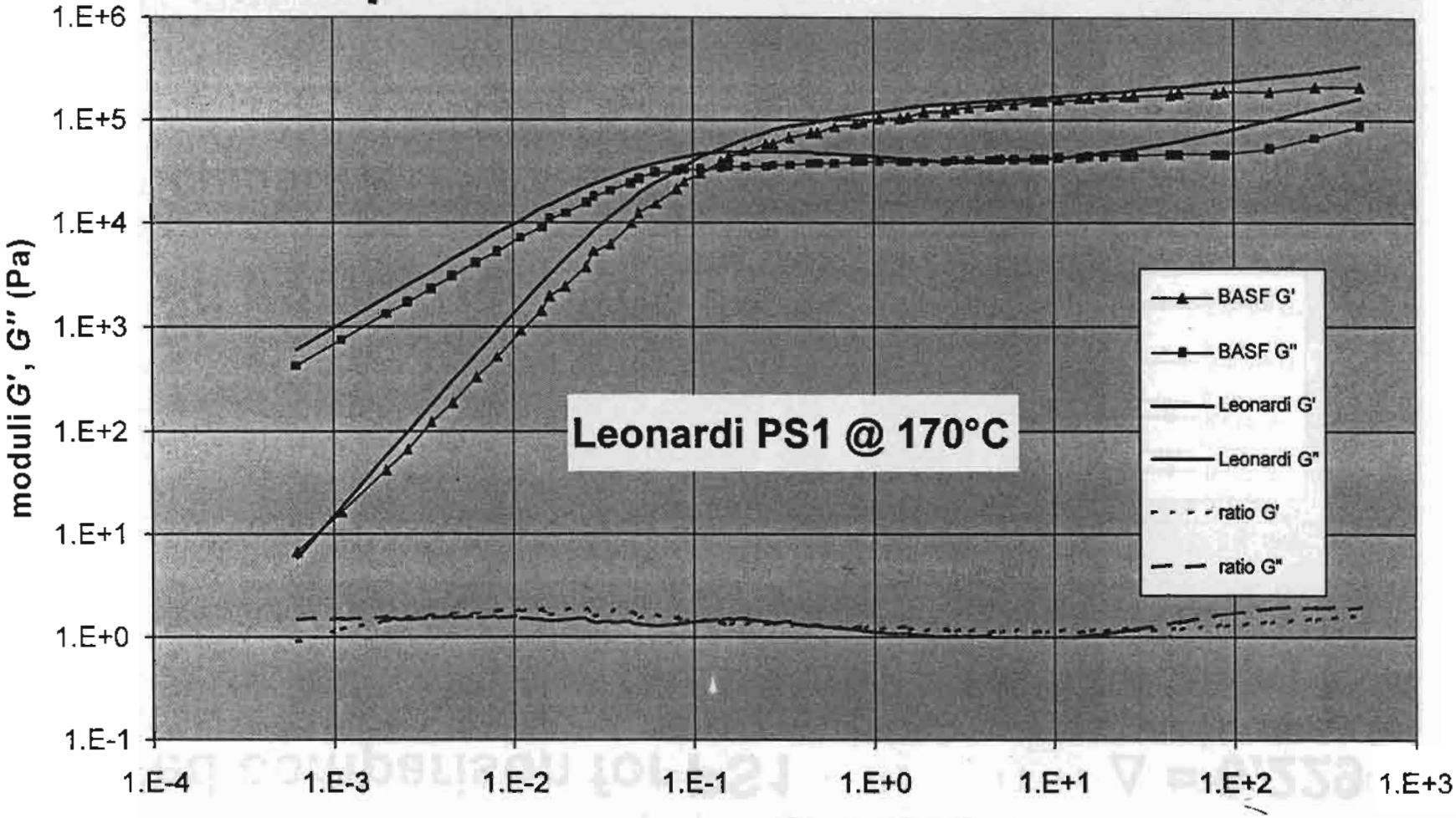
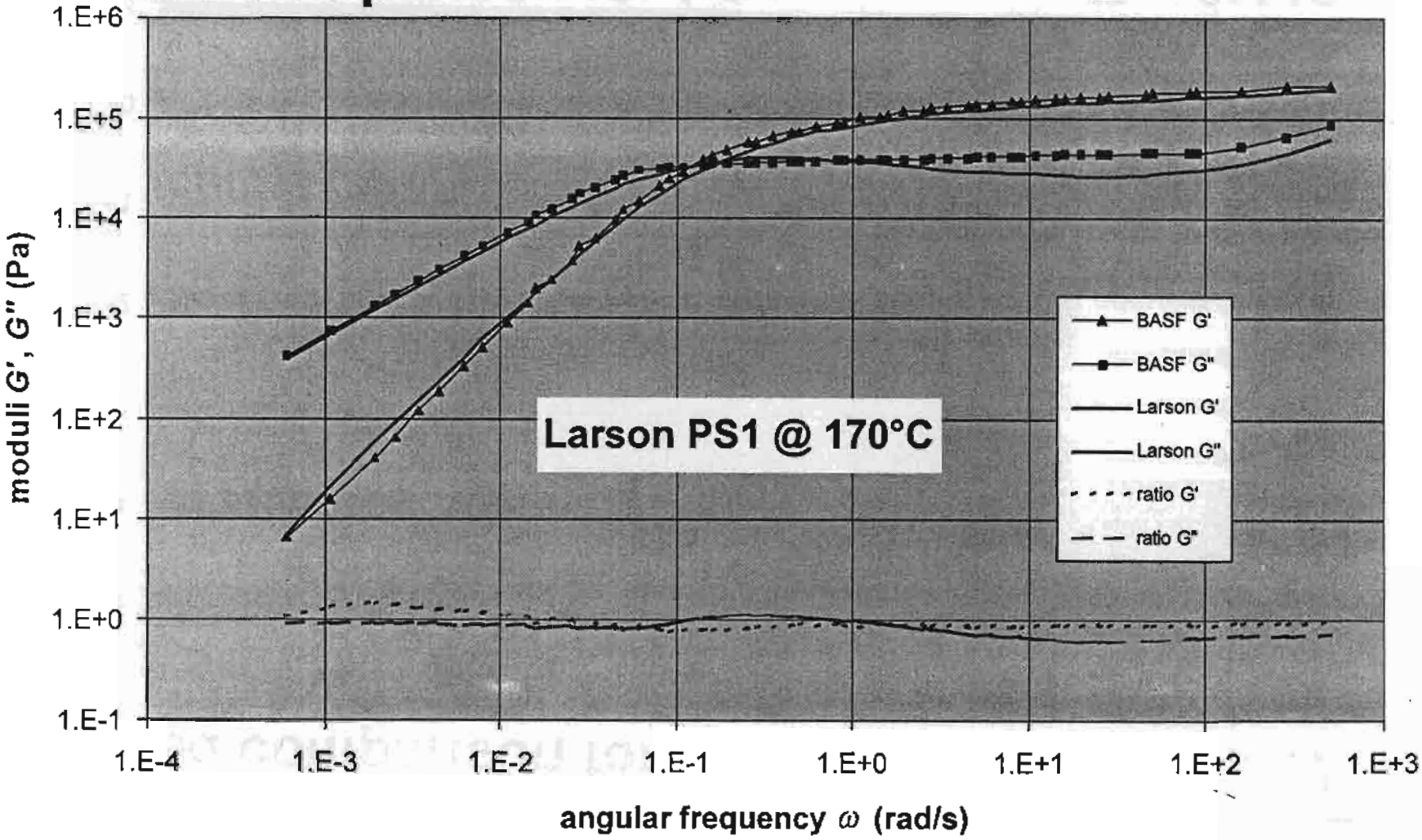
PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

Detailed comparison for PS1 $\Delta = 0.198$



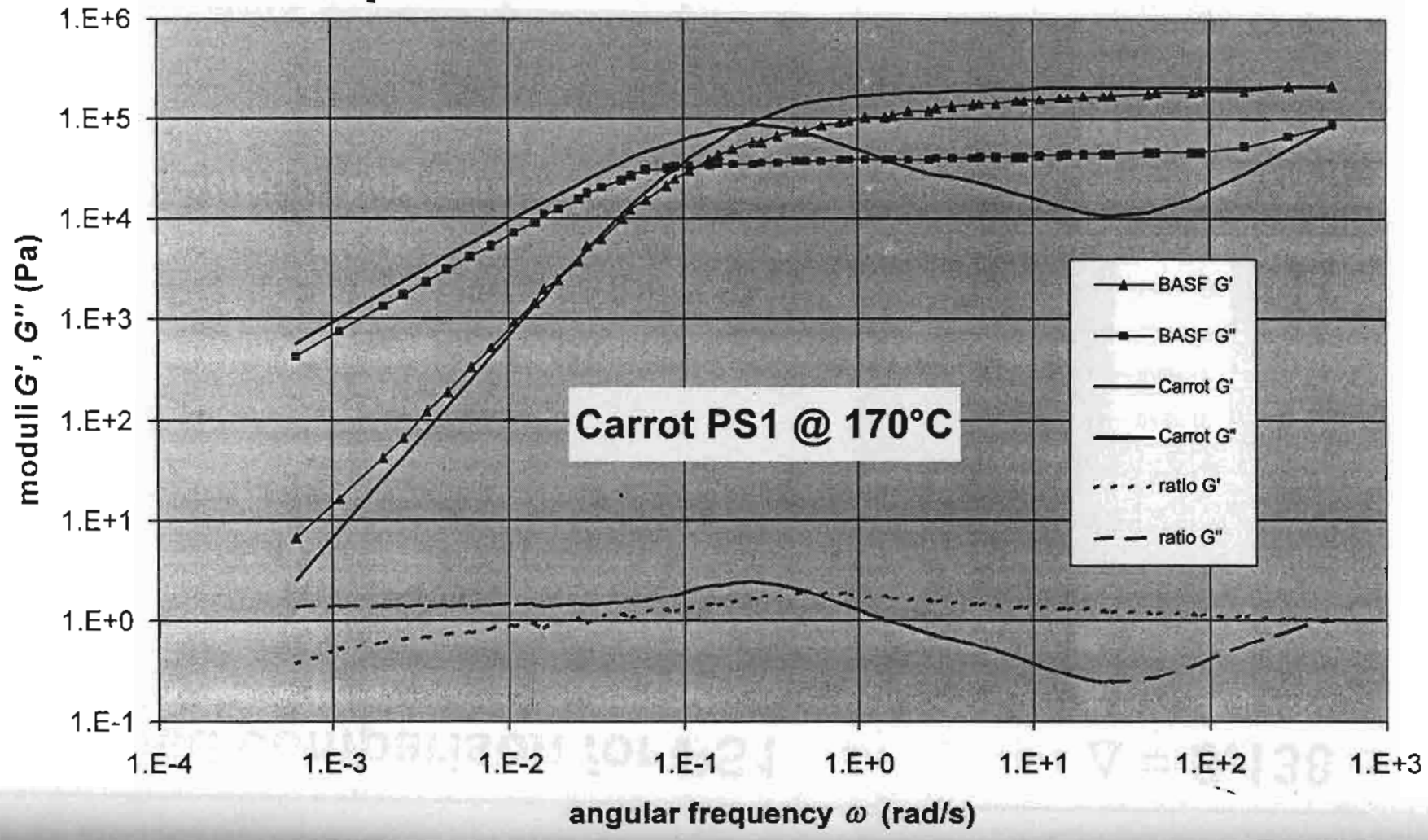
Detailed comparison for PS1

$\Delta = 0.138$



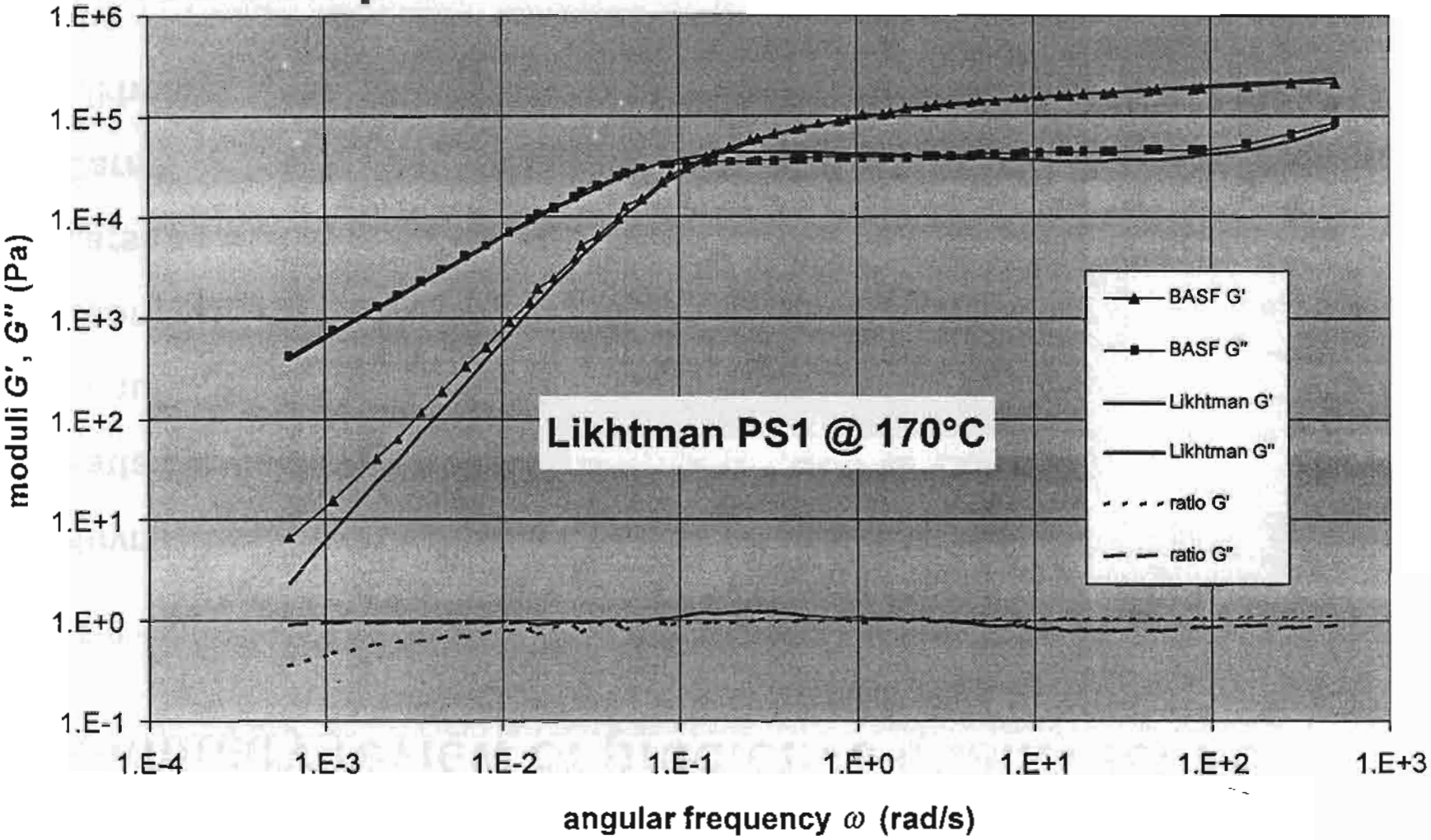
PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

Detailed comparison for PS1 $\Delta = 0.347$



Detailed comparison for PS1

$\Delta = 0.118$

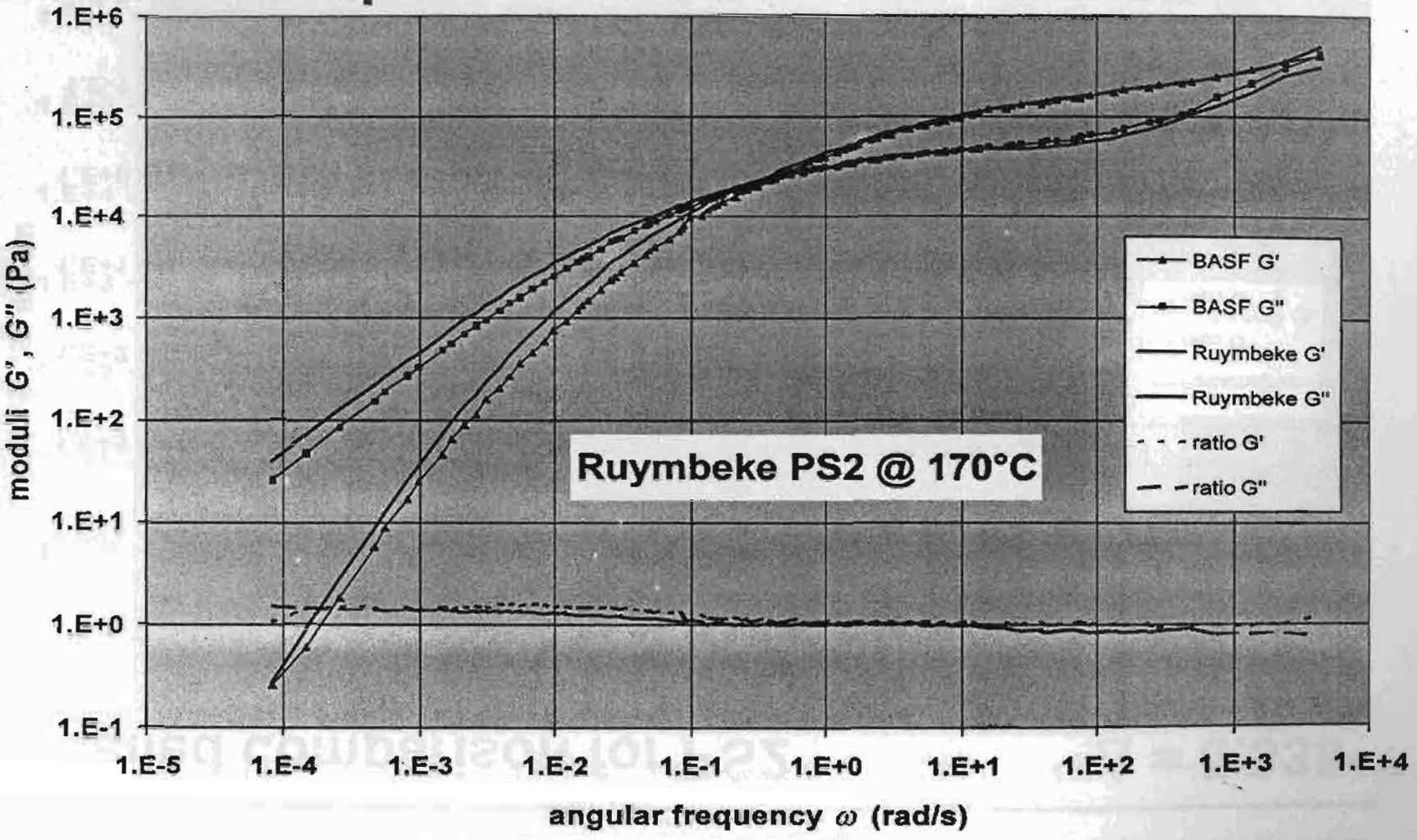


Preliminary review of predictive quality for PS1

	Δ PS1
• Ruymbeke	0.086
• Pattamaprom	0.363
• Schulze	0.229
• Leonardi	0.198
• Larson	0.138
• Carrot	0.347
• Likhtman	0.118

