Supplementary Information

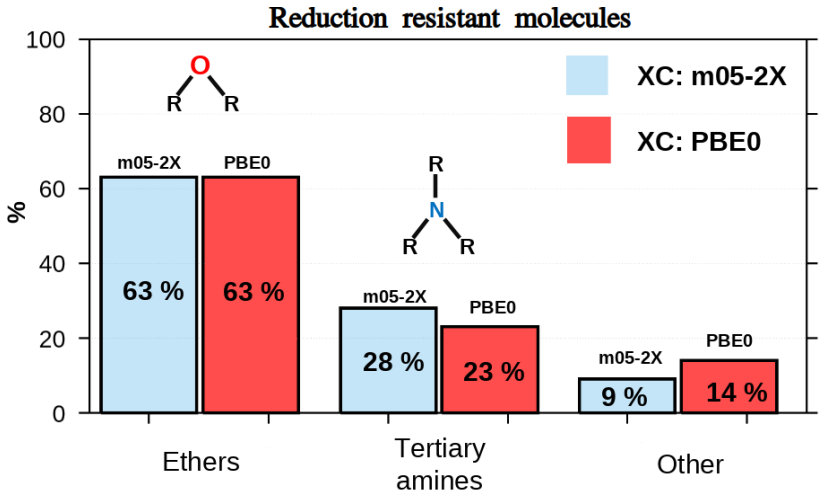

Figure S1: Comparison of the results obtained using the m05-2X and PBE0 exchange-correlation (XC) functionals. The fraction of reduction-resistant molecules in each chemical class is shown. The trend that tertiary amines constitute the second-largest family of reduction-resistant components is consistent across both functionals.

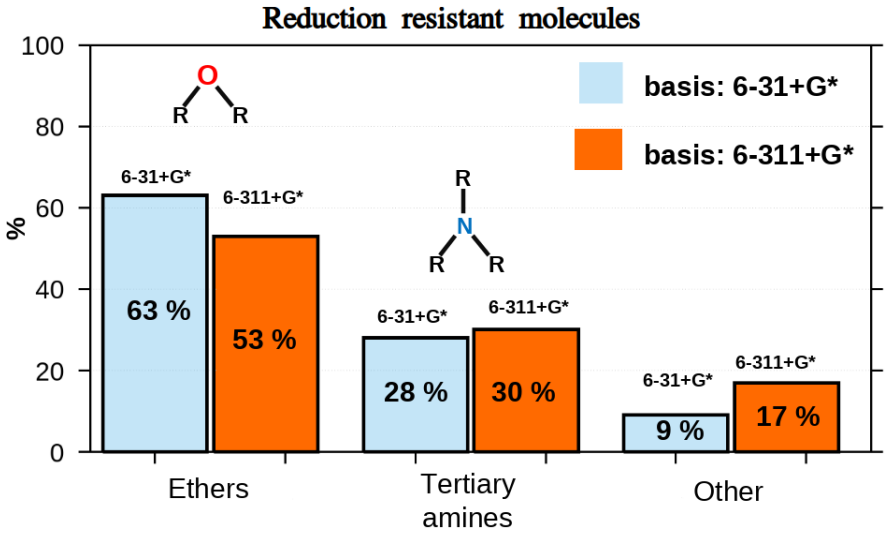

Figure S2: Comparison of the results obtained with the 6-31+G* and 6-311+G* basis sets using the m05-2X functional. The 6-311+G* calculations were performed for a smaller randomly selected subset of 300 molecules. The fraction of reduction-resistant molecules in each chemical class is shown. The trend that tertiary amines constitute the second-largest family of reduction-resistant components is consistent across the two basis sets despite their different sizes.

