LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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: BM028499.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	393	400	408	rVB	279444	397467	26.25%	5.304%
2	7.175	671	678	690	rVB2	155868	310434	20.51%	4.143%
3	7.610	744	752	760	rBV	17202	28257	1.87%	0.377%
4	8.016	814	821	828	rBV	111251	169939	11.23%	2.268%
5	9.193	1012	1021	1028	rBV	331241	533557	35.24%	7.120%
6	10.834	1292	1300	1305	rBV	141847	233131	15.40%	3.111%
7	10.881	1305	1308	1317	rVB	17719	29407	1.94%	0.392%
8	12.440	1567	1573	1578	rBV	12124	23393	1.55%	0.312%
9	13.281	1709	1716	1724	rBV	738760	1094909	72.32%	14.612%
10	13.545	1755	1761	1769	rBV	53249	77962	5.15%	1.040%
11	14.110	1851	1857	1863	rVB	50126	66301	4.38%	0.885%
12	14.657	1941	1950	1954	rBV	200414	286913	18.95%	3.829%
13	14.698	1954	1957	1969	rVB	46360	72277	4.77%	0.965%
14	16.139	2196	2202	2212	rVB	631163	859352	56.76%	11.468%
15	16.869	2321	2326	2332	rBV	11656	16341	1.08%	0.218%
16	17.386	2408	2414	2420	rBV	243175	320931	21.20%	4.283%
17	18.263	2557	2563	2572	rBV	156196	222573	14.70%	2.970%
18	19.016	2685	2691	2695	rBV	10526	16100	1.06%	0.215%
19	19.521	2772	2777	2787	rBV	97974	136240	9.00%	1.818%
20	19.745	2811	2815	2818	rBV	17424	18146	1.20%	0.242%
21	19.980	2849	2855	2860	rBV	1267400	1513878	100.00%	20.203%
22	20.274	2902	2905	2908	rVB	14381	15712	1.04%	0.210%
23	20.762	2984	2988	2992	rBV	16140	20134	1.33%	0.269%
24	21.215	3061	3065	3072	rBV	223589	264632	17.48%	3.532%
25	21.515	3111	3116	3121	rBV	313581	374272	24.72%	4.995%
26	21.651	3136	3139	3144	rVB2	19957	23009	1.52%	0.307%
27	23.798	3498	3504	3511	rVB2	200710	367986	24.31%	4.911%

