

Knowledge Discovery Database: Selection & Sampling

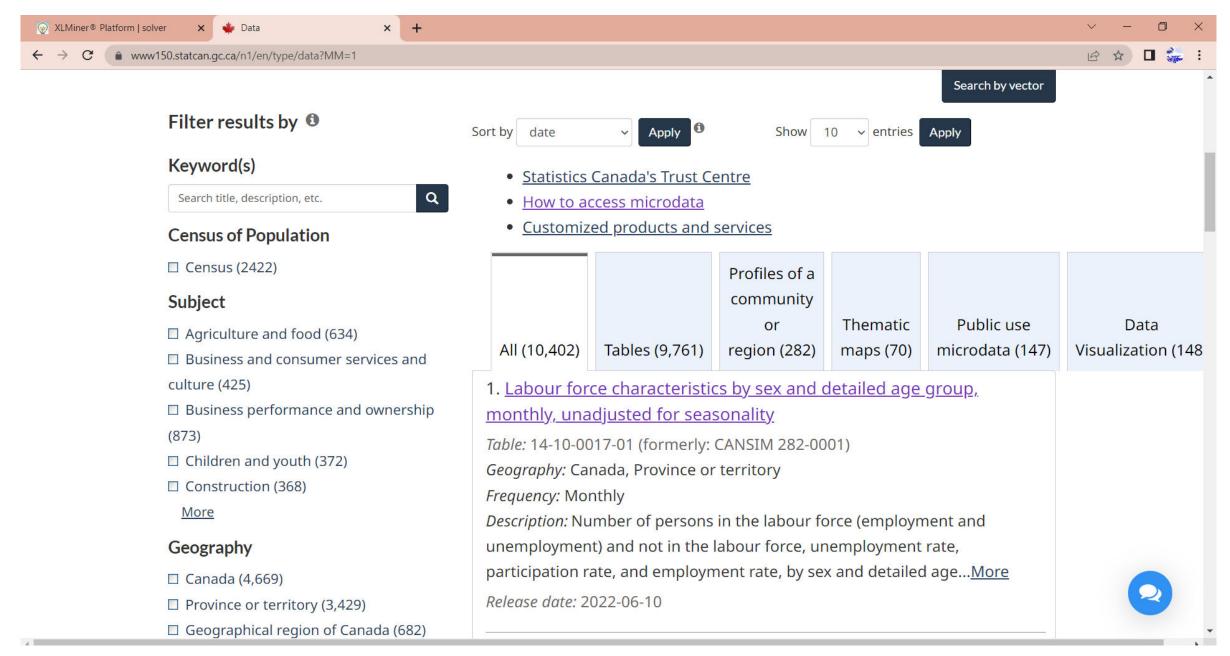
MBI304- Data Mining & Data Analytics

Mamta Sagar

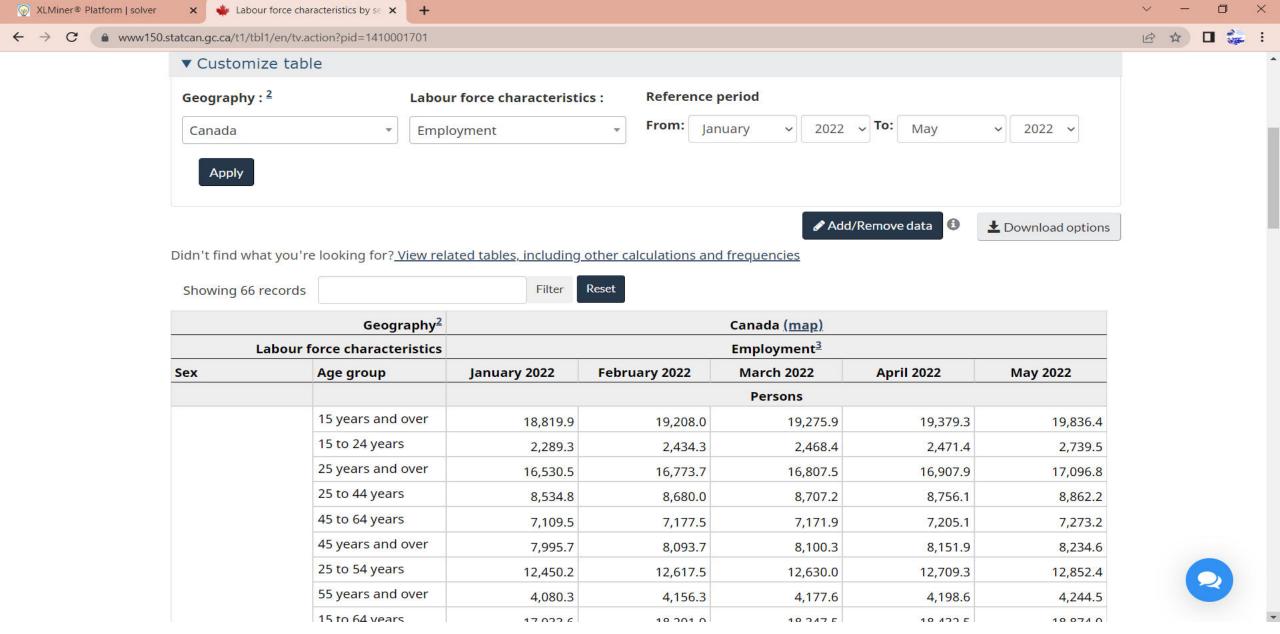
Department of Bioinformatics

University Institute of Engineering & Technology, CSJM University, Kanpur

https://www150.statcan.gc.ca/n1/en/type/data?MM=1



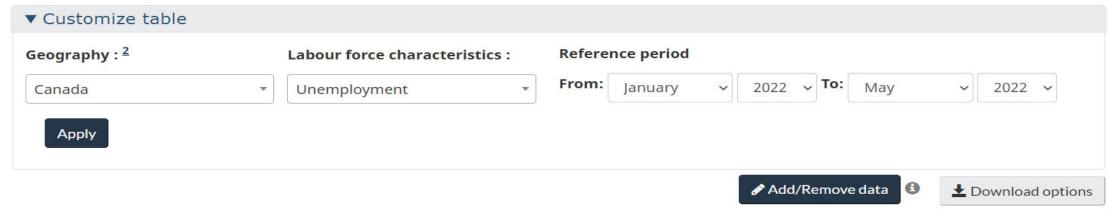
