LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-P25A

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-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.675	247	253	268	rBV	30974	120929	1.58%	0.278%
2	5.369	364	371	386	rBV	2575362	3601214	47.17%	8.275%
3	6.981	637	645	664	rBV	2387045	3760882	49.26%	8.642%
4	7.798	778	784	793	rBV	724986	1092532	14.31%	2.510%
5	8.975	976	984	1000	rBV	1475465	2404227	31.49%	5.524%
6	10.604	1253	1261	1274	rBV	903965	1477853	19.36%	3.396%
7	13.080	1675	1682	1695	rBV	3758735	5241659	68.65%	12.044%
8	13.927	1820	1826	1838	rVB	262749	378127	4.95%	0.869%
9	14.463	1910	1917	1928	rVB	1346644	1867630	24.46%	4.291%
10	15.963	2165	2172	2187	rBV	3206024	4318679	56.57%	9.923%
11	16.627	2280	2285	2297	rBV9	35468	93170	1.22%	0.214%
12	17.221	2380	2386	2391	rBV	1605682	2196731	28.77%	5.048%
13	18.004	2513	2519	2524	rBV	62147	128266	1.68%	0.295%
14	18.062	2525	2529	2535	rVV	306205	465259	6.09%	1.069%
15	18.127	2535	2540	2556	rVB	1108153	1660813	21.75%	3.816%
16	19.239	2724	2729	2734	rBV	354869	444709	5.82%	1.022%
17	19.286	2734	2737	2740	rBV	152192	202203	2.65%	0.465%
18	19.404	2753	2757	2770	rBV	322572	476429	6.24%	1.095%
19	19.651	2796	2799	2809	rVB	86713	133806	1.75%	0.307%
20	19.856	2829	2834	2842	rBV	6512703	7634841	100.00%	17.543%
21	20.498	2940	2943	2950	rBV2	73109	101097	1.32%	0.232%
22	21.133	3047	3051	3060	rBV	482349	746690	9.78%	1.716%
23	21.421	3095	3100	3105	rBV	2004937	2518864	32.99%	5.788%
24	23.792	3497	3503	3510	rVB	1304823	2453798	32.14%	5.638%

