LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055632.D
Acq On : 15 Nov 2022 21:50
Operator : CG/JU
Sample : N5431-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221178-COMP-13-MODIFIED-ELUTRIATE

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.694	231	239	244	rBV	23320	36672	1.12%	0.287%
2	5.305	337	343	351	rBV	64852	100288	3.05%	0.784%
3	5.781	418	424	437	rVB	406835	652279	19.87%	5.099%
4	7.391	690	698	709	rBV	323068	547394	16.67%	4.279%
5	8.255	838	845	852	rBV	136510	232342	7.08%	1.816%
6	9.424	1037	1044	1057	rVB	441388	797394	24.28%	6.233%
7	11.086	1318	1327	1334	rBV	186566	336306	10.24%	2.629%
8	13.501	1730	1738	1745	rBV	1123422	1775794	54.08%	13.881%
9	14.312	1870	1876	1882	rBV	32190	46499	1.42%	0.363%
10	14.876	1963	1972	1981	rBV	331531	513272	15.63%	4.012%
11	16.357	2217	2224	2236	rBV	1141828	1745263	53.15%	13.642%
12	17.620	2432	2439	2448	rVB	472144	717586	21.85%	5.609%
13	18.266	2541	2549	2554	rBV5	26659	36199	1.10%	0.283%
14	18.478	2580	2585	2594	rBV2	87608	147963	4.51%	1.157%
15	19.741	2794	2800	2812	rBV	78175	145960	4.45%	1.141%
16	20.205	2873	2879	2885	rBV	2488346	3283532	100.00%	25.667%
17	21.915	3163	3170	3178	rVB2	494127	830706	25.30%	6.493%
18	25.329	3741	3751	3763	rVB2	280207	847560	25.81%	6.625%

