LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120122\
Data File : BG055861.D
Acq On : 1 Dec 2022 18:41
Operator : CG/JU
Sample : N5814-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-113022

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.259	327	335	346	rBV	171224	277557	12.13%	2.138%
2	5.740	410	417	432	rBV	604309	1020513	44.59%	7.861%
3	7.362	685	693	705	rBV	619873	1094536	47.82%	8.431%
4	8.208	830	837	843	rBV	140418	234967	10.27%	1.810%
5	9.383	1029	1037	1048	rBV	385875	689509	30.13%	5.311%
6	11.034	1311	1318	1326	rBV	190840	342528	14.97%	2.638%
7	13.455	1723	1730	1738	rBV	1086071	1673715	73.13%	12.892%
8	14.836	1957	1965	1972	rBV	319621	495922	21.67%	3.820%
9	16.316	2211	2217	2228	rBV	885849	1342873	58.67%	10.344%
10	17.574	2425	2431	2437	rBV	394751	600504	26.24%	4.625%
11	17.615	2437	2438	2445	rVB2	21361	26080	1.14%	0.201%
12	18.202	2534	2538	2543	rVB	71366	91855	4.01%	0.708%
13	18.431	2572	2577	2585	rBV	194704	307593	13.44%	2.369%
14	19.330	2726	2730	2733	rBV	345065	416491	18.20%	3.208%
15	19.366	2733	2736	2746	rVB2	172633	251665	11.00%	1.938%
16	19.495	2754	2758	2762	rVB	41485	50463	2.20%	0.389%
17	19.612	2775	2778	2784	rVB	46304	68095	2.98%	0.525%
18	19.689	2788	2791	2800	rVV	71223	117094	5.12%	0.902%
19	19.941	2832	2834	2837	rBV3	22985	27654	1.21%	0.213%
20	19.977	2837	2840	2844	rVB	39895	50499	2.21%	0.389%
21	20.159	2866	2871	2877	rBV	1799908	2288770	100.00%	17.630%
22	20.934	3000	3003	3008	rVB	47356	53559	2.34%	0.413%
23	21.863	3155	3161	3167	rVB2	352113	599232	26.18%	4.616%
24	24.207	3556	3560	3568	rVB2	115251	257235	11.24%	1.981%
25	25.241	3730	3736	3748	rVB2	197477	603671	26.38%	4.650%

