LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

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-BM010522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.043	301	307	317	rVB2	54311	81309	1.01%	0.190%
2	5.519	381	388	396	rBV	2225598	3239685	40.35%	7.573%
3	7.125	653	661	671	rBV	2163240	3502544	43.63%	8.187%
4	7.972	799	805	812	rVB	578260	922478	11.49%	2.156%
5	9.137	995	1003	1012	rBV	1428495	2318906	28.88%	5.421%
6	10.566	1239	1246	1254	rBV	133890	210726	2.62%	0.493%
7	10.790	1275	1284	1291	rBV	807467	1334663	16.62%	3.120%
8	13.242	1694	1701	1711	rBV	3470003	5076908	63.24%	11.868%
9	14.613	1924	1934	1943	rBV	1283409	1902218	23.69%	4.447%
10	16.089	2179	2185	2198	rBV	3052793	4516182	56.25%	10.557%
11	17.348	2392	2399	2404	rBV	1635059	2367469	29.49%	5.534%
12	18.242	2544	2551	2561	rBV2	176662	282484	3.52%	0.660%
13	19.395	2740	2747	2754	rBV	137814	205421	2.56%	0.480%
14	19.512	2763	2767	2772	rBV	70508	96515	1.20%	0.226%
15	19.754	2804	2808	2812	rBV	96759	135853	1.69%	0.318%
16	19.960	2837	2843	2849	rBV	6451683	8028565	100.00%	18.767%
17	21.059	3026	3030	3037	rBV	378455	423061	5.27%	0.989%
18	21.224	3054	3058	3066	rBV	434490	555073	6.91%	1.298%
19	21.430	3089	3093	3099	rBV	158012	183381	2.28%	0.429%
20	21.512	3101	3107	3111	rBV	2165063	2906785	36.21%	6.795%
21	21.677	3132	3135	3139	rBV2	77362	88674	1.10%	0.207%
22	22.142	3211	3214	3219	rBV3	98490	137827	1.72%	0.322%
23	22.648	3297	3300	3306	rVB2	144183	200464	2.50%	0.469%
24	23.212	3392	3396	3406	rVB2	223709	429486	5.35%	1.004%
25	23.853	3502	3505	3511	rVB	219249	354734	4.42%	0.829%
26	23.936	3512	3519	3527	rVB2	1332885	2697772	33.60%	6.306%
27	24.595	3626	3631	3639	rVB	275976	580448	7.23%	1.357%

