LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-GA

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-BG061323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057712.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.131	3	7	22	rVB	125778	230970	9.96%	1.686%
2	5.052	328	334	342	rVB	49373	77507	3.34%	0.566%
3	5.517	404	413	425	rBV	943606	1475778	63.65%	10.771%
4	7.103	674	683	693	rBV	909904	1540758	66.45%	11.245%
5	7.943	819	826	833	rBV	173292	291794	12.58%	2.130%
6	9.101	1013	1023	1033	rBV	516633	893079	38.52%	6.518%
7	10.740	1295	1302	1309	rBV	228776	413039	17.81%	3.015%
8	13.202	1713	1721	1727	rVB	1176380	1858560	80.15%	13.565%
9	14.571	1947	1954	1962	rVB	336235	509613	21.98%	3.719%
10	15.928	2178	2185	2191	rBV	77836	111006	4.79%	0.810%
11	16.057	2200	2207	2214	rBV	919409	1355819	58.47%	9.896%
12	17.315	2415	2421	2427	rBV	409616	604912	26.09%	4.415%
13	18.208	2567	2573	2582	rBV2	66421	104606	4.51%	0.763%
14	19.477	2783	2789	2793	rBV5	22247	31170	1.34%	0.227%
15	19.935	2860	2867	2872	rBV	1765579	2318765	100.00%	16.924%
16	21.228	3083	3087	3096	rBV	138311	237250	10.23%	1.732%
17	21.568	3138	3145	3151	rBV	365859	605115	26.10%	4.416%
18	21.774	3166	3180	3186	rBV	54008	232254	10.02%	1.695%
19	22.391	3280	3285	3289	rBV6	17532	35479	1.53%	0.259%
20	23.037	3389	3395	3406	rBV5	35199	102170	4.41%	0.746%
21	24.735	3674	3684	3695	rBV2	220394	624932	26.95%	4.561%
22	26.040	3902	3906	3913	rVB7	19265	46668	2.01%	0.341%

