

Supplementary material for

Fast Methods for Prediction of Aldehyde Oxidase-Mediated Site-of-Metabolism

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List of supplementary material:

Table S1.	Values of Q1, median, Q3, and whiskers for the box plots shown in Fig. 2.
Fig. S1.	2D structures of compounds.
Montefiori.csv	CSV file with calculated data for SOMs and non-SOMs in the 78 compounds.
Montefiori.sdf	SDF file with coordinates of the 78 compounds and experimental SOMs.

Table S1. Values of the Q1, median, Q3, and whiskers for the box plots shown in Fig. 2.

Descriptor	Median	Q1	Q3	High Whisker	Low Whisker	Highest value	Lowest value
Chemical Shielding (SOM)	68.6	64.9	73.9	87.4	51.4	96.1	33.5
Chemical Shielding (no SOM)	47.1	42.8	51.5	63.0	35.1	63.0	35.5
Chemical Shift (SOM)	127.5	121.7	132.0	147.4	106.3	163.8	85.0
Chemical Shift (no SOM)	149.9	146.7	155.2	164.5	136.7	164.5	136.7
ESP Charges (SOM)	-0.14	-0.33	0.01	0.51	-0.70	0.68	-0.70
ESP Charges (no SOM)	0.39	0.27	0.47	0.72	-0.02	0.72	-0.20
Gasteiger Charges (SOM)	-0.04	-0.05	-0.01	0.04	-0.11	0.21	-0.20
Gasteiger Charges (no SOM)	0.06	0.03	0.10	0.19	-0.04	0.21	-0.04
Product Stability (SOM)	94.9	80.8	100.8	130.7	50.9	162.6	7.1
Product Stability (no SOM)	66.9	55.6	81.4	120.1	16.8	126.6	0.0
Relative Span (SOM)	0.82	0.74	0.90	1.00	0.53	1.00	0.53
Relative Span (no SOM)	0.86	0.75	1.00	1.00	0.55	1.00	0.55
2D-SASA (SOM)	28.8	26.1	32.7	41.1	16.5	41.2	16.5
2D-SASA (no SOM)	33.6	31.2	36.0	39.6	24.2	39.6	21.3

Fig. S1. 2D structures of compounds.

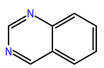
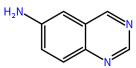
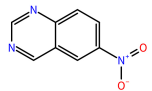
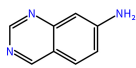
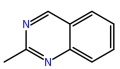
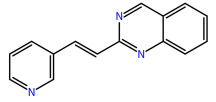
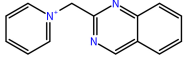
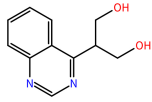
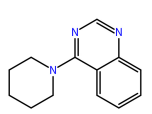
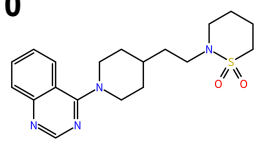
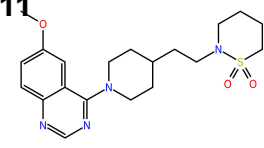
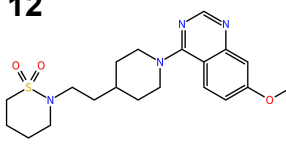
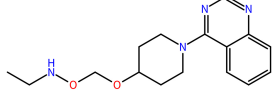
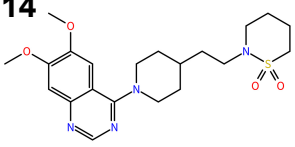
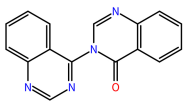
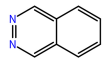
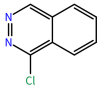
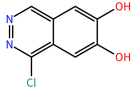
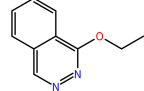
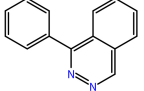
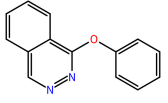
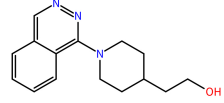
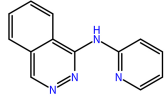
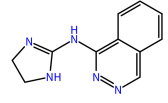
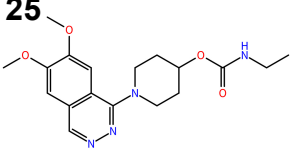
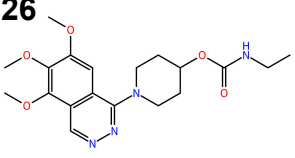
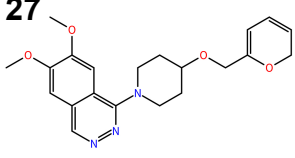
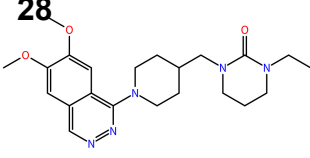
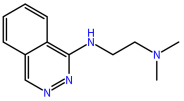
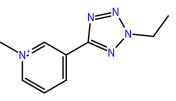
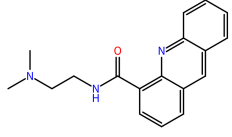
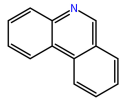
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Fig. S1. 2D structures of compounds.