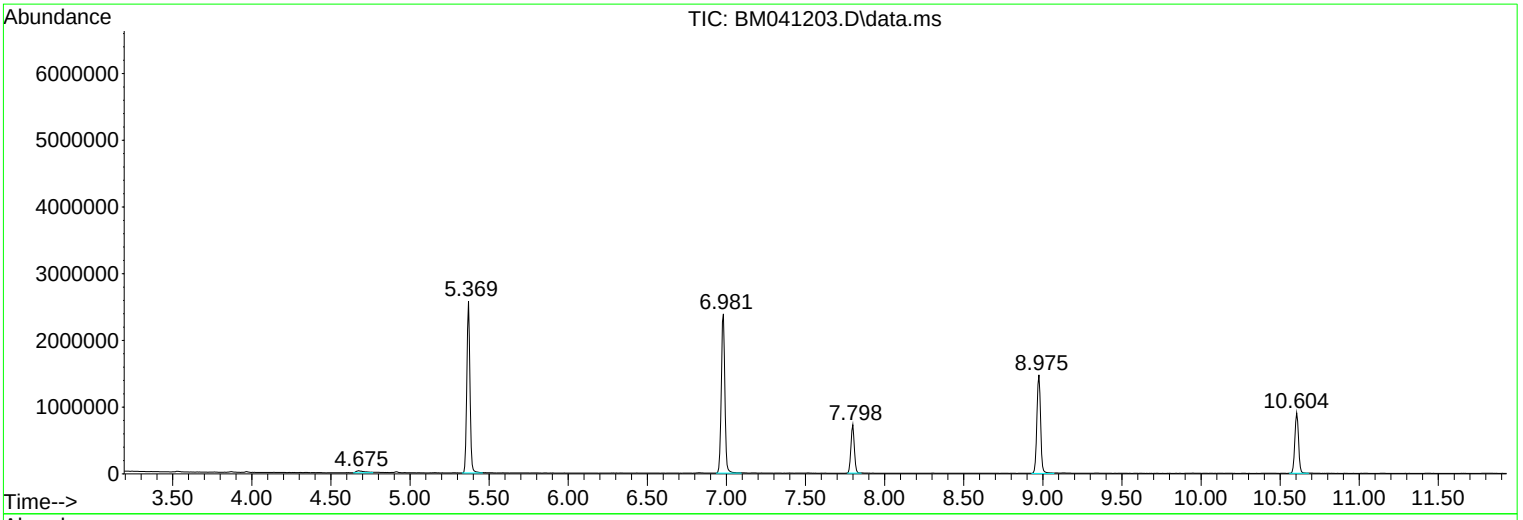
Sum of corrected areas: 43520408

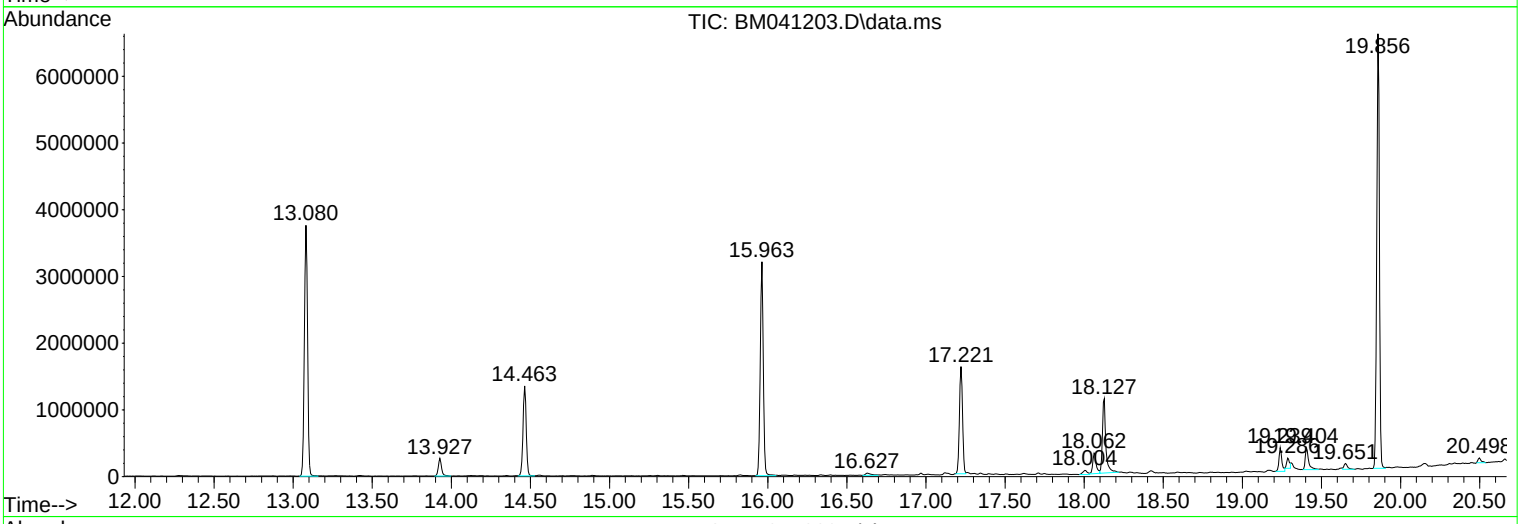
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

