Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information

Specific Nucleophile-Electrophile Interactions in Nucleophilic Aromatic Substitutions

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Table S1. Kinetic results for the reaction between FDNB and propylamine in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 10.59	**Fn = 0.33**
13.5	0.0016
33.8	0.0037
54.1	0.0065
74.5	0.0107
94.8	0.0124
115	0.0148
135	0.0184
pH = 10.89	**Fn = 0.50**
8.30	0.0016
20.7	0.0038
33.1	0.0065
45.5	0.0093
57.9	0.0112
70.3	0.0132
82.7	0.0151
pH = 11.19	**Fn = 0.67**
12.9	0.0030
32.3	0.0077
51.7	0.0140
71.1	0.0170
90.4	0.0210
110	0.0274
129	0.0335

Table S2. Kinetic results for the reaction between FDNB and glycine in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 9.46	**Fn = 0.33**
7.60	0.00038
19.0	0.00095
30.4	0.00140
41.8	0.00190
53.2	0.00257
64.6	0.00308
76.0	0.00357
pH = 9.76	**Fn = 0.50**
9.50	0.00066
23.8	0.00163
38.0	0.00268
52.3	0.00357
66.6	0.00480
80.8	0.00585
95.1	0.00656
pH = 10.06	**Fn = 0.67**
7.90	0.00071
19.7	0.00168
31.5	0.00290
43.4	0.00409
55.2	0.00525
67.0	0.00638
78.8	0.00746

Table S3. Kinetic results for the reaction between FDNB and ethanolamine in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 9.20	**Fn = 0.33**
14.0	0.00040
35.1	0.00103
56.1	0.00168
77.1	0.00242
98.1	0.00318
119	0.00412
140	0.00484
pH = 9.50	**Fn = 0.50**
11.9	0.00052
29.7	0.00138
47.5	0.00232
65.4	0.00328
83.2	0.00404
101	0.00450
119	0.00527
pH = 9.80	**Fn = 0.67**
10.1	0.00092
25.2	0.00192
40.4	0.00312
55.5	0.00402
70.6	0.00532
85.8	0.00647

Table S4. Kinetic results for the reaction between FDNB and benzylamine in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 9.04	**Fn = 0.33**
15.2	0.00081
37.9	0.00297
60.6	0.00454
83.3	0.00587
106	0.00758
129	0.00902
152	0.01095
pH = 9.34	**Fn = 0.50**
13.0	0.00147
32.5	0.00365
52.0	0.00583
71.5	0.00790
91.0	0.00947
110	0.01171
130	0.01334
pH = 9.64	**Fn = 0.67**
11.8	0.00156
29.4	0.00488
47.1	0.00789
64.8	0.01107
82.4	0.01445
100	0.01629
118	0.01977

Table S5. Kinetic results for the reaction between FDNB and glycine ethyl ester in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 7.80	**Fn = 0.33**
14.0	0.00011
34.9	0.00030
55.8	0.00049
76.8	0.00068
97.7	0.00087
119	0.00108
140	0.00128
pH = 7.68	**Fn = 0.50**
0.0089	0.00013
0.0222	0.00030
0.0354	0.00048
0.0487	0.00066
0.0620	0.00088
0.0753	0.000102
0.0886	0.00128
pH = 8.40	**Fn = 0.67**
11.5	0.00019
28.8	0.00049
46.1	0.00075
63.4	0.00106
80.7	0.00140
97.9	0.00172
115	0.00204

Table S6. Kinetic results for the reaction between FDNB and trifluoroethylamine in water at 25°C. Ionic Strenght 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 5.70	**Fn = 0.50**
13.5	0.000013
33.9	0.000030
54.2	0.000049
74.5	0.000067
94.8	0.000082
115	0.000105
135	0.000122
pH = 6.00	**Fn = 0.67**
6.40	0.000016
16.0	0.000025
25.6	0.000031
35.2	0.000042
44.8	0.000056
54.4	0.000062
64.0	0.000071

Table S7. Kinetic results for the reaction between FDNB and hydrazine in water at 25°C. Ionic Strength 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 7.80	**Fn = 0.33**
7.30	0.00139
18.3	0.00305
29.3	0.00460
40.2	0.00633
51.2	0.00814
62.2	0.00992
73.1	0.01058
pH = 8.10	**Fn = 0.50**
7.4	0.00154
18.5	0.00372
29.5	0.00566
40.6	0.00899
51.7	0.01116
62.8	0.01381
73.8	0.01636
pH = 8.40	**Fn = 0.67**
6.80	0.00169
17.1	0.00418
27.4	0.00687
37.7	0.01077
47.9	0.01313
58.2	0.01598
68.5	0.01784

Table S8. Kinetic results for the reaction between FDNB and quinuclidine in water at 25°C. Ionic Strenght 0.2 M (KCl)

$[N]_{Total}$ / mM	k_{obsd} / s^{-1}
pH = 11.1	**Fn = 0.33**
2.10	0.00015
5.30	0.00025
8.50	0.00034
11.7	0.00044
14.9	0.00056
18.0	0.00065
21.2	0.00075
pH = 11.4	**Fn = 0.50**
2.40	0.00023
3.85	0.00031
5.29	0.00036
6.73	0.00044
8.17	0.00050
9.62	0.00059
pH = 11.7	**Fn = 0.67**
5.43	0.00053
8.69	0.00070
12.0	0.00087
15.2	0.00102
18.5	0.00115
21.7	0.00127

