LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.761	379	387	401	rBV	554834	957360	66.50%	9.113%
2	7.377	654	662	677	rBV	581105	1050819	72.99%	10.003%
3	8.229	800	807	821	rBV	139315	251900	17.50%	2.398%
4	9.404	997	1007	1019	rBV	366853	681498	47.34%	6.487%
5	10.802	1237	1245	1257	rBV	26613	58246	4.05%	0.554%
6	11.055	1280	1288	1296	rBV	202793	375175	26.06%	3.571%
7	13.476	1691	1700	1708	rBV	886566	1388848	96.47%	13.220%
8	14.856	1925	1935	1944	rBV	326888	522785	36.31%	4.976%
9	15.655	2066	2071	2077	rVB3	10037	15751	1.09%	0.150%
10	16.343	2181	2188	2196	rBV	674609	1029329	71.50%	9.798%
11	16.519	2213	2218	2224	rBV2	11565	23926	1.66%	0.228%
12	17.312	2348	2353	2358	rBV	12788	20593	1.43%	0.196%
13	17.606	2396	2403	2408	rBV	354685	580249	40.30%	5.523%
14	17.706	2417	2420	2425	rVB7	12280	15039	1.04%	0.143%
15	18.053	2475	2479	2484	rVB2	13937	19048	1.32%	0.181%
16	18.229	2505	2509	2516	rVB	90471	114449	7.95%	1.089%
17	18.452	2543	2547	2556	rBV4	43070	85884	5.97%	0.818%
18	18.740	2592	2596	2599	rBV2	15645	20198	1.40%	0.192%
19	19.357	2697	2701	2704	rBV2	368437	498710	34.64%	4.747%
20	19.386	2704	2706	2718	rVB2	454366	587073	40.78%	5.588%
21	19.516	2725	2728	2732	rBV	65584	83853	5.82%	0.798%
22	20.191	2838	2843	2848	rVB	1132067	1439674	100.00%	13.704%
23	20.462	2887	2889	2894	rVB2	37912	41195	2.86%	0.392%
24	21.490	3062	3064	3074	rVB3	92895	167939	11.67%	1.599%
25	21.907	3130	3135	3144	rVB	282144	475868	33.05%	4.530%

