Supporting Material

Assessment of the Performance of DFT Functionals in the Fulfillment of Off-Diagonal Hypervirial Relationships

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1 Cartesian coordinates in Bohr used for the calculations

Table S1: Geometries used for the APFD calculations.

C_2H_6

C	0.00000	1.44480	-0.00588
C	0.00000	-1.44480	-0.00588
H	1.35400	2.20973	-1.35990
H	-1.85818	2.22113	-0.44116
H	0.55582	2.18935	1.83636
H	-1.35400	-2.20973	-1.35990
H	1.85818	-2.22113	-0.44116
H	-0.55582	-2.18935	1.83636

H_2O_2

O	-0.01493	1.34871	-0.28924
O	0.01493	-1.34871	-0.28924
H	-1.46110	-1.71931	0.70836
H	1.46110	1.71931	0.70836

CH_3NH_2

C	1.33206	-0.00074	0.03163
H	2.04162	-0.93385	1.73990
H	2.18833	-0.96194	-1.58345
H	2.03607	1.93425	0.02265
N	-1.40769	-0.00177	-0.21550
H	-2.20688	-1.55448	0.54790
H	-2.19769	1.53287	0.59169

N_2H_4

N	0.00000	1.36465	-0.20738
N	0.00000	-1.36465	-0.20738
H	-0.95917	2.02503	1.32681
H	1.80487	1.90909	0.12487
H	-1.80487	-1.90909	0.12487
H	0.95917	-2.02503	1.32681

CH_3OH

C	1.25003	0.03560	0.00408
H	2.04467	-1.59153	-0.97783
H	2.01278	0.09007	1.92707
H	1.87463	1.73312	-0.99866
O	-1.40800	-0.23159	0.00267
H	-2.16824	1.40747	0.00359

NH_2OH

N	1.30289	0.11122	-0.27029
O	-1.36282	-0.23038	0.10816
H	-2.07337	1.34785	-0.42942
H	1.99213	-1.58215	0.31331
H	1.86361	1.29876	1.14284

Table S2: Geometries used for the B3LYP calculations.

C_2H_6

C	0.00000	1.44792	-0.00580
C	0.00000	-1.44792	-0.00580
H	1.35307	2.21026	-1.35887
H	-1.85684	2.22106	-0.44188
H	0.55421	2.18984	1.83553
H	-1.35307	-2.21026	-1.35887
H	1.85684	-2.22106	-0.44188
H	-0.55421	-2.18984	1.83553

H_2O_2

O	0.00000	1.36782	-0.10932
O	0.00000	-1.36782	-0.10932
H	-1.49703	-1.71137	0.87457
H	1.49703	1.71137	0.87457

CH_3NH_2

C	1.33951	-0.00070	0.03120
H	2.04372	-0.92907	1.74153
H	2.19294	-0.96582	-1.58022
H	2.03724	1.93417	0.01895
N	-1.41358	-0.00210	-0.21485
H	-2.21316	-1.55623	0.54764
H	-2.20273	1.53584	0.58885

N_2H_4

N	0.00000	1.37708	-0.20748
N	0.00000	-1.37708	-0.20748
H	-0.96419	2.03046	1.32720
H	1.80702	1.91729	0.12516
H	-1.80702	-1.91729	0.12516
H	0.96419	-2.03046	1.32720

CH_3OH

C	1.26105	0.03603	0.00360
H	2.05037	-1.59094	-0.97676
H	2.01397	0.09183	1.92642
H	1.86966	1.73491	-0.99747
O	-1.41493	-0.23255	0.00290
H	-2.18085	1.40841	0.00303

NH_2OH

N	1.32103	0.11075	-0.26947
O	-1.37881	-0.23046	0.10707
H	-2.08376	1.35490	-0.43181
H	1.99895	-1.58788	0.31497
H	1.86810	1.30143	1.14659

Table S3: Geometries used for the B3P86 calculations.

C_2H_6

C	0.00000	1.44102	-0.00579
C	0.00000	-1.44102	-0.00579
H	1.35296	2.20217	-1.35876
H	-1.85665	2.21315	-0.44194
H	0.55408	2.18168	1.83542
H	-1.35296	-2.20217	-1.35876
H	1.85665	-2.21315	-0.44194
H	-0.55408	-2.18168	1.83542

H_2O_2

O	0.00000	1.35232	-0.11111
O	0.00000	-1.35232	-0.11111
H	-1.48085	-1.70194	0.88888
H	1.48085	1.70194	0.88888

CH_3NH_2

C	1.33132	-0.00087	0.03135
H	2.03676	-0.93482	1.73811
H	2.19038	-0.95833	-1.58192
H	2.03175	1.93297	0.02714
N	-1.40746	-0.00206	-0.21651
H	-2.20316	-1.55365	0.55103
H	-2.19143	1.53347	0.59311

N_2H_4

N	0.00000	1.36577	-0.20758
N	0.00000	-1.36577	-0.20758
H	-0.95857	2.02123	1.32828
H	1.80528	1.90709	0.12475
H	-1.80528	-1.90709	0.12475
H	0.95857	-2.02123	1.32828

CH_3OH

C	1.25082	0.03566	0.00386
H	2.04817	-1.58872	-0.97565
H	2.01059	0.09423	1.92499
H	1.86381	1.73309	-0.99885
O	-1.40744	-0.23247	0.00291
H	-2.16792	1.40720	0.00303

NH_2OH

N	1.30557	0.11121	-0.27002
O	-1.36511	-0.23058	0.10786
H	-2.07163	1.35044	-0.43038
H	1.99236	-1.58299	0.31326
H	1.86112	1.29869	1.14442

Table S4: Geometries used for the B3PW91 calculations.

C_2H_6

C	0.00000	1.44325	-0.00579
C	0.00000	-1.44325	-0.00579
H	1.35411	2.20562	-1.35991
H	-1.85821	2.21665	-0.44227
H	0.55461	2.18517	1.83694
H	-1.35411	-2.20562	-1.35991
H	1.85821	-2.21665	-0.44227
H	-0.55461	-2.18517	1.83694

H_2O_2

O	0.00000	1.35394	-0.11115
O	0.00000	-1.35394	-0.11115
H	-1.48109	-1.70354	0.88920
H	1.48109	1.70354	0.88920

CH_3NH_2

C	1.33281	-0.00082	0.03132
H	2.03972	-0.93551	1.73957
H	2.19322	-0.95946	-1.58312
H	2.03495	1.93445	0.02690
N	-1.40928	-0.00204	-0.21654
H	-2.20565	-1.55429	0.55116
H	-2.19415	1.53399	0.59330

N_2H_4

N	0.00000	1.36715	-0.20777
N	0.00000	-1.36715	-0.20777
H	-0.95833	2.02274	1.32962
H	1.80641	1.90824	0.12476
H	-1.80641	-1.90824	0.12476
H	0.95833	-2.02274	1.32962

CH_3OH

C	1.25177	0.03560	0.00385
H	2.04848	-1.59082	-0.97708
H	2.01269	0.09274	1.92680
H	1.86713	1.73439	-0.99925
O	-1.40905	-0.23240	0.00290
H	-2.16657	1.40929	0.00327

NH_2OH

N	1.30699	0.11122	-0.27019
O	-1.36665	-0.23058	0.10789
H	-2.07249	1.35132	-0.43063
H	1.99352	-1.58426	0.31347
H	1.86322	1.29903	1.14540

Table S5: Geometries used for the B97D calculations.

C_2H_6

C	0.00000	1.45587	-0.00572
C	0.00000	-1.45587	-0.00572
H	1.36305	2.21562	-1.36879
H	-1.87063	2.22585	-0.44654
H	0.55647	2.19477	1.84965
H	-1.36305	-2.21562	-1.36879
H	1.87063	-2.22585	-0.44654
H	-0.55647	-2.19477	1.84965

H_2O_2

O	0.00000	1.38280	-0.11385
O	0.00000	-1.38280	-0.11385
H	-1.48494	-1.70561	0.91079
H	1.48494	1.70561	0.91079

CH_3NH_2

C	1.34639	-0.00011	0.03150
H	2.04637	-0.96907	1.73700
H	2.20564	-0.94168	-1.60687
H	2.03723	1.94965	0.05915
N	-1.42516	-0.00240	-0.22546
H	-2.20154	-1.55684	0.57932
H	-2.18988	1.53537	0.62066

N_2H_4

N	0.00000	1.38704	-0.21195
N	0.00000	-1.38704	-0.21195
H	-0.93617	2.02687	1.35995
H	1.82348	1.90450	0.12372
H	-1.82348	-1.90450	0.12372
H	0.93617	-2.02687	1.35995

CH_3OH

C	1.26793	0.03433	0.00335
H	2.05738	-1.60733	-0.98108
H	2.02618	0.09714	1.94043
H	1.87701	1.74357	-1.00963
O	-1.42590	-0.23354	0.00368
H	-2.16095	1.42891	0.00078

NH_2OH

N	-1.32897	-0.11662	-0.28572
O	1.39410	0.23876	0.11744
H	2.08212	-1.35606	-0.43921
H	-2.00213	1.58991	0.31605
H	-1.86951	-1.30086	1.15449

Table S6: Geometries used for the B97D3 calculations.

C_2H_6

C	0.00000	1.45104	-0.00586
C	0.00000	-1.45104	-0.00586
H	1.35925	2.21419	-1.36512
H	-1.86529	2.22524	-0.44367
H	0.55690	2.19352	1.84396
H	-1.35925	-2.21419	-1.36512
H	1.86529	-2.22524	-0.44367
H	-0.55690	-2.19352	1.84396

H_2O_2

O	0.00000	1.38276	-0.11181
O	0.00000	-1.38276	-0.11181
H	-1.49772	-1.70445	0.89448
H	1.49772	1.70445	0.89448

CH_3NH_2

C	1.34310	0.00001	0.03193
H	2.05021	-0.96265	1.73427
H	2.20080	-0.94483	-1.60146
H	2.04027	1.94424	0.05071
N	-1.42162	-0.00204	-0.22357
H	-2.20450	-1.55664	0.57295
H	-2.19401	1.53406	0.61698

N_2H_4

N	0.00000	1.38514	-0.21164
N	0.00000	-1.38514	-0.21164
H	-0.93536	2.03149	1.35770
H	1.82195	1.90572	0.12375
H	-1.82195	-1.90572	0.12375
H	0.93536	-2.03149	1.35770

CH_3OH

C	1.26577	0.03494	0.00354
H	2.05468	-1.60219	-0.98068
H	2.02531	0.09287	1.93569
H	1.88026	1.73990	-1.00503
O	-1.42353	-0.23324	0.00332
H	-2.16665	1.42573	0.00218

NH_2OH

N	-1.32903	-0.11790	-0.28707
O	1.39211	0.23795	0.11772
H	2.08461	-1.35474	-0.44003
H	-2.00028	1.58799	0.31720
H	-1.87180	-1.29818	1.15524

Table S7: Geometries used for the B98 calculations.

