

Supplementary Information for

Design of Bio-based Organic Phase Change Materials Containing “Safety Valve”

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AE of the Benzoxazine Syntheses.

1. C-fa-4

$$\text{AE (\%)} = [\text{MM}_{\text{C-fa-4}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{\text{Butylamine}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 401.68 \text{ g}\cdot\text{mol}^{-1} \\ / [304.52 \text{ g}\cdot\text{mol}^{-1} + 73.14 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 85.8 \%$$

2. C-fa-8

$$\text{AE (\%)} = [\text{MM}_{\text{C-fa-8}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{\text{Octylamine}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 457.79 \text{ g}\cdot\text{mol}^{-1} \\ / [304.52 \text{ g}\cdot\text{mol}^{-1} + 129.25 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 87.4 \%$$

3. C-fa-12

$$\text{AE (\%)} = [\text{MM}_{\text{C-fa-12}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{\text{Dodecylamine}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 513.90 \text{ g}\cdot\text{mol}^{-1} \\ / [304.52 \text{ g}\cdot\text{mol}^{-1} + 185.36 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 88.6 \%$$

4. C-aa-4

$$\text{AE (\%)} = [\text{MM}_{\text{C-aa-4}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{\gamma\text{-aminobutyric acid}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 431.66 \\ \text{ g}\cdot\text{mol}^{-1} / [304.52 \text{ g}\cdot\text{mol}^{-1} + 103.12 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 86.7 \%$$

5. C-aa-8

$$\text{AE (\%)} = [\text{MM}_{\text{C-aa-8}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{8\text{-aminooctanoic acid}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 431.66 \\ \text{ g}\cdot\text{mol}^{-1} / [304.52 \text{ g}\cdot\text{mol}^{-1} + 159.23 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 88.1 \%$$

6. C-aa-12

$$\text{AE (\%)} = [\text{MM}_{\text{C-aa-12}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{12\text{-aminolauric acid}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = 487.77 \\ \text{ g}\cdot\text{mol}^{-1} / [304.52 \text{ g}\cdot\text{mol}^{-1} + 215.34 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 89.2 \%$$

7. C-ae-4

$$\text{AE (\%)} = [\text{MM}_{\text{C-ae-4}} / [\text{MM}_{\text{Cardanol}} + \text{MM}_{4\text{-aminobutyric acid methyl ester}} + 3(\text{MM}_{\text{pf}})] \times 100 \% = \\ 487.77 \text{ g}\cdot\text{mol}^{-1} / [304.52 \text{ g}\cdot\text{mol}^{-1} + 117.15 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})] \times 100 \% = 87.1 \%$$

8. C-ae-8

$$\text{AE (\%)} = \frac{[\text{MM}_{\text{C-ae-8}}]}{[\text{MM}_{\text{Cardanol}} + \text{MM}_{8\text{-Aame}} + 3(\text{MM}_{\text{pf}})]} \times 100 \% = 487.77 \text{ g}\cdot\text{mol}^{-1} \\ \frac{1}{[304.52 \text{ g}\cdot\text{mol}^{-1} + 173.26 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})} \times 100 \% = 88.3 \%$$

9. C-ae-12

$$\text{AE (\%)} = \frac{[\text{MM}_{\text{C-ae-12}}]}{[\text{MM}_{\text{Cardanol}} + \text{MM}_{12\text{-Aame}} + 3(\text{MM}_{\text{pf}})]} \times 100 \% = 487.77 \text{ g}\cdot\text{mol}^{-1} \\ \frac{1}{[304.52 \text{ g}\cdot\text{mol}^{-1} + 229.36 \text{ g}\cdot\text{mol}^{-1}] + 3(30 \text{ g}\cdot\text{mol}^{-1})} \times 100 \% = 89.4 \%$$

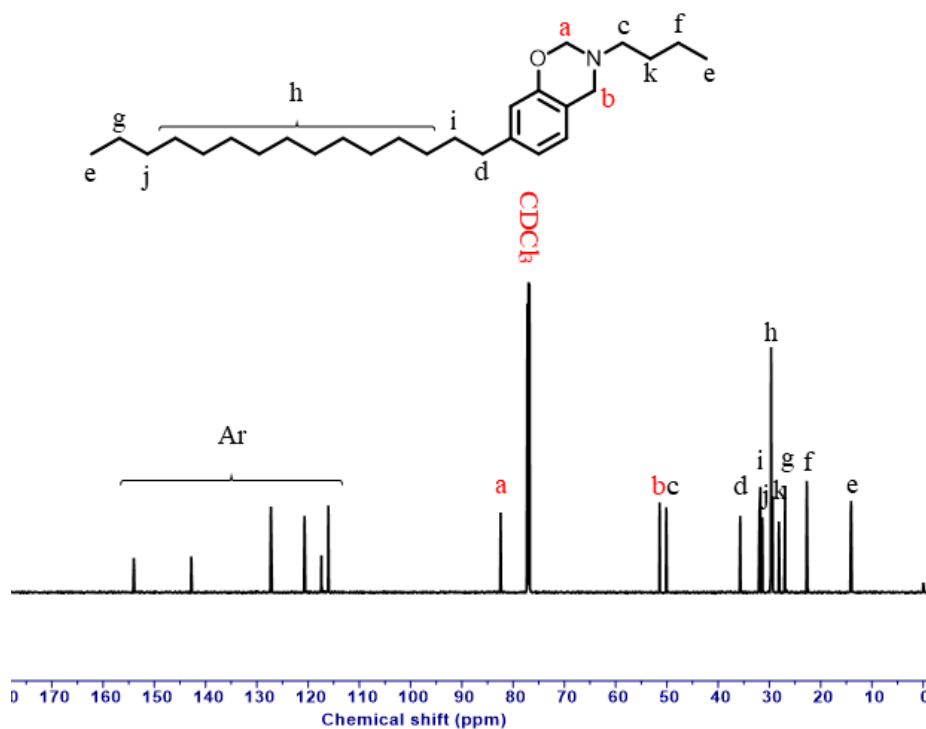


Figure S1. ¹³C NMR spectra of C-fa-4.

