

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
 Data File : BG047982.D
 Acq On : 22 Jan 2021 17:39
 Operator : CG/JU
 Sample : M1191-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0023-SITE-WATER-044

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: BG047982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.694	394	401	411	rVB	462605	710797	19.56%	4.117%
2	7.281	664	671	682	rVB2	303716	595883	16.40%	3.451%
3	8.139	811	817	824	rBV	163622	280780	7.73%	1.626%
4	9.302	1006	1015	1025	rBV	544576	965885	26.59%	5.594%
5	10.959	1289	1297	1306	rBV	212666	380018	10.46%	2.201%
6	13.391	1702	1711	1718	rBV	1425403	2194692	60.41%	12.711%
7	14.396	1875	1882	1889	rVB5	20468	38525	1.06%	0.223%
8	14.760	1938	1944	1951	rVB	352258	570490	15.70%	3.304%
9	16.247	2189	2197	2208	rBV	1432652	2147182	59.10%	12.436%
10	17.504	2405	2411	2418	rBV	513903	788653	21.71%	4.568%
11	18.391	2556	2562	2570	rBV	350553	519780	14.31%	3.010%
12	18.462	2570	2574	2578	rVB	41288	60329	1.66%	0.349%
13	18.902	2644	2649	2655	rBV	27147	50525	1.39%	0.293%
14	19.090	2677	2681	2686	rVB2	34792	45344	1.25%	0.263%
15	19.161	2686	2693	2697	rBV	218599	290596	8.00%	1.683%
16	19.243	2703	2707	2712	rBV	64743	81396	2.24%	0.471%
