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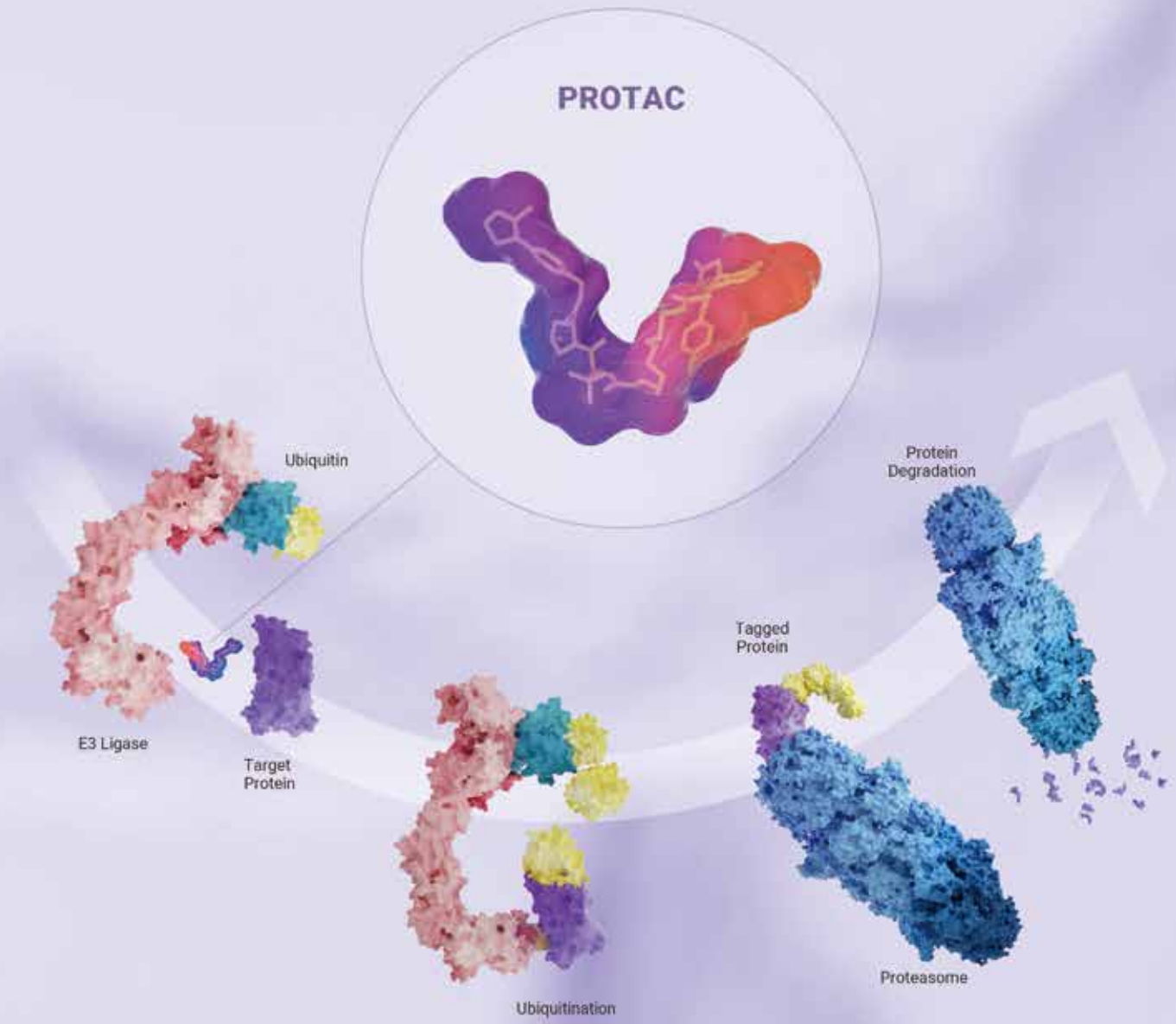
# PROTACs
## (PROteolysis-TArgeting Chimeras)
## Handbook



# PROTACs (PROteolysis-TArgeting Chimeras)

**PROTAC, short for PROteolysis-TArgeting Chimera**, is a heterobifunctional nano molecule containing two different ligands; ligand for ubiquitin E3 and ligand for target protein. The two parts are connected by a linker to form a "three-unit" polymer, target protein ligand-linker-E3 ligase ligand[1].

Once the PROTAC molecule enters the cell, ligand for protein of interest (POI) can specifically bind to the corresponding target protein, while E3 ligase ligand can recruit E3 ligase to form the trimer complex of POI-Linker-E3 ligase, in which E3 ligase mediates ubiquitination on POI by ubiquitin from enzyme E2. POI labeled by ubiquitin is recognized and degraded by the proteasome system. It is not necessary for POI ligand to occupy the binding site for a long time during this progress because of instantaneous ubiquitination after the transient formation of the ternary complex, so PROTAC can be reused many times in cells[2].

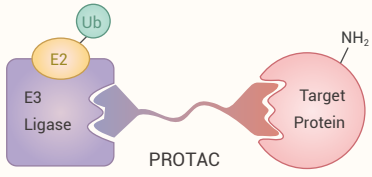



Figure 1. Composition of PROTACs[1].

