LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
Acq On : 8 Oct 2020 19:29
Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

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-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.815	244	251	261	rVB	132668	235709	4.27%	1.057%
2	5.667	389	396	407	rBV	874136	1408719	25.49%	6.317%
3	7.253	659	666	677	rBV	619637	1069333	19.35%	4.795%
4	8.105	804	811	817	rBV	237243	408762	7.40%	1.833%
5	8.164	817	821	828	rVB	43604	66120	1.20%	0.297%
6	9.268	1001	1009	1016	rVB	812524	1392560	25.20%	6.245%
7	10.919	1282	1290	1296	rBV	306337	531982	9.63%	2.386%
8	12.359	1526	1535	1540	rBV	44935	87604	1.59%	0.393%
9	12.412	1540	1544	1555	rVB	43356	79613	1.44%	0.357%
10	13.093	1655	1660	1668	rBV3	52098	84207	1.52%	0.378%
11	13.358	1696	1705	1714	rBV	1813884	2899427	52.47%	13.002%
12	14.174	1837	1844	1849	rBV	136976	200559	3.63%	0.899%
13	14.727	1932	1938	1946	rVB2	472318	745067	13.48%	3.341%
14	16.213	2184	2191	2198	rBV	1693155	2541570	45.99%	11.397%
15	17.470	2398	2405	2413	rBV	640049	965388	17.47%	4.329%
16	18.352	2549	2555	2565	rBV	391058	590118	10.68%	2.646%
17	19.621	2766	2771	2780	rBV	222212	345261	6.25%	1.548%
18	20.079	2842	2849	2857	rVB	4145895	5525801	100.00%	24.779%
19	21.383	3066	3071	3083	rBV2	331974	596204	10.79%	2.674%
20	21.748	3126	3133	3140	rVB2	760463	1232969	22.31%	5.529%
21	25.015	3679	3689	3702	rBV2	444811	1292947	23.40%	5.798%

Sum of corrected areas: 22299920

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
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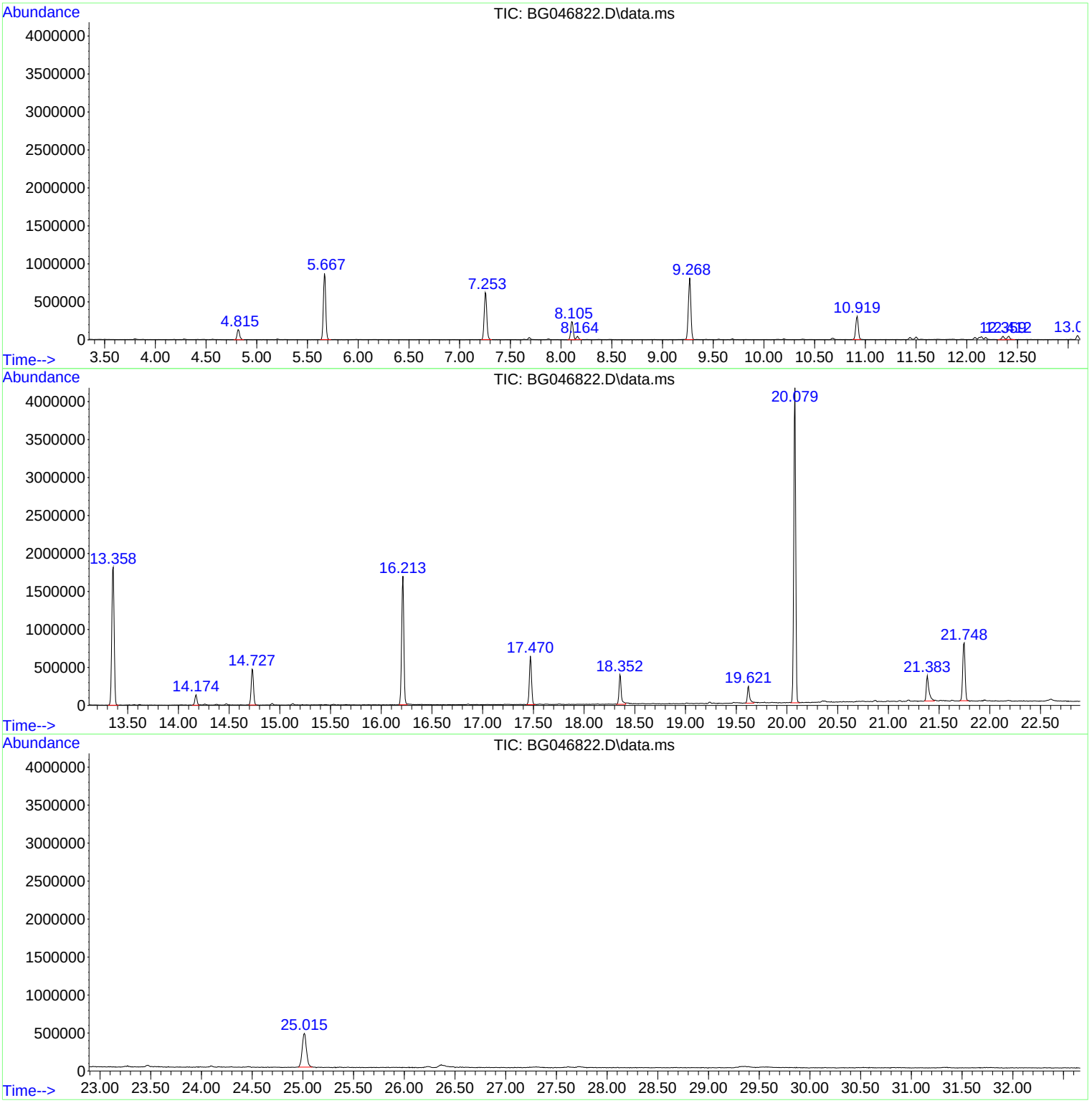
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW4D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
Acq On : 8 Oct 2020 19:29
Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

