

Supplementary Table 1: Chemical structure of tested compounds

A. Bevacizumab, humanized anti-VEGF antibody (Avastin ®)¹

>1bj1_H|Fab-12, F(ab)-12, 12-IgG1, rhuMAb-VEGF|||VH-CH1 (VH(1-123)+CH1(124-215))|||||231||||MW 24867.8|MW 24867.8|

EVQLVESGGGLVQPGGSLRLSCAASGYTFTNYGMNWVRQAPGKGLEWVGWINTYTGEPTY
AADFKRRFTFSLDTSKSTAYLQMNSLRAEDTAVYYCAKYPHYYGSSHWFYFDVWVGQGLVT
VSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVL
QSSGLYSLSSVTVPSSSLGTQTYICNVNHKPSNTKVDKKVEPKSCDKTHT

>1bj1_J|Fab-12, F(ab)-12, 12-IgG1, rhuMAb-VEGF|||L-KAPPA (V-KAPPA(1-107)+C-KAPPA(108-213))|||||214||||MW 23451.0|MW 23451.0|

DIQMTQSPSSLSASVGDRVTITCSASQDISNYLNWYQQKPGKAPKVLIIYFTSSLHSGVPS
RFSGSGSGTDFTLTISLQPEDFATYYCQQYSTVPWTFGQGTKVEIKRTVAAPSVFIFPP
SDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLT
LSKADYEKHKVYACEVTHQGLSSPVTKSFNRGEC

>1bj1_K|Fab-12, F(ab)-12, 12-IgG1, rhuMAb-VEGF|||VH-CH1 (VH(1-123)+CH1(124-215))|||||231||||MW 24867.8|MW 24867.8|

EVQLVESGGGLVQPGGSLRLSCAASGYTFTNYGMNWVRQAPGKGLEWVGWINTYTGEPTY
AADFKRRFTFSLDTSKSTAYLQMNSLRAEDTAVYYCAKYPHYYGSSHWFYFDVWVGQGLVT
VSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVL
QSSGLYSLSSVTVPSSSLGTQTYICNVNHKPSNTKVDKKVEPKSCDKTHT

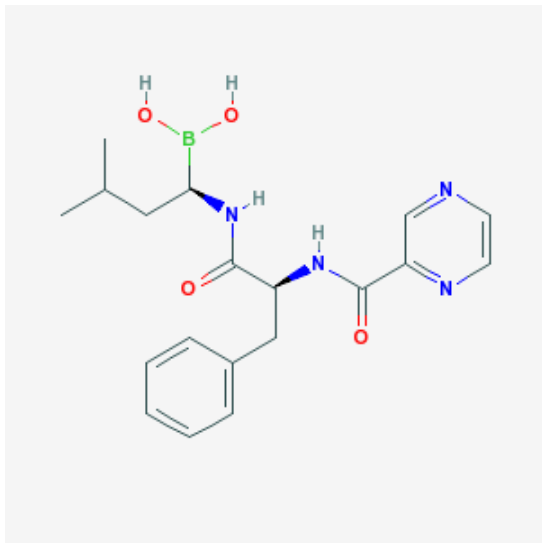
>1bj1_L|Fab-12, F(ab)-12, 12-IgG1, rhuMAb-VEGF|||L-KAPPA (V-KAPPA(1-107)+C-KAPPA(108-213))|||||214||||MW 23451.0|MW 23451.0|

DIQMTQSPSSLSASVGDRVTITCSASQDISNYLNWYQQKPGKAPKVLIIYFTSSLHSGVPS
RFSGSGSGTDFTLTISLQPEDFATYYCQQYSTVPWTFGQGTKVEIKRTVAAPSVFIFPP
SDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLT
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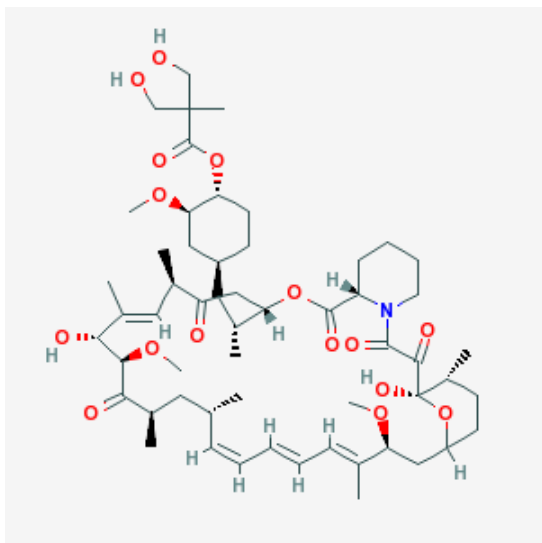
B. Bortezomib (Velcade®)²

[(1*R*)-3-methyl-1-(((2*S*)-3-phenyl-2-[(pyrazin-2-ylcarbonyl)amino]propanoyl)amino)butyl]boronic acid