Sum of corrected areas: 12982580

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Instrument :
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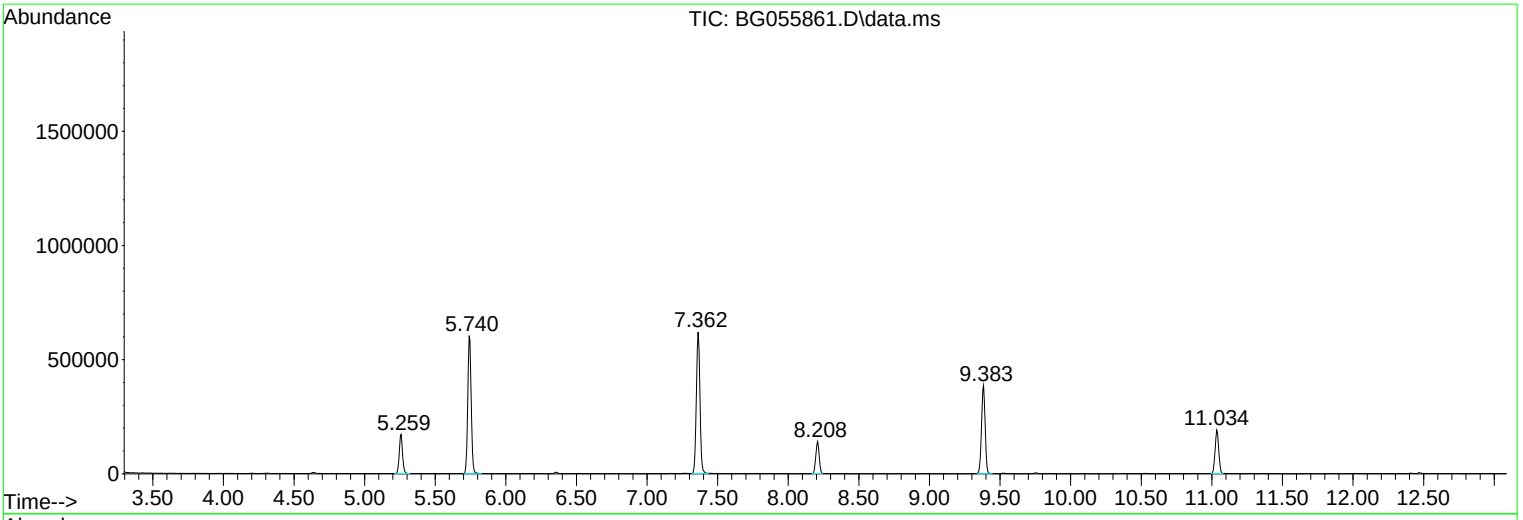
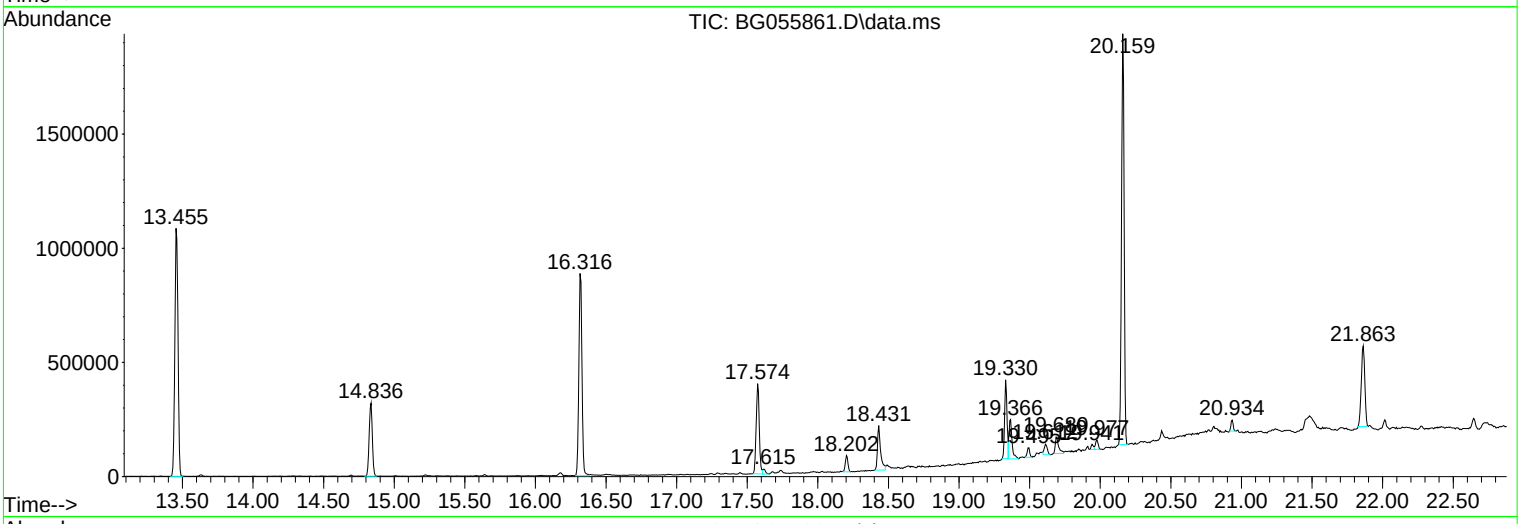
