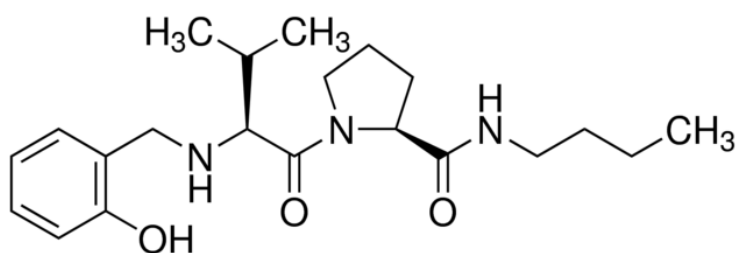


HRMS data for the *in vitro* tested compounds

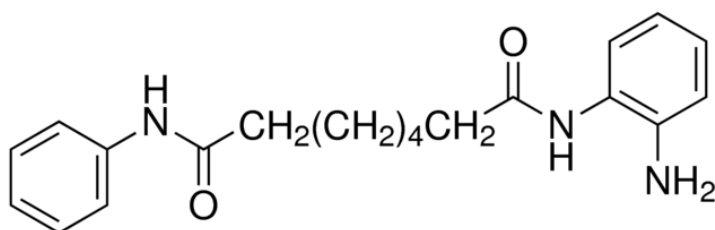
The purity of all compounds screened in biological assays was determined to be >95% by HPLC/MS analysis. HRMS were obtained on an Agilent 6540 UHD accurate-mass Q-TOF spectrometer equipped with a Dual AJS ESI source working in positive mode.



798827

(*S*)-*N*-Butyl-1-[(2-hydroxybenzyl)-*L*-valyl]pyrrolidine-2-carboxamide

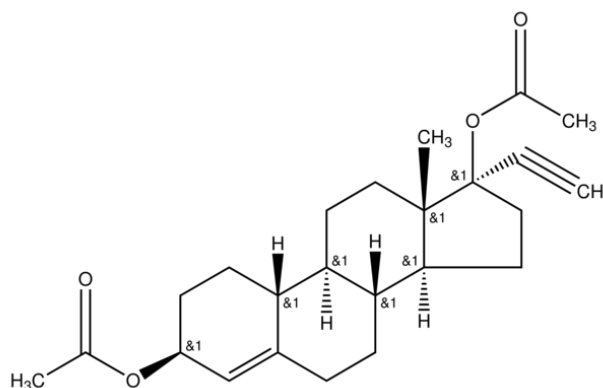
ESI-HRMS calcd for C₂₁H₃₃N₃O₃ [M+H]⁺: 375.5059; found 375.5021.



B8063

N1-(2-aminophenyl)-N8-phenyl-octanediamide

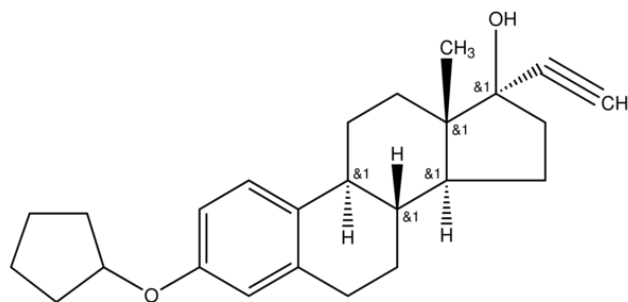
ESI-HRMS calcd for C₂₀H₂₅N₃O₂ [M+H]⁺: 339.4322; found 339.4398.



E7263

(3β, 17α)-19-Norpregn-4-en-20-yne-3,17-diol diacetate, 3β,17β-Diacetoxy-17α-ethynyl-4-estrene, Etynodiol acetate

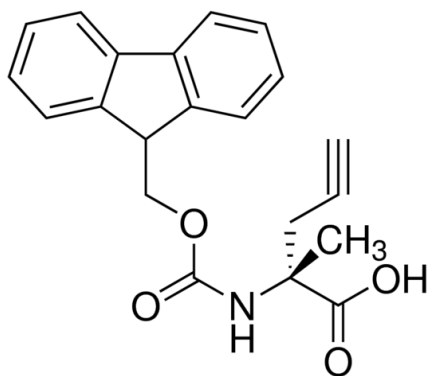
ESI-HRMS calcd for C₂₄H₃₂O₄ [M+H]⁺: 384.5095; found 384.5066.



E7887

17 α -Ethynyl-1,3,5(10)-estratriene-3,17 β -diol 3-cyclopentyl ether, Quinestrol

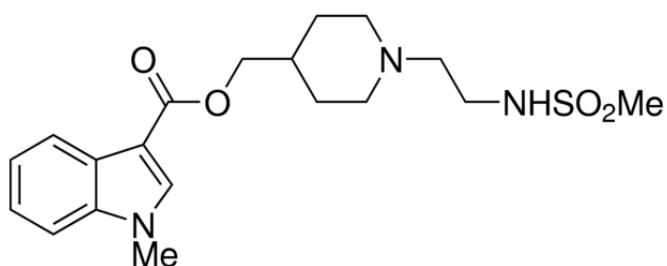
ESI-HRMS calcd for C₂₅H₃₂O₂ [M+H]⁺: 364.5214; found 364.5234.



