LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0024-SITE-WATER-045

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_G\METHODS\8270-BG012121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.691	393	400	413	rBV	495316	827601	21.00%	4.497%
2	7.284	663	671	684	rBV	344670	648264	16.45%	3.522%
3	8.142	807	817	825	rBV	193490	323279	8.20%	1.757%
4	9.305	1002	1015	1023	rBV	600413	1071109	27.18%	5.820%
5	10.956	1289	1296	1305	rBV	247056	436391	11.07%	2.371%
6	13.388	1702	1710	1717	rBV	1569280	2437901	61.86%	13.246%
7	14.763	1937	1944	1953	rVB2	409647	643083	16.32%	3.494%
8	16.244	2190	2196	2210	rVB	1499718	2303978	58.46%	12.519%
9	17.507	2404	2411	2419	rBV	550667	859310	21.81%	4.669%
10	18.388	2555	2561	2569	rBV2	329975	474115	12.03%	2.576%
11	18.459	2570	2573	2579	rVB	36458	55875	1.42%	0.304%
12	18.899	2644	2648	2653	rBV	29320	45533	1.16%	0.247%
13	19.093	2677	2681	2684	rBV3	32787	41335	1.05%	0.225%
14	19.158	2688	2692	2697	rBV	234552	283561	7.20%	1.541%
15	19.246	2702	2707	2711	rVV	65606	86028	2.18%	0.467%
16	19.652	2771	2776	2787	rBV	218561	314590	7.98%	1.709%
17	19.787	2796	2799	2807	rVB	74898	92951	2.36%	0.505%
18	20.110	2848	2854	2859	rBV	2954879	3940860	100.00%	21.412%
19	20.315	2884	2889	2895	rBV2	47459	75919	1.93%	0.413%
20	20.797	2967	2971	2975	rVB	93989	124728	3.16%	0.678%
21	20.868	2978	2983	2986	rBV5	23358	44956	1.14%	0.244%
22	21.015	3003	3008	3013	rBV	452092	545389	13.84%	2.963%
23	21.062	3013	3016	3021	rVV	101230	123570	3.14%	0.671%
24	21.132	3024	3028	3036	rVB3	39098	64248	1.63%	0.349%
25	21.420	3072	3077	3084	rBV	233153	323058	8.20%	1.755%
26	21.579	3101	3104	3111	rVB2	44223	64767	1.64%	0.352%
27	21.673	3118	3120	3124	rVB2	43240	51184	1.30%	0.278%
28	21.784	3132	3139	3147	rVB	625345	1045747	26.54%	5.682%
29	22.630	3278	3283	3292	rVB7	29719	68306	1.73%	0.371%
30	25.080	3691	3700	3710	rBV2	348054	986861	25.04%	5.362%

