LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048050.D
Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

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: BG048050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.680	391	398	409	rVB	768425	1209339	44.72%	7.847%
2	7.272	661	669	681	rVB	788492	1384319	51.19%	8.982%
3	8.124	807	814	820	rBV2	198447	325578	12.04%	2.113%
4	9.282	1004	1011	1023	rVB	439894	814137	30.11%	5.283%
5	10.938	1285	1293	1300	rBV	249328	444342	16.43%	2.883%
6	13.371	1700	1707	1715	rBV	1120801	1665591	61.60%	10.807%
7	13.635	1746	1752	1759	rVB2	59532	90291	3.34%	0.586%
8	14.188	1840	1846	1851	rBV	28072	41949	1.55%	0.272%
9	14.746	1934	1941	1949	rVB	428702	663351	24.53%	4.304%
10	16.226	2187	2193	2204	rBV	1067359	1588013	58.73%	10.304%
11	17.490	2401	2408	2414	rBV	557627	849188	31.40%	5.510%
12	18.365	2552	2557	2568	rBV	224915	327769	12.12%	2.127%
13	18.882	2640	2645	2650	rBV2	18726	30822	1.14%	0.200%
14	19.135	2684	2688	2696	rVB	117015	148957	5.51%	0.967%
15	19.223	2698	2703	2708	rBV	63149	93531	3.46%	0.607%
16	19.540	2749	2757	2762	rVB10	23256	50902	1.88%	0.330%
17	19.628	2768	2772	2780	rBV	89939	123707	4.57%	0.803%
18	19.763	2792	2795	2802	rVB4	26033	44732	1.65%	0.290%
19	20.087	2844	2850	2856	rBV	2012347	2704034	100.00%	17.545%
20	20.357	2890	2896	2900	rBV8	23224	37464	1.39%	0.243%
21	20.991	3001	3004	3009	rVB2	27802	35054	1.30%	0.227%
22	21.397	3068	3073	3081	rBV	269801	388357	14.36%	2.520%
23	21.761	3129	3135	3150	rVB2	592447	987254	36.51%	6.406%
24	22.607	3273	3279	3289	rVB2	23391	59157	2.19%	0.384%
25	23.494	3424	3430	3438	rVB	177140	344530	12.74%	2.236%
26	25.045	3684	3694	3709	rBV2	328446	959297	35.48%	6.224%

