LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1B-A-J

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-BG121323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	5	9	22	rVB	425851	759529	9.35%	2.461%
2	5.525	407	415	425	rBV	564567	889358	10.95%	2.882%
3	7.112	678	685	693	rVB	329700	563712	6.94%	1.827%
4	7.958	821	829	834	rBV2	373191	634577	7.81%	2.056%
5	9.115	1018	1026	1033	rBV	902279	1585370	19.51%	5.137%
6	10.760	1294	1306	1314	rBV	494453	967113	11.90%	3.134%
7	13.216	1715	1724	1733	rBV	2829194	4420796	54.41%	14.325%
8	14.591	1947	1958	1968	rBV2	789389	1503931	18.51%	4.873%
9	16.078	2205	2211	2217	rBV	2392748	3621109	44.56%	11.733%
10	16.877	2342	2347	2351	rBV	338311	427565	5.26%	1.385%
11	17.341	2419	2426	2432	rBV	1075806	1592665	19.60%	5.161%
12	18.128	2555	2560	2567	rBV2	192675	308778	3.80%	1.001%
13	18.234	2573	2578	2584	rBV	505511	661211	8.14%	2.143%
14	18.346	2591	2597	2601	rBV3	181860	285428	3.51%	0.925%
15	18.992	2704	2707	2711	rBV	169595	235337	2.90%	0.763%
16	19.162	2733	2736	2740	rBV2	344763	508723	6.26%	1.648%
17	19.386	2770	2774	2779	rBV3	460634	893967	11.00%	2.897%
18	19.509	2791	2795	2798	rBV2	823764	1145097	14.09%	3.710%
19	19.961	2866	2872	2878	rBV	5755611	8125587	100.00%	26.329%
20	20.461	2954	2957	2967	rBV3	833840	1731703	21.31%	5.611%

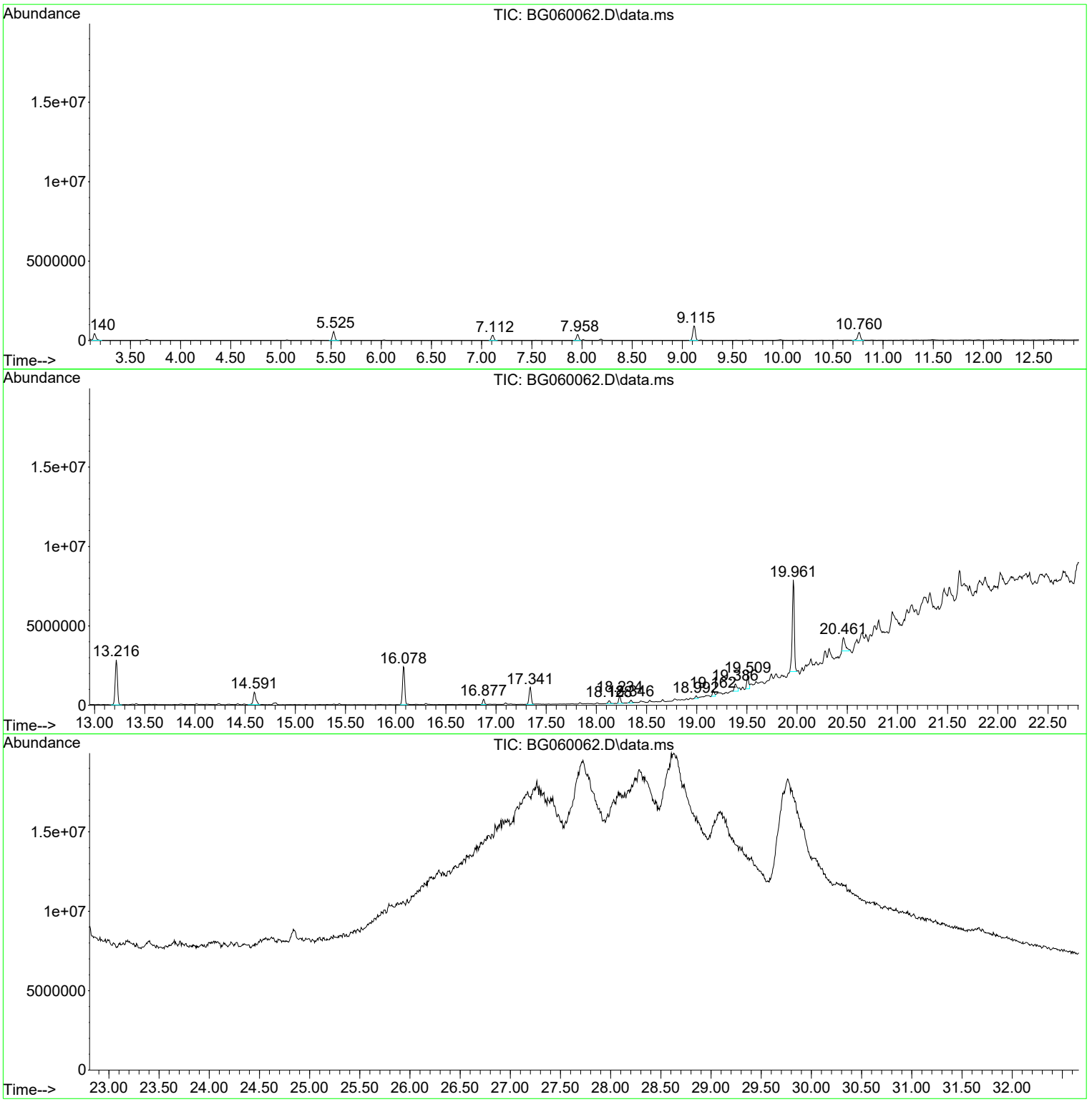
Sum of corrected areas: 30861556

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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Data File : BG060062.D
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Operator : MA/JU
Sample : 05791-10
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

