LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

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: BG048046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.677	389	398	406	rBV	550876	861464	23.78%	4.353%
2	7.269	662	669	683	rVB	408222	730330	20.16%	3.690%
3	8.121	807	814	821	rBV	192646	317979	8.78%	1.607%
4	9.284	1005	1012	1021	rBV	565863	985871	27.21%	4.981%
5	10.935	1286	1293	1304	rVB	236205	431416	11.91%	2.180%
6	13.374	1700	1708	1715	rBV	1467605	2233867	61.65%	11.287%
7	14.190	1841	1847	1852	rBV	35074	50855	1.40%	0.257%
8	14.378	1875	1879	1891	rVB5	19229	37858	1.04%	0.191%
9	14.743	1935	1941	1950	rVB2	396643	634895	17.52%	3.208%
10	16.229	2187	2194	2203	rBV	1350254	2001521	55.24%	10.113%
11	17.486	2401	2408	2416	rBV	542026	810818	22.38%	4.097%
12	17.763	2447	2455	2460	rBV	763095	986929	27.24%	4.987%
13	18.374	2553	2559	2566	rBV	697700	958688	26.46%	4.844%
14	18.444	2567	2571	2575	rVB	56467	76457	2.11%	0.386%
15	19.137	2684	2689	2693	rBV	191584	236438	6.53%	1.195%
16	19.226	2700	2704	2710	rBV	62963	79375	2.19%	0.401%
17	19.490	2745	2749	2751	rBV4	30684	38583	1.06%	0.195%
18	19.637	2768	2774	2783	rBV	527784	740778	20.44%	3.743%
19	19.766	2792	2796	2803	rVB	59980	77840	2.15%	0.393%
20	20.089	2845	2851	2856	rBV	2830850	3623279	100.00%	18.307%
21	20.295	2883	2886	2892	rVB	38291	57926	1.60%	0.293%
22	20.771	2964	2967	2972	rVB	91004	119640	3.30%	0.604%
23	20.994	3000	3005	3009	rBV	399087	495692	13.68%	2.505%
24	21.041	3009	3013	3018	rVV	95990	123233	3.40%	0.623%
25	21.112	3022	3025	3033	rVB2	38414	58775	1.62%	0.297%
26	21.394	3068	3073	3083	rBV	432143	672839	18.57%	3.400%
27	21.552	3097	3100	3104	rVB	42233	54555	1.51%	0.276%
28	21.764	3129	3136	3144	rVB	584850	966509	26.67%	4.883%
29	21.963	3167	3170	3175	rVB6	27783	37660	1.04%	0.190%
30	22.592	3273	3277	3279	rBV4	29812	52221	1.44%	0.264%
31	24.126	3533	3538	3544	rVB6	27649	55362	1.53%	0.280%
32	25.048	3684	3695	3710	rBV2	331197	990055	27.32%	5.002%
33	26.388	3917	3923	3934	rVB8	57504	192266	5.31%	0.971%

