Supporting Informations

for

DFT Approach to the Gibbs Energy of Hydride Anion in Acetonitrile by Modelling Hydricities

Zoran Glasovac*[,a], Borislav Kovačević [b], Davor Margetić [a]

a) *Division of organic chemistry and biochemistry, Ruđer Bošković Institute, Bijenička c. 54, HR-10000, Zagreb, Croatia.*

b) *Division of physical chemistry, Ruđer Bošković Institute, Bijenička c. 54, HR-10000, Zagreb, Croatia.*

Corresponding author: E-mail: glasovac@irb.hr

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S1. Correlation data for all models used in this work.

Computed electronic energies, Gibbs energies and energies of solvation used to construct these graphs are given in a separate MS Excell file (Glasovac_Hydricities_Models.xlsx).

Table S1. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M1 model for a set of the reference structures.

Structures $M^{+/0}$/$[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.52986	-0.00902	-188.53888				
$HCOO^-$	-189.25748	-0.00242	-189.25990	452.4	**45.5**	**44**	1.5
B_2H_6	-53.27271	0.03999	-53.23272				
BH_4^-	-27.35006	0.01417	-27.33589	451.5	**44.6**	**50.4**	5.8
Et_3B	-262.48814	0.16434	-262.32380				
Et_3BH^-	-263.18558	0.17193	-263.01365	432.9	**26.1**	**26**	0.1
Ph_3C^+	-732.66150	0.24124	-732.42025				
Ph_3CH	-733.46870	0.24881	-733.21989	501.8	**94.7**	**96**	1.3
$PhCH_2^+$	-270.64956	0.08914	-270.56042				
$PhCH_3$	-271.49344	0.09847	-271.39497	523.7	**116.6**	**118**	1.4
$pNO_2PhCH_2^+$	-475.07783	0.08616	-474.99168				
pNO_2PhCH_3	-475.94419	0.09677	-475.84742	537.0	**129.8**	**129**	0.8
$pOMePhCH_2^+$	-385.16473	0.11970	-385.04503				
$pOMePhCH_3$	-385.98896	0.12794	-385.86102	512.0	**105.0**	**107**	2.0
$BImH^+$	-458.82714	0.15548	-458.67166				
BImHH	-459.55835	0.16452	-459.39383	453.2	**46.3**	**45**	1.3
$BImMe^+$	-498.14379	0.17973	-497.96405				
BImMeH	-498.87185	0.19064	-498.68121	450.0	**43.1**	**43**	0.1
$BImPh^+$	-689.82178	0.23028	-689.59150				
BImPhH	-690.55343	0.23836	-690.31507	454.0	**47.1**	**50**	2.9
$MeDHP^+$	-327.27795	0.12651	-327.15144				
MeDHPH	-328.00668	0.13546	-327.87121	451.7	**44.8**	**41**	3.8
$BnDHP^+$	-558.26544	0.20174	-558.06370				
BnDHPH	-558.99730	0.21000	-558.78730	454.1	**47.2**	**43**	4.2
$HFlu^+$	-500.44717	0.14429	-500.30289				
HFluH	-501.28460	0.15580	-501.12880	518.3	**111.2**	**109**	2.2
$MeOOCFlu^+$	-728.25736	0.18006	-728.07730				
MeOOCFluH	-729.10270	0.19242	-728.91028	522.7	**115.6**	**114**	1.6
$MeOFlu^+$	-614.97345	0.17549	-614.79796				
MeOFluH	-615.77239	0.18542	-615.58698	495.1	**88.1**	**89**	0.9
$PhtrMe^+$	-595.16572	0.19049	-594.97522				
PhtrMeH	-595.92303	0.19966	-595.72337	469.5	**62.5**	**61.4**	1.1

PhtrBn$^+$	-826.15194	0.26576	-825.88618				
PhtrBnH	-826.91142	0.27400	-826.63743	471.4	**64.5**	**64.8**	0.3
BNA$^+$	-687.62135	0.19874	-687.42261				
BNAH	-688.37049	0.20636	-688.16413	465.3	**58.4**	**59**	0.6
HEHMe$^+$	-900.83479	0.28032	-900.55447				
HEHMeH	-901.58723	0.28727	-901.29995	467.8	**60.9**	**61.5**	0.6
2OM$^+$	-1148.59257	0.34965	-1148.24292				
2OMH	-1149.34042	0.35857	-1148.98185	463.7	**56.8**	**58.2**	1.4
4OM$^+$	-1284.12042	0.38250	-1283.73792				
4OMH	-1284.89115	0.39236	-1284.49879	477.5	**70.5**	**70.2**	0.3
						MUE=	1.6
						MAX=	5.8
						RMSE=	2.2

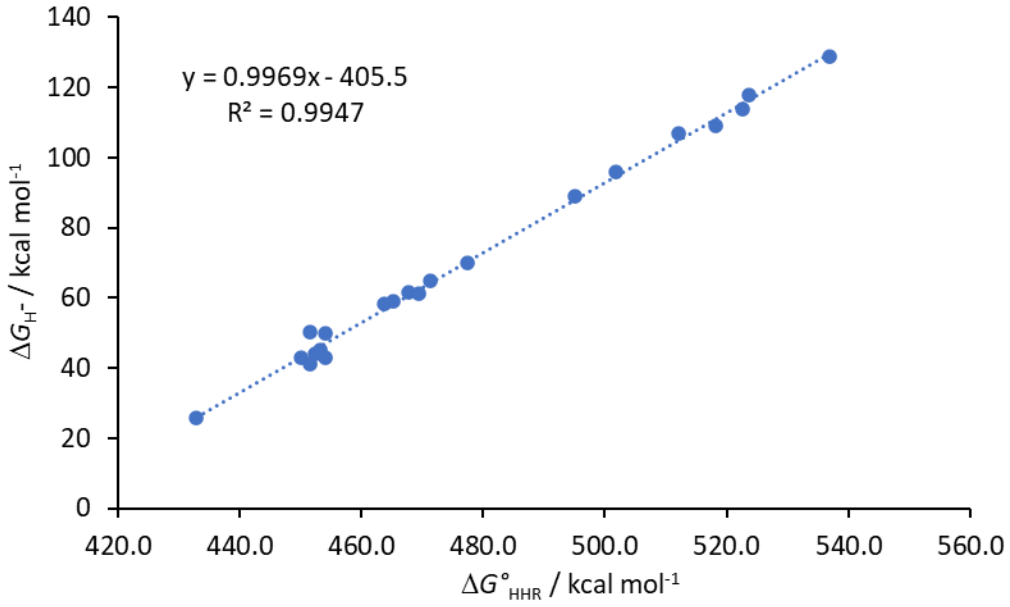

Figure S1. Correlation line obtained with the M1 model.

Table S2. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M2 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.59379	-0.00902	-188.60282				
$HCOO^-$	-189.31469	-0.00242	-189.31711	448.2	41.6	**44**	2.4
B_2H_6	-53.28304	0.03999	-53.24305				
BH_4^-	-27.35822	0.01417	-27.34404	453.4	46.8	**50.4**	3.6
Et_3B	-262.54165	0.16434	-262.37731				
Et_3BH^-	-263.24072	0.17193	-263.06879	433.9	27.4	**26**	1.4
Ph_3C^+	-732.82168	0.24124	-732.58044				
Ph_3CH	-733.62959	0.24881	-733.38078	502.2	95.3	**96**	0.7
$PhCH_2^+$	-270.70840	0.08914	-270.61926				
$PhCH_3$	-271.55280	0.09847	-271.45433	524.0	117.0	**118**	1.0
$pNO_2PhCH_2^+$	-475.20247	0.08616	-475.11631				
pNO_2PhCH_3	-476.06857	0.09677	-475.97180	536.8	129.7	**129**	0.7
$pOMePhCH_2^+$	-385.25752	0.11970	-385.13781				
$pOMePhCH_3$	-386.08119	0.12794	-385.95325	511.7	104.7	**107**	2.3
$BImH^+$	-458.93369	0.15548	-458.77821				
BImHH	-459.66411	0.16452	-459.49959	452.7	46.1	**45**	1.1
$BImMe^+$	-498.25859	0.17973	-498.07886				
BImMeH	-498.98543	0.19064	-498.79479	449.3	42.7	**43**	0.3
$BImPh^+$	-689.97955	0.23028	-689.74927				
BImPhH	-690.70992	0.23836	-690.47155	453.2	46.6	**50**	3.4
$MeDHP^+$	-327.35143	0.12651	-327.22492				
MeDHPH	-328.08155	0.13546	-327.94609	452.5	45.9	**41**	4.9
$BnDHP^+$	-558.38991	0.20174	-558.18818				
BnDHPH	-559.12294	0.21000	-558.91294	454.8	48.2	**43**	5.2
$HFlu^+$	-500.55713	0.14429	-500.41285				
HFluH	-501.39497	0.15580	-501.23917	518.5	111.5	**109**	2.5
$MeOOCFlu^+$	-728.43365	0.18006	-728.25359				
MeOOCFluH	-729.27893	0.19242	-729.08651	522.7	115.6	**114**	1.6
$MeOFlu^+$	-615.11732	0.17549	-614.94183				
MeOFluH	-615.91472	0.18542	-615.72931	494.1	87.3	**89**	1.7
$PhtrMe^+$	-595.29976	0.19049	-595.10926				
PhtrMeH	-596.05628	0.19966	-595.85662	469.0	62.3	**61.4**	0.9
$PhtrBn^+$	-826.33678	0.26576	-826.07102				
PhtrBnH	-827.09548	0.27400	-826.82148	470.9	64.2	**64.8**	0.6
BNA^+	-687.78640	0.19874	-687.58766				
BNAH	-688.53577	0.20636	-688.32941	465.5	58.8	**59**	0.2

$HEHMe^+$	-901.06452	0.28032	-900.78420				
HEHMeH	-901.81571	0.28727	-901.52844	467.0	60.3	**61.5**	1.2
$2OM^+$	-1148.86728	0.34965	-1148.51763				
2OMH	-1149.61479	0.35857	-1149.25623	463.5	56.8	**58.2**	1.4
$4OM^+$	-1284.43727	0.38250	-1284.05477				
4OMH	-1285.20799	0.39236	-1284.81563	477.4	70.7	**70.2**	0.5
						MUE=	1.8
						MAX=	5.2
						RMSE=	2.3

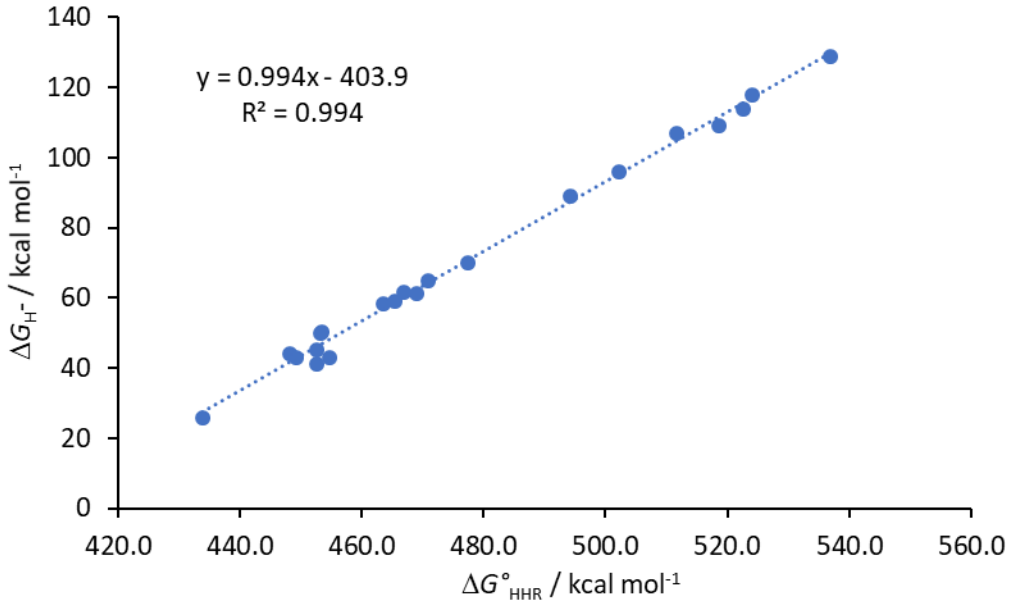

Figure S2. Correlation line obtained with the M2 model.

Table S3. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M3 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.60059	-0.00902	-188.60961				
$HCOO^-$	-189.32054	-0.00242	-189.32296	447.6	**41.6**	**44**	2.4
B_2H_6	-53.28678	0.03999	-53.24679				
BH_4^-	-27.35996	0.01417	-27.34578	453.3	**47.2**	**50.4**	3.2
Et_3B	-262.55682	0.16434	-262.39248				
Et_3BH^-	-263.25539	0.17193	-263.08347	433.6	**27.6**	**26**	1.6
Ph_3C^+	-732.85424	0.24124	-732.61300				
Ph_3CH	-733.66114	0.24881	-733.41233	501.6	**95.3**	**96**	0.7
$PhCH_2^+$	-270.72209	0.08914	-270.63295				
$PhCH_3$	-271.56575	0.09847	-271.46727	523.5	**117.2**	**118**	0.8
$pNO_2PhCH_2^+$	-475.22273	0.08616	-475.13658				
pNO_2PhCH_3	-476.08776	0.09677	-475.99099	536.2	**129.7**	**129**	0.7
$pOMePhCH_2^+$	-385.27604	0.11970	-385.15634				
$pOMePhCH_3$	-386.09880	0.12794	-385.97086	511.1	**104.8**	**107**	2.2
$BImH^+$	-458.95468	0.15548	-458.79920				
BImHH	-459.68415	0.16452	-459.51964	452.1	**46.0**	**45**	1.0
$BImMe^+$	-498.28156	0.17973	-498.10183				
BImMeH	-499.00755	0.19064	-498.81691	448.7	**42.7**	**43**	0.3
$BImPh^+$	-690.00966	0.23028	-689.77938				
BImPhH	-690.73923	0.23836	-690.50086	452.7	**46.7**	**50**	3.3
$MeDHP^+$	-327.36798	0.12651	-327.24147				
MeDHPH	-328.09713	0.13546	-327.96166	451.9	**45.9**	**41**	4.9
$BnDHP^+$	-558.41577	0.20174	-558.21404				
BnDHPH	-559.14774	0.21000	-558.93774	454.1	**48.0**	**43**	5.0
$HFlu^+$	-500.57948	0.14429	-500.43520				
HFluH	-501.41641	0.15580	-501.26061	518.0	**111.6**	**109**	2.6
$MeOOCFlu^+$	-728.46452	0.18006	-728.28446				
MeOOCFluH	-729.30867	0.19242	-729.11625	522.0	**115.6**	**114**	1.6
$MeOFlu^+$	-615.14449	0.17549	-614.96901				
MeOFluH	-615.94072	0.18542	-615.75530	493.4	**87.2**	**89**	1.8
$PhtrMe^+$	-595.32611	0.19049	-595.13562				
PhtrMeH	-596.08159	0.19966	-595.88194	468.3	**62.2**	**61.4**	0.8
$PhtrBn^+$	-826.37250	0.26576	-826.10674				
PhtrBnH	-827.13022	0.27400	-826.85622	470.3	**64.2**	**64.8**	0.6
BNA^+	-687.81594	0.19874	-687.61720				
BNAH	-688.56425	0.20636	-688.35789	464.8	**58.7**	**59**	0.3

HEHMe$^+$	-901.10371	0.28032	-900.82339				
HEHMeH	-901.85353	0.28727	-901.56626	466.2	**60.0**	**61.5**	1.5
2OM$^+$	-1148.91416	0.34965	-1148.56451				
2OMH	-1149.66082	0.35857	-1149.30226	462.9	**56.8**	**58.2**	1.4
4OM$^+$	-1284.49006	0.38250	-1284.10757				
4OMH	-1285.26005	0.39236	-1284.86769	477.0	**70.8**	**70.2**	0.6
						MUE=	1.8
						MAX=	5.0

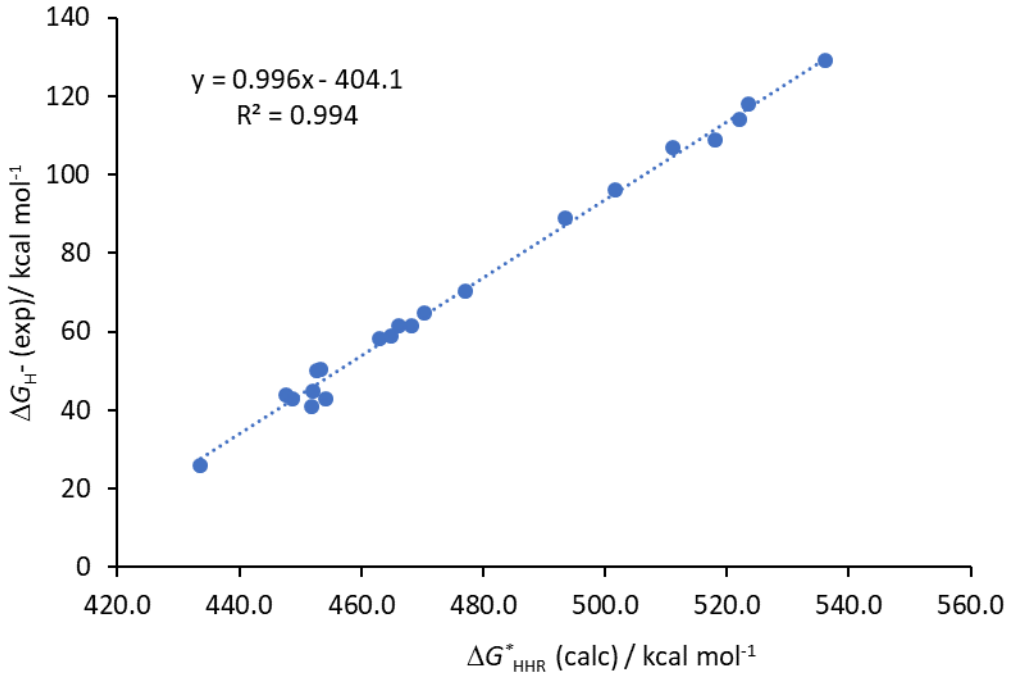

Figure S3. Correlation line obtained with the M3 model.

Table S4. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M4 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.59638	-0.00902	-188.60540				
$HCOO^-$	-189.31515	-0.00242	-189.31757	446.9	41.6	**44**	2.4
B_2H_6	-53.26217	0.03999	-53.22218				
BH_4^-	-27.34000	0.01417	-27.32583	448.5	43.2	**50.4**	7.2
Et_3B	-262.49061	0.16434	-262.32627				
Et_3BH^-	-263.18703	0.17193	-263.01510	432.2	27.3	**26**	1.3
Ph_3C^+	-732.80681	0.24124	-732.56557				
Ph_3CH	-733.61312	0.24881	-733.36431	501.2	94.6	**96**	1.4
$PhCH_2^+$	-270.69387	0.08914	-270.60473				
$PhCH_3$	-271.53802	0.09847	-271.43954	523.9	116.7	**118**	1.3
$pNO_2PhCH_2^+$	-475.19148	0.08616	-475.10533				
pNO_2PhCH_3	-476.05746	0.09677	-475.96069	536.8	129.2	**129**	0.2
$pOMePhCH_2^+$	-385.24178	0.11970	-385.12207				
$pOMePhCH_3$	-386.06513	0.12794	-385.93720	511.5	104.6	**107**	2.4
$BImH^+$	-458.91503	0.15548	-458.75955				
BImHH	-459.64411	0.16452	-459.47959	451.8	46.4	**45**	1.4
$BImMe^+$	-498.23308	0.17973	-498.05335				
BImMeH	-498.95880	0.19064	-498.76816	448.5	43.2	**43**	0.2
$BImPh^+$	-689.95916	0.23028	-689.72888				
BImPhH	-690.68869	0.23836	-690.45033	452.7	47.3	**50**	2.7
$MeDHP^+$	-327.32824	0.12651	-327.20173				
MeDHPH	-328.05713	0.13546	-327.92166	451.8	46.4	**41**	5.4
$BnDHP^+$	-558.36554	0.20174	-558.16381				
BnDHPH	-559.09798	0.21000	-558.88798	454.4	49.0	**43**	6.0
$HFlu^+$	-500.54960	0.14429	-500.40531				
HFluH	-501.38722	0.15580	-501.23142	518.4	111.3	**109**	2.3
$MeOOCFlu^+$	-728.42653	0.18006	-728.24647				
MeOOCFluH	-729.27245	0.19242	-729.08003	523.1	115.9	**114**	1.9
$MeOFlu^+$	-615.10765	0.17549	-614.93216				
MeOFluH	-615.90520	0.18542	-615.71978	494.2	87.8	**89**	1.2
$PhtrMe^+$	-595.28923	0.19049	-595.09873				
PhtrMeH	-596.04398	0.19966	-595.84432	467.9	62.1	**61.4**	0.7
$PhtrBn^+$	-826.32487	0.26576	-826.05911				
PhtrBnH	-827.08186	0.27400	-826.80787	469.9	64.0	**64.8**	0.8
BNA^+	-687.76983	0.19874	-687.57109				
BNAH	-688.51859	0.20636	-688.31223	465.1	59.3	**59**	0.3

$HEHMe^+$	-901.02536	0.28032	-900.74504				
HEHMeH	-901.77487	0.28727	-901.48759	466.0	60.2	**61.5**	1.3
$2OM^+$	-1148.85428	0.34965	-1148.50463				
2OMH	-1149.60046	0.35857	-1149.24189	462.6	57.0	**58.2**	1.2
$4OM^+$	-1284.41618	0.38250	-1284.03368				
4OMH	-1285.18888	0.39236	-1284.79652	478.7	72.6	**70.2**	2.4
						MUE=	2.1
						MAX=	7.2
						RMSE=	2.8

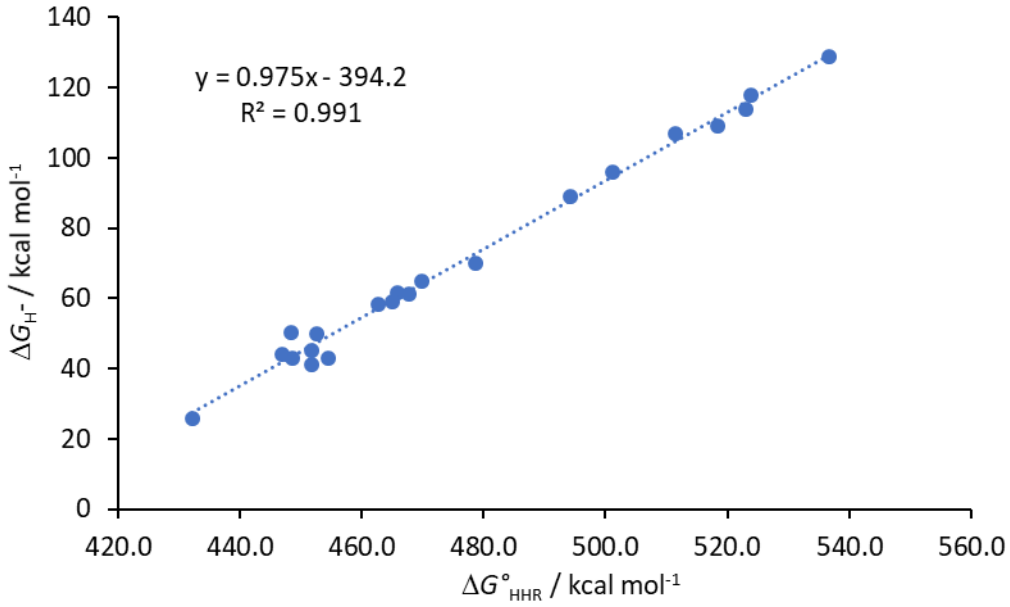

Figure S4. Correlation line obtained with the M4 model.

