A Conceptual DFT Study of the Molecular Properties of Glycating Carbonyl Compounds

Electronic Supporting Information

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Table S1A: HOMO and LUMO orbital energies (in eV), ionization potentials $I$ and electron affinities $A$ (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrophilization power ($\omega^-$), electrophilic power ($\omega^+$), and net electrophilicity $\Delta\omega^{\pm}$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the M11 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical $I$ and $A$.

| Property       | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega^+_K$ | $\omega^-_K$ | $\Delta\omega^{\pm}_K$ |
|----------------|------|------|----------|----------|------------|-------------|-------------|-----------------|
| Acetaldehyde   | -10.35 | 1.61 | 4.37     | 11.95    | 0.80       | 4.53        | 0.16        | 4.69            |
| Acetol         | -9.97 | 1.63 | 4.17     | 11.60    | 0.75       | 4.31        | 0.14        | 4.45            |
| Acetone        | -10.18 | 1.79 | 4.20     | 11.97    | 0.74       | 4.32        | 0.12        | 4.44            |
| Arabinose      | -10.11 | 1.31 | 4.40     | 11.42    | 0.85       | 4.61        | 0.21        | 4.82            |
| Glucose        | -9.98 | 1.19 | 4.40     | 11.17    | 0.87       | 4.63        | 0.23        | 4.86            |
| d-Glyceraldehyde | -10.49 | 1.33 | 4.58     | 11.82    | 0.89       | 4.80        | 0.22        | 5.02            |
| Glycolaldehyde | -10.47 | 1.31 | 4.58     | 11.78    | 0.89       | 4.81        | 0.23        | 5.04            |
| Glyoxal        | -10.33 | -0.62 | 5.47     | 9.71     | 1.54       | 6.43        | 0.95        | 7.38            |
| l-Glyceraldehyde | -10.49 | 1.33 | 4.58     | 11.82    | 0.89       | 4.80        | 0.22        | 5.02            |
| Methylglyoxal  | -10.20 | -0.40 | 5.30     | 9.79     | 1.43       | 6.13        | 0.83        | 6.96            |
| Ribose         | -10.16 | 1.15 | 4.50     | 11.31    | 0.90       | 4.75        | 0.25        | 5.00            |

| Property       | $I$   | $A$   | $\chi$   | $\eta$   | $\omega$   | $\omega^-$ | $\omega^+$ | $\Delta\omega^{\pm}$ |
|----------------|------|------|----------|----------|------------|------------|------------|-----------------|
| Acetaldehyde   | 7.39 | 1.31 | 4.35     | 6.08     | 1.56       | 5.67       | 1.32       | 6.99            |
| Acetol         | 7.23 | 1.16 | 4.19     | 6.07     | 1.45       | 5.37       | 1.18       | 6.55            |
| Acetone        | 7.23 | 1.01 | 4.12     | 6.21     | 1.37       | 5.18       | 1.06       | 6.24            |
| Arabinose      | 7.53 | 1.55 | 4.54     | 5.98     | 1.72       | 6.09       | 1.55       | 7.64            |
| Glucose        | 7.57 | 1.66 | 4.61     | 5.91     | 1.80       | 6.28       | 1.66       | 7.94            |
| d-Glyceraldehyde | 7.63 | 1.54 | 4.58     | 6.09     | 1.72       | 6.12       | 1.54       | 7.66            |
| Glycolaldehyde | 7.58 | 1.58 | 4.58     | 5.99     | 1.75       | 6.17       | 1.59       | 7.75            |
| Glyoxal        | 7.75 | 3.35 | 5.55     | 4.40     | 3.50       | 10.05      | 4.50       | 14.55           |
| l-Glyceraldehyde | 7.63 | 1.54 | 4.58     | 6.09     | 1.72       | 6.12       | 1.54       | 7.66            |
| Methylglyoxal  | 7.55 | 3.14 | 5.34     | 4.42     | 3.23       | 9.41       | 4.07       | 13.48           |
| Ribose         | 7.77 | 1.68 | 4.73     | 6.08     | 1.83       | 6.41       | 1.69       | 8.10            |
Table S1B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_{\chi}$, $J_{\eta}$, $J_{\omega}$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega^\pm}$ and $J_{D2}$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S1A

|                | $J_I$ | $J_A$ | $J_{HL}$ | $J_{\chi}$ | $J_{\eta}$ | $J_{\omega}$ | $J_{D1}$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta\omega^\pm}$ | $J_{D2}$ |
|----------------|-------|-------|----------|------------|------------|-------------|----------|----------------|----------------|--------------------------|--------|
| Acetaldehyde   | 2.96  | 2.92  | 4.16     | 0.02       | 5.88       | 0.76        | 5.93     | 1.14           | 1.16           | 2.30                     | 2.82   |
| Acetol         | 2.75  | 2.79  | 3.91     | 0.02       | 5.53       | 0.70        | 5.58     | 1.06           | 1.04           | 2.10                     | 2.57   |
| Acetone        | 2.96  | 2.80  | 4.07     | 0.08       | 5.76       | 0.63        | 5.79     | 0.86           | 0.94           | 1.80                     | 2.20   |
| Arabinose      | 2.59  | 2.86  | 3.85     | 0.14       | 5.44       | 0.87        | 5.51     | 1.48           | 1.34           | 2.82                     | 3.45   |
| Glucose        | 2.41  | 2.85  | 3.73     | 0.22       | 5.26       | 0.94        | 5.35     | 1.65           | 1.43           | 3.09                     | 3.78   |
| d-Glyceraldehyde| 2.85  | 2.87  | 4.05     | 0.01       | 5.72       | 0.84        | 5.78     | 1.32           | 1.31           | 2.63                     | 3.22   |
| Glycolaldehyde | 2.90  | 2.89  | 4.09     | 0.00       | 5.79       | 0.86        | 5.85     | 1.35           | 1.36           | 2.71                     | 3.32   |
| Glyoxal        | 2.58  | 2.73  | 3.76     | 0.07       | 5.32       | 1.96        | 5.67     | 3.62           | 3.55           | 7.17                     | 8.78   |
| l-Glyceraldehyde| 2.85  | 2.87  | 4.05     | 0.01       | 5.72       | 0.84        | 5.78     | 1.32           | 1.31           | 2.63                     | 3.22   |
| Methylglyoxal  | 2.65  | 2.73  | 3.80     | 0.04       | 5.38       | 1.80        | 5.67     | 3.28           | 3.24           | 6.52                     | 7.99   |
| Ribose         | 2.39  | 2.84  | 3.71     | 0.22       | 5.23       | 0.94        | 5.32     | 1.66           | 1.44           | 3.10                     | 3.80   |
| Average        | 2.72  | 2.83  | 3.93     | 0.08       | 5.55       | 1.01        | 5.66     | 1.70           | 1.65           | 3.35                     | 4.11   |
Table S2A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the M11L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical I and A.

