LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100720\
Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-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-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.967	102	107	112	rBV	63944	104638	2.95%	0.579%
2	4.572	204	210	219	rBV5	18725	35852	1.01%	0.198%
3	4.878	256	262	271	rBV	304164	491814	13.87%	2.721%
4	5.207	311	318	325	rBV2	18517	36269	1.02%	0.201%
5	5.577	374	381	390	rBV	64166	153637	4.33%	0.850%
6	5.671	390	397	407	rVB	778527	1224377	34.53%	6.775%
7	5.859	424	429	438	rVB2	52827	83709	2.36%	0.463%
8	6.611	551	557	562	rBV3	25509	53856	1.52%	0.298%
9	7.198	650	657	661	rBV3	34802	62885	1.77%	0.348%
10	7.257	661	667	678	rVB	806056	1387952	39.14%	7.680%
11	7.639	726	732	736	rBV3	58662	85767	2.42%	0.475%
12	7.692	736	741	750	rVB	80866	122876	3.47%	0.680%
13	7.880	766	773	782	rVB	113976	194986	5.50%	1.079%
14	8.109	803	812	820	rBV	235591	418599	11.80%	2.316%
15	9.267	1002	1009	1020	rVB	502711	910335	25.67%	5.037%
16	10.923	1283	1291	1297	rBV	305963	550820	15.53%	3.048%
17	12.627	1576	1581	1588	rVB3	45890	72364	2.04%	0.400%
18	13.356	1698	1705	1713	rBV	1287667	1974047	55.67%	10.923%
19	14.178	1839	1845	1850	rBV	132075	188089	5.30%	1.041%
20	14.572	1906	1912	1919	rBV	73383	109301	3.08%	0.605%
21	14.731	1932	1939	1947	rBV2	496237	780631	22.01%	4.319%
22	16.211	2185	2191	2204	rBV	970271	1470415	41.47%	8.136%
23	17.475	2399	2406	2412	rBV	697954	1027733	28.98%	5.687%
24	18.356	2552	2556	2560	rBV3	47413	57303	1.62%	0.317%
25	20.077	2843	2849	2856	rBV	2607172	3546129	100.00%	19.621%
26	21.388	3067	3072	3080	rBV3	122158	228815	6.45%	1.266%
27	21.752	3127	3134	3143	rVB2	824847	1343680	37.89%	7.435%
28	25.025	3680	3691	3701	rBV2	473540	1355889	38.24%	7.502%

Sum of corrected areas: 18072768

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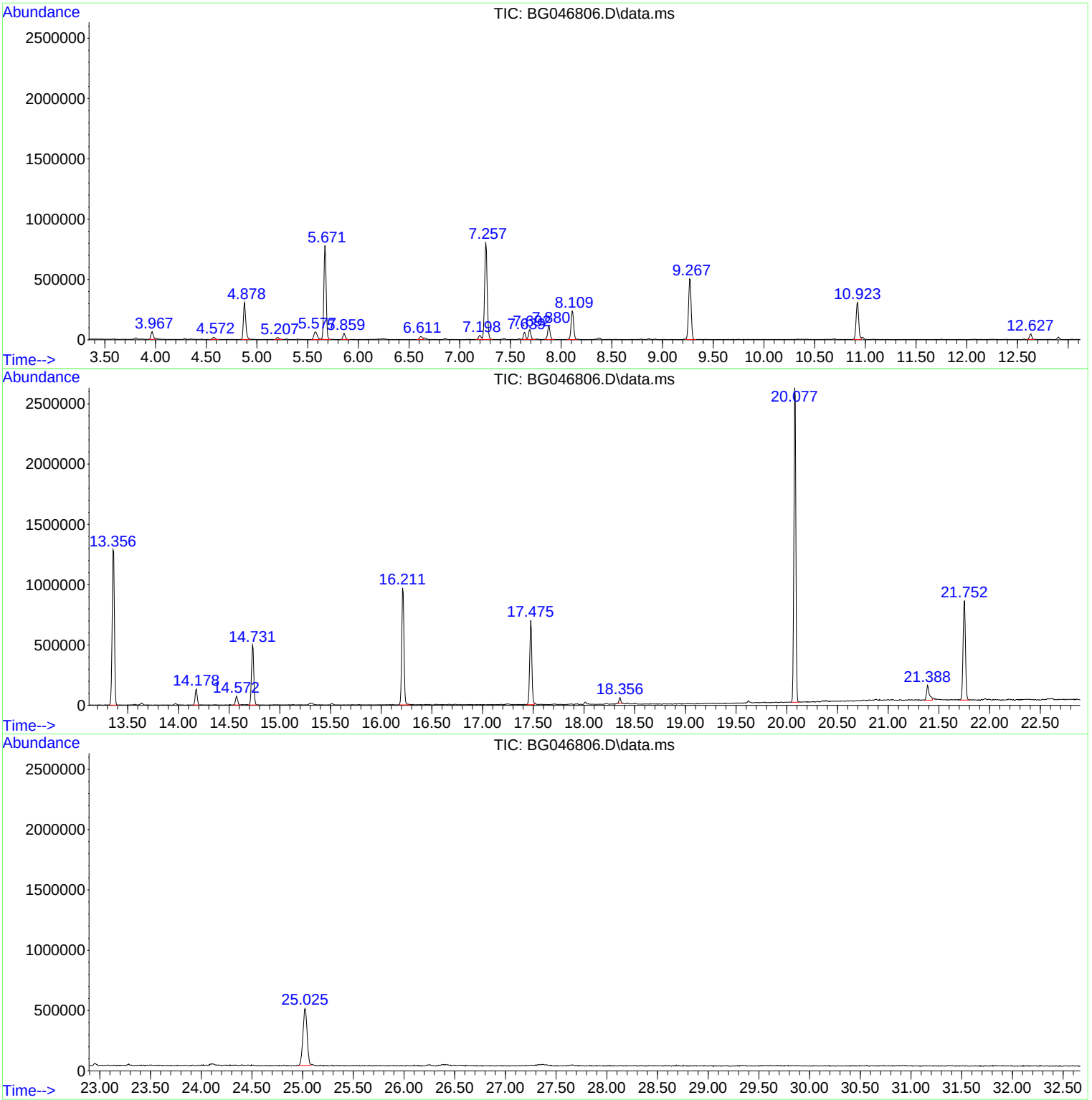
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S-2

