LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050222\
Data File : BG053408.D
Acq On : 2 May 2022 20:52
Operator : CG/JU
Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

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-BG040822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.191	302	307	316	rBV	57228	92107	3.41%	0.857%
2	5.602	371	377	382	rBV	83315	131866	4.88%	1.226%
3	5.667	382	388	396	rVV	498526	834799	30.90%	7.763%
4	5.755	396	403	408	rVB	25888	53700	1.99%	0.499%
5	7.077	622	628	634	rVB	37404	58239	2.16%	0.542%
6	7.265	652	660	667	rBV	590645	1055522	39.07%	9.816%
7	7.318	667	669	676	rVB	19646	28999	1.07%	0.270%
8	7.488	692	698	706	rVB	47990	78637	2.91%	0.731%
9	7.747	736	742	750	rVB	72922	118605	4.39%	1.103%
10	8.099	795	802	809	rBV2	94106	163507	6.05%	1.521%
11	8.481	860	867	872	rBV	20736	34480	1.28%	0.321%
12	9.262	993	1000	1010	rVB	373384	684701	25.35%	6.368%
13	10.913	1273	1281	1287	rBV	122720	231504	8.57%	2.153%
14	13.351	1688	1696	1703	rBV	972095	1548836	57.33%	14.404%
15	14.725	1923	1930	1938	rBV	217091	339213	12.56%	3.155%
16	16.212	2176	2183	2196	rBV	598539	915931	33.91%	8.518%
17	17.469	2391	2397	2402	rBV	306117	461350	17.08%	4.290%
18	20.071	2834	2840	2846	rBV	2097873	2701389	100.00%	25.122%
19	21.369	3056	3061	3069	rBV	101094	161311	5.97%	1.500%
20	21.751	3118	3126	3137	rBV2	306118	536577	19.86%	4.990%
21	25.041	3674	3686	3700	rBV2	182951	521717	19.31%	4.852%

