The datas of the title compounds

4-isopropylcyclohexa-1, 3-dienecarboxylic acid (3, $C_{10}H_{16}O_3$)

IR (cm^{-1}): 3415 (O–H); 2961, 2874 (–CH_3, –CH_2); 1700 (–C=O). ^1H NMR($CDCl_3$, δ/ppm, 300 MHz): 6.94 (d, 1H, O=C–C=CH–); 5.90 (d, 1H, –CH=C–$(Me)_2$); 2.46 (m, H, –CH–$(Me)_2$); 2.51 (t, 2H, –CH_2–C–C=O); 2.27 (t, 2H, –CH_2–C–C=C); 1.10 (d, 6H, –CH_3). TOF-ESI-MS (m/z): 167 [M + H]$^+$. Anal. calcd for $C_{10}H_{14}O_2$: C, 72.29; H, 11.67. Found: C, 73.11; H, 10.99.

4-isopropyl-N-phenyl cyclohexa-1, 3-dienecarboxamide (5a, $C_{16}H_{19}NO$)

IR (cm^{-1}): 3312 (N–H); 2957, 2870 (–CH_3, –CH_2); 1653, 1630 (–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.57 (s, 1H, CONH–); 7.07-7.55 (m, 5H, Ar–H); 6.76-6.78 (d, 1H, OC–C=CH–); 5.83-5.85 (d, 1H, –CH=C–$(Me)_2$); 2.85-3.03 (m, 1H, –CH–$(Me)_2$); 2.49-256 (t, 2H, –CH_2–C–CO); 2.23-2.29 (t, 2H, –CH_2–C–C=C); 1.04-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 242 [M+H] $^+$; 264 [M+Na] $^+$. Anal. calcd for $C_{16}H_{19}NO$: C, 79.67; H, 7.88; N, 5.81. Found: C, 80.15; H, 7.42; N, 5.99.

4-isopropyl-N-(o-methylphenyl) cyclohexa-1, 3-dienecarboxamide (5b, $C_{17}H_{21}NO$)

IR (cm^{-1}): 3248 (NH); 2963, 2858 (CH); 1650 (N–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.95 (s, 1H, CONH–); 7.02-7.43 (m, 4H, Ar–H); 6.80-6.91 (d, 1H, OC–C=CH–); 5.82-5.86 (d, 1H, –CH=C–$(Me)_2$); 2.40-2.54 (m, 1H, –CH–$(Me)_2$); 2.34-2.37 (t, 2H, –CH_2–C–CO); 2.50-2.29 (t, 2H, –CH_2–C–C=C); 2.19 (s, 3H, Ar–CH_3); 1.03-1.56 (d, 6H, –CH_3). TOF-ESI-MS (m/z): 256 [M+H] $^+$; 278 [M+Na] $^+$. Anal. calcd for C17H21NO: C, 80.00; H, 8.24; N, 5.49. Found: C, 80.12; H, 8.34; N, 5.23.

4-isopropyl-N-(m-methylphenyl) cyclohexa-1, 3-dienecarboxamide (5c, $C_{17}H_{21}NO$).

IR (cm^{-1}): 3302 (NH); 2959, 2870 (CH); 1650, 1653 (N–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300

MHz): 7.44 (s, 1H, CONH–); 7.18-7.40 (m, 4H, Ar–H); 6.91-6.93 (d, 1H, OC–C=CH–); 5.83-5.84 (d, 1H, –CH=C–$(Me)_2$); 2.85-3.02 (m, 1H, –CH–$(Me)_2$); 2.49-2.55 (t, 2H, –CH_2–C–CO); 2.23-2.29 (t, 2H, –CH_2–C–C=C); 2.35 (s, 3H, Ar–CH_3), 1.04-1.10 (d, 6H, –CH_3). TOF-ESI-MS (m/z): 256 $[M+H]^+$, 278 $[M+Na]^+$. Anal. calcd for C17H21NO: C, 80.00; H, 8.24; N, 5.49. Found: C, 80.25; H, 8.35; N, 5.37.

