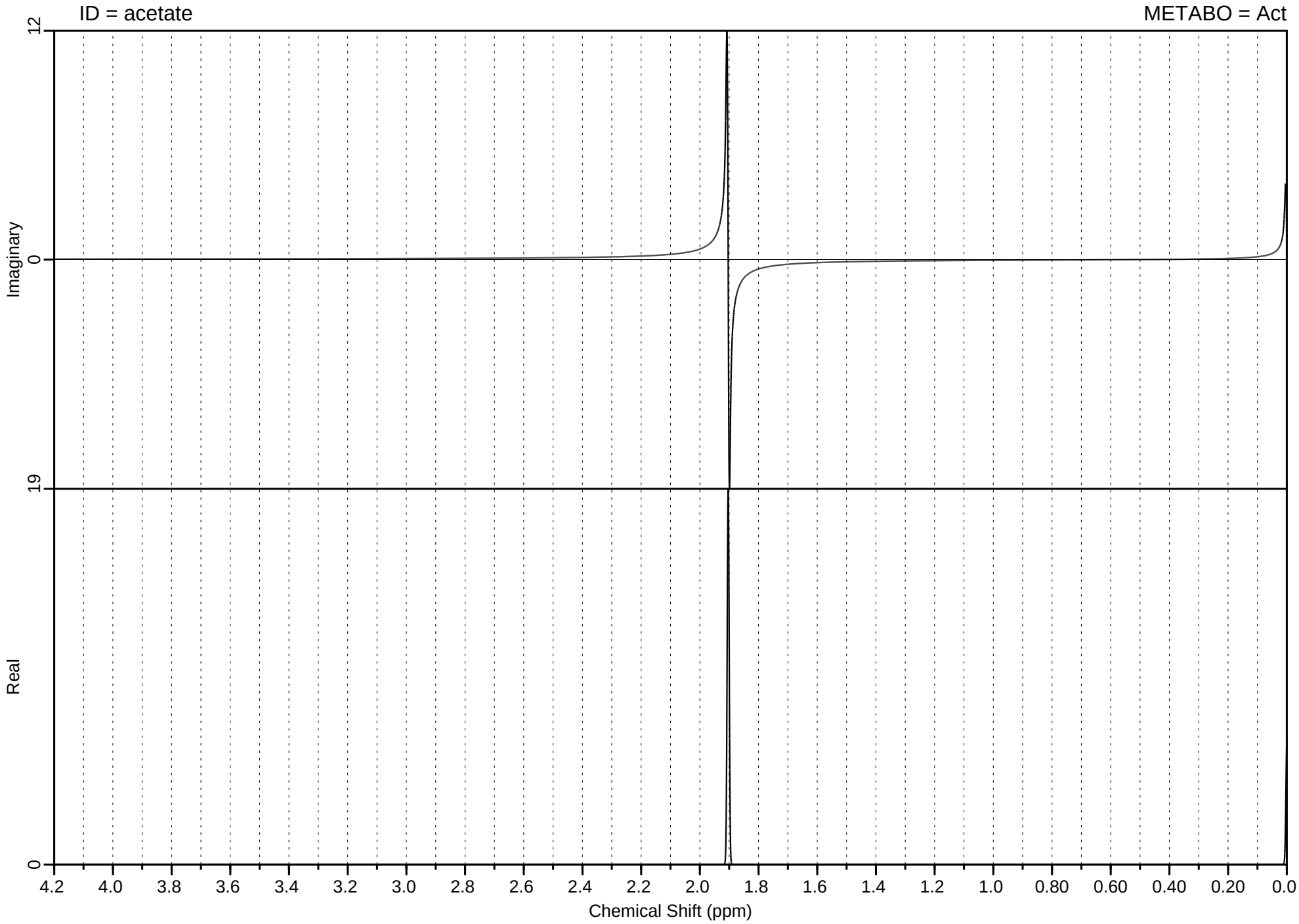
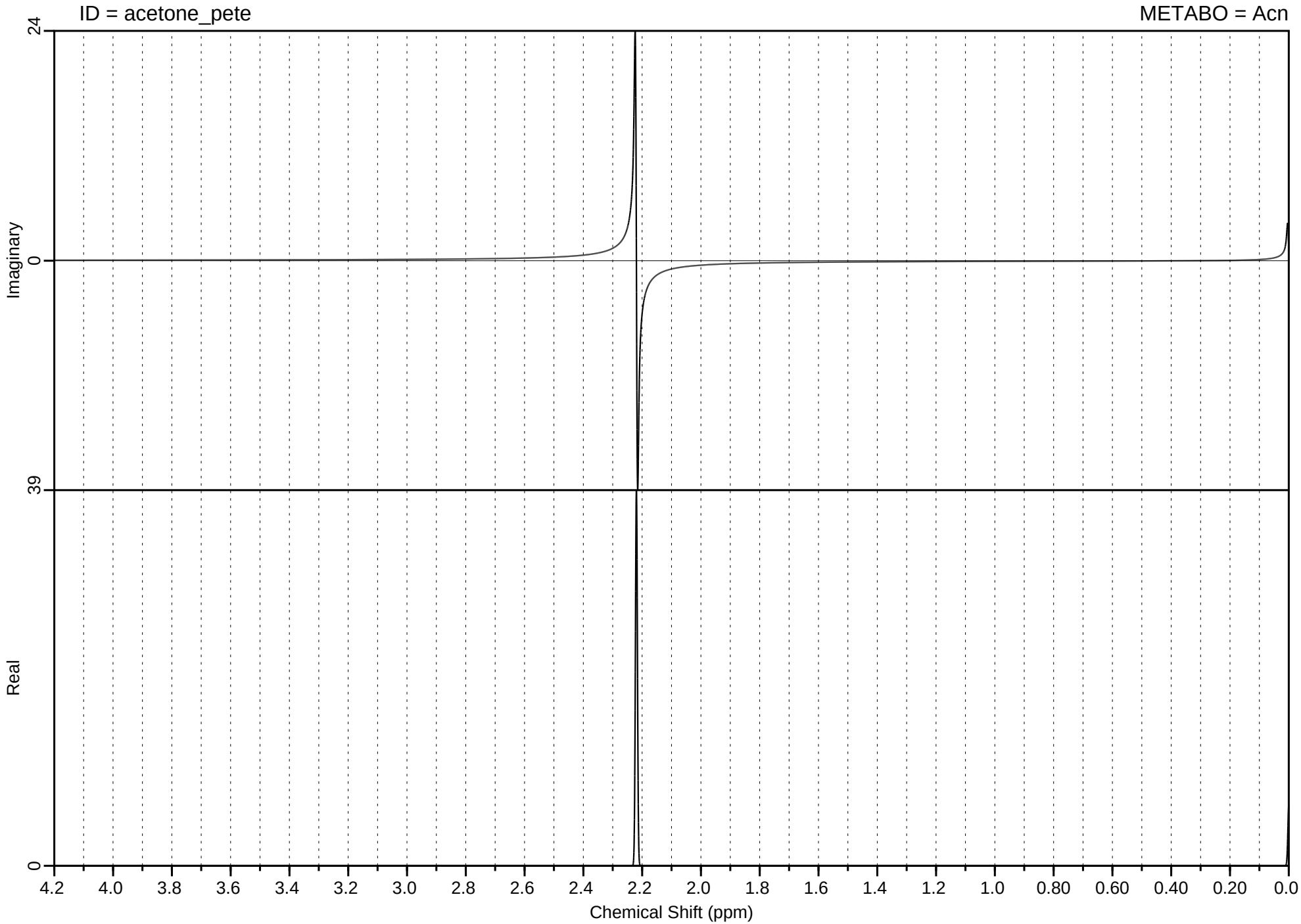
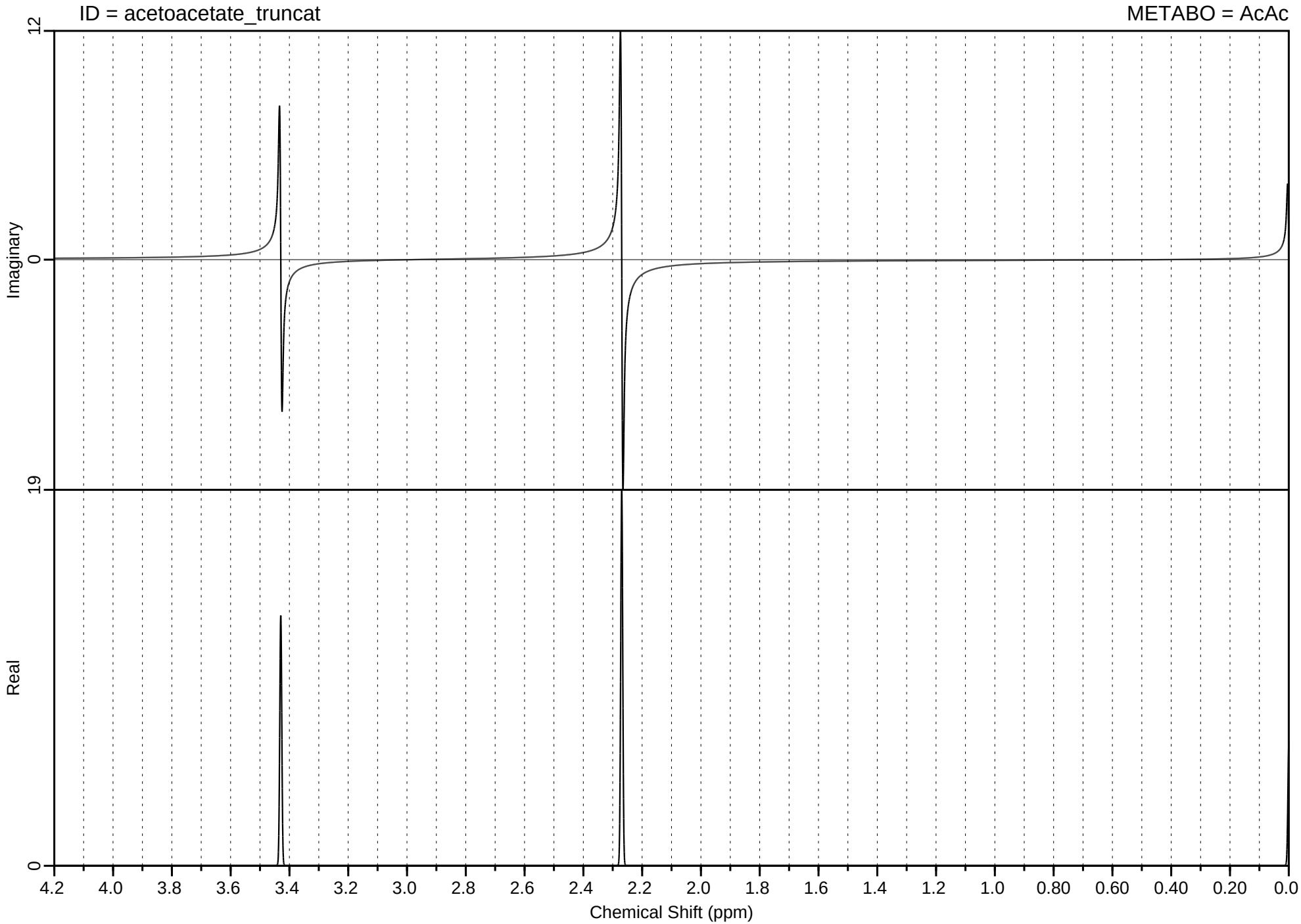
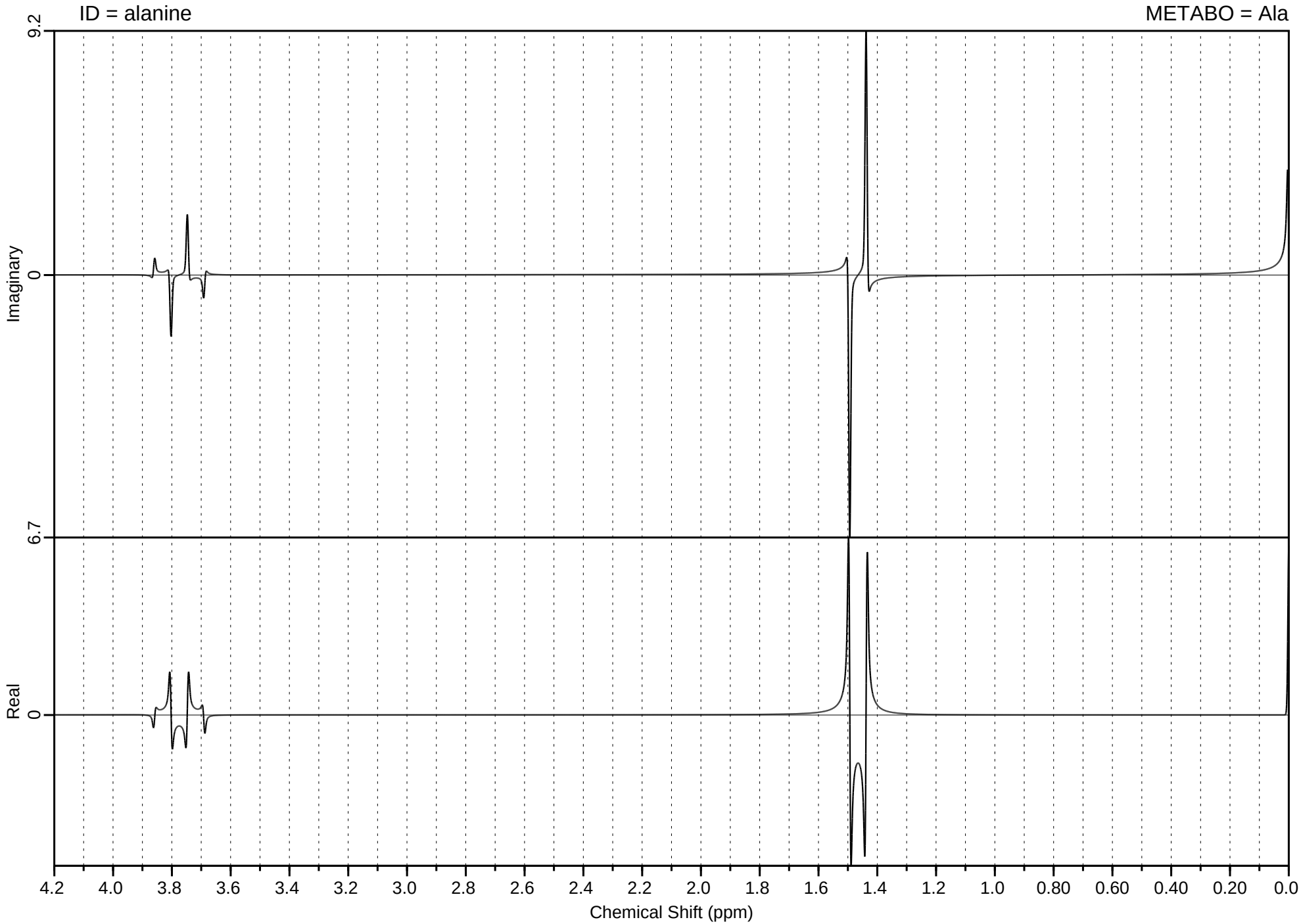
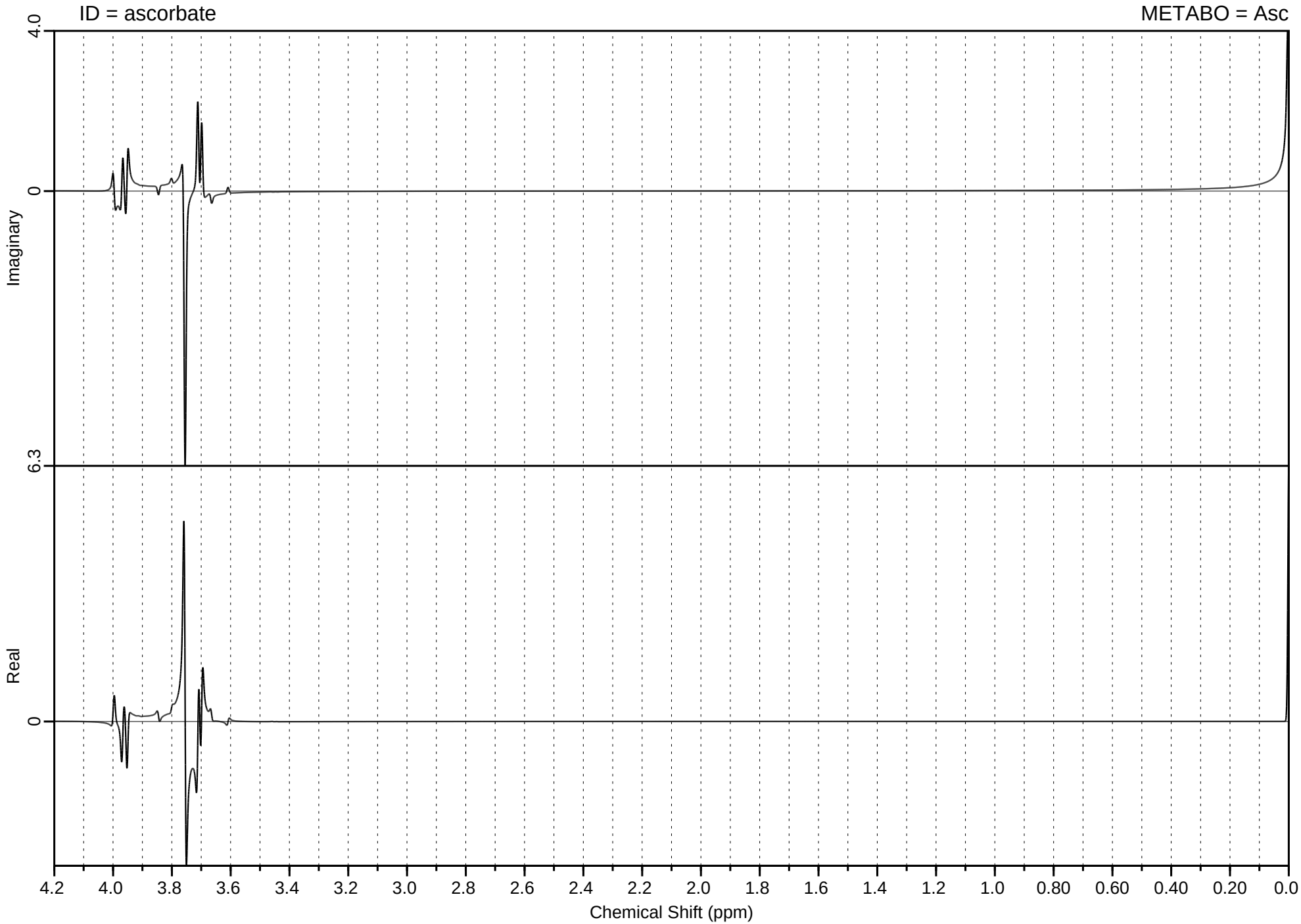
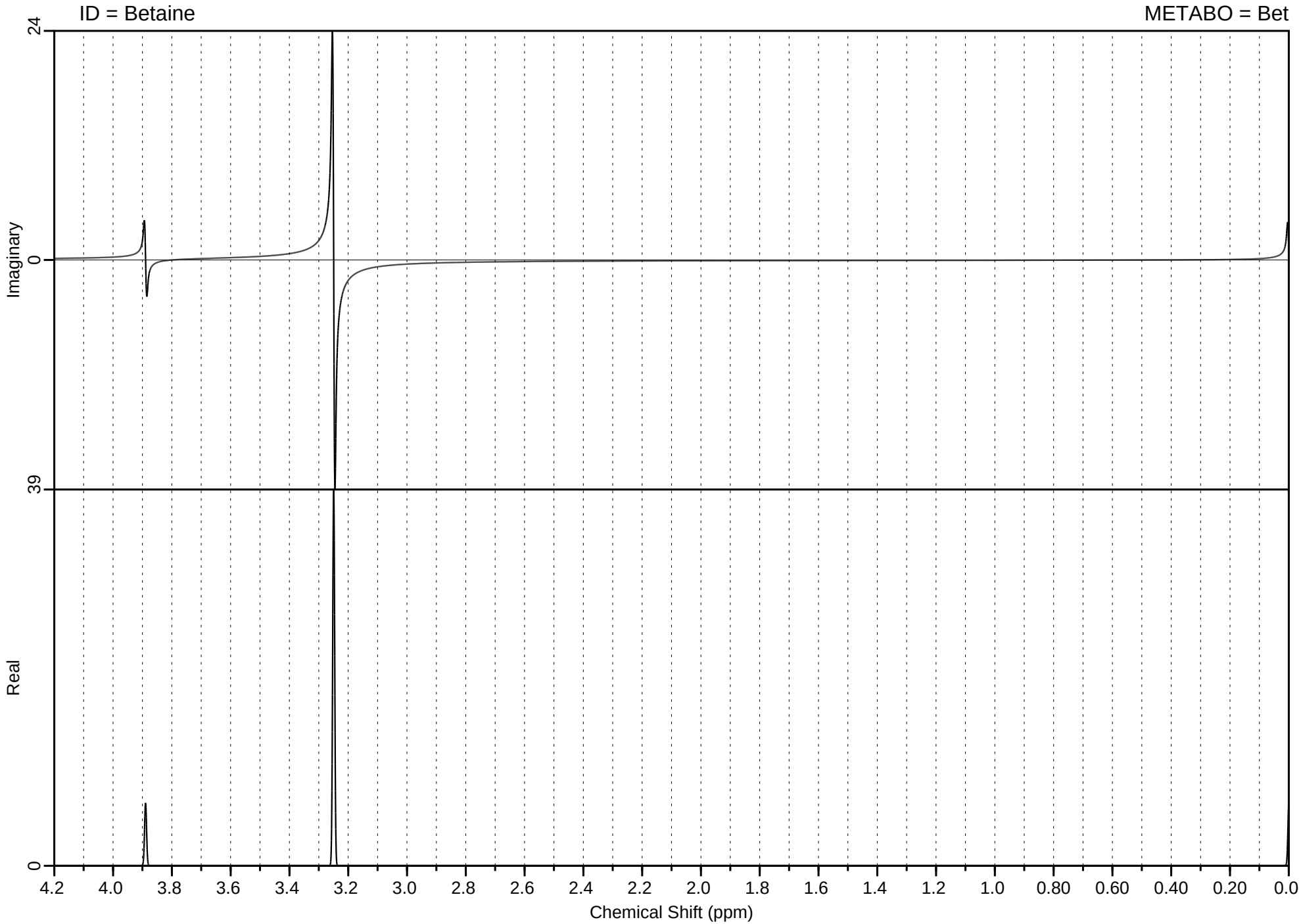