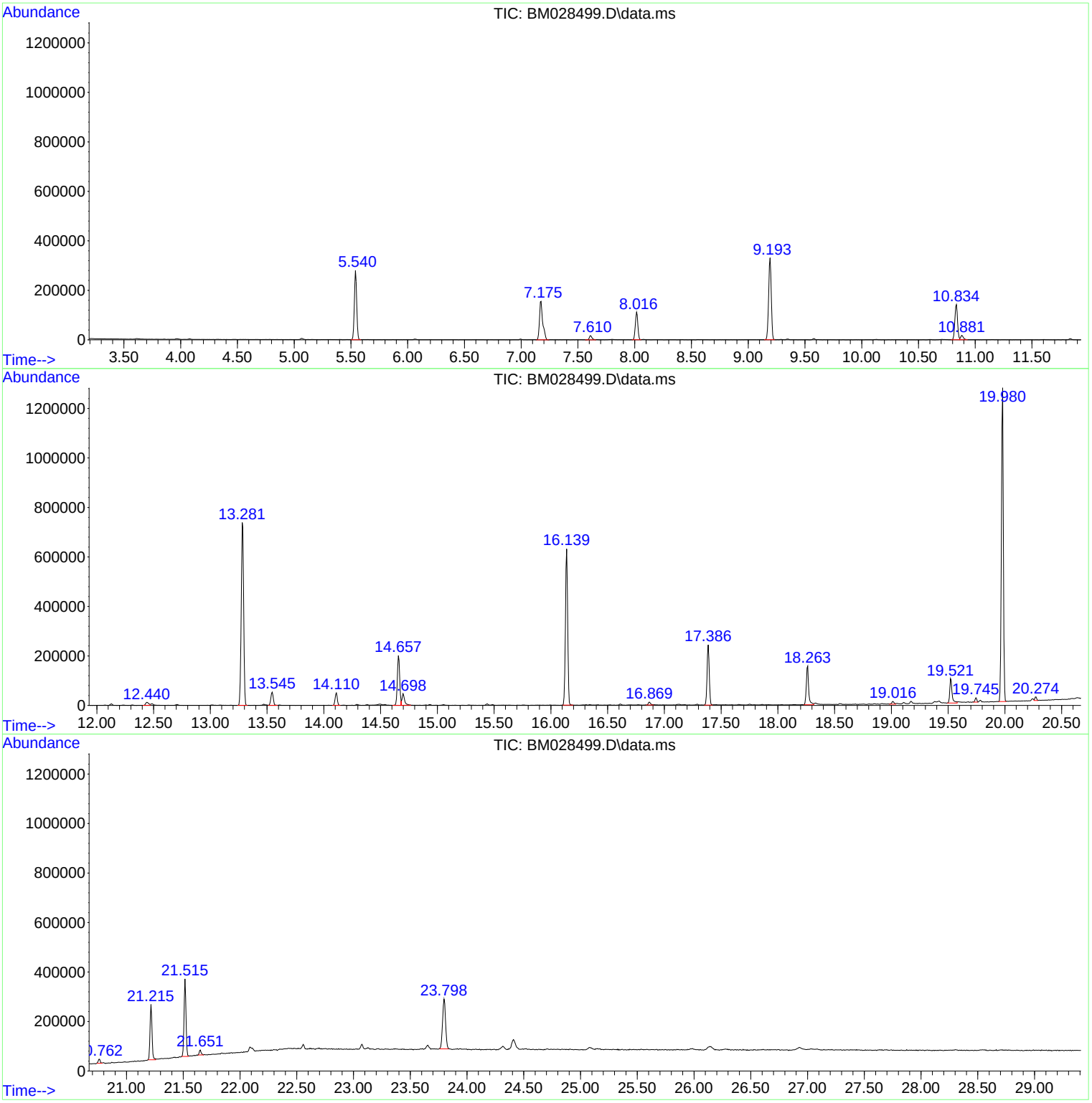
Sum of corrected areas: 7493253

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-2

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 : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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

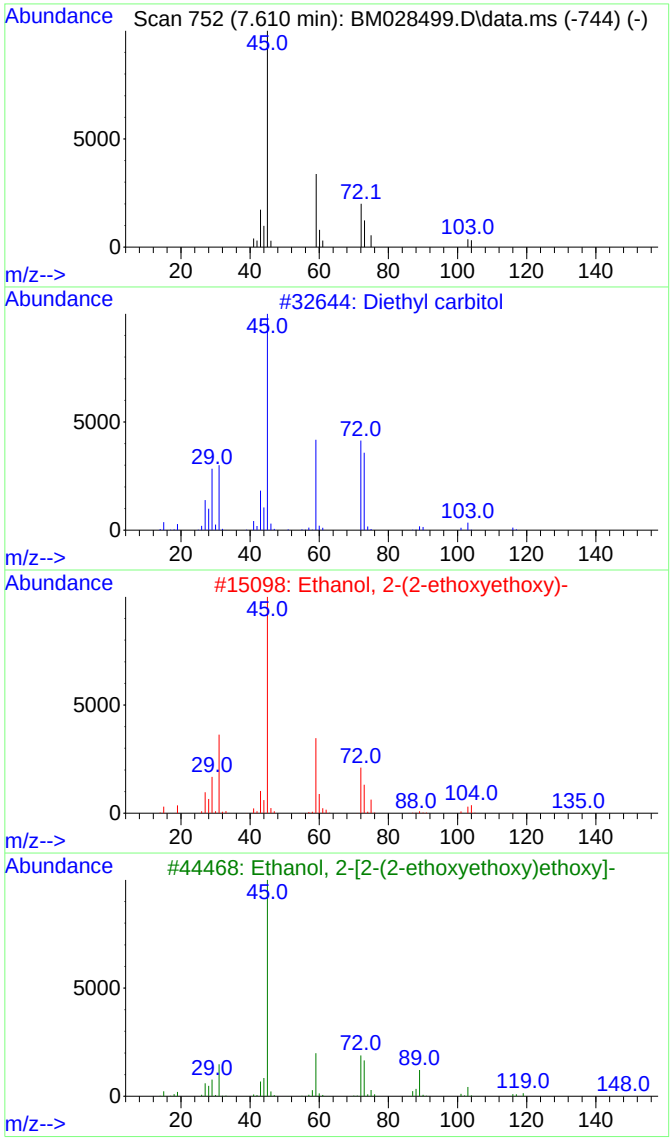
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

