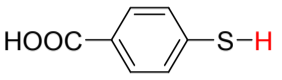
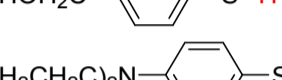
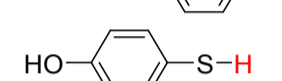
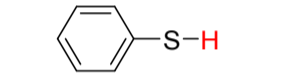
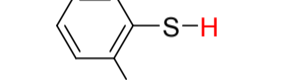
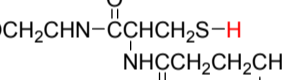
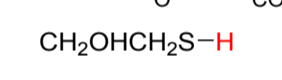
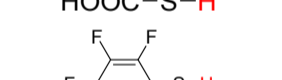
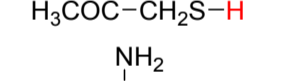
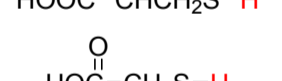
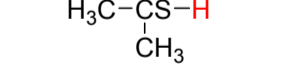
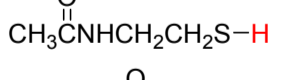
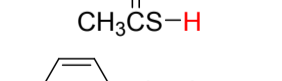
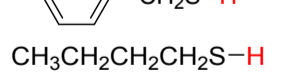
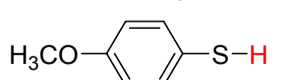



Theoretical modeling of pK_a 's of thiol compounds in aqueous solution

Yuanyuan Zheng, Wenrui Zheng*, Danfeng Zhu and Huifang Chang

College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China

Table S1 58 pK_a 's of thiols by 10 DFT methods with PCM-Bondi model in thermodynamic cycle 2.

| Entry | thiols | Exp. | M05 | M05-2X | M06 | M06-2X | M06-HF | M06-L | B3P86 | BMK | KMLY P | WB97XD |
|-------|---|-------|-------|--------|-------|--------|--------|-------|-------|-------|-----------|--------|
| 1 |  | 5.90 | 5.56 | 4.12 | 4.58 | 4.26 | 5.90 | 5.01 | 5.86 | 4.10 | 7.37 | 4.29 |
| 2 |  | 6.60 | 6.24 | 5.58 | 6.05 | 4.77 | 6.60 | 5.83 | 5.69 | 5.63 | 8.25 | 5.10 |
| 3 |  | 4.90 | 5.76 | 5.18 | 5.90 | 5.09 | 4.90 | 5.26 | 5.15 | 4.69 | 7.22 | 4.67 |
| 4 |  | 5.17 | 6.35 | 4.93 | 6.29 | 5.04 | 5.17 | 5.64 | 5.30 | 4.53 | 7.98 | 4.78 |
| 5 |  | 6.40 | 7.78 | 7.07 | 7.55 | 6.81 | 6.40 | 6.82 | 7.09 | 6.26 | 9.26 | 6.36 |
| 6 |  | 7.01 | 9.02 | 7.48 | 8.85 | 8.79 | 7.00 | 7.80 | 9.03 | 7.28 | 10.98 | 7.96 |
| 7 |  | 6.90 | 7.95 | 7.59 | 8.22 | 7.83 | 6.90 | 6.87 | 8.12 | 6.73 | 10.46 | 7.94 |
| 8 |  | 4.61 | 4.76 | 2.39 | 4.35 | 6.32 | 4.61 | 5.40 | 4.71 | 4.49 | 5.91 | 3.15 |
