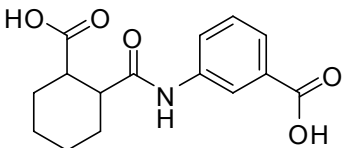
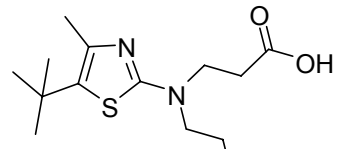
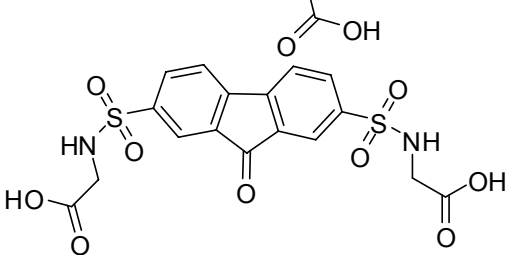
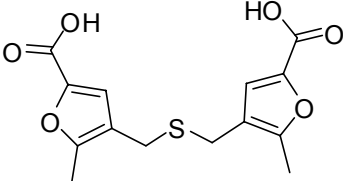
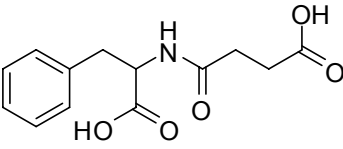
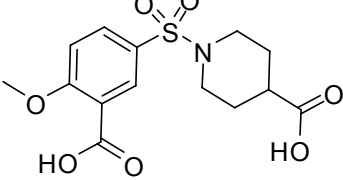
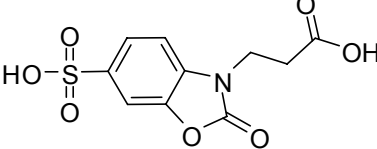
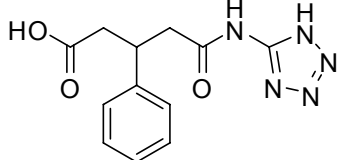
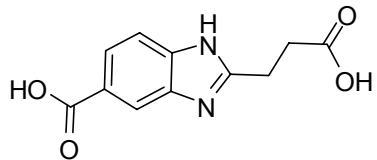


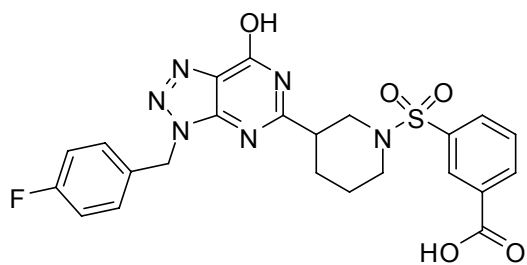
Supplementary Information

Table S1. Moderately Active Compounds Retrieved Using Pharmacophore H1NI2, A1NI2, A3NI1

S.No.	Structure	Activity IC ₅₀ (μM)
S1 H1NI2		32
S2 H1NI2		50
S3 H1NI2		27
S4 A1NI2		50
S5 A1NI2		33
S6 A1NI2		40
S7 A1NI2		40
S8 H1- A1NI2		33

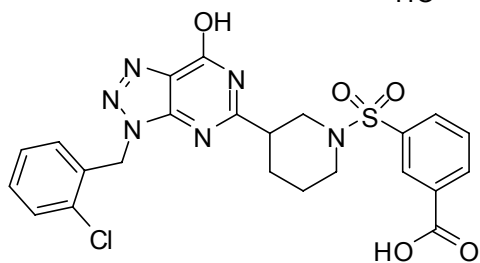
S9 H1- A1NI2		55
S10 H1- A1NI2		60
S11 H1- A1NI2		50
S12 H1- A1NI2		40
S13 H1- A1NI2		40
S14 H1- A1NI2		30
S15 H1- A1NI2		80
S16 H1- A1NI2		30 ± 2
S17 H1- A1NI2		80