Sum of corrected areas: 10505409

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
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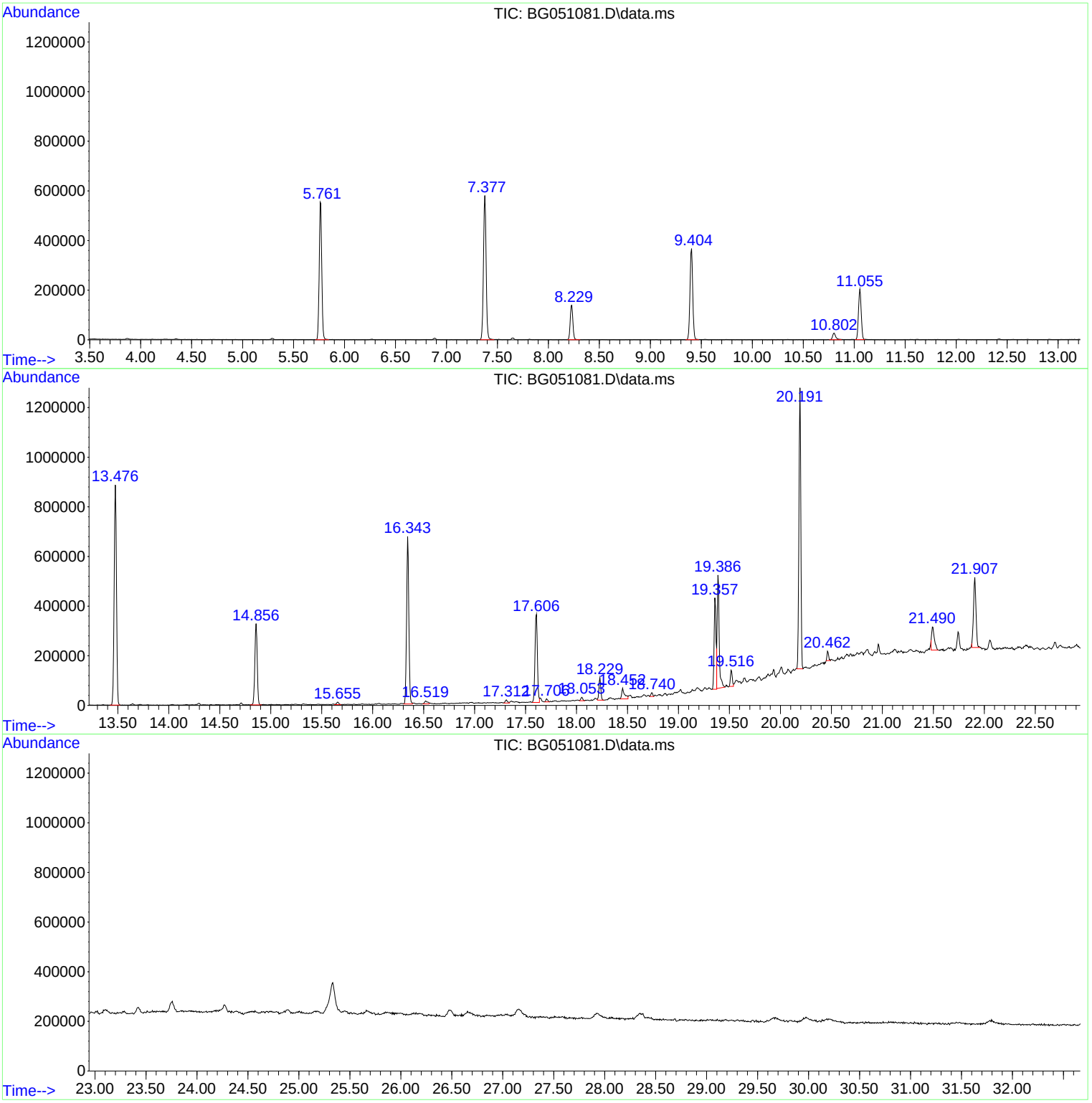
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

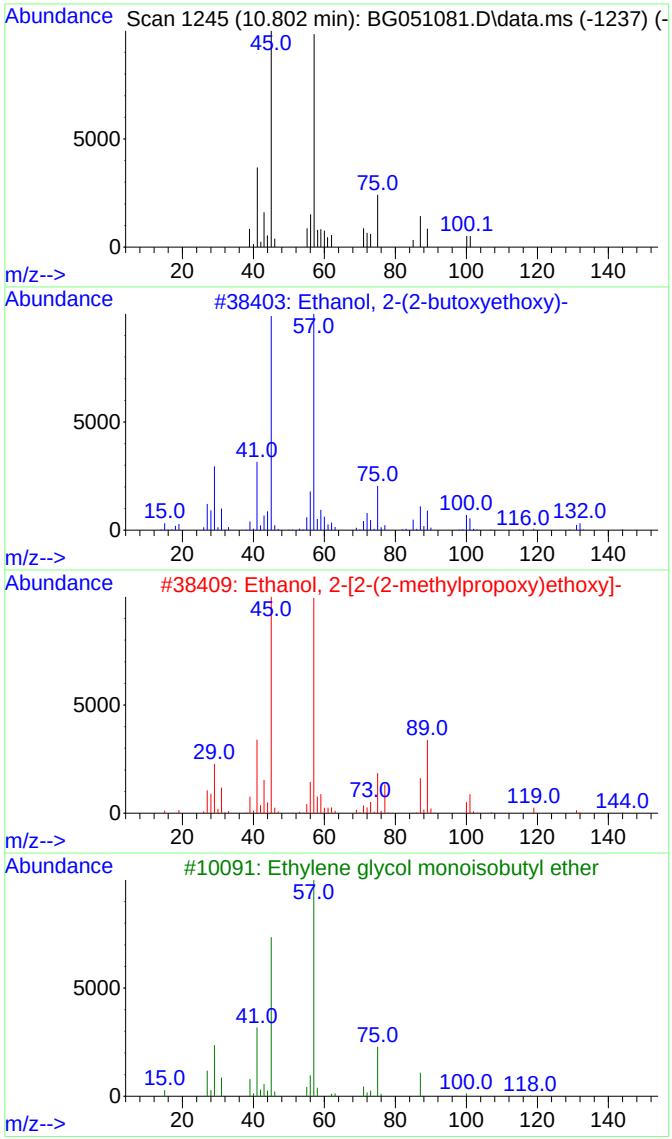
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