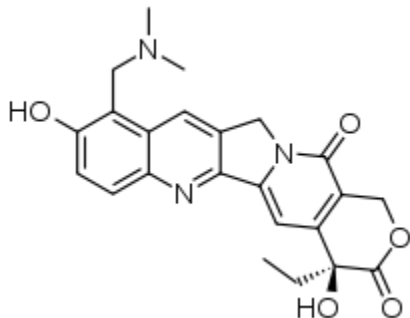
C. Temsirolimus (Torisel®)²

(1*R*,2*R*,4*S*)-4-((2*R*)-2-((3*S*,6*R*,7*E*,9*R*,10*R*,12*R*,14*S*,15*E*,17*E*,19*E*,21*S*,23*S*,26*R*,27*R*,34*aS*)-9,27-dihydroxy-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-1,5,11,28,29-pentaoxo-1,4,5,6,9,10,11,12,13,14,21,22,23,24,25,26,27,28,29,31,32,33,34,34a-tetracosahydro-3*H*-23,27-epoxy-pyrido[2,1-*c*][1,4]oxazacyclohentriacontin-3-yl)propyl)-2-methoxycyclohexyl 3-hydroxy-2-(hydroxymethyl)-2-methylpropanoate



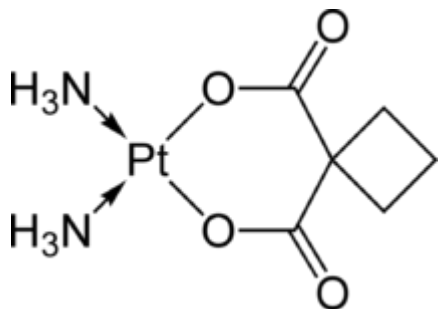
D. Topotecan (Hycamtin ®)²

(S)-10-[(dimethylamino)methyl]-4-ethyl-4,9-dihydroxy-1*H*-pyrano[3',4':6,7]indolizino[1,2-*b*]quinoline-3,14(4*H*,12*H*)-dione monohydrochloride



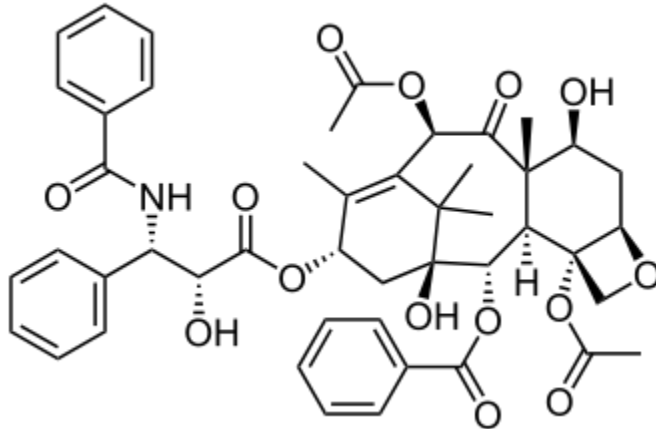
E. Carboplatin (Paraplatin ®)²

cis-diammine(1,1-cyclobutanedicarboxylato)platinum



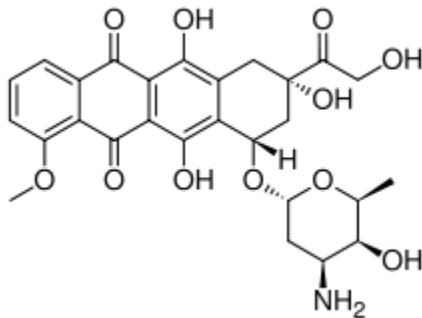
F. Paclitaxel (Taxol ®)²

(1S,2S,3R,4S,7R,9S,10S,12R,15S)-4,12-Diacetoxy-15-[[[(2R,3S)-3- (benzoylamino)-2-hydroxy-3- phenylpropanoyl]oxy]-1,9- dihydroxy-10,14,17,17-tetramethyl -11-oxo-6-oxatetracyclo [11.3.1.0~3,10~.0~4,7~] heptadec-13-en-2-yl rel-benzoate

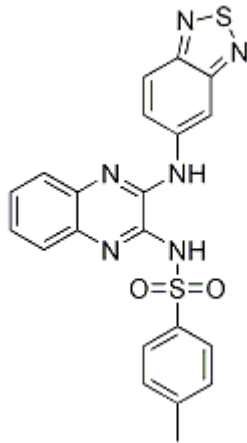


G. Pegylated liposomal doxorubicin hydrochloride (Doxil ®)²

(8S,10S)-10-(4-amino-5-hydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-7,8,9,10-tetrahydrotetracene-5,12-dione



H. XL147³



¹Drug Bank; www.drugbank.ca

²FDA; www.fda.gov

³Selleck Chemicals; www.selleckchem.com