S18
A3NI1



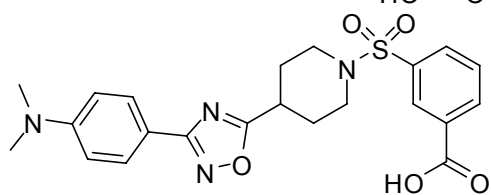
33

S19
A3NI1



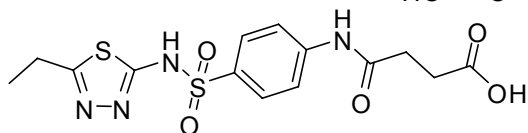
87

S20
A3NI1



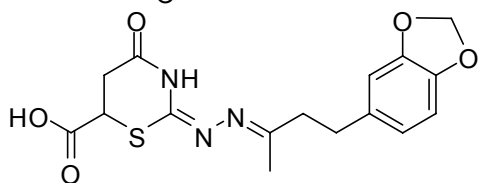
40

S21
A3NI1



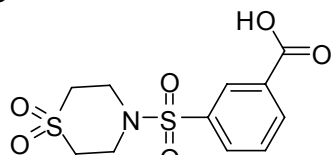
80

S22
A3NI1



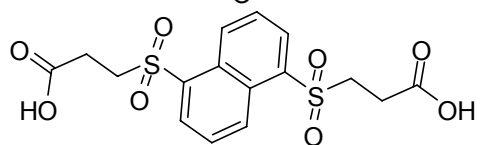
50

S23
A3NI1



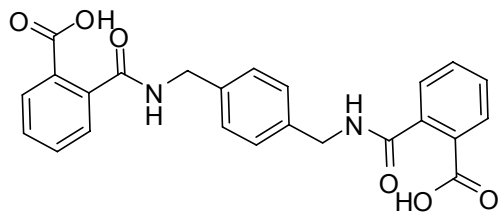
80

S24
Common



35

S25
Common

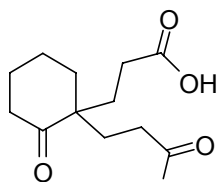


30

Table S2. Inactive Compounds Retrieved Using Pharmacophore Models H1NI2, A1NI2, A3NI1

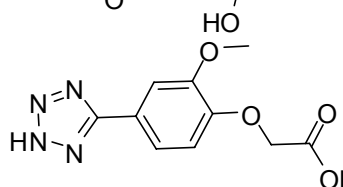
S.No.	Structure	Activity IC ₅₀ (μM)
S26 H1NI2		>100
S27 A1NI2		>100
S28 A1NI2		>100
S29 H1- A1NI2		>100
S30 H1- A1NI2		>100
S31 H1- A1NI2		>100
S32 H1- A1NI2		>100
S33 H1- A1NI2		>100

