

**Waste PET Chemical Processing to Terephthalic Amides and their Effect on Asphalt
Performance**

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27 total figures (though some have a and b, so the number is 16)

No tables

13 pages

NMR spectra: the chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from tetramethylsilane, which was used as an internal standard, and coupling constants are reported in Hertz (Hz). Samples were prepared in deuterated dimethyl sulfoxide ($(CD_3)_2SO$) or deuterated chloroform ($CDCl_3$).

Additive 1

1H NMR (500 MHz, $(CD_3)_2SO$) δ 8.54 (t, 2H, $J = 5.5$ Hz), 7.92 (s, 4H), 4.73 (t, 2H, $J = 5.5$ Hz), 3.52 (q, 4H, $J = 6.0$ Hz), 3.33 (q, 4H, $J = 6.0$ Hz). ^{13}C NMR (126 MHz, $(CD_3)_2SO$) δ 165.6, 136.6, 127.1, 59.7, 42.2.

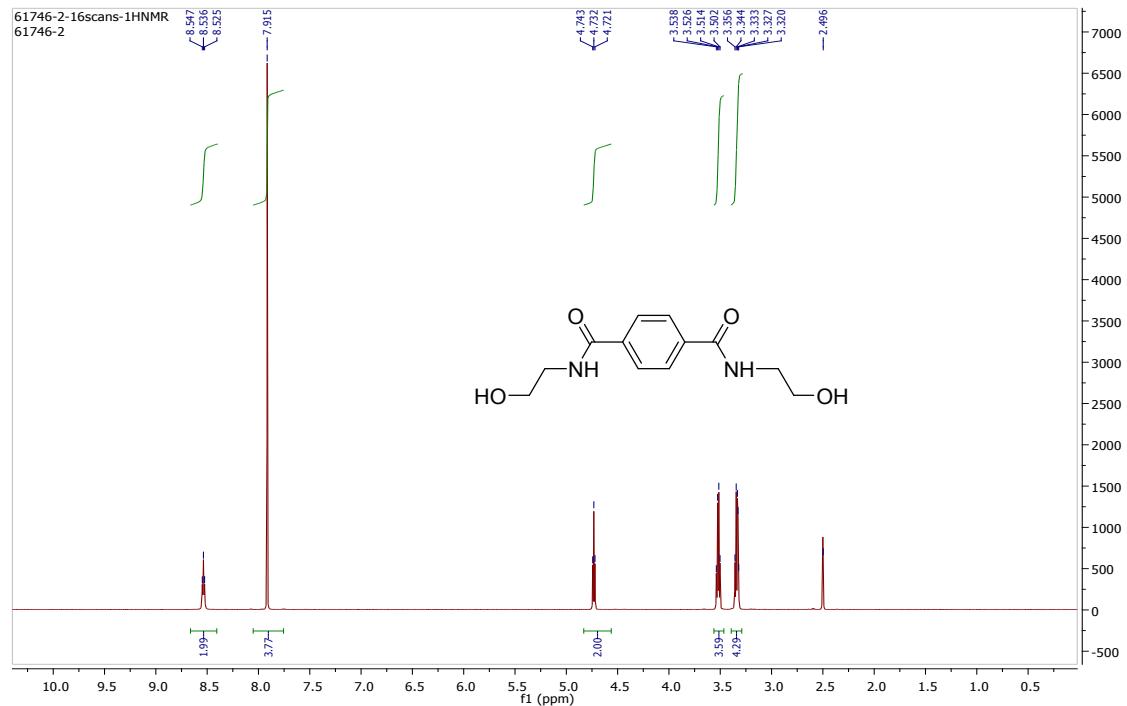


Figure S1a: 1H NMR for Additive 1

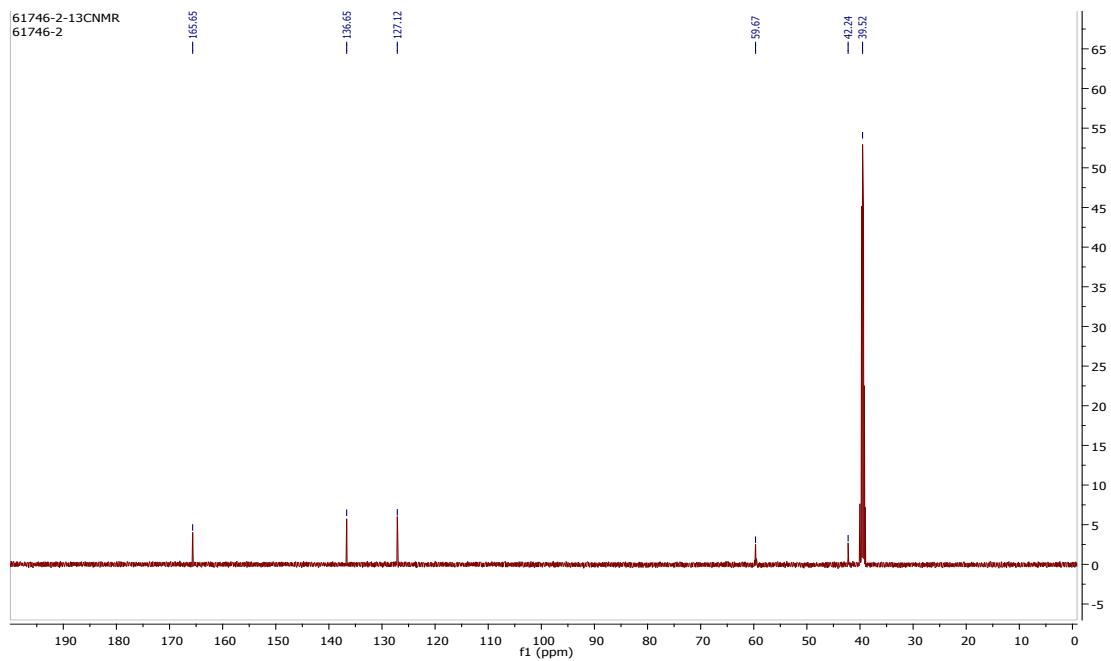


Figure S1b: ^{13}C NMR for Additive 1

Additive 2

^1H NMR (500 MHz, ((CD₃)₂SO) δ 8.54 (t, 2H, J = 5.5 Hz), 7.92 (s, 4H), 4.73 (t, 2H, J = 5.5 Hz), 3.52 (q, 4H, J = 6.0 Hz), 3.34 (q, 4H, J = 6.0 Hz). ^{13}C NMR (126 MHz, (CD₃)₂SO) δ 165.7, 136.7, 127.1, 59.7, 42.2.

