LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.540	394	400	408	rBB	245369	354136	21.62%	4.840%
2	7.169	671	677	688	rVB2	137997	279433	17.06%	3.819%
3	7.610	747	752	760	rBV	23261	35115	2.14%	0.480%
4	8.016	815	821	828	rVB	109280	167922	10.25%	2.295%
5	9.192	1013	1021	1030	rBV	332687	534607	32.63%	7.307%
6	10.833	1293	1300	1305	rBV	142796	230231	14.05%	3.147%
7	10.880	1305	1308	1319	rVB	19942	31673	1.93%	0.433%
8	13.280	1709	1716	1723	rBV	750090	1125784	68.72%	15.388%
9	13.545	1755	1761	1770	rVB	123256	178363	10.89%	2.438%
10	14.110	1851	1857	1864	rVB	57065	73790	4.50%	1.009%
11	14.657	1945	1950	1954	rBV	191951	279897	17.08%	3.826%
12	14.698	1954	1957	1969	rVB	42154	60406	3.69%	0.826%
13	15.757	2132	2137	2142	rBV	20243	25190	1.54%	0.344%
14	16.139	2196	2202	2213	rVB	641428	894375	54.59%	12.225%
15	17.386	2408	2414	2420	rBV	232198	319075	19.48%	4.361%
16	18.256	2557	2562	2569	rBV	45469	59501	3.63%	0.813%
17	19.109	2702	2707	2713	rBV2	22523	32853	2.01%	0.449%
18	19.427	2757	2761	2765	rVB2	14239	18731	1.14%	0.256%
19	19.521	2770	2777	2784	rBV3	26158	52256	3.19%	0.714%
20	19.745	2811	2815	2819	rVB	19266	20421	1.25%	0.279%
21	19.980	2849	2855	2860	rBV	1368101	1638299	100.00%	22.393%
22	20.274	2902	2905	2910	rVB	19213	20884	1.27%	0.285%
23	21.215	3061	3065	3074	rBV	121734	149028	9.10%	2.037%
24	21.515	3111	3116	3123	rBV	311017	370125	22.59%	5.059%
25	23.797	3498	3504	3513	rVB2	189590	364061	22.22%	4.976%

