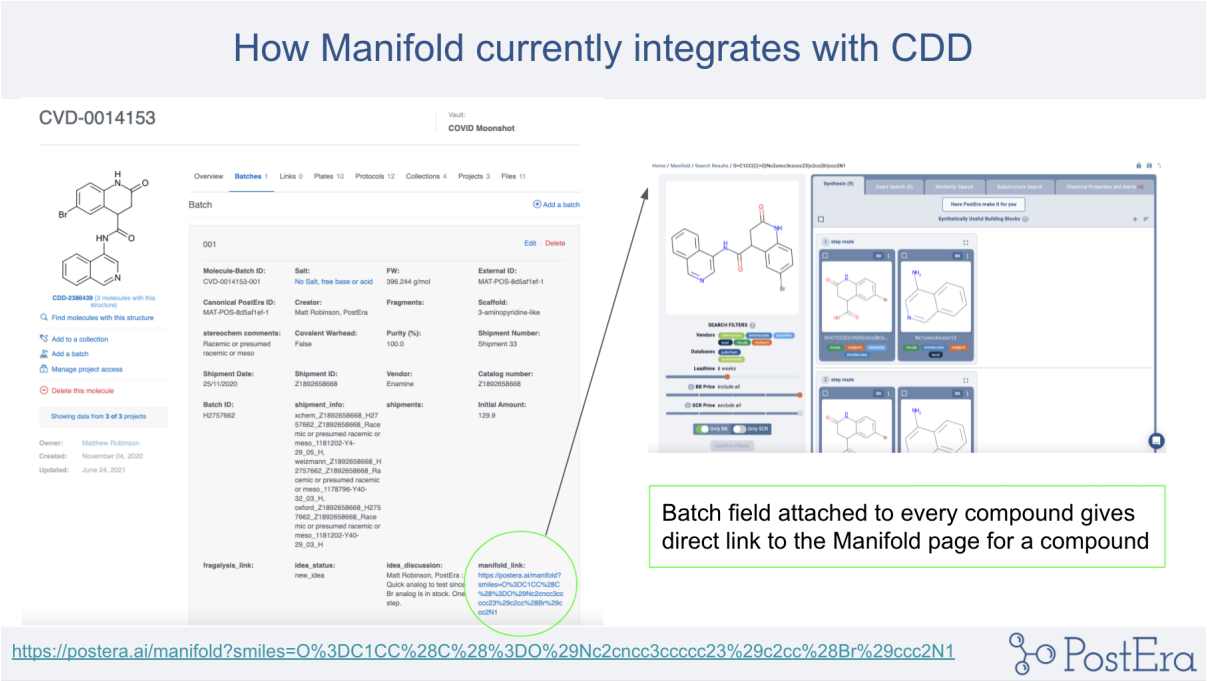
Manifold + CDD integration

PostEra's Manifold, built for synthesis and search across the world's vast collection of purchasable molecules, was originally designed for the COVID Moonshot project, which also utilized CDD Vault to store drug discovery data. Thus, interoperability between Manifold and CDD was an early priority, allowing for streamlined storage and analysis of designs and results.