ID = acetate
METABO = Act
12
Imaginary
0
19
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

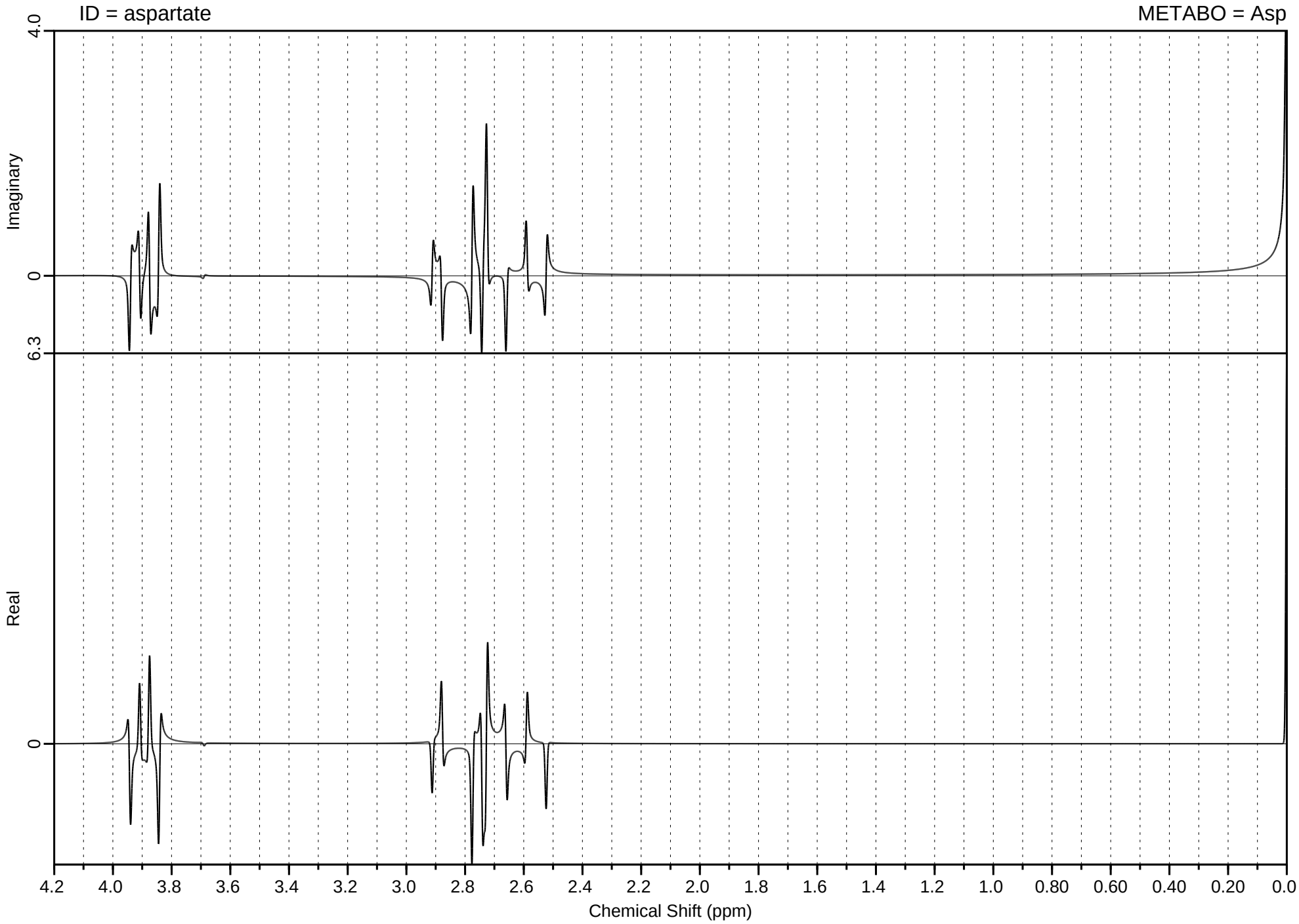

ID = acetone_pete
METABO = Acn
Imaginary
Real
24
0
39
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

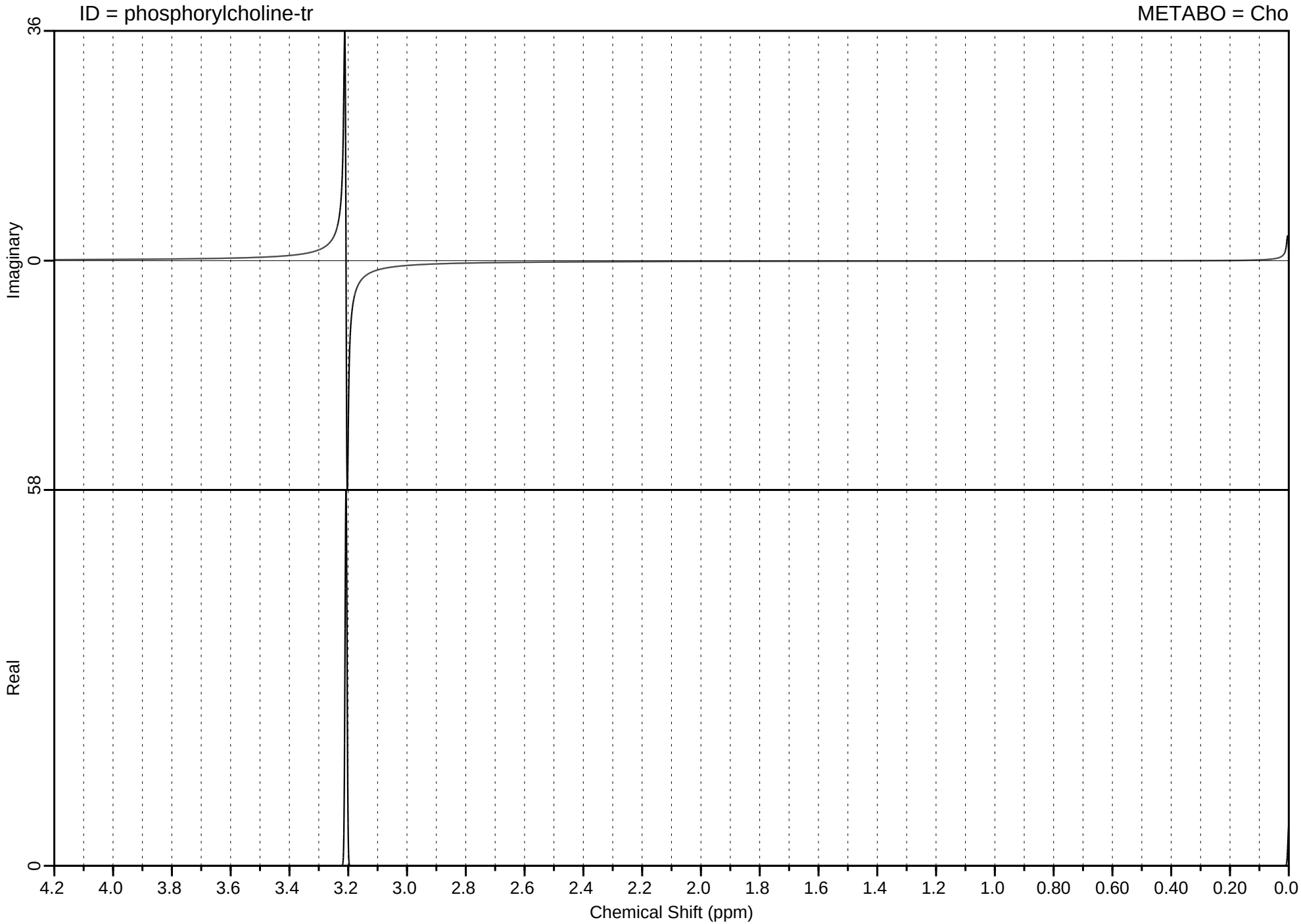

ID = acetoacetate_truncat
METABO = AcAc
Imaginary
Real
12
0
19
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

