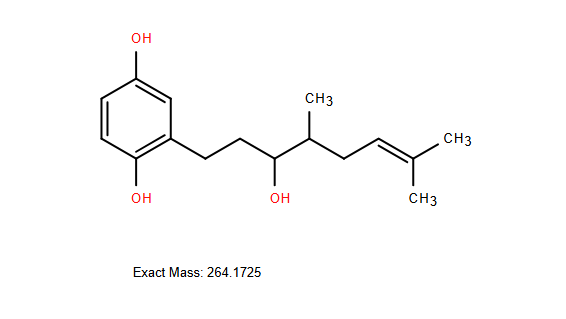
对于化合物的分析结果如下：

1. 将mol文件在AAT Bioquest平台（[MOL to SMILES Converter | AAT Bioquest](https://www.aatbio.com/tools/mol-to-smiles-converter)）转换为smi文件，其分子结构为：C1(=CC(=C(C=C1O)CCC(O)C(CC=C(C)C)C)O)



1. 使用Deepseek对化合物进行分析

### \*\*结构解析\*\*

1. \*\*核心结构\*\*：

苯环（`C1=CC=C(C=C1O)`）作为母核，带有两个羟基（`-OH`），分别在1位和3位（间苯二酚骨架）。

2. \*\*侧链\*\*：

一个羟基取代的丙基链（`CCC(O)`）连接在苯环的4位。

丙基的第二个碳上进一步连接一个分支烷基链：`C(CC=C(C)C)`，即一个含 \*\*异戊二烯单元\*\*（`CC=C(C)C`）的支链。

### \*\*可能的化合物类别\*\*

1. \*\*类黄酮或萜类酚衍生物\*\*：

异戊二烯侧链（`CC=C(C)C`）常见于 \*\*萜类化合物\*\*（如植物中的单萜或倍半萜酚）。

若苯环与其他环状结构相连，则可能属于 \*\*黄酮类\*\*（但当前结构无此特征）。

2. \*\*植物来源的酚类\*\*：

类似结构可见于天然产物，如 \*\*多酚类\*\*（如迷迭香酸衍生物）或 \*\*苯丙素类\*\*（侧链含丙烯基或烯丙基）。

### \*\*Smiles的标准化表示\*\*

修正后的Smiles：

`OC1=CC(=CC(=C1)CCC(O)C(CC=C(C)C)C)O`

### \*\*可能的天然类似物\*\*

\*\*苯丙烯衍生物\*\*（如丁子香酚类似物，但侧链更长且分支）

\*\*萜烯酚类\*\*（如某些精油成分，带异戊二烯基和酚羟基）、

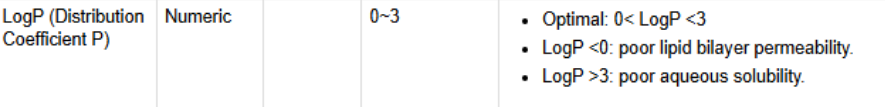
1. 化合物4作用的潜在靶点

使用化合物4smi分子结构在[SwissTargetPrediction](http://swisstargetprediction.ch/)进行潜在靶点预测，预测结果如下表：