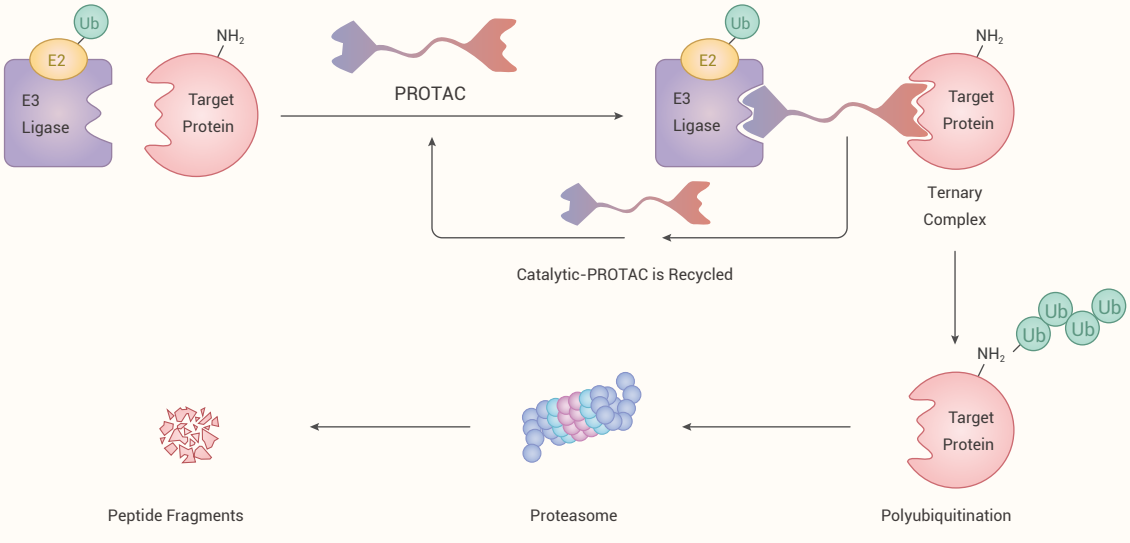



Figure 2. PROTAC-mediated degradation of target proteins through the UPS[2].

## PROTAC improves the drugability of protein

Compared with traditional small molecules which need to know the binding site and mechanism of target protein, PROTAC ignores the mechanism of the target protein itself and directly degrades target protein after ubiquitin labeling. In addition, due to its specific mechanism, it requires only a small amount to be effective, often at the nanomolar level. PROTAC is devoid of drug resistance, and has become a solution to the undruggable problem of many tumor intracellular proteins.

## Mechanism of Action

1. Ubiquitin activating enzyme E1 activates ubiquitin molecule, then the activated ubiquitin molecule is transferred to ubiquitin conjugating enzyme E2.

2. The complex of ubiquitin ligase E3 and the target protein bridged by the PROTAC molecule binds to E2 following the instructions of E3.

3. The target protein is labeled with ubiquitin because of the increased proximity and collision.

4. Repeating the labeling process above.

5. The target protein labeled with multiple ubiquitinations is eventually recognized and degraded by the proteasome.

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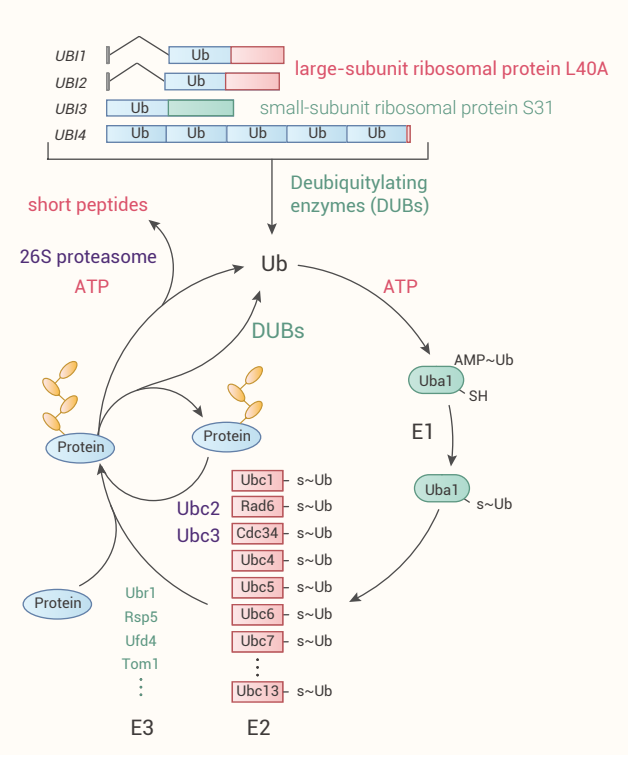
# Target Proteins for PROTACs




The protein degraded by the ubiquitin-proteasome pathway include cyclin, fusion-associated protein, cell surface receptor, transcription factor, tumor suppressor, oncogene product, abnormal protein and intracellular denatured protein under stress. In principle, PROTAC can be used for the degradation of all the above proteins.

At present, PROTAC molecules targeting AR, ER, BTK, IKZF1/3, BRD9, Bcl-xl and IRAK4 have entered the stage of clinical development[3].

Besides PROTAC, there are also other target protein degraders (TPDs) such as LYTAC, AUTAC, ATTEC, which can target proteins from lysosomal pathway[4].

Figure 3. Ubiquitin-proteasome pathway [3]

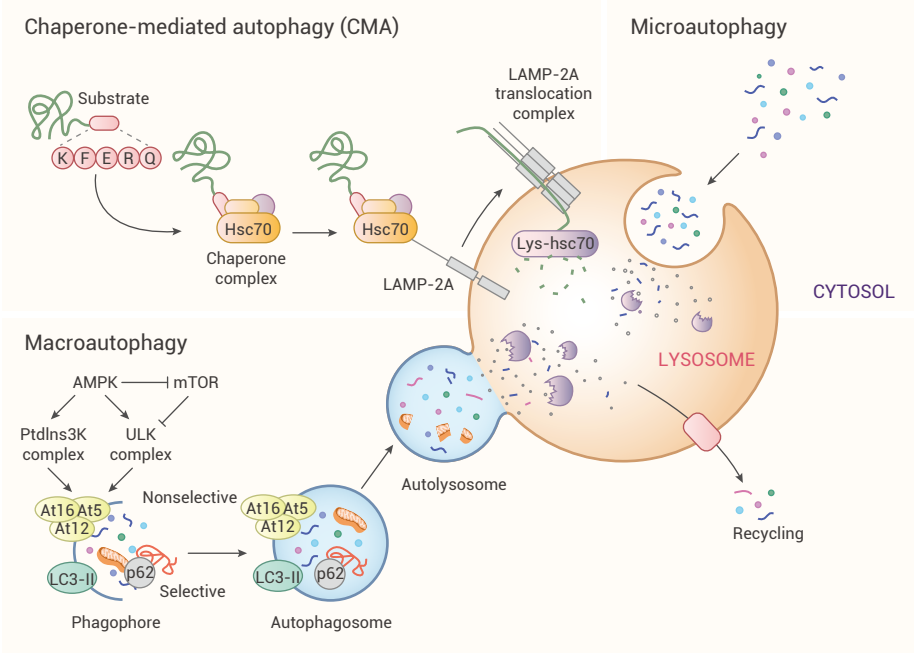
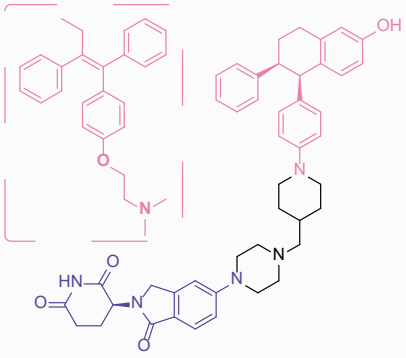