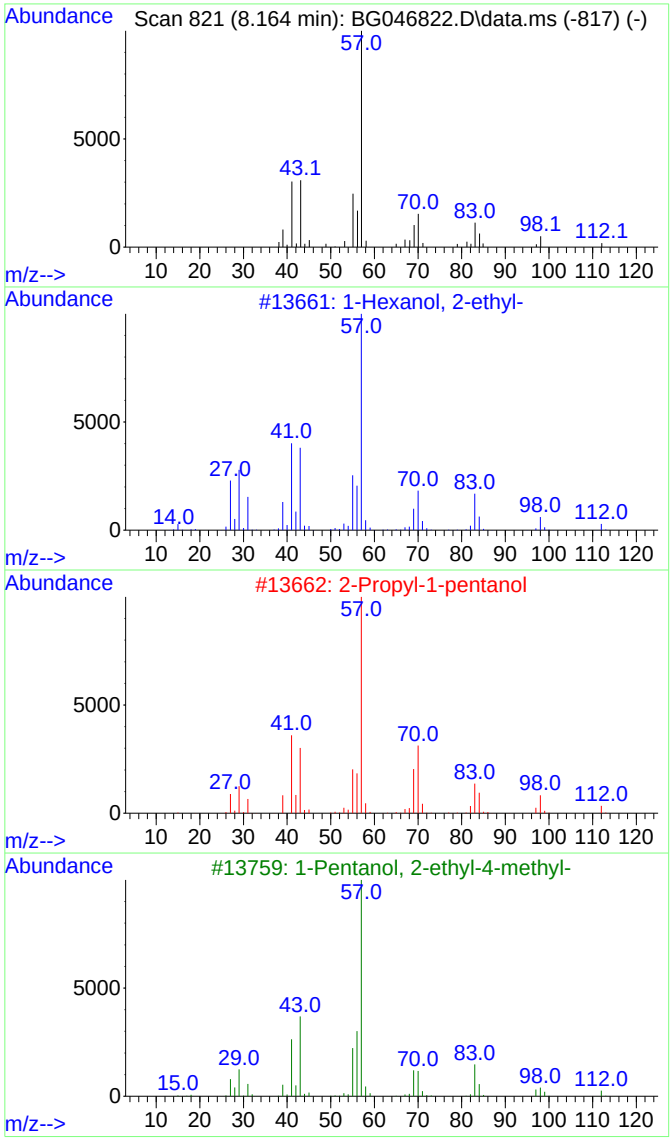
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