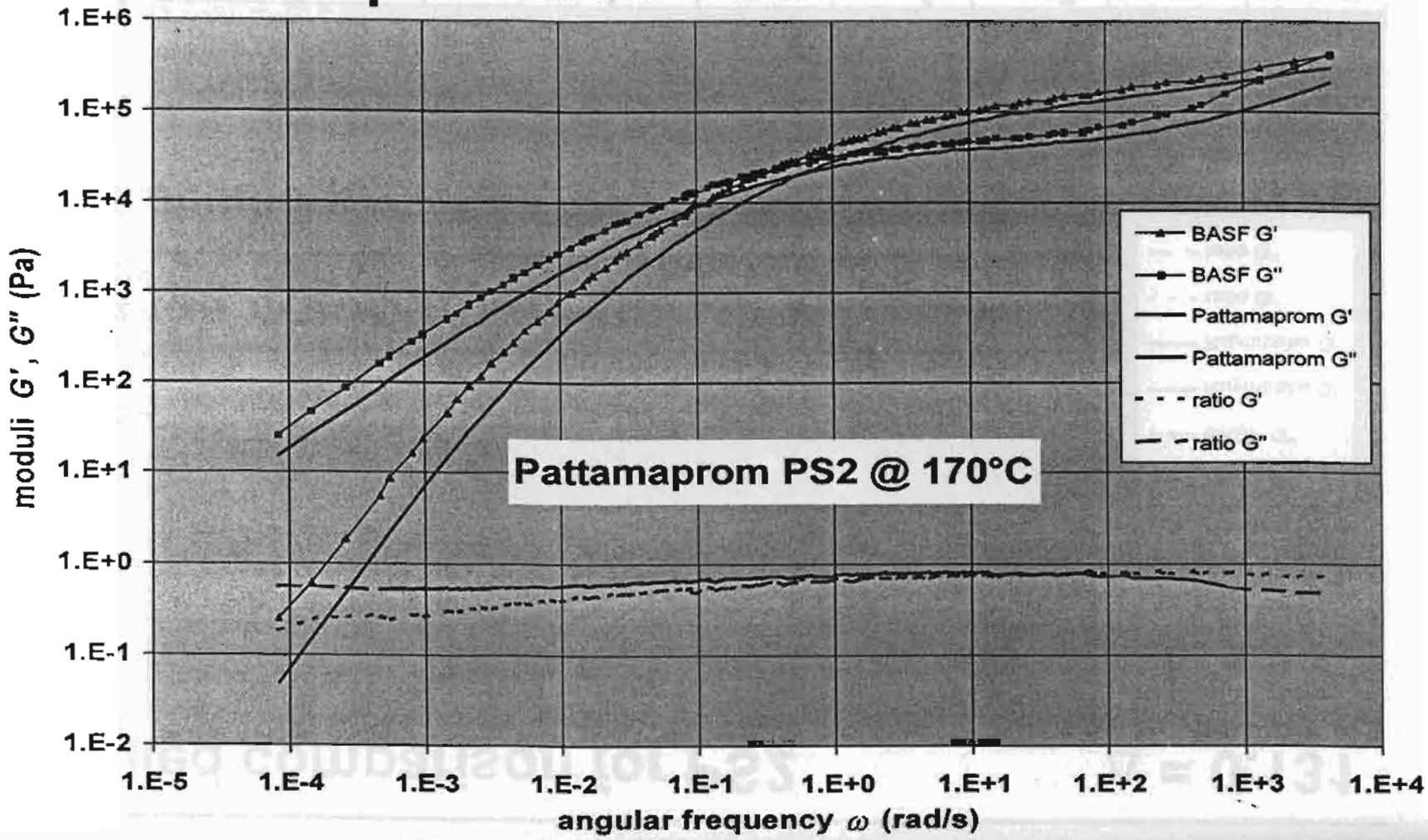
Detailed comparison for PS2

$\Delta = 0.131$



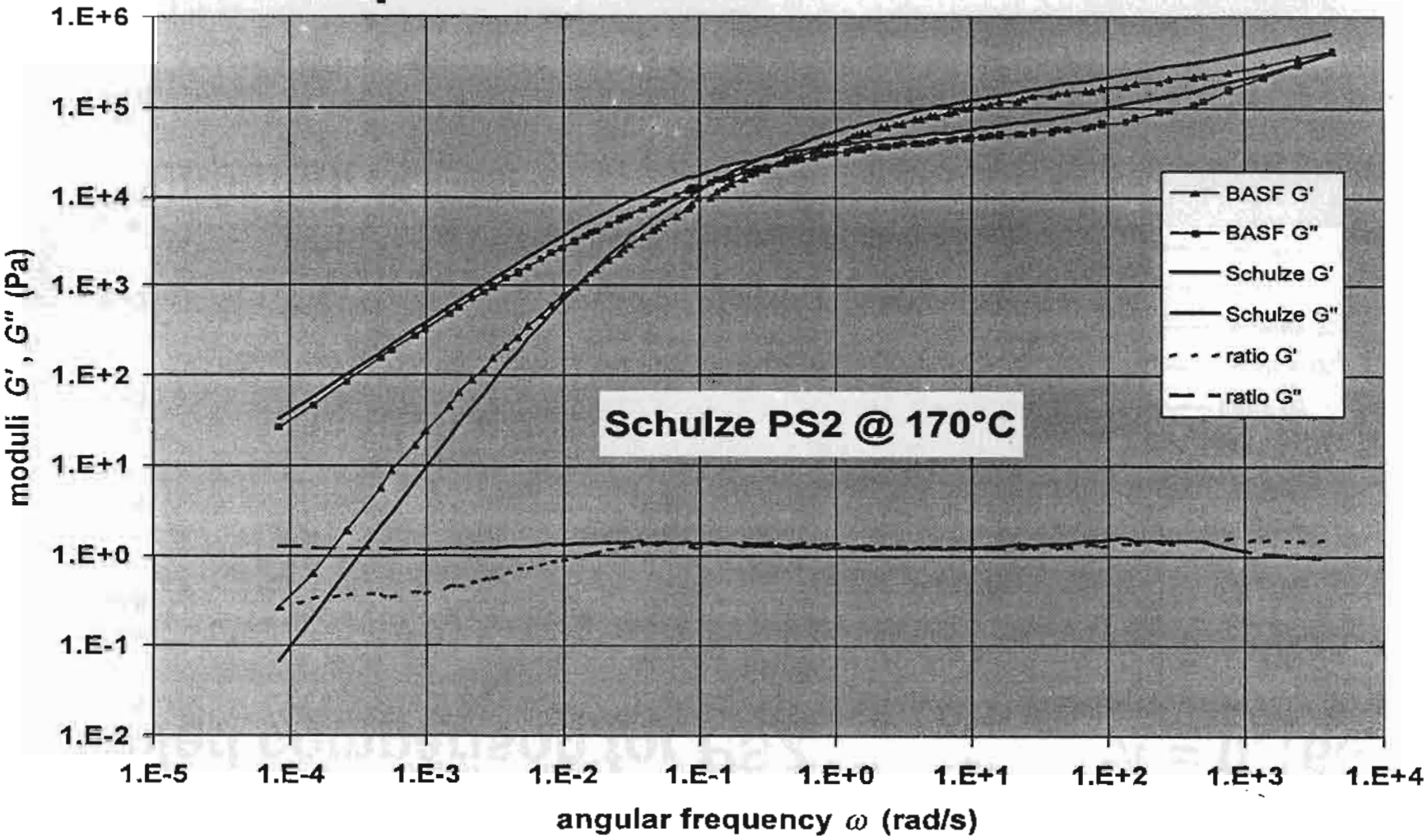
PS benchmark for direct and inverse linear viscoelasticity prediction BASF