| Property          | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega^+_K$ | $\omega^-_K$ | $\Delta\omega^\pm_K$ |
|-------------------|------|------|----------|----------|------------|--------------|--------------|---------------------|
| Acetaldehyde      | -6.65| -1.49| 4.07     | 5.16     | 1.60       | 5.56         | 1.50         | 7.06                |
| Acetol            | -6.33| -1.38| 3.86     | 4.95     | 1.50       | 5.24         | 1.38         | 6.62                |
| Acetone           | -6.55| -1.25| 3.90     | 5.31     | 1.43       | 5.15         | 1.25         | 6.39                |
| Arabinose         | -6.43| -1.72| 4.08     | 4.71     | 1.77       | 5.87         | 1.79         | 7.65                |
| Glucose           | -6.39| -1.86| 4.13     | 4.53     | 1.88       | 6.10         | 1.98         | 8.08                |
| d-Glyceraldehyde  | -6.71| -1.75| 4.23     | 4.96     | 1.80       | 6.03         | 1.80         | 7.83                |
| Glycolaldehyde    | -6.73| -1.79| 4.26     | 4.94     | 1.84       | 6.11         | 1.85         | 7.96                |
| Glyoxal           | -6.59| -3.73| 5.16     | 2.86     | 4.66       | 12.07        | 6.91         | 18.99               |
| l-Glyceraldehyde  | -6.71| -1.75| 4.23     | 4.96     | 1.80       | 6.03         | 1.80         | 7.83                |
| Methylglyoxal     | -6.48| -3.42| 4.95     | 3.06     | 4.00       | 10.67        | 5.72         | 16.39               |
| Ribose            | -6.53| -1.87| 4.20     | 4.66     | 1.90       | 6.19         | 1.98         | 8.17                |

| Property          | I    | A    | $\chi$ | $\eta$ | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta\omega^\pm$ |
|-------------------|------|------|--------|--------|----------|------------|------------|---------------------|
| Acetaldehyde      | 7.15 | 1.21 | 4.18   | 5.94   | 1.47     | 5.40       | 1.22       | 6.62                |
| Acetol            | 6.82 | 1.11 | 3.97   | 5.71   | 1.38     | 5.10       | 1.13       | 6.22                |
| Acetone           | 7.01 | 0.97 | 3.99   | 6.04   | 1.32     | 5.01       | 1.02       | 6.04                |
| Arabinose         | 6.82 | 1.45 | 4.14   | 5.37   | 1.59     | 5.59       | 1.45       | 7.04                |
| Glucose           | 6.74 | 1.56 | 4.15   | 5.18   | 1.66     | 5.72       | 1.58       | 7.30                |
| d-Glyceraldehyde  | 7.16 | 1.44 | 4.30   | 5.72   | 1.62     | 5.75       | 1.44       | 7.19                |
| Glycolaldehyde    | 7.26 | 1.51 | 4.39   | 5.75   | 1.67     | 5.90       | 1.51       | 7.41                |
| Glyoxal           | 7.16 | 3.32 | 5.24   | 3.84   | 3.58     | 10.01      | 4.77       | 14.79               |
| l-Glyceraldehyde  | 7.16 | 1.44 | 4.30   | 5.72   | 1.62     | 5.75       | 1.44       | 7.19                |
| Methylglyoxal     | 7.03 | 3.04 | 5.03   | 3.98   | 3.18     | 9.12       | 4.09       | 13.21               |
| Ribose            | 6.88 | 1.59 | 4.23   | 5.29   | 1.69     | 5.83       | 1.60       | 7.43                |
Table S2B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_X$, $J_\eta$, $J_{\omega}$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega^\pm}$ and $J_D$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S2A.

|                  | $J_I$ | $J_A$ | $J_{HL}$ | $J_X$ | $J_\eta$ | $J_{\omega}$ | $J_{D1}$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta\omega^\pm}$ | $J_D$ |
|------------------|-------|-------|----------|-------|----------|-------------|----------|----------------|----------------|---------------------|-------|
| Acetaldehyde     | 0.51  | 0.28  | 0.58     | 0.11  | 0.79     | 0.13        | 0.81     | 0.16           | 0.27           | 0.44                | 0.54  |
| Acetol           | 0.49  | 0.27  | 0.56     | 0.11  | 0.75     | 0.12        | 0.77     | 0.14           | 0.25           | 0.40                | 0.49  |
| Acetone          | 0.46  | 0.27  | 0.54     | 0.09  | 0.73     | 0.11        | 0.75     | 0.13           | 0.23           | 0.36                | 0.44  |
| Arabinose        | 0.39  | 0.27  | 0.47     | 0.06  | 0.66     | 0.17        | 0.69     | 0.28           | 0.33           | 0.61                | 0.75  |
| Glucose          | 0.35  | 0.30  | 0.46     | 0.02  | 0.64     | 0.22        | 0.68     | 0.38           | 0.40           | 0.78                | 0.96  |
| d-Glyceraldehyde | 0.45  | 0.30  | 0.55     | 0.07  | 0.76     | 0.18        | 0.78     | 0.28           | 0.36           | 0.64                | 0.78  |
| Glycolaldehyde   | 0.53  | 0.28  | 0.59     | 0.13  | 0.80     | 0.16        | 0.83     | 0.21           | 0.34           | 0.55                | 0.68  |
| Glyoxal          | 0.57  | 0.41  | 0.70     | 0.08  | 0.98     | 1.08        | 1.46     | 2.06           | 2.14           | 4.20                | 5.14  |
| l-Glyceraldehyde | 0.45  | 0.30  | 0.55     | 0.07  | 0.76     | 0.18        | 0.78     | 0.28           | 0.36           | 0.64                | 0.78  |
| Methylglyoxal    | 0.55  | 0.38  | 0.67     | 0.08  | 0.93     | 0.82        | 1.24     | 1.55           | 1.63           | 3.18                | 3.89  |
| Ribose           | 0.35  | 0.29  | 0.45     | 0.03  | 0.64     | 0.20        | 0.67     | 0.35           | 0.38           | 0.73                | 0.90  |
| Average          | 0.46  | 0.30  | 0.56     | 0.08  | 0.77     | 0.31        | 0.86     | 0.53           | 0.61           | 1.14                | 1.40  |
Table S3A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the MN12L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical I and A.

