LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

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: BM041335.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	283	291	297	rBV	58105	90095	1.43%	0.258%
2	5.357	362	369	383	rBV	2135009	3142443	49.99%	9.013%
3	6.963	635	642	661	rBV	2081754	3277575	52.13%	9.400%
4	7.404	710	717	726	rBV3	27933	64857	1.03%	0.186%
5	7.781	774	781	790	rBV	468391	722607	11.49%	2.072%
6	8.957	973	981	994	rBV	1257946	2080108	33.09%	5.966%
7	10.586	1250	1258	1273	rBV	572290	984048	15.65%	2.822%
8	13.063	1673	1679	1696	rBV	3173156	4505850	71.67%	12.923%
9	13.339	1718	1726	1739	rBV	590003	944910	15.03%	2.710%
10	14.445	1908	1914	1930	rBV	820371	1249050	19.87%	3.582%
11	15.951	2163	2170	2186	rBV	2636117	3770100	59.97%	10.813%
12	17.209	2375	2384	2389	rBV	1041806	1445051	22.99%	4.144%
13	18.115	2530	2538	2557	rBV	808842	1446433	23.01%	4.148%
14	19.056	2695	2698	2705	rVB4	65288	79005	1.26%	0.227%
15	19.280	2732	2736	2743	rVB2	59162	97456	1.55%	0.280%
16	19.392	2751	2755	2772	rBV	325856	588619	9.36%	1.688%
17	19.645	2795	2798	2807	rVB2	49429	80634	1.28%	0.231%
18	19.850	2827	2833	2843	rBV	5233353	6286754	100.00%	18.031%
19	20.544	2945	2951	2957	rBV	300738	395812	6.30%	1.135%
20	21.121	3045	3049	3056	rBV	320154	448139	7.13%	1.285%
21	21.415	3094	3099	3104	rBV	1259343	1603478	25.51%	4.599%
22	23.780	3495	3501	3513	rVB	795047	1564023	24.88%	4.486%