C_2H_6

C	0.00000	1.45032	-0.00572
C	0.00000	-1.45032	-0.00572
H	1.35567	2.21050	-1.36140
H	-1.86028	2.22110	-0.44383
H	0.55394	2.19008	1.83955
H	-1.35567	-2.21050	-1.36140
H	1.86028	-2.22110	-0.44383
H	-0.55394	-2.19008	1.83955

H_2O_2

O	0.00000	1.35866	-0.11059
O	0.00000	-1.35866	-0.11059
H	-1.48487	-1.70498	0.88475
H	1.48487	1.70498	0.88475

CH_3NH_2

C	1.33959	-0.00057	0.03157
H	2.04123	-0.94415	1.73740
H	2.19352	-0.95529	-1.58900
H	2.03647	1.93736	0.03414
N	-1.41526	-0.00195	-0.21874
H	-2.20639	-1.55483	0.55841
H	-2.19558	1.53398	0.60082

N_2H_4

N	0.00000	1.37757	-0.20880
N	0.00000	-1.37757	-0.20880
H	-0.95325	2.02524	1.33704
H	1.81088	1.91030	0.12455
H	-1.81088	-1.91030	0.12455
H	0.95325	-2.02524	1.33704

CH_3OH

C	1.25521	0.03570	0.00372
H	2.04903	-1.59273	-0.97791
H	2.01327	0.09220	1.92859
H	1.86865	1.73631	-0.99934
O	-1.41134	-0.23230	0.00290
H	-2.17147	1.40841	0.00313

NH_2OH

N	1.31564	0.11158	-0.27062
O	-1.37420	-0.23033	0.10739
H	-2.07556	1.35305	-0.43192
H	1.99533	-1.58772	0.31488
H	1.86430	1.29625	1.15226

Table S8: Geometries used for the B972 calculations.

C_2H_6

C	0.00000	1.44264	-0.00569
C	0.00000	-1.44264	-0.00569
H	1.35254	2.20337	-1.35823
H	-1.85572	2.21482	-0.44206
H	0.55426	2.18358	1.83443
H	-1.35254	-2.20337	-1.35823
H	1.85572	-2.21482	-0.44206
H	-0.55426	-2.18358	1.83443

H_2O_2

O	0.00000	1.34899	-0.11125
O	0.00000	-1.34899	-0.11125
H	-1.47195	-1.70034	0.88999
H	1.47195	1.70034	0.88999

CH_3NH_2

C	1.33105	-0.00062	0.03135
H	2.03677	-0.94027	1.73343
H	2.18880	-0.95341	-1.58370
H	2.03156	1.93187	0.03278
N	-1.40834	-0.00195	-0.21750
H	-2.19815	-1.54889	0.55459
H	-2.18688	1.52810	0.59734

N_2H_4

N	0.00000	1.36470	-0.20747
N	0.00000	-1.36470	-0.20747
H	-0.95285	2.01789	1.32805
H	1.80186	1.90298	0.12423
H	-1.80186	-1.90298	0.12423
H	0.95285	-2.01789	1.32805

CH_3OH

C	1.25050	0.03517	0.00380
H	2.04615	-1.58894	-0.97470
H	2.00968	0.09371	1.92376
H	1.86450	1.73115	-0.99822
O	-1.40782	-0.23151	0.00296
H	-2.16078	1.40510	0.00266

NH_2OH

N	1.30381	0.11121	-0.26981
O	-1.36333	-0.22968	0.10761
H	-2.06775	1.34536	-0.42918
H	1.98909	-1.57890	0.31274
H	1.85865	1.29256	1.14420

Table S9: Geometries used for the BLYP calculations.

C_2H_6

C	0.00000	1.45846	-0.00574
C	0.00000	-1.45846	-0.00574
H	1.36149	2.22399	-1.36724
H	-1.86814	2.23476	-0.44566
H	0.55649	2.20375	1.84737
H	-1.36149	-2.22399	-1.36724
H	1.86814	-2.23476	-0.44566
H	-0.55649	-2.20375	1.84737

H_2O_2

O	0.00000	1.40619	-0.10945
O	0.00000	-1.40619	-0.10945
H	-1.52917	-1.71660	0.87557
H	1.52917	1.71660	0.87557

CH_3NH_2

C	1.35384	-0.00027	0.03210
H	2.06082	-0.95779	1.73996
H	2.20823	-0.95161	-1.60228
H	2.04931	1.94750	0.04344
N	-1.42987	-0.00210	-0.22271
H	-2.22166	-1.56407	0.57108
H	-2.21069	1.54229	0.61413

N_2H_4

N	0.00000	1.40162	-0.21223
N	0.00000	-1.40162	-0.21223
H	-0.94502	2.04700	1.36082
H	1.83102	1.91960	0.12483
H	-1.83102	-1.91960	0.12483
H	0.94502	-2.04700	1.36082

CH_3OH

C	1.27928	0.03586	0.00352
H	2.06023	-1.60548	-0.98435
H	2.03351	0.08884	1.93939
H	1.89045	1.74400	-1.00470
O	-1.43408	-0.23451	0.00316
H	-2.18724	1.43360	0.00329

NH_2OH

N	-1.34898	-0.11829	-0.29027
O	1.41304	0.24232	0.11813
H	2.10506	-1.36383	-0.44428
H	-2.01083	1.59896	0.31860
H	-1.88267	-1.30404	1.16087

Table S10: Geometries used for the CAM-B3LYP calculations.

C_2H_6

C	0.00000	1.44226	-0.00574
C	0.00000	-1.44226	-0.00574
H	1.35188	2.20177	-1.35763
H	-1.85527	2.21238	-0.44200
H	0.55312	2.18138	1.83405
H	-1.35188	-2.20177	-1.35763
H	1.85527	-2.21238	-0.44200
H	-0.55312	-2.18138	1.83405

H_2O_2

O	0.00000	1.35056	-0.10911
O	0.00000	-1.35056	-0.10911
H	-1.48989	-1.71056	0.87285
H	1.48989	1.71056	0.87285

CH_3NH_2

C	1.33491	-0.00113	0.03086
H	2.03350	-0.91348	1.74783
H	2.18703	-0.97715	-1.57062
H	2.03233	1.93121	0.00329
N	-1.40666	-0.00196	-0.21051
H	-2.21279	-1.55736	0.53328
H	-2.20295	1.53731	0.57462

N_2H_4

N	0.00000	1.36600	-0.20512
N	0.00000	-1.36600	-0.20512
H	-0.98216	2.02444	1.30974
H	1.79920	1.92060	0.12609
H	-1.79920	-1.92060	0.12609
H	0.98216	-2.02444	1.30974

CH_3OH

C	1.25392	0.03657	0.00376
H	2.04733	-1.58580	-0.97646
H	2.00636	0.09135	1.92397
H	1.86062	1.73496	-0.99489
O	-1.40682	-0.23246	0.00258
H	-2.18328	1.39976	0.00418

NH_2OH

N	-1.30805	-0.10623	-0.26068
O	1.36373	0.22902	0.09972
H	2.07923	-1.35130	-0.42778
H	-1.99703	1.58800	0.31171
H	-1.86227	-1.30435	1.14009

Table S11: Geometries used for the HF calculations.

C_2H_6

C	0.00000	1.44540	-0.00580
C	0.00000	-1.44540	-0.00580
H	1.34610	2.19640	-1.35180
H	-1.84760	2.20620	-0.44010
H	0.55040	2.17530	1.82660
H	-1.34610	-2.19640	-1.35180
H	1.84760	-2.20620	-0.44010
H	-0.55040	-2.17530	1.82660

H_2O_2

O	0.00000	1.30749	-0.10823
O	0.00000	-1.30749	-0.10823
H	-1.43216	-1.71197	0.86584
H	1.43216	1.71197	0.86584

CH_3NH_2

C	1.33101	-0.00054	0.02964
H	2.01489	-0.90873	1.73946
H	2.17263	-0.97895	-1.55898
H	2.02662	1.92027	0.00228
N	-1.40275	-0.00171	-0.20840
H	-2.19560	-1.53762	0.53035
H	-2.18535	1.52020	0.56785

N_2H_4

N	0.00000	1.35037	-0.20021
N	0.00000	-1.35037	-0.20021
H	-0.98949	2.00361	1.27599
H	1.76927	1.91419	0.12549
H	-1.76927	-1.91419	0.12549
H	0.98949	-2.00361	1.27599

CH_3OH

C	1.24039	0.03557	0.00335
H	2.03753	-1.57435	-0.96644
H	1.98362	0.09647	1.91184
H	1.83931	1.72624	-0.98743
O	-1.39102	-0.22772	0.00252
H	-2.17467	1.36000	0.00181

NH_2OH

N	1.27399	0.10096	-0.25903
O	-1.33395	-0.22509	0.10739
H	-2.08200	1.29409	-0.42079
H	1.99556	-1.54353	0.32078
H	1.84015	1.34342	1.05410

Table S12: Geometries used for the LSDA calculations.

C_2H_6

C	0.00000	1.42835	-0.00640
C	0.00000	-1.42835	-0.00640
H	1.36056	2.20534	-1.36696
H	-1.86779	2.21773	-0.43886
H	0.56324	2.18323	1.84420
H	-1.36056	-2.20534	-1.36696
H	1.86779	-2.21773	-0.43886
H	-0.56324	-2.18323	1.84420

H_2O_2

O	0.00000	1.34816	-0.11290
O	0.00000	-1.34816	-0.11290
H	-1.49701	-1.70079	0.90323
H	1.49701	1.70079	0.90323

CH_3NH_2

C	1.31775	-0.00152	0.03196
H	2.05366	-0.90483	1.76539
H	2.19571	-0.98979	-1.57656
H	2.03224	1.94426	-0.01476
N	-1.39344	-0.00246	-0.20778
H	-2.22236	-1.57486	0.52034
H	-2.21168	1.55159	0.56829

N_2H_4

N	0.00000	1.35315	-0.20794
N	0.00000	-1.35315	-0.20794
H	-0.97637	2.03869	1.32907
H	1.81659	1.91815	0.12647
H	-1.81659	-1.91815	0.12647
H	0.97637	-2.03869	1.32907

CH_3OH

C	1.23804	0.03720	0.00452
H	2.05401	-1.59602	-0.98463
H	2.02178	0.09551	1.93742
H	1.86895	1.74446	-1.00833
O	-1.39925	-0.23556	0.00294
H	-2.17902	1.41732	0.00493

NH_2OH

N	1.29393	0.11331	-0.27365
O	-1.35619	-0.23400	0.11037
H	-2.07725	1.36067	-0.43229
H	2.00126	-1.59160	0.31254
H	1.86800	1.30975	1.15236

Table S13: Geometries used for the M06 calculations.

C_2H_6

C	0.00000	1.43781	-0.00571
C	0.00000	-1.43781	-0.00571
H	1.35195	2.19709	-1.35767
H	-1.85532	2.20757	-0.44248
H	0.55264	2.17650	1.83443
H	-1.35195	-2.19709	-1.35767
H	1.85532	-2.20757	-0.44248
H	-0.55264	-2.17650	1.83443

H_2O_2

O	0.00000	1.34143	-0.11126
O	0.00000	-1.34143	-0.11126
H	-1.47486	-1.70308	0.89006
H	1.47486	1.70308	0.89006

CH_3NH_2

C	1.33025	-0.00106	0.03115
H	2.03470	-0.92237	1.74235
H	2.18909	-0.96673	-1.57506
H	2.02761	1.93167	0.01481
N	-1.40451	-0.00232	-0.21319
H	-2.20649	-1.55394	0.54104
H	-2.19481	1.53399	0.58233

N_2H_4

N	0.00000	1.36448	-0.20717
N	0.00000	-1.36448	-0.20717
H	-0.96080	2.01814	1.32552
H	1.80254	1.90812	0.12465
H	-1.80254	-1.90812	0.12465
H	0.96080	-2.01814	1.32552

CH_3OH

C	1.24433	0.03605	0.00379
H	2.04676	-1.58476	-0.97513
H	2.00838	0.09331	1.92181
H	1.85939	1.73227	-0.99601
O	-1.40148	-0.23223	0.00287
H	-2.16866	1.40068	0.00371

NH_2OH

N	1.29791	0.11100	-0.26996
O	-1.35795	-0.23055	0.10845
H	-2.07515	1.34296	-0.42915
H	1.99446	-1.57733	0.31366
H	1.85888	1.30170	1.13765

Table S14: Geometries used for the M06-2X calculations.

