LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

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-BG111318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.157	313	318	326	rVB2	15810	28097	1.44%	0.327%
2	5.621	390	397	412	rBV	287845	524228	26.86%	6.097%
3	7.225	662	670	684	rBV	319603	634209	32.49%	7.376%
4	7.601	727	734	747	rBV	300781	568056	29.10%	6.606%
5	8.077	809	815	824	rVB	60977	109695	5.62%	1.276%
6	8.400	862	870	880	rBV	234279	442912	22.69%	5.151%
7	9.252	1007	1015	1024	rBV	199082	387166	19.84%	4.503%
8	10.897	1284	1295	1308	rBV	85285	165721	8.49%	1.927%
9	13.329	1703	1709	1724	rBV	554091	906140	46.42%	10.538%
10	14.158	1843	1850	1858	rBV	60680	97310	4.99%	1.132%
11	14.710	1938	1944	1953	rBV2	146962	245313	12.57%	2.853%
12	16.203	2191	2198	2207	rBV2	487736	796459	40.80%	9.263%
13	17.460	2406	2412	2420	rBV	236030	365837	18.74%	4.255%
14	18.318	2553	2558	2569	rBV2	51193	85078	4.36%	0.989%
15	19.587	2769	2774	2786	rBV3	26316	45589	2.34%	0.530%
16	20.063	2849	2855	2867	rBV	1467651	1951871	100.00%	22.700%
17	21.344	3067	3073	3081	rBV3	32978	76124	3.90%	0.885%
18	21.743	3134	3141	3149	rBV	377050	652882	33.45%	7.593%
19	24.029	3524	3530	3537	rVB8	8042	19645	1.01%	0.228%
20	25.063	3685	3706	3719	rBV2	155976	496398	25.43%	5.773%