Figure S1. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and propylamine in water at 25°C. Ionic Strength 0.2M (KCl)

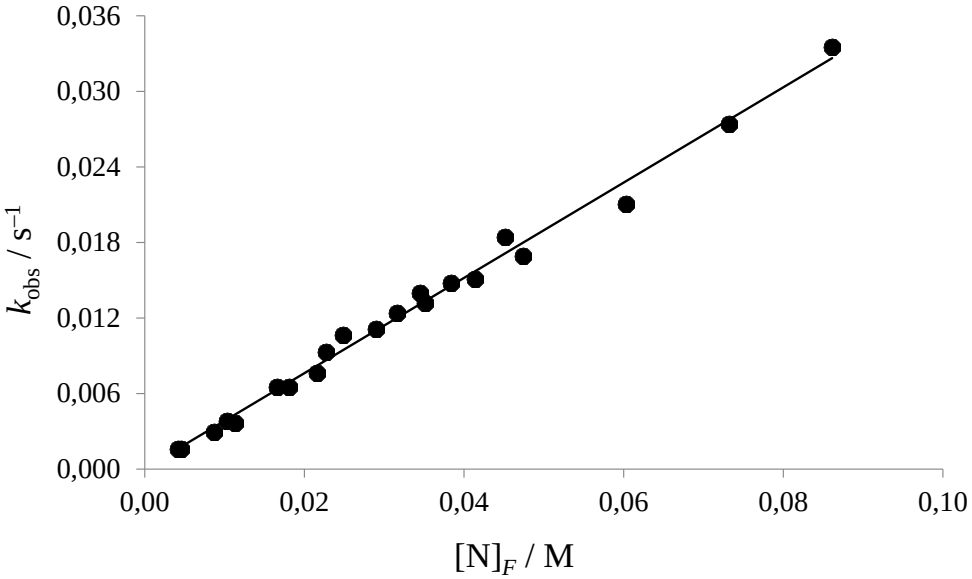


Figure S2. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and glycine in Water at 25°C. Ionic Strength 0.2M (KCl).

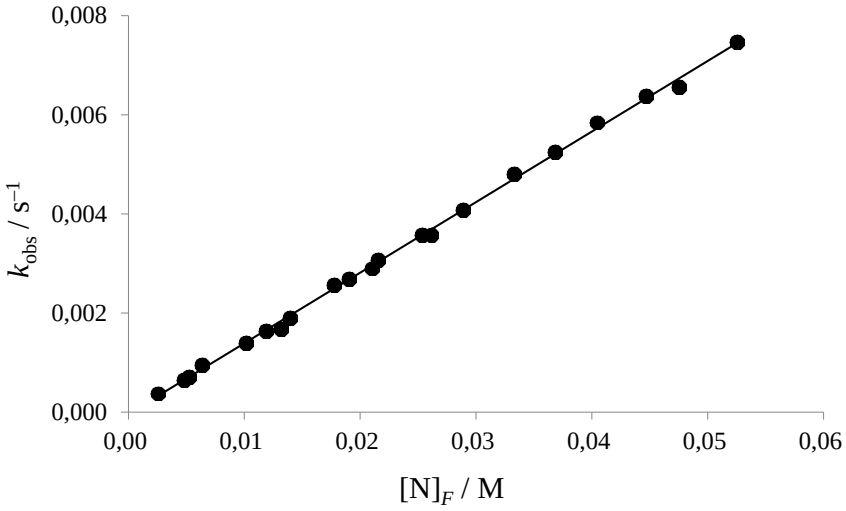


Figure S3. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and ethanolamine in water at 25°C. Ionic Strength 0.2M (KCl)

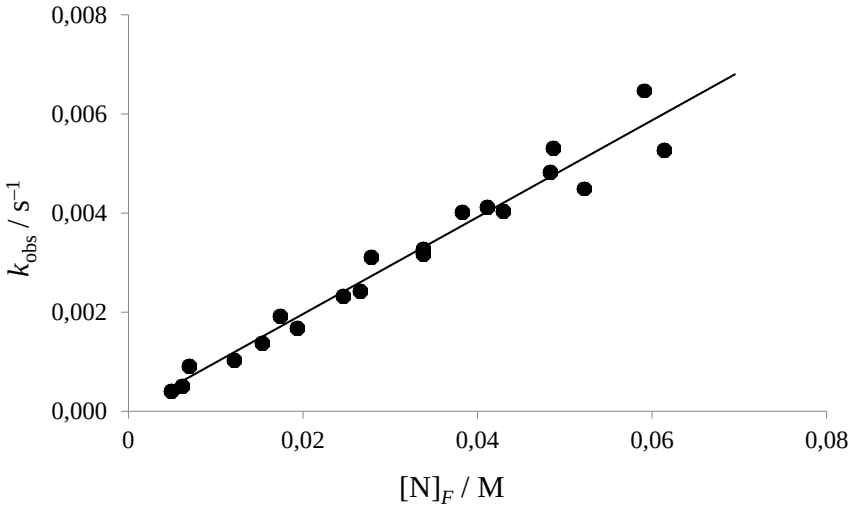


Figure S4. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and benzylamine in water at 25°C. Ionic Strength 0.2M (KCl)

