Supporting Information for

Enhanced Scale Inhibition against $Ca_3(PO_4)_2$ and Fe_2O_3 in Water Using Multi-Functional Fluorescent-Tagged Antibacterial Scale Inhibitors

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Summary

Text S1. Synthetic method of FM-AA-APEO.

After certain amounts of AA, APEO and FM (degree of polymerization: 10) with designed ratios was dissolved in 90 mL of water, the solution was kept at 70 ^{o}C under magnetic stirring and nitrogen condition for 30 min. Subsequently, initiator solution (0.3 g of ammonium persulfate dissolved in 15 mL of water) was added dropwise over a period of 1 h. The reaction mixture was heated to 80 ^{o}C and maintained at this temperature for a further 2 h. Solid scale inhibitor product was finally obtained after precipitation using excessive acetone, washing with ethanol, and vacuum drying at 45 ^{o}C for 24 h.

Text S2. Calculation methods of *X* and *Y* in AA-APEO-*X* and FM-AA-APEO-*Y*.

(1) For 1 mol of APEO repeated unit in AA-APEO-*X*, there were *X* mol of AA repeated units. Hence, mass of C and H atoms could be expressed as follows:

$M_{(C\ atoms)} = (3X+23)\ mol \times 12\ g/mol = (36X+276)\ g$;

$M_{(H\ atoms)} = (4X+46)\ mol \times 1\ g/mol = (4X+46)\ g$.

Therefore, $M_{(C\ atoms)}/M_{(H\ atoms)}$ equaled $(36X+276)/(4X+46)$, where the mass ratio of C and H was obtained from elemental analysis.

(2) Performance results of AA-APEO in Section 3.1 showed that the optimized molar ratio of AA:APEO was 8:1 in AA-APEO. Thus, the ratio of AA:APEO of 8:1 was further used in the trinary copolymers (FM-AA-APEO). For *Y* mol of FM repeated unit in FM-AA-APEO-*Y*, there were $[8\times(1-Y)/9]$ mol of AA and $(1-Y)/9$ mol of APEO units, respectively. Hence, mass of C and N atoms can be expressed as follows:

$M_{(C\ atoms)} = [3\times8\times(1-Y)/9+23\times(1-Y)/9+22Y]\times12\ g/mol=(188+604Y)/3\ g$;

$M_{(N\ atoms)} = 3\times Y\ mol \times 14\ g/mol = 42Y\ g$;

Therefore, $M_{(N\ atoms)}/M_{(C\ atoms)}$ equaled $63Y/(94+302Y)$, where the mass ratio of N and C is obtained from elemental analysis.

Text S3. Methodologies and results of structural characterization of scale inhibitors.

FTIR spectra were recorded on a Bruker Tensor 27 IR spectrometer system using samples pelletized with KBr. ^{1}H NMR spectra were recorded on a Bruker model AVANCE400 NMR spectrometer using D_2O as the solvent. UV-vis spectra were recorded on a Hitachi UH-5300 UV-vis spectrophotometer. Elemental analysis was conducted on a Vario EL III elemental analyzer. Thermogravimetric (TG) analysis was performed on a Diamond DMA spectrometer.

The FTIR spectra were shown in SI Figure S2a. Peaks at 1730 and 1107 cm^{-1} indicated C=O and C-O in FP-AA-APEO, respectively. Besides, characteristic peaks of FM monomers at 787 and 1398 cm^{-1} (C-N in N-methyl piperazine) remained slight peaks in the final FM-AA-APEO. ^{1}H NMR spectra in SI Figure S2b confirmed that the main structure of the designed inhibitor FM-AA-APEO was found. UV spectra in SI Figure S2c demonstrated that, the final FM-AA-APEO owned the main adsorption peak at 388 nm due to the existence of FM groups, while AA-APEO08 did not. TG curves in SI Figure S4d showed that, FM-AA-APEO-1.56% had better thermal stability than AA-APEO-8 without the fluorescent groups.

Table S1. Coded levels for two variables of fluorescent intensity response in binary-solute solutions containing FM-AA-APEO and calcium ions in RSM analysis.

Factors	Range and Levels				
	-2	-1	0	1	2
X_1: Ca^{2+} (mg/L)	200	400	600	800	1000
X_2: Dosage (mg/L)	2	4	6	8	10

Table S2. Coded levels for two variables of fluorescent intensity response in binary-solute solutions containing FM-AA-APEO and ferric ions in RSM analysis.

