

Supporting Information

Ortho-substituent Effects on Halogen Bond Geometry for N-Haloimide···2-Substituted pyridine Complexes

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1. General information

Pyridine (>99%) was purchased from VWR International GmbH. 2-Ethylpyridine (>98%), 2-phenylpyridine (>98%), 2-(dimethylamino)pyridine (>98%), N-iodosuccinimide (>99%), N-iodophthalimide (>98%), N-iodosaccharin (>98%), N-bromophthalimide (>95%), N-bromosaccharin (>98%) were purchased from TCI. 2-Fluoropyridine (98%), 2-cyanopyridine (99%), 2-chloropyridine (99%), 2-bromopyridine (99%), 2-methylpyridine (98%), 2-trimethylsilylpyridine (>98%), N-bromosuccinimide (>99%) and acetone (>99.9%) were purchased from sigma, whereas 2-methoxypyridine (98%) from Acros, 2-isopropylpyridine (95%) and 2-iodopyridine (97%) from Fluorochem, and 2-trifluoromethylpyridine (98%) from abcr chemicals. 2-Diphenylmethylpyridine and 2-(1,1-diphenylethyl)pyridine are synthesised following the literature. All reagents and solvents for synthesis were purchased from commercial sources and used without further purification. CDCl_3 (99.80% D, <0.01% water) was purchased from Eurisotop.

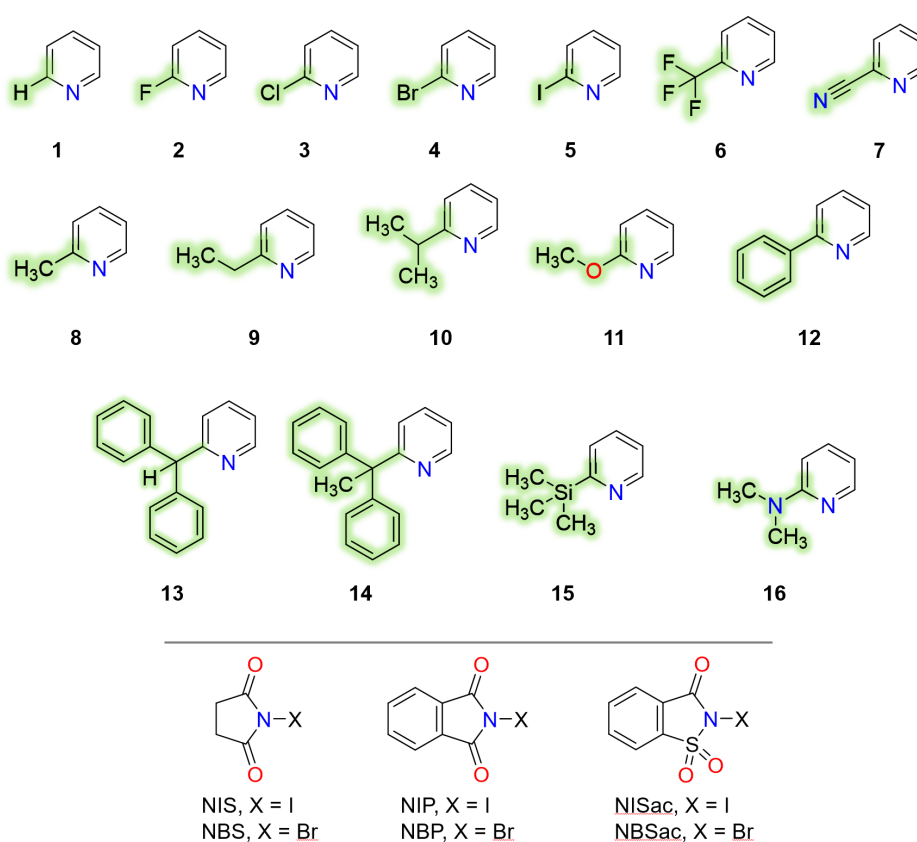


Figure S1. List of 2-substituted pyridines (1 - 16) as XB acceptors and N-halimides: N-iodosuccinimide (NIS), N-bromosuccinimide (NBS), N-iodophthalimide (NIP), and N-bromophthalimide (NBP), N-iodosaccharin (NISac), and N-bromosaccharin (NBSac) as XB donors.

2. X-Ray crystallography

The single-crystal X-ray data for NIS-1, NIS-2, NIS-5, NIS-8, NISac-6, NISac-11, NBS-1, NBS-4, NBS-8, NBS-9, NBP-3, NBP-4, NBP-8, NBP-12, NBP-13, NBSac-2, NBSac-4, NBSac-5, NBSac-5a, (NISac)₂I-12H, (NISac)₂I-15H, (NISac)₂I-15Ha, NHSac-5, NSac-1H, NSac-16H, and NSac-16Ha were measured at 170K on a Bruker-Nonius Kappa CCD diffractometer equipped with an APEX-II CCD detector using graphite-monochromated Mo-K α ($\lambda = 0.71073$ Å) radiation. Single-crystal X-ray data for NIS-3, NIS-4, NIS-6, NIS-9, NIS-11, NISac-3, NBS-3, NBP-6, NBP-7, NBSac-3, and (NISac)₂I-10H were measured either 120K or 170K on a Rigaku SuperNova Single source diffractometer equipped with an Eos CCD detector using mirror-monochromated Mo-K α ($\lambda = 0.71073$ Å) radiation. The X-ray crystal structure data for NIS-12, NIS-13, NIP-1, NIP-2, NIP-3, NIP-5, NIP-6, NIP-12, NIP-13, NISac-2, NISac-4, NBP-1, NBP-2, NBP-5, NBP-9, NBP-10, NBP-11, NBSac-6, NBSac-13, and NBSac-14 were collected at 120 K, using a Rigaku SuperNova four-circle diffractometer equipped with a Hybrid Pixel Array Detector (detector type: HyPix-Arc 100) and Cu-K α ($\lambda = 1.54184$ Å) radiation. Whereas the data for NIP-4, NIP-8, NIP-9, NIP-14, NISac-5, NISac-7, NISac-9, NBS-5, NBSac-9, and NSac-8H were collected at 120 K using an XtaLAB Synergy R four-circle diffractometer equipped with a Hybrid Pixel Array Detector (detector type: HyPix-Arc 100). Diffraction type is PhotonJet R (Cu, $\lambda = 1.54184$ Å) X-ray source. CrysAlisPro was used for the data collection and reduction, and the intensities were absorption corrected using a gaussian face index absorption correction method for the data collection carried out using Rigaku diffractometers. For the data obtained using Bruker Nonius Kappa diffractometer, the processing was performed using the program COLLECT and HKL DENZO AND SCALEPACK.⁶ The structure was solved with direct methods (SHELXS)^{7,8} and refined by full-matrix least squares on F^2 using the OLEX2 software⁹, which utilizes the SHELXL-2015 module.^{7,8} All structures were solved by intrinsic phasing (SHELXT)^[2] and refined by full-matrix least squares on F^2 using the OLEX2^[3], utilizing the SHELXL-2015 module.^[4,5] Anisotropic displacement parameters were assigned to non-H atoms and isotropic displacement parameters for all H atoms were constrained to multiples of the equivalent displacement parameters of their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{parent atom})$. Single crystal data and CCDC numbers of all new structures are included below. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html> (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44 1223 336033; E-mail: deposit@ccdc.cam.ac.uk).

1) Crystal data for NIS-1 [CCDC-2297270]: Sum formula: C₉H₉IN₂O₂, M = 304.08, colourless block, 0.28 x 0.26 x 0.26 mm³, orthorhombic, space group *Cc*ce, a = 7.6331(15) Å, b = 20.056(4) Å, c = 27.136(5) Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, V = 4154.2(14) Å³, Z = 16, D_c = 1.945 g/cm³, F₀₀₀ = 2336, $\mu = 3.059$ mm⁻¹, T = 170 K, $\theta_{\text{max}} = 25.249^\circ$, 13835 total reflections, 1738 with $I_o > 2\sigma(I_o)$, R_{int} = 0.0304, 1874 data, 131 parameters, 0 restraints, GooF = 1.217, R = 0.0209 and wR = 0.0414 [$I_o > 2\sigma(I_o)$], R = 0.0243 and wR = 0.0424 (all reflections), 0.267 < $d\Delta\rho$ < -0.292 e/Å³.

2) Crystal data for NIS-2 [CCDC-2297268]: Sum formula: C₉H₈FIN₂O₂, M = 322.07, colourless block, 0.17 x 0.12 x 0.07 mm³, orthorhombic, space group P2₁2₁2₁, a = 5.9336(12) Å, b = 8.8973(18) Å, c = 20.295(4) Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, V = 1071.4(4) Å³, Z = 4, D_c = 1.997 g/cm³, F₀₀₀ = 616, $\mu = 2.984$ mm⁻¹, T = 170 K, $\theta_{\text{max}} = 25.242^\circ$, 5237 total reflections, 1794 with $I_o > 2\sigma(I_o)$, R_{int} = 0.0371, 1934 data, 136 parameters, 0 restraints, GooF = 1.014, R = 0.0261 and wR = 0.0440 [$I_o > 2\sigma(I_o)$], R = 0.0298 and wR = 0.0448 (all reflections), 0.356 < $d\Delta\rho$ < -0.283 e/Å³.

3) Crystal data for NIS-3 [CCDC-2297274]: Sum formula: $C_9H_8ClIN_2O_2$, $M = 338.52$, colourless block, $0.103 \times 0.05 \times 0.034 \text{ mm}^3$, orthorhombic, space group $Pbca$, $a = 10.9926(11) \text{ \AA}$, $b = 7.6239(9) \text{ \AA}$, $c = 25.772(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2159.9(5) \text{ \AA}^3$, $Z = 8$, $D_c = 2.082 \text{ g/cm}^3$, $F_{000} = 1296$, $\mu = 3.193 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.246^\circ$, 13851 total reflections, 1675 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0896$, 1955 data, 124 parameters, 12 restraints, $\text{GooF} = 1.263$, $R = 0.0971$ and $wR = 0.2105 [I_o > 2\sigma(I_o)]$, $R = 0.1056$ and $wR = 0.2145$ (all reflections), $3.029 < d\Delta\rho < -3.733 \text{ e/\AA}^3$.

4) Crystal data for NIS-4 [CCDC-2297275]: Sum formula: $C_9H_8BrIN_2O_2$, $M = 382.98$, colourless block, $0.218 \times 0.113 \times 0.031 \text{ mm}^3$, orthorhombic, space group $Pbca$, $a = 11.0084(2) \text{ \AA}$, $b = 7.73508(14) \text{ \AA}$, $c = 25.9301(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2207.96(7) \text{ \AA}^3$, $Z = 8$, $D_c = 2.304 \text{ g/cm}^3$, $F_{000} = 1440$, $\mu = 6.501 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.246^\circ$, 11331 total reflections, 1776 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0389$, 1999 data, 136 parameters, 0 restraints, $\text{GooF} = 0.0193$, $R = 0.0971$ and $wR = 0.0408 [I_o > 2\sigma(I_o)]$, $R = 0.0245$ and $wR = 0.0434$ (all reflections), $0.389 < d\Delta\rho < -0.439 \text{ e/\AA}^3$.

5) Crystal data for NIS-5 [CCDC-2297273]: Sum formula: $C_9H_8I_2N_2O_2$, $M = 429.97$, colourless block, $0.24 \times 0.17 \times 0.16 \text{ mm}^3$, orthorhombic, space group $Pbca$, $a = 11.095(2) \text{ \AA}$, $b = 8.1428(16) \text{ \AA}$, $c = 26.146(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2362.3(8) \text{ \AA}^3$, $Z = 8$, $D_c = 2.418 \text{ g/cm}^3$, $F_{000} = 1584$, $\mu = 5.308 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.248^\circ$, 19077 total reflections, 1978 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0461$, 2140 data, 136 parameters, 0 restraints, $\text{GooF} = 1.087$, $R = 0.0195$ and $wR = 0.0398 [I_o > 2\sigma(I_o)]$, $R = 0.0227$ and $wR = 0.0410$ (all reflections), $0.332 < d\Delta\rho < -0.440 \text{ e/\AA}^3$.

6) Crystal data for NIS-6 [CCDC-2297267]: Sum formula: $C_{10}H_8F_3IN_2O_2$, $M = 372.08$, colourless block, $0.126 \times 0.084 \times 0.064 \text{ mm}^3$, triclinic, space group $P-1$, $a = 7.6569(5) \text{ \AA}$, $b = 8.5366(5) \text{ \AA}$, $c = 10.7553(5) \text{ \AA}$, $\alpha = 70.796(4)^\circ$, $\beta = 83.671(4)^\circ$, $\gamma = 64.566(6)^\circ$, $V = 599.15(6) \text{ \AA}^3$, $Z = 2$, $D_c = 2.062 \text{ g/cm}^3$, $F_{000} = 356$, $\mu = 2.707 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 29.032^\circ$, 10509 total reflections, 2535 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0466$, 2852 data, 163 parameters, 0 restraints, $\text{GooF} = 1.074$, $R = 0.0320$ and $wR = 0.0701 [I_o > 2\sigma(I_o)]$, $R = 0.0395$ and $wR = 0.0750$ (all reflections), $1.231 < d\Delta\rho < -0.756 \text{ e/\AA}^3$.

7) Crystal data for NIS-8 [CCDC-2297269]: Sum formula: $C_{10}H_{11}IN_2O_2$, $M = 318.11$, colourless block, $0.28 \times 0.17 \times 0.11 \text{ mm}^3$, orthorhombic, space group $P2_12_12_1$, $a = 8.7985(18) \text{ \AA}$, $b = 6.2308(12) \text{ \AA}$, $c = 20.982(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 1150.3(4) \text{ \AA}^3$, $Z = 4$, $D_c = 1.837 \text{ g/cm}^3$, $F_{000} = 616$, $\mu = 2.767 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 23483 total reflections, 2059 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0466$, 2092 data, 137 parameters, 0 restraints, $\text{GooF} = 1.053$, $R = 0.0201$ and $wR = 0.0492 [I_o > 2\sigma(I_o)]$, $R = 0.0206$ and $wR = 0.0494$ (all reflections), $0.657 < d\Delta\rho < -0.350 \text{ e/\AA}^3$.

8) Crystal data for NIS-9 [CCDC-2297265]: Sum formula: $C_{11}H_{13}IN_2O_2$, $M = 332.13$, colourless block, $0.171 \times 0.107 \times 0.064 \text{ mm}^3$, tetragonal, space group $I4_1/a$, $a = 20.4816(3) \text{ \AA}$, $b = 20.4816(3) \text{ \AA}$, $c = 11.6092(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 4870.01(19) \text{ \AA}^3$, $Z = 16$, $D_c = 1.812 \text{ g/cm}^3$, $F_{000} = 2592$, $\mu = 2.618 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.243^\circ$, 8040 total reflections, 1854 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0337$, 2199 data, 146 parameters, 0 restraints, $\text{GooF} = 1.047$, $R = 0.0214$ and $wR = 0.0428 [I_o > 2\sigma(I_o)]$, $R = 0.0287$ and $wR = 0.0461$ (all reflections), $0.361 < d\Delta\rho < -0.404 \text{ e/\AA}^3$.

9) Crystal data for NIS-11 [CCDC-2297272]: Sum formula: $C_{14}H_{15}I_2N_3O_5$, $M = 559.09$, colourless block, $0.139 \times 0.094 \times 0.078 \text{ mm}^3$, monoclinic, space group $P2_1/c$, $a = 7.620(3) \text{ \AA}$, $b = 32.311(4) \text{ \AA}$, $c = 7.808(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 116.24(4)^\circ$, $\gamma = 90^\circ$, $V = 1724.2(9) \text{ \AA}^3$, $Z = 4$, $D_c = 2.154 \text{ g/cm}^3$, $F_{000} = 1064$, $\mu = 3.677 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.249^\circ$, 9717 total reflections, 2746 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0386$, 3120 data, 218 parameters, 0 restraints, $\text{GooF} = 1.046$, $R = 0.0306$ and $wR = 0.0660 [I_o > 2\sigma(I_o)]$, $R = 0.0371$ and $wR = 0.0700$ (all reflections), $1.551 < d\Delta\rho < -0.907 \text{ e/\AA}^3$.

10) Crystal data for NIS-12 [CCDC-2297271]: Sum formula: $C_{15}H_{13}IN_2O_2$, $M = 380.17$, colourless block, $0.08 \times 0.05 \times 0.039 \text{ mm}^3$, monoclinic, space group $P2_1/n$, $a = 8.37100(10) \text{ \AA}$, $b = 14.43480(10) \text{ \AA}$, $c = 11.62240(10) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 91.1510(10)^\circ$, $\gamma = 90^\circ$, $V = 1404.09(2) \text{ \AA}^3$, $Z = 4$, $D_c = 1.798 \text{ g/cm}^3$,

F000 = 744, $\mu = 17.951 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 79.848^\circ$, 18458 total reflections, 2882 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0275$, 3007 data, 181 parameters, 0 restraints, GooF = 1.107, R = 0.0217 and wR = 0.0587 [$I_o > 2\sigma(I_o)$], R = 0.0226 and wR = 0.0594 (all reflections), $0.378 < d\Delta\rho < -0.796 \text{ e}/\text{\AA}^3$.

11) Crystal data for NIS-13 [CCDC-2297266]: Sum formula: $\text{C}_{22}\text{H}_{19}\text{IN}_2\text{O}_2$, M = 470.29, colourless block, $0.14 \times 0.13 \times 0.12 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{n}$, a = 9.3071(19) \AA , b = 14.349(3) \AA , c = 14.998(3) \AA , $\alpha = 90^\circ$, $\beta = 104.76(3)^\circ$, $\gamma = 90^\circ$, V = 1936.8(7) \AA^3 , Z = 4, Dc = 1.613 g/cm^3 , F000 = 744, $\mu = 1.673 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 25.248^\circ$, 12131 total reflections, 1921 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.1646$, 3498 data, 238 parameters, 0 restraints, GooF = 1.032, R = 0.0764 and wR = 0.1222 [$I_o > 2\sigma(I_o)$], R = 0.1637 and wR = 0.1479 (all reflections), $1.061 < d\Delta\rho < -0.844 \text{ e}/\text{\AA}^3$.

12) Crystal data for NIP-1 [CCDC-2297333]: Sum formula: $\text{C}_{13}\text{H}_9\text{IN}_2\text{O}_2$, M = 352.12, colourless block, $0.08 \times 0.05 \times 0.04 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{n}$, a = 15.5195(3) \AA , b = 4.89490(10) \AA , c = 16.2965(3) \AA , $\alpha = 90^\circ$, $\beta = 92.922(2)^\circ$, $\gamma = 90^\circ$, V = 1236.38(4) \AA^3 , Z = 4, Dc = 1.892 g/cm^3 , F000 = 680, $\mu = 20.327 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 80.006^\circ$, 8798 total reflections, 2385 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0400$, 2620 data, 163 parameters, 0 restraints, GooF = 1.079, R = 0.0302 and wR = 0.0806 [$I_o > 2\sigma(I_o)$], R = 0.0335 and wR = 0.0827 (all reflections), $0.848 < d\Delta\rho < -1.093 \text{ e}/\text{\AA}^3$.

13) Crystal data for NIP-2 [CCDC-2297327]: Sum formula: $\text{C}_{13}\text{H}_8\text{FIN}_2\text{O}_2$, M = 370.11, colourless plate, $0.13 \times 0.06 \times 0.02 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{n}$, a = 15.7548(2) \AA , b = 4.77590(10) \AA , c = 16.7152(2) \AA , $\alpha = 90^\circ$, $\beta = 93.8410(10)^\circ$, $\gamma = 90^\circ$, V = 1254.88(3) \AA^3 , Z = 4, Dc = 1.959 g/cm^3 , F000 = 712, $\mu = 20.185 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 76.239^\circ$, 8278 total reflections, 2427 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0316$, 2579 data, 151 parameters, 0 restraints, GooF = 1.107, R = 0.0366 and wR = 0.0986 [$I_o > 2\sigma(I_o)$], R = 0.0382 and wR = 0.0997 (all reflections), $1.419 < d\Delta\rho < -1.491 \text{ e}/\text{\AA}^3$.

14) Crystal data for NIP-3 [CCDC-2297334]: Sum formula: $\text{C}_{13}\text{H}_8\text{ClIN}_2\text{O}_2$, M = 386.56, colourless plate, $0.054 \times 0.049 \times 0.029 \text{ mm}^3$, triclinic, space group P-1, a = 8.0361(2) \AA , b = 8.7865(2) \AA , c = 9.9708(2) \AA , $\alpha = 100.790(2)^\circ$, $\beta = 91.074(2)^\circ$, $\gamma = 107.116(2)^\circ$, V = 658.91(3) \AA^3 , Z = 1, Dc = 1.948 g/cm^3 , F000 = 372, $\mu = 20.964 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 76.339^\circ$, 7183 total reflections, 2639 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0179$, 2703 data, 172 parameters, 0 restraints, GooF = 1.063, R = 0.0144 and wR = 0.0370 [$I_o > 2\sigma(I_o)$], R = 0.0149 and wR = 0.0372 (all reflections), $0.373 < d\Delta\rho < -0.391 \text{ e}/\text{\AA}^3$.

15) Crystal data for NIP-4 [CCDC-2297329]: Sum formula: $\text{C}_{13}\text{H}_8\text{BrIN}_2\text{O}_2$, M = 431.02, colourless block, $0.07 \times 0.054 \times 0.021 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{c}$, a = 14.2203(2) \AA , b = 13.41620(10) \AA , c = 14.1484(2) \AA , $\alpha = 90^\circ$, $\beta = 99.5010(10)^\circ$, $\gamma = 90^\circ$, V = 2662.24(6) \AA^3 , Z = 8, Dc = 2.151 g/cm^3 , F000 = 1632, $\mu = 22.426 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 76.823^\circ$, 41335 total reflections, 2639 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0446$, 5554 data, 343 parameters, 0 restraints, GooF = 1.048, R = 0.0297 and wR = 0.0768 [$I_o > 2\sigma(I_o)$], R = 0.0320 and wR = 0.0781 (all reflections), $2.616 < d\Delta\rho < -0.947 \text{ e}/\text{\AA}^3$.

16) Crystal data for NIP-5 [CCDC-2297328]: Sum formula: $\text{C}_{13}\text{H}_8\text{I}_2\text{N}_2\text{O}_2$, M = 478.01, colourless block, $0.07 \times 0.06 \times 0.03 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{n}$, a = 8.00690(10) \AA , b = 20.1482(2) \AA , c = 9.02500(10) \AA , $\alpha = 90^\circ$, $\beta = 103.3530(10)^\circ$, $\gamma = 90^\circ$, V = 1416.59(3) \AA^3 , Z = 4, Dc = 2.241 g/cm^3 , F000 = 888, $\mu = 34.880 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 79.695^\circ$, 10817 total reflections, 2761 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0380$, 3002 data, 172 parameters, 0 restraints, GooF = 1.077, R = 0.0293 and wR = 0.0783 [$I_o > 2\sigma(I_o)$], R = 0.0319 and wR = 0.0797 (all reflections), $0.984 < d\Delta\rho < -1.039 \text{ e}/\text{\AA}^3$.

17) Crystal data for NIP-6 [CCDC-2297331]: Sum formula: $\text{C}_{14}\text{H}_8\text{F}_3\text{IN}_2\text{O}_2$, M = 420.12, colourless block, $0.173 \times 0.086 \times 0.049 \text{ mm}^3$, monoclinic, space group $\text{P}2_1/\text{n}$, a = 8.06450(10) \AA , b = 16.6115(2) \AA , c = 10.93320(10) \AA , $\alpha = 90^\circ$, $\beta = 101.7350(10)^\circ$, $\gamma = 90^\circ$, V = 1434.04(3) \AA^3 , Z = 4, Dc = 1.946 g/cm^3 , F000 = 808, $\mu = 17.967 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 79.620^\circ$, 10691 total reflections, 2852 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0379$, 3034 data, 199 parameters, 0 restraints, GooF = 1.130, R = 0.0294 and wR = 0.0760 [$I_o > 2\sigma(I_o)$], R = 0.0312 and wR = 0.0772 (all reflections), $0.515 < d\Delta\rho < -0.852 \text{ e}/\text{\AA}^3$.

18) Crystal data for NIP-8 [CCDC-2297332]: Sum formula: $C_{14}H_{11}IN_2O_2$, $M = 366.15$, colourless block, $0.024 \times 0.019 \times 0.015 \text{ mm}^3$, monoclinic, space group $P2_1/c$, $a = 11.8650(8) \text{ \AA}$, $b = 4.0903(3) \text{ \AA}$, $c = 27.3208(14) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 95.799(5)^\circ$, $\gamma = 90^\circ$, $V = 1319.13(15) \text{ \AA}^3$, $Z = 4$, $D_c = 1.844 \text{ g/cm}^3$, $F_{000} = 712$, $\mu = 19.079 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.176^\circ$, 17772 total reflections, 2561 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.1193$, 2916 data, 174 parameters, 0 restraints, $\text{GooF} = 1.129$, $R = 0.0926$ and $wR = 0.2311$ [$I_o > 2\sigma(I_o)$], $R = 0.1074$ and $wR = 0.2509$ (all reflections), $3.324 < d\Delta\rho < -2.063 \text{ e/\AA}^3$.

19) Crystal data for NIP-9 [CCDC-2297336]: Sum formula: $C_{15}H_{13}IN_2O_2$, $M = 380.17$, colourless block, $0.161 \times 0.114 \times 0.075 \text{ mm}^3$, orthorhombic space group $P2_12_12_1$, $a = 8.12390(10) \text{ \AA}$, $b = 13.34730(10) \text{ \AA}$, $c = 13.42760(10) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 1455.98(2) \text{ \AA}^3$, $Z = 4$, $D_c = 1.734 \text{ g/cm}^3$, $F_{000} = 744$, $\mu = 17.311 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 78.114^\circ$, 21185 total reflections, 3077 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0257$, 3084 data, 182 parameters, 0 restraints, $\text{GooF} = 1.087$, $R = 0.0134$ and $wR = 0.0340$ [$I_o > 2\sigma(I_o)$], $R = 0.0135$ and $wR = 0.0341$ (all reflections), $0.342 < d\Delta\rho < -0.302 \text{ e/\AA}^3$.

20) Crystal data for NIP-12 [CCDC-2297330]: Sum formula: $C_{19}H_{13}IN_2O_2$, $M = 428.21$, colourless block, $0.1 \times 0.09 \times 0.07 \text{ mm}^3$, triclinic space group $P-1$, $a = 8.4879(2) \text{ \AA}$, $b = 9.0871(2) \text{ \AA}$, $c = 11.4115(4) \text{ \AA}$, $\alpha = 106.189(3)^\circ$, $\beta = 98.364(2)^\circ$, $\gamma = 93.869(2)^\circ$, $V = 830.86(4) \text{ \AA}^3$, $Z = 2$, $D_c = 1.712 \text{ g/cm}^3$, $F_{000} = 420$, $\mu = 15.254 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.563^\circ$, 9873 total reflections, 3331 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0420$, 3509 data, 217 parameters, 0 restraints, $\text{GooF} = 1.091$, $R = 0.0413$ and $wR = 0.1062$ [$I_o > 2\sigma(I_o)$], $R = 0.0429$ and $wR = 0.1072$ (all reflections), $1.911 < d\Delta\rho < -1.125 \text{ e/\AA}^3$.

