**Supporting Information for**

Structure-reactivity relationships on Michael-type additions of secondary cyclic amines with 3-cyanomethylidene-2-oxindoline derivatives

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**1. UV-Visible spectra and kinetic results**

**1.1. Reactions of piperidine with 3-cyanomethylidene-2-oxindoline derivatives (3a-e)**

* *2-(2-Oxindolin-3-ylidene)malononitrile (****3a****):*



**Figure S1.** UV–Vis absorption spectra and kinetic relaxation processes of the formation of adduct (**5a**) (max = 375; 434 nm) from the reaction of 2-(2-oxindolin-3-ylidene)malononitrile(**3a**) ( = 338 nm) with piperidine (**4a**) (c = 1 x10-2 mol dm-3) (cycle time = 100 s x 50) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-2** | **2.0 x10-2** |
| **3.0 x10-2** | **4.0 x10-2** |
| **5.0 x10-2** | **6.0 x10-2** |

**Figure S2.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 338 nm during the reaction of 2-(2-oxindolin-3-ylidene)malononitrile(**3a**)with piperidine (**4a**) (1.0x10-2 < [piperidine] < 6.0x10-2 mol dm-3) at *T* = 20 °C in MeCN.

**Table S1.** Kinetic results for reaction of piperidine (**4a**) with 2-(2-oxindolin-3-ylidene)malononitrile(**3a**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[piperidine] /mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-2 | 2.13x10-4 | **3.22x10-2** |
| 2.0x10-2 | 3.43x10-4 |
| 3.0x10-2 | 6.78x10-4 |
| 4.0x10-2 | 9.68x10-4 |
| 5.0x10-2 | 1.44x10-3 |
| 6.0x10-2 | 1.90x10-3 |

* *2-(1-Ethyl-2-oxindolin-3-ylidene)malononitrile (****3b****):*



**Figure S3.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**5b**) (max = 382; 433 nm) from the reaction of 2-(1-ethyl-2-oxindolin-3-ylidene)malononitrile (**3b**) ( = 345; 540 nm) with piperidine (**4a**) (c = 3 x10-2 mol dm-3) (cycle time = 100 s x 70) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-2** | **2.0 x10-2** |
| **3.0 x10-2** | **4.0 x10-2** |
| **6.0 x10-2** | **8.0 x10-2** |

**Figure S4.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 345 nm during the reaction of 2-(1-Ethyl-2-oxindolin-3-ylidene)malononitrile (**3b**) with piperidine (**4a**) (1.0x10-2 < [piperidine] < 8.0x10-2 mol dm-3) at T = 20 °C in MeCN.

**Table S2.** Kinetic results for reaction of piperidine (**4a**) with 2-(1-ethyl-2-oxindolin-3-ylidene)malononitrile (**3b**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[piperidine] /mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-2 | 2.59x10-4 | **2.72x10-2** |
| 2.0x10-2 | 5.71x10-4 |
| 3.0x10-2 | 8.42x10-4 |
| 4.0x10-2 | 1.13x10-3 |
| 6.0x10-2 | 1.70x10-3 |
| 8.0x10-2 | 2.15x10-3 |

* *2-(5-Chloro-2-oxindolin-3-ylidene)malononitrile (****3c****):*



**Figure S5.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**5c**) (max = 379; 432 nm) from the reaction of 2-(5-chloro-2-oxindolin-3-ylidene)malononitrile(**3c**) ( = 342 nm) with piperidine (**4a**) (c = 4 x10-2 mol dm-3) (cycle time = 100 s x 60) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-3** | **2.0 x10-3** |
| **3.0 x10-3** | **5.0 x10-3** |
| **6.0 x10-3** | **8.0 x10-3** |

**Figure S6.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 342 nm during the reaction of 2-(5-chloro-2-oxindolin-3-ylidene)malononitrile(**3c**)with piperidine (**4a**) (1.0x10-3 < [piperidine] < 8.0x10-3 mol dm-3) at *T* = 20 °C in MeCN.

