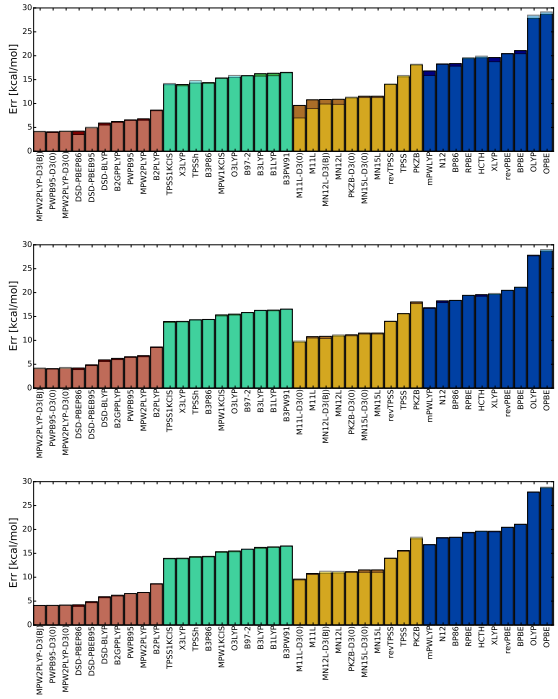
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information for "'Diet GMKTN55' offers accelerated benchmarking through a representative subset approach"

This electronic supplementary information contains:

1. Supplementary Figure 1 showing the worst cases using the $N_s = 30$, 100 and 150 element subsets.
2. Supplementary Tables 1,2 listing systems included in the $N_s = 30$ and 150 subsets, to supplement results for $N_s = 100$ in the main text.
3. Supplementary Figure 2 showing the best cases for MGCDB84 using $N_s = 30$, 100 and 150 element subsets tailored to the alternative database.
4. Description of results and files provided on Github.



Supplementary Figure 1 Comparison of errors found using $N_s = 30, 100, 150$ (top to bottom) subsets compared with the full database. Here, results are divivided into four categories: double-hybrid DFAs (reds), hybrid DFAs (greens), meta-GGAs (earth tones) and GGAs (blues). The paler colour in each category represent MADs for the subset, and the darker colour is for the full database. The blended colour represents overlap. Only the ten worst methods are shown in each category.

Supplementary Table 1 Full list of benchmark sets and specific elements used in the $N_s = 30$ diet-GMTKN55 ranking set. These structures are sufficient to reproduce the full WTMAD-2 ranking with good accuracy, using the weights W listed here.

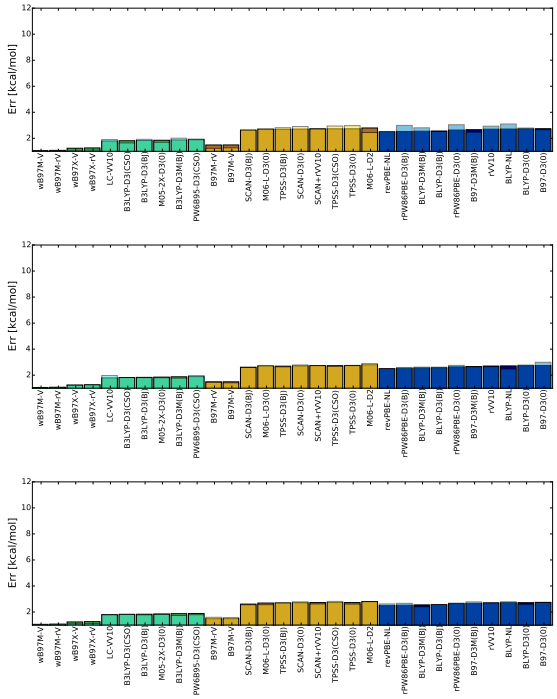
Set	W	IDs	Set	W	IDs	Set	W	IDs	Set	W	IDs
ACONF[†]	30.99	10	Amino20x4[†]	23.31	28, 54	BH76[14,15]	3.05	5	BHPERI[16]	2.72	11
BHROT27[†]	9.06	16, 26	BSR36[17]	3.51	31	BUT14DIOL[18]	20.30	13	CDIE20[19]	14.02	9
DC13[†]	1.03	1	DIPCS10[†]	0.09	7	FH51[20]	1.83	24, 30	G21EA[21]	1.69	14, 25
HAL59[24,25†]	12.38	40, 57	HEAVY28[26]	45.79	16	MB16-43[31]	0.12	10	MCONF[32]	11.43	1
PNICO23[34]	13.30	16	PX13[50]	1.70	9	S66[37]	10.40	6, 50	SIE4x4[†]	1.69	15
W4-11[40]	0.19	30, 57, 132	WCPT18[51]	1.62	15						

[†] Contains systems from one of the GMTKN databases[5,43–45]

Supplementary Table 2 As per Supplementary Table 1, but for $N_s = 150$.