Table S5. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M5 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.55137	-0.00902	-188.56039				
$HCOO^-$	-189.26657	-0.00242	-189.26899	444.7	43.1	**44**	0.9
B_2H_6	-53.23105	0.03999	-53.19106				
BH_4^-	-27.32641	0.01417	-27.31223	449.7	48.3	**50.4**	2.1
Et_3B	-262.37752	0.16434	-262.21318				
Et_3BH^-	-263.07255	0.17193	-262.90062	431.4	29.4	**26**	3.4
Ph_3C^+	-732.52341	0.24124	-732.28217				
Ph_3CH	-733.31730	0.24881	-733.06849	493.4	93.4	**96**	2.6
$PhCH_2^+$	-270.59334	0.08914	-270.50420				
$PhCH_3$	-271.42830	0.09847	-271.32983	518.1	118.9	**118**	0.9
$pNO_2PhCH_2^+$	-475.04919	0.08616	-474.96304				
pNO_2PhCH_3	-475.90491	0.09677	-475.80814	530.3	131.5	**129**	2.5
$pOMePhCH_2^+$	-385.10470	0.11970	-384.98499				
$pOMePhCH_3$	-385.91871	0.12794	-385.79077	505.6	106.0	**107**	1.0
$BImH^+$	-458.73933	0.15548	-458.58385				
BImHH	-459.46302	0.16452	-459.29850	448.5	47.0	**45**	2.0
$BImMe^+$	-498.04095	0.17973	-497.86122				
BImMeH	-498.76189	0.19064	-498.57125	445.6	44.0	**43**	1.0
$BImPh^+$	-689.69111	0.23028	-689.46084				
BImPhH	-690.41452	0.23836	-690.17616	448.9	47.4	**50**	2.6
$MeDHP^+$	-327.20488	0.12651	-327.07837				
MeDHPH	-327.92531	0.13546	-327.78985	446.5	45.0	**41**	4.0
$BnDHP^+$	-558.14880	0.20174	-557.94707				
BnDHPH	-558.87129	0.21000	-558.66129	448.2	46.7	**43**	3.7
$HFlu^+$	-500.35917	0.14429	-500.21488				
HFluH	-501.18388	0.15580	-501.02808	510.3	110.8	**109**	1.8
$MeOOCFlu^+$	-728.17150	0.18006	-727.99144				
MeOOCFluH	-729.00208	0.19242	-728.80966	513.4	114.1	**114**	0.1
$MeOFlu^+$	-614.87876	0.17549	-614.70327				
MeOFluH	-615.66664	0.18542	-615.48122	488.2	88.0	**89**	1.0
$PhtrMe^+$	-595.05900	0.19049	-594.86851				
PhtrMeH	-595.80504	0.19966	-595.60538	462.4	61.4	**61.4**	0.0
$PhtrBn^+$	-826.00193	0.26576	-825.73617				
PhtrBnH	-826.74969	0.27400	-826.47570	464.1	63.1	**64.8**	1.7
BNA^+	-687.51953	0.19874	-687.32080				
BNAH	-688.25871	0.20636	-688.05235	459.1	58.0	**59**	1.0

$HEHMe^+$	-900.71807	0.28032	-900.43775				
HEHMeH	-901.46035	0.28727	-901.17307	461.4	60.4	**61.5**	1.1
$2OM^+$	-1148.42548	0.34965	-1148.07583				
2OMH	-1149.15923	0.35857	-1148.80067	454.8	53.6	**58.2**	4.6
$4OM^+$	-1283.95252	0.38250	-1283.57003				
4OMH	-1284.71137	0.39236	-1284.31901	470.0	69.2	**70.2**	1.0
						MUE=	1.8
						MAX=	4.6
						RMSE=	2.2

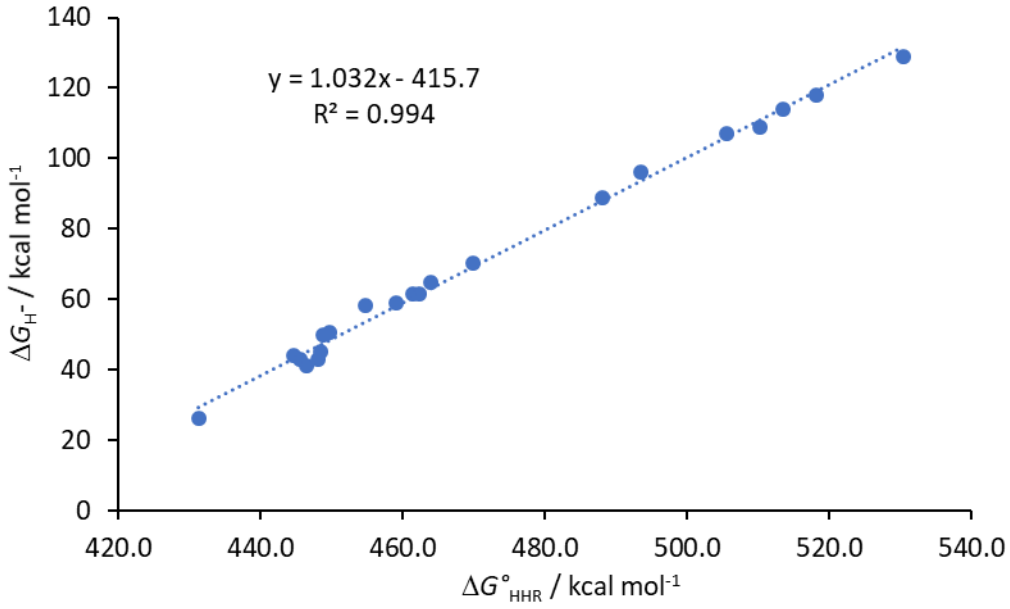

Figure S5. Correlation line obtained with the M5 model.

Table S6. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M6 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.65938	-0.00928	-188.66866				
$HCOO^-$	-189.38378	-0.00285	-189.38664	450.5	45.2	**44**	1.2
B_2H_6	-53.30953	0.03967	-53.26986				
BH_4^-	-27.37627	0.01445	-27.36181	456.1	51.1	**50.4**	0.7
Et_3B	-262.62875	0.16140	-262.46735				
Et_3BH^-	-263.32877	0.16960	-263.15917	434.1	27.8	**26**	1.8
Ph_3C^+	-733.09329	0.23745	-732.85584				
Ph_3CH	-733.89030	0.24544	-733.64486	495.1	92.5	**96**	3.5
$PhCH_2^+$	-270.81682	0.08782	-270.72900				
$PhCH_3$	-271.65569	0.09836	-271.55733	519.8	118.6	**118**	0.6
$pNO_2PhCH_2^+$	-475.37731	0.08643	-475.29088				
pNO_2PhCH_3	-476.23875	0.09631	-476.14244	534.4	134.0	**129**	5.0
$pOMePhCH_2^+$	-385.40212	0.11768	-385.28444				
$pOMePhCH_3$	-386.22002	0.12581	-386.09422	508.1	106.3	**107**	0.7
$BImH^+$	-459.09275	0.15372	-458.93903				
BImHH	-459.82163	0.16164	-459.65999	452.4	47.2	**45**	2.2
$BImMe^+$	-498.42757	0.17845	-498.24912				
BImMeH	-499.15280	0.18800	-498.96480	449.1	43.7	**43**	0.7
$BImPh^+$	-690.21780	0.22713	-689.99067				
BImPhH	-690.94599	0.23494	-690.71105	452.0	46.8	**50**	3.2
$MeDHP^+$	-327.46930	0.12522	-327.34408				
MeDHPH	-328.19660	0.13326	-328.06334	451.3	46.1	**41**	5.1
$BnDHP^+$	-558.58863	0.19919	-558.38944				
BnDHPH	-559.31786	0.20828	-559.10958	451.9	46.6	**43**	3.6
$HFlu^+$	-500.75014	0.14218	-500.60796				
HFluH	-501.57753	0.15336	-501.42417	512.2	110.5	**109**	1.5
$MeOOCFlu^+$	-728.69956	0.17680	-728.52276				
MeOOCFluH	-729.53231	0.19091	-729.34140	513.7	112.1	**114**	1.9
$MeOFlu^+$	-615.34134	0.17389	-615.16745				
MeOFluH	-616.13085	0.18225	-615.94860	490.2	87.2	**89**	1.8
$PhtrMe^+$	-595.51561	0.18881	-595.32680				
PhtrMeH	-596.26630	0.19644	-596.06986	466.3	61.9	**61.4**	0.5
$PhtrBn^+$	-826.63337	0.26310	-826.37027				
PhtrBnH	-827.38551	0.26973	-827.11578	467.8	63.5	**64.8**	1.3
BNA^+	-688.02699	0.19679	-687.83020				
BNAH	-688.77305	0.20297	-688.57007	464.3	59.8	**59**	0.8

HEHMe$^+$	-901.36127	0.27514	-901.08613				
HEHMeH	-902.10979	0.28373	-901.82606	464.3	59.8	**61.5**	1.7
2OM$^+$	-1149.25566	0.34400	-1148.91166				
2OMH	-1149.99312	0.35230	-1149.64082	457.6	52.7	**58.2**	5.5
4OM$^+$	-1284.86738	0.37538	-1284.49200				
4OMH	-1285.62767	0.38600	-1285.24168	470.4	66.3	**70.2**	3.9
						MUE=	2.3
						MAX=	5.1
						RMSE=	2.8

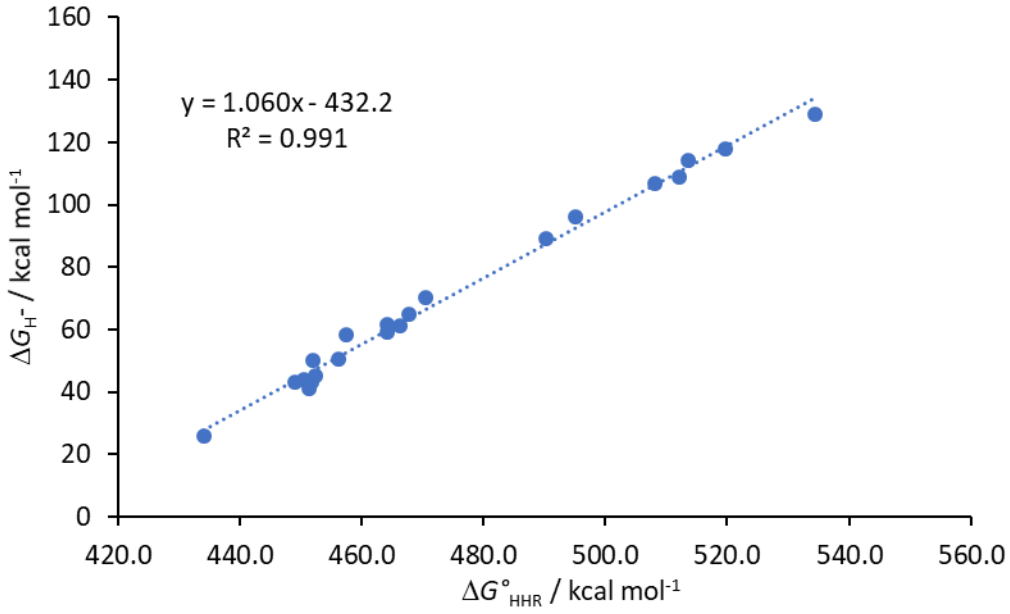

Figure S6. Correlation line obtained with the M6 model.

Table S7. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M7 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.59337	-0.00928	-188.60264				
$HCOO^-$	-189.31440	-0.00285	-189.31725	448.4	41.7	**44**	2.3
B_2H_6	-53.28305	0.03967	-53.24339				
BH_4^-	-27.35824	0.01445	-27.34379	453.1	46.3	**50.4**	4.1
Et_3B	-262.54130	0.16140	-262.37990				
Et_3BH^-	-263.24020	0.16960	-263.07060	433.4	26.7	**26**	0.7
Ph_3C^+	-732.81979	0.23745	-732.58234				
Ph_3CH	-733.62746	0.24544	-733.38202	501.8	94.9	**96**	1.1
$PhCH_2^+$	-270.70787	0.08782	-270.62005				
$PhCH_3$	-271.55224	0.09836	-271.45389	523.2	116.3	**118**	1.7
$pNO_2PhCH_2^+$	-475.20100	0.08643	-475.11457				
pNO_2PhCH_3	-476.06707	0.09631	-475.97077	537.3	130.3	**129**	1.3
$pOMePhCH_2^+$	-385.25656	0.11768	-385.13888				
$pOMePhCH_3$	-386.08036	0.12581	-385.95456	511.8	104.9	**107**	2.1
$BImH^+$	-458.93272	0.15372	-458.77900				
BImHH	-459.66310	0.16164	-459.50146	453.4	46.6	**45**	1.6
$BImMe^+$	-498.25755	0.17845	-498.07910				
BImMeH	-498.98429	0.18800	-498.79629	450.0	43.3	**43**	0.3
$BImPh^+$	-689.97773	0.22713	-689.75060				
BImPhH	-690.70812	0.23494	-690.47318	453.4	46.7	**50**	3.3
$MeDHP^+$	-327.35083	0.12522	-327.22561				
MeDHPH	-328.08095	0.13326	-327.94769	453.1	46.3	**41**	5.3
$BnDHP^+$	-558.38833	0.19919	-558.18914				
BnDHPH	-559.12129	0.20828	-558.91301	454.2	47.5	**43**	4.5
$HFlu^+$	-500.55598	0.14218	-500.41380				
HFluH	-501.39384	0.15336	-501.24048	518.7	111.8	**109**	2.8
$MeOOCFlu^+$	-728.43144	0.17680	-728.25464				
MeOOCFluH	-729.27676	0.19091	-729.08585	521.6	114.7	**114**	0.7
$MeOFlu^+$	-615.11565	0.17389	-614.94176				
MeOFluH	-615.91301	0.18225	-615.73076	495.1	88.2	**89**	0.8
$PhtrMe^+$	-595.29834	0.18881	-595.10953				
PhtrMeH	-596.05489	0.19644	-595.85845	470.0	63.1	**61.4**	1.7
$PhtrBn^+$	-826.33460	0.26310	-826.07150				
PhtrBnH	-827.09326	0.26973	-826.82353	471.9	65.1	**64.8**	0.3
BNA^+	-687.78467	0.19679	-687.58788				
BNAH	-688.53378	0.20297	-688.33081	466.2	59.4	**59**	0.4

HEHMe$^+$	-901.06233	0.27514	-900.78719				
HEHMeH	-901.81339	0.28373	-901.52967	465.9	59.1	**61.5**	2.4
2OM$^+$	-1148.86411	0.34400	-1148.52011				
2OMH	-1149.61138	0.35230	-1149.25908	463.7	56.9	**58.2**	1.3
4OM$^+$	-1284.43346	0.37538	-1284.05809				
4OMH	-1285.20404	0.38600	-1284.81804	476.9	70.0	**70.2**	0.2
						MUE=	1.8
						MAX=	5.3
						RMSE=	2.3

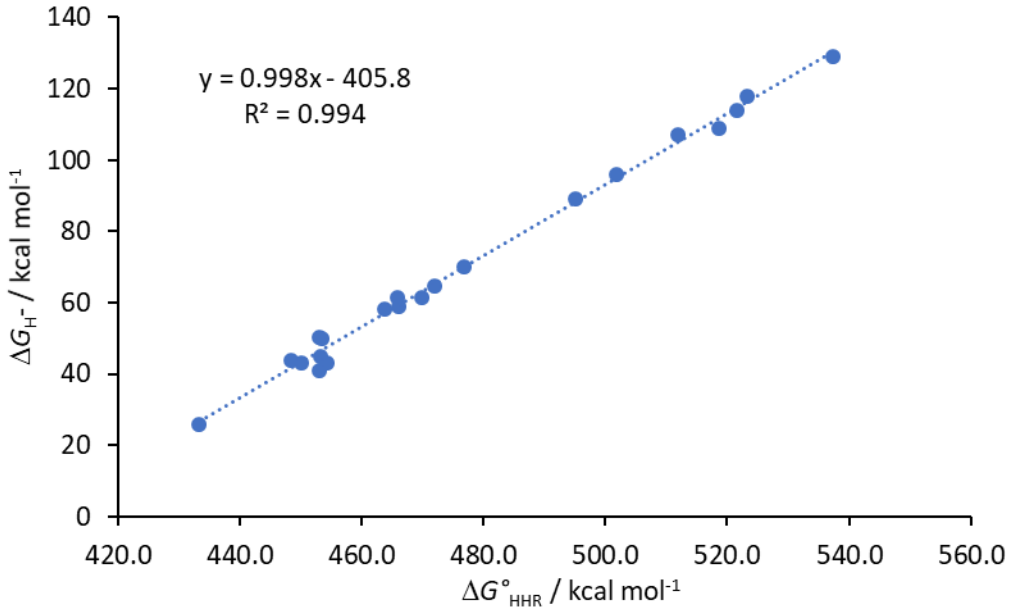

Figure S7. Correlation line obtained with the M7 model.