4-isopropyl-N-(p-methylphenyl) cyclohexa-1, 3-dienecarboxamide (5d, $C_{17}H_{21}NO$)

IR (cm^{-1}): 3315 (NH); 2963, 2870 (CH); 1650, 1635 (N–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.78 (s, 1H, CONH–); 7.18-7.40 (m, 4H, Ar–H); 6.72-6.80 (d, 1H, OC–C=CH–); 5.82-5.86 (d, 1H, –CH=C–$(Me)_2$); 2.84-3.03 (m, 1H, –CH–$(Me)_2$); 2.49-2.55 (t, 2H, –CH_2–C–CO); 2.23-2.28 (t, 2H, –CH_2–C–C=C); 2.32 (s, 3H, Ar–CH_3); 1.03-1.10 (d, 6H, –CH_3).

TOF-ESI-MS (m/z): 256 $[M+H]^+$; 278 $[M+Na]^+$. Anal. calcd for C17H21NO: C, 80.00; H, 8.24; N, 5.49. Found: C, 80.13; H, 8.06; N, 5.45.

4-isopropyl-N-(2, 4-dimethylphenyl) cyclohexa-1, 3-dienecarboxamide (5e, $C_{18}H_{23}NO$)

IR (cm^{-1}): 3256 (NH); 2960, 2856 (CH); 1643 (N–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.74 (s, 1H, CONH–); 6.97-7.34 (m, 3H, Ar–H); 6.78-6.82 (d, 1H, OC–C=CH–); 5.81-5.86 (d, 1H, –CH=C–$(Me)_2$); 2.36-2.44 (m, 1H, –CH–$(Me)_2$); 2.28 (s, 3H, Ar–CH_3); 2.15 (s, 3H, Ar–CH_3); 1.83 (t, 2H, –CH_2–C–CO); 1.75 (t, 2H, –CH_2–C–C=C); 1.03-1.5 (d, 6H, –CH_3). TOF-ESI-MS (m/z): 270 $[M+H]^+$; 292 $[M+Na]^+$. Anal. calcd for C18H23NO: C, 80.30; H, 8.55; N, 5.20. Found: C, 80.63; H, 8.19; N, 5.57.

4-isopropyl-N-(3, 5-dimethylphenyl) cyclohexa-1, 3-dienecarboxamide (5f, $C_{18}H_{23}NO$)

IR (cm^{-1}): 3285 (NH); 2960, 2870 (–CH_3, –CH_2); 1651, 1626 (N–C=O). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.78 (s, 1H, CONH–); 7.20-7.35 (m, 3H, Ar–H); 6.71-6.75 (d, 1H, OC–C=CH–);

5.83-5.85 (d, 1H, –CH=C–$(Me)_2$); 2.85-2.87 (m, 1H, –CH–$(Me)_2$); 2.48-2.54 (t, 2H, –CH_2–C–CO); 2.52-2.33 (t, 2H, –CH_2–C–C=C); 2.35 (s, 6H, Ar–CH_3), 1.03-1.10 (d, 6H, –CH_3). TOF-ESI-MS (m/z): 270 $[M+H]^+$; 292 $[M+Na]^+$. Anal. calcd for C18H23NO: C, 80.30; H, 8.55; N, 5.20. Found: C, 80.57; H, 8.23; N, 5.38.