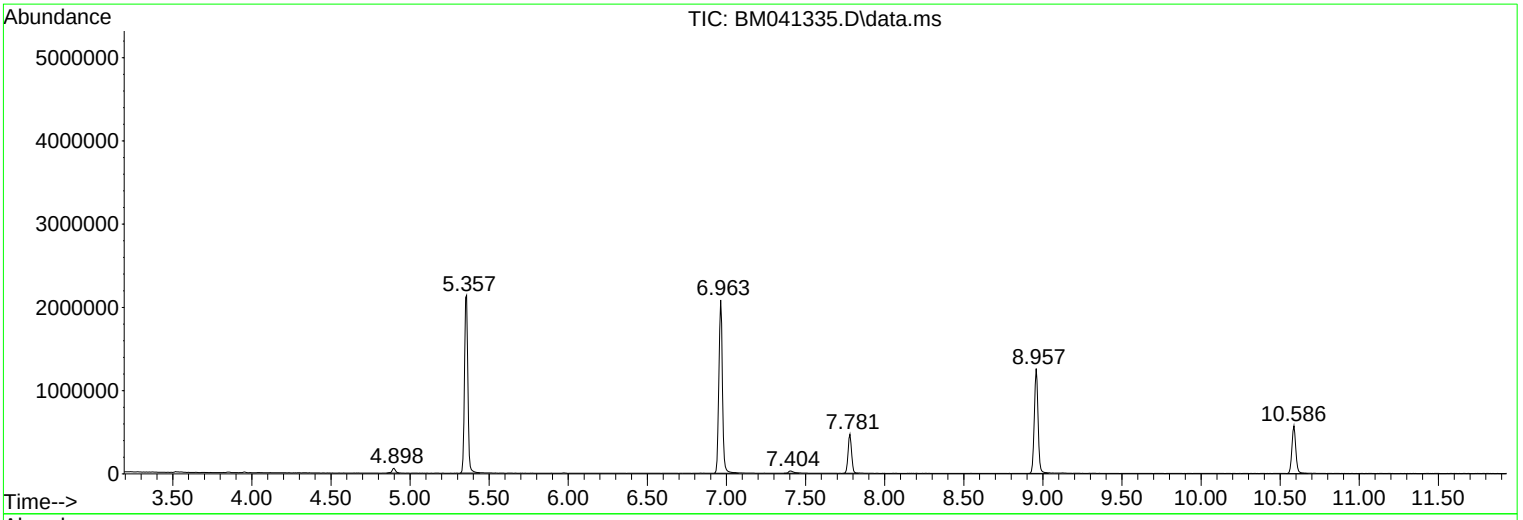
Sum of corrected areas: 34867047

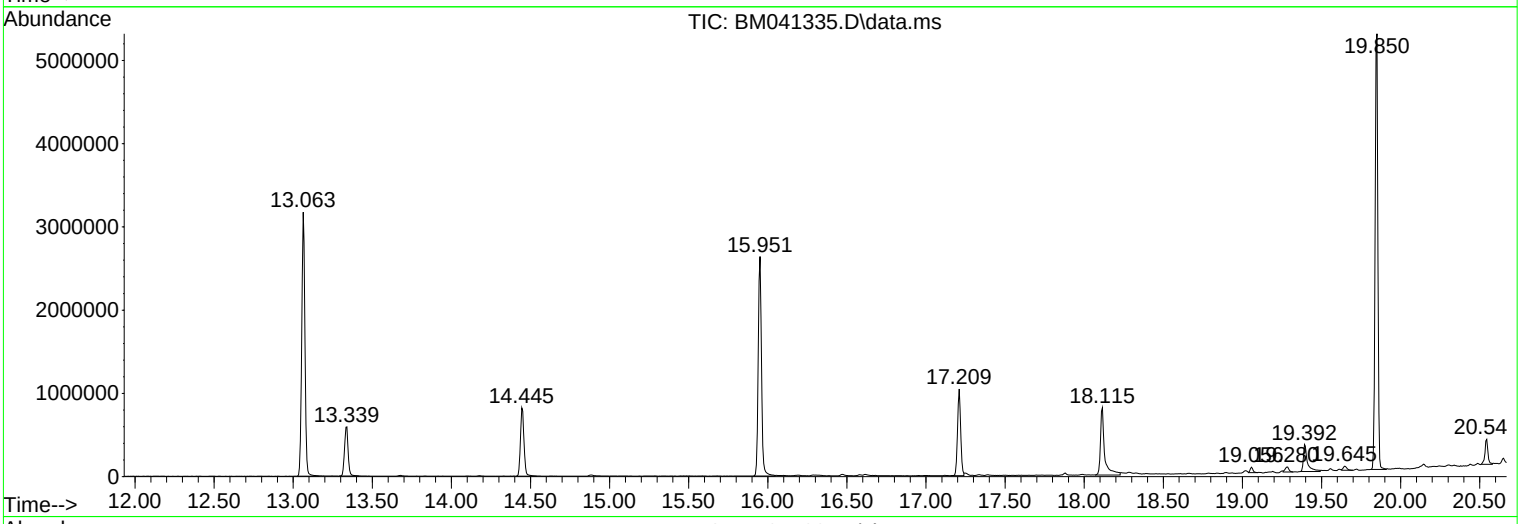
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

