Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Theoretical Study on Adiabatic Electron Affinity of Fatty Acids

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Table S1 The calculated AEA of 26 carboxylic acids by using 34 kinds of DFTs (kcal/mol)

Entry	Molecules	B3lyp	B3p86	M05	M05-2x	M06	M06-2x	B3pw91	M06-L
1	CH_3-COOH	-18.28	-8.95	-23.21	-27.49	-24.67	-27.42	-20.69	-28.18
2	CH_3CH_2-COOH	-16.37	-7.12	-20.97	-26.22	-22.79	-25.75	-18.83	-26.64
3	$CH_3CH_2CH_2$-COOH	-11.43	-2.75	-15.36	-22.47	-18.00	-20.44	-13.64	-22.20
4	CH_3HC=CH-COOH	0.84	12.88	-1.00	-1.45	-0.70	-2.48	0.33	-3.78
5	$CH_3CH_2CH_2CH_2$-COOH	-15.25	-5.96	-18.67	-25.41	-20.47	-24.19	-17.58	-24.93
6	CH_3CH_2HC=CH-COOH	3.50	14.77	1.85	-0.06	1.48	-0.83	2.44	-2.31
7	H_2C=CHCH=CH-COOH	19.17	31.85	17.59	17.60	18.05	16.48	19.16	16.14
8	CH_3CH(OH)COOH	-9.79	0.32	-14.57	-15.59	-14.15	-15.94	-12.06	-19.29
9	CH_3CH_2CH(OH)COOH	-10.27	0.13	-14.98	-15.56	-14.87	-16.30	-12.55	-19.90
10	CH_3CH(OH)CH_2COOH	-8.20	1.09	-11.88	-18.05	-14.22	-15.19	-9.85	-18.48
11	CH_3C(OH)=CHCOOH	1.34	12.49	-1.16	-1.66	-1.26	-2.92	-0.01	-5.62
12	CH_3C(=O)CH_2COOH	-2.71	8.53	-5.94	-8.96	-6.11	-9.93	-4.03	-7.74
13	CH_3CH_2C(=O)COOH	22.65	34.86	18.85	21.86	19.84	19.36	21.93	17.12
14	CH_2=CHC(=O)COOH	32.76	45.41	29.31	31.96	30.43	29.83	32.46	28.91
15	CH_3CH(NH_2)CH_2COOH	-15.80	-5.65	-19.88	-21.94	-20.27	-22.67	-17.96	-25.31
16	CH_3C(NH_2)=CHCOOH	-8.50	2.32	-11.26	-12.90	-11.30	-13.31	-9.76	-14.97
17	CH_3C(NH_2)=CHCOOH	-8.50	2.32	-11.26	-12.90	-11.30	-13.31	-9.76	-14.97
18	CH_3CH(F)CH_2COOH	-13.19	-3.35	-17.26	-18.76	-17.94	-19.71	-15.61	-23.16

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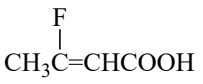
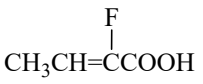
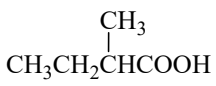
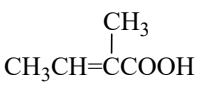
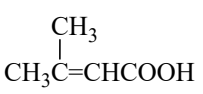
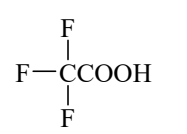
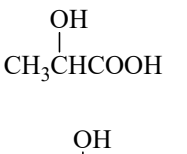
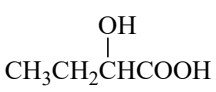
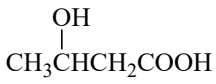
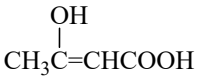
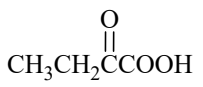
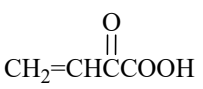
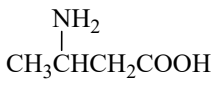
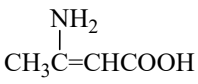
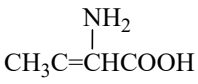
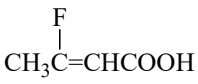
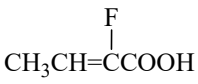
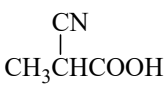
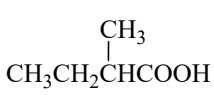
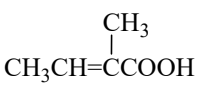
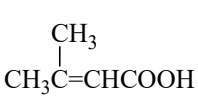
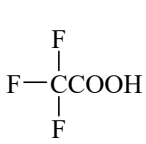
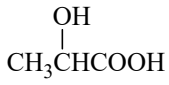
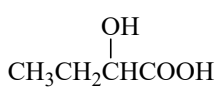
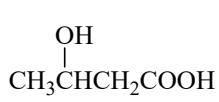
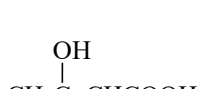
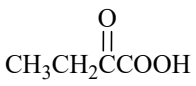
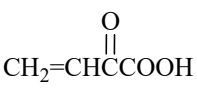
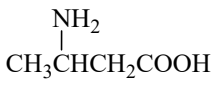
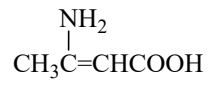
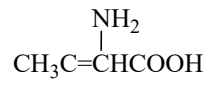
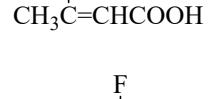
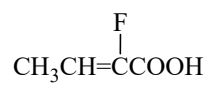
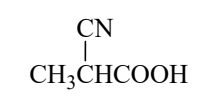
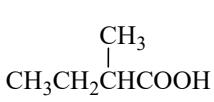
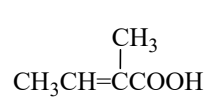
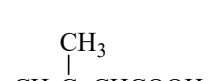
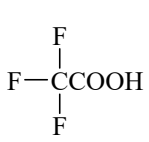
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

