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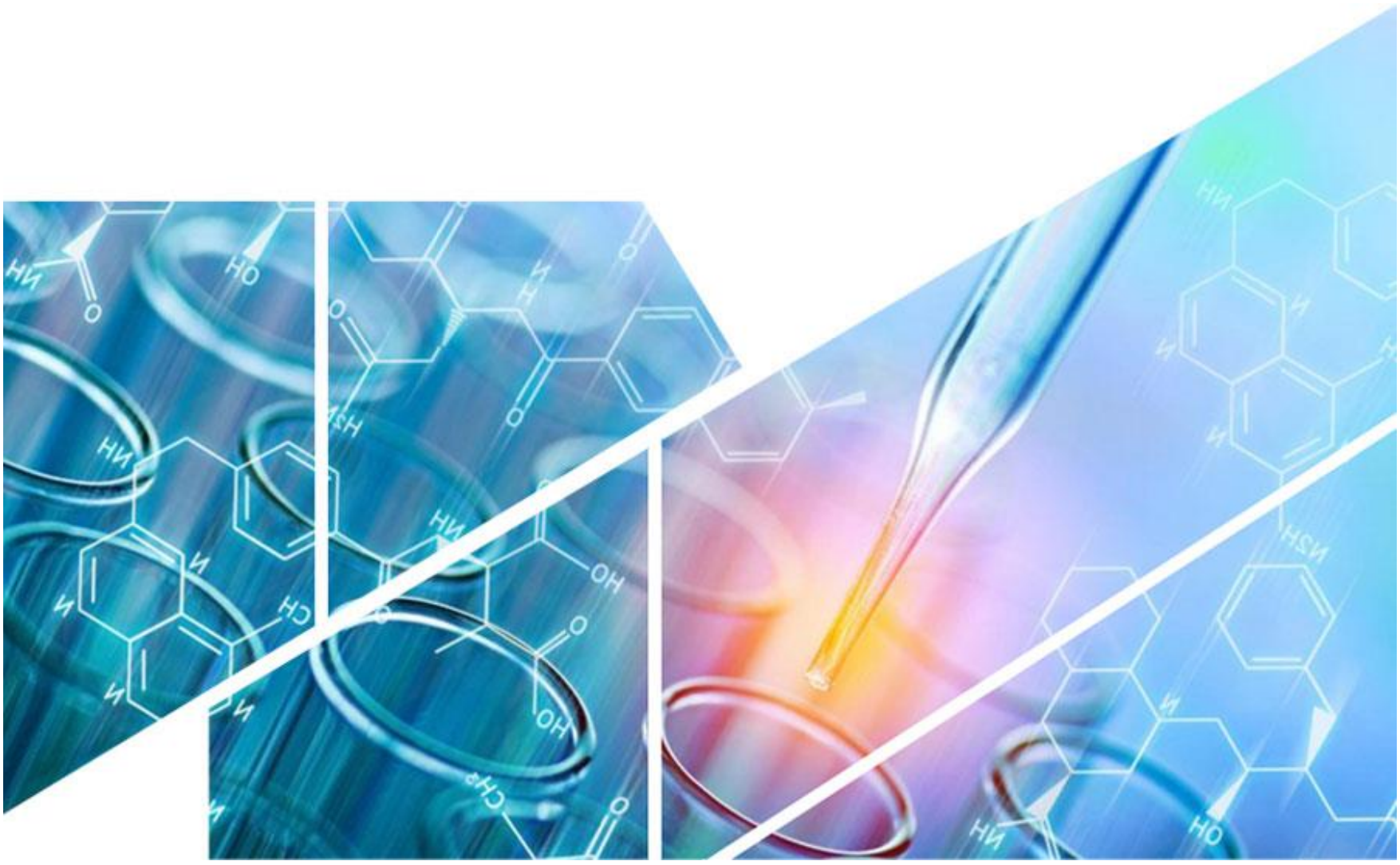
45-16 Ramsey Road Shirley, NY 11967, USA