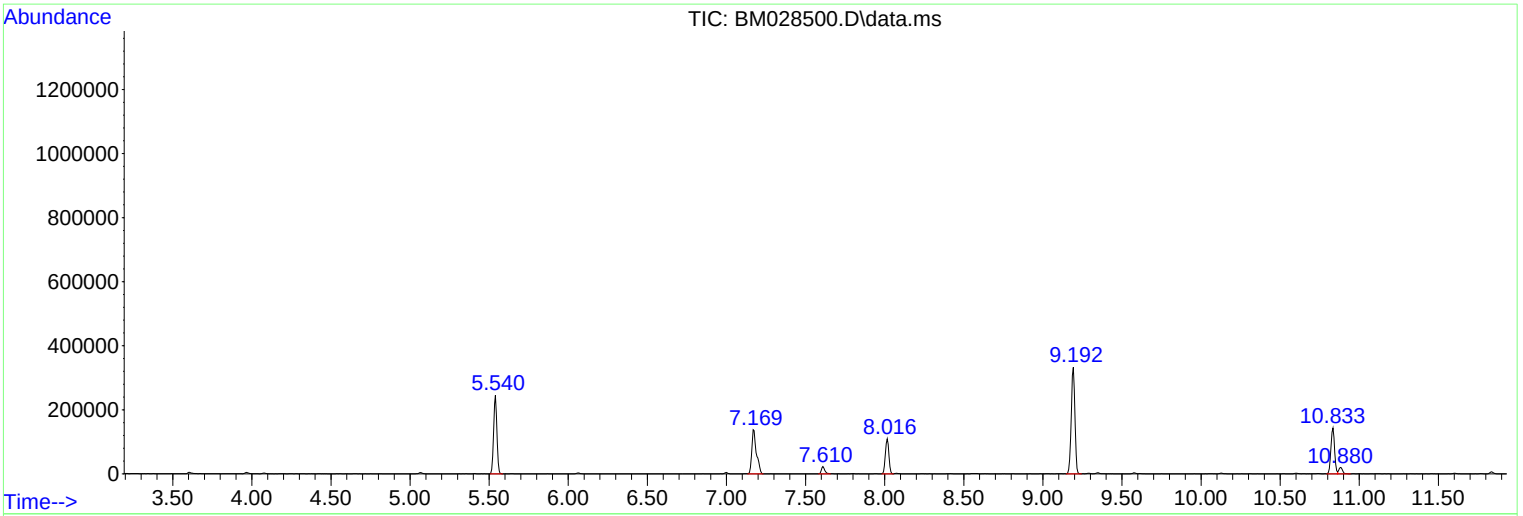
Sum of corrected areas: 7316156

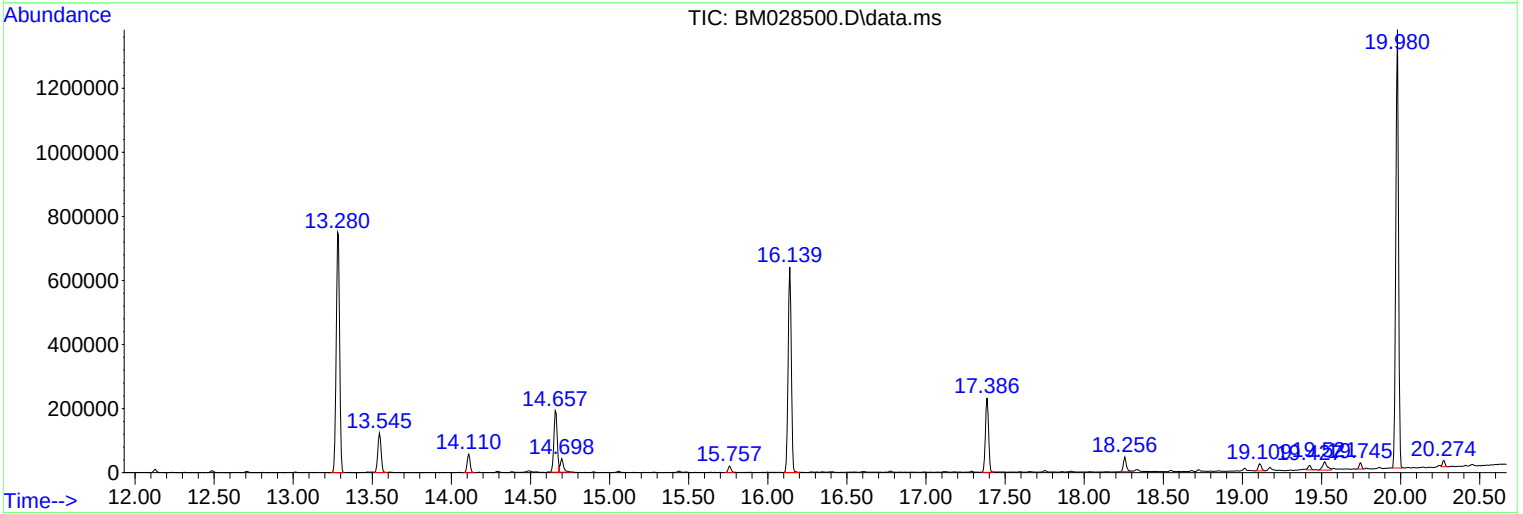
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

