Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and quantitative structure−activity relationship (QSAR) studies of novel rosin-based diamide insecticides

Jian Li,*[a] Yanqing Gao,*[b] Shibin Shang,[c] Xiaoping Rao,[c] Jie Song[d] and Zongde Wang[e]

[a] *College of Forestry, Northwest Agriculture and Forestry University, Yangling, Shaanxi 712100, People's Republic of China*

[b] *Research & Development Center of Biorational Pesticide, College of Plant Protection, Northwest Agriculture and Forestry University, Yangling, Shaanxi 712100, People's Republic of China*

[c] *Institute of Chemical Industry of Forest Products, Chinese Academy of Forestry, Nanjing, Jiangsu 210042, People's Republic of China*

[d] *Department of Chemistry and Biochemistry, University of Michigan-Flint, Flint, Michigan 48502, United States*

[e] *College of Forestry, Jiangxi Agriculture University, Nanchang, Jiangxi 330045, People's Republic of China*

*Corresponding author: Tel: +0086-029-87082392 (J. L.). Fax: +0086-029-87082392 (J. L.). E-mail: ericlee99@nwsuaf.edu.cn (J. L.). gaoyanqinggc@163.com (Y.Q. Gao).

*Data for compound **4c***. Yield: 6.6 g (60%); yellow powder; m.p. 125.7-126.9°C. IR (cm^{-1}): 3301 (N-H); 2924, 2864 (-CH_3, -CH_2); 1663 (N-C=O); 748 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.05, 7.99 (m, 2H, CONH-); 7.34-7.03 (m, 8H, Ar-H); 5.30 (S, H, C=CH-); 2.69 (S, H, -CH-C=O-); 2.20 (S, 6H, Ar-CH_3); 2.24-2.11 (m, 3H, -CH-); 2.19-2.04 (m, 14H, -CH_2-); 1.55 (m, H, -CH-$(Me)_2$); 1.21-0.62 (m, 12H, CH_3). ESI-MS m/z = 553 $[M + H]^+$. Anal. Calcd for $C_{37}H_{48}N_2O_2$: C, 80.39; H, 8.75; N, 5.07. Found: C, 80.28; H, 8.80; N, 4.84.

*Data for compound **4d***. Yield: 4.97 g (45%); white powder; m.p. 126.9-127.8°C. IR (cm^{-1}): 3338 (N-H); 2922, 2864 (-CH_3, -CH_2); 1663 (N-C=O); 778, 689 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.09, 7.98 (m, 2H, CONH-); 7.31-6.96 (m, 8H, Ar-H); 5.29 (S, H, C=CH-); 2.67 (S, H, -CH-C=O-); 2.31 (S, 6H, Ar-CH_3); 2.33-2.29 (m, 3H, -CH-); 2.17-1.27 (m, 14H, -CH_2-); 1.58 (m, H, -CH-$(Me)_2$); 1.17-0.59 (m, 12H, CH_3). ESI-MS m/z = 553 $[M + H]^+$. Anal. Calcd for $C_{37}H_{48}N_2O_2$: C, 80.39; H, 8.75; N, 5.07. Found: C, 80.19; H, 8.97; N, 4.95.

*Data for compound **4e***. Yield: 5.85 g (53%); white powder; m.p. 142.0-142.9°C. IR (cm^{-1}): 3334 (N-H); 2922, 2864 (-CH_3, -CH_2); 1662 (N-C=O); 812 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.35, 8.06 (m, 2H, CONH-); 7.35-7.04 (m, 8H, Ar-H); 5.30 (S, H, C=CH-); 2.66 (S, H, -CH-C=O-); 2.28 (S, 6H, Ar-CH_3); 2.32-2.27 (m, 3H, -CH-); 2.17-1.26 (m, 14H, -CH_2-); 1.54 (m, H, -CH-$(Me)_2$); 1.16-0.70 (m, 12H, CH_3). ESI-MS m/z = 553 $[M + H]^+$. Anal. Calcd for $C_{37}H_{48}N_2O_2$: C, 80.39; H, 8.75; N, 5.07. Found: C, 80.47; H, 8.85; N, 4.95.