HSP Inhibitors

(inhibitors, agonists and modulators)



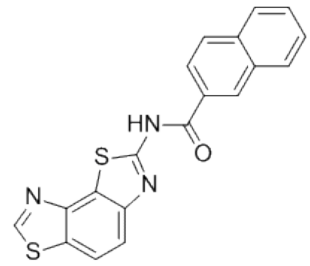
Heat-shock proteins (HSPs), or stress proteins, are highly conserved and present in all organisms and in all cells of all organisms. Selected HSPs, also known as chaperones, play crucial roles in folding/unfolding of proteins, assembly of multiprotein complexes, transport/sorting of proteins into correct subcellular compartments, cell-cycle control and signaling, and protection of cells against stress/apoptosis.

KIN1148 - CAS 1428729-56-9

Catalog Number: B0084-007650 **Price:** $398/100 mg

Molecular Weight: 361.44 **Molecular Formula:** C19H11N3OS2

Description: KIN1148, a small-molecule IRF3 agonist, associates with and activates recombinant RIG-I protein in cell-free assays. KIN1148 is a novel influenza vaccine adjuvant found to enhance flu vaccine efficacy.

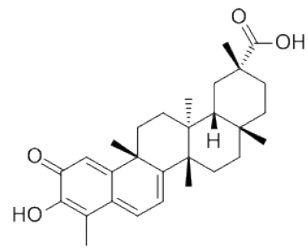


Celastrol - CAS 34157-83-0

Catalog Number: B0084-187070 **Price:** $198/10 mg; $798/1 g

Molecular Weight: 450.61 **Molecular Formula:** C29H38O4

Description: Celastrol (tripterine) is a chemical compound isolated from the root extracts of Tripterygium wilfordii (Thunder god vine) and Celastrus regelii. Celastrol is a pentacyclic triterpenoid and belongs to the family of quinone methides. In in vitro and in vivo animal experiments, celastrol exhibits antioxidant, anti-inflammatory, anticancer, and insecticidal activities. It has been shown to have obesity-controlling effects in mice.



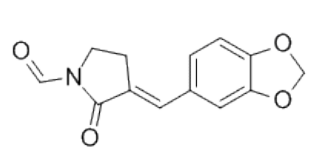
Celastrol
CAS: 34157-83-0

KNK437 - CAS 218924-25-5

Catalog Number: B0084-470906 **Price:** $278/50 mg

Molecular Weight: 245.23 **Molecular Formula:** C13H11NO4

Description: KNK437 is a pan-HSP inhibitor, which inhibits the synthesis of inducible HSPs, including HSP105, HSP72, and HSP40.

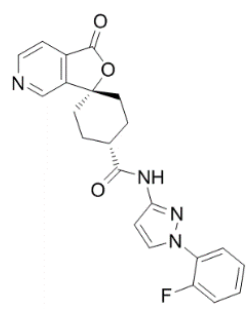


HSP70-IN-1 - CAS 1268273-90-0

Catalog Number:

Molecular Weight: 464.58 **Molecular Formula:** C24H28N6O2S

Description: HSP70-IN-1 is a heat shock protein (HSP) inhibitor that interferes with the formation of functional Hsp70-HOP-Hsp90 machinery, and it inhibits the growth of Kasumi-1 cells with an IC50 of 2.3 μM.

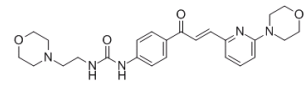


TRC051384 - CAS 867164-40-7

Catalog Number:

Molecular Weight: 465.54 **Molecular Formula:** C25H31N5O4

Description: TRC051384 is a heat shock protein 70 (HSP70) inducer.

