LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054348.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.574	365	372	384	rVB	184277	326973	21.61%	3.590%
2	7.178	638	645	660	rVB	204476	367802	24.31%	4.038%
3	7.994	777	784	791	rBV	64052	109907	7.26%	1.207%
4	9.158	973	982	993	rBV	127098	229746	15.18%	2.522%
5	10.803	1255	1262	1273	rBB	82419	153086	10.12%	1.681%
6	13.253	1672	1679	1687	rBV	411472	643259	42.52%	7.062%
7	14.634	1907	1914	1921	rBB	155406	249293	16.48%	2.737%
8	16.120	2161	2167	2180	rBV2	422011	641981	42.43%	7.048%
9	17.378	2374	2381	2386	rBV	229701	349617	23.11%	3.838%
10	17.419	2386	2388	2394	rVB	20527	24453	1.62%	0.268%
11	18.036	2488	2493	2499	rBV	244902	320888	21.21%	3.523%
12	18.265	2525	2532	2536	rBV3	28880	52248	3.45%	0.574%
13	18.300	2536	2538	2546	rVB2	13998	19974	1.32%	0.219%
14	18.447	2557	2563	2567	rBV2	9495	19323	1.28%	0.212%
15	19.175	2681	2687	2690	rBV	1141300	1513000	100.00%	16.610%
16	19.211	2690	2693	2704	rVB2	672599	918278	60.69%	10.081%
17	19.340	2710	2715	2720	rVB	150425	183451	12.12%	2.014%
18	19.428	2725	2730	2736	rVB	74105	114525	7.57%	1.257%
19	19.763	2781	2787	2788	rBV2	13803	20938	1.38%	0.230%
20	19.792	2788	2792	2799	rVV	78988	118436	7.83%	1.300%
21	19.986	2819	2825	2830	rBV	911961	1222428	80.79%	13.420%
22	20.257	2866	2871	2873	rBV6	14129	23539	1.56%	0.258%
23	20.286	2873	2876	2880	rVV2	17688	27350	1.81%	0.300%
24	20.321	2880	2882	2886	rVB5	13112	15646	1.03%	0.172%
25	20.439	2897	2902	2906	rBV4	19250	41212	2.72%	0.452%
26	20.591	2922	2928	2932	rBV2	23995	45527	3.01%	0.500%
27	21.050	3002	3006	3012	rVB2	15513	29866	1.97%	0.328%
28	21.220	3028	3035	3040	rBV4	13448	32772	2.17%	0.360%
29	21.279	3041	3045	3050	rVV6	24427	44500	2.94%	0.489%
30	21.438	3069	3072	3080	rVB6	14600	21769	1.44%	0.239%
31	21.643	3100	3107	3112	rBV	280529	507270	33.53%	5.569%
32	21.690	3112	3115	3120	rVB	40682	61268	4.05%	0.673%
33	23.306	3386	3390	3397	rVB4	20320	44256	2.93%	0.486%
34	23.829	3473	3479	3487	rBV3	29896	92355	6.10%	1.014%
35	24.698	3621	3627	3637	rVB	27151	76465	5.05%	0.839%
36	24.851	3643	3653	3664	rBV2	152682	445315	29.43%	4.889%

LSC Area Percent Report

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Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

