First Electrophilic Substitution of (-)-Agroclavine, Indoramine, Phenothiazine, Chlorpromazine, Iminodibenzyl, Imipramine, and Phenazone with Triethyl Orthoformate as an a[1]-Synthon

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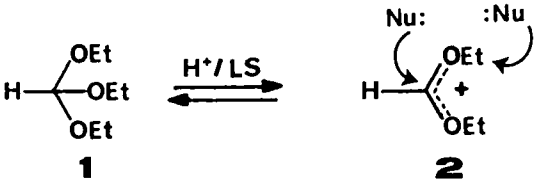
Agroclavine, imipramine hydrochloride, and phenazone reacted with triethyl orthoformate under acid catalysis in an electrophilic, tandem substitution reaction to furnish C_3-symmetrical tris(heteroaryl)methanes while indoramine, phenothiazine, and iminodibenzyl were formylated, ethylated, or ethoxymethylated. The ambident electrophilic reactivity of triethyl orthoformate as an a[1]-synthon was clearly apparent.

Erste elektrophile Substitutionen von (-)-Agroclavin, Indoramin, Phenothiazin, Chlorpromazin, Iminodibenzyl, Imipramin und Phenazon mit Orthoameisensäuretriethylester als a[1]-Synthon

Agroclavin, Imipraminhydrochlorid und Phenazon reagieren mit Orthoameisensäuretriethylester säurekatalysiert in einer elektrophilen Tandem-Substitution zu C_3-symmetrischen Trihetarylmethanen, während Indoramin, Phenothiazin und Iminodibenzyl formyliert, ethyliert oder ethoxymethyliert werden. Die ambidente elektrophile Reaktivität des Elektrophils kommt als a[1]-Synthon voll zum Tragen.

The synthetic chemistry of triethyl orthoformate (**1**) as an a[1]-synthon (formylating and alkylating reagent) towards electron-rich π-systems has been thoroughly investigated in the course of our ongoing studies[1]. The ambident diethoxycarbenium ion (**2**), generated *in situ* from **1** by the action of a *Brönsted* or a *Lewis* acid, has been discussed as the reactive species[1]; in its behaviour towards nucleophiles (Nu:), **2** can be considered as a synthetic equivalent of both the formylium ion and the ethylium ion.



1 **2**

The only reports published up to date on the subject of electrophilic substitution reactions of electron-rich drugs and structurally related systems with **1** are our preparative studies[2,3] which at the same time show that **1** also functions as an extremely selective colour reagent. The successful application of **1** as a reagent in drug analysis has been described in detail in Ref.[3].

We now report on further results from the reactions of ambident, nucleophilic drugs such as (-)-agroclavine (**3**), indoramine (**4**), phenothiazine (**5**), chlorpromazine (**6**), iminodibenzyl (**7**), imipramine (**8**), and phenazone (**9**) with **1** under *Brönsted* or *Lewis* acid catalysis.

Results and Discussion

In continuation of our investigations on the S_EAr reactions of indole derivatives[3,4], we became interested in the behaviour of the drugs agroclavine (**3**) and indoramine (as the hydrochloride; **4**) towards reactions with the electrophile **1** in the hope of acquiring new information on the reactivities of the compounds and the synthetic scope of the methodology. The relatively mild trichloroacetic acid was chosen as the catalytically active acid. Sufficient amounts of the free base molecules of the tested drugs **3** and **4** are present in the equilibrium under the selected reaction conditions.

Thus, the reaction of agroclavine (**3**) with triethyl orthoformate (**1**) proceeded regioselectively (only substrates and the one product **10a** could be detected by analysis of the reaction mixture) to furnish the novel molecular three-bladed propeller **10a**[2], a 2,2',2"-tris(indolyl)methane with C_3-symmetry. The mechanism of the reaction comprises an electrophilic tandem substitution. Work-up of **10a**, which is extremely sensitive towards oxidation on account of its leucobase structure, was performed by means of "rapid" centrifugal layer chromatography (CLC) and its constitution was unambiguously confirmed by FAB-mass and 400 MHz ^{1}H-NMR spectroscopy. Under the selected reaction conditions and within the detection limits of the NMR spectroscopic analysis, stereoisomerisation of the agroclavine skeleton in **10a** did not take place.