| 9 |  | 6.55 | 7.86 | 6.55 | 6.74 | 6.09 | 6.55 | 6.31 | 7.52 | 7.49 | 9.96 | 6.79 |
| 10 |  | 5.70 | 15.22 | 7.14 | 7.52 | 7.37 | 5.70 | 4.61 | 7.74 | 7.02 | 6.95 | 6.63 |
| 11 |  | 7.31 | 9.65 | 9.74 | 9.66 | 9.72 | 7.30 | 8.43 | 9.41 | 9.07 | 11.52 | 8.83 |
| 12 |  | 8.60 | 7.01 | 4.79 | 6.72 | 4.18 | 8.60 | 7.70 | 5.77 | 7.04 | 6.73 | 5.71 |
| 13 |  | 9.60 | 12.16 | 11.50 | 11.75 | 11.63 | 9.60 | 10.68 | 11.73 | 11.49 | 13.87 | 11.09 |
| 14 |  | 3.20 | 1.52 | 0.01 | 1.13 | 0.05 | 3.20 | 4.90 | 1.07 | 1.48 | 2.40 | 1.05 |
| 15 |  | 2.68 | 1.78 | 2.82 | 2.28 | 2.20 | 2.68 | 3.30 | 0.36 | 1.01 | 3.27 | 1.38 |
| 16 |  | 7.91 | 14.86 | 11.66 | 10.47 | 12.18 | 7.86 | 9.86 | 13.95 | 13.57 | 14.45 | 10.64 |
| 17 |  | 8.30 | 12.52 | 12.93 | 11.20 | 12.87 | 8.30 | 10.04 | 11.22 | 10.47 | 12.79 | 12.49 |
| 18 |  | 10.50 | 10.04 | 8.73 | 10.14 | 7.55 | 10.50 | 13.12 | 10.78 | 10.14 | 15.24 | 14.70 |
| 19 |  | 10.61 | 12.22 | 11.35 | 12.07 | 12.02 | 10.61 | 10.32 | 11.00 | 10.94 | 13.59 | 11.27 |
| 20 |  | 10.86 | 13.00 | 12.11 | 12.78 | 12.69 | 10.86 | 11.41 | 12.50 | 11.93 | 14.79 | 12.35 |
| 21 |  | 11.30 | 12.87 | 12.42 | 12.36 | 12.64 | 11.31 | 12.32 | 13.16 | 16.47 | 15.91 | 12.68 |
| 22 |  | 9.92 | 12.27 | 12.04 | 13.13 | 11.93 | 9.92 | 11.70 | 15.27 | 14.98 | 17.89 | 13.96 |
| 23 |  | 3.62 | 4.09 | 3.59 | 2.63 | 4.28 | 3.62 | 5.10 | 1.59 | 2.26 | 6.54 | 3.09 |
| 24 |  | 9.43 | 11.09 | 10.50 | 11.10 | 11.16 | 9.43 | 11.58 | 10.54 | 11.36 | 12.78 | 11.06 |
| 25 |  | 10.88 | 13.92 | 12.85 | 13.19 | 12.65 | 10.88 | 12.25 | 12.65 | 12.60 | 13.78 | 13.23 |
| 26 |  | 6.89 | 5.46 | 4.77 | 5.62 | 6.96 | 6.89 | 6.68 | 4.50 | 3.72 | 9.34 | 6.08 |
| 27 |  | 6.78 | 8.54 | 8.37 | 8.12 | 7.96 | 6.78 | 8.04 | 7.82 | 6.96 | 9.34 | 7.24 |

* Corresponding author. Tel.: +86 21 67791216; fax: +86 21 67791220.
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).


