Leafweb: Dataset in Support of Coupled Modeling of Photophysics, Photochemistry, and Biochemistry of Photosynthesis, December 2022 Release

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Summary:

This data set contains measurements of leaf gas exchange and Pulse-Amplitude Modulated (PAM) fluorometry of light, CO₂, O₂, and temperature responses from 26 C₃ and four C₄ species measured by independent researchers in Canada, China, Finland, The Netherlands, and USA in the field, garden, or greenhouse. Data were collected between 1987 and 2021, however data for individual species only provide coverage over a few hours to one year. Species include three lianas, three shrubs, two boreal deciduous trees, two boreal evergreen needle-leaf tree, three temperate deciduous trees, four tropical deciduous trees, three tropical evergreen trees, one C₃ grass, three C₄ grasses, and six crop varieties. These measurements are conducted according to standard protocols in gas exchange (Long and Bernacchi 2003) and PAM fluorometry (Baker 2008). The Scots pine (Pinus sylvestris) dataset contains one-year continuous fluorometry observations made at intervals of 10 or 30 minutes in the field under natural environments using Walz monitoring PAM. Measurements from all other 29 species include simultaneous PAM fluorometry and gas exchange observations. Among these 29 species, seven species were measured with light response curves only (*i.e.*, light intensity varied systematically with ambient CO₂ concentration controlled at a constant level, e.g., 400 ppm). All the other 22 species were measured with both the light response and CO₂ response (*i.e.*, ambient CO₂ concentration varied systematically with light intensity controlled at a constant level, e.g., $1200 \,\mu\text{molm}^{-2}\text{s}^{-1}$). For most species, measurements were made with temperature controlled at ~ 25 °C with the exceptions of Scots pine (natural diurnal and seasonal variations), tomato cultivar Basket Vee (~ 21 °C), and cotton which contained temperature stress experiments (9 to 40 °C). All measurements were made at ambient O₂ concentration except for the tomato cultivar Basket Vee and cotton which used two O₂ levels (2 and 21%) and rice and tomato cultivar Growdena which used five O₂ levels (2, 10, 21, 35, and 50%). This data set contains 260 comma-separated (*.csv) files contained as a compressed (*.zip) file.

Related Publication:

The measurements and results of this study have been described in the following publication:

Gu L, B Grodzinski, J Han, T Marie, Y-J Zhang, CY Song, and Y Sun. 2022. An Exploratory Steady-state Redox Model of Photosynthetic Linear Electron Transport for Use in Complete Modeling of Photosynthesis for Broad Applications. Plant Cell and Environment. (in review)

Data Citation:

Cite this data set as follows:

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Related Data Sets

Han, Jimei; Gu, Lianhong; Zhang, Yongjiang; Sun, Ying. 2022. Data from: The Physiological Basis for Estimating Photosynthesis from Chlorophyll a Fluorescence. https://ecommons.cornell.edu/handle/1813/110978

• Contains Leafweb data used in other leaf photosynthesis – related studies

Lianhong Gu, Ivan Haworth, Anna Jensen, Rich Norby, Benjamin Turner, et al. 2021. Photosynthetic parameters and nutrient content of trees at the Panama crane sites. ESS-DIVE. doi:10.15486/NGT/1255260, version: ess-dive-b77e1bd5d1a52f4-20220527T170937436. <u>https://www.osti.gov/dataexplorer/biblio/dataset/1255260</u>

• Contains Leafweb data used in other leaf photosynthesis – related studies.

Han, Jimei; Gu, Lianhong; Zhang, Yongjiang; Sun, Ying. 2022. Data from: The Physiological Basis for Estimating Photosynthesis from Chlorophyll a Fluorescence. https://ecommons.cornell.edu/handle/1813/110978

• Contains a subset of some data present in this dataset.

Data and Documentation Access

For public access to Leafweb data, please visit <u>www.leafweb.org</u>. For public access to data from the US Department of Energy Terrestrial Ecosystem Science Scientific Focus Ares (TES-SFA), please visit: <u>https://tes-sfa.ornl.gov/node/80</u>.

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1. Data Set Overview:

This data set contains measurements of leaf gas exchange and Pulse-Amplitude Modulated (PAM) fluorometry of light, CO₂, O₂, and temperature responses from 26 C₃ and four C₄ species measured by independent researchers in Canada, China, Finland, The Netherlands, and USA in the field, garden, or greenhouse. Data were collected between 1987 and 2021, however data for individual species only provide coverage over a few hours to one year. Species include three lianas, three shrubs, two boreal deciduous trees, two boreal evergreen needle-leaf tree, three temperate deciduous trees, four tropical deciduous trees, three tropical evergreen trees, one C₃ grass, three C₄ grasses, and six crop varieties. These measurements are conducted according to standard PAM fluorometry and gas exchange measurement protocols. The Scots pine dataset contains one-year continuous fluorometry observations made at intervals of 10 or 30 minutes in the field under natural environments using Walz monitoring PAM. Measurements from all other 29 species include simultaneous PAM fluorometry and gas exchange observations. Among these 29 species, 7 species were measured with light response curves only (*i.e.*, light intensity varied systematically with ambient CO₂ concentration controlled at a constant level, *e.g.*, 400 ppm). All the other 22 species were measured with both the light response and CO₂ response (*i.e.*, ambient CO₂ concentration varied systematically with light intensity controlled at a constant level, *e.g.*, 1200 μ molm⁻²s⁻¹). For most species, measurements were made with temperature controlled at ~ 25 °C with the exceptions of Scots pine (natural diurnal and seasonal variations), tomato cultivar Basket Vee ($\sim 21 \text{ °C}$), and cotton which contained temperature stress experiments (9 to 40 °C). All measurements were made at ambient O2 concentration except for the tomato cultivar Basket Vee and cotton which used two O₂ levels (2 and 21%) and rice and tomato cultivar Growdena which used five O₂ levels (2, 10, 21, 35, and 50%).

