LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

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-BG100322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055087.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.370	10	14	22	rBV	250530	379892	18.76%	3.963%
2	5.385	351	357	371	rVB	127063	209029	10.32%	2.181%
3	5.855	428	437	455	rBV	394819	651827	32.20%	6.800%
4	7.465	702	711	720	rBV	410097	708072	34.98%	7.386%
5	8.335	851	859	867	rBV	97379	165096	8.15%	1.722%
6	9.504	1049	1058	1066	rBV	239722	424674	20.98%	4.430%
7	11.167	1334	1341	1350	rBV	132353	234413	11.58%	2.445%
8	13.570	1744	1750	1759	rVB	701997	1057890	52.25%	11.036%
9	14.939	1975	1983	1990	rVB	244731	373384	18.44%	3.895%
10	16.414	2227	2234	2243	rBV	676277	1051149	51.92%	10.965%
11	17.677	2441	2449	2455	rBV	339843	522316	25.80%	5.449%
12	18.529	2589	2594	2602	rBV2	66889	109638	5.42%	1.144%
13	19.780	2803	2807	2819	rBV4	21687	43763	2.16%	0.457%
14	20.250	2881	2887	2893	rBV	1564390	2024508	100.00%	21.119%
15	21.566	3106	3111	3125	rBV	66390	108585	5.36%	1.133%
16	21.837	3152	3157	3162	rVB3	12526	21657	1.07%	0.226%
17	21.966	3172	3179	3186	rBV	349721	594165	29.35%	6.198%
18	22.818	3319	3324	3334	rVB6	15097	36511	1.80%	0.381%
19	23.934	3508	3514	3526	rVB4	25834	56587	2.80%	0.590%
20	24.434	3592	3599	3605	rBV2	22960	50756	2.51%	0.529%
21	24.492	3605	3609	3618	rVB8	15388	33820	1.67%	0.353%
22	25.415	3755	3766	3781	rVB2	198608	609504	30.11%	6.358%
23	26.719	3977	3988	3997	rVB5	37168	118819	5.87%	1.239%