S34
H1-
A1NI2



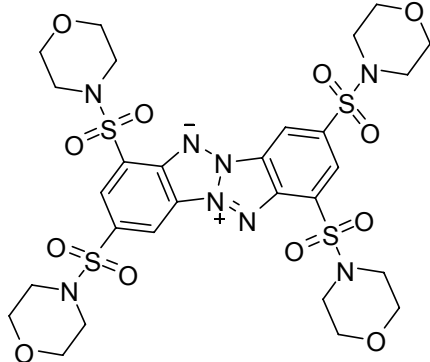
>100

S35
H1-
A1NI2



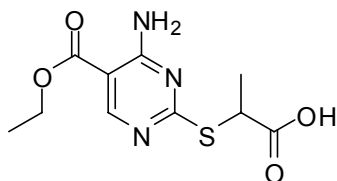
>100

S36
A3NI1



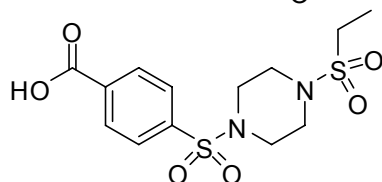
>100

S37
A3NI1



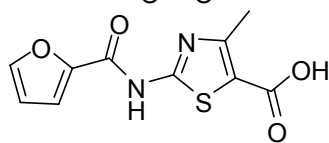
>100

S38
A3NI1



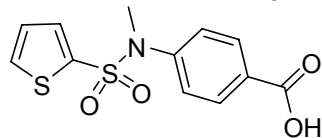
>100

S39
A3NI1



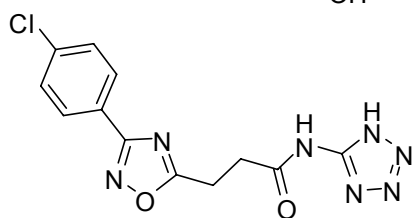
>100

S40
A3NI1

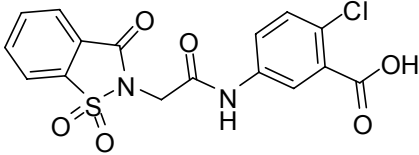
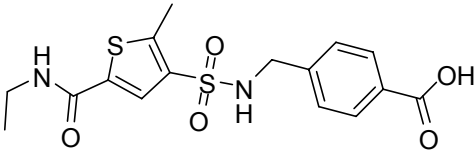
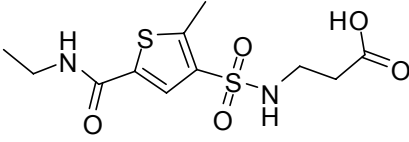
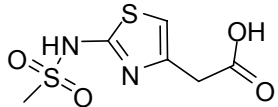
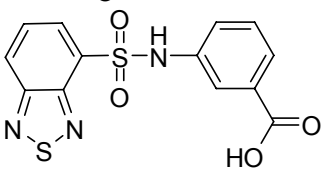
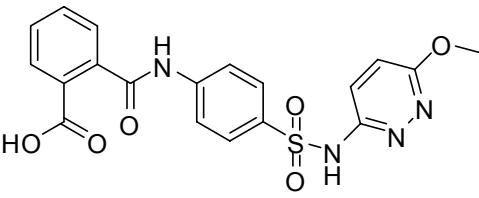
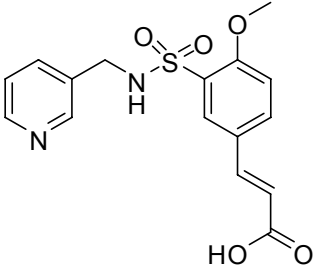
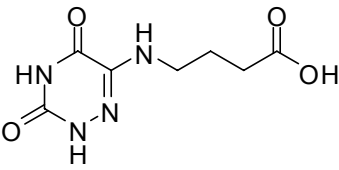
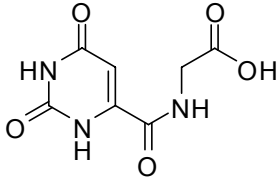
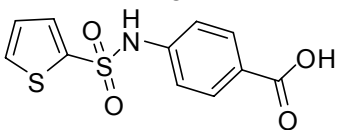


>100

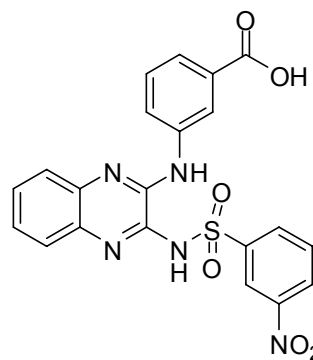
S41
A3NI1



>100

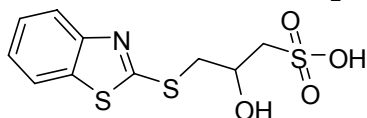
S42 A3NI1		>100
S43 A3NI1		>100
S44 A3NI1		>100
S45 A3NI1		>100
S46 A3NI1		>100
S47 A3NI1		>100
S48 A3NI1		>100
S49 A3NI1		>100
S50 A3NI1		>100
S51 A3NI1		>100

S52
A3NI1



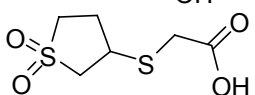
>100

S53
A3NI1



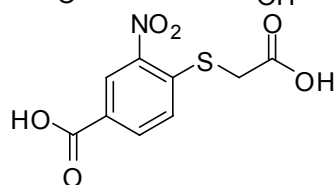
100

S54
A3NI1



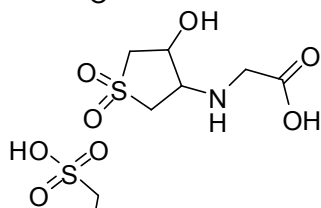
>100

S55
A3NI1



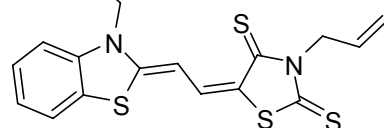
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S56
A3NI1