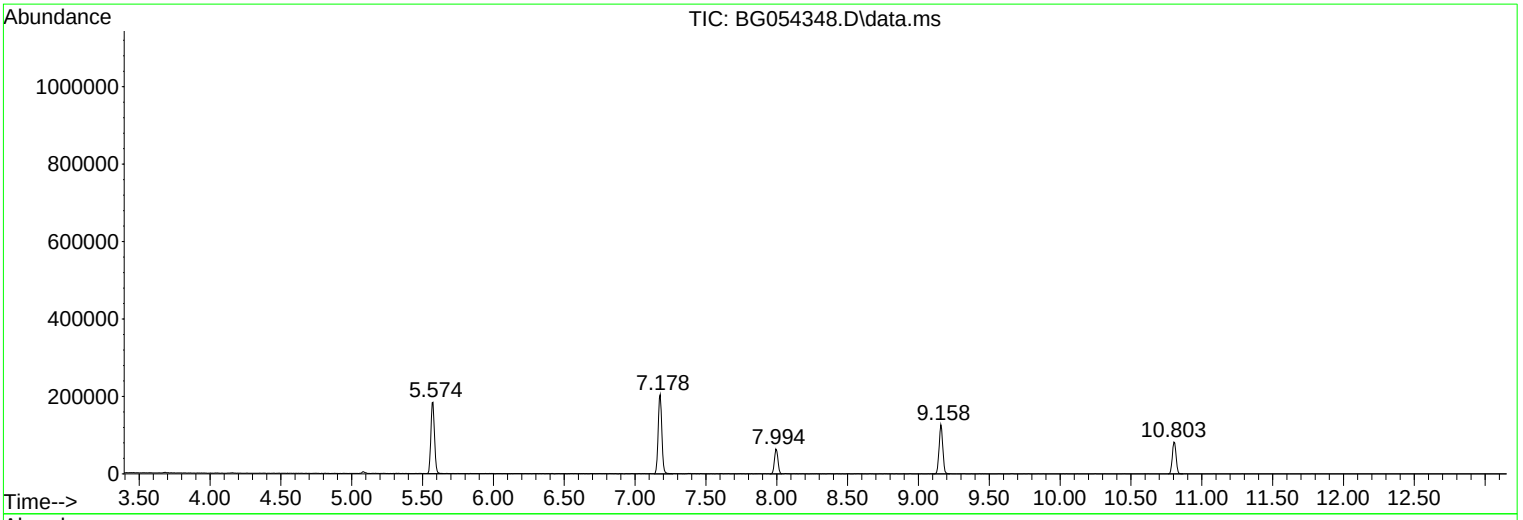
Sum of corrected areas: 9108716

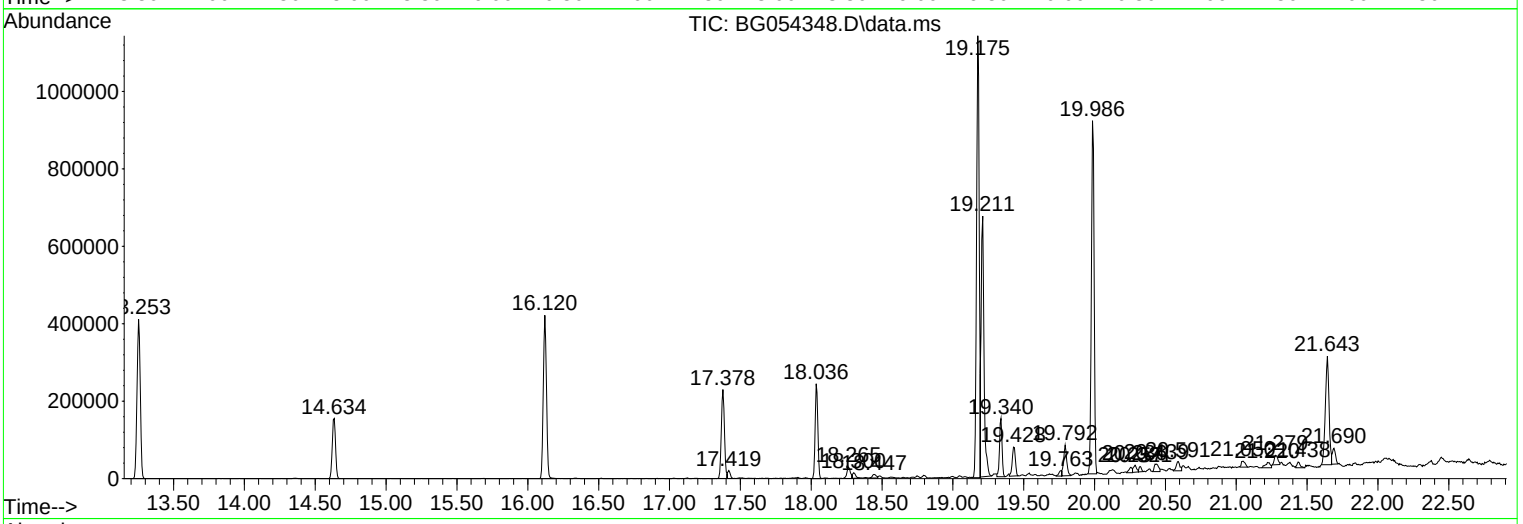
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