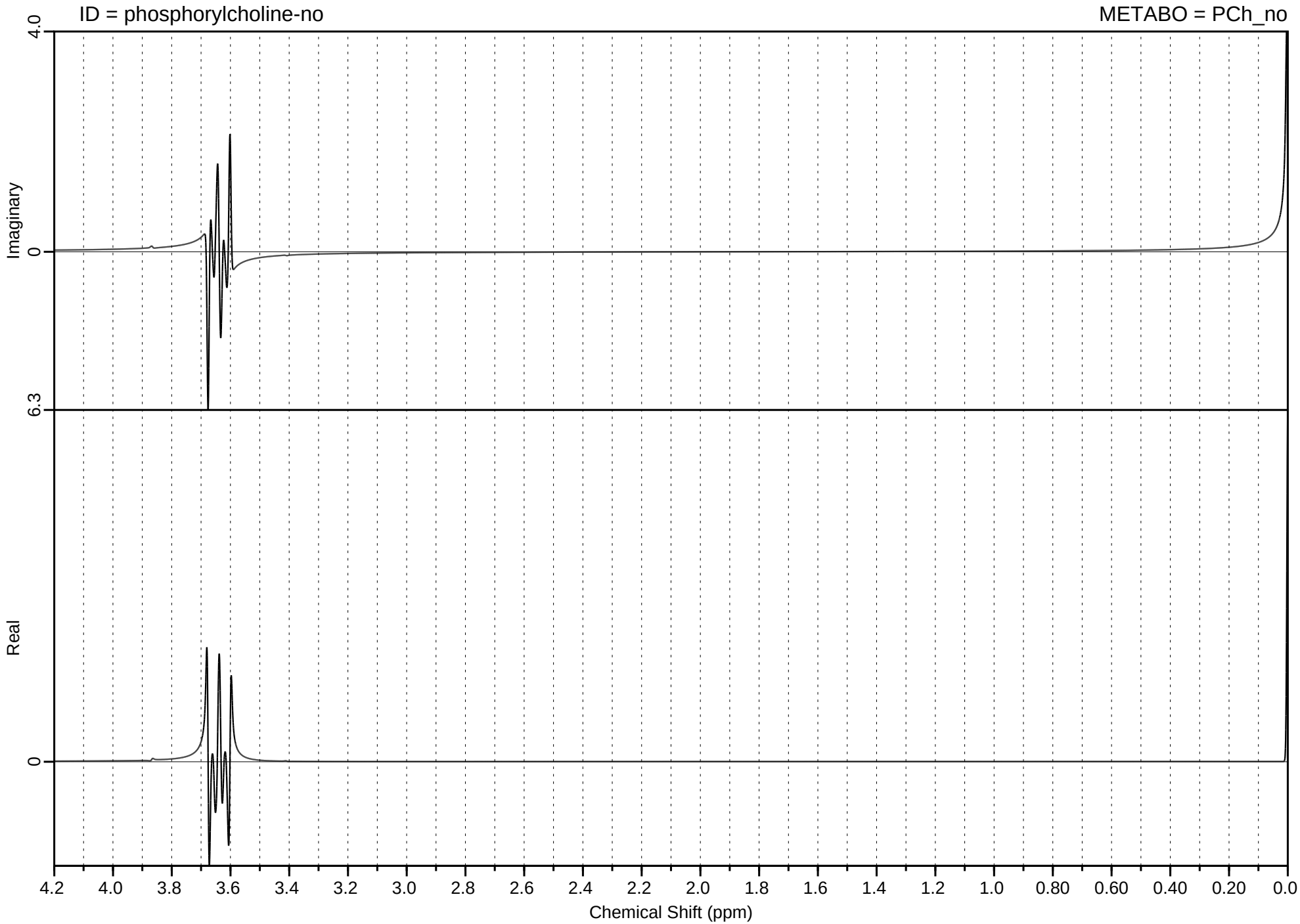

ID = alanine
METABO = Ala
9.2
Imaginary
0
6.7
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

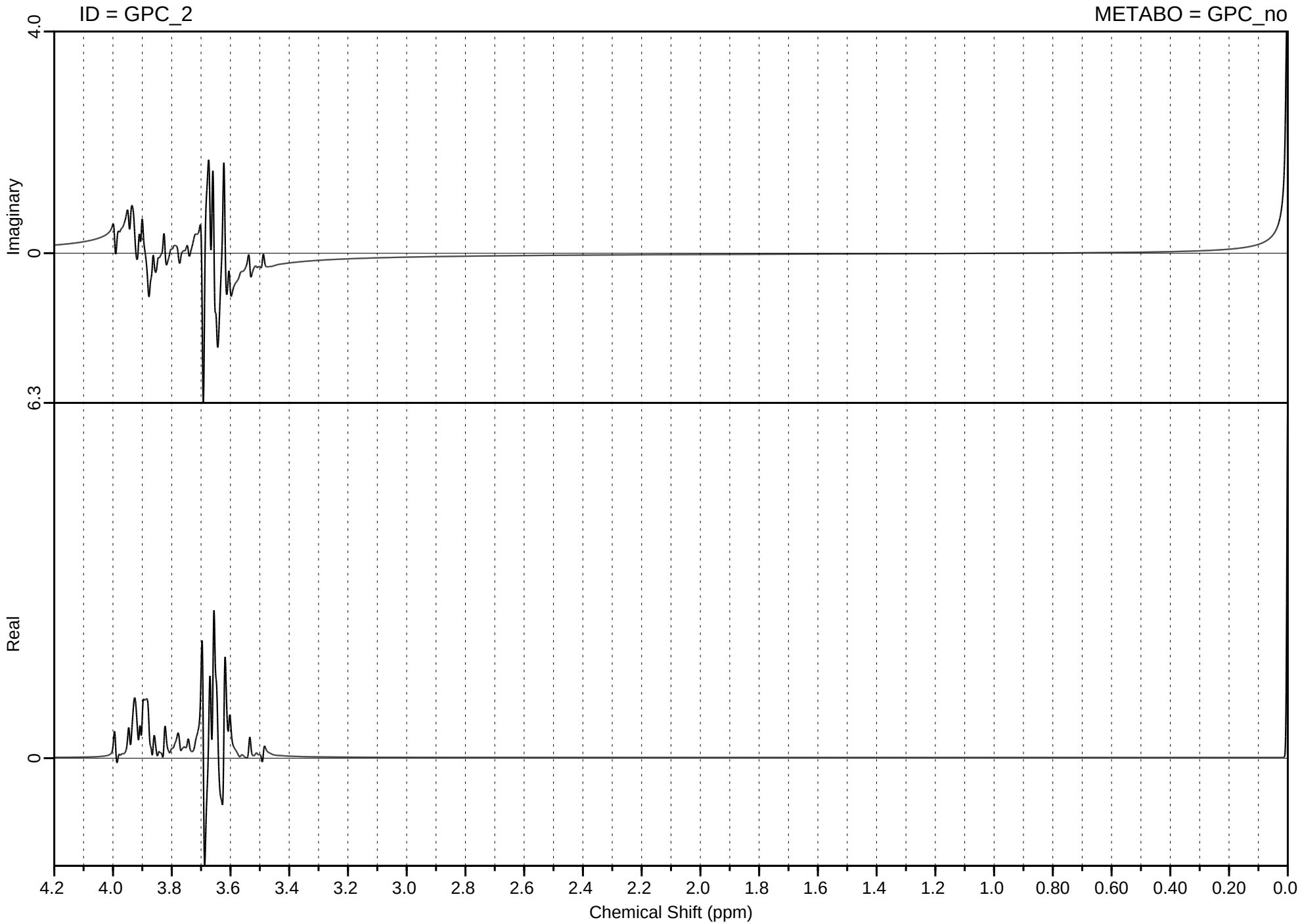

ID = ascorbate
METABO = Asc
4.0
0
Imaginary
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

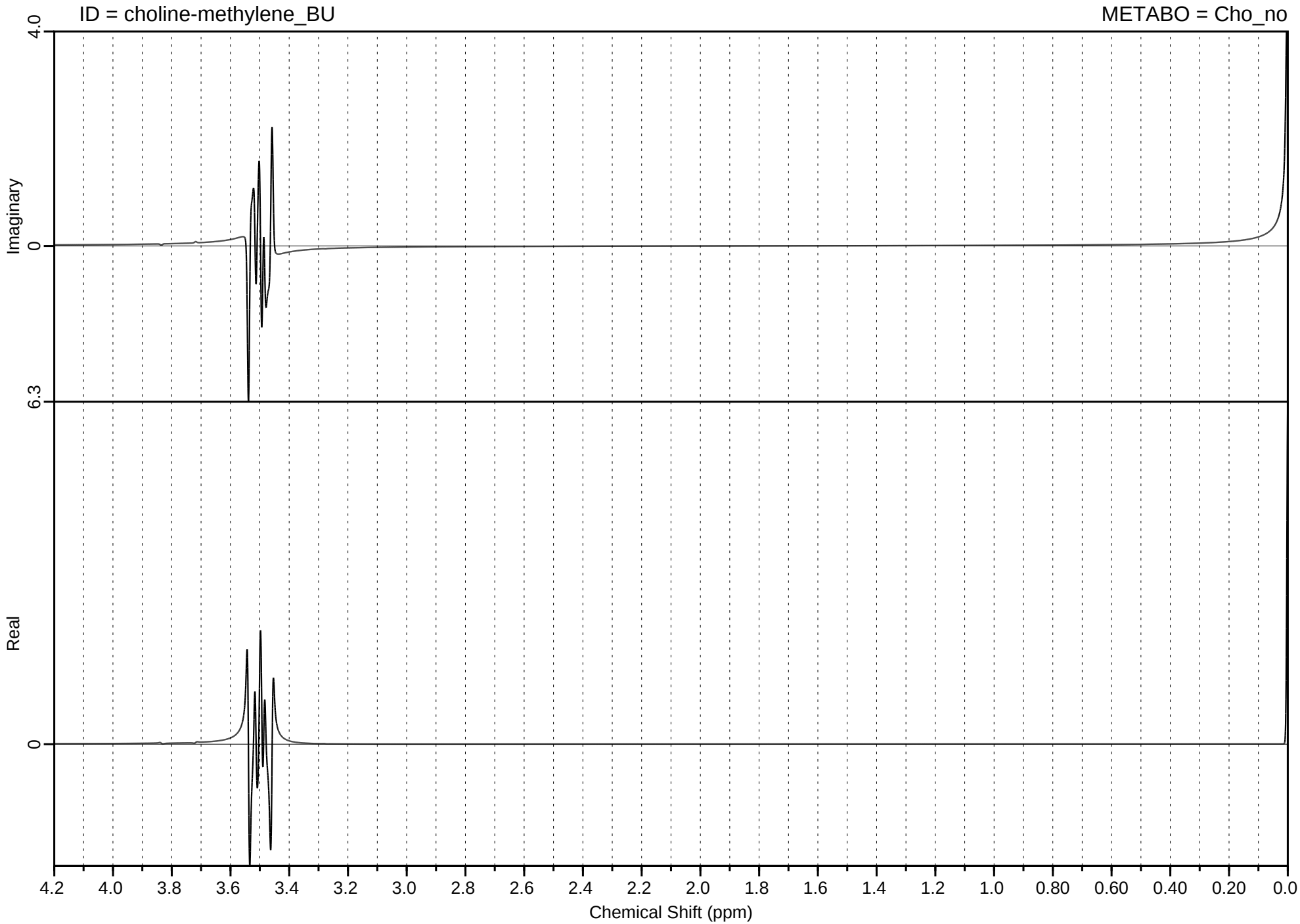

ID = Betaine
METABO = Bet
Imaginary
Real
24
0
39
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

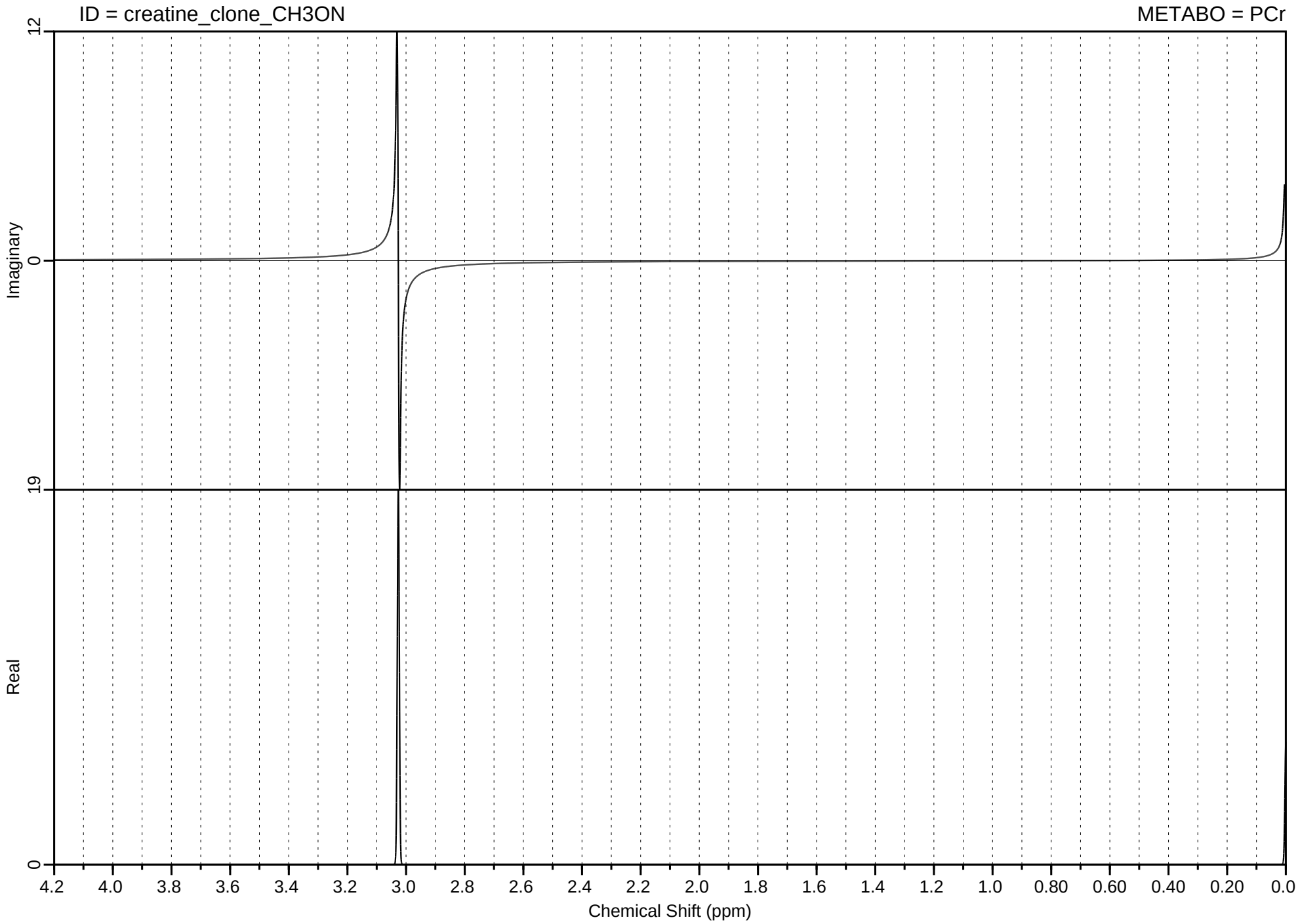

ID = aspartate
METABO = Asp
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

