We provide detailed datasets from our analysis of proteins that are identified in human liver, lung, kidney and intestine microsomes by MS-based proteomics. Also included is a set of CYP450 enzymes and microsomal glutathione-S-transferase (MGSTs) activities in human liver microsomes. The data presented in this paper support the research article “Targeted label-free approach for quantification of epoxide hydrolase and glutathione transferases in microsomes” (Song et al., 2015) [1]. We expect that the data will contribute to the study of metabolism enzymes.

© 2018 Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).
**Value of the data**

- The proteins identified in human liver, lung, kidney and intestine microsomes with high sequence coverage.
- Data from the LC-ESI-MS/MS analysis will provide researchers with detailed information on metabolism enzymes in human liver, lung, kidney and intestine microsomes.
- Data from the enzyme activity analysis will enable researchers to observe the different activities of CYP450 enzymes and MGST enzyme in human liver microsomes.

1. **Data**

The data set shows the CYP450 enzymes and MGSTs activities in individual human liver microsomes (Table 1), the identified metabolism enzymes in human liver (Fig. S1), lung (Fig. S2), kidney (Fig. S3) and intestine (Fig. S4) microsomes are also reported.

2. **Experimental design, materials and methods**

2.1. **Mass spectrometric analysis**

All of the samples were prepared following the previous study [1]. A reversed phase Waters nanoACQUITY column (1.7 µm, BEH130 C18, 100 µm i.d. × 100 µm, Waters Corp.) coupled to a Thermo LTQ Velos Orbitrap tandem mass spectrometer (Thermo Fisher Scientific) was used to identify the proteins in human liver, lung, kidney and intestine microsomes. Samples were eluted at 1.2 µL/min. t = 0–5 min 99%A/1%B, t = 5.1 min 85%A/15%B, t = 50 min 40%A/60%B, t = 55 min 15%A/85%B, t = 55.1–65 min 99%A/1%B where A = 97% water/3% acetonitrile/0.1% formic acid and B = 0.1% formic acid in acetonitrile. Peptides were ionized via a nanoelectrospray ionization (ESI) source, and their mass spectra and collisionally induced dissociation (CID) fragmentation mass spectra were recorded. High resolution (60,000 resolving power), accurate mass spectra were recorded between m/z 395-2000 in ~ 1.2 s on the orbitrap mass analyzer. While the next high-resolution mass spectrum was being acquired on the orbitrap, the LTQ Velos linear ion trap independently recorded CID fragmentation mass spectra of the 8 most abundant-S2 ions present in the previous orbitrap mass spectrum. During the course of a 60-min nano-LC-MS/MS run, this approach typically generated ~ 3000 high-resolution mass spectra and between 12,000–15,000 CID MS/MS spectra. Thermo-Finnegan Proteome Discoverer 2.0 software (Thermo Fisher Scientific) was used to interface with the Mascot (Matrix Science) protein database search engine. MS/MS spectral information was used by Mascot to search the SwissProt Protein database, and a decoy search was employed to establish a false discovery rate. MS Data processed using Mascot (S1, S2, S3, S4) are presented in the Supplementary information tables.
## Table 1
CYP450 enzymes, MEH, and MGSTs activities in human liver microsomes.