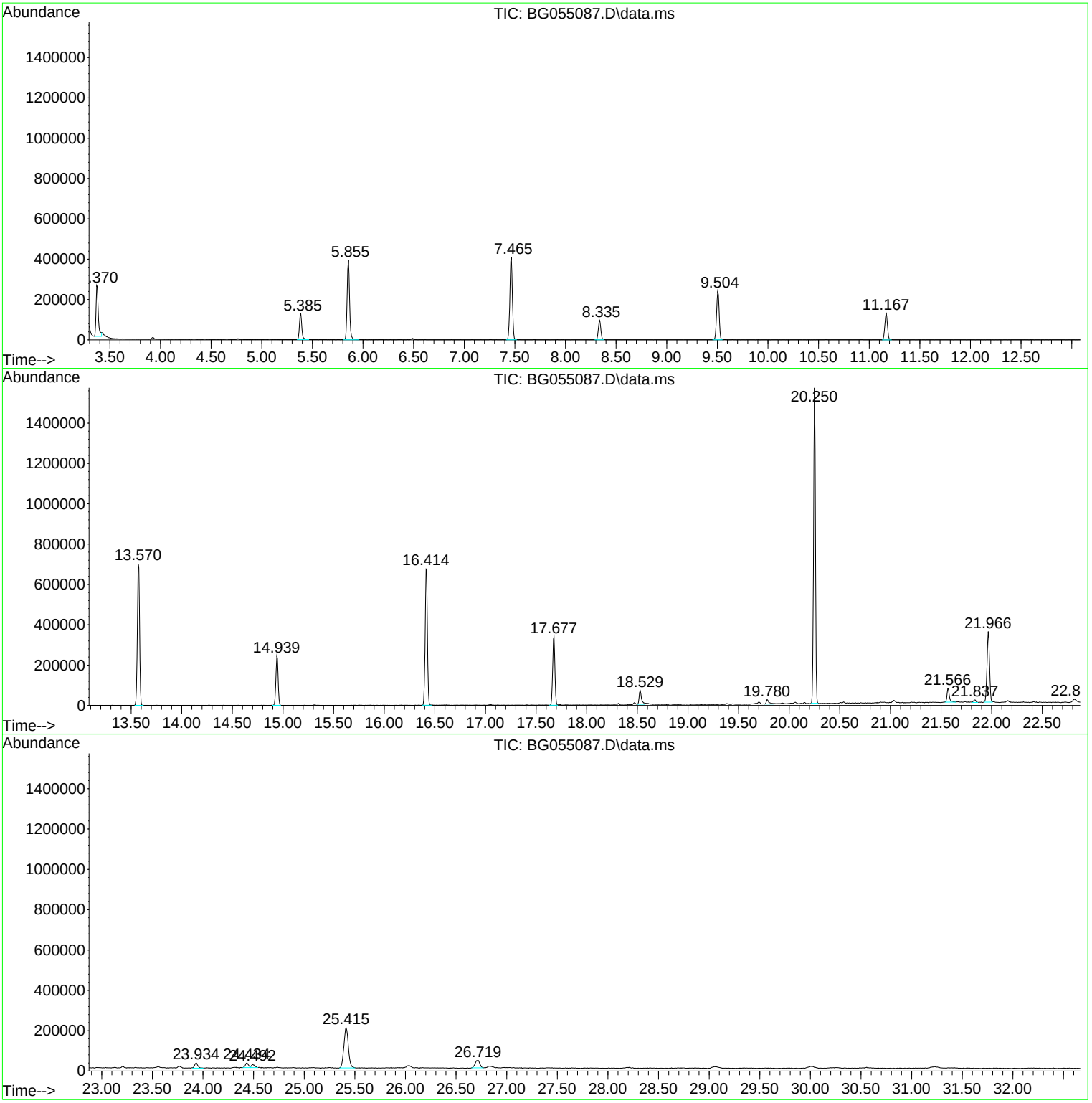
Sum of corrected areas: 9586055

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

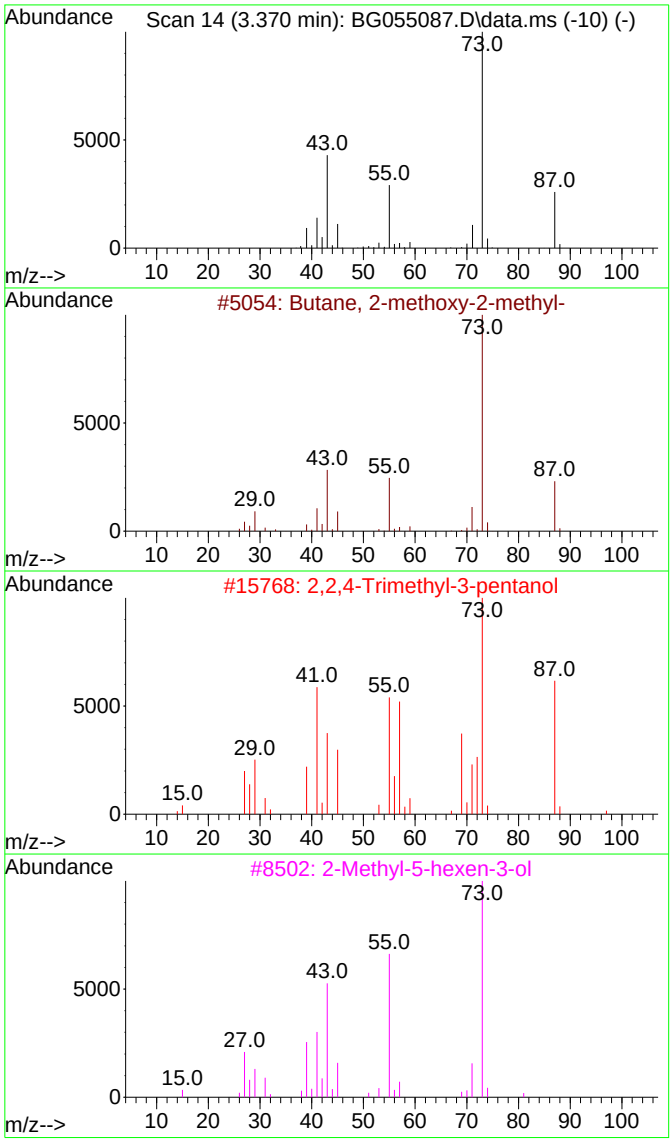
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