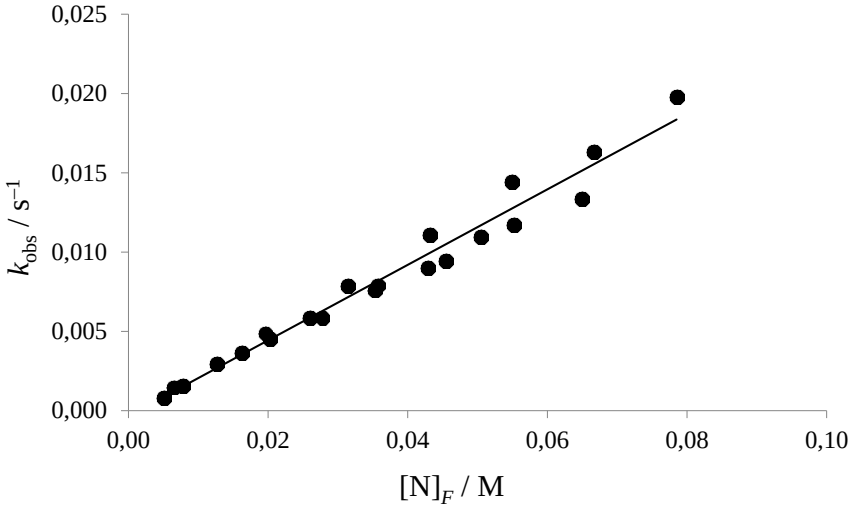


Figure S5. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and glycine ethyl ester in water at 25°C. Ionic Strength 0.2M (KCl)

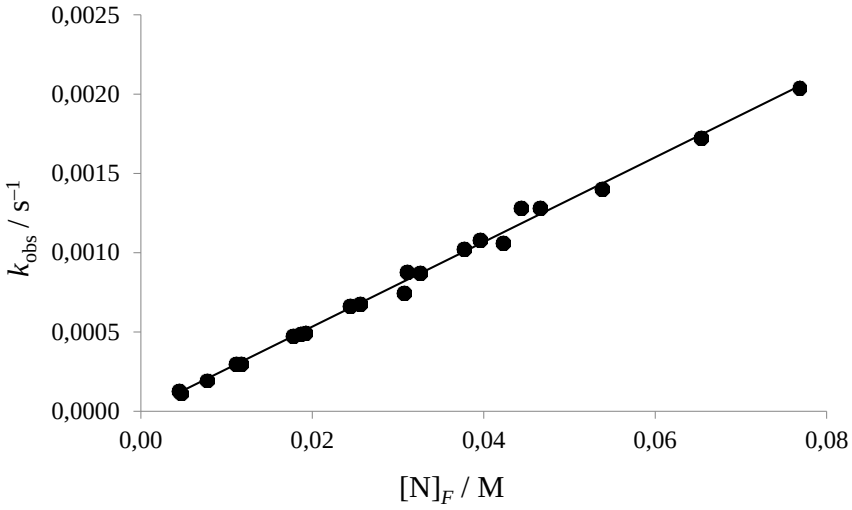


Figure S6. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and trifluoroethylamine in water at 25°C. Ionic Strength 0.2M (KCl)

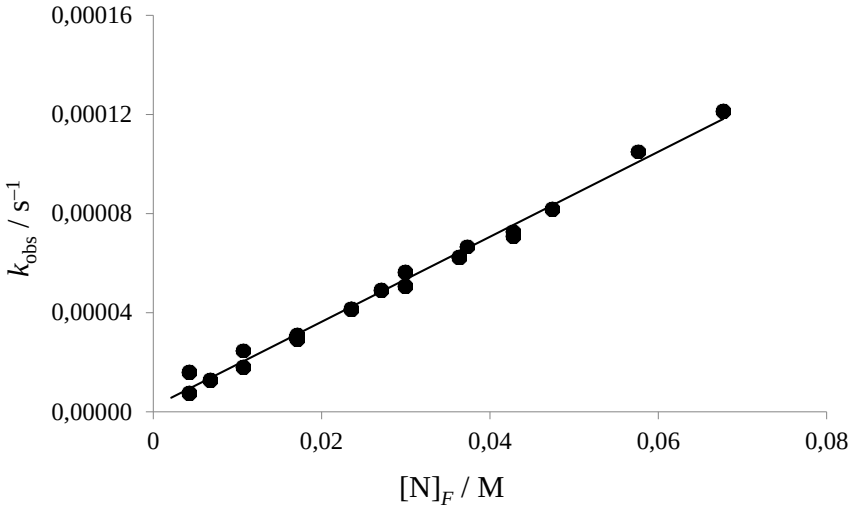


Figure S7. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and hydrazine in water at 25°C. Ionic Strength 0.2M (KCl)