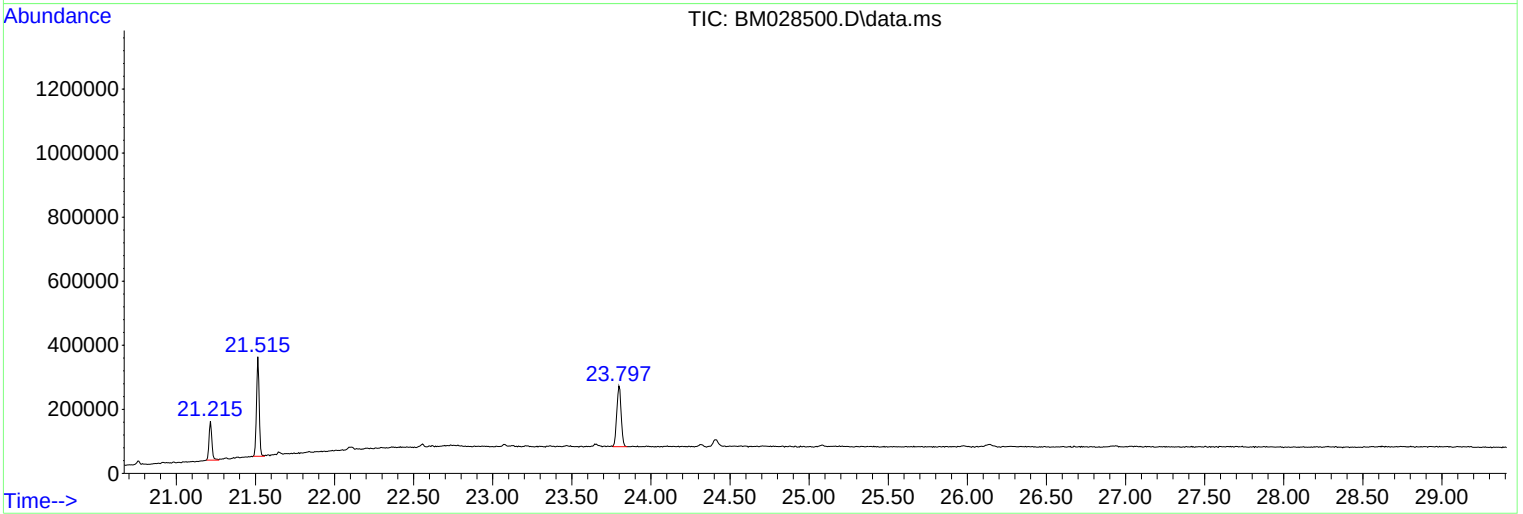
Instrument :
BNA_M
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1

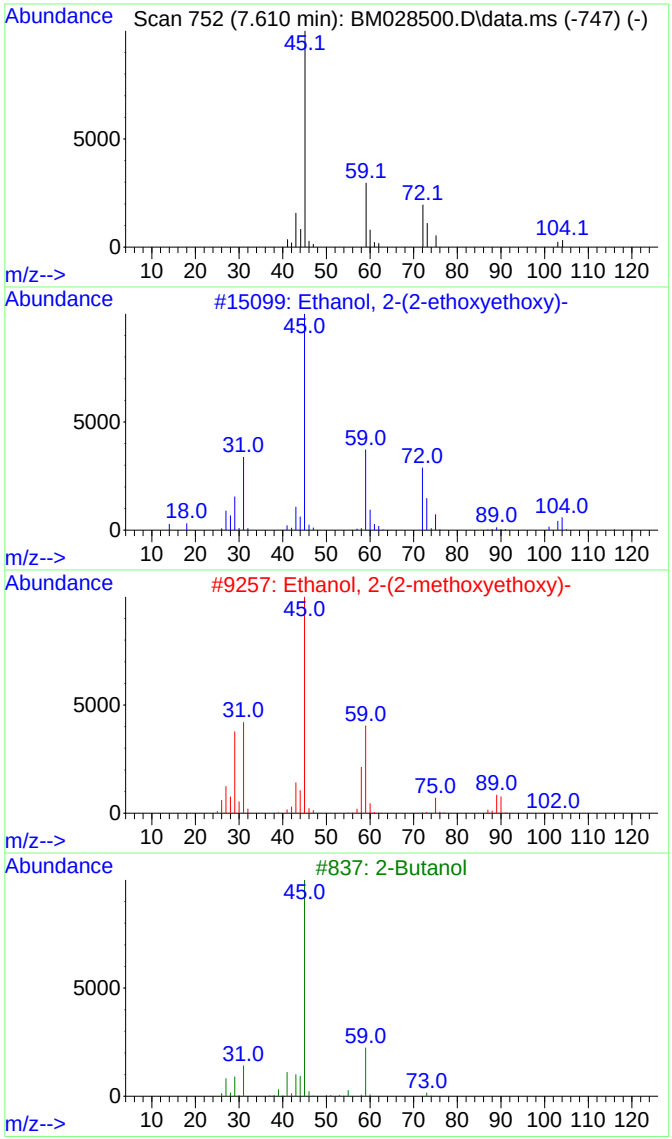
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

