Supplementary Materials: Optimizing the semi-analytical algorithms for estimating *Chlorophyll-a* and *Phycocyanin* concentrations in inland waters in Korea

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A1. Semi-analytical algorithms

The backscattering function and Y value in the IIMIW model were parametrized as

$$b_p(P_1) = \frac{b_b(778) - b_w(778)}{\left(\frac{P_1}{778}\right)^Y} \quad \text{(S1)}$$

$$Y = P_2\left(P_3 + P_4 \exp\left(P_5 \frac{r_{rs}(P_6)}{r_{rs}(P_1)}\right)\right) \quad \text{(S2)}$$

where the P_x is an interested parameter.

The additional parameters were selected in terms of the absorption coefficient of PC like below

$$a_{cdom}(P_7) = a_g(P_7) - a_{phy-pc}(P_7) \quad \text{(S3)}$$

$$a_{cdom}(P_8) = a_g(P_8) - a_{phy-pc}(P_8) \quad \text{(S4)}$$

$$\mathrm{S_{cdom}} = \frac{1}{P_9}\ln\left(\frac{a_{cdom}(P_7)}{a_{cdom}(P_8)}\right) \quad \text{(S5)}$$

$$a_{phy-pc}(P_7, P_8, P_{23}) = P_{10}a_g(675) + P_{11} \quad \text{(S6)}$$

The backscattering that was independent on the wavelength was set to parameter as

$$b_b(778) = \frac{P_{12}R_{rs}(778)}{0.082 + P_{13}R_{rs}(778)} \quad \text{(S7)}$$

Then, the bio-optical algorithms were parameterized as follows.

For the Gons algorithm,

$$Chl - a(mg\ m^{-3}) = \frac{a_g(P_{14})}{P_{15}} \quad \text{(S8)}$$

For the Gilerson algorithm,

$$Chl - a(mg\ m^{-3}) = \left(\frac{a_g(P_{14})}{P_{16}}\right)^{P_{17}} \quad \text{(S9)}$$

For the Ritchie algorithm,

$$Chl - a(mg\ m^{-3}) = P_{22}(P_{18}a_{gh}(630) + P_{19}a_{gh}(647) + P_{20}a_{gh}(P_{14}) + P_{21}a_{gh}(630)) \quad \text{(S10)}$$

For the PC algorithm,

$$PC\ (mg\ m^{-3}) = \frac{a_{pc}(P_{23})}{P_{24}} \quad \text{(S11)}$$

For the Duan algorithm,

$$a_g(\lambda_1) = \frac{R_{rs}(709)}{R_{rs}(P_{14})}(a_w(709) + b_b) - \mathrm{b_b}^{P_{25}} - a_w(P_{14}) \quad \text{(S12)}$$

$$Chl - a(mg\ m^{-3}) = \frac{a_g(P_{14})}{P_{26}} \quad \text{(S13)}$$

For the Simis algorithm,

$$a_g(\lambda_1) = \frac{1}{P_{27}}\left(\frac{R_{rs}(709)}{R_{rs}(P_{14})}(a_w(709) + b_b) - b_b - a_w(P_{14})\right) \quad \text{(S14)}$$

$$Chl - a(mg\ m^{-3}) = \frac{a_g(P_{14})}{P_{28}} \quad \text{(S15)}$$

For the Simis algorithm for PC

$$a_g(P_{23}) = \frac{1}{P_{29}}\left(\frac{R_{rs}(709)}{R_{rs}(P_{23})}(a_w(709) - b_b) - b_b - a_w(P_{23})\right)$$

$$-\left(\frac{P_{30}}{P_{27}}\left(\frac{R_{rs}(709)}{R_{rs}(P_{14})}(a_w(709) - b_b) - b_b - a_w(P_{14})\right)\right) \quad \text{(S16)}$$

$$PC(mg\ m^{-3}) = \frac{a_g(P_{23})}{P_{31}} \quad \text{(S17)}$$

Table S1. Summary of the *Chl-a* algorithms

<table>
<tr><th colspan="6">Chl-a Algorithms</th></tr>
<tr><th></th><th>Gons*</th><th>Gilerson**</th><th>Ritchie***</th><th>Simis****</th><th>Duan*****</th></tr>
<tr><td rowspan="2">Semi-analytical algorithm</td><td colspan="3" rowspan="2">$$b_b(\lambda) = b_p(560)\left(\frac{560}{\lambda}\right)^{Y} + b_w(\lambda)$$ $$b_p(560) = \frac{b_b(778) - b_w(778)}{\left(\frac{560}{778}\right)^{Y}}$$ $$b_b(778) = \frac{r_{rs}(778)a_w(778)}{0.082 - r_{rs}(778)}$$ $$Y = 2.0\left(1 - 1.2\exp\left(-0.9\frac{r_{rs}(443)}{r_{rs}(560)}\right)\right)$$ $$a_g(\lambda_1) = [\frac{R(\lambda_2)b_b(\lambda_1)}{R(\lambda_1)b_b(\lambda_2)}(\mathrm{a_w}(\lambda_2) + b_b(\lambda_2)] - b_b(\lambda_1) - a_w(\lambda_1)$$</td><td colspan="2">$$b_b(778) = \frac{1.61R_{rs}(778)}{0.082 - 0.6R_{rs}(778)}$$</td></tr>
<tr><td>$$a_g(\lambda_{chla}) = \frac{1}{0.68}\left(\frac{R_{rs}(709)}{R_{rs}(\lambda_{chla})}(a_w(709) - b_b) - b_b - a_w(\lambda_{chla})\right)$$</td><td>$$a_g(\lambda_{chla}) = \frac{R_{rs}(709)}{R_{rs}(\lambda_{chla})}(a_w(709) + b_b) - \mathrm{b_b^{1.062}} - a_w(\lambda_{chla})$$</td></tr>
<tr><td></td><td>$$\frac{a_g(\lambda_{chla})}{a_g^*(\lambda_{chla})}$$</td><td>$$\left(\frac{a_g(\lambda_{chla})}{a_g^*(\lambda_{chla})}\right)^{1.124}$$</td><td>$$4.34(-0.3319a_{gh}(630) - 1.7485a_{gh}(647) + 11.9442a_{gh}(\lambda_1) - 1.4306a_{gh}(630))$$</td><td>$$\frac{a_g(\lambda_{chla})}{a_g^*(\lambda_{chla})}$$</td><td>$$\frac{a_g(\lambda_{chla})}{a_g^*(\lambda_{chla})}$$</td></tr>
</table>