C_2H_6

C	0.00000	1.44375	-0.00586
C	0.00000	-1.44375	-0.00586
H	1.35165	2.20135	-1.35752
H	-1.85504	2.21233	-0.44094
H	0.55404	2.18022	1.83362
H	-1.35165	-2.20135	-1.35752
H	1.85504	-2.21233	-0.44094
H	-0.55404	-2.18022	1.83362

H_2O_2

O	0.00000	1.35960	-0.08977
O	0.00000	-1.35960	-0.08977
H	-1.55209	-1.83725	0.71819
H	1.55209	1.83725	0.71819

CH_3NH_2

C	1.33601	-0.00098	0.03149
H	2.03111	-0.93644	1.73525
H	2.18654	-0.95635	-1.58170
H	2.03093	1.93142	0.02949
N	-1.41009	-0.00180	-0.21709
H	-2.20230	-1.55313	0.55297
H	-2.19172	1.53298	0.59468

N_2H_4

N	0.00000	1.36701	-0.20727
N	0.00000	-1.36701	-0.20727
H	-0.96000	2.01677	1.32608
H	1.80413	1.90863	0.12484
H	-1.80413	-1.90863	0.12484
H	0.96000	-2.01677	1.32608

CH_3OH

C	1.25238	0.03602	0.00390
H	2.04624	-1.58666	-0.97388
H	2.00358	0.09486	1.92311
H	1.85921	1.73206	-0.99694
O	-1.40624	-0.23239	0.00274
H	-2.17342	1.40270	0.00240

NH_2OH

N	1.30003	0.11047	-0.26897
O	-1.35914	-0.23063	0.10809
H	-2.07930	1.34246	-0.42909
H	1.99543	-1.57836	0.31493
H	1.85676	1.30765	1.13221

Table S15: Geometries used for the MN12-SX calculations.

C_2H_6

C	0.00000	1.43830	-0.00589
C	0.00000	-1.43830	-0.00589
H	1.35180	2.19920	-1.35770
H	-1.85520	2.21039	-0.44066
H	0.55455	2.17814	1.83371
H	-1.35180	-2.19920	-1.35770
H	1.85520	-2.21039	-0.44066
H	-0.55455	-2.17814	1.83371

H_2O_2

O	0.00000	1.34823	-0.11082
O	0.00000	-1.34823	-0.11082
H	-1.47840	-1.70162	0.88658
H	1.47840	1.70162	0.88658

CH_3NH_2

C	1.32642	-0.00027	0.03190
H	2.03577	-0.94202	1.73151
H	2.18722	-0.95260	-1.58310
H	2.03001	1.93155	0.03516
N	-1.40410	-0.00210	-0.21948
H	-2.19675	-1.55361	0.55997
H	-2.18606	1.53297	0.60141

N_2H_4

N	0.00000	1.36648	-0.20906
N	0.00000	-1.36648	-0.20906
H	-0.94904	2.01893	1.33901
H	1.81135	1.90136	0.12439
H	-1.81135	-1.90136	0.12439
H	0.94904	-2.01893	1.33901

CH_3OH

C	1.24027	0.03612	0.00392
H	2.04396	-1.58789	-0.97208
H	2.00751	0.10068	1.92219
H	1.85920	1.72985	-1.00142
O	-1.39759	-0.23240	0.00341
H	-2.17155	1.39986	0.00053

NH_2OH

N	1.30297	0.11197	-0.27161
O	-1.36146	-0.23029	0.10832
H	-2.07752	1.34398	-0.42989
H	1.98936	-1.58539	0.31666
H	1.85899	1.29991	1.14798

Table S16: Geometries used for the PBEP86 calculations.

C_2H_6

C	0.00000	1.45075	-0.00595
C	0.00000	-1.45075	-0.00595
H	1.36454	2.22030	-1.37050
H	-1.87259	2.23170	-0.44469
H	0.55991	2.19936	1.85092
H	-1.36454	-2.22030	-1.37050
H	1.87259	-2.23170	-0.44469
H	-0.55991	-2.19936	1.85092

H_2O_2

O	0.00000	1.38572	-0.11263
O	0.00000	-1.38572	-0.11263
H	-1.50894	-1.70758	0.90104
H	1.50894	1.70758	0.90104

CH_3NH_2

C	1.34276	-0.00053	0.03262
H	2.05947	-0.96431	1.74138
H	2.20815	-0.94687	-1.60795
H	2.04545	1.95161	0.04915
N	-1.42177	-0.00206	-0.22422
H	-2.21446	-1.56582	0.57269
H	-2.20272	1.54300	0.61852

N_2H_4

N	0.00000	1.38596	-0.21286
N	0.00000	-1.38596	-0.21286
H	-0.93931	2.04104	1.36543
H	1.83290	1.91106	0.12456
H	-1.83290	-1.91106	0.12456
H	0.93931	-2.04104	1.36543

CH_3OH

C	1.26538	0.03564	0.00389
H	2.05970	-1.60809	-0.98584
H	2.03340	0.09249	1.94319
H	1.88708	1.74627	-1.01009
O	-1.42486	-0.23507	0.00331
H	-2.17354	1.43608	0.00296

NH_2OH

N	-1.32862	-0.11850	-0.29143
O	1.39492	0.24206	0.11943
H	2.09367	-1.36141	-0.44390
H	-2.00683	1.59667	0.31797
H	-1.87753	-1.30369	1.16099

Table S17: Geometries used for the BHandHLYP calculations.

C_2H_6

C	0.00000	1.43913	-0.00576
C	0.00000	-1.43913	-0.00576
H	1.34461	2.19320	-1.35037
H	-1.84545	2.20356	-0.43941
H	0.55020	2.17250	1.82431
H	-1.34461	-2.19320	-1.35037
H	1.84545	-2.20356	-0.43941
H	-0.55020	-2.17250	1.82431

H_2O_2

O	0.00000	1.33273	-0.10853
O	0.00000	-1.33273	-0.10853
H	-1.46407	-1.70746	0.86823
H	1.46407	1.70746	0.86823

CH_3NH_2

C	1.32936	-0.00093	0.03036
H	2.02224	-0.90881	1.73742
H	2.17516	-0.97306	-1.56112
H	2.02364	1.92001	0.00369
N	-1.40112	-0.00196	-0.20925
H	-2.19983	-1.54468	0.53159
H	-2.18953	1.52582	0.57102

N_2H_4

N	0.00000	1.35763	-0.20273
N	0.00000	-1.35763	-0.20273
H	-0.97962	2.01400	1.29369
H	1.78280	1.91226	0.12545
H	-1.78280	-1.91226	0.12545
H	0.97962	-2.01400	1.29369

CH_3OH

C	1.24615	0.03606	0.00367
H	2.03741	-1.57590	-0.96903
H	1.99341	0.09288	1.91193
H	1.84881	1.72437	-0.98890
O	-1.39785	-0.22990	0.00259
H	-2.17369	1.38154	0.00327

NH_2OH

N	1.29127	0.10528	-0.26341
O	-1.35065	-0.22768	0.10739
H	-2.07976	1.32127	-0.42565
H	1.99527	-1.56039	0.31713
H	1.85077	1.32356	1.09325

Table S18: Geometries used for the LC-BLYP calculations.

C_2H_6

C	0.00000	1.43364	-0.00585
C	0.00000	-1.43364	-0.00585
H	1.34996	2.19266	-1.35582
H	-1.85307	2.20355	-0.44007
H	0.55359	2.17190	1.83100
H	-1.34996	-2.19266	-1.35582
H	1.85307	-2.20355	-0.44007
H	-0.55359	-2.17190	1.83100

H_2O_2

O	0.00000	1.32722	-0.10842
O	0.00000	-1.32722	-0.10842
H	-1.48680	-1.71561	0.86739
H	1.48680	1.71561	0.86739

CH_3NH_2

C	1.32650	-0.00161	0.03002
H	2.02659	-0.86957	1.76666
H	2.17929	-1.01301	-1.54636
H	2.02854	1.92591	-0.04519
N	-1.39410	-0.00198	-0.19875
H	-2.22140	-1.56543	0.49725
H	-2.21330	1.54558	0.53879

N_2H_4

N	0.00000	1.34983	-0.20089
N	0.00000	-1.34983	-0.20089
H	-1.01713	2.02350	1.27821
H	1.78683	1.93474	0.12804
H	-1.78683	-1.93474	0.12804
H	1.01713	-2.02350	1.27821

CH_3OH

C	1.24601	0.03778	0.00396
H	2.04609	-1.57838	-0.97697
H	1.99703	0.09090	1.92188
H	1.84747	1.73706	-0.99151
O	-1.39644	-0.23306	0.00209
H	-2.19513	1.38822	0.00618

NH_2OH

N	1.28288	0.10462	-0.26333
O	-1.34444	-0.23102	0.10929
H	-2.09921	1.32729	-0.42671
H	2.01549	-1.56483	0.31790
H	1.85911	1.35333	1.07782

Table S19: Geometries used for the LC-B97D calculations.

C_2H_6

C	0.00000	1.44400	-0.00578
C	0.00000	-1.44400	-0.00578
H	1.35512	2.19480	-1.36092
H	-1.86056	2.20447	-0.44298
H	0.55399	2.17329	1.83861
H	-1.35512	-2.19480	-1.36092
H	1.86056	-2.20447	-0.44298
H	-0.55399	-2.17329	1.83861

H_2O_2

O	0.00000	1.33843	-0.10910
O	0.00000	-1.33843	-0.10910
H	-1.48413	-1.72196	0.87277
H	1.48413	1.72196	0.87277

CH_3NH_2

C	1.33775	-0.00128	0.02949
H	2.02281	-0.87799	1.77101
H	2.18390	-1.01366	-1.55284
H	2.02663	1.93463	-0.03758
N	-1.40361	-0.00233	-0.20097
H	-2.22184	-1.56649	0.50519
H	-2.21270	1.54749	0.54404

N_2H_4

N	0.00000	1.36008	-0.20128
N	0.00000	-1.36008	-0.20128
H	-1.01984	2.02236	1.28076
H	1.78989	1.93631	0.12821
H	-1.78989	-1.93631	0.12821
H	1.01984	-2.02236	1.28076

CH_3OH

C	1.25698	0.03732	0.00352
H	2.04995	-1.58602	-0.97716
H	1.99831	0.09597	1.92817
H	1.84572	1.74255	-0.99645
O	-1.40425	-0.23308	0.00255
H	-2.20186	1.38820	0.00395

NH_2OH

N	1.29541	0.10350	-0.26210
O	-1.35515	-0.23048	0.10823
H	-2.10278	1.33094	-0.42845
H	2.01608	-1.57043	0.32059
H	1.86005	1.35887	1.07674

Table S20: Geometries used for the LC-BP86 calculations.