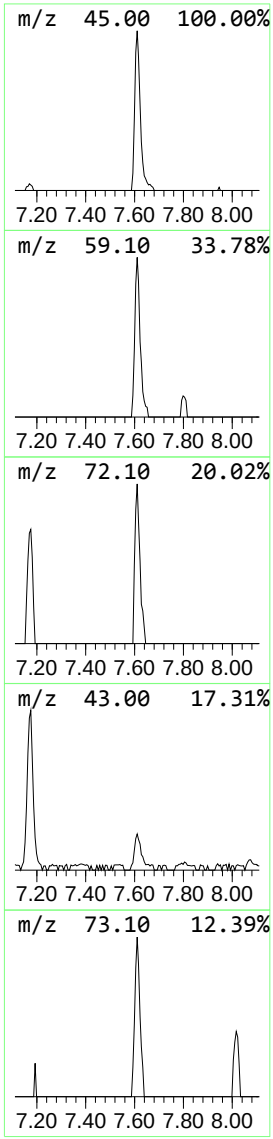
****

Peak Number 1 Diethyl carbitol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.610	3.33 ng	28257	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl carbitol	162	C8H18O3	000112-36-7	78
2	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	56
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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

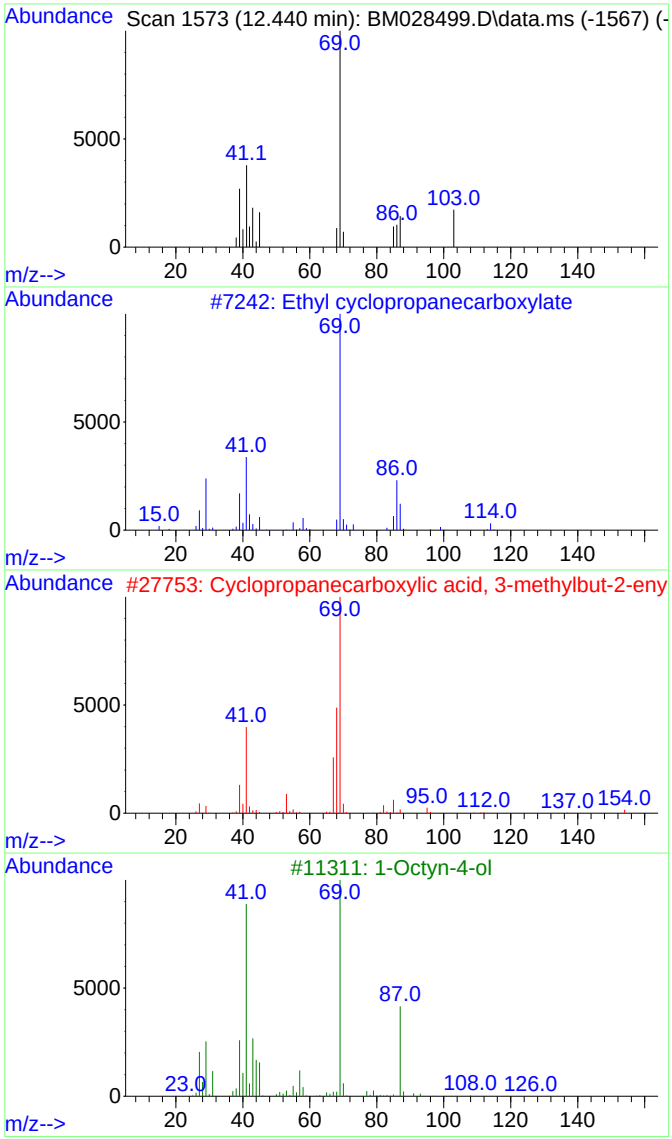
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

