COASTCOLOUR

L2 Processing for first *beta* demonstration data set

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HZG

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Overview

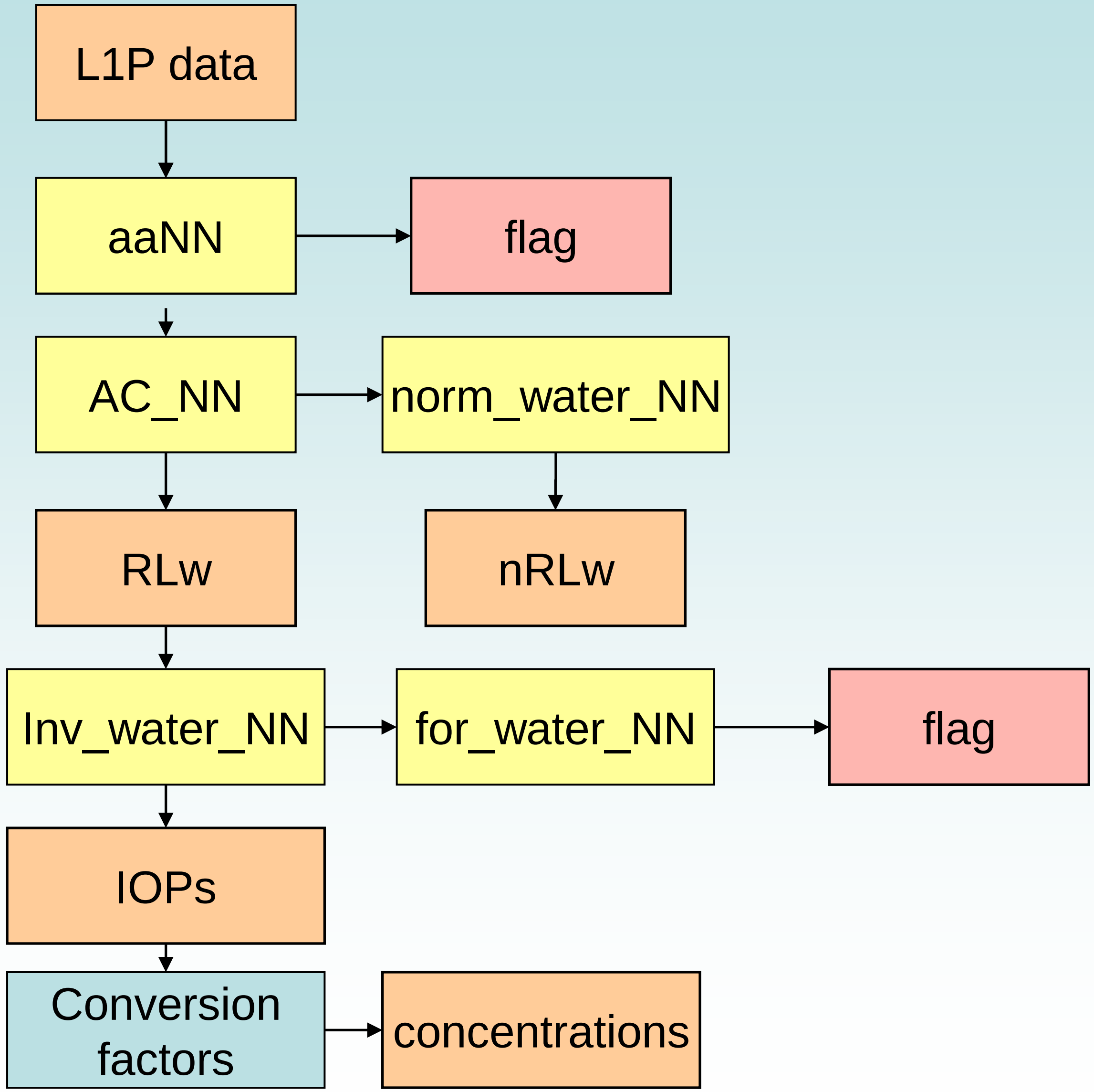
- Why this Algorithm?
- Data and bio-optical model
- Radiative transfer models used for simulations or reflectances
- Training of neural networks
- Training of neural networks using measured data
- Performance tests
- Tests using transects of different sites
- Plan for completing this work package

Why this algorithm for the demonstration data set?

- In situ Data supplied by the users were in most cases not sufficient for training the NNs
- NOMAD data set (NASA) is the most comprehensive data set for algorithm development (for which it was compiled)
- But not sufficient for all Coastcolour sites
- Thus, bio-optical model was extended for standard concentrations of TSM and for areas with extreme high TSM concentrations

- 3 sets of neural networks were trained:
  - NOMAD bio-optical model
  - Extended NOMAD model
  - High TSM model
- Atmospheric correction is not independent from water, so for each bio-optical model a separate AC NN was developed

Neural network system



Reflectances and IOPs

- ***Surface reflectances***

  RLw   Directional water leaving radiance reflectance
- RLwn Fully normalized water leaving radiance reflectance

- ***Inherent optical properties***

  a_total Total absorption coefficient of all water constituents (at 443 nm)
- b_total Total scattering or backscattering coefficient
- a_pig   Phytoplankton pigment absorption coefficient
- a_ys   Yellow substance absorption coefficient
- a_poc Absorption by particulate organic matter

Concentrations, Transparency and Indices

- ***Water constituent concentrations***
  - Chl.: Chlorophyll a concentration
  - TSM: Total suspended matter

- ***Water transparency/turbidity information***
  - Kd490: downwelling irradiance attenuation coefficient at 490 nm
  - Z90_max: Maximal signal depth
  - FNU: Formazin Nepholometric Units

- ***Chlorophyll Indices***
  - FLH: Fluorescence line height
  - MCI: Maximum chlorophyll index

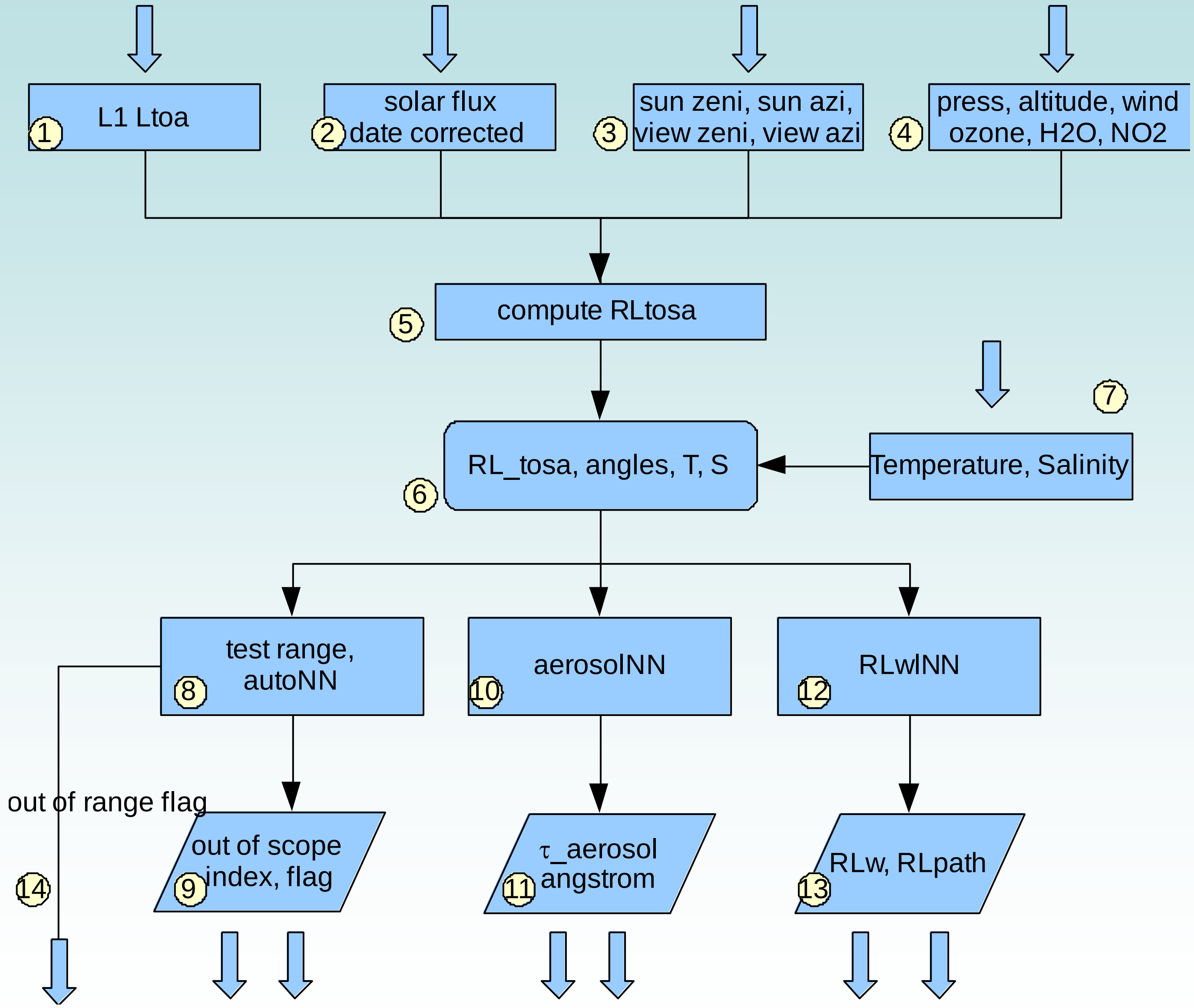
Radiative transfer models used

- Radiative tranfer model with T and S effects of pure water
  - Hydrolight for water
    - Bi-directional
    - Requires a, b and phase function as IOPs
    - Pure water IOPs T and S dependent
  - Monte Carlo photon tracing for atmosphere and specular reflectance
    - Bi-directionla
    - Aerosol optical properties, thin cirrus clouds
    - Wind dependent waves on ocean surface
    - Refractive index T and S dependent -> Fresnel reflection

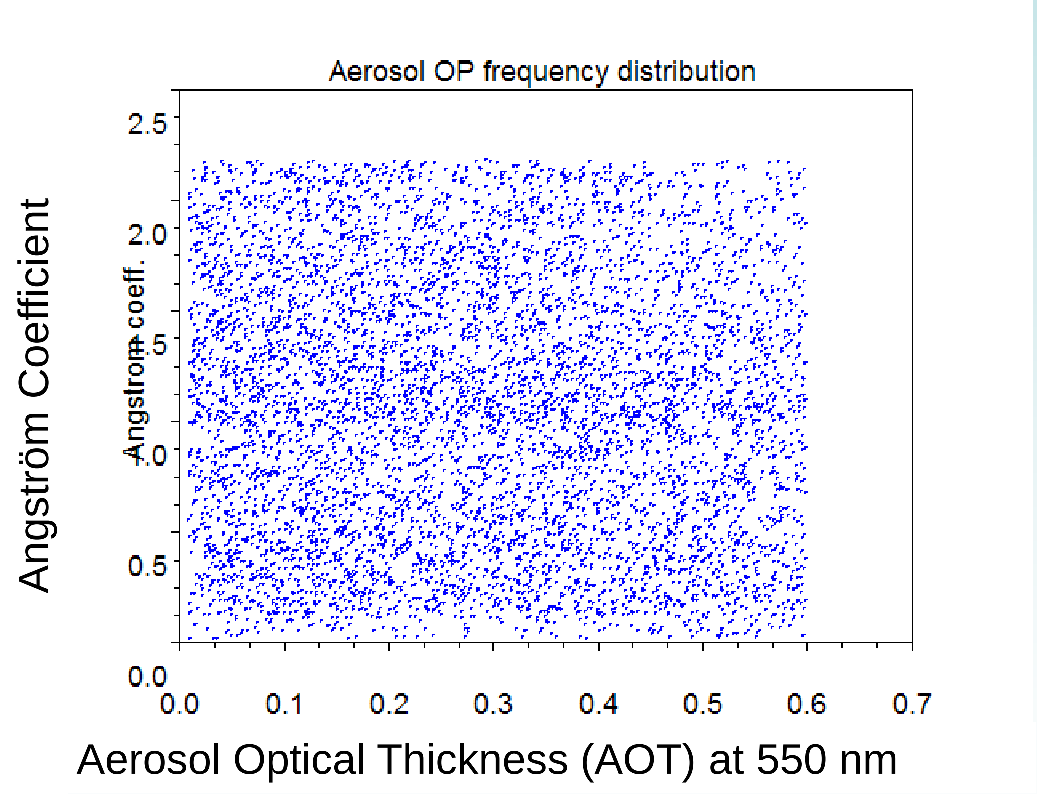
Atmospheric Correction

- Atmospheric correction is based on a combined ocean/atmosphere model
- Input to the NN are RL_tosa (standard w.r.t. surface pressure and ozone)
- Deviations from standard are pre-corrected: RL_toa -> RL_tosa
- Different AC for each class of the 3 classes of coastal waters
- Forward NN of water is used in combination with a Monte Carlo photon tracing code for simulalations
- Different forward NN for each of the 3 water classes combined with standard atmosphere part
- For each water class also autoNN for testing out of scope conditions based on RL_tosa
- No limits in glint
- Typical 1 Mio. cases simulated (incl. different sun and viewing angles)

Atmospheric Correction using NN



Aerosol Optical Properties used for NN Training data set



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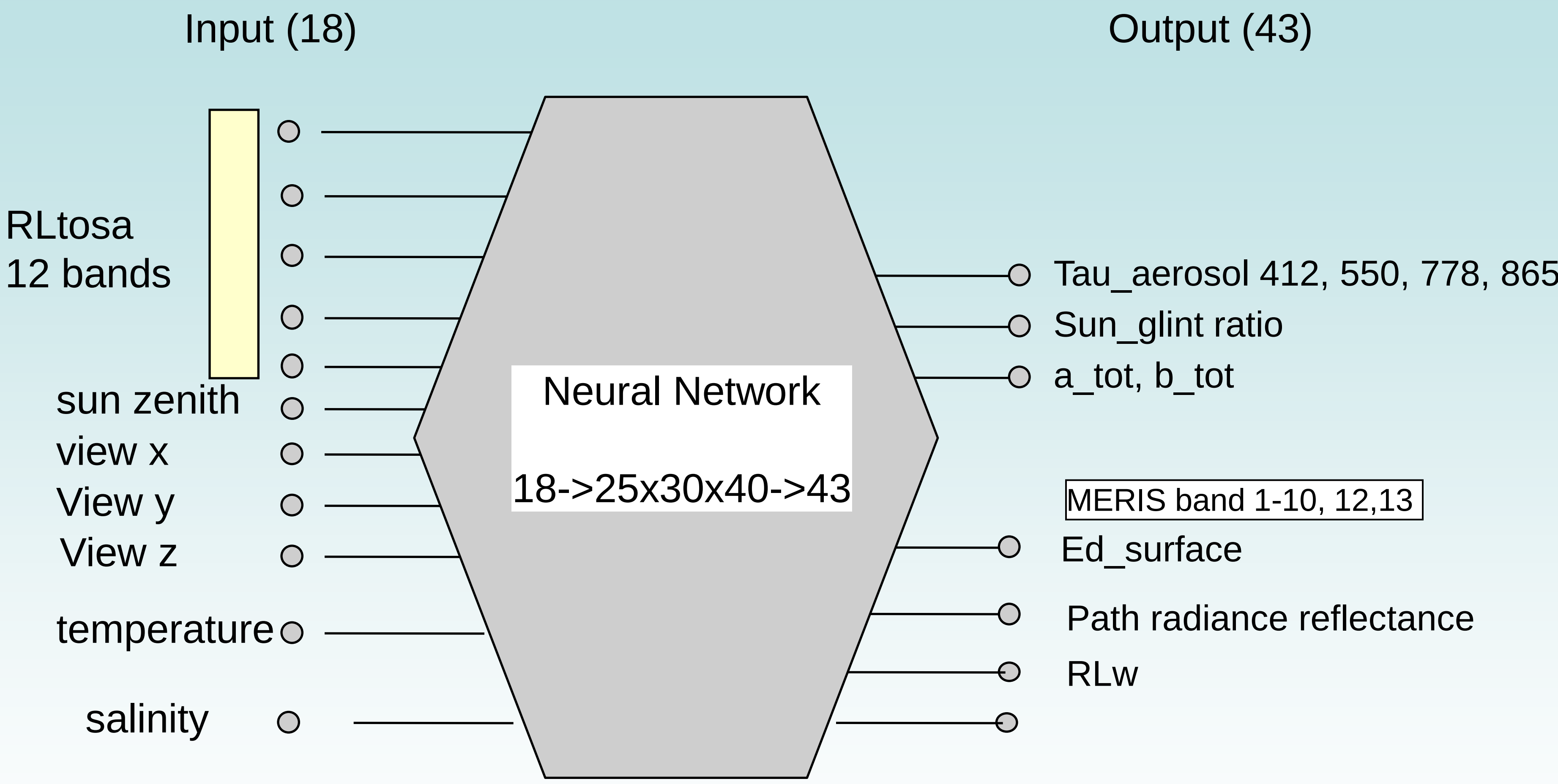
NN for atmospheric correction – CC version



$RLw(\theta,\phi) = Lw(\theta,\phi) / Ed$

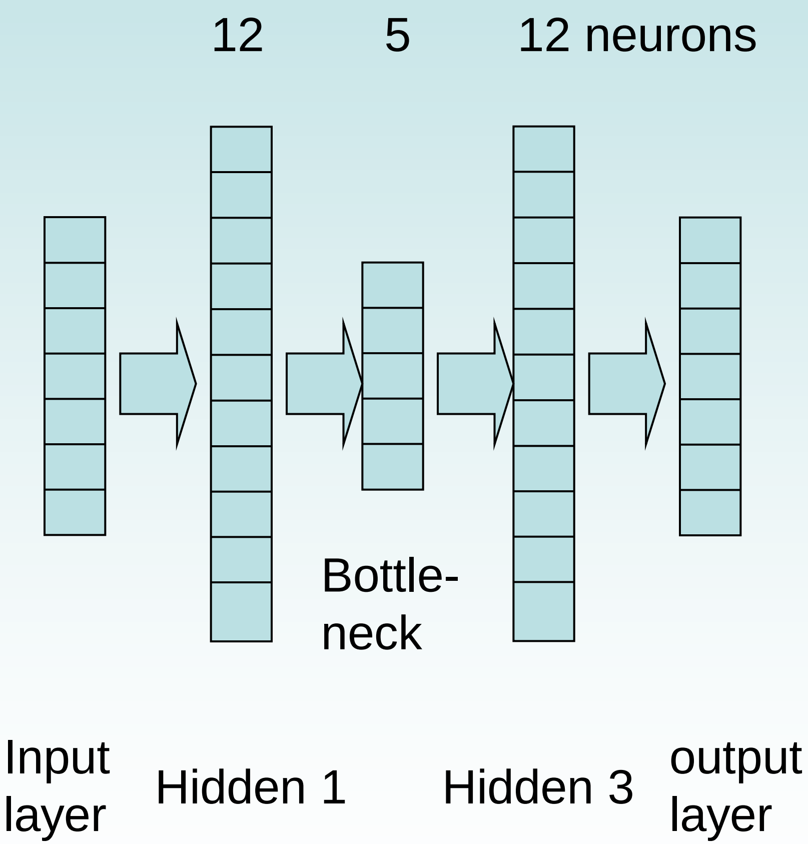
For each water type

autoNN to detect RLtosa Out of Scope spectra

- Purpose
  - Detects top of atmosphere spectra, which are out of scope of the data set used for training of the AC neural network
- Method
  - Method is an auto-associative neural network, which is trained with the same data set and has a bottleneck hidden layer to constrain the relationship between input and output spectra
  - Deviations between the input and output spectra are used as an uncertainty measure and, when above a threshold, to trigger an out of scope flag
- Status
  - Developed and implemented for each water type

Auto-associative NN

For each coastcolour water type
Includes temperature and salinity



the net has 18 inputs:
input 1 is sun_zeni_deg in [1.003,76.2]
input 2 is x in [-1.0,1.0]
input 3 is y in [-0.000005,1.0]
input 4 is z in [0.000000,0.7071]
input 5 is T_wat in [0.000151,36.0]
input 6 is S_wat in [0.000181,43.0]
Input 7-18: RL_tosa 12 bands

12 outputs:
RL_tosa‘’12 bands

Fully normalized water leaving radiance reflectances, nRLw

- Purpose
  - Determine the fully normalized water leaving radiance reflectance from bi-directional water leaving radiance reflectances
- Methods
  - Training of a neural network with bi-directional RLw and solar zenith, viewing nadir and azimuth difference angles as input and Rlw for sun in zenith and nadir view as output
- Status
  - Normalization NN has been created and implemented

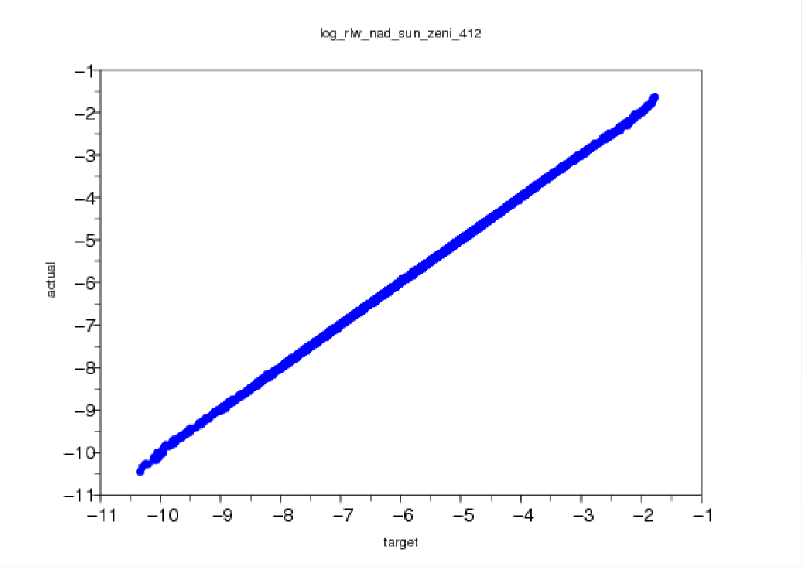
Set up of simulations

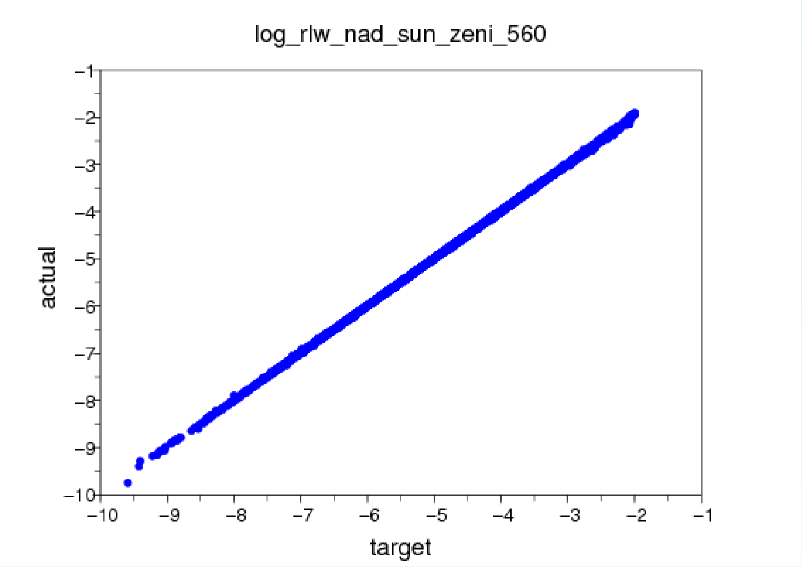
- Computation of water leaving radiance reflectances using Hydrolight
- Random variations of water optical properties according to case 2 water model
- Parameters
  - Ys absorption
  - Bleached particle absorption
  - Pigment absorption
  - Particle scattering :
  - White particle scattering: 0.005 – 30.0 m-1, exponent 0

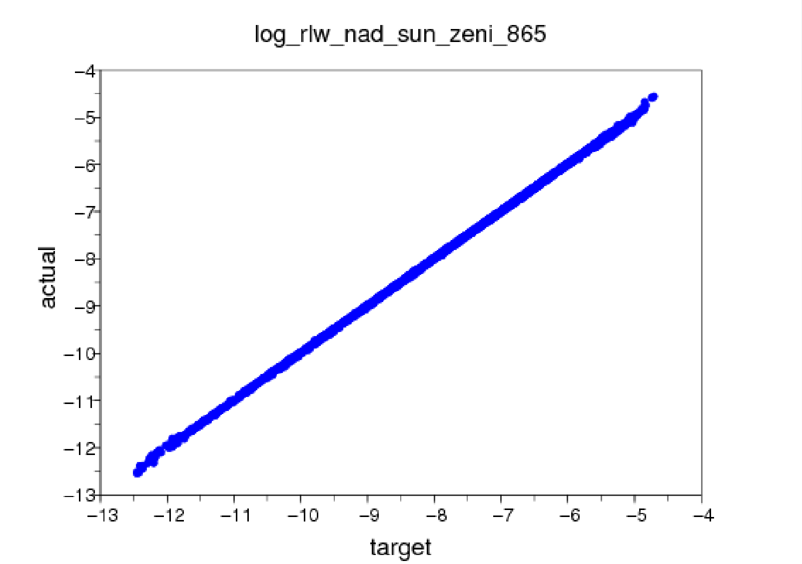
- Sun zenith angle:0 – 85 deg
- Viewing zenith angle: 0 – 45 deg
- Azimuth difference: 0 – 180 deg

- 2 runs with identical optical properties
- Sun in zenith, looking only at nadir RLw
  - Random sun and viewing angles

Result of NN







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Water algorithm

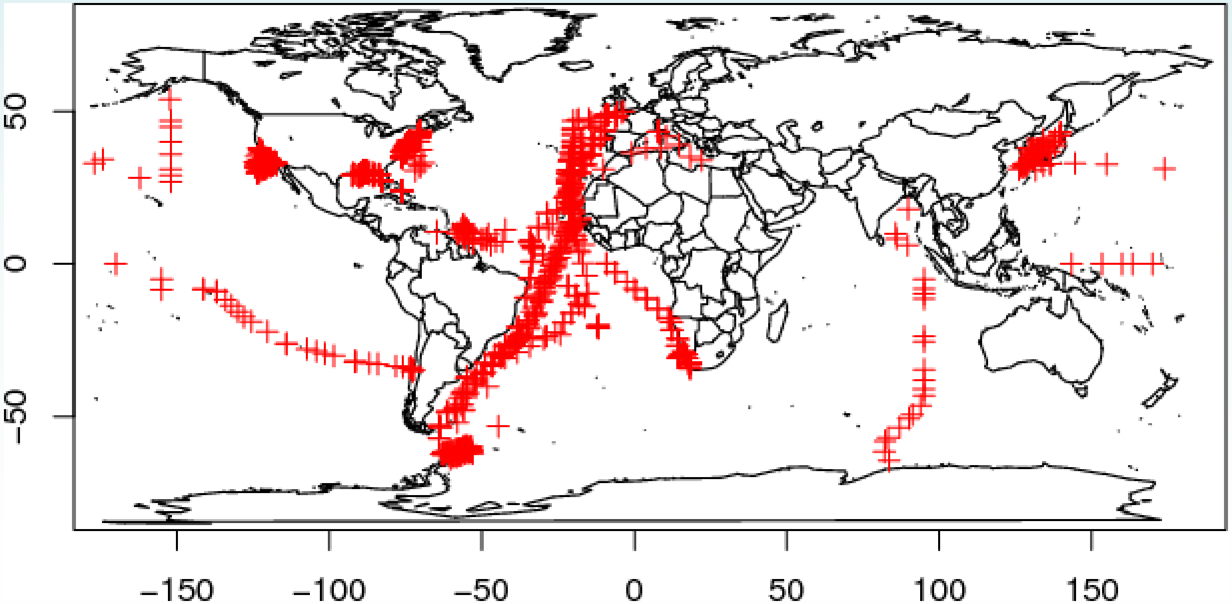
Analysis of NOMAD data set for generic algorithm

- Data set V2.0 of 2008 comprises 4359 entries with 206 variables.
  - but, not all variables are available for each entry.
- Spectral data: 20 bands in the wavelength range: 405 – 683 nm
  - But not all wavelengths are available for all stations and variables
- Data can be traced back to originator
  - flag
  - cruise
  - Year, month, day
  - Hour, minute, second
  - Lat, lon
  - id

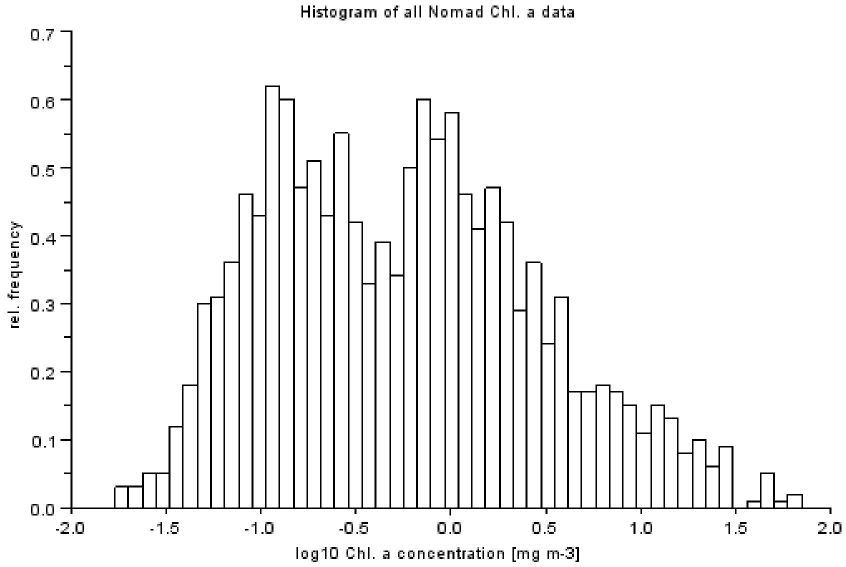
sst	Ap 405-683	wt	Chlide_a
z	Ad 405-683	sal	Mv_chl_a Dv_chl_a
Chl_f	Ag 405-683	poc	Chl_c3 Chl_c2
Chl_a	A 405-683	kpar	Chl_cl2 perid
Kd 405-683	Bb 405-683	Z_37	but-fuco hex-fuco
Lw 405-683	Bbr 405-683	Z_10	fuco pras
Eds 405-683		Z_01	viola diadino
			Allo, diato Lut, zea
		alpha-car Alpha-beta-car	chl_b beta-car

NOMAD chlorophyll

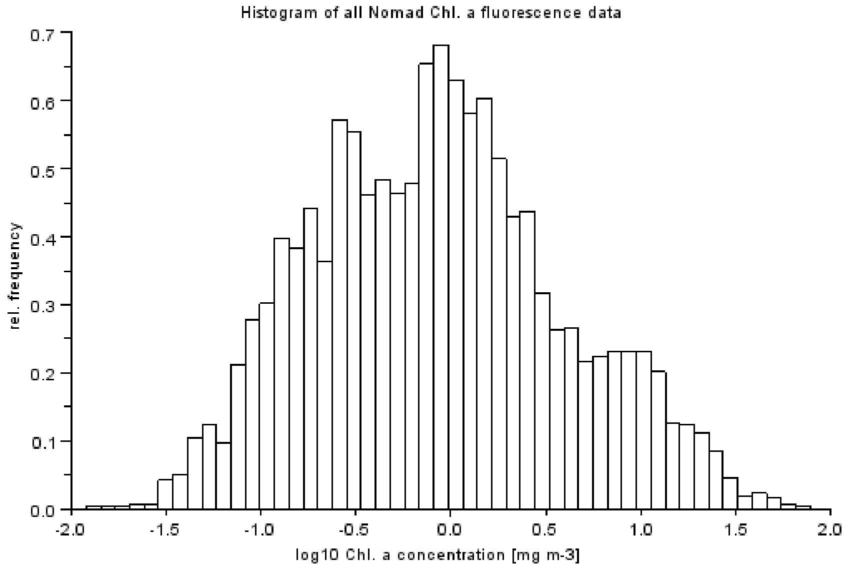
- Chlorophyll *a* from fluorometric and HPLC measurements
  - Chl_a (HPLC): 1381 stations
    - Range: 0.017 - 70.2 mg m-3,
    - 1-99% percentile: 0.03 - 28.2 mg m-3
  - Chl_f (fluorometric): 3392 stations
    - Range:0.012 – 77.9 mg m-3
    - 1-99% percentile: 0.041 – 27.7 mg m-3



NOMAD chlorophyll (log10 scale)

