Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary information

Experimental and theoretical study of intramolecular regioselective oxidations of 6-substituted 2,3-dimethylquinoxaline derivatives

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Content:

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I. General Remarks and synthesis

Scheme 1 of results and discussion section show the synthesis of compounds with a condensation of diamines with diketones and oxidation using the Wang *et. al*. procedure. The regioisomer ratio of carbaldehydes mixtures **a**:**b** was determine by δ ^{1}H NMR spectra; however the regioisomer ratio of compounds **8** and **11** were estimated through a correlation between δ ^{1}H9 of 2,3-dimethyl-6-substituted-quinoxalines and percentage of regioisomer **b** (**Figure 1S**).

Compound	R	δ ^{1}H9	Regioisomer % a	Regioisomer % b
1	H	2.7105	50	50
2	NO_2	2.7610	13	87
6	Cl	2.6809	41	59
7	Br	2.6788	46	54
8	COOH	2.6505	44	56
9	COOMe	2.7196	33	67
10	COPh	2.7183	21	79
11*	Qnx	2.7458	33	21

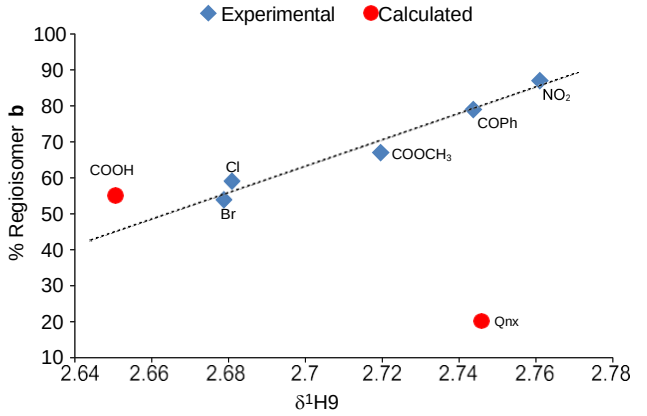
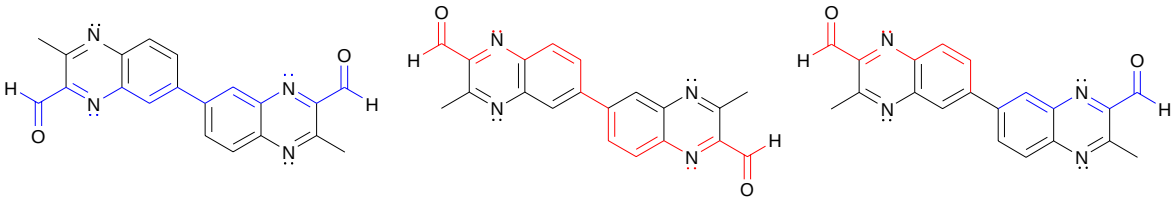


Figure 1S. Percentage ratio calculated from a linear relationship of δ ^{1}H9 vs. % regioisomers **b** obtained from synthesis. Compound **1** was not considered in the lineal regression. * In this compound the percentage of regioisomers is an approximation, only is considered a ratio of **a**:**b**.

The experimental and theoretical data analysis suggest that carbaldehydes of compound **11** is a mixture of three regioisomers **a**:**b**:**c** (**Figure 2S**) with a 5:3:7 proportional ratio respectively, however only was considered a ratio between **a** and **b** regioisomers for obtain an approximation of the regioisomer percentage, so that the regioisomer **c** was not considered.



Regioisomer **11a** (33 %)

Regioisomer **11b** (21 %)

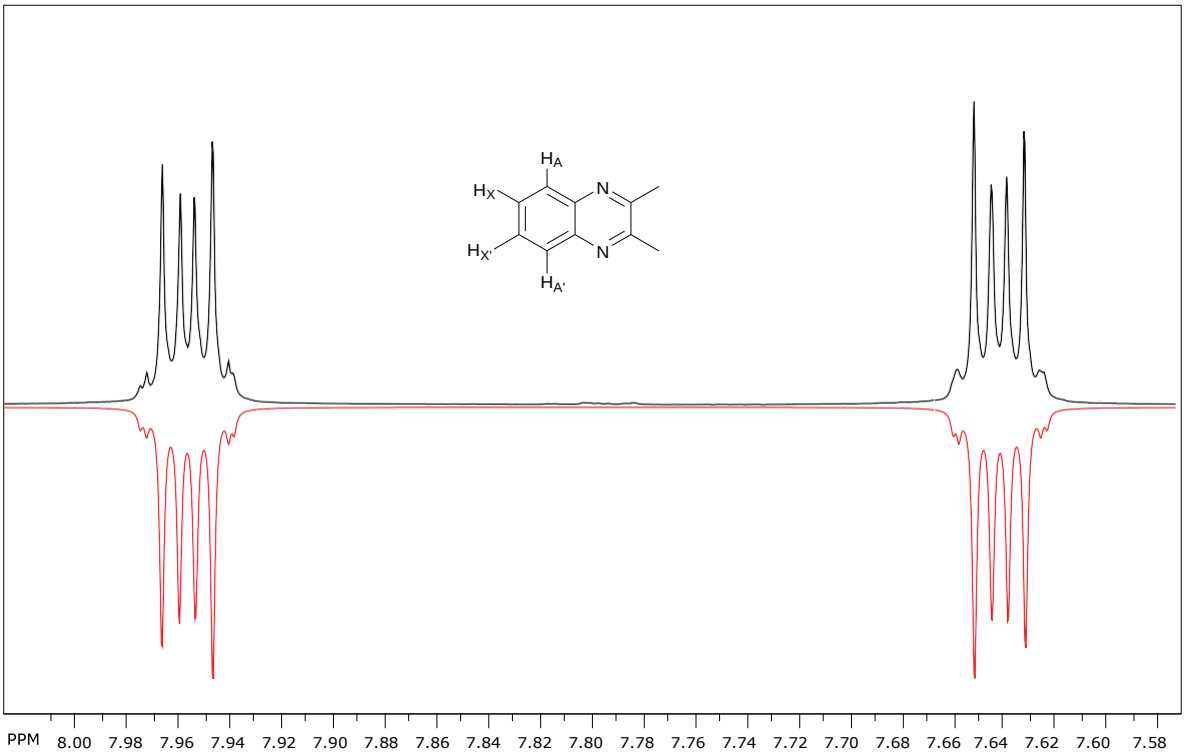
Regioisomer **11c** (46 %)

Figure 2S. Formation of the regioisomers **a**, **b** and **c** of compound **11**, suggested by experimental and theoretical analysis.

II. Spectroscopy Characterization

*II.a ^{1}H NMR spectrum analysis of Compound **1**.*

The ^{1}H NMR spectrum was assignment using the SpinWorks[1] software simulated with the NUMARIT algorithm.[2] The data reported in the experimental section were interactively fit to simulated spectrum. The second order AA'XX' spin-spin coupling system of the aromatic region is presented in above in black is the experimental spectrum and in red is the simulate one.

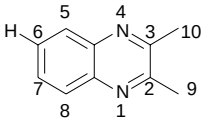


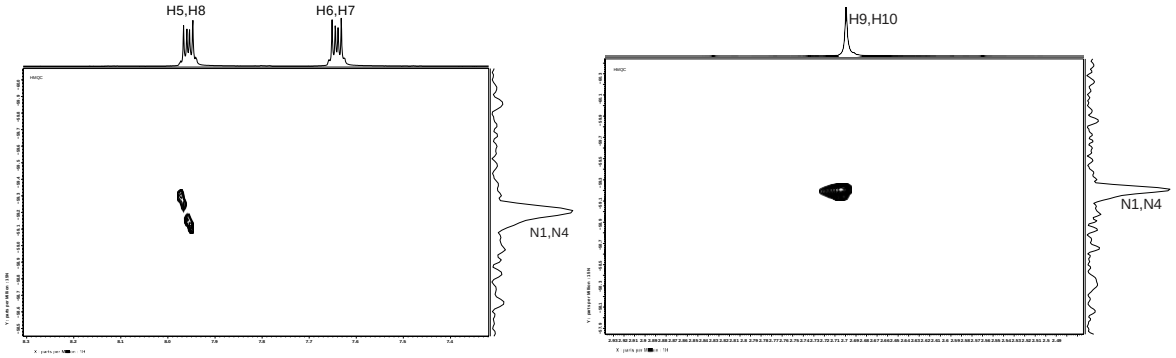
The experimental resolution of this spectrum was 0.3 Hz recorder at 500 MHz and the RMS = 0.25. δ_H = 7.95 and 7.64, $^{5}J_{H,H}$ (A,A') = 0.7±0.3, $^{3}J_{H,H}$ (A,X = A'X') = 8.6±0.3, $^{4}J_{H,H}$ (A,X' = A'X) = 1.3±0.3 and $^{3}J_{H,H}$ (X,X') = 7.0±0.3 Hz.

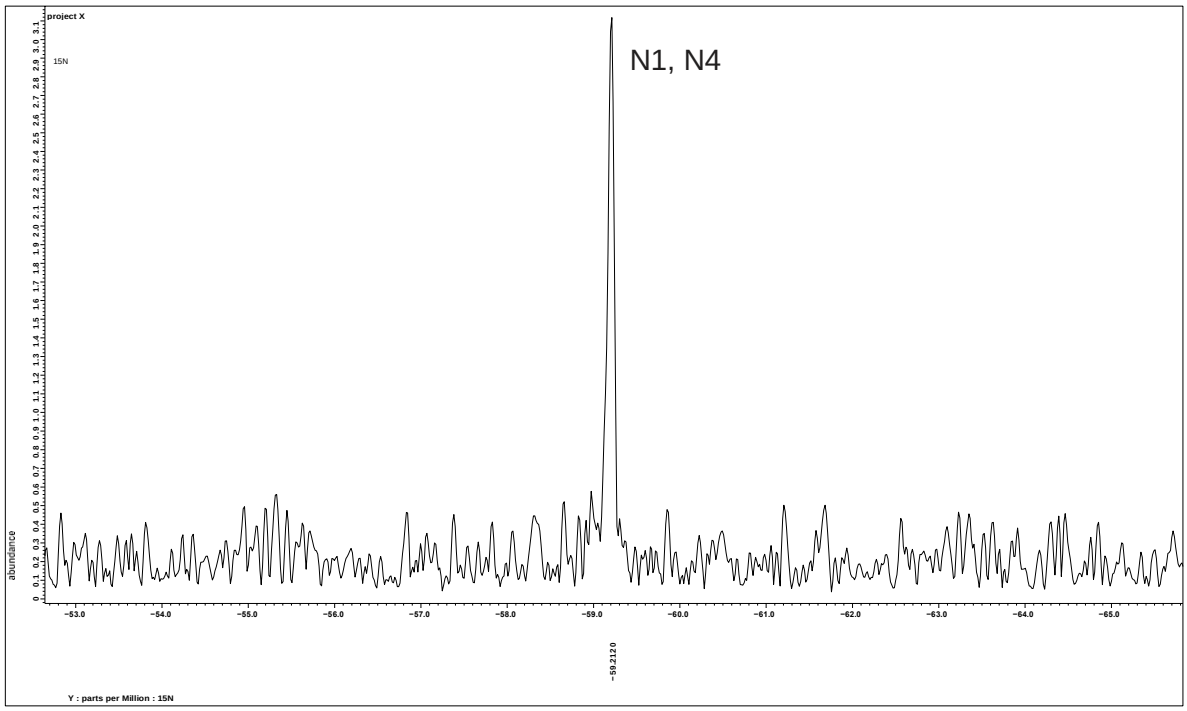
II.b ^{15}N chemical shift determination

The ^{15}N chemical shift of 2,3-dimethyl-6-substituted-quinoxalines were determined by indirect detection ^{1}H,^{15}N using the pfg-HMQC pulse sequence. In order to have a good resolution these spectra were determine in the aliphatic and aromatic regions separately in two spectra. In the methyl group region the ^{1}H resolution was better than 5 Hz while in ^{15}N the resolution was better than 2 Hz that correspond to 0.04 ppm. The best results were obtained with a $J_{H,N}$ = 5 Hz. The δ_N were determine from the slice of the 2D spectra. For the aromatic region were used the same resolution with a $J_{H,N}$ = 2 Hz. Other acquisition parameter as show as example in the spectra slice of compound **6**, **10** and **11**. In some case were recorder too the 1D ^{15}N NMR using single pulse decoupled as show for compound **2**.

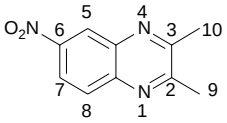
2,3-Dimethylquinoxaline (1).

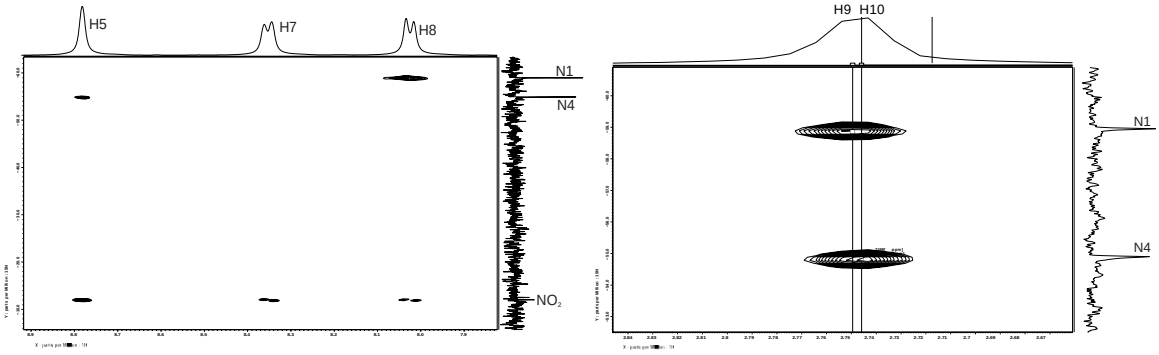


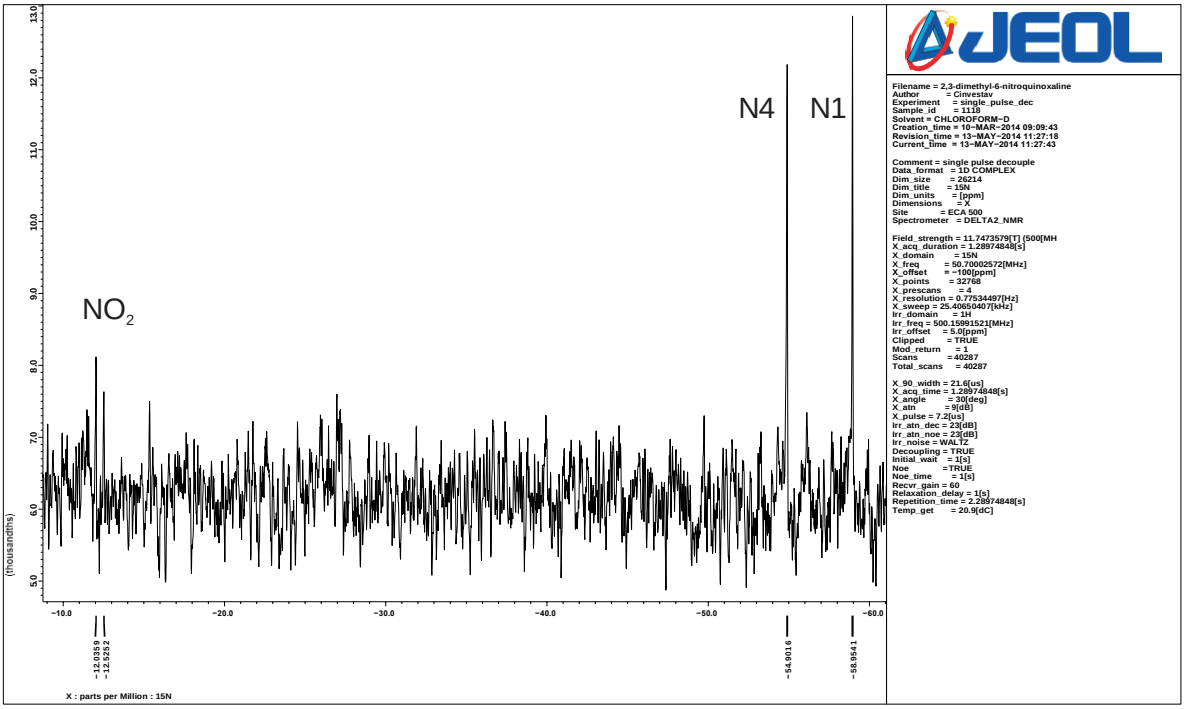




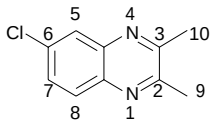
2,3-Dimethyl-6-nitroquinoxaline (2).