*Data for compound **4f***. Yield: 5.45 g (47%); white powder; m.p. 207.7-208.5°C. IR (cm^{-1}): 3265 (N-H); 2920, 2861 (-CH_3, -CH_2); 1670 (N-C=O); 804, 685 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.83, 8.71 (m, 2H, CONH-); 7.21-6.88 (m, 6H, Ar-H); 5.33 (S, H, C=CH-); 2.69 (S, H, -CH-C=O-); 2.49-1.58 (m, 14H, -CH_2-); 2.35-2.10 (S, 12H, Ar-CH_3); 2.29-2.17 (m, 3H, -CH-); 1.57 (m, H, -CH-$(Me)_2$); 1.47-0.61 (m, 12H, CH_3). ESI-MS m/z = 581 $[M + H]^+$. Anal. Calcd for $C_{39}H_{52}N_2O_2$: C, 80.64; H, 9.02; N, 4.82. Found: C, 80.52; H, 9.50; N, 4.56.

*Data for compound **4g***. Yield: 7.50 g (68%); white powder; m.p. 140.8-142.9°C. IR (cm^{-1}): 3348 (N-H); 2921, 2864 (-CH_3, -CH_2); 1664 (N-C=O); 836, 686 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.91, 8.68 (m, 2H, CONH-); 7.14-7.03 (m, 6H, Ar-H); 5.30 (S, H, C=CH-); 2.68 (S, H, -CH-C=O-); 2.54-1.26 (m, 14H, -CH_2-); 2.29-2.24 (m, 3H, -CH-); 2.28-1.42 (S, 12H, Ar-CH_3); 1.52 (m, H, -CH-$(Me)_2$); 1.14-0.61 (m, 12H, CH_3). ESI-MS m/z = 553 [M +

H]$^+$. Anal. Calcd for $C_{39}H_{52}N_2O_2$: C, 80.64; H, 9.02; N, 4.82. Found: C, 80.29; H, 9.43; N, 4.48.

*Data for compound **4h***. Yield: 8.53 g (73%); yellow powder; m.p. 129.8-130.5°C. IR (cm^{-1}): 3343 (N-H); 2929, 2866 (-CH_3, -CH_2); 1672 (N-C=O); 745 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.52, 8.34 (m, 2H, CONH-); 7.80-7.43 (m, 8H, Ar-H); 5.29 (S, H, C=CH-); 3.87 (m, 6H, -OCH_3); 2.68 (S, H, -CH-C=O-); 2.55-1.02 (m, 14H, -CH_2-); 2.16-1.87 (m, 3H, -CH-); 1.54 (m, H, -CH-$(Me)_2$); 1.16-0.67 (m, 12H, CH_3). ESI-MS m/z = 585 [M + H]$^+$. Anal. Calcd for $C_{37}H_{48}N_2O_4$: C, 75.99; H, 8.27; N, 4.79. Found: C, 76.01; H, 8.58; N, 4.45.

*Data for compound **4i***. Yield: 8.76 g (75%); white powder; m.p. 120.0-120.5°C. IR (cm^{-1}): 3349 (N-H); 2927, 2864 (-CH_3, -CH_2); 1664 (N-C=O); 770, 686 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.39, 8.22 (m, 2H, CONH-); 7.38-6.91 (m, 8H, Ar-H); 5.29 (S, H, C=CH-); 3.79 (m, 6H, -OCH_3); 2.68 (S, H, -CH-C=O-); 2.53-1.28 (m, 14H, -CH_2-); 2.19-1.87 (m, 3H, -CH-); 1.54 (m, H, -CH-$(Me)_2$); 1.21-0.65 (m, 12H, CH_3). ESI-MS m/z = 585 [M + H] $^+$. Anal. Calcd for $C_{37}H_{48}N_2O_4$: C, 75.99; H, 8.27; N, 4.79. Found: C, 75.70; H, 8.53; N, 4.43.

*Data for compound **4j***. Yield: 8.99 g (77%); white powder, m.p. 130.8-131.5°C. IR (cm^{-1}): 3324 (N-H); 2925, 2864 (-CH_3, -CH_2); 1661 (N-C=O); 825 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.38, 8.29 (m, 2H, CONH-); 7.31-7.08 (m, 8H, Ar-H); 5.31 (S, H, C=CH-); 3.17 (m, 6H, -OCH_3); 2.67 (S, H, -CH-C=O-); 2.51-1.26 (m, 14H, -CH_2-); 2.16-1.83 (m, 3H, -CH-); 1.55 (m, H, -CH-$(Me)_2$); 1.19-0.61 (m, 12H, CH_3). ESI-MS m/z = 585 [M + H] $^+$. Anal. Calcd for $C_{37}H_{48}N_2O_4$: C, 75.99; H, 8.27; N, 4.79. Found: C, 75.86; H, 8.31; N, 4.59.