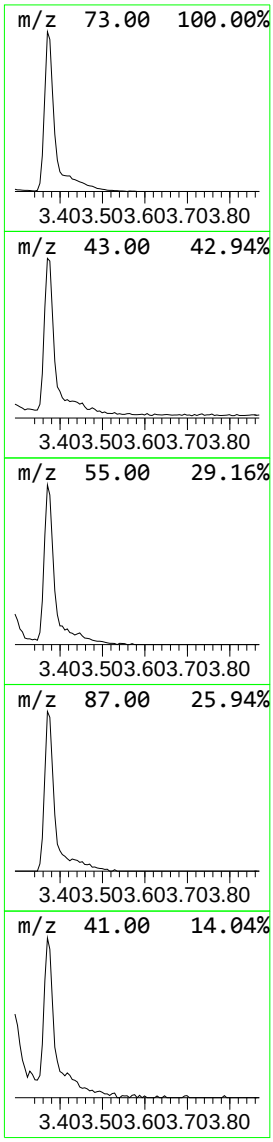
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	46.02 ng	379892	1,4-Dichlorobenzene-d4	8.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

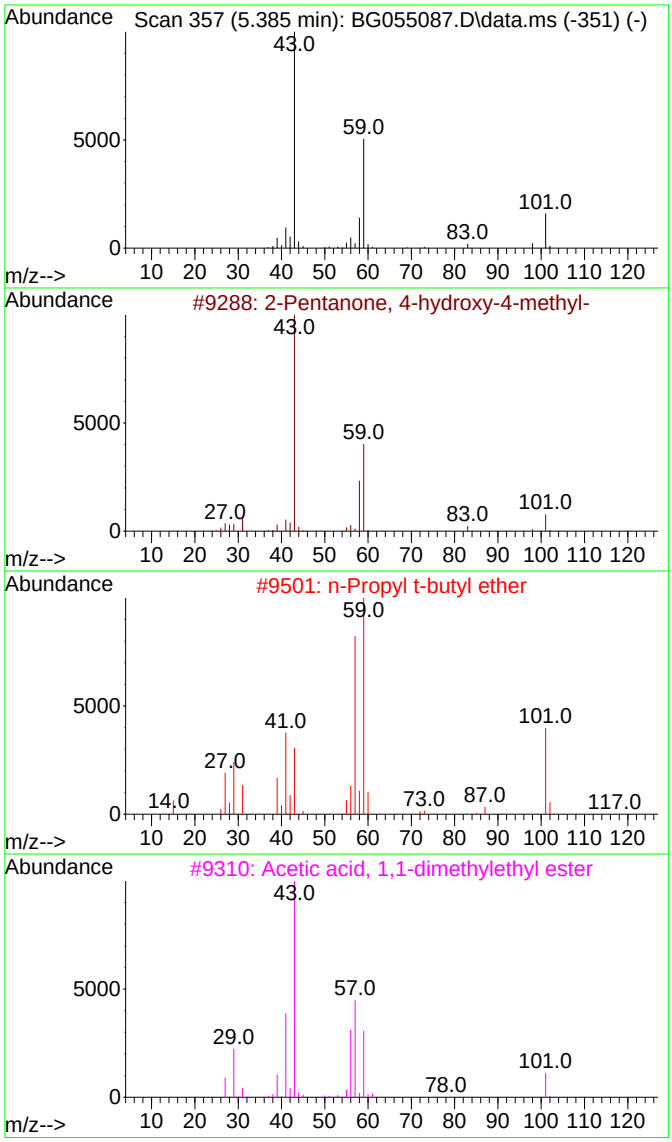
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

