LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 135-136

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050637.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.792	384	392	401	rBV	416051	691701	23.45%	4.392%
2	7.390	657	664	672	rBV	254385	458071	15.53%	2.908%
3	8.254	800	811	822	rBV	151530	269876	9.15%	1.713%
4	9.423	1001	1010	1020	rBV	578274	1059761	35.92%	6.728%
5	9.647	1020	1048	1067	rVV	442375	2185137	74.07%	13.873%
6	10.310	1155	1161	1171	rBV	20729	48019	1.63%	0.305%
7	10.827	1243	1249	1258	rBV2	28337	58237	1.97%	0.370%
8	11.080	1283	1292	1301	rBV	204006	384811	13.04%	2.443%
9	13.495	1694	1703	1710	rBV	1386323	2199907	74.57%	13.967%
10	14.376	1844	1853	1861	rBV	118577	176477	5.98%	1.120%
11	14.870	1931	1937	1944	rVB	351718	553968	18.78%	3.517%
12	15.375	2016	2023	2027	rBV2	19540	30753	1.04%	0.195%
13	16.350	2182	2189	2200	rBV	1006101	1680972	56.98%	10.673%
14	17.614	2398	2404	2413	rBV	387465	625283	21.19%	3.970%
15	18.072	2478	2482	2487	rBV2	30362	51414	1.74%	0.326%
16	18.471	2546	2550	2562	rBV	150666	258914	8.78%	1.644%
17	19.741	2761	2766	2781	rBV	454334	726503	24.62%	4.613%
18	20.205	2839	2845	2854	rVB	2219771	2950273	100.00%	18.731%
19	21.609	3081	3084	3088	rVB	24488	31500	1.07%	0.200%
20	21.914	3129	3136	3143	rVB	352244	632781	21.45%	4.018%
21	25.322	3704	3716	3729	rBV2	213883	676138	22.92%	4.293%

