

Supplementary data for the article:

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Supplementary Material

Synthesis, characterization, DFT calculations and antimicrobial activity of pentagonal-bipyramidal Zn(II) and Cd(II) complexes with 2,6-diacetylpyridine-bis(trimethylammoniumacetohydrazone)

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KATARINA ANĐELKOVIĆ*

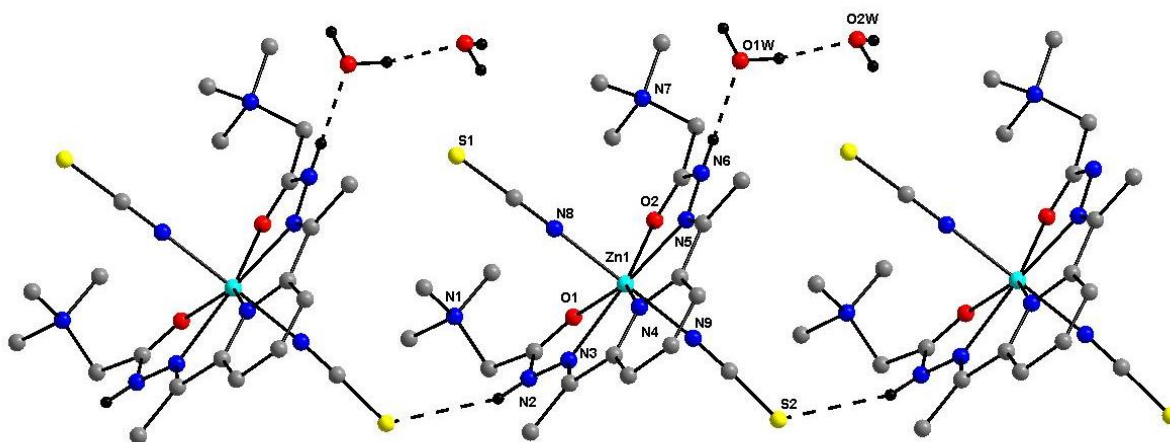
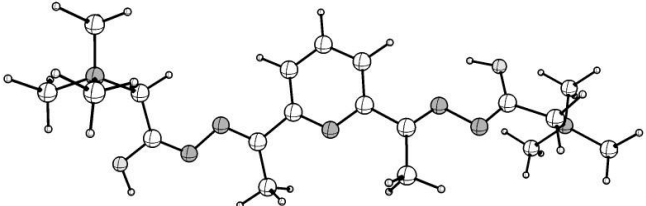
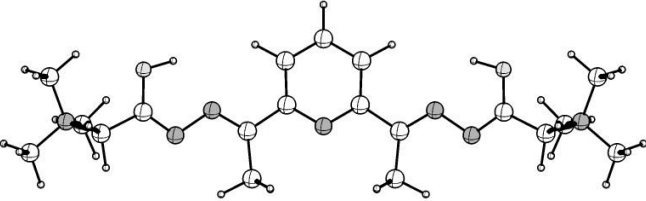
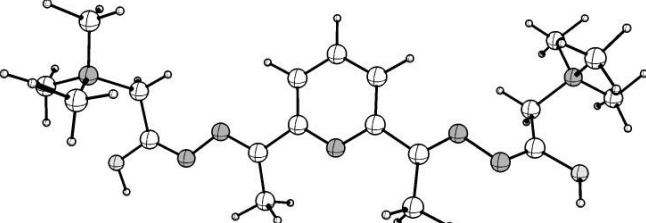
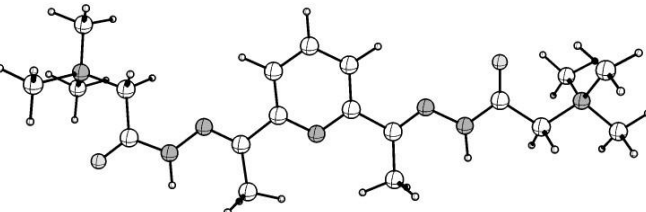
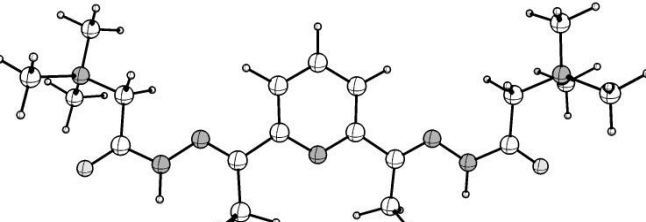
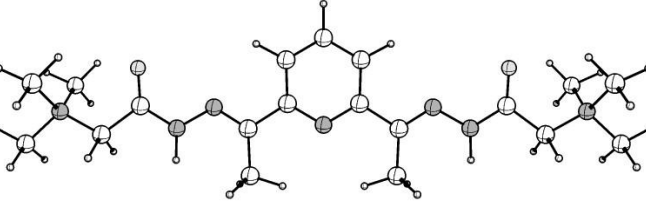