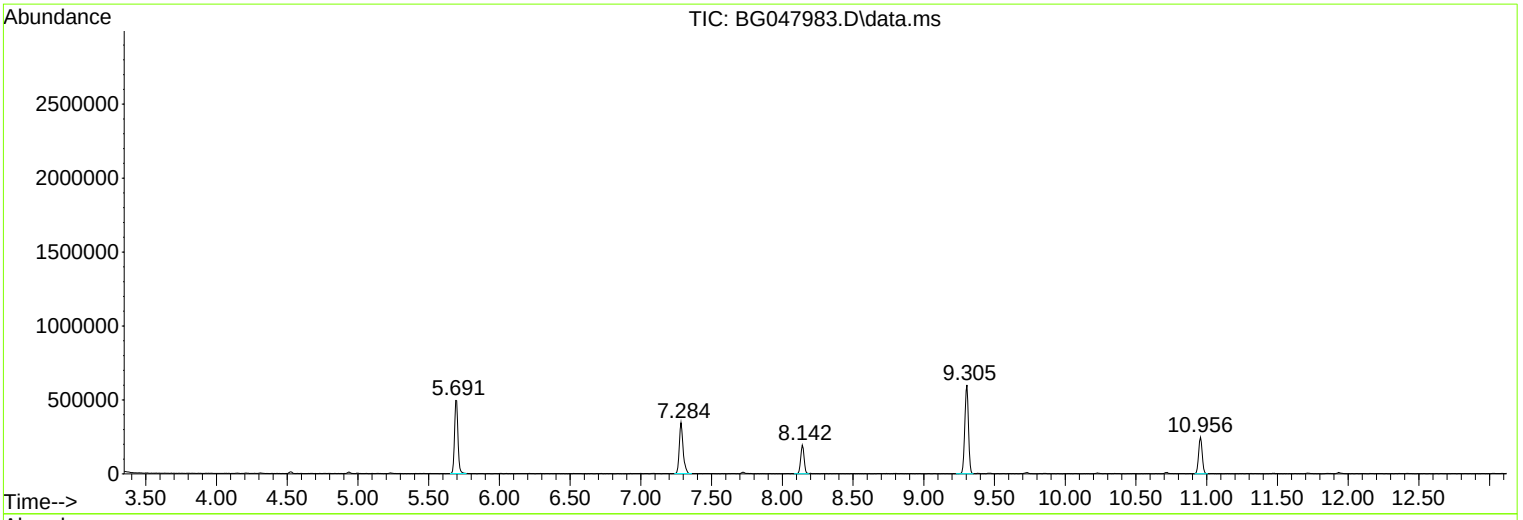
Sum of corrected areas: 18404497

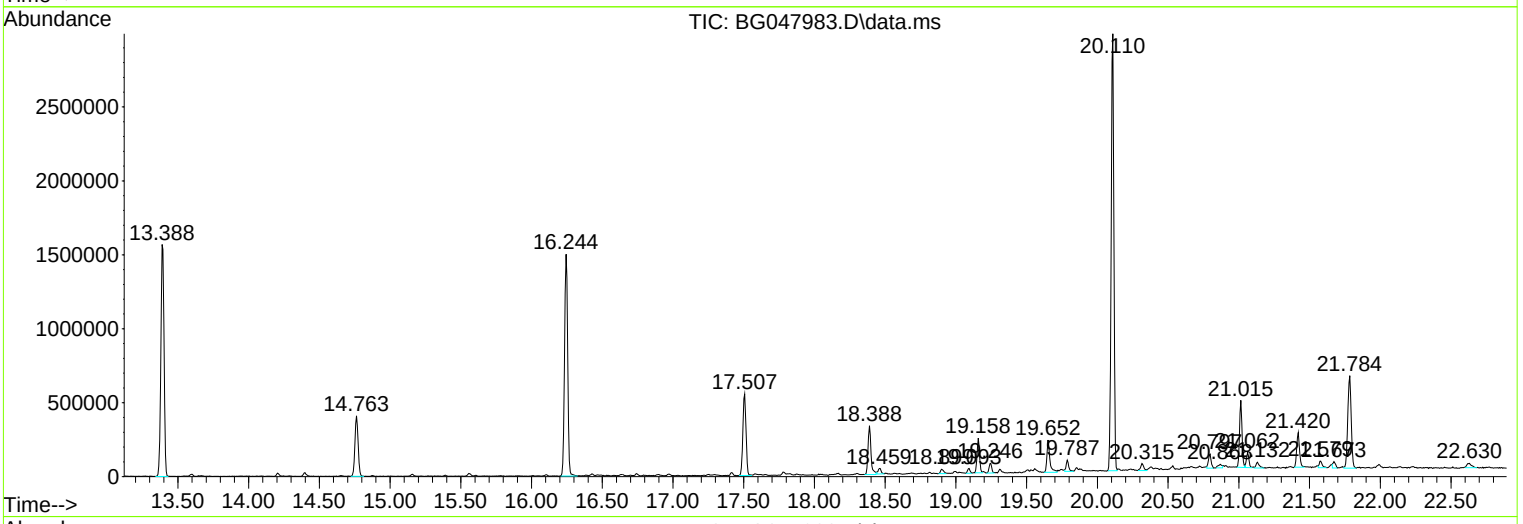
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

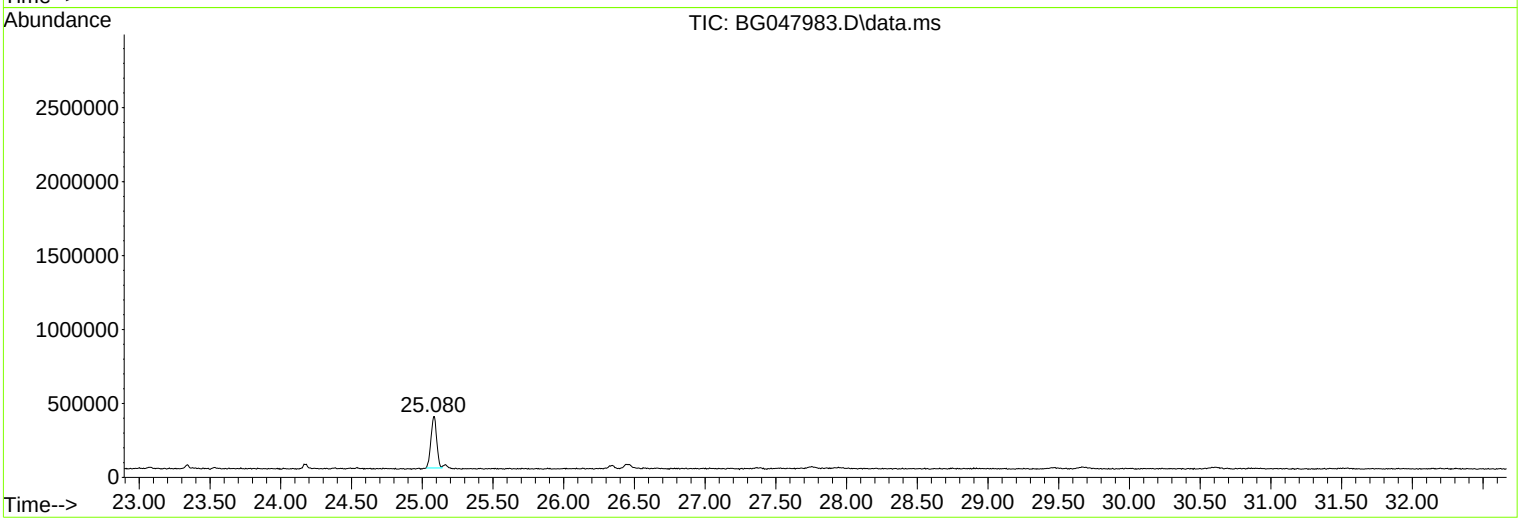
Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