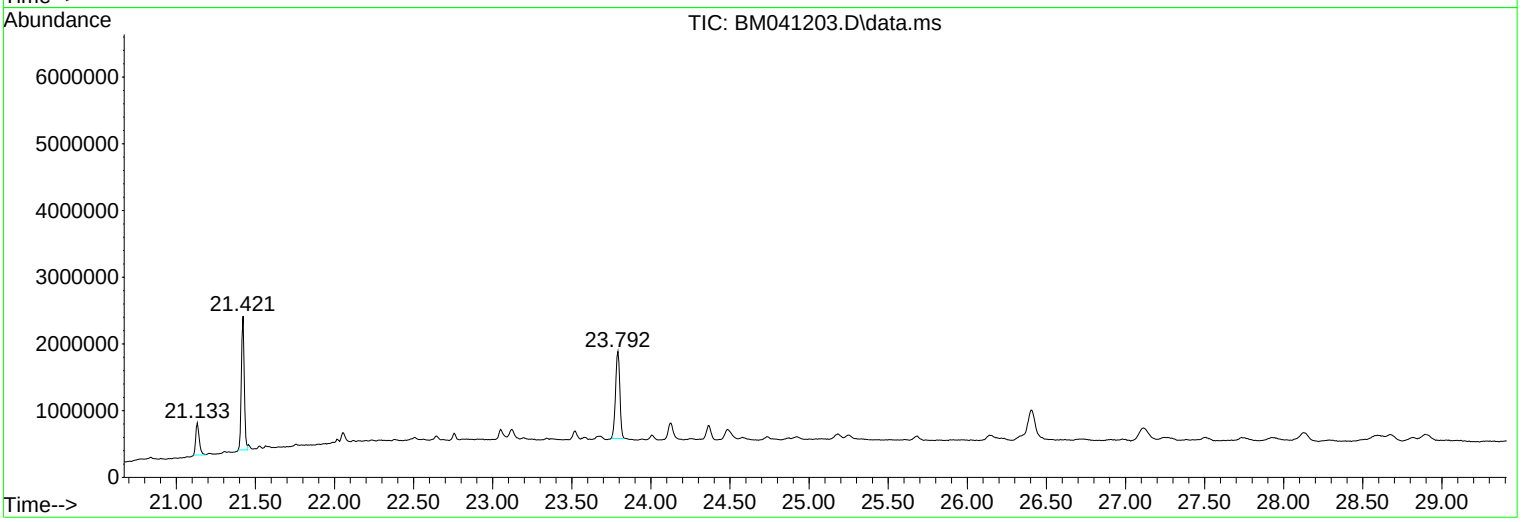
Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

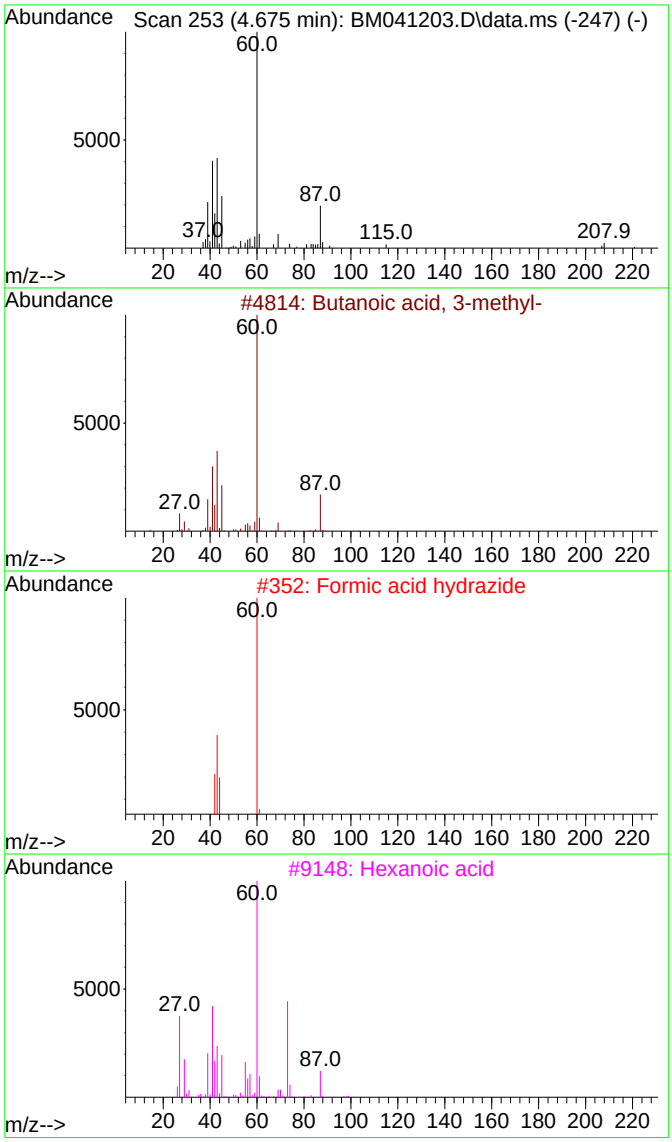
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

