LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-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_M\Methods\8270-BM102822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.569	78	82	88	rBV	89518	119441	1.29%	0.191%
2	4.969	314	320	333	rBV	540619	772100	8.31%	1.236%
3	5.434	392	399	409	rBV	4345493	6119799	65.85%	9.800%
4	7.040	664	672	689	rBV	4030795	6220412	66.93%	9.961%
5	7.863	805	812	819	rBV	1038642	1590595	17.11%	2.547%
6	9.034	1003	1011	1021	rBV	2417640	3866191	41.60%	6.191%
7	10.669	1280	1289	1300	rBV	1364042	2234243	24.04%	3.578%
8	13.127	1700	1707	1718	rBV	5203006	7517676	80.89%	12.038%
9	14.374	1915	1919	1930	rVB7	44151	125141	1.35%	0.200%
10	14.504	1934	1941	1949	rBV	1746789	2552094	27.46%	4.087%
11	14.916	2006	2011	2017	rBV	81571	129662	1.40%	0.208%
12	15.733	2140	2150	2164	rBV	123428	405565	4.36%	0.649%
13	15.992	2187	2194	2202	rBV	4205379	5778174	62.17%	9.253%
14	17.245	2401	2407	2418	rBV	1966157	2856194	30.73%	4.574%
15	17.362	2423	2427	2432	rVB4	100311	136109	1.46%	0.218%
16	18.139	2553	2559	2573	rBV	1492471	2283515	24.57%	3.657%
17	19.298	2753	2756	2766	rVB4	78220	142851	1.54%	0.229%
18	19.415	2771	2776	2791	rBV	721762	1203253	12.95%	1.927%
19	19.862	2847	2852	2863	rBV	7945649	9293858	100.00%	14.882%
20	21.127	3063	3067	3075	rBV	704263	1138019	12.24%	1.822%
21	21.415	3112	3116	3122	rBV	2972077	3857648	41.51%	6.177%
22	23.774	3511	3517	3529	rVB2	2072595	4106229	44.18%	6.575%

