LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0055-052-COMP-I-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: BG048049.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	411	rVB	610371	990040	23.50%	4.695%
2	7.268	662	669	680	rVB	462168	812188	19.28%	3.851%
3	8.125	808	815	821	rBV	189051	310599	7.37%	1.473%
4	9.283	1005	1012	1022	rVB	618580	1104826	26.23%	5.239%
5	10.934	1285	1293	1301	rBV	235634	425864	10.11%	2.019%
6	13.372	1699	1708	1717	rVB	1679498	2553683	60.63%	12.109%
7	14.189	1842	1847	1853	rBV	35360	52382	1.24%	0.248%
8	14.747	1934	1942	1949	rVB2	387563	634589	15.07%	3.009%
9	16.228	2185	2194	2209	rBV	1552720	2361745	56.07%	11.199%
10	17.491	2402	2409	2415	rVV	534744	817841	19.42%	3.878%
11	17.761	2451	2455	2458	rBV	36809	50353	1.20%	0.239%
12	18.372	2553	2559	2567	rBV	682865	902927	21.44%	4.282%
13	18.443	2567	2571	2583	rVB2	238460	372447	8.84%	1.766%
14	18.878	2641	2645	2651	rBV2	34661	58379	1.39%	0.277%
15	19.136	2684	2689	2694	rBV	265235	327035	7.76%	1.551%
16	19.224	2699	2704	2710	rBV	88358	113671	2.70%	0.539%
17	19.289	2712	2715	2722	rVB5	31366	44446	1.06%	0.211%
18	19.489	2742	2749	2751	rBV7	28969	47359	1.12%	0.225%
19	19.636	2768	2774	2785	rBV	456903	639616	15.18%	3.033%
20	19.765	2793	2796	2801	rVB	82316	95098	2.26%	0.451%
21	20.094	2845	2852	2857	rBV	3118750	4212191	100.00%	19.974%
22	20.294	2882	2886	2892	rBV	56576	74718	1.77%	0.354%
23	20.358	2892	2897	2902	rBV6	30517	65284	1.55%	0.310%
24	20.775	2964	2968	2973	rVB	116192	155466	3.69%	0.737%
25	20.993	3000	3005	3009	rBV	511589	648075	15.39%	3.073%
26	21.040	3009	3013	3017	rVV	129881	161140	3.83%	0.764%
27	21.110	3021	3025	3032	rVB2	50273	76736	1.82%	0.364%
28	21.398	3069	3074	3085	rVB	448615	648303	15.39%	3.074%
29	21.551	3096	3100	3106	rVB	58997	77378	1.84%	0.367%
30	21.762	3130	3136	3143	rVB2	588509	961109	22.82%	4.557%
31	22.961	3336	3340	3346	rVB3	47961	84843	2.01%	0.402%
32	25.041	3685	3694	3710	rVB2	327339	1002540	23.80%	4.754%
33	26.392	3917	3924	3934	rVB6	72249	205656	4.88%	0.975%

