LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

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-BG101322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	3	7	31	rVB	622766	1077913	43.72%	9.733%
2	5.349	342	351	359	rBV	49437	79366	3.22%	0.717%
3	5.825	425	432	443	rVB	207800	329095	13.35%	2.972%
4	7.435	698	706	714	rBV	120752	210187	8.52%	1.898%
5	8.305	847	854	862	rBV	104464	178992	7.26%	1.616%
6	9.474	1043	1053	1061	rBV	364876	645833	26.19%	5.832%
7	11.131	1328	1335	1342	rVB	141731	252729	10.25%	2.282%
8	13.540	1738	1745	1752	rVB	1038468	1597503	64.79%	14.425%
9	14.345	1878	1882	1887	rVB	28704	38180	1.55%	0.345%
10	14.909	1972	1978	1987	rVB	243021	390817	15.85%	3.529%
11	15.567	2075	2090	2092	rBV5	74825	251512	10.20%	2.271%
12	16.389	2223	2230	2238	rVB	804671	1227440	49.78%	11.084%
13	17.647	2438	2444	2452	rVB	317960	473055	19.19%	4.272%
14	18.499	2585	2589	2594	rBV2	34775	47747	1.94%	0.431%
15	19.750	2799	2802	2813	rVB2	71165	142472	5.78%	1.287%
16	20.220	2876	2882	2887	rBV	1849925	2465672	100.00%	22.265%
17	20.285	2888	2893	2899	rVV2	48876	89945	3.65%	0.812%
18	20.984	3007	3012	3021	rVB2	76478	150369	6.10%	1.358%
19	21.525	3101	3104	3112	rVB2	37101	61115	2.48%	0.552%
20	21.748	3138	3142	3154	rVB2	56671	127755	5.18%	1.154%
21	21.930	3167	3173	3179	rBV	294346	504420	20.46%	4.555%
22	22.635	3289	3293	3301	rVB2	49080	96337	3.91%	0.870%
23	25.355	3747	3756	3770	rVB2	194815	635819	25.79%	5.741%

