Evaluating Quality of and Enhancing Optical Chemical Structure Recognition Tools

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Previously on...

I. **Initial setup**

II. **OCSR tools' contest — OSRA was chosen**
- Generate test dataset and write checking script
- Study existing OCSR tools and choose the best

III. **Test data — first look at errors**
- Run it on test dataset
- Analyse errors & try to improve identification

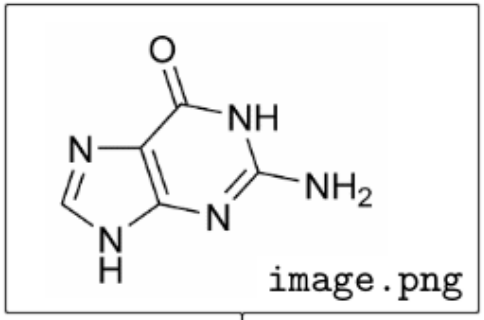
IV. **Real data — collecting errors**
- Run it on small real dataset
- Analyse errors & try to improve identification again

V. **Run it on full real dataset and estimate the error rate**

Main goal

find errors $\rightarrow$ correct them $\rightarrow$ estimate quality

Image processing with OSRA



OSRA
atoms & bonds
recognition

HO2C►COOH
CH2OH►HOH2C
spelling.txt

HOH2C►CO
C3H7►CCC
superatom.txt

...c(=O)[nH]c...
SMILE format

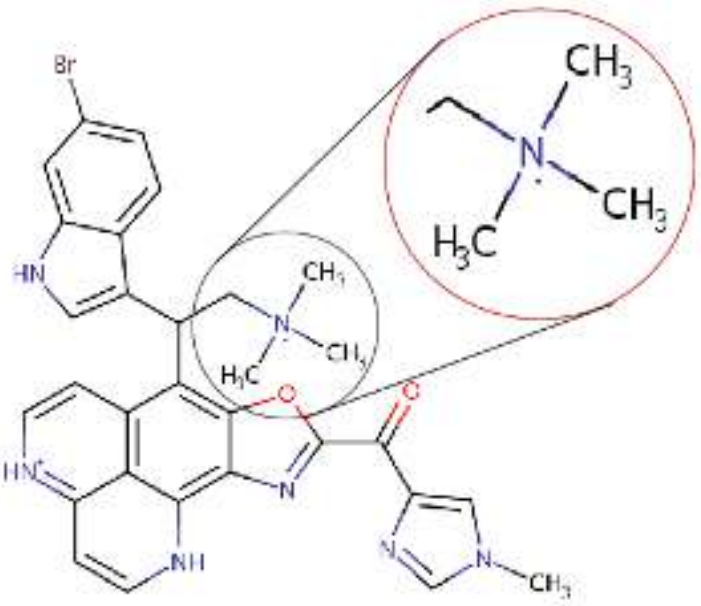
Issue: unrecognized symbols may occur:

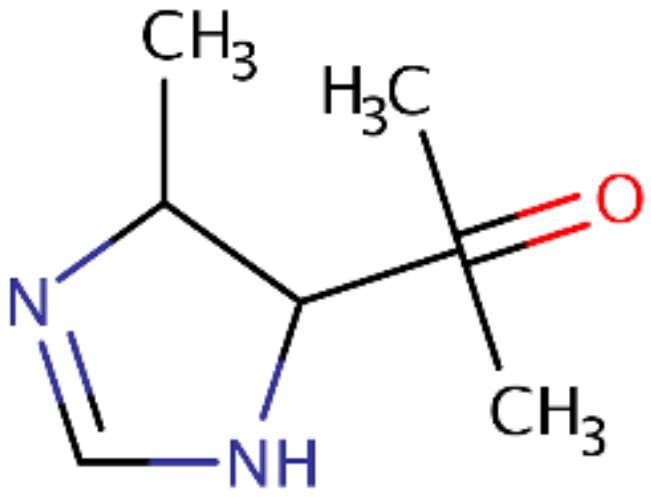
```
HoH2C --> ??
HOCH2 --> ??
```

Solution: remove hydrogen & convert to uppercase.

