

Supporting Information for the paper entitled:

Reaction Rate Constant: A Theoretical Description from Local Temperature

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Table S1. The computed values of the local temperature at the phenoxide oxygen using different approximate KEDs for all the considered phenol derivatives under study. The reference values of $\log_{10}(k_X/k_H)$ for all the systems are also provided. Also given in the last row as boldface are the Pearson correlation coefficients (R) for the correlation between the KEDs-based local temperature expressions and the reference values of the relative rate constants.

X	$\log_{10}(k_X/k_H)$	$T^{TF}(r)$	$T^W(r)$
2-Cl	-0.611	84.90076611	0.00005549283919
2-CN	-1.687	84.90339987	0.00005540859053
2-COMe	-1.863	84.90031295	0.00005317402640
2-F	-0.396	84.89916320	0.00005553261653
2-Me	0.164	84.89670623	0.00005187213542
2-NO ₂	-2.930	84.91310458	0.00005796557669
2-OMe	-0.490	84.89881635	0.00005461297115
2-OMe,4-COMe	-1.554	84.90771351	0.00005558791203
2-OMe,4-Me	-0.175	84.89835067	0.00005472507408
2-OMe,4-NO ₂	-3.356	84.91198317	0.00005641776510
3-Cl	-0.518	84.89948954	0.00005300039318
3-CN	-0.956	84.89999512	0.00005376783229
3-COMe	-0.426	84.89888996	0.00005316478053
3-F	-0.663	84.89829473	0.00005266656796
3-Me	0.412	84.89707270	0.00005187616564
3-Me,4-NO ₂	-2.518	84.90912070	0.00005380816169
3-NO ₂	-0.996	84.90025629	0.00005414394411
3-OMe	0.160	84.89719392	0.00005202142427
3-OMe,5-Cl	-0.420	84.89959343	0.00005324362493
4-Cl	-0.111	84.89796939	0.00005294272978
4-CN	-1.578	84.90394834	0.00005336954402
4-COMe	-1.246	84.90539582	0.00005297348867
4-CONH ₂	-1.629	84.90392673	0.00005294496025
4-F	-0.001	84.89605802	0.00005268185225
4-Me	0.216	84.89647952	0.00005201301837
4-NO ₂	-2.687	84.90941491	0.00005382524224
4-OMe	0.226	84.89515088	0.00005237260757
2,4-Cl	-1.196	84.90180509	0.00005635103384
2,4-NO ₂	-5.189	84.91876067	0.00005923601225
3,5-Cl	-1.164	84.90193361	0.00005408160132
3,5-Me	0.200	84.89671706	0.00005186675510
3,5-OMe	0.267	84.89728330	0.00005230894993
H	0.000	84.89700193	0.00005186117094
R		-0.9615	-0.7629

Table S1. Continued.