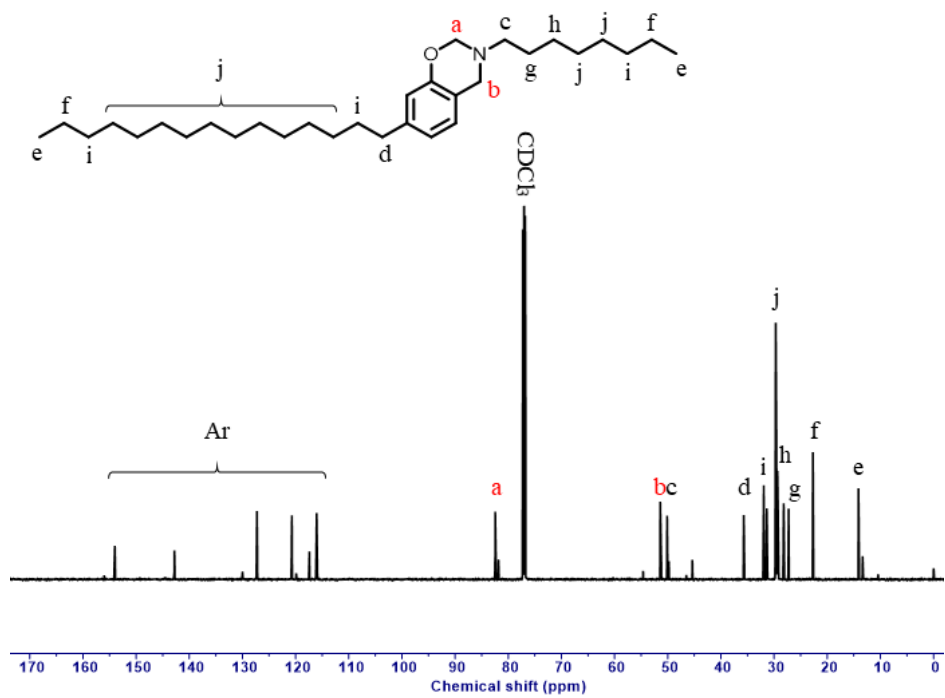


Figure S2. ^{13}C NMR spectra of C-fa-8.

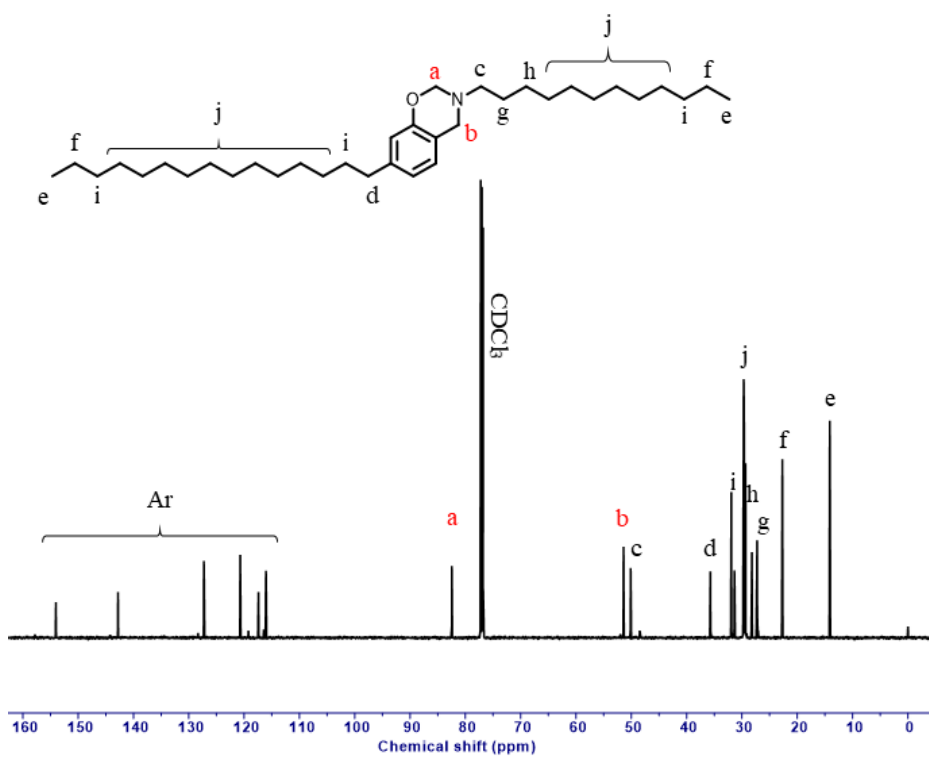


Figure S3. ^{13}C NMR spectra of C-fa-12.

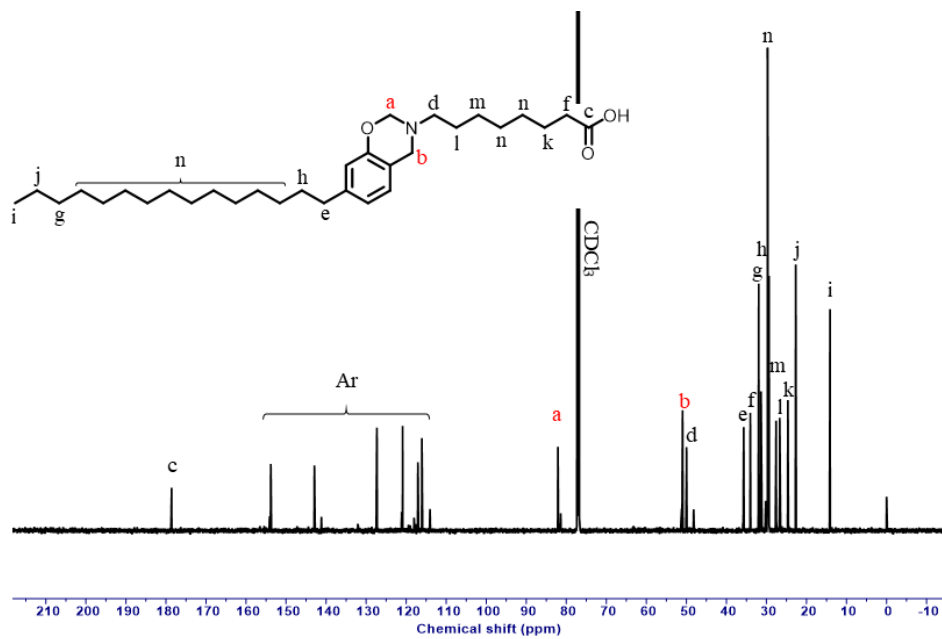


Figure S4. ^{13}C NMR spectra of C-aa-4.