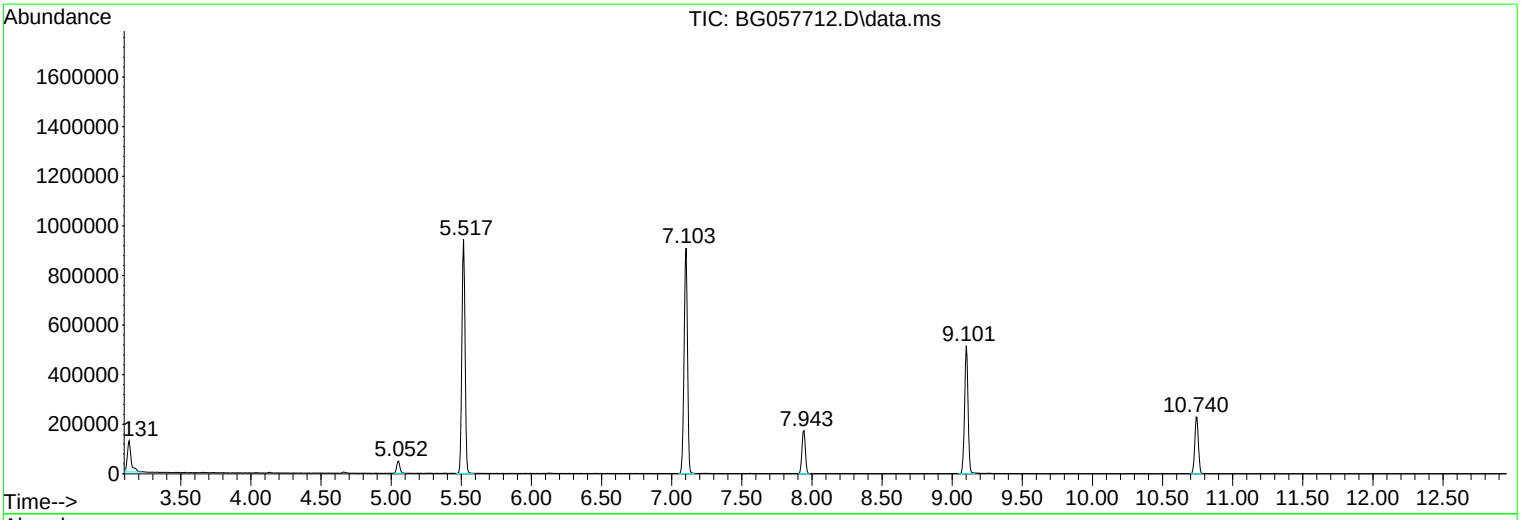
Sum of corrected areas: 13701244

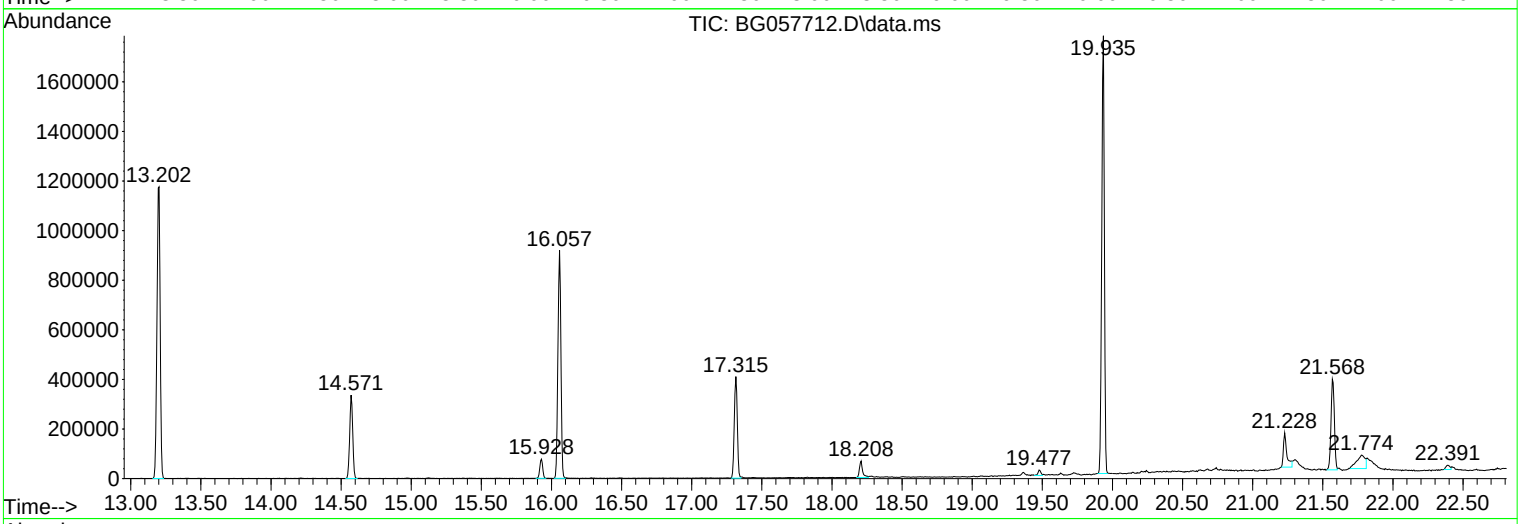
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

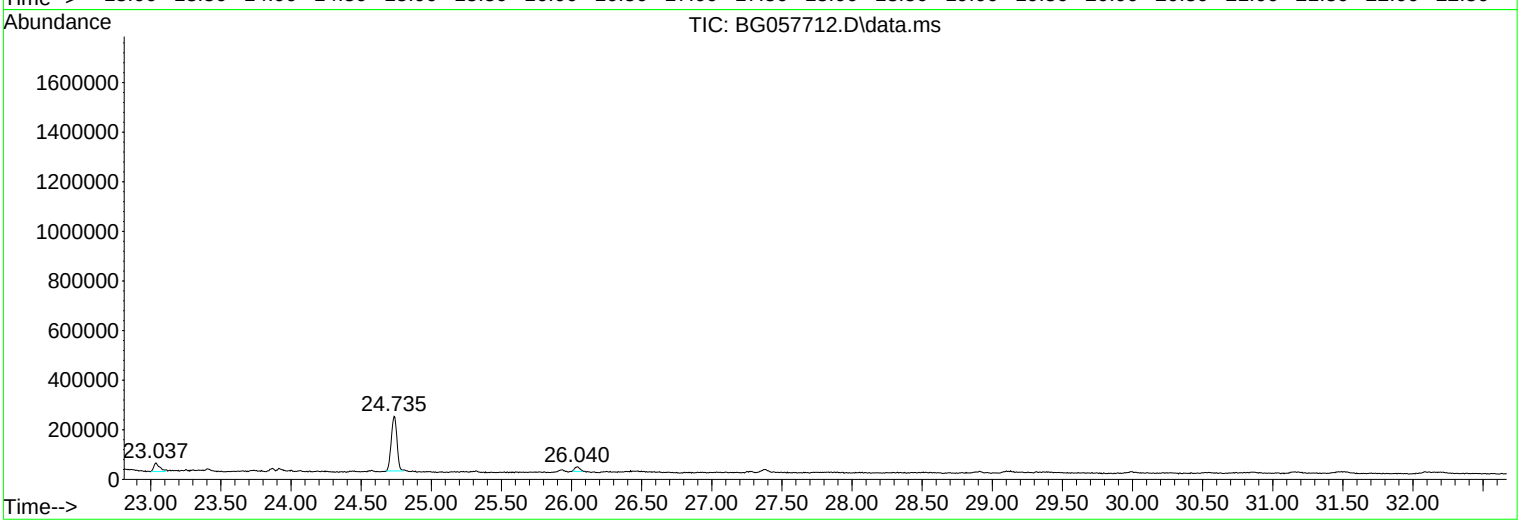
Instrument :
BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.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\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
TP-4-GA