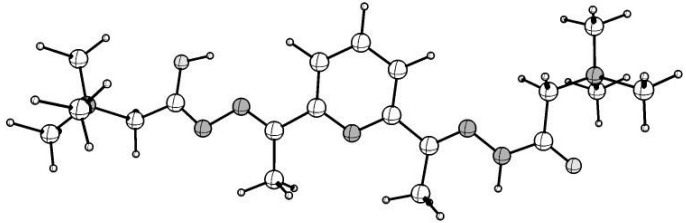
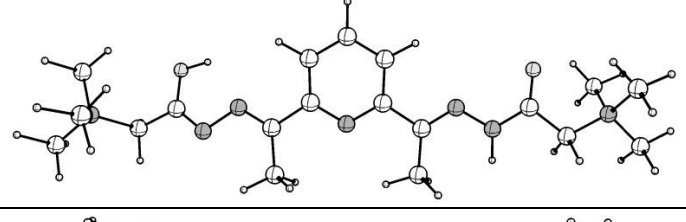
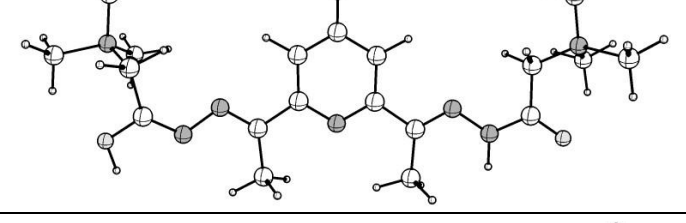
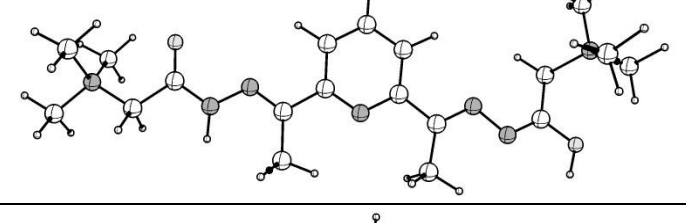
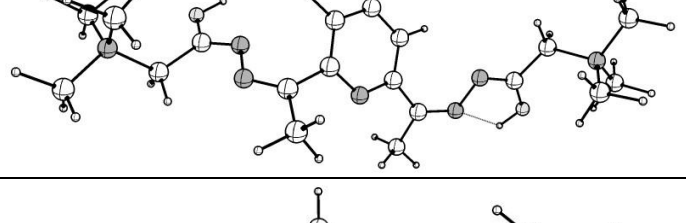
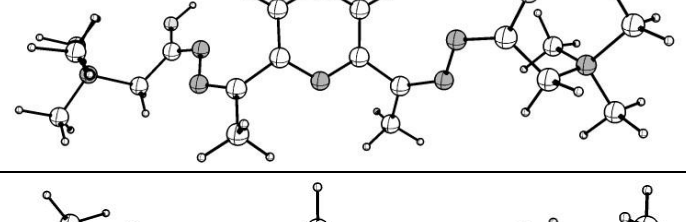
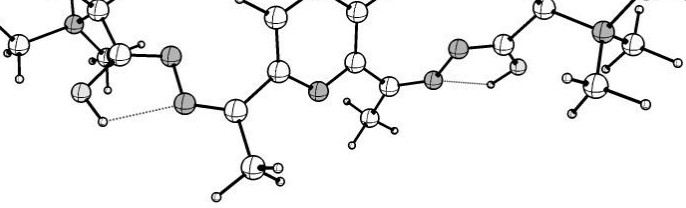
Figure S1. Fragment of the crystal structure of **1** showing N–H···S, N–H···O and O–H···O hydrogen bonding interactions between complex ions and non-coordinated water molecules. Hydrogen atoms not involved in hydrogen bonding and [Zn(NCS)]²⁻ anions have been removed for clarity.