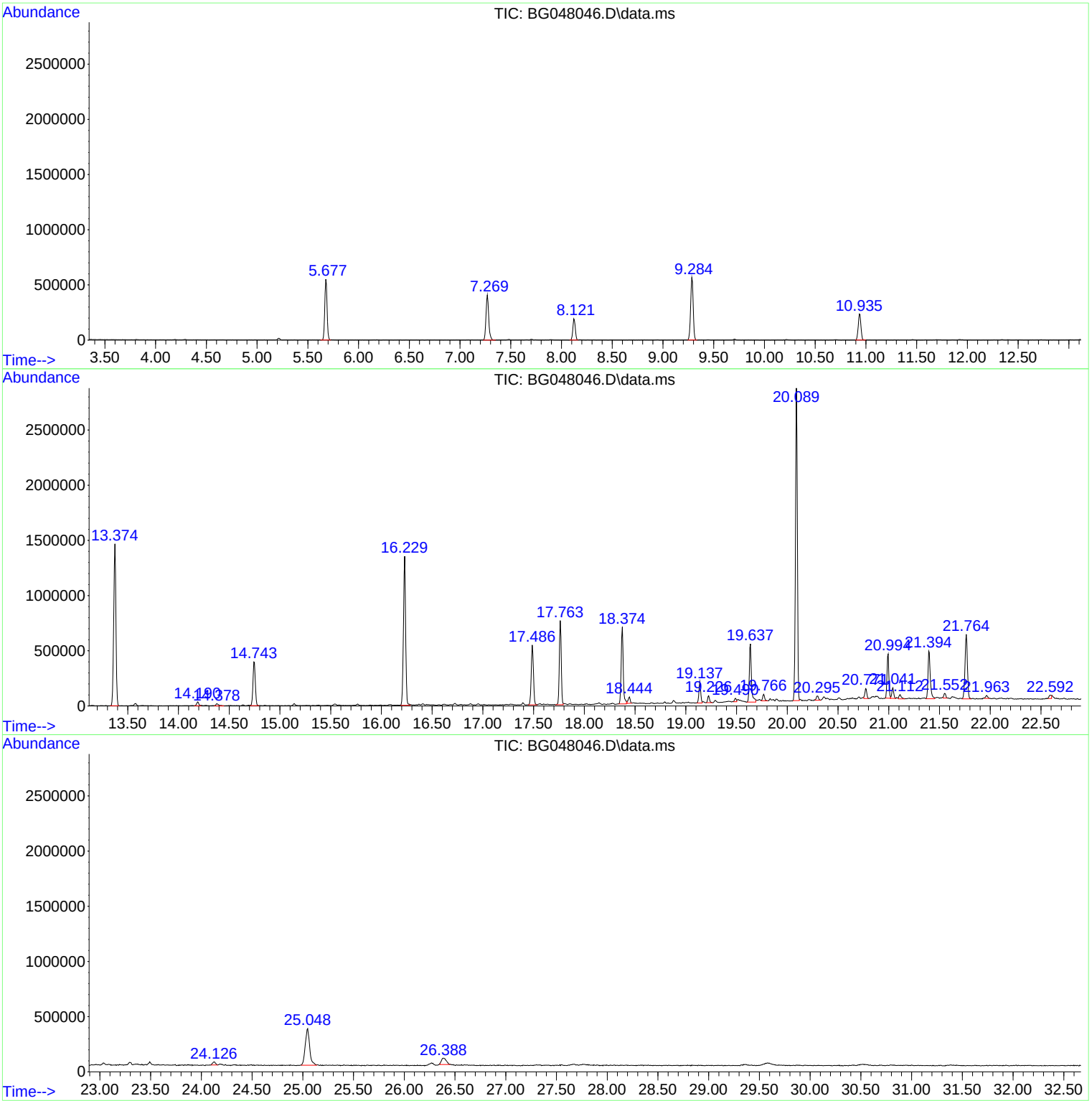
Sum of corrected areas: 19791974

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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 : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

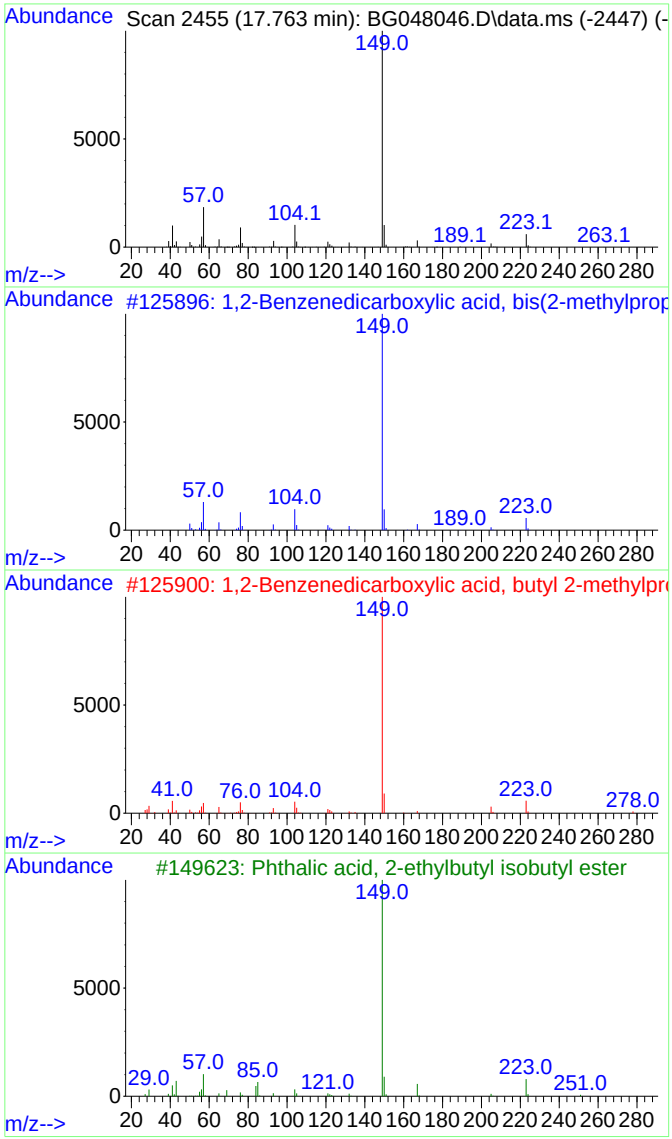
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

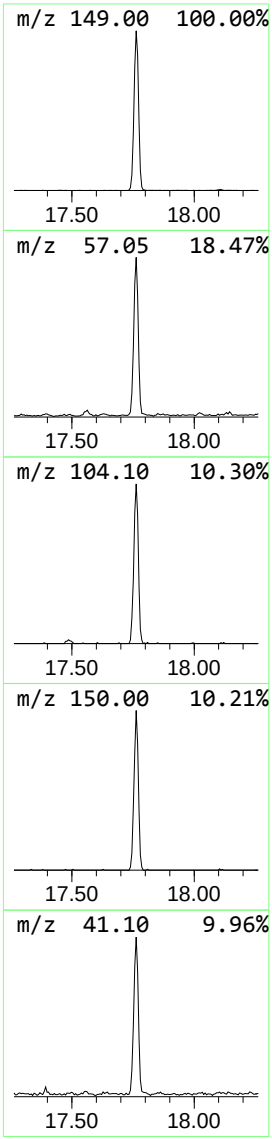
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.762	24.34 ng	986929	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	80
3	Phthalic acid, 2-ethylbutyl isob...	306	C18H26O4	1000356-88-9	72
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	72
5	Phthalic acid, isobutyl 4-methyl...	306	C18H26O4	1000356-87-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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