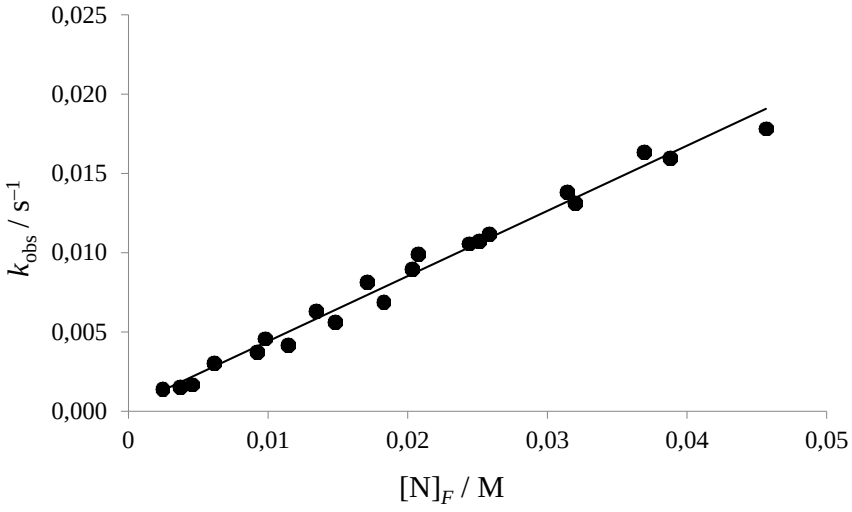


Figure S8. Plot of k_{obs} *vs.* $[N]_F$ for the reaction between FDNB and quinuclidine in water at 25°C. Ionic Strength 0.2M (KCl)

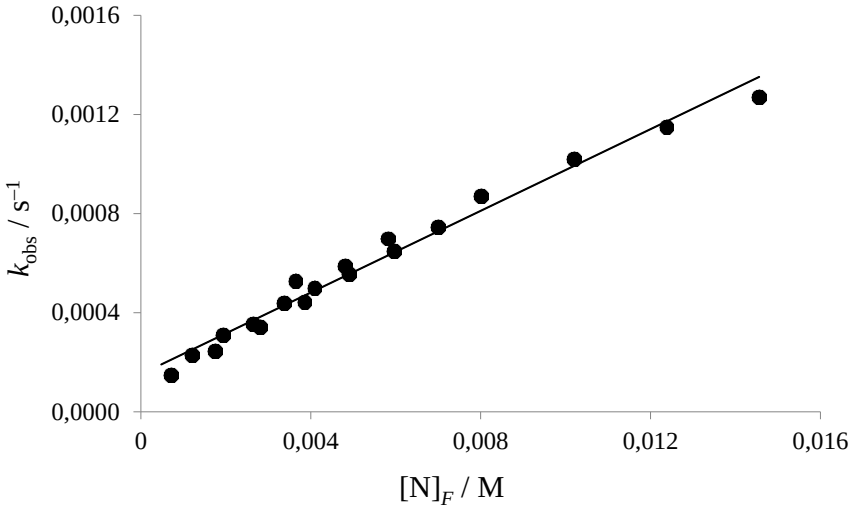
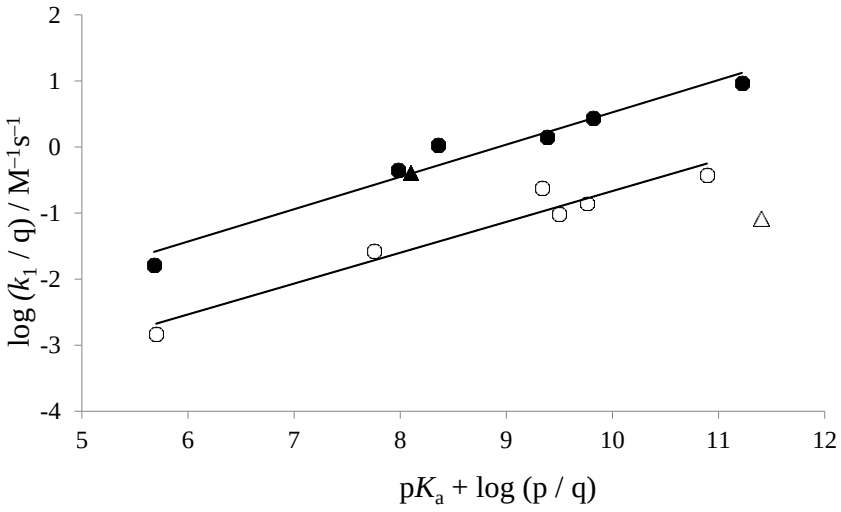


Figure S9. Brønsted-type plot for the reaction between FDNB towards primary amines, secondary alicyclic amines, hydrazine and quinuclidine



Filled circles: Secondary Alicyclic Amines. (Taken from Reference 6a)

Empty circles: Primary Amines

Filled triangle: Hydrazine

Empty triangle: Quinuclidine

Cartesian coordinates, energies (u.a.) and number of imaginary frequencies (NIMAG).