| Property         | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega^+_K$ | $\omega^-_K$ | $\Delta\omega^\pm_K$ |
|------------------|------|------|----------|----------|------------|-------------|--------------|---------------------|
| Acetaldehyde     | -6.60| -1.15| 3.88     | 5.45     | 1.38       | 5.04        | 1.16         | 6.20                |
| Acetol           | -6.24| -1.06| 3.65     | 5.18     | 1.29       | 4.72        | 1.07         | 5.79                |
| Acetone          | -6.46| -0.93| 3.69     | 5.53     | 1.23       | 4.66        | 0.96         | 5.62                |
| Arabinose        | -6.37| -1.39| 3.88     | 4.97     | 1.51       | 5.27        | 1.40         | 6.67                |
| Glucose          | -6.25| -1.49| 3.87     | 4.76     | 1.57       | 5.38        | 1.51         | 6.89                |
| d-Glyceraldehyde | -6.71| -1.40| 4.05     | 5.31     | 1.55       | 5.45        | 1.40         | 6.85                |
| Glycolaldehyde   | -6.70| -1.44| 4.07     | 5.26     | 1.58       | 5.52        | 1.45         | 6.97                |
| Glyoxal          | -6.62| -3.44| 5.03     | 3.17     | 3.99       | 10.68       | 5.65         | 16.34               |
| l-Glyceraldehyde | -6.71| -1.40| 4.05     | 5.31     | 1.55       | 5.45        | 1.40         | 6.85                |
| Methylglyoxal    | -6.49| -3.17| 4.83     | 3.32     | 3.51       | 9.65        | 4.82         | 14.47               |
| Ribose           | -6.40| -1.50| 3.95     | 4.89     | 1.59       | 5.47        | 1.52         | 6.99                |

| Property         | I    | A    | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$   | $\Delta\omega^\pm$ |
|------------------|------|------|---------|---------|----------|------------|--------------|---------------------|
| Acetaldehyde     | 6.96 | 0.92 | 3.94    | 6.04    | 1.28     | 4.92       | 0.98         | 5.89                |
| Acetol           | 6.62 | 0.79 | 3.70    | 5.83    | 1.18     | 4.57       | 0.87         | 5.44                |
| Acetone          | 6.78 | 0.65 | 3.71    | 6.14    | 1.12     | 4.49       | 0.77         | 5.26                |
| Arabinose        | 6.69 | 1.17 | 3.93    | 5.51    | 1.40     | 5.11       | 1.18         | 6.29                |
| Glucose          | 6.59 | 1.25 | 3.92    | 5.34    | 1.44     | 5.17       | 1.25         | 6.43                |
| d-Glyceraldehyde | 7.05 | 1.16 | 4.10    | 5.89    | 1.43     | 5.28       | 1.18         | 6.46                |
| Glycolaldehyde   | 7.09 | 1.23 | 4.16    | 5.87    | 1.47     | 5.40       | 1.24         | 6.63                |
| Glyoxal          | 7.11 | 3.07 | 5.09    | 4.04    | 3.21     | 9.22       | 4.13         | 13.35               |
| l-Glyceraldehyde | 7.05 | 1.16 | 4.10    | 5.89    | 1.43     | 5.28       | 1.18         | 6.46                |
| Methylglyoxal    | 6.96 | 2.83 | 4.89    | 4.13    | 2.90     | 8.50       | 3.60         | 12.10               |
| Ribose           | 6.73 | 1.28 | 4.01    | 5.45    | 1.47     | 5.29       | 1.28         | 6.57                |
Table S3B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_X$, $J_\eta$, $J_\omega$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega^\pm}$ and $J_D$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S3A.

|                  | $J_I$ | $J_A$ | $J_{HL}$ | $J_X$ | $J_\eta$ | $J_\omega$ | $J_{D1}$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta\omega^\pm}$ | $J_D$ |
|------------------|-------|-------|----------|-------|----------|------------|----------|----------------|----------------|------------------|-------|
| Acetaldehyde     | 0.36  | 0.23  | 0.43     | 0.06  | 0.59     | 0.09       | 0.60     | 0.12           | 0.18           | 0.30             | 0.37  |
| Acetol           | 0.38  | 0.27  | 0.47     | 0.06  | 0.65     | 0.11       | 0.66     | 0.15           | 0.20           | 0.35             | 0.43  |
| Acetone          | 0.32  | 0.28  | 0.43     | 0.02  | 0.60     | 0.11       | 0.61     | 0.17           | 0.19           | 0.36             | 0.44  |
| Arabinose        | 0.32  | 0.22  | 0.39     | 0.05  | 0.54     | 0.11       | 0.55     | 0.16           | 0.21           | 0.38             | 0.46  |
| Glucose          | 0.34  | 0.24  | 0.41     | 0.05  | 0.58     | 0.14       | 0.60     | 0.21           | 0.26           | 0.47             | 0.58  |
| d-Glyceraldehyde | 0.34  | 0.24  | 0.42     | 0.05  | 0.58     | 0.12       | 0.60     | 0.17           | 0.22           | 0.39             | 0.48  |
| Glycolaldehyde   | 0.39  | 0.22  | 0.45     | 0.09  | 0.61     | 0.10       | 0.62     | 0.12           | 0.21           | 0.33             | 0.41  |
| Glyoxal          | 0.50  | 0.37  | 0.62     | 0.07  | 0.87     | 0.77       | 1.16     | 1.46           | 1.53           | 2.99             | 3.66  |
| l-Glyceraldehyde | 0.34  | 0.24  | 0.42     | 0.05  | 0.58     | 0.12       | 0.60     | 0.17           | 0.22           | 0.39             | 0.48  |
| Methylglyoxal    | 0.47  | 0.34  | 0.58     | 0.06  | 0.81     | 0.62       | 1.02     | 1.15           | 1.22           | 2.37             | 2.90  |
| Ribose           | 0.34  | 0.22  | 0.40     | 0.06  | 0.56     | 0.12       | 0.57     | 0.18           | 0.24           | 0.42             | 0.51  |
| Average          | 0.37  | 0.26  | 0.46     | 0.06  | 0.63     | 0.22       | 0.69     | 0.37           | 0.43           | 0.80             | 0.98  |
Table S4A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electron donating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the MN12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical I and A.