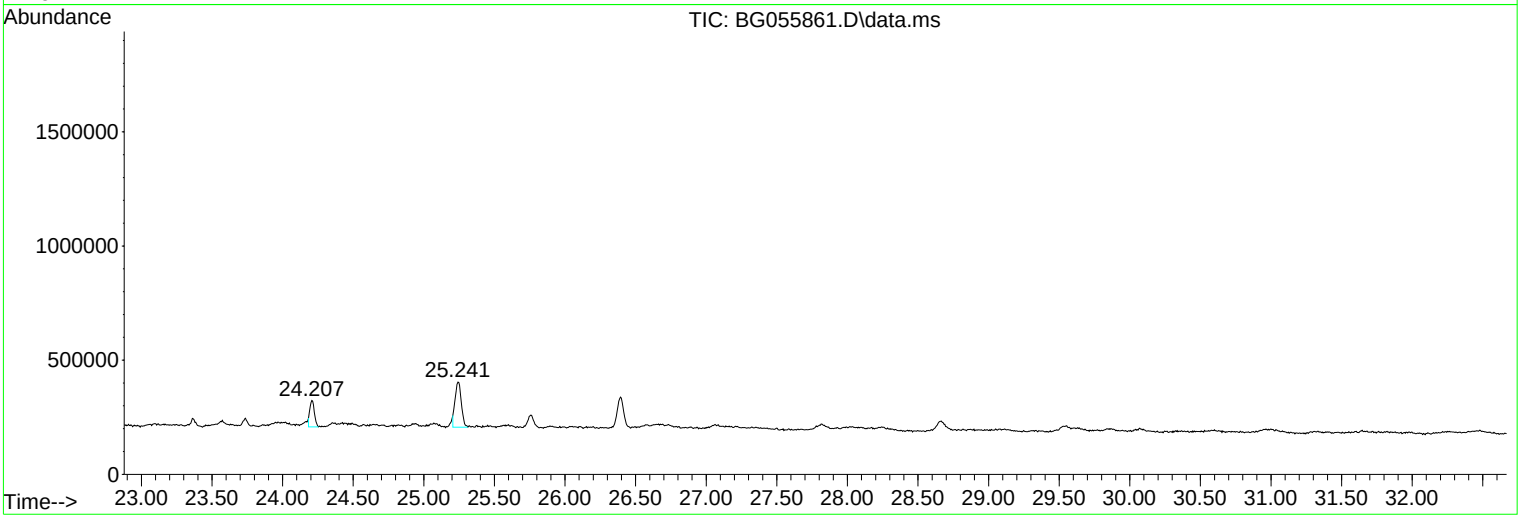
ClientSampleId :
NB-08-113022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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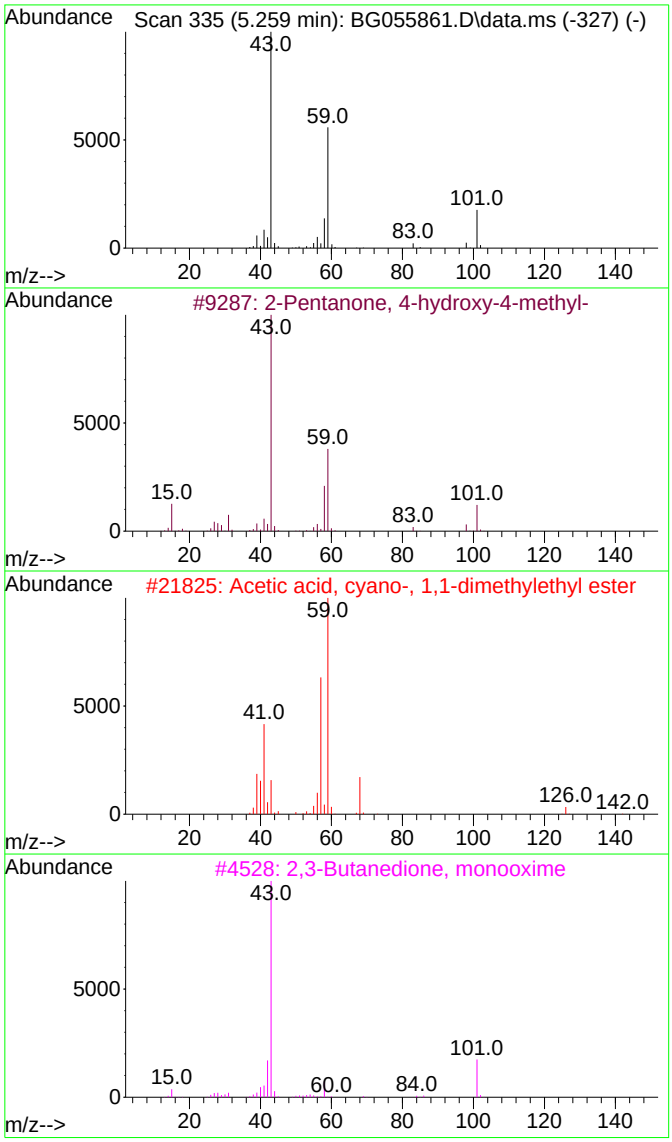
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