17	19.654	2772	2777	2789	rBV	229246	350139	9.64%	2.028%
18	19.790	2796	2800	2807	rVB	65838	85446	2.35%	0.495%
19	20.107	2848	2854	2859	rBV	2794891	3633137	100.00%	21.043%
20	20.318	2886	2890	2895	rVB	42684	52761	1.45%	0.306%
21	20.377	2895	2900	2904	rBV7	23473	41648	1.15%	0.241%
22	20.794	2967	2971	2976	rVB	87463	119072	3.28%	0.690%
23	21.012	3004	3008	3013	rBV	432645	567456	15.62%	3.287%
24	21.065	3013	3017	3022	rVV	101770	127191	3.50%	0.737%
25	21.135	3025	3029	3035	rVB4	38659	64727	1.78%	0.375%
26	21.417	3073	3077	3087	rVB	243326	345409	9.51%	2.001%
27	21.582	3101	3105	3109	rVB	52010	64116	1.76%	0.371%
28	21.670	3116	3120	3126	rVB6	40183	70549	1.94%	0.409%
29	21.781	3133	3139	3148	rVB2	605355	984910	27.11%	5.704%
30	22.627	3279	3283	3293	rVB2	29970	67900	1.87%	0.393%
31	24.179	3541	3547	3551	rBV3	24075	50787	1.40%	0.294%
32	25.089	3692	3702	3712	rBV	320855	919496	25.31%	5.326%

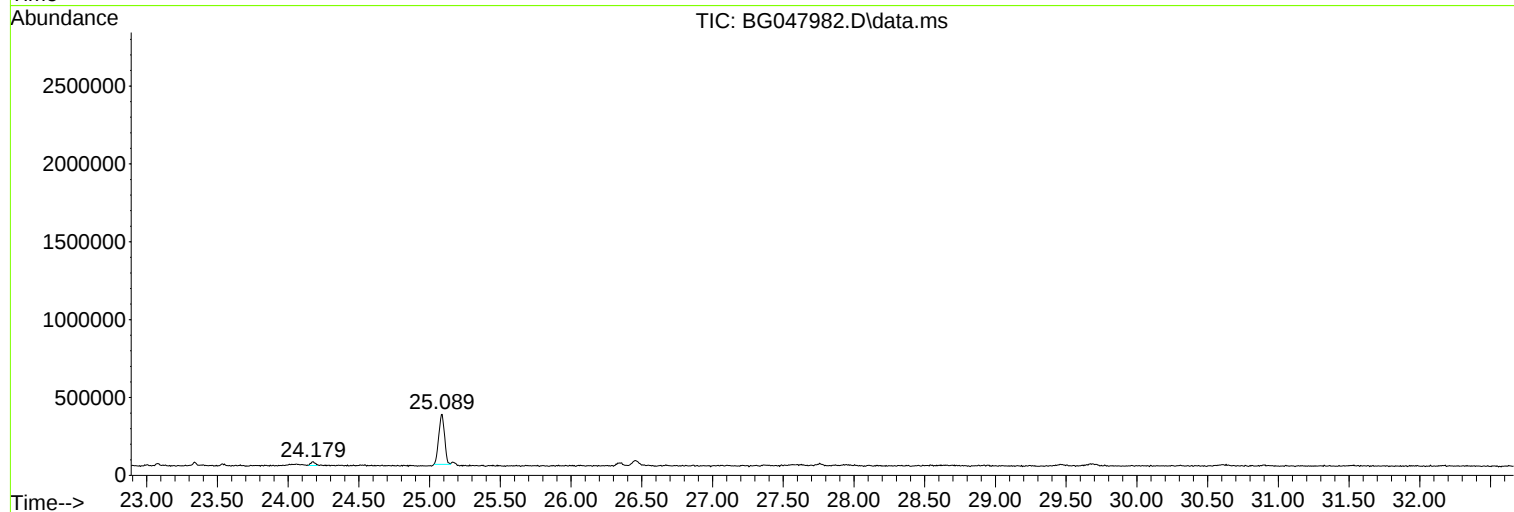
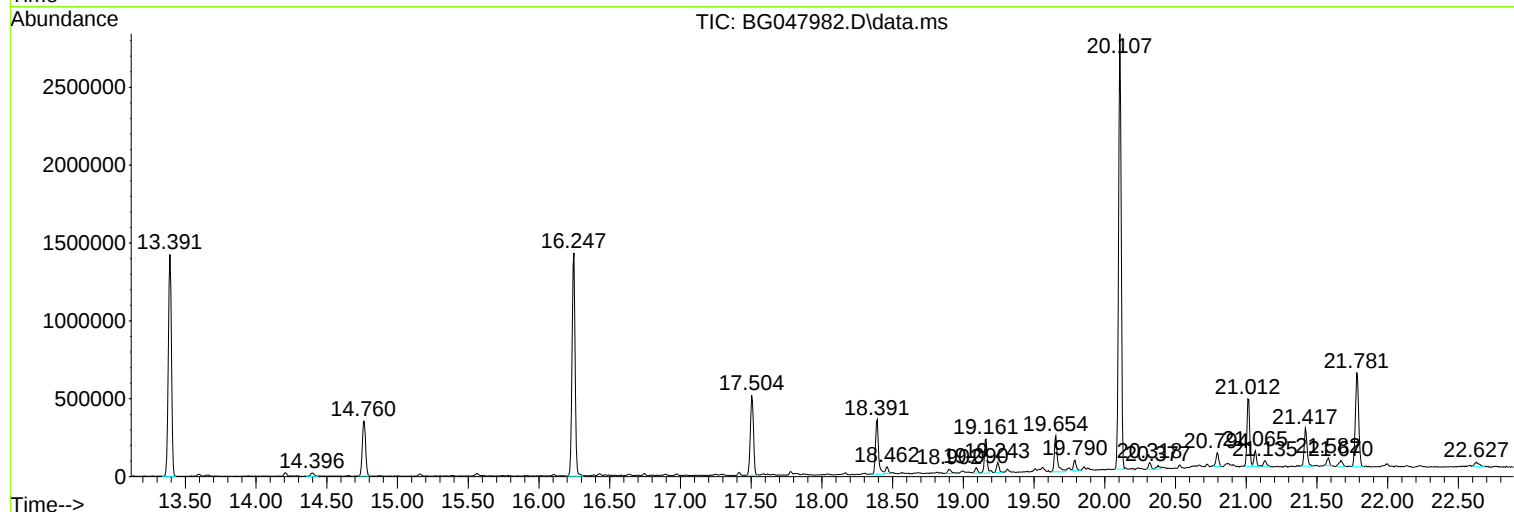
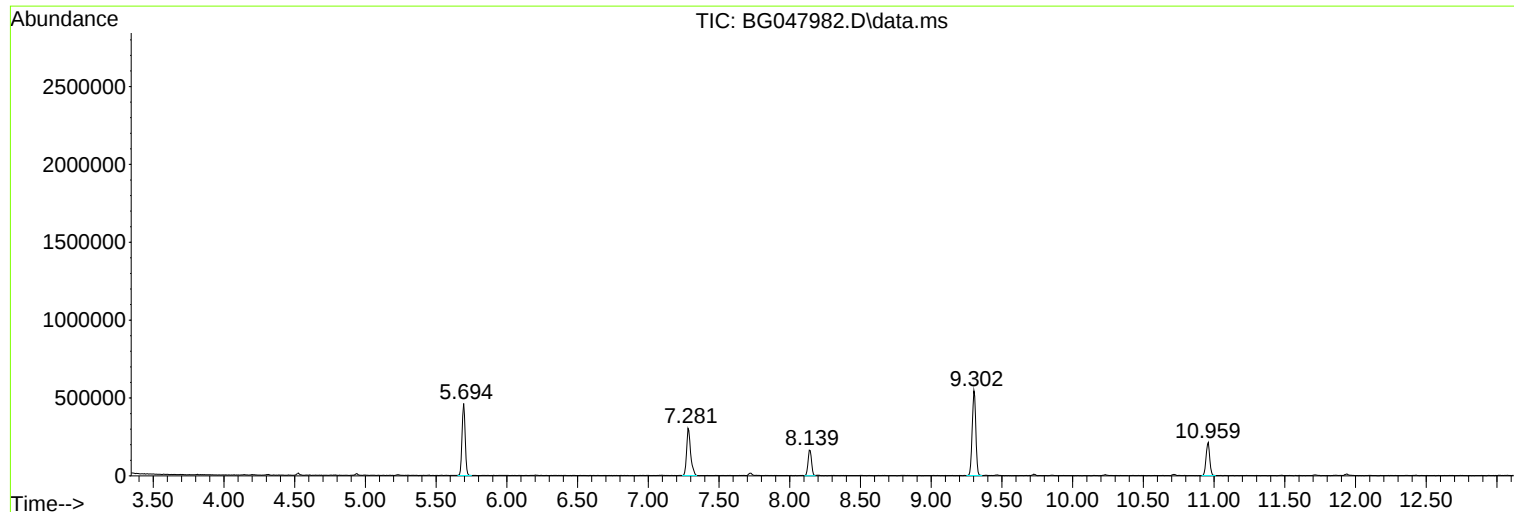
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ClientSampleId :
0023-SITE-WATER-044

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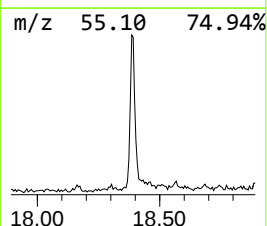