*Data for compound **4k***. Yield: 7.62 g (68%); white powder; m.p. 129.3-130.4°C. IR (cm^{-1}): 3298 (N-H); 2927, 2865 (-CH_3, -CH_2); 1647 (N-C=O); 827 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.42, 8.28 (m, 2H, CONH-); 7.37-7.19 (m, 8H, Ar-H); 5.29 (S, H, C=CH-); 2.68 (S, H, -CH-C=O-); 2.52-1.27 (m, 14H, -CH_2-); 2.08-1.93 (m, 3H, -CH-); 1.55 (m, H, -CH-$(Me)_2$); 1.16-0.65 (m, 12H, CH_3). ESI-MS m/z = 561 [M + H]$^+$. Anal. Calcd for $C_{35}H_{42}F_2N_2O_2$: C, 74.97; H, 7.55; N, 5.00. Found: C, 74.86; H, 7.53; N, 4.91.

*Data for compound **4l***. Yield: 7.71 g (65%); white powder; m.p. 156.4-157.4°C. IR (cm^{-1}): 3338 (N-H); 2925, 2865 (-CH_3, -CH_2); 1665 (N-C=O); 824 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.45, 8.39 (m, 2H, CONH-); 7.40-6.83 (m, 8H, Ar-H); 5.26 (S, H, C=CH-); 2.68 (S, H, -CH-C=O-); 2.51-1.27 (m, 14H, -CH_2-); 2.49-2.30 (m, 3H, -CH-); 1.56 (m, H, -

CH-$(Me)_2$); 1.18-0.59 (m, 12H, CH_3). ESI-MS m/z = 594 $[M + H]^+$. Anal. Calcd for $C_{35}H_{42}Cl_2N_2O_2$: C, 70.81; H, 7.13; N, 4.72. Found: C, 70.67; H, 7.07; N, 4.57.

*Data for compound **4m***. Yield: 9.55 g (70%); white powder; m.p. 140.7-141.4°C. IR (cm^{-1}): 3344 (N-H); 2924, 2864 (-CH_3, -CH_2); 1665 (N-C=O); 822 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.41, 8.35 (m, 2H, CONH-); 7.38-7.23 (m, 8H, Ar-H); 5.35 (S, H, C=CH-); 2.67 (S, H, -CH-C=O-); 2.54-1.18 (m, 14H, -CH_2-); 2.03-1.87 (m, 3H, -CH-); 1.54 (m, H, -CH-$(Me)_2$); 1.16-0.64 (m, 12H, CH_3). ESI-MS m/z = 683 $[M + H]^+$. Anal. Calcd for $C_{35}H_{42}Br_2N_2O_2$: C, 61.59; H, 6.20; N, 4.10. Found: C, 61.76; H, 6.38; N, 3.98.

*Data for compound **4n***. Yield: 5.28 g (40%); white powder; m.p. 158.9-160.2°C. IR (cm^{-1}): 3343 (N-H); 2928, 2868 (-CH_3, -CH_2); 1671 (N-C=O); 838 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300MHz): 8.64, 8.33 (m, 2H, CONH-); 7.58-7.26 (m, 8H, Ar-H); 5.31 (S, H, C=CH-); 2.69 (S, H, -CH-C=O-); 2.54-1.21 (m, 14H, -CH_2-); 2.06-1.92 (m, 3H, -CH-); 1.56 (m, H, -CH-$(Me)_2$); 1.17-0.66 (m, 12H, CH_3). ESI-MS m/z = 661 $[M + H]^+$. Anal. Calcd for $C_{37}H_{42}F_6N_2O_2$: C, 67.26; H, 6.41; N, 4.24. Found: C, 67.12; H, 6.50; N, 4.08.