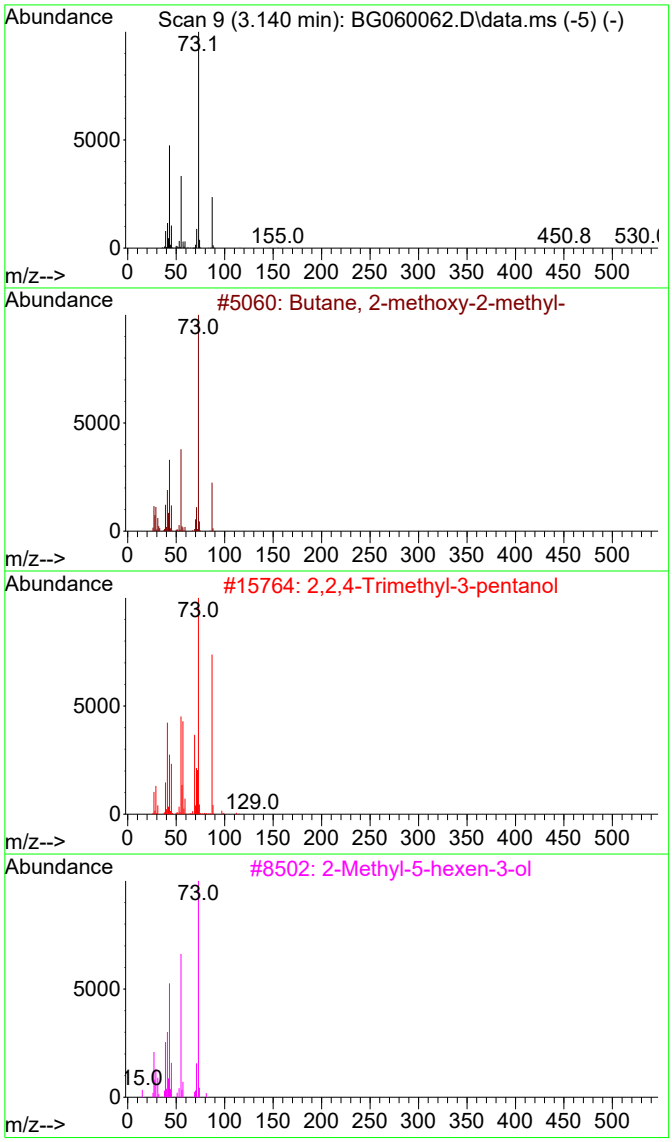
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

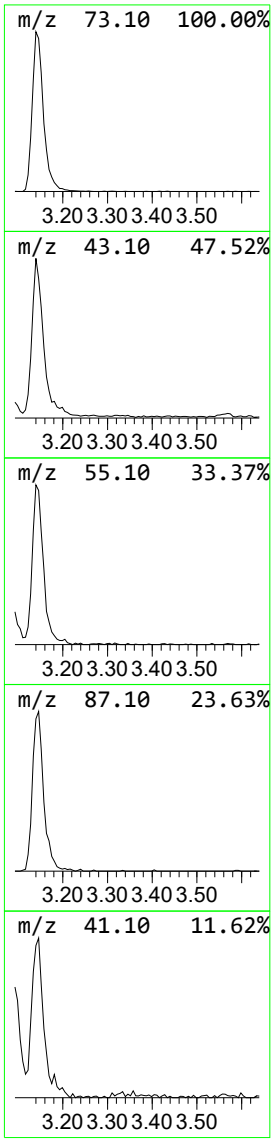
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	23.94 ng	759529	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG060062.D
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Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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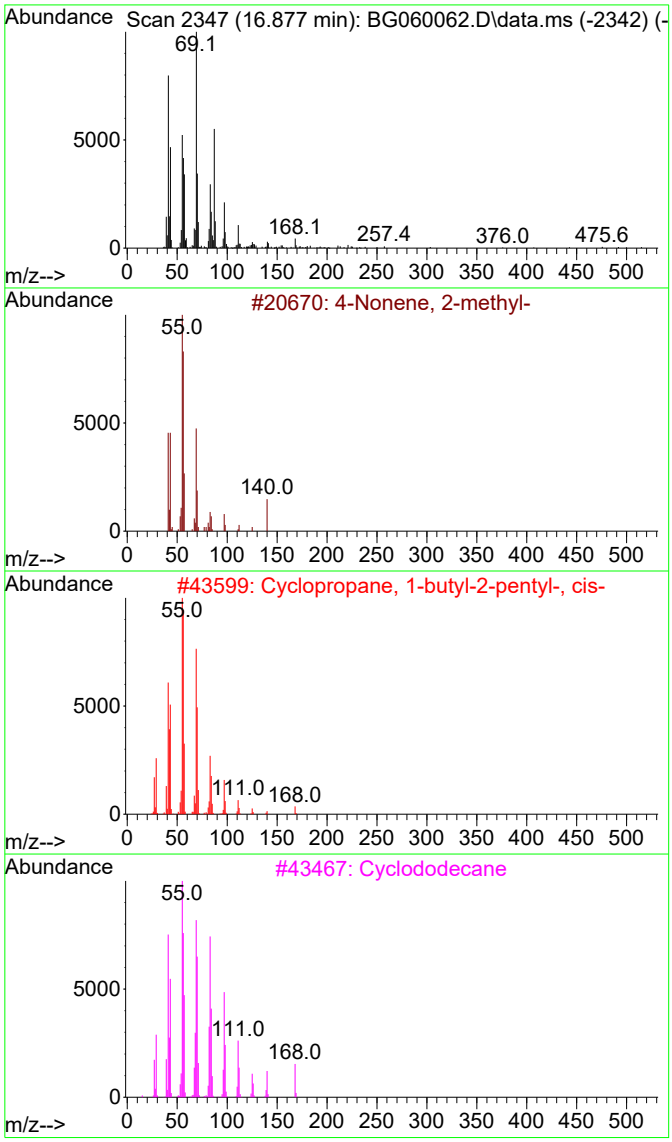
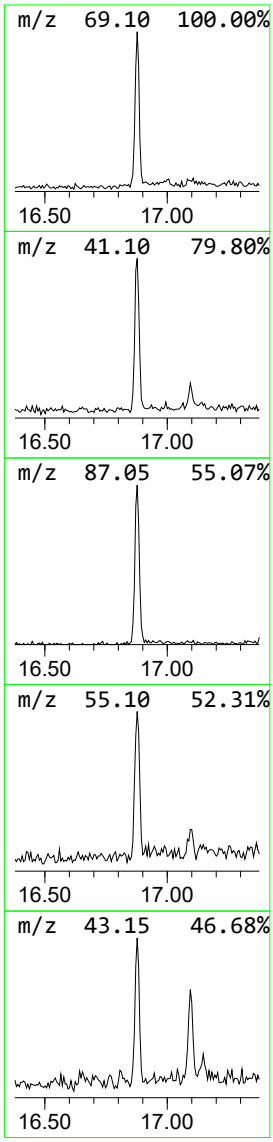
****