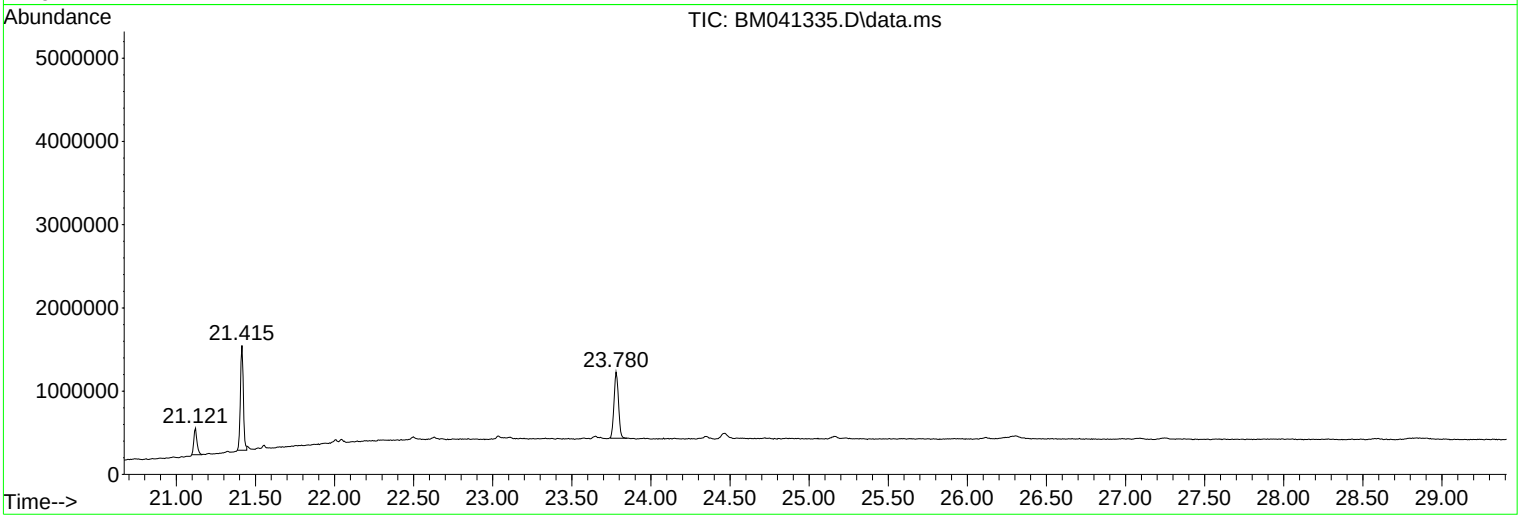
Instrument :
BNA_M
ClientSampleId :
TP-36

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\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

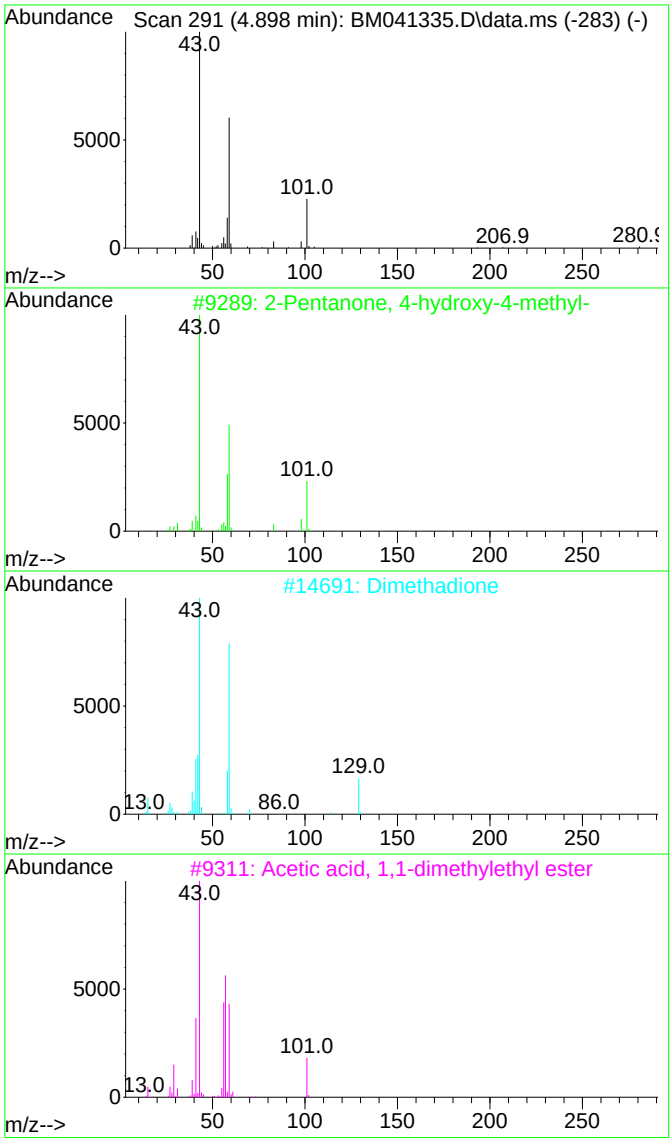
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