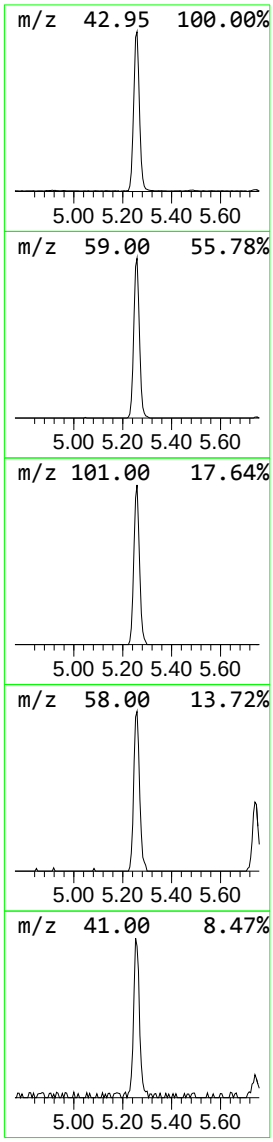
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.259	23.63 ng	277557	1,4-Dichlorobenzene-d4	8.208

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Operator : CG/JU
Sample : N5814-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
NB-08-113022

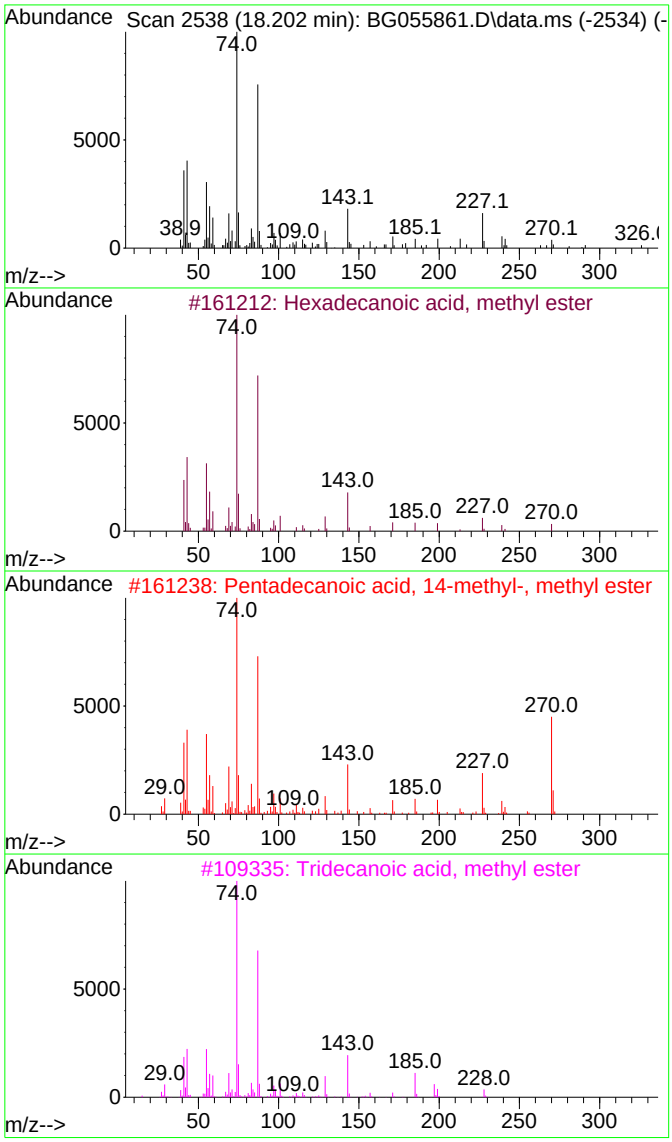
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

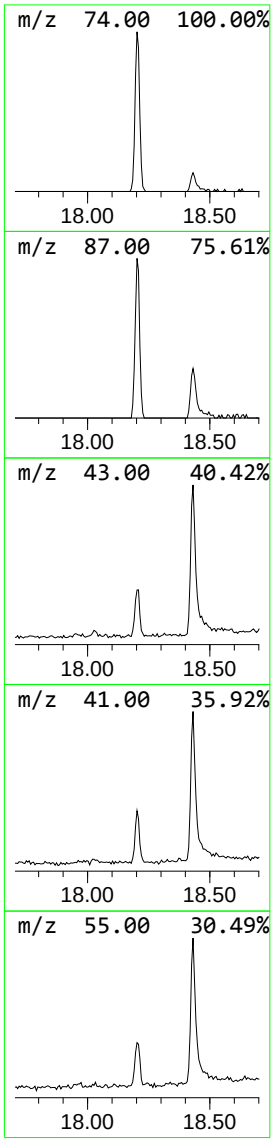
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.202	3.06 ng	91855	Phenanthrene-d10	17.573

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Methyl stearate	298	C19H38O2	000112-61-8	83





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Data File : BG055861.D
Acq On : 1 Dec 2022 18:41
Operator : CG/JU
Sample : N5814-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-113022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

