

SUPPLEMENTARY MATERIALS

Diketopiperazines: the biological and structural landscape with special focus on the anti-cancer proline-based DKP scaffold

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The overview of the structural databases.

The Research Collaboratory for Structural Bioinformatics Protein Data Bank

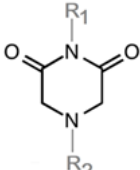
The survey of the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) revealed 42 bio-complexes related to DKP moiety, including proline-based one, signed by reference codes: 6SSG, 6SSF, 6SSE, 6SSD, 6F0B, 6F0C, 41CT, 41Q7, 41PS, 41PW, 41Q9, 5YL4, 6EZ3, 5MLQ, 5OCD, 5MLP, 4Q24, 4E0T, 4E0U, 3S7T, 3OQJ, 3OQH, 3OQI, 3OQ, 3NC6, 3NC7, 3NC3, 3NC5, 3N1A, 2X9Q, 3G5H, 3G5F, 1W1T, 1W1P, 1W1V, 1W1Y, 6VXV, 6VZB, 6WOS, 6VZA, 1O6I, 7OW9, 6VZB, 6VXV, 6VZA. Interestingly, only one complex, 1QZR, contains 2,6-DKP core.

The Cambridge Structure Database

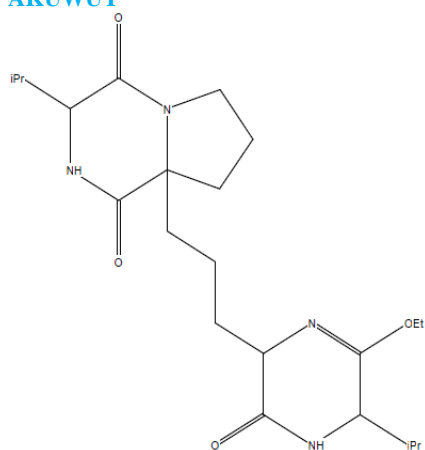
That notwithstanding, overview of the Cambridge Structure Database (CSD) to 531 (1070 without restrictions*) entries of 2,5-DKPs, 29 (43 without restrictions*) 2,3-DKPs and 37 (56 without restrictions*) hits of 2,6-DKPs. It is noteworthy that CSD collects a huge structural knowledge on potential peptide-based ligands that can be applicable at the macromolecular level. Small-molecular crystal structures, especially peptides and their derivatives, have a natural synergy with proteins. The rational design of modern effective ligands should be based not only on the 3D-structure of macromolecular target but also on potential ligands.

**restrictions: non-disordered, no errors, not polymeric, only simple crystal structures, only organics*

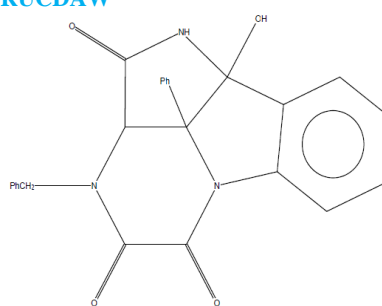
Table S1. Selected proline-based DKPs and their derivatives retrieved from the CSD (ver. May 2021).

		
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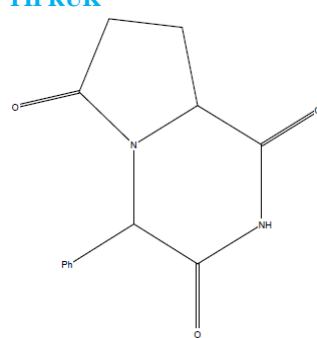
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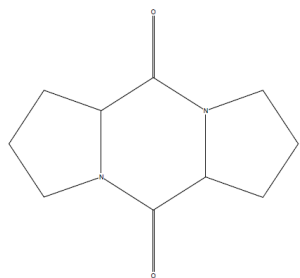
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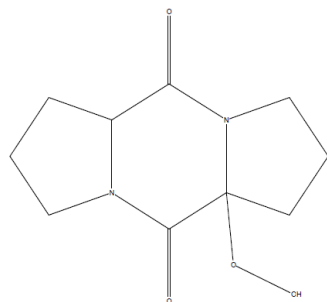
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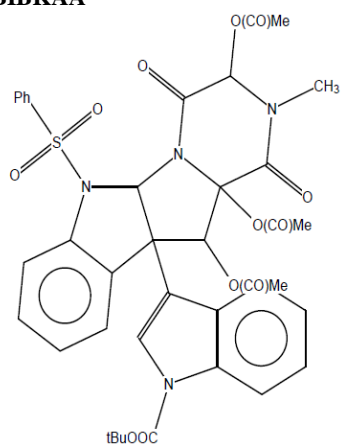
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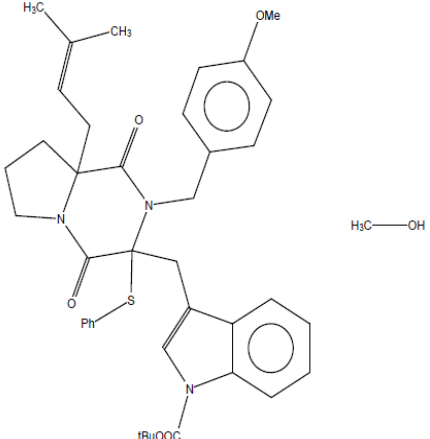
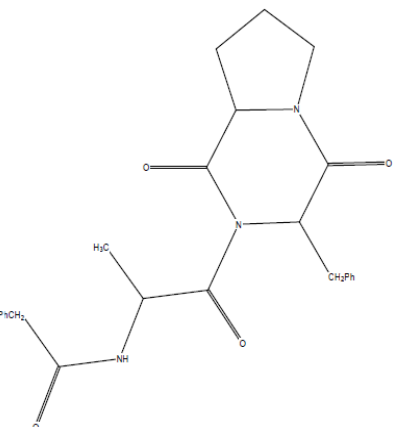
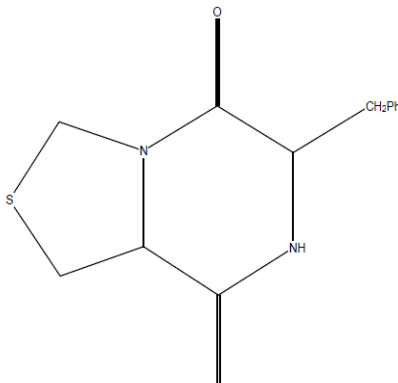
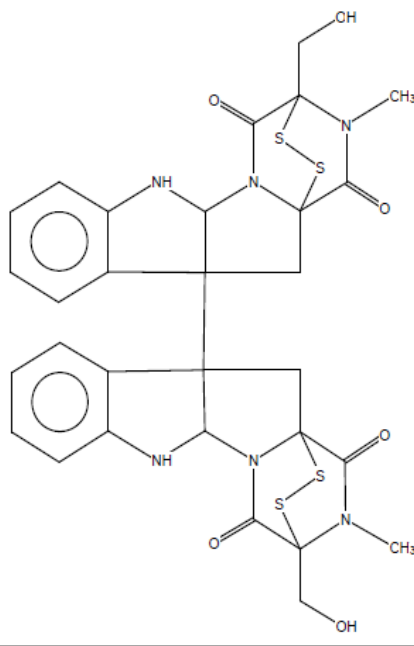
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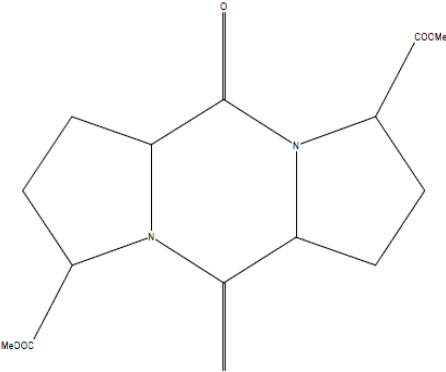
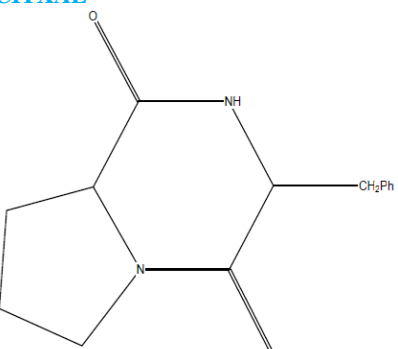
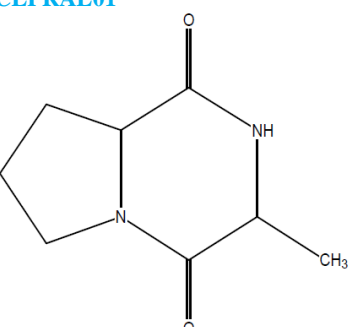
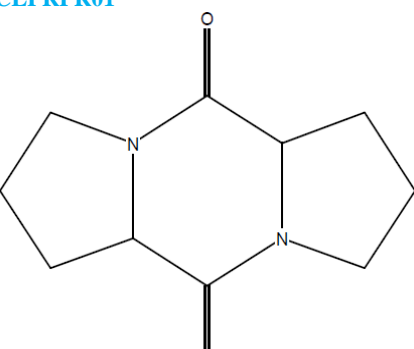


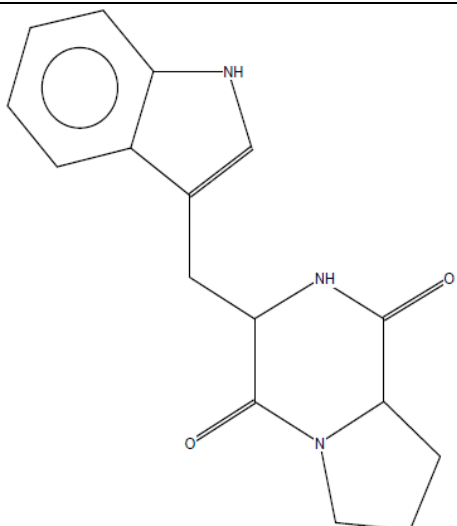
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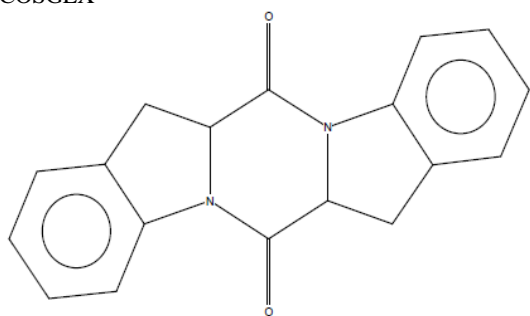
BIDDOJ

 <p>Chemical structure of a complex molecule featuring a pyrrolidine ring, a thioether, a benzothiazine system, and a 4-methoxyphenyl group. A side chain includes a vinyl group and a tert-butyl ester. A small molecule $\text{H}_3\text{C}-\text{OH}$ is also shown.</p>		
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<p>BOLWEE</p> 		
<p>CAETOC</p> 		
<p>CEWBUE</p>		