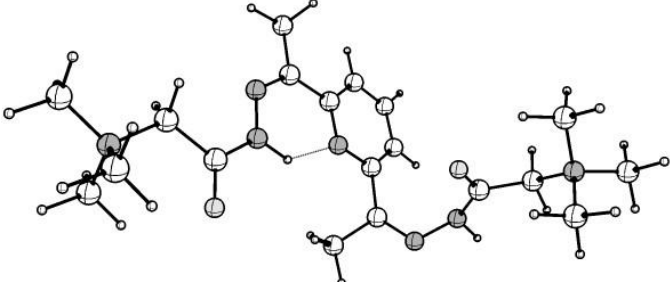
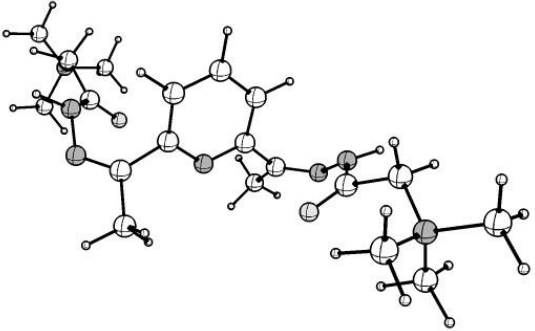
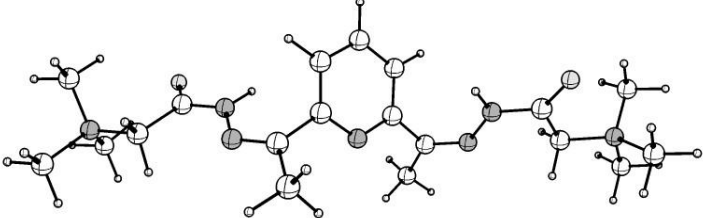
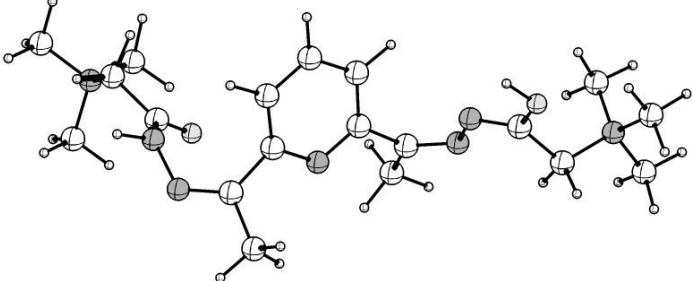
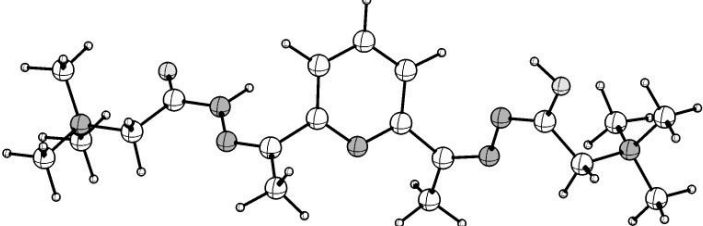
Table S1. Hydrogen bonding geometry for **1**.

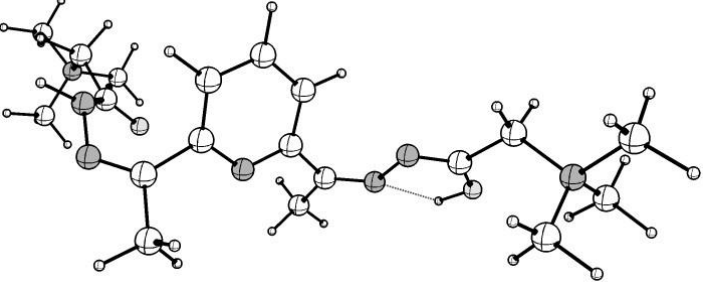
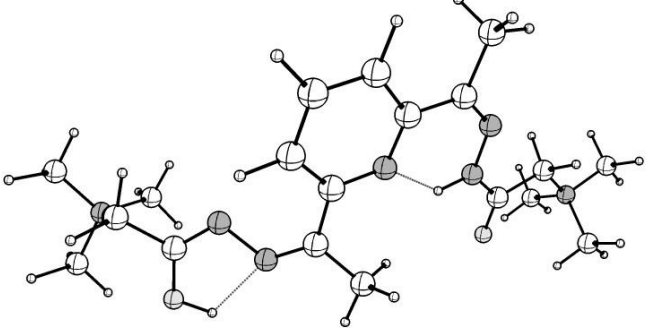
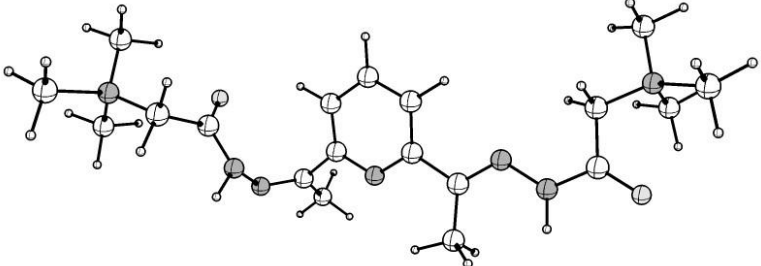
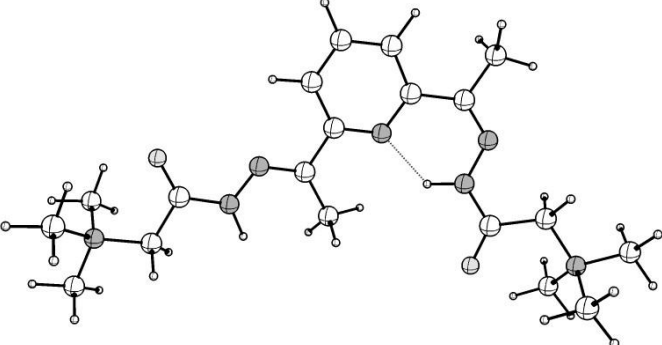
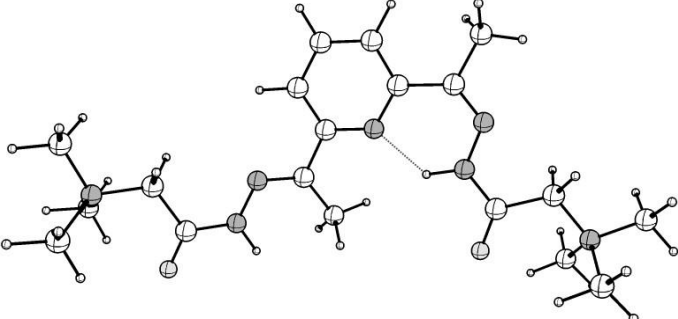
D – H ... A	<i>d</i> (D – H)/ Å	<i>d</i> (H ... A)/ Å	<i>d</i> (D ... A)/ Å	∠(DHA)/ °	Symmetry transformation for acceptors
N2-H2N···S2	0.875(18)	2.66(2)	3.485(2)	158(3)	x, y-1, z
N6-H6N···O1w	0.853(18)	1.920(19)	2.758(3)	167(3)	
O1w-H1w···O2w	0.935(19)	1.83(3)	2.734(5)	161(5)	