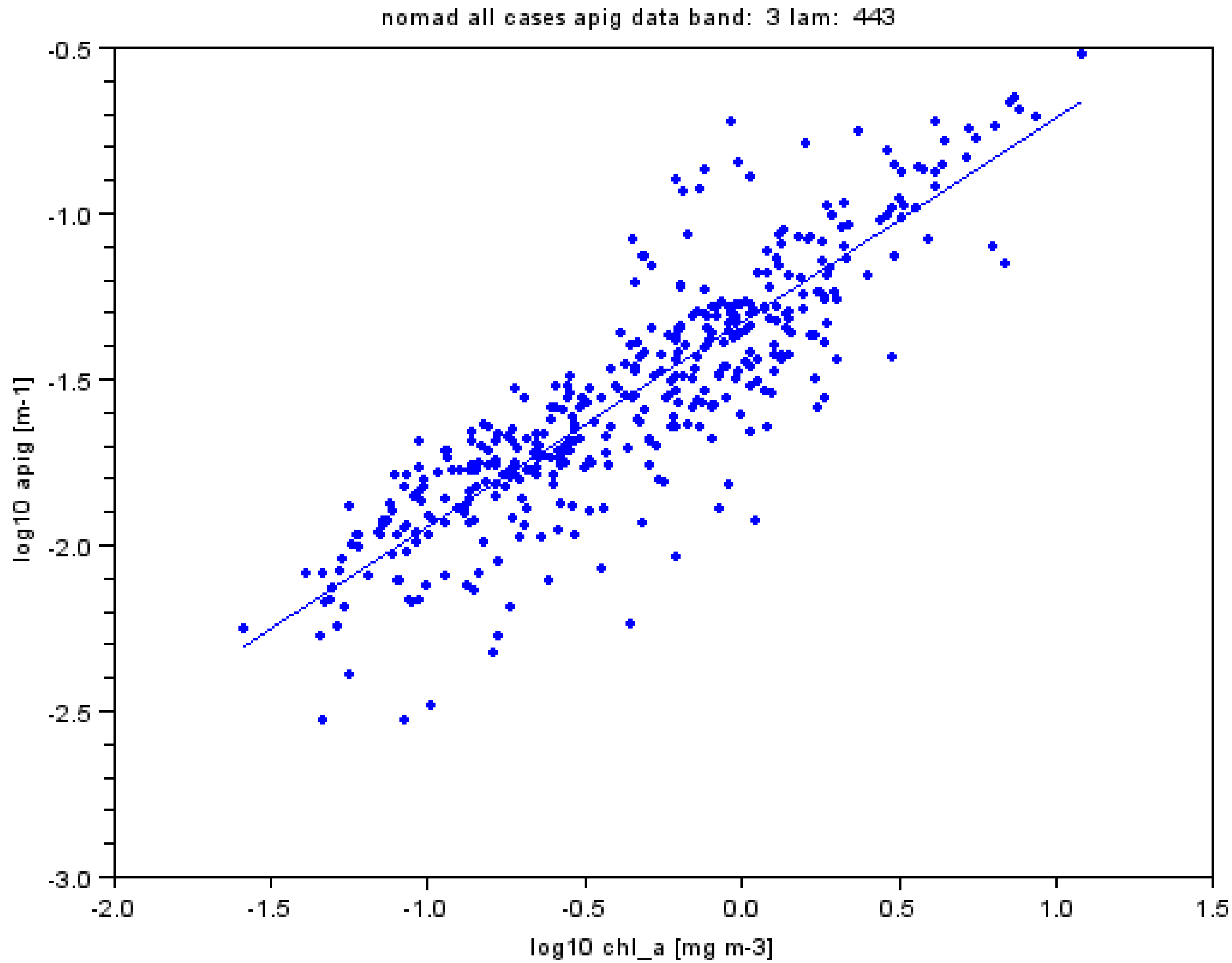


HPLC
1381 samples



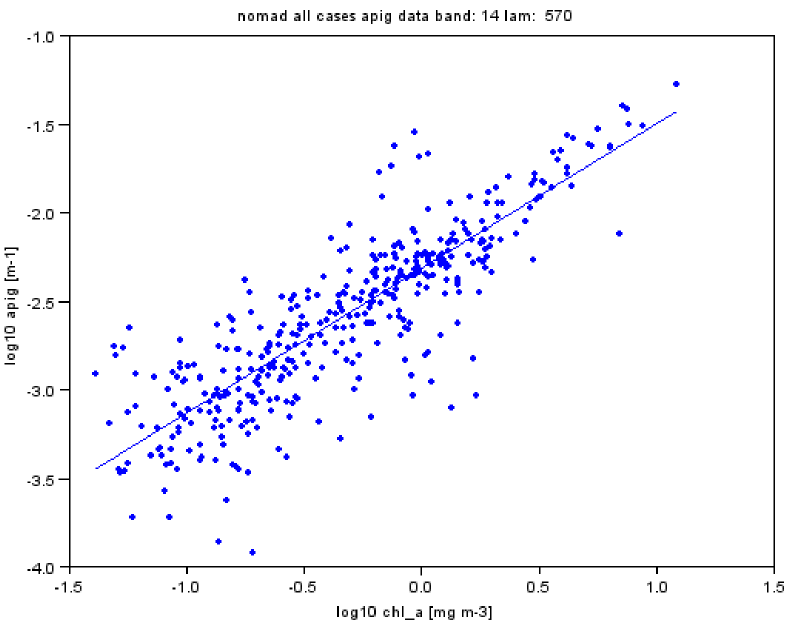
Fluorometric
3392 samples

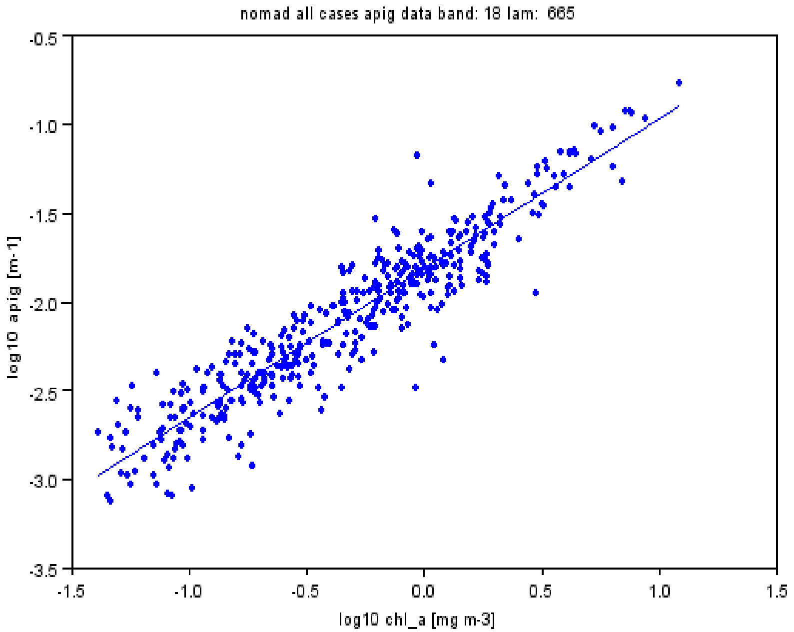
Bio-optical model: relationship between a_pig and chl_a



443 nm, log10 scale

Bio-optical model: relationship between a_pig and chl_a



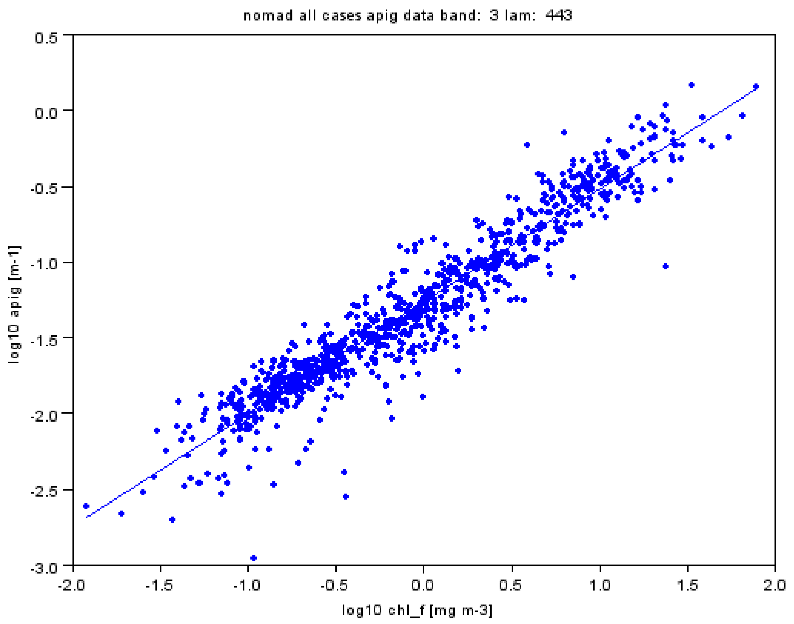


570 nm

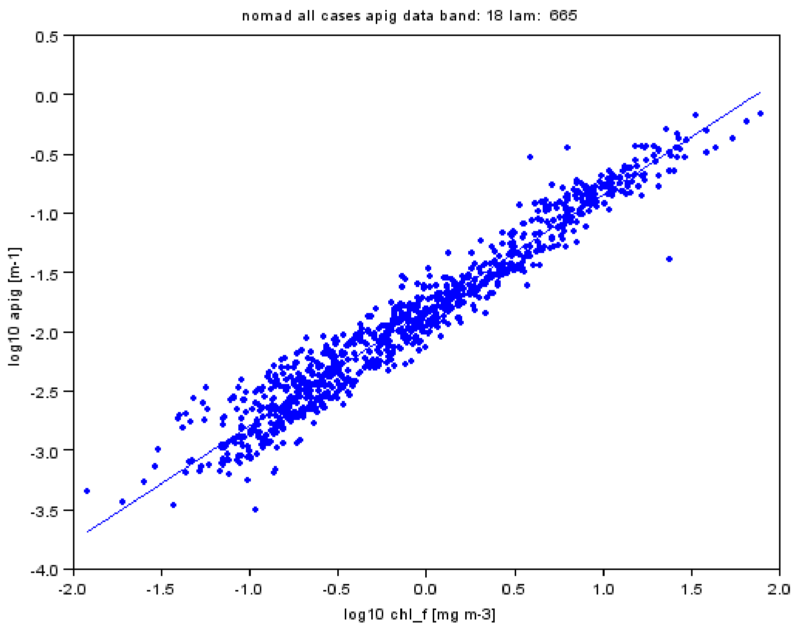
665 nm

560 nm, log10 scale

Bio-optical model: relationship between a_pig and chl_f



443 nm



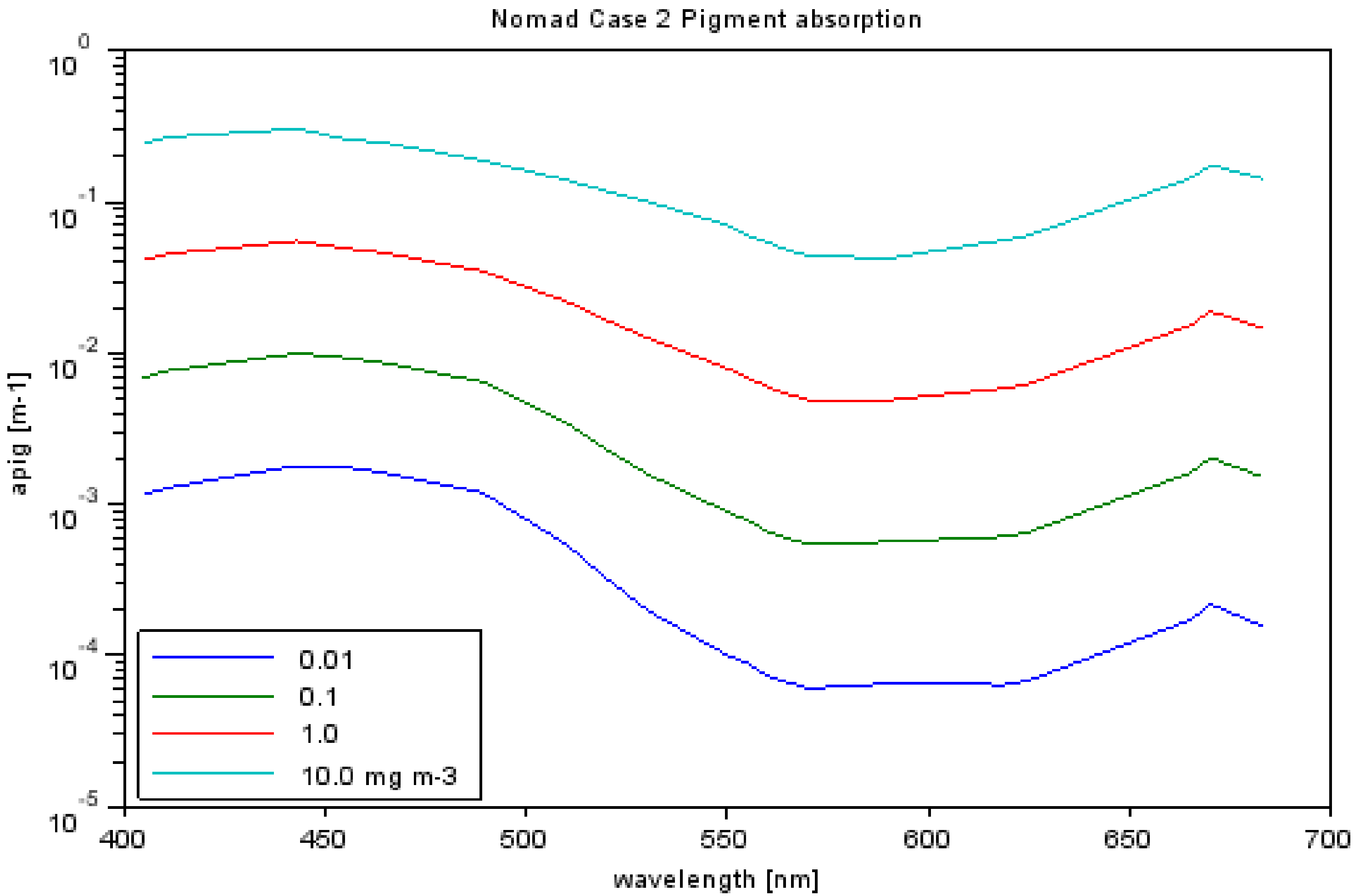
665 nm

443 nm, log10 scale, 920-956 samples for chl_f

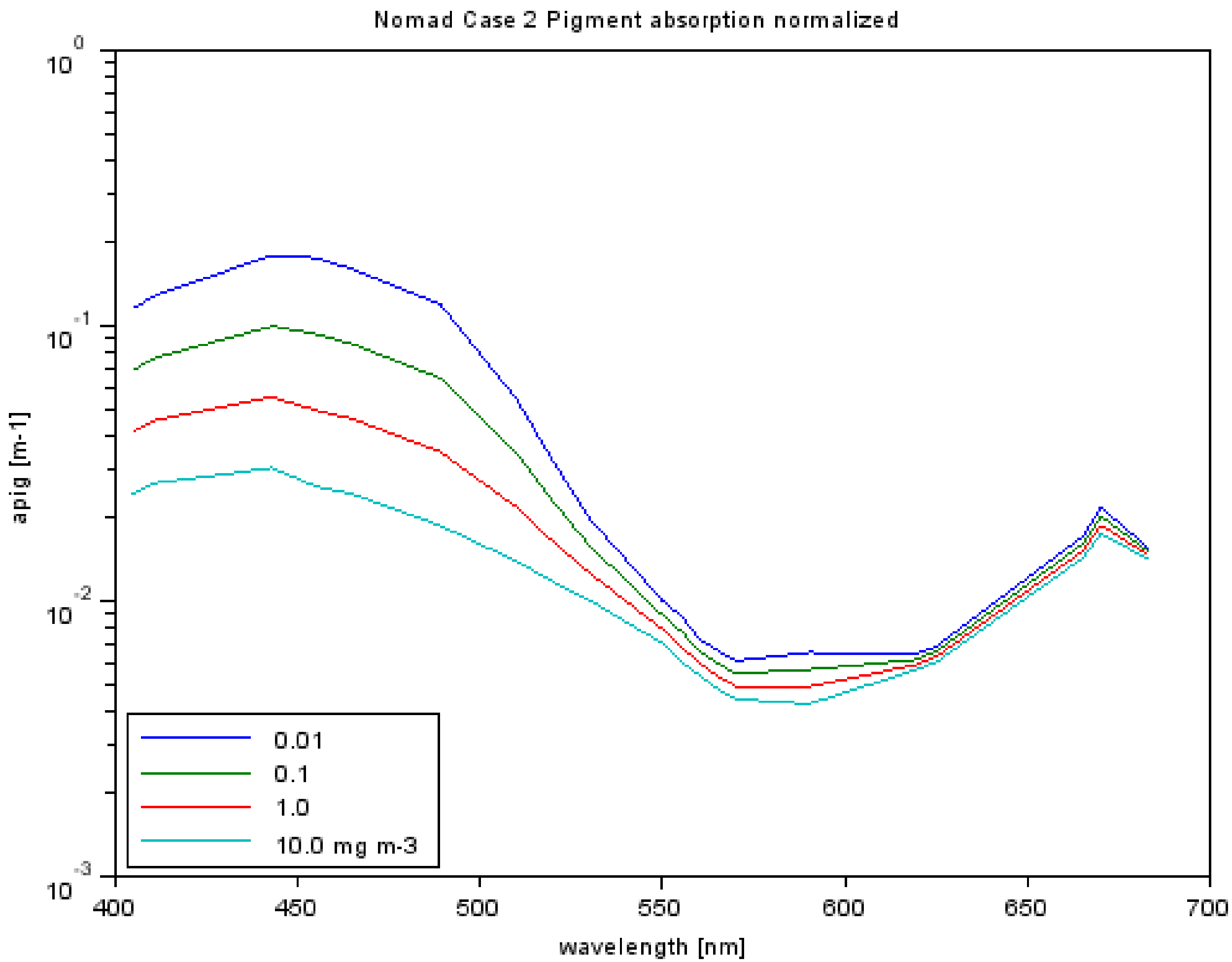
The bio-optical model

- Select chlorophyll concentration randomly from a log scale uniform distribution
- From NOMAD data analysis know the spectral relationships between chlorophyll and
  - Absorption by pigments (ap)
  - absorption by detritus (ad) with stdev
  - Absorption by gelbstoff absorption (ag) with stdev
  - Backscattering by all particles (bbp) with stdev
- Select ap, ad, ag, bbp as a function of chl., randomly within 2 stdev
- Convert bbp -> bp for Petzold phase function (factor of 55.6)
- Use Petzold phase function for all particles
- Add white scatterer, wind dependent
- Spectral shape of ad, ag, bbp directly derived from NOMAD data
- Add extra gelbstoff (spectral exponent 0.015)
- Add extra particles scattering (spectral exponent 1.0) associated with ad with spectral exponent of 0.01)

Absorption coefficient for different chlorophyll concentrations (chl_f)

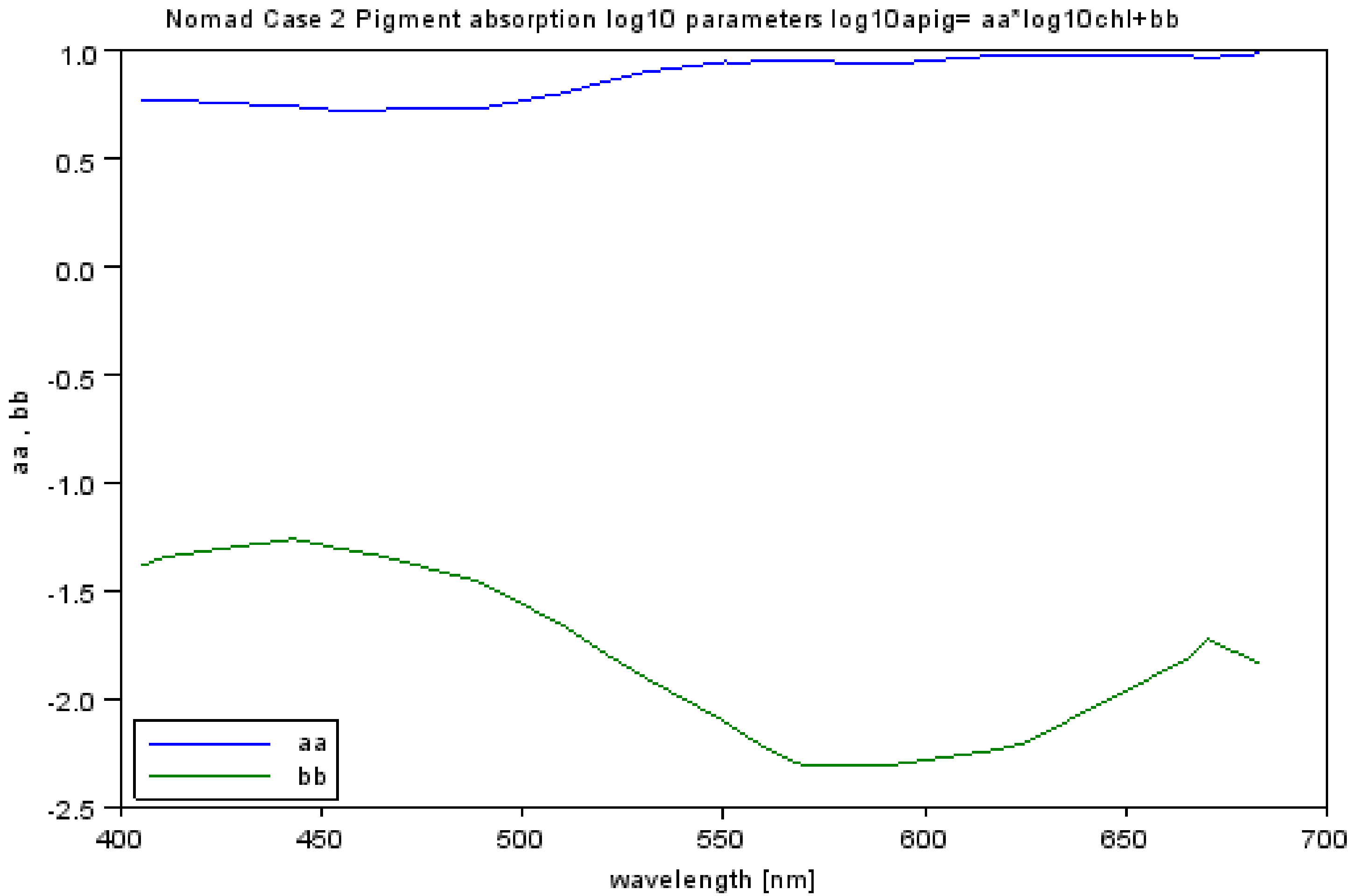


Absorption coefficient for different chlorophyll concentrations (chl_f)



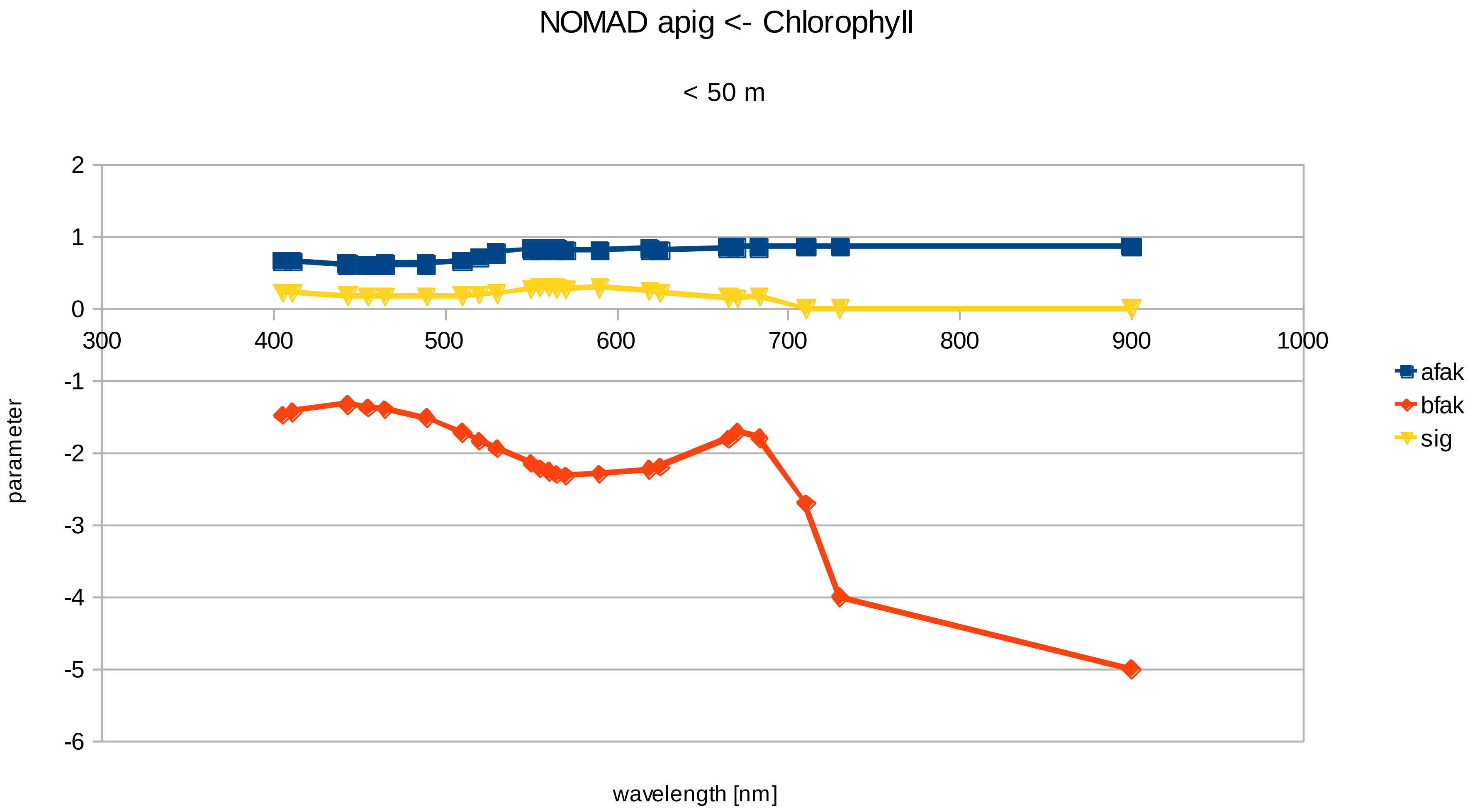
Normalized to 1 mg m-3

Regression a_pig -> chl_f

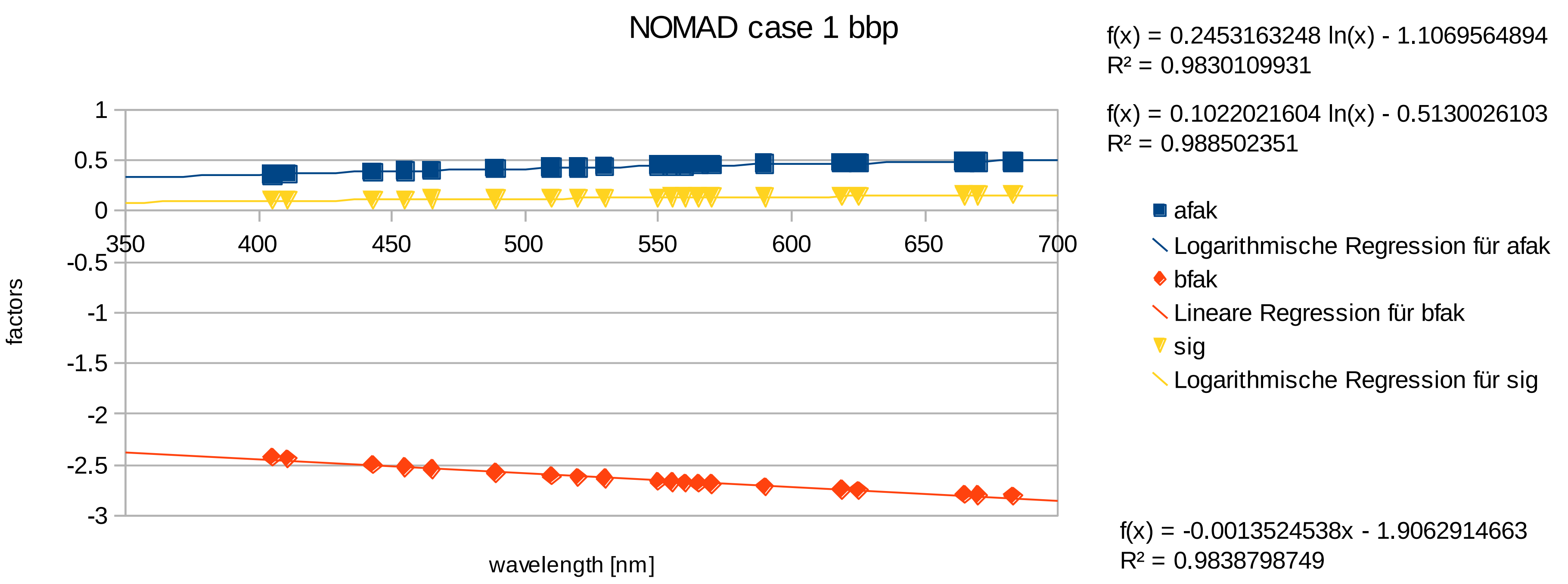


Log10 chl_f = aa + bb*log10 a_pig

Extrapolation of a_pig model



Extrapolation of bbp



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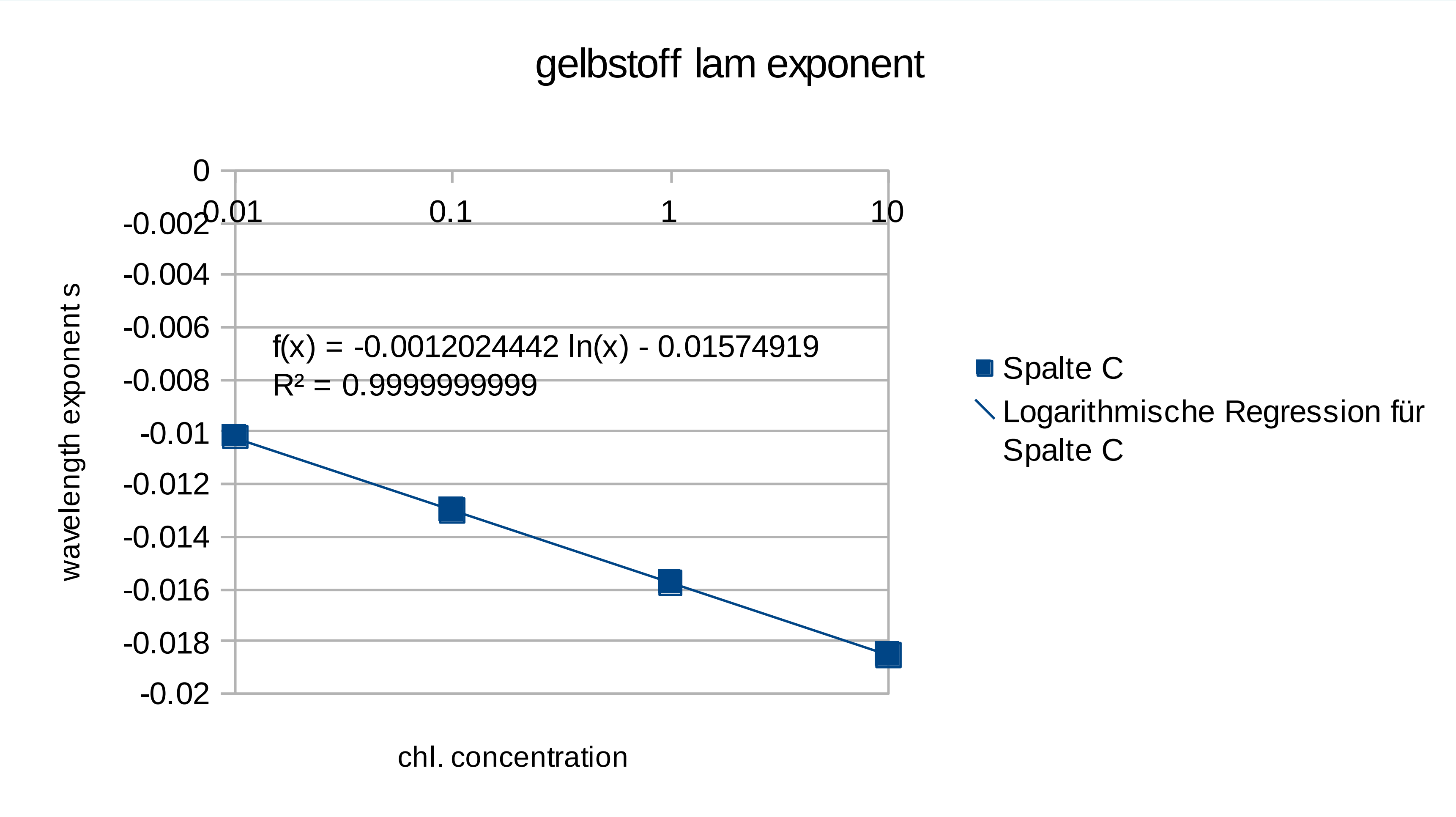
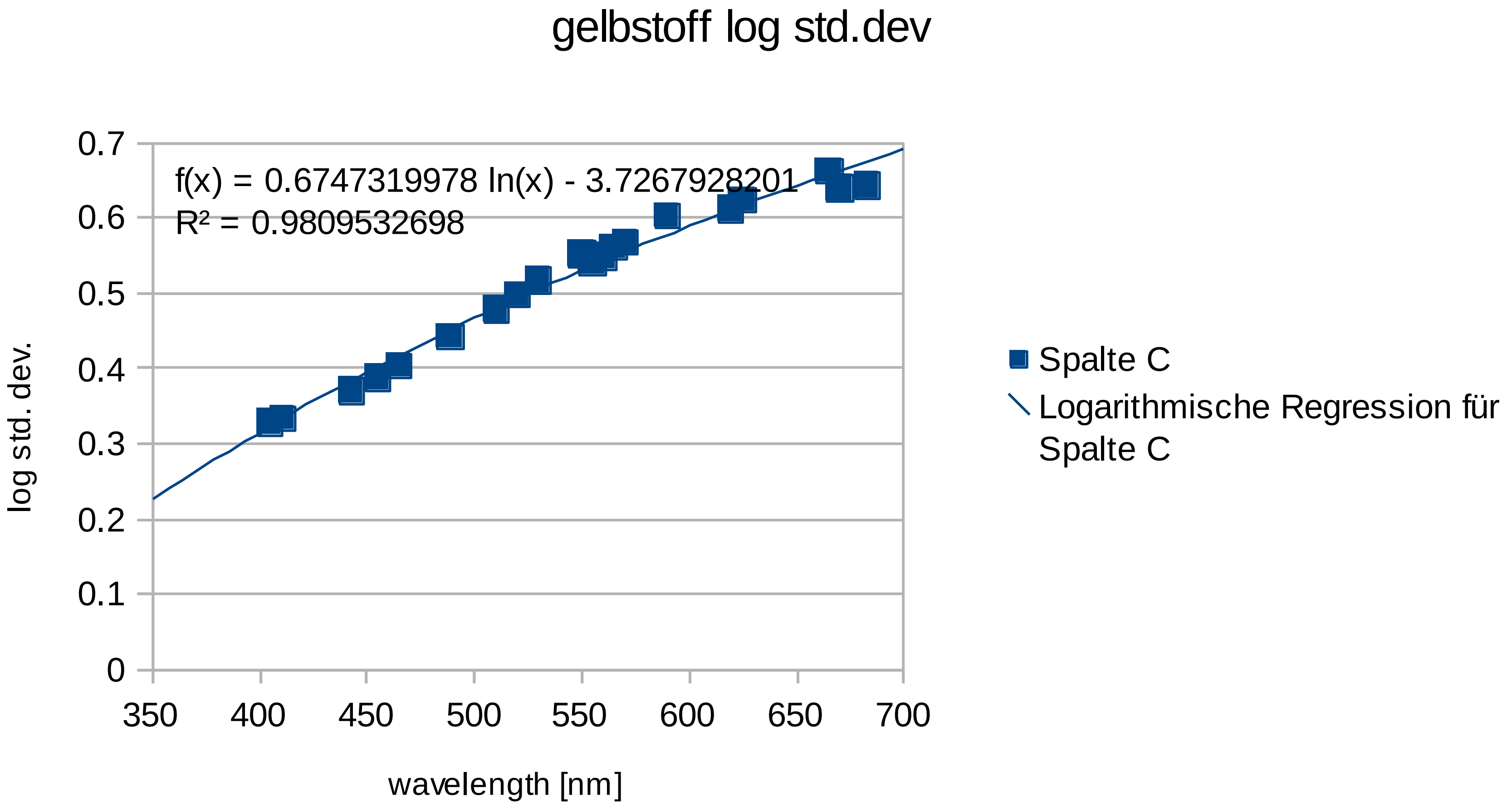
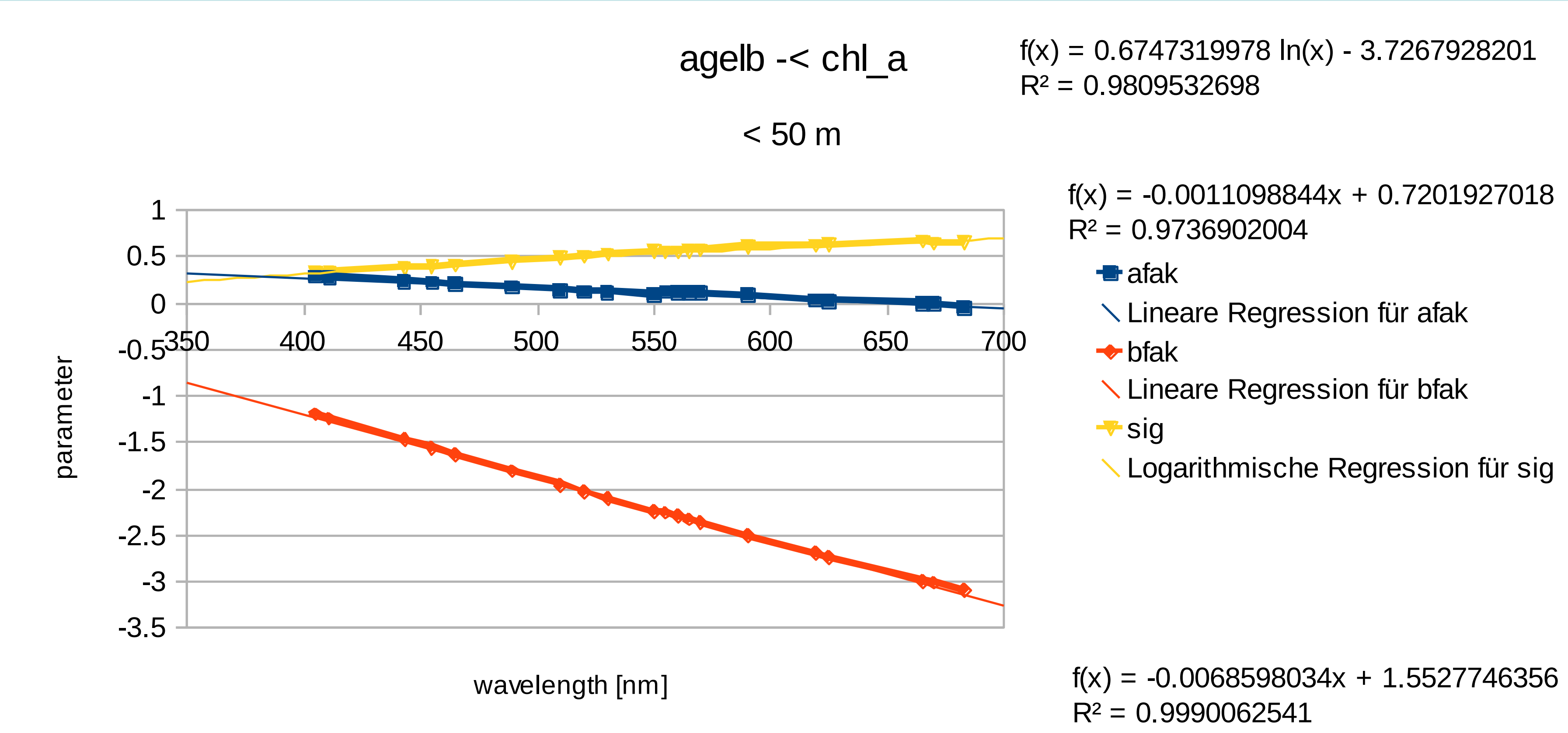
Spectral exponent of ys, function of chl. Conc.