*Data for compound **6c***. Yield: 6.12 g (85%); white powder; m.p. 212.9-213.7°C. IR (cm^{-1}): 3335, 3083 (N-H); 2959, 2879 (-CH_3, -CH_2); 1661 (N-C=O); 1633 (C=N); 1080 (C-S-C); 813 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.15, 7.99 (m, 2H, -CONH-); 7.68-7.34 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.74-1.79 (m, 5H, -CH-); 2.35-2.24 (m, 6H, Ar-CH_3); 1.92-1.28 (m, 14H, -CH_2-); 1.41-0.69 (m, 12H, CH_3). ESI-MS m/z = 721 $[M + H]^+$. Anal. Calcd for $C_{41}H_{48}N_6O_2S_2$: C, 68.30; H, 6.71; N, 11.66. Found: C, 68.33; H, 6.61; N, 11.65.

*Data for compound **6d***. Yield: 5.46 g (70%); white powder; m.p. 235.9-236.7°C. IR (cm^{-1}): 3340, 3071 (N-H); 2963, 2865 (-CH_3, -CH_2); 1660 (N-C=O); 1635 (C=N); 1298 (Ar-F); 1079 (C-S-C); 815 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.21, 8.02 (m, 2H, -CONH-); 7.59-6.90 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.81-1.79 (m, 5H, -CH-); 1.95-1.28 (m, 14H, -CH_2-); 1.37-0.55 (m, 12H, CH_3). ESI-MS m/z = 729 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_6F_2O_2S_2$: C, 64.26; H, 5.81; N, 11.53. Found: C, 64.23; H, 5.81; N, 11.45.

*Data for compound **6e***. Yield: 5.17 g (68%); white powder; m.p. 202.5-203.7°C. IR (cm^{-1}): 3341, 3069 (N-H); 2972, 2867 (-CH_3, -CH_2); 1661 (N-C=O); 1635 (C=N); 1068 (C-S-C); 829 (Ar-H); 691 (Ar-Cl). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.18, 8.02 (m, 2H, -CONH-); 7.38-7.02 (m, 8H, Ar-H); 5.27 (s, H, C=CH-); 2.94-1.76 (m, 5H, -CH-); 1.55-1.31 (m, 14H, -

CH_2-); 1.43-0.78 (m, 12H, CH_3). ESI-MS m/z = 784 $[M + Na]^+$. Anal. Calcd for $C_{39}H_{42}N_6Cl_2O_2S_2$: C, 61.49; H, 5.56; N, 11.03. Found: C, 61.63; H, 5.51; N, 11.05.

Data for compound ***6f***. Yield: 6.80 g (80%); white powder; m.p. 212.9-2213.7°C. IR (cm^{-1}): 3338, 3068 (N-H); 2968, 2871 (-CH_3, -CH_2); 1659 (N-C=O); 1638 (C=N); 1080 (C-S-C); 820 (Ar-H); 701 (Ar-Br). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.11, 7.99 (m, 2H, -CONH-); 7.62-6.94 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.89-1.69 (m, 5H, -CH-); 1.89-1.31 (m, 14H, -CH_2-); 1.41-0.88 (m, 12H, CH_3). ESI-MS m/z = 851 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_6Br_2O_2S_2$: C, 55.06; H, 4.98; N, 9.88. Found: C, 55.13; H, 5.01; N, 9.85.

Data for compound ***6g***. Yield: 6.39 g (85%); white powder; m.p. 230.8-231.9°C. IR (cm^{-1}): 3335, 3083 (N-H); 2960, 2799 (-CH_3, -CH_2); 2825 (Ar-OCH_3); 1661 (N-C=O); 1633 (C=N); 1080 (C-S-C); 813 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.13, 8.02 (m, 2H, -CONH-); 7.74-7.04 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 3.35, 3.29 (m, 6H, -OCH_3); 2.81-1.76 (m, 5H, -CH-); 1.99-1.39 (m, 14H, -CH_2-); 1.51-0.99 (m, 12H, CH_3). ESI-MS m/z = 753 $[M + H]^+$. Anal. Calcd for $C_{41}H_{48}N_6O_4S_2$: C, 65.40; H, 6.43; N, 11.16. Found: C, 65.43; H, 6.51; N, 11.05.

