

Table 1S Predicted BDE of path 1 and  $E_{a,1}$  of path 2 at the B3LYP/6-31G\* level

	Path 1	Path 2
	BDE	$E_{a,1}$
	(kJ/mol)	(kJ/mol)
A	487.544	392.922
A11	493.958	396.708
A12	495.112	401.572
A13	495.567	401.857
A14	502.968	407.116
A11'	486.316	381.659
A12'	488.105	372.095
A13'	488.473	373.145
A14'	492.081	378.038
A21	486.372	376.708
A22	488.471	378.752
A23	489.200	379.705
A24	496.031	385.754
A25	491.215	373.569
A26	497.776	380.615
A31	491.634	376.541
A32	488.839	374.316
A33	491.796	378.151
A34	495.338	385.786
A35	492.267	377.850
A36	488.863	374.976

Table 2S Predicted  $E_{a,2}$ \* at the B3LYP/6-31G\* level

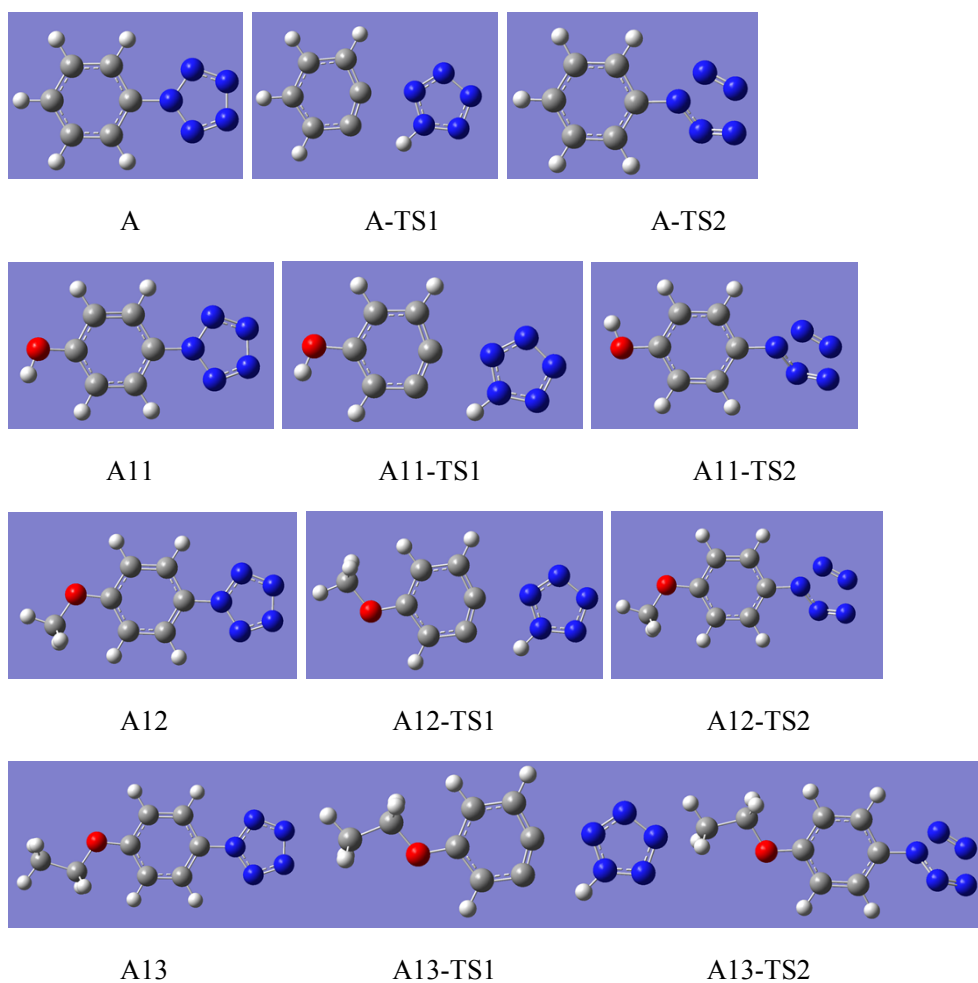
	n=1	n=2	n=3	n=4	n=5	n=6
A1n $E_{a,2}$ (kJ/mol)	92.394	92.821	92.801	94.610		
$Q_t$ (e)	-0.490	-0.491	-0.495	-0.515		
A1n' $E_{a,2}$ (kJ/mol)	89.952	91.591	91.747	93.044		
$Q_t$ (e)	-0.470	-0.477	-0.478	-0.487		
A2n $E_a$ (kJ/mol)	90.191	92.303	92.500	94.655	92.608	94.594
$Q_t$ (e)	-0.475	-0.484	-0.485	-0.503	-0.489	-0.508
A3n $E_a$ (kJ/mol)	92.611	92.089	92.927	94.834	93.908	91.578
$Q_t$ (e)	-0.492	-0.491	-0.495	-0.514	-0.503	-0.485