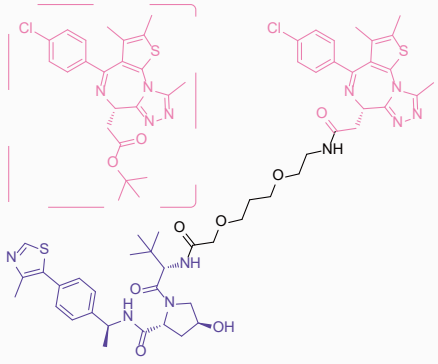

Figure 4.
Lysosomal pathway [4]

# Ligands for Target Proteins for PROTACs

Although PROTAC technology is developed to solve the druggability of some proteins, PROTAC molecules nowadays are basically developed based on known protein inhibitors, because the ligand for target protein should be highly selective to avoid off-target toxicity and it costs much to find such an appropriate molecule. For example, the known structure of PROTAC ARV-471 is derived from Tamoxifen, and ARV-766 is from (+)-JQ-1.



Tamoxifen and ARV-471



(+)-JQ-1 and ARV-110

MCE can provide you with ligands for the various target proteins to meet your needs for scientific research. We have high-quality products and services. Related popular products are listed below:

## Kinases

HY-10997

### Ibrutinib

A selective, irreversible Btk inhibitor can be used as a **BTK** ligand for the synthesis of P13I.

HY-13001

### Quizartinib

An orally active, highly selective and potent second-generation type II **FLT3** tyrosine kinase inhibitor.

## Epigenetic Factors

HY-13030

### (+)-JQ-1

A potent, specific, and reversible BET bromodomain inhibitor for the first and second bromodomain (**BRD4(1/2)**).

HY-129939

### PROTAC BRD4 ligand-1

A potent BET inhibitor, a ligand for target **BRD4** protein for PROTACT GNE-987.

## Others

HY-114872

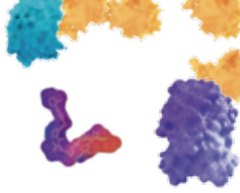
### SLF

A synthetic ligand for FK506-binding protein (**FKBP**) used in the synthesis of PROTAC.

HY-A0038

### Lasofoxifene (Tartrate)

A non-steroidal selective estrogen receptor modulator (**SERM**).



## Kinases

HY-44432
### Navitoclax-piperazine
A B-cell lymphoma extra large (**BCL-XL**) inhibitor used in the synthesis of PROTAC DT2216.

HY-126534A
### Abemaciclib metabolite M18 hydrochloride
A **CDK** inhibitor with antitumor activity to design PROTAC CDK4/6 degrader.

HY-130988
### Ipatasertib-NH2
A ligand for target protein **AKT** for PROTAC (INY-03-041).

HY-124625
### BI-4464
A highly selective ATP competitive inhibitor of **PTK2/FAK**.

HY-129967
### PROTAC IRAK4 ligand-1
A synthetic ligand for interleukin-1 receptor-associated kinase 4 (**IRAK4**).

## Epigenetic Factors

HY-130979
### EED226-COOH
An EED226-derived ligand for target protein EED ligand for PROTAC UNC6852 to degrade **PRC2**.

HY-107445
### PROTAC BRD9-binding moiety 1
A compound that binds to **BRD9**, and used for inhibiting BRD9 activity, based on PROTAC.

HY-107443
### I-BET762 carboxylic acid
An I-BET762-based warhead ligand for conjugation reactions of PROTAC targeting on BET(**BRD4**).

HY-107451
### PROTAC BET-binding moiety 1
A key intermediate for the synthesis of high-affinity **BET** inhibitors.

HY-43723
### PROTAC BET-binding moiety 2
An inhibitor of **BET bromodomain**.

## Others

HY-131388
### ABM-14
A ligand for targeting androgen receptor (**AR**) for PROTAC ARCC-4.

HY-138539
### CBP/p300 ligand 2
A ligand for target protein for PROTAC of dCBP-1. dCBP-1 is a potent and selective hetero-bifunctional degrader of **p300/CBP**.

HY-131187
### BMS-1166-N-piperidine-COOH
A potent PD-1/PD-L1 interaction inhibitor which antagonizes the inhibitory effect of PD-1/PD-L1 immune checkpoint on T cell activation.

HY-129603
### SI-109
A potent STAT3 SH2 domain inhibitor. A ligand for **STAT3** for PROTAC (SD-36).

HY-133073
### CCR7 Ligand 1
An allosteric ligand and antagonist for human CC chemokine receptor 7 (**CCR7**).