Sum of corrected areas: 10752990

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050222\
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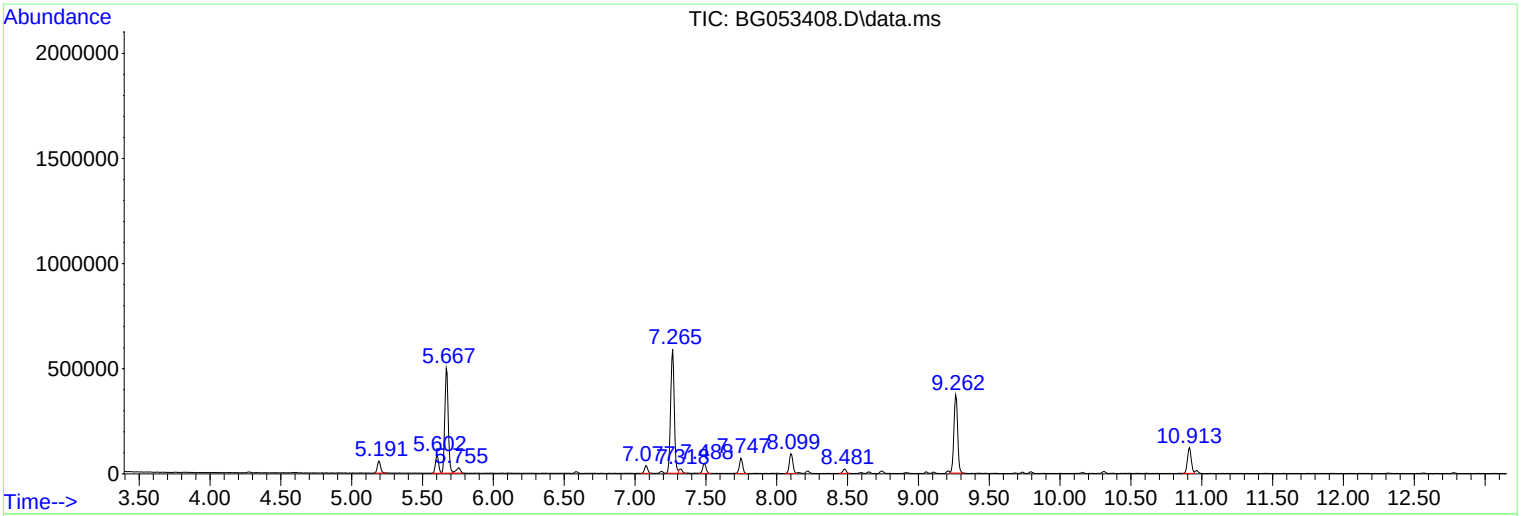
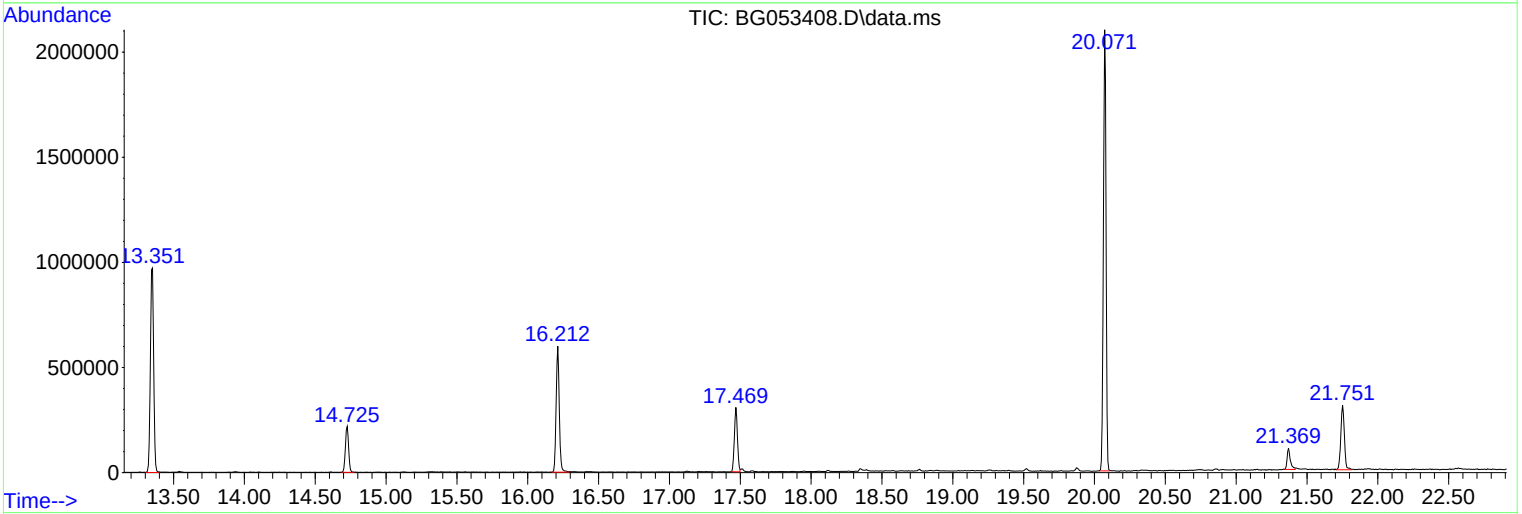
Misc :
ALS Vial : 17 Sample Multiplier: 1

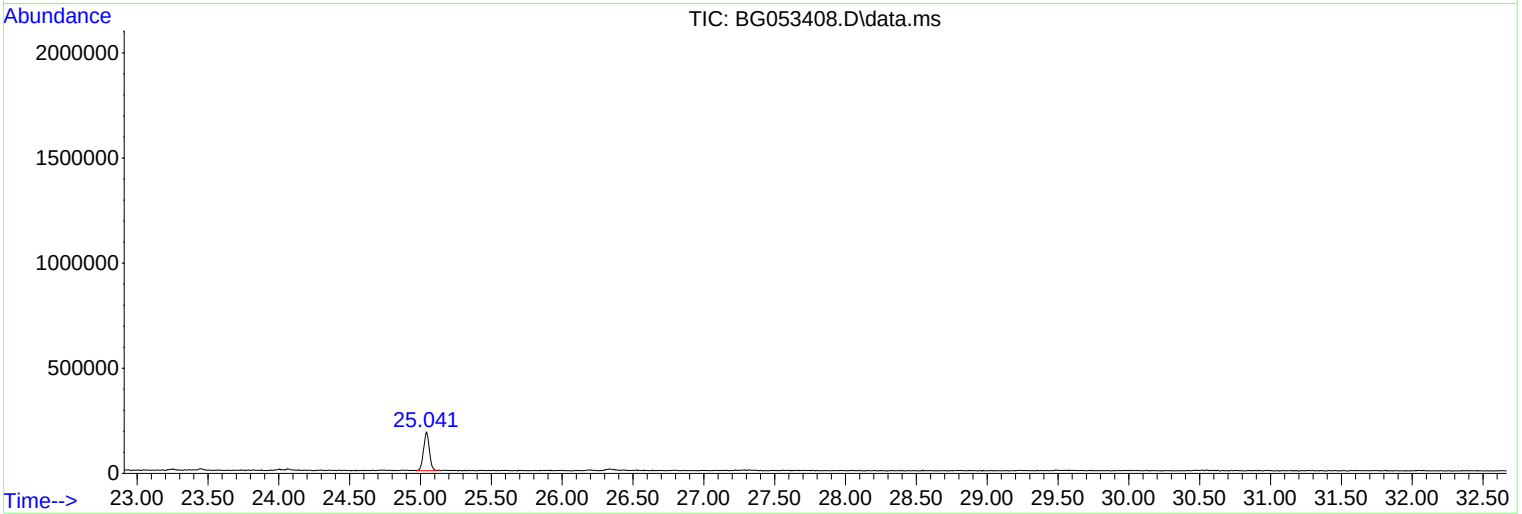
Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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 : BG053408.D
Acq On : 2 May 2022 20:52
Operator : CG/JU
Sample : N2619-07
Misc :
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Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

