LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0020-FIELD-BLANK

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-BG012521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.675	392	398	407	rVB	398164	637125	15.26%	3.974%
2	7.268	660	669	679	rVB2	253120	466110	11.17%	2.908%
3	8.126	808	815	822	rBV	164245	276257	6.62%	1.723%
4	9.283	1003	1012	1021	rBV	548518	986428	23.63%	6.153%
5	10.940	1286	1294	1301	rVB	208651	375795	9.00%	2.344%
6	13.372	1701	1708	1716	rBV	1471889	2250756	53.93%	14.040%
7	14.747	1935	1942	1949	rBV	364215	560144	13.42%	3.494%
8	16.228	2187	2194	2200	rBV	1350211	1953773	46.81%	12.188%
9	17.491	2402	2409	2416	rBV	480686	741771	17.77%	4.627%
10	18.366	2553	2558	2567	rBV	170987	244950	5.87%	1.528%
11	18.878	2641	2645	2651	rBV2	26919	48295	1.16%	0.301%
12	19.136	2685	2689	2694	rBV	189331	244887	5.87%	1.528%
13	19.224	2699	2704	2712	rBV	66486	97302	2.33%	0.607%
14	19.630	2770	2773	2780	rBV2	74614	96874	2.32%	0.604%
15	19.765	2792	2796	2800	rBV	65330	80222	1.92%	0.500%
16	20.088	2845	2851	2857	rBV	3172967	4173827	100.00%	26.036%
17	20.300	2882	2887	2892	rBV2	37269	56972	1.36%	0.355%
18	20.775	2964	2968	2973	rVB	77223	98443	2.36%	0.614%
19	20.993	3000	3005	3010	rBV	294934	363018	8.70%	2.265%
20	21.040	3010	3013	3018	rVV	73212	87895	2.11%	0.548%
21	21.398	3069	3074	3084	rBV	251282	364399	8.73%	2.273%
22	21.762	3130	3136	3143	rVB	577860	915935	21.94%	5.714%
23	25.047	3686	3695	3705	rVB	321691	863738	20.69%	5.388%
24	26.381	3917	3922	3923	rBV5	28828	45824	1.10%	0.286%

