

Supplementary Material:

A Modified Electronegativity Equalization Method for fast and accurate calculation of atomic charges in large biological molecules

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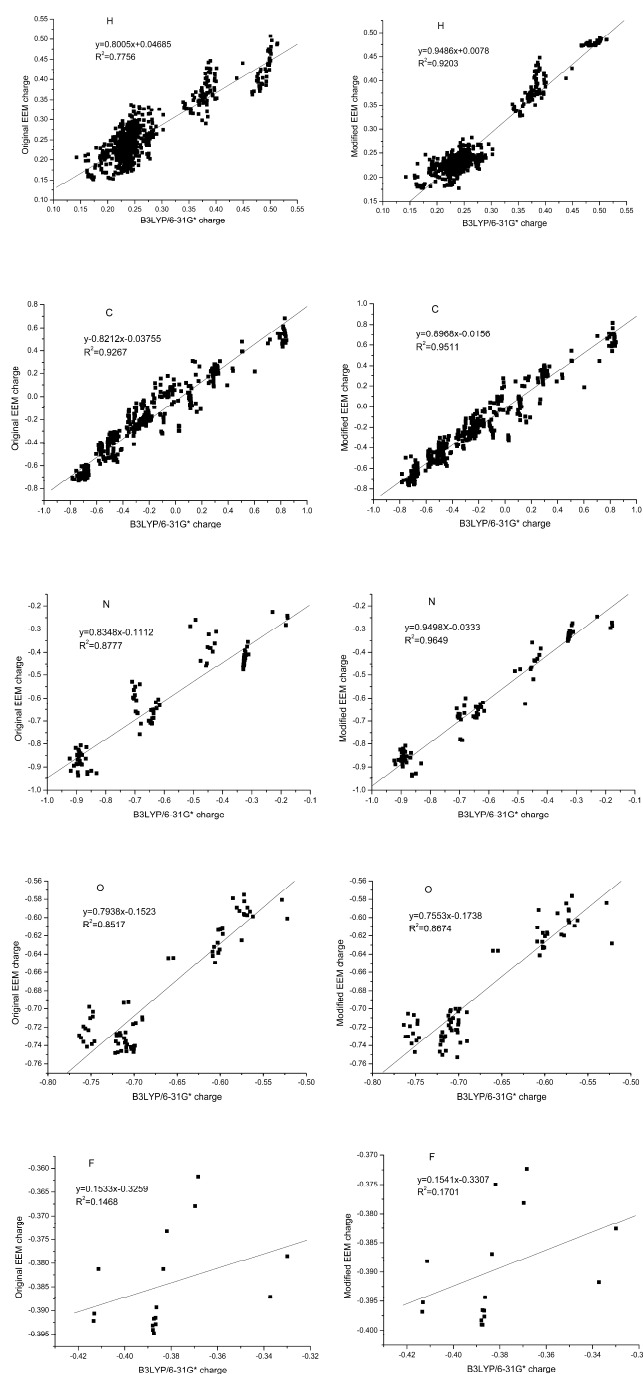