Detailed comparison for PS2 $\Delta = 0.339$



Detailed comparison for PS2

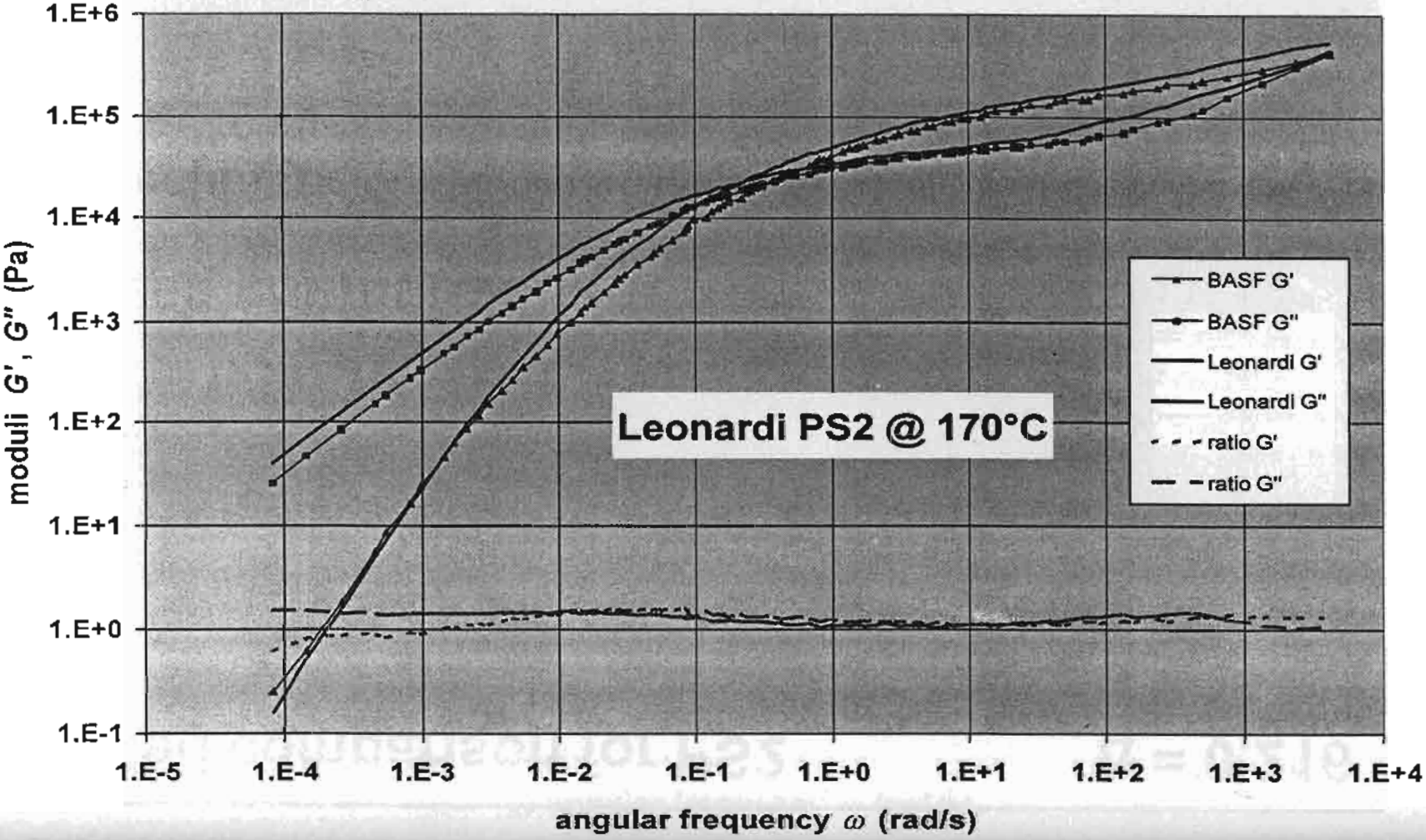
$\Delta = 0.216$



PS benchmark for direct and inverse linear viscoelasticity prediction BASF

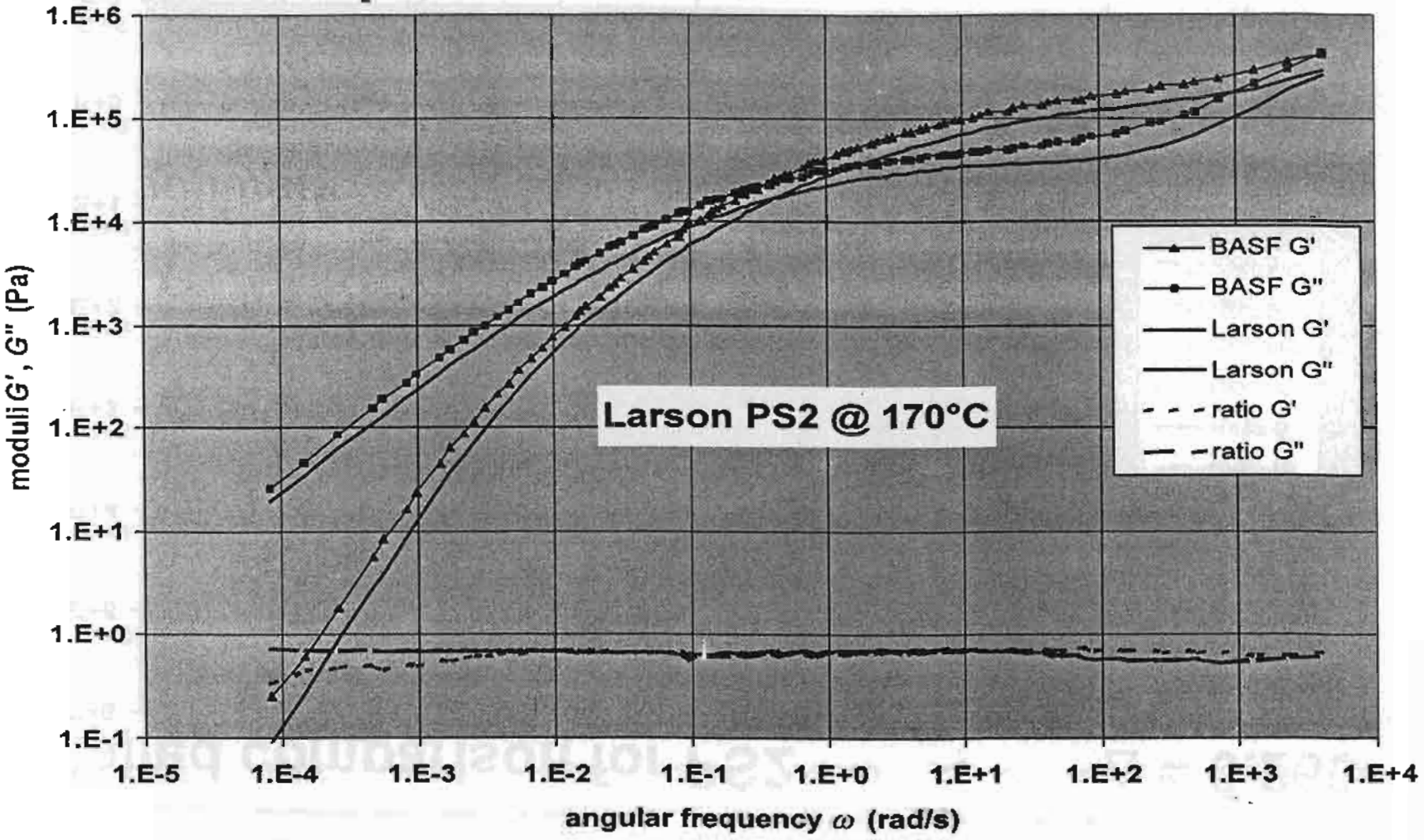
Detailed comparison for PS2

$\Delta = 0.166$



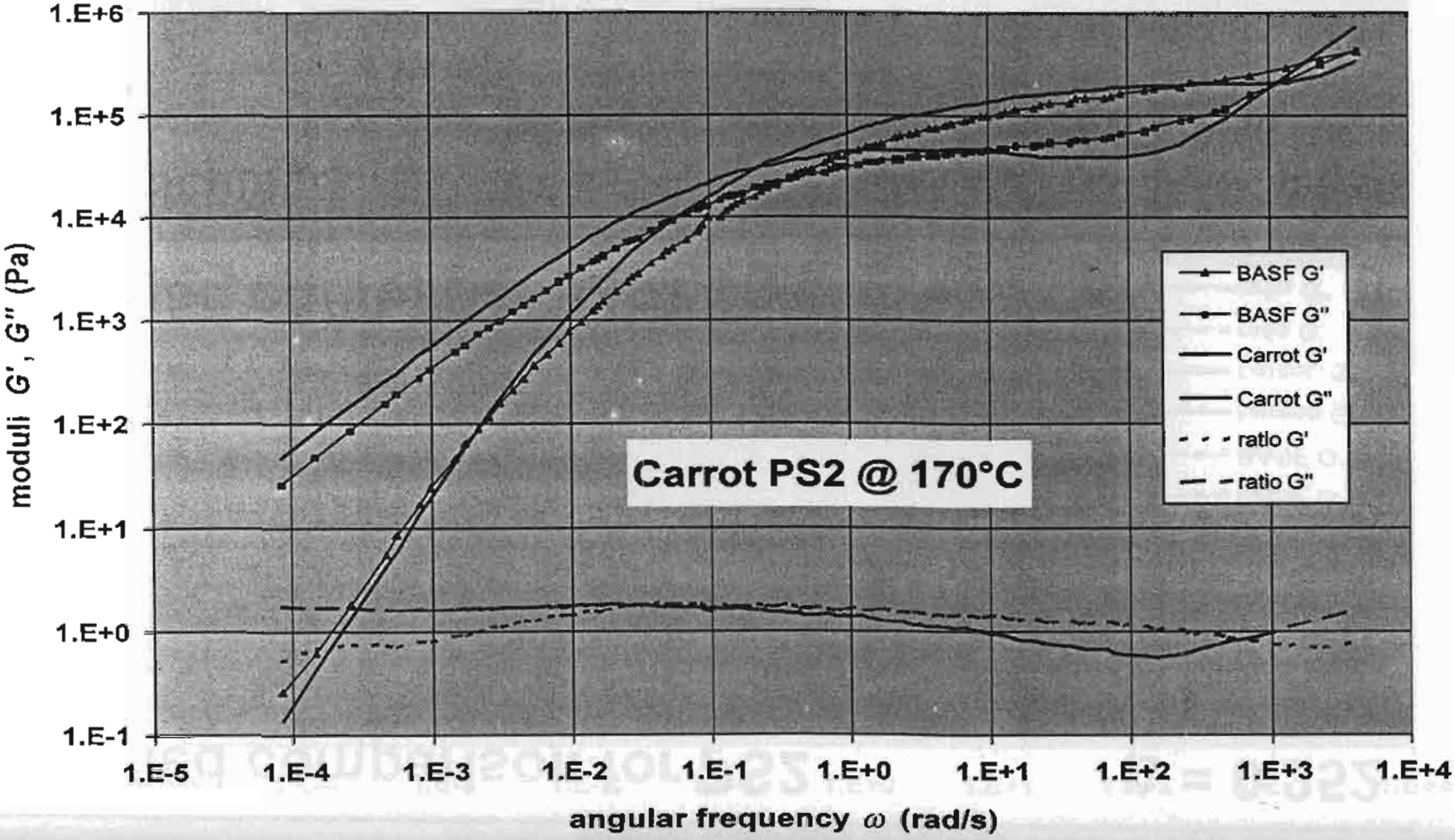
Detailed comparison for PS2

$\Delta = 0.252$



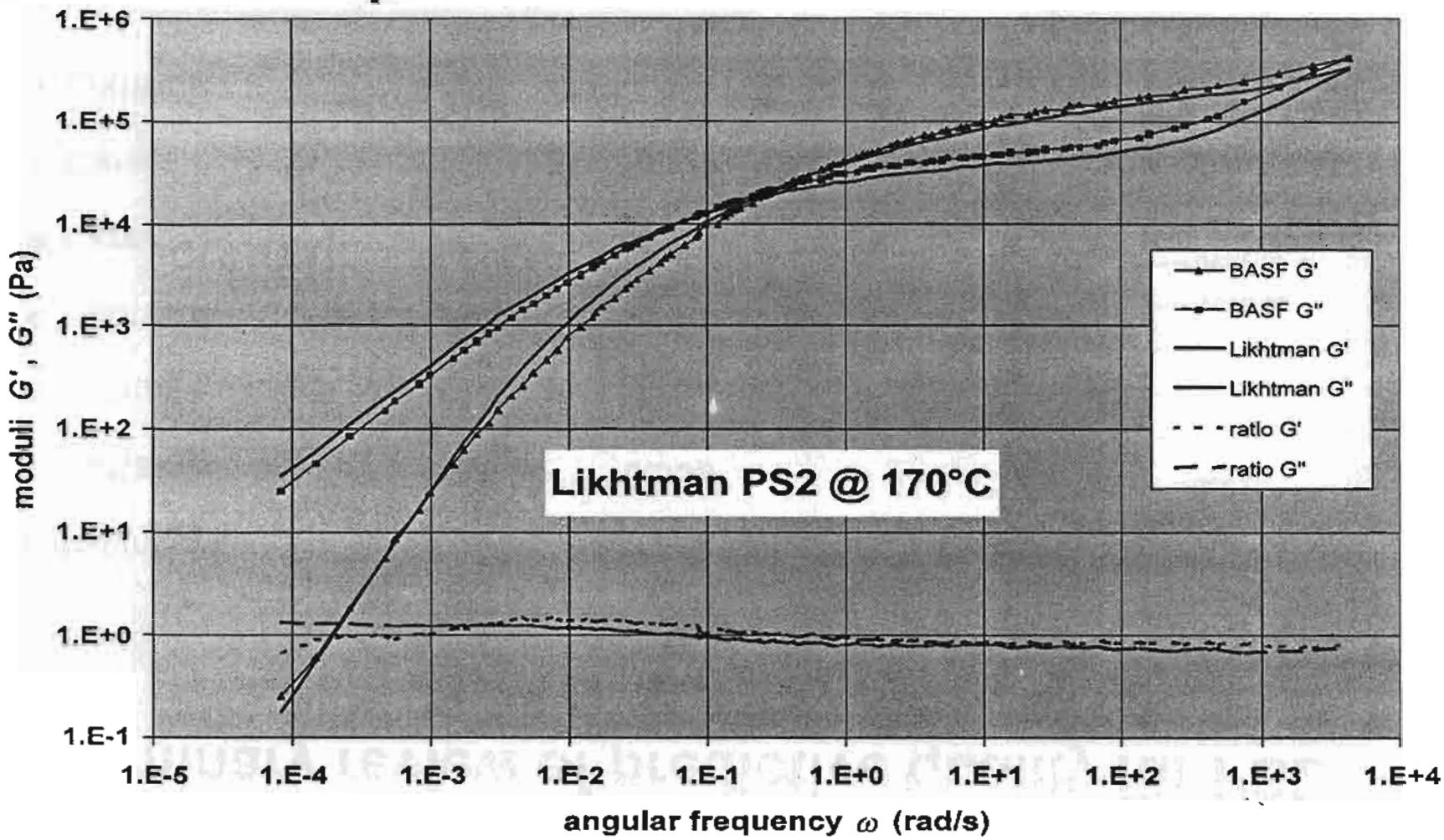
PS benchmark for direct and inverse linear viscoelasticity prediction BASF

Detailed comparison for PS2 $\Delta = 0.260$



Detailed comparison for PS2

$\Delta = 0.124$

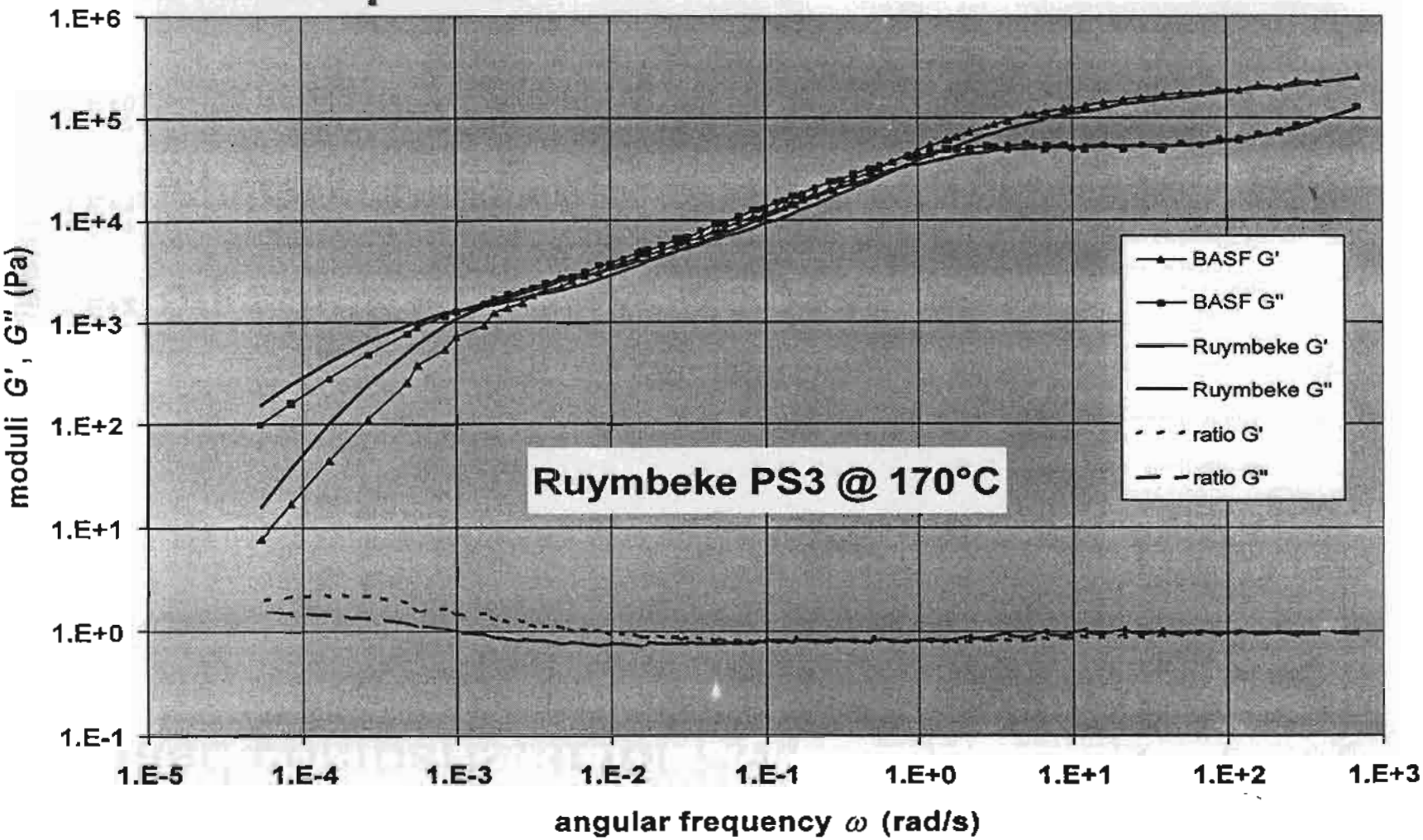


Preliminary review of predictive quality für PS2

	Δ PS2
● Ruymbeke	0.131
● Pattamaprom	0.339
● Schulze	0.216
● Leonardi	0.166
● Larson	0.252
● Carrot	0.260
● Likhtman	0.124