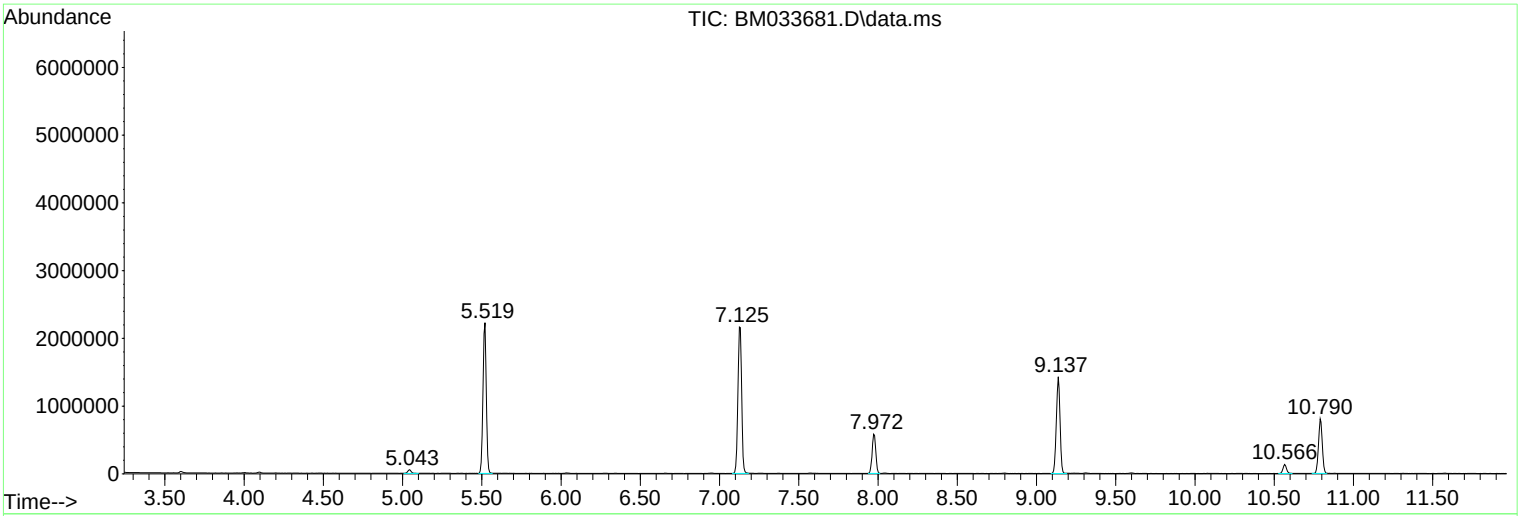
Sum of corrected areas: 42779631

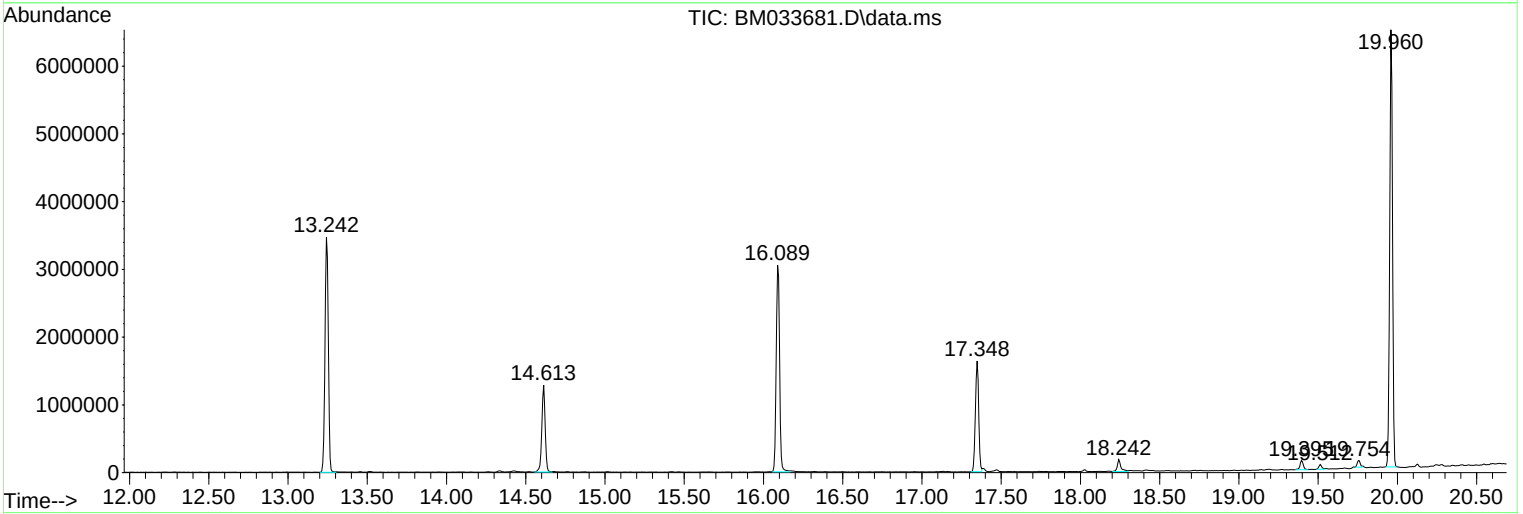
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

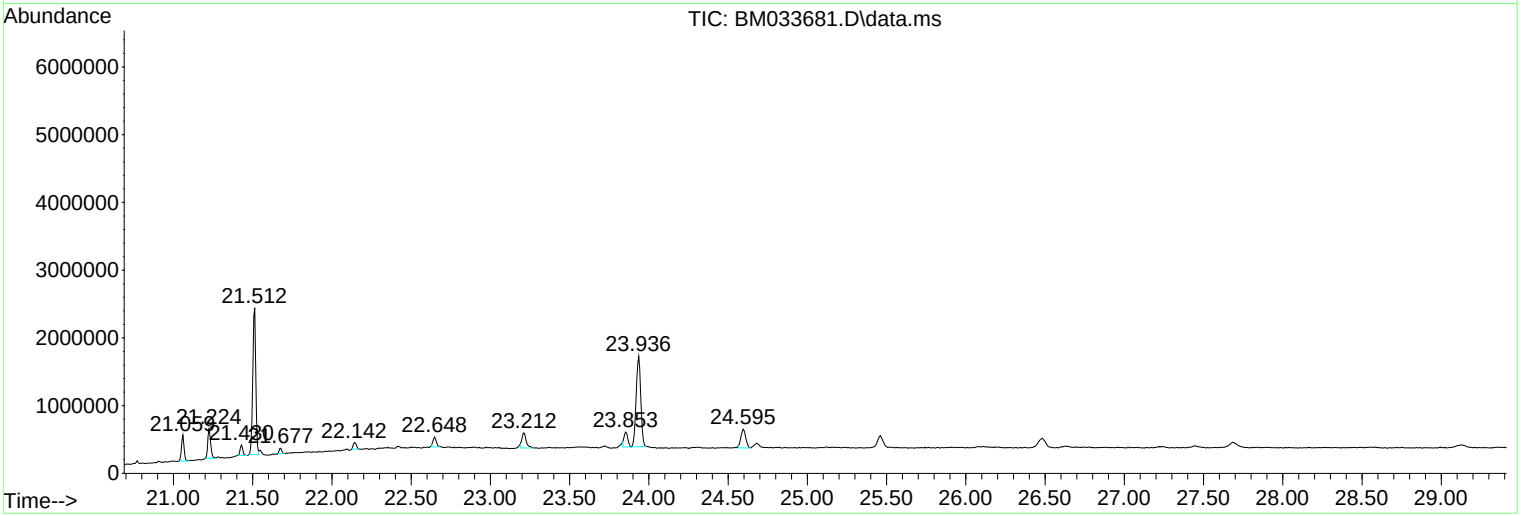
Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