Transition State for the reaction between FDNB and propylamine calculated at the B3LYP/6–31+G(d) level of theory

C	-0.35368300	0.74440400	1.17107000
C	0.36713400	-0.25673400	1.91201900
C	1.49996100	-0.84480000	1.41219800
C	2.02267000	-0.43582200	0.16243400
C	1.41796300	0.58620100	-0.55190100
C	0.25790400	1.18180000	-0.05990800
H	-0.00991200	-0.51515100	2.89722900
H	2.02612500	-1.60396400	1.97975300
H	1.83730100	0.92997000	-1.48964200
N	3.21440200	-1.07178400	-0.36156500
O	3.72505200	-1.97774900	0.31058900
O	3.65589700	-0.68328400	-1.44871600
N	-0.37094700	2.21219500	-0.85226900
O	0.29154500	2.77947000	-1.72124700
O	-1.57552700	2.45895600	-0.63871000
F	-0.91955800	1.72516600	1.96722700
C	-2.09342600	-1.15198700	-0.09415800
N	-2.08067800	0.04914200	0.75846000
H	-1.57683800	-0.88937800	-1.02390700
H	-1.49086900	-1.91640200	0.41058700
H	-2.49751100	0.86720200	0.30487800
H	-2.54262500	-0.10267800	1.65616700
C	-3.50122400	-1.68003900	-0.39405500
H	-4.01004600	-1.91655400	0.55130800
H	-4.08886300	-0.88918800	-0.87948100
C	-3.46756600	-2.92576900	-1.28822400
H	-2.90831900	-3.74207900	-0.81501200
H	-4.48164000	-3.28793900	-1.48783700
H	-2.99433800	-2.70987800	-2.25365600

E(RB+HF-LYP) -914.98490686 NIMAG = 1 , ν_I (cm^{-1}) = -235

Transition State for the reaction between FDNB and piperidine calculated at the B3LYP/6–31+G(d) level of theory

C	-0.10394200	0.41914400	1.08263000
C	0.44849800	-0.80957900	1.58977300
C	1.63021900	-1.31632900	1.11505700
C	2.37646000	-0.60040900	0.14820000
C	1.94321000	0.63836300	-0.29734300
C	0.73447400	1.15509000	0.16533000
H	-0.09370400	-1.31176000	2.38465100
H	2.02635000	-2.24955400	1.49911700
H	2.53415200	1.21153500	-1.00135400
N	3.61811200	-1.15079300	-0.35399600
O	3.97325800	-2.25630100	0.07721400
O	4.25531000	-0.49624100	-1.18719300
N	0.29520500	2.42940500	-0.34999400
O	1.12217200	3.17418100	-0.87759800
O	-0.91913200	2.70670700	-0.26419500
F	-0.76971800	1.16413500	2.03636000
H	-2.53856700	-1.58891400	-2.77369700
C	-2.78012900	-0.97922300	-1.89448800
C	-1.49512000	-0.73709500	-1.09201400
H	-3.15761300	-0.01767200	-2.27041300
C	-4.08501500	-0.87204000	0.26533800
N	-1.75248600	0.01414700	0.15419800
H	-0.76196900	-0.17569100	-1.67806400
H	-1.03365000	-1.68932700	-0.80099200
C	-2.76672000	-0.63362700	1.01639200
H	-4.54896900	0.09765800	0.03517100
H	-4.77813500	-1.40352400	0.92932800
H	-2.01502900	0.98207700	-0.05719100
H	-2.91478500	-0.00063900	1.89420700
H	-2.34332400	-1.58953600	1.35034500
C	-3.85300300	-1.66103600	-1.03169700
H	-4.79006300	-1.75430800	-1.59310700
H	-3.52951200	-2.68320200	-0.78557400

E(RB+HF-LYP) -1028.29724623 NIMAG = 1 , ν_I (cm^{-1}) = -196

Transition State for the reaction between FDNB and morpholine calculated at the B3LYP/6–31+G(d) level of theory

C	-0.13818100	0.38350600	1.05703600
C	0.42351100	-0.85330400	1.54272700
C	1.62235400	-1.33026900	1.08240300
C	2.37775200	-0.58385300	0.14516000
C	1.93431400	0.65631800	-0.28397400
C	0.70837400	1.14626100	0.16390100
H	-0.12526700	-1.38103100	2.31617100
H	2.02454000	-2.26558700	1.45505500
H	2.52971700	1.25185900	-0.96542100
N	3.63677000	-1.10595300	-0.34375400
O	4.00173800	-2.21254900	0.07561600
O	4.27747200	-0.42725300	-1.15453200
N	0.26240800	2.42372900	-0.33195700
O	1.08576700	3.19187600	-0.82885700
O	-0.95937400	2.68425300	-0.26327500
F	-0.79535100	1.11092600	2.03684200
H	-2.62069800	-1.74841500	-2.66265000
C	-2.80059500	-1.06292000	-1.83040000
O	-3.74674500	-1.69621400	-0.97836000
C	-1.49384300	-0.77869900	-1.08625600
H	-3.22377700	-0.12772000	-2.23351400
C	-4.05068600	-0.89107600	0.15211500
N	-1.74512700	0.01077000	0.13816500
H	-0.79605400	-0.22476000	-1.72120800
H	-1.01879600	-1.71698800	-0.77922400
C	-2.79495200	-0.60577600	0.98167400
H	-4.51680000	0.05449200	-0.17228500
H	-4.77837300	-1.44887200	0.74789700
H	-1.98375600	0.98190200	-0.09669400
H	-3.01549900	0.06935300	1.81183100
H	-2.39459000	-1.54441900	1.38021500

