LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

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-BG061322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.639	376	383	396	rBV	266901	471320	5.52%	1.969%
2	7.232	646	654	666	rBV	280827	513114	6.01%	2.144%
3	8.066	789	796	804	rBV	81919	148366	1.74%	0.620%
4	9.229	981	994	1001	rBV	178487	339914	3.98%	1.420%
5	10.880	1264	1275	1281	rBV	108559	240812	2.82%	1.006%
6	13.319	1681	1690	1700	rVB	553244	885598	10.37%	3.700%
7	14.693	1915	1924	1931	rVV	183577	315709	3.70%	1.319%
8	16.180	2169	2177	2186	rBV	422394	701127	8.21%	2.929%
9	16.397	2209	2214	2216	rBV	58166	85931	1.01%	0.359%
10	17.185	2343	2348	2352	rBV	62495	86966	1.02%	0.363%
11	17.437	2385	2391	2395	rBV	222376	356334	4.17%	1.489%
12	17.484	2395	2399	2405	rVB	92481	148111	1.73%	0.619%
13	18.101	2498	2504	2510	rVB	1599416	2116652	24.79%	8.843%
14	18.324	2537	2542	2546	rBV3	74894	128813	1.51%	0.538%
15	18.512	2569	2574	2586	rVB5	37035	104640	1.23%	0.437%
16	19.247	2691	2699	2702	rBV	5283059	8538382	100.00%	35.672%
17	19.276	2702	2704	2714	rVB2	3391219	4585781	53.71%	19.159%
18	19.400	2720	2725	2731	rVB	795378	991255	11.61%	4.141%
19	19.494	2736	2741	2747	rVB	251164	393722	4.61%	1.645%
20	19.852	2799	2802	2809	rVB	262293	395025	4.63%	1.650%
21	20.046	2830	2835	2841	rBV	944882	1298695	15.21%	5.426%
22	20.381	2889	2892	2899	rVB4	109445	151889	1.78%	0.635%
23	20.487	2907	2910	2917	rBV3	87574	168830	1.98%	0.705%
24	20.645	2934	2937	2941	rBV2	92228	123942	1.45%	0.518%
25	21.715	3112	3119	3124	rBV2	278207	644935	7.55%	2.694%