All PAM fluorometry measurements started with fully dark-adapted leaves to determine the minimum (F_o) and maximum (F_M) fluorescence yield. The exception is the case of Scots pine for which a monitoring PAM was used and the point in the time series where the maximum fluorescence yield peaked in night (typically before sunrise) could be treated as F_M and the corresponding steady state fluorescence yield could be treated as F_o (because there was no light in night). The F_M and F_o obtained in this way could be used as dark-adapted measurements for the following day (Porcar-Castell, 2011). F'_0 , which is the minimum fluorescence yield with all photosystem II reaction centers open but non-photochemical quenching (NPQ) unrelaxed and needed for the calculation of fractions of open reaction centers was not always measured. When needed, F'_0 could be calculated with the Oxborough – Baker approach (Oxborough and Baker, 1997). In fact, it is our view that the Oxborough – Baker approach should be used as a preferred way of determining F'_0 as it is theoretically consistent with the definition of fraction of open photosystem reaction centers and avoids potential measurement uncertainties such as the relaxation of NPQ when a far-red light is applied to drain electrons from the acceptors of photosystem II.

This data set contains 260 comma-separated (*.csv) files contained as a compressed (*.zip) file.

2. Data Characteristics:

These data are considered at **Quality Level 1**. Level 1 indicates an internally consistent data product that has been subjected to quality checks and data management procedures.

This dataset contains 260 comma-separated (*.csv) files. Data are from a variety of species, locations, and time periods (Table 1).

User note: Measurements and variables reported differ between files. Please see Section 5. Data Acquisition Materials and Methods for additional details.

Species	Туре	Data type	Temp (°C)	O ₂ conc (%)	Location	Environ- ment	Date	Subdirectory	Data contributor
Betula alleghaniens is	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 06-26	Boreal broadleaf deciduous tree dataset	Ying Sun (ys776@cornell.edu)
Betula papyrifera	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 07-01	Boreal broadleaf deciduous tree dataset	Ying Sun (ys776@cornell.edu)
Dichantheli um clandestinu m	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 07-15	C3 grass dataset	Ying Sun (ys776@cornell.edu)
<i>Cornus racemosa</i> 'Cuyzam'	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 07-03	Temperate broadleaf deciduous shrub dataset	Ying Sun (ys776@cornell.edu)
<i>Viburnum dentatum</i> 'Christom'	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 06-08	Temperate broadleaf deciduous shrub dataset	Ying Sun (ys776@cornell.edu)

Table 1. List of species, measurement types, and locations.

<i>Cornus racemosa</i> 'Ottzam'	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 07-02	Temperate broadleaf deciduous shrub dataset	Ying Sun (ys776@cornell.edu)
Juglans nigra	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 06-29	Temperate broadleaf deciduous tree dataset	Ying Sun (ys776@cornell.edu)
<i>Carya ovata</i> Wilcox'	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 07-14	Temperate broadleaf deciduous tree dataset	Ying Sun (ys776@cornell.edu)
<i>Liquidamba r styraciflua</i> 'Moraine'	C ₃	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden, USA	Garden	2020- 06-24	Temperate broadleaf deciduous tree dataset	Ying Sun (ys776@cornell.edu)
Jatropha curcas	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-16	Tropical broadleaf deciduous tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Bauhinia variegata	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-18	Tropical broadleaf deciduous tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)

Bauhinia purpurea	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-21	Tropical broadleaf deciduous tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Bombax ceiba	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-25	Tropical broadleaf deciduous tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Millettia macrostachy a	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-16	Tropical broadleaf evergreen tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Magnolia henryi	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-16	Tropical broadleaf evergreen tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Dipterocarp us turbinatus	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-18	Tropical broadleaf evergreen tree dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)

Bauhinia glauca	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-15	Tropical broadleaf deciduous liana dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Elaeagnus conferta	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-17	Tropical broadleaf deciduous liana dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Mansoa alliacea	C ₃	Light respons e	25 to 33	21	Xishuangba nna Tropical Botanical Garden, China	Garden	2020- 05-17	Tropical broadleaf deciduous liana dataset	Yong-Jiang Zhang (yongjiang.zhang@main e.edu)
Pinus sylvestris	C ₃	Natural diurnal variatio n	Natural diurnal variatio n	21	Hyytiälä Forestry Research Station, Finland	Field	2008- 08-5 to 2009- 08-15	Boreal needleleaf evergreen tree dataset	Albert Porcar-Castell (joan.porcar@helsinki.fi)
Pinus strobus	C ₃	Joint light/C O ₂ respons e	25	21	Oak Ridge National Laboratory	Greenhou se		Boreal needleleaf evergreen tree dataset	Jimei Han / Lianhong Gu (lianhong-gu@ornl.gov)
Oryza sativa 'IR64 Rice'	C ₃	Joint light/C O ₂ respons e	~ 25	2, 10, 21, 35, 50	Wageninge n University and Research,	Greenhou se		C3 crop dataset/Rice dataset	Yin, Xinyou (xinyou.yin@wur.nl)

					The Netherlands				
Solanum lycopersicu m 'Growdena'	C ₃	Joint light/C O ₂ respons e	~ 25	2, 10, 21, 35, 50	Wageninge n University and Research, The Netherlands	Greenhou se		C3 crop dataset/Tomato Growdena dataset	Yin, Xinyou (xinyou.yin@wur.nl)
Solanum lycopersicu m 'Basket Vee'	C3	Joint light/C O ₂ respons e	~ 21	2, 21	University of Guelph, Canada	Greenhou se	2021- 03-25 to 2022 1-04- 01	C3 crop dataset/Tomato Basket Vee dataset	Telesphore Marie (mariet@uoguelph.ca)
Gossypium hirsutum L. 'Upland cotton'	C ₃	Joint light/C O ₂ respons e	9 to 40	2, 21	Carnegie Institution for Science (California) , USA	Greenhou se		C3 crop dataset/Californ ia cotton dataset	Joe Berry (jberry@carnegiescience. edu)
Gossypium hirsutum L. 'Upland cotton'	C ₃	Joint light/C O ₂ respons e	25	21	Oak Ridge National Laboratory	Greenhou se		C3 crop dataset/Tenness e cotton dataset	Jimei Han / Lianhong Gu (lianhong-gu@ornl.gov)
Gossypium barbadense 'Pima'	C ₃	Joint light/C O ₂ respons e	25	21	Oak Ridge National Laboratory	Greenhou se		C3 crop dataset/Tenness e cotton dataset	Jimei Han / Lianhong Gu (lianhong-gu@ornl.gov)