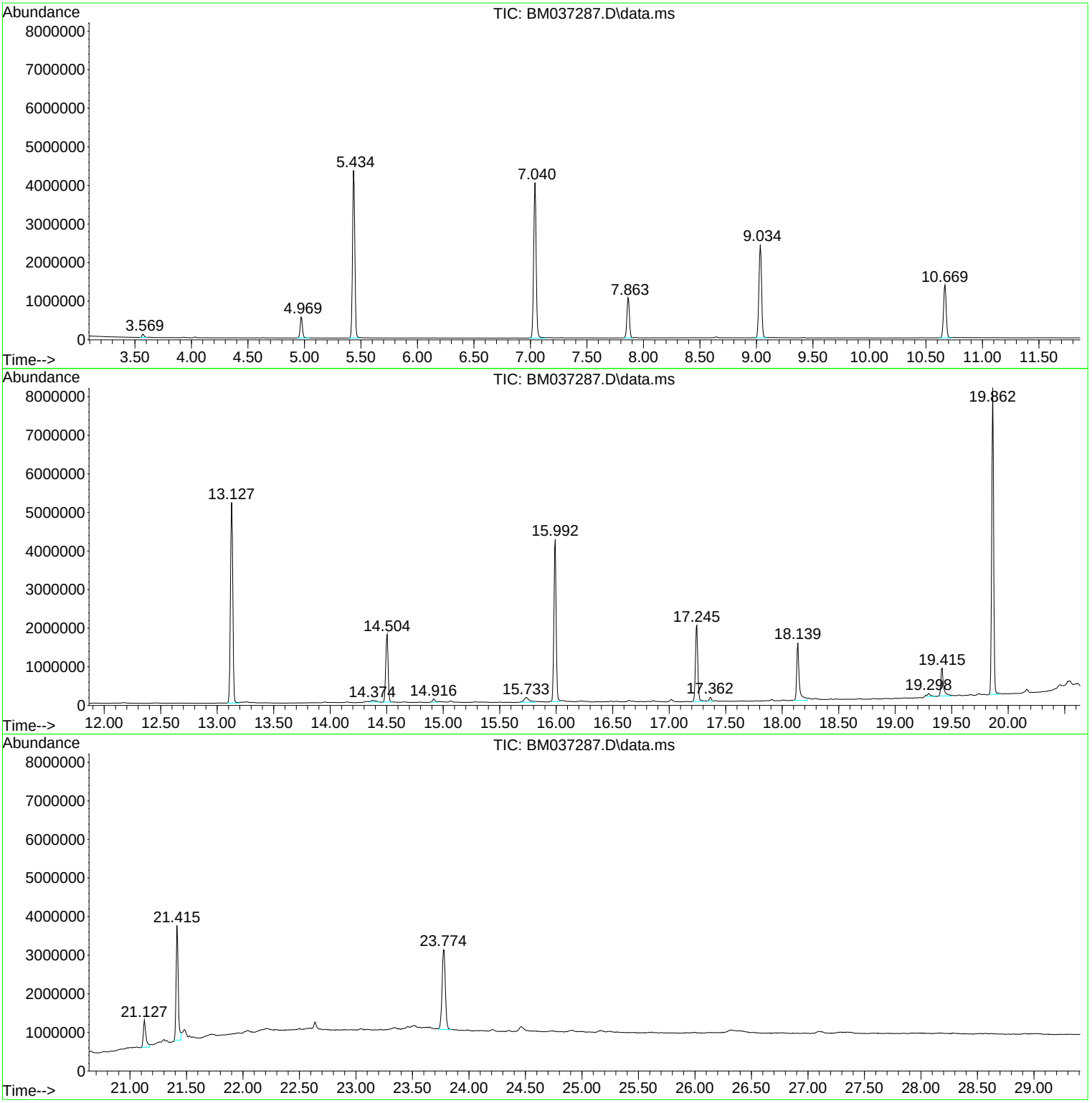
Sum of corrected areas: 62448769

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

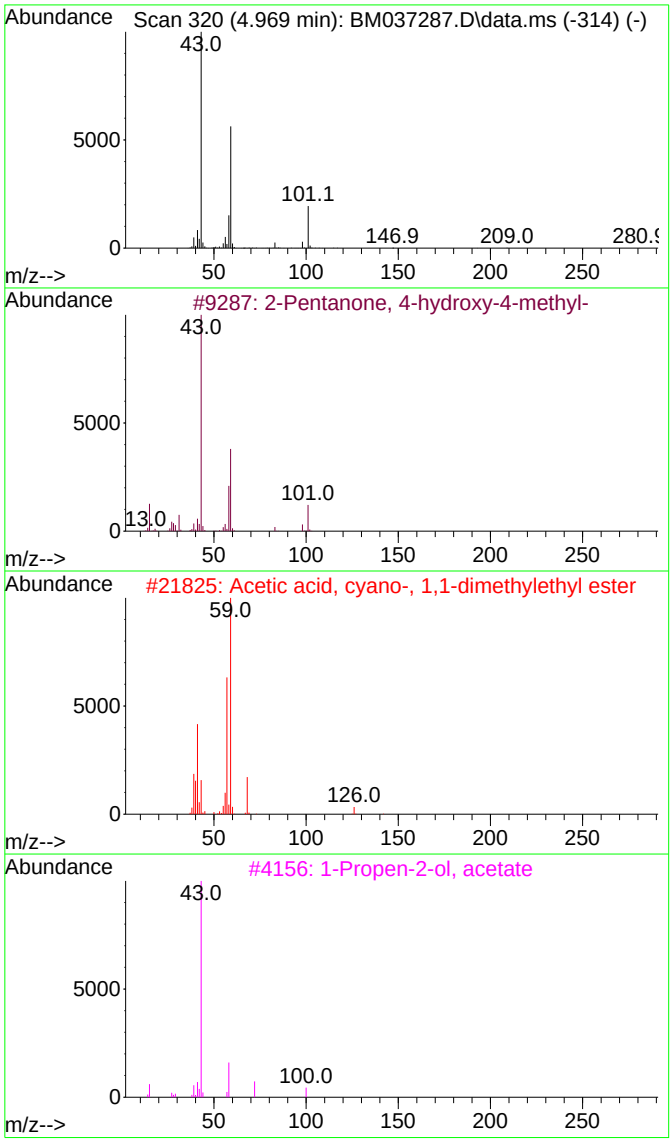
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