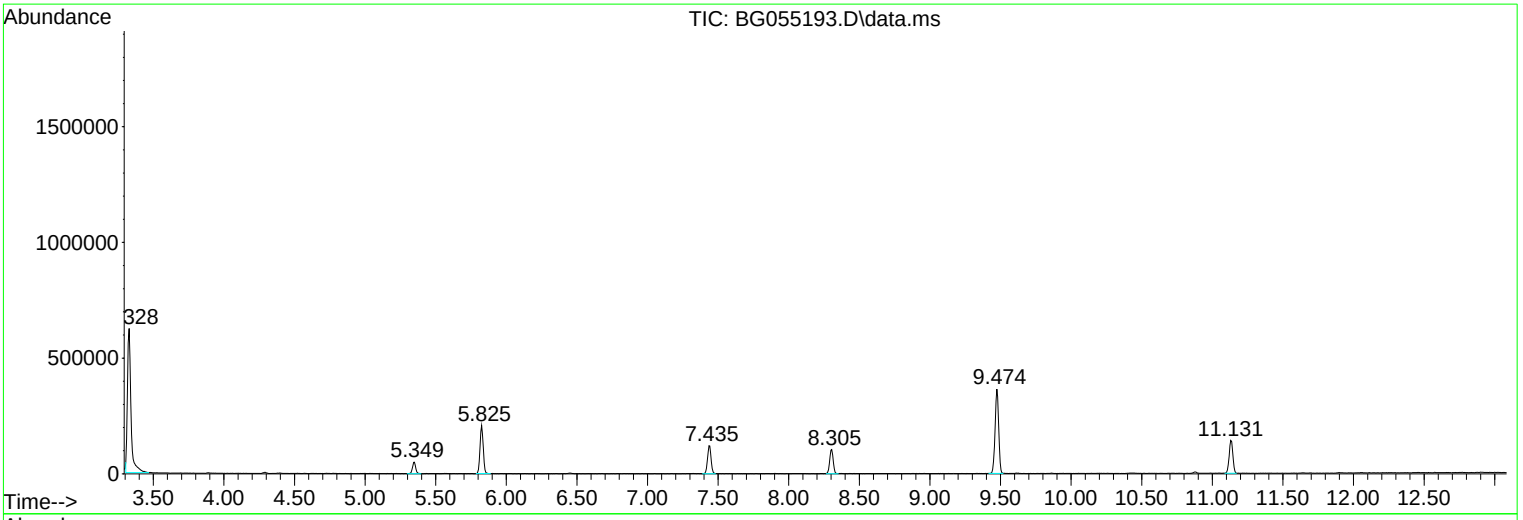
Sum of corrected areas: 11074273

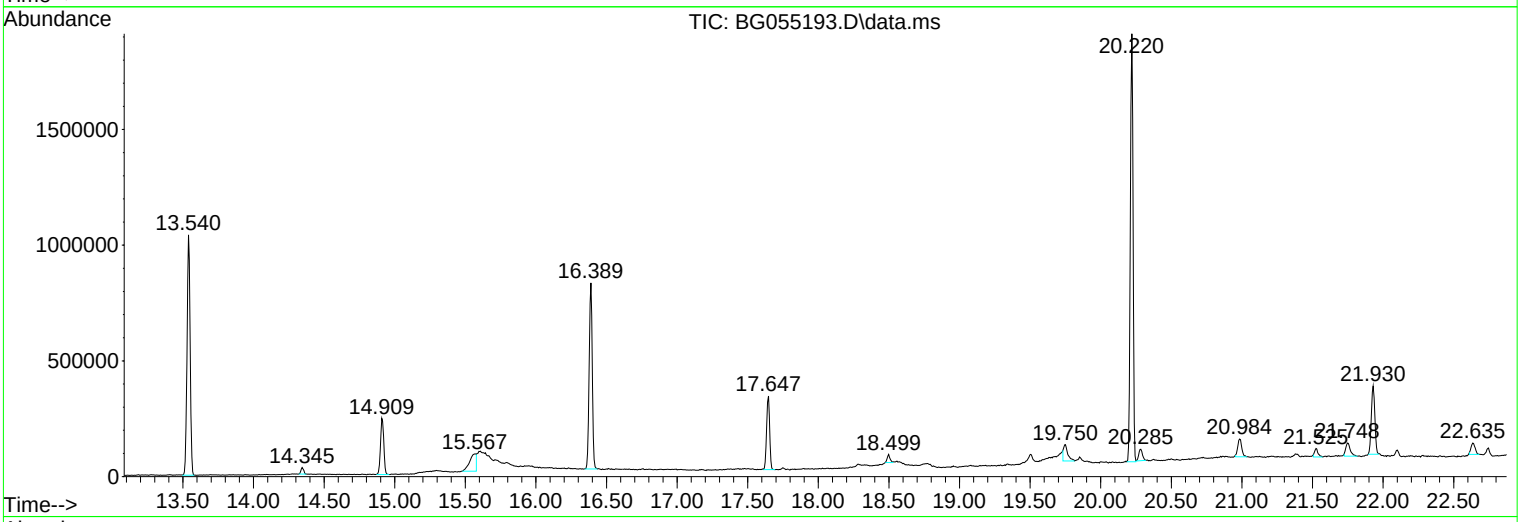
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

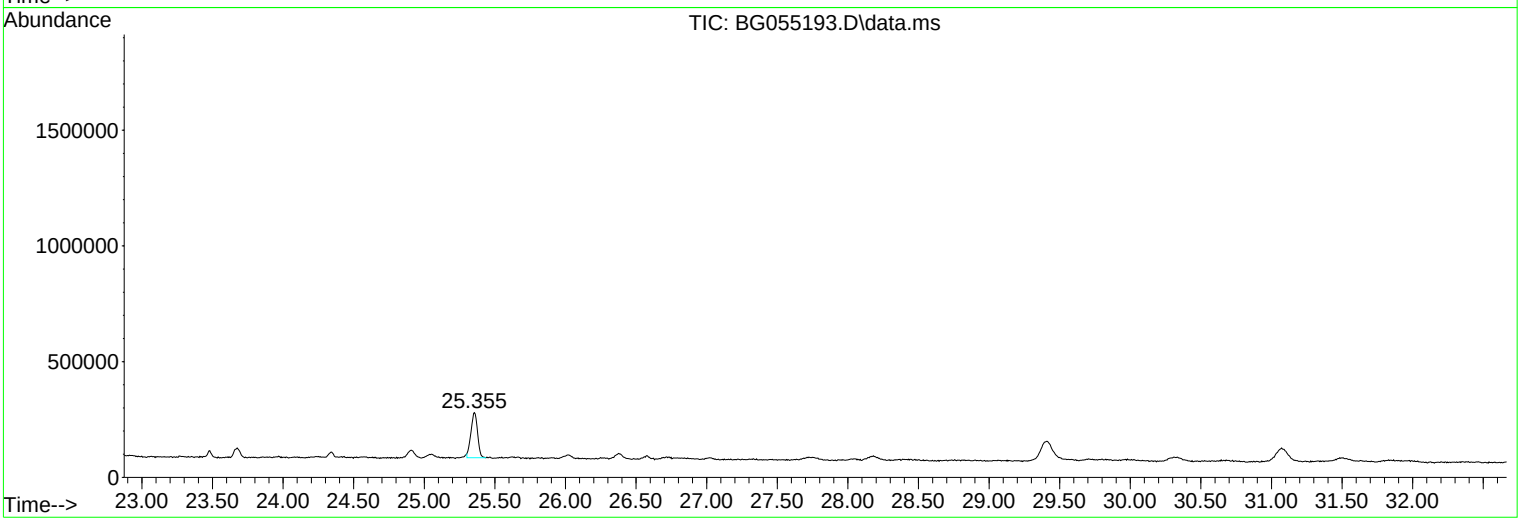
Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

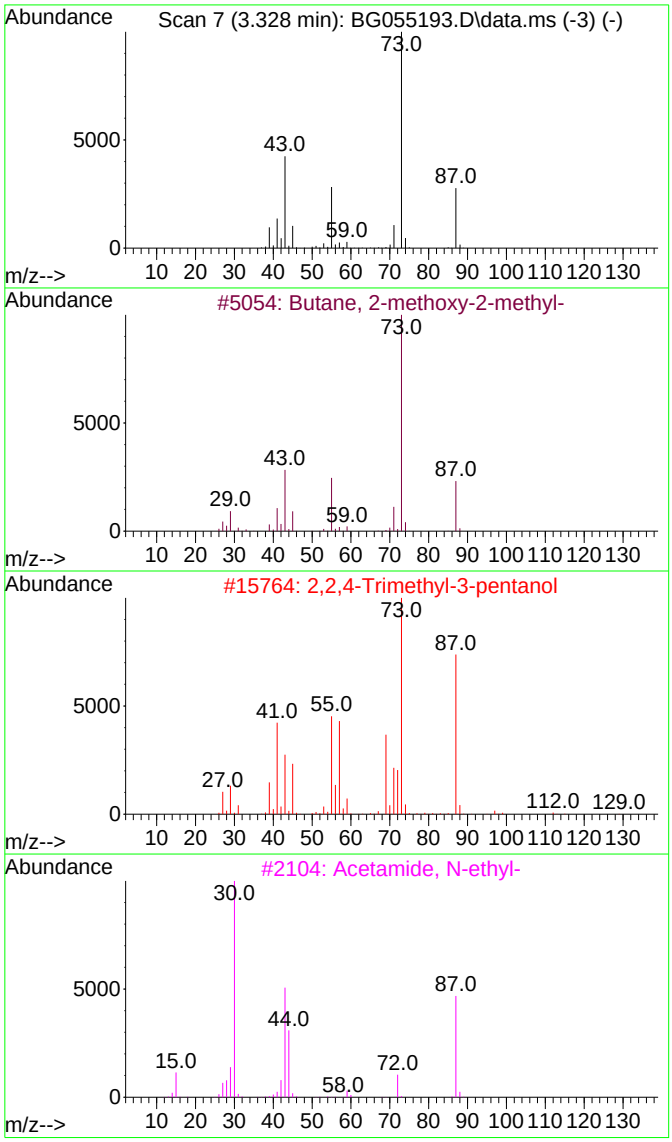
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

