

Synthesis of Ferrocene-Containing Dichalcones

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Abstract—Condensation of 1,1'-diacetylferrocene with mono- and disubstituted benzaldehydes in 96% ethanol in the presence of sodium hydroxide has afforded ferrocene-containing dichalcones.

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Many derivatives of ferrocene [1] exhibit pronounced biological activity [2–8]. Mono- and disubstituted ferrocene-containing dichalcones **III–XXXVIII** obtained via condensation of 1,1'-diacetylferrocene **I** with mono- and disubstituted benzaldehydes **II** in 96% ethanol in the presence of sodium hydroxide are of interest as compounds potentially possessing antimicrobial and fungicidal activity [9–12] (Scheme 1).

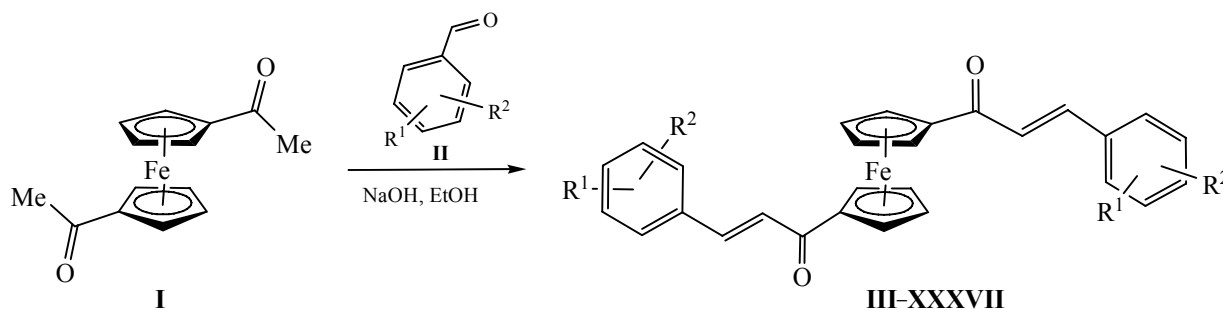
Ferrocene-containing dichalcones **III–XXXVIII** were synthesized with yields of 70–88%. Melting points and elemental analysis data of ferrocene-containing dichalcones **III–XXXVIII** are shown in

Table 1; IR and UV spectroscopy data are given in Table 2.

¹H NMR spectra of dichalcones **III–XXXVIII** contained the following proton signals confirming their structure, ppm: 4.7 br.s (4H, Cp), (4H, Cp), 5.1 br.s (4H, Cp), 7.3–7.9 m (Ar), 7.6 d (2H, =CH), and 7.4 d (2H, =CH). The signals of MeO-protons were observed at 3.7–3.9 ppm. The protons of EtO group resonated at 0.8–1.4 (3H, Me) and 3.6–4.4 ppm (2H, CH₂) [2, 13].

Further chemical modification of ferrocene dichalcones **III–XXXVIII** seems promising in view of

Scheme 1.



R¹ = R² = H (**III**); R¹ = H, 2-R² = OEt (**IV**), *n*-OBu (**V**), OCH₂Ph (**VI**); 4-R² = OMe (**VII**), *n*-OBu (**VIII**), O(CH₂)₁₄Me (**IX**), OCH₂Ph (**X**); 2-R¹ = 4-R² = OEt (**XI**), *n*-OBu (**XII**), OCH₂Ph (**XIII**); 4-R¹ = OMe, 3-R² = OEt (**XIV**); 3-R¹ = OMe, 4-R² = OMe (**XV**), OEt (**XVI**), OCHMe₂ (**XVII**), *n*-OBu (**XVIII**), OCH₂CHMe₂ (**XIX**), O(CH₂)₂CHMe₂ (**XX**), O(CH₂)₅Me (**XXI**), O(CH₂)₇Me (**XXII**), O(CH₂)₁₄Me (**XXIII**), OCH₂C≡CH (**XXIV**), *cyclo*-OC₇H₁₃ (**XXV**); 3-R¹ = OEt, 4-R² = OEt (**XXVI**), OCHMe₂ (**XXVII**), *n*-OBu (**XXVIII**), O(CH₂)₂CHMe₂ (**XXIX**), O(CH₂)₅Me (**XXX**), O(CH₂)₇Me (**XXXI**), O(CH₂)₁₄Me (**XXXII**), *cyclo*-OC₇H₁₃ (**XXXIII**), OCH₂Ph (**XXXIV**), 3-R¹ + 4-R² = OCH₂O (**XXXV**); R¹ = H, 2-R² = OH (**XXXVI**); 4-R² = OH (**XXXVII**); 3-R¹ = OMe, 4-R² = OH (**XXXVIII**).

