

Supplemental Table 1. Official chemical identification results for strict and approximate named entity recognition measures. Runs are ordered by strict F-score, descending. Highest value in each column is marked in bold. Runs marked with an asterisk are unofficial.

| Team / Run | Strict | | | Approximate | | |
|------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | Precision | Recall | F-score | Precision | Recall | F-score |
| 139 / 3 | 0.8759 | 0.8587 | 0.8672 | 0.9373 | 0.9161 | 0.9266 |
| 139 / 1 | 0.8747 | 0.8523 | 0.8633 | 0.9361 | 0.9083 | 0.9220 |
| 139 / 2 | 0.8775 | 0.8447 | 0.8607 | 0.9441 | 0.9051 | 0.9242 |
| 128 / 1 | 0.8544 | 0.8658 | 0.8600 | 0.9220 | 0.9304 | 0.9262 |
| 143 / 1 | 0.8535 | 0.8608 | 0.8571 | 0.9271 | 0.9235 | 0.9253 |
| 128 / 4 | 0.8457 | 0.8617 | 0.8536 | 0.9157 | 0.9294 | 0.9225 |
| 128 / 2 | 0.8643 | 0.8403 | 0.8521 | 0.9258 | 0.8980 | 0.9117 |
| 121 / 2 | 0.8461 | 0.8583 | 0.8521 | 0.9152 | 0.9215 | 0.9183 |
| 121 / 1 | 0.8616 | 0.8415 | 0.8515 | 0.9293 | 0.9028 | 0.9158 |
| 121 / 3 | 0.8580 | 0.8409 | 0.8494 | 0.9257 | 0.9045 | 0.9149 |
| 141 / 1 | 0.8338 | 0.8654 | 0.8493 | 0.8953 | 0.9309 | 0.9127 |
| 104 / 2 | 0.8687 | 0.8249 | 0.8463 | 0.9273 | 0.8791 | 0.9025 |
| 104 / 3 | 0.8692 | 0.8239 | 0.8459 | 0.9277 | 0.8761 | 0.9011 |
| 148 / 1 | 0.8692 | 0.8239 | 0.8459 | 0.9277 | 0.8761 | 0.9011 |
| 110 / 4 | 0.8394 | 0.8515 | 0.8454 | 0.9040 | 0.9229 | 0.9134 |
| 149 / 1 | 0.8226 | 0.8614 | 0.8416 | 0.8951 | 0.9204 | 0.9076 |
| 146 / 4 | 0.8219 | 0.8622 | 0.8415 | 0.8945 | 0.9235 | 0.9088 |
| 146 / 5 | 0.8222 | 0.8609 | 0.8411 | 0.8951 | 0.9204 | 0.9076 |
| 121 / 5 | 0.8618 | 0.8209 | 0.8409 | 0.9303 | 0.8822 | 0.9056 |
| 110 / 1 | 0.8354 | 0.8429 | 0.8392 | 0.9027 | 0.9186 | 0.9106 |
| 110 / 2 | 0.8421 | 0.8350 | 0.8386 | 0.9066 | 0.9081 | 0.9074 |
| 149 / 3 | 0.8639 | 0.8136 | 0.8380 | 0.9238 | 0.8682 | 0.8951 |