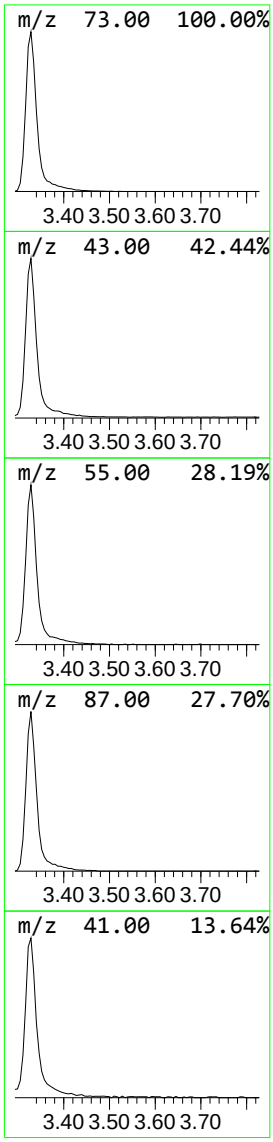
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.328	120.44 ng	1077910	1,4-Dichlorobenzene-d4	8.305

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	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

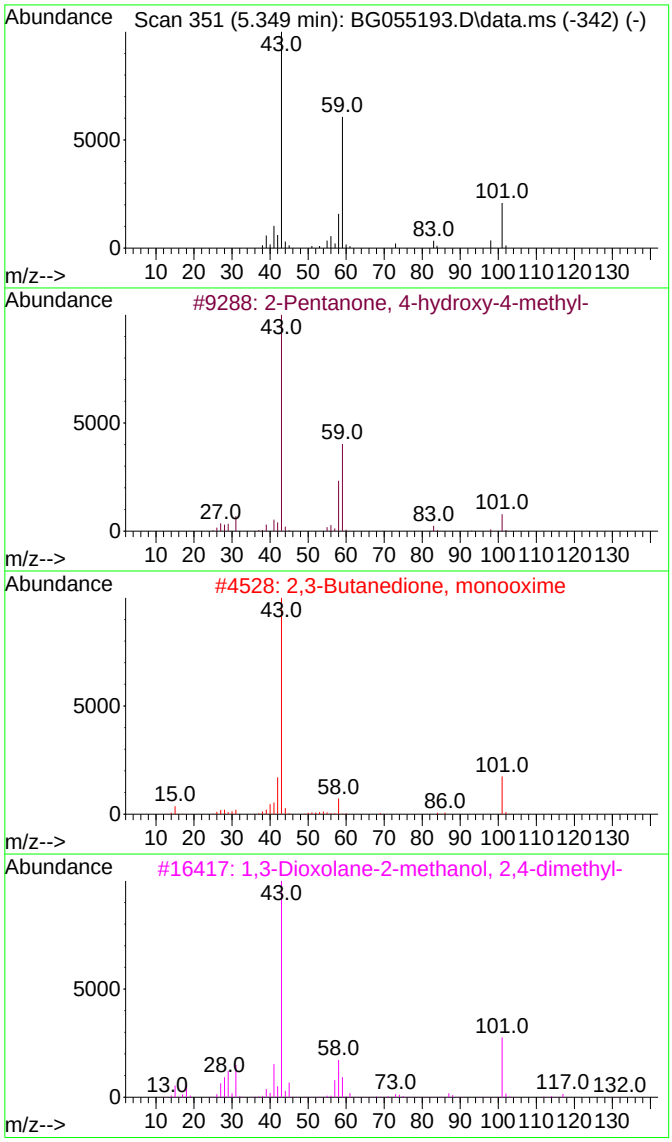
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

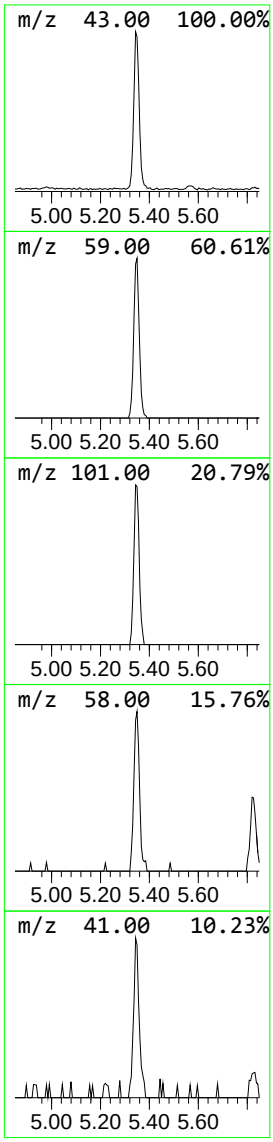
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.349	8.87 ng	79366	1,4-Dichlorobenzene-d4	8.305