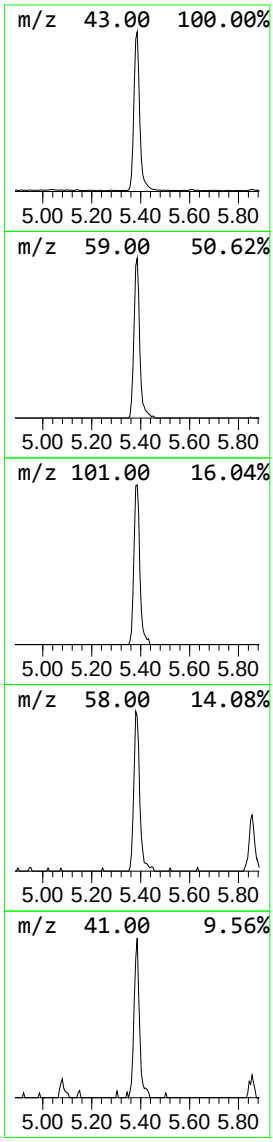
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	25.32 ng	209029	1,4-Dichlorobenzene-d4	8.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

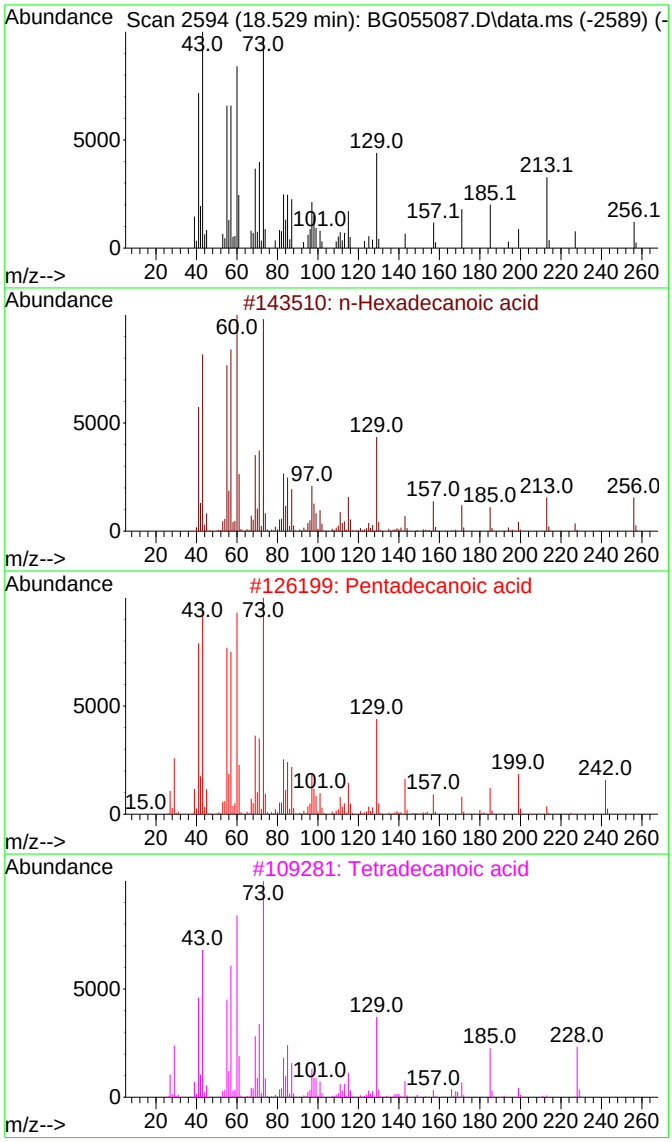
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

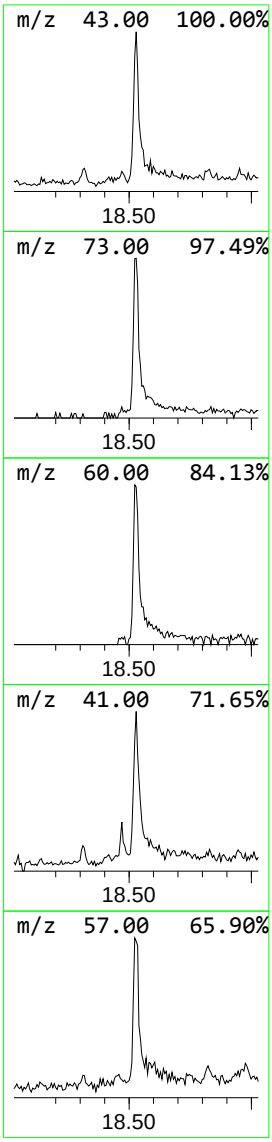
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.529	4.20 ng	109638	Phenanthrene-d10	17.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