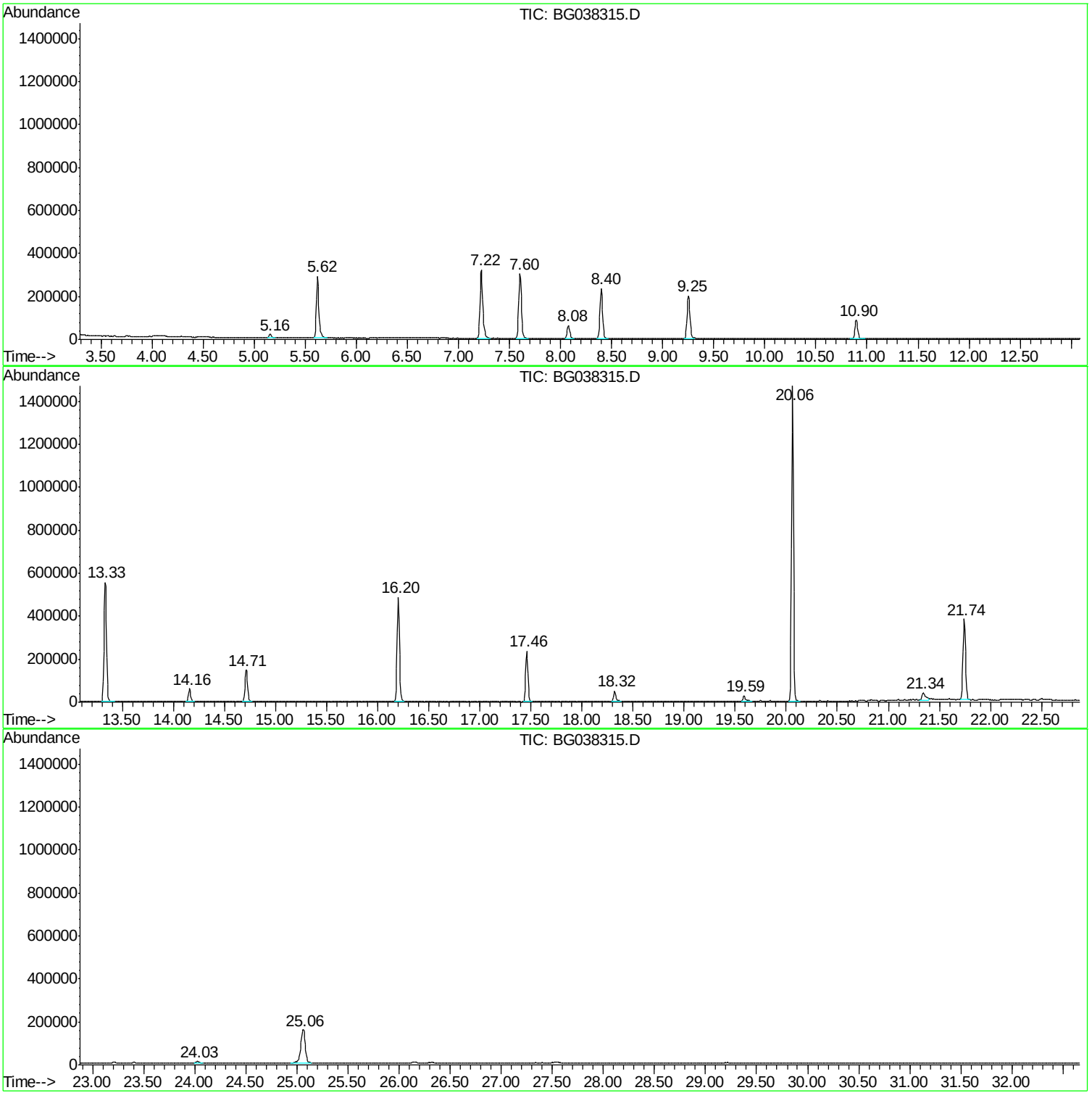
Sum of corrected areas: 8598730

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

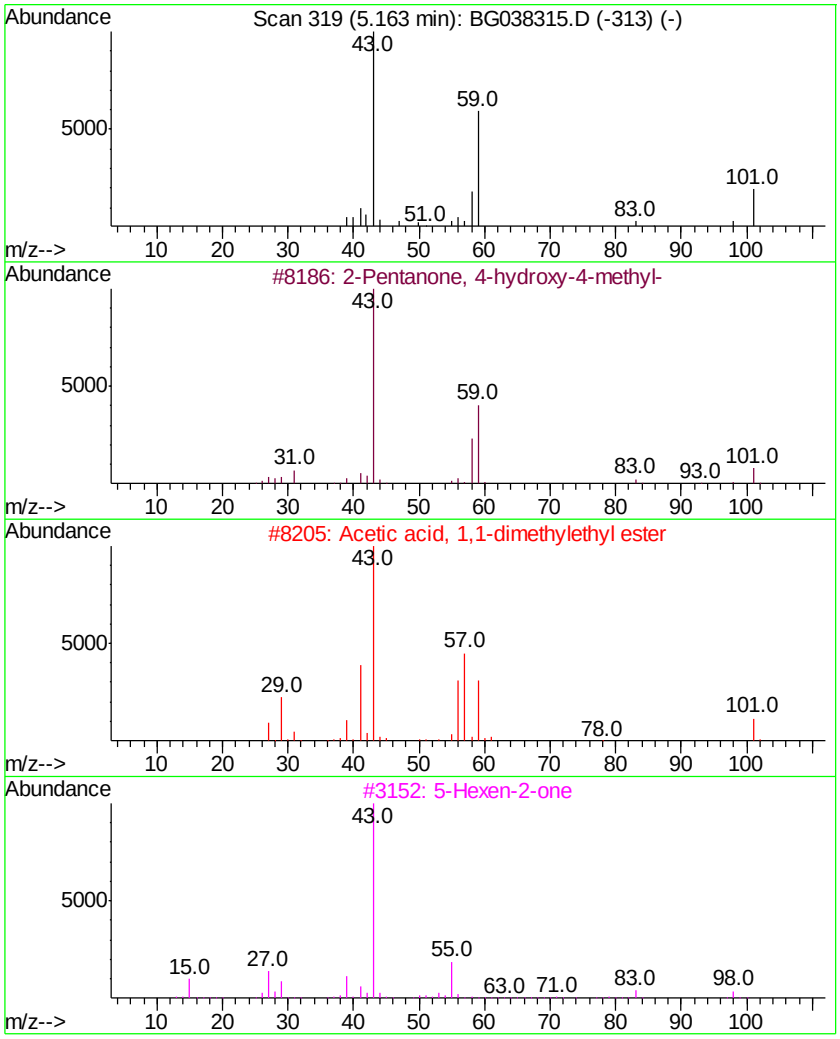
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