1-(4-isopropylcyclohexa-1, 3-dienecarbonyl)-3-phenylthiourea (7a, $C_{17}H_{20}N_2OS$)

IR (cm^{-1}): 3415, 3250 (N–H); 3038 (Ar–C–H); 1658 (C=O); 1162 (C=S). ^{1}H NMR($CDCl_3$, δ/ppm, 300 MHz): 7.83 (s, 1H, CSNH–); 7.26 (s, 1H, CONH–); 7.37-7.43 (m, 5H, Ar–H); 6.93-6.94 (d, 1H, OC–C=CH–); 5.89-5.90 (d, 1H, –CH=C–$(Me)_2$); 2.41-2.46 (m, H, –CH–$(Me)_2$); 2.47-2.51 (t, 2H, –CH_2–C–CO); 2.31-2.27 (t, 2H, –CH_2–C–C=C); 1.09-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 301$[M+H]^+$; 323$[M+Na]^+$. Anal. calcd for $C_{17}H_{19}NOS$: C, 68.00; H, 6.67; N, 9.33; S, 10.67. Found: C, 67.78; H, 6.50; N, 8.97; S, 10.01.

1-benzyl-3-(4-isopropylcyclohexa-1,3-dienecarbonyl)thiourea (7b, $C_{18}H_{22}N_2OS$)

IR (cm^{-1}): 3461 (N–H); 3039 (Ar–C–H); 1659 (C=O); 1163 (C=S). ^{1}H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.74-7.77 (t, 1H, CSNH–); 7.33 (s, 1H, CONH–); 7.24-7.40 (m, 5H, Ar–H); 6.85-6.86 (d, 1H, OC–C=CH–); 5.84-5.86 (d, 1H, –CH=C–$(Me)_2$); 2.35-2.40 (m, H, –CH–$(Me)_2$); 2.42-2.45 (t, 2H, –CH_2–C–CO); 2.20-2.26 (t, 2H, –CH_2–C–C=C); 1.06-1.08 (d, 6H, CH_3). TOF-ESI-MS (m/z): 313$[M-H]^-$. Anal. calcd for $C_{18}H_{22}N_2OS$: C, 68.79; H, 7.01; N, 8.92; S, 10.19. Found: C, 68.33; H, 7.04; N, 8.47; S, 9.87.

1-(4-isopropylcyclohexa-1,3-dienecarbonyl)-3-o-tolylthiourea (7c, $C_{18}H_{22}N_2OS$)

IR (cm^{-1}): 3420 and 3209 (N–H); 2957 and 2870 (–CH_2, –CH_3); 1653 and 1630 (–C=O); 1161(–C=S). ^{1}H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.84 (s, 1H, S=C–N–H); 7.25 (s,1H, O=C–N–H);7.20-7.29 (m, 4H, Ar–H); 6.93, 6.95 (d, 1H, OC–C=CH–); 5.89, 5.90 (d, 1H, –CH=C–$(Me)_2$);

2.41-2.45 (m, H, –CH–$(Me)_2$); 2.48-2.51 (t, 2H, –CH_2–C–CO); 2.27-2.31 (t, 2H, -CH_2-C-C=C); 2.33 (s, 3H, CH_3-Ar); 1.06-1.08 (d, 6H, CH_3). TOF-ESI-MS (m/z): 315 $[M + H]^+$; 337 $[M + Na]^+$. Anal. calcd for $C_{18}H_{22}N_2OS$: C, 68.79; H, 7.01; N, 8.92; S, 10.19. Found: C, 68.47; H, 7.11; N, 8.78; S, 9.89.

1-(4-isopropylcyclohexa-1, 3-dienecarbonyl)-3-m-tolylthiourea (7d, $C_{18}H_{22}N_2OS$)

IR (cm^{-1}): 3423 and 3210 (N–H); 2957 and 2870 (–CH_2, –CH_3); 1665 (–C=O); 1145(–C=S). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.82 (s, 1H, S=C–N–H); 7.43 (s,1H, O=C–N–H);7.25-7.52 (m, 4H, Ar–H); 6.93, 6.95 (d, 1H, OC–C=CH–); 5.87, 5.89 (d, 1H, –CH=C–$(Me)_2$); 2.31-2.45 (m, H, –CH–$(Me)_2$); 2.45-2.50 (t, 2H, –CH_2–C–CO); 2.23-2.30 (t, 2H, -CH_2-C-C=C); 2.36 (s, 3H, CH_3-Ar); 1.07-1.09 (d, 6H, CH_3). TOF-ESI-MS (m/z): 315 $[M + H]^+$; 337 $[M + Na]^+$. Anal. calcd for $C_{18}H_{22}N_2OS$: C, 68.79; H, 7.01; N, 8.92; S, 10.19. Found: C, 68.57; H, 7.06; N, 8.65; S, 9.81.