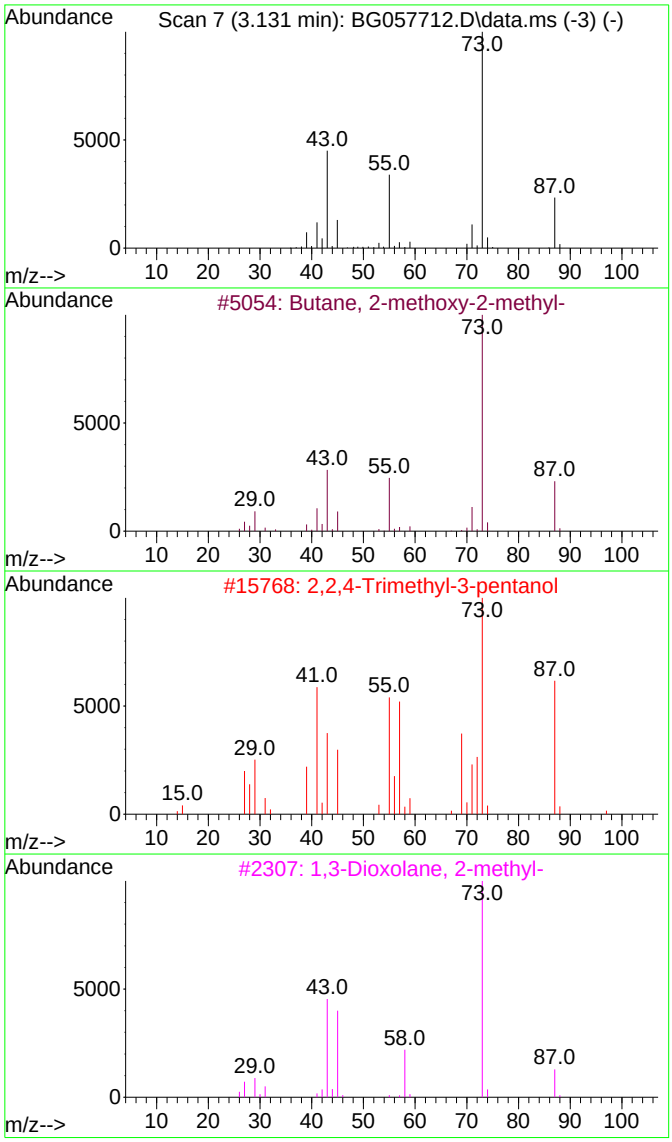
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

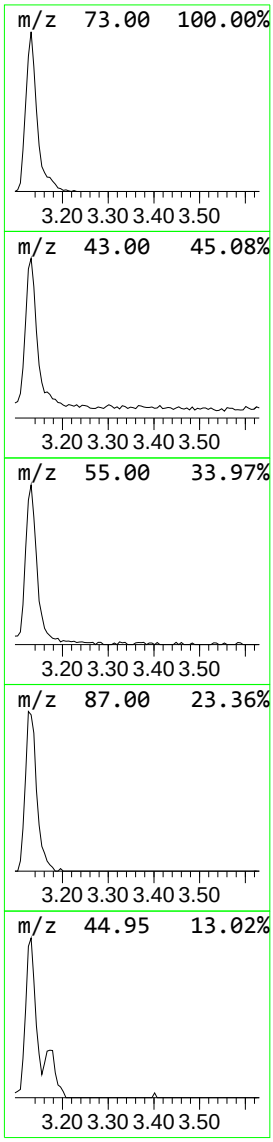
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.131	15.83 ng	230970	1,4-Dichlorobenzene-d4	7.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-GA