Labour force characteristics by sex and detailed age group, monthly, unadjusted for seasonality (x 1,000)1



Unemployment Data of Canada from Jan2022 to May 2022



Geography: Canada, Province or territory

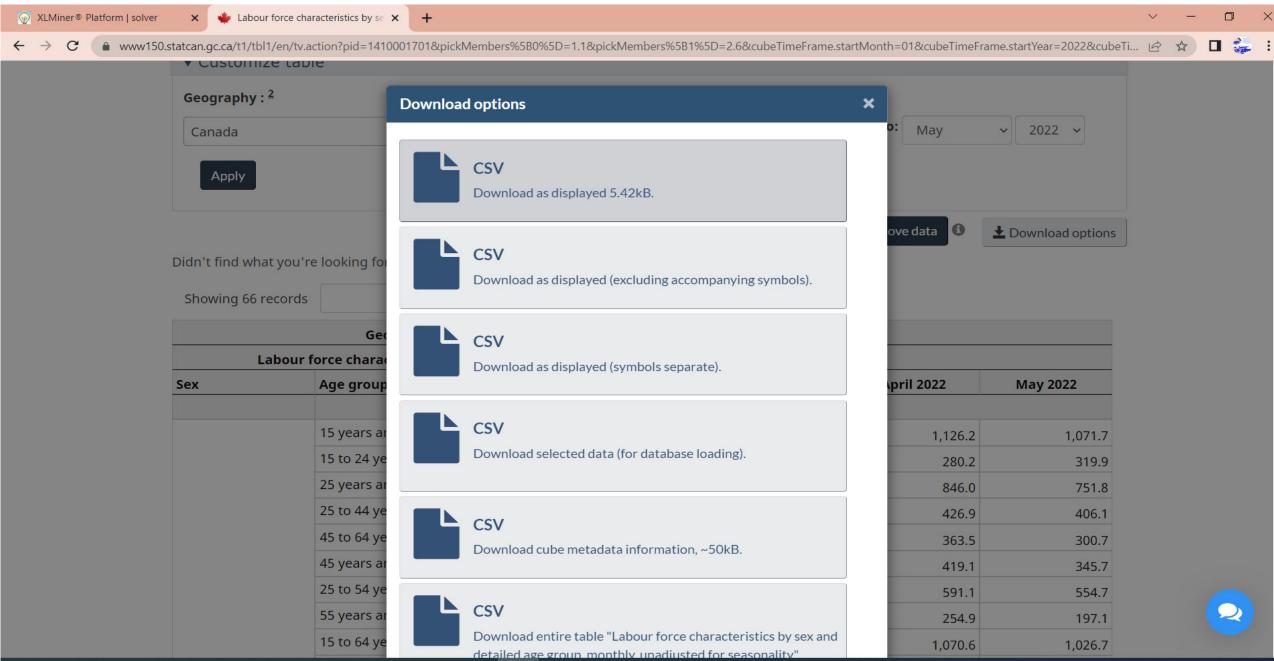


Didn't find what you're looking for? View related tables, including other calculations and frequencies

