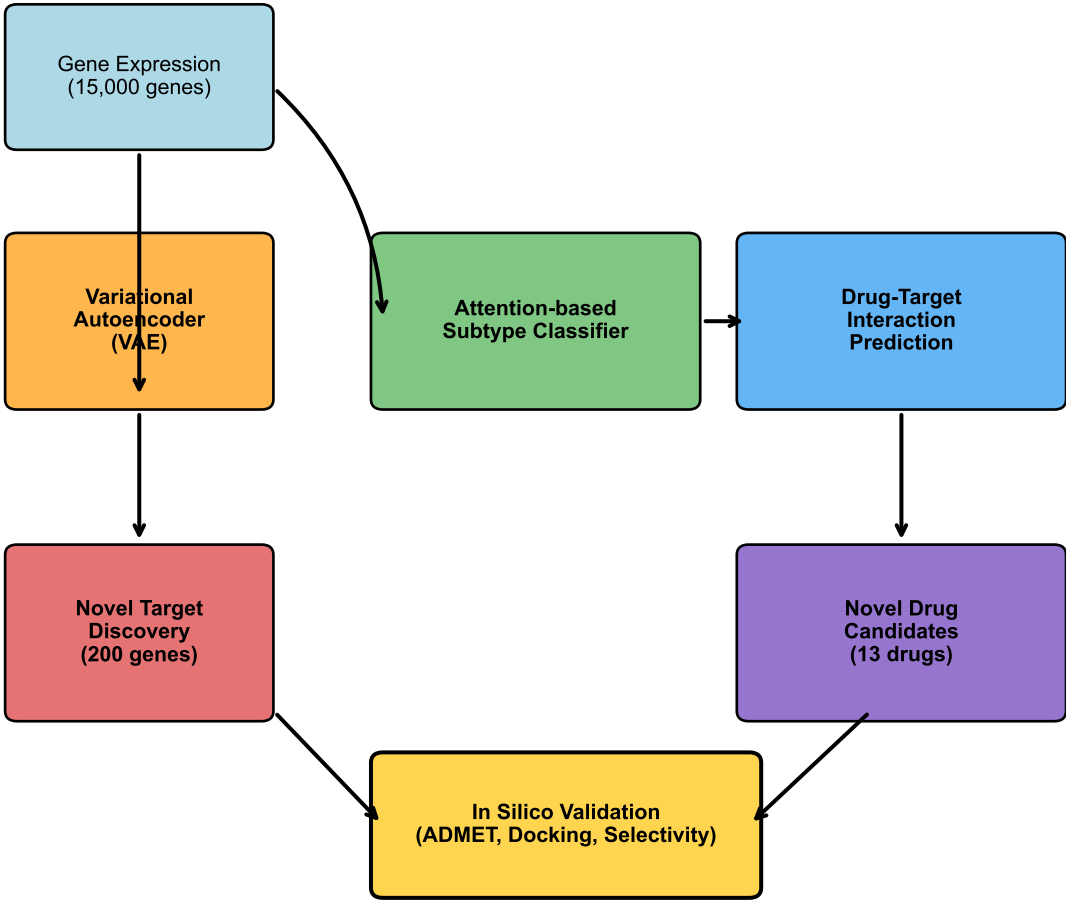


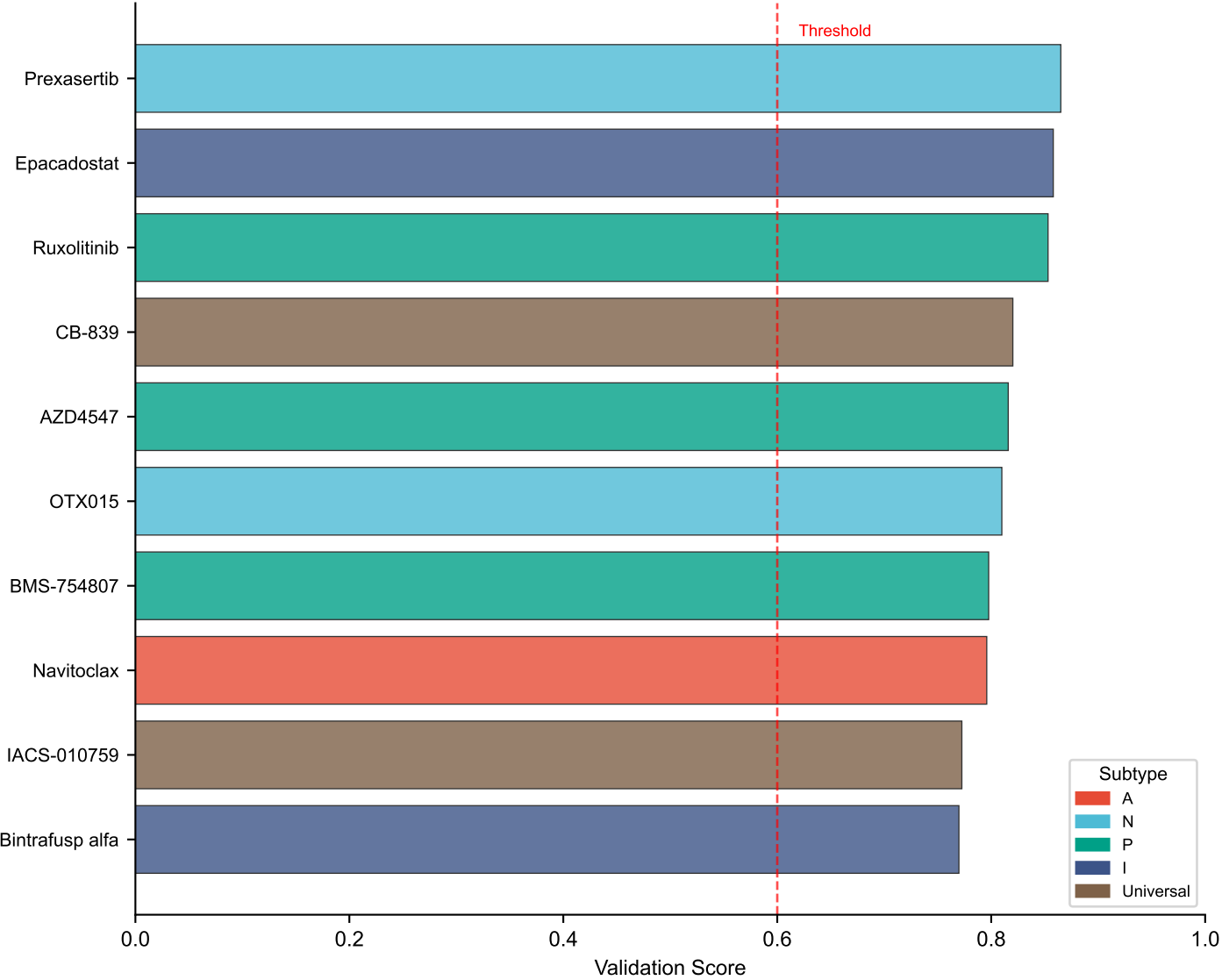
A. Deep Learning Workflow for Novel Discovery