E(RB+HF-LYP) -992.40714836 NIMAG = 1 , ν_I (cm^{-1}) = -192

Transition State for the reaction between FDNB and quinuclidine calculated at the M05–2x/6–31+G(d) level of theory

C	-0.02057000	-0.13711200	0.13618600
C	0.13834500	-0.14876800	1.57661500
C	1.36259200	-0.07070100	2.16976500
C	2.51505700	0.12128000	1.37779900
C	2.39580800	0.37530400	0.02681700
C	1.14896400	0.32388300	-0.58545100
H	-0.76624200	-0.19822500	2.16715100
H	1.46209700	-0.10854000	3.24575300
H	3.26048800	0.64777300	-0.56108500
N	3.81354100	0.16481700	2.00097000
O	3.86658200	-0.01174300	3.21024000
O	4.78831800	0.36238700	1.29293800
N	1.07462500	0.74375200	-1.96414000
O	2.11434500	1.05457200	-2.52566100
O	-0.02141100	0.77597200	-2.50565200
F	-1.24151900	0.34134900	-0.23944600
H	-2.45323500	-1.84481500	-0.17174300
C	-1.62299000	-2.36335500	0.30540100
C	-1.74753800	-3.89866500	0.17212200
H	-1.57955500	-2.05898500	1.35036700
C	0.75761300	-2.73847100	0.07504200
C	-0.55495200	-2.03055200	-1.83426000
C	-0.82685200	-4.35804800	-0.96477800
H	-1.46249400	-4.39025000	1.10594200
H	-2.78583100	-4.16417600	-0.03561200
H	1.67379000	-2.24716600	-0.25237800
H	0.74531100	-2.74752500	1.16483400
C	0.62422200	-4.16096500	-0.51138800
C	-1.07287000	-3.44804600	-2.17289700
H	0.41987600	-1.84608800	-2.28671000
H	-1.23461300	-1.24938600	-2.16211100
H	-1.01569100	-5.40161600	-1.21856500
H	1.30112100	-4.29155000	-1.35932700
H	0.90097800	-4.89727900	0.24555800
H	-0.55556700	-3.82608400	-3.05657000
H	-2.14001300	-3.41637200	-2.40702700
N	-0.38240000	-1.89589900	-0.36219600
E(RB+HF-LYP)	-1069.68053162	NIMAG = 1 , ν_I (cm^{-1}) = -184	

Transition State *with double* hydrogen bond for the reaction between FDNB and hydrazine calculated at the B3LYP/6–31+G(d) level of theory

C	1.37022400	-1.54502500	0.24017500
C	-0.94981900	-0.72355600	0.37413200
C	0.95370100	0.83856800	0.01151600
C	1.83864800	-0.22610300	0.02215700
H	2.08773200	-2.35645400	0.28561200
N	3.25312000	0.01068300	-0.17741800
O	3.63287400	1.17333900	-0.35505200
O	4.00750900	-0.97124500	-0.16114500
H	1.30761200	1.85213600	-0.13364700
N	-2.09011400	-1.13139500	-1.00200400
H	-1.89826500	-0.44454300	-1.73501500
N	-3.51373900	-1.17171900	-0.82391900
H	-3.75134600	-0.23608000	-0.48657200
H	-1.78414800	-2.04095900	-1.36011900
H	-3.68439800	-1.80503800	-0.04204400
C	0.03481000	-1.78484500	0.42385000
C	-0.41164800	0.60891700	0.17714300
F	-1.93021100	-0.84555600	1.35466100
H	-0.32395900	-2.78294700	0.66175700
N	-1.31119900	1.72565700	0.09427000
O	-2.51621700	1.47803500	-0.13844600
O	-0.86957800	2.86781600	0.21560900

E(RB+HF-LYP) -852.35689811 NIMAG = 1 , ν_I (cm^{-1}) = -146

Transition State *with single* hydrogen bond for the reaction between FDNB and hydrazine calculated at the B3LYP/6–31+G(d) level of theory

C	1.02832400	-0.70143700	-0.66412800
C	-0.00893600	-1.67060200	-0.86830000
C	-1.32388700	-1.38424500	-0.59024300
C	-1.69162600	-0.09461400	-0.14476800
C	-0.73619600	0.89976000	-0.00043600
C	0.60270600	0.61088100	-0.25757600
H	0.27824500	-2.63421500	-1.27913300
H	-2.09664600	-2.12942600	-0.74205900
H	-1.01871400	1.89843500	0.31036900
N	-3.08240100	0.19654800	0.14862300
O	-3.90165300	-0.72035500	0.01009200
O	-3.37310000	1.33724100	0.52316700
N	1.58087500	1.65646100	-0.04510100
O	1.20504200	2.82724500	-0.04932900
O	2.76042000	1.31244800	0.16786500
F	2.07722500	-0.78043400	-1.55628900
N	2.17889000	-1.39683600	0.74902500
H	2.88672600	-0.66159800	0.82877900
H	2.63459700	-2.25192800	0.42441400
N	1.58229300	-1.65084600	2.02225700
H	1.37368400	-0.74529300	2.44327000
H	0.68150900	-2.10042700	1.83568800