Sum of corrected areas: 16030740

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
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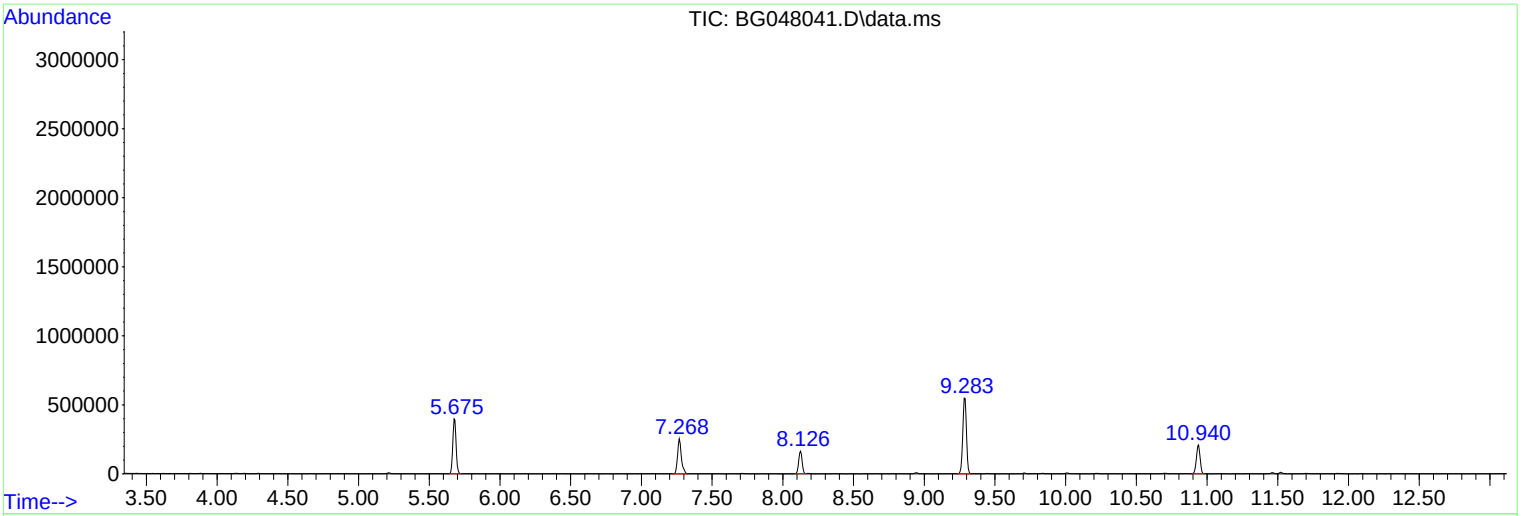
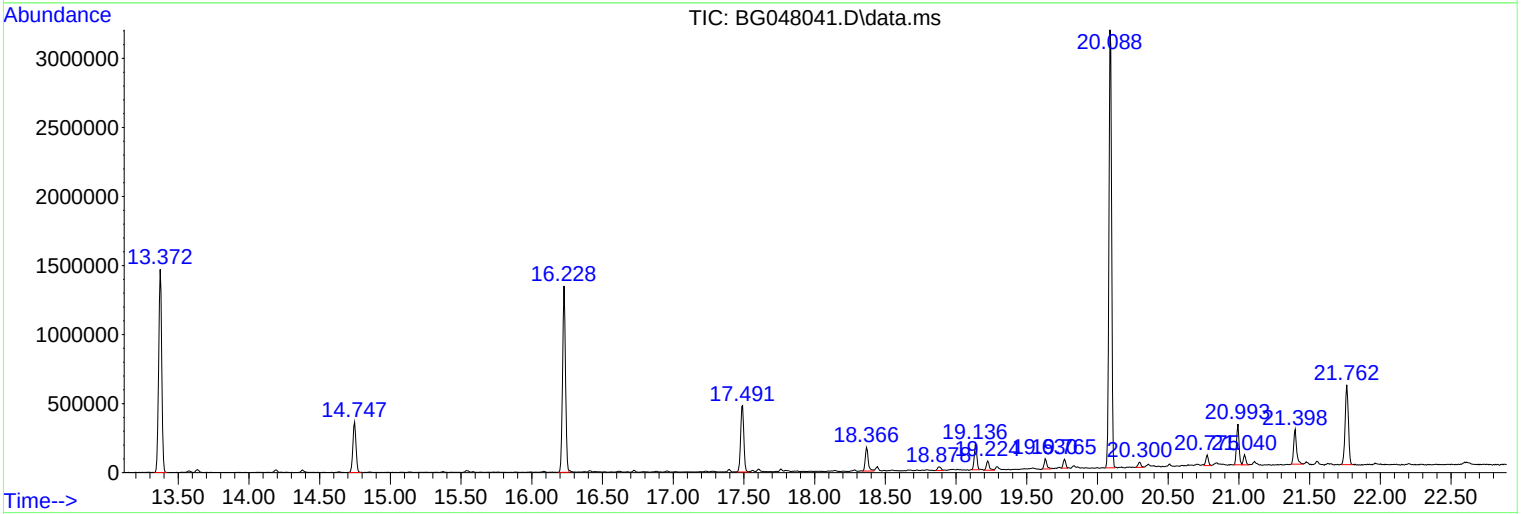
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

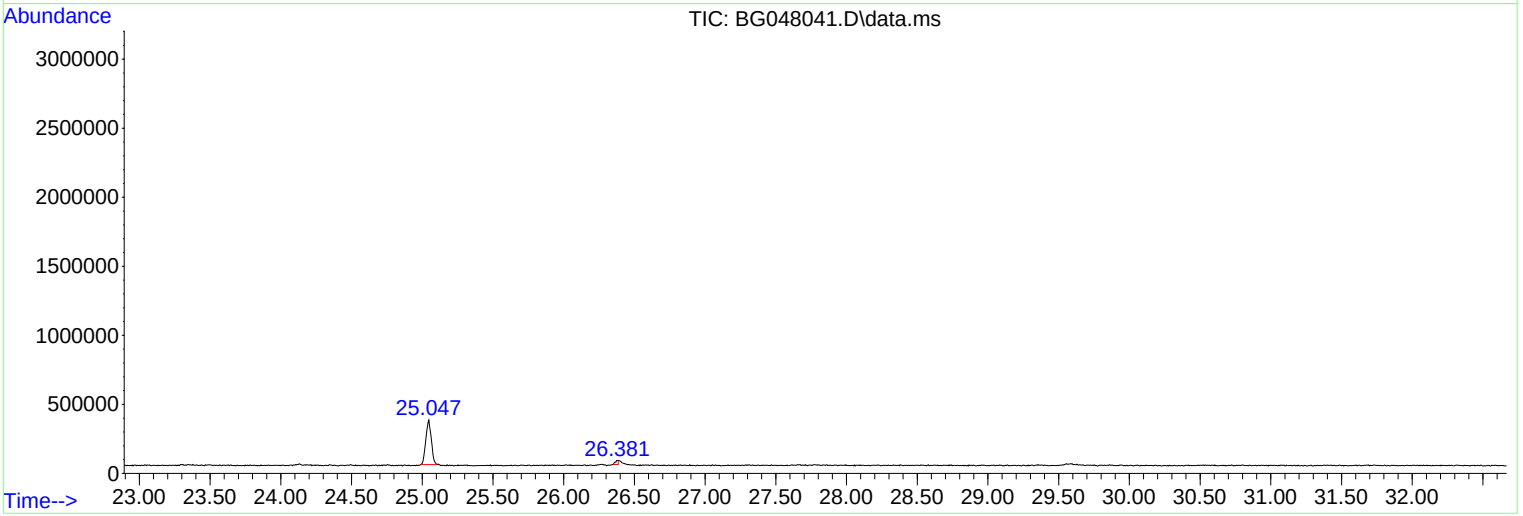
Instrument :
BNA_G
ClientSampleId :
0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

