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Group additive modeling of substituent effects in monocyclic aromatic hydrocarbon radicals — Source link

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Topics: Heat of formation group additivity, Substituent and Aromatic hydrocarbon

SUPPORTING MATERIAL

"Group Additive Modeling of Substituent Effects In Monocyclic Aromatic Hydrocarbon Radicals"

Alper Ince, Hans-Heinrich Carstensen, Maarten Sabbe
Marie-Françoise Reyniers and Guy B. Marin

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1. The Linear Regression Procedure and the Statistical Analysis

The Linear Regression and the calculation of $\overline{GAV/NNI}$ vector

As described in the text, a thermochemical property (y) of a radical is calculated through additivity of the values of GAV and NNI parameters based on how many times they occur in that radical. This leads to the following equation:

$$\sum_{i=1}^{n} X_i \beta_i = y \quad (1)$$

where X_i is the number of occurence of the parameter *i* in the radical and β_i is the value of the i^{th} parameter, which is calculated through the linear regression procedure. For each radical *j*, $\sum_{i=1}^{n} X_{ij} \beta_i$ is equal to $\hat{y}_j$, which is the group additively calculated thermochemical data of the radical whereas y_j represents the G4/BAC based thermochemical data for *j*.

Once Eq. 1 is written for all the *m* number of radicals, an overdetermined system of linear equations is obtained:

$$\sum_{j=1}^{m} X_{ij} \beta_i = y_j \text{ (i=1,2,.....n)} \quad (2)$$

Here, X_{ij} is the occurrence matrix which carries the information on how many times each of the parameters occur in each of the radicals and it has the dimensions of m x n.

Least-squares linear regression is carried out to solve this system of equations and obtain β_i vector, which contains the GAV/NNI parameters.

The difference between y_j and $\hat{y}_j$ can be called as "residual", as given in Eq. 3.

$$r_j = y_j - \sum_{i=1}^{n} X_i \beta_i \quad (3)$$

and the sum of the square of these residuals (SSQ) are given in Eq. 4.

$$SSQ = \sum_{j=1}^{m} (y_j - \hat{y}_j)^2 \quad (4)$$

The objective function SSQ, i.e. the square root of the difference between ab-initio data and the GA predictions with respect to the GAV/NNI parameters,β is minimized (argmin (SSQ)).

$$\frac{\partial SSQ}{\partial \beta} = 0 \quad (5)$$

This minimization yields the following equation:

$$(X^T X)\bar{\beta} = X^T \bar{y} \quad (6)$$

The expression in Eq. 6 can be rearranged to the following equation that yields $\bar{\beta}$, which is the $\overline{GAV/NNI}$ vector given in Eq. 15 of the text:

$$\overline{GAV/NNI} = (X^T X)^{-1} X^T \bar{y} \quad (7)$$

Since, the occurence matrix and the $\bar{y}$ vector, which contains the G4/BAC calculated thermochemical data are available, $\overline{GAV/NNI}$ vector can easily be calculated from Eq. 7 above. The $(X^T X)^{-1}$ matrix is separately calculated since it is needed for the calculation of confidence intervals, as explained below.

Calculation of Uncertainity of Parameters

First, mean squared errors (MSE) are calculated using SSQ and the degrees of freedom:

$$\text{MSE} = \frac{SSQ}{n_{molecules} - n_{parameters}} \quad (8)$$

MSE includes the variance of the residuals and the errors due to bias, i.e. systematic errors.

$$\text{MSE} = \sigma^2 + \text{Bias}^2 \quad (9)$$

These confidence intervals represent uncertainties only due to statistical errors. Several systematic sources of error exists, as explained in the text, they are not taken into consideration in this study and hence, the MSE is assumed to be equal to only σ^2.

Then, the variance-covarience matrix of parameters is calculated from the following equation:

$$\sum_{ij} Cov(X_i, X_j) = (X^T X)^{-1} * \sigma^2 \quad (10)$$

The diagonal of the covariance-variance matrix ($Cov(X_i, X_j)$) contains variances of the parameters, whereas the covariances of the parameters are obtained from the off-diagonals of this matrix.

The square root of the diagonal elements of the covariance-variance matrix, i.e. the standard deviations on the parameters, are used to calculate the confidence interval (CI_i) at 97.5% confidence level ($t_{97.5}$) of the i^{th} parameter.

$$CI_i = t_{97.5,i} * \sqrt{Cov(X_i, X_i)} \quad (11)$$

The final GAV and NNI parameters are reported with their uncertainities ($\beta_i \pm CI_i$) in Table 4 and 5, respectively.

2. List of Radicals

In this section of the Supporting Information, all the 389 radicals that appear in various sections of the article are listed.

Out of 389 radicals that appear in the article, 369 of them are monocyclic aromatic radicals (MARs) which are used for the development of GAV/NNI parameters, whereas the other 20 radicals are excluded due to the reasons described in the manuscript. The MARs within the framework of this study include unsubstituted and substituted phenyls (C_6H_5•), phenoxies (C_6H_5O•), anisyls ($C_6H_5OCH_2$•), benzoyls (C_6H_5C•=O), β-trans-styrlys (t-C_6H_5CH=CH•), β-cis-styrlys (c-C_6H_5CH=CH•), benzyls ($C_6H_5CH_2$•) and α-methylbenzyls (C_6H_5CH•CH_3).

These radicals are listed in three different sets: training set (**T**), validation set (**V**) and special cases set (**S**). Training set (**T**) includes 316 MARs that are used in the simultaneous determination of the preliminary Group Additive Values (GAVs) and non-nearest neighbor interactions (NNIs). Validation set (**V**) is used in order to test the applicability of the obtained GAVs and NNIs for the radicals that are outside the training set and this set encompasses 53 MARs. As described in the article, the final determination of these parameters are realized through the optimization of GAVs/NNIs based on the final set of 369 MARs which is formed via combination of training and validation sets. Special cases set (**S**) includes the set of 20 radicals that are excluded from the Group Additivity parameter development sets due to the reasons described in the article.

Each of these radical classes are listed in different subsets and the numbering of the radicals are based on these subset definitions. The number that corresponds to the n^{th} radical in m^{th} subset in the training set is given as "**Tm/n**", e.g. 21^{st} radical in phenyl subset (1^{st} subset) in the training set is numbered as **T1/21**. Six subsets exist in both training and test sets. These subsets are given in the following order: phenyl, phenoxy, anisyl, benzoyl, styryl and benzyl. Representations of the MARs in each of these subsets are given in the following subsections (**Figures S1**-**S14**) above the numbers and the abbreviations of the names of the corresponding MARs. In the list of molecules of the training set (**T**), these abbreviations are explained in each subsection for each subset with one example. In the validation set (**V**), the abbreviation of the radical names and the numbering method is the same, except that the numbering starts with "**V**" instead of "**T**".

In the substituted MARs of interest, the substituent groups are hydroxy (-OH), methoxy (-OCH_3), formyl (-CHO), vinyl (-$CH=CH_2$), methyl (-CH_3) and ethyl (-CH_2CH_3).

2.1 Training Set

2.1.1 Phenyl Subset

In the phenyl subset, there are 23 MARs. This subset of MARs include unsubstituted phenyl, 18 single substituted phenyls, 3 double substituted phenyls and 1 triple substituted phenyl. In the names given below, "C_6H_5•" refers to phenyl radical and single substituted phenyls are given as XC_6H_4• where X=-H,-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted phenyl (MAR no. **T1/2**) is abbreviated as o-OHC_6H_4•.

In double and triple substituted phenyls, the location of the radical site on the aryl ring is given as "C•", e.g. 1-C•-2-OH-3-OCH_3-5-CHO (MAR no. **T1/23**) represents 2-hydroxy-3-methoxy-5-formylphenyl.

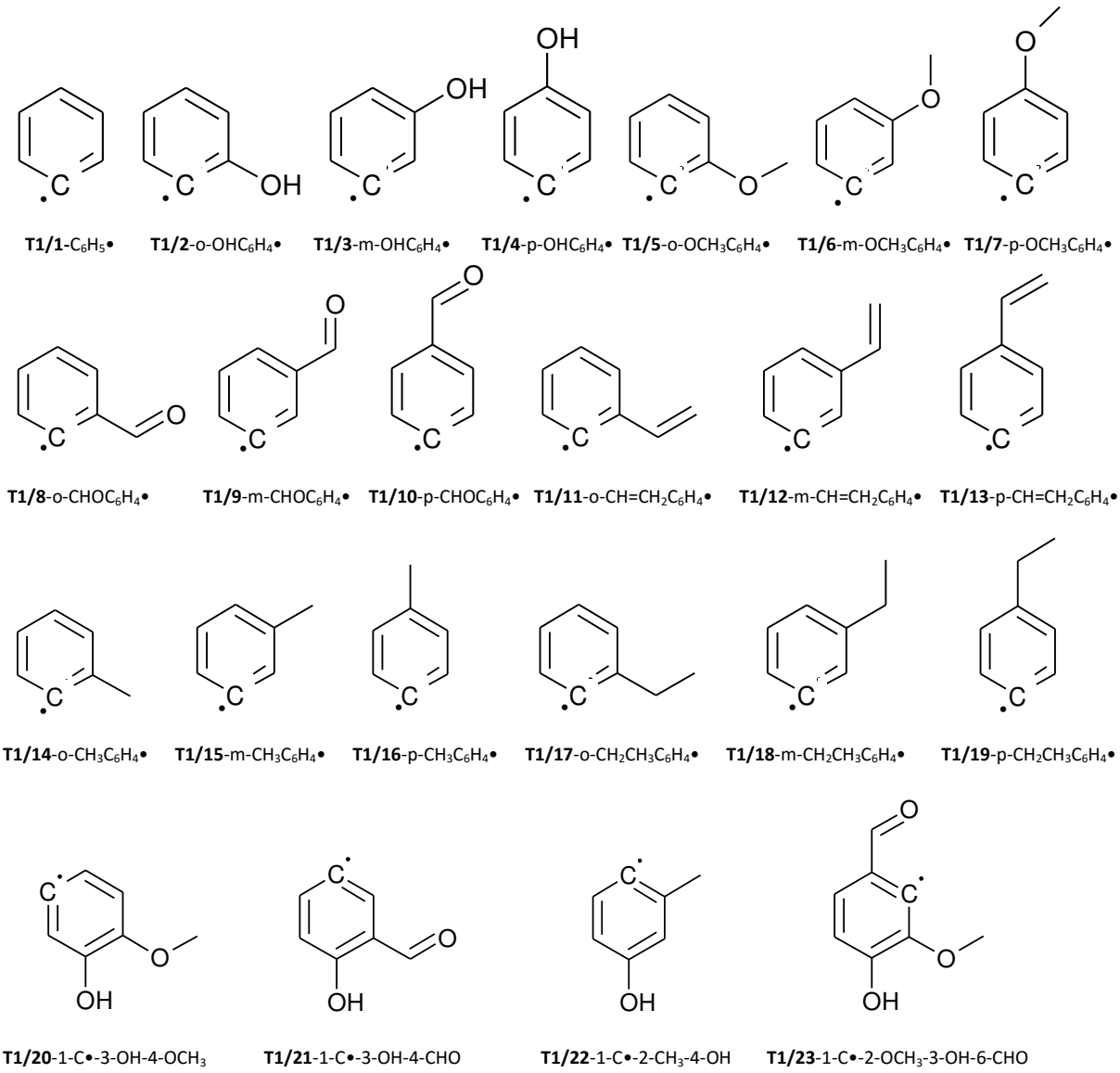
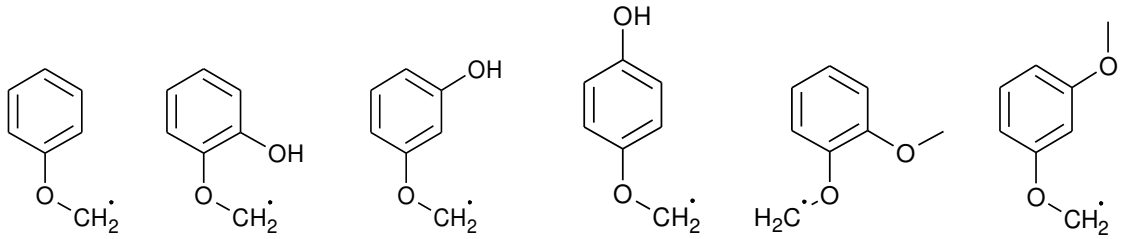


Figure S1. *List of radicals in phenyl subset of the training set.*

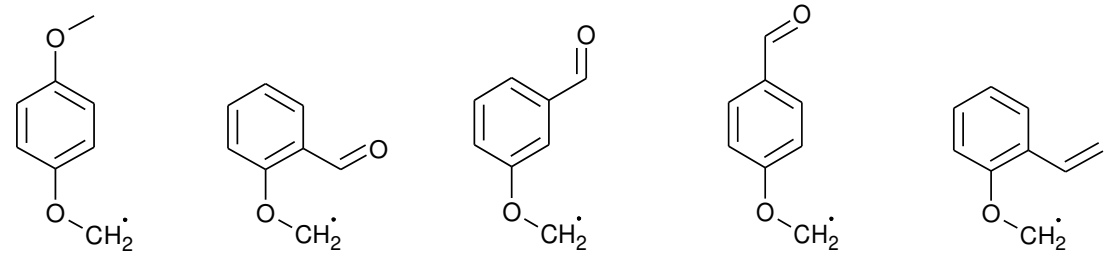
2.1.2 Anisyl Subset

There are 33 MARs in the "anisyl" subset of the training set of MARs which is composed of anisyl, 18 double substituted, 14 triple substituted anisyls. "$C_6H_5OCH_2$•" refers to anisyl radical and double substituted anisyls are given as (X)$C_6H_4OCH_2$• where X=-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted anisyl (MAR no. **T2/2**) is abbreviated as o-$OHC_6H_4OCH_2$•.

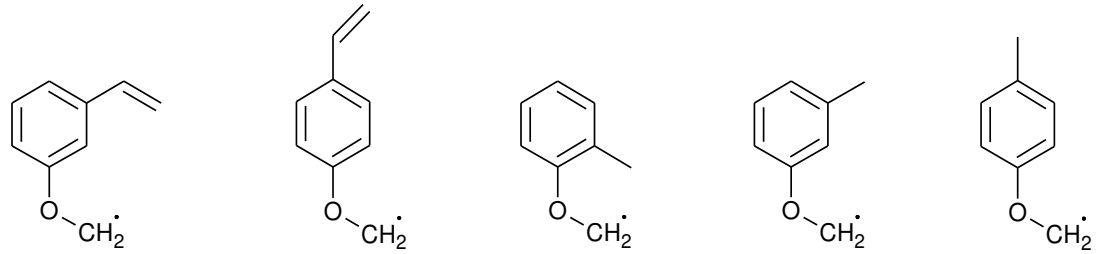
In triple substituted anisyls, "OCH_2•" is used to indicate radical substituent group. As an example; 2-hydroxy-5-vinylanisyl (MAR no. **T2/24**) is abbreviated as 1-OCH_2•-2-OH-5-$CH=CH_2$.



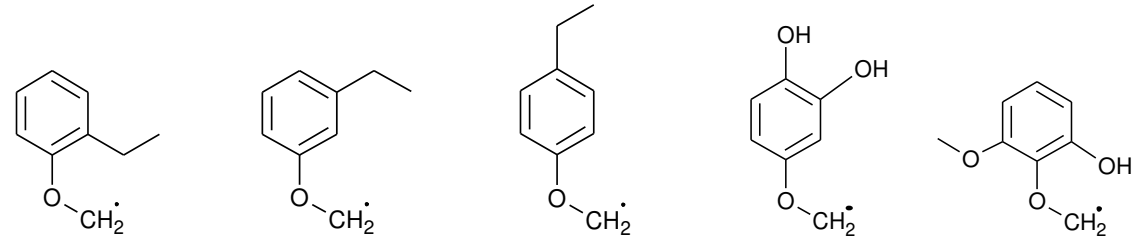
T2/1-$C_6H_5OCH_2$• **T2/2**-o-$(OH)C_6H_4OCH_2$• **T2/3**-m-$(OH)C_6H_4OCH_2$• **T2/4**-p-$(OH)C_6H_4OCH_2$• **T2/5**-o-$(OCH_3)C_6H_4OCH_2$• **T2/6**-m-$(OCH_3)C_6H_4OCH_2$•



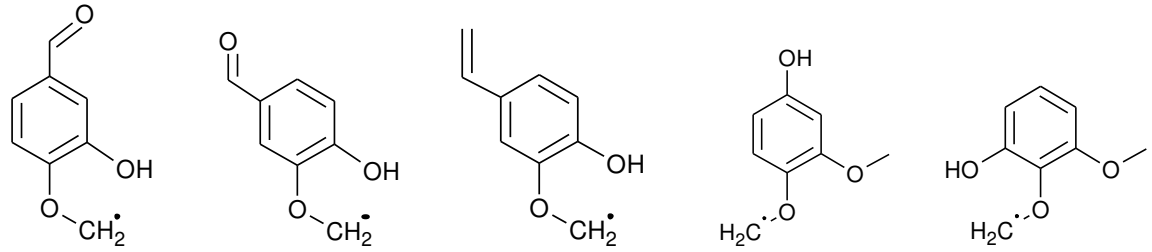
T2/7-p-$(OCH_3)C_6H_4OCH_2$• **T2/8**-o-$(CHO)C_6H_4OCH_2$• **T2/9**-m-$(CHO)C_6H_4OCH_2$• **T2/10**-p-$(CHO)C_6H_4OCH_2$• **T2/11**-o-$(CH{=}CH_2)C_6H_4OCH_2$•



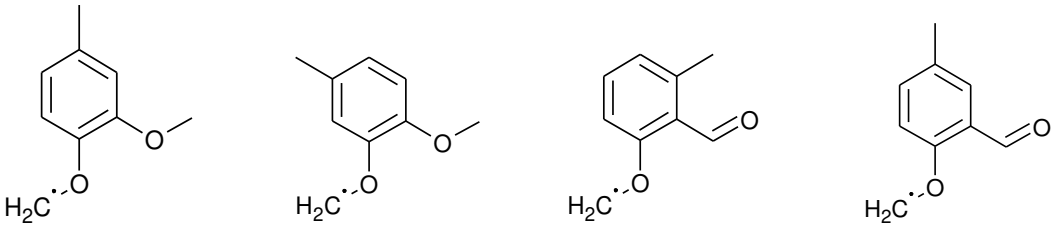
T2/12-m-$(CH{=}CH_2)C_6H_4OCH_2$• **T2/13**-p-$(CH{=}CH_2)C_6H_4OCH_2$• **T2/14**-o-$(CH_3)C_6H_4OCH_2$• **T2/15**-m-$(CH_3)C_6H_4OCH_2$• **T2/16**-p-$(CH_3)C_6H_4OCH_2$•



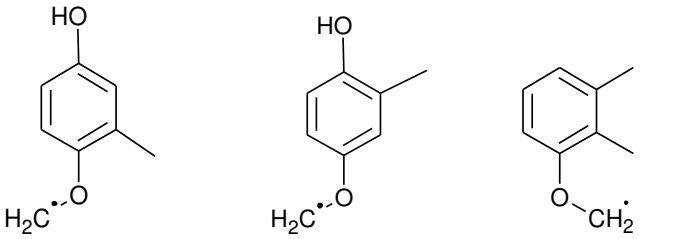
T2/17-o-$(CH_2CH_3)C_6H_4OCH_2$• **T2/18**-m-$(CH_2CH_3)C_6H_4OCH_2$•**T2/19**-p-$(CH_2CH_3)C_6H_4OCH_2$•**T2/20**-1-OCH_2•-3,4-OH **T2/21**-1-OCH_2•-2-OH-6-OCH_3



T2/22-1-OCH_2•-2-OH-4-CHO **T2/23**-1-OCH_2•-2-OH-5-CHO **T2/24**-1-OCH_2•-2-OH-5-$CH{=}CH_2$ **T2/25**-1-OCH_2•-2-OCH_3-4-OH **T2/26**-1-OCH_2•-2-OCH_3-6-OH



T2/27-1-OCH_2•-2-OCH_3-4-CH_3 **T2/28**-1-OCH_2•-2-OCH_3-5-CH_3 **T2/29**-1-OCH_2•-2-CHO-3-CH_3 **T2/30**-1-OCH_2•-2-CHO-4-CH_3



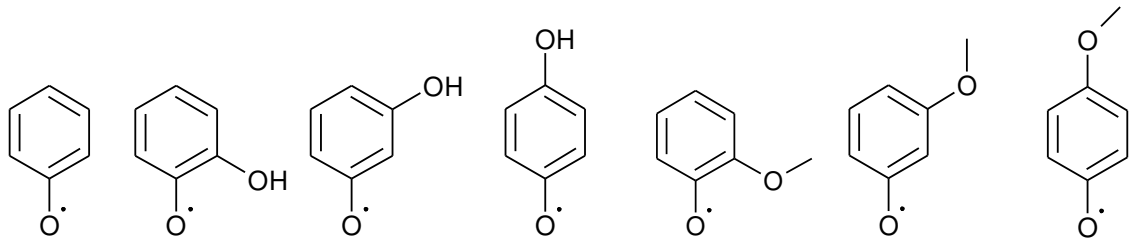
T2/31-1-OCH_2•-2-CH_3-4-OH **T2/32**-1-OCH_2•-3-CH_3-4-OH **T2/33**-1-OCH_2•-2,3-CH_3

Figure S2. *List of radicals in anisyl subset of the training set.*

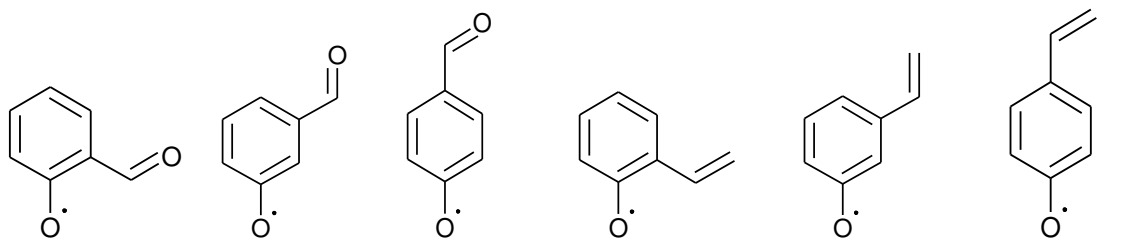
2.1.3 Phenoxy Subset

There are 68 MARs in the "phenoxy" subset of the training set of MARs which is composed of phenoxy, 18 double, 47 triple and 2 quadruple phenoxies. "C_6H_5O•" refers to phenoxy radical and double substituted phenoxies are given as (X)C_6H_4O• where X=-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted phenoxy (MAR no. **T3/2**) is abbreviated as o-OHC_6H_4O•.

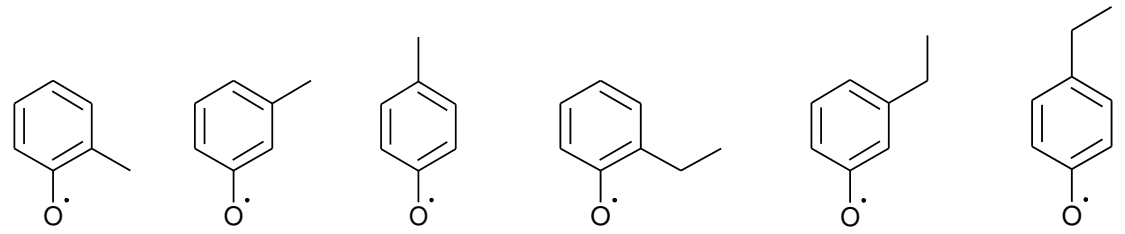
In multiple (triple and quadruple) substituted phenoxies, "O•" is used to indicate oxygen substituent with radical center. As an example; 2-formyl-4-methylphenoxy (MAR no. **T3/59**) is abbreviated as 1-O•-2-CHO-4-CH_3.



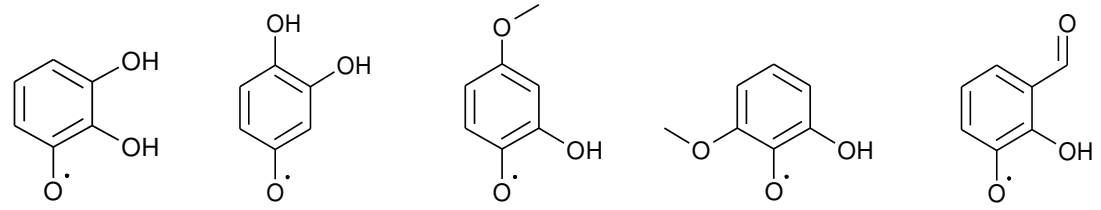
T3/1-C_6H_5O• **T3/2**-o-(OH)C_6H_4O• **T3/3**-m-(OH)C_6H_4O• **T3/4**-p-(OH)C_6H_4O• **T3/5**-o-(OCH_3)C6H4O• **T3/6**-m-(OCH_3)C6H4O• **T3/7**-p-(OCH_3)C_6H_4O•



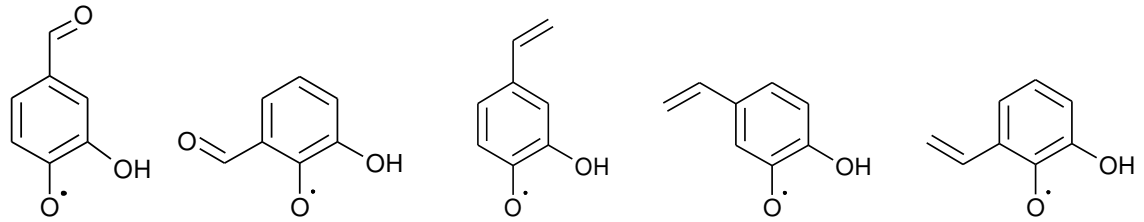
T3/8-o-(CHO)C_6H_4O• **T3/9**-m-(CHO)C_6H_4O• **T3/10**-p-(CHO)C_6H_4O• **T3/11**-o-($CH=CH_2$)C_6H_4O• **T3/12**-m-($CH=CH_2$)C_6H_4O• **T3/13**-p-($CH=CH_2$)C_6H_4O•



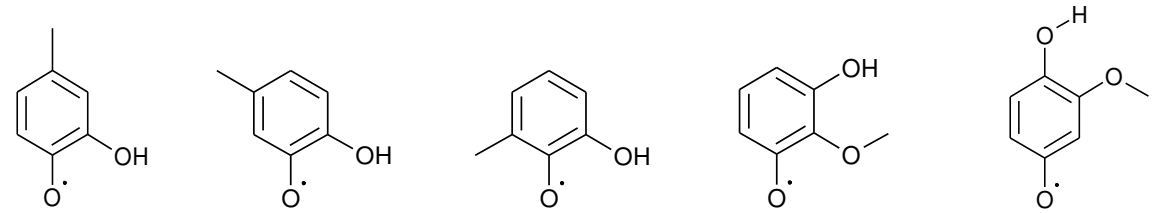
T3/14-o-$(CH_3)C_6H_4O$• **T3/15**-m-$(CH_3)C_6H_4O$• **T3/16**-p-$(CH_3)C_6H_4O$• **T3/17**-o-$(CH_2CH_3)C_6H_4O$• **T3/18**-m-$(CH_2CH_3)C_6H_4O$• **T3/19**-p-$(CH_2CH_3)C_6H_4O$•



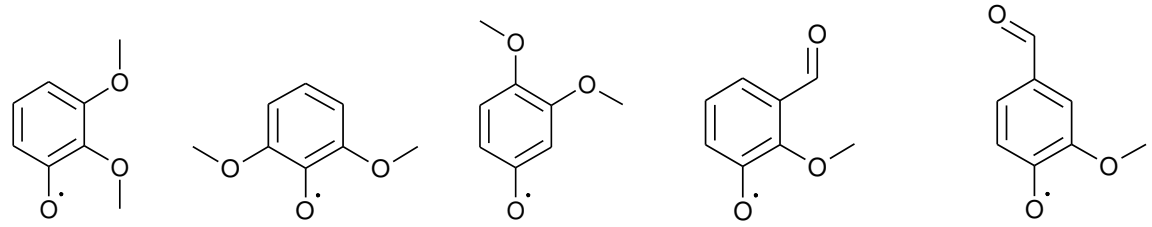
T3/20-1-O•-2,3-OH **T3/21**-1-O•-3,4-OH **T3/22**-1-O•-2-OH-4-OCH_3 **T3/23**-1-O•-2-OH-6-OCH_3 **T3/24**-1-O•-2-OH-3-CHO



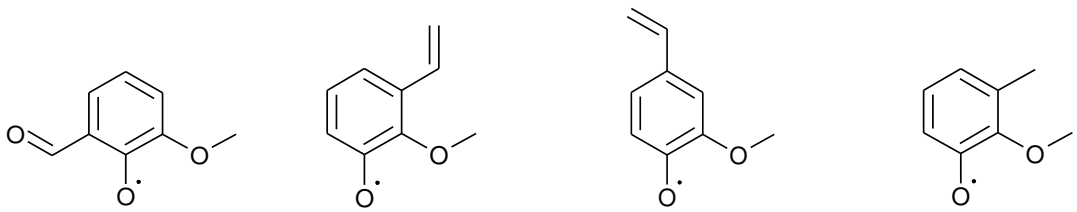
T3/25-1-O•-2-OH-4-CHO **T2/26**-1-O•-2-OH-6-CHO **T2/27**-1-O•-2-OH-4-$CH=CH_2$ **T2/28**-1-O•-2-OH-5-$CH=CH_2$ **T2/29**-1-O•-2-OH-6-$CH=CH_2$



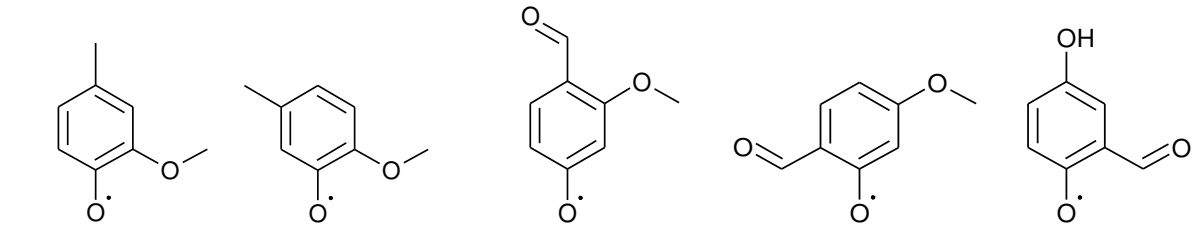
T2/30-1-O•-2-OH-4-CH_3 **T2/31**-1-O•-2-OH-5-CH_3 **T2/32**-1-O•-2-OH-6-CH_3 **T3/33**-1-O•-2-OCH_3-3-OH **T3/34**-1-O•-3-OCH_3-4-OH



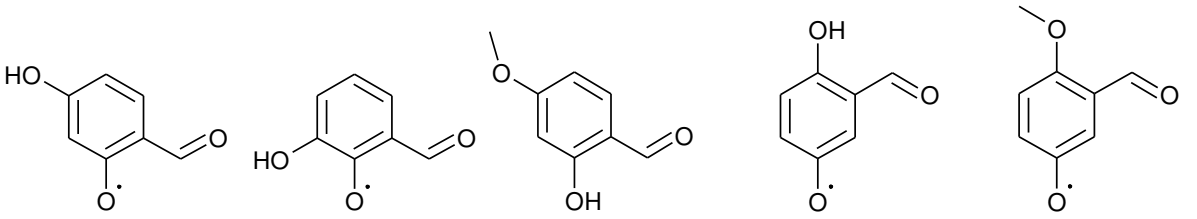
T3/35-1-O•-2,3-OCH_3 **T3/36**-1-O•-2,6-OCH_3 **T3/37**-1-O•-3,4-OCH_3 **T3/38**-1-O•-2-OCH_3-3-CHO **T3/39**-1-O•-2-OCH_3-4-CHO



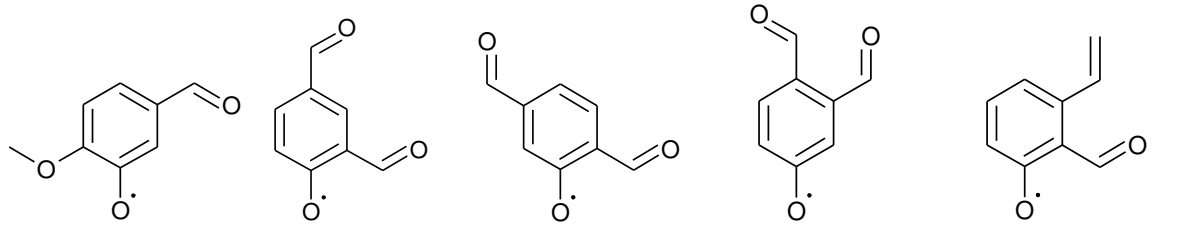
T3/40-1-O•-2-OCH_3-6-CHO **T3/41**-1-O•-2-OCH_3-3-$CH=CH_2$ **T3/42**-1-O•-2-OCH_3-4-$CH=CH_2$ **T3/43**-1-O•-2-OCH_3-3-CH_3



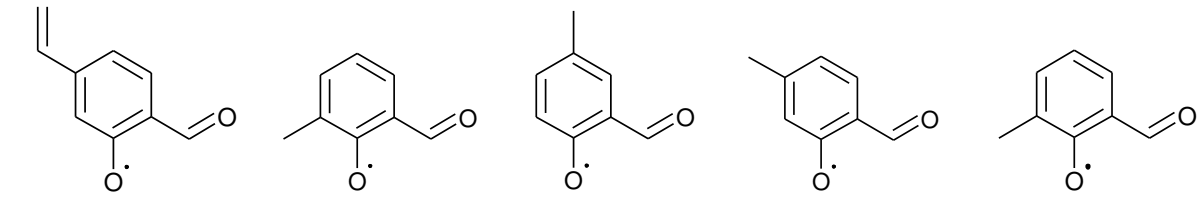
T3/44-1-O•-2-OCH_3-4-CH_3 **T3/45**-1-O•-2-OCH_3-5-CH_3 **T3/46**-1-O•-3-OCH_3-4-CHO **T3/47**-1-O•-3-OCH_3-6-CHO **T3/48**-1-O•-2-CHO-4-OH



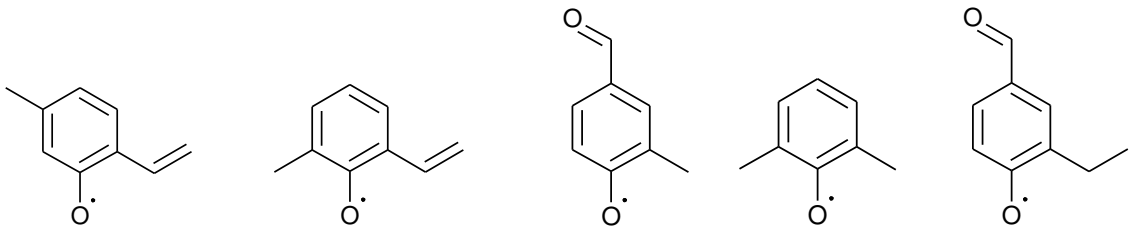
T3/49-1-O•-2-CHO-5-OH **T3/50**-1-O•-2-CHO-6-OH **T3/51**-1-O•-2-CHO-5-OCH_3 **T3/52**-1-O•-3-CHO-4-OH **T3/53**-1-O•-3-CHO-4-OCH_3



T3/54-1-O•-3-CHO-6-OCH_3 **T3/55**-1-O•-2,4-CHO **T3/56**-1-O•-2,5-CHO **T3/57**-1-O•-3,4-CHO **T3/58**-1-O•-2-CHO-3-$CH=CH_2$



T3/59-1-O•-2-CHO-5-$CH=CH_2$ **T3/60**-1-O•-2-CHO-6-CH_3 **T3/61**-1-O•-2-CHO-4-CH_3 **T3/62**-1-O•-2-CHO-5-CH_3 **T3/63**-1-O•-2-CHO-6-CH_3



T3/64-1-O•-2-$CH=CH_2$-5-CH_3 **T3/65**-1-O•-2-$CH=CH_2$-6-CH_3 **T3/66**-1-O•-2-CH_3-4-CHO **T3/67**-1-O•-2,6-CH_3 **T3/68**-1-O•-2-CH_2CH_3-4-CHO

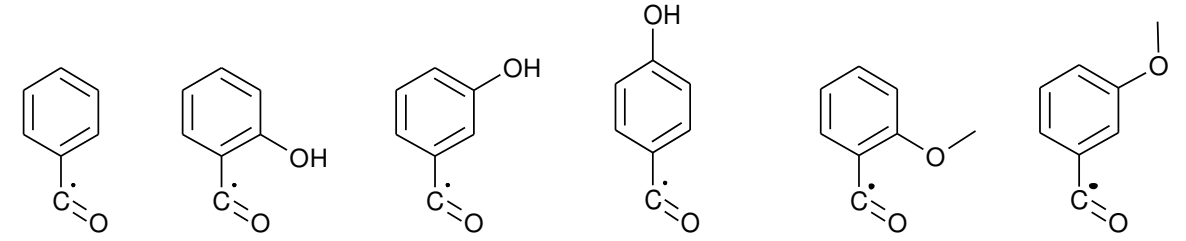
Figure S3. *List of radicals in phenoxy subset of the training set.*

2.1.4 Benzoyl Subset

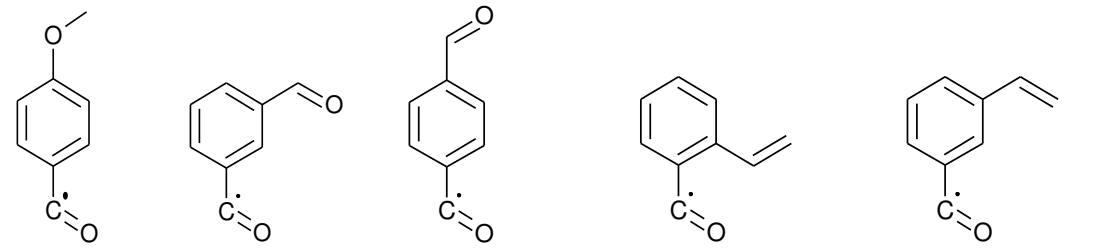
There are 42 MARs in the "benzoyl" subset of the training set of MARs which is composed of benzoyl, 18 double substituted and 23 triple substituted benzoyls. "C_6H_5C•=O" refers to benzoyl radical and

double substituted benzoyls are given as (X)$C_6H_4C\bullet=O$ where X=-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted benzoyl (MAR no. **T4/2**) is abbreviated as o-$OHC_6H_4C\bullet=O$.

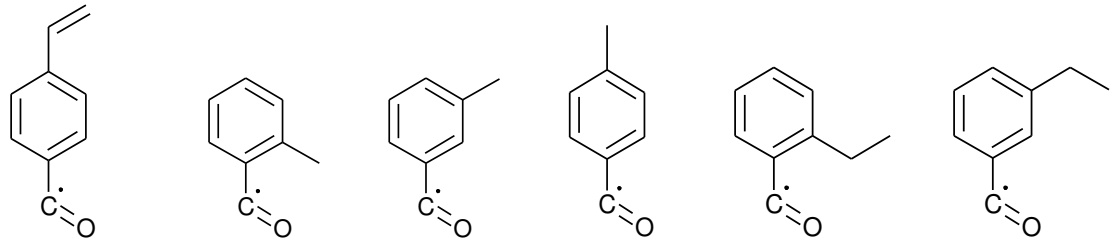
In triple substituted benzoyls, "C•=O" is used to indicate radical substituent group. As an example; 3-hydroxy-4-vinylbenzoyl (MAR no. **T4/25**) is abbreviated as 1-C•=O-3-OH-4-$CH=CH_2$.



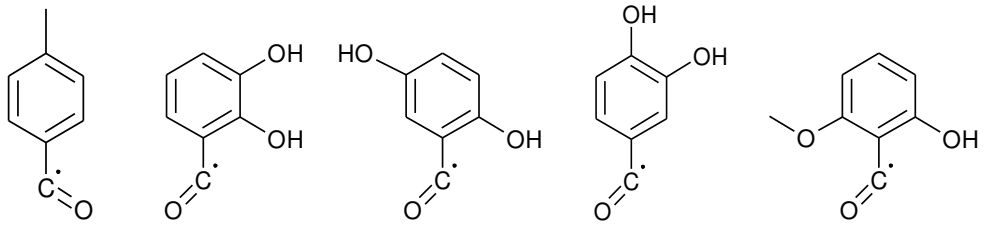
T4/1-$C_6H_5C\bullet=O$ **T4/2**-o-$(OH)C_6H_4C\bullet=O$ **T4/3**-m-$(OH)C_6H_4C\bullet=O$ **T4/4**-p-$(OH)C_6H_4C\bullet=O$ **T4/5**-o-$(OCH_3)C_6H_4C\bullet=O$ **T4/6**-m-$(OCH_3)C_6H_4C\bullet=O$



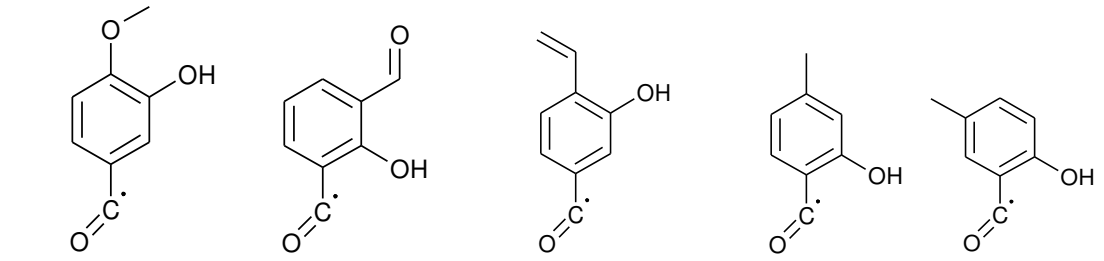
T4/7-p-$(OCH_3)C_6H_4C\bullet=O$ **T4/8**-m-$(CHO)C_6H_4C\bullet=O$ **T4/9**-p-$(CHO)C_6H_4C\bullet=O$ **T4/10**-o-$(CH=CH_2)C_6H_4C\bullet=O$ **T4/11**-m-$(CH=CH_2)C_6H_4C\bullet=O$



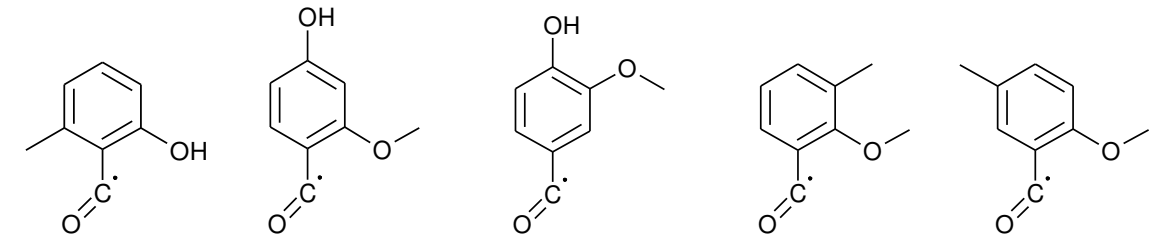
T4/12-p-$(CH=CH_2)C_6H_4C\bullet=O$ **T4/13**-o-$(CH_3)C_6H_4C\bullet=O$ **T4/14**-m-$(CH_3)C_6H_4C\bullet=O$ **T4/15**-p-$(CH_3)C_6H_4C\bullet=O$ **T4/16**-o-$(CH_2CH_3)C_6H_4C\bullet=O$ **T4/17**-m-$(CH_2CH_3)C_6H_4C\bullet=O$



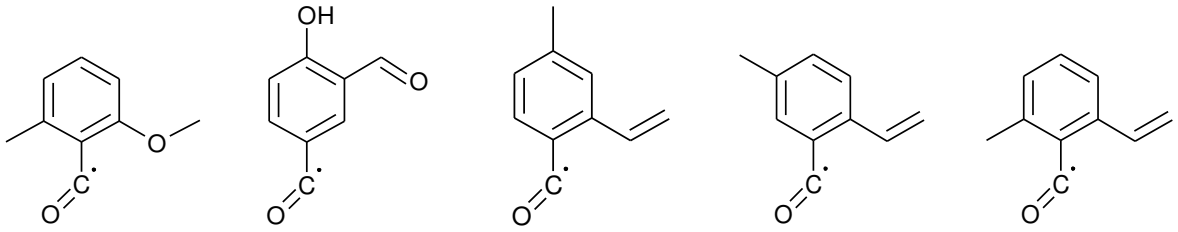
T4/18-p-$(CH_2CH_3)C_6H_4C\bullet=O$ **T4/19**-1-C•=O-2,3-OH **T4/20**-1-C•=O-2,5-OH **T4/21**-1-C•=O-3,4-OH **T4/22**-1-C•=O-2-OH-6-OCH_3



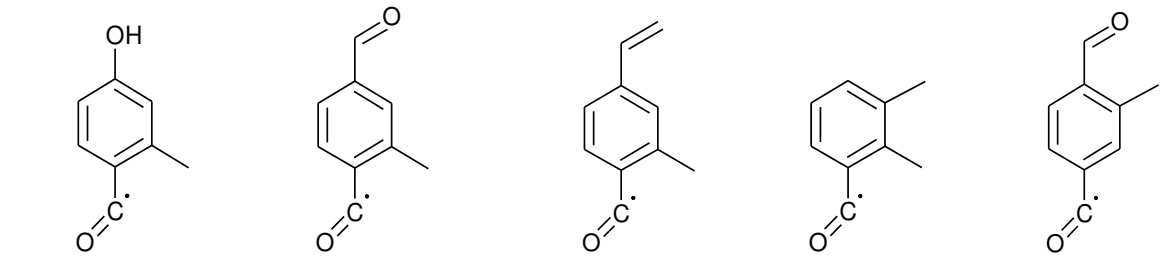
T4/23-1-C•=O-3-OH-4-OCH_3 **T4/24**-1-C•=O-2-OH-3-CHO **T4/25**-1-C•=O-3-OH-4-$CH=CH_2$ **T4/26**-1-C•=O-2-OH-4-CH_3 **T4/27**-1-C•=O-2-OH-5-CH_3



T4/28-1-C•=O-2-OH-6-CH_3 **T4/29**-1-C•=O-2-OCH_3-4-OH **T4/30**-1-C•=O-3-OCH_3-4-OH **T4/31**-1-C•=O-2-OCH_3-3-CH_3 **T4/32**-1-C•=O-2-OCH_3-5-CH_3



T4/33-1-C•=O-2-OCH_3-6-CH_3 **T4/34**-1-C•=O-3-CHO-4-OH **T4/35**-1-C•=O-2-$CH=CH_2$-4-CH_3 **T4/36**-1-C•=O-2-$CH=CH_2$-5-CH_3 **T4/37**-1-C•=O-2-$CH=CH_2$-6-CH_3



T4/38-1-C•=O-2-CH_3-4-OH **T4/39**-1-C•=O-2-CH_3-4-CHO **T4/40**-1-C•=O-2-CH_3-4-$CH=CH_2$ **T4/41**-1-C•=O-2,3-CH_3 **T4/42**-1-C•=O-3-CH_3-4-CHO

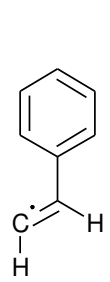
Figure S4. *List of radicals in benzoyl subset of the training set.*

2.1.5 β-Styryl Subset

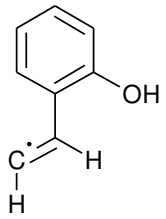
There are 80 styrlys in this subset of the training set of MARs which is composed of 38 unsubstituted and substituted trans-β-styryls and 42 unsubstituted and substituted cis-β-styryls. "t-$C_6H_5CH=CH$•" and "c-$C_6H_5CH=CH$•" refers to trans-β-styryl and cis-β-styryl radicals, respectively. The names of the double substituted radicals of trans-β-styryls and cis-β-styryls are given as (X)t-$C_6H_5CH=CH$• and (X)c-

$C_6H_5CH=CH•$, respectively where X=-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted trans-β-styryl (MAR no. **T5/2**) is abbreviated as o-(OH)t-$C_6H_4CH=CH•$.