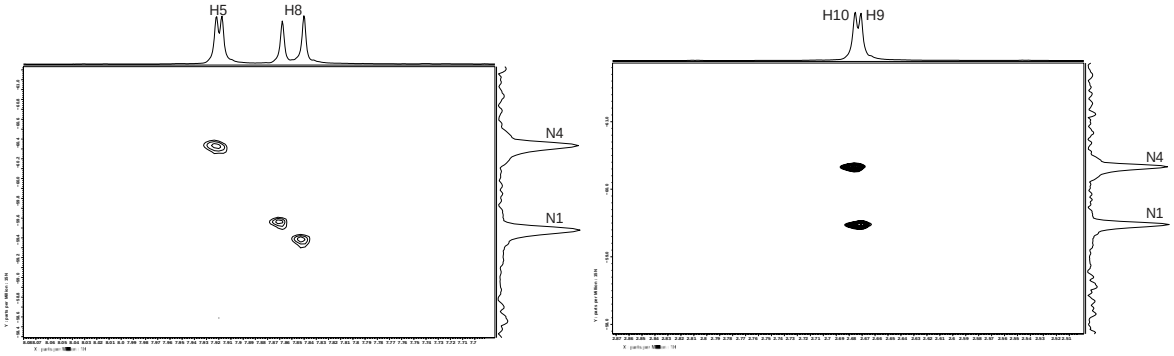


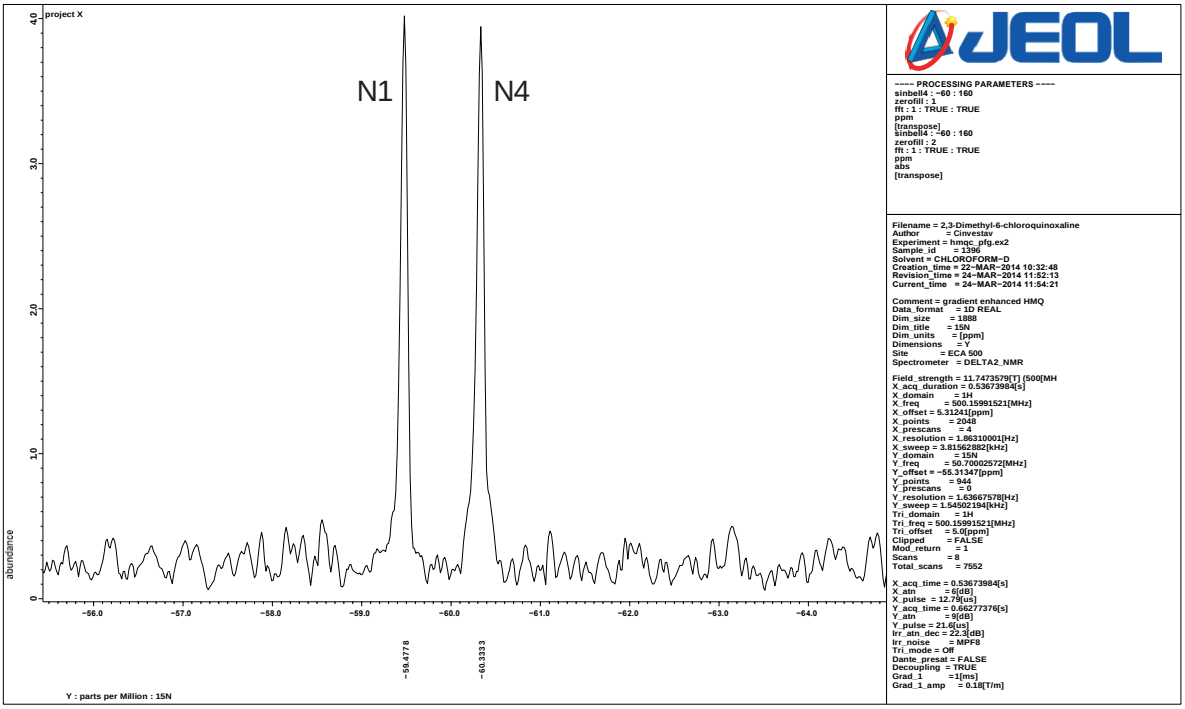




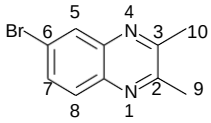
2,3-Dimethyl-6-chloroquinoxaline (6).

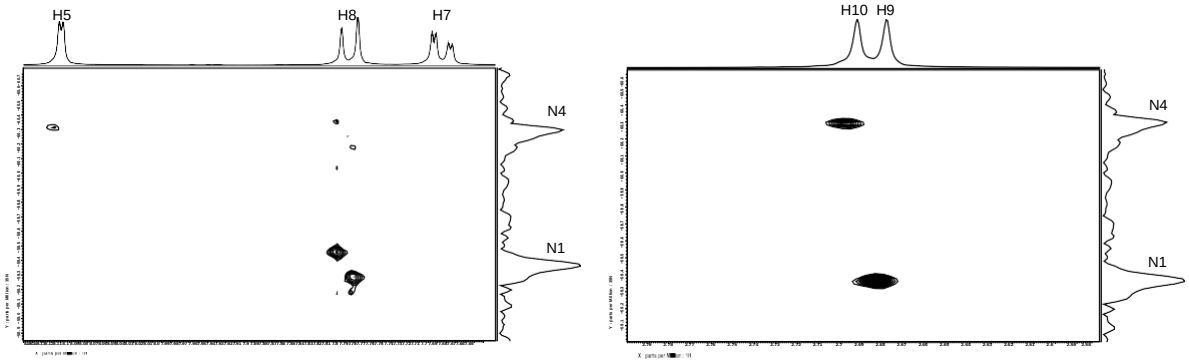


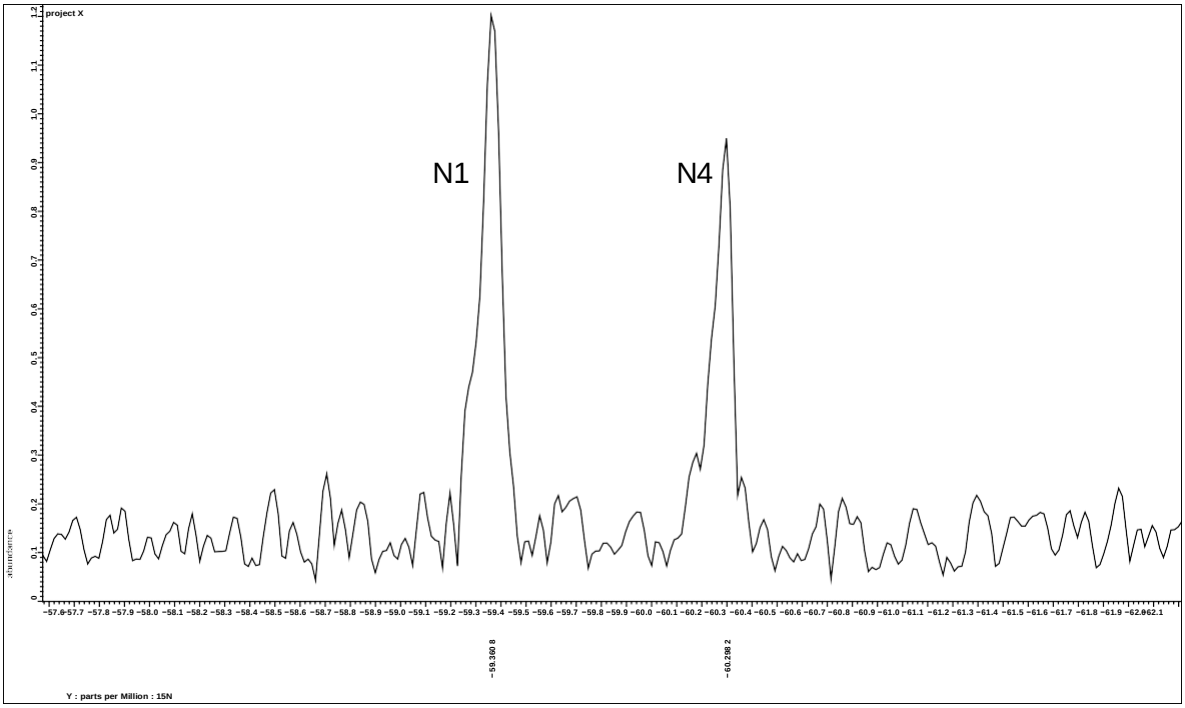




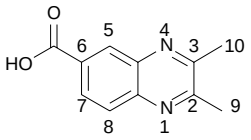
2,3-Dimethyl-6-bromoquinoxaline (7).

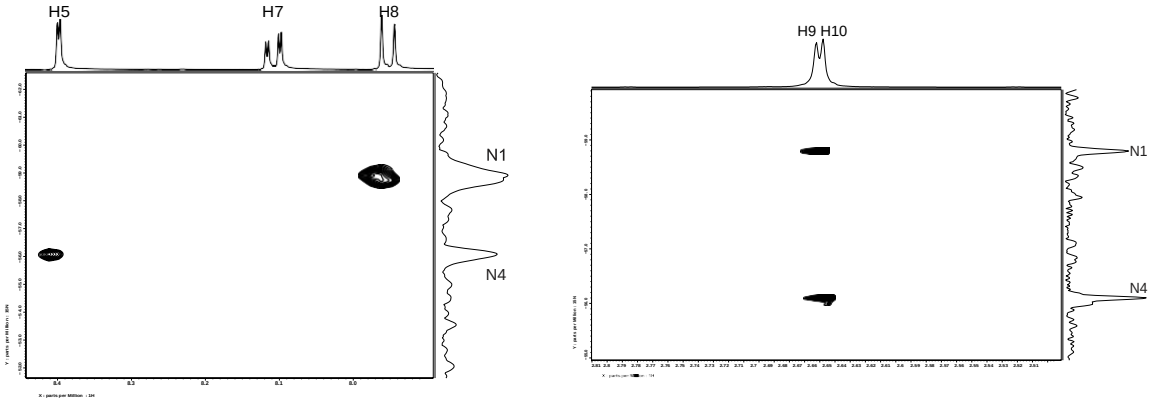


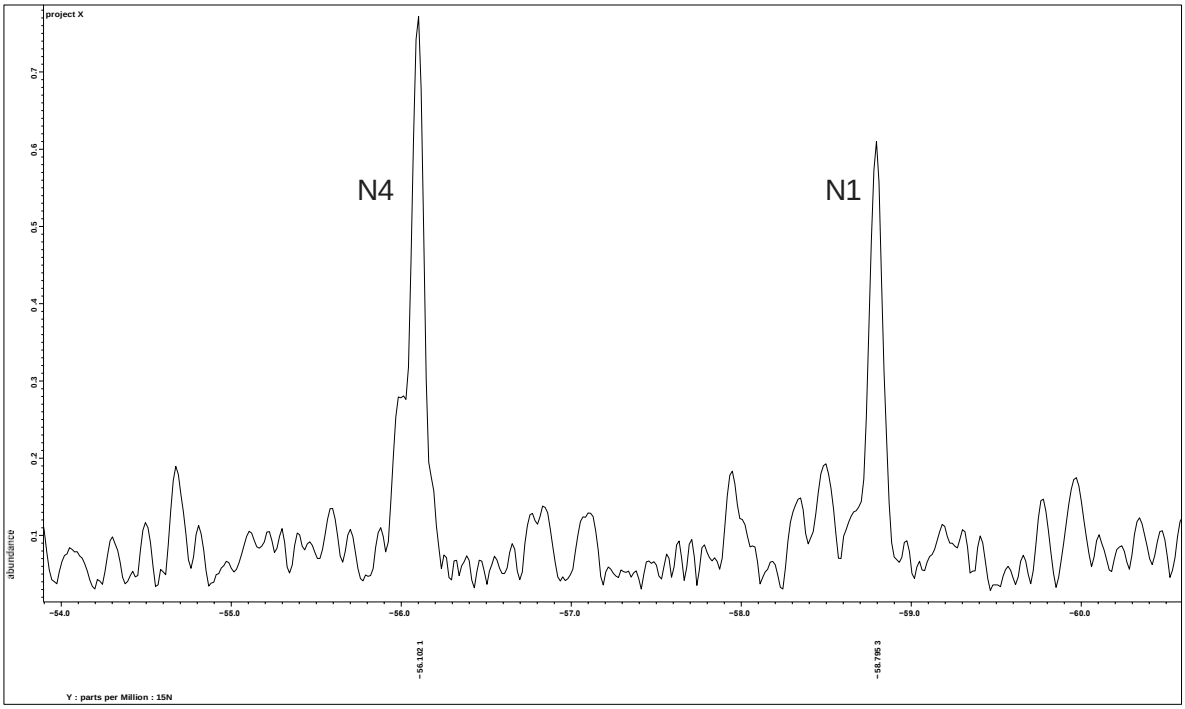




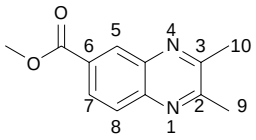
2,3-Dimethylquinoxaline-6-carboxylic acid (8).

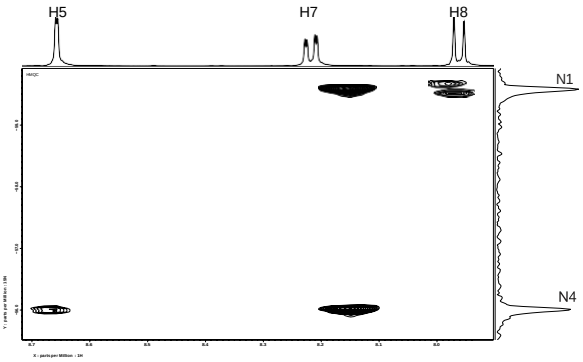


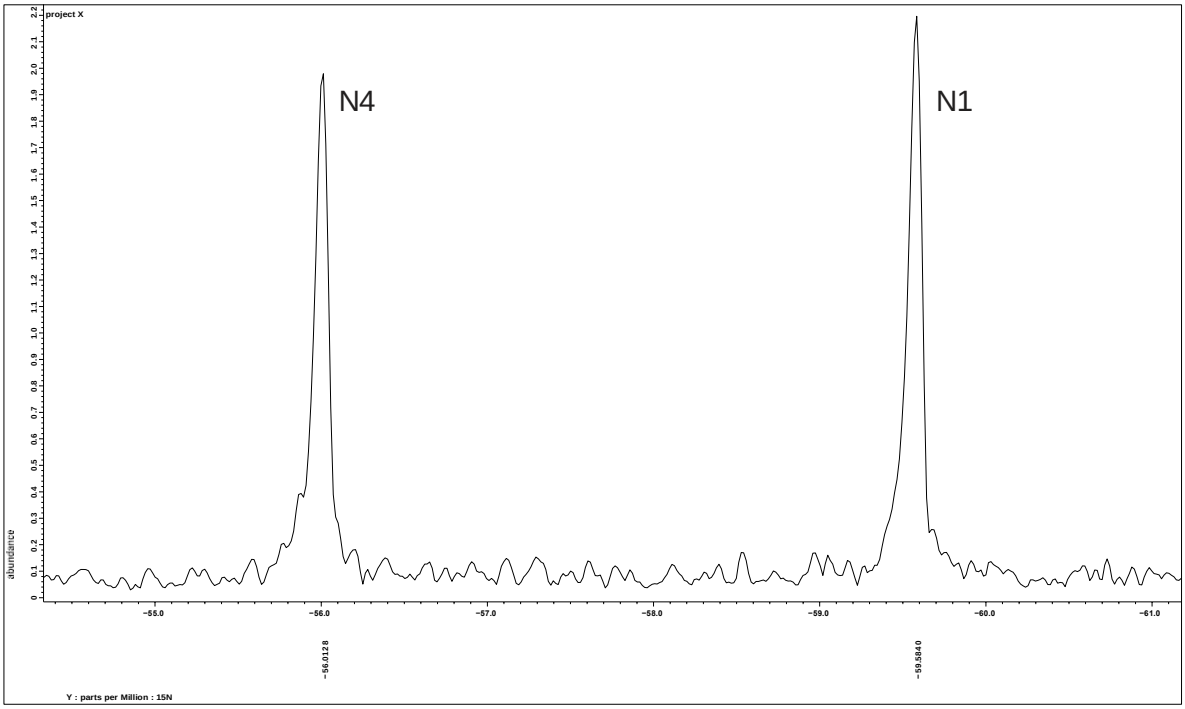




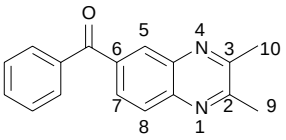
Methyl 2,3-dimethylquinoxaline-6-carboxylate (9).

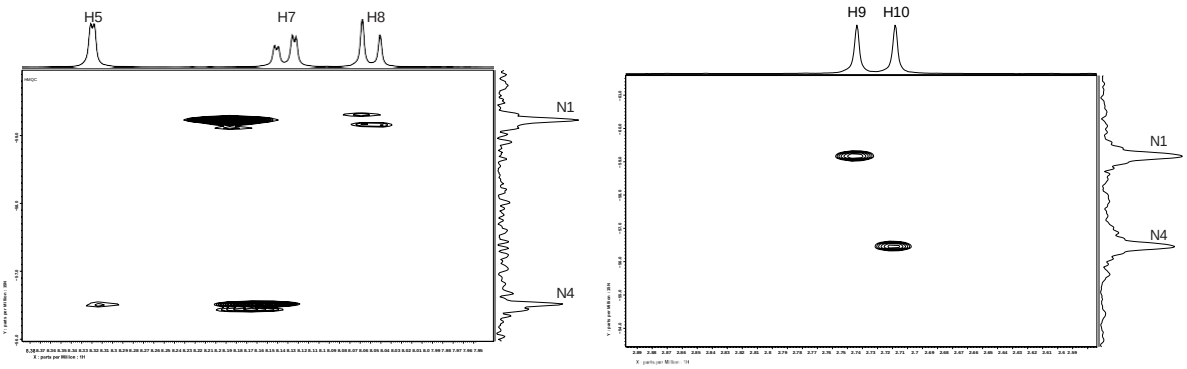


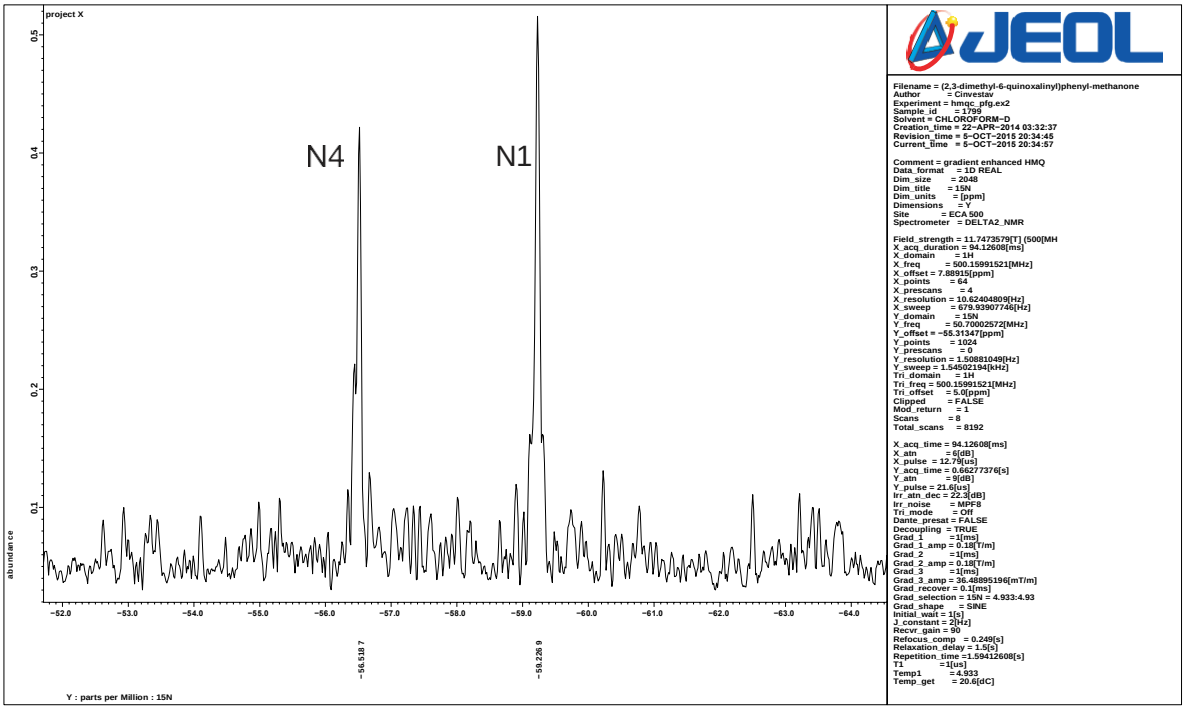




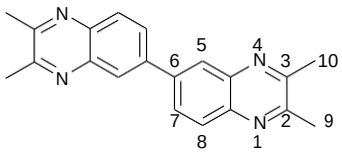
(2,3-dimethyl-6-quinoxalinyl)phenyl-methanone (10).