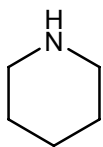
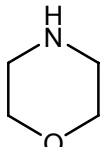
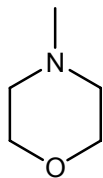
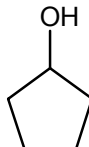
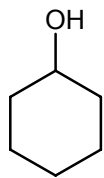
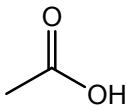
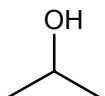
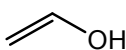
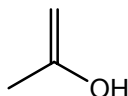
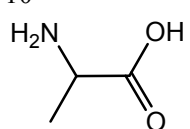
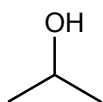
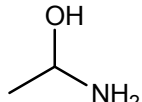
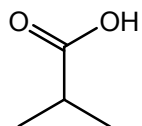
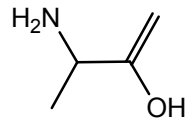
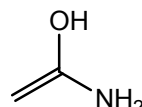
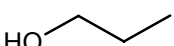
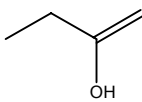
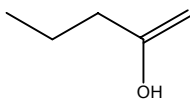
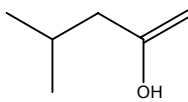
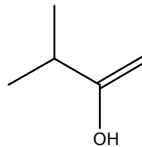
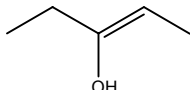
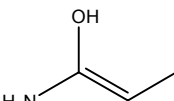
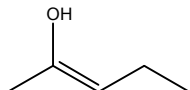
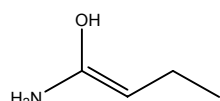
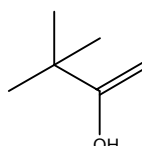
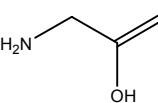
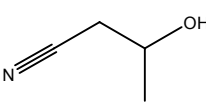
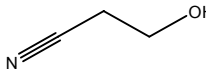
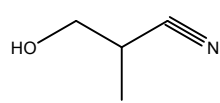
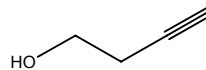
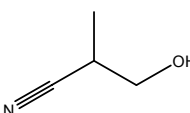
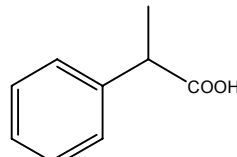
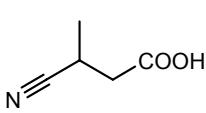
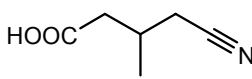
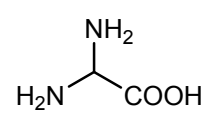
Fig. S1. Comparison of NPA charges, obtained from original and modified EEM method, with DFT charges at B3LYP/6-31G* level for all atoms in the training set, respectively. (Separate correlations are shown for H, C, N, O and F atom types). Original EEM and Modified EEM charges were obtained using the parameters calibrated in this work from table 2 and 5, respectively. Original EEM parameters are calibrated under the same condition as that of Modified EEM.

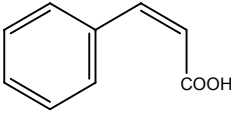
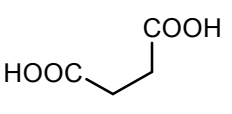
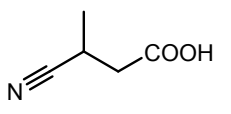
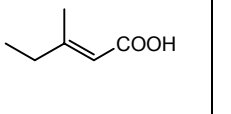
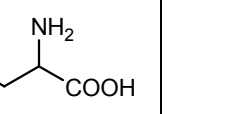
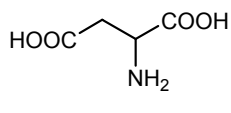
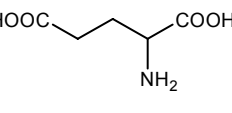
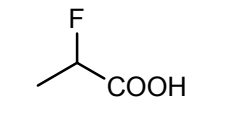
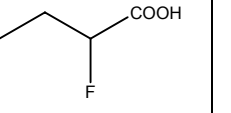
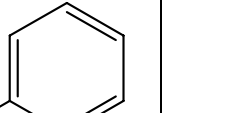
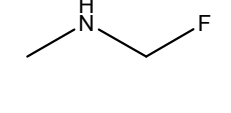
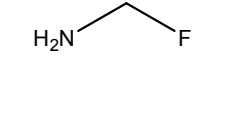
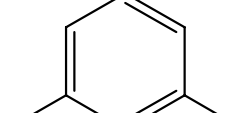
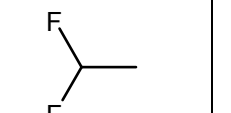
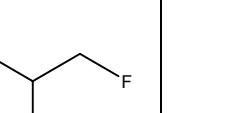
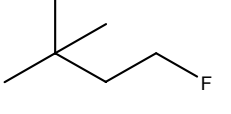
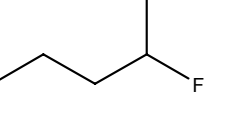
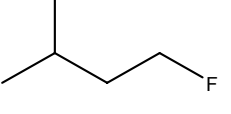
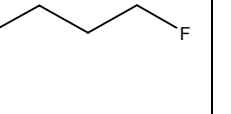
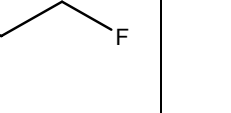
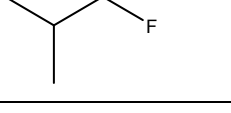
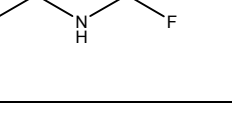
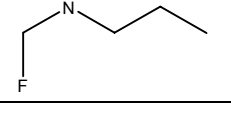
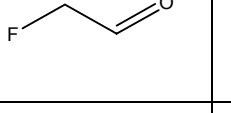
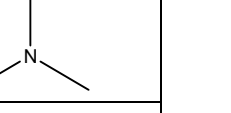
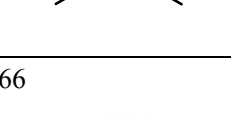

