Supplementary Data

This supplementary data is a part of paper entitled "Rotational Barrier and Bond Dissociation Energy and Enthalpy: Computational Study of the Substituent Effects in Para-Substituted Anilines and Phenols".

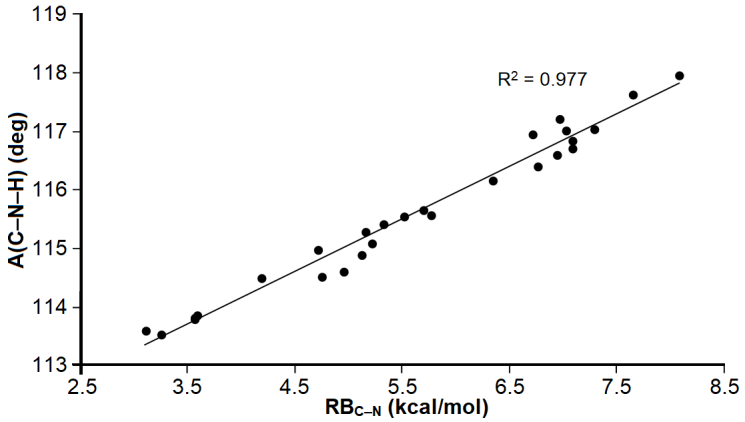

Fig S1. Phenyl–N–H bond angle vs rotational barrier around pheny–NH_2 bond in *para*-substituted anilines

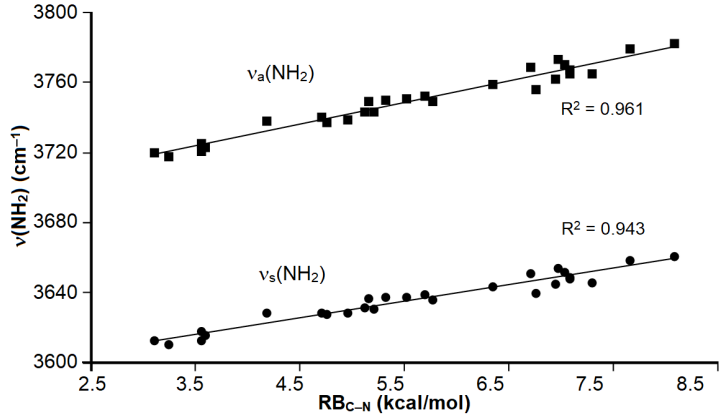

Fig S2. Symmetric and asymmetric NH_2 stretching frequencies vs rotational barrier around pheny–NH_2 bond in *para*-substituted anilines

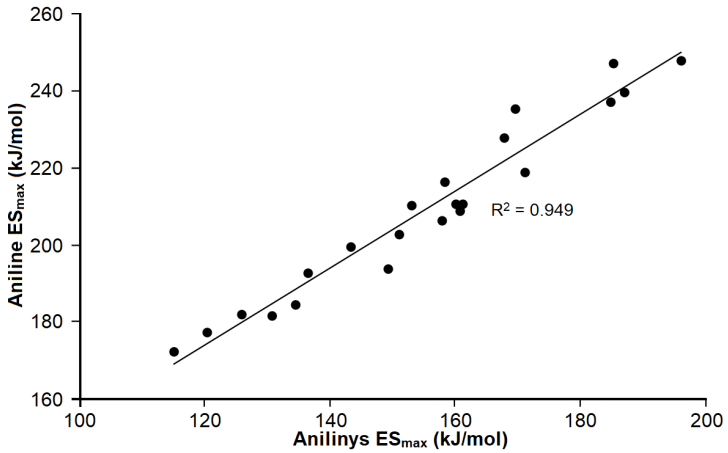

Fig S3. Maximum electrostatic potential around the amino H atom in *para*-substituted anilinic compounds vs that in *para*-substituted anilinyl radicals

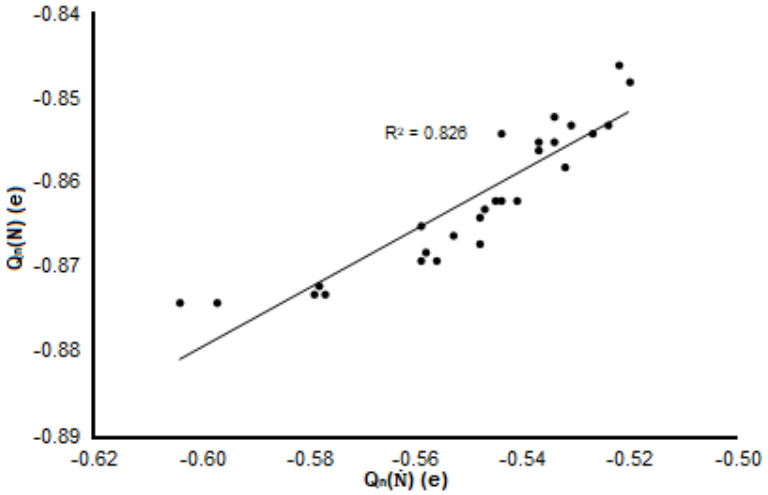

Fig S4. Natural partial charge on amino N atom of *para*-substituted anilines vs that in *para*-substituted anilinyl radicals