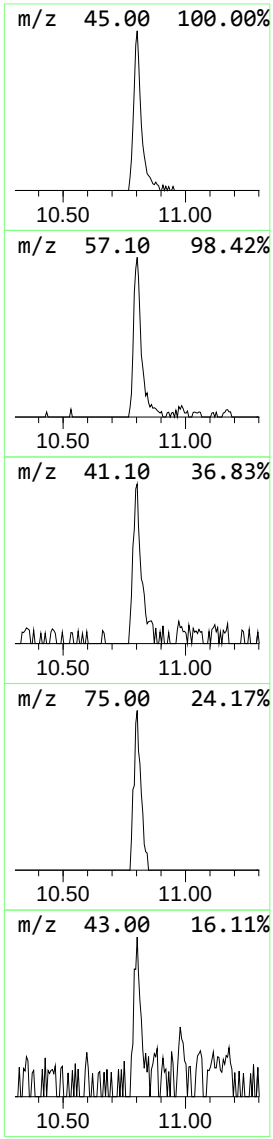
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.802	3.11 ng	58246	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	78
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

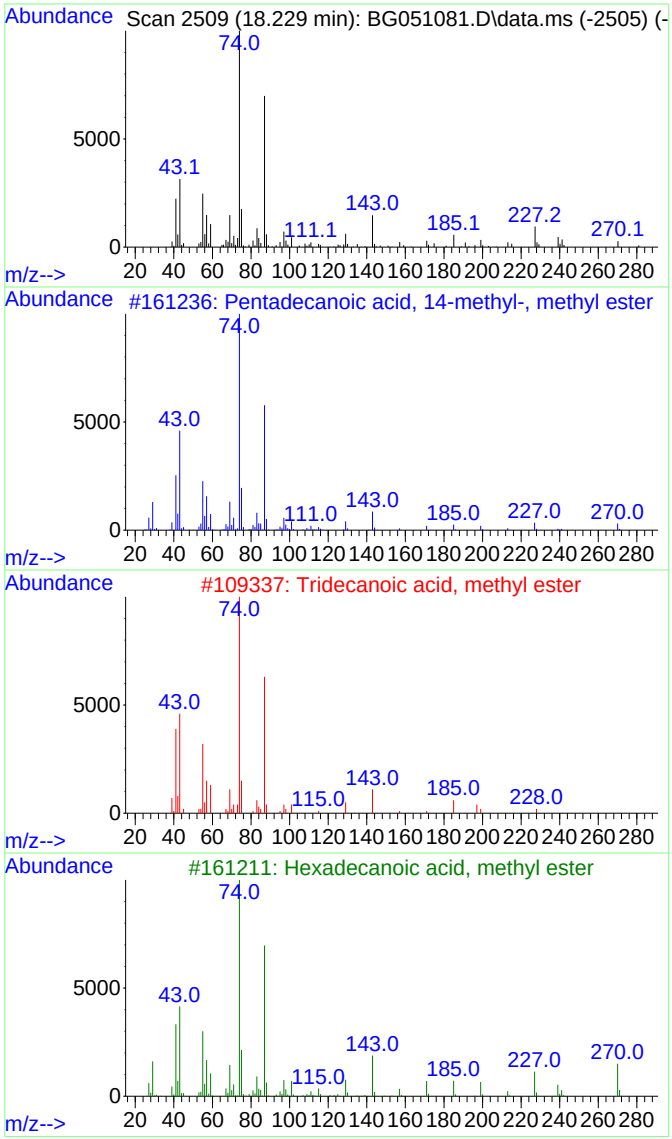
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