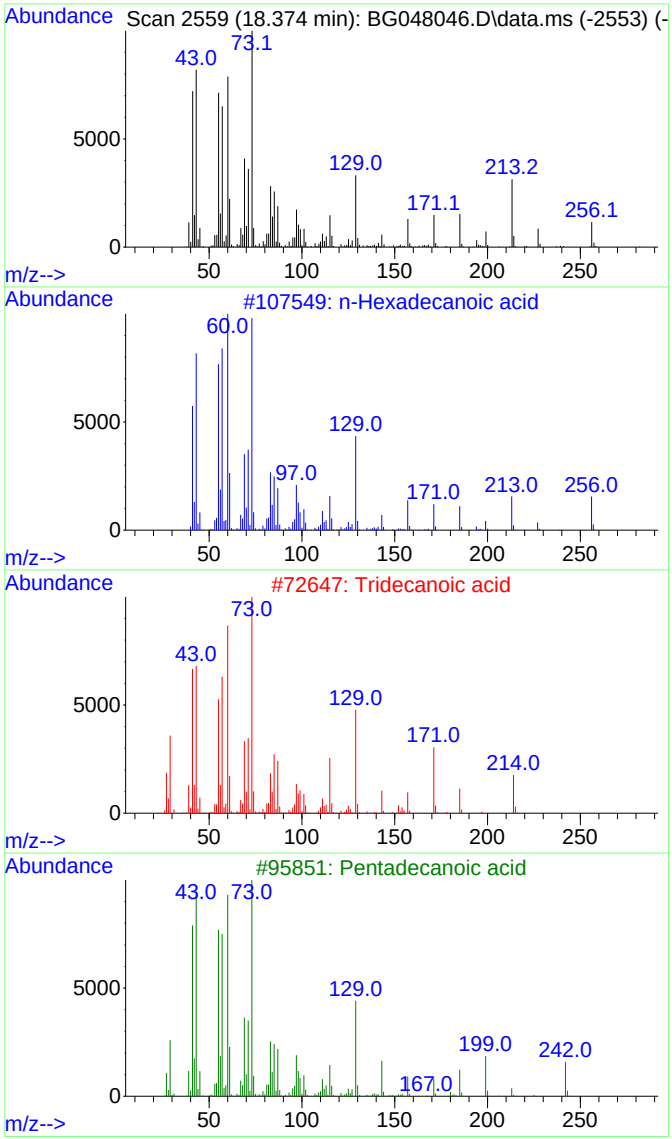
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

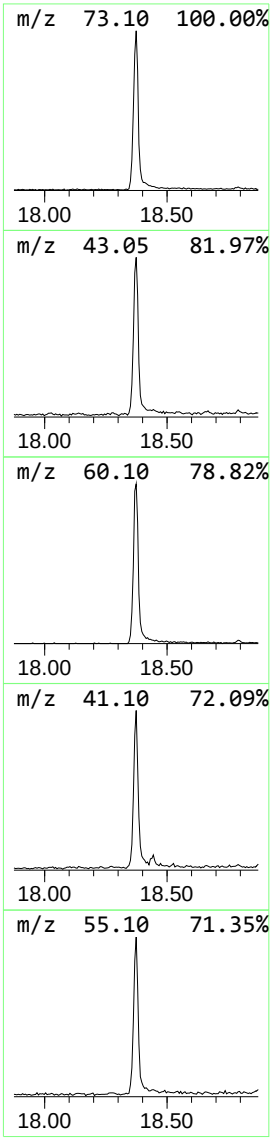
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	23.65 ng	958688	Phenanthrene-d10	17.486

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	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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