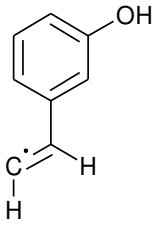
In triple substituted styryls, "t-CH=CH•" and "c-CH=CH•" represents the trans and cis radical vinyl groups, respectively. As an example; 2-hydroxy-5-vinyl trans-β-styryl (MAR no. **T5/25**) is abbreviated as 1-(t-CH=CH•)-2-OH-5-$CH=CH_2$.



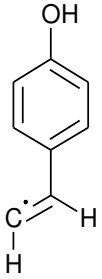
T5/1-t-$C_6H_5CH=CH•$



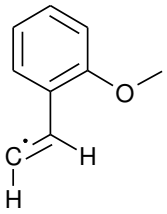
T5/2-o-(OH)t-$C_6H_4CH=CH•$



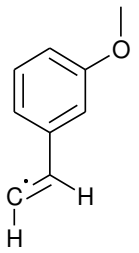
T5/3-m-(OH)t-$C_6H_4CH=CH•$



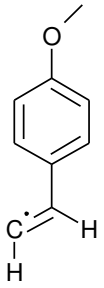
T5/4-p-(OH)t-$C_6H_4CH=CH•$



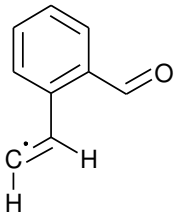
T5/5-o-(OCH_3)t-$C_6H_4CH=CH•$



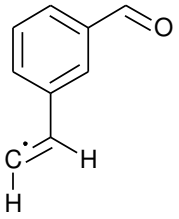
T5/6-m-(OCH_3)t-$C_6H_4CH=CH•$



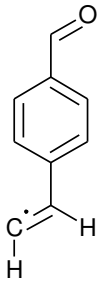
T5/7-p-(OCH_3)t-$C_6H_4CH=CH•$



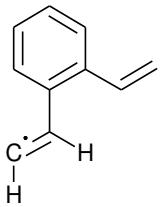
T5/8-o-(CHO)t-$C_6H_4CH=CH•$



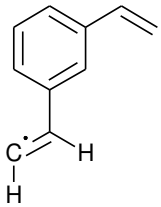
T5/9-m-(CHO)t-$C_6H_4CH=CH•$



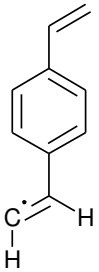
T5/10-p-(CHO)t-$C_6H_4CH=CH•$



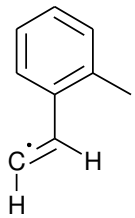
T5/11-o-($CH=CH_2$)t-$C_6H_4CH=CH•$



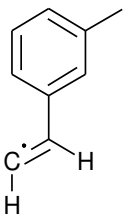
T5/12-m-($CH=CH_2$)t-$C_6H_4CH=CH•$



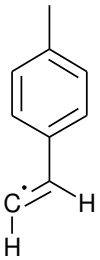
T5/13-p-($CH=CH_2$)t-$C_6H_4CH=CH•$



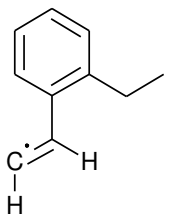
T5/14-o-(CH_3)t-$C_6H_4CH=CH•$



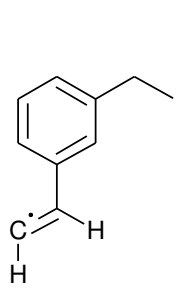
T5/15-m-(CH_3)t-$C_6H_4CH=CH•$

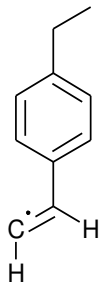


T5/16-p-(CH_3)t-$C_6H_4CH=CH•$

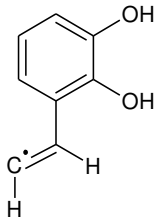


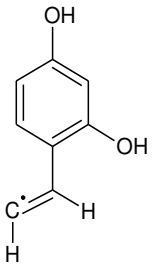
T5/17-o-(CH_2CH_3)$C_6H_4CH=CH•$

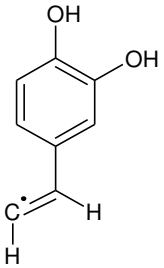


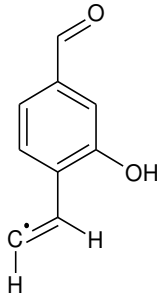


T5/18-m-$(CH_2CH_3)C_6H_4CH{=}CH\bullet$ **T5/19**-p-$(CH_2CH_3)C_6H_4CH{=}CH\bullet$

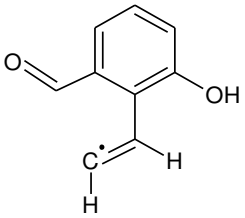


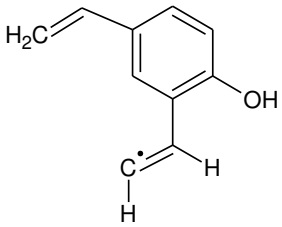


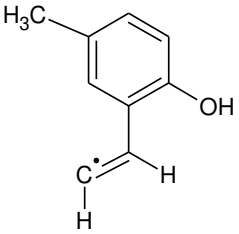




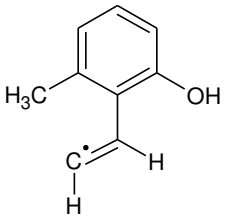
T5/20-1-(t-CH=CH•)-2,3-OH **T5/21**-1-(t-CH=CH•)-2,4-OH **T5/22**-1-(t-CH=CH•)-3,4-OH **T5/23**-1-(t-CH=CH•)-2-OH-4-CHO

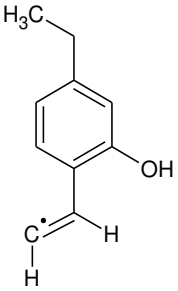


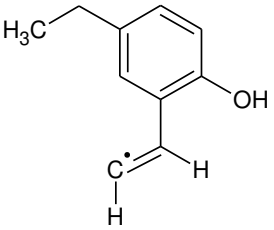


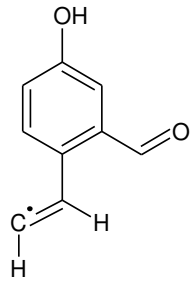


T5/24-1-(t-CH=CH•)-2-OH-6-CHO **T5/25**-1-(t-CH=CH•)-2-OH-5-$CH{=}CH_2$ **T5/26**-1-(t-CH=CH•)-2-OH-5-CH_3

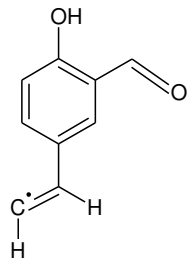


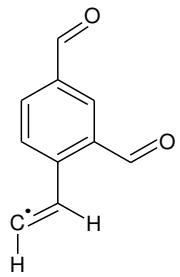


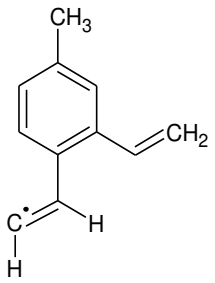


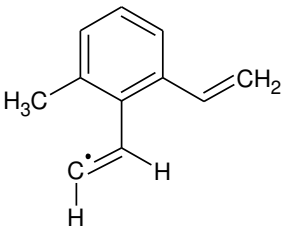


T5/27-1-(t-CH=CH•)-2-OH-6-CH_3 **T5/28**-1-(t-CH=CH•)-2-OH-4-CH_2CH_3 **T5/29**-1-(t-CH=CH•)-2-OH-5-CH_2CH_3 **T5/30**-1-(t-CH=CH•)-2-CHO-4-OH

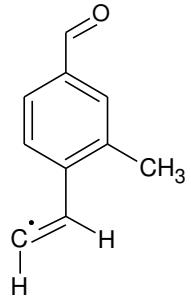




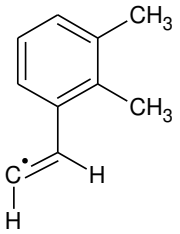




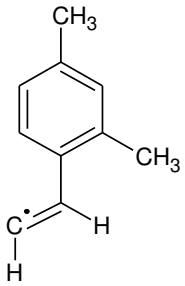
T5/31-1-(t-CH=CH•)-3-CHO-4-OH **T5/32**-1-(t-CH=CH•)-2,4-CHO **T5/33**-1-(t-CH=CH•)-2-$CH{=}CH_2$-4-CH_3 **T5/34**-1-(t-CH=CH•)-2-$CH{=}CH_2$-6-CH_3



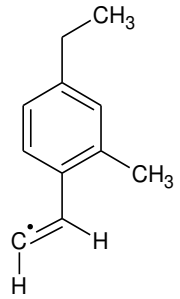
T5/35-1-(t-CH=CH•)-2-CH_3-4-CHO



T5/36-1-(t-CH=CH•)-2,3-CH_3

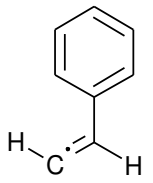


T5/37-1-(t-CH=CH•)-2,4-CH_3

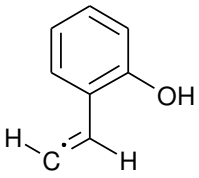


T5/38-1-(t-CH=CH•)-2-CH_3-4-CH_2CH_3

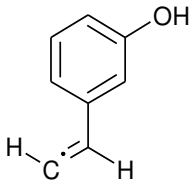
Figure S5. *Trans-β-styryl radicals in styryls subset of the training set.*



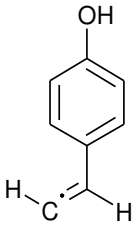
T5/39-c-C_6H_5CH=CH•



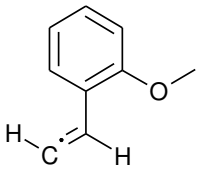
T5/40-o-(OH)c-C_6H_4CH=CH•



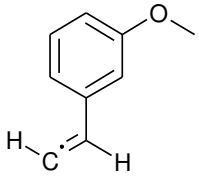
T5/41-m-(OH)c-C_6H_4CH=CH•



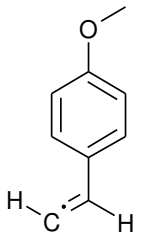
T5/42-p-(OH)c-C_6H_4CH=CH•



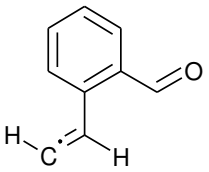
T5/43-o-(OCH_3)c-C_6H_4CH=CH•



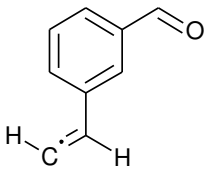
T5/44-m-(OCH_3)c-C_6H_4CH=CH•



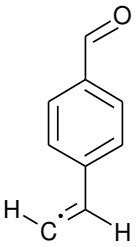
T5/45-p-(OCH_3)c-C_6H_4CH=CH•



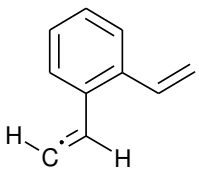
T5/46-o-(CHO)c-C_6H_4CH=CH•



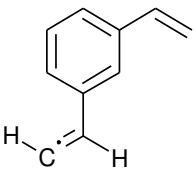
T5/47-m-(CHO)c-C_6H_4CH=CH•



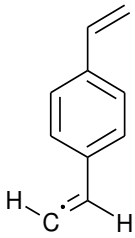
T5/48-p-(CHO)c-C_6H_4CH=CH•



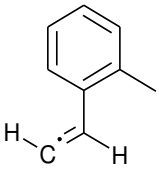
T5/49-o-($CH=CH_2$)c-C_6H_4CH=CH•



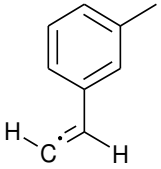
T5/50-m-($CH=CH_2$)c-C_6H_4CH=CH•



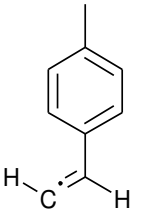
T5/51-p-($CH=CH_2$)c-C_6H_4CH=CH•



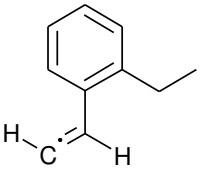
T5/52-o-(CH_3)c-C_6H_4CH=CH•



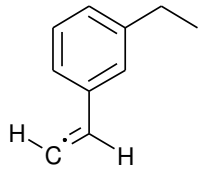
T5/53-m-(CH_3)c-C_6H_4CH=CH•



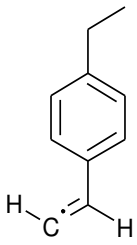
T5/54-p-(CH_3)c-C_6H_4CH=CH•



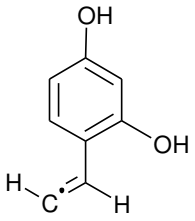
T5/55-o-(CH_2CH_3)C_6H_4CH=CH•



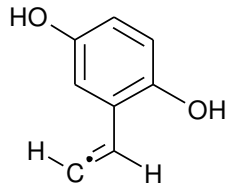
T5/56-m-(CH_2CH_3)C_6H_4CH=CH•



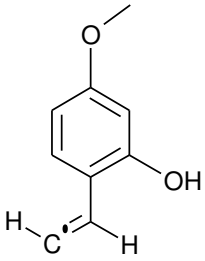
T5/57-p-(CH_2CH_3)C_6H_4CH=CH•



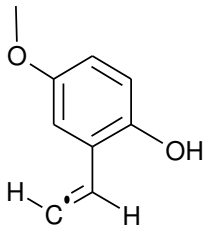
T5/58-1-(c-CH=CH•)-2,4-OH



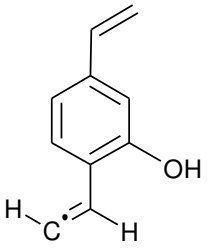
T5/59-1-(c-CH=CH•)-2,5-OH



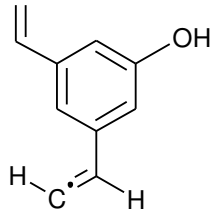
T5/60-1-(c-CH=CH•)-2-OH-4-OCH_3



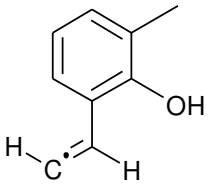
T5/61-1-(c-CH=CH•)-2-OH-5-OCH_3



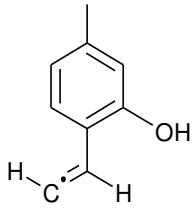
T5/62-1-(c-CH=CH•)-2-OH-4-$CH=CH_2$



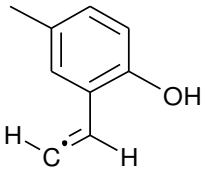
T5/63-1-(c-CH=CH•)-3-OH-5-$CH=CH_2$



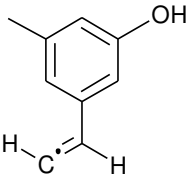
T5/64-1-(c-CH=CH•)-2-OH-3-CH_3



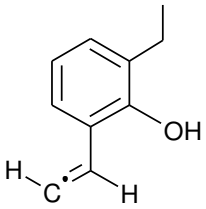
T5/65-1-(c-CH=CH•)-2-OH-4-CH_3



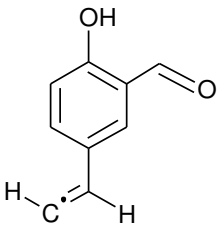
T5/66-1-(c-CH=CH•)-2-OH-5-CH_3



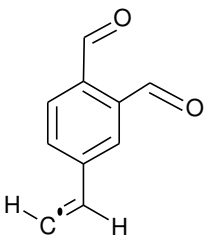
T5/67-1-(c-CH=CH•)-3-OH-5-CH_3



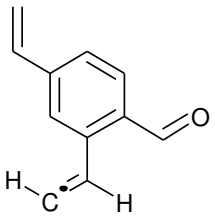
T5/68-1-(c-CH=CH•)-2-OH-3-CH_2CH_3



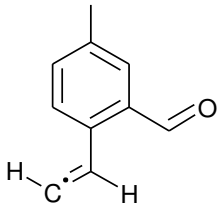
T5/69-1-(c-CH=CH•)-3-CHO-4-OH



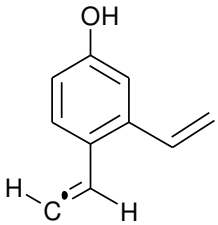
T5/70-1-(c-CH=CH•)-2,4-CHO



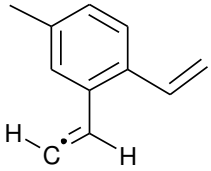
T5/71-1-(c-CH=CH•)-2-CHO-5-$CH=CH_2$

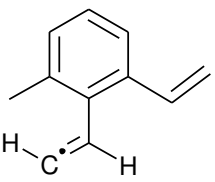


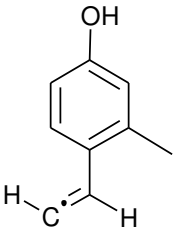
T5/72-1-(c-CH=CH•)-2-CHO-4-CH_3



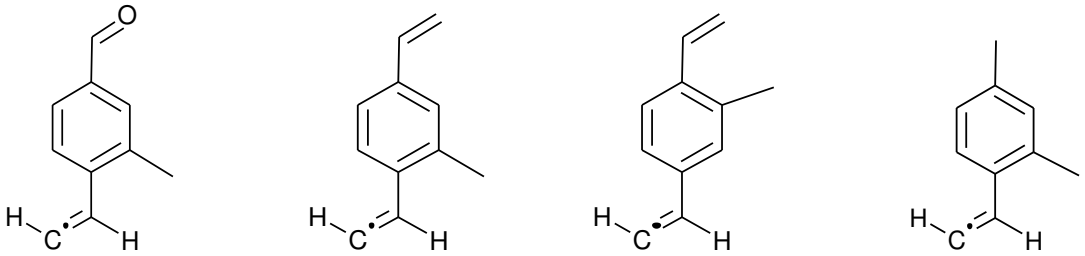
T5/73-1-(c-CH=CH•)-2-$CH=CH_2$-4-OH







T5/74-1-(c-CH=CH•)-2-CH=CH_2-5-CH_3 **T5/75**-1-(c-CH=CH•)-2-CH=CH_2-6-CH_3 **T5/76**-1-(c-CH=CH•)-2-CH_3-4-OH



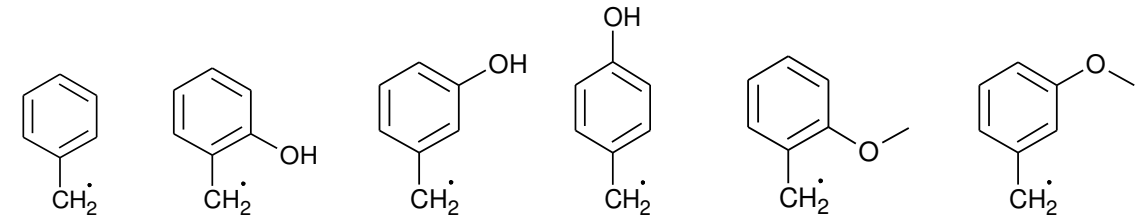
T5/77-1-(c-CH=CH•)-2-CH_3-4-CHO **T5/78**-1-(c-CH=CH•)-2-CH_3-4-CH=CH_2 **T5/79**-1-(c-CH=CH•)-3-CH_3-4-CH=CH_2 **T5/80**-1-(c-CH=CH•)-2,4-CH_3

Figure S6. *Cis-β-styryl radicals in styryls subset of the training set.*

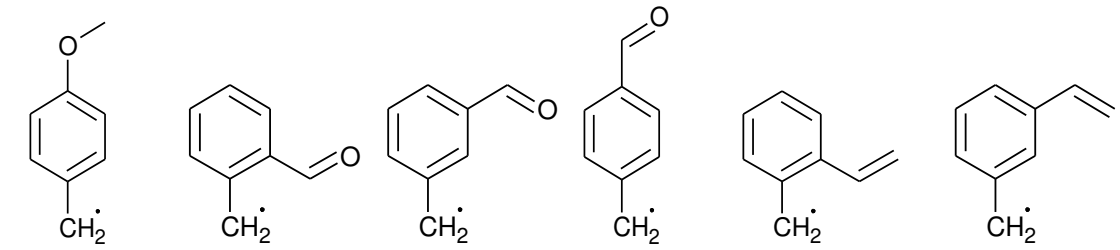
2.1.6 Benzyl/1-Phenylethyl Subset

There are 70 MARs in the "benzyl" subset of the training set of MARs which is composed of benzyl, α-methylbenzyl, 18 double substituted, 32 triple substituted benzyls and 18 double substituted α-methylbenzyls. "$C_6H_5CH_2$•" and "C_6H_5CH•CH_3" refers to benzyl and α-methylbenzyl radicals, respectively. Double substituted benzyls and α-methylbenzyls are given as (X)$C_6H_4CH_2$• and (X)C_6H_4CH•CH_3, respectively where X=-OH,-OCH_3,-CHO, -$CH=CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted benzyl (MAR no. **6/2**) is abbreviated as o-$OHC_6H_4CH_2$•.

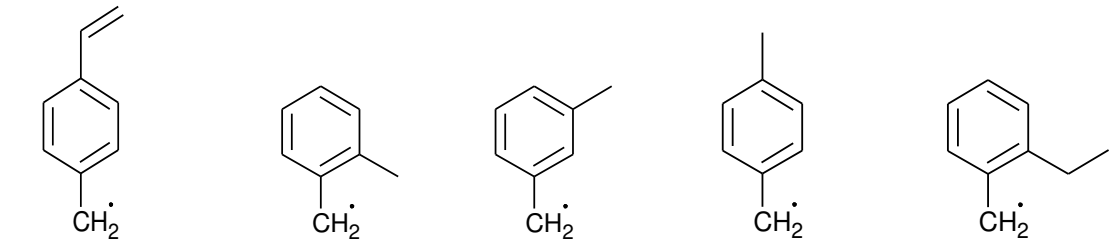
In triple substituted benzyls, "CH_2•" is used to indicate radical substituent group. As an example; 2,4-dihydroxybenzyl (MAR no. **6/21**) is abbreviated as 1-CH_2•-2,4-OH. There are no triple substituted α-methylbenzyls in the database.



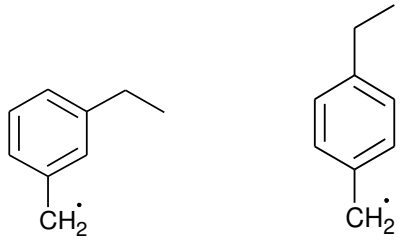
T6/1-$C_6H_5CH_2$• **T6/2**-o-$(OH)C_6H_4CH_2$• **T6/3**-m-$(OH)C_6H_4CH_2$• **T6/4**-p-$(OH)C_6H_4CH_2$• **T6/5**-o-$(OCH_3)C_6H_4CH_2$• **T6/6**-m-$(OCH_3)C_6H_4CH_2$•



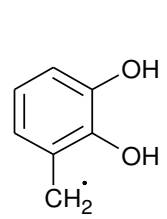
T6/7-p-$(OCH_3)C_6H_4CH_2$• **T6/8**-o-$(CHO)C_6H_4CH_2$• **T6/9**-m-$(CHO)C_6H_4CH_2$•**T6/10**-p-$(CHO)C_6H_4CH_2$• **T6/11**-o-$(CH=CH_2)C_6H_4CH_2$• **T6/12**-m-$(CH=CH_2)C_6H_4CH_2$•



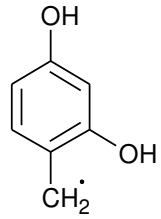
T6/13-(p-$CH=CH_2$)$C_6H_4CH_2$• **T6/14**-o-$(CH_3)C_6H_4CH_2$• **T6/15**-m-$(CH_3)C_6H_4CH_2$• **T6/16**-p-$(CH_3)C_6H_4CH_2$• **T6/17**-o-$(CH_2CH_3)C_6H_4CH_2$•



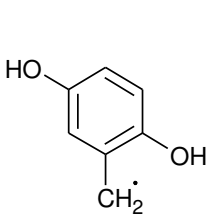
T6/18-m-$(CH_2CH_3)C_6H_4CH_2$• **T6/19**-p-$(CH_2CH_3)C_6H_4CH_2$•



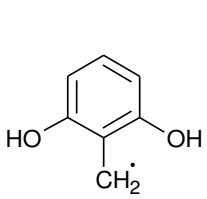
T6/20-1-CH_2•-2,3-OH



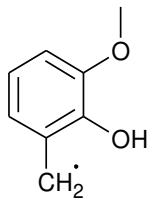
T6/21-1-CH_2•-2,4-OH



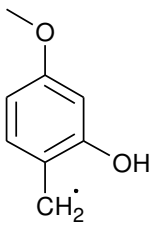
T6/22-1-CH_2•-2,5-OH



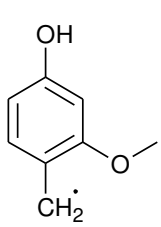
T6/23-1-CH_2•-2,6-OH



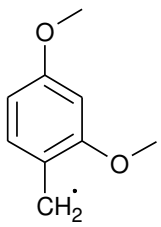
T6/24-1-CH_2•-2-OH-3-OCH_3



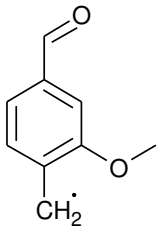
T6/25-1-CH_2•-2-OH-4-OCH_3



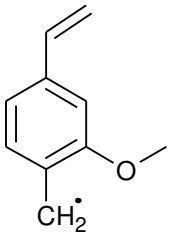
T6/26-1-CH_2•-2-OCH_3-4-OH



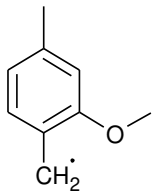
T6/27-1-CH_2•-2,4-OCH_3



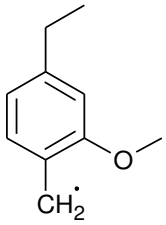
T6/28-1-CH_2•-2-OCH_3-4-CHO



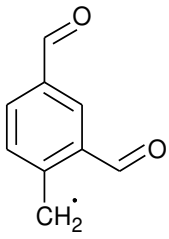
T6/29-1-CH_2•-2-OCH_3-4-CH=CH_2



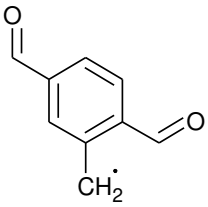
T6/30-1-CH_2•-2-OCH_3-4-CH_3



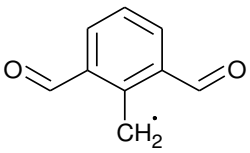
T6/31-1-CH_2•-2-OCH_3-4-CH_2CH_3



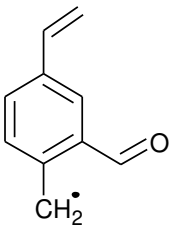
T6/32-1-CH_2•-2,4-CHO



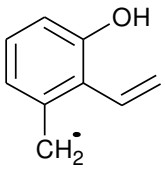
T6/33-1-CH_2•-2,5-CHO



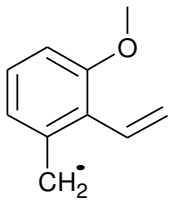
T6/34-1-CH_2•-2,6-CHO



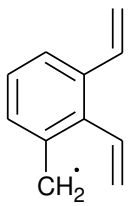
T6/35-1-CH_2•-2-CHO-4-CH=CH_2



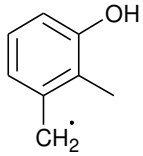
T6/36-1-CH_2•-2-CH=CH_2-3-OH



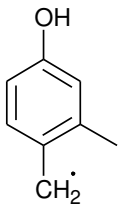
T6/37-1-CH_2•-2-CH=CH_2-3-OCH_3



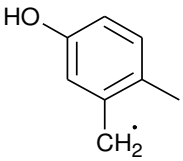
T6/38-1-CH_2•-2,3-CH=CH_2



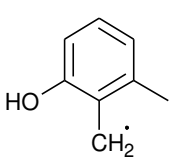
T6/39-1-CH_2•-2-CH_3-3-OH



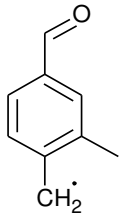
T6/40-1-CH_2•-2-CH_3-4-OH



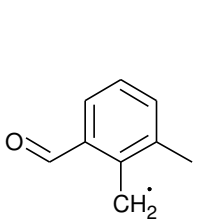
T6/41-1-CH_2•-2-CH_3-5-OH



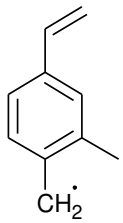
T6/42-1-CH_2•-2-CH_3-6-OH



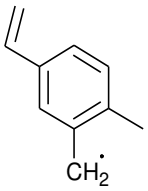
T6/43-1-CH_2•-2-CH_3-4-CHO



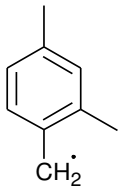
T6/44-1-CH_2•-2-CH_3-6-CHO



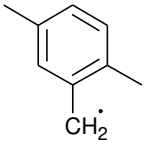
T6/45-1-CH_2•-2-CH_3-4-CH=CH_2



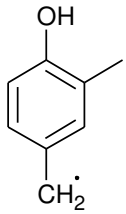
T6/46-1-CH_2•-2-CH_3-5-CH=CH_2



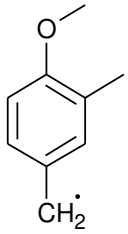
T6/47-1-CH_2•-2,4-CH_3



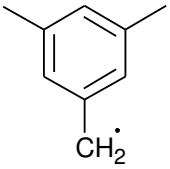
T6/48-1-CH_2•-2,5-CH_3



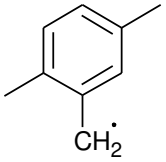
T6/49-1-CH_2•-3-CH_3-4-OH



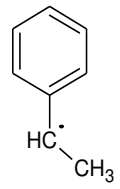
T6/50-1-CH_2•-3-CH_3-4-OCH_3



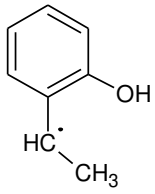
T6/51-1-CH_2•-3,5-CH_3



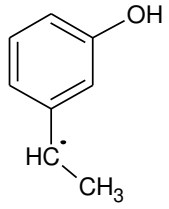
T6/52-1-CH_2•-3,6-CH_3



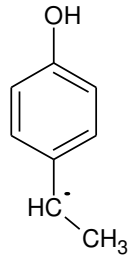
T6/53-C_6H_5CH•CH_3



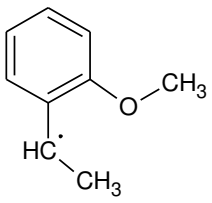
T6/54-o-(OH)C_6H_4CH•CH_3



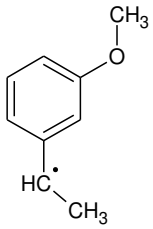
T6/55-m-(OH)C_6H_4CH•CH_3



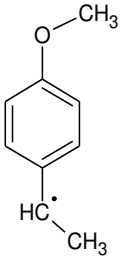
T6/56-p-(OH)C_6H_4CH•CH_3



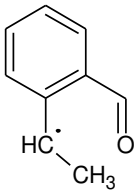
T6/57-o-(OCH_3)C_6H_4CH•CH_3



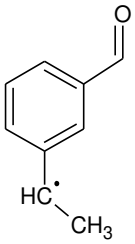
T6/58-m-(OCH_3)C_6H_4CH•CH_3



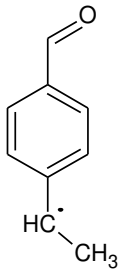
T6/59-p-(OCH_3)C_6H_4CH•CH_3



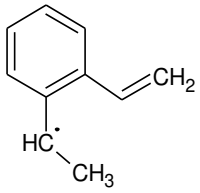
T6/60-o-(CHO)C_6H_4CH•CH_3



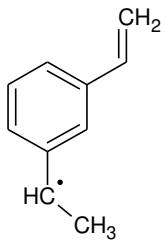
T6/61-m-(CHO)C_6H_4CH•CH_3



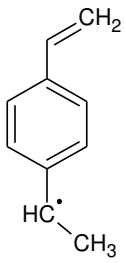
T6/62-p-(CHO)C_6H_4CH•CH_3



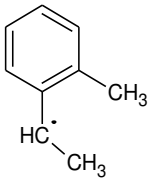
T6/63-o-($CH=CH_2$)C_6H_4CH•CH_3



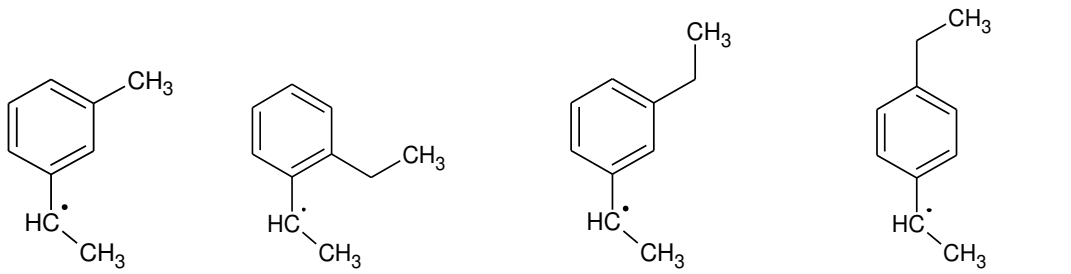
T6/64-m-($CH=CH_2$)C_6H_4CH•CH_3



T6/65-p-($CH=CH_2$)C_6H_4CH•CH_3



T6/66-o-(CH_3)C_6H_4CH•CH_3



T6/67-m-$(CH_3)C_6H_4CH•CH_3$ **T6/68**-o-$(CH_2CH_3)C_6H_4CH•CH_3$ **T6/69**-m-$(CH_2CH_3)C_6H_4CH•CH_3$ **T6/70**-p-$(CH_2CH_3)C_6H_4CH•CH_3$

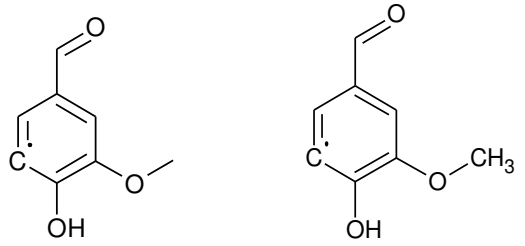
Figure S7. *List of radicals in benzyl subset of the training set.*

2.2 Validation Set

Validation set encompases 53 MARs. This set of MARs include 2 phenyls ($C_6H_5•$), 12 phenoxies ($C_6H_5O•$), 5 anisyls ($C_6H_5OCH_2•$), 9 benzoyls ($C_6H_5C•=O$), 7 β-trans-styrlys (t-$C_6H_5CH=CH•$), 8 β-cis-styrlys (c-$C_6H_5CH=CH•$), 9 benzyls ($C_6H_5CH_2•$) and 1 α-methylbenzyl ($C_6H_5CH•CH_3$). Similar to the training set, these radicals are grouped into six subsets; namely phenyl, phenoxy, anisyl, benzoyl, styryl and benzyl subsets. In the following subsections, six subsets of the validation set is given.