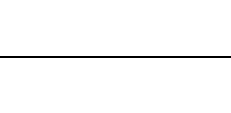
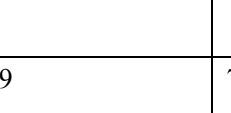

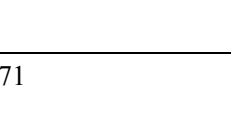
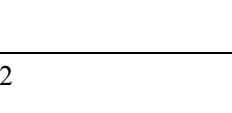
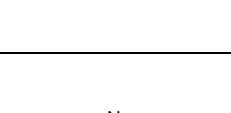

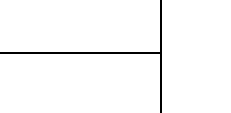
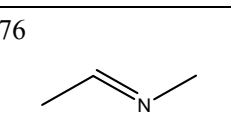
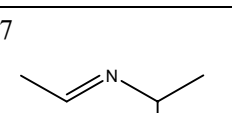
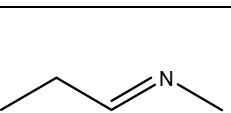
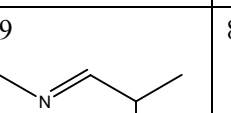
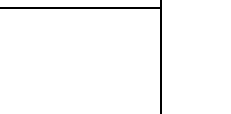





Table S1. Comparison of RMSE and DEV for modified EEM results and original EEM results in a large training set of 141 molecules^a

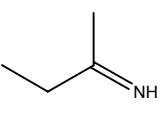
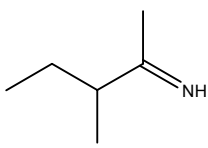
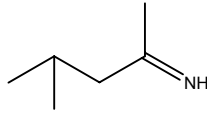
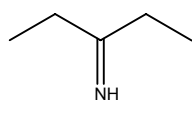
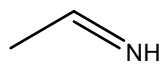
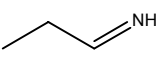
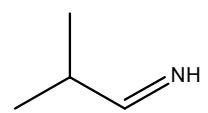
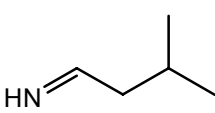
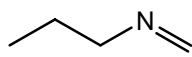
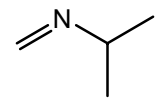
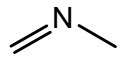
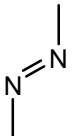
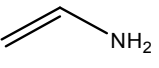
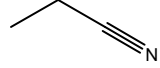
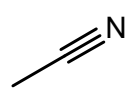
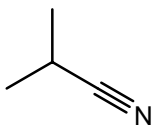
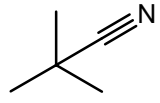
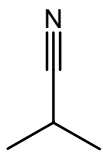
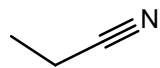
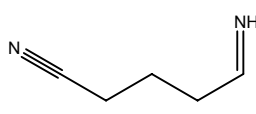
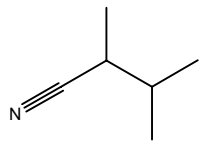
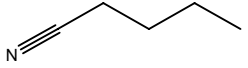
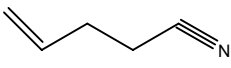
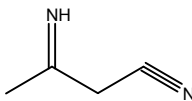
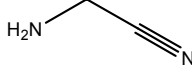
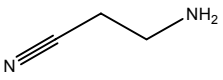
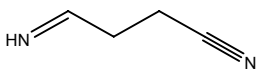
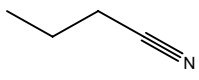
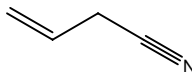
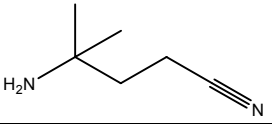
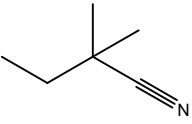