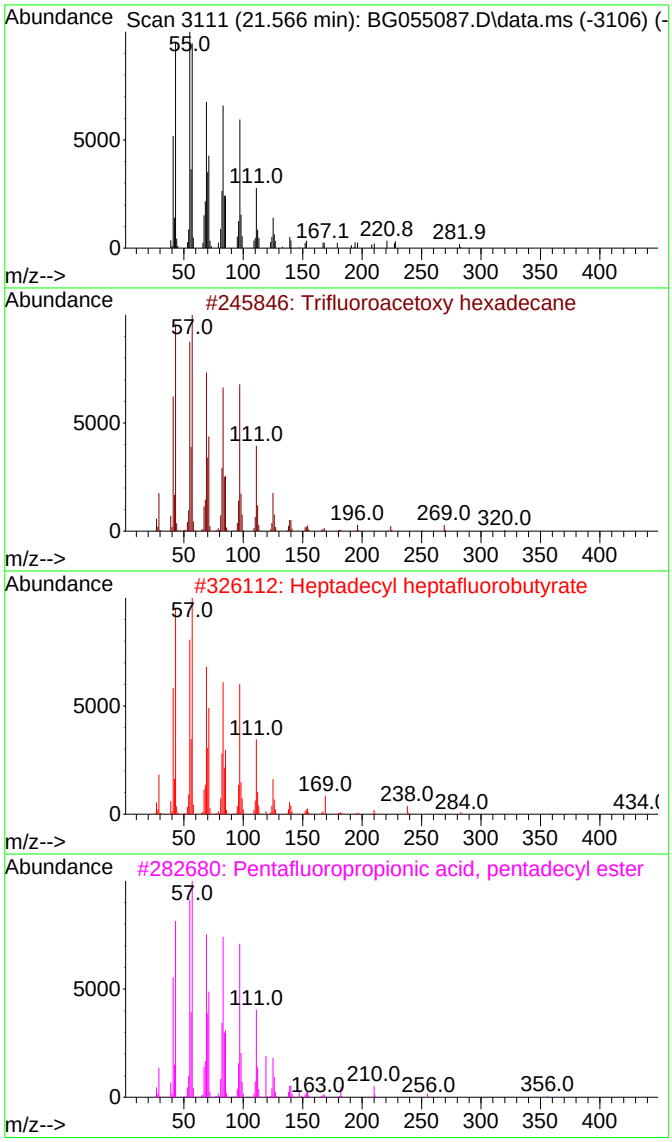
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

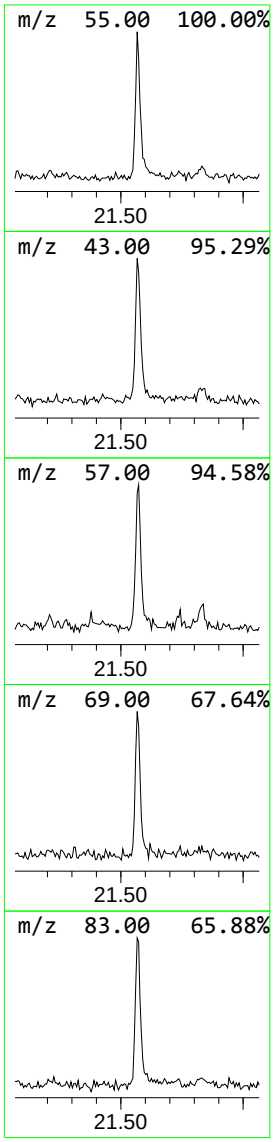
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.566	3.66 ng	108585	Chrysene-d12	21.966