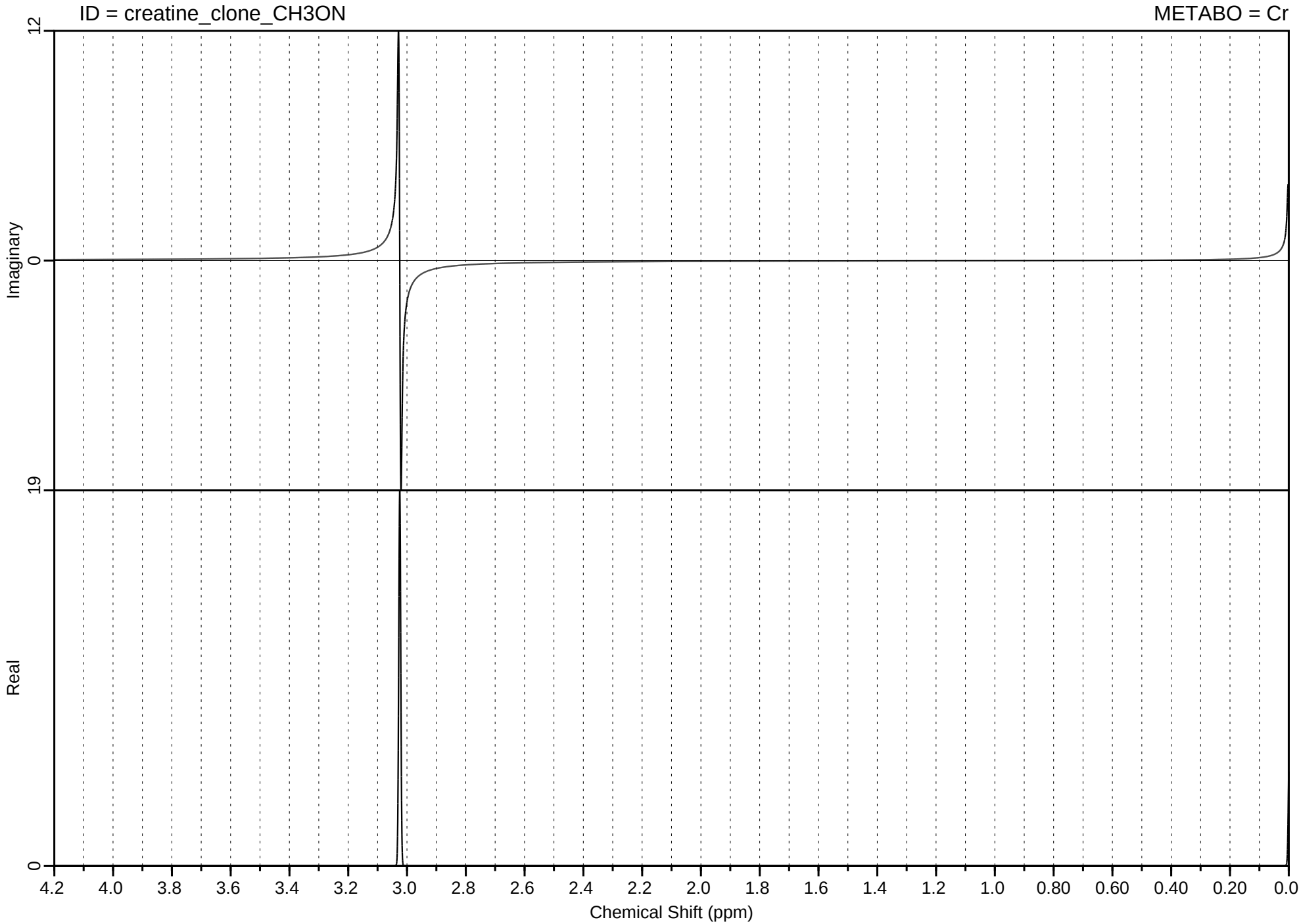

ID = phosphorylcholine-tr
METABO = Cho
36
0
Imaginary
58
0
Real
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

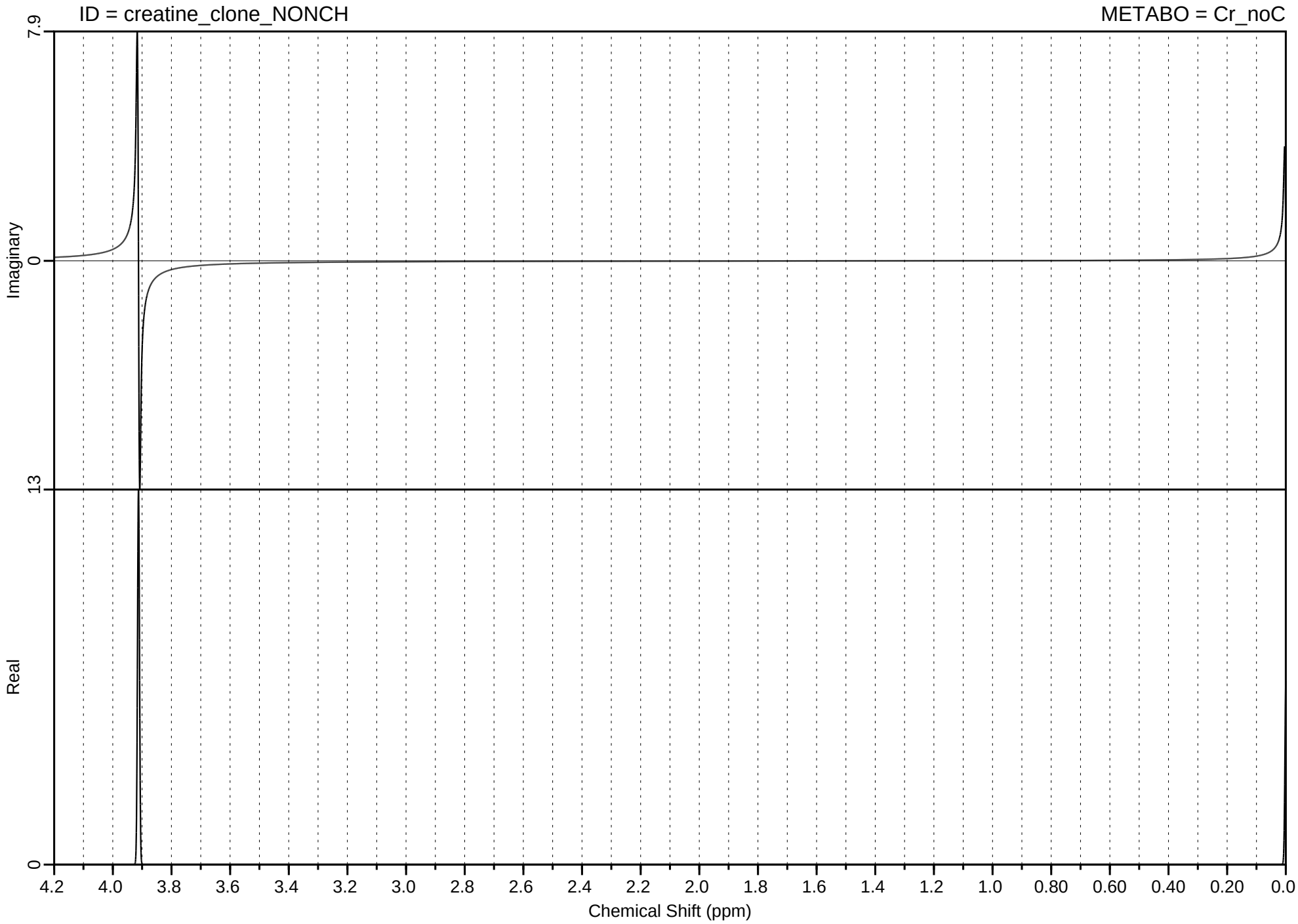

ID = phosphorylcholine-no
METABO = PCh_no
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

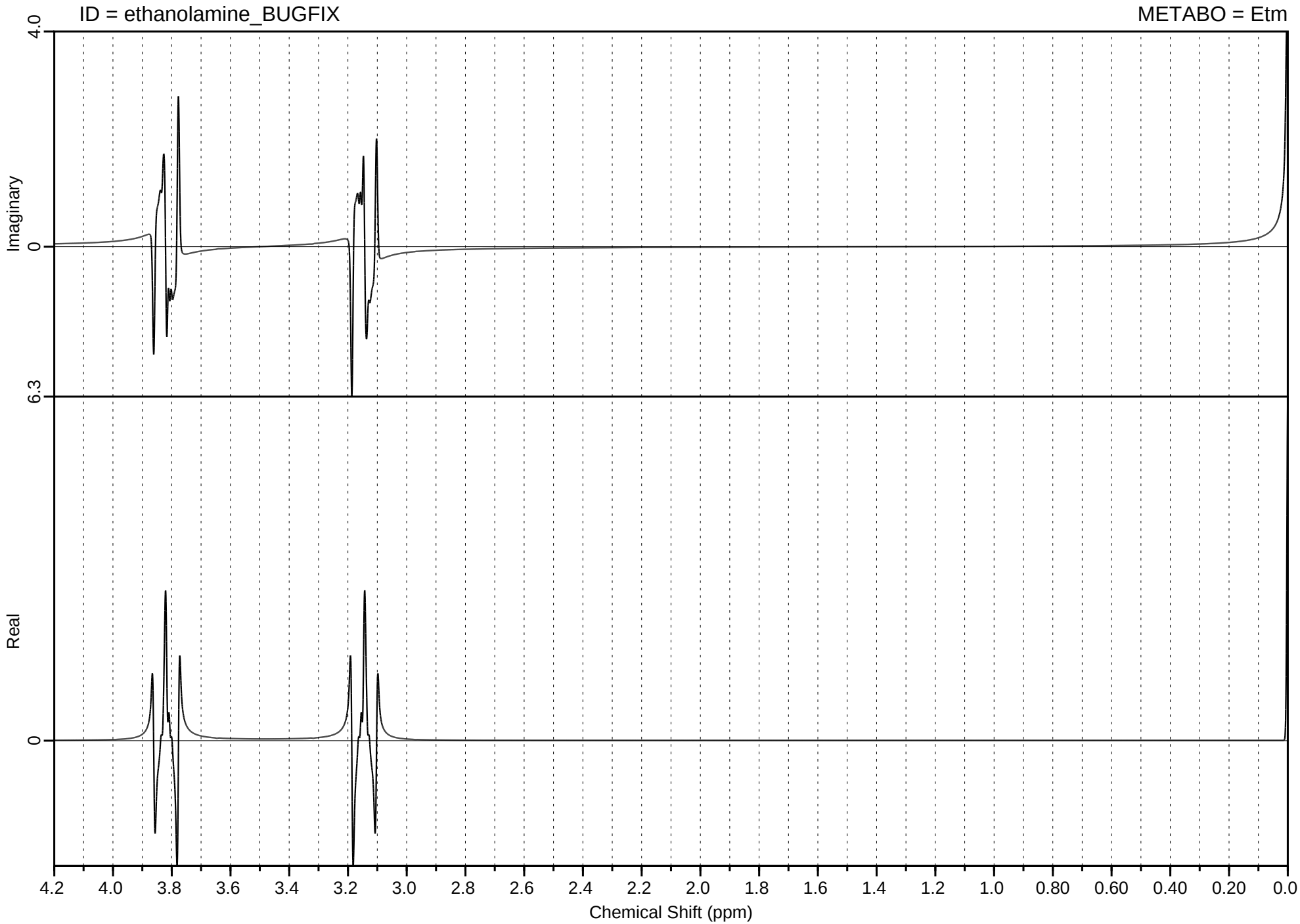

ID = GPC_2
METABO = GPC_no
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

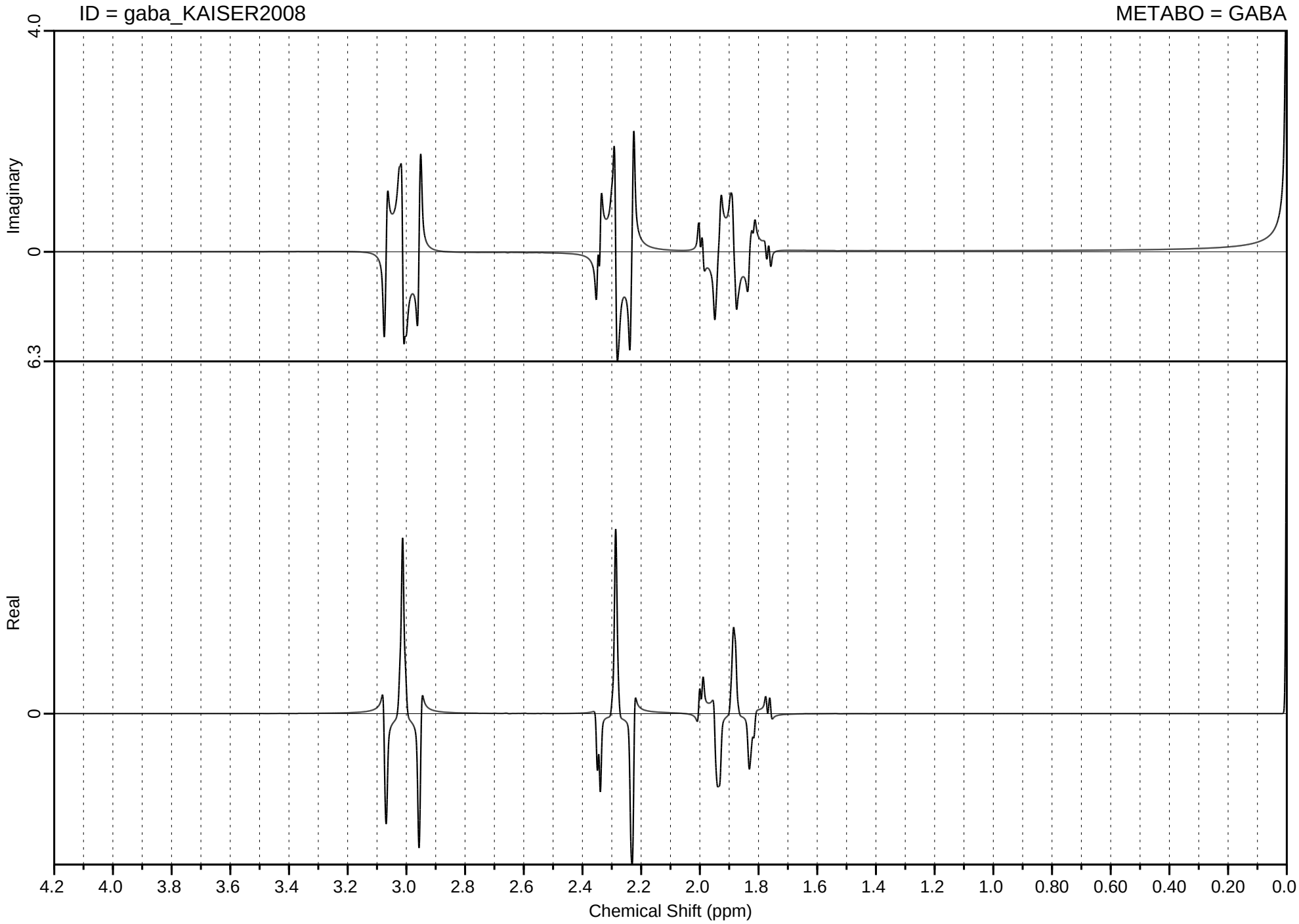

ID = choline-methylene_BU
METABO = Cho_no
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