Sum of corrected areas: 15411665

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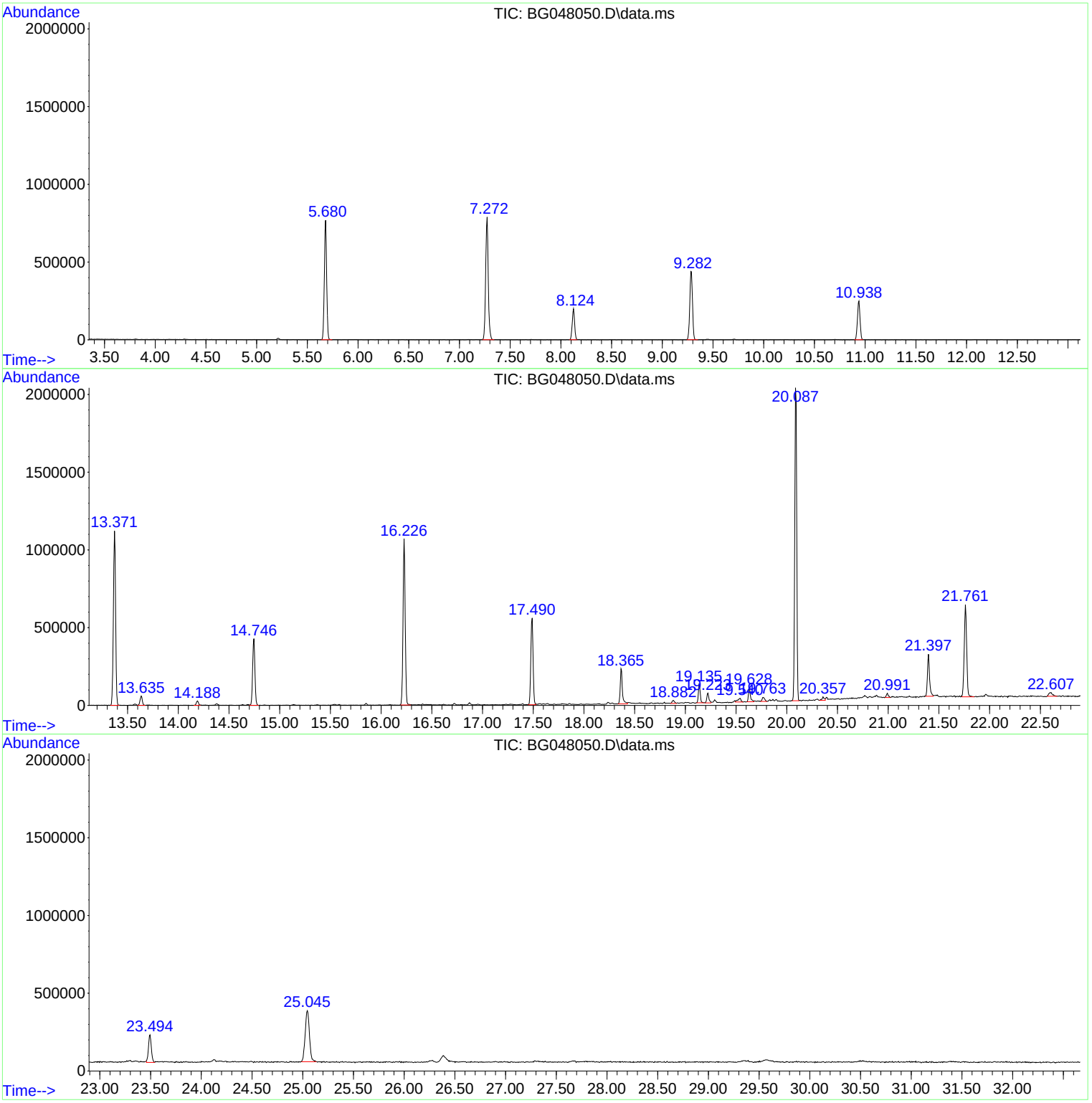
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
5

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 : BG048050.D
Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
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Instrument : BNA_G
ClientSampleId : 5

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

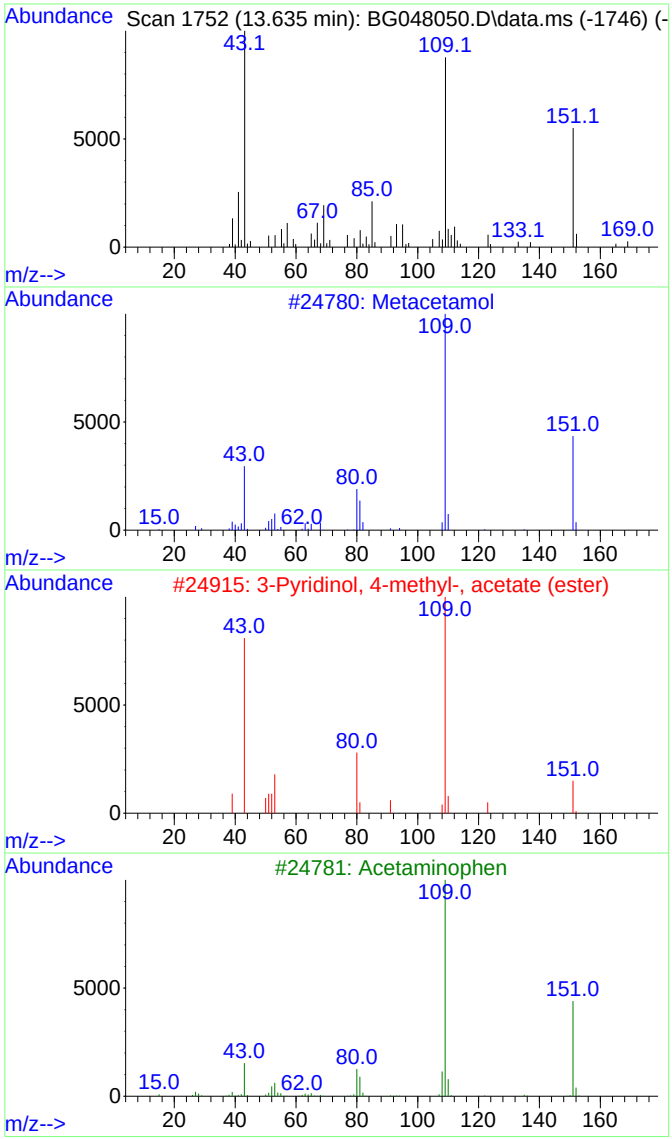
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