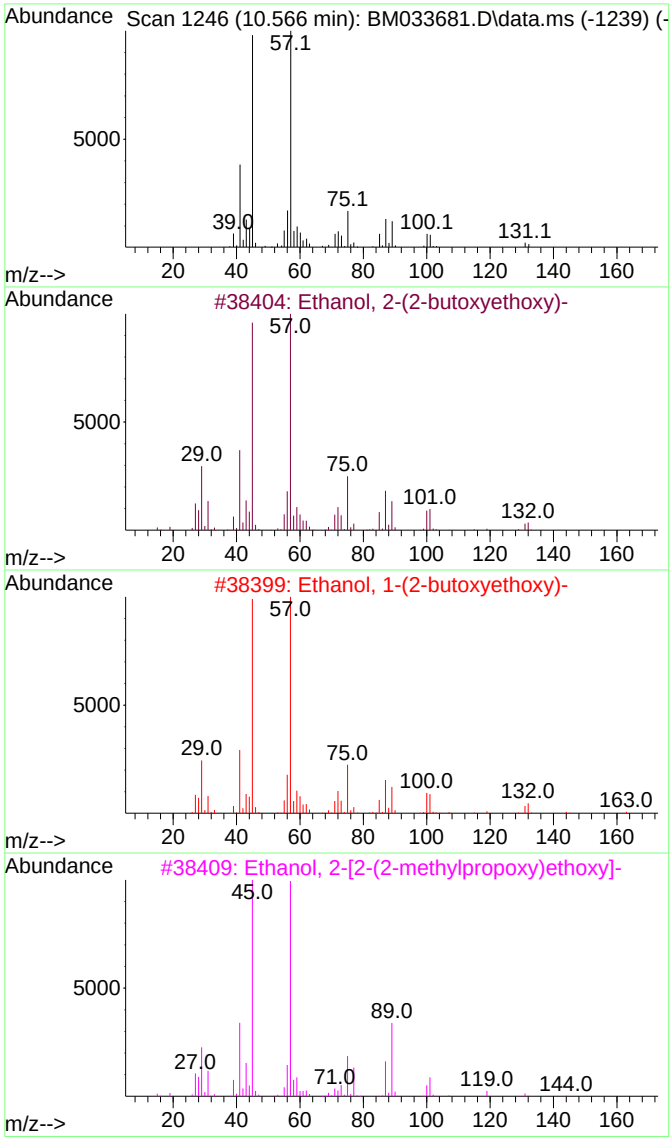
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

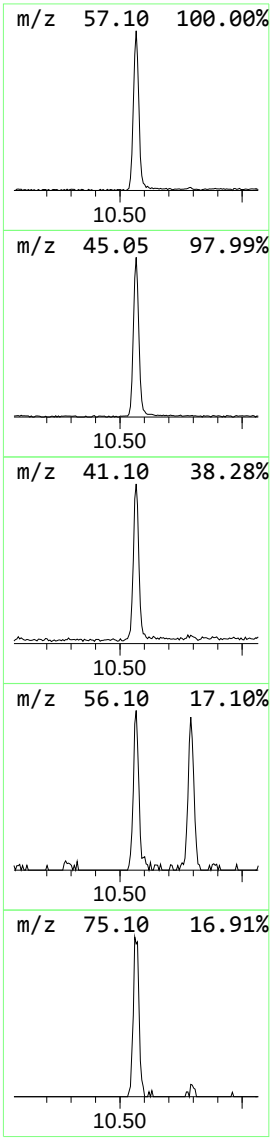
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.566	3.16 ng	210726	Naphthalene-d8	10.790