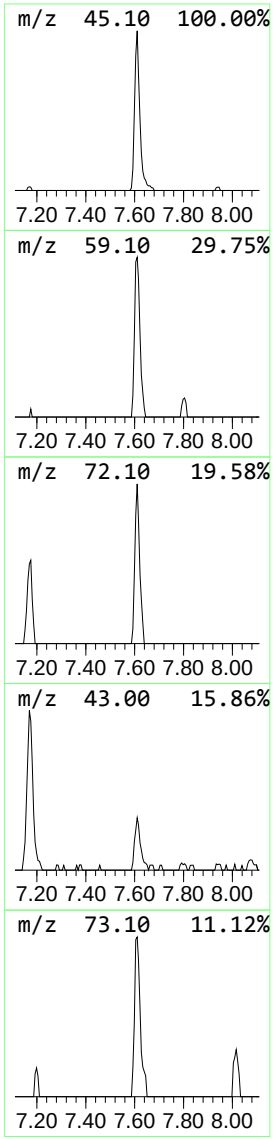
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.610	4.18 ng	35115	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
3	2-Butanol	74	C4H10O	000078-92-2	42
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1

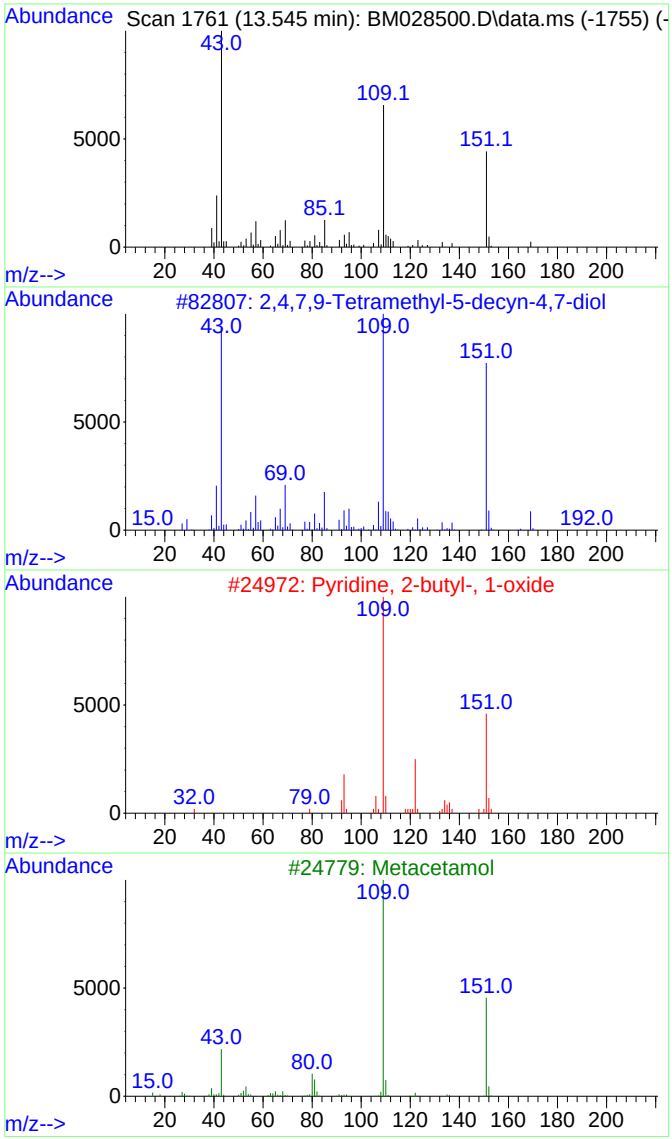
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