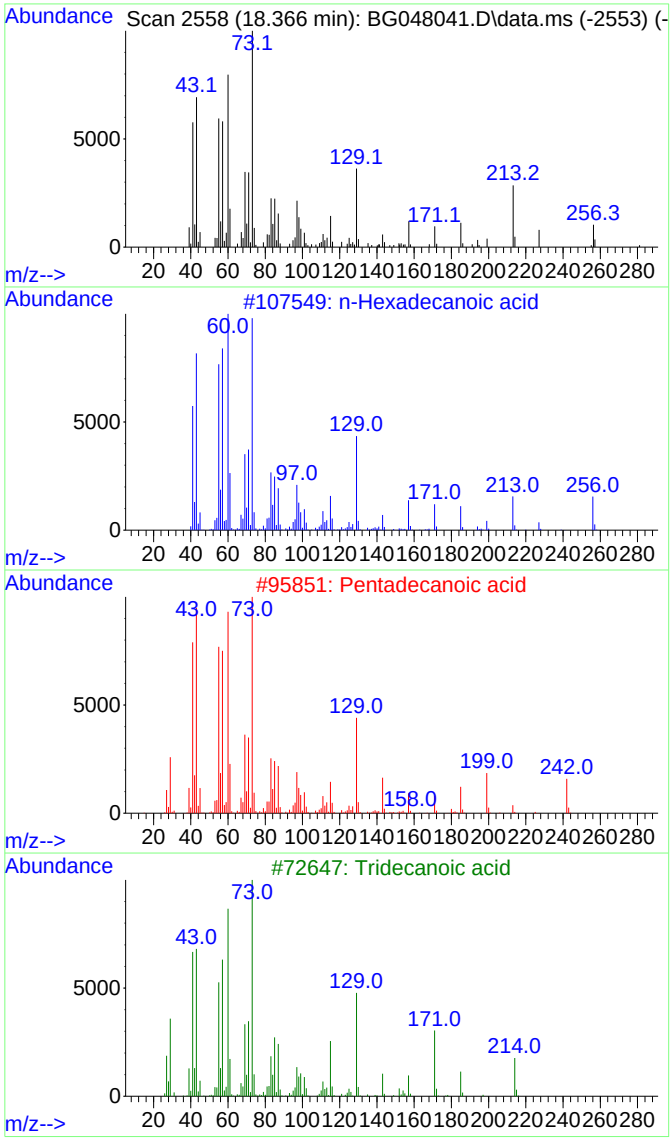
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

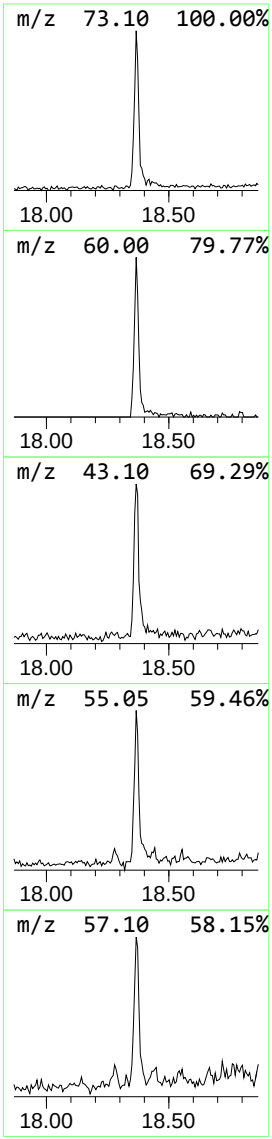
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.366	6.60 ng	244950	Phenanthrene-d10	17.491

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	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0020-FIELD-BLANK