21) Crystal data for NIP-13 [CCDC-2297337]: Sum formula: $C_{26}H_{19}IN_2O_2$, $M = 518.33$, colourless block, $0.094 \times 0.059 \times 0.036 \text{ mm}^3$, triclinic space group $P-1$, $a = 8.07700(10) \text{ \AA}$, $b = 10.56470(10) \text{ \AA}$, $c = 12.9041(2) \text{ \AA}$, $\alpha = 93.3540(10)^\circ$, $\beta = 102.5980(10)^\circ$, $\gamma = 91.6500(10)^\circ$, $V = 1071.79(2) \text{ \AA}^3$, $Z = 2$, $D_c = 1.606 \text{ g/cm}^3$, $F_{000} = 516$, $\mu = 11.943 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 76.363^\circ$, 14827 total reflections, 4373 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0172$, 4429 data, 280 parameters, 0 restraints, $\text{GooF} = 1.140$, $R = 0.0186$ and $wR = 0.0460$ [$I_o > 2\sigma(I_o)$], $R = 0.0188$ and $wR = 0.0461$ (all reflections), $0.336 < d\Delta\rho < -0.589 \text{ e/\AA}^3$.

22) Crystal data for NIP-14 [CCDC-2297335]: Sum formula: $C_{27}H_{21}IN_2O_2$, $M = 532.36$, colourless block, $0.122 \times 0.07 \times 0.058 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 11.47815(19) \text{ \AA}$, $b = 13.3347(3) \text{ \AA}$, $c = 14.7355(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 94.9703(15)^\circ$, $\gamma = 90^\circ$, $V = 2246.90(7) \text{ \AA}^3$, $Z = 4$, $D_c = 1.574 \text{ g/cm}^3$, $F_{000} = 1064$, $\mu = 11.410 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 76.711^\circ$, 8294 total reflections, 7749 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = \text{twin}$, 8294 data, 291 parameters, 0 restraints, $\text{GooF} = 1.077$, $R = 0.0448$ and $wR = 0.1203$ [$I_o > 2\sigma(I_o)$], $R = 0.0464$ and $wR = 0.1219$ (all reflections), $0.645 < d\Delta\rho < -1.058 \text{ e/\AA}^3$.

23) Crystal data for NISac-2 [CCDC-2297287]: Sum formula: $C_{12}H_8FIN_2O_3S$, $M = 406.16$, colourless plate, $0.097 \times 0.061 \times 0.021 \text{ mm}^3$, monoclinic space group $P2_1/m$, $a = 7.3022(3) \text{ \AA}$, $b = 6.6219(2) \text{ \AA}$, $c = 13.8245(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 93.769(3)^\circ$, $\gamma = 90^\circ$, $V = 667.03(4) \text{ \AA}^3$, $Z = 2$, $D_c = 2.022 \text{ g/cm}^3$, $F_{000} = 392$, $\mu = 20.542 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 78.601^\circ$, 3879 total reflections, 1413 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0528$, 1502 data, 118 parameters, 0 restraints, $\text{GooF} = 1.113$, $R = 0.0394$ and $wR = 0.1081$ [$I_o > 2\sigma(I_o)$], $R = 0.0414$ and $wR = 0.1097$ (all reflections), $1.728 < d\Delta\rho < -1.595 \text{ e/\AA}^3$.

24) Crystal data for NISac-3 [CCDC-2297289]: Sum formula: $C_{12}H_8ClIN_2O_3S$, $M = 422.61$, colourless block, $0.077 \times 0.048 \times 0.039 \text{ mm}^3$, triclinic space group $P-1$, $a = 7.6544(14) \text{ \AA}$, $b = 8.2902(12) \text{ \AA}$, $c = 11.7396(14) \text{ \AA}$, $\alpha = 89.331(11)^\circ$, $\beta = 71.252(14)^\circ$, $\gamma = 88.928(13)^\circ$, $V = 705.28(19) \text{ \AA}^3$, $Z = 2$, $D_c = 1.990 \text{ g/cm}^3$, $F_{000} = 408$, $\mu = 2.614 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 5134 total reflections, 2245 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0557$, 2550 data, 170 parameters, 18 restraints, $\text{GooF} = 1.191$, $R = 0.0954$ and $wR = 0.2577$ [$I_o > 2\sigma(I_o)$], $R = 0.1063$ and $wR = 0.2644$ (all reflections), $2.306 < d\Delta\rho < -2.485 \text{ e/\AA}^3$.

25) Crystal data for NISac-4 [CCDC-2297293]: Sum formula: $C_{12}H_8BrIN_2O_3S$, $M = 467.07$, colourless block, $0.09 \times 0.07 \times 0.04 \text{ mm}^3$, orthorhombic space group $Pbca$, $a = 7.54700(8) \text{ \AA}$, $b = 14.57493(20) \text{ \AA}$, $c = 26.1769(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2879.38(6) \text{ \AA}^3$, $Z = 8$, $D_c = 2.155 \text{ g/cm}^3$, $F_{000} = 1776$,

$\mu = 22.175 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.444^\circ$, 24371 total reflections, 2954 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0436$, 3086 data, 186 parameters, 18 restraints, $\text{GooF} = 1.096$, $R = 0.0260$ and $wR = 0.0694$ [$I_o > 2\sigma(I_o)$], $R = 0.0271$ and $wR = 0.0700$ (all reflections), $0.644 < d\Delta\rho < -0.462 \text{ e}/\text{\AA}^3$.

26) Crystal data for NISac-5 [CCDC-2297292]: Sum formula: $\text{C}_{12}\text{H}_8\text{I}_2\text{N}_2\text{O}_3\text{S}$, $M = 514.06$, colourless block, $0.06 \times 0.05 \times 0.04 \text{ mm}^3$, triclinic space group P-1, $a = 7.8104(7) \text{ \AA}$, $b = 7.8674(5) \text{ \AA}$, $c = 13.5968(12) \text{ \AA}$, $\alpha = 75.592(7)^\circ$, $\beta = 78.108(7)^\circ$, $\gamma = 64.596(8)^\circ$, $V = 726.24(11) \text{ \AA}^3$, $Z = 2$, $D_c = 2.351 \text{ g/cm}^3$, $F_{000} = 480$, $\mu = 35.446 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.444^\circ$, 10596 total reflections, 2869 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0312$, 3078 data, 181 parameters, 0 restraints, $\text{GooF} = 1.056$, $R = 0.0246$ and $wR = 0.0642$ [$I_o > 2\sigma(I_o)$], $R = 0.0266$ and $wR = 0.0652$ (all reflections), $0.640 < d\Delta\rho < -1.139 \text{ e}/\text{\AA}^3$.

27) Crystal data for NISac-6 [CCDC-2297290]: Sum formula: $\text{C}_{13}\text{H}_8\text{F}_3\text{IN}_2\text{O}_3\text{S}$, $M = 456.17$, colourless block, $0.036 \times 0.022 \times 0.019 \text{ mm}^3$, triclinic space group P-1, $a = 7.8380(16) \text{ \AA}$, $b = 8.5317(17) \text{ \AA}$, $c = 12.218(2) \text{ \AA}$, $\alpha = 83.65(3)^\circ$, $\beta = 81.29(3)^\circ$, $\gamma = 65.81(3)^\circ$, $V = 735.6(3) \text{ \AA}^3$, $Z = 2$, $D_c = 2.059 \text{ g/cm}^3$, $F_{000} = 440$, $\mu = 2.367 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.248^\circ$, 6156 total reflections, 2136 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0581$, 2670 data, 208 parameters, 0 restraints, $\text{GooF} = 1.093$, $R = 0.0569$ and $wR = 0.1020$ [$I_o > 2\sigma(I_o)$], $R = 0.0798$ and $wR = 0.1105$ (all reflections), $0.781 < d\Delta\rho < -0.767 \text{ e}/\text{\AA}^3$.

28) Crystal data for NISac-7 [CCDC-2297288]: Sum formula: $\text{C}_{13}\text{H}_8\text{IN}_3\text{O}_3\text{S}$, $M = 413.18$, colourless block, $0.03 \times 0.023 \times 0.014 \text{ mm}^3$, triclinic space group P-1, $a = 7.9971(16) \text{ \AA}$, $b = 8.0226(16) \text{ \AA}$, $c = 11.988(2) \text{ \AA}$, $\alpha = 89.73(3)^\circ$, $\beta = 71.28(3)^\circ$, $\gamma = 85.76(3)^\circ$, $V = 726.3(3) \text{ \AA}^3$, $Z = 2$, $D_c = 1.889 \text{ g/cm}^3$, $F_{000} = 400$, $\mu = 2.361 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.246^\circ$, 5963 total reflections, 2348 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0350$, 2633 data, 190 parameters, 0 restraints, $\text{GooF} = 1.087$, $R = 0.0349$ and $wR = 0.0733$ [$I_o > 2\sigma(I_o)$], $R = 0.0407$ and $wR = 0.0761$ (all reflections), $0.517 < d\Delta\rho < -0.452 \text{ e}/\text{\AA}^3$.

29) Crystal data for NISac-9 [CCDC-2297291]: Sum formula: $\text{C}_{13}\text{H}_8\text{IN}_3\text{O}_3\text{S}$, $M = 413.18$, colourless block, $0.03 \times 0.023 \times 0.014 \text{ mm}^3$, triclinic space group P-1, $a = 7.9971(16) \text{ \AA}$, $b = 8.0226(16) \text{ \AA}$, $c = 11.988(2) \text{ \AA}$, $\alpha = 89.73(3)^\circ$, $\beta = 71.28(3)^\circ$, $\gamma = 85.76(3)^\circ$, $V = 726.3(3) \text{ \AA}^3$, $Z = 2$, $D_c = 1.889 \text{ g/cm}^3$, $F_{000} = 400$, $\mu = 2.361 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.246^\circ$, 5963 total reflections, 2348 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0350$, 2633 data, 190 parameters, 0 restraints, $\text{GooF} = 1.087$, $R = 0.0349$ and $wR = 0.0733$ [$I_o > 2\sigma(I_o)$], $R = 0.0407$ and $wR = 0.0761$ (all reflections), $0.517 < d\Delta\rho < -0.452 \text{ e}/\text{\AA}^3$.

30) Crystal data for NISac-11 [CCDC-2297294]: Sum formula: $\text{C}_{13}\text{H}_{11}\text{IN}_2\text{O}_4\text{S}$, $M = 418.20$, colourless block, $0.3 \times 0.18 \times 0.13 \text{ mm}^3$, monoclinic space group $P2_1/n$, $a = 7.9337(16) \text{ \AA}$, $b = 16.262(3) \text{ \AA}$, $c = 11.312(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 91.58(3)^\circ$, $\gamma = 90^\circ$, $V = 1458.9(5) \text{ \AA}^3$, $Z = 4$, $D_c = 1.904 \text{ g/cm}^3$, $F_{000} = 816$, $\mu = 2.355 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.249^\circ$, 6447 total reflections, 2233 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0948$, 2640 data, 192 parameters, 0 restraints, $\text{GooF} = 1.085$, $R = 0.0349$ and $wR = 0.2639$ [$I_o > 2\sigma(I_o)$], $R = 0.1026$ and $wR = 0.2701$ (all reflections), $7.880 < d\Delta\rho < -2.558 \text{ e}/\text{\AA}^3$.

31) Crystal data for NBS-1 [CCDC-2297298]: Sum formula: $\text{C}_9\text{H}_9\text{BrN}_2\text{O}_2$, $M = 257.09$, colourless block, $0.3 \times 0.18 \times 0.13 \text{ mm}^3$, monoclinic space group $P2_1/n$, $a = 7.3961(15) \text{ \AA}$, $b = 21.584(4) \text{ \AA}$, $c = 24.831(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 97.97(3)^\circ$, $\gamma = 90^\circ$, $V = 3925.7(14) \text{ \AA}^3$, $Z = 16$, $D_c = 1.740 \text{ g/cm}^3$, $F_{000} = 2048$, $\mu = 4.163 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 104377 total reflections, 6162 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0494$, 7102 data, 505 parameters, 0 restraints, $\text{GooF} = 1.062$, $R = 0.0246$ and $wR = 0.0459$ [$I_o > 2\sigma(I_o)$], $R = 0.0325$ and $wR = 0.0486$ (all reflections), $0.302 < d\Delta\rho < -0.338 \text{ e}/\text{\AA}^3$.

32) Crystal data for NBS-3 [CCDC-2297296]: Sum formula: $\text{C}_9\text{H}_8\text{BrClN}_2\text{O}_2$, $M = 291.53$, colourless block, $0.1 \times 0.077 \times 0.02 \text{ mm}^3$, orthorhombic space group $Pbca$, $a = 11.5530(3) \text{ \AA}$, $b = 7.9623(2) \text{ \AA}$, $c = 23.2624(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2139.87(9) \text{ \AA}^3$, $Z = 8$, $D_c = 1.810 \text{ g/cm}^3$, $F_{000} = 1152$, $\mu = 4.072 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 29.634^\circ$, 9185 total reflections, 2101 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0278$, 2708 data, 136 parameters, 0 restraints, $\text{GooF} = 1.048$, $R = 0.0273$ and $wR = 0.0521$ [$I_o > 2\sigma(I_o)$], $R = 0.0446$ and $wR = 0.0570$ (all reflections), $0.310 < d\Delta\rho < -0.372/\text{\AA}^3$.

33) Crystal data for NBS-4 [CCDC-2297297]: Sum formula: $C_9H_8Br_2N_2O_2$, $M = 335.99$, colourless block, $0.11 \times 0.09 \times 0.025 \text{ mm}^3$, orthorhombic space group $Pbca$, $a = 11.615(2) \text{ \AA}$, $b = 7.9801(16) \text{ \AA}$, $c = 23.403(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2169.2(8) \text{ \AA}^3$, $Z = 8$, $D_c = 2.058 \text{ g/cm}^3$, $F_{000} = 1296$, $\mu = 7.455 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.244^\circ$, 10599 total reflections, 1345 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.1019$, 1960 data, 136 parameters, 0 restraints, $\text{GooF} = 1.054$, $R = 0.0543$ and $wR = 0.0959 [I_o > 2\sigma(I_o)]$, $R = 0.0921$ and $wR = 0.1087$ (all reflections), $0.717 < d\Delta\rho < -0.690 / \text{\AA}^3$.

34) Crystal data for NBS-5 [CCDC-2297300]: Sum formula: $C_9H_8BrIN_2O_2$, $M = 382.98$, colourless block, $0.077 \times 0.064 \times 0.02 \text{ mm}^3$, orthorhombic space group $Pbca$, $a = 11.7666(4) \text{ \AA}$, $b = 8.1712(2) \text{ \AA}$, $c = 23.5011(8) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2259.57(12) \text{ \AA}^3$, $Z = 8$, $D_c = 2.252 \text{ g/cm}^3$, $F_{000} = 1440$, $\mu = 26.295 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 78.483^\circ$, 21554 total reflections, 2289 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0519$, 2415 data, 136 parameters, 0 restraints, $\text{GooF} = 1.211$, $R = 0.0443$ and $wR = 0.1076 [I_o > 2\sigma(I_o)]$, $R = 0.0464$ and $wR = 0.1085$ (all reflections), $1.180 < d\Delta\rho < -1.134 / \text{\AA}^3$.

35) Crystal data for NBS-8 [CCDC-2297301]: Sum formula: $C_{10}H_{11}BrN_2O_2$, $M = 271.12$, colourless block, $0.12 \times 0.1 \times 0.1 \text{ mm}^3$, orthorhombic space group $P2_12_12_1$, $a = 5.9809(12) \text{ \AA}$, $b = 8.9612(18) \text{ \AA}$, $c = 20.756(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 1112.4(4) \text{ \AA}^3$, $Z = 4$, $D_c = 1.619 \text{ g/cm}^3$, $F_{000} = 544$, $\mu = 3.677 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 21125 total reflections, 1943 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0434$, 2009 data, 137 parameters, 0 restraints, $\text{GooF} = 1.065$, $R = 0.0204$ and $wR = 0.0450 [I_o > 2\sigma(I_o)]$, $R = 0.0220$ and $wR = 0.0455$ (all reflections), $0.252 < d\Delta\rho < -0.176 / \text{\AA}^3$.

36) Crystal data for NBS-9 [CCDC-2297299]: Sum formula: $C_{11}H_{13}BrN_2O_2$, $M = 285.14$, colourless block, $0.284 \times 0.24 \times 0.068 \text{ mm}^3$, monoclinic space group $P2_1$, $a = 9.2312(2) \text{ \AA}$, $b = 5.85165(13) \text{ \AA}$, $c = 11.3669(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 109.939(3)^\circ$, $\gamma = 90^\circ$, $V = 577.21(3) \text{ \AA}^3$, $Z = 4$, $D_c = 1.641 \text{ g/cm}^3$, $F_{000} = 288$, $\mu = 3.548 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.246^\circ$, 4253 total reflections, 1989 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0300$, 2046 data, 146 parameters, 1 restraints, $\text{GooF} = 1.063$, $R = 0.0260$ and $wR = 0.0593 [I_o > 2\sigma(I_o)]$, $R = 0.0277$ and $wR = 0.0605$ (all reflections), $0.484 < d\Delta\rho < -0.329 / \text{\AA}^3$.

37) Crystal data for NBP-1 [CCDC-2297308]: Sum formula: $C_{13}H_9BrN_2O_2$, $M = 305.13$, colourless block, $0.12 \times 0.07 \times 0.04 \text{ mm}^3$, monoclinic space group $P2_1/n$, $a = 14.2718(5) \text{ \AA}$, $b = 5.1259(2) \text{ \AA}$, $c = 16.5122(6) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 97.507(4)^\circ$, $\gamma = 90^\circ$, $V = 1197.61(8) \text{ \AA}^3$, $Z = 4$, $D_c = 1.692 \text{ g/cm}^3$, $F_{000} = 608$, $\mu = 4.652 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.591^\circ$, 7788 total reflections, 1952 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0460$, 2522 data, 163 parameters, 0 restraints, $\text{GooF} = 1.127$, $R = 0.0514$ and $wR = 0.1460 [I_o > 2\sigma(I_o)]$, $R = 0.0633$ and $wR = 0.1551$ (all reflections), $0.839 < d\Delta\rho < -1.734 / \text{\AA}^3$.

38) Crystal data for NBP-2 [CCDC-2297306]: Sum formula: $C_{13}H_8BrFN_2O_2$, $M = 323.12$, colourless block, $0.08 \times 0.04 \times 0.03 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 4.12160(10) \text{ \AA}$, $b = 25.1715(5) \text{ \AA}$, $c = 11.6335(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 92.510(2)^\circ$, $\gamma = 90^\circ$, $V = 1205.78(4) \text{ \AA}^3$, $Z = 4$, $D_c = 1.780 \text{ g/cm}^3$, $F_{000} = 640$, $\mu = 4.786 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.281^\circ$, 7798 total reflections, 2169 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0353$, 2489 data, 172 parameters, 0 restraints, $\text{GooF} = 1.132$, $R = 0.0330$ and $wR = 0.0754 [I_o > 2\sigma(I_o)]$, $R = 0.0429$ and $wR = 0.0883$ (all reflections), $0.478 < d\Delta\rho < -0.784 / \text{\AA}^3$.

39) Crystal data for NBP-3 [CCDC-2297311]: Sum formula: $C_{13}H_8BrClN_2O_2$, $M = 339.57$, colourless block, $0.024 \times 0.023 \times 0.023 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 14.079(3) \text{ \AA}$, $b = 13.204(3) \text{ \AA}$, $c = 13.898(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 100.06(3)^\circ$, $\gamma = 90^\circ$, $V = 2543.8(9) \text{ \AA}^3$, $Z = 8$, $D_c = 1.773 \text{ g/cm}^3$, $F_{000} = 1344$, $\mu = 3.440 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.248^\circ$, 18882 total reflections, 3793 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0387$, 4593 data, 343 parameters, 0 restraints, $\text{GooF} = 1.025$, $R = 0.0304$ and $wR = 0.0612 [I_o > 2\sigma(I_o)]$, $R = 0.0431$ and $wR = 0.0657$ (all reflections), $0.332 < d\Delta\rho < -0.306 / \text{\AA}^3$.

40) Crystal data for NBP-4 [CCDC-2297309]: Sum formula: $C_{13}H_8Br_2N_2O_2$, $M = 384.03$, colourless block, $0.019 \times 0.017 \times 0.017 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 14.125(3) \text{ \AA}$, $b = 13.378(3) \text{ \AA}$, $c = 13.951(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 99.81(3)^\circ$, $\gamma = 90^\circ$, $V = 2597.6(9) \text{ \AA}^3$, $Z = 8$, $D_c = 1.964 \text{ g/cm}^3$, $F_{000} = 1488$,

$\mu = 6.239 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 13993 total reflections, 2977 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0800$, 4705 data, 343 parameters, 0 restraints, $\text{GooF} = 1.065$, $R = 0.0641$ and $wR = 0.1073$ [$I_o > 2\sigma(I_o)$], $R = 0.1147$ and $wR = 0.1223$ (all reflections), $0.688 < d\Delta\rho < -0.730/\text{\AA}^3$.

41) Crystal data for NBP-5 [CCDC-2297315]: Sum formula: $\text{C}_{13}\text{H}_8\text{BrIN}_2\text{O}_2$, $M = 431.02$, colourless block, $0.012 \times 0.08 \times 0.05 \text{ mm}^3$, triclinic space group $P-1$, $a = 8.1950(3)\text{\AA}$, $b = 8.4808(3)\text{\AA}$, $c = 10.9367(3)\text{\AA}$, $\alpha = 75.266(3)^\circ$, $\beta = 76.867(3)^\circ$, $\gamma = 67.854(3)^\circ$, $V = 673.52(4)\text{\AA}^3$, $Z = 2$, $D_c = 2.125 \text{ g/cm}^3$, $F_{000} = 408$, $\mu = 22.161 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.616^\circ$, 7954 total reflections, 2744 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0349$, 2828 data, 172 parameters, 0 restraints, $\text{GooF} = 1.097$, $R = 0.0315$ and $wR = 0.0829$ [$I_o > 2\sigma(I_o)$], $R = 0.0322$ and $wR = 0.0834$ (all reflections), $0.896 < d\Delta\rho < -1.105/\text{\AA}^3$.

42) Crystal data for NBP-6 [CCDC-2297307]: Sum formula: $\text{C}_{14}\text{H}_8\text{BrF}_3\text{N}_2\text{O}_2$, $M = 373.13$, colourless block, $0.281 \times 0.141 \times 0.097 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 8.3190(4) \text{\AA}$, $b = 23.8710(7) \text{\AA}$, $c = 7.8504(4) \text{\AA}$, $\alpha = 90^\circ$, $\beta = 115.497(6)^\circ$, $\gamma = 90^\circ$, $V = 1407.11(12) \text{\AA}^3$, $Z = 4$, $D_c = 1.761 \text{ g/cm}^3$, $F_{000} = 736$, $\mu = 2.963 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 25.250^\circ$, 10235 total reflections, 2271 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0351$, 2549 data, 199 parameters, 0 restraints, $\text{GooF} = 1.040$, $R = 0.0252$ and $wR = 0.0552$ [$I_o > 2\sigma(I_o)$], $R = 0.0308$ and $wR = 0.0581$ (all reflections), $0.355 < d\Delta\rho < -0.304/\text{\AA}^3$.

43) Crystal data for NBP-7 [CCDC-2297316]: Sum formula: $\text{C}_{14}\text{H}_8\text{BrN}_3\text{O}_2$, $M = 330.14$, colourless plate, $0.021 \times 0.02 \times 0.013 \text{ mm}^3$, triclinic space group $P-1$, $a = 8.2492(16)\text{\AA}$, $b = 8.6144(17)\text{\AA}$, $c = 9.842(2)\text{\AA}$, $\alpha = 101.38(3)^\circ$, $\beta = 95.88(3)^\circ$, $\gamma = 106.01(3)^\circ$, $V = 649.9(3) \text{\AA}^3$, $Z = 2$, $D_c = 1.687 \text{ g/cm}^3$, $F_{000} = 328$, $\mu = 3.167 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.247^\circ$, 5075 total reflections, 1815 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0571$, 2348 data, 181 parameters, 0 restraints, $\text{GooF} = 1.041$, $R = 0.0621$ and $wR = 0.1162$ [$I_o > 2\sigma(I_o)$], $R = 0.0887$ and $wR = 0.1275$ (all reflections), $0.641 < d\Delta\rho < -0.595/\text{\AA}^3$.

44) Crystal data for NBP-8 [CCDC-2297312]: Sum formula: $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2$, $M = 319.16$, colourless plate, $0.17 \times 0.15 \times 0.08 \text{ mm}^3$, orthorhombic space group $Pnna$, $a = 14.223(3)\text{\AA}$, $b = 19.742(4)\text{\AA}$, $c = 18.532(4)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 5203.6(18) \text{\AA}^3$, $Z = 16$, $D_c = 1.630 \text{ g/cm}^3$, $F_{000} = 2560$, $\mu = 3.158 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.249^\circ$, 104247 total reflections, 3521 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0809$, 4718 data, 345 parameters, 0 restraints, $\text{GooF} = 1.016$, $R = 0.0307$ and $wR = 0.0629$ [$I_o > 2\sigma(I_o)$], $R = 0.0517$ and $wR = 0.0713$ (all reflections), $0.366 < d\Delta\rho < -0.285/\text{\AA}^3$.

45) Crystal data for NBP-9 [CCDC-2297318]: Sum formula: $\text{C}_{15}\text{H}_{13}\text{BrN}_2\text{O}_2$, $M = 333.18$, colourless block, $0.057 \times 0.039 \times 0.016 \text{ mm}^3$, monoclinic space group $P2_1/n$, $a = 12.7634(4)\text{\AA}$, $b = 8.6393(3)\text{\AA}$, $c = 13.1886(4)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 107.488(4)^\circ$, $\gamma = 90^\circ$, $V = 1387.05(8)\text{\AA}^3$, $Z = 4$, $D_c = 1.596 \text{ g/cm}^3$, $F_{000} = 672$, $\mu = 4.069 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.913^\circ$, 10469 total reflections, 2245 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0533$, 2938 data, 182 parameters, 0 restraints, $\text{GooF} = 1.064$, $R = 0.0400$ and $wR = 0.0885$ [$I_o > 2\sigma(I_o)$], $R = 0.0582$ and $wR = 0.0954$ (all reflections), $0.378 < d\Delta\rho < -0.625/\text{\AA}^3$.