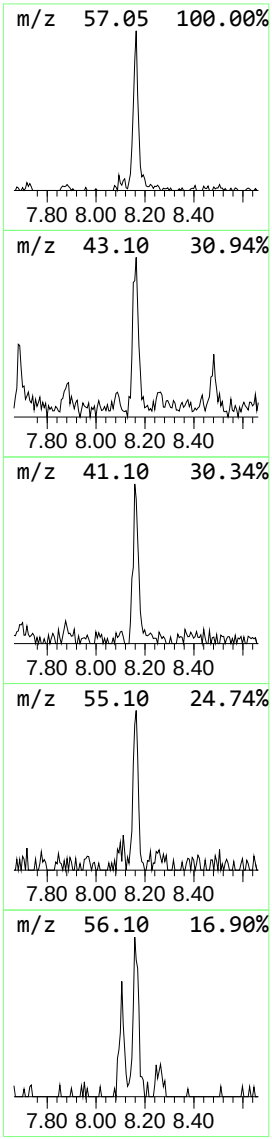
****

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.164	3.24 ng	66120	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
Acq On : 8 Oct 2020 19:29
Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

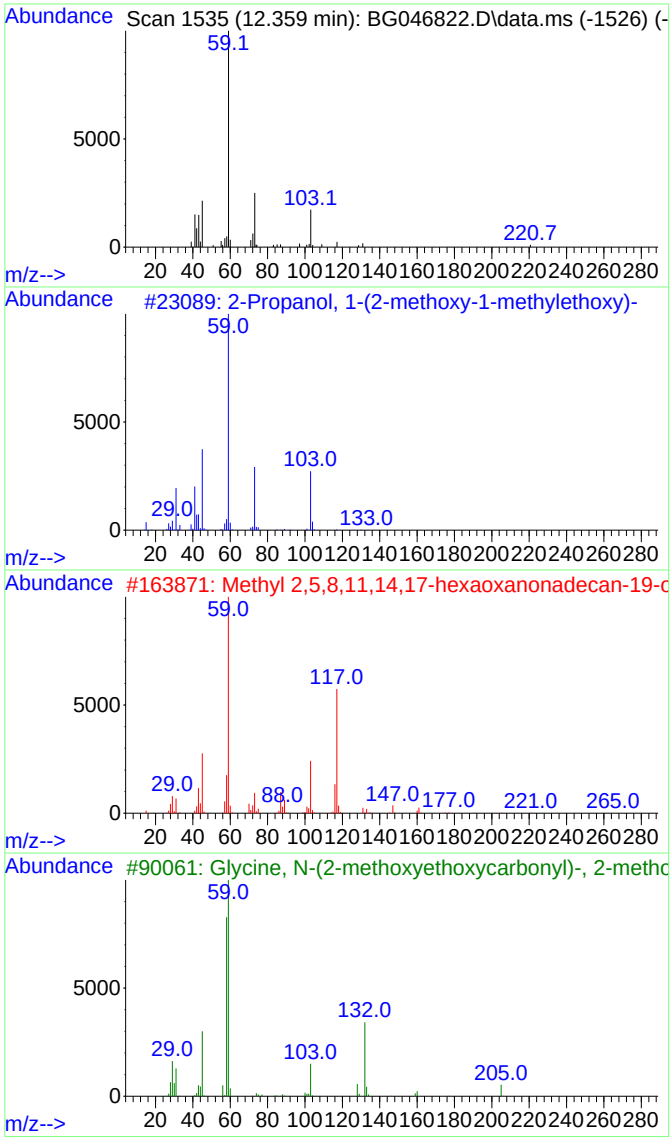
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