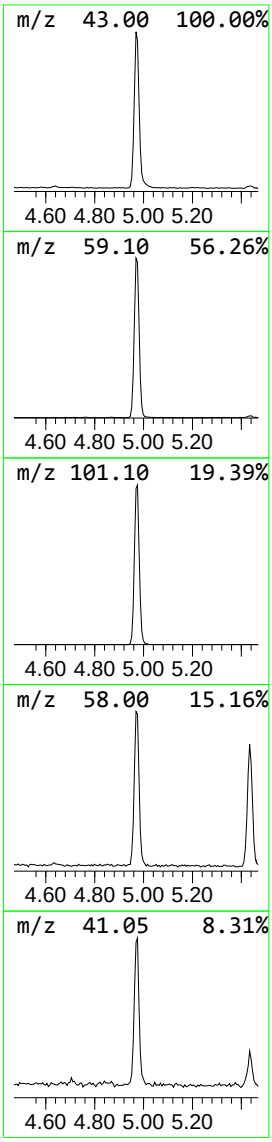
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	9.71 ng	772100	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

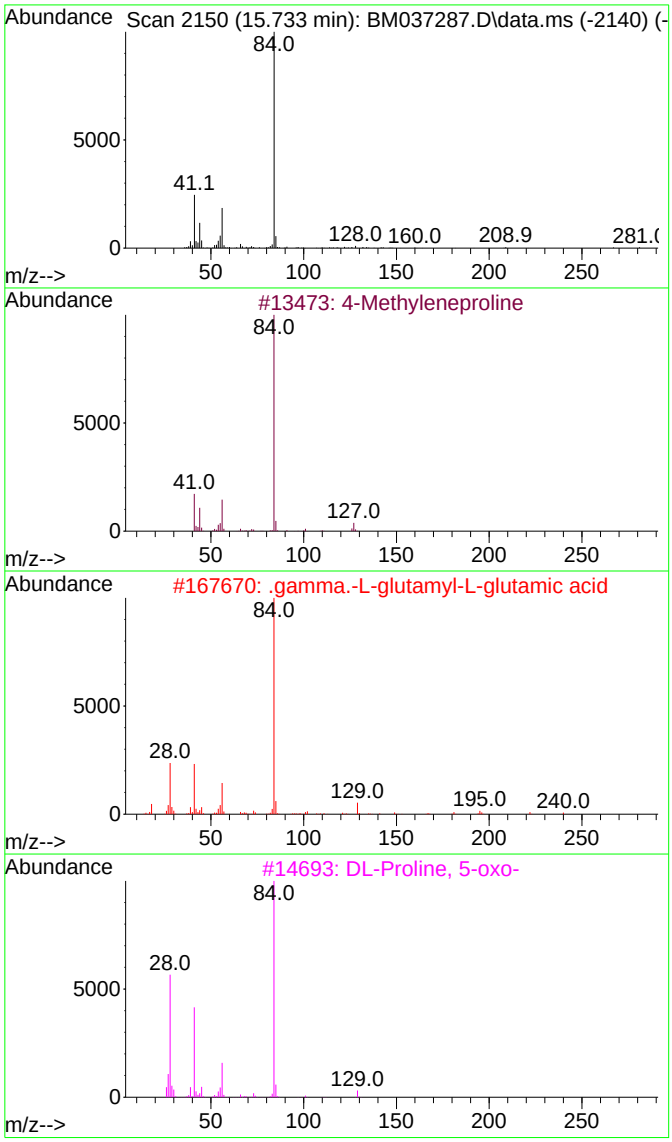
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