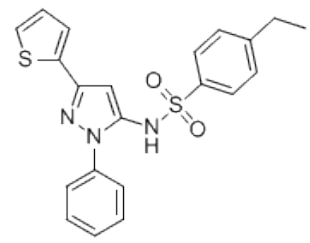


HSF1A - CAS 1196723-93-9

Catalog Number:

Molecular Weight: 409.52 **Molecular Formula:** C21H19N3O2S2

Description: HSF1A is a cell-permeable human heat shock factor protein (HSP1) activator.

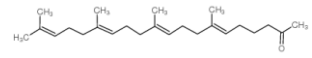


Geranylgeranylacetone - CAS 6809-52-5

Catalog Number: 6809-52-5

Molecular Weight: 330.55 **Molecular Formula:** C23H38O

Description: Geranylgeranylacetone is commonly utilized to protect the gastric mucosa in peptic ulcer disease can induce expression of HSP70, HSPB8, and HSPB1.

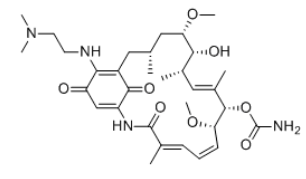


Alvespimycin - CAS 467214-20-6

Catalog Number: 467214-20-6

Molecular Weight: 616.75 **Molecular Formula:** C32H48N4O8

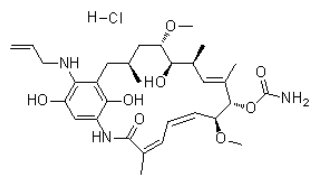
Description: Alvespimycin (17-DMAG; KOS-1022; NSC 707545) is a potent, H2O-soluble Hsp90 inhibitor with IC50 of 62 nM.17-DMAG displays ~2 times potency against human Hsp90 than 17-AAG, with IC50 of 62 nM versus 119 nM. In SKBR3 and SKOV3 cells which over-express Hsp90 client protein Her2, 17-DMAG causes down-regulation of Her2 with EC50 of 8 nM and 46 nM, respectively, as well as induction of Hsp70 with EC50 of 4 nM and 14 nM, respectively, leading to significant cytotoxicity with GI50 of 29 nM and 32 nM, respectively, consistent with Hsp90 inhibition.



Retaspimycin - CAS 857402-23-4

Catalog Number: 857402-23-4

Molecular Weight: 587.70 **Molecular Formula:** C31H45N3O8

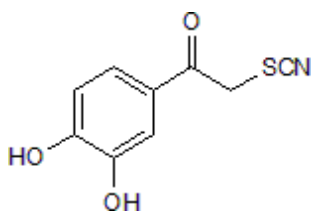


Description: Retaspimycin(IPI 504) is a small-molecule inhibitor of heat shock protein 90 (Hsp90) with antiproliferative and antineoplastic activities.Retaspimycin binds to and inhibits the cytosolic chaperone functions of Hsp90, which maintains the stability and functional shape of many oncogenic signaling proteins and may be overexpressed or overactive in tumor cells. Retaspimycin-mediated inhibition of Hsp90 promotes the proteasomal degradation of oncogenic signaling proteins in susceptible tumor cell populations, which may result in the induction of apoptosis.

BIX - CAS 101714-41-4

Catalog Number:

Molecular Weight: 209.22 **Molecular Formula:** C9H7NO3S

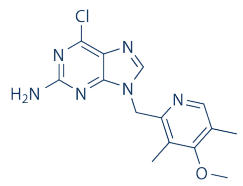


Description: BIX is a BiP (Hsp70-5) ER chaperone inducer that induces BiP expression in vitro and in vivo. BIX protects against ER-stress induced cell death in neuronal and retinal cell lines, and also protects against ischaemia-induced hippocampal cell death in vivo.