Sum of corrected areas: 12793009

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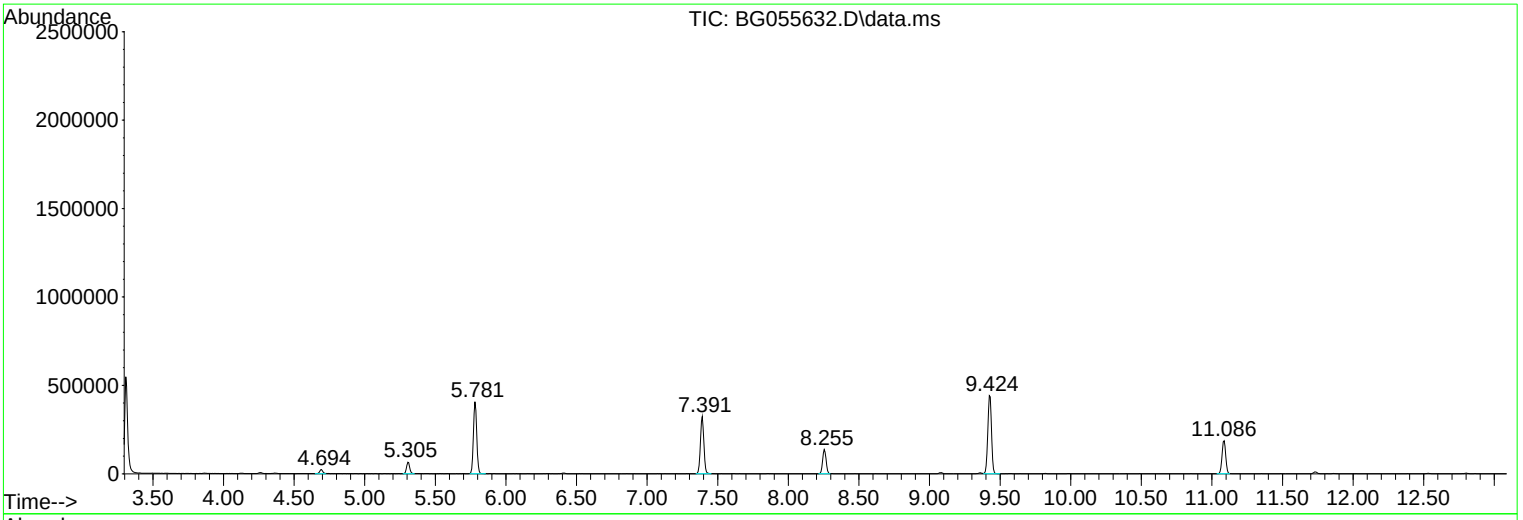
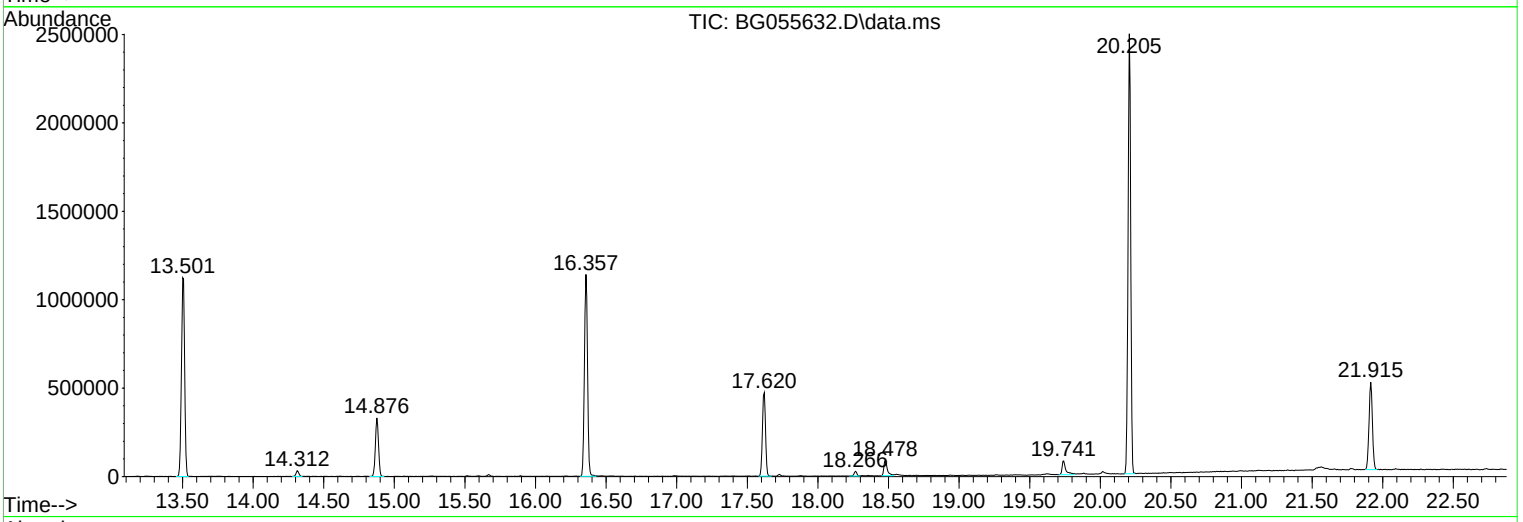
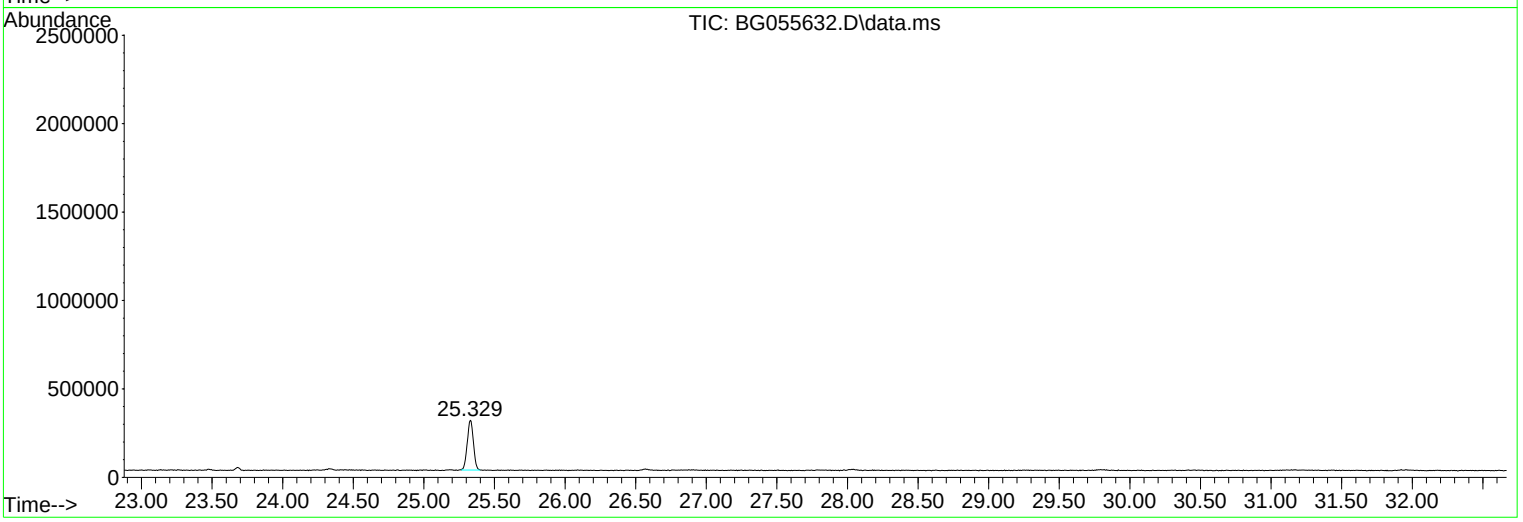
Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