| Property              | HOMO  | LUMO  | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega_K^+$ | $\Delta\omega_K^\pm$ |
|-----------------------|-------|-------|----------|----------|------------|---------------|---------------------|
| Acetaldehyde          | -7.52 | -0.94 | 4.23     | 6.58     | 1.36       | 5.25          | 1.02 6.27          |
| Acetol                | -7.14 | -0.90 | 4.02     | 6.24     | 1.29       | 4.98          | 0.97 5.95          |
| Acetone               | -7.37 | -0.75 | 4.06     | 6.63     | 1.24       | 4.93          | 0.87 5.81          |
| Arabinose             | -7.25 | -1.20 | 4.22     | 6.06     | 1.47       | 5.44          | 1.21 6.65          |
| Glucose               | -7.14 | -1.29 | 4.21     | 5.85     | 1.52       | 5.50          | 1.29 6.80          |
| d-Glyceraldehyde      | -7.62 | -1.19 | 4.40     | 6.43     | 1.51       | 5.62          | 1.22 6.84          |
| Glycolaldehyde        | -7.61 | -1.25 | 4.43     | 6.36     | 1.54       | 5.70          | 1.27 6.97          |
| Glyoxal               | -7.51 | -3.14 | 5.32     | 4.37     | 3.24       | 9.41          | 4.09 13.50         |
| l-Glyceraldehyde      | -7.62 | -1.19 | 4.40     | 6.43     | 1.51       | 5.62          | 1.22 6.84          |
| Methylglyoxal         | -7.37 | -2.90 | 5.13     | 4.47     | 2.95       | 8.74          | 3.61 12.34         |
| Ribose                | -7.28 | -1.32 | 4.30     | 5.95     | 1.55       | 5.63          | 1.33 6.96          |

| Property              | I     | A     | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta\omega^\pm$ |
|-----------------------|-------|-------|----------|----------|----------|------------|------------|---------------------|
| Acetaldehyde          | 7.21  | 1.17  | 4.19     | 6.04     | 1.45     | 5.37       | 1.19       | 6.56               |
| Acetol                | 6.96  | 1.06  | 4.01     | 5.90     | 1.36     | 5.09       | 1.09       | 6.18               |
| Acetone               | 7.04  | 0.92  | 3.98     | 6.12     | 1.29     | 4.96       | 0.98       | 5.93               |
| Arabinose             | 7.17  | 1.40  | 4.29     | 5.78     | 1.59     | 5.68       | 1.40       | 7.08               |
| Glucose               | 7.09  | 1.49  | 4.29     | 5.61     | 1.64     | 5.78       | 1.49       | 7.26               |
| d-Glyceraldehyde      | 7.37  | 1.39  | 4.38     | 5.98     | 1.60     | 5.77       | 1.39       | 7.17               |
| Glycolaldehyde        | 7.35  | 1.45  | 4.40     | 5.89     | 1.64     | 5.85       | 1.45       | 7.31               |
| Glyoxal               | 7.46  | 3.24  | 5.35     | 4.22     | 3.40     | 9.73       | 4.38       | 14.11              |
| l-Glyceraldehyde      | 7.37  | 1.39  | 4.38     | 5.98     | 1.60     | 5.77       | 1.39       | 7.17               |
| Methylglyoxal         | 7.29  | 3.01  | 5.15     | 4.28     | 3.10     | 9.04       | 3.89       | 12.93              |
| Ribose                | 7.23  | 1.52  | 4.38     | 5.72     | 1.67     | 5.89       | 1.52       | 7.41               |
Table S4B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_X$, $J_\eta$, $J_\omega$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega}^\pm$ and $J_{D2}$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S4A

|                      | $J_I$ | $J_A$ | $J_{HL}$ | $J_X$ | $J_\eta$ | $J_\omega$ | $J_{D1}$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta\omega}^\pm$ | $J_{D2}$ |
|----------------------|-------|-------|----------|-------|----------|------------|----------|----------------|----------------|---------------------|----------|
| Acetaldehyde         | 0.32  | 0.22  | 0.39     | 0.05  | 0.54     | 0.09       | 0.55     | 0.12           | 0.17           | 0.29                | 0.36     |
| Acetol               | 0.18  | 0.16  | 0.24     | 0.01  | 0.35     | 0.07       | 0.35     | 0.11           | 0.12           | 0.23                | 0.28     |
| Acetone              | 0.33  | 0.17  | 0.37     | 0.08  | 0.50     | 0.05       | 0.51     | 0.02           | 0.11           | 0.13                | 0.17     |
| Arabinose            | 0.08  | 0.20  | 0.22     | 0.06  | 0.28     | 0.12       | 0.31     | 0.25           | 0.19           | 0.43                | 0.53     |
| Glucose              | 0.04  | 0.20  | 0.20     | 0.08  | 0.24     | 0.12       | 0.28     | 0.27           | 0.19           | 0.47                | 0.57     |
| d-Glyceraldehyde     | 0.24  | 0.20  | 0.31     | 0.02  | 0.44     | 0.10       | 0.45     | 0.15           | 0.17           | 0.33                | 0.40     |
| Glycolaldehyde       | 0.27  | 0.20  | 0.33     | 0.03  | 0.47     | 0.10       | 0.48     | 0.15           | 0.18           | 0.34                | 0.41     |
| Glyoxal              | 0.04  | 0.11  | 0.12     | 0.03  | 0.15     | 0.16       | 0.22     | 0.32           | 0.29           | 0.61                | 0.75     |
| l-Glyceraldehyde     | 0.24  | 0.20  | 0.31     | 0.02  | 0.44     | 0.10       | 0.45     | 0.15           | 0.17           | 0.33                | 0.40     |
| Methylglyoxal        | 0.07  | 0.11  | 0.13     | 0.02  | 0.18     | 0.15       | 0.24     | 0.31           | 0.28           | 0.59                | 0.72     |
| Ribose               | 0.04  | 0.19  | 0.20     | 0.07  | 0.24     | 0.12       | 0.28     | 0.26           | 0.19           | 0.45                | 0.56     |
| Average              | 0.17  | 0.18  | 0.26     | 0.04  | 0.35     | 0.11       | 0.37     | 0.19           | 0.19           | 0.38                | 0.47     |
Table S5A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the N12 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical I and A.

