LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.094	12	18	30	rVB	196752	361449	29.80%	5.183%
2	5.068	349	354	363	rBV2	9105	17054	1.41%	0.245%
3	5.555	431	437	451	rBV	342669	567003	46.74%	8.131%
4	7.165	705	711	723	rBV	364209	634763	52.33%	9.102%
5	7.982	843	850	859	rBV	92842	162120	13.37%	2.325%
6	9.151	1041	1049	1063	rVB	232999	423481	34.91%	6.073%
7	10.795	1321	1329	1337	rBV	126349	227604	18.76%	3.264%
8	13.245	1739	1746	1754	rVB	584500	917357	75.63%	13.154%
9	14.620	1974	1980	1987	rVB	200527	312141	25.73%	4.476%
10	16.112	2228	2234	2249	rBV	452489	744423	61.37%	10.675%
11	17.369	2440	2448	2454	rBV	245833	371264	30.61%	5.324%
12	18.262	2595	2600	2610	rBV5	33223	91808	7.57%	1.316%
13	19.401	2786	2794	2795	rBV7	25416	50808	4.19%	0.729%
14	19.783	2856	2859	2862	rBV4	9567	15497	1.28%	0.222%
15	19.977	2887	2892	2897	rBV	951921	1213009	100.00%	17.394%
16	21.264	3107	3111	3116	rVB3	50523	71144	5.87%	1.020%
17	21.634	3168	3174	3181	rVB	249471	406817	33.54%	5.834%
18	24.829	3711	3718	3729	rVB	134606	385995	31.82%	5.535%