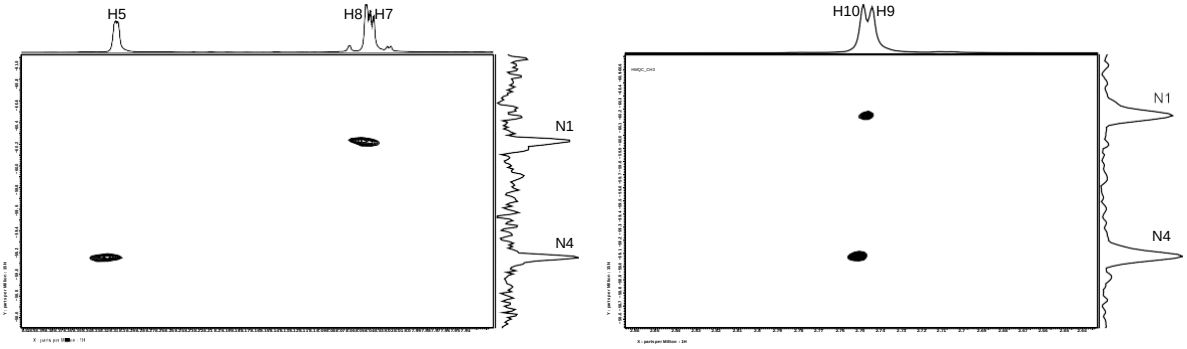


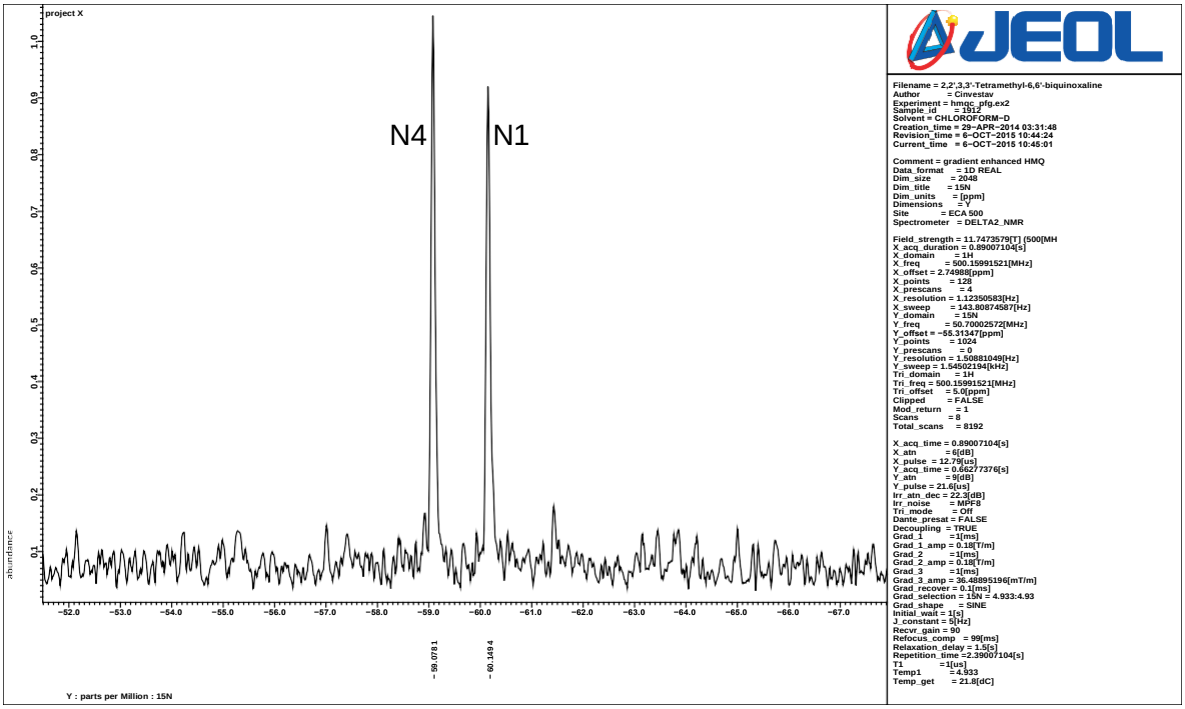




2,2',3,3'-Tetramethyl-*6,6'*-biquinoxaline (11).





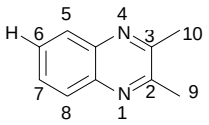


III. Spectrometric NMR titration

To evaluate the reactivity of compounds and in order to get a better accuracy and a smoother curve titration, is necessary considering the decimals values of the chemical shifts of H9 and H10. Subsequently the ***pKa*** values are getting with the semilogarithmic Henderson-Hasselbalch equation and the **Δ*K*** is obtained using the δ-diagram and the Perrin linearization. The data of 2,3-dimethyl-6R-quinoxalines are showed as follows:

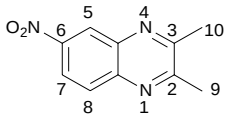
2,3-Dimethylquinoxaline (1).

pH	δH9	δH10	pH	δH9	δH10
7.54	2.5943	2.5943	0.94	2.6748	2.6748
1.82	2.6042	2.6042	0.91	2.6847	2.6847
1.53	2.6148	2.6148	0.91	2.6974	2.6974
1.4	2.6254	2.6254	0.74	2.708	2.708
1.25	2.6381	2.6381	0.66	2.7221	2.7221
1.06	2.6501	2.6501	0.63	2.7334	2.7334
1.12	2.6621	2.6621	0.57	2.7454	2.7454



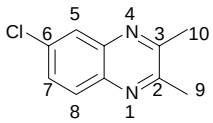
2,3-Dimethyl-6-nitroquinoxaline (2).

pH	δH9	δH10	pH	δH9	δH10
6.45	2.6557	2.6557	0.75	2.66068	2.65644
0.32	2.66279	2.65993	0.65	2.65997	2.6550
0.49	2.6642	2.66139	0.79	2.6586	2.65357
0.53	2.66419	2.66066	0.64	2.65856	2.65288
0.45	2.66377	2.66023			
0.57	2.66212	2.65821			
0.7	2.66139	2.65715			



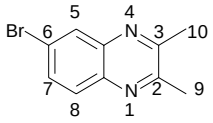
2,3-Dimethyl-6-chloroquinoxaline (6).

pH	δH9	δH10	pH	δH9	δH10
6.63	2.5512	2.5554	0.73	2.6077	2.6112
1.36	2.5547	2.5590	0.7	2.6119	2.6155
0.94	2.5689	2.5731	0.73	2.6162	2.6197
0.77	2.5809	2.5851	0.68	2.6197	2.6225
0.74	2.5900	2.5936	0.71	2.6232	2.6261
0.72	2.5971	2.6013	0.7	2.6275	2.6296
0.67	2.6028	2.6063	0.72	2.6310	2.6331



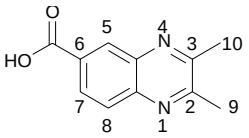
2,3-Dimethyl-6-bromoquinoxaline (7).

pH	δH9	δH10	pH	δH9	δH10
6.08	2.5484	2.5625	0.7	2.6105	2.6239
0.92	2.5625	2.5759	0.68	2.6148	2.6282
0.71	2.5759	2.5900	0.75	2.6176	2.6310
0.76	2.5865	2.5999	0.65	2.6211	2.6338
0.69	2.5950	2.6084	0.69	2.6239	2.6374
0.66	2.6013	2.6148	0.68	2.6254	2.6388
0.66	2.6063	2.6197			



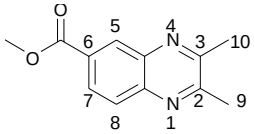
2,3-Dimethylquinoxaline-6-carboxylic acid (8).

pH	δH9	δH10	pH	δH9	δH10
5.25	2.6352	2.6324	0	2.7362	2.7306
3.27	2.6360	2.6331	0	2.7426	2.7362
0.53	2.6550	2.6522	0	2.7496	2.7433
0.19	2.6819	2.6776			
0.12	2.7002	2.6960			
0.1	2.7143	2.7094			
0	2.7263	2.7207			



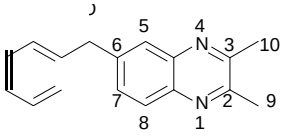
Methyl 2,3-dimethylquinoxaline-6-carboxylate (9).

pH	δH9	δH10	pH	δH9	δH10
8.43	2.5943	2.5900	0.67	2.6480	2.6423
1.4	2.6003	2.5954	0.66	2.6557	2.6501
1.12	2.6084	2.6042	0.61	2.6649	2.6586
1	2.6169	2.6119	0.58	2.6748	2.6684
0.84	2.6247	2.6197			
0.8	2.6324	2.6275			
0.74	2.6395	2.6345			



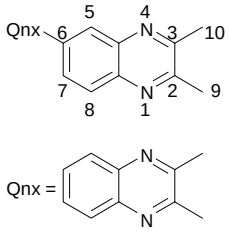
(2,3-dimethyl-6-quinoxalinyl)phenyl-methanone (10).

pH	δH9	δH10	pH	δH9	δH10
8.07	2.6480	2.6225	0.45	2.7306	2.7037
1.66	2.6515	2.6261	0.41	2.7419	2.7150
1	2.6649	2.6395	0.4	2.7525	2.7249
0.85	2.6797	2.6543	0.33	2.7595	2.7320
0.72	2.6939	2.6677	0.34	2.7673	2.7391
0.58	2.7059	2.6797	0.35	2.7779	2.7489
0.51	2.7200	2.6932			



***2,2',3,3'*-Tetramethyl-*6,6'*-biquinoxaline (11)**.

pH	δH9	δH10	pH	δH9	δH10
7.11	2.6522	2.6564	0.09	2.8111	2.8196
4.07	2.6833	2.6889	0.11	2.8196	2.8280
2.21	2.7256	2.7334			
0.26	2.7602	2.768			
0.17	2.7779	2.7857			
0.09	2.7927	2.8005			
0.00	2.8019	2.8097			



IV. Computational chemistry

The structures **1-14** were optimized with DFT ωB97XD 6-311++G (d,p) level of theory, the HOMO orbitals were get from optimized structures with HF 6-311++G (d,p) basis set. The bond lengths and angles are accord to X-ray data reported in literature. Tables **1S** and **2S** showed the values obtained for compounds **1-14**.

Table 1S. Bond length (Å) of 2,3-dimethyl-6R-quinoxalines optimized with DFT ωB97XD/6-311++(d,p) level theory.

Comp	C2C3	C2C9	C3C10	C6C7	C6R[a]	C7C8	C8C8a	C9C10	N1C2	N1C8a
1	1.442	1.501	1.501	1.413	1.084	1.369	1.413	2.964	1.305	1.362
1[b]	1.443	1.492	1.492	1.404		1.348	1.405	2.974	1.310	1.368
2	1.446	1.499	1.500	1.408	1.477	1.367	1.413	2.963	1.304	1.362
2[c]	1.447	1.496	1.494	1.401	1.466	1.372	1.409	2.942	1.311	1.371
3	1.445	1.500	1.500	1.419	1.434	1.367	1.413	2.964	1.304	1.362
4	1.443	1.500	1.500	1.416	1.503	1.366	1.414	2.963	1.305	1.361
5	1.441	1.501	1.501	1.406	1.344	1.368	1.413	2.964	1.305	1.361
6	1.442	1.500	1.500	1.411	1.746	1.368	1.413	2.963	1.305	1.361
7	1.443	1.500	1.500	1.412	1.899	1.368	1.412	2.963	1.305	1.361
8	1.445	1.500	1.500	1.417	1.488	1.368	1.413	2.963	1.304	1.362
9	1.444	1.500	1.500	1.417	1.491	1.368	1.413	2.963	1.305	1.362
10	1.443	1.500	1.500	1.419	1.498	1.366	1.414	2.964	1.305	1.361
11	1.440	1.503	1.505	1.421	1.483	1.367	1.413	3.025	1.307	1.358
11[d]	1.442	1.500	1.497	1.418	1.489	1.373	1.409	2.950	1.315	1.378
12	1.443	1.501	1.501	1.416	1.355	1.371	1.408	2.962	1.304	1.361
13	1.441	1.501	1.501	1.416	1.358	1.368	1.412	2.963	1.305	1.360
14	1.437	1.502	1.501	1.424	1.374	1.364	1.414	2.963	1.307	1.356

[a] Distance of carbon atom with substituent R. [b] X-ray of compound **1** is report in Reference 3, [c] compound 2 in reference 4 and [d] compound 11 in reference 5.

Table 2S. Angles (°, $\angle_{NCC}$) of 2,3-dimethyl-6R-quinoxalines optimized with DFT ωB97XD/6-311++(d,p) level theory.

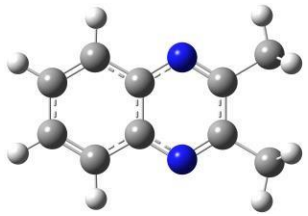
	$\angle_{N129}$	$\angle_{N123}$	$\angle_{N18a8}$	$\angle_{N18a4a}$	$\angle_{N432}$	$\angle_{2N18a}$	$\angle_{2310}$	$\angle_{329}$	$\angle_{8a87}$	$\angle_{678}$	$\angle_{567}$
1	118.0	121.4	119.6	120.7	121.4	117.7	120.4	120.4	119.8	120.5	120.5
1[b]	117.7	121.5	119.8	120.8		117.7		120.9	119.9	120.8	
2	118.0	121.6	119.4	120.7	121.4	117.6	120.4	120.3	120.2	118.8	122.9
2[c]	118.2	121.8	119.1	121.0	121.7	117.1	120.1	119.9	120.1	118.7	123.6
3	118.0	121.5	119.5	120.7	121.4	117.6	120.4	120.3	120.1	120.0	120.8
4	118.0	121.5	119.6	120.7	121.4	117.6	120.4	120.3	120.0	120.1	121.0
5	118.1	121.3	119.5	120.8	121.6	117.7	120.4	120.5	120.1	119.0	123.0
6	118.0	121.4	119.7	120.8	121.5	117.6	120.3	120.4	120.2	119.6	121.8
7	118.1	121.4	119.7	120.8	121.5	117.6	120.4	120.4	120.3	119.6	121.7
8	118.0	121.6	119.6	120.7	121.4	117.6	120.4	120.3	120.0	120.3	120.5
9	118.0	121.6	119.6	120.7	121.4	117.6	120.4	120.3	120.0	120.3	120.4
10	118.0	121.5	119.7	120.7	121.4	117.6	120.4	120.4	119.9	120.7	119.9
11	117.2	121.2	119.9	120.8	121.3	117.9	122.0	121.4	119.9	121.3	119.1
11[d]	118.6	121.7	119.9	120.8	121.8	117.1	120.7	119.6	120.0	121.1	119.0
12	118.1	121.3	119.8	121.1	121.8	117.6	120.2	120.5	120.6	120.1	120.2
13	118.1	121.2	119.7	121.1	121.7	117.6	120.3	120.6	120.1	120.4	120.6
14	118.1	121.1	120.0	121.2	121.8	117.7	120.3	120.7	120.4	121.0	119.1

See footnote in table S1 for [b], [c] and d

To calculate the heat formation of compounds was used the Spartan Pro 08 software[6] and Gaussian 09 package.[7] The initial and ending regioisomers **a**:**b**, mesomeric forms (**a1**-**a4**, **b1**-**b4**) and intermediaries (**a5**-**a6**, **b5**-**b6**) of complexes (2,3-dimethyl-6R-quinoxalines)- SeO_2 were built in Spartan pro 08 as shown in scheme 3, previously were optimized with molecular mechanics (MMFF94), the structures were exported to Gaussian 09 as MDL files, subsequently were calculated the heat formation energies with semiempirical PM6 method. The energy data obtained and the energetic diagrams were processed and built in a Microsoft excel worksheet respectively. Details of calculations for structures are shown as follows:

2,3-Dimethylquinoxaline (1).