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

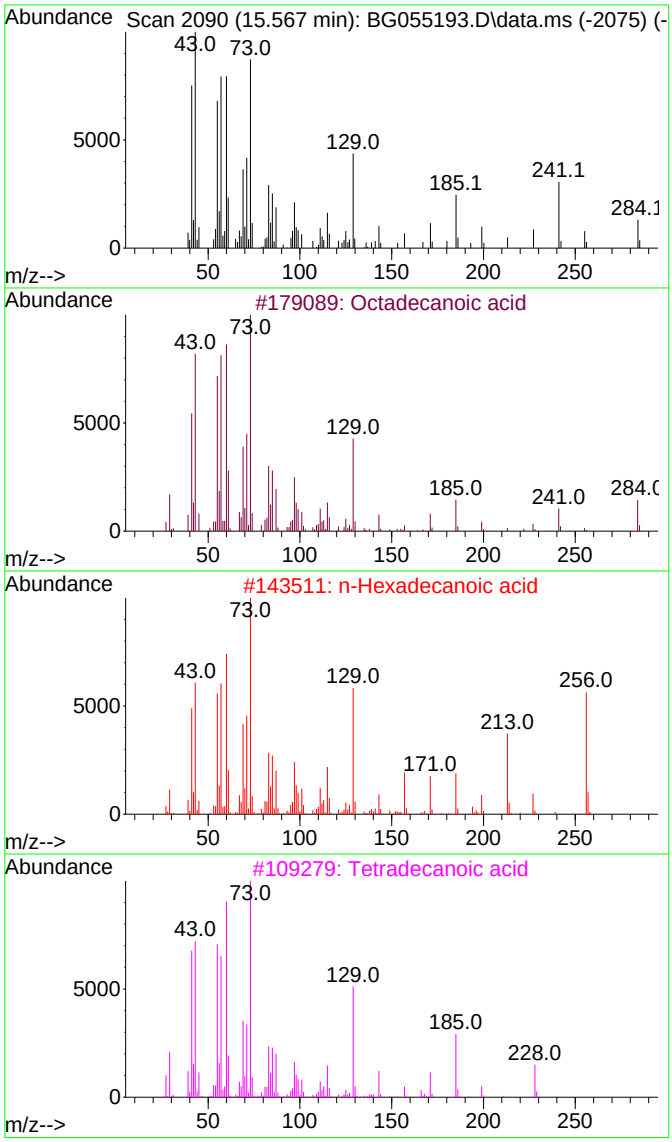
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

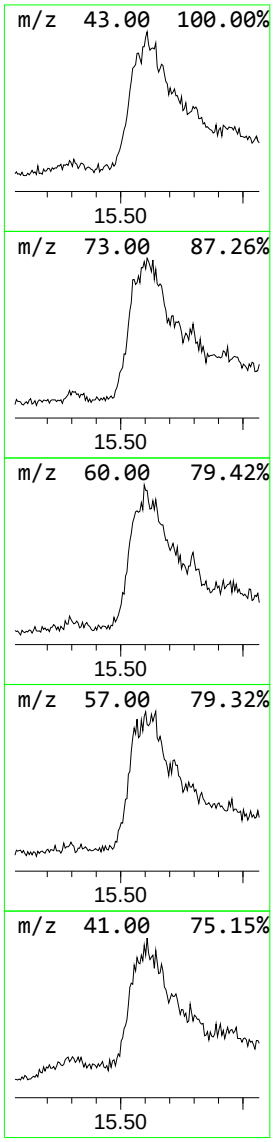
****

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.567	12.87 ng	251512	Acenaphthene-d10	14.909

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	78
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

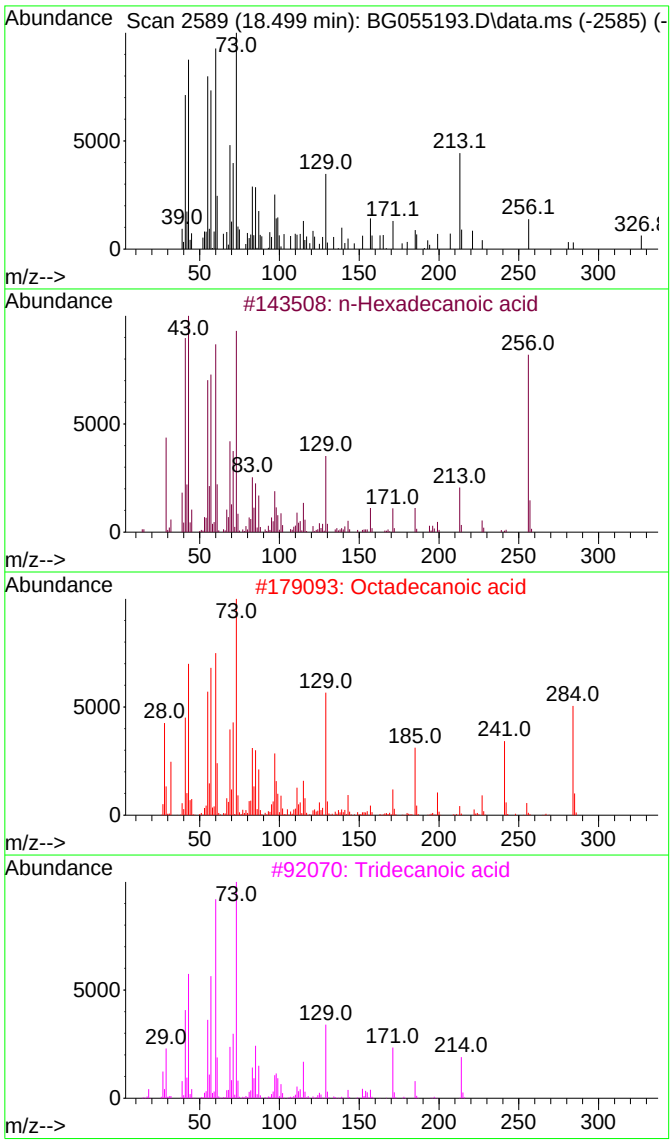
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