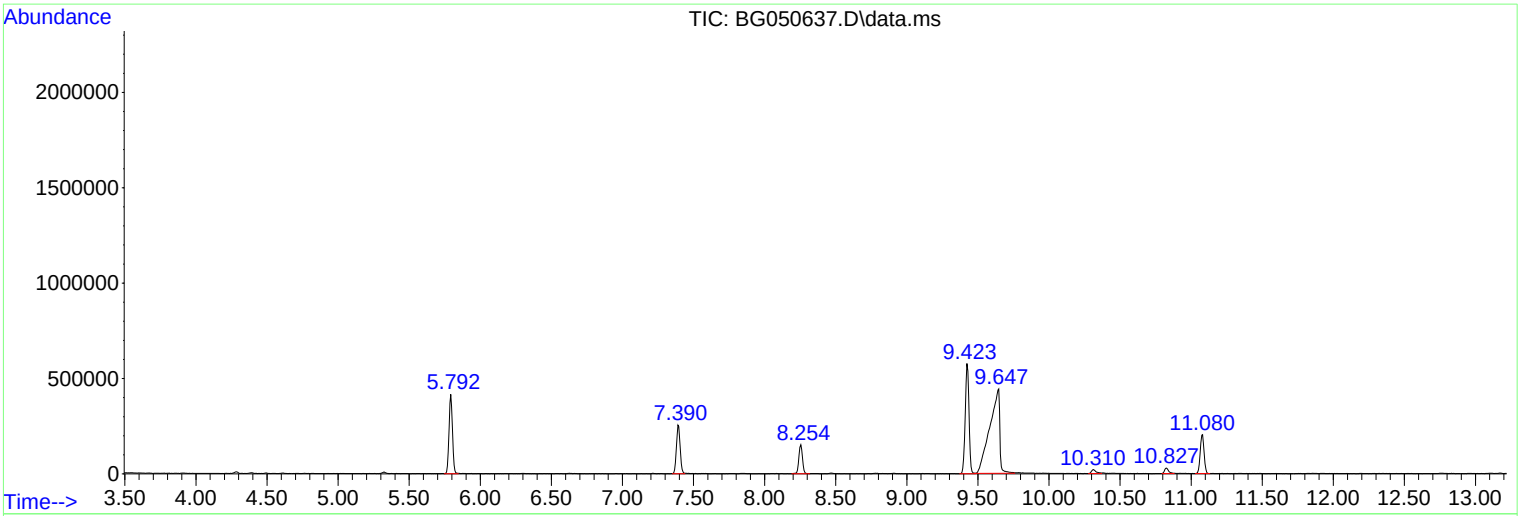
Sum of corrected areas: 15750496

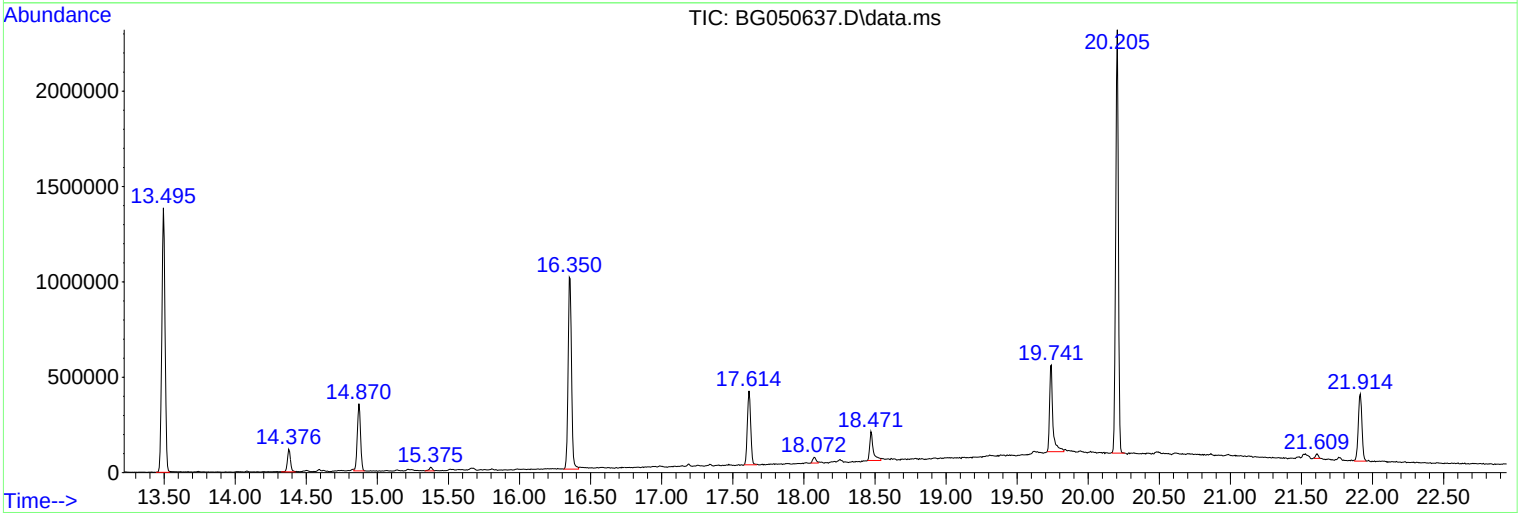
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