Unit of the bio-optical model result is mg m^{-3}. * is referenced by Gons et al., (2002),** is referenced by Gilerson et al., (2010), *** is referenced by Ritchie (2008), **** is referenced by Simis et al., (2005), and ***** is referenced by Duan et al., (2012).

Table S2. Summary of the *PC* algorithms

	***PC* Algorithms**	
	Li*	**Simis****
Semi-analytical algorithm	$a_g(\lambda_1) = [\frac{R(\lambda_2)b_b(\lambda_1)}{R(\lambda_1)b_b(\lambda_2)}(a_w(\lambda_2) + b_b(\lambda_2)] - b_b(\lambda_1) - a_w(\lambda_1)$ $a_{phy}(\lambda) = a_g(\lambda) - a_{cdom}(\lambda)$ $a_{cdom}(412) = a_g(412) - a_{phy-pc}(412)$ $a_{cdom}(510) = a_g(510) - a_{phy-pc}(510)$ $S_{cdom} = \frac{1}{98}\ln\left(\frac{a_{cdom}(412)}{a_{cdom}(510)}\right)$ $a_{cdom}(\lambda) = a_{cdom}(412)\exp(-S_{cdom}(\lambda - 412))$ $a_{phy-pc}(\lambda) = C_1(\lambda)a_g(675) + C_2(\lambda)$ $a_{pc}(\lambda) = a_{phy}(\lambda) - a_{phy-pc}(\lambda)$	$a_g(\lambda_{pc}) = \frac{1}{0.84}\left(\frac{R_{rs}(709)}{R_{rs}(\lambda_{pc})}(a_w(709) - b_b) - b_b - a_w(\lambda_{pc})\right) - \left(\frac{0.24}{0.68}\left(\frac{R_{rs}(709)}{R_{rs}(\lambda_{chla})}(a_w(709) - b_b) - b_b - a_w(\lambda_{chla})\right)\right)$
	$\frac{a_{pc}(\lambda_{pc})}{a^*_{pc}(\lambda_{pc})}$	$\frac{a_g(\lambda_{pc})}{a^*_g(\lambda_{pc})}$

Unit of the bio-optical model result is mg m^{-3}. * is referenced by Li et al., (2015),** is referenced by Simis et al., (2007).

Table S3. Sensitivity parameter ranking for the semi-analytical algorithms

Parameter	Gons	Gilerson	Ritchie	Simis	Duan	Li	Simis(PC)
P_1	6 (4.6)	7 (39.6)	9 (3.5)	-	-	9 (85.0)	-
P_2	3 (39.3)	4 (333.3)	4 (22.0)	-	-	2 (849.2)	-
P_3	2 (52.0)	2 (457.7)	1 (32.5)	-	-	1 (1185.4)	-
P_4	4 (26.7)	5 (258.2)	5 (19.2)	-	-	4 (626.8)	-
P_5	5 (7.6)	6 (69.0)	6 (6.0)	-	-	5 (167.8)	-
P_6	8 (1.2)	9 (14.0)	12 (0.9)	-	-	11 (31.2)	-
P_7	-	-	-	-	-	7 (94.7)	-
P_8	-	-	-	-	-	6 (143.8)	-
P_9	-	-	-	-	-	8 (85.7)	-
$P_{10(P_7)}$	-	-	-	-	-	14 (10.8)	-
$P_{10(P_8)}$	-	-	-	-	-	13 (14.9)	-
$P_{10(P_{23})}$	-	-	-	-	-	12 (19.8)	-
$P_{11(P_7)}$	-	-	-	-	-	17 (2.2)	-
$P_{11(P_8)}$	-	-	-	-	-	15 (3.4)	-
$P_{11(P_{23})}$	-	-	-	-	-	16 (3.0)	-
P_{12}	-	-	-	4 (1.5)	4 (0.9)	-	7 (6.9)
P_{13}	-	-	-	5 (0.4)	5 (0.3)	-	8 (1.7)
P_{14}	7 (3.7)	8 (26.2)	8 (4.2)	3 (6.7)	3 (2.2)	-	5 (35.7)
P_{15}	1 (60.6)	-	-	-	-	-	-
P_{16}	-	1 (613.9)	-	-	-	-	-
P_{17}	-	3 (393.9)	-	-	-	-	-
P_{18}	-	-	11 (2.1)	-	-	-	-
P_{19}	-	-	7 (5.4)	-	-	-	-
P_{20}	-	-	3 (25.5)	-	-	-	-
P_{21}	-	-	10 (2.2)	-	-	-	-
P_{22}	-	-	2 (28.0)	-	-	-	-
P_{23}	-	-	-	-	-	10 (41.8)	6 (8.2)
P_{24}	-	-	-	-	-	3 (824.7)	-
P_{25}	-	-	-	-	2 (13.5)	-	-
P_{26}	-	-	-	-	1 (17.5)	-	-
P_{27}	-	-	-	2 (63.4)	-	-	3 (378.1)
P_{28}	-	-	-	1 (68.9)	-	-	-
P_{29}	-	-	-	-	-	-	1 (494.5)
P_{30}	-	-	-	-	-	-	4 (273.5)
P_{31}	-	-	-	-	-	-	2 (449.7)