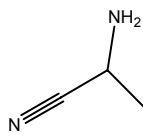
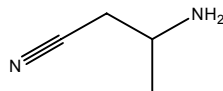
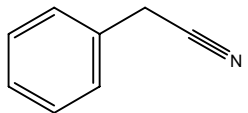
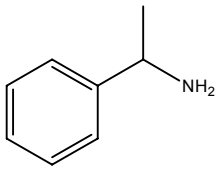
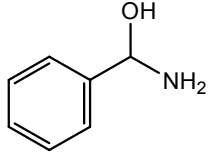
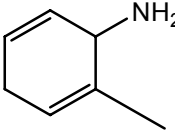
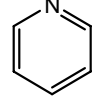
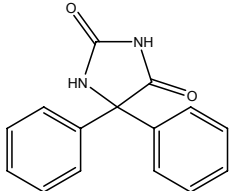
Atom type ^b	Modified EEM		Number of each atom type or atoms	EEM	
	RMSE	DEV		RMSE	DEV
H(-C)	0.0128	0.0144	1001		
H(-N)	0.0202	0.0153	92	0.0279	0.0237
H(-O)	0.0028	0.0118	46		
C _{sp} ³	0.079	0.0677	363		
C _{sp} ²	0.0876	0.0192	124		
C _{sp}	0.0335	0.0312	35	0.0889	0.0845
C(-Ar)	0.0603	0.0501	89		
N _{sp} ³	0.0512	0.0453	46		
N _{sp} ²	0.0406	0.0330	34	0.0741	0.0699
N _{sp}	0.0111	0.0118	31		
O _{sp} ³	0.0244	0.0345	49		
O _{sp} ²	0.0120	0.0266	25	0.0243	0.0271
F	0.0087	0.0177	18	0.0095	0.0159

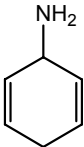
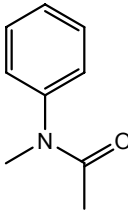
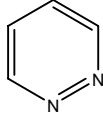
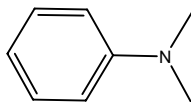
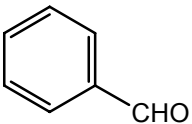

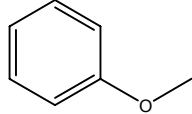
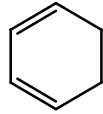
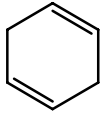
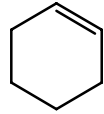




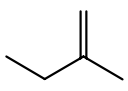

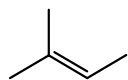
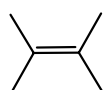
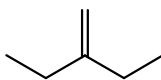

^a All values are in eV. ^b The meaning of H (-C), H (-N), H (-O), C_{sp}³, C_{sp}², C_{sp}, N_{sp}³, N_{sp}², N_{sp}, O_{sp}³ and O_{sp}² are the same as those mentioned in table 5. “EEM” represent the original EEM, which the same element is assigned to the equal parameters, but was calibrated using the same optimized method and training sets as that of distinction of different atom types in this study.

Table S2 : List of 141 number of molecules contained in the calibration set.

1 	2 	3 	4 	5 
6 	7 	8 	9 	10 
11 	12 	13 	14 	15 
16 	17 	18 	19 	20 
21 	22 	23 	24 	25 
26 	27 	28 	29 	30 
31 	32 	33 	34 	35 

36 	37 	38 	39 	40 
41 	42 	43 	44 	45 
46 	47 	48 	49 	50 
51 	52 	53 	54 	55 
56 	57 	58 	59 	60 
61 	62 	63 	64 	65 
66 	67 	68 	69 	70 
71 	72 	73 	74 	75 
76 	77 	78 	79 	80 

81 	82 	83 	84 	85 
86 	87 	88 	89 	90 
91 	92 	93 	94 	95 
96 	97 	98 	99 	100 
101 	102 	103 	104 	105 
106 	107 	108 	109 	110 
111 	112 	113 	114 	115 
116 	117 	118 	119 	120 

121 	122 	123 	124 	125 
126 	127 	128 	129 	130 
131 	132 	133 	134 	135 
136 	137 	138 	139 	140 
141 