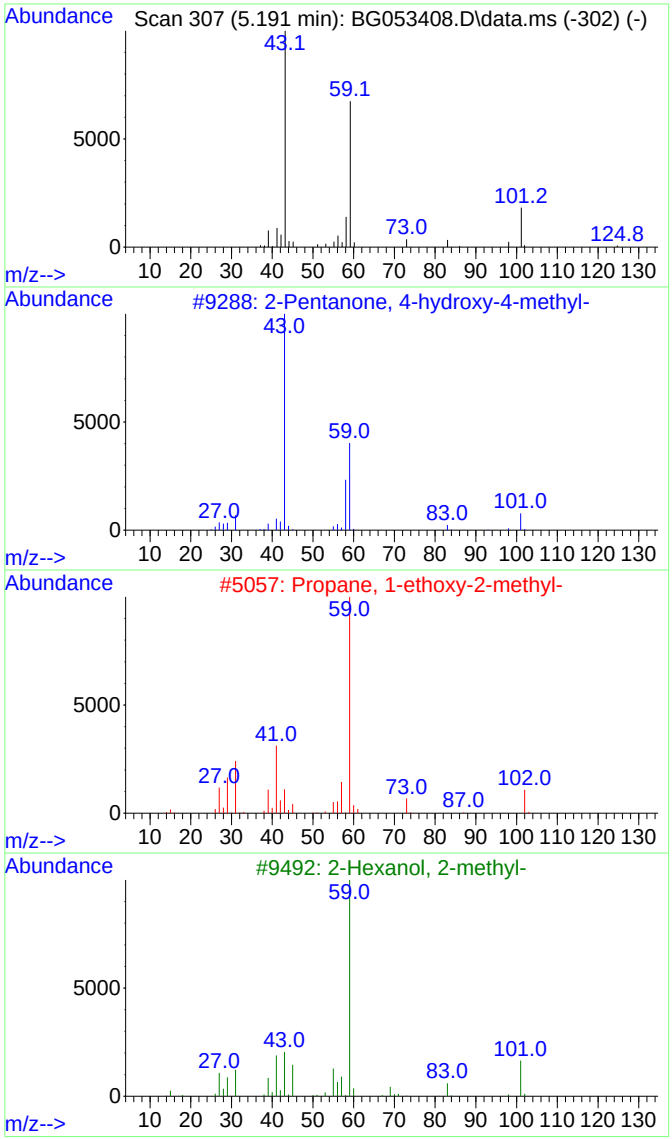
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

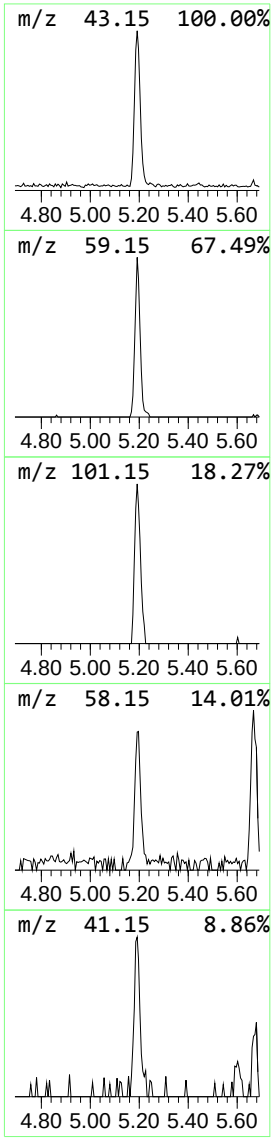
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	11.27 ng	92107	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	25





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Data File : BG053408.D
Acq On : 2 May 2022 20:52
Operator : CG/JU
Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

