**Prediction of the Glass Transition Temperatures   
of Linear Homo/heteropolymers and Cross-linked Epoxy Resins**

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**Modeling details**

Detailed explanation of ISIDA descriptors is given in the ISIDA Fragmentor2015 - User Manual which is a part of Supplementary Information.

**Table S1**. The descriptor sets producing the SVR model of maximal robustness (estimated by 12 times of 3-CV *Q*2 value) for each model.

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| Models | Descriptors | | Multiplied by molar ratio |
| Katritzky’s set |  | IIRAB--FC-1-3 | yes |
| Epoxy resin-specific |  | IIRA--P-1-4 | yes |
| Global |  | IIRA--FC-1-3 | yes |
| I: Sequences II: Atom-centered fragments | | | |
| R: Restricted A: Atom symbol B: Bond inclusion | | | |
| FC: FormalCharge P: AtomPairs  Numbers: LowerLength and UpperLength | | | |

**Table S2**. The descriptor sets involved in the SVR consensus models.

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| Models | Descriptors | | Multiplied by  molar ratio |
| Epoxy resin-specific |  | IA--FC-AP-2-6 | no |
|  | IAB--FC-AP-2-5 | no |
|  | IIA--P-FC-1-2 | no |
|  | IIRA--FC-1-3 | no |
|  | IA--2-7 | yes |
| Global |  | IIRA--1-3 | no |
|  | IIRA--1-3 | yes |
|  | IIRA--1-4 | yes |
|  | IIRA--FC-1-3 | yes |
|  | IIRAB--1-3 | yes |
| I: Sequences II: Atom-centered fragments | | | |
| R: Restricted A: Atom symbol B: Bond inclusion | | | |
| FC: FormalCharge P: AtomPairs AP: AllPaths  Numbers: LowerLength and UpperLength | | | |

**Table S3**. The complete list of 42 explored ISIDA fragmentation schemes used to search the above-selected best suited descriptor spaces. Please refer to the separately provided ISIDA Fragmentor manual for “decoding” of the schemes.

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| IA--2-7 | IA--FC-2-8 | IA--FC-AP-2-9 |
| IA--FC-AP-FC-2-6 | IA--P-2-15 | IA--P-FC-2-15 |
| IAB--2-5 | IAB--2-6 | IAB--FC-2-4 |
| IAB--FC-2-5 | IAB--FC-AP-2-5 | IAB--FC-AP-2-6 |
| IAB--FC-AP-FC-2-4 | IAB--FC-AP-FC-2-5 | IAB--P-2-14 |
| IAB--P-FC-2-14 | IAB--P-FC-AP-2-14 | IAB--P-FC-AP-FC-2-14 |
| IIA--1-2 | IIA--1-3 | IIA--FC-1-2 |
| IIA--P-1-3 | IIA--P-FC-1-2 | IIA--P-FC-1-3 |
| IIAB--1-2 | IIAB--1-3 | IIAB--FC-1-2 |
| IIAB--FC-1-3 | III--3-6 | III--FC-3-6 |
| III--FC-3-7 | IIRA--1-3 | IIRA--1-4 |
| IIRA--FC-1-3 | IIRA--P-1-4 | IIRA--P-1-5 |
| IIRA--P-FC-1-5 | IIRAB--1-2 | IIRAB--1-3 |
| IIRAB--FC-1-2 | IIRAB--FC-1-3 | IIRB--FC-1-3 |