

Supporting Information

Unusual *para*-substituent effects on the intramolecular hydrogen bond in hydrazone-based switches: insights from chemical landscape analysis and DFT

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M062X/6-31+G(d,p)

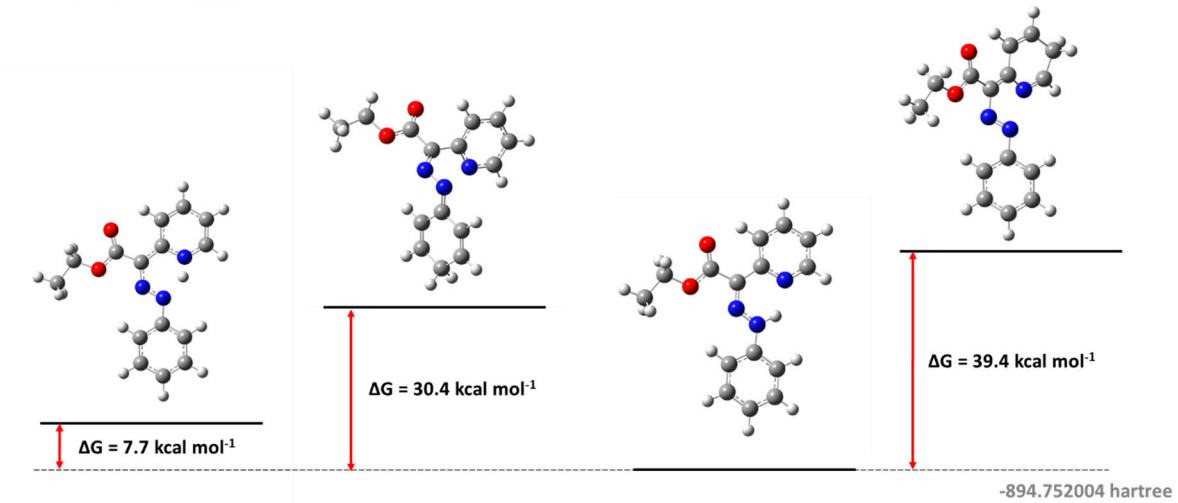


Figure S1. Relative energies of selected conventional and ring-chain tautomers of compound 1.