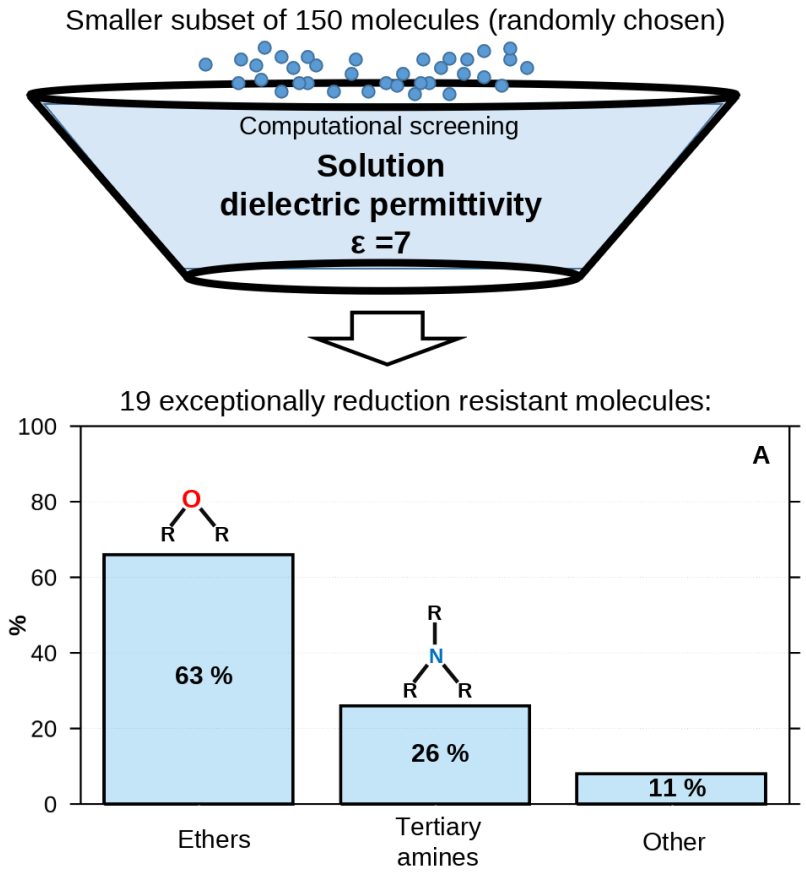

Figure S3: Sensitivity of the simulation results to the dielectric permittivity. Results at ε=7 closely match those at ε=20 reported in the main text, demonstrating no meaningful dependence on ε over a reasonable range.

1 Calculated dataset

Table 1: Dataset with SMILES and cas corresponding to molecules, maximum atomic displacement during reduction d_{max} (Å) and E_{cdft} (eV) calculated via eq. (2)

SMILES	CAS	$d_{\max}$	E_{cDFT}
CCCCN(C)C	927-62-8	0.227	-1.582
CC1(CO1)C=C	1838-94-4	2.780	2.236
CCN(CC)CC	121-44-8	0.369	-2.008
CCC(C)C(=O)C	565-61-7	0.452	0.583
B(CC)(CC)CC	97-94-9	0.891	0.146
C=CN1C=CN=C1	1072-63-5	1.157	0.409
COC(=O)OC	616-38-6	0.686	1.567
CCOC(C)(C)C	637-92-3	0.125	-1.698
CC(C)COC=C	109-53-5	1.069	0.574
CN(C)CC##N	926-64-7	0.822	1.219
C1=CON=C1	288-14-2	0.235	0.714
COCC##C	627-41-8	1.297	2.275
C1=NN=CO1	288-99-3	0.276	1.050
CCOC=O	109-94-4	1.389	1.368
CC1=CC=NC=C1	108-89-4	0.083	0.181

