LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101220\
Data File : BG046845.D
Acq On : 12 Oct 2020 13:41
Operator : CG/JU
Sample : L4358-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW

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-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.667	389	396	405	rVB	553831	873397	14.03%	3.966%
2	7.254	658	666	676	rBV	402667	712035	11.44%	3.234%
3	8.105	803	811	818	rBV2	224693	390531	6.27%	1.774%
4	9.263	1000	1008	1019	rBV	546386	970297	15.59%	4.406%
5	10.914	1281	1289	1298	rVB	287717	508608	8.17%	2.310%
6	13.352	1697	1704	1713	rBV	1382374	2132727	34.26%	9.685%
7	14.169	1838	1843	1848	rBV	72976	110908	1.78%	0.504%
8	14.727	1932	1938	1945	rVB	448360	691164	11.10%	3.139%
9	16.208	2182	2190	2207	rBV	1585330	2493471	40.05%	11.323%
10	17.471	2398	2405	2412	rBV	630484	959489	15.41%	4.357%
11	18.352	2549	2555	2569	rBV	393002	631796	10.15%	2.869%
12	18.952	2646	2657	2658	rBV10	45212	120028	1.93%	0.545%
13	19.615	2765	2770	2780	rBV2	170221	261839	4.21%	1.189%
14	20.074	2842	2848	2858	rBV	4841734	6225667	100.00%	28.272%
15	20.344	2883	2894	2896	rBV3	208580	470482	7.56%	2.137%
16	21.378	3065	3070	3080	rBV	330858	574536	9.23%	2.609%
17	21.454	3080	3083	3090	rVB2	41934	68407	1.10%	0.311%
18	21.625	3109	3112	3117	rVB2	56183	75914	1.22%	0.345%
19	21.742	3126	3132	3139	rBV	798913	1300846	20.89%	5.907%
20	22.001	3168	3176	3192	rVB3	199765	797188	12.80%	3.620%
21	23.270	3389	3392	3408	rVB10	89480	310410	4.99%	1.410%
22	25.009	3678	3688	3702	rVB2	425381	1340583	21.53%	6.088%

