Supporting Information
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Crystal data and structure refinement for 5k (CCDC 1469410)

- **Empirical formula**: C₂₆H₂₃BrN₂O₅
- **Formula weight**: 523.37
- **Temperature/K**: 100
- **Crystal system**: orthorhombic
- **Space group**: Pbca
- **a/Å**: 18.432(7)
- **b/Å**: 10.481(3)
- **c/Å**: 24.172(8)
- **α/°**: 90
- **β/°**: 90
- **γ/°**: 90
- **Volume/Å³**: 4670(3)
- **Z**: 8
- **ρ calc/g/cm³**: 1.489
- **μ/mm⁻¹**: 1.801
- **F(000)**: 2144.0
- **Crystal size/mm³**: 0.338 × 0.171 × 0.144
- **Radiation**: MoKα (λ = 0.71073)
- **2Θ range for data collection/°**: 4.42 to 51.994
- **Index ranges**: -22 ≤ h ≤ 22, -12 ≤ k ≤ 11, -29 ≤ l ≤ 29
- **Reflections collected**: 37563
- **Independent reflections**: 4585 [R_{int} = 0.0667, R_{sigma} = 0.0405]
- **Data/restraints/parameters**: 4585/0/310
- **Goodness-of-fit on F²**: 1.138
- **Final R indexes [I>=2σ (I)]**: R₁ = 0.0344, wR₂ = 0.0803
- **Final R indexes [all data]**: R₁ = 0.0549, wR₂ = 0.0969
- **Largest diff. peak/hole / e Å⁻³**: 0.47/-0.50
Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number CCDC 1469410.

**Figure 1.** Crystal structure of compound 5k
$^1$H and $^{13}$C Spectra of compound 5a
$^1$H and $^{13}$C Spectra of compound 5b

![Spectra Image](image-url)
$^1$H and $^{13}$C Spectra of compound 5c
$^1$H and $^{13}$C Spectra of compound 5d
$^1$H and $^{13}$C Spectra of compound 5e
$^1$H and $^{13}$C Spectra of compound 5f
$^1$H and $^{13}$C Spectra of compound 5g
\(^1\)H and \(^{13}\)C Spectra of compound 5h

[Diagram of chemical structure with spectra below]
$^1$H and $^{13}$C Spectra of compound 5i
$^1$H and $^{13}$C Spectra of compound 5j
$^1$H and $^{13}$C Spectra of compound 5k
\(^1\text{H and }^{13}\text{C Spectra of compound 5l}\)
$^1$H and $^{13}$C Spectra of compound 5m

[Diagram of compound 5m with corresponding spectra]
$^1$H and $^{13}$C Spectra of compound 5n
$^1$H and $^{13}$C Spectra of compound 5o
$^1$H and $^{13}$C Spectra of compound 5p
$^1$H and $^{13}$C Spectra of compound 5q

![Chemical Structure of 5q](image)

![NMR Spectra](image)
$^{1}H$ and $^{13}C$ Spectra of compound 5r

![Spectra of compound 5r]