(-) indicates the mean of the elementary effect value

Table S4. Performance analysis

Algorithms	**Referenced results**				**Single-objective optimization results**				**Multi-objective optimization results**			
	R^2	**RMSE (NRMSE)**	**R^2**	**RMSE (NRMSE)**	**R^2**	**RMSE (NRMSE)**	**R^2**	**RMSE (NRMSE)**	**R^2**	**RMSE (NRMSE)**	**R^2**	**RMSE (NRMSE)**
	Absorption coefficient*		**Concentration estimation****		**Absorption coefficient**		**Concentration estimation**		**Absorption coefficient**		**Concentration estimation**	
Gons	0.732	4.010 (1.217)	0.712	16.653 (0.428)	0.746	3.362 (1.232)	0.742	14.019 (0.360)	0.815	1.470 (0.539)	0.775	13.027 (0.335)
Gilerson	0.732	4.011 (1.218)	0.722	20.175 (0.518)	0.746	3.425 (1.255)	0.751	13.525 (0.347)	0.815	1.458 (0.534)	0.772	13.111 (0.337)
Ritchie	0.732	4.011 (1.218)	0.680	17.272 (0.444)	0.813	2.068 (0.758)	0.774	12.848 (0.330)	0.812	1.468 (0.538)	0.768	13.158 (0.338)
Simis	0.410	4.016 (1.219)	0.429	26.567 (0.682)	0.513	2.991 (1.096)	0.531	20.289 (0.521)	0.513	2.437 (0.893)	0.531	20.292 (0.521)
Duan	0.421	4.218 (1.281)	0.442	21.535 (0.553)	0.530	4.133 (1.255)	0.570	20.163 (0.518)	0.535	3.507 (1.285)	0.578	20.098 (0.517)
Li	0.002	10.805 (4.596)	0.001	1463.1 (50.186)	0.806	3.756 (1.592)	0.817	38.996 (1.338)	0.833	2.136 (0.941)	0.819	167.625 (5.750)
Simis (*PC*)	0.583	3.864 (1.644)	0.583	78.238 (2.684)	0.686	3.422 (1.456)	0.574	59.805 (2.051)	0.685	2.695 (1.187)	0.615	56.628 (1.942)

*The unit of RMSE for the absorption coefficient is m^{-1} and **the unit of RMSE for the concentration is mg m^{-3}. NRMSE is normalized root mean square error.