Table S8. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M8 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.60019	-0.00928	-188.60947				
$HCOO^-$	-189.32026	-0.00285	-189.32311	447.8	41.6	**44**	2.4
B_2H_6	-53.28680	0.03967	-53.24714				
BH_4^-	-27.36001	0.01445	-27.34555	453.1	46.8	**50.4**	3.6
Et_3B	-262.55639	0.16140	-262.39499				
Et_3BH^-	-263.25483	0.16960	-263.08524	433.1	26.9	**26**	0.9
Ph_3C^+	-732.85224	0.23745	-732.61479				
Ph_3CH	-733.65891	0.24544	-733.41347	501.2	94.9	**96**	1.1
$PhCH_2^+$	-270.72153	0.08782	-270.63371				
$PhCH_3$	-271.56514	0.09836	-271.46678	522.8	116.5	**118**	1.5
$pNO_2PhCH_2^+$	-475.22124	0.08643	-475.13481				
pNO_2PhCH_3	-476.08622	0.09631	-475.98991	536.6	130.3	**129**	1.3
$pOMePhCH_2^+$	-385.27507	0.11768	-385.15738				
$pOMePhCH_3$	-386.09793	0.12581	-385.97213	511.3	105.0	**107**	2.0
$BImH^+$	-458.95364	0.15372	-458.79992				
BImHH	-459.68308	0.16164	-459.52144	452.8	46.5	**45**	1.5
$BImMe^+$	-498.28046	0.17845	-498.10201				
BImMeH	-499.00633	0.18800	-498.81833	449.5	43.3	**43**	0.3
$BImPh^+$	-690.00778	0.22713	-689.78065				
BImPhH	-690.73735	0.23494	-690.50241	452.9	46.7	**50**	3.3
$MeDHP^+$	-327.36733	0.12522	-327.24211				
MeDHPH	-328.09647	0.13326	-327.96321	452.5	46.2	**41**	5.2
$BnDHP^+$	-558.41417	0.19919	-558.21498				
BnDHPH	-559.14604	0.20828	-558.93776	453.6	47.3	**43**	4.3
$HFlu^+$	-500.57825	0.14218	-500.43607				
HFluH	-501.41517	0.15336	-501.26181	518.2	111.9	**109**	2.9
$MeOOCFlu^+$	-728.46233	0.17680	-728.28553				
MeOOCFluH	-729.30649	0.19091	-729.11558	520.9	114.6	**114**	0.6
$MeOFlu^+$	-615.14276	0.17389	-614.96888				
MeOFluH	-615.93895	0.18225	-615.75671	494.4	88.1	**89**	0.9
$PhtrMe^+$	-595.32460	0.18881	-595.13579				
PhtrMeH	-596.08012	0.19644	-595.88367	469.3	63.1	**61.4**	1.7
$PhtrBn^+$	-826.37020	0.26310	-826.10710				
PhtrBnH	-827.12790	0.26973	-826.85817	471.3	65.0	**64.8**	0.2
BNA^+	-687.81417	0.19679	-687.61738				
BNAH	-688.56226	0.20297	-688.35929	465.6	59.3	**59**	0.3

$HEHMe^+$	-901.10148	0.27514	-900.82635				
HEHMeH	-901.85124	0.28373	-901.56752	465.1	58.8	**61.5**	2.7
$2OM^+$	-1148.91097	0.34400	-1148.56697				
2OMH	-1149.65740	0.35230	-1149.30510	463.2	56.9	**58.2**	1.3
$4OM^+$	-1284.48621	0.37538	-1284.11084				
4OMH	-1285.25609	0.38600	-1284.87009	476.4	70.2	**70.2**	0.0
						MUE=	1.8
						MAX=	5.2
						RMSE=	2.3

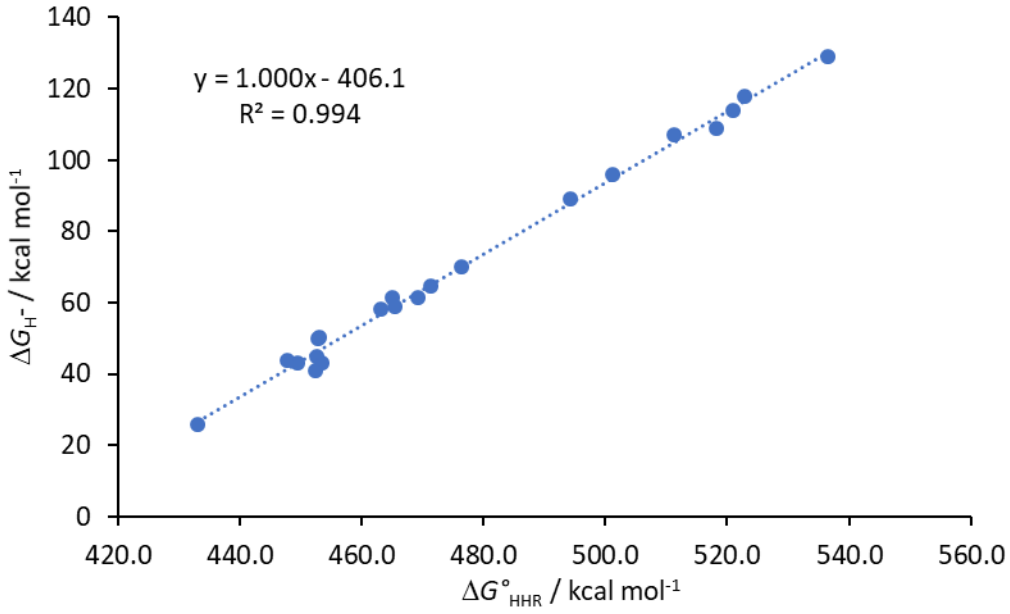

Figure S8. Correlation line obtained with the M8 model.

Table S9. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M9 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.59592	-0.00928	-188.60520				
$HCOO^-$	-189.31484	-0.00285	-189.31769	447.1	41.7	**44**	2.3
B_2H_6	-53.26225	0.03967	-53.22258				
BH_4^-	-27.34016	0.01445	-27.32571	448.3	42.9	**50.4**	7.5
Et_3B	-262.49004	0.16140	-262.32864				
Et_3BH^-	-263.18623	0.16960	-263.01663	431.7	26.7	**26**	0.7
Ph_3C^+	-732.80505	0.23745	-732.56760				
Ph_3CH	-733.61091	0.24544	-733.36547	500.7	94.1	**96**	1.9
$PhCH_2^+$	-270.69338	0.08782	-270.60557				
$PhCH_3$	-271.53746	0.09836	-271.43910	523.1	115.9	**118**	2.1
$pNO_2PhCH_2^+$	-475.18988	0.08643	-475.10345				
pNO_2PhCH_3	-476.05578	0.09631	-475.95947	537.2	129.7	**129**	0.7
$pOMePhCH_2^+$	-385.24086	0.11768	-385.12318				
$pOMePhCH_3$	-386.06431	0.12581	-385.93851	511.6	104.8	**107**	2.2
$BImH^+$	-458.91415	0.15372	-458.76043				
BImHH	-459.64306	0.16164	-459.48141	452.4	46.9	**45**	1.9
$BImMe^+$	-498.23217	0.17845	-498.05371				
BImMeH	-498.95758	0.18800	-498.76958	449.2	43.8	**43**	0.8
$BImPh^+$	-689.95779	0.22713	-689.73066				
BImPhH	-690.68689	0.23494	-690.45195	452.6	47.1	**50**	2.9
$MeDHP^+$	-327.32767	0.12522	-327.20245				
MeDHPH	-328.05648	0.13326	-327.92322	452.3	46.8	**41**	5.8
$BnDHP^+$	-558.36397	0.19919	-558.16478				
BnDHPH	-559.09608	0.20828	-558.88780	453.7	48.1	**43**	5.1
$HFlu^+$	-500.54858	0.14218	-500.40640				
HFluH	-501.38618	0.15336	-501.23281	518.6	111.6	**109**	2.6
$MeOOCFlu^+$	-728.42356	0.17680	-728.24676				
MeOOCFluH	-729.27014	0.19091	-729.07923	522.4	115.3	**114**	1.3
$MeOFlu^+$	-615.10605	0.17389	-614.93216				
MeOFluH	-615.90352	0.18225	-615.72127	495.2	88.7	**89**	0.3
$PhtrMe^+$	-595.28793	0.18881	-595.09912				
PhtrMeH	-596.04266	0.19644	-595.84622	468.8	62.9	**61.4**	1.5
$PhtrBn^+$	-826.32287	0.26310	-826.05977				
PhtrBnH	-827.07976	0.26973	-826.81003	470.8	64.9	**64.8**	0.1
BNA^+	-687.76820	0.19679	-687.57141				
BNAH	-688.51642	0.20297	-688.31344	465.6	59.8	**59**	0.8

HEHMe$^+$	-901.02288	0.27514	-900.74774				
HEHMeH	-901.77264	0.28373	-901.48891	465.1	59.3	**61.5**	2.2
2OM$^+$	-1148.85146	0.34400	-1148.50745				
2OMH	-1149.59721	0.35230	-1149.24491	462.8	57.0	**58.2**	1.2
4OM$^+$	-1284.41290	0.37538	-1284.03752				
4OMH	-1285.18509	0.38600	-1284.79909	477.9	71.8	**70.2**	1.6
						MUE=	2.2
						MAX=	7.5
						RMSE=	2.8

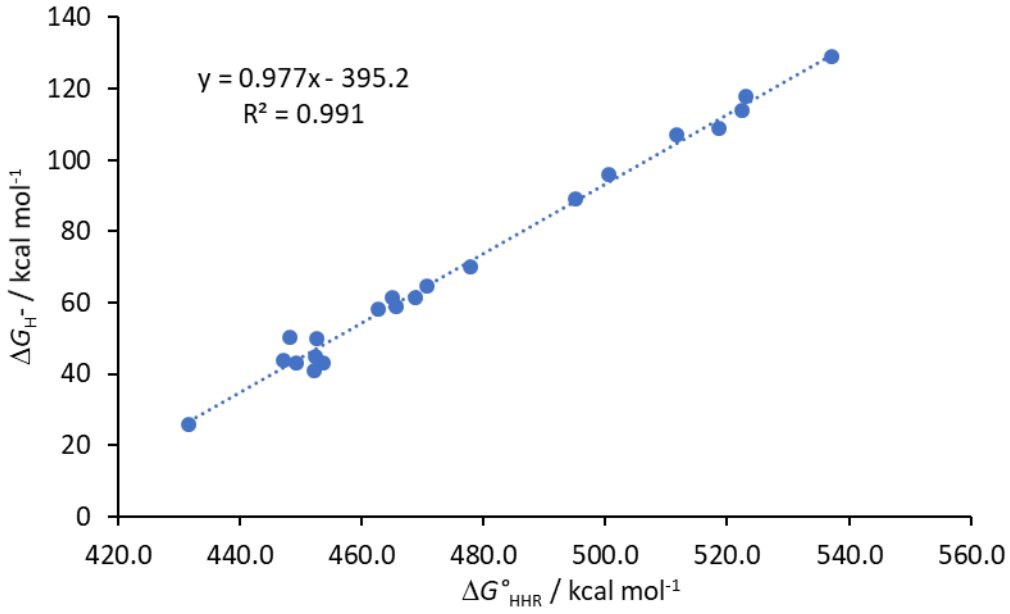

Figure S9. Correlation line obtained with the M9 model.

Table S10. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M10 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^*_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.55128	-0.00928	-188.56055				
$HCOO^-$	-189.26648	-0.00285	-189.26933	444.8	43.1	**44**	0.9
B_2H_6	-53.23113	0.03967	-53.19146				
BH_4^-	-27.32654	0.01445	-27.31209	449.5	48.0	**50.4**	2.4
Et_3B	-262.37713	0.16140	-262.21573				
Et_3BH^-	-263.07205	0.16960	-262.90246	430.9	28.8	**26**	2.8
Ph_3C^+	-732.52226	0.23745	-732.28481				
Ph_3CH	-733.31577	0.24544	-733.07033	492.9	92.9	**96**	3.1
$PhCH_2^+$	-270.59305	0.08782	-270.50523				
$PhCH_3$	-271.42794	0.09836	-271.32959	517.3	118.2	**118**	0.2
$pNO_2PhCH_2^+$	-475.04887	0.08643	-474.96244				
pNO_2PhCH_3	-475.90454	0.09631	-475.80824	530.7	132.1	**129**	3.1
$pOMePhCH_2^+$	-385.10435	0.11768	-384.98667				
$pOMePhCH_3$	-385.91830	0.12581	-385.79249	505.7	106.1	**107**	0.9
$BImH^+$	-458.73895	0.15372	-458.58523				
BImHH	-459.46246	0.16164	-459.30082	449.0	47.5	**45**	2.5
$BImMe^+$	-498.04057	0.17845	-497.86212				
BImMeH	-498.76120	0.18800	-498.57320	446.2	44.6	**43**	1.6
$BImPh^+$	-689.69037	0.22713	-689.46324				
BImPhH	-690.41347	0.23494	-690.17854	448.9	47.3	**50**	2.7
$MeDHP^+$	-327.20457	0.12522	-327.07935				
MeDHPH	-327.92489	0.13326	-327.79163	447.0	45.4	**41**	4.4
$BnDHP^+$	-558.14773	0.19919	-557.94854				
BnDHPH	-558.87003	0.20828	-558.66175	447.5	46.0	**43**	3.0
$HFlu^+$	-500.35868	0.14218	-500.21650				
HFluH	-501.18331	0.15336	-501.02994	510.4	111.1	**109**	2.1
$MeOOCFlu^+$	-728.17009	0.17680	-727.99329				
MeOOCFluH	-729.00097	0.19091	-728.81006	512.5	113.2	**114**	0.8
$MeOFlu^+$	-614.87816	0.17389	-614.70427				
MeOFluH	-615.66577	0.18225	-615.48352	489.0	88.9	**89**	0.1
$PhtrMe^+$	-595.05836	0.18881	-594.86955				
PhtrMeH	-595.80428	0.19644	-595.60783	463.3	62.3	**61.4**	0.9
$PhtrBn^+$	-826.00075	0.26310	-825.73765				
PhtrBnH	-826.74843	0.26973	-826.47869	465.0	64.0	**64.8**	0.8
BNA^+	-687.51858	0.19679	-687.32179				
BNAH	-688.25758	0.20297	-688.05461	459.8	58.7	**59**	0.3

$HEHMe^+$	-900.71707	0.27514	-900.44193				
HEHMeH	-901.45940	0.28373	-901.17567	460.4	59.3	**61.5**	2.2
$2OM^+$	-1148.42416	0.34400	-1148.08016				
2OMH	-1149.15744	0.35230	-1148.80514	454.9	53.6	**58.2**	4.6
$4OM^+$	-1283.95088	0.37538	-1283.57550				
4OMH	-1284.70916	0.38600	-1284.32316	469.2	68.3	**70.2**	1.9
						MUE=	1.9
						MAX=	4.6
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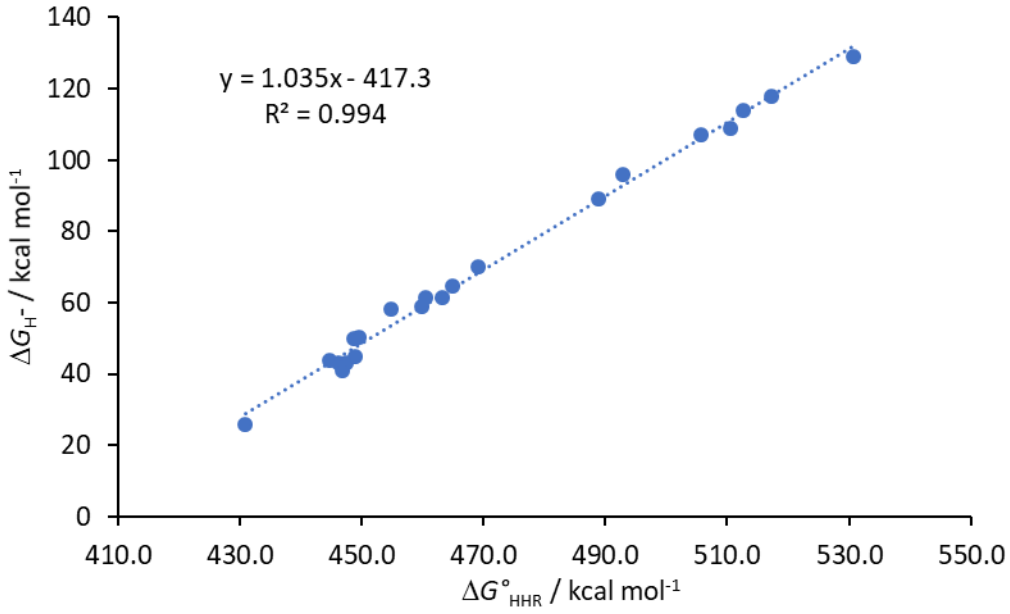

Figure S10. Correlation line obtained with the M10 model.

Table S11. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M11 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.59797	-0.00928	-188.60725				
$HCOO^-$	-189.31141	-0.00285	-189.31426	443.7	42.0	**44**	2.0
B_2H_6	-53.28637	0.03967	-53.24671				
BH_4^-	-27.36436	0.01445	-27.34991	455.9	54.5	**50.4**	4.1
Et_3B	-262.55985	0.16140	-262.39845				
Et_3BH^-	-263.26060	0.16960	-263.09100	434.6	32.7	**26**	6.7
Ph_3C^+	-732.87470	0.23745	-732.63725				
Ph_3CH	-733.67402	0.24544	-733.42858	496.6	96.3	**96**	0.3
$PhCH_2^+$	-270.73813	0.08782	-270.65031				
$PhCH_3$	-271.57130	0.09836	-271.47294	516.2	116.4	**118**	1.6
$pNO_2PhCH_2^+$	-475.23908	0.08643	-475.15265				
pNO_2PhCH_3	-476.09139	0.09631	-475.99509	528.6	129.1	**129**	0.1
$pOMePhCH_2^+$	-385.29044	0.11768	-385.17276				
$pOMePhCH_3$	-386.10378	0.12581	-385.97798	505.3	105.2	**107**	1.8
$BImH^+$	-458.97480	0.15372	-458.82108				
BImHH	-459.69305	0.16164	-459.53140	445.7	44.1	**45**	0.9
$BImMe^+$	-498.30083	0.17845	-498.12238				
BImMeH	-499.01607	0.18800	-498.82807	442.8	41.1	**43**	1.9
$BImPh^+$	-690.03057	0.22713	-689.80344				
BImPhH	-690.75080	0.23494	-690.51586	447.1	45.4	**50**	4.6
$MeDHP^+$	-327.38405	0.12522	-327.25884				
MeDHPH	-328.10313	0.13326	-327.96987	446.2	44.5	**41**	3.5
$BnDHP^+$	-558.43716	0.19919	-558.23797				
BnDHPH	-559.15827	0.20828	-558.94999	446.8	45.2	**43**	2.2
$HFlu^+$	-500.59835	0.14218	-500.45617				
HFluH	-501.42659	0.15336	-501.27323	512.7	112.8	**109**	3.8
$MeOOCFlu^+$	-728.48266	0.17680	-728.30586				
MeOOCFluH	-729.31799	0.19091	-729.12708	515.3	115.5	**114**	1.5
$MeOFlu^+$	-615.16204	0.17389	-614.98815				
MeOFluH	-615.94913	0.18225	-615.76688	488.7	88.1	**89**	0.9
$PhtrMe^+$	-595.34661	0.18881	-595.15780				
PhtrMeH	-596.09253	0.19644	-595.89608	463.3	62.1	**61.4**	0.7
$PhtrBn^+$	-826.39648	0.26310	-826.13338				
PhtrBnH	-827.14527	0.26973	-826.87554	465.7	64.6	**64.8**	0.2
BNA^+	-687.83980	0.19679	-687.64301				
BNAH	-688.57528	0.20297	-688.37230	457.6	56.3	**59**	2.7

HEHMe$^+$	-901.12227	0.27514	-900.84713				
HEHMeH	-901.86011	0.28373	-901.57638	457.6	56.3	**61.5**	5.2
2OM$^+$	-1148.93448	0.34400	-1148.59047				
2OMH	-1149.67335	0.35230	-1149.32105	458.4	57.1	**58.2**	1.1
4OM$^+$	-1284.50748	0.37538	-1284.13210				
4OMH	-1285.26954	0.38600	-1284.88354	471.5	70.6	**70.2**	0.4
						MUE=	2.2
						MAX=	6.7
						RMSE=	2.8

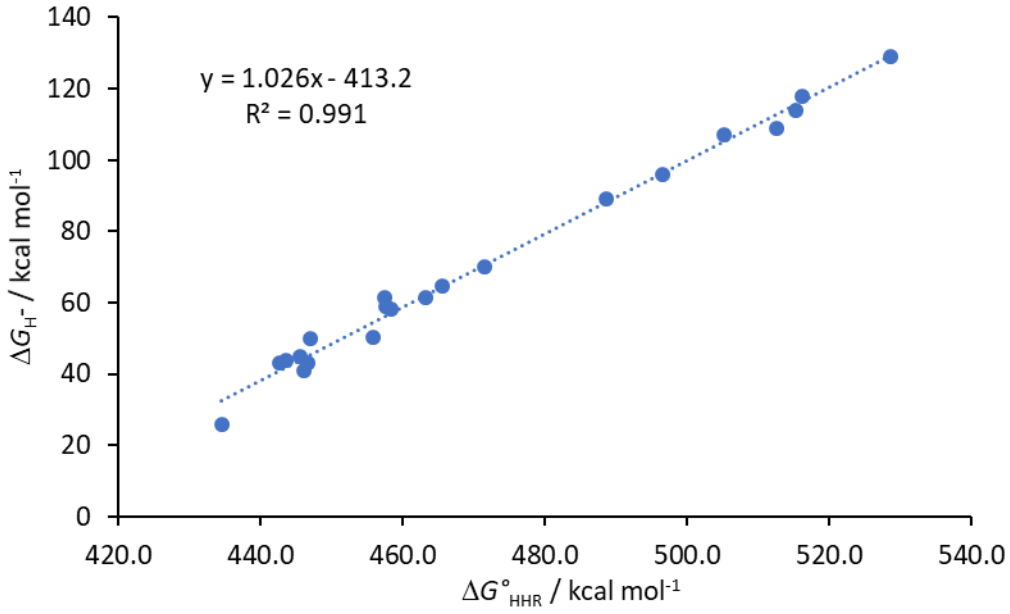

Figure S11. Correlation line obtained with the M11 model.

