

The Mass Conservation Additions to the Multisignal Sedimentation Velocity Global Parameter Window in SEDPHAT

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Standard Mass Conservation

Here, two “spectra” are being used to describe the information between 0.2 and 4 S.

The interface is divided into three segments for data entry:

- Segment 1 (highlighted with a red box):**
 - continuous ☒ segment 1
 - resolution: 75
 - lineal log ☒
 - s min: 0.200, s max: 4.000, frictional ratio: 1.498
 - ☒ spectrum 1: xt1/chr: 1.000, xt2/chr: 0.000, PP
 - ☒ spectrum 2: xt1/chr: 0.000, xt2/chr: 1.000, PP
 - ☒ fit f0
- Segment 2:**
 - ☒ segment 2
 - resolution: 75
 - lineal log ☒
 - s min: 4.100, s max: 15.000, frictional ratio: 1.543
 - ☒ spectrum 1: xt1/chr: 1.000, xt2/chr: 0.000, PP
 - ☒ spectrum 2: xt1/chr: 0.000, xt2/chr: 1.000, PP
 - ☒ fit f0
- Segment 3:**
 - ☐ segment 3
 - resolution: 0
 - lineal log ☒
 - s min: 17.000, s max: 60.000, frictional ratio: 1.200
 - ☐ spectrum 1: xt1/chr: 0.000, xt2/chr: 0.000, PP
 - ☐ spectrum 2: xt1/chr: 0.000, xt2/chr: 0.000, PP
 - ☐ fit f0

On the right side, the following options are available:

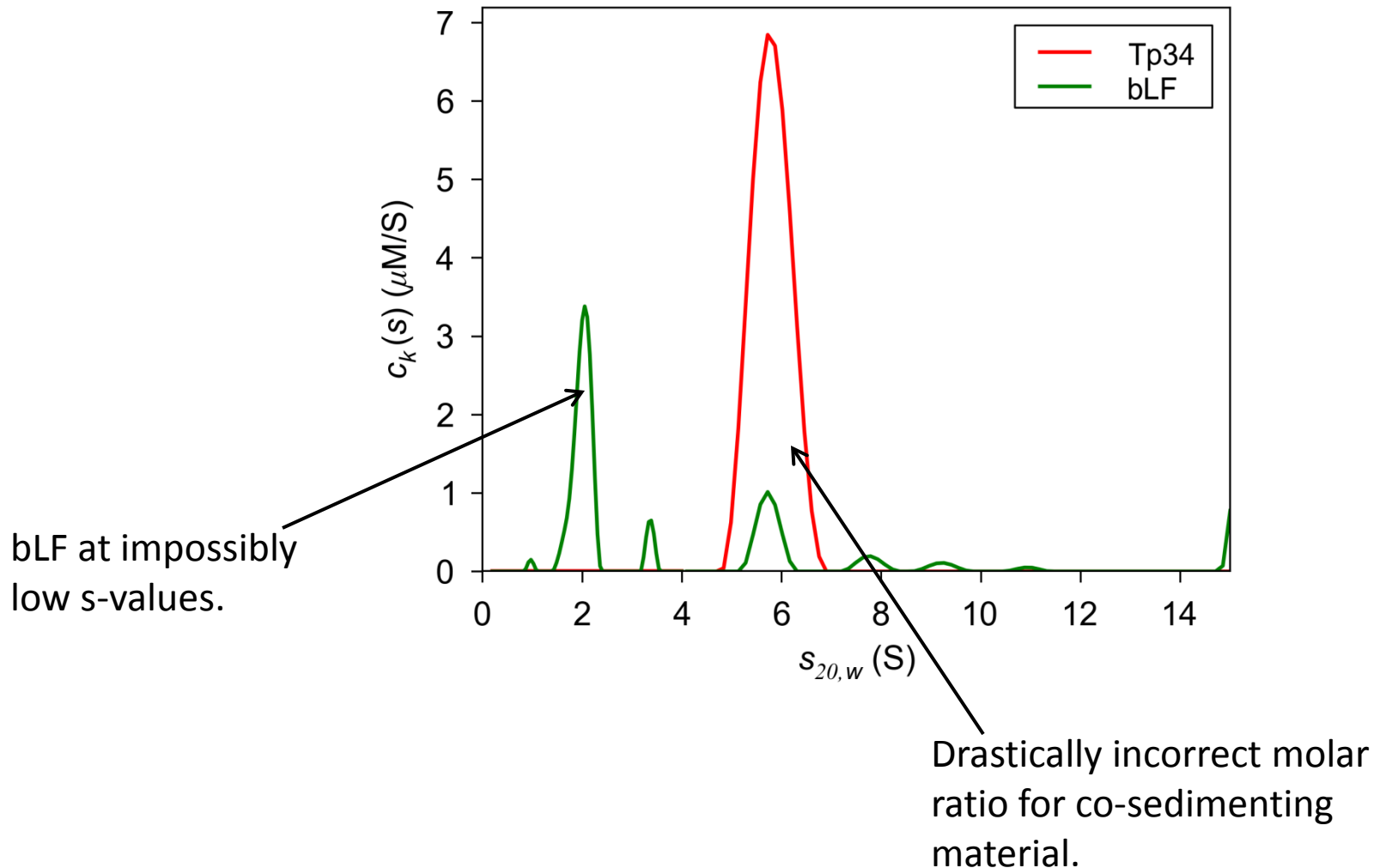
- ☒ discrete spectra in multiples of chromophore xt (except #1)
- ☒ contin. spectra in multiples of chromophore xt
- chromophore #1: xt wl 1: 65267.80, xt wl 2: 31645.00
- chromophore #2: xt wl 1: 232761.0, xt wl 2: 188280.0
- ☒ with total concentration prior knowledge
- integrate from s = 0.10 to 100.00
- ☐ penalize % defect
- ☐ auto adjust by chisq. P
- ☒ auto adjust enforce to within (%) 5.0000
- total chromophore #1 [uM]: 6.900
- total chromophore #2 [uM]: 2.300
- ☒ with Tikhonov regularization, P = 0.700
- ☒ normalize distributions
- Buttons: Cancel, OK