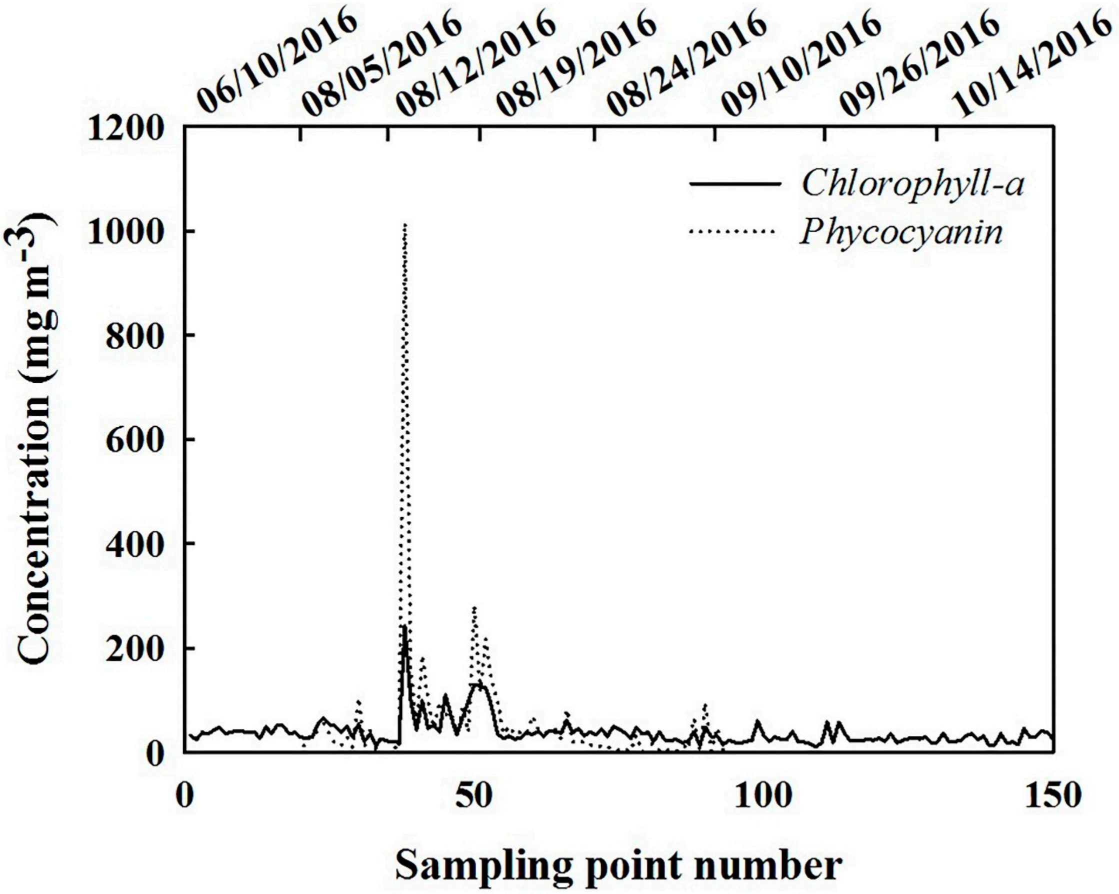

Figure S1. Temporal variation of the biomass concentrations, point number indicates the number of monitoring points.

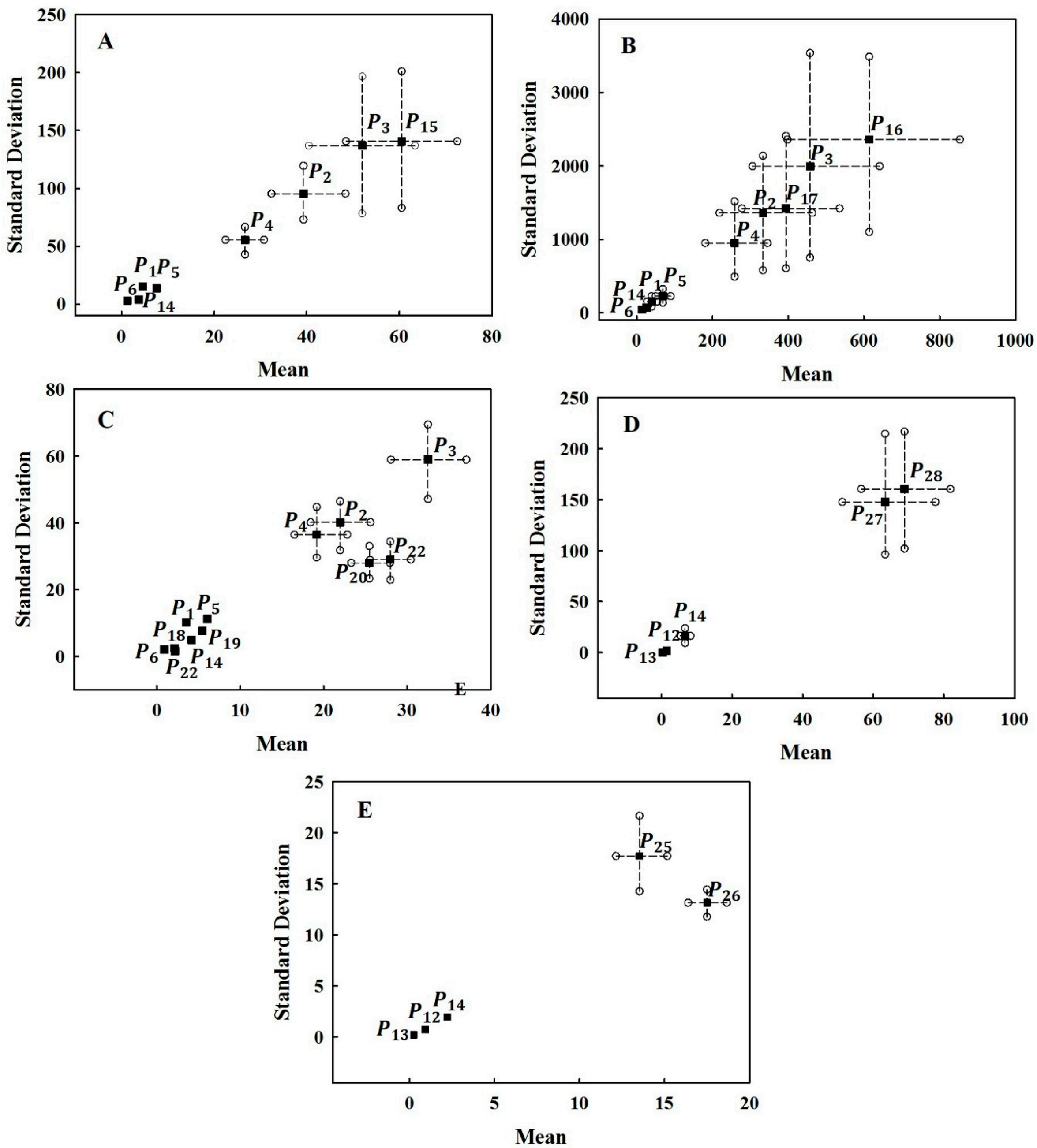

Figure S2. Sensitivity analysis results of *Chl-a* algorithms, A: Gons algorithm, B: Gilerson algorithm, C: Ritchie algorithm, D: Simis algorithm, and E: Duan algorithm