Sum of corrected areas: 22020323

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Instrument :
BNA_G
ClientSampleId :
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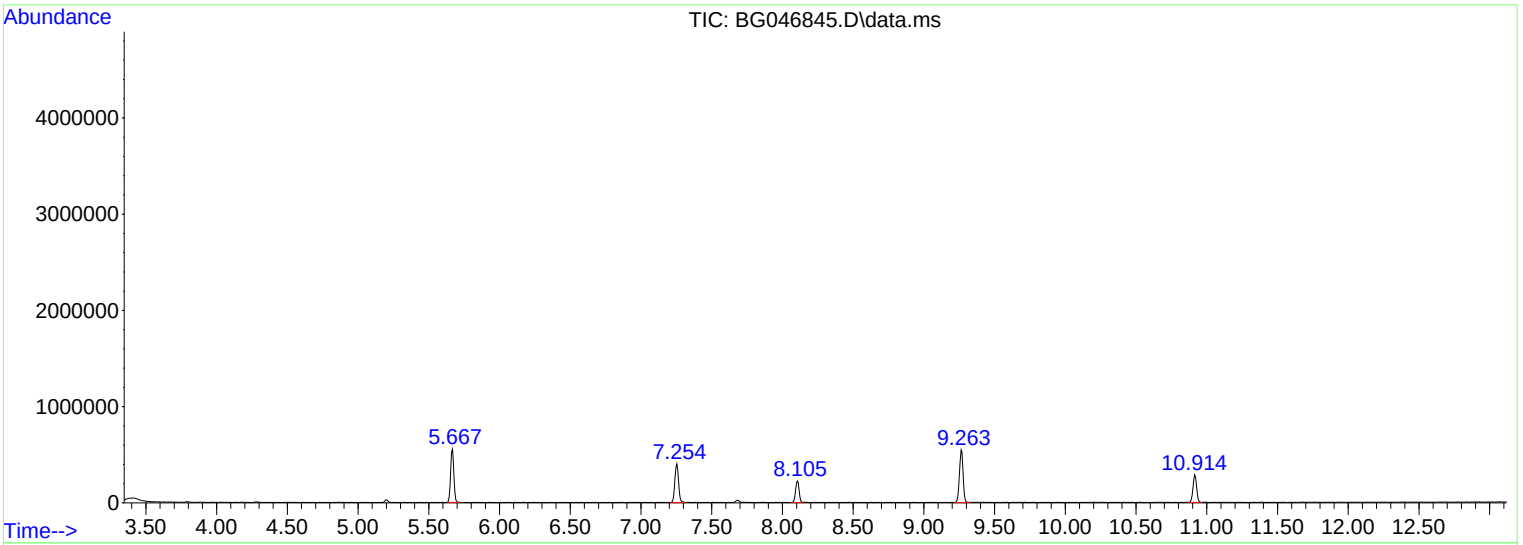
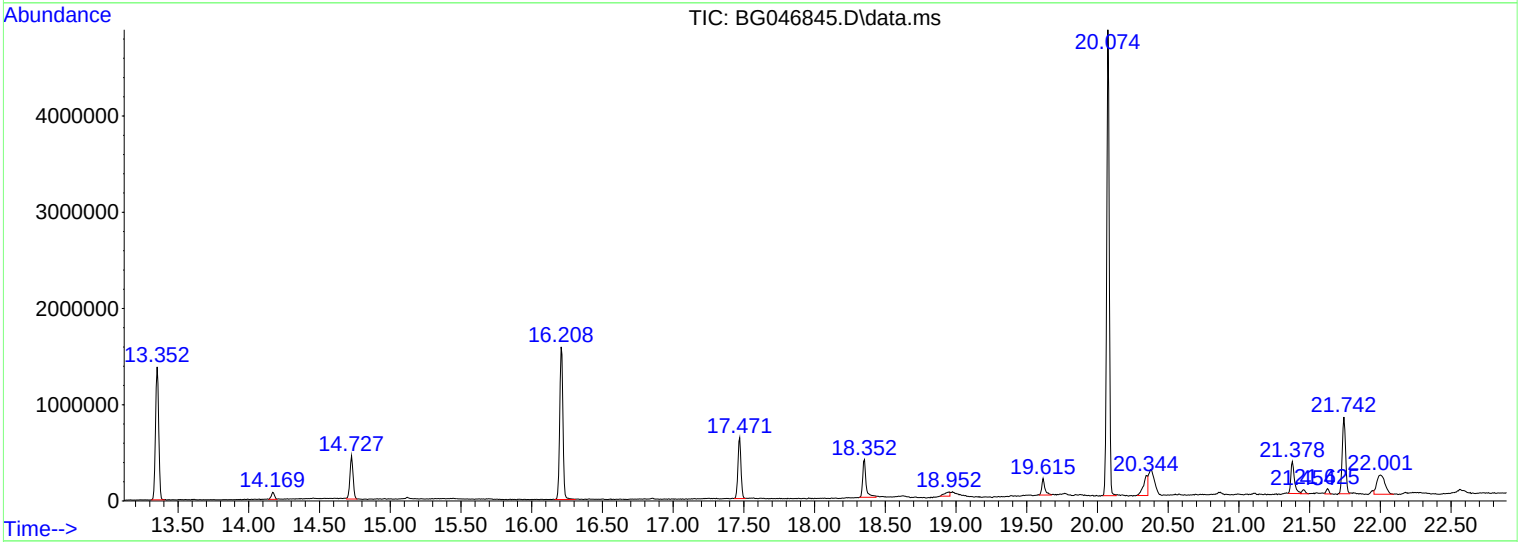
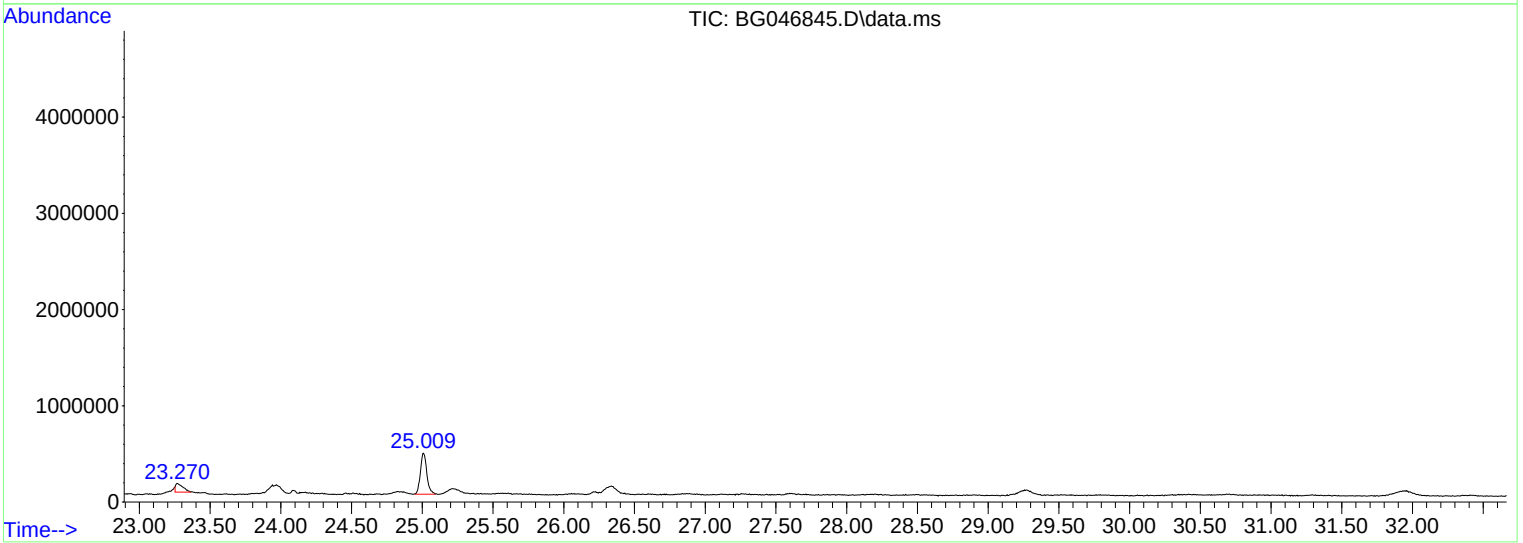
Quant Title :

