LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047968.D
Acq On : 22 Jan 2021 00:47
Operator : CG/JU
Sample : M1191-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0027-SITE-WATER-051

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: BG047968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.702	394	402	411	rBV	529050	855095	23.33%	4.779%
2	7.288	664	672	682	rBV	374987	698330	19.05%	3.903%
3	8.146	810	818	825	rBV	177912	304025	8.30%	1.699%
4	9.309	1006	1016	1024	rVB	598785	1049172	28.63%	5.863%
5	10.960	1288	1297	1304	rBV	236940	420936	11.49%	2.352%
6	13.399	1703	1712	1719	rVB	1579389	2433871	66.41%	13.602%
7	14.768	1938	1945	1952	rVB	412628	618137	16.87%	3.455%
8	16.248	2190	2197	2208	rBV	1374798	2129038	58.09%	11.898%
9	17.511	2405	2412	2420	rBV	525155	775451	21.16%	4.334%
10	18.399	2557	2563	2570	rBV	334724	475225	12.97%	2.656%
11	18.469	2570	2575	2579	rVB	39796	57837	1.58%	0.323%
12	18.910	2645	2650	2654	rBV2	33116	51907	1.42%	0.290%
13	19.168	2688	2694	2698	rBV	218987	285502	7.79%	1.596%
14	19.251	2704	2708	2712	rBV	69037	84815	2.31%	0.474%
15	19.568	2759	2762	2772	rVB2	30644	51453	1.40%	0.288%
16	19.662	2772	2778	2788	rBV	229174	351135	9.58%	1.962%
17	19.797	2797	2801	2808	rVB	66273	85594	2.34%	0.478%
18	20.114	2849	2855	2861	rBV	2894746	3664943	100.00%	20.482%
19	20.326	2887	2891	2895	rVB	47134	63698	1.74%	0.356%
20	20.802	2968	2972	2979	rVB	96700	128957	3.52%	0.721%
21	20.878	2979	2985	2990	rBV4	29181	68238	1.86%	0.381%
22	21.025	3005	3010	3014	rBV	414695	532307	14.52%	2.975%
23	21.072	3014	3018	3023	rVV	102238	125804	3.43%	0.703%
24	21.143	3026	3030	3038	rVB4	39345	59449	1.62%	0.332%
25	21.430	3074	3079	3088	rVB	245595	349314	9.53%	1.952%
26	21.589	3102	3106	3115	rVB	43493	60253	1.64%	0.337%
27	21.789	3134	3140	3149	rVB2	513757	886671	24.19%	4.955%
28	22.635	3280	3284	3292	rVB3	36162	69678	1.90%	0.389%
29	23.358	3402	3407	3412	rVB2	35335	57040	1.56%	0.319%
30	24.192	3545	3549	3556	rVB3	41787	80167	2.19%	0.448%
31	25.097	3694	3703	3713	rBV	308040	854579	23.32%	4.776%
32	25.191	3715	3719	3725	rVB6	34066	67818	1.85%	0.379%
33	26.483	3935	3939	3953	rVB6	36267	97084	2.65%	0.543%