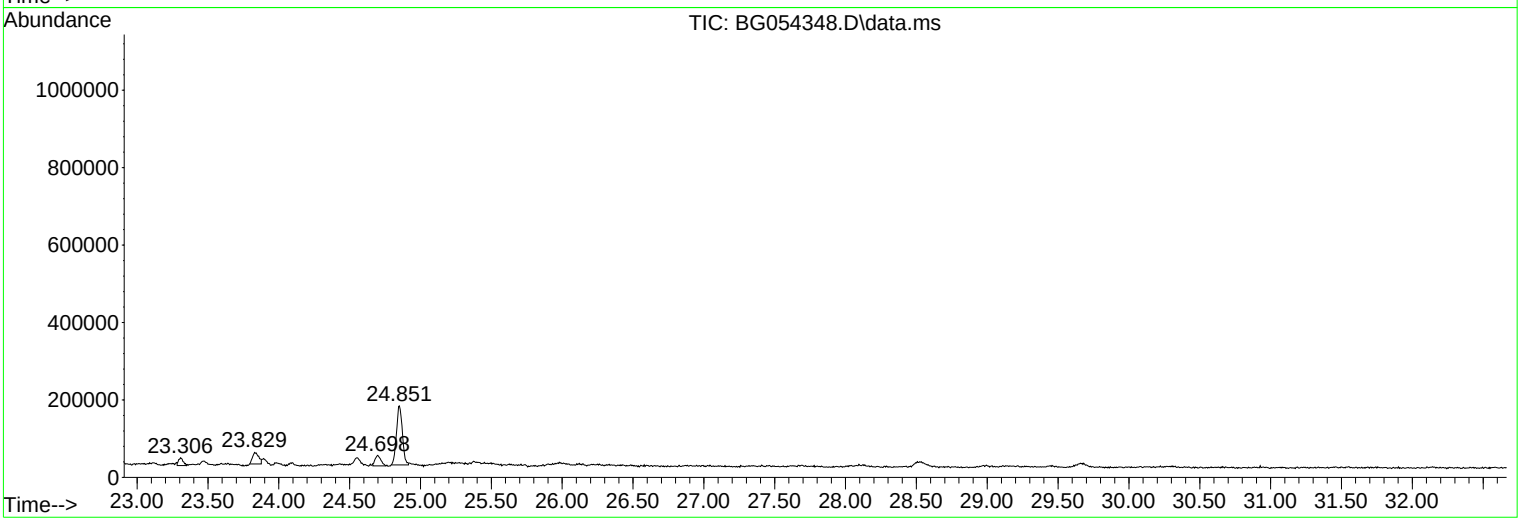
Instrument :
BNA_G
ClientSampleId :
TR-05-072022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

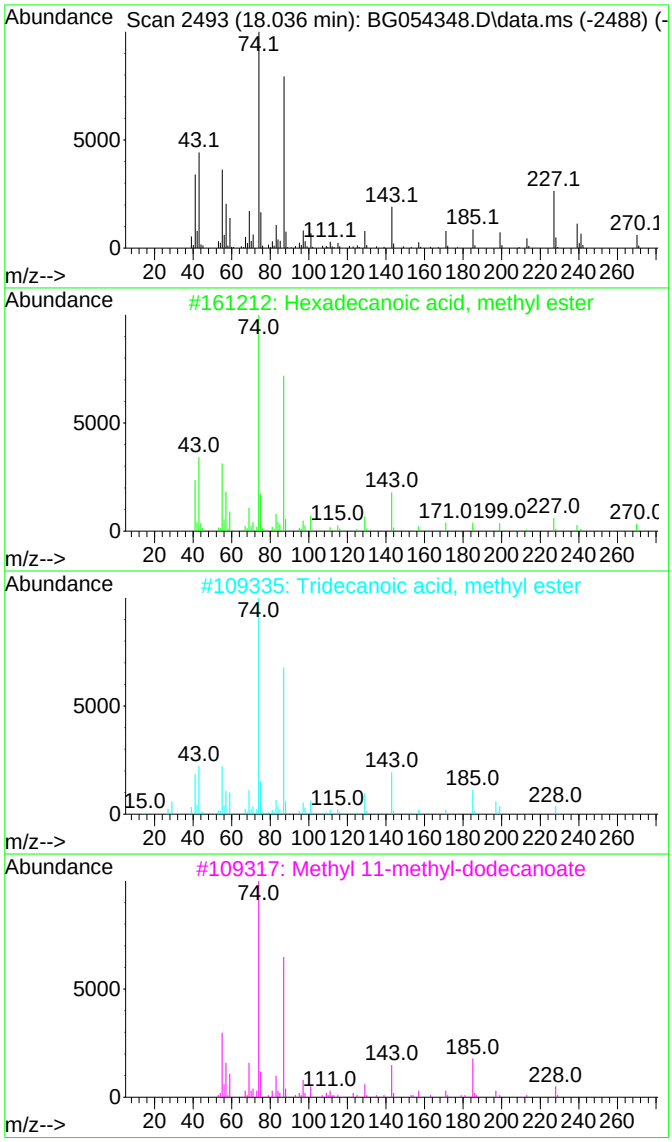
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