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

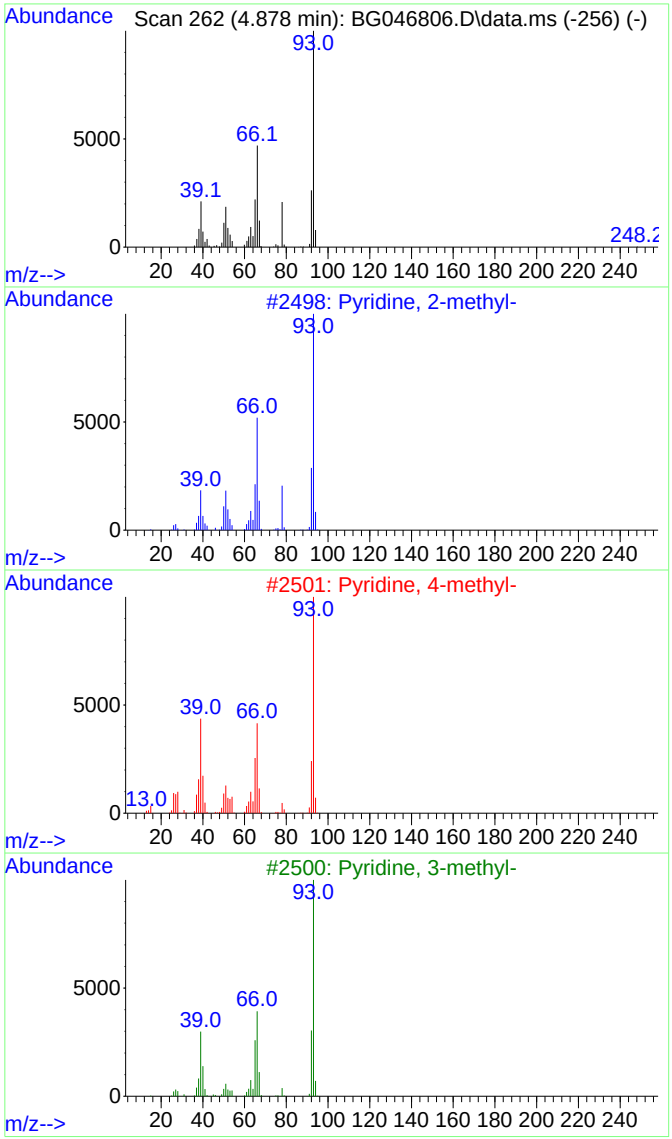
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

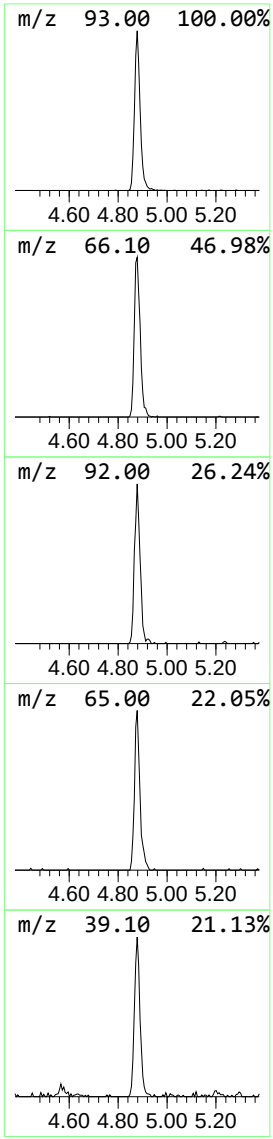
****

Peak Number 1 Pyridine, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.878	23.50 ng	491814	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-methyl-	93	C6H7N	000109-06-8	97
2	Pyridine, 4-methyl-	93	C6H7N	000108-89-4	95
3	Pyridine, 3-methyl-	93	C6H7N	000108-99-6	94
4	Aniline	93	C6H7N	000062-53-3	87
5	Silanediamine, 1,1-dimethyl-N,N'...	242	C14H18N2Si	013435-09-1	72





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Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

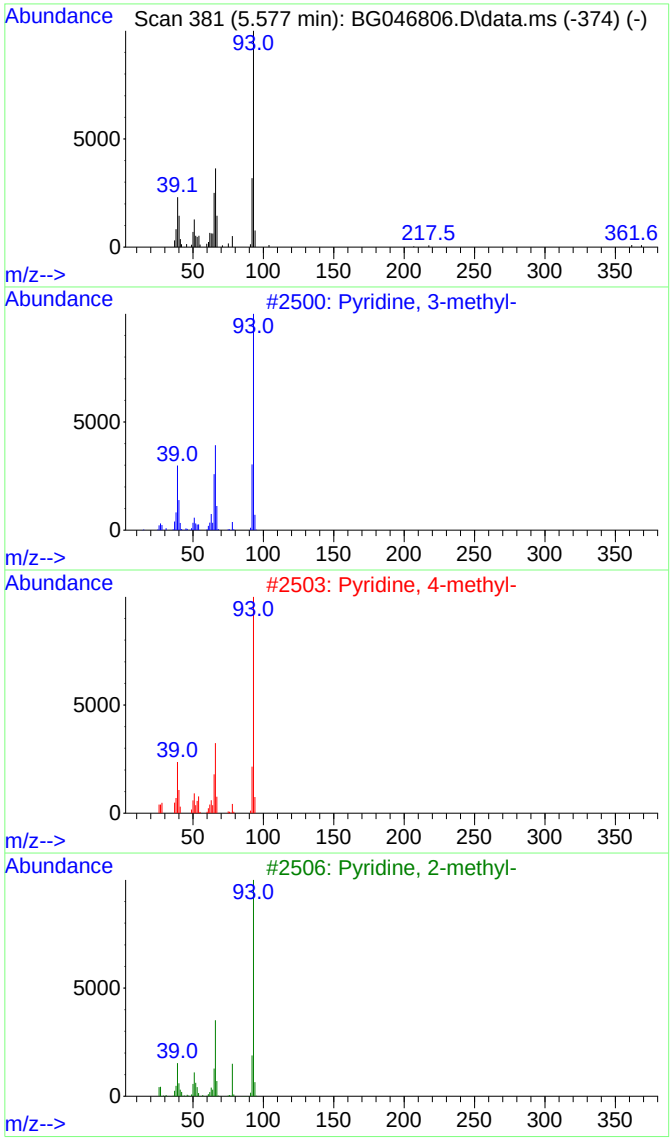
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