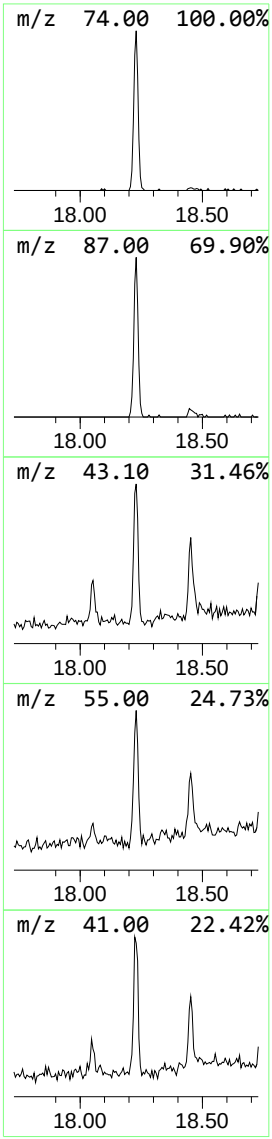
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentadecanoic acid, 14-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.229	3.94 ng	114449	Phenanthrene-d10	17.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

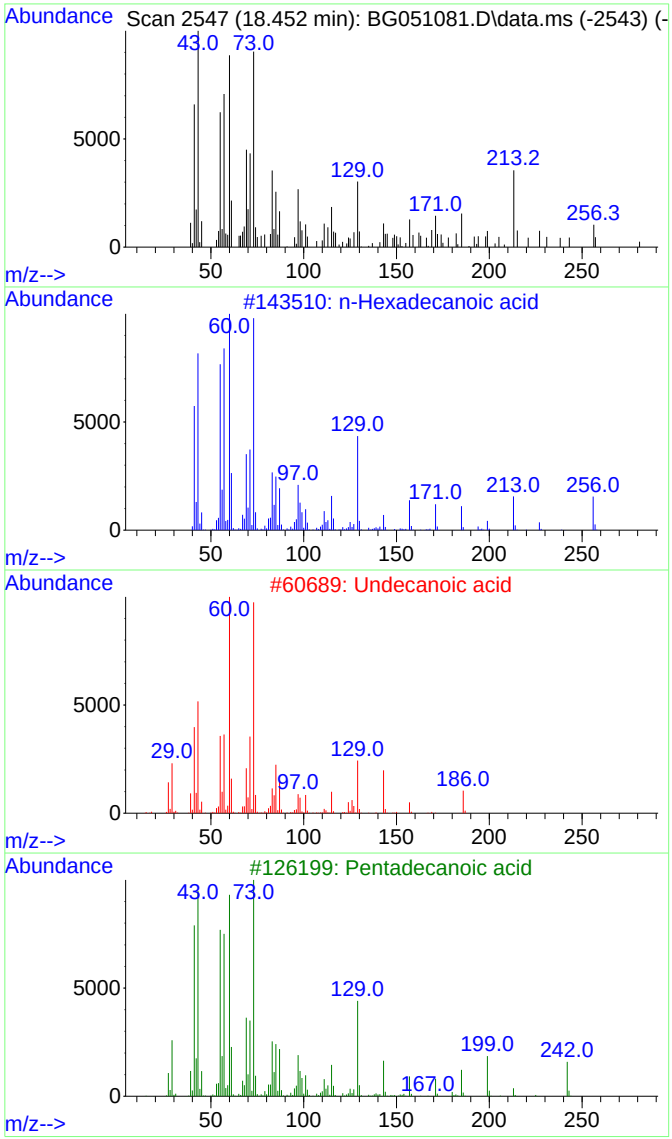
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