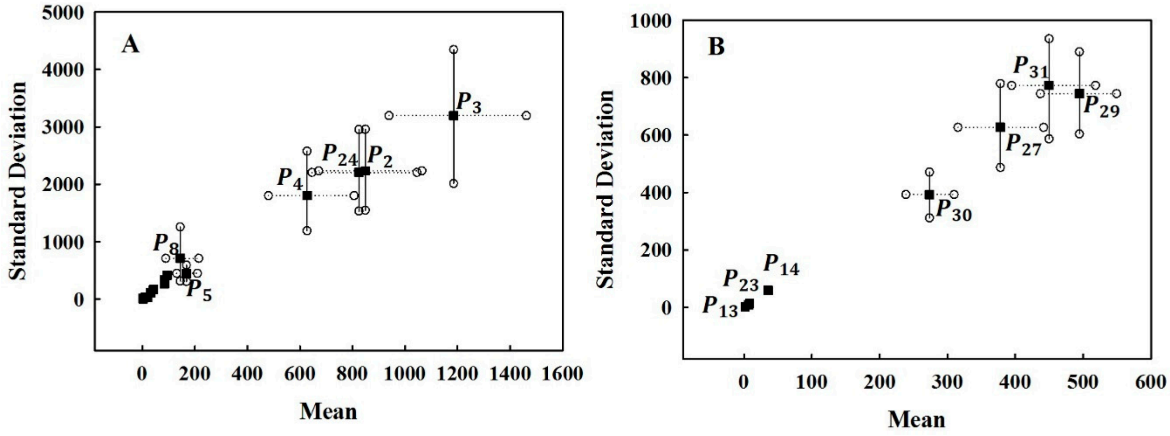

Figure S3. Sensitivity analysis of *PC* algorithms, A: Li algorithm and B:Simis algorithm

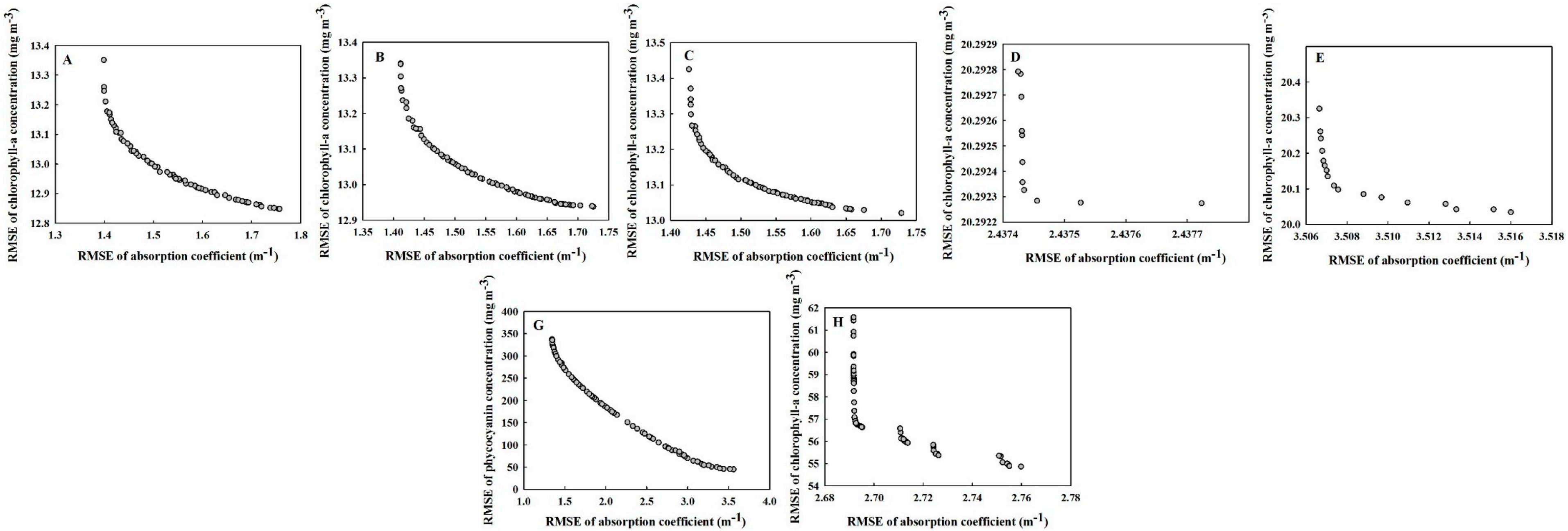

Figure S4. Pareto graph of multi-objective optimization, the top five panels are Pareto graph for Chl-a algorithm and the bottom panels are Pareto graph for PC algorithm, A is Gons algorithm, B is Gilerson algorithm, C is Ritchie algorithm, D is Simis algorithm, and E is Duan algorithm, G is Li algorithm and H is Simis algorithm