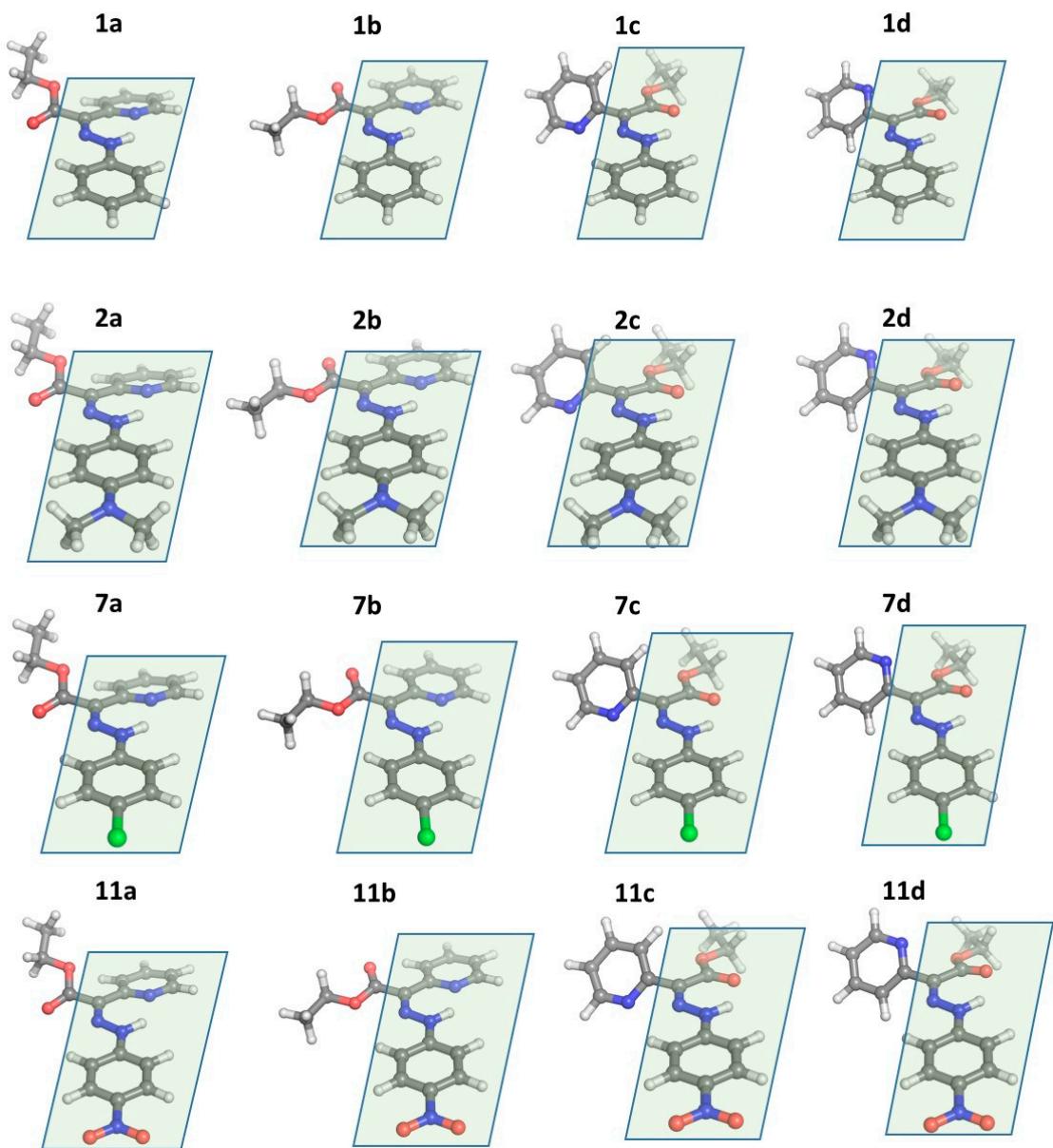


Figure S2. Optimized structures of compounds **1-11**.

Table S1. Gibbs energy differences (kcal mol^{-1}) in the gas phase (ΔG^1) and in acetonitrile (ΔG^{36}) calculated for compounds **1-11**.

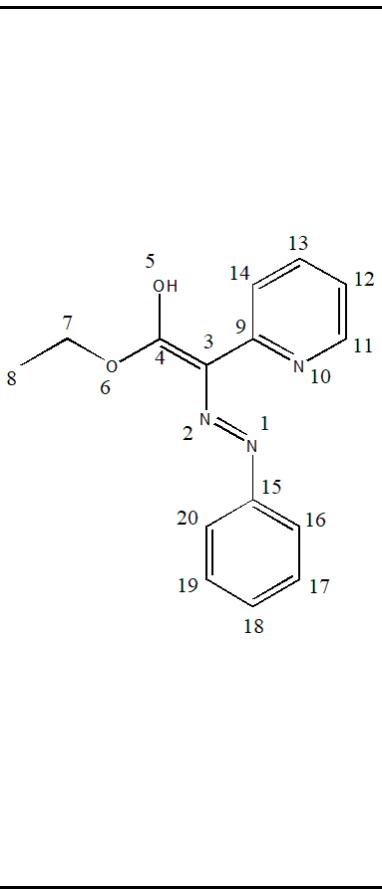
Compound	M062X/6-31+G(d,p)		MN12-SX/6-31+G(d,p)	
	$\epsilon=1$	$\epsilon=36$	$\epsilon=1$	$\epsilon=36$
1a	2.54	1.11*	2.51	1.32*
1b	0.00	0.00*	0.00	0.00*
1c	2.93	2.09*	2.82	2.35*
1d	1.09	1.49*	1.17	2.10*
2a	2.56	0.85	2.35	1.62
2b	0.00	0.00	0.00	0.00
2c	3.43	1.65	1.49	1.70
2d	1.99	1.01	0.62	1.79

3a	2.46	0.75	2.77	1.32
3b	0.00	0.00	0.00	0.00
3c	2.97	1.41	2.74	2.12
3d	1.51	0.61	1.90	1.75
4a	1.99	1.09	3.11	1.88
4b	0.00	0.00	0.00	0.00
4c	2.71	1.12	2.64	1.01
4d	1.29	2.15	2.23	1.48
5a	1.99	0.69	2.33	1.84
5b	0.00	0.00	0.00	0.00
5c	2.78	1.98	1.24	1.58
5d	1.67	1.03	0.99	2.03
6a	2.45	2.04	2.32	0.80
6b	0.00	0.00	0.00	0.00
6c	2.79	1.58	2.52	2.12
6d	1.14	0.82	1.51	1.67
7a	2.32	0.83	2.46	1.06
7b	0.00	0.00	0.00	0.00
7c	2.61	2.20	2.39	1.97
7d	1.10	1.14	1.24	1.30
8a	2.31	1.76	2.35	1.03
8b	0.00	0.00	0.00	1.00
8c	2.76	3.03	2.33	2.12
8d	1.43	1.99	1.14	1.48
9a	2.76	1.11	2.29	0.64
9b	0.00	0.00	0.00	0.00
9c	2.97	1.93	2.95	2.07
9d	1.19	0.67	1.45	1.32
10a	1.90	0.94	-	-
10b	0.00	0.00	-	-
10c	2.51	2.21	-	-
10d	1.17	1.01	-	-
11a	1.92	1.05	2.67	1.93
11b	0.00	0.00	0.00	0.00
11c	2.69	2.06	3.23	3.13
11d	0.99	1.34	1.78	2.18