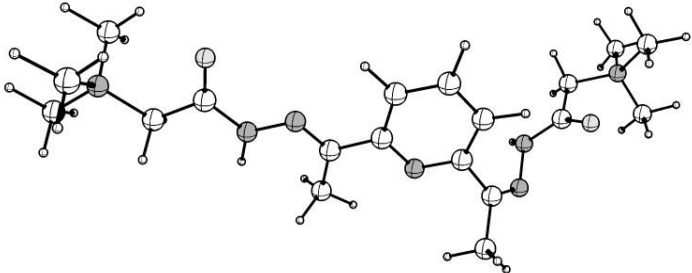
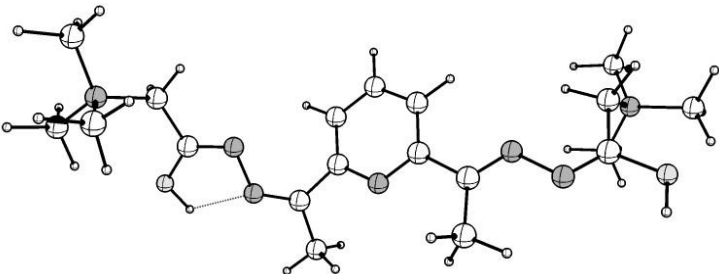
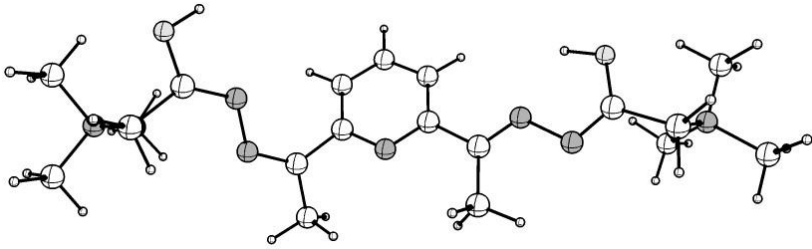
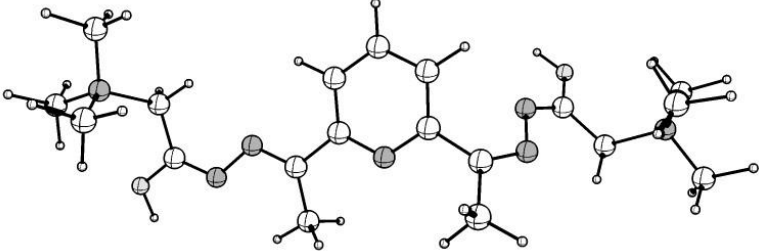
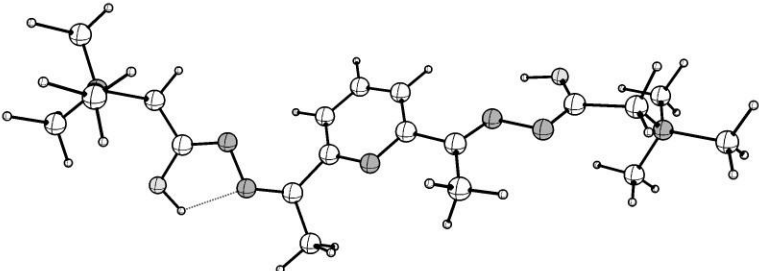
Table S2. Total energies (a. u.) and relative stability ΔE (kcal/mol) of isomers of ligand H_2LCl_2 in vacuum.