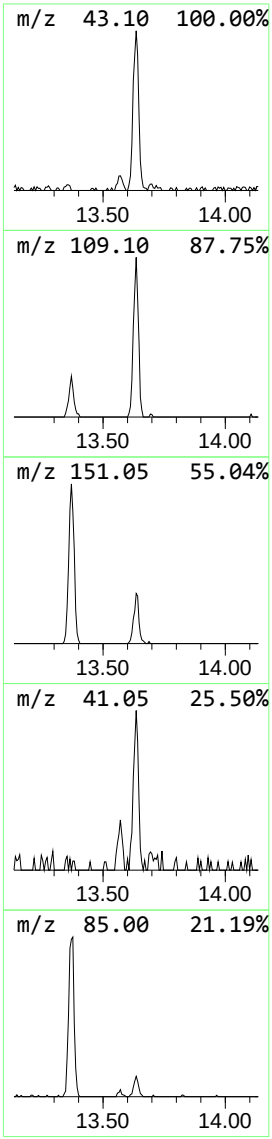
****

Peak Number 1 Metacetamol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.635	2.72 ng	90291	Acenaphthene-d10	14.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	53
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	53
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048050.D
Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

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

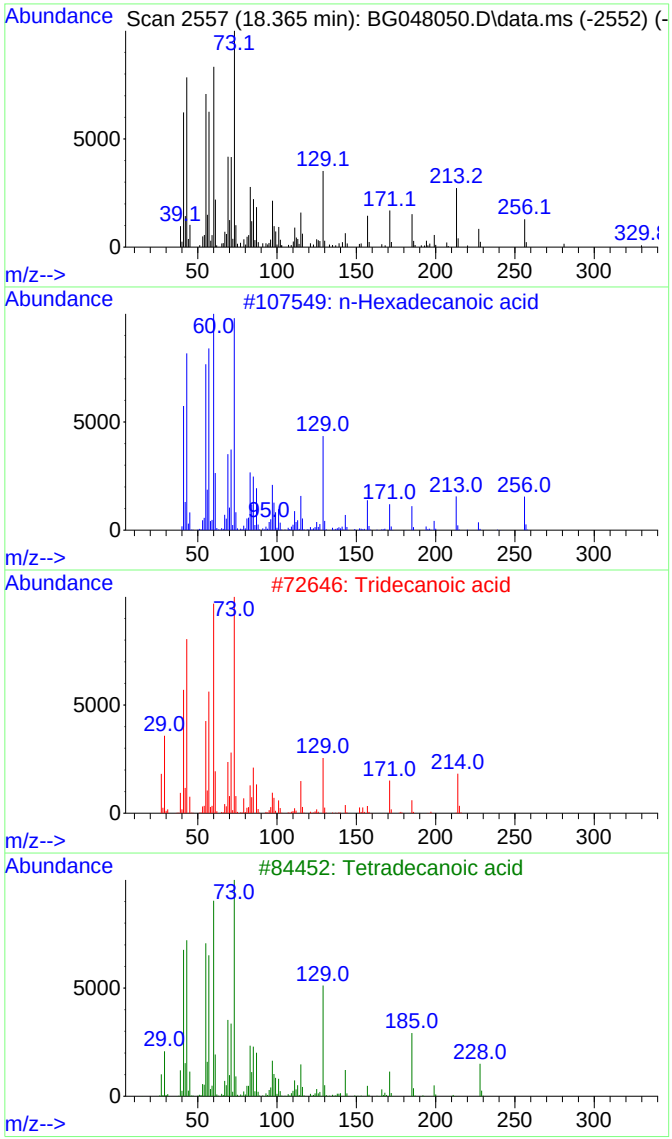
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