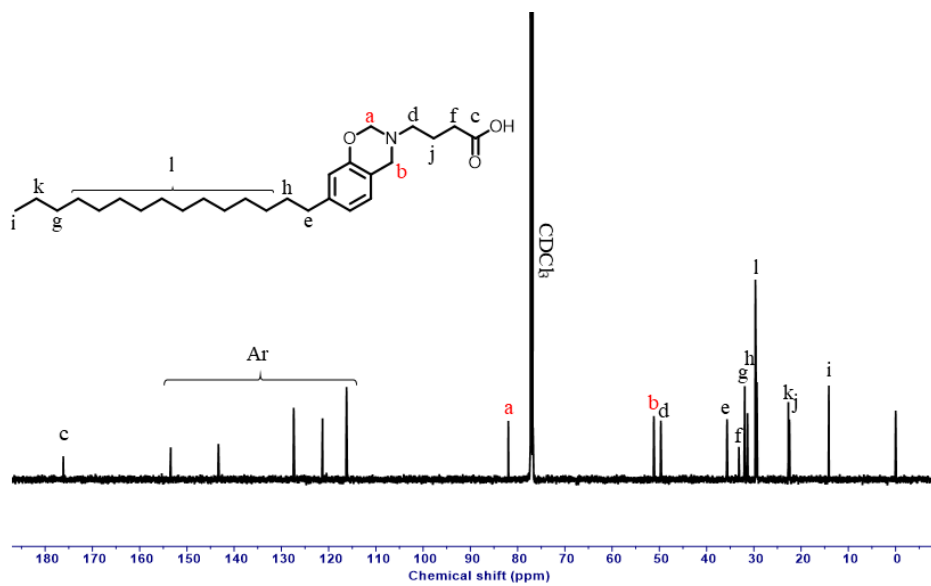


Figure S5. ^{13}C NMR spectra of C-aa-8.

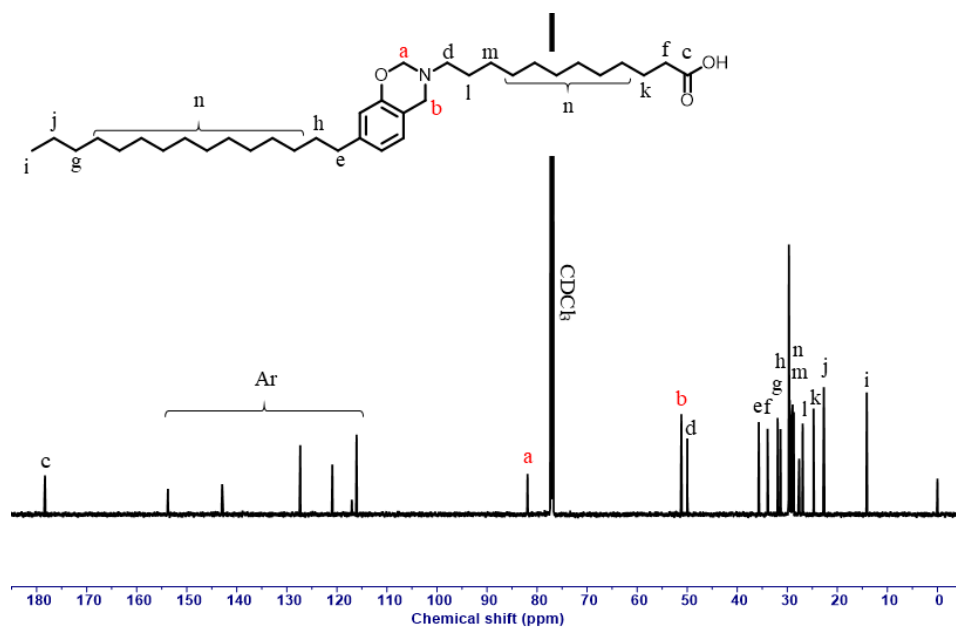


Figure S6. ^{13}C NMR spectra of C-aa-12.

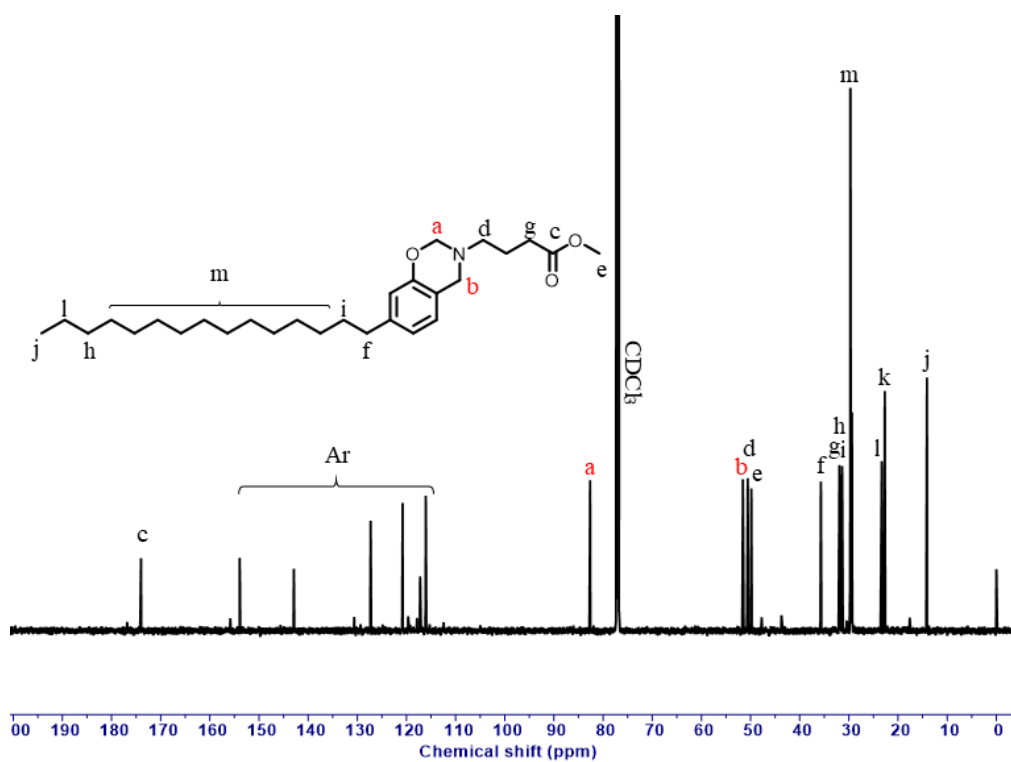


Figure S7. ^{13}C NMR spectra of C-ae-4.