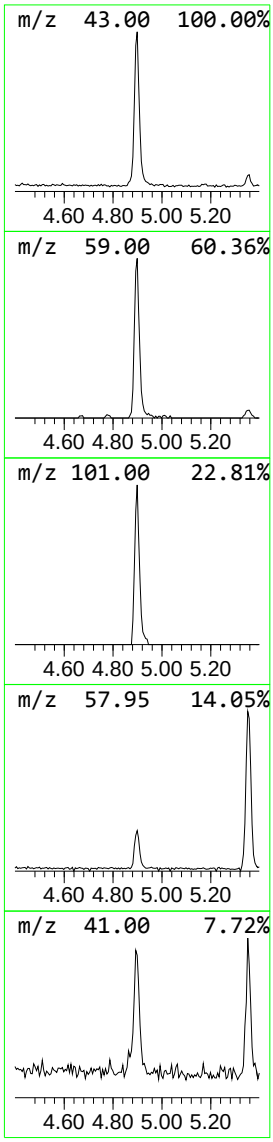
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.898	2.49 ng	90095	1,4-Dichlorobenzene-d4	7.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

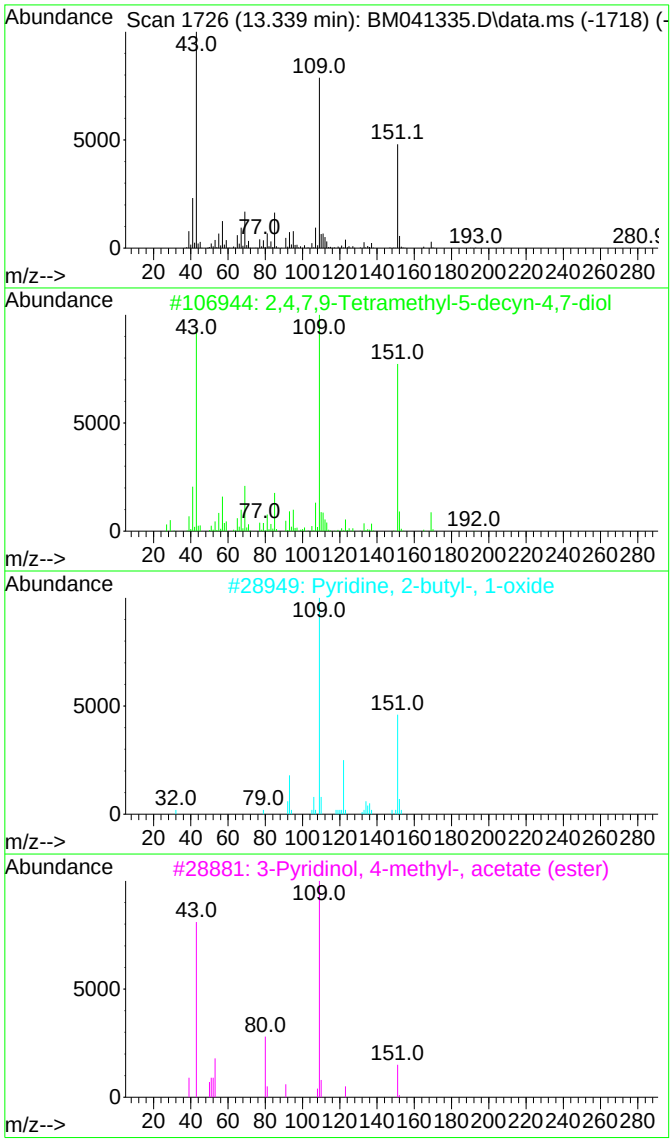
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