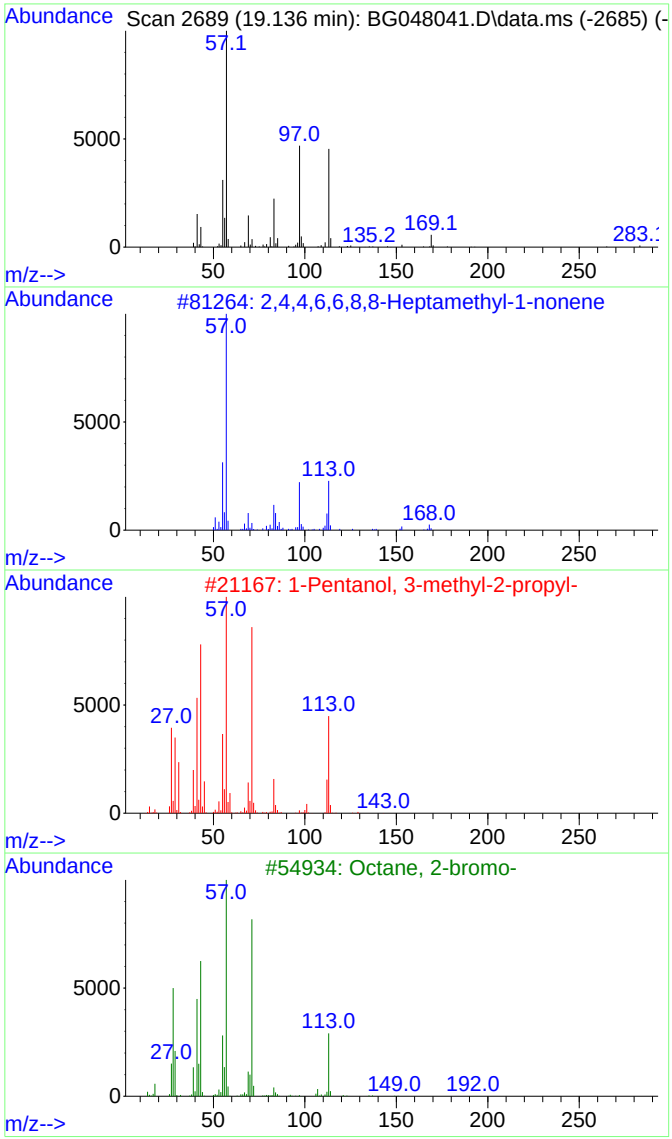
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

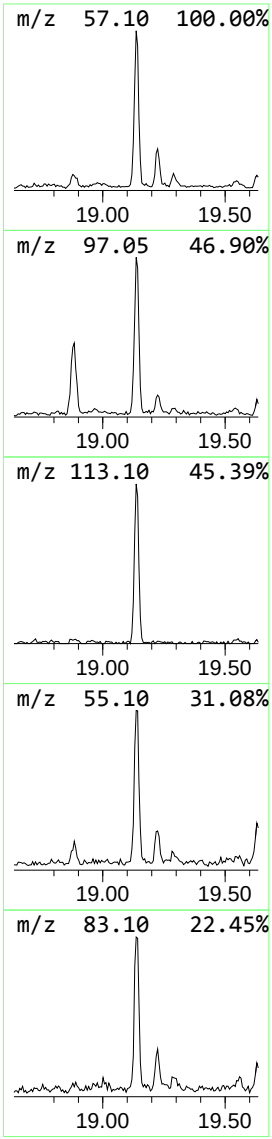
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.136	6.60 ng	244887	Phenanthrene-d10	17.491

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	64
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

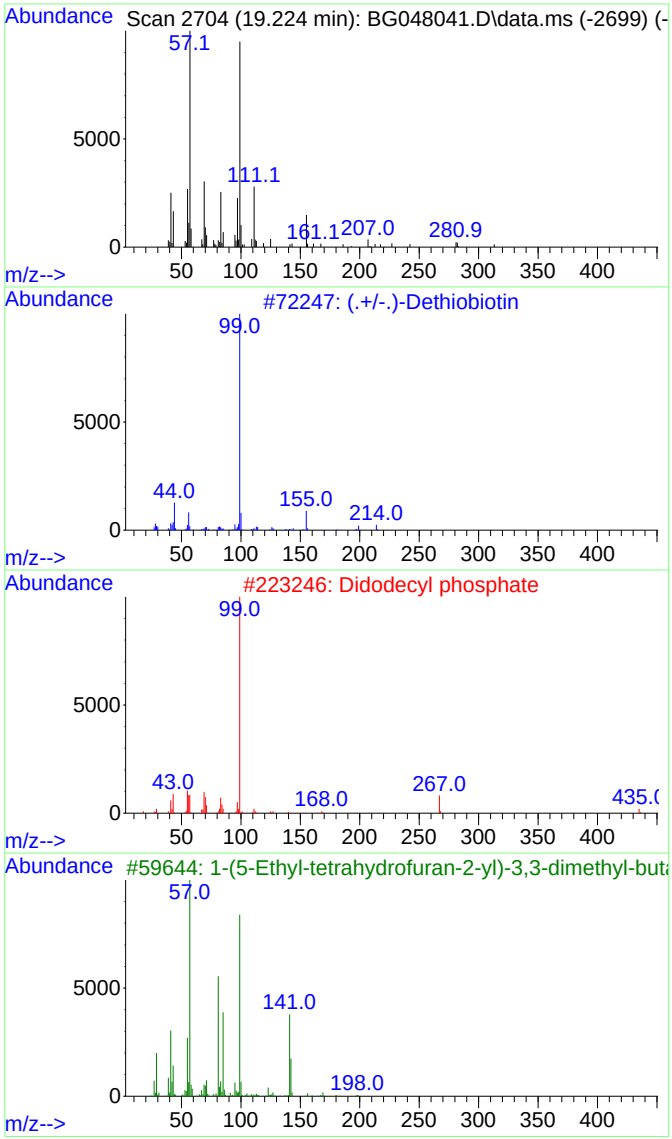
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