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

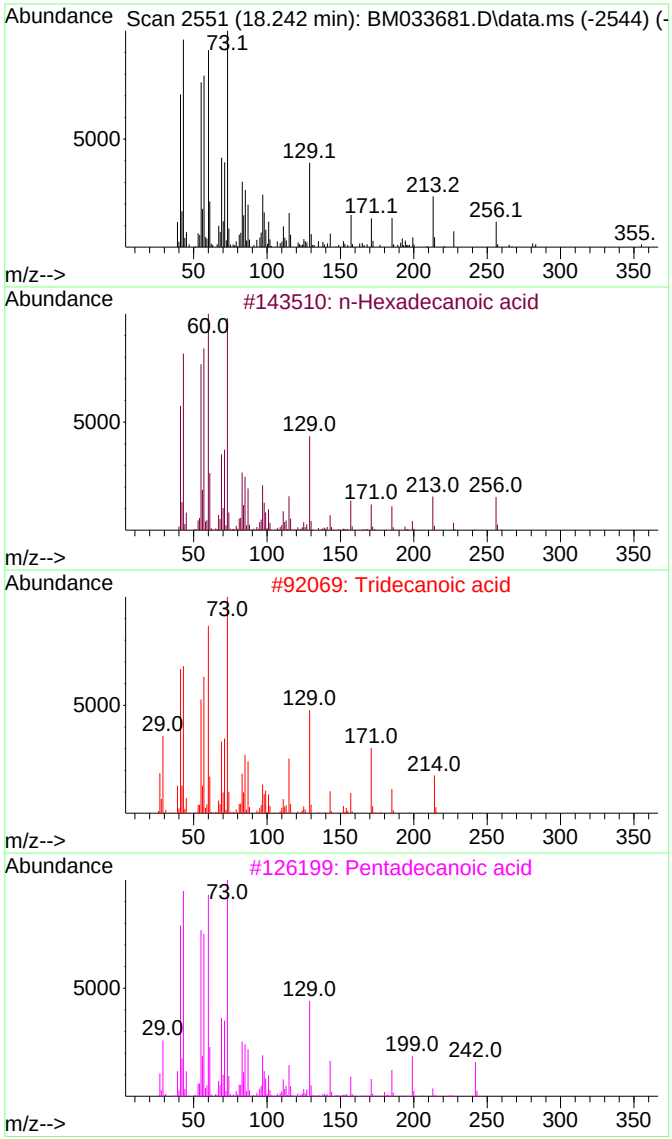
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

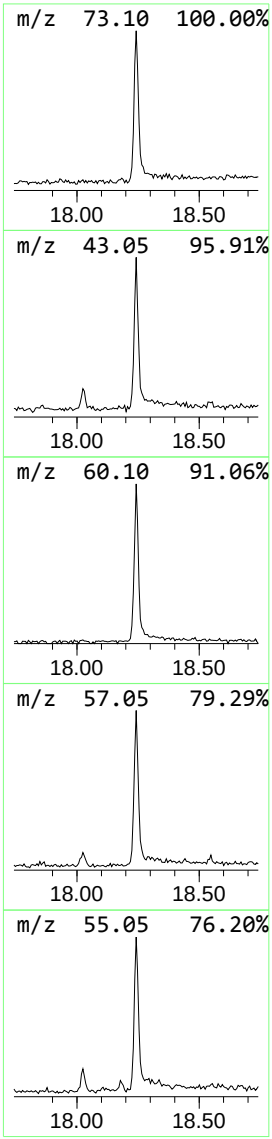
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.242	2.39 ng	282484	Phenanthrene-d10	17.348