Numbering of the MARs are exactly the same as in the training set, except that the notation starts with "**V**" instead of "**T**". As an example, the 3rd radical in the phenoxy subset of the training set (2-hydroxy-3-vinylphenoxy) is numbered as "**V2/3".**

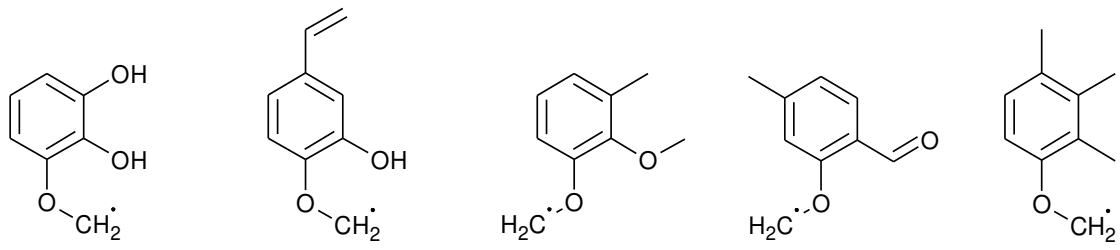
2.2.1 Phenyl Subset



V1/1-1-C•-2-OH-3-CHO-5-OCH_3 **V1/2**-1-C•-2-CHO-5-OH-6-OCH_3

Figure S8. *List of radicals in phenyl subset of the test set.*

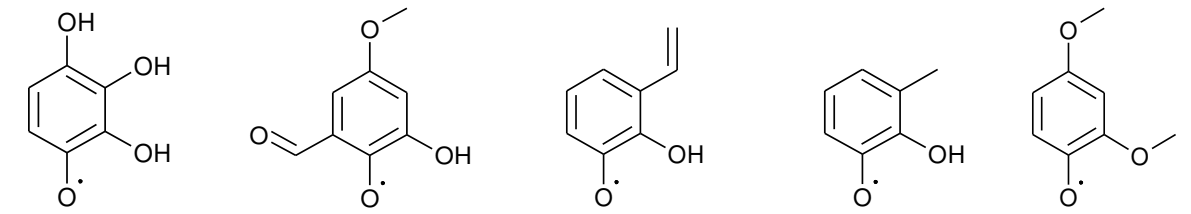
2.2.2 Anisyl Subset



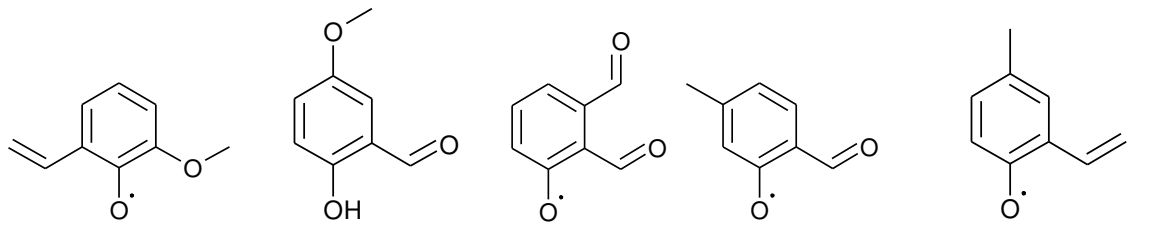
V2/1-1-OCH_2•-2,3-OH **V2/2**-1-OCH_2•-2-OH-4-$CH=CH_2$ **V2/3**-1-OCH_2•-2-OCH_3-3-CH_3 **V2/4**-1-OCH_2•-2-CHO-5-CH_3 **V2/5**-1-OCH_2•-2,3,4-CH_3

Figure S9. *List of radicals in anisyl subset of the test set.*

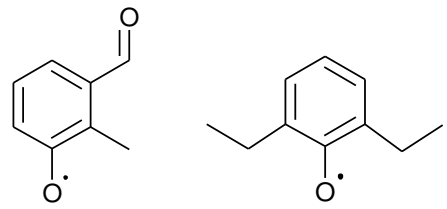
2.2.3 Phenoxy Subset



V3/1-1-O•-2,3,4-OH **V3/2**-1-O•-2-OH-4-OCH_3-6-CHO **V3/3**-1-O•-2-OH-3-$CH=CH_2$ **V3/4**-1-O•-2-OH-3-CH_3 **V3/5**-1-O•-2,4-OCH_3



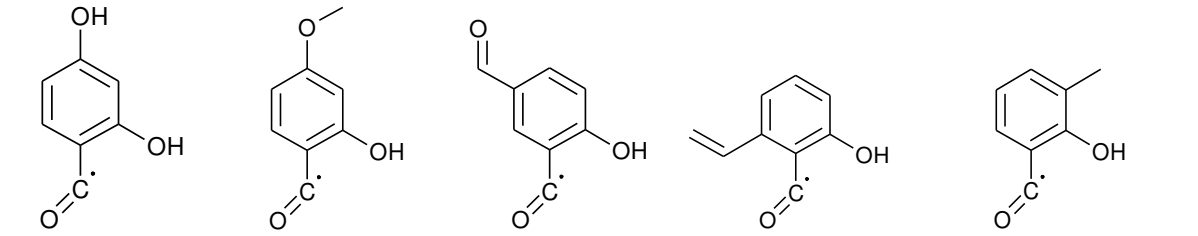
V3/6-1-O•-2-OCH_3-6-$CH=CH_2$ **V3/7**-1-O•-2-CHO-4-OCH_3 **V3/8**-1-O•-2,3-CHO **V3/9**-1-O•-2-CHO-5-CH_3 **V3/10**-1-O•-2-$CH=CH_2$-4-CH_3



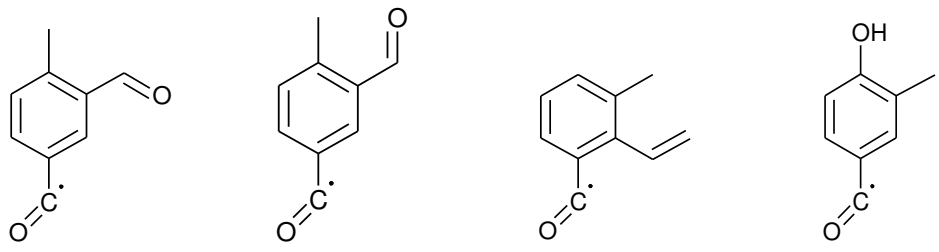
V3/11-1-O•-2-CH_3-3-CHO **V3/12**-1-O•-2,6-CH_2CH_3

Figure S10. *List of radicals in phenoxy subset of the test set.*

2.2.4 Benzoyl Subset



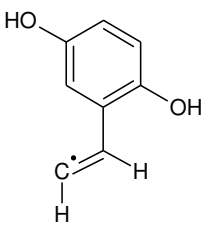
V4/1-1-C•=O-2,4-OH **V4/2**-1-C•=O-2-OH-4-OCH_3 **V4/3**-1-C•=O-2-OH-5-CHO **V4/4**-1-C•=O-2-OH-6-$CH=CH_2$ **V4/5**-1-C•=O-2-OH-3-CH_3



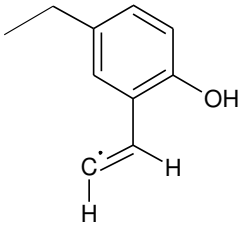
V4/6-1-C•=O-3-CHO-4-CH_3 **V4/7**-1-C•=O-3-CHO-4-CH_3 **V4/8**-1-C•=O-2-$CH=CH_2$-3-CH_3 **V4/9**-1-C•=O-3-CH_3-4-OH

Figure S11. *List of radicals in benzoyl subset of the test set.*

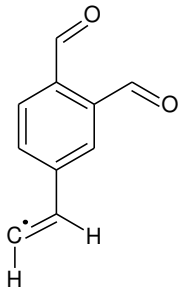
2.2.5 β-Styryl Subset



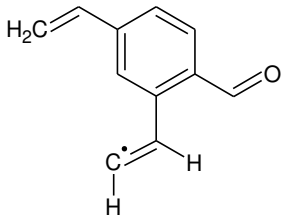
V5/1-1-(t-CH=CH•)-2,5-OH



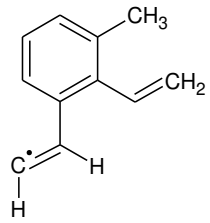
V5/2-1-(t-CH=CH•)-2-OH-5-CH_2CH_3



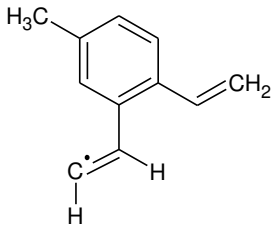
V5/3-1-(t-CH=CH•)-3,4-CHO



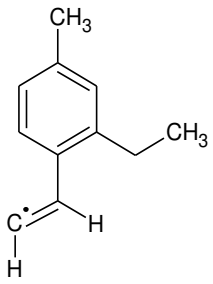
V5/4-1-(t-CH=CH•)-2-CHO-5-$CH=CH_2$



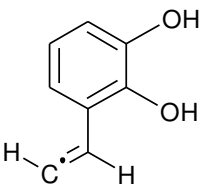
V5/5-1-(t-CH=CH•)-2-$CH=CH_2$-3-CH_3



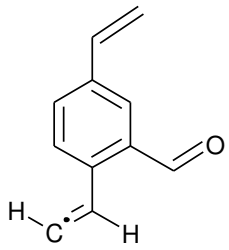
V5/6-1-(t-CH=CH•)-2-$CH=CH_2$-5-CH_3



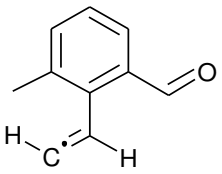
V5/7-1-(t-CH=CH•)-2-CH_2CH_3-4-CH_3



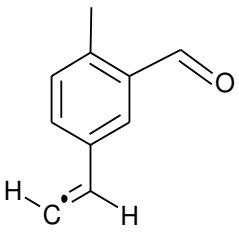
V5/8-1-(c-CH=CH•)-2,3-OH



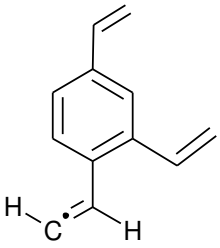
V5/9-1-(c-CH=CH•)-2-CHO-4-CH=CH



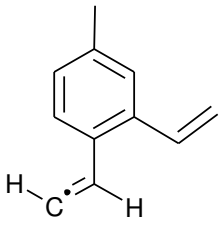
V5/10-1-(c-CH=CH•)-2-CHO-6-CH_3



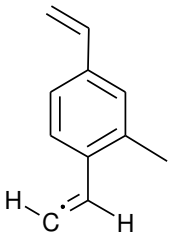
V5/11-1-(c-CH=CH•)-3-CHO-4-CH_3



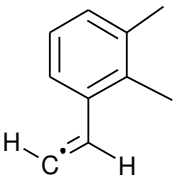
V5/12-1-(c-CH=CH•)-2,4-$CH=CH_2$



V5/13-1-(c-CH=CH•)-2-$CH=CH_2$-4-CH_3



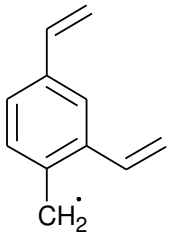
V5/14-1-(c-CH=CH•)-2-CH_3-4-$CH=CH_2$



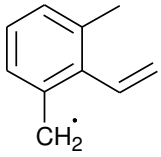
V5/15-1-(c-CH=CH•)-2,3-CH_3

Figure S12. *List of radicals in β-styryl subset of the test set.*

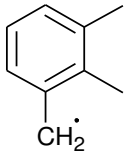
2.2.6 Benzyl/1-Phenylethyl Subset



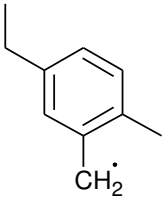
V6/1-1-CH_2•-2,4-$CH{=}CH_2$



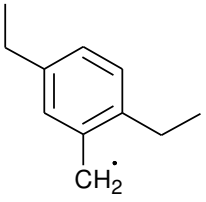
V6/2-1-CH_2•-2-$CH{=}CH_2$-3-CH_3



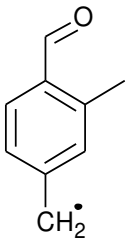
V6/3-1-CH_2•-2,3-CH_3



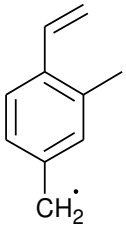
V6/4-1-CH_2•-2-CH_3-5-CH_2CH_3



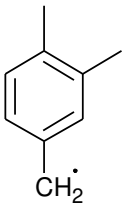
V6/5-1-CH_2•-2,5-CH_2CH_3



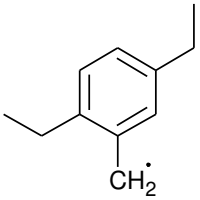
V6/6-1-CH_2•-3-CH_3-4-CHO



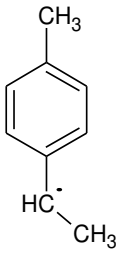
V6/7-1-CH_2•-3-CH_3-4-$CH{=}CH_2$



V6/8-1-CH_2•-3,4-CH_3



V6/9-1-CH_2•-3,6-CH_2CH_3



V6/10-p-$(CH_3)C_6H_4CH$•CH_3

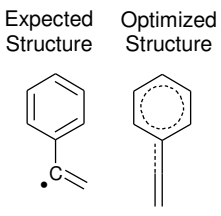
Figure S13. *List of radicals in benzyl subset of the test set.*

2.3 Special Cases Set

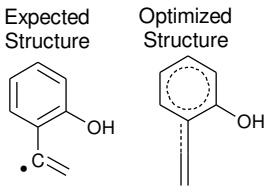
In the special cases set, there are 20 radicals which are excluded from the training set.

α-styryls can be obtained via hydrogen abstraction from the α-carbon on the vinyl substituent and these radicals prefer an allenic conformation as shown in **Figure S14** (no. **S1/1** to **S1/19**). "C•$C_5H_5{=}CH_2$" refers to α-styryl and double substituted α-styryls are given as (X)C•$C_5H_5{=}CH_2$, respectively where X=-OH,-OCH_3,-CHO, -$CH{=}CH_2$,-CH_3 or -CH_2CH_3. For instance, ortho hydroxy substituted α-styryl (**S1/2**) is abbreviated as o-(OH)C•$C_5H_5{=}CH_2$.

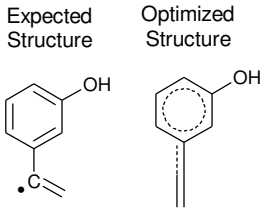
Similarly, the G4 based optimized structure of the o-formylbenzoyl radical (no. **S2/1**) is different than the expected structure where carbonyl group and the formyl group forms a five membered ring.



S1/1-C•$C_5H_5{=}CH_2$

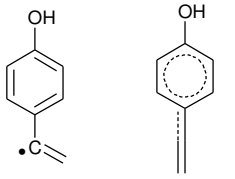


S1/2-o-(OH)C•$C_5H_4{=}CH_2$



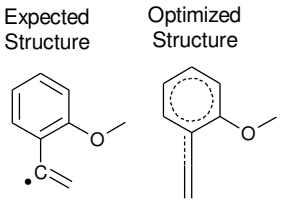
S1/3-m-(OH)C•$C_5H_4{=}CH_2$

Expected Structure Optimized Structure



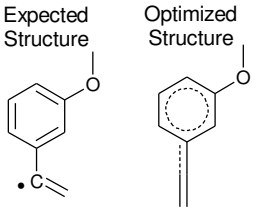
S1/4-p-(OH)C•C_5H_4=CH_2

Expected Structure Optimized Structure



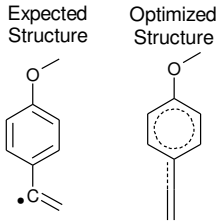
S1/5-o-(OCH_3)C•C_5H_4=CH_2

Expected Structure Optimized Structure



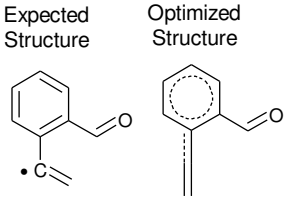
S1/6-m-(OCH_3)C•C_5H_4=CH_2

Expected Structure Optimized Structure



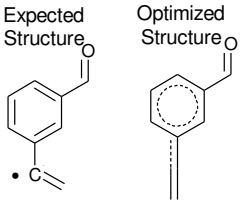
S1/7-p-(OCH_3)C•C_5H_4=CH_2

Expected Structure Optimized Structure



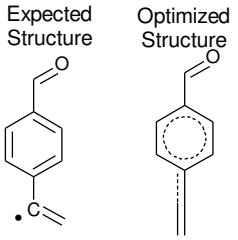
S1/8-o-(CHO)C•C_5H_4=CH_2

Expected Structure Optimized Structure



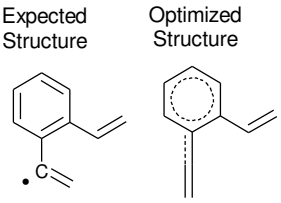
S1/9-m-(CHO)C•C_5H_4=CH_2

Expected Structure Optimized Structure



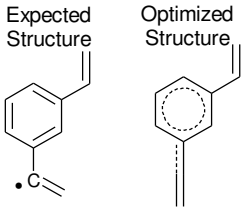
S1/10-p-(CHO)C•C_5H_4=CH_2

Expected Structure Optimized Structure



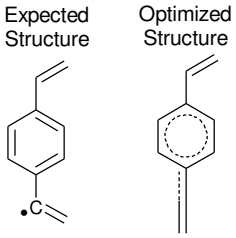
S1/11-o-($CH=CH_2$)C•C_5H_4=CH_2

Expected Structure Optimized Structure

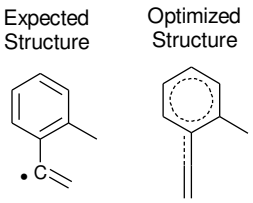


S1/12-m-($CH=CH_2$)C•C_5H_4=CH_2

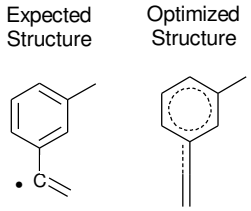
Expected Structure Optimized Structure



S1/13-p-($CH=CH_2$)C•C_5H_4=CH_2



S1/14-o-$(CH_3)C\bullet C_5H_4=CH_2$



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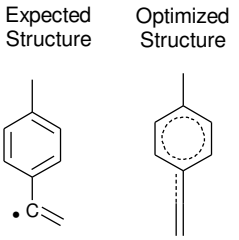
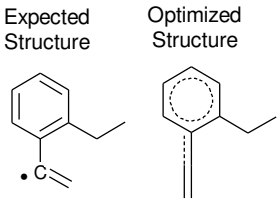
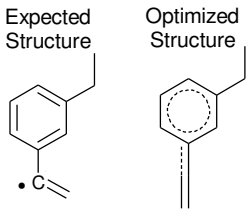


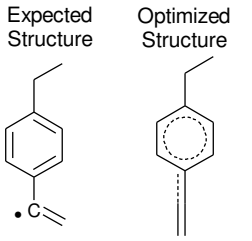
S1/16-p-$(CH_3)C\bullet C_5H_4=CH_2$



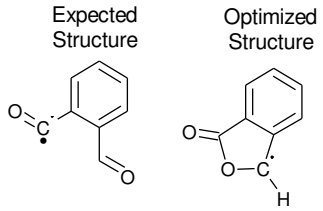
S1/17-o-$(CH_2CH_3)C\bullet C_5H_4=CH_2$



S1/18-m-$(CH_2CH_3)C\bullet C_5H_4=CH_2$



S1/19-p-$(CH_2CH_3)C\bullet C_5H_4=CH_2$



S2/1-1(3H)-Isobenzofuranonyl

Figure S14. *List of radicals in special cases set.*

3. Thermochemical Database

3.1 Thermochemical Database Used In The Training Set

All the thermochemical data obtained used for the derivation of GAVs are NNIs are given in **Table S1** respectively. In these two tables, raw standard enthalpy of formation data ($\Delta_f H^\circ$), BAC-corrected standard enthalpy of formation values ($\Delta_f H^\circ + BAC$), molecular entropy data (S°) intrinsic entropy values (S°_{int}) are given at 298 K whereas C_p values are given at 300 K, 400 K, 500 K, 600 K, 800 K, 1000 K and 1500 K. $\Delta_f H^\circ$ values are given in kJ mol^{-1} and S°_{int} and C_p values in J mol^{-1} K^{-1}. Total symmetry number (σ_{sym}) and number of optical isomers (n_{opt}) which are important in calculation of intrinsic entropy values from molecular entropy data is also provided. The numbering of the molecules is consistent with the list of molecules given in **Figure S1**.

Table S1. *Thermochemical database used as the training set for development of Group Additive Values (GAVs) and non-nearest neighbor interactions (NNIs). The units of standard enthalpy of formation ($\Delta_f H^\circ$) data is given in kJ mol^{-1} whereas the units of entropies (S°) and heat capacities (C_p) are given in J mol^{-1} K^{-1}.*

#	Training set for GAV and NNI	$\Delta_f H^\circ$ (298 K)		S° (298 K)				C_p						
		$\Delta_f H^\circ_{G4}$	$\Delta_f H^\circ_{G4/BAC}$	S°	S°_{int}	$\sigma_{tot\ sym}$	n_{opt}	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
Subset 1: Phenyl Subset														
T1/1	C_6H_5•	338.7	337.7	288.5	294.2	2	1	80.1	107.8	131.0	149.6	176.5	194.9	221.9
T1/2	o-OHC_6H_4•	167.3	162.7	319.9	319.9	1	1	104.0	134.0	157.7	176.0	201.4	218.5	243.5
T1/3	m-OHC_6H_4•	163.3	158.7	324.5	324.5	1	1	101.1	130.5	154.4	172.9	199.1	216.8	242.7
T1/4	p-OHC_6H_4•	169.6	165.0	319.1	324.8	2	1	101.2	130.4	154.0	172.4	198.7	216.4	242.4
T1/5	o-$MeOC_6H_4$•	183.0	179.2	355.1	364.2	3	1	123.2	158.6	188.2	211.7	245.4	268.5	302.7
T1/6	m-$MeOC_6H_4$•	181.6	177.8	357.5	366.6	3	1	122.4	156.7	185.4	208.4	242.4	266.2	301.5
T1/7	p-$MeOC_6H_4$•	188.2	184.4	352.5	367.4	6	1	122.3	156.3	184.7	207.7	241.8	265.7	301.3
T1/8	o-$CHOC_6H_4$•	221.7	222.7	340.3	340.3	1	1	112.0	143.1	169.0	189.9	220.3	240.8	269.4
T1/9	m-$CHOC_6H_4$•	219.8	220.8	343.1	343.1	1	1	108.5	139.6	166.0	187.4	218.7	239.8	269.2
T1/10	p-$CHOC_6H_4$•	218.5	219.5	337.2	342.9	2	1	108.3	139.5	165.9	187.3	218.5	239.7	269.3
T1/11	o-$CH{=}CH_2C_6H_4$•	405.4	405.9	351.6	351.6	1	1	120.2	155.6	185.8	210.1	245.6	269.9	305.6
T1/12	m-$CH{=}CH_2C_6H_4$•	406.5	407.0	352.9	352.9	1	1	117.2	153.7	184.3	208.9	244.6	269.1	305.1
T1/13	p-$CH{=}CH_2C_6H_4$•	407.7	408.2	347.1	352.9	2	1	117.1	153.5	184.1	208.7	244.4	269.0	305.0
T1/14	o-$CH_3C_6H_4$•	302.9	303.4	331.3	340.4	3	1	101.5	134.2	162.4	185.6	220.1	244.3	280.2
T1/15	m-$CH_3C_6H_4$•	303.0	303.5	330.8	340.0	3	1	101.6	134.3	162.6	185.8	220.3	244.5	280.3
T1/16	p-$CH_3C_6H_4$•	305.2	305.7	325.0	339.9	6	1	101.6	134.2	162.5	185.6	220.2	244.4	280.3
T1/17	o-$CH_2CH_3C_6H_4$•	281.6	281.0	366.2	381.1	6	1	124.7	163.6	197.3	225.0	266.5	295.8	339.7
T1/18	m-$CH_2CH_3C_6H_4$•	281.8	281.2	371.0	380.2	3	1	126.2	164.5	198.0	225.5	266.8	296.0	339.8
T1/19	p-$CH_2CH_3C_6H_4$•	284.0	283.4	364.7	379.6	6	1	126.6	164.8	198.2	225.6	266.9	296.1	339.9
T1/20	1-C•-3-OH-4-OCH_3	7.9	0.6	380.3	389.4	3	1	141.2	176.7	207.6	233.0	270.0	294.4	328.0
T1/21	1-C•-3-OH-4-CHO	22.0	19.5	350.2	350.2	1	1	121.9	155.6	185.5	208.0	241.6	265.7	302.4
T1/22	1-C•-2-CH_3-4-OH	132.8	129.7	361.8	371.0	3	1	122.7	156.8	185.5	208.5	242.3	265.8	300.8
T1/23	1-C•-2-OCH_3-3-OH-6-CHO	-120.6	-125.9	424.7	433.8	3	1	171.2	212.2	246.8	275.0	316.1	343.1	378.9
Subset 2: Anisyl Subset														
T2/1	$C_6H_5OCH_2$•	116.3	109.9	364.0	369.7	2	1	122.2	157.6	186.9	210.2	244.1	267.4	302.1
T2/2	o-$OHC_6H_4OCH_2$•	-59.3	-69.3	385.5	391.2	2	1	145.1	182.3	213.4	238.1	272.6	295.0	326.6
T2/3	m-$OHC_6H_4OCH_2$•	-59.5	-69.5	393.0	398.8	2	1	144.2	181.1	210.9	234.1	267.2	289.7	323.1
T2/4	p-$OHC_6H_4OCH_2$•	-50.2	-60.2	393.8	399.5	2	1	143.8	180.1	209.5	232.6	265.8	288.6	322.5
T2/5	o-$OCH_3C_6H_4OCH_2$•	-25.5	-34.7	425.4	440.3	6	1	174.5	212.0	243.5	269.7	309.5	338.1	381.4
T2/6	m-$OCH_3C_6H_4OCH_2$•	-41.6	-50.8	423.1	438.0	6	1	164.6	206.8	241.6	269.4	310.3	339.0	381.9
T2/7	p-$OCH_3C_6H_4OCH_2$•	-32.3	-41.5	427.7	442.6	6	1	165.1	206.2	240.4	268.1	309.2	338.1	381.5
T2/8	o-$CHOC_6H_4OCH_2$•	2.3	-2.1	404.8	410.6	2	1	155.9	197.3	230.6	256.4	292.7	316.9	351.2
T2/9	m-$CHOC_6H_4OCH_2$•	-3.2	-7.6	418.7	418.7	1	1	153.1	191.2	223.2	249.0	286.8	312.6	349.6
T2/10	p-$CHOC_6H_4OCH_2$•	-8.2	-12.6	402.7	417.6	6	1	150.9	189.8	222.5	248.7	286.9	312.9	350.1
T2/11	o-$CH{=}CH_2C_6H_4OCH_2$•	180.1	175.2	416.5	422.3	2	1	163.5	207.8	244.2	273.1	314.9	343.7	386.5
T2/12	m-$CH{=}CH_2C_6H_4OCH_2$•	177.7	172.8	422.0	427.8	2	1	159.9	203.9	240.4	269.6	312.2	341.7	385.4
T2/13	p-$CH{=}CH_2C_6H_4OCH_2$•	178.4	173.5	425.6	425.6	1	1	159.8	203.9	240.6	270.0	312.6	342.1	385.7
T2/14	o-$CH_3C_6H_4OCH_2$•	79.7	74.8	393.7	408.6	6	1	147.9	188.5	222.8	250.4	291.1	319.5	362.0
T2/15	m-$CH_3C_6H_4OCH_2$•	80.1	75.2	400.4	415.3	6	1	144.0	184.3	218.5	246.4	287.8	317.0	360.6
T2/16	p-$CH_3C_6H_4OCH_2$•	81.7	76.8	399.1	414.0	6	1	143.4	183.7	218.0	245.9	287.5	316.8	360.5
T2/17	o-$CH_2CH_3C_6H_4OCH_2$•	58.1	52.1	433.7	448.6	6	1	172.5	218.9	258.4	290.5	338.1	371.7	422.0
T2/18	m-$CH_2CH_3C_6H_4OCH_2$•	59.2	53.2	437.6	452.5	6	1	167.7	214.0	253.6	285.9	334.2	368.5	419.9
T2/19	p-$CH_2CH_3C_6H_4OCH_2$•	62.2	56.2	437.5	452.4	6	1	168.5	214.5	253.9	286.1	334.3	368.5	420.0
T2/20	1-OCH_2•-3,4-OH	-229.0	-242.5	418.0	423.8	2	1	163.6	201.8	233.3	258.1	292.6	314.8	346.4
T2/21	1-OCH_2•-2-OH-6-OCH_3	-202.8	-215.5	450.7	465.6	6	1	188.4	230.8	266.7	295.9	338.2	366.3	406.5
T2/22	1-OCH_2•-2-OH-4-CHO	-181.1	-189.0	435.8	441.5	2	1	174.5	216.4	250.9	278.0	315.8	340.2	373.9
T2/23	1-OCH_2•-2-OH-5-CHO	-184.9	-192.8	442.1	442.1	1	1	175.3	215.2	249.0	276.3	315.3	340.7	375.2
T2/24	1-OCH_2•-2-OH-5-$CH{=}CH_2$	1.1	-7.4	443.6	449.4	2	1	182.4	227.8	266.2	297.0	340.7	369.5	410.3

T2/25	1-OCH_2•-2-OCH_3-4-OH	-195.7	-208.4	454.1	469.0	6	1	196.9	236.0	267.7	293.4	332.2	359.9	402.2
T2/26	1-OCH_2•-2-OCH_3-6-OH	-202.8	-215.5	450.7	465.6	6	1	188.4	230.8	266.7	295.9	338.2	366.3	406.5
T2/27	1-OCH_2•-2-OCH_3-4-CH_3	-60.8	-68.5	460.7	484.7	18	1	195.7	238.2	274.9	305.8	353.4	387.8	440.0
T2/28	1-OCH_2•-2-OCH_3-5-CH_3	-60.4	-68.1	466.5	484.8	9	1	196.5	238.5	275.0	305.7	353.2	387.6	439.8
T2/29	1-OCH_2•-2-CHO-3-CH_3	-27.5	-30.4	437.8	452.7	6	1	178.9	224.5	263.1	294.1	338.6	368.4	410.5
T2/30	1-OCH_2•-2-CHO-4-CH_3	-31.7	-34.6	441.6	456.5	6	1	176.8	223.3	261.8	292.3	336.4	366.5	409.8
T2/31	1-OCH_2•-2-CH_3-4-OH	-87.7	-96.2	426.3	441.2	6	1	169.9	210.5	244.4	271.7	312.0	340.1	382.3
T2/32	1-OCH_2•-3-CH_3-4-OH	-87.3	-95.8	438.2	443.9	2	1	168.1	207.8	241.4	268.8	309.4	337.9	380.9
T2/33	1-OCH_2•-2,3-CH_3	48.7	45.3	431.0	449.3	9	1	169.9	215.3	254.3	286.3	334.5	368.9	420.5
	Subset 3: Phenoxy Subset													
T3/1	C_6H_5O•	59.9	54.1	309.8	315.5	2	1	95.6	125.5	150.4	170.2	198.6	217.9	245.8
T3/2	o-OHC_6H_4O•	-153.6	-162.9	332.6	332.6	1	1	109.7	141.7	168.1	189.1	219.1	239.4	268.7
T3/3	m-OHC_6H_4O•	-117.5	-126.8	341.7	341.7	1	1	120.2	151.8	176.9	196.1	223.1	241.1	267.3
T3/4	p-OHC_6H_4O•	-127.6	-136.9	338.2	344.0	2	1	114.5	146.3	172.4	192.9	221.8	240.9	267.9
T3/5	o-$OCH_3C_6H_4O$•	-102.4	-110.9	376.0	385.1	3	1	136.7	173.1	204.0	229.1	265.7	290.7	326.9
T3/6	m-$OCH_3C_6H_4O$•	-102.9	-111.4	374.0	383.1	3	1	140.3	179.1	210.3	234.5	268.7	292.1	326.8
T3/7	p-$OCH_3C_6H_4O$•	-110.3	-118.8	376.7	385.9	3	1	135.4	172.4	203.7	229.0	265.7	290.7	326.7
T3/8	o-$CHOC_6H_4O$•	-56.4	-60.1	364.7	364.7	1	1	124.8	158.6	187.6	211.3	245.3	267.2	295.7
T3/9	m-$CHOC_6H_4O$•	-56.8	-60.5	368.1	368.1	1	1	128.2	160.6	187.9	209.9	241.9	263.5	293.3
T3/10	p-$CHOC_6H_4O$•	-60.9	-64.6	362.0	367.7	2	1	124.1	157.5	185.5	208.1	240.8	262.8	293.3
T3/11	o-CH=$CH_2C_6H_4O$•	115.7	111.4	370.2	370.2	1	1	132.6	171.3	203.7	229.8	267.8	293.6	330.8
T3/12	m-CH=$CH_2C_6H_4O$•	124.7	120.4	373.8	373.8	1	1	133.6	171.9	204.0	229.6	266.7	292.0	329.0
T3/13	p-CH=$CH_2C_6H_4O$•	108.5	104.2	370.2	370.2	1	1	132.9	171.6	204.0	230.1	267.9	293.7	330.7
T3/14	o-$CH_3C_6H_4O$•	15.2	10.9	351.2	360.3	3	1	117.4	152.2	182.0	206.3	242.3	267.4	304.2
T3/15	m-$CH_3C_6H_4O$•	22.4	18.1	351.9	361.0	3	1	117.6	152.4	182.2	206.5	242.5	267.5	304.3
T3/16	p-$CH_3C_6H_4O$•	18.8	14.5	352.5	361.6	3	1	116.9	151.9	181.8	206.1	242.2	267.4	304.3
T3/17	o-$CH_2CH_3C_6H_4O$•	-5.3	-10.7	389.3	398.4	3	1	141.9	182.8	218.1	246.9	289.8	319.8	364.2
T3/18	m-$CH_2CH_3C_6H_4O$•	1.4	-4.0	392.1	401.2	3	1	141.5	182.2	217.3	246.0	288.8	318.9	363.6
T3/19	p-$CH_2CH_3C_6H_4O$•	-1.9	-7.3	392.9	402.0	3	1	141.1	181.7	216.8	245.6	288.5	318.7	363.6
T3/20	1-O•-2,3-OH	-326.8	-339.7	357.1	357.1	1	1	131.5	167.0	195.6	217.4	246.9	265.5	291.8
T3/21	1-O•-3,4-OH	-312.1	-325.0	361.6	361.6	1	1	134.7	169.3	197.8	220.2	251.3	270.5	294.9
T3/22	1-O•-2-OH-4-OCH_3	-325.4	-337.5	391.6	400.8	3	1	153.4	191.8	224.0	249.9	287.4	313.0	349.9
T3/23	1-O•-2-OH-6-OCH_3	-307.6	-319.7	397.5	406.6	3	1	150.0	188.3	220.7	246.8	284.9	310.9	348.7
T3/24	1-O•-2-OH-3-CHO	-269.0	-276.3	381.0	381.0	1	1	140.4	177.1	207.3	231.2	265.0	287.1	317.3
T3/25	1-O•-2-OH-4-CHO	-274.5	-281.8	382.6	382.6	1	1	139.8	174.6	203.8	227.4	261.6	284.5	316.4
T3/26	1-O•-2-OH-6-CHO	-268.4	-275.7	381.2	381.2	1	1	139.2	175.6	206.3	230.9	265.7	288.1	318.0
T3/27	1-O•-2-OH-4-CH=CH_2	-102.1	-109.9	387.9	387.9	1	1	147.2	188.0	221.9	249.1	288.4	315.1	353.3
T3/28	1-O•-2-OH-5-CH=CH_2	-89.1	-96.9	389.4	389.4	1	1	148.6	188.6	222.0	248.8	287.5	313.9	352.2
T3/29	1-O•-2-OH-6-CH=CH_2	-95.0	-102.8	384.8	384.8	1	1	147.1	187.8	221.7	249.0	288.4	315.2	353.5
T3/30	1-O•-2-OH-4-CH_3	-194.8	-202.6	369.1	378.3	3	1	131.3	168.3	199.7	225.2	262.9	289.0	327.2
T3/31	1-O•-2-OH-5-CH_3	-191.3	-199.1	368.8	377.9	3	1	132.1	168.8	200.0	225.4	263.0	289.0	327.3
T3/32	1-O•-2-OH-6-CH_3	-197.4	-205.2	368.2	377.4	3	1	132.1	168.8	200.0	225.4	263.0	289.0	327.2
T3/33	1-O•-2-OCH_3-3-OH	-280.2	-292.3	399.7	408.8	3	1	153.2	191.7	225.0	252.3	291.8	317.7	352.9
T3/34	1-O•-3-OCH_3-4-OH	-298.9	-311.0	394.5	403.6	3	1	153.1	198.0	233.0	259.0	291.7	318.4	355.0
T3/35	1-O•-2,3-OCH_3	-271.2	-282.5	433.5	451.8	9	1	180.2	223.3	260.2	290.1	333.9	363.9	407.5
T3/36	1-O•-2,6-OCH_3	-269.1	-280.4	439.9	458.2	9	1	179.7	222.3	259.0	288.9	332.9	363.2	407.4
T3/37	1-O•-3,4-OCH_3	-262.1	-273.4	435.6	453.8	9	1	185.4	224.0	260.0	288.0	336.7	364.7	407.0
T3/38	1-O•-2-OCH_3-3-CHO	-216.8	-223.3	425.6	434.7	3	1	165.3	206.2	241.5	270.3	312.5	340.6	378.1
T3/39	1-O•-2-OCH_3-4-CHO	-225.4	-231.9	429.1	438.3	3	1	168.2	206.9	240.3	267.9	308.6	336.3	374.8
T3/40	1-O•-2-OCH_3-6-CHO	-218.5	-225.0	422.9	432.0	3	1	165.8	206.0	241.2	270.1	312.3	340.0	376.8
T3/41	1-O•-2-OCH_3-3-CH=CH_2	-35.4	-42.4	432.4	441.5	3	1	171.8	216.8	255.5	287.3	334.2	366.3	412.1
T3/42	1-O•-2-OCH_3-4-CH=CH_2	-49.6	-56.6	433.9	443.0	3	1	174.5	218.8	257.0	288.1	334.0	365.5	410.8
T3/43	1-O•-2-OCH_3-3-CH_3	-140.3	-147.3	413.7	431.9	9	1	158.2	198.7	234.5	264.5	310.2	342.3	388.2
T3/44	1-O•-2-OCH_3-4-CH_3	-142.7	-149.7	412.1	430.3	9	1	158.2	199.6	235.5	265.1	309.4	340.2	385.3
T3/45	1-O•-2-OCH_3-5-CH_3	-139.8	-146.8	411.4	429.7	9	1	159.1	200.3	236.1	265.7	309.8	340.6	385.5
T3/46	1-O•-3-OCH_3-4-CHO	-219.3	-225.8	416.3	425.4	3	1	165.3	208.3	245.1	274.7	316.4	343.2	378.6
T3/47	1-O•-3-OCH_3-6-CHO	-223.0	-229.5	416.4	425.6	3	1	168.3	211.0	246.6	275.1	315.7	342.2	377.7
T3/48	1-O•-2-CHO-4-OH	-247.5	-254.8	385.8	385.8	1	1	144.4	179.5	209.0	233.1	268.1	290.8	319.6
T3/49	1-O•-2-CHO-5-OH	-236.3	-243.6	387.6	387.6	1	1	148.0	183.5	212.9	236.4	269.7	290.8	318.0
T3/50	1-O•-2-CHO-6-OH	-268.5	-275.8	381.4	381.4	1	1	139.1	175.4	206.0	230.6	265.5	288.1	318.1
T3/51	1-O•-2-CHO-5-OCH_3	-222.9	-229.4	422.2	431.3	3	1	168.5	211.1	246.7	275.1	315.7	342.2	377.7
T3/52	1-O•-3-CHO-4-OH	-272.1	-279.4	370.8	370.8	1	1	136.3	172.2	202.0	225.9	260.4	283.6	316.2
T3/53	1-O•-3-CHO-4-OCH_3	-216.0	-222.5	428.7	437.8	3	1	170.4	210.5	245.2	273.6	314.3	340.6	375.9
T3/54	1-O•-3-CHO-6-OCH_3	-224.2	-230.7	425.0	434.1	3	1	170.4	209.2	242.3	269.5	309.8	337.1	375.2
T3/55	1-O•-2,4-CHO	-174.0	-175.7	411.8	411.8	1	1	155.8	192.3	224.1	250.2	288.2	312.6	343.1
T3/56	1-O•-2,5-CHO	-169.5	-171.2	415.2	415.2	1	1	157.1	193.6	225.3	251.3	288.8	312.7	342.8
T3/57	1-O•-3,4-CHO	-164.1	-165.8	412.7	418.5	2	1	161.7	199.6	231.0	256.0	291.1	313.2	341.5
T3/58	1-O•-2-CHO-3-CH=CH_2	19.1	16.9	417.8	417.8	1	1	160.3	203.8	241.1	271.5	315.3	343.6	380.6
T3/59	1-O•-2-CHO-5-CH=CH_2	7.7	5.5	420.6	420.6	1	1	162.5	204.7	241.0	270.5	313.3	341.5	379.2
T3/60	1-O•-2-CHO-3-CH_3	-87.8	-90.0	395.0	404.1	3	1	148.4	186.3	219.5	247.3	288.9	317.0	354.8
T3/61	1-O•-2-CHO-4-CH_3	-99.8	-102.0	399.5	408.6	3	1	145.7	184.5	218.6	246.8	288.7	316.7	354.5
T3/62	1-O•-2-CHO-5-CH_3	-95.6	-97.8	398.1	407.3	3	1	146.3	185.1	219.1	247.3	289.0	316.8	354.4
T3/63	1-O•-2-CHO-6-CH_3	-101.9	-104.1	400.1	409.2	3	1	146.5	185.2	219.2	247.4	288.9	316.6	354.1
T3/64	1-O•-2-CH=CH_2-5-CH_3	77.0	74.2	405.3	414.4	3	1	155.3	198.6	235.8	266.3	311.8	343.4	389.5
T3/65	1-O•-2-CH=CH_2-6-CH_3	72.2	69.4	409.6	418.7	3	1	155.8	198.9	236.2	266.7	312.1	343.6	389.5
T3/66	1-O•-2-CH_3-4-CHO	-107.2	-109.4	403.9	413.1	3	1	146.3	184.3	217.2	244.3	284.6	312.3	351.8
T3/67	1-O•-2,6-CH_3	-29.0	-31.8	386.4	404.7	9	1	139.7	179.1	213.8	242.6	286.1	316.9	362.7
T3/68	1-O•-2-CH_2CH_3-4-CHO	-127.9	-131.3	442.5	451.7	3	1	170.3	214.6	253.0	284.6	331.8	364.5	411.5
	Subset 4: Benzoyl Subset													
T4/1	C_6H_5C•=O	119.8	118.2	340.0	345.7	2	1	109.5	140.9	167.0	187.8	217.5	237.5	266.1
T4/2	o-OHC_6H_5C•=O	-69.7	-74.8	355.3	355.3	1	1	130.0	164.9	193.6	216.5	249.4	270.5	297.0
T4/3	m-OHC_6H_5C•=O	-54.7	-59.8	373.9	373.9	1	1	132.7	165.1	191.5	212.0	240.8	259.9	287.2
T4/4	p-OHC_6H_5C•=O	-61.8	-66.9	371.5	371.5	1	1	128.7	162.2	189.7	211.3	241.7	261.5	288.9
T4/5	o-$OCH_3C_6H_5$ C•=O	-29.3	-33.7	411.3	420.4	3	1	156.0	191.7	221.8	246.2	282.5	307.8	345.1
T4/6	m-$OCH_3C_6H_5$ C•=O	-37.0	-41.4	407.3	416.4	3	1	154.9	192.4	223.6	248.6	284.9	309.8	346.3
T4/7	p-$OCH_3C_6H_5$ C•=O	-41.6	-46.0	406.0	415.1	3	1	149.9	188.6	221.4	247.7	285.7	311.2	347.7
T4/8	m-$CHOC_6H_5$ C•=O	1.3	1.8	398.8	398.8	1	1	139.3	173.6	202.6	225.9	259.8	282.3	313.4
T4/9	p-$CHOC_6H_5$ C•=O	2.3	2.8	406.6	406.6	1	1	139.8	172.6	200.6	223.5	257.3	280.2	311.9
T4/10	o-CH=$CH_2C_6H_5C$•=O	190.4	190.3	395.8	395.8	1	1	149.7	190.5	224.3	251.0	288.8	314.1	350.5
T4/11	m-CH=$CH_2C_6H_5C$•=O	182.2	182.1	404.6	404.6	1	1	146.7	186.8	220.3	247.0	285.5	311.6	349.3
T4/12	p-CH=$CH_2C_6H_5C$•=O	188.7	188.6	403.7	403.7	1	1	146.7	186.9	220.5	247.2	285.7	311.8	349.5
T4/13	o-$CH_3C_6H_5C$•=O	85.3	85.2	377.8	387.0	3	1	133.0	168.8	199.5	224.5	261.4	287.0	324.5
T4/14	m-$CH_3C_6H_5C$•=O	83.0	82.9	382.3	391.4	3	1	131.1	167.5	198.6	223.9	261.2	287.0	324.6