46) Crystal data for NBP-10 [CCDC-2297310]: Sum formula: $\text{C}_{16}\text{H}_{15}\text{BrN}_2\text{O}_2$, $M = 347.21$, colourless block, $0.1 \times 0.08 \times 0.06 \text{ mm}^3$, triclinic space group $P-1$, $a = 8.4886(2)\text{\AA}$, $b = 12.1249(3)\text{\AA}$, $c = 15.6600(4)\text{\AA}$, $\alpha = 68.744(2)^\circ$, $\beta = 88.188(2)^\circ$, $\gamma = 89.816(2)^\circ$, $V = 1501.32(7)\text{\AA}^3$, $Z = 4$, $D_c = 1.536 \text{ g/cm}^3$, $F_{000} = 704$, $\mu = 3.784 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 80.890^\circ$, 41171 total reflections, 6027 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0602$, 6355 data, 383 parameters, 0 restraints, $\text{GooF} = 1.144$, $R = 0.0828$ and $wR = 0.1999$ [$I_o > 2\sigma(I_o)$], $R = 0.0850$ and $wR = 0.2013$ (all reflections), $2.982 < d\Delta\rho < -1.050/\text{\AA}^3$.

47) Crystal data for NBP-11 [CCDC-2297314]: Sum formula: $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_3$, $M = 335.16$, colourless block, $0.052 \times 0.035 \times 0.021 \text{ mm}^3$, monoclinic space group $P2_1/m$, $a = 11.8151(2)\text{\AA}$, $b = 4.02450(10)\text{\AA}$, $c = 13.7118(2)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 91.0340(10)^\circ$, $\gamma = 90^\circ$, $V = 651.89(2)\text{\AA}^3$, $Z = 2$, $D_c = 1.707 \text{ g/cm}^3$, $F_{000} = 336$, $\mu = 4.395 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 77.929^\circ$, 7571 total reflections, 1439 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0287$, 1539 data, 149 parameters, 0 restraints, $\text{GooF} = 1.082$, $R = 0.0310$ and $wR = 0.0781$ [$I_o > 2\sigma(I_o)$], $R = 0.0335$ and $wR = 0.0792$ (all reflections), $0.599 < d\Delta\rho < -0.780/\text{\AA}^3$.

48) Crystal data for NBP-12 [CCDC-2297313]: Sum formula: $C_{19}H_{13}BrN_2O_2$, $M = 381.22$, colourless block, $0.016 \times 0.015 \times 0.015 \text{ mm}^3$, triclinic space group P-1, $a = 8.4132(17)\text{\AA}$, $b = 9.0911(18)\text{\AA}$, $c = 11.335(2)\text{\AA}$, $\alpha = 107.41(3)^\circ$, $\beta = 97.73(3)^\circ$, $\gamma = 94.77(3)^\circ$, $V = 812.8(3)\text{\AA}^3$, $Z = 2$, $D_c = 1.558 \text{ g/cm}^3$, $F_{000} = 384$, $\mu = 2.542 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.247^\circ$, 6620 total reflections, 2558 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0317$, 2930 data, 217 parameters, 0 restraints, $\text{GooF} = 1.049$, $R = 0.0310$ and $wR = 0.0621$ [$I_o > 2\sigma(I_o)$], $R = 0.0306$ and $wR = 0.0649$ (all reflections), $0.287 < d\Delta\rho < -0.293/\text{\AA}^3$.

49) Crystal data for NBP-13 [CCDC-2297317]: Sum formula: $C_{26}H_{19}BrN_2O_2$, $M = 471.34$, colourless block, $0.29 \times 0.16 \times 0.1 \text{ mm}^3$, triclinic space group P-1, $a = 8.1605(16)\text{\AA}$, $b = 10.591(2)\text{\AA}$, $c = 12.571(3)\text{\AA}$, $\alpha = 92.56(3)^\circ$, $\beta = 101.63(3)^\circ$, $\gamma = 90.74(3)^\circ$, $V = 1062.9(4)\text{\AA}^3$, $Z = 2$, $D_c = 1.473 \text{ g/cm}^3$, $F_{000} = 480$, $\mu = 2.542 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.247^\circ$, 8384 total reflections, 3223 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0332$, 3831 data, 280 parameters, 0 restraints, $\text{GooF} = 1.047$, $R = 0.0401$ and $wR = 0.0781$ [$I_o > 2\sigma(I_o)$], $R = 0.0533$ and $wR = 0.0828$ (all reflections), $0.290 < d\Delta\rho < -0.361/\text{\AA}^3$.

50) Crystal data for NBSac-2 [CCDC-2297346]: Sum formula: $C_{12}H_8BrFN_2O_3S$, $M = 359.17$, colourless block, $0.04 \times 0.034 \times 0.01 \text{ mm}^3$, orthorhombic space group $Pnma$, $a = 24.515(5)\text{\AA}$, $b = 6.7797(14)\text{\AA}$, $c = 7.8773(16)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 1309.3(5)\text{\AA}^3$, $Z = 2$, $D_c = 1.822 \text{ g/cm}^3$, $F_{000} = 712$, $\mu = 3.319 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.244^\circ$, 8081 total reflections, 1092 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0454$, 1289 data, 109 parameters, 24 restraints, $\text{GooF} = 1.058$, $R = 0.0349$ and $wR = 0.0838$ [$I_o > 2\sigma(I_o)$], $R = 0.0456$ and $wR = 0.0882$ (all reflections), $0.653 < d\Delta\rho < -0.633/\text{\AA}^3$.

51) Crystal data for NBSac-3 [CCDC-2297342]: Sum formula: $C_{12}H_8BrClN_2O_3S$, $M = 375.62$, colourless block, $0.216 \times 0.136 \times 0.087 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 8.1158(3)\text{\AA}$, $b = 23.6854(8)\text{\AA}$, $c = 7.6446(3)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 113.898(5)^\circ$, $\gamma = 90^\circ$, $V = 1343.53(10)\text{\AA}^3$, $Z = 2$, $D_c = 1.857 \text{ g/cm}^3$, $F_{000} = 744$, $\mu = 3.421 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.247^\circ$, 7356 total reflections, 2177 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0260$, 2429 data, 181 parameters, 0 restraints, $\text{GooF} = 1.057$, $R = 0.0229$ and $wR = 0.0472$ [$I_o > 2\sigma(I_o)$], $R = 0.0281$ and $wR = 0.0493$ (all reflections), $0.357 < d\Delta\rho < -0.346/\text{\AA}^3$.

52) Crystal data for NBSac-4 [CCDC-2297340]: Sum formula: $C_{12}H_8Br_2N_2O_3S$, $M = 420.08$, colourless plate, $0.01 \times 0.01 \times 0.01 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 8.1907(16)\text{\AA}$, $b = 23.803(5)\text{\AA}$, $c = 7.8308(16)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 115.31(3)^\circ$, $\gamma = 90^\circ$, $V = 1380.2(6)\text{\AA}^3$, $Z = 4$, $D_c = 2.022 \text{ g/cm}^3$, $F_{000} = 816$, $\mu = 6.032 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.250^\circ$, 10371 total reflections, 1604 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.1125$, 2503 data, 181 parameters, 6 restraints, $\text{GooF} = 1.054$, $R = 0.0698$ and $wR = 0.1132$ [$I_o > 2\sigma(I_o)$], $R = 0.1207$ and $wR = 0.1293$ (all reflections), $0.896 < d\Delta\rho < -0.711/\text{\AA}^3$.

53) Crystal data for NBSac-5 [CCDC-2297338]: Sum formula: $C_{12}H_8BrIN_2O_3S$, $M = 467.07$, colourless plate, $0.18 \times 0.14 \times 0.14 \text{ mm}^3$, triclinic space group P-1, $a = 7.6843(15)\text{\AA}$, $b = 7.9698(16)\text{\AA}$, $c = 13.624(3)\text{\AA}$, $\alpha = 75.74(3)^\circ$, $\beta = 76.07(3)^\circ$, $\gamma = 63.09(3)^\circ$, $V = 713.0(3)\text{\AA}^3$, $Z = 4$, $D_c = 2.175 \text{ g/cm}^3$, $F_{000} = 444$, $\mu = 5.201 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.250^\circ$, 5165 total reflections, 2131 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0358$, 2564 data, 181 parameters, 0 restraints, $\text{GooF} = 1.177$, $R = 0.0485$ and $wR = 0.1110$ [$I_o > 2\sigma(I_o)$], $R = 0.0623$ and $wR = 0.1159$ (all reflections), $1.007 < d\Delta\rho < -0.713/\text{\AA}^3$.

54) Crystal data for NBSac-5a [CCDC-2297344]: Sum formula: $C_{12}H_8BrIN_2O_3S$, $M = 467.07$, colourless plate, $0.016 \times 0.014 \times 0.014 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 8.3444(17)\text{\AA}$, $b = 23.800(5)\text{\AA}$, $c = 8.0893(16)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 117.32(3)^\circ$, $\gamma = 90^\circ$, $V = 1427.3(6)\text{\AA}^3$, $Z = 4$, $D_c = 2.174 \text{ g/cm}^3$, $F_{000} = 888$, $\mu = 5.196 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\max} = 25.245^\circ$, 11331 total reflections, 2097 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0566$, 2578 data, 181 parameters, 0 restraints, $\text{GooF} = 1.177$, $R = 0.0390$ and $wR = 0.0701$ [$I_o > 2\sigma(I_o)$], $R = 0.0548$ and $wR = 0.0747$ (all reflections), $0.574 < d\Delta\rho < -0.638/\text{\AA}^3$.

55) Crystal data for NBSac-6 [CCDC-2297339]: Sum formula: $C_{13}H_8BrF_3N_2O_3S$, $M = 409.18$, colourless block, $0.09 \times 0.03 \times 0.03 \text{ mm}^3$, triclinic space group P-1, $a = 7.7643(2)\text{\AA}$, $b = 8.3599(2)\text{\AA}$, $c = 12.3063(5)\text{\AA}$, $\alpha = 83.758(3)^\circ$, $\beta = 80.066(3)^\circ$, $\gamma = 64.773(3)^\circ$, $V = 711.21(4)\text{\AA}^3$, $Z = 2$, $D_c = 1.911 \text{ g/cm}^3$,

F000 = 404, $\mu = 5.820 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 79.516^\circ$, 8390 total reflections, 7909 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = \text{twin}$, 8390 data, 209 parameters, 0 restraints, GooF = 1.151, R = 0.0354 and wR = 0.0970 [$I_o > 2\sigma(I_o)$], R = 0.0373 and wR = 0.0979 (all reflections), $1.340 < d\Delta\rho < -0.620 / \text{\AA}^3$.

56) Crystal data for NBSac-9 [CCDC-2297345]: Sum formula: $\text{C}_{14}\text{H}_{13}\text{BrN}_2\text{O}_3\text{S}$, M = 369.23, colourless block, $0.14 \times 0.08 \times 0.05 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 8.55670(10) \text{\AA}$, $b = 23.9780(3) \text{\AA}$, $c = 7.75550(10) \text{\AA}$, $\alpha = 90^\circ$, $\beta = 116.634(2)^\circ$, $\gamma = 90^\circ$, $V = 1422.37(4) \text{\AA}^3$, $Z = 4$, $D_c = 1.724 \text{ g/cm}^3$, F000 = 744, $\mu = 5.426 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 78.168^\circ$, 27511 total reflections, 2926 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0343$, 3024 data, 191 parameters, 0 restraints, GooF = 1.188, R = 0.0305 and wR = 0.0691 [$I_o > 2\sigma(I_o)$], R = 0.0316 and wR = 0.0696 (all reflections), $0.665 < d\Delta\rho < -0.427 / \text{\AA}^3$.

57) Crystal data for NBSac-13 [CCDC-2297343]: Sum formula: $\text{C}_{25}\text{H}_{19}\text{BrN}_2\text{O}_3\text{S}$, M = 507.39, colourless block, $0.094 \times 0.058 \times 0.034 \text{ mm}^3$, triclinic space group P-1, $a = 8.3067(2) \text{\AA}$, $b = 9.7906(3) \text{\AA}$, $c = 14.6480(3) \text{\AA}$, $\alpha = 92.242(2)^\circ$, $\beta = 96.857(2)^\circ$, $\gamma = 112.351(2)^\circ$, $V = 1089.26(5) \text{\AA}^3$, $Z = 2$, $D_c = 1.547 \text{ g/cm}^3$, F000 = 516, $\mu = 3.725 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 80.046^\circ$, 13696 total reflections, 4179 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0350$, 4607 data, 289 parameters, 0 restraints, GooF = 1.091, R = 0.0385 and wR = 0.1046 [$I_o > 2\sigma(I_o)$], R = 0.0421 and wR = 0.1068 (all reflections), $0.946 < d\Delta\rho < -0.673 / \text{\AA}^3$.

58) Crystal data for NBSac-14 [CCDC-2297341]: Sum formula: $\text{C}_{26}\text{H}_{21}\text{BrN}_2\text{O}_3\text{S}$, M = 521.42, colourless block, $0.061 \times 0.049 \times 0.023 \text{ mm}^3$, monoclinic space group Cc, $a = 18.7927(2) \text{\AA}$, $b = 7.78420(10) \text{\AA}$, $c = 16.3844(2) \text{\AA}$, $\alpha = 90^\circ$, $\beta = 108.590(2)^\circ$, $\gamma = 90^\circ$, $V = 2271.75(5) \text{\AA}^3$, $Z = 4$, $D_c = 1.525 \text{ g/cm}^3$, F000 = 1064, $\mu = 3.588 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 79.823^\circ$, 22391 total reflections, 4144 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0455$, 4302 data, 299 parameters, 2 restraints, GooF = 1.109, R = 0.0395 and wR = 0.1020 [$I_o > 2\sigma(I_o)$], R = 0.0415 and wR = 0.1033 (all reflections), $0.484 < d\Delta\rho < -0.779 / \text{\AA}^3$.

59) Crystal data for (NSac)₂I-10H [CCDC-2297351]: Sum formula: $\text{C}_{22}\text{H}_{20}\text{IN}_3\text{O}_6\text{S}_2$, M = 613.43, colourless block, $0.403 \times 0.259 \times 0.168 \text{ mm}^3$, monoclinic space group $P2_1/n$, $a = 13.4412(3) \text{\AA}$, $b = 9.8116(3) \text{\AA}$, $c = 17.9192(4) \text{\AA}$, $\alpha = 90^\circ$, $\beta = 91.614(2)^\circ$, $\gamma = 90^\circ$, $V = 2362.24(10) \text{\AA}^3$, $Z = 4$, $D_c = 1.725 \text{ g/cm}^3$, F000 = 1224, $\mu = 1.577 \text{ mm}^{-1}$, T = 120 K, $\theta_{\text{max}} = 26.371^\circ$, 9787 total reflections, 4077 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0298$, 4831 data, 309 parameters, 0 restraints, GooF = 1.066, R = 0.0684 and wR = 0.1609 [$I_o > 2\sigma(I_o)$], R = 0.0595 and wR = 0.1718 (all reflections), $3.051 < d\Delta\rho < -1.761 / \text{\AA}^3$.

60) Crystal data for (NSac)₂I-12H [CCDC-2297348]: Sum formula: $\text{C}_{25}\text{H}_{18}\text{IN}_3\text{O}_6\text{S}_2$, M = 647.44, colourless block, $0.023 \times 0.02 \times 0.02 \text{ mm}^3$, monoclinic space group $C2/c$, $a = 12.703(3) \text{\AA}$, $b = 10.867(2) \text{\AA}$, $c = 17.869(4) \text{\AA}$, $\alpha = 90^\circ$, $\beta = 90.26(3)^\circ$, $\gamma = 90^\circ$, $V = 2466.9(9) \text{\AA}^3$, $Z = 4$, $D_c = 1.743 \text{ g/cm}^3$, F000 = 1288, $\mu = 1.516 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 28.881^\circ$, 11333 total reflections, 2682 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0318$, 3237 data, 215 parameters, 6 restraints, GooF = 1.042, R = 0.0285 and wR = 0.0597 [$I_o > 2\sigma(I_o)$], R = 0.0384 and wR = 0.0631 (all reflections), $0.316 < d\Delta\rho < -0.353 / \text{\AA}^3$.

61) Crystal data for (NSac)₂I-15H [CCDC-2297349]: Sum formula: $\text{C}_{22}\text{H}_{22}\text{IN}_3\text{O}_6\text{S}_2\text{Si}$, M = 647.44, colourless block, $0.032 \times 0.024 \times 0.02 \text{ mm}^3$, triclinic space group P-1, $a = 8.0649(10) \text{\AA}$, $b = 9.3955(11) \text{\AA}$, $c = 16.8787(14) \text{\AA}$, $\alpha = 90.644(7)^\circ$, $\beta = 90.165(7)^\circ$, $\gamma = 94.442(4)^\circ$, $V = 1275.0(2) \text{\AA}^3$, $Z = 2$, $D_c = 1.676 \text{ g/cm}^3$, F000 = 644, $\mu = 1.510 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 27.103^\circ$, 9133 total reflections, 4717 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0357$, 5494 data, 319 parameters, 0 restraints, GooF = 1.110, R = 0.0625 and wR = 0.1962 [$I_o > 2\sigma(I_o)$], R = 0.0729 and wR = 0.2069 (all reflections), $1.210 < d\Delta\rho < -2.236 / \text{\AA}^3$.

62) Crystal data for (NSac)₂I-15Ha [CCDC-2297350]: Sum formula: $\text{C}_{22}\text{H}_{22}\text{IN}_3\text{O}_6\text{S}_2\text{Si}$, M = 647.44, colourless block, $0.14 \times 0.12 \times 0.06 \text{ mm}^3$, triclinic space group P-1, $a = 9.9333(4) \text{\AA}$, $b = 10.6041(4) \text{\AA}$, $c = 13.3328(6) \text{\AA}$, $\alpha = 90.119(3)^\circ$, $\beta = 110.410(2)^\circ$, $\gamma = 102.292(2)^\circ$, $V = 1281.58(9) \text{\AA}^3$, $Z = 2$, $D_c = 1.668 \text{ g/cm}^3$, F000 = 644, $\mu = 1.502 \text{ mm}^{-1}$, T = 170 K, $\theta_{\text{max}} = 27.102^\circ$, 10295 total reflections, 4501 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0331$, 5638 data, 319 parameters, 0 restraints, GooF = 1.072, R = 0.0404 and wR = 0.0888 [$I_o > 2\sigma(I_o)$], R = 0.0579 and wR = 0.0948 (all reflections), $0.457 < d\Delta\rho < -0.606 / \text{\AA}^3$.

63) Crystal data for NHSac-5 [CCDC-2297352]: Sum formula: $C_{12}H_9IN_2O_3S$, $M = 388.17$, colourless block, $0.031 \times 0.02 \times 0.02 \text{ mm}^3$, triclinic space group P-1, $a = 7.4689(15) \text{ \AA}$, $b = 7.7102(15) \text{ \AA}$, $c = 13.155(3) \text{ \AA}$, $\alpha = 91.06(3)^\circ$, $\beta = 100.12(3)^\circ$, $\gamma = 116.40(3)^\circ$, $V = 663.9(3) \text{ \AA}^3$, $Z = 2$, $D_c = 1.942 \text{ g/cm}^3$, $F_{000} = 376$, $\mu = 2.573 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.240^\circ$, 16896 total reflections, 2169 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0452$, 2400 data, 172 parameters, 0 restraints, $\text{GooF} = 1.088$, $R = 0.0333$ and $wR = 0.0733$ [$I_o > 2\sigma(I_o)$], $R = 0.0397$ and $wR = 0.0757$ (all reflections), $1.405 < d\Delta\rho < -0.318 \text{ /\AA}^3$.

64) Crystal data for NSac-1H [CCDC-2297353]: Sum formula: $C_{24}H_{20}N_4O_6S_2$, $M = 524.56$, colourless block, $0.023 \times 0.02 \times 0.019 \text{ mm}^3$, triclinic space group P-1, $a = 7.3768(15) \text{ \AA}$, $b = 12.921(3) \text{ \AA}$, $c = 14.121(3) \text{ \AA}$, $\alpha = 65.19(3)^\circ$, $\beta = 74.93(3)^\circ$, $\gamma = 78.26(3)^\circ$, $V = 1172.8(5) \text{ \AA}^3$, $Z = 2$, $D_c = 1.485 \text{ g/cm}^3$, $F_{000} = 544$, $\mu = 0.277 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.249^\circ$, 7622 total reflections, 2706 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0435$, 4218 data, 326 parameters, 0 restraints, $\text{GooF} = 1.027$, $R = 0.0610$ and $wR = 0.1245$ [$I_o > 2\sigma(I_o)$], $R = 0.1092$ and $wR = 0.1447$ (all reflections), $0.312 < d\Delta\rho < -0.323 \text{ /\AA}^3$.

65) Crystal data for NSac-8H [CCDC-2297355]: Sum formula: $C_{13}H_{12}N_2O_3S$, $M = 276.31$, colourless block, $0.117 \times 0.093 \times 0.052 \text{ mm}^3$, triclinic space group P-1, $a = 8.5121(2) \text{ \AA}$, $b = 12.4435(2) \text{ \AA}$, $c = 13.9677(3) \text{ \AA}$, $\alpha = 107.9831(19)^\circ$, $\beta = 99.204(2)^\circ$, $\gamma = 106.347(2)^\circ$, $V = 1299.98(6) \text{ \AA}^3$, $Z = 4$, $D_c = 1.412 \text{ g/cm}^3$, $F_{000} = 576$, $\mu = 2.278 \text{ mm}^{-1}$, $T = 120 \text{ K}$, $\theta_{\text{max}} = 79.678^\circ$, 16299 total reflections, 4870 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0273$, 5412 data, 345 parameters, 0 restraints, $\text{GooF} = 1.113$, $R = 0.0413$ and $wR = 0.1174$ [$I_o > 2\sigma(I_o)$], $R = 0.0448$ and $wR = 0.1197$ (all reflections), $0.282 < d\Delta\rho < -0.579 \text{ /\AA}^3$.

66) Crystal data for NSac-16H [CCDC-2297356]: Sum formula: $C_{14}H_{15}N_3O_3S$, $M = 305.35$, colourless block, $0.42 \times 0.16 \times 0.12 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 7.1692(2) \text{ \AA}$, $b = 8.3894(2) \text{ \AA}$, $c = 23.4609(6) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 97.158(2)^\circ$, $\gamma = 90^\circ$, $V = 1400.06(6) \text{ \AA}^3$, $Z = 4$, $D_c = 1.449 \text{ g/cm}^3$, $F_{000} = 640$, $\mu = 0.245 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 27.876^\circ$, 6336 total reflections, 2582 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0402$, 3331 data, 195 parameters, 1 restraints, $\text{GooF} = 1.052$, $R = 0.0491$ and $wR = 0.1050$ [$I_o > 2\sigma(I_o)$], $R = 0.0711$ and $wR = 0.1156$ (all reflections), $0.383 < d\Delta\rho < -0.347 \text{ /\AA}^3$.

67) Crystal data for NSac-16Ha [CCDC-2297354]: Sum formula: $C_{21}H_{20}N_4O_6S_2$, $M = 488.53$, colourless block, $0.5 \times 0.28 \times 0.04 \text{ mm}^3$, triclinic space group P-1, $a = 7.1498(12) \text{ \AA}$, $b = 12.8796(19) \text{ \AA}$, $c = 13.280(2) \text{ \AA}$, $\alpha = 110.086(8)^\circ$, $\beta = 101.467(8)^\circ$, $\gamma = 95.339(8)^\circ$, $V = 1108.2(3) \text{ \AA}^3$, $Z = 2$, $D_c = 1.464 \text{ g/cm}^3$, $F_{000} = 508$, $\mu = 0.287 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 27.096^\circ$, 7913 total reflections, 3004 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0566$, 4760 data, 303 parameters, 0 restraints, $\text{GooF} = 1.078$, $R = 0.0754$ and $wR = 0.1930$ [$I_o > 2\sigma(I_o)$], $R = 0.1250$ and $wR = 0.2270$ (all reflections), $0.624 < d\Delta\rho < -0.546 \text{ /\AA}^3$.

68) Crystal data for 16-I [CCDC-2297358]: Sum formula: $C_7H_9IN_2$, $M = 248.06$, colourless block, $0.02 \times 0.019 \times 0.019 \text{ mm}^3$, monoclinic space group $P2_1/c$, $a = 5.9023(12) \text{ \AA}$, $b = 8.4518(17) \text{ \AA}$, $c = 16.929(3) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 98.55(3)^\circ$, $\gamma = 90^\circ$, $V = 835.1(3) \text{ \AA}^3$, $Z = 4$, $D_c = 1.973 \text{ g/cm}^3$, $F_{000} = 472$, $\mu = 3.762 \text{ mm}^{-1}$, $T = 170 \text{ K}$, $\theta_{\text{max}} = 25.241^\circ$, 2794 total reflections, 1300 with $I_o > 2\sigma(I_o)$, $R_{\text{int}} = 0.0489$, 1402 data, 93 parameters, 0 restraints, $\text{GooF} = 1.064$, $R = 0.0420$ and $wR = 0.1150$ [$I_o > 2\sigma(I_o)$], $R = 0.0451$ and $wR = 0.1182$ (all reflections), $1.177 < d\Delta\rho < -0.990 \text{ /\AA}^3$.