The checkbox turns Mass Conservation on.

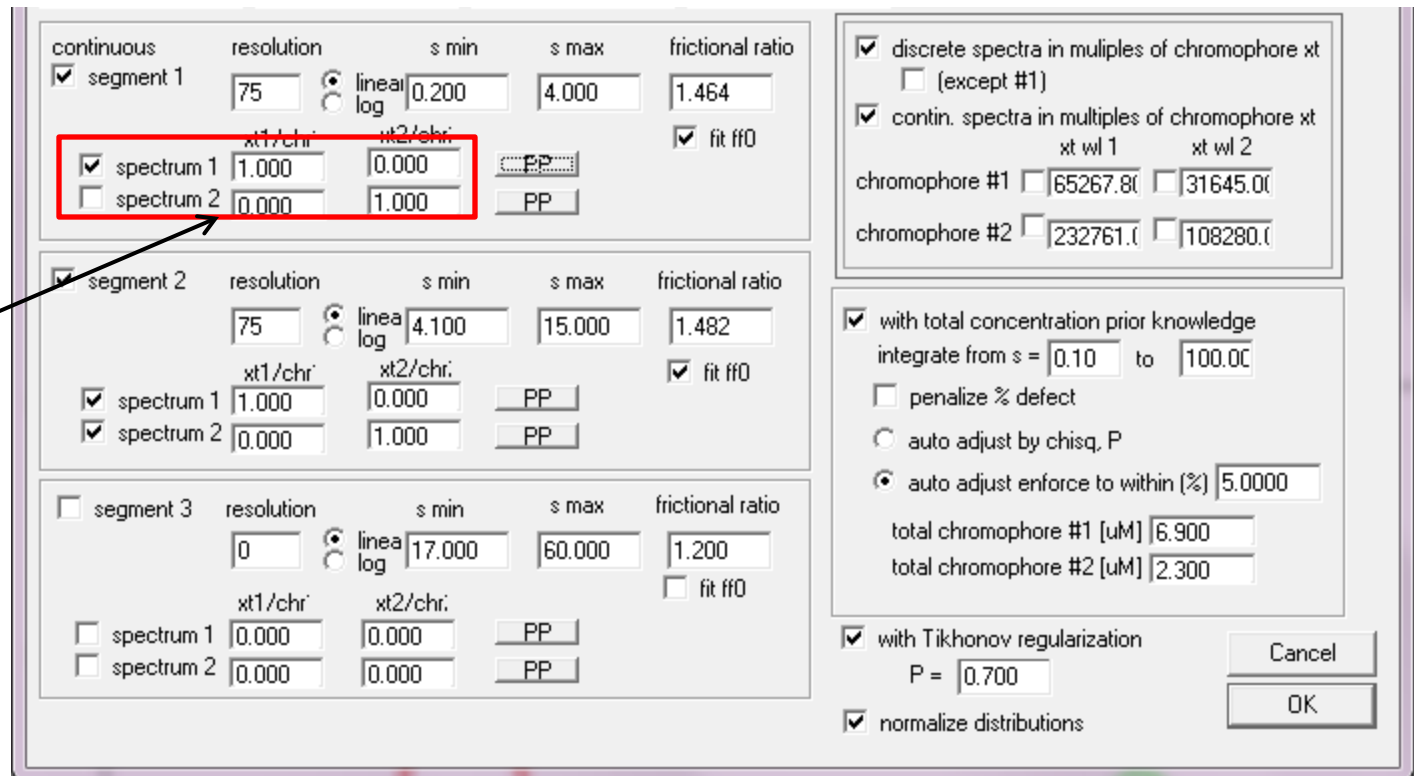
The enforce to within % option has been selected, and 5.0 has been input to the entry box. The known concentrations of chromophore #1 (Tp34) and chromophore #2 (bLF) have been input.