Data for compound ***6h***. Yield: 6.21 g (75%); white powder; m.p. 223.1-224.7°C. IR (cm^{-1}): 3345, 3079 (N-H); 2988, 2861 (-CH_3, -CH_2); 1660 (N-C=O); 1635 (C=N); 1280 (C-F); 1080 (C-S-C); 818 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.05, 7.98 (m, 2H, -CONH-); 7.72-7.03 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.94-1.71 (m, 5H, -CH-); 1.89-1.32 (m, 14H, -CH_2-); 1.41-0.73 (m, 12H, CH_3). ESI-MS m/z = 829 $[M + H]^+$. Anal. Calcd for $C_{41}H_{42}N_6F_6O_2S_2$: C, 59.41; H, 5.11; N, 10.14. Found: C, 59.43; H, 5.07; N, 10.05.

Data for compound ***6i***. Yield: 5.60 g (65%); white powder; m.p. 231.9-236.9°C. IR (cm^{-1}): 3340, 3067 (N-H); 2991, 2860 (-CH_3, -CH_2); 2813, 1266 (Ar-OCF_3, C-F); 1660 (N-C=O); 1633 (C=N); 1279 (C-F); 1080 (C-S-C); 813 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.07, 8.02 (m, 2H, -CONH-); 7.72-6.95 (m, 8H, Ar-H); 5.23 (s, H, C=CH-); 2.85-1.69 (m, 5H, -CH-); 1.90-1.41 (m, 14H, -CH_2-); 1.43-0.88 (m, 12H, CH_3). ESI-MS m/z = 861 $[M + H]^+$, 883 $[M + Na]^+$. Anal. Calcd for $C_{41}H_{42}N_6F_6O_4S_2$: C, 57.20; H, 4.92; N, 9.76. Found: C, 57.33; H, 4.81; N, 9.69.

Data for compound ***6j***. Yield: 4.54 g (58%); white powder; m.p. 235.7-236.7°C. IR (cm^{-1}): 3345, 3073 (N-H); 2993, 2875 (-CH_3, -CH_2); 1660 (N-C=O); 1635 (C=N); 1530, 1361 (Ar-

NO_2); 1079 (C-S-C); 820 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.42-8.23 (m, 8H, Ar-H); 8.10, 7.99 (m, 2H, -CONH-); 5.25 (s, H, C=CH-); 2.89-1.69 (m, 5H, -CH-); 1.89-1.31 (m, 14H, -CH_2-); 1.45-0.67 (m, 12H, CH_3). ESI-MS m/z = 783 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_8O_6S_2$: C, 59.83; H, 5.41; N, 14.31. Found: C, 59.93; H, 5.37; N, 14.25.

Data for compound ***6k***. Yield: 7.23 g (85%); white powder; m.p. 213.9-214.5°C. IR (cm^{-1}): 3341, 3070 (N-H); 2988, 2871 (-CH_3, -CH_2); 1661 (N-C=O); 1638 (C=N); 1080 (C-S-C); 819 (Ar-H); 699 (Ar-Br). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.07, 8.02 (m, 2H, -CONH-); 8.02-6.94 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.89-1.69 (m, 5H, -CH-); 1.89-1.31 (m, 14H, -CH_2-); 1.35-0.58 (m, 12H, CH_3). ESI-MS m/z = 851 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_6Br_2O_2S_2$: C, 55.06; H, 4.98; N, 9.88. Found: C, 54.93; H, 5.01; N, 9.75.

Data for compound ***6l***. Yield: 5.10 g (70%); white powder; m.p. 220.9-221.6°C. IR (cm^{-1}): 3369, 3025 (N-H); 2912, 2875 (-CH_3, -CH_2); 1660 (N-C=O); 1633 (C=N); 1238 (Ar-F); 1081 (C-S-C); 821 (Ar-H). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.19, 8.05 (m, 2H, -CONH-); 7.59-7.12 (m, 8H, Ar-H); 5.25 (s, H, C=CH-); 2.79-1.80 (m, 5H, -CH-); 1.96-1.24 (m, 14H, -CH_2-); 1.36-0.55 (m, 12H, CH_3). ESI-MS m/z = 729 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_6F_2O_2S_2$: C, 64.26; H, 5.81; N, 11.53. Found: C, 64.33; H, 5.71; N, 11.45.

