

¹Supplemental Table S1.

Stress	References	Plant species	Tissue of interest	Analytical approach
heat	Kaplan et al., 2004	<i>Arabidopsis thaliana</i>	aerial tissues	GC-MS
	Luengwilai et al., 2012	<i>Solanum lycopersicum</i>	fruit pericarp	GC-MS
	Sun et al., 2016	<i>Zea mays</i>	leaf	NMR
	Paupière et al., 2017	<i>S. lycopersicum</i>	pollen	LC-QTOF-MS
	Das et al., 2017	<i>Glycine max</i>	leaf	UPLC-MS/MS
	Sang et al., 2017	<i>Lycopersicon esculentum</i>	seedling	MALDI-TOF/TOF
	Thomason et al., 2018	<i>Triticum aestivum</i>	leaf	LC/HRMS
	Wang et al., 2018	<i>T. aestivum</i>	grain	LC-MS/MS
	Paupière et al., 2020	<i>S. lycopersicum</i>	leaf	LC-QTOF-MS
cold	Kaplan et al., 2007	<i>A. thaliana</i>	aerial tissues	GC-MS
	Welti et al., 2002	<i>A. thaliana</i>	rosettes	LC-MS/MS
	Kaplan et al., 2004	<i>A. thaliana</i>	aerial tissues	GC-MS
	Gray and Heath, 2005	<i>A. thaliana</i>	seedlings	LC-MS
	Caldana et al., 2011	<i>A. thaliana</i>	rosettes	GC-MS
	Guevara et al., 2012	<i>Thellungiella salsuginea</i>	leaf	GC-MS
	Benina et al., 2013	<i>Haberlea rhodopensis</i> , <i>Thellungiella halophyla</i> , and <i>A. thaliana</i>	leaf	GC-MS
	Zhao et al., 2019	<i>T. aestivum</i>	seedlings	LC-MS
freezing	Hannah, 2006	<i>A. thaliana</i>	leaf	GC/TOFMS
	Korn et al., 2010	<i>A. thaliana</i>	leaf	GC-MS
water-deficit	Urano et al., 2009	<i>A. thaliana</i>	aerial tissues	GC/TOFMS, CE-MS
	Yang et al., 2007	<i>Oryza sativa</i>	leaf	HPLC
	Antonio et al., 2008	<i>Lupinus albus</i>	stem	PGC-LCESI-MS
	Skirycz et al., 2010	<i>A. thaliana</i>	leaf	GC/TOFMS

	Bowne et al., 2012	<i>T. aestivum</i>	leaf	GC-MS
	Erxleben et al., 2012	<i>Physcomitrium patens</i>	Multiple tissues	GC-MS
	Witt et al., 2012	<i>Z. mays</i>	Multiple tissues	GC-TOFMS
	Sicher and Barnaby, 2012	<i>Z. mays</i>	leaf	UPLC-GC/MS
	Gechev et al., 2013	<i>H. rhodopensis</i>	leaf	GC-MS, LC-MS
	Wang et al., 2021	<i>Poa crymophila</i> Keng	seeds	LC-MS
high light exposure	Wulff-Zottele et al., 2010	<i>A. thaliana</i>	leaf	GC-MS
	Caldana et al., 2011	<i>A. thaliana</i>	rosettes	GC-MS
	Küstner et al., 2019	<i>A. thaliana</i>	rosettes	LC-MS/MS

¹Supplemental Table S1 summarizes previous metabolomics studies of plant responses to stress caused by heat, cold, freezing, water-deficit, and high light exposure. The table provides a reference to each report, the plant species, tissue studied, and the analytical approach used for the analysis.

References:

- Antonio, C., Pinheiro, C., Chaves, M.M., Ricardo, C.P., Ortuño, M.F. and Thomas-Oates, J.** (2008) Analysis of carbohydrates in *Lupinus albus* stems on imposition of water deficit, using porous graphitic carbon liquid chromatography-electrospray ionization mass spectrometry. *J. Chromatogr. A* **1187(1-2)**, 111-118. Available at: <https://doi.org/10.1016/j.chroma.2008.02.010>
- Benina, M., Obata, T., Mehterov, N., Ivanov, I., Petrov, V., Toneva, V., Fernie, A.R. and Gechev, T.S.** (2013) Comparative metabolic profiling of *Haberlea rhodopensis*, *Thellungiella halophylla*, and *Arabidopsis thaliana* exposed to low temperature. *Front. Plant Sci.* **4**, 499 Available at: <https://doi.org/10.3389/fpls.2013.00499>
- Bowne, J.B., Erwin, T.A., Juttner, J., Schnurbusch, T., Langridge, P., Bacic, A. and Roessner, U.** (2012) Drought responses of leaf tissues from wheat cultivars of differing drought tolerance at the metabolite level. *Molecular Plant* **5(2)**:418-29. Available at: <https://doi.org/10.1093/mp/ssr114>

