Supplementary Information for

# Quantum Chemistry-Informed Active Learning to Accelerate the Design and Discovery of Sustainable Energy Storage Materials

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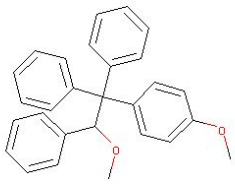
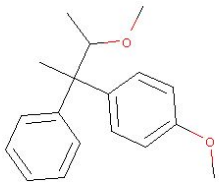
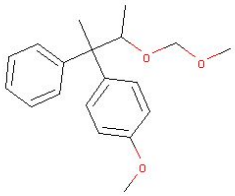
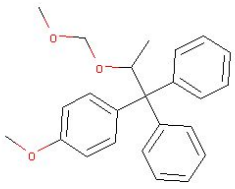
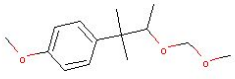
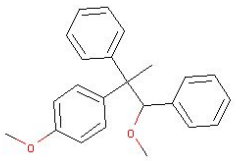
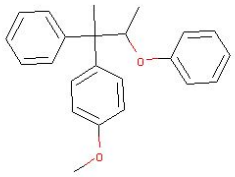
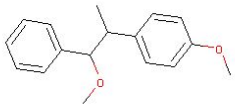
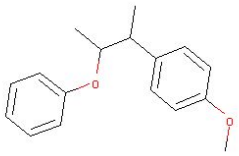
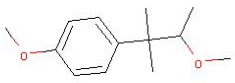
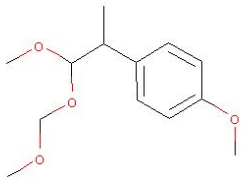
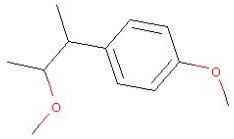
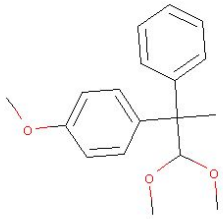
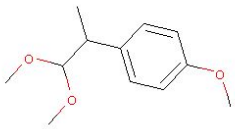
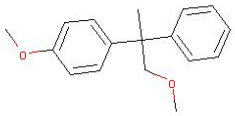
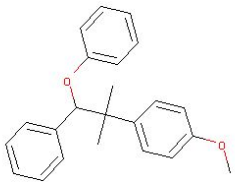
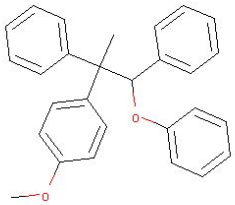
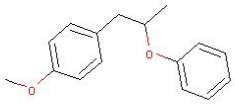
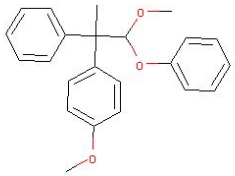
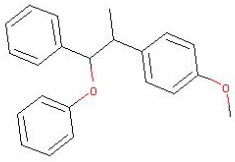
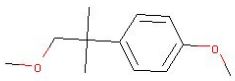
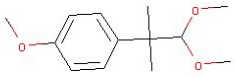
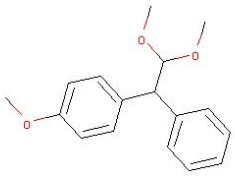
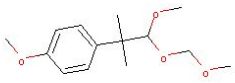
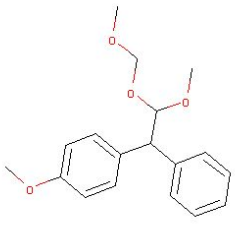
Table S1 List of 133 identified HBEs with computed oxidation potential ($E^{ox}$) in the range of 1.40 V to 1.70 V

| HBE # | SMILES | 2-D Structure | $E^{ox}$ (V vs. NHE) |
|---|---|---|---|
| 1 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C4=CC=CC=C4)OC)C=C1 |  | 1.52 |
| 2 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(C)OC)C=C1 |  | 1.52 |
| 3 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(C)OCOC)C=C1 |  | 1.53 |
| 4 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C)OCOC)C=C1 |  | 1.54 |
| 5 | O(C)C1=CC=C(C(C)(C)C(C)OCOC)C=C1 |  | 1.54 |

| | | | |
|---|---|---|---|
| 6 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(C3=CC=CC=C3)OC)C=C1 |  | 1.54 |
| 7 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(C)OC3=CC=CC=C3)C=C1 |  | 1.54 |
| 8 | O(C)C1=CC=C(C([H])(C)C(C2=CC=CC=C2)OC)C=C1 |  | 1.55 |
| 9 | O(C)C1=CC=C(C([H])(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.55 |
| 10 | O(C)C1=CC=C(C(C)(C)C(C)OC)C=C1 |  | 1.55 |

| | | | |
|---|---|---|---|
| 11 | O(C)C1=CC=C(C(C)([H])C(OC)OCOC)C=C1 |  | 1.55 |
| 12 | O(C)C1=CC=C(C([H])(C)C(C)OC)C=C1 |  | 1.56 |
| 13 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C(OC)OC)C=C1 |  | 1.56 |
| 14 | O(C)C1=CC=C(C(C)([H])C(OC)OC)C=C1 |  | 1.56 |
| 15 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C([H])OC)C=C1 |  | 1.56 |

| | | | |
|---|---|---|---|
| 16 | O(C)C1=CC=C(C(C)(C)C(C2=CC=CC=C2)OC3=CC=CC=C3)C=C1 |  | 1.56 |
| 17 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C(C3=CC=CC=C3)OC4=CC=CC=C4)C=C1 |  | 1.57 |
| 18 | O(C)C1=CC=C(C([H])([H])C(C)OC2=CC=CC=C2)C=C1 |  | 1.57 |
| 19 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(OC)OC3=CC=CC=C3)C=C1 |  | 1.57 |
| 20 | O(C)C1=CC=C(C([H])(C)C(C2=CC=CC=C2)OC3=CC=CC=C3)C=C1 |  | 1.57 |

| | | | |
|---|---|---|---|
| 21 | O(C)C1=CC=C(C(C)(C)C([H])OC)C=C1 |  | 1.57 |
| 22 | O(C)C1=CC=C(C(C)(C)C(OC)OC)C=C1 |  | 1.58 |
| 23 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(OC)OC)C=C1 |  | 1.58 |
| 24 | O(C)C1=CC=C(C(C)(C)C(OC)OCOC)C=C1 |  | 1.58 |
| 25 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(OC)OCOC)C=C1 |  | 1.58 |

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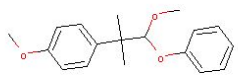
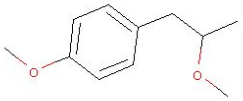
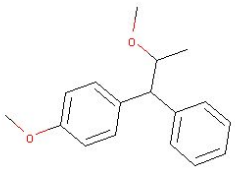
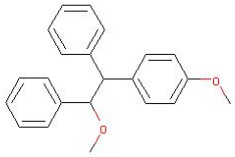
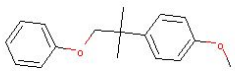
|---|---|---|---|
| 26 | O(C)C1=CC=C(C(C)(C)C(OC)OC2=CC=CC=C2)C=C1 |  | 1.58 |
| 27 | O(C)C1=CC=C(C([H])([H])C(C)OC)C=C1 |  | 1.58 |
| 28 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(C)OC)C=C1 |  | 1.58 |
| 29 | O(C)C1=CC=C(C(C2=CC=CC=C2)([H])C(C3=CC=CC=C3)OC)C=C1 |  | 1.58 |
| 30 | O(C)C1=CC=C(C(C)(C)C([H])OC2=CC=CC=C2)C=C1 |  | 1.58 |

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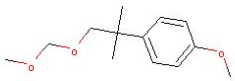
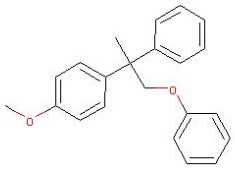
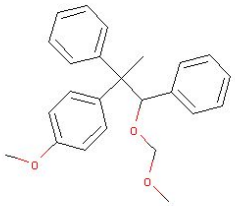
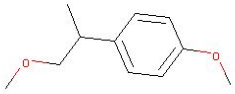
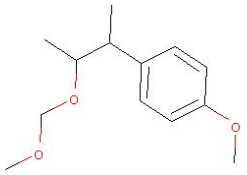
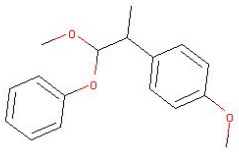
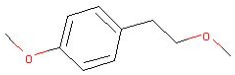
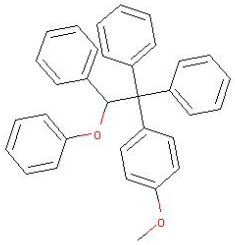
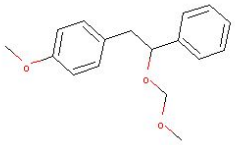
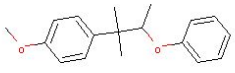
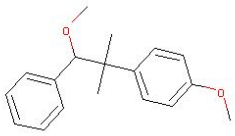
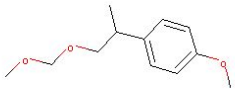
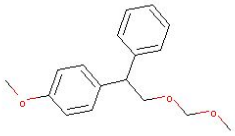
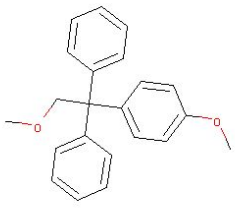
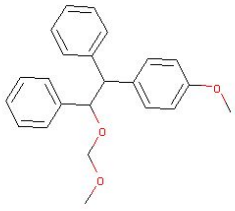
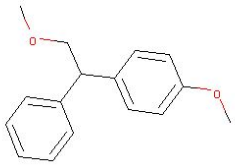
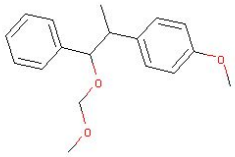
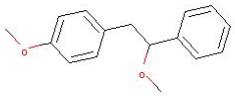
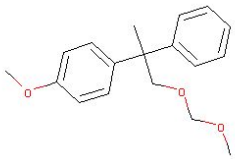
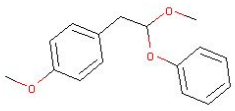
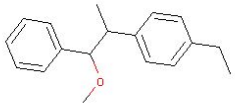
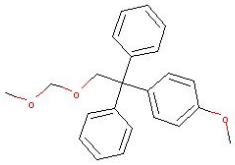
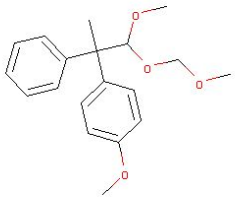
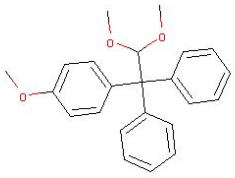
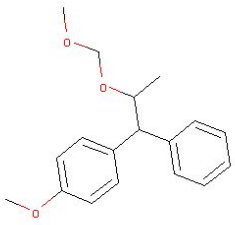
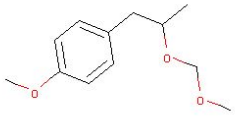
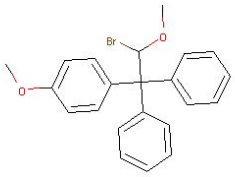
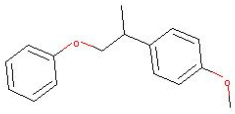
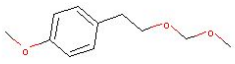
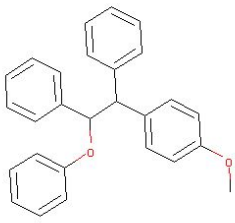
|---|---|---|---|
| 31 | O(C)C1=CC=C(C(C)(C)C([H])OCOC)C=C1 |  | 1.58 |
| 32 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C([H])OC3=CC=CC=C3)C=C1 |  | 1.58 |
| 33 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C(C3=CC=CC=C3)OCOC)C=C1 |  | 1.59 |
| 34 | O(C)C1=CC=C(C(C)([H])C([H])OC)C=C1 |  | 1.59 |
| 35 | O(C)C1=CC=C(C(C)([H])C(C)OCOC)C=C1 |  | 1.59 |