Peak Number 2 4-Nonene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.877	5.37 ng	427565	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonene, 2-methyl-	140	C10H20	055724-84-0	68
2	Cyclopropane, 1-butyl-2-pentyl-,...	168	C12H24	074663-88-0	64
3	Cyclododecane	168	C12H24	000294-62-2	50
4	2-Dodecene, (E)-	168	C12H24	007206-13-5	50
5	3-Undecene, 8-methyl-	168	C12H24	1000061-84-4	49





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Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

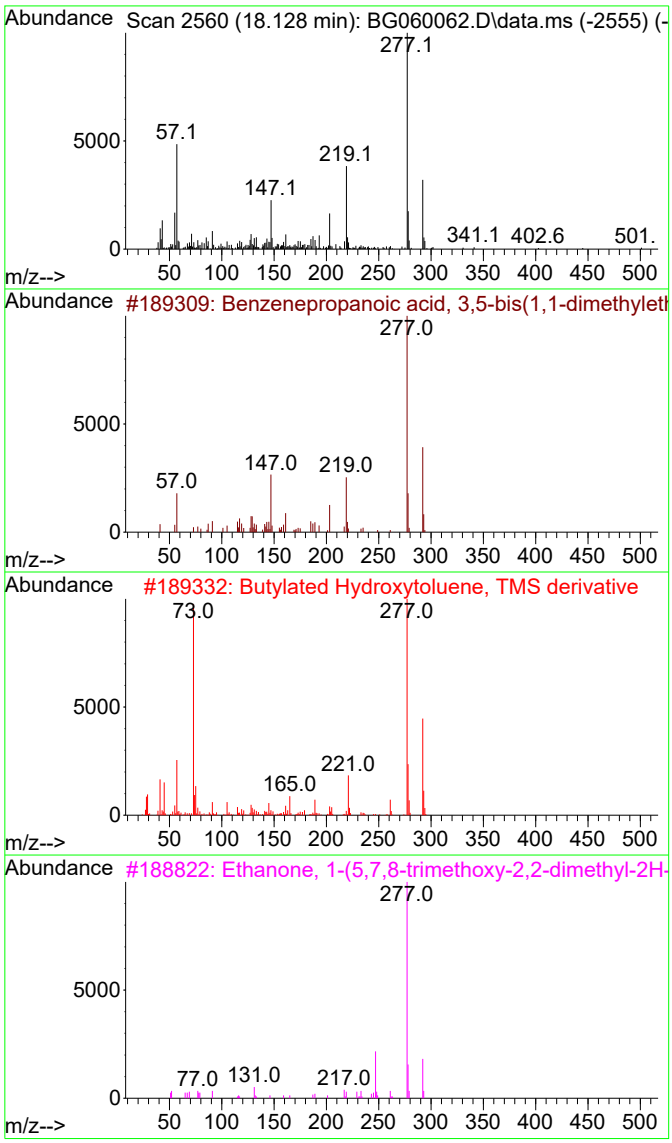
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

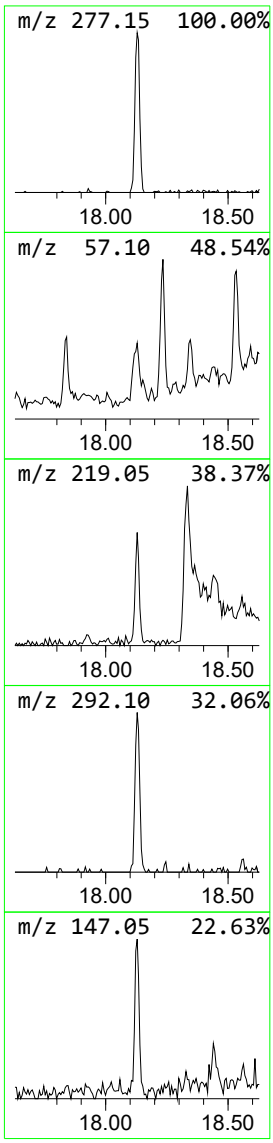
****

Peak Number 3 Benzenepropanoic acid, 3,5-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.128	3.88 ng	308778	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 3,5-bis(1...	292	C18H28O3	006386-38-5	95
2	Butylated Hydroxytoluene, TMS de...	292	C18H32OSi	018510-49-1	47
3	Ethanone, 1-(5,7,8-trimethoxy-2,...	292	C16H20O5	000482-07-5	47
4	2-Phosphabicyclo[3.1.0]hex-3-ene...	292	C20H21P	1000161-75-2	47
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	45