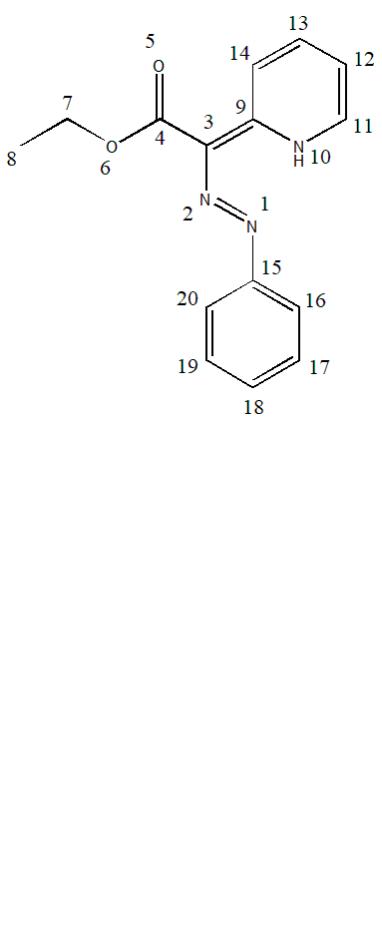
* S. Angelova, V. Paskaleva, N. Kochev, L. Antonov, DFT study of hydrazone-based molecular switches: the effect of different stators on the on/off state distribution, Mol. Phys. 117 (2019), <https://doi.org/10.1080/00268976.2018.1548717>.

Table S2. List of generated tautomers for unsubstituted and substituted (substituents H, N(CH₃)₂, NO₂) structures and their calculated rapid partial charges with Gasteiger Marsili and MMFF94 methods.

Structure	Substituent R	Tautomer №	Atom indices	Gasteiger Marsili Partial Charges	MMFF94 Partial Charges
	H	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	2	1 N	-0.15	-0.179
			2 N	-0.143	-0.171
			3 C	0.166	0.163
			4 C	0.211	0.153
			5 O	-0.339	-0.527

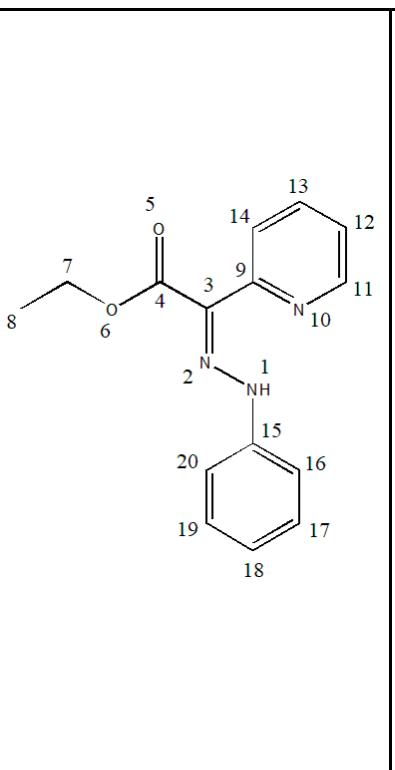
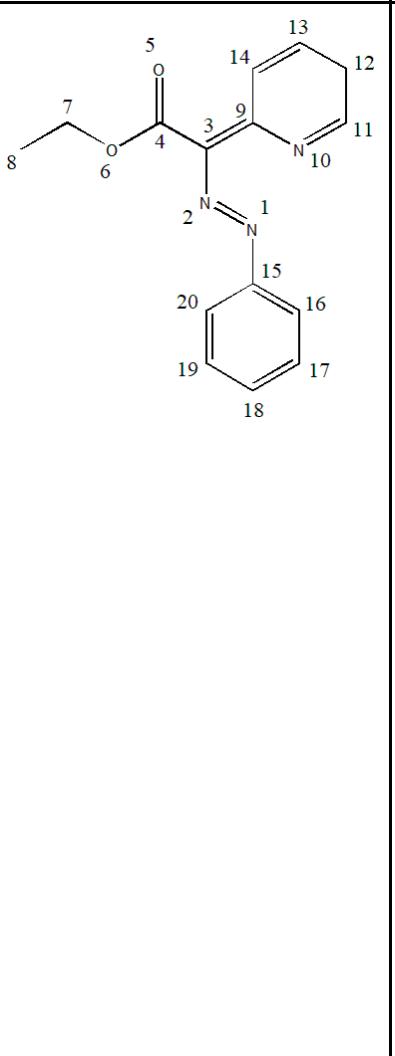


6 O	-0.324	-0.357
7 C	0.053	0.28
8 C	-0.041	0
9 C	0.095	0.318
10 N	-0.254	-0.62
11 C	0.028	0.16
12 C	-0.044	-0.15
13 C	-0.058	-0.15
14 C	-0.034	-0.15
15 C	0.086	0.179
16 C	-0.035	-0.15
17 C	-0.06	-0.15
18 C	-0.062	-0.15
19 C	-0.06	-0.15
20 C	-0.035	-0.15



H	3	1 N	-0.15	-0.179
		2 N	-0.142	-0.171
		3 C	0.176	0.185
		4 C	0.315	0.706
		5 O	-0.258	-0.57
		6 O	-0.311	-0.43
		7 C	0.054	0.28
		8 C	-0.041	0
		9 C	0.053	0.1
		10 N	-0.263	-0.6
		11 C	-0.018	-0.05
		12 C	-0.051	-0.15
		13 C	-0.059	-0.15
		14 C	-0.041	-0.15
		15 C	0.086	0.179
		16 C	-0.035	-0.15