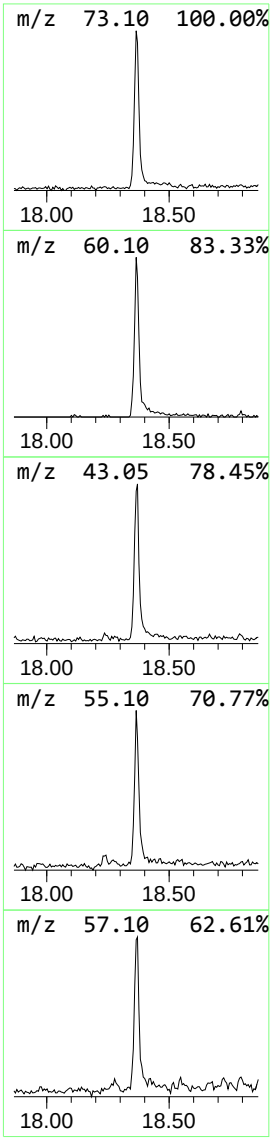
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.365	7.72 ng	327769	Phenanthrene-d10	17.490

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048050.D
Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

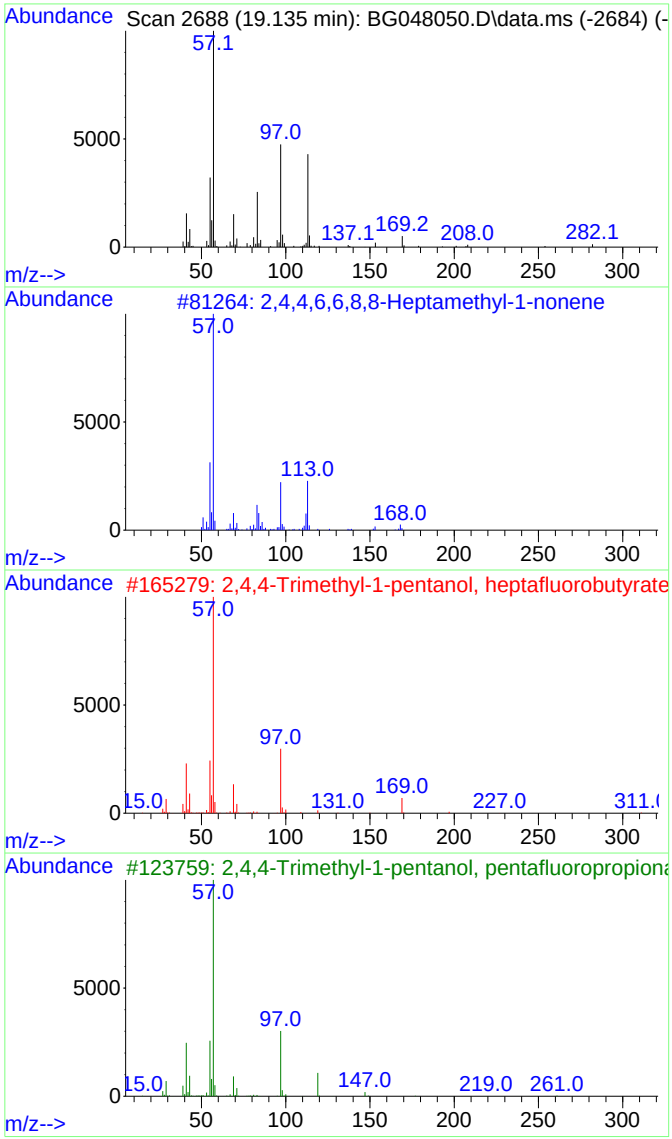
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