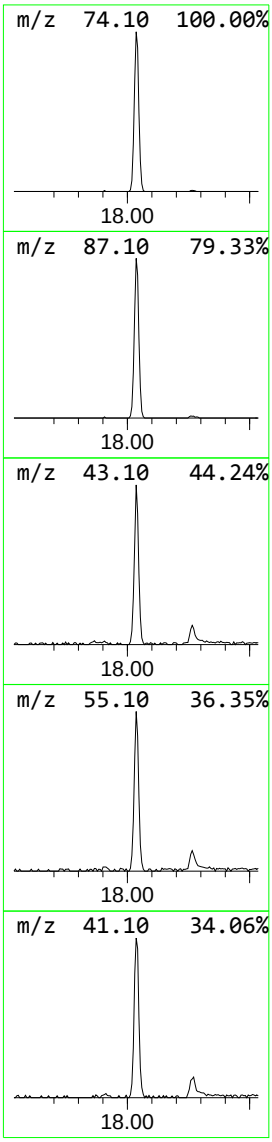
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.036	18.36 ng	320888	Phenanthrene-d10	17.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	93
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

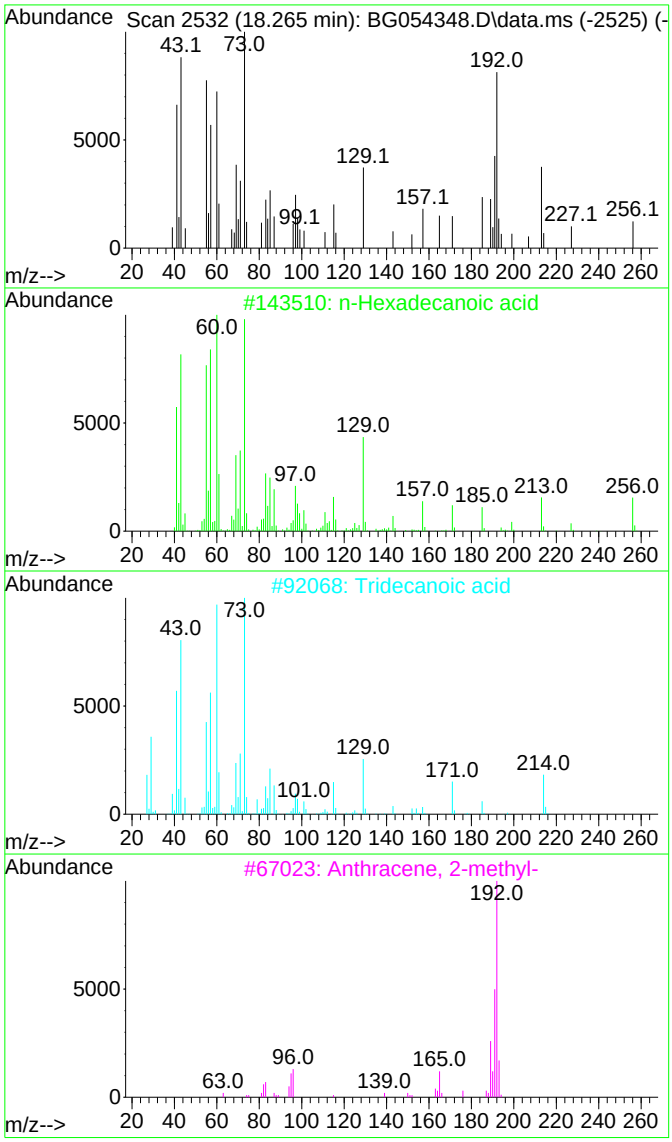
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