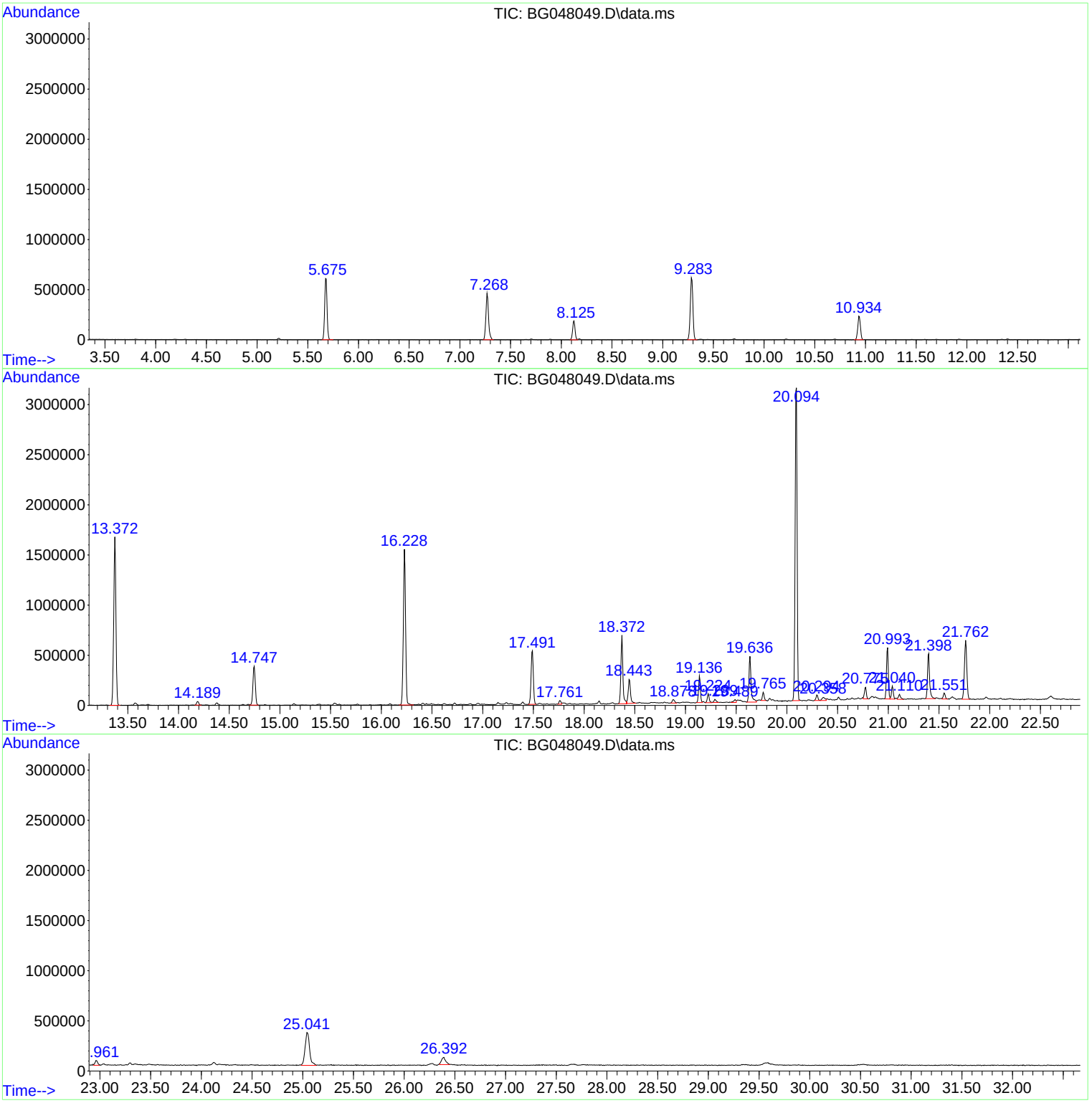
Sum of corrected areas: 21088527

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-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 : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

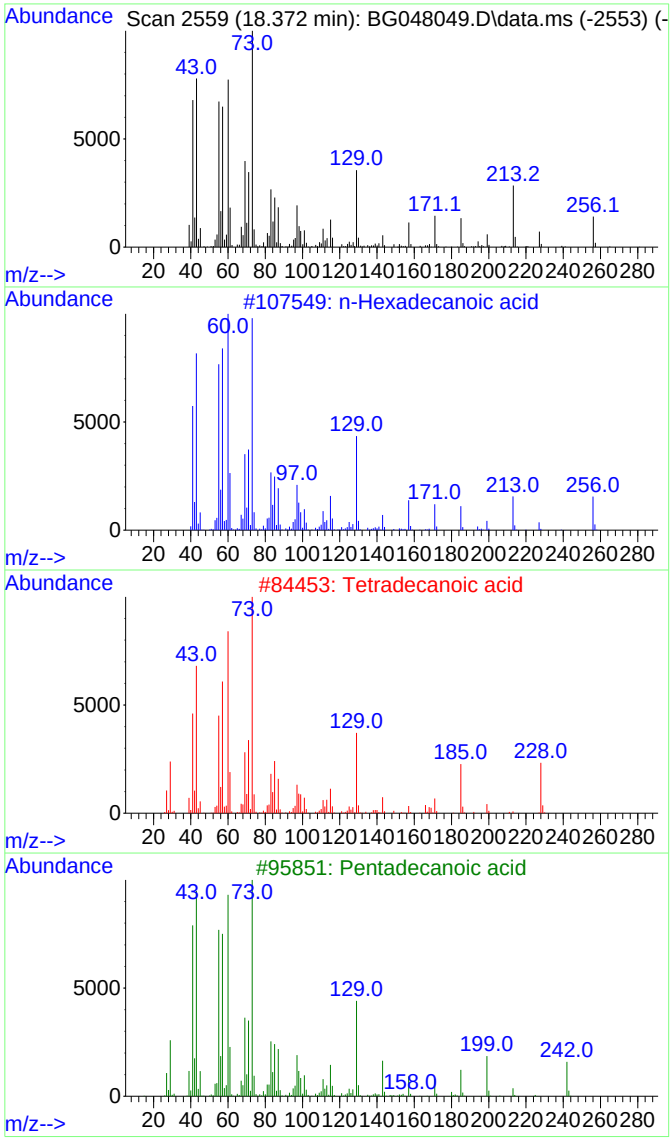
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

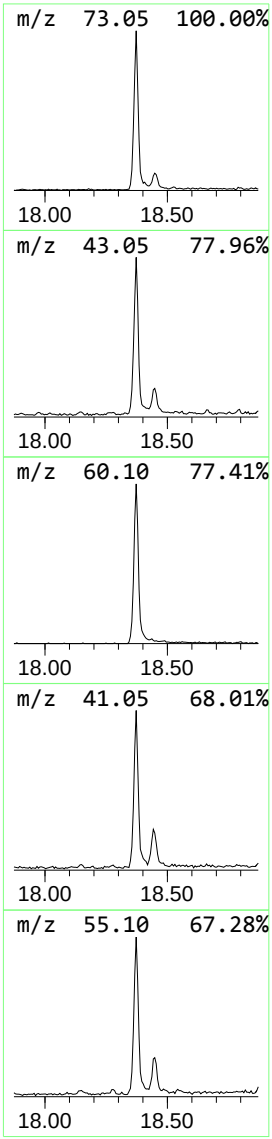
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.372	22.08 ng	902927	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