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Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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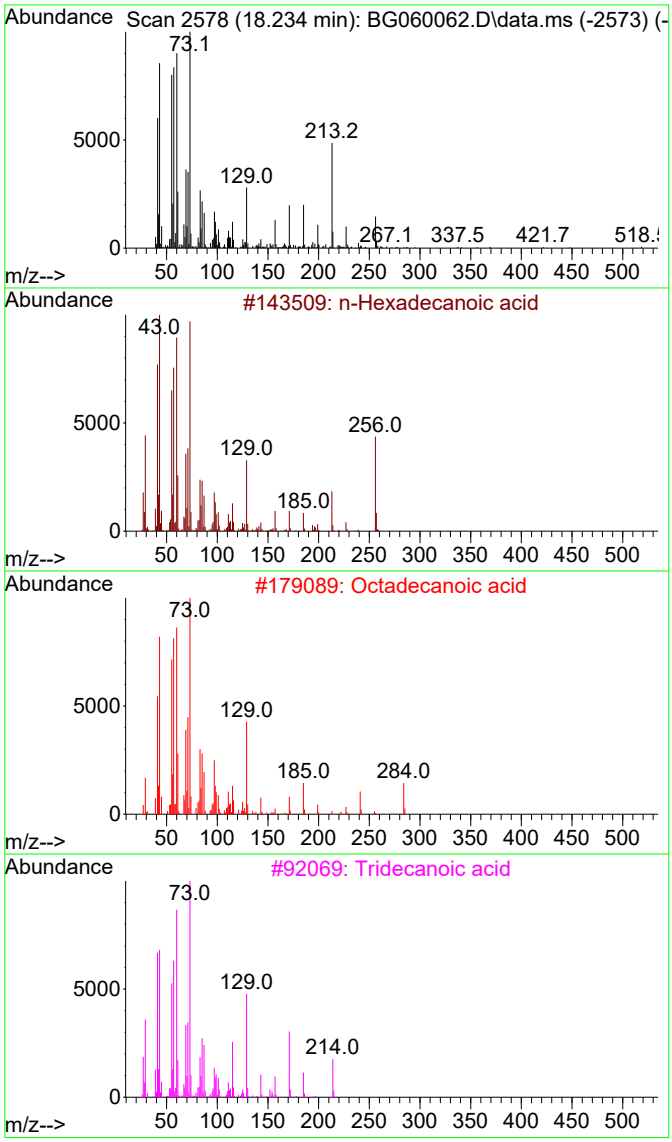
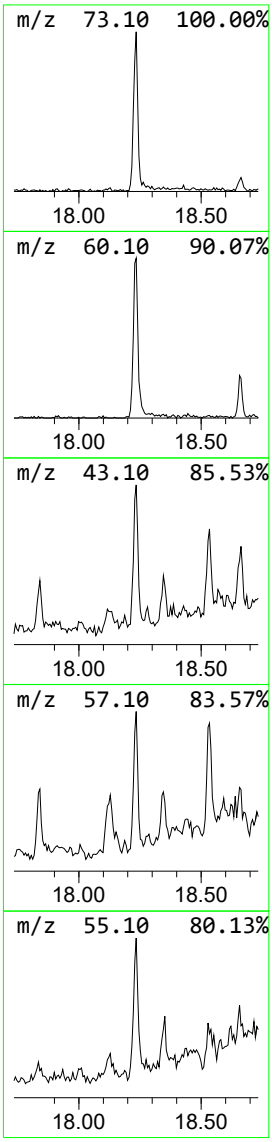
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.234	8.30 ng	661211	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Octadecanoic acid	284	C18H36O2	000057-11-4	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
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Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

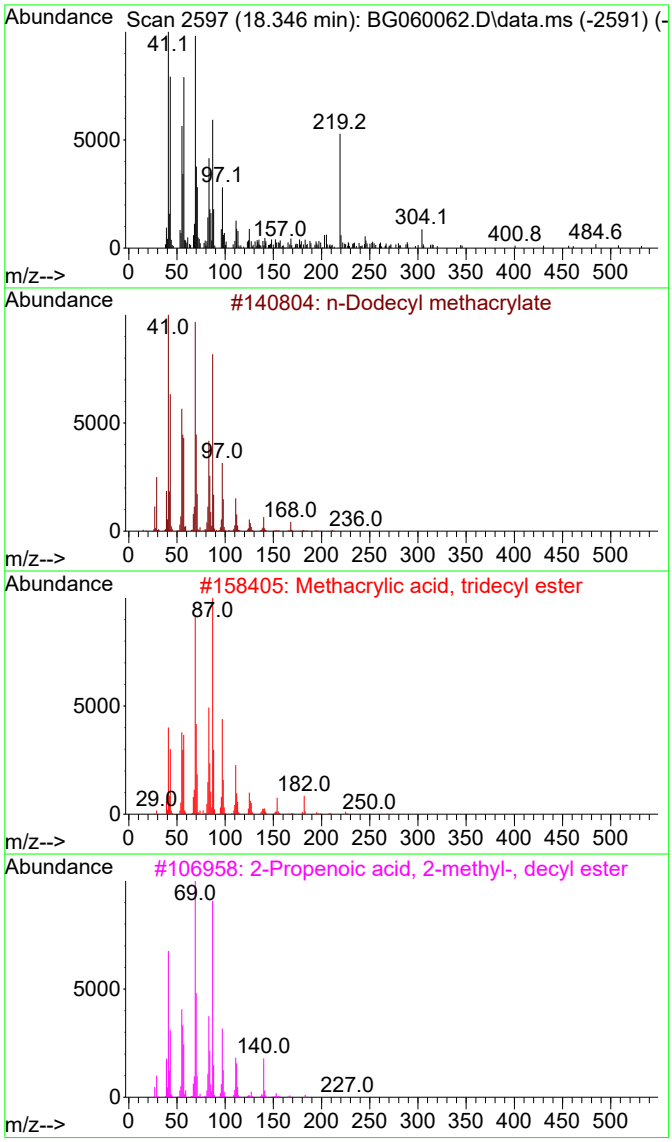
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