**Table S3.** Kinetic results for reaction of piperidine (**4a**) with 2-(5-chloro-2-oxindolin-3-ylidene)malononitrile(**3c**) in acetonitrile at 20 °C

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[piperidine]**  **/mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-3 | 4.12x10-4 | **7.85x10-1** |
| 2.0x10-3 | 1.10x10-3 |
| 3.0x10-3 | 2.04x10-3 |
| 5.0x10-3 | 3.96x10-3 |
| 6.0x10-3 | 4.72x10-3 |
| 8.0x10-3 | 6.16x10-3 |

* *2-(5-Chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile (****3d****):*



**Figure S7.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**5d**) (max = 382; 436 nm) from the reaction of 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) ( = 338; 550 nm) with piperidine (**4a**) (c = 1x10-3 mol dm-3) (cycle time = 100s x 75) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-3** | **2.0 x10-3** |
| **3.0 x10-3** | **5.0 x10-3** |
| **8.0 x10-3** |  |

**Figure S8.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 338 nm during the reaction of 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) with piperidine (**4a**) (1.0x10-3 < [piperidine] < 8.0x10-3 mol dm-3) at *T* = 20 °C in MeCN.

**Table S4.** Kinetic results for reaction of piperidine (**4a**) with 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[piperidine]**  **/mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-3 | 4.90x10-4 | **5.16x10-1** |
| 2.0x10-3 | 9.24x10-4 |
| 3.0x10-3 | 1.37x10-3 |
| 5.0x10-3 | 2.30x10-3 |
| 8.0x10-3 | 4.12x10-3 |

* *Ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate (****3e****):*



**Figure S9.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**5e**) (max = 381 nm) from the reaction of ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate(**3e**) ( = 335 nm) with piperidine (**4a**) (c = 1x10-1 mol dm-3) (cycle time = 100s x 80) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **2.0 x10-2** | **4.0 x10-2** |
| **5.0 x10-2** | **6.0 x10-2** |
| **7.0 x10-2** | **8.0 x10-2** |

**Figure S10.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 335 nm during the reaction of ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate(**3e**) with piperidine (**4a**) (2.0x10-2 < [piperidine] < 8.0x10-2 mol dm-3) at *T* = 20 °C in MeCN.

**Table S5.** Kinetic results for reaction of piperidine (**4a**) with ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate(**3e**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[piperidine]**  **/mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 2.0x10-2 | 3.93x10-4 | **1.12x10-2** |
| 4.0x10-2 | 5.75x10-4 |
| 5.0x10-2 | 6.50x10-4 |
| 6.0x10-2 | 7.41x10-4 |
| 7.0x10-2 | 8.70x10-4 |
| 8.0x10-2 | 9.36x10-4 |

**1.2. Reactions of morpholine with 3-cyanomethylidene-2-oxindoline derivatives (3a-e)**

* *2-(5-Chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile (****3d****) :*



**Figure S11.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**6d**) (max = 382; 446 nm) from the reaction of 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) ( = 338 nm) with morpholine (**4b**) (c = 1x10-1 mol dm-3) (cycle time = 200s x 25) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-2** | **3.0 x10-2** |
| **4.0 x10-2** | **6.0 x10-2** |
| **8.0 x10-2** |  |

**Figure S12.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 338 nm during the reaction 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) with morpholine (**4b**) (1.0x10-2 < [morpholine] < 8.0x10-2 mol dm-3) at *T* = 20 °C in MeCN.