T4/15	p-$CH_3C_6H_5C$•=O	81.9	81.8	380.7	389.8	3	1	130.9	167.4	198.7	224.1	261.6	287.4	324.9
T4/16	o-$CH_2CH_3C_6H_5C$•=O	63.1	61.9	419.0	428.2	3	1	158.0	200.2	236.3	265.8	309.4	339.8	384.6
T4/17	m-$CH_2CH_3C_6H_5C$•=O	61.7	60.5	423.1	432.2	3	1	155.7	197.7	234.0	263.7	307.8	338.5	383.9
T4/18	p-$CH_2CH_3C_6H_5C$•=O	60.7	59.5	420.1	429.2	3	1	155.4	197.5	233.9	263.7	308.0	338.8	384.2
T4/19	1-C•=O -2,3-OH	-251.2	-259.9	376.0	376.0	1	1	146.5	184.0	214.4	238.1	271.0	291.5	318.2
T4/20	1-C•=O -2,5-OH	-235.4	-244.1	384.4	384.4	1	1	151.4	185.9	213.5	235.5	267.9	289.9	318.6
T4/21	1-C•=O -3,4-OH	-238.8	-247.5	390.1	390.1	1	1	151.4	187.4	216.7	239.5	270.6	289.6	314.1
T4/22	1-C•=O -3-OH-4-OCH_3	-219.8	-227.7	425.0	434.1	3	1	170.9	213.0	248.2	276.1	315.0	339.7	373.2
T4/23	1-C•=O -3-OH-6-OCH_3	-196.9	-204.8	441.4	450.5	3	1	180.9	215.9	245.1	268.9	304.1	328.7	365.4
T4/24	1-C•=O -2-OH-3-CHO	-188.7	-191.8	402.5	402.5	1	1	156.9	196.0	227.9	253.1	288.7	311.7	342.2
T4/25	1-C•=O -3-OH-4-$CH=CH_2$	9.4	5.8	429.5	429.5	1	1	167.8	209.0	243.2	270.1	308.4	334.0	370.7
T4/26	1-C•=O -2-OH-4-CH_3	-112.8	-116.4	388.1	397.2	3	1	145.1	183.9	216.7	243.4	282.9	310.2	350.2
T4/27	1-C•=O -2-OH-5-CH_3	-104.0	-107.6	391.8	400.9	3	1	151.4	191.1	224.7	252.3	293.0	319.9	355.5
T4/28	1-C•=O -2-OH-6-CH_3	-109.0	-112.6	391.5	400.6	3	1	149.1	187.7	220.1	246.4	285.3	312.3	351.2
T4/29	1-C•=O -2-OCH_3-4-OH	-213.4	-221.3	432.1	441.2	3	1	177.9	215.9	247.1	272.1	308.3	332.8	368.2
T4/30	1-C•=O -3-OCH_3-4-OH	-223.0	-230.9	424.0	433.1	3	1	170.7	210.8	244.9	272.8	313.4	340.1	375.6
T4/31	1-C•=O -2-OCH_3-3-CH_3	-59.7	-62.6	443.6	461.9	9	1	177.9	221.2	258.5	288.8	333.1	363.3	407.3
T4/32	1-C•=O -2-OCH_3-5-CH_3	-63.9	-66.8	448.0	466.3	9	1	177.0	217.7	252.8	281.9	326.0	357.1	403.6
T4/33	1-C•=O -2-OCH_3-6-CH_3	-62.0	-64.9	441.1	459.4	9	1	183.3	223.2	256.6	284.2	326.6	357.2	403.3
T4/34	1-C•=O -3-CHO-4-OH	-209.0	-212.1	401.5	401.5	1	1	151.5	188.5	219.6	244.7	281.5	306.4	342.2
T4/35	1-C•=O -2-CH=CH_2-4-CH_3	151.3	152.7	430.6	439.7	3	1	171.3	217.2	256.2	287.5	333.0	364.0	409.2
T4/36	1-C•=O -2-CH=CH_2-5-CH_3	147.6	149.0	431.5	440.7	3	1	171.9	217.6	256.4	287.5	332.7	363.7	409.0
T4/37	1-C•=O -2-CH=CH_2-6-CH_3	154.1	155.5	430.7	439.8	3	1	178.7	221.6	257.7	287.0	330.8	361.6	407.6
T4/38	1-C•=O -2-CH_3-4-OH	-100.8	-104.4	403.0	412.1	3	1	152.5	190.3	222.4	248.4	286.0	311.3	347.4
T4/39	1-C•=O -2-CH_3-4-CHO	-34.1	-32.2	443.7	452.8	3	1	159.7	197.9	231.2	259.0	300.6	329.4	370.2
T4/40	1-C•=O -2-CH_3-4-$CH=CH_2$	152.9	154.3	435.2	444.3	3	1	170.3	214.9	253.0	283.9	329.6	361.3	407.8
T4/41	1-C•=O -2,3-CH_3	-29.4	-27.5	433.8	442.9	3	1	165.5	202.4	234.7	261.7	302.2	330.3	370.3
T4/42	1-C•=O -3-CH_3-4-CHO	52.7	54.1	411.2	429.4	9	1	163.1	201.8	235.8	264.2	307.3	337.9	383.6
	Subset 5: β-Styryl Subset													
T5/1	t-$C_6H_5CH=CH$•	397.8	395.7	344.8	350.6	2	1	119.7	156.7	187.4	211.8	247.1	271.2	306.4
T5/2	o-(OH)t-$C_6H_5CH=CH$•	208.2	202.5	361.9	361.9	1	1	138.6	179.1	213.4	241.4	281.2	305.8	336.7
T5/3	m-(OH)t-$C_6H_5CH=CH$•	222.8	217.1	379.3	379.3	1	1	142.3	180.5	211.5	235.7	270.2	293.4	327.4
T5/4	p-(OH)t-$C_6H_5CH=CH$•	223.1	217.4	379.6	379.6	1	1	140.5	179.3	210.8	235.3	270.0	293.4	327.5
T5/5	o-(OCH_3)t-$C_6H_5CH=CH$•	244.3	239.4	410.4	419.6	3	1	164.9	208.0	243.9	272.8	315.4	345.0	388.2
T5/6	m-(OCH_3)t-$C_6H_5CH=CH$•	240.8	235.9	414.4	423.5	3	1	164.2	207.2	242.9	271.6	313.6	342.9	386.3
T5/7	p-(OCH_3)t-$C_6H_5CH=CH$•	241.3	236.4	413.7	422.8	3	1	161.8	205.8	242.1	271.1	313.6	343.0	386.4
T5/8	o-(CHO)t-$C_6H_5CH=CH$•	286.6	286.5	393.0	393.0	1	1	152.3	194.3	228.7	255.9	294.7	320.4	356.0
T5/9	m-(CHO)t-$C_6H_5CH=CH$•	277.5	277.4	402.9	402.9	1	1	149.8	189.5	223.0	250.0	289.4	316.1	353.8
T5/10	p-(CHO)t-$C_6H_5CH=CH$•	276.8	276.7	401.6	401.6	1	1	148.2	188.5	222.4	249.6	289.3	316.1	354.0
T5/11	o-($CH=CH_2$)t-$C_6H_5CH=CH$•	469.1	468.5	408.0	408.0	1	1	159.8	204.7	242.5	272.7	316.4	346.2	390.0
T5/12	m-($CH=CH_2$)t-$C_6H_5CH=CH$•	465.3	464.7	408.8	408.8	1	1	156.9	202.7	240.7	271.1	315.1	345.3	389.6
T5/13	p-($CH=CH_2$)t-$C_6H_5CH=CH$•	465.3	464.7	407.3	407.3	1	1	156.9	202.7	240.9	271.3	315.6	345.8	390.1
T5/14	o-(CH_3)t-$C_6H_5CH=CH$•	365.8	365.2	386.7	395.8	3	1	150.3	189.6	223.5	251.2	292.5	321.7	365.2
T5/15	m-(CH_3)t-$C_6H_5CH=CH$•	362.2	361.6	387.0	396.1	3	1	141.3	183.4	219.0	248.0	290.9	320.7	364.9
T5/16	p-(CH_3)t-$C_6H_5CH=CH$•	362.5	361.9	386.3	395.5	3	1	141.3	183.3	219.0	248.0	290.9	320.8	364.9
T5/17	o-(CH_2CH_3)t-$C_6H_5CH=CH$•	345.0	343.3	423.4	432.5	3	1	172.2	218.4	258.1	290.5	339.1	373.5	425.0
T5/18	m-(CH_2CH_3)t-$C_6H_5CH=CH$•	339.7	338.0	428.2	437.3	3	1	165.3	212.9	253.9	287.3	337.2	372.2	424.2
T5/19	p-(CH_2CH_3)t-$C_6H_5CH=CH$•	341.4	339.7	430.5	439.7	3	1	166.2	213.8	254.6	287.9	337.5	372.4	424.4
T5/20	1-(t-CH=CH•)-2,3-OH	49.3	40.1	403.8	403.8	1	1	162.4	202.0	234.0	259.3	294.9	317.9	350.2
T5/21	1-(t-CH=CH•)-2,4-OH	30.4	21.2	389.7	389.7	1	1	159.3	200.8	235.3	263.2	303.2	328.4	359.4
T5/22	1-(t-CH=CH•)-3,4-OH	45.4	36.2	398.3	398.3	1	1	164.9	206.0	238.9	264.2	299.0	321.1	351.9
T5/23	1-(t-CH=CH•)-2-OH-4-CHO	89.9	86.3	409.1	409.1	1	1	167.4	211.5	249.2	280.0	323.6	350.5	383.5
T5/24	1-(t-CH=CH•)-2-OH-6-CHO	94.1	90.5	403.3	403.3	1	1	166.8	211.4	248.6	278.9	323.4	352.8	389.4
T5/25	1-(t-CH=CH•)-2-OH-5-CH=CH_2	276.2	272.0	419.9	419.9	1	1	175.9	224.9	266.7	300.7	349.3	380.3	420.3
T5/26	1-(t-CH=CH•)-2-OH-5-CH_3	176.1	171.9	398.6	407.8	3	1	160.3	205.6	244.9	277.5	324.8	355.2	395.0
T5/27	1-(t-CH=CH•)-2-OH-6-CH_3	178.1	173.9	395.0	404.1	3	1	164.0	208.6	247.2	279.0	325.1	355.1	394.9
T5/28	1-(t-CH=CH•)-2-OH-4-CH_2CH_3	150.7	145.4	439.9	449.1	3	1	184.7	235.7	280.1	317.0	371.3	407.0	454.8
T5/29	1-(t-CH=CH•)-2-OH-5-CH_2CH_3	154.8	149.5	438.0	447.1	3	1	185.0	236.0	280.6	317.5	371.5	406.9	454.4
T5/30	1-(t-CH=CH•)-2-CHO-4-OH	114.3	110.7	418.9	418.9	1	1	172.7	216.7	251.9	279.2	317.4	342.3	376.7
T5/31	1-(t-CH=CH•)-3-CHO-4-OH	73.3	69.7	408.6	408.6	1	1	162.9	205.4	240.8	269.1	310.7	339.5	381.8
T5/32	1-(t-CH=CH•)-2,4-CHO	168.1	170.1	442.3	442.3	1	1	181.2	226.6	264.0	293.8	336.7	365.1	403.4
T5/33	1-(t-CH=CH•)-2-CH=CH_2-4-CH_3	433.4	434.3	439.3	448.5	3	1	181.0	231.5	274.5	309.3	360.5	396.0	448.6
T5/34	1-(t-CH=CH•)-2-CH=CH_2-6-CH_3	437.2	438.1	441.4	450.6	3	1	182.3	231.8	273.7	307.8	358.8	394.7	448.0
T5/35	1-(t-CH=CH•)-2-CH_3-4-CHO	244.3	245.7	434.7	443.9	3	1	175.5	219.3	257.0	288.0	334.2	366.3	412.6
T5/36	1-(t-CH=CH•)-2,3-CH_3	337.6	338.5	414.7	433.0	9	1	169.7	214.6	253.7	286.0	335.1	370.1	422.9
T5/37	1-(t-CH=CH•)-2,4-CH_3	330.1	331.0	421.2	439.5	9	1	169.7	214.8	254.1	286.6	335.9	371.0	423.6
T5/38	1-(t-CH=CH•)-2-CH_3-4-CH_2CH_3	308.9	308.7	458.9	477.2	9	1	194.2	245.0	289.5	326.4	382.5	422.6	483.0
T5/39	c-$C_6H_5CH=CH$•	402.2	400.1	353.1	353.1	1	1	119.0	155.9	186.4	210.6	245.6	269.8	305.3
T5/40	o-(OH)c-$C_6H_5CH=CH$•	226.5	220.8	382.5	382.5	1	1	142.9	179.8	209.5	232.9	266.9	290.4	325.4
T5/41	m-(OH)c-$C_6H_5CH=CH$•	227.3	221.6	383.1	383.1	1	1	140.0	178.6	209.7	233.9	268.3	291.7	326.2
T5/42	p-(OH)c-$C_6H_5CH=CH$•	228.0	222.3	382.5	382.5	1	1	140.0	178.7	209.9	234.2	268.7	292.0	326.5
T5/43	o-(OCH_3)c-$C_6H_5CH=CH$•	245.2	240.3	418.6	427.7	3	1	159.7	203.9	240.9	270.6	313.8	343.6	387.2
T5/44	m-(OCH_3)c-$C_6H_5CH=CH$•	245.4	240.5	416.9	426.0	3	1	161.3	205.0	241.0	269.6	311.7	341.2	385.1
T5/45	p-(OCH_3)c-$C_6H_5CH=CH$•	246.2	241.3	416.4	425.5	3	1	161.3	205.1	241.2	270.0	312.2	341.6	385.4
T5/46	o-(CHO)c-$C_6H_5CH=CH$•	294.1	294.0	400.8	400.8	1	1	153.0	192.6	225.4	251.8	290.2	316.3	353.2
T5/47	m-(CHO)c-$C_6H_5CH=CH$•	281.7	281.6	407.0	407.0	1	1	146.8	187.1	220.6	247.3	285.8	312.0	349.8
T5/48	p-(CHO)c-$C_6H_5CH=CH$•	281.6	281.5	399.8	399.8	1	1	147.2	187.6	221.3	248.4	287.9	314.8	352.9
T5/49	o-($CH=CH_2$)c-$C_6H_5CH=CH$•	473.6	473.0	408.2	408.2	1	1	160.4	205.0	241.9	271.3	314.1	343.9	388.3
T5/50	m-($CH=CH_2$)c-$C_6H_5CH=CH$•	469.6	469.0	411.7	411.7	1	1	156.2	201.8	239.6	269.8	313.6	343.8	388.5
T5/51	p-($CH=CH_2$)c-$C_6H_5CH=CH$•	469.7	469.1	410.4	410.4	1	1	156.3	202.0	240.0	270.2	314.2	344.5	389.0
T5/52	o-(CH_3)c-$C_6H_5CH=CH$•	371.8	371.2	385.0	394.2	3	1	143.0	184.5	219.4	247.7	289.8	319.5	363.8
T5/53	m-(CH_3)c-$C_6H_5CH=CH$•	365.8	365.2	389.8	399.0	3	1	140.4	182.2	217.7	246.5	289.3	319.3	363.9
T5/54	p-(CH_3)c-$C_6H_5CH=CH$•	367.0	366.4	389.4	398.5	3	1	140.7	182.6	218.0	246.8	289.5	319.4	363.9
T5/55	o-(CH_2CH_3)c-$C_6H_5CH=CH$•	348.9	347.2	424.0	433.2	3	1	170.1	216.5	256.0	288.4	337.2	371.9	424.0
T5/56	m-(CH_2CH_3)c-$C_6H_5CH=CH$•	345.5	343.8	430.1	439.2	3	1	165.5	212.9	253.5	286.6	336.0	370.9	423.2
T5/57	p-(CH_2CH_3)c-$C_6H_5CH=CH$•	345.8	344.1	429.7	438.8	3	1	165.4	212.9	253.5	286.6	336.1	371.0	423.4
T5/58	1-(c-CH=CH•)-2,4-OH	50.1	40.9	407.8	407.8	1	1	166.6	205.1	235.2	258.5	291.4	313.8	347.2
T5/59	1-(c-CH=CH•)-2,5-OH	62.0	52.8	415.2	415.2	1	1	166.1	202.8	231.8	254.5	287.5	310.4	345.1
T5/60	1-(c-CH=CH•)-2-OH-4-OCH_3	67.7	59.2	440.1	449.3	3	1	187.8	231.5	266.6	294.4	335.0	363.3	406.0
T5/61	1-(c-CH=CH•)-2-OH-5-OCH_3	82.4	73.9	449.7	458.9	3	1	187.4	228.6	262.3	289.6	330.7	359.8	404.1
T5/62	1-(c-CH=CH•)-2-OH-4-CH=CH_2	293.5	289.3	439.1	439.1	1	1	180.5	226.1	263.2	292.5	335.3	364.8	408.9
T5/63	1-(c-CH=CH•)-3-OH-5-CH=CH_2	290.1	285.9	438.6	438.6	1	1	178.5	225.8	264.3	294.6	337.8	367.2	410.4
T5/64	1-(c-CH=CH•)-2-OH-3-CH_3	190.2	186.0	416.2	425.4	3	1	169.1	209.1	242.7	270.1	311.1	340.1	383.9
T5/65	1-(c-CH=CH•)-2-OH-4-CH_3	190.5	186.3	417.7	426.9	3	1	164.6	206.6	241.4	269.4	310.9	340.1	384.0

T5/66	1-(c-CH=CH•)-2-OH-5-CH_3	194.0	189.8	419.0	428.2	3	1	165.1	206.5	241.0	268.9	310.4	339.7	383.8
T5/67	1-(c-CH=CH•)-3-OH-5-CH_3	186.4	182.2	415.7	424.8	3	1	163.7	207.0	243.0	271.9	313.9	342.9	385.9
T5/68	1-(c-CH=CH•)-2-OH-3-CH_2CH_3	169.2	163.9	454.5	463.6	3	1	194.3	240.3	279.3	311.0	358.7	392.7	443.9
T5/69	1-(c-CH=CH•)-3-CHO-4-OH	78.4	74.8	407.9	407.9	1	1	161.7	204.2	239.4	267.5	308.2	335.9	375.9
T5/70	1-(c-CH=CH•)-2,4-CHO	176.1	178.1	445.7	445.7	1	1	181.6	224.7	260.7	289.8	332.5	361.2	400.7
T5/71	1-(c-CH=CH•)-2-CHO-5-CH=CH_2	359.2	360.6	457.1	457.1	1	1	189.6	238.1	278.4	310.8	358.1	390.3	436.5
T5/72	1-(c-CH=CH•)-2-CHO-4-CH_3	258.6	260.0	436.5	445.6	3	1	174.9	219.3	257.0	287.9	333.9	365.7	411.6
T5/73	1-(c-CH=CH•)-2-CH=CH_2-4-OH	299.1	294.9	436.1	436.1	1	1	180.2	226.6	264.5	294.3	337.0	366.2	409.5
T5/74	1-(c-CH=CH•)-2-CH=CH_2-5-CH_3	438.4	439.3	442.9	452.0	3	1	181.4	230.7	272.7	306.9	357.7	393.4	446.8
T5/75	1-(c-CH=CH•)-2-CH=CH_2-6-CH_3	441.7	442.6	439.5	448.6	3	1	191.1	238.6	278.6	311.1	359.9	394.7	447.2
T5/76	1-(c-CH=CH•)-2-CH_3-4-OH	196.2	192.0	413.6	422.7	3	1	163.9	207.3	243.0	271.5	313.0	341.9	385.0
T5/77	1-(c-CH=CH•)-2-CH_3-4-CHO	250.2	251.6	435.8	445.0	3	1	171.7	216.7	254.8	285.9	332.2	364.5	411.4
T5/78	1-(c-CH=CH•)-2-CH_3-4-CH=CH_2	438.8	439.7	442.7	451.9	3	1	180.9	230.4	272.6	306.9	357.9	393.7	447.2
T5/79	1-(c-CH=CH•)-3-CH_3-4-CH=CH_2	437.6	438.5	442.9	452.1	3	1	183.4	232.8	274.5	308.3	358.6	394.0	447.2
T5/80	1-(c-CH=CH•)-2,4-CH_3	336.2	337.1	420.6	438.9	9	1	164.7	211.2	251.1	284.0	333.7	369.1	422.4
	Subset 6: Benzyl Subset													
T6/1	$C_6H_5CH_2$•	210.3	208.2	314.5	320.3	2	1	106.3	141.1	169.9	192.8	226.5	249.9	284.8
T6/2	o-(OH)$C_6H_5CH_2$•	34.1	28.4	349.1	349.1	1	1	128.9	164.4	193.3	216.0	248.7	271.4	305.4
T6/3	m-(OH)$C_6H_5CH_2$•	35.6	29.9	350.1	350.1	1	1	127.7	164.0	193.4	216.3	249.2	271.8	305.7
T6/4	p-(OH)$C_6H_5CH_2$•	35.3	29.6	344.7	350.4	2	1	127.0	163.5	193.0	216.1	249.2	272.0	305.8
T6/5	o-(OCH_3)$C_6H_5CH_2$•	51.6	46.7	377.1	386.3	3	1	148.1	191.2	226.8	255.0	296.1	324.6	366.8
T6/6	m-(OCH_3) $C_6H_5CH_2$•	54.0	49.1	384.4	393.5	3	1	150.2	191.1	225.0	252.3	292.7	321.4	364.6
T6/7	p-(OCH_3)$C_6H_5CH_2$•	54.0	49.1	383.9	393.0	3	1	148.1	189.7	224.2	251.8	292.6	321.4	364.7
T6/8	o-(CHO)$C_6H_5CH_2$•	91.1	91.0	367.4	367.4	1	1	137.5	176.1	207.9	233.2	270.4	295.9	332.6
T6/9	m-(CHO)$C_6H_5CH_2$•	88.8	88.7	368.4	368.4	1	1	134.8	173.0	204.9	230.7	268.6	294.7	332.1
T6/10	p-(CHO)$C_6H_5CH_2$•	82.9	82.8	365.5	371.3	2	1	133.9	172.2	204.2	230.1	268.2	294.5	332.4
T6/11	o-(CH=CH_2)$C_6H_5CH_2$•	278.6	278.0	377.6	377.6	1	1	145.5	188.6	224.2	252.6	294.3	323.6	367.6
T6/12	m-(CH=CH_2)$C_6H_5CH_2$•	275.5	274.9	378.6	378.6	1	1	143.9	187.3	223.4	252.3	294.6	324.1	368.1
T6/13	p-(CH=CH_2)$C_6H_5CH_2$•	268.4	267.8	375.9	375.9	1	1	143.3	187.0	223.5	252.7	295.6	325.3	369.1
T6/14	o-(CH_3)$C_6H_5CH_2$•	175.9	175.3	352.2	361.3	3	1	131.3	170.4	203.6	230.7	271.3	300.1	343.6
T6/15	m-(CH_3)$C_6H_5CH_2$•	174.2	173.6	356.7	365.9	3	1	127.9	167.7	201.5	229.1	270.3	299.4	343.3
T6/16	p-(CH_3)$C_6H_5CH_2$•	174.7	174.1	351.4	366.3	6	1	127.8	167.5	201.3	228.9	270.2	299.4	343.3
T6/17	o-(CH_2CH_3)$C_6H_5CH_2$•	156.3	154.6	391.0	400.1	3	1	154.6	199.9	238.7	270.4	318.4	352.5	404.0
T6/18	m-(CH_2CH_3)$C_6H_5CH_2$•	153.7	152.0	396.3	405.5	3	1	152.8	198.1	237.0	268.9	316.8	351.0	402.7
T6/19	p-(CH_2CH_3)$C_6H_5CH_2$•	153.6	151.9	397.0	406.1	3	1	152.4	197.8	236.8	268.7	316.7	351.0	402.8
T6/20	1-CH_2•-2,3-OH	-144.4	-153.6	371.0	371.0	1	1	148.6	187.5	218.8	243.2	277.2	299.1	330.0
T6/21	1-CH_2•-2,4-OH	-142.1	-151.3	373.2	379.0	2	1	147.3	185.3	215.3	238.5	271.2	293.3	326.1
T6/22	1-CH_2•-2,5-OH	-133.5	-142.7	380.7	380.7	1	1	151.7	187.5	215.9	238.1	269.9	291.9	325.4
T6/23	1-CH_2•-2,6-OH	-143.0	-152.2	372.2	377.9	2	1	148.6	185.7	215.2	238.0	270.4	292.6	325.9
T6/24	1-CH_2•-2-OH-3-OCH_3	-126.0	-134.5	404.8	413.9	3	1	166.3	208.8	245.3	275.3	319.5	349.3	391.2
T6/25	1-CH_2•-2-OH-4-OCH_3	-121.8	-130.3	411.8	420.9	3	1	171.0	213.0	247.3	274.6	314.6	342.7	385.1
T6/26	1-CH_2•-2-OCH_3-4-OH	-124.0	-132.5	406.9	416.0	3	1	170.5	214.7	250.8	279.0	319.5	347.1	388.1
T6/27	1-CH_2•-2,4-OCH_3	-105.5	-113.2	438.8	457.0	9	1	191.1	240.6	281.6	314.4	362.6	396.4	446.9
T6/28	1-CH_2•-2-OCH_3-4-CHO	-80.4	-83.3	427.0	436.2	3	1	176.3	222.0	261.1	292.9	339.5	371.2	416.2
T6/29	1-CH_2•-2-OCH_3-4-CH=CH_2	107.9	104.5	432.4	441.6	3	1	184.9	237.0	280.5	315.2	365.7	400.5	451.5
T6/30	1-CH_2•-2-OCH_3-4-CH_3	15.6	12.2	414.2	432.5	9	1	170.0	218.1	258.6	291.4	340.0	374.2	425.3
T6/31	1-CH_2•-2-OCH_3-4-CH_2CH_3	-5.1	-9.6	452.4	470.6	9	1	194.4	248.2	293.9	331.0	386.4	425.6	484.6
T6/32	1-CH_2•-2,4-CHO	-33.3	-31.4	419.5	419.5	1	1	165.4	207.5	242.5	270.8	312.3	340.6	380.1
T6/33	1-CH_2•-2,5-CHO	-26.7	-24.8	419.7	419.7	1	1	167.0	209.0	243.9	272.0	313.3	341.2	379.9
T6/34	1-CH_2•-2,6-CHO	-19.2	-17.3	420.9	420.9	1	1	170.0	210.2	244.0	271.6	312.5	340.3	378.9
T6/35	1-CH_2•-2-CHO-4-CH=CH_2	148.6	150.0	422.5	422.5	1	1	174.7	222.1	261.4	293.0	339.4	371.2	416.9
T6/36	1-CH_2•-2-CH=CH_2-3-OH	100.9	96.7	398.5	404.3	2	1	169.3	216.8	254.4	283.2	323.7	351.0	391.6
T6/37	1-CH_2•-2-CH=CH_2-3-OCH_3	131.9	128.5	436.2	445.4	3	1	188.0	236.7	277.5	310.6	360.0	395.0	447.5
T6/38	1-CH_2•-2,3-CH=CH_2	350.6	351.5	431.7	431.7	1	1	187.7	238.7	281.1	315.0	364.7	399.4	451.6
T6/39	1-CH_2•-2-CH_3-3-OH	3.3	-0.9	382.9	392.0	3	1	152.7	192.4	225.5	252.3	292.2	320.5	363.5
T6/40	1-CH_2•-2-CH_3-4-OH	-0.3	-4.5	381.8	390.9	3	1	152.2	193.1	226.9	254.1	294.2	322.3	364.7
T6/41	1-CH_2•-2-CH_3-5-OH	3.2	-1.0	382.4	391.5	3	1	152.9	193.3	226.8	253.8	293.7	321.8	364.3
T6/42	1-CH_2•-2-CH_3-6-OH	-0.6	-4.8	380.3	389.4	3	1	154.8	194.5	227.5	254.2	293.8	321.7	364.2
T6/43	1-CH_2•-2-CH_3-4-CHO	47.2	48.6	403.5	412.6	3	1	159.3	201.7	238.1	268.0	313.1	344.7	391.2
T6/44	1-CH_2•-2-CH_3-6-CHO	57.5	58.9	401.7	410.9	3	1	164.0	207.0	243.0	272.3	316.1	346.7	391.6
T6/45	1-CH_2•-2-CH_3-4-CH=CH_2	233.1	234.0	407.4	416.6	3	1	168.5	216.5	257.3	290.7	340.5	375.6	428.0
T6/46	1-CH_2•-2-CH_3-5-CH=CH_2	240.7	241.6	410.3	419.4	3	1	169.0	216.6	257.1	290.1	339.4	374.3	426.9
T6/47	1-CH_2•-2,4-CH_3	140.0	140.9	388.8	407.0	9	1	152.9	196.9	235.1	266.7	315.0	349.6	402.1
T6/48	1-CH_2•-2,5-CH_3	140.4	141.3	388.7	407.0	9	1	153.0	197.0	235.1	266.8	315.0	349.6	402.1
T6/49	1-CH_2•-3-CH_3-4-OH	-1.5	-5.7	384.2	393.4	3	1	152.1	192.3	225.9	253.1	293.3	321.6	364.3
T6/50	1-CH_2•-3-CH_3-4-OCH_3	16.7	13.3	416.1	434.4	9	1	172.7	219.6	259.8	292.4	340.9	374.8	425.6
T6/51	1-CH_2•-3,5-CH_3	138.3	139.2	387.4	411.4	18	1	149.6	194.4	233.2	265.3	314.1	349.0	401.8
T6/52	1-CH_2•-3,6-CH_3	140.7	141.6	388.7	407.0	9	1	152.9	196.9	235.1	266.8	315.0	349.6	402.1
T6/53	C_6H_5CH•CH_3	178.1	174.9	359.0	368.2	3	1	124.6	164.6	199.0	227.1	269.1	298.8	343.1
T6/54	o-(OH)C_6H_5CH•CH_3	2.8	-4.0	387.3	396.4	3	1	148.7	188.9	222.9	250.4	291.3	320.1	363.6
T6/55	m-(OH)C_6H_5CH•CH_3	2.5	-4.3	389.0	398.2	3	1	145.7	187.4	222.4	250.6	291.9	320.7	364.0
T6/56	p-(OH)C_6H_5CH•CH_3	3.9	-2.9	389.4	398.5	3	1	145.5	187.2	222.2	250.4	291.8	320.8	364.1
T6/57	o-(OCH_3)C_6H_5CH•CH_3	20.1	14.1	420.0	438.2	9	1	167.5	215.2	255.8	288.8	338.1	373.0	425.1
T6/58	m-(OCH_3)C_6H_5CH•CH_3	22.0	16.0	422.0	440.3	9	1	169.9	214.9	253.7	285.8	334.5	369.5	422.4
T6/59	p-(OCH_3)C_6H_5CH•CH_3	22.8	16.8	422.0	440.3	9	1	166.7	213.3	253.2	285.9	335.1	370.1	422.9
T6/60	o-(CHO)C_6H_5CH•CH_3	58.6	57.4	407.4	416.6	3	1	156.0	200.3	238.0	268.5	313.8	345.3	391.0
T6/61	m-(CHO)C_6H_5CH•CH_3	55.5	54.3	410.1	419.2	3	1	153.4	196.7	234.2	265.1	311.4	343.7	390.5
T6/62	p-(CHO)C_6H_5CH•CH_3	53.2	52.0	405.0	414.1	3	1	153.2	196.6	234.1	265.0	311.3	343.6	390.5
T6/63	o-(CH=CH_2)C_6H_5CH•CH_3	248.1	246.4	415.6	424.7	3	1	164.7	212.6	253.4	286.8	336.8	372.3	425.7
T6/64	m-(CH=CH_2)C_6H_5CH•CH_3	243.0	241.3	417.0	426.1	3	1	162.4	210.9	252.6	286.6	337.3	373.0	426.4
T6/65	p-(CH=CH_2)C_6H_5CH•CH_3	236.5	234.8	413.7	422.9	3	1	161.8	210.7	252.7	287.1	338.3	374.1	427.4
T6/66	o-(CH_3)C_6H_5CH•CH_3	145.4	143.7	390.0	408.3	9	1	150.4	194.7	233.4	265.5	314.3	349.2	402.0
T6/67	m-(CH_3)C_6H_5CH•CH_3	142.2	140.5	395.5	413.8	9	1	146.3	191.3	230.7	263.4	313.0	348.4	401.6
T6/68	o-(CH_2CH_3)C_6H_5CH•CH_3	126.1	123.2	428.5	446.8	9	1	173.9	224.2	268.4	305.1	361.2	401.5	462.3
T6/69	m-(CH_2CH_3)C_6H_5CH•CH_3	121.8	118.9	435.6	453.9	9	1	171.3	221.8	266.3	303.2	359.5	399.9	461.0
T6/70	p-(CH_2CH_3)C_6H_5CH•CH_3	121.7	118.8	436.0	454.3	9	1	170.9	221.5	266.0	303.1	359.5	399.9	461.1

3.2 Thermochemical Database Of The Special Cases Set

Thermochemical database for the special cases set which include the molecules that are excluded from the training set for development of Group Additive Values (GAVs) and non-nearest neighbor interactions (NNIs) are given in **Table S2**.

Table S2. *Thermochemical database for the special cases set. The units of standard enthalpy of formation ($\Delta_f H^\circ$) data is given in kJ mol^{-1} whereas the units of entropies (S°) and heat capacities (C_p) are given in J mol^{-1} K^{-1}.*

Special Cases Set														
#	Radicals	$\Delta_f H^\circ$ (298 K)		S° (298 K)				C_p						
		$\Delta_f H^\circ_{G4}$	$\Delta_f H^\circ_{G4/BAC}$	S°	S°_{int}	$\sigma_{tot\ sym}$	n_{opt}	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
S1/1	C•C_5H_5=CH_2	363.1	357.4	345.9	351.7	2	1	122.4	158.4	188.2	212.2	247.5	272.1	308.5
S1/2	(o-OH)C•C_5H_5=CH_2	180.5	174.4	377.8	377.8	1	1	143.5	183.0	214.8	239.6	274.5	297.7	331.6
S1/3	(m-OH)C•C_5H_5=CH_2	188.6	182.5	381.8	381.8	1	1	143.9	181.4	211.7	235.7	270.2	294.0	329.3
S1/4	(p-OH)C•C_5H_5=CH_2	190.0	183.9	384.4	384.4	1	1	143.2	180.7	211.2	235.3	270.0	293.9	329.4
S1/5	(o-OCH_3)C•C_5H_5=CH_2	207.0	201.1	422.5	431.6	3	1	169.9	213.6	249.1	277.0	317.5	346.1	389.4
S1/6	(m-OCH_3)C•C_5H_5=CH_2	206.7	200.8	415.7	424.9	3	1	166.9	208.8	243.7	271.9	313.9	343.6	388.3
S1/7	(p-OCH_3)C•C_5H_5=CH_2	208.6	202.7	418.3	427.5	3	1	165.2	207.4	242.7	271.2	313.6	343.5	388.3
S1/8	(o-CHO)C•C_5H_5=CH_2	243.1	237.9	400.0	400.0	1	1	152.1	191.0	223.7	250.4	289.8	317.0	356.0
S1/9	(m-CHO)C•C_5H_5=CH_2	243.7	238.5	407.8	407.8	1	1	151.9	191.4	224.2	250.5	288.9	315.3	353.4
S1/10	(p-CHO)C•C_5H_5=CH_2	233.1	227.9	391.7	391.7	1	1	149.6	189.1	222.2	249.0	288.5	315.8	355.5
S1/11	(o-$CH=CH_2$)C•C_5H_5=CH_2	427.2	421.4	405.4	405.4	1	1	161.6	206.0	243.1	272.9	316.7	347.2	392.4
S1/12	(m-$CH=CH_2$)C•C_5H_5=CH_2	428.2	422.4	409.7	409.7	1	1	160.2	204.7	241.8	271.6	315.6	346.2	391.7
S1/13	(p-$CH=CH_2$)C•C_5H_5=CH_2	419.5	413.7	403.3	403.3	1	1	159.4	204.3	241.9	272.2	316.8	347.6	393.0
S1/14	(o-CH_3)C•C_5H_5=CH_2	324.8	319.0	382.0	391.1	3	1	145.5	186.0	220.6	248.9	291.6	321.8	367.1
S1/15	(m-CH_3)C•C_5H_5=CH_2	328.4	322.6	382.1	391.2	3	1	147.8	188.8	223.7	252.1	294.3	324.1	368.4
S1/16	(p-CH_3)C•C_5H_5=CH_2	327.8	322.0	388.9	398.0	3	1	143.8	184.7	219.6	248.2	291.1	321.6	367.0
S1/17	(o-CH_2CH_3)C•C_5H_5=CH_2	303.7	296.8	424.1	433.2	3	1	169.3	216.0	256.1	289.1	338.9	374.3	427.2
S1/18	(m-CH_2CH_3)C•C_5H_5=CH_2	306.4	299.5	428.1	437.2	3	1	168.9	215.4	255.4	288.2	337.8	373.2	426.3
S1/19	(p-CH_2CH_3)C•C_5H_5=CH_2	306.6	299.7	428.9	438.1	3	1	168.5	215.1	255.1	288.0	337.7	373.2	426.5
S2/1	1(3H)-Isobenzofuranonyl	-87.2	-88.5	353.7	353.7	1	1	128.4	167.2	198.8	223.7	259.1	282.5	315.5

4. Bond Dissociation Energies

In this section, the database of Bond Dissociation Energies (BDEs) and the standard enthalpy of formation ($\Delta_f H^\circ$) data used in the calculation of these BDEs are given. The calculation of the BDEs is done according to Eq. 5 described in the Methodology section of the paper.

All the $\Delta_f H^\circ$ data reported in this section of the Supporting Information is calculated with the G4/BAC method described in the Methodology section of the paper. The $\Delta_f H^\circ$ data of the monocyclic aromatic radicals (MARs) are taken from the thermochemical data in **Table S1** and **Table S2**. The standard enthalpy of formation ($\Delta_f H^\circ$) data for the closed-shell monocyclic aromatic hydrocarbons (MAHs) used in the calculation of bond dissociation energies (BDEs) are given in **Table S3**. This data is taken from the study of Ince et al..[1] where the methodology is completely consistent with the present study. The data for the small radicals are given in **Table S4**.

With the aid of the information in these **Tables S1**, **S2**,**S3** and **S4**, the database of bond dissociation energies (BDEs) are constructed. This database includes BDE for 297 bonds in 70 MAHs and it is given in **Table S5**. In this table, first, name of the molecule is given and then, the BDEs for all the bonds (available in the database) in that molecule is given one by one. In order to indicate the bond, "-" is used and besides, the smaller moiety of the molecule on one side of the bond is shown in bold. As an instance, C_6H_5-**OH** indicates the bond between ring carbon and the oxygen atom in phenol (C_6H_5OH). In double substituted MAHs, one of the substituents and its position with respect to the other substituent is given in square parenthesis "[ ]". The other substituent is the substituent which possess the bond of interest and the smaller moiety on the other side of this bond is given in bold. For example, [(m-OH)]C_6H_4O-**CH_3** represents the O-C bond in the methoxy group of the m-methoxyphenol (or m-hydroxymethoxybenzene).

The BDEs of the C_6H_5-X bonds (X=-CH=CH_2, -OCH_3, and –OH) are excluded from the discussion in the text as the trends in these BDEs can only be useful in explaining substituent interactions in MAHs which are already done by Ince et al..[1] In the text, X=-H, -CHO and -CH_3 cases are given as examples, and the information regarding the other excluded groups is given in In **Figure S15**.

Table S3. *BAC-corrected $\Delta_f H^\circ$ data at the level for G4 for monocyclic aromatic hydrocarbons (MAHs) taken from the study by Ince et al..*[1]

Mol. #	Molecule Name	$\Delta_f H^\circ_{G4/BAC}$ (kJ mol^{-1})
1	Benzene	82
2	Phenol (Hydroxybenzene)	-96
3	Anisole (Methoxybenzene)	-74.2
4	Benzaldehyde (Formylbenzene)	-37.4
5	Styrene (Vinylbenzene)	147.9
6	Toluene (Methylbenzene)	49.2
7	EthylBenzene	28.2
8	o-dihydroxybenzene	-275.8
9	m-dihydroxybenzene	-273.9
10	p-dihydroxybenzene	-266.1
11	o-dimethoxybenzene	-215.3
12	m-dimethoxybenzene	-231
13	p-dimethoxybenzene	-223.4
14	o-diformylbenzene	-136.4
15	m-diformylbenzene	-152.4
16	p-diformylbenzene	-151.3
17	o-divinylbenzene	222.2
18	m-divinylbenzene	213.9
19	p-divinylbenzene	213.2
20	o-dimethylbenzene	18.8
21	m-dimethylbenzene	16.6
22	p-dimethylbenzene	17.2
23	o-diethylbenzene	-20.4
24	m-diethylbenzene	-25.6
25	p-diethylbenzene	-24.9
26	o-methoxyphenol	-255.8
27	m-methoxyphenol	-252.6
28	p-methoxyphenol	-244.8
29	o-formylphenol	-244.1
30	m-formylphenol	-215.4
31	p-formylphenol	-219
32	o-vinylphenol	-27.8
33	m-vinylphenol	-29.9
34	p-vinylphenol	-29.7
35	o-methylphenol	-129.7
36	m-methylphenol	-129.2
37	p-methylphenol	-126.8
38	o-ethylphenol	-150.5

39	m-ethylphenol	-150.2
40	p-ethylphenol	-147.9
41	o-formylanisole	-189.5
42	m-formylanisole	-195.5
43	p-formylanisole	-198.6
44	o-vinylanisole	-5.9
45	m-vinylanisole	-8.6
46	p-vinylanisole	-8.3
47	o-methylanisole	-108.5
48	m-methylanisole	-107.2
49	p-methylanisole	-105.3
50	o-ethylanisole	-129.4
51	m-ethylanisole	-128.2
52	p-ethylanisole	-126.3
53	o-vinylbenzaldehyde	39.5
54	m-vinylbenzaldehyde	28.9
55	p-vinylbenzaldehyde	28.1
56	o-methylbenzaldehyde	-65.1
57	m-methylbenzaldehyde	-71.3
58	p-methylbenzaldehyde	-72.1
59	o-ethylbenzaldehyde	-85.8
60	m-ethylbenzaldehyde	-92.1
61	p-ethylbenzaldehyde	-92.8
62	o-methylstyrene	120.2
63	m-methylstyrene	114.9
64	p-methylstyrene	114.9
65	o-ethylstyrene	98.9
66	m-ethylstyrene	93.8
67	p-ethylstyrene	93.9
68	o-ethyltoluene	-1
69	m-ethyltoluene	-4.5
70	p-ethyltoluene	-3.9

Table S4. *BAC-corrected $\Delta_f H^\circ$ data calculated at the level for G4 for small nonaromatic radicals (H•, OH•, OCH_3•, CHO•, •$CH{=}CH_2$, •CH_3, •CH_2CH_3).*

Mol. #	Molecule Name	$\Delta_f H^\circ_{G4/BAC}$ (kJ mol^{-1})
1	Hydrogen (•H)	218.0
2	Hydroxy (•OH)	35.2
3	Methoxy(•OCH_3)	16.8
4	Formyl(•CHO)	40.2
5	Vinyl(•$CH{=}CH_2$)	294.5
6	Methyl(•CH_3)	144.7
7	Ethyl(•CH_2CH_3)	118.1

Table S5. *The database of Bond Dissociation Energies (BDEs).*

Molecule and Bond Name		**BDE (kJ mol^{-1})**
Benzene and Single Substituted MAHs		
1	**C_6H_6 (Benzene)**	
	C_6H_5-**H**	473.3
2	**C_6H_5OH (Phenol)**	
	C_6H_5-**OH**	468.5
	C_6H_5O-**H**	368.1
	C_6H_4OH[o-(C_b-**H**)]	476.1
	C_6H_4OH[m-(C_b-**H**)]	472.7
	C_6H_4OH[p-(C_b-**H**)]	479.0
3	**$C_6H_5OCH_3$ (Anisole)**	
	C_6H_5-**OCH_3**	428.6
	C_6H_5O-**CH_3**	273.1
	$C_6H_5OCH_2$-**H**	402.1
	$C_6H_4OCH_3$[o-(C_b-**H**)]	471.4
	$C_6H_4OCH_3$[m-(C_b-**H**)]	470.0
	$C_6H_4OCH_3$[p-(C_b-**H**)]	476.6
4	**C_6H_5CHO (Benzaldehyde)**	
	C_6H_5-**CHO**	415.3
	C_6H_5CO-**H**	373.6
	C_6H_4[o-(C_b-**H**)]	474.9
	C_6H_4[m-(C_b-**H**)]	476.2
	C_6H_4[p-(C_b-**H**)]	474.9
5	**$C_6H_5CH=CH_2$ (Styrene)**	
	C_6H_5-**$CH=CH_2$**	484.4
	C_6H_5C(-**H**)=CH_2	433.3
	$C_6H_5CH=CH$-**H**(trans)	470.2
	$C_6H_5CH=CH$-**H**(cis)	465.8
	$C_6H_4CH=CH_2$[o-(C_b-**H**)]	476.0
	$C_6H_4CH=CH_2$[m-(C_b-**H**)]	477.1
	$C_6H_4CH=CH_2$[p-(C_b-**H**)]	478.3
6	**$C_6H_5CH_3$ (Toluene)**	
	C_6H_5-**CH_3**	433.3
	$C_6H_5CH_2$-**H**	377.0
	$C_6H_4CH_3$[o-(C_b-**H**)]	472.2
	$C_6H_4CH_3$[m-(C_b-**H**)]	472.3
	$C_6H_4CH_3$[p-(C_b-**H**)]	474.5
7	**$C_6H_5CH_2CH_3$ (Ethyl Benzene)**	
	C_6H_5-**CH_2CH_3**	427.6
	C_6H_5(-**H**)-CH_3	364.6
	$C_6H_5CH_2$-**CH_3**	324.7
	$C_6H_4CH_3$[o-(Cb-**H**)]	470.7
	$C_6H_4CH_3$[m-(Cb-**H**)]	470.9

	$C_6H_4CH_3$[p-(Cb-**H**)]	473.1
Double Substituted Benzenes		
8	**o-dihydroxybenzene (catechol)**	
	[(o-OH)]C_6H_4-**OH**	473.8
	[(o-OH)]C_6H_4O-**H**	330.8
9	**m-dihydroxybenzene (resorcinol)**	
	[(m-OH)]C_6H_4-**OH**	467.9
	[(m-OH)]C_6H_4O-**H**	365.0
10	**p-dihydroxybenzene (hydroquinone)**	
	[(p-OH)]C_6H_4-**OH**	466.4
	[(p-OH)]C_6H_4O-**H**	347.1
11	**o-hydroxymethoxybenzene (o-guaiacol)**	
	[(o-OCH_3)]C_6H_4-**OH**	470.3
	[(o-OCH_3)]C_6H_4O-**H**	362.8
	[(o-OH)]C_6H_4-**OCH_3**	435.2
	[(o-OH)]C_6H_4O-**CH_3**	237.6
	[(o-OH)]$C_6H_4OCH_2$-**H**	404.5
12	**m-hydroxymethoxybenzene (m-guaiacol)**	
	[(m-OCH_3)]C_6H_4-**OH**	465.7
	[(m-OCH_3)]C_6H_4O-**H**	359.1
	[(m-OH)]C_6H_5-**OCH_3**	428.0
	[(m-OH)]C_6H_4O-**CH_3**	270.5
	[(m-OH)]$C_6H_4OCH_2$-**H**	401.1
13	**p-hydroxymethoxybenzene (p-guaiacol)**	
	[(p-OCH_3)]C_6H_4-**OH**	464.5
	[(p-OCH_3)]C_6H_4O-**H**	343.9
	[(p-OH)]C_6H_4-**OCH_3**	426.5
	[(p-OH)]C_6H_4O-**CH_3**	252.6
	[(p-OH)]$C_6H_4OCH_2$-**H**	402.6
14	**o-hydroxyformylbenzene**	
	[(o-CHO)]C_6H_4-**OH**	502.1
	[(o-CHO)]C_6H_4O-**H**	401.9
	[(o-OH)]C_6H_4-**CHO**	447.0
	[(o-OH)]C_6H_4CO-**H**	387.2
15	**m-hydroxyformylbenzene**	
	[(m-CHO)]C_6H_4-**OH**	471.5
	[(m-CHO)]C_6H_4O-**H**	372.8
	[(m-OH)]C_6H_4-**CHO**	414.3
	[(m-OH)]C_6H_4CO-**H**	373.5
16	**p-hydroxyformylbenzene**	
	[(p-CHO)]C_6H_4-**OH**	473.8
	[(p-CHO)]C_6H_4O-**H**	372.3
	[(p-OH)]C_6H_4-**CHO**	424.2
	[(p-OH)]C_6H_4CO-**H**	370.0
17	**o-hydroxyvinylbenzene**	