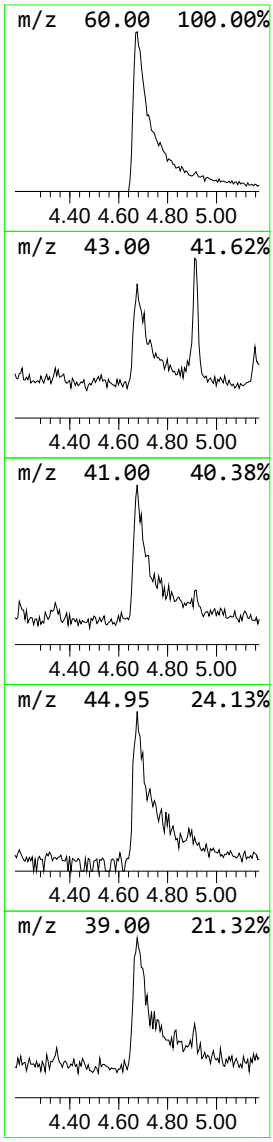
****

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.675	2.21 ng	120929	1,4-Dichlorobenzene-d4	7.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	86
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	45
4	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	40
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

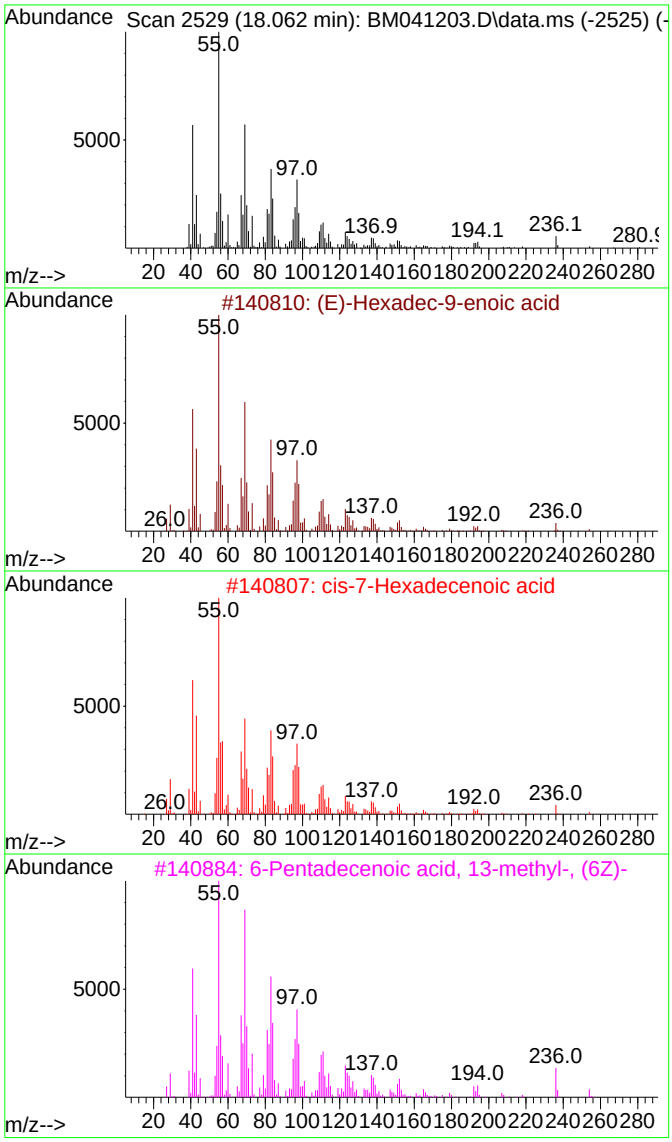
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