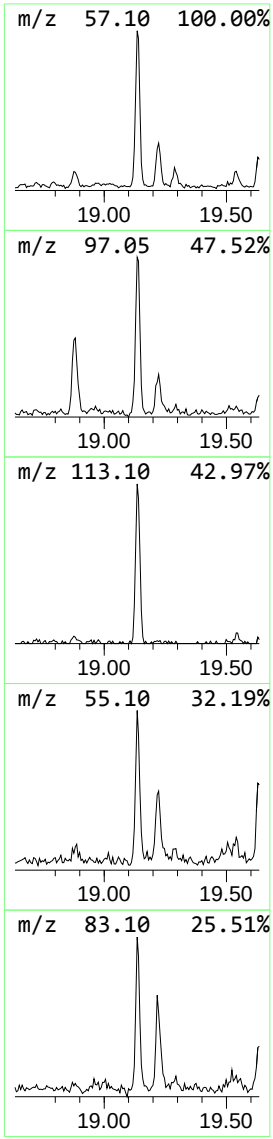
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.135	3.51 ng	148957	Phenanthrene-d10	17.490

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	78
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048050.D
Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

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

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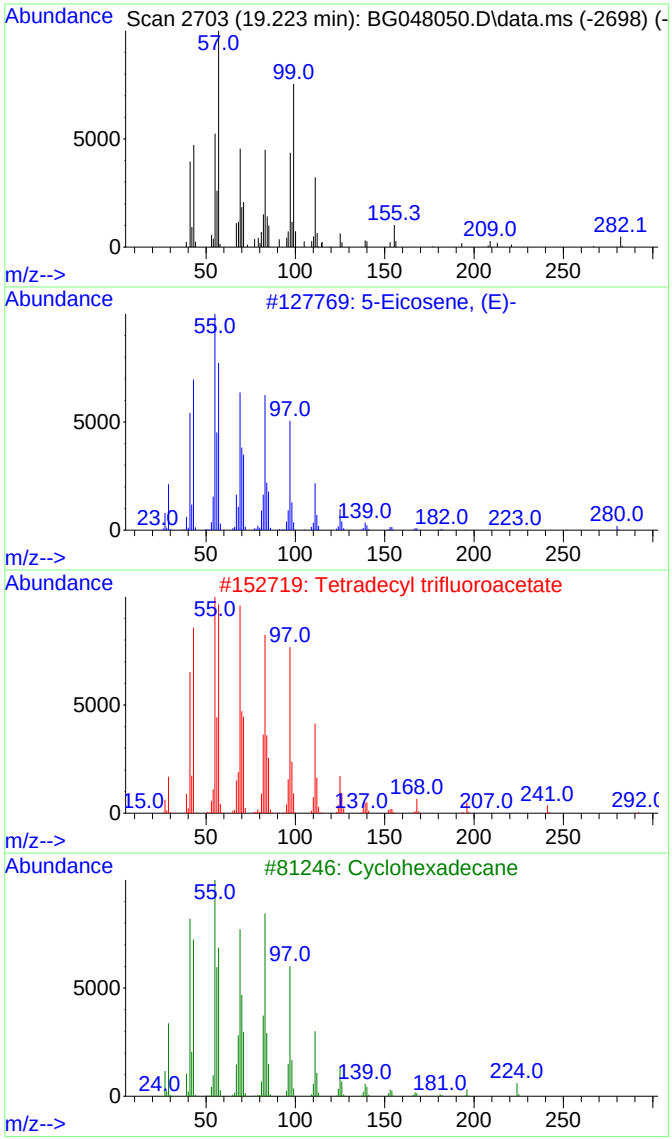
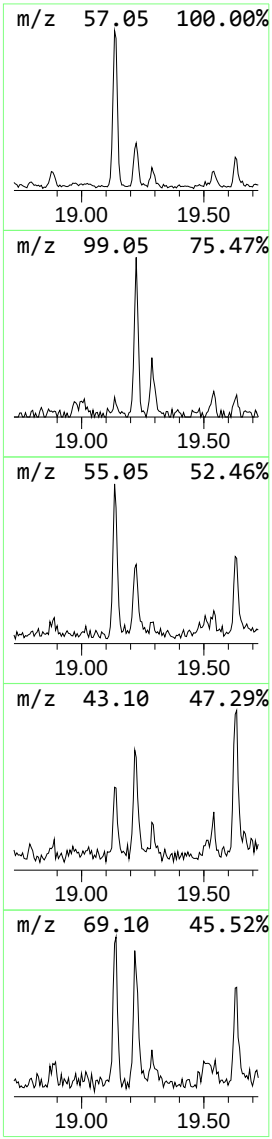
Peak Number 4 unknown19.223 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.223	2.20 ng	93531	Phenanthrene-d10	17.490