Spectrum of Standard Deviation of ag

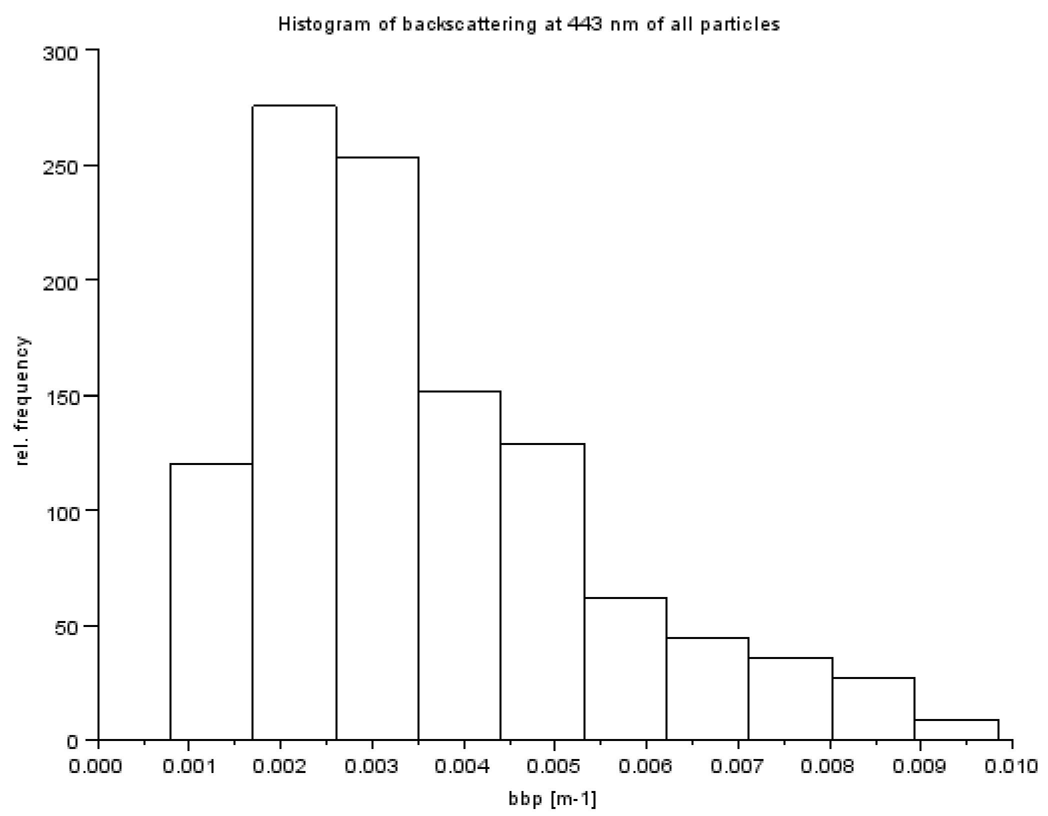


Analysis of ag as a function of chl concentration



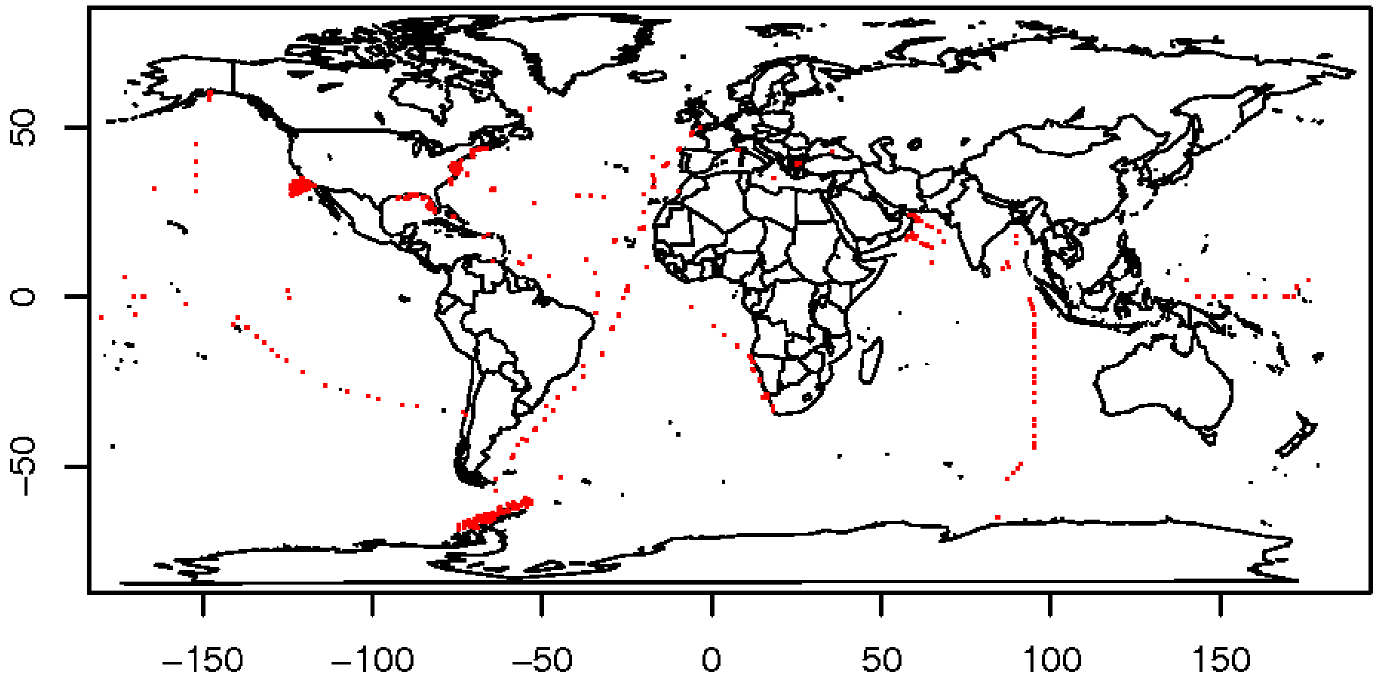
Backscattering coefficient bb

bb in NOMAD includes particles and pure water
Bb_water has been subtracted, computed with model of water radiance project



249 samples

bb distribution



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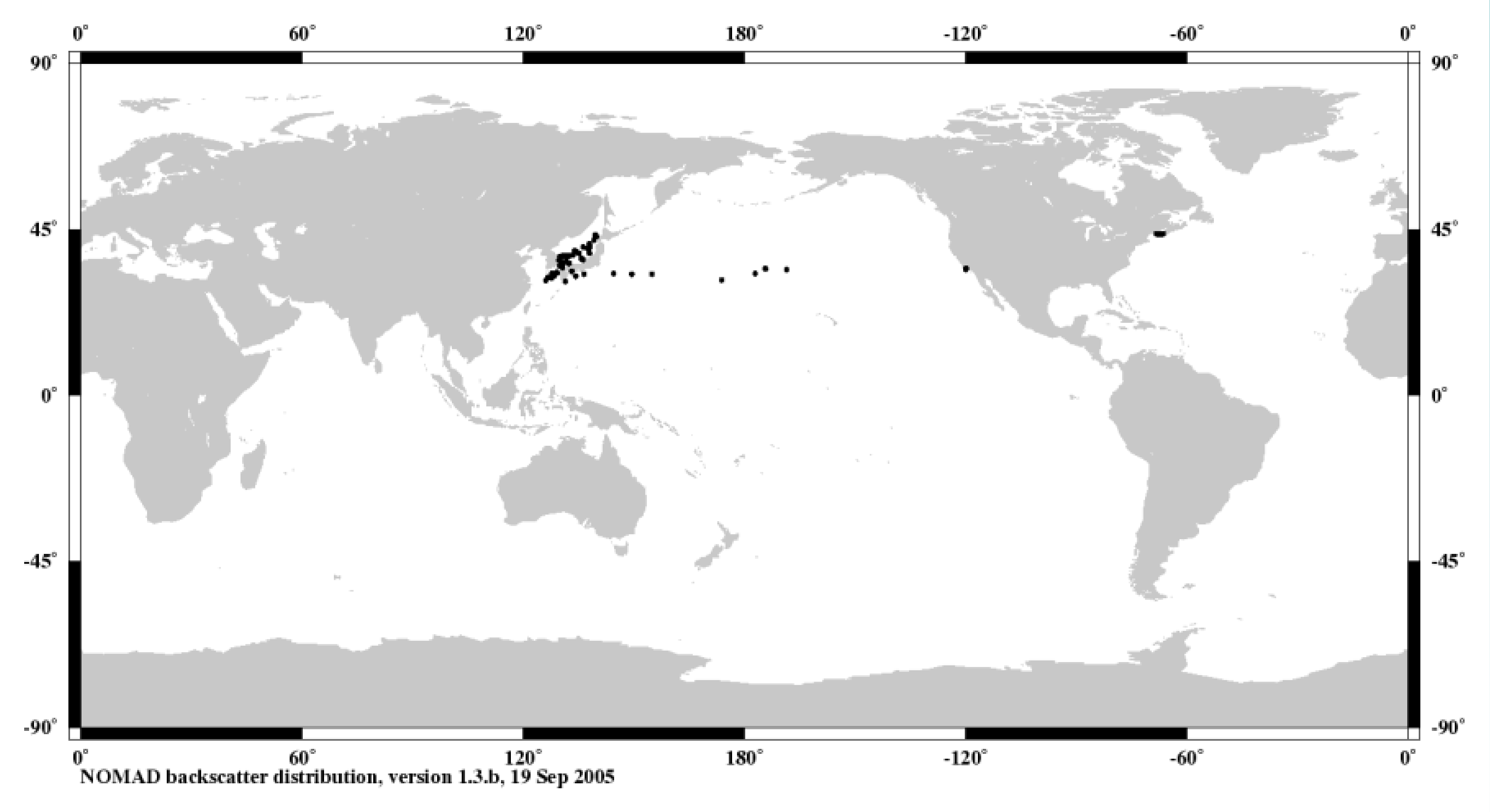
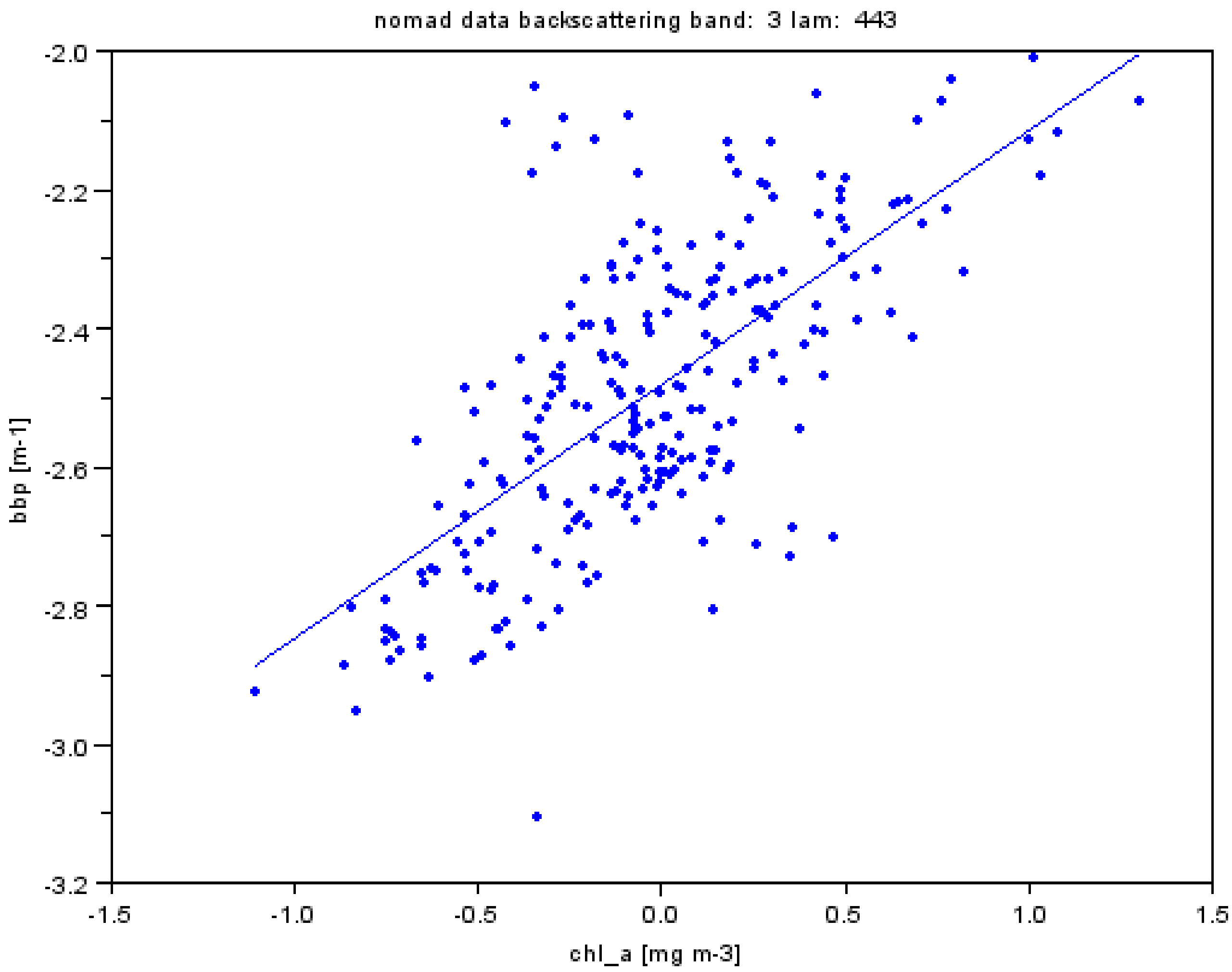
Distribution of bb all selected bands

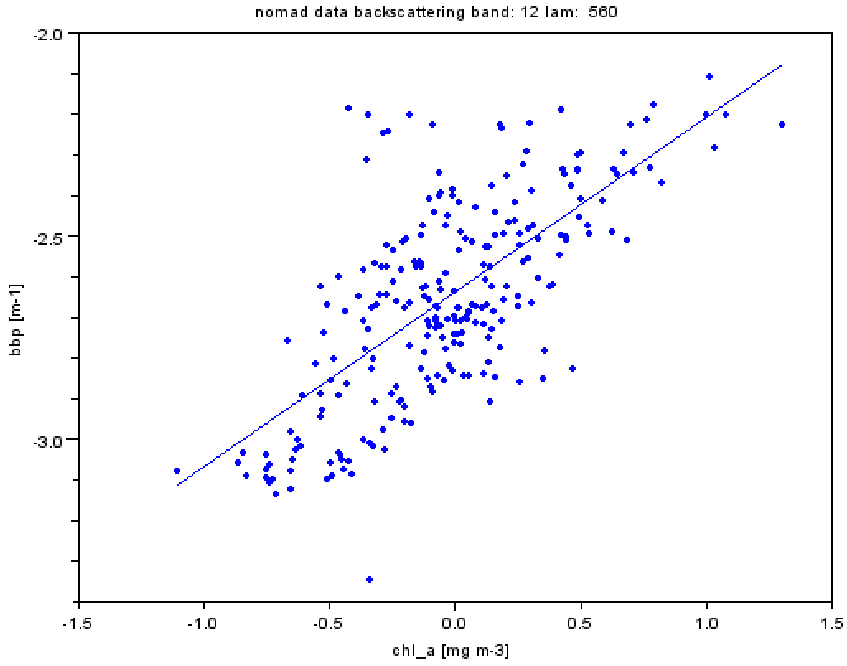


Relationship chl_f and backscattering coefficient

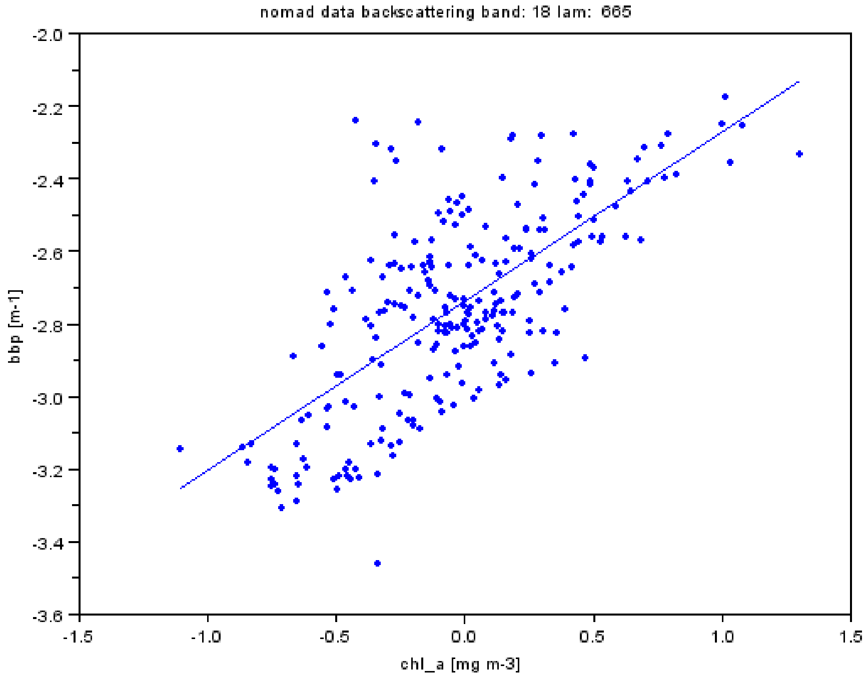


443 nm, 249 samples, log10 scale

Relationship chl_f and backscattering coefficient



560 nm



665 nm

249 samples, log10 scale

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Ranges for simulations -> scope of water NN

Standard NOMAD

chlorophyll	apig_443	adet_443	ays_443	btsm_443	bwit_443	z90_max
0.01 – 50 mg m-3	0.0012 - 1.18 m-1	0.0002 – 0.218 m-1	0.001 – 0.47 m-1	0.00718 – 0.529 m-1	0.01 – 0.1 m-1	1 – 68 m

TSM ~ 0.01 – 1.0 g m-3

extended NOMAD

chlorophyll	apig_443	adet_443	ays_443	btsm_443	bwit_443	z90_max
0.01 – 50 mg m-3	0.0012 - 1.18 m-1	0.0002 – 0.29 m-1	0.002 – 2.4 m-1	0.00718 – 55.8 m-1	0.01 – 0.1 m-1	0.38 – 66 m

TSM ~ 0.01 – 100 g m-3

extended NOMAD high tsm

chlorophyll	apig_443	adet_443	ays_443	btsm_443	bwit_443	z90_max
0.01 – 50 mg m-3	0.0012 - 1.18 m-1	0.0002 – 1.7 m-1	0.002 – 2.4 m-1	0.00718 – 556 m-1	0.01 – 0.1 m-1	0.11 – 63 m

TSM ~ 0.01 – 1000 g m-3

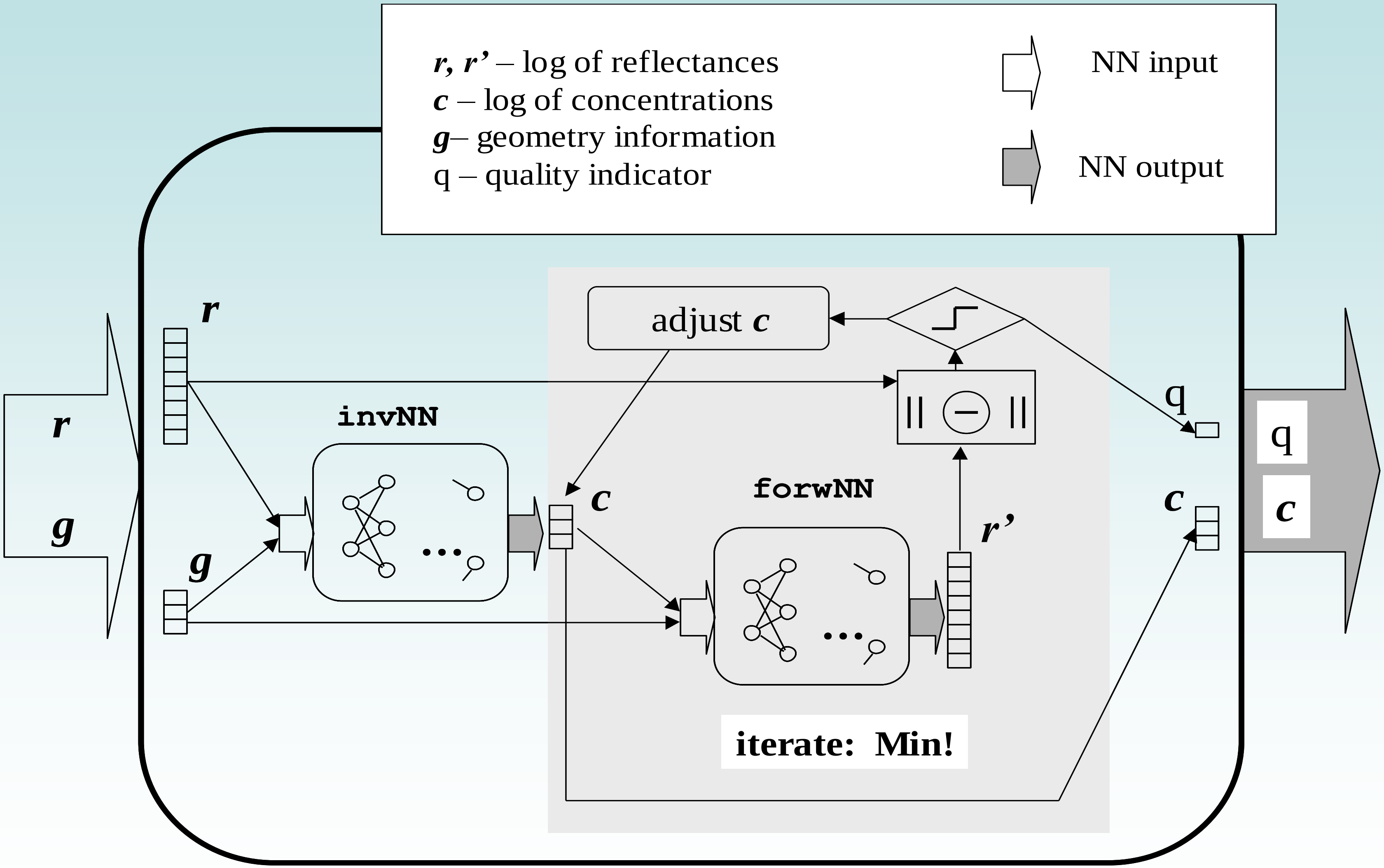
Bio-optical model for high tsm

- Absorption and scattering of pure water according to water radiance project with temperature and salinity effects
- Pigment absorption based on NOMAD bio-optical model with variable, concentration dependent spectral shapes
- Chlorophyll range 0.01 – 50 mg m-3
- Basic IOPs use covariance based on NOMAD data set with 4 std.dev. for
  - a_pig, a_g, a_d, b_tsm,
- 1/3 of all cases with background white scatterer of b=0.01 m-1
- Add white scatterer above wind dependent for wind > 7 ms-1
  - conc_bwit=conc_bwit+0.01*wind
- Additional absorption by yellow substance and particles
  - a443 of 0.01 - 2   m-1
  - btsm_443 of 0.05 - 556 m-1 (== 1000 g m-3 TSM)
  - detritus absorption ad_443:
  - ad_extra = 10**(log10_bbp_extra*1.0507611+0.4958577 + (-2.0+4.0*ran1(idumrand)*0.1731068)) (covariance from NOMAD)

Training based on a bio-optical model and simulations

- Bio-optical model is based on the following components of NOMAD data:
  - a_pig pigment absorption coefficients
  - a_g   absorption coefficient of filtered water (CDOM)
  - a_d   absorption coefficient of detritus
  - bbp   backscattering coefficient of particulate matter
- The co-variances between these components have been computed relative to the chlorophyll (chl_f) concentrations with 2 standard deviations
- Training targets are:
  - chlorophyll concentration
  - a_pig
  - a_g
  - a_d
  - bbp
  - Kd
- Input are reflectances (RLw) at MERIS bands: 412, 443, 490, 510, 560, 620, 665, 708, 753, 778, 865 nm

NN Engine with optimization



Input to inverse water NN for high TSM

- the net has 16 inputs:
- input 1 is sun_thet in [0.001169,75.0]
- input 2 is view_zeni in [0.000000,50.0]
- input 3 is azi_diff_hl in [0.000000,180.0]
- input 4 is temperature in [0.000150,36.0]
- input 5 is salinity in [0.000478,43.0]
- input 6 is log_rlw_412 in [-11.860000,-1.575]
  - *12 bands rlw*
- input 16 is log_rlw_865 in [-13.040000,-2.749]

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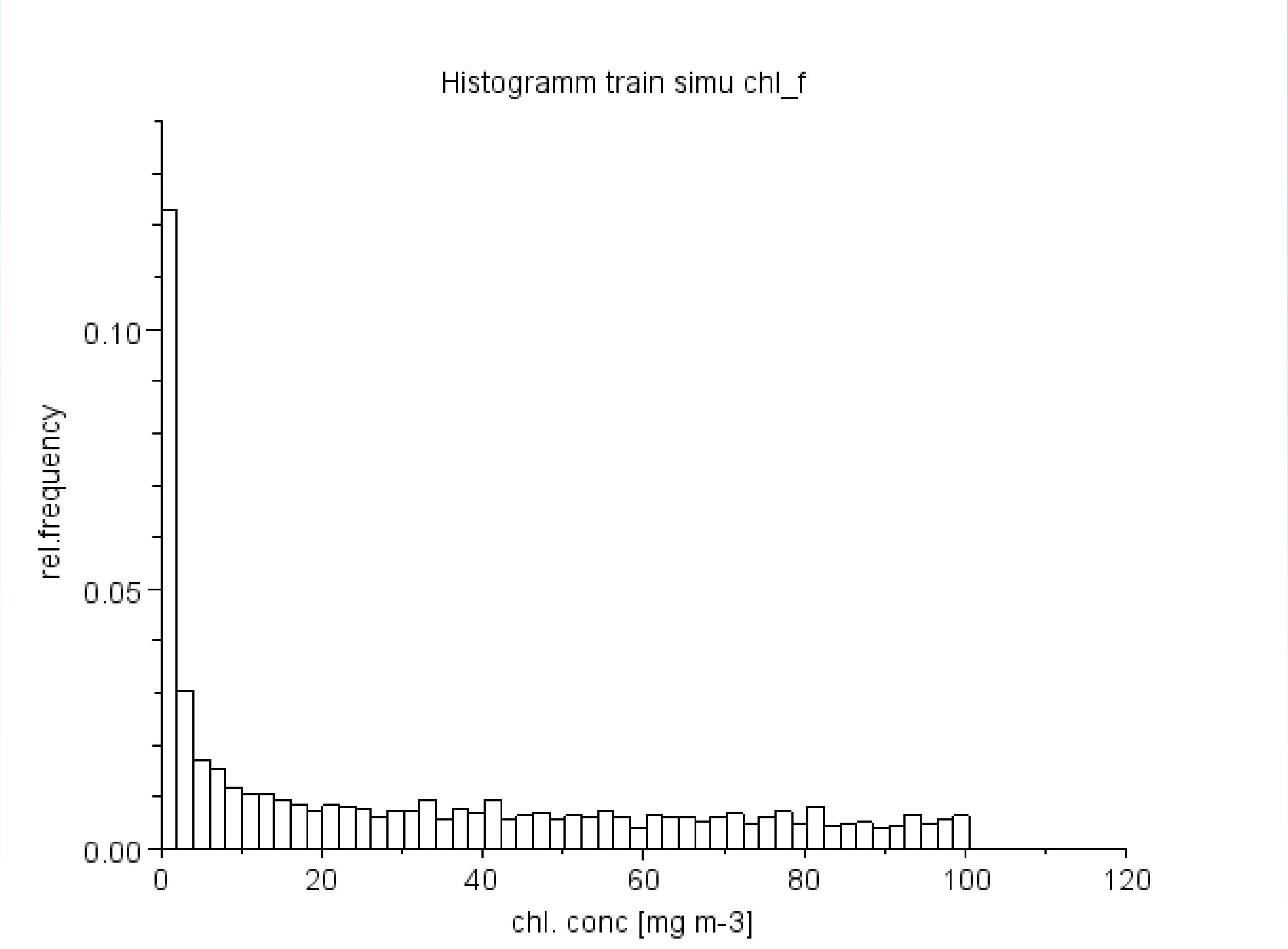
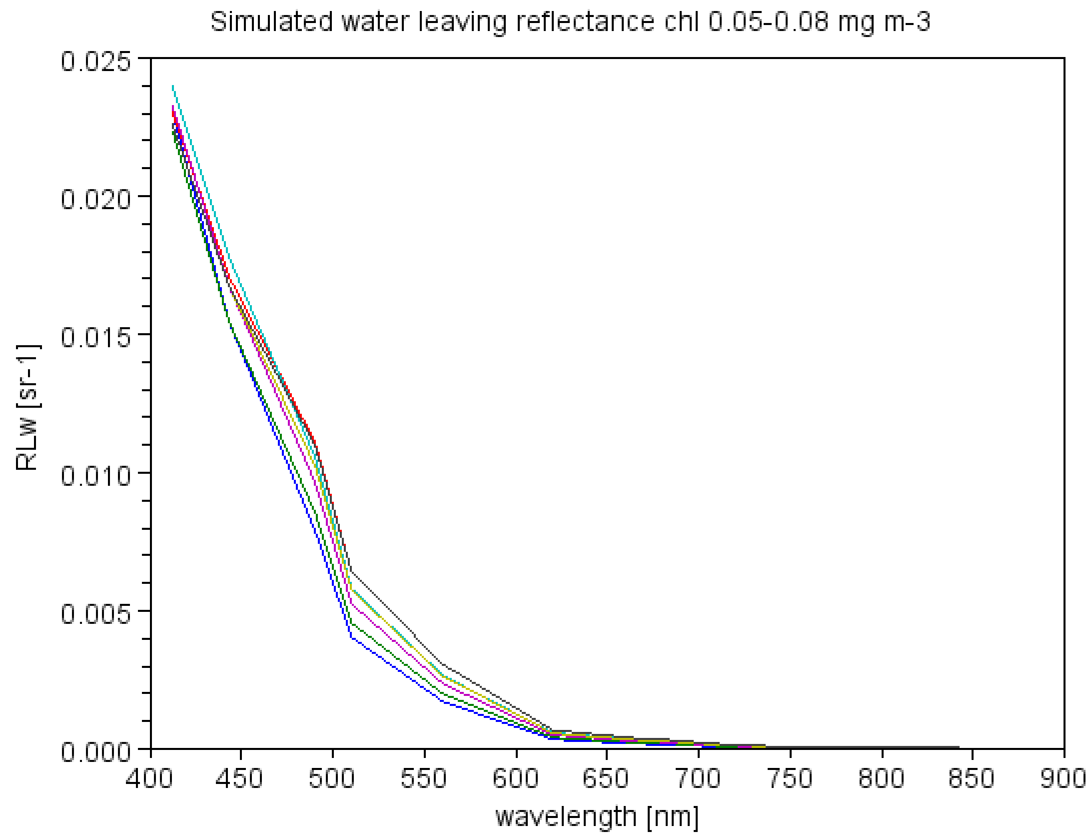
Output of inverse water NN (high tsm)