Zea mays L.	C4	Joint light/C O ₂ respons e	~ 25	21	Cornell Musgrave Research Farm	Field	2020- 08-18	C4 grass dataset	Ying Sun (ys776@cornell.edu)
Sorghastrum nutans	C ₄	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden	Garden	2020- 08-10	C4 grass dataset	Ying Sun (ys776@cornell.edu)
Andropogon gerardii	C4	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden	Garden	2020- 08-01	C4 grass dataset	Ying Sun (ys776@cornell.edu)
Panicum virgatum	C4	Joint light/C O ₂ respons e	~ 25	21	Cornell Botanic Garden	Garden	2020- 08-09	C4 grass dataset	Ying Sun (ys776@cornell.edu)

Data File Description

The variables included in the dataset, which may vary from file to file, are recognized by header names, defined according to the Standard Dictionary for Leafweb Input Data Variables, which is included below in Table 2. Not all variables listed in the Standard Dictionary are included in each file. Conversely, a file may contain instrument-specific variables not listed in the Standard Dictionary. Also, data lines don't start at the same rows. You may need to read these files with a "smart" program. It is advised to read in the whole line as a text string, and then use comma to partition this string. Use the Standard Dictionary to determine whether a row contains useful data and if so, which column is which. Note that when comparing the string and the Standard Dictionary, all letters in the string AND the Standard Dictionary should be converted to uppercases as Leafweb does not differentiate upper and lower cases for variable names. Also, ignore the exclamation mark '!' if it is placed at the beginning of a variable name or the apostrophe ''' in PAM fluorometry measurements. For example, !PARi is the same as PARi, pari, and pAri, and !FoorFs' is the same as FoorFs.

All files are in comma-separated values (CSV) format and grouped into the following subdirectories:

- 1. Tropical broadleaf deciduous liana dataset
 - This dataset consists of 9 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 3 species (*Bauhinia glauca*, *Elaeagnus conferta*, *Mansoa alliacea*). These 9 files are *Bauhinia_glauca1.csv*, *Bauhinia_glauca2.csv*, *Bauhinia_glauca3.csv*, *Elaeagnus_conferta1.csv*, *Elaeagnus_conferta2.csv*, *Elaeagnus_conferta3.csv*, *Mansoa_alliacea1.csv*, *Mansoa_alliacea2.csv*, *Mansoa_alliacea3.csv*.
- 2. Tropical broadleaf evergreen tree dataset
 - This dataset consists of 9 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 3 species (*Dipterocarpus turbinatus, Magnolia henryi, Millettia macrostachya*). These 9 files are *Dipterocarpus_turbinatus1.csv, Dipterocarpus_turbinatus2.csv, Dipterocarpus_turbinatus3.csv, Magnolia_henryi1.csv, Magnolia_henryi2.csv, Magnolia_henryi3.csv, Millettia_macrostachya1.csv, Millettia_macrostachya2.csv, Millettia_macrostachya3.csv.*
- 3. Tropical broadleaf deciduous tree dataset
 - This dataset consists of 12 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 4 species (*Jatropha curcas*, *Bauhinia variegata*, *Bauhinia purpurea*, *Bombax ceiba*). These 12 files are *Jatropha_curcas*1.csv, *Jatropha_curcas*2.csv, *Jatropha_curcas*3.csv, *Bauhinia_variegata*1.csv, *Bauhinia_variegata*2.csv, *Bauhinia_variegata*3.csv, *Bauhinia_purpurea*1.csv, *Bauhinia_purpurea*2.csv, *Bauhinia_purpurea*3.csv, *Bombax_ceiba*1.csv, *Bombax_ceiba*3.csv.
- 4. Temperate broadleaf deciduous tree dataset

- This dataset consists of 18 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 6 species (Juglans nigra, Carya ovata Wilcox, Liquidambar styraciflua Moraine, Quercus shumardii Buckl., Quercus falcata Michx., Liriodendron tulipifera L.). These 18 files are Juglans_nigra1.csv, Juglans_nigra2.csv, Juglans_nigra3.csv, Carya_ovata_Wilcox1.csv, Carya_ovata_Wilcox2.csv, Carya_ovata_Wilcox3.csv, Liquidambar_styraciflua_Moraine1.csv, Liquidambar_styraciflua_Moraine2.csv, Quercus_shumardii_Buckl1.csv, Quercus_shumardii_Buckl2.csv, Quercus_shumardii_Buckl3.csv, Quercus_falcata_Michx1.csv, Quercus_falcata_Michx3.csv, Liriodendron_tulipifera1.csv, Liriodendron_tulipifera2.csv.
- 5. Temperate broadleaf deciduous shrub dataset
 - This dataset consists of 6 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 2 species (*Cornus racemosa Cuyzam, Viburnum dentatum Christom, Cornus racemosa Ottzam*). These 6 files are *Cornus_racemosa_Cuyzam1.csv, Cornus_racemosa_Cuyzam2.csv, Cornus_racemosa_Cuyzam3.csv, Viburnum_dentatum_Christom1.csv, Viburnum_dentatum_Christom2.csv, Viburnum_dentatum_Christom3.csv*. The descriptions of the variables for each file in .csv format refer to those for the species from plant function type of Tropical broadleaf deciduous liana dataset.
- 6. Boreal broadleaf deciduous tree dataset
 - This dataset consists of 6 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates multiplied by 2 species (*Betula alleghaniensis, Betula papyrifera*). These 6 files are *Betula_alleghaniensis1.csv, Betula_alleghaniensis2.csv, Betula_alleghaniensis3.csv, Betula_papyrifera1.csv, Betula_papyrifera2.csv, Betula_papyrifera3.csv.*
- 7. Boreal needleleaf evergreen tree dataset
 - This dataset consists of data from two boreal needleleaf evergreen species: *Pinus strobus* L and *Pinus sylvestris*.
 - The *Pinus strobus* L contains 3 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates. These 3 files are *Pinus_strobus*1.csv, *Pinus_strobus*2.csv, *Pinus_strobus*2.csv.
 - The *Pinus sylvestris* dataset contains measurements of monitoring PAM and does not contain gas exchange measurements. The daily files are selected from the original dataset based on filtering criteria described in Section 2 Data Characteristics. The unfiltered data are included in a single file Original_Pinus_sylvestris_Dataset.csv
- 8. C3 crop dataset
 - This dataset includes measurements from cotton, rice, and tomato in the US (Tennessee and California), Netherlands, and Canada.