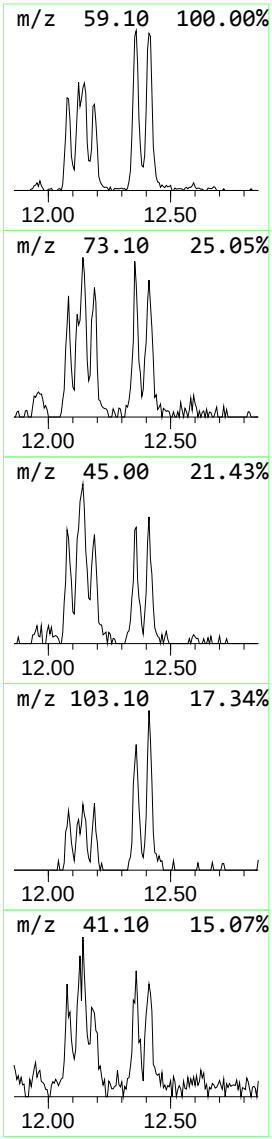
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.359	3.29 ng	87604	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	78
2	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	64
3	Glycine, N-(2-methoxyethoxycarbo...	235	C9H17NO6	1000328-06-4	59
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
Acq On : 8 Oct 2020 19:29
Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

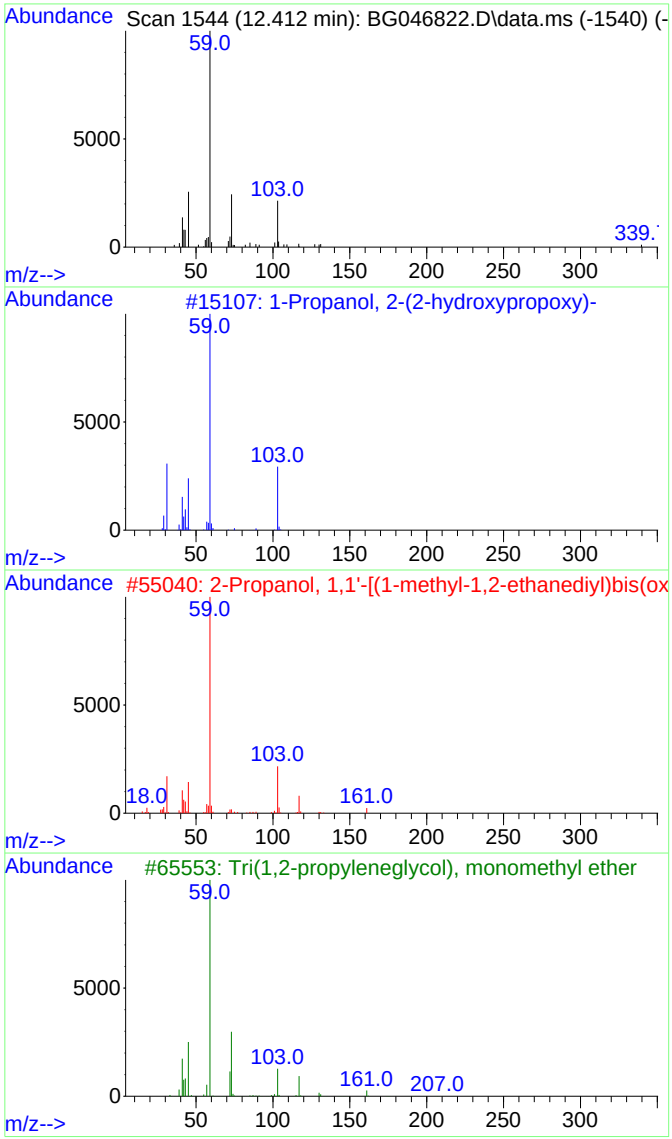
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