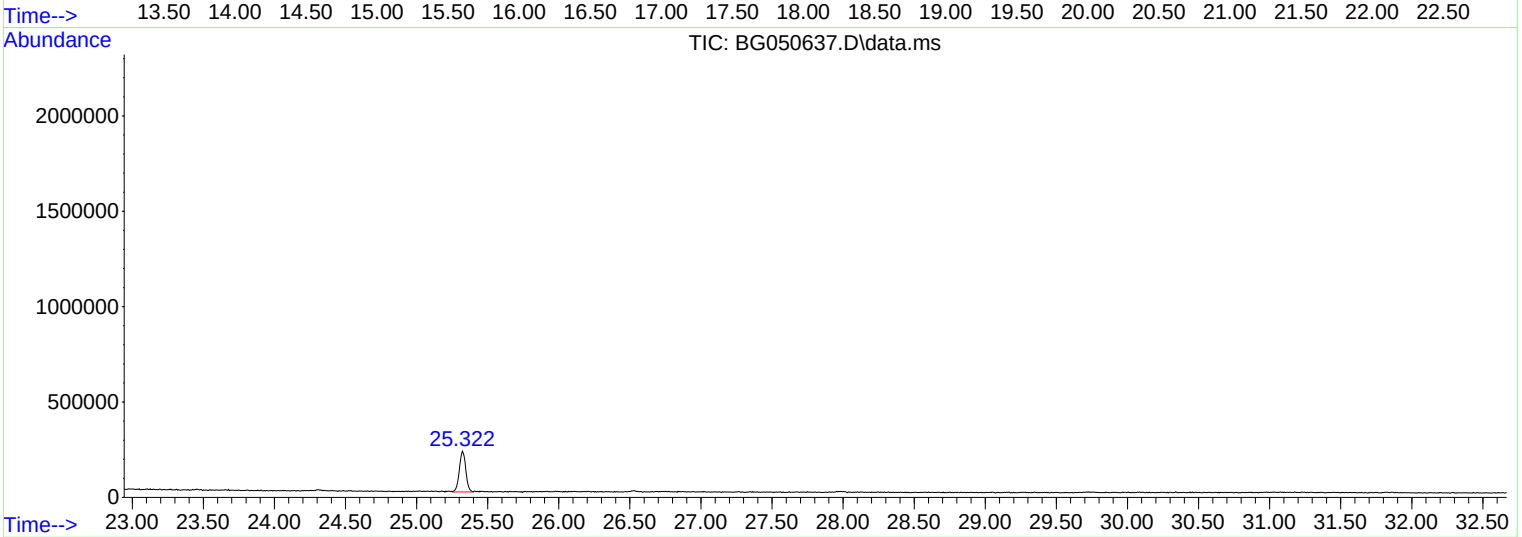
Instrument :
BNA_G
ClientSampleId :
135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

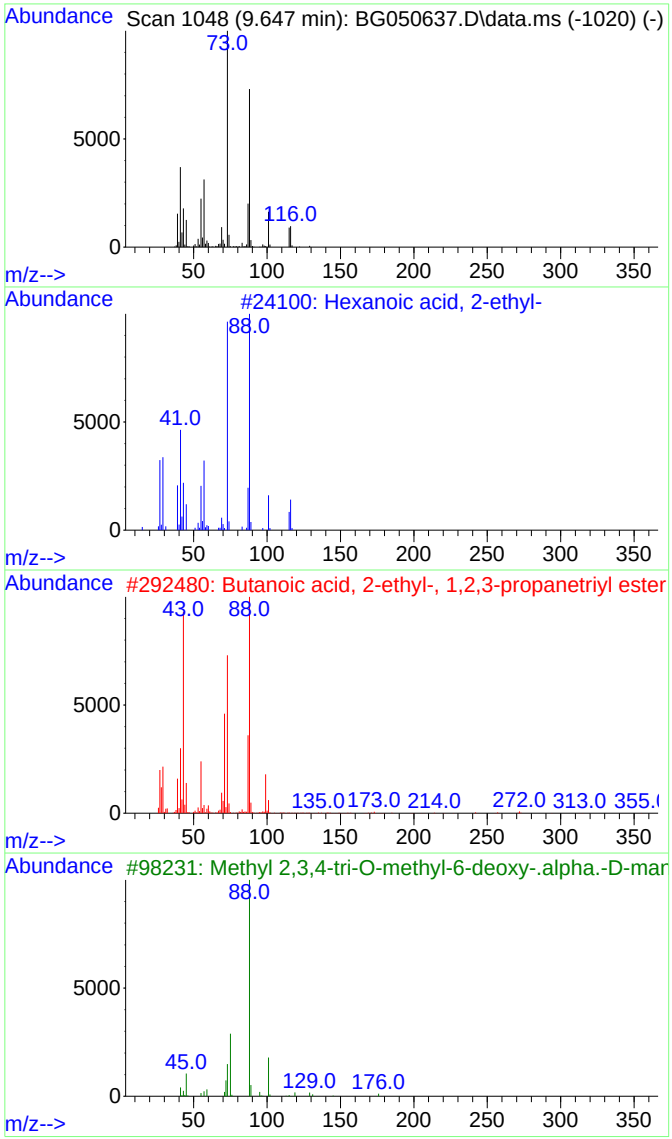
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