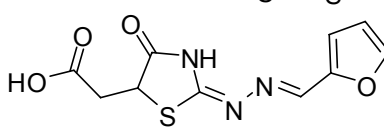
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S57
A3NI1



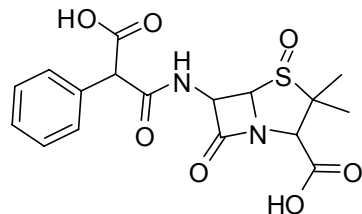
>100

S58
A3NI1



>100

S59
A3NI1



>100

Table S3. APE1 Inhibitory Activity of Compounds Retrieved
Using Pharmacophore Model A3H1

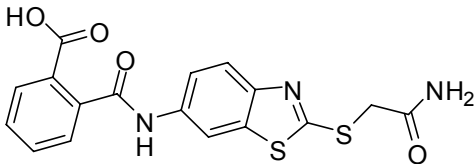
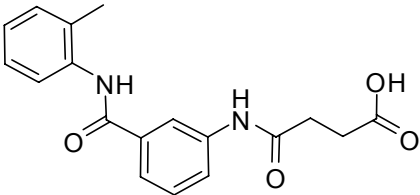
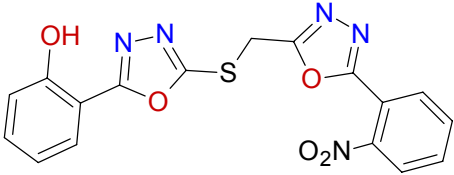
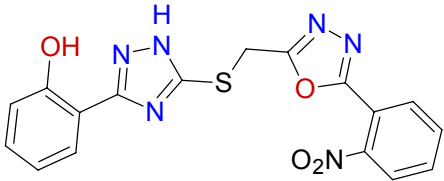
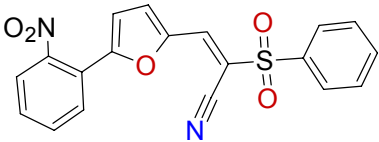
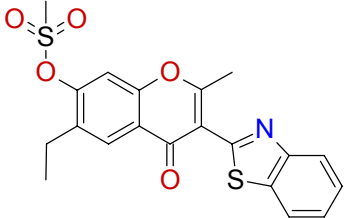
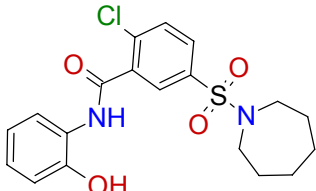
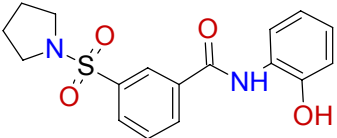
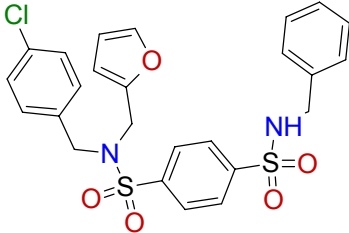
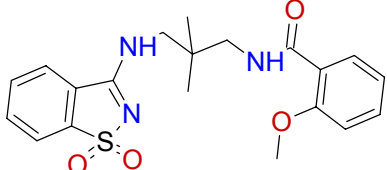
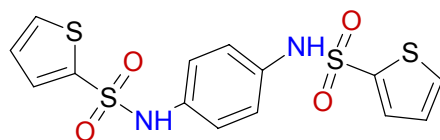
S.No.	Structure	Activity IC ₅₀ (μM)
S60		27
S61		35

Table S4. Inactive Compounds Retrieved Using Pharmacophore Model A3H1

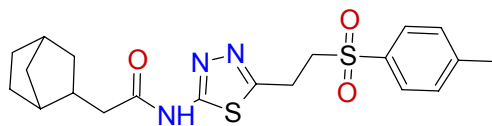
S.No.	Structure	Activity IC ₅₀ (μM)
S62		>100
S63		>100
S64		>100
S65		>100
S66		>100
S67		>100
S68		>100
S69		>100