Sum of corrected areas: 17893523

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Misc :
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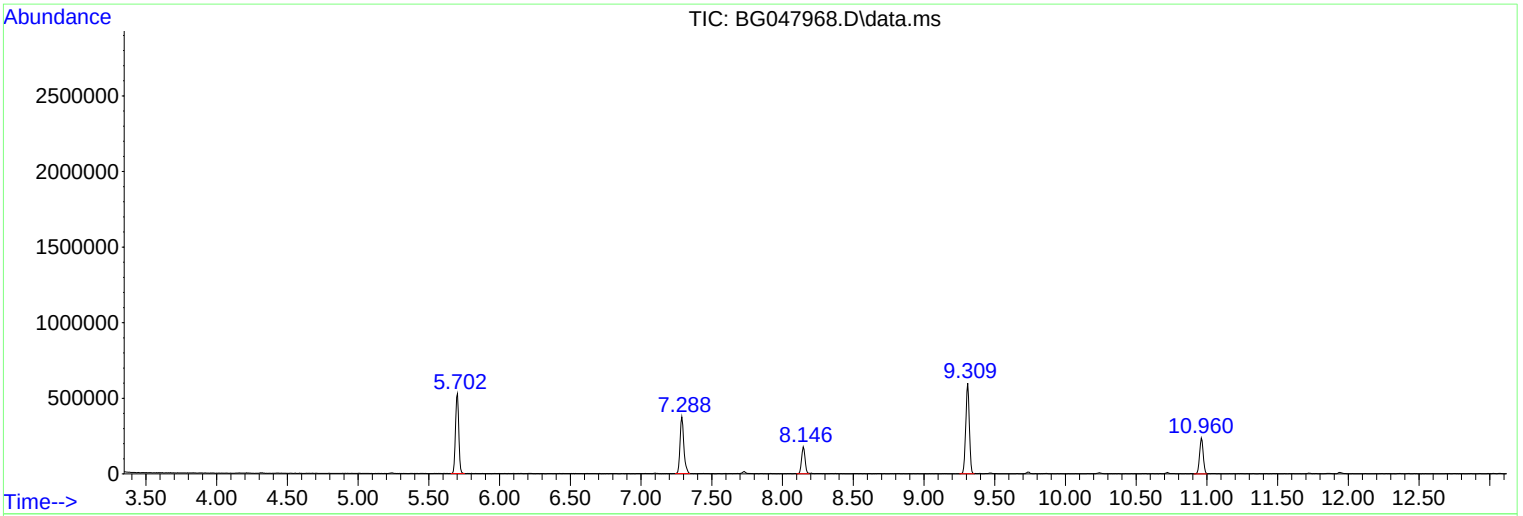
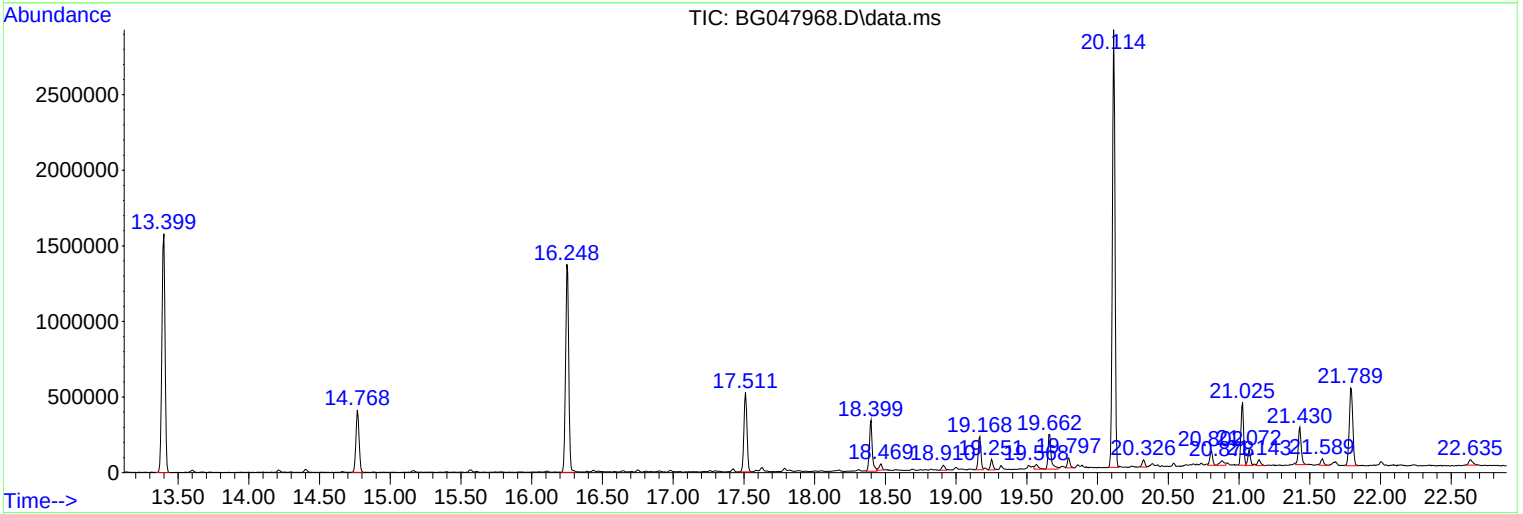
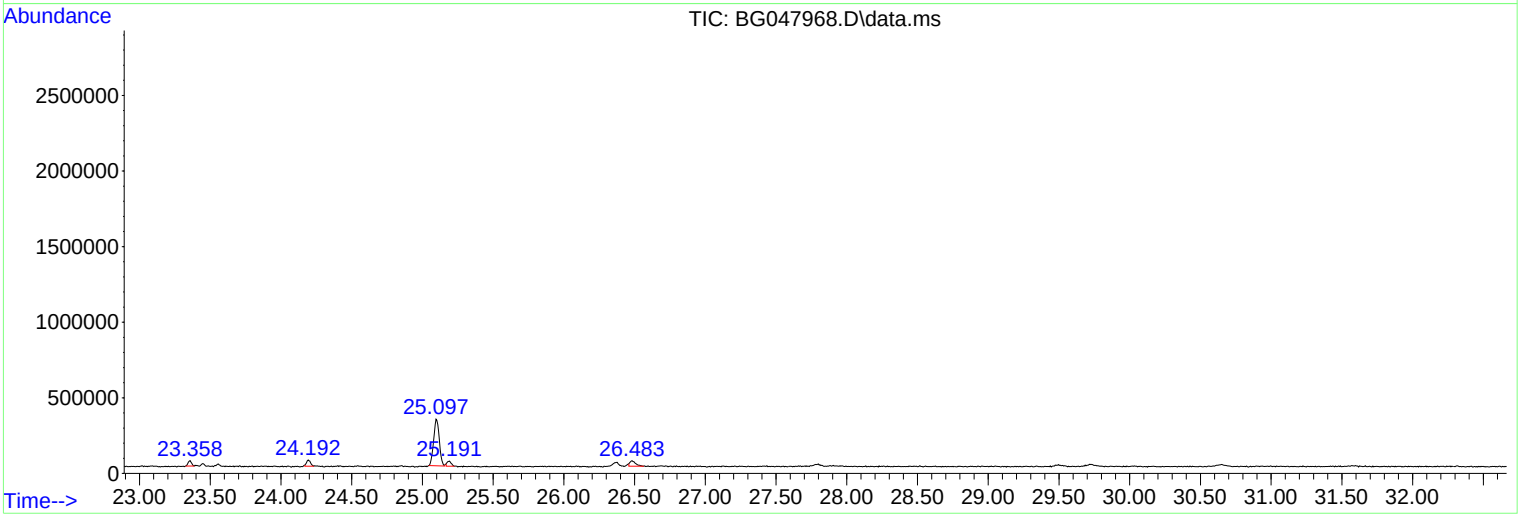
Instrument :
BNA_G
ClientSampleId :
0027-SITE-WATER-051

