chem-bla-ics

Novel QSAR and QSPR descriptors?

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For the past few weeks I have been working on a review article, which will contain a section with new QSAR/QSPR descriptors published in the period 2000-now. Here are a few:

- 2001: oxygen paths of length 3 10.1021/ci000116e
- 2002: a molecular shape descriptor 10.1021/ci000100o
- 2003: molecular signature 10.1021/ci020345w
- 2004: 4D-fingerprint 10.1021/ci049898s
- 2005: summed NMR shift difference 10.1021/ci049643e

If you know additional new descriptors, or feel like discussion one or more of the above, please leave a comment.