Table S1. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP gas-phase optimized parameters of N-iodosuccinimide complexes

| Compl | X-ray | | DFT | | I...N (Å) | | N-I-N (°) | | (C-C)-N-X (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|---------------------|----------------------|--------------------------------|----------------------|--------------------------------|-----------|-------|------------|-------|---------------|-------|----------------------------------|-----|----------------------------|-------|
| | N-I (Å) ^a | $\Delta(N-I)$ (Å) ^b | N-I (Å) ^c | $\Delta(N-I)$ (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NIS-1 ^d | 2.101(3) | 0.037 | 2.082 | 0.067 | 2.473(3) | 2.520 | 180.0 | 180.0 | 180.0 | 180.0 | 0 | 0 | 4.574 | 4.602 |
| | 2.137(3) | 0.073 | -- | -- | 2.443(3) | -- | 180.0 | -- | 180.0 | -- | 0 | -- | 4.579 | -- |
| NIS-2 | 2.082(4) | 0.018 | 2.059 | 0.044 | 2.560(4) | 2.638 | 174.55(15) | 174.7 | 179.02 | 179.8 | 0.98 | 0.2 | 4.637 | 4.693 |
| NIS-3 | 2.100(12) | 0.037 | 2.062 | 0.047 | 2.580(12) | 2.622 | 176.8(5) | 174.6 | 176.19 | 179.9 | 3.81 | 0.1 | 4.68 | 4.679 |
| NIS-4 | 2.095(2) | 0.031 | 2.062 | 0.047 | 2.578(2) | 2.625 | 176.97(9) | 174.6 | 176.79 | 179.9 | 3.21 | 0.1 | 4.672 | 4.681 |
| NIS-5 | 2.100(3) | 0.039 | 2.064 | 0.049 | 2.549(2) | 2.611 | 177.33(10) | 175.3 | 177.17 | 180.0 | 0 | 0 | 4.648 | 4.671 |
| NIS-6 | 2.094(3) | 0.03 | 2.053 | 0.038 | 2.570(3) | 2.694 | 177.95(10) | 172.5 | 179.33 | 179.7 | 0.67 | 0.3 | 4.670 | 4.737 |
| NIS-7 | - | -- | 2.056 | 0.041 | - | 2.647 | - | 177.0 | - | 179.5 | -- | 0.5 | - | 4.701 |
| NIS-8 | 2.112(4) | 0.048 | 2.085 | 0.07 | 2.481(4) | 2.523 | 175.44(17) | 177.5 | 179.59 | 179.9 | 0.41 | 0.1 | 4.588 | 4.607 |
| NIS-9 | 2.123(2) | 0.059 | 2.084 | 0.069 | 2.455(2) | 2.531 | 176.59(8) | 177.3 | 176.59 | 179.8 | 0.41 | 0.2 | 4.577 | 4.614 |
| NIS-10 | - | -- | 2.083 | 0.068 | - | 2.538 | - | 176.9 | - | 179.8 | -- | 0.2 | - | 4.619 |
| NIS-11 ^e | 2.135(4) | 0.071 | 2.077 | 0.062 | 2.422(4) | 2.566 | 174.30(15) | 175.4 | 176.96 | 179.9 | 3.04 | 0.1 | 4.552 | 4.639 |
| | 2.050(4) | -0.014 | -- | -- | 2.654(4) | -- | 170.96(12) | -- | -- | -- | -- | -- | 4.682 (N...O) ^b | -- |
| NIS-12 | 2.114(2) | 0.05 | 2.072 | 0.057 | 2.499(2) | 2.595 | 175.92(7) | 175.9 | 178.54 | 179.6 | 1.46 | 0.4 | 4.61 | 4.664 |
| NIS-13 | -- | -- | 2.086 | 0.071 | -- | 2.522 | -- | 179.9 | -- | 178.9 | -- | 1.1 | -- | 4.608 |
| NIS-14 | -- | -- | 2.067 | 0.052 | -- | 2.637 | -- | 175.4 | -- | 179.3 | -- | 0.7 | -- | 4.700 |
| NIS-15 | -- | -- | 2.088 | 0.073 | -- | 2.514 | -- | 178.2 | -- | 179.2 | -- | 0.8 | -- | 4.601 |
| NIS-16 | -- | -- | 2.072 | 0.057 | -- | 2.593 | -- | 177.2 | -- | 179.5 | -- | 0.5 | -- | 4.663 |

^a Crystal structure (N-I)_{ligand} = 2.064(6) Å; ^b $\Delta(N-I) = (N-I)_{\text{compl}} - (N-I)_{\text{ligand}}$; ^cDFT structure (N-I)_{ligand} = 2.015 Å; ^dThe asymmetric unit contains two different NIS-1 complexes. ^eTwo XB donors are present in the asymmetric unit, one of which participates in XB with imide C=O group of the 1:1 NIS:11 halogen-bonded complex.

Table S2. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP gas-phase optimized parameters of N-iodophthalimide complexes

| Compl | X-ray | | DFT | | I...N (Å) | | N-I-N (°) | | (C-C)-N-X (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|--------------------|----------------------|---------------------------------|----------------------|---------------------------------|------------|-------|------------|-------|---------------|-------|----------------------------------|-----|----------------------|-------|
| | N-I (Å) ^a | Δ (N-I) (Å) ^b | N-I (Å) ^c | Δ (N-I) (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NIP-1 | 2.130(3) | 0.093 | 2.077 | 0.07 | 2.409(3) | 2.518 | 177.68(10) | 180.0 | 177.28 | 180.0 | 2.72 | 0 | 4.538 | 4.595 |
| NIP-2 | 2.097(4) | 0.06 | 2.054 | 0.047 | 2.509(8) | 2.636 | 177.3(5) | 174.8 | 175.94 | 179.9 | 4.06 | 0.1 | 4.632 | 4.685 |
| NIP-3 | 2.0833(15) | 0.0463 | 2.057 | 0.05 | 2.553(2) | 2.620 | 176.56(5) | 174.7 | 165.21 | 179.9 | 14.79 | 0.1 | 4.634 | 4.672 |
| NIP-4 ^d | 2.078(3) | 0.041 | 2.056 | 0.049 | 2.547(3) | 2.622 | 177.52(10) | 174.7 | 170.05 | 179.9 | 9.95 | 0.1 | 4.625 | 4.673 |
| | 2.089(3) | 0.052 | -- | --- | 2.555(3) | -- | 177.13(10) | -- | 168.3 | -- | 11.7 | -- | 4.642 | -- |
| NIP-5 | 2.081(3) | 0.044 | 2.058 | 0.051 | 2.545(4) | 2.608 | 176.47(13) | 175.5 | 177.29 | 180.0 | 2.71 | 0 | 4.624 | 4.663 |
| NIP-6 | 2.076(3) | 0.039 | 2.047 | 0.04 | 2.614(4) | 2.692 | 176.74(11) | 172.7 | 177.06 | 179.7 | 2.94 | 0.3 | 4.688 | 4.729 |
| NIP-7 | -- | -- | 2.050 | 0.043 | - | 2.645 | -- | 176.8 | - | 179.6 | -- | 0.4 | -- | 4.693 |
| NIP-8 | 2.124(12) | 0.087 | 2.080 | 0.073 | 2.490(13) | 2.520 | 172.2(6) | 177.5 | 172.16 | 179.8 | 7.84 | 0.2 | 4.611 | 4.599 |
| NIP-9 | 2.122(2) | 0.085 | 2.079 | 0.072 | 2.449(2) | 2.529 | 175.22(9) | 177.4 | 176.9 | 179.8 | 3.1 | 0.2 | 4.567 | 4.607 |
| NIP-10 | -- | -- | 2.078 | 0.071 | - | 2.536 | -- | 176.9 | - | 179.8 | -- | 0.2 | -- | 4.612 |
| NIP-11 | -- | -- | 2.072 | 0.065 | - | 2.563 | -- | 175.4 | - | 179.9 | -- | 0.1 | -- | 4.631 |
| NIP-12 | 2.083(4) | 0.046 | 2.067 | 0.06 | 2.526(4) | 2.592 | 175.04(14) | 175.8 | 177.93 | 179.6 | 3.1 | 0.4 | 4.605 | 4.656 |
| NIP-13 | 2.1038(16) | 0.0668 | 2.081 | 0.074 | 2.4980(16) | 2.521 | 177.68(6) | 179.9 | 173.81 | 178.9 | 6.19 | 1.1 | 4.601 | 4.601 |
| NIP-14 | 2.091(3) | 0.054 | 2.061 | 0.054 | 2.574(3) | 2.635 | 170.05(12) | 175.4 | 170.03 | 179.0 | 9.97 | 1.0 | 4.647 | 4.693 |
| NIP-15 | -- | -- | 2.082 | 0.075 | -- | 2.515 | -- | 178.0 | -- | 179.2 | -- | 0.8 | -- | 4.596 |
| NIP-16 | -- | -- | 2.067 | 0.06 | -- | 2.592 | -- | 177.0 | -- | 179.5 | -- | 0.5 | -- | 4.657 |

^a(N-I)_{ligand} = 2.037(3) Å; ^b Δ (N-I) = (N-I)_{compl} - (N-I)_{ligand}; ^cDFT structure (N-I)_{ligand} = 2.007 Å; ^dThe asymmetric unit contains two different NIS-4 complexes.

Table S3. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP gas-phase optimized parameters of N-iodosaccharin complexes

| Compl | X-ray | | DFT | | I...N (Å) | | N-I-N (°) | | (C-C)-N-X (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|---|----------------------|---------------------------------|----------------------|---------------------------------|------------|-------|------------|-------|------------------|-------|----------------------------------|-----|----------------------|-------|
| | N-I (Å) ^a | Δ (N-I) (Å) ^b | N-I (Å) ^c | Δ (N-I) (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NISac-1 | 2.254(11) | 0.188 | 2.102 | 0.094 | 2.279(11) | 2.447 | 174.5(4) | 180.0 | 167.41 | 177.6 | 12.59 | 2.4 | 4.527 | 4.549 |
| NISac-2 | 2.105(5) | 0.039 | 2.073 | 0.065 | 2.492(6) | 2.557 | 172.8(2) | 175.4 | 173.85 | 177.4 | 6.15 | 2.6 | 4.589 | 4.626 |
| NISac-3 | 2.140(14) | 0.074 | 2.077 | 0.069 | 2.455(15) | 2.542 | 172.8(6) | 175.2 | 175.62 | 177.5 | 4.38 | 2.5 | 4.581 | 4.614 |
| NISac-4 | 2.123(3) | 0.057 | 2.076 | 0.068 | 2.441(3) | 2.544 | 176.35(10) | 175.2 | 176.34 | 177.6 | 3.66 | 2.4 | 4.561 | 4.616 |
| NISac-5 | 2.168(3) | 0.1 | 2.079 | 0.071 | 2.376(3) | 2.529 | 178.67(10) | 176.0 | 163.93 | 177.7 | | 2.3 | 4.544 | 4.606 |
| NISac-6 | 2.099(6) | 0.033 | 2.064 | 0.056 | 2.528(6) | 2.609 | 172.9(3) | 173.3 | 166.01 | 177.3 | 16.07 | 2.7 | 4.618 | 4.665 |
| NISac-7 | 2.131(4) | 0.065 | 2.068 | 0.06 | 2.440(4) | 2.562 | 175.4(2) | 175.2 | 177.62 | 177.1 | 2.38 | 2.9 | 4.568 | 4.627 |
| NISac-8 | - | | 2.106 | 0.098 | - | 2.447 | - | 177.7 | - | 177.8 | -- | 2.2 | - | 4.553 |
| NISac-9 | 2.231(19) | 0.165 | 2.107 | 0.099 | 2.325(18) | 2.449 | 175.4(7) | 177.3 | 177.9 | 177.9 | 2.1 | 2.1 | 4.544 | 4.555 |
| (NSac) ₂ I-10H | 2.218(4) | 0.152 | 2.104 | 0.096 | 2.280(4) | 2.461 | 179.21(13) | 177.2 | 169.48 169.23 | 178.0 | 10.52 10.77 | 2 | 4.497 | 4.564 |
| NISac-11 | 2.211(11) | 0.145 | 2.097 | 0.089 | 2.342(11) | 2.485 | 178.8(4) | 175.9 | 163.06 | 177.7 | 16.94 | 2.3 | 4.553 | 4.579 |
| (NSac) ₂ I-12H | 2.2639(19) | 0.198 | 2.092 | 0.084 | 2.2639(19) | 2.504 | 180.0 | 176.5 | 168.76 | 177.1 | 11.24 | 2.9 | 4.528 | 4.594 |
| NISac-13 | - | -- | 2.110 | 0.102 | - | 2.445 | - | 179.3 | - | 174.3 | -- | 5.7 | - | 4.555 |
| NISac-14 | - | -- | 2.086 | 0.078 | - | 2.553 | - | 175.5 | - | 176.5 | -- | 3.5 | - | 4.636 |
| (NSac) ₂ I-15H ^c | 2.274(5) | 0.208 | 2.115 | 0.107 | 2.214(5) | 2.419 | 178.89(18) | 179.8 | 171.83 169.67 | 179.3 | 8.17 10.33 | 0.7 | 4.487 | 4.534 |
| (NSac) ₂ I-15Ha ^c | 2.283(3) | 0.217 | -- | -- | 2.221(3) | - | 176.97(12) | - | 176.71 171.78 | - | 3.19 8.22 | -- | 4.503 | - |
| NISac-16 | - | -- | 2.093 | 0.085 | - | 2.502 | - | 177.4 | - | 176.9 | -- | 3.1 | - | 4.593 |

^a(N-I)_{ligand} = 2.066(4) Å; ^b Δ (N-I) = (N-I)_{compl} - (N-I)_{ligand}; ^cDFT structure (N-I)_{ligand} = 2.008 Å; ^dTwo different XB complexes were obtained for (NISac)₂I-15H.

Table S4. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP/PCM^a optimized parameters and free energies of complexation of N-iodosaccharin complexes in CHCl₃.

| Compl | N-I (Å) | | I...N (Å) | | N-I-N (°) | | (C-C)-N-X (°) | | Bending angle Δθ (°) | | (imide)N...N(Py) (Å) | | ΔG _{complex} (XB) (kJ mol ⁻¹) |
|----------|-----------|-------|-----------|-------|------------|-------|---------------|-------|----------------------|-----|----------------------|-------|--|
| | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | DFT |
| NISac-1 | 2.254(11) | 2.154 | 2.279(11) | 2.349 | 174.5(4) | 179.9 | 167.41 | 177.8 | 12.59 | 2.2 | 4.527 | 4.503 | -33.2 |
| NISac-2 | 2.105(5) | 2.110 | 2.492(6) | 2.453 | 172.8(2) | 176.6 | 173.85 | 177.7 | 6.15 | 2.3 | 4.589 | 4.561 | -10.8 |
| NISac-3 | 2.140(14) | 2.114 | 2.455(15) | 2.445 | 172.8(6) | 176.3 | 175.62 | 177.9 | 4.38 | 2.1 | 4.581 | 4.556 | -13.2 |
| NISac-4 | 2.123(3) | 2.112 | 2.441(3) | 2.449 | 176.35(10) | 176.3 | 176.34 | 177.9 | 3.66 | 2.1 | 4.561 | 4.559 | -11.7 |
| NISac-5 | 2.166(3) | 2.116 | 2.378(3) | 2.438 | 178.67(10) | 176.9 | 163.93 | 178.0 | | 2.0 | 4.544 | 4.552 | -14.7 |
| NISac-6 | 2.099(6) | 2.095 | 2.528(6) | 2.510 | 172.9(3) | 175.2 | 166.01 | 177.7 | 16.07 | 2.3 | 4.618 | 4.601 | -6.3 |
| NISac-7 | 2.131(4) | 2.105 | 2.440(4) | 2.457 | 175.4(2) | 177.6 | 177.62 | 177.7 | 2.38 | 2.3 | 4.568 | 4.561 | -7.5 |
| NISac-8 | - | 2.158 | - | 2.355 | - | 177.8 | - | 178.1 | -- | 1.9 | - | 4.513 | -31.1 |
| NISac-9 | 2.231(19) | 2.159 | 2.325(18) | 2.358 | 175.4(7) | 177.3 | 177.9 | 178.1 | 2.1 | 1.9 | 4.544 | 4.516 | -31.8 |
| NISac-11 | 2.211(11) | 2.153 | 2.342(11) | 2.373 | 178.8(4) | 177.2 | 163.06 | 178.1 | 16.94 | 1.9 | 4.553 | 4.525 | -29.9 |
| NISac-13 | -- | 2.147 | - | 2.380 | - | 176.3 | - | 177.9 | -- | 2.1 | - | 4.525 | -15.2 |
| NISac-14 | -- | 2.135 | - | 2.408 | - | 176.7 | - | 178.3 | -- | 1.7 | - | 4.542 | -20.8 |
| NISac-16 | -- | 2.149 | - | 2.376 | - | 178.7 | - | 176.9 | -- | 3.1 | - | 4.525 | -28.8 |

^a Polarized continuum model was used as implemented in Gaussian16. See References 15-18.

Table S5. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP optimized parameters of N-bromosuccinimide complexes

| Comp | X-ray | | DFT | | Br...N (Å) | | N-Br-N (°) | | (C-C)-N-Br (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|--------------------|-----------------------|----------------------------------|-----------------------|----------------------------------|------------|-------|------------|-------|----------------|-------|----------------------------------|-----|----------------------|-------|
| | N-Br (Å) ^a | Δ (N-Br) (Å) ^b | N-Br (Å) ^c | Δ (N-Br) (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NBS-1 ^d | 1.8923(19) | 0.0523 | 1.873 | 0.047 | 2.444(2) | 2.507 | 177.44(9) | 180.0 | 178.74 | 180.0 | 1.26 | 0 | 4.335 | 4.380 |
| | 1.8876(19) | 0.0476 | -- | -- | 2.499(2) | | 175.38(8) | | 179.26 | -- | 0.74 | -- | 4.383 | |
| | 1.8997(19) | 0.0597 | -- | -- | 2.424(2) | | 179.45(8) | | 178.29 | -- | 1.71 | -- | 4.324 | |
| | 1.9064(19) | 0.0664 | -- | -- | 2.417(2) | | 179.96(9) | | 176.56 | -- | 3.44 | -- | 4.321 | |
| NBS-2 | - | -- | 1.852 | 0.026 | -- | 2.645 | -- | 173.1 | -- | 179.7 | -- | 0.3 | -- | 4.489 |
| NBS-3 | 1.8691(17) | 0.0291 | 1.855 | 0.029 | 2.557(2) | 2.626 | 178.47(6) | 173.6 | 175.53 | 179.7 | 4.47 | 0.3 | 4.426 | 4.474 |
| NBS-4 | 1.876(6) | 0.036 | 1.854 | 0.028 | 2.545(7) | 2.629 | 179.7(3) | 173.6 | 175.91 | 179.7 | 4.09 | 0.3 | 4.427 | 4.477 |
| NBS-5 | 1.880(6) | 0.04 | 1.856 | 0.03 | 2.503(7) | 2.611 | 178.5(2) | 174.5 | 177.04 | 179.8 | 2.96 | 0.2 | 4.384 | 4.462 |
| NBS-8 | 1.898(3) | 0.058 | 1.876 | 0.05 | 2.430(3) | 2.500 | 175.92(11) | 177.8 | 179.67 | 179.9 | 0.33 | 0.1 | 4.326 | 4.375 |
| NBS-9 | 1.901(4) | 0.061 | 1.876 | 0.05 | 2.476(4) | 2.507 | 174.78(15) | 177.9 | 175.72 | 179.8 | 4.28 | 0.2 | 4.373 | 4.381 |
| NBS-11 | - | -- | 1.865 | 0.039 | -- | 2.566 | -- | 175.0 | -- | 179.9 | -- | 0.1 | -- | 4.427 |
| NBS-12 | - | -- | 1.862 | 0.036 | -- | 2.588 | -- | 176.5 | -- | 179.6 | -- | 0.4 | -- | 4.449 |

^a(N-Br)_{ligand} = 1.840(6) Å; ^b Δ (N-Br) = (N-Br)_{compl} - (N-Br)_{ligand}; ^cDFT structure (N-Br)_{ligand} = 1.826 Å; ^dThe asymmetric unit contains four crystallographically independent 1:1 XB complexes;

Table S6. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP optimized parameters of N-bromophthalimide complexes

| Comp | X-ray | | DFT | | Br...N (Å) | | N-Br-N (°) | | (C-C)-N-Br (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|---------------------|-----------------------|---------------------------------|-----------------------|---------------------------------|------------|-------|------------|-------|----------------|-------|----------------------------------|-----|----------------------|-------|
| | N-Br (Å) ^a | $\Delta(N-Br)$ (Å) ^b | N-Br (Å) ^c | $\Delta(N-Br)$ (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NBP-1 | 1.924(3) | 0.083 | 1.868 | 0.048 | 2.329(3) | 2.505 | 177.51(13) | 180.0 | 178.53 | 180.0 | 1.47 | 0 | 4.252 | 4.373 |
| NBP-2 | 1.859(5) | 0.018 | 1.848 | 0.028 | 2.607(3) | 2.644 | 168.94(10) | 173.4 | 172.75 | 179.7 | 7.25 | 0.3 | 4.44 | 4.484 |
| NBP-3 ^d | 1.867(2) | 0.026 | 1.850 | 0.03 | 2.513(3) | 2.625 | 178.06(10) | 173.9 | 171.3 | 179.7 | 7.25 | 0.3 | 4.38 | 4.469 |
| | 1.877(2) | 0.036 | -- | -- | 2.544(2) | | 177.70(9) | -- | 169.81 | -- | 10.19 | -- | 4.42 | |
| NBP-4 ^d | 1.872(7) | 0.031 | 1.850 | 0.03 | 2.506(7) | 2.628 | 177.9(3) | 173.8 | 169.9 | 179.7 | 10.1 | 0.3 | 4.379 | 4.471 |
| | 1.878(7) | 0.037 | -- | -- | 2.558(7) | | 177.4(3) | | 170.18 | -- | 9.82 | -- | 4.436 | |
| NBP-5 | 1.883(3) | 0.042 | 1.852 | 0.032 | 2.491(3) | 2.609 | 178.27(14) | 174.7 | 173.02 | 179.8 | 6.28 | 0.2 | 4.373 | 4.456 |
| NBP-6 | 1.8659(18) | 0.0249 | 1.845 | 0.025 | 2.631(2) | 2.673 | 169.92(11) | 171.4 | 169.38 | 179.6 | 10.62 | 0.4 | 4.48 | 4.506 |
| NBP-7 | 1.872(7) | 0.031 | 1.846 | 0.026 | 2.558(7) | 2.655 | 175.12(18) | 176.8 | 166.73 | 179.6 | 13.27 | 0.4 | 4.431 | 4.499 |
| NBP-8 ^d | 1.913(2) | 0.072 | 1.872 | 0.052 | 2.391(2) | 2.498 | 178.97(9) | 177.8 | 178.78 | 179.8 | 1.22 | 0.2 | 4.304 | 4.369 |
| | 1.919(2) | 0.078 | -- | -- | 2.380(3) | | 177.88(10) | | 174.28 | -- | 5.72 | -- | 4.298 | |
| NBP-9 | 1.918(3) | 0.077 | 1.871 | 0.051 | 2.408(4) | 2.505 | 176.74(12) | 177.8 | 174.89 | 179.8 | 5.11 | 0.2 | 4.325 | 4.376 |
| NBP-10 ^d | 1.894(4) | 0.053 | 1.871 | 0.051 | 2.448(5) | 2.511 | 173.41(17) | 177.4 | 174.97 | 179.8 | 5.03 | 0.2 | 4.332 | 4.381 |
| | 1.902(4) | 0.061 | --- | -- | 2.457(5) | | 174.02(17) | | 174.09 | -- | 5.91 | -- | 4.352 | |
| NBP-11 | 1.908(4) | 0.067 | 1.861 | 0.041 | 2.399(2) | 2.563 | 175.03(13) | 175.1 | 178.22 | 179.8 | 1.78 | 0.2 | 4.303 | 4.420 |
| NBP-12 | 1.880(2) | 0.039 | 1.858 | 0.038 | 2.516(2) | 2.588 | 174.52(10) | 176.3 | 178.85 | 179.6 | 1.15 | 0.4 | 4.392 | 4.443 |
| NBP-13 | 1.892(3) | 0.051 | 1.871 | 0.051 | 2.435(3) | 2.504 | 176.65(10) | 179.8 | 173.66 | 179.2 | 6.34 | 0.8 | 4.325 | 4.375 |

^a(N-Br)_{ligand} = 1.841(5) Å; ^b $\Delta(N-I) = (N-I)_{\text{compl}} - (N-I)_{\text{ligand}}$; ^cDFT structure (N-Br)_{ligand} = 1.820 Å; ^dThe asymmetric unit contains two crystallographically independent 1:1 XB complexes.

Table S7. Comparison of Solid-state X-ray crystal structure XB parameters and PBE0-D3/def2-TZVP optimized parameters of N-bromophthalimide complexes

| Comp | X-ray | | DFT | | Br...N (Å) | | N-Br-N (°) | | (C-C)-N-Br (°) | | Bending angle $\Delta\theta$ (°) | | (imide)N...N(Py) (Å) | |
|-----------------------|-----------------------|----------------------------------|-----------------------|----------------------------------|------------|-------|------------|-------|----------------|-------|----------------------------------|-----|----------------------|-------|
| | N-Br (Å) ^a | Δ (N-Br) (Å) ^b | N-Br (Å) ^c | Δ (N-Br) (Å) ^b | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT | X-ray | DFT |
| NBSac-1 | -- | -- | 1.894 | 0.072 | - | 2.401 | - | 179.7 | - | 178.2 | -- | 1.8 | -- | 4.295 |
| NBSac-2 | 1.882(4) | 0.055 | 1.862 | 0.04 | 2.442(3) | 2.555 | 177.5(2) | 174.5 | 176.79 | 177.9 | 3.21 | 2.1 | 4.323 | 4.413 |
| NBSac-3 | 1.9230(19) | 0.096 | 1.866 | 0.044 | 2.401(2) | 2.530 | 174.90(8) | 174.7 | 158.26 | 178.0 | 21.74 | 2 | 4.319 | 4.392 |
| NBSac-4 | 1.913(7) | 0.086 | 1.866 | 0.044 | 2.395(6) | 2.529 | 175.1(4) | 174.7 | 158.63 | 178.0 | 21.37 | 2 | 4.303 | 4.391 |
| NBSac-5 ^d | 1.920(4) | 0.093 | 1.870 | 0.048 | 2.392(4) | 2.506 | 175.1(2) | 176.1 | 159.52 | 178.5 | 20.48 | 1.5 | 4.308 | 4.374 |
| NBSac-5a ^d | 1.952(7) | 0.125 | -- | -- | 2.266(7) | -- | 178.4(3) | -- | 164.93 | -- | 15.07 | -- | 4.218 | |
| NBSac-6 | 1.893(3) | 0.066 | 1.858 | 0.036 | 2.463(3) | 2.591 | 172.96(19) | 172.5 | 164.15 | 177.9 | 15.85 | 2.1 | 4.349 | 4.439 |
| NBSac-7 | -- | -- | 1.858 | 0.036 | 2.438 | 2.572 | 175.48 | 173.6 | 177.04 | 177.6 | 2.96 | 2.4 | 4.564 | 4.423 |
| NBSac-9 | 1.988(2) | 0.161 | 1.902 | 0.08 | 2.266(2) | 2.385 | 173.09(10) | 177.6 | 155.73 | 178.5 | 24.27 | 1.5 | 4.246 | 4.287 |
| NBSac-13 | 1.938(2) | 0.111 | 1.904 | 0.082 | 2.316(2) | 2.387 | 174.28(9) | 179.2 | 167.9 | 172.7 | 12.1 | 7.3 | 4.249 | 4.291 |
| NBSac-14 | 1.916(5) | 0.089 | 1.876 | 0.054 | 2.474(5) | 2.517 | 169.60(16) | 174.7 | 175.25 | 174.9 | 4.75 | 5.1 | 4.372 | 4.389 |
| NBSac-15 | -- | -- | 1.917 | 0.095 | - | 2.332 | - | 179.6 | - | 179.6 | -- | 0.4 | -- | 4.250 |
| NBSac-16 | -- | -- | 1.883 | 0.061 | - | 2.466 | - | 177.9 | - | 177.4 | -- | 2.6 | -- | 4.349 |

^a(N-Br)_{ligand} = 1.827(4) Å; ^b Δ (N-Br) = (N-Br)_{compl} - (N-Br)_{ligand}; ^cDFT structure (N-Br)_{ligand} = 1.822 Å; ^dTwo different XB complexes were obtained for NISac-5.