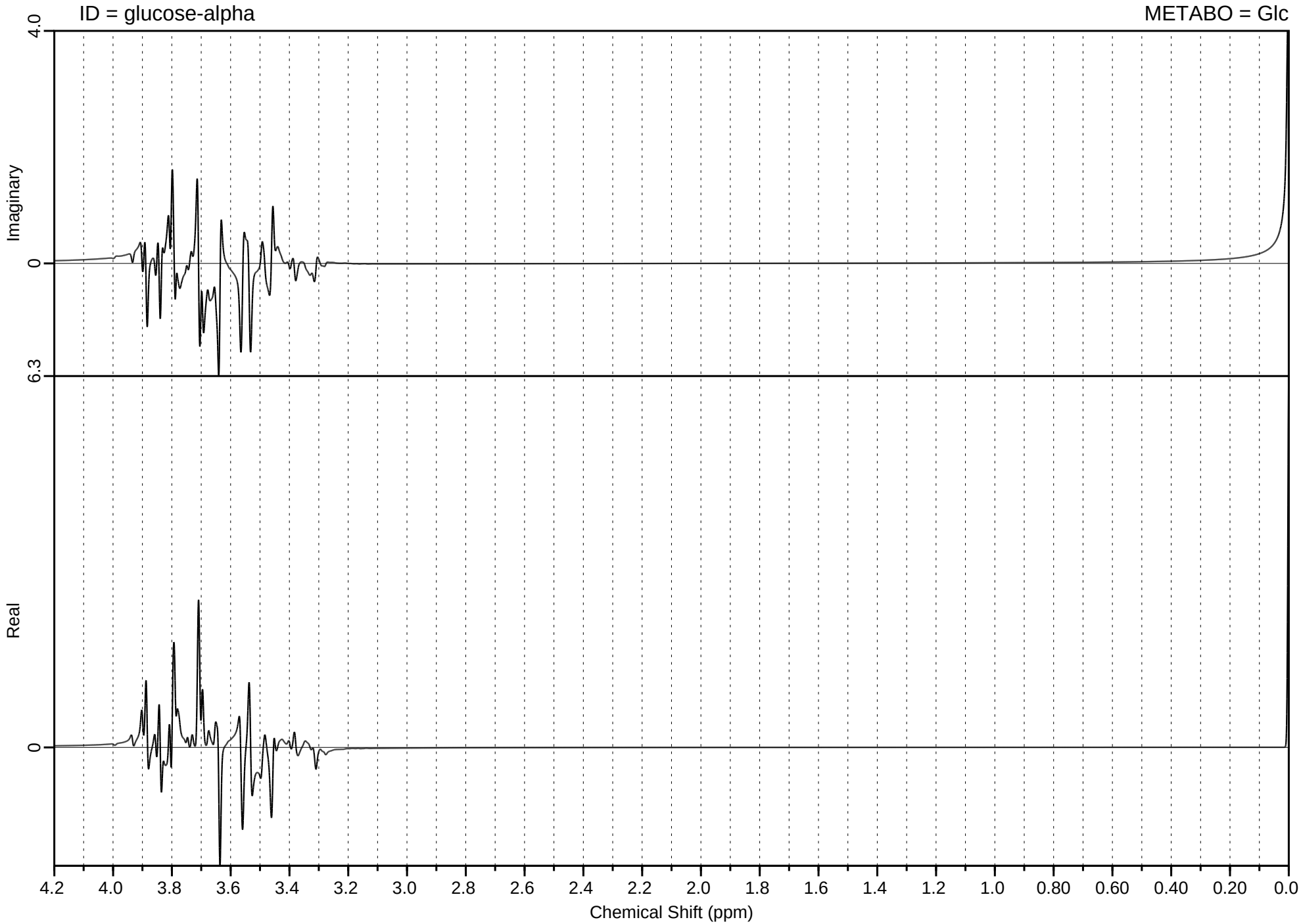

ID = creatine_clone_CH3ON
METABO = PCr
Imaginary
Real
12
0
19
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

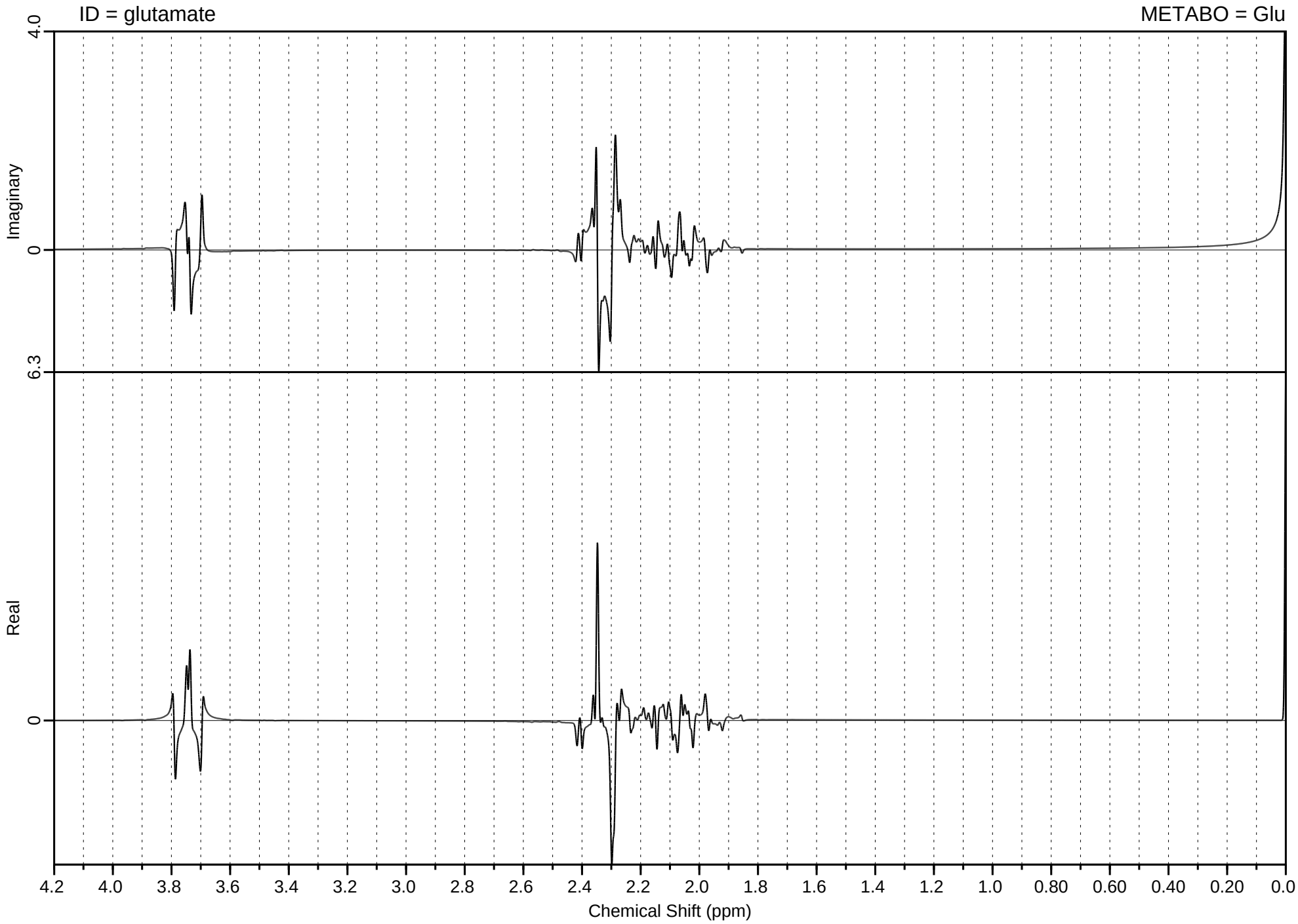

ID = creatine_clone_CH3ON
METABO = Cr
12
0
Imaginary
19
0
Real
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

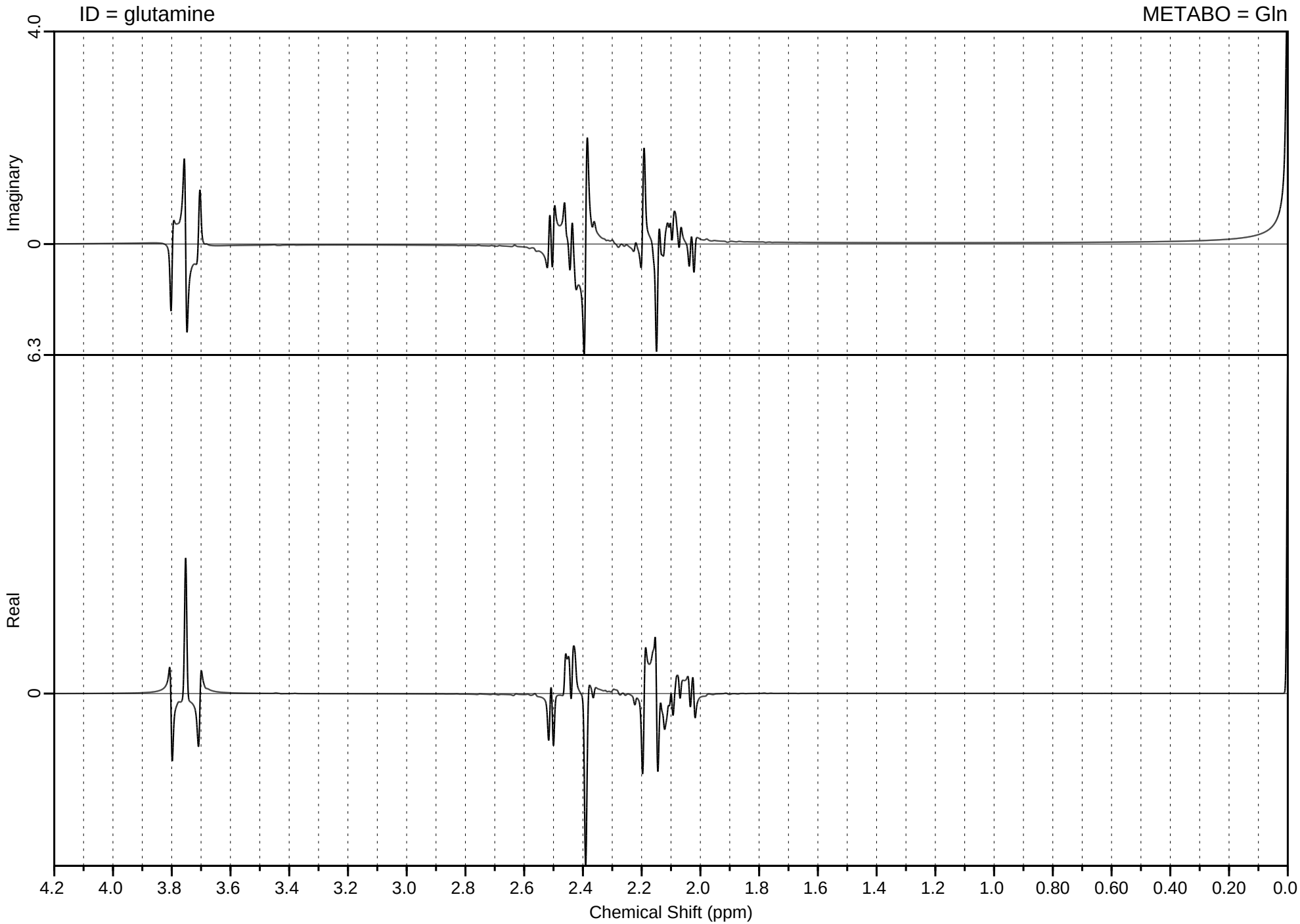

ID = creatine_clone_NONCH
METABO = Cr_noC
7.9
0
Imaginary
13
0
Real
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

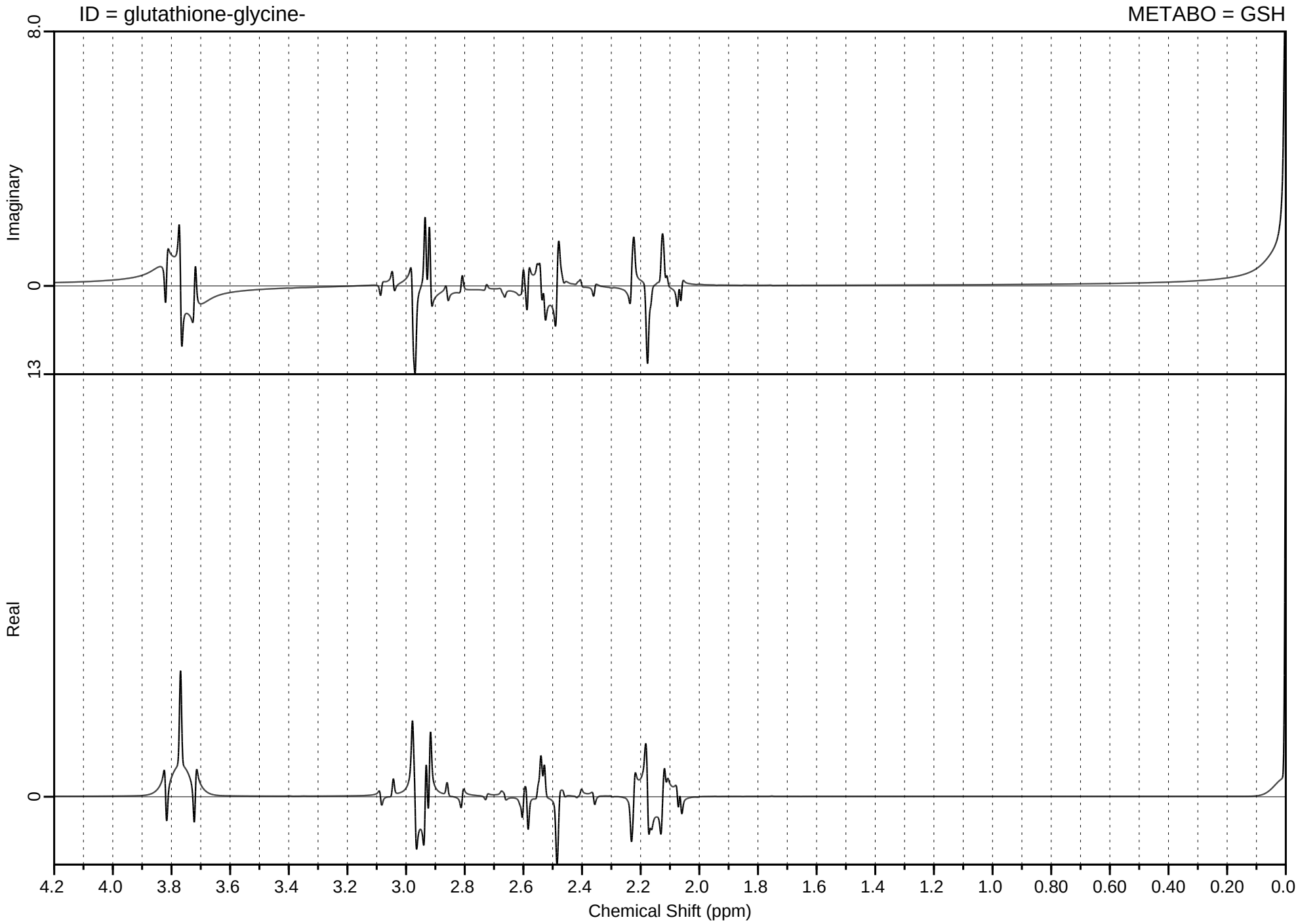

ID = ethanolamine_BUGFIX
METABO = Etm
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