221178-COMP-13-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Instrument :
BNA_G
ClientSampleId :
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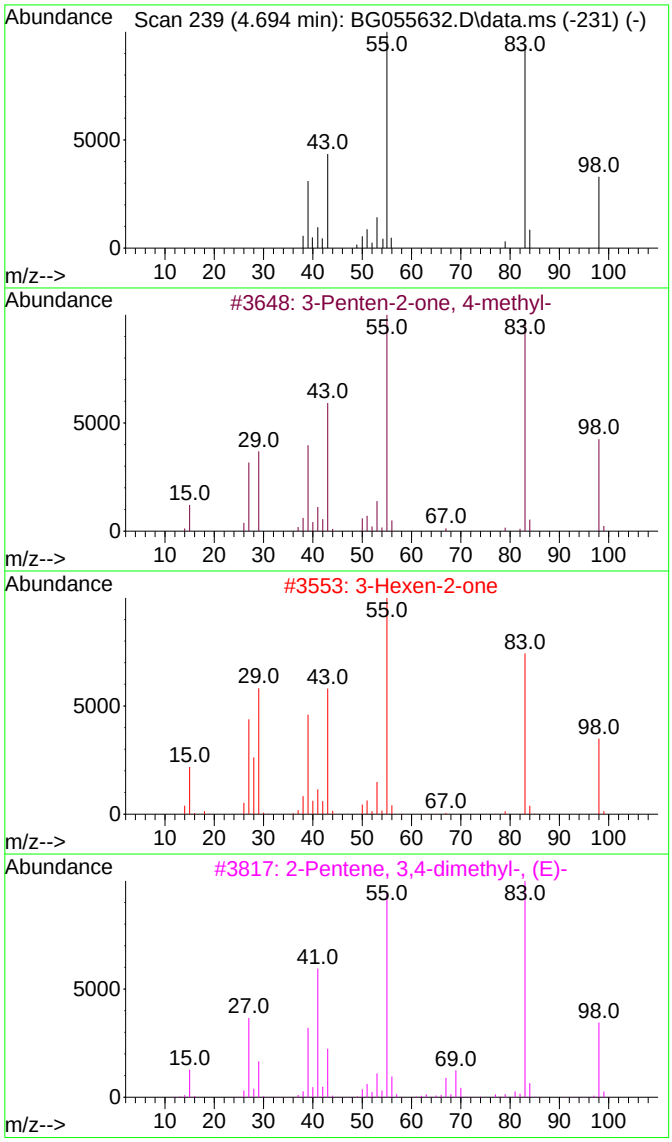
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