C_2H_6

C	0.00000	1.42861	-0.00597
C	0.00000	-1.42861	-0.00597
H	1.35257	2.19045	-1.35855
H	-1.85676	2.20177	-0.43988
H	0.55580	2.16928	1.83423
H	-1.35257	-2.19045	-1.35855
H	1.85676	-2.20177	-0.43988
H	-0.55580	-2.16928	1.83423

H_2O_2

O	0.00000	1.31510	-0.11054
O	0.00000	-1.31510	-0.11054
H	-1.47294	-1.70722	0.88430
H	1.47294	1.70722	0.88430

CH_3NH_2

C	1.31944	-0.00187	0.03046
H	2.02466	-0.87995	1.76605
H	2.18026	-1.00474	-1.55386
H	2.02621	1.92948	-0.03442
N	-1.38964	-0.00192	-0.20130
H	-2.21476	-1.56573	0.50264
H	-2.20554	1.54560	0.54597

N_2H_4

N	0.00000	1.34166	-0.20214
N	0.00000	-1.34166	-0.20214
H	-1.00696	2.01553	1.28756
H	1.79020	1.92396	0.12741
H	-1.79020	-1.92396	0.12741
H	1.00696	-2.01553	1.28756

CH_3OH

C	1.23746	0.03754	0.00426
H	2.04644	-1.58005	-0.97866
H	1.99613	0.09277	1.92531
H	1.84388	1.73942	-0.99518
O	-1.39105	-0.23359	0.00206
H	-2.18286	1.39138	0.00646

NH_2OH

N	1.27119	0.10600	-0.26516
O	-1.33422	-0.23154	0.11017
H	-2.08587	1.32778	-0.42645
H	2.00793	-1.56471	0.31621
H	1.85333	1.34724	1.08505

2 Disaggregated data

Table S21: AD_{HV}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	5.033E-05	1.953E-04	1.863E-04	2.179E-04	4.028E-04	3.039E-04
B3LYP	5.291E-05	2.082E-04	1.982E-04	2.323E-04	4.282E-04	3.656E-04
B3P86	4.731E-05	1.833E-04	1.770E-04	2.031E-04	3.784E-04	2.862E-04
B3PW91	5.113E-05	1.958E-04	1.877E-04	2.156E-04	4.025E-04	3.025E-04
B97-2	5.101E-05	1.970E-04	1.881E-04	2.199E-04	4.098E-04	3.070E-04
B97D	6.037E-05	2.271E-04	2.218E-04	2.544E-04	4.728E-04	4.012E-04
B97D3	6.010E-05	2.282E-04	2.211E-04	2.551E-04	4.728E-04	4.037E-04
B98	5.121E-05	1.954E-04	1.877E-04	2.164E-04	4.060E-04	3.049E-04
BHandHLYP	4.438E-05	1.782E-04	1.662E-04	1.964E-04	3.654E-04	2.681E-04
BLYP	6.420E-05	2.464E-04	2.405E-04	2.729E-04	4.993E-04	4.363E-04
CAM-B3LYP	4.963E-05	1.998E-04	1.925E-04	2.235E-04	4.227E-04	3.197E-04
HF	3.855E-05	1.540E-04	1.404E-04	1.663E-04	3.032E-04	2.184E-04
LC-BLYP	4.496E-05	1.868E-04	1.819E-04	2.086E-04	4.036E-04	3.068E-04
LC-B97D	4.231E-05	1.612E-04	1.519E-04	1.701E-04	3.260E-04	2.480E-04
LC-BP86	4.204E-05	1.705E-04	1.644E-04	1.883E-04	3.589E-04	2.714E-04
LSDA	5.518E-05	2.105E-04	2.006E-04	2.389E-04	4.278E-04	3.275E-04
M06	2.505E-04	4.617E-04	4.620E-04	3.593E-04	5.547E-04	3.692E-04
M06-2X	3.155E-04	5.478E-04	5.111E-04	4.336E-04	6.410E-04	4.331E-04
MN12-SX	3.236E-04	6.291E-04	6.400E-04	5.292E-04	8.143E-04	5.901E-04
PBEP86	5.904E-05	2.279E-04	2.230E-04	2.580E-04	4.758E-04	4.080E-04

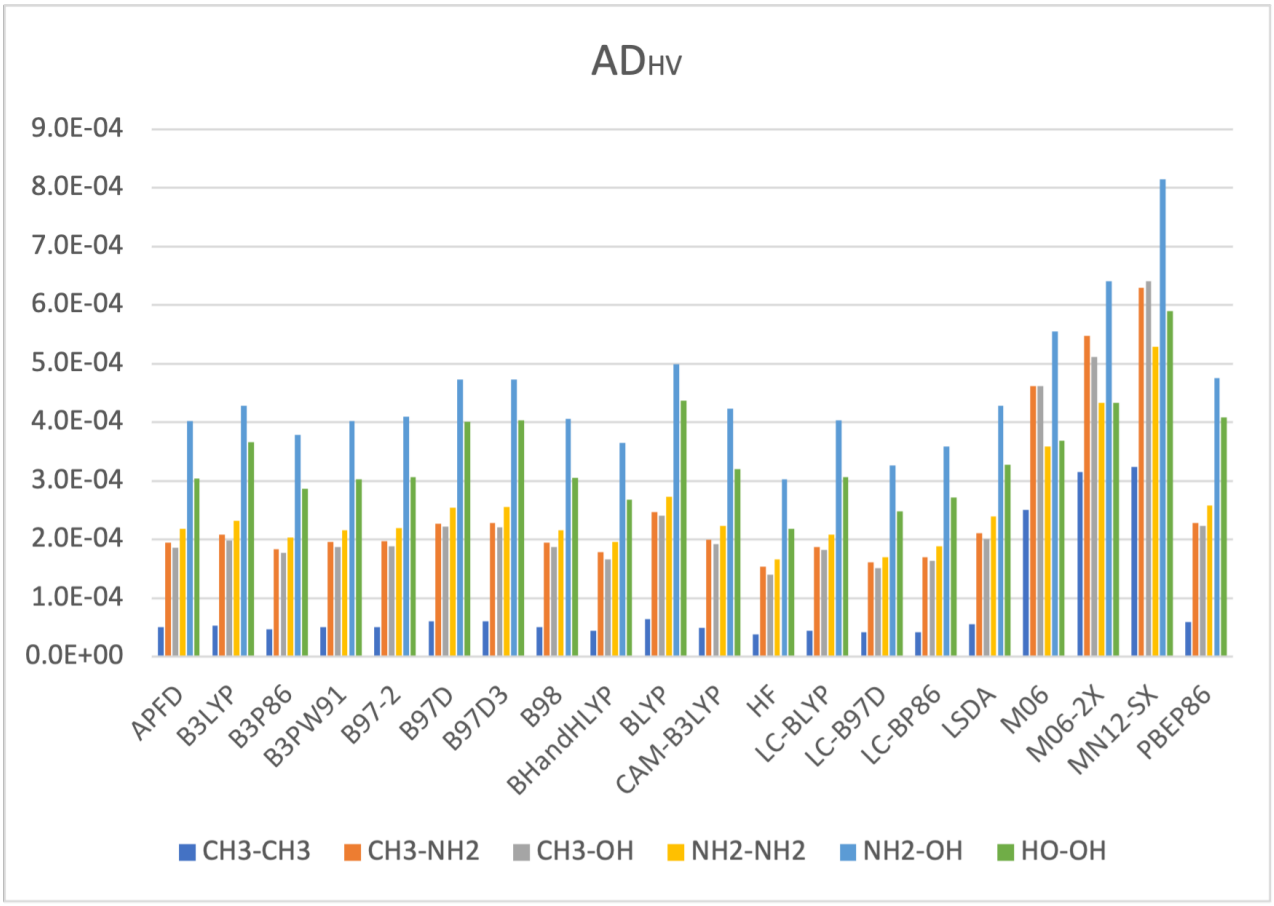

Figure S1: Histogram chart of data in Table S21.

Table S22: AD_{RR}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	3.438E-03	3.777E-02	3.411E-02	8.219E-02	1.426E-01	1.187E-01
B3LYP	4.194E-03	4.387E-02	3.893E-02	9.246E-02	1.602E-01	1.888E-01
B3P86	2.919E-03	3.333E-02	3.075E-02	7.224E-02	1.270E-01	1.068E-01
B3PW91	3.604E-03	3.720E-02	3.413E-02	8.051E-02	1.397E-01	1.169E-01
B97-2	3.968E-03	3.766E-02	3.469E-02	8.203E-02	1.438E-01	1.202E-01
B97D	6.713E-03	4.842E-02	4.584E-02	1.024E-01	1.816E-01	2.230E-01
B97D3	6.655E-03	4.890E-02	4.568E-02	1.033E-01	1.814E-01	2.237E-01
B98	3.465E-03	3.777E-02	3.459E-02	8.020E-02	1.438E-01	1.209E-01
BHandHLYP	2.239E-03	3.218E-02	2.813E-02	6.913E-02	1.199E-01	9.638E-02
BLYP	6.941E-03	5.752E-02	5.264E-02	1.187E-01	2.066E-01	2.610E-01
CAM-B3LYP	3.391E-03	4.110E-02	3.703E-02	8.719E-02	1.554E-01	1.311E-01
HF	1.419E-03	2.257E-02	1.991E-02	4.834E-02	8.280E-02	6.311E-02
LC-BLYP	2.191E-03	3.704E-02	3.323E-02	7.791E-02	1.437E-01	1.216E-01
LC-B97D	2.185E-03	2.705E-02	2.379E-02	5.301E-02	1.007E-01	8.599E-02
LC-BP86	1.798E-03	2.927E-02	2.716E-02	6.239E-02	1.159E-01	9.841E-02
LSDA	5.099E-03	5.013E-02	4.124E-02	1.085E-01	1.765E-01	1.467E-01
M06	7.943E-01	6.924E-01	5.755E-01	5.467E-01	4.084E-01	2.785E-01
M06-2X	1.722E+00	1.622E+00	1.486E+00	1.532E+00	1.383E+00	1.230E+00
MN12-SX	1.062E+00	1.338E+00	1.526E+00	1.598E+00	1.819E+00	1.970E+00
PBEP86	5.698E-03	5.106E-02	4.660E-02	1.090E-01	1.909E-01	2.352E-01