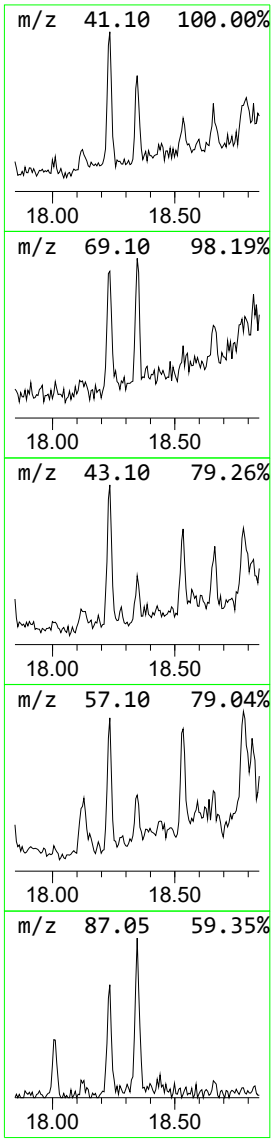
****

Peak Number 5 n-Dodecyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.346	3.58 ng	285428	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	64
2	Methacrylic acid, tridecyl ester	268	C17H32O2	1000340-28-9	53
3	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	50
4	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	41
5	5-Hexadecanol	242	C16H34O	021078-87-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
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Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

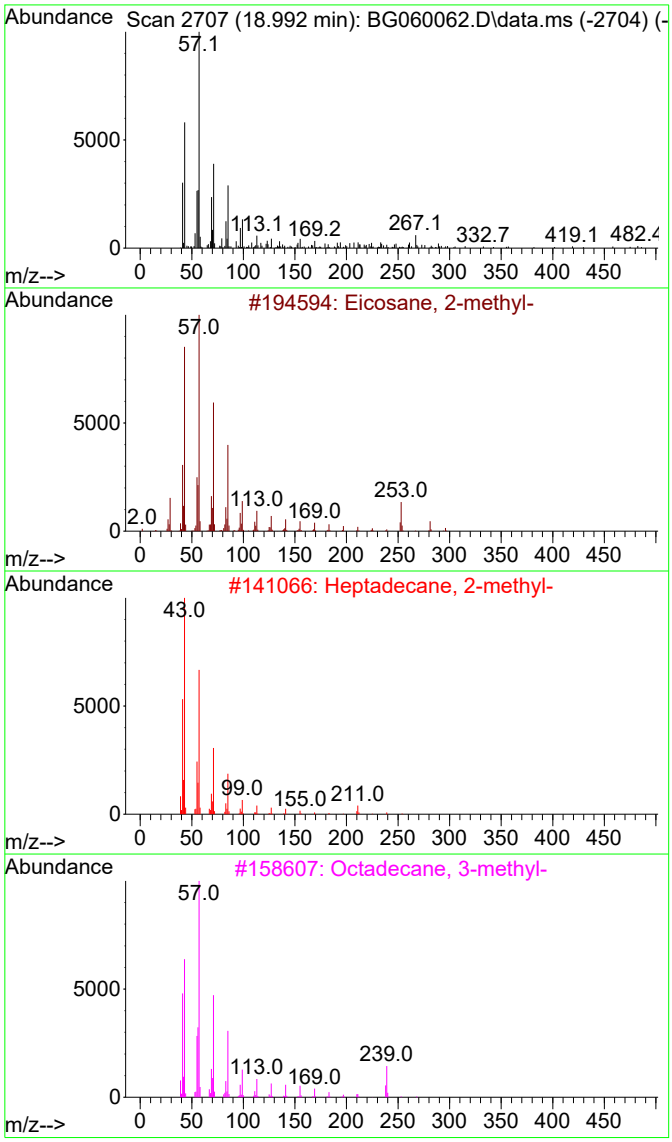
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

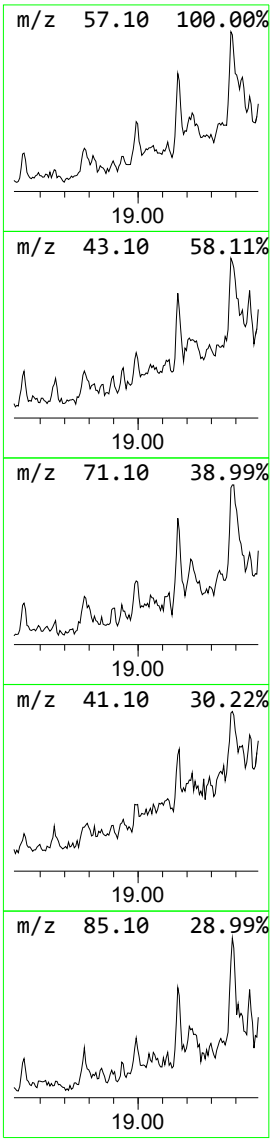
****

Peak Number 6 Eicosane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.992	2.96 ng	235337	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2-methyl-	296	C21H44	001560-84-5	89
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	80
3	Octadecane, 3-methyl-	268	C19H40	006561-44-0	78
4	Tetradecane, 6,9-dimethyl-	226	C16H34	055045-13-1	72
5	Hexatriacontane	507	C36H74	000630-06-8	72