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







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Quant Title :

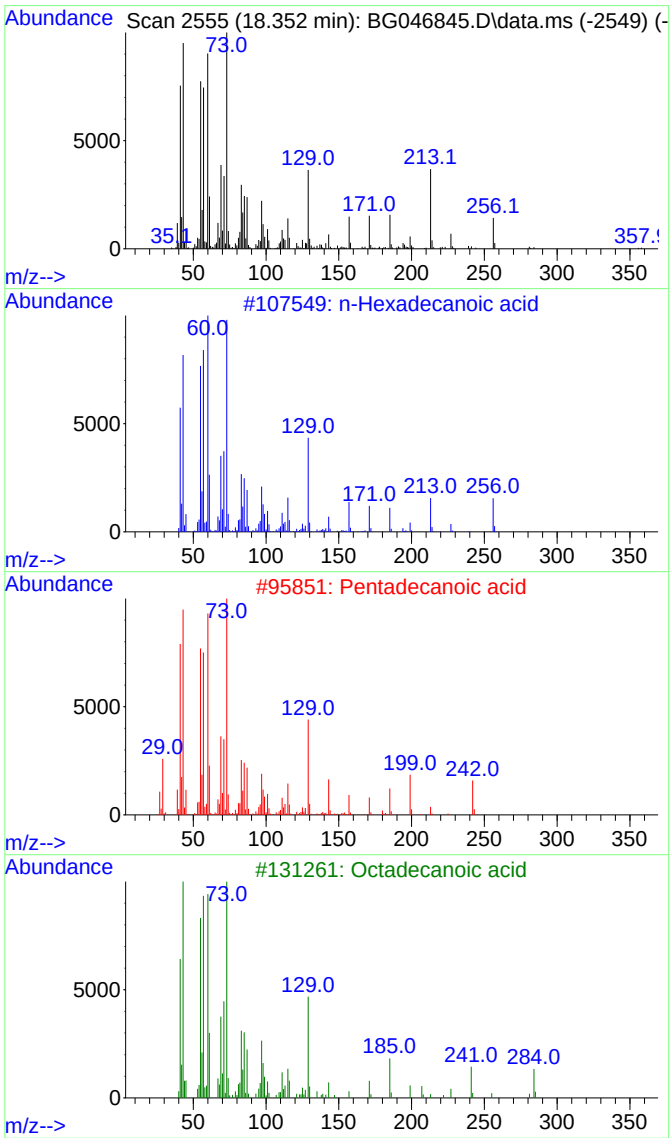
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

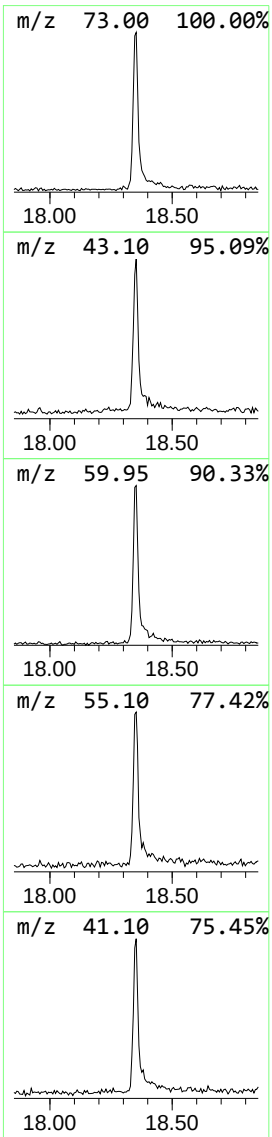
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.352	13.17 ng	631796	Phenanthrene-d10	17.471

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	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Operator : CG/JU
Sample : L4358-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW