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Target | Common name | Uniprot ID | ChEMBL ID | Target Class | Probability\* |
| Cyclooxygenase-2 | PTGS2 | P35354 | CHEMBL230 | Oxidoreductase | 0.1199 |
| Vascular endothelial growth factor receptor 2 | KDR | P35968 | CHEMBL279 | Kinase | 0.1120 |
| Estrogen receptor alpha | ESR1 | P03372 | CHEMBL206 | Nuclear receptor | 0.1120 |
| Estrogen receptor beta | ESR2 | Q92731 | CHEMBL242 | Nuclear receptor | 0.1120 |
| DNA polymerase beta (by homology) | POLB | P06746 | CHEMBL2392 | Enzyme | 0.1120 |
| Cannabinoid receptor 1 | CNR1 | P21554 | CHEMBL218 | Family A G protein-coupled receptor | 0.1120 |
| Neuropeptide Y receptor type 5 | NPY5R | Q15761 | CHEMBL4561 | Family A G protein-coupled receptor | 0.1120 |
| Insulin-like growth factor I receptor | IGF1R | P08069 | CHEMBL1957 | Kinase | 0.1120 |
| Tyrosine-protein kinase SRC | SRC | P12931 | CHEMBL267 | Kinase | 0.1120 |
| N-arachidonyl glycine receptor | GPR18 | Q14330 | CHEMBL2384898 | Family A G protein-coupled receptor | 0.1120 |
| Serine/threonine-protein kinase mTOR | MTOR | P42345 | CHEMBL2842 | Kinase | 0.1120 |
| Signal transducer and activator of transcription 3 | STAT3 | P40763 | CHEMBL4026 | Transcription factor | 0.1120 |
| Cyclin-dependent kinase 2 | CDK2 | P24941 | CHEMBL301 | Kinase | 0.1120 |
| Cannabinoid receptor 2 | CNR2 | P34972 | CHEMBL253 | Family A G protein-coupled receptor | 0.1120 |
| PI3-kinase p110-gamma subunit | PIK3CG | P48736 | CHEMBL3267 | Enzyme | 0.1120 |
| PI3-kinase p110-alpha subunit | PIK3CA | P42336 | CHEMBL4005 | Enzyme | 0.1120 |
| Vanilloid receptor | TRPV1 | Q8NER1 | CHEMBL4794 | Voltage-gated ion channel | 0.1120 |
| Cyclin-dependent kinase 1/cyclin B | CCNB3 CDK1 CCNB1 CCNB2 | Q8WWL7 P06493 P14635 O95067 | CHEMBL2094127 | Other cytosolic protein | 0.1120 |
| Glycogen synthase kinase-3 beta | GSK3B | P49841 | CHEMBL262 | Kinase | 0.1120 |
| Adenosine deaminase | ADA | P00813 | CHEMBL1910 | Hydrolase | 0.1120 |
| Glucocorticoid receptor | NR3C1 | P04150 | CHEMBL2034 | Nuclear receptor | 0.1120 |
| MAP kinase p38 alpha | MAPK14 | Q16539 | CHEMBL260 | Kinase | 0.1120 |
| Protein farnesyltransferase | FNTA FNTB | P49354 P49356 | CHEMBL2094108 | Enzyme | 0.1120 |
| DNA-dependent protein kinase | PRKDC | P78527 | CHEMBL3142 | Kinase | 0.1120 |
| Carbonic anhydrase VB | CA5B | Q9Y2D0 | CHEMBL3969 | Lyase | 0.1120 |
| Carbonic anhydrase VA | CA5A | P35218 | CHEMBL4789 | Lyase | 0.1120 |
| Serine/threonine-protein kinase Chk1 | CHEK1 | O14757 | CHEMBL4630 | Kinase | 0.1120 |
| Serine/threonine-protein kinase WEE1 | WEE1 | P30291 | CHEMBL5491 | Kinase | 0.1120 |
| ALK tyrosine kinase receptor | ALK | Q9UM73 | CHEMBL4247 | Kinase | 0.1120 |
| Heat shock protein HSP 90-beta | HSP90AB1 | P08238 | CHEMBL4303 | Other cytosolic protein | 0.1120 |
| Beta-secretase 1 | BACE1 | P56817 | CHEMBL4822 | Protease | 0.1120 |
| Sulfonylurea receptor 2 | ABCC9 | O60706 | CHEMBL1971 | Primary active transporter | 0.1120 |