	[(o-CH=CH_2)]C_6H_4-**OH**	469.0
	[(o-CH=CH_2)]C_6H_4O-**H**	357.2
	[(o-OH)]C_6H_4-**CH=CH_2**	485.1
	[(o-OH)]C_6H_4C(-**H**)=CH_2	420.2
	[(o-OH)]C_6H_4CH=CH-**H**(trans)	466.6
	[(o-OH)]C_6H_4CH=CH-**H**(cis)	448.3
18	**m-hydroxyvinylbenzene**	
	[(m-CH=CH_2)]C_6H_4-**OH**	472.2
	[(m-CH=CH_2)]C_6H_4O-**H**	368.3
	[(m-OH)]C_6H_4-**CH=CH_2**	483.2
	[(m-OH)]C_6H_4C(-**H**)=CH_2	430.4
	[(m-OH)]C_6H_4CH=CH-**H**(trans)	469.5
	[(m-OH)]C_6H_4CH=CH-**H**(cis)	465.0
19	**p-hydroxyvinylbenzene**	
	[(p-CH=CH_2)]C_6H_4-**OH**	473.2
	[(p-CH=CH_2)]C_6H_4O-**H**	351.9
	[(p-OH)]C_6H_4-**CH=CH_2**	489.3
	[(p-OH)]C_6H_4C(-**H**)=CH_2	431.6
	[(p-OH)]C_6H_4CH=CH-**H**(trans)	470.0
	[(p-OH)]C_6H_4CH=CH-**H**(cis)	465.1
20	**o-hydroxymethylbenzene (o-Cresol)**	
	[(o-CH_3)]C_6H_4-**OH**	468.4
	[(o-CH_3)]C_6H_4O-**H**	358.6
	[(o-OH)]C_6H_4-**CH_3**	437.2
	[(o-OH)]$C_6H_4CH_2$-**H**	376.1
21	**m-hydroxymethylbenzene (m-Cresol)**	
	[(m-CH_3)]C_6H_4-**OH**	468.0
	[(m-CH_3)]C_6H_4O-**H**	365.3
	[(m-OH)]C_6H_4-**CH_3**	432.7
	[(m-OH)]$C_6H_4CH_2$-**H**	377.1
22	**p-hydroxymethylbenzene (p-Cresol)**	
	[(p-CH_3)]C_6H_4-**OH**	467.8
	[(p-CH_3)]C_6H_4O-**H**	359.3
	[(p-OH)]C_6H_4-**CH_3**	436.6
	[(p-OH)]$C_6H_4CH_2$-**H**	374.4
23	**o-hydroxyethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**OH**	466.8
	[(o-CH_2CH_3)]C_6H_4O-**H**	357.8
	[(o-OH)]C_6H_4-**CH_2CH_3**	431.4
	[(o-OH)]C_6H_4CH(-**H**)CH_3	364.5
	[(o-OH)]$C_6H_4CH_2$-**CH_3**	323.7
24	**m-hydroxyethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**OH**	466.7
	[(m-CH_2CH_3)]C_6H_4O-**H**	364.2
	[(m-OH)]C_6H_4-**CH_2CH_3**	427.1

	[(m-OH)]C_6H_4CH(-**H**)CH_3	363.9
	[(m-OH)]$C_6H_4CH_2$-**CH_3**	324.9
25	**p-hydroxyethylbenzene**	
	[(p-CH_2CH_3)]C_6H_5-**OH**	466.6
	[(p-CH_2CH_3)]C_6H_5O-**H**	358.6
	[(p-OH)]C_6H_4-**CH_2CH_3**	431.1
	[(p-OH)]C_6H_4CH(-**H**)CH_3	363.0
	[(p-OH)]$C_6H_4CH_2$-**CH_3**	322.3
26	**o-dimethoxybenzene**	
	[(o-OCH_3)]C_6H_4-**OCH_3**	411.2
	[(o-OCH_3)]C_6H_4O-**CH_3**	249.1
	[(o-OCH_3)]$C_6H_4OCH_2$-**H**	398.6
27	**m-dimethoxybenzene**	
	[(m-OCH_3)]C_6H_4-**OCH_3**	425.5
	[(m-OCH_3)]C_6H_4O-**CH_3**	264.3
	[(m-OCH_3)]$C_6H_4OCH_2$-**H**	398.2
28	**p-dimethoxybenzene**	
	[(p-OCH_3)]C_6H_4-**OCH_3**	424.5
	[(p-OCH_3)]C_6H_4O-**CH_3**	249.3
	[(p-OCH_3)]$C_6H_4OCH_2$-**H**	399.9
29	**o-methoxyformylbenzene**	
	[(p-CHO)]C_6H_4-**OCH_3**	428.9
	[(p-CHO)]C_6H_4O-**CH_3**	274.1
	[(p-CHO)]$C_6H_4OCH_2$-**H**	405.4
	[(o-OCH_3)]C_6H_4-**CHO**	408.9
	[(o-OCH_3)]C_6H_4CO-**H**	373.8
30	**m-methoxyformylbenzene**	
	[(m-CHO)]C_6H_4-**OCH_3**	433.0
	[(m-CHO)]C_6H_4O-**CH_3**	279.7
	[(m-CHO)]$C_6H_4OCH_2$-**H**	405.9
	[(m-OCH_3)]C_6H_4-**CHO**	413.5
	[(m-OCH_3)]C_6H_4CO-**H**	372.1
31	**p-methoxyformylbenzene**	
	[(p-CHO)]C_6H_4-**OCH_3**	434.8
	[(p-CHO)]C_6H_4O-**CH_3**	278.7
	[(p-CHO)]$C_6H_4OCH_2$-**H**	404.0
	[(p-OCH_3)]C_6H_4-**CHO**	423.2
	[(p-OCH_3)]C_6H_4CO-**H**	370.6
32	**o-methoxyvinylbenzene**	
	[(o-$CH=CH_2$)]C_6H_4-**OCH_3**	428.5
	[(o-$CH=CH_2$)]C_6H_4O-**CH_3**	262.1
	[(o-$CH=CH_2$)]$C_6H_4OCH_2$-**H**	405.1
	[(o-OCH_3)]C_6H_4-**$CH=CH_2$**	479.7
	[(o-OCH_3)]C_6H_4C(-**H**)$=CH_2$	425.0
	[(o-OCH_3)]$C_6H_4CH=CH$-**H**(trans)	464.2

	[(o-OCH_3)]C_6H_4CH=CH-**H**(cis)	463.3
33	**m-methoxyvinylbenzene**	
	[(m-$CH=CH_2$)]C_6H_4-**OCH_3**	432.3
	[(m-$CH=CH_2$)]C_6H_4O-**CH_3**	273.8
	[(m-$CH=CH_2$)]$C_6H_4OCH_2$-**H**	405.4
	[(m-OCH_3)]C_6H_4-**$CH=CH_2$**	481.0
	[(m-OCH_3)]C_6H_4C(-**H**)=CH_2	427.4
	[(m-OCH_3)]C_6H_4CH=CH-**H**(trans)	467.1
	[(m-OCH_3)]C_6H_4CH=CH-**H**(cis)	462.5
34	**p-methoxyvinylbenzene**	
	[(p-$CH=CH_2$)]C_6H_4-**OCH_3**	433.2
	[(p-$CH=CH_2$)]C_6H_4O-**CH_3**	257.3
	[(p-$CH=CH_2$)]$C_6H_4OCH_2$-**H**	405.7
	[(p-OCH_3)]C_6H_4-**$CH=CH_2$**	487.3
	[(p-OCH_3)]C_6H_4C(-**H**)=CH_2	429.0
	[(p-OCH_3)]C_6H_4CH=CH-**H**(trans)	467.6
	[(p-OCH_3)]C_6H_4CH=CH-**H**(cis)	462.7
35	**o-methoxymethylbenzene**	
	[(o-CH_3)]C_6H_4-**OCH_3**	432.5
	[(o-CH_3)]C_6H_4O-**CH_3**	264.2
	[(o-CH_3)]$C_6H_4OCH_2$-**H**	401.3
	[(o-OCH_3)]C_6H_4-**CH_3**	432.5
	[(o-OCH_3)]$C_6H_4CH_2$-**H**	373.2
36	**m-methoxymethylbenzene**	
	[(m-CH_3)]C_6H_4-**OCH_3**	427.4
	[(m-CH_3)]C_6H_4O-**CH_3**	270.1
	[(m-CH_3)]$C_6H_4OCH_2$-**H**	400.4
	[(m-OCH_3)]C_6H_4-**CH_3**	429.8
	[(m-OCH_3)]$C_6H_4CH_2$-**H**	374.3
37	**p-methoxymethylbenzene**	
	[(p-CH_3)]C_6H_4-**OCH_3**	427.7
	[(p-CH_3)]C_6H_4O-**CH_3**	264.6
	[(p-CH_3)]$C_6H_4OCH_2$-**H**	401.8
	[(p-OCH_3)]C_6H_4-**CH_3**	434.5
	[(p-OCH_3)]$C_6H_4CH_2$-**H**	372.4
38	**o-methoxyethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**OCH_3**	427.1
	[(o-CH_2CH_3)]C_6H_4O-**CH_3**	263.5
	[(o-CH_2CH_3)]$C_6H_4OCH_2$-**H**	399.5
	[(o-OCH_3)]C_6H_4-**CH_2CH_3**	426.8
	[(o-OCH_3)]C_6H_4CH(-**H**)CH_3	361.5
	[(o-OCH_3)]$C_6H_4CH_2$-**CH_3**	320.9
39	**m-methoxyethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**OCH_3**	426.1
	[(m-CH_2CH_3)]C_6H_4O-**CH_3**	269.0

	[(m-CH_2CH_3)]$C_6H_4OCH_2$-**H**	399.4
	[(m-OCH_3)]C_6H_4-**CH_2CH_3**	424.2
	[(m-OCH_3)]C_6H_4CH(-**H**)CH_3	362.2
	[(m-OCH_3)]$C_6H_4CH_2$-**CH_3**	322.1
40	**p-methoxyethylbenzene**	
	[(p-CH_2CH_3)]C_6H_4-**OCH_3**	426.4
	[(p-CH_2CH_3)]C_6H_4O-**CH_3**	263.8
	[(p-CH_2CH_3)]$C_6H_4OCH_2$-**H**	400.5
	[(p-OCH_3)]C_6H_4-**CH_2CH_3**	428.9
	[(p-OCH_3)]C_6H_4CH(-**H**)CH_3	361.1
	[(p-OCH_3)]$C_6H_4CH_2$-**CH_3**	320.2
41	**o-diformylbenzene**	
	[(o-CHO)]C_6H_4-**CHO**	399.3
	[(o-CHO)]C_6H_4CO-**H**	267.2
42	**m-diformylbenzene**	
	[(m-CHO)]C_6H_4-**CHO**	413.4
	[(m-CHO)]C_6H_4CO-**H**	372.1
43	**p-diformylbenzene**	
	[(p-CHO)]C_6H_4-**CHO**	411.0
	[(p-CHO)]C_6H_4CO-**H**	372.0
44	**o-formylvinylbenzene**	
	[(o-$CH=CH_2$)]C_6H_4-**CHO**	406.6
	[(o-$CH=CH_2$)]C_6H_4CO-**H**	368.8
	[(o-CHO)]C_6H_4-**$CH=CH_2$**	477.8
	[(o-CHO)]C_6H_4C(-**H**)$=CH_2$	416.4
	[(o-CHO)]$C_6H_4CH=CH$-**H**(trans)	472.5
	[(o-CHO)]$C_6H_4CH=CH$-**H**(cis)	465.0
45	**m-formylvinylbenzene**	
	[(m-$CH=CH_2$)]C_6H_4-**CHO**	418.3
	[(m-$CH=CH_2$)]C_6H_4CO-**H**	371.2
	[(m-CHO)]C_6H_4-**$CH=CH_2$**	486.5
	[(m-CHO)]C_6H_4C(-**H**)$=CH_2$	427.6
	[(m-CHO)]$C_6H_4CH=CH$-**H**(trans)	470.7
	[(m-CHO)]$C_6H_4CH=CH$-**H**(cis)	466.5
46	**p-formylvinylbenzene**	
	[(p-$CH=CH_2$)]C_6H_4-**CHO**	420.3
	[(p-$CH=CH_2$)]C_6H_4CO-**H**	378.5
	[(p-CHO)]C_6H_4-**$CH=CH_2$**	486.0
	[(p-CHO)]C_6H_4C(-**H**)$=CH_2$	417.8
	[(p-CHO)]$C_6H_4CH=CH$-**H**(trans)	471.4
	[(p-CHO)]$C_6H_4CH=CH$-**H**(cis)	466.6
47	**o-formylmethylbenzene**	
	[(o-CH_3)]C_6H_4-**CHO**	408.7
	[(o-CH_3)]C_6H_4CO-**H**	368.3
	[(o-CHO)]C_6H_4-**CH_3**	432.6

	[(o-CHO)]$C_6H_4CH_2$-**H**	374.1
48	**m-formylmethylbenzene**	
	[(m-CH_3)]C_6H_4-**CHO**	415.0
	[(m-CH_3)]C_6H_4CO-**H**	372.2
	[(m-CHO)]C_6H_4-**CH_3**	436.9
	[(m-CHO)]$C_6H_4CH_2$-**H**	378.0
49	**p-formylmethylbenzene**	
	[(p-CH_3)]C_6H_4-**CHO**	418.0
	[(p-CH_3)]C_6H_4CO-**H**	371.9
	[(p-CHO)]C_6H_4-**CH_3**	436.4
	[(p-CHO)]$C_6H_4CH_2$-**H**	372.9
50	**o-formylethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**CHO**	407.0
	[(o-CH_2CH_3)]C_6H_4CO-**H**	365.7
	[(o-CHO)]C_6H_4-**CH_2CH_3**	426.7
	[(o-CHO)]C_6H_4CH(-**H**)CH_3	362.8
	[(o-CHO)]$C_6H_4CH_2$-**CH_3**	321.6
51	**m-formylethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**CHO**	413.5
	[(m-CH_2CH_3)]C_6H_4CO-**H**	370.6
	[(m-CHO)]C_6H_4-**CH_2CH_3**	431.1
	[(m-CHO)]C_6H_4CH(-**H**)CH_3	364.4
	[(m-CHO)]$C_6H_4CH_2$-**CH_3**	325.6
52	**p-formylethylbenzene**	
	[(p-CH_2CH_3)]C_6H_4-**CHO**	416.4
	[(p-CH_2CH_3)]C_6H_4CO-**H**	370.3
	[(p-CHO)]C_6H_4-**CH_2CH_3**	430.5
	[(p-CHO)]C_6H_4CH(-**H**)CH_3	365.0
	[(p-CHO)]$C_6H_4CH_2$-**CH_3**	320.4
53	**o-divinylbenzene**	
	[(o-CH=CH_2)]C_6H_4-**CH=CH_2**	478.3
	[(o-CH=CH_2)]C_6H_4C(-**H**)=CH_2	417.3
	[(o-CH=CH_2)]C_6H_4CH=CH-**H**(trans)	468.8
	[(o-CH=CH_2)]C_6H_4CH=CH-**H**(cis)	464.3
54	**m-divinylbenzene**	
	[(m-CH=CH_2)]C_6H_4-**CH=CH_2**	487.7
	[(m-CH=CH_2)]C_6H_4C(-**H**)=CH_2	426.6
	[(m-CH=CH_2)]C_6H_4CH=CH-**H**(trans)	473.1
	[(m-CH=CH_2)]C_6H_4CH=CH-**H**(cis)	468.8
55	**p-divinylbenzene**	
	[(p-CH=CH_2)]C_6H_4-**CH=CH_2**	489.6
	[(p-CH=CH_2)]C_6H_4C(-**H**)=CH_2	418.6
	[(p-CH=CH_2)]C_6H_4CH=CH-**H**(trans)	473.9
	[(p-CH=CH_2)]C_6H_4CH=CH-**H**(cis)	469.5
56	**o-vinylmethylbenzene**	

	[(o-CH_3)]C_6H_4-**$CH=CH_2$**	477.8
	[(o-CH_3)]C_6H_4C(-**H**)=CH_2	416.9
	[(o-CH_3)]C_6H_4CH=CH-**H**(trans)	469.0
	[(o-CH_3)]C_6H_4CH=CH-**H**(cis)	463.0
	[(o-$CH=CH_2$)]C_6H_4-**CH_3**	430.5
	[(o-$CH=CH_2$)]$C_6H_4CH_2$-**H**	375.8
57	**m-vinylmethylbenzene**	
	[(m-CH_3)]C_6H_4-**$CH=CH_2$**	483.2
	[(m-CH_3)]C_6H_4C(-**H**)=CH_2	425.8
	[(m-CH_3)]C_6H_4CH=CH-**H**(trans)	468.3
	[(m-CH_3)]C_6H_4CH=CH-**H**(cis)	464.7
	[(m-$CH=CH_2$)]C_6H_4-**CH_3**	436.9
	[(m-$CH=CH_2$)]$C_6H_4CH_2$-**H**	378.0
58	**p-vinylmethylbenzene**	
	[(p-CH_3)]C_6H_4-**$CH=CH_2$**	485.4
	[(p-CH_3)]C_6H_4C(-**H**)=CH_2	425.2
	[(p-CH_3)]C_6H_4CH=CH-**H**(cis)	469.5
	[(p-CH_3)]C_6H_4CH=CH-**H**(trans)	465.0
	[(p-$CH=CH_2$)]C_6H_4-**CH_3**	438.1
	[(p-$CH=CH_2$)]$C_6H_4CH_2$-**H**	370.9
59	**o-vinylethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**$CH=CH_2$**	476.6
	[(o-CH_2CH_3)]C_6H_4C(-**H**)=CH_2	415.9
	[(o-CH_2CH_3)]C_6H_4CH=CH-**H**(trans)	466.2
	[(o-CH_2CH_3)]C_6H_4CH=CH-**H**(cis)	462.3
	[(o-$CH=CH_2$)]C_6H_4-**CH_2CH_3**	425.1
	[(o-$CH=CH_2$)]C_6H_4CH(-**H**)CH_3	365.4
	[(o-$CH=CH_2$)]$C_6H_4CH_2$-**CH_3**	323.8
60	**m-vinylethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**$CH=CH_2$**	481.9
	[(m-CH_2CH_3)]C_6H_4C(-**H**)=CH_2	423.7
	[(m-CH_2CH_3)]C_6H_4CH=CH-**H**(trans)	467.9
	[(m-CH_2CH_3)]C_6H_4CH=CH-**H**(cis)	462.3
	[(m-$CH=CH_2$)]C_6H_4-**CH_2CH_3**	431.3
	[(m-$CH=CH_2$)]C_6H_4CH(-**H**)CH_3	365.4
	[(m-$CH=CH_2$)]$C_6H_4CH_2$-**CH_3**	325.8
61	**p-vinylethylbenzene**	
	[(p-CH_2CH_3)]C_6H_4-**$CH=CH_2$**	484.0
	[(p-CH_2CH_3)]C_6H_4C(-**H**)=CH_2	423.8
	[(p-CH_2CH_3)]C_6H_4CH=CH-**H**(trans)	468.1
	[(p-CH_2CH_3)]C_6H_4CH=CH-**H**(cis)	463.5
	[(p-$CH=CH_2$)]C_6H_4-**CH_2CH_3**	432.4
	[(p-$CH=CH_2$)]C_6H_4CH(-**H**)CH_3	358.8
	[(p-$CH=CH_2$)]$C_6H_4CH_2$-**CH_3**	318.6
62	**o-dimethylbenzene (o-Xylene)**	

	[(o-CH_3)]C_6H_4-**CH_3**	429.3
	[(o-CH_3)]$C_6H_4CH_2$-**H**	374.5
63	**m-dimethylbenzene (m-Xylene)**	
	[(m-CH_3)]C_6H_4-**CH_3**	431.7
	[(m-CH_3)]$C_6H_4CH_2$-**H**	375.0
64	**p-dimethylbenzene (p-Xylene)**	
	[(p-CH_3)]C_6H_4-**CH_3**	433.3
	[(p-CH_3)]$C_6H_4CH_2$-**H**	374.9
65	**o-methylethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**CH_3**	426.7
	[(o-CH_2CH_3)]$C_6H_4CH_2$-**H**	373.5
	[(o-CH_3)]C_6H_4-**CH_2CH_3**	422.5
	[(o-CH_3)]C_6H_4CH(-**H**)CH_3	362.6
	[(o-CH_3)]$C_6H_4CH_2$-**CH_3**	321.0
66	**m-methylethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**CH_3**	430.4
	[(m-CH_2CH_3)]$C_6H_4CH_2$-**H**	374.4
	[(m-CH_3)]C_6H_4-**CH_2CH_3**	426.1
	[(m-CH_3)]C_6H_4CH(-**H**)CH_3	362.9
	[(m-CH_3)]$C_6H_4CH_2$-**CH_3**	322.8
67	**p-methylethylbenzene**	
	[(p-CH_2CH_3)]C_6H_4-**CH_3**	432.0
	[(p-CH_2CH_3)]$C_6H_4CH_2$-**H**	373.7
	[(p-CH_3)]C_6H_4-**CH_2CH_3**	427.7
	[(p-CH_3)]C_6H_4CH(-**H**)CH_3	345.1
	[(p-CH_3)]$C_6H_4CH_2$-**CH_3**	322.7
68	**o-diethylbenzene**	
	[(o-CH_2CH_3)]C_6H_4-**CH_2CH_3**	419.5
	[(o-CH_2CH_3)]C_6H_4CH(-**H**)CH_3	361.6
	[(o-CH_2CH_3)]$C_6H_4CH_2$-**CH_3**	319.7
69	**m-diethylbenzene**	
	[(m-CH_2CH_3)]C_6H_4-**CH_2CH_3**	424.9
	[(m-CH_2CH_3)]C_6H_4CH(-**H**)CH_3	362.5
	[(m- CH_2CH_3)]$C_6H_4CH_2$-**CH_3**	322.3
70	**p-diethylbenzene**	
	[(p-CH_2CH_3)]C_6H_4-**CH_2CH_3**	426.4
	[(p-CH_2CH_3)]C_6H_4CH(-**H**)CH_3	361.7
	[(p-CH_2CH_3)]$C_6H_4CH_2$-**CH_3**	321.5

5. Experimental Validation of G4/BAC Data

Experimental validation of the G4/BAC data is made through the comparison of the BDE values calculated with G4/BAC method with the available experimental data. All the reported experimental BDE data in Luo's handbook and the cited literature[2-29] are plotted against the G4/BAC data in **Figure S15**. In **Figure S16**, the deviations of the G4/BAC data from the literature values are plotted against G4/BAC data for bond strengths.

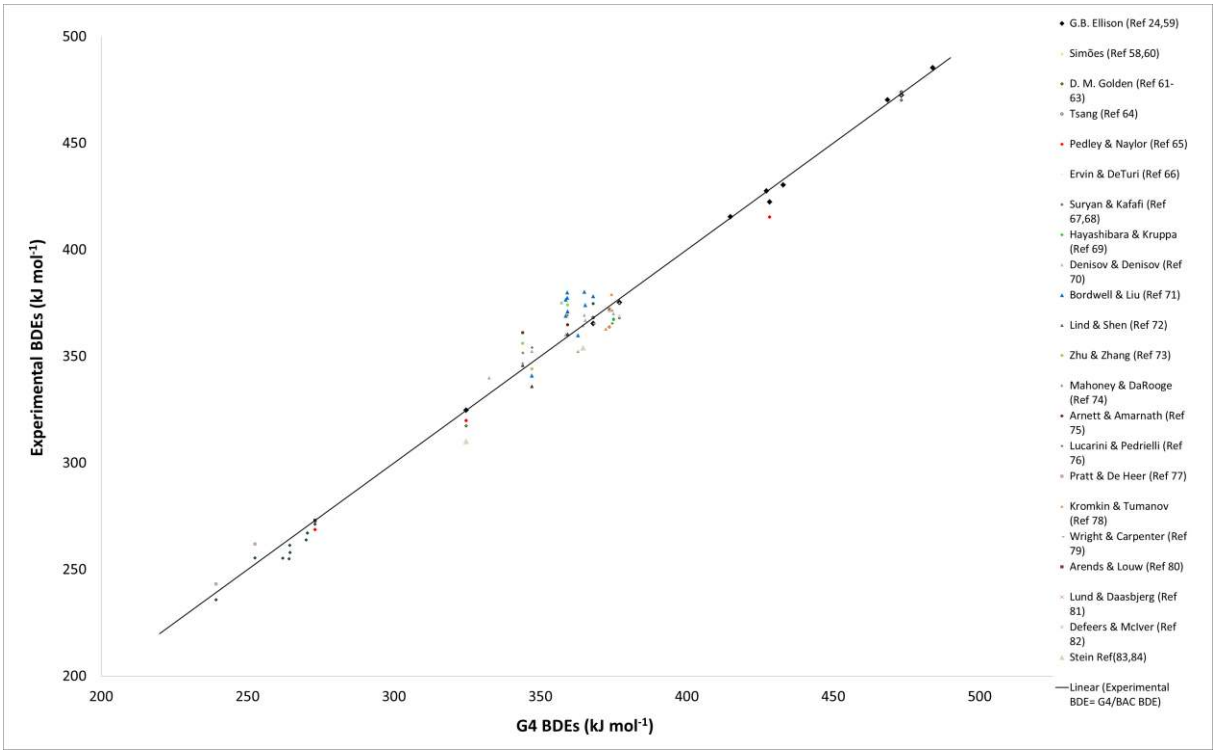


Figure S15. *Reported experimental BDE data in the literature plotted against G4/BAC data in the present study. Color code (shown on the right) is used to depict the references for the studies from where the data is taken.*[2-29]

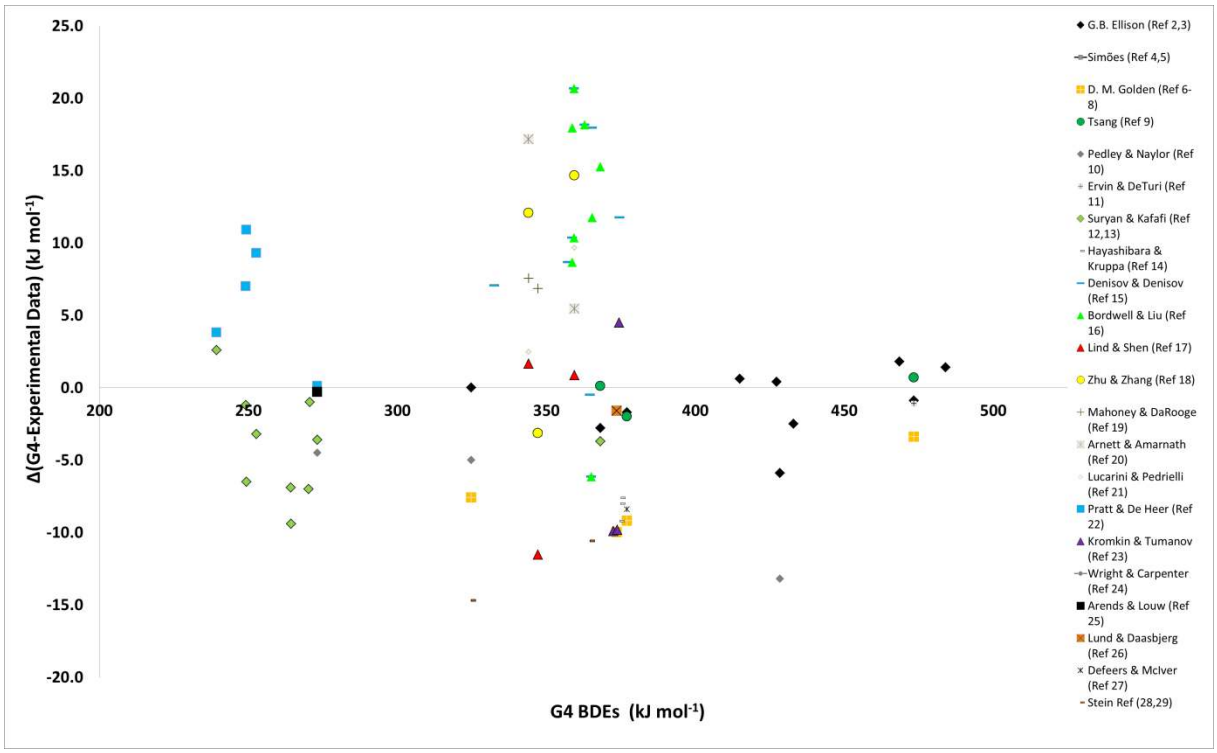


Figure S16. *Plot of the deviation of the G4/BAC data from the reported experimental values for the BDEs of the bonds in monocyclic aromatic hydrocarbons (MAHs) against G4/BAC data.*[2-29]

6. The BDE Analysis: Bond Dissociation Energy Plots

The objective of BDE Analysis is to identify substituent interactions in monocyclic aromatic radicals. This analysis uses the change of BDEs upon addition of a substituent group (ΔBDE).

With the following relation, one uses the BDE analysis to identify the substituent effects in the MARs,i.e. $NNI_{Radical}$:

$\Delta BDE = NNI_{Parent} - NNI_{Radical}$ (refer to text for the derivation of this relation)

Here, the ΔBDEs are calculated in the present study and the NNI_{Parent} values are taken from the study of Ince et al.[1] The ΔBDE plots which are not shown in the manuscript are presented in this subsection in **Figure S17**, **Figure S24** and **Figure S26**. In **Figures S18-S22** and **Figures S27-S28**, the BDEs of various bonds are plotted for varying substituent groups.

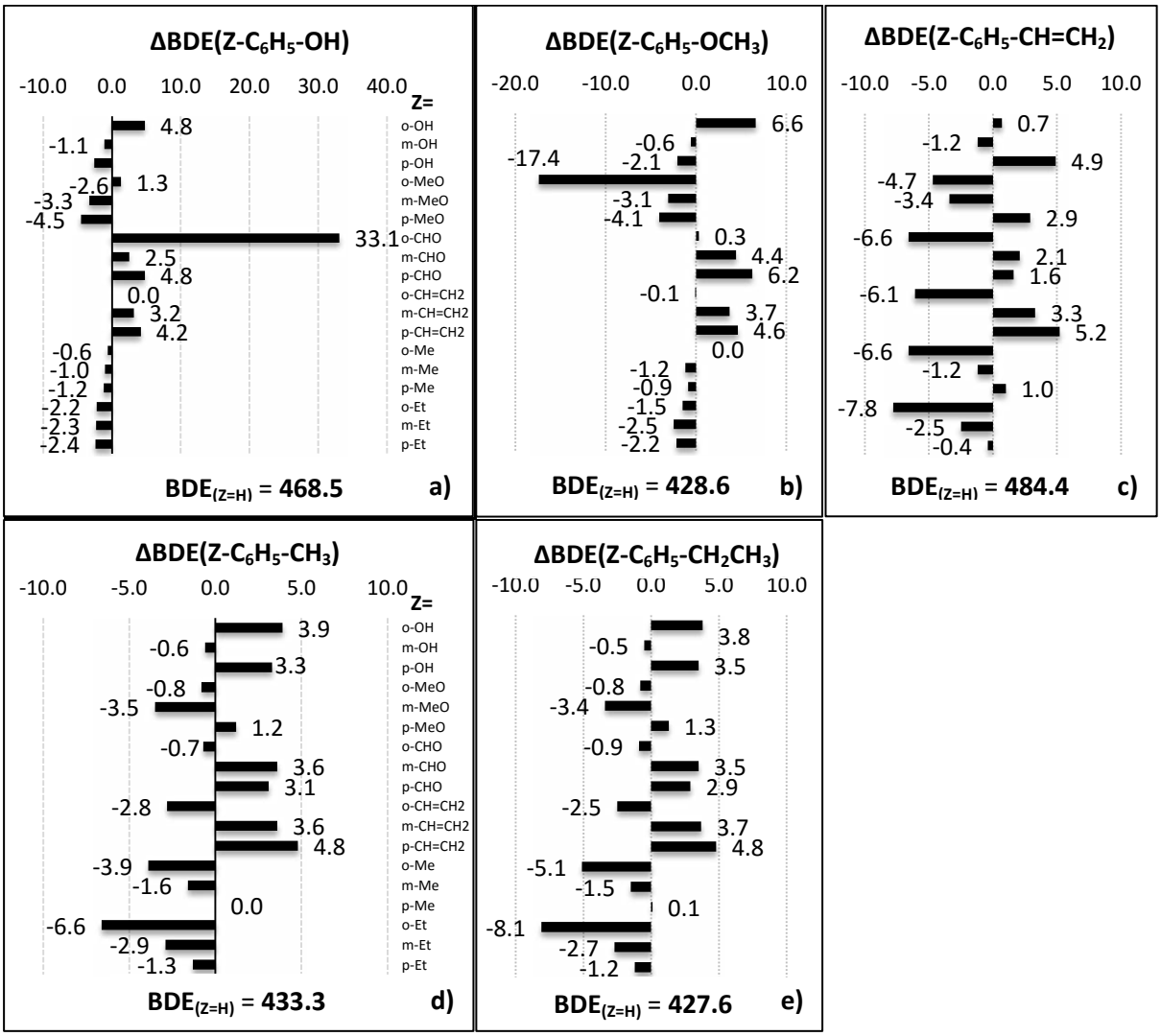


Figure S17. *ΔBDE (= $BDE_Z - BDE_H$) for the bonds in substituted C_6H_4-X molecules where X= **(a)** -OH, **(b)** -OCH_3, **(c)** -$CH=CH_2$, **(d)** -CH_3 and **(e)** -CH_2CH_3 for various Z groups. Below each plot, the BDEs of the bonds in unsubstituted MAHs (**$BDE_{(Z=H)}$**) are given. See text for the details regarding the definition of ΔBDEs. Note that the scale of the x-axis differs for the different bonds. All units are kJ mol^{-1}.*

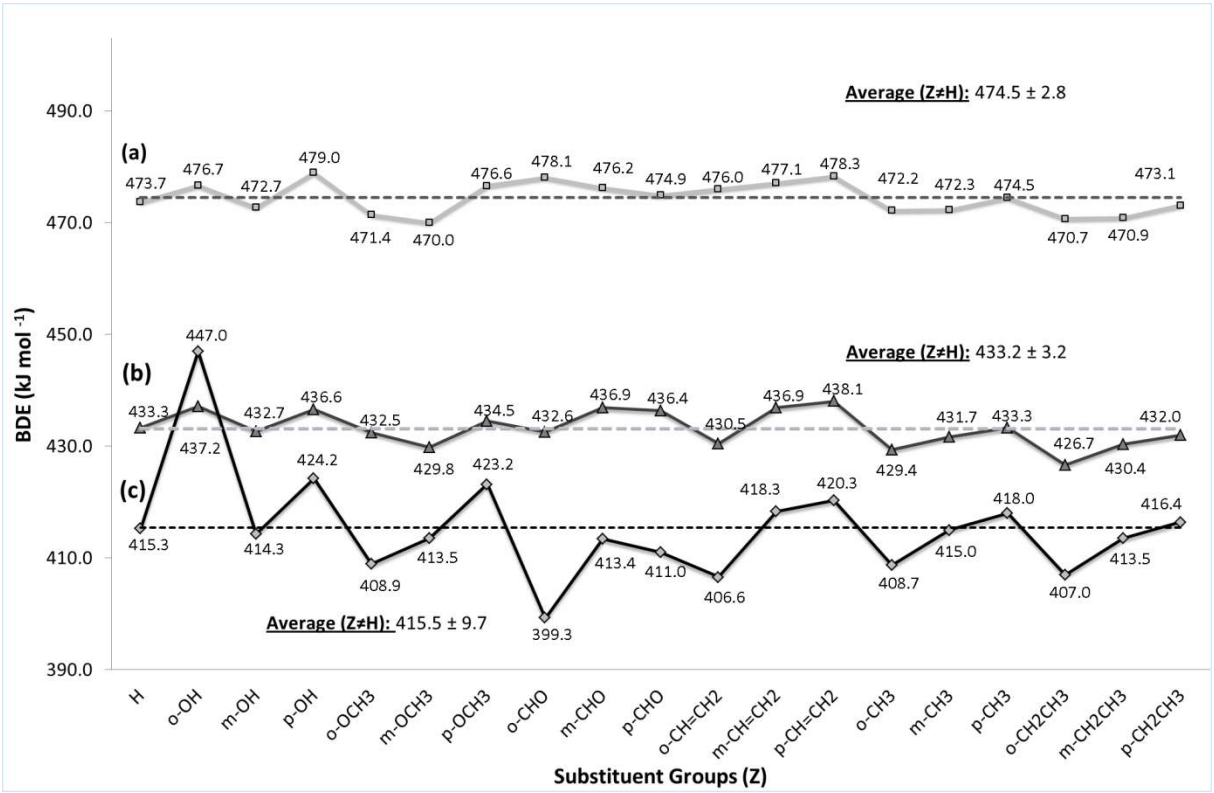


Figure S18. *BDEs for the bonds in substituted Z-C_6H_4-X molecules with X=-H* ***(a)****, -CH_3* ***(b)****, and -CHO* ***(c)****. The average values do not include the unsubstituted case (Z = H). Units are in kJ mol^{-1}.*

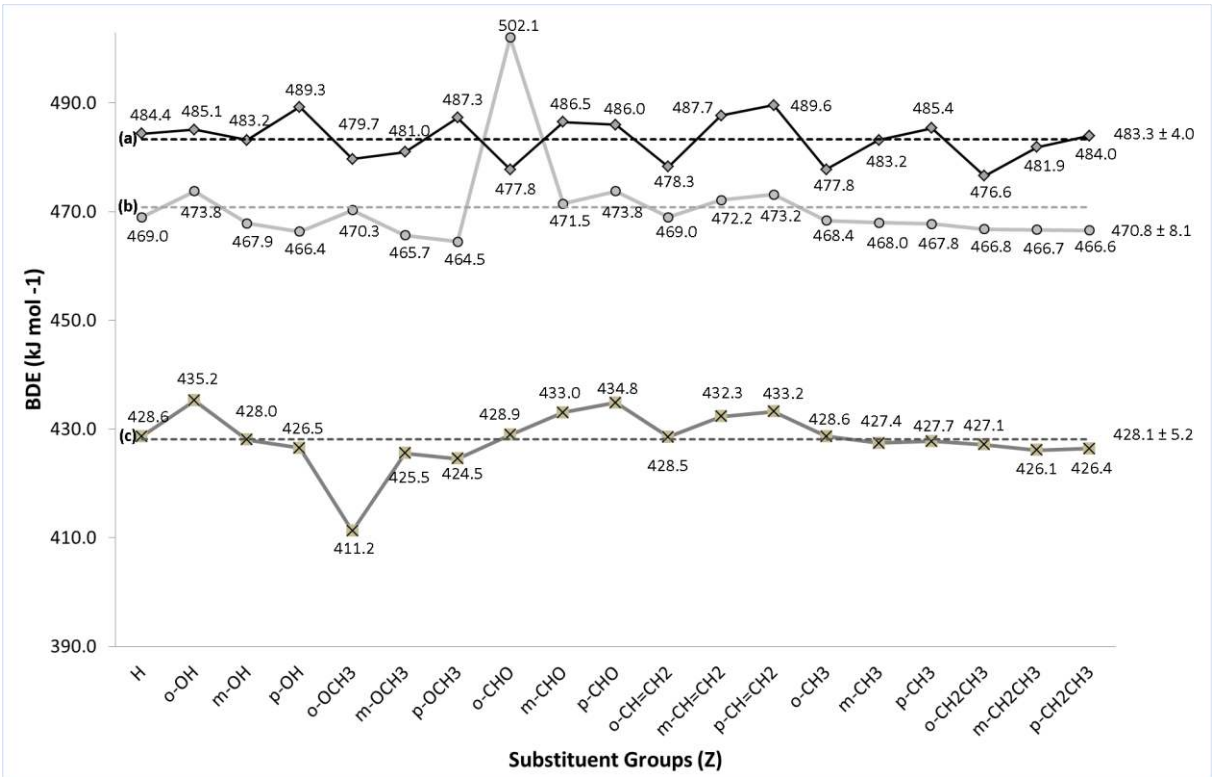


Figure S19. *BDEs of substituted Z-C_6H_4-X molecules with X= $CH=CH_2$* ***(a)****, OH* ***(b)****, and OCH_3* ***(c)****. The average values do not include the unsubstituted case (Z = H). Units are in kJ mol^{-1}.*

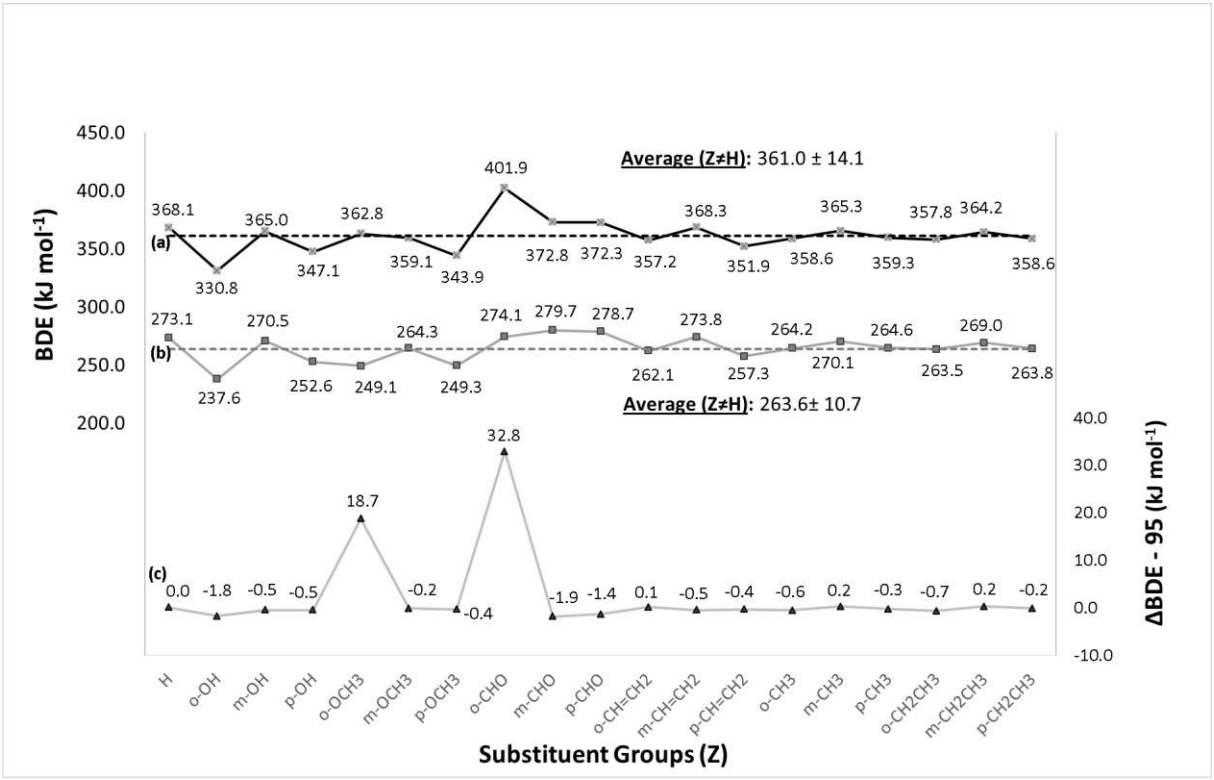


Figure S20. *BDEs for the Z-C_6H_4O-H (trace **(a)**) and Z-C_6H_4O-CH_3 (trace **(b)**) bonds in unsubstituted and substituted phenols and anisoles. Trace **(c)** presents the difference between two traces (a) and (b) corrected by 95 kJ mol^{-1} (the difference between the Z=H cases). The average values do not include the unsubstituted case (Z = H). Units are in kJ mol^{-1}.*