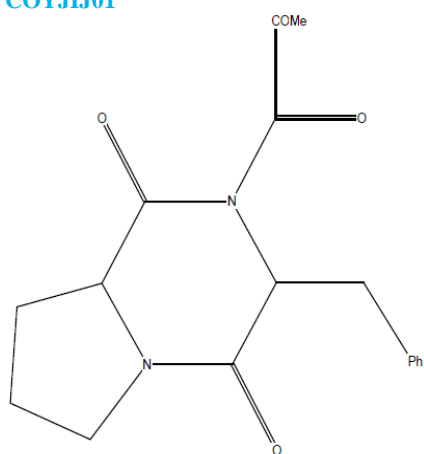
		
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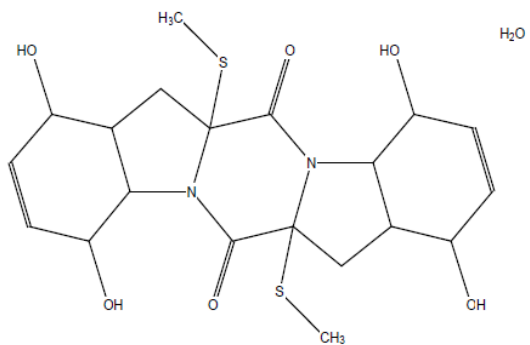
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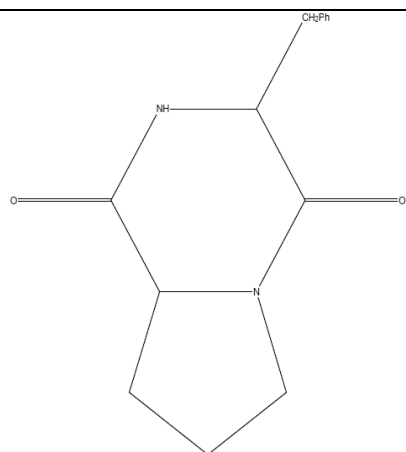
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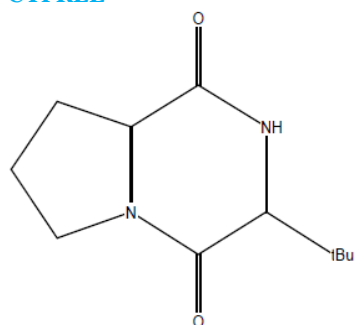
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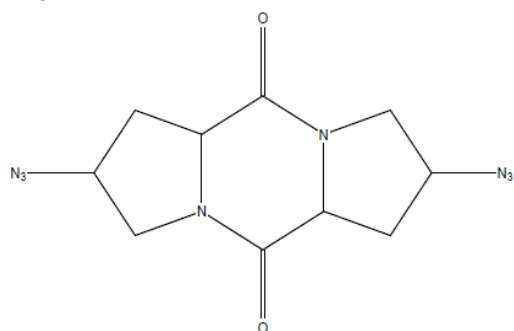
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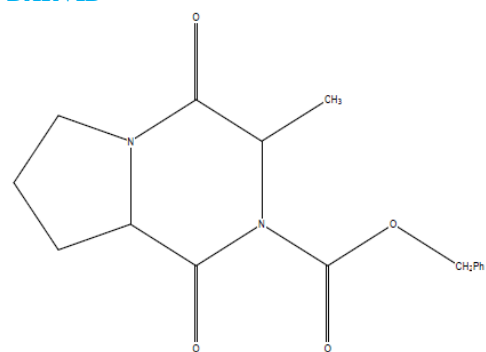
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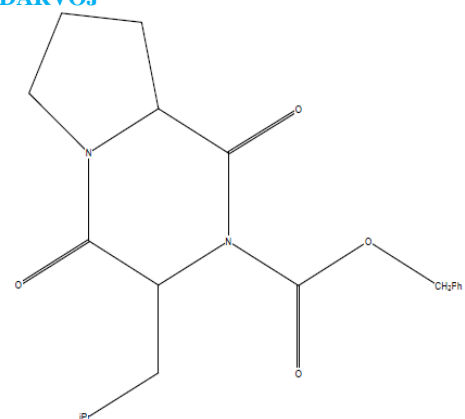
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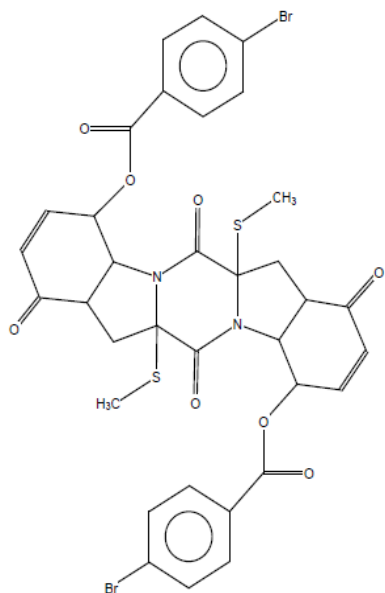
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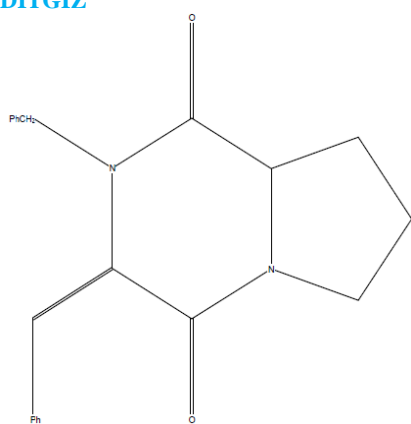
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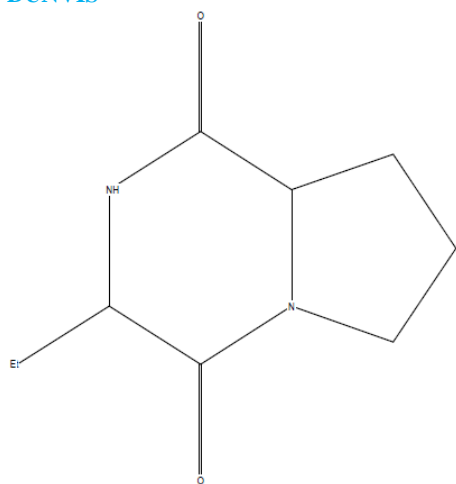
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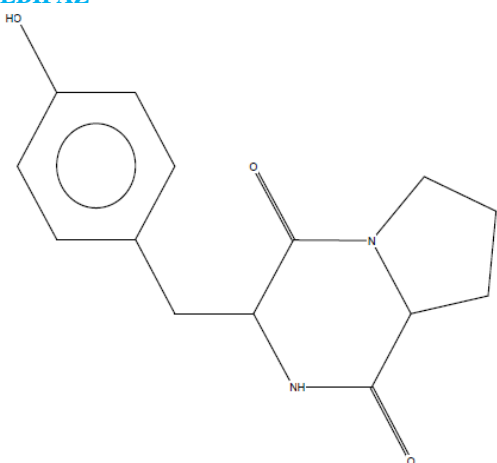
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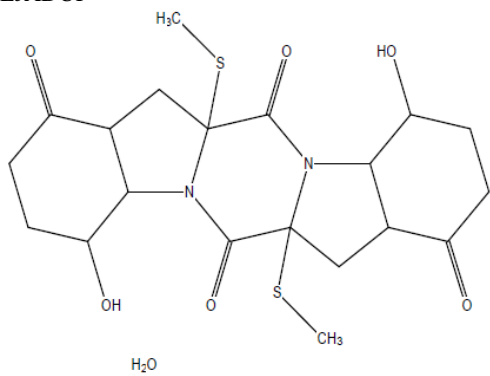
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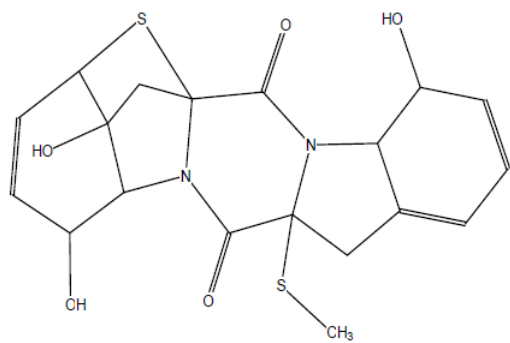
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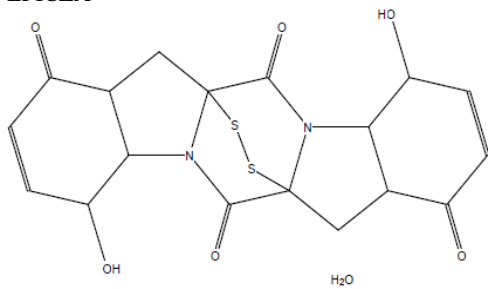
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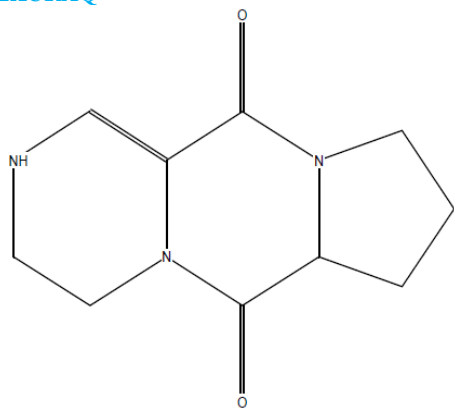
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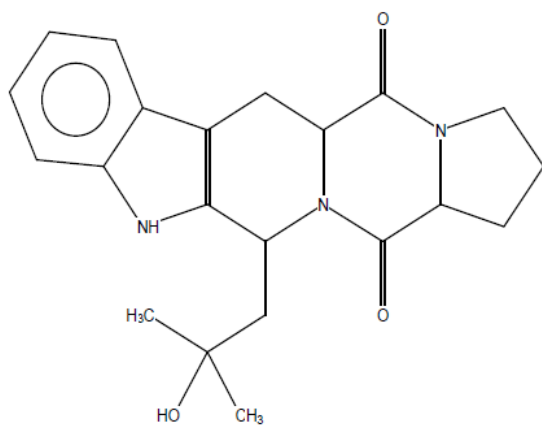
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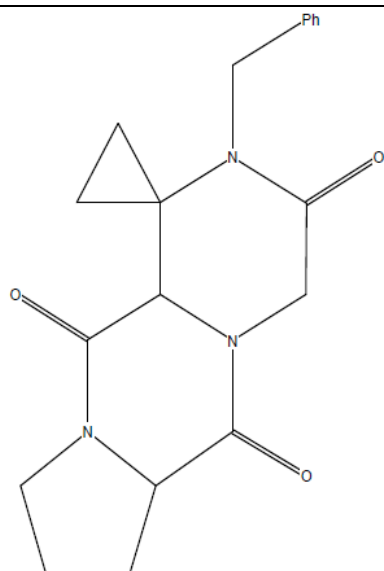
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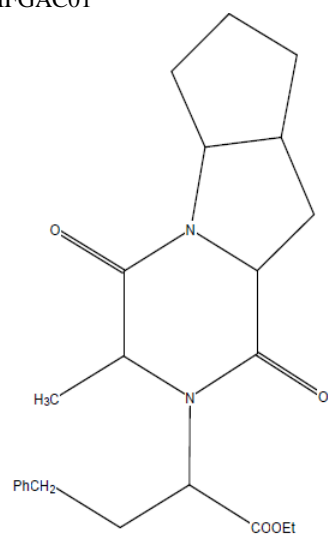
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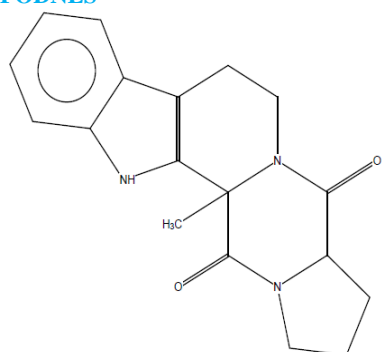
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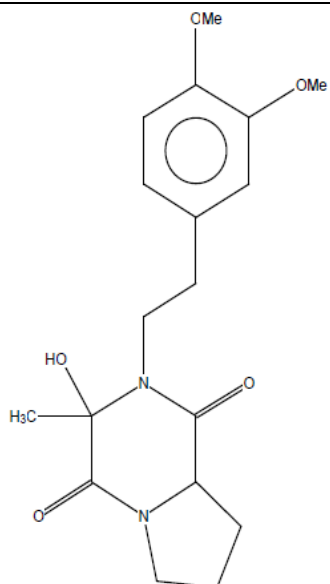
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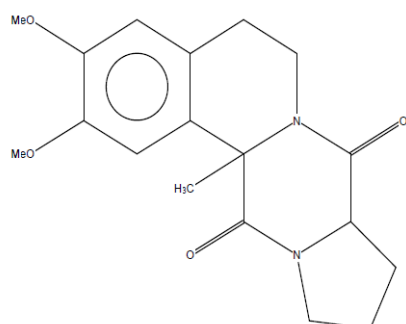
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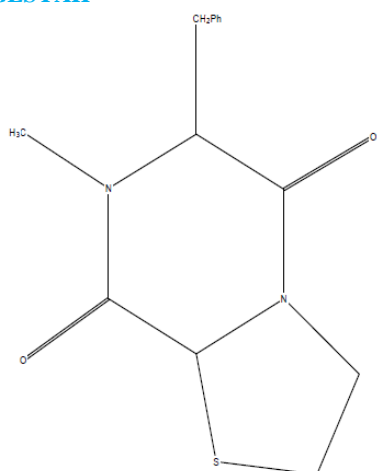
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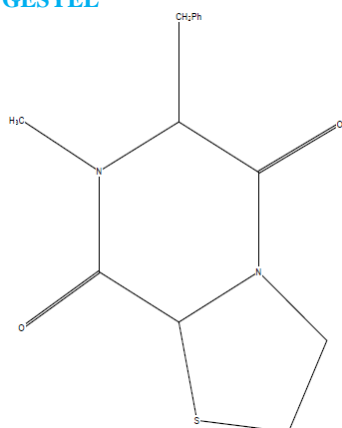
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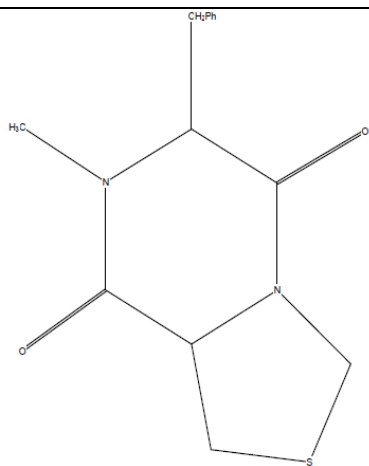
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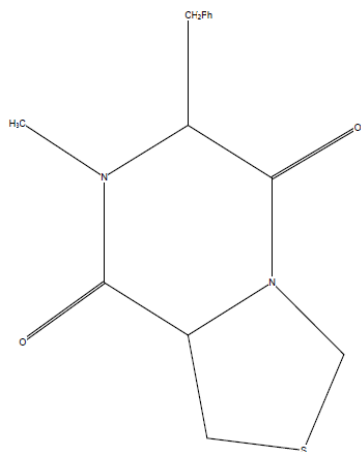
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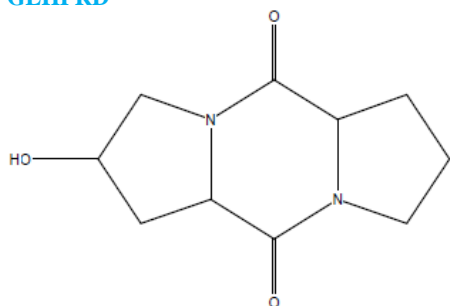
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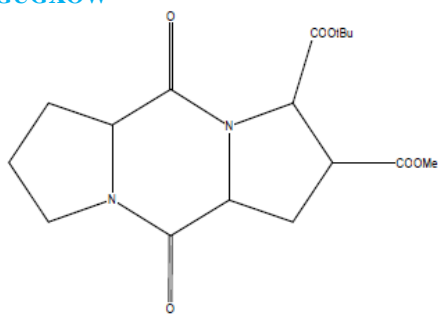
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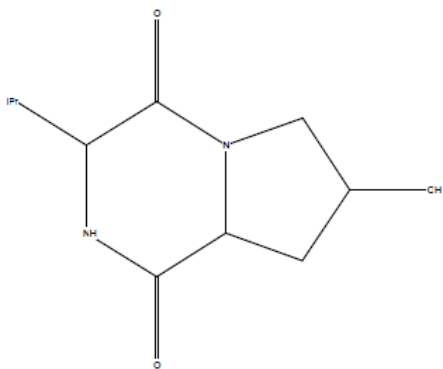
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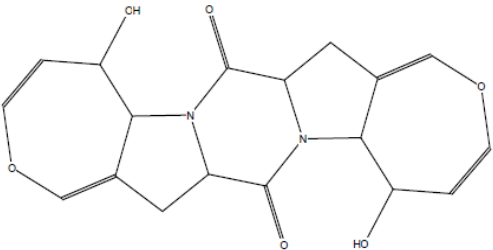
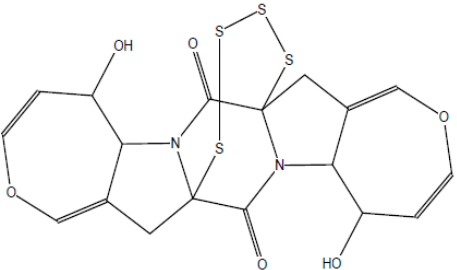
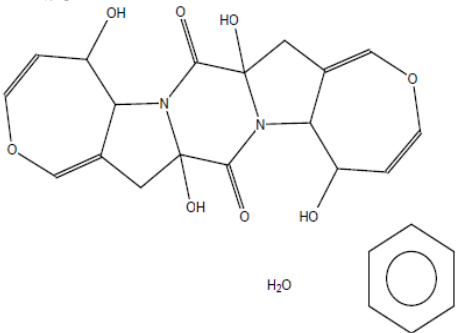
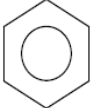
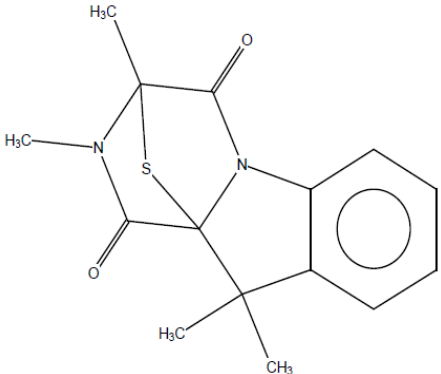
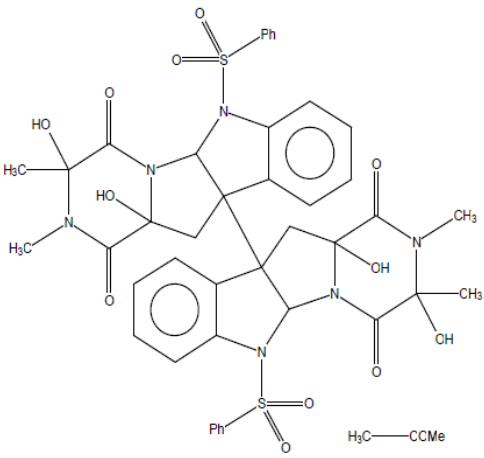
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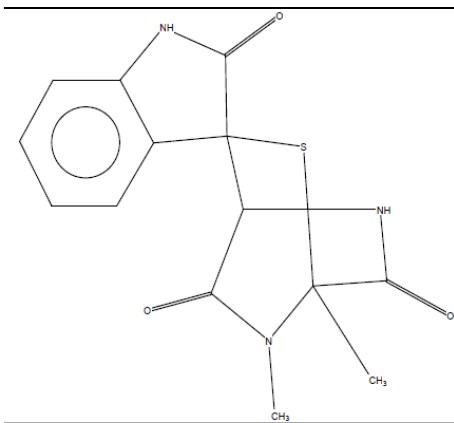


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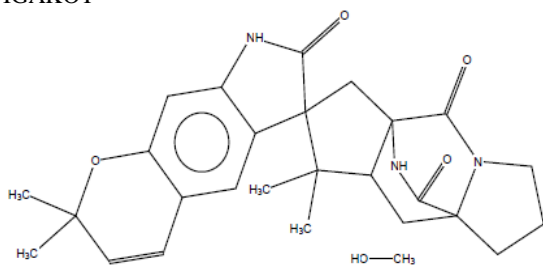


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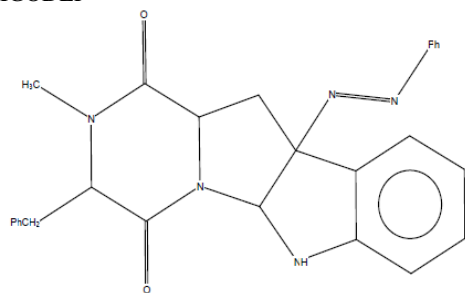
		