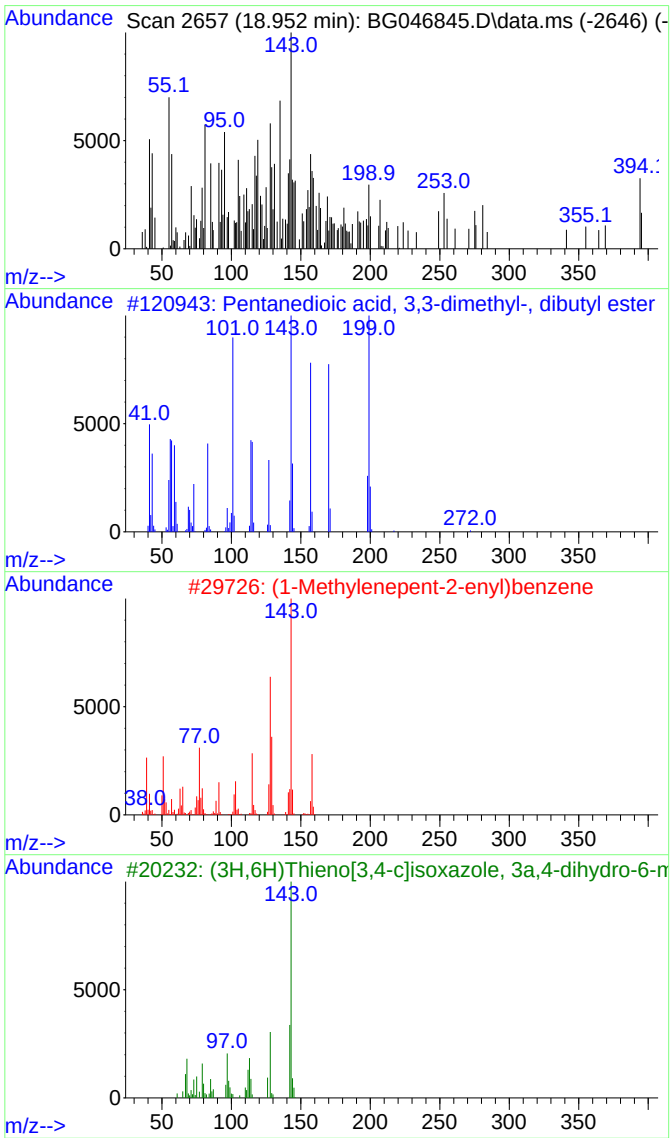
Quant Title :

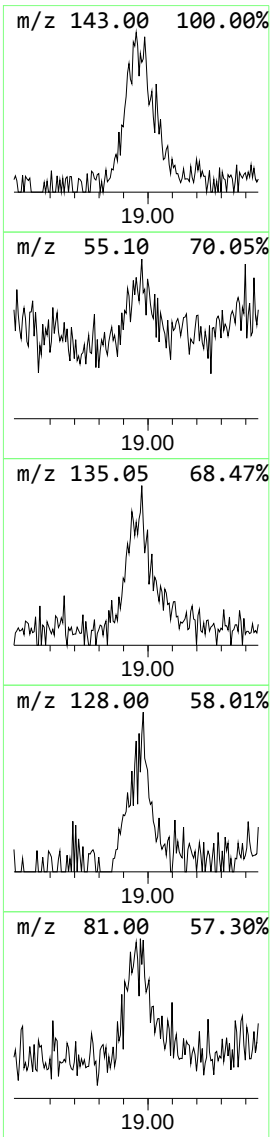
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown18.95 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.952	2.50 ng	120028	Phenanthrene-d10	17.471

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, 3,3-dimethyl-...	272	C15H28O4	056051-59-3	25
2	(1-Methylenepent-2-enyl)benzene	158	C12H14	084313-24-6	22
3	(3H,6H)Thieno[3,4-c]isoxazole, 3...	143	C6H9NOS	1000115-56-0	22
4	(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	22
5	1H-Indene, 1-methyl-3-propyl-	172	C13H16	111400-83-0	22





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Operator : CG/JU
Sample : L4358-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW

Quant Title :