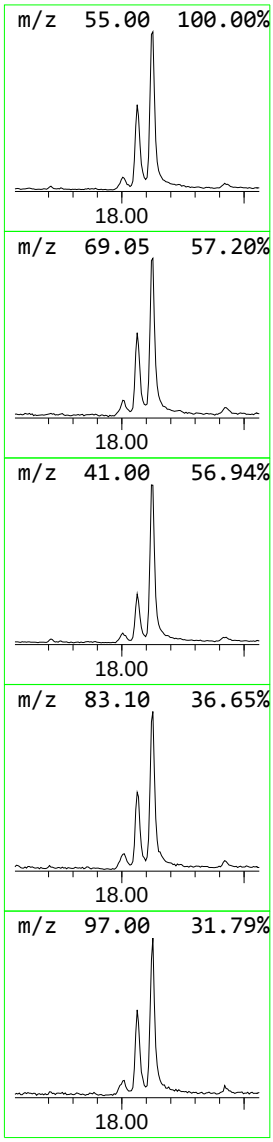
****

Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	4.24 ng	465259	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
3	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	95
4	Palmitoleic acid	254	C16H30O2	000373-49-9	94
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

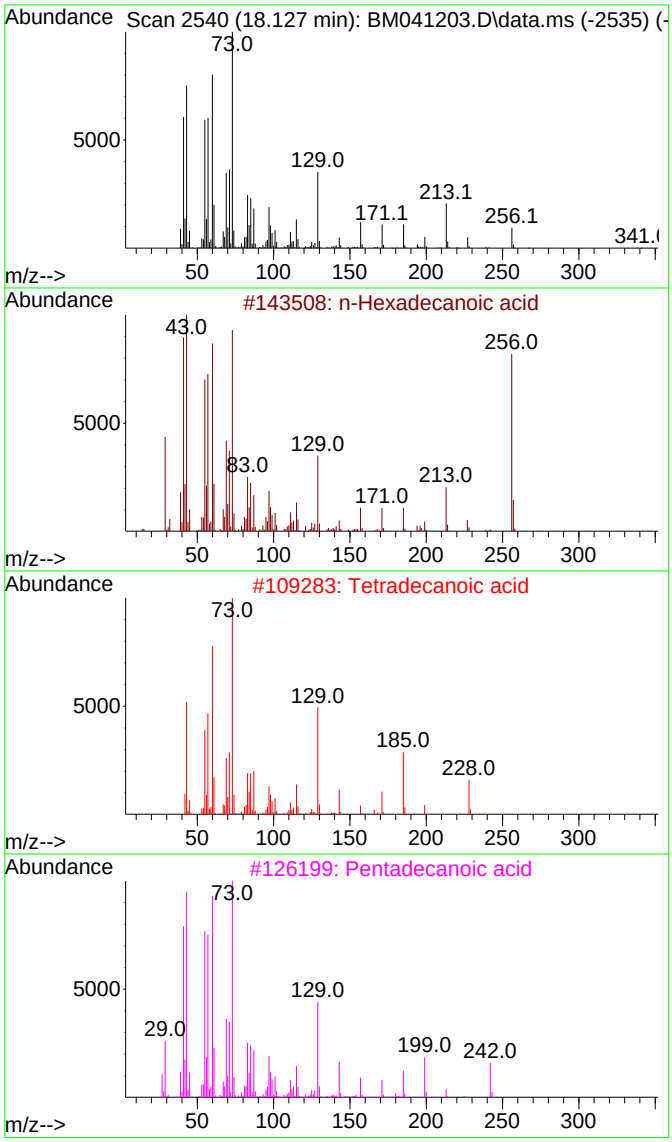
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

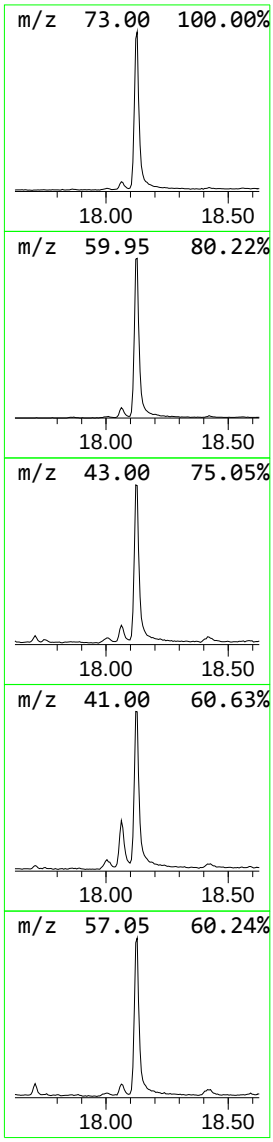
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	15.12 ng	1660810	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