Table S12. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M12 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.59372	-0.00928	-188.60299				
$HCOO^-$	-189.30584	-0.00285	-189.30870	442.8	41.9	**44**	2.1
B_2H_6	-53.26175	0.03967	-53.22208				
BH_4^-	-27.34465	0.01445	-27.33020	451.3	50.4	**50.4**	0.0
Et_3B	-262.49357	0.16140	-262.33216				
Et_3BH^-	-263.19203	0.16960	-263.02243	433.1	32.1	**26**	6.1
Ph_3C^+	-732.82781	0.23745	-732.59036				
Ph_3CH	-733.62630	0.24544	-733.38086	496.0	95.5	**96**	0.5
$PhCH_2^+$	-270.71024	0.08782	-270.62242				
$PhCH_3$	-271.54375	0.09836	-271.44539	516.4	116.0	**118**	2.0
$pNO_2PhCH_2^+$	-475.20820	0.08643	-475.12177				
pNO_2PhCH_3	-476.06111	0.09631	-475.96481	529.0	128.7	**129**	0.3
$pOMePhCH_2^+$	-385.25652	0.11768	-385.13884				
$pOMePhCH_3$	-386.07030	0.12581	-385.94449	505.6	105.1	**107**	1.9
$BImH^+$	-458.93558	0.15372	-458.78187				
BImHH	-459.65319	0.16164	-459.49155	445.3	44.4	**45**	0.6
$BImMe^+$	-498.25281	0.17845	-498.07436				
BImMeH	-498.96751	0.18800	-498.77951	442.5	41.5	**43**	1.5
$BImPh^+$	-689.98086	0.22713	-689.75373				
BImPhH	-690.70060	0.23494	-690.46566	446.7	45.8	**50**	4.2
$MeDHP^+$	-327.34466	0.12522	-327.21944				
MeDHPH	-328.06328	0.13326	-327.93002	445.9	45.0	**41**	4.0
$BnDHP^+$	-558.38723	0.19919	-558.18804				
BnDHPH	-559.10851	0.20828	-558.90023	446.9	46.0	**43**	3.0
$HFlu^+$	-500.56895	0.14218	-500.42677				
HFluH	-501.39780	0.15336	-501.24443	513.1	112.7	**109**	3.7
$MeOOCFlu^+$	-728.44426	0.17680	-728.26746				
MeOOCFluH	-729.28188	0.19091	-729.09097	516.8	116.4	**114**	2.4
$MeOFlu^+$	-615.12566	0.17389	-614.95177				
MeOFluH	-615.91390	0.18225	-615.73165	489.4	88.8	**89**	0.2
$PhtrMe^+$	-595.31030	0.18881	-595.12149				
PhtrMeH	-596.05532	0.19644	-595.85887	462.7	61.9	**61.4**	0.5
$PhtrBn^+$	-826.34954	0.26310	-826.08644				
PhtrBnH	-827.09747	0.26973	-826.82774	465.2	64.4	**64.8**	0.4
BNA^+	-687.79417	0.19679	-687.59738				
BNAH	-688.52969	0.20297	-688.32672	457.7	56.8	**59**	2.2

HEHMe$^+$	-901.04409	0.27514	-900.76895				
HEHMeH	-901.78176	0.28373	-901.49803	457.5	56.7	**61.5**	4.8
2OM$^+$	-1148.87547	0.34400	-1148.53147				
2OMH	-1149.61354	0.35230	-1149.26124	457.9	57.1	**58.2**	1.1
4OM$^+$	-1284.43472	0.37538	-1284.05934				
4OMH	-1285.19894	0.38600	-1284.81294	472.9	72.2	**70.2**	2.0
						MUE=	2.1
						MAX=	6.1
						RMSE=	2.6

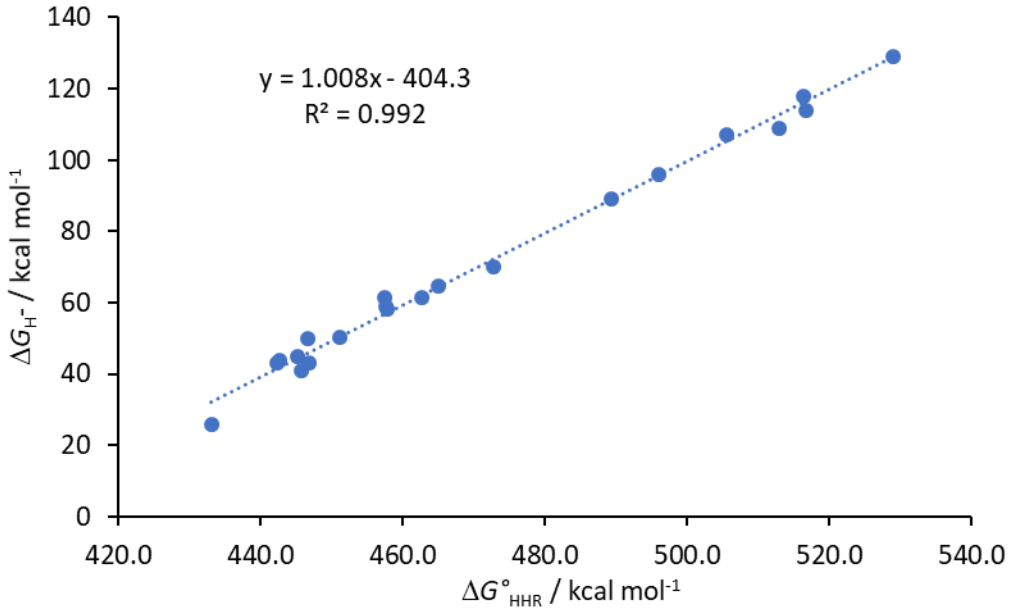

Figure S12. Correlation line obtained with the M12 model.

Table S13. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M13 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.54908	-0.00928	-188.55835				
$HCOO^-$	-189.25792	-0.00285	-189.26077	440.8	44.1	**44**	0.1
B_2H_6	-53.23075	0.03967	-53.19108				
BH_4^-	-27.33051	0.01445	-27.31606	452.1	56.1	**50.4**	5.7
Et_3B	-262.38051	0.16140	-262.21911				
Et_3BH^-	-263.07688	0.16960	-262.90728	431.8	34.6	**26**	8.6
Ph_3C^+	-732.54472	0.23745	-732.30727				
Ph_3CH	-733.33043	0.24544	-733.08500	488.0	94.2	**96**	1.8
$PhCH_2^+$	-270.60975	0.08782	-270.52193				
$PhCH_3$	-271.43392	0.09836	-271.33556	510.6	118.0	**118**	0.0
$pNO_2PhCH_2^+$	-475.06676	0.08643	-474.98033				
pNO_2PhCH_3	-475.90974	0.09631	-475.81343	522.8	131.0	**129**	2.0
$pOMePhCH_2^+$	-385.11990	0.11768	-385.00222				
$pOMePhCH_3$	-385.92404	0.12581	-385.79823	499.5	106.3	**107**	0.7
$BImH^+$	-458.76027	0.15372	-458.60655				
BImHH	-459.47231	0.16164	-459.31067	441.8	45.2	**45**	0.2
$BImMe^+$	-498.06119	0.17845	-497.88273				
BImMeH	-498.77083	0.18800	-498.58283	439.3	42.5	**43**	0.5
$BImPh^+$	-689.71334	0.22713	-689.48621				
BImPhH	-690.42664	0.23494	-690.19170	442.7	46.1	**50**	3.9
$MeDHP^+$	-327.22156	0.12522	-327.09634				
MeDHPH	-327.93136	0.13326	-327.79810	440.4	43.6	**41**	2.6
$BnDHP^+$	-558.17089	0.19919	-557.97170				
BnDHPH	-558.88191	0.20828	-558.67363	440.5	43.7	**43**	0.7
$HFlu^+$	-500.37877	0.14218	-500.23659				
HFluH	-501.19442	0.15336	-501.04106	504.8	111.9	**109**	2.9
$MeOOCFlu^+$	-728.19063	0.17680	-728.01383				
MeOOCFluH	-729.01231	0.19091	-728.82140	506.8	114.0	**114**	0.0
$MeOFlu^+$	-614.89759	0.17389	-614.72370				
MeOFluH	-615.67571	0.18225	-615.49346	483.0	88.8	**89**	0.2
$PhtrMe^+$	-595.08045	0.18881	-594.89163				
PhtrMeH	-595.81642	0.19644	-595.61997	457.0	61.3	**61.4**	0.1
$PhtrBn^+$	-826.02703	0.26310	-825.76393				
PhtrBnH	-826.76537	0.26973	-826.49564	459.2	63.5	**64.8**	1.3
BNA^+	-687.54439	0.19679	-687.34760				
BNAH	-688.27048	0.20297	-688.06750	451.7	55.7	**59**	3.3

HEHMe$^+$	-900.73824	0.27514	-900.46310				
HEHMeH	-901.46839	0.28373	-901.18466	452.8	56.8	**61.5**	4.7
2OM$^+$	-1148.44793	0.34400	-1148.10393				
2OMH	-1149.17314	0.35230	-1148.82084	449.9	53.7	**58.2**	4.5
4OM$^+$	-1283.97242	0.37538	-1283.59705				
4OMH	-1284.72233	0.38600	-1284.33633	463.9	68.6	**70.2**	1.6
						MUE=	2.2
						MAX=	8.6
						RMSE=	3.1

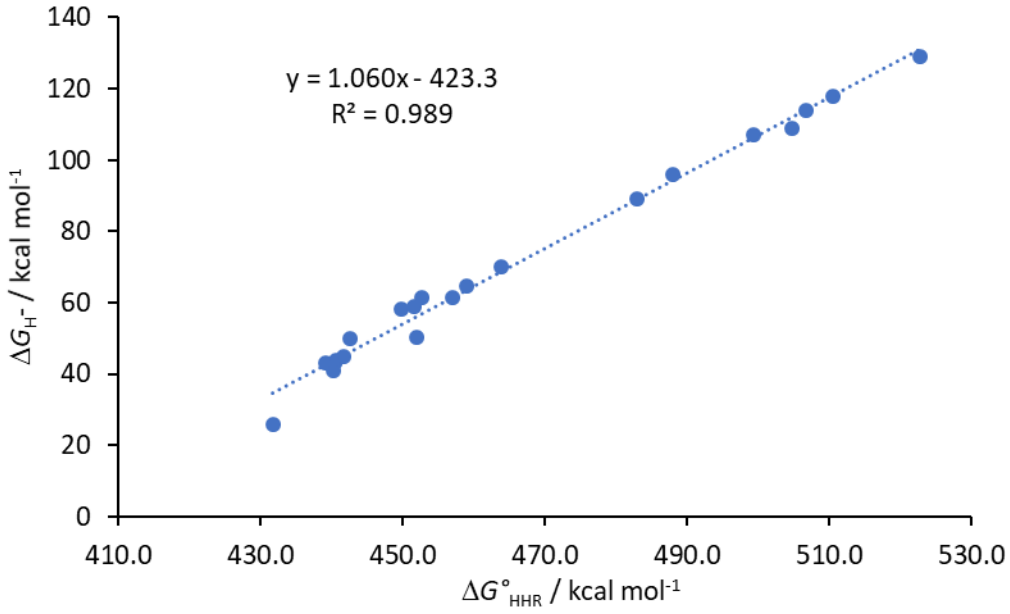

Figure S13. Correlation line obtained with the M13 model.

Table S14. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M14 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.65716	-0.00928	-188.66644				
$HCOO^-$	-189.37497	-0.00285	-189.37783	446.4	46.1	**44**	2.1
B_2H_6	-53.30916	0.03967	-53.26949				
BH_4^-	-27.37978	0.01445	-27.36533	458.4	59.2	**50.4**	8.8
Et_3B	-262.63207	0.16140	-262.47067				
Et_3BH^-	-263.33333	0.16960	-263.16374	434.9	33.7	**26**	7.7
Ph_3C^+	-733.11582	0.23745	-732.87836				
Ph_3CH	-733.90497	0.24544	-733.65953	490.2	93.6	**96**	2.4
$PhCH_2^+$	-270.83361	0.08782	-270.74579				
$PhCH_3$	-271.66166	0.09836	-271.56330	513.0	118.3	**118**	0.3
$pNO_2PhCH_2^+$	-475.39544	0.08643	-475.30901				
pNO_2PhCH_3	-476.24391	0.09631	-476.14761	526.2	132.7	**129**	3.7
$pOMePhCH_2^+$	-385.41778	0.11768	-385.30010				
$pOMePhCH_3$	-386.22575	0.12581	-386.09994	501.9	106.3	**107**	0.7
$BImH^+$	-459.11413	0.15372	-458.96041				
BImHH	-459.83147	0.16164	-459.66983	445.2	44.8	**45**	0.2
$BImMe^+$	-498.44828	0.17845	-498.26982				
BImMeH	-499.16242	0.18800	-498.97442	442.1	41.5	**43**	1.5
$BImPh^+$	-690.24083	0.22713	-690.01370				
BImPhH	-690.95913	0.23494	-690.72419	445.8	45.5	**50**	4.5
$MeDHP^+$	-327.48635	0.12522	-327.36114				
MeDHPH	-328.20307	0.13326	-328.06980	444.7	44.3	**41**	3.3
$BnDHP^+$	-558.61189	0.19919	-558.41270				
BnDHPH	-559.32974	0.20828	-559.12146	444.8	44.4	**43**	1.4
$HFlu^+$	-500.77028	0.14218	-500.62810				
HFluH	-501.58863	0.15336	-501.43526	506.5	111.3	**109**	2.3
$MeOOCFlu^+$	-728.72015	0.17680	-728.54335				
MeOOCFluH	-729.54359	0.19091	-729.35268	507.9	112.8	**114**	1.2
$MeOFlu^+$	-615.36083	0.17389	-615.18694				
MeOFluH	-616.14075	0.18225	-615.95851	484.2	87.1	**89**	1.9
$PhtrMe^+$	-595.53774	0.18881	-595.34893				
PhtrMeH	-596.27843	0.19644	-596.08199	460.0	60.9	**61.4**	0.5
$PhtrBn^+$	-826.65969	0.26310	-826.39659				
PhtrBnH	-827.40243	0.26973	-827.13270	461.9	63.0	**64.8**	1.8
BNA^+	-688.05288	0.19679	-687.85609				
BNAH	-688.78588	0.20297	-688.58291	456.1	56.6	**59**	2.4

HEHMe$^+$	-901.38249	0.27514	-901.10735				
HEHMeH	-902.11865	0.28373	-901.83492	456.6	57.1	**61.5**	4.4
2OM$^+$	-1149.27940	0.34400	-1148.93540				
2OMH	-1150.00878	0.35230	-1149.65648	452.5	52.7	**58.2**	5.5
4OM$^+$	-1284.88885	0.37538	-1284.51347				
4OMH	-1285.64079	0.38600	-1285.25480	465.2	66.5	**70.2**	3.7
						MUE=	2.9
						MAX=	8.8
						RMSE=	3.6

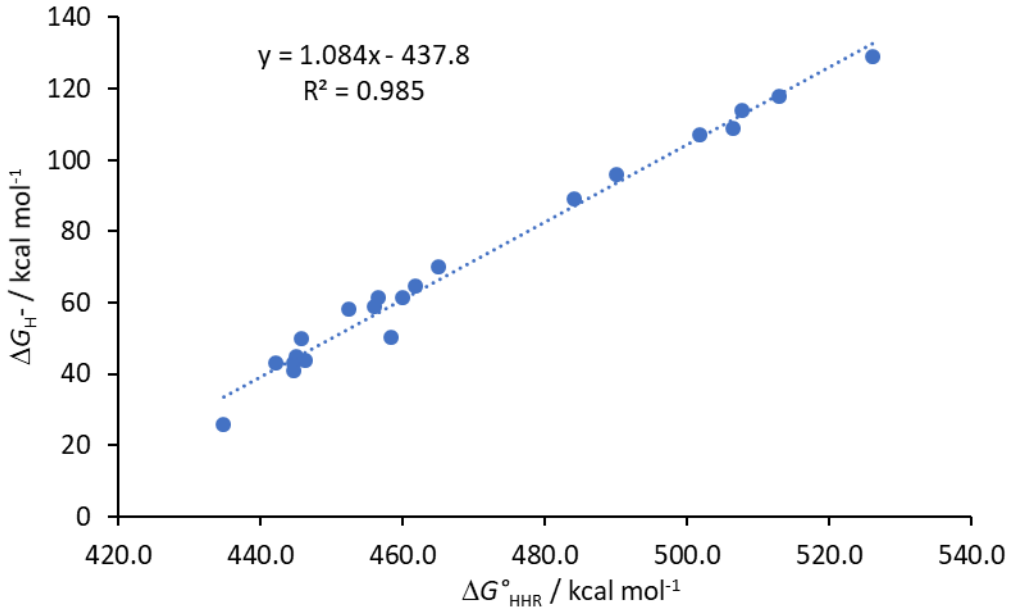

Figure S14. Correlation line obtained with the M14 model.

Table S15. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M15 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.65735	-0.00928	-188.66663				
$HCOO^-$	-189.37548	-0.00285	-189.37834	446.6	45.4	**44**	1.4
B_2H_6	-53.31112	0.03967	-53.27145				
BH_4^-	-27.38018	0.01445	-27.36573	458.1	57.9	**50.4**	7.5
Et_3B	-262.64758	0.16140	-262.48618				
Et_3BH^-	-263.35036	0.16960	-263.18076	435.9	33.6	**26**	7.6
Ph_3C^+	-733.14740	0.23745	-732.90995				
Ph_3CH	-733.93754	0.24544	-733.69210	490.8	93.5	**96**	2.5
$PhCH_2^+$	-270.84086	0.08782	-270.75304				
$PhCH_3$	-271.66951	0.09836	-271.57115	513.4	118.1	**118**	0.1
$pNO_2PhCH_2^+$	-475.40639	0.08643	-475.31996				
pNO_2PhCH_3	-476.25547	0.09631	-476.15917	526.6	132.6	**129**	3.6
$pOMePhCH_2^+$	-385.42944	0.11768	-385.31175				
$pOMePhCH_3$	-386.23793	0.12581	-386.11212	502.2	106.0	**107**	1.0
$BImH^+$	-459.12983	0.15372	-458.97611				
BImHH	-459.84931	0.16164	-459.68767	446.5	45.3	**45**	0.3
$BImMe^+$	-498.46803	0.17845	-498.28957				
BImMeH	-499.18463	0.18800	-498.99663	443.7	42.2	**43**	0.8
$BImPh^+$	-690.26975	0.22713	-690.04262				
BImPhH	-690.98975	0.23494	-690.75481	446.9	45.7	**50**	4.3
$MeDHP^+$	-327.49721	0.12522	-327.37199				
MeDHPH	-328.21518	0.13326	-328.08192	445.5	44.1	**41**	3.1
$BnDHP^+$	-558.63388	0.19919	-558.43469				
BnDHPH	-559.35324	0.20828	-559.14496	445.7	44.4	**43**	1.4
$HFlu^+$	-500.78557	0.14218	-500.64339				
HFluH	-501.60513	0.15336	-501.45177	507.3	111.5	**109**	2.5
$MeOOCFlu^+$	-728.74335	0.17680	-728.56655				
MeOOCFluH	-729.56875	0.19091	-729.37784	509.1	113.5	**114**	0.5
$MeOFlu^+$	-615.38172	0.17389	-615.20783				
MeOFluH	-616.16410	0.18225	-615.98186	485.7	88.0	**89**	1.0
$PhtrMe^+$	-595.55955	0.18881	-595.37073				
PhtrMeH	-596.30197	0.19644	-596.10553	461.1	61.2	**61.4**	0.2
$PhtrBn^+$	-826.69313	0.26310	-826.43003				
PhtrBnH	-827.43760	0.26973	-827.16786	463.0	63.2	**64.8**	1.6
BNA^+	-688.07744	0.19679	-687.88065				
BNAH	-688.81169	0.20297	-688.60872	456.9	56.6	**59**	2.4
$HEHMe^+$	-901.41891	0.27514	-901.14377				
HEHMeH	-902.15679	0.28373	-901.87306	457.6	57.4	**61.5**	4.1

2OM$^+$	-1149.33326	0.34400	-1148.98926				
2OMH	-1150.06366	0.35230	-1149.71136	453.1	52.5	**58.2**	5.7
4OM$^+$	-1284.94968	0.37538	-1284.57430				
4OMH	-1285.70524	0.38600	-1285.31925	467.5	68.1	**70.2**	2.1
						MUE=	2.6
						MAX=	7.6
						RMSE=	3.4

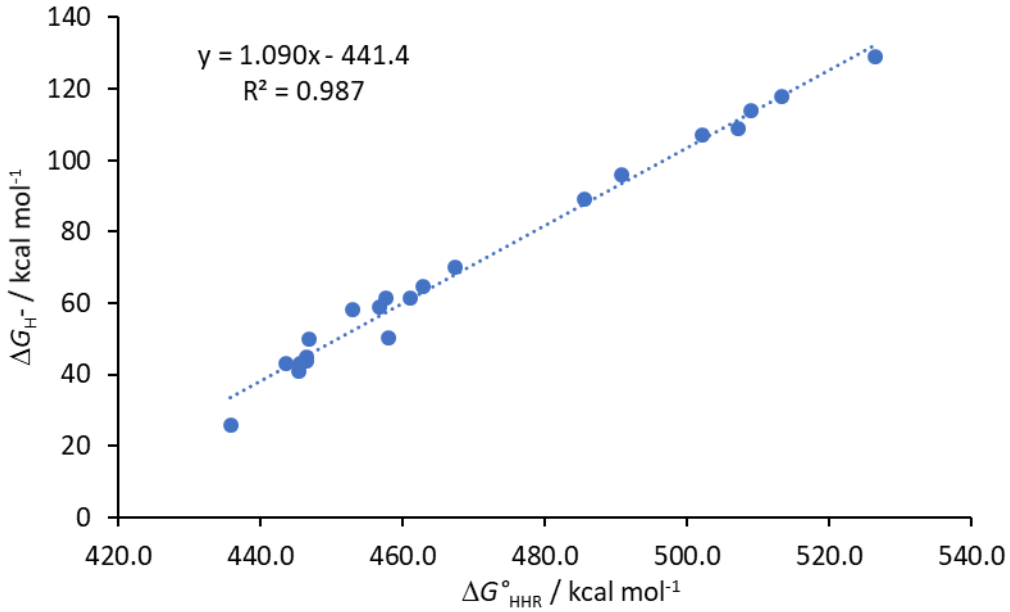

Figure S15. Correlation line obtained with the M15 model.

