

FragLites Screen (EG)

Catalogue number: 155084

Sub-type:

Images:

Contributor

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Institute: Northern Institute For Cancer Research, Newcastle University

Images:

Tool details

***FOR RESEARCH USE ONLY**

Name: FragLites Screen (EG)

Alternate name:

Class:

Conjugate:

Description: The FragLites screen consist of a set of 31 compounds designed to express a "pharmacophore doublet" of two hydrogen bond acceptors or a donor and an acceptor displayed on an aromatic scaffold and incorporating a heavy halogen atom. This set allows the mapping of a protein surface for productive drug-like interactions by X-ray crystallography and unambiguous identification of binding events by observing the anomalous dispersion. This method can be used to assess druggability and provide potential start point for lead discovery in very short timescales and with minimal screening. Validation of the approach has been established using CDK2 protein as a model system

Purpose:

Parental cell:

Organism:

Tissue:

Model:

Gender:

Isotype:

Reactivity:

Selectivity:

Host:

Immunogen:

Immunogen UNIPROT ID:

Sequence:

Growth properties:

Production details:

Formulation:

Recommended controls:

Bacterial resistance:

Selectable markers:

Additional notes: The compound set is available dispensed in an assay ready ECHO plate. Format: 10uL per compound @ 100mM in EG Library Plate Source Well Library Name SMILES FragLite Set 1 A1 FL1 BrC1=CCN=C1 FragLite Set 1 A2 FL2 IC1=CCN=C1 FragLite Set 1 A3 FL3 BrC1=CC=CC=C1 FragLite Set 1 A4 FL4 NC1=CC=CC(Br)=C1 FragLite Set 1 A5 FL5 NC1=CC=CC(I)=C1 FragLite Set 1 A6 FL6 O=C1C=CC(Br)C=CC1 FragLite Set 1 A7 FL7 O=C1C=CC(I)C=CC1 FragLite Set 1 A8 FL8 BrC1=CC=C(S(N)(=O)=O)C=CC1 FragLite Set 1 A9 FL9 IC1=CC=C(S(N)(=O)=O)C=CC1 FragLite Set 1 A10 FL10 O=C1CC2=C(C=CC(Br)C=C2)N1 FragLite Set 1 A11 FL11 BrC1=CC=C(NC(C)=O)C=CC1 FragLite Set 1 A12 FL12 IC1=CC=C(C(N)=O)C=CC1 FragLite Set 1 A13 FL13 BrC1=CC=CC=C1 FragLite Set 1 A14 FL14 IC1=CC=CC=C1 FragLite Set 1 A15 FL15 BrC1=CC(OC)=NC=CC1 FragLite Set 1 A16 FL16 BrC1=CC=NC2=CC=CC=C21 FragLite Set 1 A17 FL17 BrC1=CC=C(S(C)(=O)=O)C=CC1 FragLite Set 1 A18 FL18 BrC1=CC(CO)=NC=CC1 FragLite Set 1 A19 FL19 OC1=C(OC)C=CC(Br)C=C1 FragLite Set 1 A20 FL20 BrC1=CC(COC)=NC=CC1 FragLite Set 1 A21 FL21 OC1=C(C#N)C=CC(Br)C=C1 FragLite Set 1 A22 FL22 BrC1=CC(OC)=C(CO)C=CC1 FragLite Set 1 A23 FL23 BrC1=CC(CCO)N=CC1 FragLite Set 1 A24 FL24 BrC1=CC(O)=C(C(O)=O)C=CC1 FragLite Set 1 B1 FL25 BrC1=CC(C#N)=C(OC)C=CC1 FragLite Set 1 B2 FL26 BrC1=CC(CCO)N=CC1 FragLite Set 1 B3 FL27 BrC1=CC(CO)=O)N=CC1 FragLite Set 1 B4 FL28 O=C1N(CCO)C=CC(Br)=CC1 FragLite Set 1 B5 FL29 O=C1N(CCO)C=CC(Br)=CC1 FragLite Set 1 B6 FL30 O=C1N(CO)=O)C=CC(Br)=CC1 FragLite Set 1 B7 FL31 BrC1=CC(OC)=C(CO)=O)C=CC1

Target details

Target:

Target alternate names:

Target background:

Molecular weight:

Ic50:

Applications

Application:

Application notes:

Handling

Format:

Concentration:

Passage number:

Growth medium:

Temperature:

Atmosphere:

Volume:

Storage medium:

Storage buffer:

Storage conditions: Keep frozen ~-10° C

Shipping conditions: pound set is available dispensed in an assay ready ECHO plate. Format: 10uL per compound @ 100mM in ECLibrary Plate Source Well Library Name SMILESFragLite Set 1 A1 FL1 BrC1=CN=C1FragLite Set 1 A2 FL2 IC1=CN=C1FragLite Set 1 A3 FL3 BrC1=CON=C1FragLite Set 1 A4 FL4 NC1=NC=CC(Br)=C1FragLite Set 1 A5 FL5 NC1=NC=CC(I)=C1FragLite Set 1 A6 FL6 O=C1C=C(Br)C=CN1FragLite Set 1 A7 FL7 O=C1C=C(I)C=CN1FragLite Set 1 A8 FL8 BrC1=CC=C(S(N)(=O)=O)C=C1FragLite Set 1 A9 FL9 IC1=CC=C(S(N)(=O)=O)C=C1FragLite Set 1 A10 FL10 O=C1CC2=C(C=C(Br)C=C2)N1FragLite Set 1 A11 FL11 BrC1=CC=C(NC(C)=O)C=C1FragLite Set 1 A12 FL12 IC1=CC=C(C(N)=O)C=C1FragLite Set 1 A13 FL13 BrC1=CN=CN=C1FragLite Set 1 A14 FL14 IC1=CN=CN=C1FragLite Set 1 A15 FL15 BrC1=CC(OC)=NC=C1FragLite Set 1 A16 FL16 BrC1=CC=NC2=NC=CC=C21FragLite Set 1 A17 FL17 BrC1=CC=C(S(C)(=O)=O)C=C1FDry Ice

Related tools

Related tools:

References

References: Generation of in vivo labelling tumour cell lines by Luigi Ombrato and Ilaria Malanchi. Protocol Exchange, DOI: 10.21203/rs.2.14720/v1 ; Ombrato et al. 2019. Nature. PMID: 31462798.