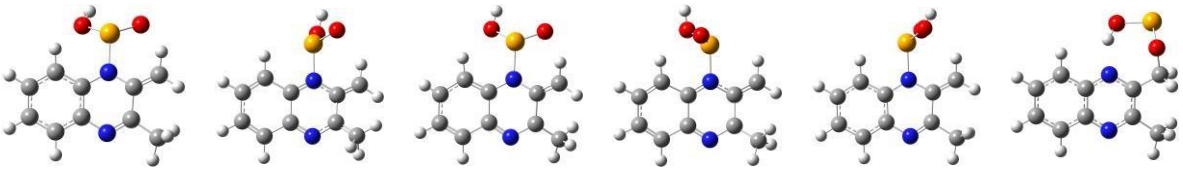
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-496.55382297 a.u
RMS Gradient Norm	0.00000451 a.u
Imaginary Freq	0
Dipole Moment	0.8639 Debye
Point Group	C1



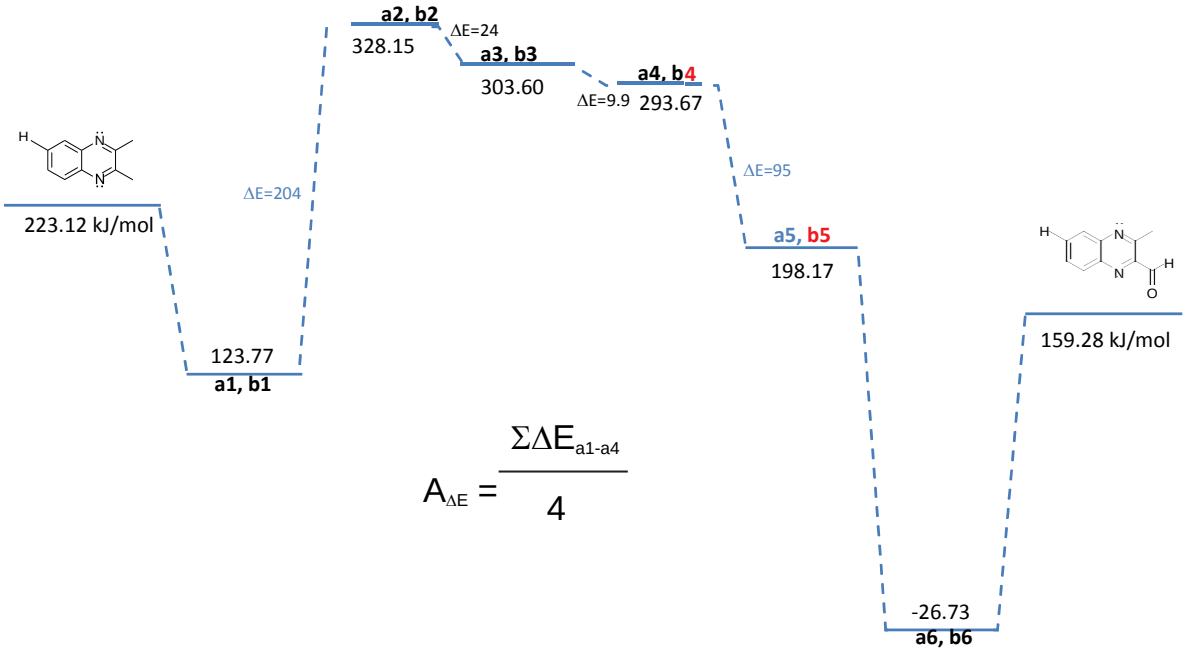
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.092271	0.706911	0.000009
2	6	0	-1.912657	1.403510	-0.000025
3	6	0	-0.683403	0.705931	-0.000016
4	6	0	-0.683402	-0.705931	-0.000007
5	6	0	-1.912656	-1.403510	0.000015
6	6	0	-3.092271	-0.706911	0.000036
7	1	0	-4.036534	1.239577	0.000019
8	1	0	-1.884877	2.486969	-0.000043
9	1	0	-1.884875	-2.486969	0.000030
10	6	0	1.600115	-0.721237	-0.000049
11	6	0	1.600113	0.721237	-0.000028
12	6	0	2.894180	-1.482040	-0.000009
13	1	0	3.496066	-1.235494	-0.880003
14	1	0	3.495127	-1.236783	0.881024
15	1	0	2.684711	-2.550634	-0.000802
16	6	0	2.894179	1.482041	0.000050
17	1	0	3.495642	1.235879	0.880457
18	1	0	3.495547	1.236399	-0.880569
19	1	0	2.684714	2.550636	0.000333
20	7	0	0.487103	-1.403194	-0.000037
21	7	0	0.487102	1.403193	-0.000016
22	1	0	-4.036533	-1.239578	0.000069

Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



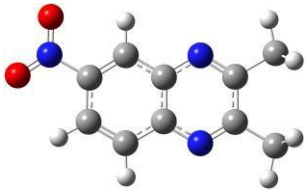
a1, b1 **a2, b2** **a3, b3** **a4, b4** **a5, b5** **a6, b6**



$$A_{\Delta E} = \frac{\Sigma \Delta E_{a1\text{-}a4}}{4}$$

2,3-Dimethyl-6-nitroquinoxaline (2).

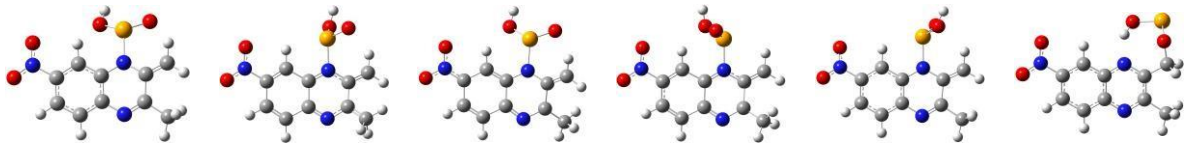
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-701.04864973 a.u
RMS Gradient Norm	0.00013478 a.u
Imaginary Freq	0
Dipole Moment	6.2709 Debye
Point Group	CS



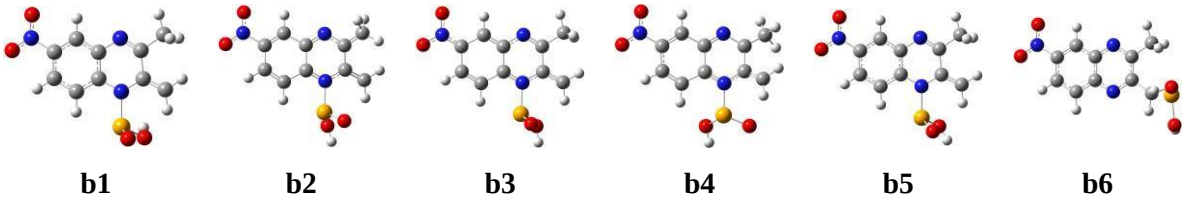
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.844497	-1.038294	0.000000
2	1	0	-2.076010	1.090417	0.000000
3	6	0	-1.392099	0.252295	0.000000
4	6	0	0.368416	-1.942075	0.000000
5	6	0	0.000000	0.473768	0.000000
6	6	0	-0.983285	-2.152372	0.000000
7	6	0	0.883894	-0.626031	0.000000
8	7	0	0.469309	1.753348	0.000000
9	1	0	-1.405770	-3.147550	0.000000
10	1	0	1.070588	-2.766851	0.000000
11	6	0	1.762090	1.921472	0.000000
12	6	0	2.669300	0.795033	0.000000
13	7	0	2.232830	-0.434436	0.000000
14	7	0	-3.302464	-1.275749	0.000000
15	8	0	-4.033923	-0.306735	0.000000
16	8	0	-3.681140	-2.430451	0.000000
17	6	0	4.152595	1.016682	0.000000
18	1	0	4.463331	1.586711	0.880514
19	1	0	4.463331	1.586711	-0.880514
20	1	0	4.661219	0.054159	0.000000
21	6	0	2.292806	3.324489	0.000000
22	1	0	2.915372	3.508079	0.880569
23	1	0	2.915372	3.508079	-0.880569
24	1	0	1.460031	4.025784	0.000000

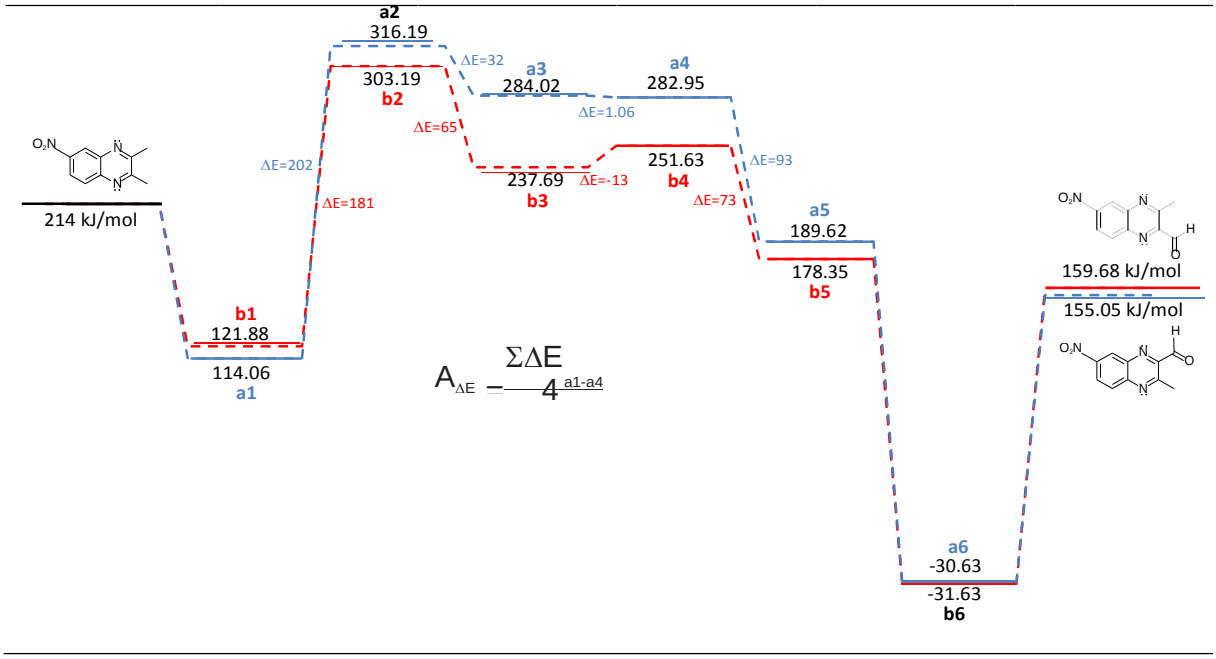
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

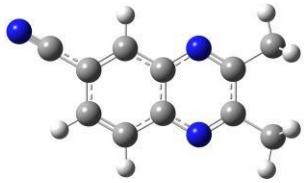


b1 **b2** **b3** **b4** **b5** **b6**



6-carbonitrile-2,3-dimethylquinoxaline (3).

Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-588.78280682 a.u
RMS Gradient Norm	0.00006290 a.u
Imaginary Freq	0
Dipole Moment	6.0776 Debye
Point Group	CS

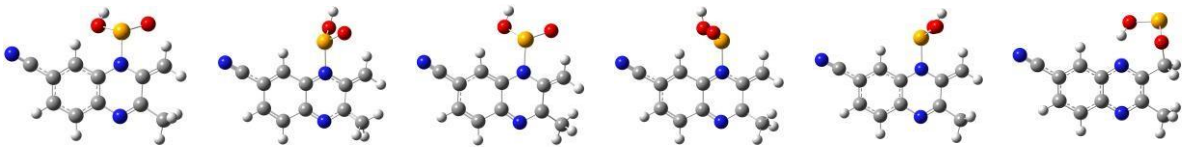


Standard orientation:

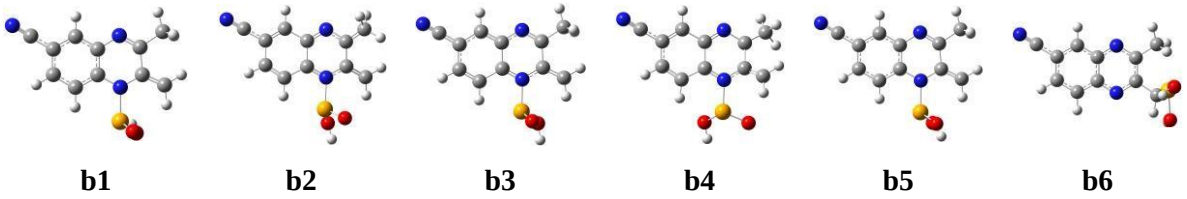
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.386994	0.798571	0.000000
2	1	0	-0.964926	2.414465	0.000000
3	6	0	-1.122938	1.342965	0.000000
4	6	0	-1.491448	-1.443203	0.000000
5	6	0	0.000000	0.490299	0.000000
6	6	0	-2.574013	-0.608422	0.000000
7	6	0	-0.183051	-0.908009	0.000000
8	7	0	1.249183	1.034944	0.000000
9	1	0	-3.580831	-1.007685	0.000000
10	1	0	-1.605648	-2.520453	0.000000
11	6	0	2.264747	0.216581	0.000000
12	6	0	2.078051	-1.216955	0.000000
13	7	0	0.887229	-1.750686	0.000000
14	6	0	3.263691	-2.135857	0.000000
15	1	0	3.890421	-1.966324	0.880465
16	1	0	3.890421	-1.966324	-0.880465
17	1	0	2.920089	-3.168976	0.000000
18	6	0	3.645279	0.803728	0.000000
19	1	0	4.208889	0.481711	0.880615
20	1	0	4.208889	0.481711	-0.880615
21	1	0	3.574399	1.890151	0.000000
22	6	0	-3.535444	1.658504	0.000000
23	7	0	-4.463409	2.340386	0.000000

-

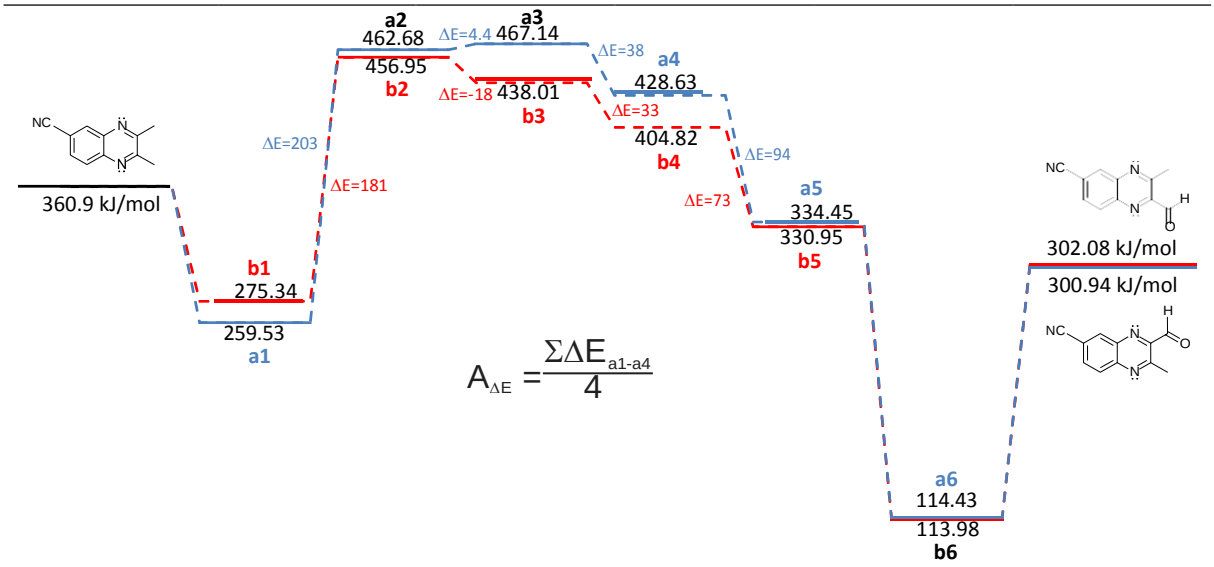
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

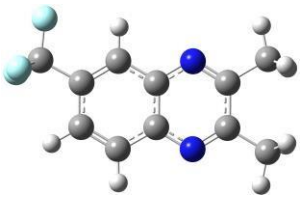


b1 **b2** **b3** **b4** **b5** **b6**



2,3-Dimethyl-6-(trifluoromethyl)quinoxaline (4).