Table S16. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M16 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^*_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.65734	-0.00928	-188.66662				
$HCOO^-$	-189.37547	-0.00290	-189.37837	446.6	**45.3**	**44**	1.3
B_2H_6	-53.31110	0.03948	-53.27162				
BH_4^-	-27.38017	0.01437	-27.36580	458.1	**57.7**	**50.4**	7.3
Et_3B	-262.64770	0.16258	-262.48512				
Et_3BH^-	-263.35051	0.16990	-263.18061	436.4	**34.3**	**26**	8.3
Ph_3C^+	-733.14751	0.23793	-732.90959				
Ph_3CH	-733.93778	0.24580	-733.69198	491.0	**93.3**	**96**	2.7
$PhCH_2^+$	-270.84084	0.08808	-270.75276				
$PhCH_3$	-271.66950	0.09592	-271.57358	515.1	**119.4**	**118**	1.4
$pNO_2PhCH_2^+$	-475.40684	0.08561	-475.32123				
pNO_2PhCH_3	-476.25547	0.09642	-476.15905	525.7	**131.0**	**129**	2.0
$pOMePhCH_2^+$	-385.42942	0.11776	-385.31166				
$pOMePhCH_3$	-386.23793	0.12587	-386.11206	502.3	**105.6**	**107**	1.4
$BImH^+$	-459.12987	0.15369	-458.97618				
BImHH	-459.84931	0.16214	-459.68718	446.2	**44.8**	**45**	0.2
$BImMe^+$	-498.46804	0.17814	-498.28990				
BImMeH	-499.18465	0.18862	-498.99604	443.1	**41.5**	**43**	1.5
$BImPh^+$	-690.26986	0.22807	-690.04179				
BImPhH	-690.98986	0.23493	-690.75493	447.5	**46.3**	**50**	3.7
$MeDHP^+$	-327.49719	0.12507	-327.37212				
MeDHPH	-328.21519	0.13343	-328.08176	445.3	**43.9**	**41**	2.9
$BnDHP^+$	-558.63398	0.19840	-558.43558				
BnDHPH	-559.35341	0.20617	-559.14724	446.6	**45.2**	**43**	2.2
$HFlu^+$	-500.78560	0.14217	-500.64343				
HFluH	-501.60518	0.15337	-501.45182	507.3	**111.0**	**109**	2.0
$MeOOCFlu^+$	-728.74351	0.17761	-728.56590				
MeOOCFluH	-729.56905	0.18879	-729.38026	511.0	**115.1**	**114**	1.1
$MeOFlu^+$	-615.38175	0.17383	-615.20792				
MeOFluH	-616.16425	0.18240	-615.98186	485.7	**87.6**	**89**	1.4
$PhtrMe^+$	-595.55954	0.18750	-595.37204				
PhtrMeH	-596.30197	0.19651	-596.10546	460.2	**60.0**	**61.4**	1.4
$PhtrBn^+$	-826.69323	0.26246	-826.43076				
PhtrBnH	-827.43779	0.26976	-827.16803	462.6	**62.6**	**64.8**	2.2
BNA^+	-688.07783	0.19618	-687.88165				
BNAH	-688.81198	0.20336	-688.60863	456.2	**55.7**	**59**	3.3

HEHMe$^+$	-901.41899	0.27736	-901.14163				
HEHMeH	-902.15700	0.28467	-901.87233	458.5	**58.2**	**61.5**	3.3
2OM$^+$	-1149.33368	0.34444	-1148.98925				
2OMH	-1150.06470	0.35361	-1149.71109	453.0	**52.2**	**58.2**	6.0
4OM$^+$	-1284.95001	0.37720	-1284.57281				
4OMH	-1285.70608	0.38666	-1285.31942	468.5	**69.0**	**70.2**	1.2
						MUE=	2.7
						MAX=	8.3
						RMSE=	3.4

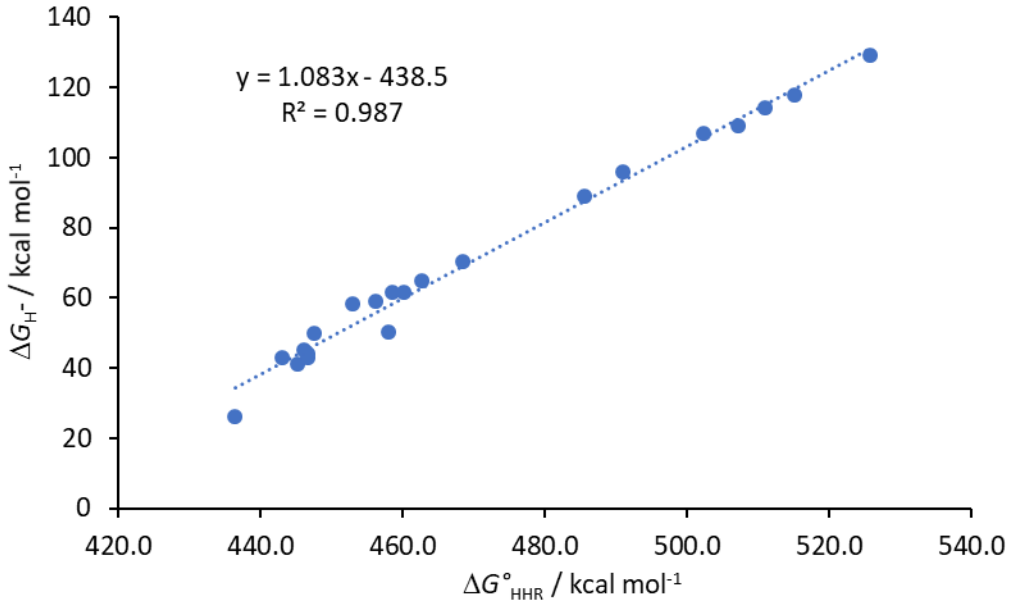

Figure S16. Correlation line obtained with the M16 model.

Table S17. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M17 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^{*}_{HHR}	ΔG_{H^-} calc.	ΔG_{H^-} exp.	$\lvert\Delta(\Delta G_{H^-})\rvert$
CO_2	-188.60059	-0.00891	-188.60950				
$HCOO^-$	-189.32022	-0.00338	-189.32360	448.1	42.0	**44**	2.0
B_2H_6	-53.28676	0.04020	-53.24657				
BH_4^-	-27.35982	0.01374	-27.34608	453.6	47.4	**50.4**	3.0
Et_3B	-262.55682	0.16474	-262.39208				
Et_3BH^-	-263.25510	0.17178	-263.08332	433.8	27.7	**26**	1.7
Ph_3C^+	-732.85415	0.24183	-732.61231				
Ph_3CH	-733.66124	0.24937	-733.41187	501.7	95.4	**96**	0.6
$PhCH_2^+$	-270.72195	0.08909	-270.63285				
$PhCH_3$	-271.56585	0.09842	-271.46743	523.7	117.3	**118**	0.7
$pNO_2PhCH_2^+$	-475.22234	0.08488	-475.13746				
pNO_2PhCH_3	-476.08778	0.09684	-475.99094	535.6	129.2	**129**	0.2
$pOMePhCH_2^+$	-385.27587	0.11924	-385.15663				
$pOMePhCH_3$	-386.09886	0.12811	-385.97075	510.9	104.5	**107**	2.5
$BImH^+$	-458.95456	0.15550	-458.79906				
BImHH	-459.68424	0.16451	-459.51973	452.2	46.1	**45**	1.1
$BImMe^+$	-498.28146	0.17963	-498.10184				
BImMeH	-499.00761	0.19071	-498.81690	448.7	42.6	**43**	0.4
$BImPh^+$	-690.00949	0.23015	-689.77933				
BImPhH	-690.73936	0.23864	-690.50071	452.7	46.5	**50**	3.5
$MeDHP^+$	-327.36780	0.12468	-327.24312				
MeDHPH	-328.09720	0.13572	-327.96149	450.8	44.6	**41**	3.6
$BnDHP^+$	-558.41448	0.20129	-558.21319				
BnDHPH	-559.14788	0.21008	-558.93779	454.7	48.6	**43**	5.6
$HFlu^+$	-500.57938	0.14427	-500.43510				
HFluH	-501.41658	0.15596	-501.26062	518.0	111.7	**109**	2.7
$MeOOCFlu^+$	-728.46389	0.18071	-728.28318				
MeOOCFluH	-729.30853	0.19263	-729.11590	522.5	116.2	**114**	2.2
$MeOFlu^+$	-615.14430	0.17559	-614.96871				
MeOFluH	-615.94084	0.18575	-615.75509	493.5	87.2	**89**	1.8
$PhtrMe^+$	-595.32598	0.19049	-595.13549				
PhtrMeH	-596.08175	0.19973	-595.88202	468.5	62.3	**61.4**	0.9
$PhtrBn^+$	-826.37241	0.26572	-826.10669				
PhtrBnH	-827.13036	0.27444	-826.85592	470.1	63.9	**64.8**	0.9
BNA^+	-687.81467	0.19840	-687.61627				
BNAH	-688.56409	0.20652	-688.35757	465.2	59.0	**59**	0.0

HEHMe$^+$	-901.10258	0.28069	-900.82189				
HEHMeH	-901.85340	0.28961	-901.56379	465.6	59.4	**61.5**	2.1
2OM$^+$	-1148.91411	0.34996	-1148.56415				
2OMH	-1149.66090	0.35832	-1149.30259	463.4	57.2	**58.2**	1.0
4OM$^+$	-1284.48998	0.38278	-1284.10720				
4OMH	-1285.26004	0.39273	-1284.86731	477.0	70.8	**70.2**	0.6
						MUE=	1.8
						MAX=	5.6
						RMSE=	2.2

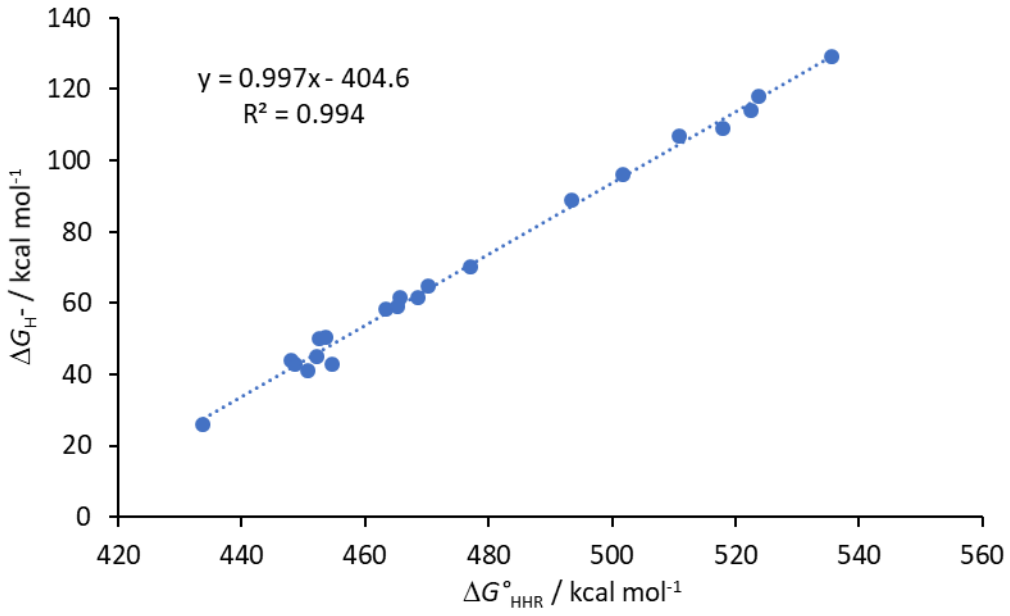

Figure S17. Correlation line obtained with the M17 model.

Table S18. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M18 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^*_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.59638	-0.00891	-188.60528				
$HCOO^-$	-189.31479	-0.00338	-189.31817	447.3	42.0	**44**	2.0
B_2H_6	-53.26216	0.04020	-53.22196				
BH_4^-	-27.33978	0.01374	-27.32603	448.7	43.3	**50.4**	7.1
Et_3B	-262.49061	0.16474	-262.32587				
Et_3BH^-	-263.18675	0.17178	-263.01497	432.4	27.5	**26**	1.5
Ph_3C^+	-732.80672	0.24183	-732.56489				
Ph_3CH	-733.61331	0.24937	-733.36394	501.4	94.8	**96**	1.2
$PhCH_2^+$	-270.69372	0.08909	-270.60463				
$PhCH_3$	-271.53810	0.09842	-271.43968	524.0	116.8	**118**	1.2
$pNO_2PhCH_2^+$	-475.19115	0.08488	-475.10627				
pNO_2PhCH_3	-476.05756	0.09684	-475.96072	536.2	128.7	**129**	0.3
$pOMePhCH_2^+$	-385.24157	0.11924	-385.12233				
$pOMePhCH_3$	-386.06517	0.12811	-385.93706	511.2	104.4	**107**	2.6
$BImH^+$	-458.91492	0.15550	-458.75942				
BImHH	-459.64405	0.16451	-459.47954	451.9	46.5	**45**	1.5
$BImMe^+$	-498.23298	0.17963	-498.05336				
BImMeH	-498.95873	0.19071	-498.76802	448.5	43.1	**43**	0.1
$BImPh^+$	-689.95889	0.23015	-689.72874				
BImPhH	-690.68872	0.23864	-690.45008	452.6	47.2	**50**	2.8
$MeDHP^+$	-327.32806	0.12468	-327.20338				
MeDHPH	-328.05716	0.13572	-327.92145	450.6	45.2	**41**	4.2
$BnDHP^+$	-558.36441	0.20129	-558.16312				
BnDHPH	-559.09807	0.21008	-558.88799	454.9	49.4	**43**	6.4
$HFlu^+$	-500.54951	0.14427	-500.40524				
HFluH	-501.38735	0.15596	-501.23139	518.4	111.4	**109**	2.4
$MeOOCFlu^+$	-728.42645	0.18071	-728.24574				
MeOOCFluH	-729.27253	0.19263	-729.07990	523.4	116.3	**114**	2.3
$MeOFlu^+$	-615.10743	0.17559	-614.93185				
MeOFluH	-615.90526	0.18575	-615.71951	494.3	87.8	**89**	1.2
$PhtrMe^+$	-595.28906	0.19049	-595.09857				
PhtrMeH	-596.04404	0.19973	-595.84431	468.0	62.1	**61.4**	0.7
$PhtrBn^+$	-826.32476	0.26572	-826.05904				
PhtrBnH	-827.08194	0.27444	-826.80750	469.7	63.8	**64.8**	1.0
BNA^+	-687.76879	0.19840	-687.57039				
BNAH	-688.51842	0.20652	-688.31190	465.3	59.5	**59**	0.5

HEHMe$^+$	-901.02475	0.28069	-900.74406				
HEHMeH	-901.77484	0.28961	-901.48522	465.1	59.3	**61.5**	2.2
2OM$^+$	-1148.85412	0.34996	-1148.50415				
2OMH	-1149.60043	0.35832	-1149.24211	463.1	57.4	**58.2**	0.8
4OM$^+$	-1284.41586	0.38278	-1284.03309				
4OMH	-1285.18873	0.39273	-1284.79600	478.7	72.7	**70.2**	2.5
						MUE=	2.1
						MAX=	7.1
						RMSE=	2.8

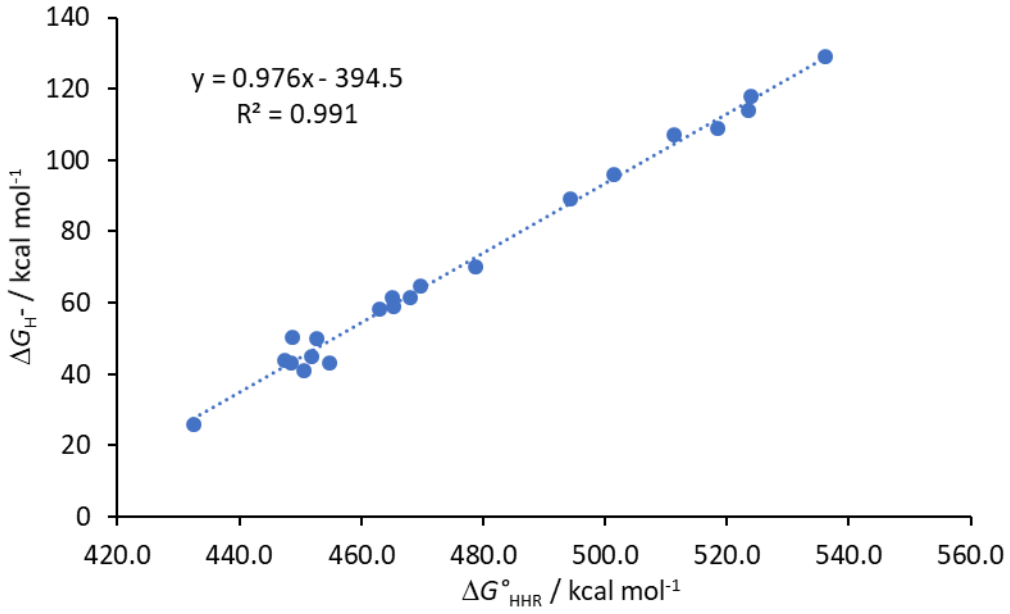

Figure S18. Correlation line obtained with the M18 model.

Table S19. Energies (in a.u.) and hydricities (in kcalmol^{-1}) obtained with M19 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	ΔG^*_{HHR}	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H)\rvert$
CO_2	-188.55137	-0.00891	-188.56028				
$HCOO^-$	-189.26618	-0.00338	-189.26956	445.1	43.6	**44**	0.4
B_2H_6	-53.23106	0.04020	-53.19087				
BH_4^-	-27.32621	0.01374	-27.31246	449.9	48.7	**50.4**	1.7
Et_3B	-262.37753	0.16474	-262.21279				
Et_3BH^-	-263.07233	0.17178	-262.90055	431.6	29.7	**26**	3.7
Ph_3C^+	-732.52334	0.24183	-732.28151				
Ph_3CH	-733.31722	0.24937	-733.06785	493.4	93.6	**96**	2.4
$PhCH_2^+$	-270.59321	0.08909	-270.50411				
$PhCH_3$	-271.42833	0.09842	-271.32991	518.2	119.2	**118**	1.2
$pNO_2PhCH_2^+$	-475.04873	0.08488	-474.96386				
pNO_2PhCH_3	-475.90475	0.09684	-475.80791	529.6	131.0	**129**	2.0
$pOMePhCH_2^+$	-385.10447	0.11924	-384.98522				
$pOMePhCH_3$	-385.91861	0.12811	-385.79050	505.3	105.9	**107**	1.1
$BImH^+$	-458.73925	0.15550	-458.58375				
BImHH	-459.46286	0.16451	-459.29836	448.4	47.1	**45**	2.1
$BImMe^+$	-498.04093	0.17963	-497.86131				
BImMeH	-498.76174	0.19071	-498.57103	445.4	43.9	**43**	0.9
$BImPh^+$	-689.69102	0.23015	-689.46087				
BImPhH	-690.41443	0.23864	-690.17578	448.6	47.3	**50**	2.7
$MeDHP^+$	-327.20476	0.12468	-327.08008				
MeDHPH	-327.92527	0.13572	-327.78955	445.2	43.8	**41**	2.8
$BnDHP^+$	-558.14772	0.20129	-557.94643				
BnDHPH	-558.87129	0.21008	-558.66121	448.5	47.2	**43**	4.2
$HFlu^+$	-500.35912	0.14427	-500.21485				
HFluH	-501.18389	0.15596	-501.02793	510.2	111.0	**109**	2.0
$MeOOCFlu^+$	-728.17128	0.18071	-727.99057				
MeOOCFluH	-729.00177	0.19263	-728.80914	513.7	114.5	**114**	0.5
$MeOFlu^+$	-614.87869	0.17559	-614.70310				
MeOFluH	-615.66653	0.18575	-615.48078	488.0	88.0	**89**	1.0
$PhtrMe^+$	-595.05894	0.19049	-594.86845				
PhtrMeH	-595.80498	0.19973	-595.60525	462.4	61.5	**61.4**	0.1
$PhtrBn^+$	-826.00191	0.26572	-825.73619				
PhtrBnH	-826.74957	0.27444	-826.47513	463.7	62.9	**64.8**	1.9
BNA^+	-687.51839	0.19840	-687.32000				
BNAH	-688.25830	0.20652	-688.05177	459.2	58.2	**59**	0.8

HEHMe$^+$	-900.71710	0.28069	-900.43641				
HEHMeH	-901.45995	0.28961	-901.17034	460.5	59.6	**61.5**	1.9
2OM$^+$	-1148.42536	0.34996	-1148.07540				
2OMH	-1149.15887	0.35832	-1148.80055	455.0	53.9	**58.2**	4.3
4OM$^+$	-1283.95219	0.38278	-1283.56942				
4OMH	-1284.71077	0.39273	-1284.31804	469.8	69.2	**70.2**	1.0
						MUE=	1.8
						MAX=	4.2
						RMSE=	2.2

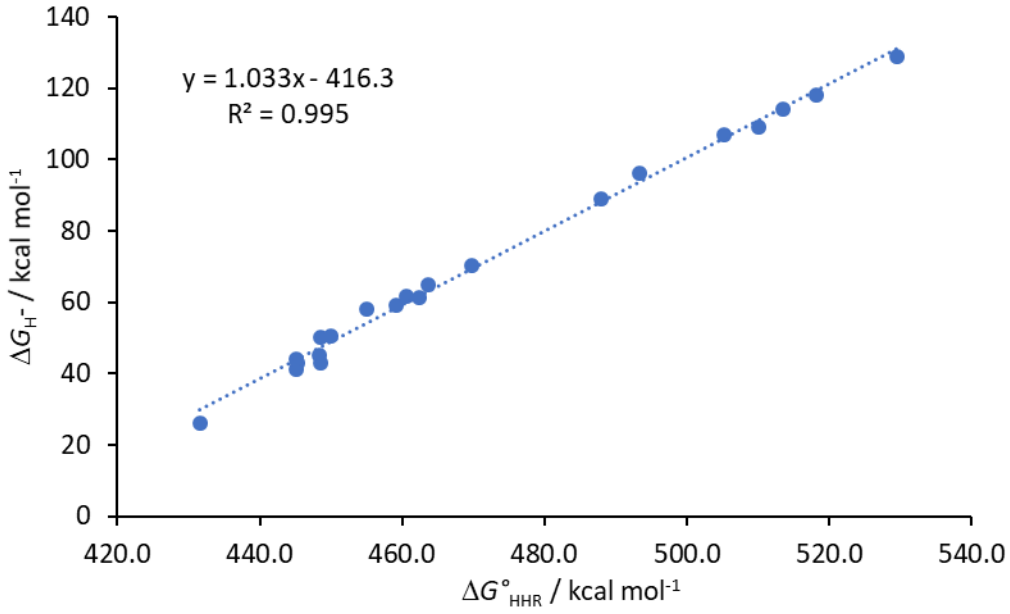

Figure S19. Correlation line obtained with the M19 model.

