LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

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-BM020123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038749.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	297	305	320	rBV	280649	397889	9.74%	2.194%
2	5.452	379	385	397	rBV	859073	1236545	30.28%	6.820%
3	7.075	653	661	674	rBV	846396	1312264	32.13%	7.237%
4	7.893	794	800	808	rBV	254634	380214	9.31%	2.097%
5	9.069	993	1000	1010	rBV	517406	814820	19.95%	4.494%
6	10.704	1269	1278	1290	rBV	321602	517136	12.66%	2.852%
7	13.163	1689	1696	1702	rBV	1772973	2404233	58.87%	13.259%
8	14.539	1923	1930	1936	rVB	528593	770384	18.86%	4.249%
9	15.898	2153	2161	2168	rVB	111215	145752	3.57%	0.804%
10	16.027	2177	2183	2192	rBV	1433891	1904684	46.64%	10.504%
11	17.280	2389	2396	2401	rBV	687166	911610	22.32%	5.028%
12	17.321	2401	2403	2411	rVB	36328	45413	1.11%	0.250%
13	18.168	2541	2547	2558	rBV	195396	312308	7.65%	1.722%
14	19.333	2741	2745	2750	rVB	92999	128003	3.13%	0.706%
15	19.439	2759	2763	2770	rBV	103154	145557	3.56%	0.803%
16	19.698	2803	2807	2812	rVB	84062	107555	2.63%	0.593%
17	19.904	2836	2842	2846	rBV	3627396	4084016	100.00%	22.523%
18	20.445	2930	2934	2939	rBV2	55497	74127	1.82%	0.409%
19	21.150	3050	3054	3066	rBV2	218907	316403	7.75%	1.745%
20	21.356	3086	3089	3094	rBV	50787	67422	1.65%	0.372%
21	21.462	3101	3107	3111	rBV	824962	1101889	26.98%	6.077%
22	23.839	3504	3511	3517	rBV2	485598	954245	23.37%	5.263%