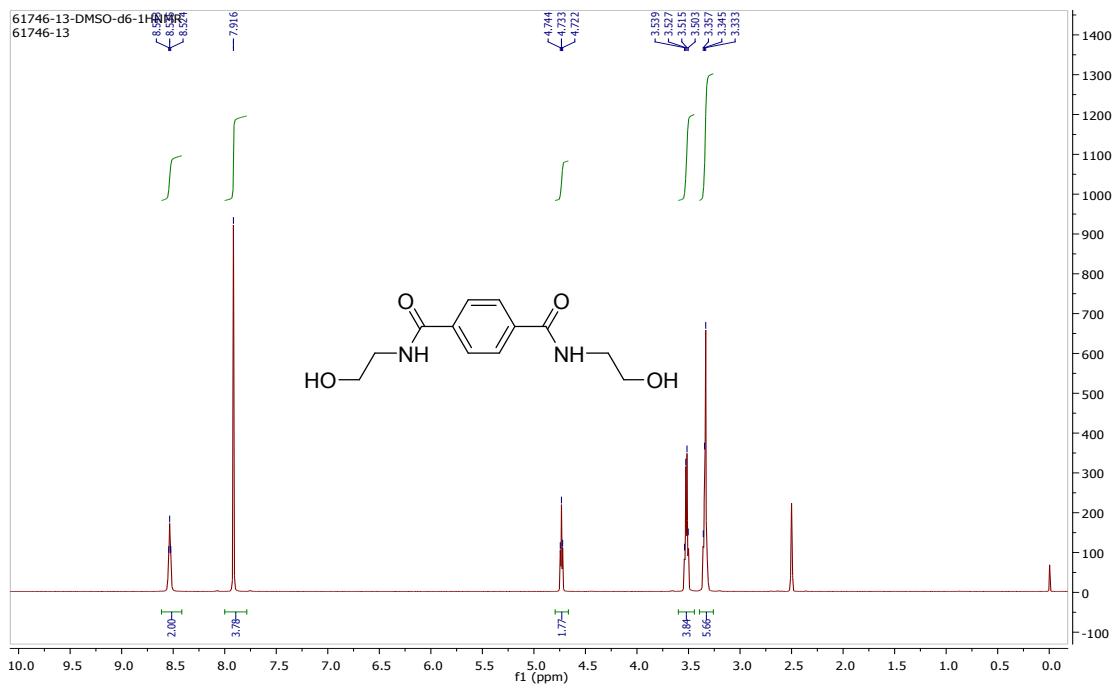


Figure S2a: ^1H NMR for Additive 2

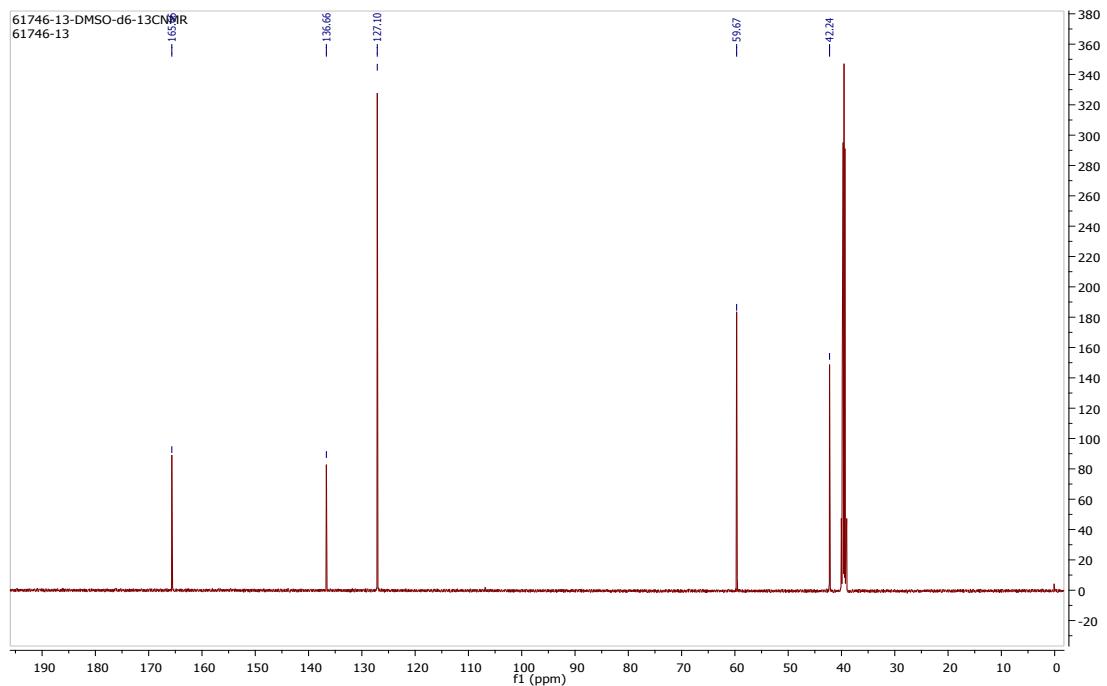


Figure S2b: ¹³C NMR for Additive 2

Additive 3 [mixture of A (47.3%) and B (52.7%)]

¹H NMR (500 MHz, CDCl₃) δ 8.10-8.15 (4H), 7.81-7.82 (4H), 6.24 (0.82H), 6.15 (1.47H), 4.69 (2H), 4.49 (2H), 3.98 (3H), 3.74 (3H), 3.46 (4H), 1.85 (4H), 1.62-1.71 (7H), 1.25 (25H), 0.87 (6H). ¹³C NMR (126 MHz, CDCl₃) δ 130.1, 127.1, 67.1, 61.5, 40.5, 32.1, 29.8, 29.7, 29.5, 27.2, 22.8, 14.3.