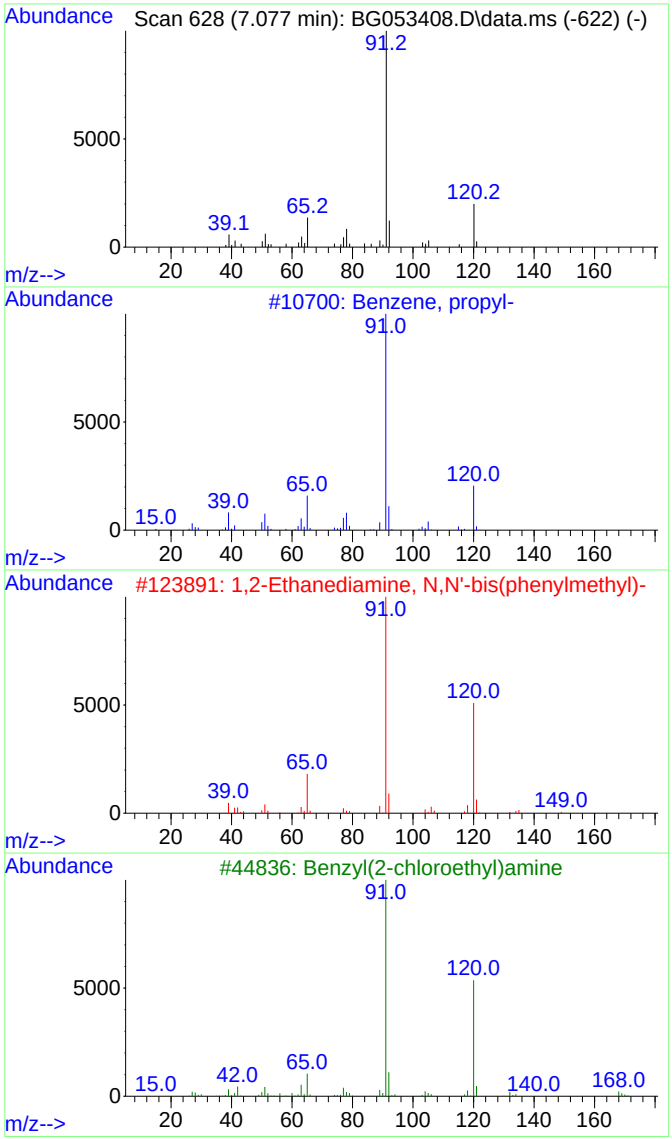
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

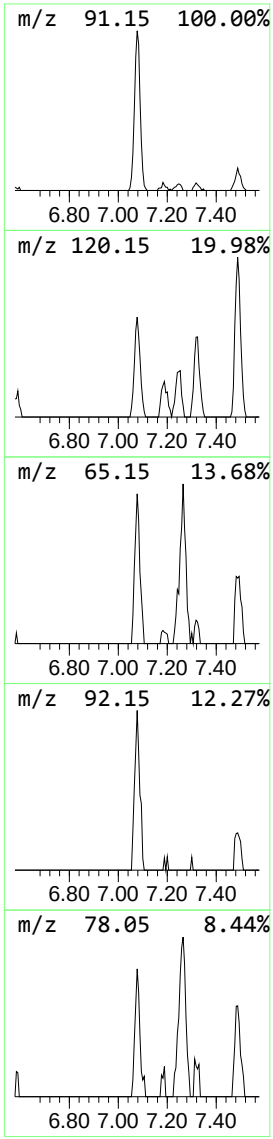
****

Peak Number 4 Benzene, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.077	7.12 ng	58239	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	94
2	1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	78
3	Benzyl(2-chloroethyl)amine	169	C9H12ClN	042074-16-8	78
4	N-Butylbenzylamine	163	C11H17N	002403-22-7	78
5	1-(Benzylamino)propan-2-ol	165	C10H15NO	1000486-84-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050222\
Data File : BG053408.D
Acq On : 2 May 2022 20:52
Operator : CG/JU
Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