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Data File : BG060062.D
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Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

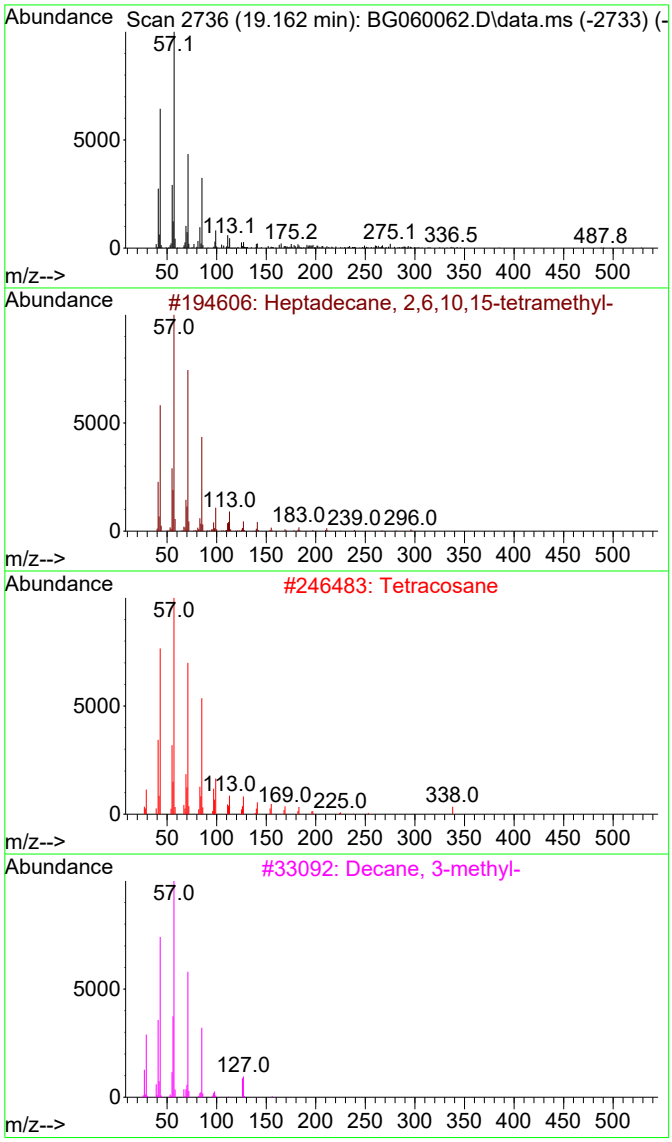
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

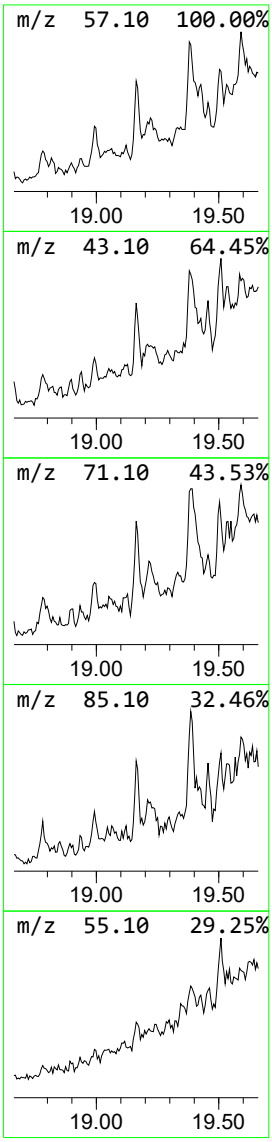
****

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.162	6.39 ng	508723	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76
2	Tetracosane	338	C24H50	000646-31-1	76
3	Decane, 3-methyl-	156	C11H24	013151-34-3	72
4	Nonadecane	268	C19H40	000629-92-5	64
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64





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Operator : MA/JU
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ALS Vial : 33 Sample Multiplier: 1