**Table S6.** Kinetic results for reaction of morpholine (**4b**) with 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[morpholine]**  **/mol dm-3** | ***kobsd***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-2 | 1.17x10-4 | **2.91x10-2** |
| 3.0x10-2 | 6.43x10-4 |
| 4.0x10-2 | 1.51x10-3 |
| 6.0x10-2 | 1.88x10-3 |
| 8.0x10-2 | 2.29x10-3 |

**1.3. Reactions of pyrolidine with 3-cyanomethylidene-2-oxindoline derivatives (3a-e)**

* *2-(5-Chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile (****3d****) :*



**Figure S13.** UV–vis absorption spectra and kinetic relaxation processes of the formation of adduct (**7d**) (max = 382; 446 nm) from the reaction of 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) ( = 338 nm) with pyrrolidine (**4c**) (c = 1x10-3 mol dm-3) (cycle time = 80s x 15) in MeCN at 20 °C.

|  |  |
| --- | --- |
| **1.0 x10-3** | **2.0 x10-3** |
| **4.0 x10-3** | **6.0 x10-3** |
| **8.0 x10-3** |  |

**Figure S14.** ln(A∞ - At) against time traces showing the processes pertaining to the exponential decay of the absorbance at 338 nm during the reaction 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) with pyrrolidine (**4c**)(1.0x10-3 < [pyrrolidine] < 8.0x10-3 mol dm-3) at *T* = 20 °C in MeCN.

**Table S7** Kinetic results for reaction of pyrrolidine (**4c**) with 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**) in acetonitrile at 20 °C.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[pyrrolidine]**  **/mol dm-3** | ***kobs***  **/s-1** | ***k1***  **/mol-1 dm3 s-1** |
| 1.0x10-3 | 6.99x10-3 | **3.06** |
| 2.0x10-3 | 1.01x10-2 |
| 4.0x10-3 | 1.55x10-2 |
| 6.0x10-3 | 1.97x10-2 |
| 8.0x10-3 | 2.53x10-2 |



**Figure S15.** Influence of the concentration of piperidine (**4a**)on the observed first-order rate constant (*k*obs) for addition to the 2-(1-ethyl-2-oxindolin-3-ylidene)malononitrile(**3b**)in acetonitrile solution at 20°C.



**Figure S16.** Influence of the concentration of piperidine (**4a**)on the observed first-order rate constant (*k*obs) for addition to the 2-(5-chloro-2-oxindolin-3-ylidene)malononitrile (**3c**)in acetonitrile solution at 20°C.



**Figure S17.** Influence of the concentration of piperidine (**4a**)on the observed first-order rate constant (*k*obs) for addition to the 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**)in acetonitrile solution at 20°C.



**Figure S18.** Influence of the concentration of piperidine (**4a**)on the observed first-order rate constant (*k*obs) for addition to the ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate (**3e**)in acetonitrile solution at 20°C.



**Figure S19.** Influence of the concentration of morpholine (**4b**)on the observed first-order rate constant (*k*obs) for addition to the 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**)in acetonitrile solution at 20°C.



**Figure S20.** Influence of the concentration of pyrolidine (**4c**)on the observed first-order rate constant (*k*obs) for addition to the 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile(**3d**)in acetonitrile solution at 20°C.

**2. Theoretical calculations**

Quantum chemical calculations were performed on several derivatives to gain a better insight of their electronic, thermodynamic and kinetic properties. The relevant points on the ground potential energy surface were located at the B3LYP/6-31G(d,p) level of theory. This functional has proved to give satisfactory results in predicting electronic and spectroscopic properties of various types of compounds (Jacquemin et al., 2009). All the calculations were performed with Gaussian03 package of programs (Frisch et al., 2003) (Table S8).

# Jacquemin, D., Wathelet, V., Perpete, E., Adamo, C., 2009. Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. J Chem Theory Comput. 5, 2420-2435.

M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian-03, Revision B.04, Gaussian, Inc., Pittsburgh PA, 2003.