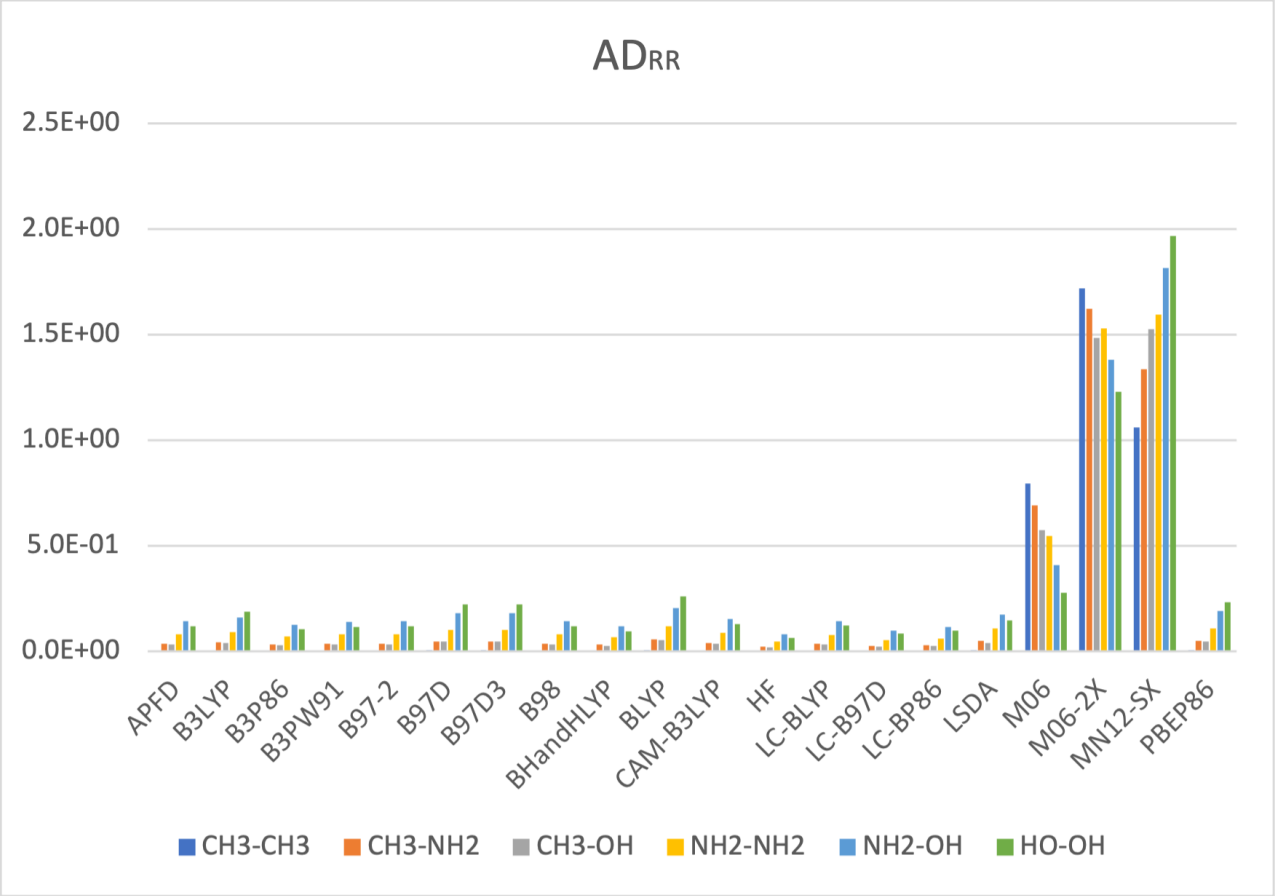

Figure S2: Histogram chart of data in Table S22.

Table S23: AD_{PR}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	3.206E-03	5.843E-03	5.296E-03	9.214E-03	1.236E-02	1.474E-02
B3LYP	3.324E-03	6.368E-03	5.776E-03	1.013E-02	1.358E-02	1.532E-02
B3P86	3.091E-03	5.415E-03	4.944E-03	8.401E-03	1.119E-02	1.330E-02
B3PW91	3.207E-03	5.810E-03	5.282E-03	9.134E-03	1.214E-02	1.447E-02
B97-2	2.965E-03	5.708E-03	5.193E-03	9.241E-03	1.247E-02	1.492E-02
B97D	3.129E-03	6.747E-03	6.215E-03	1.140E-02	1.514E-02	1.738E-02
B97D3	3.126E-03	6.775E-03	6.195E-03	1.142E-02	1.512E-02	1.751E-02
B98	3.215E-03	5.890E-03	5.355E-03	9.253E-03	1.247E-02	1.507E-02
BHandHLYP	2.945E-03	5.120E-03	4.637E-03	7.802E-03	1.069E-02	1.227E-02
BLYP	3.799E-03	7.867E-03	7.238E-03	1.287E-02	1.682E-02	1.996E-02
CAM-B3LYP	3.228E-03	6.011E-03	5.601E-03	9.476E-03	1.327E-02	1.625E-02
HF	2.594E-03	4.074E-03	3.686E-03	5.821E-03	7.872E-03	8.332E-03
LC-BLYP	3.145E-03	5.517E-03	5.297E-03	8.412E-03	1.248E-02	1.526E-02
LC-B97D	2.751E-03	4.302E-03	4.222E-03	6.186E-03	9.030E-03	1.098E-02
LC-BP86	3.006E-03	4.866E-03	4.664E-03	7.216E-03	1.045E-02	1.239E-02
LSDA	3.378E-03	6.788E-03	5.927E-03	1.123E-02	1.475E-02	1.776E-02
M06	4.331E-03	6.676E-03	6.733E-03	1.017E-02	1.333E-02	1.567E-02
M06-2X	3.202E-03	6.863E-03	5.432E-03	1.098E-02	1.288E-02	1.491E-02
MN12-SX	1.232E-03	6.732E-03	3.597E-03	1.562E-02	1.493E-02	1.410E-02
PBEP86	3.623E-03	7.247E-03	6.634E-03	1.191E-02	1.570E-02	1.830E-02

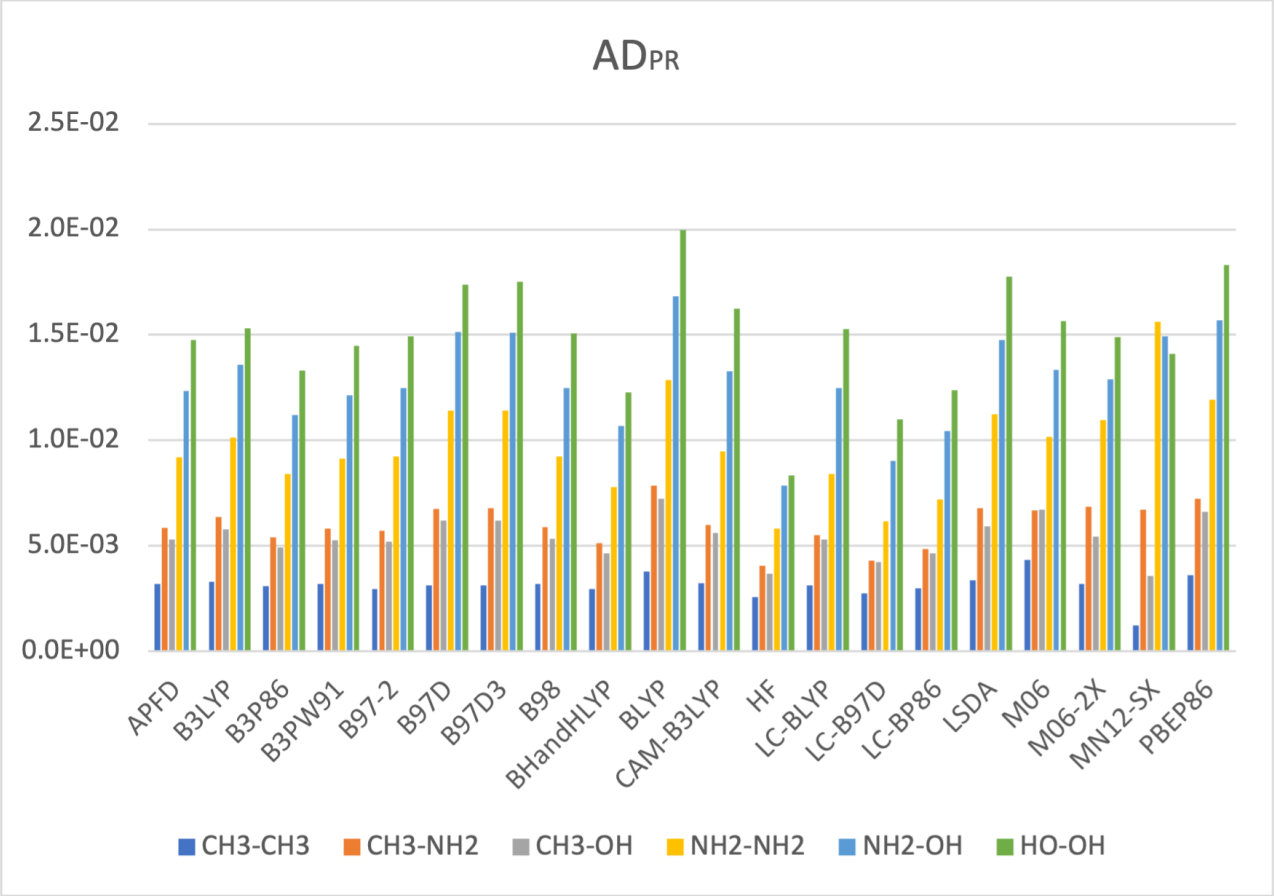

Figure S3: Histogram chart of data in Table S23.

Table S24: AD_{PP}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	6.791E-03	1.976E-02	1.974E-02	4.086E-02	5.870E-02	7.022E-02
B3LYP	7.415E-03	2.208E-02	2.196E-02	4.542E-02	6.476E-02	7.737E-02
B3P86	6.386E-03	1.819E-02	1.833E-02	3.713E-02	5.345E-02	6.429E-02
B3PW91	6.883E-03	1.966E-02	1.973E-02	4.030E-02	5.757E-02	6.911E-02
B97-2	6.799E-03	1.967E-02	1.981E-02	4.083E-02	5.882E-02	7.058E-02
B97D	8.570E-03	2.422E-02	2.437E-02	5.008E-02	7.040E-02	8.603E-02
B97D3	8.535E-03	2.432E-02	2.428E-02	5.023E-02	7.030E-02	8.650E-02
B98	6.777E-03	1.990E-02	2.000E-02	4.073E-02	5.920E-02	7.149E-02
BHandHLYP	5.779E-03	1.731E-02	1.729E-02	3.520E-02	5.177E-02	5.966E-02
BLYP	9.544E-03	2.784E-02	2.754E-02	5.690E-02	7.889E-02	9.889E-02
CAM-B3LYP	6.869E-03	2.098E-02	2.142E-02	4.294E-02	6.370E-02	7.730E-02
HF	4.793E-03	1.368E-02	1.352E-02	2.619E-02	3.877E-02	4.192E-02
LC-BLYP	6.078E-03	1.913E-02	2.008E-02	3.847E-02	6.041E-02	7.315E-02
LC-B97D	5.572E-03	1.507E-02	1.599E-02	2.892E-02	4.581E-02	5.571E-02
LC-BP86	5.651E-03	1.618E-02	1.723E-02	3.230E-02	5.059E-02	6.077E-02
LSDA	8.042E-03	2.422E-02	2.269E-02	5.077E-02	6.990E-02	8.365E-02
M06	8.549E-01	7.651E-01	6.409E-01	6.129E-01	4.782E-01	3.354E-01
M06-2X	1.800E+00	1.706E+00	1.552E+00	1.617E+00	1.467E+00	1.309E+00
MN12-SX	9.490E-01	1.200E+00	1.375E+00	1.425E+00	1.609E+00	1.792E+00
PBEP86	8.661E-03	2.535E-02	2.497E-02	5.282E-02	7.394E-02	9.115E-02