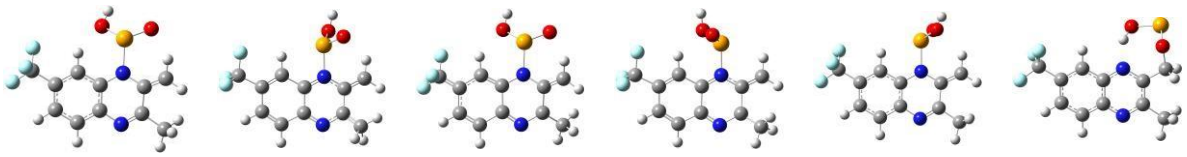
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-833.61280178 a.u
RMS Gradient Norm	0.00001019 a.u
Imaginary Freq	0
Dipole Moment	4.2572 Debye
Point Group	C1



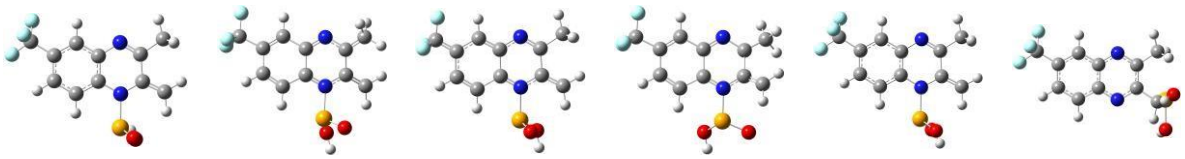
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.775458	0.128790	-0.009440
2	1	0	0.990238	-1.871244	-0.016130
3	6	0	0.779780	-0.809416	-0.011891
4	6	0	0.175668	1.933366	-0.001247
5	6	0	-0.569813	-0.390017	-0.008599
6	6	0	1.475923	1.512814	-0.003854
7	6	0	-0.874280	0.985719	-0.003136
8	7	0	-1.557697	-1.326862	-0.008876
9	1	0	2.284248	2.234419	-0.003251
10	1	0	-0.082044	2.985543	0.002197
11	6	0	-2.792322	-0.903814	-0.002712
12	6	0	-3.105194	0.505849	0.001447
13	7	0	-2.167107	1.413593	0.001061
14	6	0	-4.533149	0.966050	0.004036
15	1	0	-5.075537	0.560146	0.862840
16	1	0	-5.054325	0.627940	-0.896712
17	1	0	-4.562823	2.053727	0.043838
18	6	0	-3.889303	-1.927159	0.007014
19	1	0	-4.484561	-1.851608	0.922234
20	1	0	-4.572396	-1.784989	-0.835288
21	1	0	-3.453002	-2.923051	-0.049874
22	6	0	3.221492	-0.282144	0.001452
23	9	0	3.384383	-1.609035	-0.079283
24	9	0	3.839924	0.126163	1.126249
25	9	0	3.897721	0.265290	-1.026252

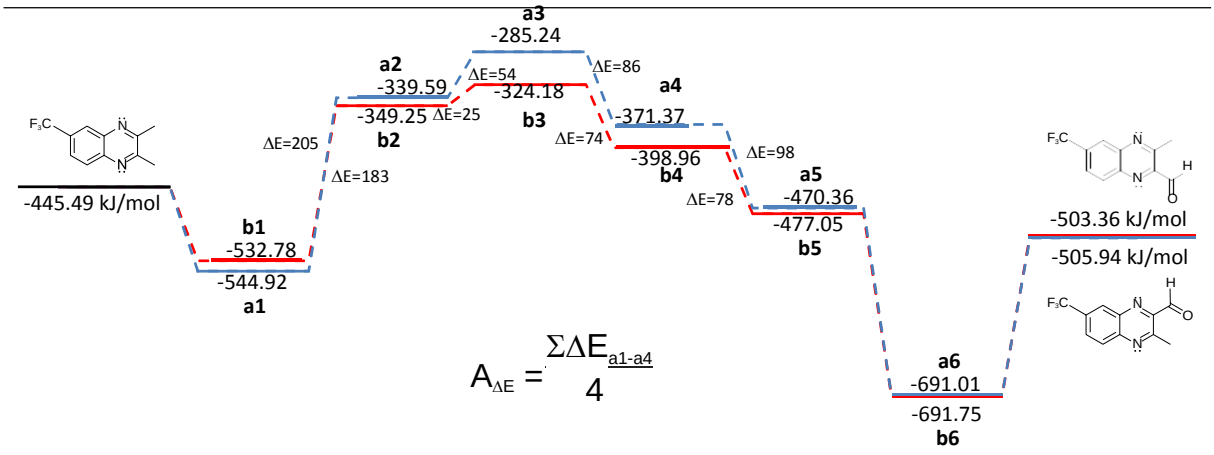
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

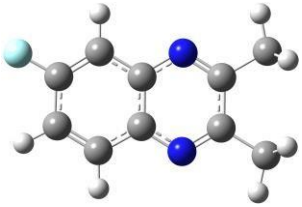


b1 **b2** **b3** **b4** **b5** **b6**



2,3-Dimethyl-6-fluoroquinoxaline (5).

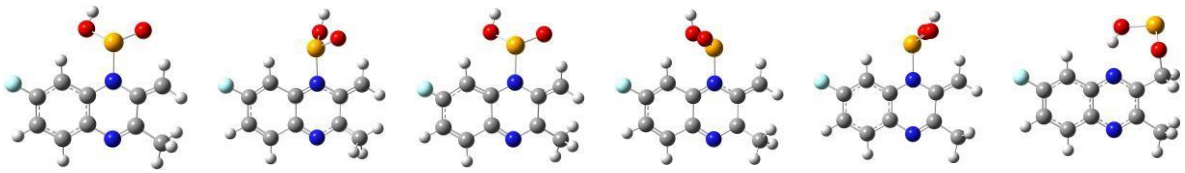
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-595.79541900 a.u
RMS Gradient Norm	0.00011526 a.u
Imaginary Freq	1
Dipole Moment	2.6078 Debye
Point Group	CS



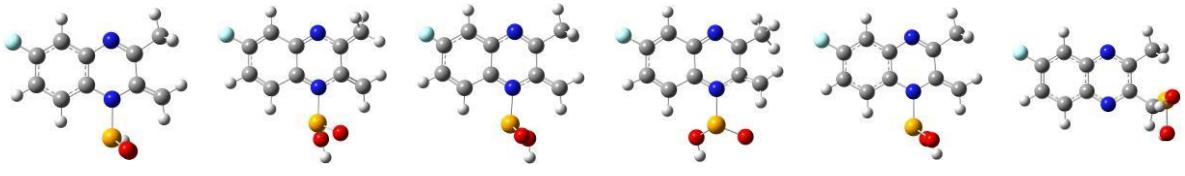
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.112441	1.770006	0.000000
2	1	0	-0.248621	2.822556	0.000000
3	6	0	-0.752343	1.864784	0.000000
4	6	0	-2.073416	-0.620806	0.000000
5	6	0	0.000000	0.669156	0.000000
6	6	0	-2.796438	0.541502	0.000000
7	6	0	-0.660303	-0.579239	0.000000
8	7	0	1.360258	0.736454	0.000000
9	1	0	-3.879336	0.541509	0.000000
10	1	0	-2.558557	-1.589326	0.000000
11	6	0	2.022605	-0.389201	0.000000
12	6	0	1.348438	-1.663635	0.000000
13	7	0	0.045368	-1.743010	0.000000
14	6	0	2.135008	-2.942370	0.000000
15	1	0	2.781031	-3.007644	0.880596
16	1	0	2.781031	-3.007644	-0.880596
17	1	0	1.447315	-3.786673	0.000000
18	6	0	3.522193	-0.322673	0.000000
19	1	0	3.937729	-0.821893	0.880410
20	1	0	3.937729	-0.821893	-0.880410
21	1	0	3.836816	0.719711	0.000000
22	9	0	-2.852704	2.892449	0.000000

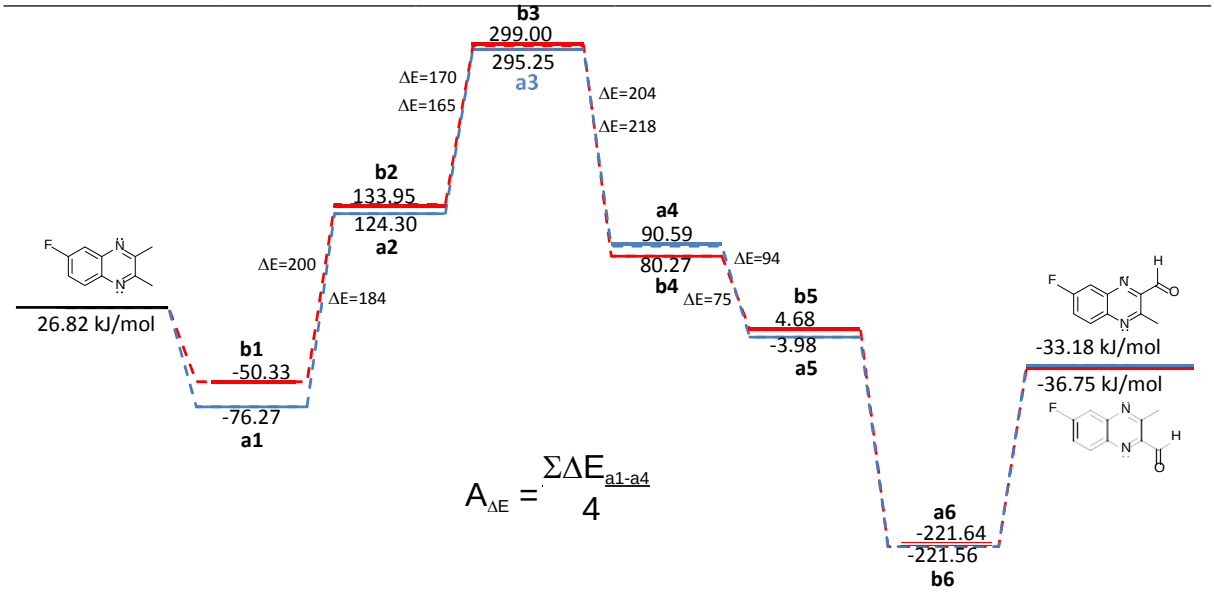
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

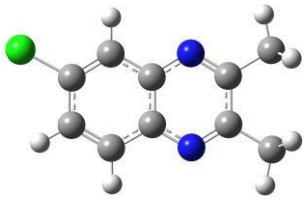


b1 **b2** **b3** **b4** **b5** **b6**



2,3-Dimethyl-6-chloroquinoxaline (6).

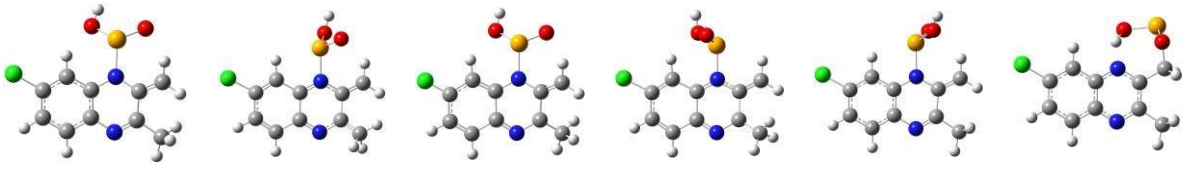
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-956.16091472 a.u
RMS Gradient Norm	0.00000882 a.u
Imaginary Freq	1
Dipole Moment	2.8323 Debye
Point Group	C1



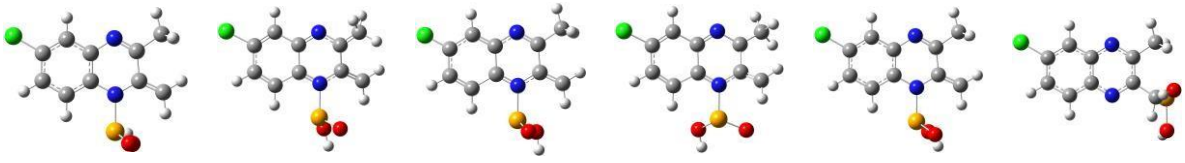
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.145938	1.360835	0.000286
2	6	0	-0.861256	1.832045	0.000279
3	6	0	0.227550	0.931147	-0.000071
4	6	0	-0.022010	-0.457196	-0.000470
5	6	0	-1.351961	-0.935329	-0.000493
6	6	0	-2.378072	-0.031939	-0.000045
7	1	0	-2.988501	2.040905	0.000586
8	1	0	-0.650101	2.894709	0.000559
9	1	0	-1.525416	-2.003802	-0.000727
10	6	0	2.221124	-0.875535	-0.000406
11	6	0	2.476507	0.544518	-0.000019
12	6	0	3.360690	-1.851946	0.000849
13	1	0	4.002741	-1.708517	-0.873274
14	1	0	3.988247	-1.721133	0.887524
15	1	0	2.965860	-2.866610	-0.009216
16	6	0	3.884438	1.064466	-0.000256
17	1	0	4.435249	0.710239	0.876149
18	1	0	4.429853	0.722580	-0.884992
19	1	0	3.866287	2.153197	0.007114
20	7	0	1.005354	-1.351242	-0.000725
21	7	0	1.500974	1.412008	0.000132
22	17	0	-4.031468	-0.596078	0.000148

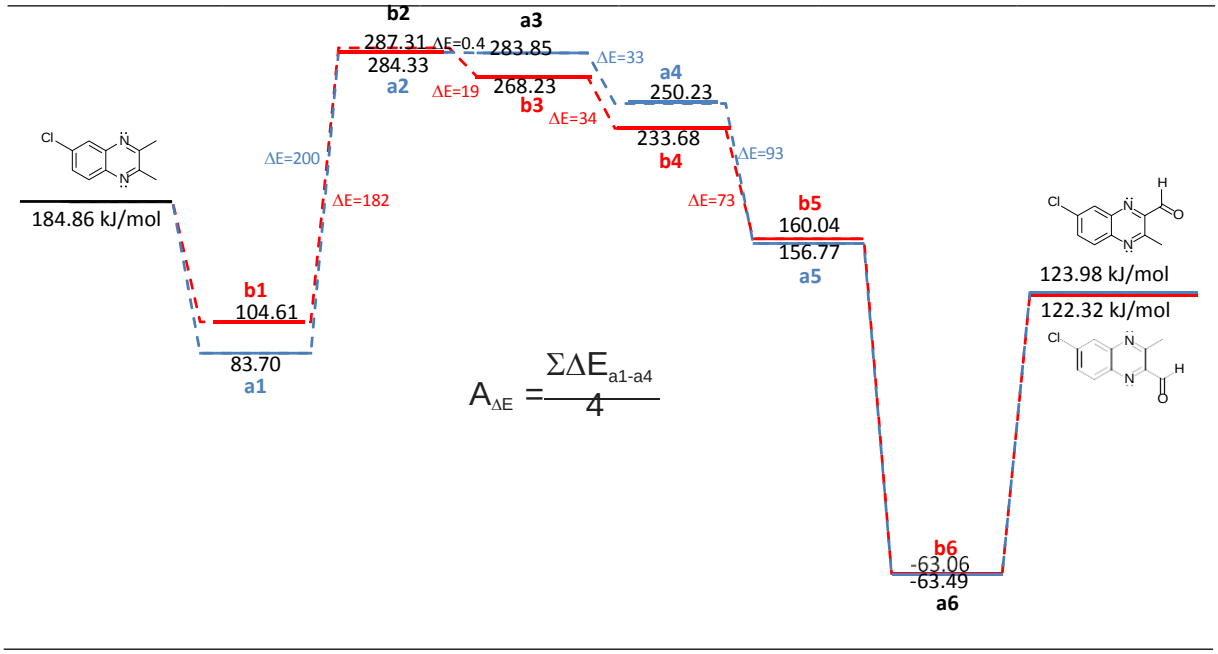
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

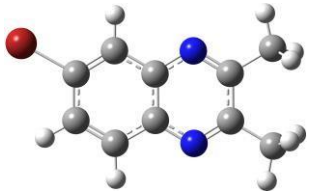


b1 **b2** **b3** **b4** **b5** **b6**


b2
287.31
ΔE=0.4
284.33
a2
a3
283.85
ΔE=33
a4
250.23
ΔE=19
268.23
b3
ΔE=34
233.68
b4
ΔE=93
ΔE=200
ΔE=182
ΔE=73
b5
160.04
156.77
a5
184.86 kJ/mol
b1
104.61
83.70
a1
b6
-63.06
-63.49
a6
123.98 kJ/mol
122.32 kJ/mol
$A_{\Delta E} = \frac{\Sigma \Delta E_{a1\text{-}a4}}{4}$

2,3-Dimethyl-6-bromoquinoxaline (7).

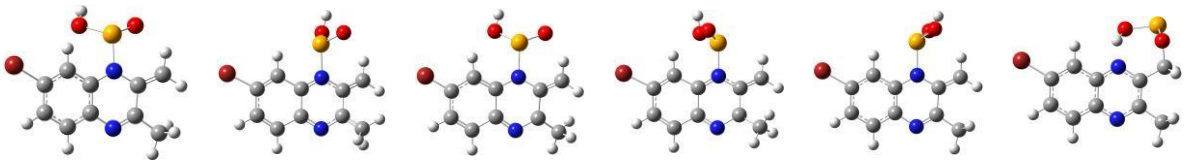
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-3070.1257740 a.u
RMS Gradient Norm	0.00001167 a.u
Imaginary Freq	0
Dipole Moment	2.7976 Debye
Point Group	C1



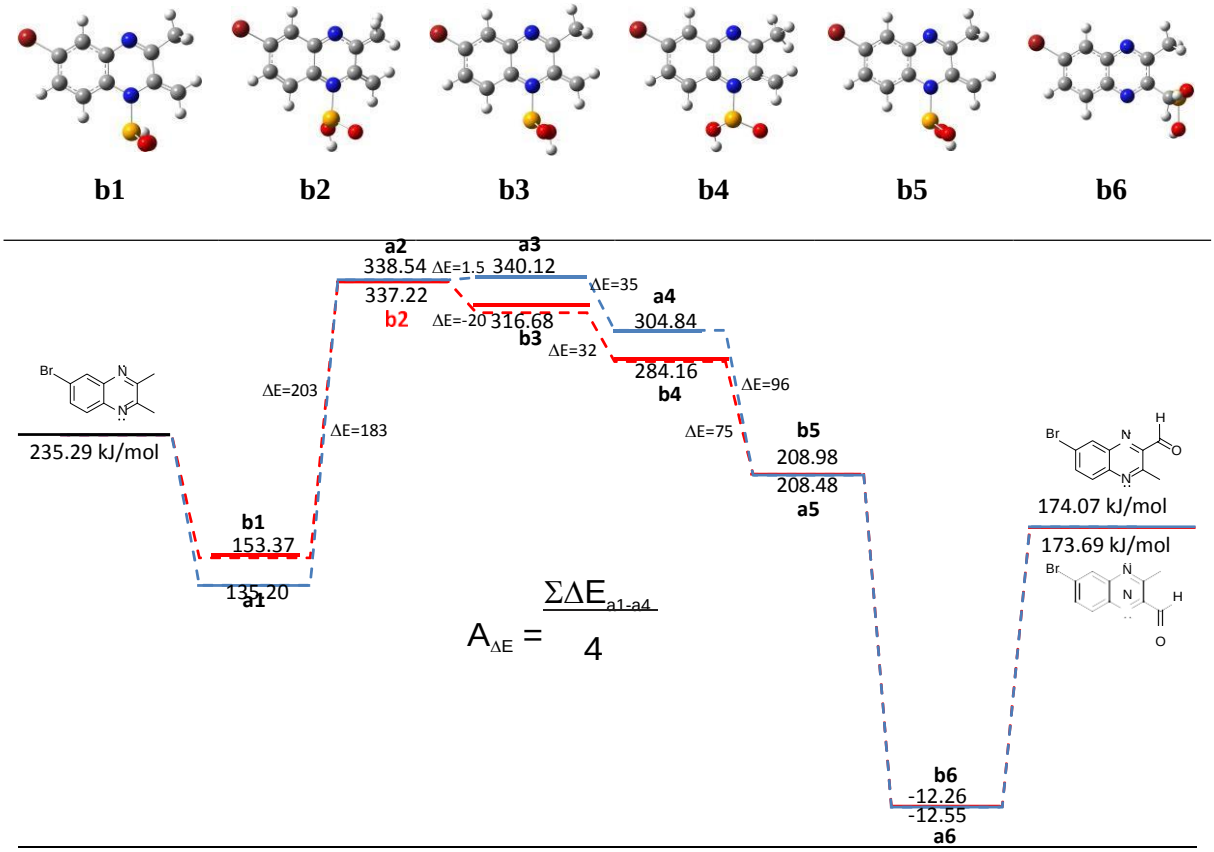
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.406947	1.546643	0.001124
2	6	0	-0.097809	1.946834	0.001111
3	6	0	0.940504	0.988627	-0.000769
4	6	0	0.616277	-0.383700	-0.003017
5	6	0	-0.738096	-0.788870	-0.003110
6	6	0	-1.715330	0.167912	-0.000627
7	1	0	-2.207490	2.275491	0.002737
8	1	0	0.170495	2.996590	0.002616
9	1	0	-0.963099	-1.847779	-0.004368
10	6	0	2.833080	-0.924185	-0.002361
11	6	0	3.165220	0.480215	0.000032
12	6	0	3.916701	-1.962069	0.004554
13	1	0	4.600385	-1.828020	-0.838671
14	1	0	4.514648	-1.895279	0.918798
15	1	0	3.467448	-2.952213	-0.052524
16	6	0	4.599497	0.922029	-0.000440
17	1	0	5.139062	0.510227	0.857439
18	1	0	5.115247	0.578257	-0.902233
19	1	0	4.642726	2.009353	0.039325
20	7	0	1.593113	-1.332501	-0.004516
21	7	0	2.238399	1.399482	0.000611
22	35	0	-3.542245	-0.350746	0.000721

Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO

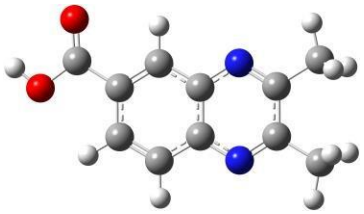


a1 **a2** **a3** **a4** **a5** **a6**


b1
b2
b3
b4
b5
b6
a2
338.54
337.22
b2
ΔE=1.5
a3
340.12
316.68
b3
ΔE=-20
ΔE=35
a4
304.84
284.16
b4
ΔE=32
ΔE=96
ΔE=75
b5
208.98
208.48
a5
b6
-12.26
-12.55
a6
ΔE=203
ΔE=183
b1
153.37
135.20
a1
235.29 kJ/mol
174.07 kJ/mol
173.69 kJ/mol
Br
N
H
O
$A_{\Delta E} = \frac{\Sigma \Delta E_{a1\text{-}a4}}{4}$

2,3-Dimethylquinoxaline-6-carboxylic acid (8).

Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-685.13023589 a.u
RMS Gradient Norm	0.00001072 a.u
Imaginary Freq	0
Dipole Moment	2.6167 Debye
Point Group	C1

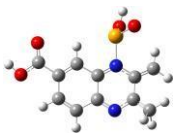


Standard orientation:

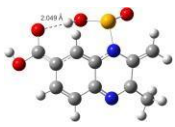
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.833720	-1.439735	-0.000157
2	6	0	0.540847	-1.886955	-0.000311
3	6	0	-0.528104	-0.962515	-0.001626
4	6	0	-0.253162	0.421408	-0.003754
5	6	0	1.084492	0.865664	-0.003730
6	6	0	2.109625	-0.049532	-0.001304
7	1	0	2.656830	-2.142456	0.001231
8	1	0	0.304065	-2.944191	0.000885
9	1	0	1.289940	1.929356	-0.004635
10	6	0	-2.487244	0.886827	-0.002170
11	6	0	-2.769047	-0.530458	0.000452
12	6	0	-3.607670	1.885091	0.004656
13	1	0	-4.283237	1.729581	-0.841387
14	1	0	-4.205404	1.794560	0.916912
15	1	0	-3.193052	2.890472	-0.048332
16	6	0	-4.186839	-1.021339	0.001215
17	1	0	-4.738416	-0.628702	0.860403
18	1	0	-4.714795	-0.692790	-0.899145
19	1	0	-4.192555	-2.109497	0.039141
20	7	0	-1.263366	1.336856	-0.004863
21	7	0	-1.812497	-1.418024	0.000381
22	6	0	3.504175	0.469892	0.000916
23	8	0	3.806399	1.634862	0.000677
24	8	0	4.427597	-0.510682	0.003781
25	1	0	5.290935	-0.081684	0.005508

Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO

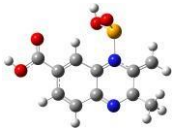
a1



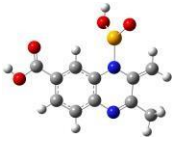
a2



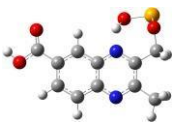
a3



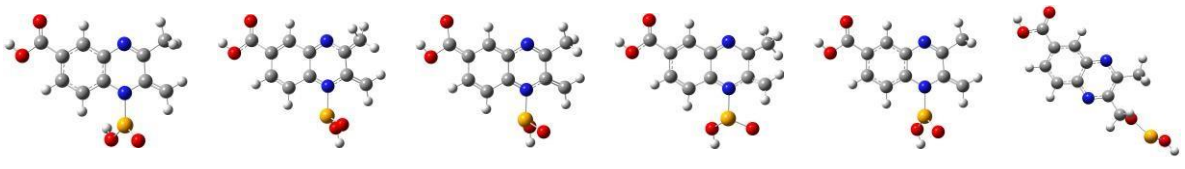
a4



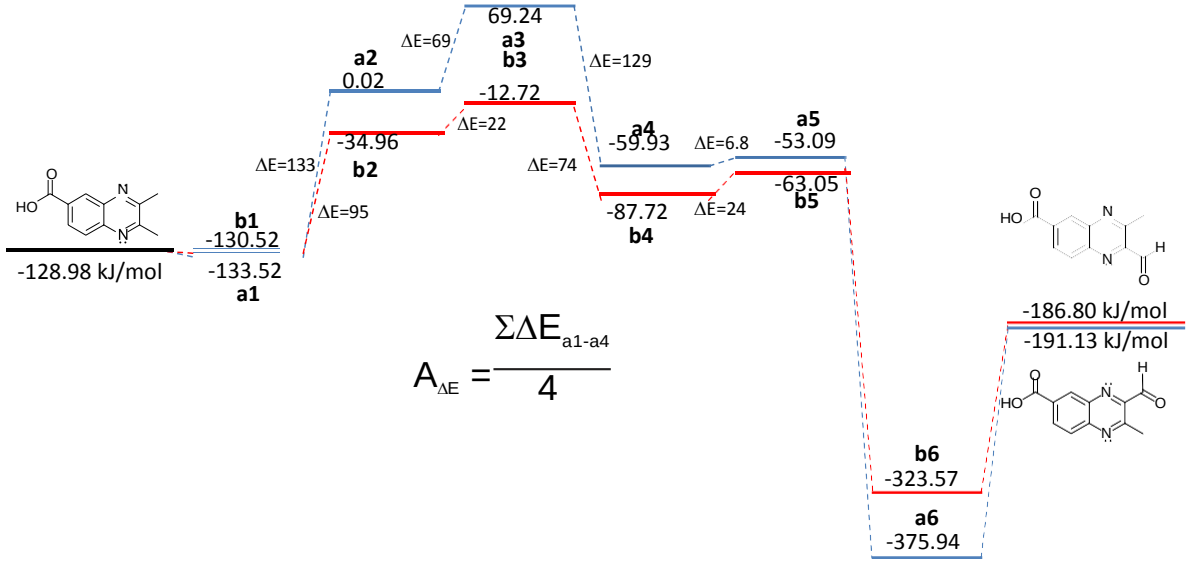
a5



a6

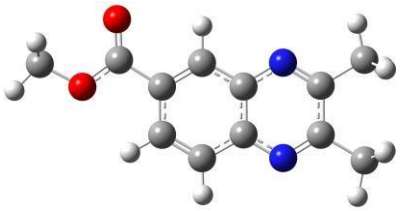


b1 **b2** **b3** **b4** **b5** **b6**



Methyl 2,3-dimethylquinoxaline-6-carboxylate (9).

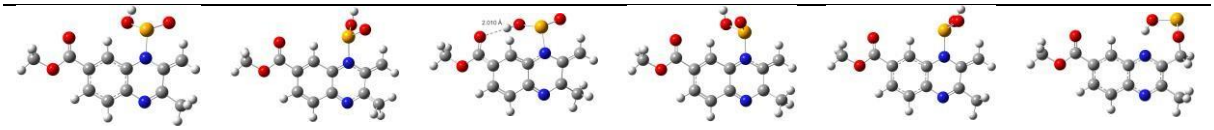
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-724.42622001 a.u
RMS Gradient Norm	0.00000603 a.u
Imaginary Freq	0
Dipole Moment	2.0624 Debye
Point Group	C1



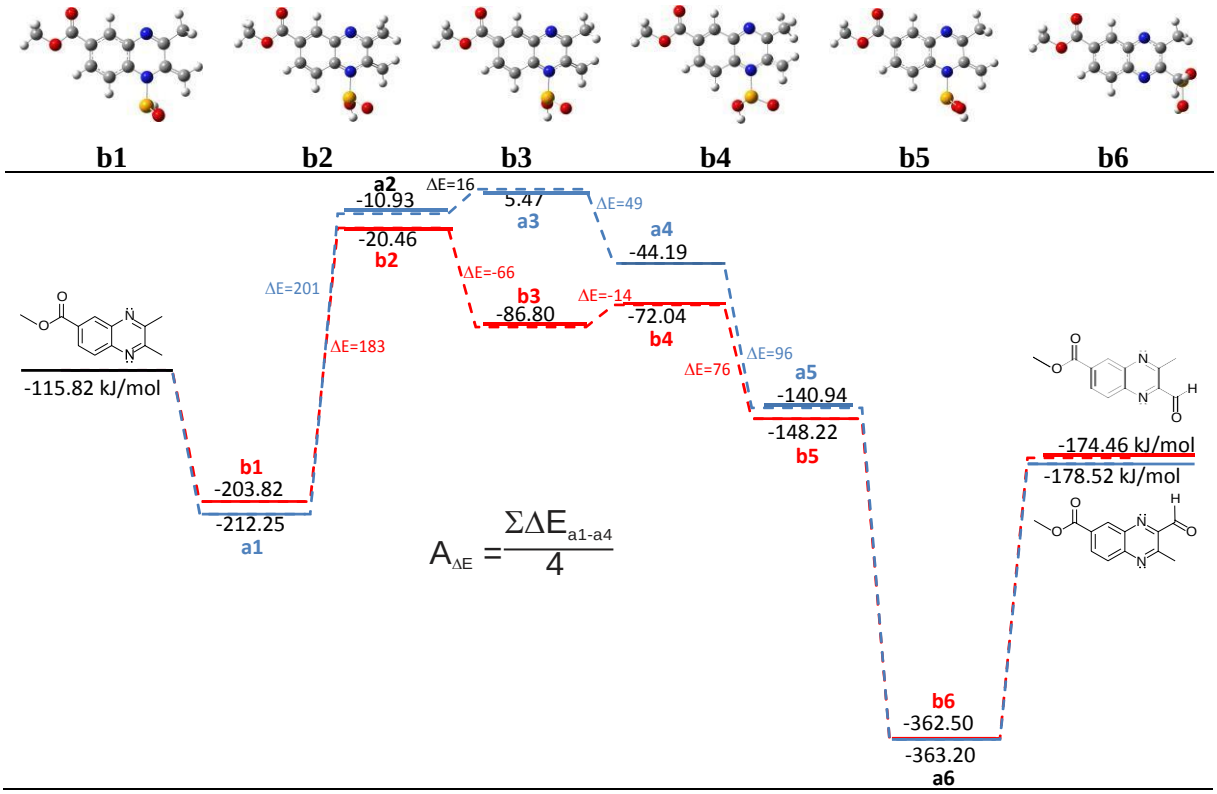
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.419535	-1.431229	-0.002563
2	6	0	0.128201	-1.882867	-0.002128
3	6	0	-0.944036	-0.962042	-0.002742
4	6	0	-0.672531	0.422601	-0.005345
5	6	0	0.664373	0.870582	-0.005991
6	6	0	1.692542	-0.040426	-0.003736
7	1	0	2.245994	-2.129891	-0.001419
8	1	0	-0.105142	-2.940945	-0.000676
9	1	0	0.866636	1.934861	-0.006890
10	6	0	-2.908205	0.881351	-0.001899
11	6	0	-3.186181	-0.536022	0.001605
12	6	0	-4.031243	1.876934	0.005566
13	1	0	-4.707593	1.719209	-0.839480
14	1	0	-4.627658	1.785879	0.918663
15	1	0	-3.619046	2.883266	-0.048810
16	6	0	-4.602772	-1.030950	0.004349
17	1	0	-5.154783	-0.639252	0.863710
18	1	0	-5.132795	-0.705059	-0.895810
19	1	0	-4.605199	-2.119114	0.043359
20	7	0	-1.685364	1.334907	-0.005858
21	7	0	-2.227034	-1.421056	0.000697
22	6	0	3.088210	0.486290	-0.000800
23	8	0	3.376791	1.655657	0.000055
24	8	0	4.001390	-0.494845	0.001690
25	6	0	5.365890	-0.074591	0.007445
26	1	0	5.579573	0.516290	0.899571
27	1	0	5.953373	-0.990175	0.005677
28	1	0	5.585286	0.523680	-0.878303

Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO

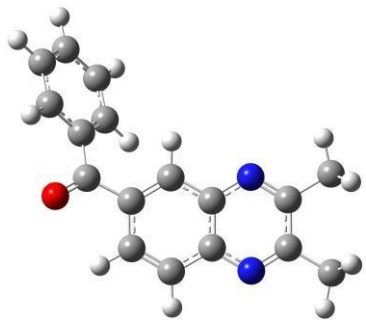


a1 **a2** **a3** **a4** **a5** **a6**


b1
b2
b3
b4
b5
b6
a2
-10.93
ΔE=16
5.47
a3
ΔE=49
a4
-44.19
-20.46
b2
ΔE=-66
ΔE=201
b3
-86.80
ΔE=-14
-72.04
b4
ΔE=183
ΔE=96
a5
-140.94
ΔE=76
-115.82 kJ/mol
b1
-203.82
-212.25
a1
-148.22
b5
-174.46 kJ/mol
-178.52 kJ/mol
b6
-362.50
-363.20
a6
$A_{\Delta E} = \frac{\Sigma \Delta E_{a1\text{-}a4}}{4}$

(2,3-dimethyl-6-quinoxalinyl)phenyl-methanone (10).

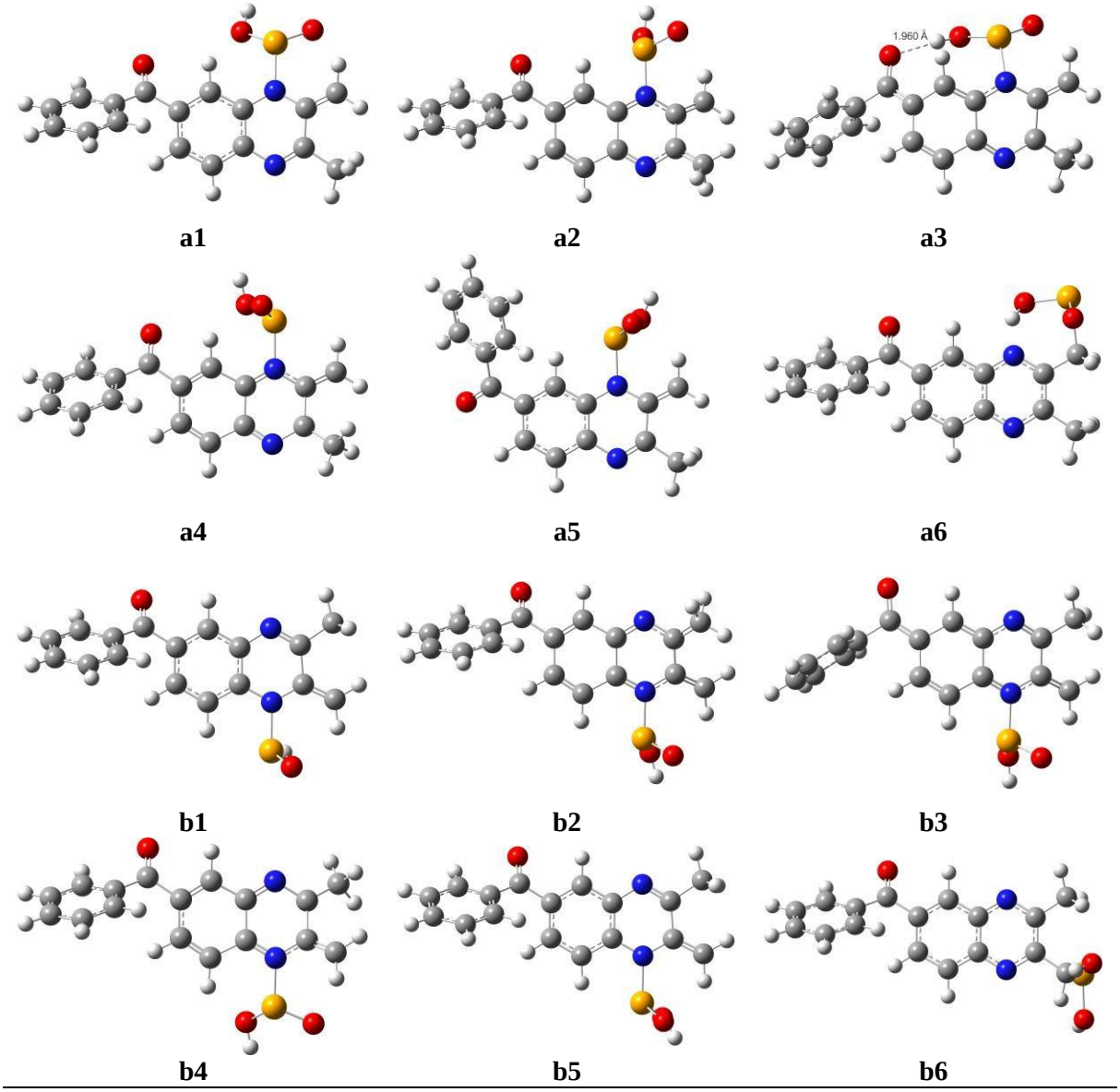
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-840.90586078 a.u
RMS Gradient Norm	0.00001100 a.u
Imaginary Freq	0
Dipole Moment	4.1587 Debye
Point Group	C1