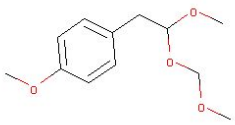
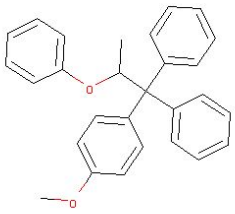
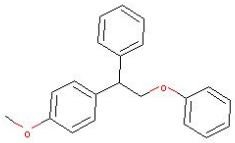
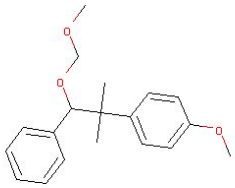
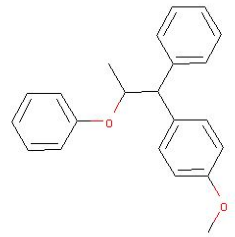
| | | | |
|---|---|---|---|
| 36 | O(C)C1=CC=C(C([H])(C)C(OC)OC2=CC=CC=C2)C=C1 |  | 1.59 |
| 37 | O(C)C1=CC=C(C([H])([H])C([H])OC)C=C1 |  | 1.59 |
| 38 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C4=CC=CC=C4)OC5=CC=CC=C5)C=C1 |  | 1.59 |
| 39 | O(C)C1=CC=C(C([H])([H])C(C2=CC=CC=C2)OCOC)C=C1 |  | 1.59 |
| 40 | O(C)C1=CC=C(C(C)(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.59 |

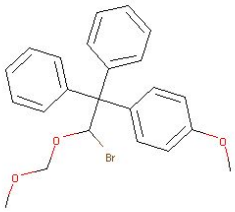
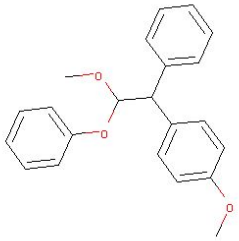
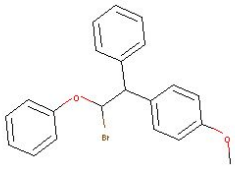
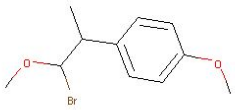
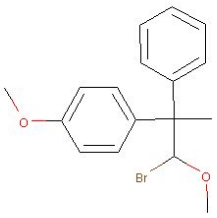
| | | | |
|---|---|---|---|
| 41 | O(C)C1=CC=C(C(C)(C)C(C2=CC=CC=C2)OC)C=C1 |  | 1.60 |
| 42 | O(C)C1=CC=C(C(C)([H])C([H])OCOC)C=C1 |  | 1.60 |
| 43 | O(C)C1=CC=C(C(C2=CC=CC=C2)([H])C([H])OCOC)C=C1 |  | 1.60 |
| 44 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C([H])OC)C=C1 |  | 1.60 |
| 45 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(C3=CC=CC=C3)OCOC)C=C1 |  | 1.6 |

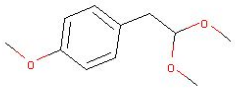
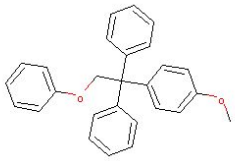
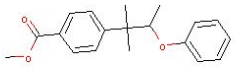
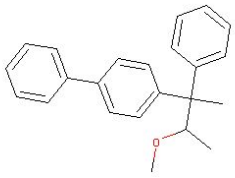
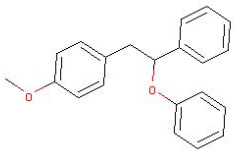
| | | | |
|---|---|---|---|
| 46 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C([H])OC)C=C1 |  | 1.60 |
| 47 | O(C)C1=CC=C(C(C)([H])C(C2=CC=CC=C2)OCOC)C=C1 |  | 1.60 |
| 48 | O(C)C1=CC=C(C([H])([H])C(C2=CC=CC=C2)OC)C=C1 |  | 1.60 |
| 49 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C([H])OCOC)C=C1 |  | 1.61 |
| 50 | O(C)C1=CC=C(C([H])([H])C(OC)OC2=CC=CC=C2)C=C1 |  | 1.61 |

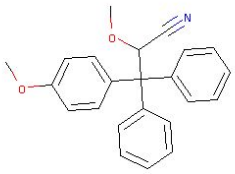
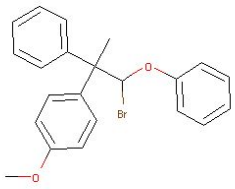
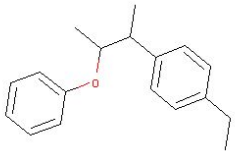
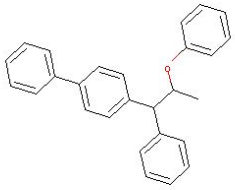
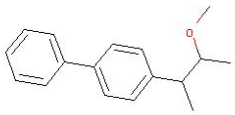
| | | | |
|---|---|---|---|
| 51 | CCC1=CC=C(C([H])(C)C(C2=CC=CC=C2)OC)C=C1 |  | 1.61 |
| 52 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C([H])OCOC)C=C1 |  | 1.61 |
| 53 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C(OC)OCOC)C=C1 |  | 1.61 |
| 54 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(OC)OC)C=C1 |  | 1.61 |
| 55 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(C)OCOC)C=C1 |  | 1.61 |

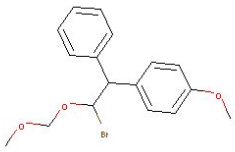
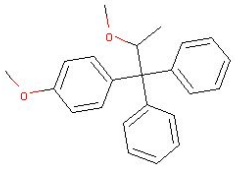
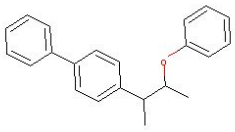
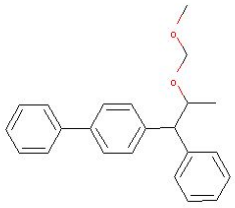
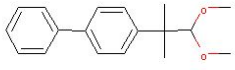
| | | | |
|---|---|---|---|
| 56 | O(C)C1=CC=C(C([H])([H])C(C)OCOC)C=C1 |  | 1.61 |
| 57 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(Br)OC)C=C1 |  | 1.61 |
| 58 | O(C)C1=CC=C(C([H])(C)C([H])OC2=CC=CC=C2)C=C1 |  | 1.62 |
| 59 | O(C)C1=CC=C(C([H])([H])C([H])OCOC)C=C1 |  | 1.62 |
| 60 | O(C)C1=CC=C(C(C2=CC=CC=C2)([H])C(C3=CC=CC=C3)OC4=CC=CC=C4)C=C1 |  | 1.62 |

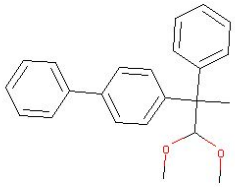
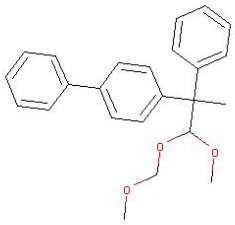
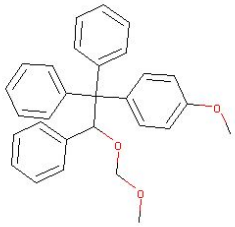
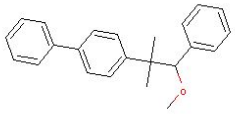
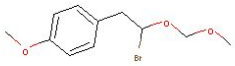
| | | | |
|---|---|---|---|
| 61 | O(C)C1=CC=C(C([H])([H])C(OC)OCOC)C=C1 |  | 1.62 |
| 62 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C)OC4=CC=CC=C4)C=C1 |  | 1.62 |
| 63 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C([H])OC3=CC=CC=C3)C=C1 |  | 1.63 |
| 64 | O(C)C1=CC=C(C(C)(C)C(C2=CC=CC=C2)OCOC)C=C1 |  | 1.63 |
| 65 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(C)OC3=CC=CC=C3)C=C1 |  | 1.63 |

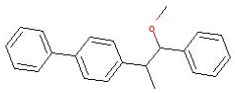
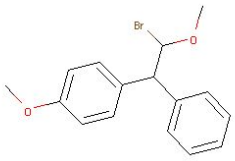
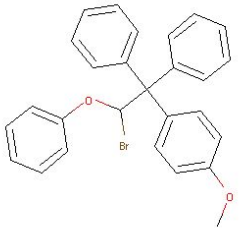
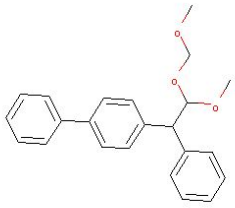
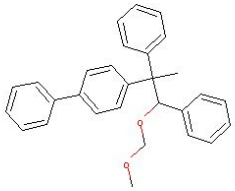
| | | | |
|---|---|---|---|
| 66 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(Br)OCOC)C=C1 |  | 1.63 |
| 67 | O(C)C1=CC=C(C(C2=CC=CC=C2)([H])C(OC)OC3=CC=CC=C3)C=C1 |  | 1.63 |
| 68 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(Br)OC3=CC=CC=C3)C=C1 |  | 1.63 |
| 69 | O(C)C1=CC=C(C([H])(C)C(Br)OC)C=C1 |  | 1.64 |
| 70 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(Br)OC)C=C1 |  | 1.64 |