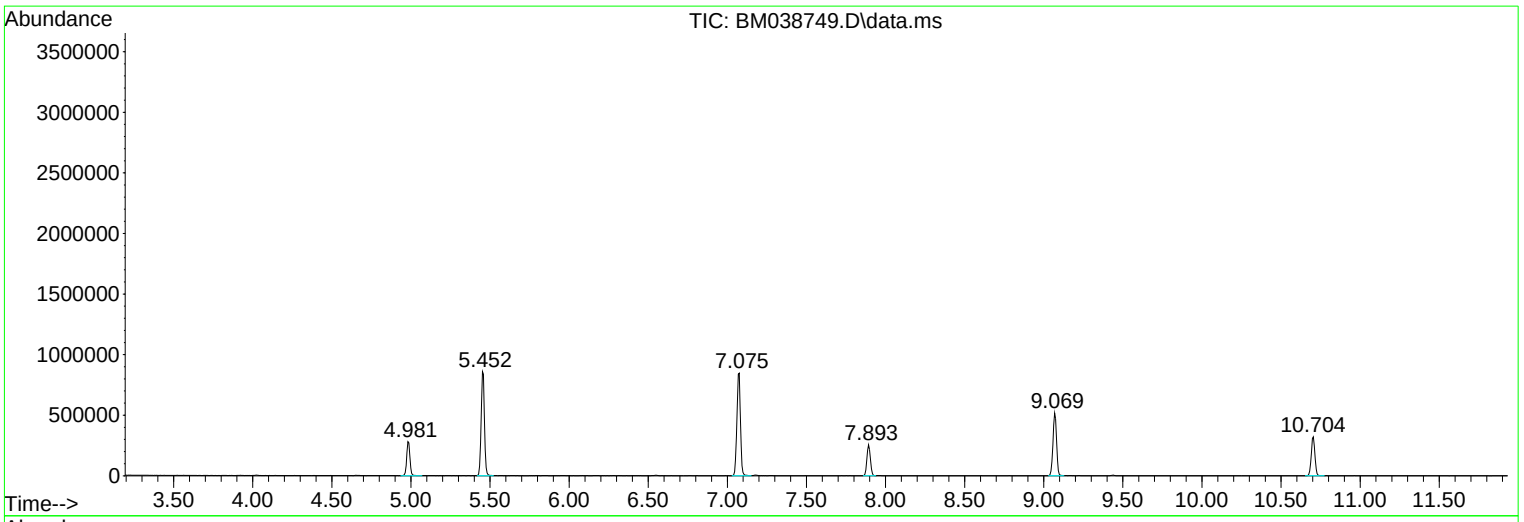
Sum of corrected areas: 18132469

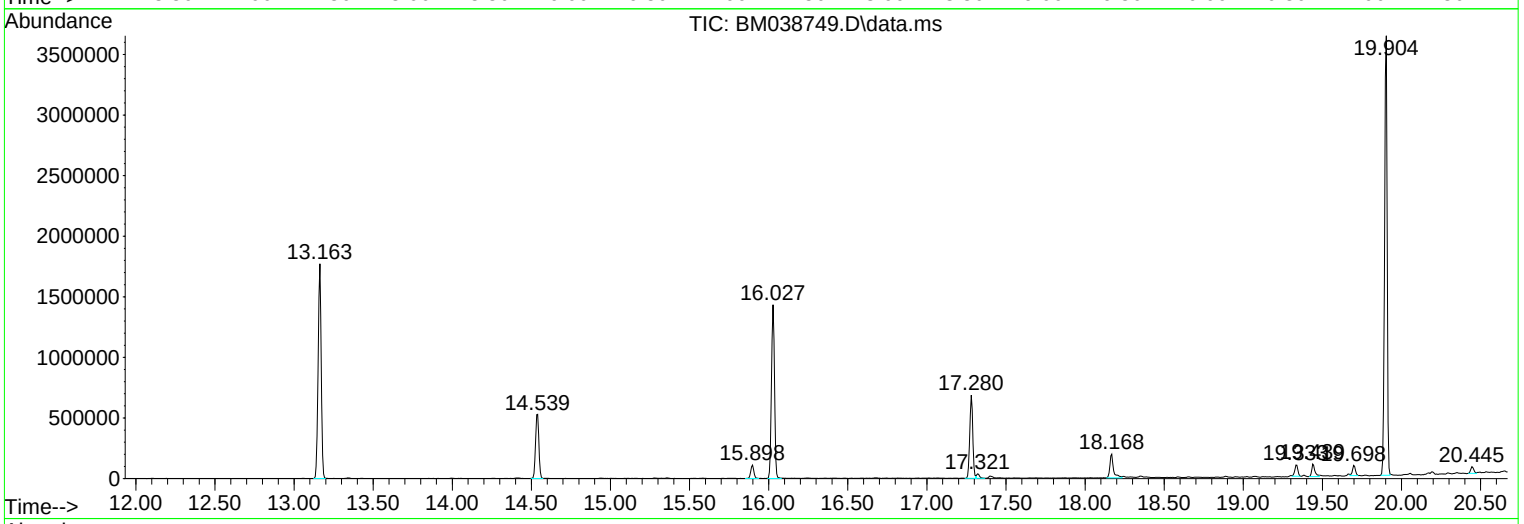
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