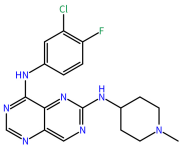
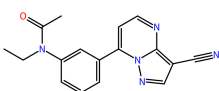
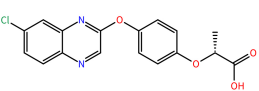
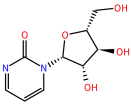
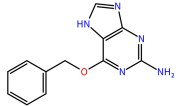
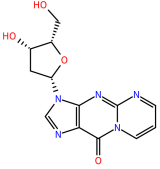
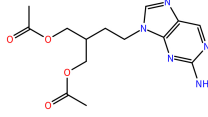
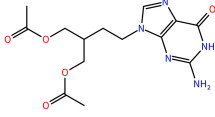
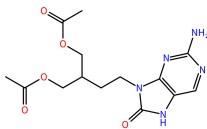
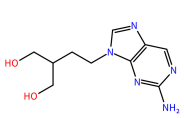
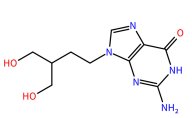
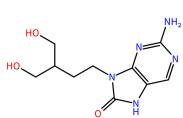

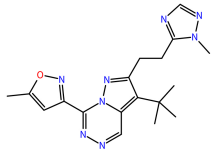
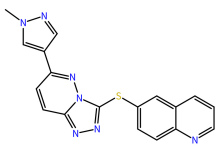
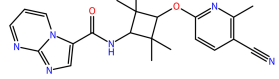
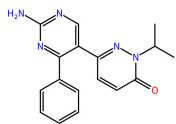
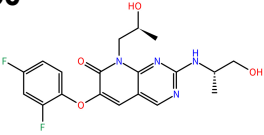
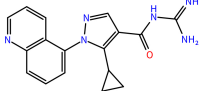
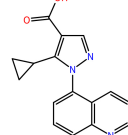
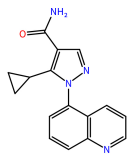
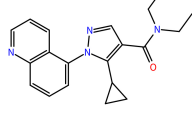
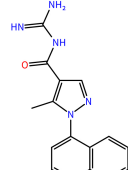
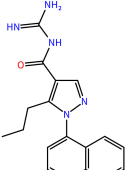
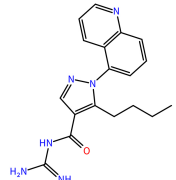
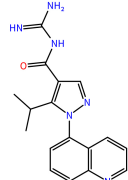
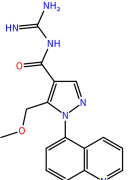
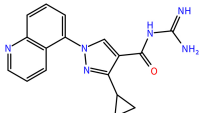
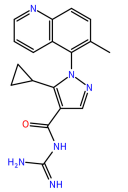
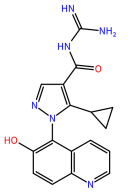
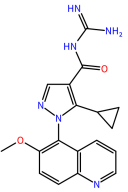
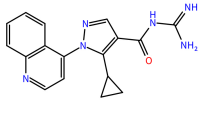
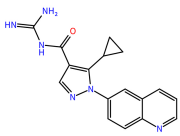
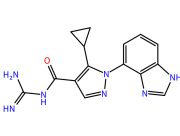
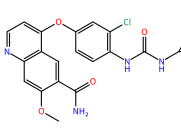
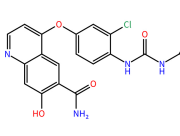
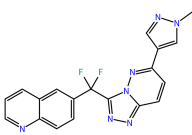
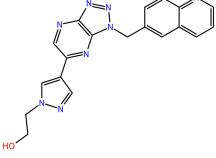
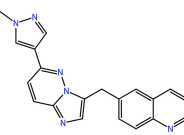
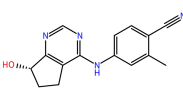
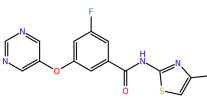