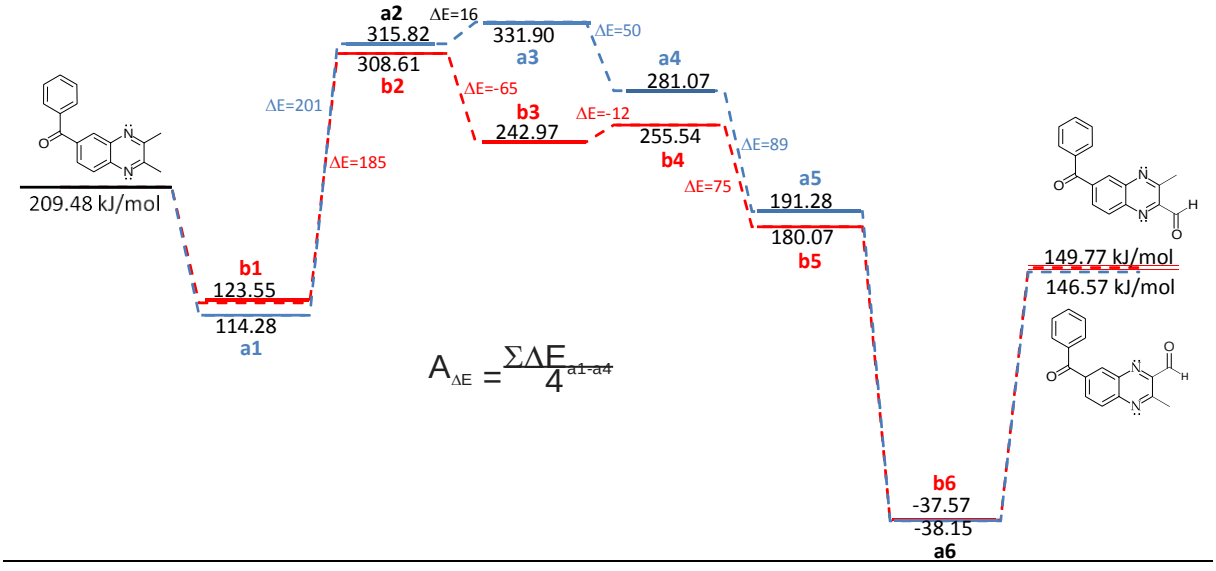


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.073697	2.339445	0.322935
2	6	0	1.431920	2.283770	0.460037
3	6	0	2.117904	1.071477	0.213003
4	6	0	1.389283	-0.072913	-0.171254
5	6	0	-0.016253	0.000332	-0.288817
6	6	0	-0.667508	1.185517	-0.041589
7	1	0	-0.465369	3.264989	0.485330
8	1	0	2.013368	3.151403	0.748745
9	1	0	-0.546161	-0.893302	-0.596747
10	6	0	3.319272	-1.284066	-0.299428
11	6	0	4.065271	-0.113335	0.095296
12	6	0	4.025054	-2.579722	-0.573682
13	1	0	4.767423	-2.465162	-1.369110
14	1	0	4.556500	-2.933045	0.315209
15	1	0	3.295864	-3.330817	-0.873067
16	6	0	5.558280	-0.174094	0.231659
17	1	0	5.856444	-0.923008	0.971346
18	1	0	6.027664	-0.452683	-0.716631
19	1	0	5.932897	0.800450	0.540759
20	7	0	2.020631	-1.252636	-0.426450
21	7	0	3.472573	1.023636	0.342012
22	6	0	-2.146319	1.337852	-0.232786
23	8	0	-2.604366	2.412213	-0.561189
24	6	0	-3.051011	0.162271	-0.026593
25	6	0	-2.789922	-0.829484	0.920185
26	6	0	-4.231653	0.109004	-0.769719
27	6	0	-3.697793	-1.863150	1.116026
28	1	0	-1.887057	-0.783984	1.518216
29	6	0	-5.126090	-0.934264	-0.587682
30	1	0	-4.433326	0.896457	-1.486376
31	6	0	-4.860703	-1.920980	0.357514
32	1	0	-3.496119	-2.622840	1.862472
33	1	0	-6.035439	-0.976883	-1.176259
34	1	0	-5.564763	-2.732243	0.506056

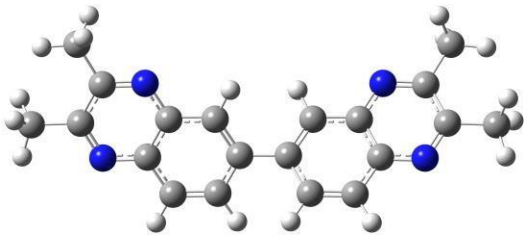
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO


1.960 Å
a1
a2
a3
a4
a5
a6
b1
b2
b3
b4
b5
b6


209.48 kJ/mol
b1
123.55
114.28
a1
ΔE=201
ΔE=185
a2
315.82
308.61
b2
ΔE=16
331.90
a3
ΔE=-65
b3
242.97
ΔE=50
a4
281.07
ΔE=-12
255.54
b4
ΔE=89
ΔE=75
a5
191.28
180.07
b5
b6
-37.57
-38.15
a6
149.77 kJ/mol
146.57 kJ/mol
$A_{\Delta E} = \frac{\Sigma \Delta E}{4}$ a1-a4

***2,2',3,3'*-Tetramethyl-*6,6'*-biquinoxaline (11)**.

Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-991.91299620 a.u
RMS Gradient Norm	0.00003795 a.u
Imaginary Freq	2
Dipole Moment	0.9521 Debye
Point Group	C1

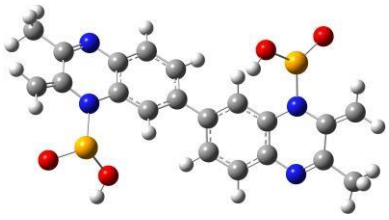


Standard orientation:

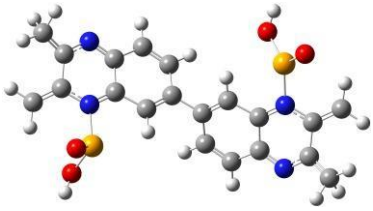
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.401378	-1.986717	-0.590949
2	6	0	-2.760150	-2.014894	-0.739513
3	6	0	-3.534940	-0.892300	-0.367547
4	6	0	-1.483312	0.255039	0.294437
5	6	0	-0.738444	-0.841489	-0.070687
6	1	0	-0.810154	-2.843260	-0.896222
7	1	0	-3.271061	-2.879341	-1.147027
8	1	0	-1.019229	1.138434	0.718149
9	6	0	-4.905725	1.299363	0.384364
10	6	0	-5.564589	0.136345	-0.153739
11	6	0	0.738415	-0.841589	0.069246
12	6	0	1.483549	0.254570	-0.296446
13	6	0	1.401025	-1.986542	0.590520
14	6	0	2.888863	0.248219	-0.153787
15	1	0	1.019717	1.137732	-0.720919
16	6	0	2.759723	-2.014729	0.739723
17	1	0	0.809587	-2.842801	0.896174
18	6	0	3.534755	-0.892402	0.367473
19	1	0	3.270371	-2.878915	1.148121
20	6	0	4.906062	1.298726	-0.385071
21	6	0	5.564519	0.136230	0.154693
22	6	0	-5.669162	2.524955	0.810286
23	1	0	-5.484563	2.719861	1.869257
24	1	0	-5.308559	3.392440	0.252892
25	1	0	-6.743150	2.434289	0.655989
26	6	0	-7.057628	0.087483	-0.321719
27	1	0	-7.569359	0.217158	0.636291
28	1	0	-7.407900	0.877574	-0.992231
29	1	0	-7.333890	-0.878489	-0.741638
30	6	0	5.669656	2.524618	-0.809877
31	1	0	5.472758	2.729501	-1.864661
32	1	0	5.320096	3.388890	-0.240413
33	1	0	6.745014	2.428001	-0.669413
34	6	0	7.057327	0.087883	0.324872
35	1	0	7.570331	0.214303	-0.632898
36	1	0	7.406762	0.880202	0.993177

37	1	0	7.332982	-0.876729	0.748300
38	7	0	3.607700	1.339488	-0.529155
39	7	0	4.885383	-0.921835	0.515050
40	7	0	-3.607249	1.340306	0.527347
41	7	0	-4.885689	-0.921903	-0.514011
42	6	0	-2.888692	0.248691	0.152464

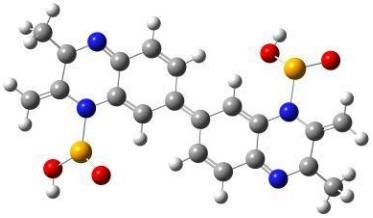
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



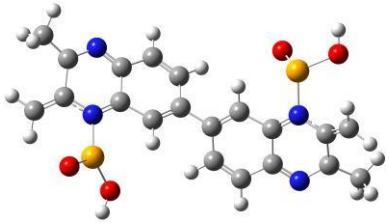
a1



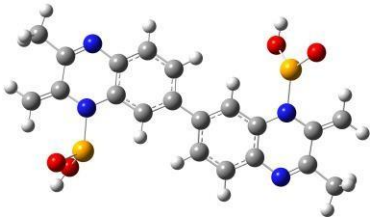
a2



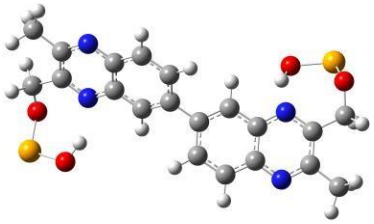
a3



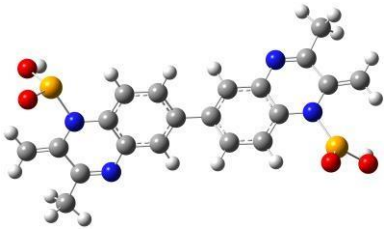
a4



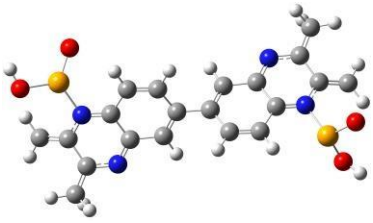
a5



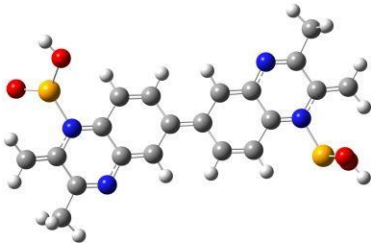
a6



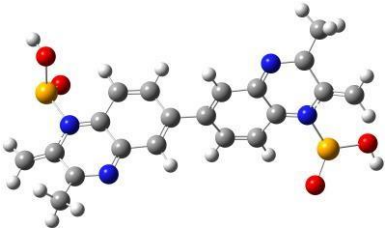
b1



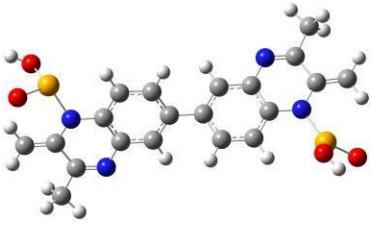
b2



b3

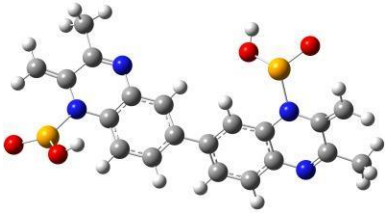


b4

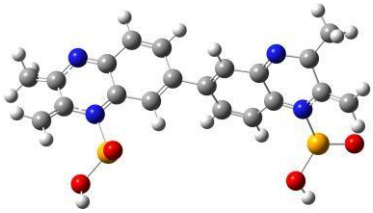


b5

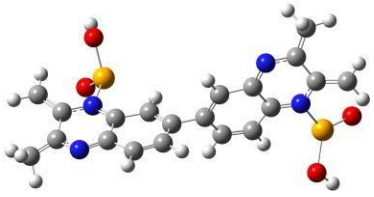
b6



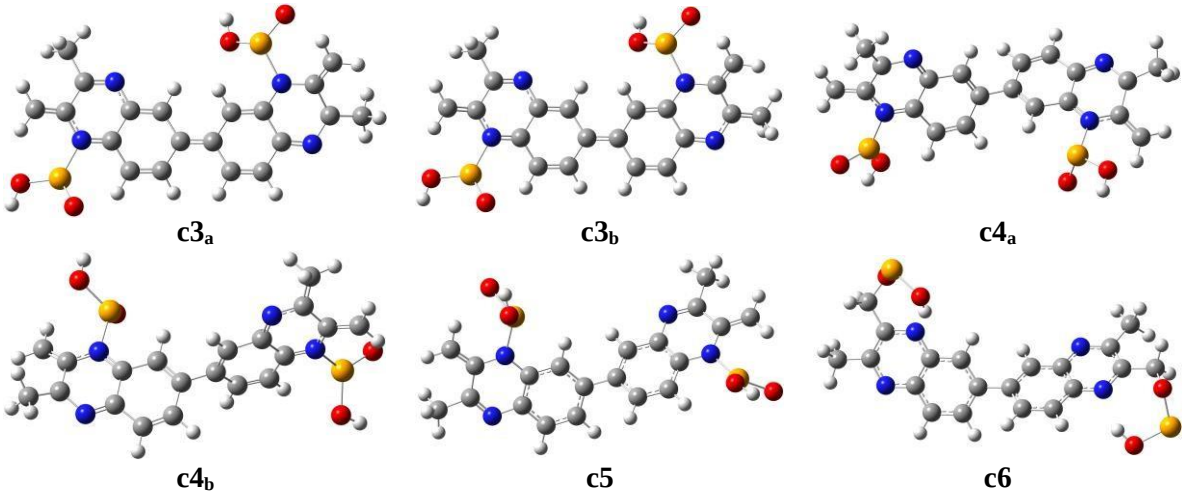
c1

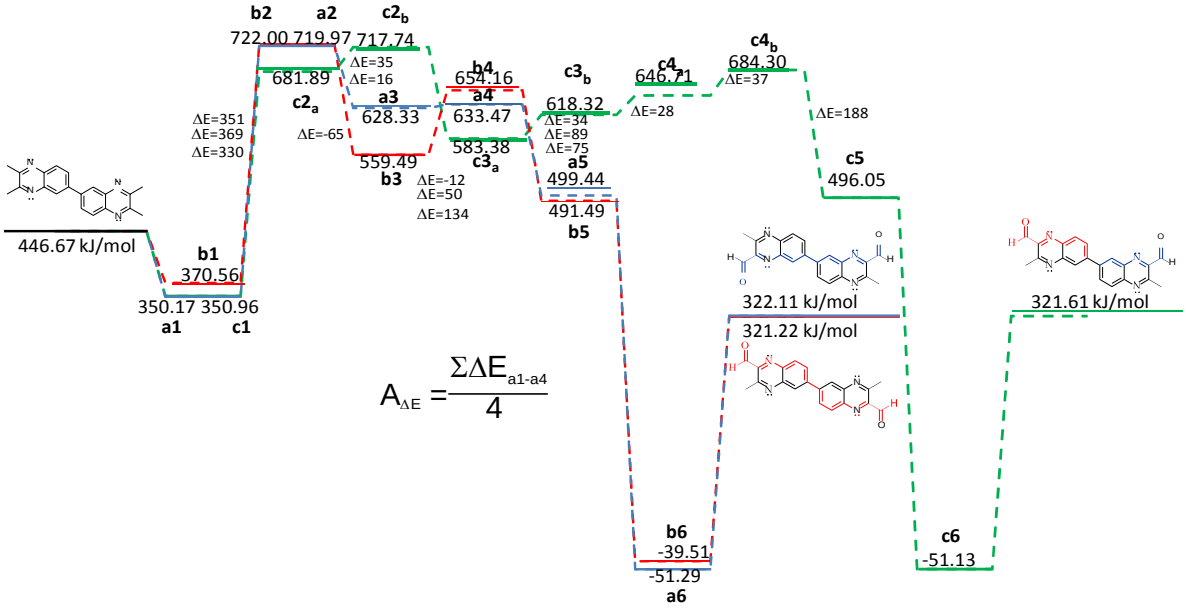


$c2_a$



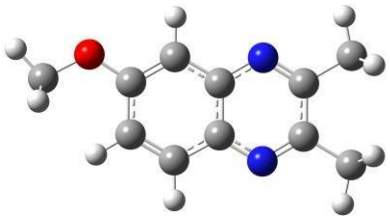
$c2_b$


c3a
c3b
c4a
c4b
c5
c6


446.67 kJ/mol
a1
350.17
b1
370.56
c1
350.96
ΔE=351
ΔE=369
ΔE=330
b2
722.00
a2
719.97
c2b
717.74
ΔE=35
ΔE=16
681.89
c2a
ΔE=-65
a3
628.33
559.49
b3
ΔE=-12
ΔE=50
ΔE=134
b4
654.16
a4
633.47
583.38
c3a
c3b
618.32
ΔE=34
ΔE=89
ΔE=75
a5
499.44
491.49
b5
c4a
646.71
ΔE=28
c4b
684.30
ΔE=37
ΔE=188
c5
496.05
322.11 kJ/mol
321.22 kJ/mol
b6
-39.51
-51.29
a6
c6
-51.13
321.61 kJ/mol
$A_{\Delta E} = \frac{\Sigma \Delta E_{a1\text{-}a4}}{4}$

2,3-Dimethyl-6-methoxyquinoxaline (12).