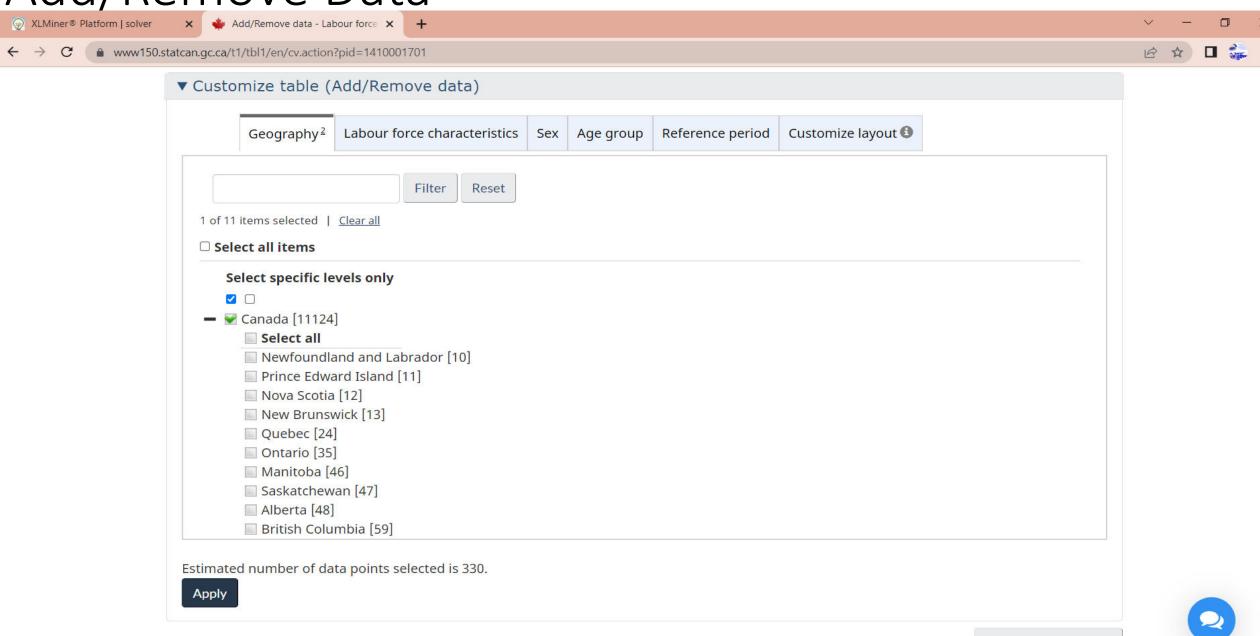
Showing 66 records Filter Reset

	Canada <u>(map)</u>						
Labour force characteristics		Unemployment ³					
Age group	January 2022	February 2022	March 2022	April 2022	May 2022		
			Persons				
15 years and over	1,369.4	1,160.4	1,171.7	1,126.2	1,071.7		
15 to 24 years	363.0	294.5	277.8	280.2	319.9		
25 years and over	1,006.4	865.9	893.9	846.0	751.8		
25 to 44 years	531.2	450.8	458.7	426.9	406.1		
45 to 64 years	409.3	354.8	373.9	363.5	300.7		
45 years and over	475.2	415.1	435.2	419.1	345.7		
	15 to 24 years 25 years and over 25 to 44 years 45 to 64 years	15 to 24 years 363.0 25 years and over 1,006.4 25 to 44 years 531.2 45 to 64 years 409.3	15 to 24 years 363.0 294.5 25 years and over 1,006.4 865.9 25 to 44 years 531.2 450.8 45 to 64 years 409.3 354.8	15 years and over 1,369.4 1,160.4 1,171.7 15 to 24 years 363.0 294.5 277.8 25 years and over 1,006.4 865.9 893.9 25 to 44 years 531.2 450.8 458.7 45 to 64 years 409.3 354.8 373.9	15 years and over 1,369.4 1,160.4 1,171.7 1,126.2 15 to 24 years 363.0 294.5 277.8 280.2 25 years and over 1,006.4 865.9 893.9 846.0 25 to 44 years 531.2 450.8 458.7 426.9 45 to 64 years 409.3 354.8 373.9 363.5		