X	$T^{GEA2}(r)$	$T^{TF5W}(r)$	$T^{TFvW}(r)$	$T^{TF9W}(r)$
2-Cl	84.90077228	84.90077721	84.90082160	84.90077269
2-CN	84.90340603	84.90341095	84.90345528	84.90340644
2-COMe	84.90031886	84.90032358	84.90036612	84.90031925
2-F	84.89916937	84.89917431	84.89921873	84.89916978
2-Me	84.89671199	84.89671660	84.89675810	84.89671238
2-NO ₂	84.91311102	84.91311617	84.91316255	84.91311145
2-OMe	84.89882242	84.89882727	84.89887096	84.89882283
2-OMe,4-COMe	84.90771968	84.90772462	84.90776909	84.90772010
2-OMe,4-Me	84.89835675	84.89836161	84.89840539	84.89835716
2-OMe,4-NO ₂	84.91198944	84.91199446	84.91203959	84.91198986
3-Cl	84.89949543	84.89950014	84.89954254	84.89949583
3-CN	84.90000109	84.90000587	84.90004889	84.90000149
3-COMe	84.89889587	84.89890060	84.89894313	84.89889627
3-F	84.89830059	84.89830527	84.89834740	84.89830098
3-Me	84.89707846	84.89708308	84.89712458	84.89707885
3-Me,4-NO ₂	84.90912668	84.90913146	84.90917451	84.90912708
3-NO ₂	84.90026230	84.90026711	84.90031043	84.90026271
3-OMe	84.89719970	84.89720432	84.89724594	84.89720009
3-OMe,5-Cl	84.89959935	84.89960408	84.89964668	84.89959974
4-Cl	84.89797527	84.89797998	84.89802233	84.89797566
4-CN	84.90395427	84.90395902	84.90400171	84.90395467
4-COMe	84.90540170	84.90540641	84.90544879	84.90540210
4-CONH ₂	84.90393262	84.90393732	84.90397968	84.90393301
4-F	84.89606387	84.89606855	84.89611070	84.89606426
4-Me	84.89648530	84.89648992	84.89653153	84.89648569
4-NO ₂	84.90942089	84.90942567	84.90946873	84.90942129
4-OMe	84.89515670	84.89516136	84.89520326	84.89515709
2,4-Cl	84.90181135	84.90181636	84.90186144	84.90181177
2,4-NO ₂	84.91876725	84.91877252	84.91881991	84.91876770
3,5-Cl	84.90193962	84.90194443	84.90198770	84.90194003
3,5-Me	84.89672282	84.89672743	84.89676893	84.89672321
3,5-OMe	84.89728912	84.89729377	84.89733561	84.89728950
H	84.89700769	84.89701230	84.89705379	84.89700808
R	-0.9615	-0.9615	-0.9615	-0.9615

Table S1. Continued.

X	$T^{TF-N}(r)$	$T^{Pear}(r)$	$T^{DK\ Pade}(r)$	$T^{LLP}(r)$
2-Cl	90.50432657	84.90077228	84.90077228	84.90077505
2-CN	90.60423841	84.90340603	84.90340603	84.90340880
2-COMe	90.37065002	84.90031886	84.90031886	84.90032152
2-F	90.70456762	84.89916937	84.89916937	84.89917215
2-Me	90.70194263	84.89671199	84.89671199	84.89671458
2-NO ₂	90.38426584	84.91311102	84.91311102	84.91311392
2-OMe	90.50224813	84.89882242	84.89882242	84.89882515
2-OMe,4-COMe	90.08007229	84.90771968	84.90771968	84.90772246
2-OMe,4-Me	90.32709324	84.89835675	84.89835675	84.89835949
2-OMe,4-NO ₂	90.08460205	84.91198944	84.91198944	84.91199226
3-Cl	90.50296575	84.89949543	84.89949543	84.89949808
3-CN	90.60060505	84.90000109	84.90000109	84.90000378
3-COMe	90.36913534	84.89889587	84.89889587	84.89889853
3-F	90.70363976	84.89830059	84.89830059	84.89830322
3-Me	90.70233417	84.89707846	84.89707846	84.89708106
3-Me,4-NO ₂	90.22178951	84.90912668	84.90912668	84.90912937
3-NO ₂	90.37058970	84.90026230	84.90026230	84.90026501
3-OMe	90.50051861	84.89719970	84.89719970	84.89720230
3-OMe,5-Cl	90.17507453	84.89959935	84.89959935	84.89960201
4-Cl	90.50134526	84.89797527	84.89797527	84.89797792
4-CN	90.60482371	84.90395427	84.90395427	84.90395694
4-COMe	90.37606039	84.90540170	84.90540170	84.90540435
4-CONH ₂	90.37449665	84.90393262	84.90393262	84.90393526
4-F	90.70125010	84.89606387	84.89606387	84.89606651
4-Me	90.70170043	84.89648530	84.89648530	84.89648790
4-NO ₂	90.38033844	84.90942089	84.90942089	84.90942358
4-OMe	90.49834073	84.89515670	84.89515670	84.89515932
2,4-Cl	90.17742362	84.90181135	84.90181135	84.90181417
2,4-NO ₂	89.99637417	84.91876725	84.91876725	84.91877022
3,5-Cl	90.17756013	84.90193962	84.90193962	84.90194233
3,5-Me	90.50001028	84.89672282	84.89672282	84.89672542
3,5-OMe	90.17262086	84.89728912	84.89728912	84.89729173
H	90.94022463	84.89700769	84.89700769	84.89701028
R	0.5783	-0.9615	-0.9615	-0.9615