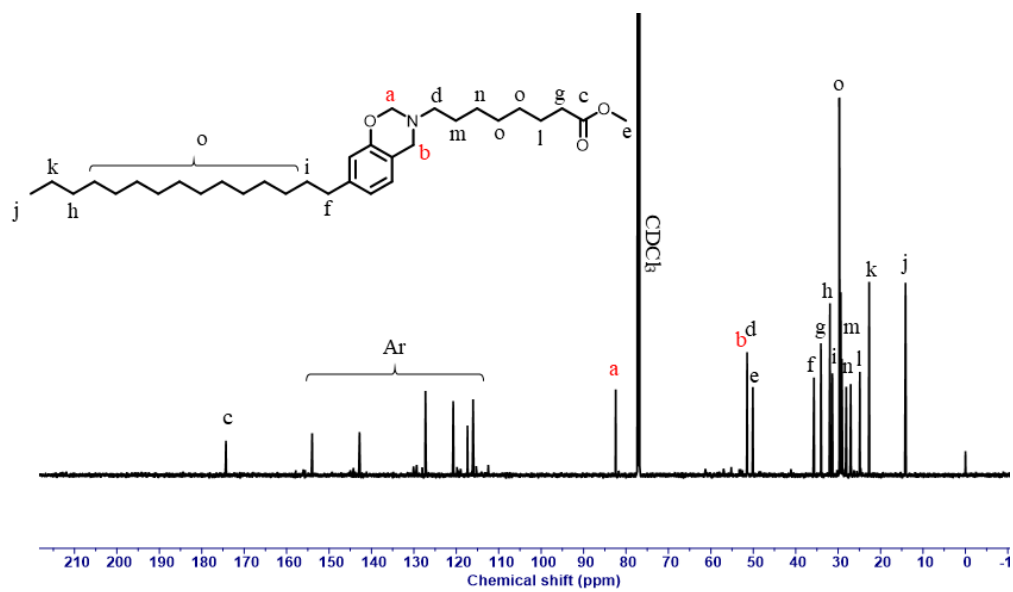


Figure S8. ^{13}C NMR spectra of C-ae-8.

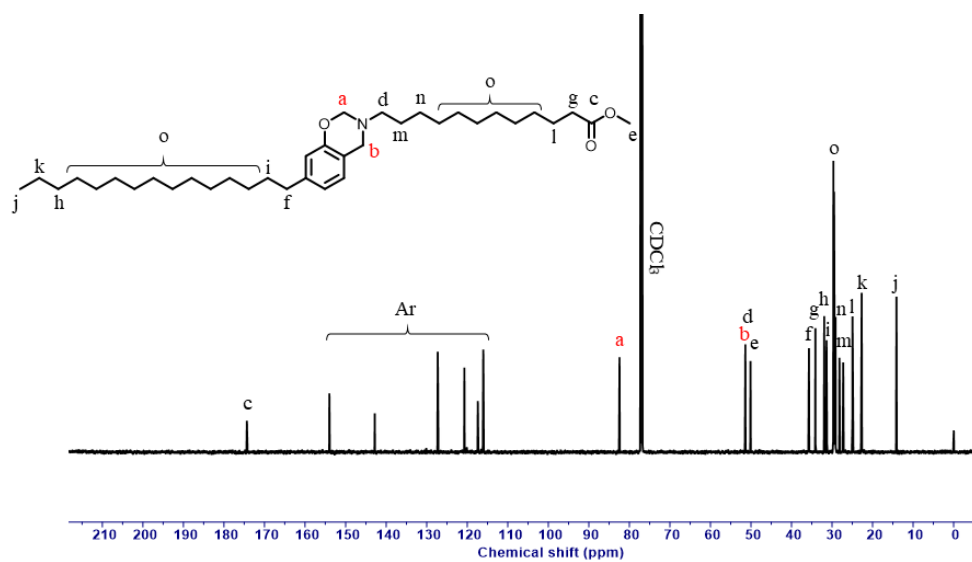


Figure S9. ^{13}C NMR spectra of C-ae-12.

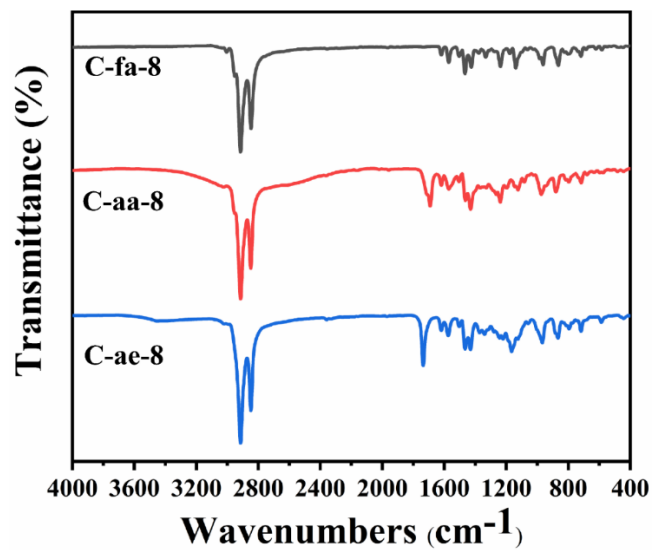


Figure S10. FT-IR curves of C-fa-8, C-aa-8, C-ae-8.

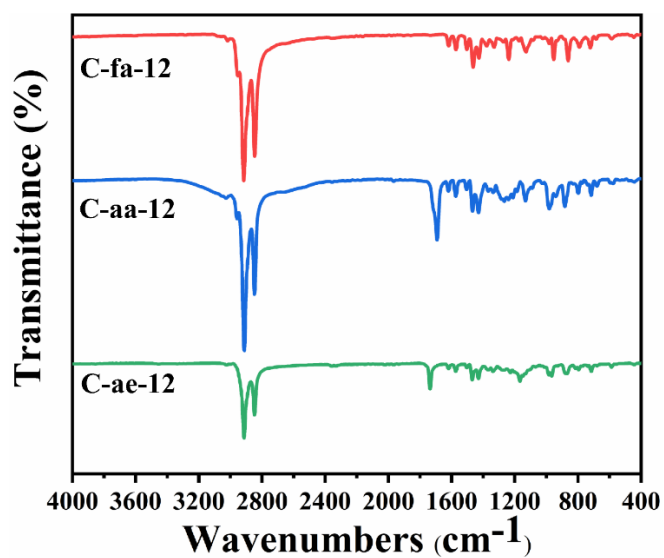


Figure S11. FT-IR results of C-fa-12, C-aa-12, C-ae-12.

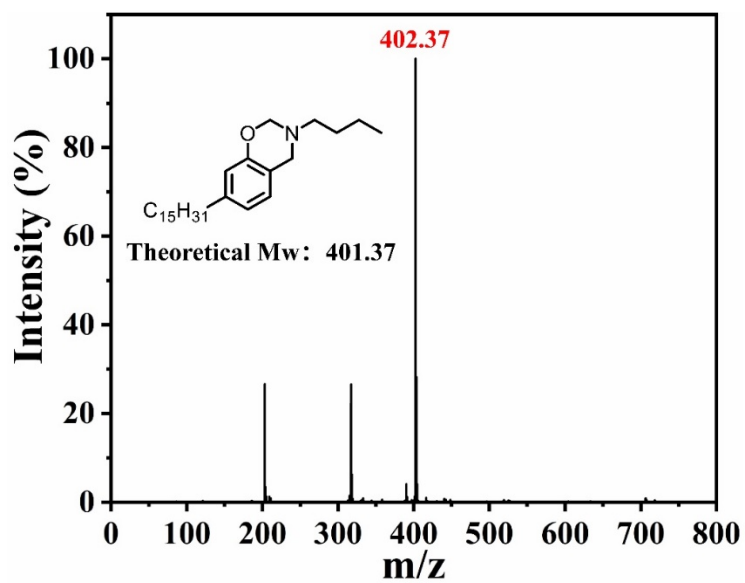


Figure S12. HRMS spectra of C-fa-4.