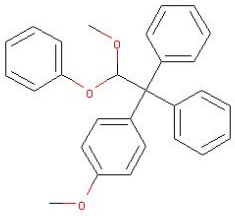
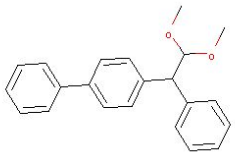
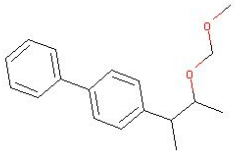
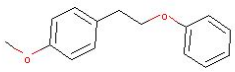
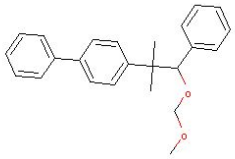
| | | | |
|---|---|---|---|
| 71 | O(C)C1=CC=C(C([H])([H])C(OC)OC)C=C1 |  | 1.64 |
| 72 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C([H])OC4=CC=CC=C4)C=C1 |  | 1.64 |
| 73 | C(OC)(=O)C1=CC=C(C(C)(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.65 |
| 74 | C1=CC=CC=C1C2=CC=C(C(C)(C3=CC=CC=C3)C(C)OC)C=C2 |  | 1.65 |
| 75 | O(C)C1=CC=C(C([H])([H])C(C2=CC=CC=C2)OC3=CC=CC=C3)C=C1 |  | 1.65 |

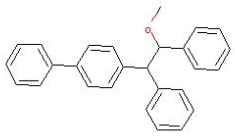
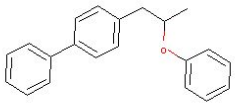
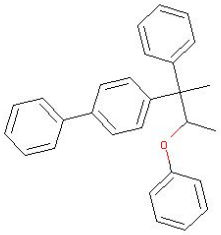
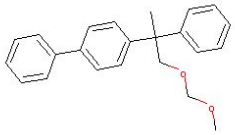
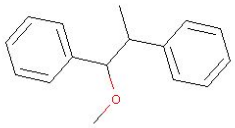
| | | | |
|---|---|---|---|
| 76 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C#N)OC)C=C1 |  | 1.65 |
| 77 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C)C(Br)OC3=CC=CC=C3)C=C1 |  | 1.65 |
| 78 | CCC1=CC=C(C([H])(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.66 |
| 79 | C1=CC=CC=C1C2=CC=C(C([H])(C3=CC=CC=C3)C(C)OC4=CC=CC=C4)C=C2 |  | 1.66 |
| 80 | C1=CC=CC=C1C2=CC=C(C(C)([H])C(C)OC)C=C2 |  | 1.66 |

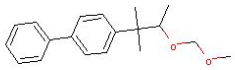
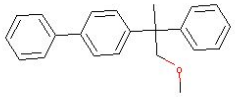
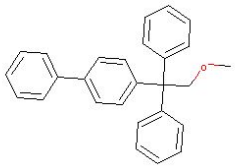
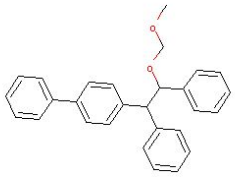
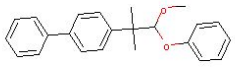
| | | | |
|---|---|---|---|
| 81 | O(C)C1=CC=C(C(C2=CC=CC=C2)([H])C(Br)OCOC)C=C1 |  | 1.66 |
| 82 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C)OC)C=C1 |  | 1.66 |
| 83 | C1=CC=CC=C1C2=CC=C(C([H])(C)C(C)OC3=CC=CC=C3)C=C2 |  | 1.66 |
| 84 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)([H])C(C)OCOC)C=C2 |  | 1.66 |
| 85 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(OC)OC)C=C2 |  | 1.66 |

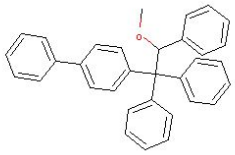
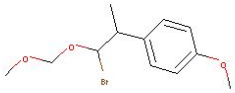
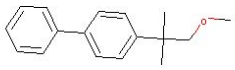
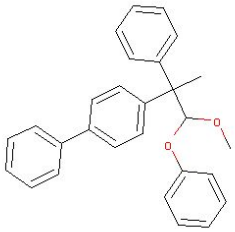
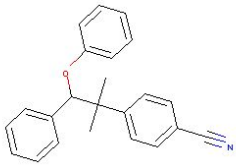
| | | | |
|---|---|---|---|
| 86 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(OC)OC)C=C2 |  | 1.67 |
| 87 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(OC)OCOC)C=C2 |  | 1.67 |
| 88 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C4=CC=CC=C4)OCOC)C=C1 |  | 1.67 |
| 89 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(C3=CC=CC=C3)OC)C=C2 |  | 1.67 |
| 90 | O(C)C1=CC=C(C([H])([H])C(Br)OCOC)C=C1 |  | 1.67 |

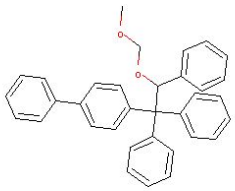
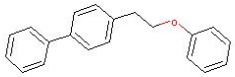
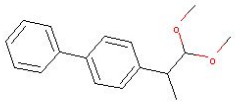
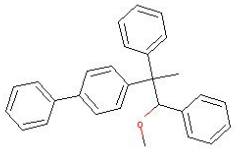
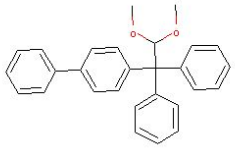
| | | | |
|---|---|---|---|
| 91 | C1=CC=CC=C1C2=CC=C(C([H])(C)C(C3=CC=CC=C3)OC)C=C2 |  | 1.67 |
| 92 | O(C)C1=CC=C(C([H])(C2=CC=CC=C2)C(Br)OC)C=C1 |  | 1.67 |
| 93 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(Br)OC4=CC=CC=C4)C=C1 |  | 1.67 |
| 94 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)([H])C(OC)OCOC)C=C2 |  | 1.68 |
| 95 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(C4=CC=CC=C4)OCOC)C=C2 |  | 1.68 |

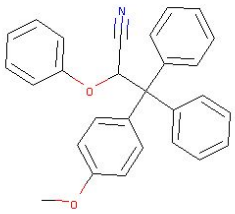
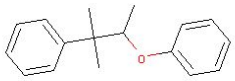
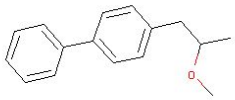
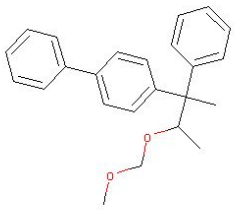
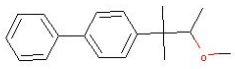
| | | | |
|---|---|---|---|
| 96 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(OC)OC4=CC=CC=C4)C=C1 |  | 1.68 |
| 97 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)([H])C(OC)OC)C=C2 |  | 1.68 |
| 98 | C1=CC=CC=C1C2=CC=C(C([H])(C)C(C)OCOC)C=C2 |  | 1.68 |
| 99 | O(C)C1=CC=C(C([H])([H])C([H])OC2=CC=CC=C2)C=C1 |  | 1.68 |
| 100 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(C3=CC=CC=C3)OCOC)C=C2 |  | 1.68 |

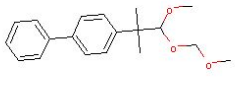
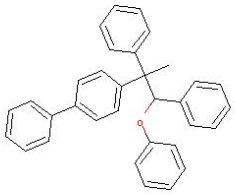
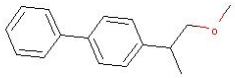
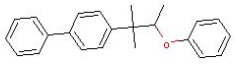
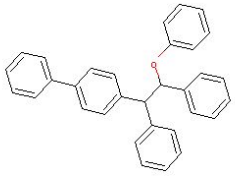
| | | | |
|---|---|---|---|
| 101 | C1=CC=CC=C1C2=CC=C(C([H])(C3=CC=CC=C3)C(C4=CC=CC=C4)OC)C=C2 |  | 1.68 |
| 102 | C1=CC=CC=C1C2=CC=C(C([H])([H])C(C)OC3=CC=CC=C3)C=C2 |  | 1.68 |
| 103 | C1=CC=CC=C1C2=CC=C(C(C)(C3=CC=CC=C3)C(C)OC4=CC=CC=C4)C=C2 |  | 1.68 |
| 104 | C1=CC=CC=C1C2=CC=C(C(C)(C3=CC=CC=C3)C([H])OCOC)C=C2 |  | 1.68 |
| 105 | [H]C1=CC=C(C(C)([H])C(C2=CC=CC=C2)OC)C=C1 |  | 1.68 |

| | | | |
|---|---|---|---|
| 106 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(C)OCOC)C=C2 |  | 1.68 |
| 107 | C1=CC=CC=C1C2=CC=C(C(C)(C3=CC=CC=C3)C([H])OC)C=C2 |  | 1.68 |
| 108 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C4=CC=CC=C4)C([H])OC)C=C2 |  | 1.68 |
| 109 | C1=CC=CC=C1C2=CC=C(C([H])(C3=CC=CC=C3)C(C4=CC=CC=C4)OCOC)C=C2 |  | 1.69 |
| 110 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(OC)OC3=CC=CC=C3)C=C2 |  | 1.69 |

| | | | |
|---|---|---|---|
| 111 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C4=CC=CC=C4)C(C5=CC=CC=C5)OC)C=C2 |  | 1.69 |
| 112 | O(C)C1=CC=C(C([H])(C)C(Br)OCOC)C=C1 |  | 1.69 |
| 113 | C1=CC=CC=C1C2=CC=C(C(C)(C)C([H])OC)C=C2 |  | 1.69 |
| 114 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(OC)OC4=CC=CC=C4)C=C2 |  | 1.69 |
| 115 | C(#N)C1=CC=C(C(C)(C)C(C2=CC=CC=C2)OC3=CC=CC=C3)C=C1 |  | 1.69 |

| | | | |
|---|---|---|---|
| 116 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C4=CC=CC=C4)C(C5=CC=CC=C5)OCOC)C=C2 |  | 1.69 |
| 117 | C1=CC=CC=C1C2=CC=C(C([H])([H])C([H])OC3=CC=CC=C3)C=C2 |  | 1.69 |
| 118 | C1=CC=CC=C1C2=CC=C(C([H])(C)C(OC)OC)C=C2 |  | 1.69 |
| 119 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(C4=CC=CC=C4)OC)C=C2 |  | 1.69 |
| 120 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C4=CC=CC=C4)C(OC)OC)C=C2 |  | 1.69 |

| | | | |
|---|---|---|---|
| 121 | O(C)C1=CC=C(C(C2=CC=CC=C2)(C3=CC=CC=C3)C(C#N)OC4=CC=CC=C4)C=C1 |  | 1.69 |
| 122 | [H]C1=CC=C(C(C)(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.69 |
| 123 | C1=CC=CC=C1C2=CC=C(C([H])([H])C(C)OC)C=C2 |  | 1.69 |
| 124 | C1=CC=CC=C1C2=CC=C(C(C)(C3=CC=CC=C3)C(C)OCOC)C=C2 |  | 1.69 |
| 125 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(C)OC)C=C2 |  | 1.69 |

| | | | |
|---|---|---|---|
| 126 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(OC)OCOC)C=C2 |  | 1.69 |
| 127 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)(C)C(C4=CC=CC=C4)OC5=CC=CC=C5)C=C2 |  | 1.69 |
| 128 | C1=CC=CC=C1C2=CC=C(C([H])(C)C([H])OC)C=C2 |  | 1.70 |
| 129 | C1=CC=CC=C1C2=CC=C(C(C)(C)C(C)OC3=CC=CC=C3)C=C2 |  | 1.70 |
| 130 | C1=CC=CC=C1C2=CC=C(C(C3=CC=CC=C3)([H])C(C4=CC=CC=C4)OC5=CC=CC=C5)C=C2 |  | 1.70 |