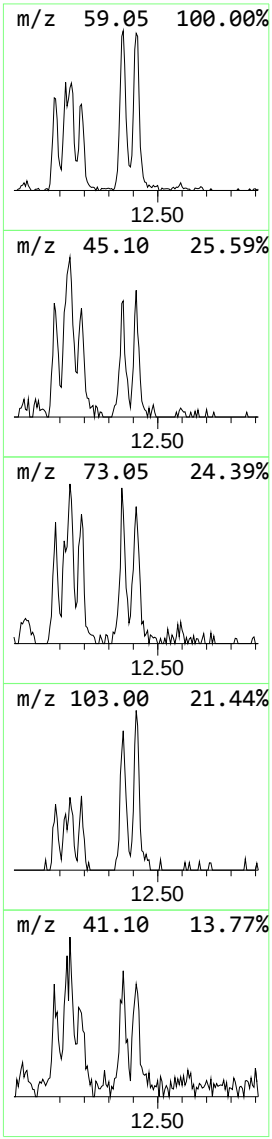
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.412	2.99 ng	79613	Naphthalene-d8	10.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
2	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53
3	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	50
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-11-4	42
5	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046822.D
Acq On : 8 Oct 2020 19:29
Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

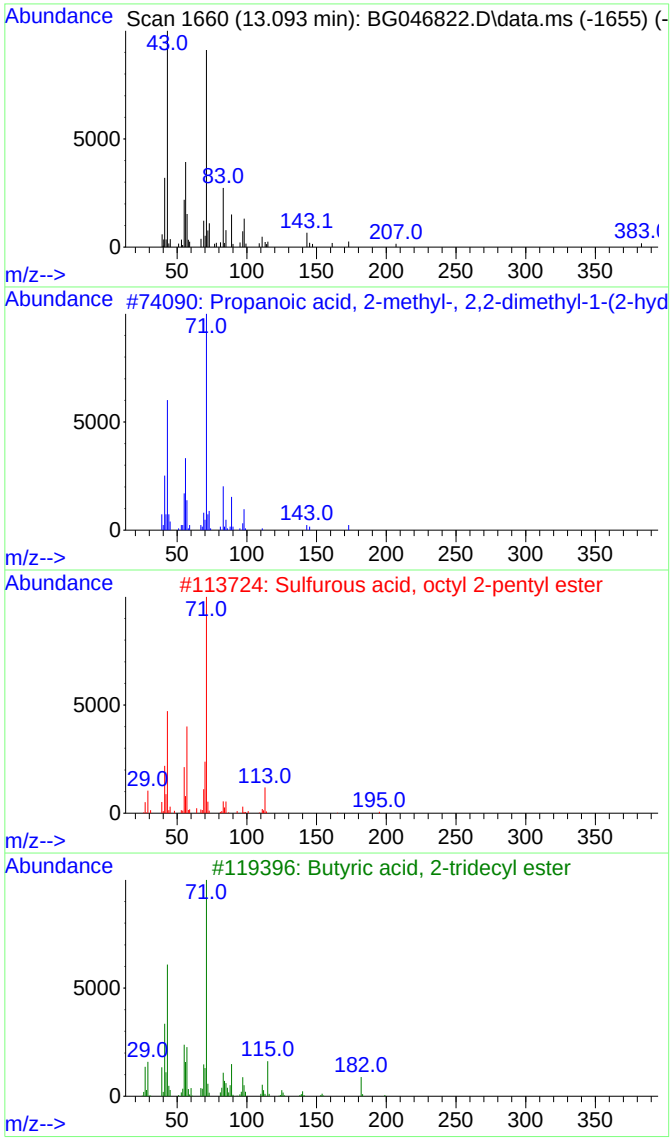
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

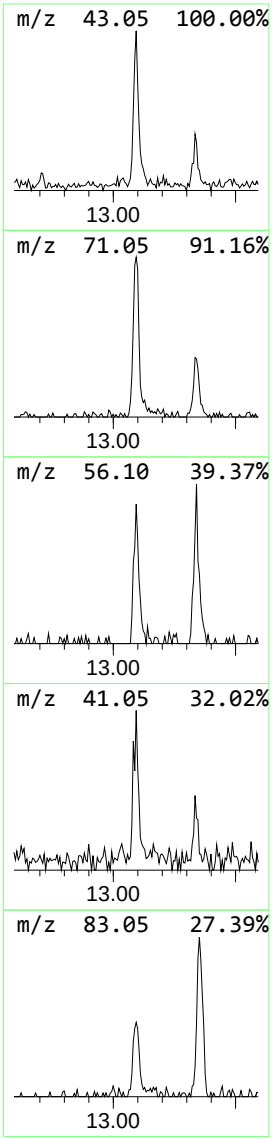
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.093	2.26 ng	84207	Acenaphthene-d10	14.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	87
2	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43
3	Butyric acid, 2-tridecyl ester	270	C17H34O2	055193-07-2	40
4	Butyric acid, 3-tetradecyl ester	284	C18H36O2	1000280-57-1	38
5	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	38