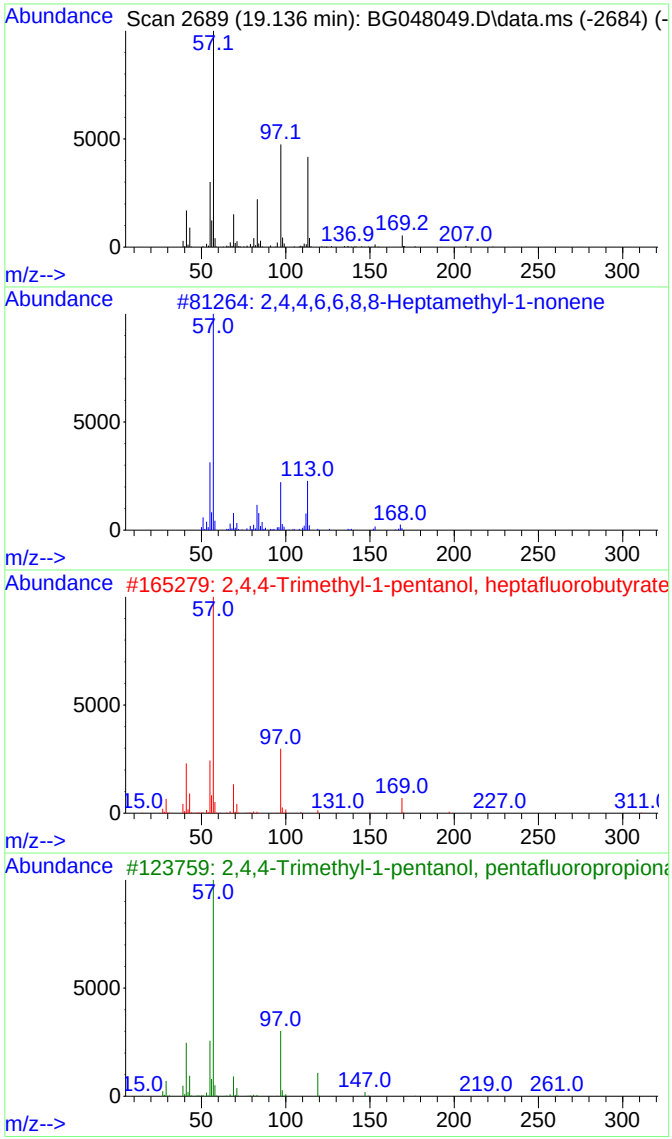
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

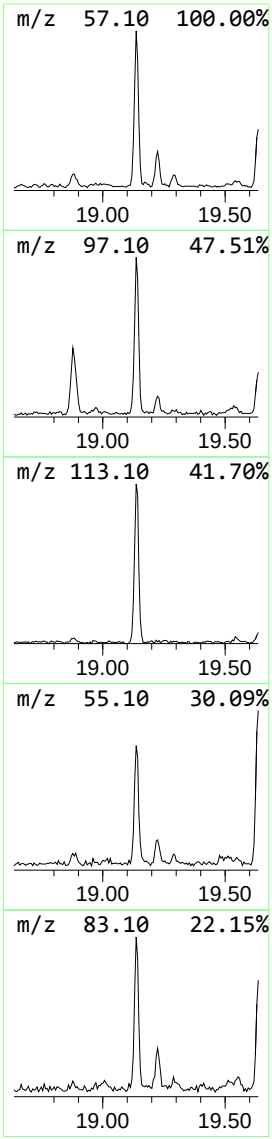
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.136	8.00 ng	327035	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	56
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