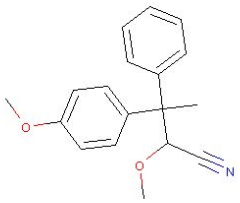
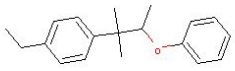
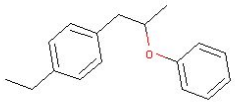
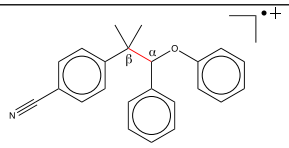
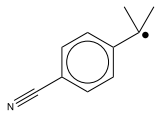
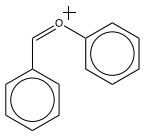
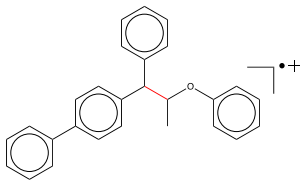
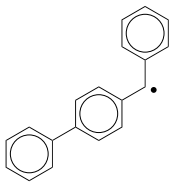
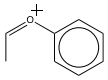
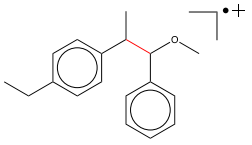
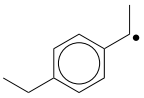
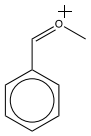
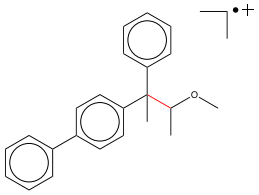
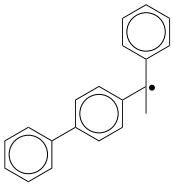
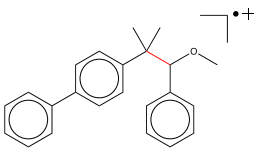
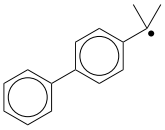
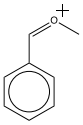
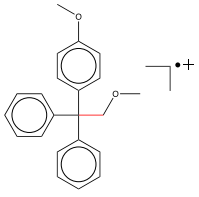
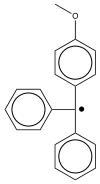
| | | | |
|---|---|---|---|
| 131 | O(C)C1=CC=C(C(C)(C2=CC=CC=C2)C(C#N)OC)C=C1 |  | 1.70 |
| 132 | CCC1=CC=C(C(C)(C)C(C)OC2=CC=CC=C2)C=C1 |  | 1.70 |
| 133 | CCC1=CC=C(C([H])([H])C(C)OC2=CC=CC=C2)C=C1 |  | 1.70 |

Table S2 Most favorable mesolytic cleavage pathways (red bonds) and their corresponding fragmentation free energy ($\Delta G_{min}^{meso}$) for 10 randomly selected molecules from the 133 identified HBEs in Table S1.

| Parent HBE | $E^{ox}$ (V vs. NHE) | Fragment 1 | Fragment 2 | $\Delta G_{min}^{meso}$ (kJ/mol) |
|---|---|---|---|---|
|  CC(C)(c1ccc(C#N)cc1)C(Oc1ccccc1)c1ccccc1 | 1.69 |  |  | -61.69 |
|  CC(Oc1ccccc1)C(c1ccccc1)c1ccc(-c2ccccc2)cc1 | 1.66 |  |  | -6.37 |
|  CCc1ccc(C(C)C(OC)c2ccccc2)cc1 | 1.61 |  |  | -62.74 |
|  COC(C)C(C)(c1ccccc1)c1ccc(-c2ccccc2)cc1 | 1.65 |  |  | -56.35 |
|  COC(c1ccccc1)C(C)(C)c1ccc(-c2ccccc2)cc1 | 1.67 |  |  | -65.74 |
|  COCC(c1ccccc1)(c1ccccc1)c1ccc(OC)cc1 | 1.60 |  |  | -23.40 |

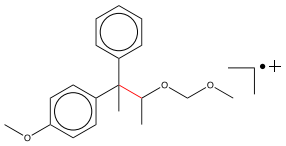
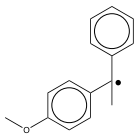
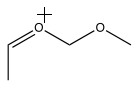
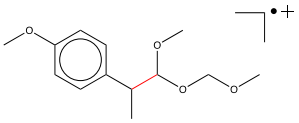
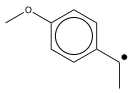
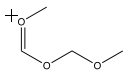
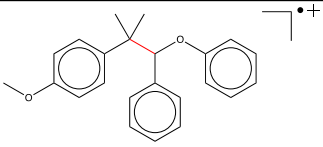
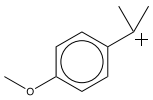
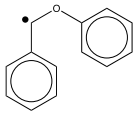
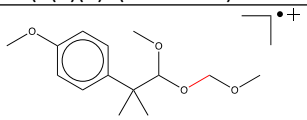
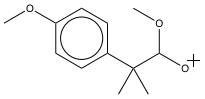
| | | | | |
|---|---|---|---|---|
|  COCOC(C)C(C)(c1ccccc1)c1ccc(OC)cc1 | 1.53 |  |  | -54.55 |
|  COCOC(OC)C(C)c1ccc(OC)cc1 | 1.55 |  |  | -32.20 |
|  COc1ccc(C(C)(C)C(Oc2ccccc2)c2ccccc2)cc1 | 1.56 |  |  | -50.14 |
|  COCOC(OC)C(C)(C)c1ccc(OC)cc1 | 1.58 |  |  | -66.96 |

Table S3 List of 49 tabulated features and their value ranges. The Pearson correlation coefficients were derived from DFT-computed oxidation potentials.

| **Feature** | **Comment** | **Unit** | **Min** | **Max** | **Pearson correlation coefficient** |
|---|---|---|---|---|---|
| sssr | Smallest set of smallest rings | | 1.0 | 6.0 | -0.30 |
| clogp[1] | Crippen's Partition Coefficient (measure of lipophilicity) | | 1.27 | 9.51 | -0.36 |
| Molar refractivity (mr)[1] | | $m^3$/mol | 42.02 | 160.9 | -0.36 |
| Molecular weight (mw) | | g/mol | 136.09 | 504.11 | -0.20 |
| tpsa[2] | Topological polar surface area | Å$^2$ | 9.23 | 132.97 | 0.57 |
| chi0n[3] | Simple molecular connectivity index (order 0) | | 6.21 | 21.73 | -0.36 |
| chi1n[3] | Simple molecular connectivity index (order 1) | | 3.46 | 13.39 | -0.34 |
| chi2n[3] | Simple molecular connectivity index (order 2) | | 2.23 | 9.71 | -0.41 |
| chi3n[3] | Simple molecular connectivity index (order 3) | | 1.44 | 7.4 | -0.33 |
| chi4n[3] | Simple molecular connectivity index (order 4) | | 0.86 | 5.58 | -0.30 |
| chi0v[3] | Valence molecular connectivity index (order 0) | | 6.21 | 21.73 | -0.34 |
| chi1v[3] | Valence molecular connectivity index (order 1) | | 3.46 | 13.39 | -0.33 |
| chi2v[3] | Valence molecular connectivity index (order 2) | | 2.23 | 9.71 | -0.39 |
| chi3v[3] | Valence molecular connectivity index (order 3) | | 1.44 | 7.4 | -0.30 |
| chi4v[3] | Valence molecular connectivity index (order 4) | | 0.86 | 5.58 | -0.28 |
| fracsp3 | Fraction of sp3 C | | 0.05 | 0.6 | 0.03 |
| hall_kier_alpha[3] | Ratio of covalent radii of atom (x) and sp3 C atom ($\alpha_x = \left({r_x}/{r_{C_{sp3}}}\right) - 1$) | | -4.88 | -0.34 | 0.05 |
| kappa1[3] | Molecular shape index (order 1) | | 7.29 | 24.46 | -0.22 |
| kappa2[3] | Molecular shape index (order 2) | | 3.72 | 11.25 | -0.21 |
| kappa3[3] | Molecular shape index (order 3) | | 1.73 | 4.88 | -0.32 |
| Labute's approximate surface area (labuteasa)[4] | | Å$^2$ | 61.64 | 230.56 | -0.26 |
| number_aromatic_rings | | | 1.0 | 6.0 | -0.30 |
| number_atom_stereocenters | | | 0.0 | 2.0 | -0.02 |
| number_HBA | | | 1.0 | 7.0 | 0.36 |
| number_hetero_atoms | | | 1.0 | 8.0 | 0.41 |
| number_rings | | | 1.0 | 6.0 | -0.30 |
| number_rotatable_bonds | | | 3.0 | 9.0 | -0.23 |
| number_heavy_atoms | | | 10.0 | 39.0 | -0.23 |
| number_n_o | | | 1.0 | 8.0 | 0.39 |
| number_valence_electrons | | | 54.0 | 188.0 | -0.27 |
| max_partial_charge | | | 0.05 | 0.34 | 0.40 |

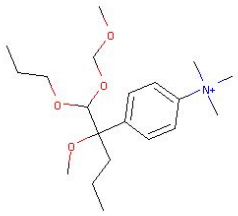
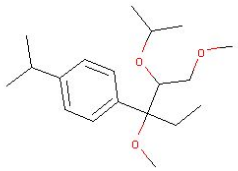
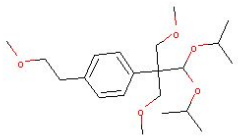
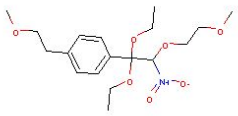
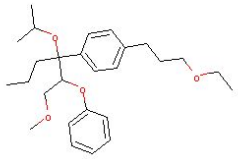
| | | | | | |
|---|---|---|---|---|---|
| min_partial_charge | | | -0.5 | -0.35 | 0.22 |
| fr_C_O | Number of -CO | | 0.0 | 1.0 | 0.24 |
| fr_C_O_noCOO | | | 0.0 | 1.0 | 0.24 |
| fr_methoxy | Number of -OCH3 | | 0.0 | 3.0 | 0.17 |
| fr_ester | | | 0.0 | 1.0 | 0.24 |
| fr_ether | | | 1.0 | 4.0 | 0.10 |
| fr_NH0 | | | 0.0 | 4.0 | 0.21 |
| fr_aniline | | | 0.0 | 1.0 | -0.76 |
| fr_nitrile | | | 0.0 | 4.0 | 0.41 |
| fr_nitro | | | 0.0 | 1.0 | 0.30 |
| fr_halogen | | | 0.0 | 1.0 | 0.06 |
| fr_alkyl_halide | | | 0.0 | 1.0 | 0.06 |
| fr_unbrch_alkane | Number of unbranched alkane | | 0.0 | 2.0 | 0.04 |
| fr_benzene | | | 1.0 | 6.0 | -0.30 |
| fr_nitro_arom | | | 0.0 | 1.0 | 0.30 |
| fr_nitro_arom_nonortho | | | 0.0 | 1.0 | 0.30 |
| fr_para_hydroxylation | | | 0.0 | 1.0 | -0.24 |
| fr_aryl_methyl | | | 0.0 | 1.0 | 0.06 |