- the net has 7 outputs:
- output 1 is log_conc_chlor in [-4.605000,3.912] *0.01 – 50 mg m-3*
- output 2 is log_conc_apart in [-8.450000,0.5441]
- output 3 is log_conc_agelb in [-6.194000,0.8829] *0.002 – 2.4 m-1*
- output 4 is log_conc_apig in [-6.735000,0.1856]
- output 5 is log_conc_bpart in [-4.926000,6.321] *0.01 – 950 g m-3*
- output 6 is log_conc_bwit in [-4.605000,-2.303]
- output 7 is log_mean_kdmin in [-4.147000,2.191] *0.016 – 9.0 m-1*

Chlorophyll frequency distribution used for simulation



Mixed lin-log distribution



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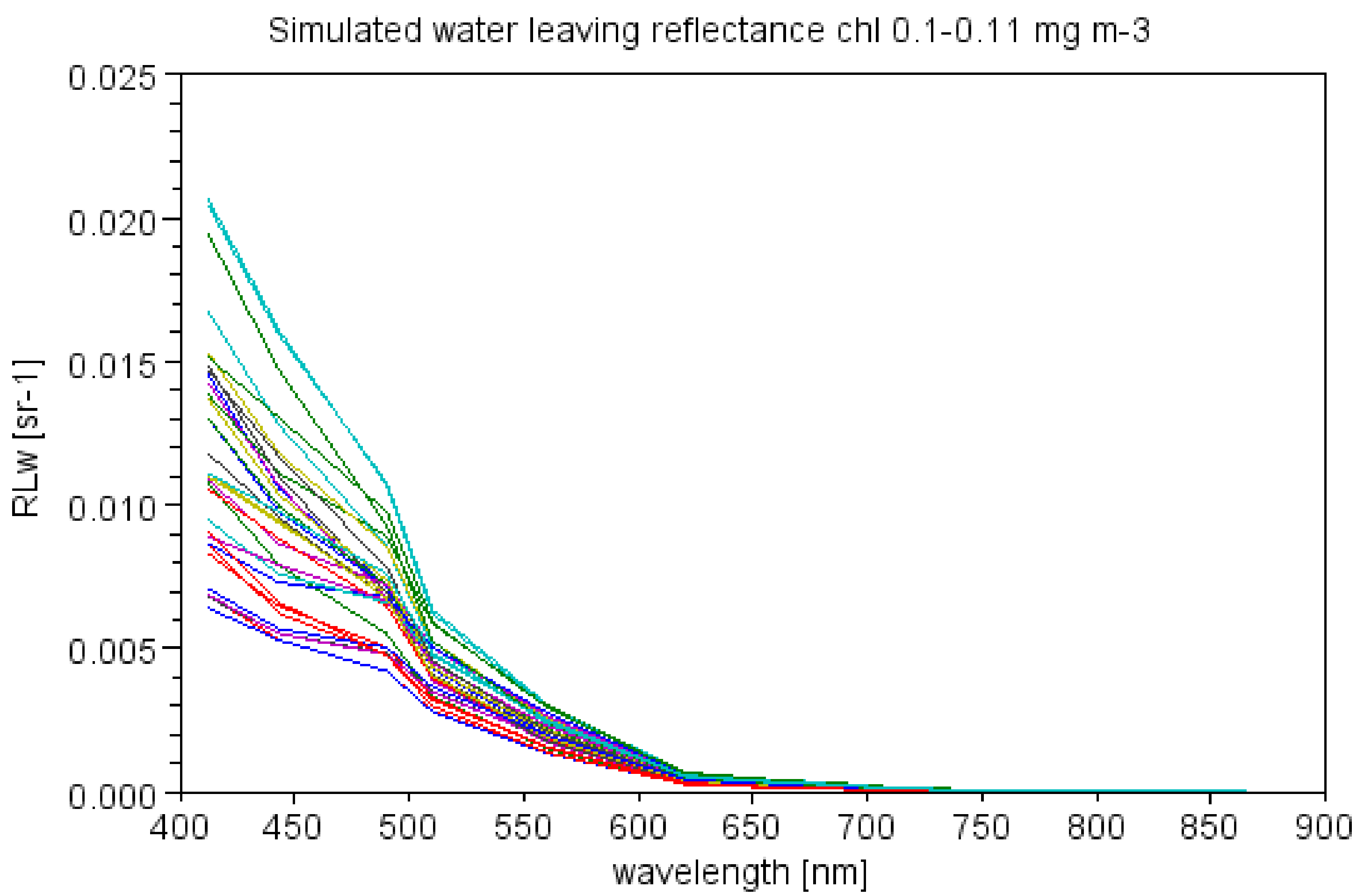
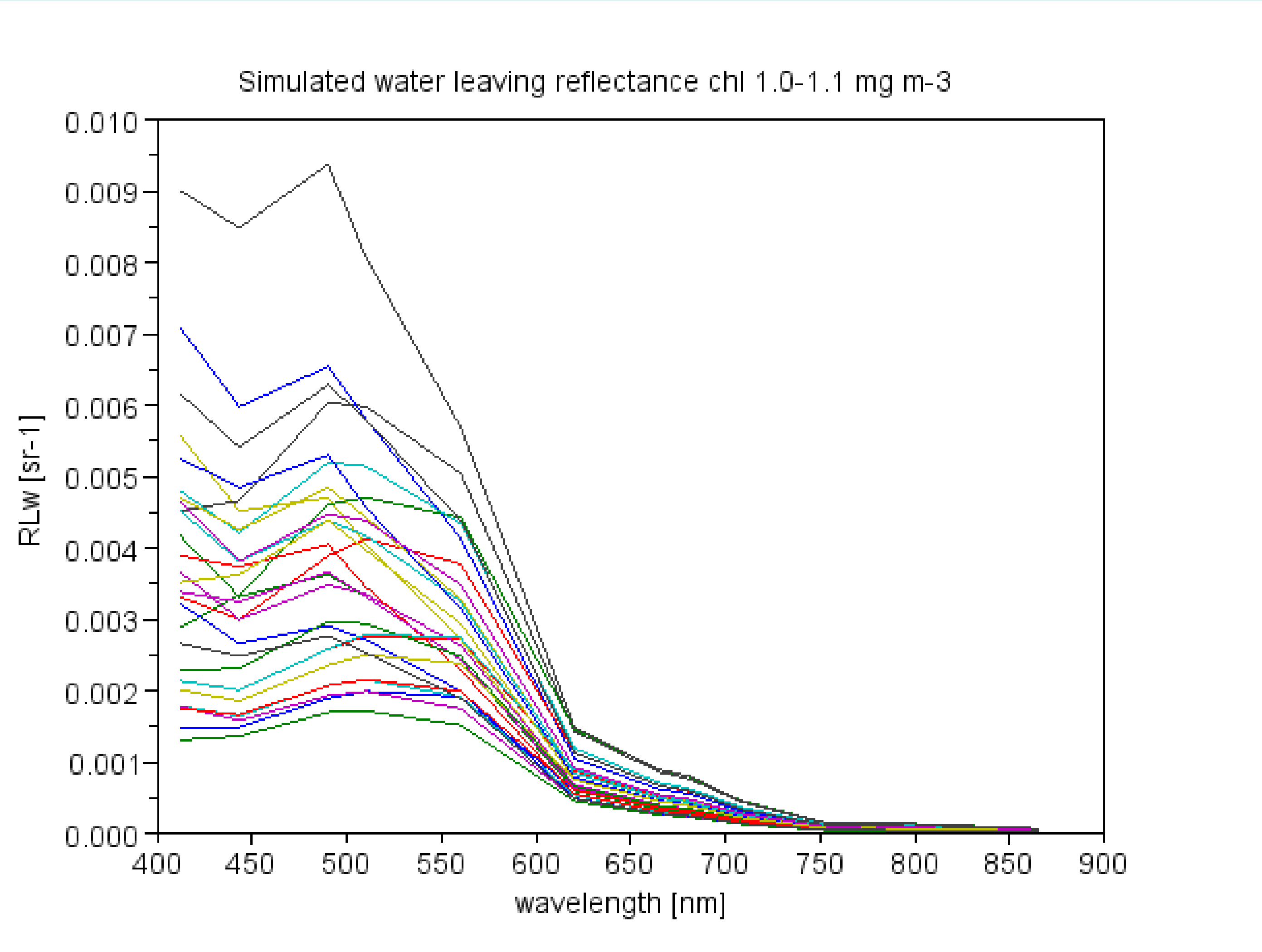
RLw from simulated data set



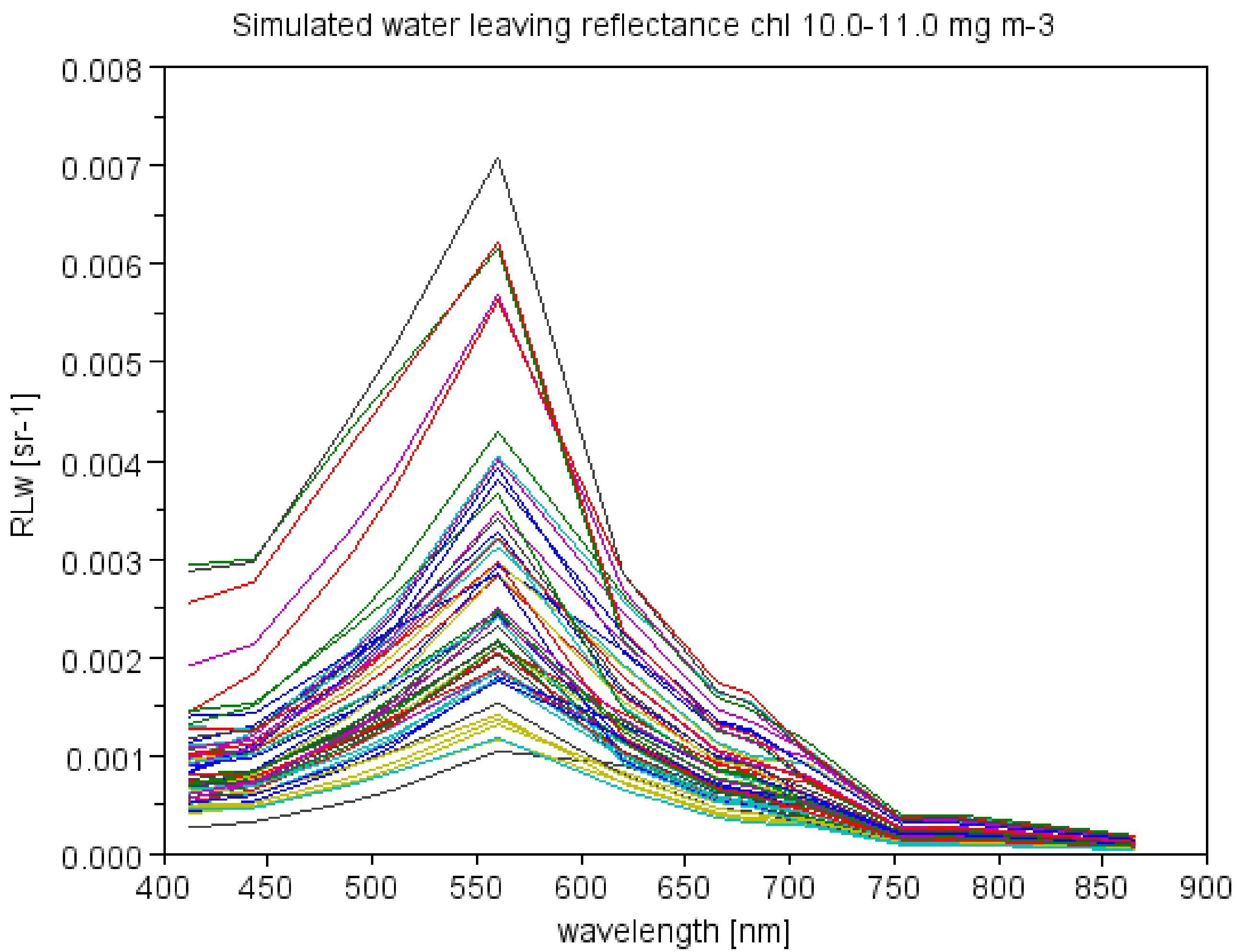
Chl_f 0.1 – 0.11 mg m-3

RLw from simulated data set



Chl_f 1.0 – 1.1 mg m-3

RLw from simulated data set



Chl_f 10.0 – 11.0 mg m-3

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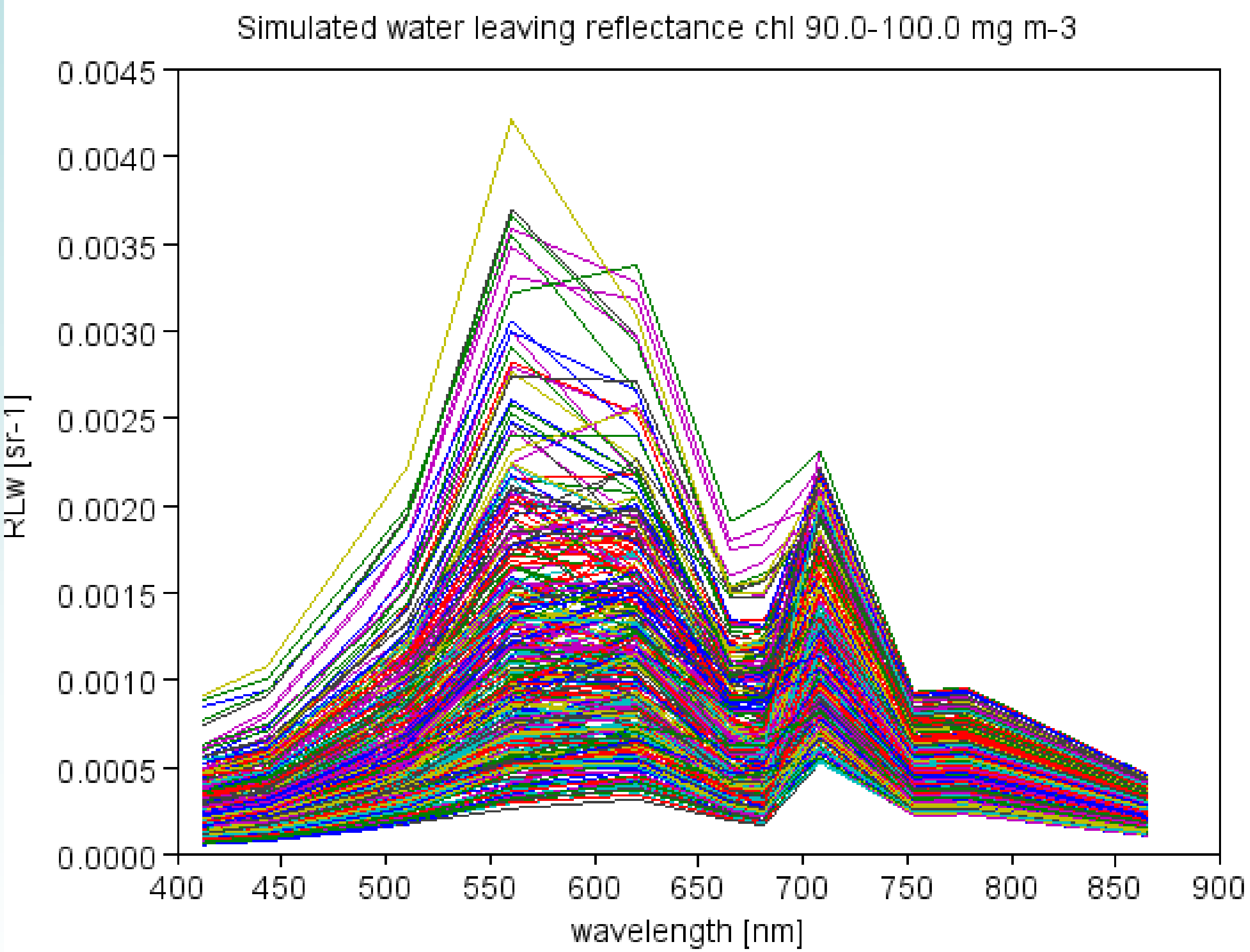
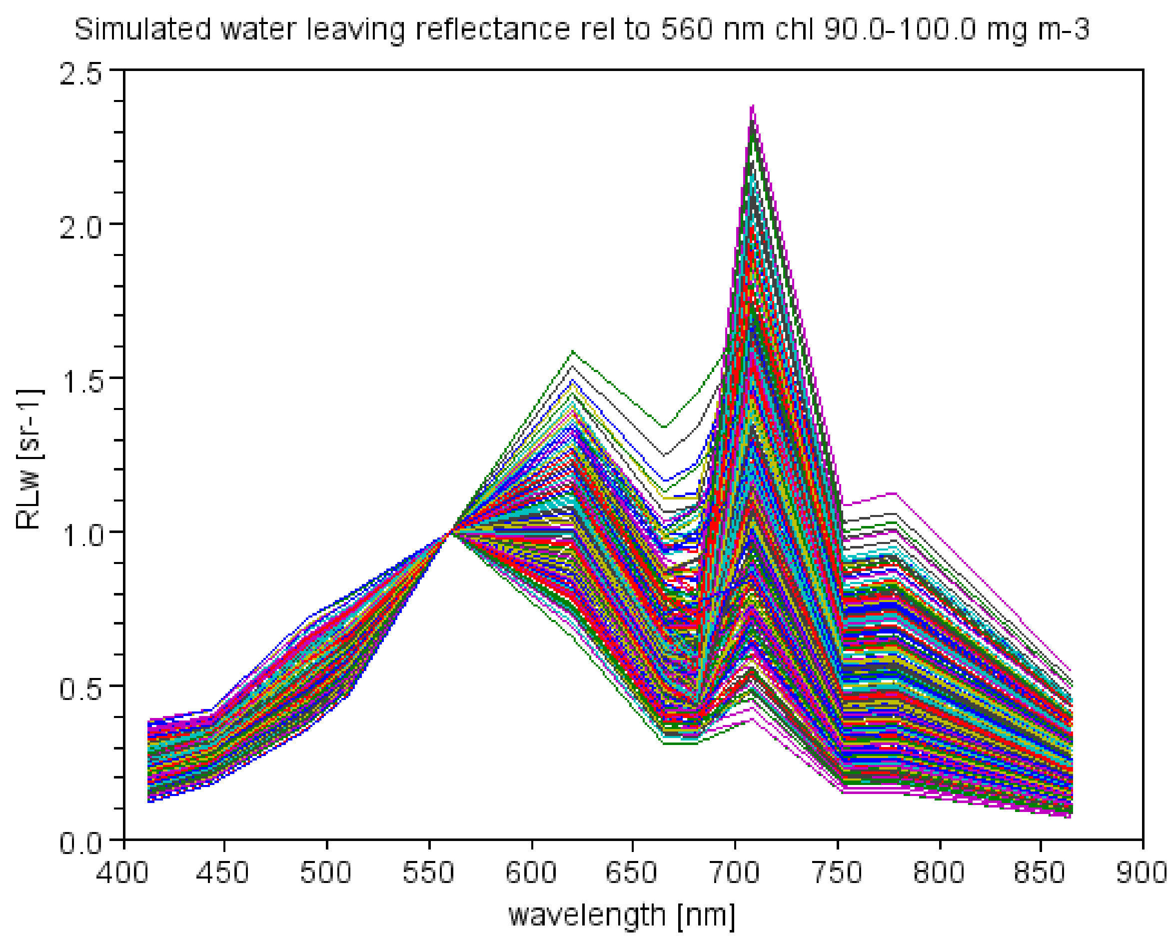
RLw from simulated data set



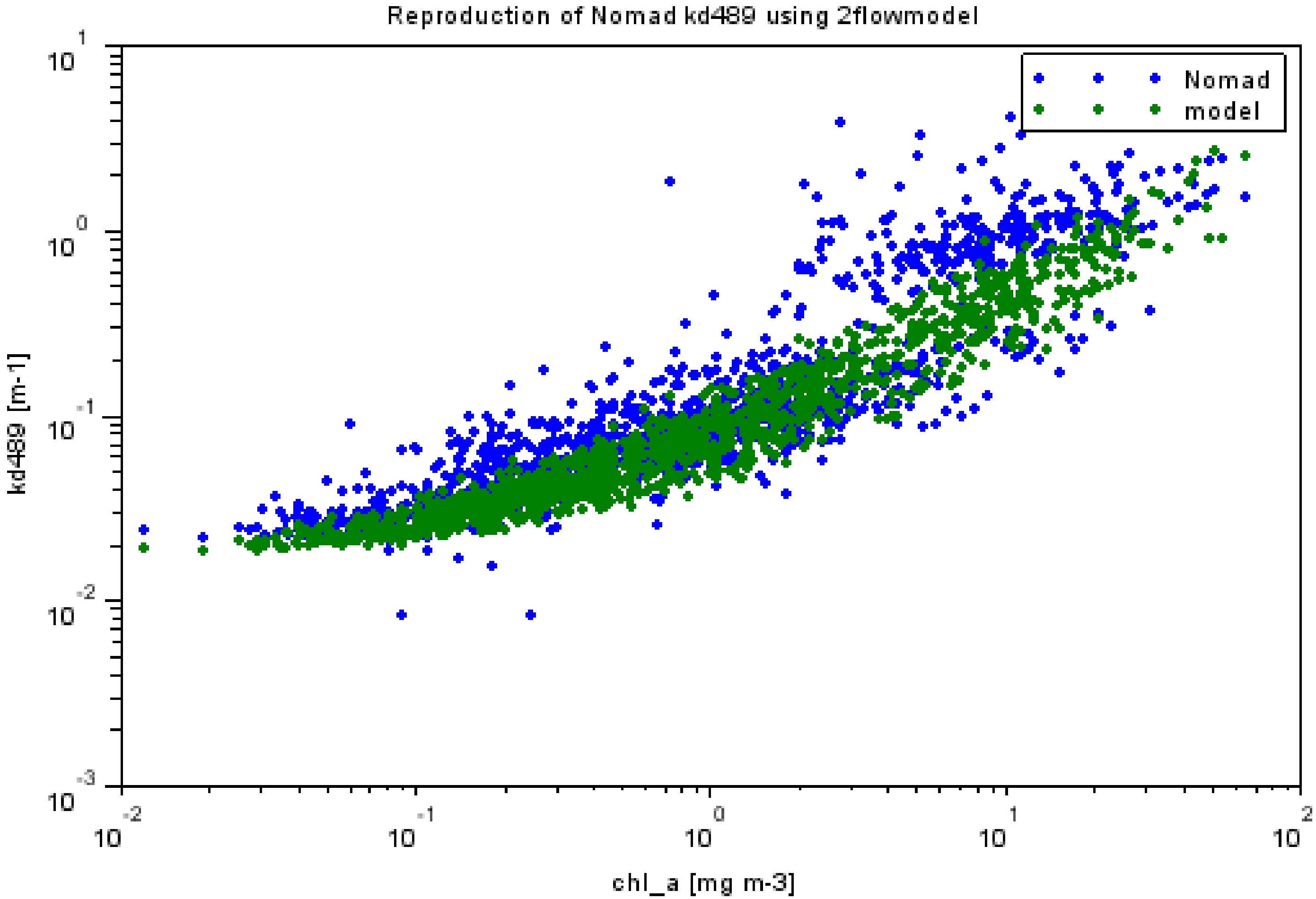
Chl_f 90.0 – 100.0 mg m-3

RLw rel to 560 nm from simulated data set



Chl_f 90.0 – 100.0 mg m-3, log scale

Reproduction of Nomad data set using model: kd489



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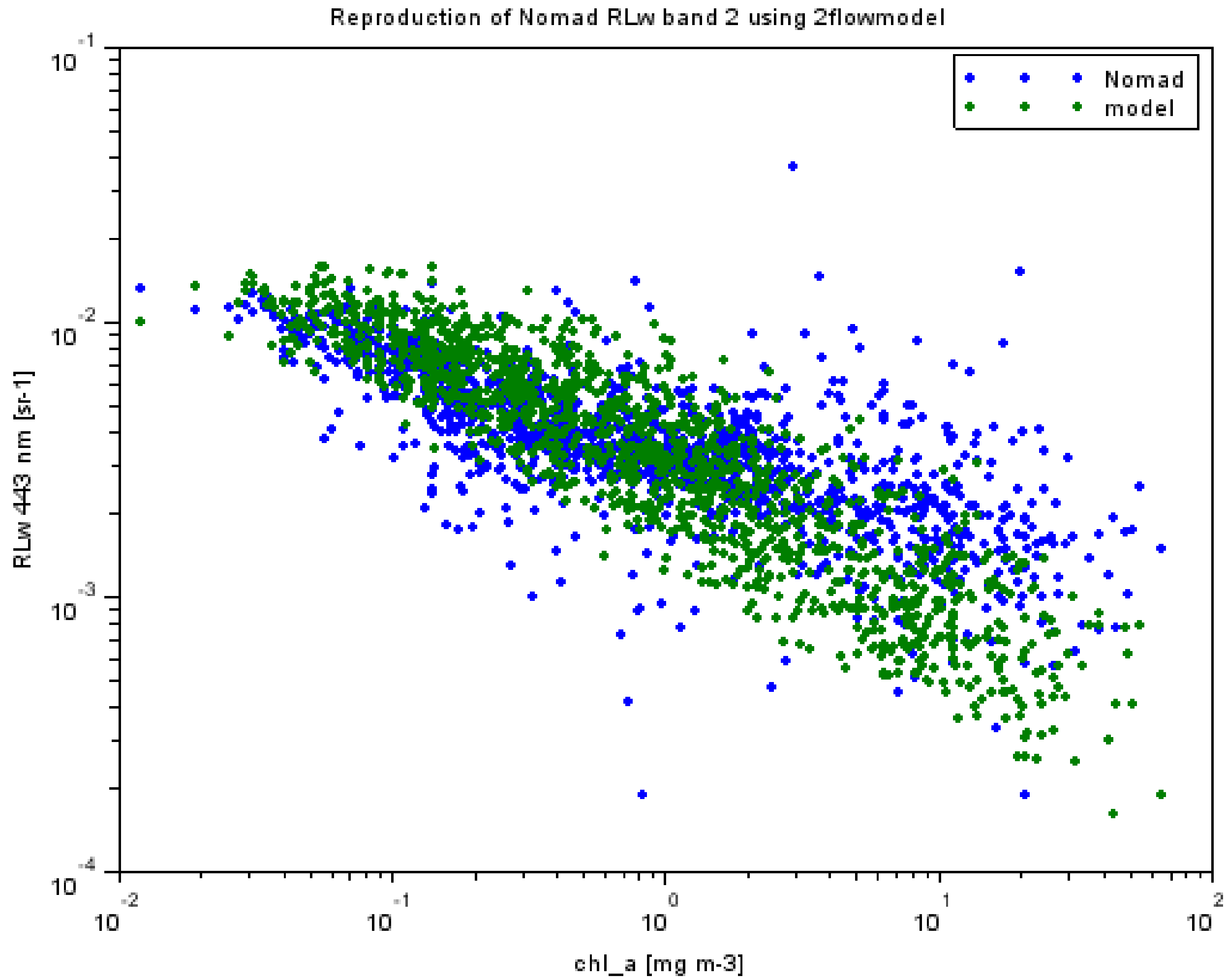
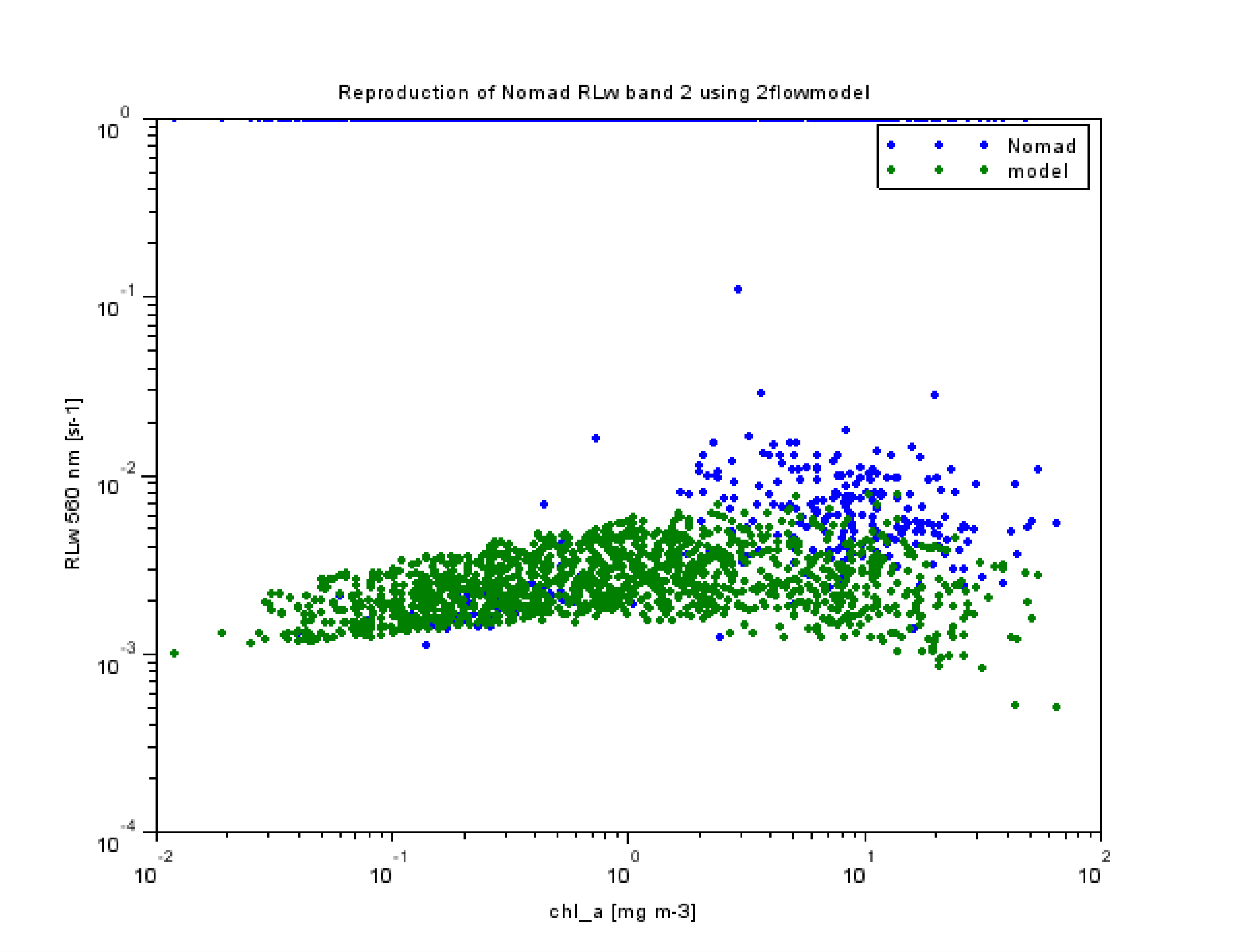
Reproduction of Nomad data set using model: RLw 443 nm



Reproduction of Nomad data set using model: RLw 560 nm



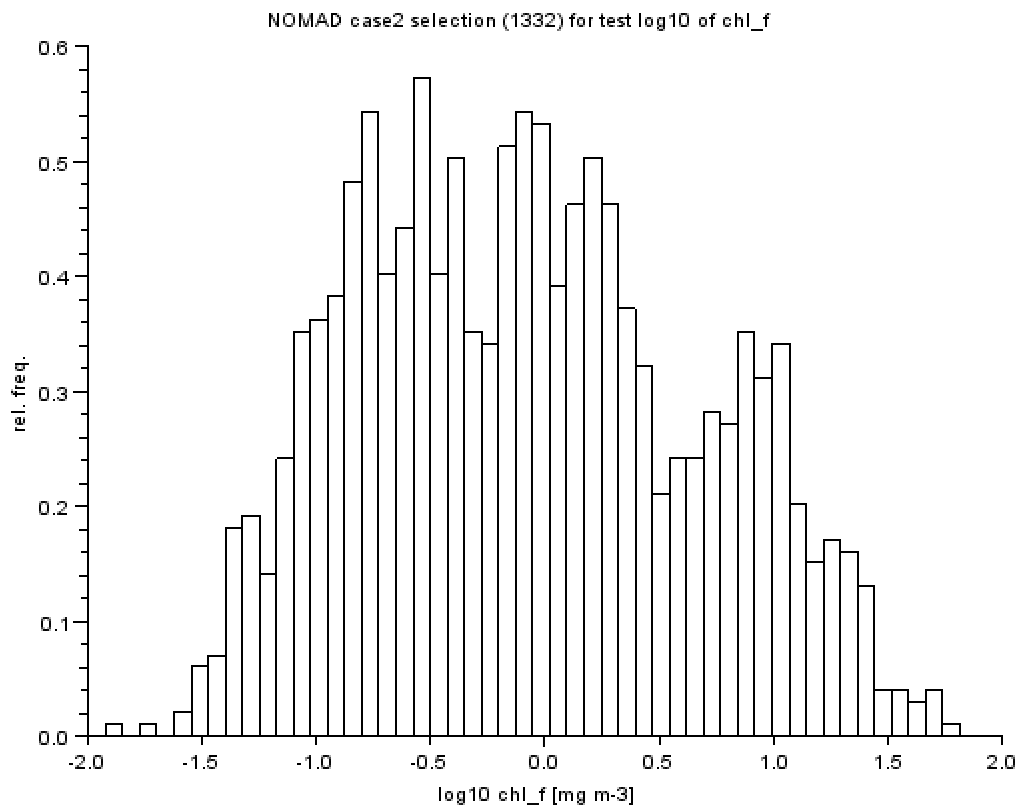
Alternative ways to use NNs

- Bio-optical model based on optical components -> atmospheric correction
- Training based directly on field data
- Inverse NN with only 1 output parameter
- Inverse NN with only 1 output parameter and adapted input band sets
- Forward NN used as forward model within an optimization loop
- s. later presentation

Questions, remarks ?