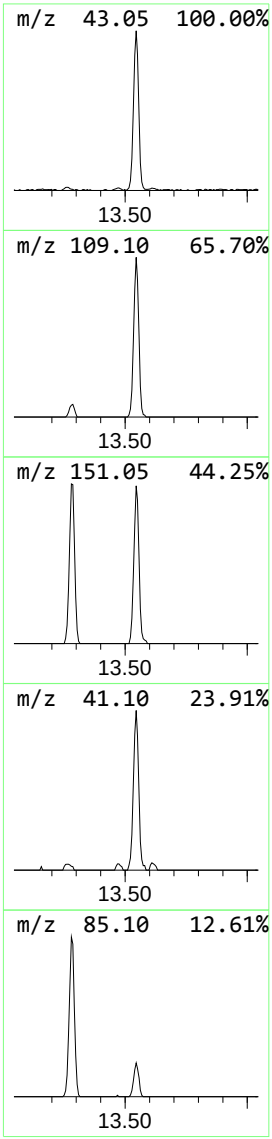
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	12.74 ng	178363	Acenaphthene-d10	14.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	58
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

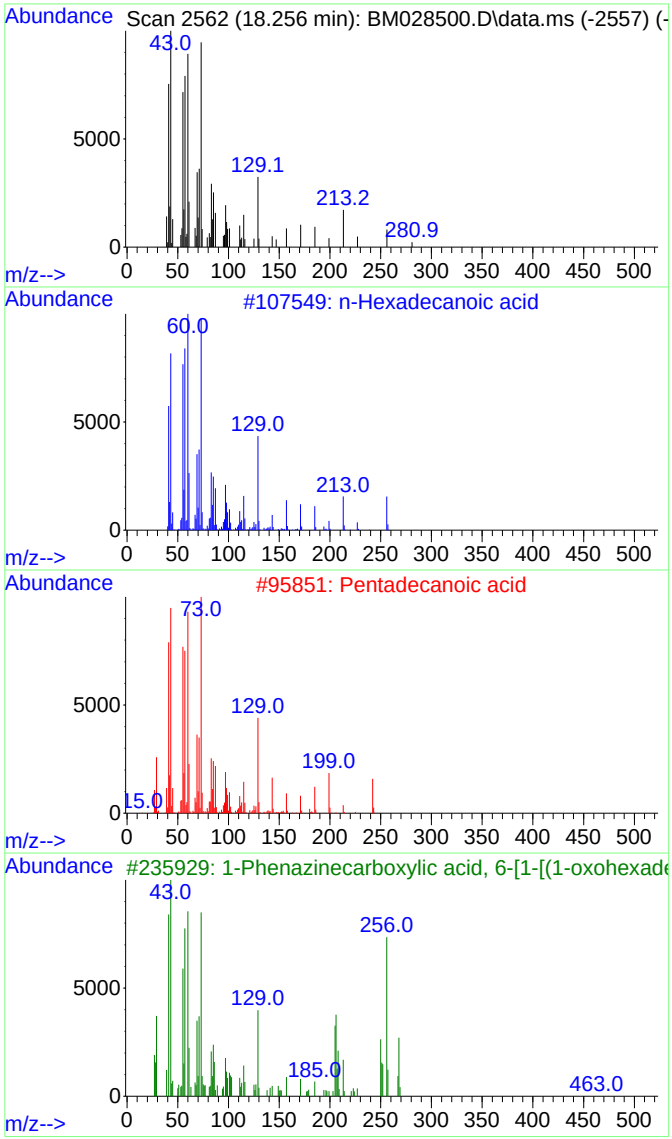
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