# Ligands for E3 Ligases

E3 ligases are usually divided into different families such as RING, HECT, RBR, and each family includes many sub-categories. The discovery of E3 ligases and their ligands promote the continuous enrichment of PROTACs. The ligands of E3 ligases mainly used nowadays focus on three ligases named cereblon (CRBN), von Hippel-Lindau (VHL) and inhibitor of apoptosis protein (IAP). CRBN ligands include thalidomide and other derived immunomodulatory imine drugs (IMiDs). VHL ligands include the long amino acid sequence of HIF-1α protein and its derivative of peptidomimetic binding part. IAP ligands mainly consist of peptidomimetic antagonists of endogenous components[5].

In addition, there are some uncommon ligands of E3 ligase, including MDM2, DCAF15, RNF114, DCAF16, KEAP1, and FEM1B.

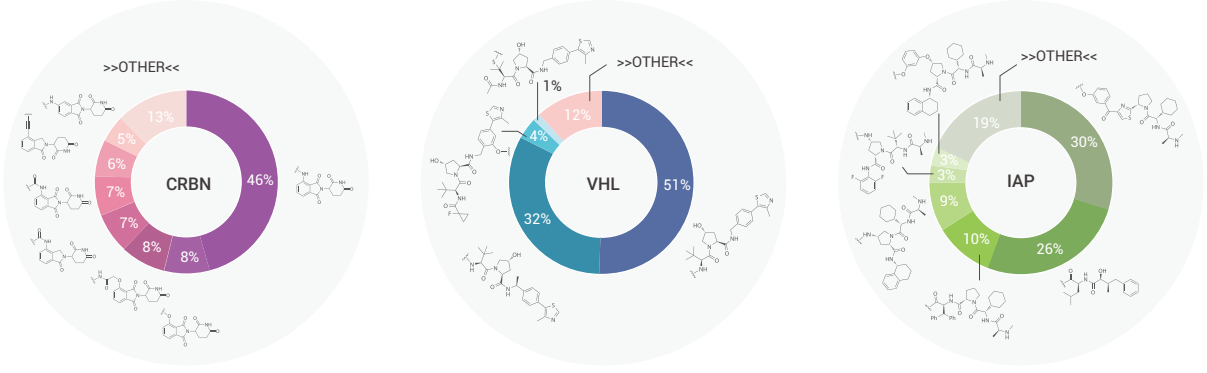
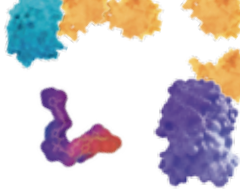



Figure 5. Common ligands for E3 Ligases[5].

MCE can provide Ligands for E3 Ligases with various structures and varieties. In addition to common categories, the unusual E3 ligands are also included. Related popular products are listed below:

| CRBN | VHL | IAP |
|---|---|---|
| HY-10984<br>**Pomalidomide**<br>A third-generation immunomodulatory agent, acts as **molecular glue**. | HY-101763A<br>**(S,R,S)-AHPC hydrochloride**<br>A VH032-based VHL ligand used in the recruitment of the **von Hippel-Lindau (VHL)** protein. | HY-128808<br>**cIAP1 ligand 1**<br>A LCL161 derivative based **IAP** ligand which can be connected to the ABL ligand for protein by a linker to form SNIPER. |



## CRBN

HY-23095
### Thalidomide-5-OH
A Thalidomide-based **cereblon** ligand used in the recruitment of CRBN protein.

HY-W072954
### Lenalidomide-5-Br
A Lenalidomide-based **cereblon** ligand used in the recruitment of CRBN protein.

HY-101291
### Iberdomide
A **cereblon** (CRBN) modulator used in the recruitment of CRBN protein.

## VHL

HY-125905
### VH032-cyclopropane-F
A VH032-based **VHL** ligand to form PROTAC 1.

HY-120217
### VH032
A VHL ligand used in the recruitment of the **von Hippel-Lindau (VHL)** protein.

HY-100947
### VH-298
A highly potent inhibitor of the VHL used in PROTAC technology.

## IAP

HY-111856
### LCL161-O-Me
A LCL161 derivative based **IAP** ligand which can be connected to the ABL ligand for protein by a linker to form SNIPER.

HY-128806
### E3 ligase Ligand 9
A ligand for E3 ubiquitin ligase to form PROTACs or SNIPERs.

HY-128810
### E3 ligase Ligand 13
A ligand for E3 ubiquitin ligase to form PROTACs.

## Others

HY-128837
### Nutlin carboxylic acid
A Nutlin 3-based **MDM2** ligand can be connected to the ligand for protein by a linker to form PROTACs.

HY-131385
### KB02-COOH
A fragment of synthesis of ubiquitin E3 ligase ligand KB02 to form KB02-JQ1 and KB02-SLF.

HY-13650
### Indisulam
A carbonic anhydrase inhibitor with anticancer activity via recruitment to **DCAF15**.

HY-130842
### β-Naphthoflavone-CH2-Br
An arylhydrocarbon receptor (**AhR**) ligand used to synthesize β-NF-JQ1.

HY-130269
### β-Naphthoflavone-CH2-OH
A ligand for arylhydrocarbon receptor (**AhR**) E3 ligase.

HY-125292
### NV03
A potent and selective antagonist of UHRF1- H3K9me3 interaction by binding to UHRF1 tandem tudor domain.

# PROTAC Linkers

The linker is a bridge connecting the E3 ligase ligand and target protein ligand. According to the composition, PROTAC Linkers can be divided into PEG, alkyl chain, heteroaryl chain and other fragments. According to the function, the linkers can be divided into ordinary, clickable, and photo-switchable linkers, etc. According to the connecting unit, the linkers can be classified into hydroxyl, amino, mercapto, carboxyl, halogen, alkynyl, and azide, etc.

There is no mature scheme for the selection of PROTAC linkers so linkers are optimized based on structure-activity relationship. It is important to get the modest chain length, because linkers with too short or too long length both decrease the degradation activity[6].