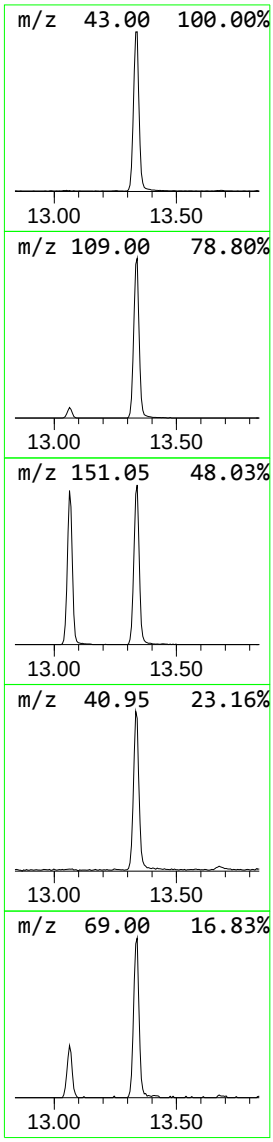
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.339	15.13 ng	944910	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	Diacetamate	193	C10H11NO3	002623-33-8	59
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

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

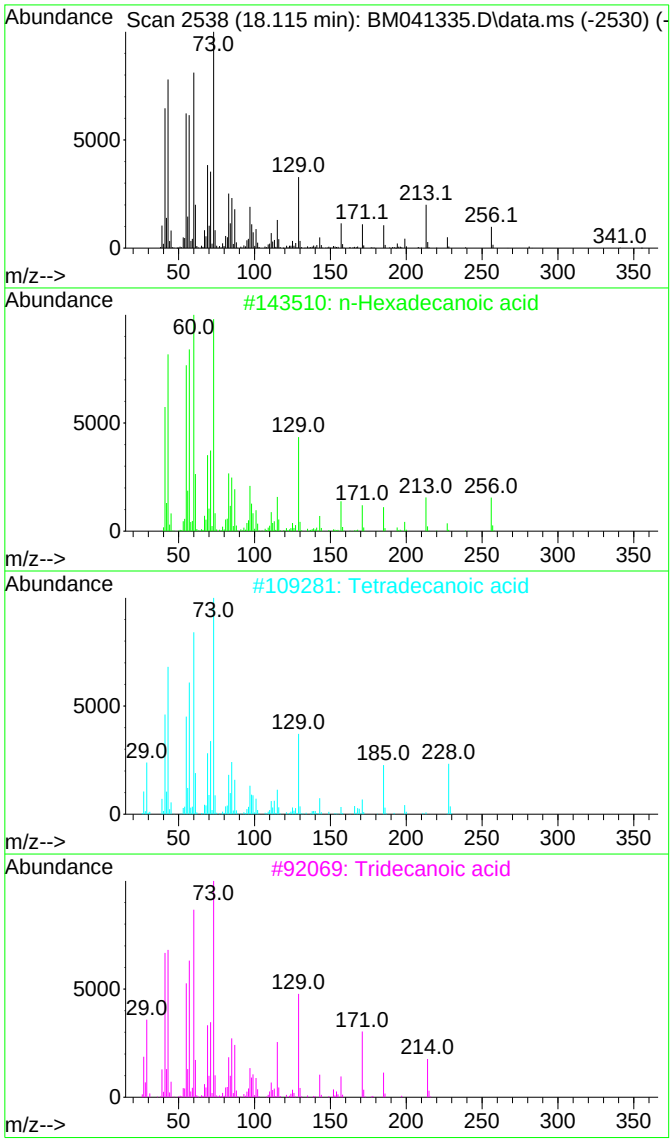
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

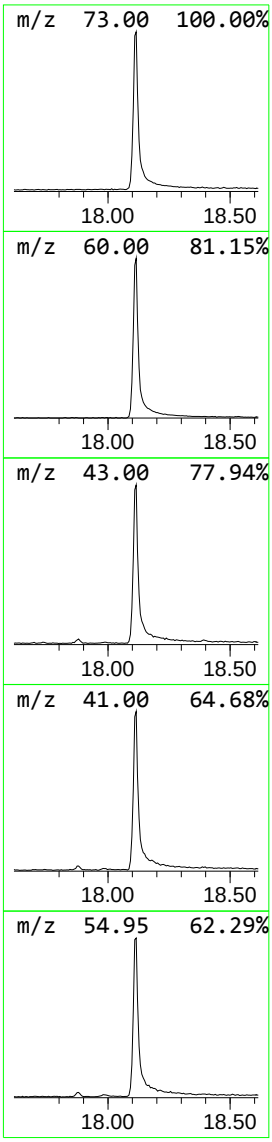
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	20.02 ng	1446430	Phenanthrene-d10	17.209