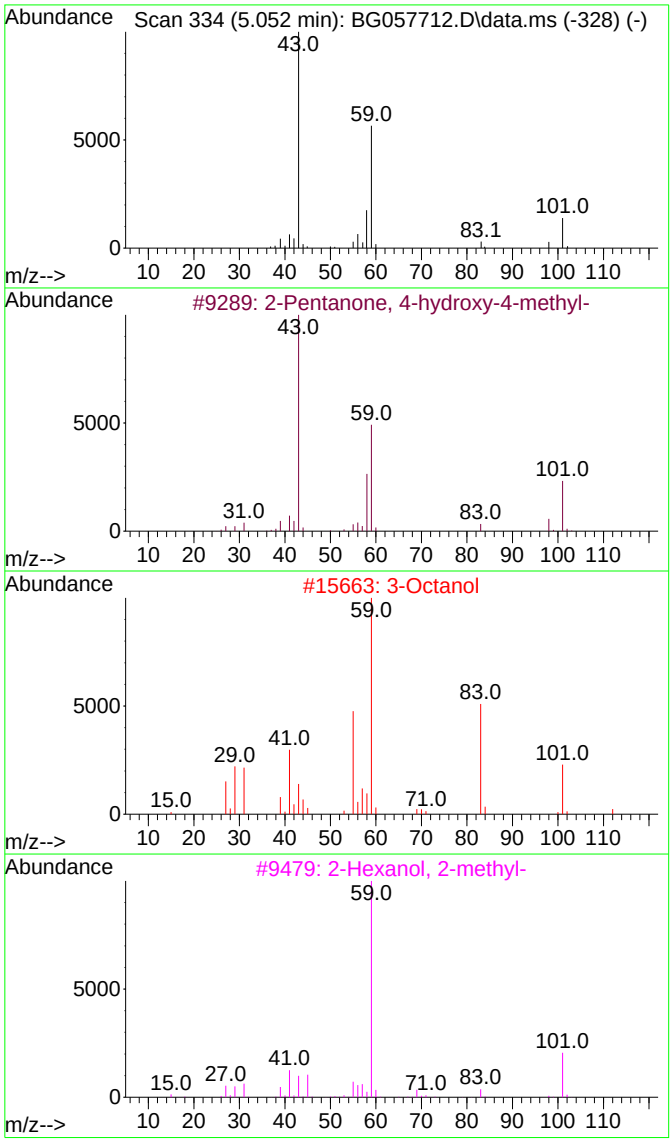
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

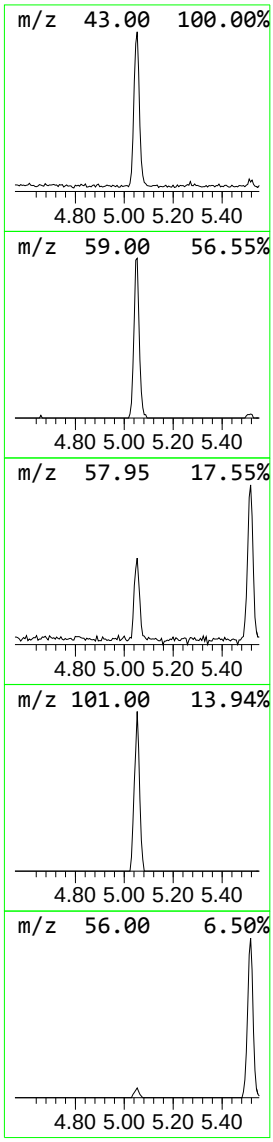
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	5.31 ng	77507	1,4-Dichlorobenzene-d4	7.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Octanol	130	C8H18O	000589-98-0	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