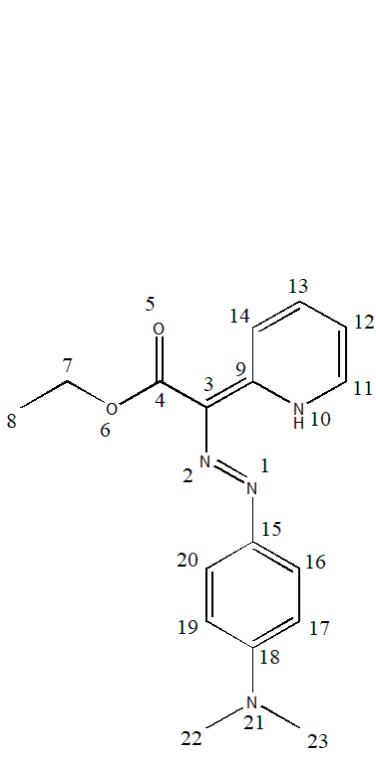
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.038	-0.136
			17 C	-0.078	-0.288
			18 C	-0.016	0.276
			19 C	-0.078	-0.288
			20 C	-0.038	-0.136
	H	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28

		8 C	-0.041	0	
		9 C	0.096	0.278	
		10 N	-0.254	-0.62	
		11 C	0.028	0.16	
		12 C	-0.044	-0.15	
		13 C	-0.058	-0.15	
		14 C	-0.034	-0.15	
		15 C	0.036	0.1	
		16 C	-0.042	-0.15	
		17 C	-0.06	-0.15	
		18 C	-0.062	-0.15	
		19 C	-0.06	-0.15	
		20 C	-0.042	-0.15	
	H	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.171
			10 N	-0.258	-0.621
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15

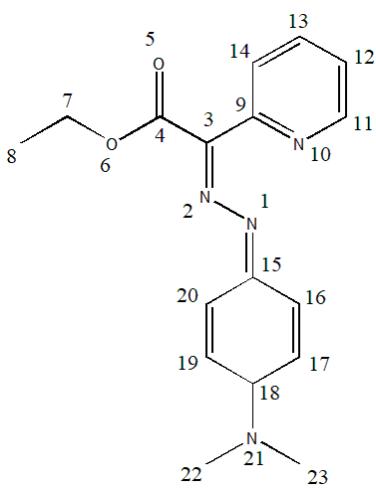
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	-0.038	-0.136
			17 C	-0.06	-0.15
			18 C	-0.066	-0.15
			19 C	-0.078	-0.288
			20 C	0.01	0.199
	H	8	1 N	-0.15	-0.179
2 N	-0.142	-0.171			
3 C	0.179	0.185			
4 C	0.316	0.706			
5 O	-0.258	-0.57			
6 O	-0.311	-0.43			
7 C	0.054	0.28			
8 C	-0.041	0			
9 C	0.078	0.033			

			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	$N(CH_3)_2$	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15

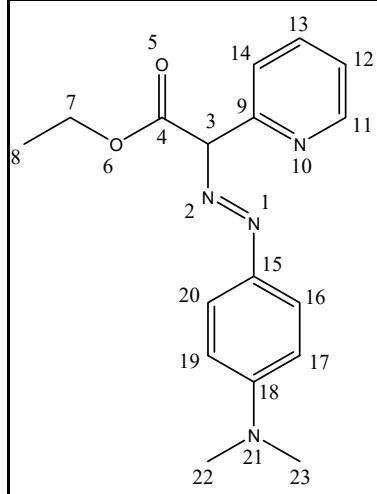
			21 N	-0.281	-0.838	
			22 C	-0.009	0.369	
			23 C	-0.009	0.369	
	$N(CH_3)_2$	2	1 N	-0.15	-0.179	
				2 N	-0.143	-0.171
				3 C	0.166	0.163
				4 C	0.211	0.153
				5 O	-0.339	-0.527
				6 O	-0.324	-0.357
				7 C	0.053	0.28
				8 C	-0.041	0
				9 C	0.095	0.318
				10 N	-0.254	-0.62
				11 C	0.028	0.16
				12 C	-0.044	-0.15
				13 C	-0.058	-0.15
				14 C	-0.034	-0.15
				15 C	0.086	0.179
				16 C	-0.033	-0.15
				17 C	-0.042	-0.15
				18 C	0.017	0.1
				19 C	-0.042	-0.15
				20 C	-0.033	-0.15
				21 N	-0.281	-0.838
				22 C	-0.009	0.369
				23 C	-0.009	0.369
	$N(CH_3)_2$	3	1 N	-0.15	-0.179	
				2 N	-0.142	-0.171
				3 C	0.176	0.185
				4 C	0.315	0.706
				5 O	-0.258	-0.57