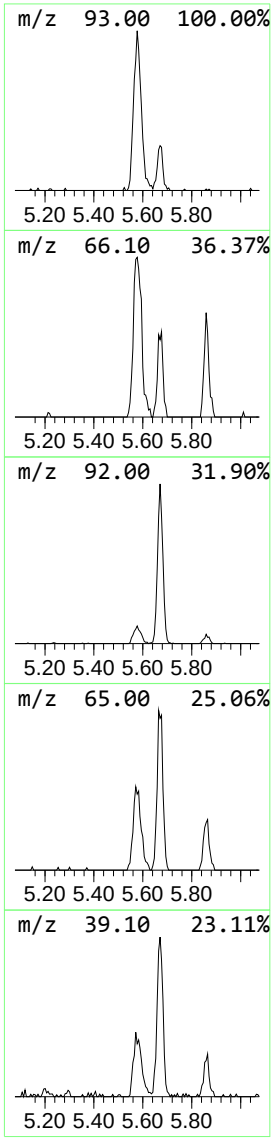
****

Peak Number 2 Pyridine, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.577	7.34 ng	153637	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3-methyl-	93	C6H7N	000108-99-6	94
2	Pyridine, 4-methyl-	93	C6H7N	000108-89-4	94
3	Pyridine, 2-methyl-	93	C6H7N	000109-06-8	87
4	2-Pyridineacetic acid	137	C7H7NO2	013115-43-0	83
5	Aniline	93	C6H7N	000062-53-3	83





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Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

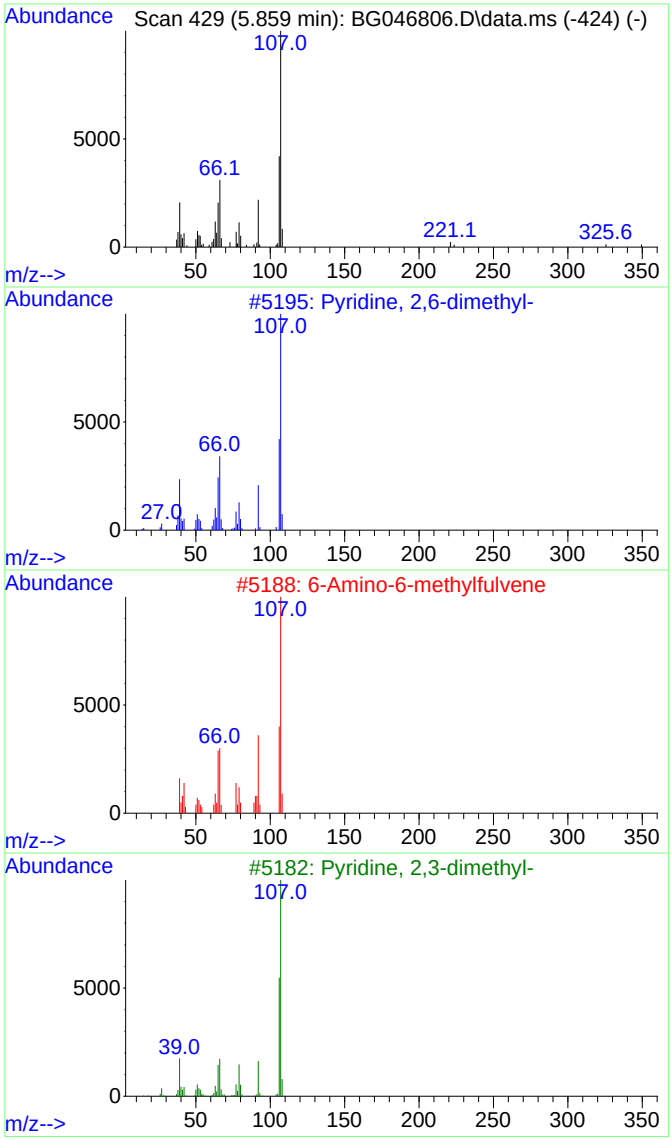
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

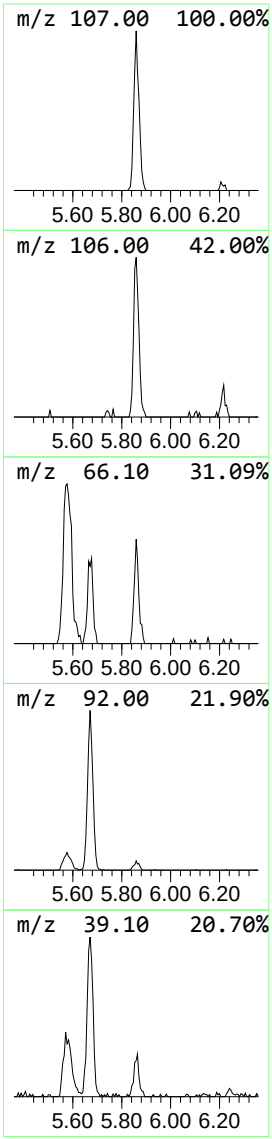
****

Peak Number 3 Pyridine, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.859	4.00 ng	83709	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2,6-dimethyl-	107	C7H9N	000108-48-5	96
2	6-Amino-6-methylfulvene	107	C7H9N	000694-74-6	74
3	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	52
4	Pyridine, 3,4-dimethyl-	107	C7H9N	000583-58-4	49
5	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	46





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Acq On : 7 Oct 2020 17:44
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Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