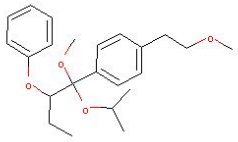
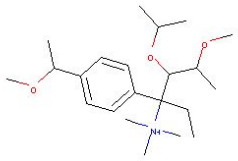
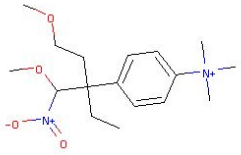
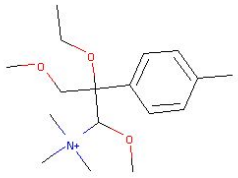
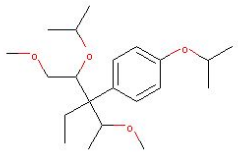
Table S4 List of functional groups and their corresponding scaffold sites used for populating HBE database of 112,000 entries

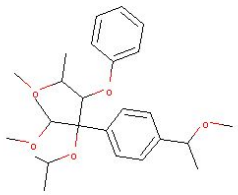
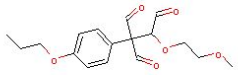
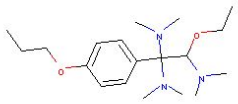
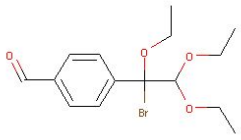
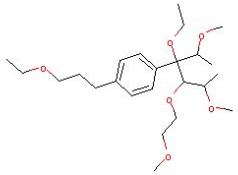
| **Scaffold Site** | **Functional group** |
|---|---|
| R1 | -Me, -Et, -Pr, -Ph, -COMe, -C(Me)Me, -EtOMe |
| R2 | -$N(Me)_3^+$, -COMe, -Et, -OCMe, $N(Me)_2$, -$NO_2$, -C(=O), -Pr, -iPr, -EtOMe, -C(Me)OMe |
| R3 | -$N(Me)_3^+$, -Me, -COMe, -Br, -C(=O), -OEth, -*Pr*, -*iPr*, -C(COMe), -C(Me)(OMe), -*OPr*, -O*iPr* |
| R4 | -$N(Me)_3^+$, -OMe, -COMe, -Br, -N(Me)Me, -Et, -OEt, -$NO_2$, -C(=O), -Pr, -C(Me)Me, -C(COMe), -C(Me)(OMe), -OPr, -OiPr) |
| R5 | -$N(Me)_3^+$, -OMe, -COMe, -Br, -N(Me)Me, -Et, -OEt, -$NO_2$, -C(=O), -Pr, -C(Me)Me, -C(COMe), -C(Me)(OMe), -OPr, -*OiPr*) |

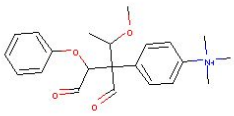
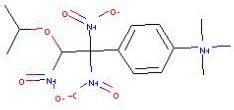
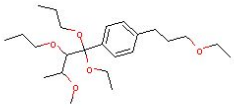
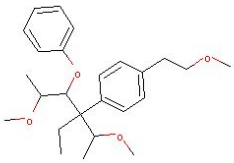
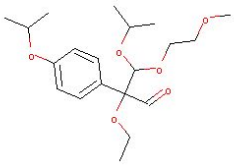
Substituent groups are, *Ph: phenyl, Et :ethyl, OMe: methoxy, iPr: isopropyl, OPr: propoxy, EtOMe: methoxy ethyl, Pr: propyl*

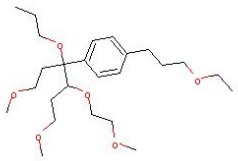
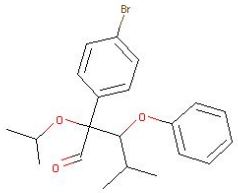
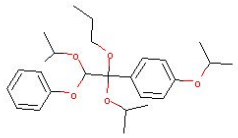
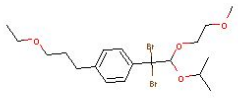
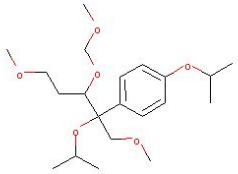
Table S5 List of HBEs evaluated during BO run #1 (BO1) and their corresponding $E^{ox}$. The initial 10 were randomly selected.

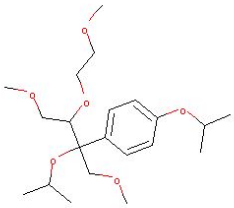
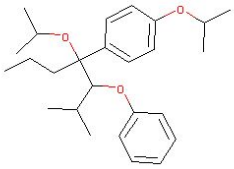
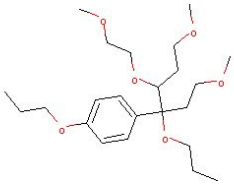
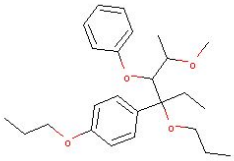
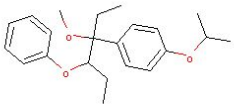
| HBE # | SMILES | 2-D Structure | DFT-computed $E^{ox}$ (V vs. NHE) | BO-predicted $E^{ox}$ (V vs. NHE) |
|---|---|---|---|---|
| 1’ | CCCOC(OCOC)C(CCC)(OC)c1ccc([N+](C)(C)C)cc1 |  | 1.14 | |
| 2’ | CCC(OC)(c1ccc(C(C)C)cc1)C(COC)OC(C)C |  | 1.87 | |
| 3’ | COCCc1ccc(C(COC)(COC)C(OC(C)C)OC(C)C)cc1 |  | 1.87 | |
| 4’ | CCOC(OCC)(c1ccc(CCOC)cc1)C(OCCOC)[N+](=O)[O-] |  | 2.23 | |
| 5’ | CCCC(OC(C)C)(c1ccc(CCOCC)cc1)C(COC)Oc1ccccc1 |  | 1.63 | |

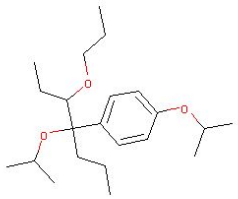
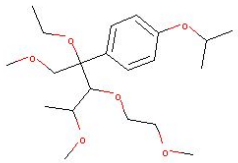
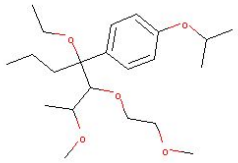
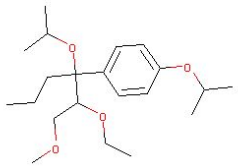
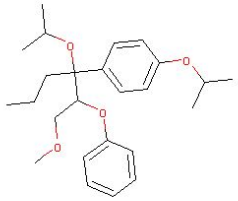
| | | | | |
|---|---|---|---|---|
| 6’ | CCC(Oc1ccccc1)C(OC)(OC(C)C)c1ccc(CCOC)cc1 |  | 1.68 | |
| 7’ | CCC(c1ccc(C(C)OC)cc1)(C(OC(C)C)C(C)OC)[N+](C)(C)C |  | 2.65 | |
| 8’ | CCC(CCOC)(c1ccc([N+](C)(C)C)cc1)C(OC)[N+](=O)[O-] |  | 2.81 | |
| 9’ | CCOC(COC)(c1ccc(C)cc1)C(OC)[N+](C)(C)C |  | 2.43 | |
| 10’ | CCC(c1ccc(OC(C)C)cc1)(C(C)OC)C(COC)OC(C)C |  | 1.49 | |

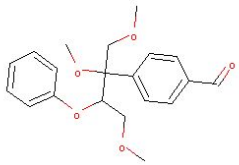
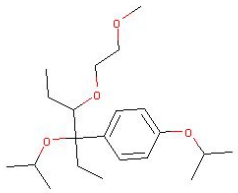
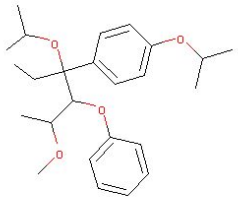
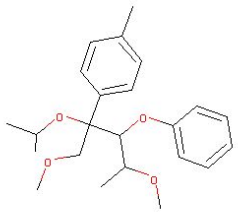
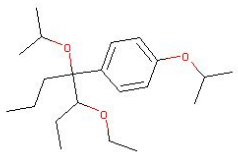
| | | | | |
|---|---|---|---|---|
| 1 | COC(C)c1ccc(C(OC(C)C)(C(C)OC)C(Oc2ccccc2)C(C)OC)cc1 |  | 1.62 | 1.62 |
| 2 | CCCOc1ccc(C(C=O)(C=O)C(C=O)OCCOC)cc1 |  | 1.92 | 1.82 |
| 3 | CCCOc1ccc(C(C(OCC)N(C)C)(N(C)C)N(C)C)cc1 |  | 0.5 | 1.25 |
| 4 | CCOC(OCC)C(Br)(OCC)c1ccc(C=O)cc1 |  | 2.74 | 1.72 |
| 5 | CCOCCCc1ccc(C(OCC)(C(C)OC)C(OCCOC)C(C)OC)cc1 |  | 1.78 | 1.76 |