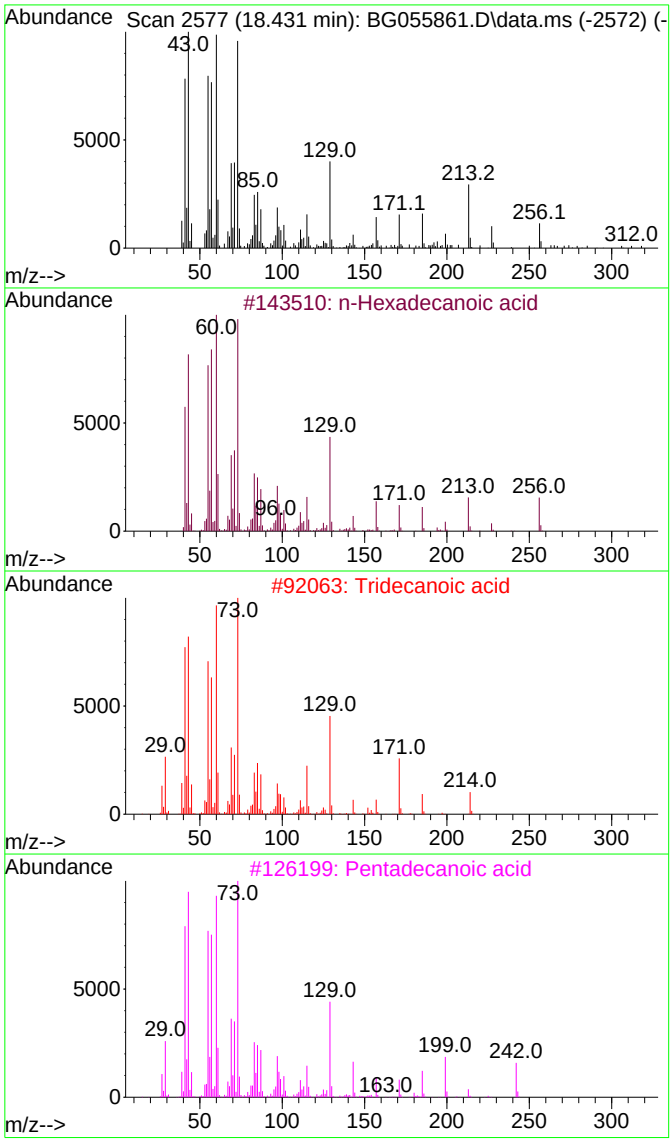
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

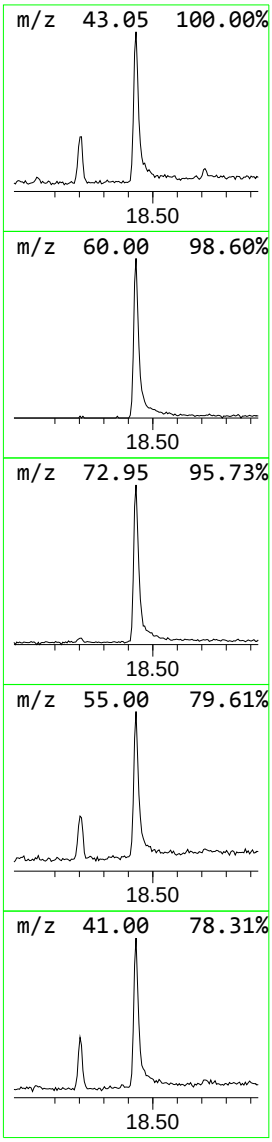
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.431	10.24 ng	307593	Phenanthrene-d10	17.573

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Sample : N5814-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-113022

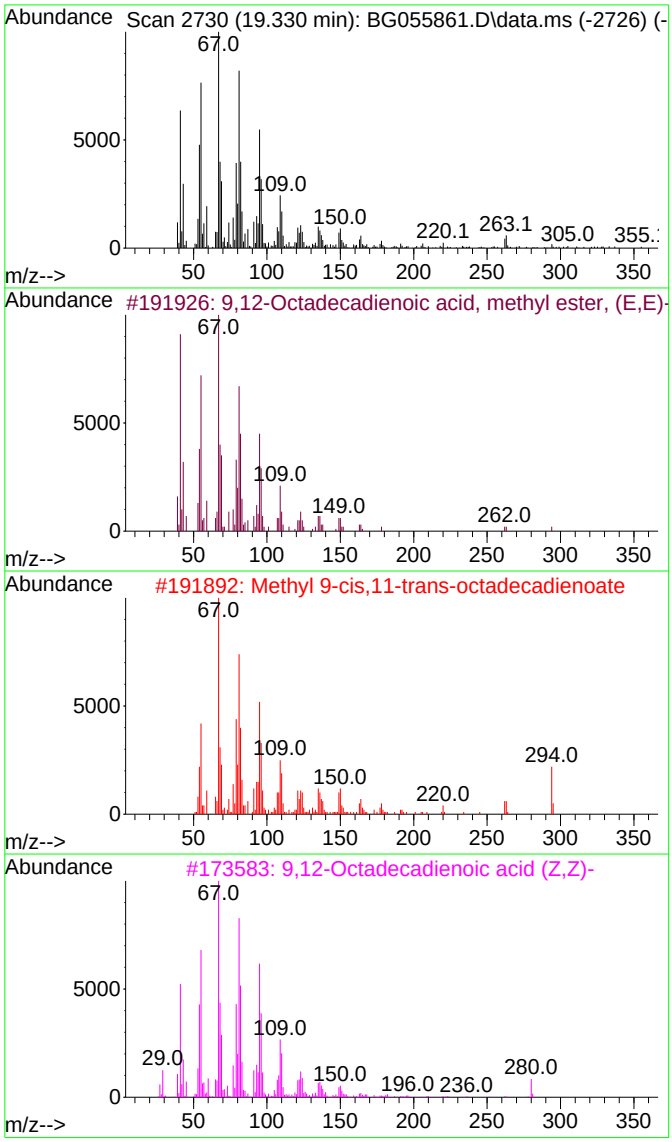
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