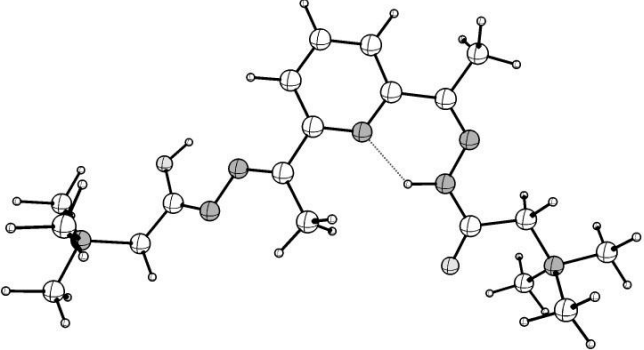
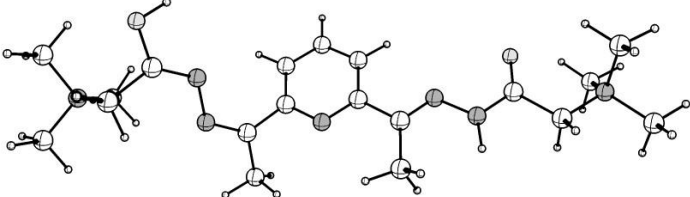
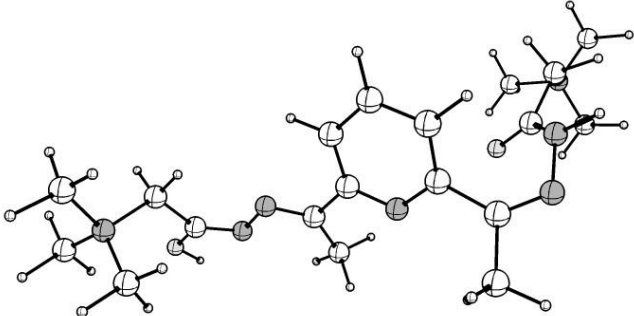
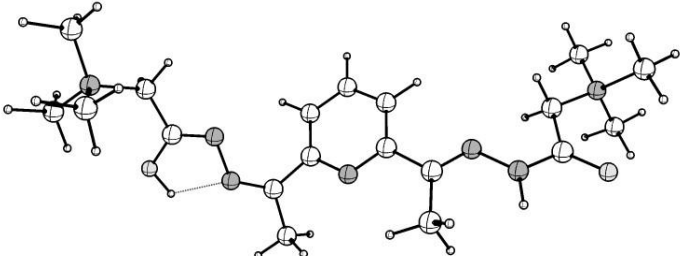
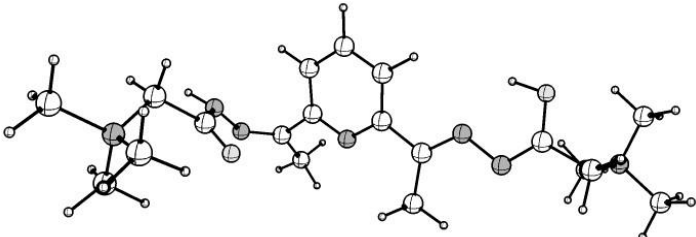
Isomers of ligand	Total energy (a.u.) vacuum	Relative energies (vacuum) ΔE kcal/mol
	-1277.3135255	26.3
	-1277.3220107	21.0
	-1277.3047975	31.8
	-1277.3479212	4.7
	-1277.3545819	0.6
	-1277.3394096	10.1

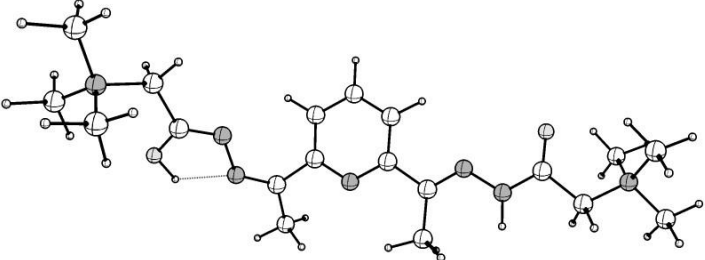
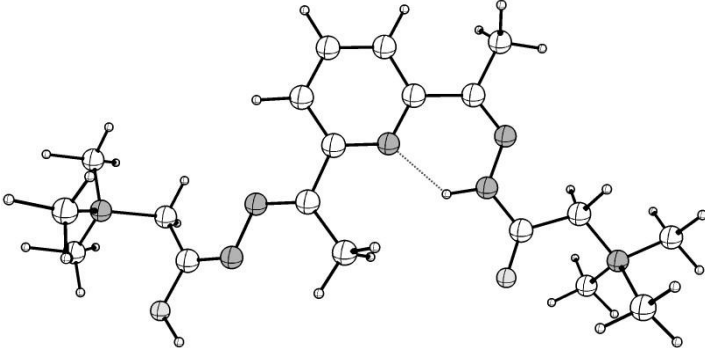
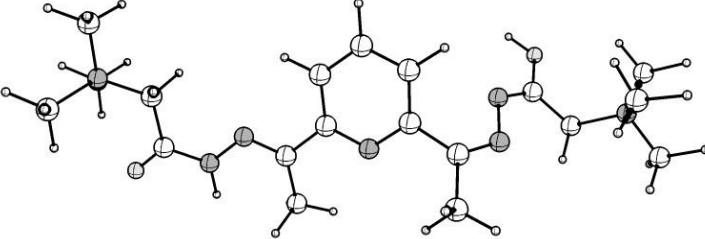
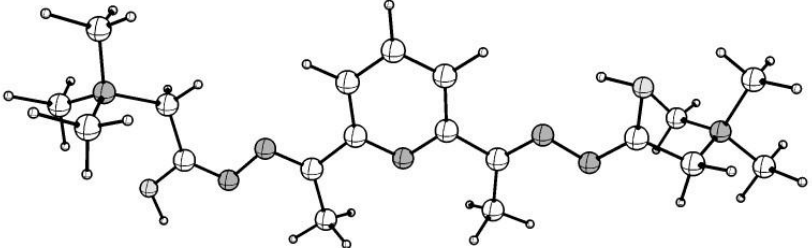
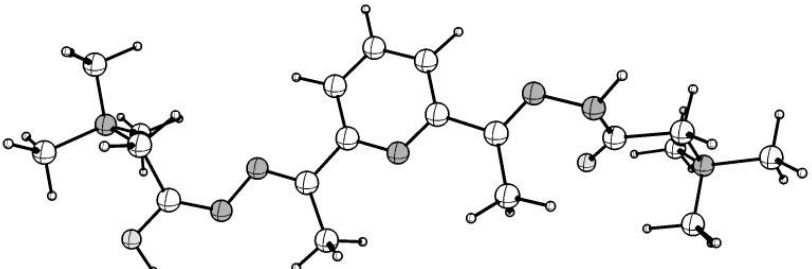
	-1277.3387479	10.5
	-1277.3312015	15.2
	-1277.3299313	16.0
	-1277.3230867	20.3
	-1277.3016073	33.8
	-1277.29602	37.3
	-1277.3072979	30.2