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

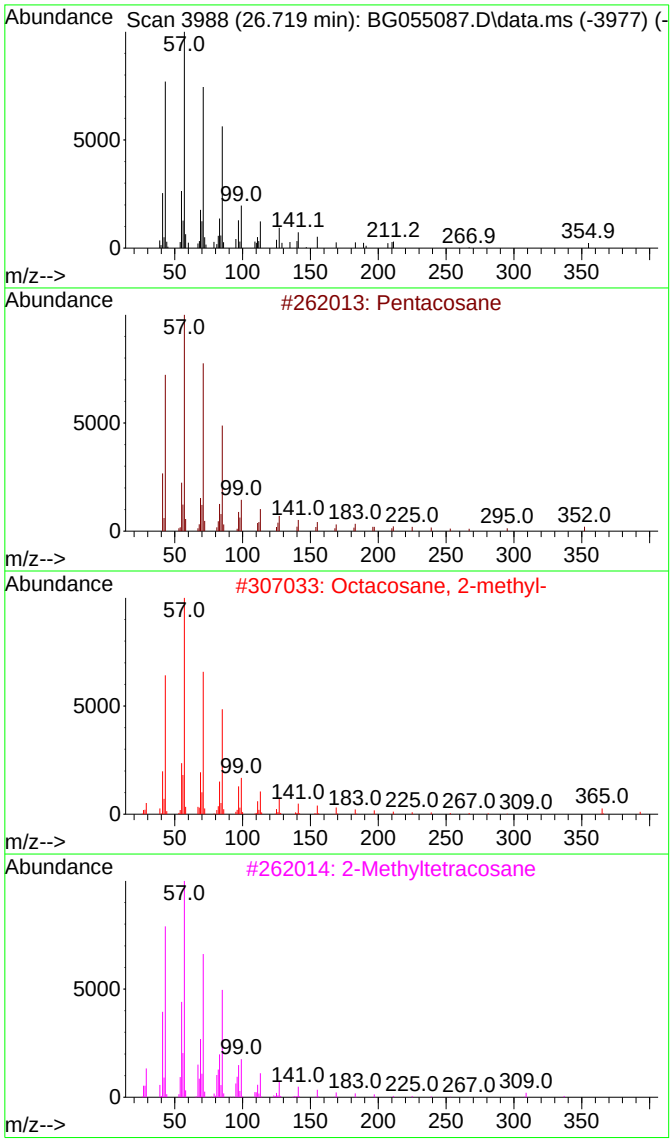
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

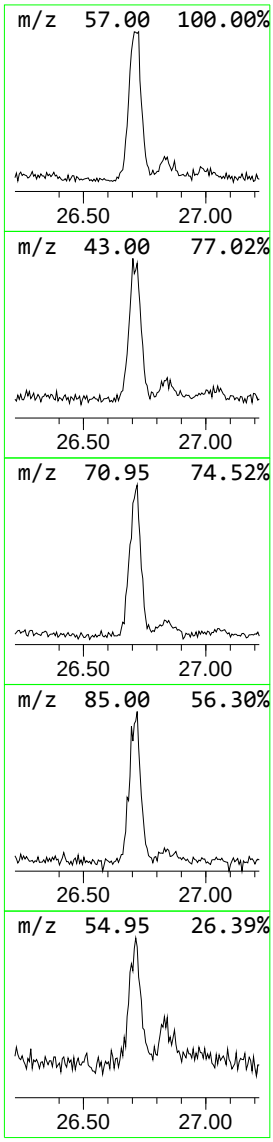
****

Peak Number 5 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.719	3.90 ng	118819	Perylene-d12	25.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	2-Methyltetracosane	352	C25H52	001560-78-7	90
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	90
5	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055087.D
Acq On : 6 Oct 2022 18:17
Operator : CG/JU
Sample : N5014-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-2.0-4.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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...	3.370	46.0	ng	379892	1	8.341	165096	20.0
2-Pentanone, 4-...	5.385	25.3	ng	209029	1	8.341	165096	20.0
n-Hexadecanoic ...	18.529	4.2	ng	109638	4	17.677	522316	20.0
Trifluoroacetox...	21.566	3.7	ng	108585	5	21.966	594165	20.0
Pentacosane	26.719	3.9	ng	118819	6	25.409	609504	20.0