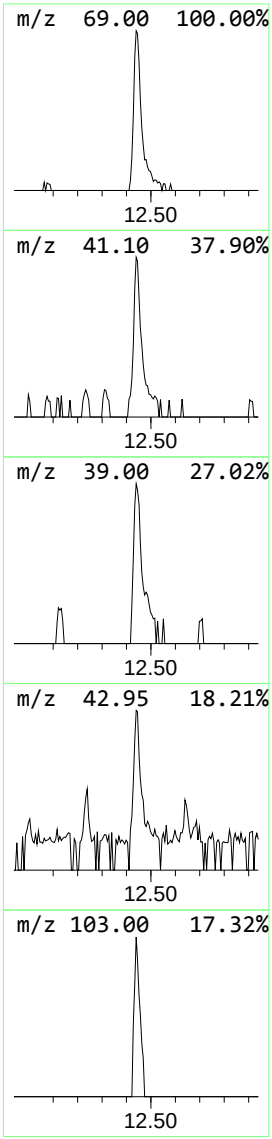
****

Peak Number 2 unknown12.440 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.440	2.01 ng	23393	Naphthalene-d8	10.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
2	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
3	1-Octyn-4-ol	126	C8H14O	052517-92-7	9
4	1,6-Hexanediamine	116	C6H16N2	000124-09-4	9
5	meso-5,6-Decanediol	174	C10H22O2	003266-25-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-2

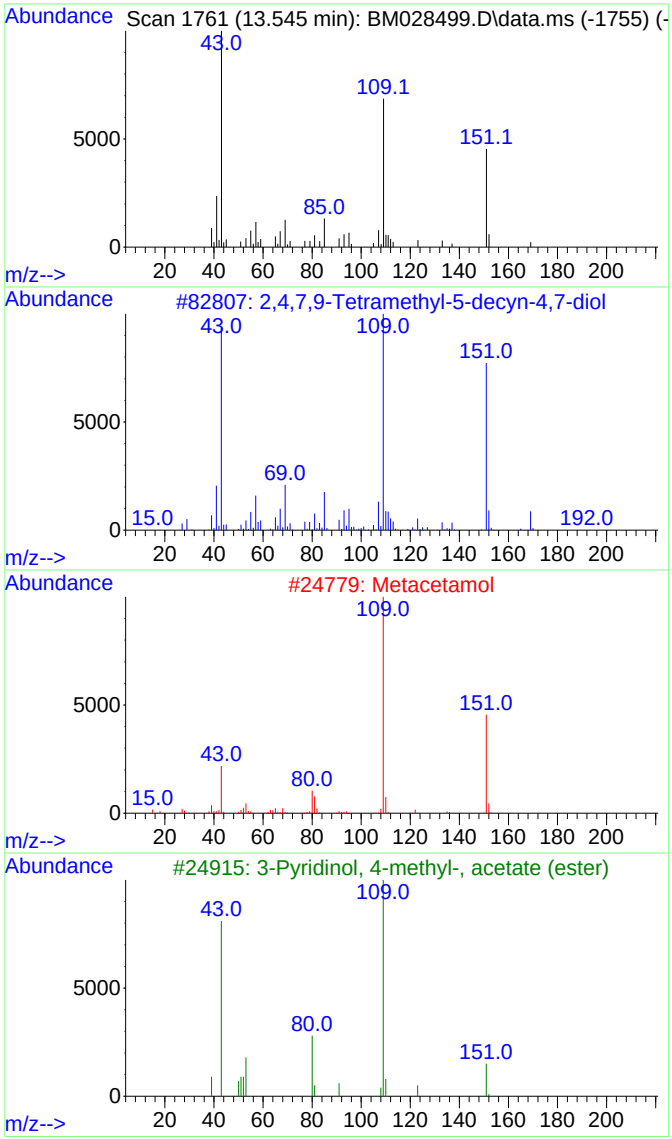
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