1-(4-isopropylcyclohexa-1, 3-dienecarbonyl)-3-p-tolylthiourea (7e, $C_{18}H_{22}N_2OS$)

IR (cm^{-1}): 3415, 3203 (N–H); 3030 (Ar–C–H); 1666 (C=O); 1162 (C=S). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.58 (s, 1H, CSNH–); 7.26 (s, 1H, CONH–); 7.18-7.22 (m, 4H, Ar–H); 6.93-6.94 (d, 1H, OC–C=CH–); 5.88-5.89 (d, 1H, –CH=C–$(Me)_2$); 2.41-2.44 (m, H, –CH–$(Me)_2$); 2.46-2.50 (t, 2H, –CH_2–C–CO); 2.26-2.30 (t, 2H, –CH_2–C–C=C); 2.35 (s, 3H, CH_3–Ar); 1.08-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 315 $[M+H]^+$; 337$[M+Na]^+$. Anal. calcd for $C_{18}H_{22}N_2OS$: C, 68.79; H, 7.01; N, 8.92; S, 10.19. Found: C, 69.34; H, 7.06; N, 9.05; S, 9.78.

1-(2,4-dimethylphenyl)-3-(4-isopropylcyclohexa-1,3-dienecarbonyl)thiourea(7f, $C_{19}H_{24}N_2OS$)

IR (cm^{-1}): 3416, 3198 (N–H); 3030 (Ar–C–H); 1662 (C=O), 1151 (C=S). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.57 (s, 1H, CSNH–); 7.26 (s, 1H, CONH–), 7.04-7.09 (m, 3H, Ar–H); 6.95-6.96 (d, 1H, OC–C=CH–); 5.89-5.90 (d, 1H, –CH=C–$(Me)_2$); 2.40-2.44 (m, H, –CH–$(Me)_2$);

2.47-2.51 (t, 2H, –CH_2–C–CO); 2.30-2.34 (t, 2H, –CH_2–C–C=C); 2.32 (s, 3H, 2–CH_3–Ar); 2.27 (s, 3H, 4–CH_3–Ar); 1.09-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 329$[M+H]^+$; 351 $[M+Na]^+$. Anal. calcd for $C_{19}H_{24}N_2OS$: C, 69.51; H, 7.32; N, 8.54; S, 9.76. Found: C, 69.55; H, 7.14; N, 8.62; S, 9.30.

1-(funan-2-yl) ethanone oximyl 4-isopropylcyclohexa-1,3-dienecarboxylate (8a, $C_{16}H_{19}NO_3$)

IR (cm^{-1}): 1729 (–O–C=O); 1606 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.54, 7.57 (d, 1H, furan–α–C-H); 7.14,7.13 (d, 1H, OC–C=CH–); 6.93-6.94 (d, 2H, furan–β–C–H); 5.89, 5.90 (d, 1H, –CH=C–$(Me)_2$); 2.89-2.91 (m, H, –CH–$(Me)_2$); 2.52-2.58 (t, 2H, –CH_2–C–CO); 2.35 (s, 3H, –N=C–CH_3); 2.22-2.29 (t, 2H, –CH_2–C–C=C); 1.07-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 295 $[M+Na]^+$. Anal. calcd for $C_{16}H_{19}NO_3$: C, 70.33; H, 6.96; N, 5.13. Found: C, 70.21; H, 7.03; N, 5.18.