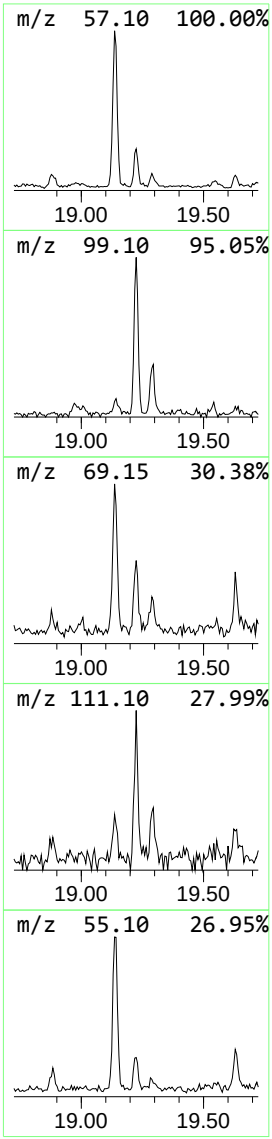
****

Peak Number 3 unknown19.224 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.224	2.62 ng	97302	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	43
2	Didodecyl phosphate	434	C24H51O4P	007057-92-3	38
3	1-(5-Ethyl-tetrahydrofuran-2-yl)...	198	C12H22O2	343942-34-7	38
4	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	38
5	Phosphoric acid, nonyl propyl un...	420	C23H49O4P	1000309-00-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

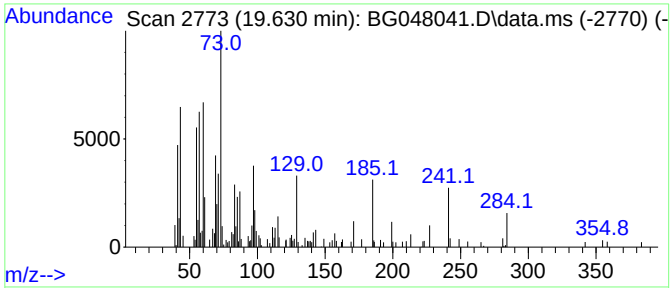
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

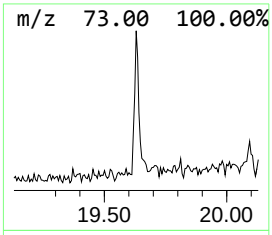
****

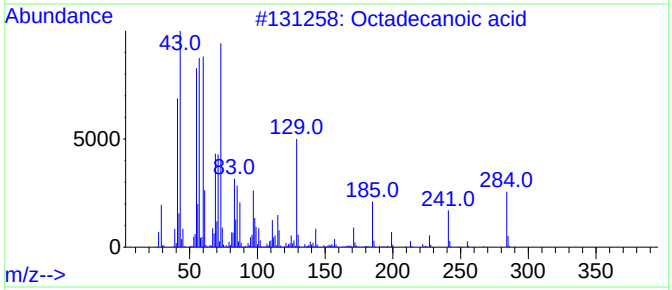
Peak Number 4 Octadecanoic acid Concentration Rank 7

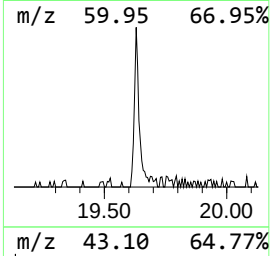
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.630	2.12 ng	96874	Chrysene-d12	21.762