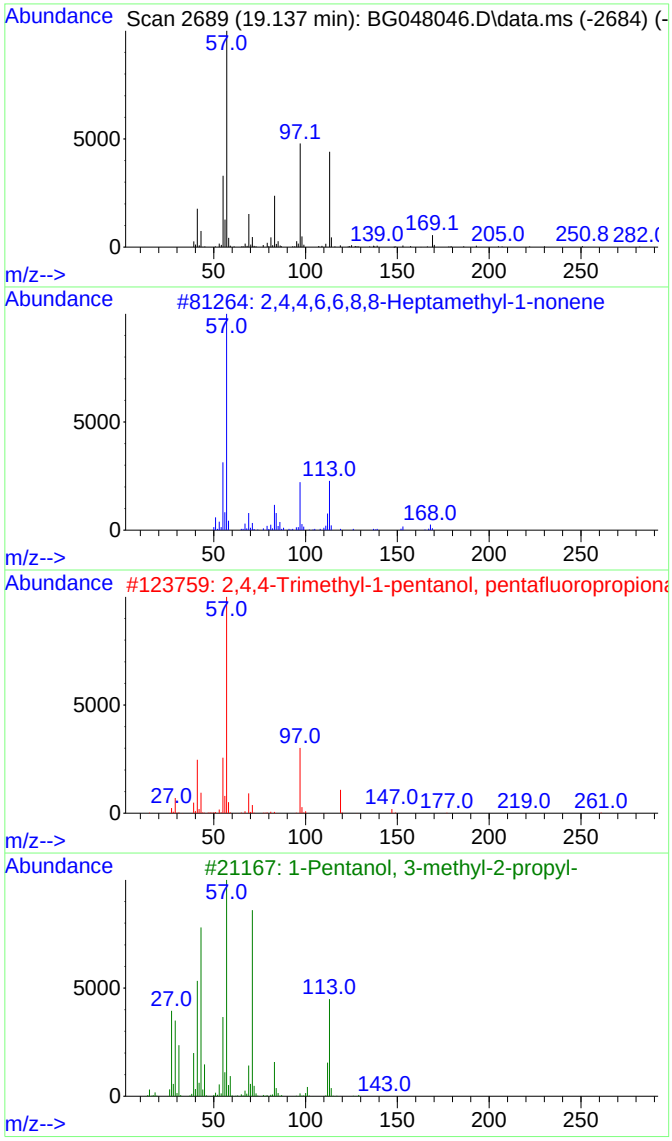
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

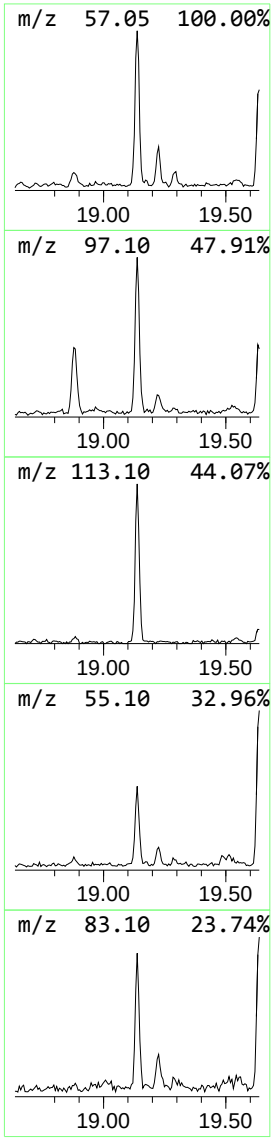
****

Peak Number 3 unknown19.137 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.137	5.83 ng	236438	Phenanthrene-d10	17.486

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	40
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25
5	4-Hepten-3-one, 5-methyl-, (Z)-	126	C8H14O	020685-43-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

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

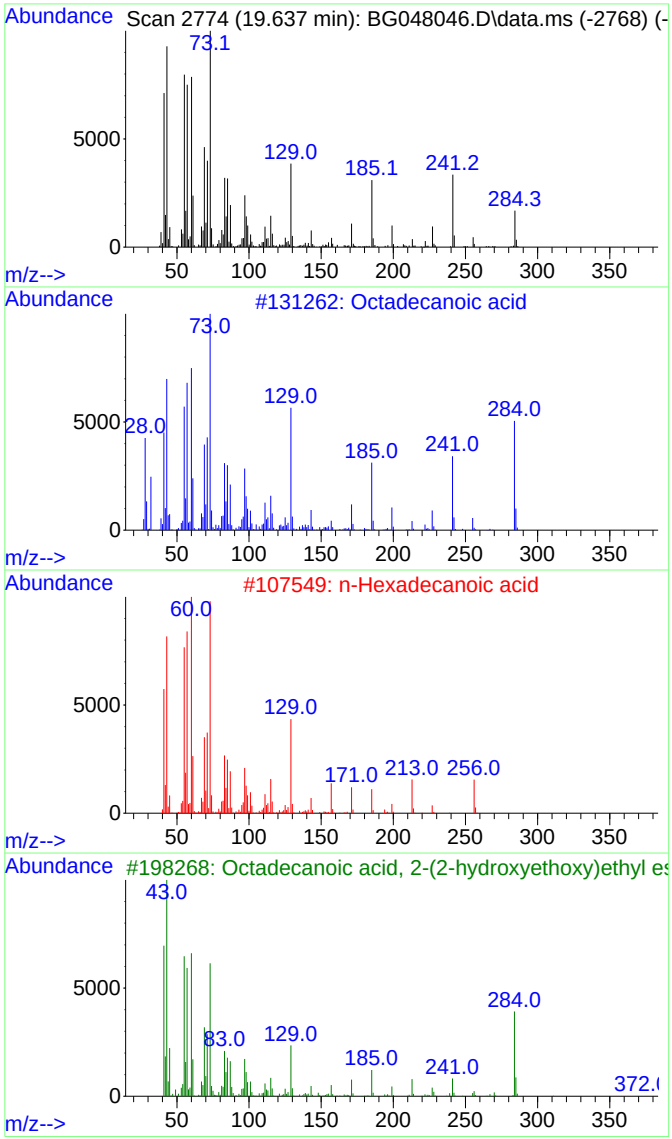
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