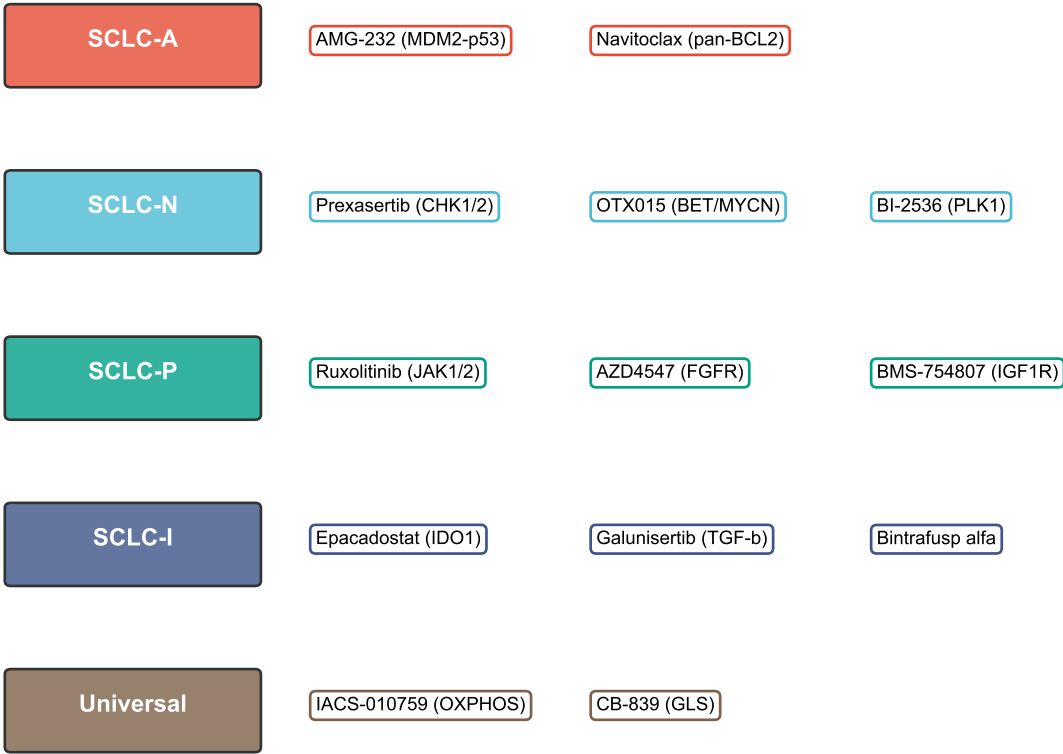
B. Novel Drug Candidates with In Silico Validation

Drug	Subtype	Mechanism	Valid.	ADMET
Prexasertib	N	CHK1/2 inhibitor, replication stres...	0.87	1.0
Epacadostat	I	IDO1 inhibitor, restores T-cell fun...	0.86	0.8
Ruxolitinib	P	JAK1/2 inhibitor, blocks cytokine s...	0.85	1.0
CB-839	Universal	Glutaminase inhibitor, metabolic ta...	0.82	0.8
AZD4547	P	Selective FGFR inhibitor	0.82	1.0
OTX015	N	BET inhibitor, downregulates MYCN	0.81	1.0
BMS-754807	P	IGF1R/IR inhibitor	0.80	1.0
Navitoclax	A	Pan-BCL2 family inhibitor	0.80	0.6
IACS-010759	Universal	Complex I inhibitor, OXPHOS targeti...	0.77	1.0
Bintrafusp alfa	I	Bifunctional TGF-β trap + anti-PD-L...	0.77	0.7

C. Validation Scores



D. Subtype-Specific Novel Therapeutic Recommendations



All candidates passed in silico validation (score > 0.6)