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Data File : BG046822.D
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Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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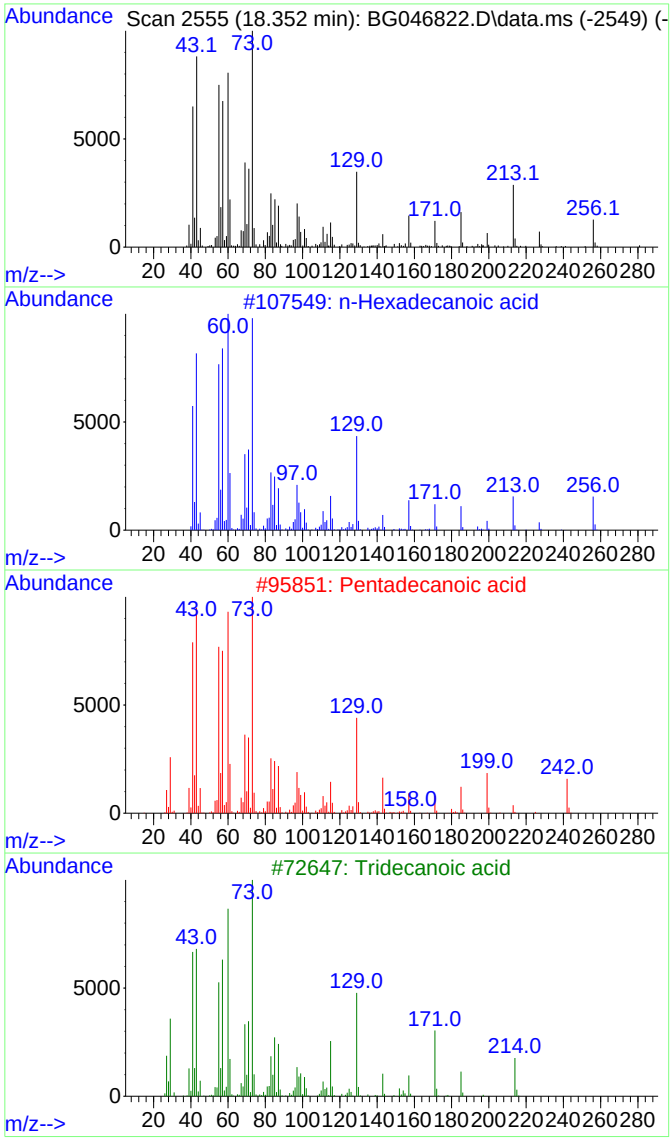
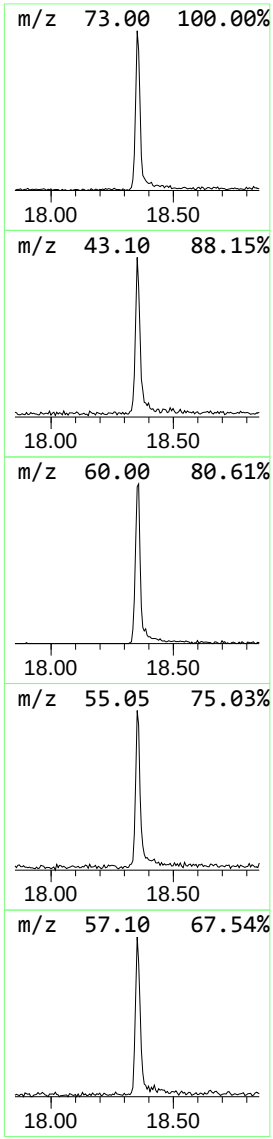
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.352	12.23 ng	590118	Phenanthrene-d10	17.470