Table 1. Yields, melting points, and elemental analysis data for ferrocene-containing dichalcones **III–XXXVIII**

Comp. no.	Yield, %	mp, °C	Found, %			Formula	Calculated, %		
			C	H	Fe		C	H	Fe
III	88	154–155	75.69	5.13	12.14	C ₂₈ H ₂₂ FeO ₂	75.35	4.97	12.51
IV	85	176–177	72.28	5.75	10.19	C ₃₂ H ₃₀ FeO ₄	71.92	5.66	10.45
V	81	113–115	73.57	6.61	9.20	C ₃₆ H ₃₈ FeO ₄	73.22	6.49	9.46
VI	82	93–94	76.88	5.34	8.23	C ₄₂ H ₃₄ FeO ₄	76.60	5.20	8.48
VII	85	146–148	71.48	5.24	10.75	C ₃₀ H ₂₆ FeO ₄	71.16	5.18	11.03
VIII	84	122–124	73.50	6.64	9.25	C ₃₆ H ₃₈ FeO ₄	73.22	6.49	9.46
IX	80	58–60	77.77	9.38	6.05	C ₅₈ H ₈₂ FeO ₄	77.48	9.19	6.21
X	81	61–63	76.93	5.34	8.19	C ₄₂ H ₃₄ FeO ₄	76.60	5.20	8.48
XI	83	68–69	69.85	6.29	8.63	C ₃₆ H ₃₈ FeO ₆	69.46	6.15	8.97
XII	84	161–163	72.21	7.66	7.25	C ₄₄ H ₅₄ FeO ₆	71.93	7.41	7.60
XIII	84	79–81	77.48	5.16	7.22	C ₅₆ H ₄₆ FeO ₆	77.24	5.32	6.41
XIV	83	72–73	69.01	5.94	9.07	C ₃₄ H ₃₄ FeO ₆	68.69	5.76	9.39
XV	84	159–160	68.10	5.63	9.45	C ₃₂ H ₃₀ FeO ₆	67.85	5.34	9.86
XVI	82	154–156	68.96	6.04	8.98	C ₃₄ H ₃₄ FeO ₆	68.69	5.76	9.39
XVII	82	120–122	69.90	6.25	8.56	C ₃₆ H ₃₈ FeO ₆	69.46	6.15	8.97
XVIII	86	95–97	70.58	6.73	8.24	C ₃₈ H ₄₂ FeO ₆	70.15	6.51	8.58
XIX	80	100–102	70.73	6.82	8.20	C ₃₈ H ₄₂ FeO ₆	70.15	6.51	8.58
XX	84	86–88	71.05	7.12	7.90	C ₄₀ H ₄₆ FeO ₆	70.79	6.83	8.23
XXI	82	63–65	71.49	7.31	7.32	C ₄₂ H ₅₀ FeO ₆	71.38	7.13	7.90
XXII	80	114–116	72.72	7.87	7.05	C ₄₆ H ₅₈ FeO ₆	72.43	7.66	7.32
XXIII	81	125–127	75.40	9.04	5.39	C ₆₀ H ₈₆ FeO ₆	75.13	9.04	5.82
XXIV	82	63–64	70.68	5.18	8.88	C ₃₆ H ₃₀ FeO ₆	70.37	4.92	9.09
XXV	82	129–131	72.70	7.13	7.24	C ₄₄ H ₅₀ FeO ₆	72.32	6.90	7.64
XXVI	80	117–119	69.85	6.35	8.61	C ₃₆ H ₃₈ FeO ₆	69.46	6.15	8.97
XXVII	81	153–155	70.38	6.67	8.33	C ₃₈ H ₄₂ FeO ₆	70.15	6.51	8.58
XXVIII	80	101–103	71.00	6.98	7.90	C ₄₀ H ₄₆ FeO ₆	70.79	6.83	8.23
XXIX	84	78–80	71.65	7.36	7.64	C ₄₂ H ₅₀ FeO ₆	71.38	7.13	7.90
XXX	79	79–81	72.21	7.67	7.32	C ₄₄ H ₅₄ FeO ₆	71.93	7.41	7.60
XXXI	84	75–77	73.32	8.14	6.89	C ₄₈ H ₆₂ FeO ₆	72.90	7.90	7.06
XXXII	82	57–59	75.79	9.30	5.23	C ₆₂ H ₉₀ FeO ₆	75.43	9.19	5.66
XXXIII	82	145–147	73.23	7.38	7.06	C ₄₆ H ₅₄ FeO ₆	72.81	7.17	7.36
XXXIV	80	96–98	74.30	5.73	7.22	C ₄₆ H ₄₂ FeO ₆	73.99	5.67	7.48
XXXV	81	200–202	67.76	4.12	10.05	C ₃₀ H ₂₂ FeO ₆	67.43	4.15	10.45
XXXVI	74	198–200	70.57	4.90	11.39	C ₂₈ H ₂₂ FeO ₆	70.31	4.64	11.68
XXXVII	71	128–129	70.63	4.95	11.27	C ₂₈ H ₂₂ FeO ₆	70.31	4.64	11.68
XXXVIII	70	164–166	67.28	4.99	10.04	C ₃₀ H ₂₆ FeO ₆	66.93	4.87	10.37