Data for compound ***6m***. Yield: 5.71 g (75%); white powder; m.p. 212.2-213.2°C. IR (cm^{-1}): 3389, 3025 (N-H); 2957, 2834 (-CH_3, -CH_2); 1660 (N-C=O); 1633 (C=N); 1068 (C-S-C); 825 (Ar-H); 689 (Ar-Cl). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.28, 8.11 (m, 2H, -CONH-); 7.68-7.02 (m, 8H, Ar-H); 5.27 (s, H, C=CH-); 2.93-1.66 (m, 5H, -CH-); 1.85-1.31 (m, 14H, -CH_2-); 1.33-0.76 (m, 12H, CH_3). ESI-MS m/z = 762 $[M + H]^+$. Anal. Calcd for $C_{39}H_{42}N_6Cl_2O_2S_2$: C, 61.49; H, 5.56; N, 11.03. Found: C, 61.43; H, 5.51; N, 11.05.

Data for compound ***6n***. Yield: 5.81 g (70%); white powder; m.p. 229.9-231.2°C. IR (cm^{-1}): 3367, 3031 (N-H); 2953, 2855 (-CH_3, -CH_2); 1660 (N-C=O); 1633 (C=N); 1065 (C-S-C); 877, 811 (Ar-H); 679 (Ar-Cl). ^{1}H NMR (DMSO-d_6. δ/ppm. 300 MHz): 8.18, 8.01 (m, 2H, -CONH-); 7.63-7.32 (m, 6H, Ar-H); 5.27 (s, H, C=CH-); 2.88-1.61 (m, 5H, -CH-); 1.86-1.40 (m, 14H, -CH_2-); 1.50-0.99 (m, 12H, CH_3). ESI-MS m/z = 831 $[M + H]^+$. Anal. Calcd for $C_{39}H_{40}N_6Cl_4O_2S_2$: C, 56.39; H, 4.85; N, 10.12. Found: C, 56.43; H, 4.81; N, 10.05.