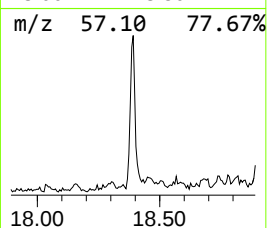
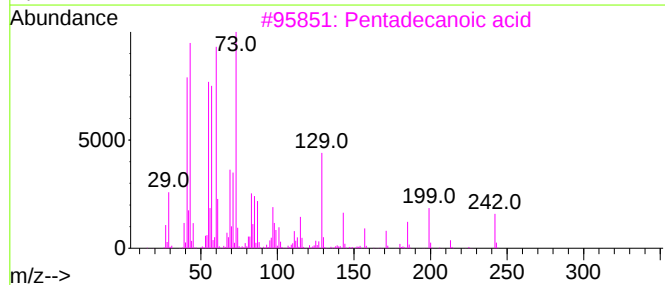
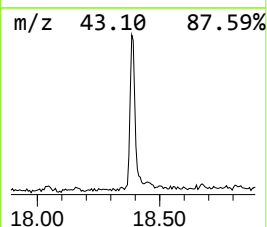
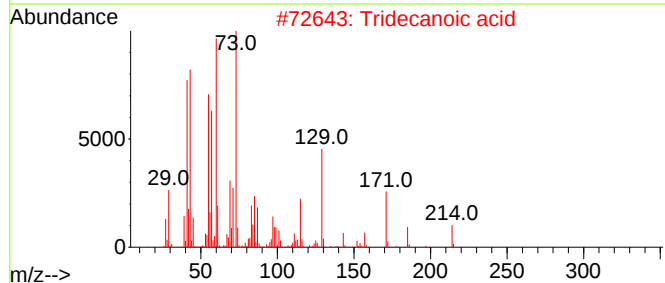
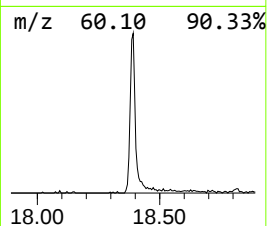
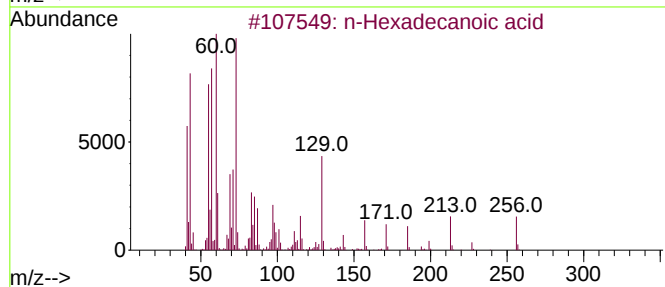
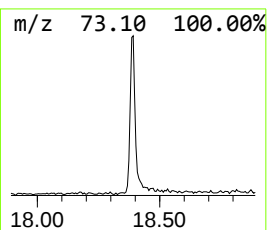
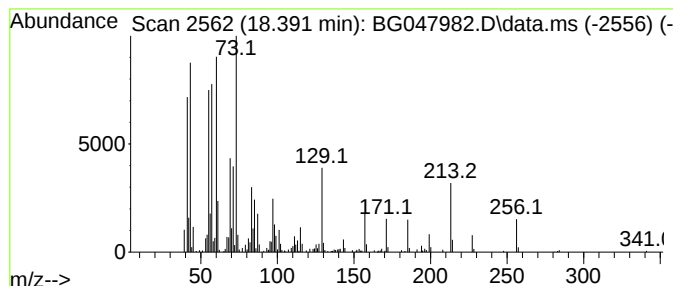
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.391	13.18 ng	519780	Phenanthrene-d10	17.504

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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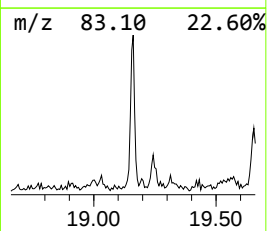
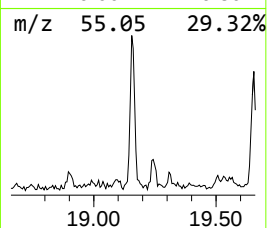
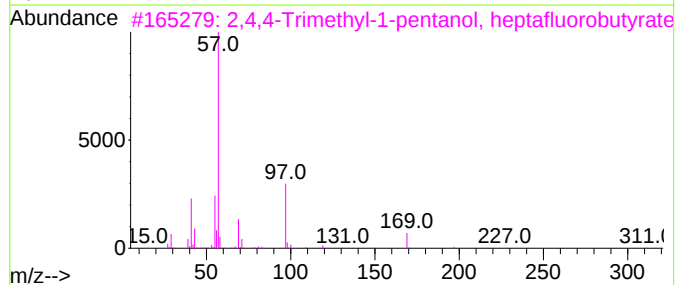
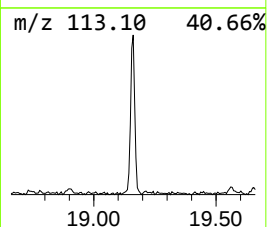
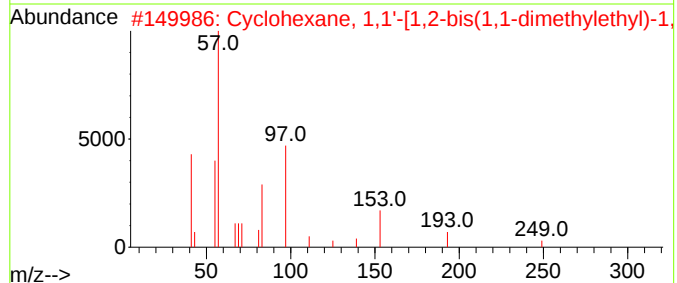
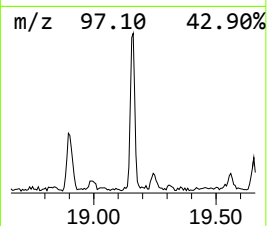
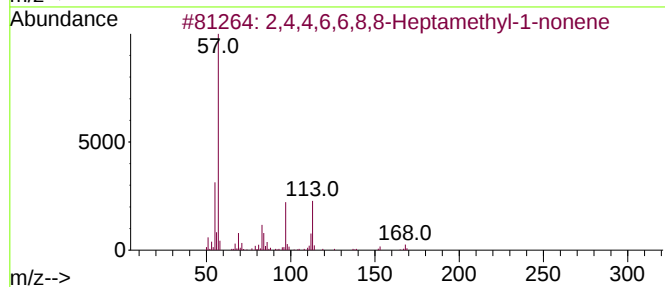
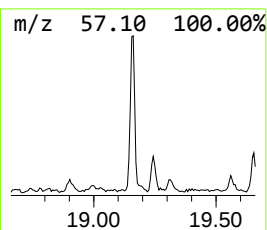
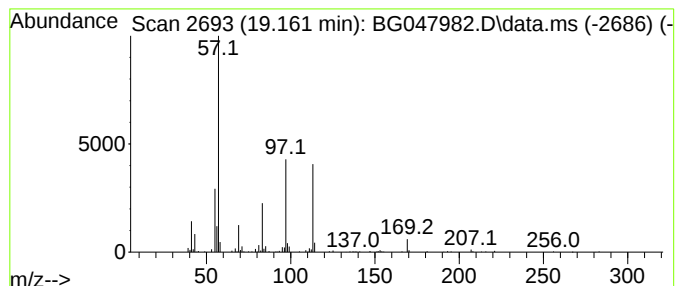
Instrument :
BNA_G
ClientSampleId :
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Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.161	7.37 ng	290596	Phenanthrene-d10	17.504	
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	72