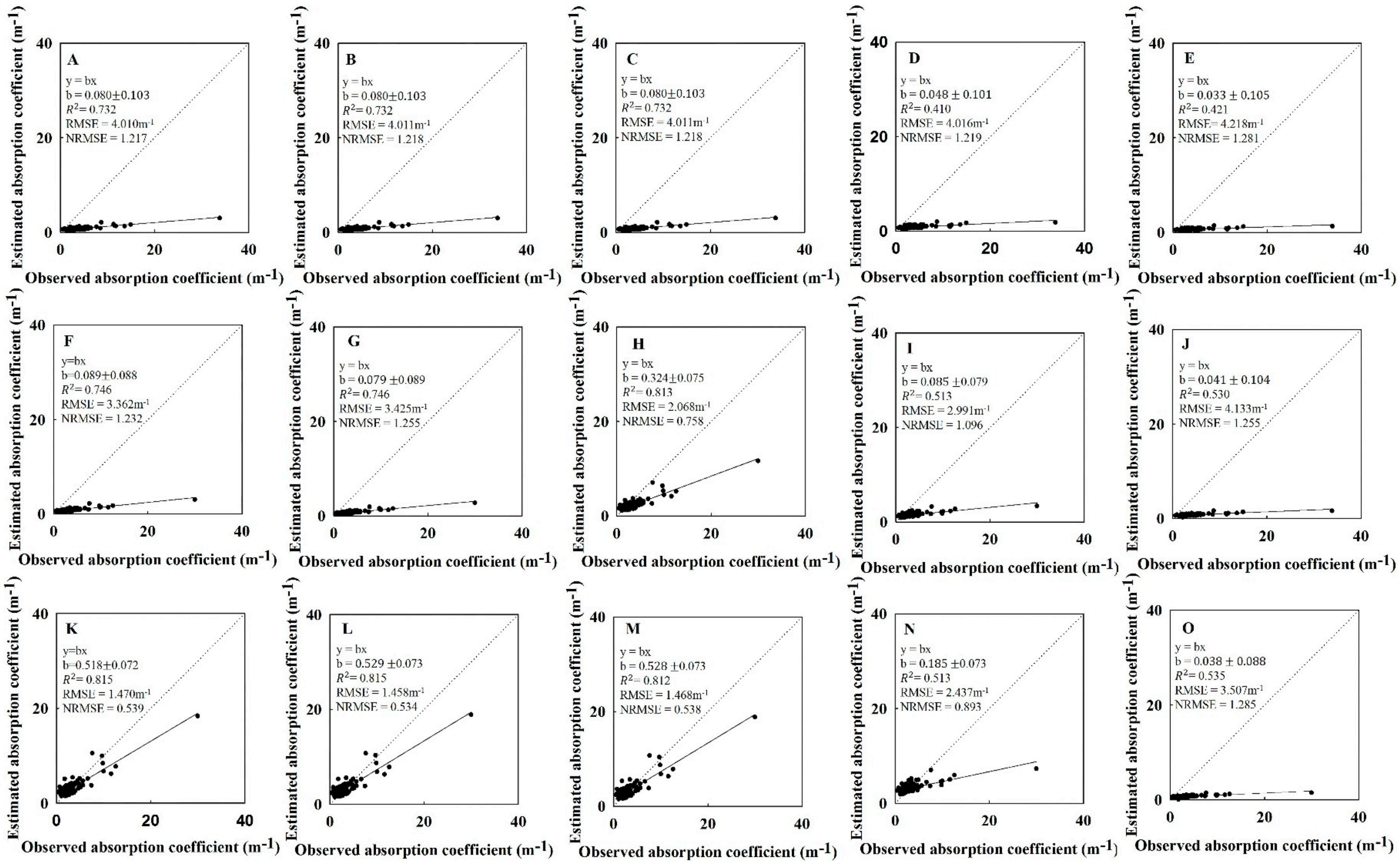

Figure S5. Comparison of measured, published and estimated from the single-objective and multi-objective optimization absorption coefficients in *Chl-a* algorithms. The top five panels are developed with published values, the middle five panels are developed with the single-objective optimization, and the bottom five panels are developed with the multi-objective optimization. A, F and K are Gons algorithm results, B, G, and L are Gons algorithm results, C, H, and M are Ritchie algorithm results, D, I, and N are Simis algorithm results, and E, J, and O are Duan algorithm results