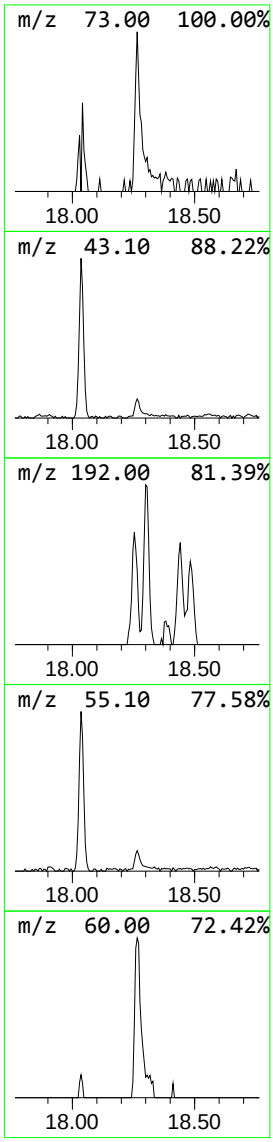
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.265	2.99 ng	52248	Phenanthrene-d10	17.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	74
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	30
5	[1,2,4]Triazole-3-thione, 5-amin...	192	C8H8N4S	1010303-72-9	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

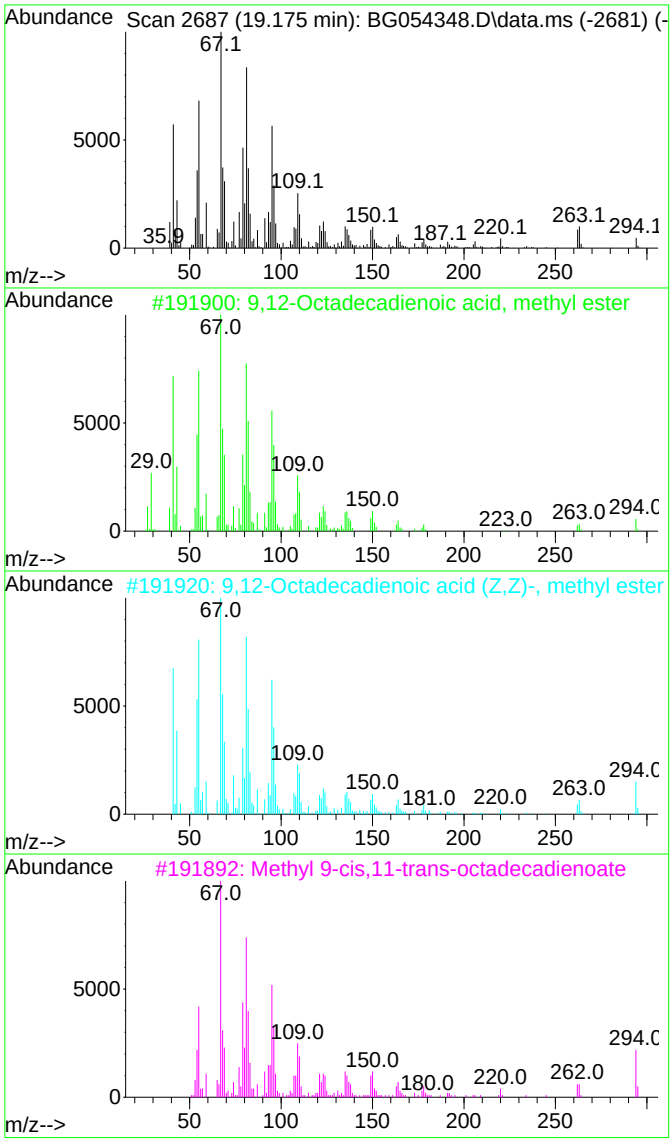
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