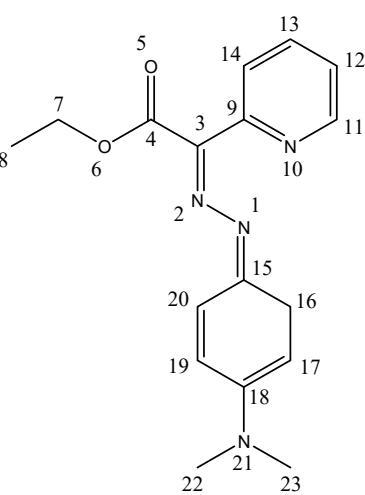
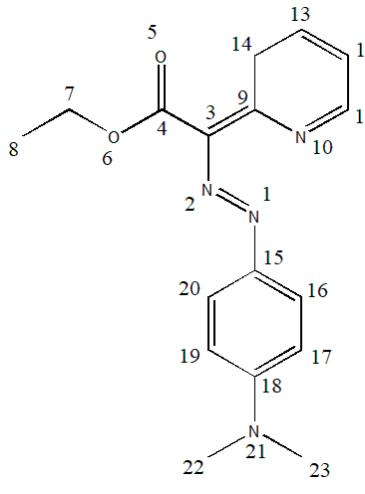
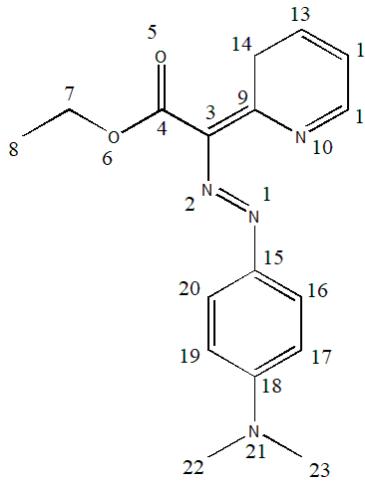
6 O	-0.311	-0.43
7 C	0.054	0.28
8 C	-0.041	0
9 C	0.053	0.1
10 N	-0.263	-0.6
11 C	-0.018	-0.05
12 C	-0.051	-0.15
13 C	-0.059	-0.15
14 C	-0.041	-0.15
15 C	0.086	0.179
16 C	-0.033	-0.15
17 C	-0.042	-0.15
18 C	0.017	0.1
19 C	-0.042	-0.15
20 C	-0.033	-0.15
21 N	-0.281	-0.838
22 C	-0.009	0.369
23 C	-0.009	0.369



N(CH ₃) ₂	4	1 N	-0.15	-0.45
		2 N	-0.141	-0.45
		3 C	0.183	0.482
		4 C	0.316	0.72
		5 O	-0.258	-0.57
		6 O	-0.311	-0.43
		7 C	0.054	0.28
		8 C	-0.041	0
		9 C	0.097	0.278
		10 N	-0.254	-0.62
		11 C	0.028	0.16
		12 C	-0.044	-0.15
		13 C	-0.058	-0.15

			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.037	-0.136
			17 C	-0.061	-0.288
			18 C	0.047	0.546
			19 C	-0.061	-0.288
			20 C	-0.037	-0.136
			21 N	-0.299	-0.81
			22 C	-0.013	0.27
			23 C	-0.013	0.27
 <p>Chemical structure of compound 5:</p> <pre> graph TD A1((1)) --- A2((2)) A2 --- A3((3)) A3 --- A4((4)) A4 --- A5((5)) A5 --- A6((6)) A6 --- A7((7)) A7 --- A8((8)) A8 --- A9((9)) A9 --- A10((10)) A10 --- A11((11)) A11 --- A12((12)) A12 --- A13((13)) A13 --- A14((14)) A14 --- A15((15)) A15 --- A16((16)) A16 --- A17((17)) A17 --- A18((18)) A18 --- A19((19)) A19 --- A20((20)) A20 --- A15 A21((21)) --- A22((22)) A21 --- A23((23)) </pre>	N(CH₃)₂ 5	1 N -0.182 -0.458 2 N -0.188 -0.492 3 C 0.175 0.482 4 C 0.315 0.72 5 O -0.258 -0.57 6 O -0.311 -0.43 7 C 0.054 0.28 8 C -0.041 0 9 C 0.096 0.278 10 N -0.254 -0.62 11 C 0.028 0.16 12 C -0.044 -0.15 13 C -0.058 -0.15 14 C -0.034 -0.15 15 C 0.036 0.1 16 C -0.041 -0.15 17 C -0.042 -0.15 18 C 0.017 0.1 19 C -0.042 -0.15 20 C -0.041 -0.15 21 N -0.281 -0.838			

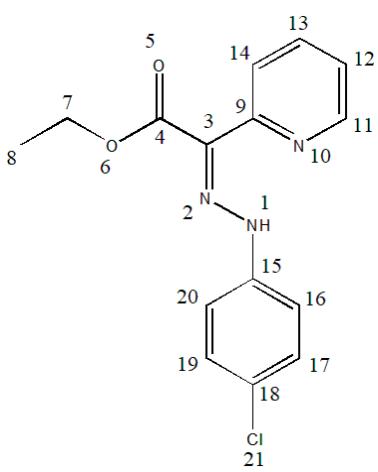
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	N(CH ₃) ₂	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.171
			10 N	-0.258	-0.621
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	N(CH ₃) ₂	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43