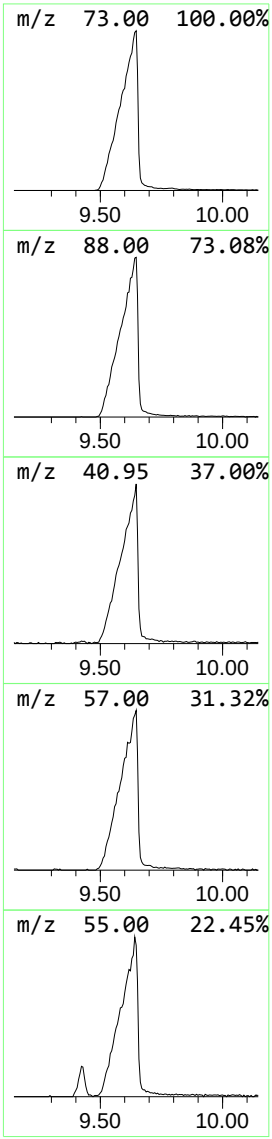
****

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.647	161.94 ng	2185140	1,4-Dichlorobenzene-d4	8.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	32
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	32
5	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

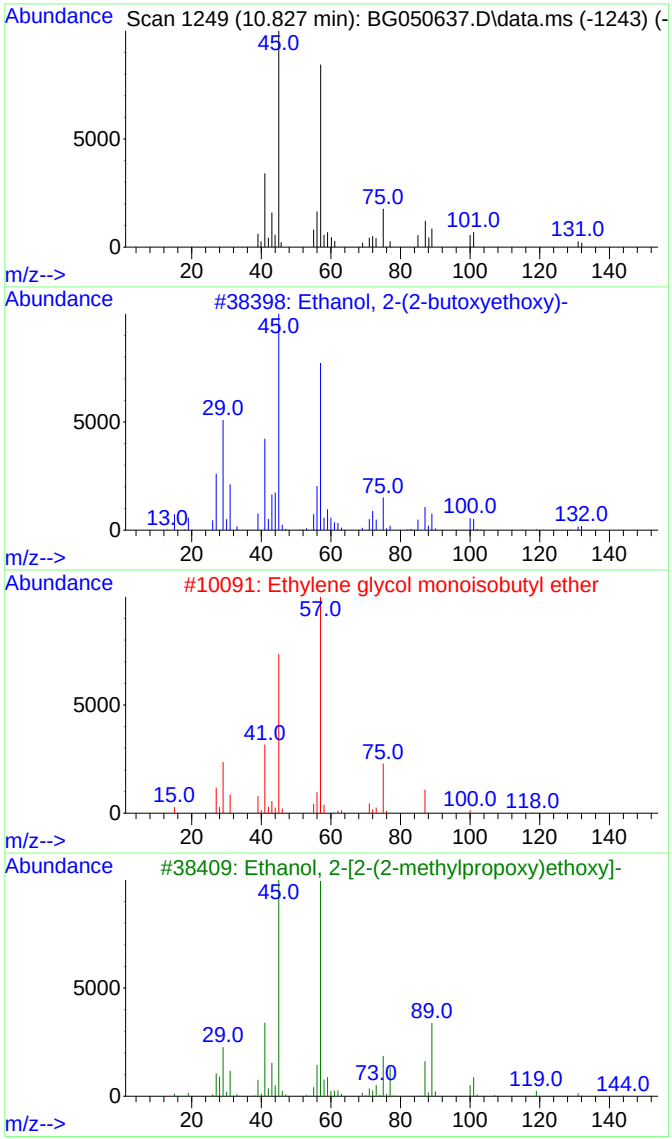
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