The Resulting Distribution

The preceding parameters could work for a better-behaved case, but there are pathologies present for these data:



Low-s-Constrained Mass Conservation



The screenshot shows a software interface with three segments for configuring mass conservation constraints. Segment 1 is active, and its parameters are as follows:

continuous	resolution	s min	s max	frictional ratio
<input checked="" type="checkbox"/> segment 1	75	linear log	0.200 4.000	1.464
<input checked="" type="checkbox"/> spectrum 1	xt1/chr: 1.000	xt2/chr: 0.000	PP	<input checked="" type="checkbox"/> fit ffo
<input type="checkbox"/> spectrum 2	0.000	1.000	PP	

Segment 2 parameters:

resolution	s min	s max	frictional ratio
75	linear log	4.100 15.000	1.482
<input checked="" type="checkbox"/> spectrum 1	xt1/chr: 1.000	xt2/chr: 0.000	PP
<input checked="" type="checkbox"/> spectrum 2	0.000	1.000	PP

Segment 3 parameters:

resolution	s min	s max	frictional ratio
0	linear log	17.000 60.000	1.200
<input type="checkbox"/> spectrum 1	xt1/chr: 0.000	xt2/chr: 0.000	PP
<input type="checkbox"/> spectrum 2	0.000	0.000	PP

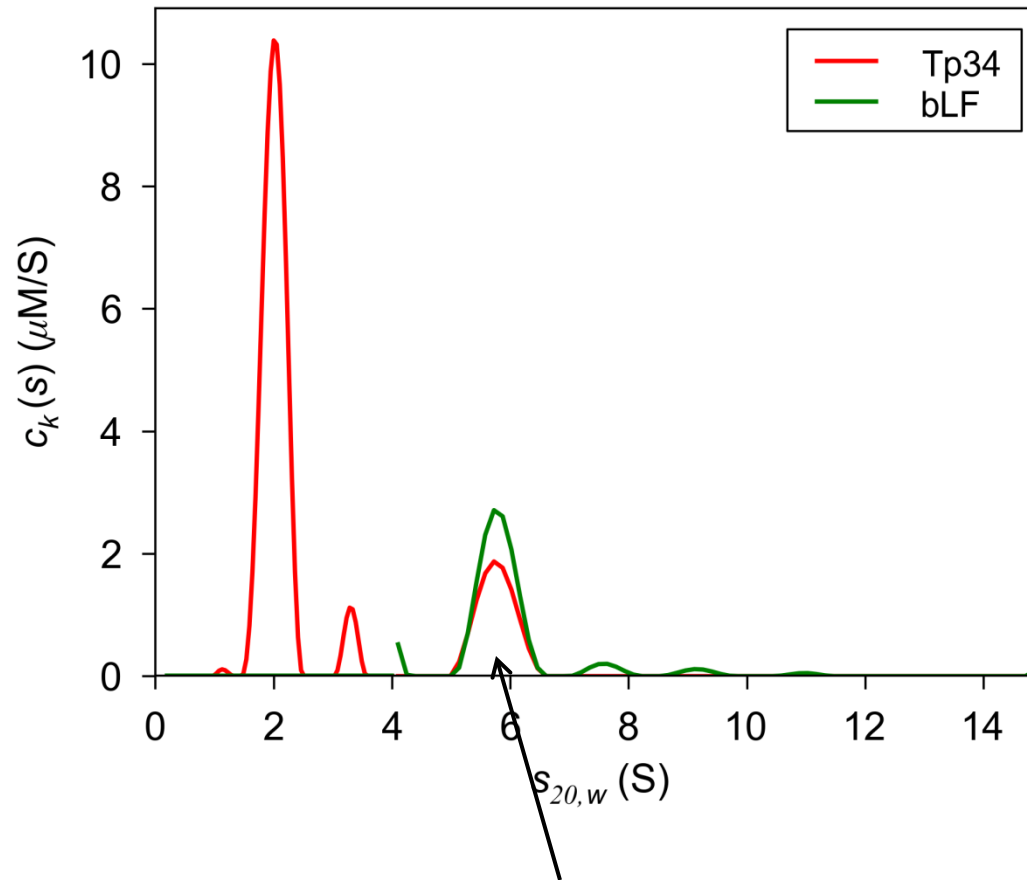
Global settings on the right:

- ☒ discrete spectra in multiples of chromophore xt
☐ (except #1)
- ☒ contin. spectra in multiples of chromophore xt
- chromophore #1: xt wl 1 65267.80, xt wl 2 31645.00
- chromophore #2: 232761.0, 108280.0
- ☒ with total concentration prior knowledge
integrate from s = 0.10 to 100.00
- ☐ penalize % defect
- ☐ auto adjust by chisq, P
- ☒ auto adjust enforce to within (%) 5.0000
- total chromophore #1 [uM] 6.900
- total chromophore #2 [uM] 2.300
- ☒ with Tikhonov regularization
P = 0.700
- ☒ normalize distributions

Buttons: Cancel, OK

Here, spectrum 2 , which accounts for bLF, has been turned off, forcing all of the low-s material to be Tp34.

The Final Distribution



Now, a reasonable ratio of Tp34:bLF is found.