Downloading data as displayed

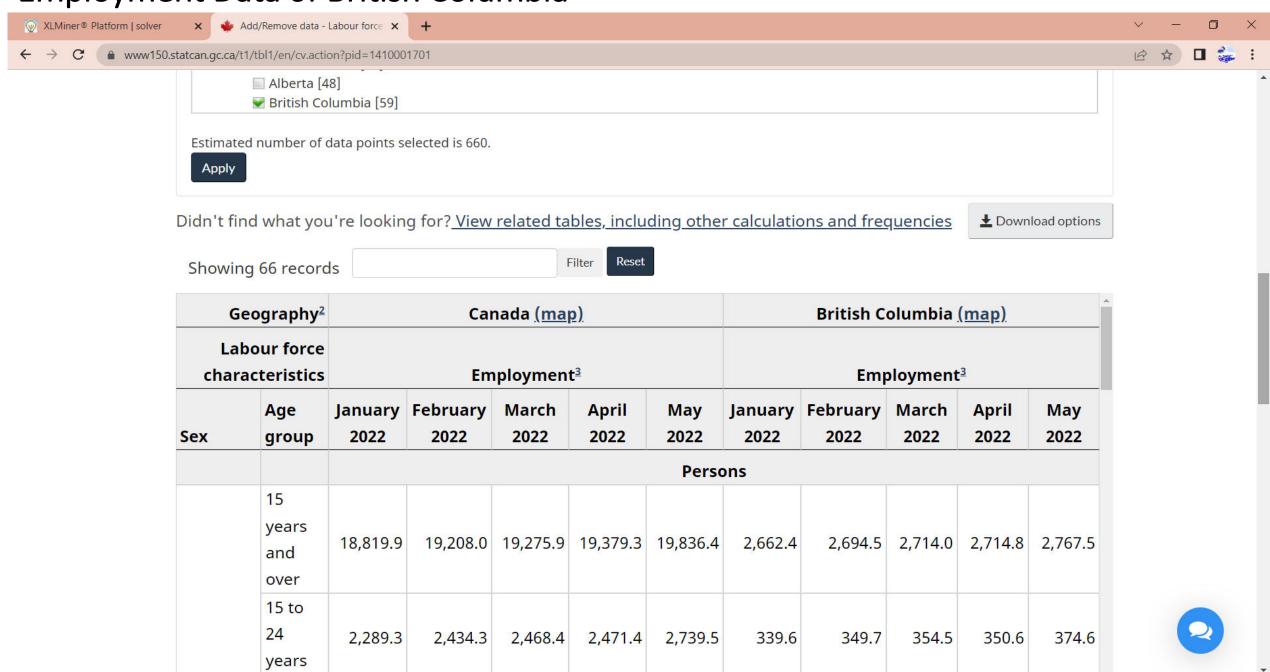


Add/Remove Data

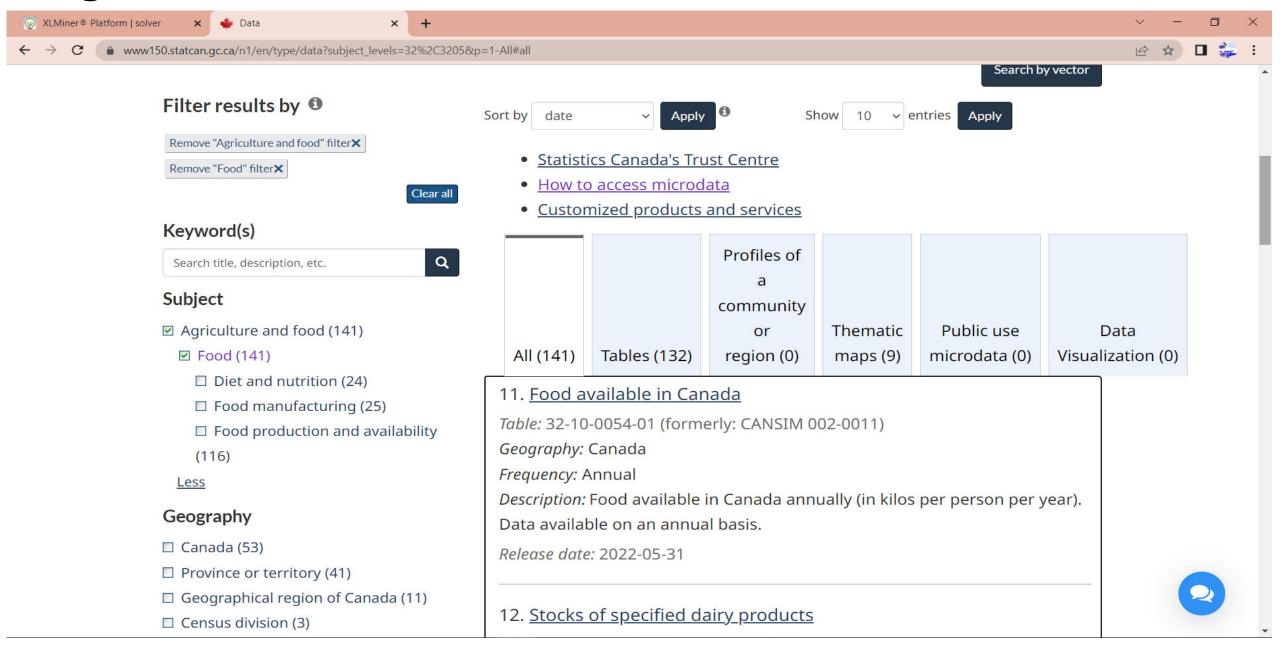


Didn't find what you're looking for? <u>View related tables, including other calculations and frequencies</u> **★** Do