Indoramine (as the hydrochloride; **4**) reacted only in pure **1**, acting as both solvent and electrophile, in the presence of trichloroacetic acid. As a consequence of the steric control of the reaction, the N-formylated derivative **10b** was the only product obtained. In this case also, CLC was highly suitable for the isolation and purification of the derivatised drug.

^{1}H-NMR spectroscopy of **10b** (D_6-DMSO) revealed a mixture of (*E*)- and (*Z*)- rotamers in a 4:6 ratio in a thermodynamic equilibrium at 20°C. The stereochemical assignments were clarified by differential ^{1}H,^{1}H-NOE measurements (Fig. 1).

The phenothiazine parent compound **5**, which is sensitive towards oxidation, reacted sluggishly with **1** in CH_2Cl_2

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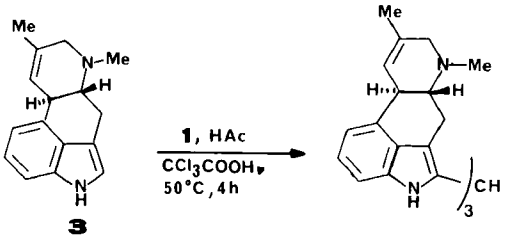
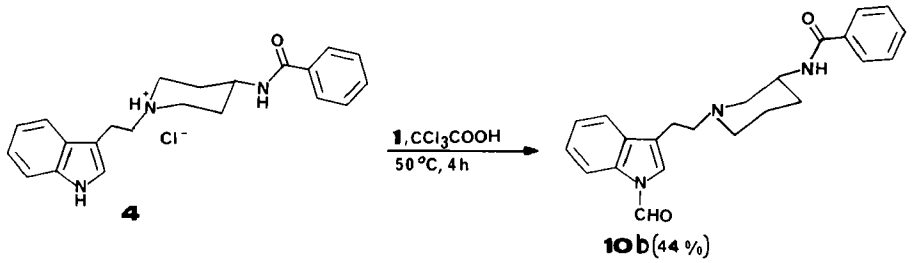