1-(thiophene-2-yl) ethanone oximyl 4-isopropylcyclohexa-1,3-dienecarboxylate (8b, $C_{16}H_{19}NO_2S$)

IR (cm^{-1}): 1738 (–C=O); 1584 (–C=S). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 8.05, 8.03 (d, 1H, thiophene–α–C–H); 7.49, 7.50 (d, 2H, thiophene–β–C–H); 7.09, 7.11 (d, 1H, OC–C=CH–); 5.87, 5.89 (d, 1H, –CH=C–$(Me)_2$); 2.50-2.59 (m, H, –CH–$(Me)_2$); 2.40-2.43 (t, 2H, –CH_2–C–CO); 2.31 (s, 3H, –N=C–CH_3); 2.23-2.24 (t, 2H, –CH_2–C–C=C); 1.06-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 289 $[M + H]^+$. Anal. calcd for $C_{16}H_{19}NO_2S$: C, 66.44; H, 6.57; N, 9.69. Found: C, 66.88; H, 6.34; N, 9.48.

1-(4-chlorophenyl) ethanone oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8c, $C_{18}H_{20}ClNO_2$)

IR (cm^{-1}): 1734 (–O–C=O); 1592 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.70, 7.72 (d, 2H, *o*–C–H); 7.33-7.36 (d, 2H, *m*–C–H); 7.13, 7.14 (d, 1H, OC–C=CH–); 5.91, 5.92 (d, 1H, –CH=C–$(Me)_2$); 2.53-2.55 (m, H, –CH-$(Me)_2$); 2.40-2.41 (t, 2H, –CH_2-C-CO); 2.30 (s, 3H, –N=C–CH_3); 2.20-2.23 (t, 2H, –CH_2–C–C=C); 1.04-1.08 (d, 6H, CH_3). TOF-ESI-MS (m/z): 317 $[M+H]^+$. Anal. calcd for $C_{18}H_{20}ClNO_2$: C, 68.03; H, 6.30; N: 4.41. Found: C, 67.86; H, 6.31; N, 4.51.

1-(*p*-tolyl) ethanone oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8d, $C_{19}H_{23}NO_2$)

IR (cm^{-1}): 1734 (–O–C=O); 1592 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.64, 7.79 (d, 2H, *o*–C–H), 7.51, 7.54 (d, 2H, *m*–C–H); 7.12, 7.17 (d, 1H, OC–C=CH–), 5.87, 5.88 (d, 1H, –CH=C–$(Me)_2$); 2.50-2.58 (m, H, –CH–$(Me)_2$); 2.40-2.41 (t, 2H, –CH_2–C–CO); 2.21-2.23 (t, 2H, –CH_2–C–C=C); 2.27 (s, 3H, Ar–H); 1.80 (s, 3H, –N=C–CH_3); 1.04-1.08 (d, 6H, CH_3). TOF-ESI-MS (m/z): 297 $[M+H]^+$. Anal. calcd for $C_{19}H_{23}NO_2$: C, 76.77; H, 7.74; N, 4.71. Found: C, 75.86; H, 8.15; N, 5.21.

Dicyclohexylmethanone oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8e, $C_{23}H_{35}NO_2$)

IR (cm^{-1}): 1735 (–O–C=O); 1608 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.04, 7.05 (d, 1H, OC–C=CH–); 5.83, 5.85 (d, 1H, –CH=C–$(Me)_2$); 2.51-2.57 (m, H, –CH–$(Me)_2$); 2.35-2.40 (t, 2H, –CH_2–C–CO); 2.20-2.26 (t, 2H, –CH_2–C–C=C); 1.66-1.78 (m, 10H, cyclehexyl–C–H); 1.02-1.06 (d, 6H, CH_3). TOF-ESI-MS (m/z): 261$[M+H]^+$. Anal. calcd for $C_{23}H_{35}NO_2$: C, 77.31; H, 9.80; N, 3.92. Found: C, 77.65; H, 9.63; N, 3.35.