Table S20a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M20 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.58544	-0.00882	-188.59426	-188.51604	-188.51896
$HCOO^-$	-189.20095	-0.00261	-189.20356	-189.13615	-189.23986
B_2H_6	-53.25869	0.04072	-53.21797	-53.24467	-53.24569
BH_4^-	-27.23887	0.01402	-27.22485	-27.23061	-27.32986
Et_3B	-262.47972	0.16473	-262.31499	-262.40772	-262.40844
Et_3BH^-	-263.10487	0.17291	-262.93196	-263.03191	-263.10441
Ph_3C^+	-732.71992	0.24063	-732.47929	-732.52745	-732.58538
Ph_3CH	-733.57839	0.24834	-733.33006	-733.38377	-733.39074
$PhCH_2^+$	-270.60584	0.08871	-270.51714	-270.53389	-270.61105
$PhCH_3$	-271.52446	0.09769	-271.42677	-271.45101	-271.45425
$pNO_2PhCH_2^+$	-475.08250	0.08605	-474.99645	-474.93952	-475.02895
pNO_2PhCH_3	-476.03015	0.09686	-475.93329	-475.88645	-475.89458
$pOMePhCH_2^+$	-385.15476	0.11907	-385.03568	-385.04368	-385.11520
$pOMePhCH_3$	-386.04491	0.12842	-385.91649	-385.93322	-385.93839
$BImH^+$	-458.82556	0.15507	-458.67049	-458.69810	-458.77012
BImHH	-459.61963	0.16423	-459.45540	-459.49099	-459.49860
$BImMe^+$	-498.14491	0.17798	-497.96694	-498.00655	-498.07581
BImMeH	-498.93308	0.19030	-498.74278	-498.79432	-498.80171
$BImPh^+$	-689.86951	0.23007	-689.63945	-689.68145	-689.74482
BImPhH	-690.65499	0.23805	-690.41695	-690.46646	-690.47440
$MeDHP^+$	-327.24162	0.12476	-327.11686	-327.15128	-327.22530
MeDHPH	-328.04106	0.13553	-327.90553	-327.94809	-327.95216
$BnDHP^+$	-558.27534	0.19963	-558.07571	-558.12441	-558.19218
BnDHPH	-559.07134	0.21007	-558.86127	-558.91790	-558.92382
$HFlu^+$	-500.46256	0.14367	-500.31889	-500.33212	-500.39888
HFluH	-501.36206	0.15530	-501.20676	-501.22990	-501.23556
$MeOOCFlu^+$	-728.33235	0.18034	-728.15201	-728.12782	-728.19133
MeOOCFluH	-729.23280	0.19188	-729.04092	-729.02620	-729.03631
$MeOFlu^+$	-615.01781	0.17501	-614.84280	-614.84854	-614.91347
MeOFluH	-615.87447	0.18515	-615.68932	-615.70499	-615.71153
$PhtrMe^+$	-595.19901	0.19000	-595.00901	-595.03904	-595.10577
PhtrMeH	-596.01382	0.19918	-595.81465	-595.85316	-595.86065
$PhtrBn^+$	-826.23104	0.26458	-825.96647	-826.01062	-826.07203
PhtrBnH	-827.04173	0.27340	-826.76833	-826.82067	-826.82912

BNA^+	-687.66460	0.19798	-687.46662	-687.46944	-687.54675
BNAH	-688.47574	0.20627	-688.26947	-688.27862	-688.29444
$HEHMe^+$	-900.91913	0.28150	-900.63764	-900.64814	-900.71748
HEHMeH	-901.72680	0.28853	-901.43827	-901.45533	-901.46750
$2OM^+$	-1148.75397	0.34940	-1148.40457	-1148.43085	-1148.48661
2OMH	-1149.54379	0.35858	-1149.18521	-1149.21879	-1149.23192
$4OM^+$	-1284.31015	0.38248	-1283.92767	-1283.93782	-1283.99370
4OMH	-1285.12434	0.39405	-1284.73029	-1284.75021	-1284.76572

Table S20b. Energies of solvation as well as the hydricity data obtained with M20 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2		-1.83	63.25				
$HCOO^-$	382.3	-65.08		445.6	**40.5**	**44**	3.5
B_2H_6		-0.64	61.64				
BH_4^-	386.5	-62.29		448.1	**43.0**	**50.4**	7.4
Et_3B		-0.4	45.05				
Et_3BH^-	387.2	-45.5		432.2	**27.6**	**26**	1.6
Ph_3C^+		-36.35	-31.97				
Ph_3CH	533.9	-4.38		501.9	**94.9**	**96**	1.1
$PhCH_2^+$		-48.42	-46.38				
$PhCH_3$	570.8	-2.04		524.4	**116.7**	**118**	1.3
$pNO_2PhCH_2^+$		-56.11	-51.01				
pNO_2PhCH_3	587.9	-5.10		536.9	**128.7**	**129**	0.3
$pOMePhCH_2^+$		-44.88	-41.63				
$pOMePhCH_3$	552.7	-3.25		511.1	**103.8**	**107**	3.2
$BImH^+$		-45.19	-40.42				
BImHH	492.5	-4.77		452.1	**46.8**	**45**	1.8
$BImMe^+$		-43.47	-38.83				
BImMeH	486.8	-4.63		448.0	**42.9**	**43**	0.1
$BImPh^+$		-39.76	-34.78				
BImPhH	487.9	-4.98		453.1	**47.8**	**50**	2.2
$MeDHP^+$		-46.45	-43.90				
MeDHPH	494.9	-2.55		451.0	**45.8**	**41**	4.8
$BnDHP^+$		-42.53	-38.81				
BnDHPH	492.9	-3.71		454.1	**48.8**	**43**	5.8
$HFlu^+$		-41.89	-38.35				
HFluH	557.1	-3.55		518.8	**111.3**	**109**	2.3

MeOOCFlu$^+$		-39.85	-33.51				
MeOOCFluH	557.8	-6.34		524.3	**116.6**	**114**	2.6
MeOFlu$^+$		-40.75	-36.65				
MeOFluH	531.2	-4.10		494.6	**87.8**	**89**	1.2
PhtrMe$^+$		-41.88	-37.18				
PhtrMeH	505.5	-4.70		468.4	**62.5**	**61.4**	1.1
PhtrBn$^+$		-38.53	-33.23				
PhtrBnH	503.2	-5.30		469.9	**64.0**	**64.8**	0.8
BNA$^+$		-48.51	-38.59				
BNAH	503.8	-9.93		465.2	**59.5**	**59**	0.5
HEHMe$^+$		-43.51	-35.87				
HEHMeH	502.4	-7.64		466.5	**60.8**	**61.5**	0.7
2OM$^+$		-34.99	-26.75				
2OMH	489.9	-8.24		463.1	**57.4**	**58.2**	0.8
4OM$^+$		-35.07	-25.33				
4OMH	503.7	-9.73		478.3	**72.1**	**70.2**	1.9
						MUE=	2.1
						MAX=	7.4
						RMSE=	2.8

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas;}$ Δ(ΔE_{sol}) = ΔE_{sol} ([M+H]$^{0/-}$) - ΔE_{sol} ([M]$^{+/0}$); all energies are given in the Table S20a.

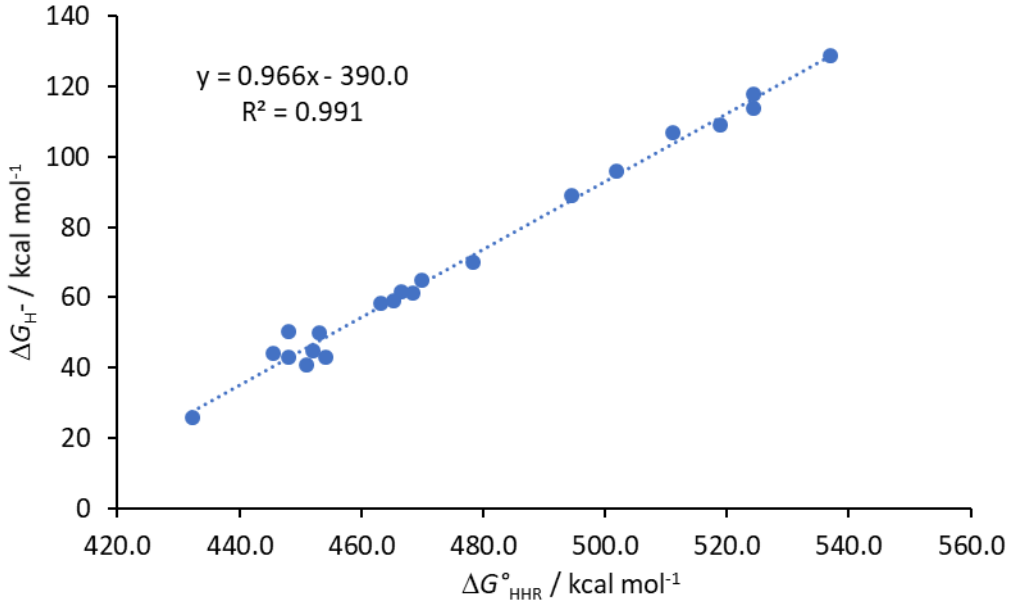

Figure S20. Correlation line obtained with the M20 model.

Table S21a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M21 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.59397	-0.00882	-188.60279	-188.51604	-188.51896
$HCOO^-$	-189.21164	-0.00261	-189.21425	-189.13615	-189.23986
B_2H_6	-53.26120	0.04072	-53.22048	-53.24439	-53.24542
BH_4^-	-27.24007	0.01402	-27.22605	-27.23052	-27.32965
Et_3B	-262.48995	0.16473	-262.32522	-262.40772	-262.40844
Et_3BH^-	-263.11451	0.17291	-262.94160	-263.03191	-263.10441
Ph_3C^+	-732.74902	0.24063	-732.50839	-732.52745	-732.58538
Ph_3CH	-733.60658	0.24834	-733.35824	-733.38377	-733.39074
$PhCH_2^+$	-270.61684	0.08871	-270.52813	-270.53389	-270.61105
$PhCH_3$	-271.53503	0.09769	-271.43734	-271.45101	-271.45425
$pNO_2PhCH_2^+$	-475.10295	0.08605	-475.01690	-474.93952	-475.02895
pNO_2PhCH_3	-476.04992	0.09686	-475.95307	-475.88645	-475.89458
$pOMePhCH_2^+$	-385.17055	0.11907	-385.05148	-385.04368	-385.11520
$pOMePhCH_3$	-386.06048	0.12842	-385.93205	-385.93322	-385.93839
$BImH^+$	-458.84317	0.15507	-458.68810	-458.69810	-458.77012
BImHH	-459.63716	0.16423	-459.47294	-459.49099	-459.49860
$BImMe^+$	-498.16388	0.17798	-497.98591	-498.00655	-498.07581
BImMeH	-498.95194	0.19030	-498.76164	-498.79432	-498.80171
$BImPh^+$	-689.89592	0.23007	-689.66585	-689.68145	-689.74482
BImPhH	-690.68129	0.23805	-690.44324	-690.46646	-690.47440
$MeDHP^+$	-327.25425	0.12476	-327.12949	-327.15128	-327.22530
MeDHPH	-328.05343	0.13553	-327.91790	-327.94809	-327.95216
$BnDHP^+$	-558.29692	0.19963	-558.09729	-558.12441	-558.19218
BnDHPH	-559.09254	0.21007	-558.88246	-558.91790	-558.92382
$HFlu^+$	-500.48302	0.14367	-500.33935	-500.33212	-500.39888
HFluH	-501.38203	0.15530	-501.22673	-501.22990	-501.23556
$MeOOCFlu^+$	-728.36263	0.18034	-728.18228	-728.12782	-728.19133
MeOOCFluH	-729.26258	0.19188	-729.07069	-729.02620	-729.03631
$MeOFlu^+$	-615.04299	0.17501	-614.86798	-614.84854	-614.91347
MeOFluH	-615.89920	0.18515	-615.71405	-615.70499	-615.71153
$PhtrMe^+$	-595.22275	0.19000	-595.03274	-595.03904	-595.10577
PhtrMeH	-596.03716	0.19918	-595.83798	-595.85316	-595.86065
$PhtrBn^+$	-826.26375	0.26458	-825.99917	-826.01062	-826.07203
PhtrBnH	-827.07398	0.27340	-826.80058	-826.82067	-826.82912

BNA^+	-687.69231	0.19798	-687.49433	-687.46944	-687.54675
BNAH	-688.50328	0.20627	-688.29701	-688.27862	-688.29444
$HEHMe^+$	-900.95581	0.28150	-900.67431	-900.64814	-900.71748
HEHMeH	-901.76321	0.28853	-901.47468	-901.45533	-901.46750
$2OM^+$	-1148.79909	0.34940	-1148.44969	-1148.43085	-1148.48661
2OMH	-1149.58854	0.35858	-1149.22996	-1149.21879	-1149.23192
$4OM^+$	-1284.36094	0.38248	-1283.97846	-1283.93782	-1283.99370
4OMH	-1285.17467	0.39405	-1284.78062	-1284.75021	-1284.76572

Table S21b. Energies of solvation as well as the hydricity data obtained with M21 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2	383.7	-1.83	63.25				
$HCOO^-$		-65.08		446.9	41.9	**44**	2.1
B_2H_6	386.4	-0.64	61.56				
BH_4^-		-62.20		448.0	42.9	**50.4**	7.5
Et_3B	386.8	-0.4	45.05				
Et_3BH^-		-45.5		431.8	27.2	**26**	1.2
Ph_3C^+	533.3	-36.35	-31.97				
Ph_3CH		-4.38		501.3	94.7	**96**	1.3
$PhCH_2^+$	570.5	-48.42	-46.38				
$PhCH_3$		-2.04		524.2	116.8	**118**	1.2
$pNO_2PhCH_2^+$	587.5	-56.11	-51.01				
pNO_2PhCH_3		-5.10		536.4	128.8	**129**	0.2
$pOMePhCH_2^+$	552.6	-44.88	-41.63				
$pOMePhCH_3$		-3.25		510.9	104.0	**107**	3.0
$BImH^+$	492.5	-45.19	-40.42				
BImHH		-4.77		452.1	46.8	**45**	1.8
$BImMe^+$	486.8	-43.47	-38.83				
BImMeH		-4.63		447.9	42.8	**43**	0.2
$BImPh^+$	487.8	-39.76	-34.78				
BImPhH		-4.98		453.0	47.8	**50**	2.2
$MeDHP^+$	494.7	-46.45	-43.90				
MeDHPH		-2.55		450.8	45.7	**41**	4.7
$BnDHP^+$	492.7	-42.53	-38.81				
BnDHPH		-3.71		453.9	48.6	**43**	5.6
$HFlu^+$	556.8	-41.89	-38.35				
HFluH		-3.55		518.5	111.3	**109**	2.3

MeOOCFlu$^+$	557.5	-39.85	-33.51				
MeOOCFluH		-6.34		524.0	116.7	**114**	2.7
MeOFlu$^+$	530.9	-40.75	-36.65				
MeOFluH		-4.10		494.3	87.8	**89**	1.2
PhtrMe$^+$	505.3	-41.88	-37.18				
PhtrMeH		-4.70		468.1	62.4	**61.4**	1.0
PhtrBn$^+$	502.9	-38.53	-33.23				
PhtrBnH		-5.30		469.7	63.9	**64.8**	0.9
BNA$^+$	503.7	-48.51	-38.59				
BNAH		-9.93		465.1	59.5	**59**	0.5
HEHMe$^+$	502.2	-43.51	-35.87				
HEHMeH		-7.64		466.4	60.7	**61.5**	0.8
2OM$^+$	489.6	-34.99	-26.75				
2OMH		-8.24		462.9	57.3	**58.2**	0.9
4OM$^+$	503.4	-35.07	-25.33				
4OMH		-9.73		478.0	72.1	**70.2**	1.9
						MUE=	2.1
						MAX=	7.5
						RMSE=	2.7

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas;}$ $\Delta(\Delta E_{sol}) = \Delta E_{sol}$ ([M+H]$^{0/-}$) - ΔE_{sol} ([M]$^{+/0}$); all energies are given in the Table S21a.

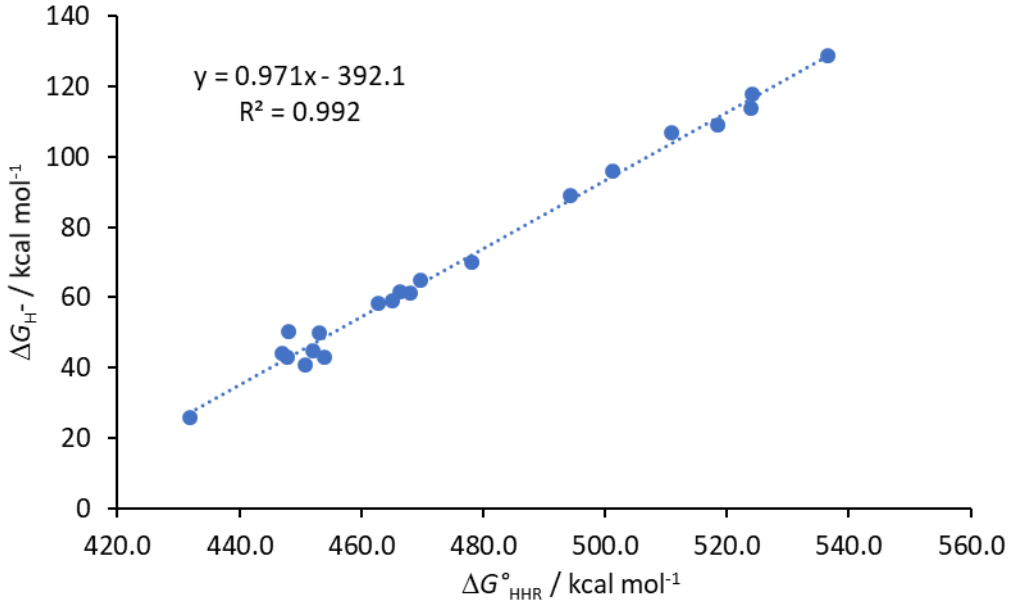

Figure S21. Correlation line obtained with the M21 model.