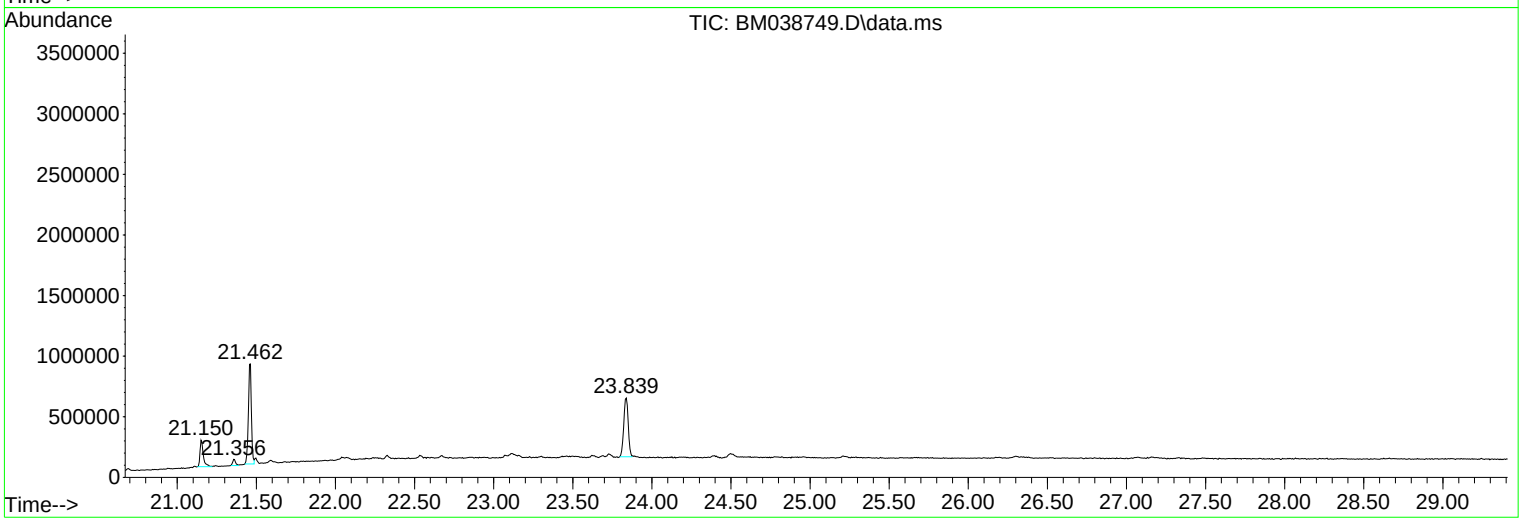
Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

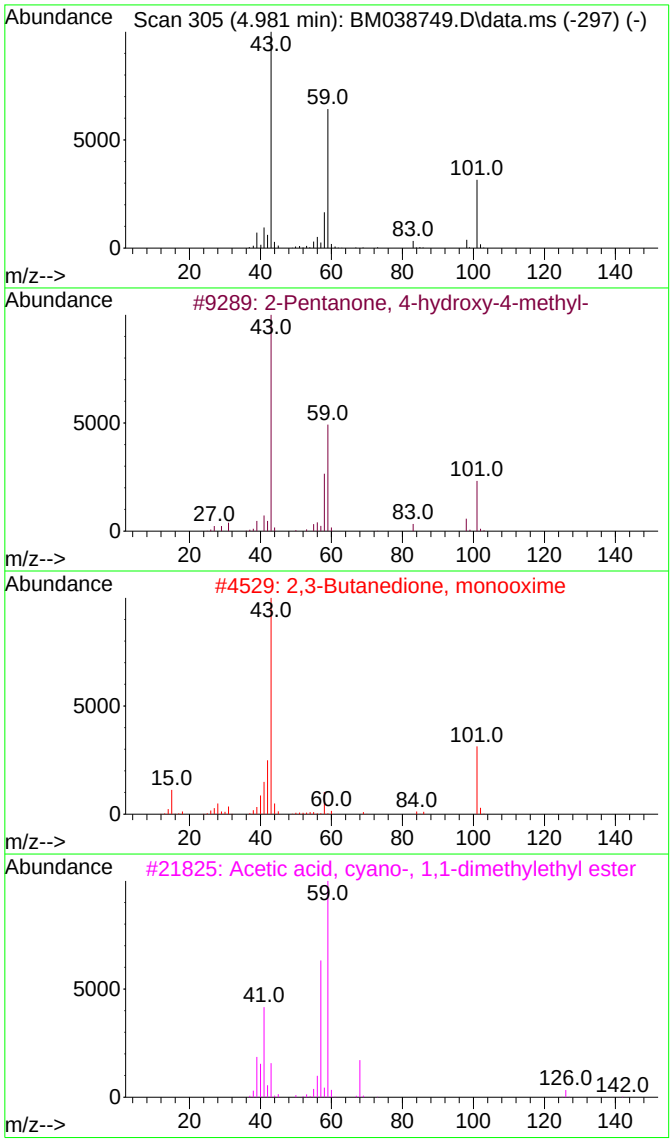
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