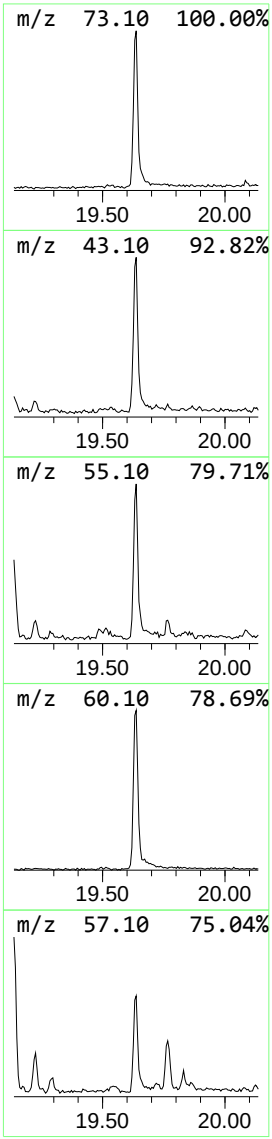
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.637	15.33 ng	740778	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

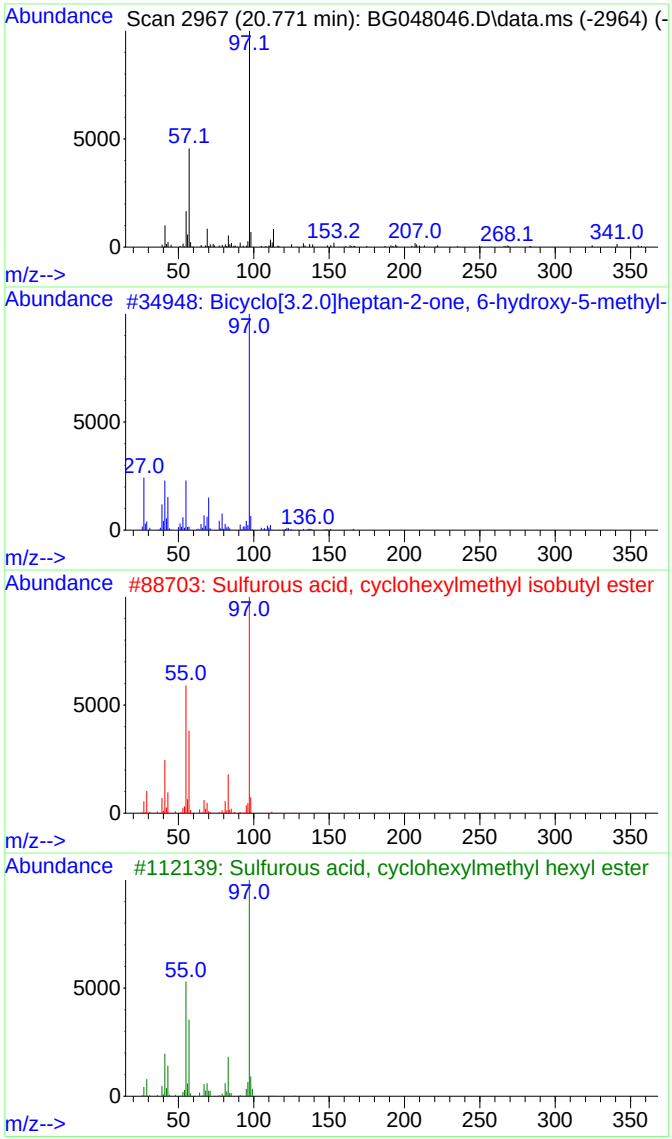
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

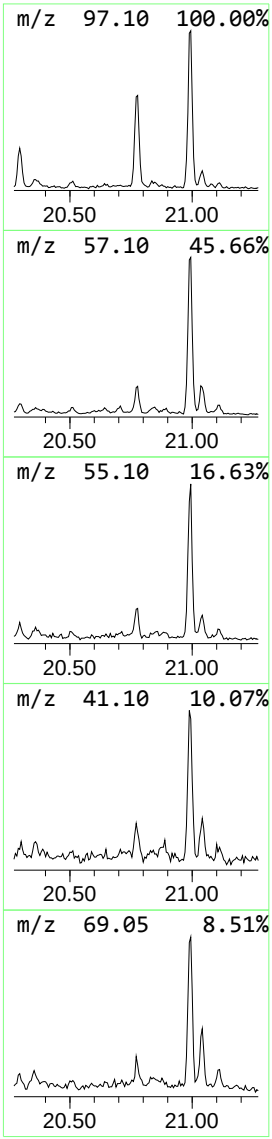
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Bicyclo[3.2.0]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.771	2.48 ng	119640	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.2.0]heptan-2-one, 6-hy...	166	C10H14O2	1000154-96-8	59
2	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	39
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	38
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	38
5	2-Hexenoic acid, 2-hexenyl ester...	196	C12H20O2	054845-28-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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