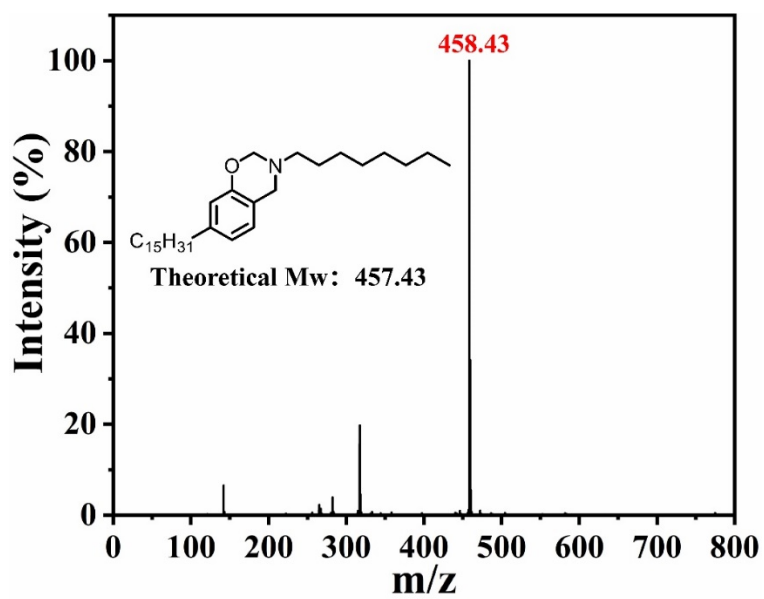


Figure S13. HRMS results of C-fa-8.

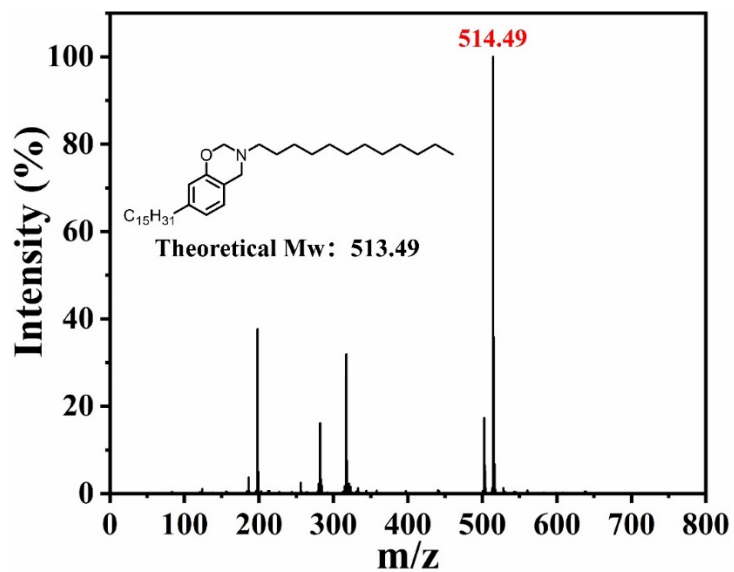


Figure S14. HRMS spectra of C-fa-12.

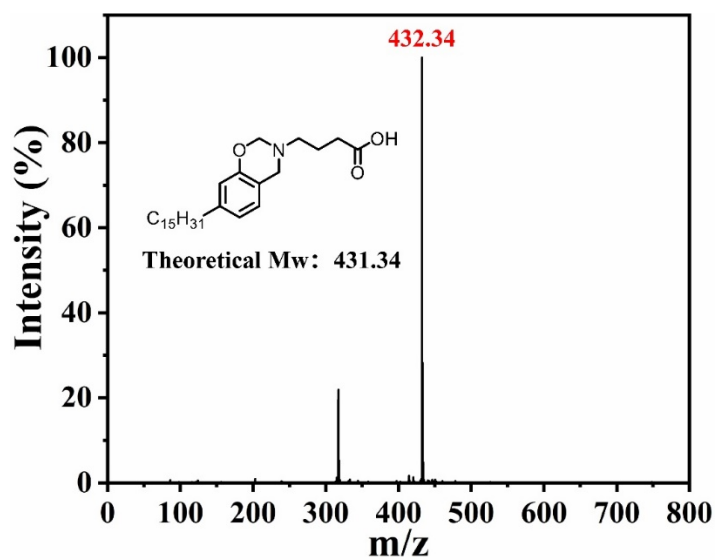


Figure S15. HRMS results of C-aa-4.

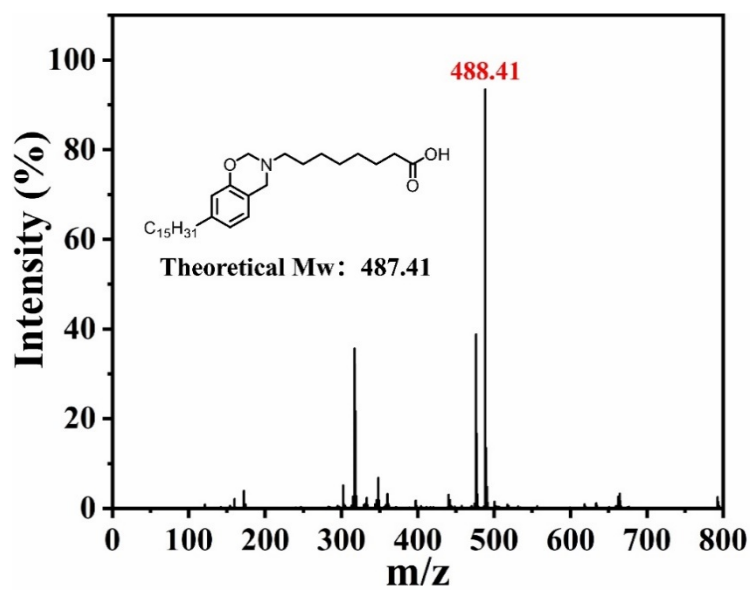


Figure S16. HRMS spectra of C-aa-8.