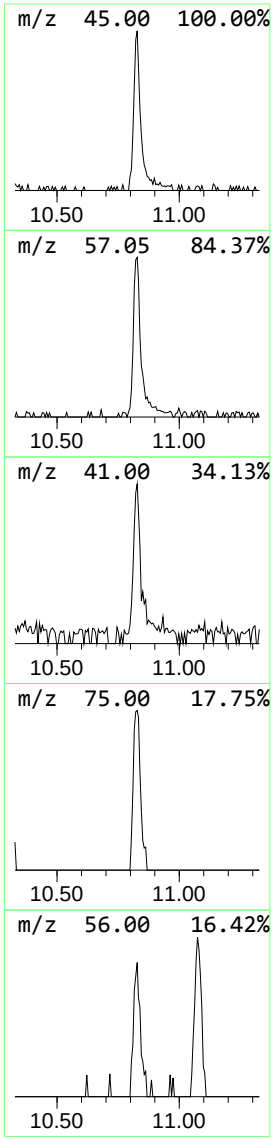
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	3.03 ng	58237	Naphthalene-d8	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 135-136

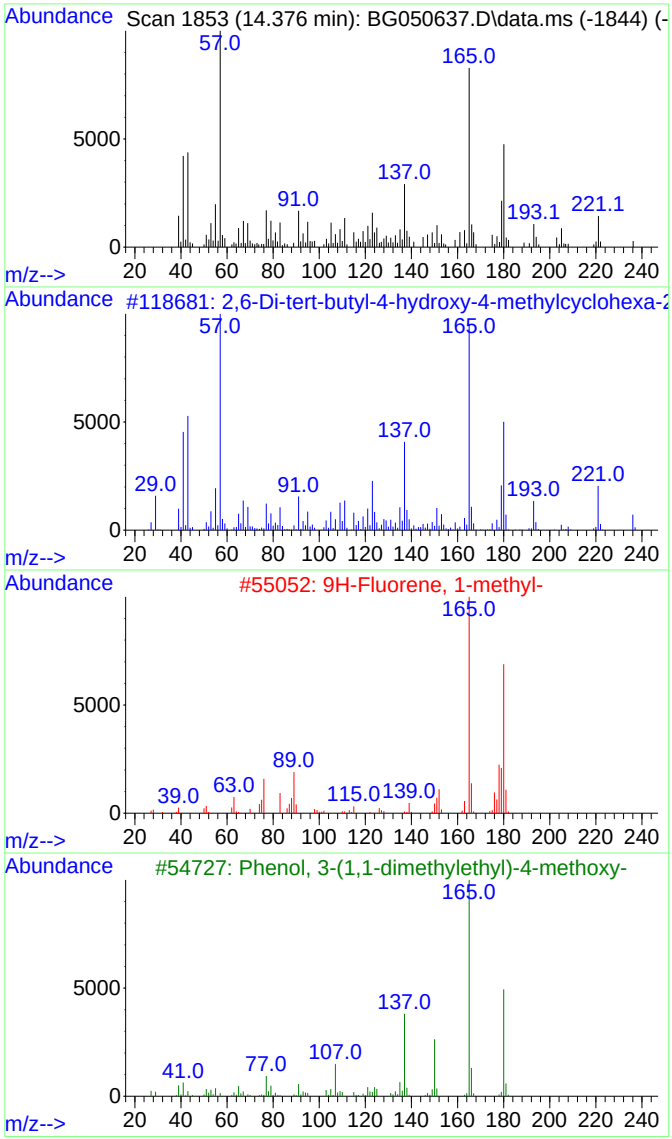
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

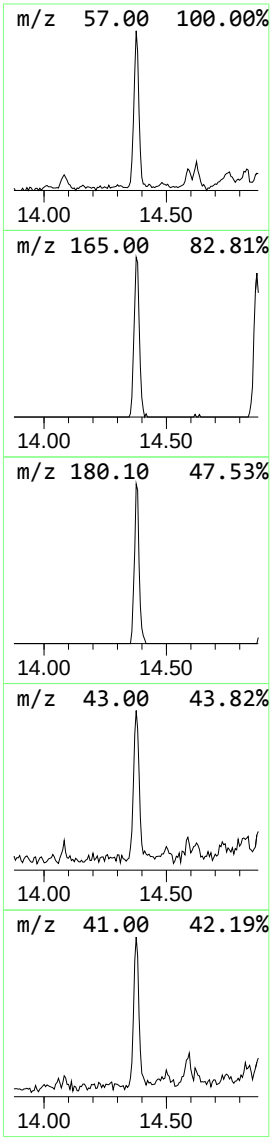
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,6-Di-tert-butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.376	6.37 ng	176477	Acenaphthene-d10	14.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	90
2	9H-Fluorene, 1-methyl-	180	C14H12	001730-37-6	68
3	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	62
4	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	58
5	5-tert-Butyl-2-methylbenzenethiol	180	C11H16S	007340-90-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