| Enzymes | Individual human liver microsomes (n = 16) | Age < 60 (n = 10) | Age > 65 (n = 6) | Male (n = 8) | Female (n = 8) |
|---------|------------------------------------------|------------------|-----------------|-------------|--------------|
|         | Max (pmol/mg protein/min) | Min (pmol/mg protein/min) | Max/min pmol/mg protein/min | pmol/mg protein/min | pmol/mg protein/min | pmol/mg protein/min | pmol/mg protein/min |
| CYP1A2  | 498 | 137 | 3.64 | 280 ± 130 | 259 ± 42.5 | 261 ± 121 | 285 ± 100 |
| CYP2A6  | 1710 | 71.8 | 23.8 | 1188 ± 535 | 472 ± 333 | 1254 ± 498 | 646 ± 520 |
| CYP2B6  | 1330 | 76.3 | 17.4 | 570 ± 453 | 111 ± 35.0 | 498 ± 475 | 336 ± 399 |
| CYP2C8  | 4370 | 629 | 6.95 | 2521 ± 956 | 1252 ± 486 | 2009 ± 674 | 2188 ± 1344 |
| CYP2C9  | 3340 | 1710 | 1.95 | 2544 ± 780 | 2072 ± 591 | 2457 ± 635 | 2317 ± 899 |
| CYP2C19 | 167 | 4.18 | 40.0 | 56.0 ± 64.4 | 25.8 ± 38.7 | 57.6 ± 67.9 | 39.6 ± 50.2 |
| CYP2D6  | 651 | 120 | 5.43 | 397 ± 207 | 246 ± 93.6 | 260 ± 107 | 433 ± 219 |
| CYP2E1  | 3770 | 730 | 5.16 | 2321 ± 1160 | 1750 ± 658 | 1908 ± 1006 | 2353 ± 1089 |
| CYP3A4  | 5220 | 429 | 12.2 | 2779 ± 1403 | 1070 ± 448 | 1943 ± 457 | 2475 ± 2014 |
| MEH     | 0.774 | 0.509 | 1.52 | 0.638 ± 0.0768 | 0.646 ± 0.0566 | 0.659 ± 0.0679 | 0.622 ± 0.0694 |
| MGSTs   | 0.744 | 0.509 | 1.52 | 0.638 ± 0.0768 | 0.646 ± 0.0566 | 0.659 ± 0.0679 | 0.622 ± 0.0694 |
2.2. Assessment of the activities of CYP450 enzymes and MGST in human liver microsomes

To assess the activities of CYP450 enzymes and MGST in human liver microsomes, known substrates specific for each enzyme were used. Briefly, liver microsomes (0.5 mg/mL), NADPH (1 mM) and known substrate were mixed with phosphate buffer (50 mM, pH 7.4) in a total volume of 200 µL. The CYP450 substrates used were phenacetin (20 µM) for CYP1A2-catalyzed phenacetin O-dealkylation, coumarin (4 µM) CYP2A6-catalyzed coumarin 7-hydroxylation, S-mephenytoin (10 µM) CYP2B6-catalyzed S-mephenytoin N-demethylation, amodiaquine (10 µM) CYP2C8-catalyzed amodiaquine N-dealkylation, tolbutamide (50 µM) for CYP2C9-catalyzed tolbutamide 4-methylhydroxylation, S-mephenytoin (50 µM) for CYP2C19-catalyzed S-mephenytoin 4’-hydroxylation, dextromethorphan (10 µM) for CYP2D6-catalyzed dextromethorphan O-demethylation, chlorzoxazone (10 µM) for CYP2E1-catalyzed chlorzoxazone 6-hydroxylation, and midazolam (10 µM) for CYP3A4-catalyzed 1′-Hydroxymidazolam. The substrate concentrations used were below their respective Km values. After preincubation at 37 °C for 5 min, 10 µL of NADPH (20 mM) was added to initiate the reaction. After incubation, 400 µL acetonitrile containing internal standard was added to stop the reaction. The samples were centrifuged at 10,000 g for 10 min and the supernatants were concentrated by drying in vacuo. The residue was re-dissolved in 100 µL acetonitrile/water (50/50, v/v) and analyzed following the previous study [2,3].

Gutathione S-transferase activity was assayed following the method of Habig et al. [4] with 1 mM CDNB and 5 mM glutathione as the substrates.

Acknowledgements

The study was supported by Science Foundation for the Youth Scholars of Hubei Provincial Department of Education for Science and technology research program (No.: Q2017007).

Transparency document. Supplementary material

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.03.124.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.03.124.

References

[1] W. Song, L. Yu, Z. Peng Targeted, label-free approach for quantification of epoxide hydrolase and glutathione transferases in microsomes, Anal. Biochem. 478 (2015) 8–13.
[2] P.G. Alden, R.S. Plumb, M.D. Jones, P.D. Rainville, D. Shave, A rapid ultra-performance liquid chromatography/tandem mass spectrometric methodology for the in vitro analysis of Pooled and Cocktail cytochrome P450 assays, Rapid Commun. Mass Spectrom. 24 (2010) 147–154.
[3] D. Spaggiari, L. Geiser, Y. Daali, S. Rudaz, Phenotyping of CYP450 in human liver microsomes using the cocktail approach, Anal. Bioanal. Chem. 406 (2014) 4875–4887.
[4] W.H. Habig, M.J. Pabst, W.B. Jakoby, Glutathione S-transferases. The first enzymatic step in mercapturic acid formation, J. Biol. Chem. 249 (1974) 7130–7139.