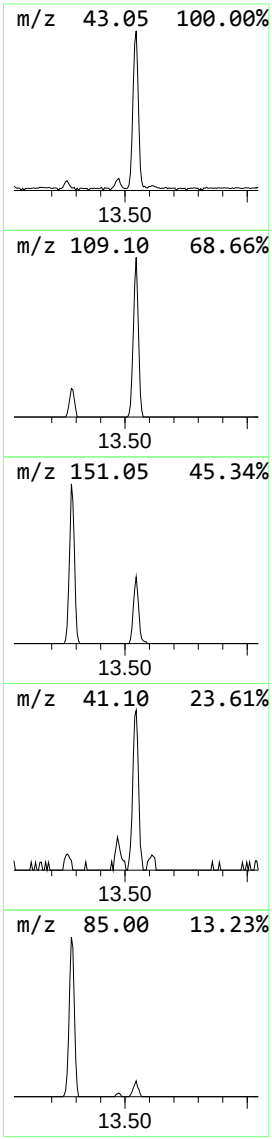
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	5.43 ng	77962	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	87
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	45
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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

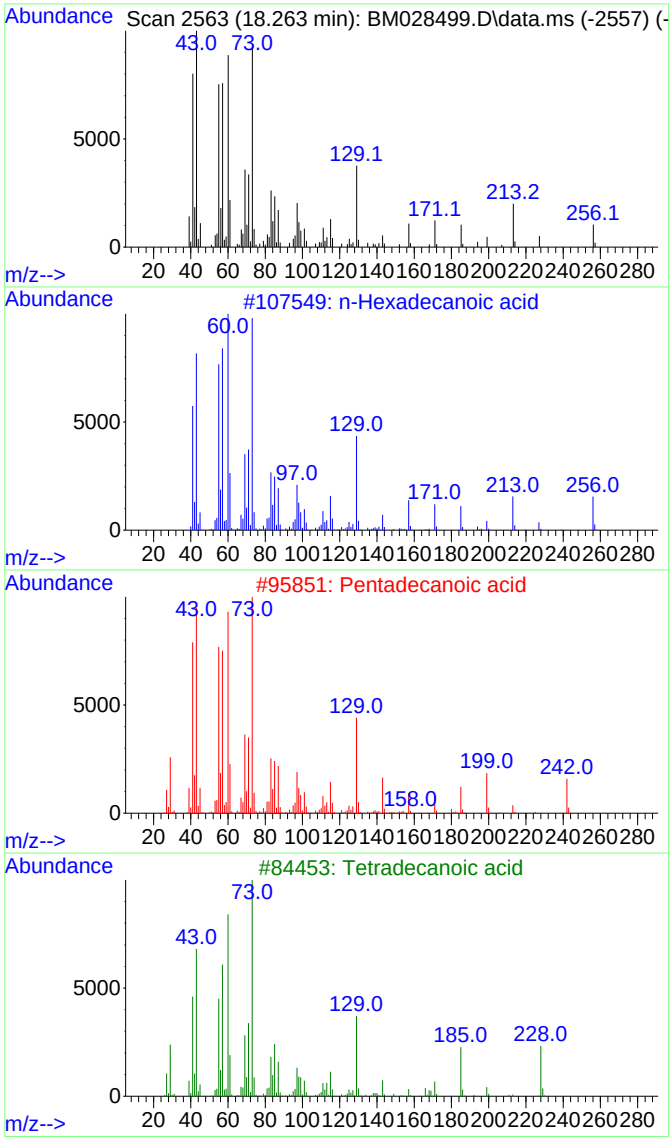
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

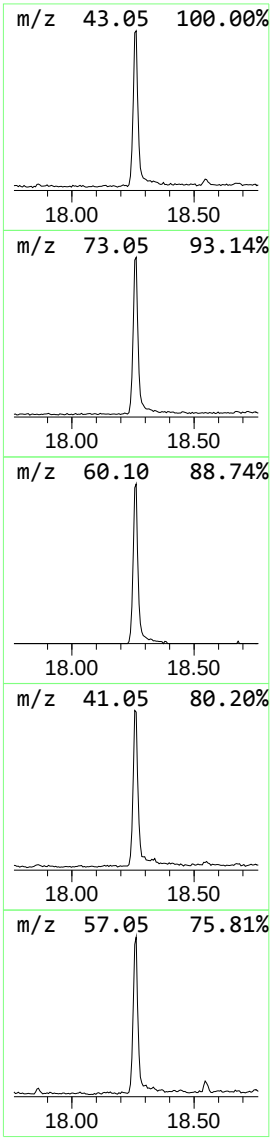
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.263	13.87 ng	222573	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	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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