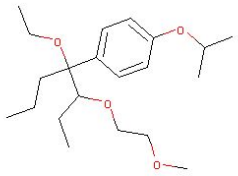
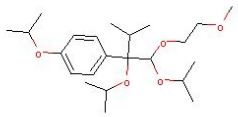
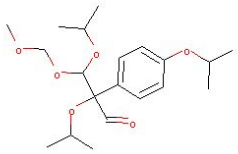
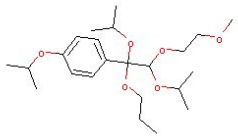
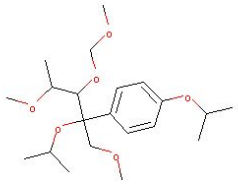
| | | | | |
|---|---|---|---|---|
| 6 | COC(C)C(C=O)(c1ccc([N+](C)(C)C)cc1)C(C=O)Oc1ccccc1 |  | 2.02 | 1.56 |
| 7 | CC(C)OC([N+](=O)[O-])C(c1ccc([N+](C)(C)C)cc1)([N+](=O)[O-])[N+](=O)[O-] |  | 3.44 | 1.23 |
| 8 | CCCOC(C(C)OC)C(OCC)(OCCC)c1ccc(CCCOCC)cc1 |  | 1.77 | 1.67 |
| 9 | CCC(c1ccc(CCOC)cc1)(C(C)OC)C(Oc1ccccc1)C(C)OC |  | 1.77 | 1.64 |
| 10 | CCOC(C=O)(c1ccc(OC(C)C)cc1)C(OCCOC)OC(C)C |  | 1.62 | 1.69 |

| | | | | |
|---|---|---|---|---|
| 11 | CCCOC(CCOC)(c1ccc(CCCOCC)cc1)C(CCOC)OCCOC |  | 1.64 | 1.55 |
| 12 | CC(C)OC(C=O)(c1ccc(Br)cc1)C(Oc1ccccc1)C(C)C |  | 1.73 | 1.67 |
| 13 | CCCOC(OC(C)C)(c1ccc(OC(C)C)cc1)C(Oc1ccccc1)OC(C)C |  | 1.60 | 1.62 |
| 14 | CCOCCCc1ccc(C(Br)(Br)C(OCCOC)OC(C)C)cc1 |  | 2.31 | 1.33 |
| 15 | COCCC(OCOC)C(COC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.50 | 1.72 |

| | | | | |
|---|---|---|---|---|
| 16 | COCCOC(COC)C(COC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.53 | 1.70 |
| 17 | CCCC(OC(C)C)(c1ccc(OC(C)C)cc1)C(Oc1ccccc1)C(C)C |  | 1.55 | 1.60 |
| 18 | CCCOc1ccc(C(CCOC)(OCCC)C(CCOC)OCCOC)cc1 |  | 1.63 | 1.57 |
| 19 | CCCOc1ccc(C(CC)(OCCC)C(Oc2ccccc2)C(C)OC)cc1 |  | 1.58 | 1.63 |
| 20 | CCC(Oc1ccccc1)C(CC)(OC)c1ccc(OC(C)C)cc1 |  | 1.53 | 1.57 |

| | | | | |
|---|---|---|---|---|
| 21 | CCCOC(CC)C(CCC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.43 | 1.60 |
| 22 | CCOC(COC)(c1ccc(OC(C)C)cc1)C(OCCOC)C(C)OC |  | 1.54 | 1.59 |
| 23 | CCCC(OCC)(c1ccc(OC(C)C)cc1)C(OCCOC)C(C)OC |  | 1.57 | 1.56 |
| 24 | CCCC(OC(C)C)(c1ccc(OC(C)C)cc1)C(COC)OCC |  | 1.57 | 1.55 |
| 25 | CCCC(OC(C)C)(c1ccc(OC(C)C)cc1)C(COC)Oc1ccccc1 |  | 1.52 | 1.55 |

| | | | | |
|---|---|---|---|---|
| 26 | COCC(Oc1ccccc1)C(COC)(OC)c1ccc(C=O)cc1 |  | 1.83 | 1.51 |
| 27 | CCC(OCCOC)C(CC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.50 | 1.55 |
| 28 | CCC(OC(C)C)(c1ccc(OC(C)C)cc1)C(Oc1ccccc1)C(C)OC |  | 1.53 | 1.56 |
| 29 | COCC(OC(C)C)(c1ccc(C)cc1)C(Oc1ccccc1)C(C)OC |  | 1.72 | 1.69 |
| 30 | CCCC(OC(C)C)(c1ccc(OC(C)C)cc1)C(CC)OCC |  | 1.50 | 1.54 |

| | | | | |
|---|---|---|---|---|
| 31 | CCCC(OCC)(c1ccc(OC(C)C)cc1)C(CC)OCCOC |  | 1.34 | 1.54 |
| 32 | COCCOC(OC(C)C)C(OC(C)C)(c1ccc(OC(C)C)cc1)C(C)C |  | 1.46 | 1.59 |
| 33 | COCOC(OC(C)C)C(C=O)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.68 | 1.53 |
| 34 | CCCOC(OC(C)C)(c1ccc(OC(C)C)cc1)C(OCCOC)OC(C)C |  | 1.54 | 1.51 |
| 35 | COCOC(C(C)OC)C(COC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.55 | 1.57 |

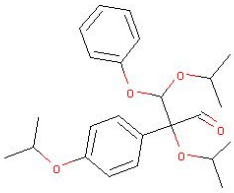
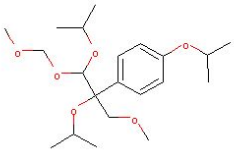
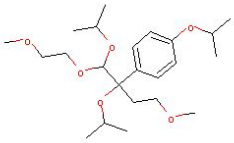
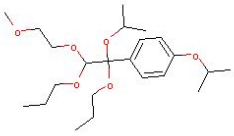
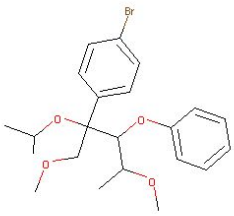
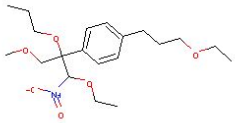
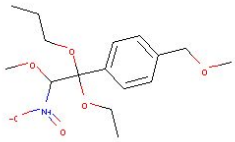
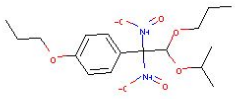
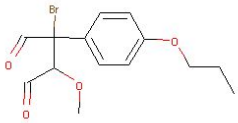
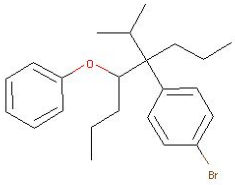
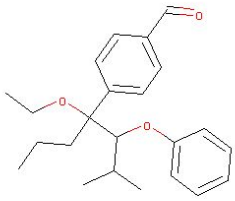
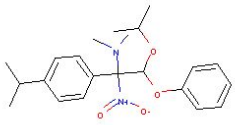
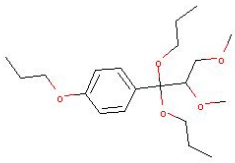
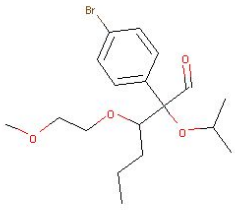
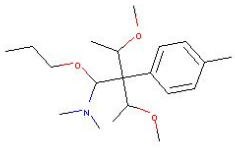
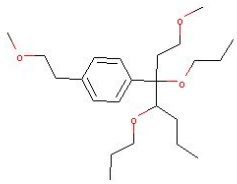
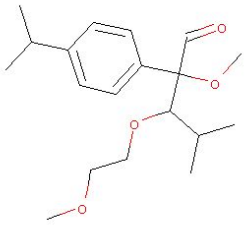
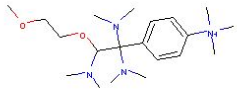
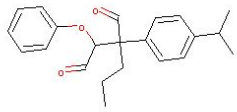
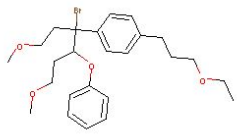
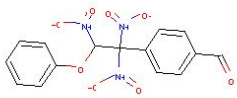
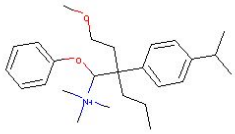
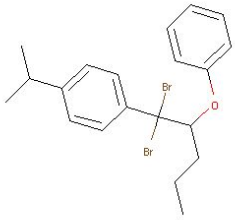
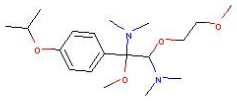
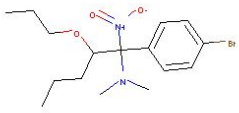
| | | | | |
|---|---|---|---|---|
| 36 | CC(C)Oc1ccc(C(C=O)(OC(C)C)C(Oc2ccccc2)OC(C)C)cc1 |  | 1.66 | 1.59 |
| 37 | COCOC(OC(C)C)C(COC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.53 | 1.53 |
| 38 | COCCOC(OC(C)C)C(CCOC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.53 | 1.52 |
| 39 | CCCOC(OCCOC)C(OCCC)(OC(C)C)c1ccc(OC(C)C)cc1 |  | 1.63 | 1.52 |
| 40 | COCC(OC(C)C)(c1ccc(Br)cc1)C(Oc1ccccc1)C(C)OC |  | 1.75 | 1.56 |

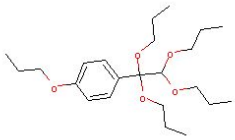
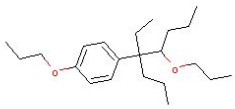
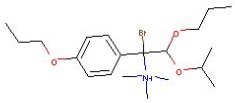
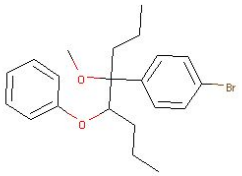
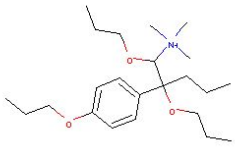
Table S6 List of HBEs evaluated during BO run #2 (BO2) and their corresponding $E^{ox}$. The initial 10 were randomly selected.

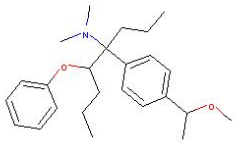
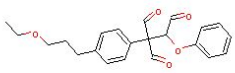
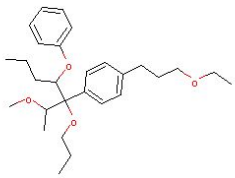
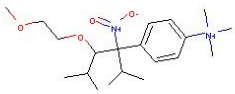
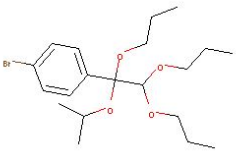
| HBE # | SMILES | 2-D Structure | DFT-computed $E^{ox}$ (V vs. NHE) | BO-computed $E^{ox}$ (V vs. NHE) |
|---|---|---|---|---|
| 1’ | CCCOC(COC)(c1ccc(CCCOCC)cc1)C(OCC)[N+](=O)[O-] |  | 2.08 | |
| 2’ | CCCOC(OCC)(c1ccc(COC)cc1)C(OC)[N+](=O)[O-] |  | 2.29 | |
| 3’ | CCCOc1ccc(C(C(OCCC)OC(C)C)([N+](=O)[O-])[N+](=O)[O-])cc1 |  | 2.07 | |
| 4’ | CCCOc1ccc(C(Br)(C=O)C(C=O)OC)cc1 |  | 1.94 | |
| 5’ | CCCC(Oc1ccccc1)C(CCC)(c1ccc(Br)cc1)C(C)C |  | 1.70 | |