2	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	37
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28



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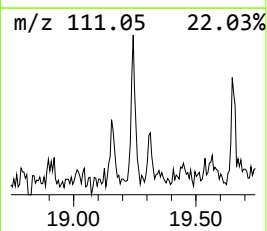
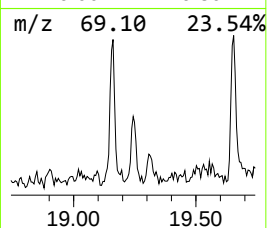
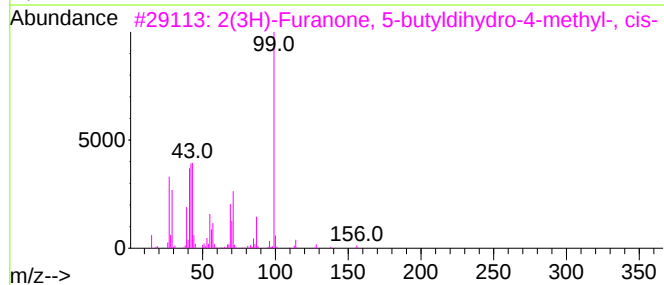
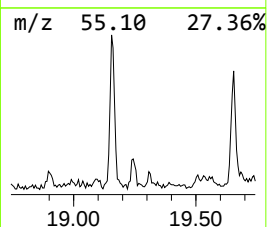
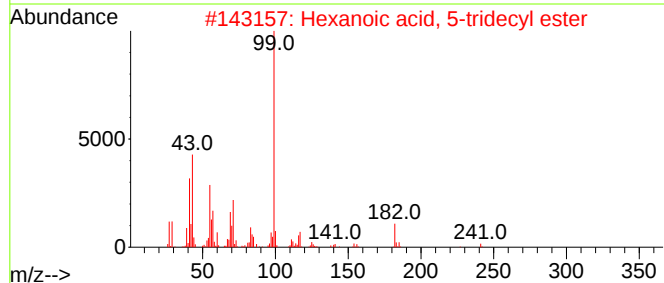
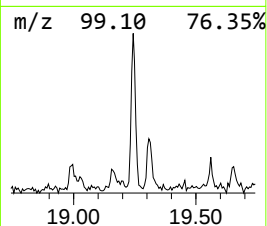
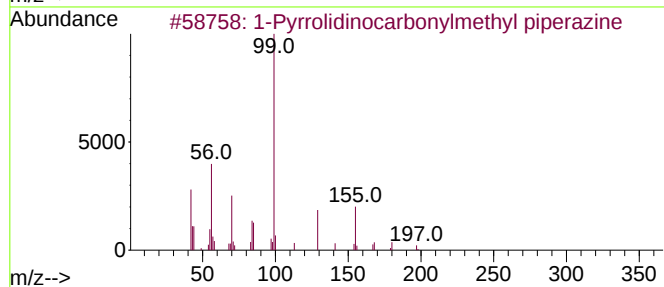
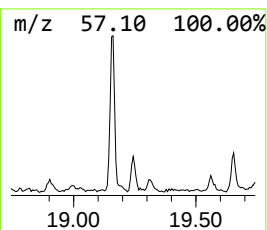
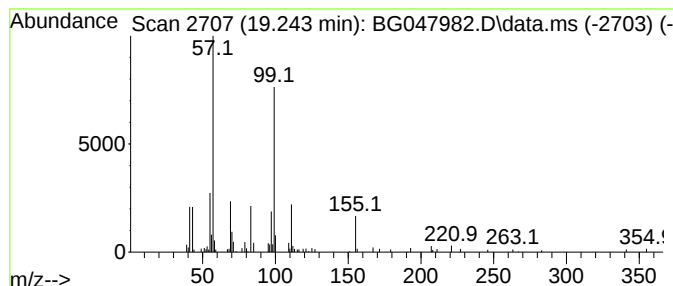
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Peak Number 3 unknown19.243 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.243	2.06 ng	81396	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	43
2			Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	38
3			2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	38
4			Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	37
5			Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	37



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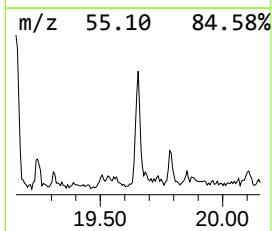
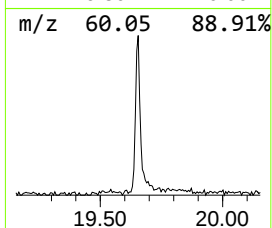
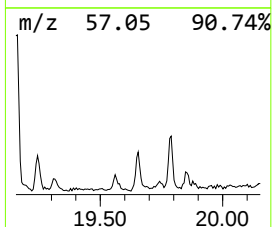
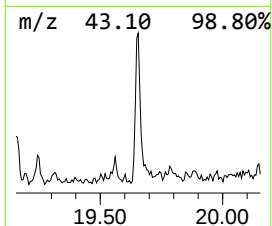