TIC Library : C:\Database\NIST11.L
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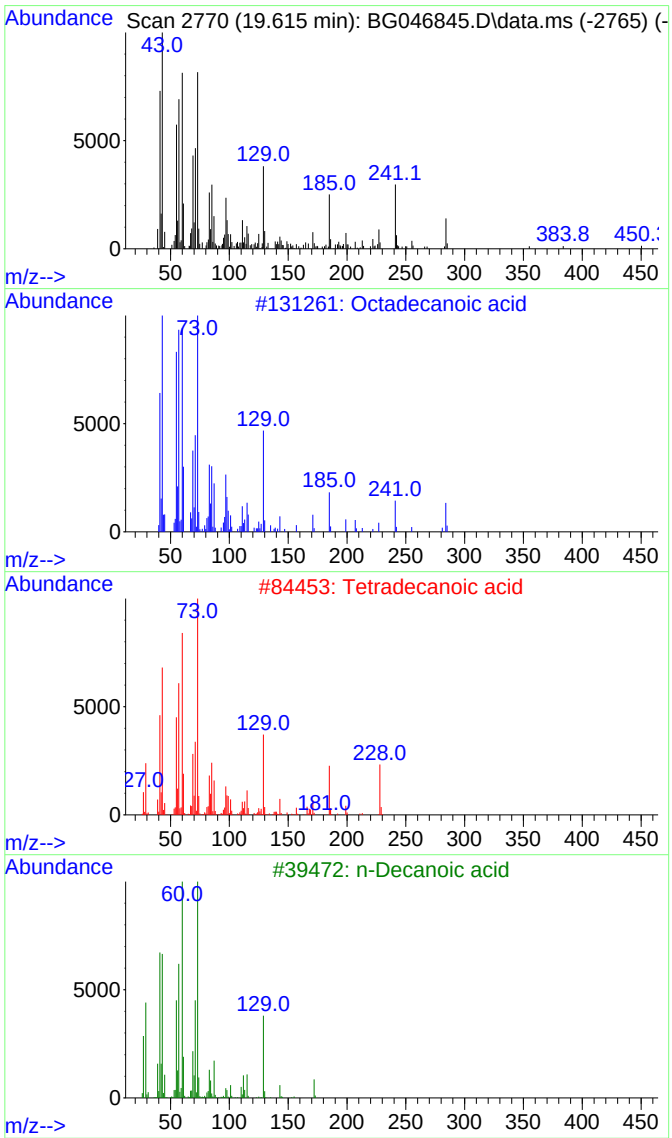
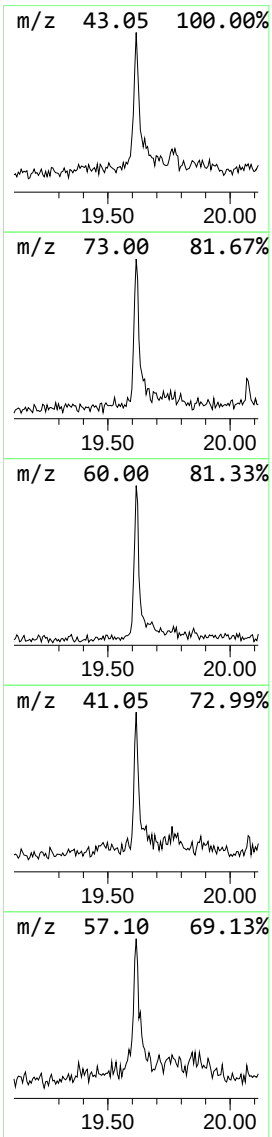
Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.616	4.03 ng	261839	Chrysene-d12	21.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Operator : CG/JU
Sample : L4358-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW

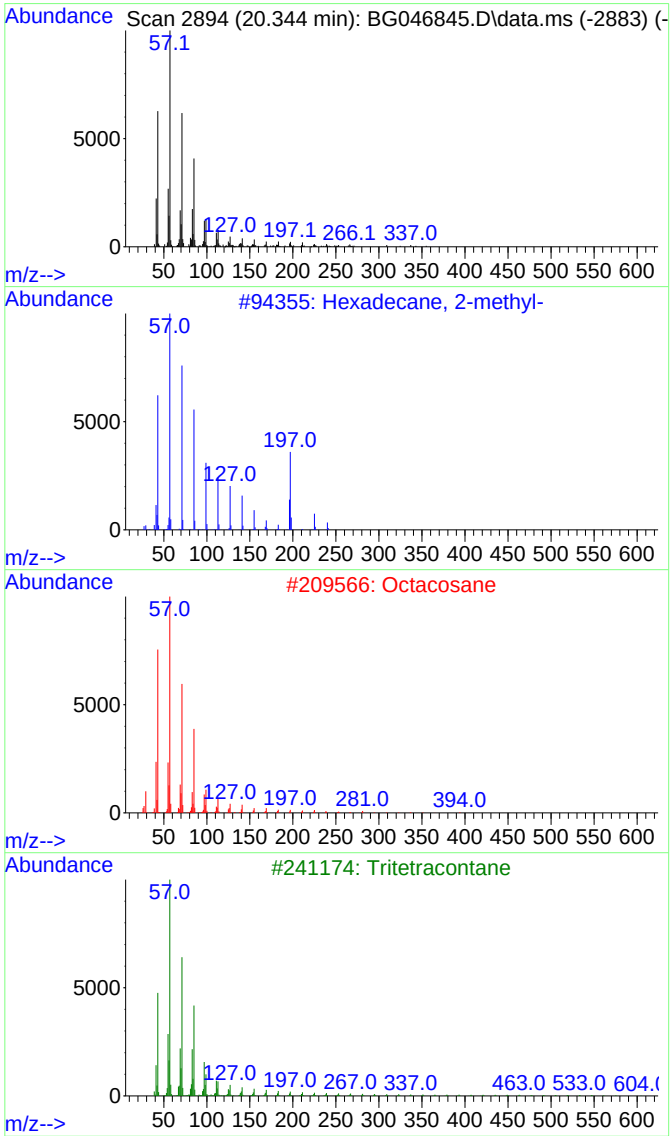
Quant Title :