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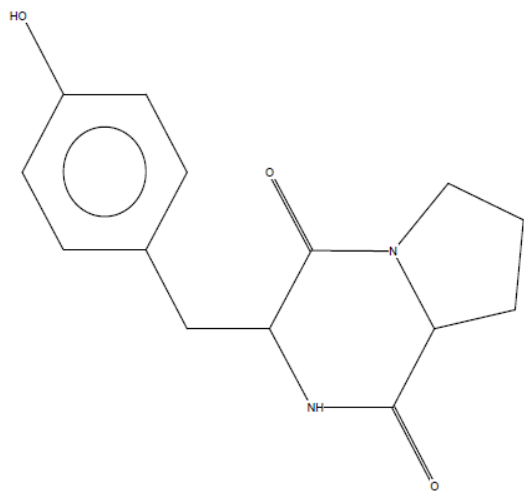
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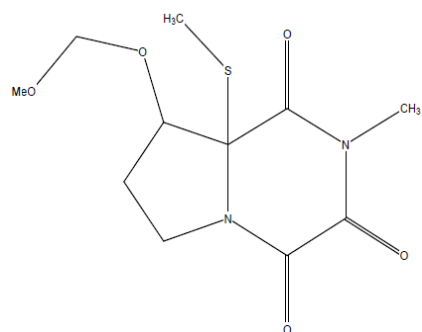
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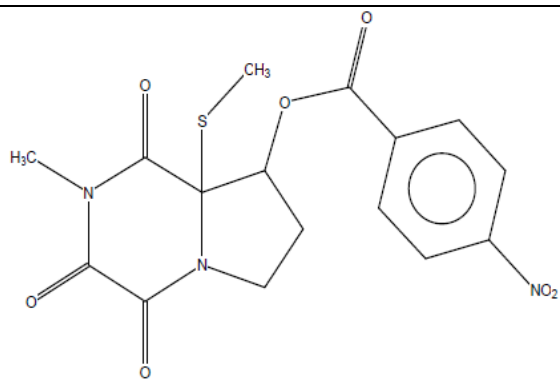
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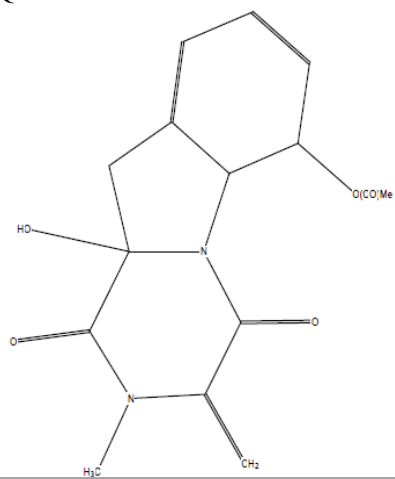
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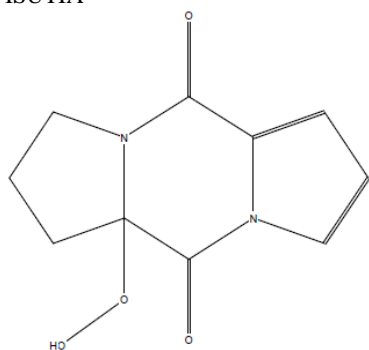
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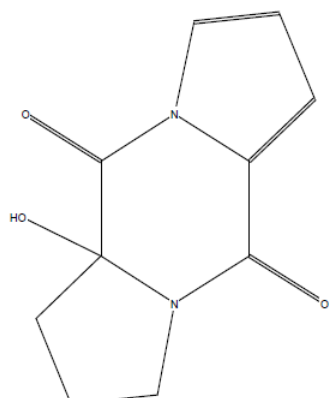
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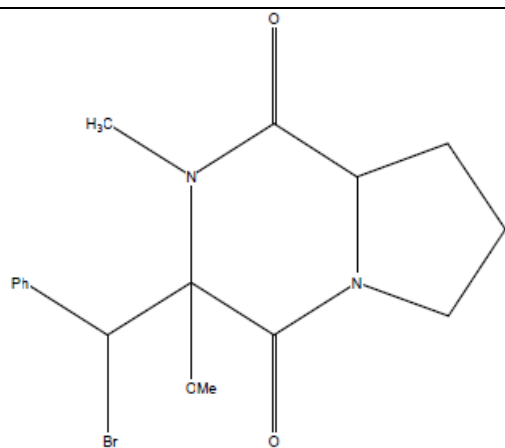
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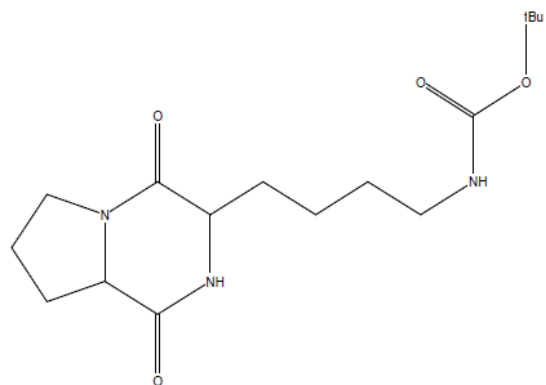
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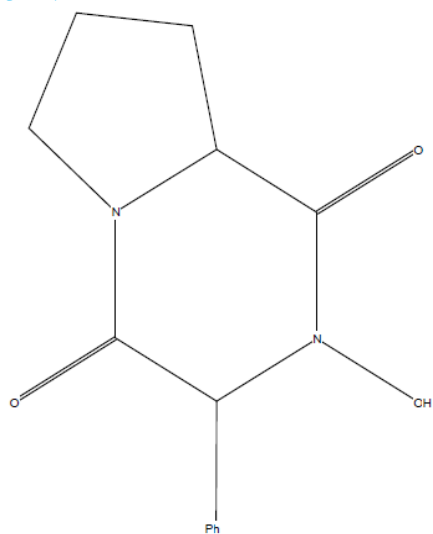
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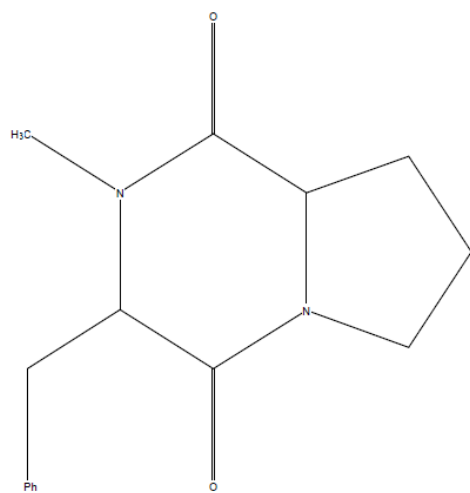
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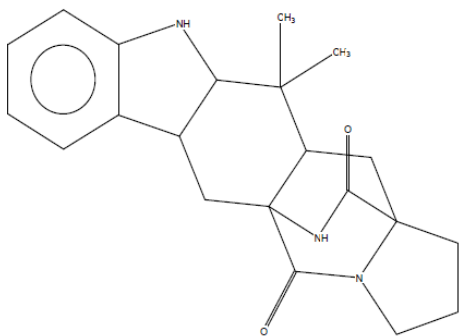
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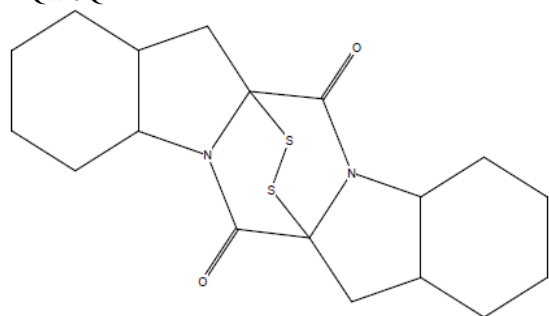
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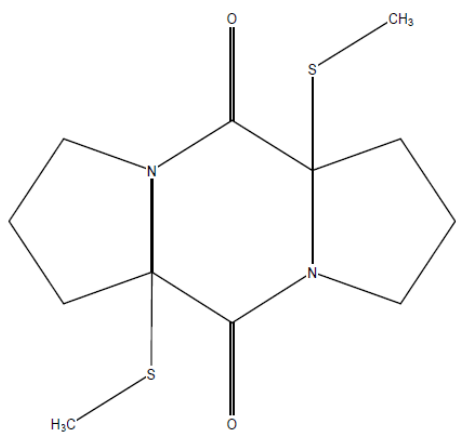
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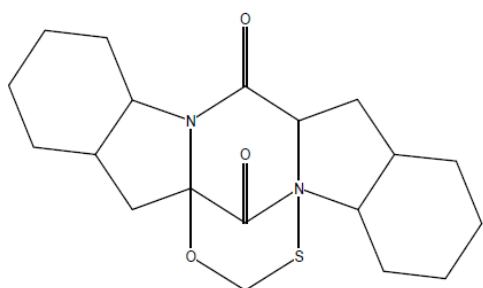
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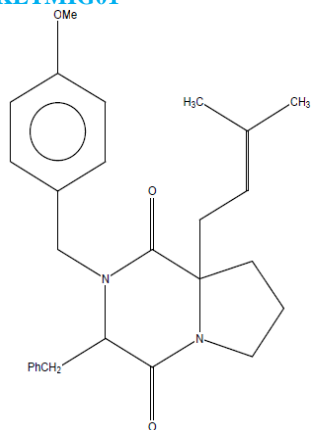
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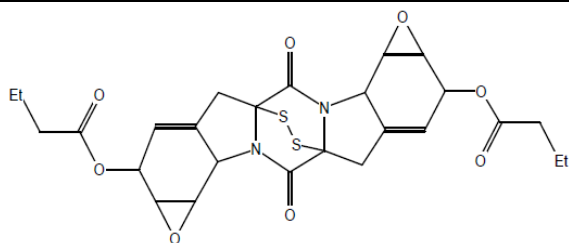
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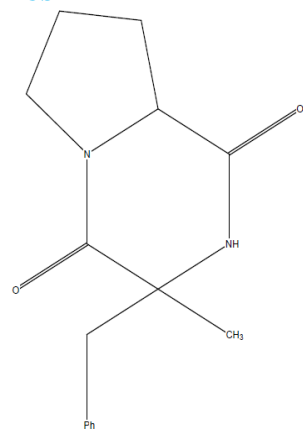
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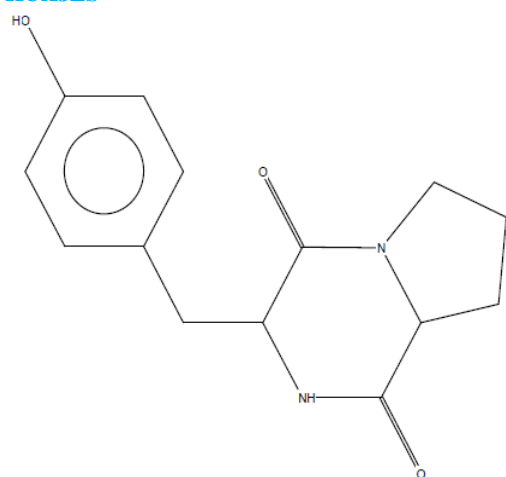
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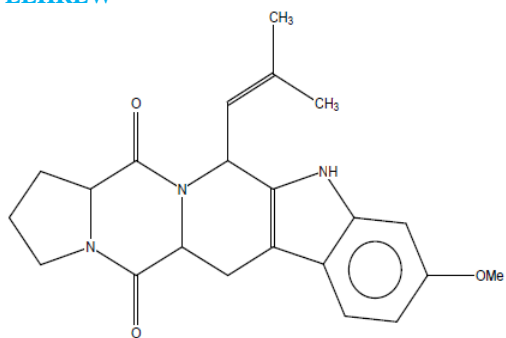
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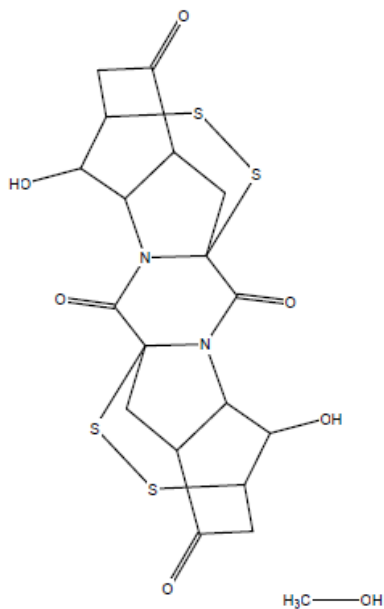
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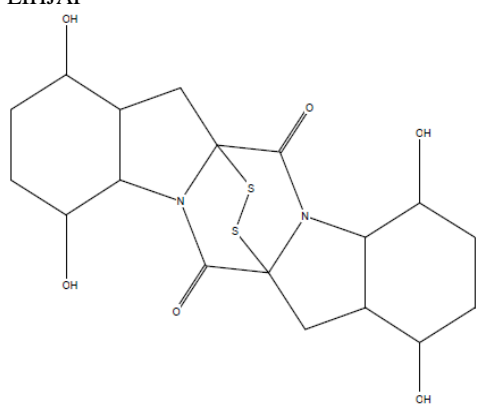
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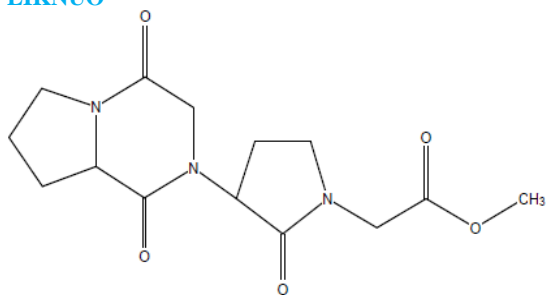
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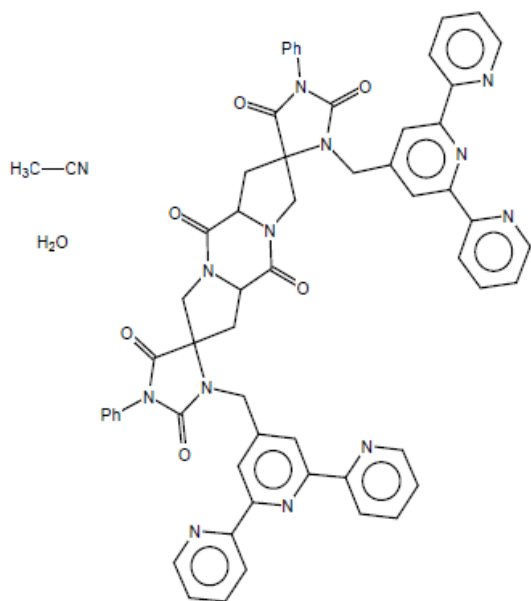
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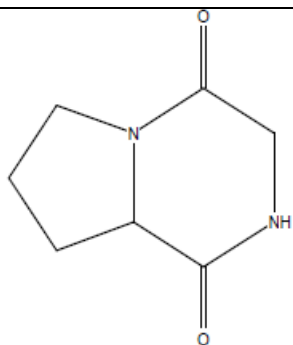
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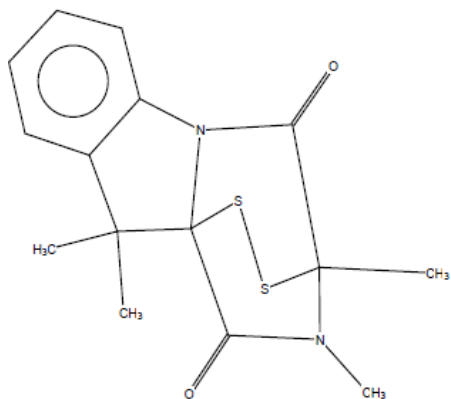
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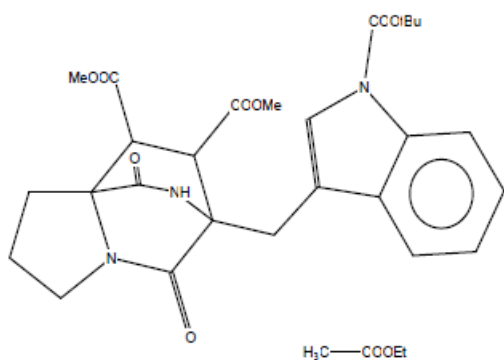
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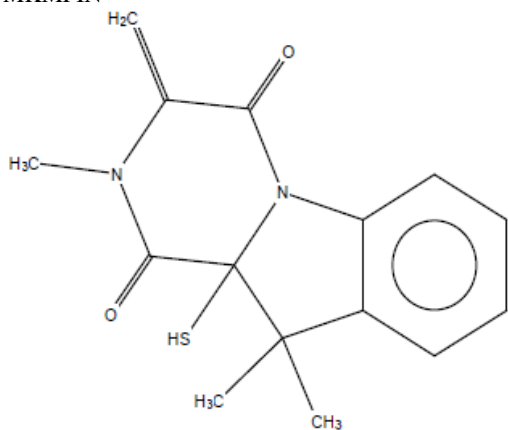
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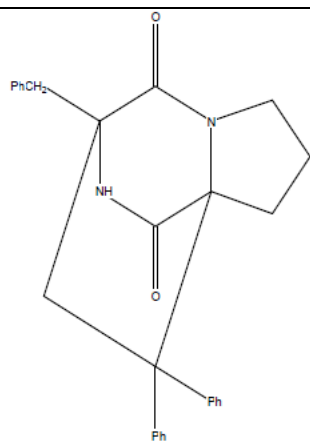
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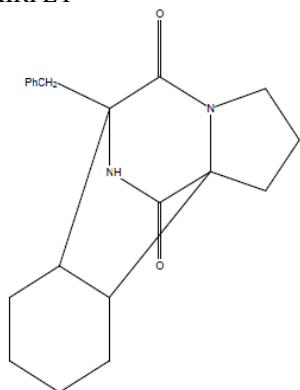
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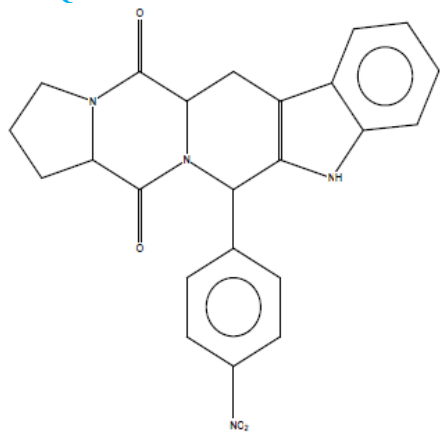
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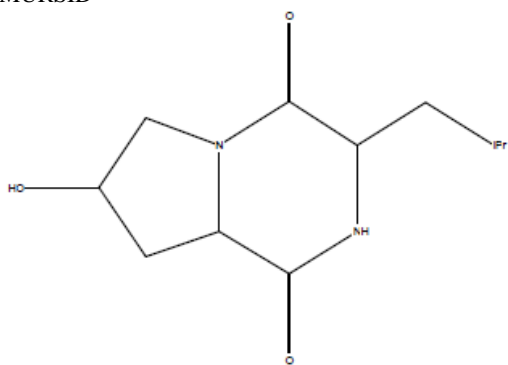
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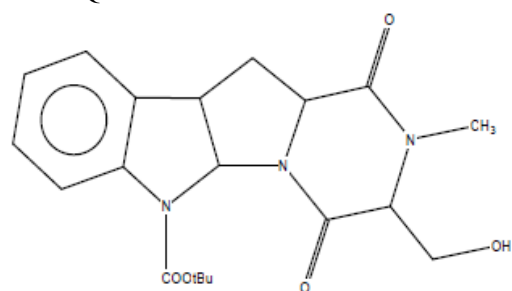
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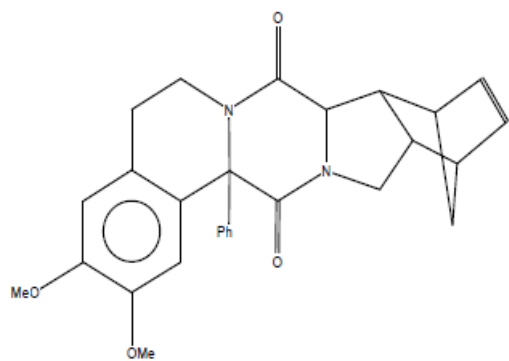
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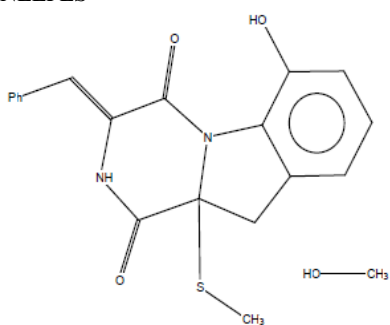
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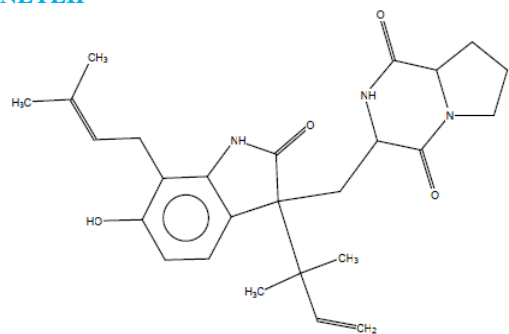
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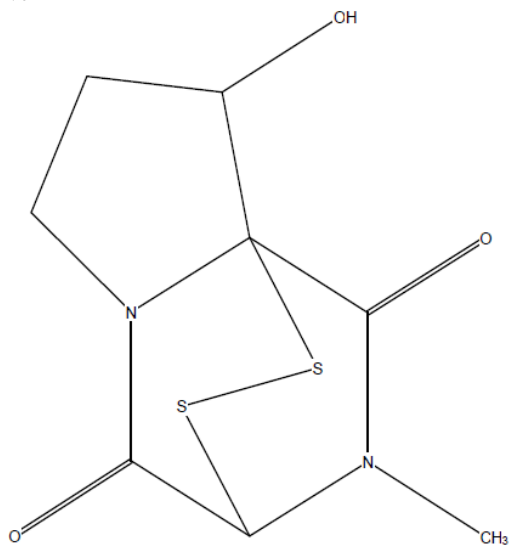
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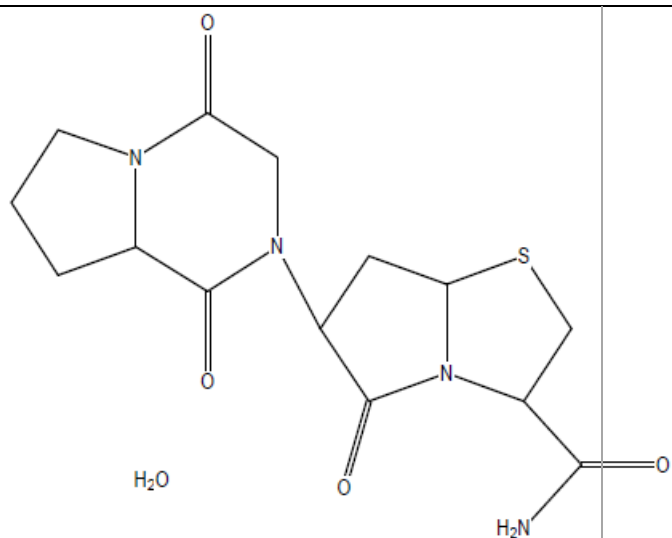
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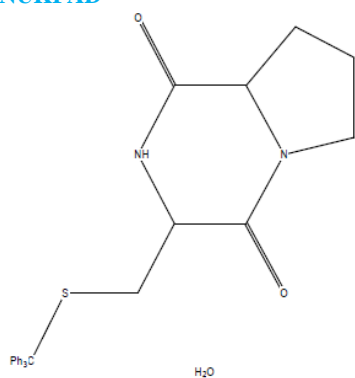
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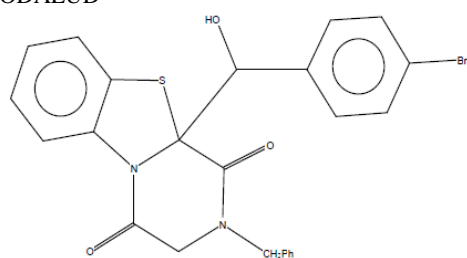
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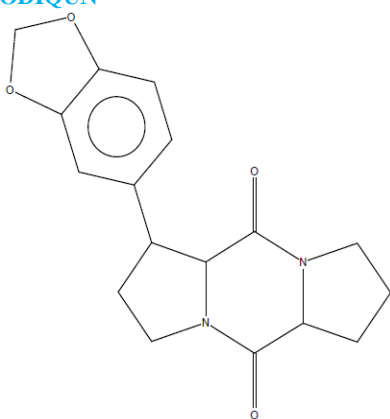
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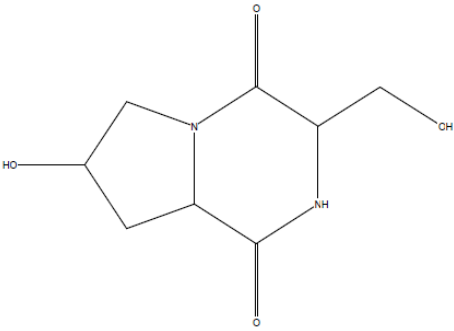
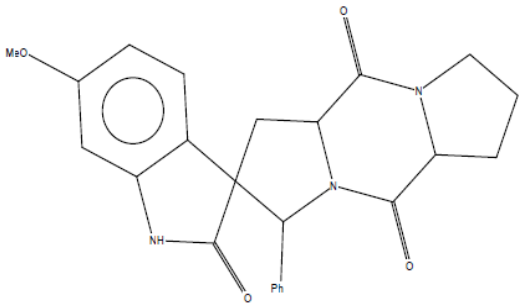
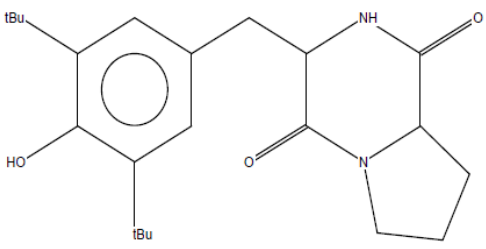
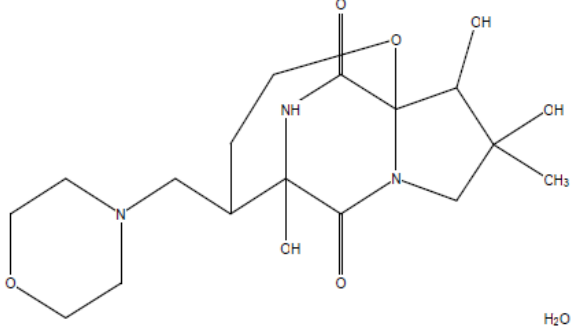
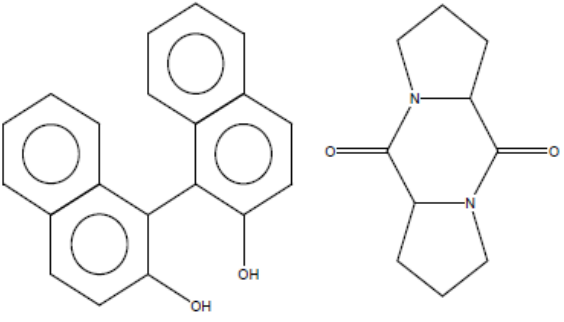
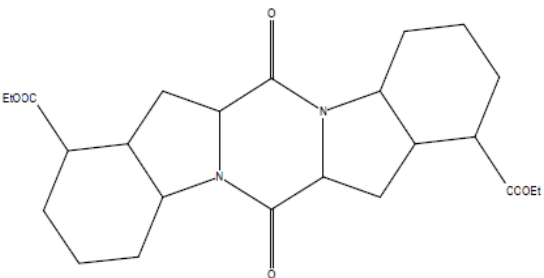
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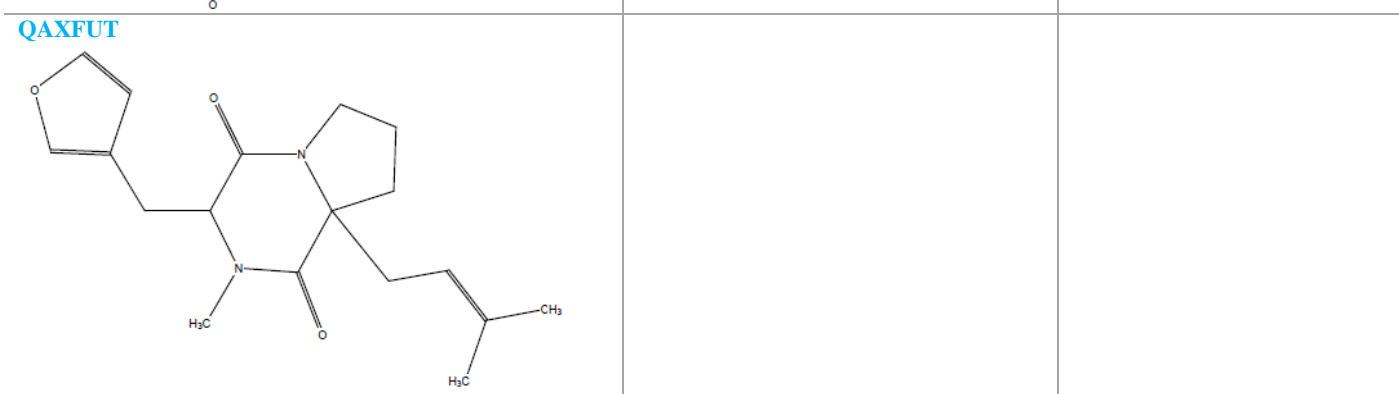
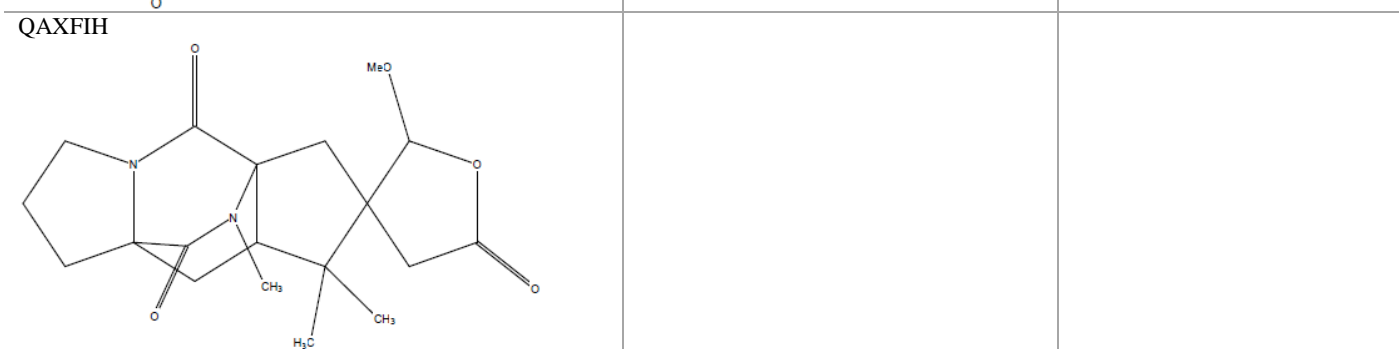
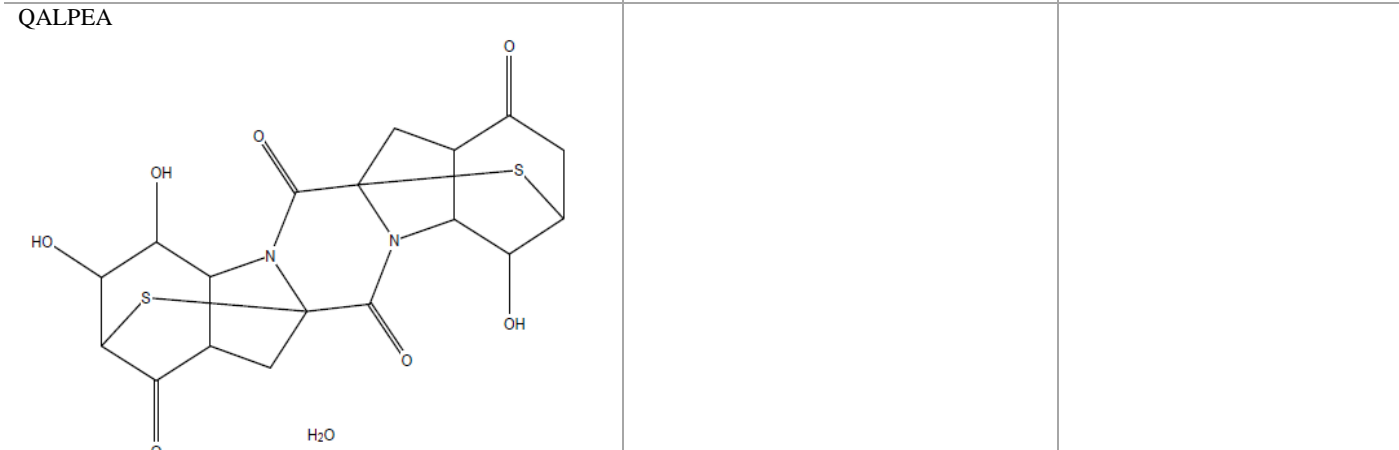
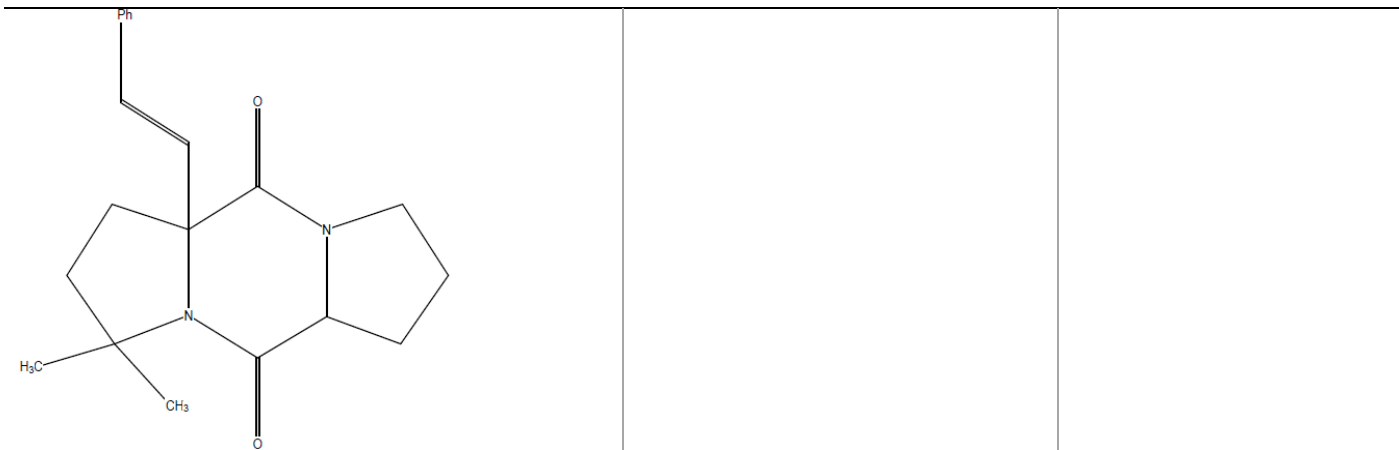