| Tyrosine kinase non-receptor protein 2 | TNK2 | Q07912 | CHEMBL4599 | Kinase | 0.1120 |
| Thrombin | F2 | P00734 | CHEMBL204 | Protease | 0.1120 |
| Mitogen-activated protein kinase kinase kinase 14 | MAP3K14 | Q99558 | CHEMBL5888 | Kinase | 0.1120 |
| Tyrosine-protein kinase JAK1 | JAK1 | P23458 | CHEMBL2835 | Kinase | 0.1120 |
| Monoamine oxidase A (by homology) | MAOA | P21397 | CHEMBL1951 | Oxidoreductase | 0.1120 |
| Monoamine oxidase B (by homology) | MAOB | P27338 | CHEMBL2039 | Oxidoreductase | 0.1120 |
| Endothelin receptor ET-A | EDNRA | P25101 | CHEMBL252 | Family A G protein-coupled receptor | 0.1120 |
| Histone deacetylase 6 | HDAC6 | Q9UBN7 | CHEMBL1865 | Eraser | 0.1120 |
| PI3-kinase p110-alpha/p85-alpha | PIK3CA PIK3R1 | P42336 P27986 | CHEMBL2111367 | Enzyme | 0.1120 |
| Histone deacetylase 1 | HDAC1 | Q13547 | CHEMBL325 | Eraser | 0.1120 |
| dUTP pyrophosphatase | DUT | P33316 | CHEMBL5203 | Enzyme | 0.1120 |
| Tyrosine-protein kinase JAK2 | JAK2 | O60674 | CHEMBL2971 | Kinase | 0.1120 |
| Tyrosine-protein kinase JAK3 | JAK3 | P52333 | CHEMBL2148 | Kinase | 0.1120 |
| Matrix metalloproteinase 3 | MMP3 | P08254 | CHEMBL283 | Protease | 0.1120 |
| Matrix metalloproteinase 1 | MMP1 | P03956 | CHEMBL332 | Protease | 0.1120 |
| Matrix metalloproteinase 2 | MMP2 | P08253 | CHEMBL333 | Protease | 0.1120 |
| Tyrosine-protein kinase TYK2 | TYK2 | P29597 | CHEMBL3553 | Kinase | 0.1120 |
| Matrix metalloproteinase 7 | MMP7 | P09237 | CHEMBL4073 | Protease | 0.1120 |
| Matrix metalloproteinase 8 | MMP8 | P22894 | CHEMBL4588 | Protease | 0.1120 |
| Complement factor D | CFD | P00746 | CHEMBL2176771 | Protease | 0.1120 |
| Rho-associated protein kinase 2 | ROCK2 | O75116 | CHEMBL2973 | Kinase | 0.1120 |
| Beta-galactoside alpha-2,6-sialyltransferase 1 | ST6GAL1 | P15907 | CHEMBL3596075 | Transferase | 0.1120 |
| Serine/threonine-protein kinase PIM3 | PIM3 | Q86V86 | CHEMBL5407 | Kinase | 0.1120 |
| Liver glycogen phosphorylase | PYGL | P06737 | CHEMBL2568 | Enzyme | 0.1120 |
| c-Jun N-terminal kinase 3 | MAPK10 | P53779 | CHEMBL2637 | Kinase | 0.1120 |
| Eukaryotic translation initiation factor 2-alpha kinase 3 | EIF2AK3 | Q9NZJ5 | CHEMBL6030 | Kinase | 0.1120 |
| Tyrosine-protein kinase SYK | SYK | P43405 | CHEMBL2599 | Kinase | 0.1120 |
| Mammalian target of Rapamycin (mTORC1) | FKBP1A MTOR | P62942 P42345 | CHEMBL2221341 | Kinase | 0.1120 |
| Endothelin receptor ET-B | EDNRB | P24530 | CHEMBL1785 | Family A G protein-coupled receptor | 0.1120 |
| Cyclin-dependent kinase 1/cyclin B1 | CDK1 CCNB1 | P06493 P14635 | CHEMBL1907602 | Other cytosolic protein | 0.1120 |
| Cyclin-dependent kinase 2/cyclin E1 | CCNE1 CDK2 | P24864 P24941 | CHEMBL1907605 | Kinase | 0.1120 |
| Thrombin and coagulation factor X | F10 | P00742 | CHEMBL244 | Protease | 0.1120 |
| Phosphodiesterase 2A | PDE2A | O00408 | CHEMBL2652 | Phosphodiesterase | 0.1120 |
| Matrix metalloproteinase 13 | MMP13 | P45452 | CHEMBL280 | Protease | 0.1120 |
| Matrix metalloproteinase 9 | MMP9 | P14780 | CHEMBL321 | Protease | 0.1120 |