E(RB+HF-LYP) -852.35860427 NIMAG = 1 , ν_I (cm^{-1}) = -225

Transition State for the reaction between FDNB and piperidine with a water molecule calculated at the B3LYP/6–31+G(d) level of theory

C	0.11740000	0.02410000	0.04970000
C	0.04250000	0.13030000	1.48490000
C	1.16580000	0.19640000	2.26510000
C	2.44680000	0.24110000	1.66170000
C	2.57120000	0.28320000	0.28430000
C	1.43210000	0.21090000	-0.52030000
H	-0.94640000	0.17670000	1.92830000
H	1.08920000	0.25650000	3.34480000
H	3.54450000	0.38130000	-0.18020000
N	3.63250000	0.29230000	2.49290000
O	3.47410000	0.26820000	3.72100000
O	4.73590000	0.35100000	1.93870000
N	1.61480000	0.26890000	-1.94590000
O	2.70920000	0.61780000	-2.39450000
O	0.65850000	-0.06280000	-2.67550000
F	-0.93980000	0.62260000	-0.59480000
H	0.89970000	-4.90080000	-0.38520000
C	0.08870000	-4.19480000	-0.60330000
C	0.55090000	-2.77960000	-0.22940000
H	-0.08990000	-4.24010000	-1.68660000
C	-2.27720000	-3.51080000	-0.05540000
N	-0.51500000	-1.77510000	-0.42430000
H	1.41430000	-2.47820000	-0.82900000
H	0.84490000	-2.73760000	0.82730000
C	-1.75670000	-2.11250000	0.30870000
H	-2.60670000	-3.50670000	-1.10270000
H	-3.16140000	-3.72740000	0.55740000
H	-0.74620000	-1.68130000	-1.42100000
H	-2.49720000	-1.34300000	0.07580000
H	-1.52780000	-2.06450000	1.38060000
C	-1.19220000	-4.57740000	0.15250000
H	-1.55240000	-5.55820000	-0.18060000
H	-0.96920000	-4.67090000	1.22570000
O	-1.84920000	-1.32830000	-3.07390000
H	-1.22600000	-0.59360000	-3.21650000
H	-1.93040000	-1.77080000	-3.93210000

E(RB+HF-LYP) -1068.84171927 NIMAG = 1 , ν_I (cm^{-1}) = -174

Transition State for the reaction between FNB and piperidine molecule calculated at the B3LYP/6–31+G(d) level of theory

C	0.00666700	-0.15569200	0.02291500
C	0.04302500	-0.13367800	1.46834300
C	1.22086800	0.02186400	2.15871600
C	2.46207900	0.20176600	1.49493000
C	2.46910300	0.24781200	0.11762600
C	1.28167200	0.07721100	-0.62609700
H	1.18802300	0.03899000	3.24612500
H	3.38425800	0.41500700	-0.43957300
N	1.35998500	0.10159100	-2.04783200
O	2.38675400	0.52587700	-2.59432200
O	0.38855000	-0.34528500	-2.71277600
F	-1.07382300	0.58265600	-0.49760600
H	0.46127700	-4.97709900	-0.56602600
C	-0.23288900	-4.18110600	-0.86245800
C	0.25418100	-2.85635500	-0.26524600
H	-0.19283900	-4.11965600	-1.95924400
C	-2.60043200	-3.32422500	-0.70489000
N	-0.67469100	-1.74160900	-0.56524900
H	1.23828500	-2.58050900	-0.65289100
H	0.33051400	-2.91913300	0.82728800
C	-2.06029300	-2.01656000	-0.11030200
H	-2.71816800	-3.20472300	-1.79132300
H	-3.60291200	-3.50670900	-0.29783000
H	-0.65227500	-1.52267000	-1.57060100
H	-2.67787400	-1.16204900	-0.39171700
H	-2.03353400	-2.07700000	0.98471800
C	-1.66424800	-4.50464100	-0.40867200
H	-2.02615700	-5.41241100	-0.90586300
H	-1.66764900	-4.71257300	0.67159400
H	-0.90771200	-0.19149300	1.99019000
H	3.37989800	0.32654600	2.05951900