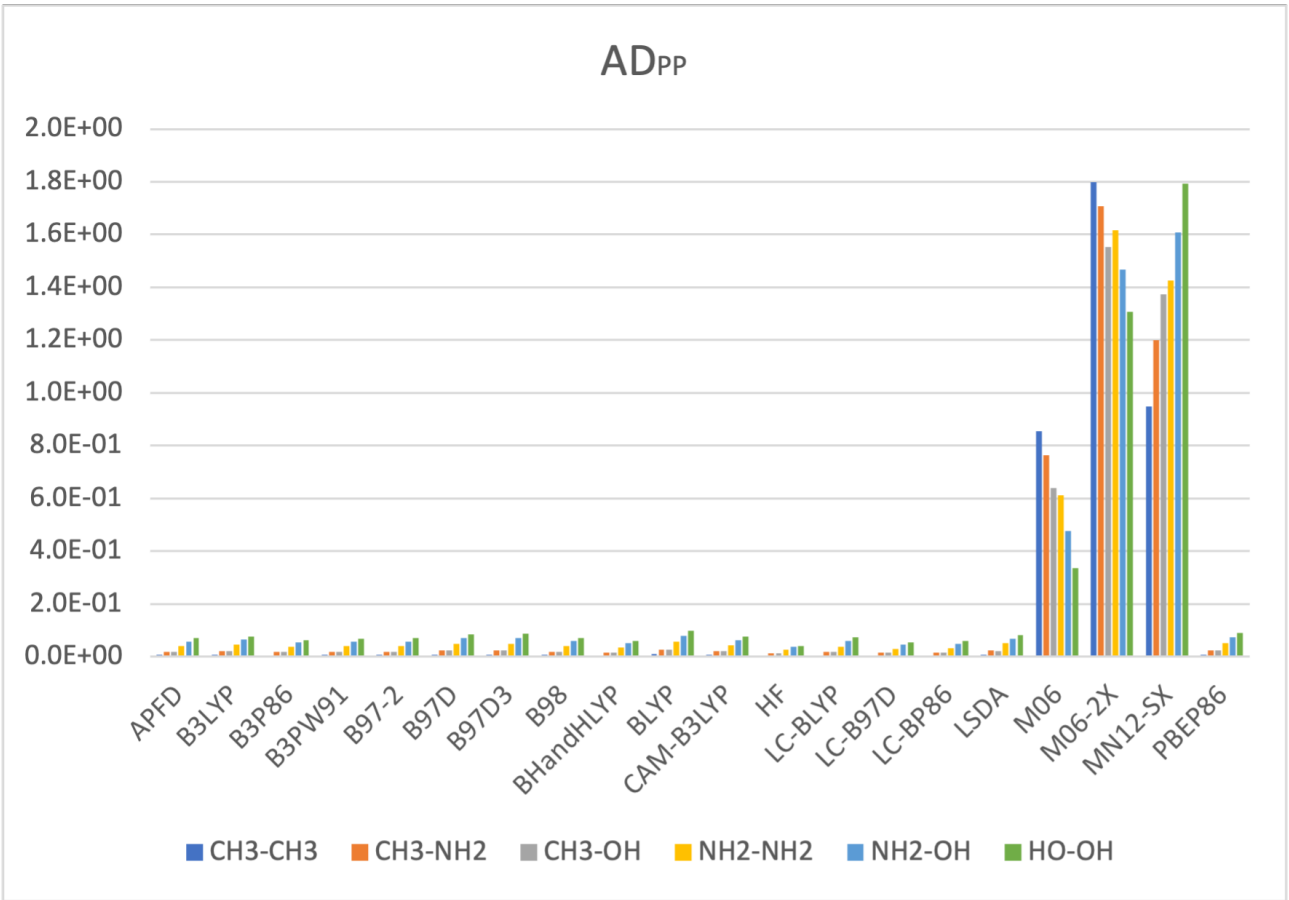

Figure S4: Histogram chart of data in Table S24.

Table S25: AD_{RL}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	3.337E-04	2.898E-03	2.266E-03	6.740E-03	5.071E-03	7.471E-03
B3LYP	3.720E-04	3.350E-03	2.721E-03	7.541E-03	5.887E-03	6.714E-03
B3P86	2.914E-04	2.563E-03	2.075E-03	5.933E-03	4.501E-03	6.717E-03
B3PW91	3.653E-04	2.824E-03	2.232E-03	6.653E-03	4.991E-03	7.352E-03
B97-2	3.281E-04	2.997E-03	2.458E-03	6.741E-03	5.175E-03	7.544E-03
B97D	4.663E-04	4.002E-03	3.366E-03	8.951E-03	6.786E-03	7.551E-03
B97D3	4.478E-04	4.049E-03	3.390E-03	8.999E-03	6.809E-03	7.624E-03
B98	3.258E-04	3.038E-03	2.454E-03	6.602E-03	5.292E-03	7.622E-03
BHandHLYP	2.460E-04	2.417E-03	1.950E-03	5.224E-03	4.184E-03	6.128E-03
BLYP	5.386E-04	4.570E-03	3.916E-03	1.035E-02	8.036E-03	8.687E-03
CAM-B3LYP	3.406E-04	3.082E-03	2.687E-03	6.692E-03	5.772E-03	8.286E-03
HF	1.702E-04	1.662E-03	1.224E-03	3.371E-03	2.800E-03	3.994E-03
LC-BLYP	2.529E-04	2.647E-03	2.408E-03	5.479E-03	5.494E-03	7.722E-03
LC-B97D	1.246E-04	1.873E-03	1.785E-03	3.591E-03	4.043E-03	5.458E-03
LC-BP86	2.205E-04	2.056E-03	1.769E-03	4.447E-03	4.287E-03	6.180E-03
LSDA	4.379E-04	3.634E-03	2.723E-03	9.026E-03	6.606E-03	9.199E-03
M06	5.363E-04	3.469E-03	2.310E-03	9.045E-03	6.949E-03	8.191E-03
M06-2X	3.436E-04	3.898E-03	2.328E-03	5.532E-03	4.172E-03	6.923E-03
MN12-SX	7.544E-04	7.431E-03	3.551E-03	1.145E-02	8.086E-03	9.034E-03
PBEP86	4.874E-04	4.094E-03	3.304E-03	9.418E-03	7.247E-03	7.995E-03

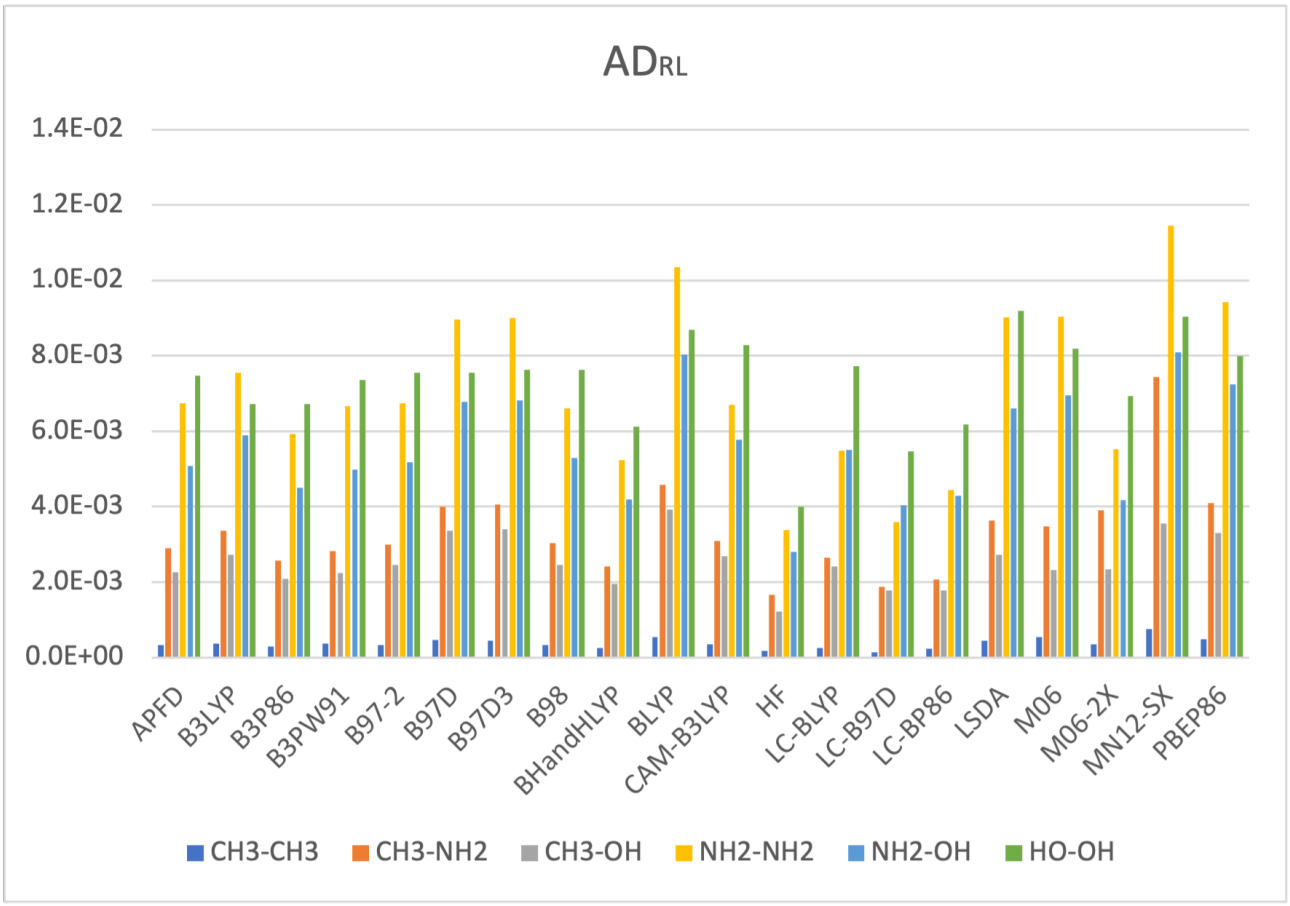

Figure S5: Histogram chart of data in Table S25.