F5312

(*R*)-*N*-Fmoc- α -propargyl-Ala-OH, (*R*)-*N*-Fmoc- α -propargylalanine

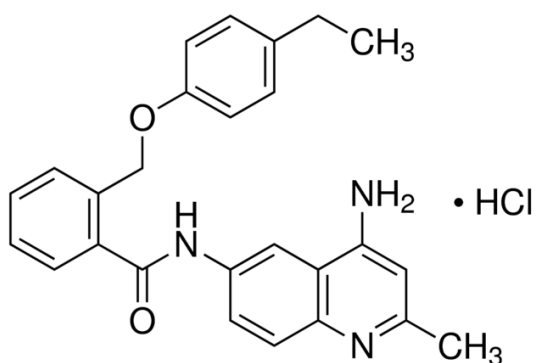
ESI-HRMS calcd for C₂₁H₁₉NO₄ [M+H]⁺: 349.3807; found 349.3789.



G5918

1-[2-[(Methylsulfonyl)-amino]ethyl]-4-piperidinyl]methyl 1-methyl-1H-indole-3-carboxylate

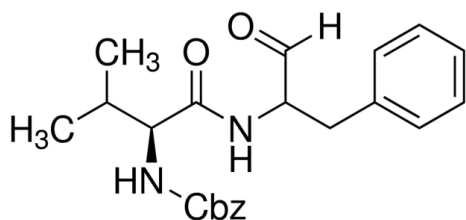
ESI-HRMS calcd for C₁₉H₂₇N₃O₄S [M+H]⁺: 393.5010; found 393.4991.



J3955

N-(4-amino-2-methylquinolin-6-yl)-2-(4-ethylphenoxy)methylbenzamide hydrochloride

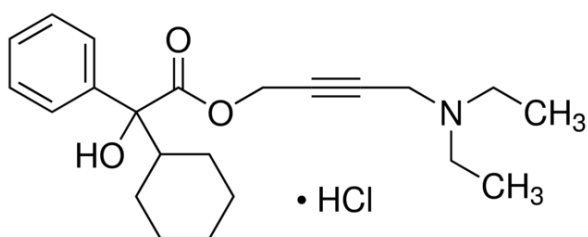
ESI-HRMS calcd for $C_{26}H_{25}N_3O_2 \cdot HCl$ $[M+H]^+$: 447.9575; found 447.9533.



M6690

Calpain Inhibitor III

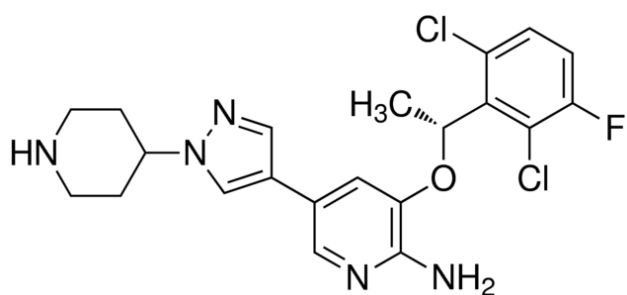
ESI-HRMS calcd for $C_{22}H_{26}N_2O_4$ $[M+H]^+$: 382.4538; found 382.4576.



O0288000

**α -Phenylcyclohexaneglycolic acid 4-(diethylamino)-2-butyne ester hydrochloride,
Oxybutynin chloride**

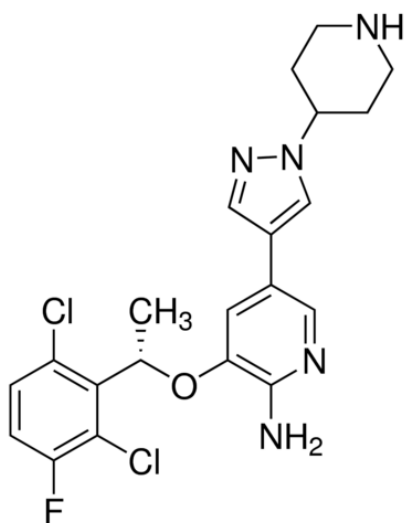
ESI-HRMS calcd for $C_{22}H_{31}NO_3 \cdot HCl$ $[M+H]^+$: 393.9482; found 393.9421.



PZ0191

Crizotinib

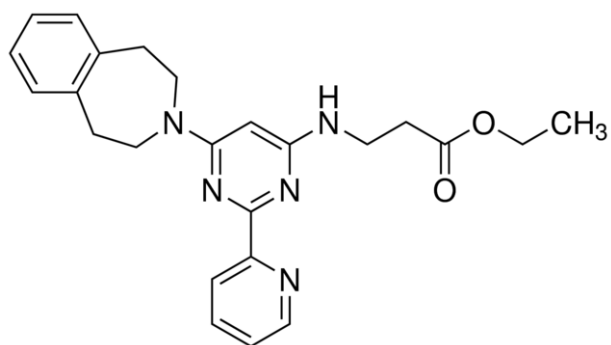
ESI-HRMS calcd for $C_{21}H_{22}Cl_2FN_5O$ $[M+H]^+$: 450.3374; found 450.3362.



PZ0240

(S)-Crizotinib

ESI-HRMS calcd for $C_{21}H_{22}Cl_2FN_5O$ $[M+H]^+$: 450.3374; found 450.3351.



SML0701

GSK-J4

Ethyl 3-(((6-(4,5-dihydro-1H-benzo[d]azepin-3(2H)-yl)-2-(pyridin-2-yl)pyrimidin-4-yl)amino)propanoate

ESI-HRMS calcd for $C_{24}H_{27}N_5O_2$ $[M+H]^+$: 417.5045; found 417.5011.