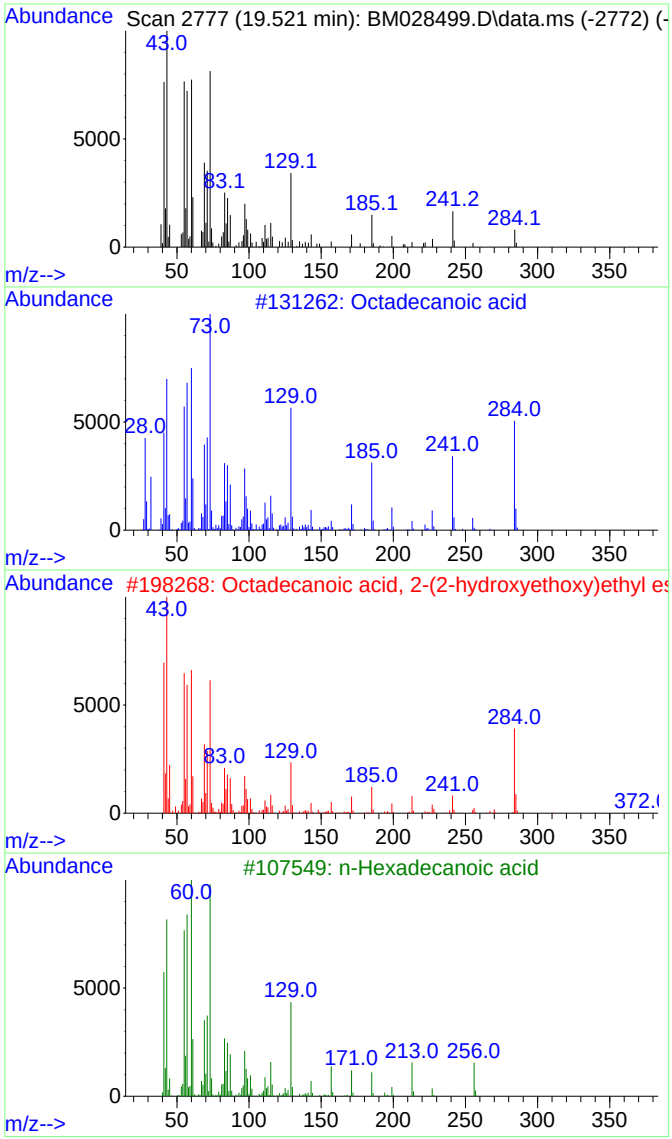
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

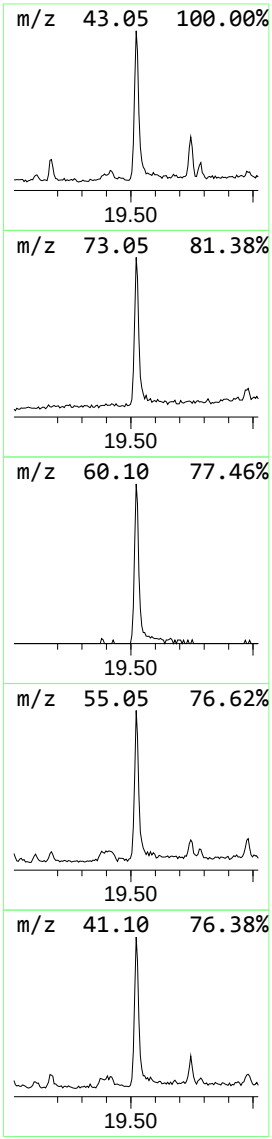
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	7.28 ng	136240	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-2