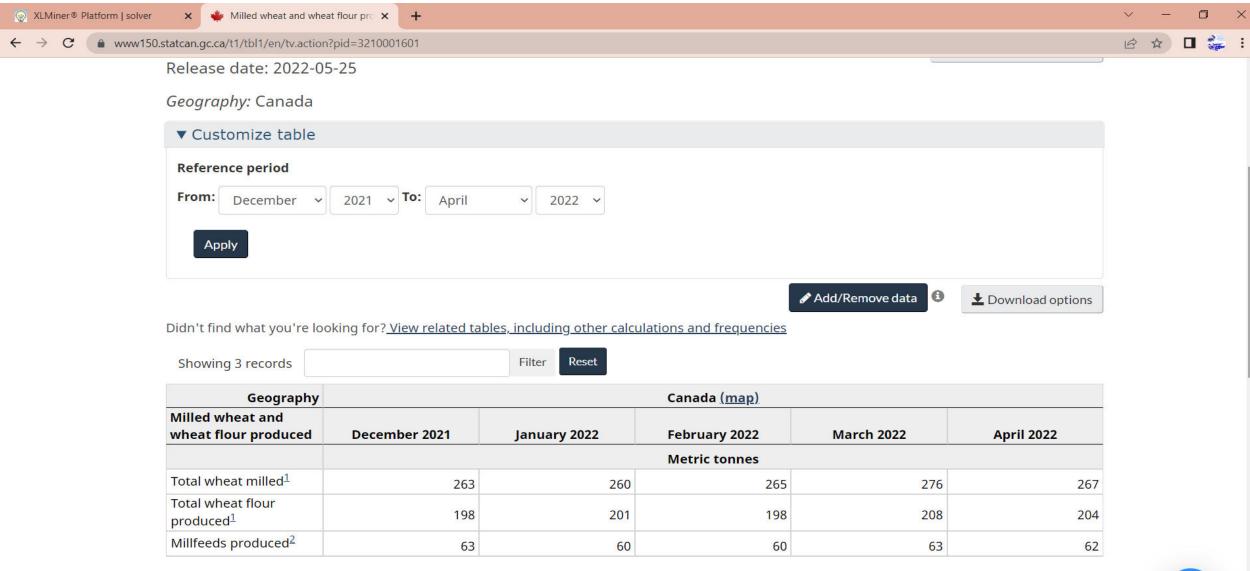
Employment Data Of British Columbia



Agriculture & Food Data

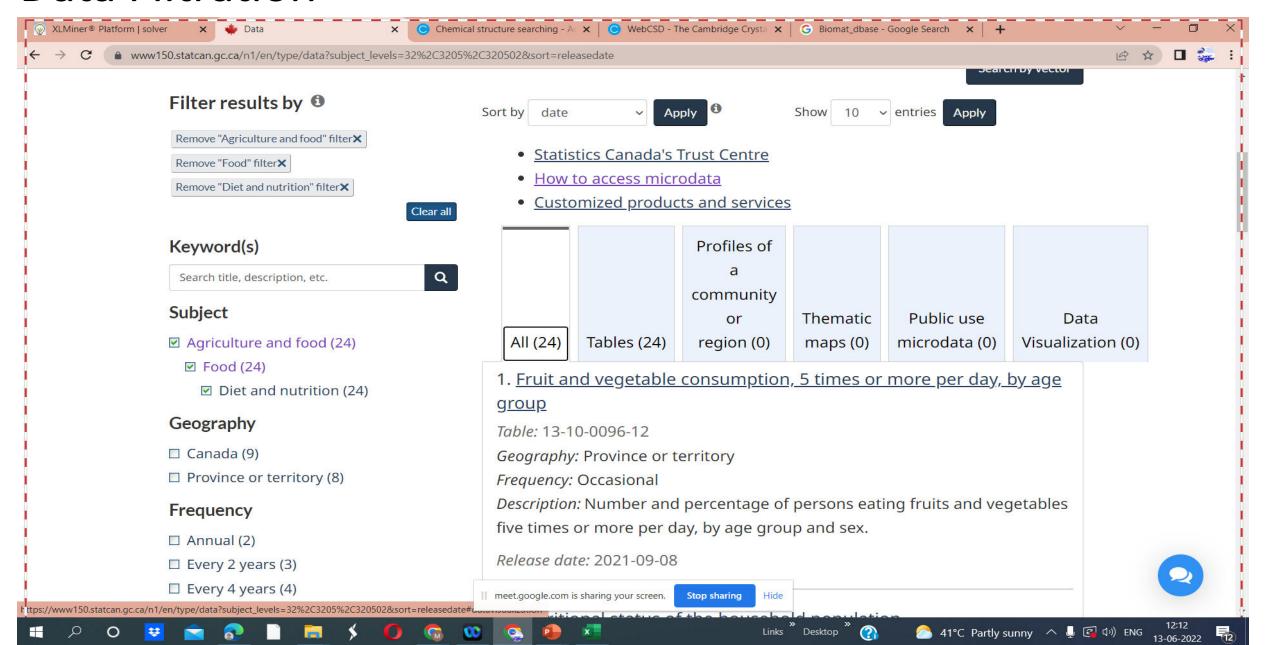


Milled wheat and wheat flour produced (x 1,000)