Detailed comparison for PS3

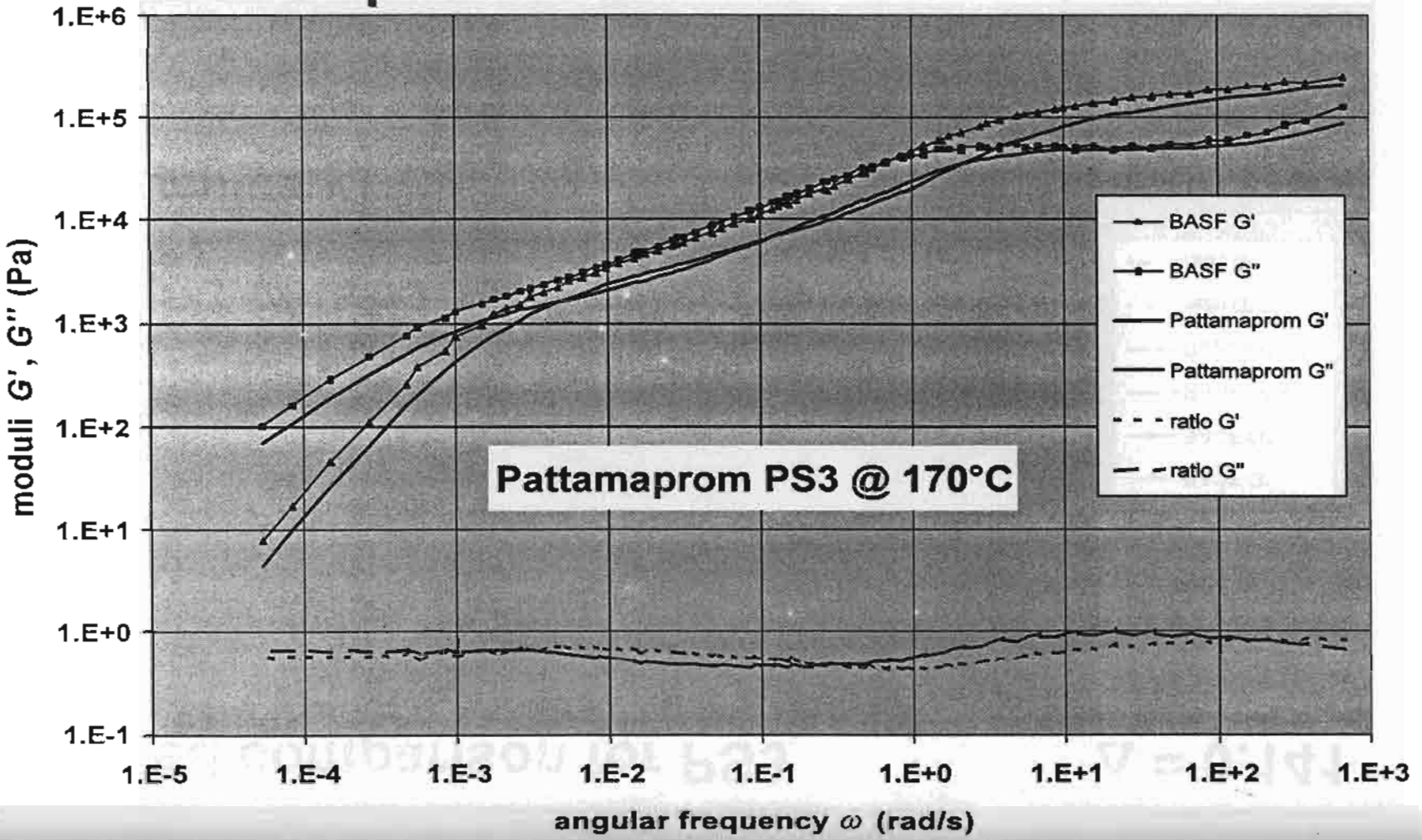
$\Delta = 0.141$



PS benchmark for direct and inverse linear viscoelasticity prediction BASF

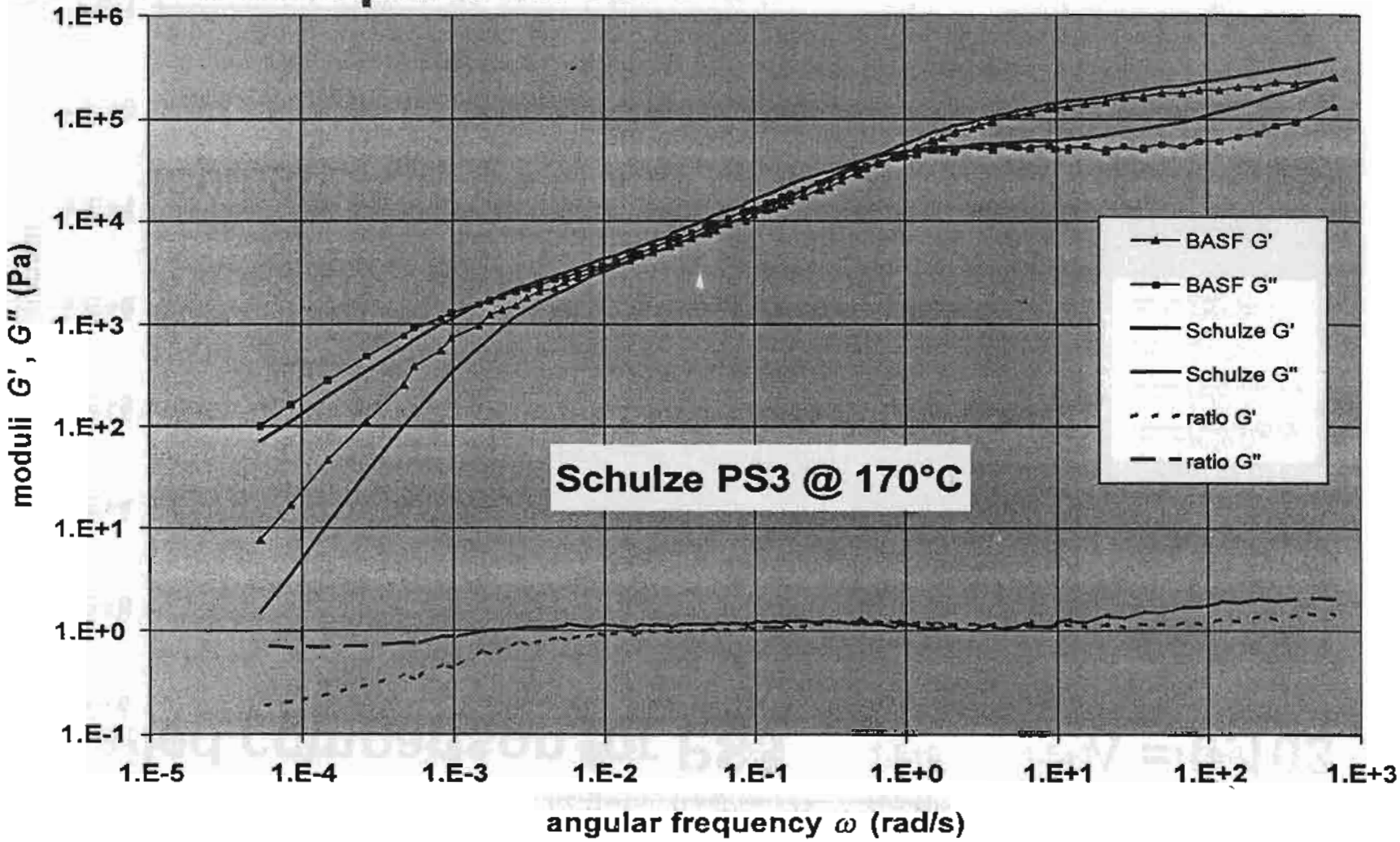
Detailed comparison for PS3

$\Delta = 0.332$



Detailed comparison for PS3

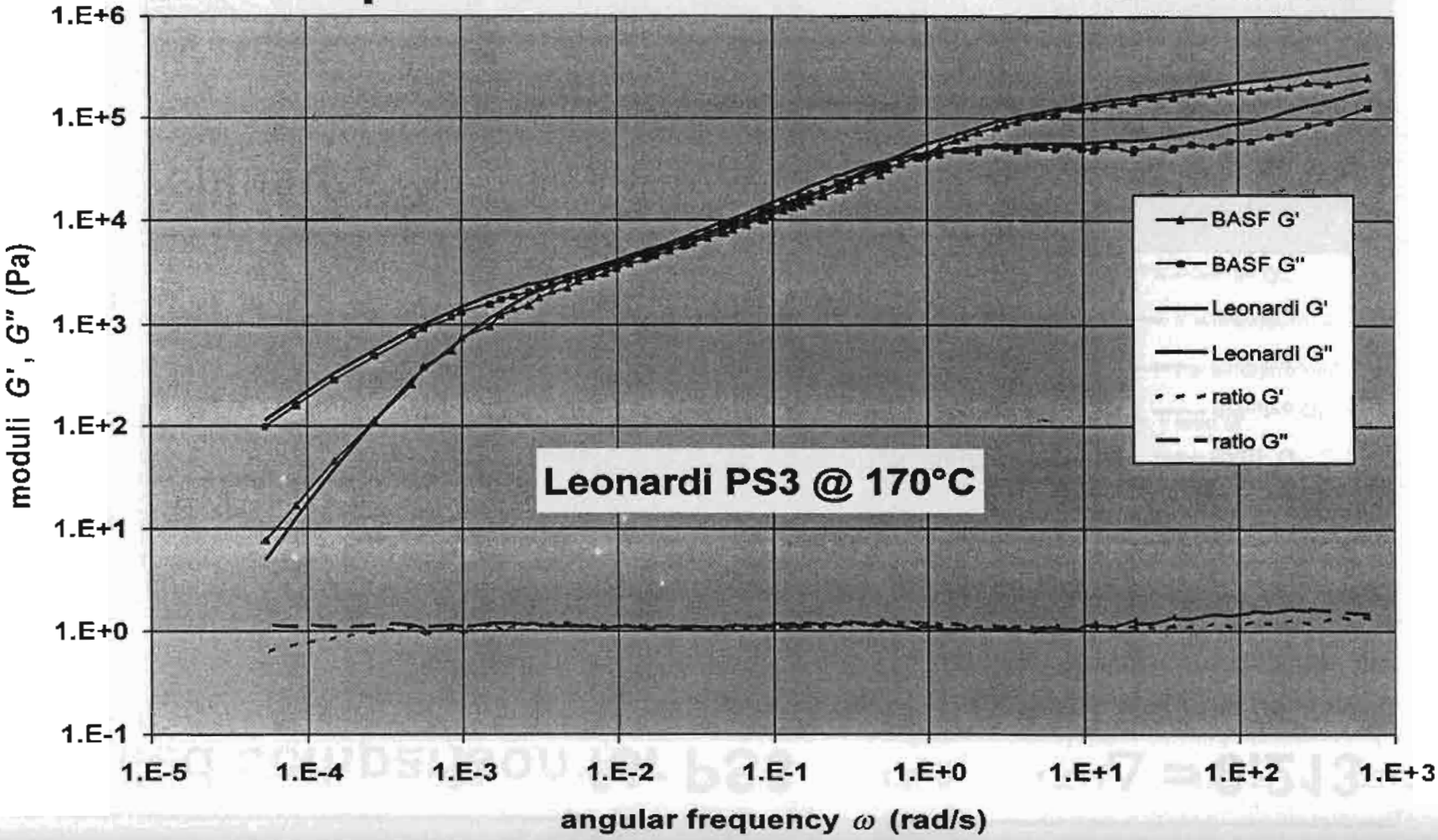
$\Delta = 0.213$



PS benchmark for direct and inverse linear viscoelasticity prediction BASF

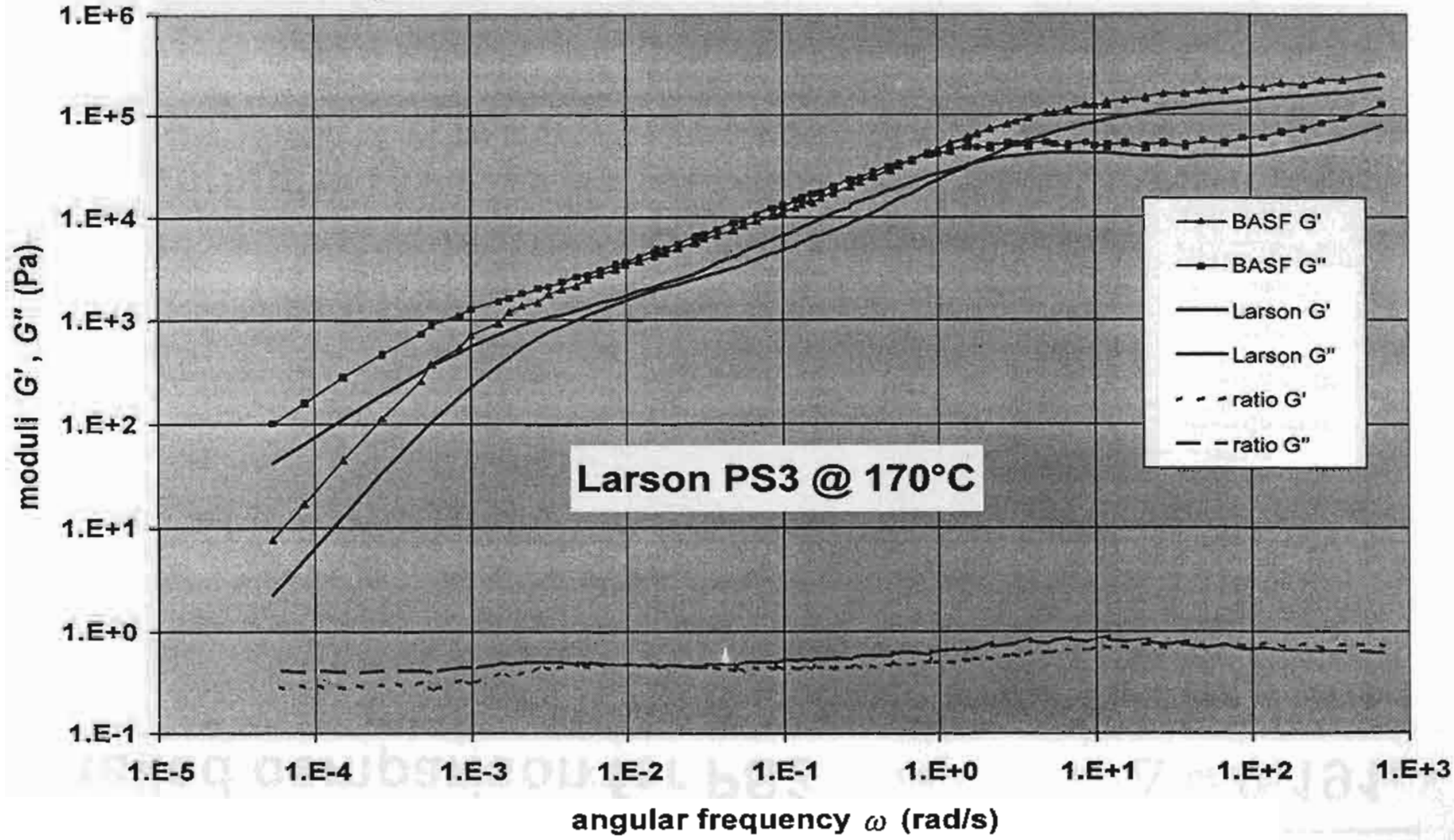
Detailed comparison for PS3

$\Delta = 0.103$



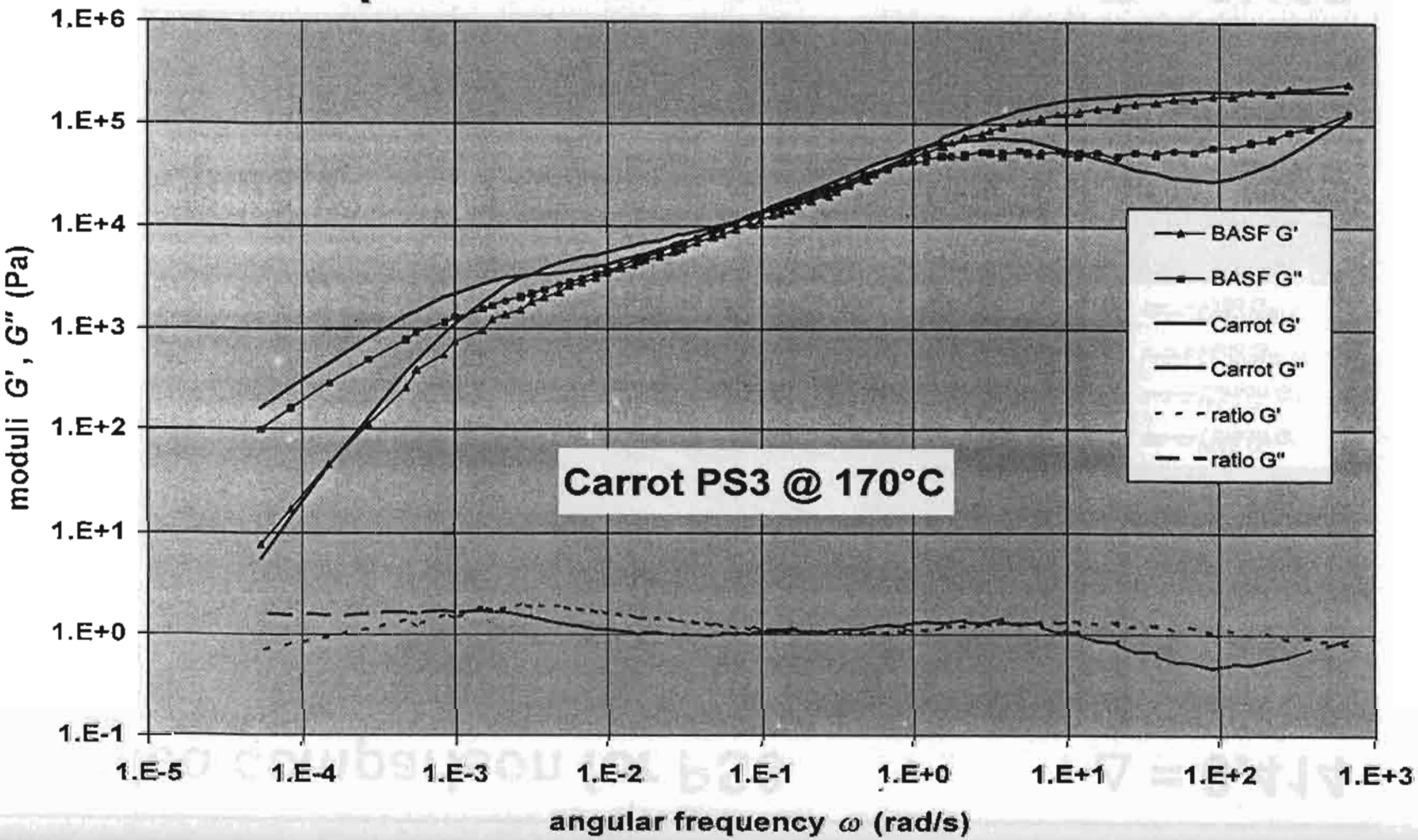
Detailed comparison for PS3

$\Delta = 0.414$



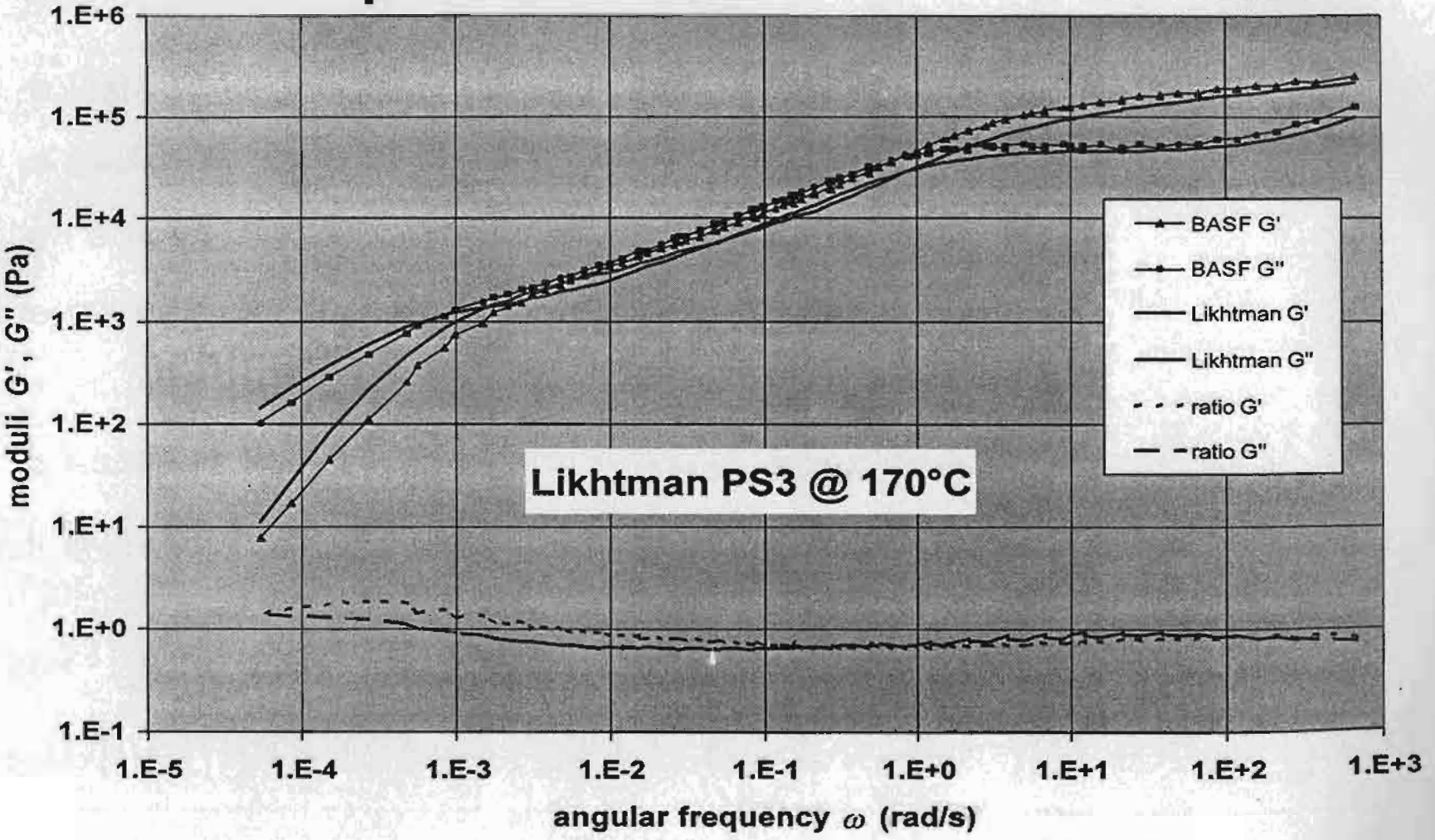
PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