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SMILES	CAS	$d_{\max}$	E_{cDFT}
CCC(C)Cl	78-86-4	1.388	3.376
CC(C)CCC##N	542-54-1	0.842	0.884
CN1CCCCC1	626-67-5	0.042	-1.964
CC(C)OC=O	625-55-8	1.363	1.256
CCC(=O)OC	554-12-1	0.601	1.196
CCCOC=O	110-74-7	1.416	1.359
CCCCCC##N	628-73-9	0.726	0.946
COC=O	107-31-3	1.111	1.507
CCN1CCCC1=O	2687-91-4	2.176	0.499
CCN(CC)C(=O)C	685-91-6	0.443	0.394
CC1=C(OC(=N1)C)C	20662-84-4	1.442	0.537
CC1COC(=O)O1	108-32-7	1.714	3.730
C1CCN(CC1)C=O	2591-86-8	0.890	0.577
CC1=C(N=CC=C1)C	583-61-9	0.571	0.410
CCC1=CC=NC=C1	536-75-4	0.237	0.251
CN(C)[Si](C)(C)C	2083-91-2	0.169	-1.383
CC1C(=NC(O1)C)C	22694-96-8	0.773	0.528
CC1=CN=C(C=C1)C	589-93-5	1.019	0.427
CC1=NC(=CC=C1)C	108-48-5	1.830	0.355
CC1=C(C=NC=C1)C	583-58-4	0.111	0.109
CC1=NCCS1	2346-00-1	0.364	0.763
CCOCC=C(C)C	22094-00-4	1.434	2.333
CC1=NCSC1	52558-99-3	0.582	0.445
CN(C)CCN(C)C	110-18-9	0.594	-2.237
CO[Si](C)(C)C	1825-61-2	0.165	-1.386
CC1=CC(=NC=C1)C	108-47-4	0.353	0.083
B(OC)(OC)OC	121-43-7	2.011	0.771
COC(C=C)OC	6044-68-4	0.620	-0.132
CCC1COC(=O)O1	4437-85-8	0.405	1.709
CC(C)C1=CC=NC=C1	696-30-0	0.434	0.352
COCCC(=O)OC	3852-09-3	1.996	1.064
CO[Si](C)(C)OC	1112-39-6	1.342	0.467
CC(=O)OCCOC	110-49-6	1.698	1.200
C1=CC=C(C=C1)Cl	108-90-7	1.078	4.184
CCCC1=CC=CC=N1	622-39-9	0.364	0.446
C1COCCN1C=O	4394-85-8	1.559	0.951
CCC1=CN=C(C=C1)C	536-88-9	1.324	0.411
CN(C)C(OC)OC	4637-24-5	3.560	2.966
CC1=C(N=C(C=C1)C)C	1462-84-6	0.917	0.276
C1CCC(CC1)Cl	542-18-7	1.842	3.433
CN(C)CC(=O)OC	7148-06-3	1.869	0.982
CC(=O)OCCCC=C	1576-85-8	0.635	1.244
CCCCOC(=O)CC	590-01-2	1.419	0.972
CCC=CCCOC=O	2315-09-5	0.611	1.329
CC/C=C/CC(=O)OC	2396-78-3	1.812	1.175
CCCC(=O)OCCC	105-66-8	1.814	1.163
CCCC1CCC(=O)O1	105-21-5	0.371	0.978
CC(C)(C)OCC1CO1	7665-72-7	2.008	2.563
CC(=C)CCOC(=O)C	5205-07-2	1.024	0.994
CCCCOCC1CO1	2426-08-6	0.927	-1.509
CCCC(C)C(=O)OC	2177-77-7	2.363	1.027
CCOS(=O)(=O)C	62-50-0	0.561	3.359
CC1COC(O1)CC(C)C	18433-93-7	0.867	-1.496
COC1=CC(=CC=C1)OC	151-10-0	1.070	0.044
CCCCCC(=O)OCC	123-66-0	0.385	0.974