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







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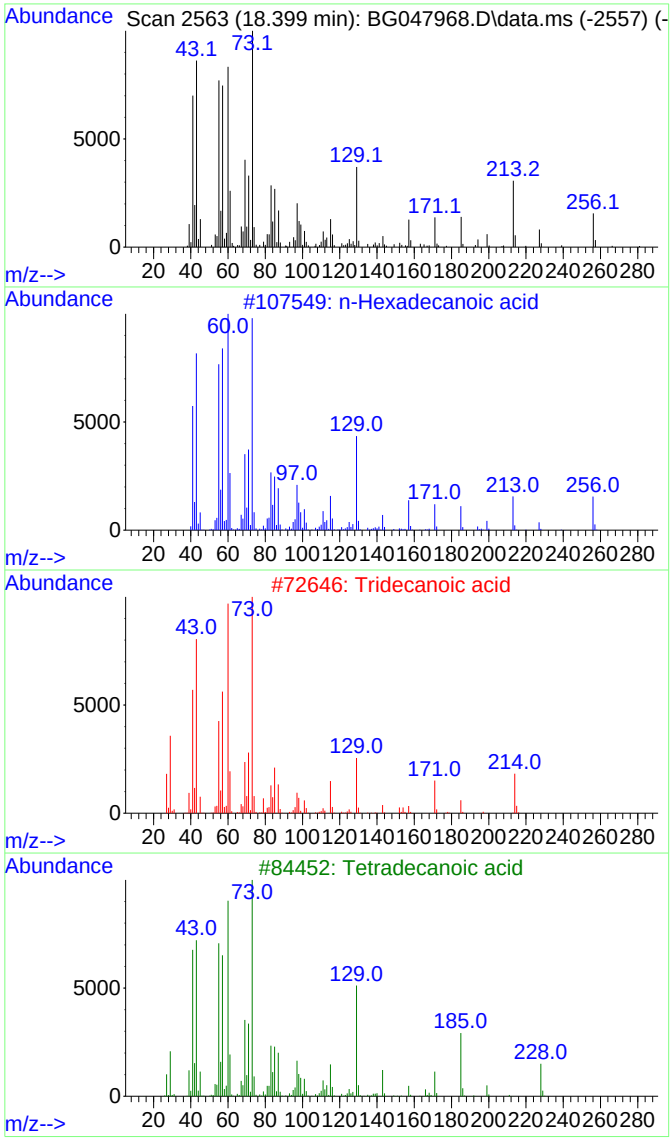
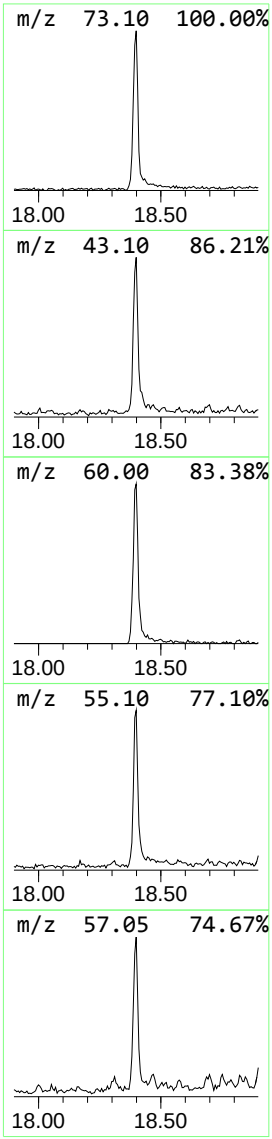
Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.399	12.26 ng	475225	Phenanthrene-d10	17.512

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Data File : BG047968.D
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Operator : CG/JU
Sample : M1191-09
Misc :
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Instrument : BNA_G
ClientSampleId : 0027-SITE-WATER-051

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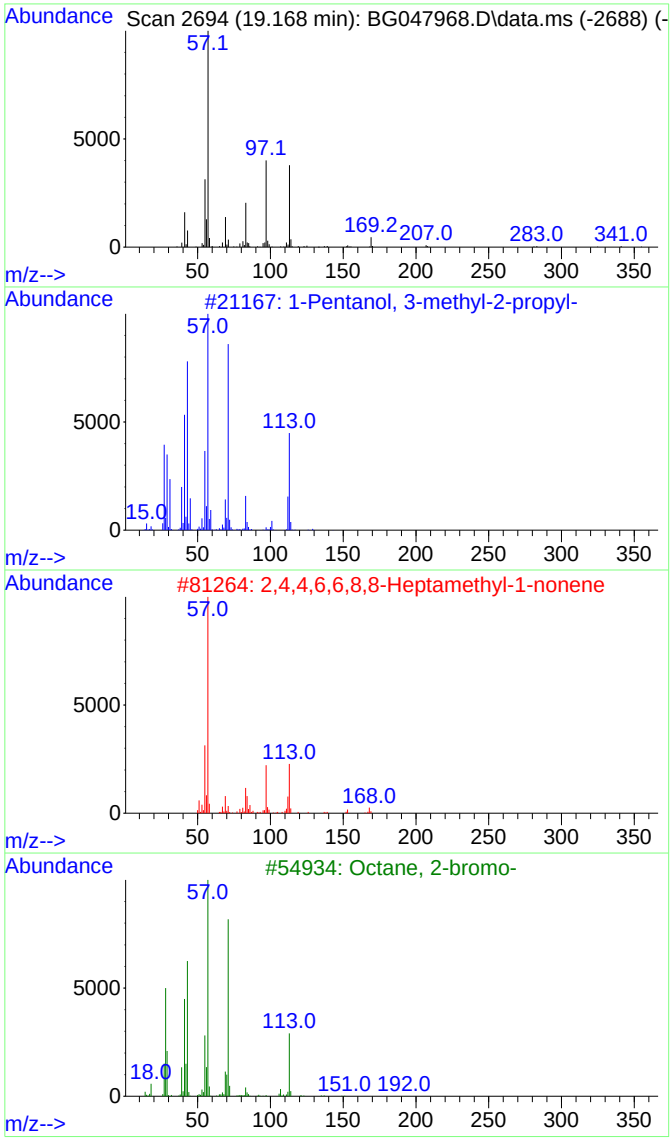
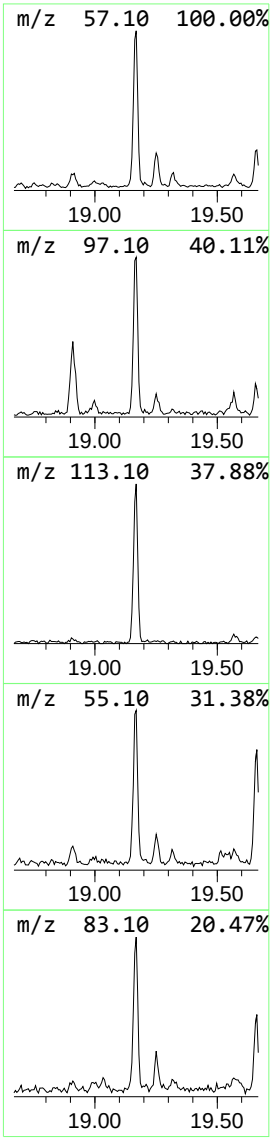
Peak Number 2 unknown19.168 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.168	7.36 ng	285502	Phenanthrene-d10	17.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	47
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	43
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38