Table S1. Continued.

X	$T^{OL1}(r)$	$T^{OL2}(r)$	$T^{Thak}(r)$	$T^{B86A}(r)$
2-Cl	84.90154734	84.91077190	84.87139060	84.90077400
2-CN	84.90418052	84.91339833	84.87404586	84.90340775
2-COMe	84.90107756	84.91011046	84.87154830	84.90032051
2-F	84.89994471	84.90917242	84.86977761	84.89917110
2-Me	84.89746133	84.90638455	84.86829114	84.89671360
2-NO ₂	84.91390322	84.92332832	84.88308986	84.91311282
2-OMe	84.89959131	84.90874354	84.86967136	84.89882412
2-OMe,4-COMe	84.90849544	84.91772815	84.87831201	84.90772141
2-OMe,4-Me	84.89912642	84.90828786	84.86917633	84.89835845
2-OMe,4-NO ₂	84.91277099	84.92207145	84.88236573	84.91199120
3-Cl	84.90025288	84.90927122	84.87077132	84.89949708
3-CN	84.90076401	84.90984638	84.87107283	84.90000277
3-COMe	84.89965450	84.90868655	84.87012802	84.89889752
3-F	84.89905565	84.90804593	84.86966592	84.89830222
3-Me	84.89782783	84.90675142	84.86865647	84.89708008
3-Me,4-NO ₂	84.90988993	84.91897613	84.88018615	84.90912835
3-NO ₂	84.90102789	84.91014146	84.87123453	84.90026399
3-OMe	84.89795012	84.90688599	84.86873851	84.89720132
3-OMe,5-Cl	84.90035854	84.90939722	84.87081038	84.89960100
4-Cl	84.89873230	84.90774573	84.86926681	84.89797692
4-CN	84.90471438	84.91376380	84.87513104	84.90395593
4-COMe	84.90615899	84.91517539	84.87668376	84.90540335
4-CONH ₂	84.90468969	84.91370363	84.87522254	84.90393426
4-F	84.89681903	84.90581048	84.86742549	84.89606551
4-Me	84.89723565	84.90617078	84.86802650	84.89648692
4-NO ₂	84.91018426	84.91927190	84.88047579	84.90942256
4-OMe	84.89590964	84.90487503	84.86660140	84.89515833
2,4-Cl	84.90259239	84.91188687	84.87220669	84.90181310
2,4-NO ₂	84.91956812	84.92909451	84.88842307	84.91876910
3,5-Cl	84.90270478	84.91181327	84.87292802	84.90194131
3,5-Me	84.89747212	84.90639489	84.86830342	84.89672443
3,5-OMe	84.89804160	84.90700175	84.86875054	84.89729074
H	84.89775695	84.90667926	84.86858975	84.89700930
R	-0.9616	-0.9620	-0.9581	-0.9615

Table S1. Continued.

