Which cat does this compound look like?

Group: cytohackR

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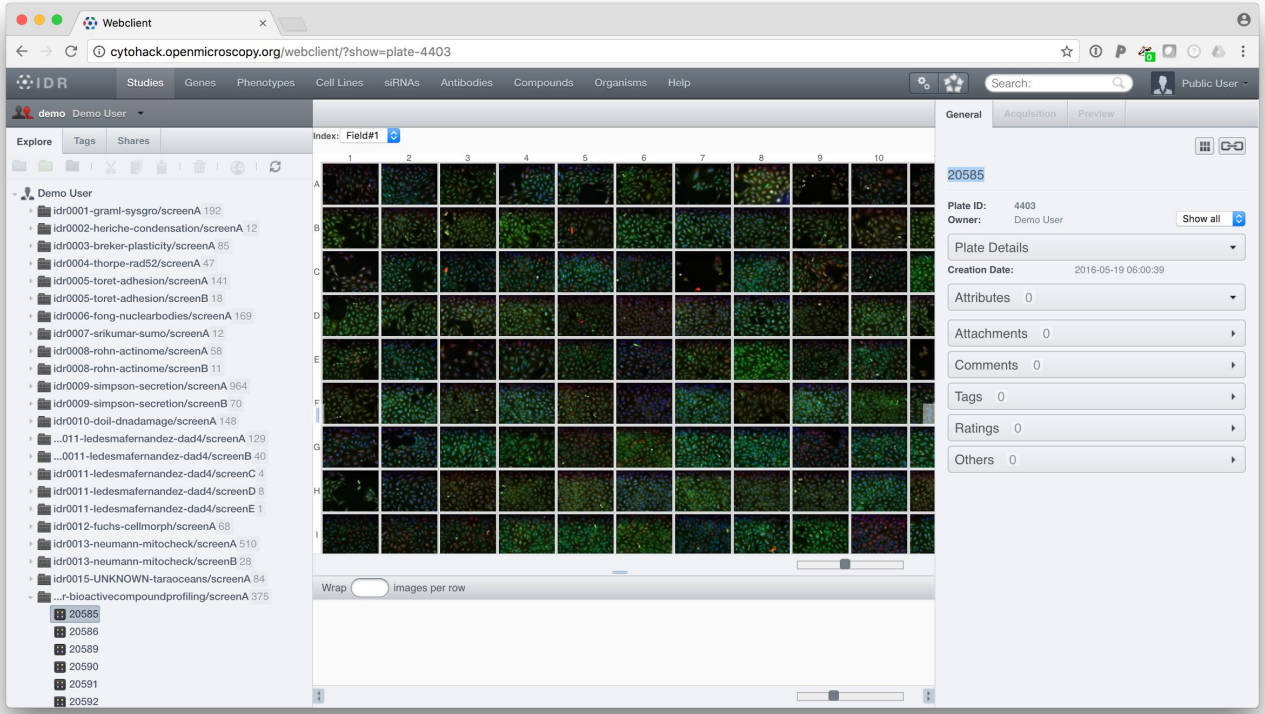
Extract images from IDR