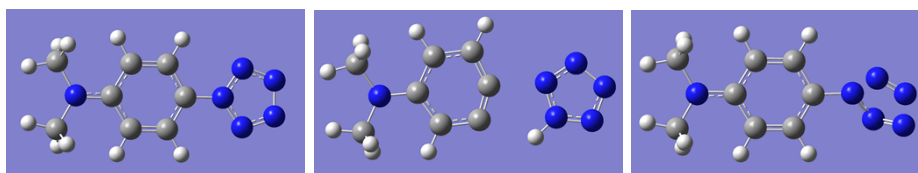
\*  $E_{a,2}$  and  $Q_t$  of A are 90.466 and -0.470 e, respectively.

Table 3S Predicted  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and  $E_{\text{g}}$  at the B3LYP/6-31G\* level \*

		n=1	n=2	n=3	n=4	n=5	n=6
A1n	$E_{\text{HOMO}}$	-6.69	-6.56	-6.52	-5.69		
	$E_{\text{LUMO}}$	-1.87	-1.82	-1.79	-1.54		
	$E_{\text{g}}$	4.82	4.74	4.72	4.15		
A1n'	$E_{\text{HOMO}}$	-6.81	-6.65	-6.60	-5.71		
	$E_{\text{LUMO}}$	-2.04	-2.02	-1.99	-1.77		
	$E_{\text{g}}$	4.77	4.63	4.61	3.93		
A2n	$E_{\text{HOMO}}$	-6.65	-6.56	-6.48	-5.32	-6.51	-5.63
	$E_{\text{LUMO}}$	-2.05	-1.98	-1.93	-1.54	-1.97	-1.69
	$E_{\text{g}}$	4.60	4.58	4.56	3.78	4.54	3.94
A3n	$E_{\text{HOMO}}$	-6.33	-6.48	-6.29	-5.26	-5.58	-6.39
	$E_{\text{LUMO}}$	-1.88	-1.92	-1.79	-1.60	-1.78	-1.89
	$E_{\text{g}}$	4.45	4.56	4.50	3.67	3.80	4.50

\* $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and  $E_{\text{g}}$  of A are -7.36, -2.07 and 5.29 eV, respectively.