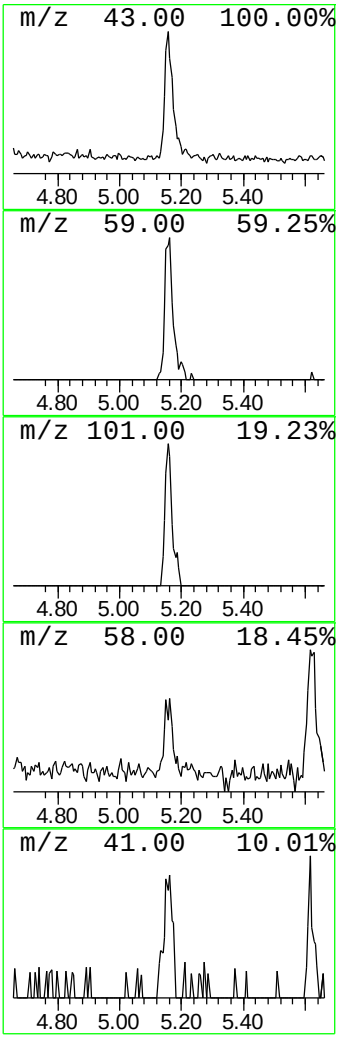
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	5.12 ng	28097	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

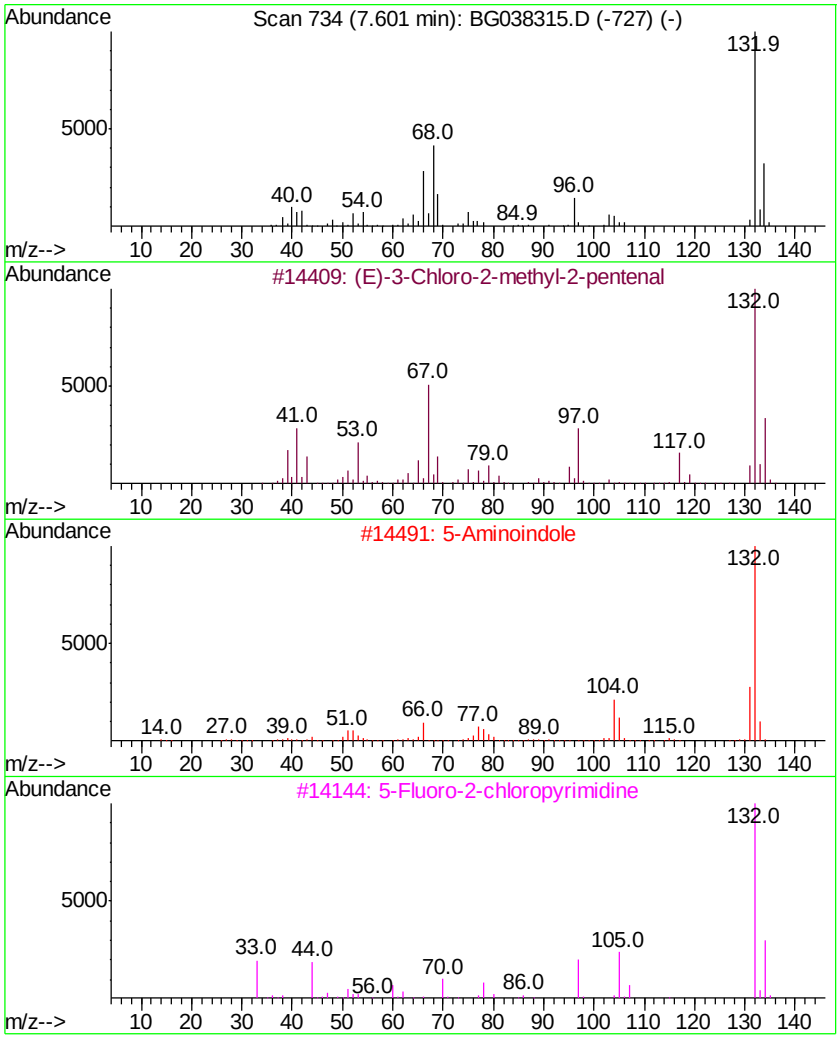
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