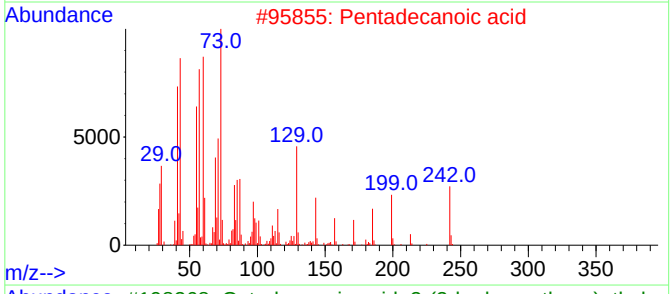
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	38

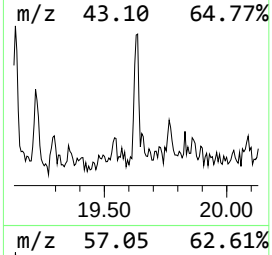


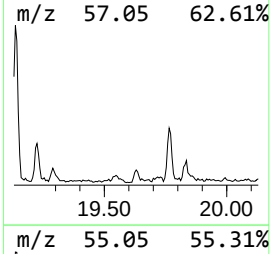


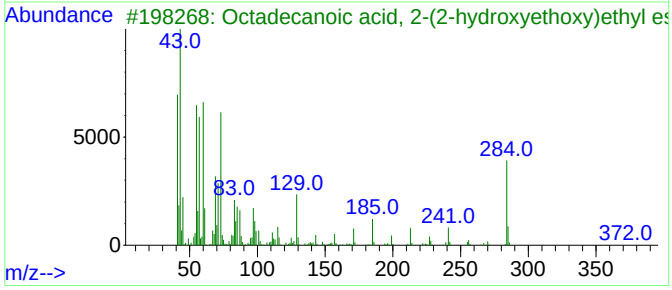


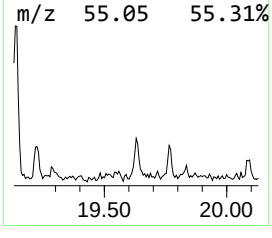












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0020-FIELD-BLANK

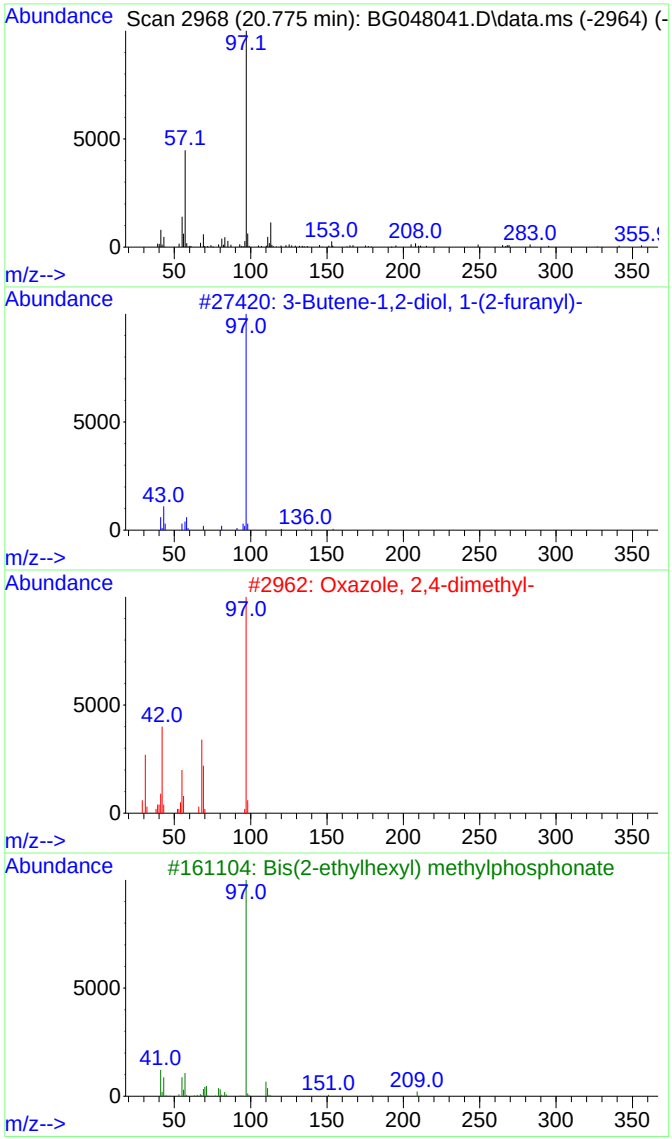
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