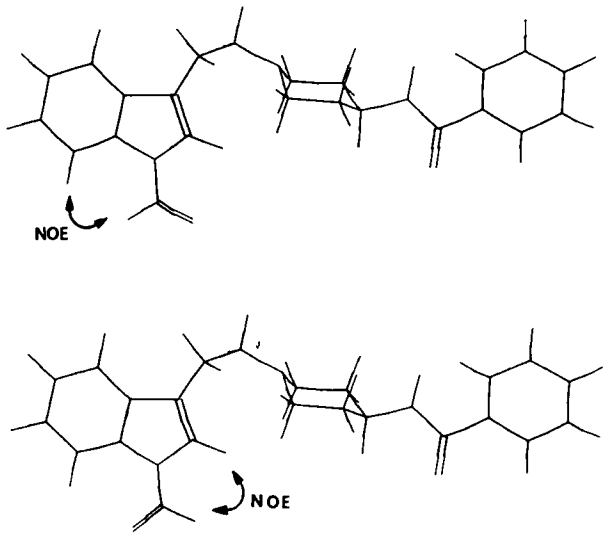


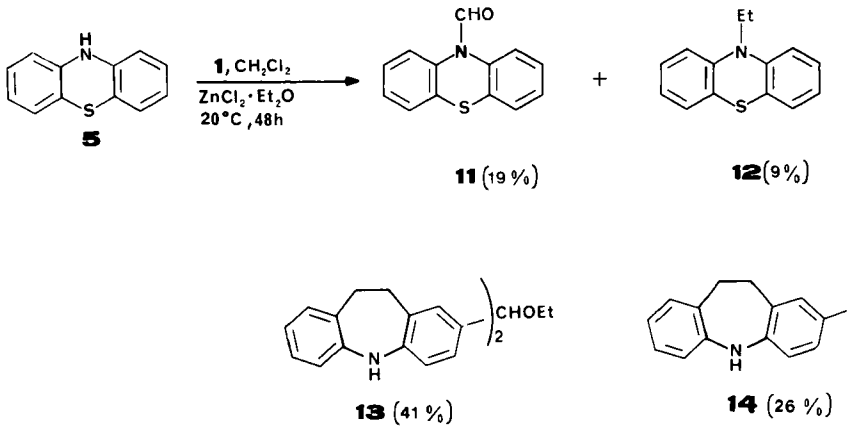
Figure 1. Geometry-optimised and energy-minimised predominant configurations of (*E*)- and (*Z*)-**10b** according to force field calculations. [$E_{(E)}$ = 18.7 kcal · mol^{-1}; $E_{(Z)}$ = 19.1 kcal · mol^{-1}; programme: Alchemy II TM, TRIPOS Associates, St. Louis, MO/USA]. The diagnostically relevant ^{1}H,^{1}H-NOE's are also shown.

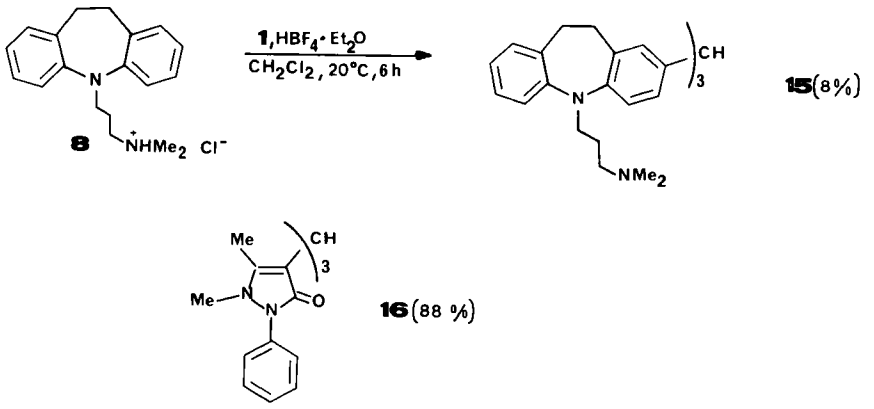
under $ZnCl_2$-diethyl etherate catalysis and anhydrous conditions to give the phenothiazine derivatives **11** and **12**. The ambident electrophilic reactivity of the electrophile **2**, generated *in situ* from **1**, is well known from the lit. and is clearly apparent in this reaction[1].

In the reaction of **1** with chlorpromazine (as the hydrochloride; **6**) and in spite of variations in the reaction conditions, no definable and analytically characterisable products could be isolated in a pure form although TLC analysis of the reaction mixture did indicate that a derivatisation had occurred.

Iminodibenzyl (**7**), the parent compound of the iminodibenzyl pharmaceuticals, reacted with **1** under mild conditions and $ZnCl_2$ diethyl etherate catalysis to the bis(aryl)ethoxymethane **13**. The regiochemistry of the electrophilic C2-attack at **7** is in accordance with reported data[5]. The constitution of **13** was confirmed by differential ^{1}H,^{1}H-NOE measurements and INDOR spectra. When this reaction was performed with a 10 molar excess of **1**, the iminodibenzyl-2-carbaldehyde (**14**) was formed in addition.