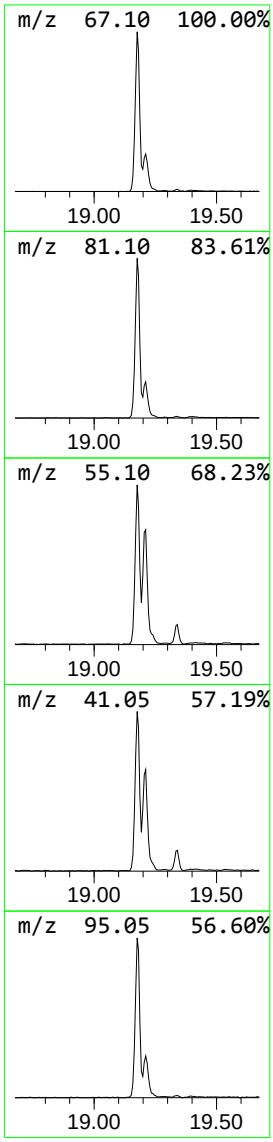
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.176	86.55 ng	1513000	Phenanthrene-d10	17.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

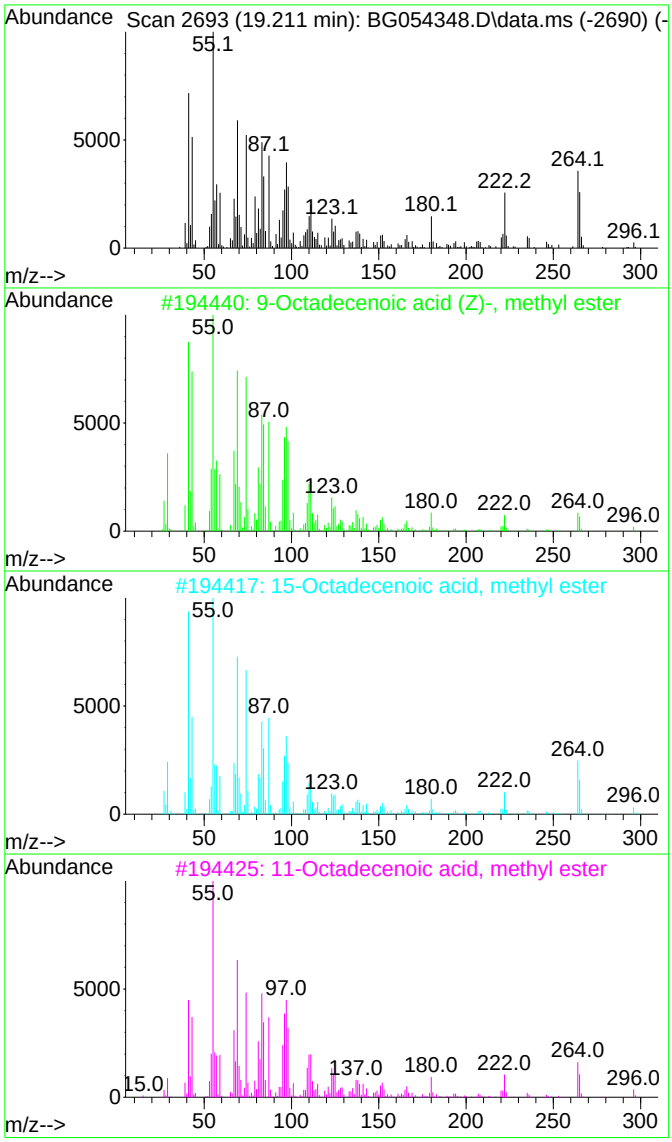
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

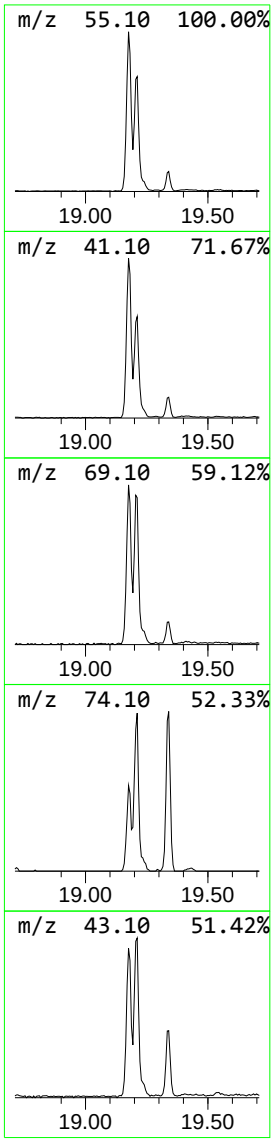
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.211	52.53 ng	918278	Phenanthrene-d10	17.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	98
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
Data File : BG054348.D
Acq On : 21 Jul 2022 17:03
Operator : CG/JU
Sample : N3816-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-072022

