Table S1: Allometric equations of species used for the calculation of tree biomass.

Species name	Biomass equation			
	Stem	Branch	Leave	Root
Quercus mongolica	W=0.2053*D^2.2928	W=0.0098*D^2.7006	W=0.0257*D^1.9377	W=0.0772*D^2.2983
Larix gmelinii	W=0.0625*D^2.5525	W=0.0122*D^2.4563	W=0.0600*D^1.7714	W=0.0160*D^2.5912
Ulmus macrocarpa	W=0.0607*D^2.5990	W=0.0678*D^1.9623	W=0.0148*D^1.9816	W=0.0633*D^2.1362
Sorbus alnifolia	W=0.0607*D^2.5990	W=0.0678*D^1.9623	W=0.0148*D^1.9816	W=0.0633*D^2.1362
Tilia amurensis	W=0.1256*D^2.1210	W=0.0193*D^2.0701	W=0.0734*D^1.2285	W=0.0977*D^1.9056
Syringa reticulata	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Acer truncatum	W=0.0464*D^2.6008	W=0.0110*D^2.9347	W=0.0085*D^2.3421	W=0.0670*D^2.3783
Tilia mongolica	W=0.1256*D^2.1210	W=0.0193*D^2.0701	W=0.0734*D^1.2285	W=0.0977*D^1.9056
Fraxinus rhynchophylla	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Abelia biflora	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Populus davidiana	W=0.2538*D^1.1815	W=0.0470*D^1.9739	W=0.0222*D^2.1885	W=0.2501*D^1.6022
Tilia mandshurica	W=0.1256*D^2.1210	W=0.0193*D^2.0701	W=0.0734*D^1.2285	W=0.0977*D^1.9056
Betula dahurica	W=0.1795*D^2.0440	W=0.0094*D^2.7151	W=0.082*D^2.1970	W=0.565*D^2.1311
Betula platyphylla	W=0.1951*D^2.2398	W=0.0228*D^2.2723	W=0.0111*D^1.9708	W=0.0322*D^2.3600
Malus baccata	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Ulmus davidiana var. japonica	W=0.0607*D^2.5990	W=0.0678*D^1.9623	W=0.0148*D^1.9816	W=0.0633*D^2.1362
Pinus tabuliformis	W=0.2000*D^1.9441	W=0.0055*D^2.3134	W=0.0599*D^1.9368	W=0.0308*D^2.2204
Armeniaca sibirica	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Pyrus ussuriensis	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730
Juglans mandshurica	W=0.1030*D^2.2110	W=0.0150*D^2.5840	W=0.0150*D^2.0930	W=0.0970*D^2.2730

Table S2: Allometric equations of species used for the calculation of shrub biomass.

Species name	Biomass equation	Biomass equation	Biomass equation	Biomass equation
Components	Stem	Branch	Leave	Root
Leptopus chinensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Fraxinus rhynchophylla	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Spiraea pubescens	M=1.0434*V_c^0.9868	M=1.1322*V_c^0.9033	M=0.0984*V_c^0.5541	M=-0.0057+0.8109*M_a
Lespedeza bicolor	M=-0.0021+0.8790*V_c	M=-0.0024+1.0686*V_c	M=-0.0001+0.1791*V_c	M=0.0072+0.5644*M_a
Quercus mongolica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Viburnum burejaeticum	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Tilia mongolica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Deutzia scabra	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Ulmus macrocarpa	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Corylus heterophylla	M=0.0317*(D^2*H)^0.8184	M=0.0474*(D^2*H)^0.8038	M=0.0185*(D^2*H)^0.6651	M=0.4305*M_a^0.7827
Rubus crataegifolius	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Rhododendron micranthum	M=0.0274*D^2*H)^0.6120	M=0.0274*(D^2*H)^0.6120	M=0.0121*(D^2*H)^0.5376	M=0.0213*(D^2*H)^0.6477
Deutzia hamata	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Lonicera maximowiczii	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Vitis amurensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7400	M=0.0202*(D^2*H)^0.7401	M=0.0202*(D^2*H)^0.7402
Abelia biflora	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Syringa reticulata var. amurensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Cerasus tomentosa	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Rosa davurica	M=-0.0027+0.0393*(D^2*H)	M=-0.0011+0.0524*(D^2*H)	M=0.0013+0.0133*(D^2*H)	M=0.0342*(D^2*H)^0.6695
Tilia amurensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Corylus heterophylla	M=0.0317*(D^2*H)^0.8184	M=0.0474*(D^2*H)^0.8038	M=0.0185*(D^2*H)^0.6651	M=0.4305*M_a^0.7827
Acer truncatum	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Juglans mandshurica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Philadelphus schrenkii	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Ulmus davidiana var. japonica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Salix chaenomeloides	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Schisandra chinensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Betula platyphylla	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Acer mono	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Adeinophora stricta	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Syzygium aromaticum	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Pinus tabuliformis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H