In contrast but in analogy to the reaction of **3** with **1**, imipramine (as the hydrochloride; **8**) reacted with **1** under HBF_4 diethyl etherate catalysis to furnish the C_3 symmetrical triarylmethane derivative **15** in 8% yield as the sole,





preparatively characterisable product. **15** was purified by flash chromatography and its constitution confirmed by FD-mass and ^{1}H-NMR spectroscopy.

Phenazone (**9**) also reacted with **1** to a completely C_3 symmetrical product. The reaction was performed in pure **1** as both solvent and electrophile under trichloroacetic acid catalysis and gave rise to the tris(pyrazolyl)methane **16** - a "leucobase" which is extremely stable towards oxidation. The regiochemistry of the attack (exclusive C-4-subsitution) is in accordance with the reported chemistry of **9**[6].

A plausible explanation for this attack of the electrophile at the C-4 of **9** is the presence of the electronically integrated "push-pull" alkene structure in **9**.

The present investigations have shown that, in addition to its reactions with anilines[3], indoles[2], and pyrroles[4] which all exhibit high charge densities and high HOMO energies, triethyl orthoformate (**1**) is also able to take part in electrophilic substitutions with significantly less electron-rich arenes and heterocyclic systems. Specially designed and selective reaction conditions, above all, are essential for the success of these reactions and for the preparative isolation of novel derivatives of the tested drugs and their parent skeletons.

We are grateful to the Deutsche Forschungsgemeinschaft, Bonn, for financial support of this work and to Dr. *Camran Flo*, University of Mainz, for computer-assisted molecular modeling.

Experimental Part

For chromatographic techniques, analytical apparatus, and methods of structure elucidation: Ref.[2]; petroleum ether: boiling range 40-60°C.

Reaction of (-)-Agroclavine (**3**) *with Triethyl Orthoformate* (**1**) *to form the 2,2',2"-Tris(indolyl)methane* (**10a**)

Agroclavine (**3**; 238 mg, 1 mmol) in a mixture of triethyl orthoformate (**1**; 296 mg, 2 mmol), trichloroacetic acid (1 g, 6.14 mmol), and 9 ml glacial acetic acid was stirred at 50°C (water bath). After an initial violet colouration, the mixture became dark blue. The reaction was quenched after 4 h by basification with a mixture of NH_3 and ice/water and the resultant mixture was extracted with three 50 ml portions of CH_2Cl_2. The combined org. phases were dried, evaporated, and the resultant crude product was separated by CLC[2] (chloroform, under an NH_3 atmosphere). **10a** was then obtained as a fine crystalline, light beige-coloured precipitate from MeOH. Yield 75 mg (31 %). - M.p. 270°C (decomp.). - $C_{49}H_{52}N_6$ (725.0). - Pos. FAB-MS: m/z (%) = 726 ($M^{+\cdot}$ + 1, 100), 725 (51), 724 (27). - IR (KBr): ν (cm^{-1}) = 3600-2600 (broad, highly overlapped bands), 1650 (m, br.), 1600 (s, br.), 1450 (s), 1335 (s), 1230 (m), 1195 (w), 1165 (w), 1130 (m), 1070 (w), 1020 (w), 970 (w), 810 (w), 780 (w), 750 (s). - ^{1}H-NMR (400 MHz, D_6-DMSO): δ (ppm) = 1.65 (s, 9H, CH_3), 1.74 (s, 9H, CH_3), 1.96-2.11 (m, 6H, H-5, H-4), 2.29 (br. d, J = 12 Hz, 3H, H-4), 2.53 (br. d, ^{2}J = 16.4 Hz, 3H, H-7), 2.99 (br. d, ^{2}J = 16.3 Hz, 3H), 3.39 (mc, 3H, H-10; hidden by H_2O signal in room temp. spectrum, visible in spectrum recorded at 50°C), 6.02 (s, 1H, central methine H), 6.07 (s, 3H, H-9), 6.84 (d, ^{3}J = 7 Hz, 3H, H-12 or H-14), 6.96 ("t", ^{3}J = 7.5 Hz, 3H, H-13), 7.08 (d, ^{3}J = 8 Hz, H-14 or H-12), 10.74 (s, 3H, NH).