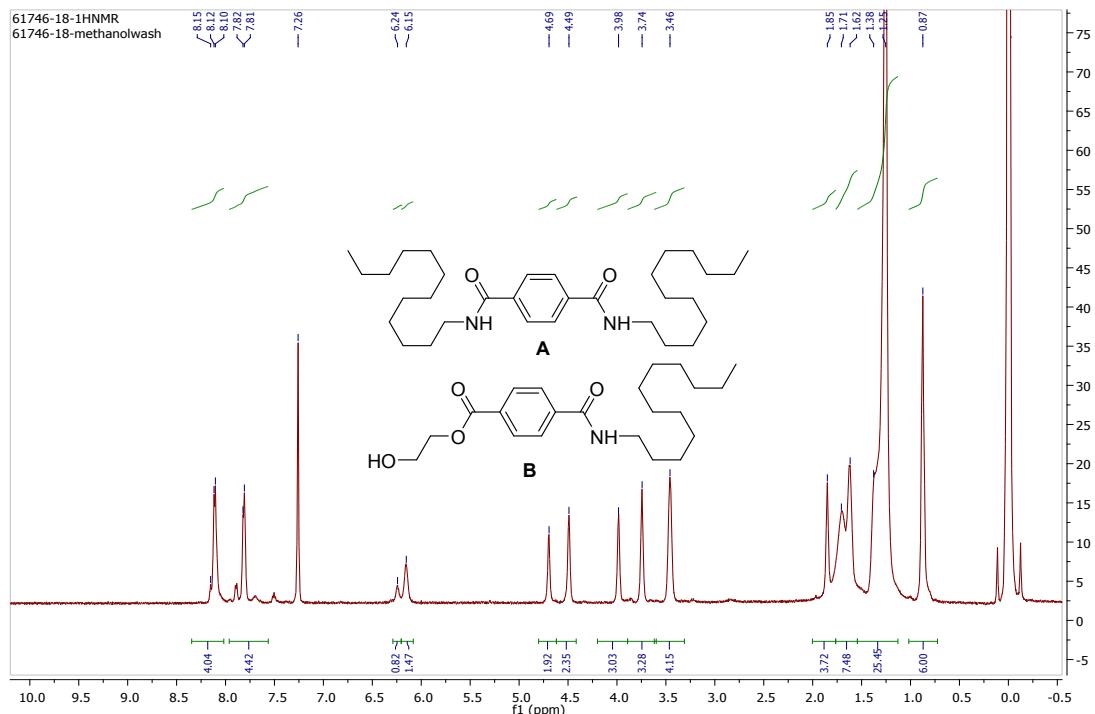


Figure S3a: ^1H NMR for Additive 3

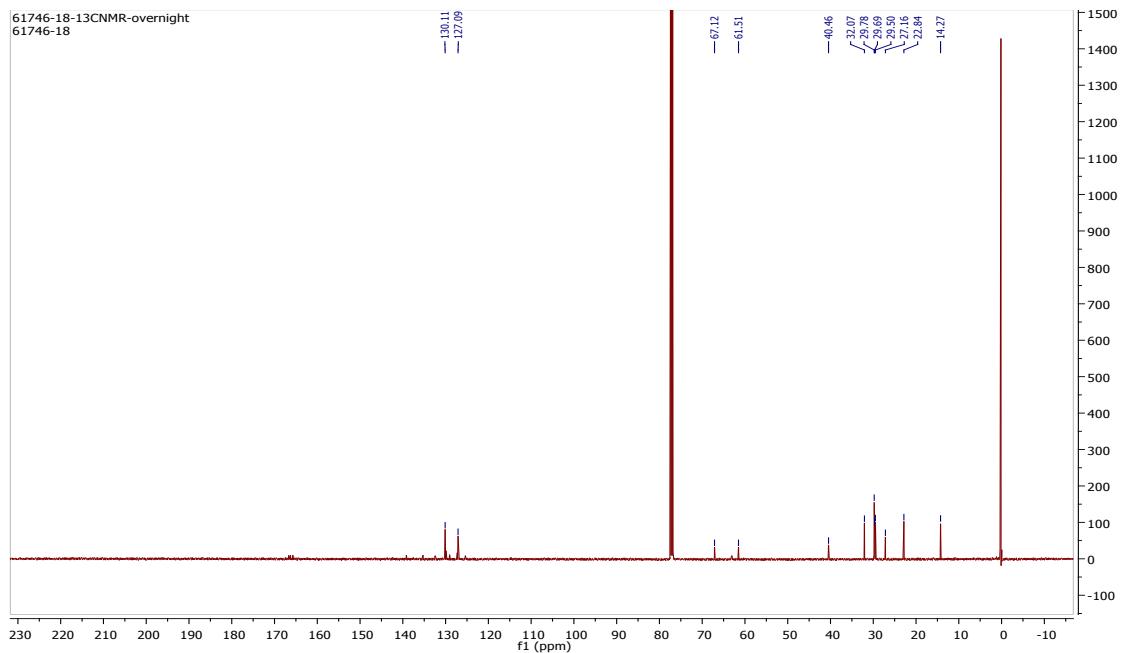


Figure S3b: ^{13}C NMR for Additive 3

Additive 4 [mixture of C (62.1%) and D (37.9%)]

^1H NMR (500 MHz, CDCl_3) δ 8.08-8.13 (2H), 7.80 (3H), 6.26 (0.57H), 6.16 (1.87H), 4.7 (2H), 4.49 (2H), 3.98 (2H), 3.74 (2H), 3.44-3.48 (5H), 1.85 (2H), 1.61-1.64 (10H), 1.32-1.40 (11H), 0.90 (6H). ^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{SO}$ and $((\text{CD}_3)_2\text{CO})$) δ 139.9, 137.7, 77.4, 70.4, 50.1, 42.0, 37.1, 32.9, 24.0.