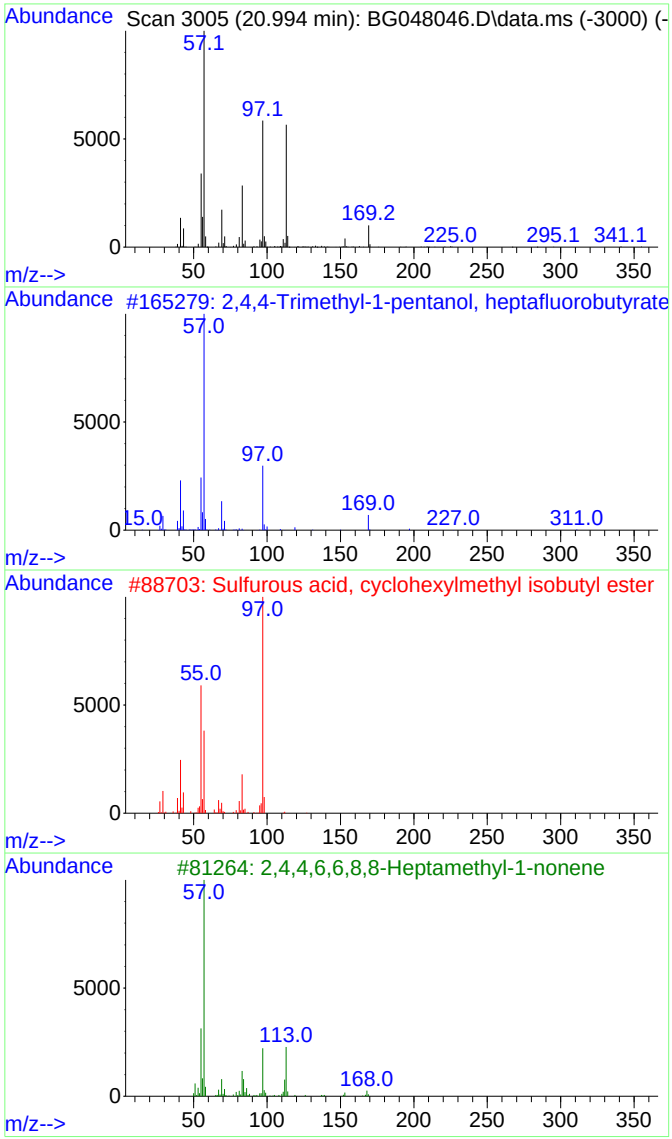
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

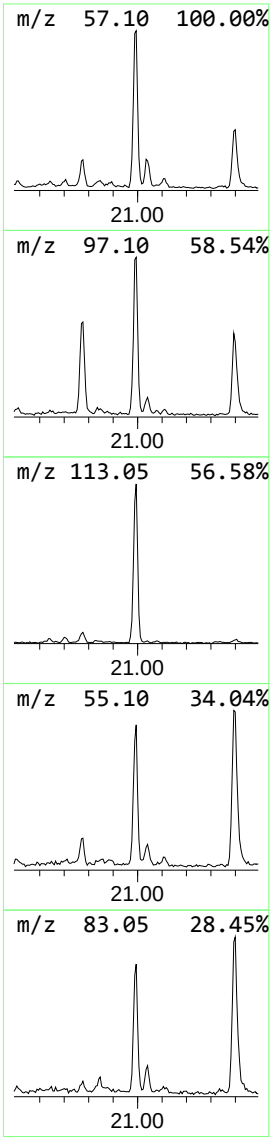
****

Peak Number 6 unknown20.994 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.994	10.26 ng	495692	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
2	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	27
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25
4	7-Ethyl-4,6-undecandione	212	C13H24O2	1000374-11-8	17
5	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

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

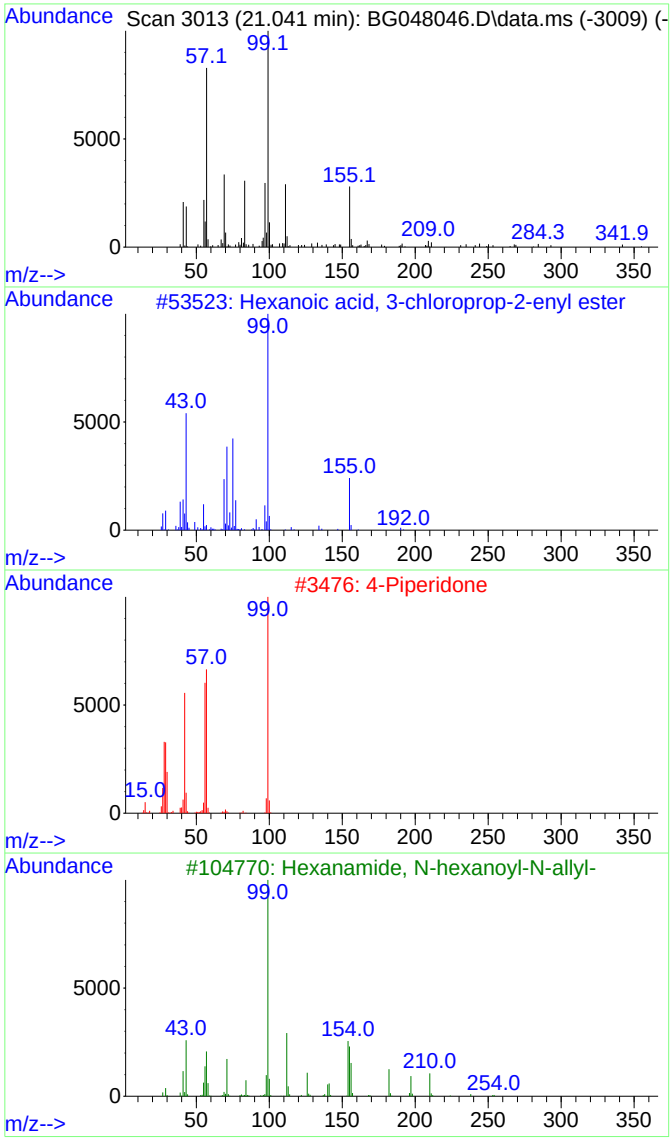
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