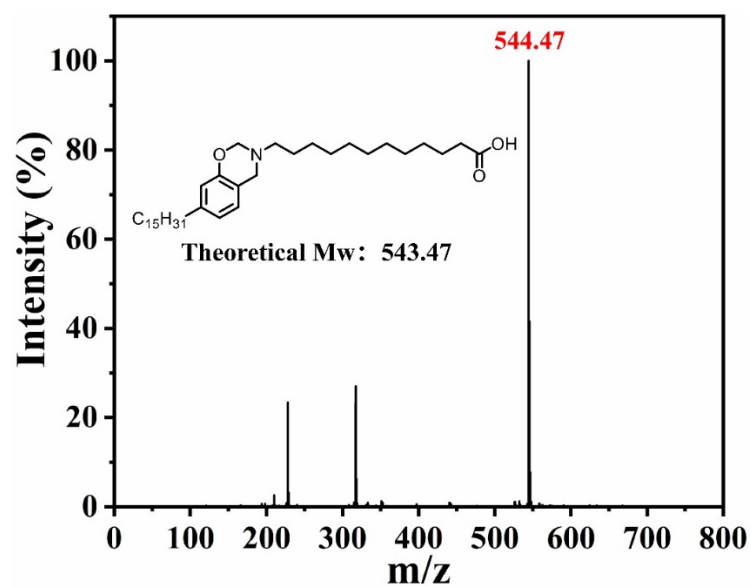


Figure S17. HRMS results of C-aa-12.

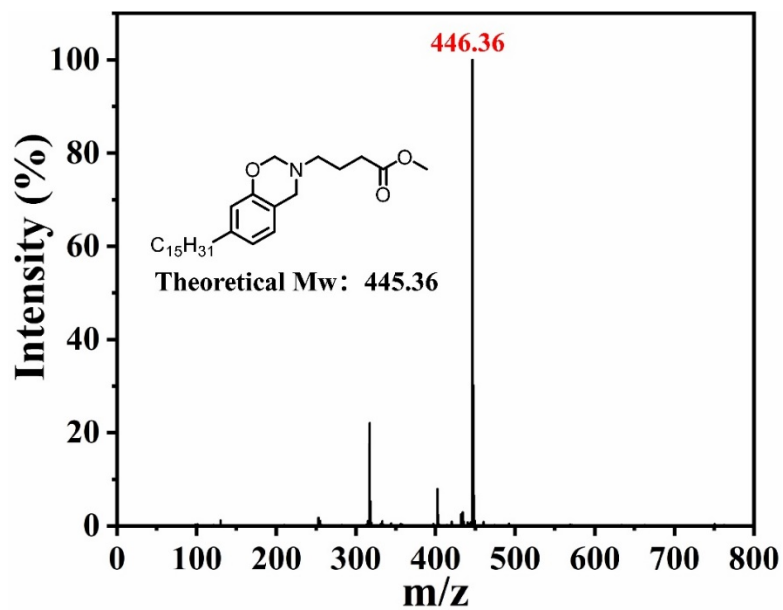


Figure S18. HRMS spectra of C-ae-4.

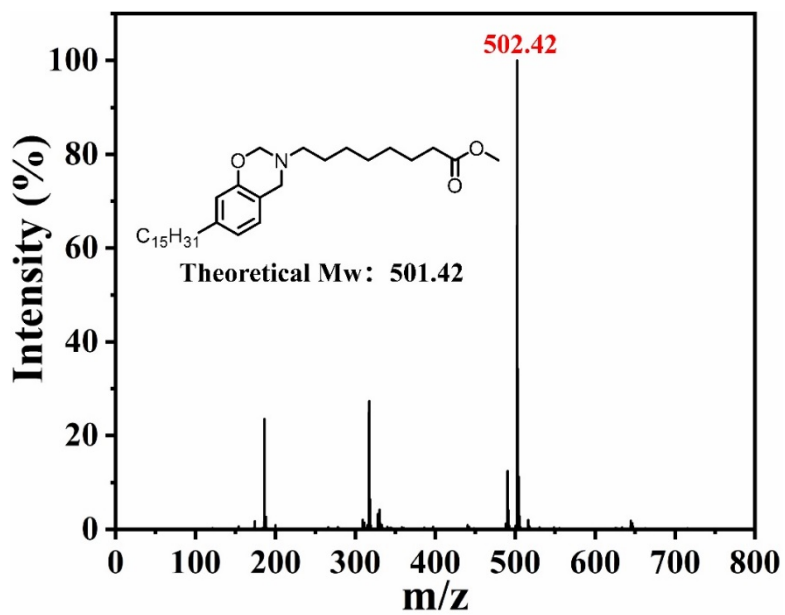


Figure S19. HRMS results of C-ae-8.

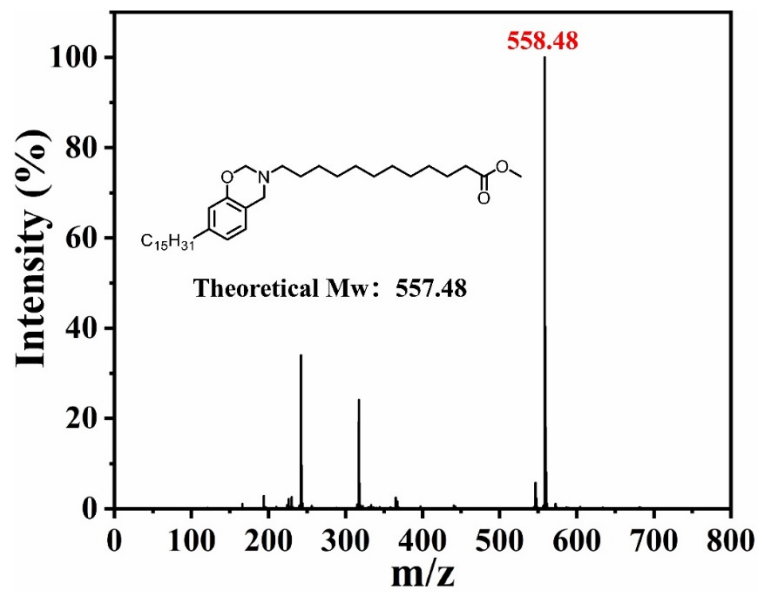


Figure S20. HRMS spectra of C-ae-12.