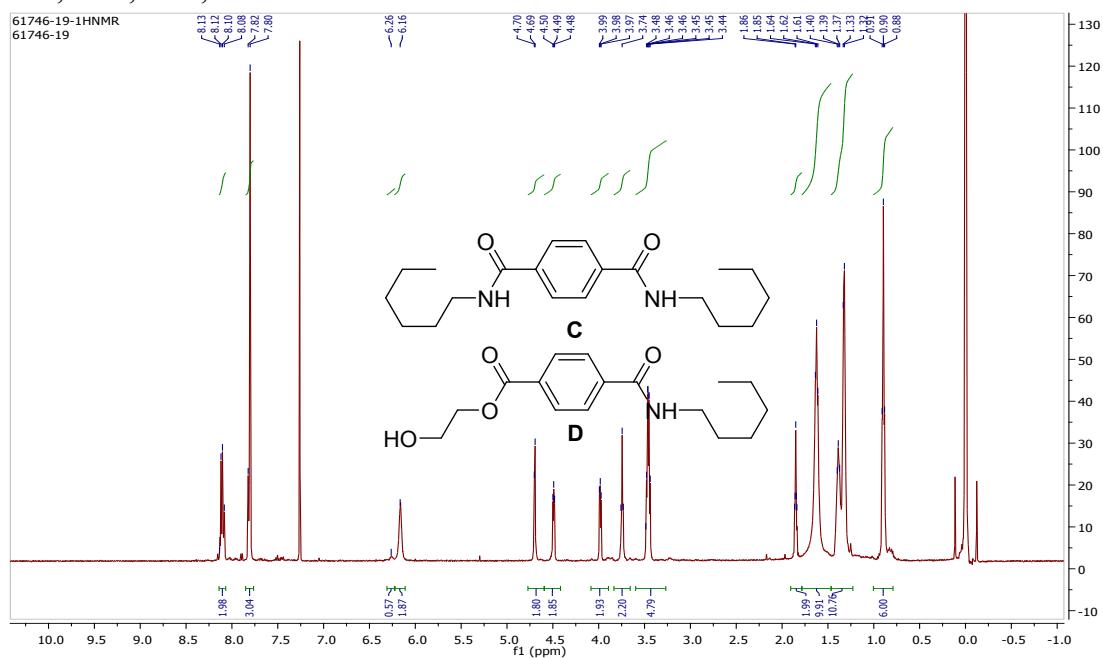


Figure S4a: ^1H NMR for Additive 4

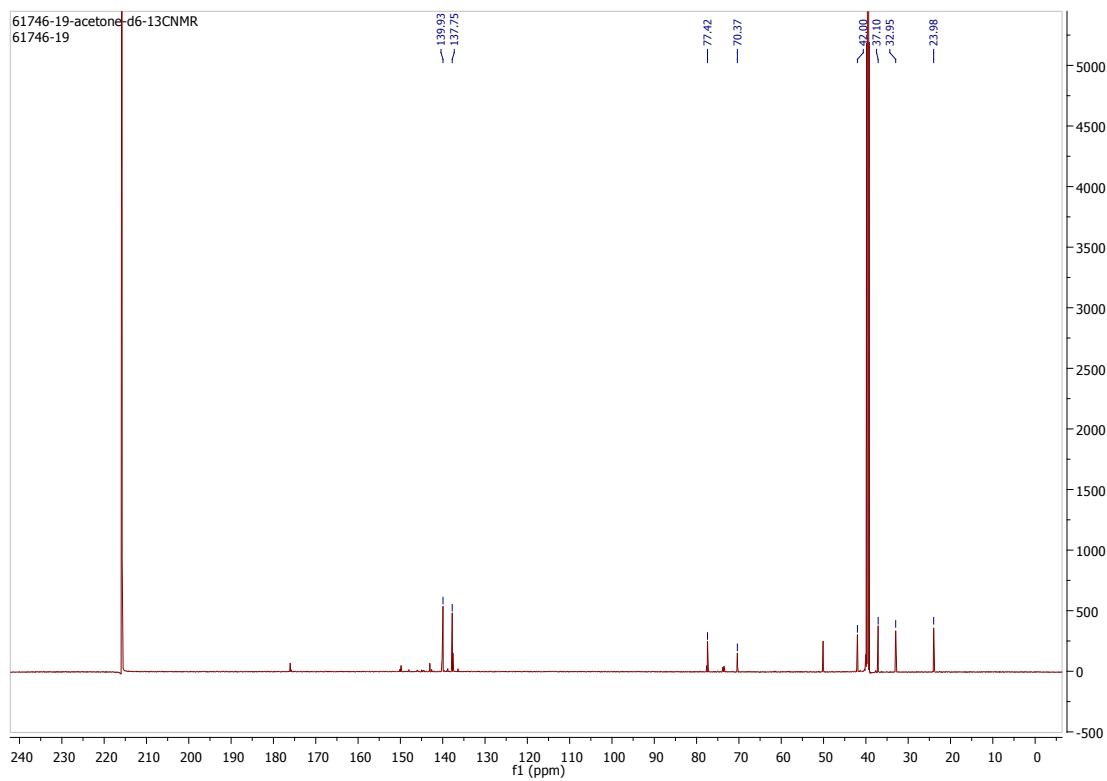


Figure S4b: ¹³C NMR for additive 4

Additive 6

¹H NMR (500 MHz, (CD₃)₂SO) δ 8.54 (t, 2H, J = 5.5 Hz), 7.89 (s, 4H), 4.47 (t, 2H, J = 5.5 Hz), 3.46 (q, 4H, J = 6.0 Hz), 3.33(q, 4H, J = 6.0 Hz). ¹³C NMR (126 MHz, (CD₃)₂SO) δ 165.5, 136.6, 127.1, 58.7, 36.7, 32.4.

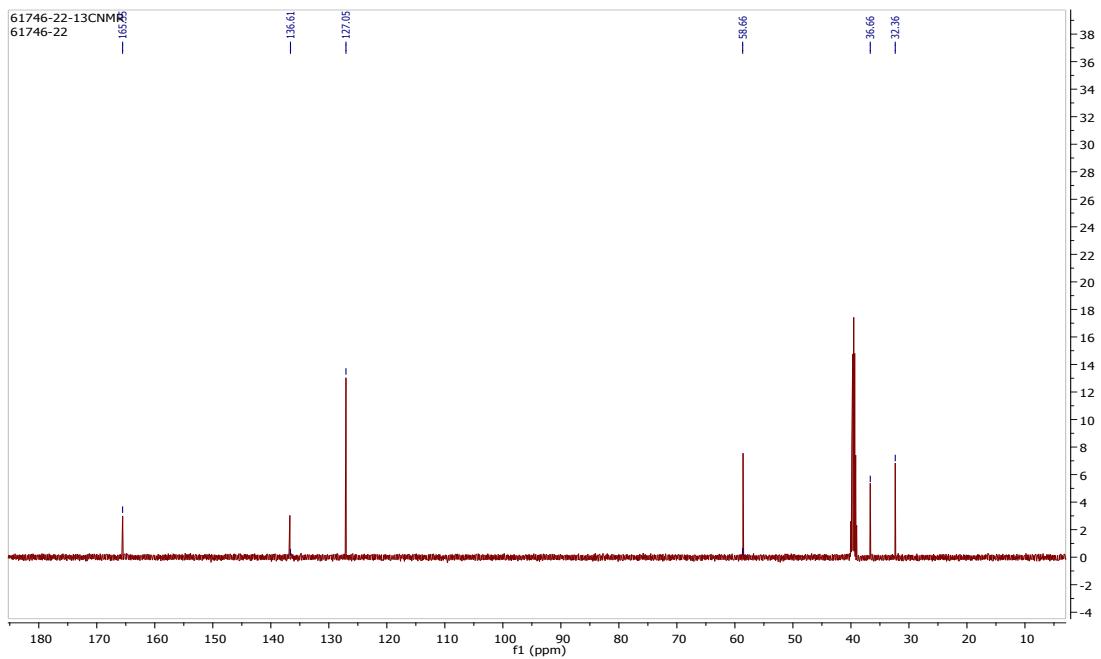
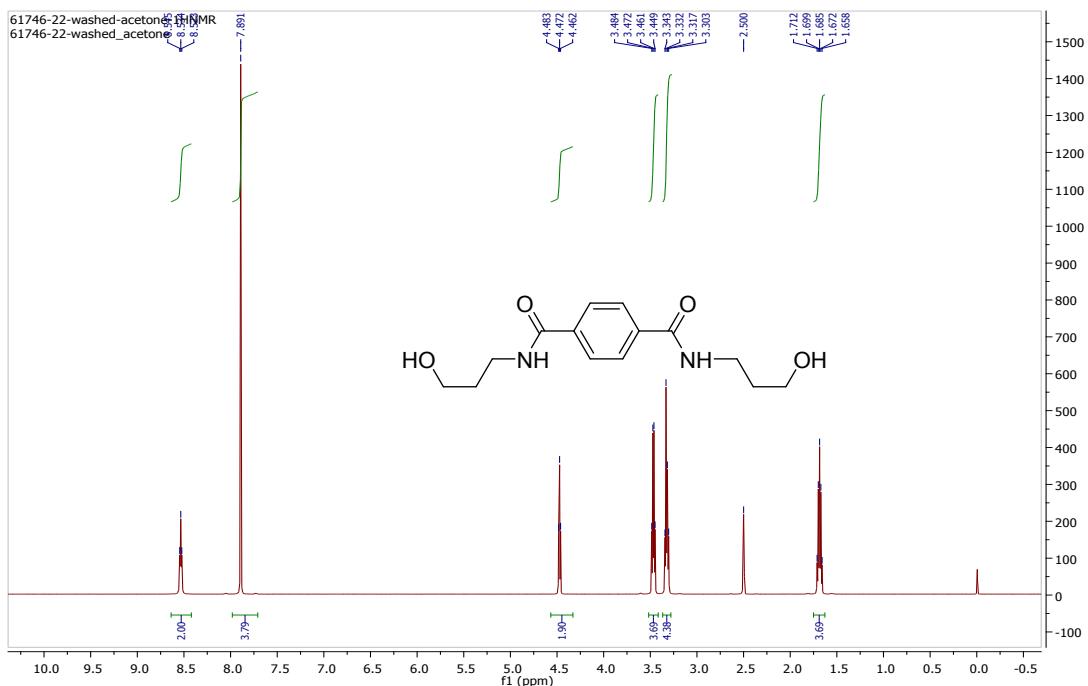