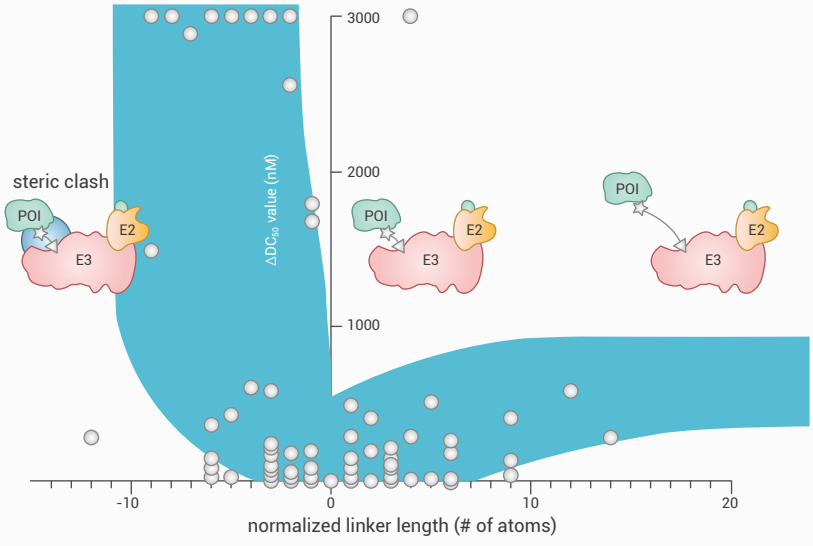



Figure 6. Effect of Linker length on PROTAC's activity[6].

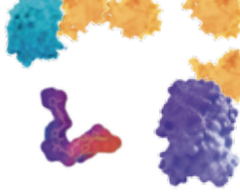
MCE can provide Ligands for E3 ligases with various structures and varieties. In addition to common categories, the unusual E3 ligands are also included. Related popular products are listed below:

## Alkyl Motifs

HY-30105
**N-Boc-piperazine**
Amino/amino connector.

HY-107608
**Leukotriene B4**
Carboxyl/hydroxyl/double bond connector.

HY-133405
**Boc-NH-O-C1-NHS ester**
Carboxyl/amino connector.



## Alkyl Motifs

HY-W004701
**Br-C3-methyl ester**
Halogen/carboxyl connector.

HY-113336B
**(±)15-HETE**
Carboxyl/hydroxyl/double bond connector.

HY-W014099
**Boc-NH-C4-acid**
Carboxyl/amino connector.

HY-40171
**NH2-C2-NH-Boc**
Amino/amino connector.

HY-W018464
**N-Boc-serinol**
Hydroxyl/amino connector.

HY-W014831
**11-Aminoundecanoic acid**
Amino/carboxyl connector.

## PEG Motifs

HY-W008005
**Amino-PEG4-alcohol**
Amino/hydroxyl connector

HY-W017772
**Boc-NH-PEG3**
Hydroxyl/amino connector

HY-130541
**Propargyl-PEG2-OH**
Alkyne /hydroxyl connector

HY-W007713
**Fmoc-8-amino-3,6-dioxaoctanoic acid**
Carboxyl/amino connector

HY-42488
**Hydroxy-PEG3-(CH2)2-Boc**
Hydroxyl/carboxyl connector

HY-W040246
**Fmoc-NH-PEG6-CH2CH2COOH**
Carboxyl/amino connector

HY-W004896
**Boc-NH-PEG2**
Hydroxyl/amino connector

HY-22335
**Amino-PEG4-C2-amine**
Amino/amino connector

HY-W016735
**Azido-PEG3-alcohol**
Azide/hydroxyl connector

## Aryl and Heteraryl Motifs

HY-141263
**Methyltetrazine-acid**
Carboxyl connector.

HY-W008574
**TGN-020**
Amino connector.

HY-113697
**Mal-amido-PEG2-C2-amido-Ph-C2-CO-AZD**
Mal connector.

# Building Blocks of Conjugates

MCE can also provide you with Target Protein Ligand-Linker Conjugates of hot target protein to meet your needs for scientific research. We have high-quality products and services. Related popular products are listed below:

## Target Protein Ligand-Linker Conjugates

HY-44148

### FAK ligand-Linker Conjugate 1

Extensively used for PROTAC-mediated protein degradation of **FAK**.

HY-141486

### Dual PARP EGFR ligand for PROTAC

Used in the synthesis of DP-C-4, which is CRBN-based dual PROTAC for simultaneous degradation of **EGFR** and **PARP**.

HY-139403

### MRTX849 ethoxypropanoic acid

Used in the synthesis of PROTAC LC-2 targeting **$KRAS^{G12C}$**.

MCE also provides E3 Ligase Ligand Linker Conjugates with novel and diverse structures derived from commonly used E3 ligands for rapid conjugation with relevant target protein ligands. Related popular products are listed below:

## E3 Ligase Ligand Linker Conjugates

HY-130737

### Pomalidomide 4'-alkylC5-acid

A synthesized E3 ligase ligand-linker conjugate based on **cereblon** ligand.

HY-103615

### Thalidomide-O-amido-C4-N3

A synthesized E3 ligase ligand-linker conjugate based on **cereblon** ligand.

HY-122725

### Lenalidomide-C5-NH2

A synthesized E3 ligase ligand-linker conjugate based on **cereblon** ligand.

HY-103608

### (*S*,*R*,*S*)-AHPC-(C3-PEG)2-C6-Cl

A synthesized E3 ligase ligand-linker conjugate based on **VHL** ligand.

HY-103600

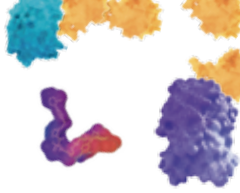
### (*S*,*R*,*S*)-AHPC-PEG1-N3

A synthesized E3 ligase ligand-linker conjugate based on **VHL** ligand.

HY-128812

### cIAP1 Ligand-Linker Conjugates 11

A synthesized E3 ligase ligand-linker conjugate based on **IAP** ligand.