Sum of corrected areas: 23935863

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Misc :
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Instrument :
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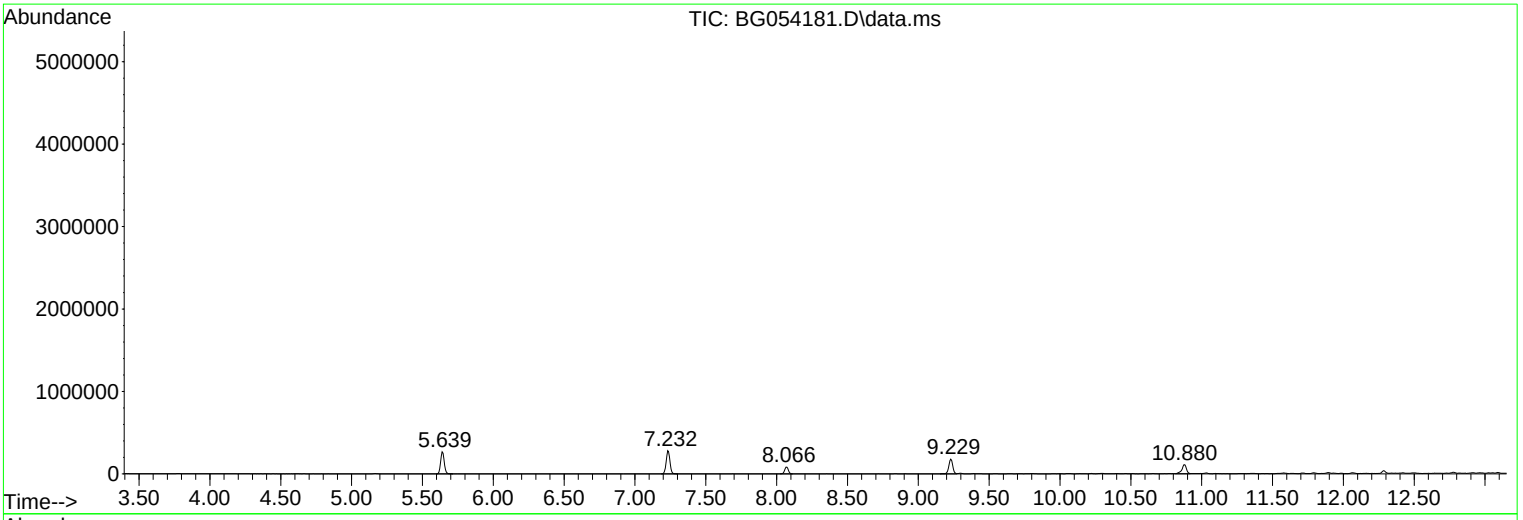
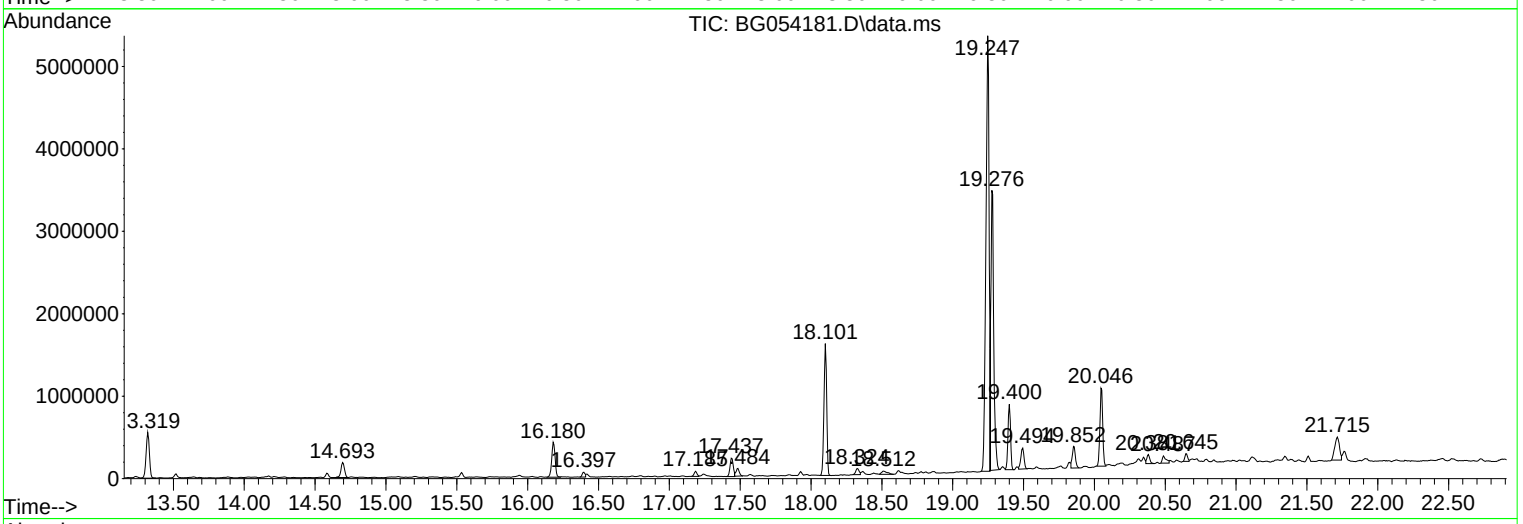
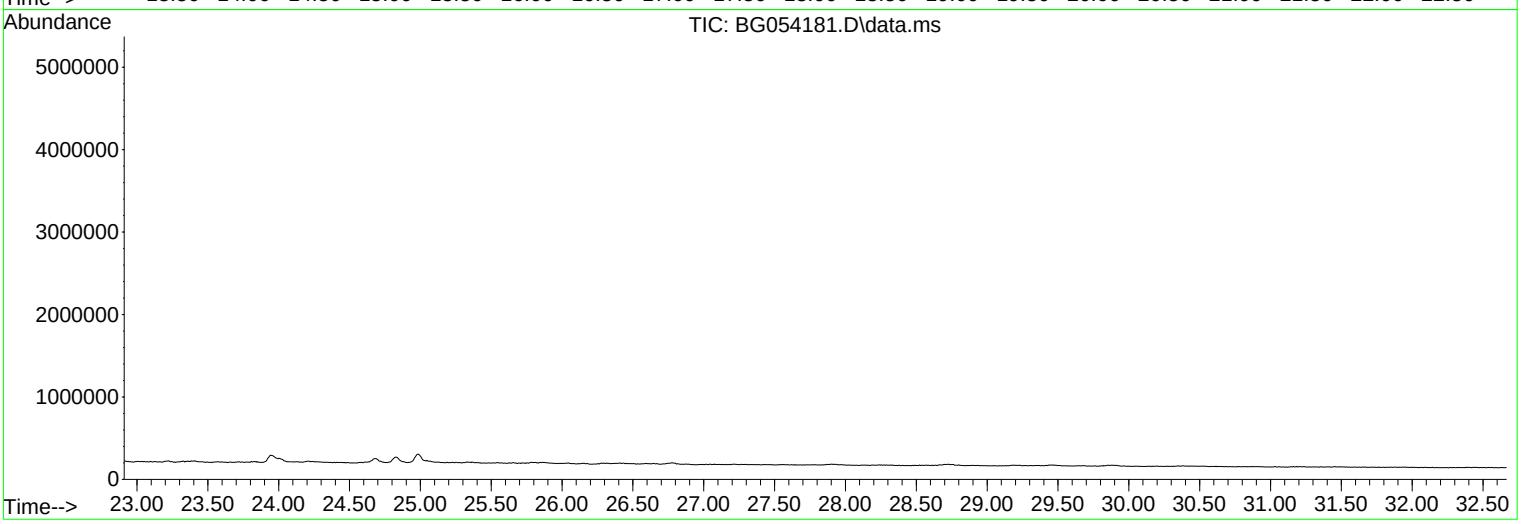
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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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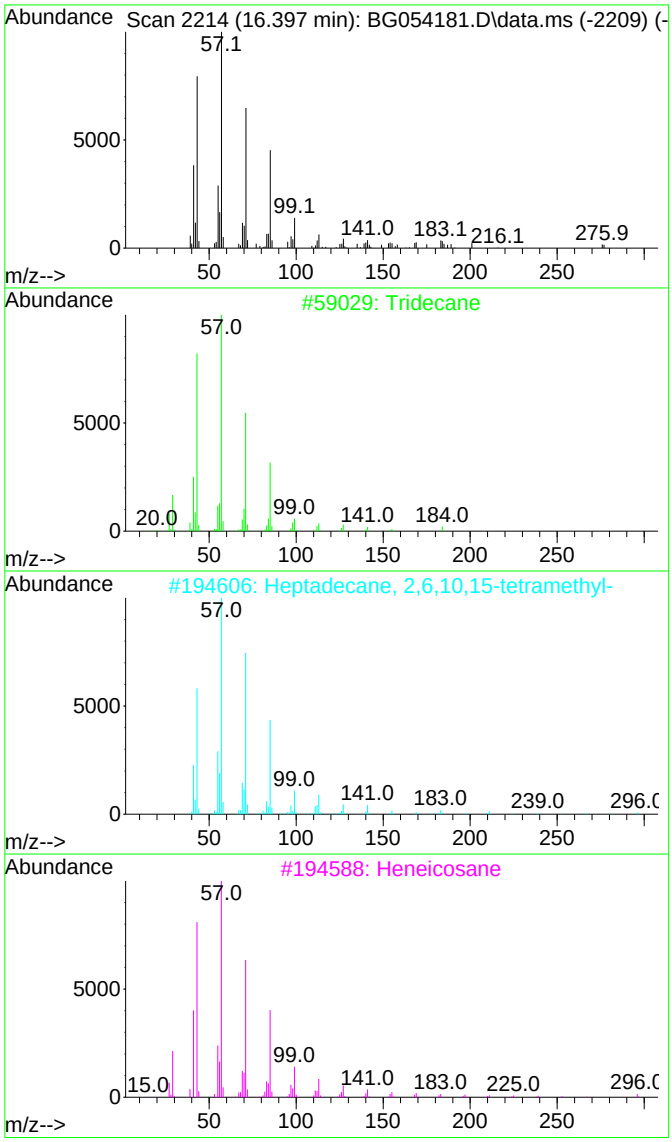
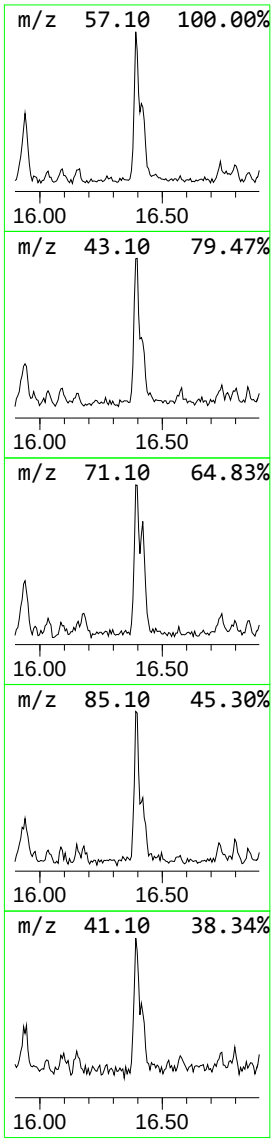
****