| 139 / 5 | 0.8706 | 0.8068 | 0.8375 | 0.9286 | 0.8566 | 0.8912 |
| 149 / 4 | 0.8644 | 0.8123 | 0.8375 | 0.9242 | 0.8650 | 0.8936 |
| 149 / 5 | 0.8641 | 0.8121 | 0.8373 | 0.9242 | 0.8651 | 0.8937 |
| 148 / 4 | 0.8835 | 0.7893 | 0.8337 | 0.9367 | 0.8341 | 0.8824 |
| 148 / 2 | 0.8824 | 0.7898 | 0.8335 | 0.9363 | 0.8371 | 0.8839 |
| 148 / 3 | 0.8828 | 0.7890 | 0.8333 | 0.9367 | 0.8345 | 0.8826 |
| 146 / 3 | 0.8280 | 0.8382 | 0.8330 | 0.8996 | 0.9031 | 0.9013 |
| 148 / 5 | 0.8270 | 0.8388 | 0.8328 | 0.8993 | 0.9061 | 0.9027 |
| 146 / 1 | 0.8273 | 0.8375 | 0.8324 | 0.8996 | 0.9031 | 0.9013 |
| 157 / 1 | 0.8476 | 0.8101 | 0.8284 | 0.9128 | 0.8670 | 0.8893 |
| 157 / 2 | 0.8476 | 0.8101 | 0.8284 | 0.9128 | 0.8670 | 0.8893 |
| 157 / 3 | 0.8476 | 0.8101 | 0.8284 | 0.9128 | 0.8670 | 0.8893 |
| 157 / 4 | 0.8476 | 0.8101 | 0.8284 | 0.9128 | 0.8670 | 0.8893 |
| 157 / 5 | 0.8476 | 0.8101 | 0.8284 | 0.9128 | 0.8670 | 0.8893 |
| 139 / 4 | 0.8720 | 0.7885 | 0.8282 | 0.9345 | 0.8359 | 0.8825 |
| 146 / 2 | 0.9082 | 0.7436 | 0.8177 | 0.9561 | 0.7809 | 0.8597 |
| 104 / 1 | 0.9077 | 0.7435 | 0.8174 | 0.9562 | 0.7812 | 0.8599 |
| 149 / 2 | 0.9069 | 0.7437 | 0.8173 | 0.9559 | 0.7835 | 0.8611 |
| 128 / 3 | 0.8440 | 0.7896 | 0.8159 | 0.9187 | 0.8541 | 0.8852 |
| Benchmark | 0.8440 | 0.7877 | 0.8149 | 0.9156 | 0.8492 | 0.8811 |
| 155 / 1 | 0.8312 | 0.7967 | 0.8136 | 0.9009 | 0.8596 | 0.8798 |
| 110 / 3 | 0.8505 | 0.7662 | 0.8062 | 0.9231 | 0.8295 | 0.8738 |
| 110 / 5 | 0.8372 | 0.7416 | 0.7865 | 0.9150 | 0.8081 | 0.8583 |
| 121 / 4 | 0.8345 | 0.7374 | 0.7830 | 0.9123 | 0.7993 | 0.8521 |
| 155 / 3* | 0.7676 | 0.6886 | 0.7259 | 0.8881 | 0.8041 | 0.8440 |
| 155 / 2* | 0.7541 | 0.6011 | 0.6690 | 0.8682 | 0.6964 | 0.7729 |
| 143 / 2 | 0.7817 | 0.5552 | 0.6493 | 0.8544 | 0.5990 | 0.7043 |
| 114 / 1 | 0.7219 | 0.5897 | 0.6492 | 0.8348 | 0.6919 | 0.7567 |