# Target Protein Degraders

PROTAC (PROteolysis-TArgeting Chimera) is a heterobifunctional nano molecule containing two different ligands, ligand for ubiquitin E3 and ligand for the target protein. The two parts are connected by the linker to form a trimer complex, target protein ligand-linker-E3 ligase ligand. The polymer works by targeting protein, using organism's protein-degradation pathway.

Along with PROTAC, there are also other target protein degraders similar to the structure and mechanism of PROTAC like LYTAC, AUTAC and SNIPER.

Lysosome targeting chimera (LYTAC) degrades target proteins via the lysosomal pathway rather than the common proteasome pathway. LYTAC degrades target proteins by binding to the asialoglycoprotein receptor on lysosome through its asialoglycoprotein receptor ligand. Another side of LYTAC is usually an antibody so it can bind to the target protein for degradation[7].

Autophagy-targeting chimera (AUTAC) degrades target proteins via the lysosomal pathway rather than the common proteasome pathway. One end of AUTAC is the target protein ligand, the other end is a site of K63 ubiquitin modification, and the two parts are connected by a linker. AUTAC induces recognition of LC3 receptors of autophagosomes by K63-linked polyubiquitination and then the Target-AUTAC complex is phagocytosed and transferred into lysosomes for degradation[8].

Specific and Non-genetic inhibitors of apoptosis protein [IAP]-dependent Protein Erasers (SNIPERs), a class of small-molecule degraders, are designed to induce IAP-mediated ubiquitylation and proteasomal degradation of target proteins[9].

MCE can provide you with novel and diverse PROTACs, LYTACs, AUTACs and SNIPERs to meet your needs for scientific research. Related popular products are listed below:

## PROTAC

HY-112588
### dBET6
A highly potent, selective and cell-permeable degrader of **BET** based on PROTAC with antitumor activity.

HY-111556
### BSJ-03-123
A potent and novel **CDK6**-selective small-molecule degrader (PROTAC).

HY-129523
### PROTAC K-Ras Degrader-1
A potent **K-Ras** degrader based PROTAC, exhibits ≥70% degradation efficacy in SW1573 cells.

## PROTAC

HY-16954
### ARV-825
A **BRD4** degrader based on PROTAC technology which binds to BD1 and BD2 of BRD4.

HY-129602
### SD-36
A potent and efficacious PROTAC **STAT3** degrader.

HY-112155
### MS4078
An anaplastic lymphoma kinase (**ALK**) PROTAC.

HY-139039
### BSJ-4-116
A highly potent and selective **CDK12** degrader.

HY-130615
### PROTAC EED degrader-2
A polycomb repressive complex 2 (**PRC2**) inhibitor targeting the EED subunit.

HY-141438
### SIM1
A potent von Hippel-Lindau (VHL)-based trivalent PROTAC capable of degradation for all **BET** family members.

## LYTAC

HY-139482
### tri-GalNAc-COOH
An asialoglycoprotein receptor (ASGPR) ligand that can be used for LYTAC research.

HY-145013
### tri-GalNAc-COOH (acetylation)
The acetylated and modified form of tri-GalNAc-COOH. Can be used for the synthesis of LYTAC.

## AUTAC

HY-133869
### cGMP-HTL
A molecule contains a HT-ligand, a linker and the Cys-S-cGMP (autophagy tag).

HY-129652
### Halo PROTAC 1
A ligand having activity to bind to an intracellular proteins fused with HaloTag and a structure having activity to induce autophagy.

HY-134640
### AUTAC4
An AUTAC which can downregulate cytosolic proteins and promote targeted mitochondrial turnover via mitophagy.

## SNIPER

HY-111875
### SNIPER(BRD)-1
A degrader of both **BRD4**, **cIAP1** , **cIAP2** and **XIAP**.

HY-111872
### SNIPER(ABL)-020
A degrader of **Bcr-Abl** via Dasatinib (ABL inhibitor) and Bestatin (IAP ligand).

HY-111876
### SNIPER(TACC3)-1
A degrader targets the **TACC3** protein for degradation based on IAP ligand.

HY-122825
### SNIPER(ER)-110
A degrader targets estrogen receptor (**ER**) for degradation based on IAP ligand.

HY-111858
### SNIPER(ABL)-050
A PROTAC conjugating Imatinib (ABL inhibitor) to MV-1 (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111861
### SNIPER(ABL)-024
A PROTAC conjugating GNF5 (ABL inhibitor) to LCL161 derivative (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111842
### PROTAC CRABP-II Degrader-3
A potent cellular retinoic acid binding protein (**CRABP-II**) degrader based on IAP ligand.

HY-111851
### SNIPER(ABL)-049
A PROTAC conjugating Imatinib (ABL inhibitor) to Bestatin (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111879
### Biotin-BS
A PROTAC contains two different ligands, methyl-bestatin (MeBS) for cIAP1 and biotin.

HY-111871
### SNIPER(ABL)-033
A PROTAC conjugating HG-7-85-01 (ABL inhibitor) to LCL161 derivative (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111863
### SNIPER(ABL)-047
A PROTAC conjugating HG-7-85-01 (ABL inhibitor) to MV-1 (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-129619
### SNIPER(ER)-87
A PROTAC conjugated to the estrogen receptor α (**ERα**) ligand 4-hydroxytamoxifen by a PEG linker, efficiently degrades the ERα protein.

HY-111854
### SNIPER(ABL)-015
A PROTAC conjugating GNF5 (ABL inhibitor) to MV-1 (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111874
### SNIPER(ABL)-039
A PROTAC conjugating Dasatinib (ABL inhibitor) to LCL161 derivative (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

HY-111859
### SNIPER(ABL)-058
A PRTAC conjugating Imatinib (ABL inhibitor) to LCL161 derivative (IAP ligand) with a linker, induces the reduction of **BCR-ABL** protein.

# Molecular Glues as Target Protein Degraders

Protein degradation agents based on the ubiquitin-proteasome pathway include a part of molecular glues. Molecular glues are a class of small molecule compounds that can induce or stabilize the interaction between proteins. If one of the proteins is ubiquitin ligase, molecular glue can cause another protein to undergo ubiquitin modification and degradation through the proteasome pathway, which is similar to PROTAC[10].