S70



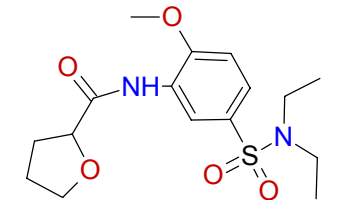
>100

S71



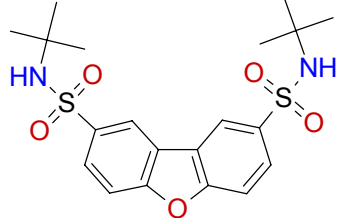
>100

S72



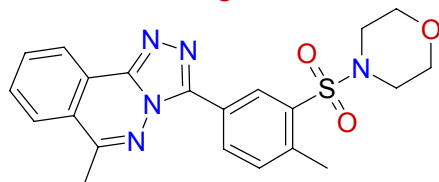
>100

S73



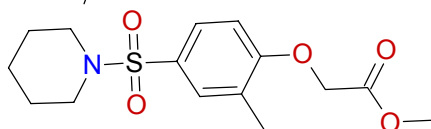
>100

S74



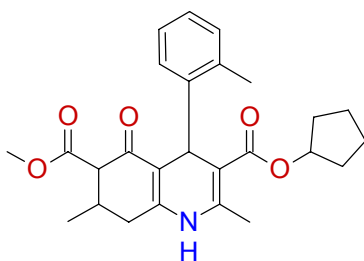
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S75



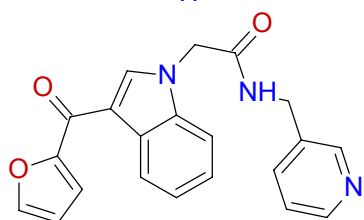
>100

S76



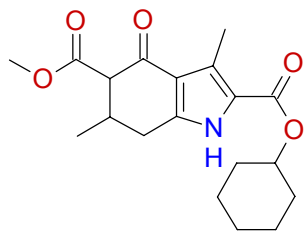
>100

S77



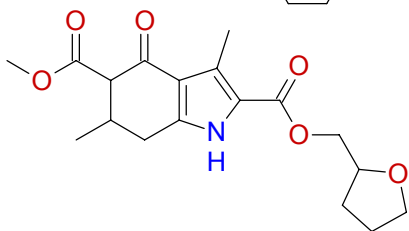
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S78



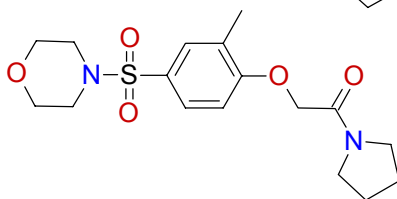
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S79



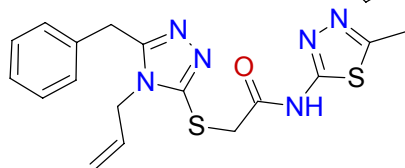
>100

S80



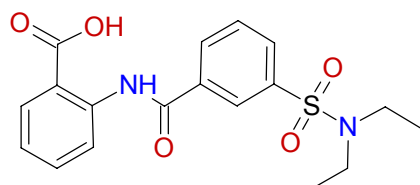
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S81



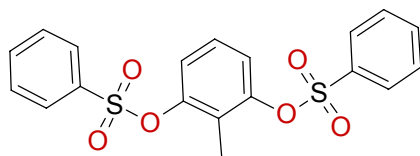
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S82