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

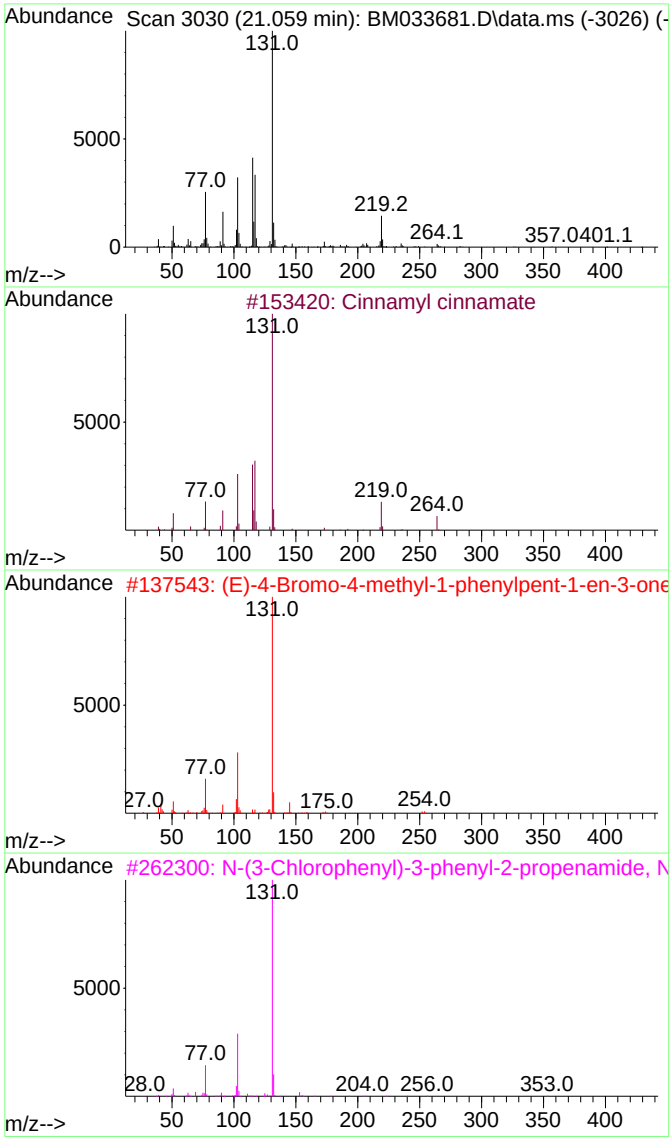
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

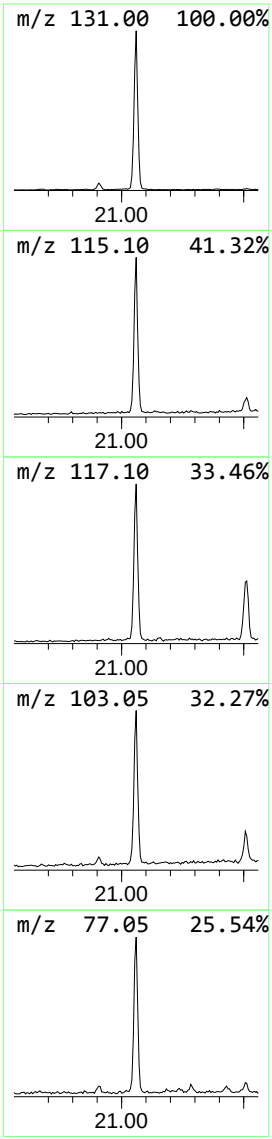
****

Peak Number 3 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.060	2.91 ng	423061	Chrysene-d12	21.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
3	N-(3-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-37-1	47
4	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
5	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

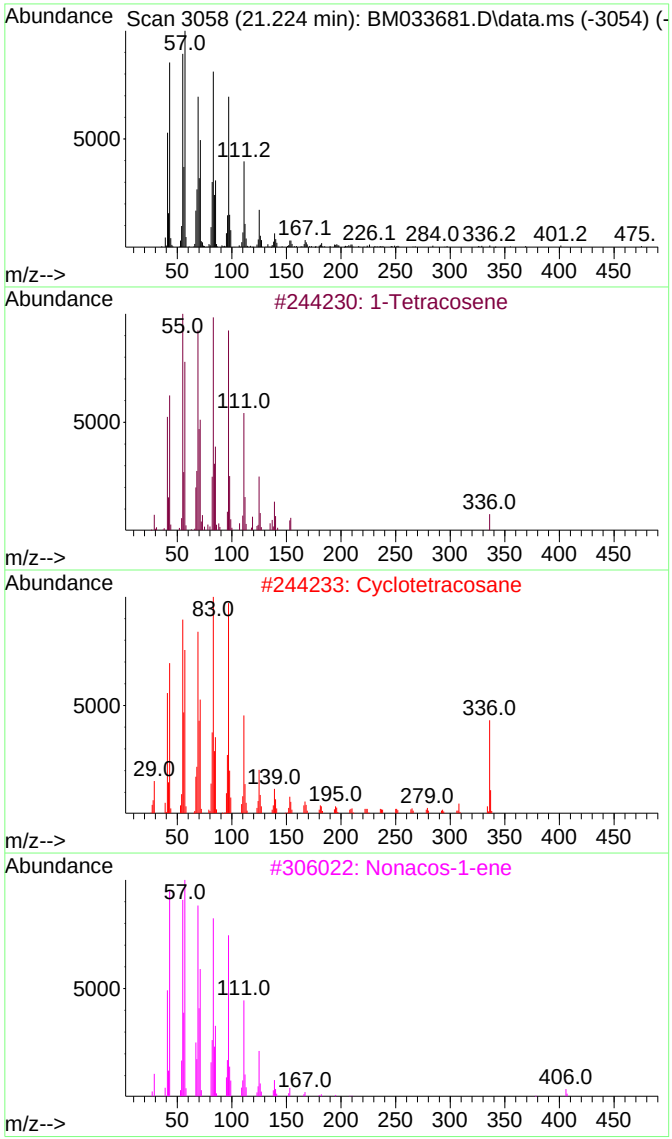
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