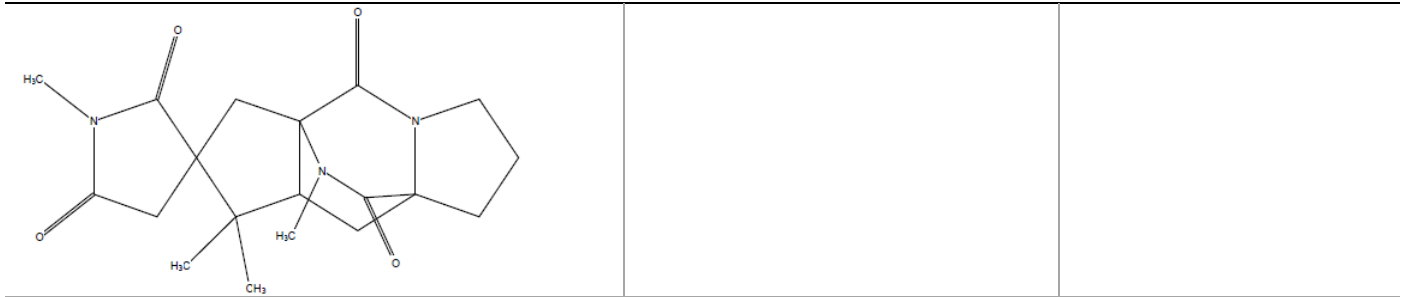
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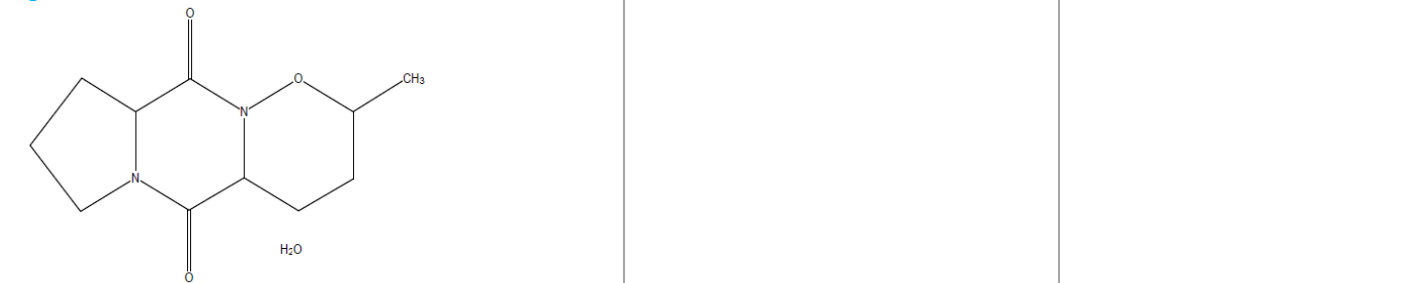
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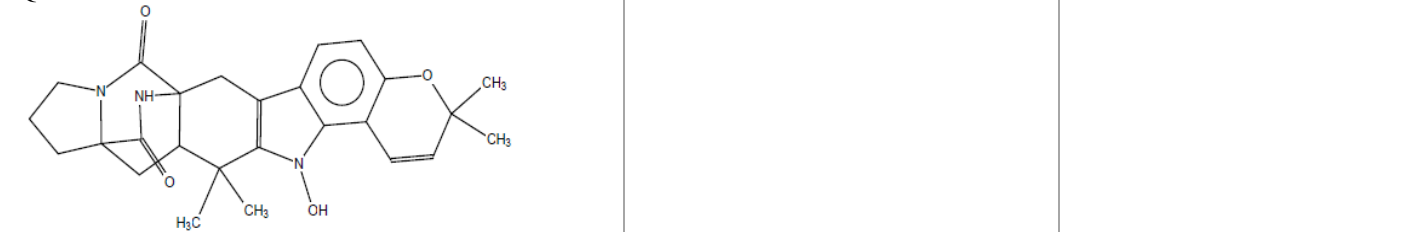