- Tennessee cotton dataset: It consists of 6 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates of 2 species (Gossypium hirsutum L., Gossypium barbadense L.). These 6 files are Gossypium_hirsutum1.csv, Gossypium_hirsutum2.csv, Gossypium_hirsutum3.csv, Gossypium_barbadense1.csv, Gossypium_barbadense2.csv, Gossypium_barbadense3.csv.
- California cotton dataset: It consists of 7 files, which include gas exchange and chlorophyll a fluorescence data from different leaves of *Gossypium hirsutum* with different combinations of environmental conditions. These 7 files are California_cotton1 to California_cotton7.
- Rice dataset: It consists of 20 files, which include gas exchange and chlorophyll a fluorescence data from different leaves of *Oryza sativa* 'IR64 Rice' with different combinations of environmental conditions. These 20 files are RicePot42234O235.csv, RicePot42234O250.csv, RicePot42235O210.csv, RicePot42235O221.csv, RicePot42236O22.csv, RicePot42236O250.csv, RicePot42237O22.csv, RicePot42237O235.csv, RicePot42238O210.csv, RicePot42238O221.csv, RicePot42241O235.csv, RicePot42241O250.csv, RicePot42242O210.csv, RicePot42241O235.csv, RicePot42243O221.csv, RicePot42243O22.csv, RicePot42244O221.csv, RicePot42243O221.csv, RicePot42243O22.csv, RicePot42244O221.csv, RicePot42243O221.csv, RicePot42243O22.csv, RicePot42244O221.csv, RicePot42244O235.csv, RicePot42243O22.csv, RicePot42244O221.csv, RicePot42244O235.csv,
- Tomato Growdena dataset: It consists of 24 files, which include gas exchange and chlorophyll a fluorescence data from different leaves of *Solanum lycopersicum* 'Growdena' with different combinations of environmental conditions. These 24 files are Tomatao15Oxygen50.csv, Tomatao26Oxygen50.csv, Tomatao37Oxygen50.csv, Tomatao480xygen50.csv, Tomato15Oxygen10.csv, Tomato15Oxygen21.csv, Tomato15Oxygen2.csv, Tomato15Oxygen35.csv, Tomato26Oxygen10.csv, Tomato26Oxygen21.csv, Tomato26Oxygen2.csv, Tomato26Oxygen35.csv, Tomato37Oxygen10.csv, Tomato37Oxygen21.csv, Tomato37Oxygen21.csv, Tomato480xygen35.csv, Tomato480xygen10.csv, Tomato480xygen2.csv, Tomato480xygen35.csv, Tomato480xygen2.csv, Tomato480xygen35.csv, Tomato480xygen2.csv, Tomato480xygen35.csv, Tomato480xygen2.csv, Tomato480xygen2.csv, TomatoAPAR10xygen2.csv, TomatoAPAR20xygen2.csv.
- Tomato Basket Vee dataset: It consists of 6 files, which include gas exchange and chlorophyll a fluorescence data from different leaves of *Solanum lycopersicum* 'Basket Vee' with different combinations of environmental conditions and photoperiod treatments. These 6 files are 20210325_12hr_rep_1_tomato_Basket_Vee.csv, 20210329_12hr_rep_2_tomato_Basket_Vee.csv, 20210331_12hr_rep_3_tomato_Basket_Vee.csv, 20210327_24hr_rep_1_tomato_Basket_Vee.csv, 20210330_24hr_rep_2_tomato_Basket_Vee.csv, 20210401_24hr_rep_3_tomato_Basket_Vee.csv
- 9. C3 grass dataset

- This dataset consists of 3 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates of one species (*Dichanthelium clandestinum*). These 3 files are *Dichanthelium_clandestinum1.csv*, *Dichanthelium_clandestinum2.csv*, *Dichanthelium_clandestinum3.csv*.
- 10. C4 crop dataset
 - This dataset consists of 3 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates of one species (*Zea mays L.*). These 3 files are *Zea_mays1.csv*, *Zea_mays2.csv*, *Zea_mays3.csv*.
- 11. C4 grass dataset
 - This dataset consists of 9 files, which include gas exchange and chlorophyll a fluorescence data from 3 replicates of 3 species (*Sorghastrum nutans, Andropogon gerardii, Panicum virgatum*). These 3 files are *Sorghastrum_nutans1.csv, Sorghastrum_nutans2.csv, Sorghastrum_nutans3.csv, Andropogon_gerardii1.csv, Andropogon_gerardii2.csv, Andropogon_gerardii3.csv, Panicum_virgatum1.csv, Panicum_virgatum2.csv, Panicum_virgatum3.csv.*

Using Leafweb

Leafweb uses the following naming conventions for input variables, if provided. These conventions must be strictly followed for Leafweb algorithms to recognize them. Variables starting with '!' are must-have variables for Leafweb to do analyses. If no '!' data are provided, no analyses will be done by Leafweb unless PAM fluorometry data are provided. Fill any missing data with '-9999'. Ideally the gas exchange and PAM fluorometry should be measured simultaneously for the same leaf. But if they are measured in sequence, these two types of data can still be put into the same file so that photophysical, photochemical and biochemical parameters can be estimated. In sequential measurements, fill any missing gas exchange variables with -9999 when PAM fluorometry is measured; likewise, fill any missing PAM fluorometry measurements with -9999 when gas exchange measurements are made. Use LeafwebInputDataFileFormat.csv as an input data file template. Contact <u>lianhong-gu@ornl.gov</u> and james.kolpack@gmail.com for any Leafweb-related questions.