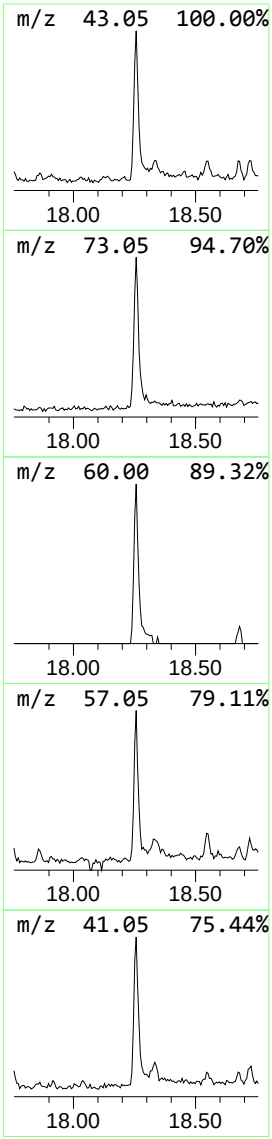
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.256	3.73 ng	59501	Phenanthrene-d10	17.386

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	87
3	1-Phenazinecarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

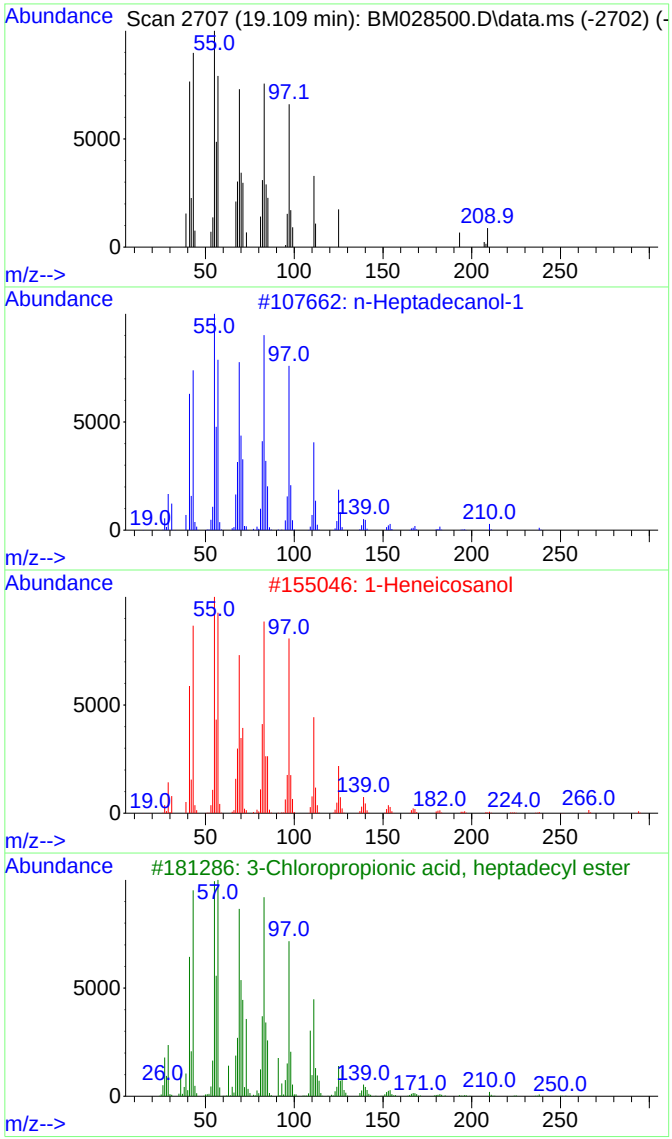
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

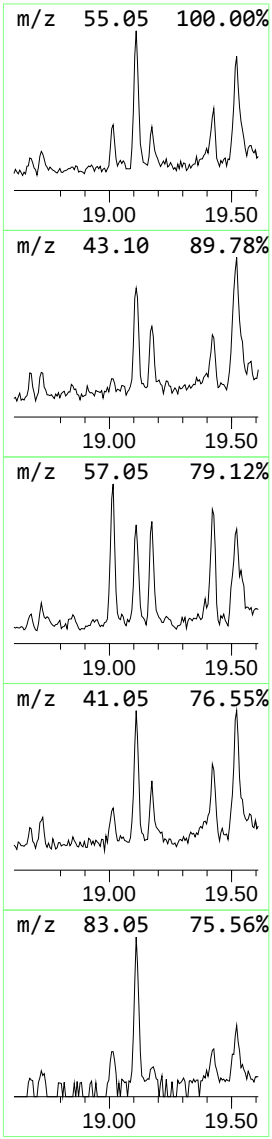
****

Peak Number 4 n-Heptadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.109	2.06 ng	32853	Phenanthrene-d10	17.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5	1-Octadecene	252	C18H36	000112-88-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