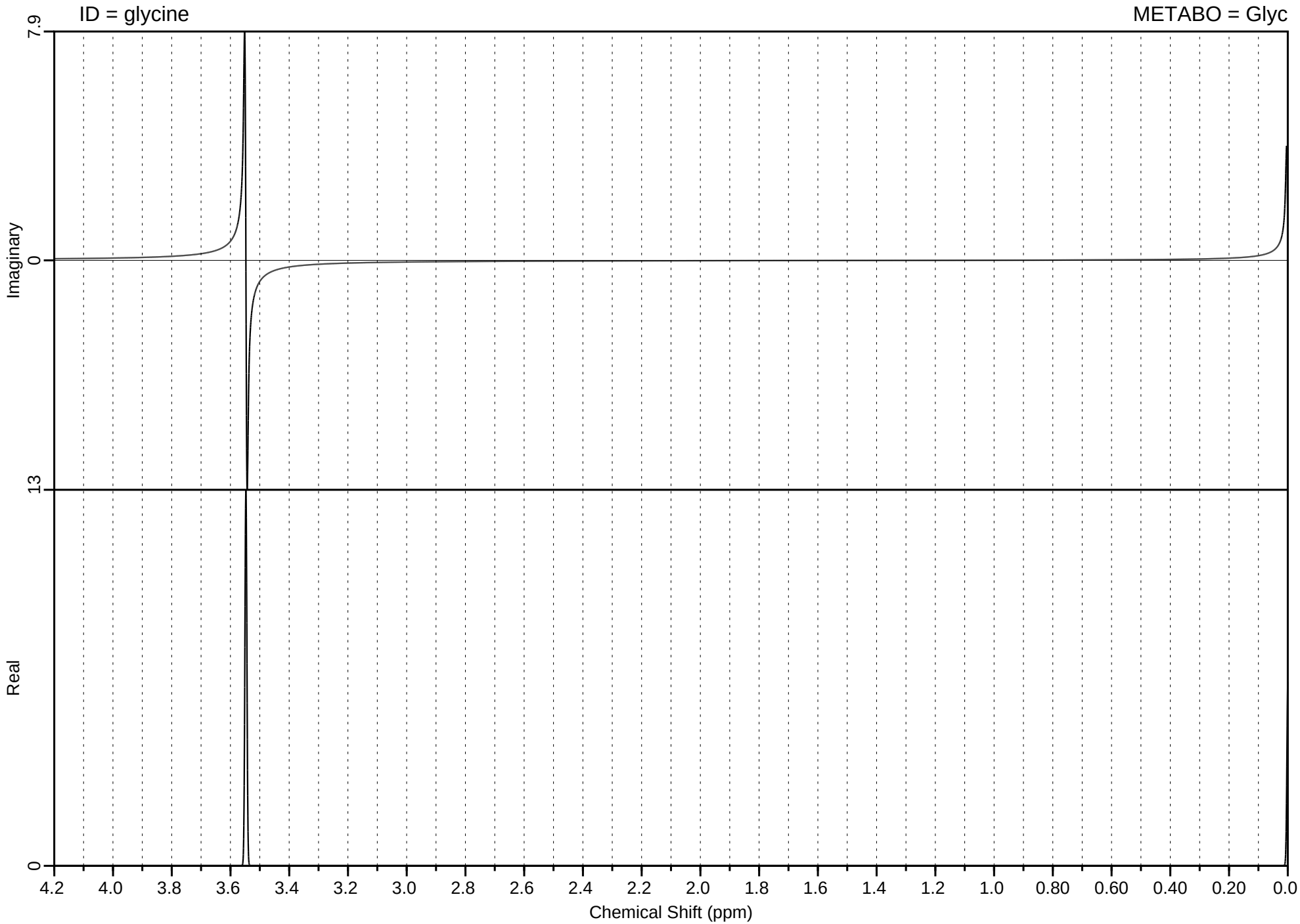

ID = gaba_KAISER2008
METABO = GABA
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

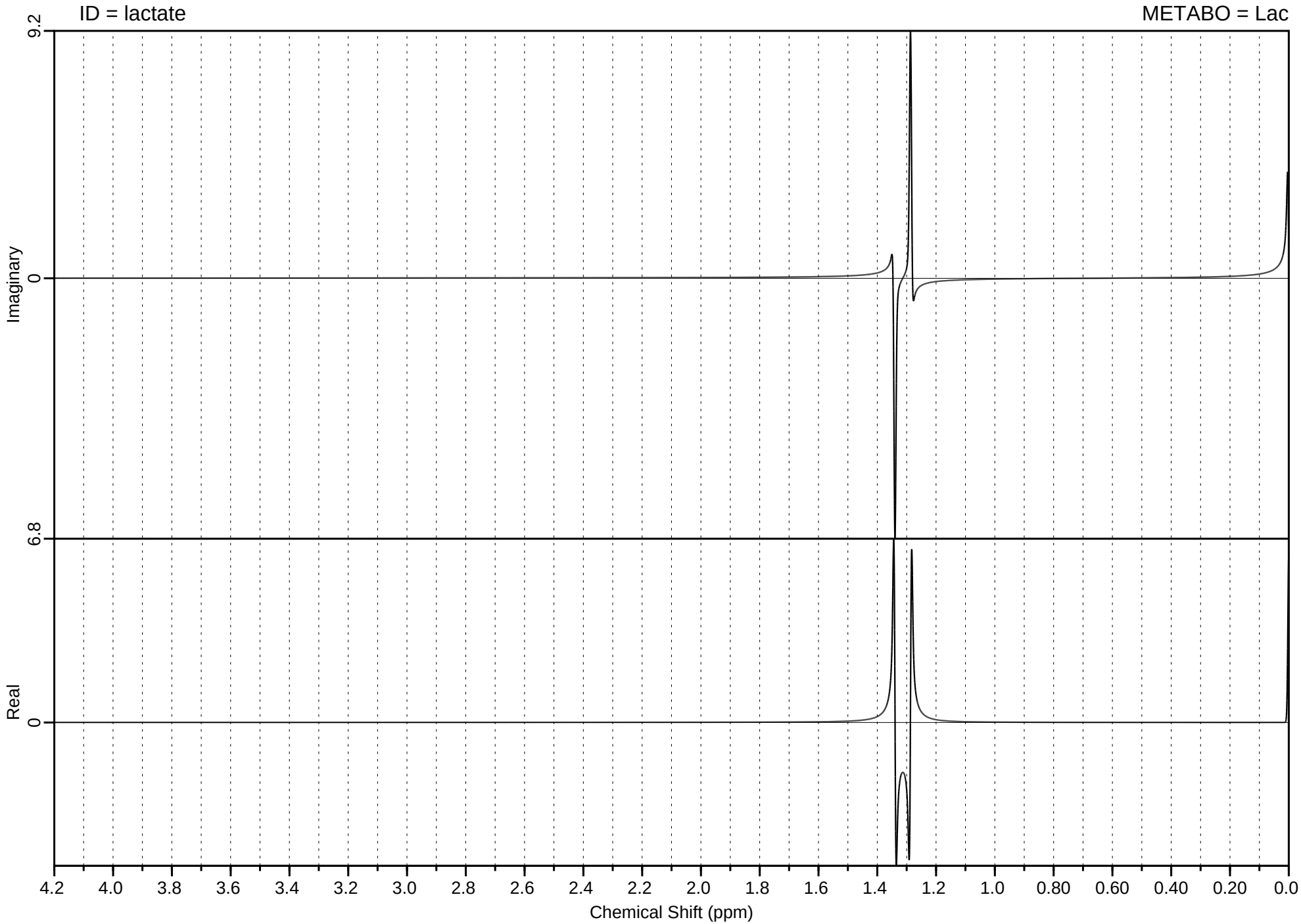

ID = glucose-alpha
METABO = Glc
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

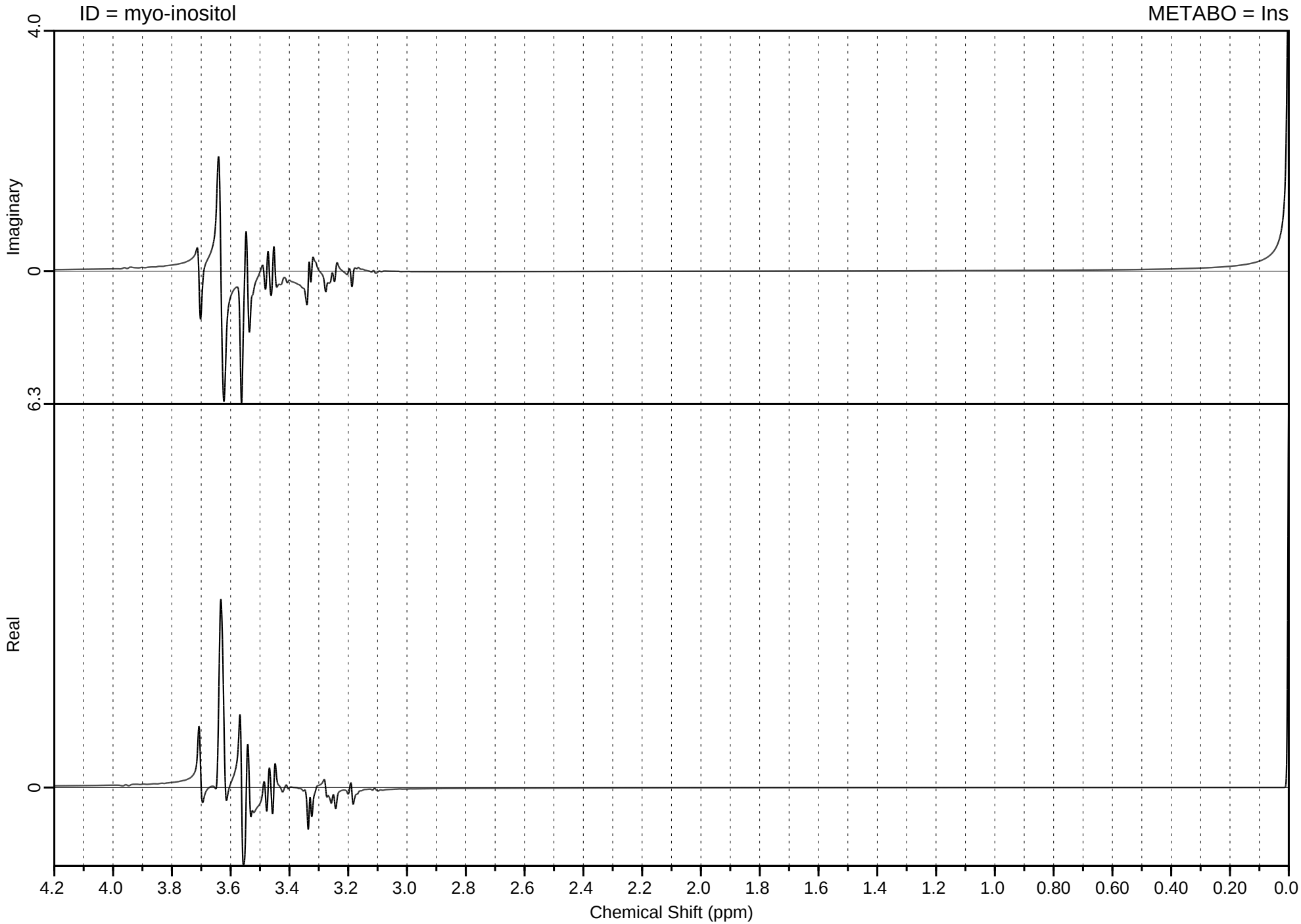

ID = glutamate
METABO = Glu
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

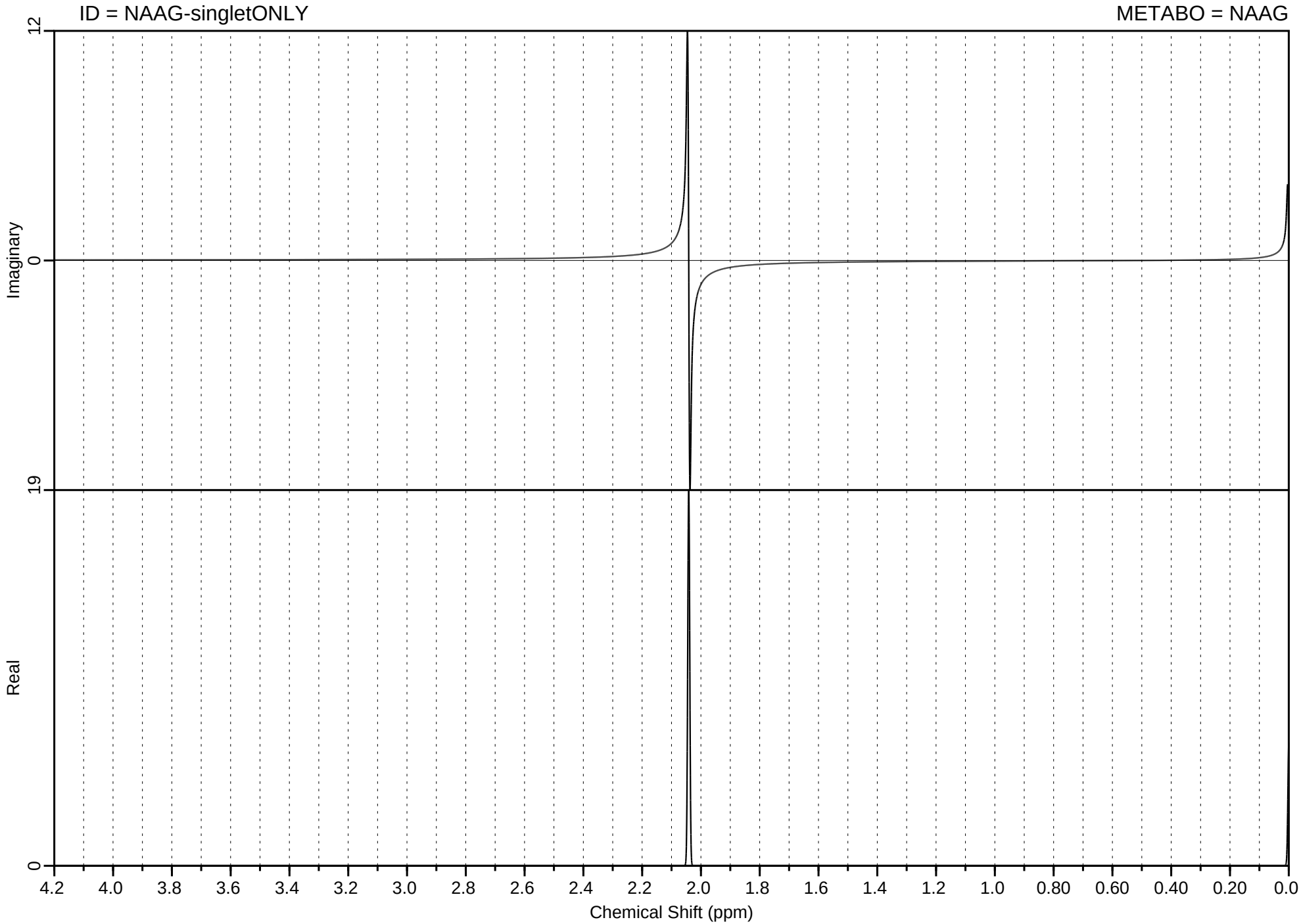

ID = glutamine
METABO = Gln
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