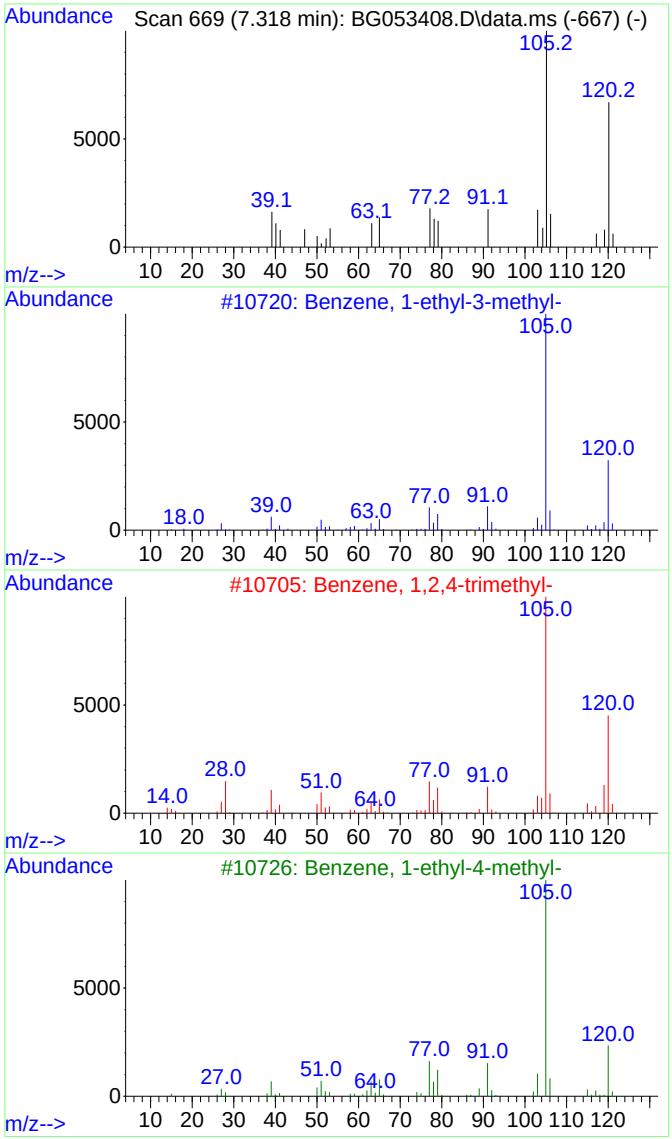
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

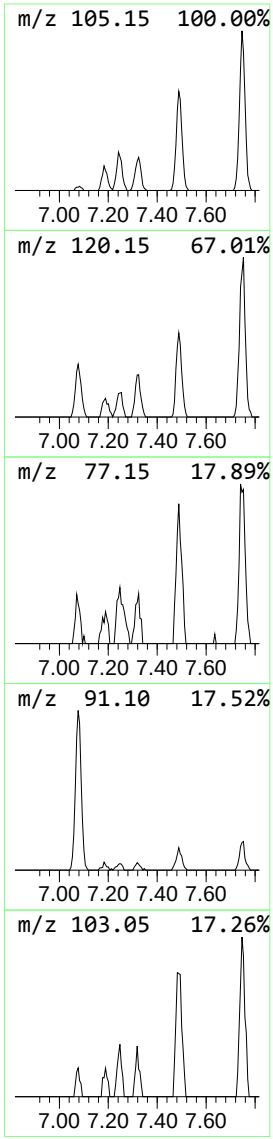
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.318	3.55 ng	28999	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	86
5	Mesitylene	120	C9H12	000108-67-8	80





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Data File : BG053408.D
Acq On : 2 May 2022 20:52
Operator : CG/JU
Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

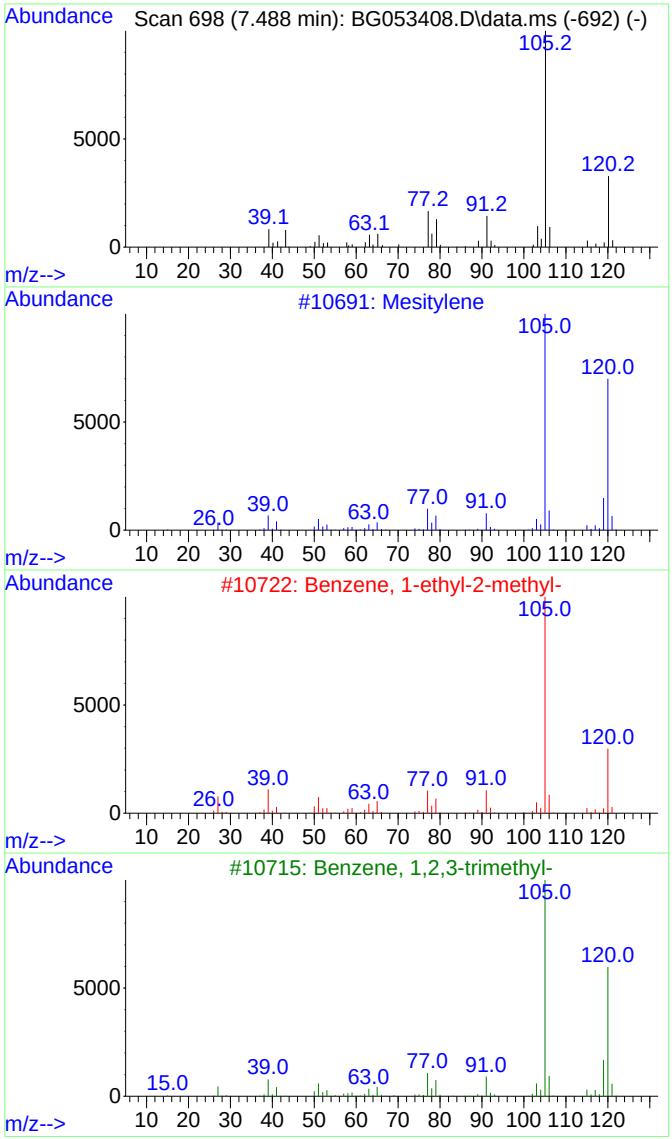
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