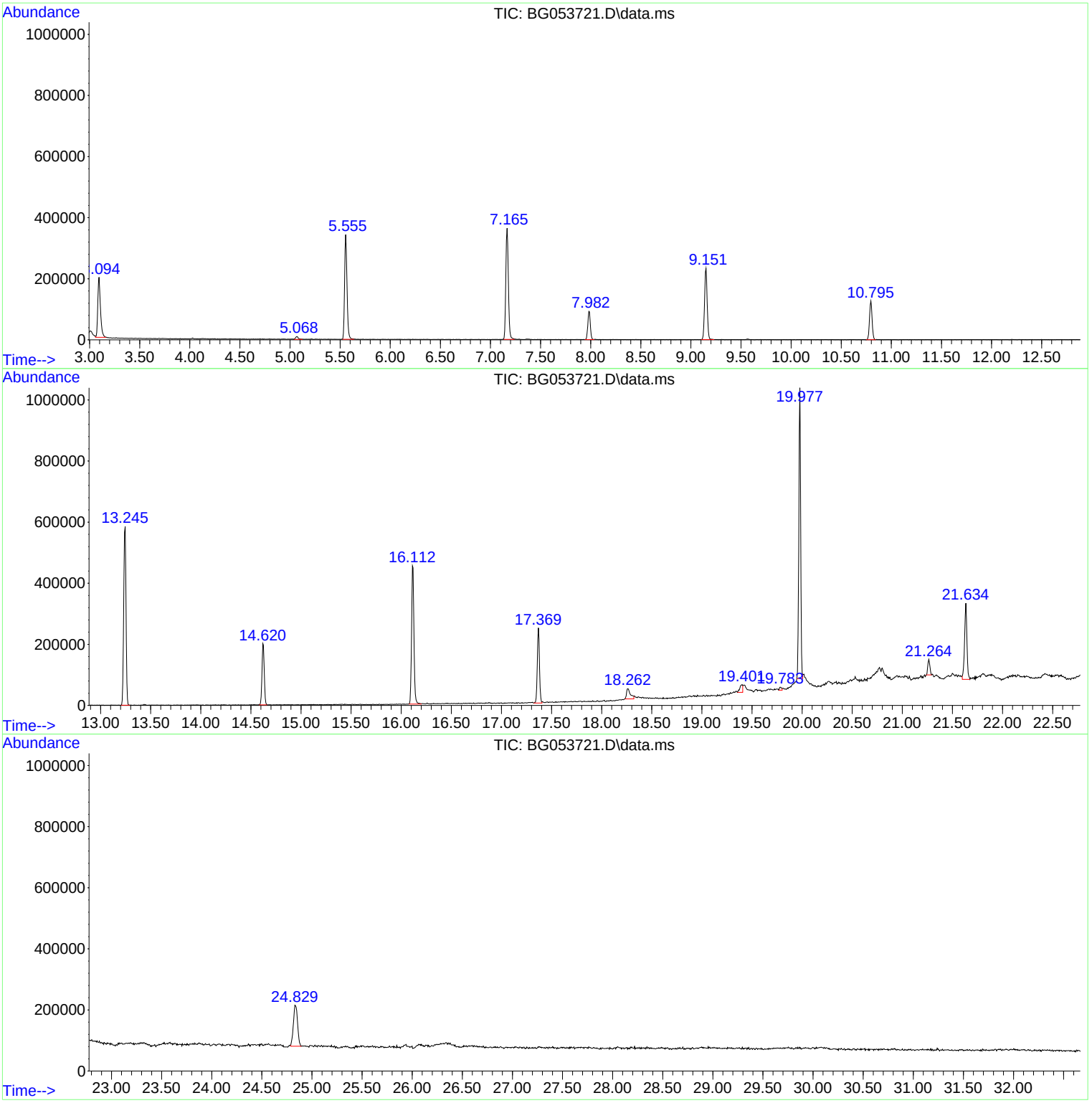
Sum of corrected areas: 6973737

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

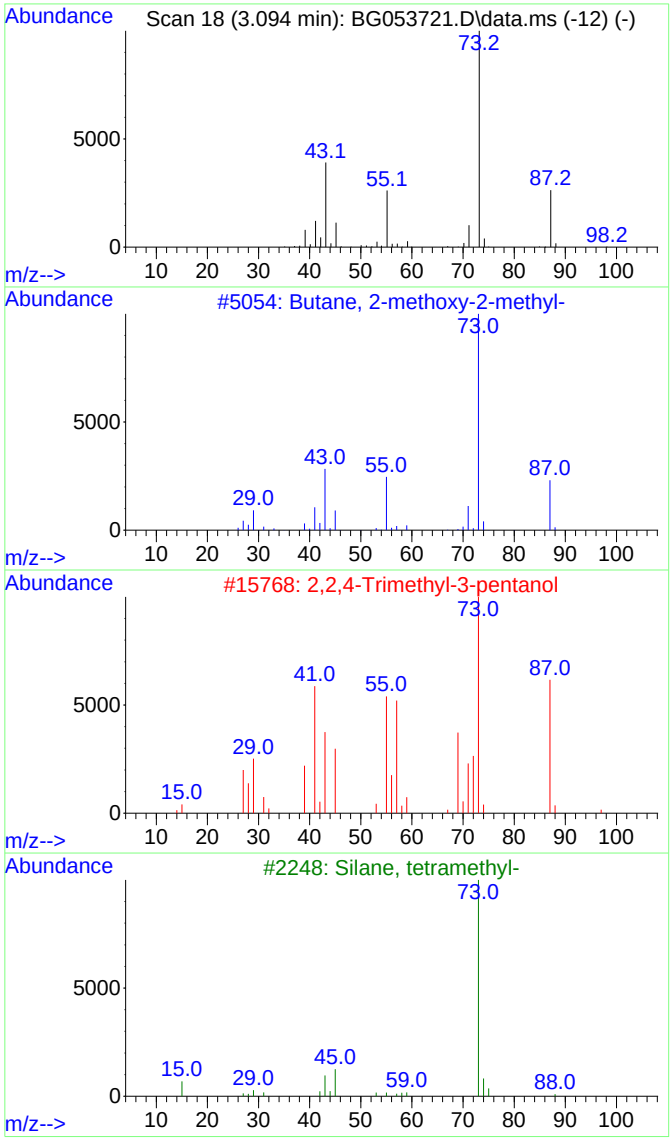
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