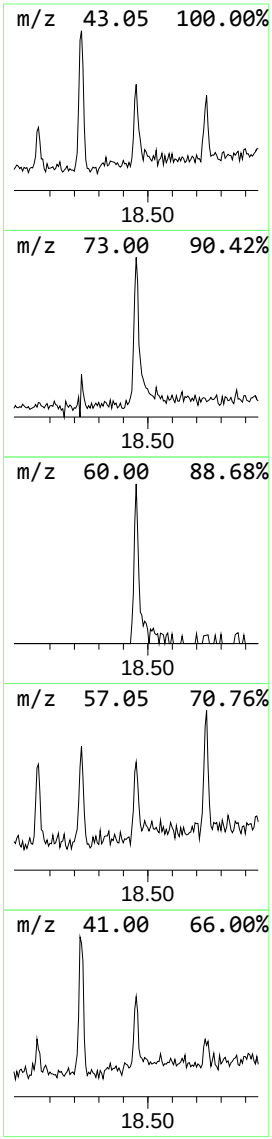
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.452	2.96 ng	85884	Phenanthrene-d10	17.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

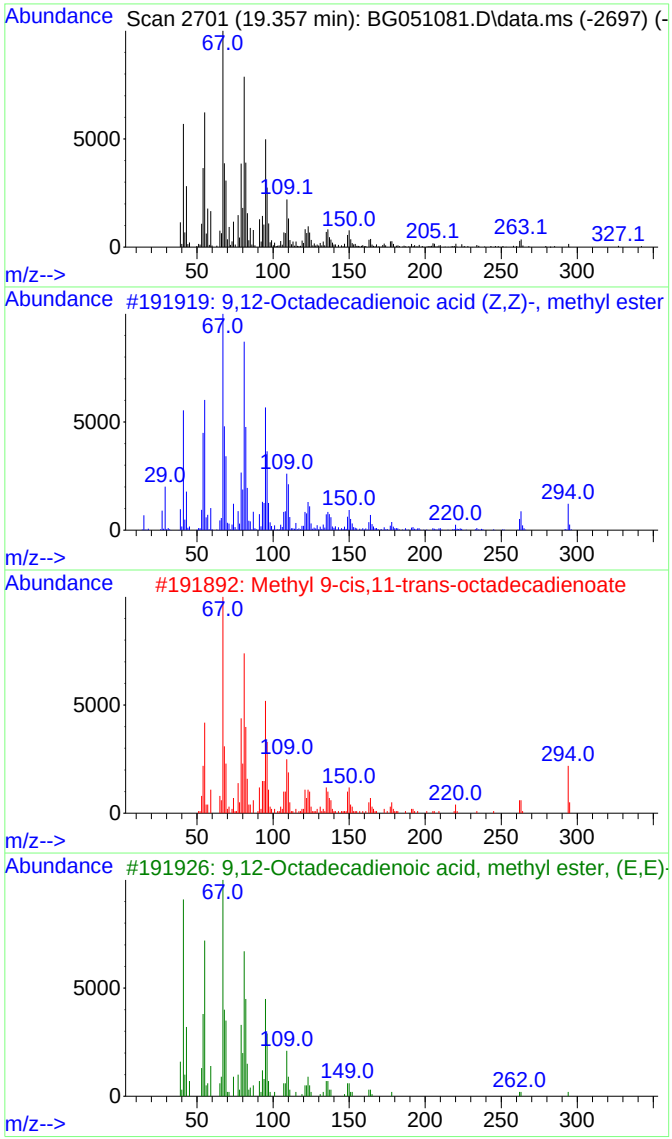
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

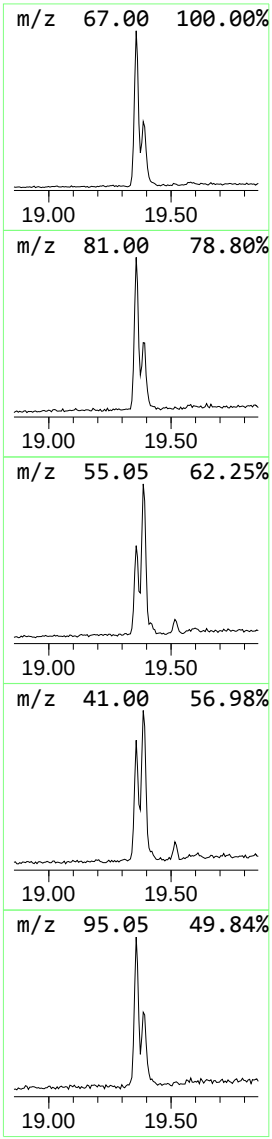
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	17.19 ng	498710	Phenanthrene-d10	17.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051081.D
Acq On : 17 Nov 2021 00:42
Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