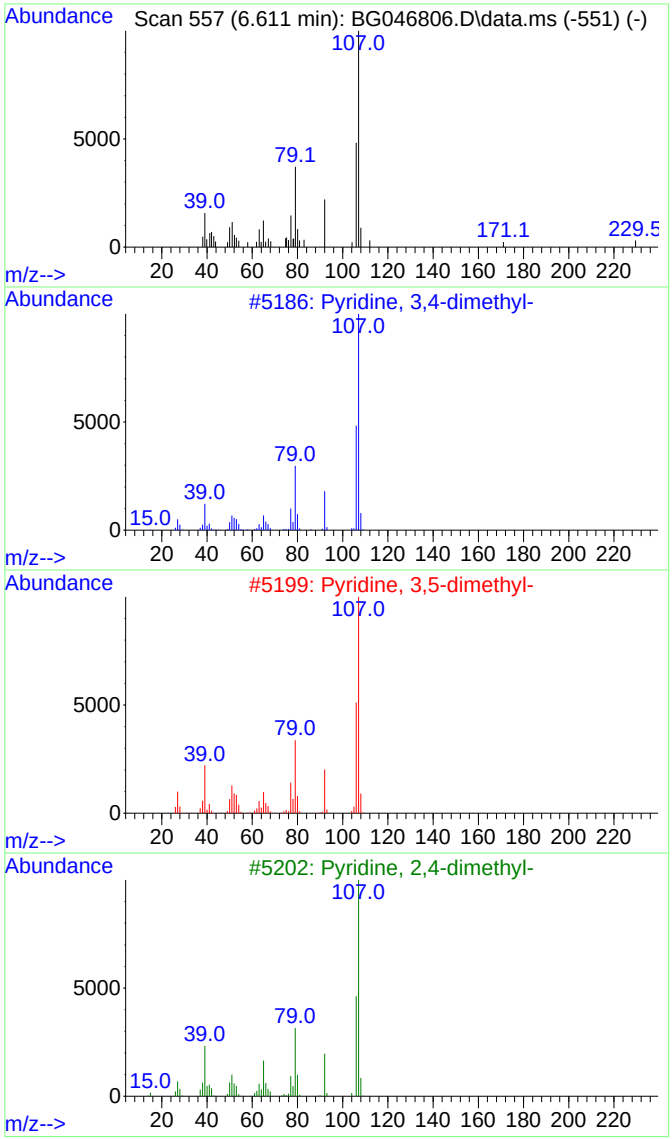
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

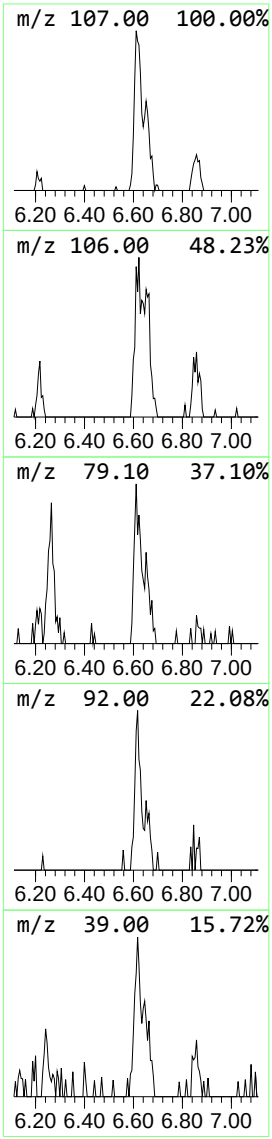
****

Peak Number 4 Pyridine, 3,4-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.611	2.57 ng	53856	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3,4-dimethyl-	107	C7H9N	000583-58-4	94
2	Pyridine, 3,5-dimethyl-	107	C7H9N	000591-22-0	94
3	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	91
4	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	90
5	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	74





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Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

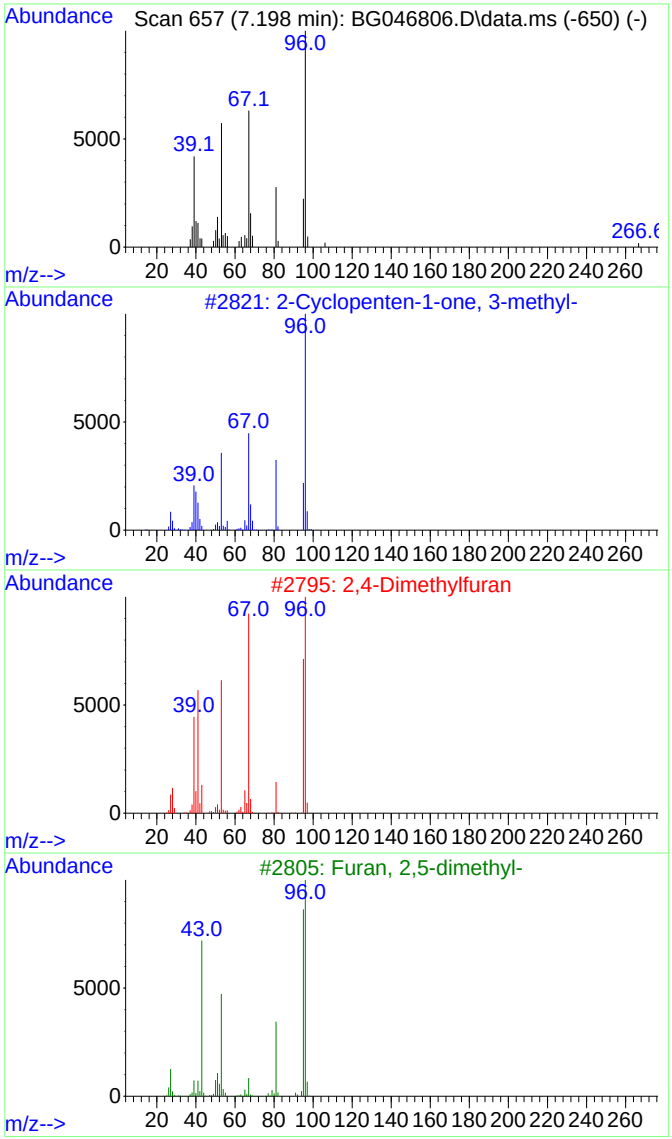
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