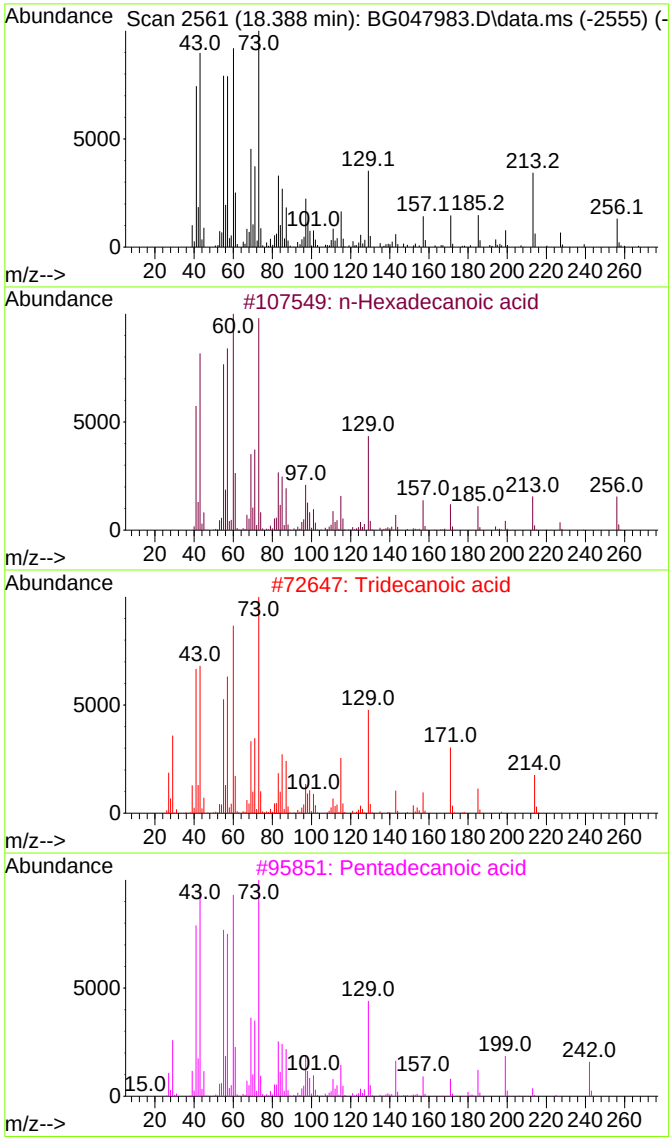
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

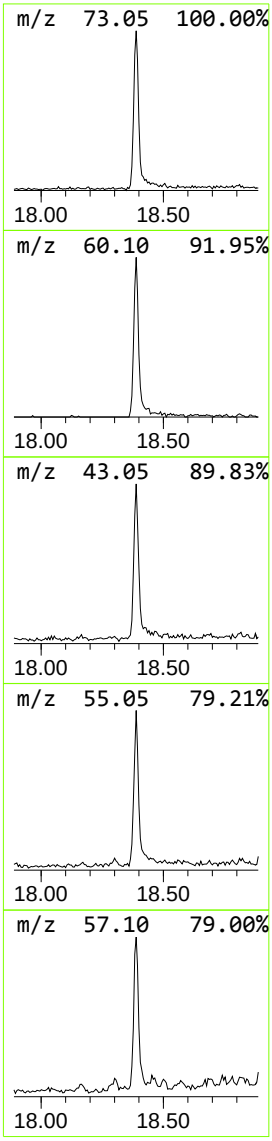
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.388	11.03 ng	474115	Phenanthrene-d10	17.507

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	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