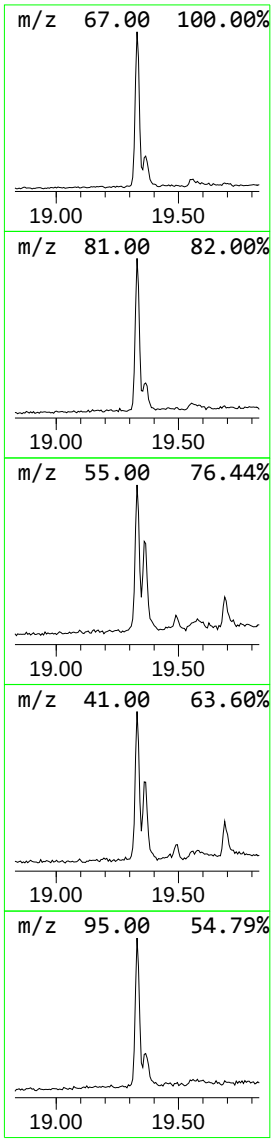
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.330	13.87 ng	416491	Phenanthrene-d10	17.573

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	95
3	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	94
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
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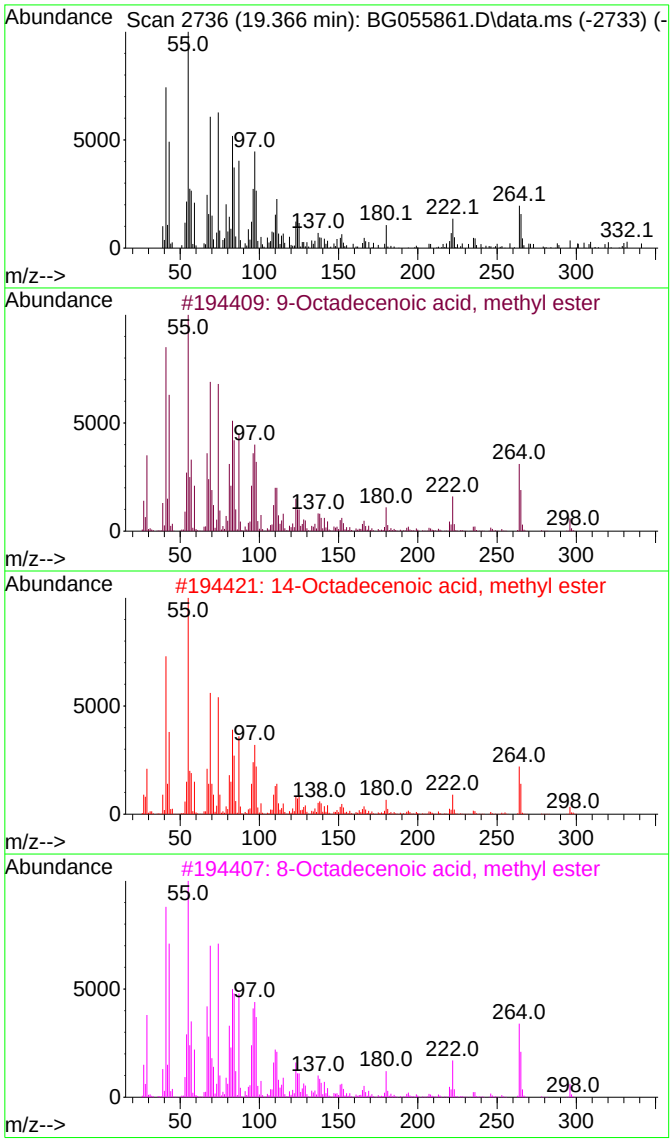
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