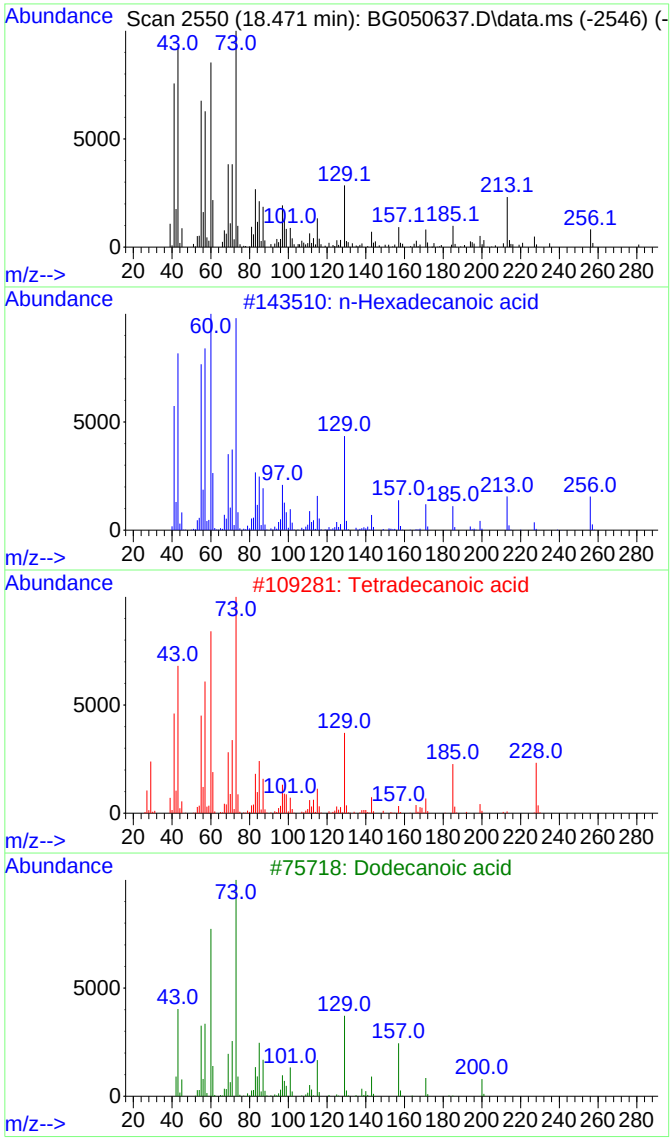
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

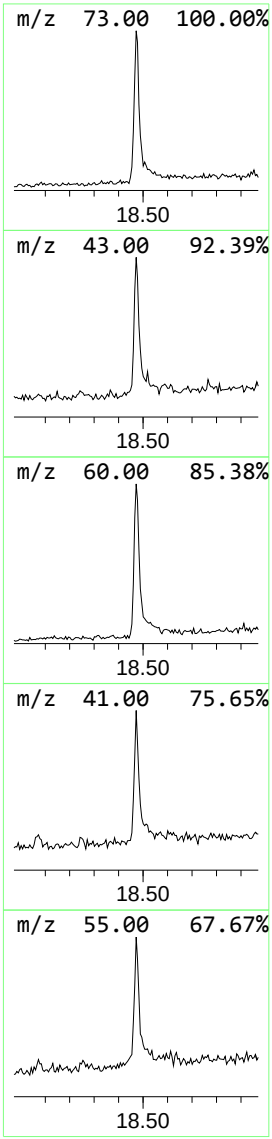
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.471	8.28 ng	258914	Phenanthrene-d10	17.614

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	95
3	Dodecanoic acid	200	C12H24O2	000143-07-7	92
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