Peak Number 1 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	4.82 ng	85931	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	95
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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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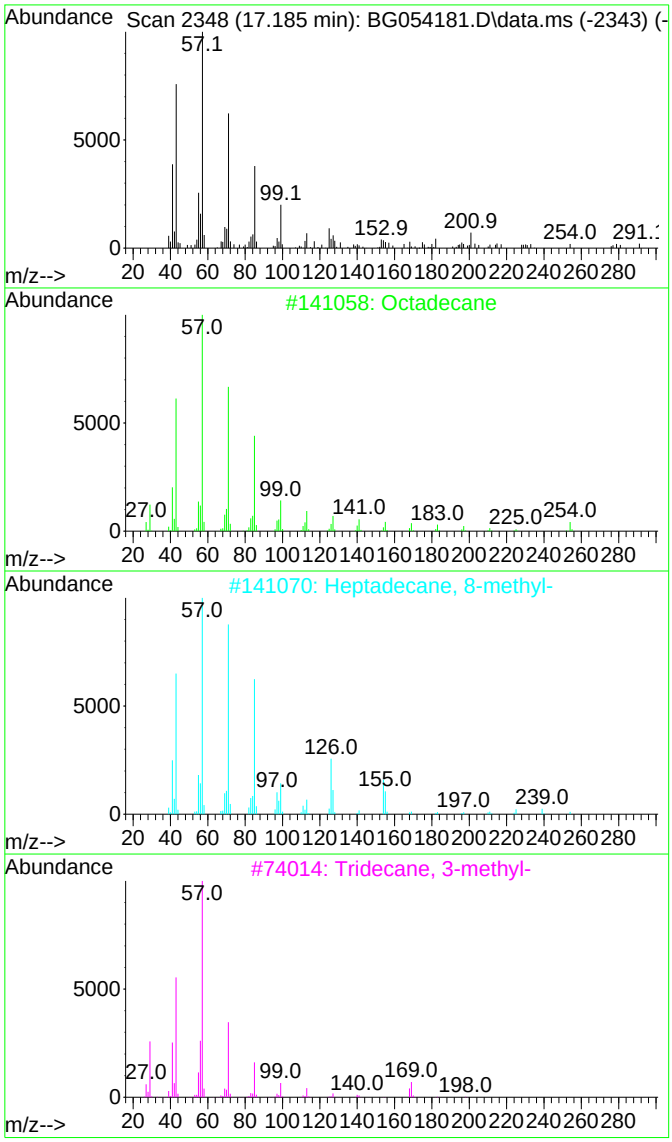
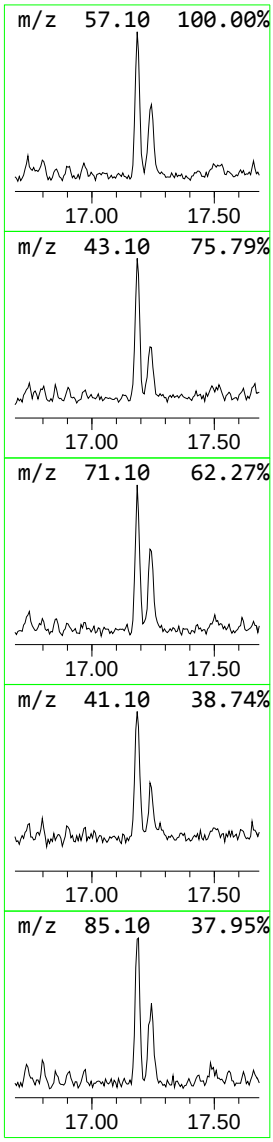
Peak Number 2 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.185	4.88 ng	86966	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	76
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	70
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	64
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
5	Pentadecane	212	C15H32	000629-62-9	58





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Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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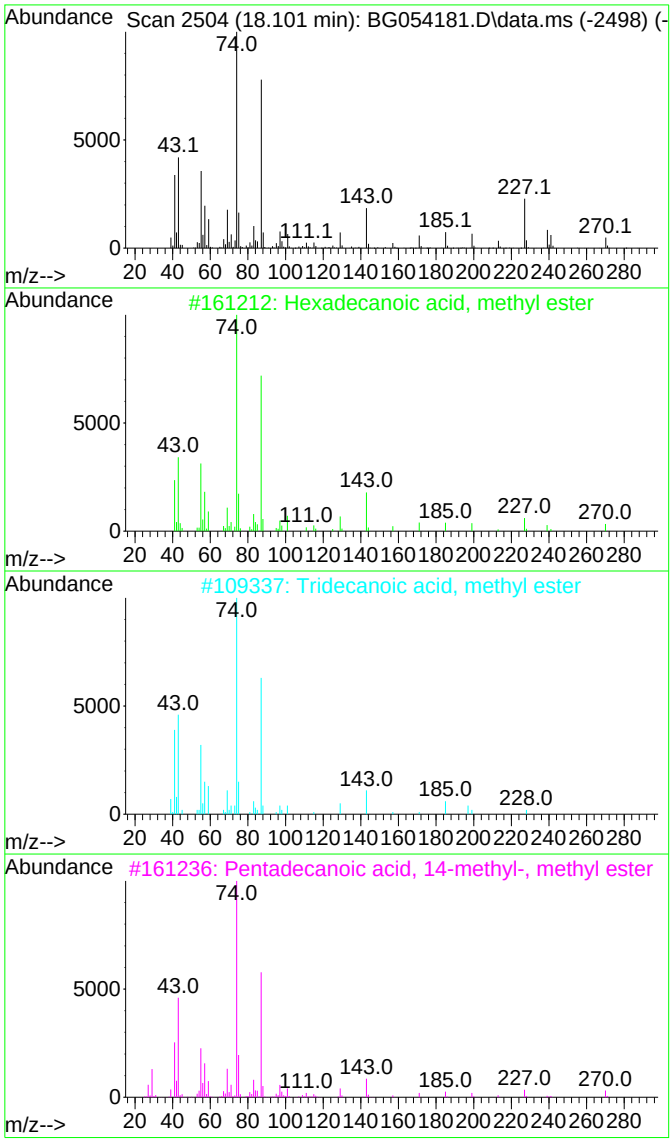
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