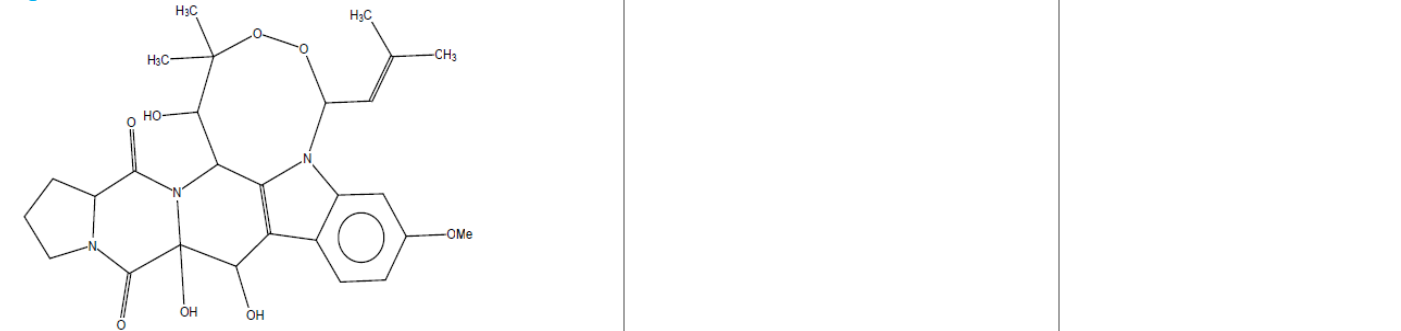
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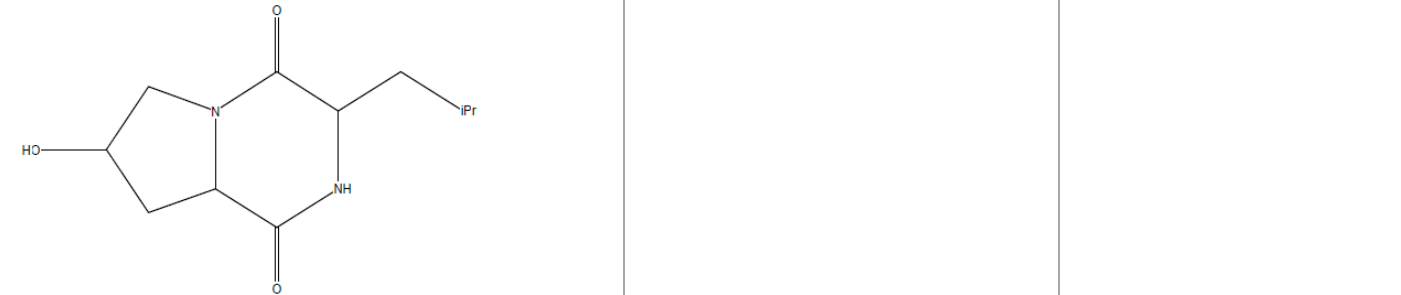
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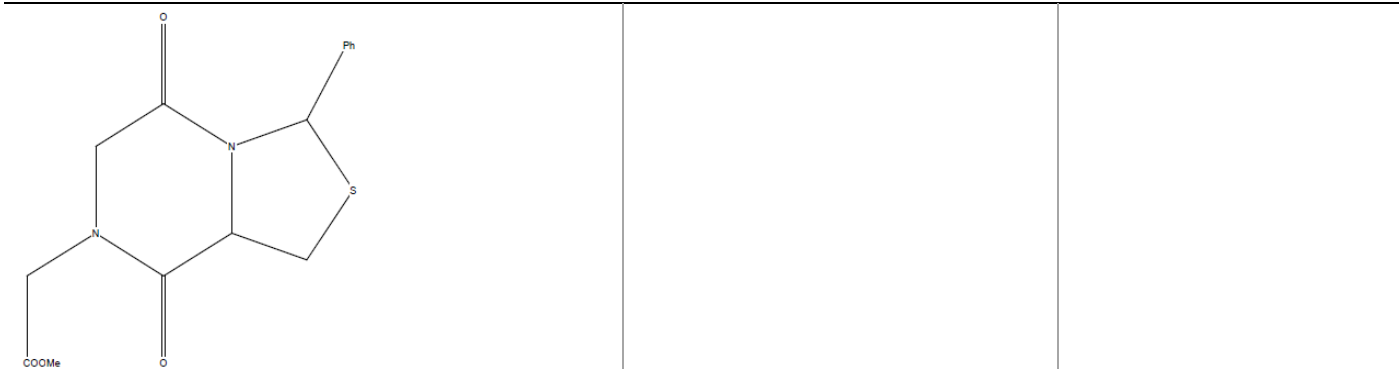
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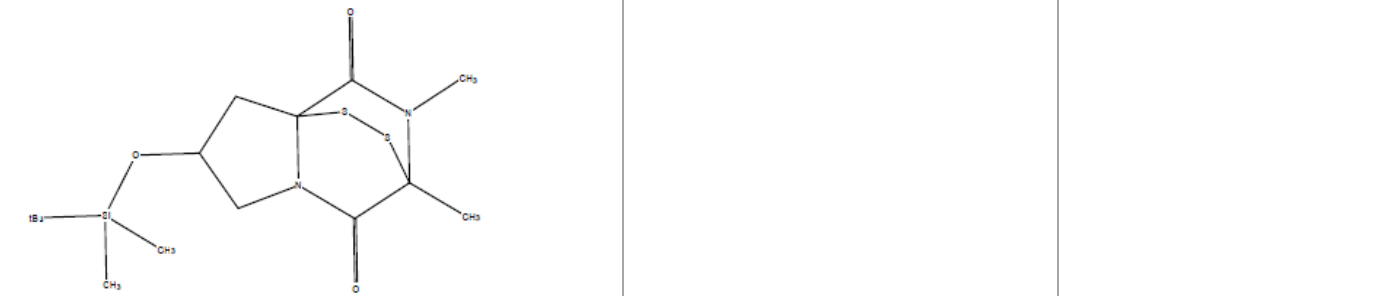
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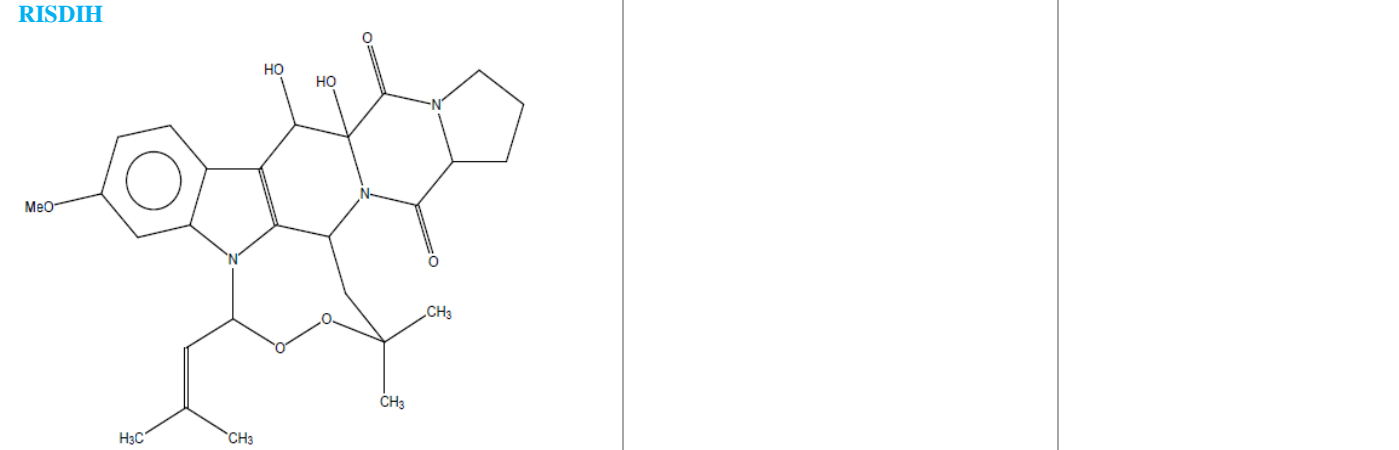
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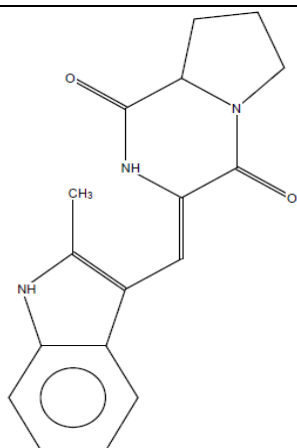
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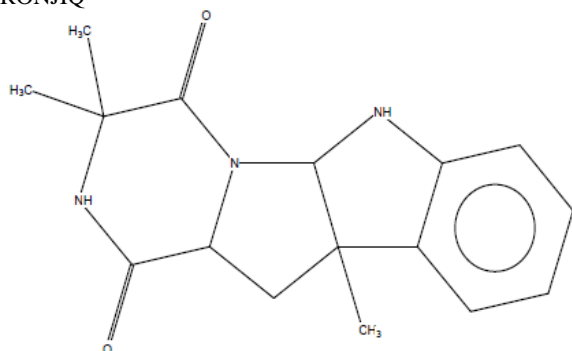
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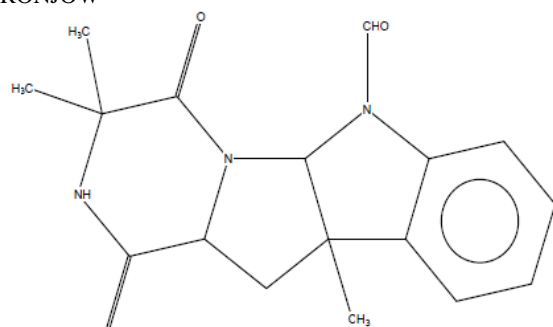
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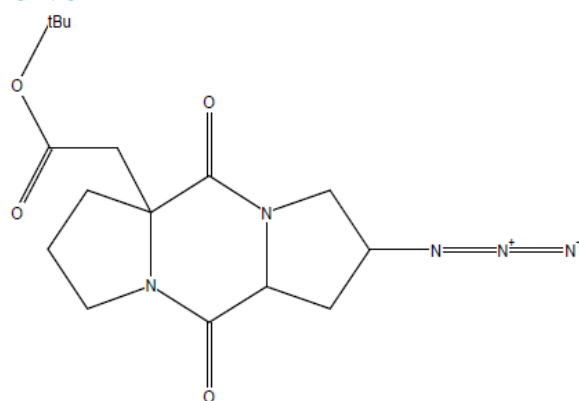
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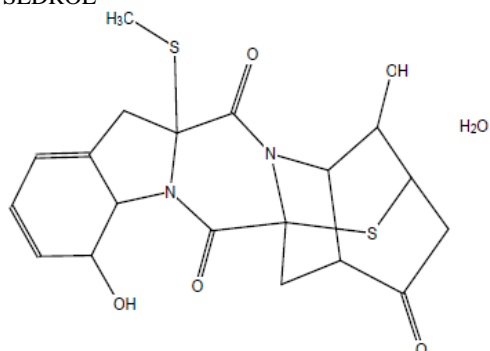
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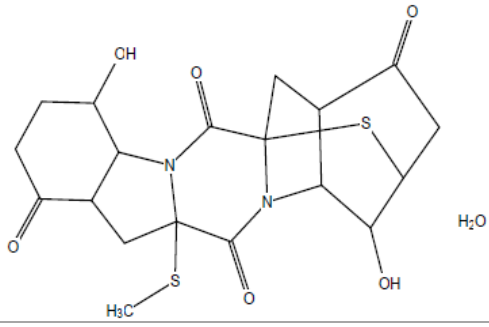
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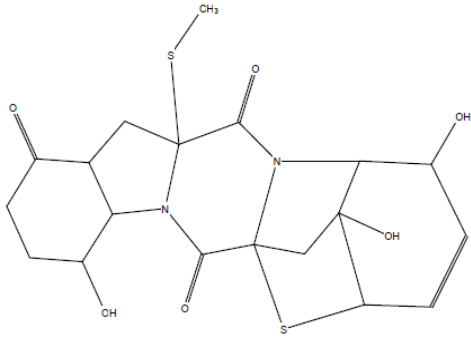
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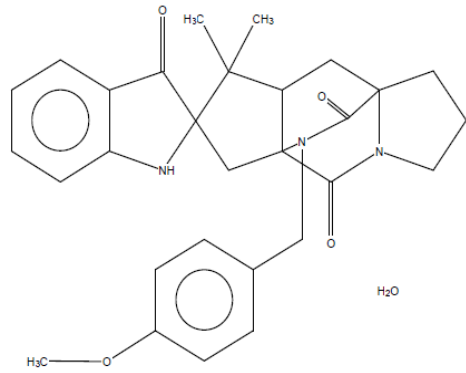
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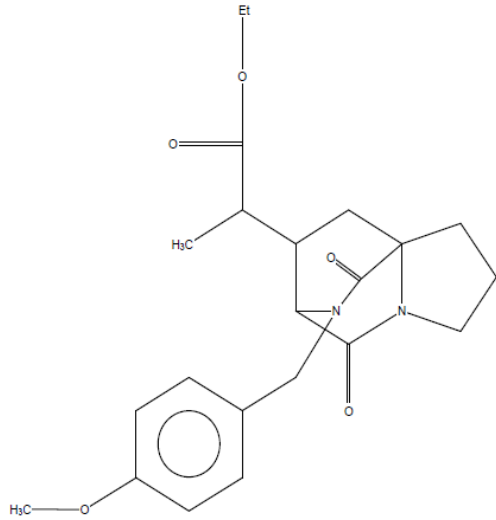
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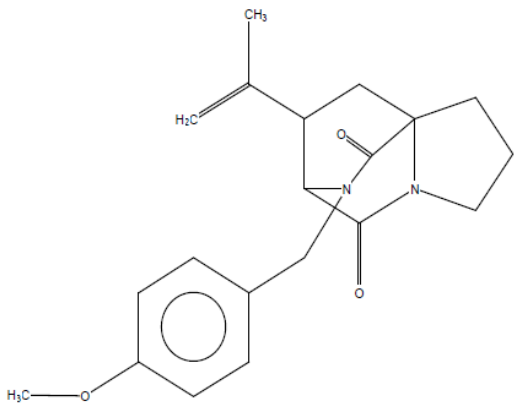
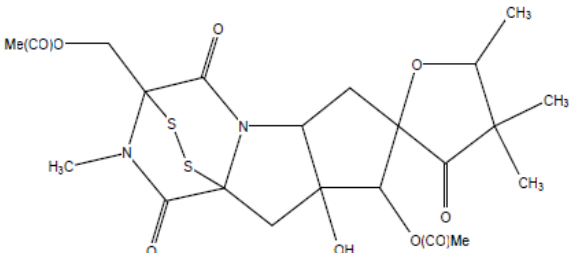
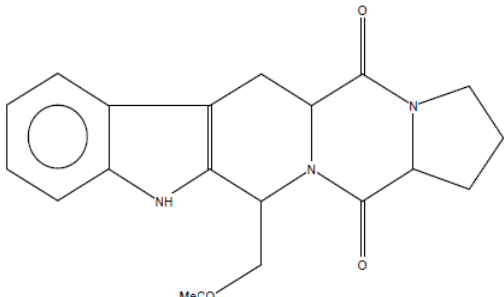
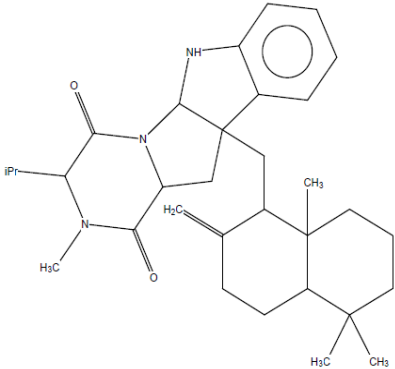
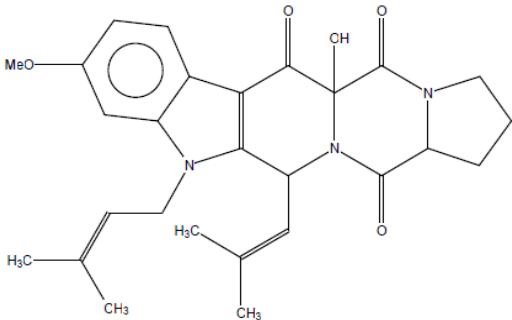
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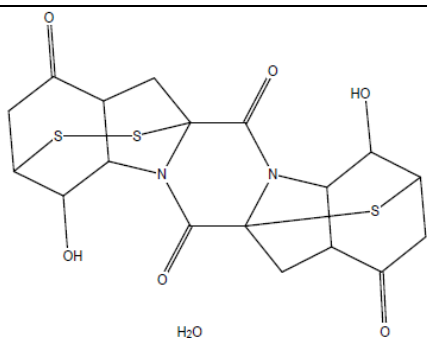


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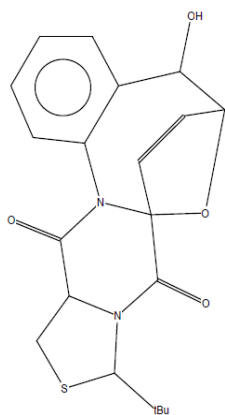


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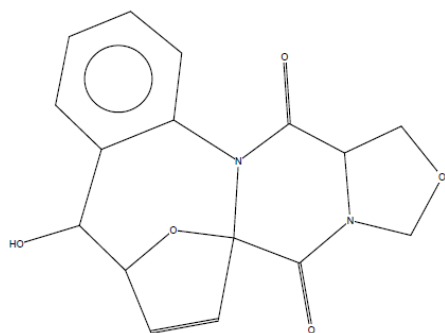
		
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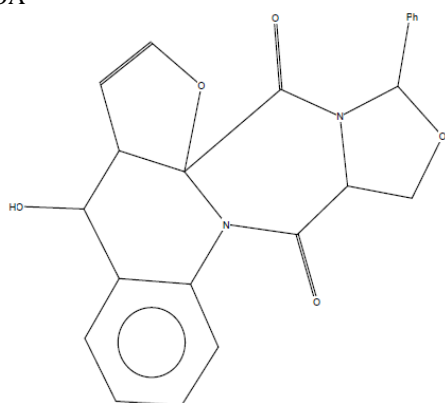
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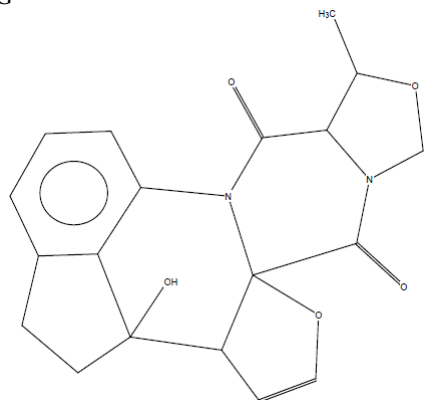
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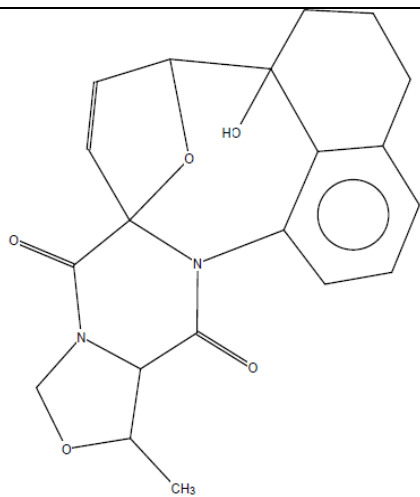


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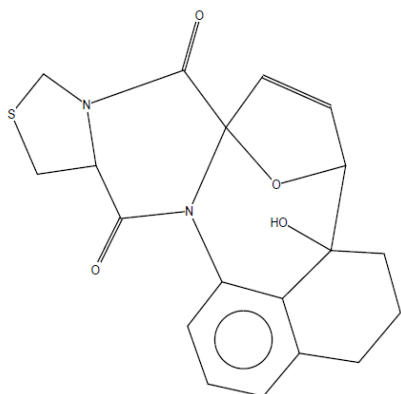