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Operator : CG/JU
Sample : M1191-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0027-SITE-WATER-051

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
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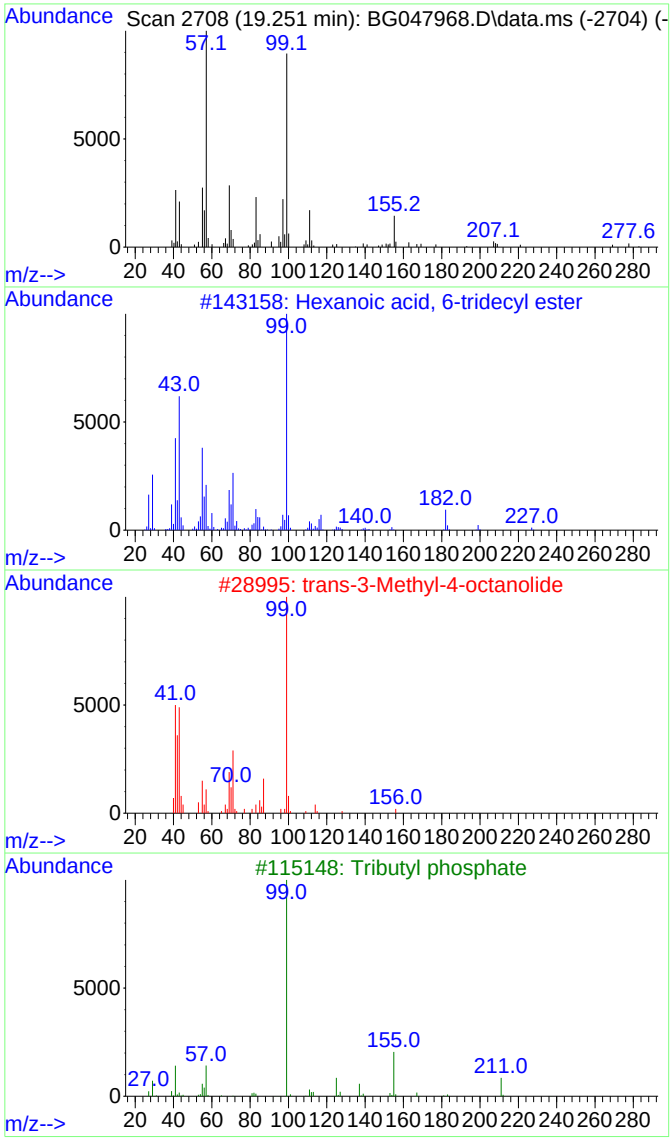
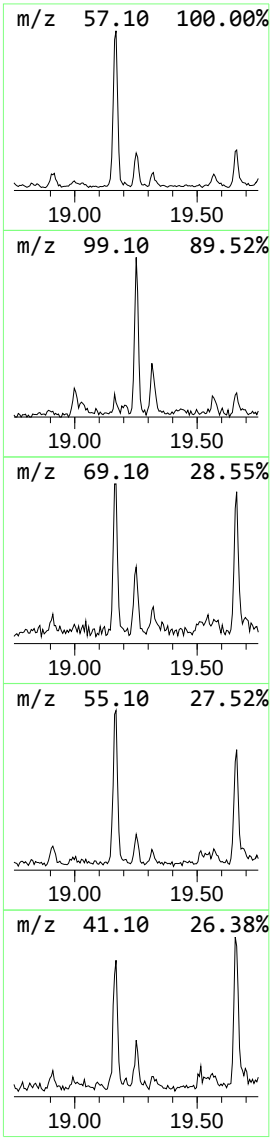
Peak Number 3 unknown19.251 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	2.19 ng	84815	Phenanthrene-d10	17.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	43
2	trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	43
3	Tributyl phosphate	266	C12H27O4P	000126-73-8	38
4	Formaldehyde, dipropylhydrazone	128	C7H16N2	054253-56-4	38
5	Pyrazol-3-one, 5-amino-1-(1-ethy...	169	C8H15N3O	1000316-44-2	38





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Sample : M1191-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0027-SITE-WATER-051