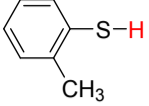
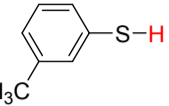
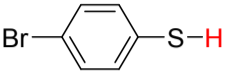
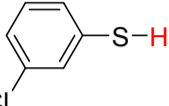
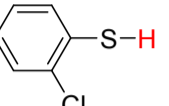
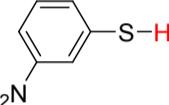
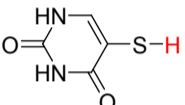
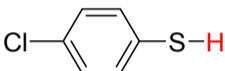
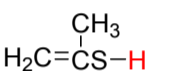
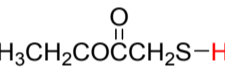
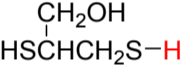
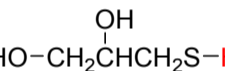
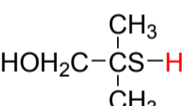
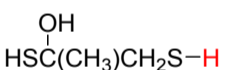
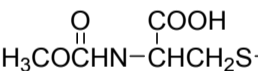
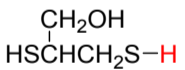
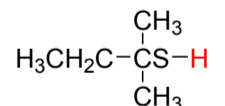
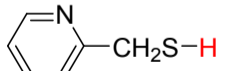
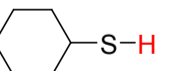
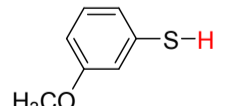
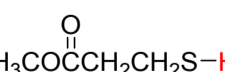
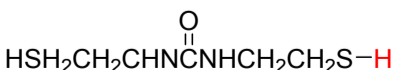
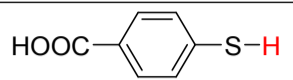
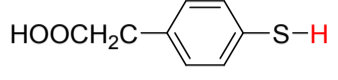
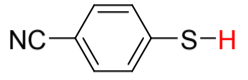
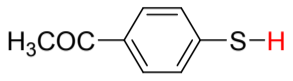
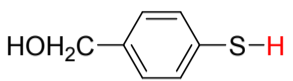
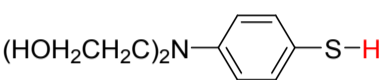
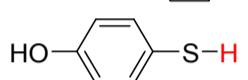
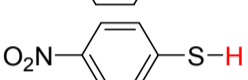
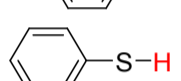
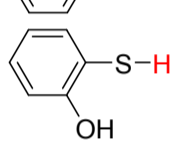
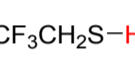
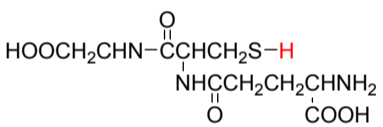
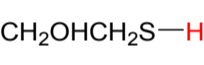
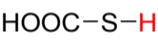
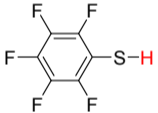
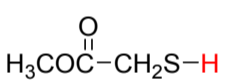
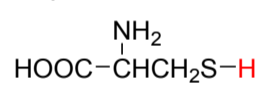
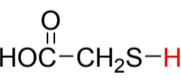
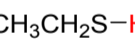
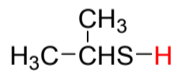
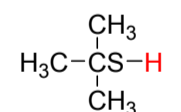
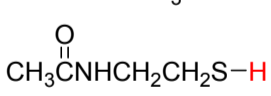
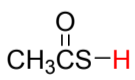
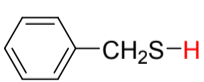
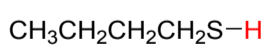
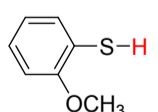
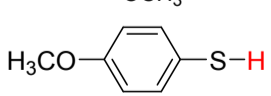
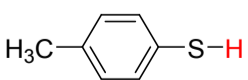
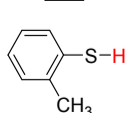
| | | | | | | | | | | | | |
|----|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 28 |  | 6.82 | 7.82 | 7.57 | 6.62 | 7.63 | 6.82 | 7.37 | 8.02 | 7.19 | 10.48 | 6.75 |