- Caldana, C., Degenkolbe, T., Cuadros-Inostroza, A., Klie, S., Sulpice, R., Leisse, A., Steinhauser, D., Fernie, A.R., Willmitzer, L. and Hannah, M.A.** (2011) High-density kinetic analysis of the metabolomic and transcriptomic response of Arabidopsis to eight environmental conditions. *Plant J.* **67**, 869–884. Available at: <https://doi.org/10.1111/j.1365-313X.2011.04640.x>
- Das, A., Rushton, P.J. and Rohila, J.S.** (2017) Metabolomic profiling of soybeans (*Glycine max* L.) reveals the importance of sugar and nitrogen metabolism under drought and heat stress. *Plants (Basel, Switzerland)* **6(2)**, 21. Available at: <https://doi.org/10.3390/plants6020021>
- Erxleben, A., Gessler, A., Vervliet-Scheebaum, M. and Reski, R.** (2012) Metabolite profiling of the moss *Physcomitrella patens* reveals evolutionary conservation of osmoprotective substances. *Plant Cell Rep.* **31(2)**, 427–436 Available at: <https://doi.org/10.1007/s00299-011-1177-9>
- Gechev, T.S., Benina, M., Obata, T., Tohge, T., Sujeeth, N., Minkov, I., Hille, J., Temanni, M.R., Marriott, A.S., Bergström, E., Thomas-Oates, J., Antonio, C., Mueller-Roeber, B., Schippers, J.H., Fernie, A.R., and Toneva, V.** (2013) Molecular mechanisms of desiccation tolerance in the resurrection glacial relic *Haberlea rhodopensis*. *Cell Mol Life Sci.* **70(4)**, 689–709. Available at: <https://doi.org/10.1007/s00018-012-1155-6>
- Gray, G.R. and Heath, D.** (2005) A global reorganization of the metabolome in Arabidopsis during cold acclimation is revealed by metabolic fingerprinting. *Physiol. Plant.* **124**, 236–248. Available at: <https://doi.org/10.1111/j.1399-3054.2005.00507.x>
- Guevara, D. R., Champigny, M. J., Tattersall, A., Dedrick, J., Wong, C. E., Li, Y., Labbe, A., Ping, C. L., Wang, Y., Nuin, P., Golding, G. B., McCarry, B. E., Summers, P. S., Moffatt, B. A., and Weretilnyk, E. A.** (2012) Transcriptomic and metabolomic analysis of Yukon *Thellungiella* plants grown in cabinets and their natural habitat show phenotypic plasticity. *BMC Plant Biol.* **12**, 175. Available at: <https://doi.org/10.1186/1471-2229-12-175>
- Hannah, M.A.** (2006) Natural genetic variation of freezing tolerance in Arabidopsis. *Plant Physiol.* **142**, 98–112. Available at: <https://doi.org/10.1104/pp.106.081141>.
- Kaplan, F., Kopka, J., Haskell, D.W., Zhao, W., Schiller, K.C., Gatzke, N., Sung, D.Y. and Guy, C.L.** (2004) Exploring the temperature-stress metabolome. *Plant Physiol.* **136**, 4159–4168. Available at: <https://doi.org/10.1104/pp.104.052142>
- Kaplan, F., Kopka, J., Sung, D.Y., Zhao, W., Popp, M., Porat, R. and Guy, C.L.** (2007) Transcript and metabolite profiling during cold acclimation of Arabidopsis reveals an intricate relationship of cold-regulated gene expression with modifications in metabolite content. *Plant J.* **50**, 967–981. Available at: <https://doi.org/10.1111/j.1365-313X.2007.03100.x>

- Korn, M., Gärtner, T., Erban, A., Kopka, J., Selbig, J. and Hinch, D.K.** (2010) Predicting Arabidopsis freezing tolerance and heterosis in freezing tolerance from metabolite composition. *Mol. Plant* **3**, 224–235. Available at: <http://dx.doi.org/10.1093/mp/ssp105>.
- Küstner, L., Fürtauer, L., Weckwerth, W., Nägele, T. and Heyer, A.G.** (2019) Subcellular dynamics of proteins and metabolites under abiotic stress reveal deferred response of the *Arabidopsis thaliana* hexokinase-1 mutant gin2-1 to high light. *Plant J.* **100**(3), 456–472. Available at: <https://doi.org/10.1111/tpj.14491>
- Luengwilai, K., Saltveit, M. and Beckles, D.M.** (2012) Metabolite content of harvested Micro-Tom tomato (*Solanum lycopersicum* L.) fruit is altered by chilling and protective heat-shock treatments as shown by GC-MS metabolic profiling. *Postharvest Biol. Technol.* **63**(1), 116–122 Available at: <https://doi.org/10.1016/j.postharvbio.2011.05.014>
- Paupière, M.J., Müller, F., Li, H., Rieu, I., Tikunov, Y.M., Visser, R.G.F. and Bovy, A.G.** (2017) Untargeted metabolomic analysis of tomato pollen development and heat stress response. *Plant Reprod.* **30**(2), 81–94. Available at: <https://doi.org/10.1007/s00497-017-0301-6>
- Paupière, M.J., Tikunov, Y., Schleiff, E., Bovy, A. and Fragkostefanakis, S.** (2020) Reprogramming of tomato leaf metabolome by the activity of heat stress transcription factor HsfB1. *Front. Plant Sci.* **11**, 610599 Available at: <https://doi.org/10.3389/fpls.2020.610599>
- Sang, Q., Shan, X., An, Y., Shu, S., Sun, J. and Guo, S.** (2017) Proteomic analysis reveals the positive effect of exogenous spermidine in tomato seedlings' response to high-temperature stress. *Front. Plant Sci.* **8**, 120. Available at: <https://doi.org/10.3389/fpls.2017.00120>
- Sicher, R.C. and Barnaby, J.Y.** (2012) Impact of carbon dioxide enrichment on the responses of maize leaf transcripts and metabolites to water stress. *Physiol. Plant.* **144**(3), 238–53. Available at: <https://doi.org/10.1111/j.1399-3054.2011.01555.x>.
- Skirycz, A., De Bodt, S., Obata, T., De Clercq, I., Claeys, H., De Rycke, R., Andriankaja, M., Van Aken, O., Van Breusegem, F., Fernie, A.R. and Inzé, D.** (2010) Developmental stage specificity and the role of mitochondrial metabolism in the response of Arabidopsis leaves to prolonged mild osmotic stress. *Plant Physiol.* **152**, 226–244. Available at: <https://doi.org/10.1104/pp.109.148965>.
- Sun, C.X., Gao, X.X., Li, M.Q., Fu, J.Q. and Zhang, Y.L.** (2016) Plastic responses in the metabolome and functional traits of maize plants to temperature variations. *Plant Biol.* **18**(2), 249–261 Available at: <https://doi.org/10.1111/plb.12378>