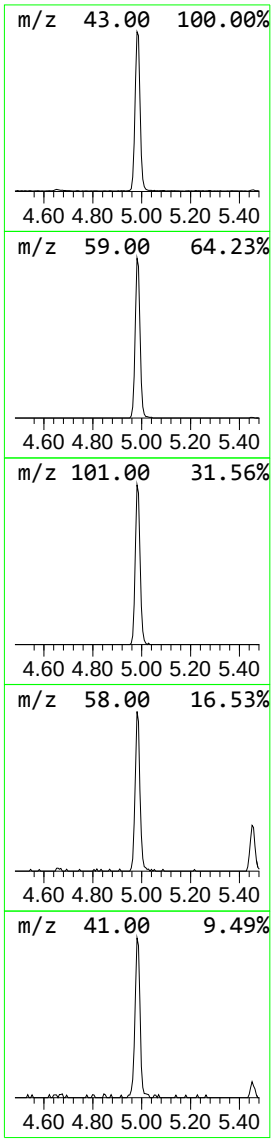
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	20.93 ng	397889	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

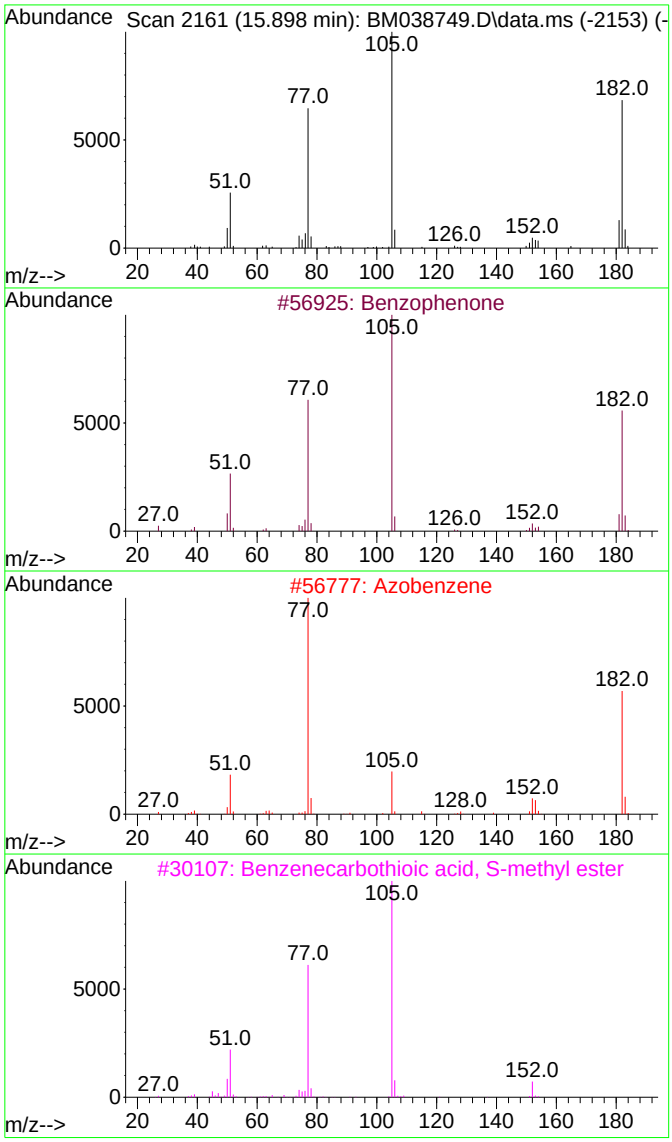
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