| | | | | | | |
|----------|--------|--------|--------|--------|--------|--------|
| 130 / 1* | 0.7208 | 0.5211 | 0.6049 | 0.8933 | 0.6331 | 0.7410 |
| 116 / 3 | 0.8234 | 0.1916 | 0.3109 | 0.9196 | 0.215 | 0.3485 |
| 116 / 1 | 0.8207 | 0.1853 | 0.3023 | 0.9143 | 0.2072 | 0.3378 |
| 116 / 2 | 0.8419 | 0.1734 | 0.2876 | 0.9291 | 0.1925 | 0.3189 |

Supplemental Table 2. Official chemical identification results for strict and approximate normalization measures. Runs are ordered by strict F-score, descending. Highest value in each column is marked in bold. Runs marked with an asterisk are unofficial.

| Team / Run | Strict | | | Approximate | | |
|------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | Precision | Recall | F-score | Precision | Recall | F-score |
| 110 / 4 | 0.8621 | 0.7702 | 0.8136 | 0.8302 | 0.7867 | 0.8030 |
| 128 / 2 | 0.7792 | 0.8434 | 0.8101 | 0.7258 | 0.8679 | 0.7864 |
| 110 / 1 | 0.8582 | 0.7641 | 0.8084 | 0.8246 | 0.7709 | 0.7910 |
| 128 / 1 | 0.7833 | 0.8339 | 0.8078 | 0.7400 | 0.8595 | 0.7909 |
| 121 / 1 | 0.7874 | 0.8281 | 0.8072 | 0.7530 | 0.8643 | 0.8015 |
| 121 / 3 | 0.7876 | 0.8272 | 0.8069 | 0.7462 | 0.8606 | 0.7959 |
| 110 / 2 | 0.8221 | 0.7898 | 0.8056 | 0.7760 | 0.8040 | 0.7849 |
| 128 / 4 | 0.7755 | 0.8318 | 0.8027 | 0.7250 | 0.8591 | 0.7822 |
| 121 / 2 | 0.7748 | 0.8315 | 0.8021 | 0.7341 | 0.8669 | 0.7914 |
| 121 / 5 | 0.7821 | 0.8226 | 0.8019 | 0.7468 | 0.8569 | 0.7936 |
| 128 / 3 | 0.7780 | 0.8257 | 0.8011 | 0.7316 | 0.8517 | 0.7827 |
| 157 / 3 | 0.7338 | 0.8683 | 0.7954 | 0.6954 | 0.8976 | 0.7760 |
| 110 / 3 | 0.8124 | 0.7760 | 0.7938 | 0.7759 | 0.8017 | 0.7828 |
| 157 / 5 | 0.7306 | 0.8658 | 0.7925 | 0.6782 | 0.8919 | 0.7625 |
| Benchmark | 0.8151 | 0.7644 | 0.7889 | 0.7917 | 0.7889 | 0.7857 |
| 141 / 1 | 0.7890 | 0.7849 | 0.7870 | 0.7192 | 0.8254 | 0.7628 |
| 110 / 5 | 0.8310 | 0.7411 | 0.7835 | 0.8051 | 0.7648 | 0.7781 |
| 139 / 2 | 0.7256 | 0.8505 | 0.7831 | 0.7113 | 0.8966 | 0.7883 |
| 139 / 4 | 0.7383 | 0.8281 | 0.7806 | 0.7365 | 0.8777 | 0.7957 |
| 157 / 2 | 0.7078 | 0.8698 | 0.7805 | 0.6612 | 0.9018 | 0.7554 |
| 139 / 1 | 0.7212 | 0.8471 | 0.7791 | 0.7107 | 0.8916 | 0.7850 |
| 157 / 4 | 0.7038 | 0.8670 | 0.7769 | 0.6424 | 0.8961 | 0.7399 |
| 157 / 1 | 0.7038 | 0.8670 | 0.7769 | 0.6421 | 0.8959 | 0.7395 |
| 155 / 1 | 0.7886 | 0.7644 | 0.7763 | 0.7309 | 0.7917 | 0.7551 |
| 139 / 3 | 0.7120 | 0.8499 | 0.7749 | 0.6924 | 0.8969 | 0.7757 |
| 121 / 4 | 0.7571 | 0.7886 | 0.7725 | 0.7311 | 0.8441 | 0.7774 |
| 139 / 5 | 0.7300 | 0.8159 | 0.7705 | 0.7257 | 0.8676 | 0.7837 |
| 155 / 3* | 0.7836 | 0.7243 | 0.7527 | 0.7083 | 0.7499 | 0.7227 |
| 155 / 2* | 0.7634 | 0.7050 | 0.7330 | 0.7012 | 0.7323 | 0.7094 |
| 104 / 1 | 0.6720 | 0.7475 | 0.7078 | 0.6319 | 0.8097 | 0.7039 |
| 149 / 2 | 0.6645 | 0.7451 | 0.7025 | 0.6260 | 0.8174 | 0.7033 |
| 148 / 4 | 0.6481 | 0.7629 | 0.7008 | 0.6043 | 0.8281 | 0.6923 |
| 148 / 3 | 0.6477 | 0.7626 | 0.7004 | 0.6044 | 0.8284 | 0.6925 |
| 148 / 2 | 0.6401 | 0.7607 | 0.6952 | 0.5984 | 0.8348 | 0.6909 |
| 149 / 4 | 0.6306 | 0.7730 | 0.6946 | 0.5825 | 0.8385 | 0.6811 |
| 149 / 5 | 0.6303 | 0.7727 | 0.6943 | 0.5828 | 0.8392 | 0.6815 |
| 104 / 2 | 0.6248 | 0.7699 | 0.6898 | 0.5778 | 0.8466 | 0.6813 |
| 149 / 3 | 0.6225 | 0.7708 | 0.6887 | 0.5765 | 0.8456 | 0.6793 |
| 146 / 1 | 0.5931 | 0.7816 | 0.6744 | 0.5418 | 0.8558 | 0.6581 |
| 148 / 5 | 0.5871 | 0.7806 | 0.6702 | 0.5396 | 0.8616 | 0.6580 |
| 146 / 2 | 0.6298 | 0.7105 | 0.6677 | 0.5816 | 0.7806 | 0.6617 |
| 148 / 1 | 0.5939 | 0.7344 | 0.6567 | 0.5424 | 0.8156 | 0.6473 |
| 104 / 3 | 0.5939 | 0.7344 | 0.6567 | 0.5417 | 0.8153 | 0.6468 |
| 146 / 3 | 0.5587 | 0.7445 | 0.6384 | 0.5081 | 0.8312 | 0.6262 |