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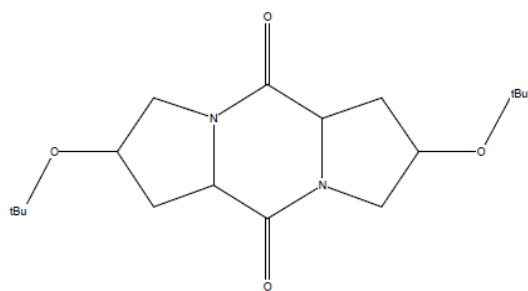
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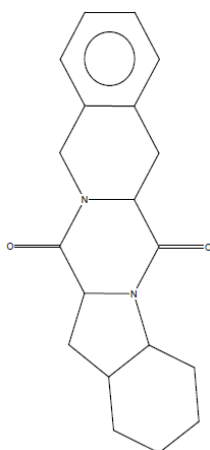
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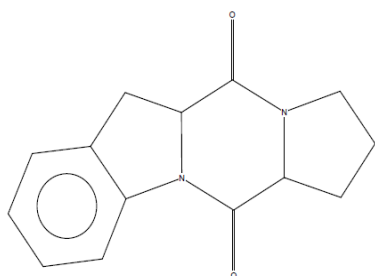
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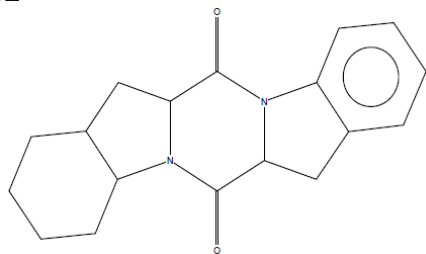
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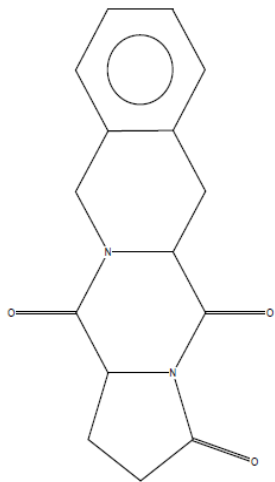
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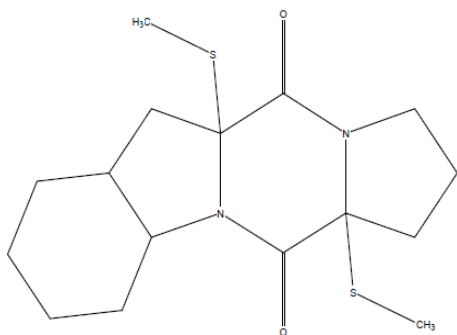
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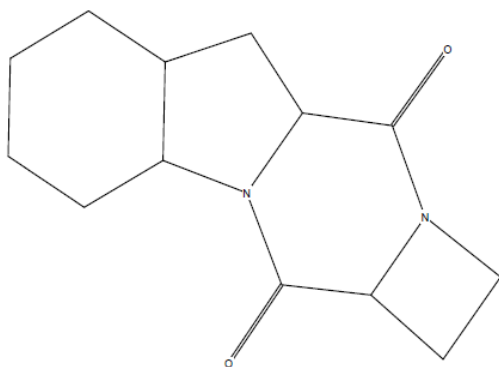
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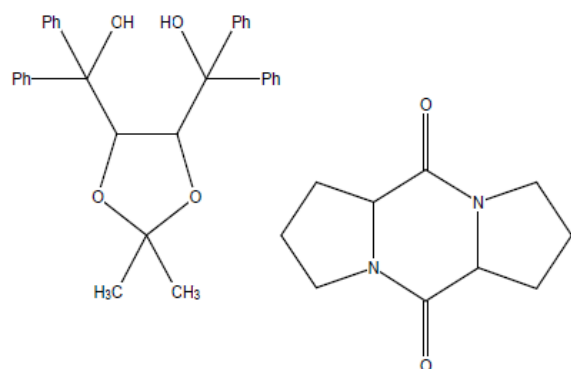
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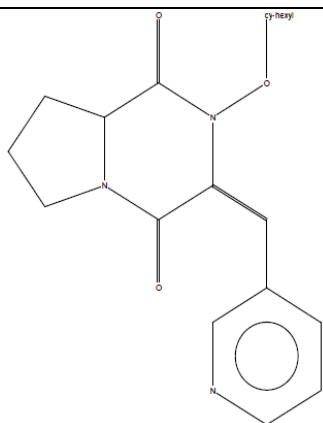
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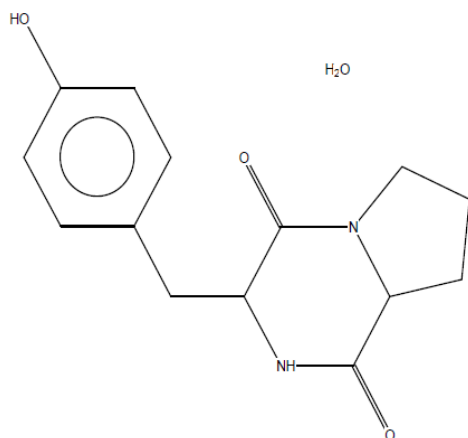
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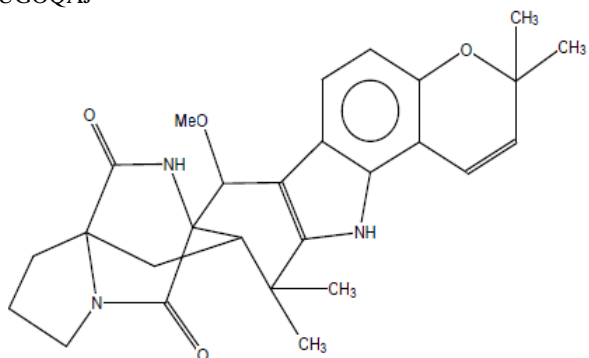
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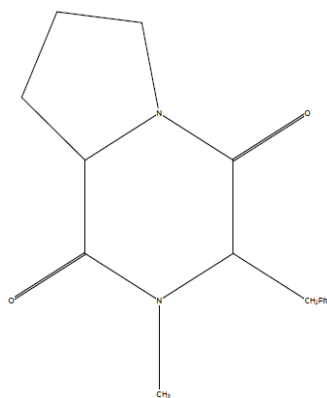
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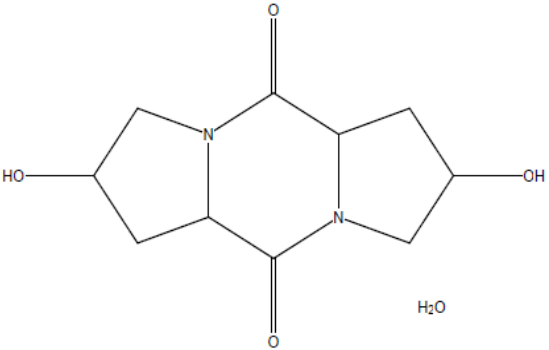
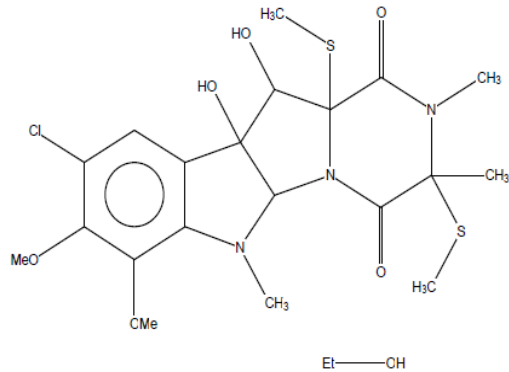
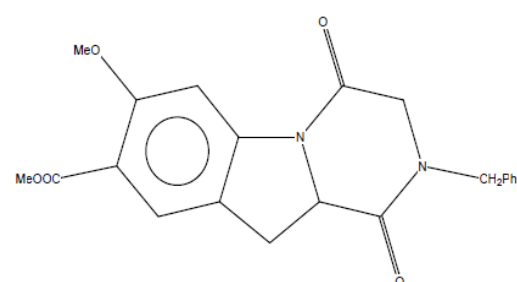
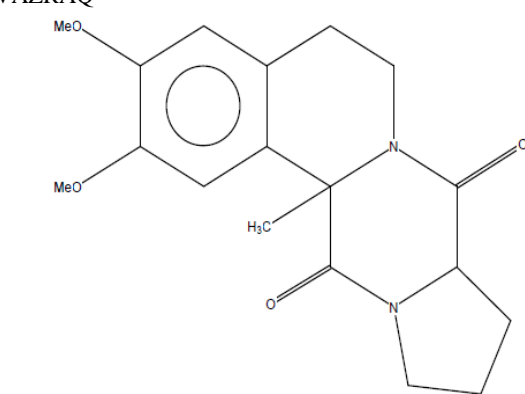
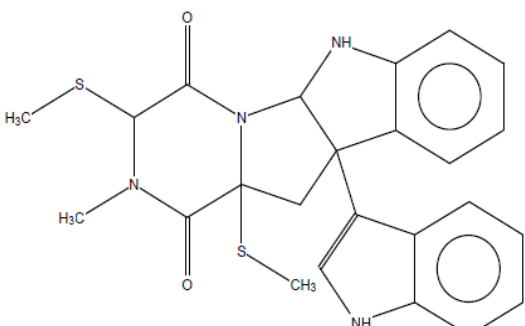
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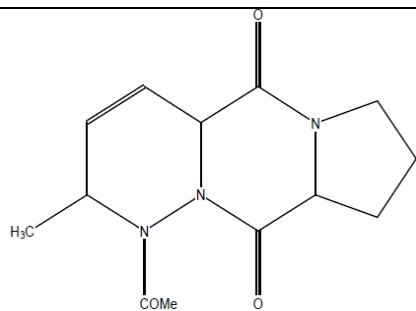


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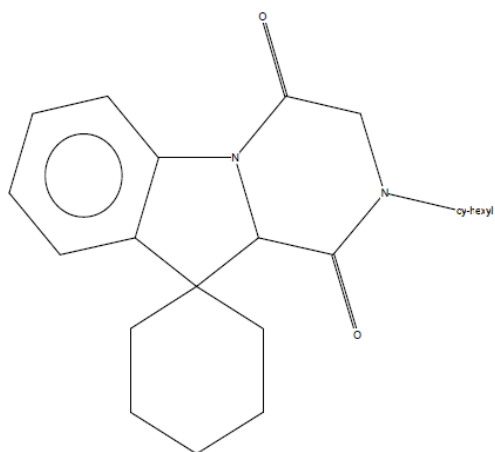


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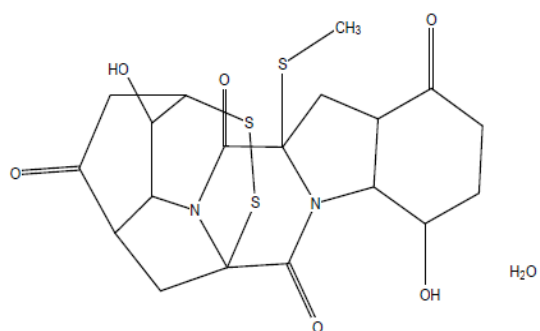
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<p>VAVZUP</p>  <p>O</p>		
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<p>VEVXEB</p>  <p>H₃C</p>		
<p>VIDRAB</p>		



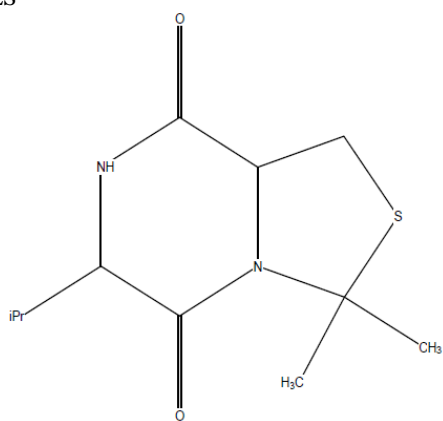
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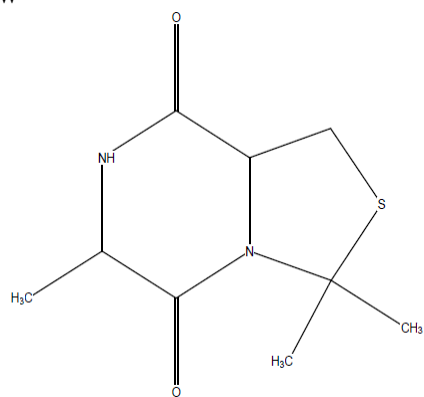
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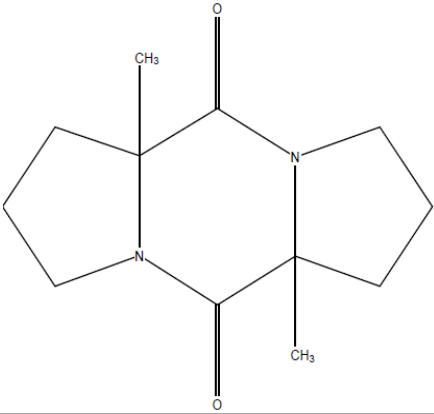
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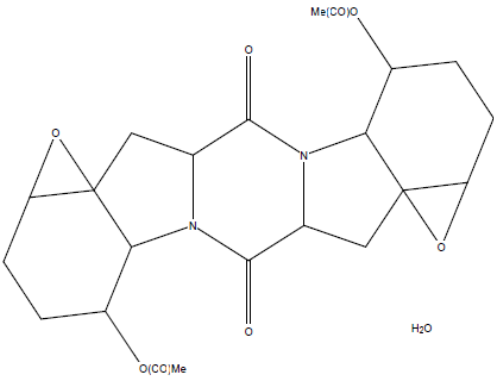
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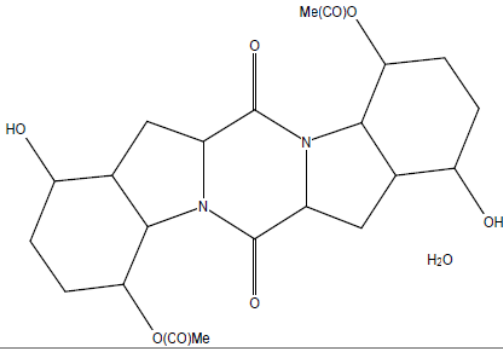
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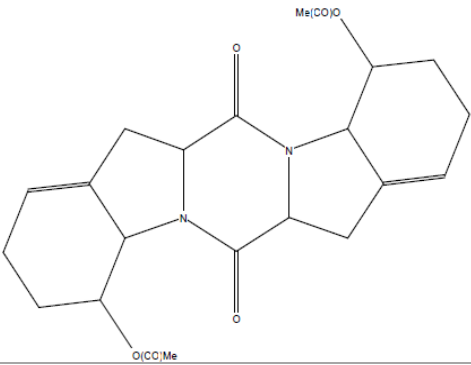
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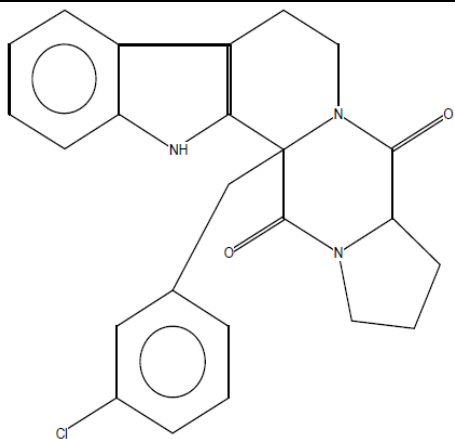
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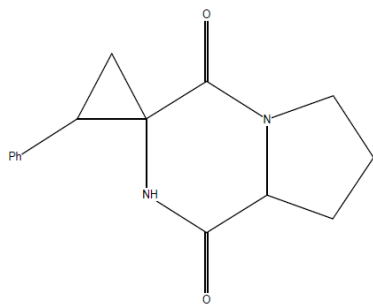
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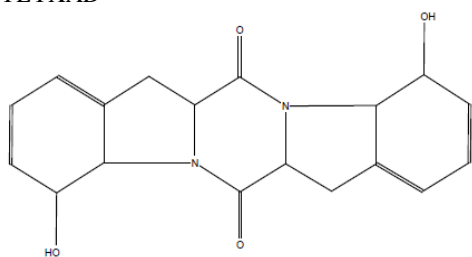
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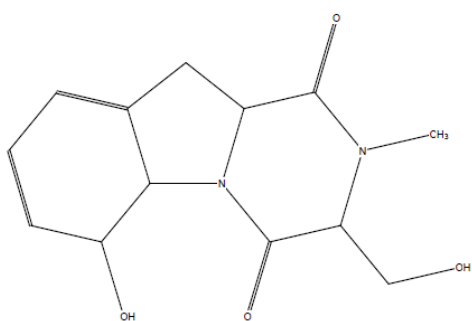
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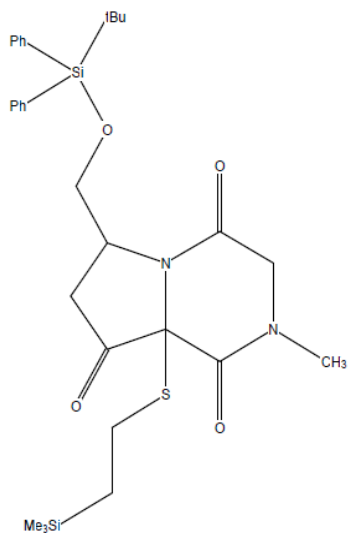
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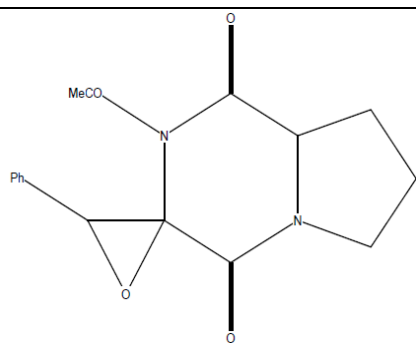
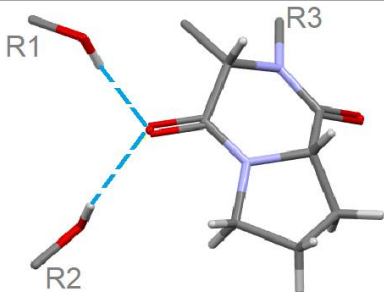
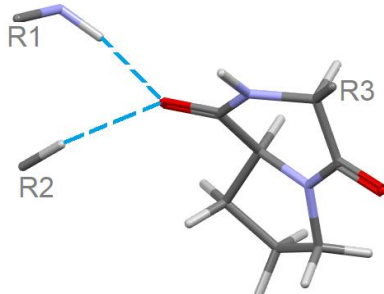
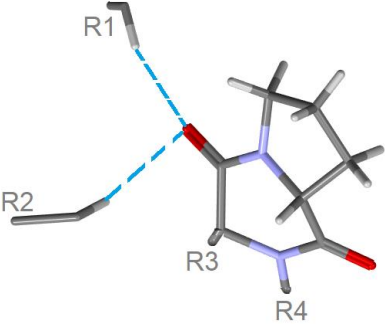
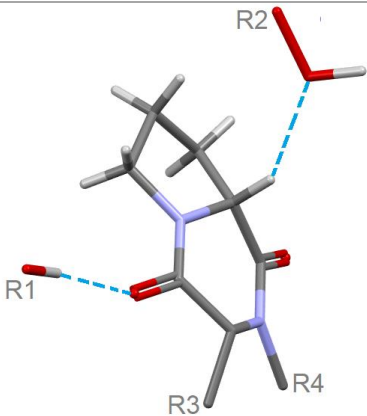
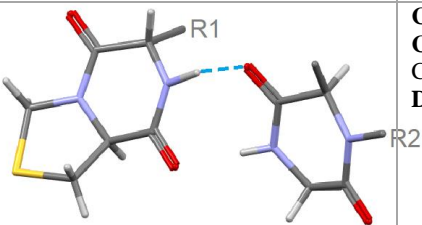
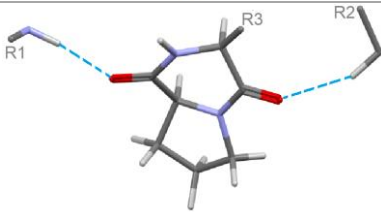
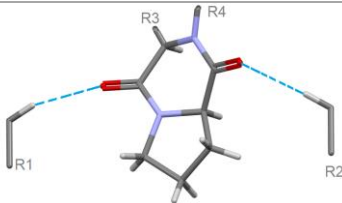
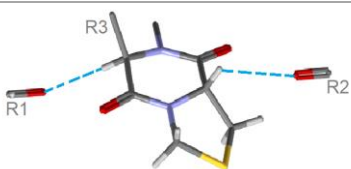
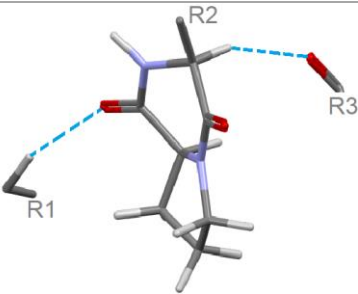
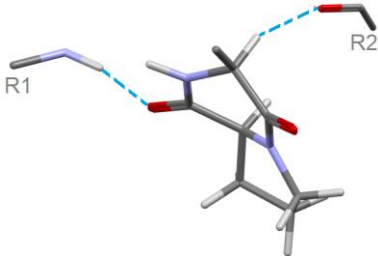
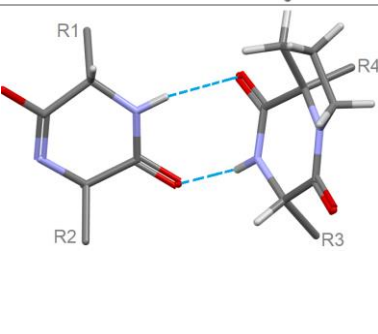
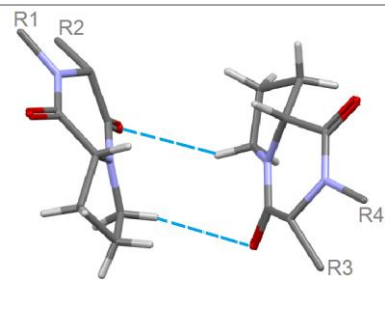
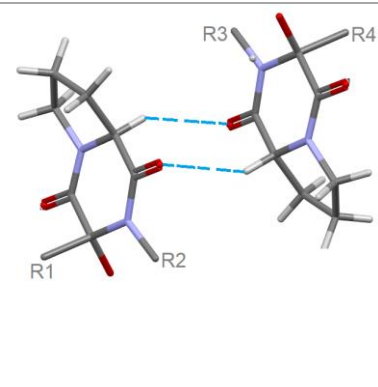
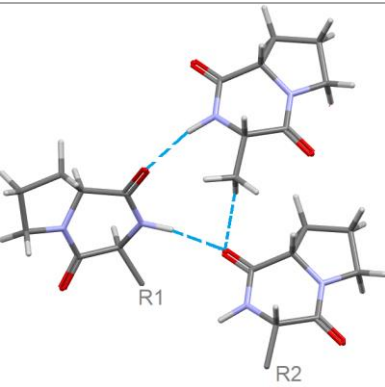
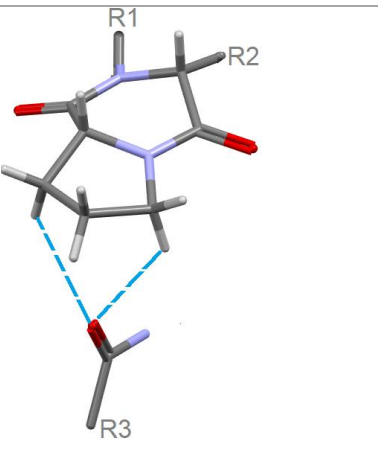
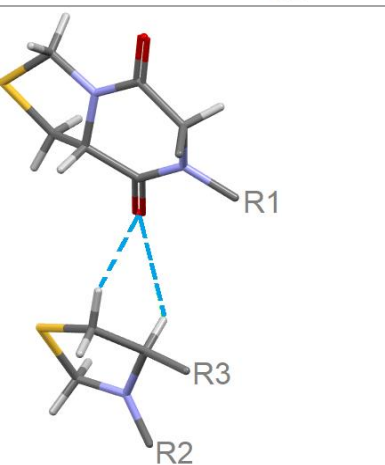
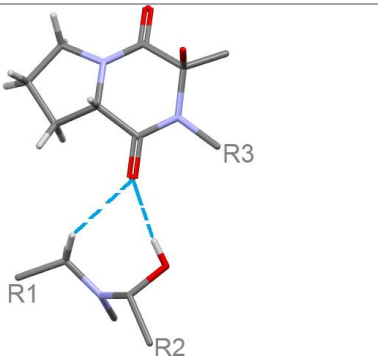
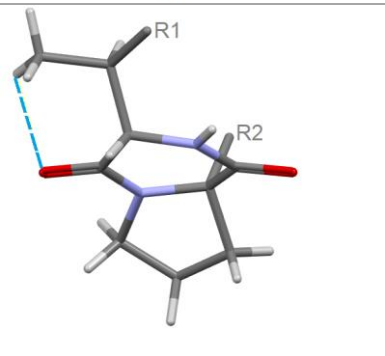