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	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

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

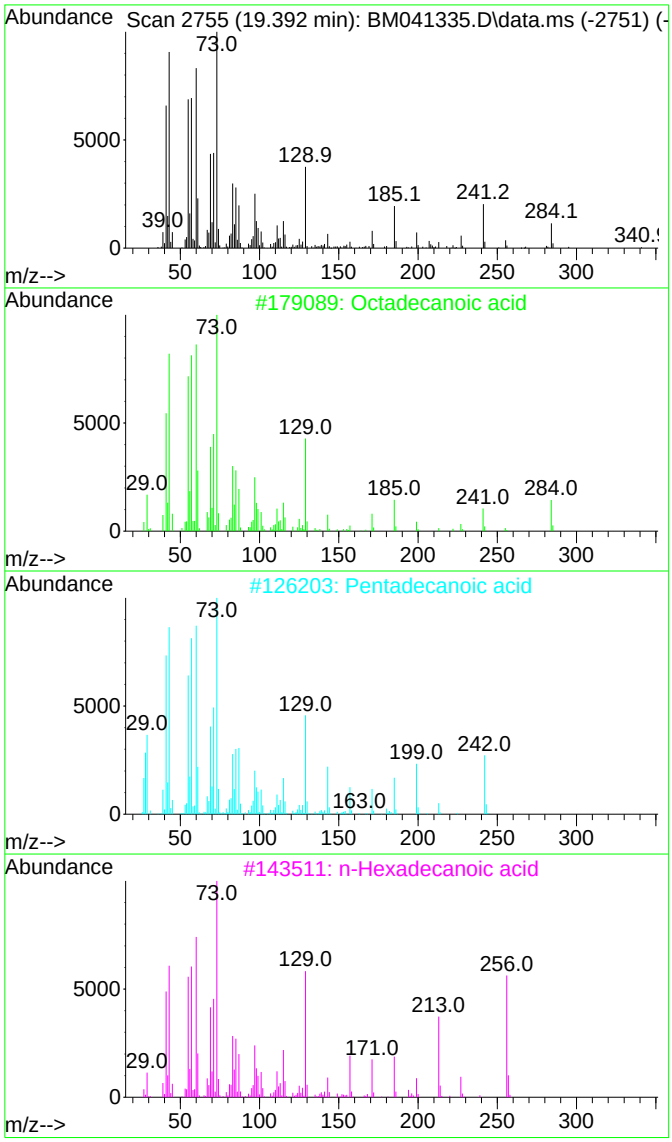
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

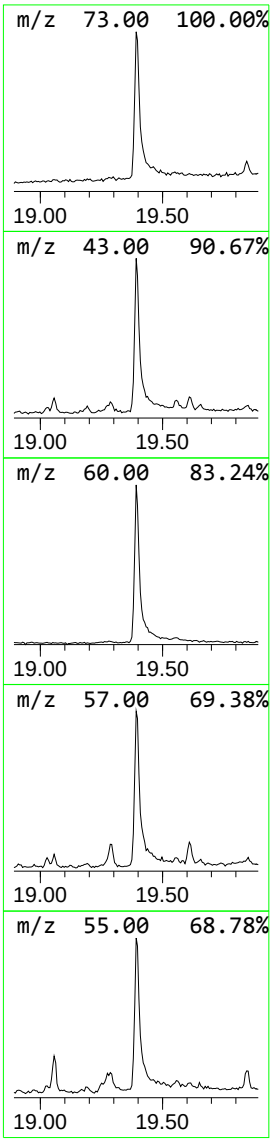
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	7.34 ng	588619	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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