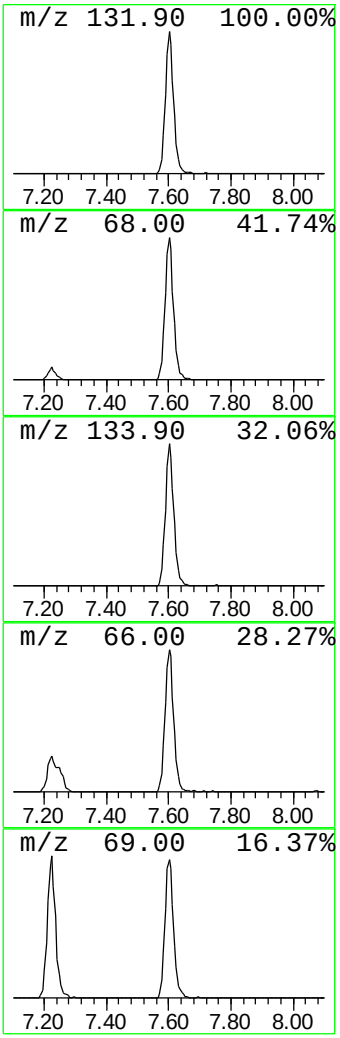
****

Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	103.57 ng	568056	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

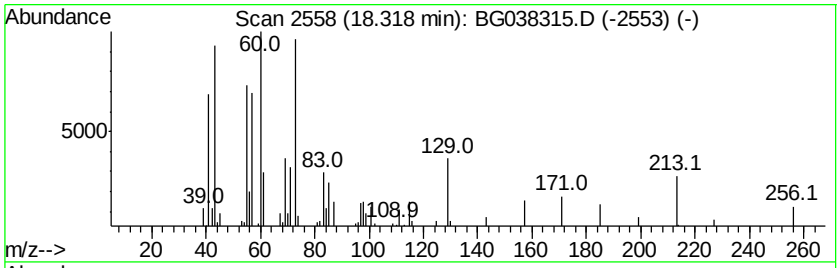
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

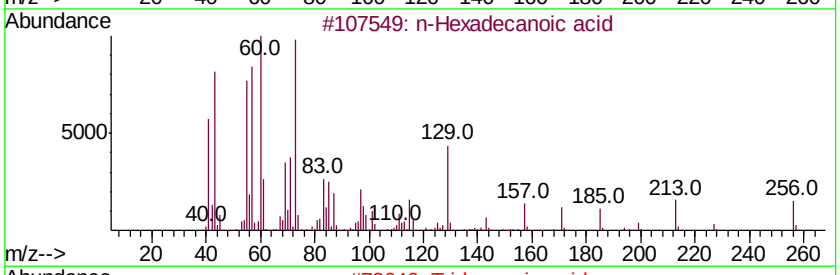
****

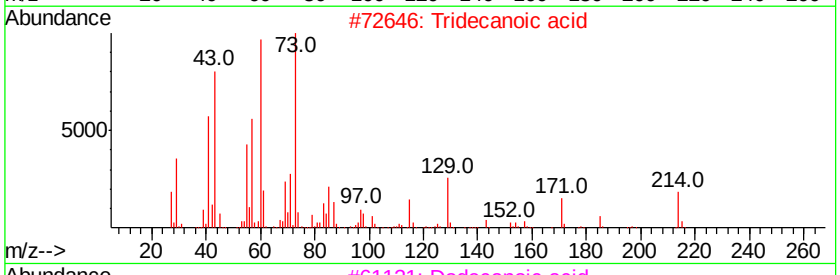
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