N-{1-[2-(1-Formyl-1H-indol-3-yl)-ethyl]-4-piperidinyl}benzamide (**10b**)

Indoramine hydrochloride (**4**; 380 mg, 1 mmol) was suspended in trichloroacetic acid (800 mg, 4.9 mmol) and 4.5 ml triethyl orthoformate (**1**). The mixture was warmed to 50°C whereupon **4** slowly dissolved. After 4 h, the yellow-orange coloured mixture was treated with 10 ml water, stirred for further 10 min, then cooled in ice, and carfully made alkaline by addition of conc. NH_3. The aqueous solution was extracted with three 20 ml portions of CH_2Cl_2, the org. extracts were dried with Na_2SO_4 and concentrated. The residue was taken up in a small volume of eluent and purified by CLC[2] ($CHCl_3$/MeOH, 95/5, NH_3 atmosphere). The pure product (TLC analysis) was obtained as a white, amorphous precipitate from CH_2Cl_2/petroleum ether. Yield 166 mg (44 %). - M.p. 170°C. - EI-MS (70 eV m/z (%) = 218 (13), 217 (100), 174 (25), 130 (11), 105 (62). - IR (KBr): ν (cm^{-1}) = 3300 (s, NH), 3100 (w), 3060 (s), 2950 (m), 2850 (w), 2800 (m), 2770 (w), 1710 (s), 1630 (s), 1600 (w), 1575 (w), 1530 (s), 1485 (w), 1455 (s), 1375 (s), 1335 (m), 1310 (w), 1285 (w), 1245 (w), 1225 (w), 1185 (m), 1160 (w), 1140 (w), 1120 (m), 1080 (m), 1060 (w), 790 (m), 750 (m), 700 (m). - ^{1}H-NMR (400 MHz, D_6-DMSO): δ (ppm) = 1.59 (mc, 2H, CH_2), 1.79 (br. d, 2H, CH_2), 2.06 (br. t, 2H, CH_2), 2.63 (br. t, 2H, CH_2), 2.84 (br. t, 2H, CH_2), 2.99 (br. d, 2H, CH_2), 3.78 (mc, 1H, piperidine methine H), 7.3-7.36 (m, 2H, indole H-5 or indole H-6, CONH), 7.43 (t, ^{3}J = 7.3 Hz, 2H, arom. H), 7.50 (t, ^{3}J = 7.2 Hz, 1H, arom. H), 7.62-7.68 (m, 2H, indole H-6 or indole H-5, indole H-5), 7.84 (d, ^{3}J = 7.2 Hz, 2H, arom. H), 8.0, 8.2 (2 br. d, 1H, indole H-7), 8.25 (d, ^{3}J = 7.5 Hz, 1H, indole H-4), 9.22, 9.62 (2 br. s, 1H, CHO). - $C_{23}H_{25}N_3O_2$ (375.5) Calcd. C 73.6 H 6.71 N 11.2 Found C 73.6 H 6.74 N 11.1.

N-Formylphenothiazine (**11**) *and N-Ethylphenothiazine* (**12**)

Phenothiazine (**5**; 2 g, 10 mmol) together with **1** (1.5 g, 10 mmol) and $ZnCl_2 \cdot Et_2O$ (4.5 ml of a 2.2 molar solution in CH_2Cl_2, 10 mmol) was dissolved in 35 ml CH_2Cl_2. The mixture got dark blue. After 6 h at room temp., further portions of **1** (1.5 g) and $ZnCl_2 \cdot Et_2O$ solution (4.5 ml) were added and after a further 24 h again 1.5 g **1** (1.5 g) were added. After a total of 48 h, the mixture was made basic by 5% aqueous NaOH and extracted several times with CH_2Cl_2. The combined org. extracts were

concentrated and the crude products **11**, **12** were separated by column chromatography (cc) (petroleum ether/ethyl acetate, 9/1): Small, colourless, matted needles from petroleum ether.