| Property         | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega_K^-$ | $\omega_K^+$ | $\Delta\omega_K^\pm$ |
|------------------|------|------|----------|----------|------------|--------------|--------------|-------------------|
| Acetaldehyde     | -6.01| -1.66| 3.84     | 4.34     | 1.69       | 5.58         | 1.74         | 7.32              |
| Acetol           | -5.70| -1.52| 3.61     | 4.17     | 1.56       | 5.19         | 1.58         | 6.77              |
| Acetone          | -5.84| -1.40| 3.62     | 4.44     | 1.47       | 5.03         | 1.41         | 6.44              |
| Arabinose        | -5.87| -1.87| 3.87     | 4.00     | 1.87       | 5.94         | 2.06         | 8.00              |
| Glucose          | -5.76| -2.07| 3.91     | 3.70     | 2.07       | 6.33         | 2.42         | 8.75              |
| d-Glyceraldehyde | -6.10| -1.88| 3.99     | 4.22     | 1.89       | 6.03         | 2.04         | 8.08              |
| Glycolaldehyde   | -6.14| -1.93| 4.03     | 4.21     | 1.93       | 6.14         | 2.11         | 8.25              |
| Glyoxal          | -6.12| -3.89| 5.01     | 2.23     | 5.62       | 13.89        | 8.88         | 22.77             |
| l-Glyceraldehyde | -6.10| -1.88| 3.99     | 4.22     | 1.89       | 6.03         | 2.04         | 8.08              |
| Methylglyoxal    | -5.96| -3.57| 4.77     | 3.76     | 4.76       | 12.05        | 7.28         | 19.33             |

| Property         | I    | A    | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta\omega^\pm$ |
|------------------|------|------|---------|---------|----------|------------|------------|-------------------|
| Acetaldehyde     | 6.90 | 0.99 | 3.95    | 5.91    | 1.32     | 4.97       | 1.03       | 6.00              |
| Acetol           | 6.38 | 0.88 | 3.63    | 5.50    | 1.20     | 4.55       | 0.92       | 5.47              |
| Acetone          | 6.69 | 0.74 | 3.71    | 5.95    | 1.16     | 4.55       | 0.83       | 5.38              |
| Arabinose        | 6.31 | 1.20 | 3.76    | 5.11    | 1.38     | 4.96       | 1.20       | 6.16              |
| Glucose          | 6.16 | 1.37 | 3.76    | 4.79    | 1.48     | 5.14       | 1.38       | 6.51              |
| d-Glyceraldehyde | 6.71 | 1.20 | 3.95    | 5.52    | 1.42     | 5.16       | 1.20       | 6.36              |
| Glycolaldehyde   | 6.94 | 1.27 | 4.11    | 5.66    | 1.49     | 5.38       | 1.28       | 6.66              |
| Glyoxal          | 6.87 | 3.23 | 5.05    | 3.64    | 3.50     | 9.76       | 4.71       | 14.47             |
| l-Glyceraldehyde | 6.71 | 1.20 | 3.95    | 5.52    | 1.42     | 5.16       | 1.20       | 6.36              |
| Methylglyoxal    | 6.66 | 2.94 | 4.80    | 3.72    | 3.10     | 8.84       | 4.03       | 12.87             |
| Ribose           | 6.35 | 1.41 | 3.88    | 4.94    | 1.52     | 5.29       | 1.41       | 6.71              |
Table S5B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_\chi$, $J_\eta$, $J_\omega$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega^\pm}$ and $J_{D2}$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S5A.

|                   | $J_I$ | $J_A$ | $J_{HL}$ | $J_\chi$ | $J_\eta$ | $J_\omega$ | $J_{D1}$ | $J_{\omega^-}$ | $J_{\omega^+}$ | $J_{\Delta\omega^\pm}$ | $J_{D2}$ |
|-------------------|-------|-------|----------|----------|----------|------------|----------|----------------|----------------|------------------------|--------|
| Acetaldehyde      | 0.90  | 0.68  | 1.12     | 0.11     | 1.57     | 0.38       | 1.62     | 0.60           | 0.71           | 1.32                   | 1.61   |
| Acetol            | 0.68  | 0.65  | 0.94     | 0.02     | 1.32     | 0.37       | 1.37     | 0.64           | 0.66           | 1.30                   | 1.59   |
| Acetone           | 0.86  | 0.66  | 1.08     | 0.10     | 1.51     | 0.31       | 1.55     | 0.48           | 0.58           | 1.06                   | 1.31   |
| Arabinose         | 0.44  | 0.67  | 0.80     | 0.12     | 1.11     | 0.49       | 1.22     | 0.98           | 0.86           | 1.84                   | 2.25   |
| Glucose           | 0.40  | 0.70  | 0.80     | 0.15     | 1.09     | 0.59       | 1.25     | 1.19           | 1.04           | 2.24                   | 2.74   |
| d-Glyceraldehyde  | 0.61  | 0.69  | 0.92     | 0.04     | 1.30     | 0.47       | 1.38     | 0.88           | 0.84           | 1.72                   | 2.11   |
| Glycolaldehyde    | 0.80  | 0.65  | 1.03     | 0.07     | 1.45     | 0.44       | 1.52     | 0.76           | 0.83           | 1.59                   | 1.95   |
| Glyoxal           | 0.74  | 0.66  | 1.00     | 0.04     | 1.41     | 2.12       | 2.55     | 4.13           | 4.17           | 8.31                   | 10.17  |
| l-Glyceraldehyde  | 0.61  | 0.69  | 0.92     | 0.04     | 1.30     | 0.47       | 1.38     | 0.88           | 0.84           | 1.72                   | 2.11   |
| Methylglyoxal     | 0.70  | 0.63  | 0.94     | 0.04     | 1.33     | 1.66       | 2.13     | 3.21           | 3.25           | 6.47                   | 7.92   |
| Ribose            | 0.40  | 0.68  | 0.79     | 0.14     | 1.08     | 0.57       | 1.23     | 1.13           | 1.00           | 2.13                   | 2.61   |
| Average           | 0.65  | 0.67  | 0.94     | 0.08     | 1.32     | 0.72       | 1.56     | 1.35           | 1.34           | 2.70                   | 3.31   |
Table S6A: HOMO and LUMO orbital energies (in eV), ionization potentials $I$ and electron affinities $A$ (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta \omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the N12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical $I$ and $A$.