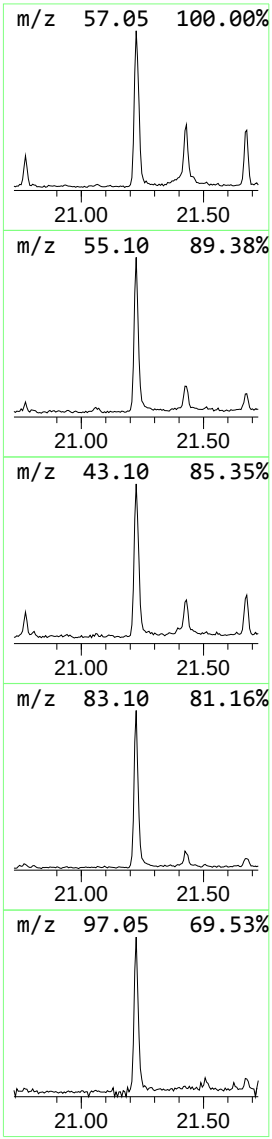
****

Peak Number 4 1-Tetracosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.224	3.82 ng	555073	Chrysene-d12	21.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	99
2	Cyclotetracosane	336	C24H48	000297-03-0	98
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

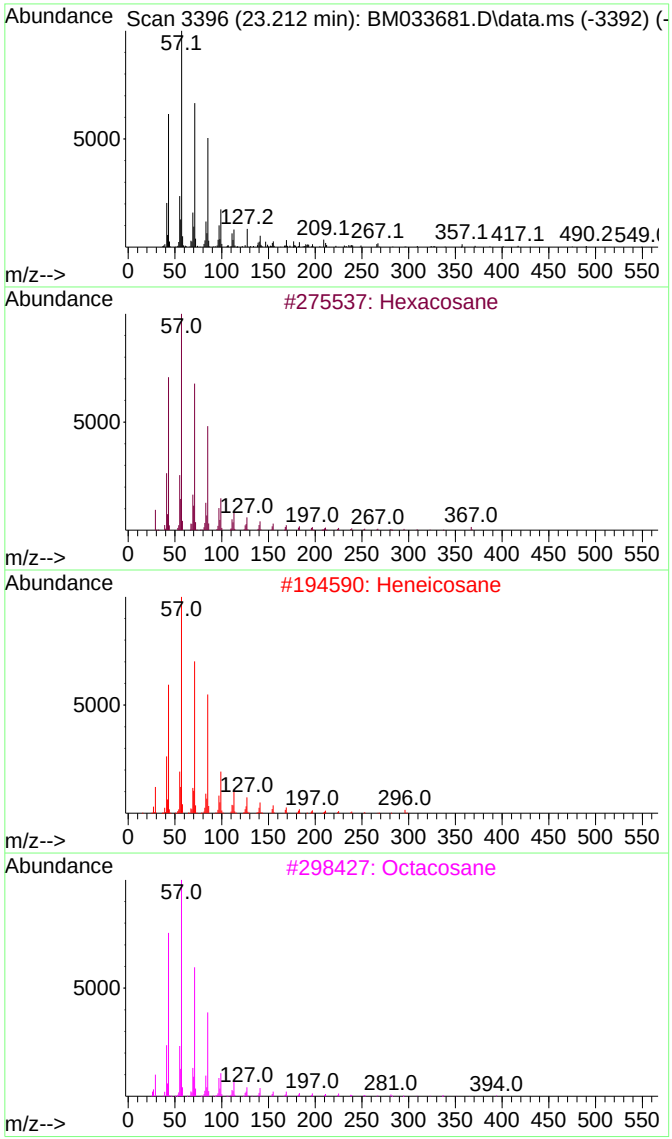
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