Table S8. Literature X-ray crystal structure XB parameters of N-haloimide complexes

| CSD Code | Donor | N–X (Å)^a | X...N (Å) | N–X–N (°) | (C–C)–N–X (°) | bending angle (°) | (imide)N...N(Py) (Å) |
|-----------------|--------------|--------------------------------|----------------------|----------------------|--------------------------|------------------------------|---------------------------------|
| SECYIL | NBS | 1.898 | 2.439 | 176.24 | 178.8 | 1.2 | 4.334 |
| SECYOR | NBS | 1.885 | 2.501 | 174.22 | 179.11 | 0.89 | 4.381 |
| SECYUX | NBS | 1.897 | 2.418 | 175 | 179.28 | 0.72 | 4.31 |
| SECZAE | NBS | 1.844 | 2.558 | 171.72 | 176.28 | 3.72 | 4.39 |
| SECZEI | NBS | 1.873 | 2.491 | 176.07 | 179.29 | 0.71 | 4.362 |
| SECZIM | NBS | 1.868 | 2.597 | 176.27 | 176.49 | 3.51 | 4.462 |
| MUPFUB | NBS | 1.932 | 2.319 | 179.96 | 177.8 | 2.2 | 4.251 |
| DEGTIW | NBS | 1.885 | 2.471 | 176.36 | 177.06 | 2.94 | 4.354 |
| VELVIU | NBP | 1.88 | 2.494 | 174.58 | 171.92 | 8.08 | 4.369 |
| VELVOA | NBP | 1.906 | 2.425 | 179.26 | 178.1 | 1.9 | 4.331 |
| | | 1.904 | 2.404 | 178.34 | 175.13 | 4.87 | 4.308 |
| VELVUG | NBP | 1.898 | 2.449 | 179.92 | 179.45 | 0.55 | 4.347 |
| VELWAN | NBP | 1.87 | 2.487 | 178.28 | 179.02 | 0.98 | 4.356 |
| VELWER | NBP | 1.888 | 2.454 | 175.42 | 171.22 | 8.78 | 4.338 |
| VELWUH | NBP | 1.894 | 2.476 | 179.2 | 178.14 | 1.86 | 4.37 |
| VELXES | NBP | 1.885 | 2.454 | 175.96 | 175.96 | 4.04 | 4.336 |
| VELXIW | NBP | 1.91 | 2.38 | 178.6 | 179.29 | 0.71 | 4.294 |
| KECJAG | NBSac | 2.0727 | 2.098 | 178.77 | 177.76 | 2.24 | 4.171 |
| KUWHAN | NIS | 2.116 | 2.484 | 180 | 180 | 0 | 4.599 |
| | | 2.142 | 2.428 | 180 | 180 | 0 | 4.57 |
| KUWHER | NIS | 2.146 | 2.407 | 178.94 | 176.85 | 3.15 | 4.553 |
| OGIWOS | NIS | 2.117 | 2.493 | 180 | 180 | 0 | 4.609 |
| | | 2.144 | 2.429 | 180 | 180 | 0 | 4.574 |
| SECXEG | NIS | 2.12 | 2.412 | 177.16 | 173.27 | 6.73 | 4.532 |
| | | 2.145 | 2.408 | 177.67 | 178.85 | 1.15 | 4.552 |
| SECXOQ | NIS | 2.1 | 2.5 | 173.88 | 178.04 | 1.96 | 4.594 |
| SECYAD | NIS | 2.109 | 2.474 | 176.1 | 178.29 | 1.71 | 4.584 |
| DECGUQ | NIS | 2.086 | 2.502 | 175.86 | 178.96 | 1.04 | 4.585 |
| DEGTAO | NIS | 2.103 | 2.539 | 177.44 | 178.39 | 1.61 | 4.641 |
| DEGTES | NIS | 2.092 | 2.498 | 176.71 | 176.74 | 3.26 | 4.589 |
| KUWHIV | NISac | 2.22 | 2.305 | 178.18 | 174.19 | 5.81 | 4.523 |
| KUWHUH | NISac | 2.293 | 2.28 | 178.84 | 173.17 | 6.83 | 4.521 |
| MUGDAU | NISac | 2.254 | 2.279 | 174.5 | 167.41 | 12.59 | 4.527 |
| OGIWUY | NISac | 2.292 | 2.218 | 178.56 | 172.49 | 7.51 | 4.509 |

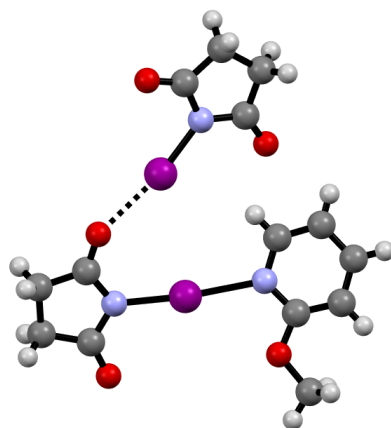


Figure S2. X-ray crystal structure of NIS-11. Two XB donors are present in the asymmetric unit, one of which participates in XB with imide C=O group of the NIS-11 halogen-bonded complex.

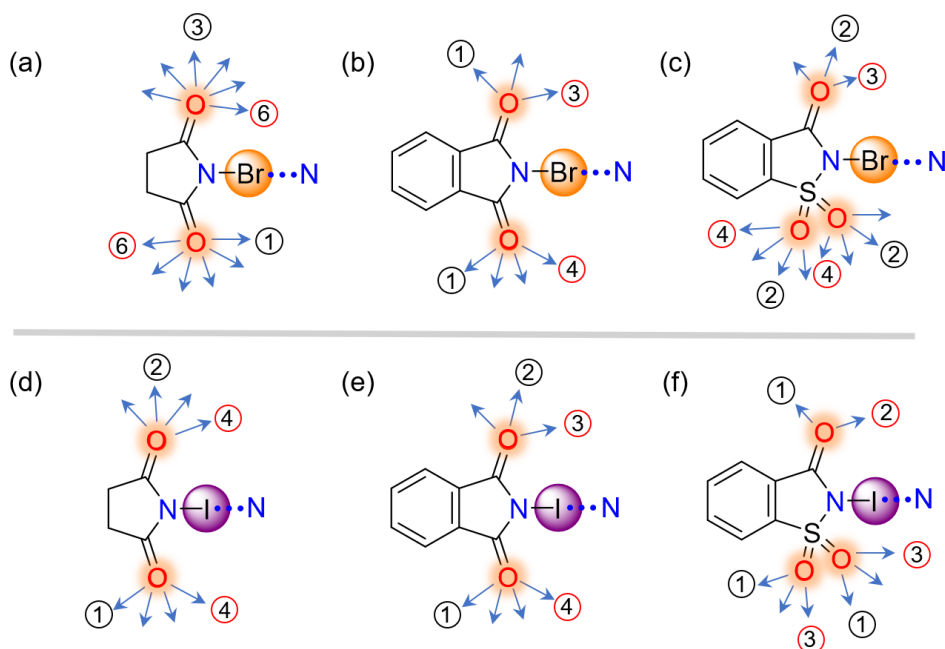


Figure S3. Polydentate coordination nature of XB donors in halogen-bonded complexes. The numbers inside black circles represent minimum denticity whereas those inside red circles represent maximum denticity. For instance, as seen in Figure S3d, the iodosuccinimide's first oxygen displays bidentate (minimum) and tetradentate (maximum) coordination modes, whereas the second oxygen displays monodentate (minimum) and tetradentate (maximum) coordination modes.

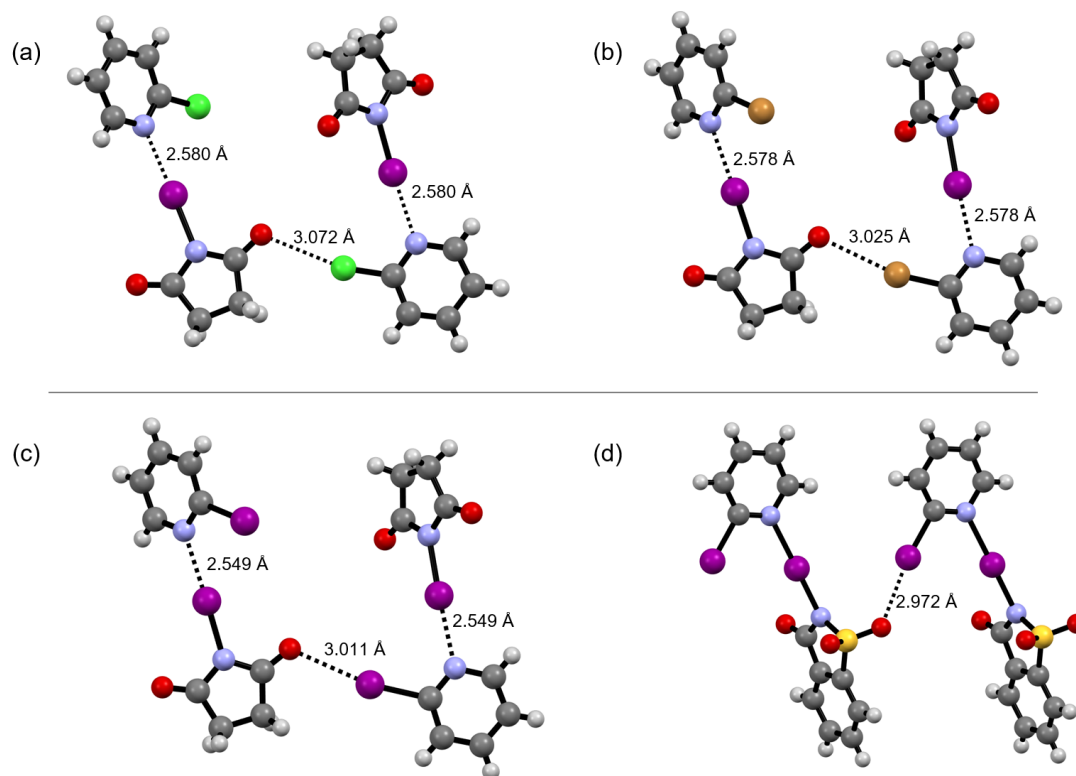


Figure S4. X-ray crystal structure of (a) NIS-3, (b) NIS-4, (c) NIS-5, and (d) NISac-5 in ball and stick model displaying the C–X···O=C halogen bonding interactions

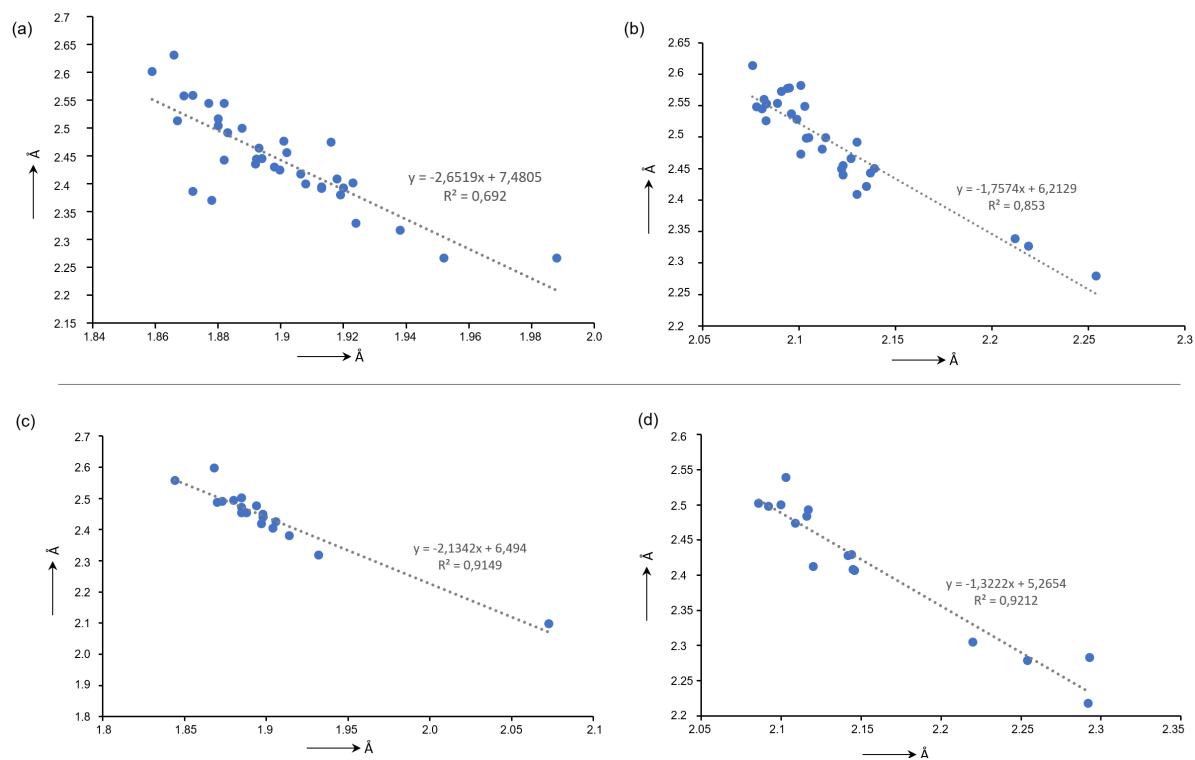


Figure S5. Correlation between N–X and X···N distances of (a) bromoimide-2-*ortho*-substituted pyridine complexes (b) iodoimide-2-*ortho*-substituted pyridine complexes and (c) bromoimide-2-*meta/para*-substituted pyridine complexes and (d) iodoimide-2-*meta/para*-substituted pyridine complexes.

3. Computational results

Optimized geometries and harmonic vibrational frequencies of all structures were derived by DFT calculations performed with PBE0 hybrid functional¹⁰ employing def2-TZVP basis sets.¹¹ Dispersion interactions in the complex structures were treated with Grimme's empirical D3 correction version that used Becke-Johnson dampening.¹² Complexation energies corrected for basis set superposition errors were derived from counterpoise calculations.¹³ Effect of solvent to XB structures in CHCl₃ solutions was modelled using polarized continuum model (PCM) calculations.¹⁵⁻¹⁸ All calculations were run on Gaussian 16 program package.¹⁴

Table S9. Computed (PBE0-D3/def2-TZVP) halogen bonding interaction energies ΔE_{XB} [kJ mol⁻¹].

| Compl | ΔE_{XB} | Compl | ΔE_{XB} | Compl | ΔE_{XB} | Compl | ΔE_{XB} | Compl | ΔE_{XB} | Compl | ΔE_{XB} |
|--------------|-----------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|
| NIS-1 | -65.5 | NIP-1 | -65.1 | NISac-1 | -81.3 | NBSac-1 | -56.9 | NBP-1 | -43.1 | NBS-1 | -43.1 |
| NIS-2 | -47.7 | NIP-2 | -47.3 | NISac-2 | -58.7 | NBSac-2 | -38.4 | NBP-2 | -30.4 | NBS-2 | -30.5 |
| NIS-3 | -51.1 | NIP-3 | -50.6 | NISac-3 | -62.8 | NBSac-3 | -41.8 | NBP-3 | -33.0 | NBS-3 | -33.1 |
| NIS-4 | -50.8 | NIP-4 | -50.2 | NISac-4 | -62.3 | NBSac-4 | -41.5 | NBP-4 | -32.8 | NBS-4 | -32.9 |
| NIS-5 | -52.5 | NIP-5 | -51.9 | NISac-5 | -64.6 | NBSac-5 | -43.5 | NBP-5 | -34.1 | NBS-5 | -34.2 |
| NIS-6 | -44.9 | NIP-6 | -44.4 | NISac-6 | -54.2 | NBSac-6 | -37.2 | NBP-6 | -30.1 | NBS-8 | -47.2 |
| NIS-7 | -44.4 | NIP-7 | -43.8 | NISac-7 | -53.8 | NBSac-7 | -35.1 | NBP-7 | -28.3 | NBS-9 | -48.4 |
| NIS-8 | -70.0 | NIP-8 | -69.5 | NISac-8 | -87.0 | NBSac-8 | -62.8 | NBP-8 | -47.1 | NBS-11 | -40.4 |
| NIS-9 | -71.3 | NIP-9 | -70.5 | NISac-9 | -88.1 | NBSac-9 | -63.8 | NBP-9 | -48.2 | NBS-12 | -42.0 |
| NIS-10 | -71.3 | NIP-10 | -70.5 | NISac-10 | -88.0 | NBSac-10 | -64.1 | NBP-10 | -48.4 | | |
| NIS-11 | -63.1 | NIP-11 | -62.7 | NISac-11 | -79.3 | NBSac-11 | -53.3 | NBP-11 | -40.4 | | |
| NIS-12 | -63.1 | NIP-12 | -62.3 | NISac-12 | -79.4 | NBSac-12 | -55.3 | NBP-12 | -41.8 | | |
| NIS-13 | -78.9 | NIP-13 | -77.7 | NISac-13 | -98.0 | NBSac-13 | -73.1 | NBP-13 | -55.1 | | |
| NIS-14 | -68.0 | NIP-14 | -67.7 | NISac-14 | -86.5 | NBSac-14 | -62.3 | | | | |
| NIS-15 | -77.3 | NIP-15 | -76.1 | NISac-15 | -99.3 | NBSac-15 | -77.1 | | | | |
| NIS-16 | -63.0 | NIP-16 | -62.2 | NISac-16 | -79.5 | NBSac-16 | -55.1 | | | | |

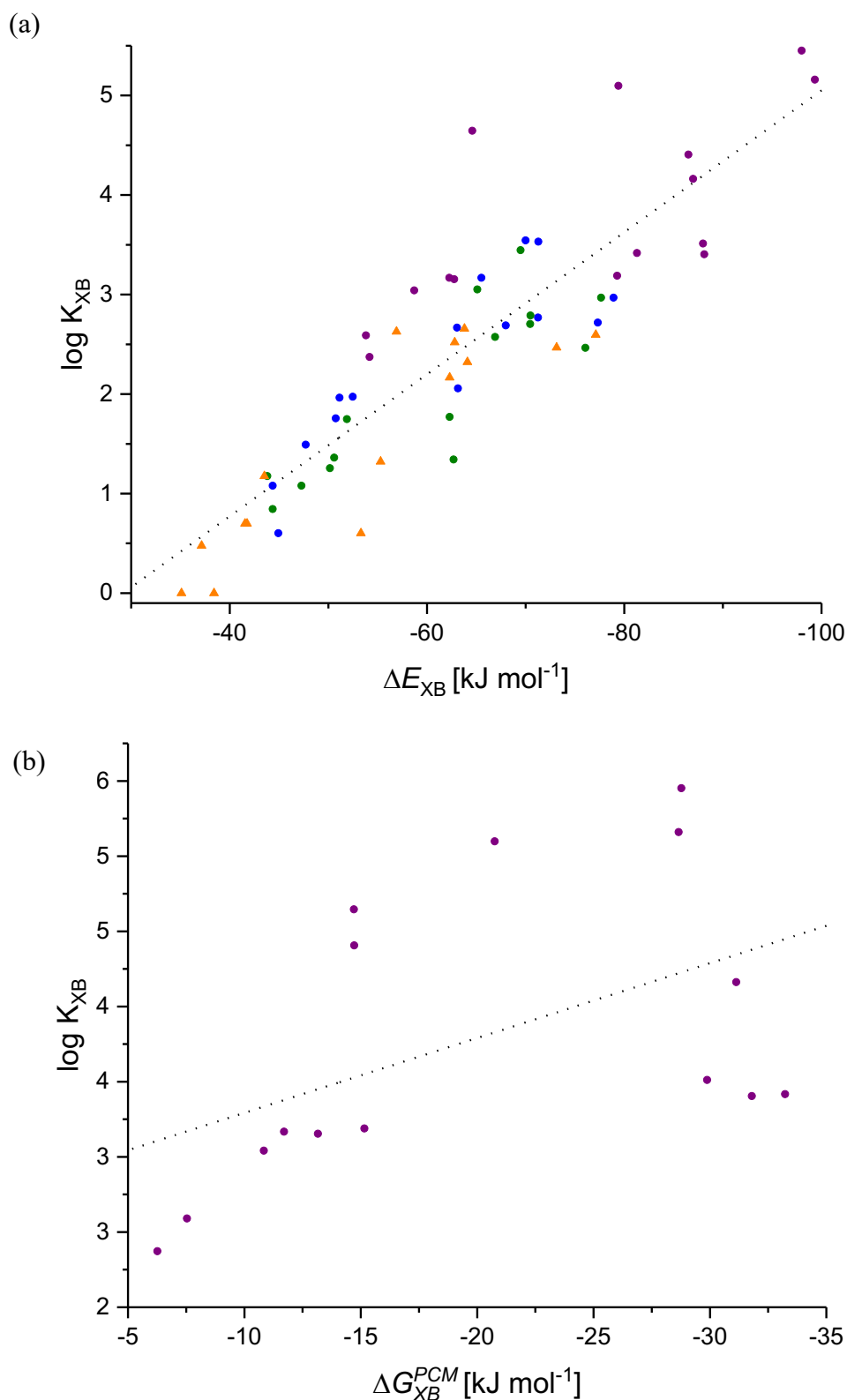


Figure S5. a) Linear correlation between solution ^1H NMR association constants, $\log K_{\text{XB}}$ and a) calculated complexation energies, ΔE_{XB} ($R^2 = 0.760$) for 60 XB complexes of NIS-**Z** (blue dots), NIP-**Z** (green dots), NISac-**Z** (purple dots) and NBSac-**Z** (orange triangles), b) calculated complexation free energies $\Delta G_{\text{XB}}^{\text{PCM}}$ ($R^2 = 0.189$) for fifteen NISac-**Z** complexes in CHCl_3 solution. Calculated values have been determined with PBE0-D3/def2-TZVP method.

4. Solution NMR

All the ^{15}N NMR spectra were obtained by mixing 1:1 molar ratio of respective XB donor and acceptor molecules in CDCl_3 and were recorded on a Bruker Avance III 500 MHz spectrometer equipped with prodigy probe. External ^{15}N reference used was 90% ^{15}N enriched nitromethane in a sealed tube. The ^{15}N spectra could be measured with one scan/increment. The signal was calibrated to 0 ppm, and the other samples were measured using the same parameters. Only the number of scans and the receiver gain were altered. When the sealed internal reference tube was measured inside the sample, the signal from the enriched reference was too strong, while the signal from the sample was too weak. Sine bell window function with zero shifts was used for apodization before Fourier transformation, and all the measurements were made either with 64 or 128 scans. The HMBC ^1H - ^{15}N chemical shift changes for NIP, NBP, NISac and NBSac could not be obtained.

The titrations were performed in CDCl_3 at the temperatures. In an NMR tube, a 10 mM sample solution (volume 600 μL) of N-haloimide were prepared, and all titrations were performed with at least 20 data points up to 4.5-5.0 equivalents of the guest added, using 0.15 M stock solutions of pyridines dissolved in CDCl_3 . Titration experiments were conducted using Bruker Avance III 500 MHz spectrometer. Titration data was fitted into a 1:1 binding model using online Bindfit software.¹⁹ The association constants are summarized in Table S11. The chemical shifts of protons in donor were used to calculate the binding constants.

Table S10. Solution ^{15}N NMR of N-haloimide XB complexes (CDCl_3 , 298.0K).

| Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ | Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ | Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ | Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ | Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ | Comp | $\Delta\delta\text{N}_{\text{coord}}^{\text{a}}$ |
|-------------|--|-------------|--|-------------|--|-------------|--|-------------|--|-------------|--|
| NIS-1 | -41.5 | NIP-1 | -0.7 | NISac-1 | -63.1 | NBS-1 | -2.0 | NBP-1 | -0.7 | NBSac-1 | -23.2 |
| NIS-2 | -13.5 | NIP-2 | -2.6 | NISac-2 | -33.7 | NBS-2 | -1.0 | NBP-2 | -2.6 | NBSac-2 | -2.5 |
| NIS-3 | -16.9 | NIP-3 | -1.6 | NISac-3 | -40.8 | NBS-3 | -2.5 | NBP-3 | -1.6 | NBSac-3 | -3.7 |
| NIS-4 | -15.3 | NIP-4 | -2.5 | NISac-4 | -41.4 | NBS-4 | -1.6 | NBP-4 | -2.5 | NBSac-4 | -3.8 |
| NIS-5 | -20.2 | NIP-5 | -2.2 | NISac-5 | -46.6 | NBS-5 | -2.9 | NBP-5 | -2.2 | NBSac-5 | -8.6 |
| NIS-6 | -5.9 | NIP-6 | -2.4 | NISac-6 | -21.6 | NBS-6 | -5.9 | NBP-6 | -2.4 | NBSac-6 | -0.9 |
| NIS-7 | -10.1 | NIP-7 | -2.4 | NISac-7 | -25.6 | NBS-7 | -0.4 | NBP-7 | -2.4 | NBSac-7 | -1.7 |
| NIS-8 | -42 | NIP-8 | -4.5 | NISac-8 | -62.8 | NBS-8 | -7.2 | NBP-8 | -4.5 | NBSac-8 | -38.5 |
| NIS-9 | -40.2 | NIP-9 | -1.7 | NISac-9 | -62.2 | NBS-9 | -6.2 | NBP-9 | -1.7 | NBSac-9 | -32.6 |
| NIS-10 | -37.2 | NIP-10 | -4.1 | NISac-10 | -59.5 | NBS-10 | -3.7 | NBP-10 | -4.1 | NBSac-10 | -32.3 |
| NIS-11 | -14 | NIP-11 | -12.3 | NISac-11 | -42.8 | NBS-11 | -1.6 | NBP-11 | -1.0 | NBSac-11 | -2.8 |
| NIS-12 | -24 | NIP-12 | -24.0 | NISac-12 | -47.7 | NBS-12 | -0.9 | NBP-12 | -0.5 | NBSac-12 | -47.7 |
| NIS-13 | -35.6 | NIP-13 | -37.4 | NISac-13 | -51.5 | NBS-13 | -3.0 | NBP-13 | -3.0 | NBSac-13 | -24.7 |
| NIS-14 | -8.2 | NIP-14 | 3.1 | NISac-14 | -43.7 | NBS-14 | 0.5 | NBP-14 | 0.08 | NBSac-14 | -4.1 |
| NIS-15 | -40.5 | NIP-15 | -37.8 | NISac-15 | -72.2 | NBS-15 | -5.3 | NBP-15 | -3.8 | NBSac-15 | -50.2 |
| NIS-16 | -2.6 | NIP-16 | -0.8 | NISac-16 | -50.2 | NBS-16 | -2.5 | NBP-16 | -0.7 | NBSac-16 | -73.5 |

$$^{\text{a}}\Delta\delta\text{N}_{\text{coord}} = \Delta\delta\text{N}_{\text{complex}} - \Delta\delta\text{N}_{\text{pyridine}}$$

Table S11. Solution ¹H NMR association constants of N-haloimide XB complexes (CDCl₃, 298.0K)

| Compl | Ka (M ⁻¹) | Compl | Ka (M ⁻¹) | Compl | Ka (M ⁻¹) | Compl | Ka (M ⁻¹) | Compl | Ka (M ⁻¹) | Compl | Ka (M ⁻¹) |
|--------|-----------------------|--------|-----------------------|----------|-----------------------|--------|----------------------------|------------------------------|-----------------------|----------|--------------------------------|
| NIS-1 | 1471±718 | NIP-1 | 1124±157 | NISac-1 | 2610 ± 313 | NBS-1 | 4±1 | NBP-1 | 2 | NBSac-1 | 424±18 |
| NIS-2 | 31 ± 1 | NIP-2 | 12±0.1 | NISac-2 | 1100±21 | NBS-2 | 1 ^a | NBP-2 | 1 ^a | NBSac-2 | 1 ^a |
| NIS-3 | 92 ± 1 | NIP-3 | 23±1 | NISac-3 | 1424±47 | NBS-3 | 1 ^a | NBP-3 | 1 ^a | NBSac-3 | 5±1 |
| NIS-4 | 57 ± 1 | NIP-4 | 18±1 | NISac-4 | 1472±38 | NBS-4 | 1 ^a | NBP-4 | 1 ^a | NBSac-4 | 5±1 |
| NIS-5 | 94 ± 5 | NIP-5 | 56±1 | NISac-5 | 4427 ^b | NBS-5 | 1 ^a | NBP-5 | 1 ^a | NBSac-5 | 15±1 |
| NIS-6 | 4 ± 1 | NIP-6 | 7±1 | NISac-6 | 236±5 | NBS-6 | 2 ^a | NBP-6 | 1 ^a | NBSac-6 | 3±1 |
| NIS-7 | 12±1 | NIP-7 | 15±1 | NISac-7 | 389±7 | NBS-7 | 1 ^a | NBP-7 | 1 ^a | NBSac-7 | 1 ^a |
| NIS-8 | 3494±1555 | NIP-8 | 2790±391 | NISac-8 | 14522±3776 | NBS-8 | 5±2 (21±1) ^c | NBP-8 (19±1) ^c | 4±1 | NBSac-8 | 331±8 (423±23) ^c |
| NIS-9 | 3398±1611 | NIP-9 | 506±37 | NISac-9 | 2536±185 | NBS-9 | 4±3 | NBP-9 | 2 ^a | NBSac-9 | 455±9 |
| NIS-10 | 588±159 | NIP-10 | 617±35 | NISac-10 | 3250±374 | NBS-10 | 2 | NBP-10 | 1 ^a | NBSac-10 | 210±4 |
| NIS-11 | 114 ± 2 | NIP-11 | 22±1 | NISac-11 | 1545±142 | NBS-11 | 1 ^a | NBP-11 | 1 ^a | NBSac-11 | 4±1 |
| NIS-12 | 465 ± 32 | NIP-12 | 59±1 | NISac-12 | 125282 ^b | NBS-12 | 1 ^a | NBP-12 | 1 ^a | NBSac-12 | 21±1 |
| NIS-13 | 931±13 | NIP-13 | 932±14 | NISac-13 | 282807 ^b | NBS-13 | 1 ^a | NBP-13 | 2 ^a | NBSac-13 | 294±2 |
| NIS-14 | 490±59 | NIP-14 | 375±11 | NISac-14 | 25495 ^b | NBS-14 | 1 ^a | NBP-14 | 2 ^a | NBSac-14 | 147±1 |
| NIS-15 | 522±79 | NIP-15 | 291±16 | NISac-15 | 144459 ^b | NBS-15 | 2 ^a | NBP-15 | 2 ^a | NBSac-15 | 394±12 |
| NIS-16 | -- | NIP-16 | -- | NISac-16 | -- | NBS-16 | -- | NBP-16 | -- | NBSac-16 | -- |

^aWeak binding, values are shown for reference. ^b>100% excessive error, values are for reference only. ^cAssociation constants obtained by using 1M pyridine stock solutions.