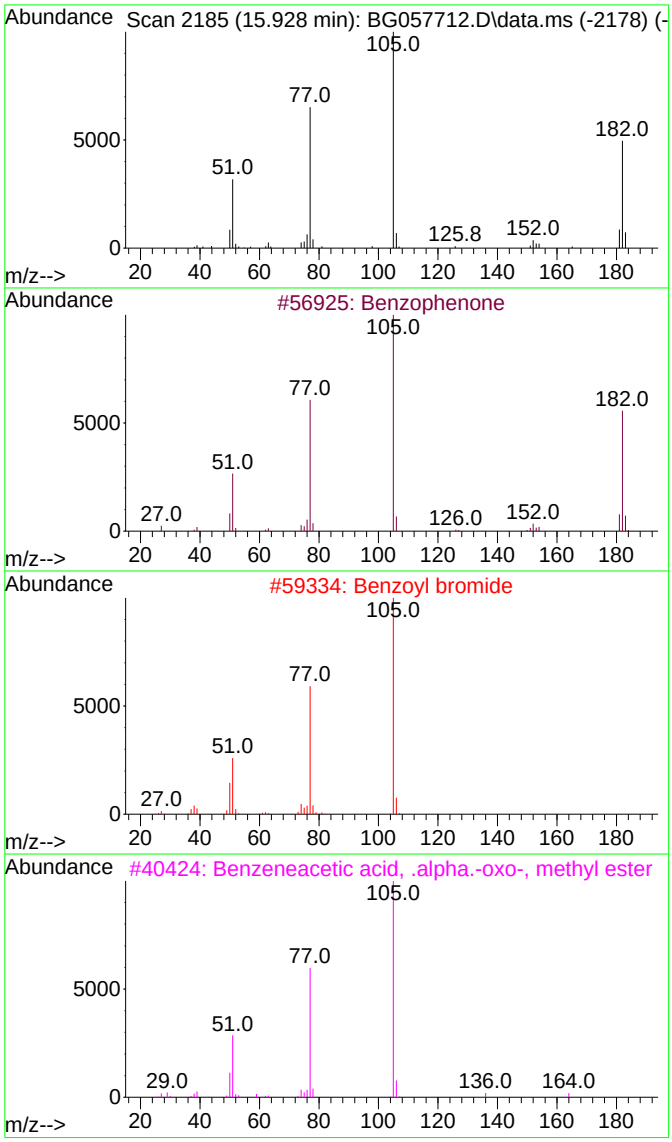
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

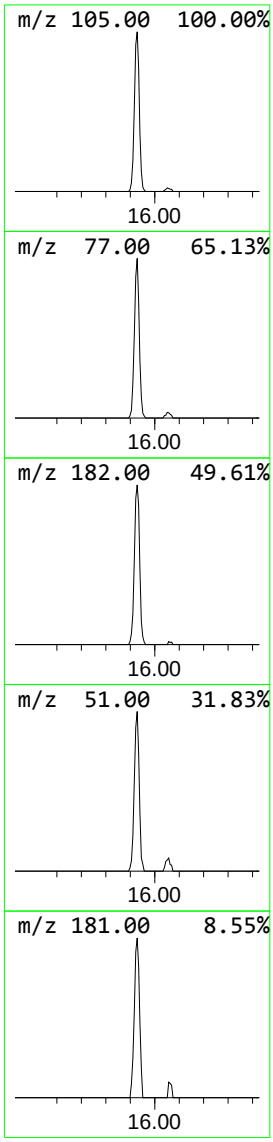
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.928	4.36 ng	111006	Acenaphthene-d10	14.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

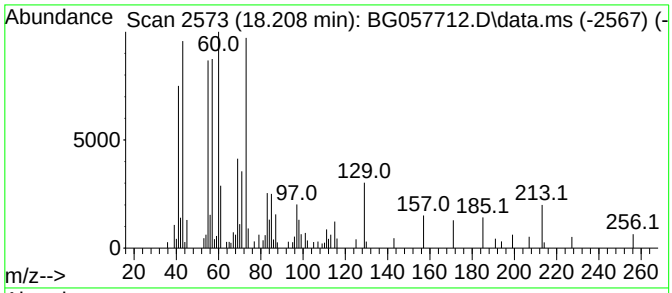
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

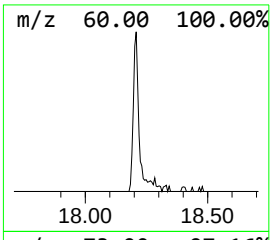
****

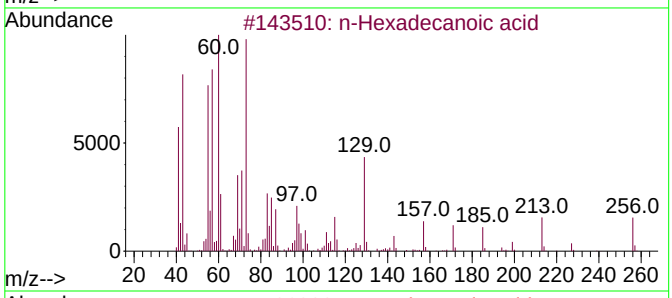
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

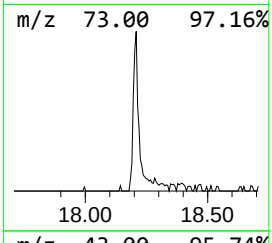
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.208	3.46 ng	104606	Phenanthrene-d10	17.314