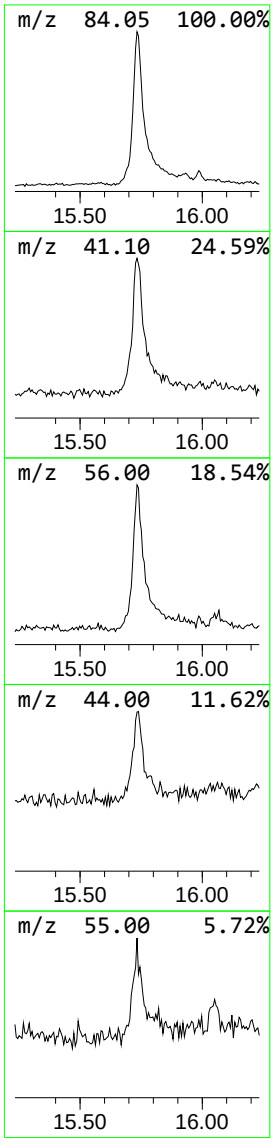
****

Peak Number 2 4-Methyleneproline Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	3.18 ng	405565	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyleneproline	127	C6H9NO2	1000131-14-7	78
2	.gamma.-L-glutamyl-L-glutamic acid	276	C10H16N2O7	001116-22-9	72
3	DL-Proline, 5-oxo-	129	C5H7NO3	000149-87-1	72
4	1,3,2-Dioxaborolan-4-one, 2-ethy...	128	C5H9BO3	074646-14-3	64
5	L-Glutamic acid	147	C5H9NO4	000056-86-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

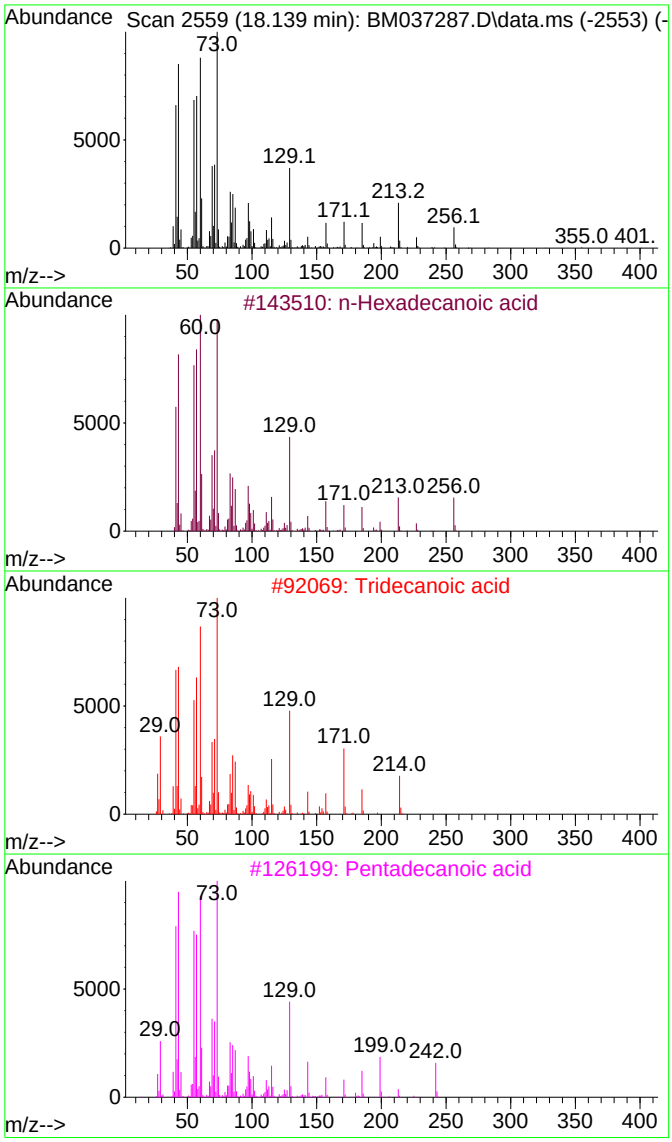
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

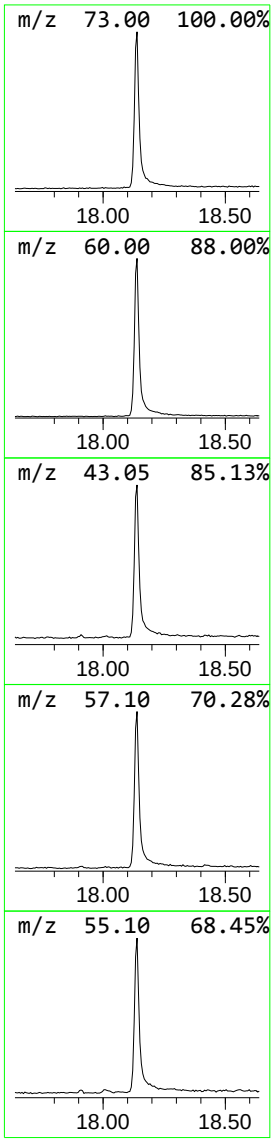
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	15.99 ng	2283520	Phenanthrene-d10	17.245