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
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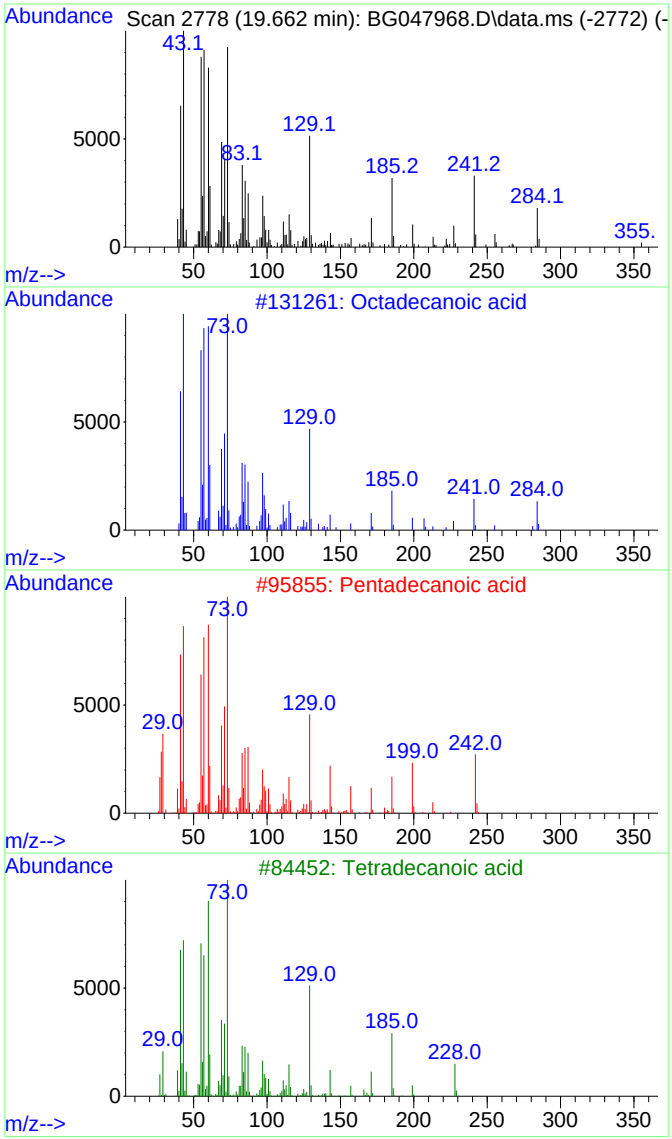
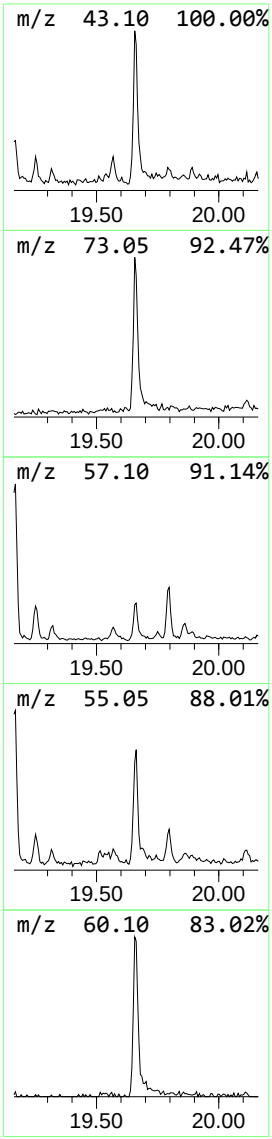
Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.662	7.92 ng	351135	Chrysene-d12	21.789

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	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Instrument :
BNA_G
ClientSampleId :
0027-SITE-WATER-051

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
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TIC Library : C:\Database\NIST11.L
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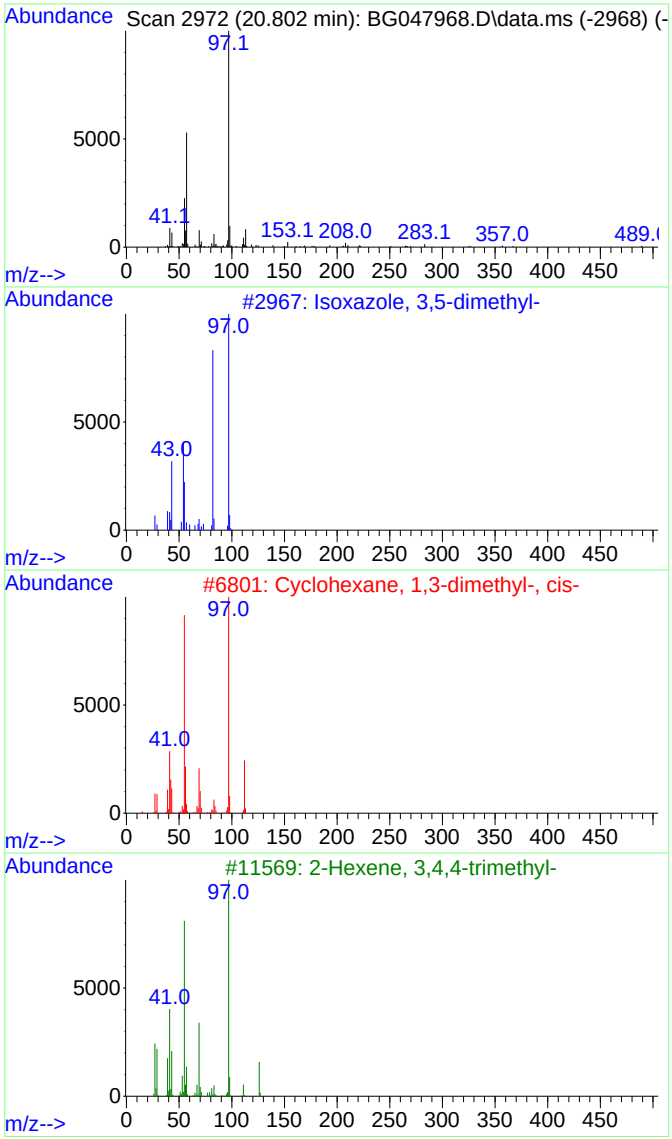
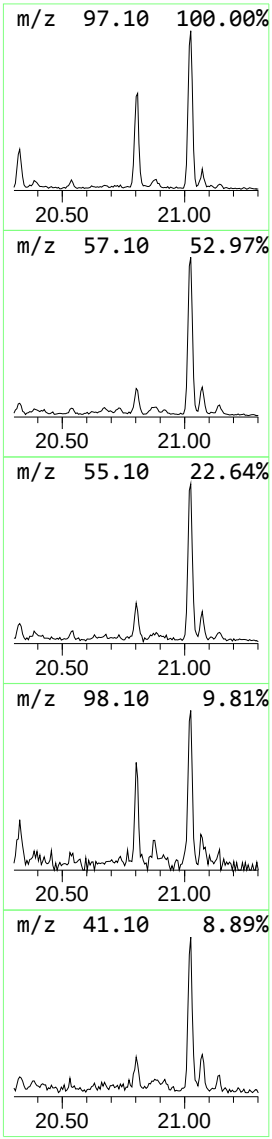
Peak Number 5 Isoxazole, 3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.802	2.91 ng	128957	Chrysene-d12	21.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	64
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	56
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	53
5	4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	53