| Cytochrome P450 11B1 | CYP11B1 | P15538 | CHEMBL1908 | Cytochrome P450 | 0.1120 |
| Neprilysin | MME | P08473 | CHEMBL1944 | Protease | 0.1120 |
| Tyrosine-protein kinase receptor FLT3 | FLT3 | P36888 | CHEMBL1974 | Kinase | 0.1120 |
| Cyclin-dependent kinase 2/cyclin A | CDK2 CCNA1 CCNA2 | P24941 P78396 P20248 | CHEMBL2094128 | Other cytosolic protein | 0.1120 |
| Adenosine A1 receptor (by homology) | ADORA1 | P30542 | CHEMBL226 | Family A G protein-coupled receptor | 0.1120 |
| Protein kinase C beta | PRKCB | P05771 | CHEMBL3045 | Kinase | 0.1120 |
| ADAM17 | ADAM17 | P78536 | CHEMBL3706 | Protease | 0.1120 |
| Matrix metalloproteinase 14 | MMP14 | P50281 | CHEMBL3869 | Protease | 0.1120 |
| Serine/threonine-protein kinase RIPK2 | RIPK2 | O43353 | CHEMBL5014 | Kinase | 0.1120 |
| Melatonin receptor 1A | MTNR1A | P48039 | CHEMBL1945 | Family A G protein-coupled receptor | 0.1120 |
| Cytochrome P450 11B2 | CYP11B2 | P19099 | CHEMBL2722 | Cytochrome P450 | 0.1120 |
| Gamma-secretase | PSEN2 PSENEN NCSTN APH1A PSEN1 APH1B | P49810 Q9NZ42 Q92542 Q96BI3 P49768 Q8WW43 | CHEMBL2094135 | Protease | 0.1120 |
| Dual-specificity tyrosine-phosphorylation regulated kinase 1A | DYRK1A | Q13627 | CHEMBL2292 | Kinase | 0.1120 |
| PI3-kinase p110-delta subunit | PIK3CD | O00329 | CHEMBL3130 | Enzyme | 0.1120 |
| Dual specificity protein kinase CLK4 | CLK4 | Q9HAZ1 | CHEMBL4203 | Kinase | 0.1120 |
| Dual specificty protein kinase CLK1 | CLK1 | P49759 | CHEMBL4224 | Kinase | 0.1120 |
| Dual specificity protein kinase CLK2 | CLK2 | P49760 | CHEMBL4225 | Kinase | 0.1120 |
| Dual specificity protein kinase CLK3 | CLK3 | P49761 | CHEMBL4226 | Kinase | 0.1120 |
| Dual specificity tyrosine-phosphorylation-regulated kinase 1B | DYRK1B | Q9Y463 | CHEMBL5543 | Kinase | 0.1120 |
| Anandamide amidohydrolase | FAAH | O00519 | CHEMBL2243 | Enzyme | 0.1120 |
| Cytochrome P450 17A1 | CYP17A1 | P05093 | CHEMBL3522 | Cytochrome P450 | 0.1120 |
| Phenylethanolamine N-methyltransferase | PNMT | P11086 | CHEMBL4617 | Enzyme | 0.1120 |
| 5-lipoxygenase activating protein | ALOX5AP | P20292 | CHEMBL4550 | Other cytosolic protein | 0.1120 |
| Poly [ADP-ribose] polymerase-1 | PARP1 | P09874 | CHEMBL3105 | Enzyme | 0.1120 |
| Rho-associated protein kinase 1 | ROCK1 | Q13464 | CHEMBL3231 | Kinase | 0.1120 |
| Dual specificity mitogen-activated protein kinase kinase 1 | MAP2K1 | Q02750 | CHEMBL3587 | Kinase | 0.1120 |
| Proteinase activated receptor 4 | F2RL3 | Q96RI0 | CHEMBL4691 | Family A G protein-coupled receptor | 0.1120 |
| Muscarinic acetylcholine receptor M5 | CHRM5 | P08912 | CHEMBL2035 | Family A G protein-coupled receptor | 0.1120 |
| Prostatic acid phosphatase | ACPP | P15309 | CHEMBL2633 | Enzyme | 0.1120 |
| Cytochrome P450 2C9 | CYP2C9 | P11712 | CHEMBL3397 | Cytochrome P450 | 0.1120 |
| Cytochrome P450 2C19 | CYP2C19 | P33261 | CHEMBL3622 | Cytochrome P450 | 0.1120 |
| TGF-beta receptor type I | TGFBR1 | P36897 | CHEMBL4439 | Kinase | 0.1120 |
| c-Jun N-terminal kinase 1 | MAPK8 | P45983 | CHEMBL2276 | Kinase | 0.1120 |