Table 2. IR and UV spectral data for compounds **I** and **III–XXXVIII**

Comp. no.	ν , cm^{-1}	λ_{max} , nm (ϵ)
I	3104, 3089, 3074 (CH_{Cp}); 2960, 2923, 2853 (CH_{Me}); 1660 (C=O); 1456, 1375, 1354, 1279 (C=C_{Cp}); 892, 860, 843, 830, 621 (CH_{Cp})	224 (18000), 264 (13000), 464 (500)
III	3115, 3110, 3085, 3057, 3026 (CH_{Ar} and CH_{Cp}); 1657 (C=O); 1599, 1575, 1497, 1458, 1449, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 870, 830, 770, 760, 730, 687 (CH_{Ar} and CH_{Cp})	229 (15000), 317 (23000)
IV	2112, 3094, 3060, 3032 (CH_{Ar} and CH_{Cp}); 2876, 2923, 2875, 2840 (CH_{Alk}); 1661, 1649 (C=O); 1595, 1491, 1455, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 870, 860, 831, 802, 762, 750 (CH_{Ar} and CH_{Cp})	282 (17000), 310 (16000)
V	3120, 3093, 3080, 3035 (CH_{Ar} and CH_{Cp}); 2956, 2929, 2869 (CH_{Alk}); 1659 (C=O); 1598, 1490, 1456, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 870, 860, 834, 802, 755 (CH_{Ar} and CH_{Cp})	283 (17000), 310 (17000)
VI	3102, 3090, 3063, 3032 (CH_{Ar} and CH_{Cp}); 2924, 2854 (CH_{Alk}); 1665, 1647 (C=O); 1597, 1497, 1484, 1454, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 865, 854, 832, 801, 755, 750, 699, 660 (CH_{Ar} and CH_{Cp})	203 (55000), 255 (14000), 320 (10000)
VII	3117, 3096, 3058, 3040, 3035, 3005 (CH_{Ar} and CH_{Cp}); 2960, 2927, 2838 (CH_{Alk}); 1655 (C=O); 1593, 1573, 1513, 1460, 1423, 1381 (C=C , C=C_{Ar} and C=C_{Cp}); 1294, 1259, 1239, 1173, 1030 (C-O); 825, 818, 800, 720 (CH_{Ar} and CH_{Cp})	224 (24000), 247 (23000), 280 (23000), 292 (25000), 345 (34000)
VIII	3119, 3091, 3080, 3030, 3006 (CH_{Ar} and CH_{Cp}); 2958, 2933, 2872 (CH_{Alk}); 1665, 1659 (C=O); 1595, 1573, 1511, 1462, 1425, 1490, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 870, 827, 804, 730 (CH_{Ar} and CH_{Cp})	224 (24000), 248 (23000), 280 (24000), 293 (25000), 345 (35000)
IX	3121, 3092, 3055, 3030 (CH_{Ar} and CH_{Cp}); 2955, 2918, 2850 (CH_{Alk}); 1664, 1651 (C=O); 1590, 1572, 1512, 1461, 1379 (C=C , C=C_{Ar} and C=C_{Cp}); 1239, 1175, 1082 (C-O); 870, 860, 829, 818, 805, 730, 719 (CH_{Ar} and CH_{Cp})	223 (22000), 246 (23000), 280 (22000), 292 (25000), 344 (34000)
X	3111, 3090, 3055, 3035, 3005 (CH_{Ar} and CH_{Cp}); 2957, 2925, 2865, 2853, 2829, 2805 (CH_{Alk}); 1688 (C=O); 1601, 1575, 1510, 1394 (C=C , C=C_{Ar} and C=C_{Cp}); 1260, 1164, 1019 (C-O); 867, 831, 750, 696, 655 (CH_{Ar} and CH_{Cp})	298 (16000), 359 (19000)
XI	3115, 3092, 3076, 3035, 3010 (CH_{Ar} and CH_{Cp}); 2978, 2927, 2900, 2857 (CH_{Alk}); 1671, 1658 (C=O); 1602, 1504, 1455, 1393 (C=C , C=C_{Ar} and C=C_{Cp}); 1261, 1187, 1116, 1094, 1043 (C-O); 855, 843, 820, 807, 790, 760, 730, 680 (CH_{Ar} and CH_{Cp})	298 (17000), 359 (19000)
XII	3110, 3097 (CH_{Ar} and CH_{Cp}); 2957, 2930, 2869 (CH_{Alk}); 1662 (C=O); 1607, 1586, 1504, 1461, 1432, 1381 (C=C , C=C_{Ar} and C=C_{Cp}); 1329, 1290, 1259, 1182, 1124, 1027 (C-O); 860, 855, 832, 794, 770, 760, 740 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XIII	3108, 3090, 3070, 3031, 3005 (CH_{Ar} and CH_{Cp}); 2960, 2924, 2870, 2849 (CH_{Alk}); 1670 (C=O); 1605, 1579, 1501, 1453, 1436, 1381 (C=C , C=C_{Ar} and C=C_{Cp}); 1261, 1177, 1120, 1100, 1017 (C-O); 832, 820, 796, 731, 697, 680 (CH_{Ar} and CH_{Cp})	204 (58000), 255 (16000), 320 (12000)
XIV	3106, 3092, 3060, 3005 (CH_{Ar} and CH_{Cp}); 2975, 2928, 2837 (CH_{Alk}); 1664, 1650 (C=O); 1587, 1512, 1455, 1380 (C=C , C=C_{Ar} and C=C_{Cp}); 1260, 1222, 1139, 1079, 1027 (C-O); 823, 806, 770, 710 (CH_{Ar} and CH_{Cp})	299 (17000), 359 (19000)
XV	3105, 3088, 3045, 3030, 3002 (CH_{Ar} and CH_{Cp}); 2959, 2923, 2852, 2840 (CH_{Alk}); 1656, 1650 (C=O); 1590, 1515, 1457, 1378 (C=C , C=C_{Ar} and C=C_{Cp}); 1261, 1137, 1081, 1023 (C-O); 840, 830, 812, 760, 710 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XVI	3110, 3090, 3080, 3040, 3010 (CH_{Ar} and CH_{Cp}); 2985, 2923, 2840 (CH_{Alk}); 1664, 1648 (C=O); 1589, 1517, 1458, 1379 (C=C , C=C_{Ar} and C=C_{Cp}); 1260, 1139, 1082, 1031 (C-O); 850, 830, 800, 780, 711 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)

Table 2. (Contd.)