Column Name	Units	Description				
Metadata: information to make the gas exchange and PAM fluorometry data useful in synthesis						
SiteID		Name for the place where data are collected				
Latitude(Degrees)	Degrees	Latitude of the site, north is positive				
Longitude(Degrees)	Degrees	Longitude of the site, east is positive				
Elevation	m	Elevation of the site				
SampleYear		The year when the measurement is made				
SampleDayOfYear	Day of year	The day when the measurement is made; January 1 is				
		day 1				
GrowSeasonStart	Day of year	The start day of the growing season				
GrowSeasonEnd	Day of year	The end day of the growing season				

 Table 2. Leafweb data variable descriptions.

StandAge	Years	The number of years since the site was cleared
CanopyHeight	m	The mean canopy height
LeafAreaIndex	m^2m^2	Leaf area index of the canopy at the time of
		measurement
SpeciesSampled		Name of species measured
Environment		Characterize the general growing environment of the
		plant into Nature, Garden, Greenhouse, or Farm
AveTimeResolution	Minutes	The average time between two consecutive gas
		exchange sample points
SampleHeight	m	The height above floor of the leaf measured
LeafAge	days	The age of the leaf measured
SpecificLeafArea	cm^2g^{-1}	Specific leaf area
LfNitrogenContent	%	Leaf nitrogen content
LfCarbonContent	%	Leaf carbon content
LfPhosphorusContent	%	Leaf phosphorus content
WoodPorosity	Ring or diffuse	Wood porosity
	porous	
Sapwooddensity	gcm ⁻³	Sapwood density
LeafLength	cm	Leaf length
LeafWidth	cm	Leaf width
User-preferred parame	eter values: if provided,	the values will be used by Leafweb in fitting
Gamma*25	Pa	CO ₂ compensation point at 25 °C
KC25	Pa	Michaelis-Menten constant for RuBP carboxylation at
		25 °C
KO25	Pa	Michaelis-Menten constant for RuBP oxygenation at
		25 °C
AlphaTPU		Fraction of glycolate carbon remained outside of
		chloroplast (i.e., not returned to stroma)
Rd25	µmolm ⁻² s ⁻¹	Day respiration at 25 °C
Resistwpbs25	µmol ⁻¹ m ² sPa	Cell wall / plasmalemma resistance for C ₃ species or
		bundle sheath resistance for C ₄ species to CO ₂
		diffusion
Resistchm25	µmol ⁻¹ m ² sPa	Chloroplast envelope resistance for C ₃ species or
		mesophyll resistance for C ₄ species to CO ₂ diffusion
Gas exchange and PA	M fluorometry data: th	is is the main data section

DataType		Data type indicator:
7 1		=0, dark-adapted measurements
		=5, carboxylation is known to be limited by Rubisco,
		don't use if not sure
		=6, carboxylation is known to be limited by RuBP
		regeneration, don't use if not sure
		=7, carboxylation is known to be limited by triose
		phosphate utilization (TPU)
		= 11 to 25, A/Ci curves. Each different number
		represents a different A/Ci curve (i.e., the same leaf
		measured at different PAR levels). For example, if five
		different PAR levels are used to measure five different
		A/Ci curves, use 11, 12, 13, 14 and 15 to identify the
		points of each curve. All points in the first A/Ci curve
		should be given the DataType '11'. All points in the
		second A/Ci curve should be given the DataType '12',
		and so on. Maximum 15 A/Ci curves for each input
		file. The curves must be ordered consecutively.
		= 31 to 45, A/Light curves. Each different number
		represents a different A/PAR curve (i.e., the same leaf
		measured at different ambient CO_2 levels). For
		example, if five different ambient CO ₂ levels are used
		to measure five different A/PAR curves, use 31, 32, 33,
		34 and 35 to identify the points of each curve. All
		points in the first A/PAR curve should be given the
		DataType '31', all points in the second A/Ci curve
		should be given the DataType '32', and so on.
		Maximum 15 A/PAR curves for each input file. The
		curves must be ordered consecutively.
		=-9999, all other types of measurement.
ObsNo		The data point No.
ObsDate	YYYY-MM-DD	The date of observation
HHMMSS	hh:mm:ss	clock time
!AnetCO2	µmolm ⁻² s ⁻¹	Net CO ₂ assimilation rate, must have variable, any
		leaks must have been corrected.
AnetO2	µmolm ⁻² s ⁻¹	Net O ₂ evolving rate
AnetVOC	nmolm ⁻² s ⁻¹	VOC emission rate. Specify the VOC species in 'Extra
		info' in the header section of the input data file
!StomCond	molm ⁻² s ⁻¹	Stomatal conductance to water vapor diffusion
!CO2i	µmolmol ⁻¹	Intercellular CO ₂ concentration in ppm
!Trmmol	mmolm ⁻² s ⁻¹	Transpiration rate
!VpdL	kPa	Water vapor pressure deficit at the leaf surface,
	2	calculated based on leaf temperature
LeatAreaMeasured	cm ²	The area of the leaf covered by the chamber. When the
		leaf is larger than the chamber, this is also the chamber
		area. When the leaf is smaller than the chamber, this is
		the total leaf area; in this case, all the flux /conductance
		variables must have been already corrected to a per leaf
		area basis.