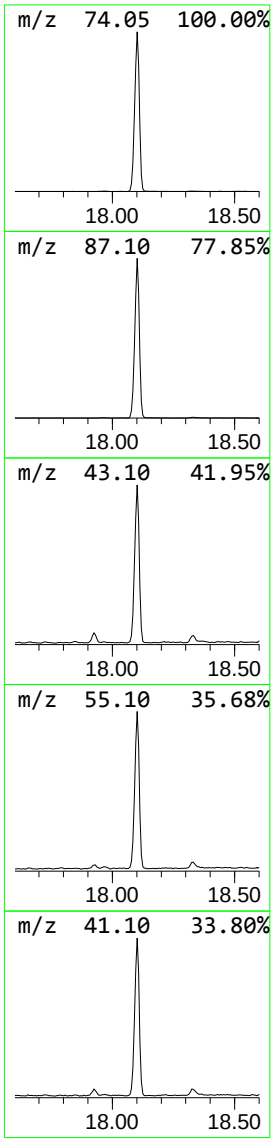
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.101	118.80 ng	2116650	Phenanthrene-d10	17.437

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	95
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	76
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	74





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Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

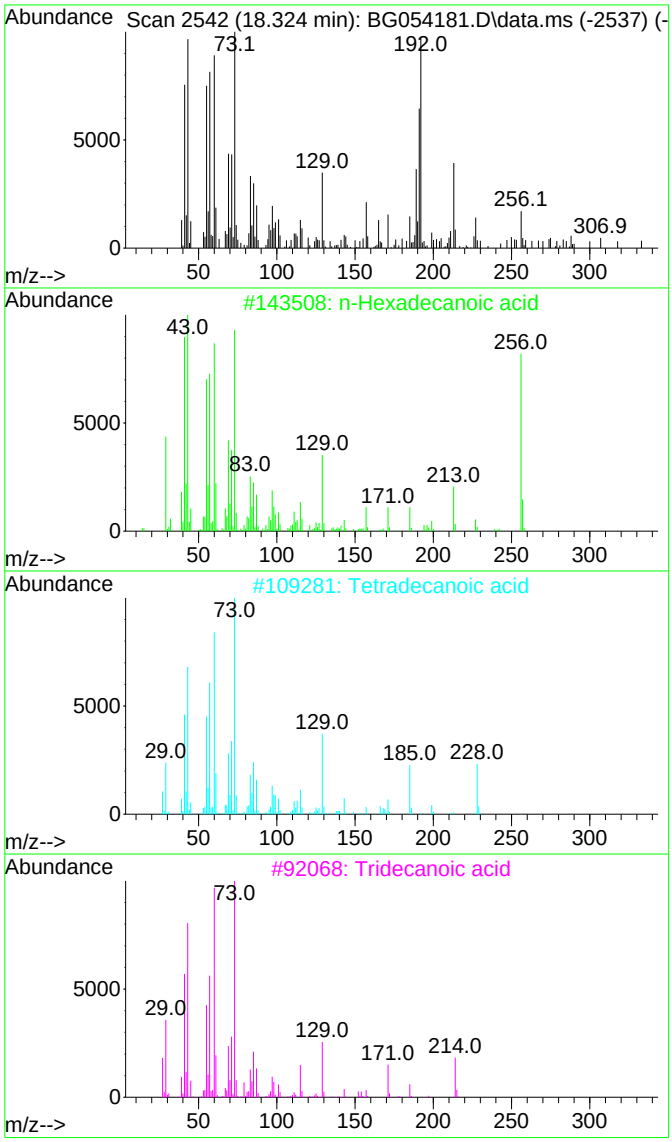
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

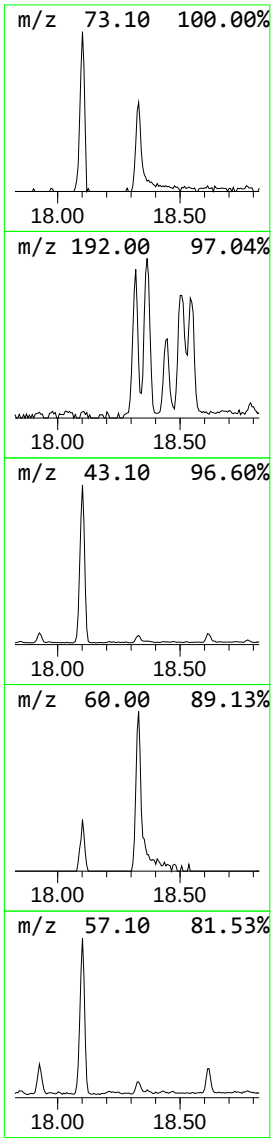
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.325	7.23 ng	128813	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	84
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	46
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38