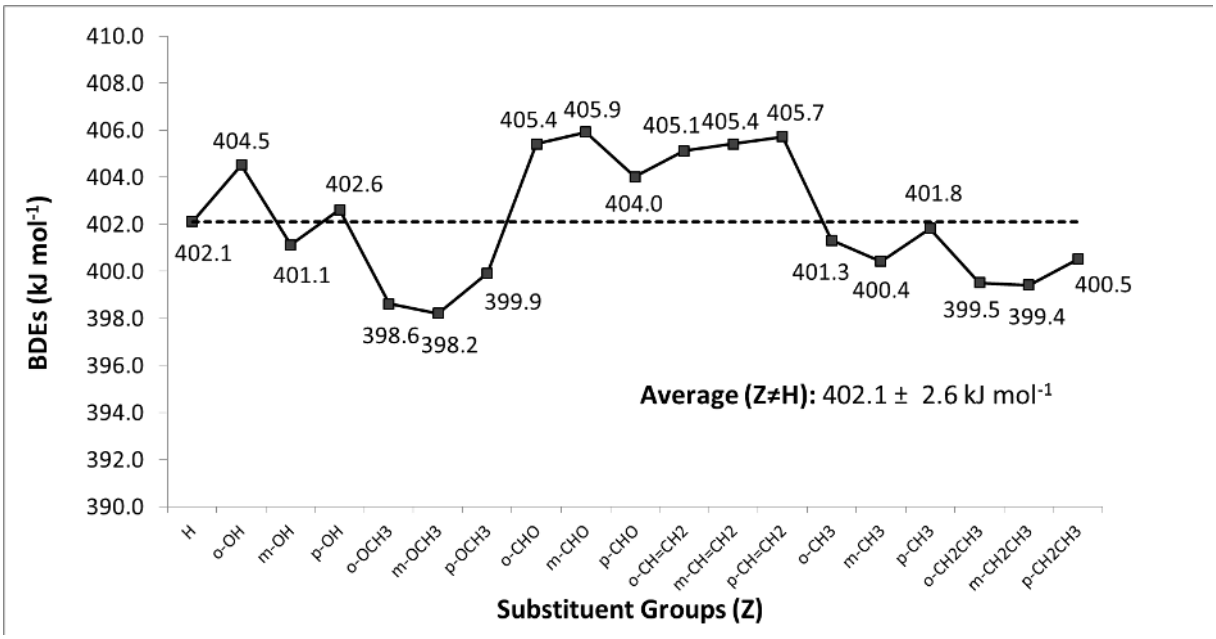


Figure S21. *BDE changes for Z-$C_6H_4OCH_2$-H bonds in substituted anisoles with respect to varying Z groups. The average value does not include the unsubstituted case (Z = H). Units are in kJ mol^{-1}.*

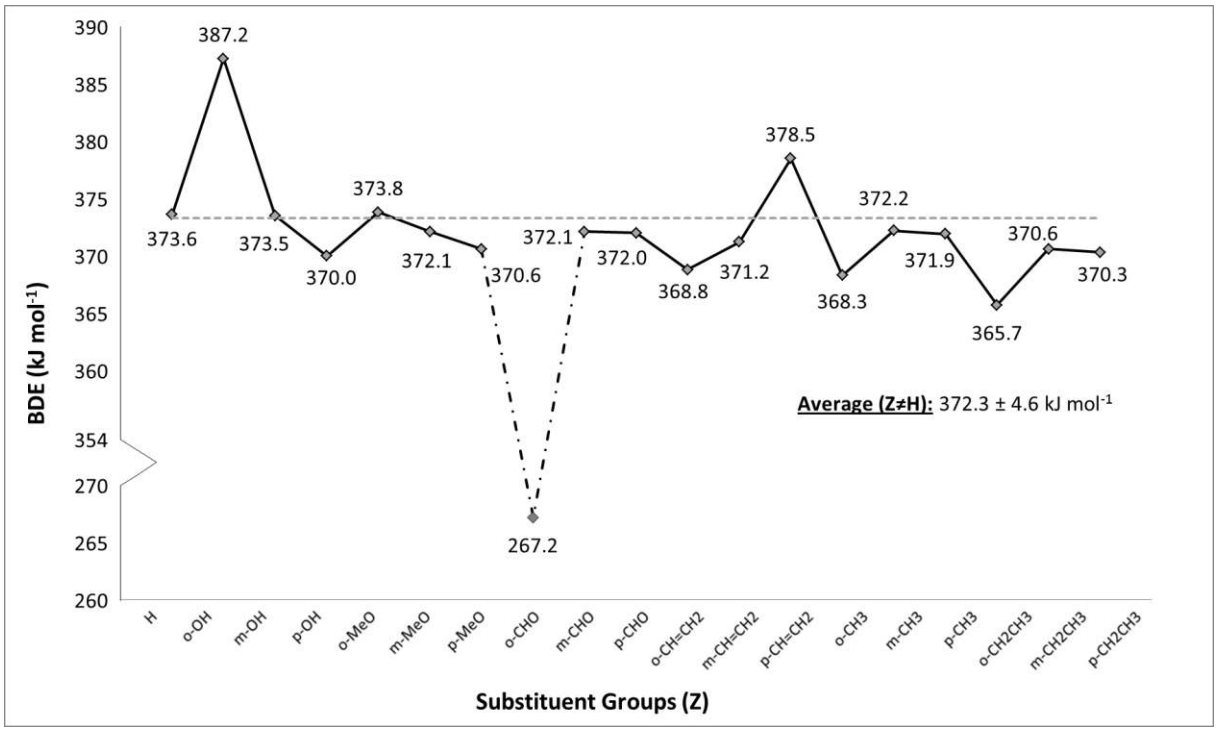


Figure S22. *BDE changes for Z-$C_6H_4C(=O)$-H bonds in substituted benzaldehydes with respect to varying Z substituents. The average value does not include the unsubstituted (Z = H) and the outlier case (Z = o-CHO). Units are in kJ mol^{-1}.*

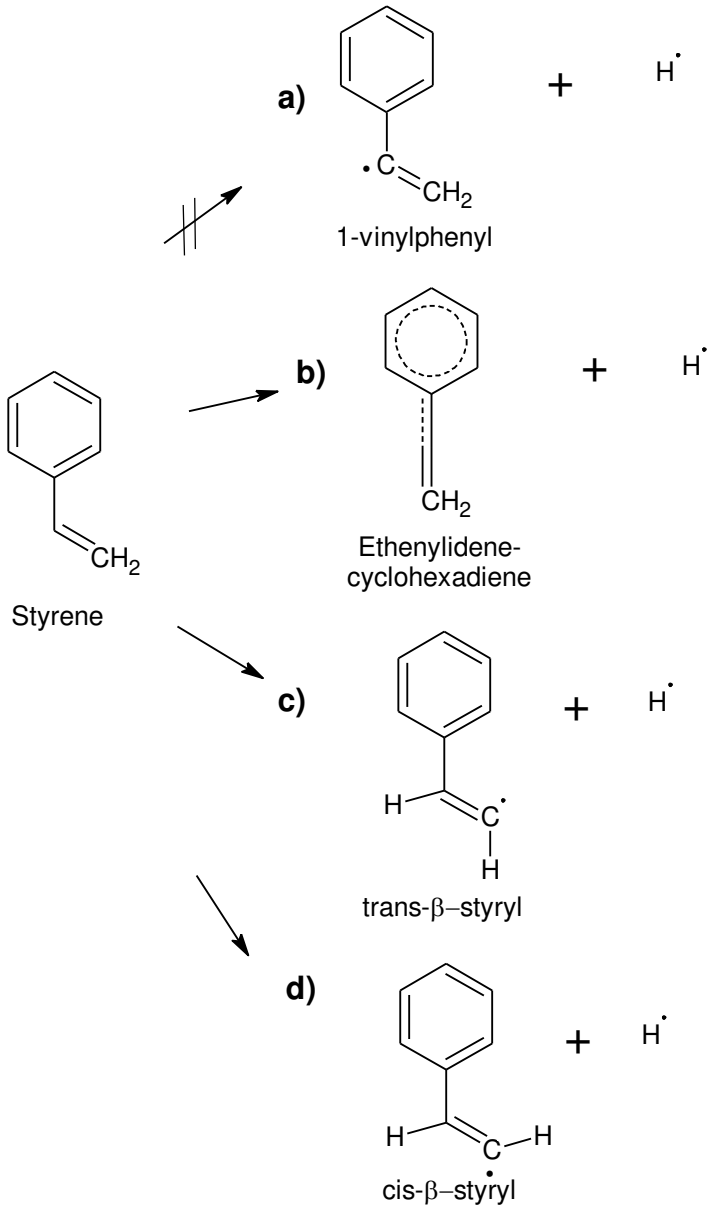


Figure S23. *Prototypical reactions that yield* ***a)*** *α-styryl ($C_5H_5C\bullet=CH_2$),* ***b)*** *ethenylidene-cyclohexadiene,* ***c)*** *trans-β-styryl (t-β-styryl) and* ***d)*** *cis-β-styryl (c-β-styryl) radicals.*

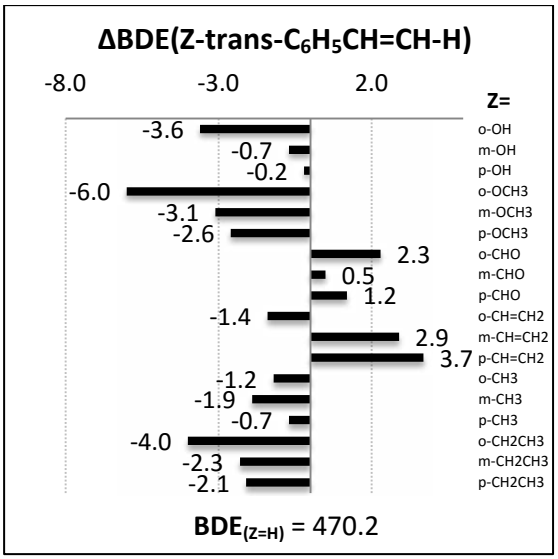


Figure S24. *ΔBDEs (*= $BDE_Z - BDE_H$) *for Z-trans-C_6H_4CH=CH-H for 18 different Z groups. Below the plot, the BDE of the bond in unsubstituted styrene (**$BDE_{(Z=H)}$**) is given. See text for the details regarding the definition of ΔBDEs. Note that the scale of the x-axis differs for the different bonds. All units are kJ mol^{-1}.The ΔBDEs are given in kJ mol^{-1}.*

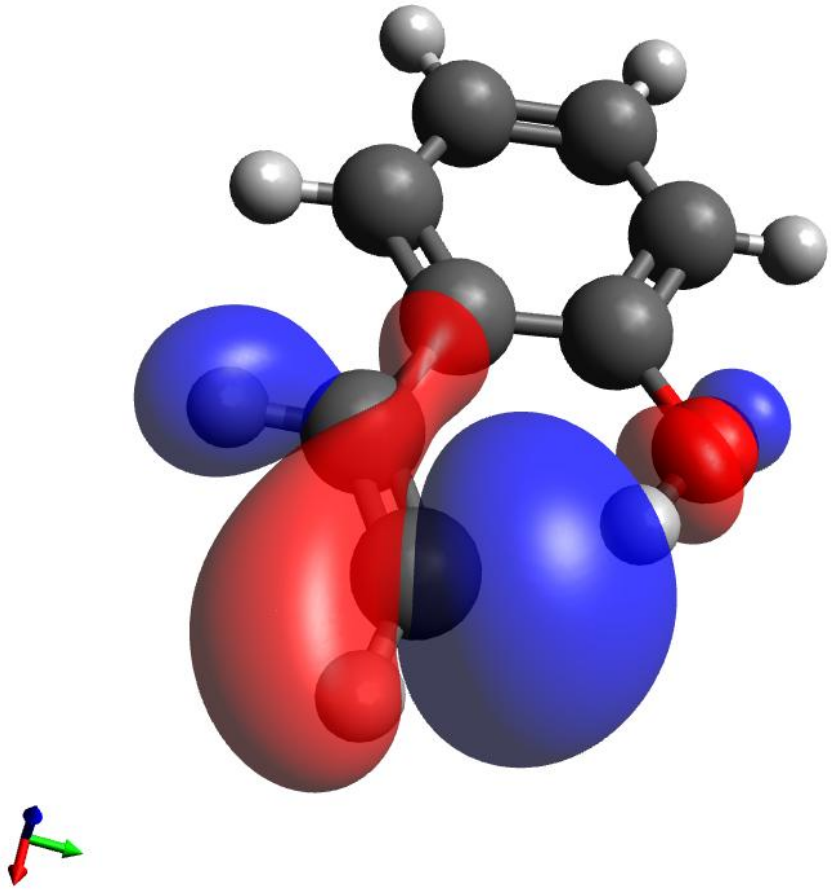


Figure S25. *3D molecular orbital representation of the substituent interaction in o-OH substituted trans-β-styryl radical.*

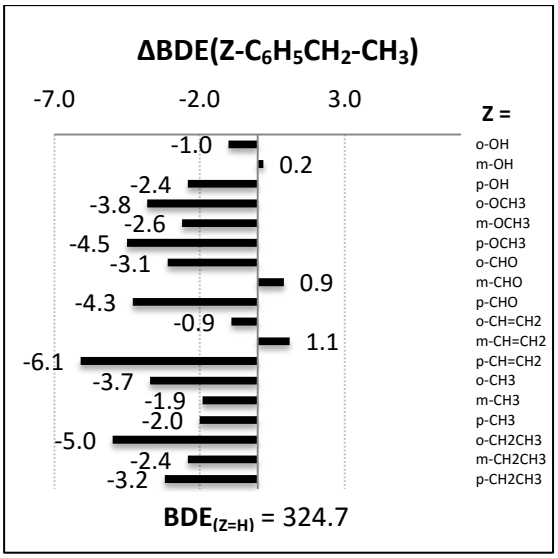


Figure S26. *ΔBDEs (*= $BDE_Z - BDE_H$*) for Z-$C_6H_4CH_2$-CH_3 for 18 different Z groups. Below the plot, the BDE of the bond in unsubstituted ethyl benzene (**$BDE_{(Z=H)}$**) is given. See text for the details regarding the definition of ΔBDEs. Note that the scale of the x-axis differs for the different bonds. All units are kJ mol^{-1}.The ΔBDEs are given in kJ mol^{-1}.*

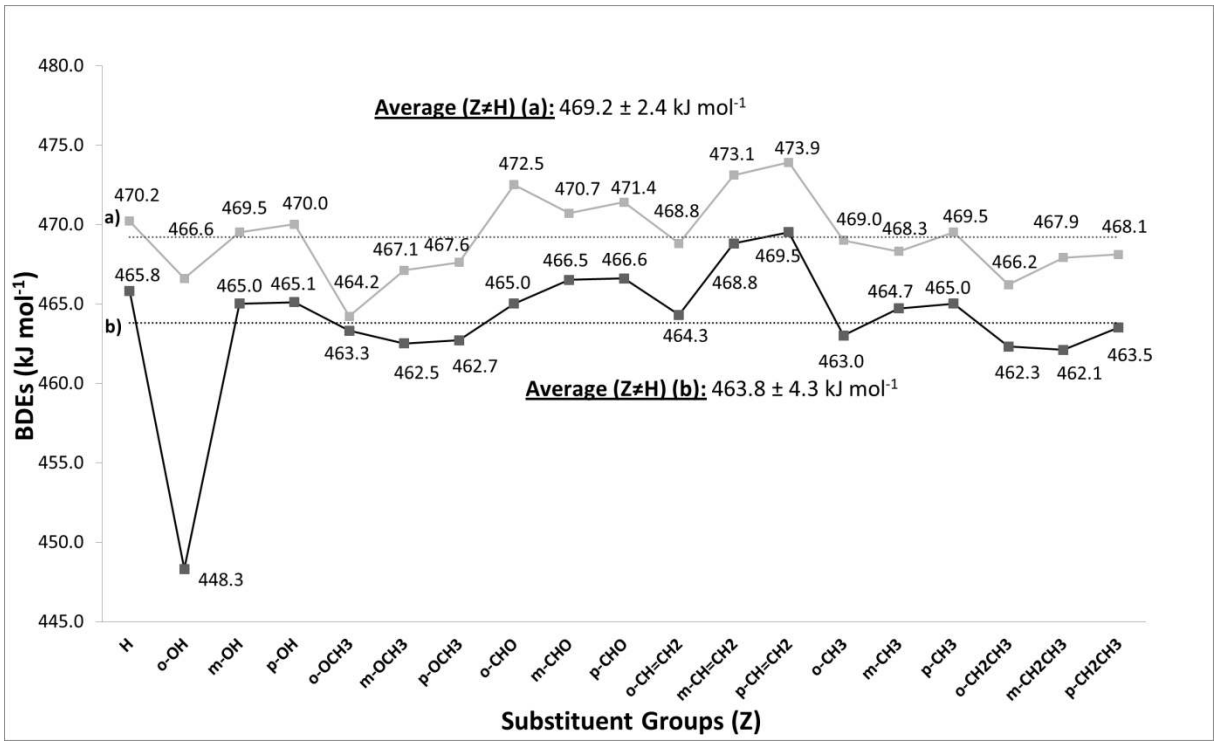


Figure S27. *The variation of BDEs with respect to varying Z groups in cases where* ***(a)*** *Z-cis-$C_6H_4CH=CH•$ (dissociation of the trans C-H bond in styrene) and* ***(b) Z****-trans-$C_6H_4CH=CH•$ (dissociation of the cis C-H bond in styrene) is formed. The average values do not include the unsubstituted case (Z = H).*

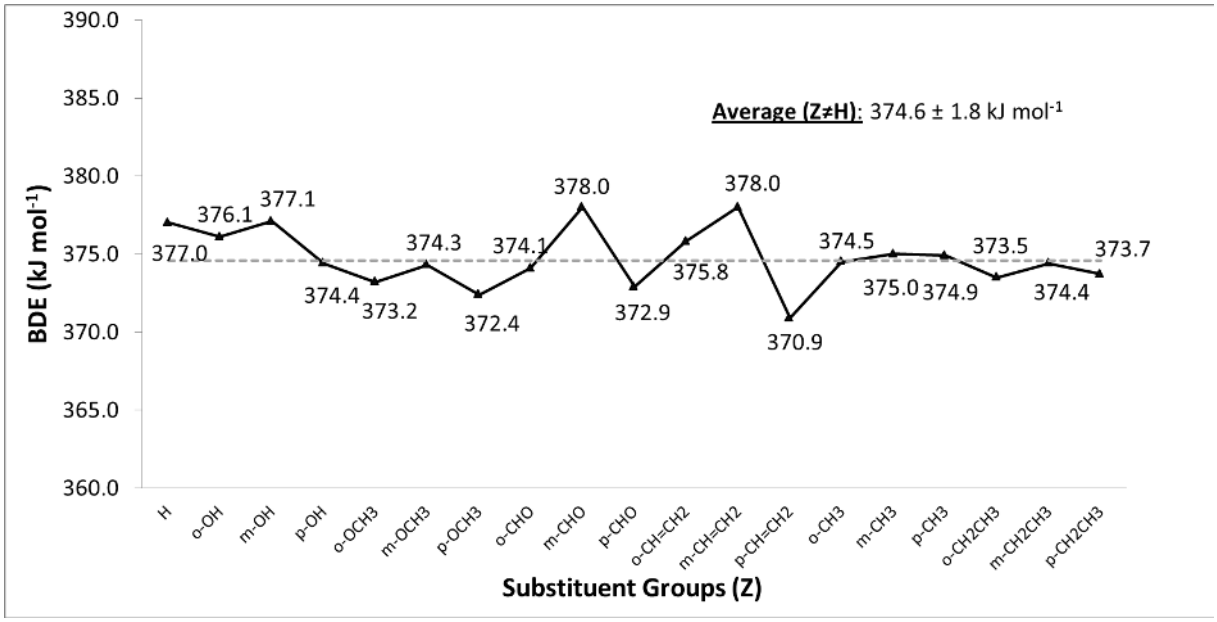


Figure S28. *BDE changes for Z-$C_6H_4CH_2$-H bonds in substituted toluenes with respect to varying Z groups. The average values do not include the unsubstituted case (Z = H).*

7. Definition and Physical Origins of the Non-Nearest Neighbor Interactions

The physical origins of the substituent effects in MARs and the definition of these NNIs are given in **Table S6**.

Table S6. *Definitions of NNIs for the prediction of thermodynamic properties in MARs and an explanation of the cause of the interaction.*

NNI #	Interaction	Contributing physical effects
Anisyl Radicals ($C_6H_4OCH_2$•) + Substituent		
NNI1	$C_6H_4OCH_2$• — *p*-OH/OCH_3	* destabilizing mesomeric effects +M (OCH_2•) with +M (OH)
NNI2	$C_6H_4OCH_2$• — *o*-CHO	* destabilizing neighboring electron withdrawing groups (-I effects)
NNI3	$C_6H_4OCH_2$• — *o*-OCH_3	* destabilizing anomeric effect (Lone Pair Repulsion)
Phenoxyl Radicals (C_6H_4O•) + Substituent		
NNI4	C_6H_4O• — *o*-OH	* Hydrogen bond * stabilizing mesomeric effects +M (OH) with -M (C_6H_5O•)
NNI5	C_6H_4O• — *o*-OCH_3	* stabilizing mesomeric effects +M (OCH_3) with -M (C_6H_5O•) * steric interaction
NNI6	C_6H_4O• — *m*-OCH_3	* likely a combination of inductive and electrostatic effects because the orientation of the OCH_3 group is crucial
NNI7	C_6H_4O• — *p*-OH/OCH_3	* stabilizing mesomeric effects +M (OH/OCH_3) with -M (C_6H_5O•)
NNI8	C_6H_4O• — *o*-CHO	* steric interaction * destabilizing mesomeric effects -M (CHO) with -M (C_6H_5O•)
NNI9	C_6H_5O• — *m*-CHO	* destabilizing inductive effects -I (OCH_3) with -I (C_6H_5O•)
NNI10	C_6H_4O• — *o*-CH=CH_2	* destabilizing steric interaction * stabilizing mesomeric effects +M (CH=CH_2) with -M (C_6H_5O•)
NNI11	C_6H_4O• — *p*-CH=CH_2	* stabilizing mesomeric effects +M (CH=CH_2) with -M (C_6H_5O•)
NNI12	C_6H_4O• — *o*-CH_3/CH_2CH_3	* hyperconjugation
NNI13	C_6H_4O• — *p*-CH_3/CH_2CH_3	* hyperconjugation
Benzoyl Radicals (C_6H_4C•=O) + Substituent		
NNI14	C_6H_4C•=O — *o*-OH	* stabilizing mesomeric effects +M (OH) with -M (C•=O) * H-bond
NNI15	C_6H_4C•=O — *p*-OH/OCH_3	* stabilizing mesomeric effects +M (OH) with -M (C•=O)
NNI16	C_6H_4C•=O — *o*-OCH_3	* destabilizing anomeric effect (Repulsion between lone pair and single electron on (C•=O))
NNI17	C_6H_4C•=O — *m*-CHO	* destabilizing inductive effects

		-I (CHO) with -I (C•=O) similar to m-CHO—CHO[1]
NNI18	$C_6H_4C•=O$ — *p*-CHO	* destabilizing inductive effects -I (CHO) with -I (C•=O) * destabilizing mesomeric effects -M (CHO) with -M (C•=O)
NNI19	$C_6H_4C•=O$ — *o*-$CH=CH_2$	* weak steric interaction * destabilizing mesomeric effects -M ($CH=CH_2$) with -M (C•=O)
Styryl Radicals ($C_6H_4CH=CH•$) + Substituent		
NNI20	trans-$C_6H_4CH=CH•$ — *o*-OH	* 3-center, 3-electron bond (O-H---C•)
NNI21	trans/cis-$C_6H_4CH=CH•$ — *o*-CHO	* steric interaction
NNI22	trans/cis-$C_6H_4CH=CH•$) — *o*-$CH=CH_2$	* steric interaction
NNI23	trans/cis-$C_6H_4CH=CH•$) — *o*-CH_3/CH_2CH_3	* steric interaction
NNI24	cis-$C_6H_4CH=CH•$	* cis correction
Benzyl ($C_6H_4CH=CH•$)/ 1-Phenylethyl Radicals ($C_6H_4C•HCH_3$) + Substituent		
NNI25	$C_6H_4CH_2•$/$C_6H_5C•HCH_3$ — *p*-$CH=CH_2$	* stabilizing mesomeric effects -M ($CH=CH_2$) with +M ($C_6H_5C•$)
NNI26	$C_6H_4CH_2•$/$C_6H_5C•HCH_3$ — *o*-$CH=CH_2$	* steric interaction preventing resonance
NNI27	$C_6H_4CH_2•$/$C_6H_5C•HCH_3$ — *p*-CHO	* stabilizing mesomeric effects -M (CHO) with +M ($C_6H_5C•$)
NNI28	$C_6H_4CH_2•$/$C_6H_5C•HCH_3$ — *o*-CHO	* steric interaction
NNI29	*o*-$C_6H_4CH_2•$—CH_3/CH_2CH_3 *o*-$C_6H_4CH•CH_3$—CH_3/CH_2CH_3	* steric interaction restricting internal rotation * hyperconjugation

8. Initial Determination of GAV and NNI Parameters

As described in the paper, the GAV and the NNI parameters are determined simultaneously based on a least squares linear regression minimization procedure of the differences between Group Additivity calculations and the first principles data for the reference thermochemical database that possess 316 MARs. The NNIs that account for the substituent interactions between nonradical substituents are defined by Ince et al. and they are given in **Table S7**.

The GAVs and the NNIs that are obtained from the linear regression are tabulated in **Table S8** and **Table S9**, respectively. The statistics of the linear regression is given in **Table S10**.

Table S7. *NNIs taken from Ince et al. that are required for the NNIs in substituted MAHs.*[1]

NNIs of Nonradical Substituent Interactions	$\Delta_f H^\circ$	S°	C_p [J mol^{-1} K^{-1}]						
	[kJ mol^{-1}]	[J mol^{-1} K^{-1}]	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
o-OH+ OH/OCH_3	-3.0	-5.6	-2.7	-1.5	0.2	2.0	4.2	4.8	3.7
o-OH+CHO	-27.4	-21.3	-10.4	-9.0	-7.4	-6.0	-3.4	-1.4	1.8
o-CHO+CHO	21.1	6.4	1.7	1.7	1.6	1.4	0.4	-0.8	-2.5
o-Anomeric Effect (OCH_3+OCH_3)	14.7	7.8	0.0	-3.4	-4.7	-5.0	-4.4	-3.7	-2.2
o-OCH_3+CHO	7.9	-1.7	-2.6	0.3	2.6	3.9	4.1	3.3	1.3
o-CH_3/CH_2CH_3+CH_3/CH_2CH_3	4.2	-6.6	3.3	2.9	2.6	2.5	2.3	2.0	1.5
o-CH_3/CH_2CH_3+CHO	8.1	-2.4	4.0	3.0	2.0	1.1	0.0	-0.6	-0.9
o-CH=CH_2+OH/OCH_3	2.6	-3.3	2.5	2.7	2.6	2.5	2.1	1.8	1.2
o-CH=CH_2+CHO	11.9	-2.6	1.3	1.6	2.1	2.5	2.4	1.8	0.3
o-CH=CH_2+CH=CH_2	8.1	-2.3	4.6	3.2	2.1	1.3	0.2	-0.2	-0.5
o-CH=CH_2+ CH_3/CH_2CH_3	4.6	-5.7	-5.7	5.6	4.9	4.2	2.9	2.1	1.0
m-CHO+CHO	4.8	0.1	1.7	1.0	0.5	0.1	-0.4	-0.7	-0.8
p-CHO+CHO	9.9	-0.8	1.8	1.4	1.0	0.7	0.1	-0.3	-0.9
p-OH/OCH_3+OH/OCH_3	7.3	4.0	1.7	0.4	-0.8	-1.7	-2.3	-2.3	-1.7
p-CHO+OH/OCH_3	-4.6	-0.8	-1.6	-1.0	-0.3	0.2	0.9	1.2	1.5

Table S8. *GAVs for standard enthalpy of formation ($\Delta_f H^\circ$) and entropy (S°) at 298 K, and heat capacity (C_p) at various temperatures for the MARs derived from the reference database, given with 97.5% confidence intervals.*

GAVs	$\Delta_f H^\circ$	S°	C_p [J mol^{-1} K^{-1}]						
	[kJ mol^{-1}]	[J mol^{-1} K^{-1}]	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
$\dot{C}_b$	270.4 ± 1.1	52.6 ± 0.9	12.2 ± 0.8	14.9	16.7	18.0	19.6	20.6	21.3
C_b-($\dot{O}$)	-16.3 ± 1.4	73.6 ± 1.2	28 ± 1	32.8	36.4	39.0	42.2	44.1	45.5
O-(C_b)($\dot{C}$)	-130.2 ± 1.1	28.5 ± 1	15.7 ± 0.8	20.0	21.1	21.4	20.9	20.8	20.3
C_b-($C\dot{O}$)	48.4 ± 1.3	102.7 ± 1.1	42.7 ± 0.9	48.5	53.2	56.5	60.8	63.3	65.5
$\dot{C}$-(C_b)(H)$_2$	112.9 ± 0.9	111.6 ± 0.8	27.2 ± 0.7	33.7	38.8	42.6	48.0	52.2	58.6
$\dot{C}$-(C_b)(C)(H)	124.8 ± 1.2	32.5 ± 1.1	21.7 ± 0.9	26.0	30.1	32.9	36.9	40.1	44.0

Table S9. *The NNIs that are determined from the simultaneous linear regression (along with GAVs) from the training dataset.*[a]

NNIs	$\Delta_f H^\circ$	S°	C_p [J mol^{-1} K^{-1}]						
	[kJ mol^{-1}]	[J mol^{-1} K^{-1}]	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
NNI1	6.1 ± 2.3	3.7 ± 2.0	0.1 ± 1.7	-1.0	-2.0	-2.5	-2.7	-2.4	-1.4
NNI2	8 ± 3.1	-4.2 ± 2.7	2 ± 2.2	4.9	6.0	6.0	4.6	3.1	0.8
NNI3	11 ± 2.3	1.1 ± 2.0	4.7 ± 1.7	1.8	-0.2	-0.8	-0.8	-0.7	-0.3
NNI4	-36.9 ± 1.6	-10.9 ± 1.4	-8.2 ± 1.2	-7.3	-6.3	-5.0	-2.9	-1.3	1.4
NNI5	-7.2 ± 1.6	-0.1 ± 1.3	-2.5 ± 1.1	-2.7	-2.3	-1.5	-0.3	0.2	0.6
NNI6	-8.3 ± 2.3	-4.8 ± 2.0	0.7 ± 1.7	2.7	3.7	3.6	3.0	2.1	1.0
NNI7	-15.4 ± 2.0	-3 ± 1.7	-2.7 ± 1.4	-2.2	-1.5	-1.0	0.2	0.8	1.8
NNI8	6.2 ± 1.6	-0.4 ± 1.3	-1 ± 1.1	-0.3	0.6	1.6	2.7	2.8	1.7

NNI9	4.6 ± 2.0	2.8 ± 1.7	2.2 ± 1.5	2.3	2.1	1.9	1.4	0.9	0.6
NNI10	-8 ± 2.8	-4.3 ± 2.4	0.4 ± 2.0	0.2	0.3	0.5	1.2	1.6	1.8
NNI11	-12.9 ± 3.1	-3.1 ± 2.6	0.2 ± 2.2	0.1	0.1	0.4	0.9	1.2	1.3
NNI12	-8.4 ± 1.7	0.4 ± 1.4	-0.2 ± 1.2	-0.3	-0.2	-0.1	0.0	0.0	0.1
NNI13	-5.8 ± 2.5	0.1 ± 2.1	-0.7 ± 1.8	-0.6	-0.5	-0.5	-0.3	-0.2	-0.1
NNI14	-16.5 ± 2.3	-19.6 ± 2.0	-5.9 ± 1.7	-3.6	-1.6	0.7	4.5	6.8	8.2
NNI15	-8.1 ± 2.1	-3.7 ± 1.8	-2.8 ± 1.5	-1.9	-0.9	0.2	1.7	2.4	2.7
NNI16	6.7 ± 2.4	2.4 ± 2.0	3.1 ± 1.7	1.7	0.5	0.0	-0.5	-0.8	-0.5
NNI17	5.4 ± 3.1	4.4 ± 2.6	0.5 ± 2.2	0.6	0.4	0.1	-0.5	-0.6	0.4
NNI18	5.3 ± 3.2	13.4 ± 2.7	-0.7 ± 2.3	-2.1	-3.1	-3.6	-4.0	-3.7	-2.7
NNI19	3.7 ± 2.8	-8.4 ± 2.4	4.1 ± 2.0	4.5	4.4	4.1	3.1	2.2	1.1
NNI20	-14.7 ± 1.9	-17.7 ± 1.7	-5.5 ± 1.4	-2.9	0.5	4.4	10.1	12.1	9.7
NNI21	13.5 ± 1.8	-5.3 ± 1.6	1.9 ± 1.3	3.2	3.5	3.2	2.4	1.9	1.3
NNI22	7.2 ± 2.0	-5.3 ± 1.7	1.8 ± 1.4	2.8	2.4	2.0	1.2	0.8	0.4
NNI23	3.7 ± 1.4	-4 ± 1.2	3 ± 1.0	2.9	2.3	1.7	0.8	0.5	0.1
NNI24	-3.9 ± 1.0	-3.7 ± 0.9	1.5 ± 0.7	1.6	2.1	2.3	2.2	2.1	1.6
NNI25	-6.2 ± 2.4	-4.8 ± 2.0	0.3 ± 1.7	0.8	1.2	1.5	1.9	1.8	1.4
NNI26	6.4 ± 2.4	-1.1 ± 2.0	2.3 ± 1.7	2.1	1.5	1.0	0.4	-0.1	-0.3
NNI27	-5.1 ± 2.4	0.8 ± 2.0	-1.6 ± 1.7	-1.2	-0.8	-0.6	-0.4	-0.2	0.2
NNI28	5.5 ± 1.7	2.1 ± 1.5	1.8 ± 1.2	2.1	1.8	1.2	0.3	-0.2	-0.6
NNI29	2.9 ± 1.5	-3.8 ± 1.3	3.8 ± 1.1	2.9	2.1	1.4	0.7	0.4	0.1

[a] The interactions pertaining to the NNIs given here can be found in **Table 3**.

Table S10. *Statistical analysis for the linear regression analysis of the GAVs and NNIs for the standard enthalpies of formation ($\Delta_f H^\circ$) and entropies (S°) at 298 K and heat capacities (C_p) at various temperatures for MARs.*[a]

	$\Delta_f H^\circ$	S°	C_p [J mol^{-1} K^{-1}]						
	[kJ mol^{-1}]	**[J mol^{-1} K^{-1}]**	**300 K**	**400 K**	**500 K**	**600 K**	**800 K**	**1000 K**	**1500 K**
MAD	1.92	1.66	1.26	1.09	1.02	1.01	1.01	0.93	0.74
RMS	2.39	2.03	1.71	1.48	1.39	1.39	1.45	1.32	1.05
MAX	6.66	4.91	5.85	5.03	5.17	5.54	5.96	5.74	4.60
F	14924	9340	1599	2999	4236	4986	5544	7434	13420

[a] **F:**Significance; **MAD:** mean average deviation ; **RMS:** root mean square ; **MAX:** maximum deviation.

9. Thermochemical Data Of The Validation Set

The transferability of the preliminary GAV/NNI parameters (See **Table S7** and **Table S8**) to the MARs outside the training set are tested on a set of 53 triple and quadruple substituted MARs (See **Figures S8-S13**). The thermochemical data for the validation set is given in **Table S11.**

The NNI parameters defined for the MARs bring a significant improvement to the GA based predictions which can be seen in **Table S12**. In this table, GA predictions with and without $NNI_{Radical}$ parameters are given. Below the table, there is a statistical comparison of these two cases where the sharp decrease in deviations upon the addition of NNIs can be seen.

Table S11. *Thermochemical database used as the validation set for the preliminary Group Additive Values (GAVs) and non-nearest neighbor interactions (NNIs). The units of standard enthalpy of formation ($\Delta_f H^\circ$) data is given in kJ mol^{-1} whereas the units of entropies (S°) and heat capacities (C_p) are given in J mol^{-1} K^{-1}.*

Validation Set

#	Radicals	$\Delta_f H^\circ$ (298 K)		S° (298 K)				C_p						
		$\Delta_f H^\circ_{G4}$	$\Delta_f H^\circ_{G4/BAC}$	S°	S°_{int}	$\sigma_{tot\ sym}$	n_{opt}	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
V-1/1	1-C•-2-CHO-5-OH-6-OCH_3	-116.2	-121.5	428.0	437.1	3	1	168.9	207.8	242.0	270.5	312.2	339.8	376.8
V-1/2	1-C•-2-OH-3-OCH_3-5-CHO	-116	-121.3	424.3	433.4	3	1	170.3	210.9	244.8	272.2	311.7	338.1	375.0
V-2/1	1-OCH_2•-2,3-OH	-236.5	-250.0	409.5	415.2	2	1	164.3	203.8	236.6	262.3	297.5	319.3	349.3
V-2/2	1-OCH_2•-2-OH-4-CH=CH_2	7.6	-0.9	443.0	448.7	2	1	183.1	229.3	267.7	298.2	341.1	369.4	410.0
V-2/3	1-OCH_2•-2-OCH_3-3-CH_3	-57.3	-65.0	459.2	483.3	18	1	187.3	230.6	269.5	302.2	352.0	387.4	440.3
V-2/4	1-OCH_2•-2-CHO-5-CH_3	-37	-39.9	437.5	452.4	6	1	177.0	223.2	261.4	291.8	335.9	366.0	409.6
V-2/5	1-OCH_2•-2,3,4-CH_3	21.6	19.7	465.3	492.7	27	1	194.3	243.5	286.8	323.0	378.4	418.3	478.8
V-3/1	1-O•-2,3,4-OH	-519.7	-536.2	377.2	377.2	1	1	147.7	184.2	214.0	237.8	271.1	292.1	318.7
V-3/2	1-O•-2-OH-4-OCH_3-6-CHO	-443.1	-453.2	440.3	449.4	3	1	178.8	221.5	258.4	288.7	332.9	362.0	400.7
V-3/3	1-O•-2-OH-3-CH=CH_2	-88.9	-96.7	387.4	387.4	1	1	146.2	187.1	221.2	248.3	287.5	314.0	352.4
V-3/4	1-O•-2-OH-3-CH_3	-192.6	-200.4	368.3	377.4	3	1	132.1	168.7	199.9	225.3	262.9	289.0	327.2
V-3/5	1-O•-2,3-OCH_3	-243.3	-254.6	444.2	462.5	9	1	183.2	224.4	260.6	290.3	333.6	363.1	406.5
V-3/6	1-O•-2-OCH_3-6-CH=CH_2	-39.4	-46.4	434.8	443.9	3	1	172.6	217.2	255.7	287.1	333.2	364.8	410.5
V-3/7	1-O•-2-CHO-4-OCH_3	-232.8	-239.3	419.1	428.2	3	1	167.5	207.0	241.3	269.9	312.4	340.9	378.7
V-3/8	1-O•-2,3-CHO	-158.8	-160.5	413.7	419.5	2	1	158.9	196.4	228.2	254.0	291.1	314.5	343.5
V-3/9	1-O•-2-CHO-6-CH=CH_2	0	-2.2	416.4	416.4	1	1	161.6	204.2	240.8	270.7	314.3	342.9	380.8
V-3/10	1-O•-2-CH=CH_2-4-CH_3	74.8	72.0	406.3	415.5	3	1	154.3	197.8	235.2	265.9	311.5	343.2	389.3
V-3/11	1-O•-2-CH_3-3-CHO	-92.5	-94.7	407.2	416.4	3	1	146.5	184.6	217.5	244.6	284.6	312.0	350.9
V-3/12	1-O•-2,6-CH_2CH_3	-70.5	-75.5	461.8	485.8	18	1	189.6	240.8	286.2	323.9	381.0	421.7	482.6
V-4/1	1-C•=O-2,4-OH	-256.7	-265.4	379.3	379.3	1	1	143.6	179.1	207.9	230.6	262.7	283.8	313.7
V-4/2	1-C•=O-2-OH-4-OCH_3	-239.5	-247.4	409.0	418.1	3	1	165.6	206.2	240.3	267.6	307.1	333.9	372.6
V-4/3	1-C•=O-2-OH-5-CHO	-198.1	-201.2	403.4	403.4	1	1	151.4	188.5	219.3	244.2	280.3	304.6	338.9
V-4/4	1-C•=O-2-OH-6-CH=CH_2	-0.5	-4.1	409.5	409.5	1	1	167.0	210.3	245.1	272.5	311.9	338.6	376.8
V-4/5	1-C•=O-2-OH-3-CH_3	-107.6	-111.2	389.6	398.7	3	1	151.9	190.4	222.8	249.4	289.5	317.8	357.2
V-4/6	1-C•=O-2-OCH_3-3-CHO	-135.5	-137.8	456.8	466.0	3	1	182.8	226.7	263.6	292.8	333.7	360.2	396.4
V-4/7	1-C•=O-3-CHO-4-CH_3	-30.7	-28.8	428.0	437.1	3	1	167.0	205.3	238.3	265.5	305.9	333.5	372.4
V-4/8	1-C•=O-2-CH=CH_2-3-CH_3	154.4	155.8	432.5	441.6	3	1	177.1	221.2	258.1	287.7	331.3	361.8	407.6
V-4/9	1-C•=O-3-CH_3-4-OH	-98.7	-102.3	404.2	413.4	3	1	154.7	191.8	223.4	249.0	286.3	311.4	347.5
V-5/1	1-(t-CH=CH•)-2,5-OH	44.4	35.2	394.5	394.5	1	1	161.1	202.9	237.6	265.1	302.8	325.7	355.2
V-5/2	1-(t-CH=CH•)-2-OH-5-CH_2CH_3	154.8	149.5	439.4	448.5	3	1	185.3	236.2	280.7	317.5	371.5	406.9	454.4
V-5/3	1-(t-CH=CH•)-3,4-CHO	176.2	178.2	451.4	451.4	1	1	181.6	225.1	262.1	292.3	336.0	364.3	401.6
V-5/4	1-(t-CH=CH•)-2-CHO-5-CH=CH_2	353.1	354.5	450.8	450.8	1	1	189.2	240.1	281.9	315.0	362.6	394.5	439.3
V-5/5	1-(t-CH=CH•)-2-CH=CH_2-3-CH_3	440.5	441.4	439.3	448.5	3	1	186.6	234.9	276.0	309.5	359.6	394.9	447.8
V-5/6	1-(t-CH=CH•)-2-CH=CH_2-5-CH_3	433.7	434.6	440.5	449.6	3	1	180.5	231.0	274.1	309.0	360.3	395.9	448.5
V-5/7	1-(t-CH=CH•)-2-CH_2CH_3-4-CH_3	308.5	308.3	461.3	479.6	9	1	195.4	246.7	291.2	327.9	383.7	423.6	483.7
V-5/8	1-(c-CH=CH•)-2,3-OH	49.3	40.1	403.8	403.8	1	1	162.4	202.0	234.0	259.3	294.8	317.9	350.2
V-5/9	1-(c-CH=CH•)-2-CHO-4-CH=CH_2	361.6	363.0	452.7	452.7	1	1	190.4	238.8	279.1	311.4	358.6	390.7	436.7
V-5/10	1-(c-CH=CH•)-2-CHO-6-CH_3	267.9	269.3	434.9	444.0	3	1	177.0	220.7	257.6	287.7	332.8	364.3	410.3
V-5/11	1-(c-CH=CH•)-3-CHO-4-CH_3	251.4	252.8	435.8	444.9	3	1	174.6	218.3	255.9	286.8	332.8	364.8	411.1
V-5/12	1-(c-CH=CH•)-2,4-CH=CH_2	540.5	541.4	463.5	463.5	1	1	197.4	250.9	295.4	330.9	382.7	418.6	471.9
V-5/13	1-(c-CH=CH•)-2-CH=CH_2-4-CH_3	437.8	438.7	443.7	452.9	3	1	180.9	231.0	273.6	308.0	358.7	394.2	447.2
V-5/14	1-(c-CH=CH•)-2-CH_3-4-CH=CH_2	438.6	439.5	441.8	450.9	3	1	180.4	230.8	273.2	307.5	358.5	394.2	447.5
V-5/15	1-(c-CH=CH•)-2,3- CH_3	342.9	343.8	419.6	437.9	9	1	164.4	210.2	249.8	282.6	332.4	368.0	421.7
V-6/1	1-CH_2•-2,4-CH=CH_2	335.9	336.8	433.2	433.2	1	1	182.8	234.5	277.6	312.3	363.2	398.8	451.8
V-6/2	1-CH_2•-2-CH=CH_2-3-CH_3	251.2	252.1	411.6	420.7	3	1	169.2	215.2	254.9	287.6	337.0	372.2	425.5
V-6/3	1-CH_2•-2,3-CH_3	147.5	148.4	385.7	403.9	9	1	152.7	196.6	234.8	266.5	314.7	349.4	401.9
V-6/4	1-CH_2•-2-CH_3-5-	119.8	119.6	428.4	446.7	9	1	177.7	227.4	270.7	306.6	361.6	401.2	461.5
V-6/5	1-CH_2•-2,5-CH_2CH_3	100.1	98.7	467.3	485.6	9	1	200.9	256.8	305.7	346.4	408.6	453.6	521.8
V-6/6	1-CH_2•-3-CH_3-4-CHO	52.1	53.5	401.8	410.9	3	1	161.7	203.2	239.1	268.8	313.5	345.0	391.1
V-6/7	1-CH_2•-3-CH_3-4-CH=CH_2	239.3	240.2	404.8	419.7	6	1	172.7	220.3	260.4	293.0	341.7	376.2	428.1
V-6/8	1-CH_2•-3,4-CH_3	141.1	142.0	388.3	406.6	9	1	154.8	197.9	235.7	267.1	315.2	349.8	402.2
V-6/9	1-CH_2•-3,6-CH_2CH_3	100.1	98.7	466.9	485.1	9	1	200.7	256.7	305.6	346.3	408.5	453.5	521.6