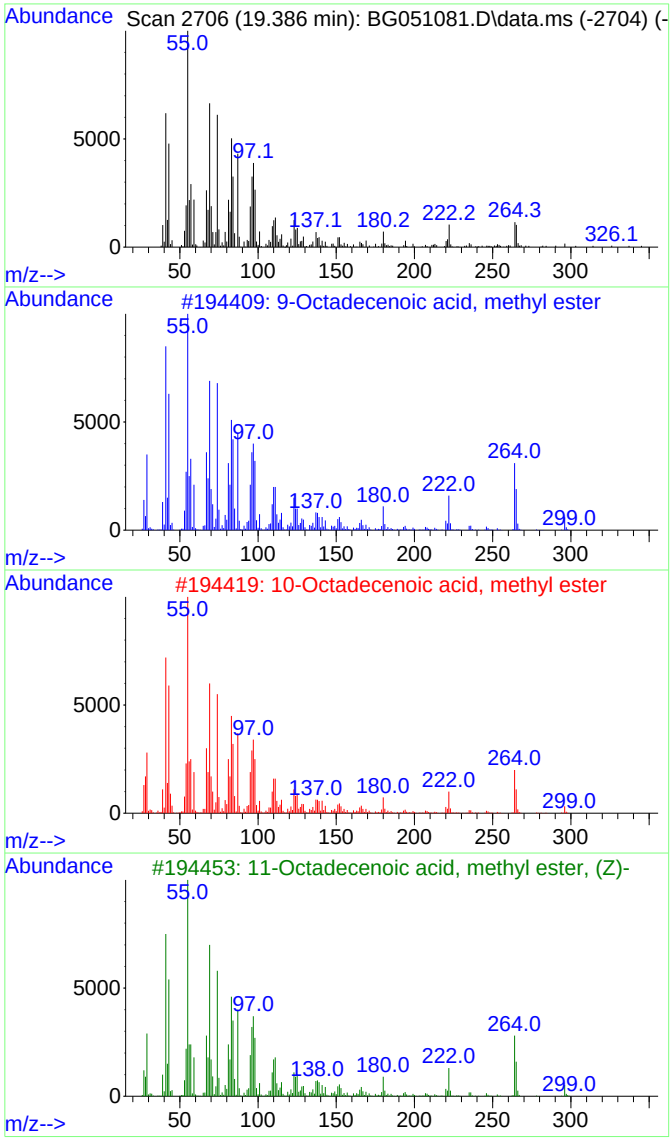
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

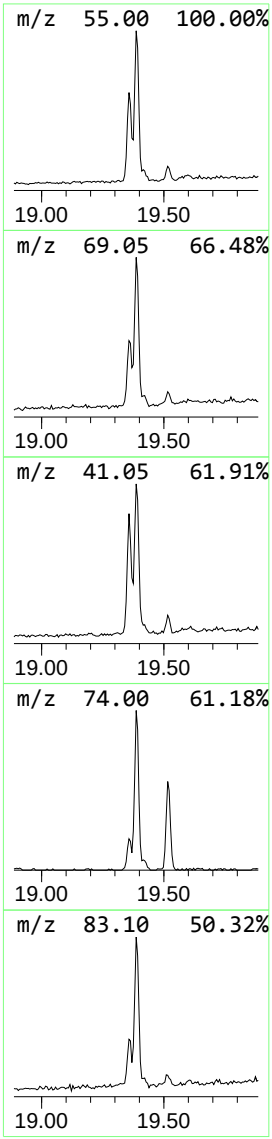
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	20.24 ng	587073	Phenanthrene-d10	17.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
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Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