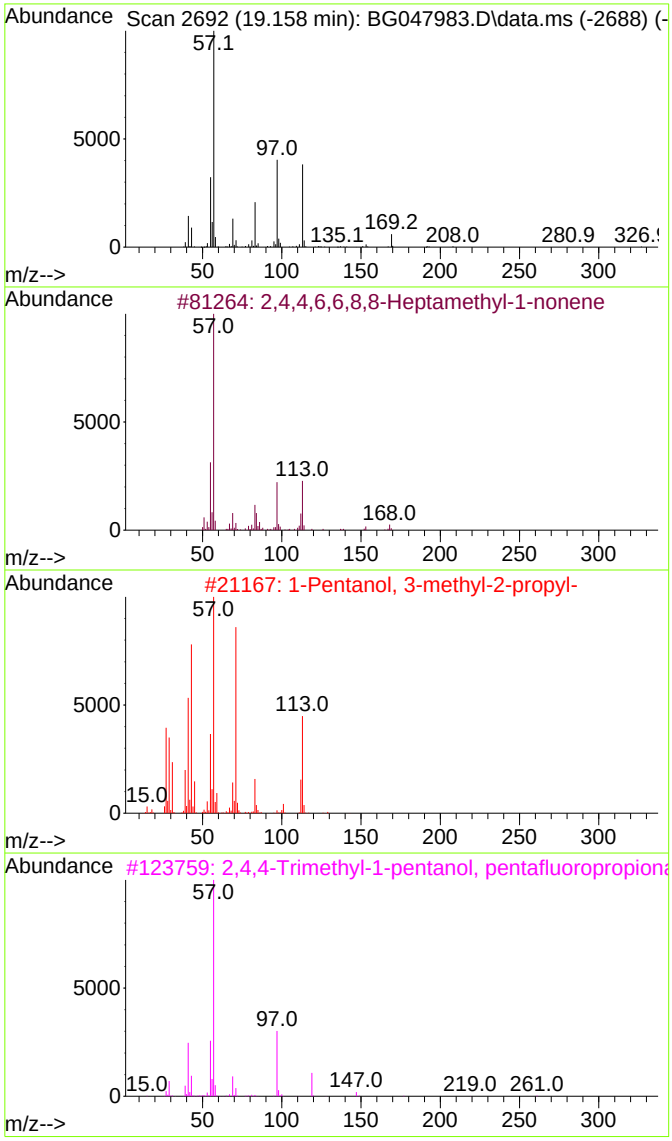
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

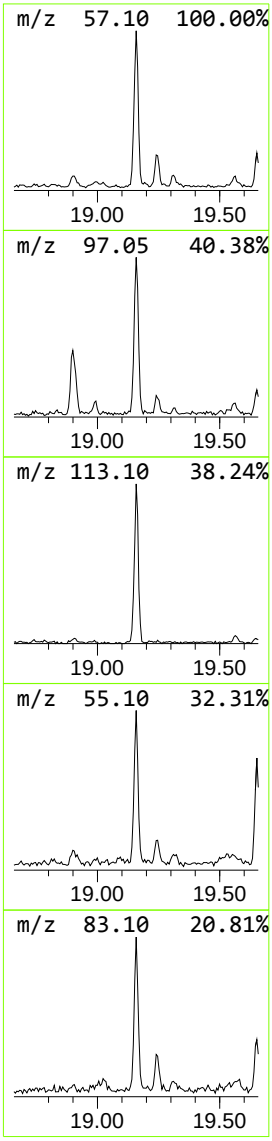
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.158	6.60 ng	283561	Phenanthrene-d10	17.507

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	59
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	50
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	43
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

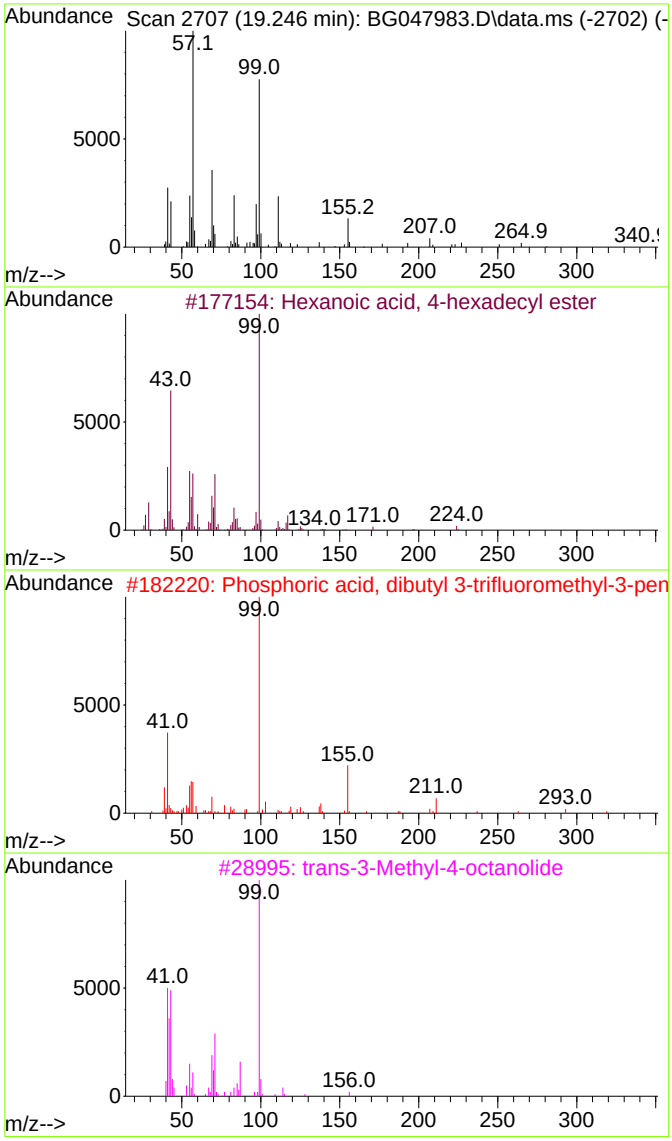
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