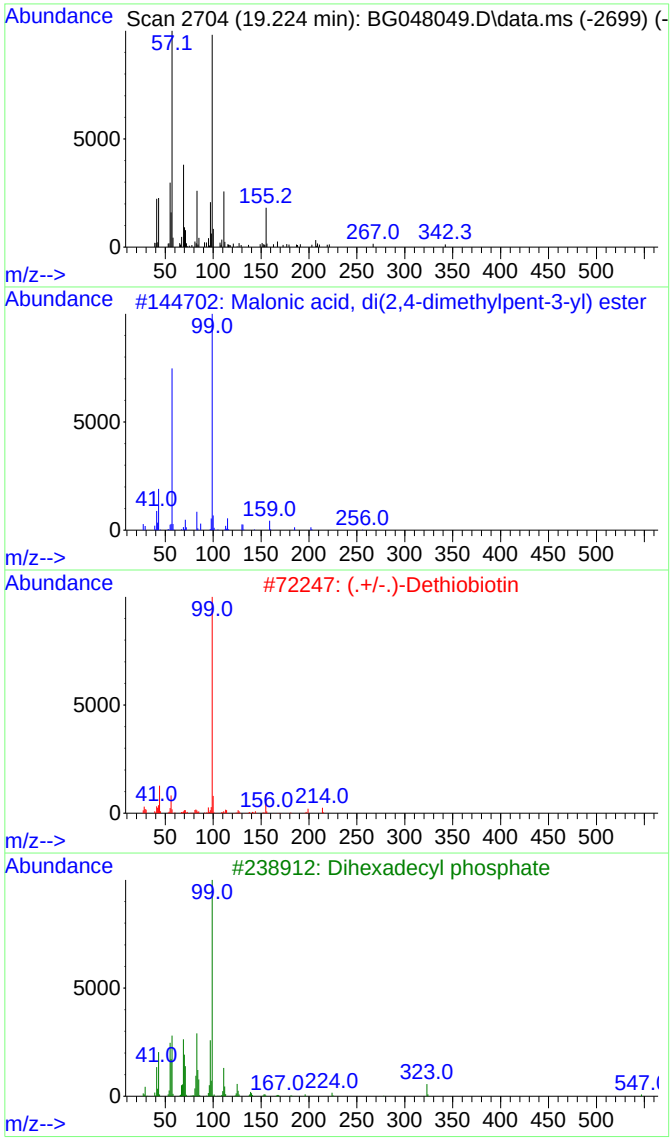
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

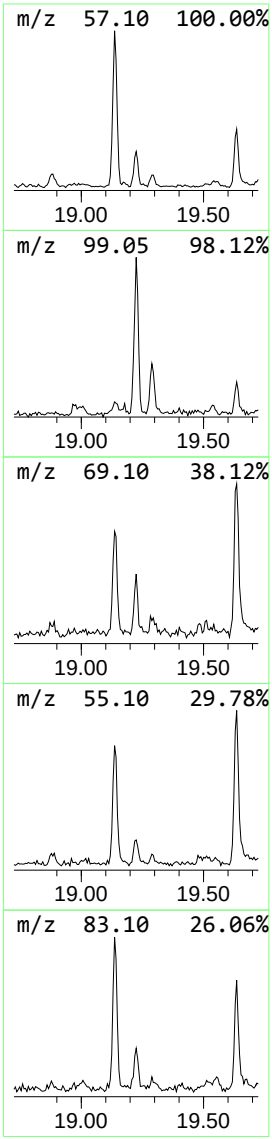
****

Peak Number 3 unknown19.224 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.224	2.78 ng	113671	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	47
2	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	43
3	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	42
4	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	38
5	Phthalic acid, di(2,4-dimethylpe...	362	C22H34O4	1000356-85-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

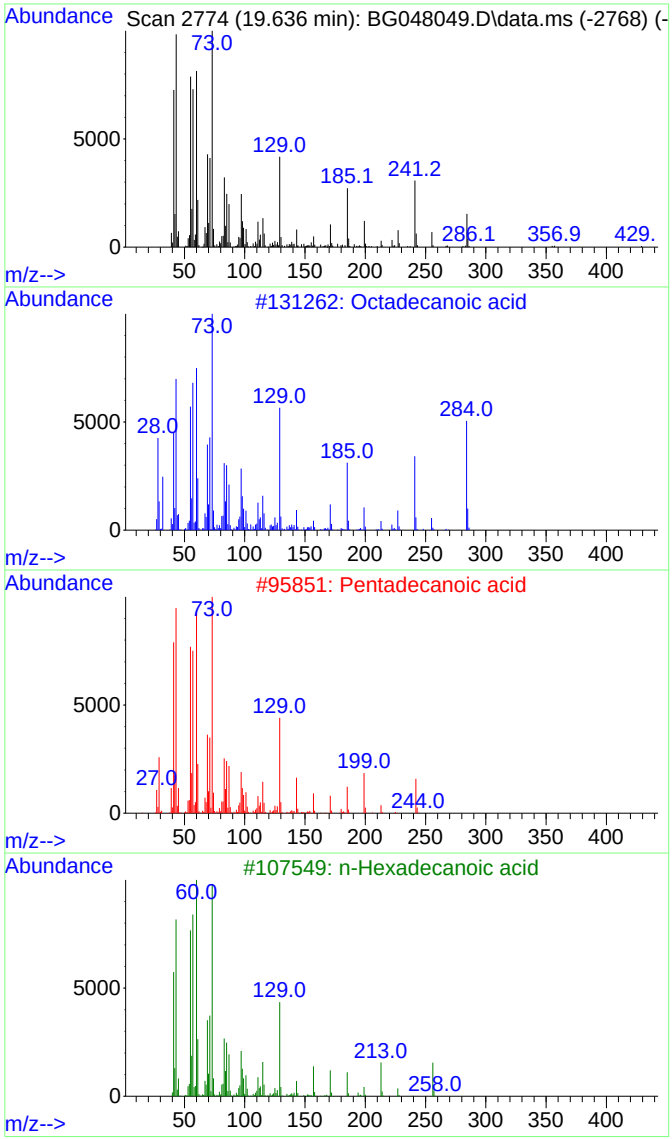
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