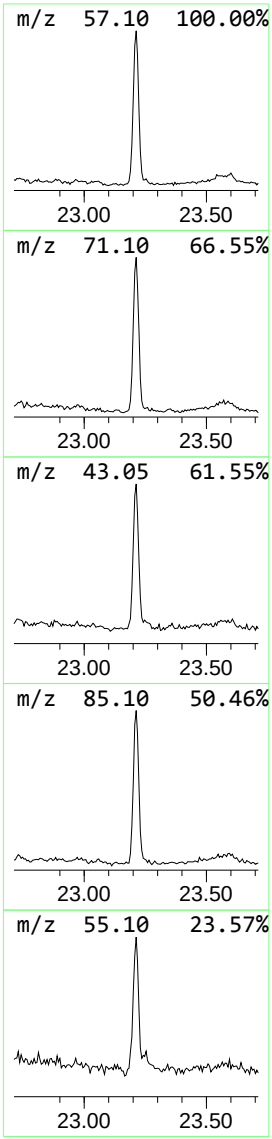
****

Peak Number 5 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.212	3.18 ng	429486	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

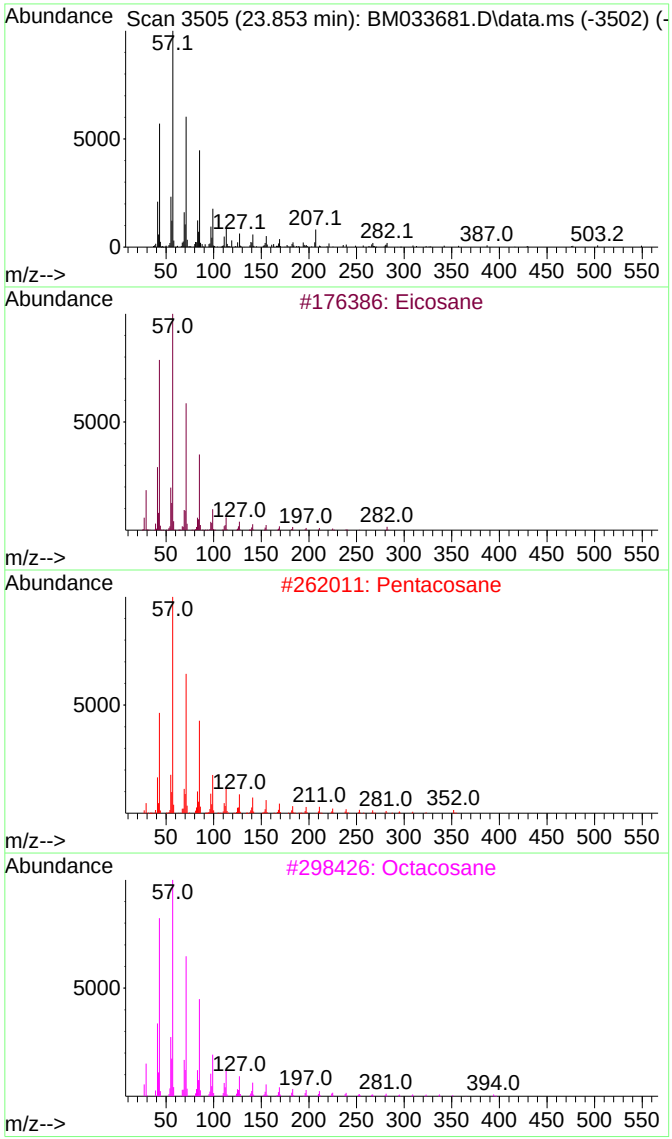
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

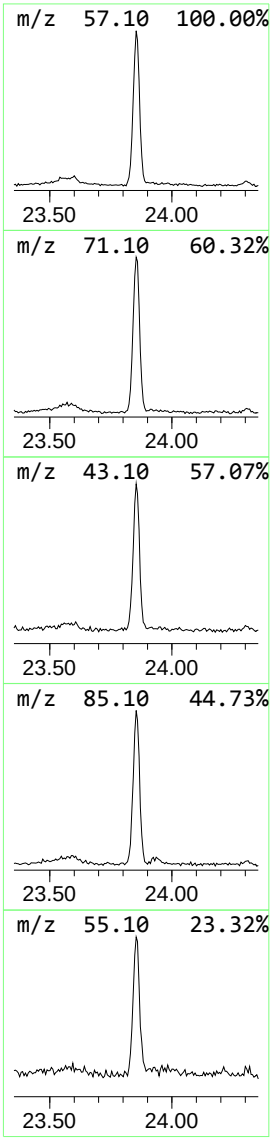
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.853	2.63 ng	354734	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentacosane	352	C25H52	000629-99-2	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