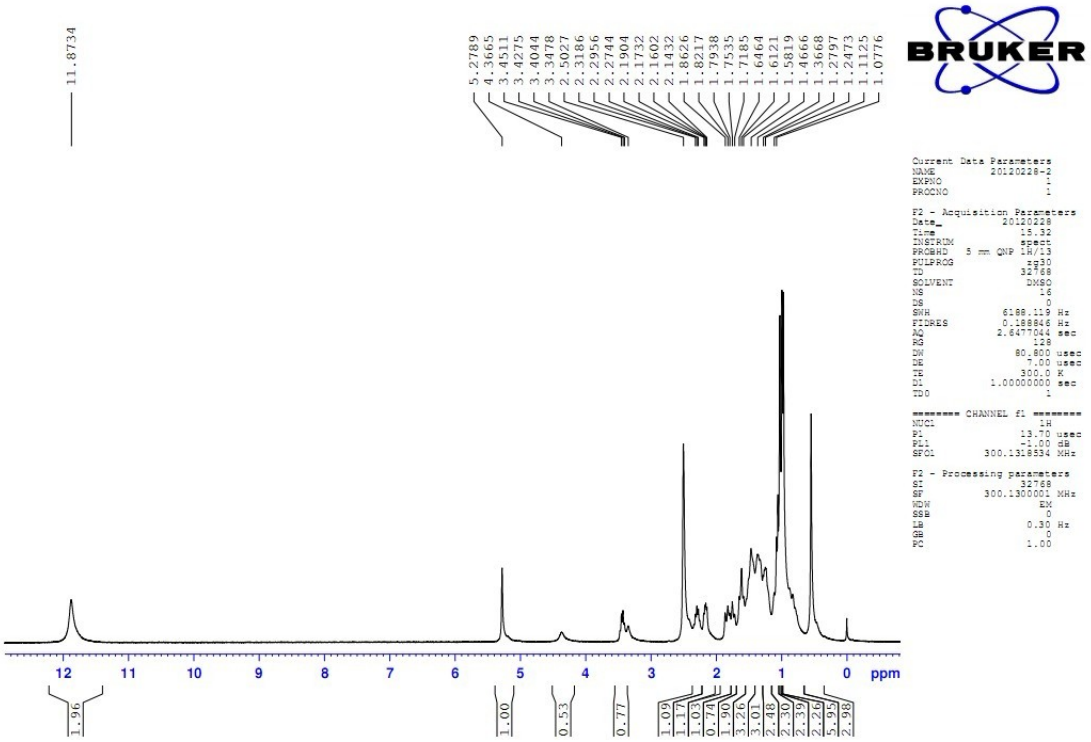

Fig. S1. [1]H NMR spectrum of the compound 1b

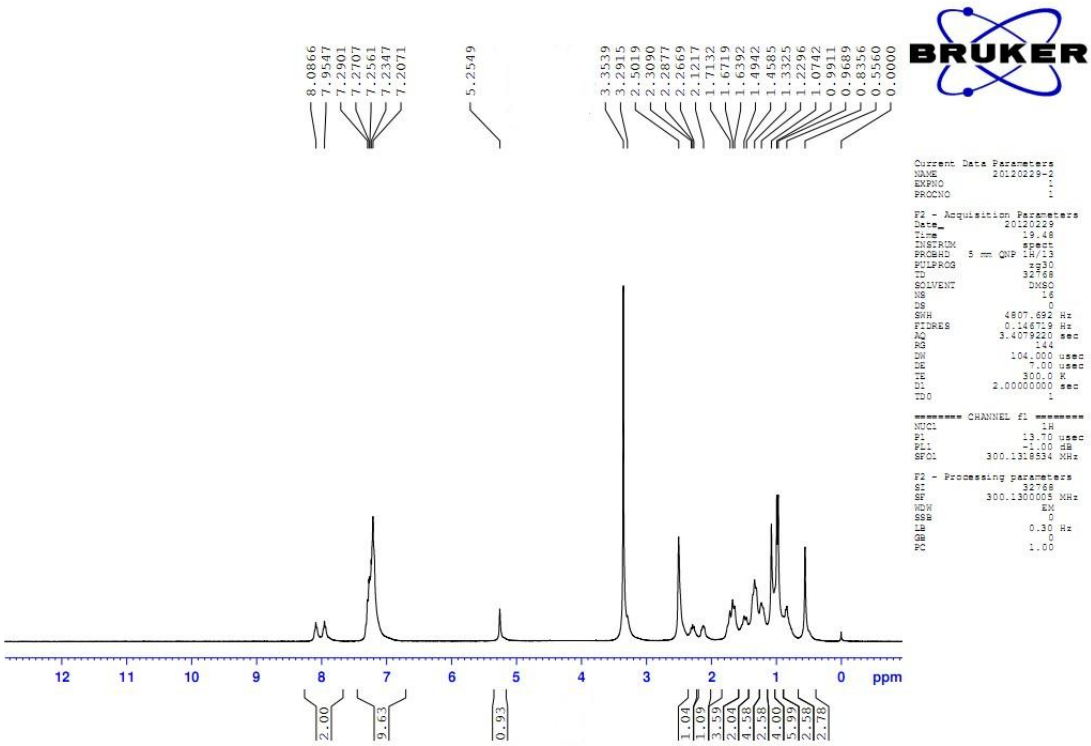

Fig. S2. [1]H NMR spectrum of the compound **4b**

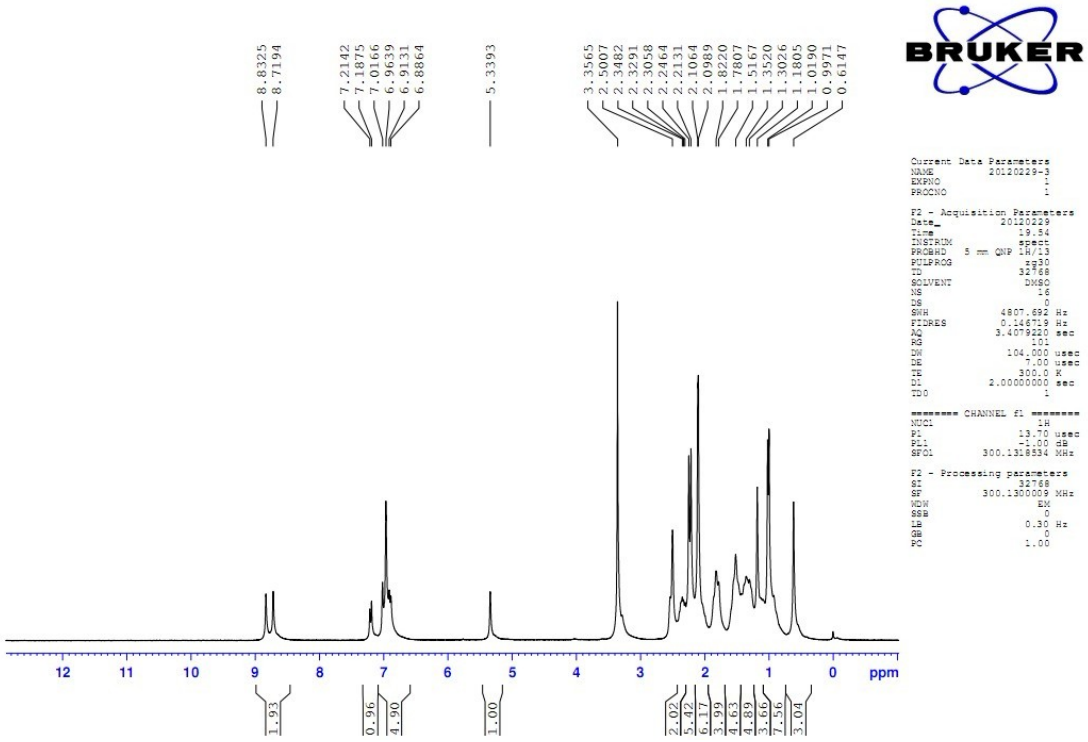

Fig. S3. ^{1}H NMR spectrum of the compound **4f**

Table S1. Values of log LC_{50} and descriptors of rosin-based diamides

Compd.	log LC_{50}	HOMO[a]	DM[b]	q^{O}_{max}[c]	q^{N}_{min}[d]	μ_h[e]
3	0.441	-0.1912	0.8980	-0.3779	-0.4376	0.9790
4a	0.470	-0.2178	4.4970	-0.3635	-0.3776	1.3960
4b	0.470	-0.2134	5.0120	-0.3360	-0.3329	1.7510
4c	0.459	-0.2116	5.2830	-0.3373	-0.3331	1.5500
4d	0.466	-0.2122	5.0690	-0.3360	-0.3330	1.7190
4e	0.455	-0.2073	4.7230	-0.3360	-0.3320	1.7780
4f	0.399	-0.2050	4.9600	-0.3362	-0.3323	1.7100
4g	0.470	-0.2092	4.5760	-0.3368	-0.3330	1.7950
4h	0.792	-0.2050	5.1960	-0.3211	-0.2331	1.8260
4i	0.805	-0.2127	3.1540	-0.3333	-0.2148	1.3240
4j	0.802	-0.2055	6.5240	-0.3305	-0.2098	2.3430
4k	0.329	-0.2169	7.5030	-0.3354	-0.3318	1.6630