**Table S8.** HOMO and LUMO frontier orbitals of 3-cyanomethylidene-2-oxindoline derivatives **(3a-e).**

|  |  |  |
| --- | --- | --- |
|  | **HOMO** | **LUMO** |
| C:\Users\EHD\Desktop\calcul DFT (sheima)\N-H Di-CN isatin.jpg**(3a)** | C:\Users\EHD\Desktop\calcul DFT (sheima)\HOMO N-H Di-CN isatin.jpg | C:\Users\EHD\Desktop\calcul DFT (sheima)\LUMO N-H Di-CN isatin.jpg |
| C:\Users\EHD\Desktop\calcul DFT (sheima)\N-Ethyl Di-CN isatin.jpg**(3b)** | C:\Users\EHD\Desktop\calcul DFT (sheima)\HOMO N-Ethyl Di-CN isatin.jpg | C:\Users\EHD\Desktop\calcul DFT (sheima)\LUMO N-Ethyl Di-CN isatin.jpg |
| C:\Users\EHD\Desktop\calcul DFT (sheima)\5-Cl N-H Di-CN isatin.jpg**(3c)** | C:\Users\EHD\Desktop\calcul DFT (sheima)\HOMO 5-Cl N-H Di-CN isatin.jpg | C:\Users\EHD\Desktop\calcul DFT (sheima)\LUMO 5-Cl N-H Di-CN isatin.jpg |
| C:\Users\EHD\Desktop\calcul DFT (sheima)\5-Cl N-Me Di-CN isatin.jpg**(3d)** | C:\Users\EHD\Desktop\calcul DFT (sheima)\HOMO 5-Cl N-Me Di-CN isatin.jpg | C:\Users\EHD\Desktop\calcul DFT (sheima)\LUMO 5-Cl N-Me Di-CN isatin.jpg |
| C:\Users\EHD\Desktop\calcul DFT (sheima)\5-Cl N-Me CN-CO2Et isatin.jpg**(3e)** | C:\Users\EHD\Desktop\calcul DFT (sheima)\HOMO 5-Cl N-Me CN-CO2Et isatin.jpg | C:\Users\EHD\Desktop\calcul DFT (sheima)\LUMO 5-Cl N-Me CN-CO2Et isatin.jpg |