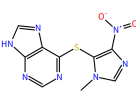
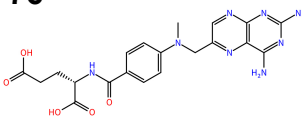
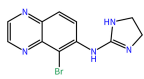
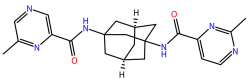
<p>33</p>  <p>BIBX1382</p>	<p>34</p>  <p>Zaleplon</p>	<p>35</p>  <p>XK469</p>	<p>36</p>  <p>Zebularine</p>
<p>37</p>  <p>O6-Benzylguanine</p>	<p>38</p>  <p>M1dG</p>	<p>39</p>  <p>Famciclovir</p>	<p>40</p>  <p>6-Oxo-Famciclovir</p>
<p>41</p>  <p>8-Oxo-Famciclovir</p>	<p>42</p>  <p>6-Deoxypenciclovir</p>	<p>43</p>  <p>6-Oxo-6-Deoxypenciclovir</p>	<p>44</p>  <p>8-Oxo-6-Deoxypenciclovir</p>
<p>45</p>  <p>6-Mercaptopurine</p>	<p>46</p>  <p>OConnor_1</p>	<p>47</p>  <p>SGX523</p>	<p>48</p>  <p>Linton_1</p>
<p>49</p>  <p>FK3453</p>	<p>50</p>  <p>Zhang_Ro1</p>	<p>51</p>  <p>Zoniporide</p>	<p>52</p>  <p>Quinoline_Dalvie_2</p>
<p>53</p>  <p>Quinoline_Dalvie_3</p>	<p>54</p>  <p>Quinoline_Dalvie_4</p>	<p>55</p>  <p>Quinoline_Dalvie_5</p>	<p>56</p>  <p>Quinoline_Dalvie_6</p>
<p>57</p>  <p>Quinoline_Dalvie_7</p>	<p>58</p>  <p>Quinoline_Dalvie_8</p>	<p>59</p>  <p>Quinoline_Dalvie_9</p>	<p>60</p>  <p>Quinoline_Dalvie_10</p>
<p>61</p>  <p>Quinoline_Dalvie_11</p>	<p>62</p>  <p>Quinoline_Dalvie_12</p>	<p>63</p>  <p>Quinoline_Dalvie_13</p>	<p>64</p>  <p>Quinoline_Dalvie_14</p>

Fig. S1. 2D structures of compounds.

<p>65</p>  <p>Quinoline_Dalvie_15</p>	<p>66</p>  <p>Quinoline_Dalvie_16</p>	<p>67</p>  <p>Lenvatinib</p>	<p>68</p>  <p>Desmethyl_Lenvatinib</p>
<p>69</p>  <p>Loikema_JNJ_38877605</p>	<p>70</p>  <p>Zientek_PF_4217903</p>	<p>71</p>  <p>Xu_7</p>	<p>72</p>  <p>Itoh_RS_8359</p>
<p>73</p>  <p>Morrison_VU0409106</p>	<p>74</p>  <p>6-Methylpurine</p>	<p>75</p>  <p>Azathioprine</p>	<p>76</p>  <p>Methotrexate</p>
<p>77</p>  <p>Brimonidine</p>	<p>78</p>  <p>Lu_AF09535</p>		