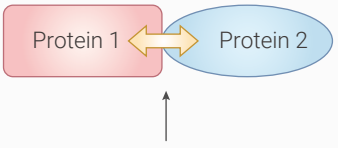



Figure 7. Molecular glue mechanism

Autophagosome-tethering compound (ATTEC) degrades target proteins via the lysosomal pathway rather than the common proteasome pathway. ATTEC degrades target proteins by molecular glue mechanism, and its molecular weight is smaller than AUTAC. ATTECs shorten the distance between LC3 receptor and target protein and then the target protein is phagocytosed and transferred into lysosome for degradation[11].

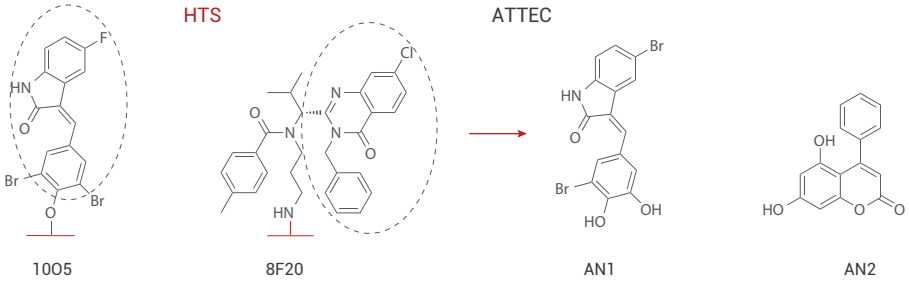



Figure 8. Structure of ATTECs[11].

MCE can provide you with molecular glues and ATTECs to meet your needs for scientific research. Related popular products are listed below:

## Molecular Glues

HY-129395
### Mezigdomide
A **cereblon** E3 ubiquitin ligase modulating drug, acts as a molecular glue.

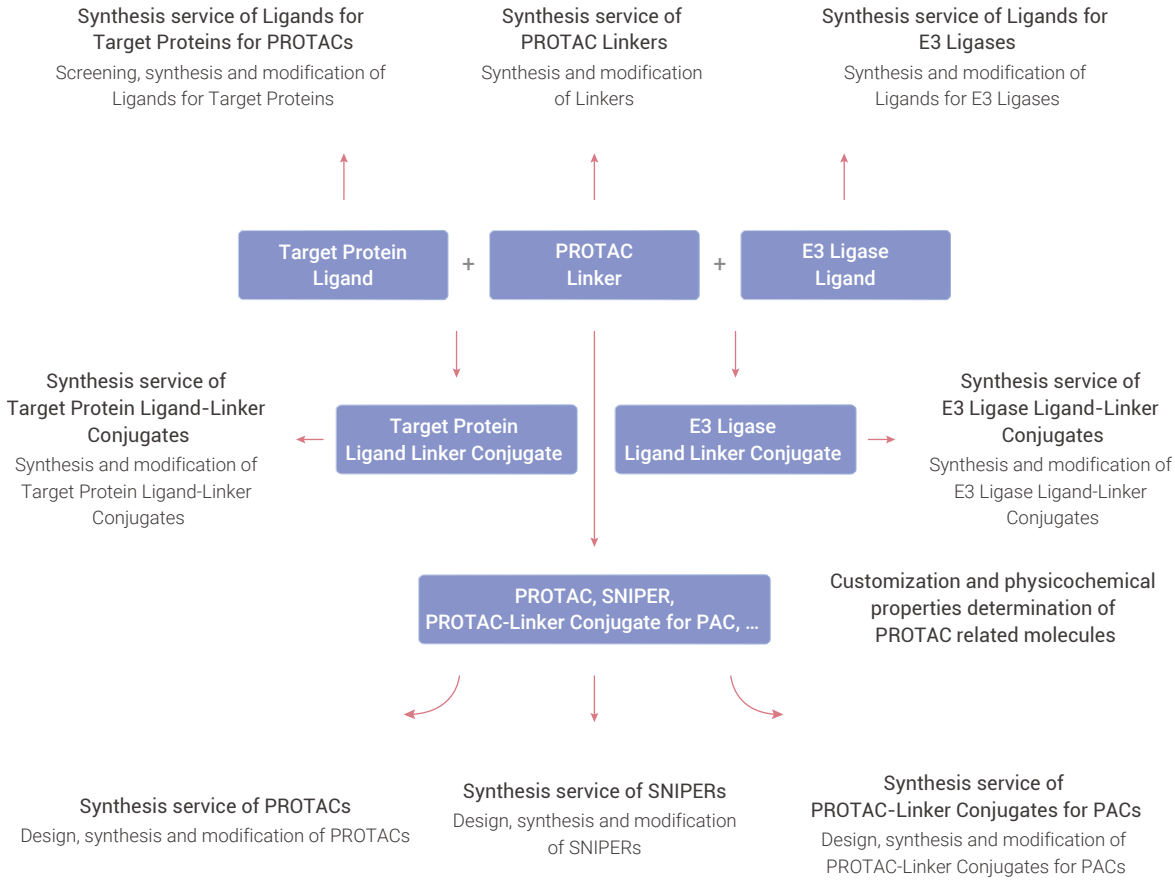
HY-130800
### Eragidomide
A first-in-class **GSPT1**-selective cereblon E3 ligase modulator, acts as a molecular glue.

## ATTEC

HY-130258
### LC3-mHTT-IN-AN1
A mHTT-LC3 linker compound, which interacts with both mutant huntingtin protein (mHTT) and LC3B but not with wtHTT or irrelevant control proteins.