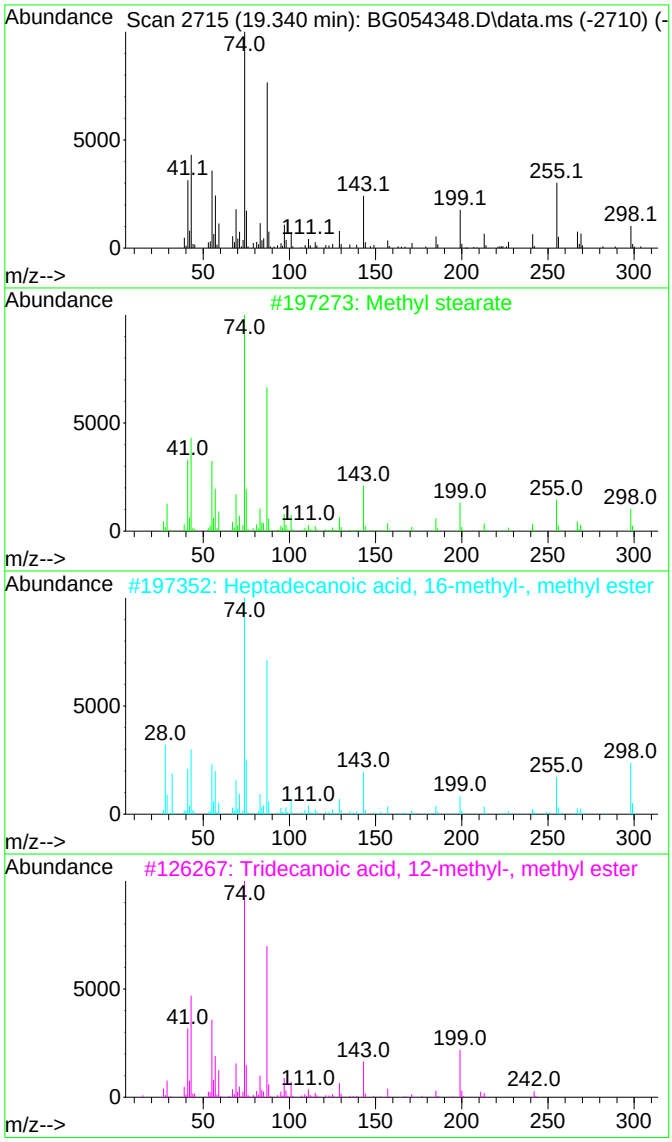
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

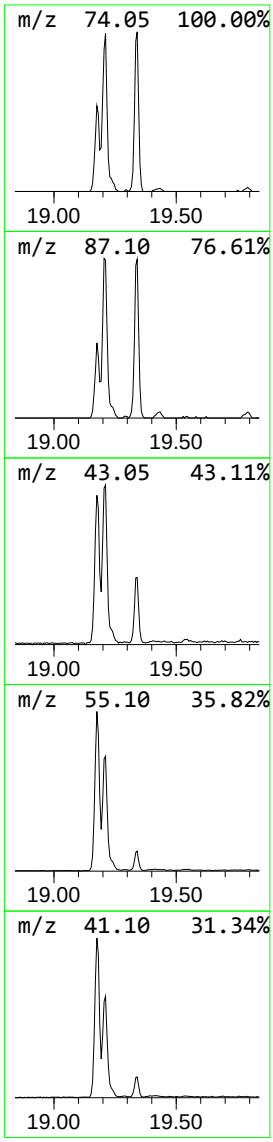
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.340	10.49 ng	183451	Phenanthrene-d10	17.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	99
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	96
3	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	94
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072122\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Hexadecanoic ac...	18.036	18.4	ng	320888	4	17.378	349617	20.0
n-Hexadecanoic ...	18.265	3.0	ng	52248	4	17.378	349617	20.0
9,12-Octadecadi...	19.176	86.5	ng	1513000	4	17.378	349617	20.0
9-Octadecenoic ...	19.211	52.5	ng	918278	4	17.378	349617	20.0
Methyl stearate	19.340	10.5	ng	183451	4	17.378	349617	20.0