BIIB021 - CAS 848695-25-0

Catalog Number: 848695-25-0

Molecular Weight: 318.76 **Molecular Formula:** C14H15ClN6O

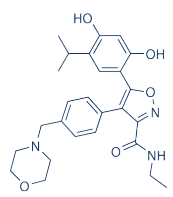


Description: BIIB021 is An orally active, purine-scaffold, small-molecule inhibitor of heat shock protein 90 (Hsp90) with potential antineoplastic activity. BIIB021 that is currently undergoing Phase II testing, may have broader application against tumors with acquired multidrug resistance or tumors located in organs protected by MDR proteins, such as the adrenal glands, brain and testis.

Luminespib - CAS 747412-49-3

Catalog Number: 747412-49-3

Molecular Weight: 465.54 **Molecular Formula:** C26H31N3O5

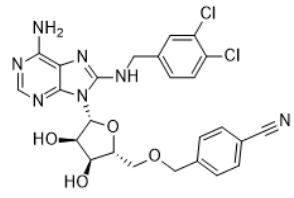


Description: Luminespib, also known as AUY-922 (or NVP-AUY922), is a derivative of 4,5-diarylisoxazole and a third-generation heat shock protein 90 (Hsp90) inhibitor with potential antineoplastic activity. Hsp90 inhibitor AUY922 has been shown to bind with high affinity to and inhibit Hsp90, resulting in the proteasomal degradation of oncogenic client proteins.

VER-155008 - CAS 1134156-31-2

Catalog Number: 1134156-31-2

Molecular Weight: 556.40 **Molecular Formula:** C25H23Cl2N7O4

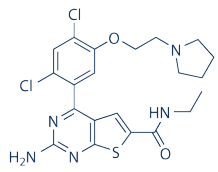


Description: VER-155008 is an adenosine-derived inhibitor of heat shock protein 70 (Hsp70; IC50 = 0.5 μM) that is selective over Hsp90.It targets the nucleotide-binding domain (NBD) of Hsp70 and similarly binds the NBDs of Hsp70 cognates Hsc70 (Ki = 10 μM) and glucose-regulated protein 78 (Grp78; KD = 80 nM).VER-155008 inhibits the proliferation of human breast and colon cancer cell lines, inducing apoptosis or caspase-independent cell death.It induces the proteasome-dependent degradation of Hsp90 client proteins and potentiates the apoptotic activity of Hsp90 inhibitors.VER-15508 also triggers paraptosis in anaplastic thyroid carcinoma cells.

NVP-BEP800 - CAS 847559-80-2

Catalog Number: 847559-80-2

Molecular Weight: 480.41 **Molecular Formula:** C21H23Cl2N5O2S

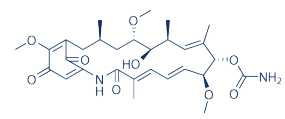


Description: NVP-BEP800 is a novel, fully synthetic Hsp90β inhibitor with IC50 of 58 nM, exhibits >70-fold selectivity against Hsp90 family members Grp94 and Trap-1.

Geldanamycin - CAS 30562-34-6

Catalog Number: 30562-34-6

Molecular Weight: 560.64 **Molecular Formula:** C29H40N2O9

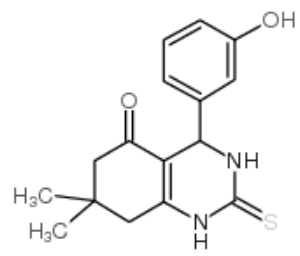


Description: Geldanamycin is a benzoquinone ansamycin antibiotic that binds to Hsp90 (Heat Shock Protein 90) and inhibits its function. Hsp90 client proteins play important roles in the regulation of the cell cycle, cell growth, cell survival, apoptosis, angiogenesis and oncogenesis. Hsp90-geldanamycin complex. PDB 1yet Geldanamycin induces the degradation of proteins that are mutated in tumor cells such as v-Src, Bcr-Abl and p53 preferentially over their normal cellular counterparts. This effect is mediated via Hsp90. Despite its potent antitumor potential, geldanamycin presents several major drawbacks as a drug candidate (namely, hepatotoxicity) that have led to the development of geldanamycin analogues.