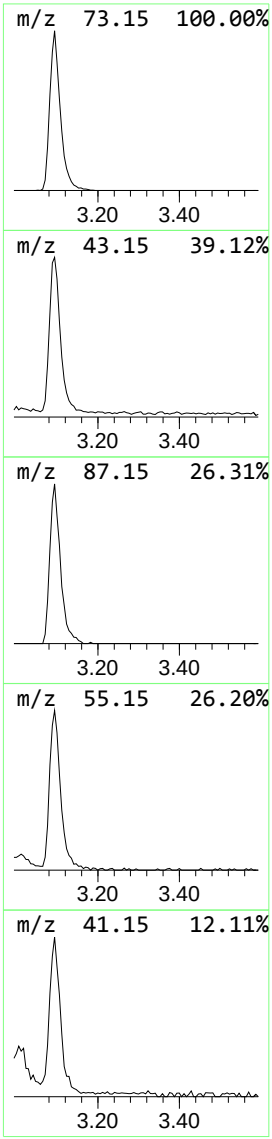
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.094	44.59 ng	361449	1,4-Dichlorobenzene-d4	7.987

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	64
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

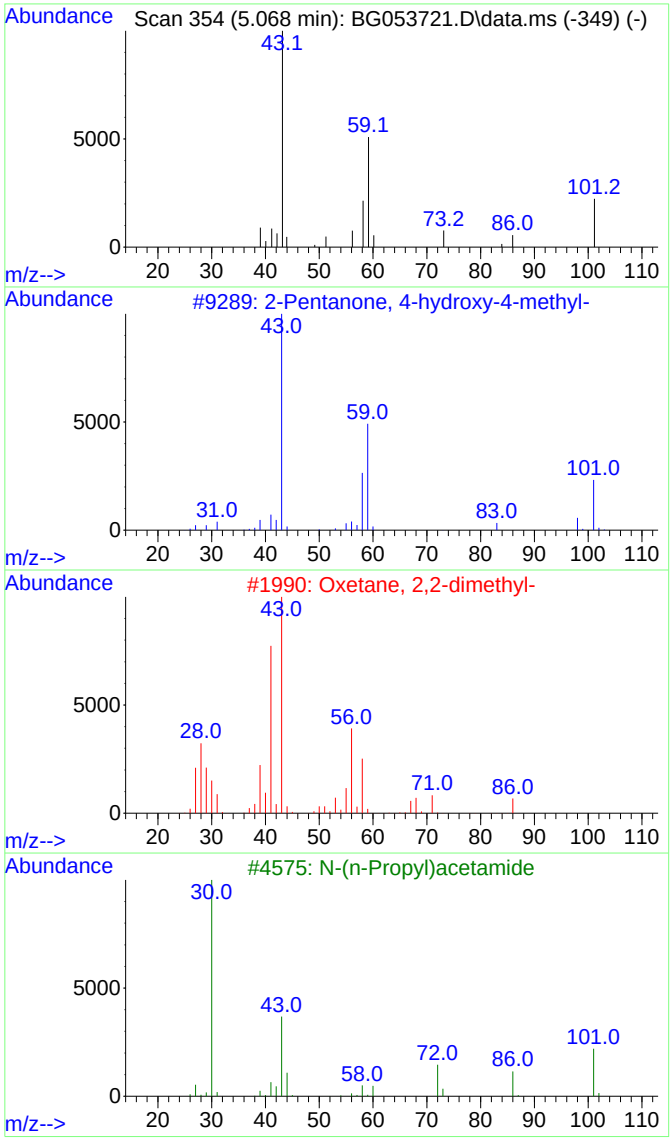
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

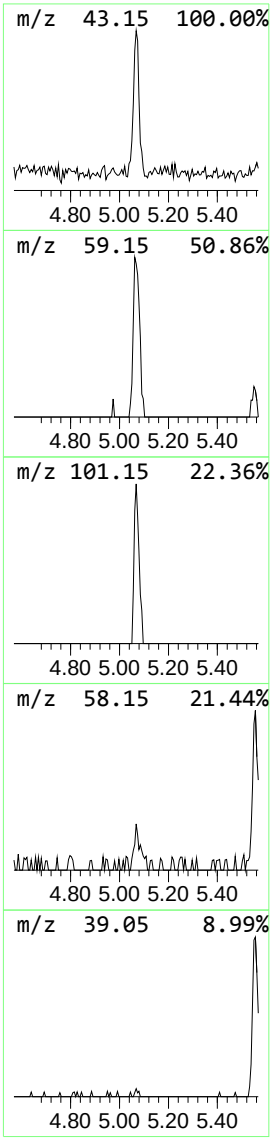
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.068	2.10 ng	17054	1,4-Dichlorobenzene-d4	7.987