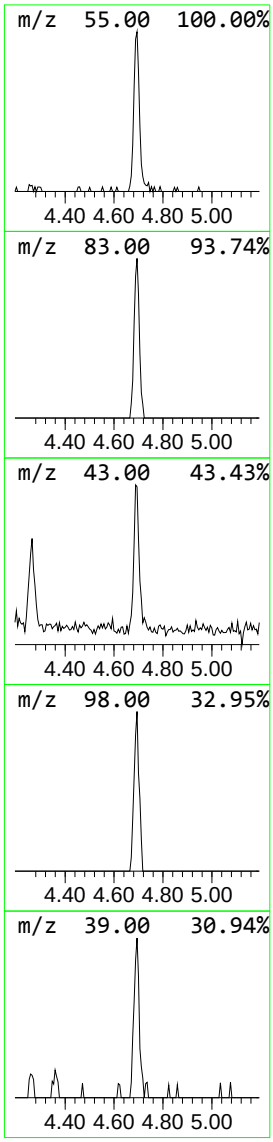
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.694	3.16 ng	36672	1,4-Dichlorobenzene-d4	8.255

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





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Operator : CG/JU
Sample : N5431-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221178-COMP-13-MODIFIED-ELUTRIATE

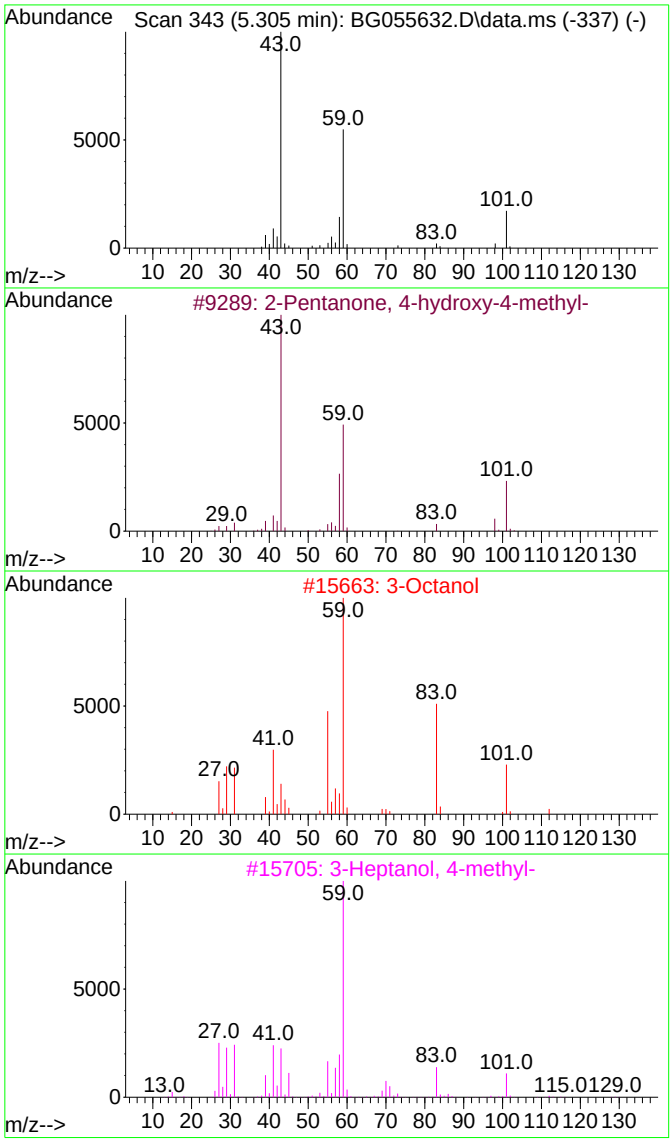
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

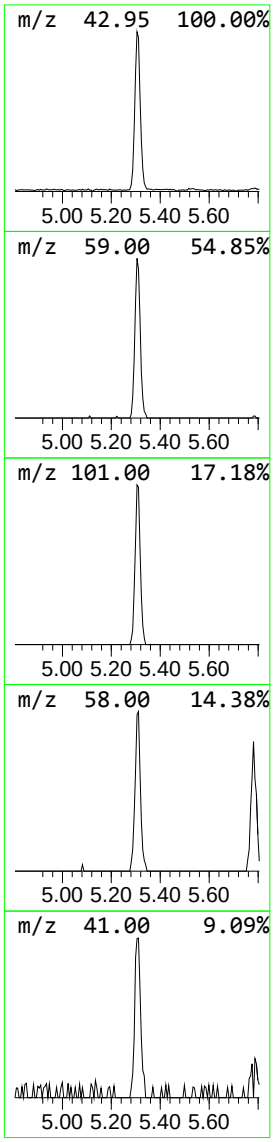
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.305	8.63 ng	100288	1,4-Dichlorobenzene-d4	8.255