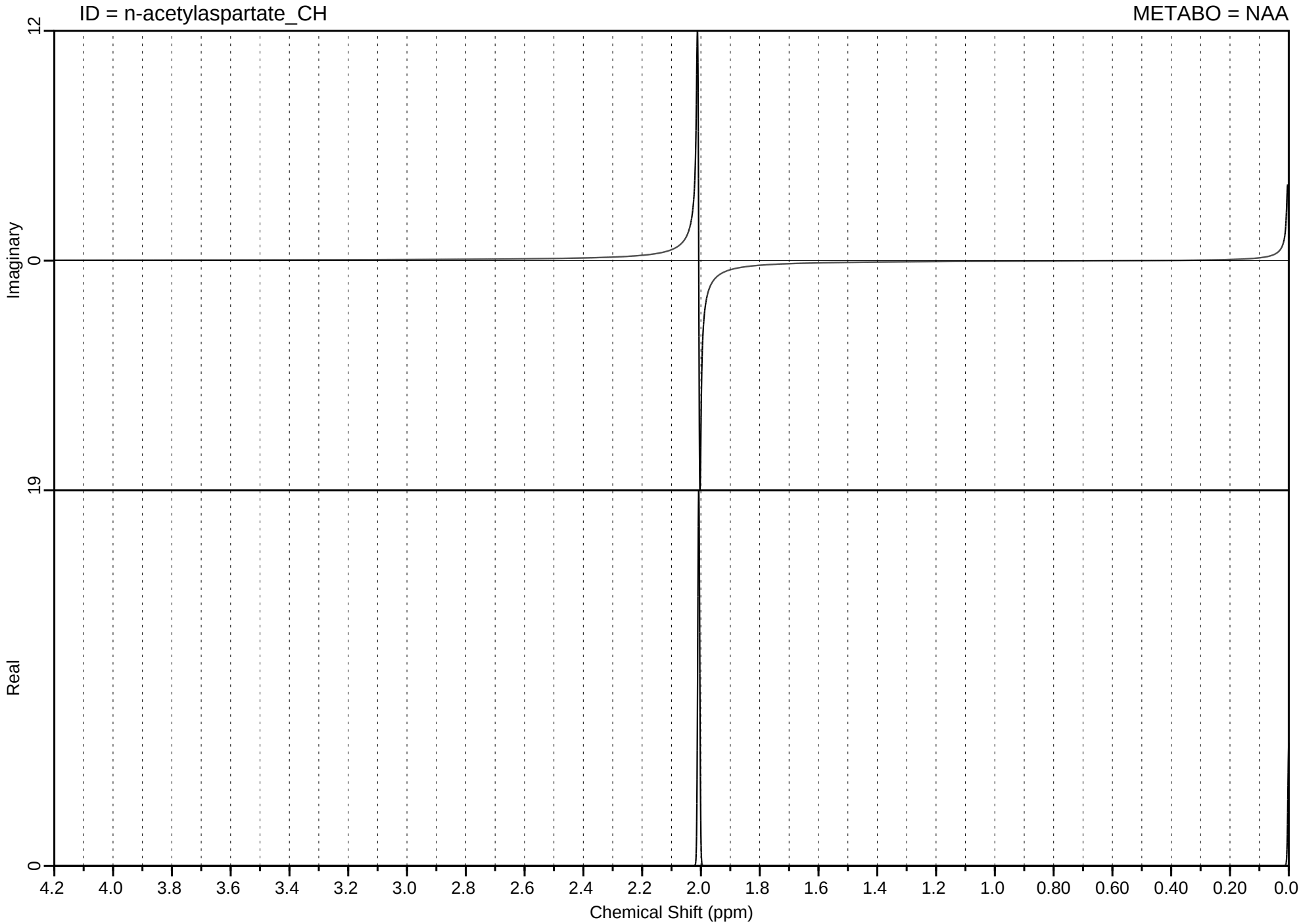

ID = glutathione-glycine-
METABO = GSH
8.0
Imaginary
0
13
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

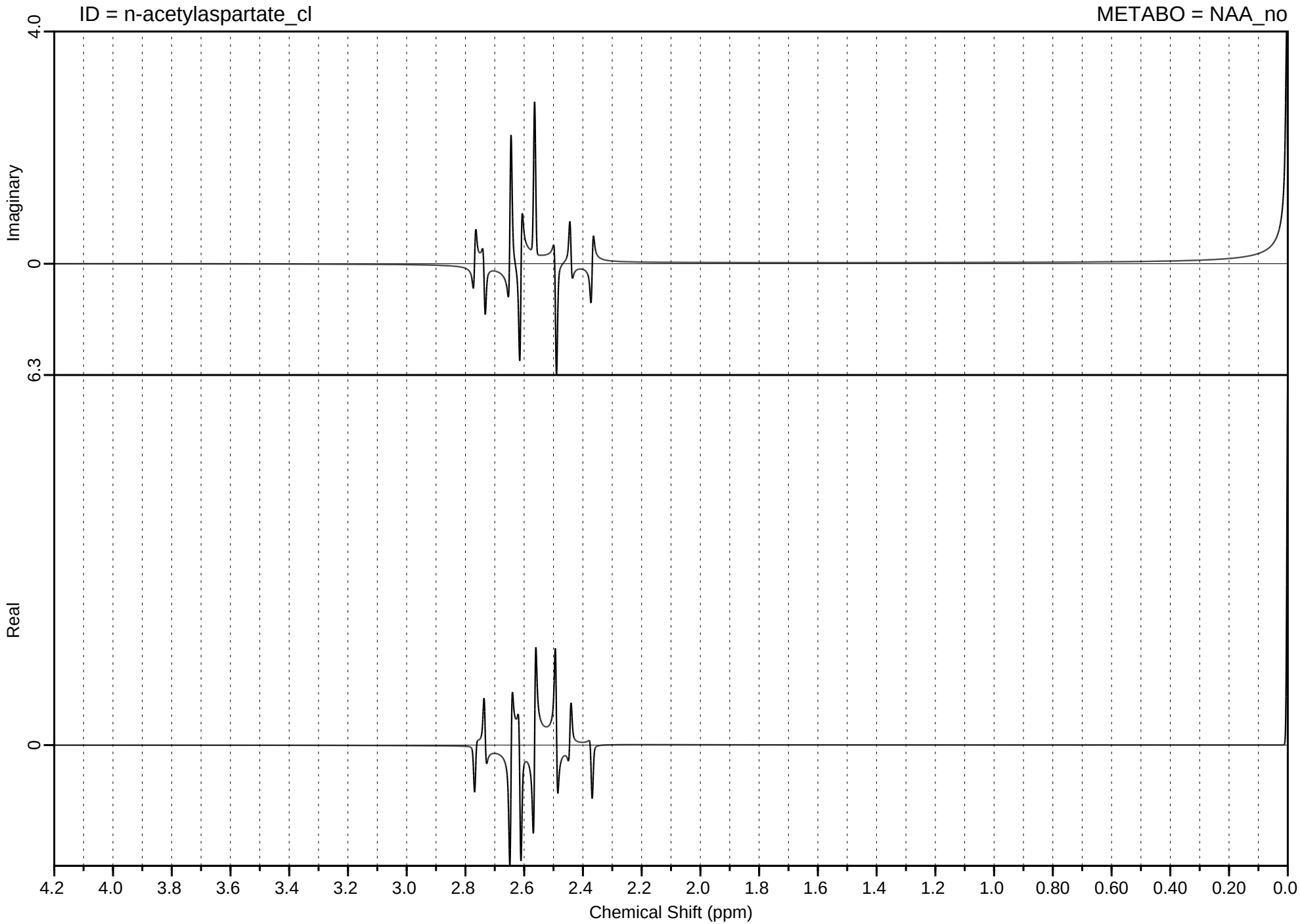

ID = glycine
METABO = Glyc
7.9
Imaginary
0
13
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

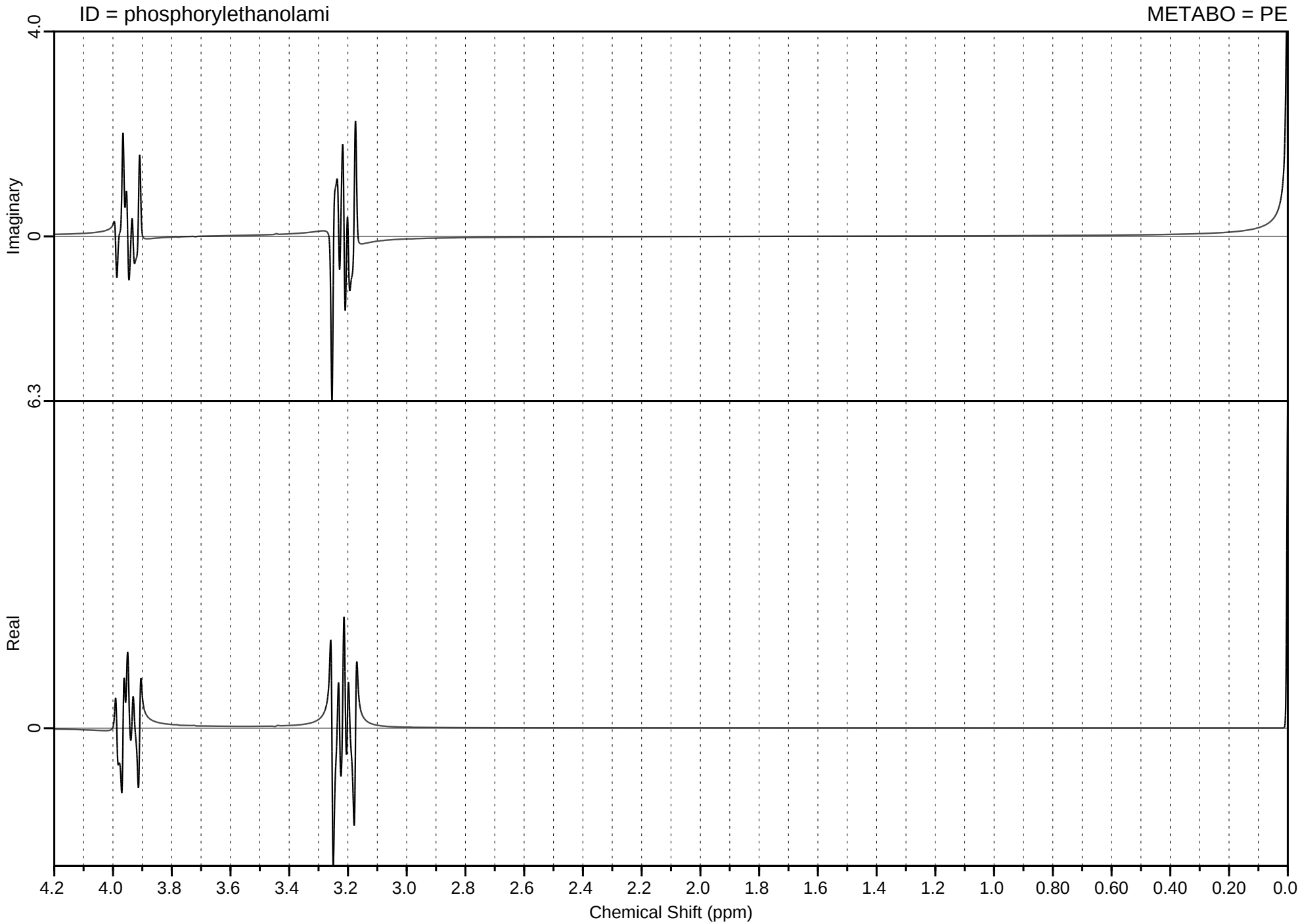

ID = lactate
METABO = Lac
9.2
Imaginary
0
6.8
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

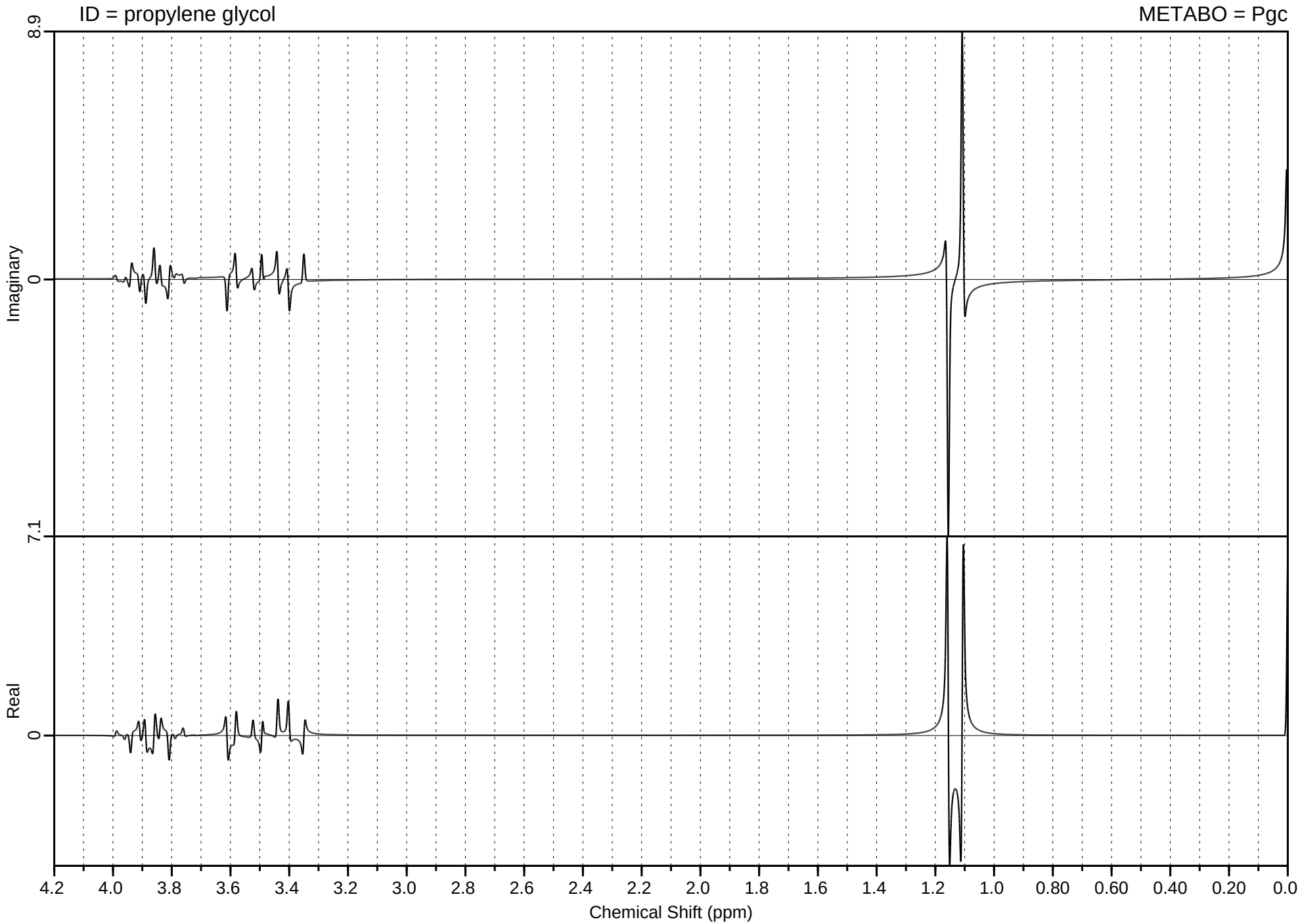

ID = myo-inositol
METABO = Ins
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