Picolinaldehyde oximyl 4-isopropylcyclohexa-1,3-dienecarboxylate (8f, $C_{16}H_{18}N_2O_2$)

IR (cm^{-1}): 1728 (–O–C=O); 1646 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 8.66-8.68 (d, 1H, pyridine–*α*–C–H); 7.75-7.80 (m, 1H, pyridine–*γ*–C–H); 7.35-7.37 (m, 2H, pyridine–*β*–C–H); 7.18, 7.20 (d, 1H, OC–C=CH–), 5.83, 5.85 (d, 1H, –CH=C–$(Me)_2$); 2.89 (s, 1H, –N=C–H);

2.40-2.45 (m, H, –CH–$(Me)_2$); 2.40-2.41 (t, 2H, –CH_2–C–CO); 2.20-2.23 (t, 2H, –CH_2–C–C=C); 1.04-1.08 (d, 6H, CH_3). TOF-ESI-MS (m/z): 270$[M+H]^+$. Anal. calcd for $C_{16}H_{18}N_2O_2$: C, 71.11; H, 6.67; N, 10.37. Found: C, 71.22; H, 6.87; N, 10.58.

Propan-2-one oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8g, $C_{13}H_{19}NO_2$)

IR (cm^{-1}): 1735 (–O–C=O); 1643 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.04, 7.06 (d, 1H, OC–C=CH–); 5.83, 5.85 (d, 1H, –CH=C–$(Me)_2$); 2.42-2.54 (m, H, –CH–$(Me)_2$); 2.39-2.41 (t, 2H, –CH_2–C–CO); 2.20-2.26 (t, 2H, –CH_2–C–C=C); 2.00 (s, 6H, –N=C–$(Me)_2$); 1.02-1.06 (d, 6H, CH_3). TOF-ESI-MS (m/z): 221$[M+H]^+$. Anal. calcd for $C_{13}H_{19}NO_2$: C, 70.59; H, 8.60; N, 6.33. Found: C, 71.11; H, 8.68; N, 5.73.

Butan-2-one oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8h, $C_{14}H_{21}NO_2$)

IR (cm^{-1}): 1729 (–O–C=O); 1643 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.04, 7.07 (d, 1H, OC–C=CH–); 5.84, 5.86 (d, 1H, –CH=C–$(Me)_2$); 2.57-2.60 (m, H, –CH–$(Me)_2$); 2.39-2.41 (t, 2H, –CH_2–C–CO); 2.15-2.17 (t, 2H, –CH_2–C–C=C); 2.00 (s, 3H, –N=C–CH_3); 1.37-1.41 (m, 2H, –N=C–CH_2–); 1.03-1.05 (d, 6H, CH_3); 0.90-1.00 (t, 3H, –CH_2–CH_3). TOF-ESI-MS (m/z): 236$[M+H]^+$; 258$[M+Na]^+$. Anal. calcd for $C_{14}H_{21}NO_2$: C, 71.49; H, 8.94; N, 5.96. Found: C, 70.79; H, 9.00; N, 6.60.

***E*)-benzaldehyde oximyl 4-isopropylcyclohexa-1,3-dienecarboxylate (8i, $C_{17}H_{19}NO_2$)**

IR (cm^{-1}): 3395 (H–C=N); 1725 (–O–C=O); 1646 (C=N). ^1H NMR ($CDCl_3$, δ/ppm, 300 MHz): 8.43 (s, 1H, –N=CH); 7.76, 7.78 (d, 2H, *o*–C–H); 7.33, 7.43 (m, 3H, *m, p*–C–H); 7.15, 7.16 (d, 1H, OC–C=CH–); 5.84, 5.85 (d, 1H, –CH=C–$(Me)_2$); 2.52-2.58 (m, H, –CH–$(Me)_2$); 2.40-2.41 (t, 2H, –CH_2–C–CO); 2.21-2.29 (t, 2H, –CH_2–C–C=C); 1.04-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z):

269[M+H]$^{+}$. Anal. calcd for $C_{17}H_{19}NO_2$: C, 76.12; H, 7.06 ; N, 5.20. Found: C, 75.92; H, 7.16; N, 5.30.