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SMILES	CAS	$d_{\max}$	E_{cDFT}
CCCCCC(=O)N(C)C	5830-30-8	0.687	0.467
CC(=O)OCCSC	5862-47-5	2.125	1.183
CN(C=O)C1=CC=CC=C1	93-61-8	1.089	0.598
CCCCN1CCCC1=O	3470-98-2	0.378	0.288
CCN(CC)[Si](C)(C)C	996-50-9	0.621	-1.499
CC(C)CC(C)CC(=O)C	19549-80-5	0.627	0.518
CN(CCC##N)CCC##N	1555-58-4	1.813	1.046
CCOCC(C)OC(=O)C	54839-24-6	2.924	1.012
CCC(=O)OC(C)COC	148462-57-1	2.455	1.006
C(CSCCC##N)C##N	111-97-7	0.755	1.153
C[Si](C)(CCl)Cl	1719-57-9	1.263	4.351
CC(CCOC(=O)C)OC	4435-53-4	1.133	0.951
CCOCCOCCOC	1002-67-1	0.441	-1.986
CC1=C(C=C(C=C1)Cl)C	615-60-1	1.597	4.586
C(C(F)F)(F)F	359-35-3	1.579	1.898
C1=CC=C(C(=C1)F)F	367-11-3	1.068	1.531
CC1=CC(=CC=C1)F	352-70-5	0.435	0.115
CC1CCC(CC1)C(=O)OC	51181-40-9	1.486	0.937
C=COCC(F)(F)F	406-90-6	0.631	2.622
CCCCOC(=O)CC(C)C	109-19-3	0.324	1.086
CCCCC1CCCC(=O)O1	3301-94-8	0.697	0.804
CN(C)CCOCCN(C)C	3033-62-3	0.780	-1.551
CCCCC(CC)OC(=O)C	5921-83-5	2.435	0.999
CC1=CC=C(C=C1)F	352-32-9	0.051	-0.614
C1C(O1)CF	503-09-3	0.827	2.803
CC1(COC1=O)C	1955-45-9	0.714	3.026
CC1CCOC1=O	1679-47-6	0.318	0.989
CCCCOC=C	111-34-2	1.093	0.119
CCCCOC=O	592-84-7	1.426	1.331
COCCOC=C	1663-35-0	1.705	0.068
C=CCOCC=C	557-40-4	1.620	2.600
CCC(C)(C)OC	994-05-8	0.126	-1.946
CC(C)(OC)OC	77-76-9	0.472	-1.629
CC(C)OC(=O)C	108-21-4	0.306	1.188
CC(C)(C)OC=O	762-75-4	1.528	1.216
CC(=C)OC(=O)C	108-22-5	1.189	2.679
CC(C)C(=O)OC	547-63-7	1.517	0.922
CCCOCCC	111-43-3	0.275	-1.805
CCOCC1CO1	4016-11-9	0.669	2.784
CCOCOCC	462-95-3	2.213	-1.694
CC(C)COC=O	542-55-2	1.688	1.330
CCCC(=O)OC	623-42-7	1.461	0.969
CC(=O)OCC=C	591-87-7	0.459	1.307
CCC(=O)OCC	105-37-3	0.693	1.166
CCCOC(=O)CC	106-36-5	0.711	0.837
CN(C)C(=O)N(C)C	632-22-4	1.979	0.619
COCC1=CC=CO1	13679-46-4	1.942	1.808
CCC(=O)OC(C)C	637-78-5	0.598	1.132
CCOC(C)OCC	105-57-7	1.932	-1.715
CC(C)OCC1CO1	4016-14-2	0.292	-1.703
COC1CCC=CO1	4454-05-1	2.016	-0.032
CC(C)(C)C(=O)OC	598-98-1	1.493	0.986
CCC1CCC(=O)O1	695-06-7	0.313	1.005
CCOCCOCC	629-14-1	0.562	-1.953
CC(C)CCOC=O	110-45-2	0.467	-1.470