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Data File : BG054181.D
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Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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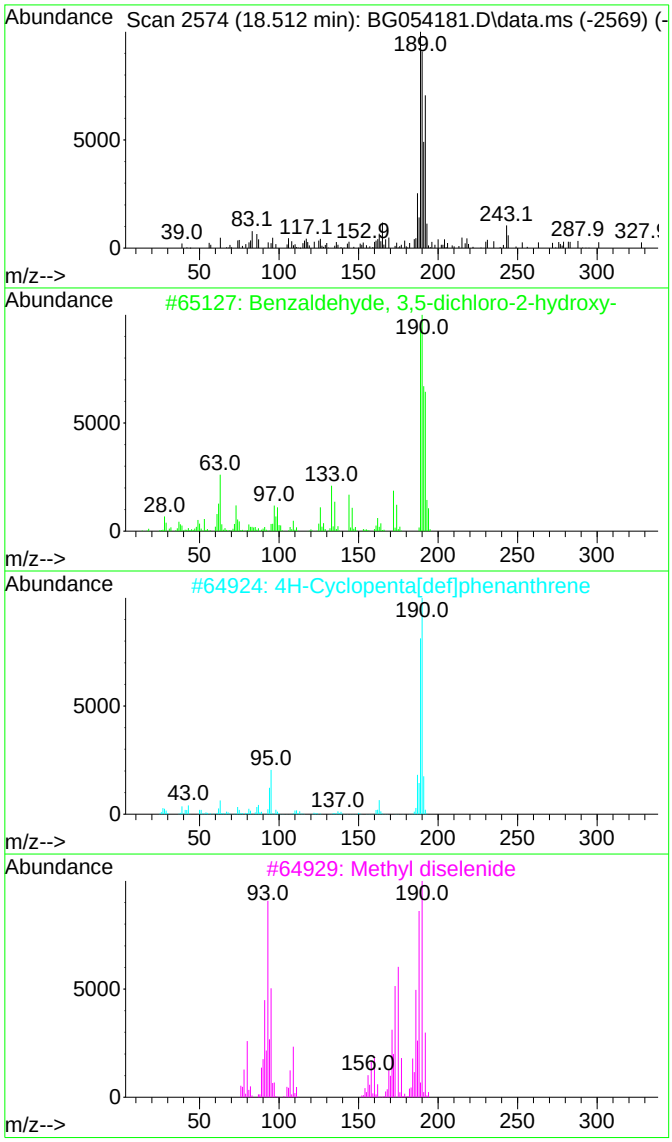
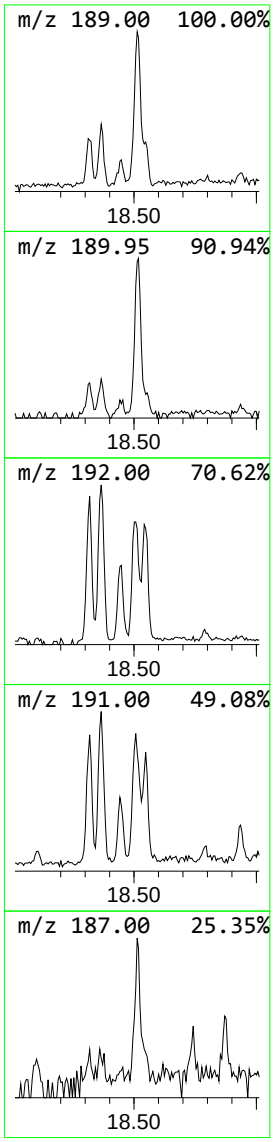
****
Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.512	5.87 ng	104640	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	Methyl diselenide	190	C2H6Se2	007101-31-7	38
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	35





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Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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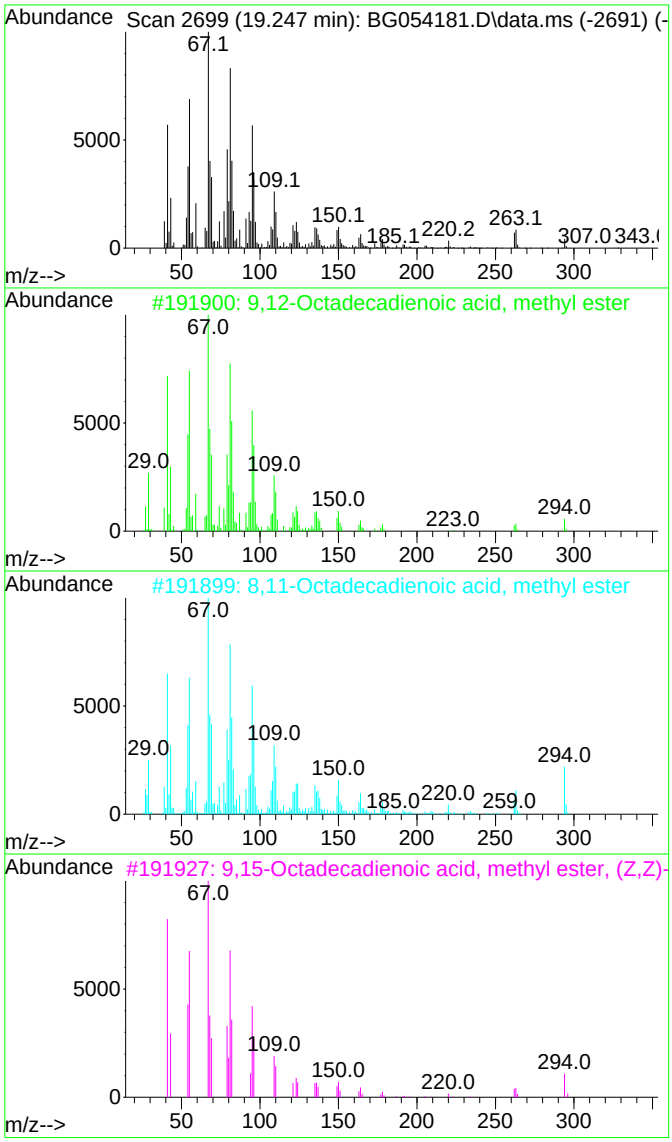
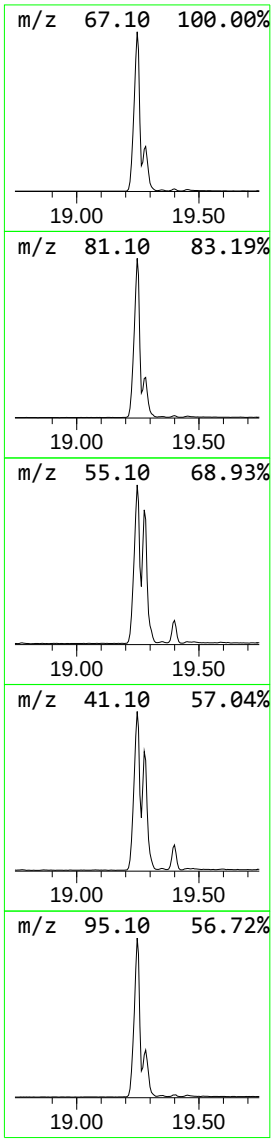
****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.247	479.24 ng	8538380	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	95