Dimethylenastron - CAS 863774-58-7

Catalog Number: 863774-58-7

Molecular Weight: 302.39 **Molecular Formula:** C16H18N2O2S

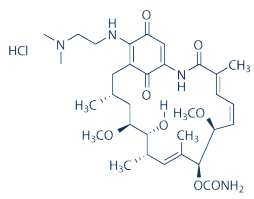


Description: Dimethylenastron is an inhibitor of mitotic motor kinesin Eg5 (IC50 = 200 nM).The inhibition of kinesin Eg5 by small molecules such as monastrol is currently evaluated as an approach to develop a novel class of antiproliferative drugs for the treatment of malignant tumours. .

Alvespimycin HCl - CAS 467214-21-7

Catalog Number: 467214-21-7

Molecular Weight: 653.21 **Molecular Formula:** C32H48N4O8•HCl

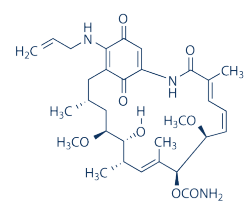


Description: Alvespimycin hydrochloride is the hydrochloride salt of alvespimycin, an analogue of the antineoplastic benzoquinone antibiotic geldanamycin. Alvespimycin binds to Hsp90, a chaperone protein that aids in the assembly, maturation and folding of proteins. Subsequently, the function of Hsp90 is inhibited, leading to the degradation and depletion of its client proteins such as kinases and transcription factors involved with cell cycle regulation and signal transduction.

Tanespimycin - CAS 75747-14-7

Catalog Number: 75747-14-7

Molecular Weight: 585.69 **Molecular Formula:** C31H43N3O8

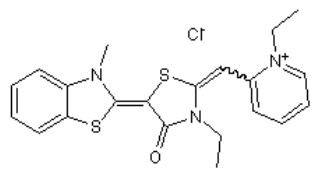


Description: 17-AAG is an orally bioavailable, small-molecule inhibitor of several receptor protein tyrosine kinases with potential antiangiogenic and antineoplastic activitie, binds to and inhibits the vascular endothelial growth factor receptors (VEGFRs) type 2 and 3, platelet-derived growth factor receptor beta (PDGFRb) and c-Kit, which may result in the inhibition of angiogenesis and cellular proliferation in tumors in which these receptors are upregulated. These telatinib-inhibited receptor protein tyrosine kinases are overexpressed or mutated in many tumor cell types and may play key roles in tumor angiogenesis and tumor cell proliferation. 17-AAG is a synthetic analogue of the benzoquinone ansamycin antibiotic geldanamycin and has also been found to inhibit the molecular chaperone Hsp90.

MKT 077 - CAS 147366-41-4

Catalog Number:

Molecular Weight: 432 **Molecular Formula:** C21H22ClN3OS2



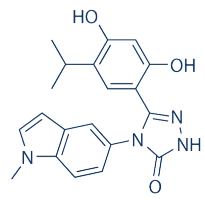
Description: MKT-077 is a cationic rhodacyanine dye. It shows antiproliferative activity against cancer cell lines with EC50s value of 1.4-2.2 μM in vitro through its ability to inhibit members of the heat shock protein 70 family of molecular chaperones.

Ganetespib - CAS 888216-25-9

Catalog Number: 888216-25-9

Molecular Weight: 364.40 **Molecular Formula:** C20H20N4O3

Description: Ganetespib, also known as STA-9090, is a synthetic small-molecule inhibitor of heat shock protein 90 (Hsp90) with potential antineoplastic activity. Hsp90 inhibitor STA-9090 binds to and inhibits Hsp90, resulting in the proteasomal degradation of oncogenic client proteins, the inhibition of cell proliferation and the elevation of heat shock protein 72 (Hsp72); it may inhibit the activity of multiple kinases, such as c-Kit, EGFR, and Bcr-Abl, which as client proteins depend on functional Hsp90 for maintenance. Hsp90, a 90 kDa molecular chaperone upregulated in a variety of tumor cells, plays a key role in the conformational maturation, stability and function of "client" proteins within the cell, many of which are involved in signal transduction, cell cycle regulation and apoptosis, including kinases, transcription factors and hormone receptors. Hsp72 exhibits anti-apoptotic functions; its up-regulation may be used as a surrogate marker for Hsp90 inhibition.