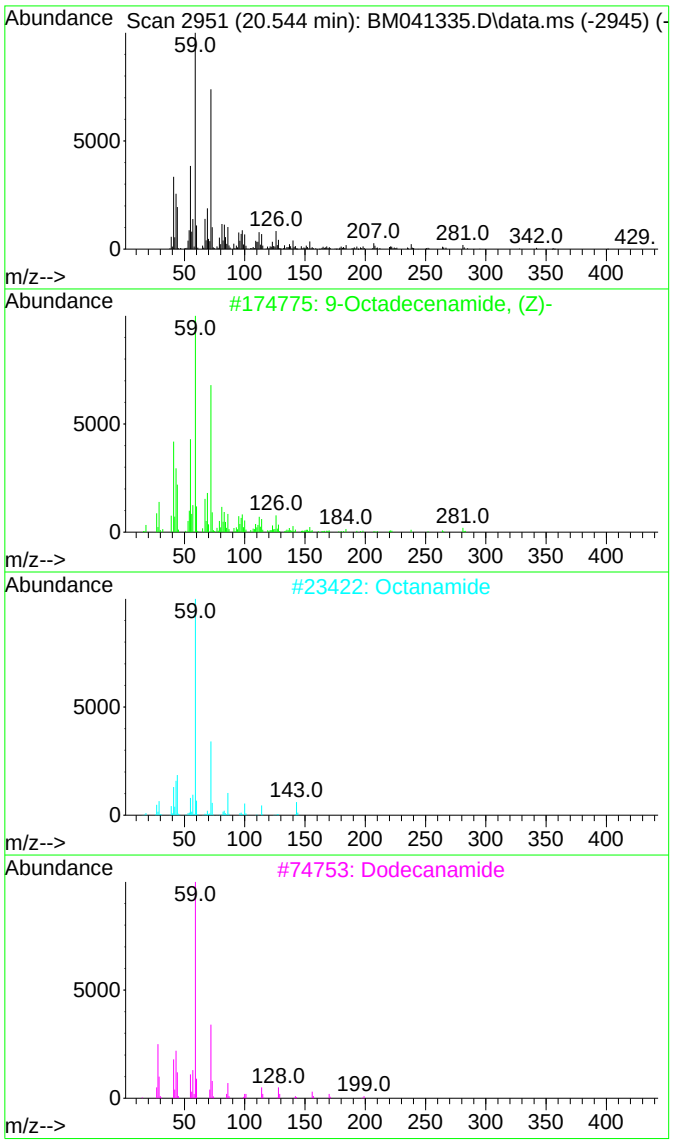
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

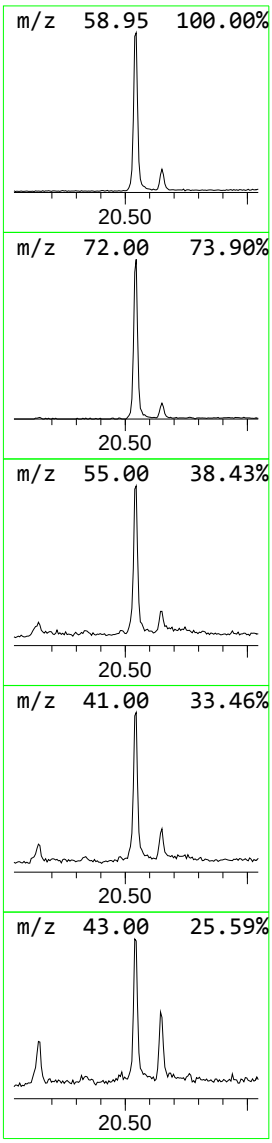
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.544	4.94 ng	395812	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Octanamide	143	C8H17NO	000629-01-6	53
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	Butan-2-yl(ethyl)amine	101	C6H15N	021035-44-9	43
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