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Oxetane, 2,2-dimethyl-	86	C5H10O	006245-99-4	9
3	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

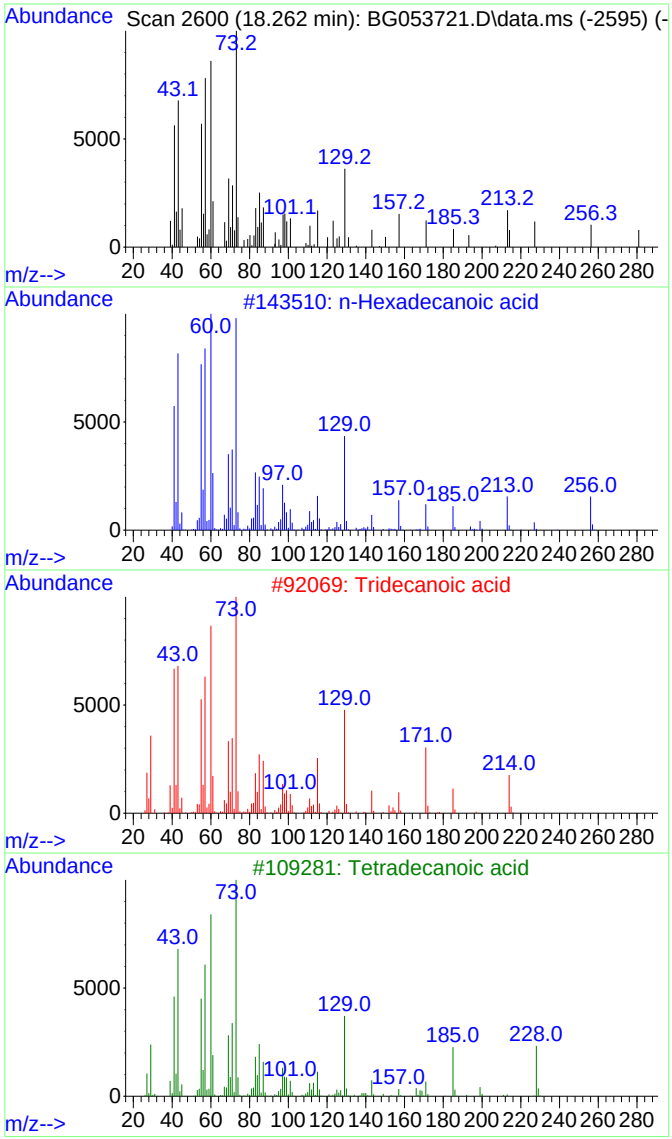
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

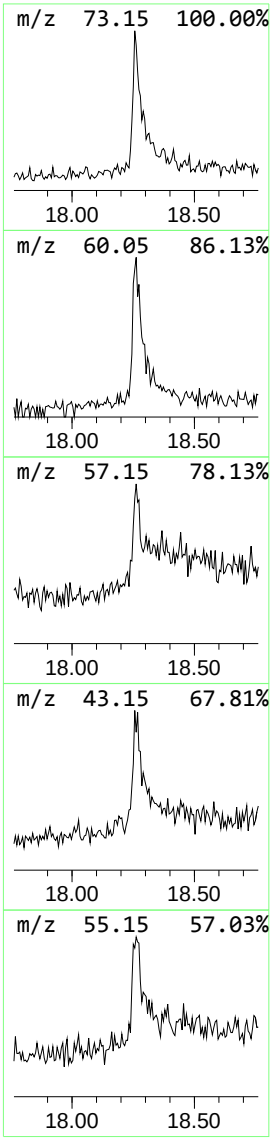
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.262	4.95 ng	91808	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