Vitex negundo var. heterophylla	M=0.1389*A_c^1.0343	M=0.2709*A_c^1.0354	M=0.1225*A_c^1.0370	M=-0.0104+1.2420*M_a
Lespedeza floribunda	M=-0.0021+0.8790*V_c	M=-0.0024+1.0686*V_c	M=-0.0001+0.1791*V_c	M=0.0072+0.5644*M_a
Cerasus humilis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Deutzia parviflora	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Armeniaca sibirica	M=0.0895*(D^2*H)^0.219	M=0.1114*(D^2*H)^0.7267	M=0.0160*(D^2*H)^0.8205	M=0.0798*(D^2*H)^0.8316
Rhamnus davurica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Caragana sinica	M=0.3164*V_c^0.7296	M=0.3493*V_c^0.7136	M=0.0306*V_c^0.6026	M=0.1953*M_a^0.7579
Deutzia scabra	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Betula dahurica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Tilia mandshurica	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Celtis koraiensis	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Lonicera villosa	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Ostryopsis davidiana	M=0.0263+0.0238*D^2*H	M=0.046*(D^2*H)^0.6299	M=0.012*(D^2*H)^0.3315	M=-0.0034+0.0495*D^2*H
Berberis poiretii	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Ailanthus altissima	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H
Amorpha fruticosa	M=0.0202*(D^2*H)^0.7399	M=0.0202*(D^2*H)^0.7399	M=0.0051+0.0065*D^2*H	M=-0.0026+0.0225*D^2*H

Note: 'D' indicates basal area; 'H' height; 'Vc' Vc=(crown/2)^2*π*H; and 'M' and 'W' represent total biomass of each specie.

Table S3: A summary of 24 plot variables is used in SEM for Beijing temperate forest, including stand factors (grey), species diversity (italic), and environmental variables (bold).

Variables	**Unit**	**Minimum**	**Maximum**	**Mean**
Dependent variables				
Tree C storage (TC)	t ha^{-1}	50.96	130.19	95.66
Shrub C storage (SC)		0.01	0.41	0.11
Herb C storage (HC)		0.01	0.70	0.26
Explanatory indicators				
Forest types		0.00	1.00	0.25
Basal area (stand indicator)	m^2 ha^{-1}	19.48	43.98	30.21
stand density (stand indicator)	ind. ha^{-1}	800.00	3175.00	1727.08
Mean height (stand indicator)	m	6.12	14.95	8.96
Mean DBH	cm	10.22	20.55	14.05
maximum height (stand indicator)	m	9.60	30.40	16.67
Tree Species richness (diversity indicator)		1.00	8.00	5.33
Tree Shannon-Weaver (diversity indicator)		0.00	2.57	1.46
Simpson index (diversity indicator)		0.00	0.80	0.49
Pielou index (diversity indicator)		0.00	0.87	0.57
Canopy openness (Environmental indicator)		9.19	16.34	12.39
Elevation (Environmental indicator)	m	1100.00	1400.00	1246.41
Shrub species richness (diversity indicator)		9.19	16.34	12.39
Shrub Shannon-Weaver (diversity indicator)		5.00	12.00	8.04
Simpson index (diversity indicator)		2.32	3.58	2.95
Pielou's index (diversity indicator)		0.98	1.00	0.99
Herb species richness (diversity indicator)		4.00	14.00	7.50
Herb Shannon-Weaver (diversity indicator)		1.95	3.77	2.78
Simpson index (diversity indicator)		0.73	0.92	0.84
Pielou's index (diversity indicator)		0.96	1.00	0.98

Assessed-re-assessed process of SEMs

In this study, we performed confirmatory factor analyses to assess the validity and reliability of the models using data obtained from a field inventory. Stand variables, such as mean diameter at breast height (DBH), mean height, maximum height, basal area and stem density were constructed based on the primary collected data. However, upon reassessing the model fit of structural equation model (SEM), we found it to be poor. This poor fit can be attributed to multicollinearity, where some variables were highly correlated and redundant in their meaning. To improve the carbon storage model for trees, we identified the mean DBH and the basal area as two strong factors, while other biotic characteristics (tree density, mean height, and maximum height) were removed as indicators due to their weak correlation loadings with the variable of the carbon storage construct tree layer. On the other hand, mean height and maximum height were found to be powerful predictors for the understory carbon storage models. Covariance indicators with poor fit were ignored based on bootstrap-based model fit evaluation (SRMR < 0.08) and the development of discriminant and convergent validity of SEM. Indicator loadings with a correlation coefficient (*r*) greater than 0.70 were considered standard, and any indicators with non-significant weight and loading estimates were dropped from further analysis of the SEM .