X	$T^{B86B}(r)$	$T^{DK87}(r)$	$T^{PW86}(r)$	$T^{PW91}(r)$
2-Cl	84.90077427	84.90076880	84.90076899	84.90077022
2-CN	84.90340802	84.90340256	84.90340275	84.90340398
2-COMe	84.90032076	84.90031553	84.90031571	84.90031689
2-F	84.89917136	84.89916589	84.89916608	84.89916732
2-Me	84.89671385	84.89670874	84.89670892	84.89671007
2-NO ₂	84.91311310	84.91310739	84.91310759	84.91310888
2-OMe	84.89882438	84.89881900	84.89881918	84.89882040
2-OMe,4-COMe	84.90772167	84.90771620	84.90771639	84.90771762
2-OMe,4-Me	84.89835871	84.89835332	84.89835351	84.89835472
2-OMe,4-NO ₂	84.91199146	84.91198591	84.91198610	84.91198735
3-Cl	84.89949733	84.89949211	84.89949229	84.89949347
3-CN	84.90000302	84.89999773	84.89999791	84.89999910
3-COMe	84.89889778	84.89889254	84.89889272	84.89889390
3-F	84.89830247	84.89829729	84.89829746	84.89829864
3-Me	84.89708032	84.89707521	84.89707539	84.89707654
3-Me,4-NO ₂	84.90912861	84.90912331	84.90912349	84.90912469
3-NO ₂	84.90026424	84.90025891	84.90025909	84.90026030
3-OMe	84.89720156	84.89719644	84.89719662	84.89719778
3-OMe,5-Cl	84.89960126	84.89959601	84.89959619	84.89959738
4-Cl	84.89797717	84.89797195	84.89797213	84.89797331
4-CN	84.90395618	84.90395093	84.90395111	84.90395230
4-COMe	84.90540360	84.90539838	84.90539856	84.90539974
4-CONH ₂	84.90393451	84.90392930	84.90392948	84.90393066
4-F	84.89606576	84.89606057	84.89606075	84.89606192
4-Me	84.89648716	84.89648204	84.89648222	84.89648338
4-NO ₂	84.90942282	84.90941752	84.90941770	84.90941890
4-OMe	84.89515858	84.89515342	84.89515360	84.89515477
2,4-Cl	84.90181337	84.90180782	84.90180801	84.90180926
2,4-NO ₂	84.91876938	84.91876354	84.91876374	84.91876506
3,5-Cl	84.90194156	84.90193623	84.90193642	84.90193762
3,5-Me	84.89672468	84.89671957	84.89671975	84.89672090
3,5-OMe	84.89729099	84.89728584	84.89728602	84.89728718
H	84.89700955	84.89700444	84.89700462	84.89700577
R	-0.9615	-0.9615	-0.9615	-0.9615

Table S1. Continued.

X	$T^{LG94}(r)$	$T^{ABSP}(r)$	$T^{GR}(r)$	$T^{GEA4}(r)$
2-Cl	85.07241300	55.23668853	55.92958533	287.2241224
2-CN	85.07492418	54.61369183	55.26687620	287.2221647
2-COMe	85.06847121	56.08440194	56.82748381	287.2253718
2-F	85.07086755	53.93010513	54.53733736	287.2272118
2-Me	85.06286651	53.92854074	54.53575539	287.2304537
2-NO ₂	85.08839910	56.09285676	56.83605059	287.2081015
2-OMe	85.06914703	55.23541913	55.92830001	287.2272385
2-OMe,4-COMe	85.07950902	57.95391011	58.79183337	287.2151616
2-OMe,4-Me	85.06884893	56.34507898	57.10276278	287.2282126
2-OMe,4-NO ₂	85.08501139	57.95682521	58.79479060	287.2092909
3-Cl	85.06738250	55.23585550	55.92874188	287.2246709
3-CN	85.06905396	54.61150010	55.26465827	287.2250165
3-COMe	85.06703269	56.08346192	56.82653134	287.2263021
3-F	85.06567672	53.92955059	54.53677661	287.2264062
3-Me	85.06323957	53.92877353	54.53599081	287.2285652
3-Me,4-NO ₂	85.07824997	57.08478072	57.88119116	287.2122631
3-NO ₂	85.06988327	56.08436548	56.82744686	287.2242261
3-OMe	85.06358474	55.23436098	55.92722862	287.2281213
3-OMe,5-Cl	85.06785682	57.30642840	58.11409385	287.2247976
4-Cl	85.06577286	55.23486643	55.92774039	287.2272334
4-CN	85.07240757	54.61404259	55.26723118	287.2190388
4-COMe	85.07325381	56.08775943	56.83088579	287.2170916
4-CONH ₂	85.07173971	56.08678894	56.82990245	287.2190745
4-F	85.06346110	53.92812979	54.53533981	287.2299270
4-Me	85.06285667	53.92839687	54.53560990	287.2293923
4-NO ₂	85.07857031	56.09041526	56.83357680	287.2115025
4-OMe	85.06207936	55.23303213	55.92588310	287.2313821
2,4-Cl	85.07472413	57.30792435	58.11561084	287.2229715
2,4-NO ₂	85.09589629	58.54767049	59.41098146	287.2005500
3,5-Cl	85.07146836	57.30800884	58.11569655	287.2213207
3,5-Me	85.06286905	55.23405058	55.92691433	287.2293029
3,5-OMe	85.06411626	57.30486815	58.11251162	287.2282060
H	85.06314560	52.35809022	52.84930133	287.2282454
R	-0.9454	-0.5931	-0.5919	0.9532