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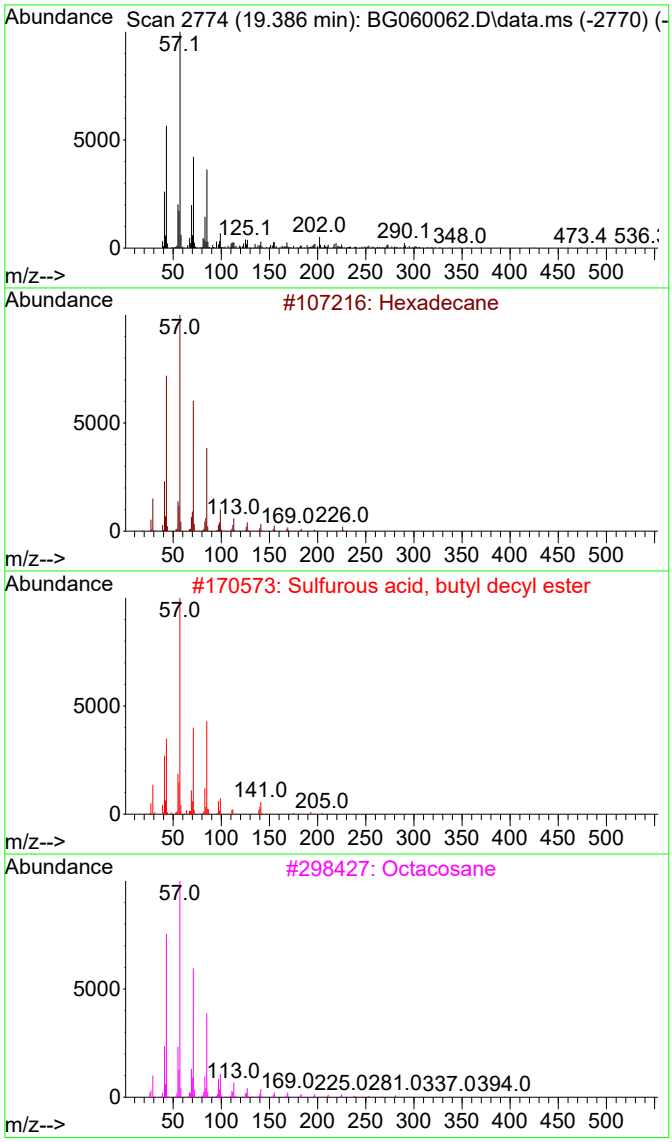
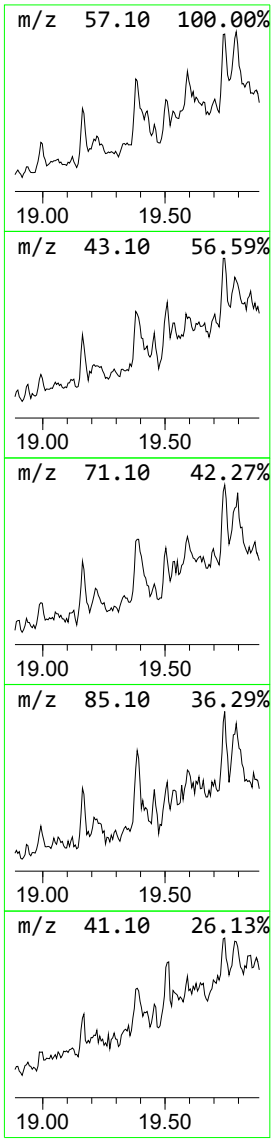
Peak Number 8 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	11.23 ng	893967	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	72
2	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
3	Octacosane	394	C28H58	000630-02-4	62
4	Decane, 1-iodo-	268	C10H21I	002050-77-3	62
5	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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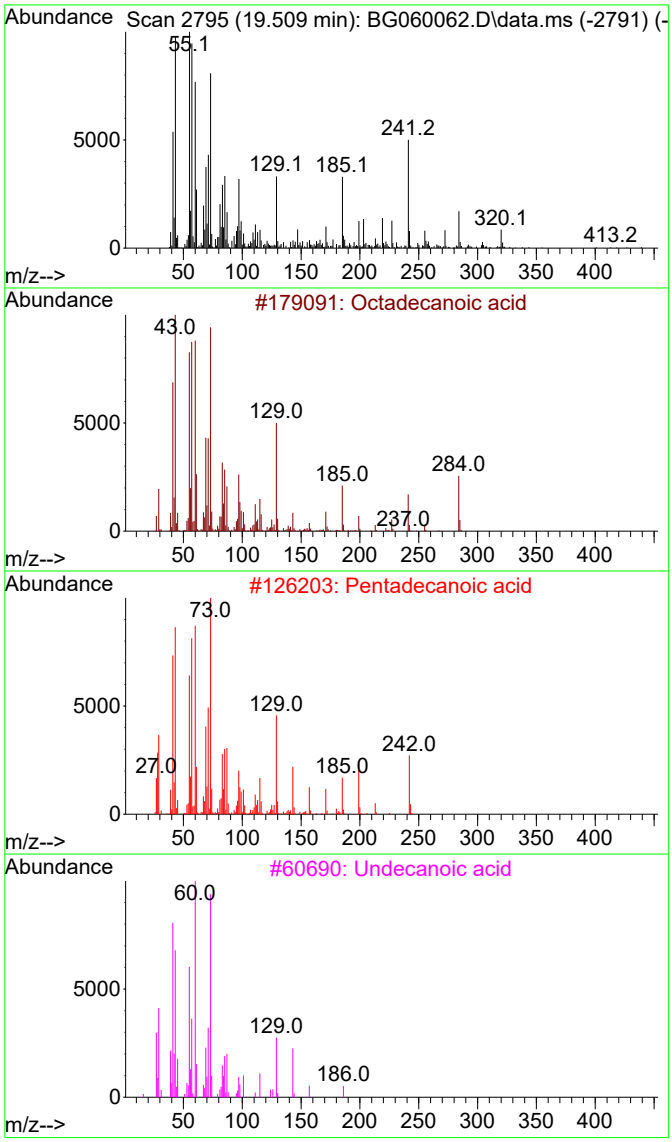
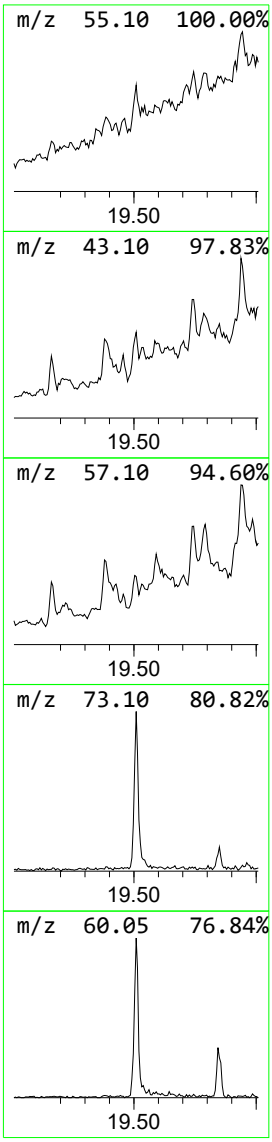
Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	13.23 ng	1145100	Chrysene-d12	21.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	45
4	n-Decanoic acid	172	C10H20O2	000334-48-5	45
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43