To calculate the species diversity indices for the vegetation component (tree, shrub, and herb), we used the 'Vegan' package in the R software. Subsequently, we employed PLS-SEM analysis to examine the direct and indirect effects of species diversity on carbon storage in trees, shrubs, and herbs. However, we found that Pielou's evenness correlation loads ($r = 0.26$) were insufficient and did not meet the standard indicator loading threshold ($r > 0.70$). Similarly, Shannon-Wiener, Simpson, and richness indicators exhibited high multicollinearity with latent variables (species diversity), with loadings ranging from 0.90 to 0.95. Among these, the Shannon-Wiener index was selected as a robust indicator of species diversity in the SEM to analyze its direct and indirect effects on carbon storage in trees, shrubs, and herbs.

Here, we regarded forest types as a categorical fixed factor in a numerical way (from mixed to conifer forest types as ordered and detailed in table 1). To determine the influence on overstory, shrub and herb carbon storage, we analyzed 24 sample plots across four forest types, investigating whether measured factors (stand, species indices, and environmental factors) or the categorical fixed variable (forest type) can explain for the observed changes (carbon storage). Furthermore, we considered elevation and canopy openness as environmental indicators. SEM was used to investigate the relationship between carbon storage in trees, shrubs, and herbs and various ecological variables. The inclusion of the elevation covariance indicator as an environmental factor was designed to account for additional computationally independent effects on carbon storage. However, we observed strong collinearity between canopy openness loads and elevation indicators (with correlation coefficients of 0.81 and 0.85, respectively) within the environmental factor construct. This multicollinearity among indicator loadings, which conveyed similar meanings, restricted the significance, direction, and magnitude of other indicators, making it challenging to interpret the best-fit model of the SEM.

Table S4: We chose the best-fit SEMs for carbon storage in trees, shrubs, and herbs using model fit criteria (SRMR, dULS, dG), with R2 indicating the proportion explained by independent variables in TC, SC and HC (TC indicated tree carbon, SC, shrub carbon and HC herb carbon).

Overview of models	Numbers of stand factors	Numbers of Diversity indicators	Number of Environmental variables	Forest types	Model fit summary				Best fit SEM Model selection assessed-re-assessed based on SRMR
					SRMR	d-ULS	dG	R2	
1a(TC)	**2.00**	**1.00**	**1.00**	**1.00**	**0.07**	**0.11**	**0.10**	**0.75**	**Accepted**
1b(SC)	**2.00**	**1.00**	**1.00**	**1.00**	**0.07**	**0.29**	**0.19**	**0.16**	**Accepted**
1c(HC)	**2.00**	**1.00**	**1.00**	**1.00**	**0.07**	**0.13**	**0.06**	**0.36**	**Accepted**
2a(TC)	3.00	2.00	1.00	1.00	0.14	0.71	0.46	0.75	Rejected
2b(SC)	3.00	2.00	1.00	1.00	0.19	2.01	0.91	0.20	Rejected
3a(TC)	4.00	2.00	2.00	1.00	0.18	1.69	1.32	0.69	Rejected
3b(SC)	4.00	2.00	2.00	1.00	0.19	1.98	0.93	0.19	Rejected
3c(HC)	4.00	2.00	2.00	1.00	0.11	0.35	0.14	0.37	Rejected
4a(TC)	5.00	3.00	2.00	1.00	0.18	2.63	1.82	0.71	Rejected
4b(SC)	5.00	3.00	2.00	1.00	0.20	3.03	1.87	0.36	Rejected
4c(HC)	5.00	3.00	2.00	1.00	0.22	3.79	8.66	0.41	Rejected
5a(TC)	6.00	4.00	2.00	1.00	0.20	4.15	3.68	0.68	Rejected
5b(SC)	6.00	4.00	2.00	1.00	0.19	3.77	8.24	0.48	Rejected
5c(HC)	6.00	4.00	2.00	1.00	0.16	_	_	0.37	Bad