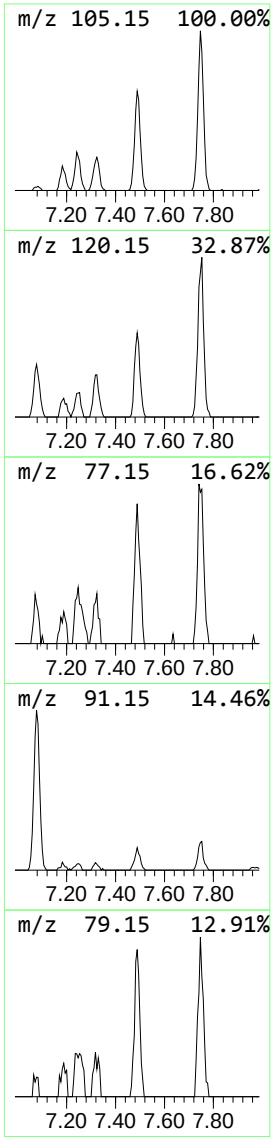
****

Peak Number 6 Mesitylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.488	9.62 ng	78637	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	91
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	2,4-Nonadiyne	120	C9H12	063621-15-8	90





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Operator : CG/JU
Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

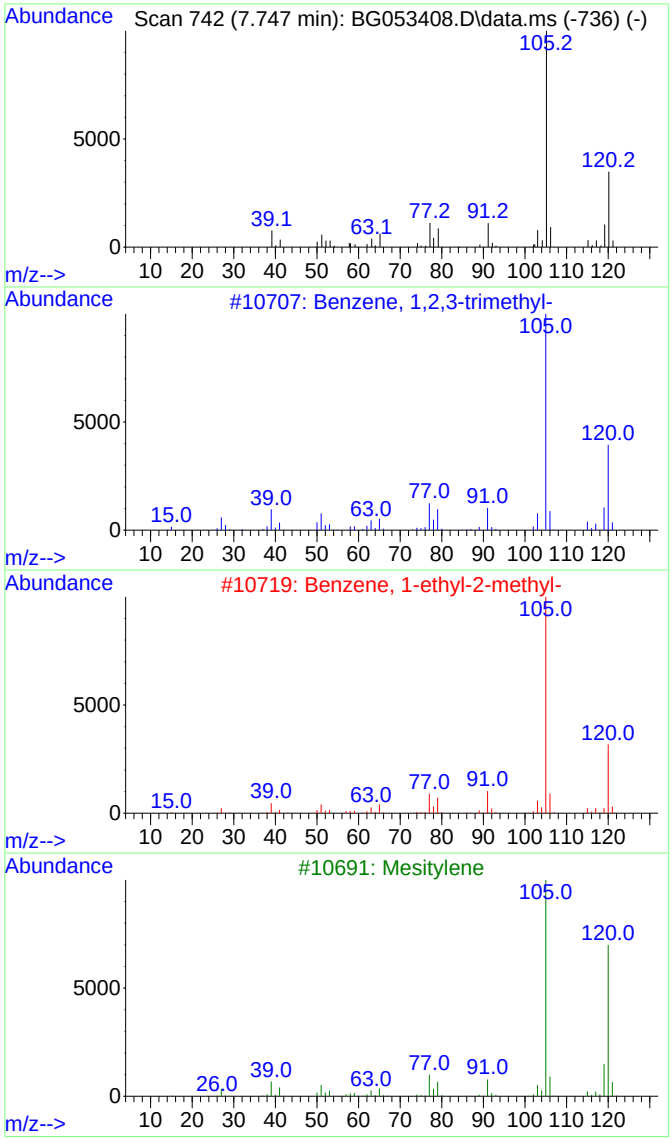
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