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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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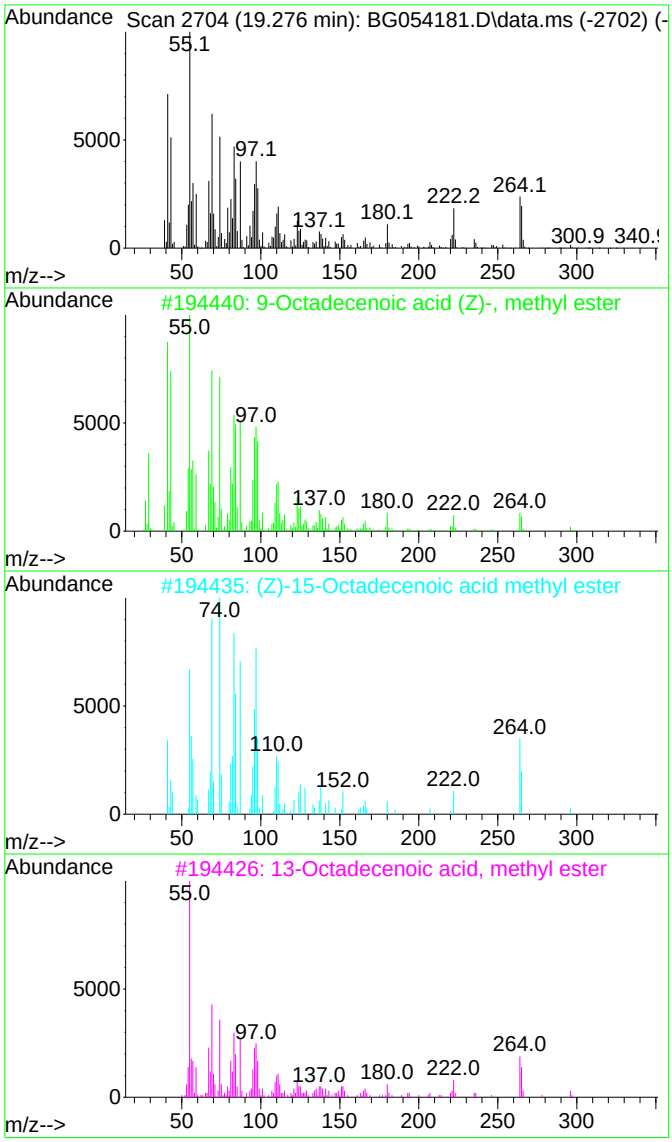
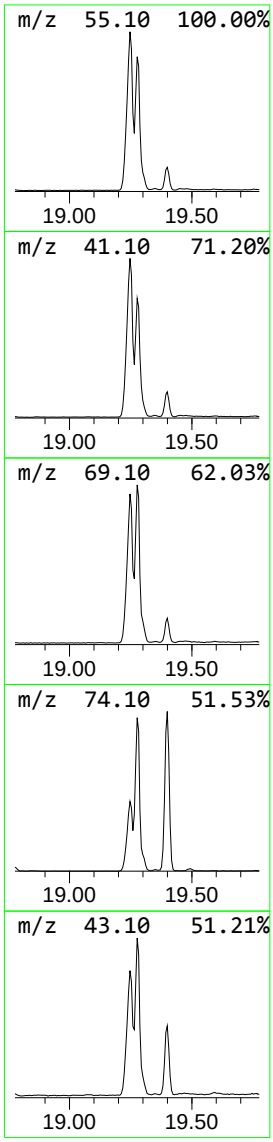
Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.276	257.39 ng	4585780	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	95
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	94
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94





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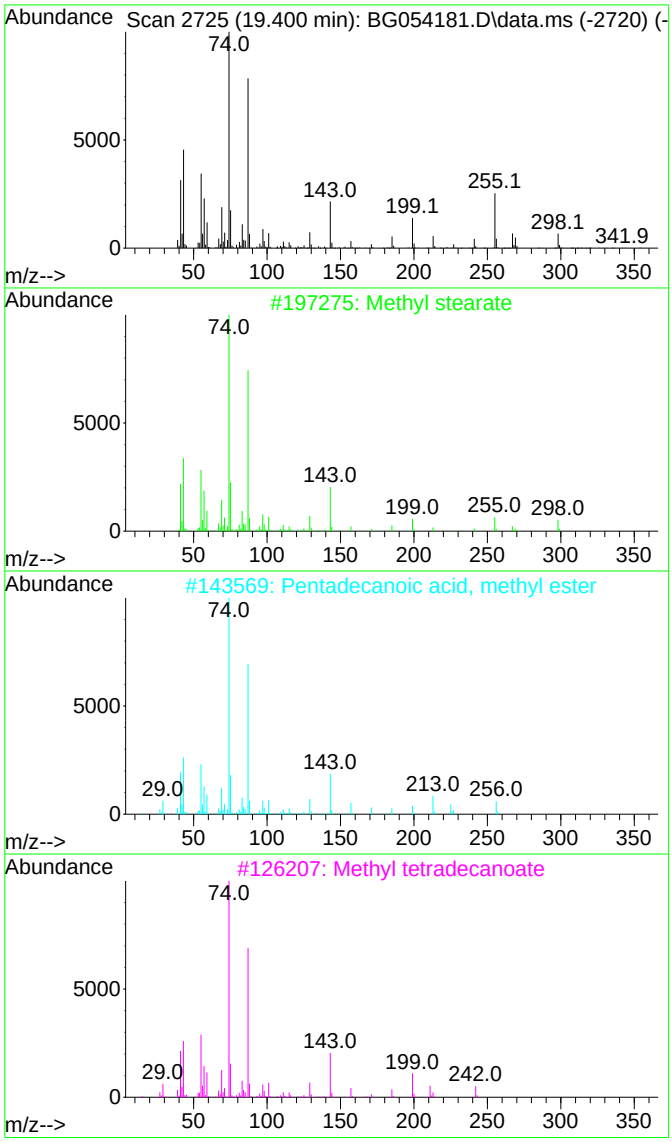
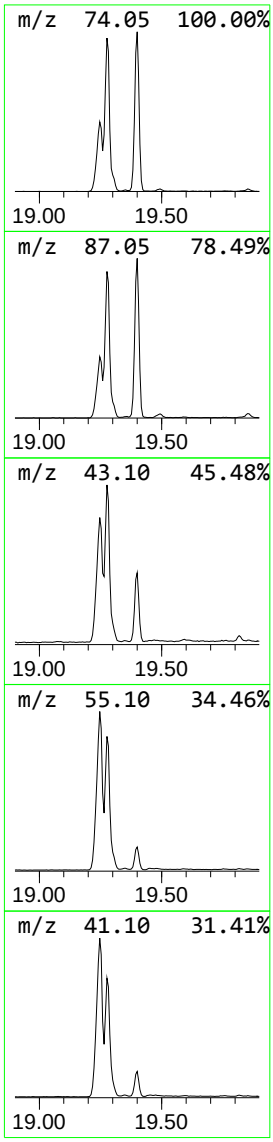
****