| Property         | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega^-_K$ | $\omega^+_K$ | $\Delta \omega^\pm_K$ |
|------------------|------|------|----------|----------|------------|--------------|--------------|----------------------|
| Acetaldehyde     | -7.21| -0.98| 4.10     | 6.23     | 1.35       | 5.13         | 1.03         | 6.16                 |
| Acetol           | -6.88| -0.89| 3.88     | 5.99     | 1.26       | 4.83         | 0.95         | 5.78                 |
| Acetone          | -7.05| -0.73| 3.89     | 6.31     | 1.20       | 4.74         | 0.85         | 5.59                 |
| Arabinose        | -7.04| -1.22| 4.13     | 5.82     | 1.47       | 5.36         | 1.23         | 6.60                 |
| Glucose          | -6.91| -1.36| 4.14     | 5.55     | 1.54       | 5.50         | 1.36         | 6.86                 |
| d-Glyceraldehyde | -7.33| -1.22| 4.28     | 6.11     | 1.50       | 5.52         | 1.24         | 6.75                 |
| Glycolaldehyde   | -7.34| -1.27| 4.30     | 6.08     | 1.52       | 5.58         | 1.28         | 6.86                 |
| Glyoxal          | -7.31| -3.27| 5.29     | 4.04     | 3.46       | 9.81         | 4.53         | 14.34                |
| l-Glyceraldehyde | -7.33| -1.22| 4.28     | 6.11     | 1.50       | 5.52         | 1.24         | 6.75                 |
| Methylglyoxal    | -7.15| -3.00| 5.07     | 4.15     | 3.10       | 9.00         | 3.93         | 12.93                |
| Ribose           | -7.09| -1.40| 4.25     | 5.70     | 1.58       | 5.64         | 1.40         | 7.04                 |

| Property         | I    | A    | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta \omega^\pm$ |
|------------------|------|------|----------|----------|----------|------------|------------|----------------------|
| Acetaldehyde     | 7.12 | 1.16 | 4.14     | 5.96     | 1.44     | 5.32       | 1.18       | 6.50                 |
| Acetol           | 6.83 | 1.03 | 3.93     | 5.81     | 1.33     | 4.98       | 1.06       | 6.04                 |
| Acetone          | 6.93 | 0.88 | 3.90     | 6.05     | 1.26     | 4.84       | 0.94       | 5.79                 |
| Arabinose        | 7.03 | 1.37 | 4.20     | 5.66     | 1.56     | 5.57       | 1.37       | 6.94                 |
| Glucose          | 6.91 | 1.50 | 4.20     | 5.40     | 1.64     | 5.71       | 1.51       | 7.22                 |
| d-Glyceraldehyde | 7.28 | 1.37 | 4.33     | 5.91     | 1.58     | 5.70       | 1.37       | 7.07                 |
| Glycolaldehyde   | 7.28 | 1.44 | 4.36     | 5.83     | 1.63     | 5.80       | 1.44       | 7.24                 |
| Glyoxal          | 7.37 | 3.33 | 5.35     | 4.04     | 3.54     | 10.0       | 14.67      | 14.68                |
| l-Glyceraldehyde | 7.28 | 1.37 | 4.33     | 5.91     | 1.58     | 5.70       | 1.37       | 7.07                 |
| Methylglyoxal    | 7.17 | 3.08 | 5.12     | 4.10     | 3.20     | 7.23       | 4.10       | 13.33                |
| Ribose           | 7.09 | 1.54 | 4.31     | 5.56     | 1.68     | 5.86       | 1.54       | 7.40                 |
Table S6B: Descriptors $J_I$, $J_A$, $J_{HL}$, $J_\chi$, $J_\eta$, $J_\omega$, $J_{D1}$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta \omega^\pm}$ and $J_{D2}$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S6A.

|                | $J_I$ | $J_A$ | $J_{HL}$ | $J_\chi$ | $J_\eta$ | $J_\omega$ | $J_{D1}$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta \omega^\pm}$ | $J_{D2}$ |
|----------------|-------|-------|----------|----------|----------|------------|----------|----------------|----------------|--------------------------|----------|
| Acetaldehyde   | 0.09  | 0.18  | 0.20     | 0.04     | 0.28     | 0.09       | 0.19     | 0.15           | 0.33           | 0.41                     |
| Acetol         | 0.05  | 0.14  | 0.15     | 0.05     | 0.19     | 0.07       | 0.20     | 0.15           | 0.11           | 0.26                     | 0.32     |
| Acetone        | 0.12  | 0.14  | 0.18     | 0.01     | 0.26     | 0.06       | 0.27     | 0.11           | 0.10           | 0.20                     | 0.25     |
| Arabinose      | 0.01  | 0.15  | 0.15     | 0.07     | 0.16     | 0.09       | 0.20     | 0.21           | 0.14           | 0.35                     | 0.43     |
| Glucose        | 0.01  | 0.14  | 0.14     | 0.07     | 0.15     | 0.09       | 0.19     | 0.21           | 0.15           | 0.36                     | 0.44     |
| d-Glyceraldehyde| 0.05  | 0.15  | 0.16     | 0.05     | 0.20     | 0.09       | 0.22     | 0.18           | 0.14           | 0.32                     | 0.39     |
| Glycolaldehyde | 0.07  | 0.18  | 0.19     | 0.05     | 0.24     | 0.10       | 0.27     | 0.22           | 0.16           | 0.38                     | 0.47     |
| Glyoxal        | 0.06  | 0.06  | 0.09     | 0.06     | 0.00     | 0.08       | 0.10     | 0.20           | 0.14           | 0.34                     | 0.42     |
| l-Glyceraldehyde| 0.05  | 0.15  | 0.16     | 0.05     | 0.20     | 0.09       | 0.22     | 0.18           | 0.14           | 0.32                     | 0.39     |
| Methylglyoxal  | 0.02  | 0.08  | 0.08     | 0.05     | 0.06     | 0.10       | 0.13     | 0.23           | 0.18           | 0.40                     | 0.49     |
| Ribose         | 0.00  | 0.14  | 0.14     | 0.07     | 0.14     | 0.09       | 0.18     | 0.21           | 0.14           | 0.36                     | 0.44     |
| Average        | 0.05  | 0.14  | 0.15     | 0.05     | 0.17     | 0.09       | 0.21     | 0.19           | 0.14           | 0.33                     | 0.41     |
Table S7A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^{\pm}$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the SOGGA11 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical I and A.

