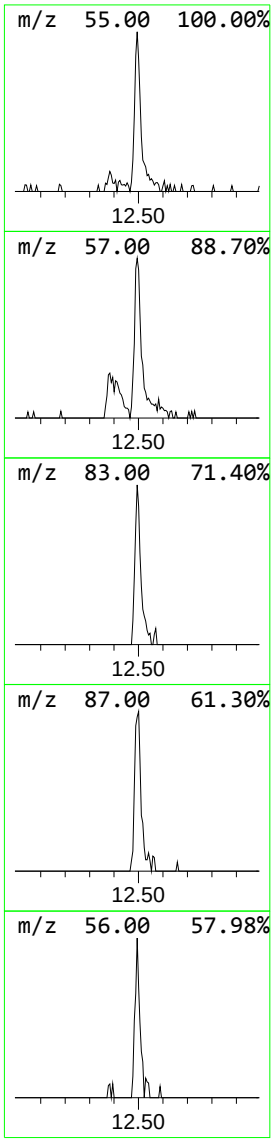
****

Peak Number 5 unknown12.494 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.494	2.50 ng	50922	Naphthalene-d8	10.614

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Butanediol, 3,3-dimethyl-	118	C6H14O2	059562-82-2	37
2	3-Octanol, 1,1,2,2-tetrafluoro-	202	C8H14F4O	074810-72-3	32
3	1-Pentanamine	87	C5H13N	000110-58-7	27
4	Cyclopropanecarboxylic acid, 1-a...	101	C4H7NO2	022059-21-8	27
5	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

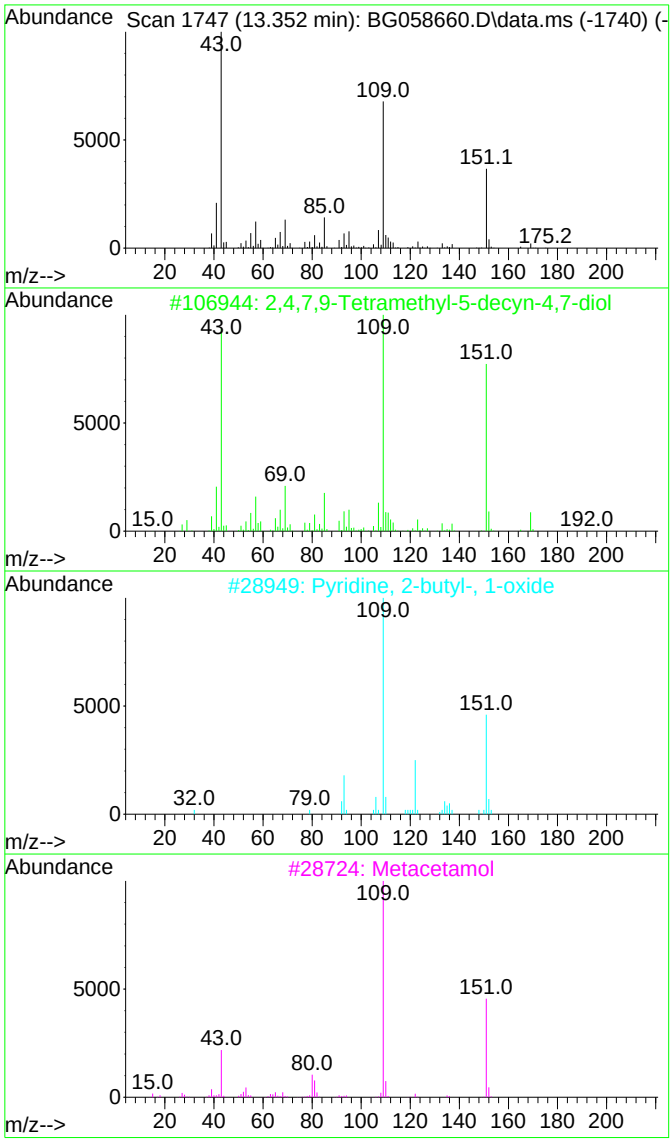
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

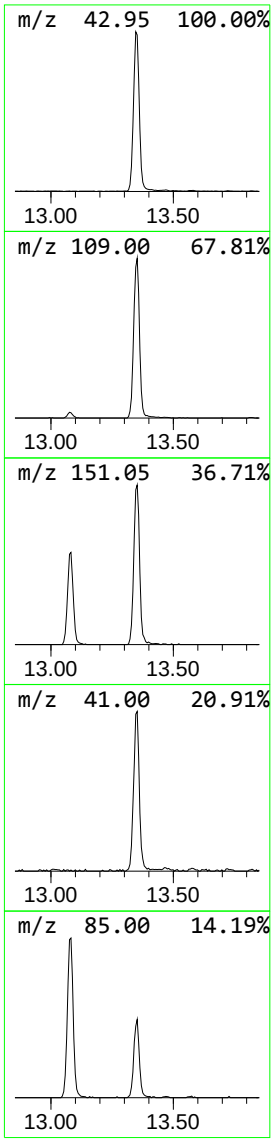
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.352	25.53 ng	773329	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	Acetaminophen	151	C8H9NO2	000103-90-2	47
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