StmRat	NA	The ratio of stomatal density of the adaxial (upper) side
		to the abaxial (lower) side
BLCond	molm ⁻² s ⁻¹	Leaf boundary layer conductance to water vapor
		diffusion
Tair	°C	Air temperature in sample chamber
!Tleaf	°C	Temperature of leaf thermocouple
TBlk	°C	Temperature of cooler block
CO2R	µmolmol ⁻¹	Reference CO ₂ concentration
CO2S	µmolmol ⁻¹	Sample CO ₂ concentration
H2OR	mmolmol ⁻¹	Reference CO ₂ concentration
H2OS	mmolmol ⁻¹	Sample CO ₂ concentration
RH_R	%	Reference chamber air relative humidity
RH_S	%	Sample chamber air relative humidity
FlowRate	µmols ⁻¹	Air flow rate through the chambers
!PARi	µmolmol ⁻¹ s ⁻¹	PAR measured by the in-chamber quantum sensor; this
		is the light intensity driving gas exchange or PAM
		fluorometry. PARi should be very close to PARi@Fs.
PARo	µmolmol ⁻¹ s ⁻¹	PAR measured by a quantum sensor outside of the leaf
		chamber
!AirPress	kPA	Ambient air pressure
OxygenLevel%	%	Oxygen level in the sample chamber
TissueArea	cm ²	The green tissue area inside the sample chamber (for
		non-leaf green issues such as sphagnum)
TissueMass	g	The green tissue mass inside the sample chamber
		(for non-leaf green issues such as sphagnum)
PARi@Fs	µmolmol ⁻¹ s ⁻¹	PAR measured by the in-chamber quantum sensor at
Ŭ		the time of PAM fluorometry. PARi@Fs is very close
		to PARi.
!FoorFs [']	Arbitrary unit	Minimum fluorescence yield under fully dark-adapted
		conditions (Fo) or steady fluorescence under actinic
		light (Fs'). If it is Fo, both PARi and DataType must be
		zero.
!FmorFm [']	Arbitrary unit	Maximum fluorescence yield under fully dark-
		adapted conditions (Fm) or under actinic light
		(Fm'). If it is Fm, both PARi and DataType must
		be zero.
FoDark	Arbitrary unit	Minimum fluorescence vield under fully dark-adapted
1 02 000		conditions. When provided, the cells of this column
		should contain the same value for all the actinic
		measurements made after the dark adaptation.
		Alternatively this value could be placed as the first
		value in the !FoorFs' column (preferred).
FmDark	Arbitrary unit	Maximum fluorescence yield under fully dark-adapted
		conditions. When provided, the cells of this column
		should contain the same value for all the actinic
		measurements made after the dark adaptation.
		Alternatively this value could be placed as the first
		value in the !FmorFm' column (preferred).

3 Applications and Derivation

The Leafweb: December 2022 dataset is unique in that it contains simultaneous measurements of leaf gas exchange and pulse – amplitude modulated (PAM) fluorometry across plant functional types, photosynthetic pathways, and climates. Another key feature of this dataset is that it includes multi-type response curves (light, CO₂, temperature, and O₂). This dataset supports complete modeling of photosynthesis at the leaf scale, including photophysical, photochemical, and biochemical reactions. It will be particularly useful for research in the applications of remotely sensed solar induced chlorophyll fluorescence and the responses of energy dissipation pathways to environmental variations across species and climates.

4. Quality Assessment:

These data are considered at **Quality Level 1**. Level 1 indicates an internally consistent data product that has been subjected to quality checks and data management procedures. Data included in Leafweb-Sept2022 were obtained following standard protocols in gas exchange (Long and Bernacchi 2003) and PAM fluorometry (Baker 2008). The dataset has been evaluated in different modeling studies (Han et al. 2022a and b, Gu et al. 2022) and found to be of high quality.

5. Data Acquisition Materials and Methods:

The measurements used in this study were collected by different groups in different locations / countries for different objectives (Table 1). Some of the datasets used were already fully described elsewhere and generously shared by their owners. These datasets include 'Growdena' tomato and rice measured by Dr. Xinyou Yin of Wageningen University and Research (Yin *et al.*, 2020), Scots pine by Dr. Albert Porcar-Castell of University of Helsinki (Porcar-Castell, 2011), and cotton by Dr. Joseph Berry of Carnegie Institution for Science at Stanford (Weis and Berry, 1987). Some of the rest species were also used in other publications (Han *et al.*, 2022a &b). All measurements followed commonly accepted protocols of PAM fluorometry (Baker, 2008) and gas exchange (Long and Bernacchi, 2003) for stability and steady state.

Both the 'Growdena' tomato and rice datasets consisted of light response and CO₂ response curves measured on young but fully expanded leaves of four replicate plants (Yin *et al.*, 2020). Simultaneous PAM fluorescence and gas exchange measurements were made. For each replicate plant, one light response curve and one CO₂ response curve were measured at each of the five oxygen levels (2, 10, 21, 35 and 50%). The light response curves had PAR ranging from 20 to 1500 μ molm⁻²s⁻¹ while the CO₂ response curves had ambient CO₂ concentration ranging from 50 to 1500 ppm. The leaf temperature was controlled around 25°C ± 0.5°C. Some minor adjustments to this overall measurement design were detailed in Yin *et al.* (2020).