* *2-(2-Oxindolin-3-ylidene)malononitrile (****3a****):*

6 2.845371 1.535520 -0.000007

6 3.599056 0.356283 0.000012

6 2.988421 -0.903345 0.000021

6 1.602110 -0.944990 -0.000001

6 0.817689 0.237497 -0.000020

6 1.451459 1.486652 -0.000020

7 0.764064 -2.059955 0.000013

6 -0.573157 -1.699199 -0.000070

6 -0.572238 -0.176284 -0.000015

8 -1.526003 -2.449247 -0.000024

6 -1.730231 0.548672 0.000006

6 -3.039185 -0.034821 0.000005

7 -4.144189 -0.398407 0.000044

6 -1.708750 1.980429 0.000023

7 -1.679608 3.143973 0.000024

1 3.348188 2.496461 -0.000008

1 4.683207 0.414843 0.000026

1 3.580441 -1.812583 0.000041

1 0.871730 2.401886 -0.000028

1 1.059339 -3.024394 0.000003

* *2-(1-Ethyl-2-oxindolin-3-ylidene)malononitrile (****3b****):*

6 1.224386 3.126770 0.035947

6 2.467230 2.498661 -0.094802

6 2.579052 1.106689 -0.201400

6 1.408575 0.360070 -0.174434

6 0.137744 0.980098 -0.044446

6 0.050503 2.372918 0.061723

7 1.261450 -1.027224 -0.273903

6 -0.077455 -1.381421 -0.205873

6 -0.848833 -0.080449 -0.058888

8 -0.523260 -2.511465 -0.258119

6 -2.211628 -0.049389 0.031100

6 -3.042793 -1.216600 -0.002312

7 -3.811393 -2.089698 -0.017731

6 -2.917910 1.188648 0.169108

7 -3.482130 2.200488 0.281188

1 1.170861 4.206902 0.117844

1 3.370748 3.100646 -0.113507

1 3.549753 0.634385 -0.301090

1 -0.911284 2.861574 0.161774

6 2.333482 -2.010129 -0.392923

6 3.018871 -2.318378 0.940551

1 3.053579 -1.641668 -1.131578

1 1.869604 -2.911177 -0.800632

1 3.815549 -3.053015 0.788981

1 3.462852 -1.421704 1.382957

1 2.301592 -2.734095 1.653205

* *2-(5-Chloro-2-oxindolin-3-ylidene)malononitrile (****3c****):*

6 -2.573239 0.121016 -0.000129

6 -2.832833 -1.253484 0.000092

6 -1.783820 -2.177779 0.000179

6 -0.485140 -1.690058 -0.000075

6 -0.214712 -0.298161 -0.000281

6 -1.271407 0.619449 -0.000274

7 0.714565 -2.399350 0.000033

6 1.812422 -1.553626 -0.000834

6 1.229292 -0.147221 -0.000153

8 2.979390 -1.881274 0.000132

6 2.019785 0.965876 0.000134

6 3.452466 0.927430 0.000053

7 4.612427 1.013919 -0.000017

6 1.451221 2.280136 0.000441

7 0.977535 3.343147 0.000702

1 -3.859605 -1.601360 0.000255

1 -1.989490 -3.242763 0.000409

1 -1.096061 1.687706 -0.000340

1 0.810780 -3.403403 0.000553

17 -3.920979 1.243796 -0.000110

* *2-(5-Chloro-1-methyl-2-oxindolin-3-ylidene)malononitrile (****3d****) :*

6 -2.650556 -0.177851 -0.000132

6 -2.801318 1.211868 -0.000162

6 -1.682405 2.051784 -0.000230

6 -0.424840 1.464308 -0.000325

6 -0.267078 0.054699 -0.000288

6 -1.390794 -0.777127 -0.000167

7 0.822128 2.091259 -0.000381

6 1.843283 1.151676 -0.000627

6 1.160088 -0.205391 -0.000139

8 3.035164 1.386785 0.000231

6 1.864470 -1.374680 0.000109

6 3.296030 -1.445491 0.000121

7 4.445816 -1.621516 0.000184

6 1.197867 -2.642175 0.000310

7 0.645267 -3.666376 0.000440

1 -3.797821 1.639024 -0.000102

1 -1.806351 3.128697 -0.000233

1 -1.299912 -1.855929 -0.000075

17 -4.081645 -1.192850 0.000029

6 1.058863 3.521919 0.000542

1 0.628809 3.988676 -0.891544

1 0.628913 3.987537 0.893278

1 2.138875 3.671362 0.000553

* *Ethyl 2-(5-chloro-1-methyl-2-oxindolin-3-ylidene)-2-cyanoacetate (****3e****):*

6 -2.735962 -1.334059 0.010491

6 -3.612609 -0.312790 0.381858

6 -3.156032 1.004470 0.493402

6 -1.815629 1.256660 0.234458

6 -0.918119 0.222161 -0.132303

6 -1.388973 -1.087292 -0.259390

7 -1.151918 2.484037 0.279141

6 0.185974 2.329809 -0.048181

6 0.391089 0.845166 -0.308574

6 -1.749954 3.764965 0.597524

8 1.014447 3.218848 -0.098124

6 1.626045 0.341471 -0.574081

17 -3.348984 -2.974674 -0.134333

6 1.863692 -1.134274 -0.844386

8 1.226043 -1.723568 -1.686635

8 2.811514 -1.773326 -0.145386

6 3.953070 -2.363334 1.868371

6 3.479693 -1.203548 1.013366

6 2.785973 1.168434 -0.703958

7 3.815505 1.696067 -0.840704

1 -4.653738 -0.544720 0.575942

1 -3.838013 1.799332 0.773519

1 -0.740783 -1.890711 -0.581424

1 -2.542156 4.014415 -0.116270

1 -0.960589 4.514766 0.536934

1 -2.168266 3.759426 1.609568

1 4.487547 -1.979540 2.742665

1 3.109073 -2.966987 2.212458

1 4.632203 -3.006710 1.303133

1 2.782202 -0.562759 1.562073

1 4.314569 -0.590447 0.665592