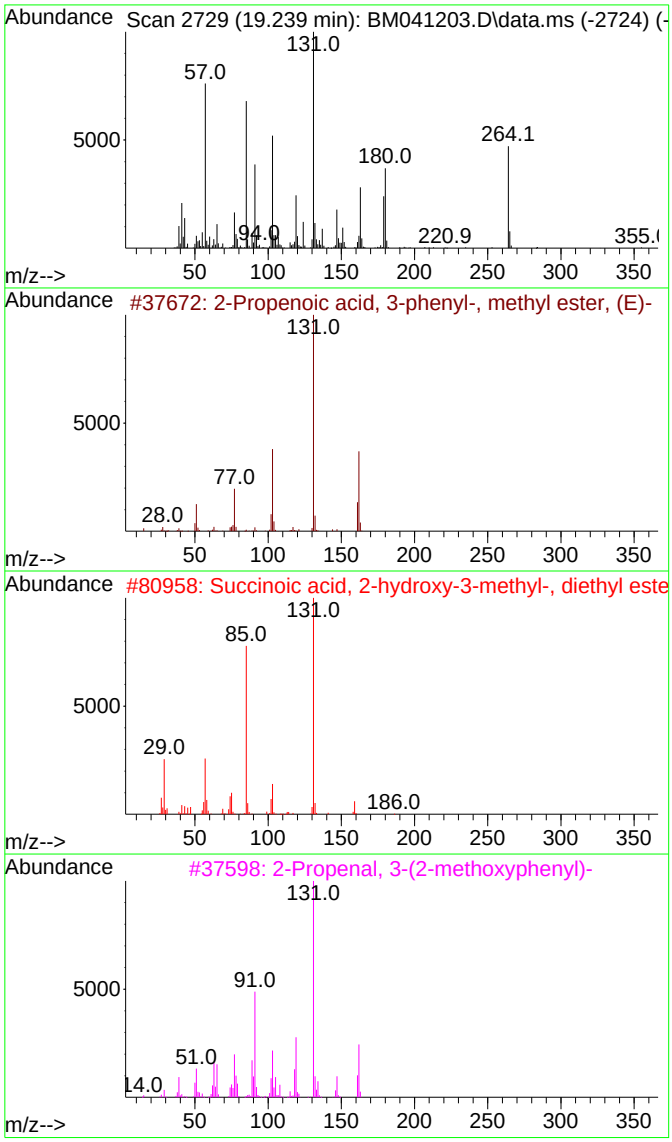
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

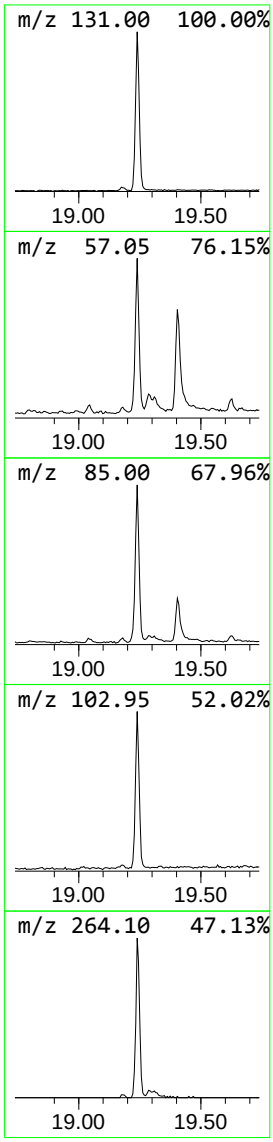
****

Peak Number 4 unknown19.239 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.239	4.05 ng	444709	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	42
2	Succinoic acid, 2-hydroxy-3-meth...	204	C9H16O5	1000196-85-6	35
3	2-Propenal, 3-(2-methoxyphenyl)-	162	C10H10O2	001504-74-1	27
4	(Z)-2-Methoxycinnamaldehyde	162	C10H10O2	076760-43-5	27
5	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