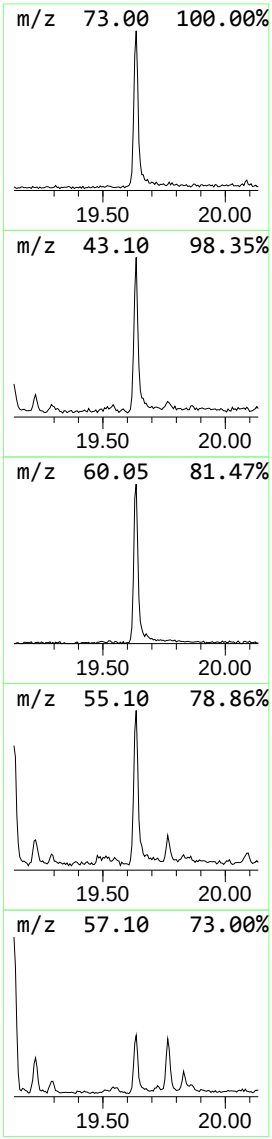
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.636	13.31 ng	639616	Chrysene-d12	21.762

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

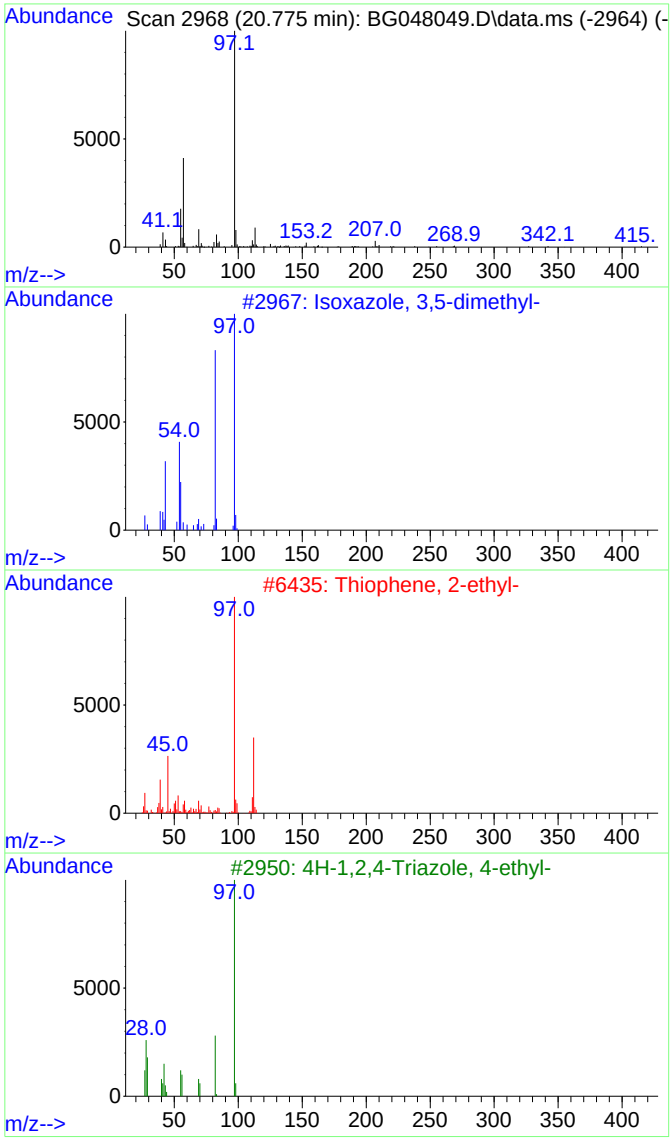
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

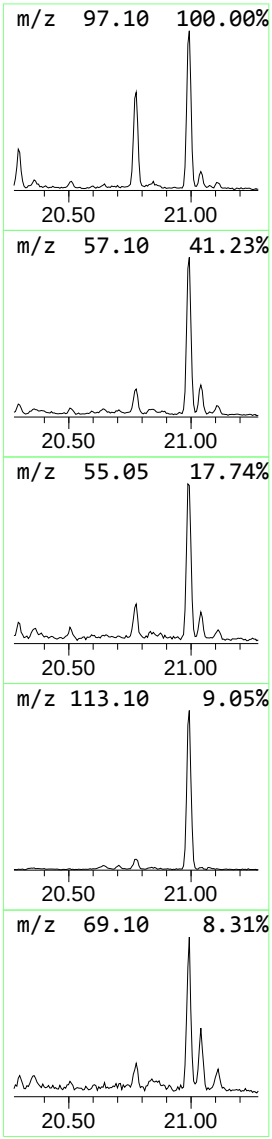
****

Peak Number 5 Isoxazole, 3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.775	3.24 ng	155466	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
2	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	42
3	4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	42
4	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	39
5	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