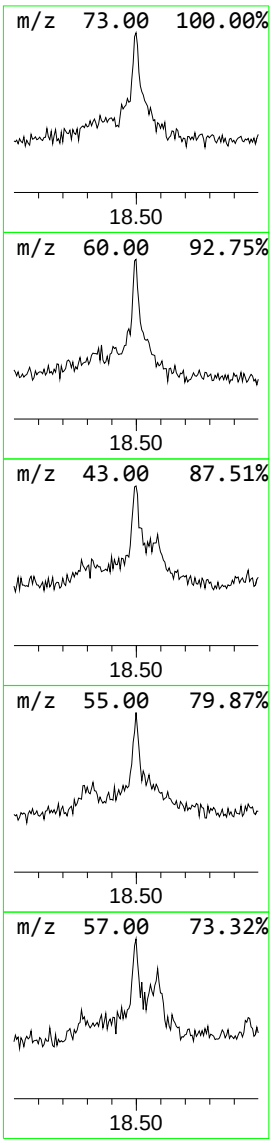
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	2.02 ng	47747	Phenanthrene-d10	17.647

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

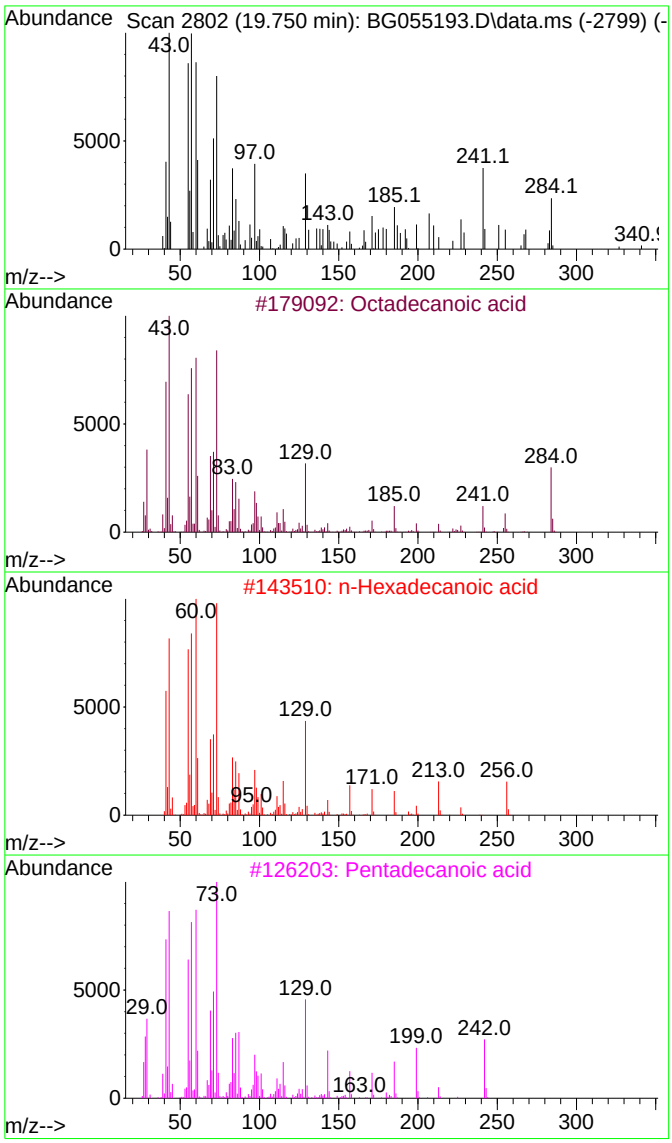
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

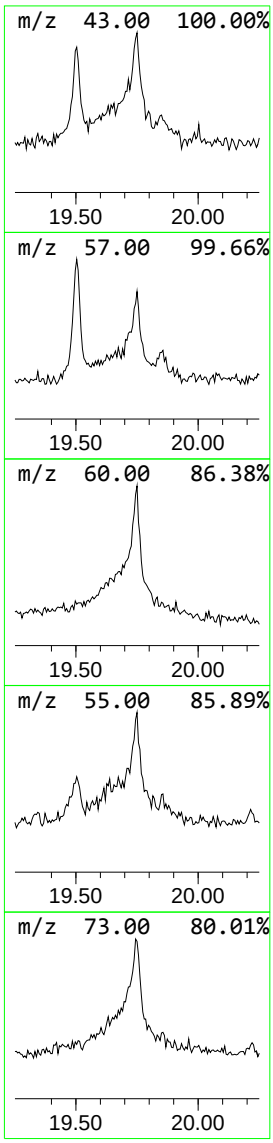
****

Peak Number 5 unknown19.750 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.750	6.02 ng	142472	Phenanthrene-d10	17.647

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	60
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

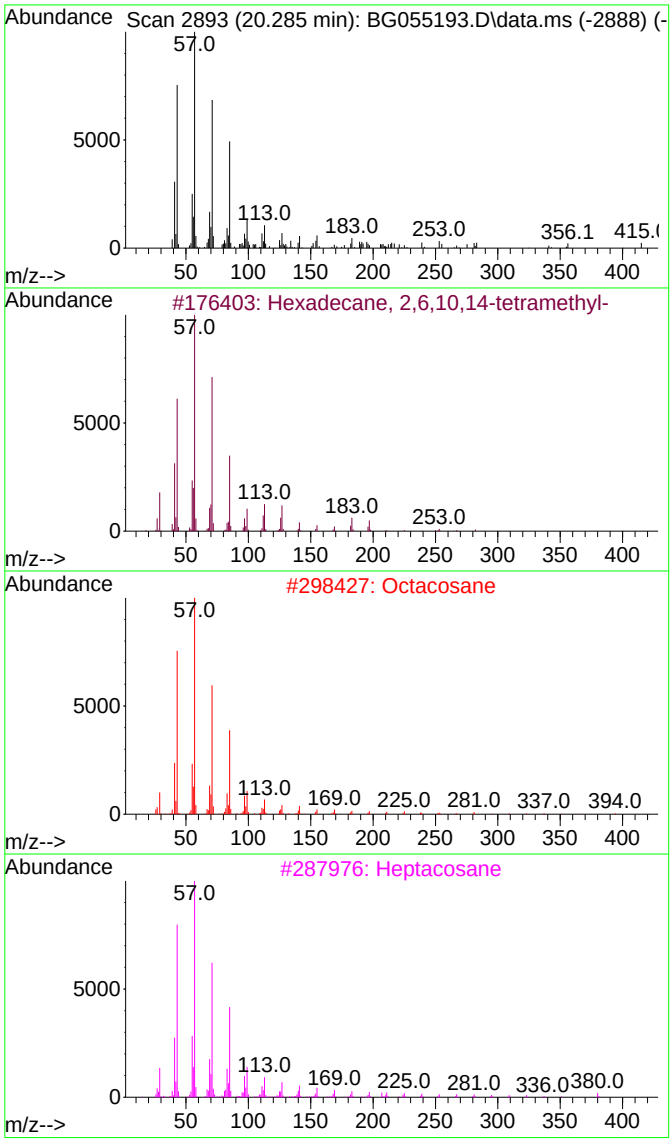
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

