Supplementary Table 1: Results of Hyde calculations for the ligand molecules performed by SeeSAR v9.2

S.No.	Ligands Name	LLE	LE	Estimated Affinity				Torsion
				pM	nM	µM	mM	
1.	Ligand-1							
2.	Ligand-9							
3.	Ligand-7							
4.	Ligand-17							
5.	Ligand-11							
6.	Ligand-10							
7.	Ligand-5							
8.	Ligand-3							
9.	Ligand-16							
10.	Ligand-15							
11.	Ligand-13							
12.	Ligand-4							
13.	Ligand-8							
14.	Ligand-14							
15.	Ligand-12							
16.	Ligand-2							
17.	Ligand-6							
18.	Flumazenil							

Supplementary Table 2: Binding energy contituents for different time fragments

48-50 ns	Binding Energy	Van der Waal's Energy	Electrostatic Energy	Polar Solvation Energy	SASA Energy
FYP	-213.029	-244.404	-12.319	59.597	-15.903
Ligand 1	-215.409	-275.072	-17.025	95.891	-19.202
Ligand 7	-209.469	-242.735	-7.044	57.462	-17.152
Ligand 9	-225.522	-261.716	-6.233	61.086	-18.660
Ligand 17	-229.364	-260.982	-7.966	57.634	-18.051
148-150 ns					
FYP	-223.405	-254.795	-14.200	61.243	-15.653
Ligand 1	-270.784	-316.719	-16.838	82.299	-19.526
Ligand 7	-165.474	-205.831	-6.367	62.905	-16.182
Ligand 9	-209.839	-246.813	-9.761	65.056	-18.322
Ligand 17	-240.001	-271.979	-4.383	55.311	-18.951
248-250 ns					
FYP	-226.585	-260.621	-10.124	59.485	-15.653
Ligand 1	-262.330	-299.052	-17.700	74.235	-19.812
Ligand 7	-190.378	-238.576	-9.061	75.327	-18.068
Ligand 9	-223.888	-257.371	-16.165	67.594	-17.946
Ligand 17	-239.739	-267.899	-5.248	51.771	-18.363
348-350 ns					
FYP	-226.020	-260.170	-12.291	61.795	-15.354
Ligand 1	-222.208	-272.030	-6.489	76.476	-20.165
Ligand 7	-207.425	-244.581	-2.568	56.933	-17.208
Ligand 9	-218.309	-269.405	-10.069	79.990	-18.825
Ligand 17	-236.315	-274.744	-5.917	62.691	-18.345
448-450 ns					
FYP	-228.647	-264.594	-11.686	63.712	-16.079
Ligand 1	-208.196	-277.504	-5.426	94.960	-20.226
Ligand 7	-208.769	-246.905	0.491	55.039	-17.394
Ligand 9	-216.707	-258.072	-4.849	65.042	-18.827
Ligand 17	-255.836	-293.404	-6.474	62.722	-18.679

Supplementary Table 3: Contribution energies of binding pocket residues at different time fragments.

$GABA_A$ Rs	48-50 ns		148-150 ns		248-250 ns		348-350 ns		448-450 ns	
α1-subunit	FYP	Ligand-17	FYP	Ligand-17	FYP	Ligand-17	FYP	Ligand-17	FYP	Ligand-17
Phe100	-5.5361	-4.0888	-6.5843	-4.8200	-5.1172	-4.4057	-5.7201	-4.8331	-6.6078	-5.3261
His102	-6.8749	-9.4694	-6.8019	-6.8018	-6.9461	-7.5058	-7.6851	-7.0911	-7.4626	-6.2328
Tyr160	-5.8403	-7.1327	-8.9861	-4.6164	-7.9399	-4.6756	-7.2858	-4.5247	-7.7489	-4.8112
Val203	-6.4392	-7.1493	-6.0054	-7.8894	-5.2475	-8.0615	-4.3311	-7.2795	-7.9448	-7.7411
Tyr210	-12.3789	-6.9399	-14.4341	-9.2493	-15.055	-8.7083	-14.808	-7.1389	-13.4917	-8.6000
Val212	-5.6497	-6.3438	-4.8641	-5.6685	-6.4998	-5.1959	-6.5691	-5.0223	-3.2042	-4.6821
γ2-Subunit										
Tyr58	-5.4686	-1.3826	-5.7879	-8.9735	-5.7240	-9.9728	-8.3821	-9.2605	-8.3533	-9.8188
Asn60	-	-0.0555	-	-1.3457	-	-1.0910	-	-1.3882	-	-1.3112
Phe77	-17.9415	-12.7429	-17.6219	-15.3973	-18.4165	-13.1408	-18.319	-14.4355	-18.1627	-13.8003
Ala79	-	-	-2.4311	-3.2400	-1.8225	-3.4603	-1.7868	-3.3513	-1.7513	-3.3893
Arg132	-	-1.0638	-	-	-	-	-	-	-	-
Thr142	-1.6687	-5.2574	-3.3898	-4.7106	-1.9887	-4.8394	-1.8560	-4.6086	-1.7789	-4.6247
Lys184	-	-	-1.7882	-	-1.7261	-	-2.5057	-	-0.9786	-
Glu189	-	-	-	-1.0710	-	-1.7644	-	-1.8693	-	-1.1320
Asp192	-	-	-	-1.1708	-	-1.2764	-	-1.2614	-	-1.3684

- Residues depicted in bold are present in the crystal structure of $GABA_A$Rs with Flumazenil.
- Residues not showing any interaction are indicated by '-' symbol.