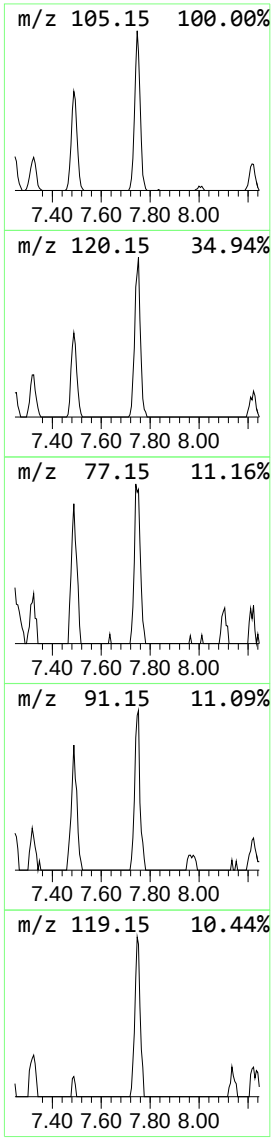
****

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.747	14.51 ng	118605	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : BG053408.D
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Sample : N2619-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

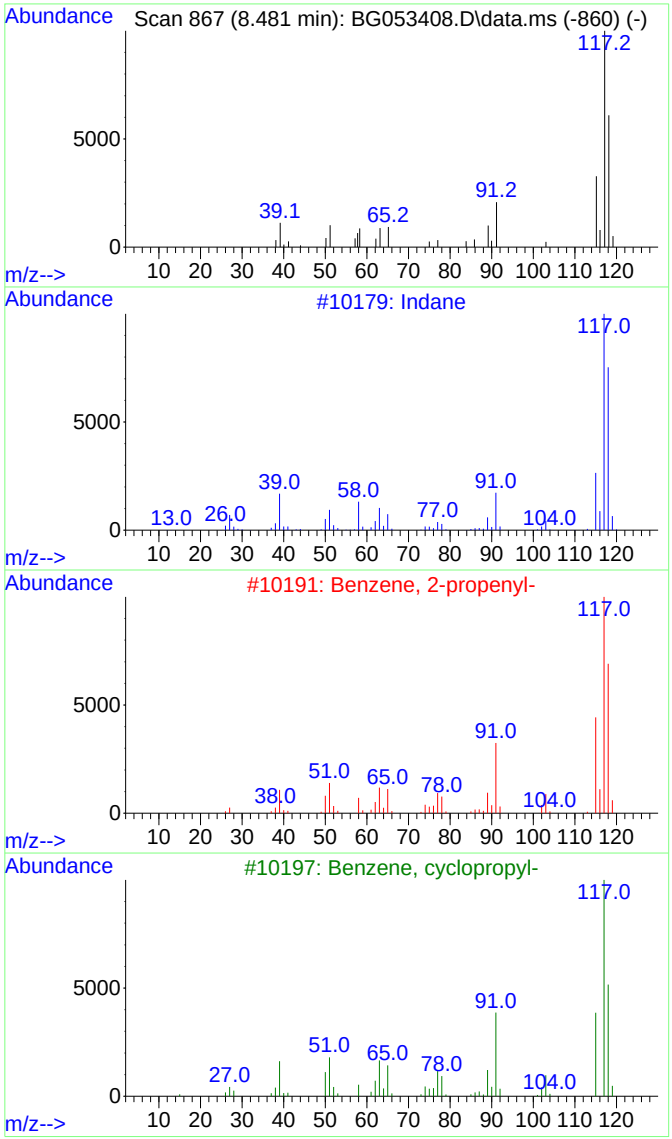
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

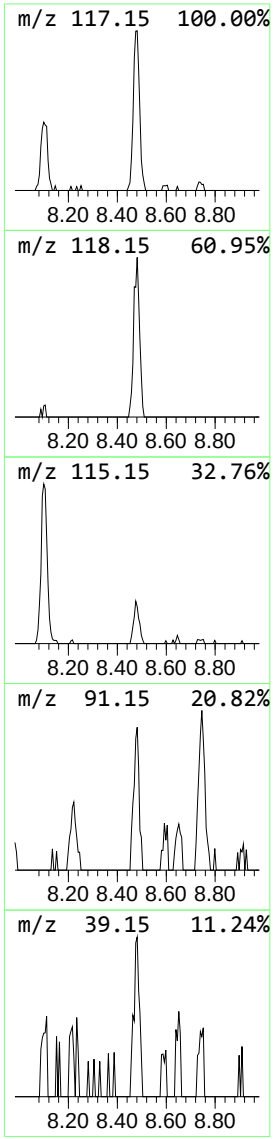
****

Peak Number 8 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	4.22 ng	34480	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64