11. - Yield 427 mg (19 %). - M.p. 144°C, Ref.[7]: 144-145°C. EI-MS (70 eV): m/z (%) = 227 ($M^{+\cdot}$, 66), 198 (100). - IR (KBr): ν (cm^{-1}) = 1690 (s), 1590 (w), 1485 (w), 1470 (s), 1445 (m), 1410 (w), 1380 (s), 1300 (m), 1290 (w), 1260 (s), 1240 (m), 1160 (w), 1150 (m), 1130 (w), 1040 (w), 955 (w), 930 (w), 790 (w), 765 (m), 750 (s), 725 (m), 705 (w). - ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.17-7.40 (m, 7H, aromatic H), 7.73 (d, ^3J = 7.6 Hz, 1H, arom. H), 8.65 (s, 1H, CHO). - $C_{13}H_9NOS$ (227.3) Calcd. C 68.7 H 3.99 N 6.2 S 14.1 Found C 68.7 H 4.10 N 6.2 S 14.1.

12. - Yield 204 mg (9 %). - M.p. 102°C, Ref.[7]: 103-105°C. - EI-MS (70 eV): m/z (%) = 227 ($M^{+\cdot}$, 70), 212 (16), 198 (100). - IR (KBr) ν (cm^{-1}) = 3070 (w), 3000 (w), 2950 (w), 2880 (w), 1590 (m), 1570 (w), 1490 (w), 1460 (s), 1440 (s), 1390 (w), 1330 (m), 1280 (m), 1255 (s), 1235 (m), 1145 (w), 1135 (m), 1115 (w), 1060 (w), 1040 (w), 895 (w), 765 (s), 740 (m). - ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.41 (t, ^3J = 7.0 Hz, 3H, CH_2CH_3), 3.92 (mc, 2H, CH_2CH_3), 6.88 (mc, 4H, arom. H), 7.14 (mc, 4H, arom. H). - $C_{14}H_{13}NS$ (227.3) Cacld. C 74.0 H 5.76 N 6.2 S 14.1 Found C 73.9 H 5.86 N 6.3 S 14.1.

Bis(10,11-dihydro-5H-dibenz[b,f]azepin-2-yl)methyl ethyl ether (**13**)

Iminodibenzyl (**7**; 975 mg, 5 mmol) and (3 g, 20 mmol) were dissolved in 30 ml CH_2Cl_2, then $ZnCl_2 \cdot Et_2O$ (4.5 ml of a 2.2 molar solution in CH_2Cl_2, 10 mmol) was added dropwise. After an initial yellow-brown colouration the mixture soon became dark green. After 14 h at room temp. the mixture was treated with 20 ml EtOH whereupon the formed dark-coloured precipitate dissolved almost completely. The mixture was then made alkaline with NH_3/ice/water and extracted with CH_2Cl_2. The org. extracts were dried, evaporated, and the crude product was separated by flash chromatography (petroleum ether/ethyl acetate, 85/15). Product **13** was obtained from petroleum ether as a beige, amorphous solid. Yield 457 mg (41 %). - M.p. 66-68°C. - HR-MS (70 eV): m/z = 446.5921 (calcd. for $C_{31}H_{30}N_2O$: 446.5910). - EI-MS (70 eV): m/z (%) = 446 ($M^{+\cdot}$, 13), 401 (34), 58 (100). - IR (KBr) ν (cm^{-1}) = 3380, 3350 (w, NH), 3020 (w), 2970 (w), 2900 (w), 2840 (w), 1610 (w), 1590 (m), 1490 (s), 1440 (m), 1340 (m), 1330 (m), 1285 (w), 1250 (w), 1125 (w), 1065 (m), 1020 (w), 940 (w), 905 (w), 890 (w), 815 (w), 765 (m), 750 (m), 720 (w). - ^{1}H-NMR (400 MHz, C_6D_6): δ (ppm) = 1.26 (^3J = 7.0 Hz, 3H, OCH_2CH_3), 2.82 (mc, 8H, CH_2CH_2), 3.51 (q, ^3J = 7.0 Hz, 2H, OCH_2CH_3), 5.27 (s, 1H, central methine H), 5.48 (s, 2H, NH), 6.28 (br. d, ^3J = 7.9 Hz, 2H, H-6 or H-9), 6.30 (d, ^3J = 8.2 Hz, 2H, H-4), 6.72 (dd, ^3J = 7.4 Hz, ^4J = 0.9 Hz, 2H, H-7 or H-8), 6.84 (br. d, ^3J = 7.4 Hz, 2H, H-9 or H-6), 6.97 (dd, ^3J = 7.6 Hz, ^4J = 1.5 Hz, 2H, H-8 or H-7), 7.17 (d, ^4J = 1.6 Hz, 2H, H-1), 7.26 (dd, ^3J = 8.2 Hz, ^4J = 1.9 Hz, 2H, H-3).