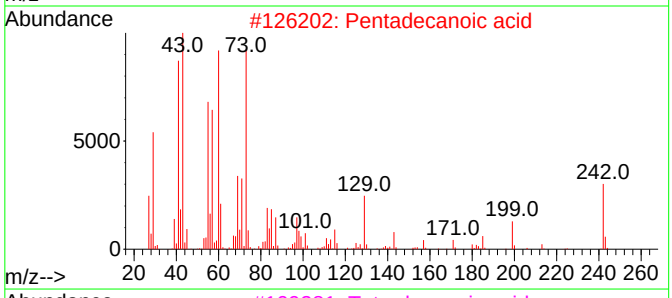
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53

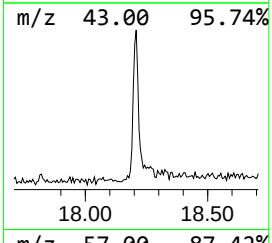


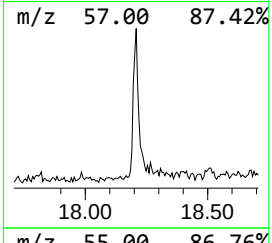


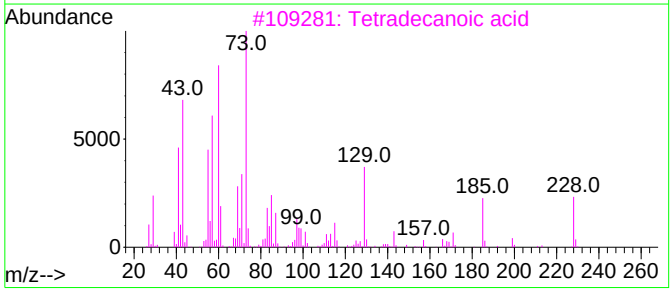


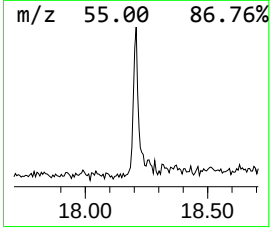












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
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Misc :
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BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

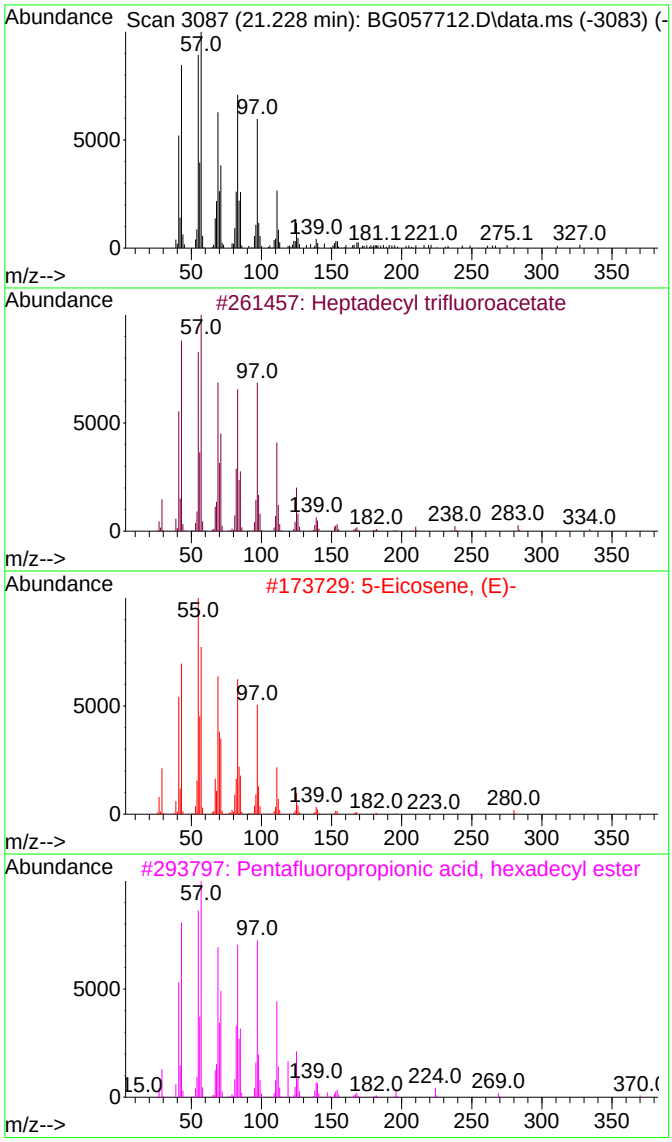
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