Atom charge

Issue: OSRA may fail to detect atom charge.





Solution: store expected degrees for each atom type, correct or mark incorrect recognitions.

C	N	O	H	Cl	Br
4	3	2	1	1	1

Table 1: Expected degrees of atom degrees

Quality assessment

Atom quality q_i:

Value	Description
0	unrecognized atom
0.5	wrong degree
0.75	spelling correction
1	otherwise

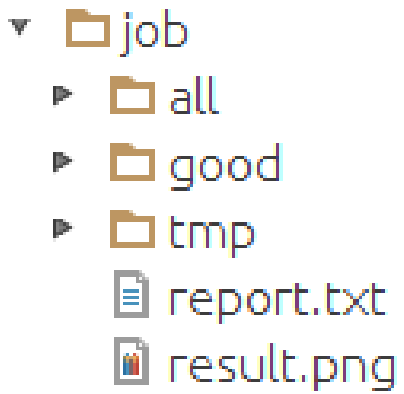
Overall quality Q:

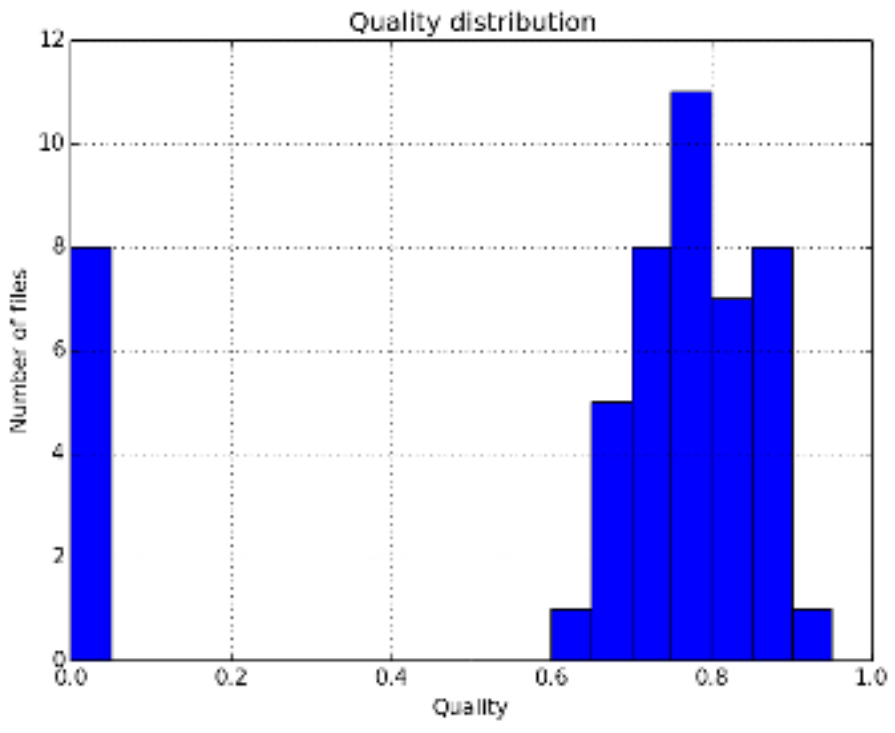
$$Q = \frac{1}{N} \sum_{i=1}^{N} q_i$$

Output format

report.txt

```
  filename    | unrec | spell | deg | qual
-----------------------------------------
00000102.png |   5   |   10  |  0  |  0.6
00000103.png |   1   |    3  |  1  |  0.7
```





Future plans

- Quality metric improvement & threshold value adjustment for better classification of recognition results.
- Add some situational tests for specific cases (e.g. limits for cycle length)

Acknowledgements

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Questions?

Thanks for your attention!