Set	W	IDs	Set	W	IDs
ACONF[†]	30.99	11, 14	AHB21[12]	2.53	6, 10, 15
AL2X6[†]	1.58	5	Amino20x4[†]	23.31	4, 6, 15, 25, 39, 41, 46, 68
BH76[14,15]	3.05	8, 36, 37, 47, 50, 53, 66	BH76RC[†]	2.66	5
BHPERI[16]	2.72	2, 8, 25	BHROT27[†]	9.06	3, 11, 14, 21
BSR36[17]	3.51	17, 22	BUT14DIOL[18]	20.30	2, 29, 32, 38, 39, 42, 43, 53
C60ISO[49]	0.58	7, 9	CDIE20[19]	14.02	1, 18, 20
CHB6[12]	2.12	2	DARC[†]	1.75	11
DC13[†]	1.03	10, 13	DIPCS10[†]	0.09	2
FH51[20]	1.83	26, 27, 40, 48	G21EA[21]	1.69	17, 20, 23
G21IP[21,22]	0.22	6, 15, 31	G2RC[23]	1.11	16, 24, 25
HAL59[24,25†]	12.38	7, 11, 16, 28, 32, 56	HEAVY28[26]	45.79	3, 16, 24
ICONF[†]	17.40	16	IDISP[22,29,47,52,53]	4.00	3
IL16[12,27]	0.52	11, 14	INV24[28]	1.78	1, 14, 15
ISO34[29]	3.90	21	ISOL24[30]	2.59	2, 4, 20
MB16-43[31]	0.12	14	MCONF[32]	11.43	11, 20, 30
NBPRC[22,48]	2.30	1	PA26[†]	0.30	20, 25
PArel[†]	12.28	13	PCONF21[33]	35.05	3
PNICO23[34]	13.30	7, 11, 13, 21	PX13[50]	1.70	8
RC21[35]	1.59	5, 6, 8, 16, 20	RG18[†]	98.00	11, 13, 15
RSE43[36]	7.48	14, 40	S22[46,54]	7.78	3, 8, 11
S66[37]	10.40	8, 17, 25, 28, 42, 47, 61	SCONF[38]	12.36	16
SIE4x4[†]	1.69	15	TAUT15[†]	18.66	5, 13
UPU23[39]	9.93	2, 4, 9, 15	W4-11[40]	0.19	2, 7, 30, 31, 38, 58, 63, 73, 77, 85, 86, 95, 102, 106, 129
WATER27[41]	0.70	2, 17	WCPT18[51]	1.62	6, 8, 9, 18
YBDE18[42]	1.15	6, 8, 9, 13, 16			

[†] Contains systems from one of the GMTKN databases[5,43–45]



Supplementary Figure 2 Comparison of errors found using $N_s = 30, 100, 150$ (top to bottom) subsets compared with the full database for MGCDB84. Here, results are divivided into three categories: hybrid DFAs (greens), meta-GGAs (earth tones) and GGAs (blues). The paler colour in each category represent MADs for the subset, and the darker colour is for the full database. The blended colour represents overlap. Only the ten best methods are shown in each category. Scale is kept consistent with plots in the main text.

Description of results and files provided on Github

In addition to the tabulated data presented here, key results were collated into "yaml" files (`http://yaml.org/`) containing the structural data required to use the diet databases reported in the text. These files, are available at `https://github.com/gambort/DietGMTKN55`.

As an example of how to use these files, a python script is also provided that generates the structural part of Gaussian Input Files. This file is primarily designed to serve as a software-ambivalent template for generating structures for any quantum chemistry code, and for processing the outputs therefrom.

Additional files are provided for the diet versions of MGCDB84[9], which were used to generate Supplementary Figure 2.

Supplementary References

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