Comp. no.	ν , cm^{-1}	λ_{max} , nm (ϵ)
XVII	3109, 3090, 3085, 3040, 3010 (CH_{Ar} and CH_{Cp}); 2973, 2928, 2880, 2840, 2830 (CH_{Alk}); 1663, 1652 ($\text{C}=\text{O}$); 1586, 1507, 1460, 1420, 1379 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1262, 1240, 1136, 1109, 1078, 1029 ($\text{C}-\text{O}$); 860, 845, 826, 812, 770, 730, 710, 660 (CH_{Ar} and CH_{Cp})	299 (15000), 359 (19000)
XVIII	3109, 3099, 3080, 3060, 3040, 3002 (CH_{Ar} and CH_{Cp}); 2958, 2923, 2871, 2855 (CH_{Alk}); 1662, 1650 ($\text{C}=\text{O}$); 1590, 1512, 1463, 1422, 1379 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1263, 1241, 1137, 1082, 1027 ($\text{C}-\text{O}$); 870, 840, 820, 810, 796, 730, 713, 660 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XIX	3110, 3100, 3099, 3060, 3040, 3015 (CH_{Ar} and CH_{Cp}); 2958, 2930, 2871, 2850, 2835 (CH_{Alk}); 1664, 1650 ($\text{C}=\text{O}$); 1588, 1513, 1467, 1423, 1396, 1379 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1260, 1243, 1138, 1082, 1022 ($\text{C}-\text{O}$); 870, 845, 827, 812, 800, 780, 730, 710, 650 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XX	3101, 3070, 3008 (CH_{Ar} and CH_{Cp}); 2954, 29923, 2866, 2854, 2830 (CH_{Alk}); 1661 ($\text{C}=\text{O}$); 1586, 1511, 1462, 1420, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1261, 1222, 1140, 1028 ($\text{C}-\text{O}$); 870, 860, 811, 760, 735, 716, 660 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XXI	3112, 3088, 3060, 3004 (CH_{Ar} and CH_{Cp}); 2960, 2925, 2855 (CH_{Alk}); 1656 ($\text{C}=\text{O}$); 1588, 1513, 1464, 1424, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1263, 1137, 1082, 1028 ($\text{C}-\text{O}$); 870, 845, 803, 733, 710, 660 (CH_{Ar} and CH_{Cp})	328 (18000)
XXII	3115, 3098, 3080, 3060, 3040, 2999 (CH_{Ar} and CH_{Cp}); 2923, 2852 (CH_{Alk}); 1651 ($\text{C}=\text{O}$); 1589, 1516, 1461, 1423, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1263, 1241, 1137, 1092, 1030 ($\text{C}-\text{O}$); 860, 833, 802, 730, 710, 660 (CH_{Ar} and CH_{Cp})	330 (17000)
XXIII	3120, 3096, 3080, 2998 (CH_{Ar} and CH_{Cp}); 2918, 2850 (CH_{Alk}); 1655 ($\text{C}=\text{O}$); 1586, 1513, 1466, 1425, 1381 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1270, 1236, 1139, 1028 ($\text{C}-\text{O}$); 870, 840, 830, 806, 730, 720, 660 (CH_{Ar} and CH_{Cp})	329 (17000)