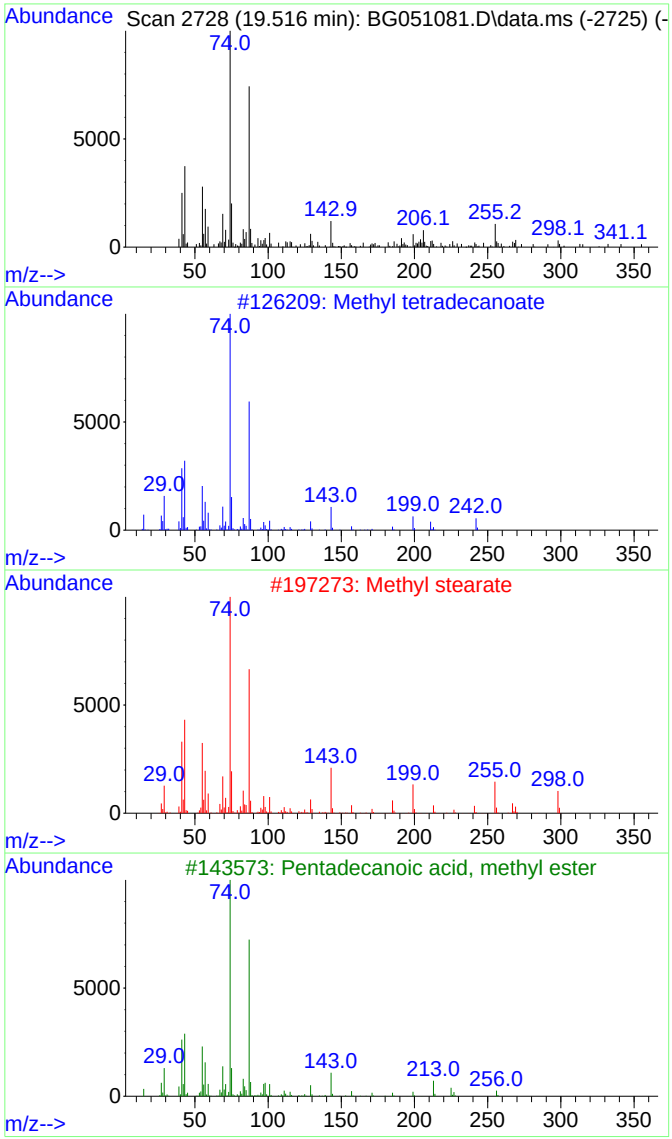
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

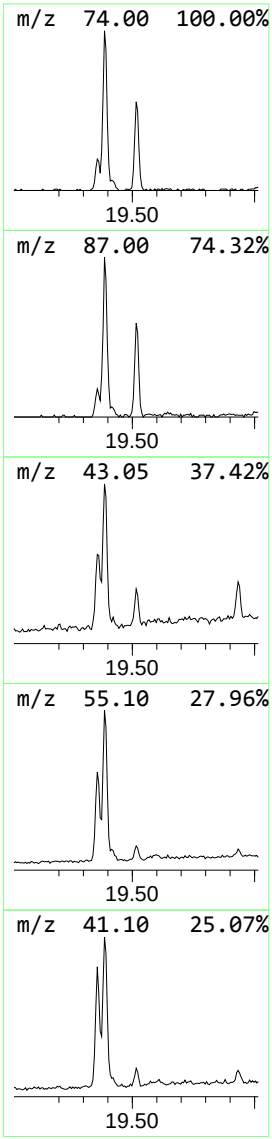
****

Peak Number 6 Methyl tetradecanoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	2.89 ng	83853	Phenanthrene-d10	17.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
2	Methyl stearate	298	C19H38O2	000112-61-8	89
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86





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Operator : CG/JU
Sample : M4684-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-111221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