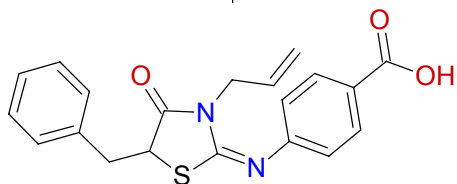
100

S83



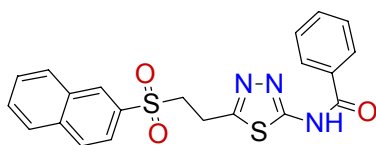
>100

S84



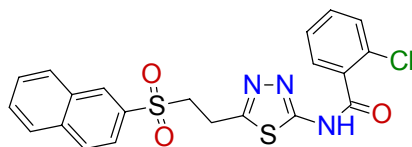
100

S85



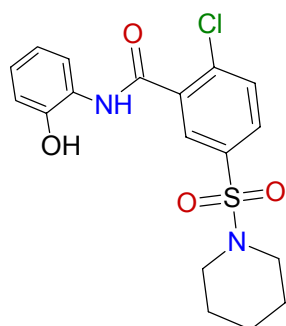
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S86



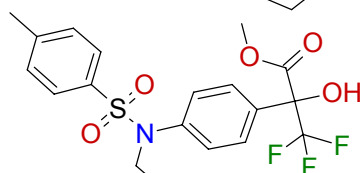
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S87



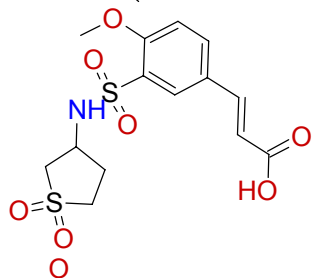
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S88



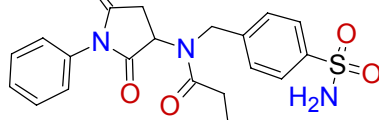
>100

S89



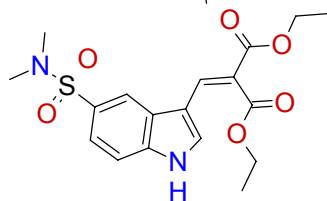
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S90



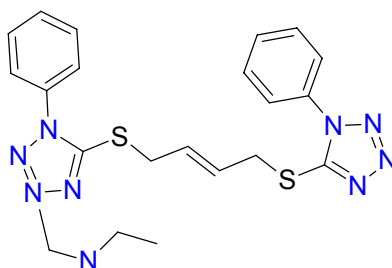
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S91



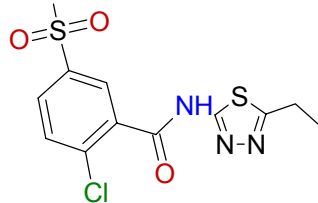
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S92

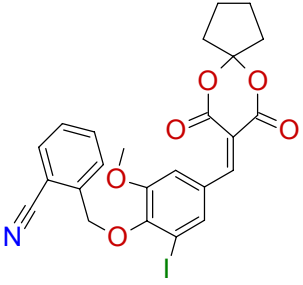
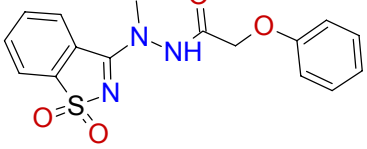
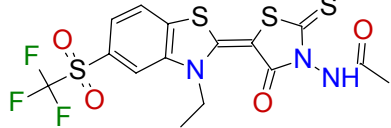
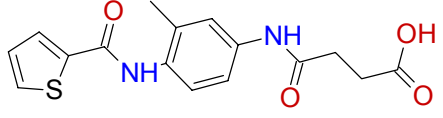
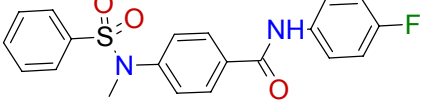
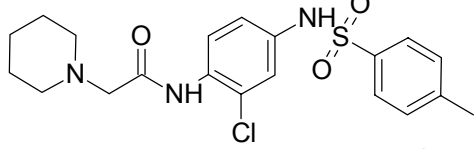
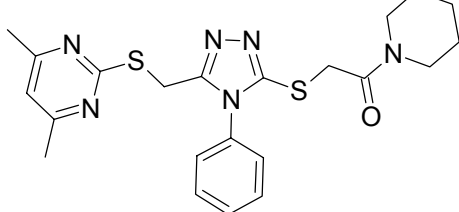
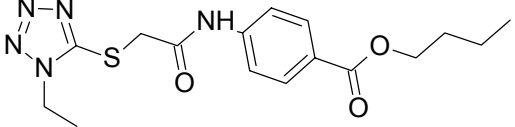
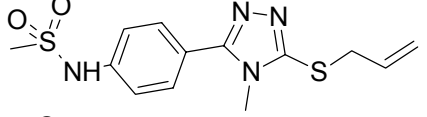
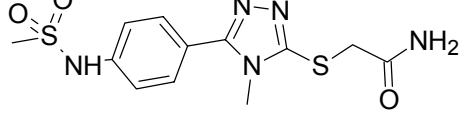