# Technical Service Related to PROTACs

MCE can provide one-stop services for the design, synthesis, analysis, purification, optimization, detection and evaluation of PROTAC-related products (Ligands for E3 Ligases, PROTAC Linkers, Ligands for Target Protein for PROTACs, E3 Ligase Ligand-Linker Conjugates, Target Protein Ligand-Linker Conjugates, PROTACs, SNIPERs, PROTAC-Linker Conjugates for PAC). For the target proteins with unknown ligands, we have a variety of compound libraries and virtual screening libraries as the basis to screen protein-related ligands and construct appropriate PROTAC molecules.




## Online Consulting:

The corresponding scheme and price for PROTAC shall be determined after evaluation. For further information on service pricing or technical details, please email sales@MedChemExpress.com or contact MCE sales staff directly.

## Elements of PROTACs

PROTAC molecules are generally composed of three parts: Ligand for Target Protein, Linker and Ligand for E3 Ligase.

### 1. Selection of Ligand for E3 Ligase

E3 ligase is a key structure for target protein ubiquitination. Its ligands include many types, among which CRBN (Cereblon), VHL (von Hippel-Lindau), IAP and MDM2 are now frequently used. Ligands of CRBN with good drug-likeness are generally preferred, followed by VHL and IAP derived from endogenous ligand peptides. Consideration should also be given to the abundance of the corresponding E3 ligase in the cell where the specific target protein is located and the physical and chemical parameters of the final PROTAC.

### 2. Selection of Linker

Linkers are molecules that connect ligand for E3 ligase and ligand for the target protein. The properties of linkers have a great influence on the membrane permeability, efficacy and metabolic distribution of PROTAC. The ideal linker length should be able to maintain the lowest binding entropy of the two proteins without affecting their binding in space. There are also studies on multiple connectors and photoswitchable linkers.

### 3. Selection of Ligand for Target Protein

As the guiding group of PROTAC, the target protein ligand is responsible for capturing the target protein, which requires high coordination ability and selectivity. In practical applications, existing inhibitors and activators of proteins can be used as ligand candidates, while proteins without related molecule reports can be searched for ligands by high-throughput screening (HTS) and Virtual Screening. It is not necessary for ligands to be inhibitor or agonist, but it should be highly specific to the target protein.

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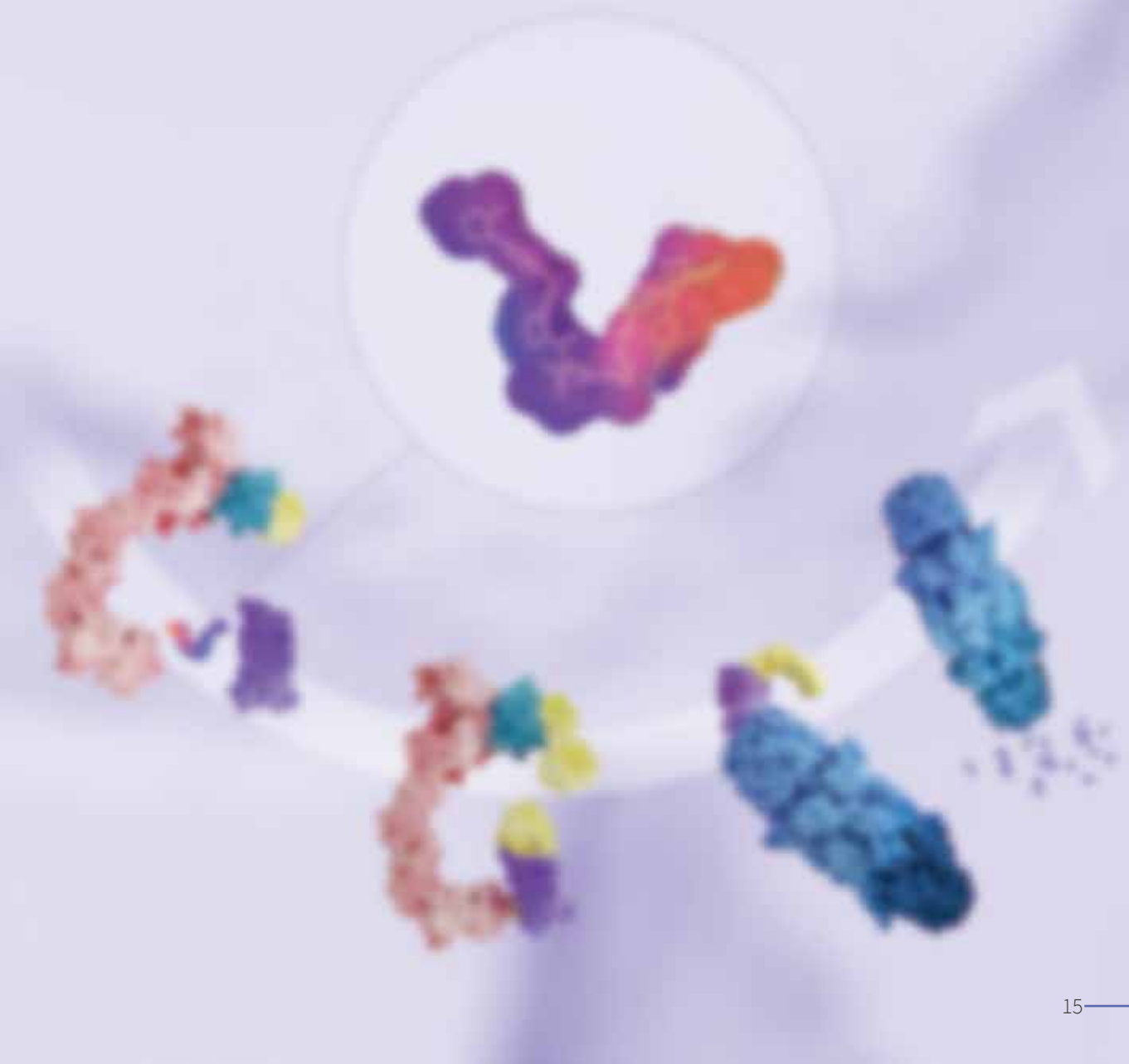

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