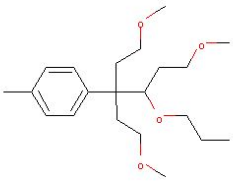
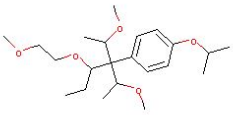
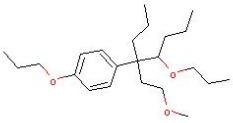
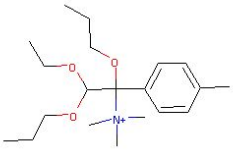
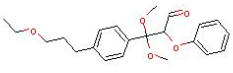
| | | | | |
|---|---|---|---|---|
| 6’ | CCCC(OCC)(c1ccc(C=O)cc1)C(Oc1ccccc1)C(C)C |  | 1.75 | |
| 7’ | CC(C)OC(Oc1ccccc1)C(c1ccc(C(C)C)cc1)(N(C)C)[N+](=O)[O-] |  | 1.67 | |
| 8’ | CCCOc1ccc(C(OCCC)(OCCC)C(COC)OC)cc1 |  | 1.63 | |
| 9’ | CCCC(OCCOC)C(C=O)(OC(C)C)c1ccc(Br)cc1 |  | 1.32 | |
| 10’ | CCCOC(N(C)C)C(c1ccc(C)cc1)(C(C)OC)C(C)OC |  | 0.86 | |

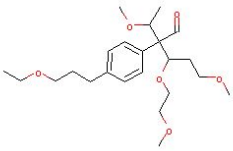
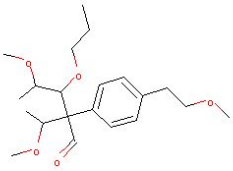
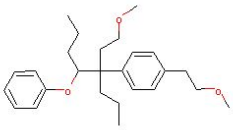
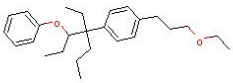
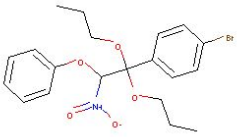
| | | | | |
|---|---|---|---|---|
| 1 | CCCOC(CCC)C(CCOC)(OCCC)c1ccc(CCOC)cc1 |  | 1.65 | 1.81 |
| 2 | COCCOC(C(C)C)C(C=O)(OC)c1ccc(C(C)C)cc1 |  | 1.99 | 1.69 |
| 3 | COCCOC(N(C)C)C(c1ccc([N+](C)(C)C)cc1)(N(C)C)N(C)C |  | -0.47 | 1.67 |
| 4 | CCCC(C=O)(c1ccc(C(C)C)cc1)C(C=O)Oc1ccccc1 |  | 1.89 | 1.73 |
| 5 | CCOCCCc1ccc(C(Br)(COC)C(CCOC)Oc2ccccc2)cc1 |  | 1.70 | 1.65 |

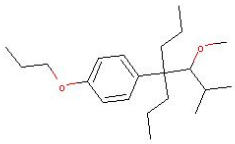
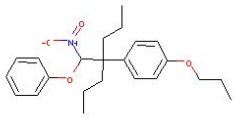
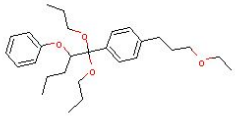
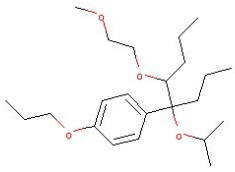
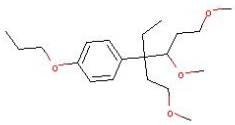
| | | | | |
|---|---|---|---|---|
| 6 | O=Cc1ccc(C(C(Oc2ccccc2)[N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])cc1 |  | 2.53 | 1.68 |
| 7 | CCCC(CCOC)(c1ccc(C(C)C)cc1)C(Oc1ccccc1)[N+](C)(C)C |  | 2.29 | 1.68 |
| 8 | CCCC(Oc1ccccc1)C(Br)(Br)c1ccc(C(C)C)cc1 |  | 1.86 | 1.66 |
| 9 | COCCOC(N(C)C)C(OC)(c1ccc(OC(C)C)cc1)N(C)C |  | -0.33 | 1.70 |
| 10 | CCCOC(CCC)C(c1ccc(Br)cc1)(N(C)C)[N+](=O)[O-] |  | 1.91 | 1.56 |

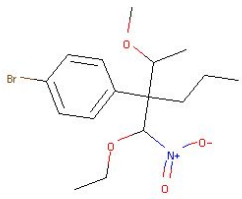
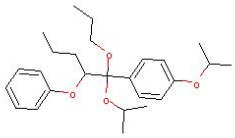
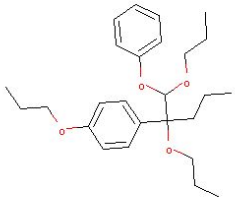
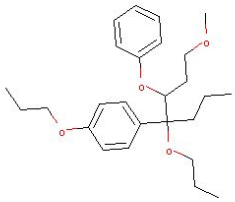
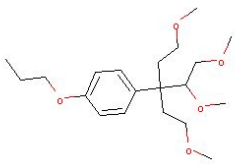
| | | | | |
|---|---|---|---|---|
| 11 | CCCOc1ccc(C(OCCC)(OCCC)C(OCCC)OCCC)cc1 |  | 1.68 | 1.81 |
| 12 | CCCOc1ccc(C(CC)(CCC)C(CCC)OCCC)cc1 |  | 1.50 | 1.90 |
| 13 | CCCOc1ccc(C(Br)(C(OCCC)OC(C)C)[N+](C)(C)C)cc1 |  | 2.31 | 1.65 |
| 14 | CCCC(Oc1ccccc1)C(CCC)(OC)c1ccc(Br)cc1 |  | 1.72 | 1.88 |
| 15 | CCCOc1ccc(C(CCC)(OCCC)C(OCCC)[N+](C)(C)C)cc1 |  | 1.92 | 1.72 |

| | | | | |
|---|---|---|---|---|
| 16 | CCCC(Oc1ccccc1)C(CCC)(c1ccc(C(C)OC)cc1)N(C)C |  | 1.02 | 1.71 |
| 17 | CCOCCCc1ccc(C(C=O)(C=O)C(C=O)Oc2ccccc2)cc1 |  | 1.90 | 1.77 |
| 18 | CCCOC(c1ccc(CCCOCC)cc1)(C(C)OC)C(CCC)Oc1ccccc1 |  | 1.64 | 1.63 |
| 19 | COCCOC(C(C)C)C(c1ccc([N+](C)(C)C)cc1)(C(C)C)[N+](=O)[O-] |  | 2.61 | 1.73 |
| 20 | CCCOC(OCCC)C(OCCC)(OC(C)C)c1ccc(Br)cc1 |  | 2.26 | 1.59 |

| | | | | |
|---|---|---|---|---|
| 21 | CCCOC(CCOC)C(CCOC)(CCOC)c1ccc(C)cc1 |  | 1.99 | 1.75 |
| 22 | CCC(OCCOC)C(c1ccc(OC(C)C)cc1)(C(C)OC)C(C)OC |  | 1.45 | 1.63 |
| 23 | CCCOc1ccc(C(CCC)(CCOC)C(CCC)OCCC)cc1 |  | 1.45 | 1.62 |
| 24 | CCCOC(OCC)C(OCCC)(c1ccc(C)cc1)[N+](C)(C)C |  | 2.53 | 1.63 |
| 25 | CCOCCCc1ccc(C(OC)(OC)C(C=O)Oc2ccccc2)cc1 |  | 1.89 | 1.65 |

| | | | | |
|---|---|---|---|---|
| 26 | CCOCCCc1ccc(C(C=O)(C(C)OC)C(CCOC)OCCOC)cc1 |  | 1.99 | 1.63 |
| 27 | CCCOC(C(C)OC)C(C=O)(c1ccc(CCOC)cc1)C(C)OC |  | 2.01 | 1.73 |
| 28 | CCCC(Oc1ccccc1)C(CCC)(CCOC)c1ccc(CCOC)cc1 |  | 1.67 | 1.68 |
| 29 | CCCC(CC)(c1ccc(CCCOCC)cc1)C(CC)Oc1ccccc1 |  | 1.69 | 1.86 |
| 30 | CCCOC(OCCC)(c1ccc(Br)cc1)C(Oc1ccccc1)[N+](=O)[O-] |  | 2.01 | 1.60 |

| | | | | |
|---|---|---|---|---|
| 31 | CCCOc1ccc(C(CCC)(CCC)C(OC)C(C)C)cc1 |  | 1.47 | 1.70 |
| 32 | CCCOc1ccc(C(CCC)(CCC)C(Oc2ccccc2)[N+](=O)[O-])cc1 |  | 1.72 | 1.81 |
| 33 | CCCOC(OCCC)(c1ccc(CCCOCC)cc1)C(CCC)Oc1ccccc1 |  | 1.72 | 1.56 |
| 34 | CCCOc1ccc(C(CCC)(OC(C)C)C(CCC)OCCOC)cc1 |  | 1.64 | 1.65 |
| 35 | CCCOc1ccc(C(CC)(CCOC)C(CCOC)OC)cc1 |  | 1.52 | 1.70 |

| | | | | |
|---|---|---|---|---|
| 36 | CCCC(c1ccc(Br)cc1)(C(C)OC)C(OCC)[N+](=O)[O-] |  | 2.31 | 1.80 |
| 37 | CCCOC(OC(C)C)(c1ccc(OC(C)C)cc1)C(CCC)Oc1ccccc1 |  | 1.54 | 1.85 |
| 38 | CCCOc1ccc(C(CCC)(OCCC)C(OCCC)Oc2ccccc2)cc1 |  | 1.60 | 1.65 |
| 39 | CCCOc1ccc(C(CCC)(OCCC)C(CCOC)Oc2ccccc2)cc1 |  | 1.61 | 1.56 |
| 40 | CCCOc1ccc(C(CCOC)(CCOC)C(COC)OC)cc1 |  | 1.54 | 1.81 |

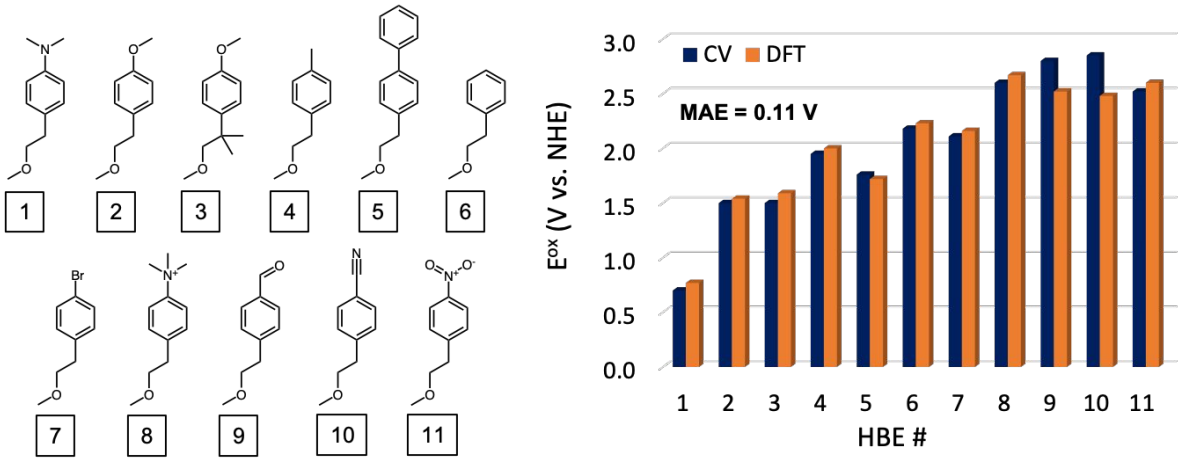



Figure S1 Comparison between DFT-computed oxidation potentials (orange) and cyclic voltammetry measurements (blue) for 11 randomly selected homobenzylic ether molecules