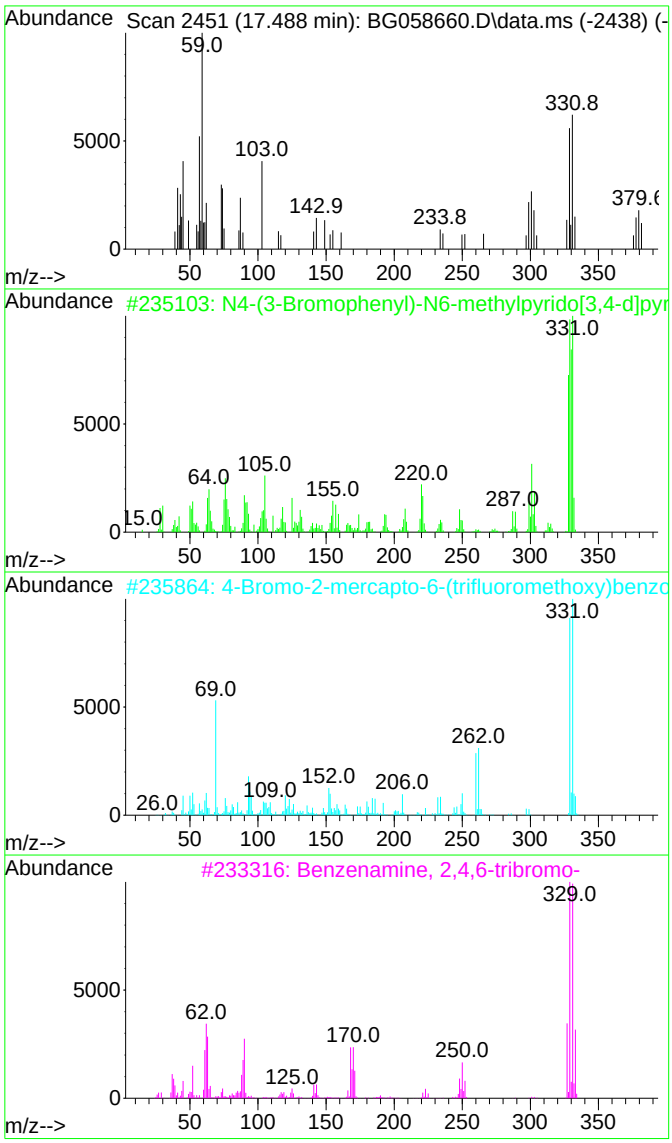
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

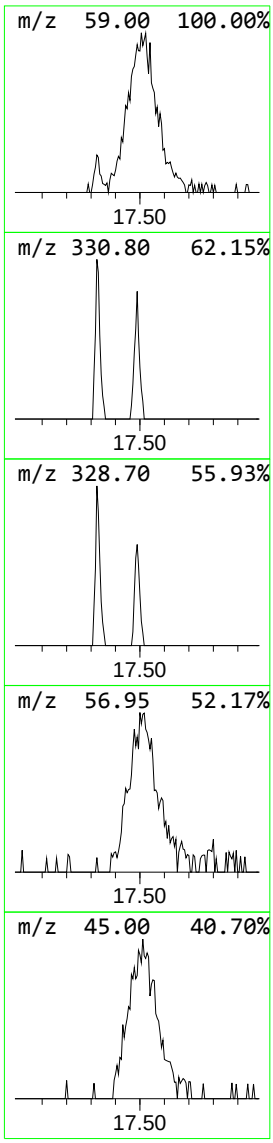
****

Peak Number 7 unknown17.488 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.488	2.67 ng	107207	Phenanthrene-d10	17.206

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N4-(3-Bromophenyl)-N6-methylpyri...	329	C14H12BrN5	171179-06-9	14
2	4-Bromo-2-mercapto-6-(trifluorom...	329	C8H3BrF3NOS2	1000502-92-7	11
3	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	10
4	N-Methyl bromoazepam	329	C15H12BrN3O	001812-33-5	10
5	1-Cyclohexyl-6-methyl-4-(thiophe...	333	C16H19N3OS2	1000435-84-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080923\
Data File : BG058660.D
Acq On : 9 Aug 2023 15:54
Operator : MA/JU
Sample : 03917-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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-Hexanone	3.581	5.7	ng	79554	1	7.811	279131	20.0
2-Pentanone, 4-...	4.909	11.3	ng	158076	1	7.811	279131	20.0
1-Propanol, 2-(...	11.137	15.9	ng	323790	2	10.614	406901	20.0
2-Propanol, 1-(...	11.202	20.9	ng	426155	2	10.614	406901	20.0
unknown12.494	12.494	2.5	ng	50922	2	10.614	406901	20.0
2,4,7,9-Tetrame...	13.352	25.5	ng	773329	3	14.463	605714	20.0
unknown17.488	17.488	2.7	ng	107207	4	17.206	802381	20.0