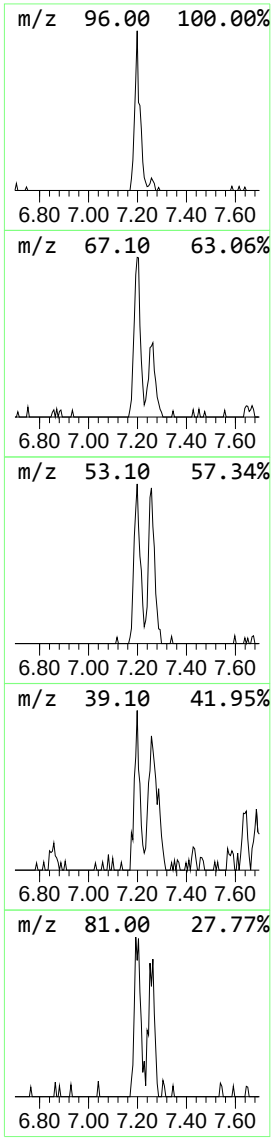
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclopenten-1-one, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.198	3.00 ng	62885	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	87
2	2,4-Dimethylfuran	96	C6H8O	003710-43-8	64
3	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	53
4	4-Vinyl-4,5-dihydro-3H-pyrazole	96	C5H8N2	063438-33-5	53
5	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	47





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Instrument : BNA_G
ClientSampleId : S-2

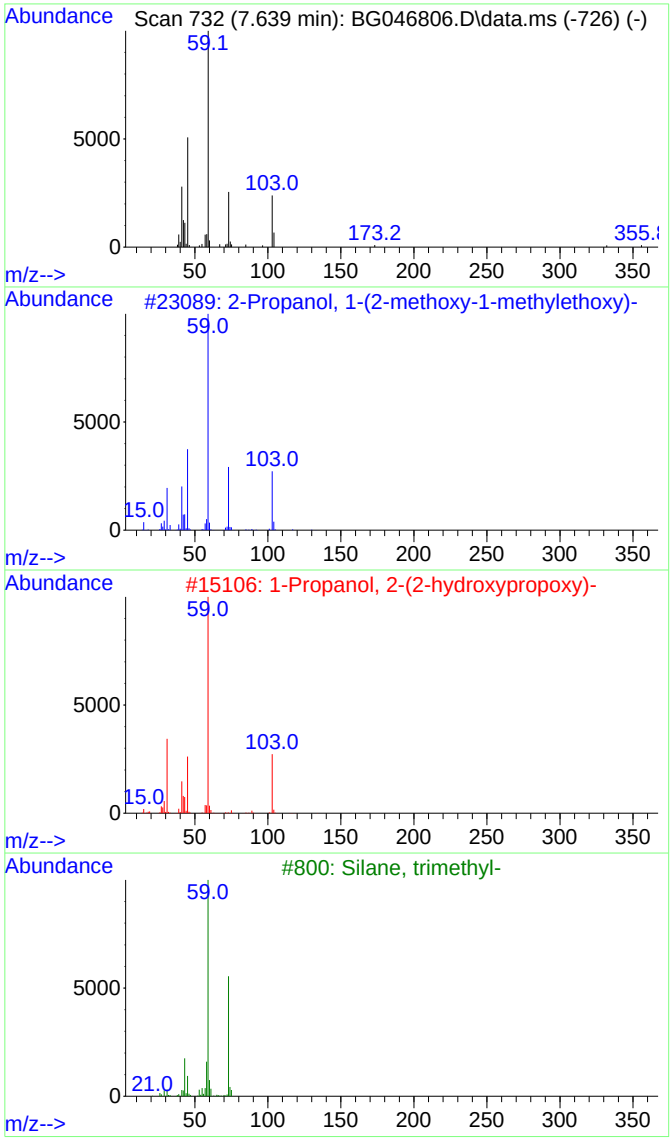
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

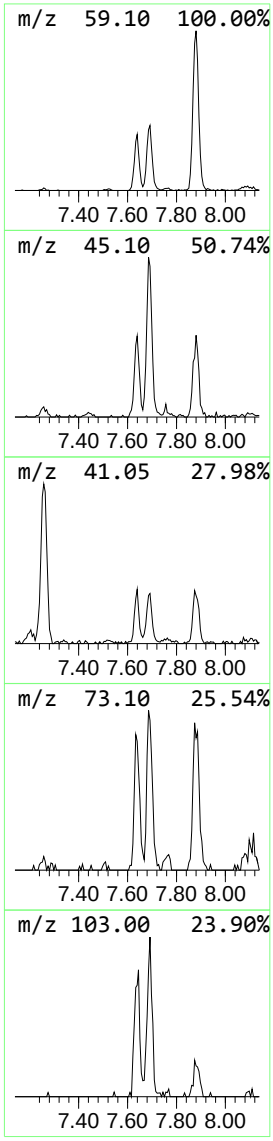
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.639	4.10 ng	85767	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	50
4	Ethyl 2,5,8,11,14,17-hexaoxanona...	338	C15H30O8	1000366-80-6	50
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	47





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

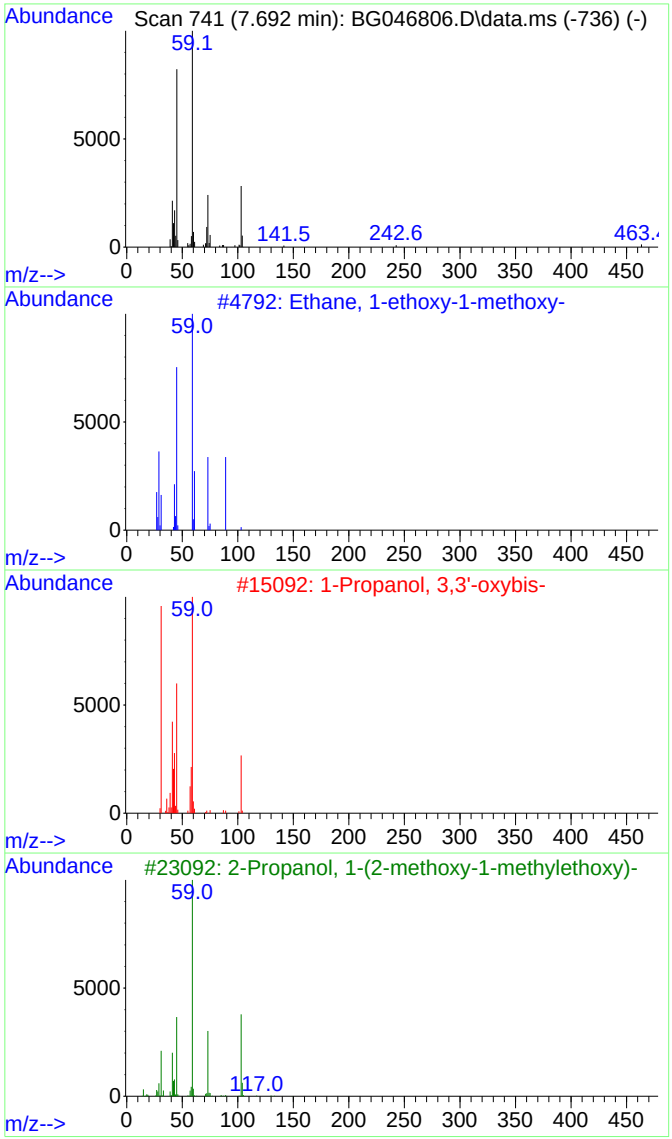
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