Table S22a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M22 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.59409	-0.00874	-188.60283	-188.51601	-188.51893
$HCOO^-$	-189.21130	-0.00284	-189.21414	-189.13580	-189.23891
B_2H_6	-53.26074	0.04001	-53.22073	-53.24439	-53.24542
BH_4^-	-27.23989	0.01394	-27.22595	-27.23052	-27.32965
Et_3B	-262.48926	0.16345	-262.32581	-262.40740	-262.40813
Et_3BH^-	-263.11371	0.17207	-262.94163	-263.03159	-263.10409
Ph_3C^+	-732.74820	0.23988	-732.50832	-732.52717	-732.58508
Ph_3CH	-733.60580	0.24801	-733.35780	-733.38349	-733.39046
$PhCH_2^+$	-270.61643	0.08838	-270.52805	-270.53374	-270.61084
$PhCH_3$	-271.53465	0.09768	-271.43697	-271.45086	-271.45411
$pNO_2PhCH_2^+$	-475.10277	0.08606	-475.01671	-474.93928	-475.02837
pNO_2PhCH_3	-476.04972	0.09651	-475.95321	-475.88619	-475.89413
$pOMePhCH_2^+$	-385.17009	0.11874	-385.05135	-385.04347	-385.11497
$pOMePhCH_3$	-386.05997	0.12802	-385.93195	-385.93300	-385.93813
$BImH^+$	-458.84258	0.15451	-458.68807	-458.69787	-458.76986
BImHH	-459.63655	0.16330	-459.47325	-459.49073	-459.49825
$BImMe^+$	-498.16323	0.17858	-497.98465	-498.00627	-498.07551
BImMeH	-498.95120	0.18914	-498.76206	-498.79401	-498.80130
$BImPh^+$	-689.89513	0.22934	-689.66579	-689.68115	-689.74447
BImPhH	-690.68046	0.23713	-690.44333	-690.46611	-690.47399
$MeDHP^+$	-327.25378	0.12538	-327.12840	-327.15107	-327.22505
MeDHPH	-328.05291	0.13472	-327.91819	-327.94785	-327.95188
$BnDHP^+$	-558.29624	0.19961	-558.09663	-558.12415	-558.19185
BnDHPH	-559.09184	0.20960	-558.88224	-558.91762	-558.92354
$HFlu^+$	-500.48247	0.14364	-500.33883	-500.33195	-500.39868
HFluH	-501.38147	0.15502	-501.22645	-501.22973	-501.23540
$MeOOCFlu^+$	-728.36176	0.17994	-728.18182	-728.12745	-728.19054
MeOOCFluH	-729.26176	0.19167	-729.07009	-729.02583	-729.03543
$MeOFlu^+$	-615.04240	0.17496	-614.86744	-614.84830	-614.91323
MeOFluH	-615.89856	0.18469	-615.71387	-615.70472	-615.71119
$PhtrMe^+$	-595.22212	0.18980	-595.03232	-595.03880	-595.10551
PhtrMeH	-596.03653	0.19858	-595.83794	-595.85292	-595.86038
$PhtrBn^+$	-826.26292	0.26439	-825.99853	-826.01033	-826.07172
PhtrBnH	-827.07312	0.27305	-826.80007	-826.82037	-826.82878

BNA^+	-687.69165	0.19755	-687.49410	-687.46900	-687.54627
BNAH	-688.50249	0.20667	-688.29582	-688.27814	-688.29359
$HEHMe^+$	-900.95461	0.27922	-900.67538	-900.64733	-900.71625
HEHMeH	-901.76218	0.28811	-901.47407	-901.45462	-901.46646
$2OM^+$	-1148.79794	0.34846	-1148.44948	-1148.43032	-1148.48602
2OMH	-1149.58736	0.35721	-1149.23015	-1149.21831	-1149.23131
$4OM^+$	-1284.35932	0.38197	-1283.97735	-1283.93712	-1283.99291
4OMH	-1285.17333	0.39298	-1284.78035	-1284.74963	-1284.76498

Table S22b. Energies of solvation as well as the hydricity data obtained with M22 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2		-1.83	62.87				
$HCOO^-$	383.6	-64.70		446.5	**41.4**	**44**	2.6
B_2H_6		-0.64	61.56				
BH_4^-	386.3	-62.20		447.8	**42.7**	**50.4**	7.7
Et_3B		-0.46	45.04				
Et_3BH^-	386.4	-45.50		431.5	**26.8**	**26**	0.8
Ph_3C^+		-36.34	-31.96				
Ph_3CH	533.1	-4.37		501.1	**94.4**	**96**	1.6
$PhCH_2^+$		-48.38	-46.34				
$PhCH_3$	570.4	-2.04		524.0	**116.6**	**118**	1.4
$pNO_2PhCH_2^+$		-55.90	-50.92				
pNO_2PhCH_3	587.7	-4.98		536.7	**129.0**	**129**	0.0
$pOMePhCH_2^+$		-44.86	-41.64				
$pOMePhCH_3$	552.6	-3.22		510.9	**104.0**	**107**	3.0
$BImH^+$		-45.17	-40.46				
BImHH	492.7	-4.72		452.2	**47.0**	**45**	2.0
$BImMe^+$		-43.45	-38.88				
BImMeH	487.8	-4.57		449.0	**43.8**	**43**	0.8
$BImPh^+$		-39.73	-34.79				
BImPhH	487.9	-4.94		453.1	**47.8**	**50**	2.2
$MeDHP^+$		-46.42	-43.90				
MeDHPH	495.6	-2.52		451.7	**46.5**	**41**	5.5
$BnDHP^+$		-42.48	-38.77				
BnDHPH	493.0	-3.72		454.2	**48.9**	**43**	5.9
$HFlu^+$		-41.87	-38.31				
HFluH	557.0	-3.56		518.7	**111.5**	**109**	2.5

$MeOOCFlu^+$		-39.59	-33.56				
MeOOCFluH	557.4	-6.02		523.8	**116.5**	**114**	2.5
$MeOFlu^+$		-40.74	-36.68				
MeOFluH	531.1	-4.06		494.5	**88.0**	**89**	1.0
$PhtrMe^+$		-41.86	-37.18				
PhtrMeH	505.5	-4.68		468.4	**62.6**	**61.4**	1.2
$PhtrBn^+$		-38.52	-33.24				
PhtrBnH	503.0	-5.28		469.7	**64.0**	**64.8**	0.8
BNA^+		-48.49	-38.79				
BNAH	503.1	-9.70		464.3	**58.7**	**59**	0.3
$HEHMe^+$		-43.25	-35.82				
HEHMeH	501.2	-7.43		465.4	**59.7**	**61.5**	1.8
$2OM^+$		-34.95	-26.79				
2OMH	489.9	-8.16		463.1	**57.5**	**58.2**	0.7
$4OM^+$		-35.01	-25.37				
4OMH	503.9	-9.64		478.5	**72.5**	**70.2**	2.3
						MUE=	2.2
						MAX=	7.7
						RMSE=	2.9

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas}$; $\Delta(\Delta E_{sol}) = \Delta E_{sol}$ ($[M+H]^{0/-}$) - ΔE_{sol} ($[M]^{+/0}$); all energies are given in the Table S22a.

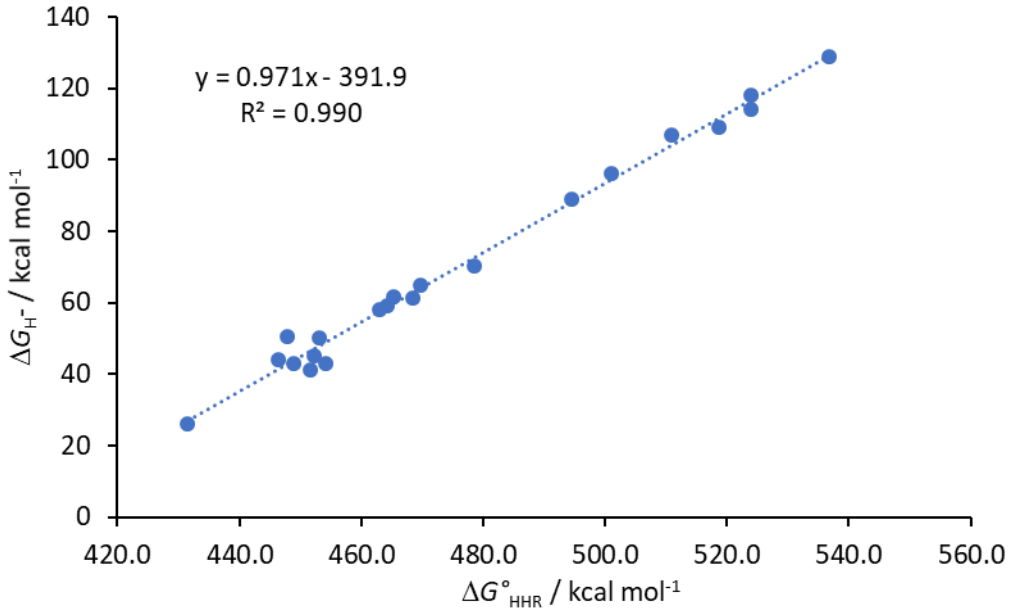

Figure S22. Correlation line obtained with the M22 model.

Table S23a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M23 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.59409	-0.00874	-188.60283	-188.51601	-188.51666
$HCOO^-$	-189.21130	-0.00284	-189.21414	-189.13580	-189.23000
B_2H_6	-53.26074	0.04001	-53.22073	-53.24439	-53.24484
BH_4^-	-27.23989	0.01394	-27.22595	-27.23052	-27.33427
Et_3B	-262.48926	0.16345	-262.32581	-262.40740	-262.41146
Et_3BH^-	-263.11371	0.17207	-262.94163	-263.03158	-263.10906
Ph_3C^+	-732.74820	0.23988	-732.50832	-732.52717	-732.60851
Ph_3CH	-733.60580	0.24801	-733.35780	-733.38349	-733.40595
$PhCH_2^+$	-270.61643	0.08838	-270.52805	-270.53374	-270.62820
$PhCH_3$	-271.53465	0.09768	-271.43697	-271.45086	-271.46052
$pNO_2PhCH_2^+$	-475.10277	0.08606	-475.01671	-474.93928	-475.04670
pNO_2PhCH_3	-476.04972	0.09651	-475.95321	-475.88619	-475.89945
$pOMePhCH_2^+$	-385.17009	0.11874	-385.05135	-385.04347	-385.13118
$pOMePhCH_3$	-386.05997	0.12802	-385.93195	-385.93300	-385.94423
$BImH^+$	-458.84258	0.15451	-458.68807	-458.69787	-458.79198
BImHH	-459.63655	0.16330	-459.47325	-459.49073	-459.50866
$BImMe^+$	-498.16323	0.17858	-497.98465	-498.00627	-498.09676
BImMeH	-498.95120	0.18914	-498.76206	-498.79401	-498.81148
$BImPh^+$	-689.89513	0.22934	-689.66579	-689.68115	-689.76808
BImPhH	-690.68046	0.23713	-690.44333	-690.46611	-690.48788
$MeDHP^+$	-327.25378	0.12538	-327.12840	-327.15107	-327.24258
MeDHPH	-328.05291	0.13472	-327.91819	-327.94785	-327.95878
$BnDHP^+$	-558.29624	0.19961	-558.09663	-558.12415	-558.21400
BnDHPH	-559.09184	0.20960	-558.88224	-558.91762	-558.93592
$HFlu^+$	-500.48247	0.14364	-500.33883	-500.33195	-500.41969
HFluH	-501.38147	0.15502	-501.22645	-501.22973	-501.24729
$MeOOCFlu^+$	-728.36176	0.17994	-728.18182	-728.12745	-728.20988
MeOOCFluH	-729.26176	0.19167	-729.07009	-729.02583	-729.04703
$MeOFlu^+$	-615.04240	0.17496	-614.86744	-614.84830	-614.93355
MeOFluH	-615.89856	0.18469	-615.71387	-615.70472	-615.72171
$PhtrMe^+$	-595.22212	0.18980	-595.03232	-595.03880	-595.12875
PhtrMeH	-596.03653	0.19858	-595.83794	-595.85292	-595.87337
$PhtrBn^+$	-826.26292	0.26439	-825.99853	-826.01033	-826.09924
PhtrBnH	-827.07312	0.27305	-826.80007	-826.82037	-826.84674

BNA^+	-687.69165	0.19755	-687.49410	-687.46900	-687.57206
BNAH	-688.50249	0.20667	-688.29582	-688.27814	-688.30725
$HEHMe^+$	-900.95461	0.27922	-900.67538	-900.64733	-900.73610
HEHMeH	-901.76218	0.28811	-901.47407	-901.45462	-901.47550
$4OM^+$	-1284.35932	0.38197	-1283.97735	-1283.93712	-1284.01565
4OMH	-1285.17333	0.39298	-1284.78035	-1284.74963	-1284.77904
$2OM^+$	-1148.79794	0.34846	-1148.44948	-1148.43032	-1148.51105
2OMH	-1149.58736	0.35721	-1149.23015	-1149.21831	-1149.24831

Table S23b. Energies of solvation as well as the hydricity data obtained with M23 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2		-0.41	58.70				
$HCOO^-$	383.6	-59.11		442.3	**41.7**	**44**	2.3
B_2H_6		-0.28	64.83				
BH_4^-	386.3	-65.11		451.1	**50.5**	**50.4**	0.1
Et_3B		-2.55	46.07				
Et_3BH^-	386.4	-48.62		432.5	**31.9**	**26**	5.9
Ph_3C^+		-51.04	-36.95				
Ph_3CH	533.1	-14.09		496.1	**95.5**	**96**	0.5
$PhCH_2^+$		-59.28	-53.22				
$PhCH_3$	570.4	-6.06		517.1	**116.6**	**118**	1.4
$pNO_2PhCH_2^+$		-67.40	-59.08				
pNO_2PhCH_3	587.7	-8.32		528.6	**128.0**	**129**	1.0
$pOMePhCH_2^+$		-55.04	-47.99				
$pOMePhCH_3$	552.6	-7.05		504.6	**104.0**	**107**	3.0
$BImH^+$		-59.06	-47.80				
BImHH	492.7	-11.25		444.9	**44.3**	**45**	0.7
$BImMe^+$		-56.79	-45.82				
BImMeH	487.8	-10.96		442.0	**41.4**	**43**	1.6
$BImPh^+$		-54.55	-40.89				
BImPhH	487.9	-13.66		447.0	**46.5**	**50**	3.5
$MeDHP^+$		-57.43	-50.57				
MeDHPH	495.6	-6.86		445.0	**44.5**	**41**	3.5
$BnDHP^+$		-56.38	-44.90				
BnDHPH	493.0	-11.48		448.1	**47.5**	**43**	4.5
$HFlu^+$		-55.06	-44.04				
HFluH	557.0	-11.02		513.0	**112.4**	**109**	3.4

MeOOCFlu$^+$		-51.72	-38.42				
MeOOCFluH	557.4	-13.31		519.0	**118.4**	**114**	4.4
MeOFlu$^+$		-53.49	-42.83				
MeOFluH	531.1	-10.67		488.3	**87.8**	**89**	1.2
PhtrMe$^+$		-56.44	-43.61				
PhtrMeH	505.5	-12.83		461.9	**61.4**	**61.4**	0.0
PhtrBn$^+$		-55.79	-39.24				
PhtrBnH	503.0	-16.55		463.7	**63.2**	**64.8**	1.6
BNA$^+$		-64.67	-46.41				
BNAH	503.1	-18.26		456.7	**56.1**	**59**	2.9
HEHMe$^+$		-55.71	-42.60				
HEHMeH	501.2	-13.10		458.6	**58.0**	**61.5**	3.5
2OM$^+$		-50.66	-31.83				
2OMH	489.9	-18.83		458.0	**57.5**	**58.2**	0.7
4OM$^+$		-49.28	-30.82				
4OMH	503.9	-18.45		473.1	**72.5**	**70.2**	2.3
						MUE=	2.3
						MAX=	5.9

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas}$; $\Delta(\Delta E_{sol})$ = ΔE_{sol} ([M+H]$^{0/-}$) - ΔE_{sol} ([M]$^{+/0}$); all energies are given in the Table S23a.

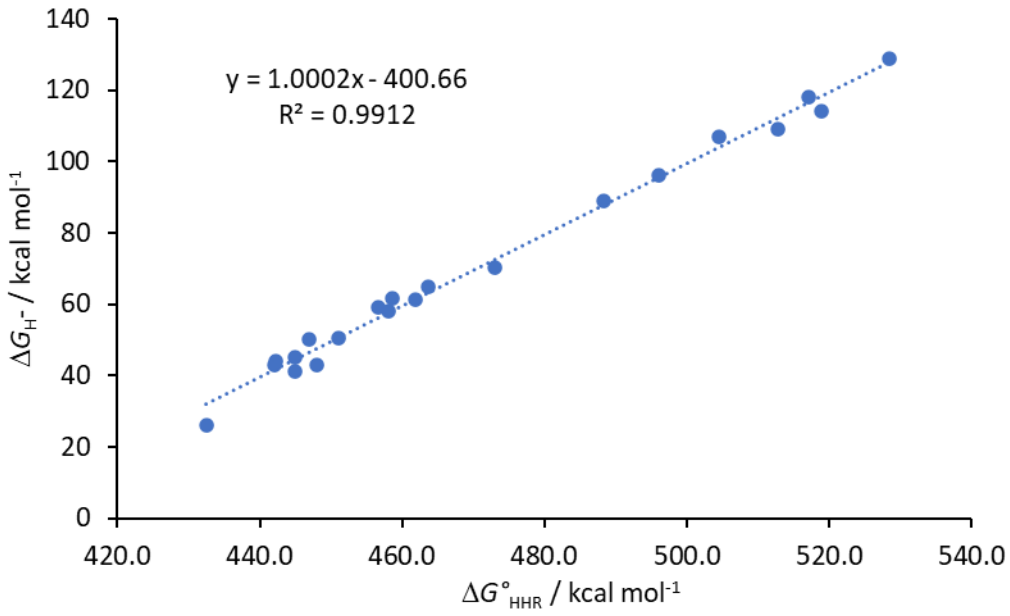

Figure S23. Correlation line obtained with the M23 model.

Table S24a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M24 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.30110	-0.00874	-188.30984	-188.51601	-188.51666
$HCOO^-$	-188.90175	-0.00284	-188.90459	-189.13580	-189.23000
B_2H_6	-53.07950	0.04001	-53.03949	-53.24439	-53.24484
BH_4^-	-27.14061	0.01394	-27.12667	-27.23052	-27.33427
Et_3B	-261.83618	0.16332	-261.67287	-262.40740	-262.41146
Et_3BH^-	-262.45543	0.17180	-262.28362	-263.03158	-263.10906
Ph_3C^+	-731.14317	0.23988	-730.90329	-732.52717	-732.60851
Ph_3CH	-731.99197	0.24801	-731.74397	-733.38349	-733.40595
$PhCH_2^+$	-270.01037	0.08838	-269.92199	-270.53374	-270.62820
$PhCH_3$	-270.92223	0.09768	-270.82454	-271.45086	-271.46052
$pNO_2PhCH_2^+$	-474.20123	0.08606	-474.11517	-474.93928	-475.04670
pNO_2PhCH_3	-475.13701	0.09651	-475.04051	-475.88619	-475.89945
$pOMePhCH_2^+$	-384.35640	0.11874	-384.23767	-385.04347	-385.13118
$pOMePhCH_3$	-385.24124	0.12802	-385.11322	-385.93300	-385.94423
$BImH^+$	-457.86880	0.15451	-457.71429	-458.69787	-458.79198
BImHH	-458.65019	0.16330	-458.48690	-459.49073	-459.50866
$BImMe^+$	-497.09630	0.17858	-496.91772	-498.00627	-498.09676
BImMeH	-497.87382	0.18914	-497.68468	-498.79401	-498.81148
$BImPh^+$	-688.41961	0.22934	-688.19028	-689.68115	-689.76808
BImPhH	-689.19349	0.23713	-688.95636	-690.46611	-690.48788
$MeDHP^+$	-326.53933	0.12538	-326.41396	-327.15107	-327.24258
MeDHPH	-327.32118	0.13472	-327.18647	-327.94785	-327.95878
$BnDHP^+$	-557.07822	0.19961	-556.87862	-558.12415	-558.21400
BnDHPH	-557.85581	0.20960	-557.64621	-558.91762	-558.93592
$HFlu^+$	-499.39079	0.14364	-499.24716	-500.33195	-500.41969
HFluH	-500.28173	0.15502	-500.12670	-501.22973	-501.24729
$MeOOCFlu^+$	-726.87842	0.17994	-726.69848	-728.12745	-728.20988
MeOOCFluH	-727.76902	0.19167	-727.57735	-729.02583	-729.04703
$MeOFlu^+$	-613.74547	0.17496	-613.57052	-614.84830	-614.93355
MeOFluH	-614.59522	0.18469	-614.41054	-615.70472	-615.72171
$PhtrMe^+$	-593.93928	0.18980	-593.74948	-595.03880	-595.12875
PhtrMeH	-594.74242	0.19858	-594.54384	-595.85292	-595.87337
$PhtrBn^+$	-824.47741	0.26439	-824.21302	-826.01033	-826.09924
PhtrBnH	-825.27649	0.27305	-825.00344	-826.82037	-826.84674

BNA^+	-686.27424	0.19755	-686.07668	-687.46900	-687.57206
BNAH	-687.06739	0.20667	-686.86072	-688.27814	-688.30725
$HEHMe^+$	-899.16951	0.27922	-898.89029	-900.64733	-900.73610
HEHMeH	-899.96514	0.28811	-899.67702	-901.45462	-901.47550
$2OM^+$	-1146.42340	0.34846	-1146.07493	-1148.43032	-1148.51105
2OMH	-1147.20506	0.35721	-1146.84784	-1149.21831	-1149.24831
$4OM^+$	-1281.75798	0.38197	-1281.37601	-1283.93712	-1284.01565
4OMH	-1282.56234	0.39298	-1282.16936	-1284.74963	-1284.77904

Table S24b. Energies of solvation as well as the hydricity data obtained with M24 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2		-0.41	58.70				
$HCOO^-$	373.2	-59.11		431.9	**39.4**	**44**	4.6
B_2H_6		-0.28	64.83				
BH_4^-	380.9	-65.11		445.7	**52.6**	**50.4**	2.2
Et_3B		-2.55	46.07				
Et_3BH^-	383.3	-48.62		429.3	**36.9**	**26**	10.9
Ph_3C^+		-51.04	-36.95				
Ph_3CH	527.5	-14.09		490.6	**95.7**	**96**	0.3
$PhCH_2^+$		-59.28	-53.22				
$PhCH_3$	566.4	-6.06		513.1	**117.4**	**118**	0.6
$pNO_2PhCH_2^+$		-67.40	-59.08				
pNO_2PhCH_3	580.7	-8.32		521.6	**125.4**	**129**	3.6
$pOMePhCH_2^+$		-55.04	-47.99				
$pOMePhCH_3$	549.4	-7.05		501.4	**106.1**	**107**	0.9
$BImH^+$		-59.06	-47.80				
BImHH	484.8	-11.25		437.0	**44.3**	**45**	0.7
$BImMe^+$		-56.79	-45.82				
BImMeH	481.3	-10.96		435.5	**42.8**	**43**	0.2
$BImPh^+$		-54.55	-40.89				
BImPhH	480.7	-13.66		439.8	**47.0**	**50**	3.0
$MeDHP^+$		-57.43	-50.57				
MeDHPH	484.8	-6.86		434.2	**41.5**	**41**	0.5
$BnDHP^+$		-56.38	-44.90				
BnDHPH	481.7	-11.48		436.8	**44.0**	**43**	1.0
$HFlu^+$		-55.06	-44.04				
HFluH	551.9	-11.02		507.9	**112.3**	**109**	3.3

$MeOOCFlu^+$		-51.72	-38.42				
MeOOCFluH	551.5	-13.31		513.1	**117.3**	**114**	3.3
$MeOFlu^+$		-53.49	-42.83				
MeOFluH	527.1	-10.67		484.3	**89.6**	**89**	0.6
$PhtrMe^+$		-56.44	-43.61				
PhtrMeH	498.5	-12.83		454.9	**61.4**	**61.4**	0.0
$PhtrBn^+$		-55.79	-39.24				
PhtrBnH	496.0	-16.55		456.8	**63.2**	**64.8**	1.6
BNA^+		-64.67	-46.41				
BNAH	492.0	-18.26		445.6	**52.5**	**59**	6.5
$HEHMe^+$		-55.71	-42.60				
HEHMeH	493.7	-13.10		451.1	**57.8**	**61.5**	3.7
$2OM^+$		-50.66	-31.83				
2OMH	485.0	-18.83		453.2	**59.8**	**58.2**	1.6
$4OM^+$		-49.28	-30.82				
4OMH	497.8	-18.45		467.0	**73.1**	**70.2**	2.9
						MUE=	2.5
						MAX=	10.9
						RMSE=	3.5

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas;}$ $\Delta(\Delta E_{sol}) = \Delta E_{sol}$ ([M+H]$^{0/-}$) - ΔE_{sol} ([M]$^{+/0}$); all energies are given in the Table S24a.