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Operator : CG/JU
Sample : L4276-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW4D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

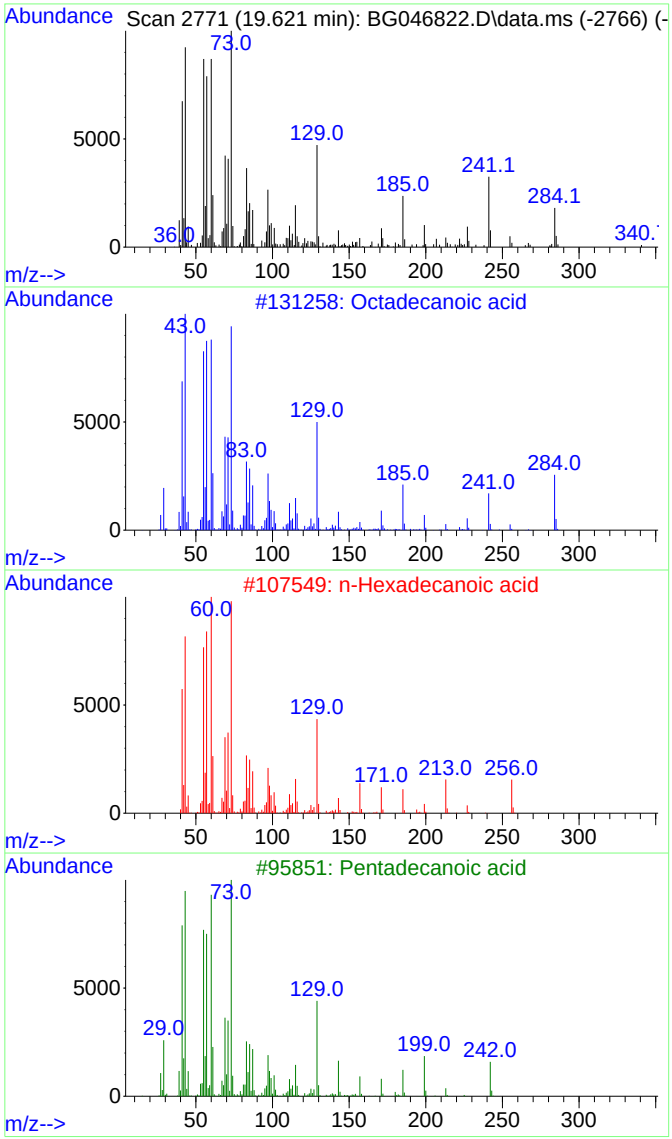
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

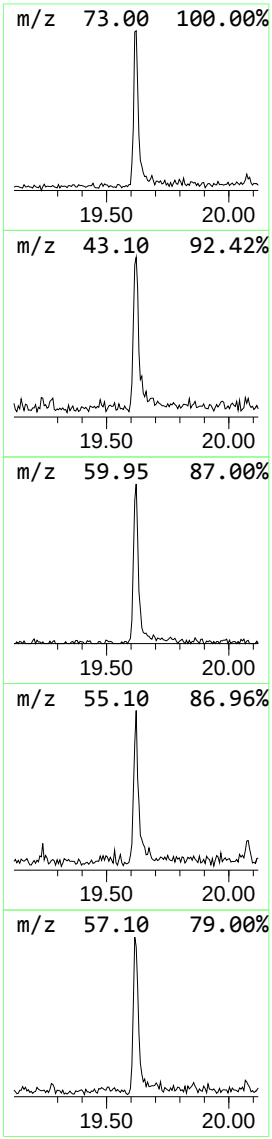
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.621	5.60 ng	345261	Chrysene-d12	21.748

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Sample : L4276-01
Misc :
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Instrument : BNA_G
ClientSampleId : MW4D