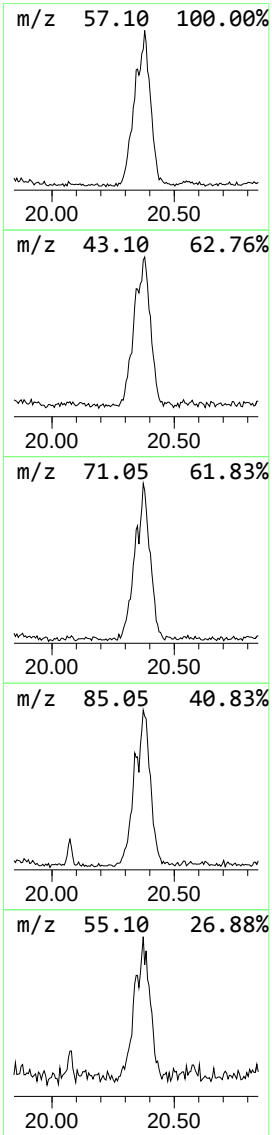
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.344	7.23 ng	470482	Chrysene-d12	21.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Tritetracontane	605	C43H88	007098-21-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Sample : L4358-01
Misc :
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Instrument : BNA_G
ClientSampleId : GW

Quant Title :

TIC Library : C:\Database\NIST11.L
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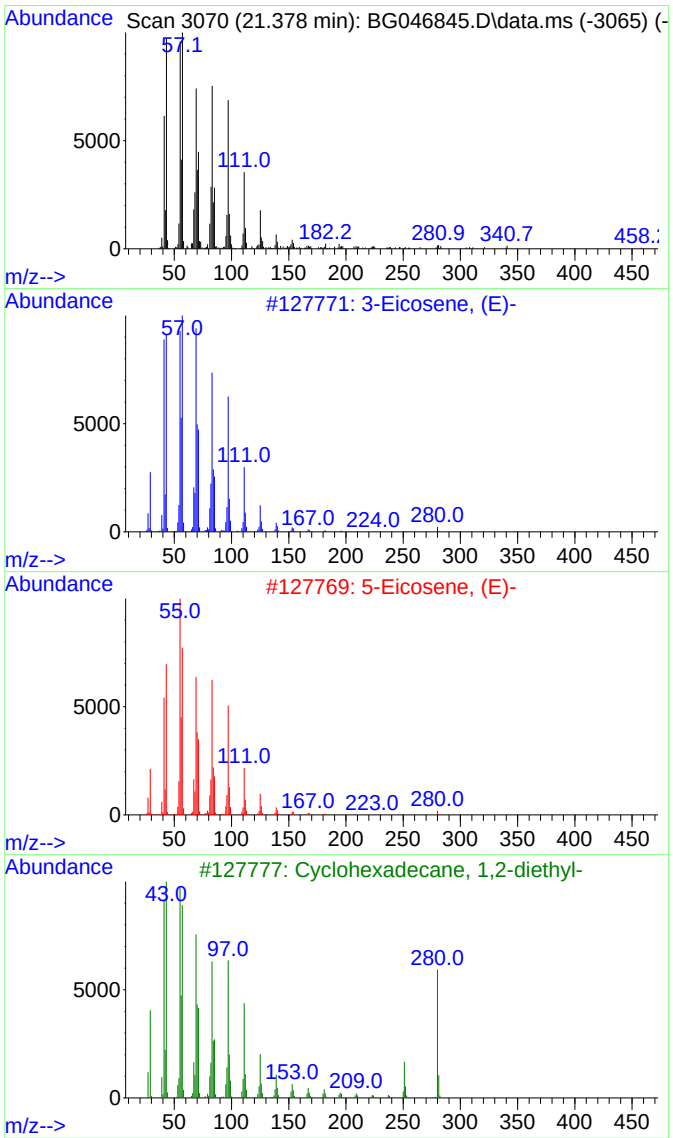
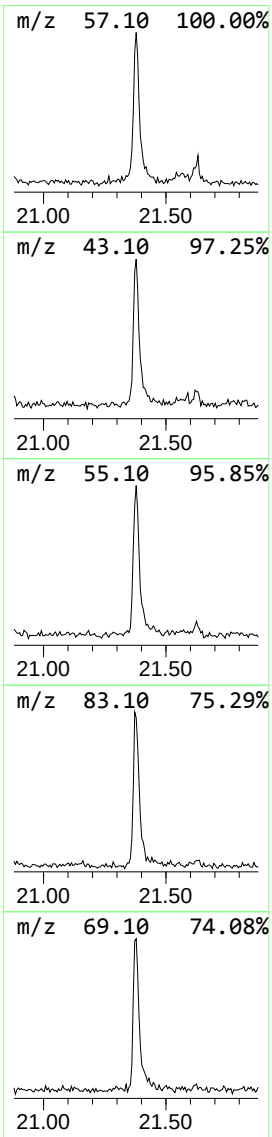
****
Peak Number 5 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.378	8.83 ng	574536	Chrysene-d12	21.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	96
4	1-Docosene	308	C22H44	001599-67-3	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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Instrument : BNA_G
ClientSampleId : GW