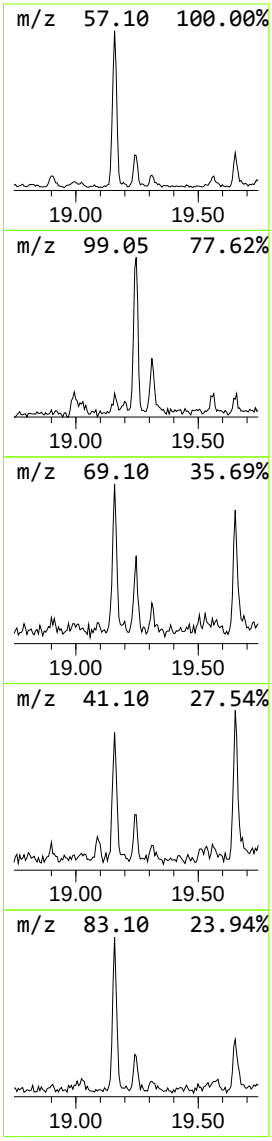
****

Peak Number 3 unknown19.246 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.246	2.00 ng	86028	Phenanthrene-d10	17.507

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	38
2	Phosphoric acid, dibutyl 3-trifl...	348	C14H28F3O4P	1000298-93-8	38
3	trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	38
4	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1000279-29-7	37
5	4-Octen-3-ol, 2,2-dimethyl-	156	C10H20O	053960-44-4	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

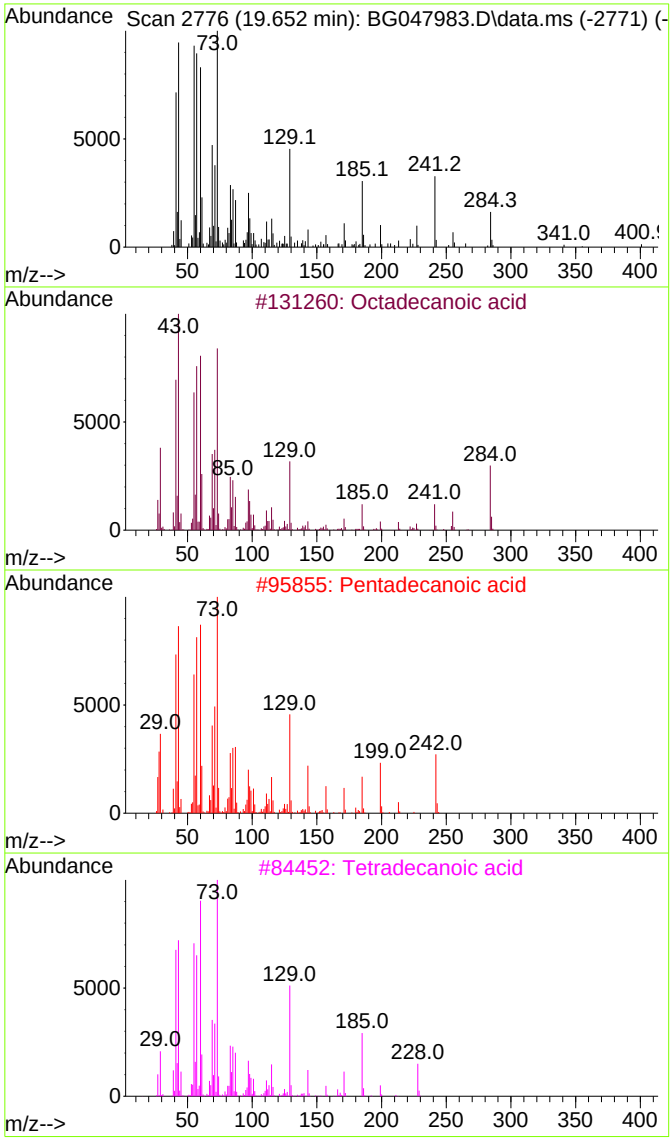
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

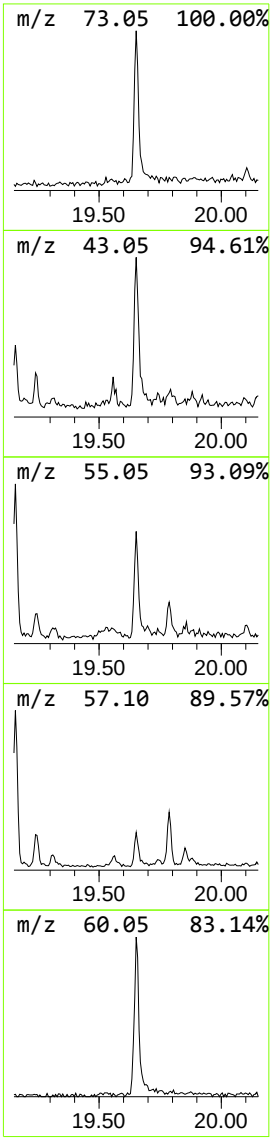
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.651	6.02 ng	314590	Chrysene-d12	21.784