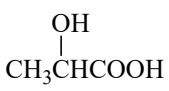
19		3.73	14.89	0.85	1.44	1.12	-0.25	2.41	-2.56
20		4.80	16.35	2.09	2.82	2.80	1.15	3.76	-0.80
21		-2.23	8.57	-6.04	-7.31	-6.20	-8.24	-4.02	-9.32
22		-13.84	-4.28	-17.71	-23.80	-18.53	-21.83	-15.97	-22.34
23		-1.21	10.70	-2.99	-3.30	-2.38	-4.16	-1.87	-5.92
24		0.69	12.40	-0.92	-2.22	-1.05	-3.07	0.01	-4.60
25	HCOOH	-22.40	-12.11	-27.84	-26.51	-27.61	-27.97	-24.43	-31.41
26		4.68	15.02	-1.40	2.91	-0.53	0.08	2.39	-4.38

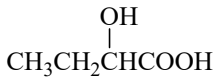
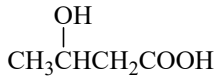
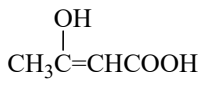
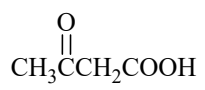
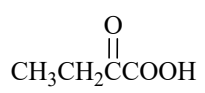
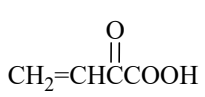
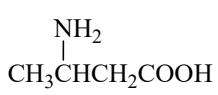
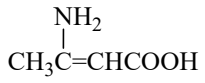
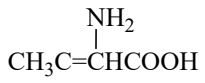
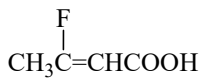
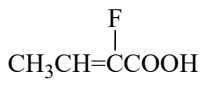
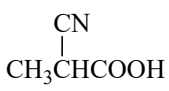
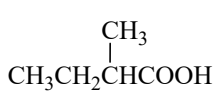
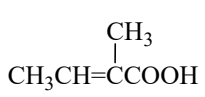
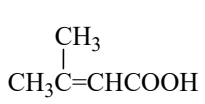
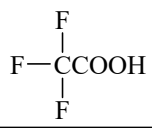
Entry	Molecules	M06-HF	B3LYP-D3	CAM-B3LYP	BP86-D3	B97-D3	B97D	BP86	ωB97
1	CH_3-COOH	-23.97	-18.28	-22.43	-13.50	-20.28	-20.23	-13.52	-28.31
2	CH_3CH_2-COOH	-22.06	-16.47	-21.08	-11.53	-18.15	-18.05	-11.42	-27.54
3	$CH_3CH_2CH_2$-COOH	-13.40	-11.55	-17.22	-7.41	-14.19	-14.11	-7.23	-26.10
4	CH_3HC=CH-COOH	-0.57	0.80	-0.35	4.36	-0.10	-0.02	4.40	-2.58
5	$CH_3CH_2CH_2CH_2$-COOH	-20.62	-15.13	-20.55	-9.96	-15.97	-15.89	-10.07	-27.39
6	CH_3CH_2HC=CH-COOH	1.57	3.35	0.99	7.88	3.09	3.11	8.02	-1.70
7	H_2C=CHCH=CH-COOH	17.57	19.04	18.01	22.43	18.24	18.19	22.55	15.88
8		-11.96	-9.87	-12.43	-5.56	-11.77	-11.88	-5.50	-17.12
9		-12.50	-10.53	-12.23	41.28	-12.83	-13.15	-6.07	-16.20
10		-9.56	-8.25	-13.02	-4.28	-11.86	-11.85	-4.24	-20.24
11		0.49	1.12	-0.06	4.60	-0.27	-0.48	4.85	-2.81
12		-8.89	-0.30	-7.67	4.66	-0.96	-0.66	3.90	-12.79
13		22.83	22.38	21.88	24.68	20.70	20.61	25.03	19.04
14		32.26	32.67	31.40	35.63	31.40	31.23	35.72	28.09