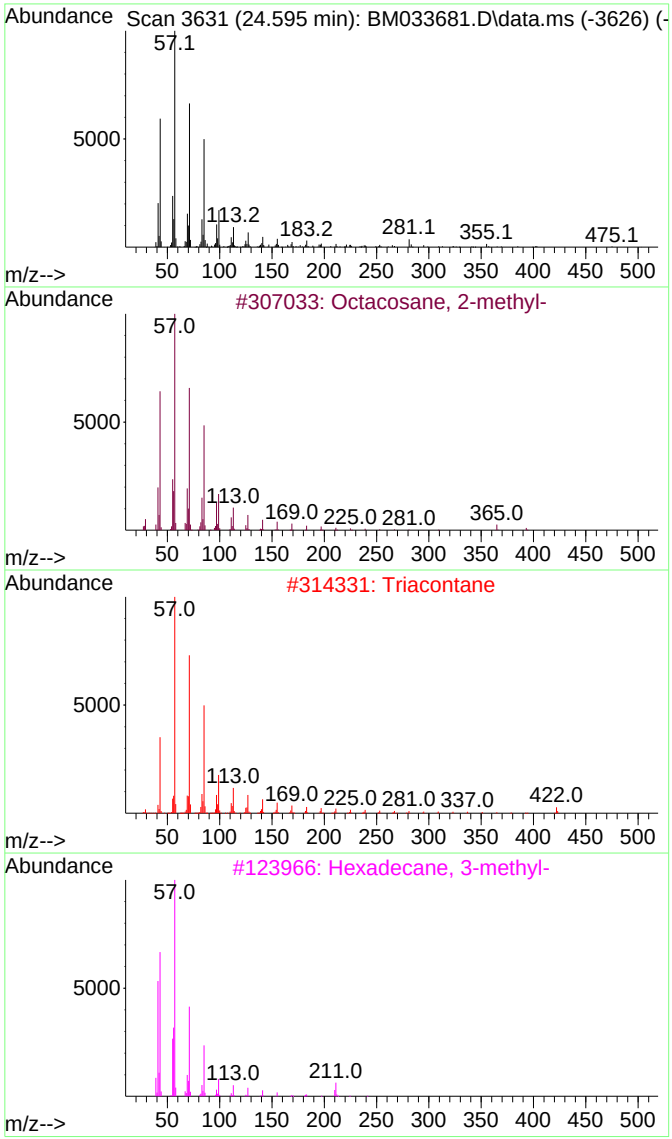
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

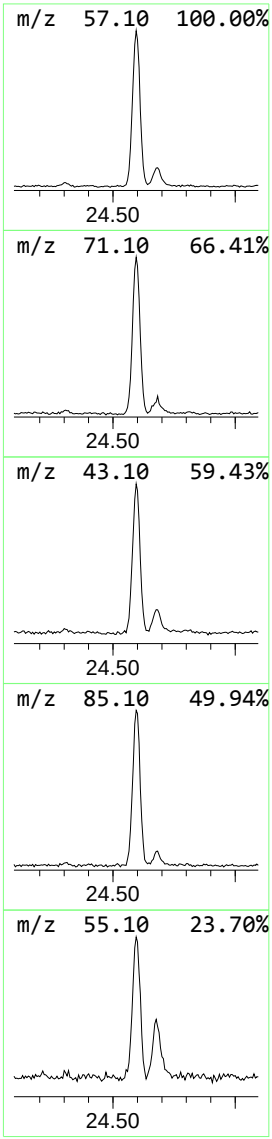
****

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.595	4.30 ng	580448	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Triacontane	422	C30H62	000638-68-6	90
3	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	89
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033681.D
Acq On : 07 Jan 2022 22:29
Operator : CG/JU
Sample : N1065-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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
Ethanol, 2-(2-b...	10.566	3.2	ng	210726	2	10.790	1334660	20.0
n-Hexadecanoic ...	18.242	2.4	ng	282484	4	17.348	2367470	20.0
Cinnamyl cinnamate	21.060	2.9	ng	423061	5	21.512	2906790	20.0
1-Tetracosene	21.224	3.8	ng	555073	5	21.512	2906790	20.0
Hexacosane	23.212	3.2	ng	429486	6	23.936	2697770	20.0
Eicosane	23.853	2.6	ng	354734	6	23.936	2697770	20.0
Octacosane, 2-m...	24.595	4.3	ng	580448	6	23.936	2697770	20.0