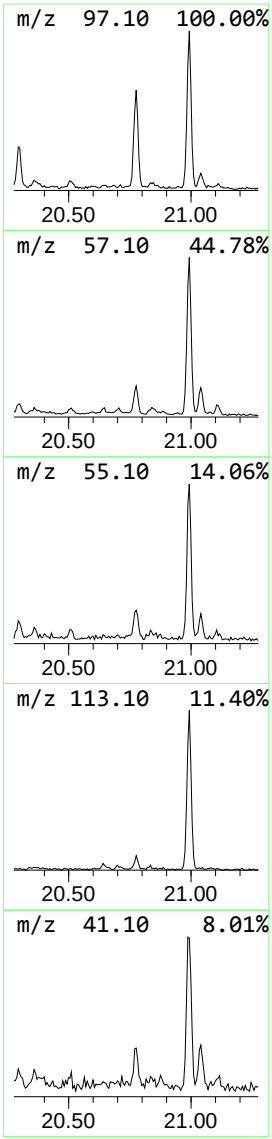
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Butene-1,2-diol, 1-(2-fur... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.775	2.15 ng	98443	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Butene-1,2-diol, 1-(2-furanyl)-	154	C8H10O3	019261-13-3	53
2	Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	42
3	Bis(2-ethylhexyl) methylphosphonate	320	C17H37O3P	1000298-35-3	39
4	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	39
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

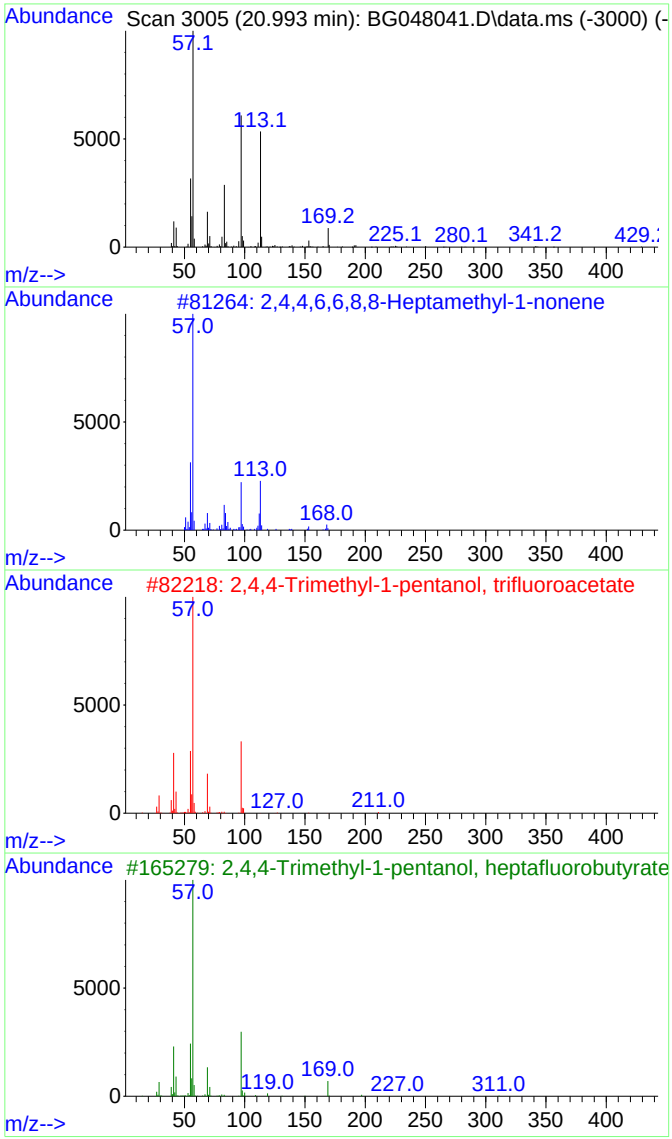
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

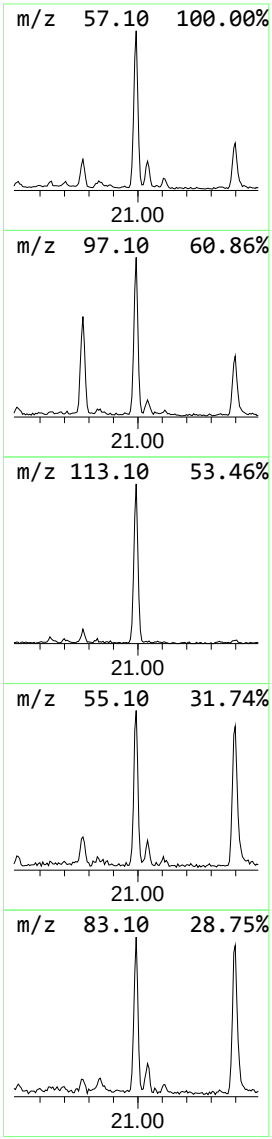
****

Peak Number 6 unknown20.993 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.993	7.93 ng	363018	Chrysene-d12	21.762