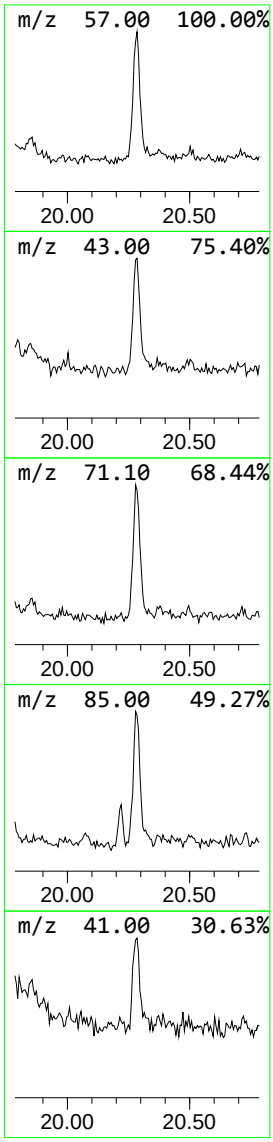
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.285	3.57 ng	89945	Chrysene-d12	21.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

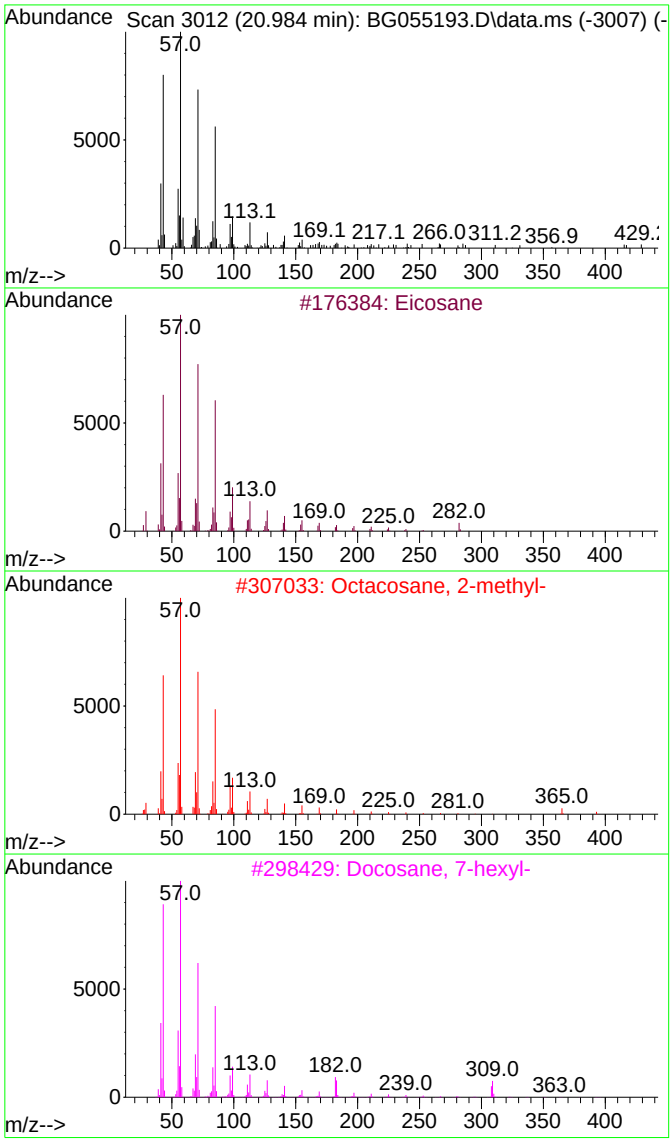
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

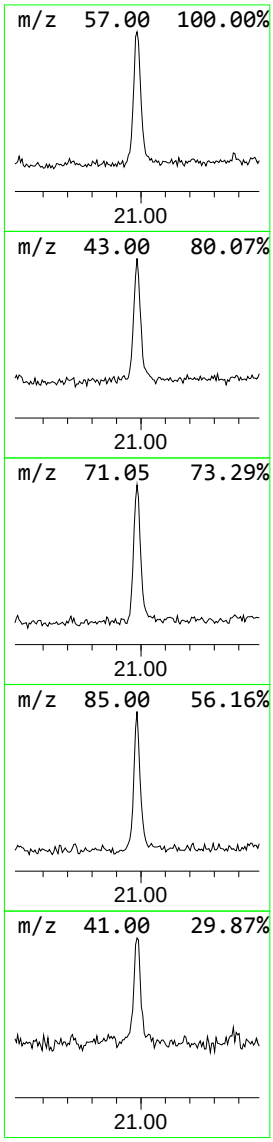
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.984	5.96 ng	150369	Chrysene-d12	21.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