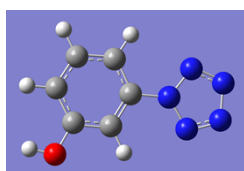




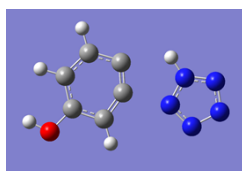
A14

A14-TS1

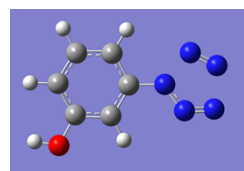
A14-TS2



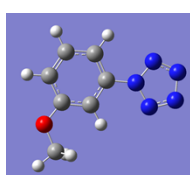
A15



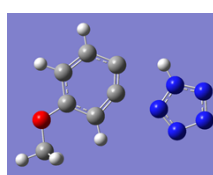
A15-TS1



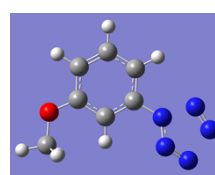
A15-TS2



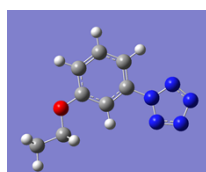
A16



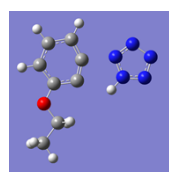
A16-TS1



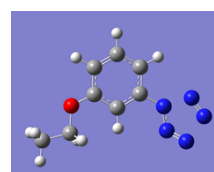
A16-TS2



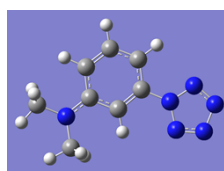
A17



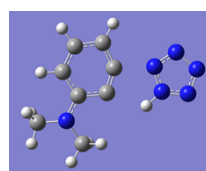
A17-TS1



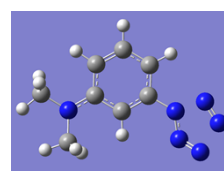
A17-TS2



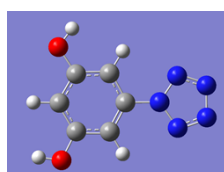
A18



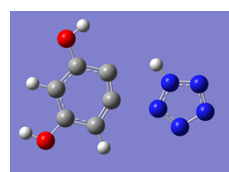
A18-TS1



A18-TS2



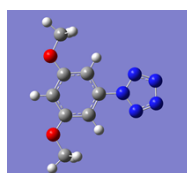
A21



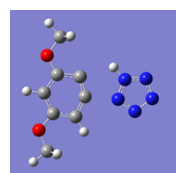
A21-TS1



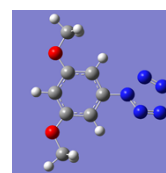
A21-TS2



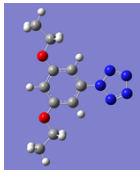
A22



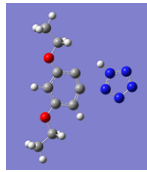
A22-TS1



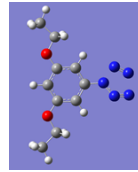
A22-TS2



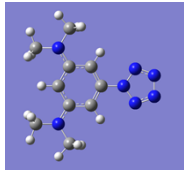
A23