Figure S5b: ¹³C NMR for Additive 6

Additive 7

¹H NMR (500 MHz, (CD₃)₂SO) δ 8.1 (d, 2H, J = 8 Hz), 7.92 (s, 4H), 4.67 (t, 2H, J = 5.0 Hz), 3.84-3.90 (m, 2H), 3.45-3.49 (m, 2H), 3.39-3.42 (m, 2H), 1.62-1.70 (m, 2H), 1.41-1.50 (m, 2H), 0.87 (t, 6H, J = 7.5 Hz). ¹³C NMR (126 MHz, (CD₃)₂SO) δ 165.6, 136.9, 127.2, 63.0, 53.2, 23.7, 10.7.

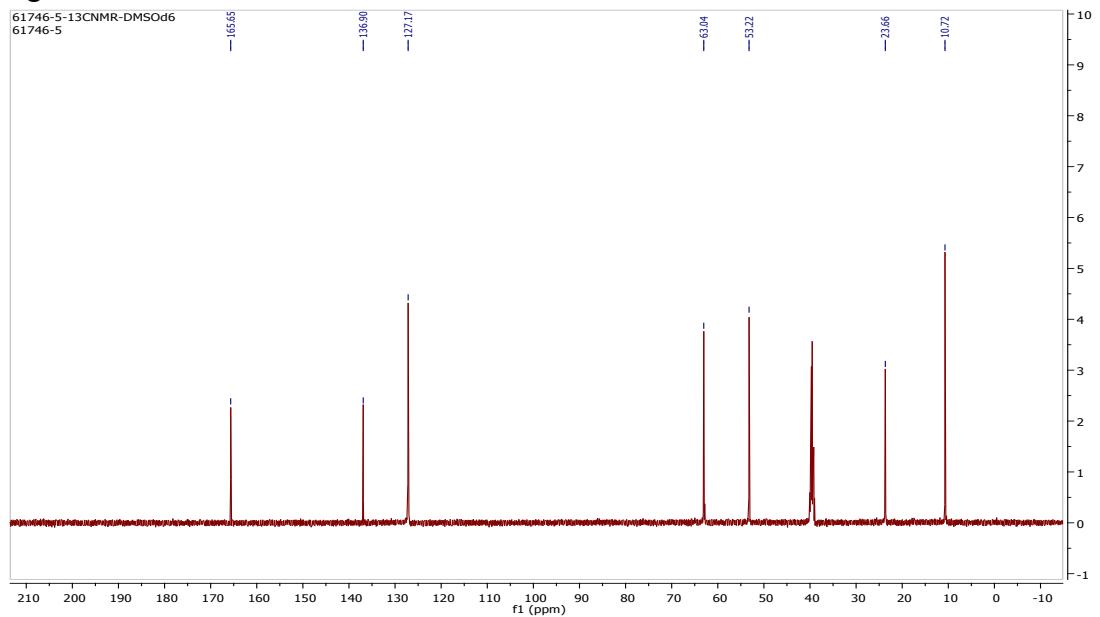
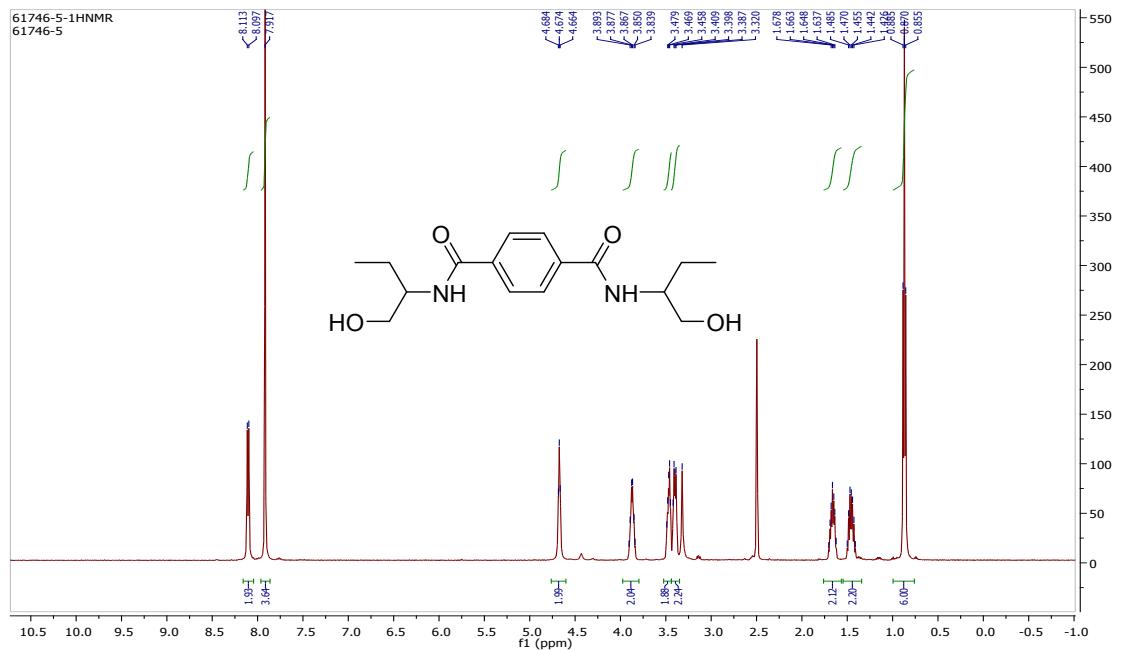


Figure S6b: ^{13}C NMR for Additive 7

Additive 8

^1H NMR (500 MHz, $(\text{CD}_3)_2\text{SO}$) 8.54 (t, 2H, $J = 5.0$ Hz), 7.89 (s, 4H), 4.28 (bs, 2H), 3.39 (m, 4H), 3.21-3.28 (m, 4H), 1.28-1.55 (m, 12H). ^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{SO}$) δ 165.4, 136.8, 127.1, 60.6, 32.3, 29.0, 23.1.