	7 C	0.054	0.28
	8 C	-0.041	0
	9 C	0.097	0.278
	10 N	-0.254	-0.62
	11 C	0.028	0.16
	12 C	-0.044	-0.15
	13 C	-0.058	-0.15
	14 C	-0.034	-0.15
	15 C	0.067	0.375
	16 C	-0.037	-0.136
	17 C	-0.042	-0.15
	18 C	0.014	0.1
	19 C	-0.06	-0.288
	20 C	0.011	0.199
	21 N	-0.281	-0.838
	22 C	-0.009	0.369
	23 C	-0.009	0.369
	N(CH ₃) ₂	8	
	1 N	-0.15	-0.179
	2 N	-0.142	-0.171
	3 C	0.179	0.185
	4 C	0.316	0.706
	5 O	-0.258	-0.57
	6 O	-0.311	-0.43
	7 C	0.054	0.28
	8 C	-0.041	0
	9 C	0.078	0.033
	10 N	-0.258	-0.621
	11 C	0.027	0.376
	12 C	-0.047	-0.136
	13 C	-0.077	-0.288
	14 C	0.01	0.276

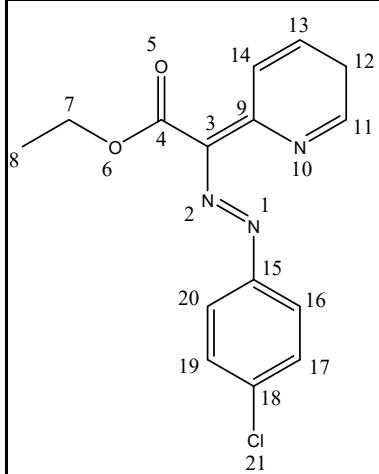
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	Cl	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
			1 N	-0.15	-0.179

	Cl	2	2 N	-0.143	-0.171
			3 C	0.166	0.163
	Cl	3	4 C	0.211	0.153
			5 O	-0.339	-0.527
	Cl	2	6 O	-0.324	-0.357
			7 C	0.053	0.28
	Cl	3	8 C	-0.041	0
			9 C	0.095	0.318
	Cl	2	10 N	-0.254	-0.62
			11 C	0.028	0.16
	Cl	3	12 C	-0.044	-0.15
			13 C	-0.058	-0.15
	Cl	2	14 C	-0.034	-0.15
			15 C	0.086	0.179
	Cl	3	16 C	-0.033	-0.15
			17 C	-0.035	-0.15
	Cl	2	18 C	0.073	0.177
			19 C	-0.035	-0.15
	Cl	3	20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	2	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
	Cl	3	3 C	0.176	0.185
			4 C	0.315	0.706
	Cl	2	5 O	-0.258	-0.57
			6 O	-0.311	-0.43
	Cl	3	7 C	0.054	0.28
			8 C	-0.041	0
	Cl	2	9 C	0.053	0.1
			10 N	-0.263	-0.6
	Cl	3	11 C	-0.018	-0.05

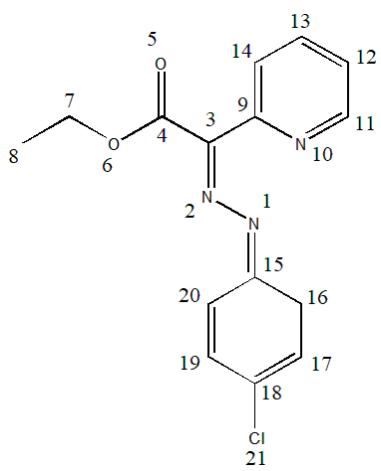
			12 C	-0.051	-0.15
			13 C	-0.059	-0.15
			14 C	-0.041	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.036	-0.136
			17 C	-0.055	-0.288
			18 C	0.097	0.566
			19 C	-0.055	-0.288
			20 C	-0.036	-0.136
			21 Cl	-0.161	-0.29



Cl	5	1 N	-0.182	-0.458
		2 N	-0.188	-0.492
		3 C	0.175	0.482
		4 C	0.315	0.72
		5 O	-0.258	-0.57
		6 O	-0.311	-0.43
		7 C	0.054	0.28
		8 C	-0.041	0
		9 C	0.096	0.278
		10 N	-0.254	-0.62
		11 C	0.028	0.16
		12 C	-0.044	-0.15
		13 C	-0.058	-0.15
		14 C	-0.034	-0.15
		15 C	0.036	0.1
		16 C	-0.04	-0.15
		17 C	-0.036	-0.15
		18 C	0.073	0.177
		19 C	-0.036	-0.15
		20 C	-0.04	-0.15
		21 Cl	-0.13	-0.177