V-6/10	p-$(CH_3)C_6H_5CH•CH_3$	142.8	142.2	395.8	414.0	9	1	146.2	191.1	230.5	263.2	312.9	348.3	401.6

Table S12. *Comparison of the predictive capability (deviations between G4/BAC and GA calculated values) of GA parameters before and after the application of $NNI_{Radical}$ parameters for standard enthalpy of formations ($\Delta_f H^\circ$), entropies (S°) at 298 K and heat capacities (C_p) at 300K.*[a][b]

		$\Delta_f H^\circ$ [kJ mol^{-1}]		S° [J mol^{-1} K^{-1}]		C_p [J mol^{-1} K^{-1}] (300K)	
#	**MAR Name**[b]	**Before $NNI_{Radical}$**[c]	**After $NNI_{Radical}$**	**Before $NNI_{Radical}$**[c]	**After $NNI_{Radical}$**	**Before $NNI_{Radical}$**[c]	**After $NNI_{Radical}$**
V1/1	1-C•-2-OCH_3-3-OH-5-CHO	-2.2	2.2	-2.9	2.9	3.7	-3.7
V1/2	1-C•-2-OH-3-OCH_3-5-CHO	-2.4	2.4	0.8	-0.8	2.2	-2.2
V2/1	1-OCH_2•-2,3-OH	0.9	-0.9	2.3	-2.3	1.6	-1.6
V2/2	1-OCH_2•-2-OH-4-CH=CH_2	-1.3	1.3	4.6	-4.6	-0.1	0.1
V2/3	1-OCH_2•-2-OCH_3-3-CH_3	-15.3	4.3	-0.5	-0.6	1.4	-6.1
V2/4	1-OCH_2•-2-CHO-5-CH_3	-4.2	-3.8	7.5	-3.3	-2.3	0.3
V2/5	1-OCH_2•-2,3,4-CH_3	-1.1	1.1	-3.2	3.2	1.7	-1.7
V3/1	1-O•-2,3,4-OH	49.0	3.3	0.4	2.6	11.6	-0.7
V3/2	1-O•-2-OH-4-OCH_3-6-CHO	50.4	-4.3	1.3	2.1	13.9	-2.0
V3/3	1-O•-2-OH-3-CH=CH_2	39.8	-2.9	0.6	-0.6	12.1	-3.9
V3/4	1-O•-2-OH-3-CH_3	41.7	-4.8	1.0	-1.0	8.3	-0.1
V3/5	1-O•-2,3-OCH_3	8.1	7.4	2.0	2.8	0.1	1.7
V3/6	1-O•-2-OCH_3-6-CH=CH_2	8.0	7.2	0.6	3.7	4.0	-1.9
V3/7	1-O•-2-CHO-4-OCH_3	14.3	-5.1	5.7	-2.3	1.8	1.9
V3/8	1-O•-2,3-CHO	-7.2	-3.6	-2.1	-0.3	-1.8	0.6
V3/9	1-O•-2-CHO-6-CH=CH_2	0.0	1.8	5.3	-0.6	1.1	-0.5
V3/10	1-O•-2-CH=CH_2-4-CH_3	13.2	0.6	4.0	0.2	0.5	-0.2
V3/11	1-O•-2-CH_3-3-CHO	1.4	2.4	-10.0	6.8	4.9	-6.9
V3/12	1-O•-2,6-CH_2CH_3	20.3	-3.5	-2.2	1.4	0.3	0.1
V4/1	1-C•=O-2,4-OH	26.7	-2.1	21.8	1.5	12.7	-4.0
V4/2	1-C•=O-2-OH-4-OCH_3	29.8	-5.2	25.4	-2.1	11.7	-3.0
V4/3	1-C•=O-2-OH-5-CHO	14.1	-3.0	16.4	-1.2	5.1	0.3
V4/4	1-C•=O-2-OH-6-CH=CH_2	9.3	3.5	21.8	6.2	3.7	-1.9
V4/5	1-C•=O-2-OH-3-CH_3	17.2	-0.7	19.7	-0.1	3.6	2.3
V4/6	1-C•=O-3-OCH_3-4-CH_3	-14.6	2.5	-4.7	-2.1	-1.2	-2.4
V4/7	1-C•=O-3-CHO-4-CH_3	0.2	-5.6	-1.6	-2.8	-0.6	0.1
V4/8	1-C•=O-2-CH=CH_2-3-CH_3	-1.3	-2.4	1.3	-7.1	-1.6	-2.5
V4/9	1-C•=O-3-CH_3-4-OH	8.3	-0.2	5.0	-1.3	0.7	2.1
V5/1	1-(t-CH=CH•)-2,5-OH	15.4	3.2	21.3	0.1	5.0	-0.9
V5/2	1-(t-CH=CH•)-2-OH-5-CH_2CH_3	17.9	0.7	19.1	2.3	3.4	0.7
V5/3	1-(t-CH=CH•)-3,4-CHO	0.8	3.1	5.8	-2.1	-1.5	0.4
V5/4	1-(t-CH=CH•)-2-CHO-5-CH=CH_2	-10.0	0.4	10.7	-1.7	-3.5	0.4
V5/5	1-(t-CH=CH•)-2-CH=CH_2-3-CH_3	-4.9	1.6	5.1	3.9	-3.0	-1.4
V5/6	1-(t-CH=CH•)-2-CH=CH_2-5-CH_3	-2.7	-0.6	9.7	-0.7	-2.6	-1.8
V5/7	1-(t-CH=CH•)-2-CH_2CH_3-4-CH_3	3.8	-3.6	5.3	2.4	-7.6	2.9
V5/8	1-(c-CH=CH•)-2,3-OH	0.2	-0.2	2.4	-2.4	-0.7	0.7

V5/9	1-(c-CH=CH•)-2-CHO-4-CH=CH_2	-18.5	5.0	8.8	-3.5	-4.6	2.6
V5/10	1-(c-CH=CH•)-2-CHO-6-CH_3	-24.0	6.8	4.6	4.7	-6.5	0.9
V5/11	1-(c-CH=CH•)-3-CHO-4-CH_3	0.6	-0.6	1.3	-1.3	-0.1	0.1
V5/12	1-(c-CH=CH•)-2,4-CH=CH_2	-10.3	3.1	8.7	-3.4	-4.2	0.9
V5/13	1-(c-CH=CH•)-2-CH=CH_2-4-CH_3	-6.8	-0.4	6.4	-1.1	-3.0	-0.3
V5/14	1-(c-CH=CH•)-2-CH_3-4-CH=CH_2	-7.6	3.9	8.4	-4.4	-2.5	-1.1
V5/15	1-(c-CH=CH•)-2,3-CH_3	-6.9	3.2	1.9	2.1	1.5	-5.1
V6/1	1-CH_2•-2,4-CH=CH_2	0.3	-0.5	3.6	2.3	-3.2	0.6
V6/2	1-CH_2•-2-CH=CH_2-3-CH_3	-9.6	3.2	-2.5	3.6	0.8	-3.1
V6/3	1-CH_2•-2,3-CH_3	-5.5	2.6	0.5	3.3	-0.4	0.4
V6/4	1-CH_2•-2-CH_3-5-CH_2CH_3	-1.5	-1.4	2.8	1.0	-3.5	3.5
V6/5	1-CH_2•-2,5-CH_2CH_3	-1.2	-1.7	2.4	1.4	-1.5	1.5
V6/6	1-CH_2•-3-CH_3-4-CHO	5.9	-1.3	-0.1	-0.7	-0.8	2.4
V6/7	1-CH_2•-3-CH_3-4-CH=CH_2	2.3	3.9	-1.5	6.3	-2.6	2.3
V6/8	1-CH_2•-3,4-CH_3	-3.3	0.4	4.4	-0.6	-5.8	5.8
V6/9	1-CH_2•-3,6-CH_2CH_3	-1.2	-1.7	2.9	0.9	-1.3	1.3
V6/10	p-(CH_3)C_6H_5CH•CH_3	-1.3	1.3	0.0	0.0	0.0	0.0
Statistics		$\Delta_f H^\circ$ [kJ mol^{-1}]		S° [J mol^{-1} K^{-1}]		C_p [J mol^{-1} K^{-1}] (300K)	
Mean Absolute Deviation (MAD)		10.7	2.7	5.9	2.3	3.5	1.8
Maximum Absolute Deviation (MAX)		50.4	7.4	25.1	7.1	13.9	6.9

[a] The ab-initio and the GA based thermochemical databases for the validation set is given in **Table S11** of the Supporting Information.
[b] The full names and the numbering of the MARs in the validation set are described in Section 2.2 of the Supporting Information. In order to avoid any confusion, the depictions of these MARs are also given in **Figures S8-S13** of the Supporting Information.
[c] This term includes GA predictions based on the GAVs for the closed and open shell groups and the NNIs that describe the interactions between non-radical groups which are defined by Ince et al..[1] and excludes the NNIs that are defined in this paper.

10. Deviations between GA and Ab-Initio Calculated Datasets

The GAVs and the NNIs for the heat capacities (C_p) at 400 K, 500 K , 600 K , 800 K, 1000K and 1500K are given along with their 97.5% confidence intervals in **Table S13** and **Table S14**, respectively. In **Table S15**, the deviations between Group Additivity (GA) and ab-initio based data for the final thermochemical database is given for the full database (369 MARs). The histograms for the differences between two datasets for $\Delta_f H^\circ$ and S° at 298K and C_p at various temperatures (300K, 400K, 500K, 600K, 800K, 1000K and 1500K) are given in **Figure S29**, **Figure S30** and **Figure S31**, respectively.

Table S13. *GAVs for heat capacity (C_p) at various temperatures for the MARs of the final database. The standard deviations relate to 97.5% confidence intervals.*

GAVs	C_p [J mol^{-1} K^{-1}]					
	400 K	500 K	600 K	800 K	1000 K	1500 K
$\dot{C}_b$	14.7 ± 0.67	16.4 ± 0.64	17.7 ± 0.64	19.4 ± 0.66	20.5 ± 0.61	21.3 ± 0.47
C_b-($\dot{O}$)	32.8 ± 0.89	36.4 ± 0.85	38.9 ± 0.85	42.2 ± 0.88	44.1 ± 0.81	45.5 ± 0.63
O-($\dot{C}$)(C_b)	19.8 ± 0.7	21.1 ± 0.67	21.4 ± 0.67	21 ± 0.69	20.9 ± 0.64	20.3 ± 0.5
C_b-($C\dot{O}$)	48.9 ± 0.81	53.6 ± 0.77	57 ± 0.77	61.4 ± 0.8	63.9 ± 0.73	65.9 ± 0.57
$\dot{C}$-(C_b)(H)$_2$	33.6 ± 0.6	38.7 ± 0.58	42.5 ± 0.58	48 ± 0.59	52.1 ± 0.55	58.5 ± 0.42
$\dot{C}$-(C_b)(C)(H)	26 ± 0.79	30.1 ± 0.76	33 ± 0.76	37 ± 0.78	40.1 ± 0.72	44 ± 0.56

Table S14. *Correction values for non-nearest neighbor interactions (NNIs) derived based on full G4/BAC radical set for the heat capacities (C_p) at various temperatures.* [a] *The standard deviations relate to 97.5% confidence intervals.*

NNI #	Description of Interaction	C_p [J mol^{-1} K^{-1}]					
		400 K	500 K	600 K	800 K	1000 K	1500 K
NNI1	$C_6H_5OCH_2$•—*p*-OH/OCH_3	-0.8 ± 1.51	-1.8 ± 1.44	-2.4 ± 1.44	-2.7 ± 1.48	-2.5 ± 1.36	-1.4 ± 1.06
NNI2	$C_6H_5OCH_2$•—*o*-OCH_3	5 ± 1.82	6 ± 1.74	5.8 ± 1.74	4.2 ± 1.79	2.6 ± 1.64	0.6 ± 1.28
NNI3	$C_6H_5OCH_2$•—*o*-CHO	0.9 ± 1.42	-0.9 ± 1.36	-1.5 ± 1.36	-1.4 ± 1.4	-1.2 ± 1.29	-0.6 ± 1
NNI4	C_6H_5O• —*o*-OH	-7.7 ± 0.99	-6.7 ± 0.94	-5.3 ± 0.94	-3.1 ± 0.97	-1.4 ± 0.89	1.4 ± 0.69
NNI5	C_6H_5O• —*o*-OCH_3	-2.7 ± 0.97	-2.2 ± 0.92	-1.4 ± 0.92	-0.3 ± 0.95	0.2 ± 0.87	0.6 ± 0.68
NNI6	C_6H_5O• —*m*-OCH_3	3 ± 1.42	4.1 ± 1.36	4.1 ± 1.36	3.4 ± 1.4	2.4 ± 1.28	1 ± 1
NNI7	C_6H_5O•—*p*-OH/OCH_3	-2.4 ± 1.12	-1.8 ± 1.07	-1.3 ± 1.07	0 ± 1.1	0.7 ± 1.01	1.8 ± 0.79
NNI8	C_6H_5O•—*o*-CHO	-0.2 ± 0.94	0.8 ± 0.89	1.8 ± 0.89	2.9 ± 0.92	3 ± 0.85	1.8 ± 0.66
NNI9	C_6H_5O•—*m*-CHO	1.8 ± 1.21	1.8 ± 1.16	1.7 ± 1.16	1.2 ± 1.19	0.8 ± 1.09	0.6 ± 0.85
NNI10	C_6H_5O•—*o*-$CH{=}CH_2$	0 ± 1.4	0.1 ± 1.33	0.4 ± 1.33	1.1 ± 1.37	1.4 ± 1.26	1.6 ± 0.98
NNI11	C_6H_5O•—*p*-$CH{=}CH_2$	0.2 ± 2.05	0.2 ± 1.95	0.5 ± 1.95	1 ± 2.01	1.3 ± 1.85	1.3 ± 1.44
NNI12	C_6H_5O•—*o*-CH_3/CH_2CH_3	-0.5 ± 0.97	-0.4 ± 0.92	-0.2 ± 0.92	-0.1 ± 0.95	-0.1 ± 0.87	-0.1 ± 0.68
NNI13	C_6H_5O•—*p*-CH_3/CH_2CH_3	-0.6 ± 1.5	-0.4 ± 1.43	-0.4 ± 1.43	-0.3 ± 1.47	-0.2 ± 1.35	-0.1 ± 1.05
NNI14	C_6H_5C•=O—*o*-OH	-4.5 ± 1.17	-2.9 ± 1.12	-1 ± 1.12	2.3 ± 1.15	4.7 ± 1.06	6.9 ± 0.82

NNI15	$C_6H_5C\bullet{=}O$— *p*-OH/OCH_3	-2.7 ± 1.2	-2 ± 1.15	-1 ± 1.15	0.2 ± 1.18	0.8 ± 1.08	1.5 ± 0.84
NNI16	$C_6H_5C\bullet{=}O$— *o*-OCH_3	1.4 ± 1.45	0.4 ± 1.39	0 ± 1.39	-0.6 ± 1.43	-0.8 ± 1.31	-0.7 ± 1.02
NNI17	$C_6H_5C\bullet{=}O$— *m*-CHO	0.7 ± 1.49	0.7 ± 1.42	0.5 ± 1.42	0 ± 1.46	-0.3 ± 1.34	0.1 ± 1.05
NNI18	$C_6H_5C\bullet{=}O$— *p*-CHO	-2.4 ± 2.1	-3.5 ± 2	-4.1 ± 2	-4.5 ± 2.06	-4.3 ± 1.9	-3.2 ± 1.48
NNI19	$C_6H_5C\bullet{=}O$— *o*-$CH{=}CH_2$	3.5 ± 1.55	3.2 ± 1.48	2.6 ± 1.48	1.5 ± 1.52	0.6 ± 1.4	0.1 ± 1.09
NNI20	trans/cis-$C_6H_5CH{=}CH\bullet$— *o*-OH	-2.9 ± 1.18	0.6 ± 1.12	4.6 ± 1.13	10.1 ± 1.16	12 ± 1.06	9.4 ± 0.83
NNI21	trans/cis-$C_6H_5CH{=}CH\bullet$— *o*-CHO	3.4 ± 1.04	3.6 ± 0.99	3.3 ± 0.99	2.4 ± 1.02	1.8 ± 0.94	1 ± 0.73
NNI22	trans/cis-$C_6H_5CH{=}CH\bullet$— *o*-$CH{=}CH_2$	2.5 ± 1.05	2.2 ± 1	1.8 ± 1	1.1 ± 1.03	0.7 ± 0.95	0.3 ± 0.74
NNI23	trans/cis-$C_6H_5CH{=}CH\bullet$— *o*-CH_3/CH_2CH_3	2.7 ± 0.81	2.1 ± 0.78	1.5 ± 0.78	0.6 ± 0.8	0.3 ± 0.74	-0.1 ± 0.57
NNI24	$C_6H_5CH{=}CH\bullet$ Cis Correction	1.6 ± 0.64	2.2 ± 0.61	2.4 ± 0.61	2.4 ± 0.62	2.2 ± 0.57	1.7 ± 0.45
NNI25	$C_6H_5CH_2\bullet$ /$C_6H_5C\bullet HCH_3$— *p*-$CH{=}CH_2$	2.1 ± 1.12	1.8 ± 1.07	1.2 ± 1.07	0.4 ± 1.1	-0.2 ± 1.02	-0.5 ± 0.79
NNI26	$C_6H_5CH_2\bullet$ /$C_6H_5C\bullet HCH_3$— *o*-$CH{=}CH_2$	1.2 ± 1.37	0.6 ± 1.31	0.1 ± 1.31	-0.5 ± 1.35	-0.7 ± 1.24	-0.7 ± 0.97
NNI27	$C_6H_5CH_2\bullet$ /$C_6H_5C\bullet HCH_3$— *p*-CHO	1.1 ± 1.34	1.2 ± 1.28	1.4 ± 1.28	1.6 ± 1.32	1.6 ± 1.21	1.3 ± 0.94
NNI28	$C_6H_5CH_2\bullet$ /$C_6H_5C\bullet HCH_3$— *o*-CHO	-0.9 ± 1.44	-0.6 ± 1.38	-0.4 ± 1.38	-0.3 ± 1.42	-0.1 ± 1.3	0.3 ± 1.02
NNI29	$C_6H_5CH_2\bullet$ /$C_6H_5C\bullet HCH_3$— *o*-CH_3/CH_2CH_3	2.6 ± 0.91	1.8 ± 0.87	1.2 ± 0.87	0.5 ± 0.9	0.3 ± 0.82	0 ± 0.64

Table S15. *Differences between group additively and ab-initio calculated values for standard enthalpy of formation ($\Delta_f H°$), entropy (S°) and heat capacity (C_p) of the final dataset of MARs. Standard enthalpies of formation ($\Delta_f H°$) are given in kJ mol^{-1}, whereas entropies (S°) and heat capacities (C_p) are in J mol^{-1} K^{-1}.*

	Group additivity calculated (GA) - Ab-Initio calculated values (AI)								
#	**Training and validation set for GAV and NNI**	$\Delta_f H^\circ$	S°	C_p					
		298 K	**298 K**	**300 K**	**400 K**	**500 K**	**600 K**	**800 K**	**1000 K**	**1500 K**
T1/1	$C_6H_5\bullet$	1.4	1.5	-1.6	-1.1	-1.1	-0.9	-0.6	-0.4	-0.1
T1/2	o-$OHC_6H_4\bullet$	-1.4	3.5	-2.1	-2.8	-3.0	-2.9	-2.2	-1.7	-0.8
T1/3	m-$OHC_6H_4\bullet$	2.6	-1.1	0.8	0.7	0.3	0.2	0.1	0.0	0.0
T1/4	p-$OHC_6H_4\bullet$	-3.7	-1.4	0.7	0.8	0.7	0.7	0.5	0.4	0.3
T1/5	o-$MeOC_6H_4\bullet$	3.2	1.6	-0.3	-1.4	-2.5	-2.9	-2.4	-1.6	-0.5
T1/6	m-$MeOC_6H_4\bullet$	4.6	-0.8	0.5	0.5	0.3	0.4	0.6	0.7	0.7
T1/7	p-$MeOC_6H_4\bullet$	-2.0	-1.6	0.6	0.9	1.0	1.1	1.2	1.2	0.9
T1/8	o-$CHOC_6H_4\bullet$	-4.1	2.6	-3.1	-3.0	-2.7	-2.1	-1.0	-0.3	0.5
T1/9	m-$CHOC_6H_4\bullet$	-2.2	-0.2	0.4	0.5	0.3	0.4	0.6	0.7	0.7
T1/10	p-$CHOC_6H_4\bullet$	-0.9	0.0	0.6	0.6	0.4	0.5	0.8	0.8	0.6
T1/11	o-$CH{=}CH_2C_6H_4\bullet$	-0.7	2.0	-3.9	-2.6	-2.3	-2.0	-1.6	-1.2	-0.6
T1/12	m-$CH{=}CH_2C_6H_4\bullet$	-1.8	0.7	-0.9	-0.7	-0.8	-0.8	-0.6	-0.4	-0.1
T1/13	p-$CH{=}CH_2C_6H_4\bullet$	-3.0	0.7	-0.8	-0.5	-0.6	-0.6	-0.4	-0.3	0.0
T1/14	o-$CH_3C_6H_4\bullet$	2.6	0.3	-0.5	-0.3	-0.5	-0.5	-0.4	-0.3	0.0
T1/15	m-$CH_3C_6H_4\bullet$	2.5	0.7	-0.6	-0.4	-0.7	-0.7	-0.6	-0.5	-0.1
T1/16	p-$CH_3C_6H_4\bullet$	0.3	0.8	-0.6	-0.3	-0.6	-0.5	-0.5	-0.4	-0.1
T1/17	o-$CH_2CH_3C_6H_4\bullet$	4.4	-1.9	1.5	1.3	0.8	0.7	0.7	0.6	0.7

T1/18	m-$CH_2CH_3C_6H_4$•	4.2	-1.0	0.0	0.4	0.1	0.2	0.4	0.4	0.6
T1/19	p-$CH_2CH_3C_6H_4$•	2.0	-0.4	-0.4	0.1	-0.1	0.1	0.3	0.3	0.5
T1/20	1-C•-3-OH-4-OCH_3	1.0	-1.5	2.4	3.5	3.1	2.2	0.5	-0.4	-1.2
T1/21	1-C•-3-OH-4-CHO	-6.1	-0.9	0.0	-3.8	0.0	0.0	0.3	0.4	0.2
T1/22	1-C•-2-CH_3-4-OH	-1.5	-2.6	1.7	1.6	1.2	1.0	0.7	0.5	0.3
T1/23	1-C•-2-OCH_3-3-OH-6-CHO	2.4	0.5	1.2	0.4	0.0	-0.5	-1.3	-1.9	-2.5
T2/1	$C_6H_5OCH_2$•	-0.3	-2.2	-0.6	-0.1	0.5	1.0	1.4	1.4	0.9
T2/2	o-$OHC_6H_4OCH_2$•	1.1	4.0	-0.1	-0.3	-1.2	-2.5	-3.8	-3.9	-2.7
T2/3	m-$OHC_6H_4OCH_2$•	1.3	-3.6	0.8	0.9	1.3	1.5	1.6	1.4	0.8
T2/4	p-$OHC_6H_4OCH_2$•	-2.1	-0.5	1.6	1.2	0.8	0.6	0.3	0.1	0.0
T2/5	o-$OCH_3C_6H_4OCH_2$•	-0.9	-1.5	-4.6	-3.1	-1.3	0.1	1.7	2.0	1.5
T2/6	m-$OCH_3C_6H_4OCH_2$•	3.7	-0.4	1.4	1.2	1.6	1.9	2.3	2.2	1.5
T2/7	p-$OCH_3C_6H_4OCH_2$•	0.3	-1.2	1.3	1.1	0.9	0.8	0.7	0.7	0.5
T2/8	o-$CHOC_6H_4OCH_2$•	-1.9	-0.7	-1.6	-1.4	-0.9	-0.3	0.4	0.6	0.5
T2/9	m-$CHOC_6H_4OCH_2$•	-3.3	-4.0	-1.1	-0.3	0.6	1.3	2.1	2.2	1.5
T2/10	p-$CHOC_6H_4OCH_2$•	1.7	-2.9	1.1	1.1	1.3	1.6	2.0	1.9	1.0
T2/11	o-$CH=CH_2C_6H_4OCH_2$•	-5.5	3.1	-4.1	-4.0	-3.2	-2.5	-1.3	-0.7	-0.3
T2/12	m-$CH=CH_2C_6H_4OCH_2$•	-3.1	-2.4	-0.5	-0.1	0.6	1.0	1.4	1.3	0.8
T2/13	p-$CH=CH_2C_6H_4OCH_2$•	-3.7	-0.2	-0.4	-0.1	0.4	0.6	1.0	0.9	0.5
T2/14	o-$CH_3C_6H_4OCH_2$•	1.7	3.9	-3.8	-3.8	-3.4	-2.8	-1.8	-1.2	-0.6
T2/15	m-$CH_3C_6H_4OCH_2$•	1.3	-2.8	0.1	0.4	0.9	1.2	1.5	1.3	0.8
T2/16	p-$CH_3C_6H_4OCH_2$•	-2.0	-1.5	0.7	1.0	1.4	1.7	1.8	1.5	0.9
T2/17	o-$CH_2CH_3C_6H_4OCH_2$•	3.8	2.4	-3.2	-3.2	-2.8	-2.3	-1.3	-1.0	-0.4
T2/18	m-$CH_2CH_3C_6H_4OCH_2$•	2.7	-1.5	1.6	1.7	2.0	2.3	2.6	2.2	1.7
T2/19	p-$CH_2CH_3C_6H_4OCH_2$•	-0.3	-1.4	0.8	1.2	1.7	2.1	2.5	2.2	1.6
T2/20	1-OCH_2•-3,4-OH	-0.6	-2.7	2.5	2.5	2.0	1.5	1.0	1.0	0.7
T2/21	1-OCH_2•-2-OH-6-OCH_3	2.1	0.9	4.9	2.6	0.3	-1.7	-3.7	-3.9	-2.7
T2/22	1-OCH_2•-2-OH-4-CHO	0.3	0.9	0.9	-1.0	-2.3	-3.3	-3.6	-3.1	-1.9
T2/23	1-OCH_2•-2-OH-5-CHO	-4.5	1.4	-0.4	-0.3	-0.8	-1.8	-3.3	-3.7	-3.2
T2/24	1-OCH_2•-2-OH-5-$CH=CH_2$	5.3	3.7	0.4	0.5	-0.4	-2.0	-3.8	-4.2	-3.2
T2/25	1-OCH_2•-2-OCH_3-4-OH	1.0	1.3	-3.2	-3.3	-2.5	-1.6	-0.4	0.0	0.2
T2/26	1-OCH_2•-2-OCH_3-6-OH	2.1	0.9	4.9	2.6	0.3	-1.7	-3.7	-3.9	-2.7
T2/27	1-OCH_2•-2-OCH_3-4-CH_3	-0.2	-0.9	-3.3	-2.1	-0.7	0.4	1.6	1.8	1.3
T2/28	1-OCH_2•-2-OCH_3-5-CH_3	-0.6	-1.0	-4.1	-2.4	-0.8	0.5	1.8	2.0	1.5
T2/29	1-OCH_2•-2-CHO-3-CH_3	1.5	-0.2	1.9	1.6	0.6	-0.5	-1.8	-2.0	-1.3
T2/30	1-OCH_2•-2-CHO-4-CH_3	-2.5	-1.6	0.0	-0.2	-0.1	0.2	0.5	0.5	0.3
T3/31	1-OCH_2•-2-CH_3-4-OH	0.8	2.8	-2.0	-2.0	-2.1	-2.1	-2.1	-1.9	-1.4
T2/32	1-OCH_2•-3-CH_3-4-OH	0.4	0.1	-0.2	0.7	0.9	0.8	0.5	0.3	0.0
T2/33	1-OCH_2•-2,3-CH_3	2.3	1.6	0.0	-0.5	-0.3	0.2	0.9	0.9	0.8
T3/1	C_6H_5O•	-2.1	0.8	-1.1	-0.7	-0.5	-0.3	0.1	0.2	0.2
T3/2	o-OHC_6H_4O•	0.0	0.8	-0.3	-0.1	-0.1	-0.1	-0.3	-0.4	-0.4
T3/3	m-OHC_6H_4O•	1.0	2.3	-2.3	-2.5	-2.2	-1.8	-1.1	-0.7	-0.4
T3/4	p-OHC_6H_4O•	-4.7	-2.8	0.7	0.6	0.4	0.2	0.1	0.2	0.8
T3/5	o-$OCH_3C_6H_4O$•	-0.1	1.6	-0.2	-0.5	-0.5	-0.4	-0.2	0.0	0.1
T3/6	m-$OCH_3C_6H_4O$•	-0.2	-0.9	-0.5	-0.8	-0.6	-0.4	0.4	0.7	0.6
T3/7	p-$OCH_3C_6H_4O$•	-1.7	-2.3	0.8	0.5	0.1	-0.2	0.0	0.5	1.5
T3/8	o-$CHOC_6H_4O$•	-2.7	-1.7	-0.7	-0.6	-0.6	-0.5	-0.3	-0.1	0.2
T3/9	m-$CHOC_6H_4O$•	-3.3	-1.1	-1.7	-0.6	0.2	0.8	1.4	1.4	1.4
T3/10	p-$CHOC_6H_4O$•	-3.9	-4.2	0.8	0.7	0.8	0.9	1.3	1.3	0.8
T3/11	o-$CH=CH_2C_6H_4O$•	0.3	0.3	-0.2	-0.2	-0.1	0.0	0.0	0.1	0.0
T3/12	m-$CH=CH_2C_6H_4O$•	-2.3	0.4	-1.3	-0.8	-0.5	-0.3	0.1	0.3	0.2
T3/13	p-$CH=CH_2C_6H_4O$•	1.0	1.0	-0.3	-0.3	-0.3	-0.3	-0.1	-0.1	-0.2
T3/14	o-$CH_3C_6H_4O$•	-0.6	2.1	-0.9	-0.7	-0.5	-0.2	0.0	0.1	0.1
T3/15	m-$CH_3C_6H_4O$•	0.8	0.3	-0.6	-0.4	-0.3	-0.2	0.0	0.1	0.1
T3/16	p-$CH_3C_6H_4O$•	-1.4	-0.1	-0.5	-0.5	-0.3	-0.2	0.0	0.0	0.0
T3/17	o-$CH_2CH_3C_6H_4O$•	0.4	2.5	-0.2	-0.3	-0.4	-0.2	0.0	0.1	0.3
T3/18	m-$CH_2CH_3C_6H_4O$•	2.3	-1.4	0.7	0.8	0.8	0.9	1.2	1.1	1.0
T3/19	p-$CH_2CH_3C_6H_4O$•	-0.2	-2.0	0.5	0.7	0.9	0.9	1.2	1.1	0.9
T3/20	1-O•-2,3-OH	-4.0	-1.6	-1.4	-2.4	-2.6	-2.0	-0.6	0.6	1.1
T3/21	1-O•-3,4-OH	2.6	1.7	1.2	0.6	0.0	-0.7	-1.9	-2.3	-1.6
T3/22	1-O•-2-OH-4-OCH_3	2.1	-0.1	-2.4	-2.1	-2.0	-2.1	-1.5	-0.9	0.6
T3/23	1-O•-2-OH-6-OCH_3	-6.3	-2.8	1.3	1.1	1.0	0.9	0.8	0.7	0.5
T3/24	1-O•-2-OH-3-CHO	-2.4	3.2	1.0	-0.3	-1.1	-1.5	-1.5	-1.3	-0.3
T3/25	1-O•-2-OH-4-CHO	4.1	-2.4	-0.9	0.2	1.4	2.4	3.5	3.5	1.8
T3/26	1-O•-2-OH-6-CHO	-2.0	-1.0	-0.3	-0.8	-1.1	-1.1	-0.6	-0.1	0.2
T3/27	1-O•-2-OH-4-$CH=CH_2$	0.2	0.4	0.2	0.1	0.0	-0.2	-0.5	-0.6	-0.5
T3/28	1-O•-2-OH-5-$CH=CH_2$	0.1	1.9	-1.4	-0.7	-0.4	-0.4	-0.6	-0.7	-0.7
T3/29	1-O•-2-OH-6-$CH=CH_2$	-0.4	2.8	0.1	0.1	0.0	-0.2	-0.4	-0.6	-0.4
T3/30	1-O•-2-OH-4-CH_3	0.8	0.4	-0.1	-0.1	-0.1	-0.2	-0.5	-0.7	-0.6
T3/31	1-O•-2-OH-5-CH_3	3.1	0.5	-0.2	0.0	0.0	0.0	-0.4	-0.5	-0.6
T3/32	1-O•-2-OH-6-CH_3	0.6	2.1	-0.8	-0.5	-0.3	-0.3	-0.5	-0.6	-0.6

T3/33	1-O•-2-OCH_3-3-OH	0.5	0.0	4.0	3.9	3.5	2.8	1.2	0.1	-1.3
T3/34	1-O•-3-OCH_3-4-OH	2.8	-2.1	4.7	**0.9**	**-0.1**	**0.3**	4.9	2.3	-1.2
T3/35	1-O•-2,3-OCH_3	-1.1	2.2	-2.1	-2.6	-2.7	-2.6	-1.3	-0.1	1.7
T3/36	1-O•-2,6-OCH_3	6.3	-1.0	-1.3	-1.8	-1.9	-1.5	-0.5	0.1	0.5
T3/37	1-O•-3,4-OCH_3	4.0	3.5	-3.9	**-1.0**	**-1.0**	**0.0**	-4.9	-2.4	0.4
T3/38	1-O•-2-OCH_3-3-CHO	4.3	1.1	0.6	2.0	2.8	3.0	1.8	0.2	-1.1
T3/39	1-O•-2-OCH_3-4-CHO	0.4	-4.4	-1.3	-0.9	-0.4	-0.1	0.3	0.4	0.3
T3/40	1-O•-2-OCH_3-6-CHO	-0.8	1.5	0.2	-0.1	-0.5	-0.6	-0.5	-0.2	0.1
T3/41	1-O•-2-OCH_3-3-$CH=CH_2$	-2.5	3.1	2.5	2.1	1.6	0.8	-0.6	-1.4	-1.9
T3/42	1-O•-2-OCH_3-4-$CH=CH_2$	-1.3	-1.4	0.0	0.3	0.3	0.5	0.6	0.7	0.7
T3/43	1-O•-2-OCH_3-3-CH_3	3.2	-0.2	0.8	1.1	1.0	0.6	-0.9	-2.1	-2.8
T3/44	1-O•-2-OCH_3-4-CH_3	-0.3	1.7	0.1	-0.3	-0.4	-0.4	-0.3	-0.1	0.0
T3/45	1-O•-2-OCH_3-5-CH_3	2.7	2.0	-0.1	-0.5	-0.6	-0.6	-0.5	-0.4	-0.1
T3/46	1-O•-3-OCH_3-4-CHO	1.6	2.3	2.3	3.7	3.6	2.4	0.2	-1.1	-1.8
T3/47	1-O•-3-OCH_3-6-CHO	-1.4	2.5	-0.5	-0.5	0.0	0.1	0.6	0.9	1.1
T3/48	1-O•-2-CHO-4-OH	-1.6	2.2	0.3	0.6	1.0	0.8	0.1	-0.6	-1.0
T3/49	1-O•-2-CHO-5-OH	-1.6	2.3	-2.1	-2.0	-1.4	-1.0	-0.5	-0.2	0.3
T3/50	1-O•-2-CHO-6-OH	-1.9	-1.2	-0.2	-0.6	-0.8	-0.8	-0.4	-0.1	0.1
T3/51	1-O•-2-CHO-5-OCH_3	-1.5	-3.2	-0.7	-0.6	-0.1	0.1	0.6	0.9	1.1
T3/52	1-O•-3-CHO-4-OH	-5.4	-0.1	0.5	0.9	1.6	1.9	2.8	2.9	-0.9
T3/53	1-O•-3-CHO-4-OCH_3	2.0	-0.7	0.5	0.0	-1.3	-2.8	-3.9	-3.3	-0.8
T3/54	1-O•-3-CHO-6-OCH_3	-0.8	2.6	-3.5	-2.3	-0.9	0.1	1.3	1.6	2.0
T3/55	1-O•-2,4-CHO	-2.8	-1.5	0.4	0.1	-0.2	-0.2	-0.2	-0.2	0.1
T3/56	1-O•-2,5-CHO	2.5	-2.2	0.8	1.1	0.9	0.9	0.9	1.0	0.9
T3/57	1-O•-3,4-CHO	2.6	2.1	-3.1	-4.5	-4.9	-4.8	-4.0	-3.1	-1.2
T3/58	1-O•-2-CHO-3-$CH=CH_2$	-1.7	0.5	2.9	2.1	1.6	1.2	0.2	-0.5	-1.2
T3/59	1-O•-2-CHO-5-$CH=CH_2$	-2.2	0.3	-0.6	-0.4	-0.4	-0.3	-0.2	-0.2	-0.1
T3/60	1-O•-2-CHO-3-CH_3	2.2	1.5	2.2	1.9	1.5	1.0	-0.1	-1.0	-1.4
T3/61	1-O•-2-CHO-4-CH_3	0.3	-0.3	0.2	0.2	0.0	0.0	-0.2	-0.2	-0.2
T3/62	1-O•-2-CHO-5-CH_3	1.9	0.7	0.3	0.1	-0.1	-0.1	-0.2	-0.2	-0.1
T3/63	1-O•-2-CHO-6-CH_3	-0.4	0.0	-0.5	-0.5	-0.5	-0.5	-0.3	0.0	0.1
T3/64	1-O•-2-$CH=CH_2$-5-CH_3	4.4	1.1	-0.4	-0.3	-0.2	-0.1	-0.2	-0.2	-0.3
T3/65	1-O•-2-$CH=CH_2$-6-CH_3	0.6	-2.1	-1.5	-1.2	-1.0	-0.8	-0.6	-0.5	-0.4
T3/66	1-O•-2-CH_3-4-CHO	-0.8	-3.5	0.6	0.6	0.7	0.9	1.1	1.2	0.6
T3/67	1-O•-2,6-CH_3	0.4	3.8	-1.3	-1.0	-0.6	-0.4	-0.1	0.0	-0.1
T3/68	1-O•-2-CH_2CH_3-4-CHO	0.5	-3.6	1.8	1.3	1.1	1.2	1.4	1.4	1.1
T4/1	C_6H_5C•=O	-1.4	-0.2	0.0	0.0	0.1	0.2	0.4	0.4	0.3
T4/2	o-OHC_6H_5C•=O	-3.0	-1.2	-3.6	-4.1	-4.7	-5.2	-5.9	-5.5	-2.7
T4/3	m-OHC_6H_5C•=O	-1.2	-0.7	0.2	0.3	0.4	0.4	0.4	0.3	0.1
T4/4	p-OHC_6H_5C•=O	-2.7	-2.0	0.9	0.5	0.2	0.0	-0.3	-0.5	-0.1
T4/5	o-$OCH_3C_6H_5C$•=O	1.2	-2.4	0.4	1.1	1.5	1.8	1.9	1.7	1.0
T4/6	m-$OCH_3C_6H_5C$•=O	1.5	-0.8	-1.0	-1.0	-0.7	-0.5	0.1	0.5	0.5
T4/7	p-$OCH_3C_6H_5C$•=O	-2.5	-3.2	0.7	0.1	-0.5	-0.7	-0.5	-0.1	0.6
T4/8	m-$CHOC_6H_5C$•=O	-0.9	-2.7	0.9	1.4	1.5	1.6	1.4	1.3	1.2
T4/9	p-$CHOC_6H_5C$•=O	-1.1	-0.3	-0.9	-0.7	-0.6	-0.5	-0.6	-0.6	-0.5
T4/10	o-$CH=CH_2C_6H_5C$•=O	-3.4	1.8	0.8	0.2	-0.5	-1.0	-1.3	-1.3	-0.8
T4/11	m-$CH=CH_2C_6H_5C$•=O	0.8	-1.2	0.6	0.4	0.4	0.4	0.5	0.5	0.3
T4/12	p-$CH=CH_2C_6H_5C$•=O	-5.7	-0.3	0.6	0.3	0.2	0.2	0.3	0.3	0.1
T4/13	o-$CH_3C_6H_5C$•=O	-1.5	3.5	-1.0	-0.7	-0.4	-0.1	0.3	0.4	0.3
T4/14	m-$CH_3C_6H_5C$•=O	0.8	-0.9	0.9	0.6	0.5	0.5	0.5	0.4	0.2
T4/15	p-$CH_3C_6H_5C$•=O	1.9	0.7	1.1	0.7	0.4	0.3	0.1	0.0	-0.1
T4/16	o-$CH_2CH_3C_6H_5C$•=O	1.2	0.8	-0.8	-1.1	-1.0	-0.8	-0.2	0.0	0.4
T4/17	m-$CH_2CH_3C_6H_5C$•=O	2.6	-3.2	1.5	1.4	1.3	1.3	1.4	1.3	1.1
T4/18	p-$CH_2CH_3C_6H_5C$•=O	3.6	-0.2	1.8	1.6	1.4	1.3	1.2	1.0	0.8
T4/19	1-C•=O-2,3-OH	1.3	0.2	0.6	-0.2	-0.5	-0.4	0.0	0.6	0.7
T4/20	1-C•=O-2,5-OH	-4.2	1.4	0.1	-0.2	-0.6	-1.5	-3.4	-4.9	-5.1
T4/21	1-C•=O-3,4-OH	-2.9	1.5	-1.1	-1.7	-1.8	-1.8	-1.7	-1.5	-0.7
T4/22	1-C•=O-3-OH-4-OCH_3	-1.6	-0.1	0.4	-1.3	-2.3	-2.7	-2.3	-1.5	-0.3
T4/23	1-C•=O-3-OH-6-OCH_3	1.8	-0.8	0.6	1.8	2.2	1.8	1.3	0.8	-0.1
T4/24	1-C•=O-2-OH-3-CHO	-1.9	2.2	0.3	-1.1	-1.9	-2.2	-1.8	-1.0	0.2
T4/25	1-C•=O-3-OH-4-$CH=CH_2$	1.9	-1.7	5.4	5.4	4.9	4.2	3.0	2.2	1.0
T4/26	1-C•=O-2-OH-4-CH_3	5.5	1.9	3.8	4.1	4.2	4.3	4.4	4.3	2.5
T4/27	1-C•=O-2-OH-5-CH_3	-3.3	-1.8	-2.5	-3.1	-3.8	-4.6	-5.7	-5.4	-2.8
T4/28	1-C•=O-2-OH-6-CH_3	1.7	-1.5	-0.2	0.3	0.8	1.3	2.0	2.2	1.5
T4/29	1-C•=O-2-OCH_3-4-OH	2.4	0.8	-1.4	-1.3	-1.0	-0.7	-0.4	-0.2	0.3
T4/30	1-C•=O-3-OCH_3-4-OH	1.6	0.9	0.6	0.9	1.0	0.6	-0.7	-1.9	-2.7
T4/31	1-C•=O-2-OCH_3-3-CH_3	-3.0	1.1	1.0	-1.2	-3.2	-4.4	-4.9	-4.3	-2.8
T4/32	1-C•=O-2-OCH_3-5-CH_3	1.2	-3.3	1.9	2.3	2.5	2.5	2.2	1.9	0.9
T4/33	1-C•=O-2-OCH_3-6-CH_3	-0.7	3.6	-4.4	-3.2	-1.3	0.2	1.6	1.8	1.2
T4/34	1-C•=O-3-CHO-4-OH	-0.8	-2.7	-1.6	-0.7	0.0	0.2	-0.2	-1.1	-3.4
T4/35	1-C•=O-2-$CH=CH_2$-4-CH_3	1.1	2.9	1.7	0.7	-0.4	-1.1	-1.7	-1.7	-1.1