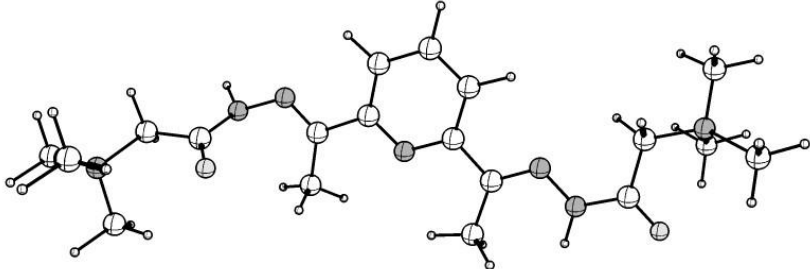
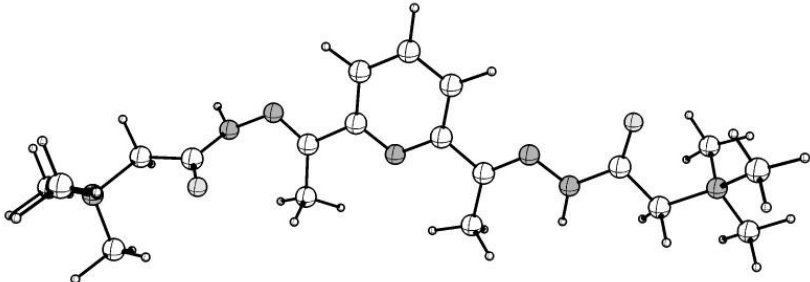
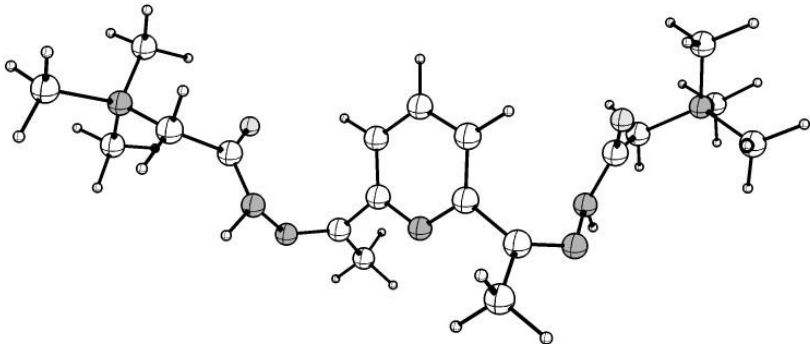
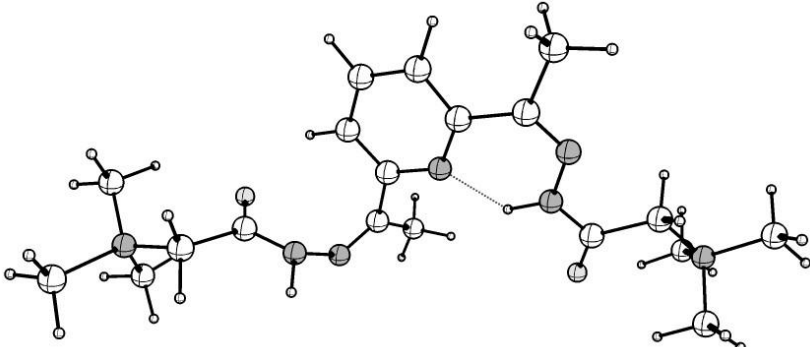
	-1277.3323112	14.5
	-1277.306337	30.8
	-1277.3439438	7.2
	-1277.3004991	34.5
	-1277.320415	22.0