Table S26: AD_{PL}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	2.064E-03	1.857E-02	1.406E-02	5.163E-02	4.285E-02	3.768E-02
B3LYP	2.262E-03	2.111E-02	1.638E-02	5.732E-02	4.686E-02	4.055E-02
B3P86	1.813E-03	1.668E-02	1.289E-02	4.530E-02	3.726E-02	3.378E-02
B3PW91	2.097E-03	1.794E-02	1.376E-02	5.024E-02	4.161E-02	3.673E-02
B97-2	2.025E-03	1.843E-02	1.423E-02	5.174E-02	4.328E-02	3.766E-02
B97D	2.687E-03	2.276E-02	1.763E-02	6.544E-02	5.407E-02	4.446E-02
B97D3	2.670E-03	2.278E-02	1.754E-02	6.582E-02	5.401E-02	4.459E-02
B98	2.004E-03	1.917E-02	1.477E-02	5.083E-02	4.220E-02	3.839E-02
BHandHLYP	1.545E-03	1.666E-02	1.285E-02	4.238E-02	3.528E-02	3.240E-02
BLYP	3.159E-03	2.622E-02	2.068E-02	7.458E-02	5.978E-02	5.162E-02
CAM-B3LYP	1.980E-03	2.061E-02	1.650E-02	5.339E-02	4.527E-02	4.240E-02
HF	1.048E-03	1.251E-02	9.422E-03	2.947E-02	2.486E-02	2.275E-02
LC-BLYP	1.556E-03	1.909E-02	1.598E-02	4.666E-02	4.452E-02	4.074E-02
LC-B97D	1.003E-03	1.435E-02	1.241E-02	3.190E-02	3.411E-02	3.009E-02
LC-BP86	1.377E-03	1.531E-02	1.260E-02	3.797E-02	3.539E-02	3.290E-02
LSDA	2.734E-03	2.277E-02	1.582E-02	6.893E-02	5.581E-02	4.592E-02
M06	8.575E-03	1.845E-01	3.420E-01	4.667E-02	1.886E-01	3.429E-02
M06-2X	1.310E-03	6.541E-02	1.529E-01	7.343E-02	1.513E-01	5.439E-02
MN12-SX	1.798E-02	3.191E-01	5.125E-01	1.336E-01	2.721E-01	9.613E-02
PBEP86	2.918E-03	2.410E-02	1.832E-02	7.063E-02	5.708E-02	4.756E-02

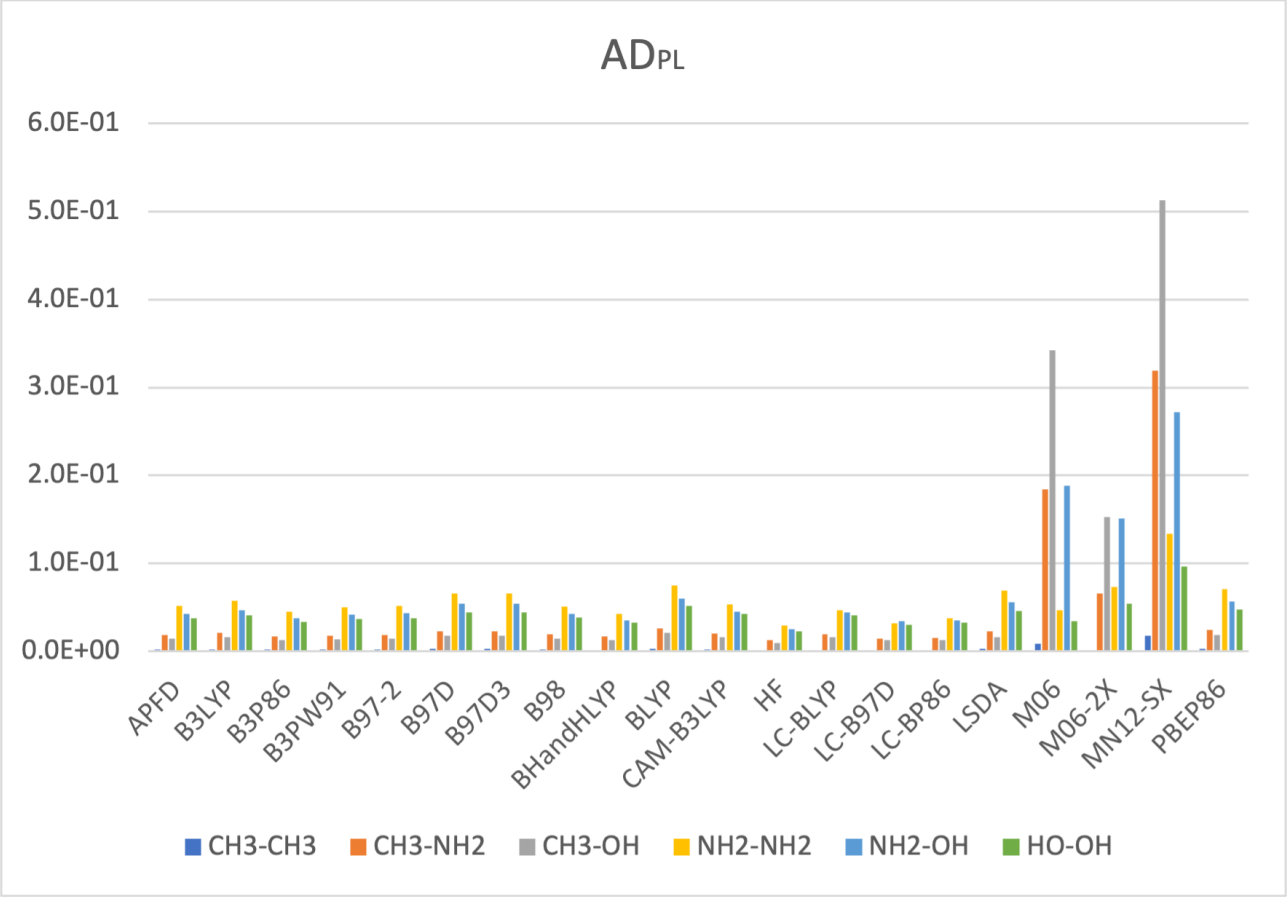

Figure S6: Histogram chart of data in Table S26.

Table S27: AD_{α}

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	1.562E-01	4.887E-01	3.267E-01	9.259E-01	9.056E-01	8.811E-01
B3LYP	1.746E-01	5.503E-01	3.654E-01	1.028E+00	9.870E-01	9.802E-01
B3P86	1.429E-01	4.520E-01	2.982E-01	8.704E-01	8.464E-01	8.306E-01
B3PW91	1.581E-01	4.873E-01	3.253E-01	9.174E-01	8.910E-01	8.708E-01
B97-2	1.556E-01	4.861E-01	3.277E-01	9.215E-01	9.080E-01	8.848E-01
B97D	2.126E-01	6.332E-01	4.248E-01	1.150E+00	1.099E+00	1.089E+00
B97D3	2.115E-01	6.346E-01	4.233E-01	1.155E+00	1.098E+00	1.094E+00
B98	1.535E-01	4.917E-01	3.309E-01	9.283E-01	9.145E-01	9.011E-01
BHandHLYP	1.189E-01	4.026E-01	2.697E-01	7.732E-01	7.699E-01	7.400E-01
BLYP	2.436E-01	7.138E-01	4.829E-01	1.286E+00	1.188E+00	1.206E+00
CAM-B3LYP	1.550E-01	5.081E-01	3.492E-01	9.532E-01	9.599E-01	9.699E-01
HF	8.470E-02	2.887E-01	2.031E-01	5.481E-01	5.599E-01	5.114E-01
LC-BLYP	1.230E-01	4.476E-01	3.261E-01	8.387E-01	8.963E-01	9.261E-01
LC-B97D	7.834E-02	3.502E-01	2.497E-01	6.495E-01	7.125E-01	7.533E-01
LC-BP86	1.086E-01	3.774E-01	2.705E-01	7.181E-01	7.718E-01	7.950E-01
LSDA	2.016E-01	6.393E-01	4.057E-01	1.221E+00	1.138E+00	1.066E+00
M06	1.003E+00	8.748E+00	6.703E+00	6.512E+00	4.832E+00	2.605E+00
M06-2X	1.345E+00	1.147E+00	8.944E+00	9.625E+00	7.534E+00	5.478E+00
MN12-SX	1.253E+00	1.045E+00	1.135E+00	2.396E+00	2.999E+00	4.207E+00
PBEP86	2.232E-01	6.625E-01	4.450E-01	1.229E+00	1.158E+00	1.150E+00

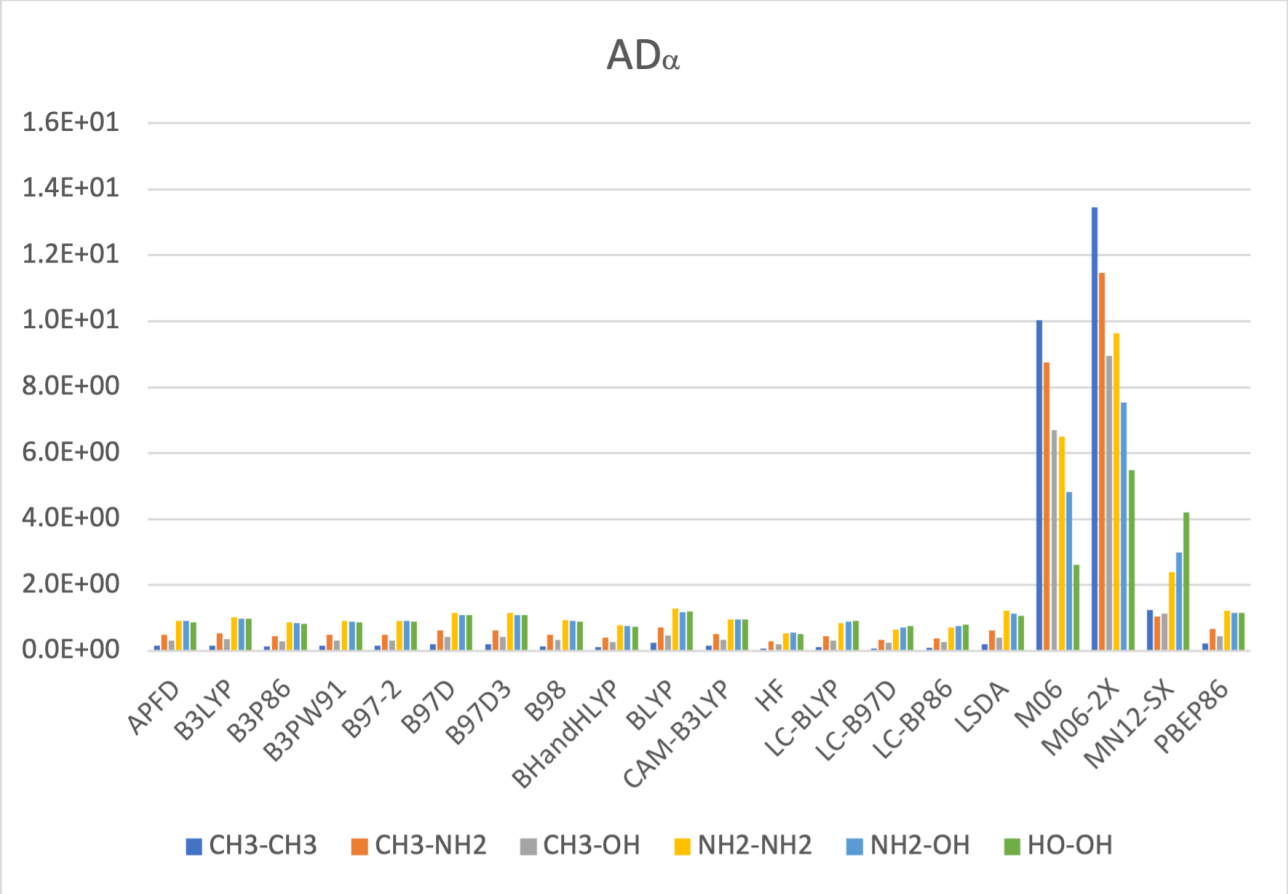

Figure S7: Histogram chart of data in Table S27.