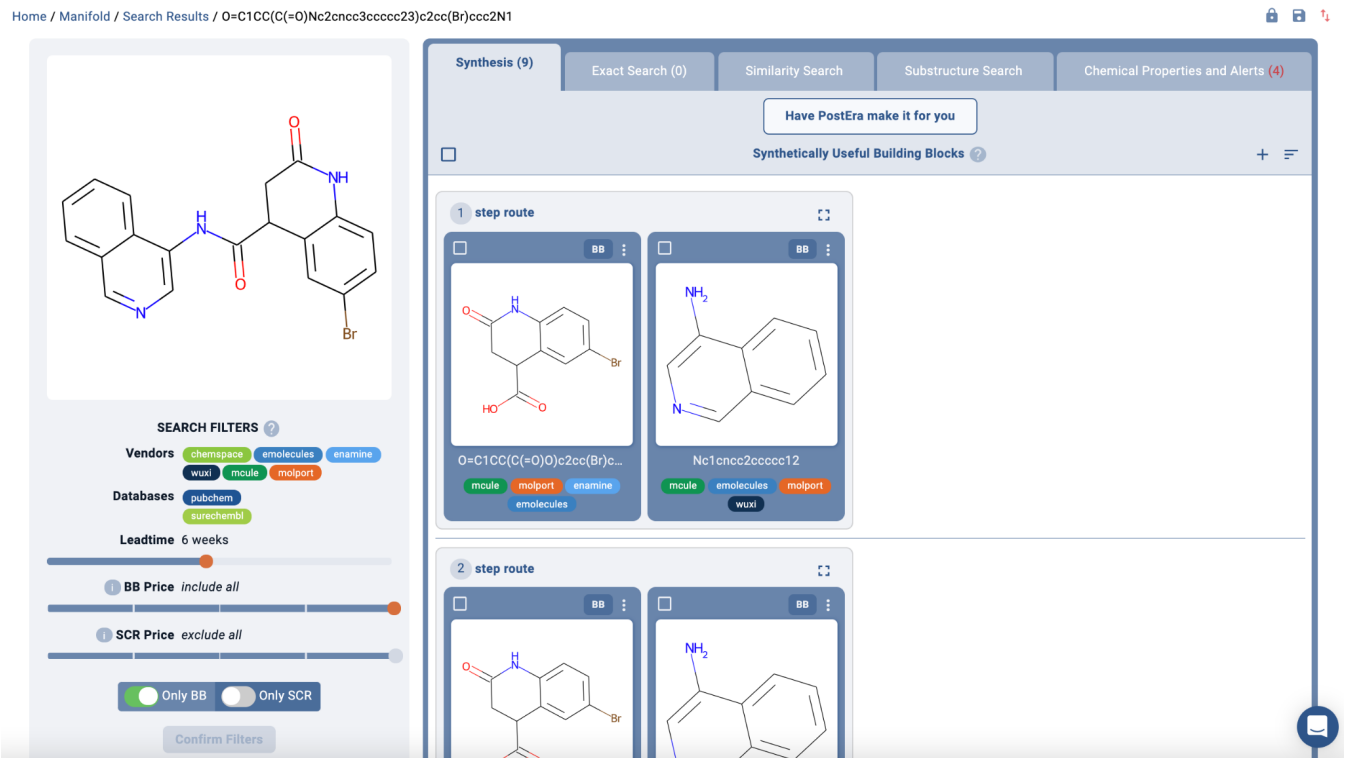
Integrating using a CDD batch field with direct Manifold link

One easy way to integrate with CDD is to create a CDD batch field that gives a direct link to a Manifold page for every compound. For example, in the image below, you can see that the batch field is constructed as `postera.ai/manifold?smiles=<url_encoded_SMILES>` to give a valid direct link such as https://postera.ai/manifold?smiles=O%3DC1CC%28C%28%3DO%29Nc2cncc3ccccc23%29c2cc%28Br%29ccc2N1, which will take you directly to a Manifold page for the molecule.