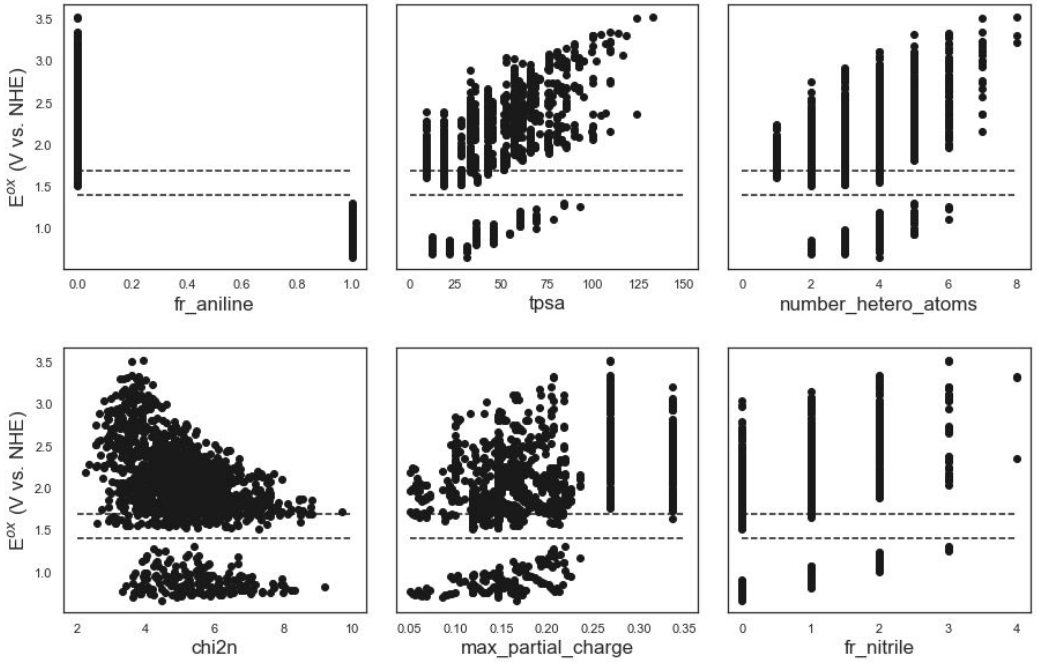



Figure S2 DFT-computed $E^{ox}$ as a function of 6 different features with highest Pearson correlation coefficient values.

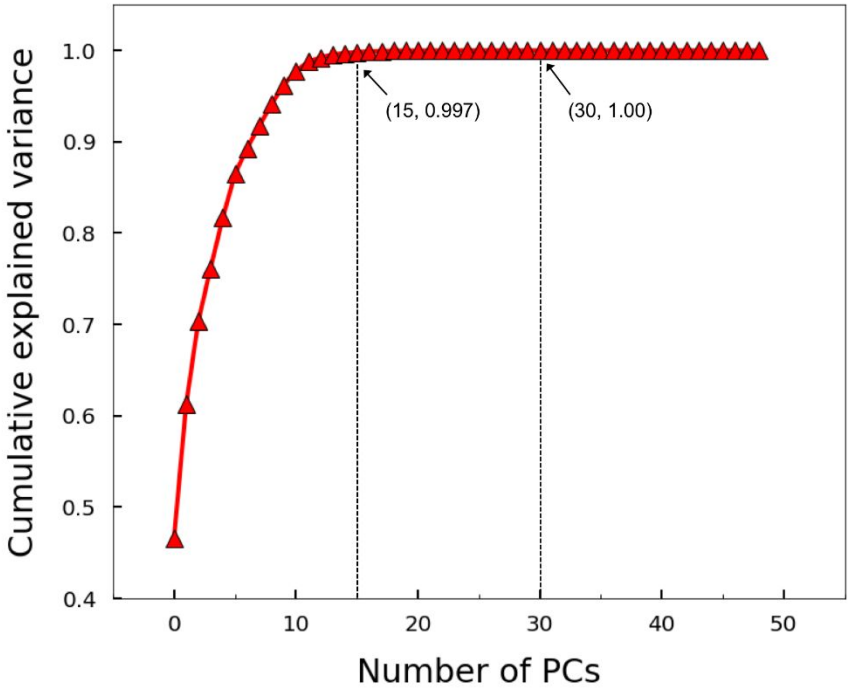



Figure S3 PCA analysis of 49 generated features for 1,400 HBE data set

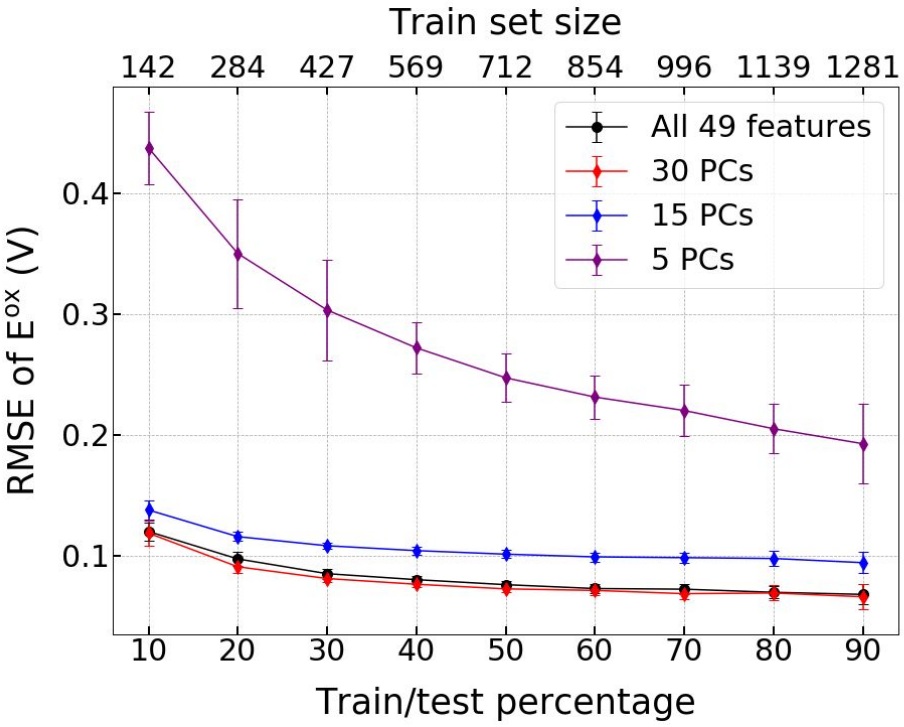



Figure S4 Learning curves of Gaussian Process Regression using various feature sets

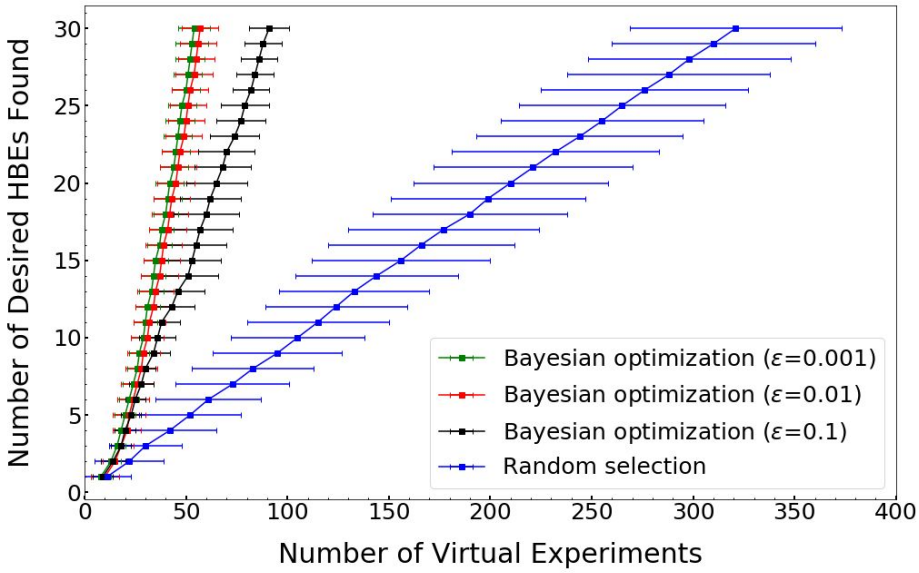



Figure S5 Comparison of sampling efficiency between random selection and Bayesian optimizations with different values of epsilon

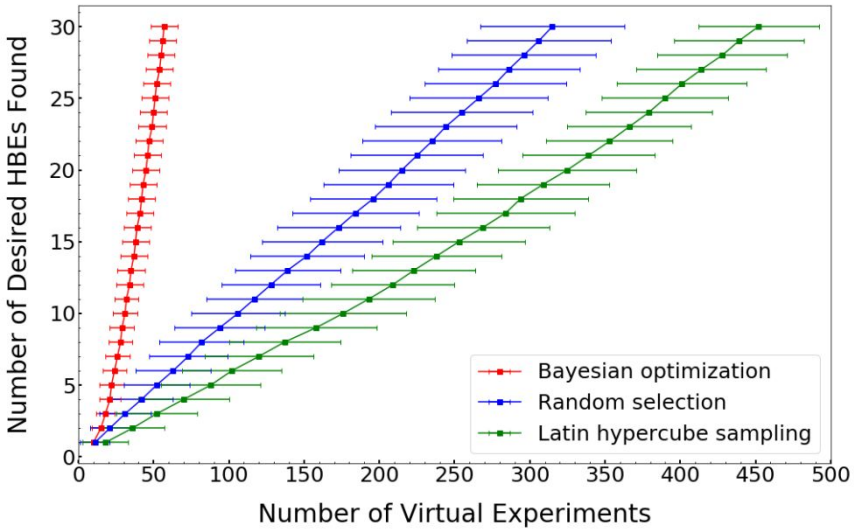



Figure S6 Comparison of efficiency between Bayesian optimization, random selection and Latin hypercube sampling

## References

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