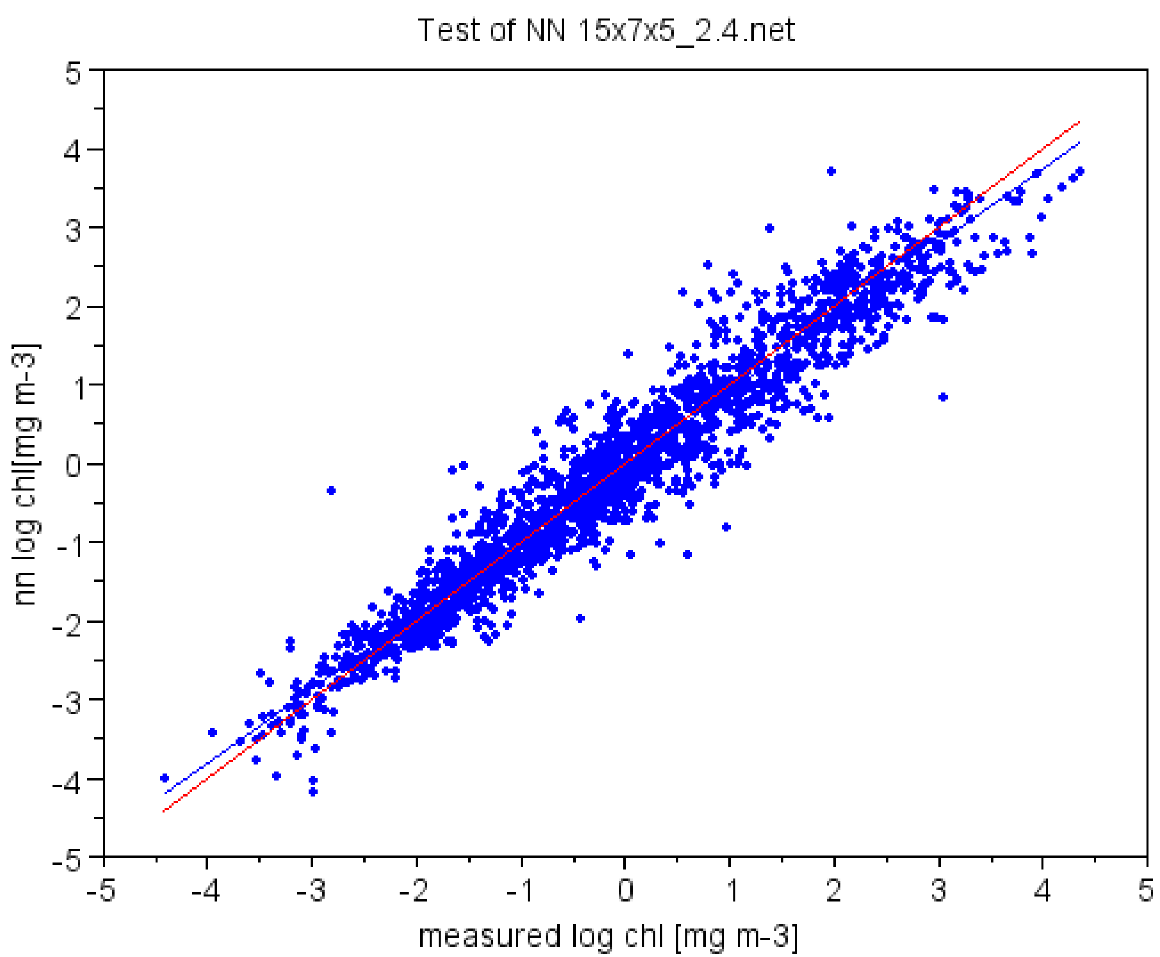
Training of NN using measured reflectance spectra

- 2 types of NN
  - Reflectances as input MERIS bands 412, 443, 490, 560, 665 nm
  - Reflectances normalized to band 560 nm



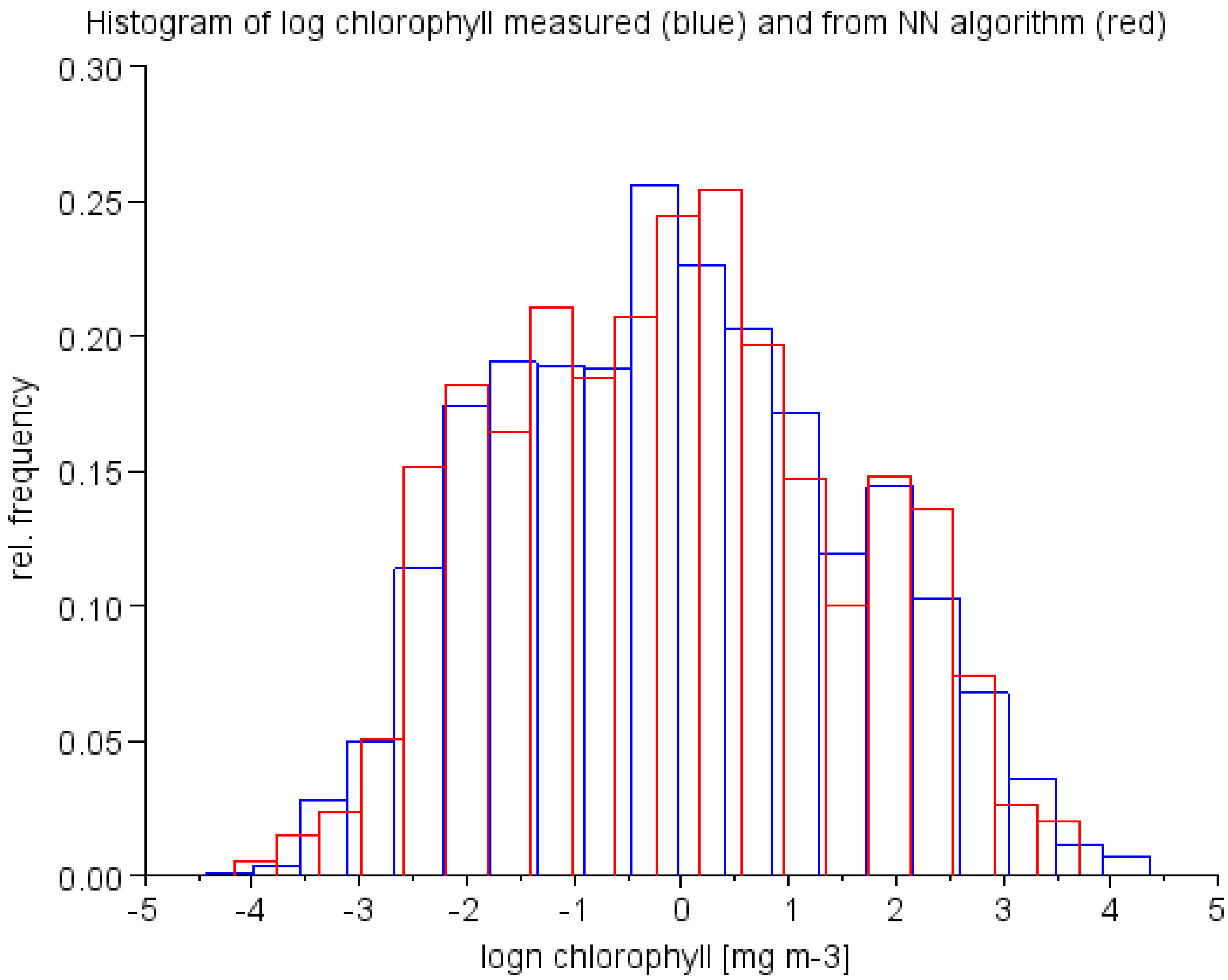
Data for testing the NN

Test of NN based on measurements for chlorophyll

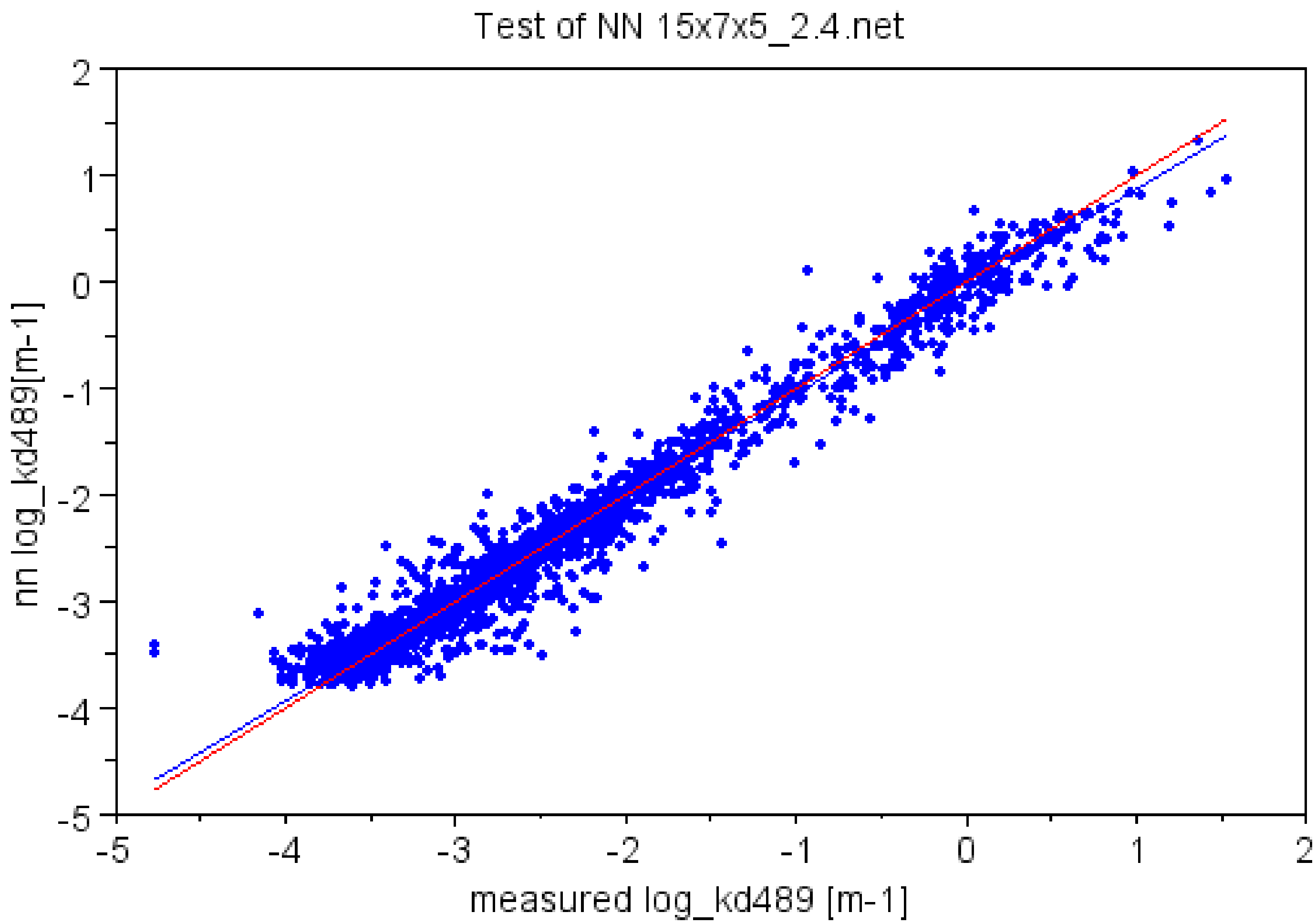


Log10 scale, red: 1 by 1 line

Comparison of histograms: measured, NN computed

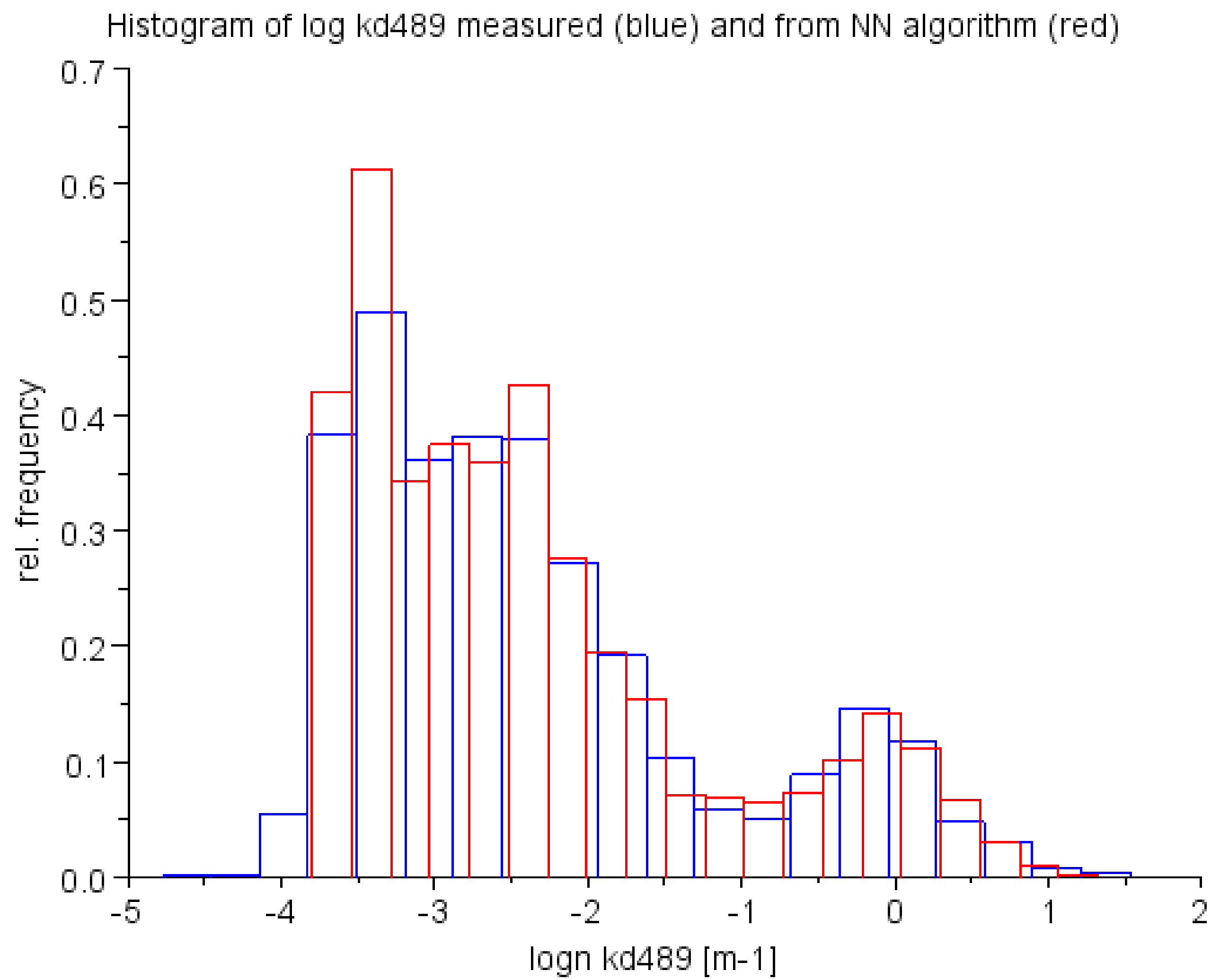


NN for kd489



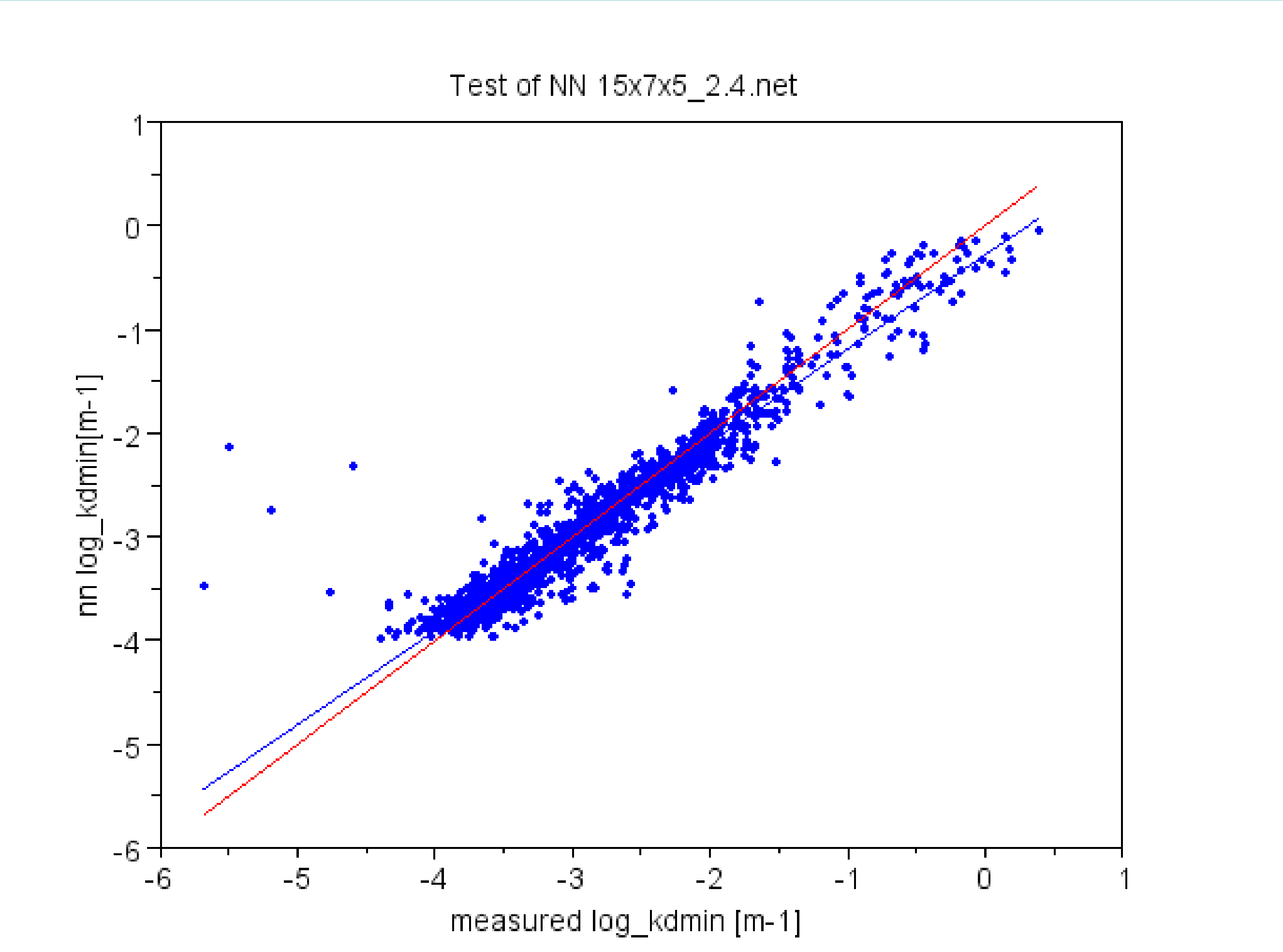
Test of NN 15x7x5_2.4.net
nn log_kd489[m-1]
measured log_kd489 [m-1]
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2

Histogram kd489 measured and NN derived

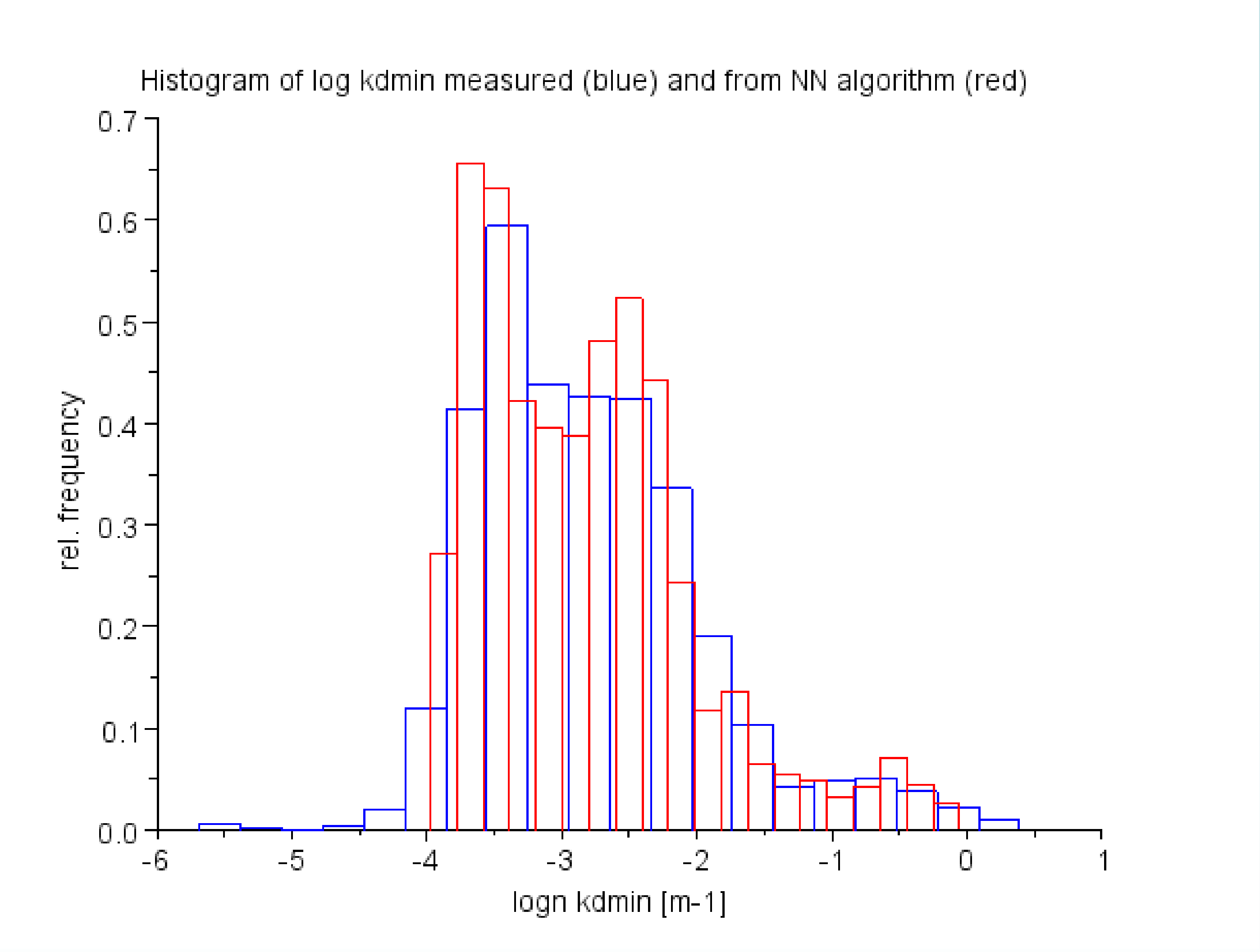


Neural network for kd_min

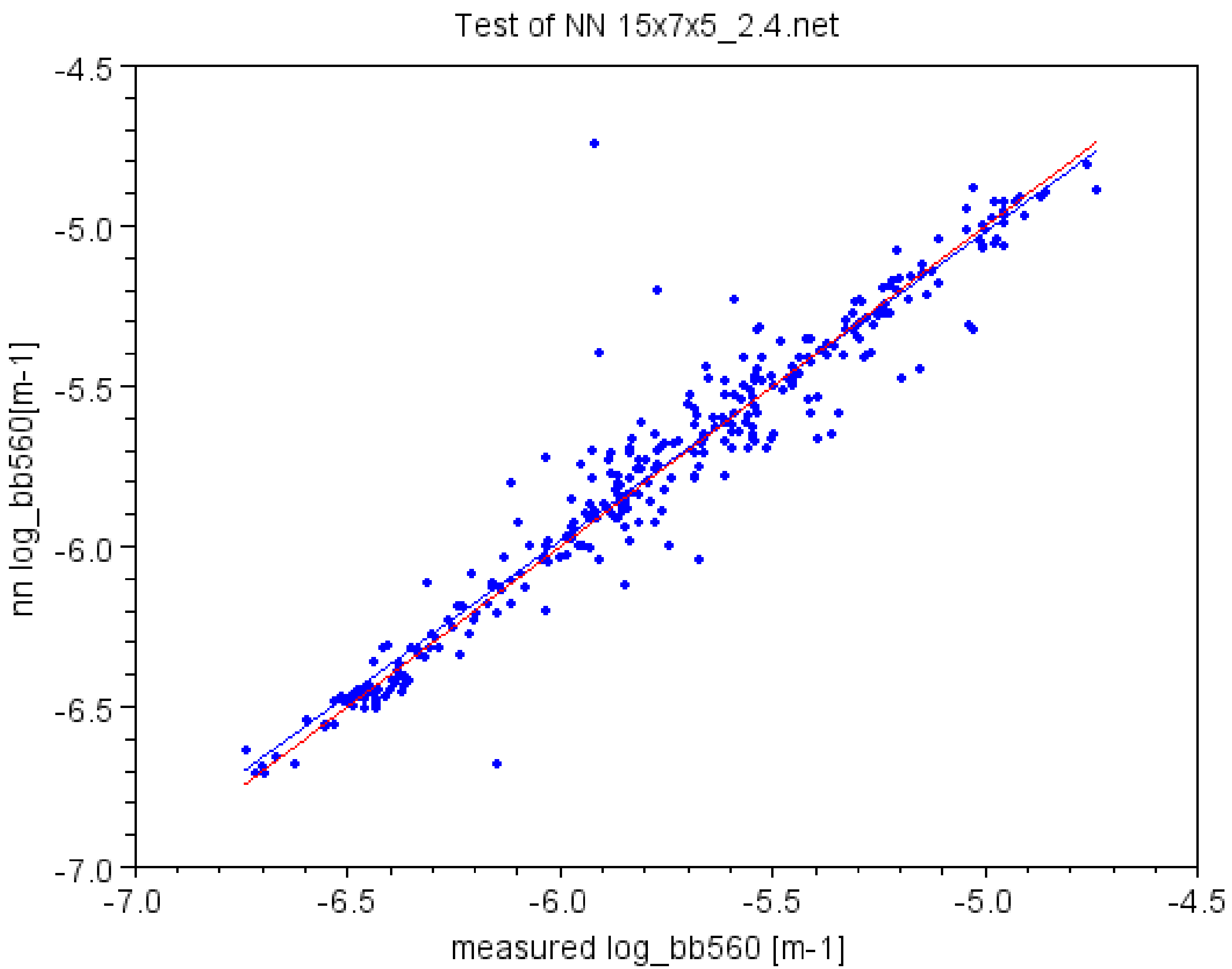
- measured from bands 411, 443, 489, 510, 555



Histogram kd_min measured and NN derived

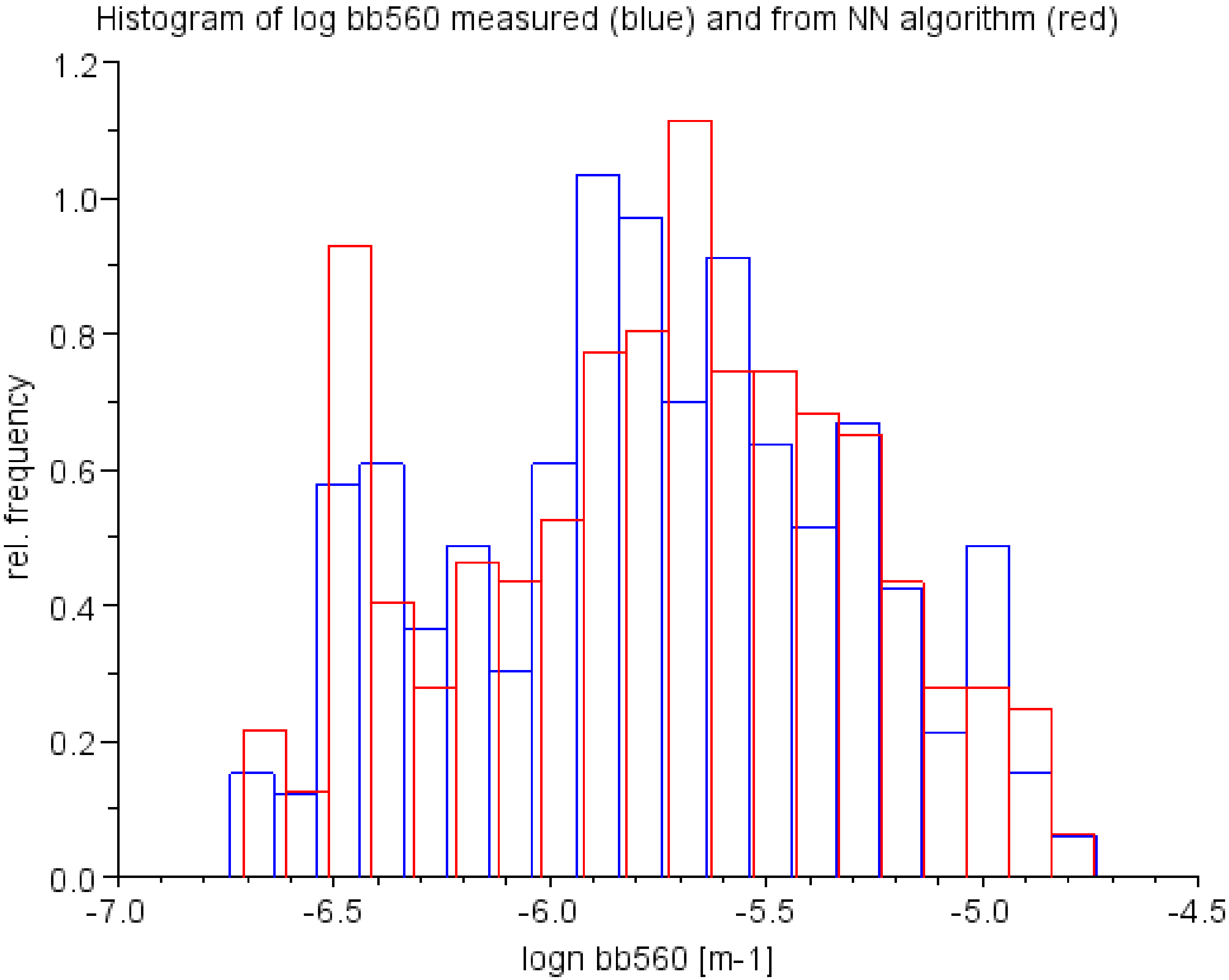


NN for backscattering coefficient bb

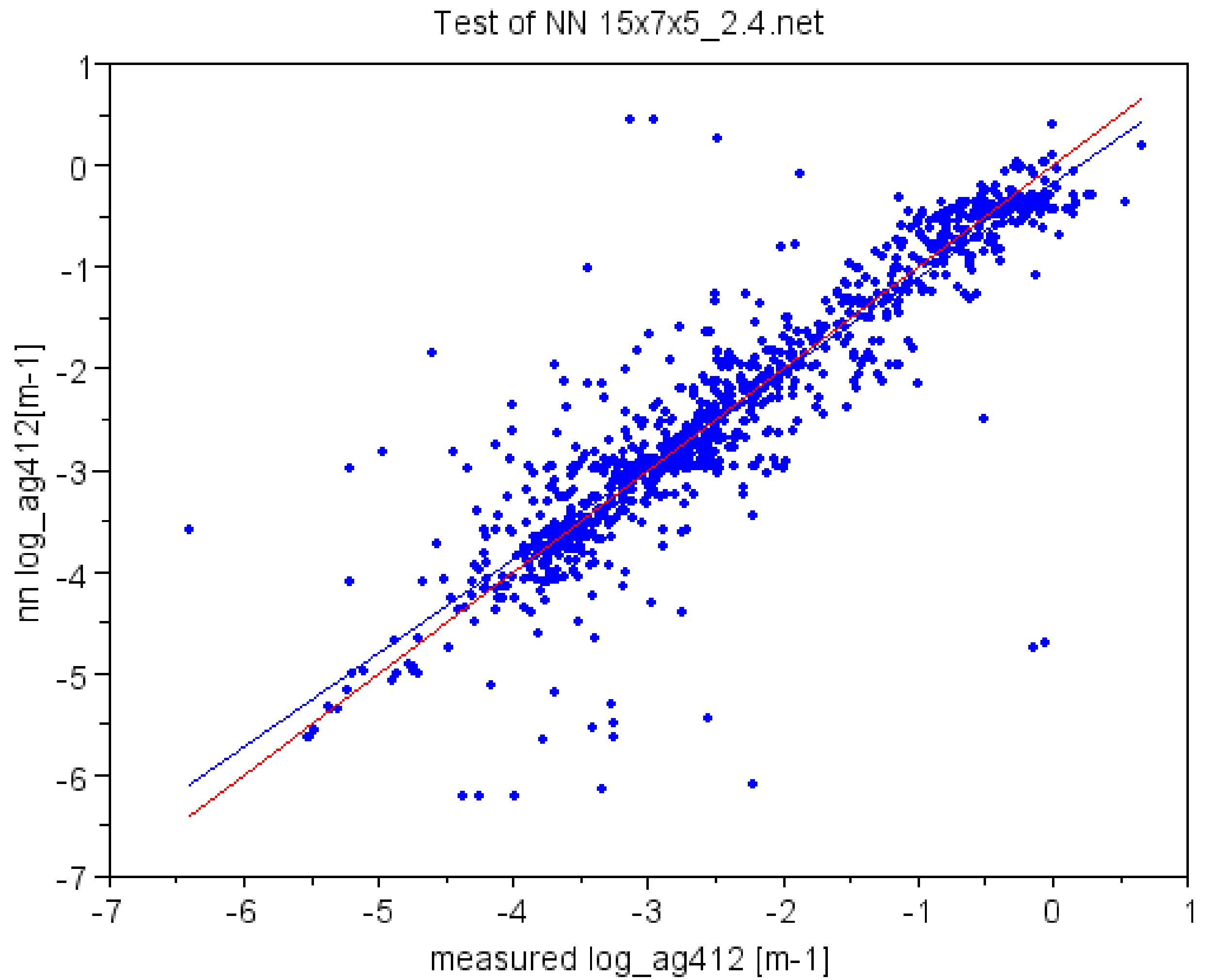


bb_560

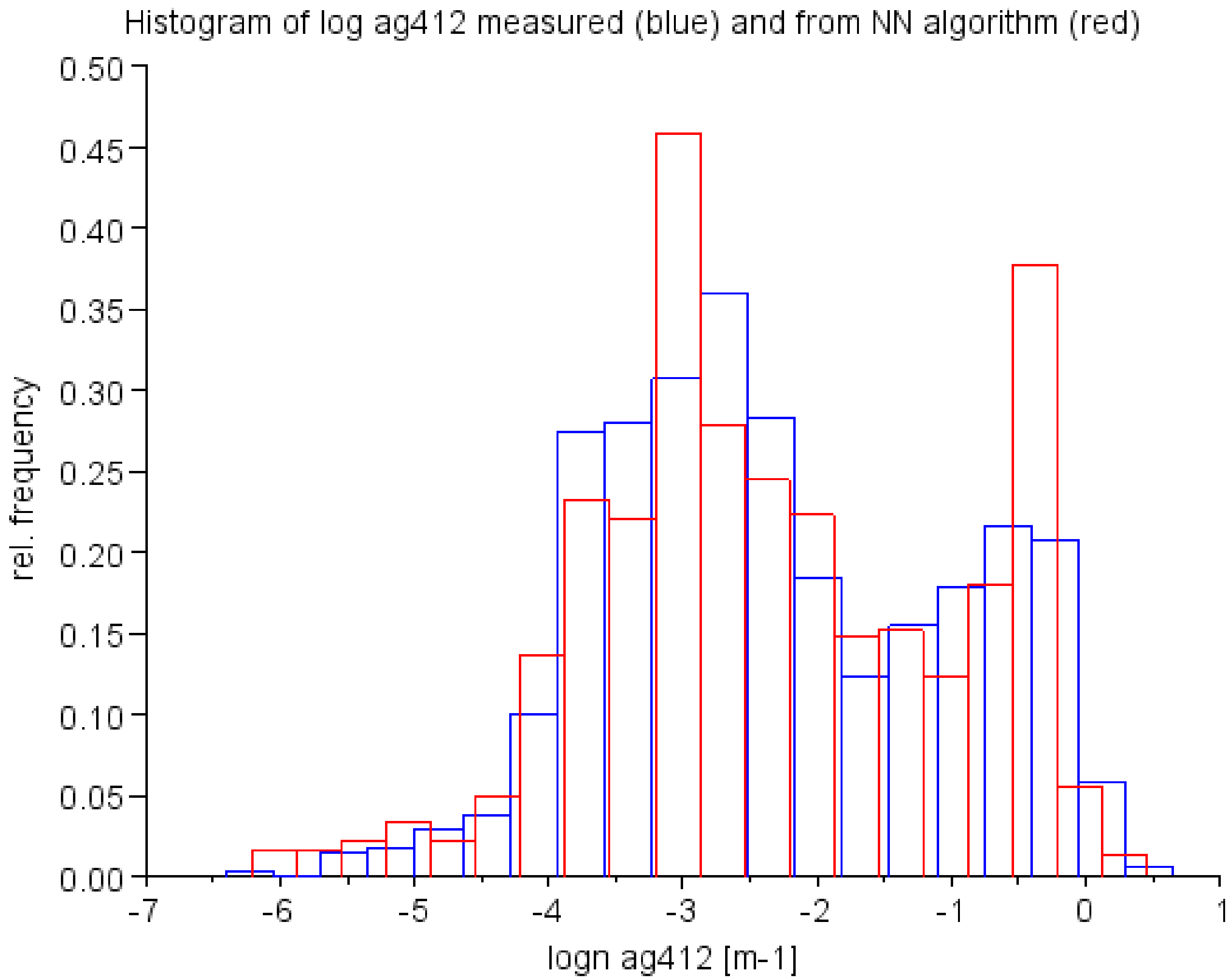
Histograms of measured and NNderived bb



NN for yellow substance (ag_412)