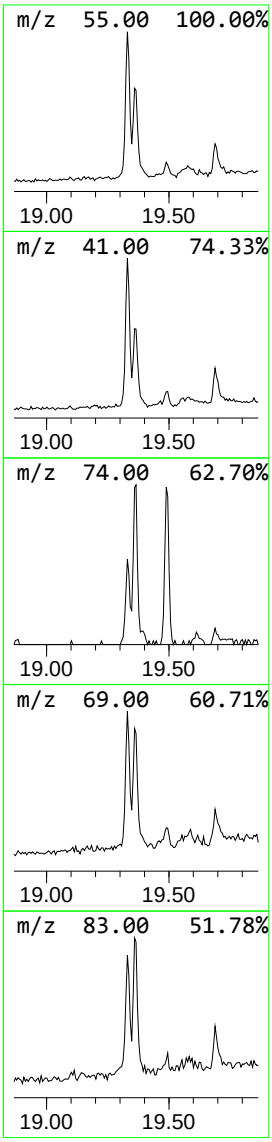
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.366	8.38 ng	251665	Phenanthrene-d10	17.573

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	97
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	96
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	96
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	95





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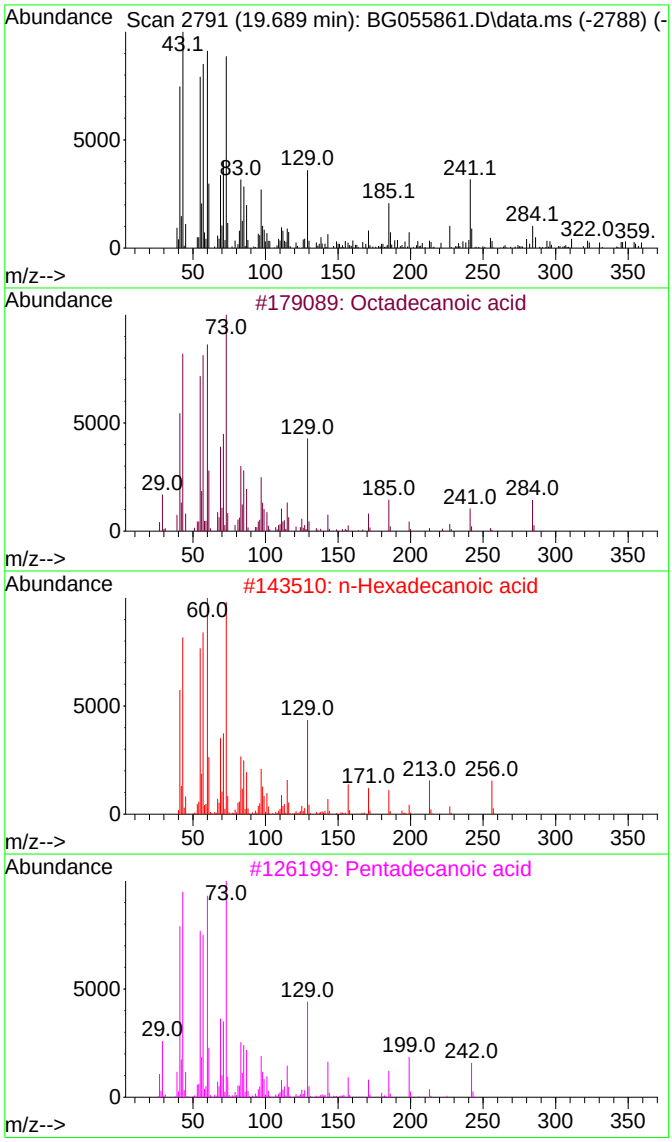
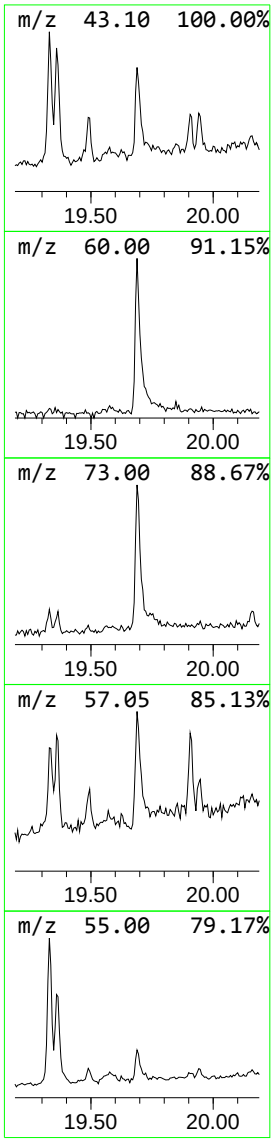
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.689	3.90 ng	117094	Phenanthrene-d10	17.573