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	43
2	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	43
3	Cyclohexadecane	224	C16H32	000295-65-8	41
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	38
5	1,4-Dioxaspiro[4.5]decane-6-carb...	213	C11H19NO3	1000191-48-0	35





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Acq On : 28 Jan 2021 5:43
Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

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

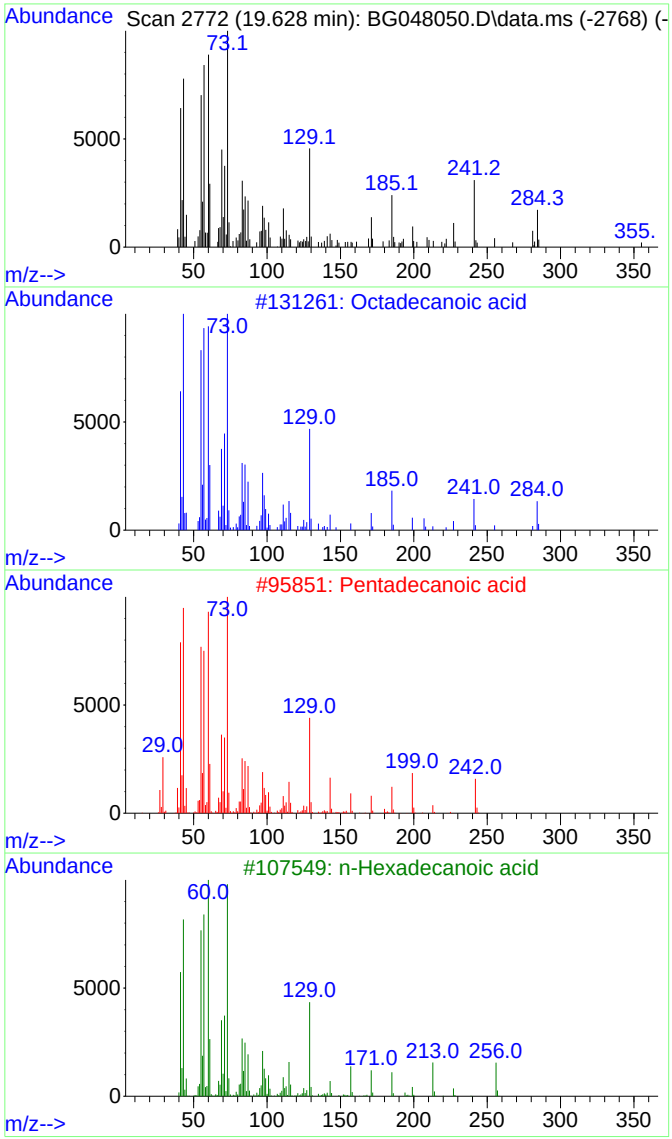
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

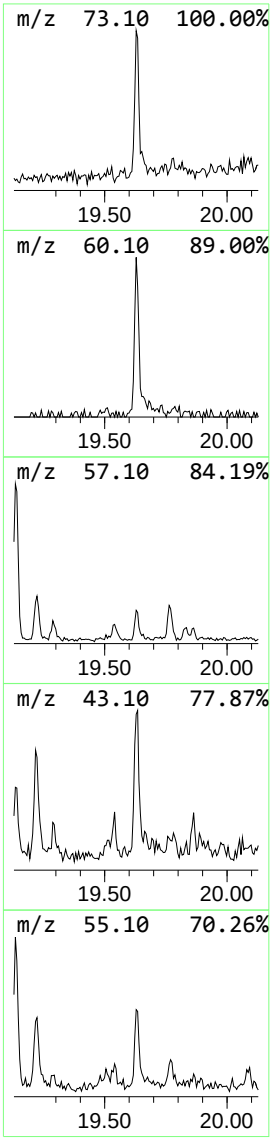
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.628	2.51 ng	123707	Chrysene-d12	21.761