XXIV	3271 ($\equiv\text{CH}$); 3110, 3094, 3040, 3001 (CH_{Ar} and CH_{Cp}); 2955, 2922, 2853 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 2119 ($\text{C}\equiv\text{C}$); 1664, 1649 ($\text{C}=\text{O}$); 1588, 1509, 1452, 1421, 1378 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1260, 1213, 1138, 1078, 1018 ($\text{C}-\text{O}$); 872, 844, 830, 806, 759, 730, 709, 688, 646 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XXV	3115, 3090, 3080, 3065, 3040, 3002 (CH_{Ar} and CH_{Cp}); 2923, 2853 (CH_{Alk}); 1659, 1649 ($\text{C}=\text{O}$); 1590, 1510, 1453, 1414, 1375 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1263, 1239, 1162, 1132, 1082, 1028, 1001 ($\text{C}-\text{O}$); 870, 855, 831, 819, 805, 785, 725, 710, 650 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XXVI	3115, 3100, 3087, 3060, 3008 (CH_{Ar} and CH_{Cp}); 2979, 2923, 2870 (CH_{Alk}); 1667, 1649 ($\text{C}=\text{O}$); 1582, 1574, 1509, 1475, 1459, 1429, 1394, 1382 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1261, 1237, 1141, 1084, 1043 ($\text{C}-\text{O}$); 865, 828, 820, 802, 790, 780, 740, 720, 660 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XXVII	3117, 3083, 3060, 3040, 3004 (CH_{Ar} and CH_{Cp}); 2976, 2921, 2880 (CH_{Alk}); 1667, 1649 ($\text{C}=\text{O}$); 1581, 1504, 1460, 1428, 1382 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1262, 1135, 1109, 1084, 1043 ($\text{C}-\text{O}$); 860, 828, 810, 780, 740, 715, 660 (CH_{Ar} and CH_{Cp})	299 (16000), 359 (19000)
XXVIII	3106, 3099, 3084, 3060, 3036, 3005 (CH_{Ar} and CH_{Cp}); 2958, 2926, 2871 (CH_{Alk}); 1663, 1648 ($\text{C}=\text{O}$); 1581, 1508, 1461, 1428, 1394, 1381 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1260, 1219, 1141, 1084, 1043, 1028 ($\text{C}-\text{O}$); 870, 825, 811, 780, 740, 720, 660 (CH_{Ar} and CH_{Cp})	328 (19000)
XXIX	3110, 3098, 3080, 3060, 3040, 3010 (CH_{Ar} and CH_{Cp}); 2955, 2926, 2870 (CH_{Alk}); 1664 ($\text{C}=\text{O}$); 1584, 1510, 1463, 1432, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1262, 1220, 1138, 1079, 1042 ($\text{C}-\text{O}$); 870, 860, 825, 812, 745, 720, 660 (CH_{Ar} and CH_{Cp})	329 (19000)
XXX	3108, 3101, 3084, 3070, 3040, 3006 (CH_{Ar} and CH_{Cp}); 2980, 2950, 2928, 2869, 2856 (CH_{Alk}); 1663, 1648 ($\text{C}=\text{O}$); 1582, 1508, 1467, 1460, 1433, 1394, 1381 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1263, 1220, 1172, 1138, 1084, 1042 ($\text{C}-\text{O}$); 870, 823, 814, 780, 735, 720, 710, 660 (CH_{Ar} and CH_{Cp})	329 (18000)