T4/36	1-C•=O-2-CH=CH_2-5-CH_3	4.8	1.9	1.1	0.3	-0.6	-1.1	-1.4	-1.4	-0.9
T4/37	1-C•=O-2-CH=CH_2-6-CH_3	-1.7	2.8	-5.7	-3.7	-1.9	-0.6	0.5	0.7	0.5
T4/38	1-C•=O-2-CH_3-4-OH	1.7	2.4	-0.4	-0.4	-0.5	-0.7	-0.8	-0.8	-0.2
T4/39	1-C•=O-2-CH_3-4-CHO	0.8	-1.5	1.7	1.2	0.8	0.4	-0.1	-0.3	-0.4
T4/40	1-C•=O-2-CH_3-4-CH=CH_2	-4.5	4.1	-0.5	-0.5	-0.3	-0.1	0.2	0.3	0.2
T4/41	1-C•=O-2,3-CH_3	0.3	1.8	-0.8	-0.4	-0.1	0.2	0.6	0.8	1.0
T4/42	1-C•=O-3-CH_3-4-CHO	0.7	-0.5	-5.3	-3.6	-2.1	-0.9	0.5	1.0	1.1
T5/1	t-C_6H_5CH=CH•	-1.0	2.2	-0.5	-0.6	-0.5	-0.3	-0.1	-0.1	0.1
T5/2	o-(OH)t-C_6H_5CH=CH•	0.2	1.0	-1.5	-1.4	-1.1	-1.0	-0.8	-0.4	0.1
T5/3	m-(OH)t-C_6H_5CH=CH•	-0.2	1.2	0.3	0.1	0.2	0.2	0.1	0.0	0.0
T5/4	p-(OH)t-C_6H_5CH=CH•	-0.5	0.9	2.1	1.3	0.9	0.6	0.3	0.0	-0.1
T5/5	o-(OCH_3)t-C_6H_5CH=CH•	-1.4	3.3	-1.3	-1.4	-1.2	-1.2	-1.3	-1.5	-1.3
T5/6	m-(OCH_3)t-C_6H_5CH=CH•	2.1	-0.6	-0.6	-0.6	-0.2	0.0	0.5	0.6	0.6
T5/7	p-(OCH_3)t-C_6H_5CH=CH•	1.6	0.1	1.8	0.8	0.6	0.5	0.5	0.5	0.5
T5/8	o-(CHO)t-C_6H_5CH=CH•	2.3	1.5	-0.4	-1.4	-1.9	-2.1	-2.0	-1.5	-0.4
T5/9	m-(CHO)t-C_6H_5CH=CH•	-3.2	-2.9	-0.2	0.0	0.3	0.6	1.0	1.0	0.8
T5/10	p-(CHO)t-C_6H_5CH=CH•	-2.5	-1.6	1.4	1.0	0.9	1.0	1.1	1.0	0.6
T5/11	o-($CH=CH_2$)t-C_6H_5CH=CH•	-0.1	-2.8	-0.7	0.2	0.1	0.0	-0.2	-0.2	0.0
T5/12	m-($CH=CH_2$)t-C_6H_5CH=CH•	-3.9	1.9	0.1	-0.3	-0.2	-0.2	0.0	0.0	0.1
T5/13	p-($CH=CH_2$)t-C_6H_5CH=CH•	-3.9	3.4	0.1	-0.3	-0.4	-0.4	-0.5	-0.5	-0.4
T5/14	o-(CH_3)t-C_6H_5CH=CH•	0.6	-1.8	-5.7	-3.5	-2.5	-1.9	-1.1	-0.8	-0.4
T5/15	m-(CH_3)t-C_6H_5CH=CH•	0.0	1.7	0.4	-0.1	-0.1	-0.1	-0.1	-0.1	0.0
T5/16	p-(CH_3)t-C_6H_5CH=CH•	-0.3	2.3	0.4	0.0	-0.1	-0.1	-0.1	-0.2	0.0
T5/17	o-(CH_2CH_3)t-C_6H_5CH=CH•	1.9	0.0	-2.4	-1.3	-0.9	-0.6	-0.2	-0.2	0.0
T5/18	m-(CH_2CH_3)t-C_6H_5CH=CH•	3.0	-1.0	1.6	1.4	1.2	1.2	1.1	0.8	0.9
T5/19	p-(CH_2CH_3)t-C_6H_5CH=CH•	1.3	-3.4	0.7	0.5	0.5	0.6	0.8	0.6	0.7
T5/20	1-(t-CH=CH•)-2,3-OH	-4.0	-1.2	0.9	1.6	2.7	3.0	2.9	2.6	1.8
T5/21	1-(t-CH=CH•)-2,4-OH	3.7	0.9	1.2	1.4	1.8	1.6	0.5	-0.7	-1.7
T5/22	1-(t-CH=CH•)-3,4-OH	-0.1	4.3	-1.6	-2.4	-2.2	-1.9	-1.2	-0.6	0.1
T5/23	1-(t-CH=CH•)-2-OH-4-CHO	-4.1	1.0	0.1	-0.4	-0.5	-0.5	0.2	0.9	1.4
T5/24	1-(t-CH=CH•)-2-OH-6-CHO	6.3	1.4	2.9	3.1	3.6	3.9	2.7	0.4	-3.5
T5/25	1-(t-CH=CH•)-2-OH-5-CH=CH_2	-3.2	0.9	-1.0	-0.9	-0.8	-0.9	-0.8	-0.7	-0.3
T5/26	1-(t-CH=CH•)-2-OH-5-CH_3	-2.3	0.1	-0.7	-0.7	-0.6	-0.7	-0.6	-0.3	0.2
T5/27	1-(t-CH=CH•)-2-OH-6-CH_3	-4.3	3.8	-4.4	-3.7	-2.9	-2.2	-0.9	-0.2	0.3
T5/28	1-(t-CH=CH•)-2-OH-4-CH_2CH_3	3.6	-2.7	0.1	0.2	0.4	0.4	0.4	0.3	0.6
T5/29	1-(t-CH=CH•)-2-OH-5-CH_2CH_3	3.7	-4.5	2.7	2.7	2.0	1.4	0.7	0.7	0.9
T5/30	1-(t-CH=CH•)-2-CHO-4-OH	0.3	3.3	2.6	0.7	-0.3	-1.0	-1.4	-1.1	-0.2
T5/31	1-(t-CH=CH•)-3-CHO-4-OH	-0.7	-2.2	-0.3	-0.4	-0.1	-0.1	-0.4	-1.5	-4.5
T5/32	1-(t-CH=CH•)-2,4-CHO	3.0	-0.5	2.8	0.7	-0.3	-0.8	-1.0	-0.9	-0.5
T5/33	1-(t-CH=CH•)-2-CH=CH_2-4-CH_3	1.0	1.7	0.6	0.6	0.1	-0.2	-0.5	-0.5	-0.2
T5/34	1-(t-CH=CH•)-2-CH=CH_2-6-CH_3	1.4	-4.1	2.2	3.1	3.1	2.7	1.8	1.1	0.3
T5/35	1-(t-CH=CH•)-2-CH_3-4-CHO	-0.4	-2.7	-0.5	0.2	0.4	0.4	0.6	0.6	0.3
T5/36	1-(t-CH=CH•)-2,3-CH_3	-1.6	-0.6	0.7	1.6	1.9	2.2	2.4	2.3	1.8
T5/37	1-(t-CH=CH•)-2,4-CH_3	1.7	-0.5	-2.6	-1.5	-1.1	-0.9	-0.7	-0.6	-0.4
T5/38	1-(t-CH=CH•)-2-CH_3-4-CH_2CH_3	3.4	0.3	-1.9	-0.7	-0.3	-0.1	0.2	0.2	0.4
T5/39	c-C_6H_5CH=CH•	-1.2	3.3	-1.2	-1.4	-1.7	-1.5	-1.0	-0.9	-0.5
T5/40	o-(OH)c-C_6H_5CH=CH•	0.3	1.6	-1.7	-0.8	0.0	0.6	1.0	0.8	0.3
T5/41	m-(OH)c-C_6H_5CH=CH•	-0.5	1.0	1.2	0.4	-0.2	-0.4	-0.4	-0.5	-0.5
T5/42	p-(OH)c-C_6H_5CH=CH•	-1.2	1.6	1.2	0.3	-0.4	-0.7	-0.8	-0.8	-0.8
T5/43	o-(OCH_3)c-C_6H_5CH=CH•	1.9	-1.2	2.5	1.1	-0.4	-1.4	-2.1	-2.3	-2.0
T5/44	m-(OCH_3)c-C_6H_5CH=CH•	1.7	0.5	0.9	0.0	-0.5	-0.4	0.0	0.1	0.1
T5/45	p-(OCH_3)c-C_6H_5CH=CH•	0.9	1.0	0.9	-0.1	-0.7	-0.8	-0.5	-0.3	-0.2
T5/46	o-(CHO)c-C_6H_5CH=CH•	-1.0	-2.6	-2.6	-1.3	-0.7	-0.3	0.2	0.4	0.7
T5/47	m-(CHO)c-C_6H_5CH=CH•	-3.2	-3.4	1.4	0.8	0.5	0.9	2.2	2.9	3.1
T5/48	p-(CHO)c-C_6H_5CH=CH•	-3.1	3.8	1.0	0.3	-0.2	-0.2	0.1	0.1	0.0
T5/49	o-($CH=CH_2$)c-C_6H_5CH=CH•	-0.4	0.6	-2.8	-1.7	-1.4	-1.0	-0.3	-0.1	0.0
T5/50	m-($CH=CH_2$)c-C_6H_5CH=CH•	-4.0	2.6	-0.6	-1.0	-1.3	-1.3	-0.9	-0.7	-0.5
T5/51	p-($CH=CH_2$)c-C_6H_5CH=CH•	-4.1	3.9	-0.7	-1.2	-1.7	-1.7	-1.5	-1.4	-1.0
T5/52	o-(CH_3)c-C_6H_5CH=CH•	-1.2	3.4	0.2	-0.1	-0.6	-0.7	-0.8	-0.8	-0.7
T5/53	m-(CH_3)c-C_6H_5CH=CH•	0.6	2.4	-0.1	-0.5	-1.0	-1.0	-0.9	-0.9	-0.7
T5/54	p-(CH_3)c-C_6H_5CH=CH•	-0.6	2.9	-0.4	-0.9	-1.3	-1.3	-1.1	-1.0	-0.7
T5/55	o-(CH_2CH_3)c-C_6H_5CH=CH•	2.2	2.9	-1.7	-1.1	-1.0	-0.8	-0.7	-0.8	-0.7
T5/56	m-(CH_2CH_3)c-C_6H_5CH=CH•	1.4	0.7	0.0	-0.2	-0.6	-0.5	-0.1	-0.1	0.2
T5/57	p-(CH_2CH_3)c-C_6H_5CH=CH•	1.1	1.1	0.1	-0.2	-0.6	-0.5	-0.2	-0.2	0.0
T5/58	1-(c-CH=CH•)-2,4-OH	2.4	4.0	-2.0	-1.6	-0.9	-0.6	-0.2	-0.3	-0.6
T5/59	1-(c-CH=CH•)-2,5-OH	-2.2	0.6	0.2	1.1	1.7	1.7	1.4	0.8	-0.2
T5/60	1-(c-CH=CH•)-2-OH-4-OCH_3	5.2	4.9	-2.2	-2.0	-1.3	-0.8	0.0	0.3	0.1
T5/61	1-(c-CH=CH•)-2-OH-5-OCH_3	-2.2	-0.7	-0.1	1.3	2.2	2.3	2.0	1.5	0.3
T5/62	1-(c-CH=CH•)-2-OH-4-CH=CH_2	-2.1	2.9	-1.5	-0.8	-0.1	0.4	0.7	0.6	0.0
T5/63	1-(c-CH=CH•)-3-OH-5-CH=CH_2	1.3	3.4	0.5	-0.5	-1.2	-1.7	-1.8	-1.8	-1.5
T5/64	1-(c-CH=CH•)-2-OH-3-CH_3	2.0	3.7	-5.4	-2.9	-1.2	-0.2	0.6	0.6	0.2

T5/65	1-(c-CH=CH•)-2-OH-4-CH_3	1.7	2.2	-0.9	-0.4	0.1	0.5	0.8	0.6	0.1
T5/66	1-(c-CH=CH•)-2-OH-5-CH_3	-1.8	0.9	-1.4	-0.3	0.5	1.0	1.3	1.0	0.3
T5/67	1-(c-CH=CH•)-3-OH-5-CH_3	5.8	4.3	0.0	-0.8	-1.5	-2.0	-2.2	-2.2	-1.8
T5/68	1-(c-CH=CH•)-2-OH-3-CH_2CH_3	3.5	4.0	-5.4	-3.1	-1.6	-0.5	0.5	0.4	0.4
T5/69	1-(c-CH=CH•)-3-CHO-4-OH	-1.6	2.1	-0.5	-0.8	-0.9	-0.9	-0.3	-0.1	-0.3
T5/70	1-(c-CH=CH•)-2,4-CHO	-0.8	-0.2	0.9	1.0	0.9	0.9	0.9	0.8	0.5
T5/71	1-(c-CH=CH•)-2-CHO-5-CH=CH_2	-1.5	-1.0	-1.4	-0.5	-0.1	0.1	0.4	0.6	0.6
T5/72	1-(c-CH=CH•)-2-CHO-4-CH_3	-0.1	-2.4	-2.0	-0.8	-0.3	0.0	0.3	0.5	0.7
T5/73	1-(c-CH=CH•)-2-CH=CH_2-4-OH	-0.1	0.4	0.8	1.2	0.8	0.4	0.1	-0.1	-0.3
T5/74	1-(c-CH=CH•)-2-CH=CH_2-5-CH_3	0.2	1.8	-1.3	-0.2	-0.2	-0.2	-0.1	-0.1	-0.1
T5/75	1-(c-CH=CH•)-2-CH=CH_2-6-CH_3	1.1	1.5	2.3	-5.4	-4.0	-2.9	-1.7	-1.1	-0.6
T5/76	1-(c-CH=CH•)-2-CH_3-4-OH	0.2	2.6	2.7	1.6	0.6	-0.1	-0.7	-0.9	-1.0
T5/77	1-(c-CH=CH•)-2-CH_3-4-CHO	-2.1	-0.2	1.9	1.1	0.4	0.2	0.2	0.2	-0.2
T5/78	1-(c-CH=CH•)-2-CH_3-4-CH=CH_2	-3.6	3.6	0.1	0.3	-0.2	-0.5	-0.8	-0.8	-0.9
T5/79	1-(c-CH=CH•)-3-CH_3-4-CH=CH_2	-2.0	1.5	0.4	0.8	0.7	0.8	0.8	0.7	0.2
T5/80	1-(c-CH=CH•)-2,4-CH_3	-0.2	3.7	1.0	0.4	-0.3	-0.6	-0.9	-0.9	-0.9
T6/1	$C_6H_5CH_2$•	-3.2	0.8	-2.3	-1.7	-1.2	-0.6	-0.1	0.0	0.2
T6/2	o-(OH)$C_6H_5CH_2$•	-1.2	-0.3	-1.5	-0.5	0.2	0.6	1.0	0.8	0.5
T6/3	m-(OH)$C_6H_5CH_2$•	-2.7	-1.3	-0.3	-0.1	0.1	0.3	0.5	0.4	0.2
T6/4	p-(OH)$C_6H_5CH_2$•	-2.4	-1.6	0.4	0.4	0.5	0.5	0.5	0.2	0.1
T6/5	o-(OCH_3)$C_6H_5CH_2$•	1.6	4.9	0.3	-1.3	-2.3	-2.7	-2.6	-2.3	-1.4
T6/6	m-(OCH_3) $C_6H_5CH_2$•	-0.8	-2.3	-1.8	-1.2	-0.5	0.0	0.8	0.9	0.8
T6/7	p-(OCH_3)$C_6H_5CH_2$•	-0.8	-1.8	0.3	0.2	0.3	0.5	0.9	0.9	0.7
T6/8	o-(CHO)$C_6H_5CH_2$•	-1.0	2.9	-1.3	-1.2	-1.0	-0.6	-0.3	-0.1	0.0
T6/9	m-(CHO)$C_6H_5CH_2$•	-4.2	-0.1	-0.4	-0.2	0.2	0.6	1.2	1.2	1.0
T6/10	p-(CHO)$C_6H_5CH_2$•	-3.5	-2.4	-0.7	-0.3	0.3	0.8	1.3	1.3	1.0
T6/11	o-($CH=CH_2$)$C_6H_5CH_2$•	-0.2	0.9	-1.9	-1.7	-1.3	-0.9	-0.3	-0.2	0.0
T6/12	m-($CH=CH_2$)$C_6H_5CH_2$•	-3.8	0.4	-2.1	-1.6	-1.1	-0.7	-0.1	0.0	0.1
T6/13	p-($CH=CH_2$)$C_6H_5CH_2$•	-2.5	-0.6	-0.6	-0.2	0.0	0.4	0.5	0.4	0.4
T6/14	o-(CH_3)$C_6H_5CH_2$•	-0.7	1.2	-1.4	-1.2	-1.0	-0.9	-0.6	-0.4	-0.2
T6/15	m-(CH_3)$C_6H_5CH_2$•	-1.7	0.2	-1.4	-1.1	-0.8	-0.5	-0.1	0.0	0.1
T6/16	p-(CH_3)$C_6H_5CH_2$•	-2.2	-0.2	-1.3	-0.9	-0.6	-0.3	0.0	0.0	0.1
T6/17	o-(CH_2CH_3)$C_6H_5CH_2$•	-0.6	0.9	0.5	0.3	0.1	0.0	-0.2	-0.4	-0.4
T6/18	m-(CH_2CH_3)$C_6H_5CH_2$•	-0.7	-0.9	-1.1	-0.5	-0.1	0.3	0.9	0.8	0.9
T6/19	p-(CH_2CH_3)$C_6H_5CH_2$•	-0.6	-1.5	-0.7	-0.2	0.1	0.5	1.0	0.8	0.8
T6/20	1-CH_2•-2,3-OH	0.0	-0.1	-0.5	-0.6	-0.3	-0.2	0.0	0.2	0.5
T6/21	1-CH_2•-2,4-OH	0.7	-2.5	3.5	3.1	3.0	2.5	1.8	1.2	0.7
T6/22	1-CH_2•-2,5-OH	-0.6	-0.2	0.8	1.3	1.6	1.2	0.8	0.3	-0.3
T6/23	1-CH_2•-2,6-OH	1.6	-1.4	2.2	2.7	3.1	3.0	2.6	1.9	0.9
T6/24	1-CH_2•-2-OH-3-OCH_3	2.0	-0.6	2.8	4.1	4.2	3.4	1.5	0.1	-1.2
T6/25	1-CH_2•-2-OH-4-OCH_3	0.8	-2.0	0.8	1.4	2.0	2.1	2.2	1.9	1.2
T6/26	1-CH_2•-2-OCH_3-4-OH	3.0	2.9	1.3	-0.3	-1.5	-2.3	-2.7	-2.5	-1.8
T6/27	1-CH_2•-2,4-OCH_3	4.8	4.3	1.7	-0.2	-1.3	-2.0	-2.0	-1.7	-1.1
T6/28	1-CH_2•-2-OCH_3-4-CHO	5.9	2.8	1.3	0.4	-0.8	-1.9	-2.9	-3.0	-2.4
T6/29	1-CH_2•-2-OCH_3-4-CH=CH_2	4.1	3.8	2.2	0.3	-1.2	-2.0	-2.5	-2.4	-1.6
T6/30	1-CH_2•-2-OCH_3-4-CH_3	3.0	3.7	0.9	-1.0	-2.1	-2.7	-2.7	-2.4	-1.5
T6/31	1-CH_2•-2-OCH_3-4-CH_2CH_3	4.2	4.1	1.7	-0.1	-1.2	-1.7	-1.6	-1.4	-0.6
T6/32	1-CH_2•-2,4-CHO	0.4	-1.3	1.7	1.0	0.7	0.6	0.5	0.3	0.1
T6/33	1-CH_2•-2,5-CHO	4.2	-3.0	1.4	0.7	0.4	0.4	0.3	0.3	-0.1
T6/34	1-CH_2•-2,6-CHO	-3.0	-1.4	0.1	1.2	1.6	1.4	1.0	0.6	0.5
T6/35	1-CH_2•-2-CHO-4-CH=CH_2	0.2	2.0	0.1	0.2	0.3	0.4	0.4	0.4	0.2
T6/36	1-CH_2•-2-CH=CH_2-3-OH	5.9	-1.4	0.2	-2.7	-4.1	-4.6	-4.3	-3.5	-1.9
T6/37	1-CH_2•-2-CH=CH_2-3-OCH_3	-4.8	-0.1	2.5	3.4	3.8	3.7	3.2	2.6	1.7
T6/38	1-CH_2•-2,3-CH=CH_2	0.5	2.4	-1.7	-2.3	-2.5	-2.6	-2.4	-2.0	-1.3
T6/39	1-CH_2•-2-CH_3-3-OH	-2.3	-1.8	0.6	1.3	1.9	1.9	1.8	1.5	0.8
T6/40	1-CH_2•-2-CH_3-4-OH	1.3	-0.7	1.1	0.6	0.5	0.1	-0.2	-0.3	-0.4
T6/41	1-CH_2•-2-CH_3-5-OH	-2.2	-1.3	0.4	0.4	0.6	0.4	0.3	0.2	0.0
T6/42	1-CH_2•-2-CH_3-6-OH	1.6	0.8	-1.5	-0.8	-0.1	0.0	0.2	0.3	0.1
T6/43	1-CH_2•-2-CH_3-4-CHO	0.3	-2.3	-0.1	0.0	0.2	0.5	0.7	0.9	0.6
T6/44	1-CH_2•-2-CH_3-6-CHO	0.7	0.8	-1.9	-2.3	-2.3	-2.1	-1.7	-1.1	-0.6
T6/45	1-CH_2•-2-CH_3-4-CH=CH_2	0.9	0.1	0.1	0.1	0.1	0.0	-0.1	-0.1	-0.1
T6/46	1-CH_2•-2-CH_3-5-CH=CH_2	-0.9	1.0	-1.3	-1.1	-0.9	-0.9	-0.6	-0.4	-0.3
T6/47	1-CH_2•-2,4-CH_3	0.6	0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.4	-0.3
T6/48	1-CH_2•-2,5-CH_3	0.2	0.5	-0.6	-0.6	-0.5	-0.6	-0.5	-0.4	-0.3
T6/49	1-CH_2•-3-CH_3-4-OH	-0.2	0.4	-2.2	-1.2	-0.4	-0.1	0.2	0.1	0.0
T6/50	1-CH_2•-3-CH_3-4-OCH_3	1.9	1.8	-1.8	-2.5	-3.3	-3.7	-3.6	-3.0	-1.8
T6/51	1-CH_2•-3,5-CH_3	-0.4	-0.3	-0.6	-0.6	-0.5	-0.3	-0.1	-0.1	0.0
T6/52	1-CH_2•-3,6-CH_3	-0.1	0.5	-0.5	-0.5	-0.5	-0.6	-0.5	-0.4	-0.3
T6/53	C_6H_5CH•CH_3	-1.0	0.7	-0.9	-0.7	-0.6	-0.4	-0.3	-0.3	-0.1
T6/54	o-(OH)C_6H_5CH•CH_3	0.1	0.2	-1.6	-0.5	0.3	0.7	0.8	0.7	0.3
T6/55	m-(OH)C_6H_5CH•CH_3	0.4	-1.6	1.4	1.0	0.8	0.5	0.2	0.1	-0.1

T6/56	p-(OH)$C_6H_5CH•CH_3$	-1.0	-1.9	1.6	1.2	1.0	0.7	0.3	0.0	-0.2
T6/57	o-(OCH_3)$C_6H_5CH•CH_3$	3.1	0.8	0.6	-0.8	-1.6	-2.0	-2.2	-2.1	-1.7
T6/58	m-(OCH_3)$C_6H_5CH•CH_3$	1.2	-1.3	-1.8	-0.5	0.5	1.0	1.4	1.4	1.0
T6/59	p-(OCH_3)$C_6H_5CH•CH_3$	0.4	-1.3	1.4	1.1	1.0	0.9	0.8	0.8	0.5
T6/60	o-(CHO)$C_6H_5CH•CH_3$	1.5	1.5	-0.1	-0.9	-1.4	-1.4	-1.2	-0.9	-0.4
T6/61	m-(CHO)$C_6H_5CH•CH_3$	-0.9	-3.1	0.7	0.6	0.6	0.7	0.8	0.8	0.6
T6/62	p-(CHO)$C_6H_5CH•CH_3$	-3.8	2.6	-0.3	-0.1	0.1	0.4	0.7	0.8	0.9
T6/63	o-($CH=CH_2$)$C_6H_5CH•CH_3$	0.3	1.6	-1.4	-1.1	-0.8	-0.6	-0.3	-0.3	-0.1
T6/64	m-($CH=CH_2$)$C_6H_5CH•CH_3$	-1.3	0.7	-0.9	-0.7	-0.6	-0.5	-0.4	-0.3	-0.2
T6/65	p-($CH=CH_2$)$C_6H_5CH•CH_3$	-0.6	0.2	0.6	0.6	0.6	0.4	0.2	0.2	0.1
T6/66	o-(CH_3)$C_6H_5CH•CH_3$	-0.1	2.0	-0.8	-1.0	-1.1	-1.2	-1.1	-0.9	-0.6
T6/67	m-(CH_3)$C_6H_5CH•CH_3$	0.3	0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.4	-0.2
T6/68	o-(CH_2CH_3)$C_6H_5CH•CH_3$	-0.2	2.0	0.9	0.5	0.1	-0.2	-0.5	-0.8	-0.7
T6/69	m-(CH_2CH_3)$C_6H_5CH•CH_3$	1.3	-1.5	0.1	0.3	0.3	0.5	0.6	0.5	0.6
T6/70	p-(CH_2CH_3)$C_6H_5CH•CH_3$	1.4	-1.9	0.5	0.6	0.6	0.6	0.6	0.5	0.5
V1/1	1-C•-2-OH-3-CHO-5-OCH_3	-2.0	-2.8	3.5	4.8	4.8	4.0	2.6	1.4	-0.4
V1/2	1-C•-2-CHO-5-OH-6-OCH_3	-2.2	0.9	2.1	1.7	2.0	2.3	3.1	3.1	1.4
V2/1	1-OCH_2•-2,3-OH	1.0	2.1	1.4	1.2	0.6	-0.3	-1.2	-1.1	-0.8
V2/2	1-OCH_2•-2-OH-4-$CH=CH_2$	-1.2	4.4	-0.3	-1.0	-1.9	-3.2	-4.2	-4.1	-2.9
V2/3	1-OCH_2•-2-OCH_3-3-CH_3	-3.7	0.5	5.1	5.5	4.7	4.0	3.0	2.2	1.0
V2/4	1-OCH_2•-2-CHO-5-CH_3	2.9	2.5	-0.2	-0.1	0.3	0.7	1.0	1.0	0.5
V2/5	1-OCH_2•-2,3,4-CH_3	-1.0	-3.4	1.4	1.4	1.8	2.4	3.1	3.0	2.4
V3/1	1-O•-2,3,4-OH	-4.1	-2.4	0.3	1.0	2.2	2.7	2.7	1.8	0.6
V3/2	1-O•-2-OH-4-OCH_3-6-CHO	3.0	-1.9	1.8	1.4	0.7	0.0	-0.7	-0.8	-0.3
V3/3	1-O•-2-OH-3-$CH=CH_2$	2.5	0.6	3.5	3.5	3.0	2.6	1.5	1.0	0.3
V3/4	1-O•-2-OH-3-CH_3	4.4	1.0	-0.2	0.1	0.1	0.1	-0.3	-0.5	-0.5
V3/5	1-O•-2,4-OCH_3	-5.3	-2.1	-1.4	-1.7	-1.9	-2.4	-2.0	-1.3	-0.3
V3/6	1-O•-2-OCH_3-6-$CH=CH_2$	-5.0	-3.0	1.7	1.7	1.5	1.4	1.5	1.5	1.3
V3/7	1-O•-2-CHO-4-OCH_3	4.0	2.2	-1.8	-0.9	-0.3	-0.3	-0.4	-0.6	-0.6
V3/8	1-O•-2,3-CHO	3.0	0.7	-1.1	-1.4	-1.4	-1.1	-1.1	-1.3	-1.4
V3/9	1-O•-2-CHO-6-$CH=CH_2$	-0.9	0.8	0.3	0.1	-0.1	-0.1	-0.2	-0.2	-0.1
V3/10	1-O•-2-$CH=CH_2$-4-CH_3	0.8	0.2	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1
V3/11	1-O•-2-CH_3-3-CHO	-2.7	-5.7	6.0	5.1	4.2	3.3	2.4	1.7	1.2
V3/12	1-O•-2,6-CH_2CH_3	2.9	-0.3	-0.8	-0.7	-0.6	-0.5	0.0	0.0	0.4
V4/1	1-C•=O-2,4-OH	1.2	-1.2	2.9	3.5	3.9	4.1	4.3	4.2	3.0
V4/2	1-C•=O-2-OH-4-OCH_3	4.3	2.4	1.9	2.4	2.5	2.8	3.7	4.2	3.6
V4/3	1-C•=O-2-OH-5-CHO	1.8	0.5	-1.0	0.0	1.2	2.1	3.2	3.5	3.0
V4/4	1-C•=O-2-OH-6-$CH=CH_2$	-3.6	-3.3	0.5	0.3	0.6	0.9	1.2	1.2	0.8
V4/5	1-C•=O-2-OH-3-CH_3	0.3	0.4	-3.0	-2.4	-1.9	-1.7	-2.2	-3.3	-4.5
V4/6	1-C•=O-3-OCH_3-4-CH_3	-2.7	0.9	1.8	0.5	-0.6	-1.3	-1.8	-1.7	-0.8
V4/7	1-C•=O-3-CHO-4-CH_3	4.7	1.6	-0.3	-0.1	-0.2	-0.5	-0.9	-1.0	-0.3
V4/8	1-C•=O-2-$CH=CH_2$-3-CH_3	2.6	-6.2	1.6	2.3	2.6	2.9	2.9	2.6	1.5
V4/9	1-C•=O-3-CH_3-4-OH	-0.4	1.1	-2.6	-1.9	-1.5	-1.3	-1.1	-0.9	-0.3
V5/1	1-(t-CH=CH•)-2,5-OH	-3.0	0.1	1.1	-0.3	-1.3	-2.0	-1.4	-0.3	0.8
V5/2	1-(t-CH=CH•)-2-OH-5-CH_2CH_3	-0.5	-2.1	-0.5	-0.3	-0.2	-0.1	0.2	0.4	1.0
V5/3	1-(t-CH=CH•)-3,4-CHO	-3.4	2.2	0.1	-0.5	-0.8	-1.2	-1.8	-2.0	-1.4
V5/4	1-(t-CH=CH•)-2-CHO-5-$CH=CH_2$	0.4	1.6	0.5	-0.9	-1.5	-1.8	-1.8	-1.4	-0.5
V5/5	1-(t-CH=CH•)-2-$CH=CH_2$-3-CH_3	-1.5	-4.0	0.7	2.8	3.5	3.8	3.3	2.7	1.6
V5/6	1-(t-CH=CH•)-2-$CH=CH_2$-5-CH_3	0.7	0.6	1.1	1.1	0.5	0.1	-0.3	-0.4	-0.1
V5/7	1-(t-CH=CH•)-2-CH_2CH_3-4-CH_3	3.8	-2.1	-3.1	-2.4	-2.0	-1.6	-1.0	-0.8	-0.3
V5/8	1-(c-CH=CH•)-2,3-OH	0.2	2.4	-0.5	0.0	0.5	0.6	0.6	0.4	0.1
V5/9	1-(c-CH=CH•)-2-CHO-4-$CH=CH_2$	-3.9	3.4	-2.2	-1.2	-0.8	-0.5	-0.1	0.2	0.4
V5/10	1-(c-CH=CH•)-2-CHO-6-CH_3	-5.2	-4.6	-1.2	0.5	1.2	1.6	1.9	2.1	1.9
V5/11	1-(c-CH=CH•)-3-CHO-4-CH_3	0.6	1.3	0.1	-0.2	-0.8	-1.1	-1.0	-1.0	-0.7
V5/12	1-(c-CH=CH•)-2,4-$CH=CH_2$	-2.7	3.2	-2.0	-1.3	-1.3	-1.2	-0.8	-0.6	-0.4
V5/13	1-(c-CH=CH•)-2-$CH=CH_2$-4-CH_3	0.8	0.9	-0.8	-0.5	-1.1	-1.3	-1.1	-0.9	-0.5
V5/14	1-(c-CH=CH•)-2-CH_3-4-$CH=CH_2$	-3.4	4.6	0.6	-0.1	-0.8	-1.1	-1.4	-1.3	-1.2
V5/15	1-(c-CH=CH•)-2,3-CH_3	-2.7	-1.9	4.6	4.3	3.6	3.3	2.7	2.2	1.3
V6/1	1-CH_2•-2,4-$CH=CH_2$	1.3	-0.5	-0.5	-0.2	0.1	0.2	0.5	0.4	0.3
V6/2	1-CH_2•-2-$CH=CH_2$-3-CH_3	-2.8	-2.9	2.6	4.5	4.9	4.7	3.7	2.8	1.5
V6/3	1-CH_2•-2,3-CH_3	-2.7	-3.0	3.0	2.7	2.4	2.2	2.1	1.8	1.4
V6/4	1-CH_2•-2-CH_3-5-CH_2CH_3	1.3	-0.7	-0.1	0.0	0.1	0.2	0.4	0.4	0.5
V6/5	1-CH_2•-2,5-CH_2CH_3	1.6	-1.1	1.9	1.6	1.3	1.0	0.9	0.4	0.4
V6/6	1-CH_2•-3-CH_3-4-CHO	0.8	0.6	-2.0	-1.1	-0.6	-0.4	-0.2	-0.3	-0.2
V6/7	1-CH_2•-3-CH_3-4-$CH=CH_2$	-3.4	-5.1	-1.8	-0.7	0.0	0.7	1.1	1.1	0.8
V6/8	1-CH_2•-3,4-CH_3	-0.5	0.9	-2.4	-1.5	-1.1	-0.9	-0.7	-0.6	-0.4
V6/9	1-CH_2•-3,6-CH_2CH_3	1.6	-0.6	2.1	1.7	1.4	1.1	1.0	0.5	0.6
V6/10	p-(CH_3)$C_6H_5CH•CH_3$	-1.4	-0.1	0.0	0.0	-0.1	-0.1	-0.3	-0.3	-0.2

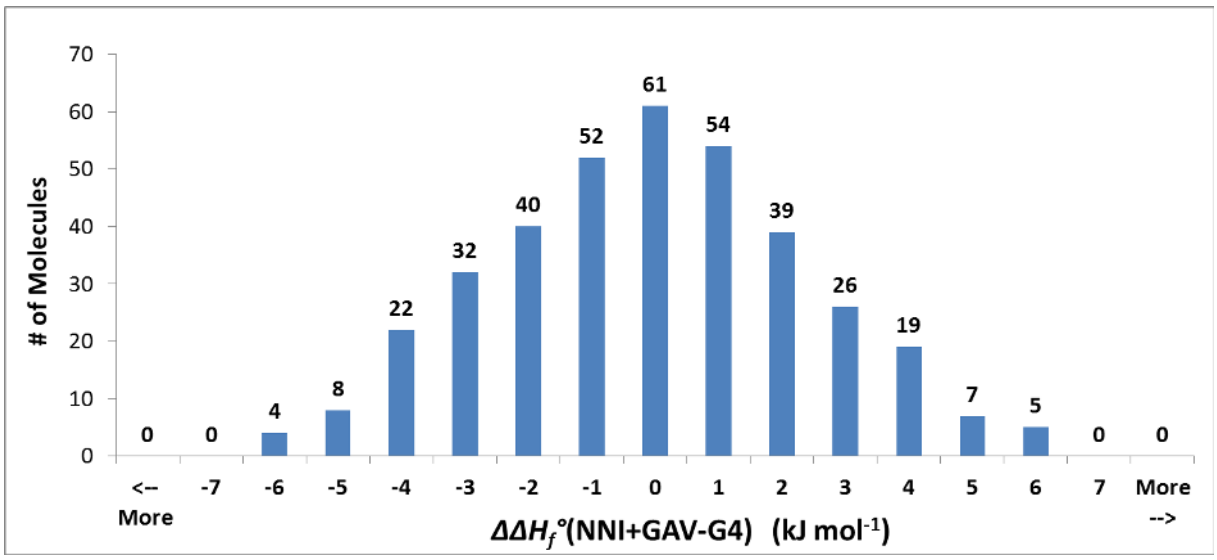


Figure S29. *Distribution of the differences between the final thermochemical data calculated with GA parameters and G4/BAC method for $\Delta_f H^\circ$ values of the MARs in the final set, $\Delta\Delta_f H°$((NNI+GAV)-G4).*

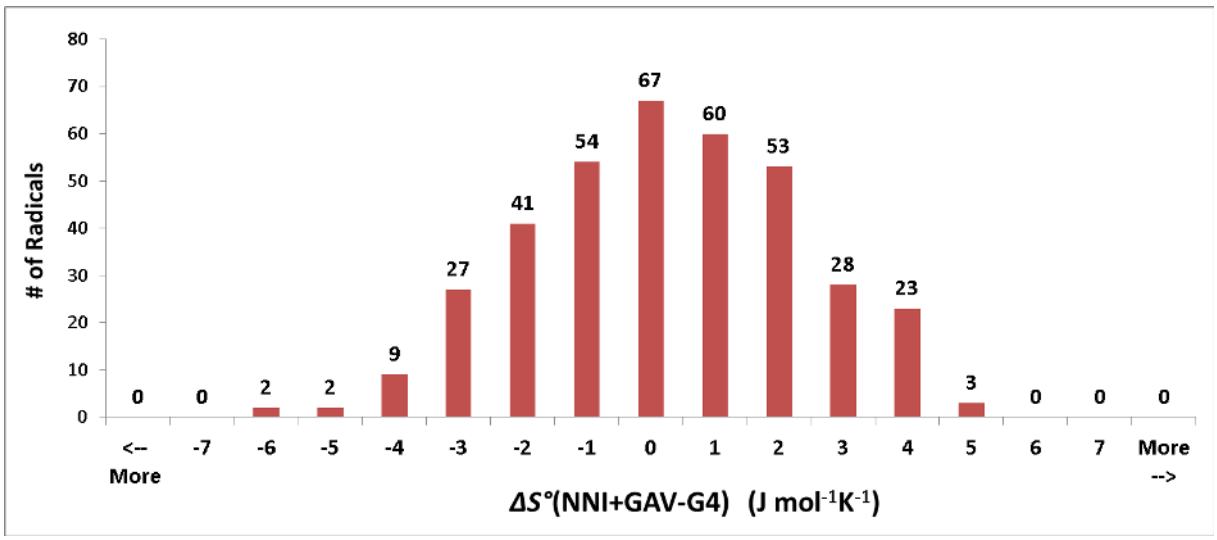


Figure S30. *Distribution of the differences between the final thermochemical data calculated with GA parameters and G4/BAC method for S° values of the MARs in the final set, $\Delta S°$((NNI+GAV)-G4).*

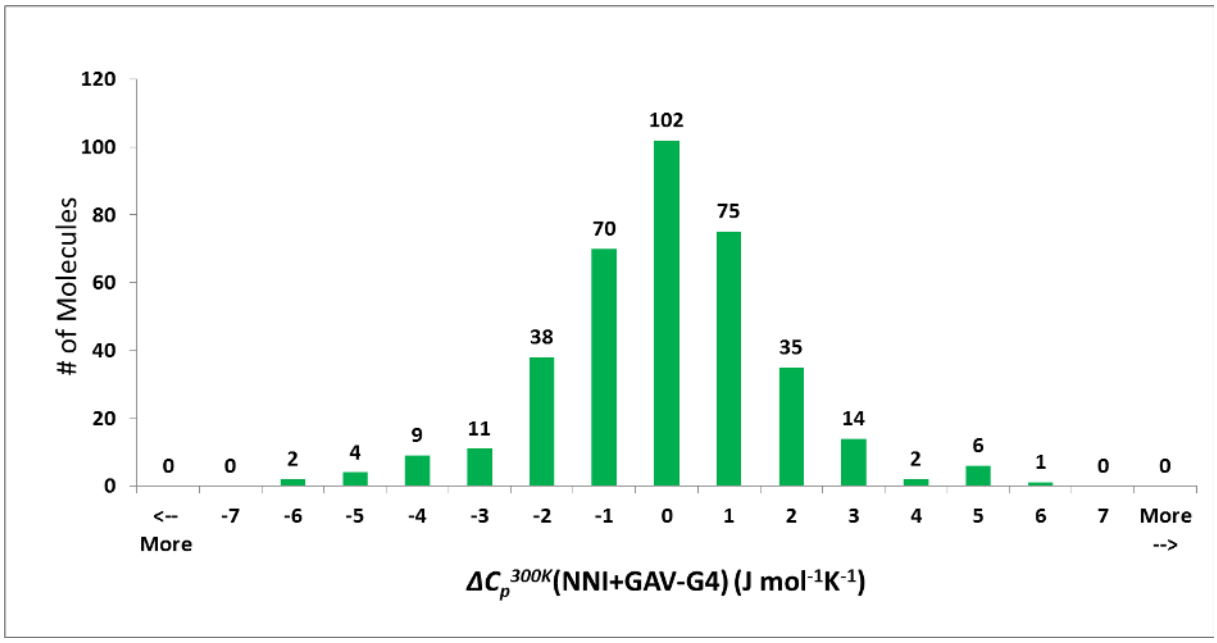


Figure S31. *Distribution of the differences between the final thermochemical data calculated with GA parameters and G4/BAC method for* C_p^{300K} *values of the MARs in the final set,* ΔC_p^{300K} *((NNI+GAV)-G4).*

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