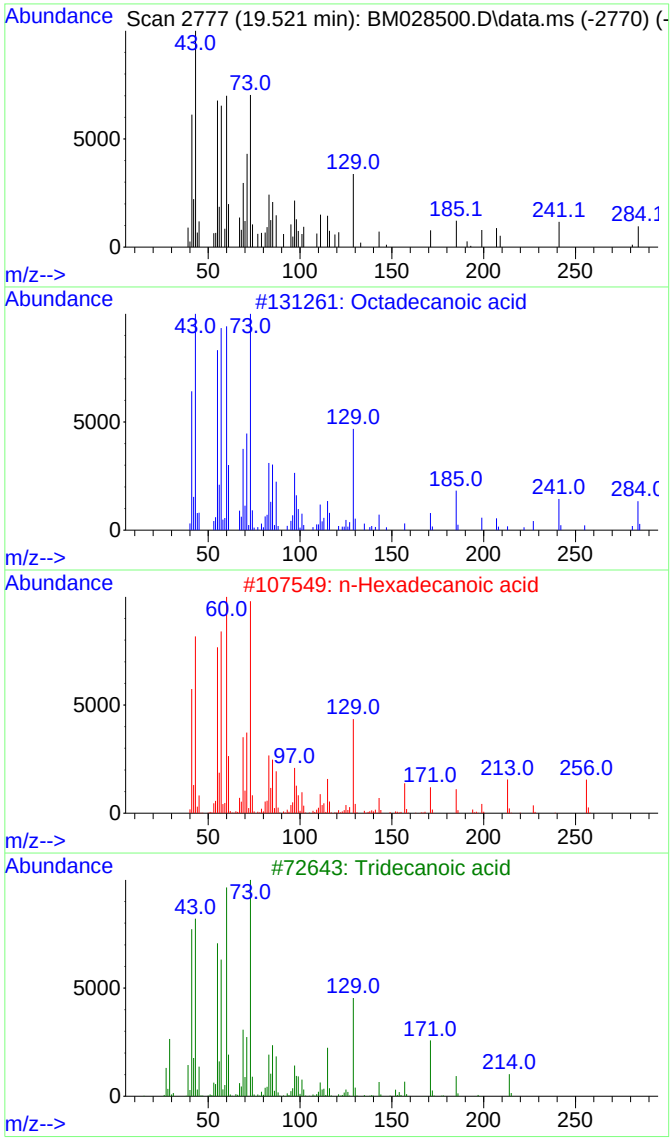
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

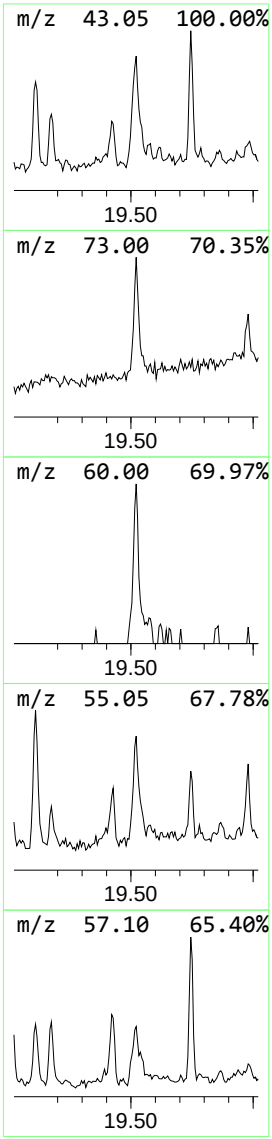
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	2.82 ng	52256	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