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.400	55.64 ng	991255	Phenanthrene-d10	17.437

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	95
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
4	2-Methylpentadecanoic acid	256	C16H32O2	025354-92-1	81
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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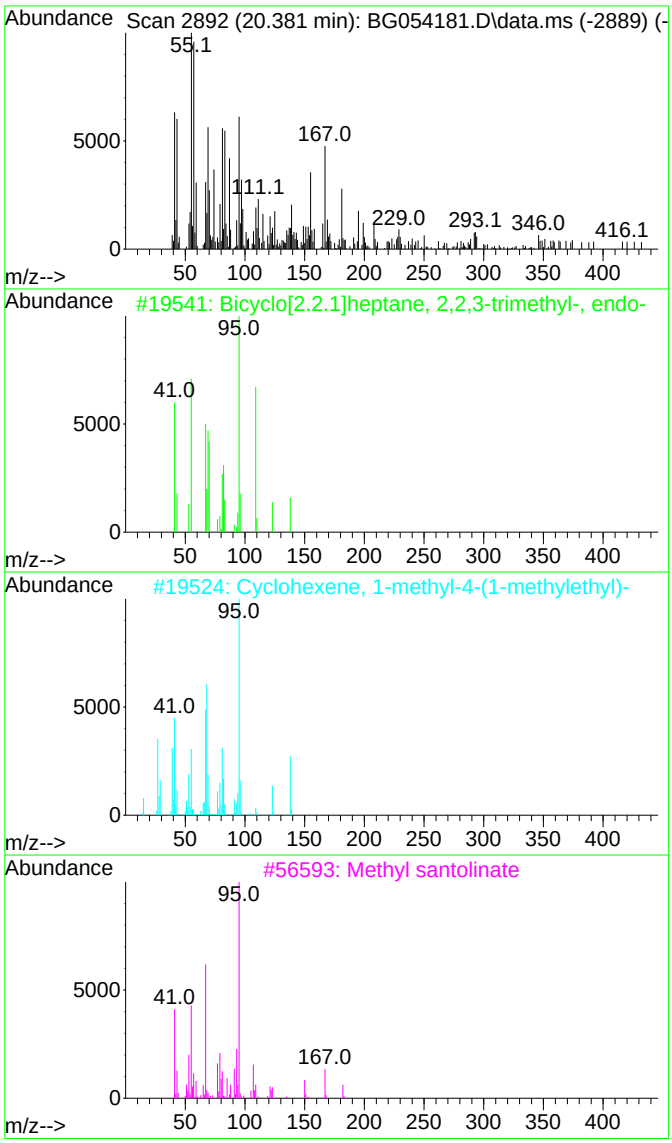
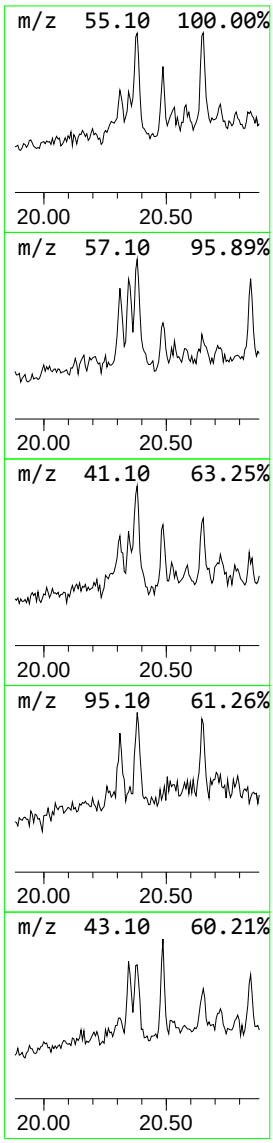
Peak Number 9 unknown20.381 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.381	4.71 ng	151889	Chrysene-d12	21.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	25
2	Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	005502-88-5	15
3	Methyl santolinate	182	C11H18O2	053163-37-4	15
4	2-Heptenoic acid, methyl ester	142	C8H14O2	022104-69-4	15
5	Methyl 18-fluoro-octadec-9-enoate	314	C19H35FO2	1000336-48-7	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

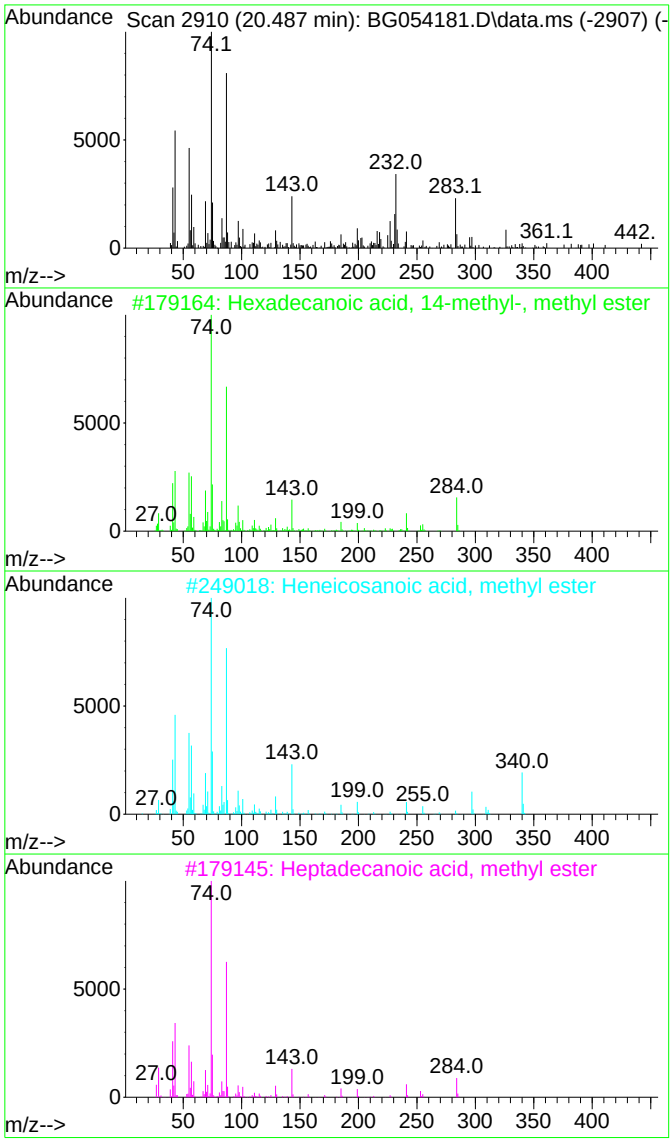
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