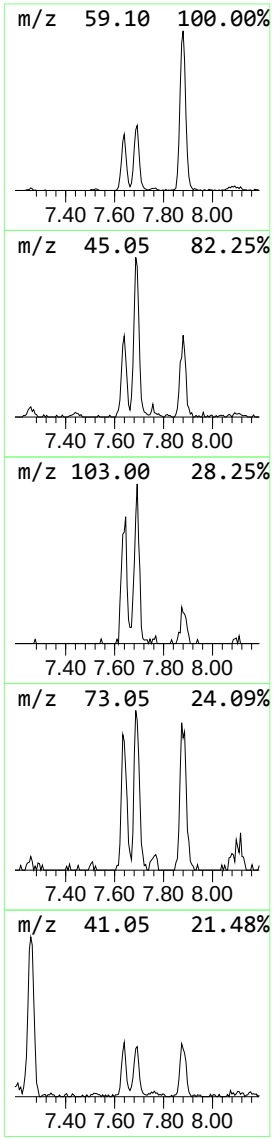
****

Peak Number 7 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.692	5.87 ng	122876	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64
2	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	50
3	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	50
4	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	50
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	43





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Instrument : BNA_G
ClientSampleId : S-2

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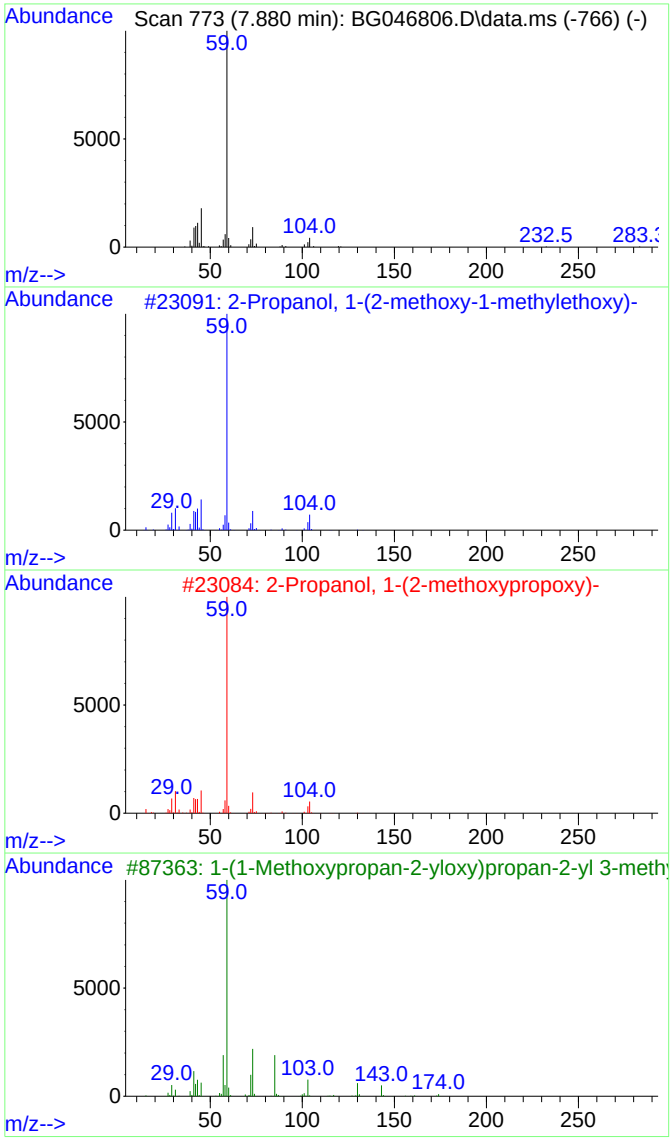
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

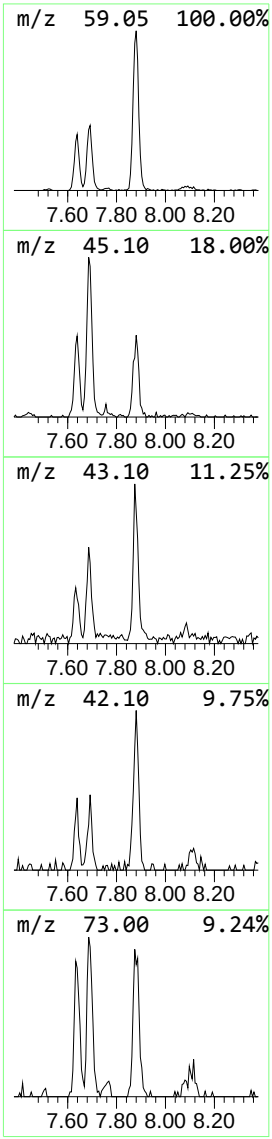
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.880	9.32 ng	194986	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
3	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	72
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	64
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