Table S2. Graphical schemes of proline-DKP-based supramolecular synthons (CSD, ver. May 2021).

<i>H-bonding Interaction forming synthon</i>	<i>Synthons and CSD entries, containing these motifs</i>	<i>H-bonding Interaction forming synthon</i>	<i>Synthons and CSD entries, containing these motifs</i>
	D(2): BUDDOJ, FODNEC, PESYUK, TUTSOR, UDALUJ C(5): QOJXIY, RISDIH C(6): BAMCEZ, JIFNER C(8): FEMWAV C(10): IMIHAP, KUXJES		C(4): PABRAM C(5): CYPRLE, DUNVIS, EBIFAZ, JEHPUH, LPROGL, UDALUJ, YERPIU C(6): CYPRLE, EXURAQ, OSELEU C(7): CYPRLE, MOPQUF C(8): LEHREW, NEYLIP, OSELEU C(9): OSELEU, RIXXIG C(10): AKUWUJ, JEHPUH D(2): EXURAQ, FODNES, KUSXIF, RIMTUE, RIXXIG D²₃(9): EXURAQ
	C(4): CLPRAL, DARVOJ, FEXXAH, ODIQUN, QAXFUT, ROPVOH C(5): APUHOJ, BAMCEZ, CLPRPR, EBIFAZ, GESYAH, GESYEL, GESYIP, GLHPRD, JEHPUH, JUCSAB, KETMIG, LPROGL, PABRAM, PUYNUS, RIMTUE, ROPVOH, UKOCON, XOLQUL C(6): APUHOJ, BAMCEZ, CLPRAL, CLPRPR, FODNUI, GESYAH, GESYEL, GESYOV, GUGXOW, JIFNER, JUCSAB, KAXQAD, KUSXIF, LEHREW, LPROGL,		C¹₂(8): JIFNER C¹₂(9): BAMCEZ C¹₂(10): EBIFAZ

	MOPQUF, NEYLIP, ODIQUN, PABRAM, PUYNUS, QAXFUT, REFYIK, ROPVOH, UCOBEV, UKOCON, VAZRAQ, XOLQUL, YERPIU, ZAJZOZ C(7) : FEXXAH, FODNOC, FODNUI, JAFEC, JIFNER, MOPQUF, NEYLIP, NOVCIK, LIKNUO, PUYNUS C(8) : BUDDOJ, DARVID, EBIFAZ, FODNUI, JIFNER, KETMIG, KUXJES, ODOQUN, PUYNUS, QAXFUT, YERPIU C(9) : DITGIZ, FODNES, GESYEL, GESYIP, GUGXOW, KETMIG, KUSXIF, KUXJES, MOPQUF, REFYIK, RIXXIG, ROPVOH, UCOBEV, UKOCON, ZAJZOZ C(10) : JUCSAB, DARVOJ, FEMWAV, NEYLIP, NOVCIK C₂(10) : BOLWEE, GESYEL D(2) : EXURAQ, FODNES, FODNOC, GESYOV, GLHPRD, KETMIG, KUSXIF, KUXJES, PESYUK, RIXXIG, TUTSOR D₂(5) : GESYOV D₂(10) : GESYOV		
	D12(3) : PESYUK, UDALUJ		
	C₁(5) : EXURAQ C₁(6) : CLPRAL, LPROGL C12(7) : NOVCIK, PABRAM C₁(8) : CLPRAL, CYPRLE, JEHPUH, YERPIU C₁(9) : EBIFAZ, KUXJES, NOVCIK, OSULEU C12(10) : OSULEU D12(3) : RIXXIG D23(7) : KUXJES D23(8) : RIMTUE D23(9) : KUSFIF		C12(4) : LPROGL, XOLQUL C12(5) : BAMCEZ, KAQKAD, ODIQUN, ROPVOH, XOLQUL C₁(6) : BOLWEE, DARVOJ, JEHPUH, ODIQUN, ROPVOH, XOLQUL C₁(7) : DARVID, NOVCIK, YERPIU, XOLQUL C₁(8) :

			CLPRAL, CLPRPR, GESYEL, GESYIP, LPROGL, PUYNUS, REFYIK, UKOCON, XOLQUL $C^1_2(9)$: APUHOJ, CLPRPR, DARVID, FODNUI, PABRAM, RIXXIG, XOLQUL $C^1_2(10)$: FODNOC, FODNUI $D^1_2(3)$: GESYOV, RIXXIG $D^2_3(8)$: GLHPRD $D^2_3(9)$: GESYOV $D^2_3(10)$: FODNOC
	$C^2_2(7)$: BAMCEZ $C^2_2(9)$: FODNOC		$C(4)$: CLPRAL $C^2_2(10)$: CLPRAL $D(2)$: BOLWEE
	$C^2_2(10)$: CLPRAL, EBIFAZ, LPROGL, MOPQUF, UDALUJ $D22(8)$: RIXXIG		$C^2_2(9)$: APUHOJ, BAMCEZ, CLPRPE, GESYOV, XOLQUL $C^2_2(10)$: CLPRAL, LIKNUO, MOPQUF, XOLQUL $D^2_2(8)$: GESYOV, NOVCIK, RIXXIG, REFYIK, TUTSOR
	$D^2_2(8)$: GESYOV		$C^2_2(10)$: CLPRAL, FODNOC $D^2_2(7)$: GESYOV $D^2_2(8)$: GESYOV

	<p>C₂²(10): CLPRAL, CYPRLE D₂²(7): GESYOV</p>		
	<p>R₂²(8): AKUWUY, BOLWEE, EBIFAZ, IMIHP</p>		<p>R₂²(10): BAMCEZ, FODNUI, GESYIP, GESYOV, JAFEC</p>
	<p>R₂²(8): JAFEC</p>		<p>R₂³(10): CLPRAL</p>
	<p>R₁¹(6): APUHOJ, CLPRPR, JEHPUH</p>		<p>R₁¹(5): GESYOV</p>
	<p>R₁¹(7): FODNOC, GESYOV</p>		<p>S(6): AKUWUY, FODNUI</p>

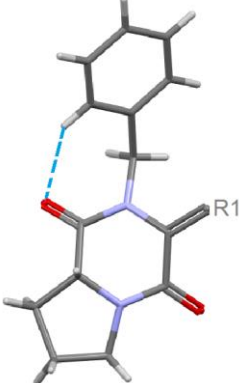
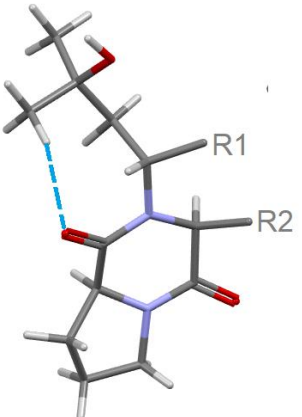
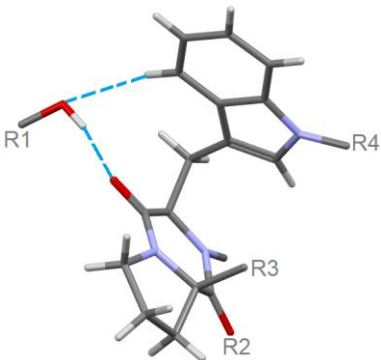
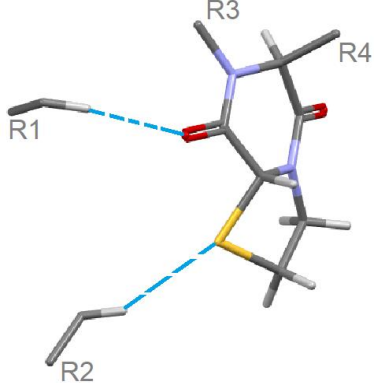
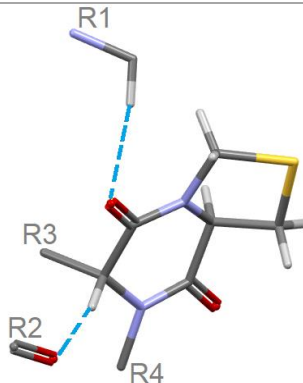
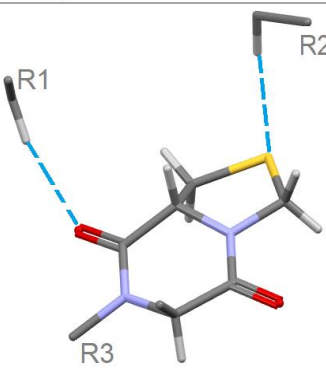
	S(7): BUDDOJ, DITGIZ		S(8): FEMWAY
	R²₂(10): BIDDOJ		C²₂(10): GESYEL D²₂(7): GESYOV
	D²₂(6): GESYOV		D²₂(7): GESYOV

Table S3. Library of proline-DKP-based supramolecular synthons (CSD, ver. May 2021, see blue entries in Tb. S1), up to 10-membered H-bonding motifs.

CSD code	ref.	Synthon	Interactions forming synthon
AKUWUY	C(10)		$(\text{DKP-NH})\text{N-H}\cdots\text{O}_{(\text{C=O-DKP})}$
	S(6)		$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	R ² ₂ (8)		$[(\text{DKP-NH})\text{N-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
APUHOJ	C(5)		$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)		$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C ¹ ₂ (9)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	C ² ₂ (9)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	R ¹ ₂ (6)		$[(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
BAMCEZ	C(6)		$(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)		$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C ¹ ₂ (5)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	C ¹ ₂ (9)		$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$ & $(\text{OH})\text{O-H}\cdots\text{C-H}_{(\text{CH-Pro})}$
	C ² ₂ (7)		$(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$ & $(\text{OH})\text{O-H}\cdots\text{C-H}_{(\text{CH-Pro})}$
	C ² ₂ (9)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	C ² ₂ (10)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	R ² ₂ (10)		$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	R ² ₂ (10)		$[(\text{OH})\text{O-H}\cdots\text{C-H}_{(\text{CH-DKP})}]_2$
BIDDOJ	S(7)		$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	D(2)		$(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(8)		$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$

	$R_2^2(10)$	$(OH)O-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O-H_{(OH)}$
BOLWEE	D(2)	$(DKP-NH)N-H\cdots O=C_{(DKP)}$
	D(2)	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(6)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$C_2^2(10)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$R_2^2(8)$	$[(DKP-NH)N-H\cdots O=C_{(DKP)}]_2$
CLPRAL	C(4)	$(Pro-NH)N-H\cdots O=C_{(DKP)}$
	C(4)	$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	C(6)	$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(6)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(8)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$[DKP-CH)C-H\cdots O=C_{(DKP)}]_2$
		$(CH)C-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(DKP-CH)C-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C_2^2(10)$	$(Pro-CH)C-H\cdots O=C_{(DKP)} \& (DKP-NH)N-H\cdots O=C_{(DKP)}$
		$(CH)C-H\cdots O=C_{(DKP)} \& (DKP-NH)N-H\cdots O=C_{(DKP)}$
		$[Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
		$[DKP-CH)C-H\cdots O=C_{(DKP)}]_2$
		$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$R_2^2(10)$	$(Pro-CH)C-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
		$[(DKP-NH)N-H\cdots O=C_{(DKP)}]_2$
CLPRPR	C(5)	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	C(6)	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(9)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$C_2^2(9)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$R_2^1(6)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
CYPRLE	C(5)	$(DKP-NH)N-H\cdots O=C_{(DKP)}$
	C(6)	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	C(7)	$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(8)$	$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$C_2^2(10)$	$(NH)N-H\cdots O=C_{(DKP)}$
DARVID	C(8)	$(Pro-CH)C-H\cdots O=C$
		$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(7)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$C_2^1(9)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$C_2^2(8)$	$(CH)C-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(C-O-C)}$
	$R_2^2(10)$	$[(DKP-CH)C-H\cdots O=C_{(DKP)}]_2$
DARWOJ	C(4)	$(Pro-CH)C-H\cdots O=C$
		$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	C(6)	$(DKP-CH)C-H\cdots O=C$
	C(10)	$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(6)$	$(Pro-CH)C-H\cdots O=C \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
	$C_2^2(10)$	$(DKP-CH)C-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C$
	$R_2^2(6)$	$(DKP-CH)C-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C$
	DITGIZ	$(CH)C-H\cdots O=C_{(DKP)}$
	C(9)	$(CH)C-H\cdots O=C_{(DKP)}$
	DUNVIS	$(DKP-NH)N-H\cdots O=C_{(DKP)}$
EBIFAZ	C(5)	$(DKP-NH)N-H\cdots O=C_{(DKP)}$
	C(5)	$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	C(8)	$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(9)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$C_2^1(10)$	$(OH)O-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
	$C_2^2(10)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
	$R_2^2(8)$	$(DKP-CH)C-H\cdots O=C_{(DKP)} \& (DKP-NH)N-H\cdots O=C_{(DKP)}$
	EXURAZ	$(NH)N-H\cdots O=C_{(DKP)}$
		$(CH)C-H\cdots O=C_{(DKP)}$
		$(DKP-NH)N-H\cdots O=C_{(DKP)}$
	C(6)	$(NH)N-H\cdots O=C_{(DKP)}$
	$C_2^1(5)$	$(NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$D_2^3(9)$	$[(NH)N-H\cdots O=C_{(DKP)}]_2$
FEMWAV	S(7)	$(CH)C-H\cdots O=C_{(DKP)}$
	S(8)	$(CH)C-H\cdots O=C_{(DKP)}$
	C(8)	$(OH)O-H\cdots O=C_{(DKP)}$
FEXXAH	C(4)	$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	C(7)	$(CH)C-H\cdots O=C_{(DKP)}$
	$C_2^2(9)$	$(CH)C-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(C=O)}$
FODNES	D(2)	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(NH)N-H\cdots O=C_{(DKP)}$
	C(9)	$(CH)C-H\cdots O=C_{(DKP)}$
FODNOC	D(2)	$(OH)O-H\cdots O=C_{(DKP)}$