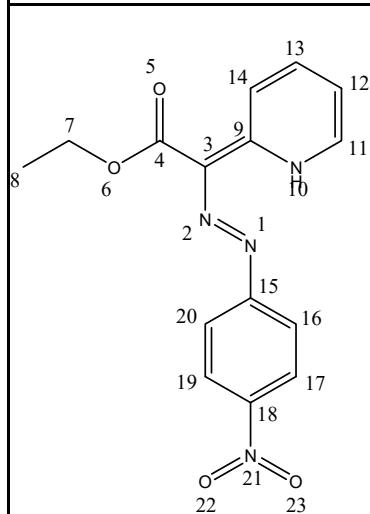


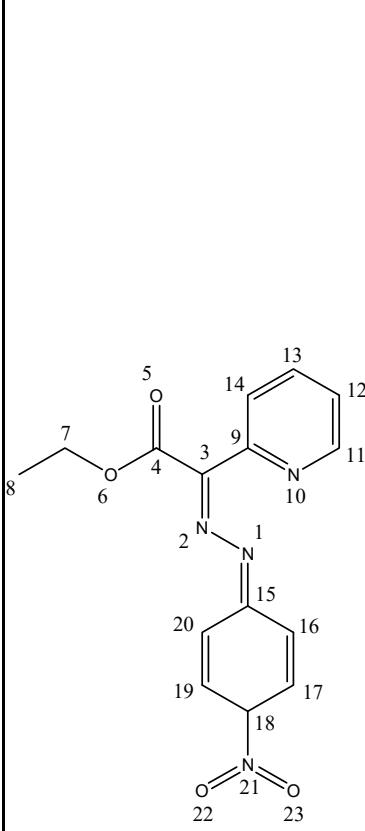
Cl	6	1 N	-0.15	-0.179
		2 N	-0.141	-0.171
		3 C	0.183	0.185
		4 C	0.316	0.706
		5 O	-0.258	-0.57
		6 O	-0.311	-0.43
		7 C	0.054	0.28
		8 C	-0.041	0
		9 C	0.096	0.171
		10 N	-0.258	-0.621

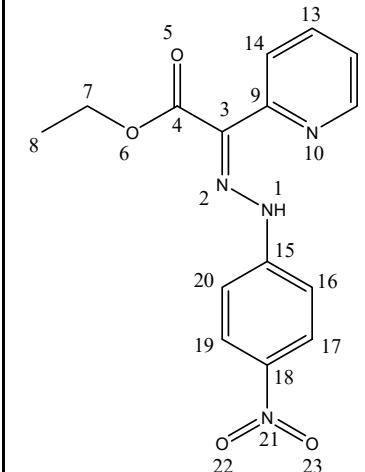
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	-0.036	-0.136
			17 C	-0.036	-0.15
			18 C	0.069	0.14
			19 C	-0.054	-0.288
			20 C	0.012	0.199

			21 Cl	-0.131	-0.14
<p>Detailed description: The chemical structure shows a complex molecule with multiple rings. A central pyridine ring is substituted at position 2 with a 2-pyridylmethyl group. This group consists of a pyridine ring fused to a methyl group (labeled 7, 8, 9). The pyridine ring has atoms labeled 1 through 6. A methylene bridge connects the 2-position of the central pyridine to the 4-position of a 4-chlorophenyl ring. The 4-chlorophenyl ring has atoms labeled 15 through 21. A chlorine atom (Cl) is explicitly labeled at position 18.</p>	Cl	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.078	0.033
			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
<p>Detailed description: The chemical structure shows a phenyl ring with a nitro group (NO2) at the top position (labeled 1) and a 4-chlorophenyl group at the bottom-right position (labeled 4).</p>	NO ₂	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167

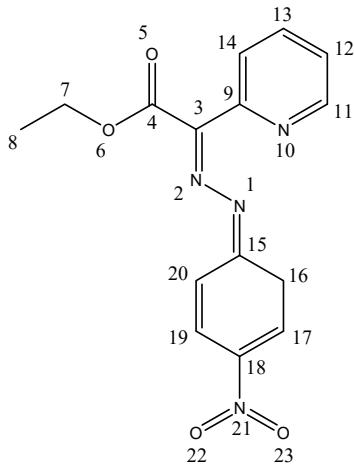
		10 N	-0.258	-0.62	
		11 C	0.028	0.16	
		12 C	-0.044	-0.15	
		13 C	-0.059	-0.15	
		14 C	-0.038	-0.15	
		15 C	0.086	0.179	
		16 C	-0.032	-0.15	
		17 C	-0.029	-0.15	
		18 C	0.127	0.133	
		19 C	-0.029	-0.15	
		20 C	-0.032	-0.15	
		21 N	0.056	0.907	
		22 O	-0.127	-0.52	
		23 O	-0.127	-0.52	
	NO ₂	2	1 N	-0.15	-0.179
		2 N	-0.143	-0.171	
		3 C	0.166	0.163	
		4 C	0.211	0.153	
		5 O	-0.339	-0.527	
		6 O	-0.324	-0.357	
		7 C	0.053	0.28	
		8 C	-0.041	0	
		9 C	0.095	0.318	
		10 N	-0.254	-0.62	
		11 C	0.028	0.16	
		12 C	-0.044	-0.15	
		13 C	-0.058	-0.15	
		14 C	-0.034	-0.15	
		15 C	0.086	0.179	
		16 C	-0.032	-0.15	
		17 C	-0.029	-0.15	