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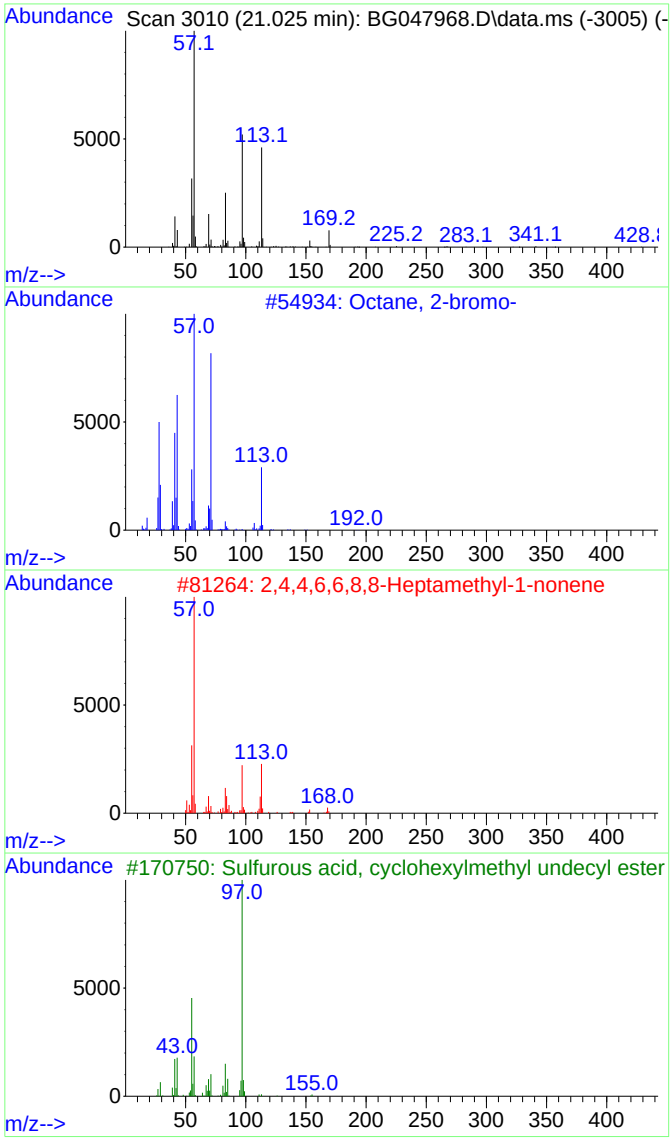
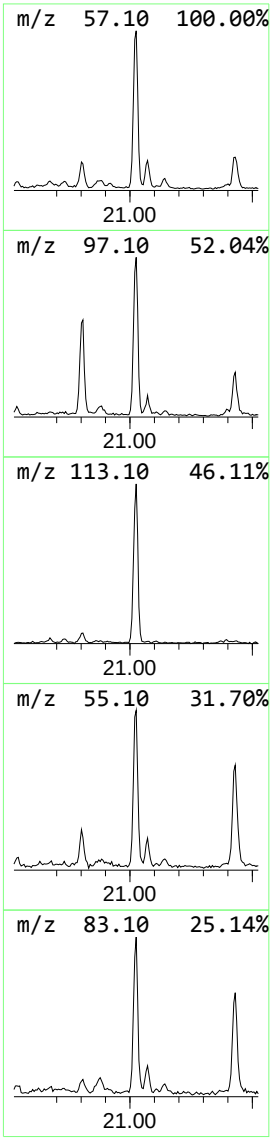
Peak Number 6 unknown21.025 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.025	12.01 ng	532307	Chrysene-d12	21.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
3	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	37
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32