| Property         | HOMO  | LUMO  | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega_K^-$ | $\omega_K^+$ | $\Delta\omega_K^{\pm}$ |
|------------------|-------|-------|----------|----------|------------|--------------|--------------|---------------------|
| Acetaldehyde     | -5.98 | -1.86 | 3.92     | 4.12     | 1.87       | 5.95         | 2.03         | 7.99               |
| Acetol           | -5.68 | -1.73 | 3.70     | 3.95     | 1.74       | 5.57         | 1.87         | 7.44               |
| Acetone          | -5.83 | -1.62 | 3.73     | 4.21     | 1.65       | 5.42         | 1.70         | 7.12               |
| Arabinose        | -5.87 | -2.16 | 4.02     | 3.71     | 2.18       | 6.60         | 2.58         | 9.17               |
| Glucose          | -5.89 | -2.33 | 4.11     | 3.56     | 2.38       | 7.03         | 2.92         | 9.95               |
| d-Glyceraldehyde | -6.03 | -2.20 | 4.12     | 3.83     | 2.21       | 6.72         | 2.60         | 9.32               |
| Glycolaldehyde   | -6.13 | -2.13 | 4.13     | 4.00     | 2.13       | 6.58         | 2.45         | 9.03               |
| Glyoxal          | -6.09 | -4.09 | 5.09     | 2.00     | 6.48       | 15.63        | 10.54        | 26.17              |
| l-Glyceraldehyde | -6.03 | -2.20 | 4.12     | 3.83     | 2.21       | 6.72         | 2.60         | 9.32               |
| Methylglyoxal    | -5.91 | -3.75 | 4.83     | 2.15     | 5.42       | 13.39        | 8.56         | 21.96              |
| Ribose           | -5.79 | -2.14 | 3.96     | 3.65     | 2.15       | 6.51         | 2.54         | 9.05               |

| Property         | I     | A     | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta\omega^{\pm}$ |
|------------------|-------|-------|---------|---------|----------|------------|------------|---------------------|
| Acetaldehyde     | 7.06  | 1.21  | 4.13    | 5.85    | 1.46     | 5.35       | 1.22       | 6.57               |
| Acetol           | 6.47  | 1.09  | 3.78    | 5.37    | 1.33     | 4.89       | 1.11       | 5.99               |
| Acetone          | 6.86  | -3.48 | 1.69    | 10.34   | 0.14     | 1.76       | 0.08       | 1.84               |
| Arabinose        | 6.29  | 1.39  | 3.84    | 4.90    | 1.50     | 5.23       | 1.40       | 6.63               |
| Glucose          | 6.28  | 1.52  | 3.90    | 4.76    | 1.60     | 5.44       | 1.54       | 6.98               |
| d-Glyceraldehyde | 6.59  | 1.41  | 4.00    | 5.18    | 1.54     | 5.41       | 1.41       | 6.82               |
| Glycolaldehyde   | 7.03  | 1.47  | 4.25    | 5.56    | 1.62     | 5.72       | 1.47       | 7.19               |
| Glyoxal          | 6.96  | 3.42  | 5.19    | 3.53    | 3.81     | 10.44      | 5.25       | 15.69              |
| l-Glyceraldehyde | 6.59  | 1.41  | 4.00    | 5.18    | 1.54     | 5.41       | 1.41       | 6.82               |
| Methylglyoxal    | 6.72  | 3.12  | 4.92    | 3.60    | 3.37     | 9.42       | 4.50       | 13.91              |
| Ribose           | 6.32  | 1.37  | 3.85    | 4.95    | 1.50     | 5.23       | 1.38       | 6.61               |
Table S7B: Descriptors $J_I$, $J_A$, $J_HL$, $J_X$, $J_\eta$, $J_\omega$, $J_D1$, $J_{\omega^+}$, $J_{\omega^-}$, $J_{\Delta\omega^\pm}$ and $J_{D2}$ for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S7A

|                | $J_I$ | $J_A$ | $J_HL$ | $J_X$ | $J_\eta$ | $J_\omega$ | $J_D1$ | $J_{\omega^+}$ | $J_{\omega^-}$ | $J_{\Delta\omega^\pm}$ | $J_{D2}$ |
|----------------|-------|-------|--------|-------|---------|-----------|-------|----------------|----------------|-------------------|--------|
| Acetaldehyde   | 1.07  | 0.65  | 1.26   | 0.21  | 1.73    | 0.41      | 1.79  | 0.60           | 0.81           | 1.41              | 1.74   |
| Acetol         | 0.79  | 0.63  | 1.01   | 0.08  | 1.42    | 0.41      | 1.48  | 0.68           | 0.76           | 1.44              | 1.77   |
| Acetone        | 1.02  | 5.10  | 5.20   | 2.04  | 6.12    | 1.51      | 6.63  | 3.66           | 1.62           | 5.27              | 6.62   |
| Arabinose      | 0.42  | 0.77  | 0.88   | 0.18  | 1.19    | 0.67      | 1.38  | 1.18           | 2.54           | 3.12              |        |
| Glucose        | 0.39  | 0.81  | 0.90   | 0.21  | 1.20    | 0.78      | 1.45  | 1.59           | 1.38           | 2.97              | 3.64   |
| d-Glyceraldehyde | 0.55 | 0.79  | 0.97   | 0.12  | 1.34    | 0.67      | 1.51  | 1.31           | 1.19           | 2.50              | 3.07   |
| Glycolaldehyde | 0.91  | 0.66  | 1.12   | 0.12  | 1.57    | 0.51      | 1.65  | 0.86           | 0.98           | 1.83              | 2.25   |
| Glyoxal        | 0.87  | 0.67  | 1.09   | 0.10  | 1.53    | 2.67      | 3.08  | 5.19           | 5.29           | 10.48             | 12.84  |
| l-Glyceraldehyde | 0.55 | 0.79  | 0.97   | 0.12  | 1.34    | 0.67      | 1.51  | 1.31           | 1.19           | 2.50              | 3.07   |
| Methylglyoxal  | 0.81  | 0.63  | 1.03   | 0.09  | 1.45    | 2.06      | 2.52  | 3.98           | 4.07           | 8.05              | 9.85   |
| Ribose         | 0.53  | 0.76  | 0.93   | 0.11  | 1.29    | 0.65      | 1.45  | 1.28           | 1.16           | 2.44              | 3.00   |
| Average        | 0.72  | 1.12  | 1.40   | 0.31  | 1.84    | 1.00      | 2.22  | 1.98           | 1.79           | 3.77              | 4.63   |
Table S8A: HOMO and LUMO orbital energies (in eV), ionization potentials $I$ and electron affinities $A$ (in eV), and global electronegativity $\chi$, total hardness $\eta$, global electrophilicity $\omega$, electrodonating power ($\omega^-$), electroaccepting power ($\omega^+$), and net electrophilicity $\Delta\omega^\pm$ of Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose calculated with the SOGGA11X density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of KID procedure and the lower part shows the results derived from the calculated vertical $I$ and $A$.