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SMILES	CAS	$d_{\max}$	E_{cDFT}
CCC1=C(OC(=N1)C)C	30408-61-8	0.981	0.470
C1COC2=CC=CC=C21	496-16-2	0.162	-0.071
CC(C)N1CCOCC1	1004-14-4	0.245	-1.506
CC(C)CC(=O)C(C)C	1888-57-9	0.573	0.514
CCCCCCC1CO1	2984-50-1	0.591	2.391
CCCCC(=O)C(C)C	13019-20-0	0.603	0.409
CCCCC1=CC=CO1	4466-24-4	0.762	0.049
CCCCOCCCC	142-96-1	0.146	-2.106
CCCCN1C=CN=C1	4316-42-1	1.116	-0.120
CCC1CCC(O1)CC	41239-48-9	0.278	-1.652
CC1=CC(=CC=C1)OC	100-84-5	0.469	-0.110
CN1CN(CN(C1)C)C	108-74-7	0.486	-1.739
CCC1=NC(=C(O1)C)C	53833-30-0	1.351	0.501
C1[C@@H](O1)C2=CC=CC=C2	20780-54-5	2.095	2.143
CC1=CC=C(C=C1)OC	104-93-8	1.728	-0.088
CC1=C(SC(=N1)C)C	13623-11-5	1.255	0.505
COC1C=CC(O1)OC	332-77-4	2.579	0.419
CC1=CC=C(C=C1)Cl	106-43-4	1.279	4.213
CCC1=NC(=CS1)C	15679-12-6	0.863	0.696
CCC1N=C(CS1)C	41803-21-8	0.866	0.336
CO[Si](C)(C=C)OC	16753-62-1	1.972	0.432
CC1=C(C=CO1)SC	63012-97-5	0.556	0.120
CC(C)C(=O)OC(C)C	617-50-5	1.788	0.851
CC(C)CCC(=O)OC	2412-80-8	1.776	0.899
CN1CCCN(C1=O)C	7226-23-5	0.639	0.528
CC1=CC(=CC=C1)Cl	108-41-8	1.828	4.975
CCCCCC(=O)OC	106-70-7	1.894	0.937
CCCC(C)OC(=O)C	626-38-0	0.633	1.136
CCOCCOC(=O)C	111-15-9	2.698	0.773
CCCOC(=O)CC(C)C	557-00-6	1.209	0.608
CCC/C=C/C(OC)OC	18318-83-7	1.564	1.812
CCC(C)C(=O)OC(C)C	66576-71-4	2.388	0.844
CCC(C)CC(=O)OCC	5870-68-8	0.665	1.056
CCCCOCCOC=C	4223-11-4	1.664	0.195
CCOC(=O)CCCC=C	54653-25-7	0.661	1.112
CCCC(=O)OCC(=C)C	7149-29-3	3.428	2.860
CCC(CC)C(=O)OCC	2983-38-2	0.938	0.733
CCCCCOC(=O)CCC	540-18-1	2.109	0.832
CC=C(C)C1CCC(O1)(C)C	7416-35-5	1.167	1.673
CC(CC(=O)OC)SC	207983-28-6	0.850	1.308
CC1=CCOC(C1)C=C(C)C	1786-08-9	0.430	-0.383
C[C@@H]1CO[C@@H]2[C@H]1CCC(=C2)C	74410-10-9	1.385	1.575
C1CCC(C1)C2CCCC2=O	4884-24-6	0.312	0.354
CC1CCC(C(=O)C1)C(C)C	491-07-6	0.210	0.475
CC(C)CCOCCC(C)C	544-01-4	0.118	-1.959
C[C@H]1CC[C@@H](CC1=O)C(C)C	13163-73-0	0.157	0.320
CC(=C)C1CCC2(C(C1)O2)C	1195-92-2	0.329	-1.539
CC1=C(OC(=N1)CC(C)C)C	26131-91-9	2.038	0.385
CC(OC)OC	534-15-6	0.611	-1.870
CC1(COC1)C	6921-35-3	1.317	2.531
COCCOC	110-71-4	0.186	-1.758
C1COCOC1	505-22-6	0.065	-1.847
C1C[C@@H]2[C@H](C1)O2	285-67-6	0.283	-2.093
CC1COCO1	1072-47-5	0.642	-1.518
C1CCOCC1	142-68-7	0.060	-2.048