5). ^1H - ^{15}N HMBC-NMR Spectra for complexes NBS-1 - NISac-15

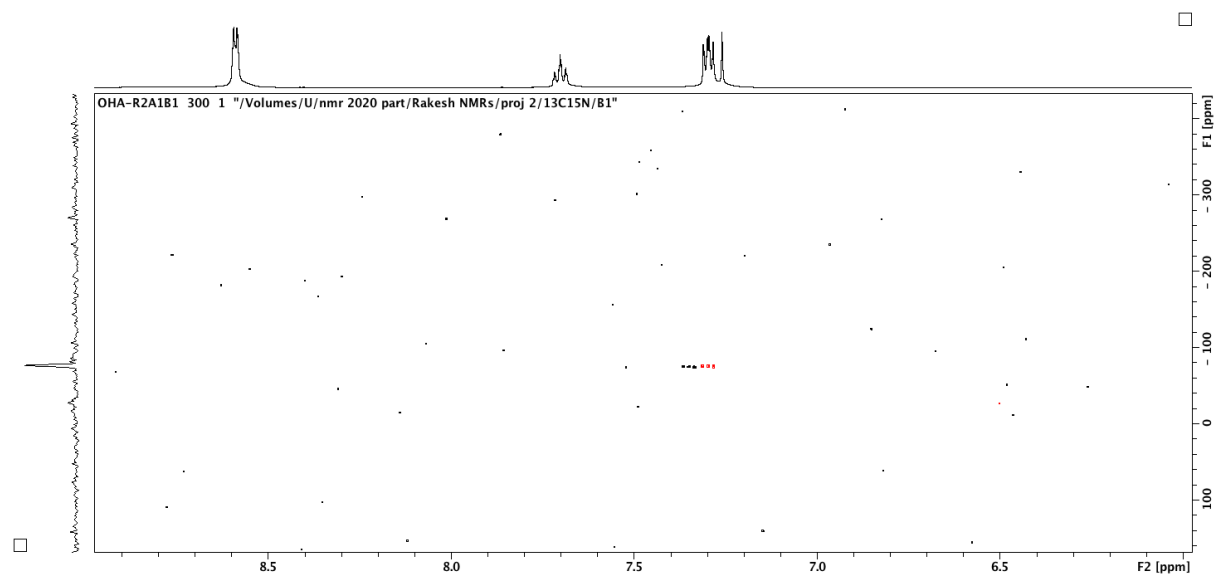


Figure S6. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NBS-1 in red contour in CDCl_3 at 303K.

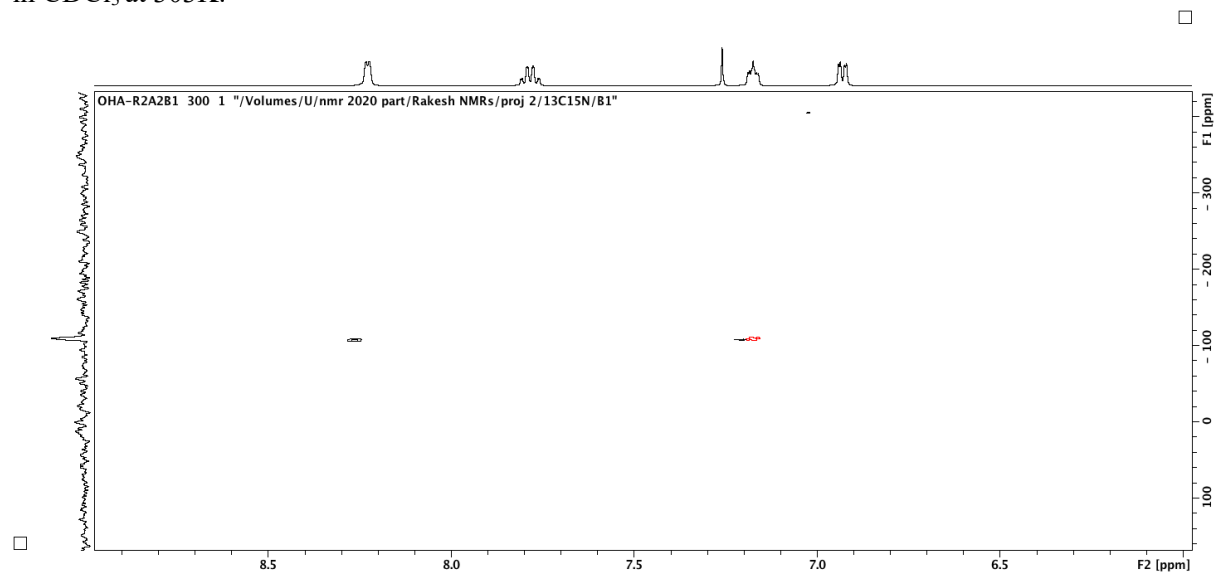


Figure S7. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NBS-2 in red contour in CDCl_3 at 303K.

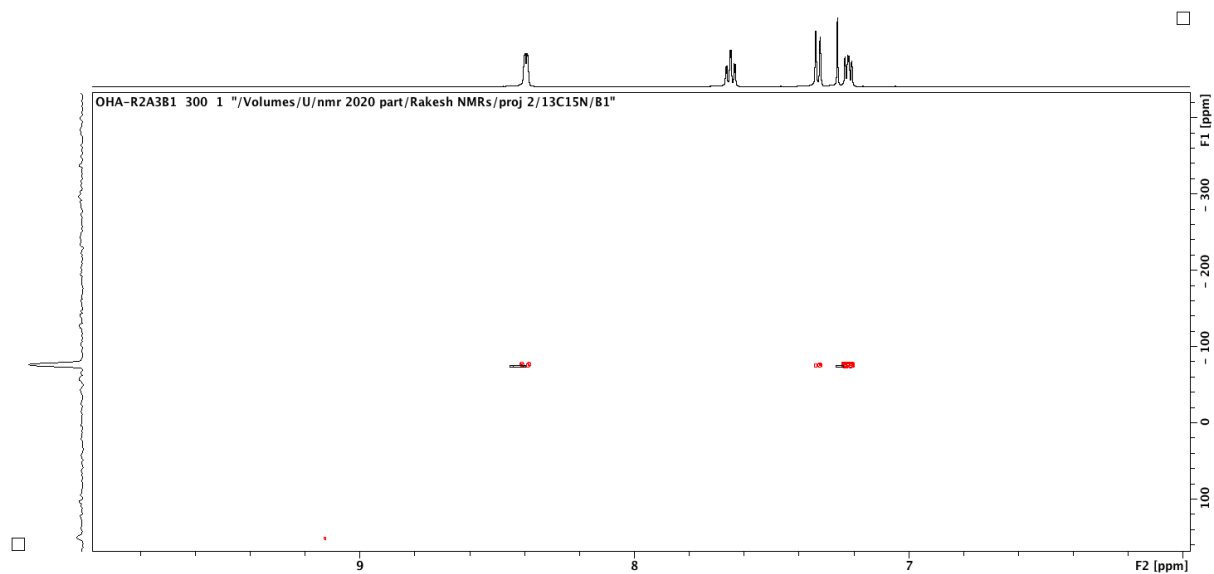


Figure S8. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NBS-**3** in red contour in CDCl_3 at 303K.

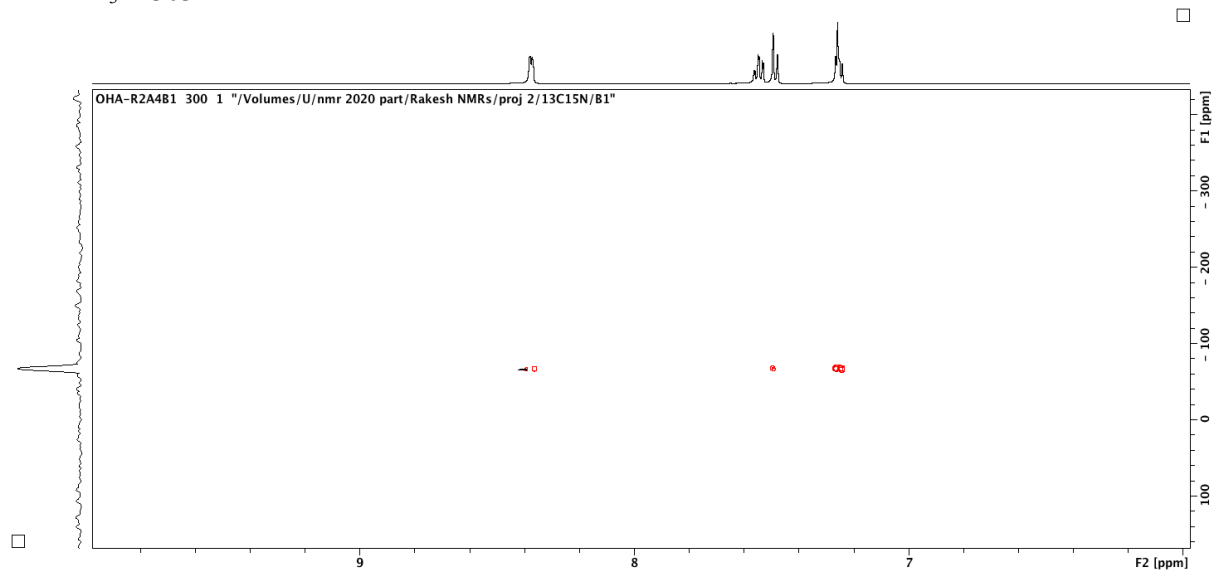


Figure S9. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NBS-**4** in red contour in CDCl_3 at 303K.

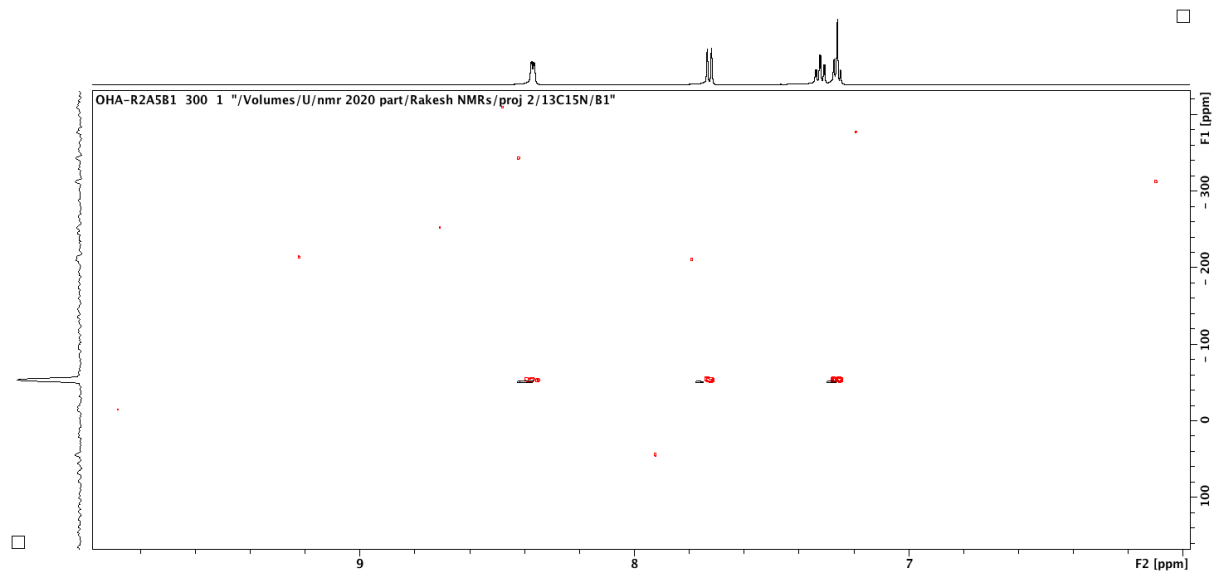


Figure S10. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex NBS-**5** in red contour in CDCl_3 at 303K.

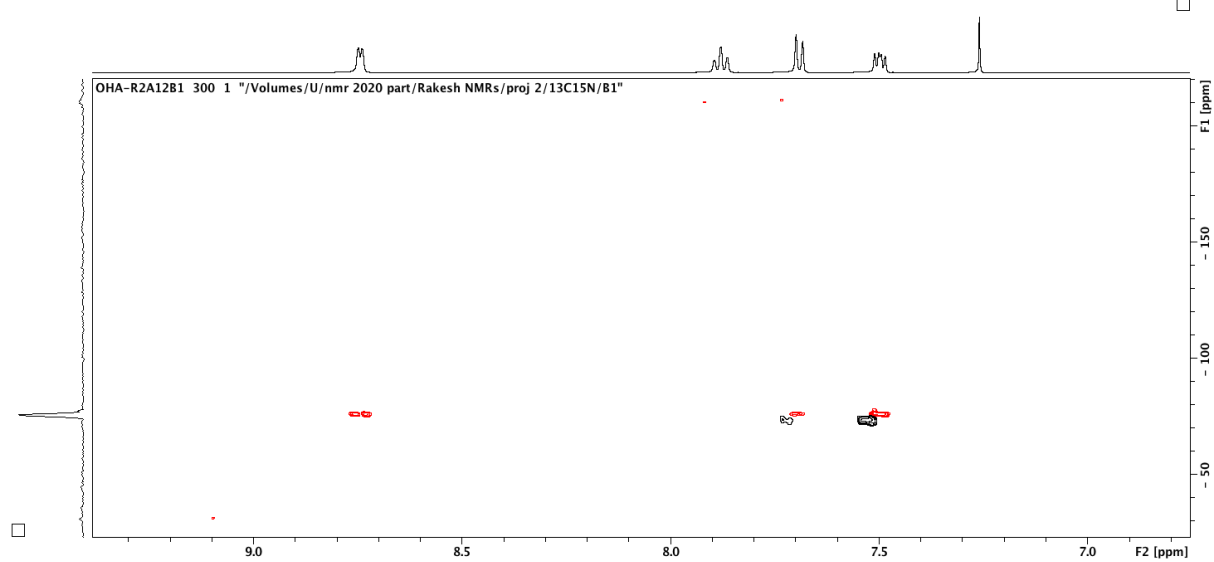


Figure S11. ^1H - ^{15}N HMBC-NMR Spectra of **6** in black contour and 1:1 complex NBS-**6** in red contour in CDCl_3 at 303K.

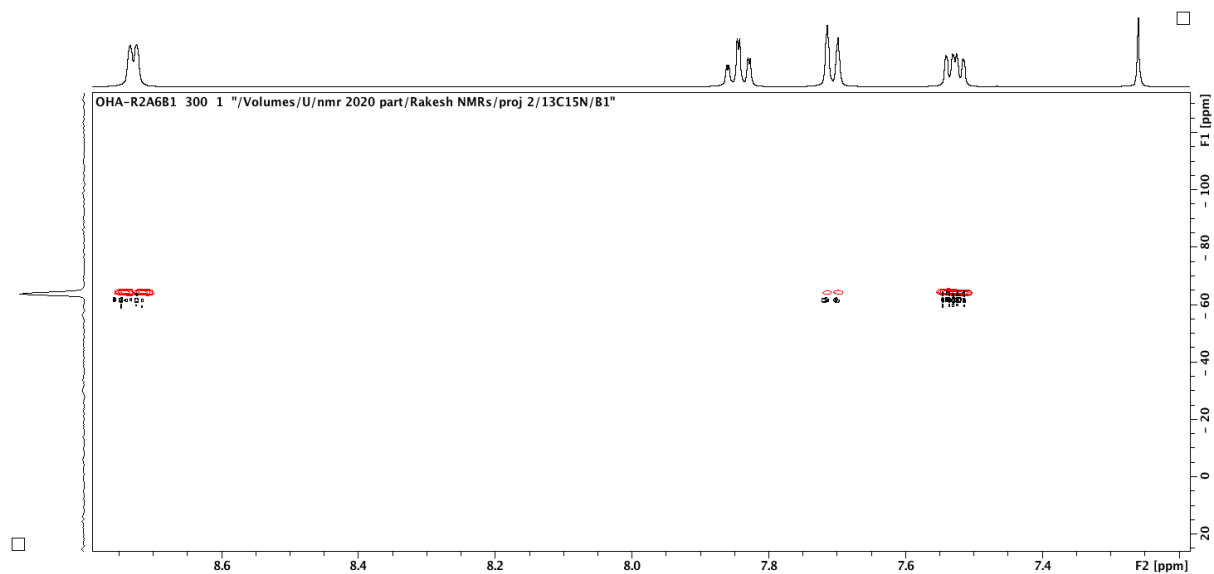


Figure S12. ^1H - ^{15}N HMBC-NMR Spectra of **7** in black contour and 1:1 complex NBS-**7** in red contour in CDCl_3 at 303K.

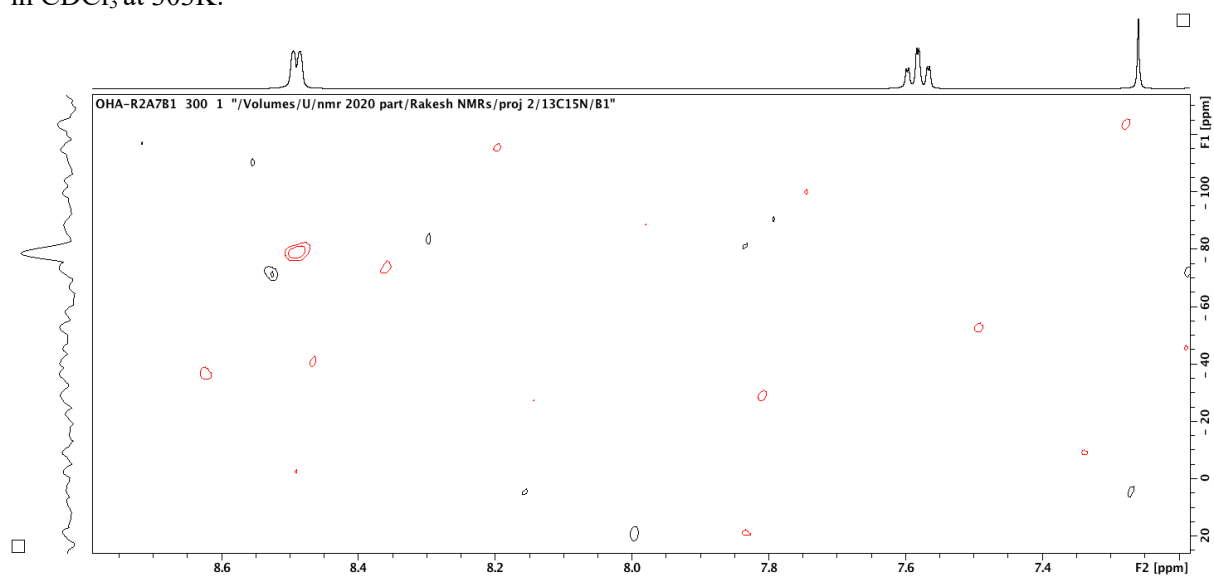


Figure S13. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NBS-**8** in red contour in CDCl_3 at 303K.

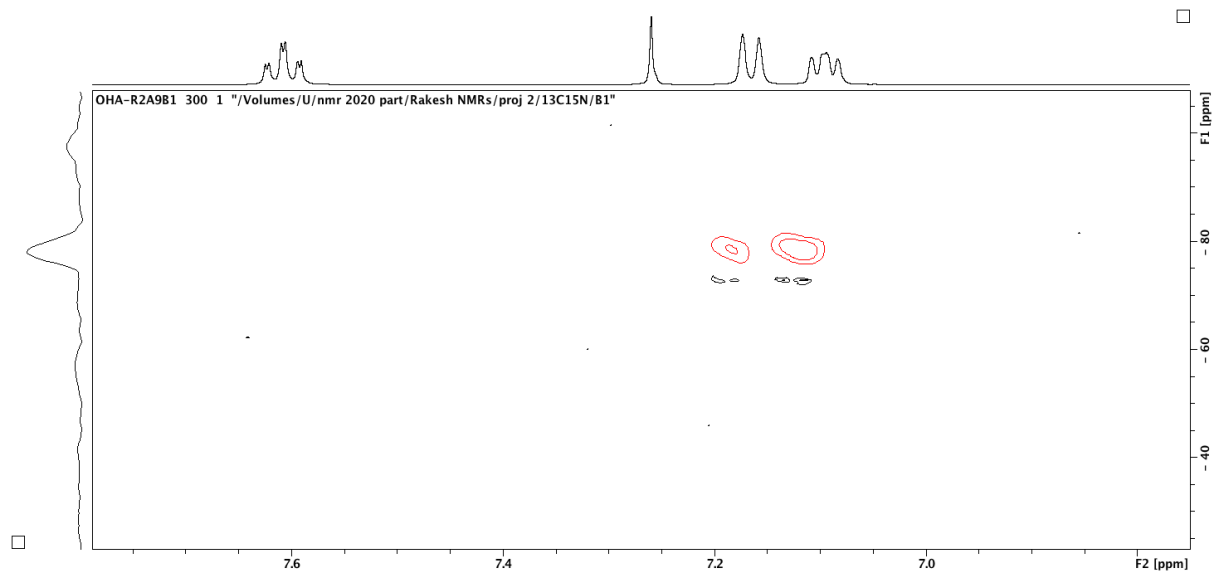


Figure S14. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NBS-**9** in red contour in CDCl_3 at 303K.

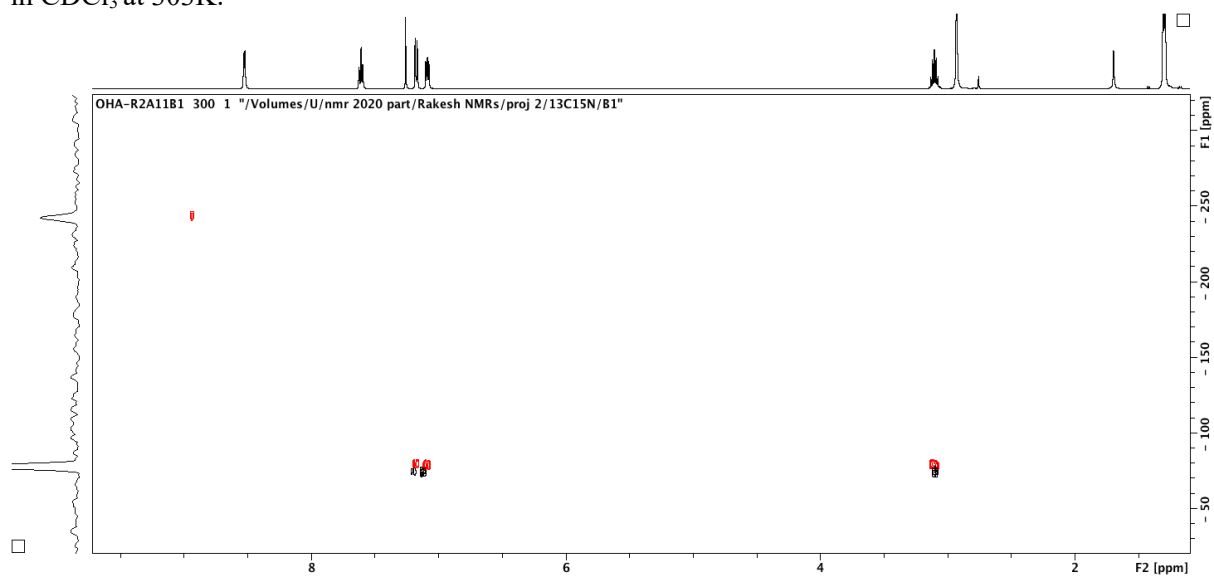


Figure S15. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NBS-**10** in red contour in CDCl_3 at 303K.