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

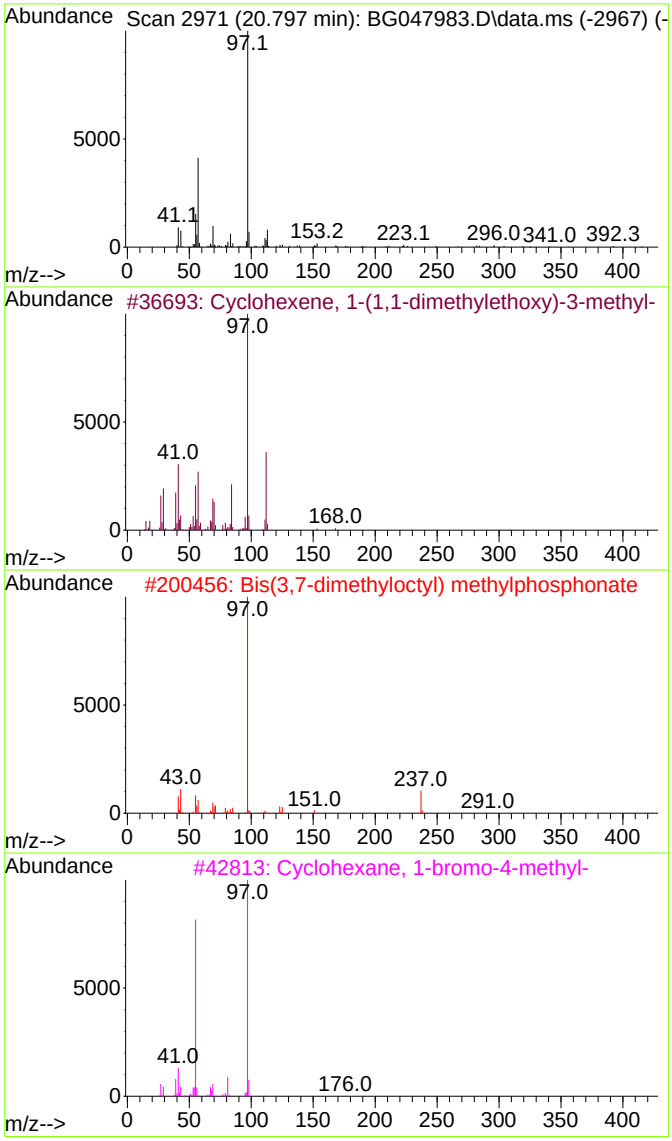
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

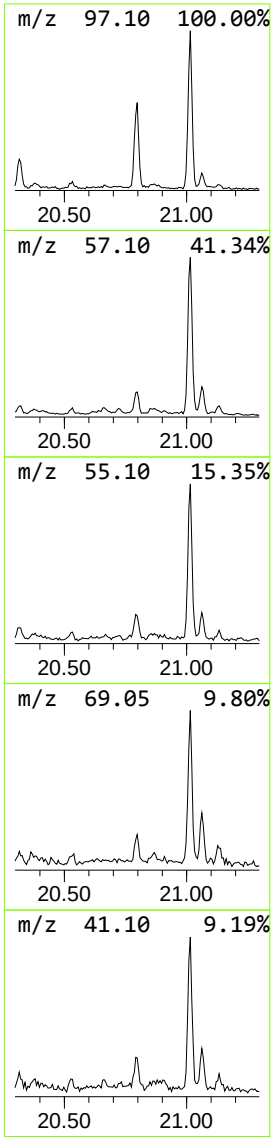
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexene, 1-(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.797	2.39 ng	124728	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-(1,1-dimethyletho...	168	C11H20O	040648-24-6	64
2	Bis(3,7-dimethyloctyl) methylpho...	376	C21H45O3P	1000298-35-2	64
3	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	59
4	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
5	2-Pyrazoline, 1-isobutyl-3-methyl-	140	C8H16N2	026964-53-4	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

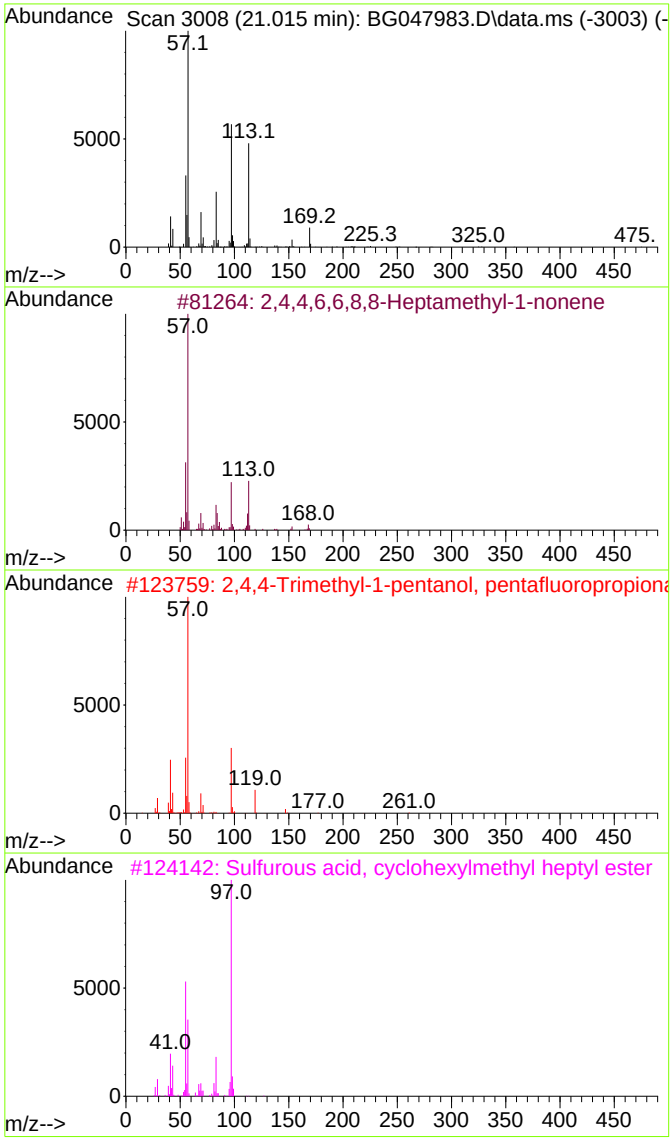
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