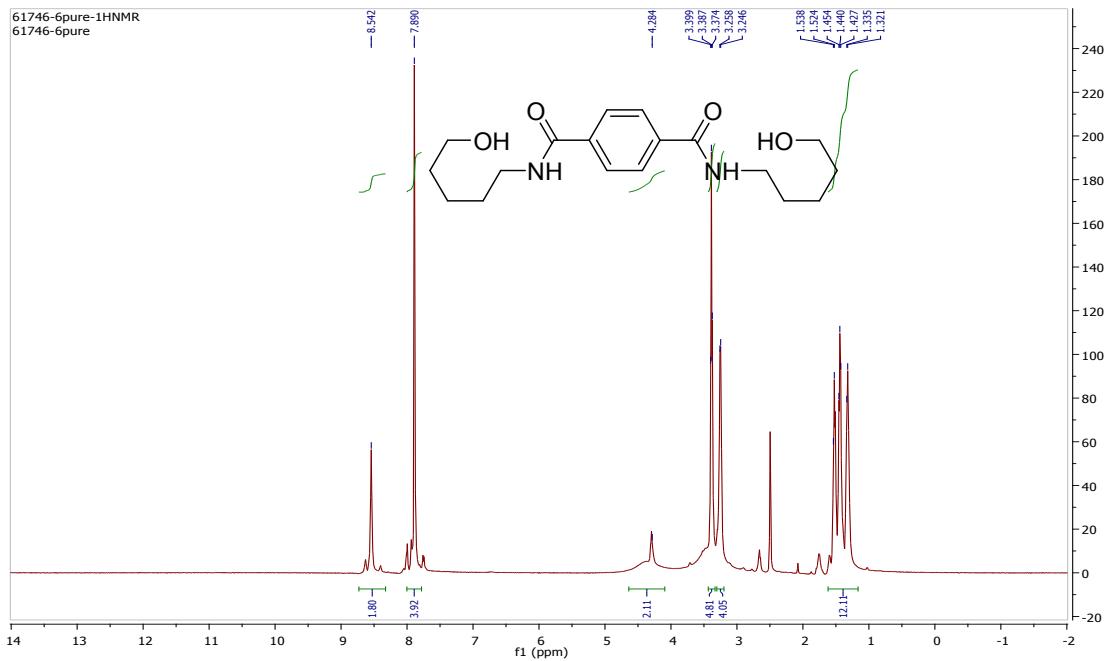


Figure S7a: ^1H NMR for Additive 8

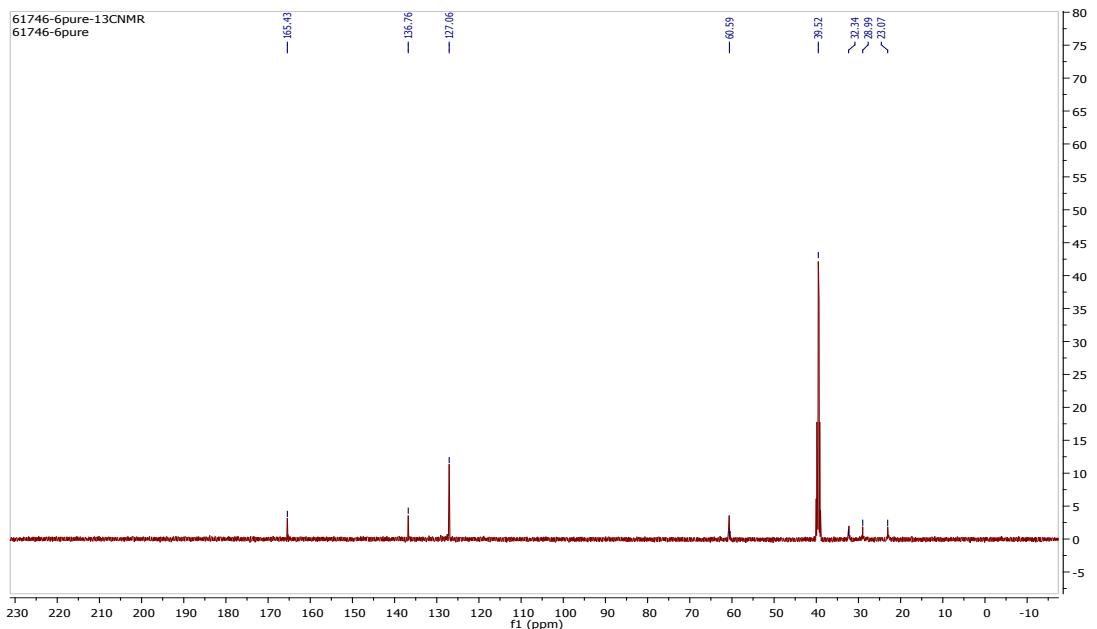


Figure S7b: ^{13}C NMR for Additive 8

Additive 9

^1H NMR (500 MHz, CDCl_3) δ 8.09-8.12 (2H, m), 7.81 (3H, s), 6.11 (2H), 4.70 (1H), 3.75 (4H), 3.45 (2H), 1.86 (5H), 1.59-1.66 (4H), 1.56 (12H), 1.26-1.41 (14H), 0.88 (6H).