4l	0.351	-0.2192	7.1530	-0.3335	-0.3328	1.7120
4m	0.351	-0.2190	7.5130	-0.3320	-0.3336	2.2810
4n	0.339	-0.2230	11.0270	-0.3275	-0.3343	1.6730
6a	0.317	-0.2112	7.0140	-0.3245	-0.3042	0.7010
6b	0.297	-0.2194	7.5630	-0.3131	-0.2982	0.5570
6c	0.274	-0.2194	7.6390	-0.3140	-0.2984	0.5520
6d	0.040	-0.2213	7.2530	-0.3111	-0.2972	0.5570
6e	0.050	-0.2229	7.4000	-0.3106	-0.2968	0.5600
6f	-0.652	-0.2247	7.9160	-0.3185	-0.2998	2.0310
6g	0.466	-0.2194	6.8450	-0.2064	-0.2977	0.7770
6h	0.073	-0.2290	9.9300	-0.3144	-0.2989	0.9230
6i	0.487	-0.1407	7.3160	-0.2494	-0.2965	0.6960
6j	0.470	-0.1478	11.9830	-0.3066	-0.2877	0.3770
6k	0.050	-0.1464	6.3940	-0.3109	-0.2962	0.9340
6l	0.083	-0.1431	7.0260	-0.3014	-0.2958	0.6320
6m	0.040	-0.1504	7.2680	-0.3035	-0.2979	0.6000
6n	-0.670	-0.2229	7.2260	-0.3015	-0.2970	0.5380

[a] Energy of the highest occupied molecular orbit in atomic units. [b] Dipole moment. [c] Max net atomic charge for a O atom. [d] Min net atomic charge for a N atom. [e] Tot hybridization composite of the molecular dipole.