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Operator : CG/JU
Sample : M1249-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 5

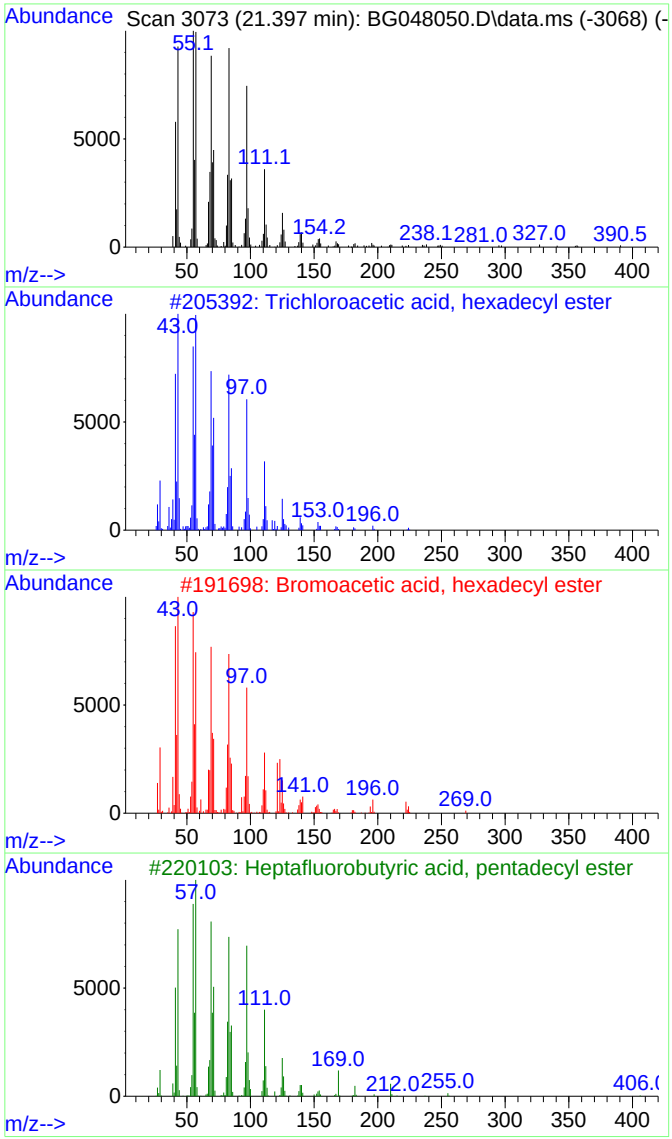
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

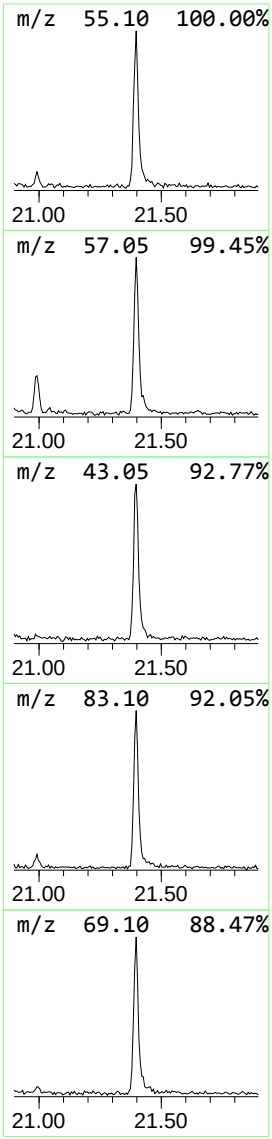
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.397	7.87 ng	388357	Chrysene-d12	21.761

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Operator : CG/JU
Sample : M1249-04
Misc :
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Instrument : BNA_G
ClientSampleId : 5