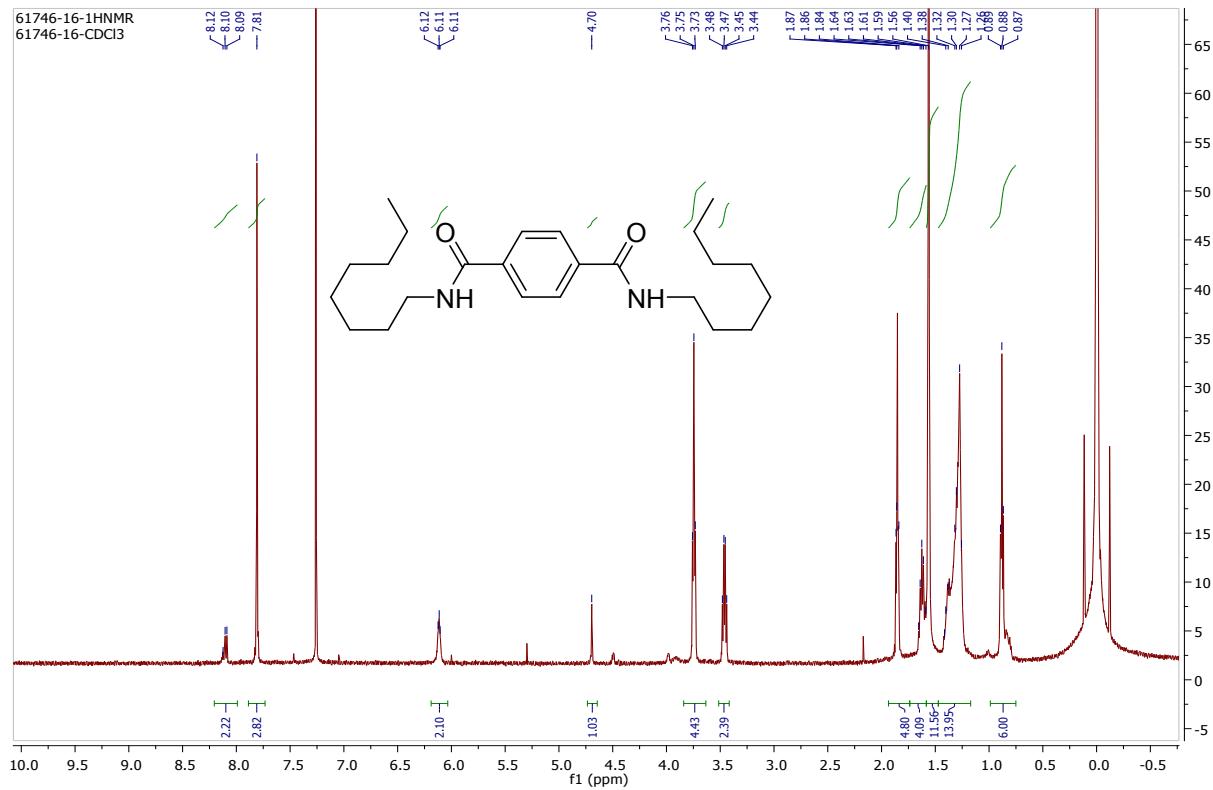


Figure S8a: ¹H NMR for Additive 9

Differential Scanning Calorimetry

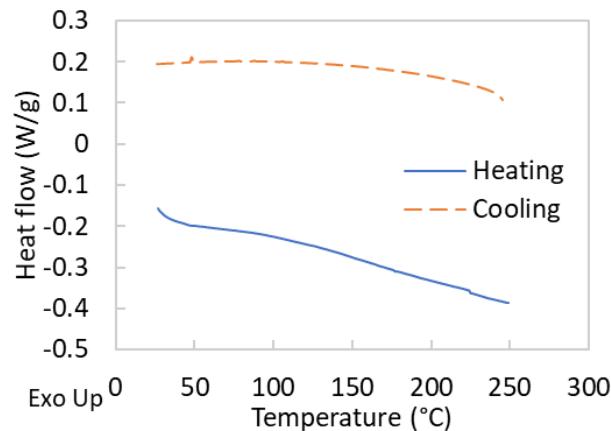


Figure S9. DSC heating and cooling thermographs of neat asphalt.

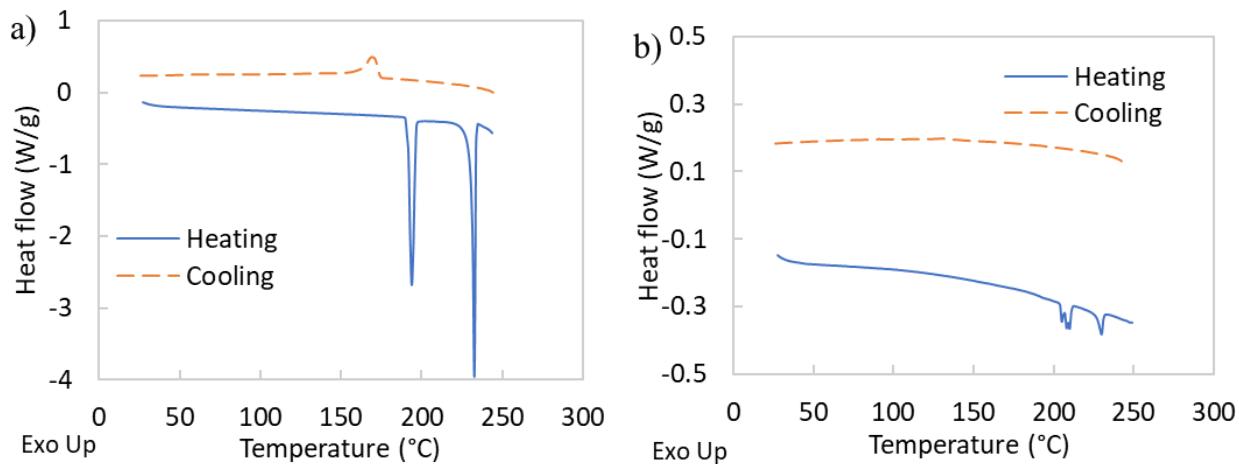


Figure S10. DSC heating and cooling thermographs of (a) additive 1 (N^1,N^4 -bis(2-hydroxyethyl)terephthalamide from clean PET source) and (b) asphalt with 5 wt% additive 1.

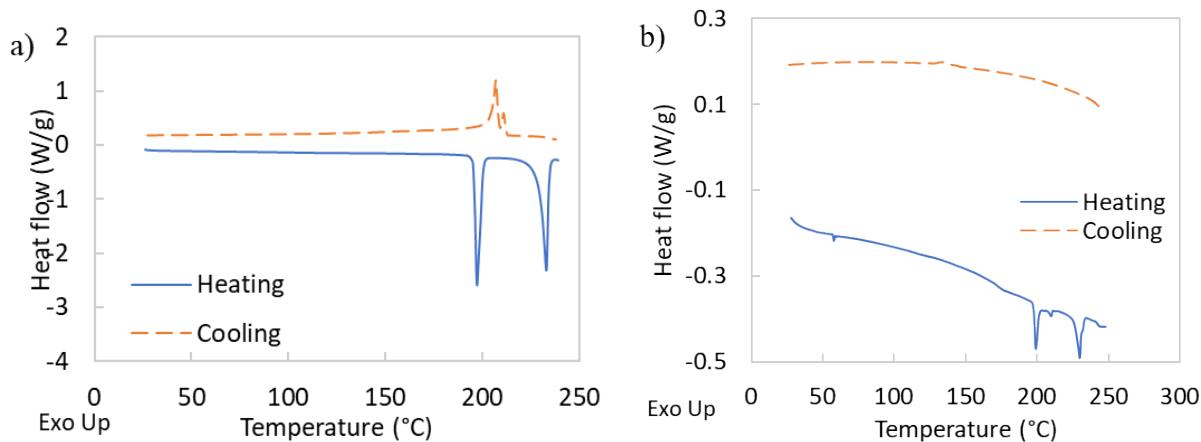


Figure S11: DSC heating and cooling thermographs of (a) additive 2 (N^1,N^4 -bis(2-hydroxyethyl)terephthalamide from mixed-waste PET source) and (b) asphalt with 5 wt% additive 2.