Acetophenone oximyl 4-isopropylcyclohexa-1, 3-dienecarboxylate (8j, $C_{18}H_{21}NO_2$)

IR (cm^{-1}): 1727 (–O–C=O); 1641 (C=N). ^{1}H NMR ($CDCl_3$, δ/ppm, 300 MHz): 7.77, 7.79 (d, 2H, *o*–C–H); 7.37-7.42 (m, 3H, *m, p*–C–H); 7.14, 7.17 (d, 1H, OC–C=CH–); 5.83, 5.85 (d, 1H, –CH=C–$(Me)_2$); 2.52-2.57 (m, H, –CH–$(Me)_2$); 2.40-2.42 (t, 2H, –CH_2–C–CO); 2.21-2.23 (t, 2H, –CH_2–C–C=C); 2.30 (s, 3H, –N=C–CH_3); 1.04-1.10 (d, 6H, CH_3). TOF-ESI-MS (m/z): 283[M+H]$^{+}$. Anal. calcd for $C_{18}H_{21}NO_2$: C, 76.33; H, 7.42; N, 4.95. Found: C, 76.35; H, 7.57; N, 4.78.

The representative calculations/plots

Table 2 Fungicidal activity of compounds against *R. solani*

NO.	Compd.	Fungicidal activity (%) at a concentration of (μg/mL)					IC_{50}	y=*a*x+*b*	R^2	log IC_{50}
		256	128	64	32	16				
1	**3**	100	67	40	20	0	92.712	y = 0.236 x - 2.722	0.977	1.967
2	**5a**	100	70	53	31	24	69.777	y = 0.175 x - 1.445	0.952	1.844
3	**5b**	100	70	50	30	23	72.485	y = 0.177 x - 1.528	0.971	1.860
4	**5c**	100	72	53	30	25	68.481	y = 0.177 x - 1.456	0.964	1.836
5	**5d**	100	70	50	30	23	72.485	y = 0.177 x - 1.528	0.971	1.860
6	**5e**	100	70	48	30	24	73.144	y = 0.177 x - 1.525	0.986	1.864
7	**5f**	100	72	54	33	25	66.345	y = 0.174 x - 1.382	0.961	1.822
8	**7a**	100	98	89	76	58	3.017	y = 0.235x - 0.102	0.990	0.480
9	**7b**	100	98	89	77	58	2.439	y = 0.236 x - 0.083	0.987	0.387
10	**7c**	100	97	87	73	57	3.284	y = 0.221 x - 0.099	0.990	0.516
11	**7d**	100	98	89	78	58	1.857	y = 0.237 x - 0.063	0.983	0.269
12	**7e**	100	97	87	73	57	3.284	y = 0.221 x - 0.099	0.990	0.516
13	**7f**	100	97	86	72	57	3.770	y = 0.218 x - 0.112	0.994	0.576
14	**8a**	100	95	75	53	33	32.604	y = 0.206 x - 1.089	0.991	1.513
15	**8b**	100	95	76	55	33	31.371	y = 0.207 x - 1.051	0.985	1.497
16	**8c**	100	95	80	61	33	27.470	y = 0.211 x - 0.948	0.957	1.439
17	**8d**	100	95	76	57	33	30.444	y = 0.206 x - 1.011	0.980	1.484
18	**8e**	100	93	70	50	30	36.840	y = 0.200 x - 1.155	0.984	1.567
19	**8f**	100	95	75	54	33	32.146	y = 0.206 x - 1.069	0.989	1.507
20	**8g**	100	95	74	52	32	33.902	y = 0.207 x - 1.138	0.992	1.530
21	**8h**	100	94	72	51	32	35.174	y = 0.201 x - 1.114	0.992	1.546
22	**8i**	100	95	79	60	32	28.749	y = 0.211 x - 0.995	0.960	1.459
23	**8j**	100	95	77	58	32	30.230	y = 0.208 x - 1.026	0.972	1.480
24	**Thiadimenol**	100	98	89	76	59	1.945	y = 0.235 x - 0.065	0.992	0.289