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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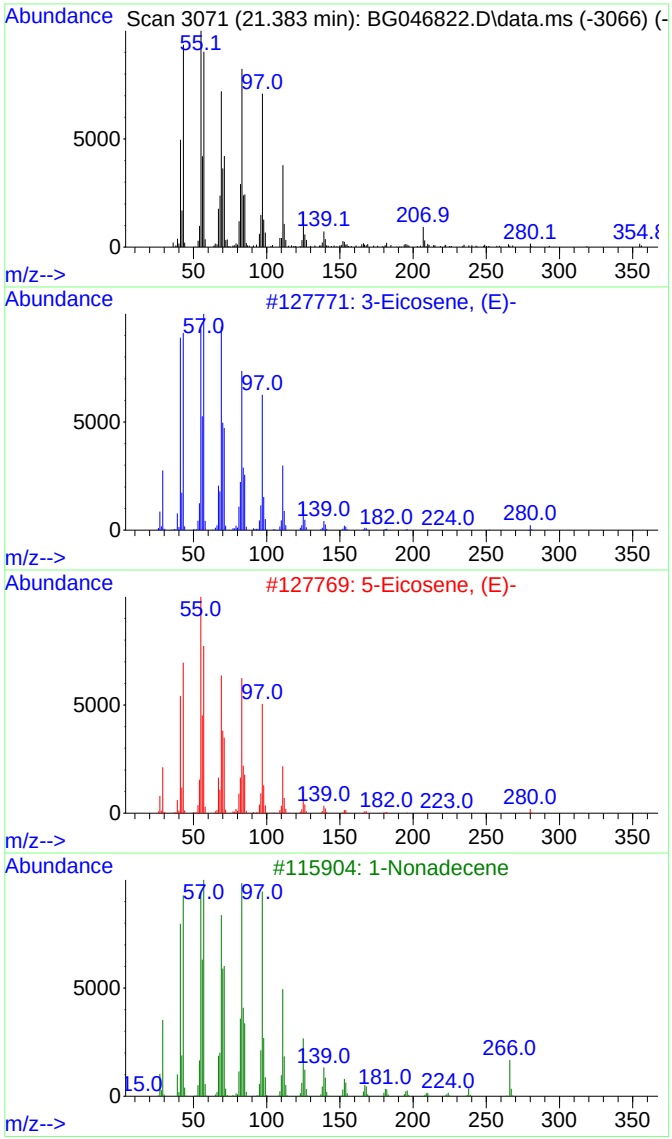
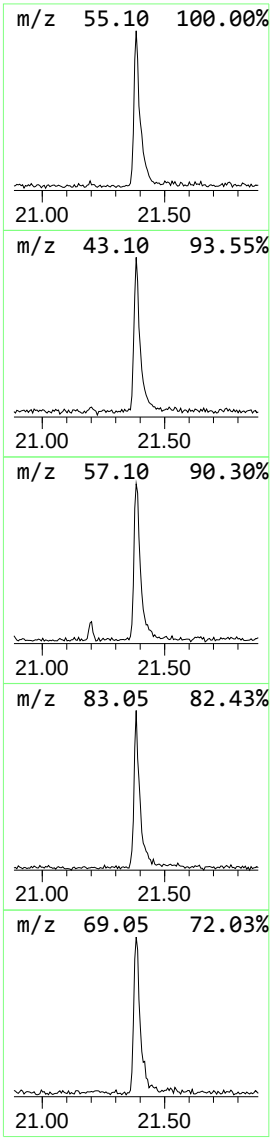
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.384	9.67 ng	596204	Chrysene-d12	21.748

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	8.164	3.2	ng	66120	1	8.111	408762	20.0
2-Propanol, 1-(...	12.359	3.3	ng	87604	2	10.919	531982	20.0
1-Propanol, 2-(...	12.412	3.0	ng	79613	2	10.919	531982	20.0
Propanoic acid,...	13.093	2.3	ng	84207	3	14.727	745067	20.0
n-Hexadecanoic ...	18.352	12.2	ng	590118	4	17.470	965388	20.0
Octadecanoic acid	19.621	5.6	ng	345261	5	21.748	1232970	20.0
3-Eicosene, (E)-	21.384	9.7	ng	596204	5	21.748	1232970	20.0