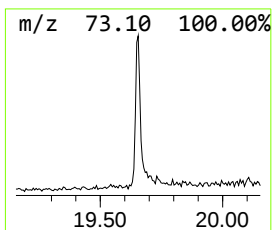
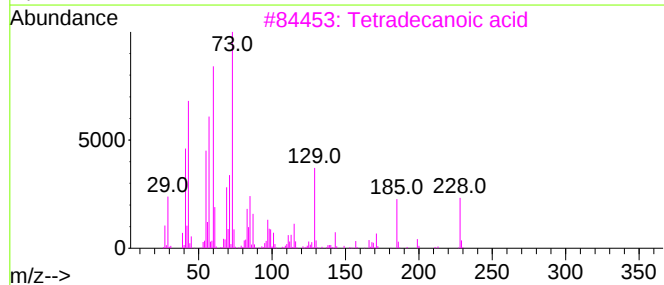
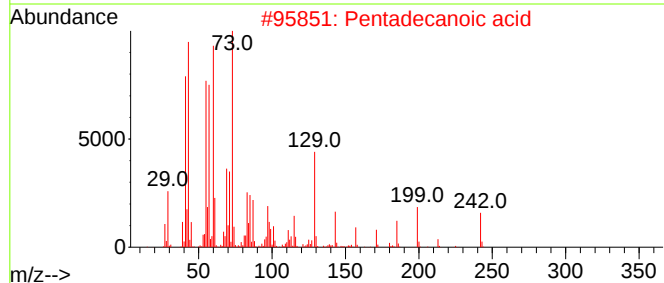
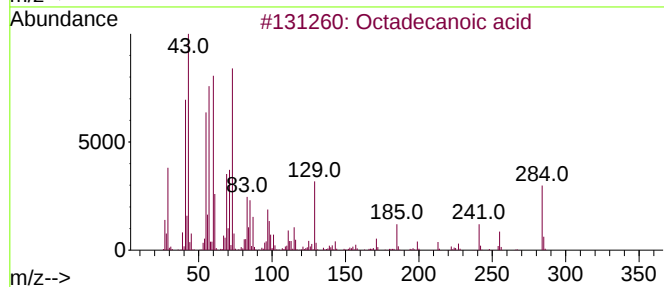
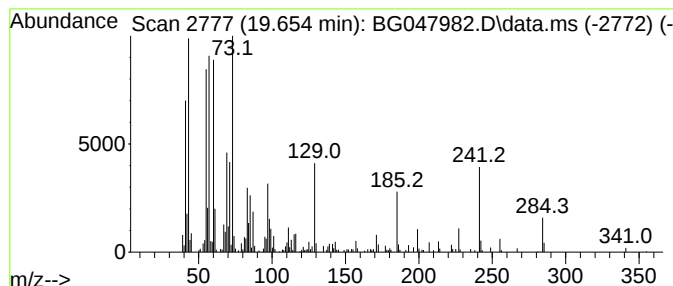
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	7.11 ng	350139	Chrysene-d12	21.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59



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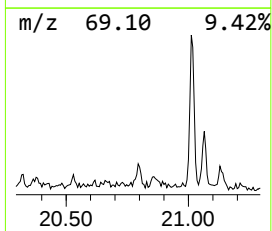
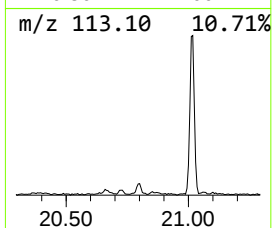
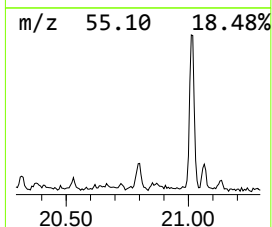
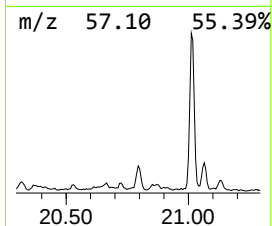
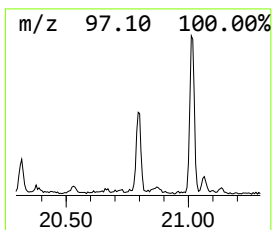
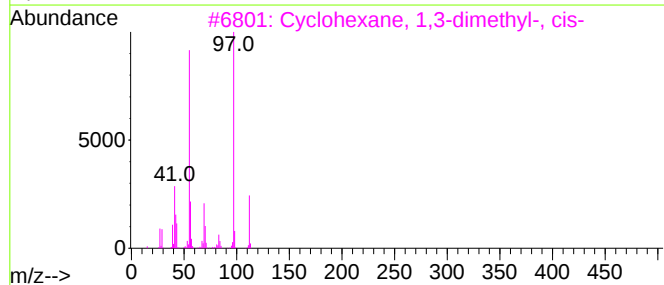
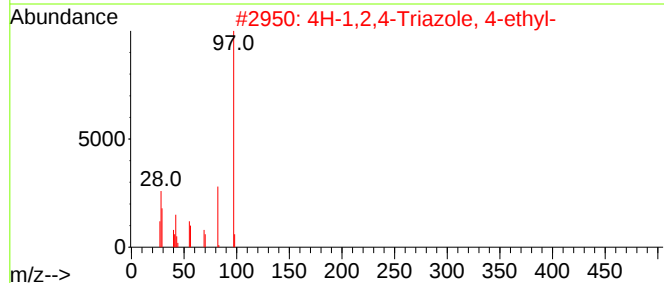
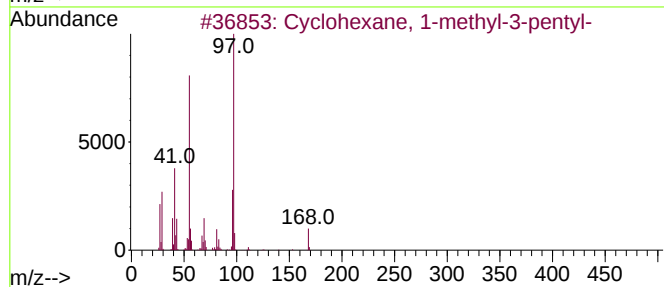
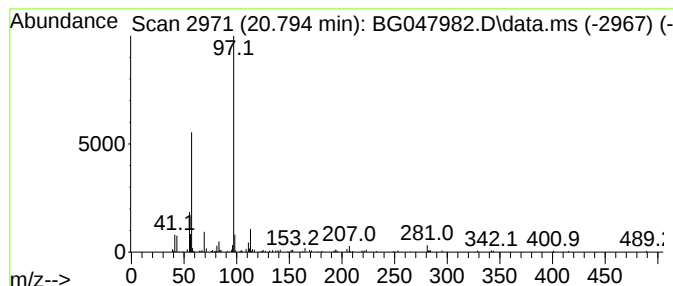
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Peak Number 5 Cyclohexane, 1-methyl-3-pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	2.42 ng	119072	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	64
2			4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	59
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
4			Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