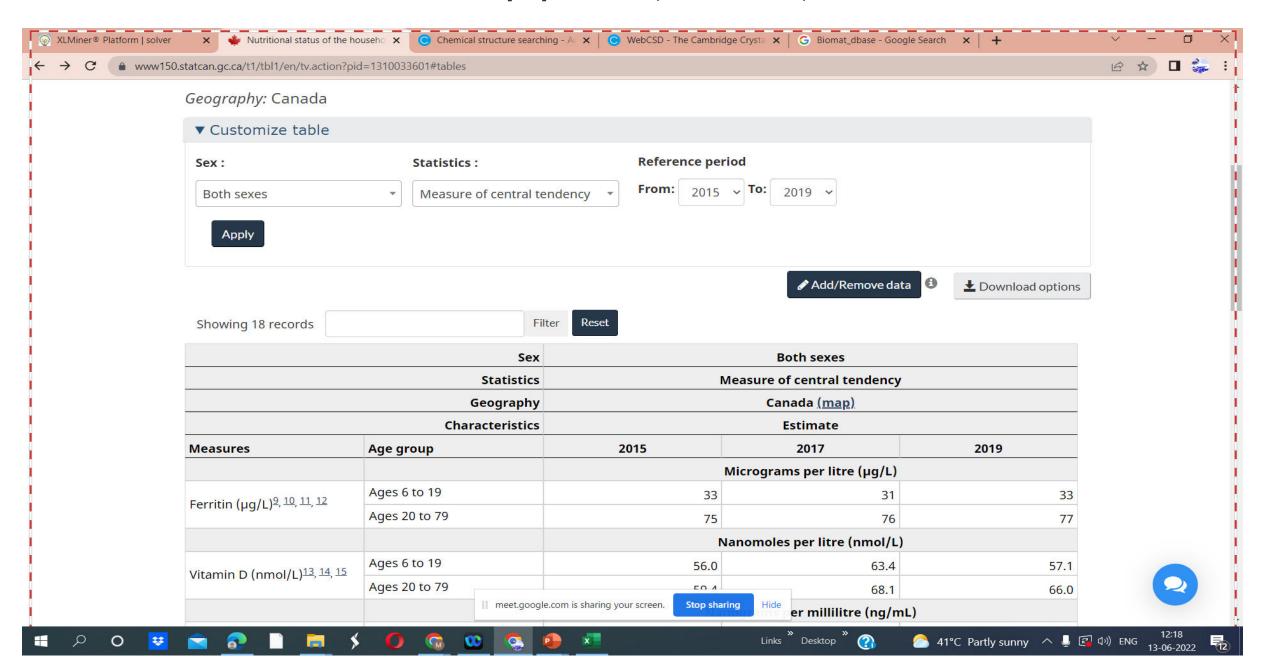




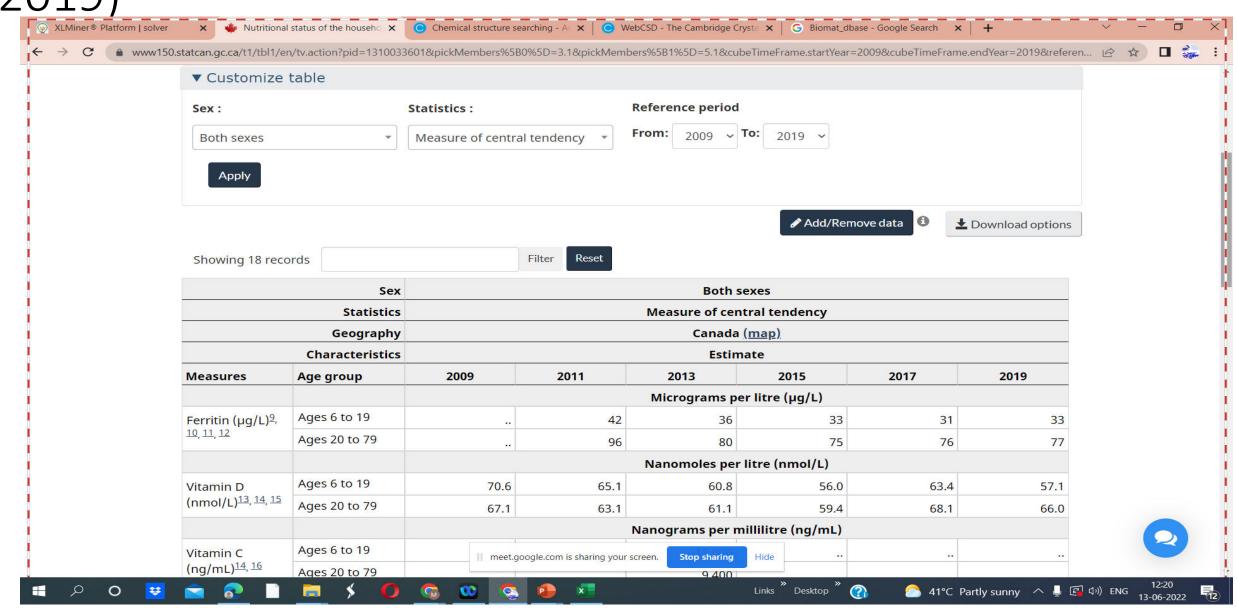
Data Filtration



Nutritional status of the household population (2015-2019)