Detailed comparison for PS3 $\Delta = 0.191$



Detailed comparison for PS3

$\Delta = 0.185$



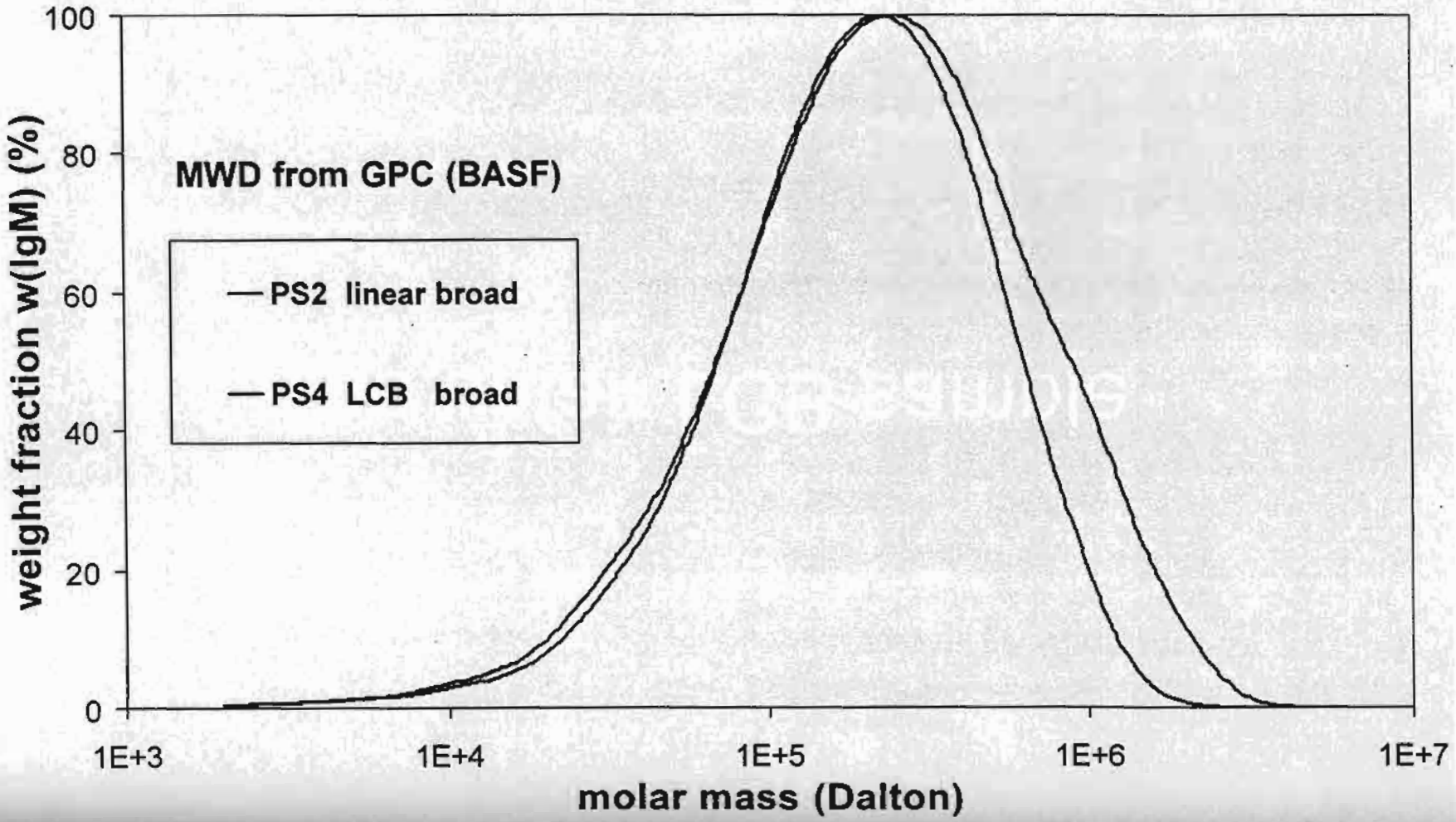
Preliminary review of predictive quality for PS3

	Δ PS3
● Ruymbeke	0.141
● Pattamaprom	0.332
● Schulze	0.213
● Leonardi	0.103
● Larson	0.414
● Carrot	0.191
● Likhtman	0.185

The unfair LCB sample

PS benchmark for direct and inverse linear viscoelasticity prediction BASF

MWD of samples PS2 and PS4

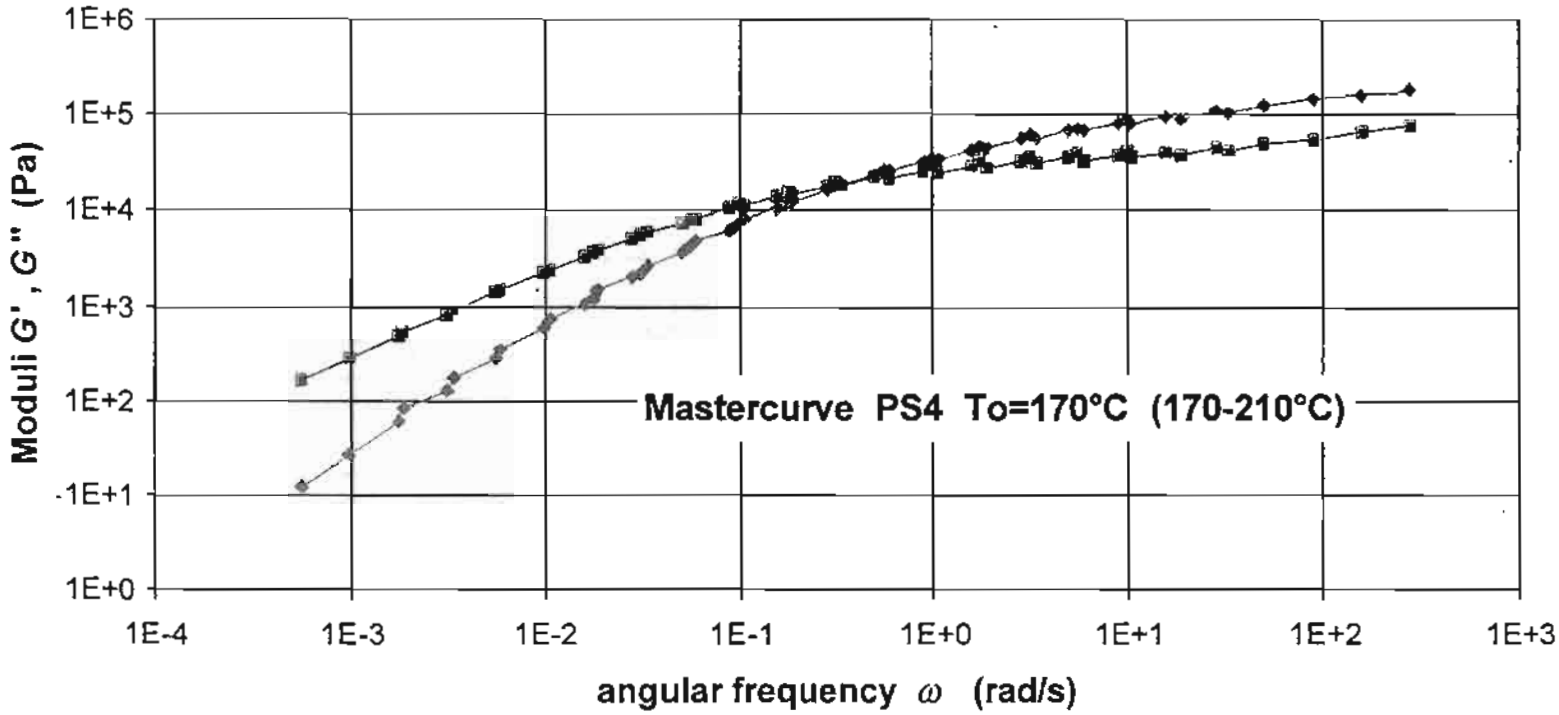


Parameters of the MWD für PS2 and PS4

- BASF GPC using Refractive Index (RI) detector

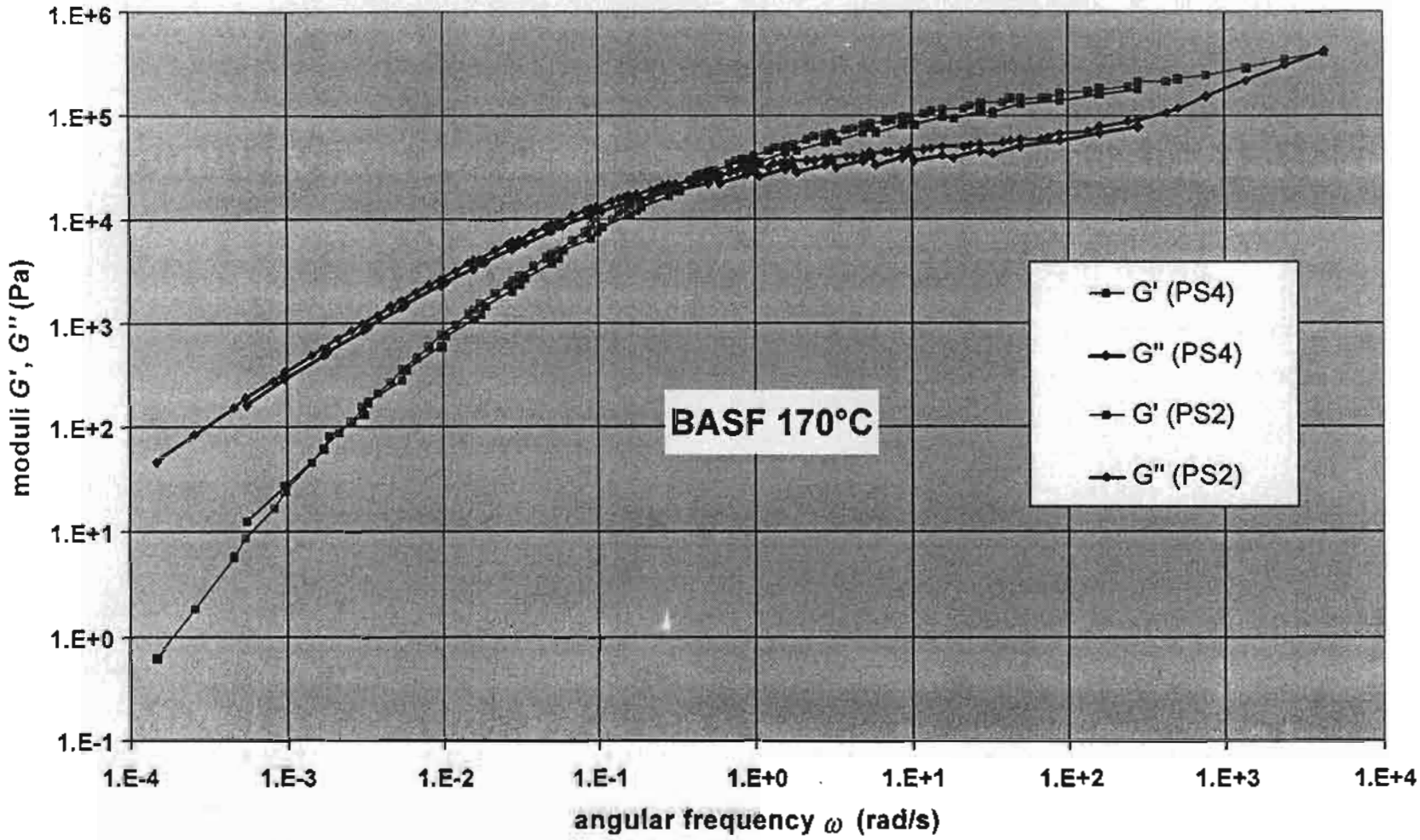
	PS2	PS4
M_n (kD)	101	107
M_w (kD)	274	370
M_z (kD)	500	820
M_w/M_n	2.72	3.47
M_z/M_w	1.82	2.22
$[\eta]$ (mL/g)	96.7	117

Mastercurve of PS4 (contains LCB)



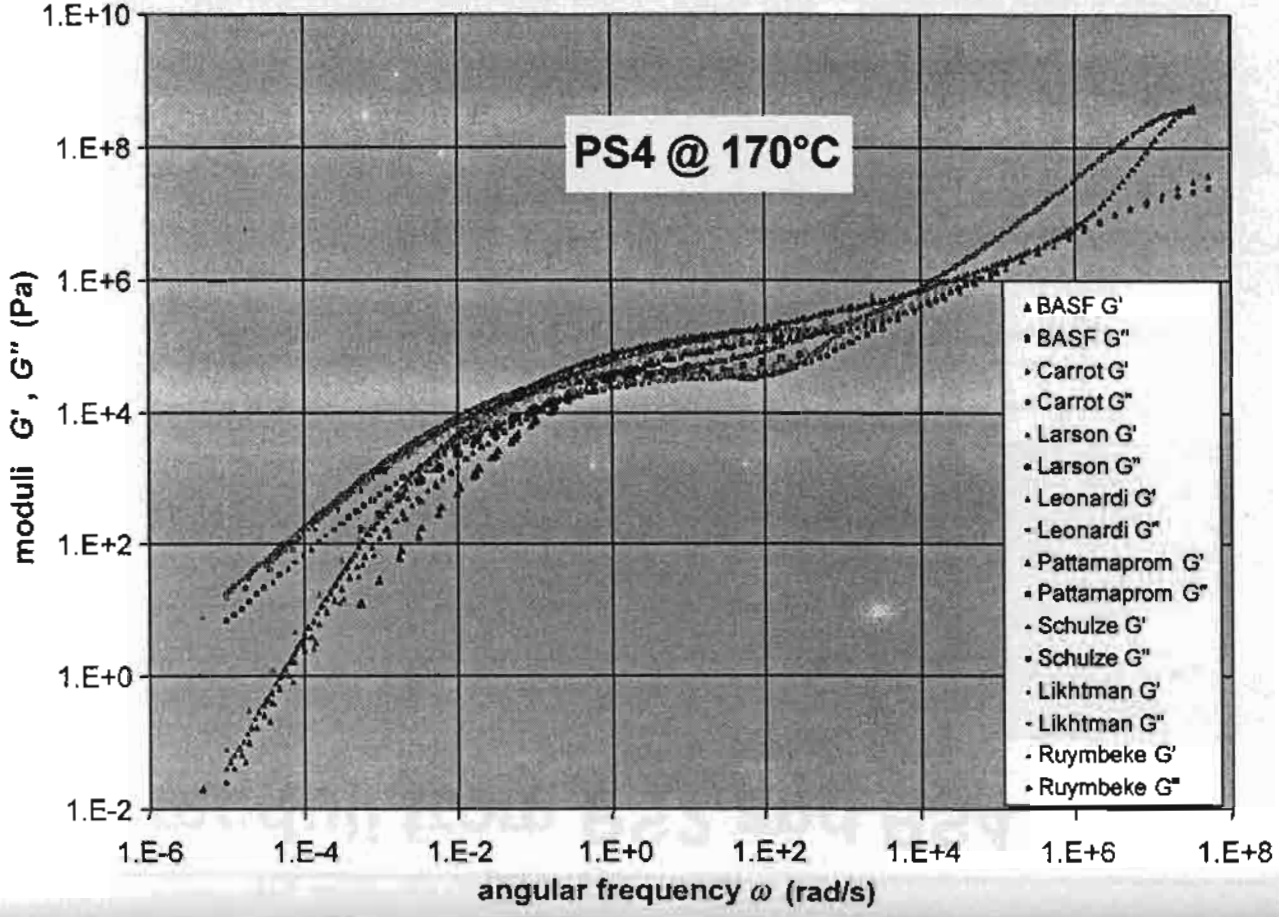
PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