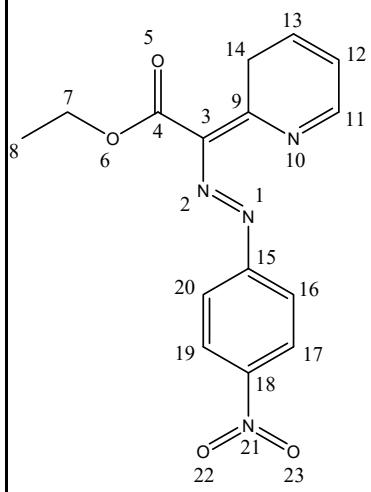
			18 C	0.127	0.133
			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
 <p>The chemical structure shows a complex molecule with two 2,6-dioxo-3-oxa-4-azabicyclo[3.1.0]hex-7-en-7-yl groups attached to a central carbon atom (C3). One group is at the 2-position and the other is at the 4-position of a 4-nitrophenyl ring. The phenyl ring has substituents at positions 2, 4, and 6.</p>	NO ₂	3	1 N	-0.15	-0.179
	NO ₂	4	2 N	-0.142	-0.171
	NO ₂	4	3 C	0.176	0.185
	NO ₂	4	4 C	0.315	0.706
	NO ₂	4	5 O	-0.258	-0.57
	NO ₂	4	6 O	-0.311	-0.43
	NO ₂	4	7 C	0.054	0.28
	NO ₂	4	8 C	-0.041	0
	NO ₂	4	9 C	0.053	0.1
	NO ₂	4	10 N	-0.263	-0.6
	NO ₂	4	11 C	-0.018	-0.05
	NO ₂	4	12 C	-0.051	-0.15
	NO ₂	4	13 C	-0.059	-0.15
	NO ₂	4	14 C	-0.041	-0.15
	NO ₂	4	15 C	0.086	0.179
	NO ₂	4	16 C	-0.032	-0.15
	NO ₂	4	17 C	-0.029	-0.15
	NO ₂	4	18 C	0.127	0.133
	NO ₂	4	19 C	-0.029	-0.15
	NO ₂	4	20 C	-0.032	-0.15
	NO ₂	4	21 N	0.056	0.907
	NO ₂	4	22 O	-0.127	-0.52
	NO ₂	4	23 O	-0.127	-0.52

		3 C	0.183	0.482
		4 C	0.316	0.72
		5 O	-0.258	-0.57
		6 O	-0.311	-0.43
		7 C	0.054	0.28
		8 C	-0.041	0
		9 C	0.097	0.278
		10 N	-0.254	-0.62
		11 C	0.028	0.16
		12 C	-0.044	-0.15
		13 C	-0.058	-0.15
		14 C	-0.034	-0.15
		15 C	0.085	0.421
		16 C	-0.036	-0.136
		17 C	-0.049	-0.288
		18 C	0.147	0.517
		19 C	-0.049	-0.288
		20 C	-0.036	-0.136
		21 N	0.033	0.8
		22 O	-0.131	-0.52
		23 O	-0.131	-0.52

	NO ₂	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.278
			10 N	-0.254	-0.62

			11 C	0.028	0.16	
			12 C	-0.044	-0.15	
			13 C	-0.058	-0.15	
			14 C	-0.034	-0.15	
			15 C	0.036	0.1	
			16 C	-0.04	-0.15	
			17 C	-0.03	-0.15	
			18 C	0.127	0.133	
			19 C	-0.03	-0.15	
			20 C	-0.04	-0.15	
			21 N	0.056	0.907	
			22 O	-0.127	-0.52	
			23 O	-0.127	-0.52	
		NO ₂	1 N	-0.15	-0.179	
			2 N	-0.141	-0.171	
			3 C	0.183	0.185	
			4 C	0.316	0.706	
			5 O	-0.258	-0.57	
			6 O	-0.311	-0.43	
			7 C	0.054	0.28	
			8 C	-0.041	0	
			9 C	0.096	0.171	
			10 N	-0.258	-0.621	
			11 C	0.009	0.329	
			12 C	0.001	0.199	
			13 C	-0.077	-0.288	
			14 C	-0.038	-0.15	
			15 C	0.086	0.179	
			16 C	-0.032	-0.15	
			17 C	-0.029	-0.15	
			18 C	0.127	0.133	

			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
 <p>The chemical structure shows a central carbon atom (3) bonded to a carbonyl group (C=O, labeled 4), a methylene group (CH₂, labeled 5), and two nitrogen atoms (labeled 1 and 2). Nitrogen 1 is part of a pyridine ring (labeled 9, 10, 11, 12, 13) which is further substituted with a nitro group (NO₂, labeled 14). Nitrogen 2 is part of a second pyridine ring (labeled 15, 16, 17, 18, 19) which is substituted with a 2-nitro-4-pyridyl group. A trifluoroethyl ester side chain (-CF₃-CH₂-COO-, labeled 6, 7, 8) is attached to the carbonyl carbon (3).</p>	NO ₂	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	0.012	0.199
			17 C	-0.048	-0.288
			18 C	0.123	0.204
			19 C	-0.03	-0.15
			20 C	-0.036	-0.136
			21 N	0.056	0.836
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO ₂	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185



4 C	0.316	0.706
5 O	-0.258	-0.57
6 O	-0.311	-0.43
7 C	0.054	0.28
8 C	-0.041	0
9 C	0.078	0.033
10 N	-0.258	-0.621
11 C	0.027	0.376
12 C	-0.047	-0.136
13 C	-0.077	-0.288
14 C	0.01	0.276
15 C	0.086	0.179
16 C	-0.032	-0.15
17 C	-0.029	-0.15
18 C	0.127	0.133
19 C	-0.029	-0.15
20 C	-0.032	-0.15
21 N	0.056	0.907
22 O	-0.127	-0.52
23 O	-0.127	-0.52