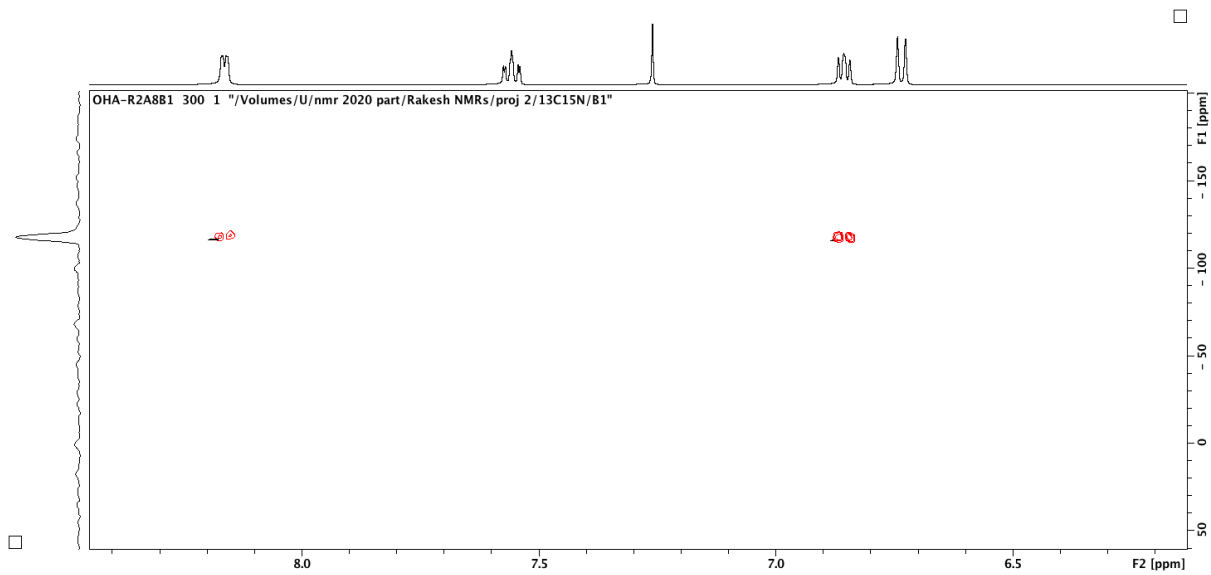


Figure S16. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NBS-**11** in red contour in CDCl_3 at 303K.

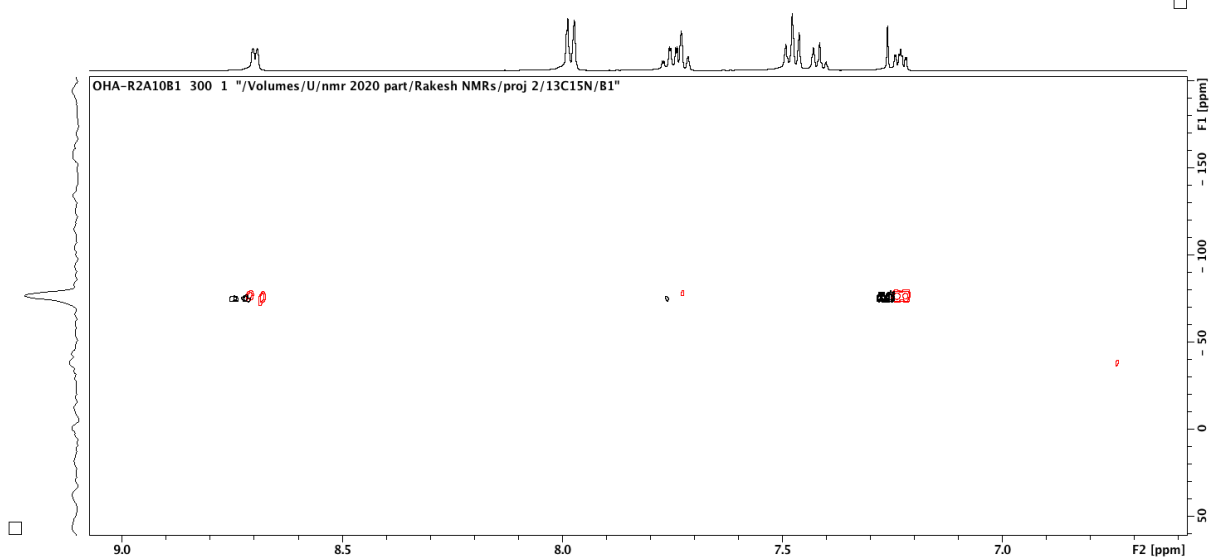


Figure S17. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour and 1:1 complex NBS-**12** in red contour in CDCl_3 at 303K.

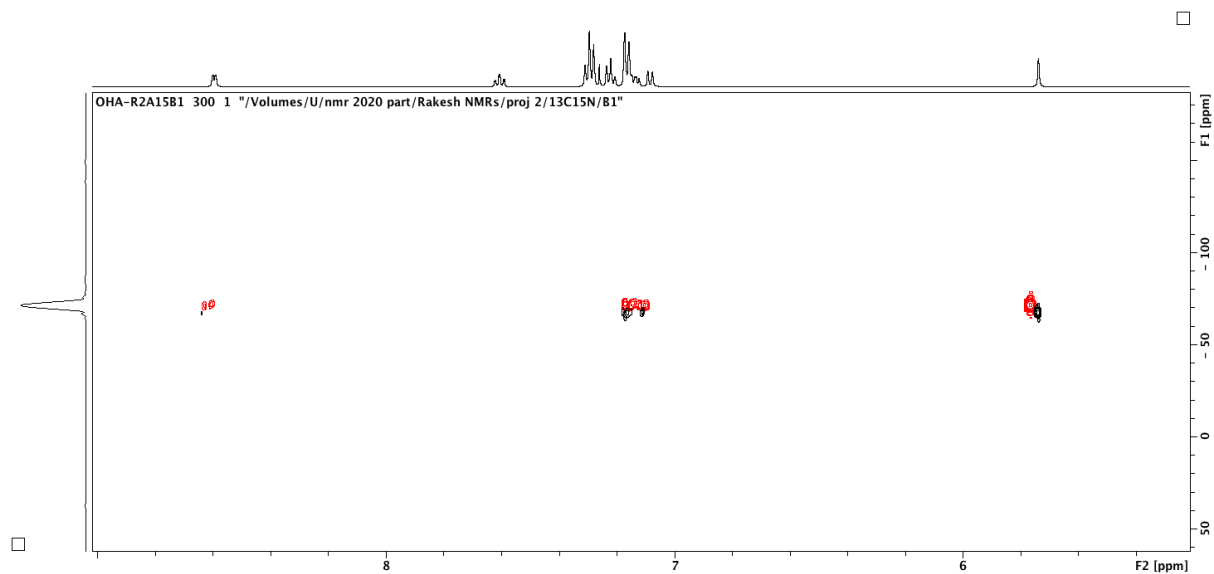


Figure S18. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NBS-**13** in red contour in CDCl_3 at 303K.

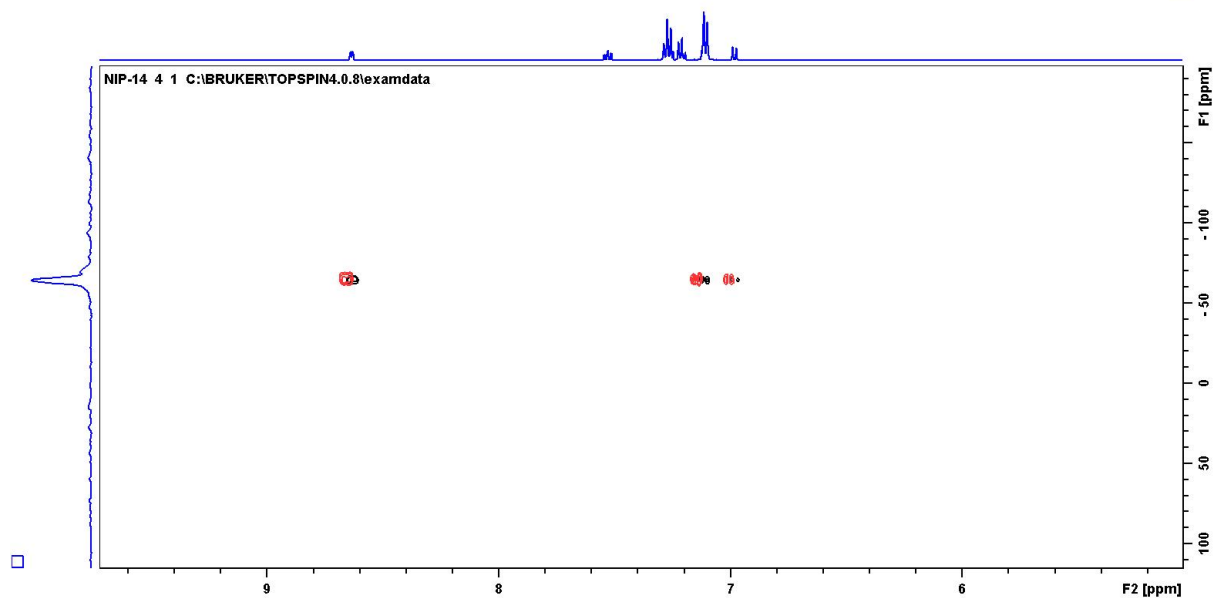


Figure S19. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NBS-**14** in red contour in CDCl_3 at 303K, 500MHz.

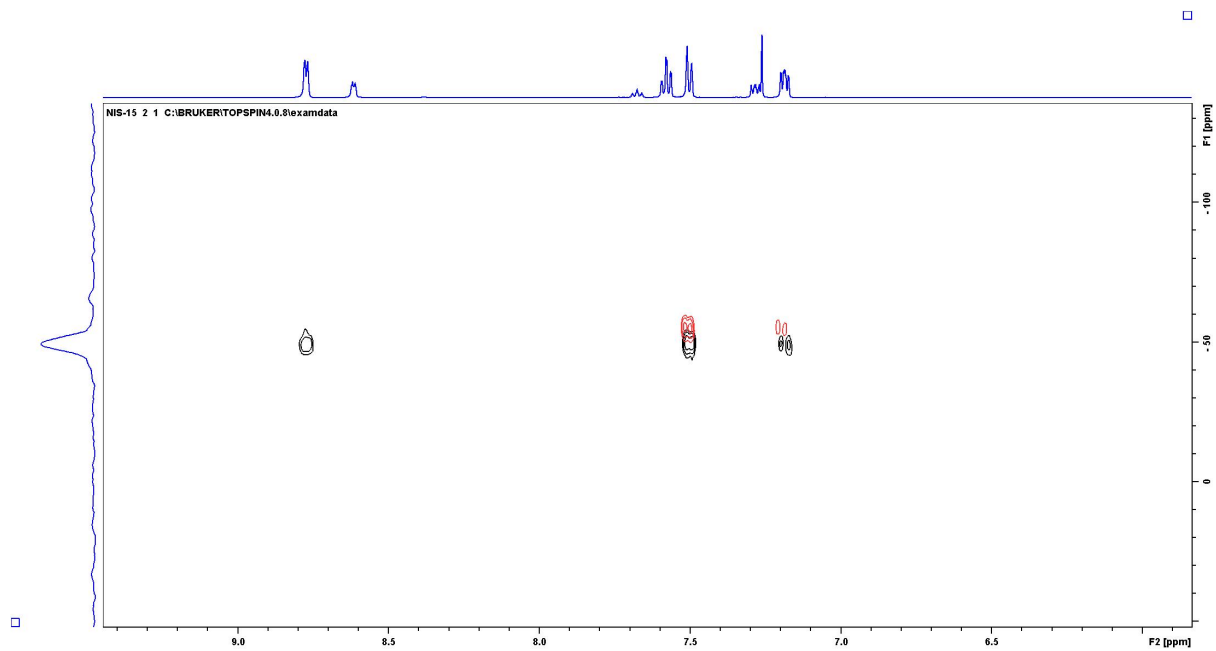


Figure S20. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NBS-**15** in red contour in CDCl_3 at 303K, 500MHz.

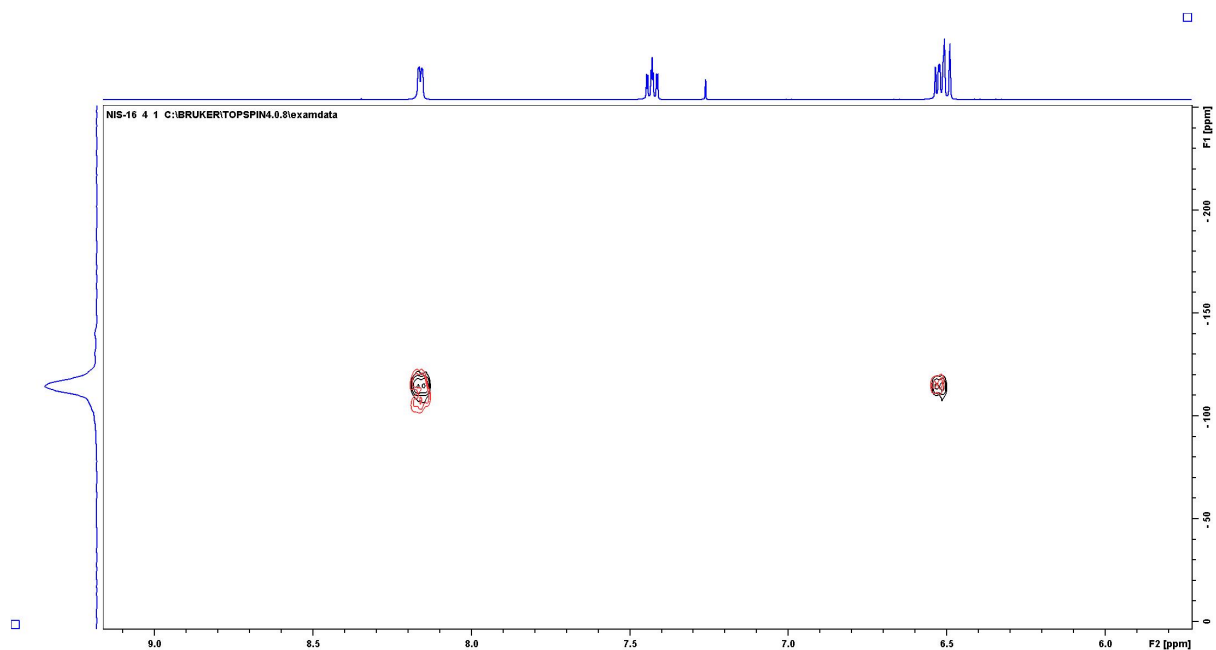


Figure S21. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NBS-**16** in red contour in CDCl_3 at 303K, 500MHz.

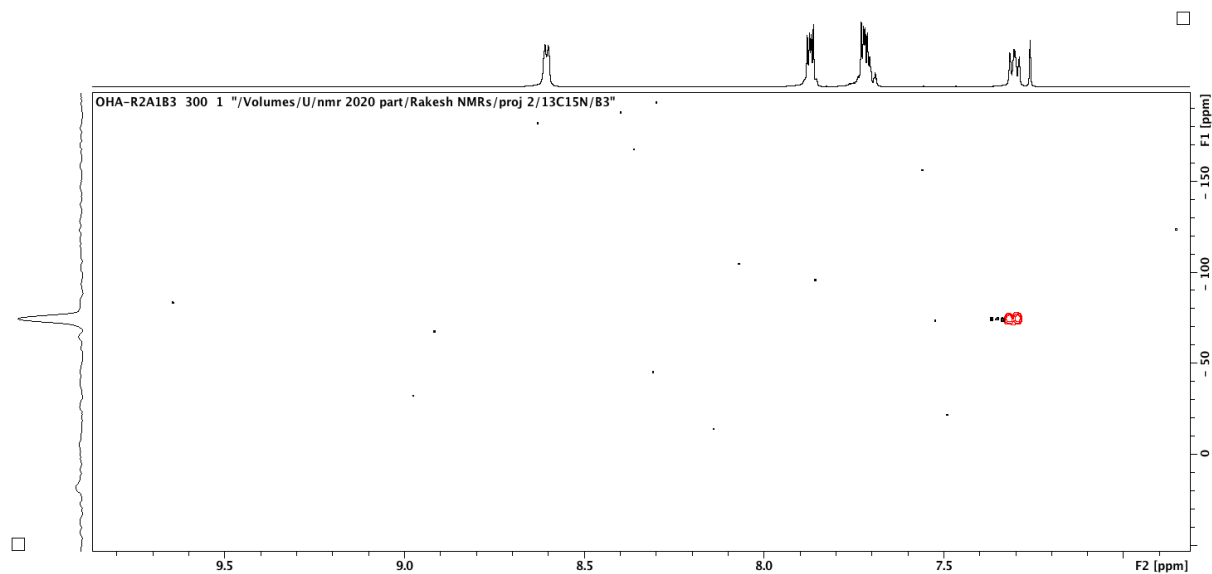


Figure S22. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NBP-**1** in red contour in CDCl_3 at 303K.

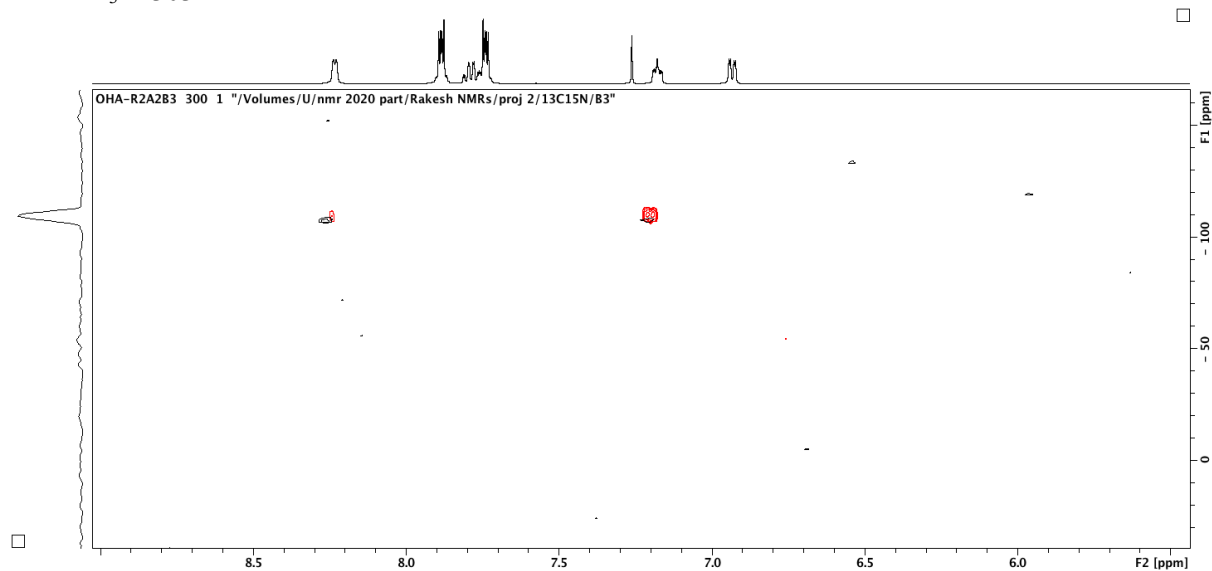


Figure S23. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NBP-**2** in red contour in CDCl_3 at 303K.

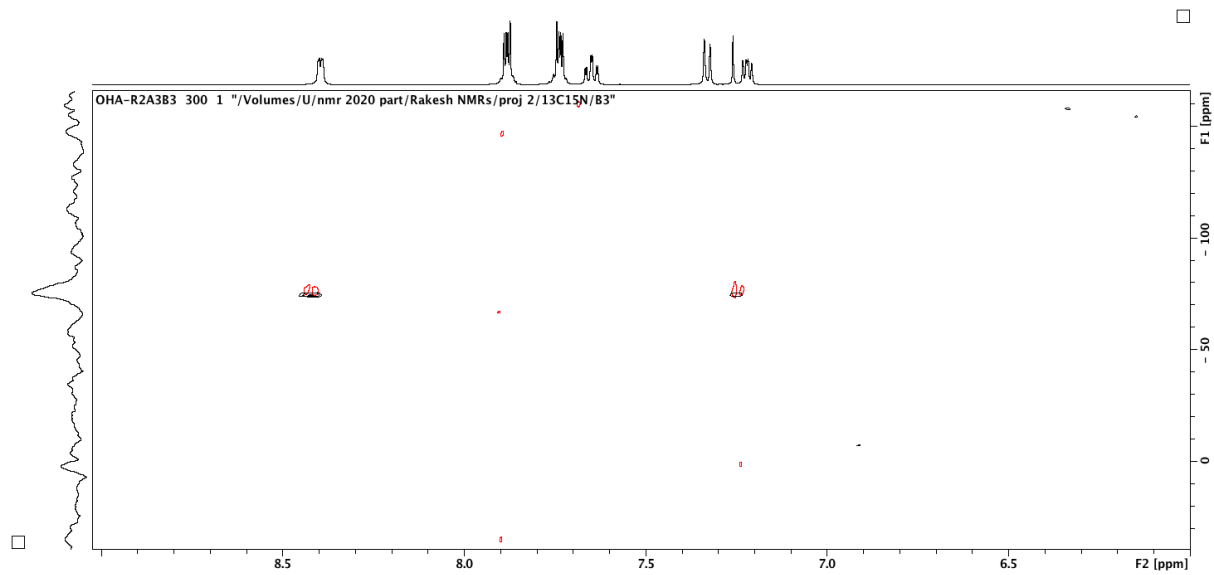


Figure S24. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NBP-**3** in red contour in CDCl_3 at 303K.

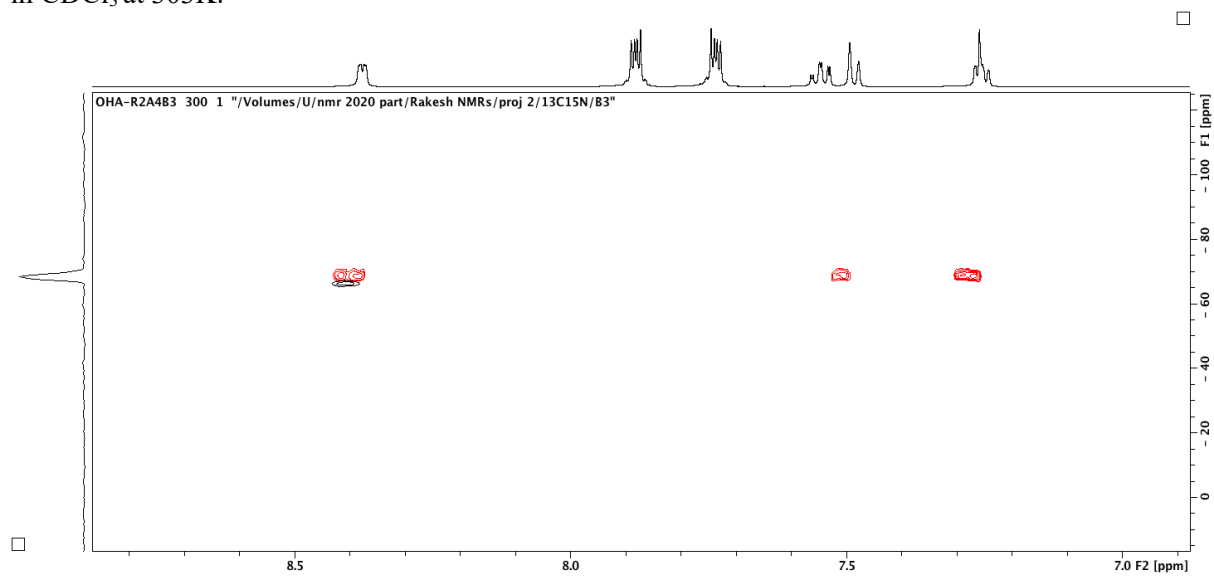


Figure S25. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NBP-**4** in red contour in CDCl_3 at 303K.

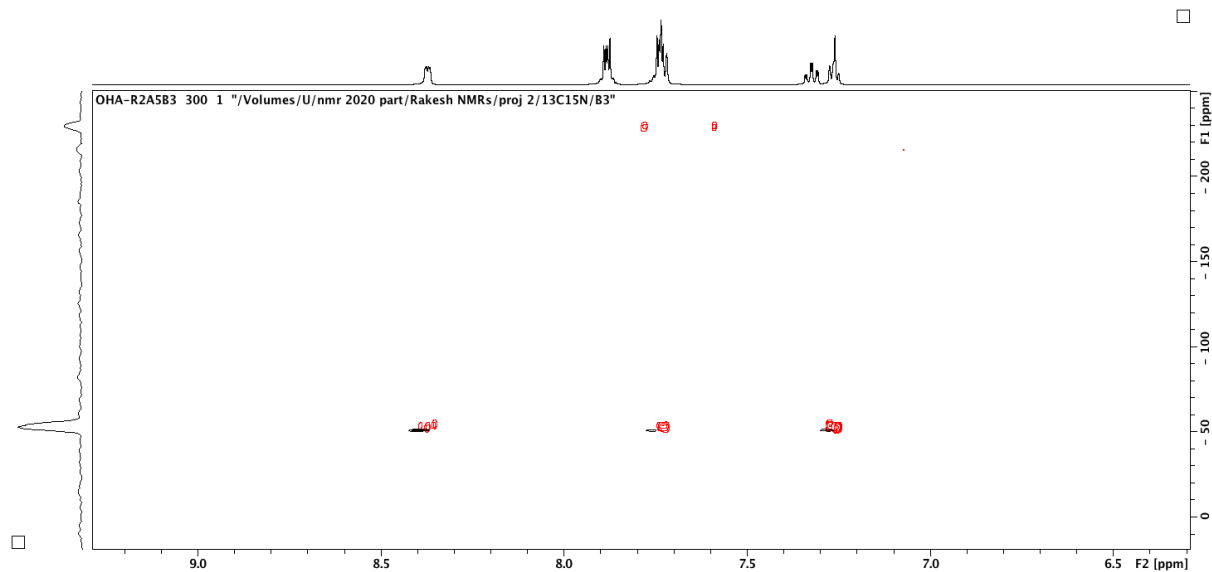


Figure S26. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex NBP-**5** in red contour in CDCl_3 at 303K.

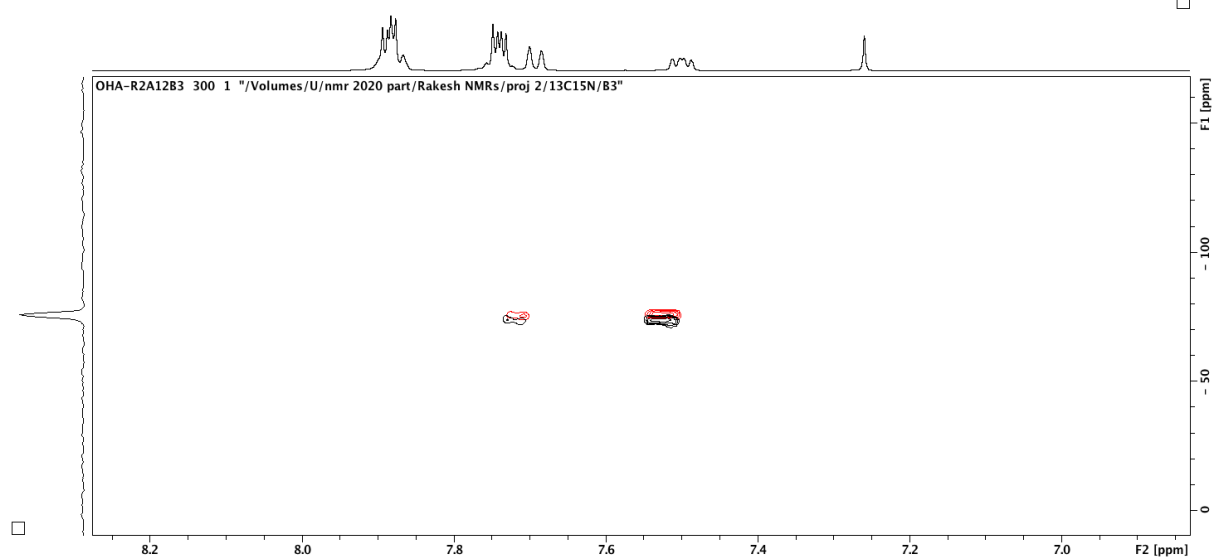


Figure S27. ^1H - ^{15}N HMBC-NMR Spectra of **6** in black contour and 1:1 complex NBP-**6** in red contour in CDCl_3 at 303K.