Comparison of moduli from PS2 and PS4



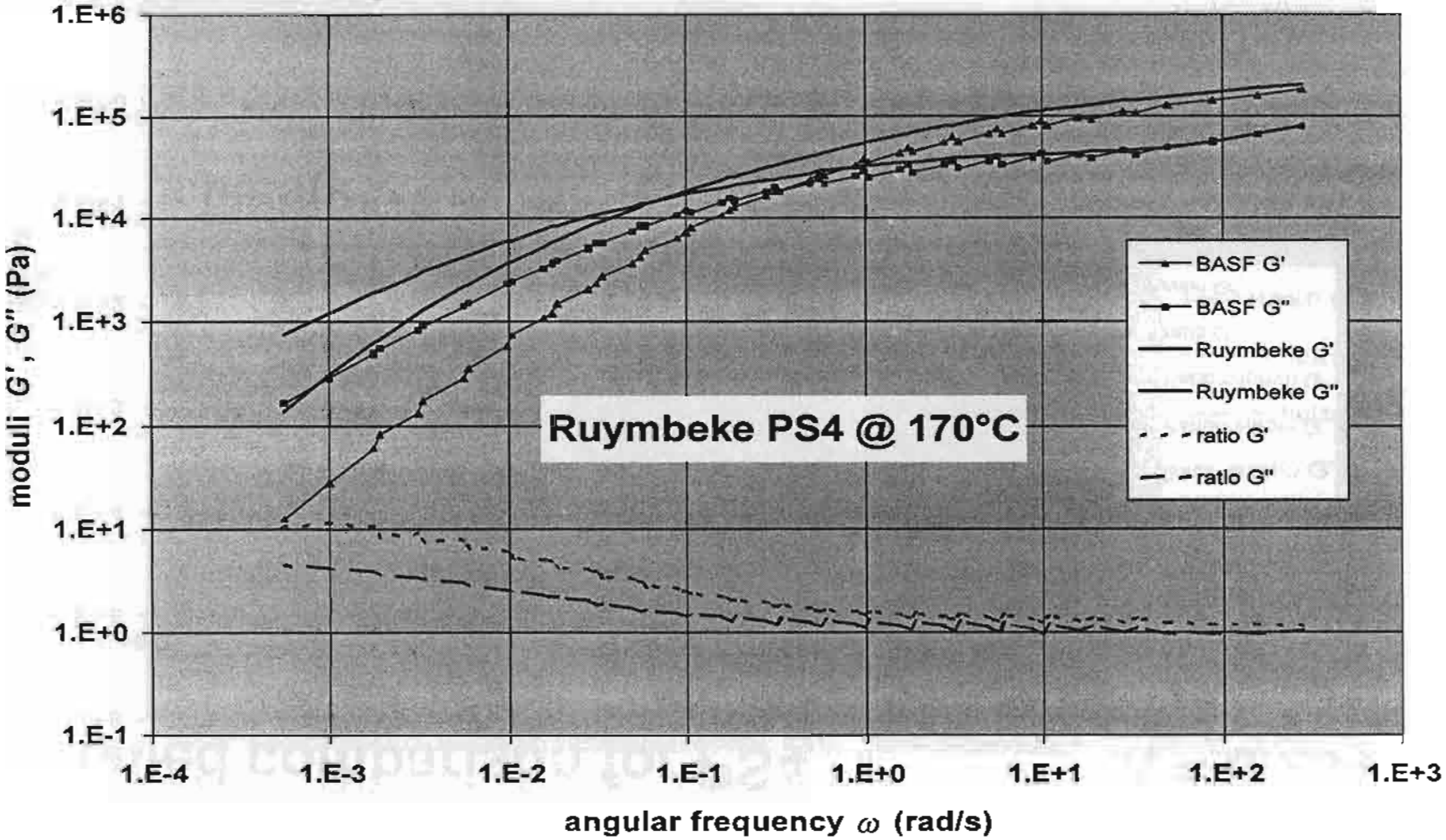
Results

- Overview on moduli predictions for PS4



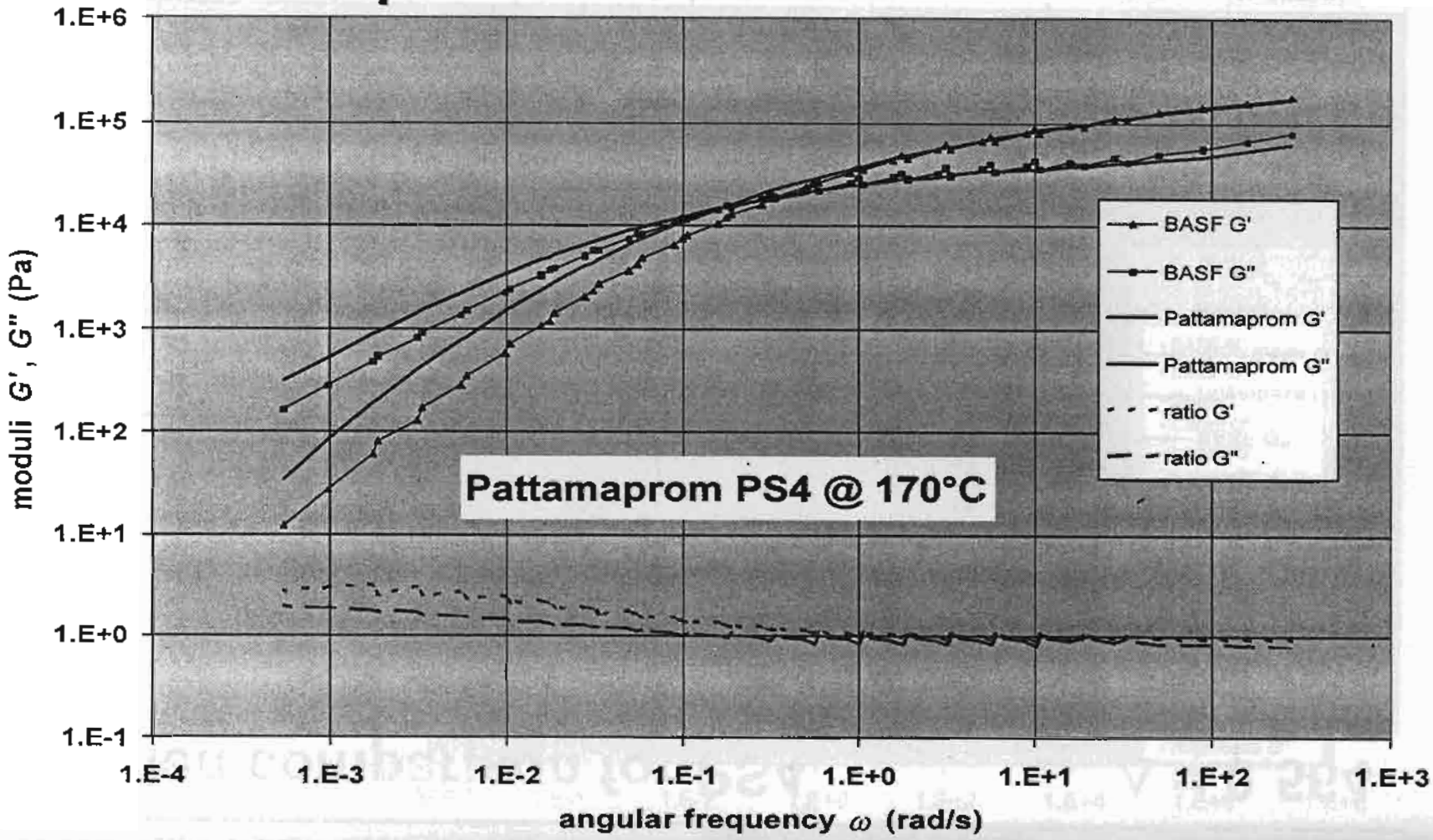
Detailed comparison for PS4

$\Delta = 0.564$



PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

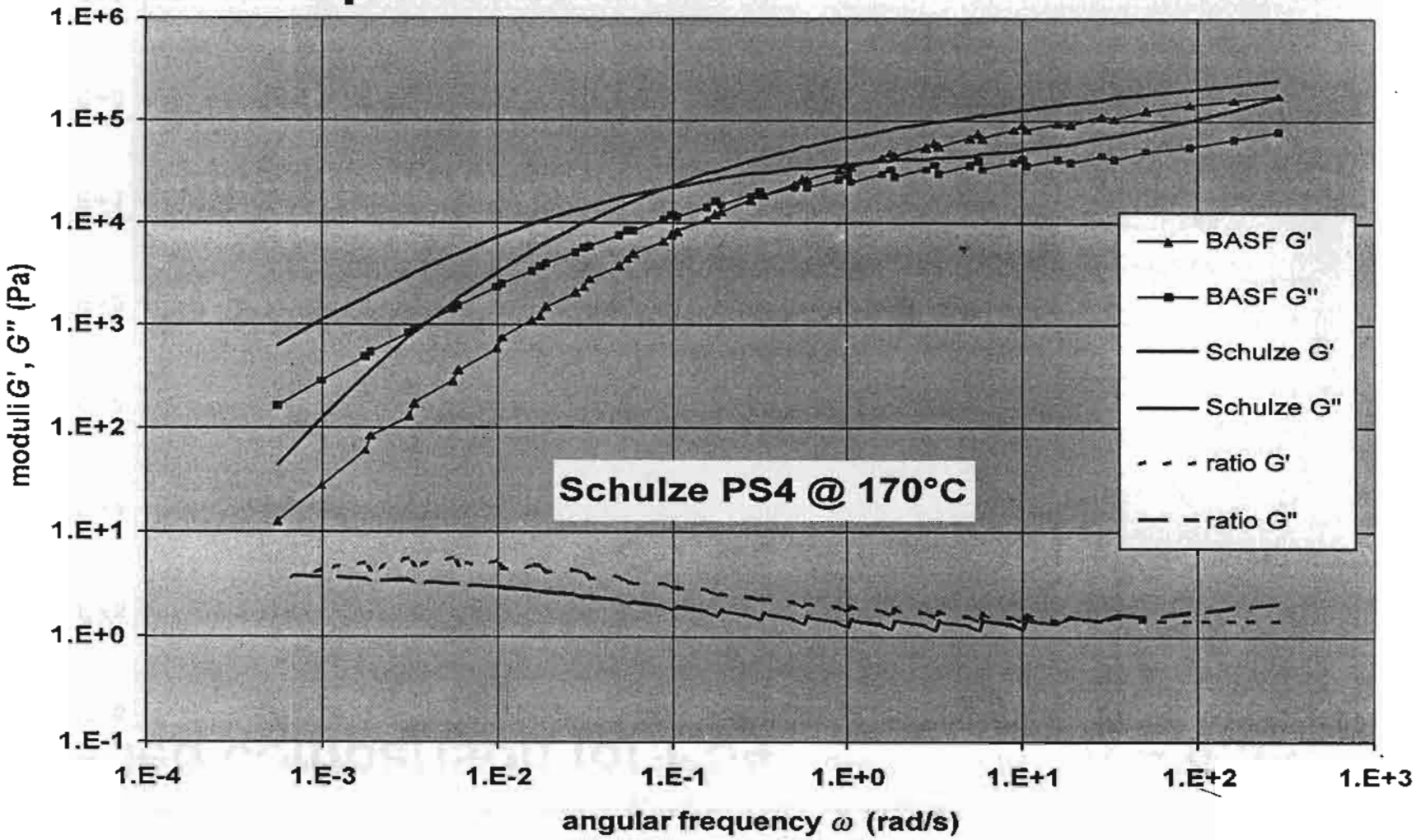
Detailed comparison for PS4 $\Delta = 0.254$