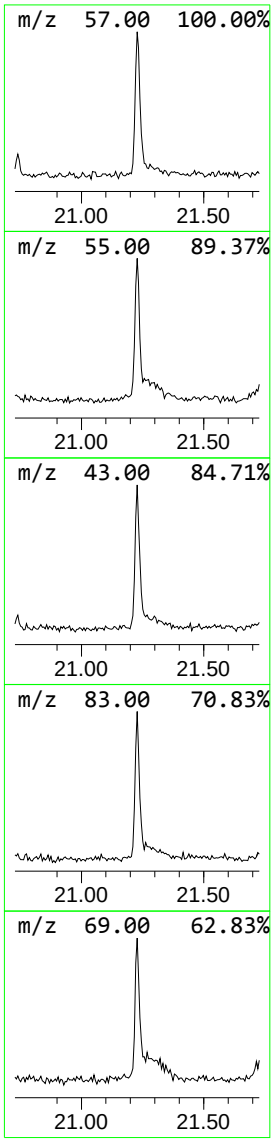
****

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.228	7.84 ng	237250	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
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Sample : 03167-01
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BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

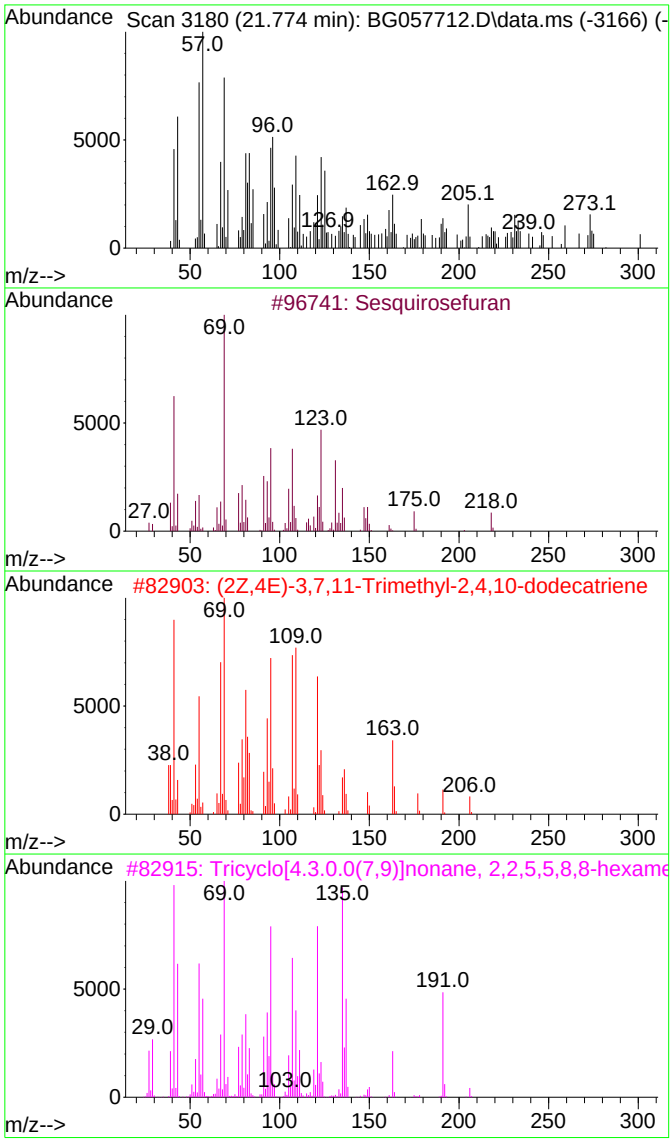
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

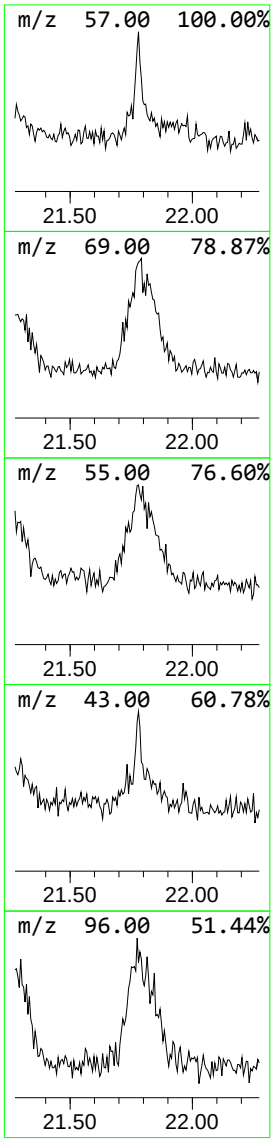
****

Peak Number 6 Sesquirosefuran Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.774	7.68 ng	232254	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sesquirosefuran	218	C15H22O	039007-93-7	81
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	47
3	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	35
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	30
5	.beta.-Bisabolenol	220	C15H24O	147126-90-7	22