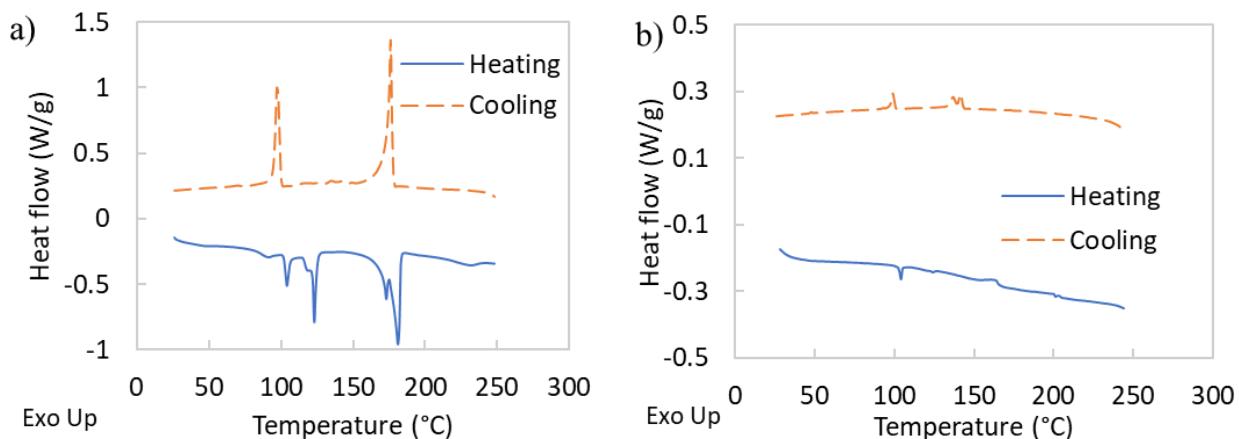


Figure S12. DSC heating and cooling thermographs of (a) additive 3 (N^1,N^4 -didodecylterephthalamide) and (b) asphalt with 5 wt% additive 3.

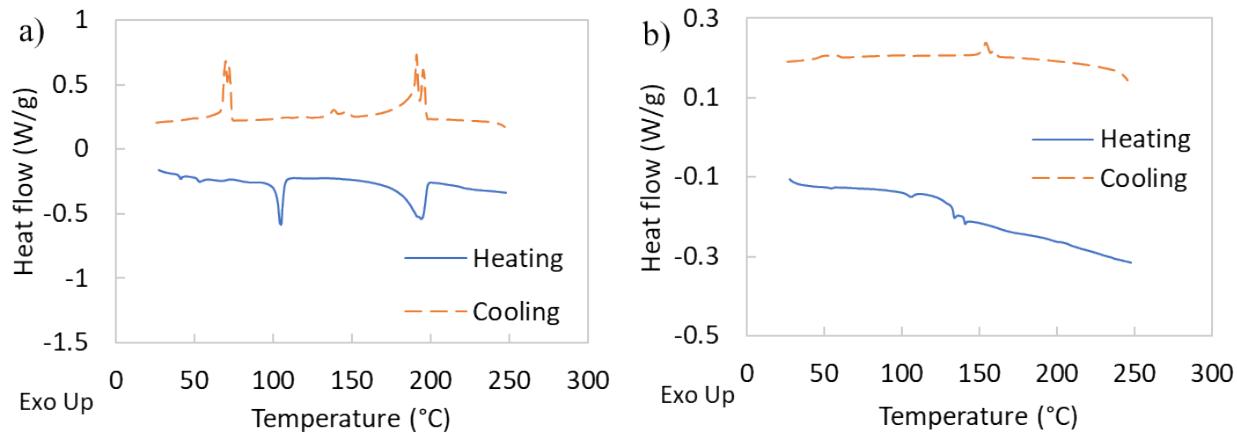


Figure S13. DSC heating and cooling thermographs of (a) additive 4 (N^1,N^4 -dihexylterephthalamide) and (b) asphalt with 5 wt% additive 4.

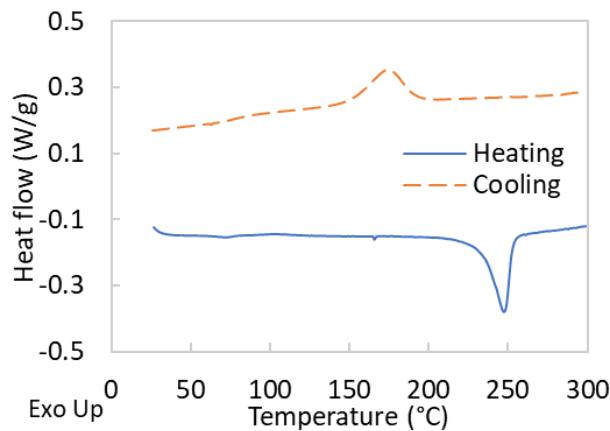


Figure S14. DSC heating and cooling thermographs of neat PET (additive 5).

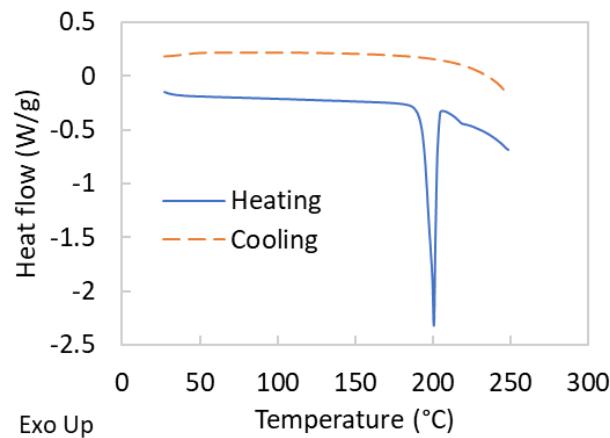


Figure S15. DSC heating and cooling thermographs of additive 7 (N^1,N^4 -diethyl- N^1,N^4 -bis(2-hydroxyethyl)terephthalamide).

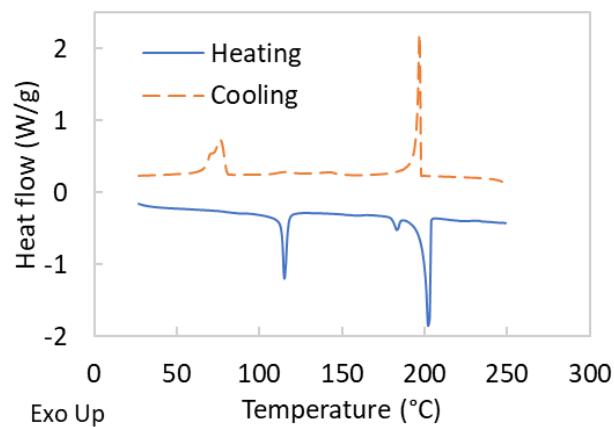


Figure S16. DSC heating and cooling thermographs of additive 9 (N^1,N^4 -diethylterephthalamide).