Table S28: $AD_{\hat{\kappa}}$

Functional	CH_3-CH_3	CH_3-NH_2	CH_3-OH	NH_2-NH_2	NH_2-OH	HO-OH
APFD	8.175E-02	4.381E-01	3.277E-01	1.897E+00	2.220E+00	8.637E-01
B3LYP	9.206E-02	5.060E-01	3.718E-01	2.105E+00	2.495E+00	9.512E-01
B3P86	7.013E-02	3.964E-01	2.794E-01	1.683E+00	1.940E+00	7.865E-01
B3PW91	8.104E-02	4.283E-01	3.357E-01	1.797E+00	2.210E+00	8.463E-01
B97-2	8.061E-02	4.492E-01	3.325E-01	1.919E+00	2.224E+00	8.673E-01
B97D	1.129E-01	7.474E-01	5.770E-01	2.595E+00	3.319E+00	1.122E+00
B97D3	1.142E-01	7.643E-01	5.728E-01	2.603E+00	3.315E+00	1.119E+00
B98	8.001E-02	4.736E-01	3.194E-01	1.922E+00	2.155E+00	8.831E-01
BHandHLYP	5.823E-02	4.350E-01	2.723E-02	1.546E+00	1.538E+00	6.959E-01
BLYP	1.361E-01	1.096E+00	6.982E-01	3.003E+00	3.932E+00	1.287E+00
CAM-B3LYP	7.903E-02	5.596E-01	2.862E-01	2.060E+00	2.204E+00	9.959E-01
HF	3.700E-02	3.620E-01	1.691E-01	1.019E+00	9.044E-01	4.488E-01
LC-BLYP	5.956E-02	5.800E-01	3.142E-01	1.832E+00	1.855E+00	9.567E-01
LC-B97D	3.407E-02	4.606E-01	2.561E-01	1.326E+00	1.228E+00	7.302E-01
LC-BP86	5.083E-02	4.612E-01	2.320E-01	1.482E+00	1.512E+00	7.830E-01
LSDA	1.164E-01	8.045E-01	5.423E-01	2.903E+00	3.489E+00	1.141E+00
M06	1.526E-01	3.097E+00	5.595E+00	4.073E+00	5.242E+00	9.658E-01
M06-2X	2.559E-01	2.130E+00	4.392E+00	6.787E+00	5.695E+00	2.646E+00
MN12-SX	5.844E-01	2.531E+00	4.142E+00	2.396E+00	4.865E+00	2.305E+00
PBEP86	1.259E-01	8.910E-01	6.447E-01	2.981E+00	3.711E+00	1.212E+00

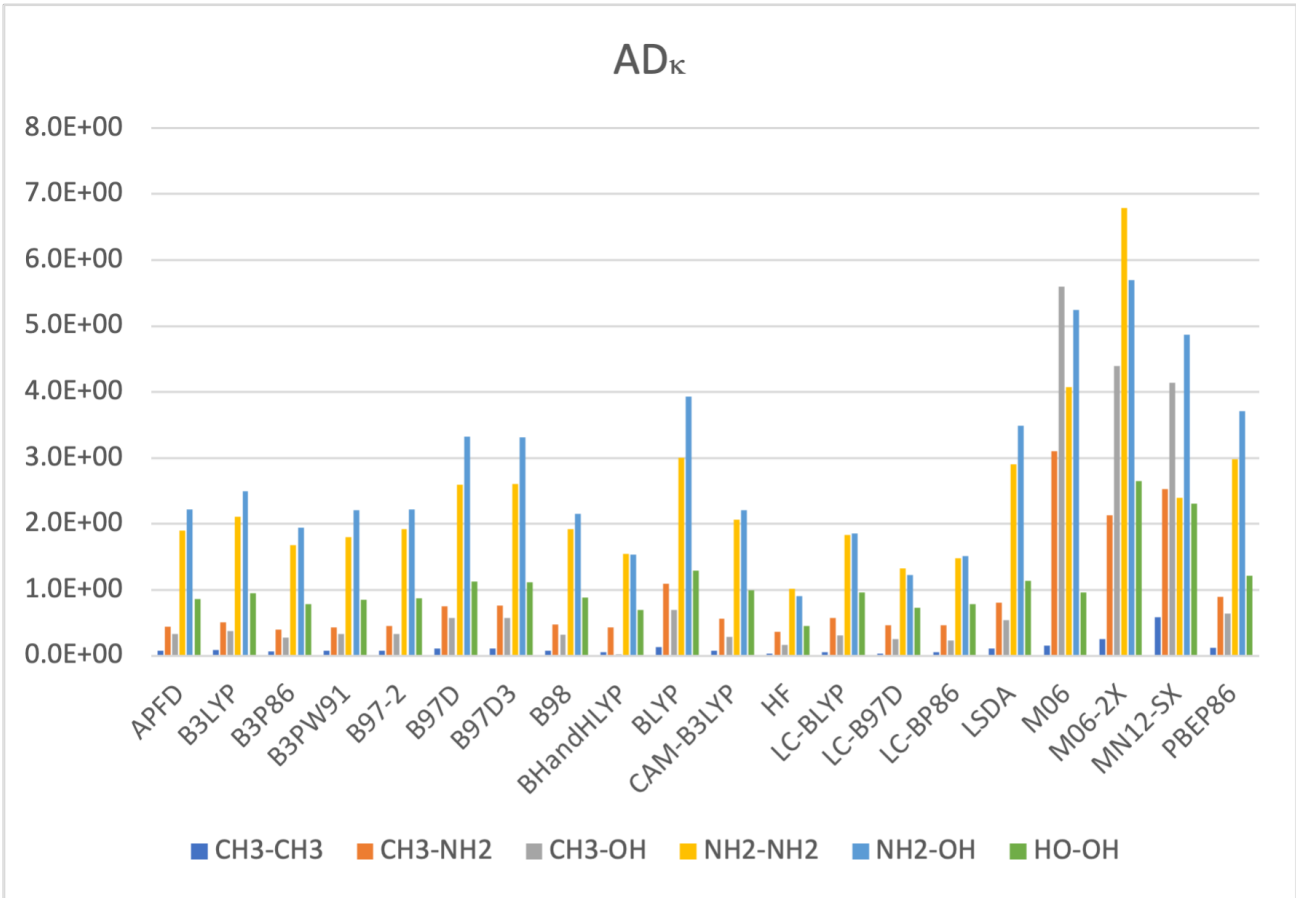

Figure S8: Histogram chart of data in Table S28.

3 Isotropic Component of the Static Dipole Polarizabilities of C_2H_6 (in a_0^3)

	RR	PR	PP
APFD	28.728	28.715	28.703
B3LYP	28.948	28.933	28.919
B3P86	28.635	28.623	28.611
B3PW91	28.685	28.672	28.659
B972	28.553	28.540	28.528
B97D	29.871	29.853	29.836
B97D3	29.745	29.727	29.710
B98	28.889	28.876	28.864
BHandHLYP	27.633	27.623	27.613
BLYP	30.189	30.168	30.149
CAMB3LYP	28.518	28.506	28.493
HF	26.953	26.946	26.940
LCBLYP	27.877	27.867	27.857
LCB97D	28.440	28.433	28.427
LCBP86	27.919	27.910	27.901
LSDA	30.147	30.131	30.114
M06	28.261	29.081	29.930
M062X	28.435	29.531	30.672
MN12SX	29.047	29.142	29.256
PBEP86	30.452	30.433	30.415

4 Isotropic Component of the Static Dipole Polarizabilities of CH_3NH_2 (in a_0^3)

	RR	PR	PP
APFD	25.848	25.809	25.774
B3LYP	26.216	26.173	26.134
B3P86	25.826	25.790	25.757
B3PW91	25.870	25.832	25.798
B972	25.698	25.660	25.625
B97D	27.183	27.134	27.090
B97D3	27.134	27.085	27.041
B98	26.024	25.986	25.950
BHandHLYP	24.645	24.613	24.583
BLYP	27.720	27.666	27.619
CAMB3LYP	25.668	25.628	25.591
HF	23.567	23.544	23.521
LCBLYP	24.906	24.871	24.837
LCB97D	25.392	25.364	25.338
LCBP86	24.859	24.829	24.801
LSDA	27.503	27.454	27.410
M06	25.452	26.150	26.876
M062X	25.397	26.322	27.286
MN12SX	26.142	26.105	26.096
PBEP86	27.874	27.823	27.778

5 Isotropic Component of the Static Dipole Polarizabilities of CH_3OH (in a_0^3)

	RR	PR	PP
APFD	21.271	21.246	21.223
B3LYP	21.544	21.517	21.492
B3P86	21.260	21.237	21.216
B3PW91	21.290	21.266	21.243
B972	21.140	21.115	21.092
B97D	22.366	22.336	22.310
B97D3	22.315	22.286	22.260
B98	21.367	21.342	21.318
BHandHLYP	20.201	20.179	20.158
BLYP	22.808	22.775	22.747
CAMB3LYP	21.167	21.140	21.114
HF	19.221	19.204	19.188
LCBLYP	20.629	20.602	20.577
LCB97D	20.993	20.972	20.953
LCBP86	20.594	20.571	20.550
LSDA	22.572	22.540	22.511
M06	20.925	21.465	22.026
M062X	20.782	21.497	22.238
MN12SX	21.349	21.259	21.189
PBEP86	22.923	22.889	22.859

6 Isotropic Component of the Static Dipole Polarizabilities of H_2O_2 (in a_0^3)

	RR	PR	PP
APFD	14.817	14.742	14.673
B3LYP	15.256	15.172	15.096
B3P86	14.894	14.823	14.758
B3PW91	14.898	14.824	14.756
B972	14.748	14.672	14.604
B97D	15.765	15.671	15.586
B97D3	15.763	15.668	15.583
B98	14.981	14.904	14.834
BHandHLYP	14.127	14.065	14.007
BLYP	16.375	16.269	16.175
CAMB3LYP	14.916	14.833	14.758
HF	13.219	13.177	13.137
LCBLYP	14.408	14.330	14.258
LCB97D	14.776	14.713	14.654
LCBP86	14.211	14.145	14.083
LSDA	15.575	15.483	15.400
M06	14.680	14.873	15.076
M062X	14.670	15.073	15.494
MN12SX	14.914	14.589	14.287
PBEP86	16.210	16.109	16.020

7 Isotropic Component of the Static Dipole Polarizabilities of N_2H_4 (in a_0^3)

	RR	PR	PP
APFD	22.996	22.919	22.850
B3LYP	23.492	23.407	23.331
B3P86	23.027	22.956	22.890
B3PW91	23.053	22.978	22.909
B972	22.877	22.801	22.733
B97D	24.462	24.367	24.284
B97D3	24.459	24.363	24.279
B98	23.249	23.172	23.103
BHandHLYP	21.805	21.741	21.683
BLYP	25.178	25.071	24.979
CAMB3LYP	22.847	22.768	22.697
HF	20.529	20.484	20.442
LCBLYP	21.933	21.864	21.801
LCB97D	22.411	22.357	22.307
LCBP86	21.780	21.721	21.667
LSDA	24.613	24.512	24.423
M06	22.707	23.230	23.779
M062X	22.452	23.223	24.030
MN12SX	23.399	23.195	23.030
PBEP86	25.183	25.082	24.992

8 Isotropic Component of the Static Dipole Polarizabilities of NH_2OH (in a_0^3)

	RR	PR	PP
APFD	18.646	18.579	18.519
B3LYP	19.103	19.029	18.964
B3P86	18.704	18.641	18.584
B3PW91	18.719	18.653	18.594
B972	18.558	18.491	18.430
B97D	19.825	19.744	19.673
B97D3	19.816	19.735	19.664
B98	18.863	18.794	18.733
BHandHLYP	17.728	17.670	17.617
BLYP	20.469	20.381	20.306
CAMB3LYP	18.655	18.582	18.517
HF	16.649	16.607	16.568
LCBLYP	17.981	17.913	17.850
LCB97D	18.395	18.340	18.290
LCBP86	17.813	17.754	17.701
LSDA	19.707	19.624	19.552
M06	18.451	18.815	19.197
M062X	18.189	18.768	19.375
MN12SX	18.862	18.616	18.400
PBEP86	20.376	20.291	20.217