Want images? Easy D

- Query using Python API
- Create list of files
- Use imagedata/download

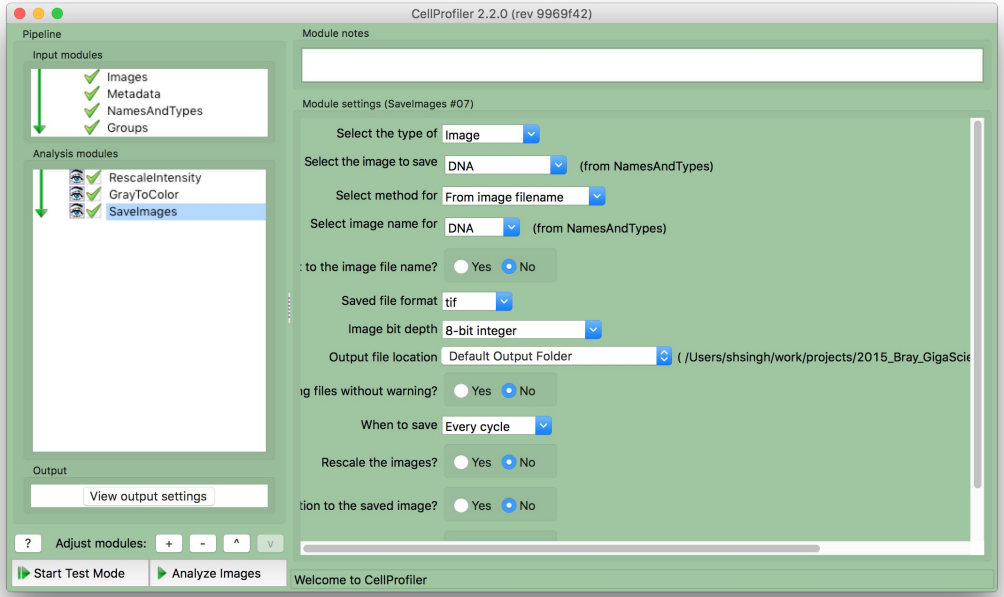
```
In [4]: omit = "uod/idr/incoming/idr0016-wawer-bioactivecompoundprofiling/"
well = "_A01_"
field = "_s1_"
for x in list_files():
    if "Hoechst" in x[0] and field in x[0]:
        print x[0][len(omit):]

Connected to IDR...
2016-01-19-screens-bbbc022/20585-Hoechst/IXMtest_A01_s1_w164FBEEF7-F77C-4892-86F5-72D0160D4FB2.tif
2016-01-19-screens-bbbc022/20585-Hoechst/IXMtest_A02_s1_w17C9F8BDB-79F0-4F8B-852B-71161631F236.tif
2016-01-19-screens-bbbc022/20585-Hoechst/IXMtest_A03_s1_w1073D64AC-9B57-43E1-A34E-1C7C986DEEFA.tif
2016-01-19-screens-bbbc022/20585-Hoechst/IXMtest_A04_s1_w195151D27-9F95-44DE-A514-2ED183E548C9.tif
```

```
while read x; do docker run --rm -v
/tmp/cytohackR:/data imagedata/download idr0016 $x
/data/; done < ~/Desktop/DNA.txt
```

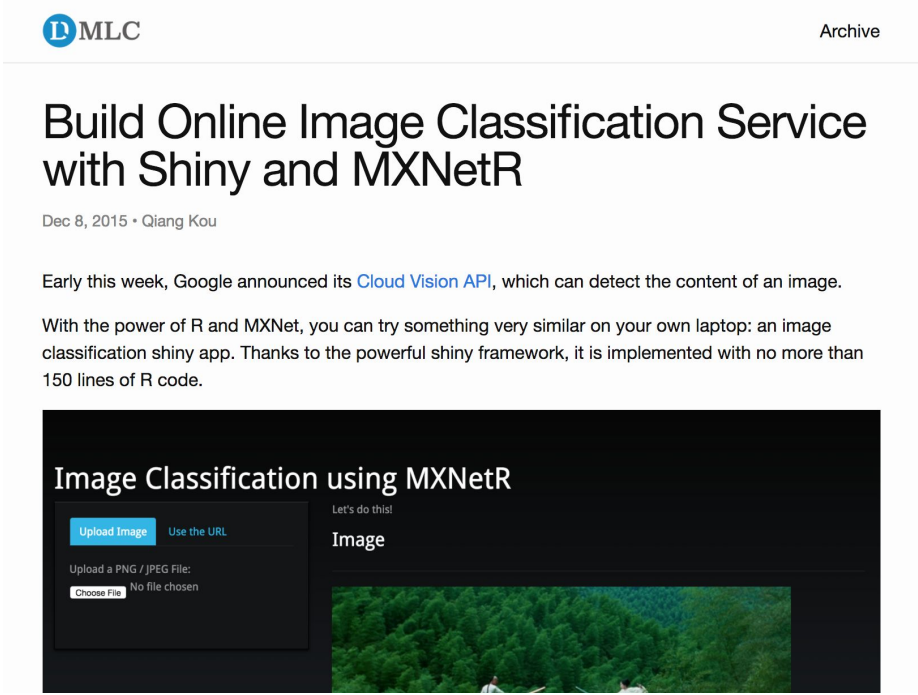
CellProfiler to convert images

- Read in all images
- Rescale to max intensity
- Make pseudo RGB



Extract features

- Use pre-trained Inception-BN network
- Use input to fully connected layer as features