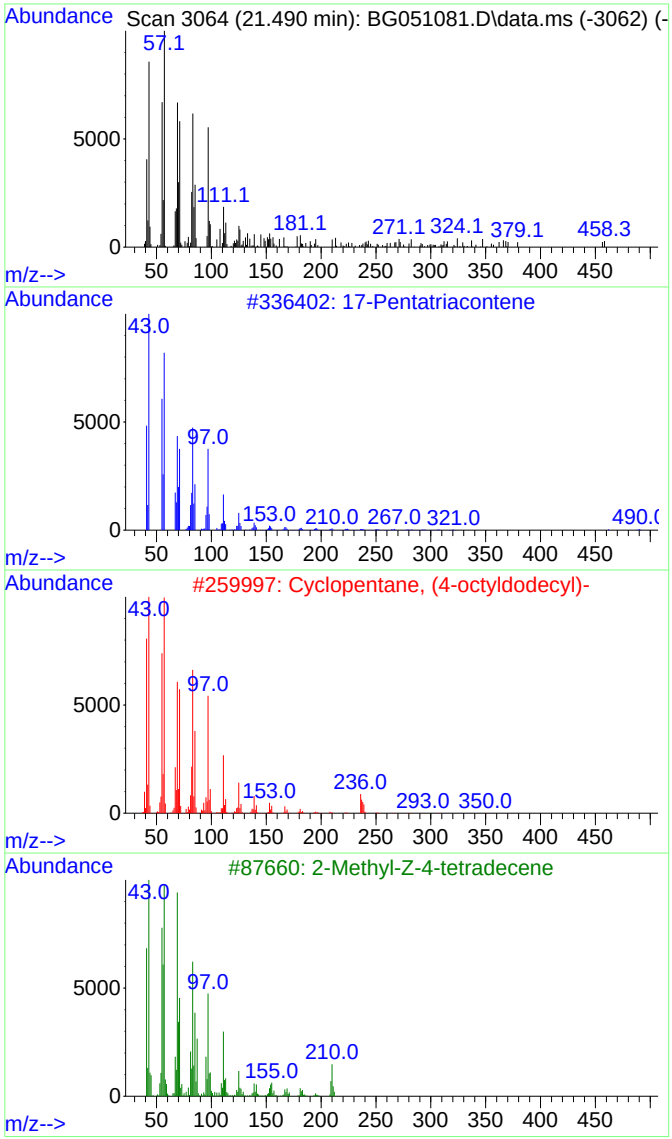
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

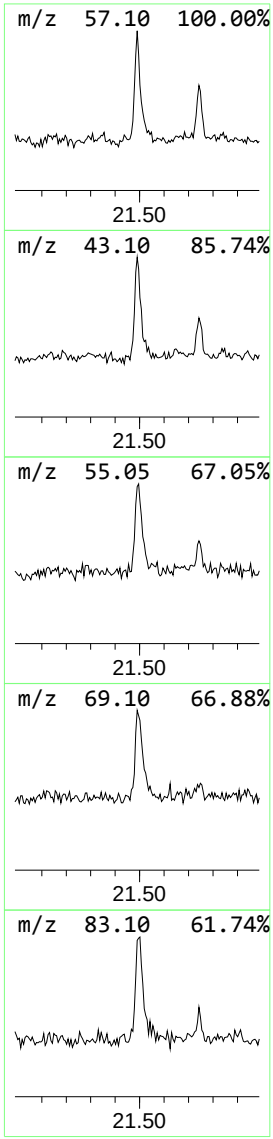
****

Peak Number 7 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	7.06 ng	167939	Chrysene-d12	21.907

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	83
2	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	83
3	2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	78
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
5	1-Hexacosanol	382	C26H54O	000506-52-5	64





Tentatively Identified Compound (LSC) summary

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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
Ethanol, 2-(2-b...	10.802	3.1	ng	58246	2	11.055	375175	20.0
Pentadecanoic a...	18.229	3.9	ng	114449	4	17.606	580249	20.0
n-Hexadecanoic ...	18.452	3.0	ng	85884	4	17.606	580249	20.0
9,12-Octadecadi...	19.357	17.2	ng	498710	4	17.606	580249	20.0
9-Octadecenoic ...	19.386	20.2	ng	587073	4	17.606	580249	20.0
Methyl tetradec...	19.516	2.9	ng	83853	4	17.606	580249	20.0
17-Pentatriacon...	21.490	7.1	ng	167939	5	21.907	475868	20.0