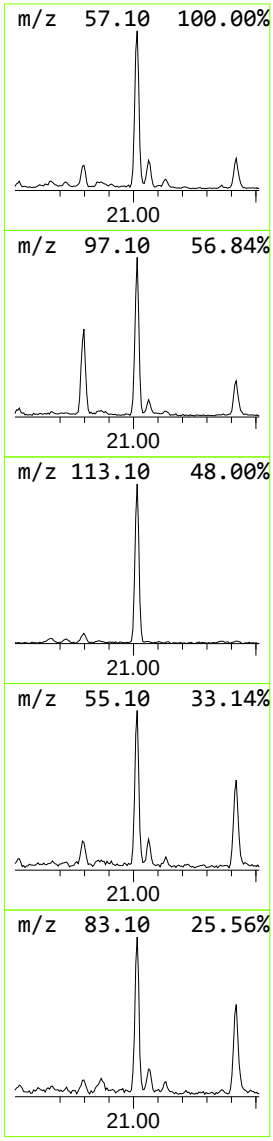
****

Peak Number 6 unknown21.015 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.015	10.43 ng	545389	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	35
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27
5	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

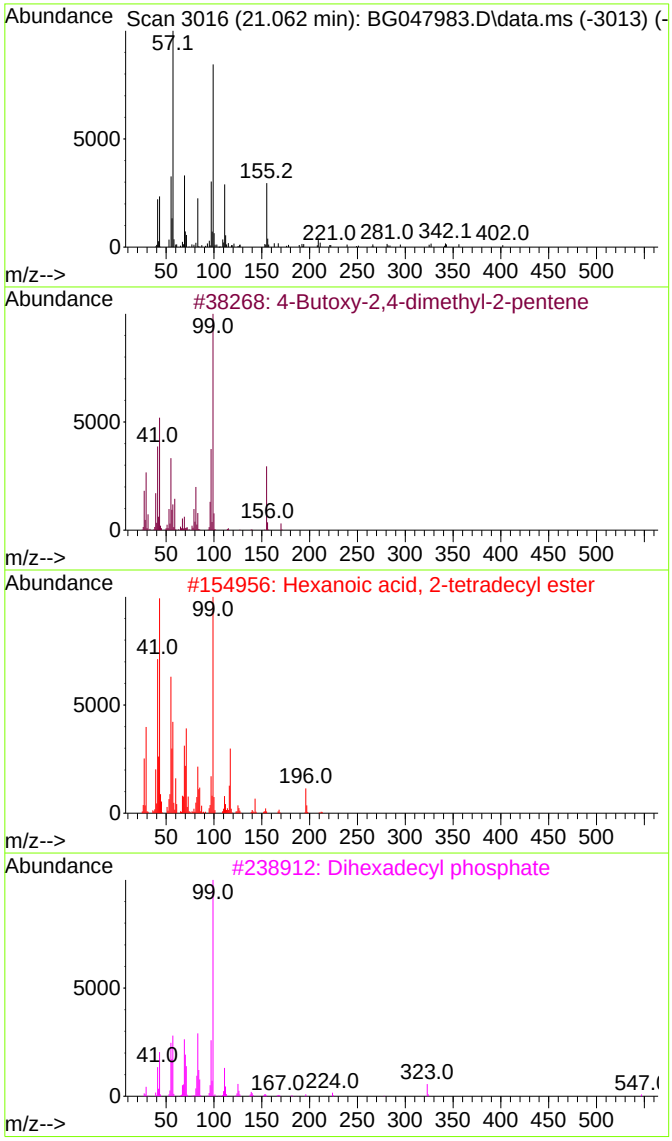
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