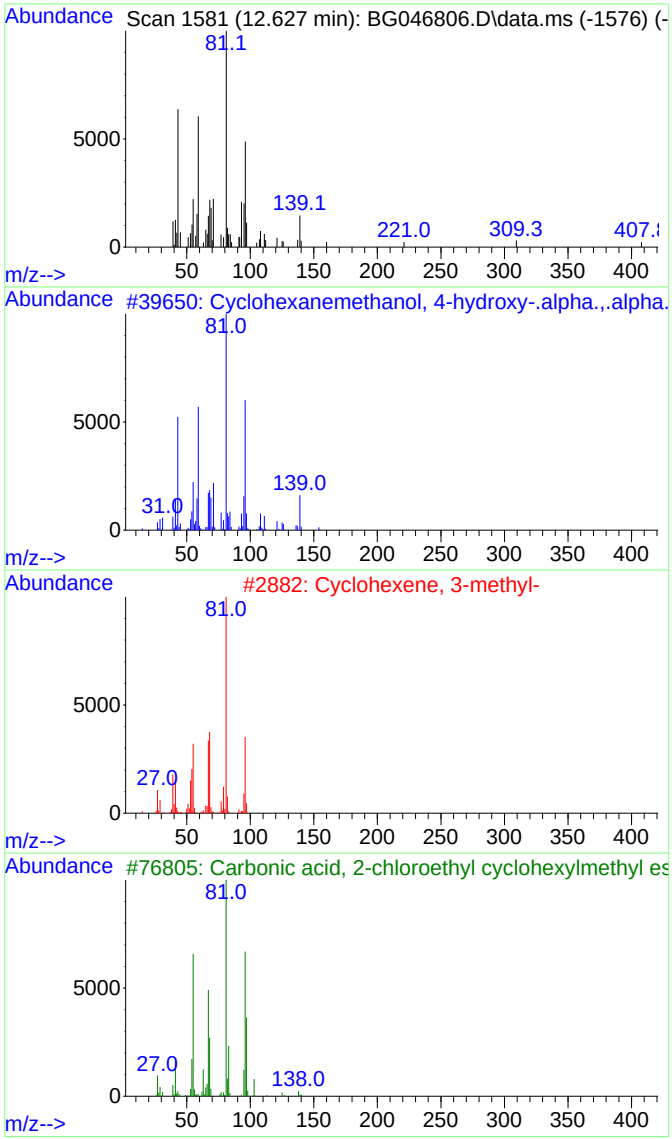
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

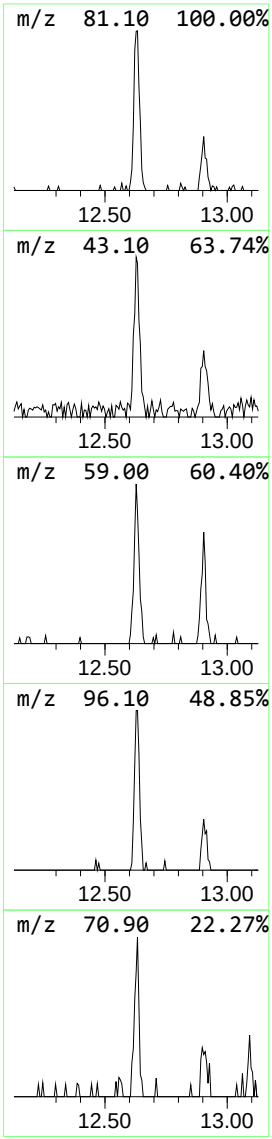
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexanemethanol, 4-hydr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.63 ng	72364	Naphthalene-d8	10.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-hydroxy-....	172	C10H20O2	000080-53-5	72
2	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	47
3	Carbonic acid, 2-chloroethyl cyc...	220	C10H17ClO3	1000357-88-3	43
4	4-Methylcyclohexanol acetate	156	C9H16O2	022597-23-5	43
5	Cyclopentane, 1-methyl-2-methylene-	96	C7H12	041158-41-2	43





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Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

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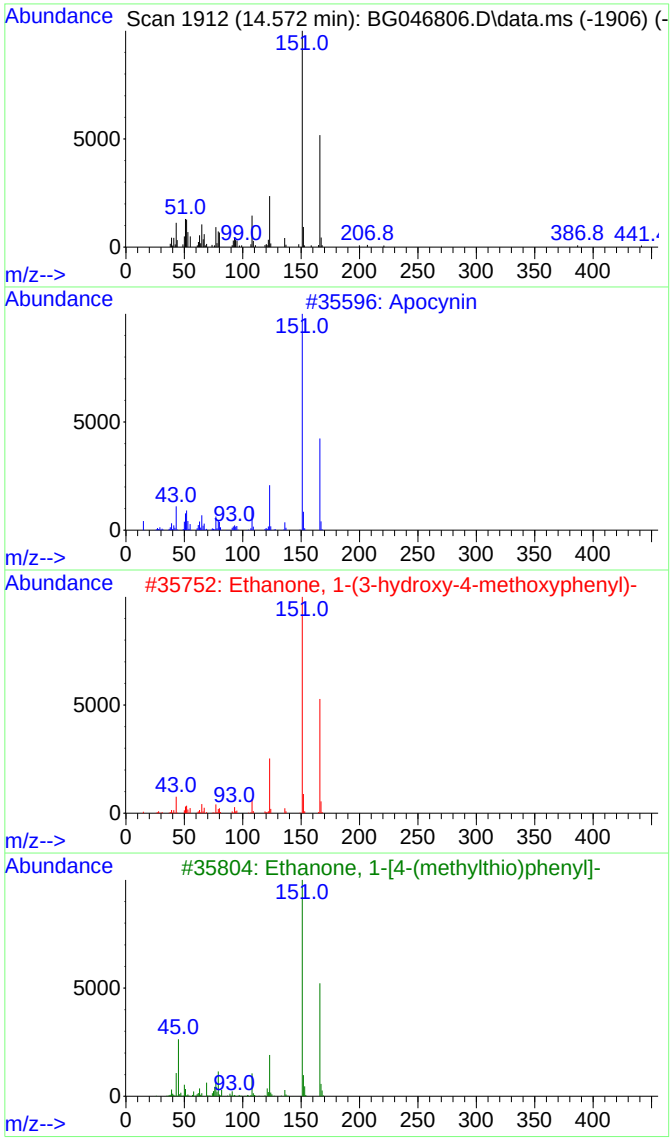
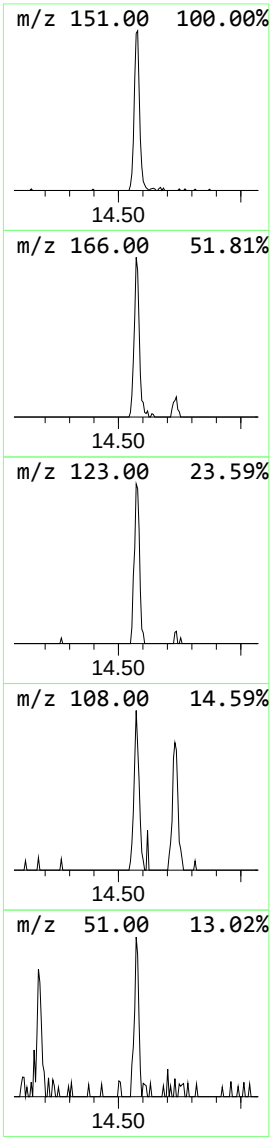
Peak Number 10 Apocynin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.572	2.80 ng	109301	Acenaphthene-d10	14.731