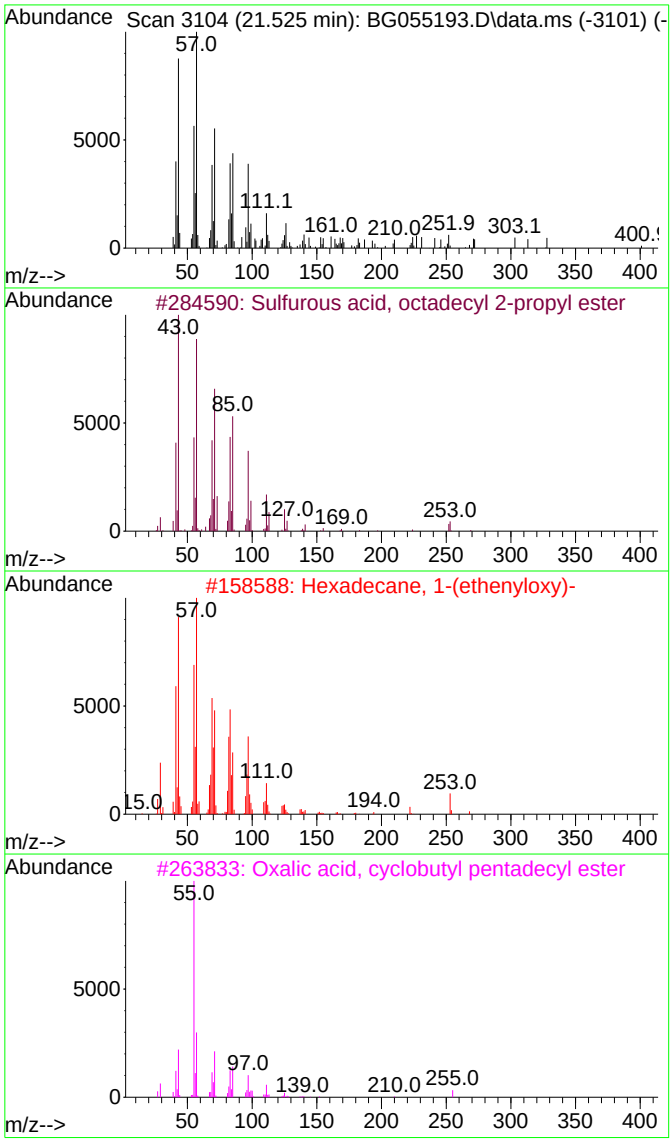
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

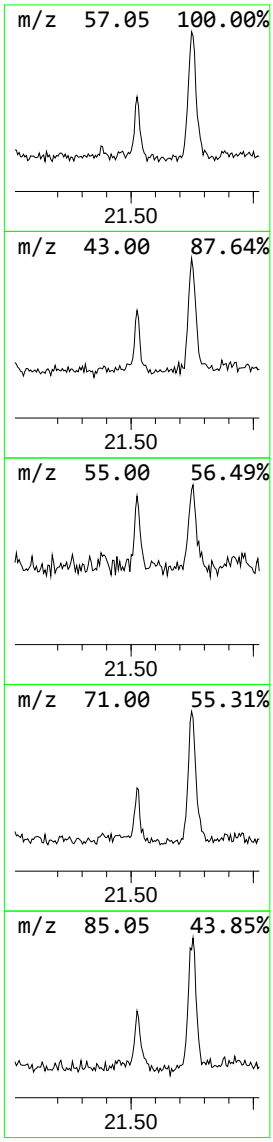
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Sulfurous acid, octadecyl 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	2.42 ng	61115	Chrysene-d12	21.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83
2	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	76
3	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	64
4	E-7-Octadecene	252	C18H36	1000130-92-0	50
5	1-Octadecene	252	C18H36	000112-88-9	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

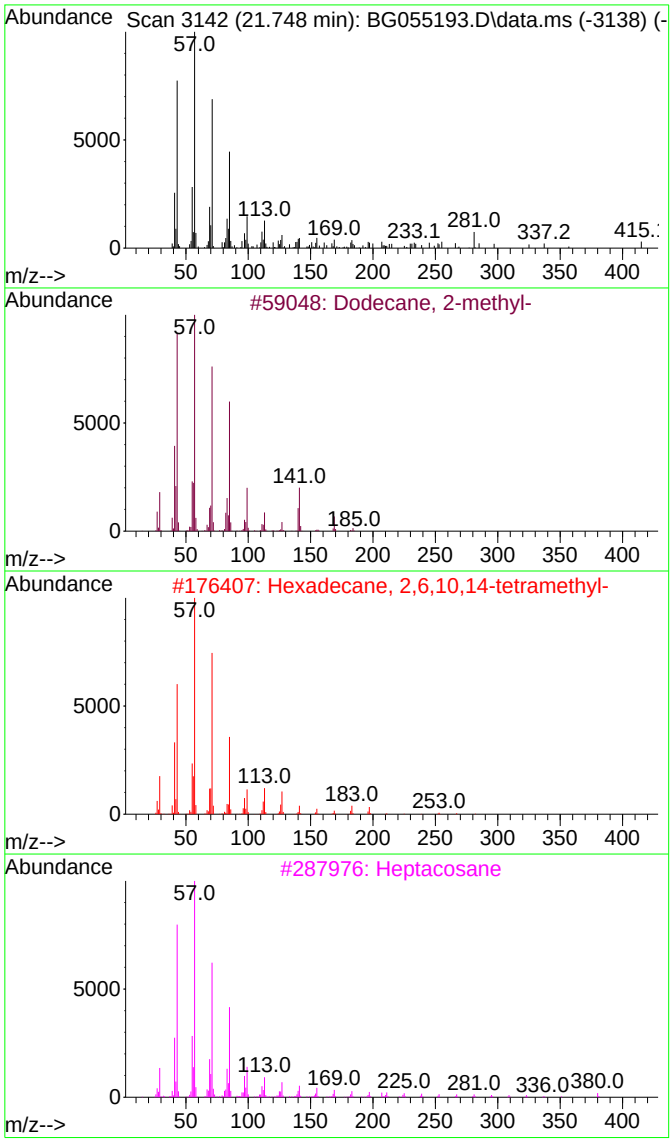
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