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ALS Vial : 17 Sample Multiplier: 1

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BNA_G
ClientSampleId :
SS04-1.5-2.5-FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

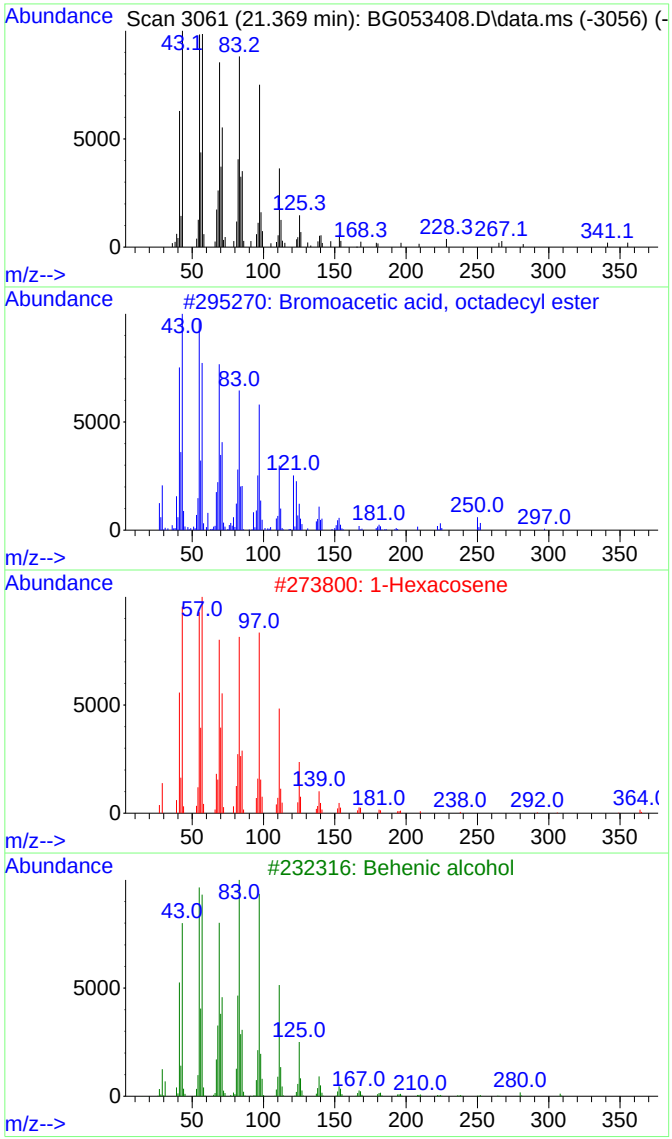
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

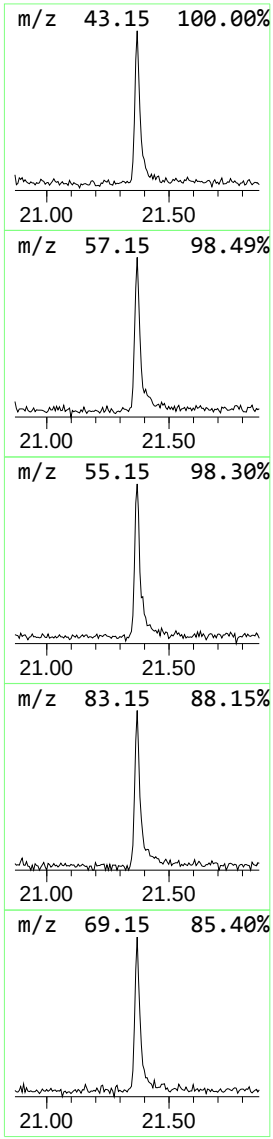
****

Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	6.01 ng	161311	Chrysene-d12	21.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.191	11.3	ng	92107	1	8.105	163507	20.0
Benzene, propyl-	7.077	7.1	ng	58239	1	8.105	163507	20.0
Benzene, 1-ethy...	7.318	3.5	ng	28999	1	8.105	163507	20.0
Mesitylene	7.488	9.6	ng	78637	1	8.105	163507	20.0
Benzene, 1,2,3-...	7.747	14.5	ng	118605	1	8.105	163507	20.0
Indane	8.481	4.2	ng	34480	1	8.105	163507	20.0
Bromoacetic aci...	21.369	6.0	ng	161311	5	21.751	536577	20.0