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	96
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	91
3	Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	87
4	Benzenethiol, 4-(1,1-dimethyleth...	166	C10H14S	002396-68-1	72
5	1,4-Dimethoxy-2,3-dimethylbenzene	166	C10H14O2	039021-83-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100720\
Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

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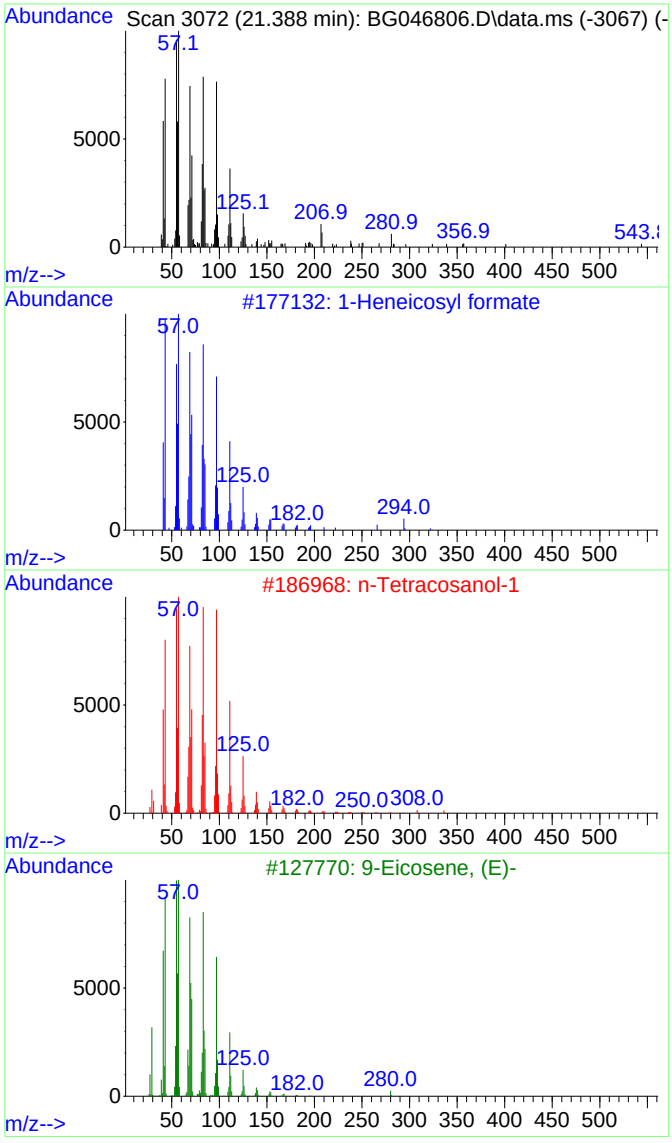
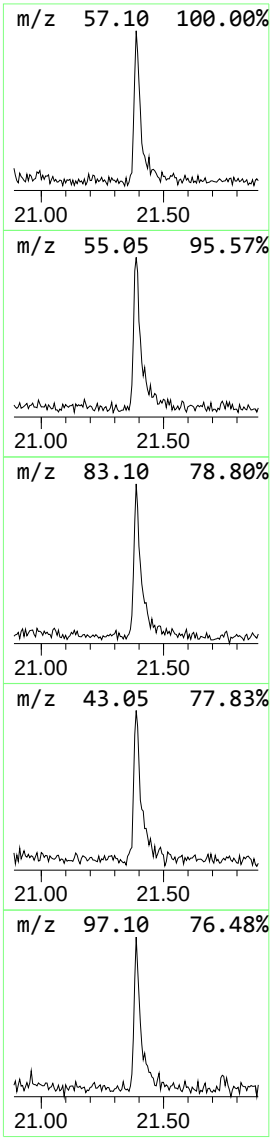
Peak Number 11 1-Heneicosyl formate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.388	3.41 ng	228815	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4	1-Nonadecene	266	C19H38	018435-45-5	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100720\
Data File : BG046806.D
Acq On : 7 Oct 2020 17:44
Operator : CG/JU
Sample : L4279-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyridine, 2-met...	4.878	23.5	ng	491814	1	8.115	418599	20.0
Pyridine, 3-met...	5.577	7.3	ng	153637	1	8.115	418599	20.0
Pyridine, 2,6-d...	5.859	4.0	ng	83709	1	8.115	418599	20.0
Pyridine, 3,4-d...	6.611	2.6	ng	53856	1	8.115	418599	20.0
2-Cyclopenten-1...	7.198	3.0	ng	62885	1	8.115	418599	20.0
1-Propanol, 2-(...	7.639	4.1	ng	85767	1	8.115	418599	20.0
Ethane, 1-ethox...	7.692	5.9	ng	122876	1	8.115	418599	20.0
2-Propanol, 1-(...	7.880	9.3	ng	194986	1	8.115	418599	20.0
Cyclohexanemeth...	12.627	2.6	ng	72364	2	10.923	550820	20.0
Apocynin	14.572	2.8	ng	109301	3	14.731	780631	20.0
1-Heneicosyl fo...	21.388	3.4	ng	228815	5	21.752	1343680	20.0