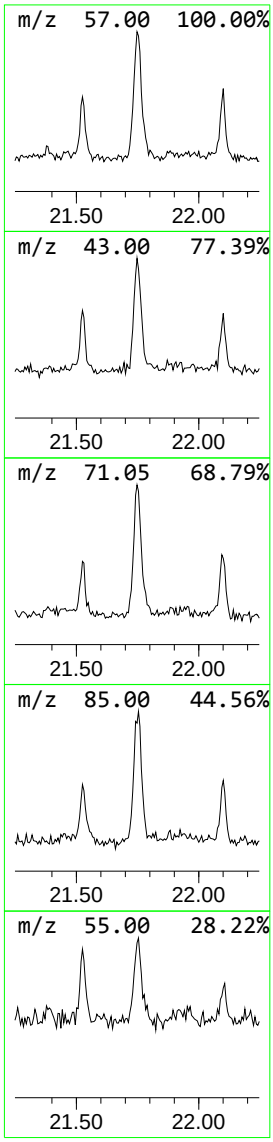
****

Peak Number 9 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.748	5.07 ng	127755	Chrysene-d12	21.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

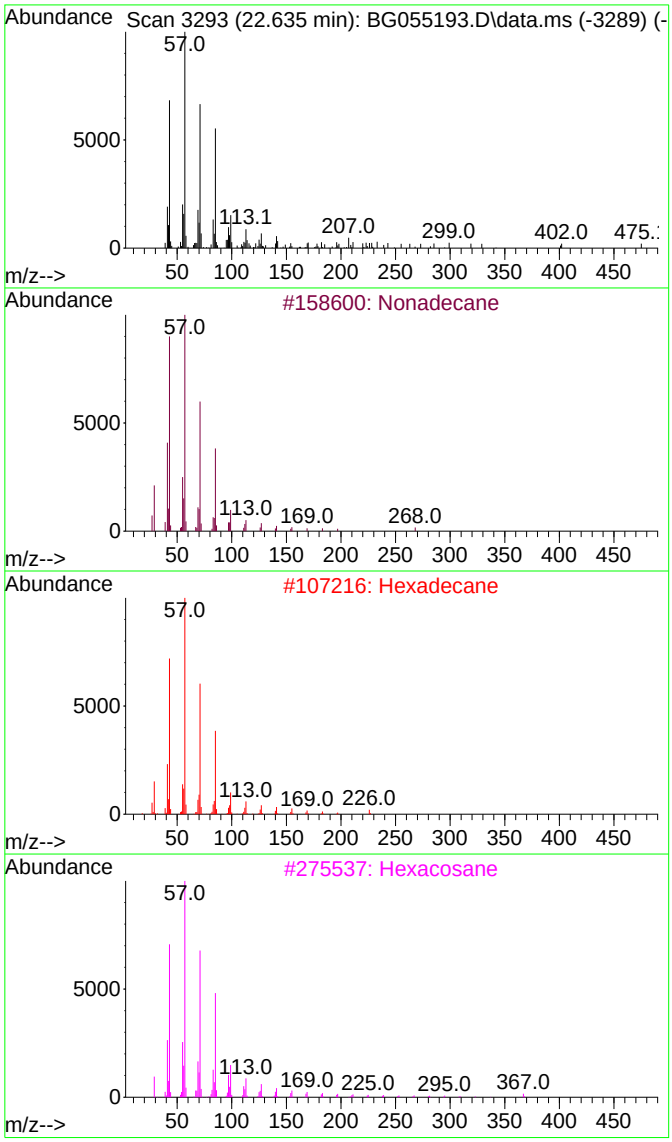
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

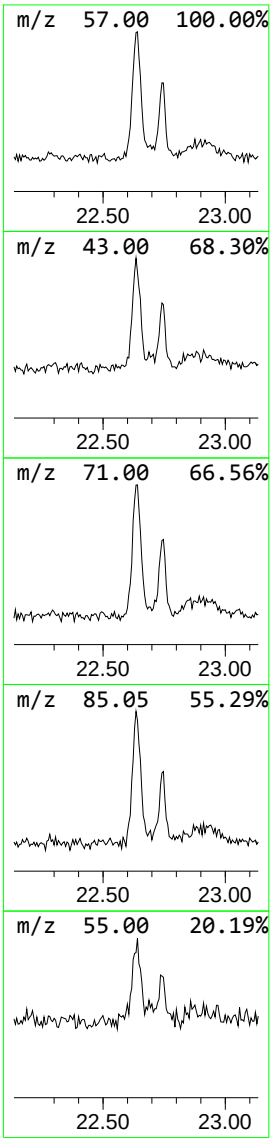
****

Peak Number 10 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.635	3.82 ng	96337	Chrysene-d12	21.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexadecane	226	C16H34	000544-76-3	93
3	Hexacosane	366	C26H54	000630-01-3	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055193.D
Acq On : 17 Oct 2022 15:16
Operator : CG/JU
Sample : N5147-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
557-E-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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...	3.328	120.4	ng	1077910	1	8.305	178992	20.0
2-Pentanone, 4-...	5.349	8.9	ng	79366	1	8.305	178992	20.0
Octadecanoic acid	15.567	12.9	ng	251512	3	14.909	390817	20.0
n-Hexadecanoic ...	18.499	2.0	ng	47747	4	17.647	473055	20.0
unknown19.750	19.750	6.0	ng	142472	4	17.647	473055	20.0
Hexadecane, 2,6...	20.285	3.6	ng	89945	5	21.930	504420	20.0
Eicosane	20.984	6.0	ng	150369	5	21.930	504420	20.0
Sulfurous acid,...	21.525	2.4	ng	61115	5	21.930	504420	20.0
Dodecane, 2-met...	21.748	5.1	ng	127755	5	21.930	504420	20.0
Nonadecane	22.635	3.8	ng	96337	5	21.930	504420	20.0