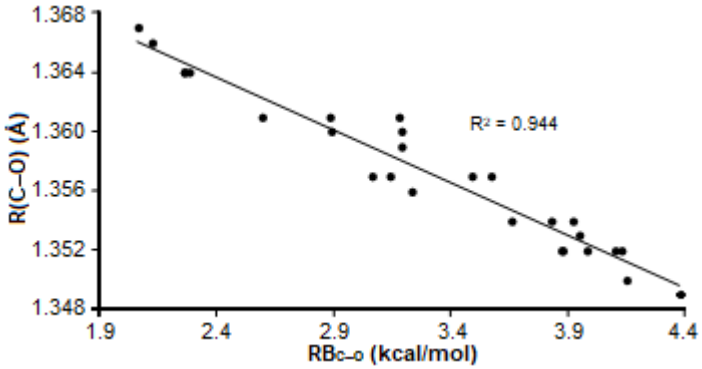

Fig S5. Phenyl–OH bond distance vs rotational barrier around phenyl–OH bond in *para*-substituted phenols

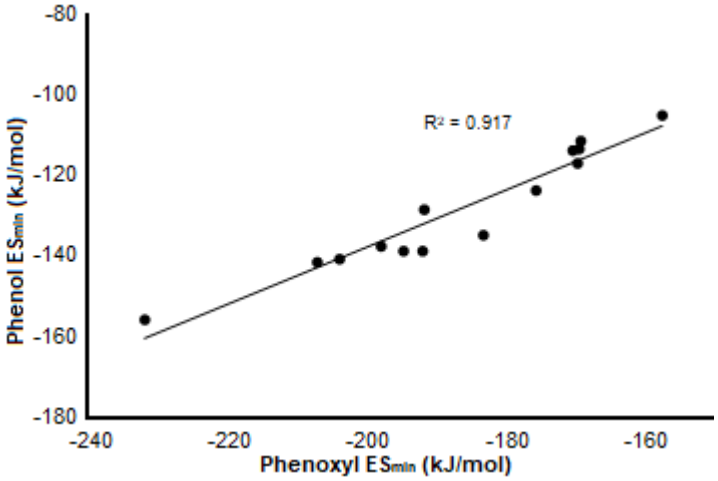

Fig S6. Minimum electrostatic potential around the hydroxyl O atom in *para*-substituted phenolic compounds vs that in *para*-substituted phenoxyl radicals

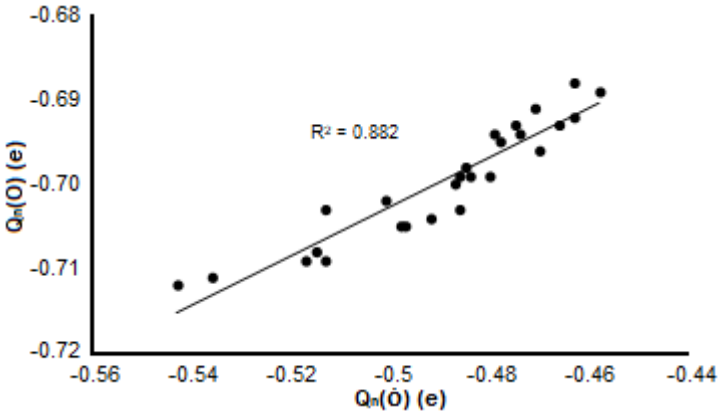

Fig S7. Natural partial charge on hydroxyl O atom of *para*-substituted phenols vs that in *para*-substituted phenoxyl radicals

Table S1. Symmetric and asymmetric NH_2 stretching frequencies, $\nu_s(NH_2)$ and $\nu_a(NH_2)$, respectively, for neutral anilinic compounds and the ṄH stretching frequency, ν(ṄH), of the corresponding anilinyl radicals

Substituent	Anilines		Anilinyls
	$\nu_s(NH_2)$ (cm^{-1})	$\nu_a(NH_2)$ (cm^{-1})	ν(ṄH)
COCl	3661	3782	3487
NO_2	3659	3779	3493
CHO	3646	3765	3492
COOH	3648	3765	3491
SiF_3	3649	3767	3489
CN	3652	3770	3493
SO_2CH_3	3654	3773	3491
$COCH_3$	3645	3762	3491
CO_2CH_3	3640	3756	3486
SCN	3651	3769	3494
CF_3	3644	3759	3490
SCH_3	3636	3749	3489
SH	3639	3752	3489
I	3638	3751	3491
Br	3638	3750	3491
Phenyl	3631	3743	3483
Cl	3637	3749	3491
H	3632	3743	3484
$C(CH_3)_3$	3629	3739	3485
CH_3	3628	3737	3486
OPhenyl	3629	3740	3490
F	3629	3738	3491
OCH_3	3616	3723	3490
OH	3618	3725	3490
OCH_2CH_3	3613	3721	3491
$N(CH_3)_2$	3611	3718	3488
NH_2	3613	3720	3489