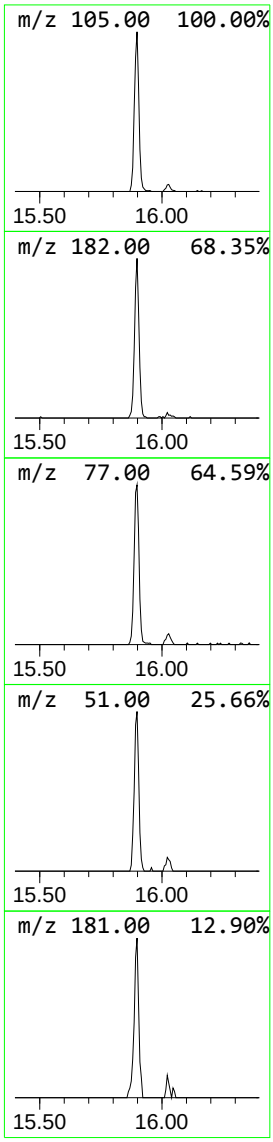
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	3.78 ng	145752	Acenaphthene-d10	14.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

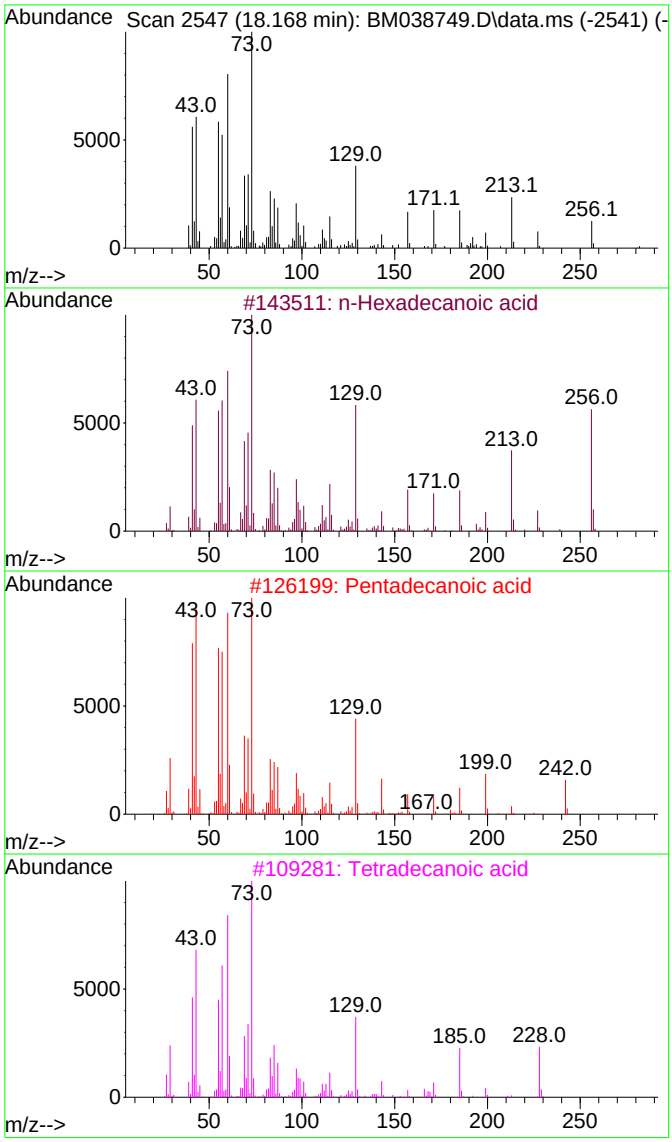
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

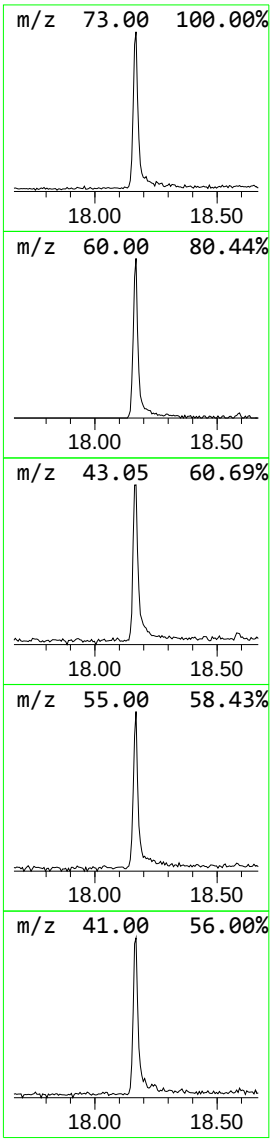
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	6.85 ng	312308	Phenanthrene-d10	17.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