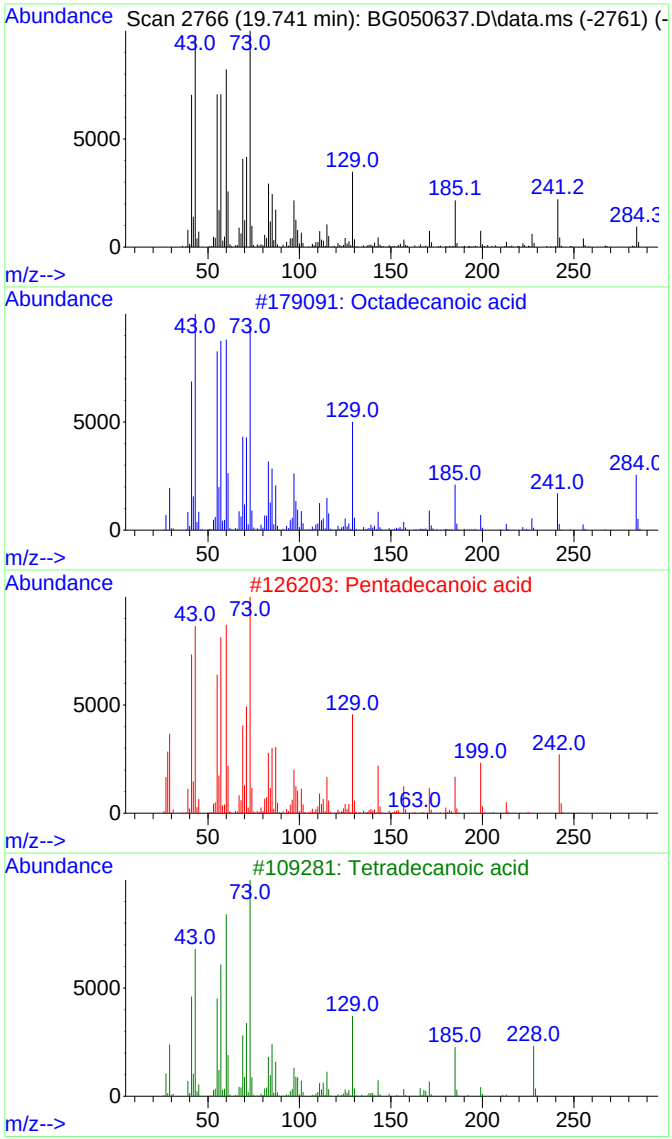
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

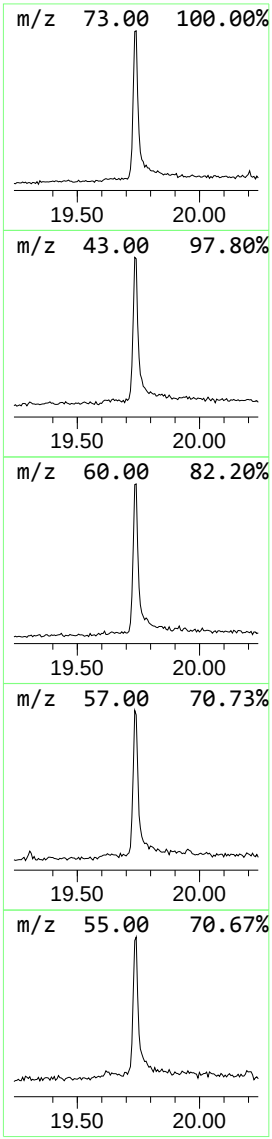
****

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.741	23.24 ng	726503	Phenanthrene-d10	17.614

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	Tridecane	184	C13H28	000629-50-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101921\
Data File : BG050637.D
Acq On : 19 Oct 2021 16:27
Operator : CG/JU
Sample : M4253-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 135-136

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanoic acid, ...	9.647	161.9	ng	2185140	1	8.254	269876	20.0
Ethanol, 2-(2-b...	10.828	3.0	ng	58237	2	11.080	384811	20.0
2,6-Di-tert-but...	14.376	6.4	ng	176477	3	14.870	553968	20.0
n-Hexadecanoic ...	18.471	8.3	ng	258914	4	17.614	625283	20.0
Octadecanoic acid	19.741	23.2	ng	726503	4	17.614	625283	20.0