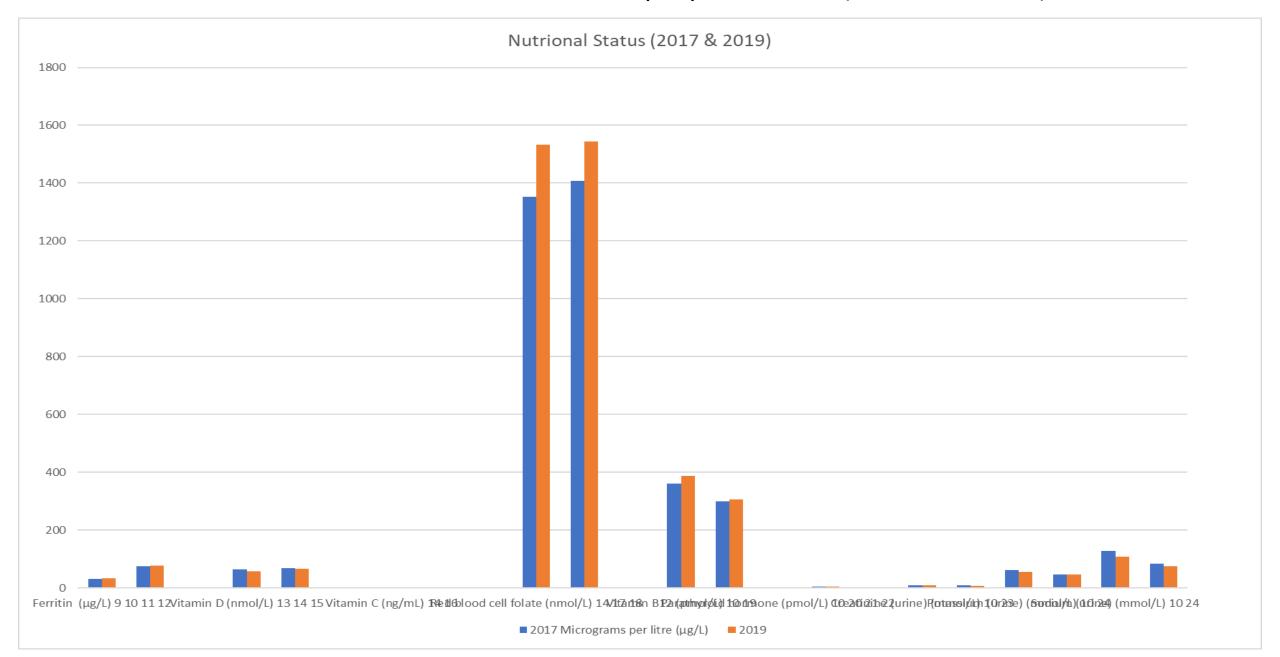
Nutritional status of the household population (2009-2019)



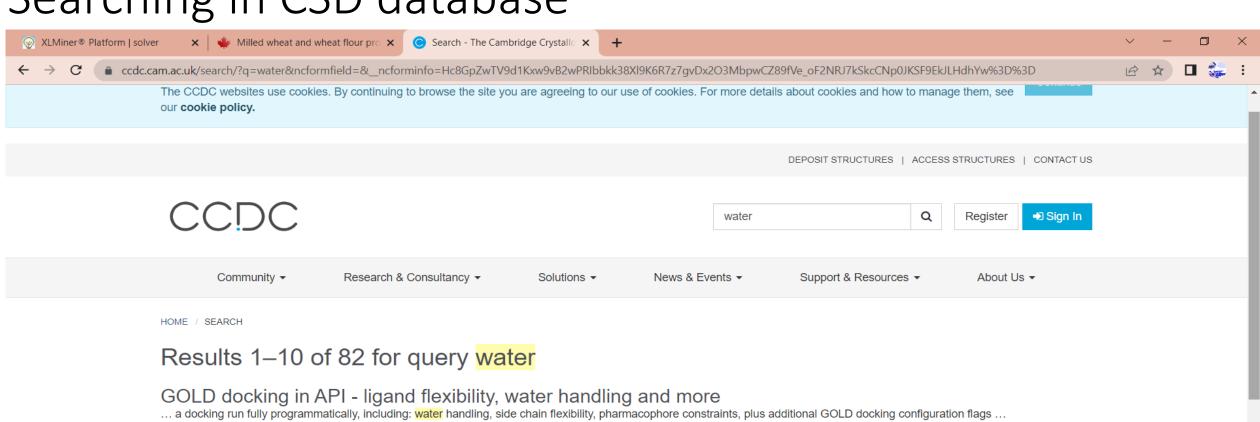
Nutrition status (in different age group)