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	36
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055632.D
Acq On : 15 Nov 2022 21:50
Operator : CG/JU
Sample : N5431-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221178-COMP-13-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

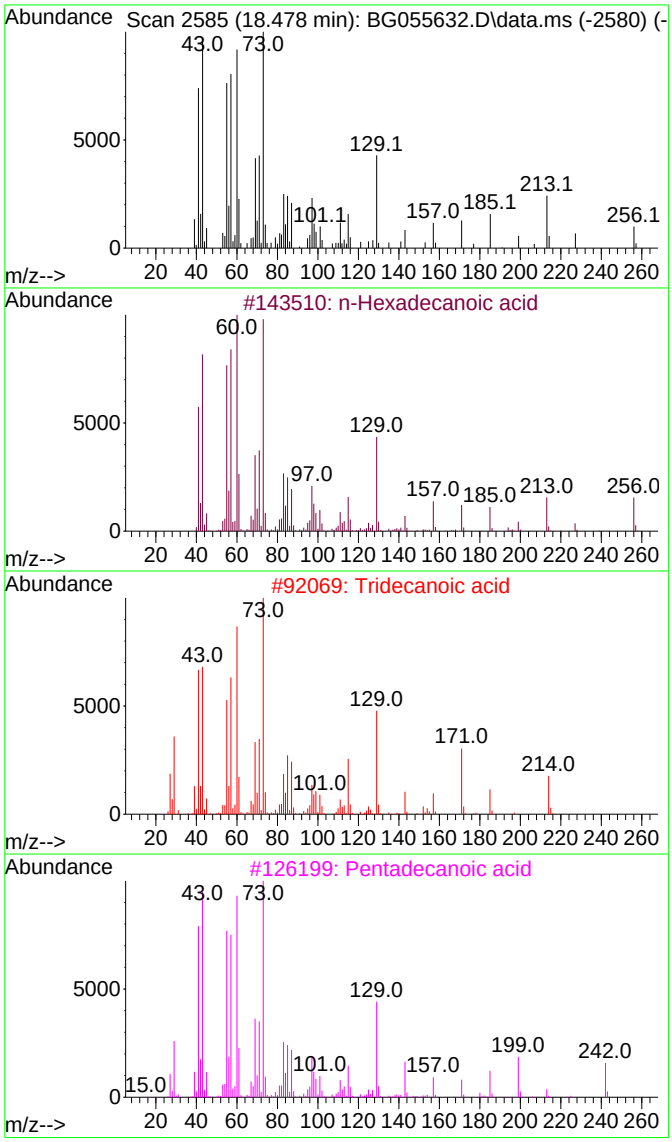
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

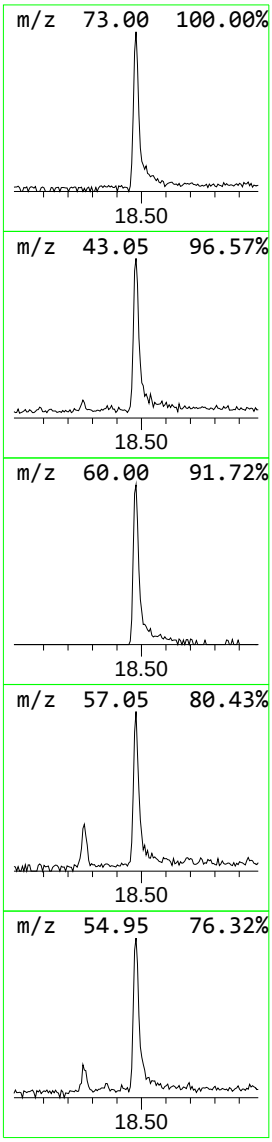
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.478	4.12 ng	147963	Phenanthrene-d10	17.620