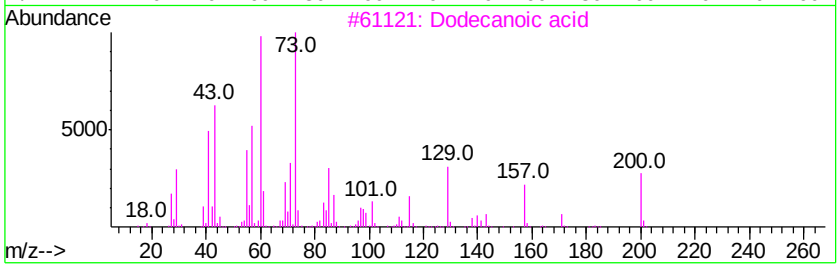
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.65 ng	85078	Phenanthrene-d10	17.46

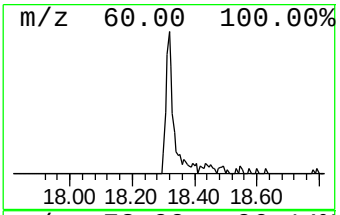
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59

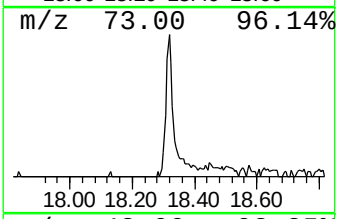


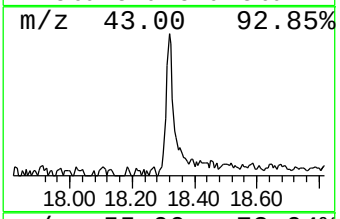


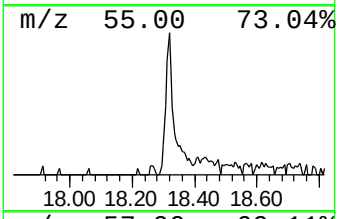


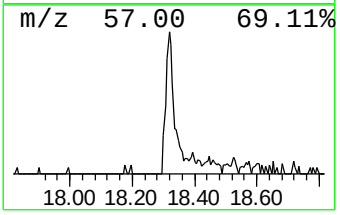












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

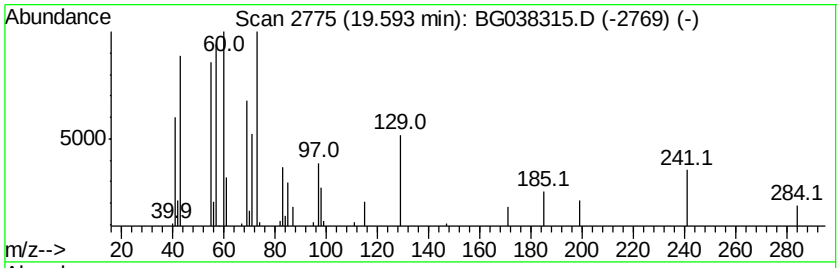
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