10,11-Dihydro-5H-dibenz[b,f]azepine-2-carbaldehyde (**14**)

Iminodibenzyl (**7**; 500 mg, 2.56 mmol) together with **1** (4 g, 27 mmol) and $ZnCl_2 \cdot Et_2O$ (6.1 ml of a 2.2 molar solution in CH_2Cl_2, 13.5 mmol) were dissolved in 30 ml CH_2Cl_2. The mixture was stirred at room temp. for 4 h, then made alkaline by NH_3/ice/water, and extracted with CH_2Cl_2. The crude product was purified by cc (petroleum ether/ethyl acetate, 85/15): Greenish-coloured crystals from petroleum ether. Yield 150 mg (26 %). - M.p. 119-120°C. - HR-MS (70 eV): m/z = 223.2729 (calcd. for $C_{15}H_{13}NO$: 223.2715). - EI-MS (70 eV): m/z (%) = 223 ($M^{+\cdot}$, 100). - IR (KBr): ν (cm^{-1}) = 3320 (m), 3210 (w), 3140 (w), 3040 (w), 2940 (w), 2910 (w), 2810 (w), 2730 (w), 1665 (s), 1630 (m), 1580 (s), 1535 (m), 1490 (s), 1440 (m), 1400 (w), 1350 (s), 1320 (m), 1295 (m), 1260 (w), 1230 (m), 1215 (m), 1180 (m), 1125 (m), 990 (w), 940 (m), 900 (w), 835 (w), 820 (m), 760 (s), 720 (w). - ^{1}H-NMR (400 MHz, C_6D_6): δ (ppm) = 2.64 (mc, 4H, CH_2CH_2), 6.06 (s, 1H, NH), 6.12 (d, ^3J = 8.3 Hz, 1H, H-4), 6.39 (d, ^3J = 7.9 Hz, 1H, H-6 or H-9), 6.75 (dd, ^3J = 7.4 Hz, ^4J = 0.9 Hz, 1H, H-7 or H-8), 6.83 (br. d, ^3J = 7 Hz, 1H, H-9 or H-6), 6.97 (dd, ^3J = 7.6 Hz, ^4J = 1.5 Hz, 1H, H-8 or H-7), 7.24 (s, 1H, H-1), 7.49 (dd, ^3J = 8.3 Hz, ^4J = 1.5 Hz, 1H, H-3), 9.73 (s, 1H, CHO).