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Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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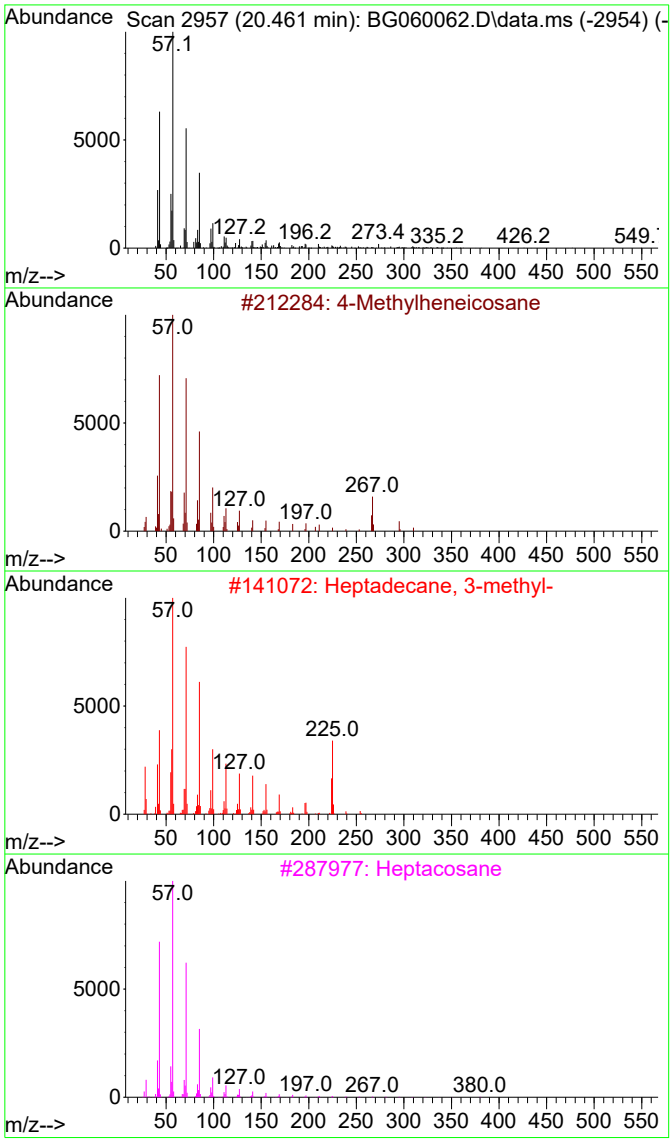
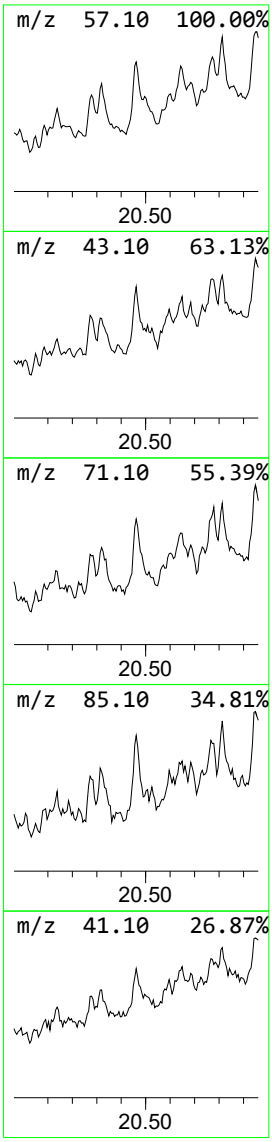
Peak Number 10 4-Methylheneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.461	20.00 ng	1731700	Chrysene-d12	21.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylheneicosane	310	C22H46	025117-29-7	91
2	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	81
5	Hexadecane	226	C16H34	000544-76-3	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060062.D
Acq On : 16 Dec 2023 9:24
Operator : MA/JU
Sample : 05791-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-A-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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
Butane, 2-metho...	3.140	23.9	ng	759529	1	7.958	634577	20.0
4-Nonene, 2-met...	16.877	5.4	ng	427565	4	17.341	1592670	20.0
Benzenepropanoi...	18.128	3.9	ng	308778	4	17.341	1592670	20.0
n-Hexadecanoic ...	18.234	8.3	ng	661211	4	17.341	1592670	20.0
n-Dodecyl metha...	18.346	3.6	ng	285428	4	17.341	1592670	20.0
Eicosane, 2-met...	18.992	3.0	ng	235337	4	17.341	1592670	20.0
Heptadecane, 2,...	19.162	6.4	ng	508723	4	17.341	1592670	20.0
Hexadecane	19.386	11.2	ng	893967	4	17.341	1592670	20.0
Octadecanoic acid	19.509	13.2	ng	1145100	5	21.618	1731700	20.0
4-Methylheneico...	20.461	20.0	ng	1731700	5	21.618	1731700	20.0