The Scots pine dataset consisted of year-round (15 August 2008 to 15 August 2009) continuous fluorescence observations under natural conditions on needles of Scots pine with a

monitoring PAM at a field site in southern Finland (Porcar-Castell, 2011). Accessed with a permanent scaffold tower, the needles were selected from the top of the canopy and parallelly arranged inside the PAM leaf clip. The same needles were used throughout the study period. The measurement interval was 10 minutes during the summer months and 30 minutes during other months. The measuring light was switched off between measuring intervals. The incident PAR and ambient air temperature were recorded simultaneously with the PAM measurements. However, no gas exchange measurements were taken, and no CO₂ responses were observed. Dark-adapted measurements were taken from nighttime. We filtered the Scots pine dataset based on the diurnal variations of the measured photochemical quantum yield of PSII (Φ_{PSII}) and PAR. This filtering ensured that the diurnal variations of environmental variables were large enough for robustly estimating model parameters. We removed days when the diurnal variation in Φ_{PSII} was less than 0.3, or when the diurnal maximum Φ_{PSII} was less than 0.5, or when the daily maximum incident PAR was less than 500 µmol m-2 s-1. The application of these thresholds removed days in which in-situ PAM monitoring may have been compromised by hazardous atmospheric conditions (e.g., rains) or PAM parameters may have too narrow diurnal variations for reliable daily fitting (e.g., whole heavily overcast days). After the filtering, the data remained were from day 228 to day 282 in 2008 (Aug 15 to Oct 8, 2008) and from day 116 to day 225 in 2009 (April 26 to August 13, 2009) with all winter days removed. 52% of the days within the 2008 measurement period and 73% of the days within the 2009 measurement period survived the data filtering and were thus used in the study. We did not partially filter a day (i.e., all data of a day were either all included, or all excluded) because partial filtering is difficult to be carried out objectively.

The cotton dataset provided by Dr. Joe Berry was environmentally controlled response curves made at either 2% or 21% ambient O₂ concentration (Weis and Berry, 1987). PAM fluorescence and gas exchange measurements were taken simultaneously. Among the curves made at 2% O₂ concentration, there were light response curves (PAR from 0 to 2500 μ molm⁻²s⁻¹) made at either 26 °C or 38 °C, CO₂ response curves (intercellular CO₂ concentration ranged from 10 to 600 ppm) and temperature response curves (10 to 40 °C) made at saturating light levels. Among the curves made at 21% O₂ concentration, there were temperature response curves (10 to 45 °C) made at saturating light levels, and light response curves (PAR from 0 to 2800 μ molm⁻²s⁻¹) made at 25 °C and 40 °C ambient temperature, respectively.

The other datasets cover 26 species (22 C_3 and 4 C_4) in five locations in the US, Canada, and China, using gas exchange systems equipped with PAM fluorometry (Table 1). The species include lianas, shrubs, boreal deciduous trees, temperate deciduous trees, tropical deciduous trees, tropical evergreen trees, C_3 and C_4 grasses, and crop varieties. Measurements were taken at Cornell Botanic Gardens (42°26'N; 76°28'W), Cornell Musgrave Research Farm (42°43'N; 76°40'W) and Oak Ridge National Laboratory, Tennessee in the US, Xishuangbanna Tropical Botanical Garden (21°41'N; 101°25'E) in China, and the University of Guelph in Canada.

Nine C₃ and four C₄ species at Cornell Botanic Gardens and Cornell Musgrave Research Farm were measured with both light and CO₂ response curves, while only light response curves were collected on C₃ species at Xishuangbanna Tropical Botanical Garden. For each light or CO₂ response curve, 3-4 healthy and fully expanded sunlit leaves were selected as replicates of each species. At Cornell Botanic Gardens and Cornell Musgrave Research Farm, joint light and CO₂ response curves were measured with GFS-3000 (Walz, Effeltrich, Germany) equipped with fluorescence measuring head (3010-S, Walz). At Xishuangbanna Tropical Botanical Garden, light response curves were measured with LI-6800 (LI-COR Inc., Lincoln, NE, USA) equipped with leaf multiphase flash fluorometer chamber (6800-01A, LI-COR Inc). For GFS-3000, relative humidity was kept between 50% and 60%, the flow rate at 700 mL min⁻¹, and the leaf temperature at 25 °C. Prior to actual measurements of light and CO₂ response curves, photosynthesis was first induced with a saturating light intensity. Once the steady state was reached (usually within 20 minutes), the gas exchange and ChIF parameters were recorded. For LI-6800, the relative humidity was set to 60%, and the flow rate to 500 mL min⁻¹. For the species in Xishuangbanna Tropical Botanical Garden, it was challenging to control leaf temperatures to a standard reference temperature of 25 °C utilized for the species at other locations because of the high ambient air temperatures and the actual leaf temperatures may be up to 33 °C.

Light response curves were automatically performed following a sequence of PAR intensities: 2000, 1800, 1500, 1200, 1000, 800, 500, 300, 200, 150, 100, 50 µmol photon m⁻² s⁻¹ for all species at Cornell Botanic Gardens, Cornell Musgrave Research Farm, and Xishuangbanna Tropical Botanical Garden. For all measurements, the ambient CO₂ concentration within the cuvette was maintained at 400 ppm. The automated measurement program met the standard stability criteria (the changes of Fs within 20s, the stability of the differences in H₂O and CO₂ concentrations between reference and sample chambers within 20s) of LI-6800 or GFS-3000. The time interval between measurements at different light intensities was restricted to 120–240 seconds for LI-6800 and 120 seconds for GFS-3000. Following the GFS-3000 protocol, a waiting period of at least 10 minutes was used, depending on the temperature difference between the ambient environment and the leaf chamber, after the set leaf temperature was achieved, prior to our actual measurements.

CO₂ response curves were automatically collected following a sequence of CO₂ concentrations: 400, 300, 200, 150, 100, 50, 0, 380, 550, 800, 1000, 1200, 1500 ppm under the saturated light intensity (2000 µmol photon $m^2 s^{-1}$ for species at Cornell Botanic Gardens and Cornell Musgrave Research Farm). The stability criteria were identical to that followed by the light response curves. The time interval between measurements at different CO₂ concentrations was restricted to 120–240 seconds for LI-6800 and 200 seconds for GFS-3000. Gas exchange variables, steady-state and maximum ChIF under light (Fs and Fm') were obtained from light and CO₂ response curves. To measure the maximum and minimum ChIF under fully dark-adapted conditions (F_M and F₀) for each leaf replicate, the measured area of each leaf was first marked to keep the same measuring position for measurements of light response curves and ChIF in dark-adapted leaves. We wrapped the measured leaf with aluminum foil, dark-adapted it for half an hour, and then recorded F_M and F₀ of the same measured area at the same position as the light or CO₂ response curves. Similar procedures were applied to species measured at Oak Ridge National Laboratory by the same researcher (Dr. Jimei Han).