Factors	Range and Levels				
	-2	-1	0	1	2
X_1: Fe^{3+} (mg/L)	5	10	15	20	25
X_2: Dosage (mg/L)	2	10	18	26	34

Table S3. RSM experimental design and results for fluorescent intensity response in binary-solute solutions containing FM-AA-APEO and calcium ions.

	Ca^{2+} concentration [a]	Dosage [a]	Experimental value	Predicted value
1	2 (1000)	-2 (2)	138.6	158.44
2	-2 (200)	2 (10)	1310	1294.16
3	-1 (400)	0 (6)	731.9	747.73
4	1 (800)	1 (8)	962.6	958.09
5	0 (600)	0 (6)	711.8	726.14
6	0 (600)	1 (8)	978.7	988.56
7	2 (1000)	0 (6)	668.0	656.2
8	0 (600)	-2 (2)	232.9	228.54
9	1 (800)	-1 (4)	465.1	442.25
10	1 (800)	0 (6)	688.3	695.63
11	0 (600)	2 (10)	1247	1260.06
12	0 (600)	-1 (4)	484.2	472.8
13	-2 (200)	-2 (2)	260.7	262.96
14	-1 (400)	1 (8)	1020	1010.11
15	2 (1000)	2 (10)	1192	1190.28
16	-1 (400)	-1 (4)	509.1	494.43
17	-2 (200)	0 (6)	746.1	760.4

[a] Values outside and inside brackets are encoded and actual (unit for dosage and Ca^{2+} concentration: mg/L) values, respectively.

Table S4. RSM experimental design and results for fluorescent intensity response in binary-solute solutions containing FM-AA-APEO and ferric ions.

	Fe^{3+} [a]	Dosage [a]	Experimental value	Predicted value
1	-2 (5)	2 (34)	3177.31	3008.88
2	2 (25)	-2 (2)	24.14	198.8
3	0 (15)	-1 (10)	973.30	996.64
4	1 (20)	1 (26)	2335.90	2532.24
5	0 (15)	0 (18)	1889.62	1822.88
6	1 (20)	0 (18)	1851.40	1878.4
7	0 (615)	2 (34)	3016.79	2998.48
8	-2 (5)	0 (18)	1930.96	1779.52
9	-1 (10)	1 (26)	2603.21	2470.64
10	0 (15)	1 (26)	2424.37	2490.16
11	2 (25)	0 (18)	1801.89	1956.48
12	-1 (10)	0 (18)	1920.68	1789.92
13	-2 (5)	-2 (2)	81.07	-85.68
14	1 (20)	-1 (10)	912.30	1065.6
15	2 (25)	2 (34)	2928.48	3078.32
16	-1 (10)	-1 (10)	1033.25	950.24
17	0 (15)	-2 (2)	38.28	11.44

[a] Values outside and inside brackets are encoded and actual (unit for Fe^{2+} concentration and dosage: mg/L) values, respectively.

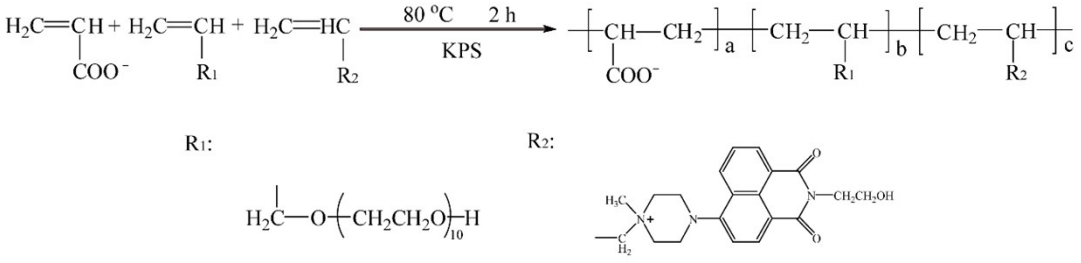

Fig. S1. Synthetic route of scale inhibitor FM-AA-APEO.