Table S2. Numerical results of the total kinetic energy (au) from integration of the accurate and approximate KEDs for the systems under study.

X	H	L	TF	W	GEA2	TF5W	TFvW	TF9W
2-Cl	764.281	764.281	703.175	515.024	760.400	806.180	1218.200	764.234
2-CN	397.662	397.662	360.603	315.571	395.667	423.718	676.175	398.016
2-COMe	457.833	457.833	415.341	361.071	455.460	487.555	776.412	458.148
2-F	404.753	404.753	367.495	314.291	402.416	430.353	681.785	404.756
2-Me	344.819	344.819	312.804	273.949	343.243	367.594	586.753	345.283
2-NO ₂	509.731	509.731	462.243	397.430	506.402	541.729	859.673	509.361
2-OMe	419.847	419.847	380.877	330.267	417.573	446.930	711.143	420.032
2-OMe,4-COMe	571.988	571.988	518.920	448.852	568.792	608.690	967.772	572.134
2-OMe,4-Me	458.964	458.964	416.367	361.727	456.559	488.713	778.095	459.252
2-OMe,4-NO ₂	623.894	623.894	565.848	485.139	619.752	662.875	1050.986	623.364
3-Cl	764.282	764.282	703.175	515.047	760.402	806.184	1218.222	764.237
3-CN	397.660	397.660	360.592	315.589	395.657	423.709	676.180	398.006
3-COMe	457.825	457.825	415.318	361.132	455.443	487.544	776.450	458.132
3-F	404.757	404.757	367.506	314.299	402.428	430.366	681.805	404.768
3-Me	344.819	344.819	312.802	273.981	343.245	367.599	586.784	345.284
3-Me,4-NO ₂	548.861	548.861	497.764	428.835	545.412	583.531	926.599	548.605
3-NO ₂	509.728	509.728	462.240	397.433	506.400	541.727	859.674	509.358
3-OMe	419.851	419.851	380.891	330.282	417.589	446.948	711.174	420.048
3-OMe,5-Cl	878.434	878.434	806.760	602.805	873.739	927.321	1409.565	878.226
4-Cl	764.278	764.278	703.167	515.032	760.392	806.173	1218.199	764.227
4-CN	397.669	397.669	360.611	315.572	395.674	423.725	676.183	398.024
4-COMe	457.840	457.840	415.343	361.121	455.468	487.567	776.464	458.156
4-CONH ₂	473.907	473.907	429.938	372.310	471.306	504.400	802.248	474.077
4-F	404.749	404.749	367.483	314.295	402.405	430.342	681.778	404.745
4-Me	344.816	344.816	312.793	273.986	343.236	367.591	586.779	345.276
4-NO ₂	509.747	509.747	462.272	397.408	506.429	541.754	859.681	509.387
4-OMe	419.844	419.844	380.868	330.286	417.566	446.925	711.154	420.025
2,4-Cl	1222.859	1222.859	1129.035	787.529	1216.538	1286.541	1916.564	1222.401
2,4-NO ₂	713.766	713.766	647.192	552.328	708.562	757.658	1199.520	712.674
3,5-Cl	1222.864	1222.864	1129.043	787.558	1216.550	1286.555	1916.601	1222.413
3,5-Me	383.937	383.937	348.298	305.441	382.236	409.386	653.739	384.510
3,5-OMe	534.004	534.004	484.478	418.042	530.927	568.087	902.520	534.039
H	305.698	305.698	277.304	242.522	304.250	325.808	519.826	306.056