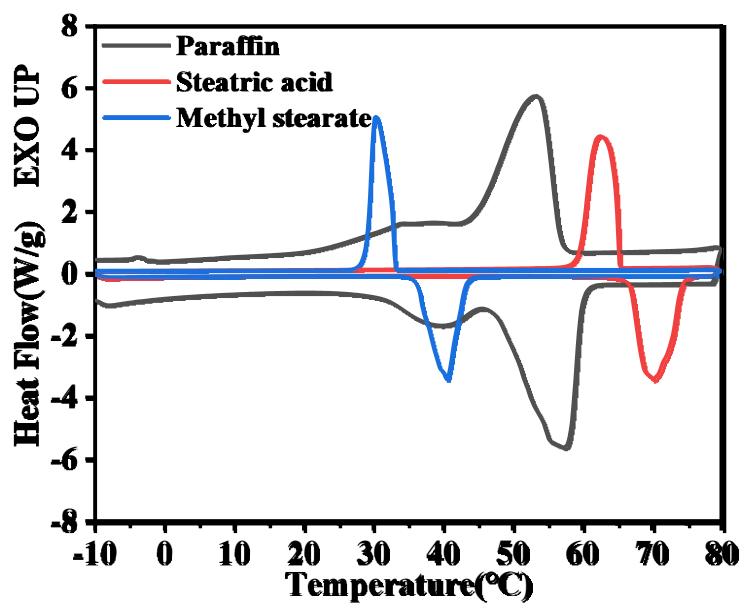


Figure S21. DSC curves of commercial PCM (paraffin, stearic acid, methyl stearate).

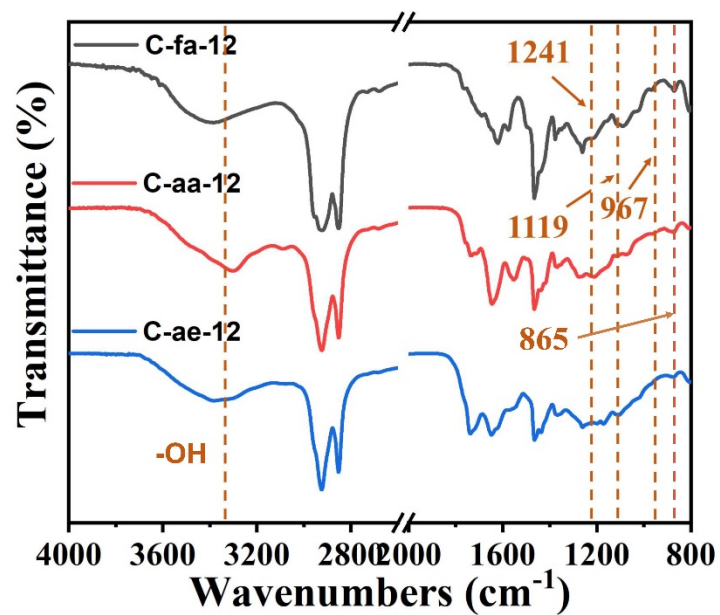


Figure S22. FT-IR spectra of cured C-fa-12, C-aa-12 and C-ae-12.

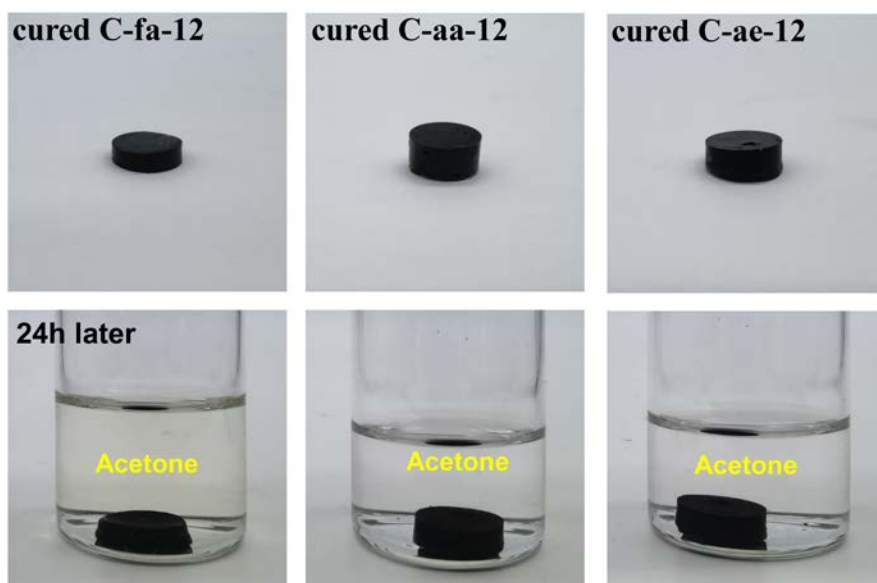


Figure S23. Digital photos of cured samples before and after acetone immersion.

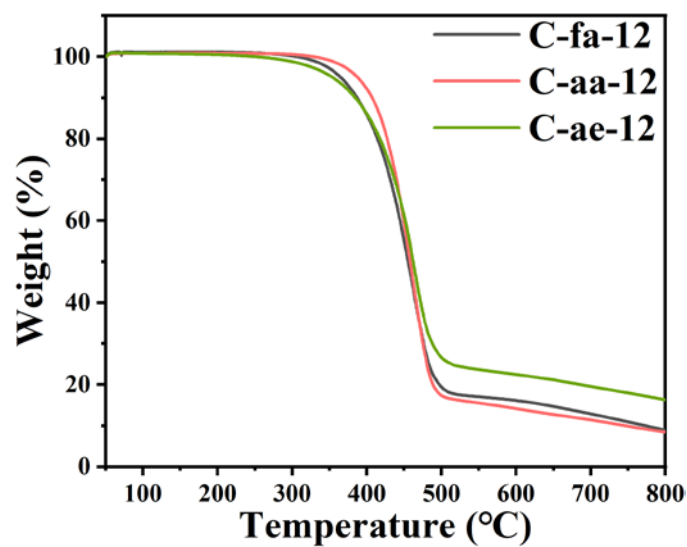


Figure S24. TGA curves of cured C-fa-12, C-aa-12 and C-ae-12.

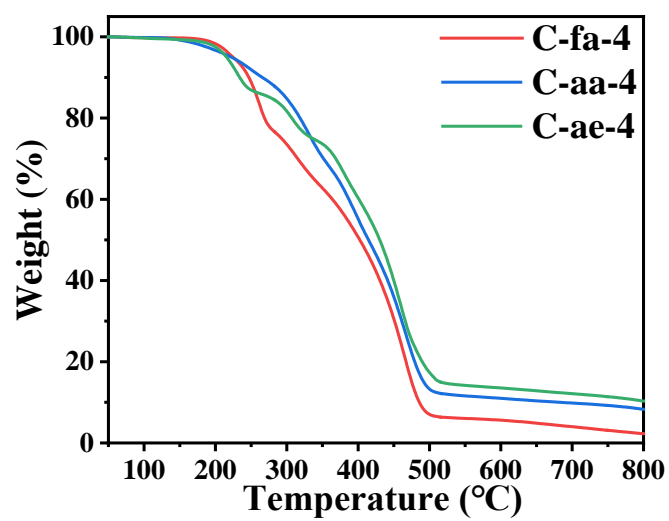


Figure S25. TGA curves of different groups of the same carbon chain (4C).