| Property         | HOMO | LUMO | $\chi_K$ | $\eta_K$ | $\omega_K$ | $\omega^-_K$ | $\omega^+_K$ | $\Delta\omega^\pm_K$ |
|------------------|------|------|----------|----------|-------------|---------------|---------------|---------------------|
| Acetaldehyde     | -8.65| 0.09 | 4.28     | 8.74     | 1.05        | 4.78          | 0.50          | 5.28                |
| Acetol           | -8.28| 0.14 | 4.07     | 8.42     | 0.98        | 4.52          | 0.46          | 4.98                |
| Acetone          | -8.48| 0.31 | 4.08     | 8.79     | 0.95        | 4.49          | 0.40          | 4.89                |
| Arabinose        | -8.69| -0.42| 4.56     | 8.27     | 1.25        | 5.30          | 0.75          | 6.05                |
| Glucose          | -8.29| -0.40| 4.34     | 7.90     | 1.19        | 5.05          | 0.71          | 5.77                |
| d-Glyceraldehyde | -8.76| -0.17| 4.46     | 8.59     | 1.16        | 5.09          | 0.62          | 5.71                |
| Glycolaldehyde   | -8.76| -0.21| 4.49     | 8.55     | 1.18        | 5.13          | 0.64          | 5.78                |
| Glyoxal          | -8.67| -2.17| 5.42     | 6.49     | 2.26        | 7.64          | 2.22          | 9.86                |
| l-Glyceraldehyde | -8.76| -0.17| 4.46     | 8.59     | 1.16        | 5.09          | 0.62          | 5.71                |
| Methylglyoxal    | -8.52| -1.95| 5.23     | 6.57     | 2.08        | 7.20          | 1.96          | 9.16                |
| Ribose           | -8.30| -0.08| 4.19     | 8.22     | 1.07        | 4.75          | 0.56          | 5.31                |

| Property         | $I$  | $A$  | $\chi$  | $\eta$  | $\omega$ | $\omega^-$ | $\omega^+$ | $\Delta\omega^\pm$ |
|------------------|------|------|----------|----------|----------|------------|------------|---------------------|
| Acetaldehyde     | 7.23 | 1.19 | 4.21     | 6.04     | 1.47     | 5.42       | 1.21       | 6.63                |
| Acetol           | 7.04 | 1.04 | 4.04     | 6.00     | 1.36     | 5.12       | 1.08       | 6.19                |
| Acetone          | 7.06 | 0.88 | 3.97     | 6.17     | 1.28     | 4.92       | 0.95       | 5.88                |
| Arabinose        | 7.47 | 1.62 | 4.55     | 5.84     | 1.77     | 6.18       | 1.63       | 7.80                |
| Glucose          | 7.35 | 1.65 | 4.50     | 5.71     | 1.77     | 6.15       | 1.65       | 7.81                |
| d-Glyceraldehyde | 7.43 | 1.41 | 4.42     | 6.02     | 1.63     | 5.84       | 1.42       | 7.25                |
| Glycolaldehyde   | 7.40 | 1.48 | 4.44     | 5.92     | 1.66     | 5.92       | 1.48       | 7.40                |
| Glyoxal          | 7.61 | 3.31 | 5.46     | 4.30     | 3.46     | 9.92       | 4.46       | 14.38               |
| l-Glyceraldehyde | 7.43 | 1.41 | 4.42     | 6.02     | 1.63     | 5.84       | 1.42       | 7.25                |
| Methylglyoxal    | 7.42 | 3.07 | 5.24     | 4.35     | 3.16     | 9.21       | 3.97       | 13.18               |
| Ribose           | 7.13 | 1.28 | 4.21     | 5.85     | 1.51     | 5.50       | 1.29       | 6.79                |
Table S8B: Descriptors \( J_I, J_A, J_{HL}, J_{\chi}, J_\eta, J_\omega, J_{D1}, J_{\omega^+}, J_{\omega^-}, J_{\Delta\omega^\pm} \) and \( J_{D2} \) for the Acetaldehyde, Acetol, Acetone, Arabinose, Glucose, d-Glyceraldehyde, Glyoxal, l-Glyceraldehyde, Methylglyoxal and Ribose molecules calculated from the results of Table S8A

| Molecule          | \( J_I \) | \( J_A \) | \( J_{HL} \) | \( J_{\chi} \) | \( J_\eta \) | \( J_\omega \) | \( J_{D1} \) | \( J_{\omega^+} \) | \( J_{\omega^-} \) | \( J_{\Delta\omega^\pm} \) | \( J_{D2} \) |
|-------------------|----------|----------|-------------|-------------|-------------|-------------|-------------|---------------|---------------|----------------|---------------|
| Acetaldehyde      | 1.42     | 1.29     | 1.91        | 0.07        | 2.70        | 0.42        | 2.74        | 0.64          | 0.71          | 1.35           | 1.66          |
| Acetol            | 1.24     | 1.18     | 1.71        | 0.03        | 2.42        | 0.38        | 2.45        | 0.59          | 0.62          | 1.21           | 1.48          |
| Acetone           | 1.42     | 1.20     | 1.86        | 0.11        | 2.62        | 0.33        | 2.64        | 0.44          | 0.55          | 0.99           | 1.21          |
| Arabinose         | 1.23     | 1.21     | 1.72        | 0.01        | 2.43        | 0.51        | 2.49        | 0.87          | 0.88          | 1.75           | 2.15          |
| Glucose           | 0.94     | 1.25     | 1.56        | 0.16        | 2.19        | 0.58        | 2.27        | 1.10          | 0.94          | 2.04           | 2.50          |
| d-Glyceraldehyde  | 1.33     | 1.25     | 1.82        | 0.04        | 2.58        | 0.47        | 2.62        | 0.75          | 0.79          | 1.55           | 1.89          |
| Glycolaldehyde    | 1.37     | 1.27     | 1.87        | 0.05        | 2.64        | 0.49        | 2.68        | 0.78          | 0.83          | 1.62           | 1.98          |
| Glyoxal           | 1.06     | 1.13     | 1.55        | 0.04        | 2.19        | 1.20        | 2.50        | 2.28          | 2.24          | 4.52           | 5.54          |
| l-Glyceraldehyde  | 1.33     | 1.25     | 1.82        | 0.04        | 2.58        | 0.47        | 2.62        | 0.75          | 0.79          | 1.55           | 1.89          |
| Methylglyoxal     | 1.10     | 1.12     | 1.57        | 0.01        | 2.22        | 1.07        | 2.46        | 2.02          | 2.00          | 4.02           | 4.92          |
| Ribose            | 1.17     | 1.20     | 1.68        | 0.01        | 2.37        | 0.44        | 2.41        | 0.75          | 0.73          | 1.48           | 1.81          |
| Average           | 1.24     | 1.21     | 1.73        | 0.06        | 2.45        | 0.58        | 2.53        | 1.00          | 1.01          | 2.01           | 2.46          |