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

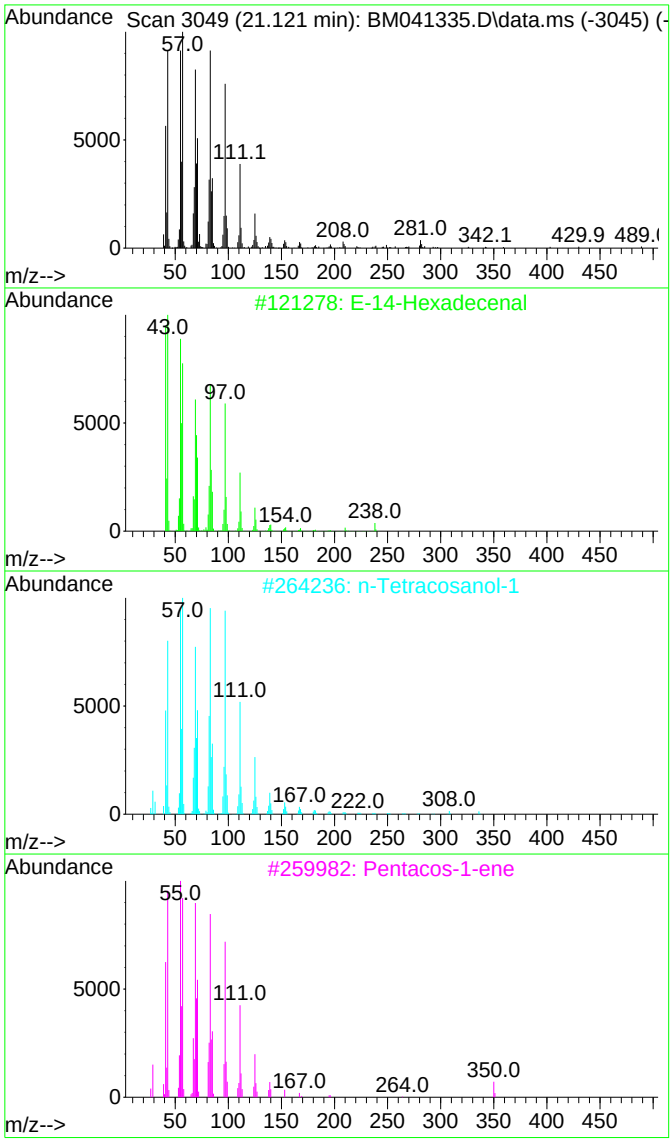
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

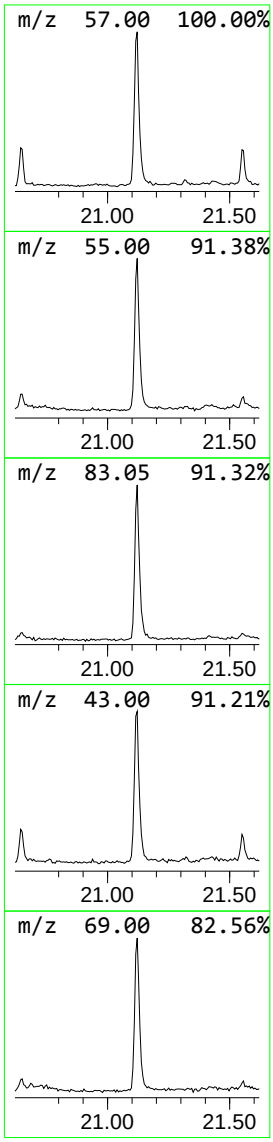
****

Peak Number 6 E-14-Hexadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	5.59 ng	448139	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080823\
Data File : BM041335.D
Acq On : 08 Aug 2023 19:13
Operator : MA/JU
Sample : 03919-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-36

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
2-Pentanone, 4-...	4.898	2.5	ng	90095	1	7.781	722607	20.0
2,4,7,9-Tetrame...	13.339	15.1	ng	944910	3	14.445	1249050	20.0
n-Hexadecanoic ...	18.115	20.0	ng	1446430	4	17.209	1445050	20.0
Octadecanoic acid	19.392	7.3	ng	588619	5	21.415	1603480	20.0
9-Octadecenamid...	20.544	4.9	ng	395812	5	21.415	1603480	20.0
E-14-Hexadecenal	21.121	5.6	ng	448139	5	21.415	1603480	20.0