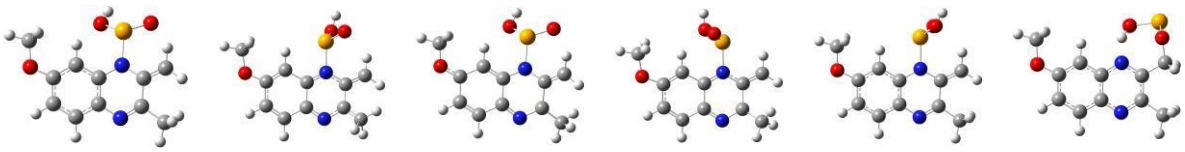
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-611.07313689 a.u
RMS Gradient Norm	0.00001243 a.u
Imaginary Freq	0
Dipole Moment	1.1334 Debye
Point Group	C1



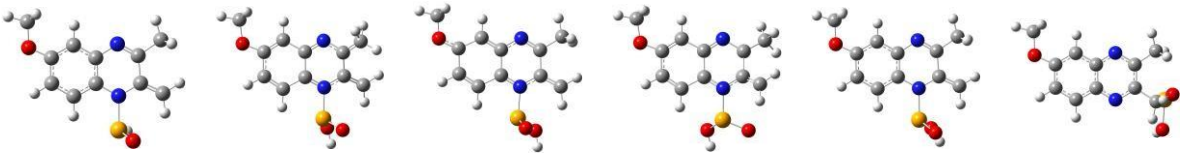
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.341429	-0.275585	-0.000443
2	1	0	-1.357860	-2.176158	-0.002059
3	6	0	-1.238496	-1.100089	-0.001480
4	6	0	-0.923453	1.681653	0.000468
5	6	0	0.052471	-0.545019	-0.001258
6	6	0	-2.180061	1.131884	0.000354
7	6	0	0.219778	0.858542	-0.000226
8	7	0	1.139916	-1.370783	-0.001772
9	1	0	-3.042493	1.785360	0.001052
10	1	0	-0.781770	2.756107	0.001156
11	6	0	2.321001	-0.816664	-0.000914
12	6	0	2.488641	0.616972	0.000018
13	7	0	1.460334	1.419925	0.000373
14	6	0	3.861852	1.224702	-0.000587
15	1	0	4.424315	0.929327	-0.891694
16	1	0	4.440055	0.898801	0.869338
17	1	0	3.773307	2.310014	0.018309
18	6	0	3.521526	-1.718652	0.002359
19	1	0	4.162878	-1.524973	-0.862554
20	1	0	4.129533	-1.557453	0.897832
21	1	0	3.192999	-2.756593	-0.021835
22	8	0	-3.551938	-0.886217	-0.000307
23	6	0	-4.718441	-0.091705	0.001301
24	1	0	-4.777923	0.538398	-0.893173
25	1	0	-5.553265	-0.790319	0.001452
26	1	0	-4.776357	0.536991	0.896880

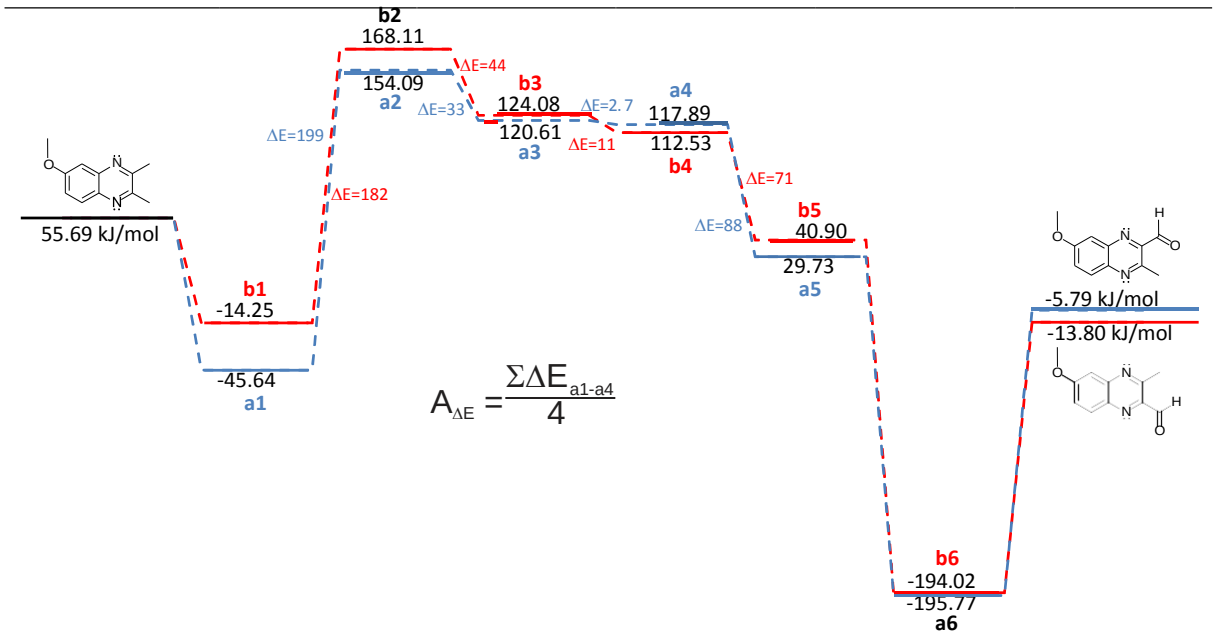
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**

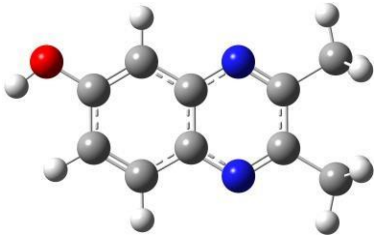


b1 **b2** **b3** **b4** **b5** **b6**



6-Hydroxy-2,3-dimethylquinoxaline (13).

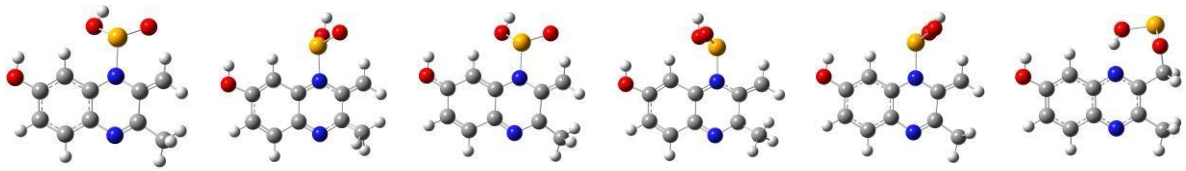
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-571.77845033 a.u
RMS Gradient Norm	0.00001115 a.u
Imaginary Freq	0
Dipole Moment	1.4121 Debye
Point Group	C1



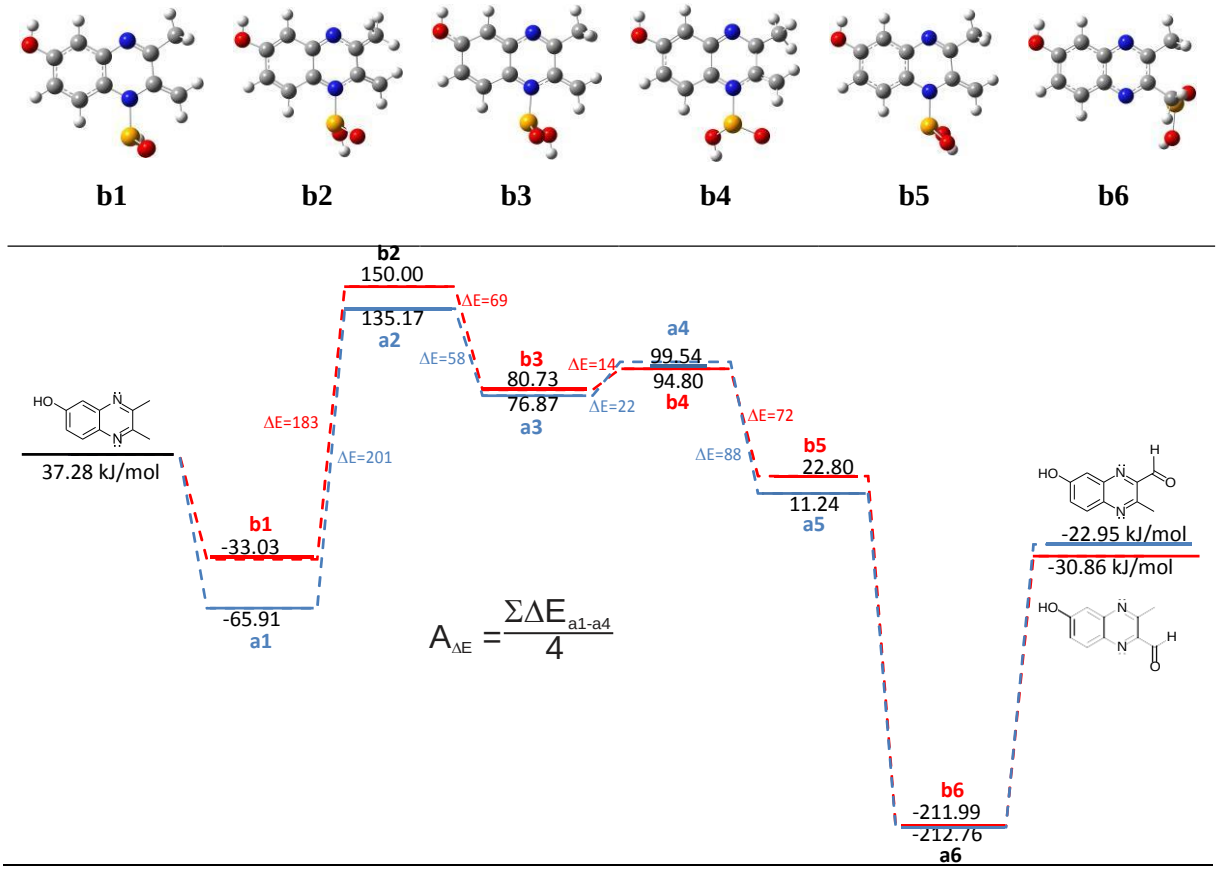
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.757641	-0.296872	-0.000099
2	1	0	-1.769637	-2.195564	-0.000044
3	6	0	-1.658913	-1.118709	-0.000037
4	6	0	-1.358002	1.673482	0.000002
5	6	0	-0.368614	-0.551956	0.000011
6	6	0	-2.605249	1.111153	-0.000006
7	6	0	-0.209339	0.851935	-0.000016
8	7	0	0.722211	-1.370045	0.000016
9	1	0	-3.487933	1.744601	0.000071
10	1	0	-1.221407	2.748404	0.000040
11	6	0	1.901514	-0.809331	0.000054
12	6	0	2.060787	0.623347	0.000060
13	7	0	1.026387	1.420152	0.000033
14	6	0	3.429731	1.240275	-0.000037
15	1	0	4.001823	0.933757	-0.881069
16	1	0	4.002409	0.932840	0.880285
17	1	0	3.334081	2.325138	0.000540
18	6	0	3.106176	-1.705473	-0.000020
19	1	0	3.730371	-1.524324	-0.880218
20	1	0	3.729777	-1.525152	0.880773
21	1	0	2.782702	-2.745255	-0.000591
22	8	0	-3.989820	-0.870079	0.000070
23	1	0	-4.666508	-0.191673	-0.000158

Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO

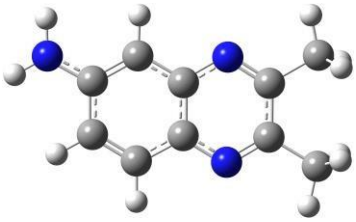


a1 **a2** **a3** **a4** **a5** **a6**


b1
b2
b3
b4
b5
b6
b2
150.00
ΔE=69
135.17
a2
ΔE=58
b3
80.73
76.87
a3
ΔE=14
ΔE=22
a4
99.54
94.80
b4
ΔE=72
b5
22.80
11.24
a5
ΔE=88
ΔE=183
ΔE=201
37.28 kJ/mol
b1
-33.03
-65.91
a1
b6
-211.99
-212.76
a6
-22.95 kJ/mol
-30.86 kJ/mol
$A_{\Delta E} = \frac{\Sigma \Delta E_{a1-a4}}{4}$

6-Amino-2,3-dimethylquinoxaline (14).

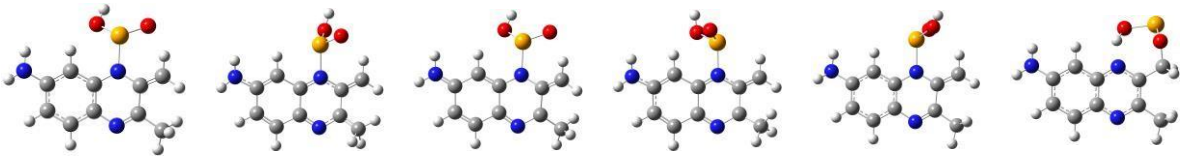
Calculation Type	OPT + FREQ
Calculation Method	RωB97XD
Basis Set	6-311++G(d,p)
Charge	0
Spin	Singlet
E(RωB97XD)	-551.91373315 a.u
RMS Gradient Norm	0.00003059 a.u
Imaginary Freq	1
Dipole Moment	1.5761 Debye
Point Group	CS



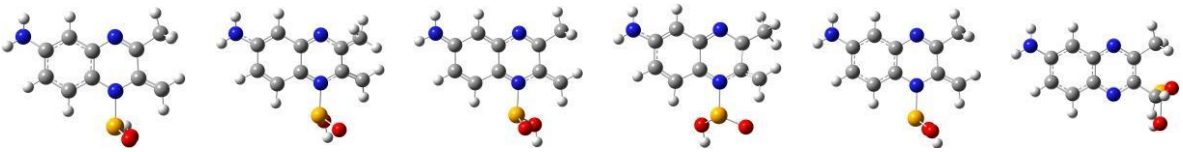
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.143062	1.774001	0.000000
2	1	0	-0.238830	2.783798	0.000000
3	6	0	-0.764103	1.835065	0.000000
4	6	0	-2.053268	-0.653530	0.000000
5	6	0	0.000000	0.651882	0.000000
6	6	0	-2.781883	0.500316	0.000000
7	6	0	-0.639099	-0.608545	0.000000
8	7	0	1.360518	0.731756	0.000000
9	1	0	-3.866626	0.456270	0.000000
10	1	0	-2.535487	-1.624158	0.000000
11	6	0	2.035284	-0.388530	0.000000
12	6	0	1.381030	-1.668523	0.000000
13	7	0	0.076371	-1.761503	0.000000
14	7	0	-2.917678	2.909317	0.000000
15	6	0	2.182004	-2.939328	0.000000
16	1	0	2.828834	-3.001074	0.880685
17	1	0	2.828834	-3.001074	-0.880685
18	1	0	1.502554	-3.790693	0.000000
19	6	0	3.534765	-0.303052	0.000000
20	1	0	3.957441	-0.796900	0.880327
21	1	0	3.957441	-0.796900	-0.880327
22	1	0	3.836257	0.743429	0.000000
23	1	0	-2.496698	3.819263	0.000000
24	1	0	-3.918210	2.852509	0.000000

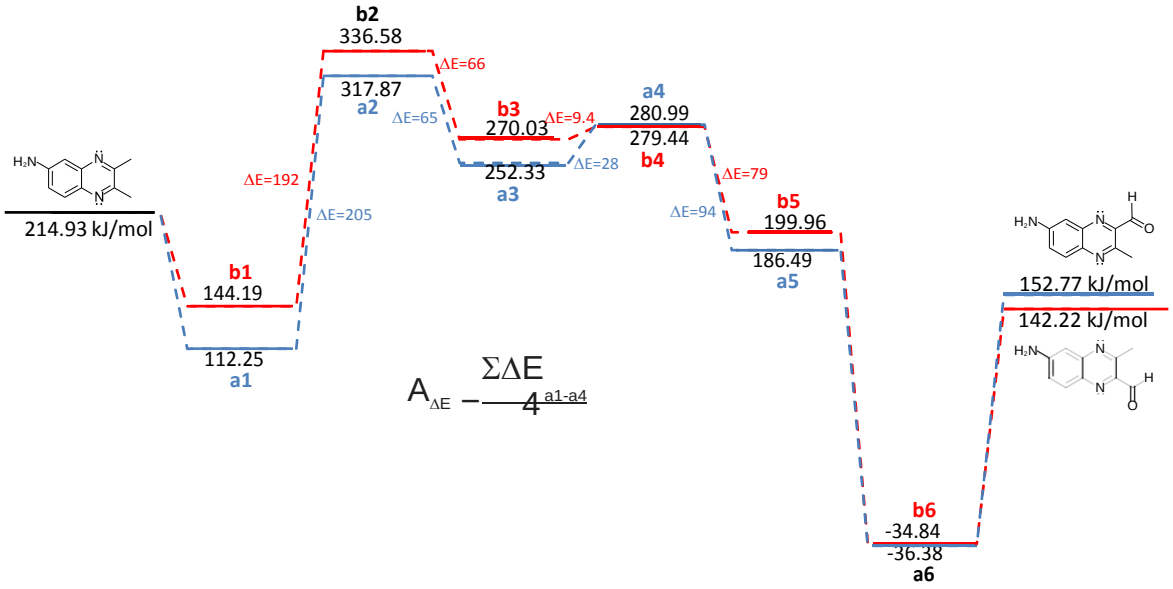
Calculation Type	SP
Calculation Method	RPM6
Basis Set	ZDO



a1 **a2** **a3** **a4** **a5** **a6**



b1 **b2** **b3** **b4** **b5** **b6**



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