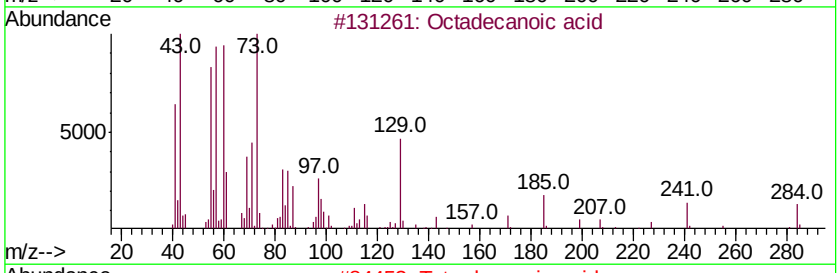
****

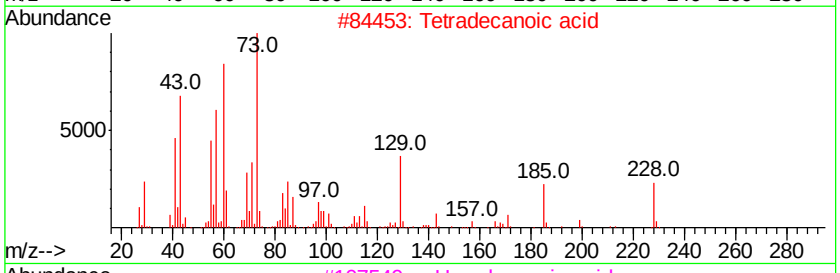
Peak Number 5 Octadecanoic acid Concentration Rank 5

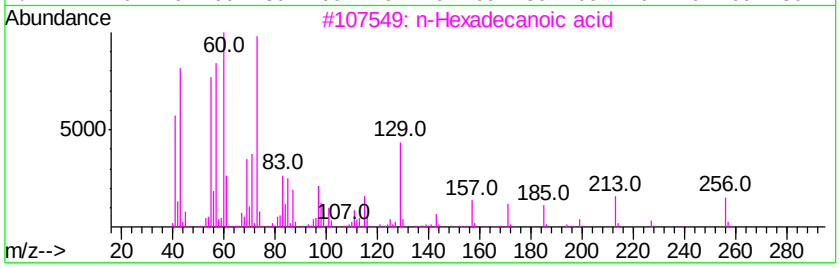
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.49 ng	45589	Phenanthrene-d10	17.46

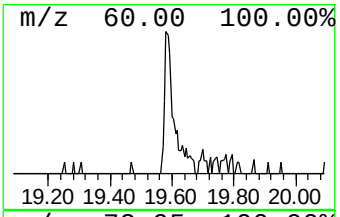
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	81
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Lactose	342	C12H22O11	000063-42-3	53