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

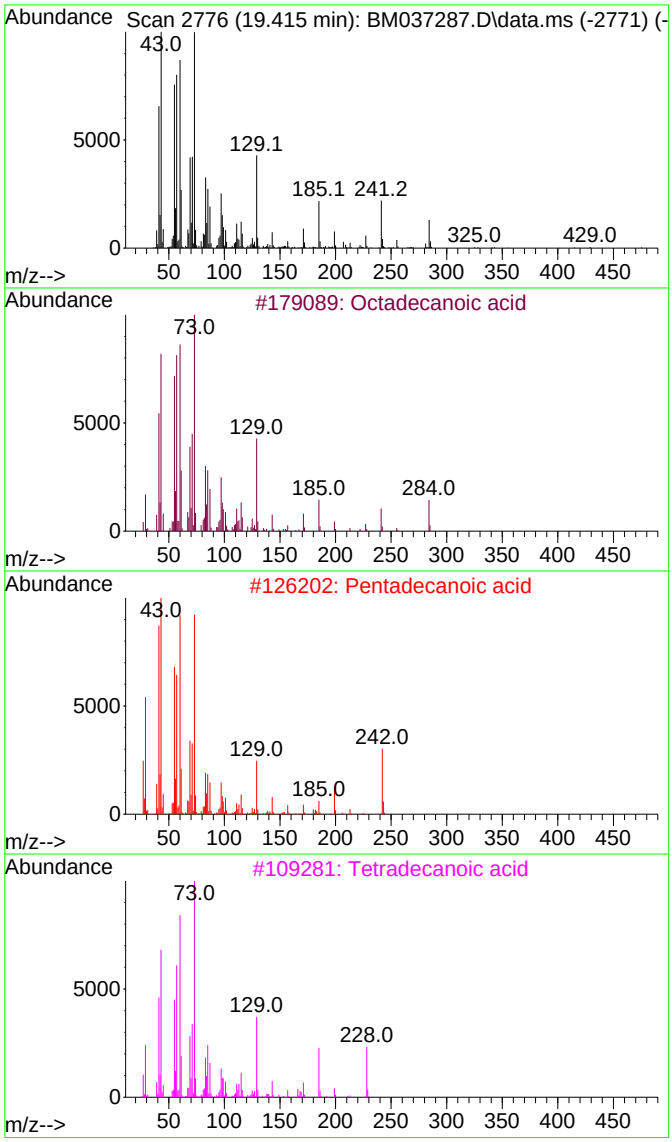
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

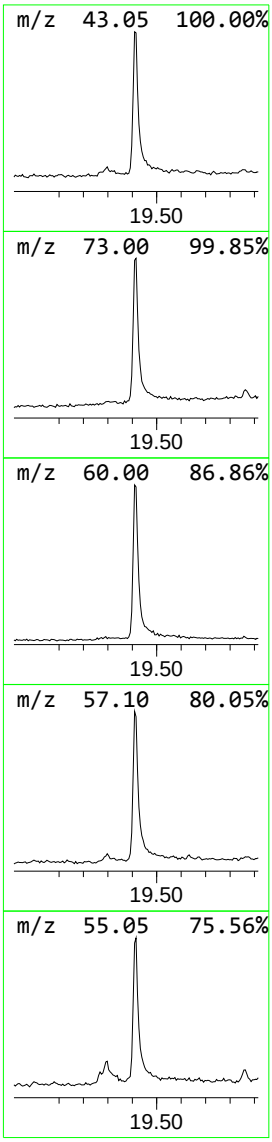
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.415	6.24 ng	1203250	Chrysene-d12	21.415