PS benchmark for direct and inverse linear viscoelasticity prediction **BASF**

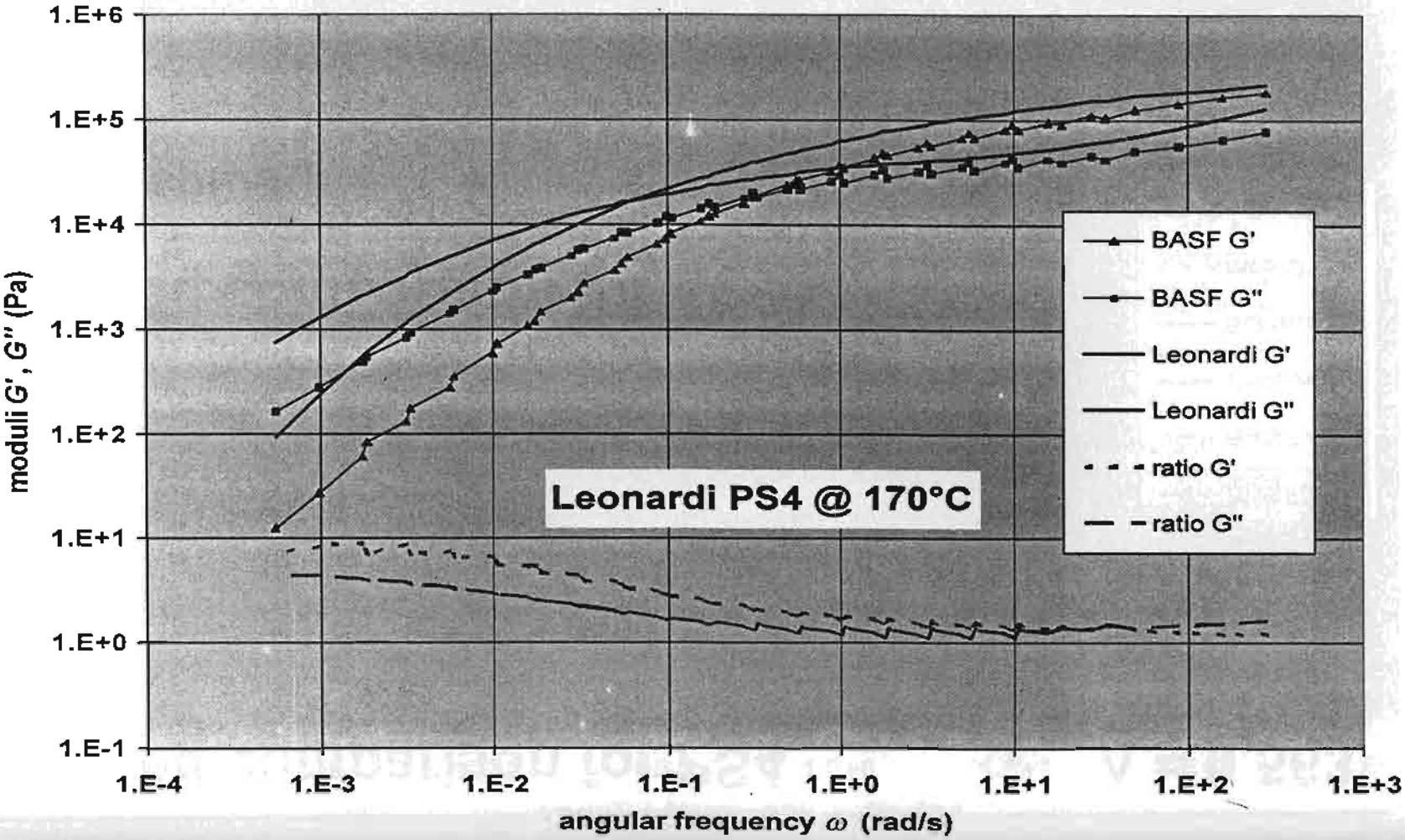
Detailed comparison for PS4

$\Delta = 0.563$



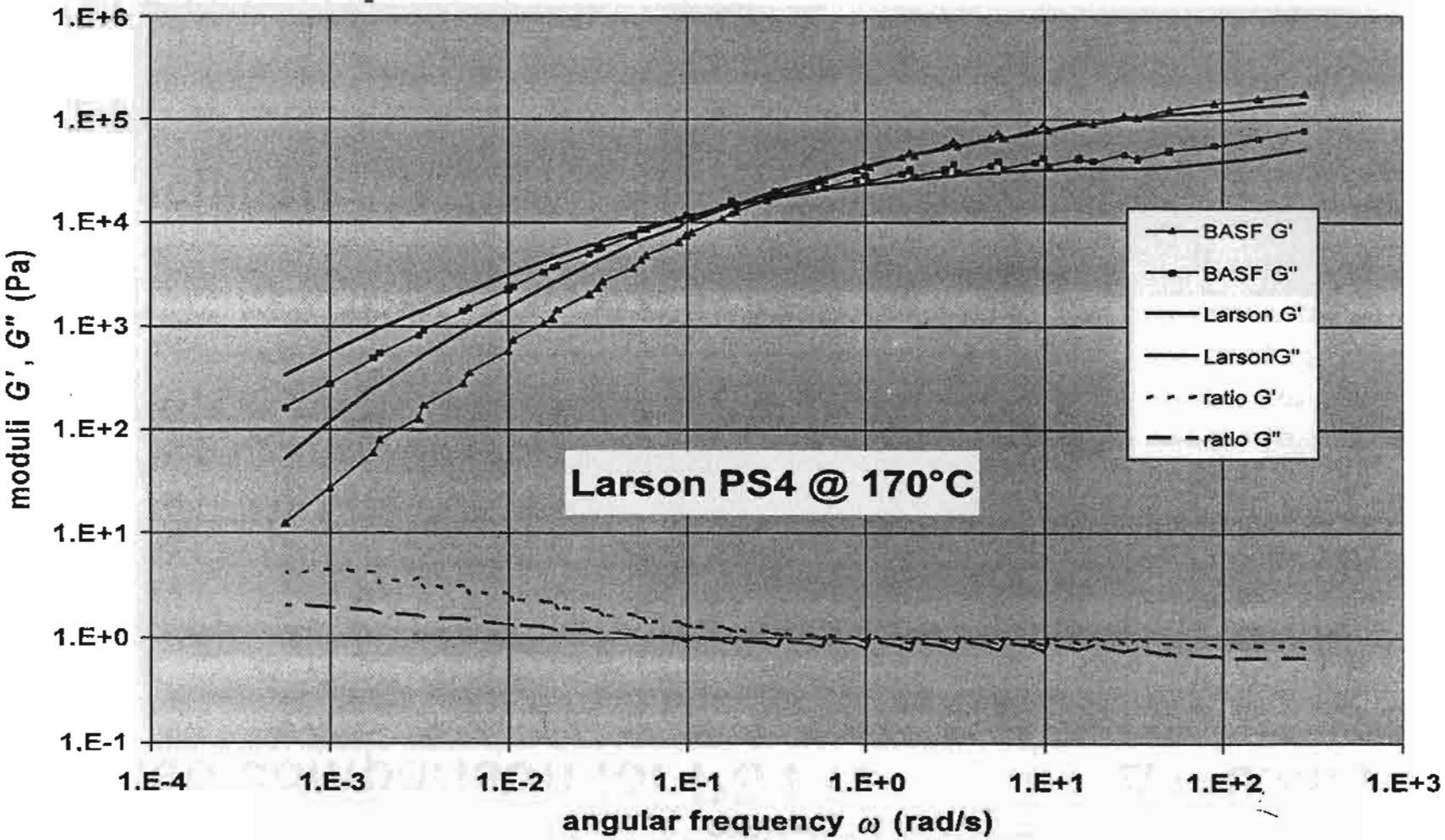
Detailed comparison for PS4

$\Delta = 0.597$



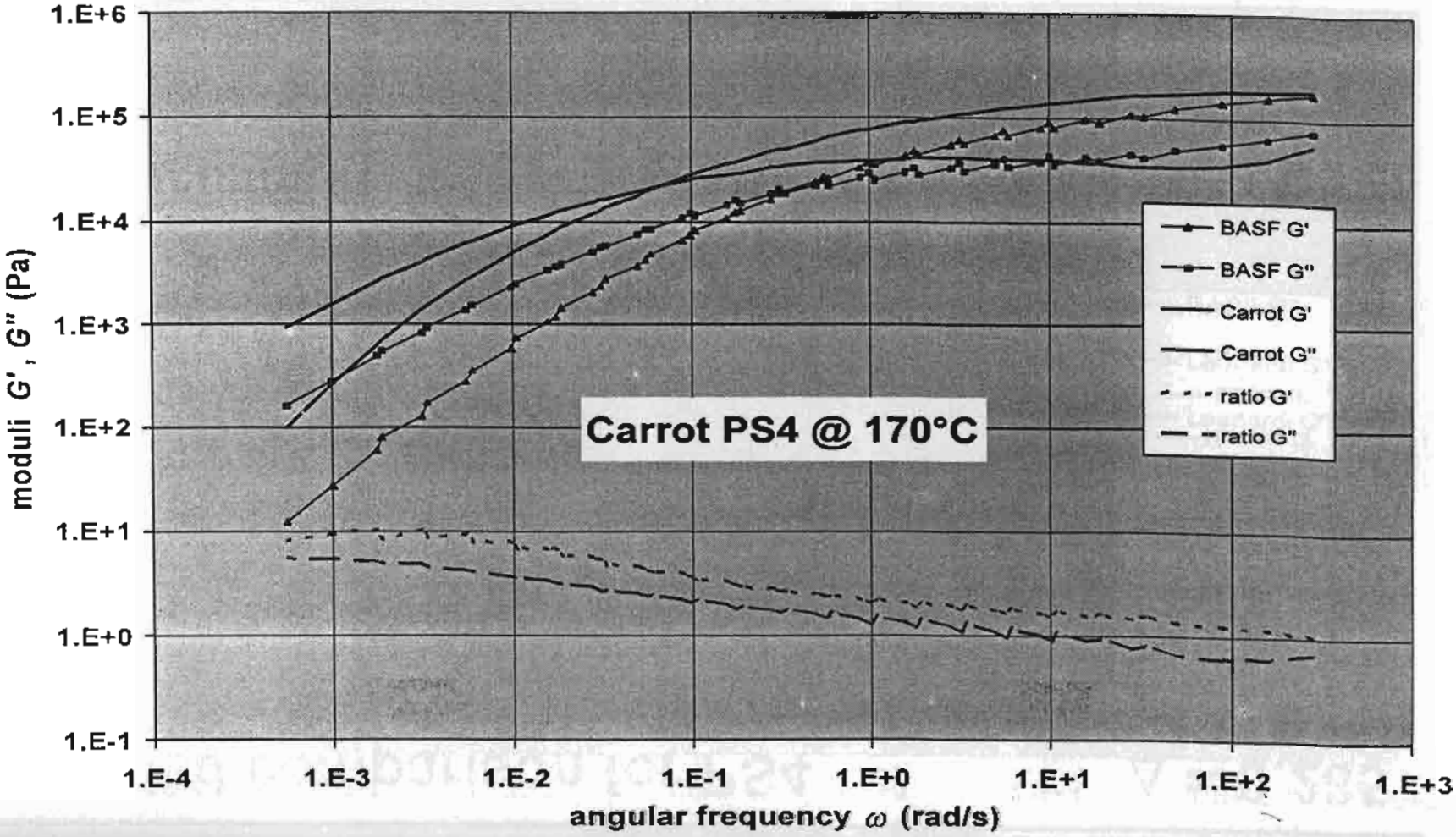
Detailed comparison for PS4

$\Delta = 0.285$



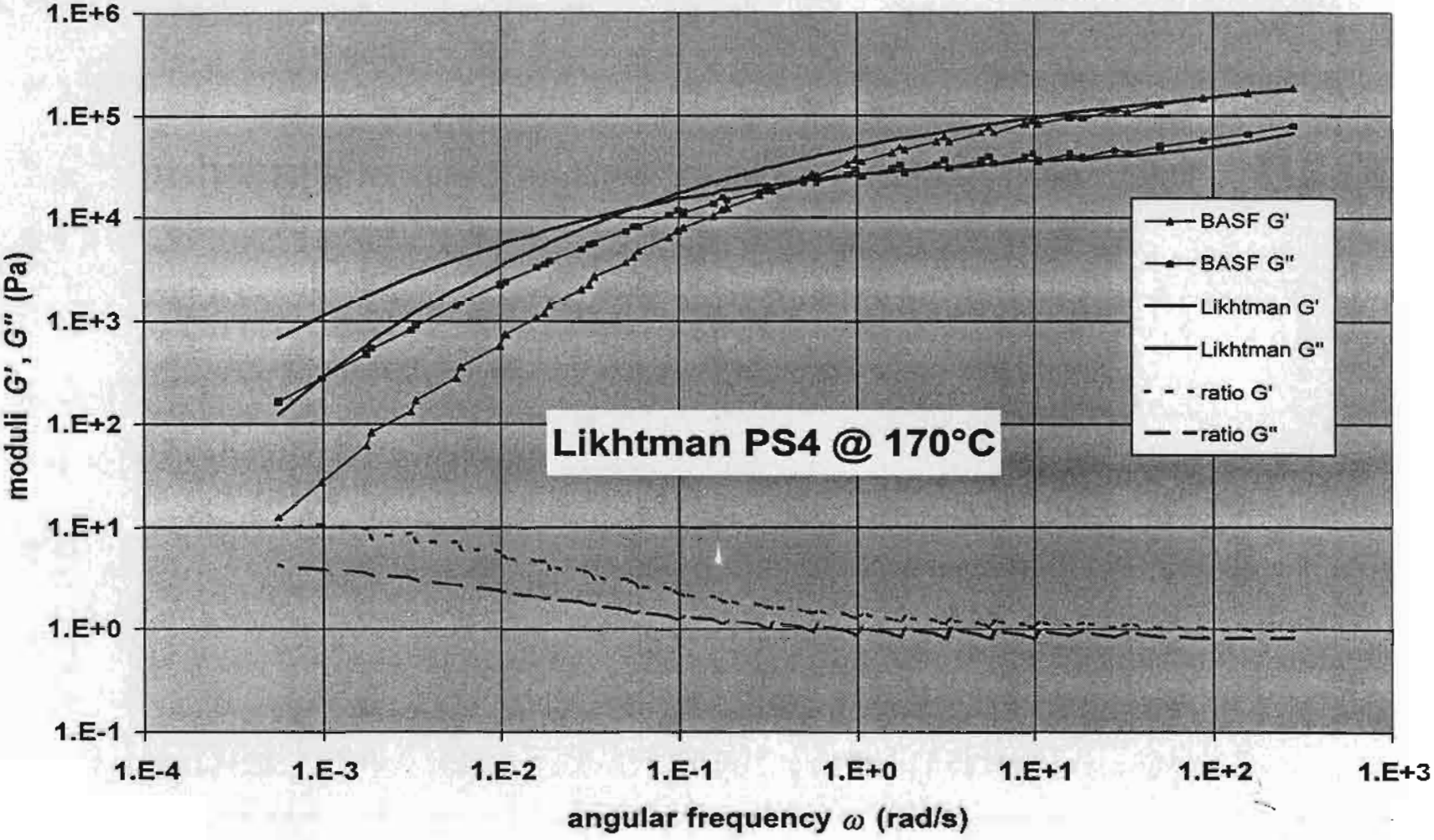
Detailed comparison for PS4

$\Delta = 0.695$



Detailed comparison for PS4

$\Delta = 0.531$



Preliminary review of predictive quality (all)

	Δ PS4
• Ruymbeke	0.564
• Pattamaprom	0.254
• Schulze	0.563
• Leonardi	0.597
• Larson	0.285
• Carrot	0.695
• Likhtman	0.531

Summary for direct prediction

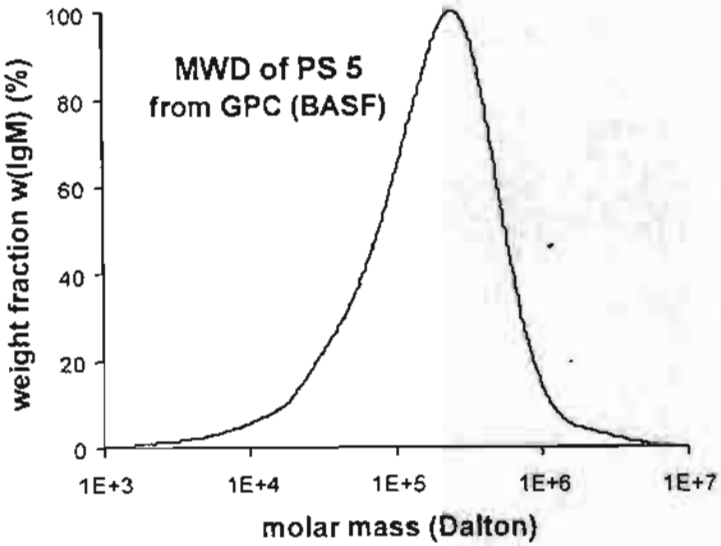
Preliminary review of predictive quality (all)

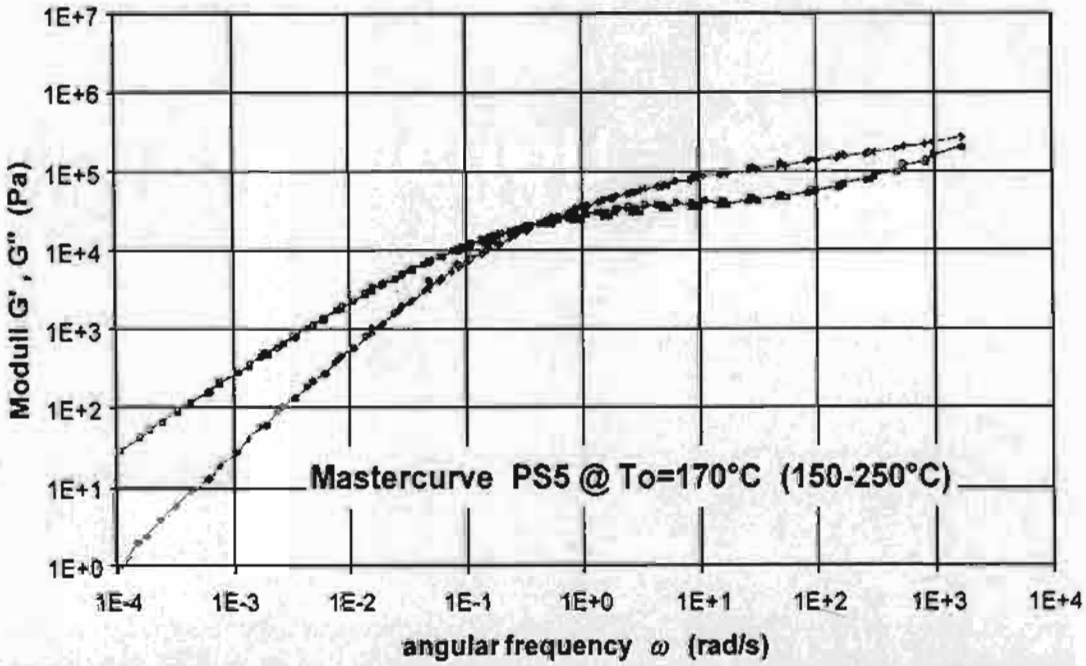
	ΔPS1	ΔPS2	ΔPS3	ΔPS4
• Ruymbeke	0.086	0.131	0.141	0.564
• Pattamaprom	0.363	0.339	0.332	0.254
• Schulze	0.229	0.216	0.213	0.563
• Leonardi	0.198	0.166	0.103	0.597
• Larson	0.138	0.252	0.414	0.285
• Carrot	0.347	0.260	0.191	0.695
• Likhtman	0.118	0.124	0.185	0.531

Inverse prediction

Test of inverse linear viscoelasticity prediction

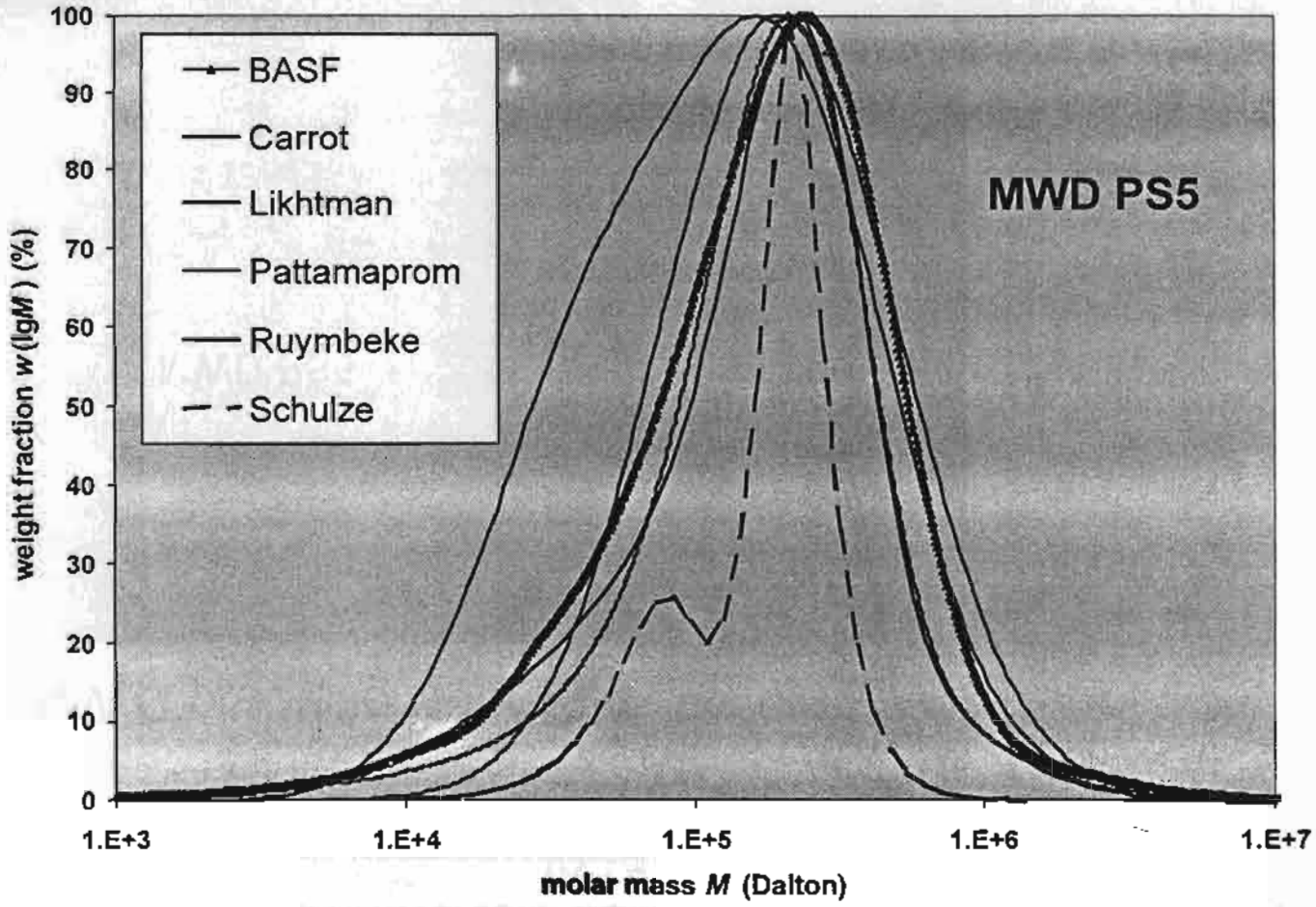
- Mastercurve of dynamic moduli @ 170°C from BASF distributed
- Participants predict MWD based on theory
- Experimental MWD from BASF GPC used as reference