Table S2. Continued.

X	TF-N	Pear	DK Pade	LLP	OL1	OL2	Thak	B86A
2-Cl	749.586	747.383	761.896	763.990	766.866	765.468	763.978	766.952
2-CN	384.816	384.273	393.917	396.414	399.268	398.277	397.506	398.536
2-COMe	442.102	442.584	453.613	456.382	459.595	458.465	457.591	458.799
2-F	392.624	391.626	401.219	403.388	406.051	405.075	404.356	405.468
2-Me	334.194	333.299	341.661	343.868	346.366	345.507	344.817	345.710
2-NO ₂	492.026	492.597	504.774	507.579	510.986	509.747	508.841	510.224
2-OMe	406.015	405.858	415.950	418.444	421.362	420.330	419.536	420.651
2-OMe,4-COMe	550.531	552.961	566.684	570.015	573.949	572.548	571.480	573.010
2-OMe,4-Me	442.992	443.660	454.712	457.484	460.703	459.573	458.689	459.904
2-OMe,4-NO ₂	600.318	603.005	617.871	621.233	625.357	623.847	622.751	624.456
3-Cl	749.585	747.383	761.898	763.991	766.869	765.470	763.980	766.953
3-CN	384.803	384.261	393.905	396.404	399.258	398.267	397.496	398.525
3-COMe	442.078	442.558	453.593	456.363	459.579	458.449	457.573	458.780
3-F	392.636	391.639	401.232	403.401	406.064	405.088	404.369	405.481
3-Me	334.192	333.296	341.660	343.868	346.367	345.508	344.817	345.710
3-Me,4-NO ₂	528.908	530.434	543.567	546.647	550.351	549.014	548.022	549.505
3-NO ₂	492.024	492.593	504.772	507.576	510.983	509.745	508.838	510.221
3-OMe	406.031	405.875	415.968	418.461	421.378	420.346	419.552	420.667
3-OMe,5-Cl	856.891	857.769	874.973	877.629	881.226	879.556	877.874	881.168
4-Cl	749.577	747.375	761.890	763.982	766.859	765.460	763.970	766.943
4-CN	384.824	384.281	393.926	396.422	399.275	398.284	397.514	398.543
4-COMe	442.105	442.585	453.621	456.388	459.603	458.474	457.598	458.806
4-CONH ₂	457.640	458.145	469.534	472.310	475.580	474.417	473.534	474.798
4-F	392.612	391.616	401.211	403.378	406.040	405.064	404.346	405.457
4-Me	334.182	333.287	341.652	343.859	346.359	345.500	344.808	345.701
4-NO ₂	492.058	492.630	504.809	507.608	511.013	509.774	508.869	510.253
4-OMe	406.006	405.851	415.945	418.437	421.355	420.323	419.529	420.644
2,4-Cl	1199.191	1199.268	1220.892	1223.148	1226.703	1224.666	1222.289	1227.442
2,4-NO ₂	685.890	689.717	706.669	710.346	714.962	713.246	712.035	714.007
3,5-Cl	1199.200	1199.277	1220.901	1223.158	1226.714	1224.678	1222.300	1227.453
3,5-Me	371.286	371.104	380.428	382.914	385.714	384.757	383.976	384.968
3,5-OMe	514.583	516.263	529.045	532.100	535.737	534.434	533.448	534.884
H	297.043	295.486	302.890	304.820	307.018	306.257	305.655	306.449