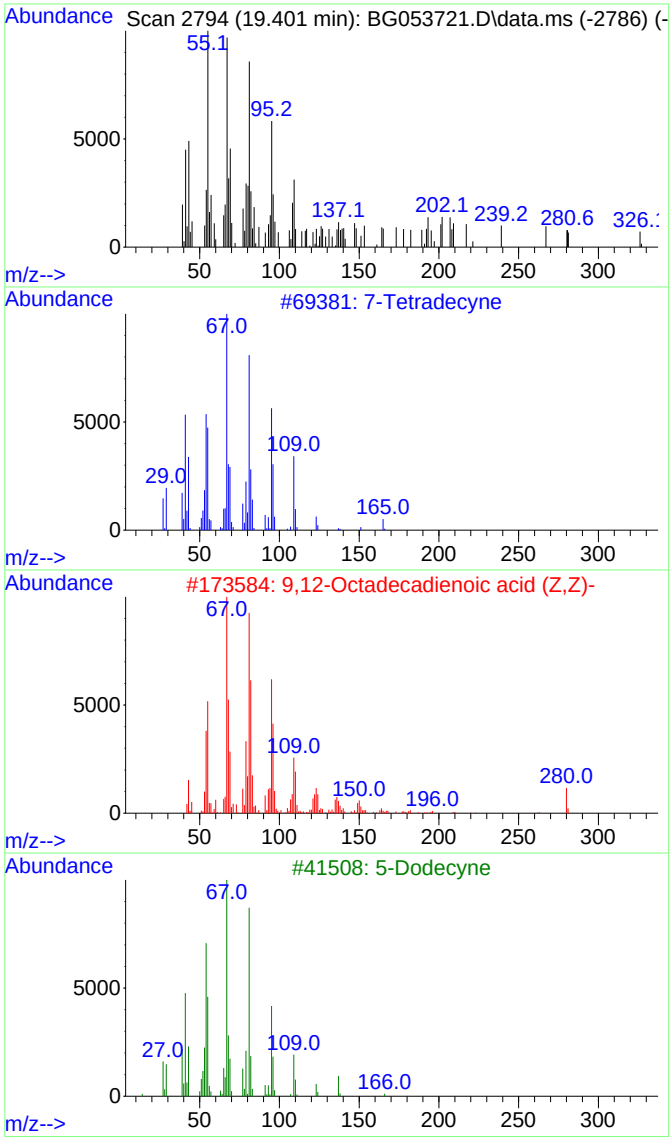
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

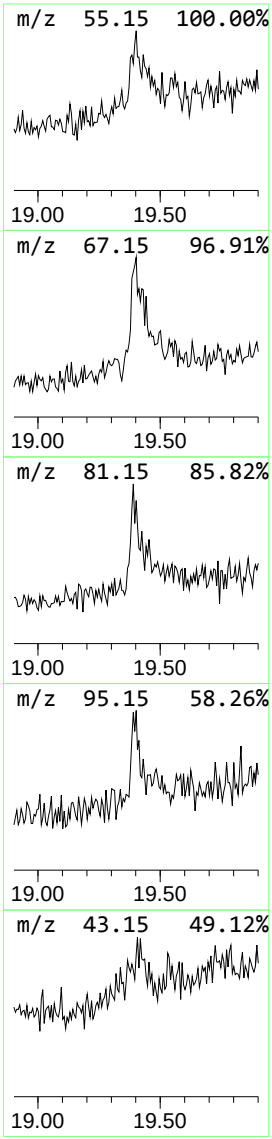
****

Peak Number 4 7-Tetradecyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.401	2.74 ng	50808	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tetradecyne	194	C14H26	035216-11-6	50
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	47
3	5-Dodecyne	166	C12H22	019780-12-2	47
4	Methyl 9,12-heptadecadienoate	280	C18H32O2	1000336-36-2	46
5	Cyclopentene, 1-pentyl-	138	C10H18	004291-98-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