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

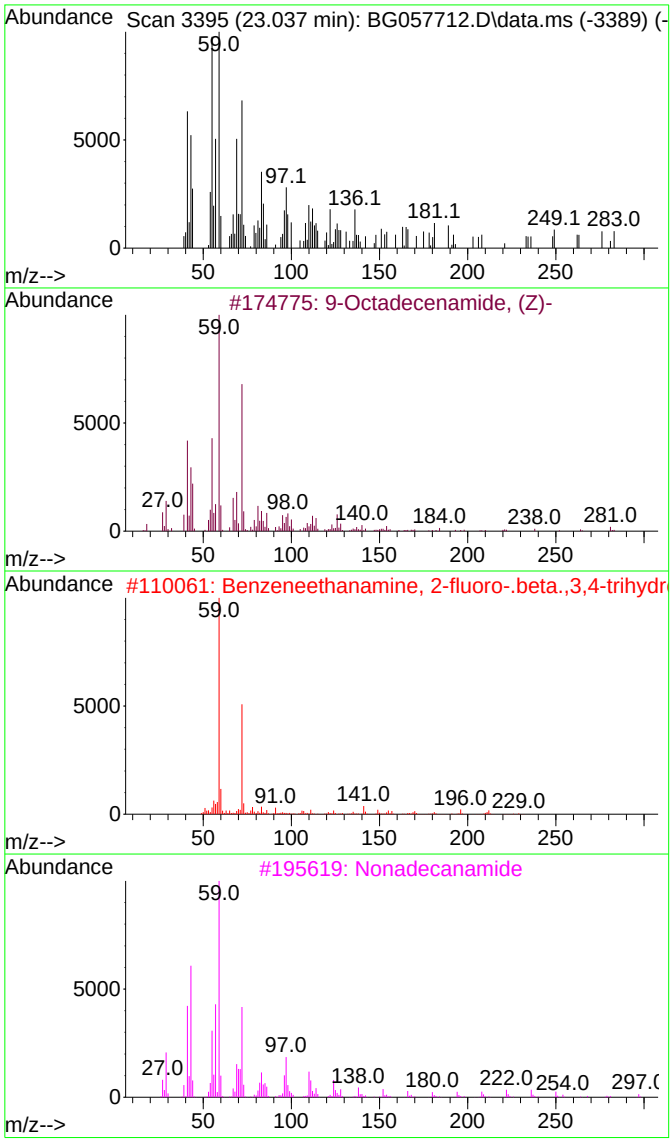
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

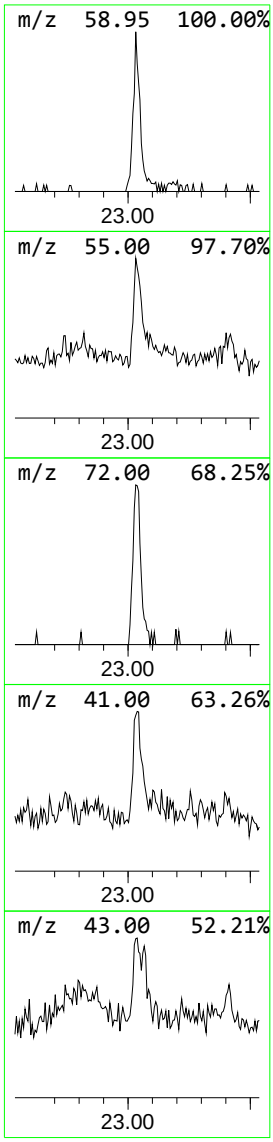
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.037	3.38 ng	102170	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	43
3	Nonadecanamide	297	C19H39NO	058185-32-3	30
4	Acetamide, N-propyl-N-(3-methylb...	171	C10H21NO	1010438-05-0	25
5	Myristoleic acid	226	C14H26O2	000544-64-9	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061423\
Data File : BG057712.D
Acq On : 14 Jun 2023 17:57
Operator : CG/JU
Sample : 03167-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-GA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.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...	3.131	15.8	ng	230970	1	7.943	291794	20.0
2-Pentanone, 4-...	5.052	5.3	ng	77507	1	7.943	291794	20.0
Benzophenone	15.928	4.4	ng	111006	3	14.571	509613	20.0
n-Hexadecanoic ...	18.208	3.5	ng	104606	4	17.314	604912	20.0
Heptadecyl trif...	21.228	7.8	ng	237250	5	21.568	605115	20.0
Sesquirosefuran	21.774	7.7	ng	232254	5	21.568	605115	20.0
9-Octadecenamid...	23.037	3.4	ng	102170	5	21.568	605115	20.0