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SMILES	CAS	$d_{\max}$	E_{cDFT}
COCC1CO1	930-37-0	0.289	-1.614
CC(C)(C)OC	1634-04-4	0.090	-1.998
CC1CCOC1	13423-15-9	0.154	-1.615
CCCOCC	628-32-0	0.616	-1.858
CCCCOC	628-28-4	0.129	-1.698
CC1CC(=O)O1	3068-88-0	0.341	1.488
CN1C=CN=C1	616-47-7	1.159	0.142
CC1CCCO1	96-47-9	0.124	-1.620
CC1=NCCO1	1120-64-5	0.829	0.819
C1CC(=O)OC1	96-48-0	1.337	2.966
CCOCC=C	557-31-3	1.471	2.557
CN1C=CC=N1	930-36-9	0.892	0.108
C1CC=COC1	110-87-2	0.484	0.040
C1C(O1)C2CO2	298-18-0	0.640	2.898
CC1=CC=CO1	534-22-5	0.417	0.025
CC1COC(O1)C	3390-12-3	0.474	-1.595
CCN(CC)C=O	617-84-5	1.390	0.735
C[Si](C)(C)C##N	7677-24-9	0.536	0.588
CC1(COC1=O)C	1955-45-9	0.743	2.975
CC1N=C(CO1)C	77311-02-5	0.685	0.739
CCC1=NCCO1	10431-98-8	0.765	0.561
CCC(C)OCC	2679-87-0	0.103	-2.018
CN(C)CCC##N	1738-25-6	0.745	1.087
CCC1=CC=CO1	3208-16-0	1.158	-0.013
CC(C)OC(C)C	108-20-3	0.241	-1.819
CN1CCOCC1	109-02-4	0.100	-1.680
CC1=CC=C(O1)C	625-86-5	0.680	-0.018
CCCCOCC	628-81-9	0.225	-1.778
CC1(C(O1)(C)C)C	5076-20-0	0.082	-2.120
C1CC[C@H]2[C@@H](C1)O2	286-20-4	0.627	2.292
C1CCN(C1)C=O	3760-54-1	0.776	0.592
C=CCN1C=CN=C1	31410-01-2	1.692	0.356
COC1=CC=CC=C1	100-66-3	1.387	-0.123
CC(CCC##N)C##N	4553-62-2	0.771	1.098
C[Si](C)(C)Cl	75-77-4	1.019	2.832
C1CC=C(C1)CC##N	22734-04-9	0.927	1.020
CCCC1=CC=CO1	4229-91-8	2.184	0.049
COC(OC)OC	149-73-5	0.468	-1.837
C1CCS(=O)C1	1600-44-8	0.671	1.928
CCOC(=O)OC	623-53-0	0.681	1.452
CN1CCN(CC1)C	106-58-1	0.139	-1.817
CCN1CCCCC1	766-09-6	0.473	-1.932
CCCCCCOC	4747-07-3	0.107	-1.613
CCCCCCC##N	629-08-3	0.670	0.946
CC(=O)OC(C)(C)C	540-88-5	0.476	1.158
CCCCCOC=O	638-49-3	1.784	1.348
CC(C)CC(=O)OC	556-24-1	0.982	0.929
CCC(C)C(=O)OC	868-57-5	0.715	1.304
COC(=O)CCC=C	818-57-5	2.037	1.299
CCCCC(=O)OC	624-24-8	1.460	0.984
CCC(C)OC(=O)C	105-46-4	2.179	0.960
CCO[Si](C)(C)C	1825-62-3	0.151	-1.497
C1CCC(=O)OCC1	502-44-3	0.338	0.806
CCN(C(C)C)C(C)C	7087-68-5	0.545	-2.044
CC1=CC(=NC(=C1)C)C	108-75-8	0.181	-0.133