Quant Title :

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TIC Integration Parameters: LSCINT.P

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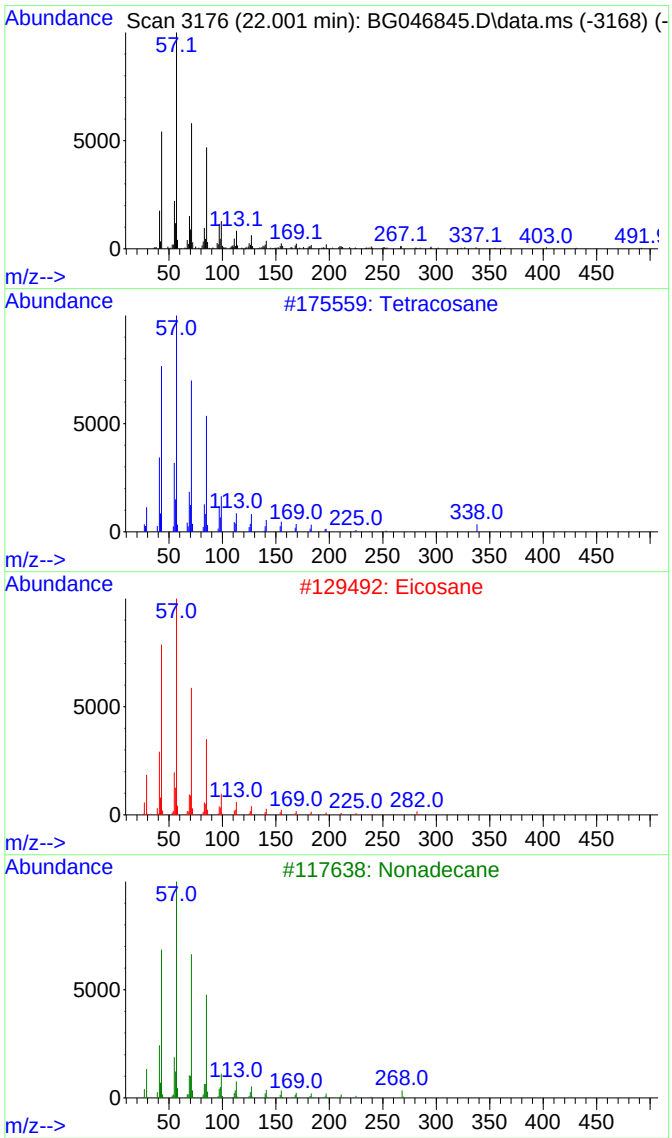
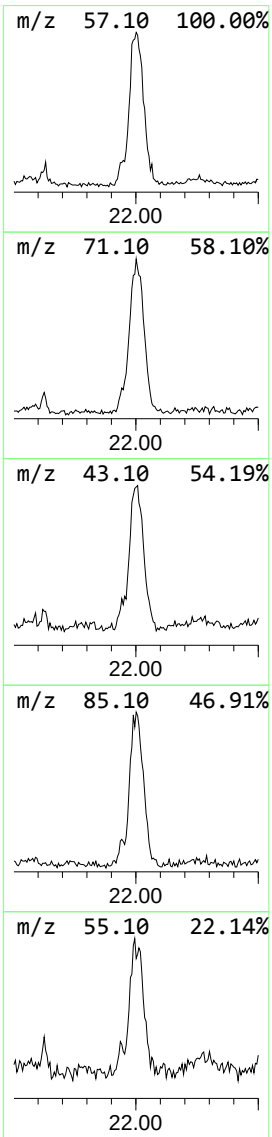
Peak Number 6 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.001	12.26 ng	797188	Chrysene-d12	21.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	86
2	Eicosane	282	C20H42	000112-95-8	83
3	Nonadecane	268	C19H40	000629-92-5	83
4	1-Iodoundecane	282	C11H23I	004282-44-4	81
5	Heneicosane	296	C21H44	000629-94-7	81





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Misc :
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ClientSampleId : GW

Quant Title :

