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Ionization potentials of fluoroindoles and the origin of nonexponential tryptophan fluorescence decay in proteins

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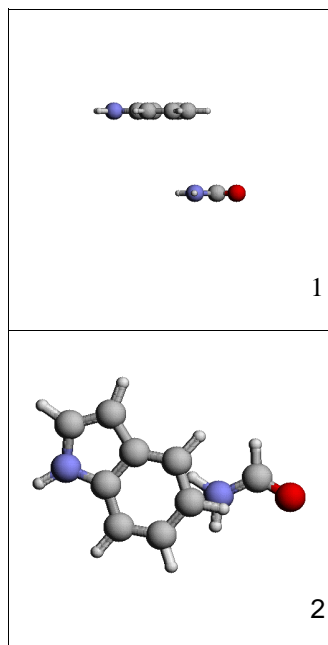
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Supporting Information for Table 2 of**Liu et al, Ionization Potentials of Fluoroindoles and the Origin of Non-Exponential Tryptophan Fluorescence Decay in Proteins**

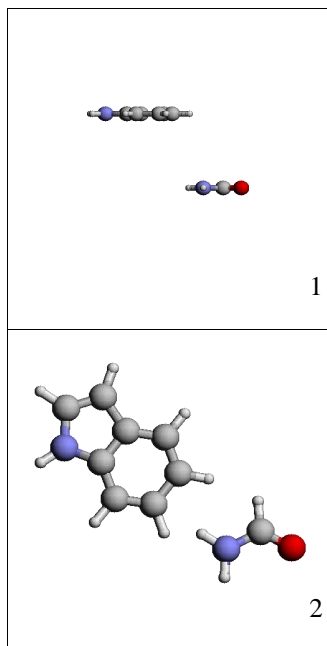
Cartesian coordinates of indole-formamide (1) and its side and top view.

N	-1.89743	0.00000	0.04940
C	-1.89743	0.00000	1.43914
C	-0.62697	0.00000	1.89071
C	0.23802	0.00000	0.73327
C	1.62202	0.00000	0.56427
C	2.13934	0.00000	-0.70795
C	1.29637	0.00000	-1.82653
C	-0.07061	0.00000	-1.68468
C	-0.59267	0.00000	-0.39727
H	-2.71071	0.00000	-0.52195
H	-2.81202	0.00000	1.98225
H	-0.32191	0.00000	2.91065
H	2.26722	0.00000	1.41988
H	3.20186	0.00000	-0.84644
H	1.71814	0.00000	-2.81076
H	-0.70879	0.00000	-2.54534
O	4.80079	4.50000	-0.48600
C	3.70629	4.50000	0.03448
H	3.57522	4.50000	1.11007
N	2.52334	4.50000	-0.61832
H	1.65734	4.50000	-0.12857
H	2.50989	4.50000	-1.61592



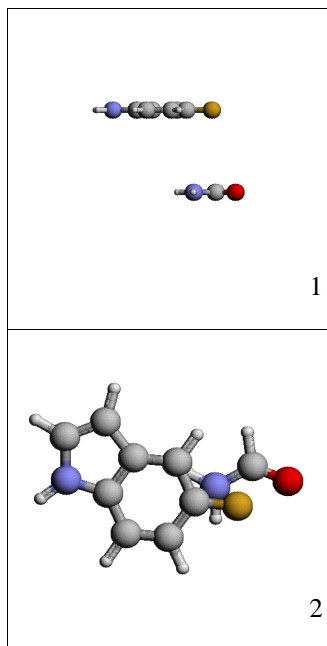
Cartesian coordinates of indole-formamide (2) its side and top view.

N	-1.89743	0.00000	0.04940
C	-1.89743	0.00000	1.43914
C	-0.62697	0.00000	1.89071
C	0.23802	0.00000	0.73327
C	1.62202	0.00000	0.56427
C	2.13934	0.00000	-0.70795
C	1.29637	0.00000	-1.82653
C	-0.07061	0.00000	-1.68468
C	-0.59267	0.00000	-0.39727
H	-2.71071	0.00000	-0.52195
H	-2.81202	0.00000	1.98225
H	-0.32191	0.00000	2.91065
H	2.26722	0.00000	1.41988
H	3.20186	0.00000	-0.84644
H	1.71814	0.00000	-2.81076
H	-0.70879	0.00000	-2.54534
O	6.30079	4.50000	-2.98600
C	5.20629	4.50000	-2.46552
H	5.07522	4.50000	-1.38993
N	4.02334	4.50000	-3.11832
H	3.15734	4.50000	-2.62857
H	4.00989	4.50000	-4.11592



Cartesian coordinates of 5- and 6-fluoroindole-formamide (1) its side and top view.

N	-1.89743	0.00000	0.04940
C	-1.89743	0.00000	1.43914
C	-0.62697	0.00000	1.89071
C	0.23802	0.00000	0.73327
C	1.62202	0.00000	0.56427
C	2.13934	0.00000	-0.70795
C	1.29637	0.00000	-1.82653
C	-0.07061	0.00000	-1.68468
C	-0.59267	0.00000	-0.39727
H	-2.71071	0.00000	-0.52195
H	-2.81202	0.00000	1.98225
H	-0.32191	0.00000	2.91065
H	2.26722	0.00000	1.41988
F	3.49289	0.00000	-0.88437
H	1.71814	0.00000	-2.81076
H	-0.70879	0.00000	-2.54534
O	4.80079	4.50000	-0.48600
C	3.70629	4.50000	0.03448
H	3.57522	4.50000	1.11007
N	2.52334	4.50000	-0.61832
H	1.65734	4.50000	-0.12857
H	2.50989	4.50000	-1.61592



Cartesian coordinates of 5- and 6-fluoroindole-formamide (2) its side and top view.

N	-1.89743	0.00000	0.04940
C	-1.89743	0.00000	1.43914
C	-0.62697	0.00000	1.89071
C	0.23802	0.00000	0.73327
C	1.62202	0.00000	0.56427
C	2.13934	0.00000	-0.70795
C	1.29637	0.00000	-1.82653
C	-0.07061	0.00000	-1.68468
C	-0.59267	0.00000	-0.39727
H	-2.71071	0.00000	-0.52195
H	-2.81202	0.00000	1.98225
H	-0.32191	0.00000	2.91065
H	2.26722	0.00000	1.41988
F	3.49289	0.00000	-0.88437
H	1.71814	0.00000	-2.81076
H	-0.70879	0.00000	-2.54534
O	6.30079	4.50000	-2.98600
C	5.20629	4.50000	-2.46552
H	5.07522	4.50000	-1.38993
N	4.02334	4.50000	-3.11832
H	3.15734	4.50000	-2.62857
H	4.00989	4.50000	-4.11592