| 29 |  | 7.00 | 8.73 | 7.82 | 8.06 | 8.60 | 7.00 | 7.68 | 7.66 | 7.16 | 10.09 | 8.05 |
| 30 |  | 6.60 | 8.28 | 7.73 | 7.40 | 5.91 | 6.60 | 7.79 | 7.15 | 6.83 | 10.15 | 6.97 |
| 31 |  | 6.02 | 7.06 | 5.79 | 6.35 | 6.20 | 6.02 | 6.22 | 6.48 | 6.19 | 8.26 | 6.07 |
| 32 |  | 5.78 | 5.49 | 6.38 | 6.47 | 5.71 | 5.78 | 6.17 | 6.68 | 5.24 | 8.78 | 6.13 |
| 33 |  | 5.68 | 8.70 | 5.96 | 5.09 | 8.16 | 5.24 | 5.76 | 9.38 | 7.58 | 8.83 | 5.33 |
| 34 | $\text{CH}_3\text{S-H}$ | 10.33 | 14.49 | 11.92 | 12.16 | 12.03 | 10.30 | 11.17 | 11.96 | 11.89 | 13.81 | 11.80 |
| 35 | $\text{CH}_3\text{CH}_2\text{CH}_2\text{S-H}$ | 10.70 | 12.40 | 12.47 | 12.46 | 12.62 | 10.70 | 11.78 | 11.85 | 12.29 | 14.33 | 12.17 |
| 36 |  | 5.24 | 8.70 | 5.96 | 5.09 | 8.16 | 6.85 | 5.76 | 9.38 | 7.58 | 8.83 | 5.33 |
| 37 |  | 5.30 | 5.67 | 4.61 | 4.09 | 3.66 | 5.30 | 6.40 | 0.33 | 1.48 | 4.76 | 3.65 |
| 38 |  | 6.14 | 7.58 | 7.09 | 6.66 | 5.86 | 6.14 | 5.81 | 6.60 | 5.36 | 8.97 | 6.63 |
| 39 |  | 7.86 | 8.36 | 7.75 | 7.92 | 8.28 | 7.86 | 6.79 | 8.38 | 7.43 | 12.04 | 7.93 |
| 40 |  | 7.95 | 10.63 | 8.75 | 6.71 | 5.14 | 7.95 | 8.80 | 7.52 | 7.65 | 9.31 | 10.21 |
| 41 |  | 8.62 | 11.75 | 9.16 | 13.65 | 11.50 | 8.62 | 7.20 | 13.81 | 10.16 | 12.97 | 11.09 |
| 42 | $\text{H}_3\text{CH}_2\text{C-OCH}_2\text{CH}_2\text{S-H}$ | 9.38 | 9.50 | 9.46 | 10.08 | 10.00 | 9.38 | 8.62 | 9.42 | 8.78 | 11.70 | 9.55 |
| 43 |  | 9.51 | 6.73 | 2.11 | 6.09 | 7.45 | 9.51 | 8.30 | 6.27 | 5.79 | 8.76 | 5.87 |
| 44 |  | 9.85 | 11.47 | 11.58 | 10.98 | 11.29 | 9.85 | 10.55 | 11.62 | 11.72 | 13.92 | 10.98 |
| 45 | $\text{H}_2\text{C=CHCH}_2\text{S-H}$ | 9.96 | 10.22 | 11.30 | 11.65 | 11.61 | 9.96 | 11.90 | 8.84 | 10.95 | 11.60 | 11.68 |
| 46 |  | 9.04 | 3.92 | 3.87 | 2.70 | 3.60 | 9.04 | 8.68 | 3.44 | 1.67 | 6.01 | 0.68 |
| 47 |  | 8.55 | 9.47 | 10.40 | 10.20 | 9.52 | 8.55 | 9.28 | 9.37 | 8.98 | 12.11 | 9.52 |
| 48 | $\text{H}_2\text{N-CH}_2\text{CH}_2\text{S-H}$ | 10.53 | 10.82 | 10.63 | 12.00 | 10.45 | 10.53 | 10.53 | 10.63 | 10.84 | 13.01 | 10.55 |
| 49 |  | 10.57 | 7.35 | 7.67 | 7.94 | 6.97 | 10.57 | 9.20 | 8.91 | 6.88 | 10.46 | 7.59 |