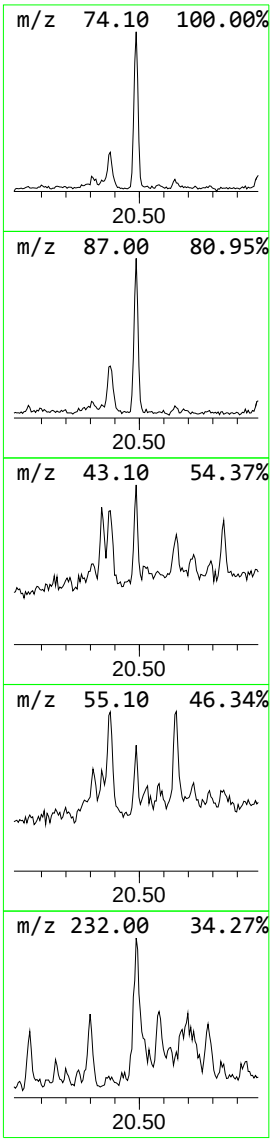
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Hexadecanoic acid, 14-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.487	5.24 ng	168830	Chrysene-d12	21.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	94
2	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	93
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
5	Tetracosanoic acid, methyl ester	382	C25H50O2	002442-49-1	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

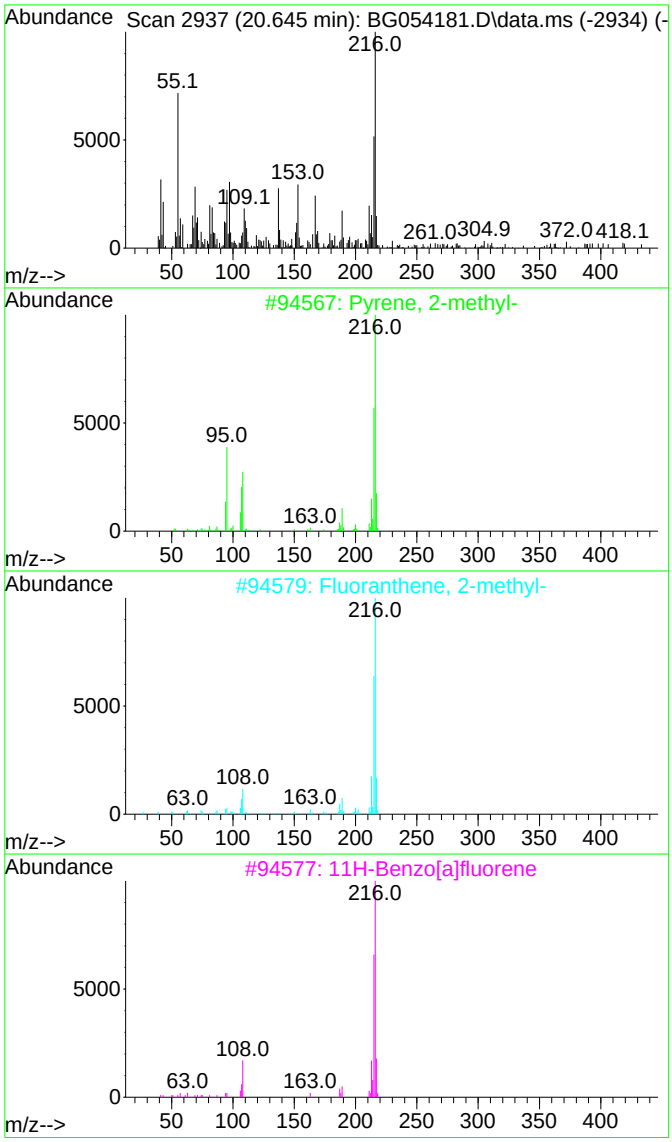
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

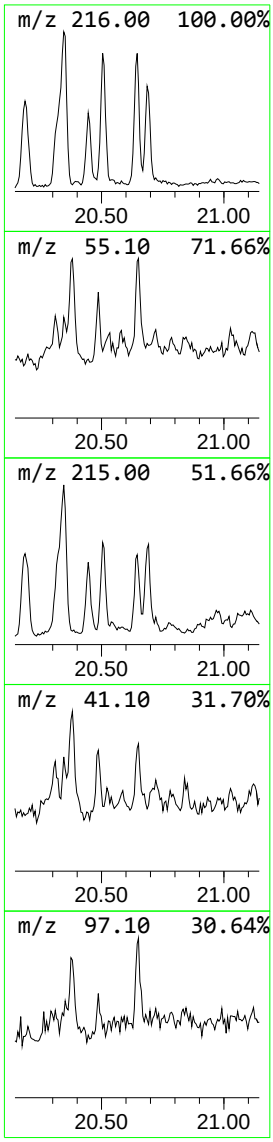
****

Peak Number 11 Pyrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.645	3.84 ng	123942	Chrysene-d12	21.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	55
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	50
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	45
4	Pyrene, 4-methyl-	216	C17H12	003353-12-6	38
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063022\
Data File : BG054181.D
Acq On : 30 Jun 2022 22:44
Operator : CG/JU
Sample : N3550-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-06292022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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
Tridecane	16.397	4.8	ng	85931	4	17.437	356334	20.0
Octadecane	17.185	4.9	ng	86966	4	17.437	356334	20.0
Hexadecanoic ac...	18.101	118.8	ng	2116650	4	17.437	356334	20.0
n-Hexadecanoic ...	18.325	7.2	ng	128813	4	17.437	356334	20.0
Benzaldehyde, 3...	18.512	5.9	ng	104640	4	17.437	356334	20.0
9,12-Octadecadi...	19.247	479.2	ng	8538380	4	17.437	356334	20.0
9-Octadecenoic ...	19.276	257.4	ng	4585780	4	17.437	356334	20.0
Methyl stearate	19.400	55.6	ng	991255	4	17.437	356334	20.0
unknown20.381	20.381	4.7	ng	151889	5	21.721	644935	20.0
Hexadecanoic ac...	20.487	5.2	ng	168830	5	21.721	644935	20.0
Pyrene, 2-methyl-	20.645	3.8	ng	123942	5	21.721	644935	20.0