Table 2. (Contd.)

Comp. no.	ν , cm^{-1}	λ_{max} , nm (ϵ)
XXXI	3108, 3100, 3085, 3060, 3010 (CH_{Ar} and CH_{Cp}); 2975, 2955, 2923, 2853 (CH_{Alk}); 1663, 1648 ($\text{C}=\text{O}$); 1583, 1509, 1460, 1430, 1395, 1381 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1264, 1220, 1138, 1084 ($\text{C}-\text{O}$); 865, 822, 809, 740, 725, 660 (CH_{Ar} and CH_{Cp})	329 (18000)
XXXII	3110, 3096, 3080, 2999 (CH_{Ar} and CH_{Cp}); 2920, 2850 (CH_{Alk}); 1656 ($\text{C}=\text{O}$); 1586, 1513, 1466, 1425, 1382 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1270, 1236, 1139, 1028 ($\text{C}-\text{O}$); 870, 840, 830, 806, 730, 720, 660 (CH_{Ar} and CH_{Cp})	330 (18000)
XXXIII	3110, 3100, 3077, 3040, 3003 (CH_{Ar} and CH_{Cp}); 2976, 2925, 2854 (CH_{Alk}); 1659 ($\text{C}=\text{O}$); 1583, 1510, 1460, 1379 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1259, 1243, 1141, 1094, 1044, 1004 ($\text{C}-\text{O}$); 860, 831, 812, 798, 765, 660 (CH_{Ar} and CH_{Cp})	330 (17000)
XXXIV	3010, 3099, 3086, 3060, 3030, 3010 (CH_{Ar} and CH_{Cp}); 2973, 2922, 2853 (CH_{Alk}); 1661, 1647 ($\text{C}=\text{O}$); 1583, 1509, 1454, 1430, 1396, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1260, 1138, 1081, 1041, 1027, 1011 ($\text{C}-\text{O}$); 860, 850, 827, 807, 754, 739, 710, 700, 670 (CH_{Ar} and CH_{Cp})	204 (52000), 255 (14000), 322 (10000)
XXXV	3116, 3095, 3070, 3030, 3008 (CH_{Ar} and CH_{Cp}); 2960, 2920, 2860 (CH_{Alk}); 1658 ($\text{C}=\text{O}$); 1588, 1499, 1449, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1258, 1079, 1036 ($\text{C}-\text{O}$); 834, 811, 750, 740, 720, 660 (CH_{Ar} and CH_{Cp})	298 (16000), 360 (21000)
XXXVI	3315 (OH); 3111, 3098, 3055, 3035, 3009 (CH_{Ar} and CH_{Cp}); 1657, 1633 ($\text{C}=\text{O}$); 1603, 1595, 1503, 1456, 1382 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1280, 1246, 1212, 1108, 1089, 1042 ($\text{C}-\text{O}$); 870, 828, 810, 747, 720, 645 (CH_{Ar} and CH_{Cp})	298 (16000), 359 (18000)
XXXVII	3377 (OH); 3112, 3100, 3093, 3020 (CH_{Ar} and CH_{Cp}); 1651 ($\text{C}=\text{O}$); 1607, 1579, 1514, 1454, 1382 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1279, 1238, 1215, 1170, 1112, 1082, 1044 ($\text{C}-\text{O}$); 890, 830, 780, 740, 670, 645, 625 (CH_{Ar} and CH_{Cp})	297 (18000), 359 (18000)
XXXVIII	3505 (OH); 3110, 3101, 3055, 3010 (CH_{Ar} and CH_{Cp}); 2970, 2922, 2845 (CH_{Alk}); 1661 ($\text{C}=\text{O}$); 1581, 1514, 1459, 1430, 1398, 1380 ($\text{C}=\text{C}$, $\text{C}=\text{C}_{\text{Ar}}$ and $\text{C}=\text{C}_{\text{Cp}}$); 1270, 1244, 1212, 1185, 1159, 1125, 1094, 1079, 1031 ($\text{C}-\text{O}$); 900, 829, 780, 770, 720, 660, 645, 625 (CH_{Ar} and CH_{Cp})	297 (18000), 360 (20000)