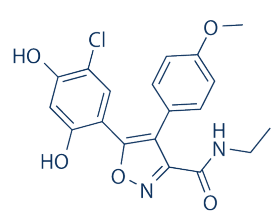


VER-50589 - CAS 747413-08-7

Catalog Number: 747413-08-7

Molecular Weight: 388.80 **Molecular Formula:** C19H17ClN2O5

Description: VER-50589 is a potent Hsp90 inhibitor with IC50 of 21 nM for Hsp90β.

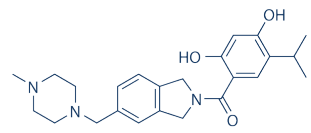


Onalespib - CAS 912999-49-6

Catalog Number: 912999-49-6

Molecular Weight: 409.52 **Molecular Formula:** C24H31N3O3

Description: Onalespib, also known as AT13387, is a synthetic, orally bioavailable, small-molecule inhibitor of heat shock protein 90 (Hsp90) with potential antineoplastic activity. AT13387 selectively binds to Hsp90, thereby inhibiting its chaperone function and promoting the degradation of oncogenic signaling proteins involved in tumor cell proliferation and survival.

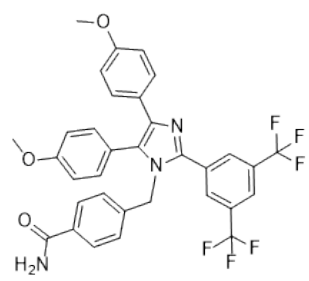


Apoptozole - CAS 1054543-47-3

Catalog Number:

Molecular Weight: 625.57 **Molecular Formula:** C33H25F6N3O3

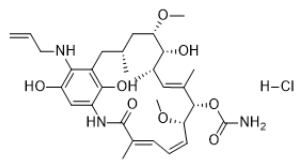
Description: Apoptozole, also known as Apoptosis Activator VII, is an apoptosis-inducing small molecule that inhibits the ATPase activity of heat shock cognate 70 (Hsc70) and Hsp70 (Kd = 210 and 140 nM, respectively). Apoptozole dose-dependently induces apoptosis in cancer cells (IC50 = 5-7 μM).



Retaspimycin Hydrochloride - CAS 857402-63-2

Catalog Number: 857402-63-2

Molecular Weight: 626.17 **Molecular Formula:** C31H48ClN3O8

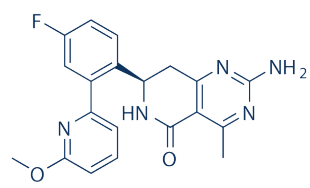


Description: Retaspimycin HCl(IPI504 HCl) is the hydrochloride salt of a small-molecule inhibitor of Hsp90 with antineoplastic and antiproliferative activities. Retaspimycin binds to and inhibits the cytosolic chaperone functions of Hsp90, which maintains the stability and functional shape of many oncogenic signaling proteins and has the possibililty to be overexpressed or overactive in tumor cells. Retaspimycin-mediated inhibition of Hsp90 promotes the proteasomal degradation of oncogenic signaling proteins in susceptible tumor cell populations, which may lead to the induction of apoptosis.