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BNA_G
ClientSampleId :
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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
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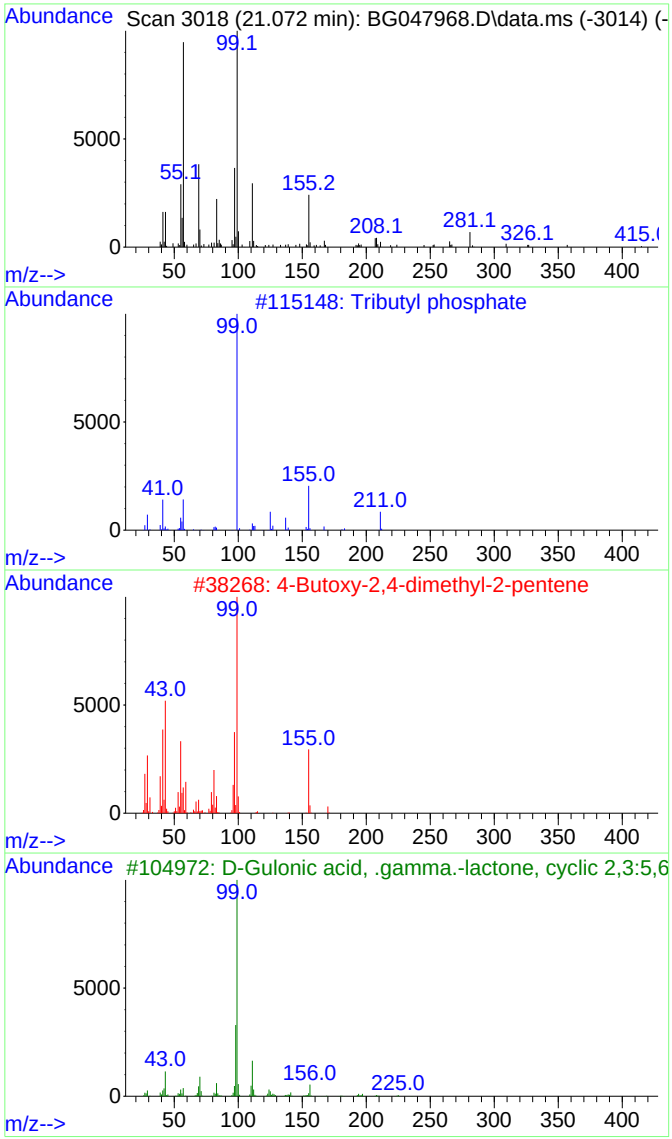
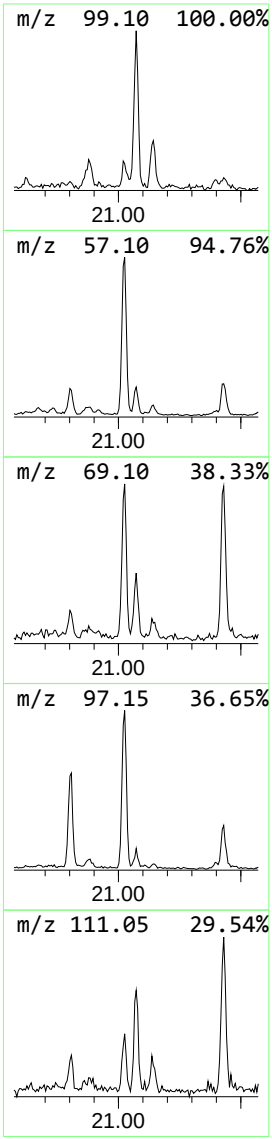
Peak Number 7 unknown21.072 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.072	2.84 ng	125804	Chrysene-d12	21.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	37
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	33
3	D-Gulonic acid, .gamma.-lactone,...	254	C10H16B2O6	074128-60-2	32
4	Ethanedicarboxamide, N-(3,5-dime...	304	C16H24N4O2	346596-53-0	27
5	2H-Pyran-2-one, tetrahydro-4-(2-...	154	C9H14O2	1000153-91-9	25