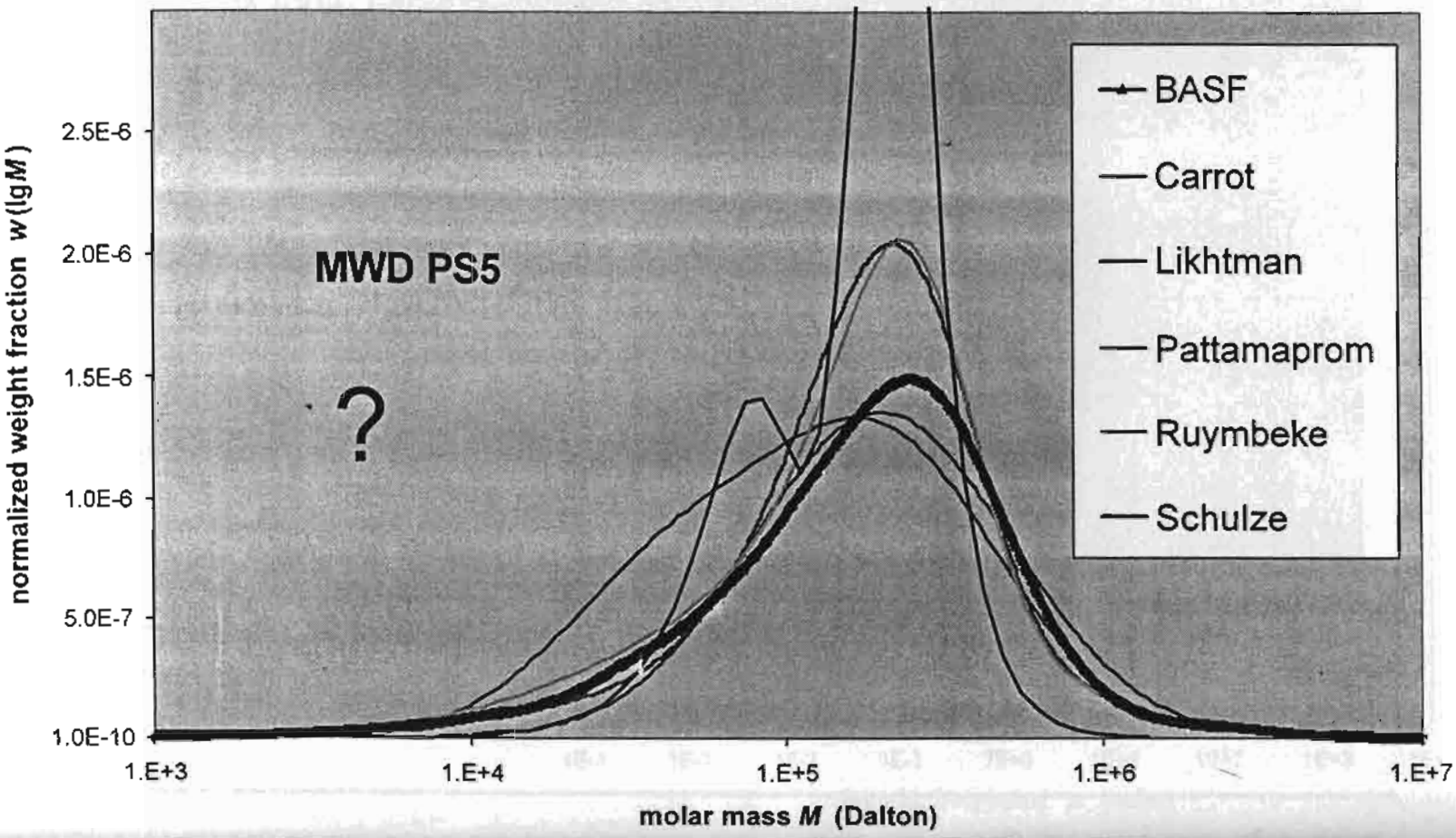
Results

- Overview on MWD prediction for PS5



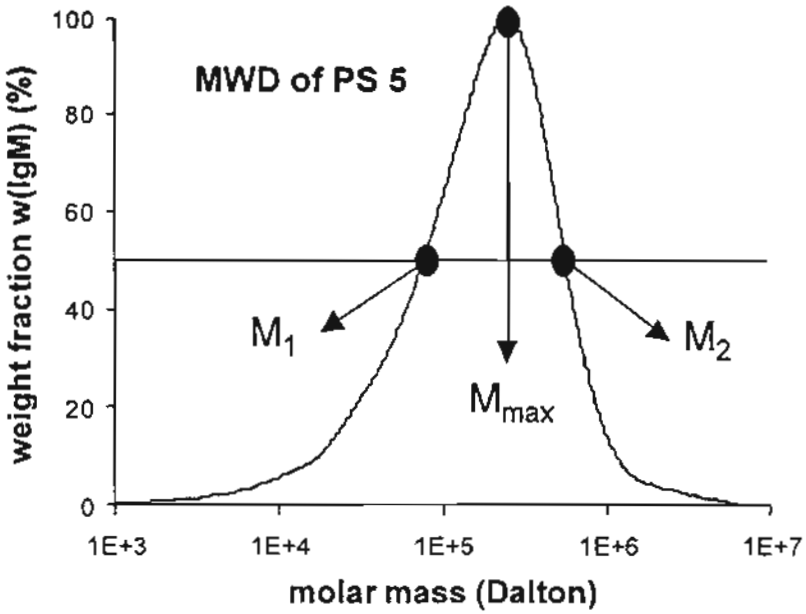
Results

- Normalized MWD predictions for PS5



Preliminary quantification of predictive quality

- 3 typical values of the predicted MWD defined:



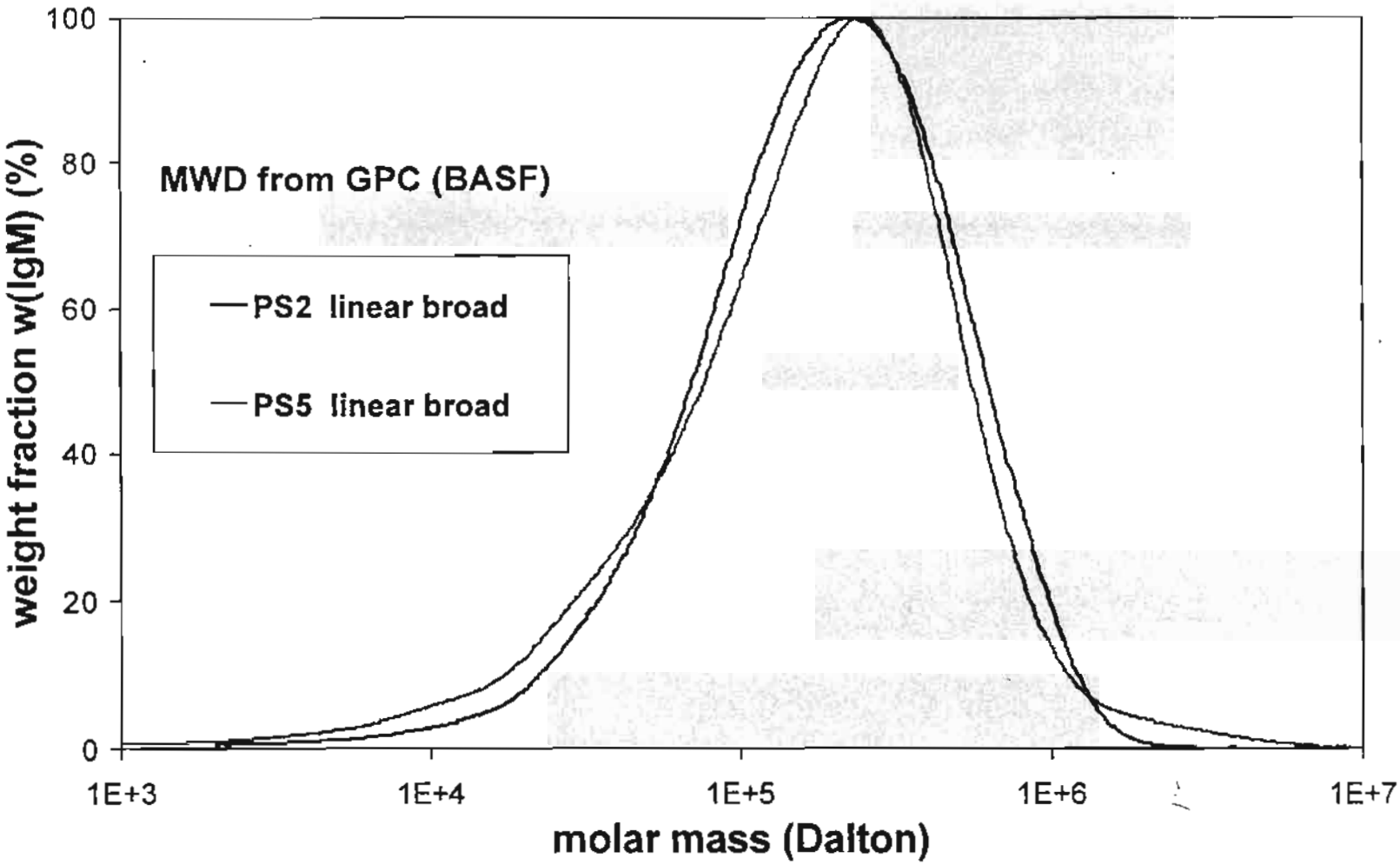
→ Deviation expressed by ratios

$M_{max}/(M_{max})_{ref}$ $(M_2/M_1)/(M_2/M_1)_{ref}$

Preliminary review of reverse predictive quality

	absolute (kD)			ratio	
	M_1	M_{max}	M_2	M_{max}	breadth
• BASF GPC	76.6	243	557		
• Carrot	28.3	168	517	0.69	2.5
• Likhtman	89.8	222	448	0.91	0.69
• Pattamaprom	65.5	200	610	0.82	1.28
• Ruymbeke	99.8	229	437	0.94	0.60
• Schulze (bimodal)	162	216	300	0.89	0.25

Comparison of PS2 and PS5 MWD

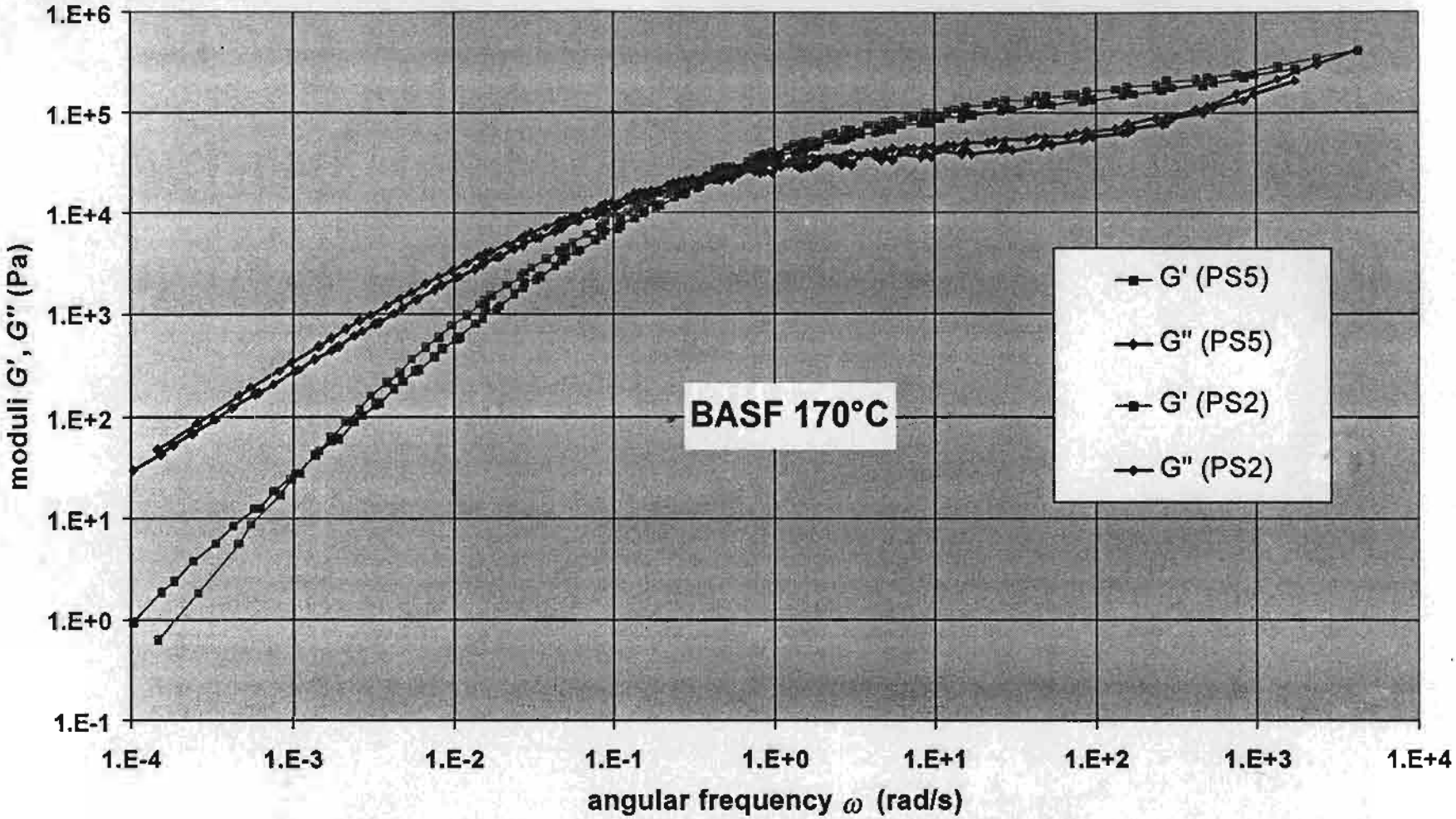


Parameters of the MWD für PS2 and PS5

- BASF GPC using Refractive Index (RI) detector

	PS2	PS5
M_n (kD)	101	69.5
M_w (kD)	274	290
M_z (kD)	500	885
M_w/M_n	2.72	4.17
M_z/M_w	1.82	3.05
$[\eta]$ (mL/g)	96.7	97.3

Comparison of PS2 and PS5 moduli



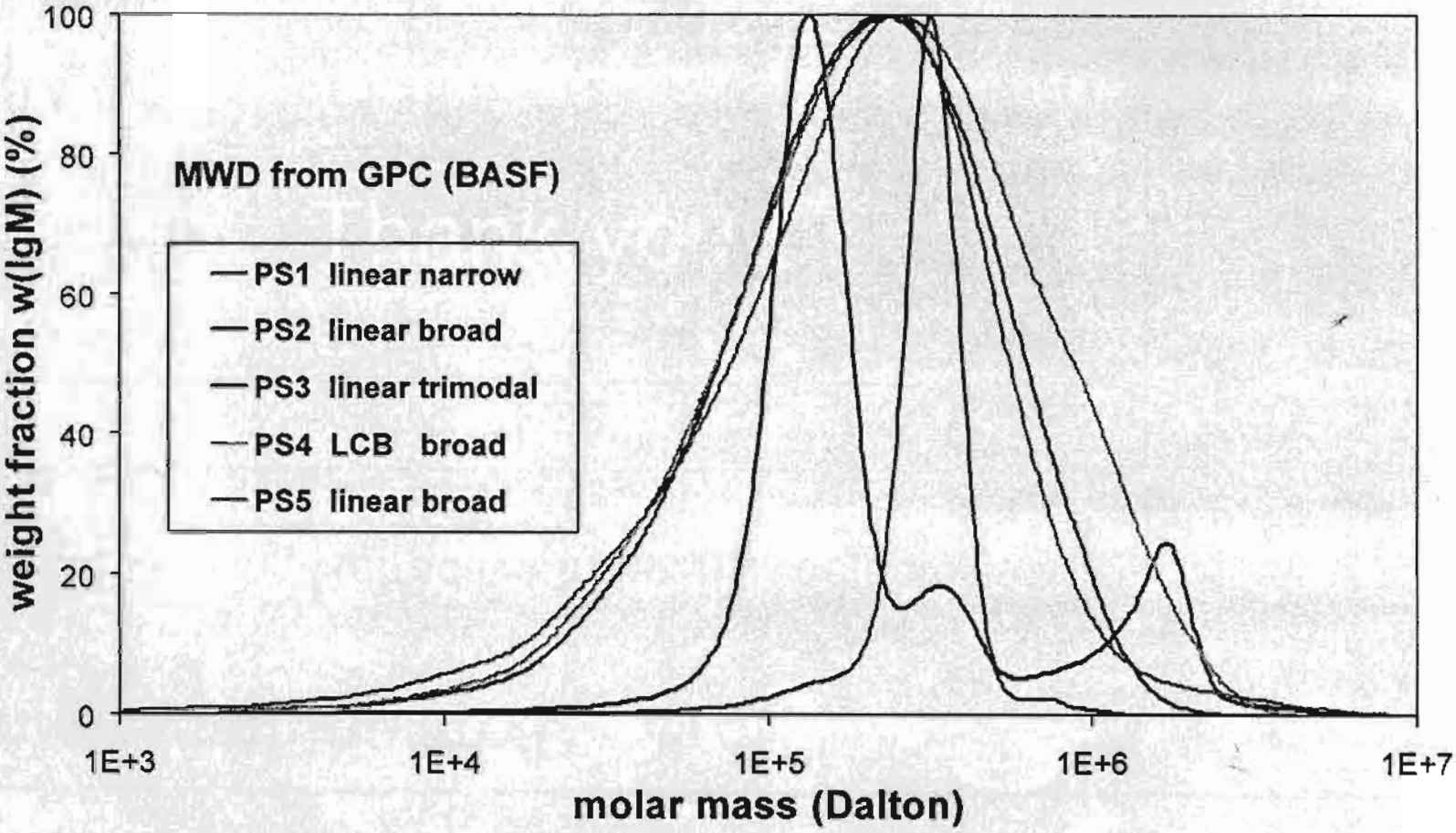
PS benchmark for direct and inverse linear viscoelasticity prediction

BASF

All samples

Samples

- 5 polystyrene samples from Dr. Christian Schade, BASF



Parameters of the MWD

- BASF GPC using Refractive Index (RI) detector

	PS1	PS2	PS3	PS4	PS5
M_n (kD)	270	101	143	107	69.5
M_w (kD)	320	274	407	370	290
M_z (kD)	355	500	1265	820	885
M_w/M_n	1.18	2.72	2.83	3.47	4.17
M_z/M_w	1.11	1.82	3.11	2.22	3.05
$[\eta]$ (mL/g)	115	96.7	120	117	97.3

Thank you !