	D ₃ ² (10)	(CH) ₃ C-H···O=C _(DKP)
	C(7)	[_{(CH)3} C-H···O=C _(DKP)] ₂ & (Pro-CH) ₃ C-H···O=C _(DKP)
	C ₂ ¹ (10)	[_{(CH)3} C-H···O=C _(DKP)] ₂
	C ₂ ² (9)	(OH) ₃ O-H···O=C _(DKP) & (DKP-CH) ₃ C-H···O=C _(DKP)
	C ₂ ² (10)	(Pro-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
		[_{(Pro-CH)3} C-H···O=C _(DKP)] ₂
	R ₂ ¹ (7)	(OH) ₃ O-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
	R ₂ ² (8)	(CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O _(C-O-C)
	R ₂ ² (10)	(OH) ₃ O-H···O=C _(DKP) & (CH) ₃ C-H···O-H _(OH)
		(OH) ₃ O-H···O=C _(DKP) & (CH) ₃ C-H···O-H _(OH)
FODNUI	S(6)	(CH) ₃ C-H···O=C _(DKP)
	C(6)	(CH) ₃ C-H···O=C _(DKP)
	C(7)	(CH) ₃ C-H···O=C _(DKP)
	C(8)	(CH) ₃ C-H···O=C _(DKP)
	C ₂ ¹ (9)	(CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	C ₂ ¹ (10)	(CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	R ₂ ² (10)	[_{(Pro-CH)3} C-H···O=C _(DKP)] ₂
GESYAH	C(5)	(CH) ₃ C-H···O=C _(DKP)
	C(6)	(CH) ₃ C-H···O=C _(DKP)
GESYEI	C(5)	(DKP-CH) ₃ C-H···O=C _(DKP)
	C(6)	(Pro-CH) ₃ C-H···O=C _(DKP)
		(CH) ₃ C-H···O=C _(DKP)
	C(9)	(CH) ₃ C-H···O=C _(DKP)
		(CH) ₃ C-H···S _(Pro)
	C ₂ ¹ (8)	(CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	C ₂ ² (10)	(DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···S _(Pro)
		(DKP) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···S _(Pro)
	R ₂ ² (9)	(DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
GESYIP	C(5)	(Pro-CH) ₃ C-H···O=C _(DKP)
		(CH) ₃ C-H···O=C _(DKP)
	C(9)	(CH) ₃ C-H···O=C _(DKP)
	C ₂ ¹ (8)	(CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	R ₂ ² (10)	(Pro-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
GESYOV	D(2)	(DKP-CH) ₃ C-H···O=C _(DKP)
		(Pro-CH) ₃ C-H···O=C _(DKP)
		(Pro-CH) ₃ C-H···O=C _(DKP)
	D ₂ ¹ (3)	(Pro-CH) ₃ C-H···O=C _(DKP) & (DKP-CH) ₃ C-H···O=C _(DKP)
	D ₂ ² (5)	(Pro-CH) ₃ C-H···S _(Pro) & (Pro-CH) ₃ C-H···O=C _(DKP)
		(Pro-CH) ₃ C-H···O=C _(DKP) & (DKP/Pro-CH) ₃ C-H···S _(Pro)
	D ₂ ² (6)	(CH) ₃ C-H···O=C _(DKP) & (DKP-CH) ₃ C-H···O=C _(DKP)
		(Pro-CH) ₃ C-H···S _(Pro) & (DKP/Pro-CH) ₃ C-H···O=C _(DKP)
	D ₂ ² (7)	(DKP-CH) ₃ C-H···S _(Pro) & (DKP-CH) ₃ C-H···O=C _(DKP)
		(DKP/Pro-CH) ₃ C-H···O=C _(DKP) & (CH-Pro/DKP) ₃ C-H···S _(Pro)
		(DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
	D ₂ ² (8)	[_{(DKP-CH)3} C-H···O=C _(DKP)] ₂
		(Pro-CH) ₃ C-H···O=C _(DKP)] ₂
		(Pro-CH) ₃ C-H···O=C _(DKP) & (DKP-CH) ₃ C-H···O=C _(DKP)
		(DKP-CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	D ₂ ² (9)	(CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···S _(Pro)
	D ₃ ² (9)	[_{(CH)3} C-H···O=C _(DKP)] ₂ & (CH-Pro) ₃ C-H···O=C _(DKP)
	D ₂ ² (10)	(Pro-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
		(DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···S _(Pro)
		(DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···S _(Pro)
	C(9)	(Pro-CH) ₃ C-H···S _(Pro)
	C ₂ ¹ (8)	(DKP-CH) ₃ C-H···S _(Pro) & (Pro-CH) ₃ C-H···S _(Pro)
	C ₂ ² (9)	(Pro-CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···S _(Pro)
		[_{(CH)3} C-H···O=C _(DKP)] ₂
	C ₂ ² (10)	(Pro-CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
		(Pro-CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···S _(Pro)
	R ₂ ¹ (5)	(Pro-CH) ₃ C-H···O=C _(DKP) & (Pro-CH) ₃ C-H···O=C _(DKP)
	R ₂ ¹ (7)	[_{(CH)3} C-H···O=C _(DKP)] ₂
	R ₂ ¹ (9)	[_{(CH)3} C-H···O=C _(DKP)] ₂
	R ₂ ² (7)	(Pro-CH) ₃ C-H···O=C _(DKP) & (DKP-CH) ₃ C-H···S _(Pro)
	R ₂ ² (9)	(Pro/DKP-CH) ₃ C-H···O=C _(DKP) & (CH) ₃ C-H···O=C _(DKP)
	R ₂ ² (10)	(CH) ₃ C-H···O=C _(DKP) & (CH-Pro) ₃ C-H···O=C _(DKP)

	D ₂ ² (5)	(Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(H ₂ O)
	D ₂ ² (6)	(Pro-CH) ₂ C-H...O=C(Pro) & (Pro-CH) ₂ C-H...O(H ₂ O)
		(Pro-CH) ₂ C-H...O(C=O) & (Pro-CH) ₂ C-H...O(H ₂ O)
	D ₂ ² (7)	(DKP/Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(H ₂ O)
	D ₂ ² (8)	(Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(H ₂ O)
	D ₂ ² (9)	(DKP/Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(H ₂ O)
	D ₃ ² (8)	(Pro/DKP-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O=C(DKP) & (DKP-CH) ₂ C-H...O=C(DKP)
	C ₂ ² (9)	[_(DKP-CH) C-H...O=C(DKP)] ₂
	C ₂ ² (10)	(Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(C=O)
GUGXOW	C(6)	(Pro-CH) ₂ C-H...O(C=O)
		(DKP/Pro-CH) ₂ C-H...O(C-O-C)
	C(9)	(Pro-CH) ₂ C-H...O(C=O)
	C ₂ ² (10)	(Pro-CH) ₂ C-H...O=C(DKP) & (Pro-CH) ₂ C-H...O(C=O)
	R ₂ ² (8)	(Pro-CH) ₂ C-H...O=C(DKP) & (DKP-CH) ₂ C-H...O(C-O-C)
IMIHP	D(2)	(DKP-CH) ₂ C-H...O=C(DKP)
	D ₃ ² (7)	[_(CH) C-H...O=C(DKP)] ₂ & (DKP-NH) ₂ N-H...O=C(DKP)
	C(9)	(CH) ₂ C-H...O=C(DKP)
	C(10)	(OH) ₂ O-H...O=C(DKP)
	C ₂ ¹ (9)	(CH) ₂ C-H...O=C(DKP) & (DKP/NH) ₂ N-H...O=C(DKP)
	R ₂ ² (8)	[_(DKP-NH) N-H...O=C(DKP)] ₂
JAFFEC	C(7)	(CH) ₂ C-H...O=C(DKP)
	R ₂ ² (8)	[_(Pro/DKP-CH) C-H...O=C(DKP)] ₂
	R ₂ ² (10)	[_(Pro/DKP-CH) C-H...O=C(DKP)] ₂
JEHPUH	C(5)	(DKP-NH) ₂ N-H...O=C(DKP)
		(CH) ₂ C-H...O=C(DKP)
	C(10)	(NH) ₂ N-H...O=C(DKP)
	C ₂ ¹ (8)	(CH) ₂ C-H...O=C(DKP) & (NH) ₂ N-H...O=C(DKP)
	C ₂ ² (8)	(DKP/Pro-CH) ₂ C-H...O=C(DKP) & (NH) ₂ N-H...O=C(DKP)
	C ₂ ² (10)	(Pro-CH) ₂ C-H...O=C(DKP) & (DKP/NH) ₂ N-H...O=C(DKP)
	R ₂ ¹ (6)	(CH) ₂ C-H...O=C(DKP) & (DKP-NH) ₂ N-H...O=C(DKP)
JIFNER	C(6)	(OH) ₂ O-H...O=C(DKP)
		(Pro-CH) ₂ C-H...O=C(DKP)
	C(7)	(CH) ₂ C-H...O=C(DKP)
	C ₂ ¹ (8)	(Pro-CH) ₂ C-H...O=C(DKP) & (OH) ₂ O-H...O=C(DKP)
	C ₂ ² (9)	(CH) ₂ C-H...O=C(DKP) & (CH) ₂ C-H...O(OH)
	C ₂ ² (10)	(CH) ₂ C-H...O(OH) & (OH) ₂ O-H...O=C(DKP)
JUCSAB	C(5)	(DKP-CH) ₂ C-H...O=C(DKP)
	C(6)	(CH) ₂ C-H...O=C(DKP)
	C(10)	(CH) ₂ C-H...O=C(DKP)
KAQXAD	S(6)	(CH) ₂ C-H...O=C(DKP)
	C(6)	(Pro-CH) ₂ C-H...O=C(DKP)
	C ₂ ¹ (5)	[_(Pro-CH) C-H...O=C(DKP)] ₂
KETMIG	D(2)	(Pro-CH) ₂ C-H...O=C(DKP)
	C(5)	(Pro-CH) ₂ C-H...O=C(DKP)
	C(8)	(CH) ₂ C-H...O=C(DKP)
	C(9)	(CH) ₂ C-H...O=C(DKP)
	R ₂ ¹ (7)	[_(CH) C-H...O=C(DKP)] ₂
KUSXIF	D(2)	(DKP-NH) ₂ N-H...O=C(DKP)
		(CH) ₂ C-H...O=C(DKP)
	D ₃ ² (9)	(CH) ₂ C-H...O=C(DKP) & (NH) ₂ N-H...O=C(DKP)
		(CH) ₂ C-H...O=C(DKP) & (DKP-NH) ₂ N-H...O=C(DKP)
	C(6)	(CH) ₂ C-H...O=C(DKP)
	C(9)	(CH) ₂ C-H...O=C(DKP)
	S(7)	(CH) ₂ C-H...O=C(DKP)
	R ₂ ² (8)	[_(DKP-NH) N-H...O=C(DKP)] ₂
KUXJES	D(2)	(Pro-CH) ₂ C-H...O=C(DKP)
	D ₃ ² (7)	(DKP-CH) ₂ C-H...O=C(DKP) & (CH) ₂ C-H...O=C(DKP) & (NH) ₂ N-H...O=C(DKP)
		(Pro-CH) ₂ C-H...O=C(DKP)
	C(8)	(CH) ₂ C-H...O=C(DKP)
	C(9)	(CH) ₂ C-H...O=C(DKP)
	C(10)	(OH) ₂ O-H...O=C(DKP)
	C ₂ ¹ (9)	(DKP-NH) ₂ N-H...O=C(DKP) & (CH) ₂ C-H...O=C(DKP)
	R ₂ ¹ (6)	(CH) ₂ C-H...O=C(DKP) & (OH) ₂ O-H...O=C(DKP)
	R ₂ ² (8)	[_(NH) N-H...O=C(DKP)] ₂
LEHREW	C(6)	(CH) ₂ C-H...O=C(DKP)
	C(8)	(NH) ₂ N-H...O=C(DKP)
LIKNUO	C(7)	(Pro-CH) ₂ C-H...O=C(DKP)
	C(10)	(CH) ₂ C-H...O(C=O)
	C ₂ ³ (10)	(DKP-CH) ₂ C-H...O(C=O) & (Pro-CH) ₂ C-H...O=C(DKP)
		[_(Pro-CH) C-H...O=C(DKP)] ₂

[illegible]

		$(CH)C-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O-H_{(OH)}$
	$D^2_2(8)$	$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O-H_{(OH)}$
		$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$D^2_2(9)$	$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O-H_{(OH)}$
	$D^2_2(10)$	$[(OH)O-H\cdots O=C_{(DKP)}]_2$
		$[(OH)O-H\cdots O=C_{(DKP)}]_2$
		$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-CH)C-H\cdots O-H_{(OH)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C^2_2(10)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$R^2_2(7)$	$(OH)O-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O-H_{(OH)}$
PUYNUS	$C(5)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(6)$	$(DKP/Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(7)$	$(CH)C-H\cdots O=C_{(DKP)}$
	$C(8)$	$(DKP/Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C^1_2(8)$	$[(DKP/-CH)C-H\cdots O=C_{(DKP)}]_2$
	$C^2_2(10)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
QAXRUT	$C(4)$	$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	$C(6)$	$(CH)C-H\cdots O=C_{(DKP)}$
	$C(8)$	$(CH)C-H\cdots O=C_{(DKP)}$
	$C^2_2(10)$	$(CH)C-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
	$R^1_2(6)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
QOJXIY	$S(6)$	$(OH)O-H\cdots O=C_{(DKP)}$
	$R^1_2(6)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
REFYIK	$C(6)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(7)$	$(DKP-CH)C-H\cdots O=C_{(C=O)}$
	$C(9)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C^1_2(8)$	$(DKP-CH)C-H\cdots O=C_{(C=O)} \& (DKP-CH)C-H\cdots O=C_{(C=O)}$
	$C^2_2(9)$	$(CH)C-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(C=O)}$
	$C^2_2(10)$	$(CH)C-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(C=O)}$
RIMTUE	$D(2)$	$(DKP-NH)N-H\cdots O=C_{(DKP)}$
	$C(5)$	$(DKP-CH)C-H\cdots O=C_{(DKP)}$
	$R^1_2(6)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$R^2_2(8)$	$[(DKP-NH)N-H\cdots O=C_{(DKP)}]_2$
	$D^2_3(8)$	$(DKP)N-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(C=O)}$
	$D^3_3(10)$	$(NH)N-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
RISDIH	$S(6)$	$(OH)O-H\cdots O=C_{(DKP)}$
	$C(5)$	$(OH)O-H\cdots O=C_{(DKP)}$
	$C^2_2(10)$	$(CH)C-H\cdots O-H_{(OH)} \& (CH)C-H\cdots O=C_{(DKP)}$
RIXSIG	$D(2)$	$(DKP)N-H\cdots O=C_{(DKP)}$
		$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(9)$	$(DKP)N-H\cdots O=C_{(DKP)}$
		$(CH)C-H\cdots O=C_{(DKP)}$
	$C^1_2(9)$	$[(CH)C-H\cdots O=C_{(DKP)}]_2$
	$D^1_2(3)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-CH)C-H\cdots C=O_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$D^2_2(6)$	$(Pro/DKP-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
		$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (DKP-CH)C-H\cdots O=C_{(DKP)}$
		$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$D^2_2(7)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$D^2_2(8)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (DKP-NH)N-H\cdots O=C_{(DKP)}$
		$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$D^2_2(9)$	$(DKP-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
	$D^2_2(10)$	$(Pro-CH)C-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (Pro-CH)C-H\cdots O=C_{(DKP)}$
		$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$R^1_2(6)$	$(Pro-NH)N-H\cdots O=C_{(DKP)} \& (CH)C-H\cdots O=C_{(DKP)}$
	$R^2_2(8)$	$[(DKP-NH)N-H\cdots O=C_{(DKP)}]_2$
	$R^2_2(9)$	$[(DKP-CH)C-H\cdots O=C_{(DKP)}]_2$
	$R^2_2(10)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
ROPVOH	$C(4)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(5)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(6)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C(9)$	$(Pro-CH)C-H\cdots O=C_{(DKP)}$
	$C^1_2(5)$	$[(Pro-CH)C-H\cdots O=C_{(DKP)}]_2$
	$C^1_2(6)$	$[(DKP/Pro-CH)C-H\cdots O=C_{(DKP)}]_2$

	$C_2^2(9)$	$(\text{Pro-CH})\text{C-H}\cdots\text{N} \text{ \& } (\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$C_2^2(10)$	$(\text{Pro-CH})\text{C-H}\cdots\text{C}=\text{O}_{(\text{DKP})} \text{ \& } (\text{Pro/DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
		$(\text{Pro-CH})\text{C-H}\cdots\text{N} \text{ \& } (\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$R_{2(6)}^1$	$[(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$R_{2(8)}^1$	$[(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$R_{3(10)}^2$	$[(\text{DKP-CH})\text{C-H}\cdots\text{C}=\text{O}_{(\text{DKP})}]_2 \text{ \& } (\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
TUTSOR	D(2)	$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
		$(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$D_{2(8)}^2$	$[(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
		$(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
		$[(\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$D_{2(9)}^2$	$(\text{CH})\text{C-H}\cdots\text{O-H}_{(\text{OH})} \text{ \& } (\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
UCOBEB	$R_{2(7)}^1$	$(\text{CH})\text{C-H}\cdots\text{C}=\text{O}_{(\text{DKP})} \text{ \& } (\text{OH})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(9)	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$C_2^2(10)$	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{DKP/Pro-CH})\text{C-H}\cdots\text{O}_{(\text{C-O-C})}$
		$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{DKP/Pro-CH})\text{C-H}\cdots\text{O}_{(\text{C-O-C})}$
UDALUJ	D(2)	$(\text{Pro/DKP-CH})\text{C-H}\cdots\text{O}_{(\text{H}_2\text{O})}$
	$D_{2(3)}^1$	$[(\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$D_{2(4)}^2$	$(\text{H}_2\text{O})\text{O-H}\cdots\text{O}_{(\text{H}_2\text{O})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$D_{2(6)}^2$	$(\text{DKP/Pro-CH})\text{C-H}\cdots\text{O}_{(\text{H}_2\text{O})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$D_{2(7)}^2$	$(\text{DKP/Pro-CH})\text{C-H}\cdots\text{C}=\text{O}_{(\text{DKP})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$D_{2(8)}^2$	$(\text{Pro-CH})\text{C-H}\cdots\text{O}_{(\text{H}_2\text{O})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
		$[(\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$D_{2(10)}^2$	$(\text{CH})\text{C-H}\cdots\text{O}_{(\text{H}_2\text{O})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$D_{3(8)}^2$	$(\text{DKP-NH})\text{N-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } [(\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
		$[(\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2 \text{ \& } (\text{DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(5)	$(\text{DKP-NH})\text{N-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
		$(\text{DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$C_2^2(6)$	$(\text{DKP/Pro-CH})\text{C-H}\cdots\text{O}_{(\text{H}_2\text{O})} \text{ \& } (\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$C_2^2(9)$	$[(\text{H}_2\text{O})\text{O-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_2^2(10)$	$(\text{DKP-NH})\text{N-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
UKOCON	$R_{2(8)}^2$	$(\text{DKP-NH})\text{N-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(5)	$(\text{DKP-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(9)	$(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
WAZRAQ	$C_{2(8)}^1$	$(\text{DKP})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)	$(\text{DKP-CH})\text{C-H}\cdots\text{H-C}_{(\text{CH-Pro})}$
	C(10)	$(\text{DKP-CH})\text{C-H}\cdots\text{O}_{(\text{C-O-C})}$
	$C_2^2(10)$	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{Pro-CH})\text{C-H}\cdots\text{O}_{(\text{C-O-C})}$
		$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})} \text{ \& } (\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
XOLQUL	C(5)	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	C(6)	$(\text{Pro-CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}$
	$C_{2(4)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(5)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(6)}^1$	$[(\text{CH})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(7)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(8)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(9)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$C_{2(10)}^2$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\text{C}_{(\text{DKP})}]_2$
	$R_{2(5)}^1$	$[(\text{Pro})\text{C-H}\cdots\text{O}=\$