| 50 |  | 11.22 | 13.10 | 12.58 | 13.65 | 12.40 | 11.22 | 12.33 | 13.17 | 13.70 | 15.95 | 12.23 |
| 51 | $\text{HS-(CH}_2)_2\text{S-H}$ | 9.05 | 10.93 | 11.15 | 9.62 | 9.45 | 9.05 | 8.41 | 10.34 | 9.52 | 16.12 | 11.07 |
| 52 |  | 8.82 | 9.78 | 9.91 | 10.33 | 9.35 | 8.82 | 10.07 | 9.82 | 10.32 | 11.91 | 9.68 |
| 53 |  | 10.69 | 12.48 | 12.80 | 12.66 | 12.49 | 10.69 | 11.74 | 12.24 | 11.58 | 14.49 | 11.95 |
| 54 |  | 6.39 | 6.60 | 6.47 | 8.21 | 8.82 | 6.39 | 6.09 | 6.84 | 6.77 | 9.31 | 7.12 |
| 55 | $\text{HO-(CH}_2)_4\text{S-H}$ | 10.19 | 12.54 | 12.35 | 12.15 | 12.09 | 10.19 | 11.69 | 11.91 | 12.28 | 14.07 | 12.75 |
| 56 |  | 9.33 | 9.52 | 9.92 | 8.73 | 9.32 | 9.33 | 8.12 | 8.94 | 9.31 | 11.26 | 9.70 |
| 57 | $\text{HS-(CH}_2)_4\text{S-H}$ | 9.88 | 13.02 | 12.15 | 11.68 | 12.02 | 9.88 | 11.57 | 10.33 | 11.24 | 13.90 | 10.94 |
| 58 |  | 9.26 | 11.35 | 13.21 | 12.59 | 9.99 | 9.26 | 8.90 | 13.19 | 11.94 | 13.67 | 11.99 |

Table S2 58 pK_a 's of thiols by M06-L and M06-2X methods with PCM-Bondi and SMD_{SSAS} models in thermodynamic cycles 1 and 2.

| Entry | thiols | Exp. | PCM-Bondi | | SMD _{SSAS} | | |
|-------|---|-------|-----------|---------|---------------------|---------|---------|
| | | | M06-L | M06-L | M06-2X | | |
| | | | Cycle 1 | Cycle 1 | Cycle 2 | Cycle 1 | Cycle 2 |
| 1 |  | 5.90 | 9.6 | 7.9 | 10.0 | 5.1 | 3.5 |
| 2 |  | 6.60 | 11.7 | 9.1 | 11.9 | 6.4 | 4.7 |
| 3 |  | 4.90 | 9.3 | 7.1 | 9.9 | 5.1 | 3.5 |
| 4 |  | 5.17 | 9.4 | 8.7 | 9.7 | 5.1 | 4.2 |
| 5 |  | 6.40 | 11.7 | 10.6 | 11.2 | 6.1 | 8.0 |
| 6 |  | 7.01 | 9.4 | 12.0 | 14.9 | 7.0 | 5.5 |
| 7 |  | 6.90 | 5.5 | 9.7 | 12.3 | 7.1 | 7.8 |
| 8 |  | 4.61 | 7.8 | 6.4 | 8.2 | 3.9 | 3.3 |
| 9 |  | 6.55 | 5.6 | 8.9 | 12.2 | 6.7 | 4.8 |
| 10 |  | 5.70 | 11.0 | 8.8 | 11.6 | 6.9 | 6.9 |
| 11 |  | 7.31 | 12.7 | 10.6 | 12.7 | 7.9 | 6.7 |
| 12 |  | 8.60 | 12.3 | 12.8 | 12.8 | 9.2 | 11.2 |
| 13 |  | 9.60 | 5.8 | 12.1 | 15.2 | 10.6 | 8.1 |
| 14 |  | 3.20 | 6.1 | 4.4 | 5.9 | 2.5 | 0.6 |
| 15 |  | 2.68 | 6.7 | 4.8 | 8.3 | 2.0 | -0.3 |
| 16 |  | 7.91 | 5.9 | 11.3 | 13.6 | 8.1 | 7.8 |
| 17 |  | 8.30 | 6.2 | 11.9 | 14.2 | 10.2 | 7.6 |
| 18 |  | 10.50 | 13.2 | 10.1 | 14.5 | 9.5 | 6.0 |
| 19 |  | 10.61 | 14.0 | 13.1 | 15.4 | 11.1 | 10.3 |
| 20 |  | 10.86 | 8.8 | 14.4 | 16.0 | 11.5 | 10.4 |