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

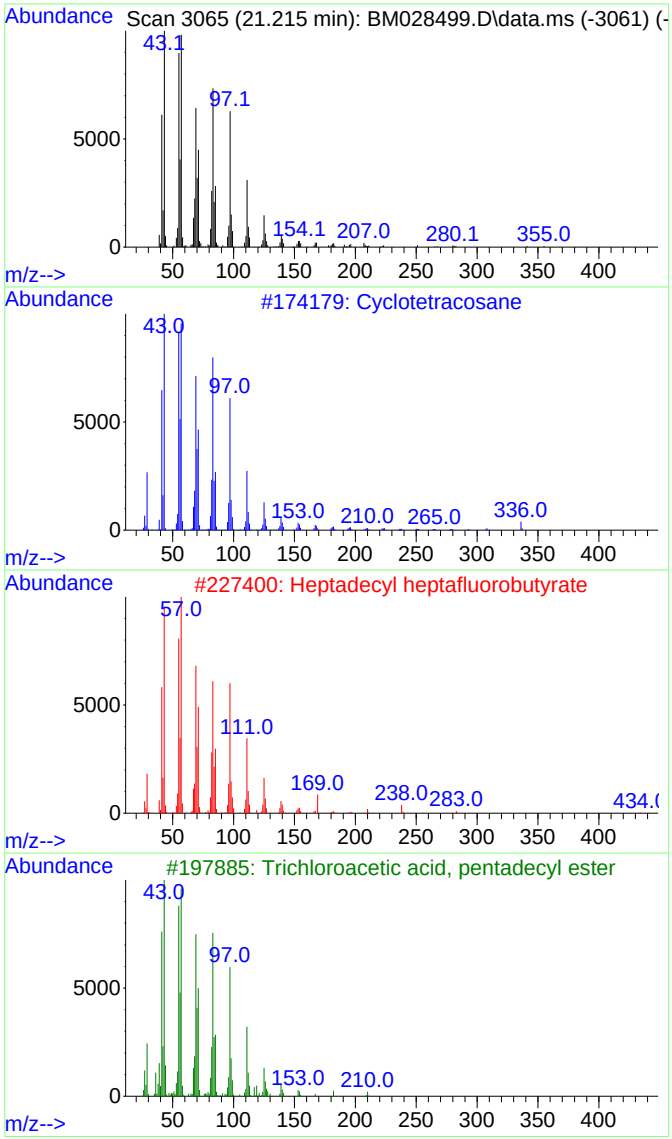
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

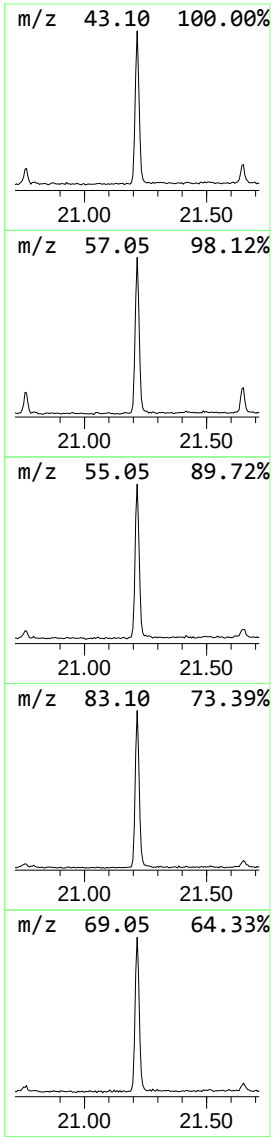
****

Peak Number 6 Cyclotetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	14.14 ng	264632	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028499.D
Acq On : 21 Jan 2021 21:44
Operator : CG/JU
Sample : M1157-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2

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
Diethyl carbitol	7.610	3.3	ng	28257	1	8.016	169939	20.0
unknown12.440	12.440	2.0	ng	23393	2	10.834	233131	20.0
2,4,7,9-Tetrame...	13.545	5.4	ng	77962	3	14.657	286913	20.0
n-Hexadecanoic ...	18.263	13.9	ng	222573	4	17.386	320931	20.0
Octadecanoic acid	19.521	7.3	ng	136240	5	21.515	374272	20.0
Cyclotetracosane	21.215	14.1	ng	264632	5	21.515	374272	20.0