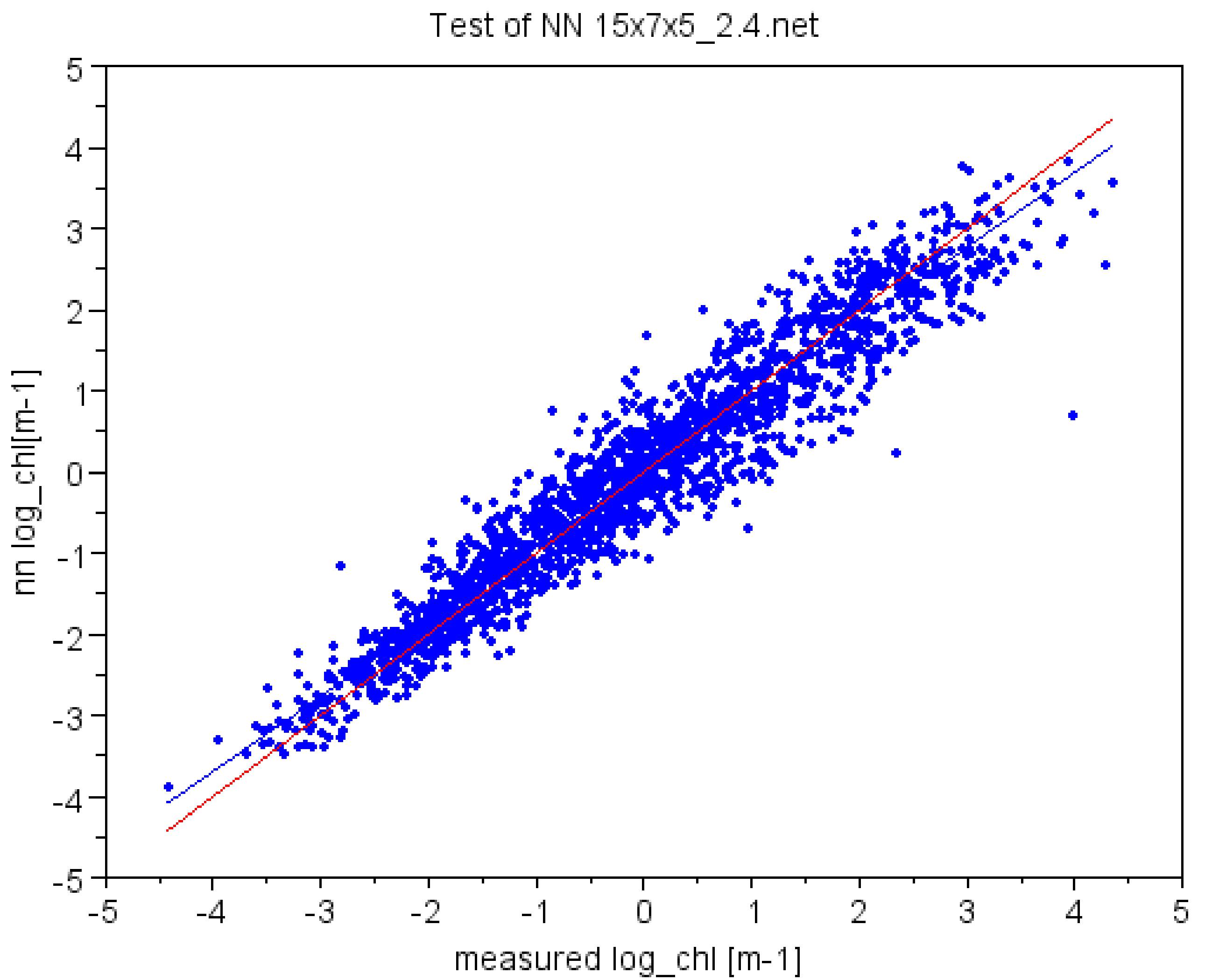


Histograms for measured and NN derived ag_412



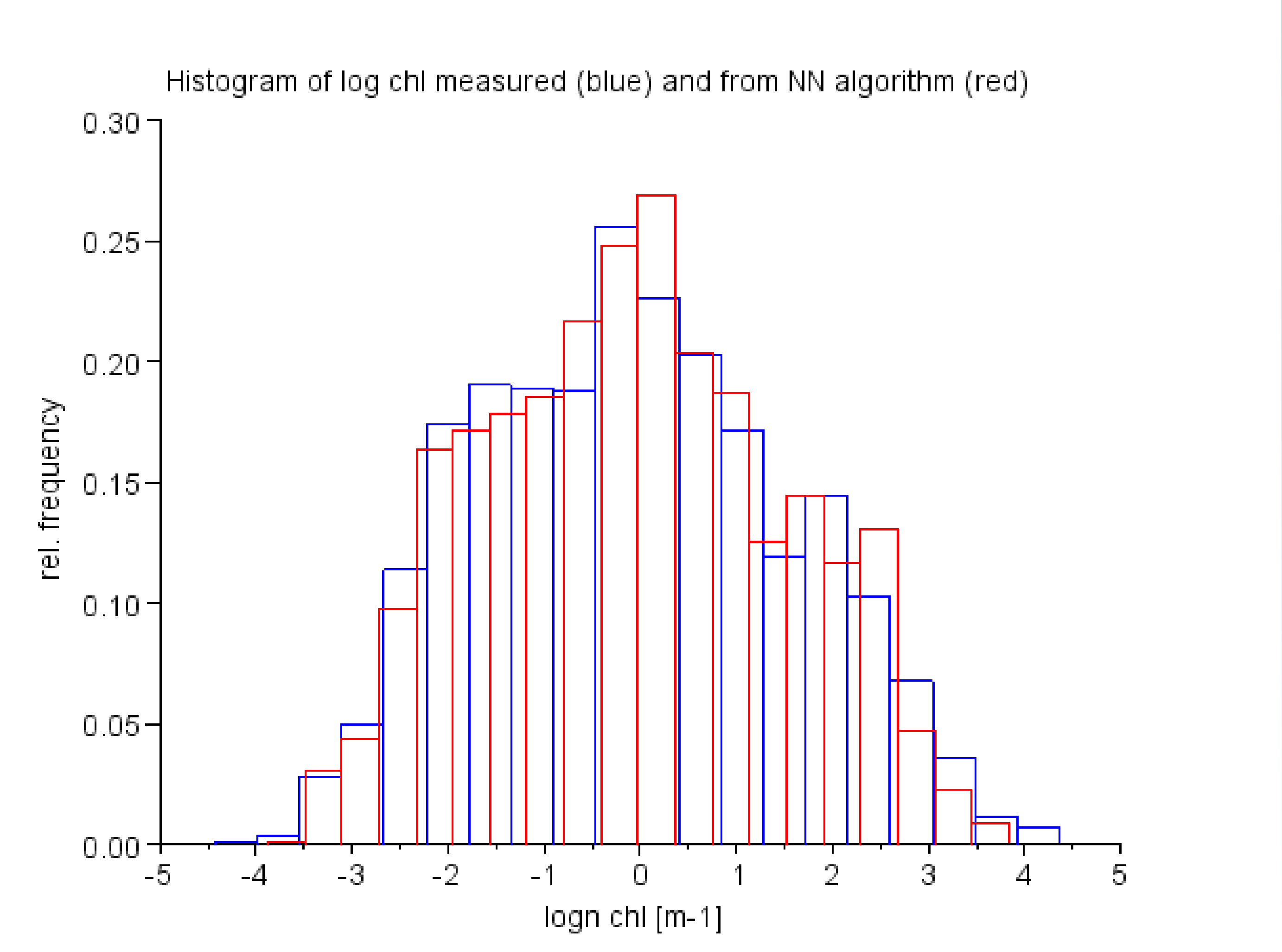
coastcolour

NN for chlorophyll for normalized reflectances (560 nm)

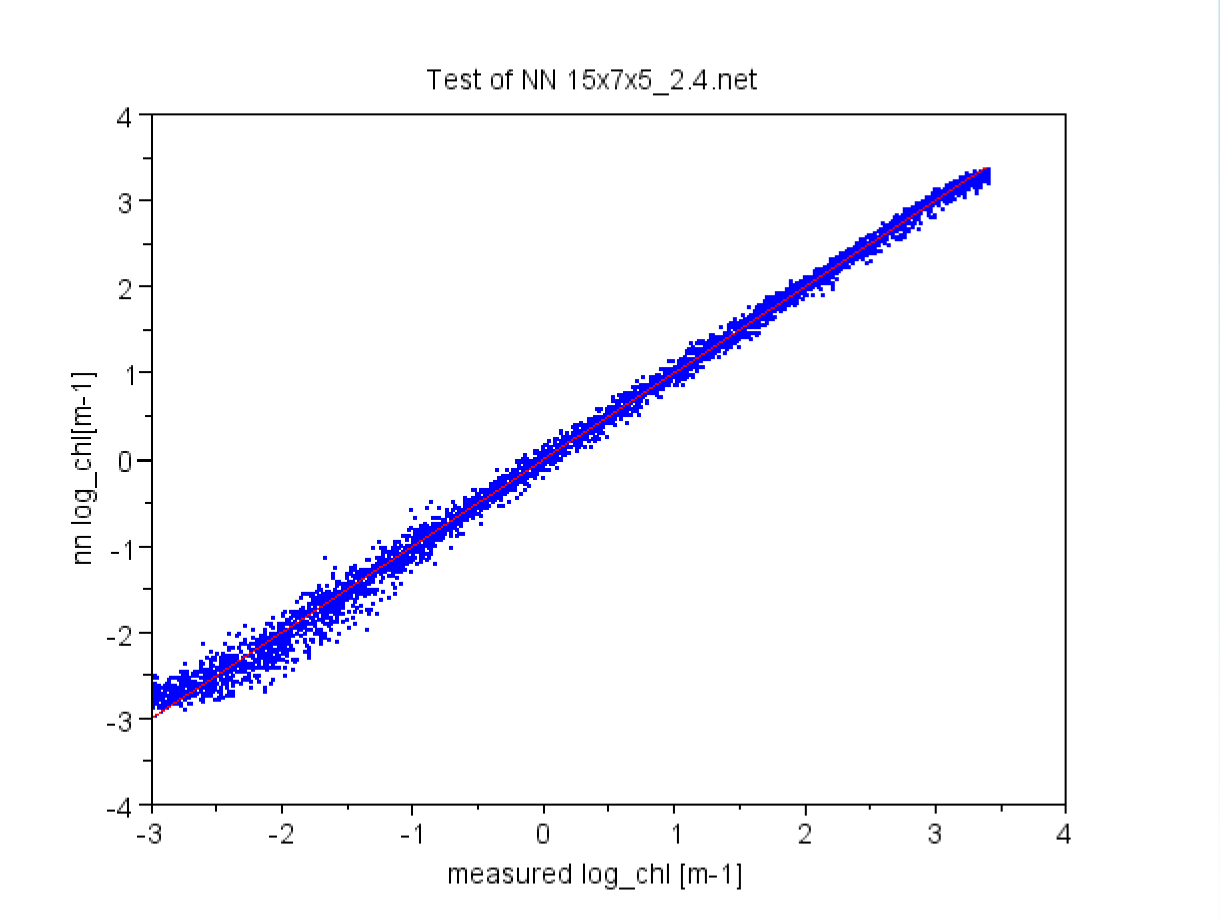


coastcolour

Histograms measured chl and NN derived from norm. Refl.

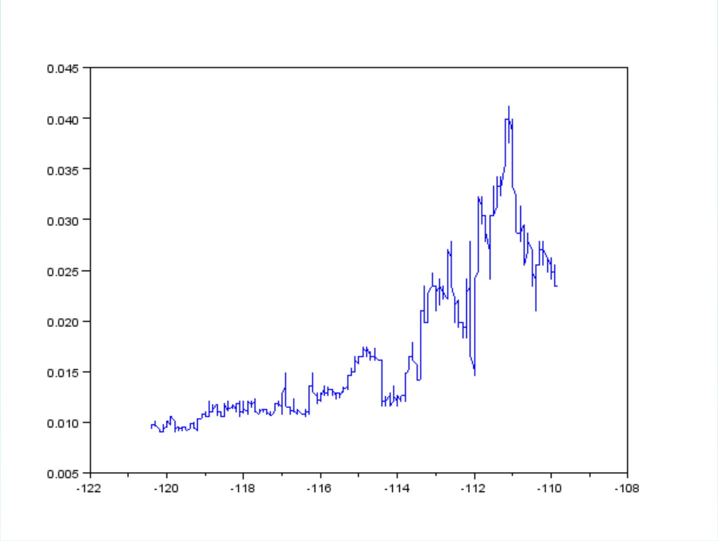


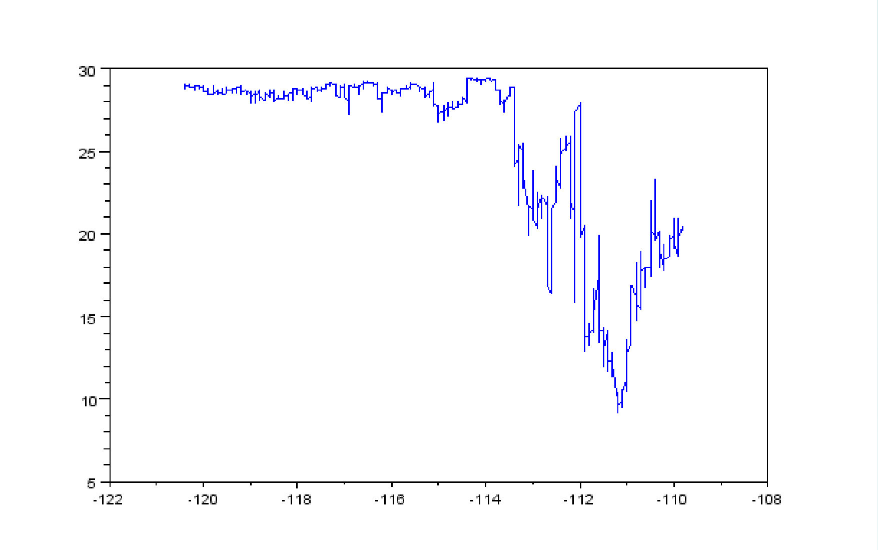
Test of training results: chlorophyll

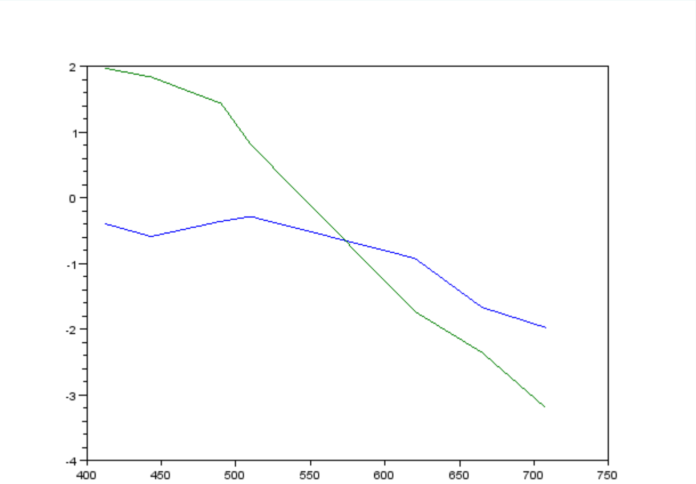


Chlorophyll, logn scale

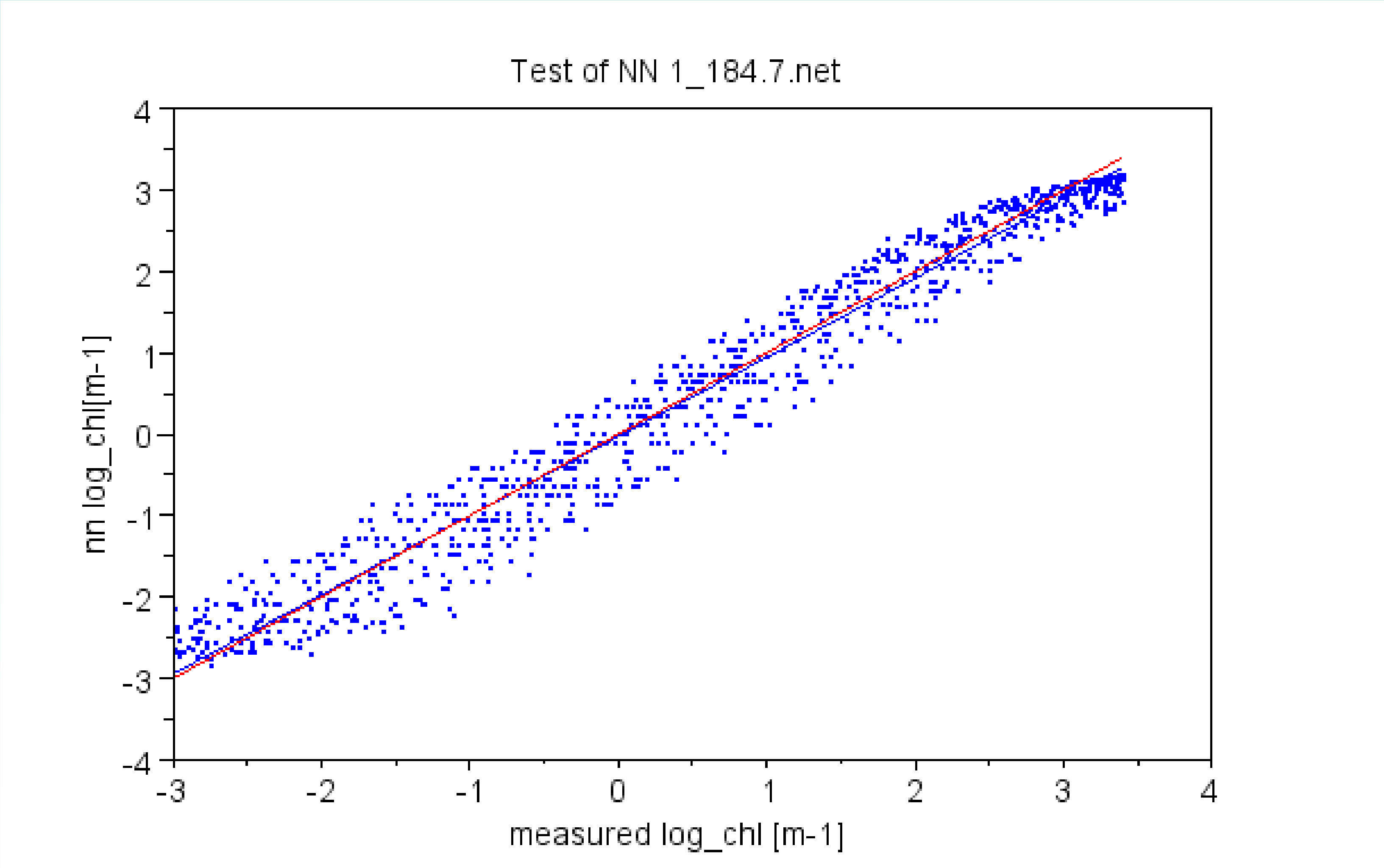
Overtrained NN





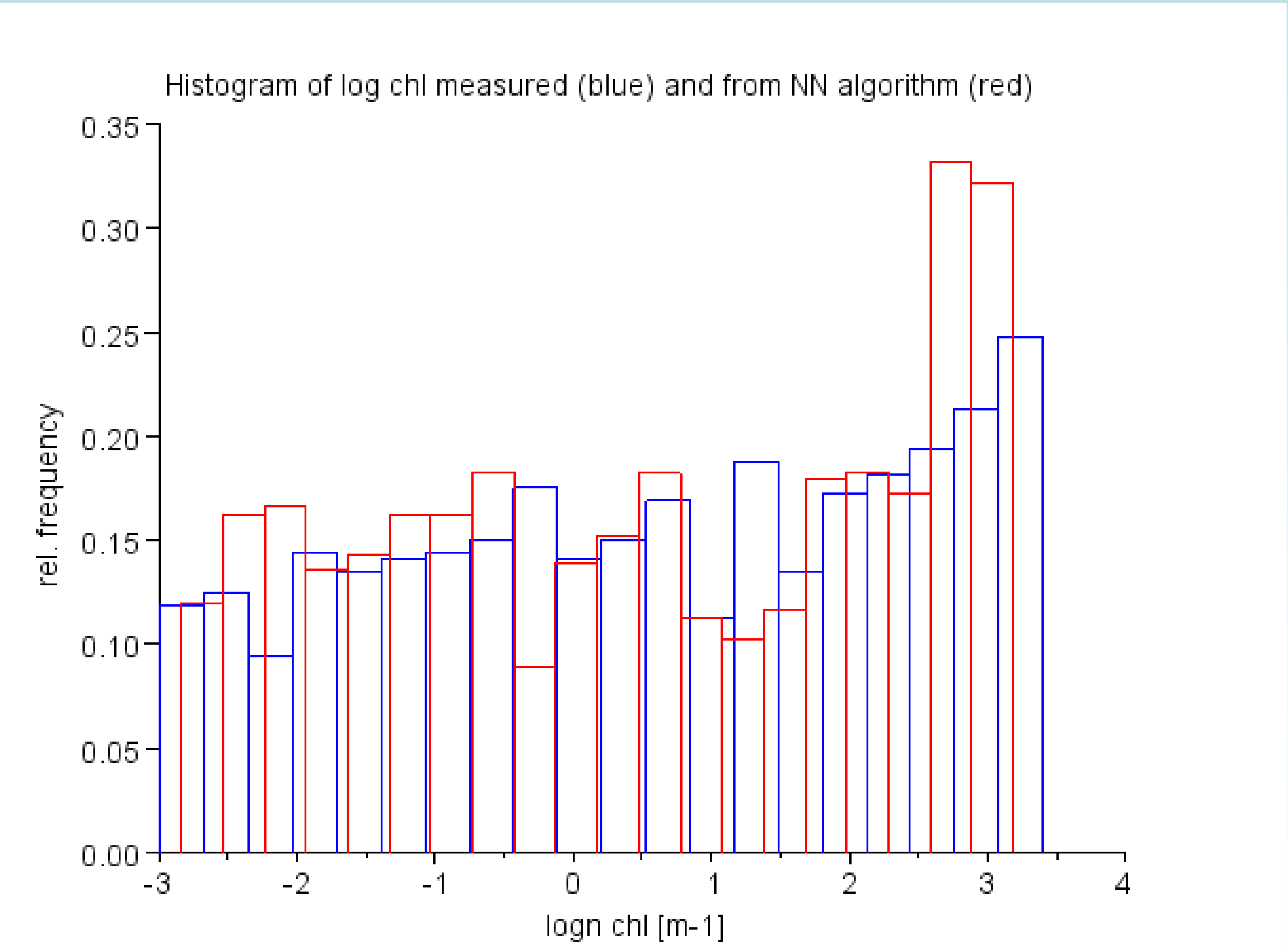


Test of training results: chlorophyll



Chlorophyll, logn scale

Reproduction of frequency distribution

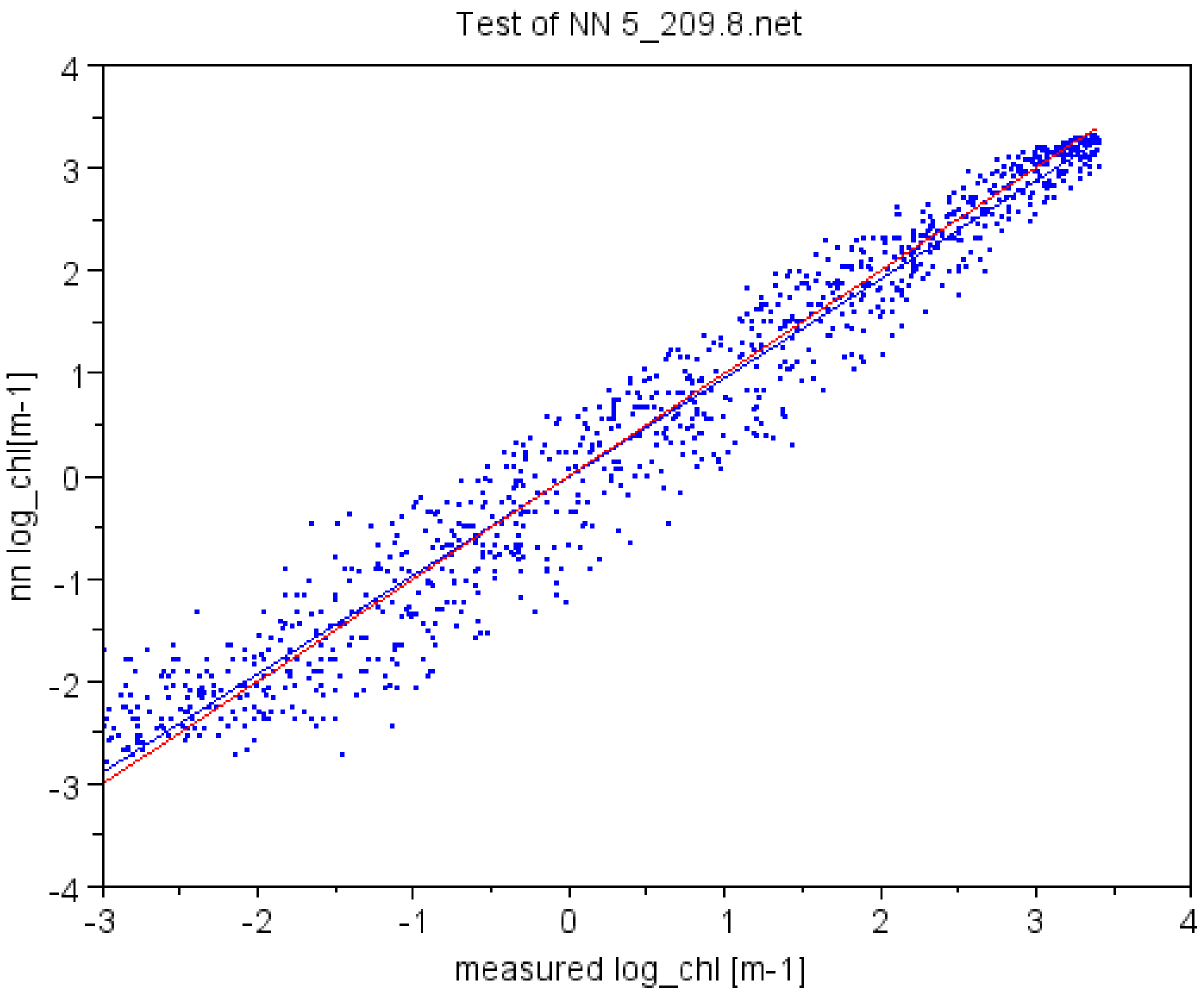


NIR NN algorithm

- Uses bands 560, 620, 665, 708 nm
- Normalized to band 560, i.e. 3 inputs to NN

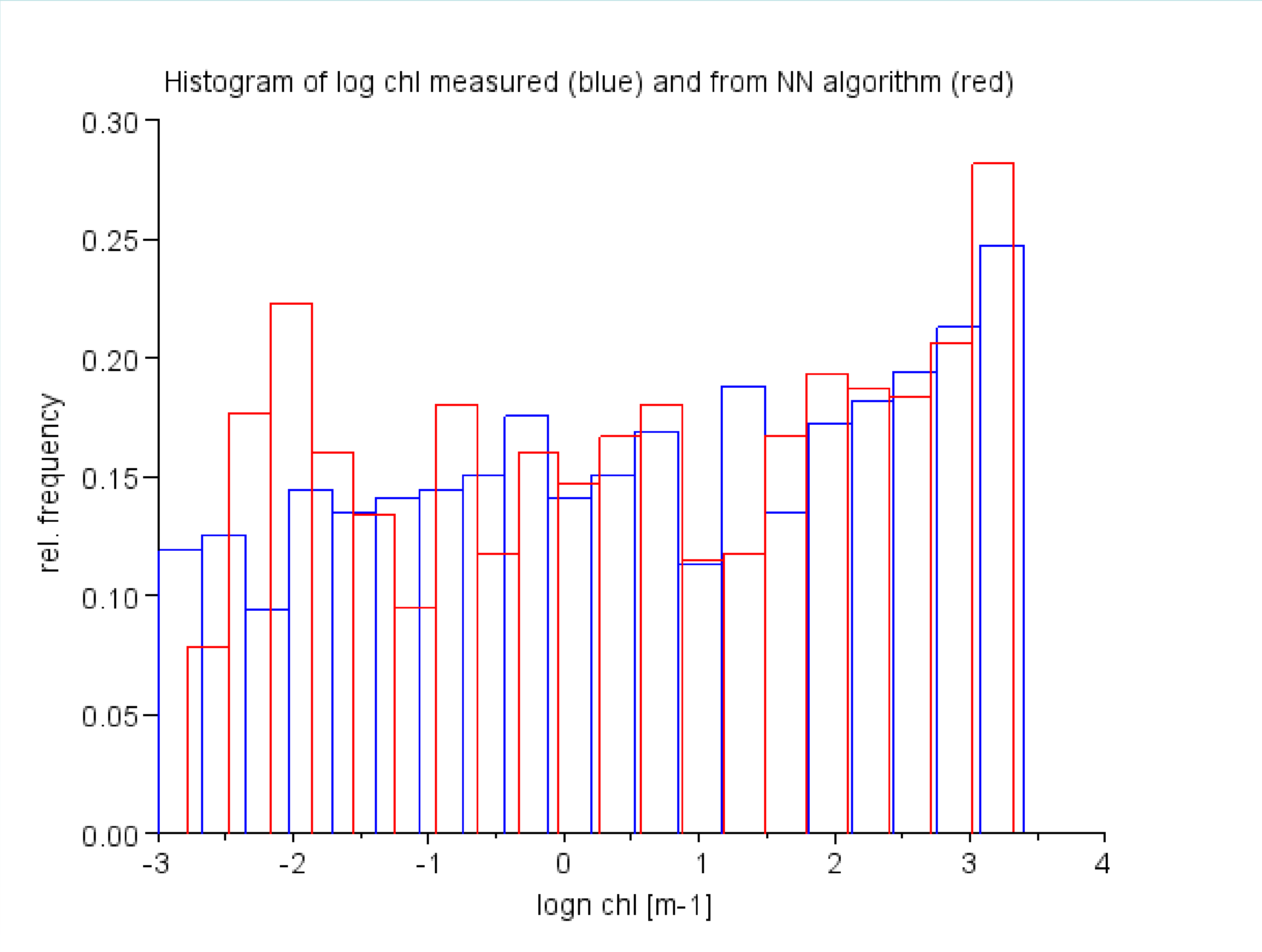
- Advantage:
  - Shallow water application
  - Better separation from yellow substance
  - Works also at very high chl. concentrations
- Disadvantage
  - Less sensitive at low chl. Concentrations (<0.1 mg m-3)

