methylphenyl-3,4,6,7,9,10-hexahydro 1,8 (2H,5H) aminine
dian. (C$_{12}$H$_{13}$NO$_{2}$) Crystal data: Space group Pbnm, a=10.899,
b=12.272, c=10.618 A, Z=8. Trial structure re\-nued to R=0.11. 
Structural and conformational features in these three
aminines will be presented.

PS-06.05.07 STRUCTURE OF 6(R)-6-(TETRA-O-ACETYL-D-0-ARA
BINO-TETROIL-1-YL)-3-(4-CHLOROPHENYL)-1,2-BIS(ETHY
CARBONYL)-1,3-0HETHYDROBISTRAZINE. By M. J.
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Departamento de Fisica de la Materia Condensada. Universidad de Sevilla. Apdo. 
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The crystal structure of the 6(r)-6[tetra-o-acetyl-D-
0-arabino-tetrol-1-yl]-3-(4-chlorophenyl)-1,2-bis 
(ethoxycarbonyl)-1,3-0hethyldisazatetrazine has
been re\-nued as a part of a structural investigations of some tetrahydrobistetrazine 
derivative compounds in order to obtain detailed 
conformational and configurational information.

C$_{24}$H$_{24}$N$_{4}$O$_{12}$(Cl$_{2}$)(Avalon, Babian, Cintas, Giménez, Molina, 
Pacillas and Sánchez, Tetrahedros Lett. 32 (1987) 2513-2516)

Intensities were measured on a CAD-4 diffractometer 
with MoKα radiation, graphite monochromator, w/2θ 
scan. The structure was solved by direct methods 
sing SIR (Burz, Camalli Cazzano, Giacovazzo, 
22 (1989) 309-323) and the non-H atoms were
re\-nued by full matrix least squares method. Refinement 
with anisotropic thermal parameters converged to a final 
R=0.067 (Rw=0.063) for 3471 reflections. D(21)=1.15.

The H-atoms were calculated from the geometry of the 
atom and assigned isotropic temperature factors 
fixed positions with the Us=values.

The tetrahydrotriazine ring adopts a twist conformation 
with ring-puckering coordinates (Cramer and Pople, J.
Am. Chem. Soc. 97 (1975) 1254-1258) Φ=41°(2)°, Ψ=36°(2)°, 
and Θ=20°(2)° for the sequence

\[ \text{1-Me,-N=N-C=N-C}=C=N \]

The substituents C1, C4, C5 and C8 are at -1503(10), 
140(10), -1504(10) and 0.7001(A) from the best calculated plane. 
The asymmetric parameters (Nardelli, Acta Crystallogr.
C39 (1982) 1411-1422) are ΔC(OC)=-1.115(15) and 
ΔC(N)=0.70(1). The terminal carbon of the sugar chaine 
deviates from planarity due to steric hindrance. The sugar configuration is in accordance 
with the title compound structure. 
The packing is governed by van der Waals contacts.

PS-06.05.08 THE CRYSTAL STRUCTURE OF THE 1:2 ADDUCT OF OCTAFLUORONAPHTALENE AND INDENE.
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The crystal structure of the title compound was determined 
by the means of the 2D X-ray structure analysis. The crystals 
were kindly supplied by Prof. B. Šmahel and Dr N.Zupancič, Laboratory of Organic Chemistry, Dept. of Chemistry and Chemical 
Technology, University of Ljubljana. The conventional crystal 
data are: C$_{42}$H$_{24}$N$_{4}$O$_{12}$, M=504.3, triclinic, P, a=7.546(1), 
b=6.629(1), c=15.876(2), α=83.16(1), β=81.17(1), γ=71.23(1), 
V=1076.3 A$^3$. The final conventional R-value was 0.0461 for 
3067 observed reflections. Enraf-Nonius diffractometer. 
SHELXS86, SHELX76, ORTEP programmes, all H 
atoms located.

The stereochemistry and peculiar geometry of this adduct as 
well as the reaction pathway will be presented in details.

PS-06.05.09 STRUCTURE OF 6(R)-6-(TETRA-O-ACETYL-D-0-ARA
BINO-TETROIL-1-YL)-3-PHENYL-2-[CYANO-CH, CH, CH, O-]
TRITHYDROPYRIDAZINE. By M. J. Díaz, M. D. Guitart, 
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Ciencias de Materiales de Sevilla, CSIC, and 
Departamento de Fisica de la Materia Condensada. Universidad de Sevilla. Apdo. 1065, E-41080, Sevilla, Spain.

The title compound is a product of the reaction of the 
sodium 4-kynzo-2-benzylideneacetone, with the 
acrylonitrile. The compound crystallizes in the space 
group P21/c, with the following cell dimensions:
a=11.76(1), b=24.269(7), c=8.433(4), \( \alpha = 90°, \beta = 90°, \)
and four molecules per unit cell. \( \mu = 0.9325 \mathrm{m}, \)
\( \rho = 1.20 \mathrm{~g} \mathrm{~cm}^{-3}, \) \( F(000) = 1000, \) \( \lambda (MoKα) = 0.7107 \mathrm{~A}, \) \( T = 293 \mathrm{~K}. \)

Altogether, 3971 reflections were collected on a single 
crystal CAD4 Enraf-Nonius diffractometer using graphite 
monochromated MoKα radiation, of which 2903 with 
\( 2\theta > I \) were considered in the structure refinement. 
The structure was solved by direct methods using SIR, 
and refinement of the non-H atoms by full matrix 
least-squares methods. H atoms were calculated from 
the geometry of the molecule and assigned isotropic 
temperature factors in fixed positions with the Us=values 
corresponding to those of the carrier atoms. 
The final cycles of the refinement gave \( R = 0.06, \) 
\( wR = 0.08. \)

The conformation of the tetrahydropyridazine ring is 
intermediate between the boat and twist-boat. 
Puckering Cramer and Pople parameter are: \( \delta = 35(1)°, \) 
\( \Psi = 0.480(2)°, \) \( \theta = 156(1)°, \) and 
Nardelli, asymmetric parameters \( 
\Delta C(N)=0.07(1) \) and \( \Delta C(\text{C})=0.056(2) \)

The last carbon of the aromatic chain deviates 
significantly from planarity. 
The configurations of the sugar chaine agree with the title structure. 
The crystal cohesion is governed by van der Waals forces.

PS-06.05.10 X-RAY STUDY OF 2-METHYL-3-ALKOXY-
CARBONYL-4-ARYL-SUBSTITUTED, DIFFERENTIALLY 
SATURATED PYRIDINES AND 1,2-NAPHTHYRIDINES. By 
Pharmaceutical and Chemical Works Ltd, Budapest, POB 110, 
H-1325, Hungary.