At the University of Guelph, Ontario, Canada, tomato 'Basket Vee' was 5-6 weeks old, grown in a standard potting mix (Sungro professional growing mix #1, Soba Beach, AB, Canada), fertigated with 20-8-20 fertilizer (Plant Products Inc., Leamington, ON, Canada) mixed in regular tap water (Guelph, Ontario tap water is relatively high in Calcium and magnesium carbonates) and adjusted to a pH of 5.5 with phosphoric acid to a final EC of 2.3 mS/cm. Plants were grown in a growth chamber at 21°C and 200 μ mol m⁻² s⁻¹ under either 12 hr light/ 12 hr dark or 24 hr light / 0 hr dark photoperiods (Biochamber, Winnipeg Canada) at the time of the experiment. The third true leaf was chosen as it was mature, fully expanded, and could fit the fluorometer gasket with no major obstructing veins. Simultaneous gas exchange and chlorophyll

fluorescence were performed using the LiCor 6400 with the 6400-40 leaf chamber fluorometer head. An intensive series of protocols were modified from Bellasio *et al.* (2016) and A/Ci curve protocol was modified from Sharkey (2019). Prior to running protocols, fluorescence measurement parameters were calibrated (Measuring intensity = 2, Light frequency = 10kHz, filter = 5, Gain = 10) and (Multi-phase flash intensity = 9, ramp depth 40%, frequency = 20kHz, filter 50kHz). Grease was applied to the gas exchange gaskets to ensure minimal leakage. CO₂ mixer calibration and other standard preparations were performed before each day of measurements. Block temperature was set to 20 °C and relative humidity was maintained at 70-80% throughout the measurement period (to mimic growing conditions). On a single leaf over the course of 10 hours, a series of protocols modified from Belassio *et al.* (2016) and Sharkey (2019) were performed in the following order: Dark respiration, survey measurement, ambient oxygen A/Ci curve, ambient oxygen light curve, low oxygen survey measurement, low oxygen A/Ci curve, low oxygen light curve, low oxygen dark respiration. This yielded four curves with Φ_{PSII} and CO₂ assimilation simultaneously, survey measurements at growing conditions, Fv/Fm, and quenching dynamics. Protocols for different types of measurements are as follows:

- Ambient O₂ dark-adapted respiration and Fv/Fm. Leaf was clamped and dark-adapted for 30 min with fluorescence measuring light off. Flow rate was set at 50µmol/s, CO2R ~ambient (440ppm), block temperature 20 C, RH 70-80%. 10 repeated readings of dark respiration were made at 20sec apart. Then fluorescence measuring light was put on for ~ 4min to stabilize, and Fo and Fm were measured for dark-adapted max photochemical quantum yield of PSII.
- Ambient O₂ A/Ci curve. The light intensity was kept at 200 μmol m⁻² s⁻¹ (low light) and flow rate at 120 μmol s⁻¹. CO2R was auto-programmed to start low and incrementally increase concentration every 150-180 seconds (50, 75, 100, 125, 150, 200, 300, 350, 400, 450, 500, 550, 600, 700, 800, 1000, 1200, 1500, 440) based on recommendations from Sharkey (2019). Fs and Fm' were measured at each CO₂ concentration point.
- 3. Ambient O₂ light curve. PAR was set to saturating level (determined to be 1200 μmol m⁻² s⁻¹ in tomato 'Basket Vee'), flow rate at 150μmols⁻¹, and CO2S at 430 ppm for up to 45 min for stabilization. The light intensity was then auto-programmed to incrementally lower PAR every 5-6min (1200, 1000, 750, 500, 300, 200, 150, 100, 75, 50, 40, 30, 20, 10 μmol m⁻² s⁻¹). At each light intensity Fs, Fm', and Fo' were measured.
- Low O₂ A/Ci curve. Light intensity was kept at 200 μmol m⁻² s⁻¹ (low light) and flow rate at 120μmol s⁻¹. CO2R was auto-programmed to start low and incrementally increase concentration every 150-180 seconds (50, 75, 100, 125, 150, 200, 300, 350, 400, 450, 500, 550, 600, 700, 800, 1000, 1200, 1500, 440 ppm) based on recommendations from Sharkey (2019). At each CO₂ concentration point, Fs and Fm² (but not Fo²) were measured.
- 5. Low O₂ light curve. PAR was set to saturating level (determined to be 1200 μmol m⁻² s⁻¹ in tomato 'Basket Vee'), flow rate at 150μmol s⁻¹, and CO2S at 430 ppm. After waiting for up to 45 min for stabilization. Light intensity was auto-programmed to incrementally lower PAR every 5-6min (1200, 1000, 750, 500, 300, 200, 150, 100, 75, 50, 40, 30, 20, 10). At each light intensity, Fs, Fm', and Fo' (not used in this study) were measured.
- 6. Low O₂ dark respiration and Fv/Fm. Leaf was dark-adapted for 30min with fluorescence measuring light off. Flow rate was set at 50 μmol s⁻¹, CO2R at ~ambient (440 ppm), block temperature at 20 C, and RH 70-80%. 10 repeated measurements of dark respiration were made at 20sec apart. Fluorescence measuring light was then turned on

for ~4min to stabilize. Dark-adapted max photochemical quantum yield of PSII was then measured.

6. Related References:

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7. Data Access:

For public access to Leafweb data, please visit the Leafweb site: www.leafweb.org

Contact for Data Access Information: https://www.leafweb.org/contact/