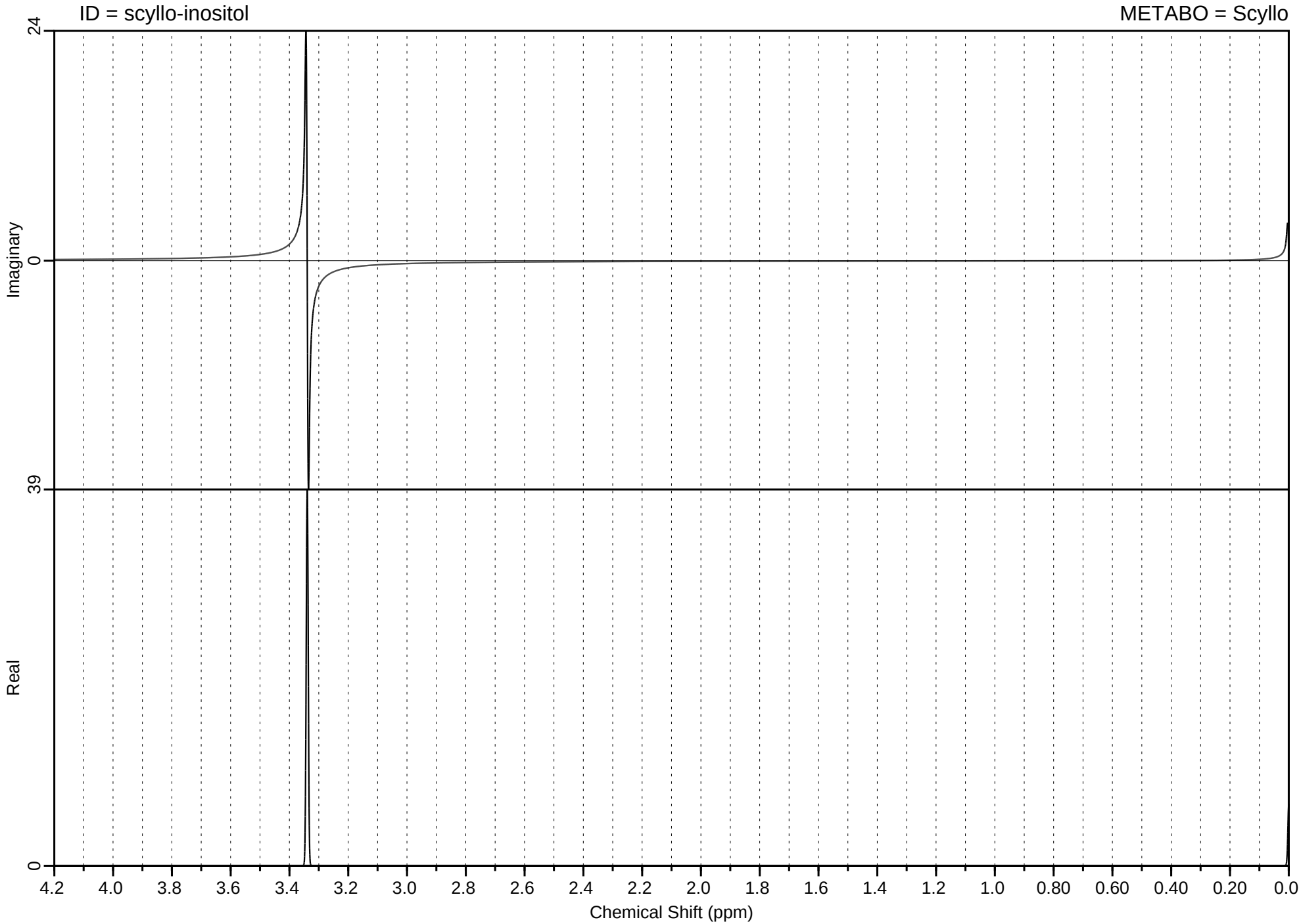

ID = NAAG-singletONLY
METABO = NAAG
Imaginary
Real
12
0
19
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

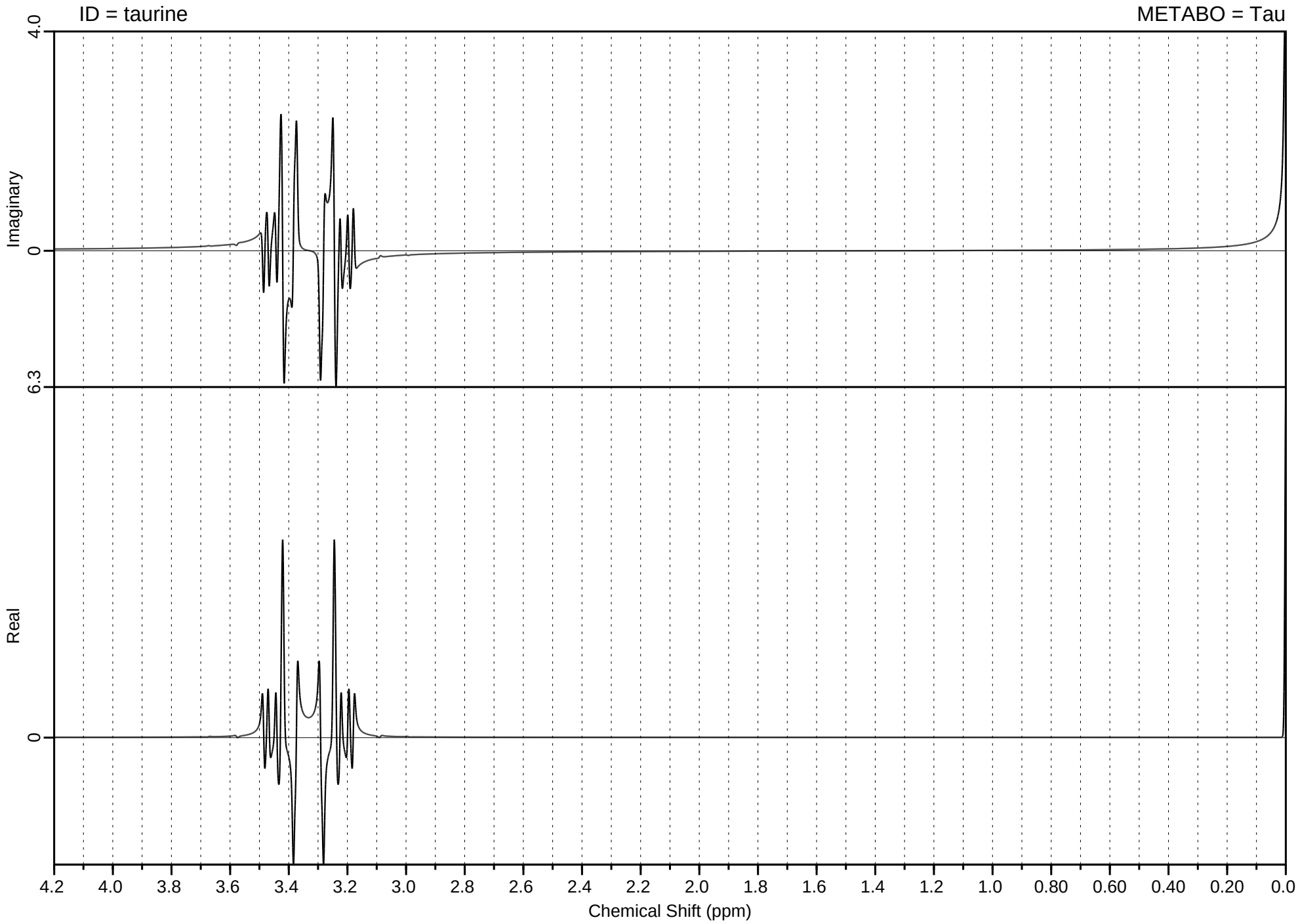

ID = n-acetylaspartate_CH
METABO = NAA
Imaginary
12
0
19
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

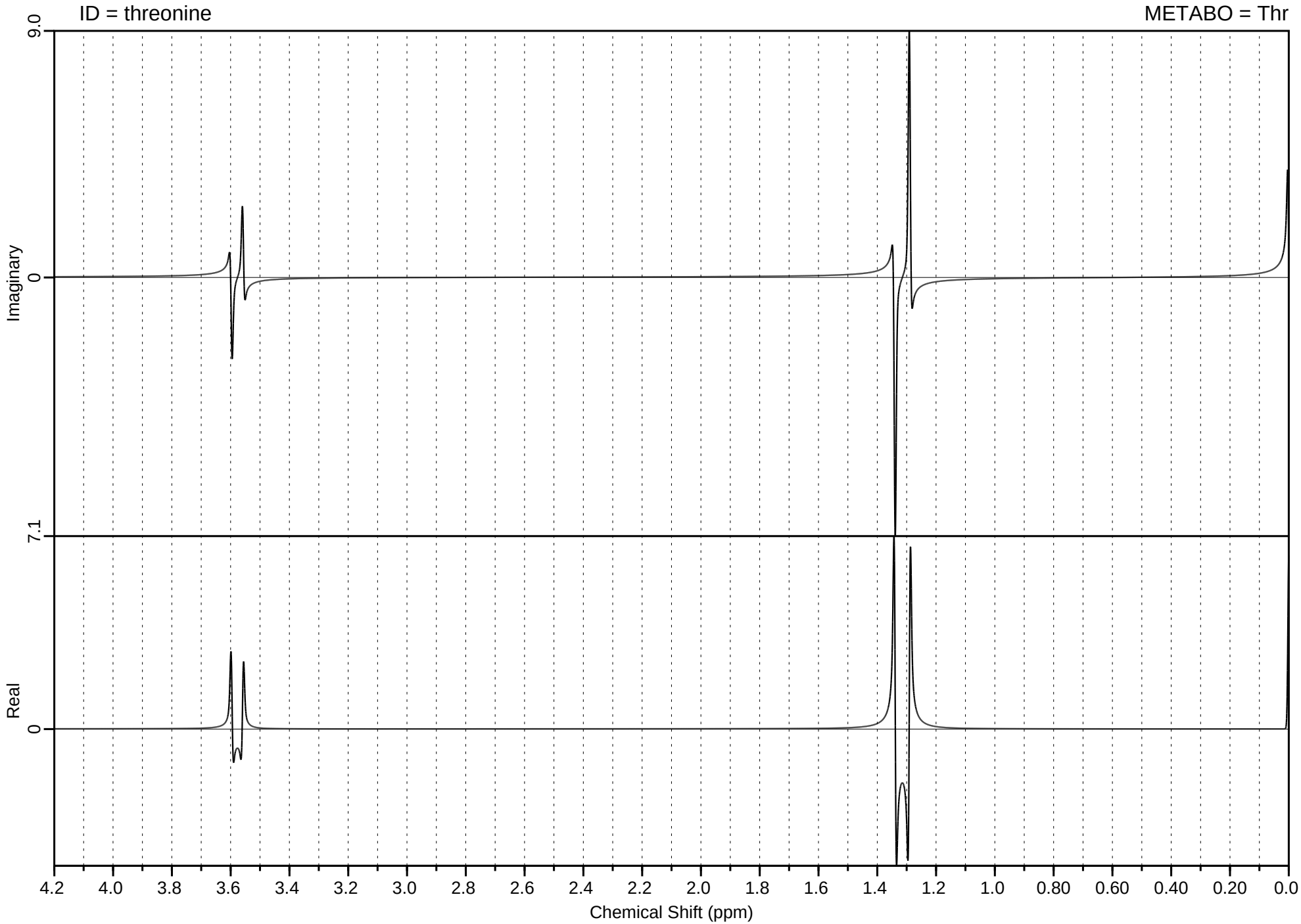

ID = n-acetylaspartate_cl
METABO = NAA_no
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)

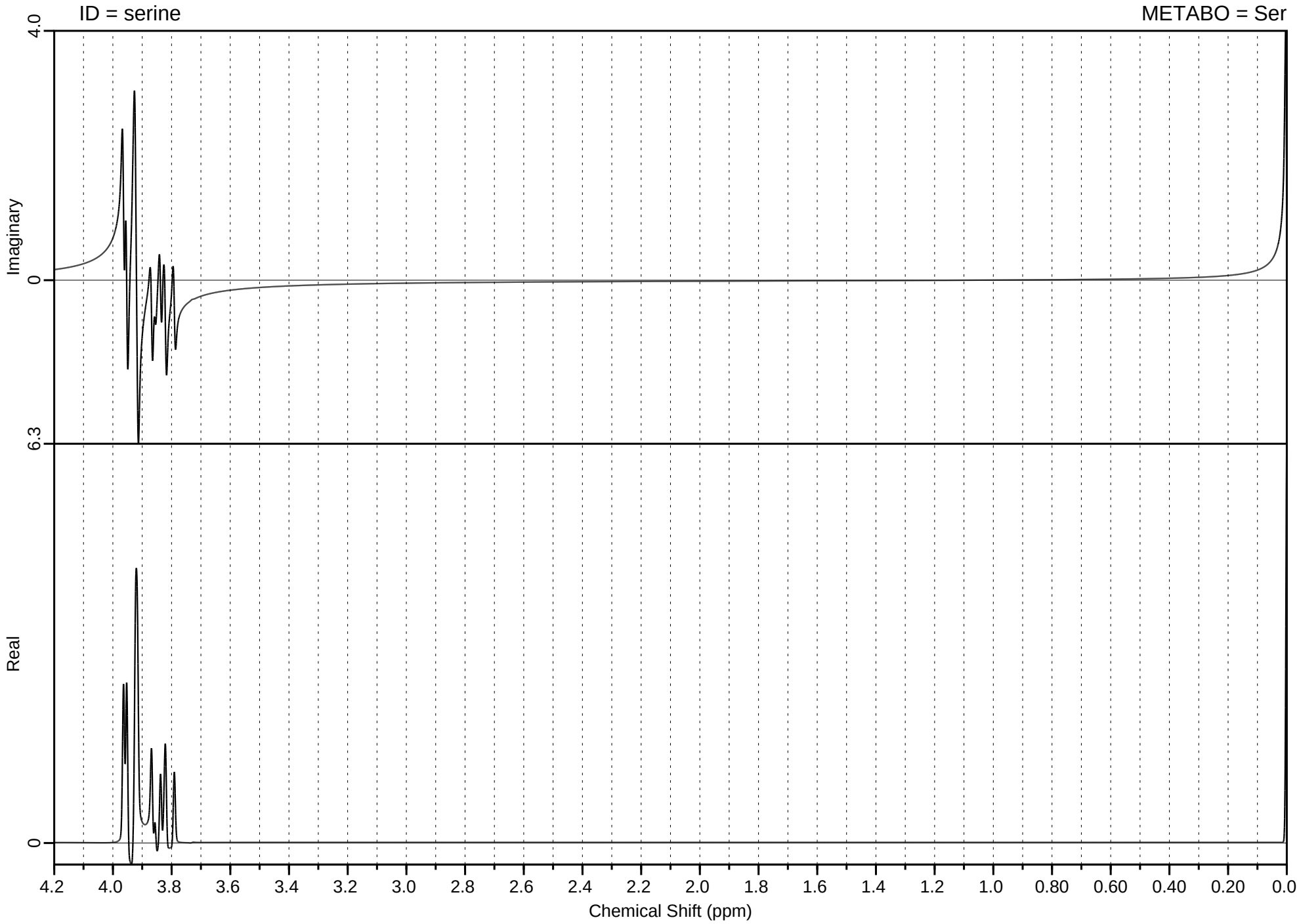

ID = phosphorylethanolami
METABO = PE
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)


ID = propylene glycol
METABO = Pgc
8.9
Imaginary
0
7.1
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)


ID = scyllo-inositol
METABO = Scyllo
Imaginary
Real
24
0
39
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)


ID = taurine
METABO = Tau
Imaginary
4.0
0
6.3
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)


ID = threonine
METABO = Thr
9.0
Imaginary
0
7.1
Real
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)


ID = serine
METABO = Ser
Imaginary
Real
4.0
0
6.3
0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0.20
0.0
Chemical Shift (ppm)