1. 进行ADMET性质预测

ADMET性质指分子在有机体内的吸收(absorption)、分布(distribution)、代谢(metabolism)、排泄(excretion)和毒性(toxicity)等性质。

这里关注化合物的脂溶性，即LogP。

使用neurosnap（[🧬 Neurosnap | Easy Online Bioinformatics Tools & Services](https://neurosnap.ai/services)）、ADMETlab3.0（[ADMETlab 3.0](https://admetlab3.scbdd.com/)）、CBDD GROUP（[CBDD-Group|Computational Biology and Drug Design Group](http://www.scbdd.com/)）进行ADMET性质预测。三个平台的LogP值分别为：3.3837、3.5924、3.384，结果均显示LogP>3，说明化合物4的脂溶性强，水溶性差。

1. 与化合物4相似的已上市药物

在DRUGBANK[Chemical Structure Search | DrugBank Online](https://go.drugbank.com/structures/search/small_molecule_drugs/structure)查找与化合物4相似度最高的上市药物，设置相似度阈值0.5，共获得8种药物，相似度集中在50%-60%。最后进行了相似药物对应疾病的查找。

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **drugname** | **NameCh** | **alias** | **similarity** | **disease** |
| **Amylmetacresol** | 戊间甲酚 |  | 0.585 | 主要用作含漱液或含片，治疗口腔炎症 |
| **Cannabidiol** | 大麻二酚 |  | 0.568 | A、神经退行性疾病：如阿尔兹海默症、帕金森等；B、精神类疾病：如抑郁症、焦虑症、创伤后应激障碍等；C、神经系统疾病：如癫痫、脑炎、脑膜炎等；D、各种疼痛：如痛经、偏头痛、癌症导致的疼痛等。 |
| **Latanoprost acid** | 拉坦前列素 | 沙拉坦、适利达 | 0.529 | 开角型青光眼，眼压过高患者的局部治疗 |
| **Latanoprost** | 同上 | 同上 | 0.509 | 同上 |
| **Vitamin E** | 维他命E | 生育酚或产妊酚 | 0.519 | 心血管病、帕金森症患者、高血压或心脑血管疾病、胎儿和婴儿的发育与生长 |
| **DL-alpha-Tocopherol** | 同上 | 同上 | 0.519 | 同上 |
| **Hexylresorcinol** | 4-己基间苯二酚 |  | 0.516 | 细菌性感染之中耳炎、外耳炎及疥藓、白藓、湿疹；具有抗菌、驱虫、防腐和抗肿瘤活性。Hexylresorcinol 可诱导鳞癌细胞凋亡 |
| **Dronabinol** | 屈大麻酚 |  | 0.509 | 用于治疗与AIDS患者体重减轻相关的神经性厌食症，以及化疗引起的恶心和呕吐 |