Get metadata

- Fetched mechanism by querying IDR

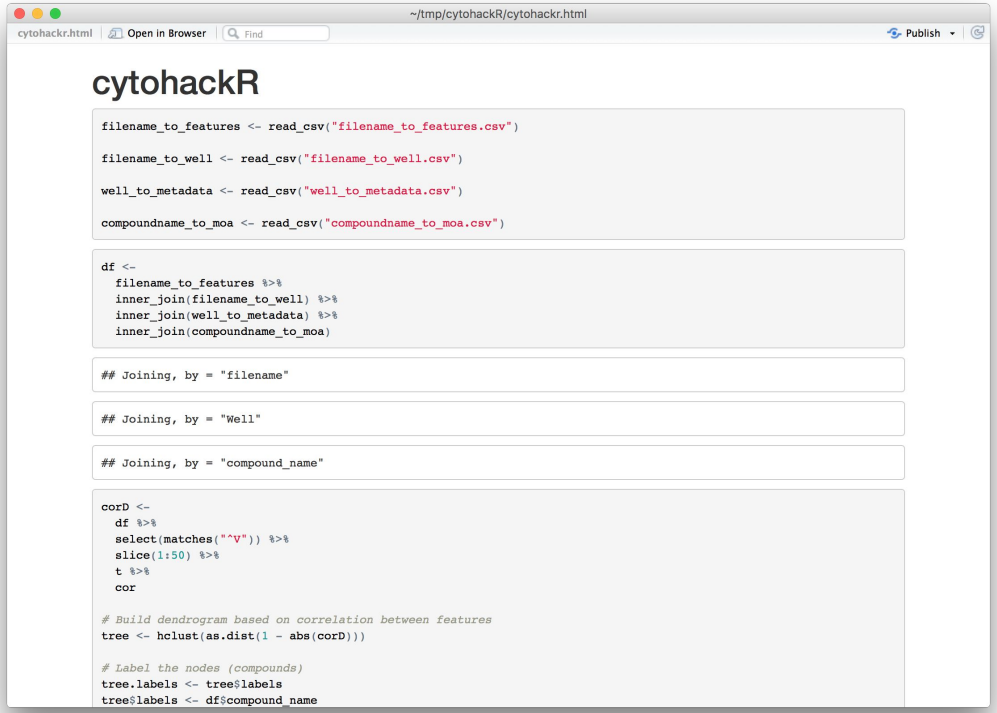
query.py

```
import omero
compounds = unwrap(q.projection(("select distinct mv1.value, mv2.value from Image i "
                         "join i.annotationLinks l1 join l1.child as a1 join a1.mapValue as mv1 "
                         "join i.annotationLinks l2 join l2.child as a2 join a2.mapValue as mv2 "
              "join i.wellSamples ws join ws.well w join w.plate p "
              "where p.id = 4403 and mv1.name = 'Product Use Annotation' and mv2.name = 'Compound Name'"), None))
```

	Well	compound_name	mechanism
1	A01	NIFLUMIC ACID	analgesic
2	A03	NICARDIPINE	vasodilator
3	A04	6-Furfurylaminopurine	auxin
4	A06	Suxibuzone	analgesic
5	A07	LIDOCAINE	anesthetic
6	A11	GLYBURIDE	vasoconstrictor
7	A12	Mepenzolate bromide	cns agent
8	A17	FLUNARIZINE	neuroprotective agent
9	A19	FLUFENAMIC ACID	analgesic

Cluster compounds

- All data was exported as CSVs
- Read into R and analyzed
  - Use tidyverse!



Cluster compounds