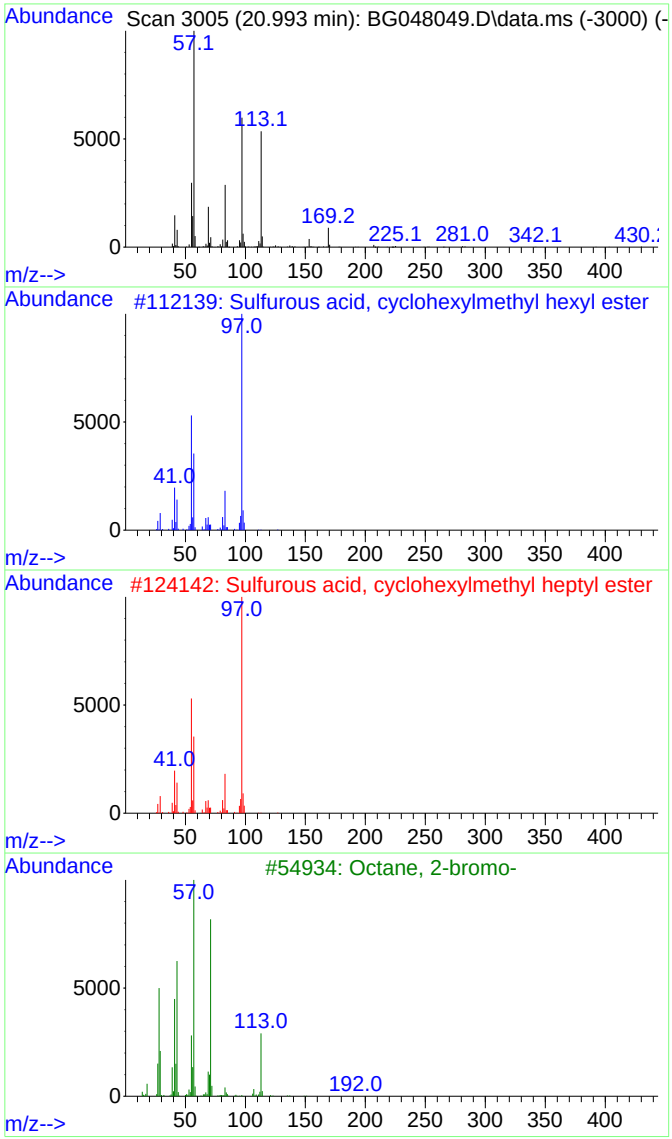
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

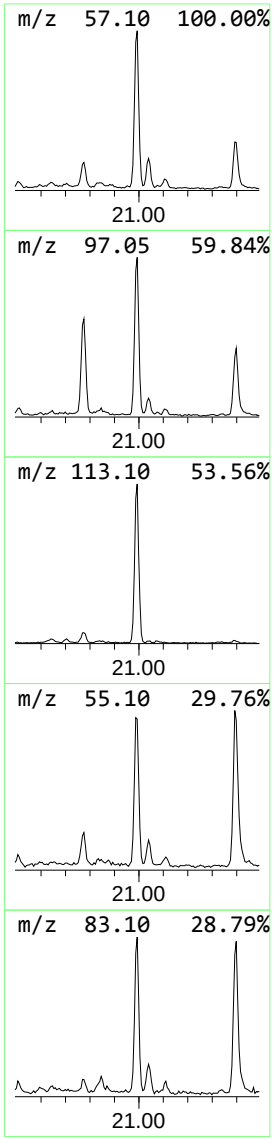
****

Peak Number 6 unknown20.933 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.993	13.49 ng	648075	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	43
2	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
4	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	35
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

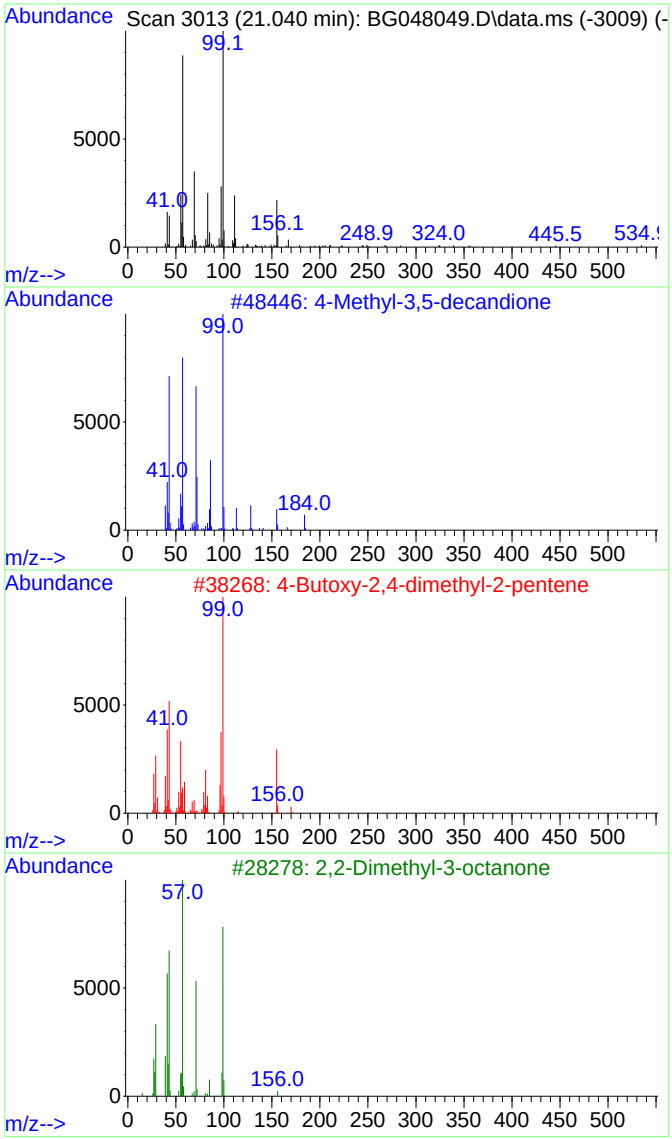
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