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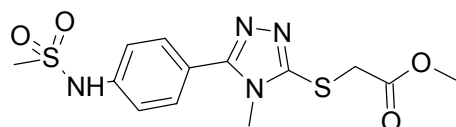
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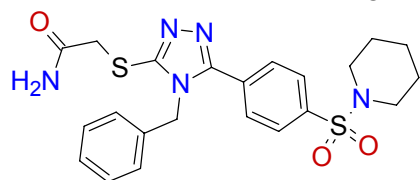
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S102		>100
S103		>100

S104



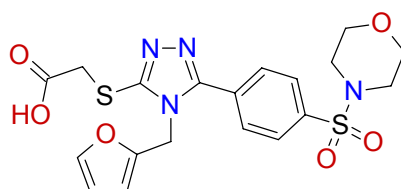
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S105



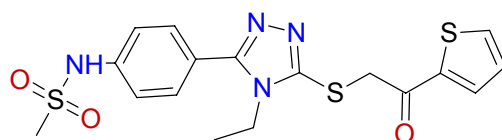
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S106



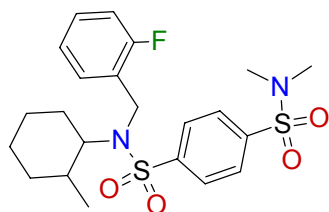
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S107



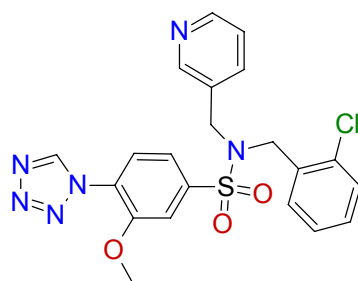
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S108



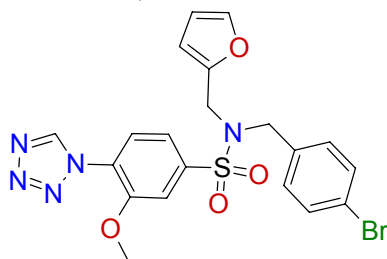
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S109



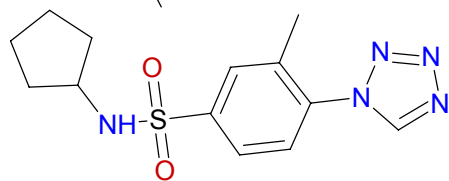
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S110



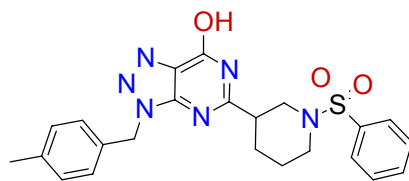
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S111



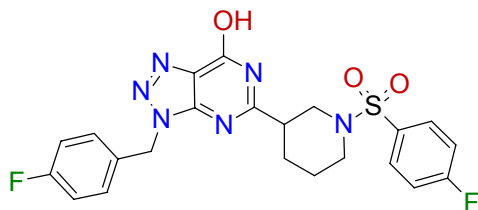
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S120



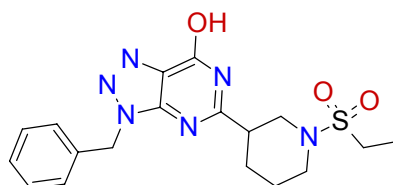
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S121



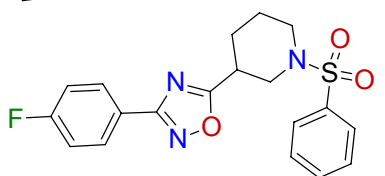
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S122