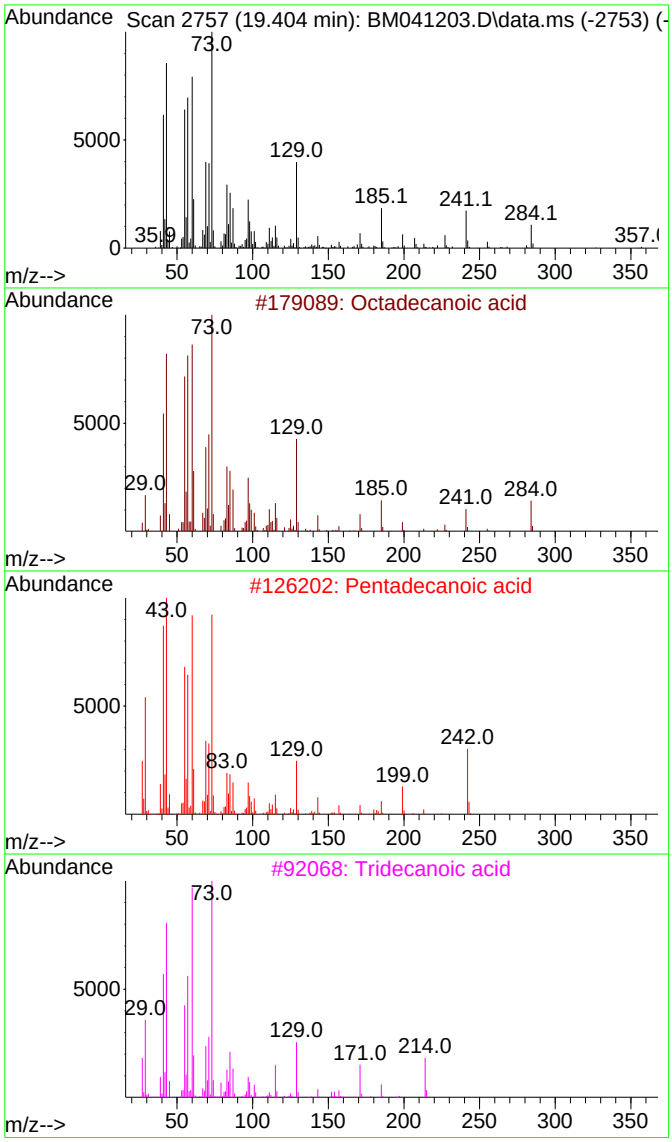
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

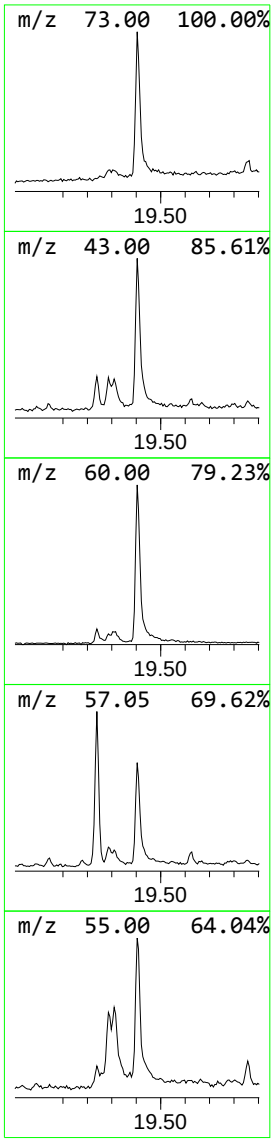
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	3.78 ng	476429	Chrysene-d12	21.421

