Supporting Information

Leveraging Efficiency Metrics for the Optimization of CELMoDs™ as Cereblon-based Molecular Glue Degraders

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Table of Content

Data Availability Statement:

Internal program data was used for the purpose of this retrospective analysis. Profiles of 5 early-stage, 8 middle-stage and 2 late-stage lead compounds were used to track progress during LO phase of the program. The early, middle and late stage were defined by the chronological order of lead optimization progress. Structural data for 8 compounds, include 4 early-stage, 3 middle-stage and 1 late-stage (CC-99282), are disclosed in Table S1.

Table S1: Disclosed Structures

ID	Lead_Stage	SMILES	Formula
Compound 1	Early-stage	FC1=CC(F)=C(C=C1)N1CCN(CC2=CC=C(CNC3=C4C(=O)N(C5CCC(=O)NC5=O)C(=O)C4=CC=C3)C=C2)CC1	C31H29F2N5O4
Compound 2	Early-stage	FC1=CC=C(C=C1)N1CCN(CC2=CC=C(CNC3=C4C(=O)N(C5CCC(=O)NC5=O)C(=O)C4=CC=C3)C=C2)CC1	C31H30FN5O4
Compound 3	Early-stage	ClC1=CC=C(C=C1)N1CCN(CC2=CC=C(CNC3=C4C(=O)N(C5CCC(=O)NC5=O)C(=O)C4=CC=C3)C=C2)CC1	C31H30ClN5O4
Compound 4	Early-stage	FC1=C(C=CC(=C1)C#N)N1CCN(CC2=CC=C(CNC3=CC=CC4=C3C(=O)N(C3CCC(=O)NC3=O)C4=O)C=C2)CC1	C32H29FN6O4
Compound 5	Middle-stage	NC(=O)C1=NC=C(C=C1)N1CCN(CC2=CC=C(CNC3=CC=CC4=C3C(=O)N(C3CCC(=O)NC3=O)C4=O)C=C2)CC1	C31H31N7O5
Compound 6	Middle-stage	FC1=CN=C(C=C1)N1CCN(CC2=CC=C(CNC3=CC=CC4=C3C(=O)N(C3CCC(=O)NC3=O)C4=O)C=C2)CC1	C30H29FN6O4
Compound 7	Middle-stage	FC1=CC(CN2CC3(CCC3)C2)=CC=C1CNC1=C2C(=O)N(C3CCC(=O)NC3=O)C(=O)C2=CC=C1	C27H27FN4O4
CC-99282	Late-stage	O=C1CC[C@H](N2C(=O)C3=CC=CC(NCC4=CC=C(CN5CC(N6CCOCC6)C5)C=C4F)=C3C2=O)C(=O)N1	C28H30FN5O5