5			2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	53



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ClientSampleId :
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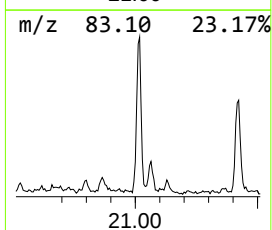
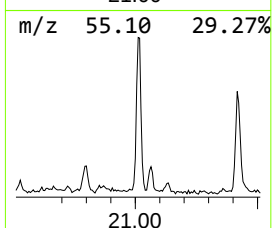
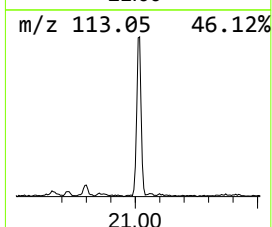
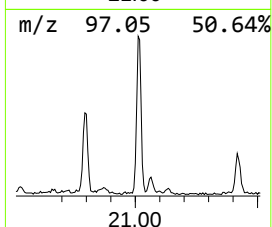
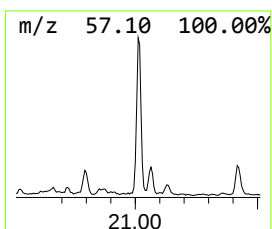
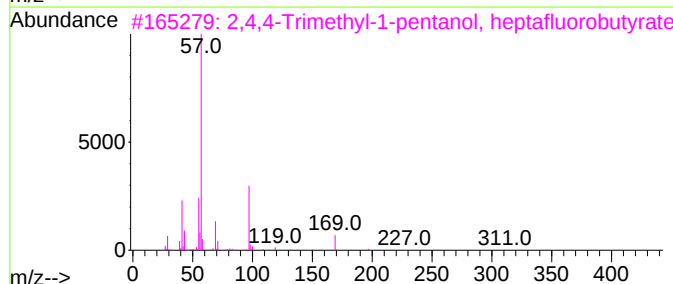
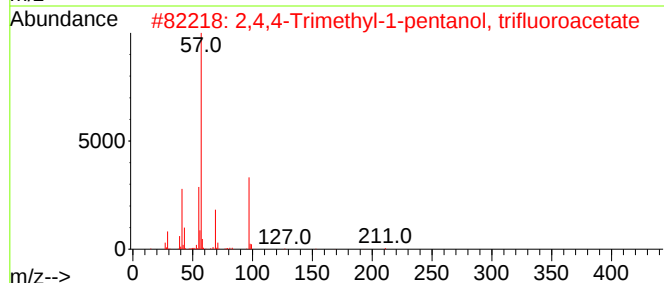
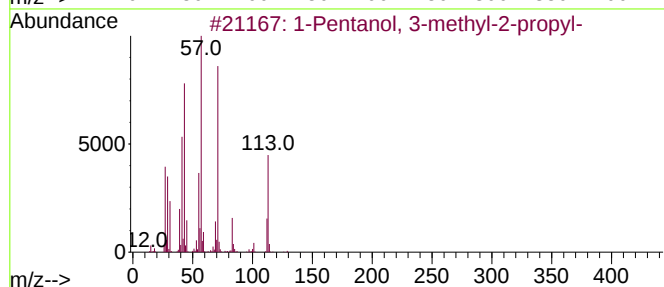
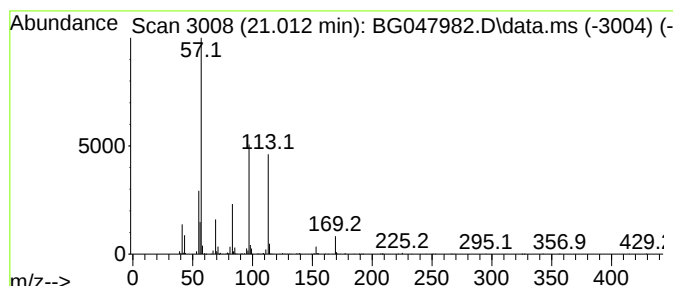
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.012 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.012	11.52 ng	567456	Chrysene-d12	21.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O		054004-40-9	40
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2		1000365-19-5	38
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2		1000365-01-4	37
4	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32		015796-04-0	37
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2		1000368-95-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047982.D
Acq On : 22 Jan 2021 17:39
Operator : CG/JU