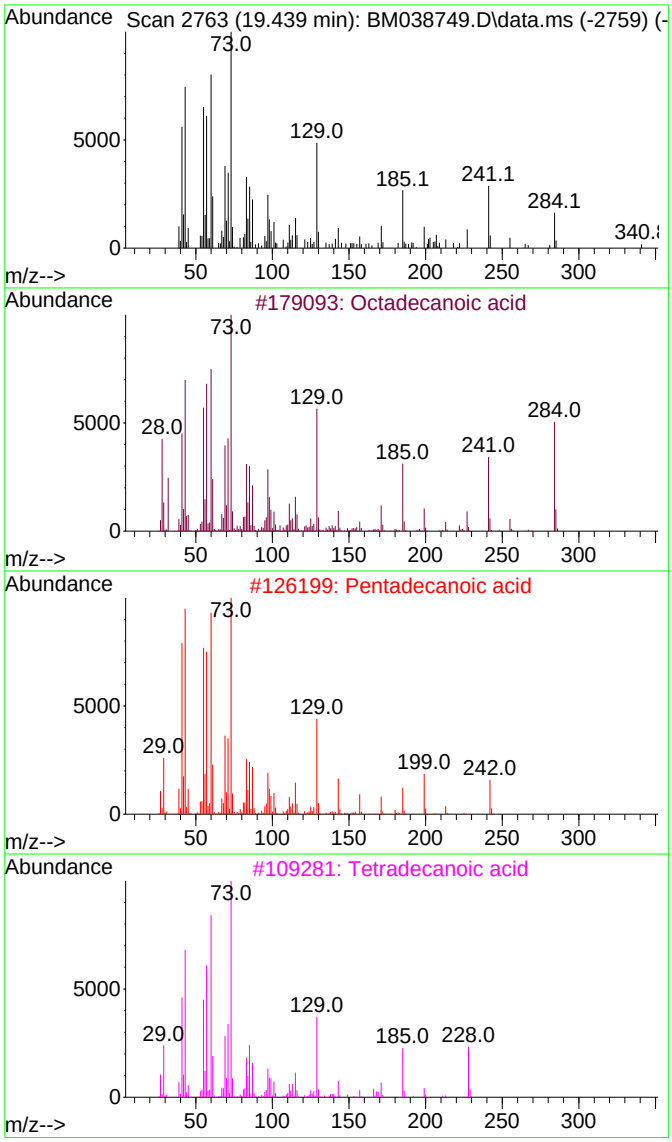
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

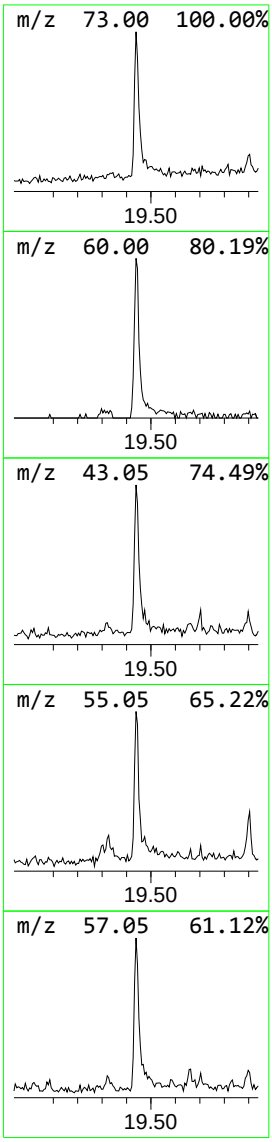
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	2.64 ng	145557	Chrysene-d12	21.462

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	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