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

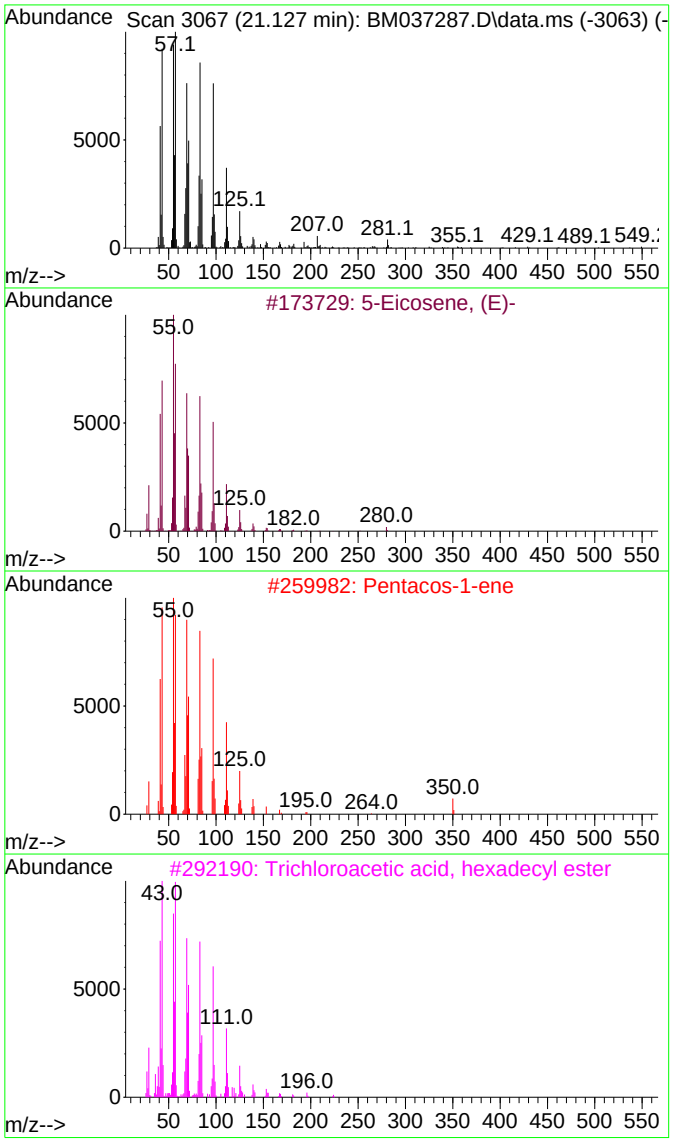
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

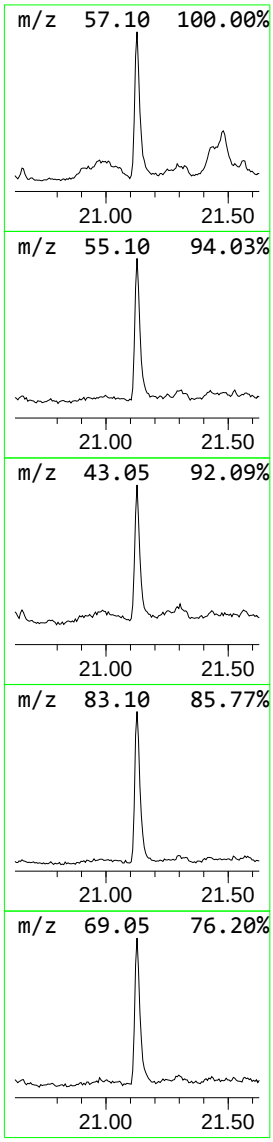
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	5.90 ng	1138020	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037287.D
Acq On : 31 Oct 2022 13:28
Operator : CG/JU
Sample : N5272-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221102-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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
2-Pentanone, 4-...	4.969	9.7	ng	772100	1	7.863	1590600	20.0
4-Methyleneproline	15.733	3.2	ng	405565	3	14.504	2552090	20.0
n-Hexadecanoic ...	18.139	16.0	ng	2283520	4	17.245	2856190	20.0
Octadecanoic acid	19.415	6.2	ng	1203250	5	21.415	3857650	20.0
5-Eicosene, (E)-	21.127	5.9	ng	1138020	5	21.415	3857650	20.0