X	B86B	DK87	PW86	PW91	LG94	ABSP	GR	GEA4
2-Cl	766.299	761.563	769.992	764.735	796.767	972.512	978.251	771.299
2-CN	397.899	394.965	400.448	396.760	412.328	547.527	550.302	402.754
2-COMe	458.081	454.726	460.993	456.783	474.757	635.441	639.077	463.567
2-F	404.869	401.956	407.406	403.751	419.704	547.732	550.361	409.399
2-Me	345.154	342.606	347.360	344.166	357.682	472.650	474.887	349.424
2-NO ₂	509.456	505.767	512.673	508.035	528.085	702.783	706.829	515.257
2-OMe	419.998	416.930	422.660	418.813	435.307	578.066	581.174	424.985
2-OMe,4-COMe	572.128	567.959	575.748	570.519	593.006	803.042	808.163	578.855
2-OMe,4-Me	459.184	455.823	462.097	457.885	475.914	638.060	641.776	464.697
2-OMe,4-NO ₂	623.525	619.023	627.449	621.793	646.357	871.359	876.943	630.561
3-Cl	766.300	761.565	769.993	764.736	796.768	972.535	978.273	771.302
3-CN	397.888	394.955	400.438	396.749	412.316	547.537	550.312	402.744
3-COMe	458.062	454.706	460.974	456.764	474.736	635.487	639.122	463.551
3-F	404.882	401.969	407.419	403.764	419.717	547.748	550.376	409.412
3-Me	345.154	342.606	347.360	344.165	357.682	472.681	474.918	349.426
3-Me,4-NO ₂	548.671	544.689	552.138	547.136	568.721	763.484	768.153	554.992
3-NO ₂	509.453	505.764	512.669	508.032	528.081	702.785	706.831	515.254
3-OMe	420.014	416.946	422.677	418.830	435.323	578.091	581.200	425.001
3-OMe,5-Cl	880.353	874.803	884.753	878.478	915.022	1147.360	1155.035	886.594
4-Cl	766.291	761.555	769.984	764.726	796.758	972.514	978.253	771.292
4-CN	397.906	394.973	400.456	396.767	412.336	547.533	550.307	402.761
4-COMe	458.087	454.731	460.999	456.789	474.762	635.492	639.128	463.575
4-CONH ₂	474.064	470.605	477.070	472.728	491.353	656.323	660.086	479.639
4-F	404.858	401.946	407.396	403.741	419.692	547.729	550.358	409.388
4-Me	345.145	342.597	347.351	344.156	357.673	472.680	474.917	349.418
4-NO ₂	509.485	505.797	512.701	508.064	528.115	702.781	706.827	515.283
4-OMe	419.991	416.923	422.654	418.806	435.298	578.080	581.188	424.978
2,4-Cl	1226.626	1219.410	1232.057	1224.372	1276.455	1549.616	1560.357	1232.882
2,4-NO ₂	712.961	707.838	717.439	710.993	739.112	998.538	1005.117	720.815
3,5-Cl	1226.637	1219.421	1232.068	1224.383	1276.466	1549.651	1560.392	1232.894
3,5-Me	384.346	381.504	386.803	383.243	398.295	532.044	534.887	389.143
3,5-OMe	534.068	530.187	537.438	532.573	553.579	745.060	749.669	540.295
H	305.959	303.705	307.914	305.085	317.067	413.542	415.146	309.706

Table S2. Continued.