| 21 |  | 11.30 | 9.9 | 13.4 | 16.5 | 10.9 | 10.4 |
| 22 |  | 9.92 | 14.6 | 15.2 | 14.4 | 10.8 | 9.5 |
| 23 |  | 3.62 | 8.9 | 6.7 | 8.7 | 3.2 | 3.4 |
| 24 |  | 9.43 | 15.1 | 14.4 | 14.7 | 9.2 | 9.6 |
| 25 |  | 10.88 | 16.0 | 13.2 | 15.3 | 11.4 | 9.6 |
| 26 |  | 6.89 | 12.2 | 10.8 | 12.1 | 6.9 | 6.3 |
| 27 |  | 6.78 | 12.2 | 9.8 | 12.2 | 7.7 | 6.6 |
| 28 |  | 6.82 | 10.9 | 9.4 | 12.3 | 6.8 | 6.9 |
| 29 |  | 7.00 | 12.0 | 9.8 | 11.9 | 7.0 | 8.0 |

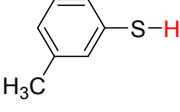
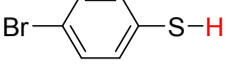
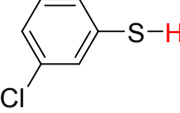
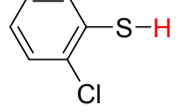
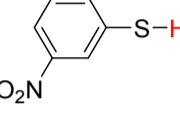
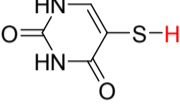
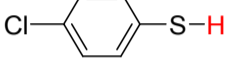
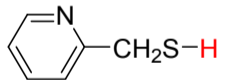
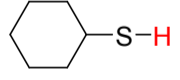
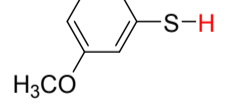
| | | | | | | | |
|----|---|-------|------|------|------|------|------|
| 30 |  | 6.60 | 11.7 | 9.3 | 11.9 | 6.6 | 5.2 |
| 31 |  | 6.02 | 11.2 | 7.6 | 11.1 | 6.2 | 4.1 |
| 32 |  | 5.78 | 5.0 | 8.0 | 10.6 | 5.8 | 5.2 |
| 33 |  | 5.68 | 10.2 | 7.9 | 10.2 | 5.5 | 4.3 |
| 34 | $\text{CH}_3\text{S}-\text{H}$ | 10.33 | 6.2 | 12.9 | 15.9 | 11.3 | 10.7 |
| 35 | $\text{CH}_3\text{CH}_2\text{CH}_2\text{S}-\text{H}$ | 10.70 | 6.1 | 13.4 | 16.1 | 11.4 | 10.3 |
| 36 |  | 5.24 | 6.1 | 7.7 | 10.2 | 6.60 | 3.7 |
| 37 |  | 5.30 | 10.4 | 9.8 | 10.3 | 5.4 | 4.5 |
| 38 |  | 6.14 | 5.2 | 8.8 | 11.2 | 7.6 | 4.4 |
| 39 | $\text{H}_2\text{C}=\overset{\text{CH}_3}{\text{C}}\text{S}-\text{H}$ | 7.86 | 12.3 | 9.4 | 12.6 | 7.6 | 5.7 |
| 40 | $\text{H}_3\text{CH}_2\text{COCCH}_2\text{S}-\text{H}$ | 7.95 | 6.0 | 12.0 | 13.5 | 8.4 | 7.3 |
| 41 | $\text{HSC}(\text{CH}_2\text{OH})\text{CH}_2\text{S}-\text{H}$ | 8.62 | 5.8 | 10.4 | 13.8 | 10.2 | 9.0 |
| 42 | $\text{H}_3\text{CH}_2\text{C}-\text{OCH}_2\text{CH}_2\text{S}-\text{H}$ | 9.38 | 6.2 | 13.0 | 15.1 | 9.5 | 7.7 |
| 43 | $\text{HO}-\text{CH}_2\overset{\text{OH}}{\text{C}}\text{HCH}_2\text{S}-\text{H}$ | 9.51 | 12.5 | 12.5 | 14.7 | 10.4 | 9.0 |
| 44 | $\text{HOH}_2\text{C}-\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{C}}}\text{S}-\text{H}$ | 9.85 | 5.3 | 12.5 | 15.1 | 10.3 | 8.9 |