15		-17.90	-16.14	-18.81	-10.93	-16.63	-16.89	-10.52	-22.98
16		-10.71	-8.47	-11.22	-3.91	-9.51	-9.37	-3.97	-13.49
17		-10.71	-8.47	-11.22	-3.91	-9.51	-9.37	-3.97	-13.48
18		-14.80	-13.31	-15.74	-9.30	-14.75	-14.65	-9.14	-19.66
19		3.23	3.69	2.69	5.95	2.09	2.18	5.97	0.42
20		3.41	4.76	3.76	7.38	3.42	3.51	7.40	1.49
21		-4.84	-2.15	-5.29	2.30	-2.41	-2.23	2.24	-9.66
22		-17.72	-13.66	-19.10	-8.66	-15.96	-15.81	-8.86	-26.53
23		-1.90	-1.12	-2.46	2.41	-1.90	-1.93	2.26	-4.65
24		-0.90	0.63	-1.02	4.51	-0.32	-0.24	4.56	-3.48
25	HCOOH	-24.86	-22.36	-23.51	-19.14	-24.47	-24.44	-19.17	-26.87
26		7.03	4.68	4.04	6.29	2.13	2.19	6.28	1.18

Entry	Molecules	ωB97XD	SOGGA11	SOGGA11-X	N12-SX	M11	M11-L	MN12-SX	MN12-L
1	CH_3-COOH	-26.45	-74.22	-23.77	-24.93	-26.33	-15.28	-22.46	-26.05
2	CH_3CH_2-COOH	-25.37	-8.09	-23.17	-22.86	-25.41	-12.37	-19.74	-24.07
3	$CH_3CH_2CH_2$-COOH	-22.01	0.55	-17.89	-17.06	-21.31	41.75	-12.69	-17.03
4	CH_3HC=CH-COOH	-2.55	-0.46	-1.27	-2.42	-0.19	2.85	-17.34	-5.42
5	$CH_3CH_2CH_2CH_2$-COOH	-24.46	-1.13	-22.08	-21.01	-24.77	-9.21	-15.88	-21.27
6	CH_3CH_2HC=CH-COOH	-1.48	10.32	0.29	0.01	0.94	7.36	3.27	-1.93
7	H_2C=CHCH=CH-COOH	16.13	17.08	17.67	16.39	18.39	20.29	18.36	13.50
8		-16.65	-3.51	-15.01	-15.74	-14.88	-9.40	-12.82	-18.14
9		-16.60	-4.72	-14.72	-15.78	-14.00	-9.63	-13.00	-18.96
10		-16.72	4.14	-13.51	-13.44	-15.60	-0.33	-8.33	-10.77
11		-3.31	4.83	-1.77	-2.25	0.06	1.38	-0.44	-6.18

