

Supporting Information

Supporting Information Figure 1. Determination of the Kinetic Constants for GABA-AT catalyzed elimination of HF from (*R*)-**2**. The equations that represent these data and the association constant are displayed on the graphs.

[R-3-F-GABA] (mM) (S)	$\delta A/\text{min}$ (v)	1/[S]	$\delta \text{NADPH}/\text{min}$ (umol/min)	1/v (min/umol)	[S]/v (mM*min/umol)
0.5000	0.024970	2	0.15531340	6.438594481	3.21929724
0.2500	0.022000	4	0.13684000	7.307804735	1.826951184
0.1250	0.018740	8	0.11656280	8.579066392	1.072383299
0.0500	0.013150	20	0.08179300	12.22598511	0.611299255
0.0250	0.007910	40	0.04920020	20.32512063	0.508128016
0.0125	0.005277	80	0.03282045	30.46880646	0.380860081

[GABA-AT] = 9.81mg/mL

so each rxn contains

0.032667mg

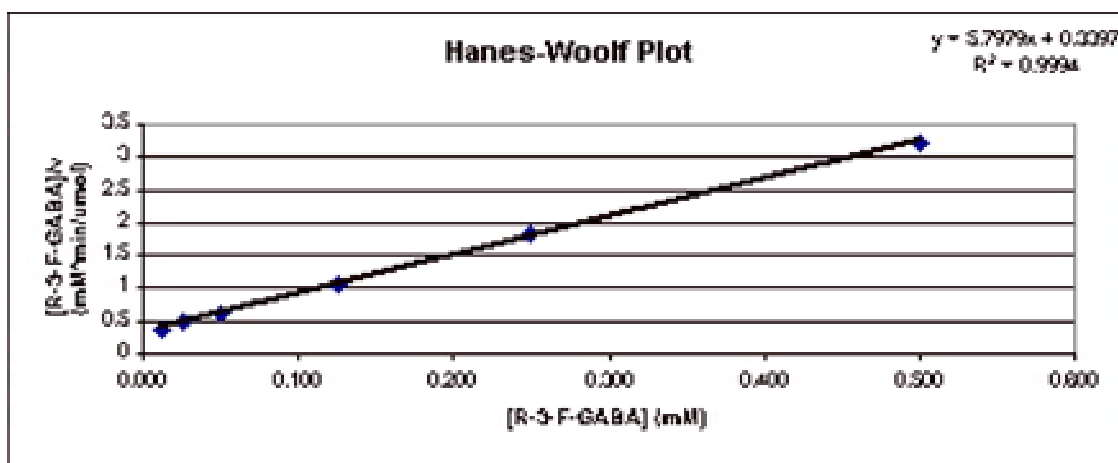
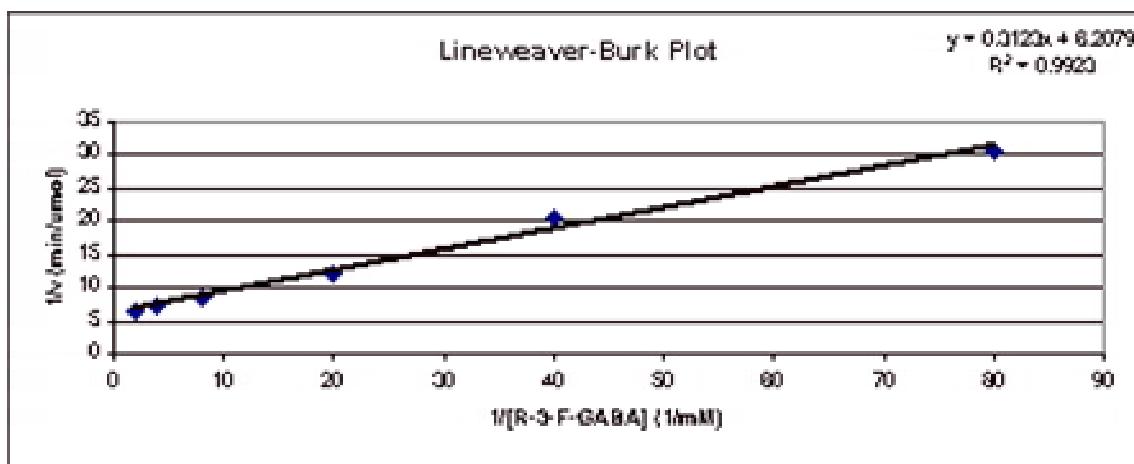
$\delta \text{Abs}/\text{min} * 6.22 \text{mM}/\text{cm}^{-1}$

accounts for conversion to

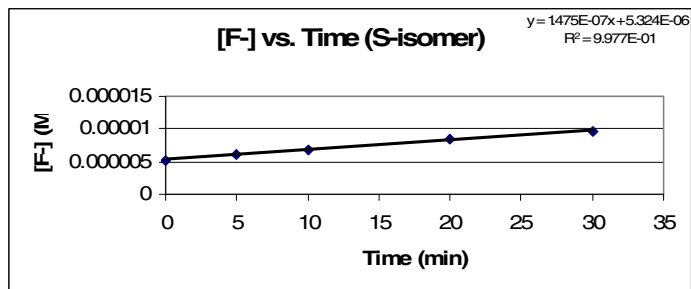
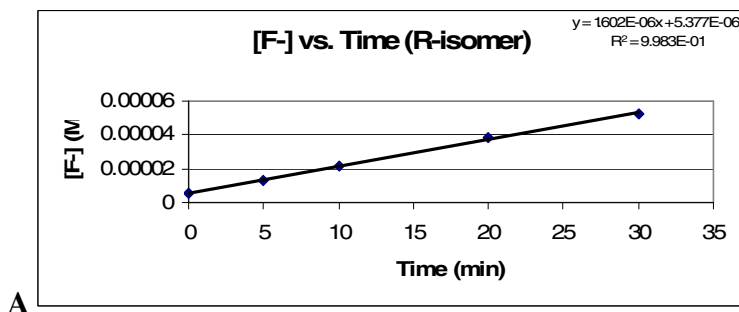
umol (divide by 1000 to convert mL to L then