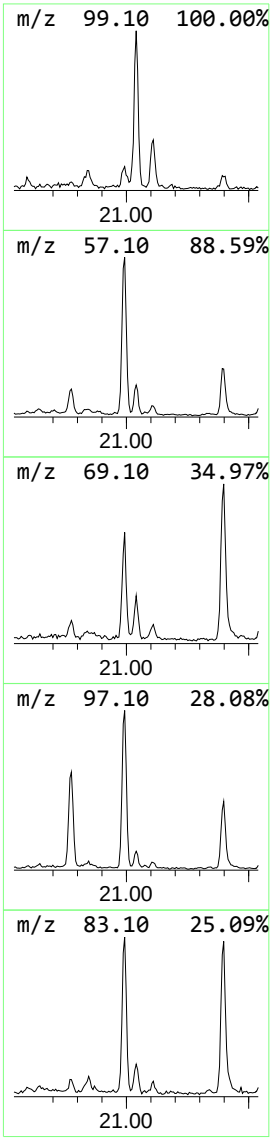
****

Peak Number 7 unknown21.040 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.040	3.35 ng	161140	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3,5-decandione	184	C11H20O2	1000374-13-1	40
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	40
3	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	32
4	D-Gulonic acid, .gamma.-lactone,...	254	C10H16B2O6	074128-60-2	25
5	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

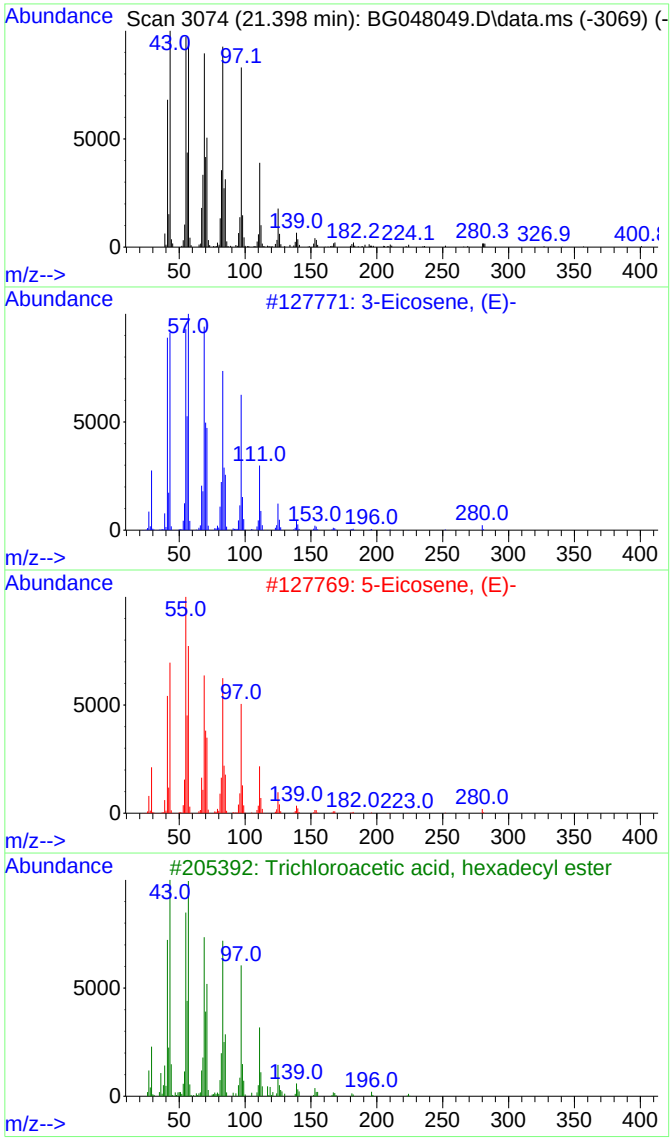
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

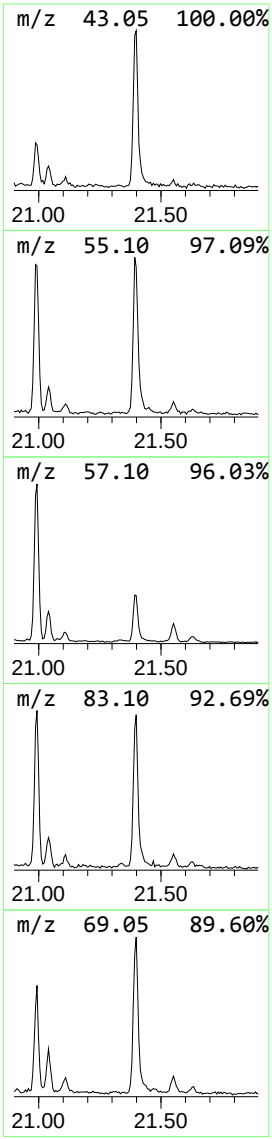
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	13.49 ng	648303	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