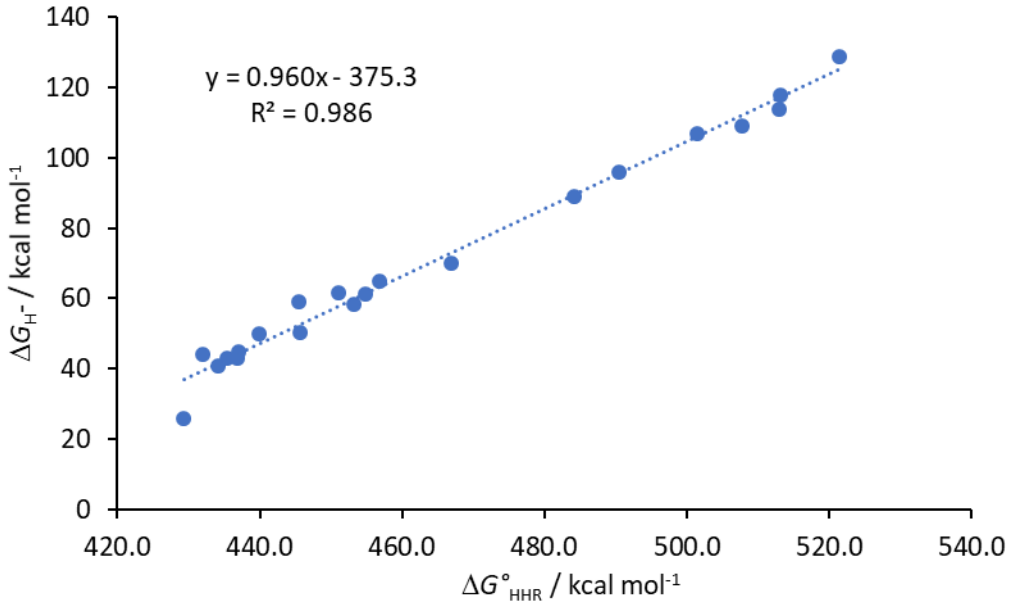

Figure S24. Correlation line obtained with the M24 model.

Table S25a. The gas-phase energies (E_{scf}(M), G_{corr}(M) and G_{tot}(M), in a.u.) as well as the electronic energies ($E_{scf}(M)_{gas}$ and $E_{scf}(M)_{sol}$, in a.u.) obtained using solvation approach within the M25 model for a set of the reference structures.

Structures $M^{+/0}/[M+H]^{0/-}$	E_{scf}(M)	G_{corr}(M)	G_{tot}(M)	E_{scf}(M) gas	E_{scf}(M) sol
CO_2	-188.30129	-0.00913	-188.31041	-188.64664	-188.63657
$HCOO^-$	-188.90209	-0.00289	-188.90498	-189.27253	-189.36820
B_2H_6	-53.07974	0.04039	-53.03935	-53.30443	-53.30506
BH_4^-	-27.14073	0.01427	-27.12646	-27.27500	-27.33624
Et_3B	-261.83616	0.16428	-261.67188	-262.61814	-262.61862
Et_3BH^-	-262.45524	0.17234	-262.28290	-263.24680	-263.31447
Ph_3C^+	-731.14258	0.23915	-730.90343	-732.99473	-733.04993
Ph_3CH	-731.99084	0.24652	-731.74432	-733.84460	-733.84944
$PhCH_2^+$	-270.01033	0.08849	-269.92184	-270.72490	-270.80008
$PhCH_3$	-270.92226	0.09746	-270.82480	-271.63874	-271.64110
$pNO_2PhCH_2^+$	-474.20220	0.08715	-474.11505	-475.26012	-475.34611
pNO_2PhCH_3	-475.13766	0.09596	-475.04170	-476.20339	-476.21161
$pOMePhCH_2^+$	-384.35637	0.11826	-384.23811	-385.30843	-385.37771
$pOMePhCH_3$	-385.24119	0.12701	-385.11418	-386.19430	-386.19832
$BImH^+$	-457.86873	0.15401	-457.71472	-458.99454	-459.06332
BImHH	-458.64947	0.16276	-458.48671	-459.79070	-459.79611
$BImMe^+$	-497.09623	0.17780	-496.91842	-498.33018	-498.39630
BImMeH	-497.87304	0.18887	-497.68418	-499.12064	-499.12581
$BImPh^+$	-688.41942	0.22831	-688.19111	-690.11499	-690.17497
BImPhH	-689.19253	0.23638	-688.95615	-690.90211	-690.90757
$MeDHP^+$	-326.53930	0.12479	-326.41450	-327.37746	-327.44923
MeDHPH	-327.32091	0.13486	-327.18605	-328.17643	-328.17915
$BnDHP^+$	-557.07778	0.19952	-556.87826	-558.48985	-558.55421
BnDHPH	-557.85470	0.20776	-557.64694	-559.28315	-559.28702
$HFlu^+$	-499.39079	0.14321	-499.24758	-500.65455	-500.71833
HFluH	-500.28167	0.15435	-500.12733	-501.54453	-501.54850
$MeOOCFlu^+$	-726.87895	0.17899	-726.69996	-728.59370	-728.65486
MeOOCFluH	-727.76964	0.19028	-727.57936	-729.48224	-729.49035
$MeOFlu^+$	-613.74521	0.17385	-613.57137	-615.24037	-615.30233
MeOFluH	-614.59481	0.18380	-614.41101	-616.09121	-616.09602
$PhtrMe^+$	-593.93916	0.18895	-593.75020	-595.41463	-595.47752
PhtrMeH	-594.74190	0.19770	-594.54420	-596.22717	-596.23229
$PhtrBn^+$	-824.47687	0.26274	-824.21413	-826.52489	-826.58198
PhtrBnH	-825.27565	0.27143	-825.00421	-827.33279	-827.33834

BNA^+	-686.27377	0.19633	-686.07744	-687.91169	-687.98501
BNAH	-687.06614	0.20452	-686.86162	-688.72134	-688.73455
$HEHMe^+$	-899.16922	0.27806	-898.89116	-901.24344	-901.30895
HEHMeH	-899.96466	0.28787	-899.67679	-902.05230	-902.06259
$2OM^+$	-1146.42204	0.34667	-1146.07536	-1149.13364	-1149.18539
2OMH	-1147.20367	0.35509	-1146.84859	-1149.91661	-1149.92542
$4OM^+$	-1281.75688	0.37949	-1281.37740	-1284.73845	-1284.78968
4OMH	-1282.55959	0.39002	-1282.16958	-1285.54138	-1285.55116

Table S25b. Energies of solvation as well as the hydricity data obtained with M25 model for a set of the reference structures. All data are given in kcal mol^{-1}.

Structures $M^{+/0}/[M+H]^{0/-}$	ΔG^*_{HHR} (gas)	ΔE_{sol} [a]	$\Delta(\Delta E_{sol})$ [a]	ΔG^*_{HHR} (sol)	ΔG_H- calc.	ΔG_H- exp.	$\lvert\Delta(\Delta G_H\text{-})\rvert$
CO_2		6.32	66.35				
$HCOO^-$	373.1	-60.03		439.4	41.3	**44**	2.7
B_2H_6		-0.40	38.0				
BH_4^-	380.8	-38.43		418.8	22.0	**50.4**	28.4
Et_3B		-0.30	42.16				
Et_3BH^-	393.5	-42.46		425.6	28.4	**26**	2.4
Ph_3C^+		-34.64	-31.60				
Ph_3CH	527.7	-3.04		496.1	94.3	**96**	1.7
$PhCH_2^+$		-47.17	-45.69				
$PhCH_3$	566.6	-1.48		520.9	117.5	**118**	0.5
$pNO_2PhCH_2^+$		-53.96	-48.80				
pNO_2PhCH_3	581.5	-5.16		532.7	128.5	**129**	0.5
$pOMePhCH_2^+$		-43.47	-40.95				
$pOMePhCH_3$	549.7	-2.52		508.8	106.2	**107**	0.8
$BImH^+$		-43.16	-39.76				
BImHH	484.4	-3.40		444.7	46.2	**45**	1.2
$BImMe^+$		-41.49	-38.25				
BImMeH	480.5	-3.24		442.3	44.0	**43**	1.0
$BImPh^+$		-37.63	-34.20				
BImPhH	480.1	-3.43		445.9	47.3	**50**	2.7
$MeDHP^+$		-45.04	-43.33				
MeDHPH	484.2	-1.71		440.8	42.6	**41**	1.6
$BnDHP^+$		-40.39	-37.96				
BnDHPH	482.4	-2.43		444.4	46.0	**43**	3.0
$HFlu^+$		-40.02	-37.53				
HFluH	552.0	-2.49		514.5	111.6	**109**	2.6

$MeOOCFlu^+$		-38.37	-33.29				
MeOOCFluH	551.8	-5.09		518.5	115.3	**114**	1.3
$MeOFlu^+$		-38.88	-35.86				
MeOFluH	526.9	-3.02		491.0	89.6	**89**	0.6
$PhtrMe^+$		-39.46	-36.25				
PhtrMeH	498.2	-3.22		462.0	62.4	**61.4**	1.0
$PhtrBn^+$		-35.82	-32.34				
PhtrBnH	495.8	-3.48		463.4	63.8	**64.8**	1.0
BNA^+		-46.01	-37.72				
BNAH	492.1	-8.29		454.4	55.3	**59**	3.7
$HEHMe^+$		-41.11	-34.65				
HEHMeH	493.0	-6.46		458.3	59.0	**61.5**	2.5
$2OM^+$		-32.47	-26.95				
2OMH	485.2	-5.53		458.3	58.9	**58.2**	0.7
$4OM^+$		-32.14	-26.01				
4OMH	497.1	-6.14		471.1	70.9	**70.2**	0.7
						MUE=	1.6[b]
						MAX=	3.7[b]
						RMSE=	1.9[b]

[a] ΔE_{sol} (M) = E(M)$_{sol}$ – E(M)$_{gas}$; $\Delta(\Delta E_{sol}) = \Delta E_{sol}$ ($[M+H]^{0/-}$) - ΔE_{sol} ($[M]^{+/0}$); all energies are given in the Table S25a; [b] the data obtained for borohydrides were excluded from correlation and the error calculations.

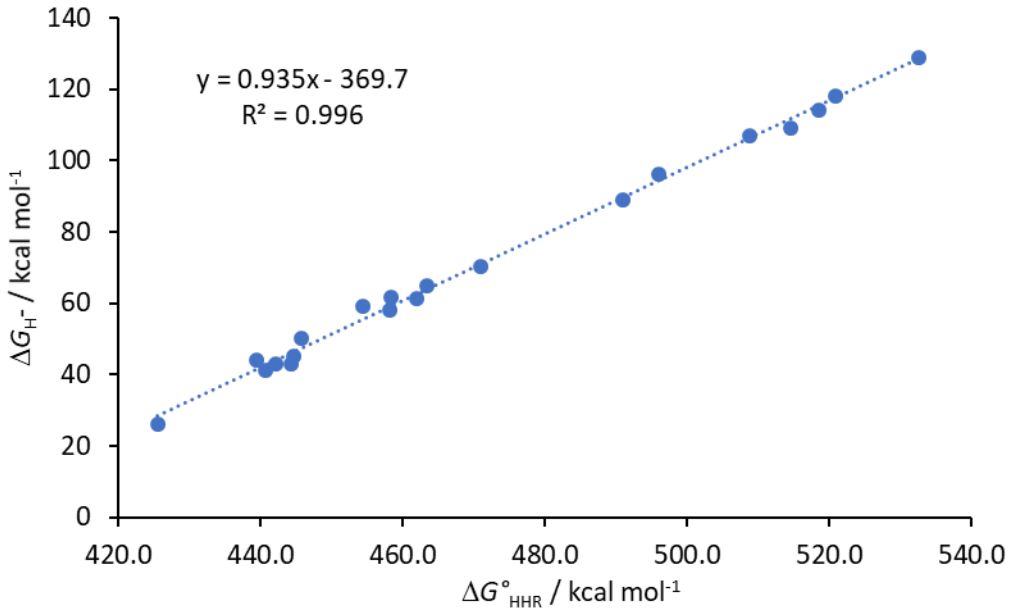

Figure S25. Correlation line obtained with the M25 model.

S2. Calculation of the Gibbs energy of hydride anion in acetonitrile

Table S26. Correlation data obtained by the computational models M1 – M25.[a,b]

Model	CSM	*a*	*b*	σ(*b*)	Model	CSM	*a*	*b*	σ(*b*)
M1	CPCM	0.997	-405.5	8.0	M14	SMD	1.084	-437.8	14.5
M2	CPCM	0.994	-403.9	8.4	M15	SMD	1.090	-441.4	13.4
M3	CPCM	0.996	-404.1	8.3	M16	SMD	1.083	-438.5	13.5
M4	CPCM	0.975	-394.2	10.1	M17	CPCM//g.p.	0.997	-404.6	8.2
M5	CPCM	1.032	-415.7	8.4	M18	CPCM//g.p.	0.976	-394.5	10.0
M6	CPCM//SMD	1.060	-432.2	10.8	M19	CPCM//g.p.	1.033	-416.3	8.2
M7	CPCM//SMD	0.998	-405.8	8.6	M20	CPCM//g.p.	0.966	-390.0	10.1
M8	CPCM//SMD	1.000	-406.1	8.5	M21	CPCM//g.p.	0.971	-392.1	9.9
M9	CPCM//SMD	0.977	-395.2	10.3	M22	CPCM//g.p.	0.970	-391.9	10.5
M10	CPCM//SMD	1.035	-417.3	8.8	M23	SMD//g.p.	1.000	-400.7	10.2
M11	SMD	1.026	-413.2	10.7	M24	SMD//g.p.	0.960	-375.3	12.3
M12	SMD	1.008	-404.3	9.8	M25	IPCM//g.p.	0.935	-369.7	6.5
M13	SMD	1.060	-423.3	12.0					

[a] Slopes are given as dimensionless units while intercepts and their errors (σ(*b*)) are in kcal mol^{-1}

[b] Three worst correlations were marked in bold, while the three best ones are marked in blue; these data were removed from the error calculations as commented below.

From the data given in Table S26 we constructed the second plot of the form given in equation (S1)

$$b = m \times a + n \quad \text{(S1)}$$

where the values of *a* and *b* were obtained by models M1 – M25. In the ideal case of *a* = 1, sum of *m* and *n* equals $\Delta G^*_{H^-,ACN}$

Table S27. The second plot correlation data (Figure S26)

	All	CPCM	SMD/IPCM
slope (*m*)	-429.5	-413.99	-470.3
intercept (*n*)	26.4	9.0	71.6
$\Delta G^*_{H^-,ACN}$	-403.1	-405.0	-398.7

Here, we can see that large variations in the chosen set of the data changes the estimated $\Delta G^*_{H^-,ACN}$ value by less than 5 kcal mol^{-1}.

Calculation of error in $\Delta G^*_{H^-,ACN}$:

The error in $\Delta G^*_{H^-,ACN}$ was calculated according to the procedure defined for calculating average value of the result. The standard errors on the intercept for each particular model is given in Table S26 ($\sigma(b)$).

$$\delta(\Delta G^*_{H,ACN}) = \sqrt{\frac{\sum_1^n \sigma(b)^2}{n}}$$

By employing this approach, an error in $\Delta G^*_{H^-,ACN}$ was estimated to 10.2 kcal mol^{-1}.

Comparison of *$\Delta G^*_{H^-,ACN}$ evaluated using only selected data:*

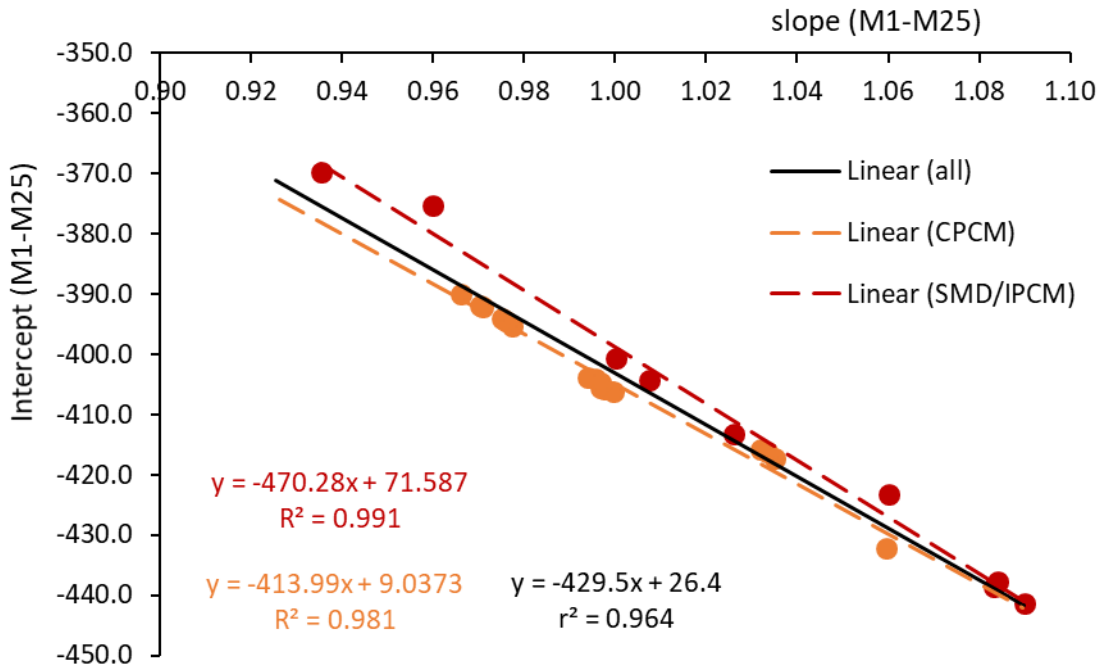

Figure S26. Correlation of the intercepts against slopes obtained for the models M1–M25 and the comparison of CPCM and SMD/IPCM results. Only the correlation over all models was used for the determination of $\Delta G^*(H^-)_{ACN}$.

$\Delta G^*(H^-)_{ACN}$ (all) = -429.5 + 26.4 = -403.1 kcal mol^{-1}

$\Delta G^*(H^-)_{ACN}$ (CPCM) = -414.0 + 9.0 = -405.0 kcal mol^{-1}

$\Delta G^*(H^-)_{ACN}$ (SMD/IPCM) = -470.3 + 71.6 = -398.7 kcal mol^{-1}

S3. Cartesian coordinates

Cartesian coordinates of the structures optimized within the model M1 are given as the separate Mercury or Molden readable file.