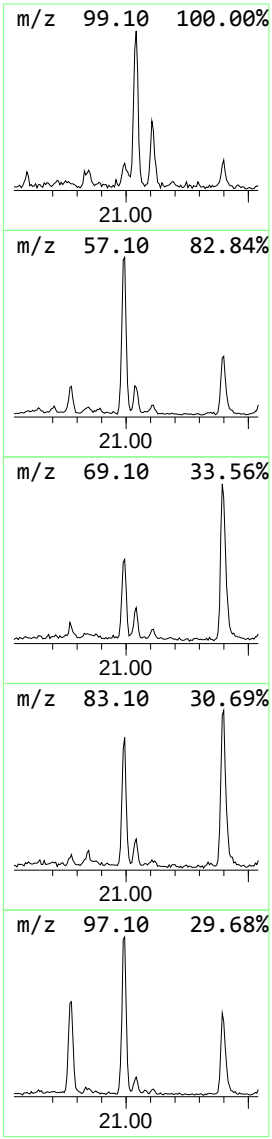
****

Peak Number 7 unknown21.041 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.041	2.55 ng	123233	Chrysene-d12	21.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	47
2	4-Piperidone	99	C5H9NO	041661-47-6	43
3	Hexanamide, N-hexanoyl-N-allyl-	253	C15H27NO2	1000340-15-1	43
4	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	43
5	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

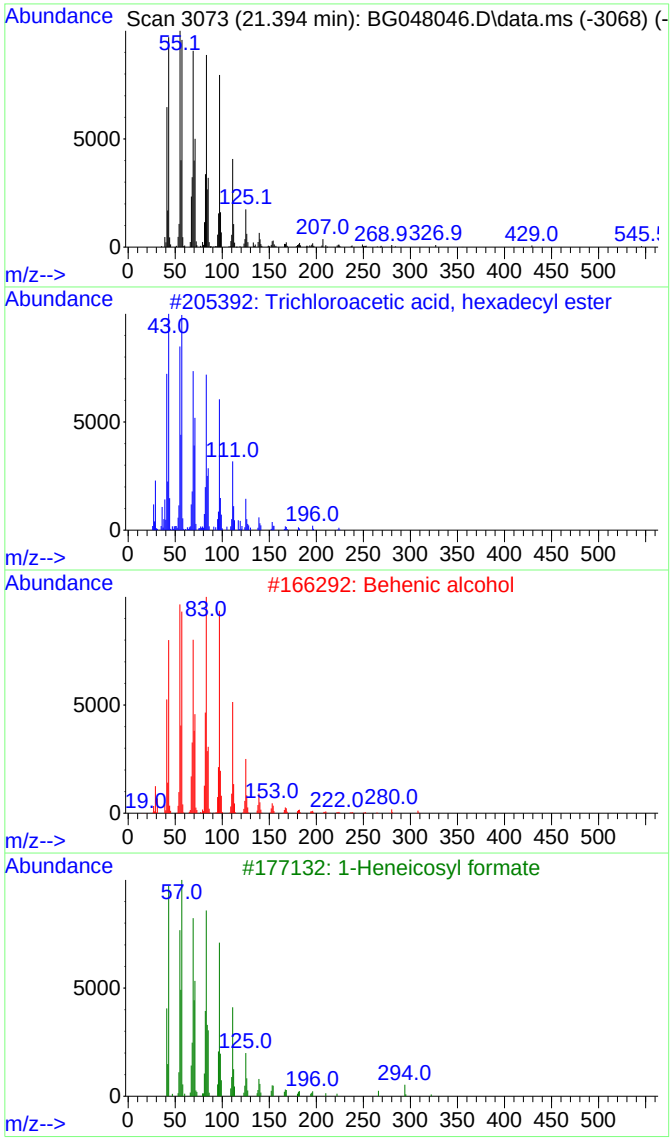
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

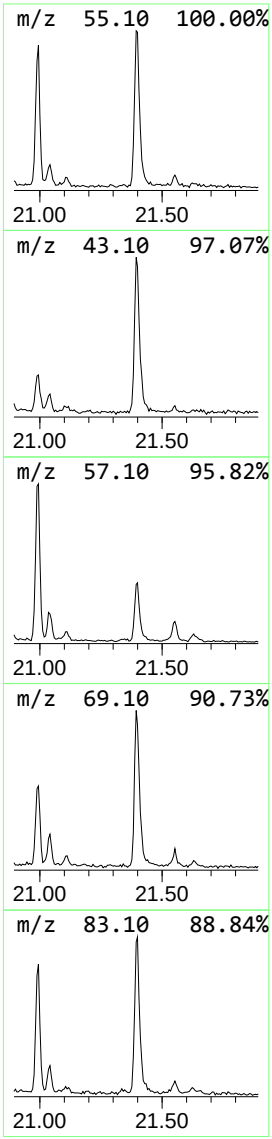
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.394	13.92 ng	672839	Chrysene-d12	21.764