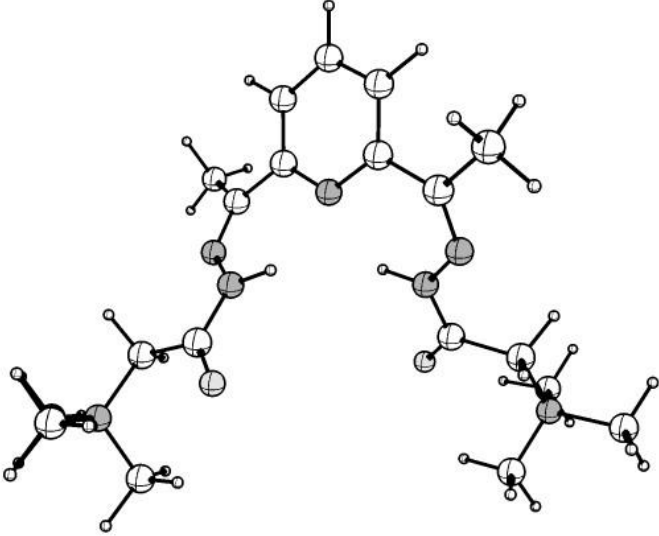
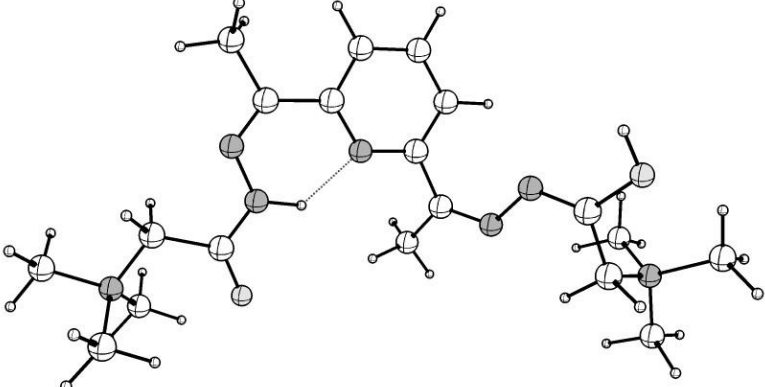
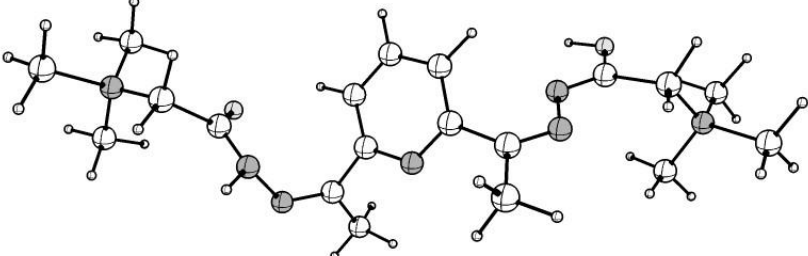
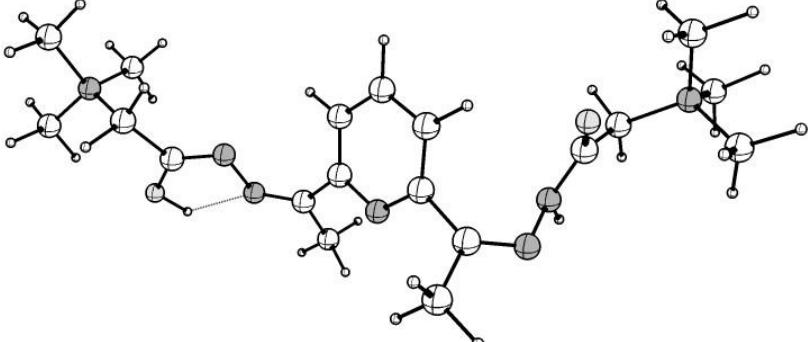
	-1277.3066858	30.6
	-1277.3329708	14.1
	-1277.3294263	16.3
	-1277.3472907	5.1
	-1277.355469	0.0