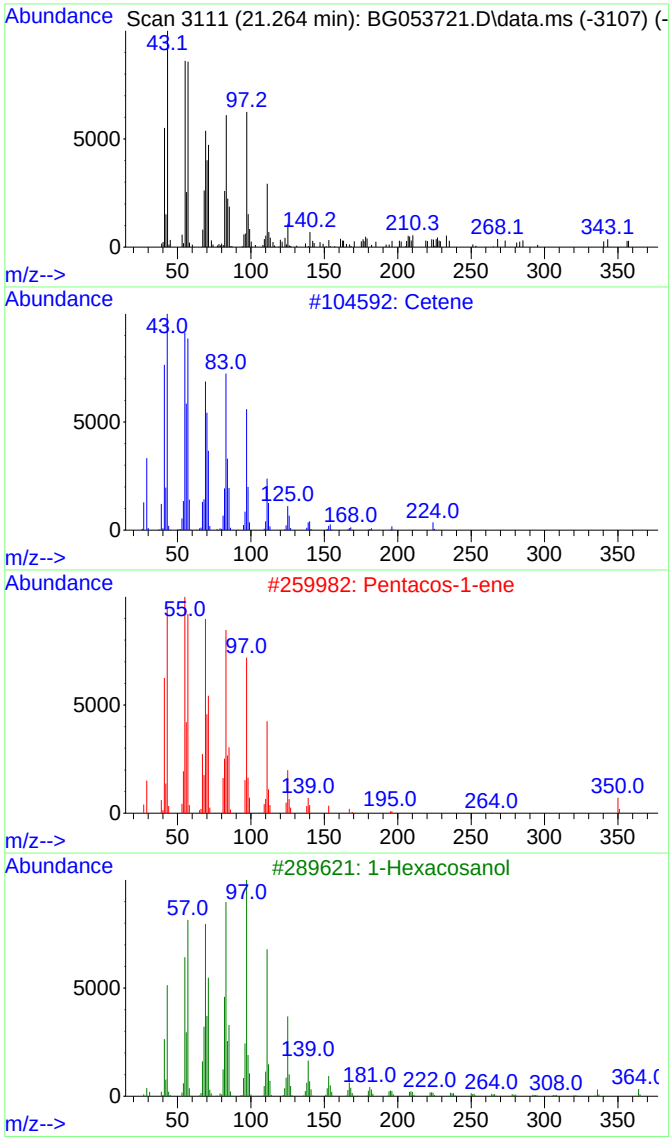
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

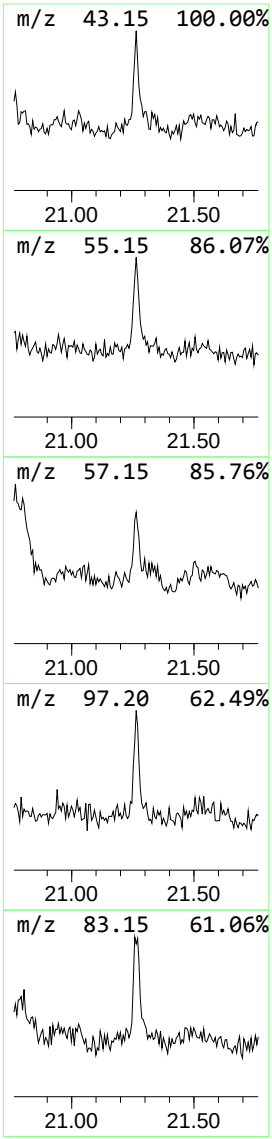
****

Peak Number 5 Cetene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.264	3.50 ng	71144	Chrysene-d12	21.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	86
2	Pentacos-1-ene	350	C25H50	016980-85-1	86
3	1-Hexacosanol	382	C26H54O	000506-52-5	68
4	1-Hexacosene	364	C26H52	018835-33-1	64
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053721.D
Acq On : 26 May 2022 17:43
Operator : CG/JU
Sample : N2985-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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...	3.094	44.6	ng	361449	1	7.987	162120	20.0
2-Pentanone, 4-...	5.068	2.1	ng	17054	1	7.987	162120	20.0
n-Hexadecanoic ...	18.262	5.0	ng	91808	4	17.369	371264	20.0
7-Tetradecyne	19.401	2.7	ng	50808	4	17.369	371264	20.0
Cetene	21.264	3.5	ng	71144	5	21.634	406817	20.0