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

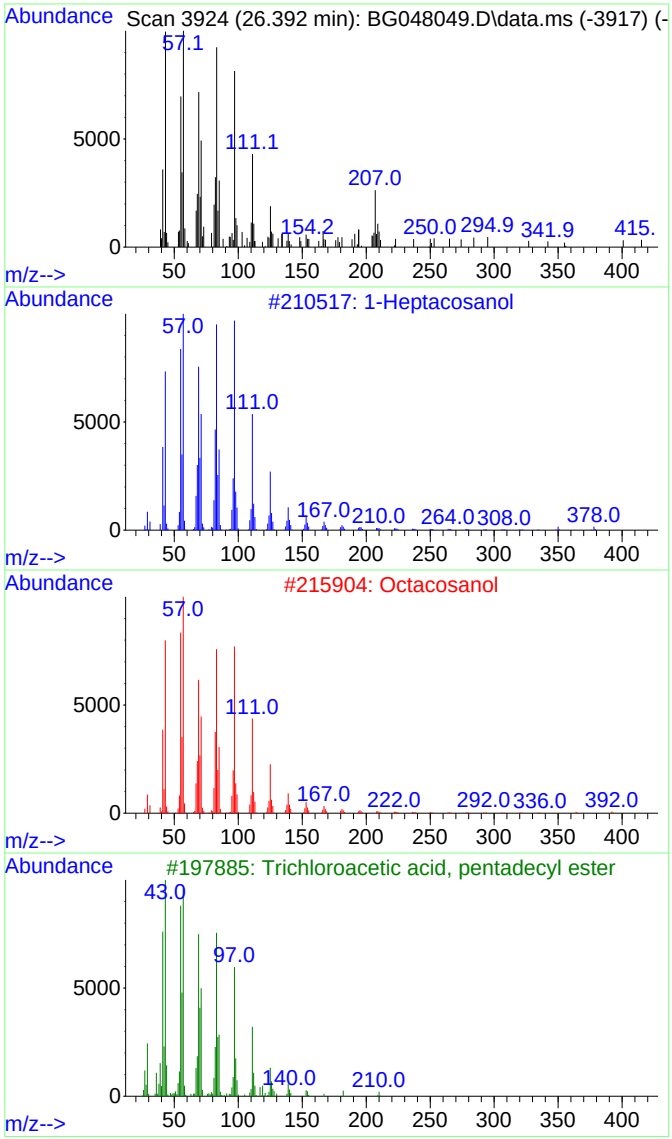
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

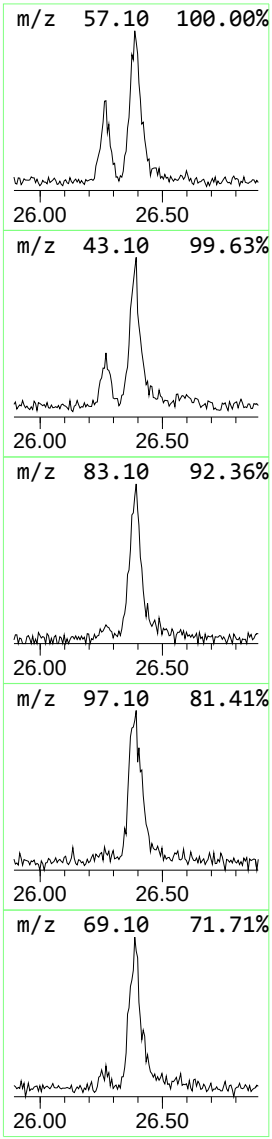
****

Peak Number 9 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.392	4.10 ng	205656	Perylene-d12	25.041

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	70
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048049.D
Acq On : 28 Jan 2021 5:02
Operator : CG/JU
Sample : M1226-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0055-052-COMP-I-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
n-Hexadecanoic ...	18.372	22.1	ng	902927	4	17.491	817841	20.0
2,4,4,6,6,8,8-H...	19.136	8.0	ng	327035	4	17.491	817841	20.0
unknown19.224	19.224	2.8	ng	113671	4	17.491	817841	20.0
Octadecanoic acid	19.636	13.3	ng	639616	5	21.762	961109	20.0
Isoxazole, 3,5-...	20.775	3.2	ng	155466	5	21.762	961109	20.0
unknown20.933	20.993	13.5	ng	648075	5	21.762	961109	20.0
unknown21.040	21.040	3.4	ng	161140	5	21.762	961109	20.0
3-Eicosene, (E)-	21.398	13.5	ng	648303	5	21.762	961109	20.0
1-Heptacosanol	26.392	4.1	ng	205656	6	25.041	1002540	20.0