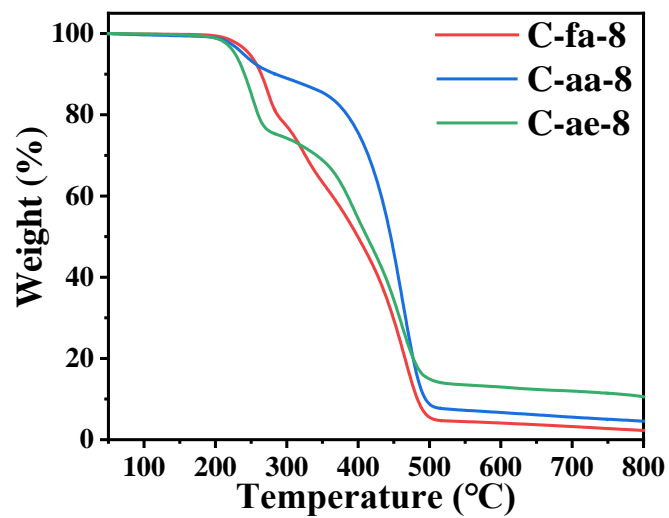


Figure S26. TGA curves of different groups of the same carbon chain (8C).

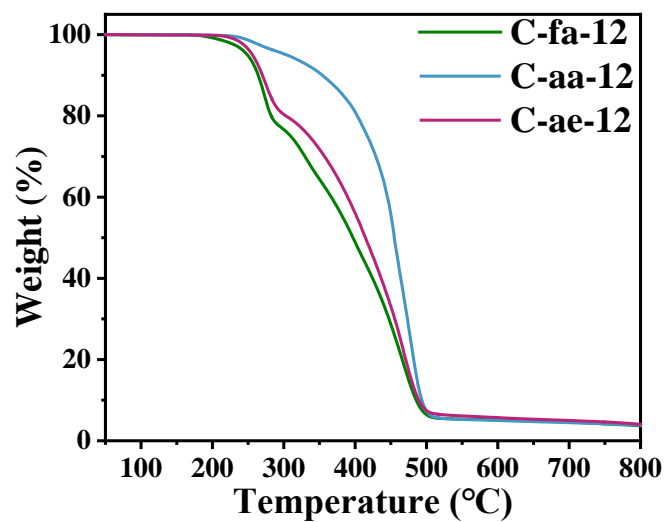


Figure S27. TGA curves of different groups of the same carbon chain (12C).

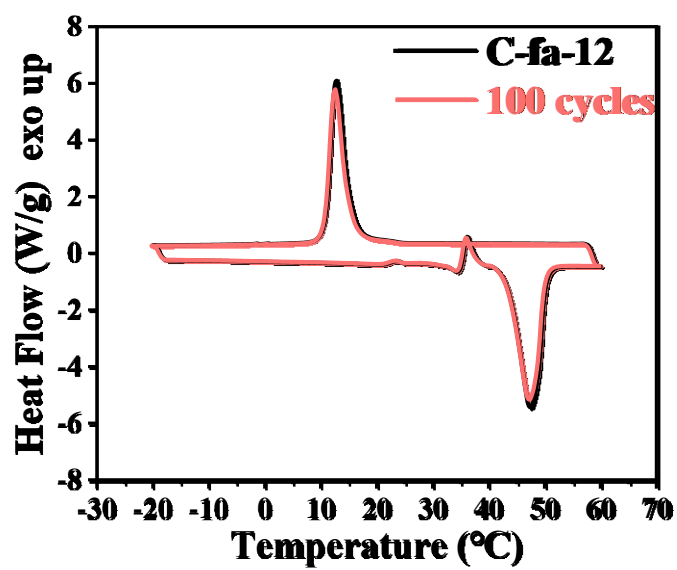


Figure S28. DSC curves of C-fa-12 before and after cycle-used 100 times.

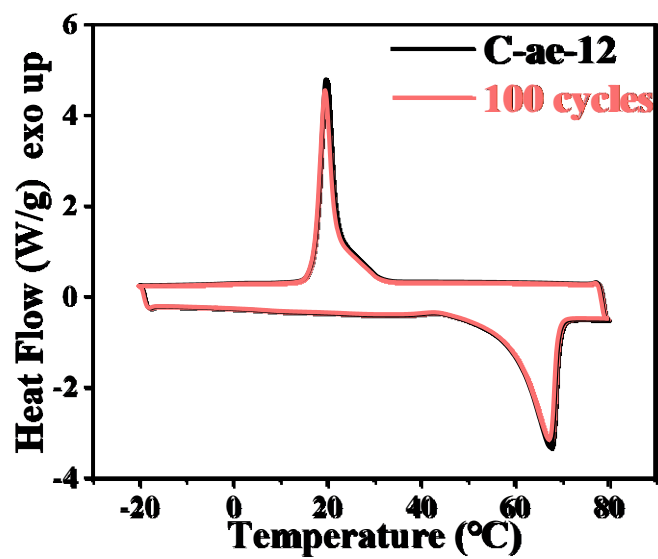


Figure S29. DSC curves of C-ae-12 before and after cycle-used 100 times.

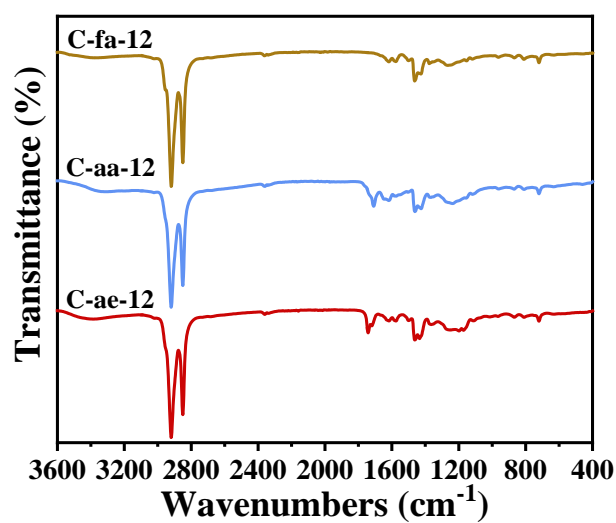


Figure S30. FT-IR spectra of the as-synthesized after ignition test.

Table S1 Samples curing temperature and evaporation before curing.

Samples	Curing temperature (°C)	Evaporation before curing (%)
C-fa-4	252	11
C-fa-8	257	9
C-fa-12	265	8
C-aa-4	173	2
C-aa-8	194	1
C-aa-12	224	1
C-ae-4	209	4
C-aa-8	219	3
C-aa-12	250	4