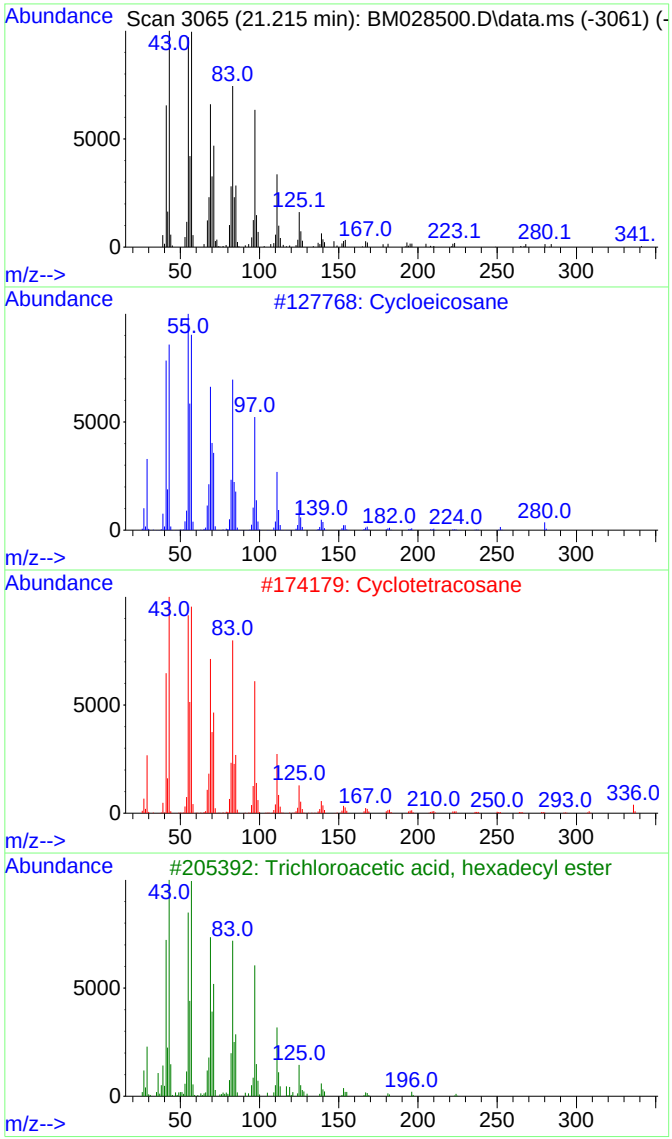
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

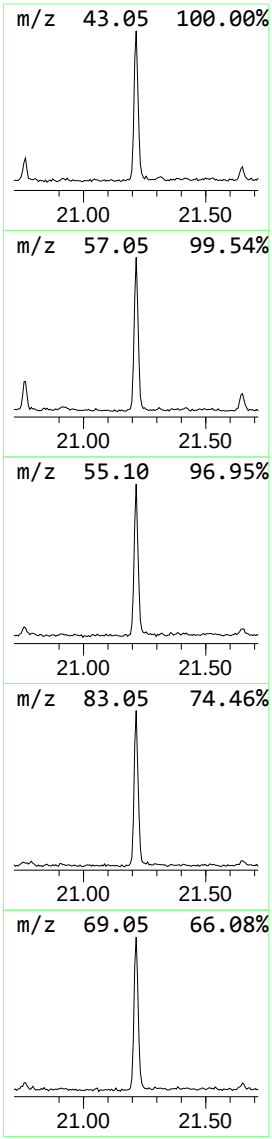
****

Peak Number 6 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	8.05 ng	149028	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	98
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028500.D
Acq On : 21 Jan 2021 22:20
Operator : CG/JU
Sample : M1157-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-e...	7.610	4.2	ng	35115	1	8.016	167922	20.0
2,4,7,9-Tetrame...	13.545	12.7	ng	178363	3	14.657	279897	20.0
n-Hexadecanoic ...	18.256	3.7	ng	59501	4	17.386	319075	20.0
n-Heptadecanol-1	19.109	2.1	ng	32853	4	17.386	319075	20.0
Octadecanoic acid	19.521	2.8	ng	52256	5	21.515	370125	20.0
Cycloeicosane	21.215	8.1	ng	149028	5	21.515	370125	20.0