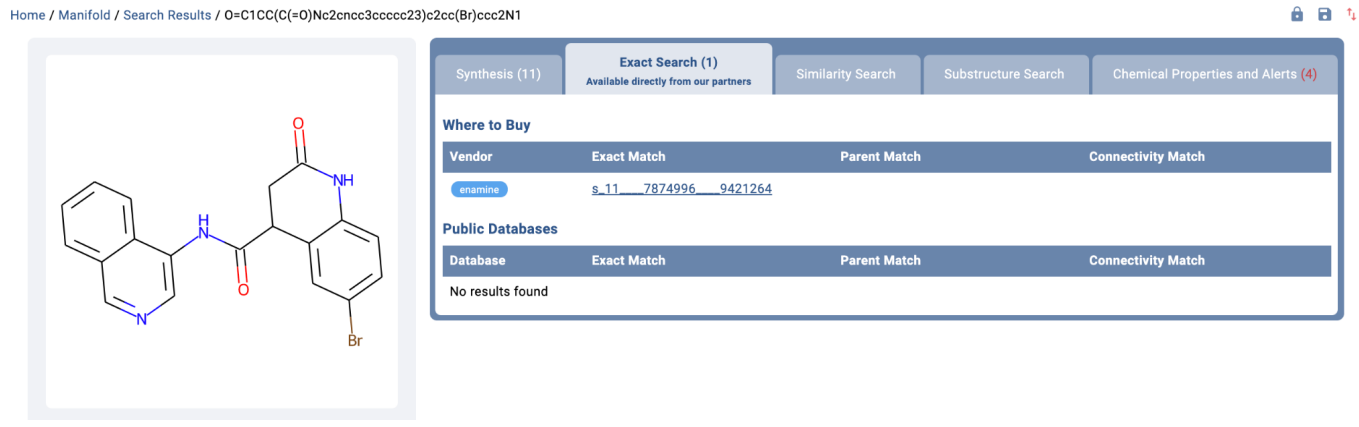


Once in Manifold, information can be gathered regarding retrosynthetic routes, useful in-stock building blocks, purchasing information, and even information such as medicinal chemistry alerts.

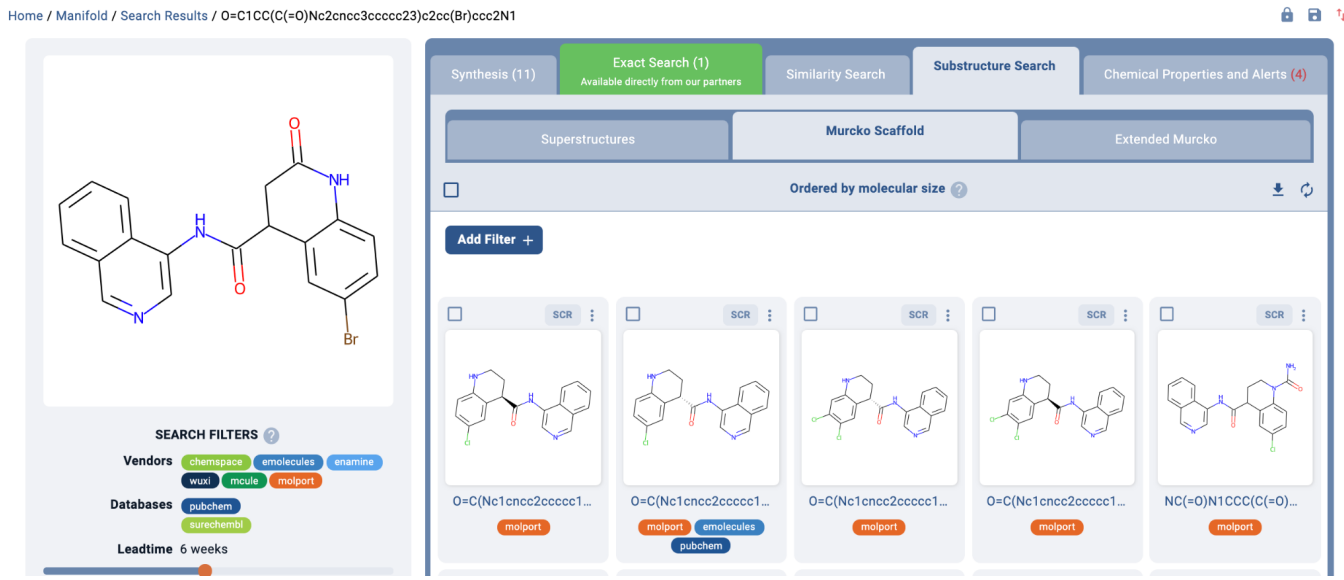
Information regarding synthetic routes and useful building blocks can be seen in the "Synthesis" tab:



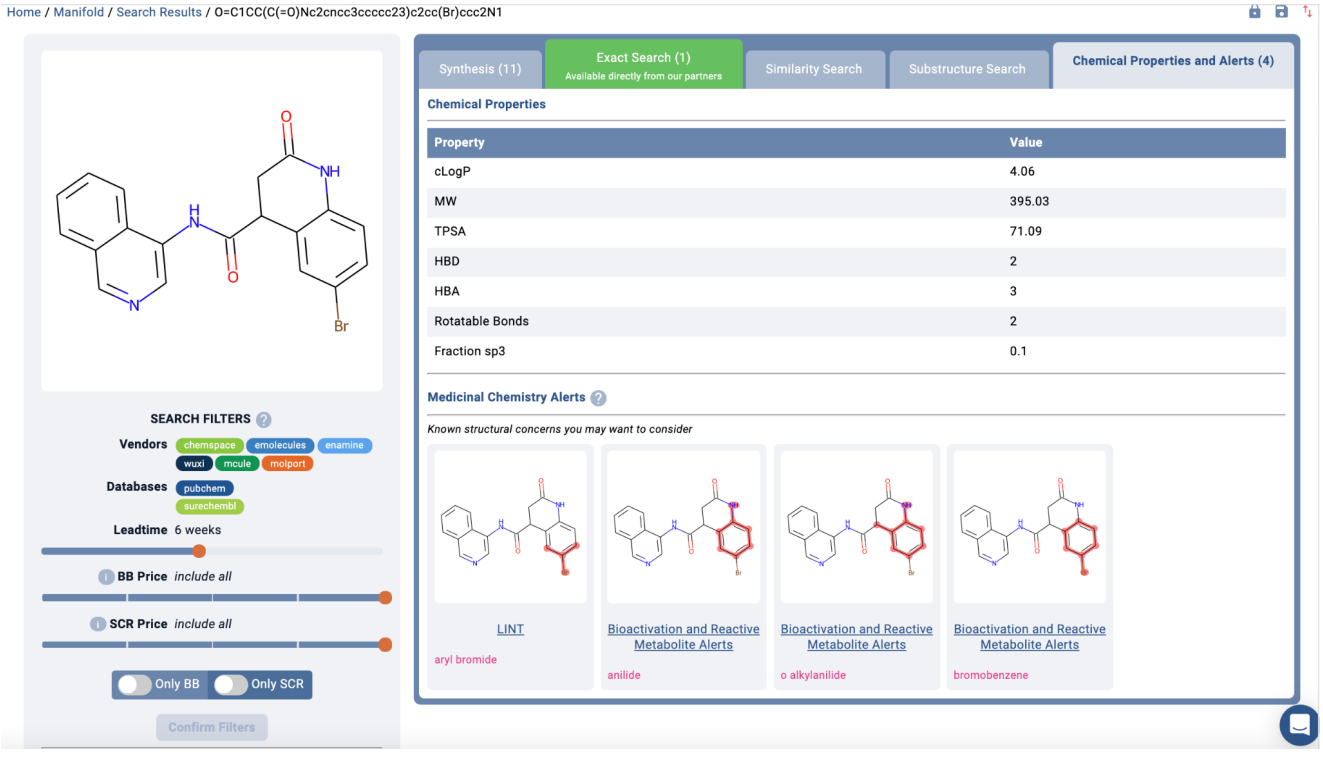
Information regarding of the vendor availability of the compound can be found in the "Exact Search" tab:



Information regarding vendor availability of similar analogs to the searched molecule are available in the "Similarity Search" and "Substructure Search" tab:

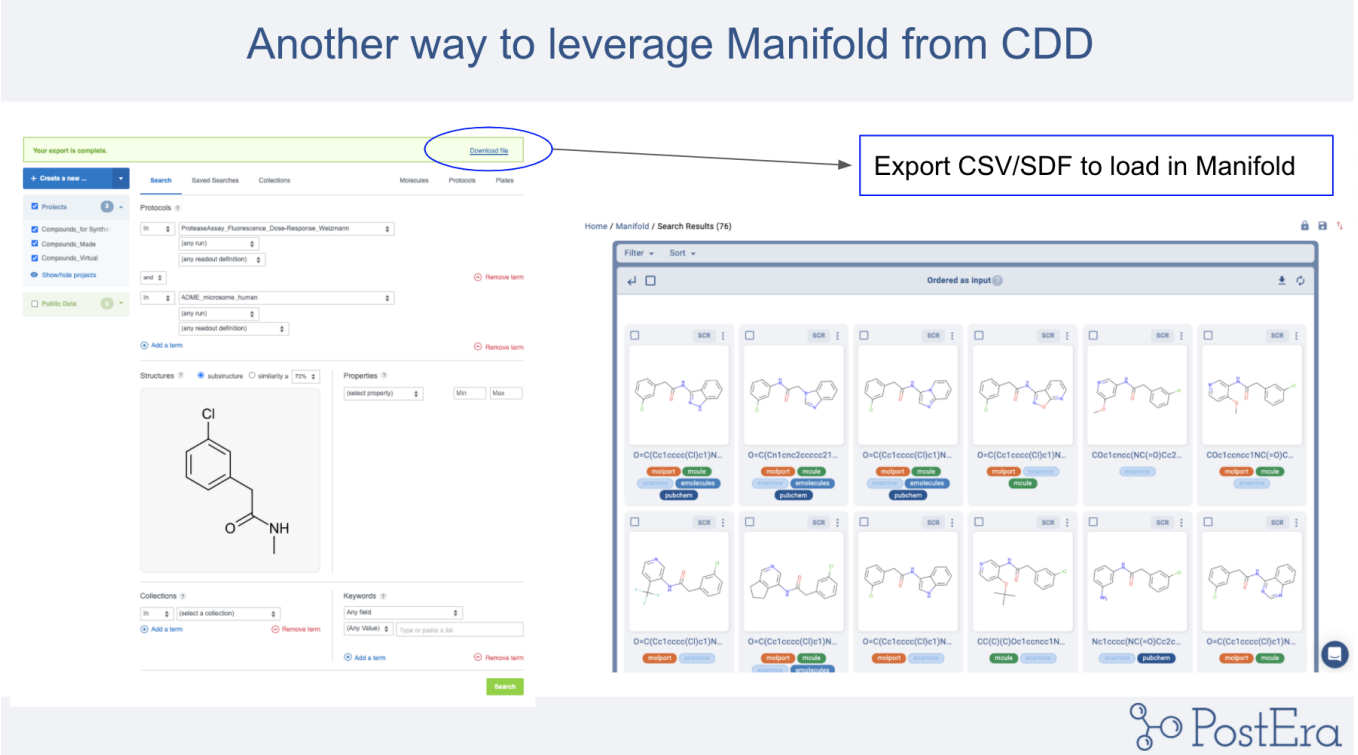


Information regarding additional information such as "Medicinal Chemistry alerts" are available in the "Chemical Properties and Alerts" tab:

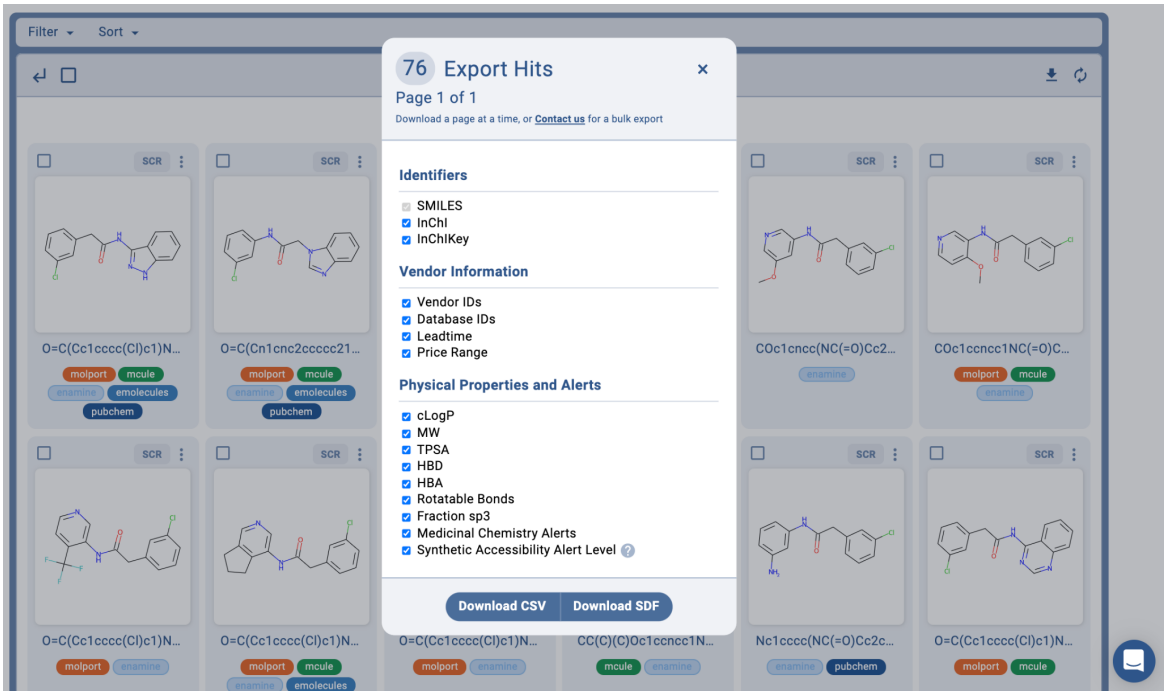


Another way of integrating with CDD

Additionally, one can always export a CDD search and enter that list of molecules in Manifold for further evaluation of synthetic feasibility and vendor availability.

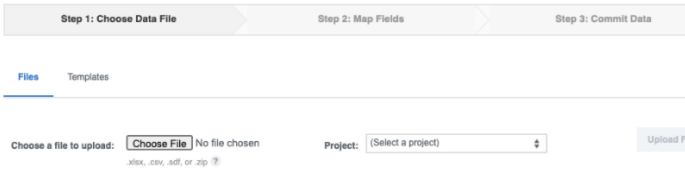


After searching a list of molecules, one can bulk export vendor availability information such as in the image below. This information can then be uploaded to CDD as either protocol information or a batch field.



smiles	pubchem	molport	enamine	mcule	emolecules	surechembl
O=C(Nc1cncc2cccc12)N1CCOc2ccc(Cl)cc21		MolPort-047-837-815				
O=C1CC(Oc2cc(Cl)cc(N(CCC3CCCCC3)C(=O)Nc3cncc4ccccc34)c2)N1						
Cc1ccncc1NC(=O)N(CCC1CCCCC1)c1cc(Cl)cc(OC(C)C)c1		MolPort-047-629-829		MCULE-4530766567	324552998	
O=C(Nc1cncc2cccc12)N(CCC1CCCCC1)c1cccc(Cl)c1						
Cc1ccncc1N1CCN(c2cccc(Cl)c2)C1=O	49872153	MolPort-047-567-650		MCULE-6378015700	324258779	SCHEMBL3782127
Cc1ccncc1NC(=O)N(C)c1cccc(Cl)c1	154875987	MolPort-047-567-644		MCULE-2476040110	324256220	
Cc1ccncc1NC(=O)N(Cc1ccccc1)c1ccc(Cl)c1	154875998	MolPort-047-567-656		MCULE-9980739925	324256476	
N#Cc1cc(Cl)cc(NC(=O)Nc2cccnc2)c1					330938350	
Cc1ccncc1NC(=O)Nc1cccc(C#N)c1	146125035	MolPort-047-314-817	BBV-182581128	MCULE-7150128297	324196832	
Cc1ccncc1NC(=O)Nc1cccc(Cl)c1	146125036	MolPort-047-314-818		MCULE-8249205061	324197088	
O=C(Nc1cccnc1)N(CCC1CCCCC1)c1cccc(Cl)c1						
N#Cc1cccc(NC(=O)Nc2cncc(N)c2)c1	154851706	MolPort-047-479-854		MCULE-3751543471	324226514	

For example, vendor availability as shown, can be added to CDD.



All of this, including scores such as synthetic accessibility, can also be done via Manifold's API.