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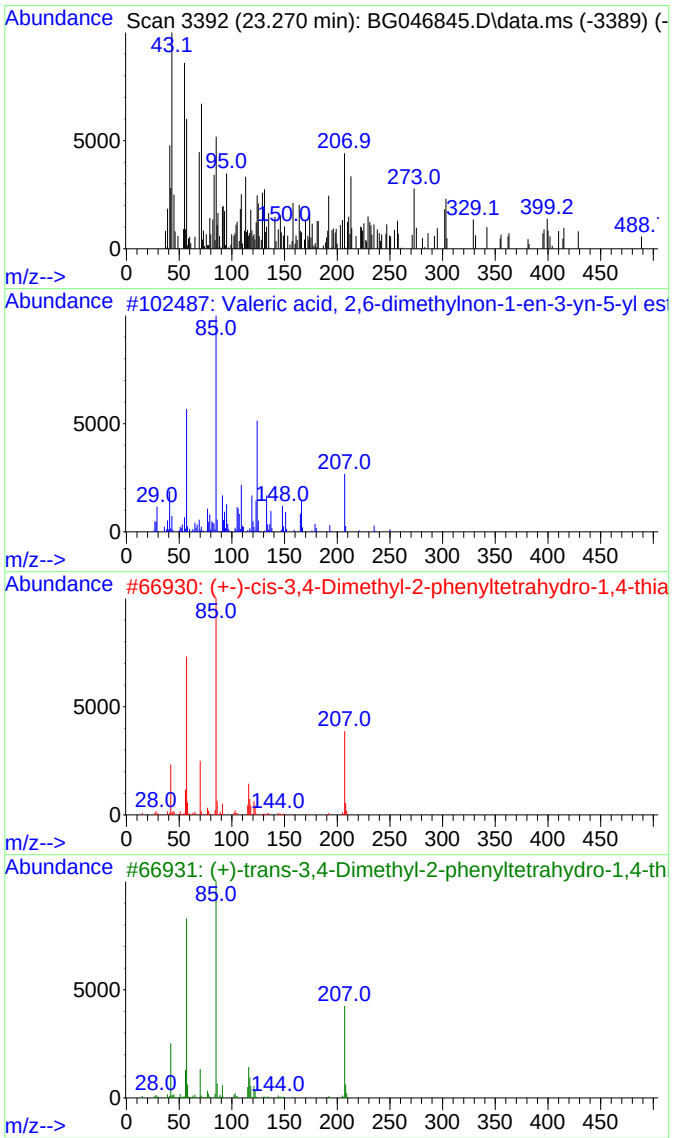
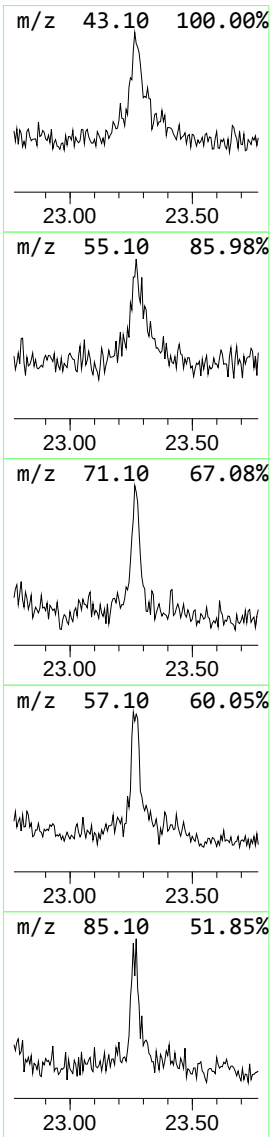
Peak Number 7 unknown23.27 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.270	4.77 ng	310410	Chrysene-d12	21.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valeric acid, 2,6-dimethylnon-1-...	250	C16H26O2	1000292-49-0	41
2	(+-)-cis-3,4-Dimethyl-2-phenylte...	207	C12H17NS	092772-63-9	35
3	(+)-trans-3,4-Dimethyl-2-phenylt...	207	C12H17NS	1000244-64-9	35
4	Di-n-decylsulfone	346	C20H42O2S	111530-37-1	25
5	1,3-Propanediamine, N,N,N'-trime...	192	C12H20N2	055667-48-6	12





Tentatively Identified Compound (LSC) summary

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Quant Title :

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
n-Hexadecanoic ...	18.352	13.2	ng	631796	4	17.471	959489	20.0
unknown18.95	18.952	2.5	ng	120028	4	17.471	959489	20.0
Octadecanoic acid	19.616	4.0	ng	261839	5	21.742	1300850	20.0
Hexadecane, 2-m...	20.344	7.2	ng	470482	5	21.742	1300850	20.0
3-Eicosene, (E)-	21.378	8.8	ng	574536	5	21.742	1300850	20.0
Tetracosane	22.001	12.3	ng	797188	5	21.742	1300850	20.0
unknown23.27	23.270	4.8	ng	310410	5	21.742	1300850	20.0