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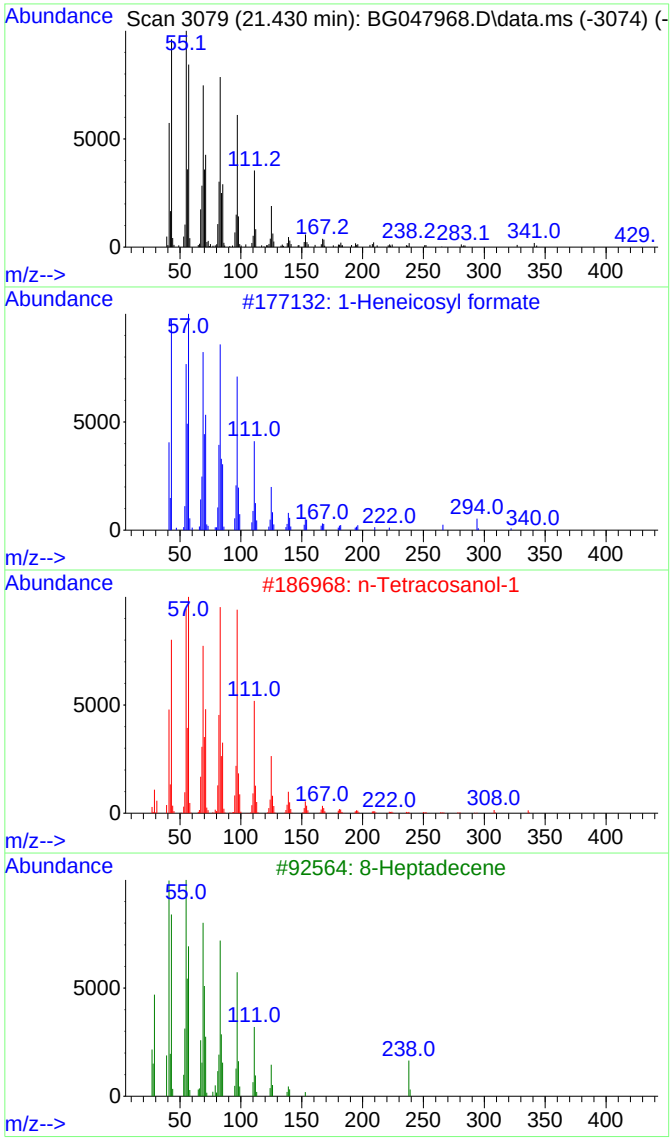
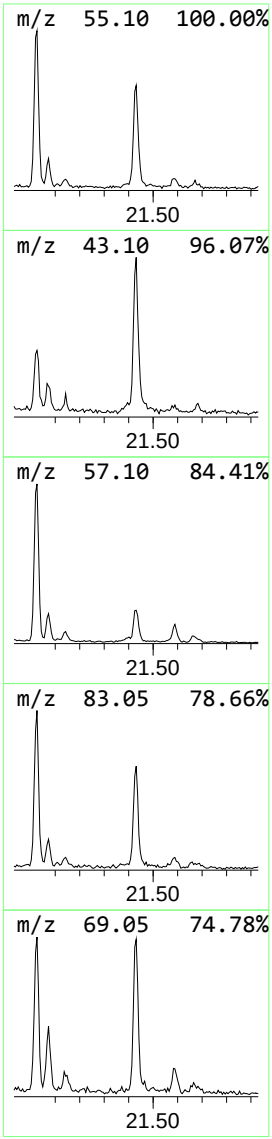
Peak Number 8 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.430	7.88 ng	349314	Chrysene-d12	21.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	8-Heptadecene	238	C17H34	002579-04-6	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047968.D
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Operator : CG/JU
Sample : M1191-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
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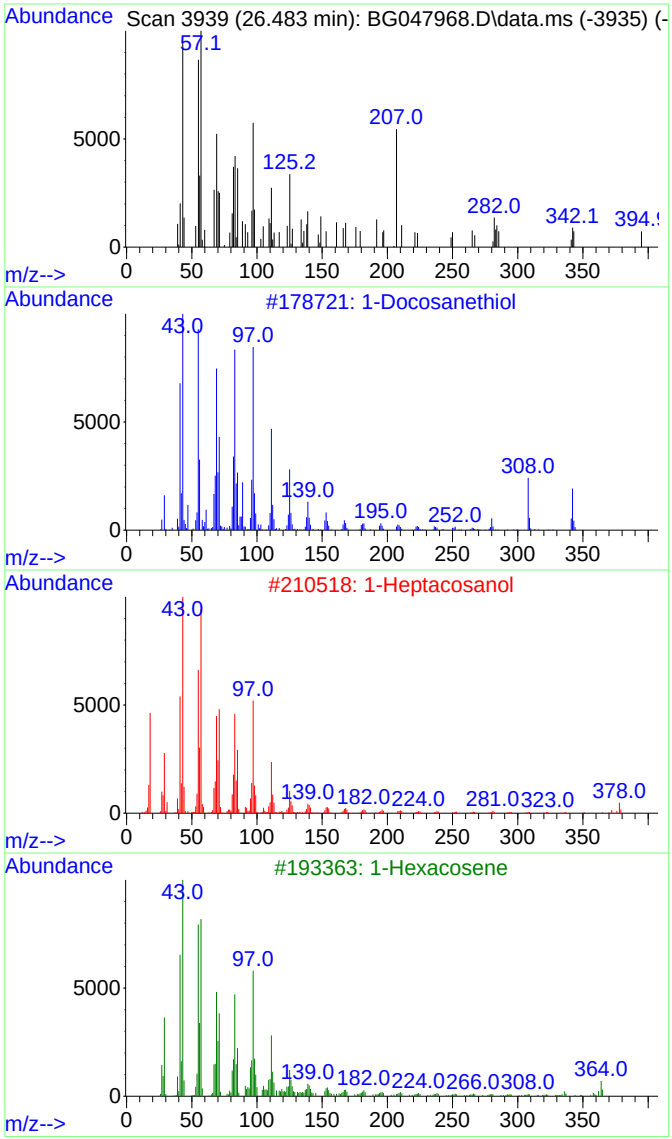
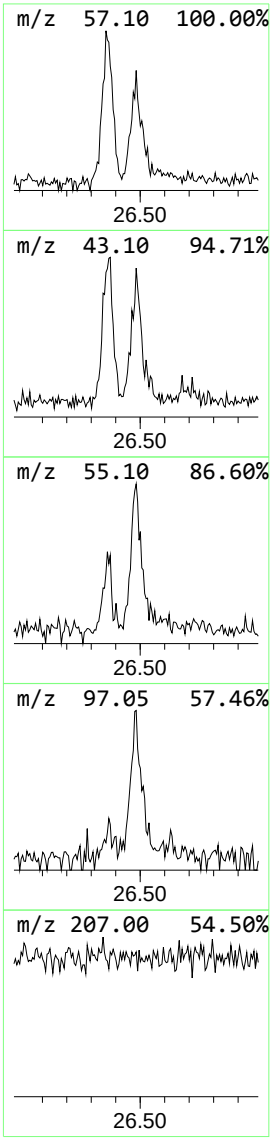
Peak Number 9 1-Docosanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.483	2.27 ng	97084	Perylene-d12	25.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	53
2	1-Heptacosanol	396	C27H56O	002004-39-9	49
3	1-Hexacosene	364	C26H52	018835-33-1	49
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	47
5	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047968.D
Acq On : 22 Jan 2021 00:47
Operator : CG/JU
Sample : M1191-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0027-SITE-WATER-051

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 ...	18.399	12.3	ng	475225	4	17.512	775451	20.0
unknown19.168	19.168	7.4	ng	285502	4	17.512	775451	20.0
unknown19.251	19.251	2.2	ng	84815	4	17.512	775451	20.0
Octadecanoic acid	19.662	7.9	ng	351135	5	21.789	886671	20.0
Isoxazole, 3,5-...	20.802	2.9	ng	128957	5	21.789	886671	20.0
unknown21.025	21.025	12.0	ng	532307	5	21.789	886671	20.0
unknown21.072	21.072	2.8	ng	125804	5	21.789	886671	20.0
1-Heneicosyl fo...	21.430	7.9	ng	349314	5	21.789	886671	20.0
1-Docosanethiol	26.483	2.3	ng	97084	6	25.097	854579	20.0