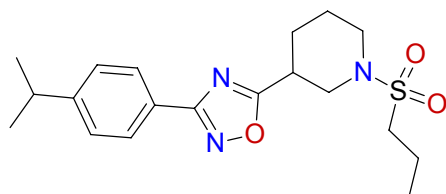
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S123



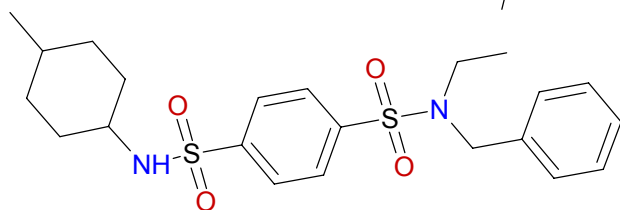
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S124



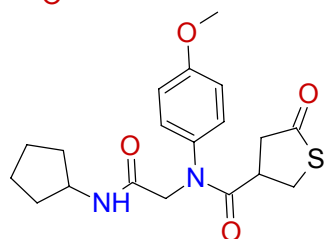
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S125



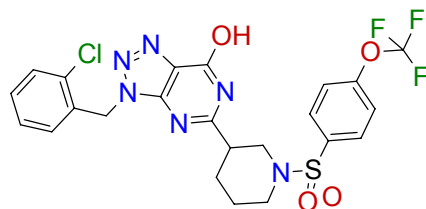
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S126

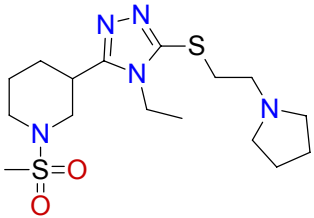
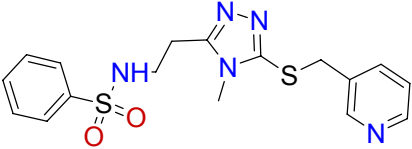
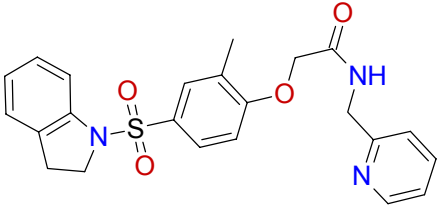
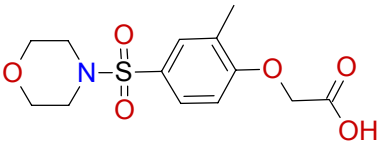
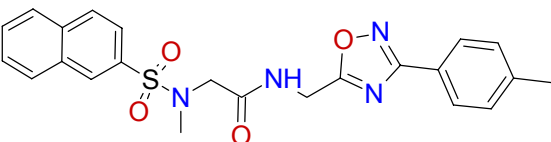
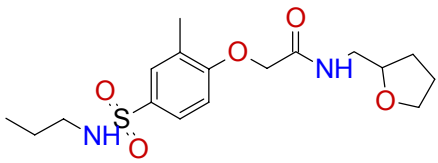
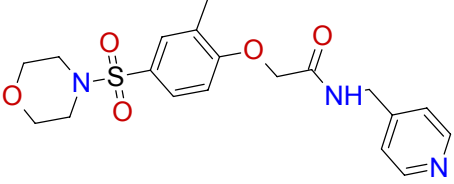
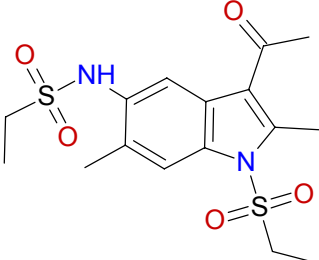


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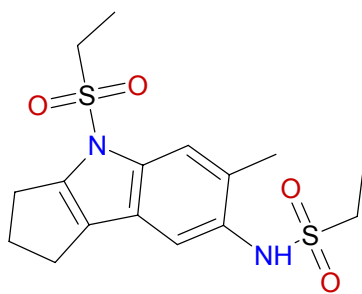
S127



>100

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S135		>100

S136



>100