| 45 | $\text{H}_2\text{C}=\text{CHCH}_2\text{S}-\text{H}$ | 9.96 | 14.7 | 12.0 | 14.4 | 9.8 | 8.7 |
| 46 | $\text{HSC}(\text{CH}_3)(\text{OH})\text{CH}_2\text{S}-\text{H}$ | 9.04 | 5.3 | 11.5 | 13.9 | 9.7 | 7.6 |
| 47 | $\text{H}_3\text{COCHN}-\overset{\text{COOH}}{\text{C}}\text{HCH}_2\text{S}-\text{H}$ | 8.55 | 5.7 | 9.5 | 13.8 | 8.9 | 8.4 |
| 48 | $\text{H}_2\text{N}-\text{CH}_2\text{CH}_2\text{S}-\text{H}$ | 10.53 | 15.2 | 12.8 | 14.8 | 10.1 | 8.5 |
| 49 | $\text{HSC}(\text{CH}_2\text{OH})\text{CH}_2\text{S}-\text{H}$ | 10.57 | 14.3 | 12.0 | 13.4 | 9.1 | 7.7 |
| 50 | $\text{H}_3\text{CH}_2\text{C}-\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{C}}}\text{S}-\text{H}$ | 11.22 | 8.7 | 13.8 | 15.8 | 12.0 | 10.7 |
| 51 | $\text{HS}-(\text{CH}_2)_2\text{S}-\text{H}$ | 9.05 | 14.2 | 12.3 | 14.5 | 9.2 | 8.9 |
| 52 |  | 8.82 | 5.4 | 10.8 | 14.0 | 9.3 | 6.8 |
| 53 |  | 10.69 | 6.0 | 13.4 | 15.9 | 12.7 | 10.0 |
| 54 |  | 6.39 | 5.1 | 8.3 | 11.5 | 6.6 | 5.9 |
| 55 | $\text{HO}-(\text{CH}_2)_4\text{S}-\text{H}$ | 10.19 | 6.6 | 12.2 | 15.5 | 10.7 | 9.8 |
| 56 | $\text{H}_3\text{COCCH}_2\text{CH}_2\text{S}-\text{H}$ | 9.33 | 6.4 | 11.6 | 14.7 | 10.8 | 8.5 |
| 57 | $\text{HS}-(\text{CH}_2)_4\text{S}-\text{H}$ | 9.88 | 5.6 | 13.5 | 15.1 | 10.3 | 8.4 |
| 58 | $\text{HSH}_2\text{CH}_2\text{CHNCO}\overset{\text{O}}{\parallel}\text{NHCH}_2\text{CH}_2\text{S}-\text{H}$ | 9.26 | 6.5 | 13.1 | 13.6 | 8.9 | 9.3 |

Table S3 The pK_a 's and molecular $V_{S,\min}$ (kcal/mol) of fluoromethyl and fluoroethyl thiol.

| R | Entry | thiols | pK_a | $V_{S,\min}$ (kcal/mol) |
|--------------|-------|---------------------------------------|--------|-------------------------|
| fluoromethyl | 1 | HS-CH ₂ F | 8.8 | -31.50 |
| | 2 | HS-CHF ₂ | 3.1 | -23.57 |
| | 3 | HS-CF ₃ | -0.8 | -12.65 |
| fluoroethyl | 4 | HS-CH ₂ CH ₂ F | 10.9 | -40.19 |
| | 5 | HS-CHF-CH ₃ | 8.9 | -33.20 |
| | 6 | HS-CH ₂ CHF ₂ | 9.9 | -34.41 |
| | 7 | HS-CHF-CH ₂ F | 6.6 | -27.48 |
| | 8 | HS-CF ₂ -CH ₃ | 4.8 | -21.72 |
| | 9 | HS-CH ₂ CF ₃ | 7.6 | -21.85 |
| | 10 | HS-CF ₂ -CH ₂ F | 1.3 | -20.69 |
| | 11 | HS-CHF-CF ₃ | 3.7 | -22.20 |
| | 12 | HS-CF ₂ -CHF ₂ | 0.3 | -17.03 |
| | 13 | HS-CF ₂ CF ₃ | -1.1 | -10.60 |