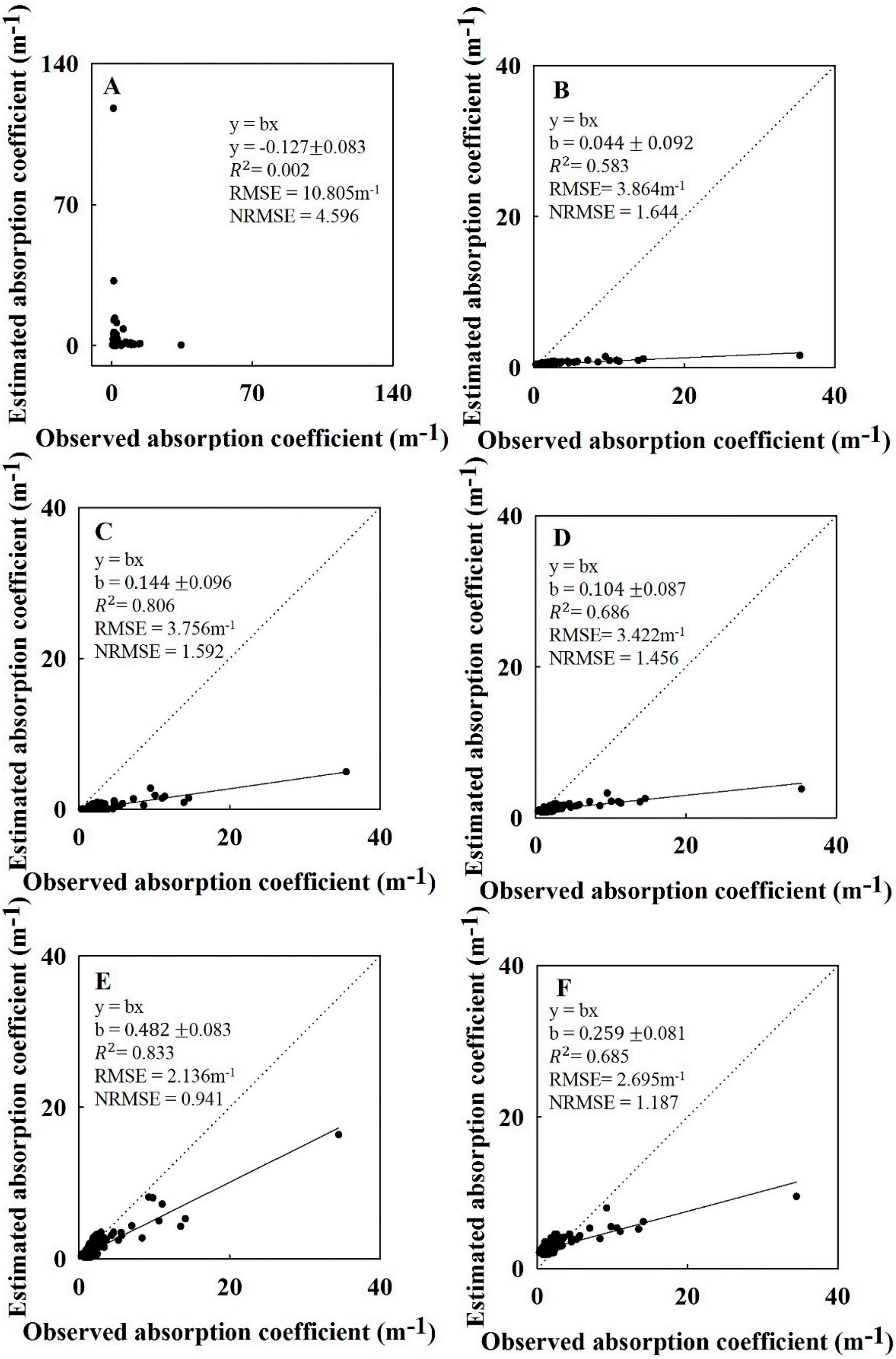

Figure S6. Comparison of measured, published and estimated from the single-objective and multi-objective optimization absorption coefficients in *PC* algorithms. The top two panels are developed with published values, the middle two panels are developed with single-objective optimization the bottom two panels are developed with the multi-objective optimization. A, C, and E are Li algorithm results, and B, D,and F are Simis algorithm results