Test of training results NIR bands: chlorophyll

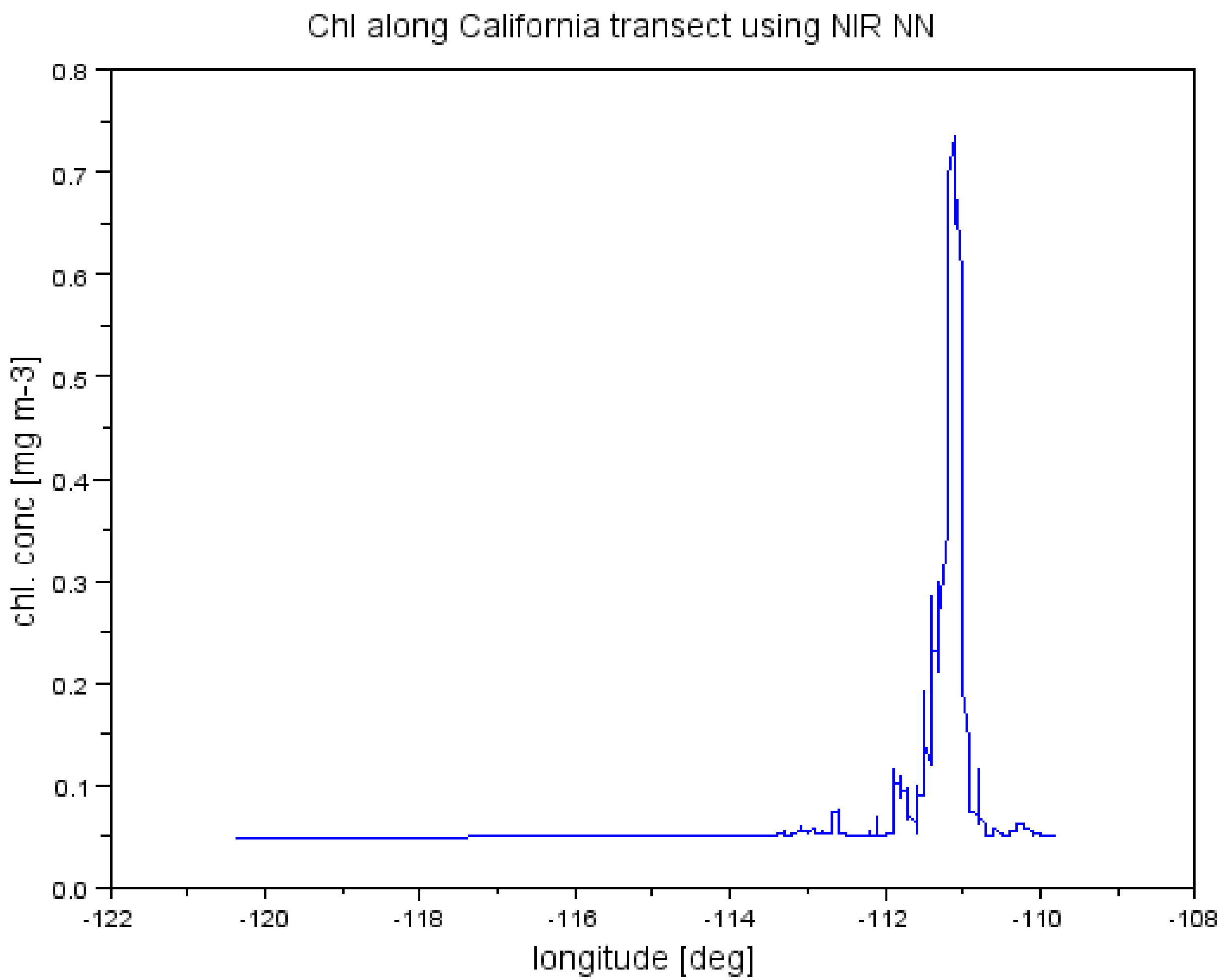


Chlorophyll, logn scale

Reproduction of frequency distribution

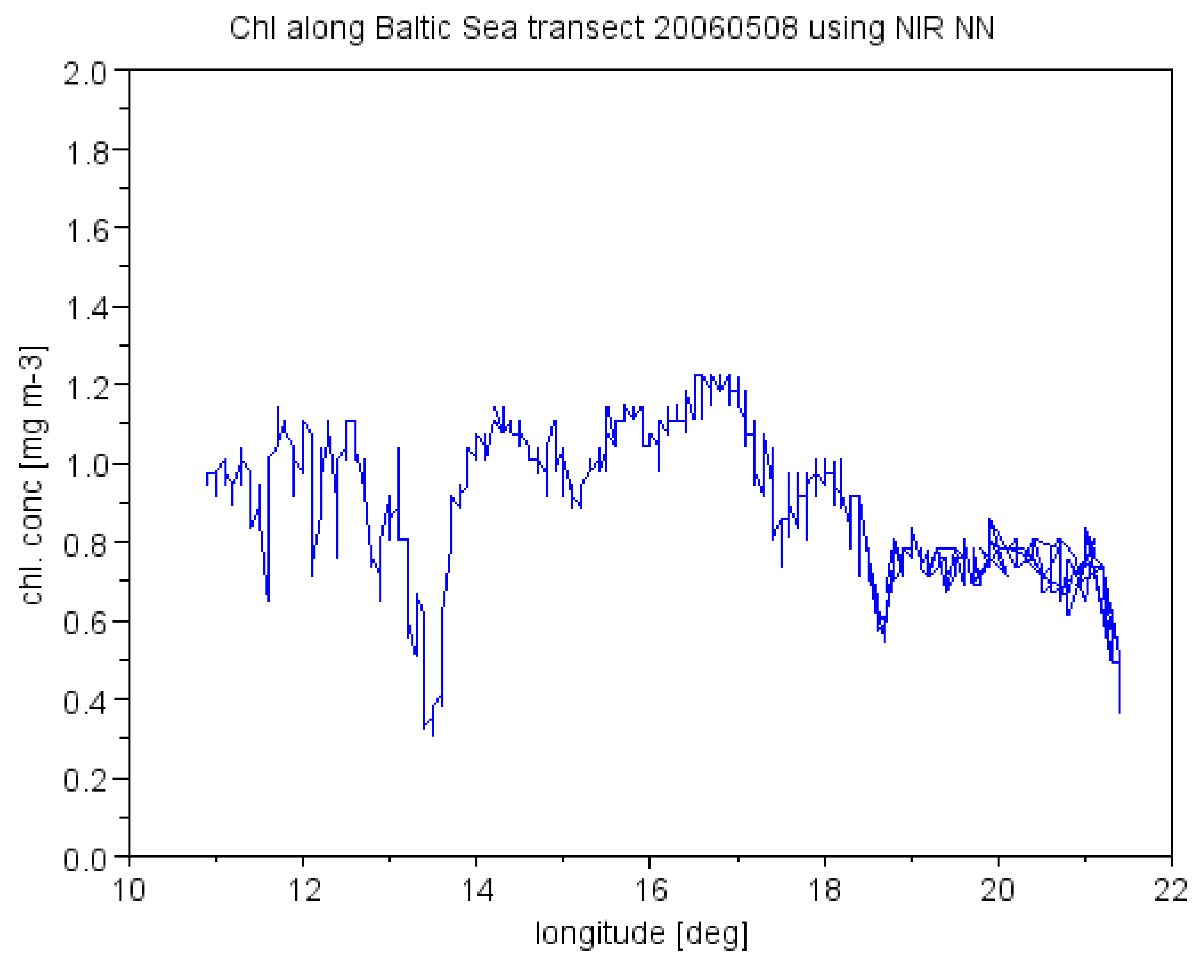


Transect test for NIR NN (California case 1)



Lower limit of NN is 0.05 mg m-3

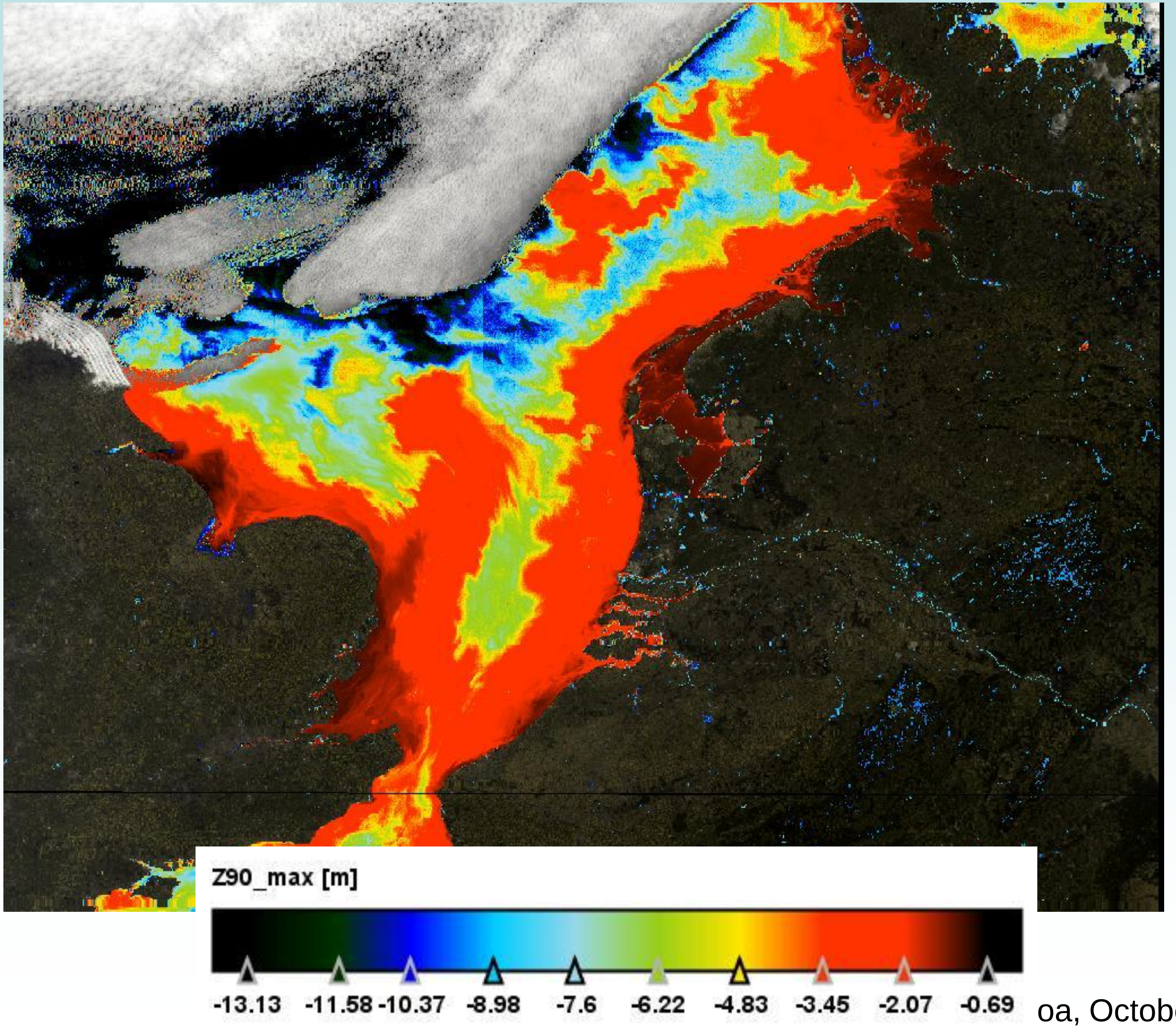
Transect test for NIR NN (Baltic Sea May 8, 2006)



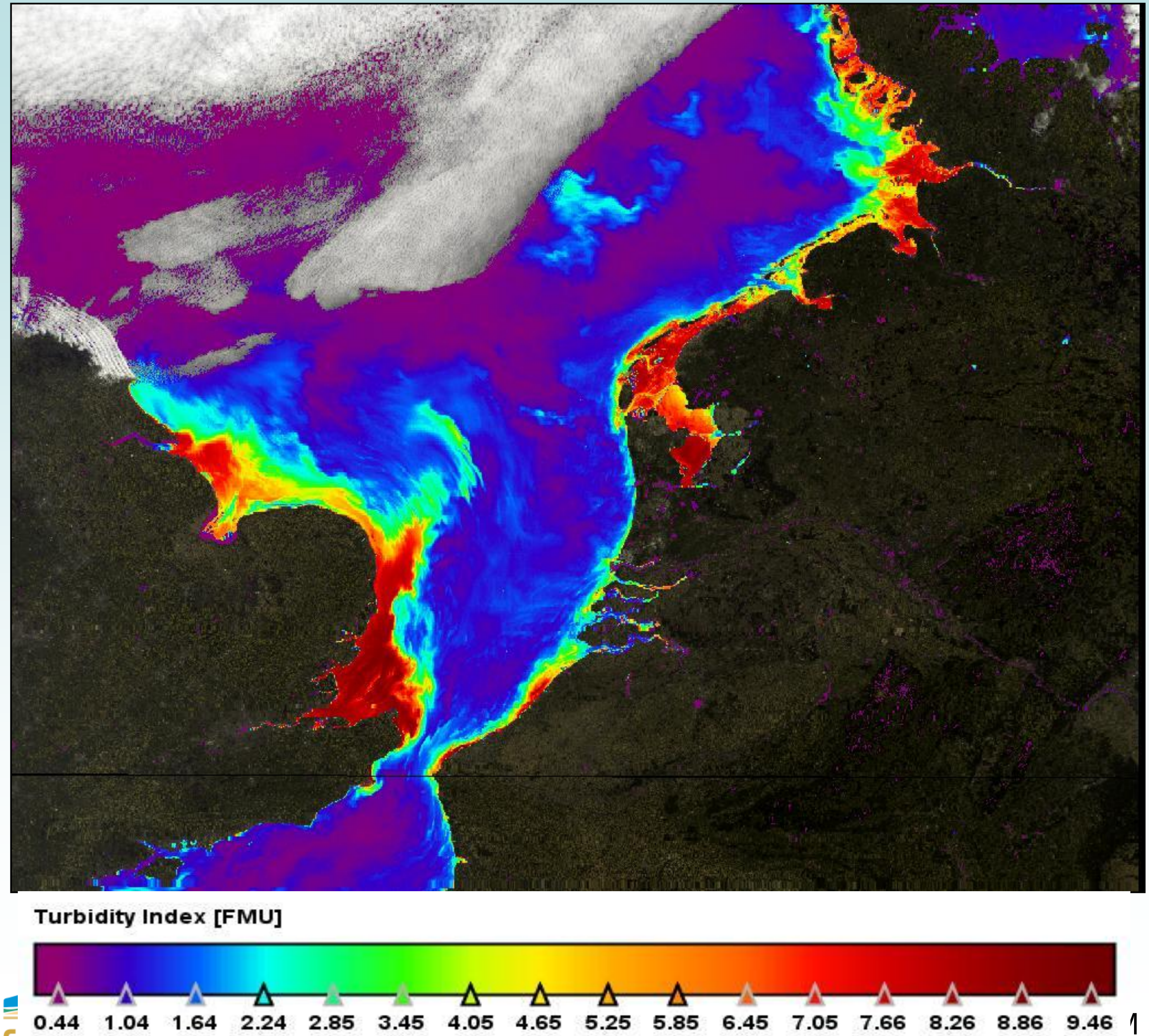
Lower limit of NN is 0.05 mg m-3

coastcolour

Visibility Depth (z90) MERIS 20070501



Turbidity Index



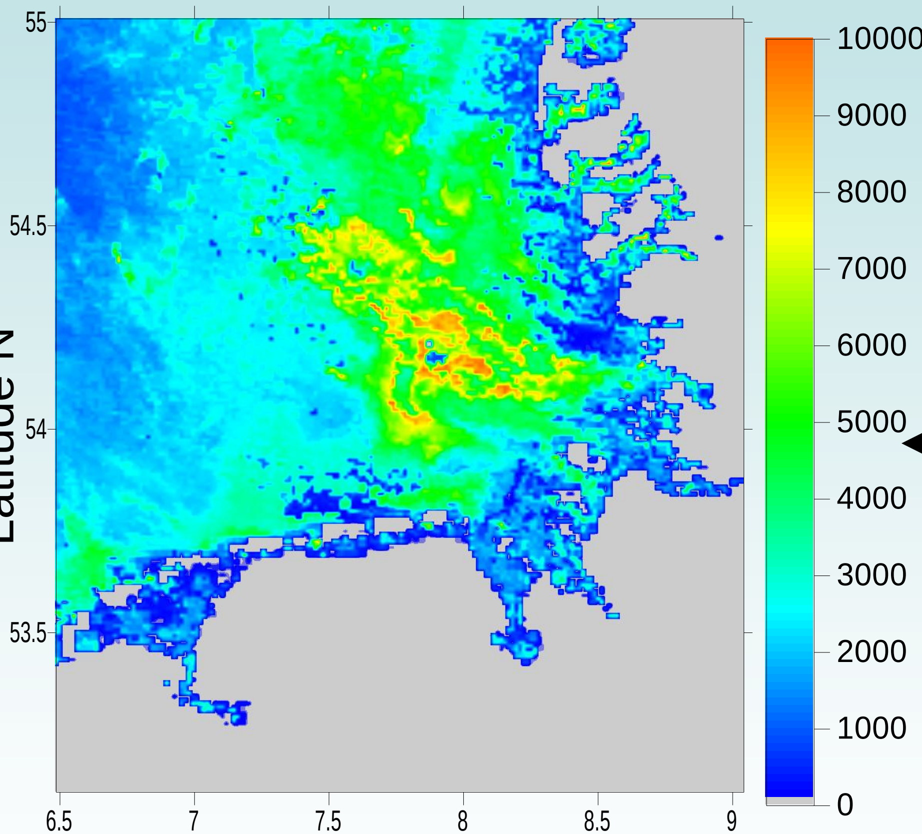
Index as defined in the standard ISO7027 Formazin Nephelometric Units (FNU)

FNU algorithm by Nechard et al.2009 Proc. of SPIE Vol. 7473 74730H-1

based on MERIS reflectance band 6 (620 nm)
Using C2R AC

MERIS FR
20070501

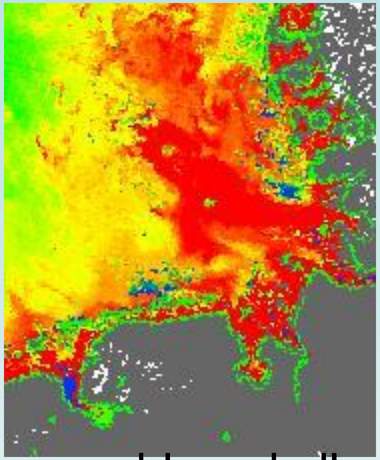
Netto PP derived from MERIS data



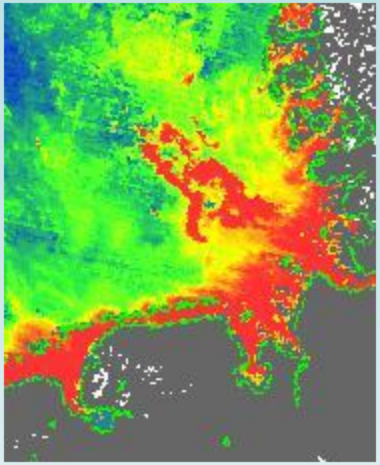
Latitude N

Longitude E

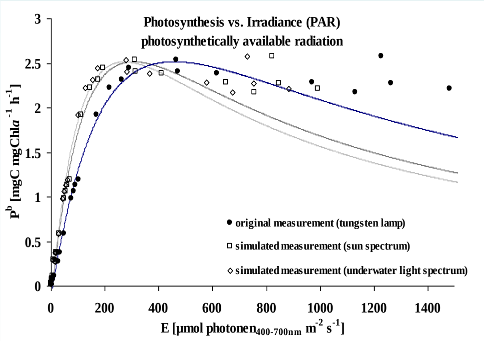
mgC m^{-2} d^{-1}



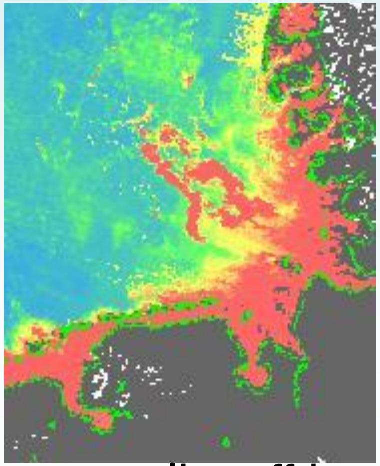
chlorophyll



TSM k



PI



gelbstoff k

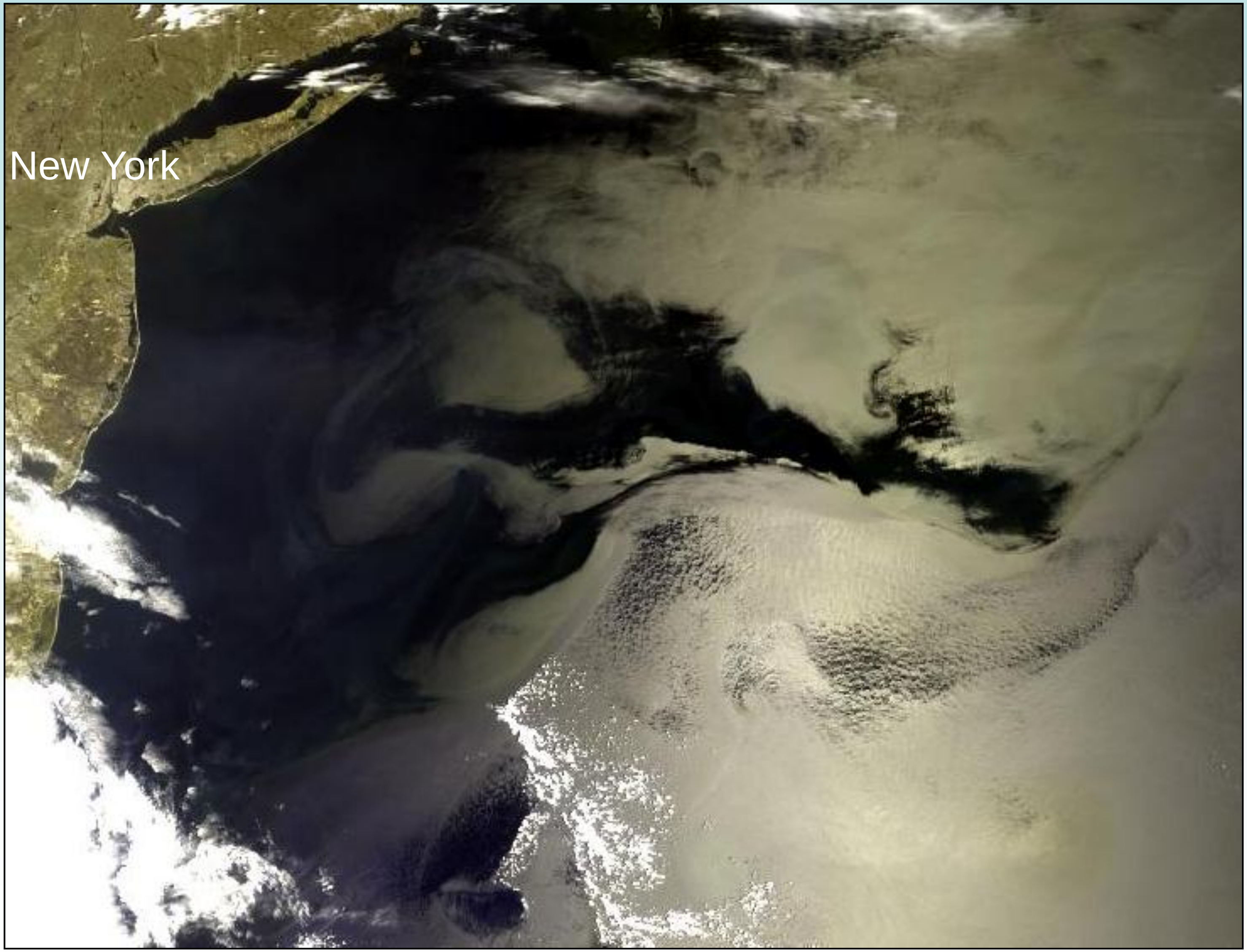
Water depth, PAR(λ) series for 24 h

Roadmap further development of water Algorithms

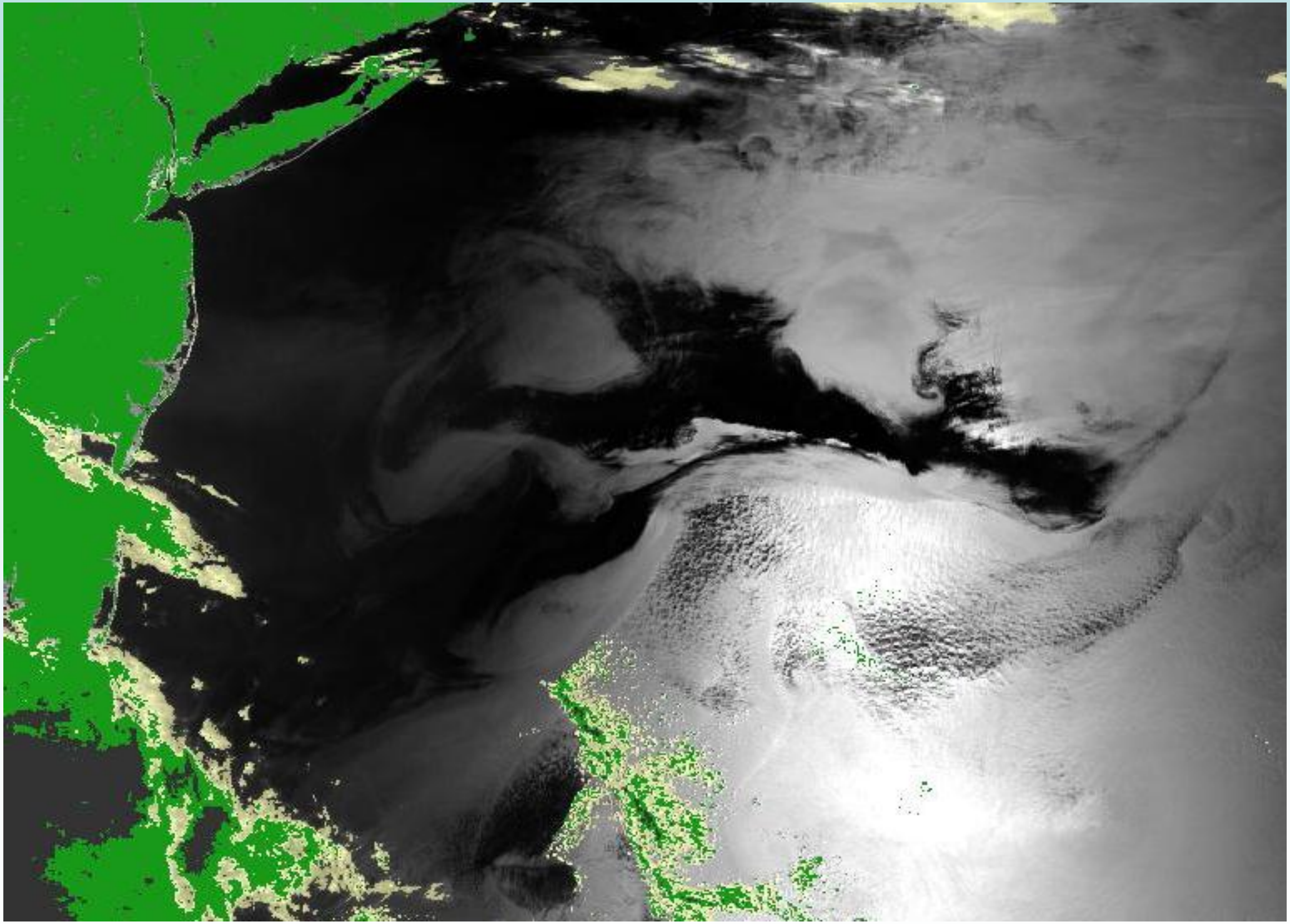
- Train NNs based on measured and simulated reflectances for
  - East Asia
  - East Pacific
- Adapt training range to concentrations of other sites
- Create NN for very high TSM (> 100 g m-3)
- Test various NNs for all sites
- Include uncertainty calculations

- Complete experimental algorithms

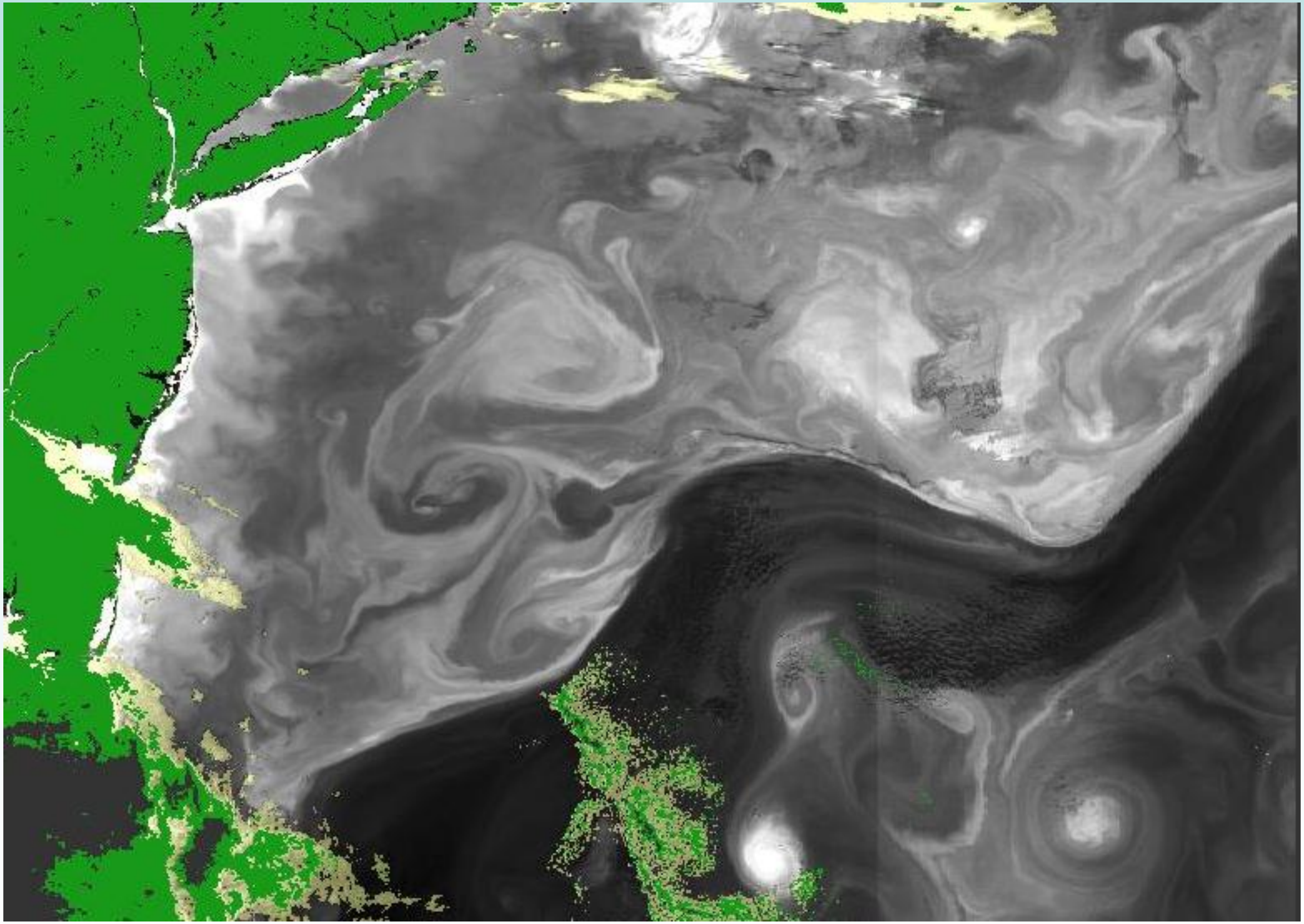
MERIS 20070505
Top of atmosphere radiance reflectance RLtoa RGB



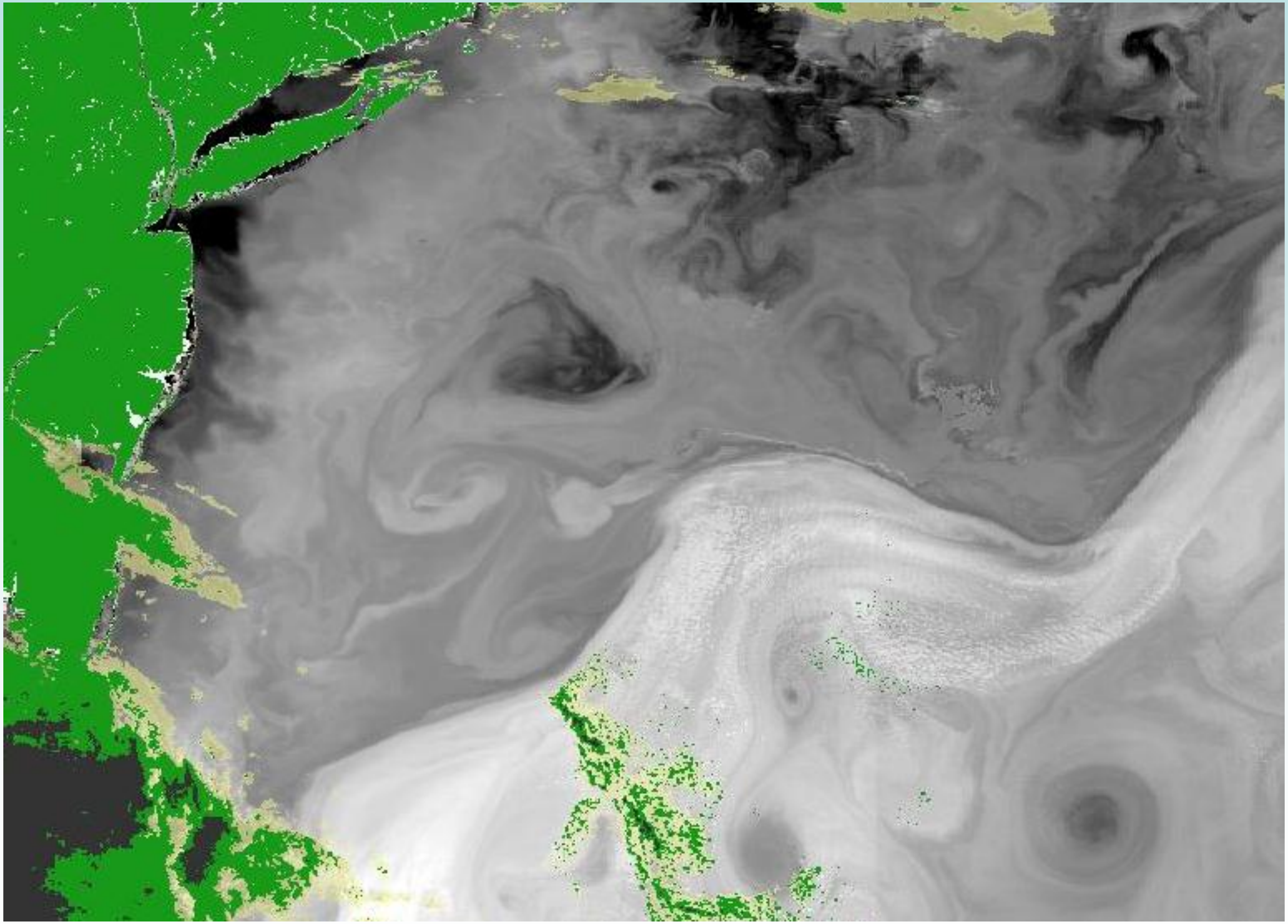
Path radiance+ Fresnel reflectance RLpath MERIS band 5 (560 nm)