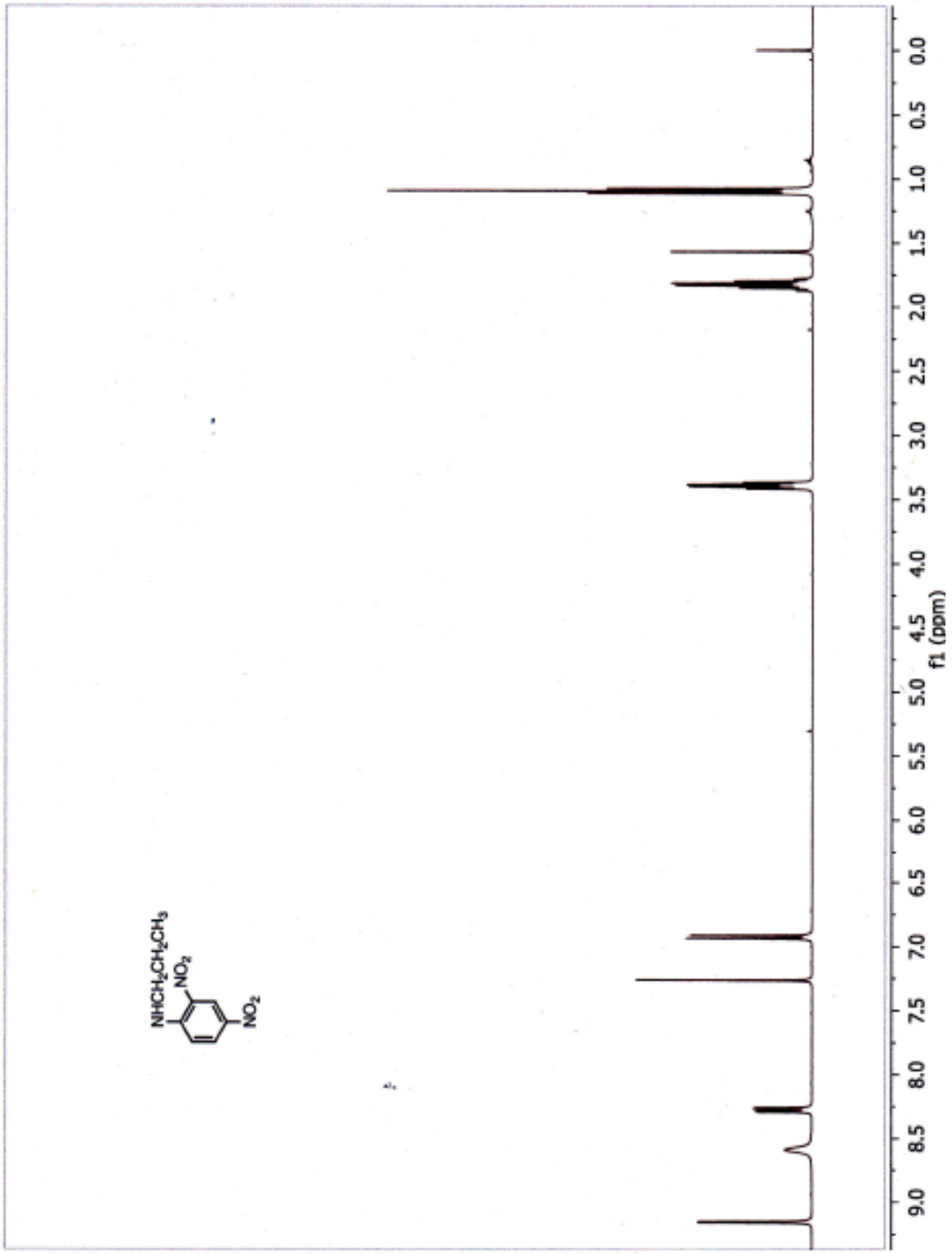
E(RB+HF-LYP) -787.89098096 NIMAG = 1 , ν_I (cm^{-1}) = -203

Transition State for the reaction between FTNB and piperidine molecule calculated at the B3LYP/6–31+G(d) level of theory

C	-0.05557800	0.05671900	0.17771900
C	0.16564400	-0.00342100	1.59873200
C	1.43525200	0.01051400	2.15098900
C	2.54961800	0.14999900	1.32549300
C	2.39890000	0.33162100	-0.04919300
C	1.13122700	0.31089600	-0.60101800
H	1.55093900	-0.06639300	3.22535600
H	3.26140400	0.50227300	-0.68234300
N	3.88618800	0.14077900	1.90857600
O	3.97691700	-0.00900000	3.12931500
O	4.84376100	0.27829000	1.14293700
N	1.02109200	0.50541100	-2.04336900
O	1.91090300	1.13697800	-2.60883600
O	0.05057900	-0.00599400	-2.61958400
F	-1.19200700	0.63715000	-0.25579600
H	0.15514700	-5.07316500	0.37002600
C	-0.28288400	-4.31426600	-0.29030500
C	-0.03514100	-2.92259000	0.31375600
H	0.24470200	-4.38881200	-1.25245900
C	-2.41829600	-3.42557800	-1.31128900
N	-0.67460100	-1.85201900	-0.47432900
H	1.03733500	-2.70773500	0.37783400
H	-0.44848300	-2.87318400	1.32829900
C	-2.13097500	-2.06022200	-0.66690000
H	-2.02628100	-3.43615200	-2.33898300
H	-3.50484000	-3.55800100	-1.38742300
H	-0.24604400	-1.78851300	-1.39960400
H	-2.50277300	-1.23945100	-1.28486800
H	-2.60484200	-1.98221000	0.31443700
C	-1.78420200	-4.56534000	-0.49893400
H	-1.94023100	-5.52700300	-1.00232500
H	-2.28112600	-4.63627000	0.47954300
N	-0.96446200	-0.12119800	2.51544600
O	-0.76073500	0.10697200	3.70889700
O	-2.05340900	-0.46155600	2.04484100

E(RB+HF-LYP) -1196.90528061 NIMAG = 1 , ν_I (cm^{-1}) = -129

^{1}H spectra for the final product 2,4-dinitro-*N*-*n*-propylaniline



^{13}C NMR spectra for the final product 2,4-dinitro-*N*-*n*-propylaniline