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tricosanoic acid	354	C23H46O2	002433-96-7	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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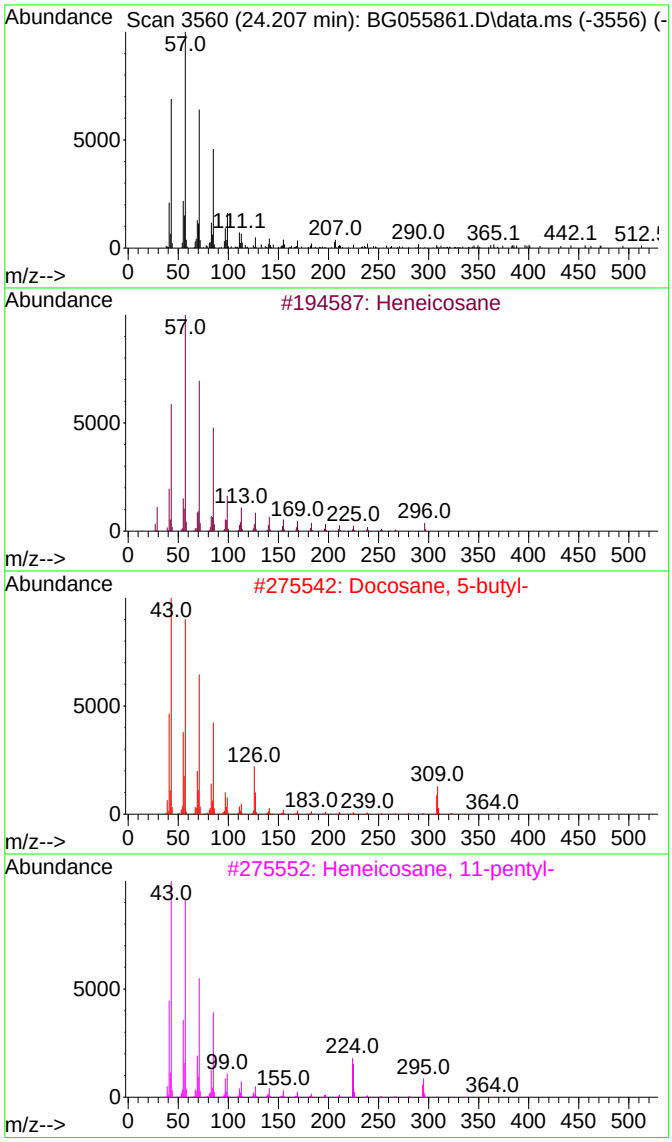
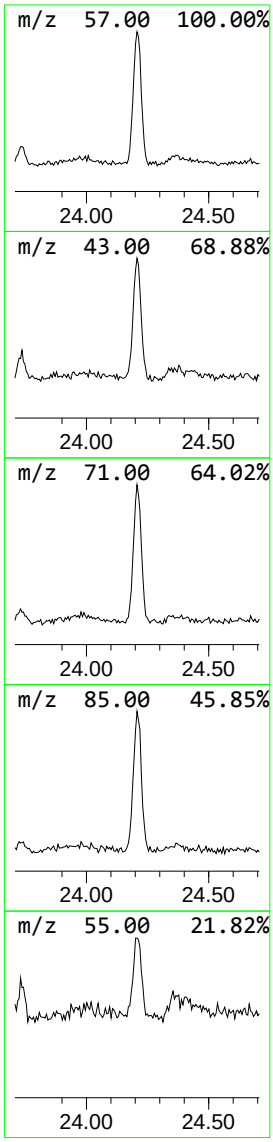
****

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.207	8.52 ng	257235	Perylene-d12	25.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
3	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
4	Docosane, 9-butyl-	366	C26H54	055282-14-9	81
5	Octacosane	394	C28H58	000630-02-4	81





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.259	23.6	ng	277557	1	8.208	234967	20.0
Hexadecanoic ac...	18.202	3.1	ng	91855	4	17.573	600504	20.0
n-Hexadecanoic ...	18.431	10.2	ng	307593	4	17.573	600504	20.0
9,12-Octadecadi...	19.330	13.9	ng	416491	4	17.573	600504	20.0
9-Octadecenoic ...	19.366	8.4	ng	251665	4	17.573	600504	20.0
Octadecanoic acid	19.689	3.9	ng	117094	4	17.573	600504	20.0
Heneicosane	24.207	8.5	ng	257235	6	25.247	603671	20.0