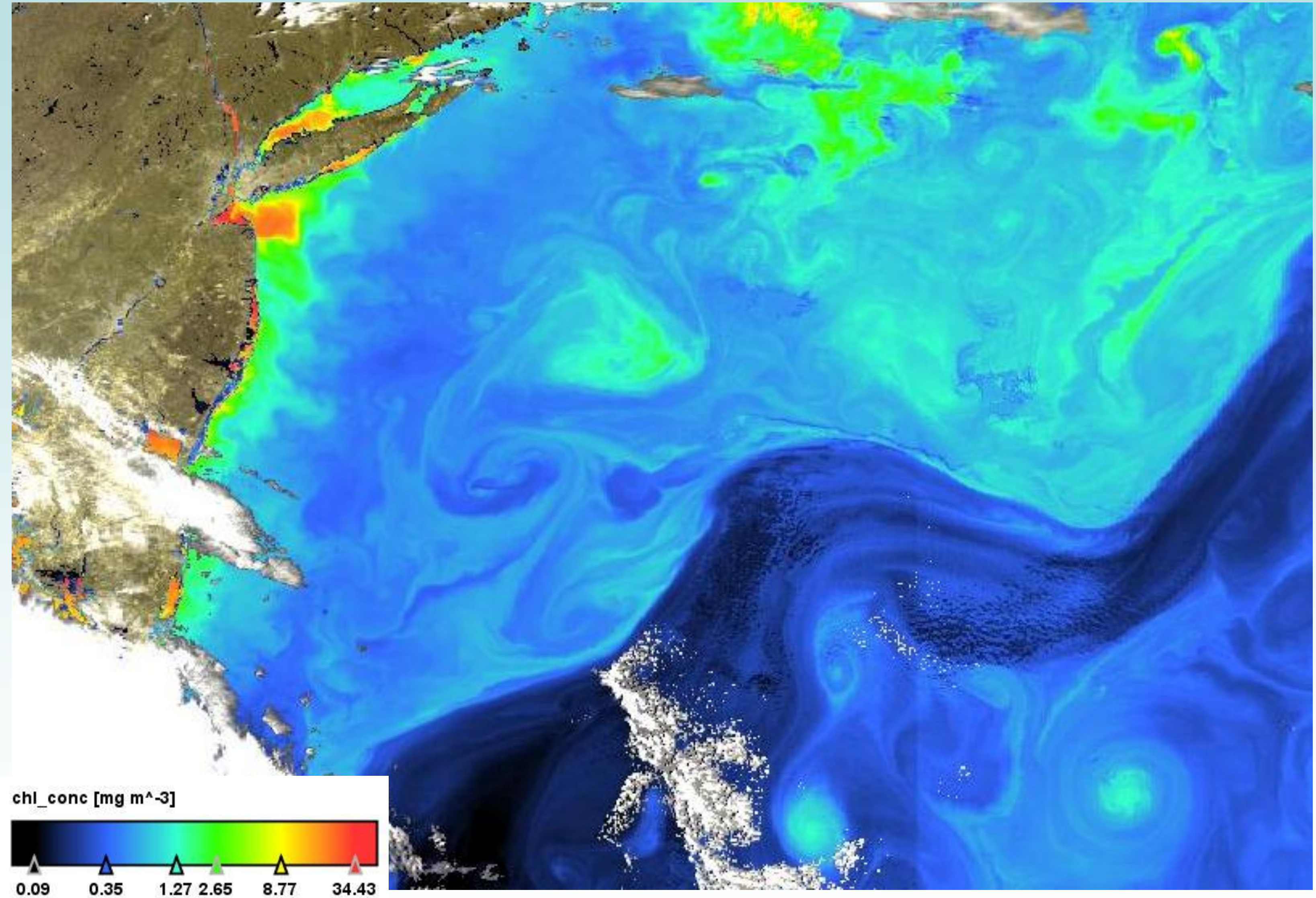
Water leaving radiance reflectance RLw MERIS band 5 (560 nm)



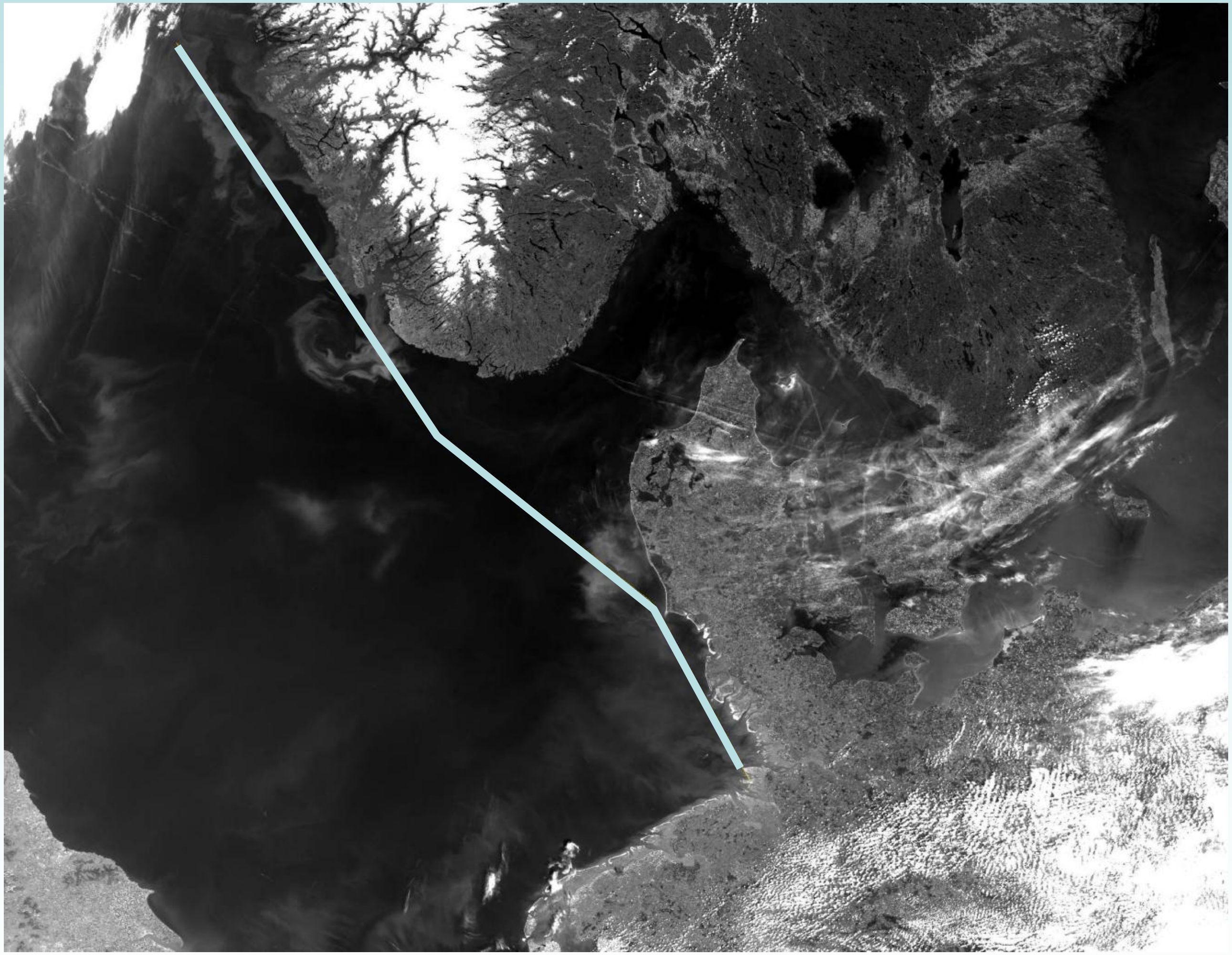
Water leaving radiance reflectance RLw MERIS band 2 (443 nm)



Chlorophyll

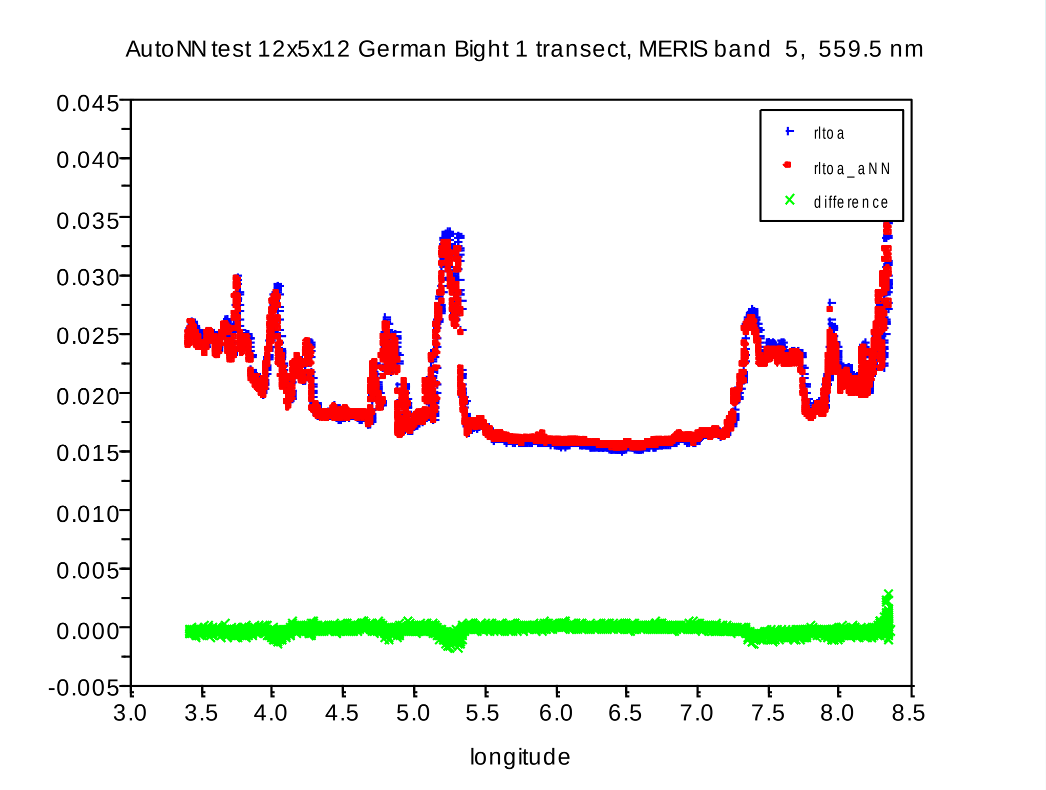


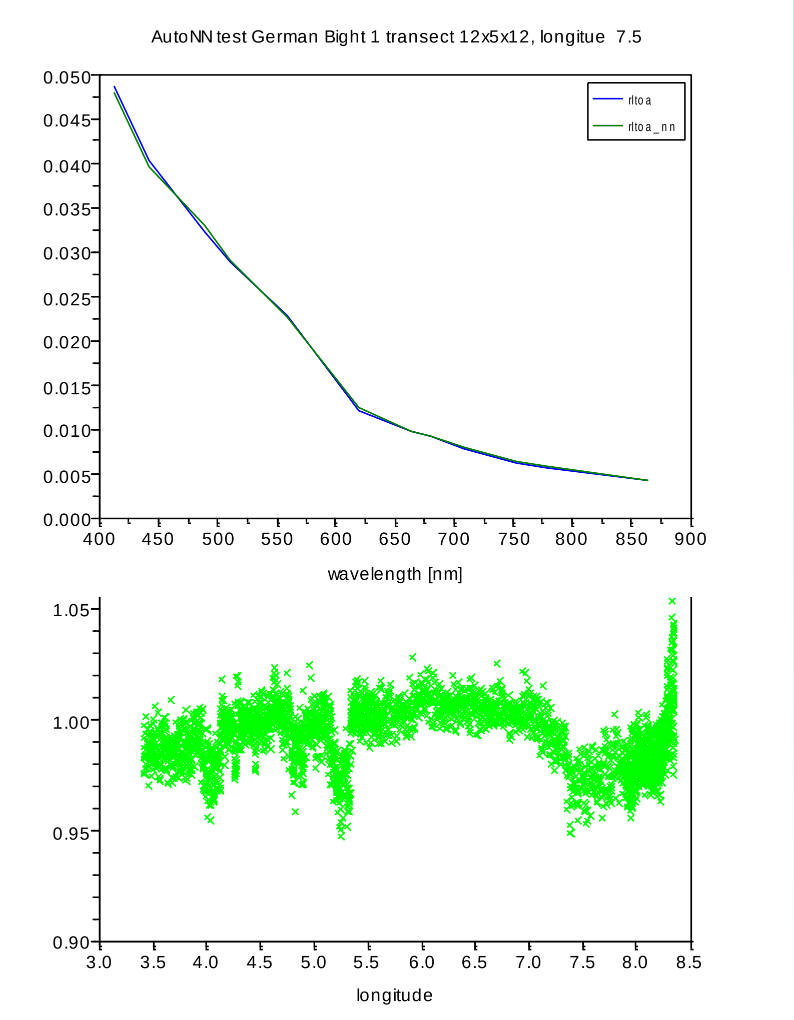
MERIS FR Scene 31.5.2009



MERIS L_toa
band 5 (560 nm)

Out of Scope Test of input spectrum with aaNN

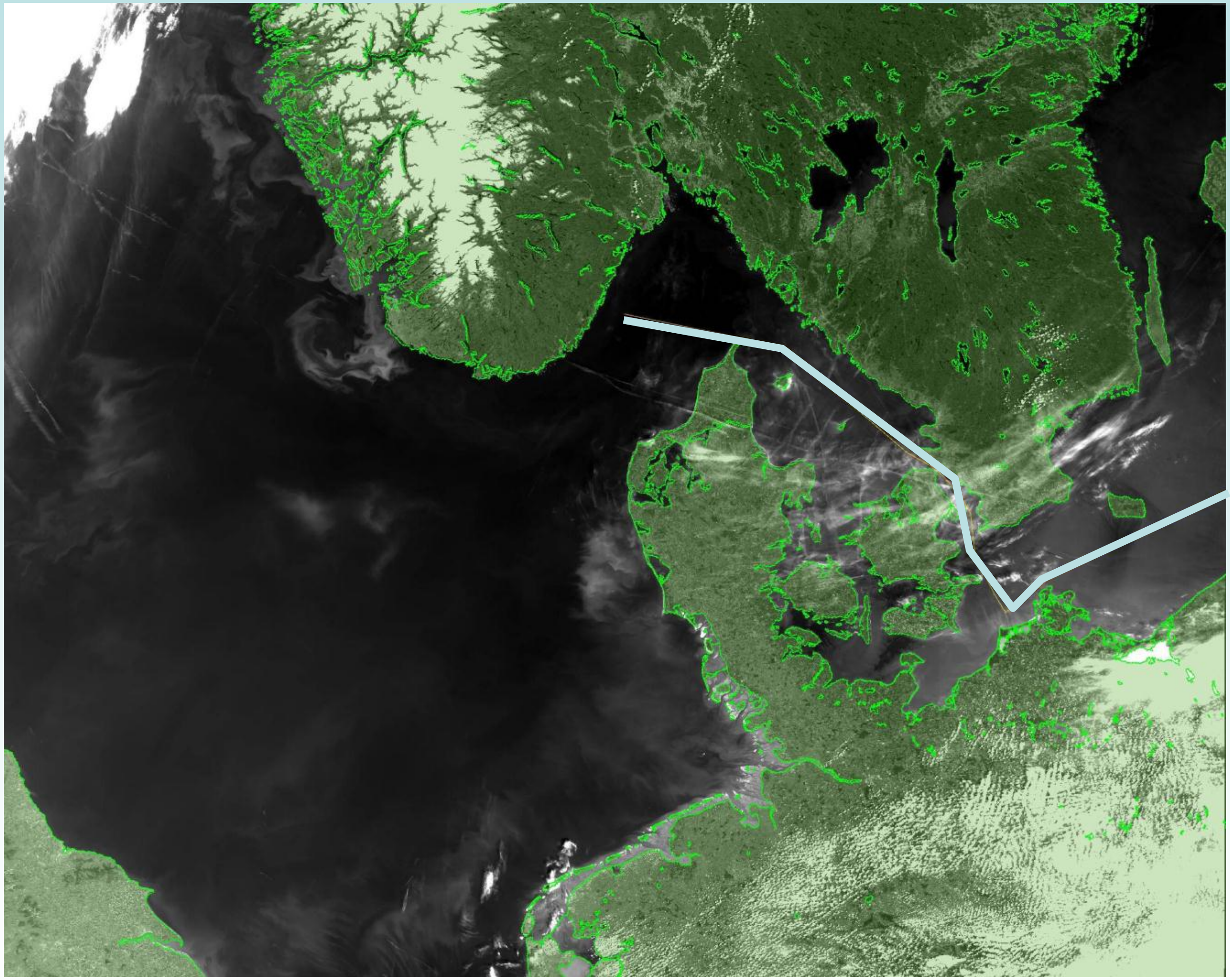




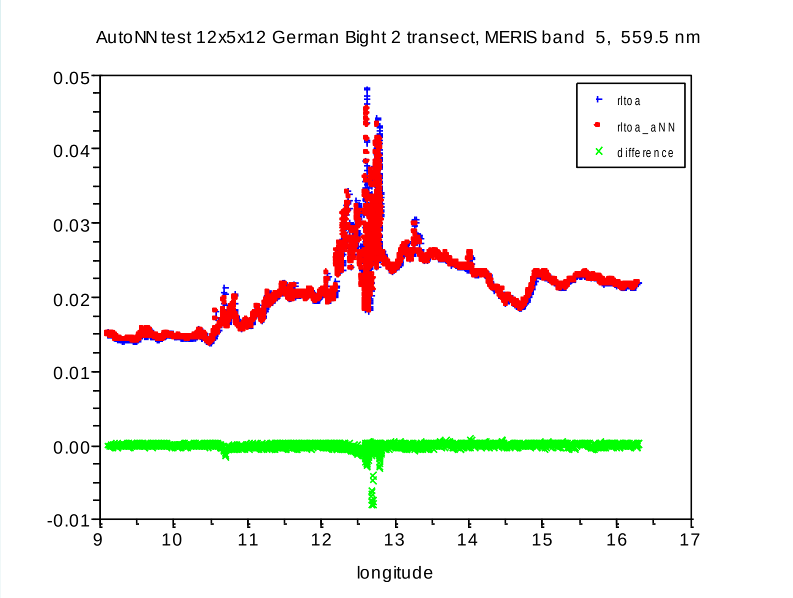
Blue = RL_toa, red =RL_aaNN, green = difference

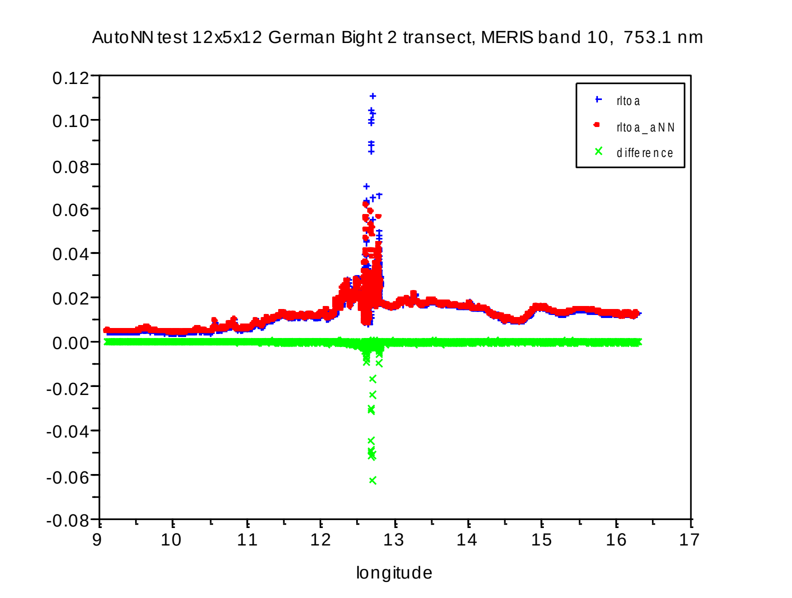
Rel. deviation

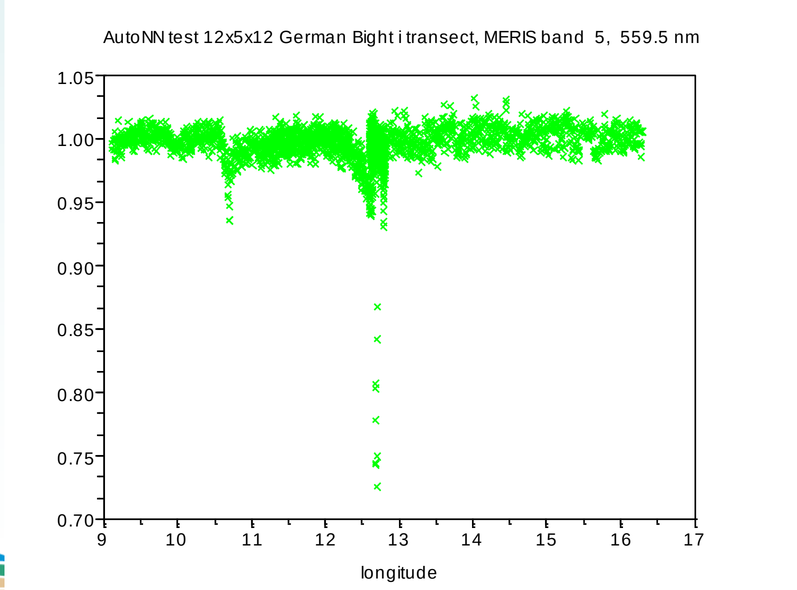
Transect with expected out of scope spectra



Out of Scope test





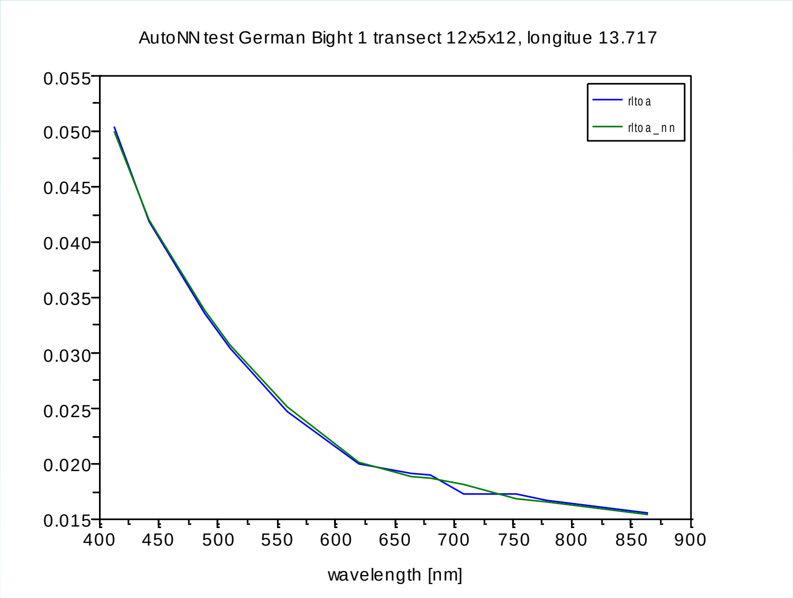


Top of atmosphere radiance reflectance along transect, band 5 and 10, blue orignal MERIS data, red output of aaNN, green difference

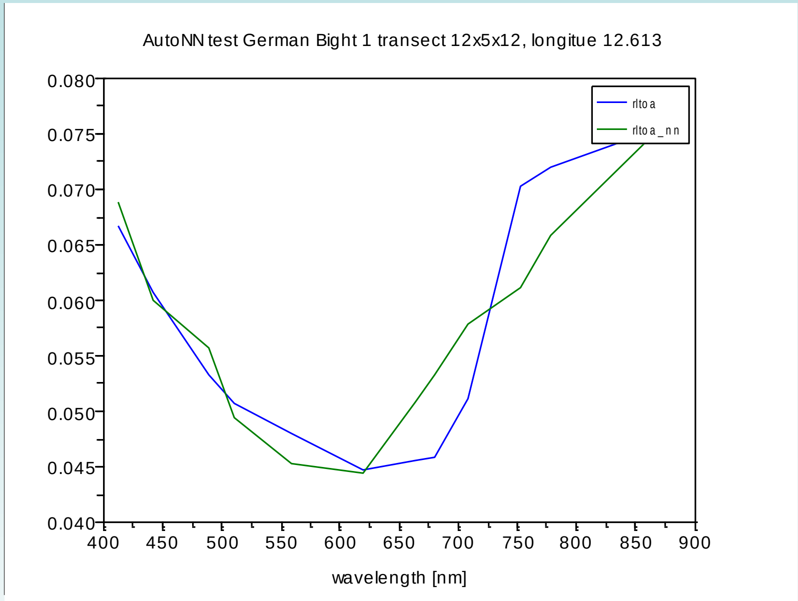
ratio toa radiiance reflectance / to radiance reflectance as output of aaNN

coastcolour

Spectra in scope and out of scope



Spectra Meris and aaNN at transect position 12.717 deg (sun glint !), where the aaNN indicates in scope



Spectra Meris and aaNN at transect position 12.613 deg, where the aaNN indicates out of scope

Experimental Products

- An attempt will be made to generate additional experimental, site specific products, including (provisional list):

- ***Acronym *Product Algorithm***
- 1% depth of PAR
- PPPPrimary Productivity or Potential Primary Productivity
  - requires the knowledge of PI parameters, PPP is without nutrient limitations
- Phytoplankton Biomass estimates in gC m-3 or gC m-2 units
- Concentrations of some taxonomic of functional groups such as coccolithophorides, Cyanobacteria etc, if abundant in dominating concentrations
- Effective Fluorescence: Derived from difference of water leaving radiance reflectance between direct output of neural network and difference between top of atmosphere reflectance (RLtoa) and path radiance reflectance (RLpath).

Strategy for Water Algorithms Development

- Neural Network
  - Training with measured reflectances, if sufficiently available
  - Training with simulated reflectances, base on bio-optical model
- Generic NN based on NOMAD data set -> bio-optical model
- Regional NN
  - Based on generic, but constrained using regional concentration / IOP ranges
  - NN generation using measured reflectances
  - NN based on regional bio-optical model
- Floating cyanobacteria (Baltic Sea)
  - Linear spectral unmixing -> coverage index

Present Status of water algorithm

Available

- Generic NNs generated based on NOMAD data set
  - NN with measured data (incl. T and S)
  - NN based on bio-optical model for different wavelength sets,
  - Reflectances and normalized reflectances (ratios)
  - Normalisation NN
  - Standard Products:
    - IOPs: a_pig, a_g, a_d, bbp
    - AOPs: kd490, kd_min, z90_490, z90_max
    - FNU Formazin Nepholometric Units
    - FLH Fluorescence line height
    - MCI   Maximum chlorophyll index

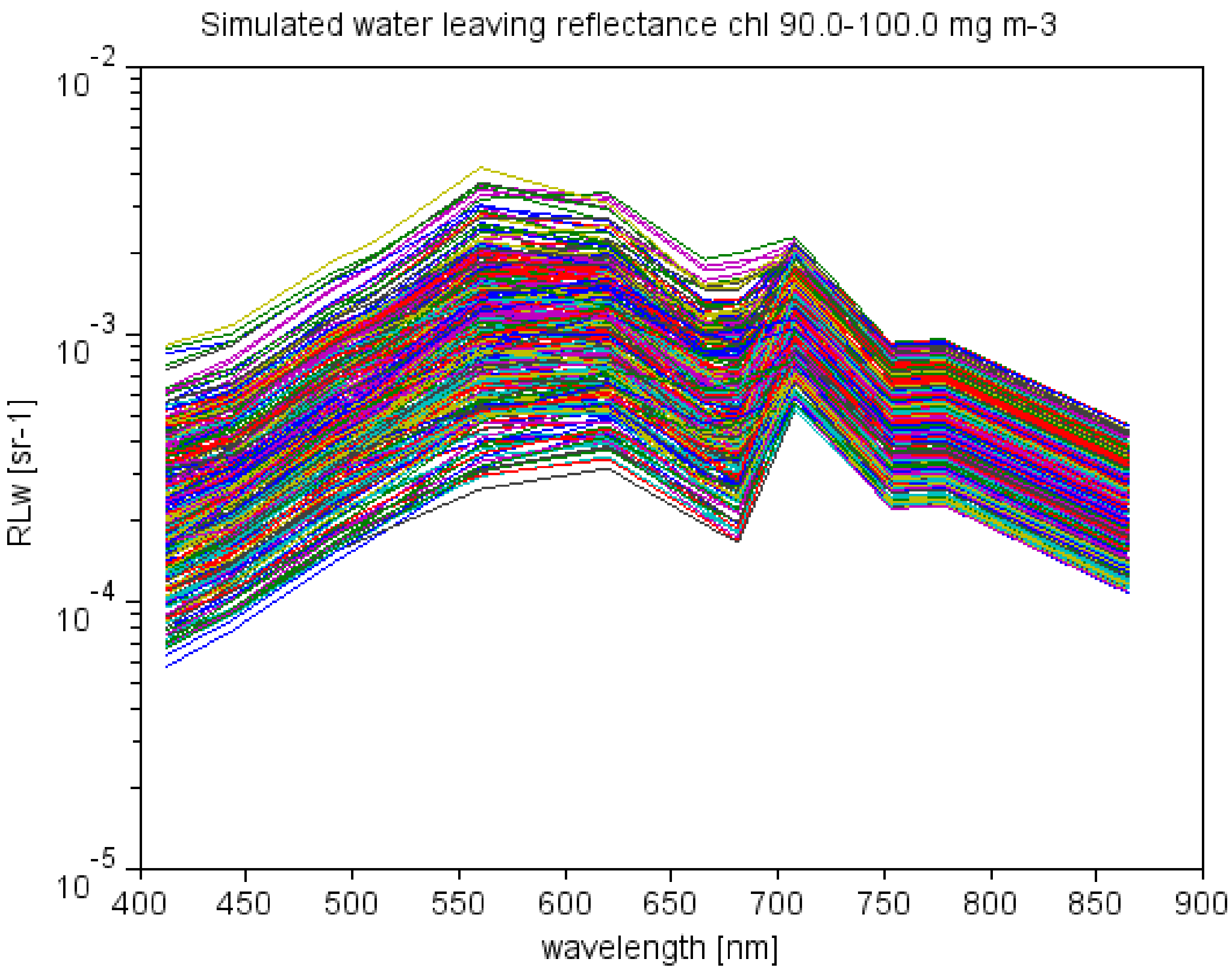
TODO

- Products: z_eu, z_sd

Data and bio-optical models

- Provided data set has many gaps
- Needs careful analysis site by site
- Most complete for NN training
  - North Sea
  - Baltic Sea (more data expected)
  - East Asia
  - East Pacific
  - Benguela
  - Australia

RLw from simulated data set



Chl_f 90.0 – 100.0 mg m-3, log scale

coastcolour

Example for AC NN for high tsm (23x25x45_37237.9.net)

- problem: /coastcolour_hlsimu_step2_hitsm/simu_test_20110604_hl_sel_rltosa_transupnn_hitsm
- saved at Thu Jun 16 08:09:03 2011
- trainings sample has total sum of error^2=37237.947867
- average of residues:
- training 37237.947867/750157/18=0.001154
- test 11044.503256/221843/43 =0.001158
- ratio avg.train/avg.test=0.997087

Input to AC net

- the net has 18 inputs:
- input 1 is sun_zeni_deg in [1.003000,76.200000]
- input 2 is x in [-1.000000,1.000000]
- input 3 is y in [-0.000005,1.000000] viewing in x,y,z coordinates
- input 4 is z in [0.000000,0.7071000]
- input 5 is T_wat in [0.000151,36.000000] water temperature
- input 6 is S_wat in [0.000181,43.000000] salinity
- input 7 is log_rl_tosa_412 in [-3.239000,-1.009000]
- - - - - - 12 bands log rl_tosa - - - - -
- input 18 is log_rl_tosa_865 in [-6.278000,-0.330300]

Output of AC net

- the net has 43 outputs:
- output 1 is log_rlw_412 in [-9.136000,-1.605000]
  - 12 bands water leaving radiance reflectance
- output 12 is log_rlw_865 in [-12.870000,-2.956000]

- output 13 is log_RL_path_412 in [-3.341000,-1.090000]
  - - 12 bands path radiance reflectance
- output 24 is log_RL_path_865 in [-6.281000,-0.372100]

- output 25 is log_Ed_boa_412 in [-2.555000,-0.143900]
  - - 12 bands downwelling irradiance at sea surface
- output 36 is log_Ed_boa_865 in [-1.981000,-0.009041]

- output 37 is tau_443aero in [0.000006,0.948000] *aerosol optical thickness*
- output 38 is tau_550_aero in [0.000005,0.610400]
- output 39 is tau_778aero in [0.000004,0.600000]
- output 40 is tau_865aero in [0.000004,0.599000]
- output 41 is log_btot in [-3.991000,6.325000] *total scattering and absorption water*
- output 42 is log_atot in [-5.637000,1.698000]
- output 43 is glintrat in [1.000000,192.300000] *glint ratio*