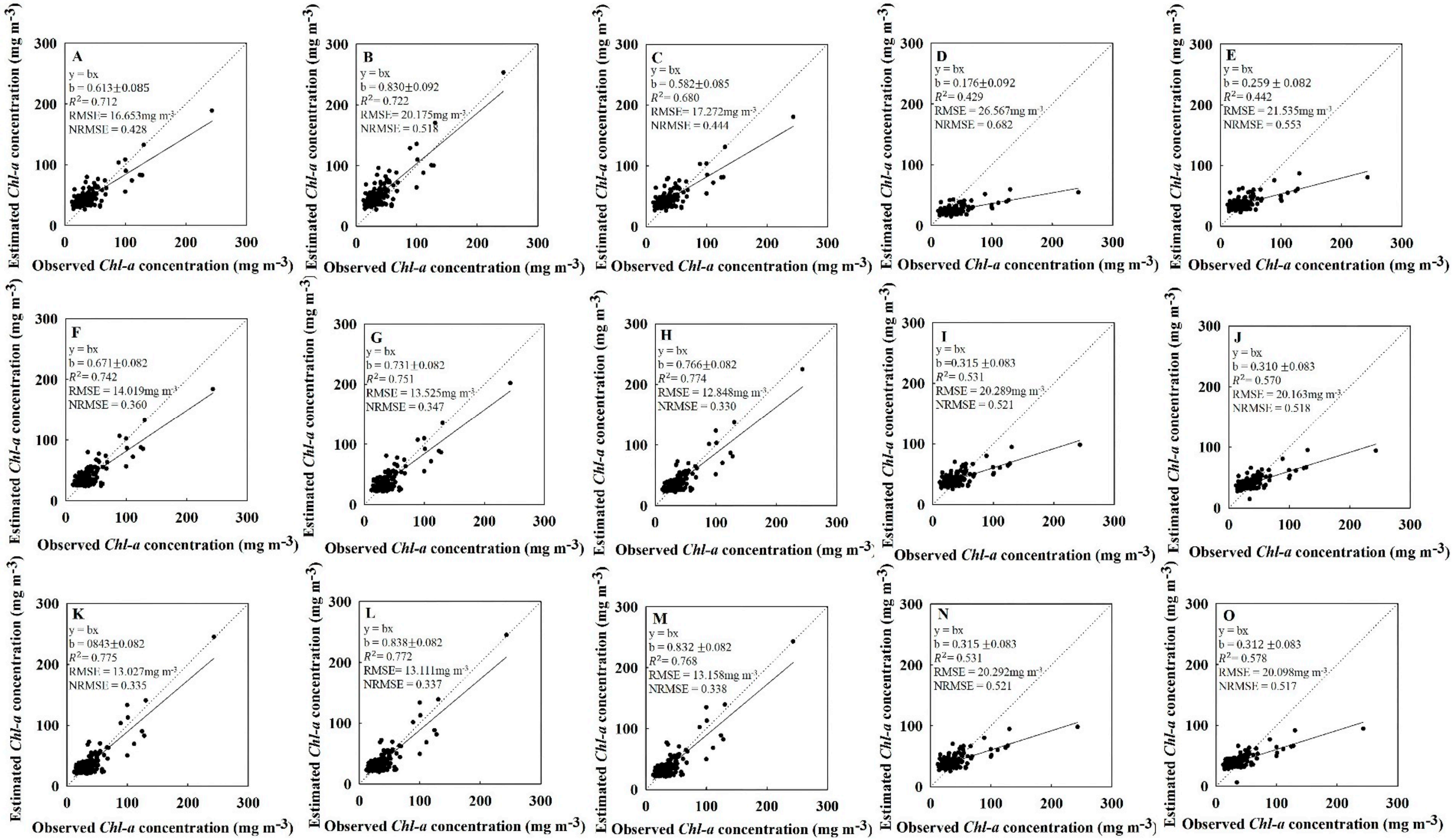

Figure S7. Comparison of measured, published and estimated from the single-objective and multi-objective optimization *Chl-a* concentration in *Chl-a* algorithms. The top five panels are developed with published values, the middle five panels are developed with the single-objective optimization, and the bottom five panels are developed with the multi-objective optimization. A, F and K are Gons algorithm results, B, G, and L are Gons algorithm results, C, H, and M are Ritchie algorithm results, D, I, and N are Simis algorithm results, and E, J, and O are Duan algorithm results

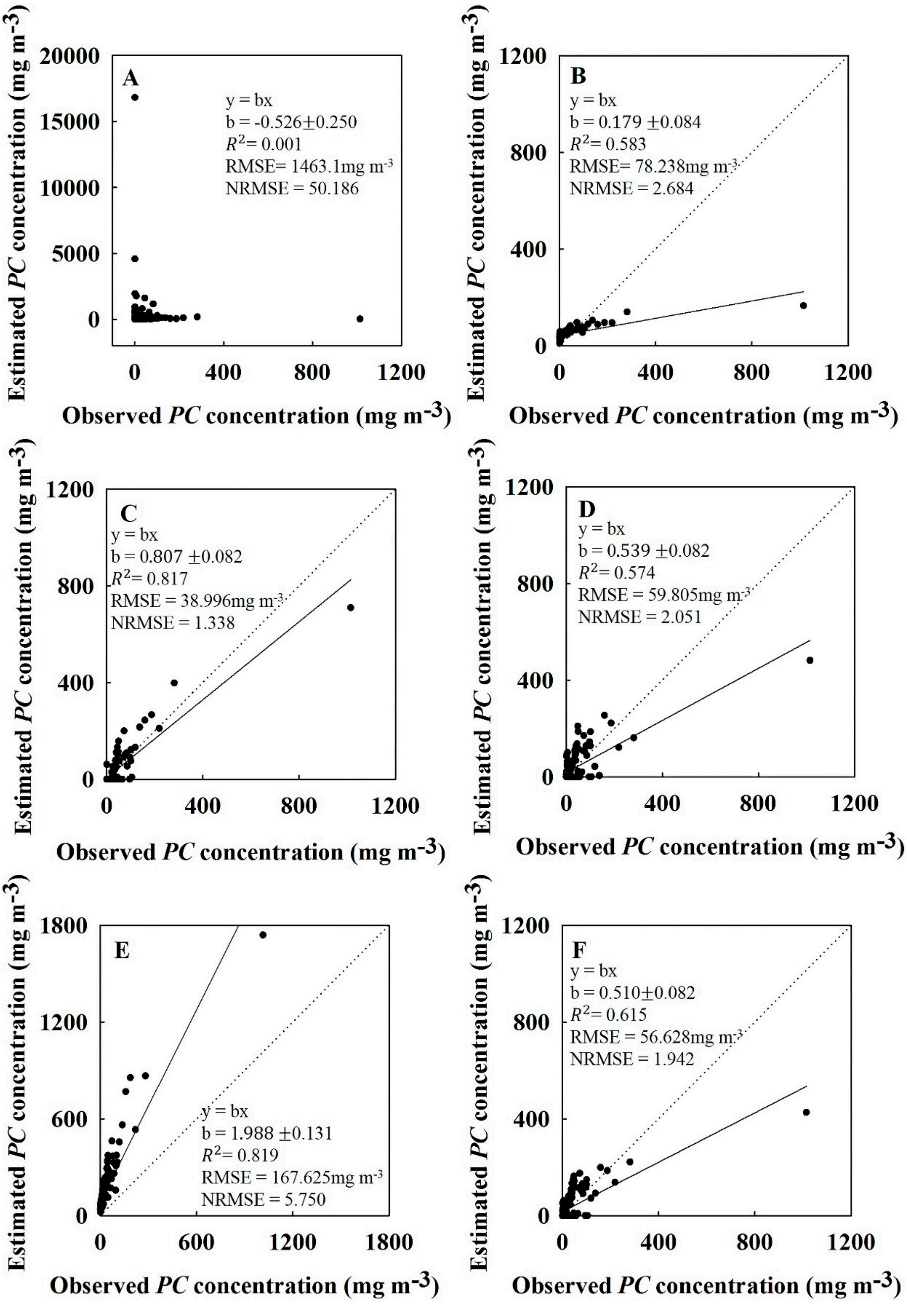

Figure S8. Comparison of measured, published and estimated from the single-objective and multi-optimization *PC* concentration in *PC* algorithms. The top two panels are developed with published values, the middle two panels are developed with single-objective optimization the bottom two panels are developed with the multi-objective optimization. A, C, and E are Li algorithm results, and B, D, and F are Simis algorithm results