Sample : M1191-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0023-SITE-WATER-044

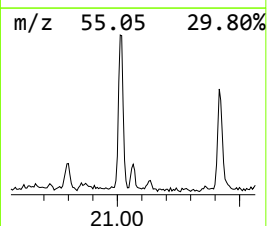
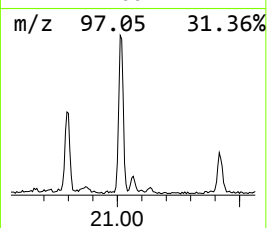
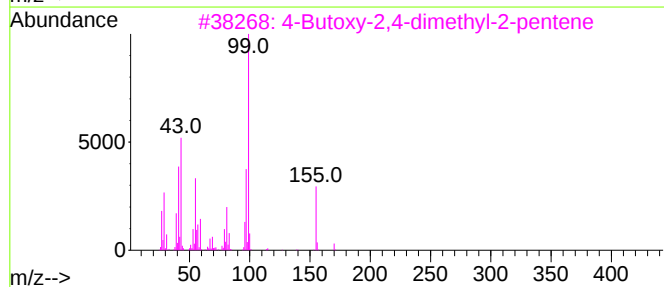
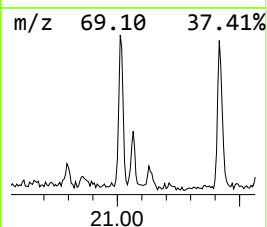
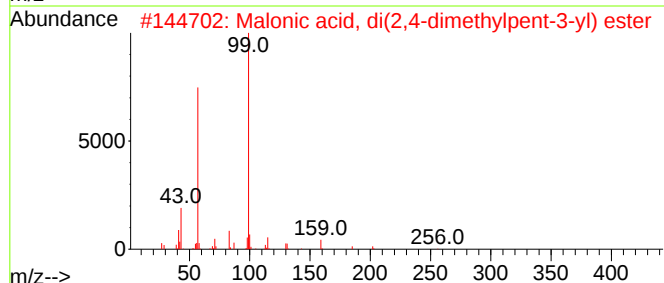
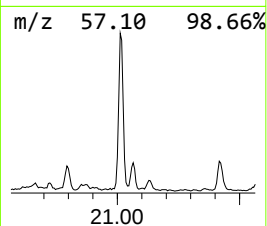
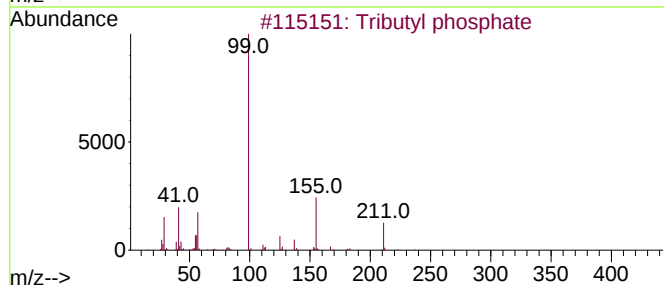
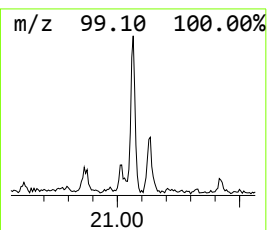
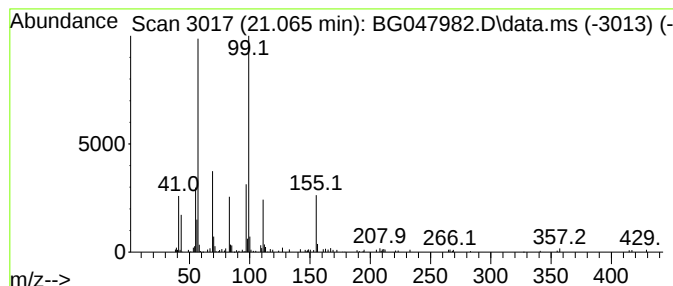
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.065 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.065	2.58 ng	127191	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tributyl phosphate	266	C12H27O4P	000126-73-8	47
2			Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	43
3			4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42
4			1,4-Dioxaspiro[4.5]decan-8-one	156	C8H12O3	004746-97-8	35
5			N-(4-Bromo-3-methyl-phenyl)-N'-(...	368	C15H21BrN4O2	1000294-59-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047982.D
Acq On : 22 Jan 2021 17:39
Operator : CG/JU
Sample : M1191-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

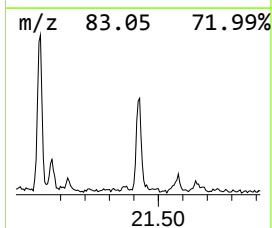
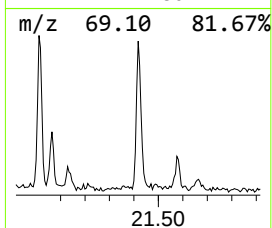
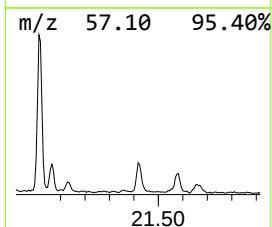