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

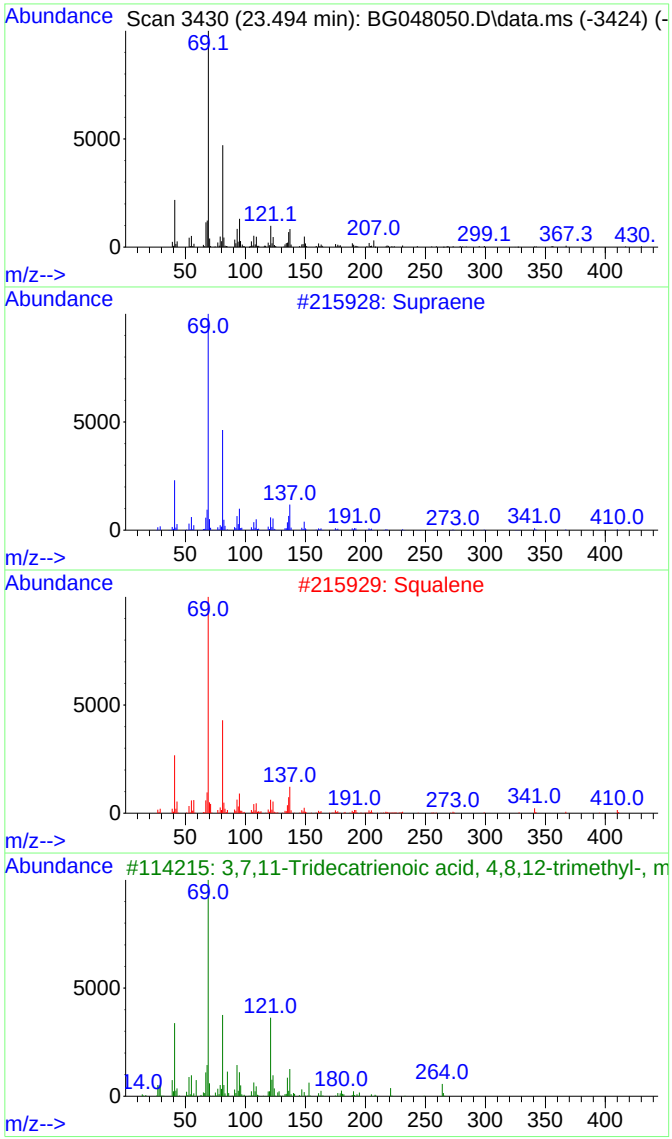
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

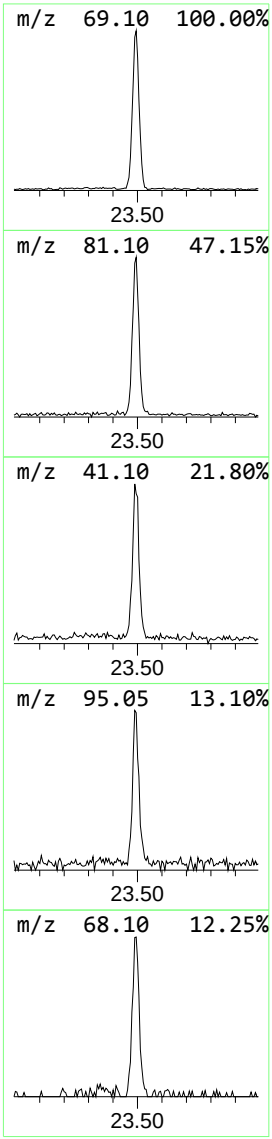
****

Peak Number 7 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.494	7.18 ng	344530	Perylene-d12	25.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	86
3	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	53





Tentatively Identified Compound (LSC) summary

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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
Metacetamol	13.635	2.7	ng	90291	3	14.746	663351	20.0
n-Hexadecanoic ...	18.365	7.7	ng	327769	4	17.490	849188	20.0
2,4,4,6,6,8,8-H...	19.135	3.5	ng	148957	4	17.490	849188	20.0
unknown19.223	19.223	2.2	ng	93531	4	17.490	849188	20.0
Octadecanoic acid	19.628	2.5	ng	123707	5	21.761	987254	20.0
Trichloroacetic...	21.397	7.9	ng	388357	5	21.761	987254	20.0
Supraene	23.494	7.2	ng	344530	6	25.045	959297	20.0