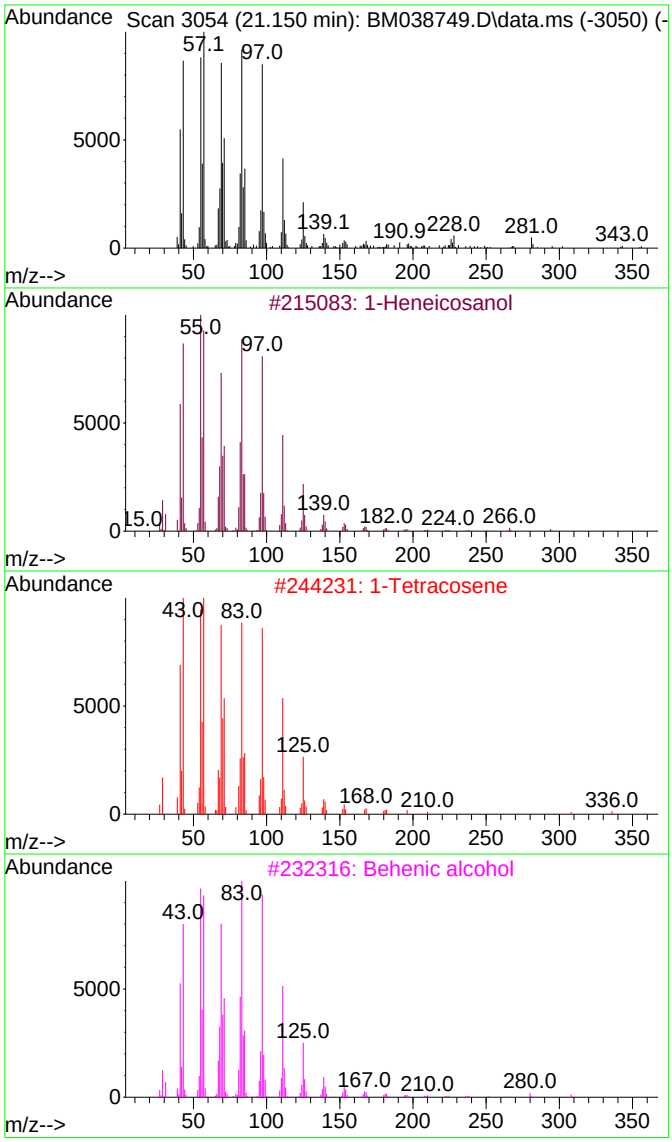
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

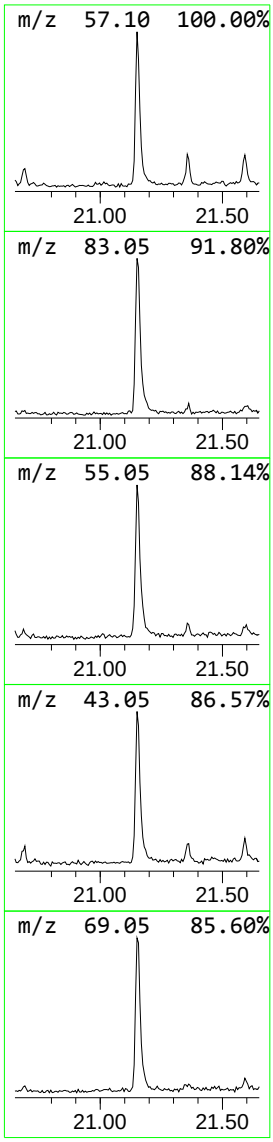
****

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.151	5.74 ng	316403	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Tetracosene	336	C24H48	010192-32-2	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
Data File : BM038749.D
Acq On : 15 Feb 2023 15:42
Operator : CG/JU
Sample : 01537-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PIT-6-(TP6)-COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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-...	4.981	20.9	ng	397889	1	7.893	380214	20.0
Benzophenone	15.898	3.8	ng	145752	3	14.539	770384	20.0
n-Hexadecanoic ...	18.168	6.8	ng	312308	4	17.280	911610	20.0
Octadecanoic acid	19.439	2.6	ng	145557	5	21.462	1101890	20.0
1-Heneicosanol	21.151	5.7	ng	316403	5	21.462	1101890	20.0