their covalent binding with pharmacophores derived from 1,2-azoles and carborane-*C*-carboxylic acid [2, 11, 12].

EXPERIMENTAL

IR spectra (pellets with KBr) were recorded using a Nicolet Protégé-460 FTIR spectrophotometer. UV spectra (1×10^{-4} mol/L solutions in methanol) were registered with a Varian Cary-300 UV spectrophotometer. ^1H NMR spectra (CDCl_3) were recorded on a Bruker Avance-500 relative to the residual signals of CHCl_3 .

Physico-chemical characteristics of 1,1'-diacetylferrocene **I** and substituted benzaldehydes **II** corresponded to the available reference data [1, 2, 13].

(2*E*,21*E*)-Ferrocenyl-1,1'-bis(3-arylprop-2-en-1-ones) (III–XXXV). A mixture of 0.033 mol of 1,1'-diacetylferrocene **I**, 0.01 mol of benzaldehyde or

substituted alkoxybenzaldehyde **II**, and 0.005 mol of NaOH in 50 mL of 96% ethanol was stirred at 20–23°C during 24 h. The reaction mixture was diluted with 150 mL of water, and the precipitate was filtered off, washed with large amount of distilled water (1.5–2 L), and dried at 35–40°C in air. Compounds **III–XXXV** were purified via low-temperature recrystallization from 80% ethanol.

(2*E*,21*E*)-Ferrocenyl-1,1'-bis[3-(hydroxyaryl)-prop-2-en-1-ones] (XXXVI–XXXVIII). A mixture of 0.01 mol of 1,1'-diacetylferrocene **I**, 0.03 mol of 2- or 4-hydroxybenzaldehyde or vanillin, and 0.05 mol of NaOH in 50 mL of 96% ethanol was stirred at 20–23°C during 24 h. The reaction mixture was diluted with 150 mL of water, and 30 mL of aqueous solution of 0.05 mol of HCl was slowly added dropwise upon vigorous stirring. The precipitate was filtered off at a porous glass filter, washed with large amount of distilled water (1.5–2 L), and dried at 35–40°C in air.

Compounds **XXXVI–XXXVIII** were purified via low-temperature recrystallization from 70% ethanol.

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