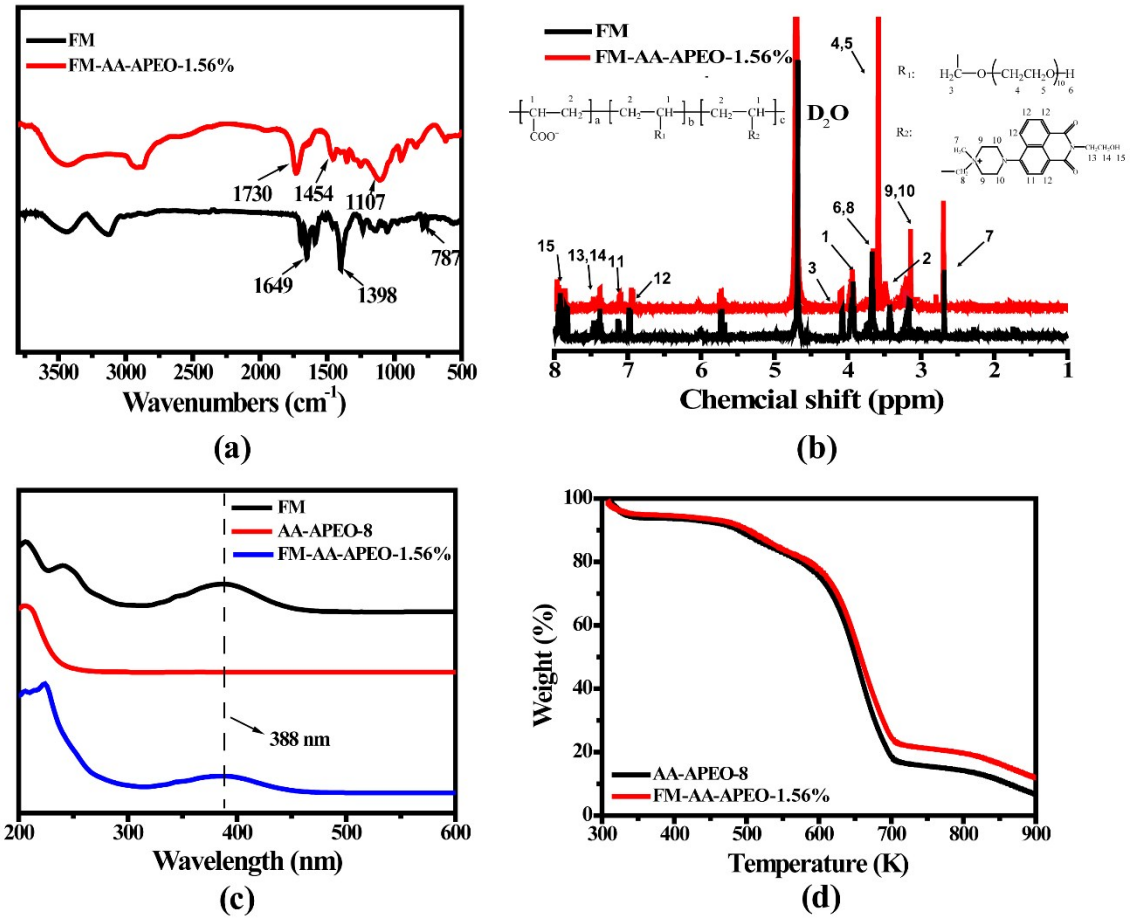

Fig. S2. (a) FTIR, (b) ^{1}H NMR, (c) UV-vis spectra and (d) TG curves of different samples.

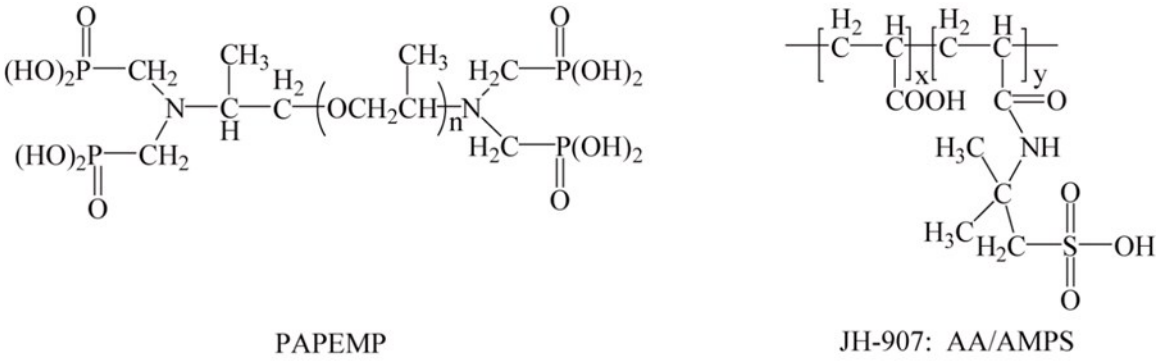

Fig. S3. Chemical structure of two commercial scale inhibitors (PAPEMP and JH-907).