Measures	33601&pickMembers%5B0%5D=3.1&pickMembers Age group	2017	2019	
		Micrograms per litre (μg/L)		
Ferritin (µg/L) ^{9, 10, 11, 12}	Ages 6 to 19	31	33	
	Ages 20 to 79	76	77	
		Nanomoles per litre (nmol/L)		
Vitamin D (nmol/L) ¹³ , ¹⁴ , ¹⁵	Ages 6 to 19	63.4	57.1	
	Ages 20 to 79	68.1	66.0	
		Nanograms per millilitre (ng/mL)		
Vitamin C (ng/mL) ¹⁴ , ¹⁶	Ages 6 to 19		***	
	Ages 20 to 79			
		Nanomoles per litre (nmol/L)		
Red blood cell folate (nmol/L) ¹⁴ , ¹⁷ ,	Ages 6 to 19	1,352	1,533	
18	Ages 20 to 79	1,407	1,543	
		Picomoles per litre		
Vitamin B12 (pmol/L) ¹⁰ , ¹⁹	Ages 6 to 19	360	387	
	Ages 20 to 79	299	306	
Parathyroid hormone (pmol/L) ¹⁰ , ²⁰ , ²¹ , ²²	2, Ages 6 to 19	3.5	3.4	
	Ages 20 to 79	4.1	4.1	
		Millimoles per litre		
Creatinine (urine) (mmol/L) ¹⁰ , ²³	Ages 6 to 19	9.9	9.2	
	Ages 20 to 79	8.5	7.9	
Potassium (urine) (mmol/L) ¹⁰ , ²⁴	Ages 6 to 19	61	56	

Nutritional status of the household population (2017-2019)



Searching in CSD database



... a docking run fully programmatically, including: water handling, side chain flexibility, pharmacophore constraints, plus additional GOLD docking configuration flags ...

Blogs http://www.ccdc.cam.ac.uk/Community/blog/gold-docking-python-api/

RE: how to change HbondCoordination settings?

... Water H-bond coordination type, molecular to the Na + and the water molecule closest to the center of mass for each configuration. firstcallonline ...

Forums http://www.ccdc.cam.ac.uk/forum/csd_python_api/Crystallography/d7d8136e-9fbf-e911-bdb3-005056975d8a#2161497a-85ca-eb11-9690-00505695c114

Other than the library size, are there any other major factors that influence the docking time?

... chains or explicit water molecules will take longer) the number of GA runs per ligand whether or not "allow early termination" is switched on the chosen GA ...

Help Desk http://www.ccdc.cam.ac.uk/support-and-resources/support/case/?caseid=71b82a1e-b4b3-4a5c-b5e2-c9c5110ee13f

Why is it not possible to return the crystallographic binding pose of the ligand?

... being docked. Water mediated hydrogen bonding is important and all the waters have been removed during protein preparation. If so, identify and extract important ...

Help Desk http://www.ccdc.cam.ac.uk/support-and-resources/support/case/?caseid=f82e1fcd-c968-45cd-b59e-e14db1385cb2

Can GOLD handle metals?

GOLD docking in API - ligand flexibility, water handling and more

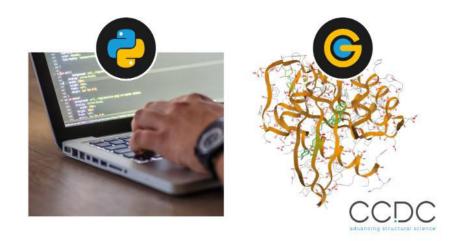


Ilenia Giangreco - July 15, 2021

More advanced settings are now available when docking with GOLD programmatically through the API. Here's what has changed in the 2021.1 release.

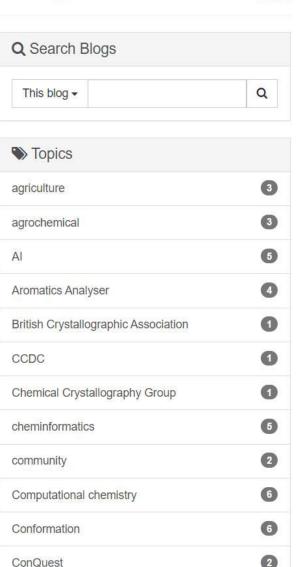
Docking with GOLD - genetically optimised ligand docking - is well validated and trusted across academia and industry. The ability to perform docking programmatically through the API further opens this functionality for computational chemists to use GOLD docking in workflows. Previously some advanced features in GOLD were only accessible in the graphical user interface Hermes, but in this release they are now accessible in the API.

You can now configure a docking run fully programmatically, including: water handling, side chain flexibility, pharmacophore constraints, plus additional GOLD docking configuration flags.



Which parameters can be controlled in the GOLD API?

It is now possible to specify water molecules that are important to ligand binding.



References

- https://www150.statcan.gc.ca/n1/en/type/data?MM=1
- CSD database
- https://www.ccdc.cam.ac.uk/solutions/csdcore/components/webcsd/