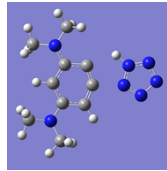
A23-TS1



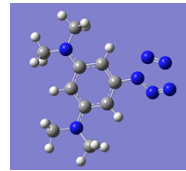
A23-TS2



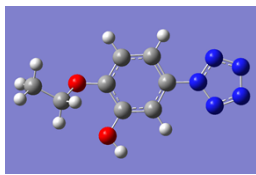
A24



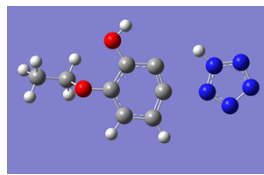
A24-TS1



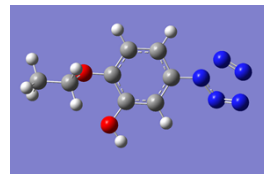
A24-TS2



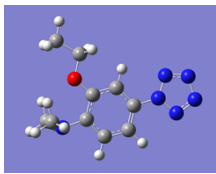
A25



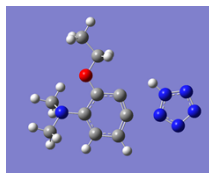
A25-TS1



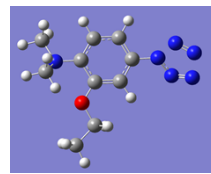
A25-TS2



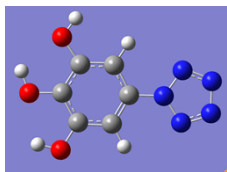
A26



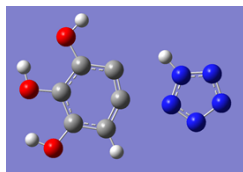
A26-TS1



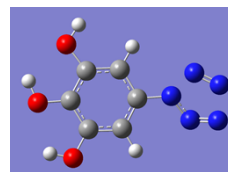
A26-TS2



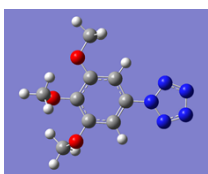
A31



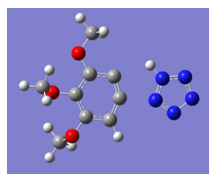
A31-TS1



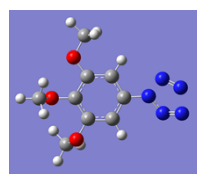
A31-TS2



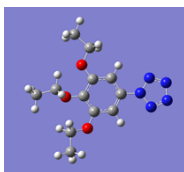
A32



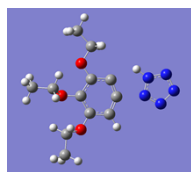
A32-TS1



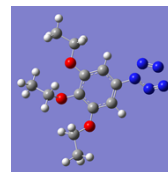
A32-TS2



A33



A33-TS1



A33-TS2

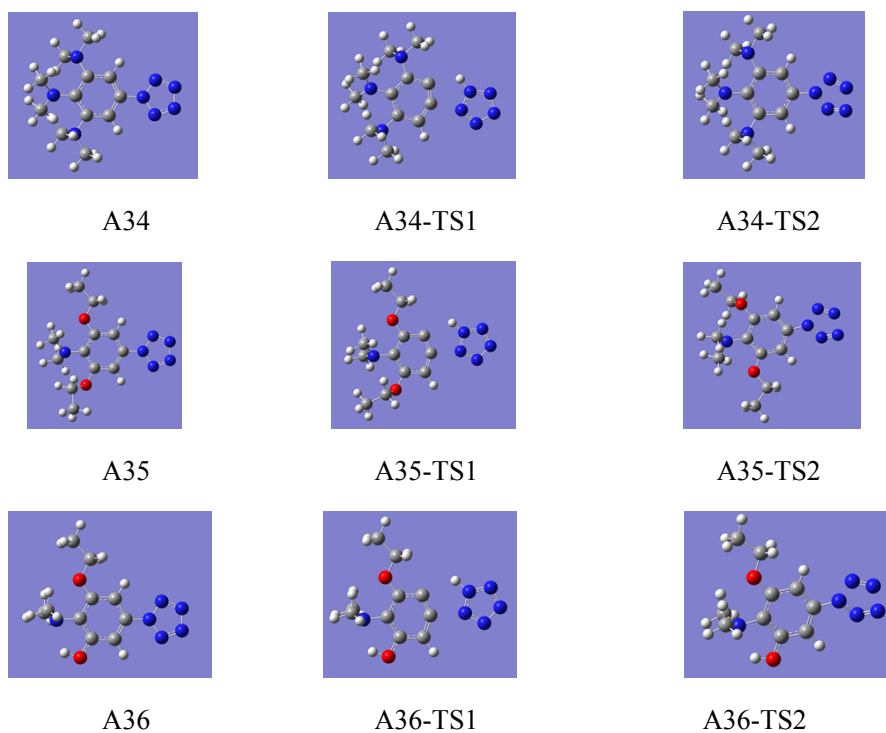


Figure 1S Structures of A, derivatives and TS1s and TS2s

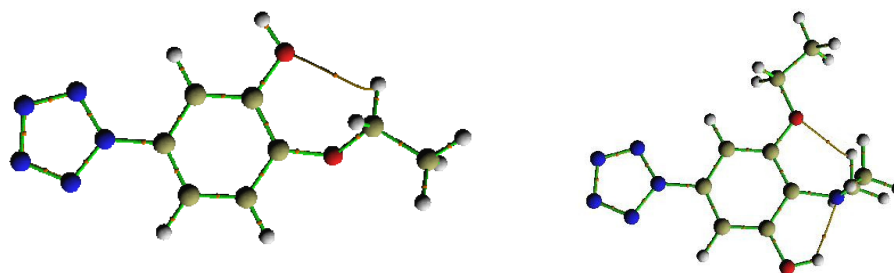


Figure 2S structures of A25 and A36 with hydrogen bond paths