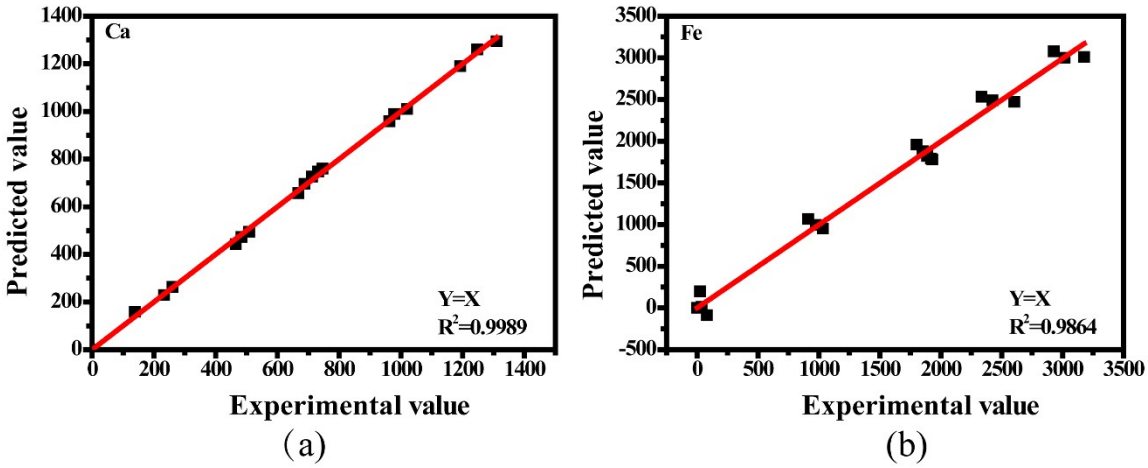

Fig. S4. Comparison between experimental and predicted values from RSM regression equations.

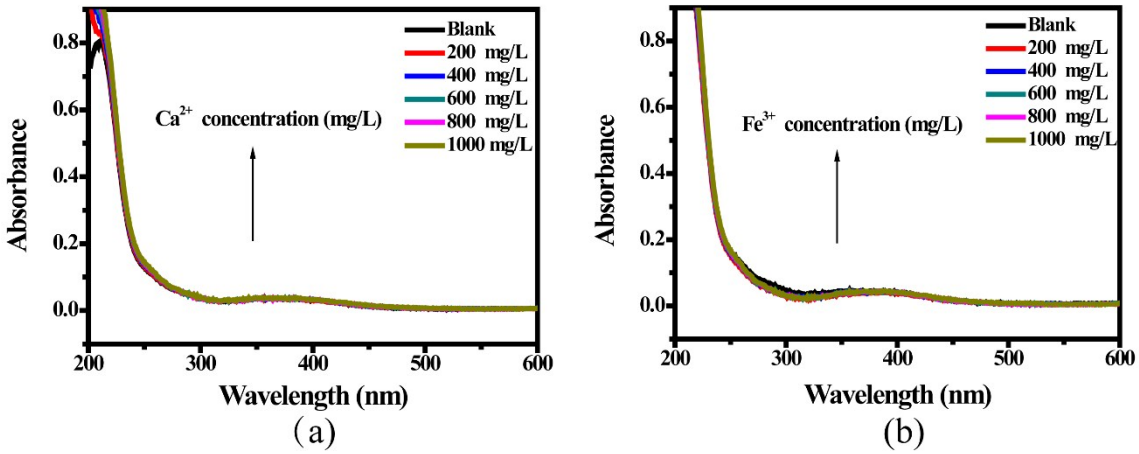

Fig. S5. UV spectra of AA-APEO-1.56% solution with the coexistence of different concentrations of (a) Ca^{2+} and (b) Fe^{3+}.

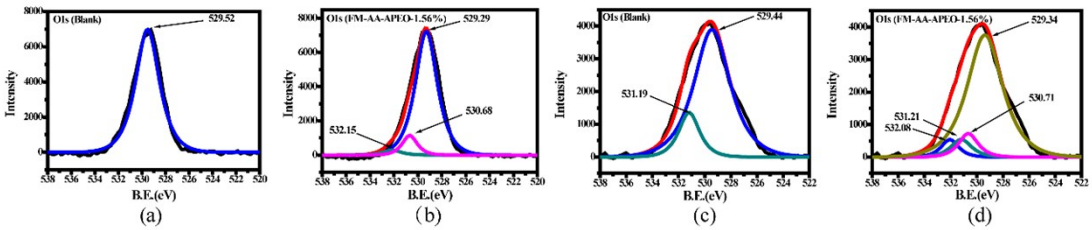

Fig. S6. O1s XPS spectra of (a and b) $Ca_3(PO_4)_2$ and (c and d) Fe_2O_3 precipitates (a and c) without and (b and d) with the coexistence of FM-AA-APEO.