Hsp990 - CAS 934343-74-5

Catalog Number: 934343-74-5

Molecular Weight: 379.39 **Molecular Formula:** C20H18FN5O2

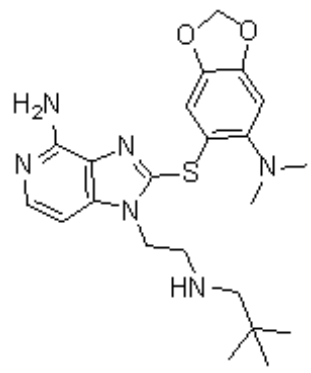


Description: Hsp980 is an orally bioavailable inhibitor of human heat-shock protein 90 (Hsp90) with potential antineoplastic activity. Hsp980 binds to and inhibits the activity of Hsp90, which may result in the proteasomal degradation of oncogenic client proteins, including HER2/ERBB2, and the inhibition of tumor cell proliferation. Hsp90, upregulated in a variety of tumor cells, is a molecular chaperone that plays a key role in the conformational maturation, stability and function of oncogenic signaling proteins, such as HER2/ERBB2, AKT, RAF1, BCR-ABL, and mutated p53, as well as many other molecules that are important in cell cycle regulation and/or immune responses.

Debio 0932 - CAS 1061318-81-7

Catalog Number: 1061318-81-7

Molecular Weight: 442.58 **Molecular Formula:** C22H30N6O2S



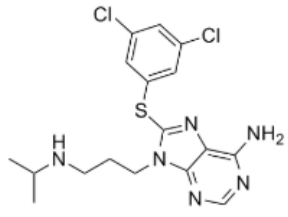
Description: Debio 0932, also known as CUDC-305, is a novel Hsp90 inhibitor with strong affinity for Hsp90 alpha/beta, high oral bioavailability and potent anti-proliferative activity against a broad range of cancer cell lines (with a mean IC50 of 220 nmol/L), including many non-small cell lung cancer (NSCLC) cell lines which are resistant to standard-of-care (SOC) agents. Debio 0932 potently inhibits tumour growth in subcutaneous xenograft models of a number of solid and haematological malignancies, including models of NSCLC which harbour mutations conferring acquired or primary erlotinib resistance. Furthermore, Debio 0932 is able to extend animal survival in models of brain metastasis due to its ability to cross the blood-brain barrier, and it enhances the activity of several standard-of-care agents in animal models of cancer.

PU-WS13 - CAS 1454619-14-7

Catalog Number: 1454619-14-7

Molecular Weight: 411.35 **Molecular Formula:** C17H20Cl2N6S

Description: PU-WS13 is a cell-permeable inhibitor of Grp94 (EC50 = 220 nM).It shows selectivity for Grp94 over the related Hsps Trap-1, Hsp90α, and Hsp90β. PU-WS13 blocks the proliferation of HER2 over-expressing SK-BR-3 cells in the sub-G1 phase and induces apoptosis, but does not affect the survival of normal cells significantly.It induces both necrosis and apoptosis in multiple myeloma cells but does not induce death in pre-B leukemic cells. Unlike pan-Hsp90 inhibitors, PU-WS13 inactivate a feedback heat-shock response.

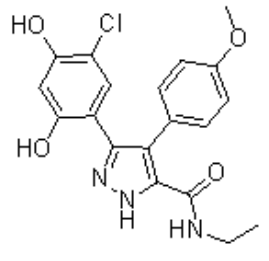


VER-49009 - CAS 558640-51-0

Catalog Number: 558640-51-0

Molecular Weight: 387.82 **Molecular Formula:** C19H18ClN3O4

Description: VER-49009 a protein 90 (HSP90) inhibitor(IC50= 47 nM).



ML346 - CAS 100872-83-1

Catalog Number: 100872-83-1

Molecular Weight: 272.26 **Molecular Formula:** C14H12N2O4

Description: ML346, a barbituric acid skeleton compound, is a novel activator of Hsp70 which could induce HSF-1-dependent chaperone expression and repair protein folding in both cellular and animal models. It has no obvious cytotoxicity and shows some extent of specif