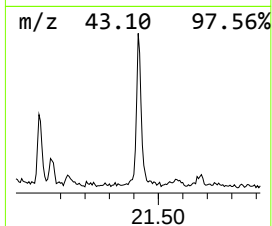
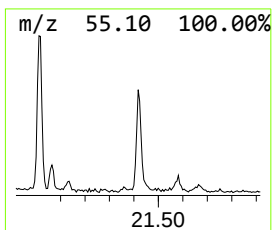
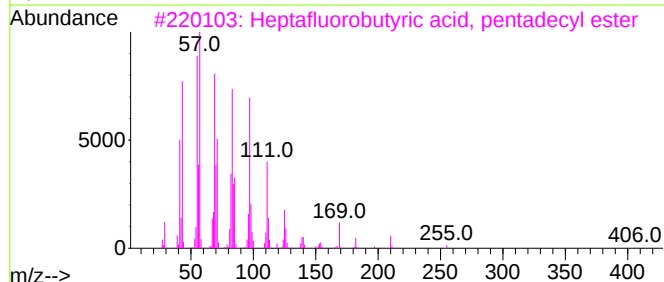
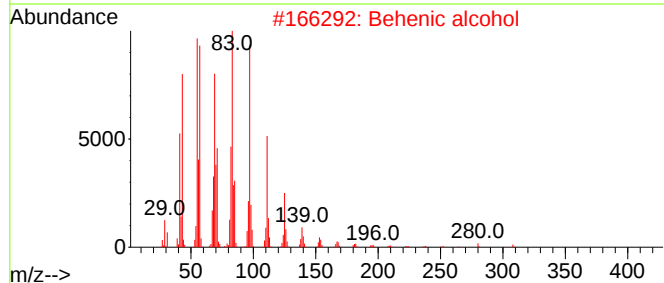
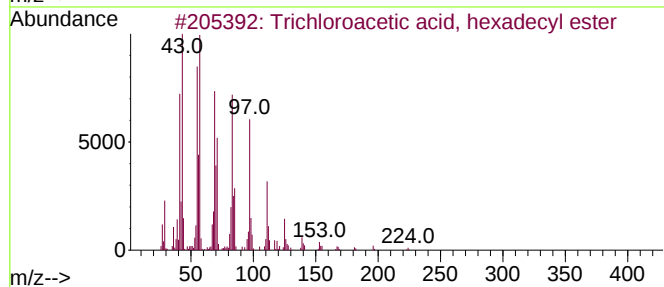
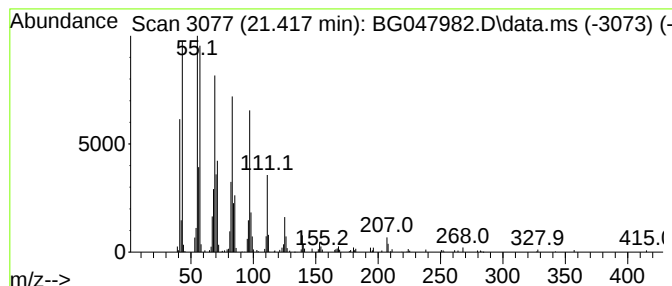
Instrument :
BNA_G
ClientSampleId :
0023-SITE-WATER-044

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, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.417	7.01 ng	345409	Chrysene-d12	21.781	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012221\
Data File : BG047982.D
Acq On : 22 Jan 2021 17:39
Operator : CG/JU
Sample : M1191-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0023-SITE-WATER-044

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.391	13.2	ng	519780	4	17.504	788653	20.0
2,4,4,6,6,8,8-H...	19.161	7.4	ng	290596	4	17.504	788653	20.0
unknown19.243	19.243	2.1	ng	81396	4	17.504	788653	20.0
Octadecanoic acid	19.654	7.1	ng	350139	5	21.781	984910	20.0
Cyclohexane, 1-...	20.794	2.4	ng	119072	5	21.781	984910	20.0
unknown21.012	21.012	11.5	ng	567456	5	21.781	984910	20.0
unknown21.065	21.065	2.6	ng	127191	5	21.781	984910	20.0
Trichloroacetic...	21.417	7.0	ng	345409	5	21.781	984910	20.0