Reaction of Imipramine Hydrochloride (**8**) *with Triethyl Orthoformate* (**1**) *to* **15**

Imipramine hydrochloride (**8**; 1.902 g, 6 mmol) was dissolved in 6 ml CH_2Cl_2 and 6 ml **1**. The solution was cooled in ice and $HBF_4 \cdot Et_2O$ (1.08 ml of a 54 % solution in Et_2O, 7.8 mmol) was added. The mixture was stirred at room temp. for 6 h, made alkaline by NH_3/ice/water, and extracted several times with CH_2Cl_2/isopropanol (4/1). The combined org. extracts were dried and evaporated. The crude product was purified by flash chromatography (petroleum ether/toluene/Et_2NH, 60/30/10). Product **15** was obtained as a white, fine crystalline precipitate. Yield 136 mg (8 %). - M.p. 164°C. - HR-MS (70 eV): m/z = 851.2351 (calcd. for $C_{58}H_{70}N_6$: 851.2322). - FD-MS: m/z (%) = 850 ($M^{+\cdot}$, 100), 766 (5), 765 (7). - IR (KBr): ν (cm^{-1}) = 3020 (w), 2940 (s), 2820 (m), 2760 (s), 1595 (w), 1485 (s), 1465 (m), 1375 (w), 1330 (m), 1315 (m), 1295 (w), 1255 (m), 1230 (s), 1170 (w), 1150 (w), 1135 (w), 1115 (m), 1100 (w), 1065 (w), 1040 (w), 975 (w), 915 (w), 830 (w), 750 (s). - ^{1}H-NMR (400 MHz, D_6-DMSO): δ (ppm) = 1.52 (mc, 6H, CH_2), 2.0 (s, 18H, $N(CH_3)_2$), 2.16 (t, ^3J = 6.9 Hz, 6H, CH_2), 2.97 (q, AA'BB', ^3J = 7.3 Hz, 12H, iminodibenzyl CH_2CH_2), 3.62 (t, ^3J = 6.9 Hz, 6H, CH_2), 5.19 (s, 1H, central methine H), 6.75 (d, ^3J = 8.2 Hz, 3H, arom H), 6.81 (s, 3H, H-1), 6.87 (d, ^3J = 8.1 Hz, 3H, arom. H), 6.95 (d, ^3J = 8.4 Hz, 3H, arom. H), 7.04-7.11 (m, 9H, arom. H).

4,4',4"-Tris (1,5-dimethyl-3-oxo-2-phenyl-1,2-dihydro-3H-pyrazolyl)-methane (**16**)

A mixture of phenazone (**9**; 377 mg, 2 mmol), **1** (2 ml, 12.1 mmol) and trichloroacetic acid (2 g, 12.3 mmol) was warmed at 50°C. The mixture became orange; after 12 h, it was treated with NH_3/ice/water, and extracted three times with CH_2Cl_2. The combined org. phases were dried and evaporated. The crude product was purified by cc ($CHCl_3$/MeOH, 95/5). **16** precipitated from acetone as white needles. Yield 340 mg (88 %). - M.p.: transformation to a highly viscous state at about 160°C, clear melt at about 235°C; Ref.[9]: m.p. 238°C (decomp.). - EI-MS (70 eV): m/z (%) = 574 ($M^{+\cdot}$, 15), 56 (100). - IR (KBr): ν (cm^{-1}) = 3080 (w), 3020 (w), 2990 (w), 2930 (w), 1670 (s), 1620 (m), 1595 (s), 1495 (s), 1455 (m), 1400 (m), 1365 (w), 1340 (m), 1310 (s), 1240 (m), 1165 (m), 1135 (w), 1045 (w), 850 (w), 780 (m), 760 (s), 735 (w), 715 (w), 695 (m). - ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 2.26 (s, 9H, CH_3), 2.98 (s, 9H, CH_3), 5.06 (s, 1H, central methine H), 7.2 (mc, 3H, arom. H), 7.38 (br. d, 12H, arom. H). - $C_{34}H_{34}N_6O_3$ (574.7) Calcd. C 71.1 H 5.96 N 14.6 Found C 71.2 H 6.12 N 14.3.

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