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	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0050-044-COMP-D-ELUTRIATE

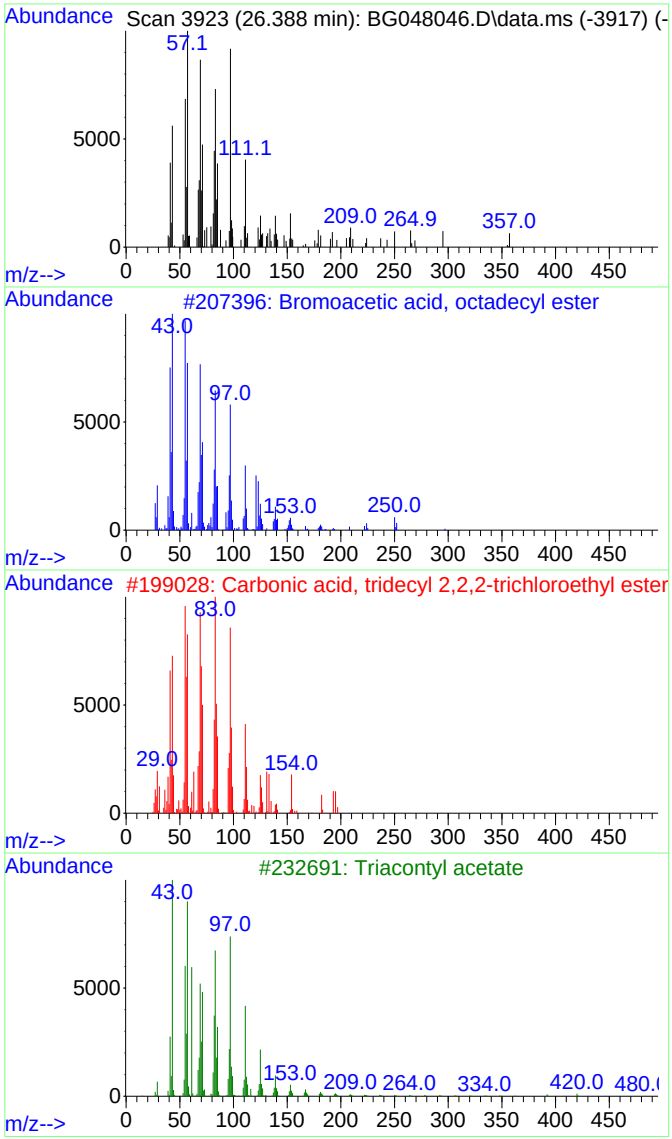
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

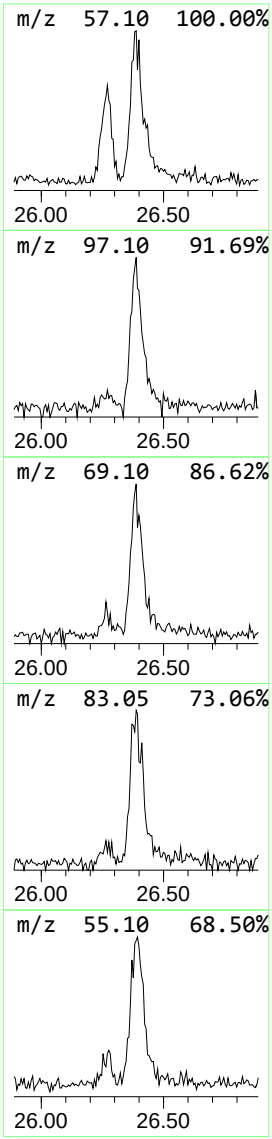
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.388	3.88 ng	192266	Perylene-d12	25.048

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
2	Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	86
3	Triacontyl acetate	480	C32H64O2	041755-58-2	76
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	53
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048046.D
Acq On : 28 Jan 2021 3:01
Operator : CG/JU
Sample : M1226-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0050-044-COMP-D-ELUTRIATE

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
1,2-Benzenedica...	17.762	24.3	ng	986929	4	17.486	810818	20.0
n-Hexadecanoic ...	18.374	23.6	ng	958688	4	17.486	810818	20.0
unknown19.137	19.137	5.8	ng	236438	4	17.486	810818	20.0
Octadecanoic acid	19.637	15.3	ng	740778	5	21.764	966509	20.0
Bicyclo[3.2.0]h...	20.771	2.5	ng	119640	5	21.764	966509	20.0
unknown20.994	20.994	10.3	ng	495692	5	21.764	966509	20.0
unknown21.041	21.041	2.5	ng	123233	5	21.764	966509	20.0
Trichloroacetic...	21.394	13.9	ng	672839	5	21.764	966509	20.0
Bromoacetic aci...	26.388	3.9	ng	192266	6	25.048	990055	20.0