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

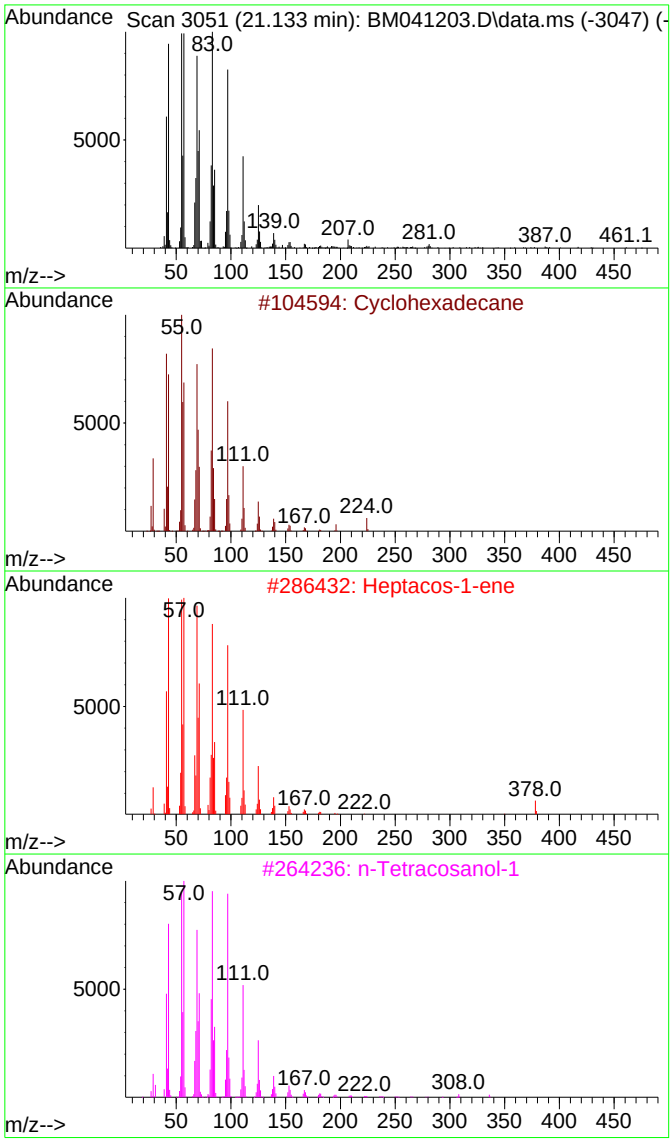
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

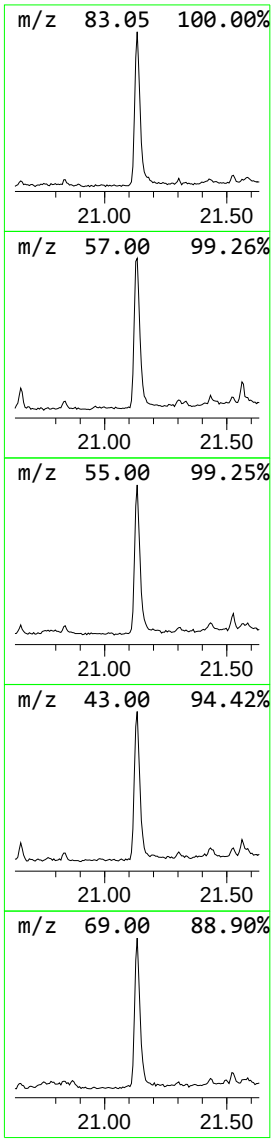
****

Peak Number 6 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	5.93 ng	746690	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041203.D
Acq On : 01 Aug 2023 00:51
Operator : MA/JU
Sample : 03741-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P25A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
Butanoic acid, ...	4.675	2.2	ng	120929	1	7.798	1092530	20.0
(E)-Hexadec-9-e...	18.063	4.2	ng	465259	4	17.221	2196730	20.0
n-Hexadecanoic ...	18.127	15.1	ng	1660810	4	17.221	2196730	20.0
unknown19.239	19.239	4.0	ng	444709	4	17.221	2196730	20.0
Octadecanoic acid	19.404	3.8	ng	476429	5	21.421	2518860	20.0
Cyclohexadecane	21.133	5.9	ng	746690	5	21.421	2518860	20.0