multiply by 1000 to convert mmol to umol)

pathlength is 1cm

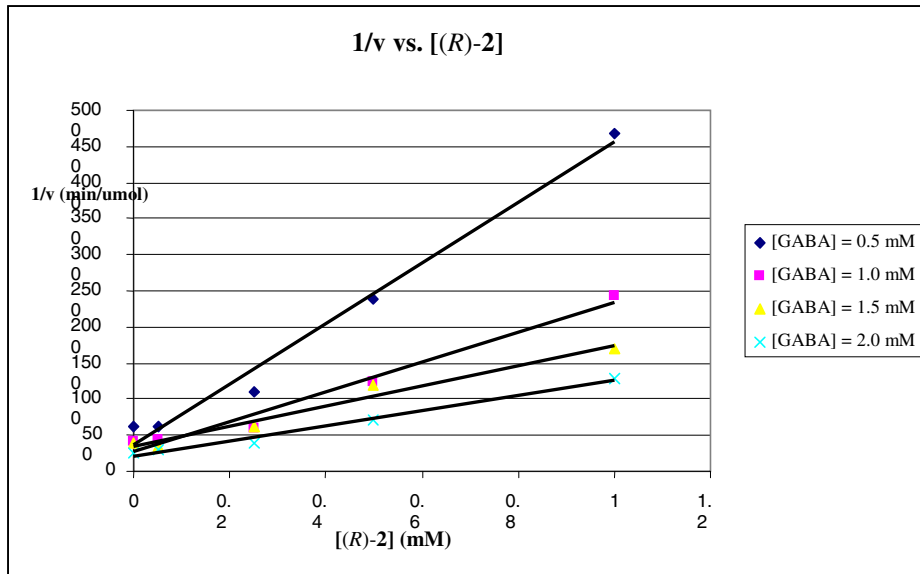


Supporting Information Figure 2. Representative plots of the increase in $[F^-]$ (as determined from the electric potential across a calibrated electrode) as a function of time for (*R*)-**2** (**A**) and (*S*)-**2** (**B**). The equations that represent these data and the association constant are displayed on the graphs.

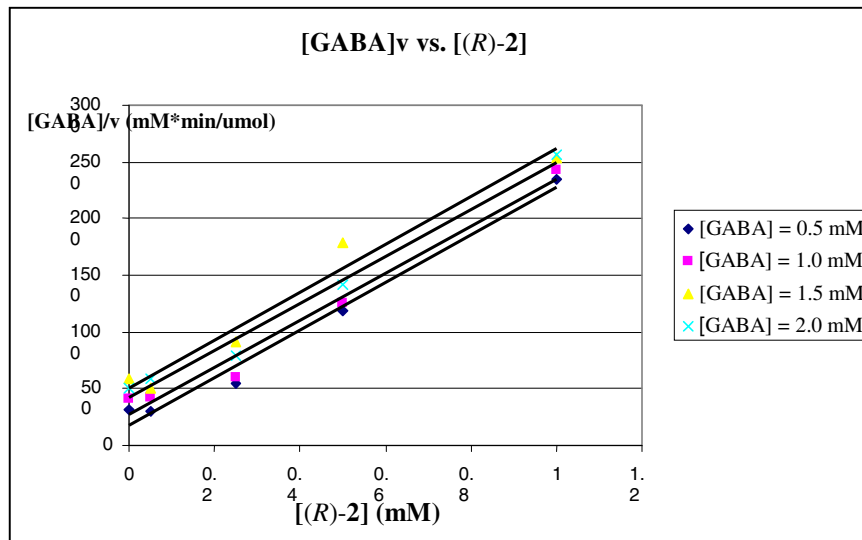


Supporting Information Figure 3. Dixon (A) and Cornish-Bowden (B) plots constructed with the data shown in Supporting Information Table 1 below. The equations for the least-square regression lines are omitted but all r^2 values are greater than 0.98 in the case of the Dixon plot ($1/v$ vs. [Inhibitor]) and greater than 0.97 in the case of the Cornish-Bowden plot ($[\text{Substrate}]/v$ vs. [Inhibitor]).

A



B



Supporting Information Table 1. Summary of the data collected to determine the (R)-2 mediated inhibition of GABA transamination.

[GABA] (mM)	0.500	1.000	1.500	2.000
[(R)-2] (mM)	Rate (v)	Rate (v)	Rate (v)	Rate (v)
0.000	0.001615	0.002436	0.002532	0.003923
0.050	0.001636	0.002337	0.002973	0.003405
0.250	0.000913	0.001683	0.001633	0.002509
0.500	0.000420	0.000800	0.000843	0.001413
1.000	0.000214	0.000413	0.000591	0.000781

Supporting Information Figure 4. Crystal structure of the active site of GABA-AT. PDB code 1OHV; SYBYL Molecular Modeling Package, version 6.9, Tripos; St. Louis, MO, 2002. <http://www.tripos.com>

QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.