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SMILES	CAS	$d_{\max}$	E_{cDFT}
CCCCN(CC)CC	4444-68-2	0.392	-1.852
C1=CC=C(C=C1)CC##N	140-29-4	0.314	-0.120
CN(C)C1CCCCC1	98-94-2	0.113	-1.933
C1CC(OC1)CCl	3003-84-7	2.444	4.101
CCOC(=O)OCC	105-58-8	0.940	1.516
CC1=C(N=C(C=C1)C)C	1462-84-6	1.051	0.308
CC(OC)(OC)OC	1445-45-0	0.281	-1.680
CCCCCCCCC##N	2243-27-8	0.750	0.873
CC1=CC=C(C=C1)N(C)C	99-97-8	0.358	-0.308
CN(C)CC1=CC=CC=C1	103-83-3	0.514	-0.322
C1=CC=C(C=C1)CCC##N	645-59-0	0.679	1.020
C[Si](C)(CC=C)Cl	4028-23-3	1.731	3.096
CN1C=CC2=CC=CC=C21	603-76-9	0.723	-0.043
CC1=CC=CC=C1N(C)C	609-72-3	1.582	-0.251
CC([Si](C)(C)C)Cl	7787-87-3	1.251	3.650
CC1=CC(=CC=C1)N(C)C	121-72-2	0.442	-0.319
CCCCC(=O)OCCC	141-06-0	0.706	1.107
CCCCC1OCC(O1)C	74094-60-3	1.995	-1.515
CCCC1CCCC(=O)O1	698-76-0	0.520	0.709
CN(C)[Si](C)(C)N(C)C	3768-58-9	2.510	-1.251
CCCCCCCCCC##N	1975-78-6	0.748	0.962
CC(C)CCN=CCC(C)C	35448-31-8	1.279	0.073
CC1(CCCC(N1C)(C)C)C	79-55-0	0.213	-1.938
CCOC(OCC)OCC	122-51-0	0.739	-1.709
CC1(CO1)C	558-30-5	1.875	2.531
CC1(CO1)C=C	1838-94-4	2.789	2.317
C1CC1C##N	5500-21-0	0.555	1.134
C1CO1	75-21-8	0.045	-1.863
COC	115-10-6	0.045	-1.837
C/C=C/CC##N	16529-66-1	0.780	1.049
C=COC=C	109-93-3	0.454	0.720
CN(C)C##N	1467-79-4	0.966	1.517
[2H]C([2H])([2H])C##N	2206-26-0	0.407	1.086
CC(=C)OC	116-11-0	0.895	-0.125
C1=COC=C1	110-00-9	0.310	0.139
CC##N	75-05-8	0.406	1.015
CCC1CO1	106-88-7	0.594	2.507
CC(C)Cl	75-29-6	1.553	3.559
CCN(C)C	598-56-1	0.063	-2.111
CC(C)C##N	78-82-0	0.718	0.985
CN1C=CC=C1	96-54-8	1.289	-0.352
CN(C)CC##C	7223-38-3	0.658	1.216
C1COCO1	646-06-0	0.839	2.968
C1C=CCO1	1708-29-8	0.274	0.141
COCOC	109-87-5	0.252	-1.587
C1COC1	503-30-0	0.080	-1.734
CC(C=C)C##N	16529-56-9	0.733	1.157
CCOC=C	109-92-2	1.346	0.077
CCCCC##N	110-59-8	0.827	0.915
CCCC##N	109-74-0	0.602	0.962
C=CCCC##N	592-51-8	0.821	0.959
COOC	690-02-8	0.471	2.891
C1CCOC1	109-99-9	0.064	-2.102
CC1CO1	75-56-9	0.061	-1.459
CCC##N	107-12-0	0.603	1.011

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SMILES	CAS	$d_{\max}$	E_{cDFT}
CN1CCCC1	120-94-5	0.101	-1.896
CCOC	540-67-0	0.522	-1.738
C1COC=C1	1191-99-7	0.624	0.392
CC(C)N(C)C	996-35-0	0.167	-2.079
C1COC1=O	57-57-8	0.884	3.182
CCCOC	557-17-5	0.261	-2.053
CCCN(C)C	926-63-6	0.256	-1.618
CCOCC	60-29-7	0.114	-1.924
C=CCC##N	109-75-1	0.694	1.107
CC1C(O1)C	3266-23-7	0.157	-1.875
CS(=O)C	67-68-5	0.120	-1.969
COC=C	107-25-5	1.064	0.102
CCCCC(=O)OCCCC	591-68-4	0.673	1.106
CCCCC(CC)C(=O)OC	816-19-3	1.819	0.850
CCCCCCC(OC)OC	10032-05-0	0.160	-1.822