- Thomason, K., Babar, M.A., Erickson, J.E., Mulvaney, M., Beecher, C. and MacDonald, G.** (2018) Comparative physiological and metabolomics analysis of wheat (*Triticum aestivum* L.) following post-anthesis heat stress. *PLoS One* **13(6)**, e0197919. Available at: <https://doi.org/10.1371/journal.pone.0197919>
- Urano, K., Maruyama, K., Ogata, Y., Morishita, Y., Takeda, M., Sakurai, N., Suzuki, H., Saito, K., Shibata, D., Kobayashi, M., Yamaguchi-Shinozaki, K. and Shinozaki, K.** (2009) Characterization of the ABA-regulated global responses to dehydration in *Arabidopsis* by metabolomics. *Plant J.* **57**, 1065–1078. Available at: <https://doi.org/10.1111/j.1365-313X.2008.03748.x>
- Wang, X., Hou, L., Lu, Y., Wu, B., Gong, X., Liu, M., Wang, J., Sun, Q., Vierling, E. and Xu, S.** (2018) Metabolic adaptation of wheat grain contributes to a stable filling rate under heat stress. *J. Exp. Bot.* **69(22)**, 5531-5545. Available at: <https://doi.org/10.1093/jxb/ery303>.
- Wang, Y., Li, X.Y., Li, C.X., He, Y., Hou, X.Y. and Ma, X.R.** (2021) The regulation of adaptation to cold and drought stresses in *Poa crymophila* Keng revealed by integrative transcriptomics and metabolomics analysis. *Front. Plant Sci.* **12**, 631117. Available at: <https://doi.org/10.3389/fpls.2021.631117>
- Welti, R., Li, W., Li, M., Sang, Y., Biesiada, H., Zhou, H.-E., Rajashekar, C.B., Williams, T.D. and Wang, X.** (2002) Profiling membrane lipids in plant stress responses. *J. Biol. Chem.* **277(35)**, 31994-2002. Available at: <https://doi.org/10.1074/jbc.M205375200>
- Witt, S., Galicia, L., Lisec, J., Cairns, J., Tiessen, A., Araus, J.L., Palacios-Rojas, N. and Fernie, A.R.** (2012) Metabolic and phenotypic responses of greenhouse-grown maize hybrids to experimentally controlled drought stress. *Mol. Plant* **5**, 401–417. Available at: <http://dx.doi.org/10.1093/mp/ssr102>.
- Wulff-Zottele, C., Gatzke, N., Kopka, J., Orellana, A., Hoefgen, R., Fisahn, J. and Hesse, H.** (2010) Photosynthesis and metabolism interact during acclimation of *Arabidopsis thaliana* to high irradiance and sulphur depletion. *Plant, Cell Environ.* **33**, 1974–1988. Available at: <https://doi.org/10.1111/j.1365-3040.2010.02199.x>
- Yang, J., Zhang, J., Liu, K., Wang, Z. and Liu, L.** (2007) Involvement of polyamines in the drought resistance of rice. *J. Exp. Bot.* **58(6)**, 1545-1555. Available at: <https://doi.org/10.1093/jxb/erm032>
- Zhao, Y., Zhou, M., Xu, K., Li, J., Li, S., Zhang, S. and Yang, X.** (2019) Integrated transcriptomics and metabolomics analyses provide insights into cold stress response in wheat. *Crop J.* **7(6)**, 857-866 Available at: <https://doi.org/10.1016/j.cj.2019.09.002>