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	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	38
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

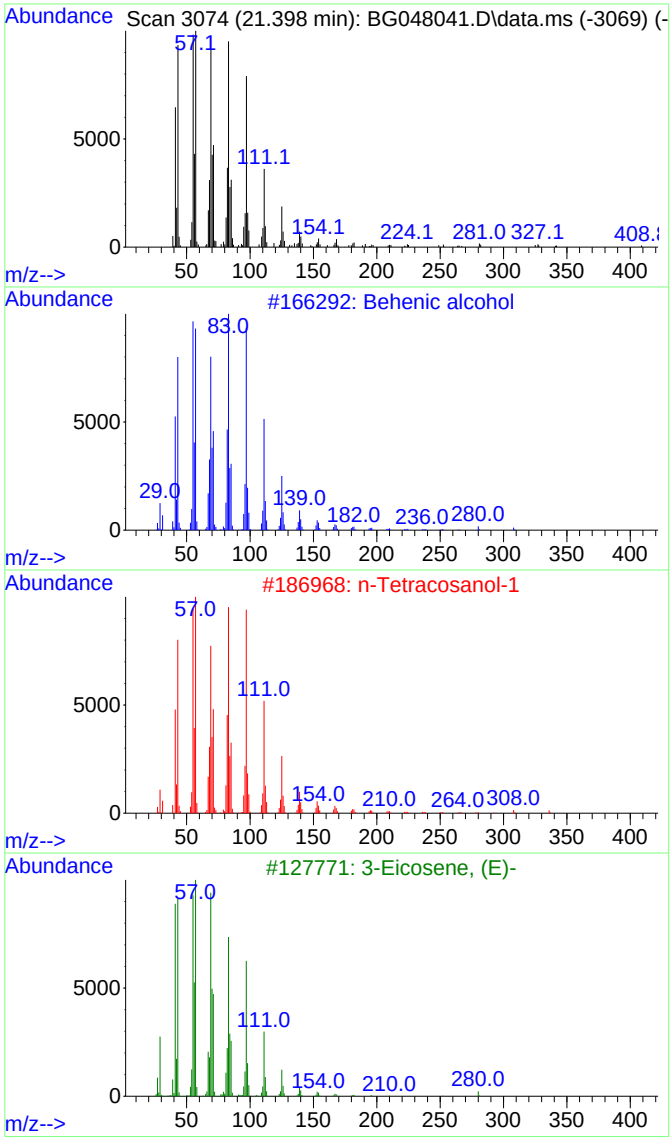
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

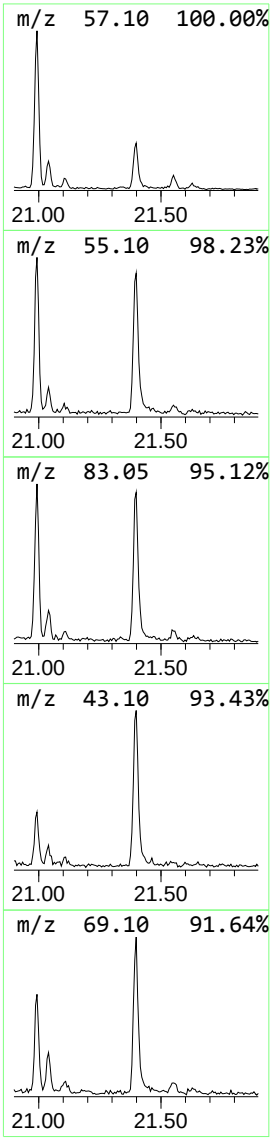
****

Peak Number 7 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	7.96 ng	364399	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	92
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048041.D
Acq On : 27 Jan 2021 23:39
Operator : CG/JU
Sample : M1212-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0020-FIELD-BLANK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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 ...	18.366	6.6	ng	244950	4	17.491	741771	20.0
2,4,4,6,6,8,8-H...	19.136	6.6	ng	244887	4	17.491	741771	20.0
unknown19.224	19.224	2.6	ng	97302	4	17.491	741771	20.0
Octadecanoic acid	19.630	2.1	ng	96874	5	21.762	915935	20.0
3-Butene-1,2-di...	20.775	2.1	ng	98443	5	21.762	915935	20.0
unknown20.993	20.993	7.9	ng	363018	5	21.762	915935	20.0
Behenic alcohol	21.398	8.0	ng	364399	5	21.762	915935	20.0