| | | | | | | |
|----------|--------|--------|--------|--------|--------|--------|
| 146 / 5 | 0.5497 | 0.7454 | 0.6328 | 0.5005 | 0.8337 | 0.6206 |
| 149 / 1 | 0.5496 | 0.7457 | 0.6328 | 0.4998 | 0.8334 | 0.6201 |
| 146 / 4 | 0.5467 | 0.7491 | 0.6321 | 0.4992 | 0.8402 | 0.6216 |
| 114 / 1 | 0.8334 | 0.4645 | 0.5965 | 0.8273 | 0.5279 | 0.6368 |
| 143 / 1 | 0.4326 | 0.6541 | 0.5208 | 0.4418 | 0.8108 | 0.5664 |
| 143 / 2 | 0.4393 | 0.5392 | 0.4842 | 0.4843 | 0.7222 | 0.5736 |
| 130 / 1* | 0.4575 | 0.4449 | 0.4511 | 0.5461 | 0.6093 | 0.5662 |

Supplemental Table 3. Official chemical indexing results with both strict and approximate measures using the updated indexing. The Increase column shows the increase in F-score for the run compared with the F-score using the original MeSH indexing. Runs are ordered by strict F-score, descending. Highest value in each column is marked in bold. Runs marked with an asterisk are unofficial.

| Team / Run | Strict | | | | Approximate | | |
|------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | Precision | Recall | F-score | Increase | Precision | Recall | F-score |
| 110 / 1 | 0.7417 | 0.5141 | 0.6073 | 0.1409 | 0.7526 | 0.6779 | 0.6743 |
| 110 / 8* | 0.6150 | 0.5808 | 0.5974 | 0.1384 | 0.7248 | 0.7513 | 0.6938 |
| 110 / 5 | 0.7463 | 0.4816 | 0.5854 | 0.1417 | 0.7594 | 0.6587 | 0.6680 |
| 110 / 9* | 0.7309 | 0.4859 | 0.5837 | 0.1186 | 0.7496 | 0.6532 | 0.6591 |
| 128 / 1* | 0.5506 | 0.5867 | 0.5681 | 0.0864 | 0.6437 | 0.7545 | 0.6507 |
| 128 / 2* | 0.5458 | 0.5921 | 0.5680 | 0.0855 | 0.6396 | 0.7591 | 0.6503 |
| 110 / 10* | 0.4921 | 0.6619 | 0.5645 | 0.1227 | 0.6066 | 0.8171 | 0.6502 |
| 110 / 7* | 0.6335 | 0.4870 | 0.5507 | 0.1293 | 0.7163 | 0.6419 | 0.6278 |
| 110 / 4 | 0.7343 | 0.4121 | 0.5279 | 0.1298 | 0.7782 | 0.6036 | 0.6400 |
| 110 / 6* | 0.5095 | 0.5396 | 0.5241 | 0.1280 | 0.6421 | 0.6915 | 0.6070 |
| Benchmark | 0.4057 | 0.7005 | 0.5138 | 0.0997 | 0.5233 | 0.8536 | 0.6135 |
| 110 / 3 | 0.6812 | 0.4048 | 0.5078 | 0.1177 | 0.7523 | 0.6020 | 0.6303 |
| 110 / 2 | 0.6721 | 0.4062 | 0.5064 | 0.1137 | 0.7372 | 0.5949 | 0.6192 |
| 157 / 1* | 0.3553 | 0.7137 | 0.4745 | 0.0939 | 0.4614 | 0.8729 | 0.5687 |
| 128 / 4* | 0.4624 | 0.4105 | 0.4349 | 0.0540 | 0.5257 | 0.5876 | 0.5030 |
| 128 / 3* | 0.4580 | 0.4060 | 0.4304 | 0.0525 | 0.5212 | 0.5817 | 0.4981 |
| 141 / 1* | 0.4958 | 0.3061 | 0.3785 | 0.0451 | 0.5459 | 0.4626 | 0.4687 |
| 157 / 2* | 0.3930 | 0.3527 | 0.3718 | 0.0447 | 0.4599 | 0.5483 | 0.4537 |
| 157 / 3* | 0.2719 | 0.2752 | 0.2736 | 0.0239 | 0.3812 | 0.4705 | 0.3785 |