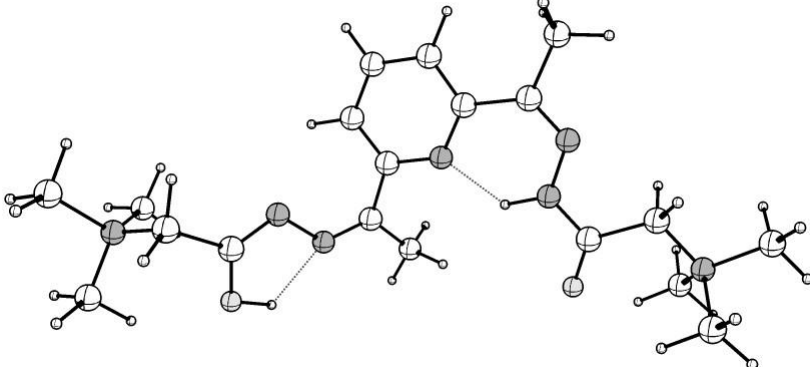
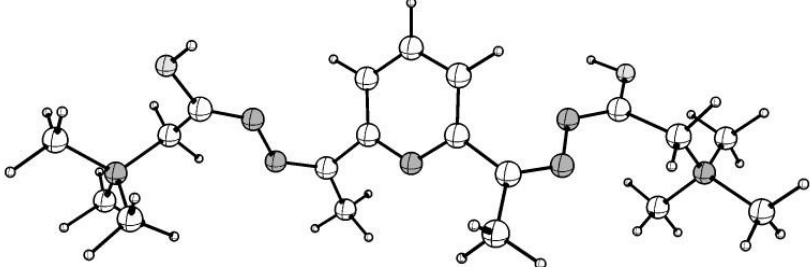
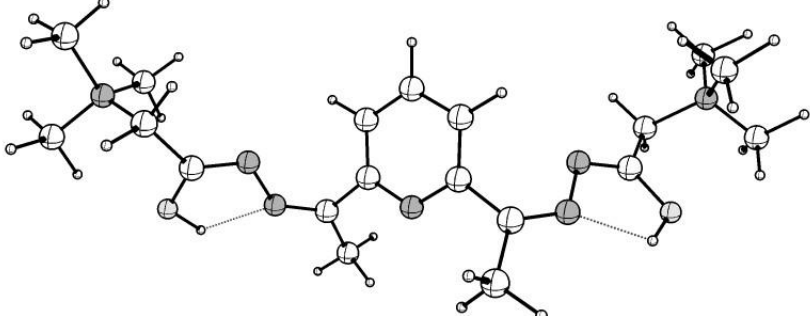
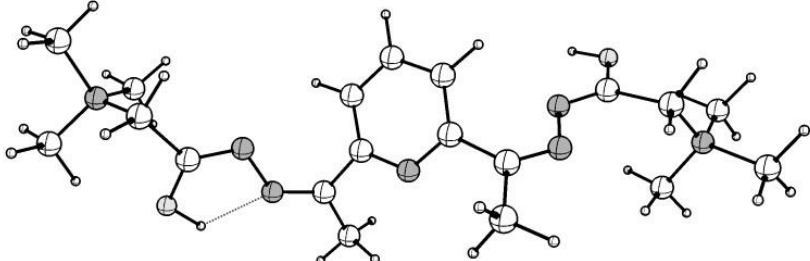
	-1277.3228446	20.5
	-1277.3059588	31.1
	-1277.3090527	29.1
	-1277.3005082	34.5
	-1277.3145603	25.7

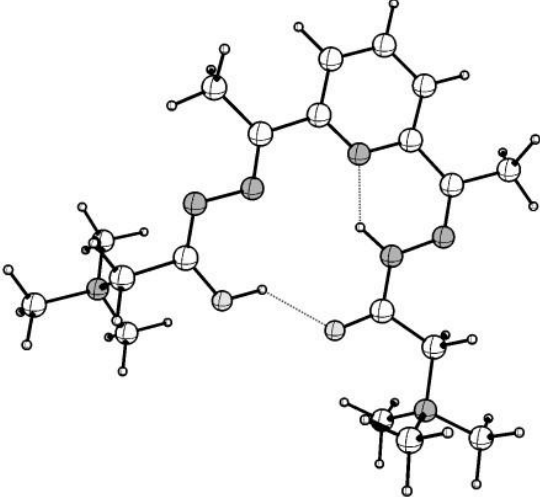
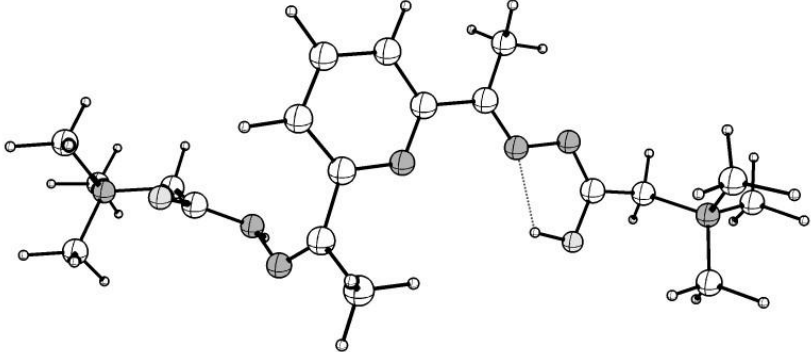
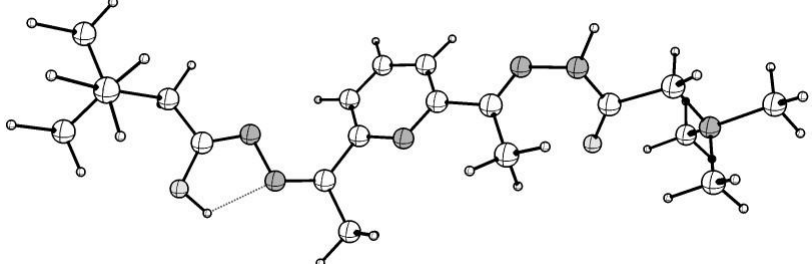
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	-1277.3182447	23.4
	-1277.3051375	31.6
	-1277.3307145	15.5
	-1277.3135488	26.3

	-1277.3237021	19.9
	-1277.3324046	14.5
	-1277.3255257	18.8
	-1277.3135528	26.3
	-1277.3191541	22.8

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	-1277.3048124	31.8
	-1277.3319221	14.8

	-1277.3479066	4.7
	-1277.3270454	17.8
	-1277.3010687	34.1
	-1277.3051552	31.6

	-1277.332975	14.1
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	-1277.3056036	31.3
	-1277.3015899	33.8

	-1277.3353948	12.6
	-1277.3083253	29.6
	-1277.3201689	22.2