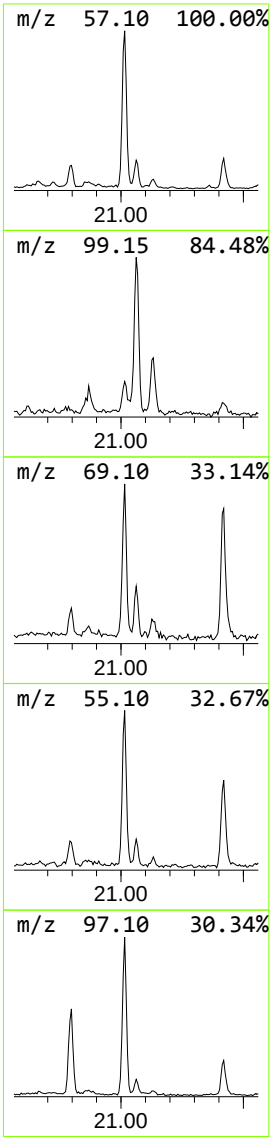
****

Peak Number 7 unknown21.062 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	2.36 ng	123570	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42
2	Hexanoic acid, 2-tetradecyl ester	312	C20H40O2	055193-21-0	38
3	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	37
4	N-Phenyl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	35
5	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0024-SITE-WATER-045

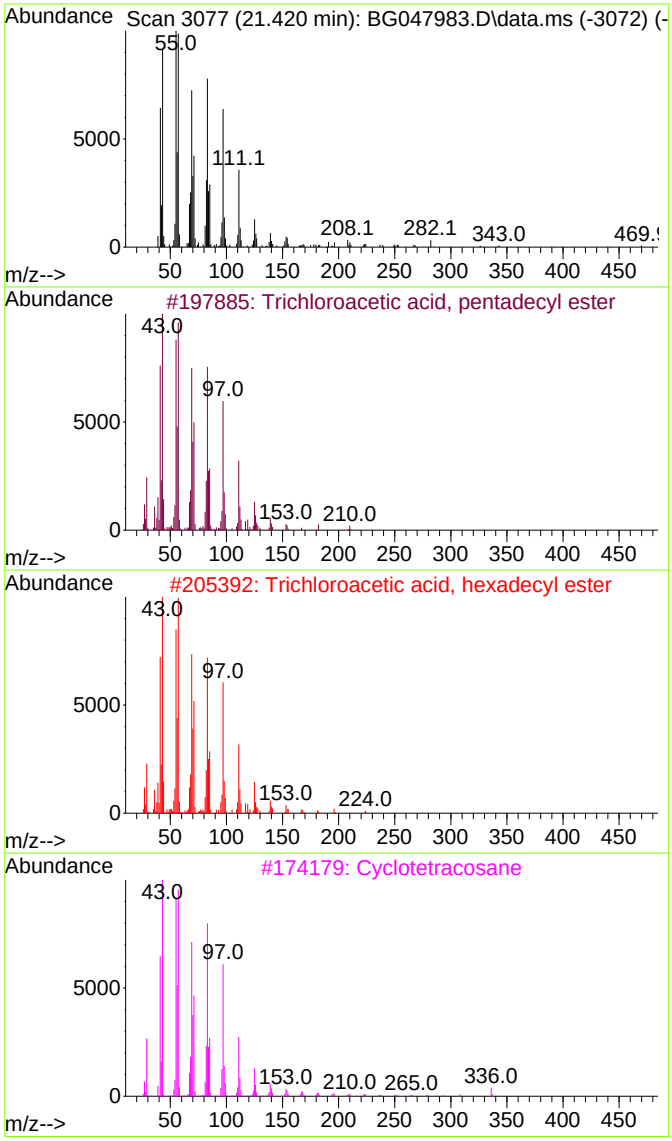
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

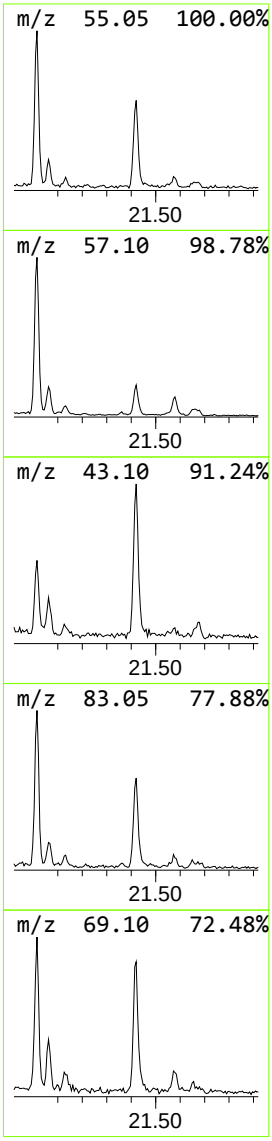
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.420	6.18 ng	323058	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047983.D
Acq On : 22 Jan 2021 18:19
Operator : CG/JU
Sample : M1191-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0024-SITE-WATER-045

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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
n-Hexadecanoic ...	18.388	11.0	ng	474115	4	17.507	859310	20.0
2,4,4,6,6,8,8-H...	19.158	6.6	ng	283561	4	17.507	859310	20.0
unknown19.246	19.246	2.0	ng	86028	4	17.507	859310	20.0
Octadecanoic acid	19.651	6.0	ng	314590	5	21.784	1045750	20.0
Cyclohexene, 1-...	20.797	2.4	ng	124728	5	21.784	1045750	20.0
unknown21.015	21.015	10.4	ng	545389	5	21.784	1045750	20.0
unknown21.062	21.062	2.4	ng	123570	5	21.784	1045750	20.0
Trichloroacetic...	21.420	6.2	ng	323058	5	21.784	1045750	20.0