12		-9.85	5.20	-8.41	-7.07	-8.82	-0.86	-20.08	-8.53
13		18.93	20.53	21.00	19.69	21.00	18.84	20.57	14.98
14		28.91	27.99	31.30	30.17	30.81	31.18	31.36	26.96
15		-22.60	-5.16	-21.13	-21.32	-20.69	-13.03	-17.96	-23.32
16		-13.64	-2.16	-11.87	-13.75	-11.82	-4.87	-9.66	-14.68
17		-13.64	-2.16	-11.86	-13.74	-11.82	-4.87	-9.66	-14.67
18		-19.65	-5.12	-18.13	-18.72	-17.34	-13.02	-15.66	-21.69
19		-0.13	4.32	1.12	0.28	2.89	1.81	1.69	-4.31
20		1.08	-0.38	2.35	1.54	3.88	3.34	3.08	-3.00
21		-8.39	2.56	-6.55	-7.15	-6.84	-2.17	-4.68	-9.95
22		-23.34	-1.65	-20.05	-19.44	-22.50	-5.64	-13.91	-17.07
23		-4.62	5.09	-3.41	-4.51	-2.00	1.31	-1.23	-6.93
24		-3.31	7.00	-1.93	-2.66	-0.74	3.52	-16.69	-5.27
25		-27.16	-24.45	-26.13	-27.69	-25.01	-24.62	-26.88	-32.18
26		-0.17	-4.50	1.08	0.62	4.28	-4.95	0.29	-6.77

Entry	Molecules	N12	MPW1P86	BMK	MPW1B95	MPW1K	MPW1KCIS	MPW3LYP	MPWB1K	BB1K	TPSS
1	CH_3-COOH	-17.07	-18.93	-28.55	-25.13	-26.02	-19.57	-17.32	-28.33	-28.65	-17.71
2	CH_3CH_2-COOH	-14.05	-17.04	-27.30	-23.18	-24.51	-17.33	-15.31	-26.62	-26.97	-15.66
3	$CH_3CH_2CH_2$-COOH	-6.72	-11.98	-22.78	-17.01	-18.61	-11.92	-10.36	-19.84	-20.21	-11.42
4	CH_3HC=CH-COOH	-1.82	2.42	-4.59	-3.82	-1.62	-0.32	1.63	-5.02	-5.45	0.33
5	$CH_3CH_2CH_2CH_2$-COOH	-23.32	-15.75	-25.99	-21.52	-23.39	-15.70	-14.01	-25.14	-25.54	-14.08
6	CH_3CH_2HC=CH-COOH	3.12	4.43	-3.33	-1.68	-0.35	2.82	4.46	-3.45	-3.94	3.77
7	H_2C=CHCH=CH-COOH	14.16	21.24	14.66	15.09	17.39	18.33	19.89	14.03	13.63	18.24
8		-10.08	-9.83	-19.22	-16.16	-16.10	-11.23	-8.65	-18.72	-19.24	-9.57

9		-10.74	-10.00	-18.76	-16.43	-15.93	-12.14	-9.12	-18.59	-19.17	-10.07
10		-3.69	-8.02	-16.72	-13.06	-13.56	-8.63	-7.12	-15.31	-15.78	-8.48
11		0.07	2.16	-5.33	-4.18	-2.13	-0.42	2.28	-5.56	-6.05	1.21
12		-1.76	-2.39	-11.42	-8.81	-9.82	-3.28	-1.66	-12.26	-12.57	-0.14
13		17.74	24.16	17.09	18.20	20.42	20.68	23.47	17.38	16.88	21.64
14		27.85	34.71	27.85	28.74	30.96	31.37	33.56	27.88	27.38	31.81
15		-13.70	-15.74	-25.24	-22.50	-21.99	-16.91	-14.61	-25.12	-25.65	-14.49
16		-82.41	-7.87	-16.02	-14.14	-12.83	-9.56	-7.70	-16.02	-16.38	-8.20
17		-10.00	-7.87	-16.01	-14.14	-12.83	-9.56	-7.70	-16.02	-16.38	-8.20
18		-12.44	-13.48	-22.03	-19.90	-19.21	-14.86	-12.03	-22.21	-22.74	-12.65
19		0.12	4.48	-2.22	-1.59	0.68	1.57	4.59	-2.69	-3.17	2.88
20		1.38	5.76	-0.92	-0.31	1.78	2.93	5.60	-1.49	-1.91	3.89
21		-2.83	-1.92	-9.58	-8.69	-7.81	-3.77	-1.16	-11.03	-11.48	-1.52
22		-9.50	-13.83	-24.41	-19.14	-21.51	-14.22	-12.57	-22.52	-22.99	-13.13
23		-2.83	0.28	-6.60	-5.82	-3.90	-2.39	-0.33	-7.09	-7.54	-1.58
24		-1.18	2.01	-5.43	-4.03	-2.23	-0.32	1.52	-5.44	-5.87	0.51
25	HCOOH	-26.13	-22.41	-29.70	-28.86	-26.87	-24.89	-21.61	-30.31	-30.72	-22.95
26		-0.36	4.43	-1.89	-1.58	0.16	1.42	5.59	-2.89	-3.39	3.79