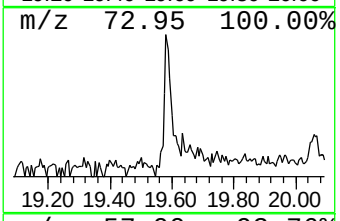


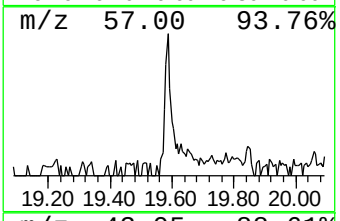


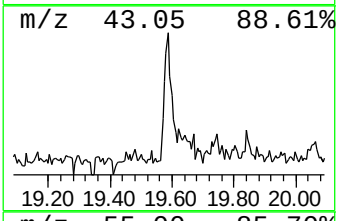


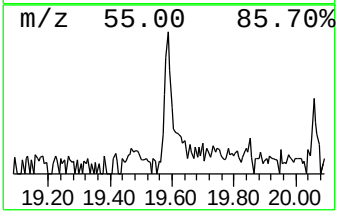












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

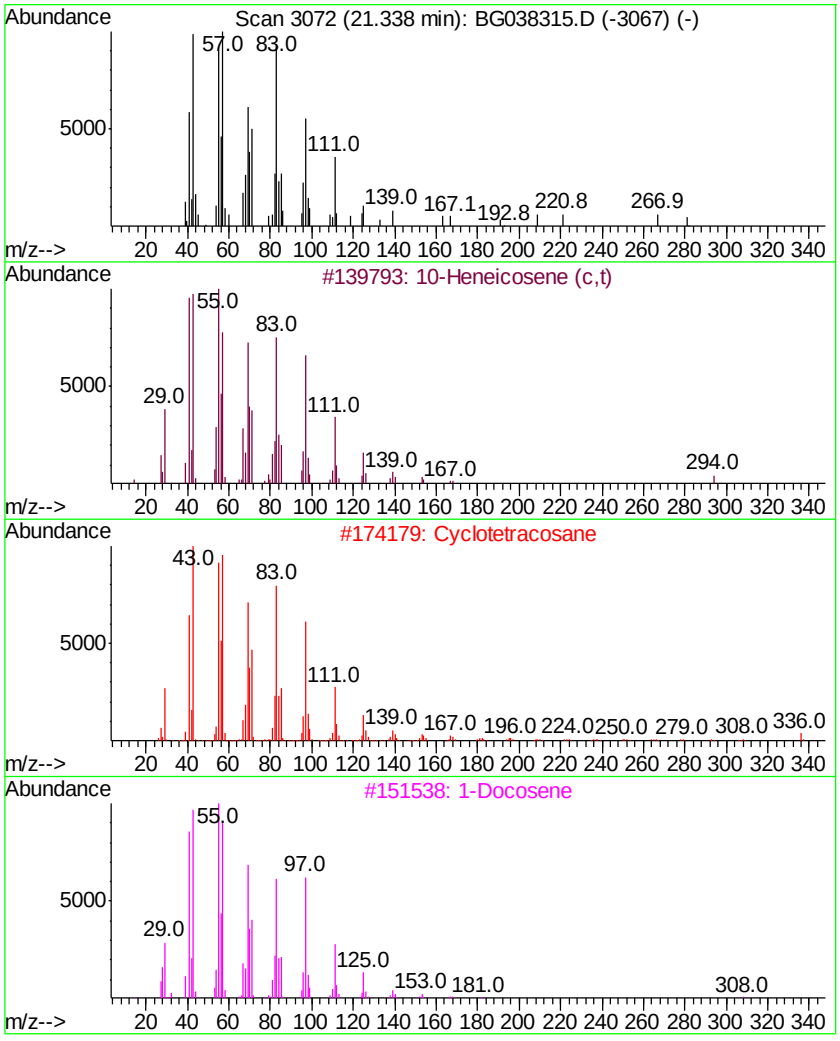
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

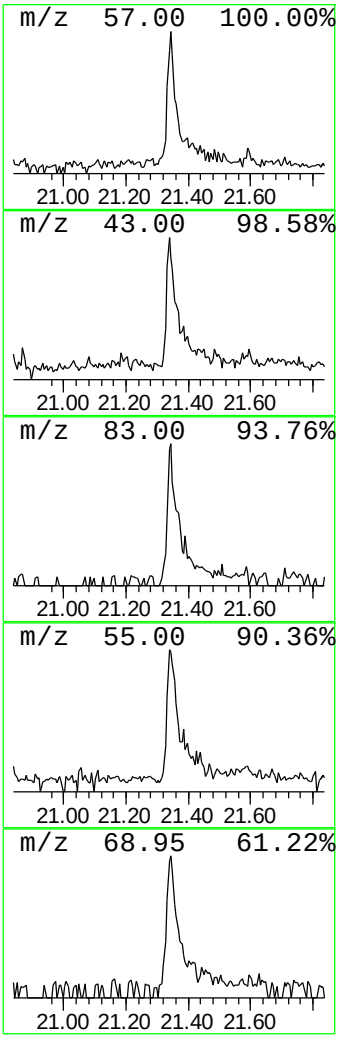
****

Peak Number 6 10-Heneicosene (c,t) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	2.33 ng	76124	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Heneicosene (c,t)	294	C21H42	095008-11-0	87
2	Cyclotetracosane	336	C24H48	000297-03-0	80
3	1-Docosene	308	C22H44	001599-67-3	60
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	58
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG120318\
Data File : BG038315.D
Acq On : 4 Dec 2018 00:56
Operator : JU/SJ
Sample : J6179-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S6-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	5.1	ng	28097	1	8.08	109695	20.0
unknown7.60	7.60	103.6	ng	568056	1	8.08	109695	20.0
n-Hexadecanoic acid	18.32	4.7	ng	85078	4	17.46	365837	20.0
Octadecanoic acid	19.59	2.5	ng	45589	4	17.46	365837	20.0
10-Heneicosene (c,t)	21.34	2.3	ng	76124	5	21.74	652882	20.0