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221178-COMP-13-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

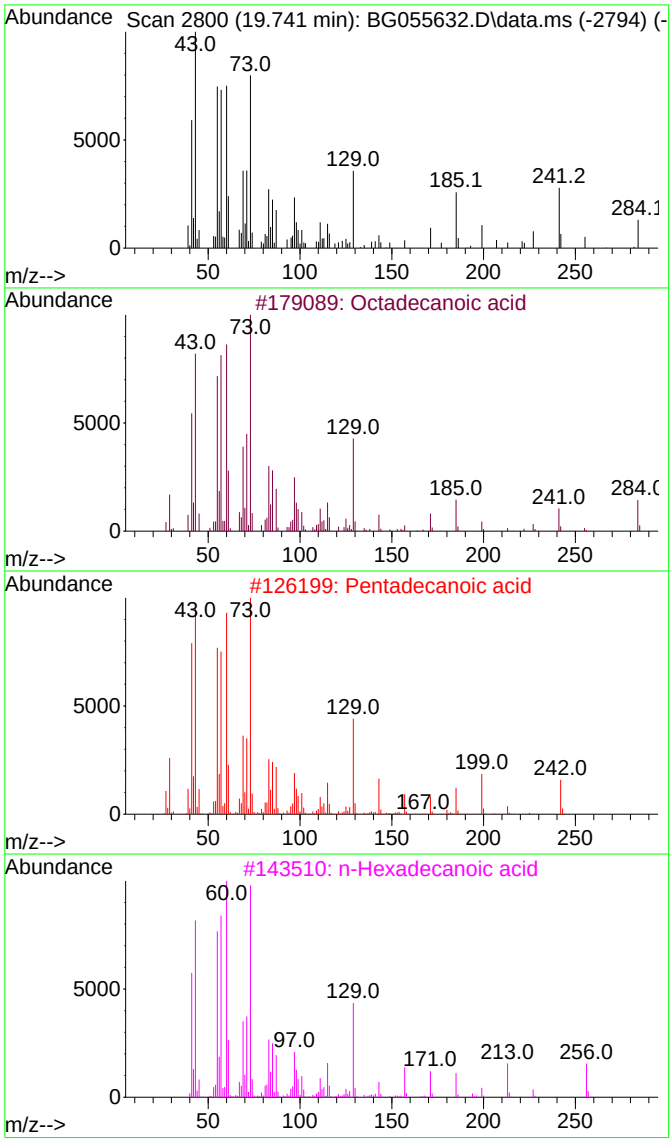
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

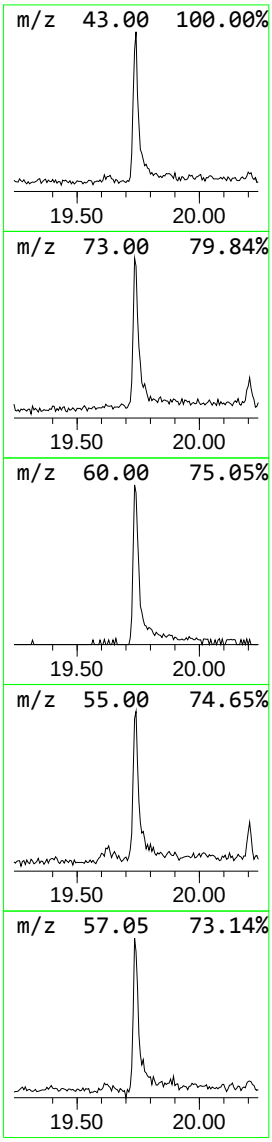
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.741	4.07 ng	145960	Phenanthrene-d10	17.620

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Tentatively Identified Compound (LSC) summary

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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
3-Penten-2-one,...	4.694	3.2	ng	36672	1	8.255	232342	20.0
2-Pentanone, 4-...	5.305	8.6	ng	100288	1	8.255	232342	20.0
n-Hexadecanoic ...	18.478	4.1	ng	147963	4	17.620	717586	20.0
Octadecanoic acid	19.741	4.1	ng	145960	4	17.620	717586	20.0