Arrival of equation 2

$$\log IC_{50} = -8.3866 - 39.598 \times HOMO - 19.346 \times DM + 8.8104 \times q^{O}_{max} + 30.670 \times q_{min} \quad (2)$$

$$N = 22,\ R^2 = 0.9879,\ F = 348.41,\ S^2 = 0.0047$$

Table 5 Fungicidal activity and structure descriptors of title compounds

No.	Compd.	log IC_{50}	Structure descriptors			
			HOMO	DM	q^{O}_{max}	q_{min}
1	**5a**	1.844	-0.3512	-0.2067	0.3524	-0.3512
2	**5b**	1.860	-0.3534	-0.2067	0.3523	-0.3534
3	**5c**	1.836	-0.3523	-0.2067	0.3524	-0.3523
4	**5d**	1.860	-0.3525	-0.2067	0.3520	-0.3525
5	**5e**	1.864	-0.3546	-0.2066	0.3519	-0.3546
6	**5f**	1.822	-0.3534	-0.2067	0.3521	-0.3534
7	**7a**	0.480	-0.2713	-0.2072	0.2748	-0.2713
8	**7b**	0.387	-0.2710	-0.2070	0.2522	-0.2768
9	**7c**	0.516	-0.2725	-0.2072	0.2745	-0.2725
10	**7d**	0.269	-0.2718	-0.2072	0.2748	-0.2718
11	**7e**	0.516	-0.2718	-0.2072	0.2749	-0.2718
12	**7f**	0.576	-0.2731	-0.2072	0.2746	-0.2731
13	**8a**	1.513	-0.2896	-0.2095	0.3705	-0.2896
14	**8b**	1.497	-0.2917	-0.4339	0.3685	-0.4339
15	**8c**	1.439	-0.2922	-0.2071	0.3706	-0.2922
16	**8d**	1.484	-0.2950	-0.2070	0.3696	-0.2950
17	**8e**	1.567	-0.2963	-0.2070	0.3697	-0.2963
18	**8f**	1.507	-0.2873	-0.2073	0.3706	-0.2873
19	**8g**	1.530	-0.2945	-0.2086	0.3698	-0.2945
20	**8h**	1.546	-0.2970	-0.2071	0.3691	-0.2970
21	**8i**	1.459	-0.2907	-0.2072	0.3697	-0.2907
22	**8j**	1.480	-0.2940	-0.2071	0.3697	-0.2940

Table 6 The best four-descriptor model

Descriptor No.	*X*	±Δ*X*	*t*-Test	Descriptor
0	-8.3866	1.5216	-5.5119	Intercept
1	-3.9598×10^{1}	1.1968×10^{1}	-3.3086	HOMO[a]
2	-1.9346×10^{1}	7.4859	-2.5843	DM[b]
3	8.8104	4.5244×10^{-1}	19.4733	q^{O}_{max}[c]
4	3.0670×10^{1}	1.1916×10^{1}	2.5738	q_{min}[d]

[a] Energy of the highest occupied molecular orbit in atomatic units. [b] Dipole moment. [c] Max net atomic charge for a O atom. [d] Min net atomic charge.

Table 8 Internal validation of the QSAR model

Training set	*N*	R^2	*F*	S^2	Test set	*N*	R^2	*F*	S^2
A+B	15	0.9800	340.78	0.0043	C	7	0.9843	345.90	0.0045
B+C	14	0.9711	339.58	0.0041	A	8	0.9814	343.25	0.0044
A+C	15	0.9724	339.63	0.0050	B	7	0.9793	341.47	0.0043
Average		0.9745	340.00	0.0045	Average		0.9817	343.54	0.0044

[a] Compounds A: **1, 4, 7, 10, 13, 16, 19, 22,** Compounds B: **2, 5, 8, 11, 14, 17, 20,** Compounds C: **3, 6, 9, 12, 15, 18, 21.**