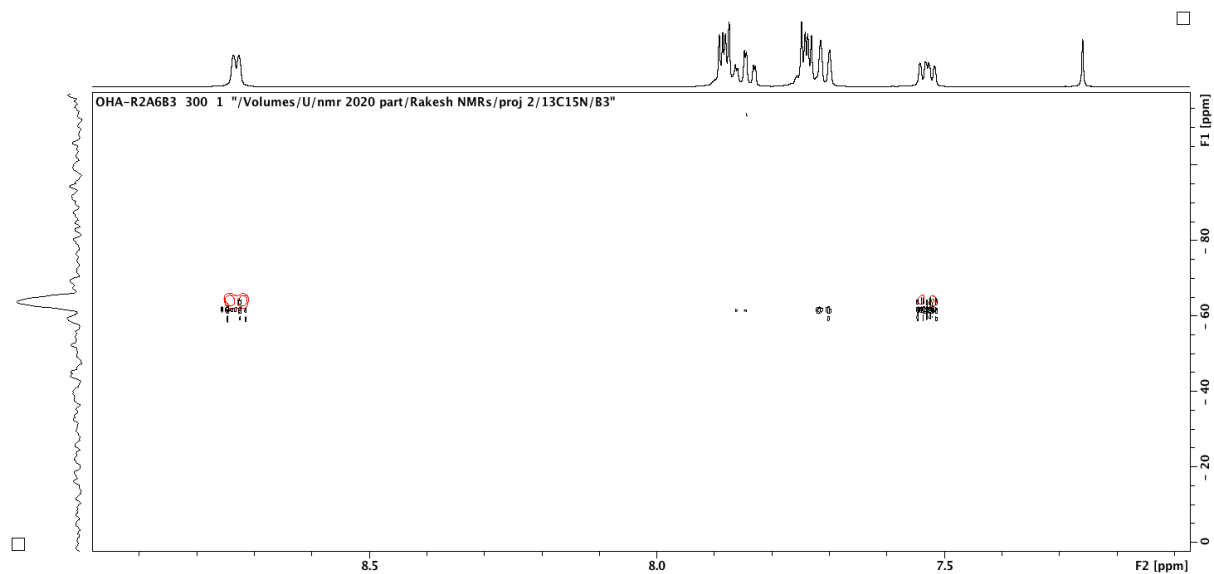


Figure S28. ^1H - ^{15}N HMBC-NMR Spectra of **7** in black contour and 1:1 complex NBP-**7** in red contour in CDCl_3 at 303K.

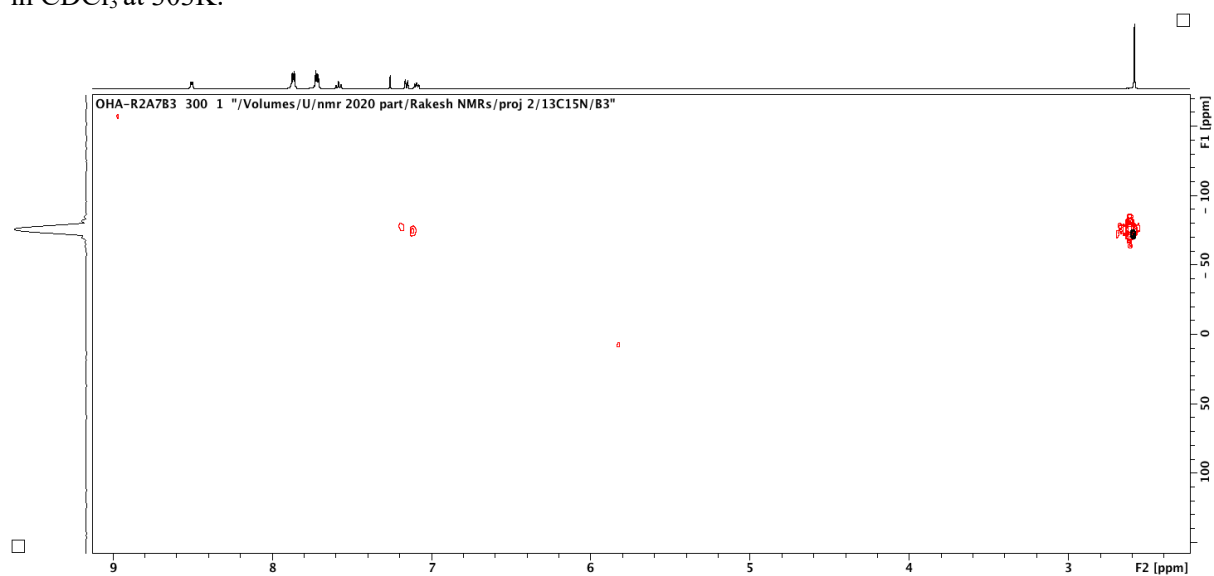


Figure S29. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NBP-**8** in red contour in CDCl_3 at 303K.

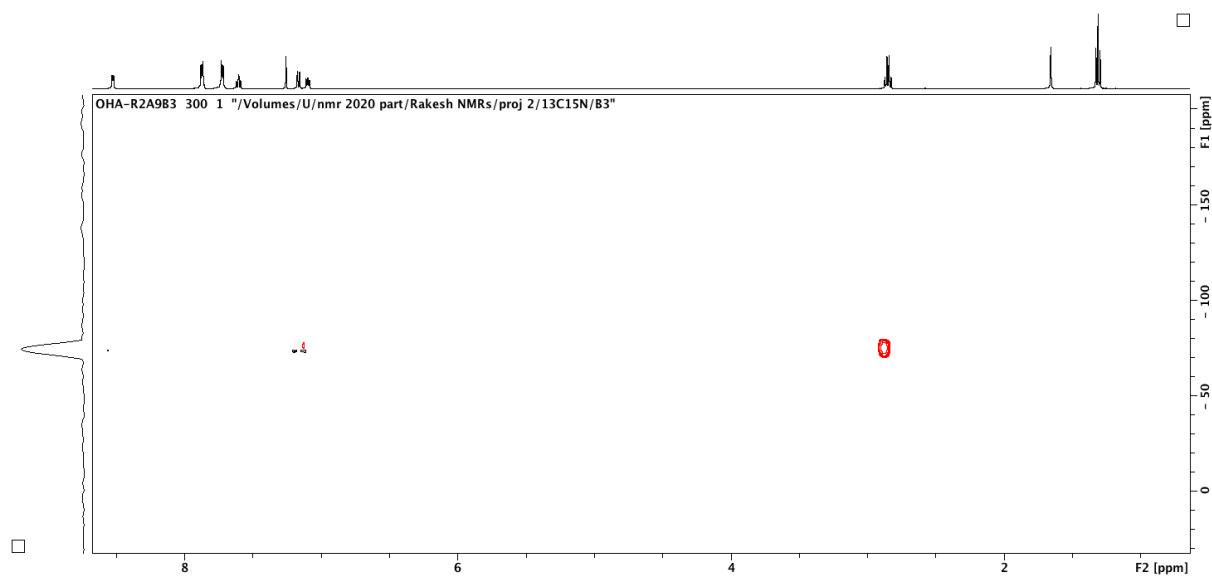


Figure S30. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NBP-**9** in red contour in CDCl_3 at 303K.

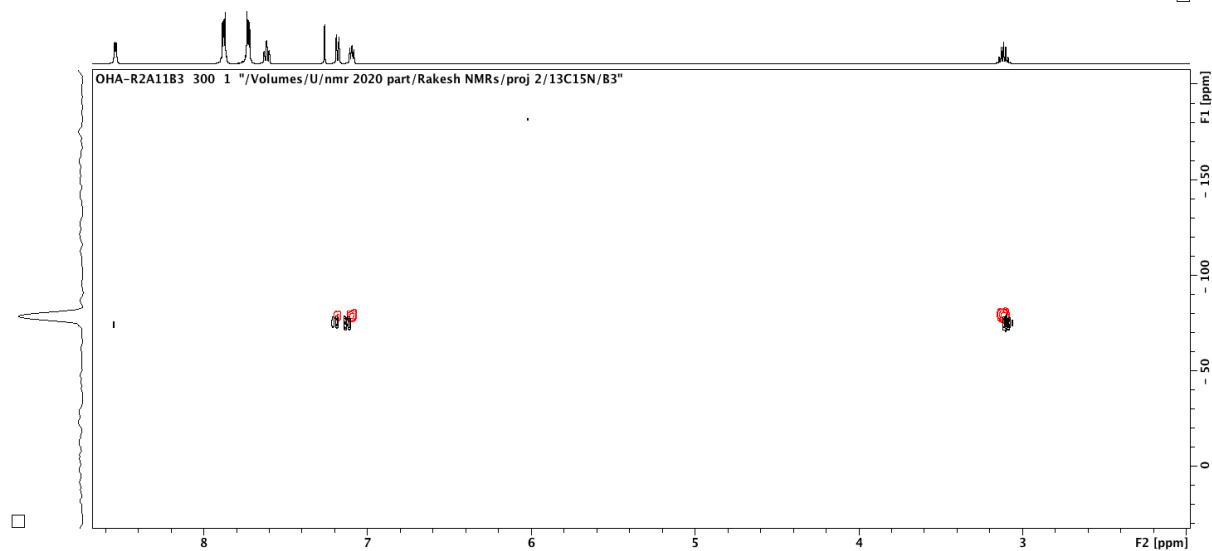


Figure S31. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NBP-**10** in red contour in CDCl_3 at 303K.

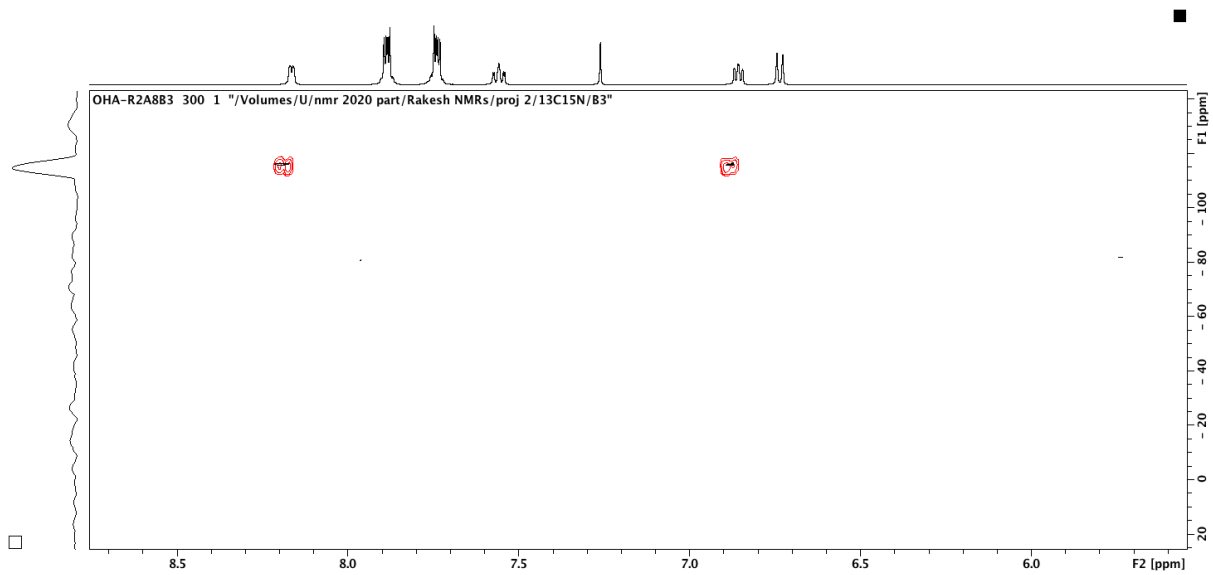


Figure S32. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NBP-**11** in red contour in CDCl_3 at 303K.

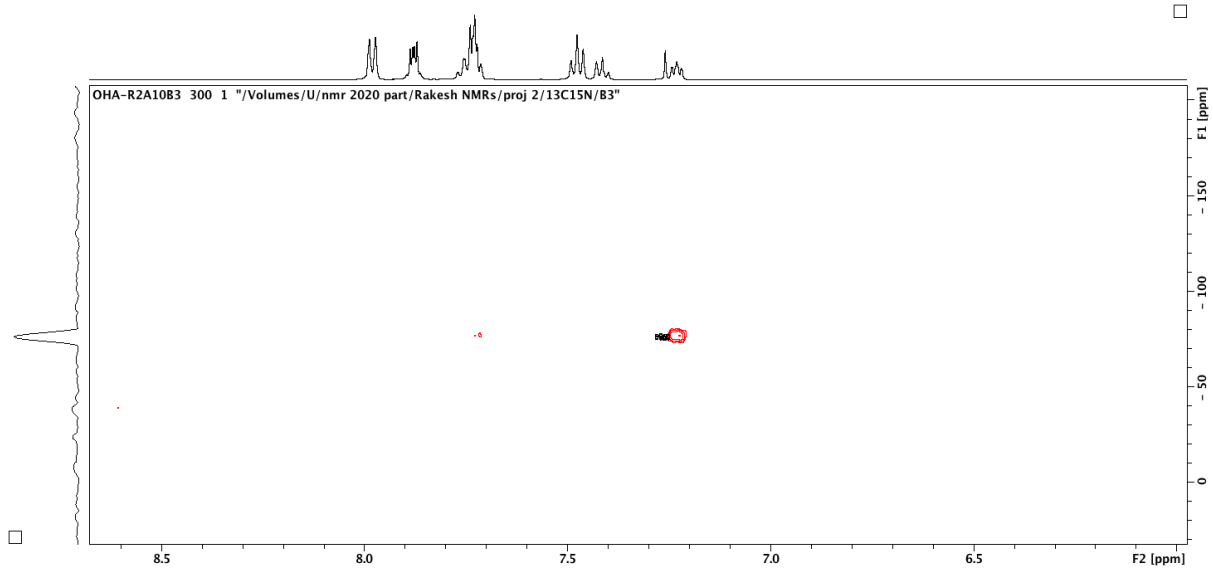


Figure S33. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour and 1:1 complex NBP-**12** in red contour in CDCl_3 at 303K.

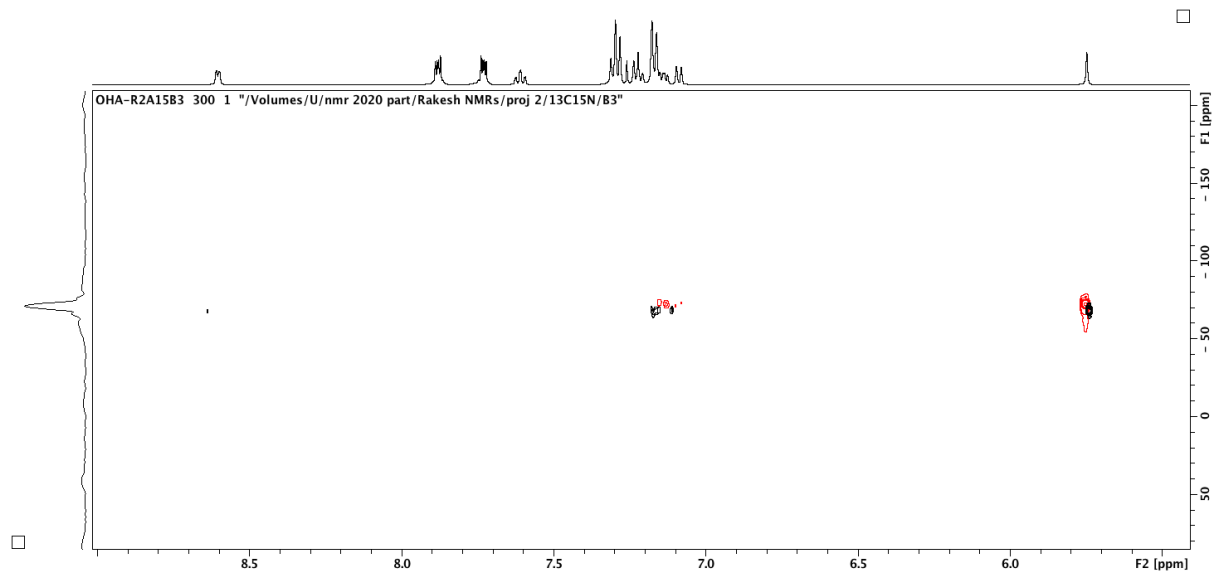


Figure S34. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NBP-**13** in red contour in CDCl_3 at 303K.

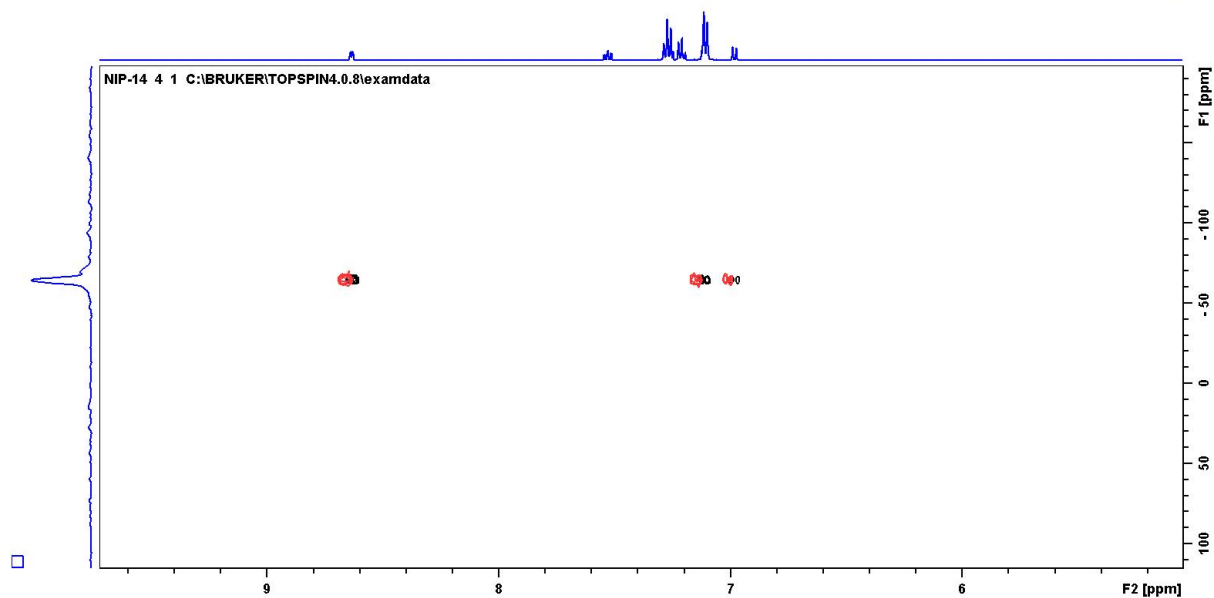


Figure S35. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NBP-**14** in red contour in CDCl_3 at 303K.

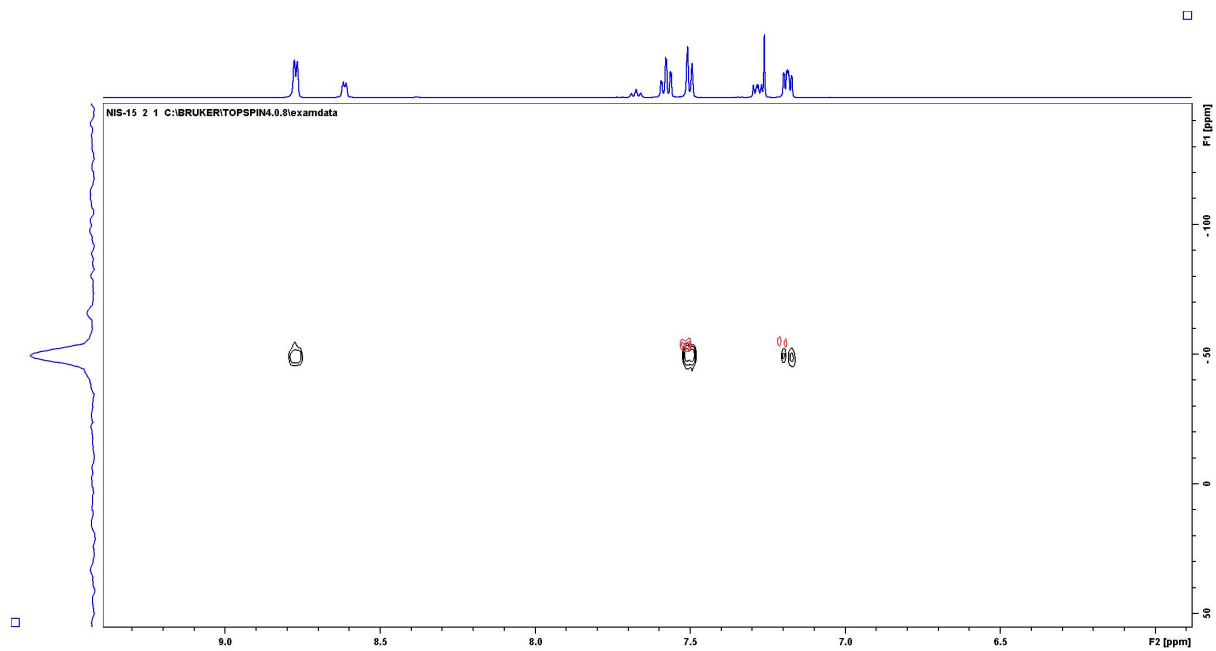


Figure S36. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NBP-**15** in red contour in CDCl_3 at 303K.

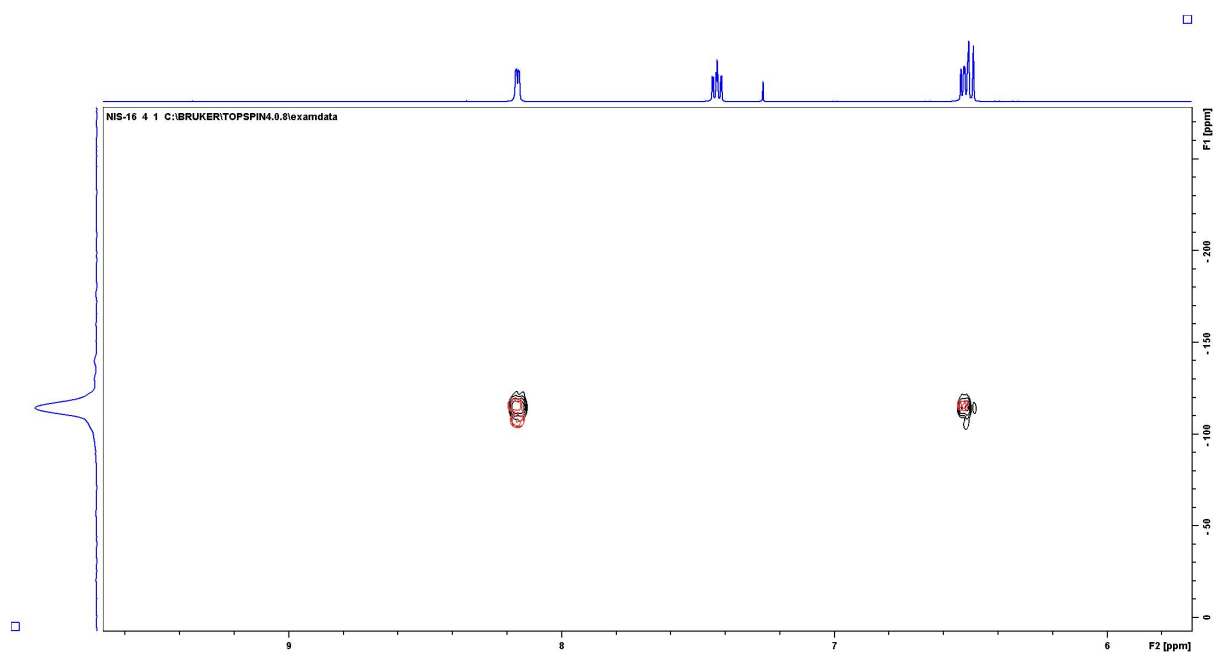


Figure S37. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NBP-**16** in red contour in CDCl_3 at 303K.

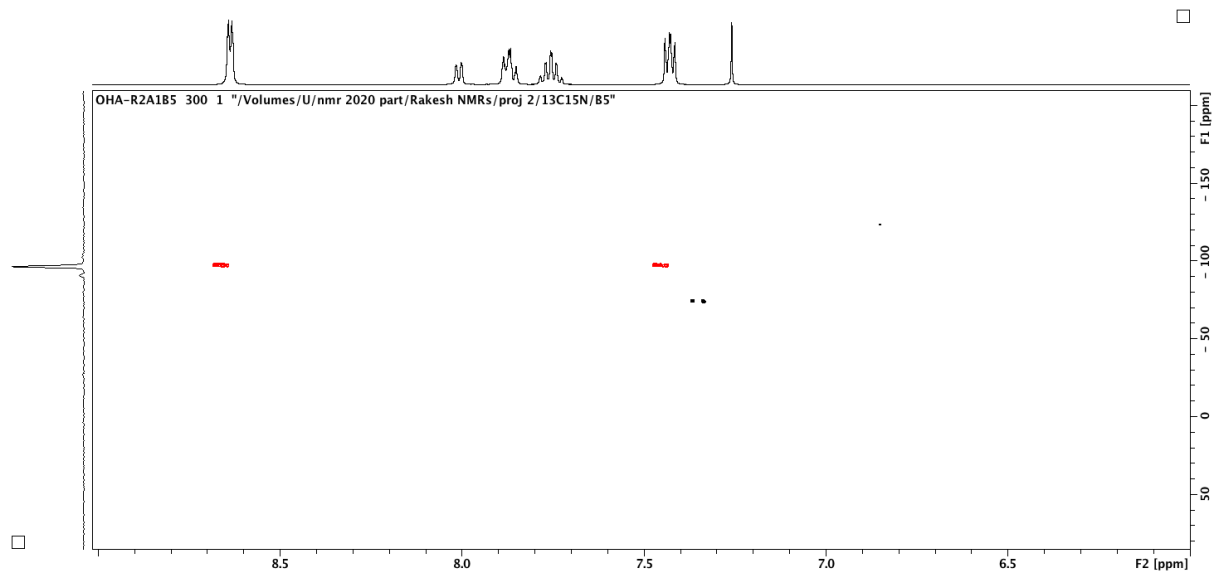


Figure S38. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NBSac-1 in red contour in CDCl_3 at 303K.

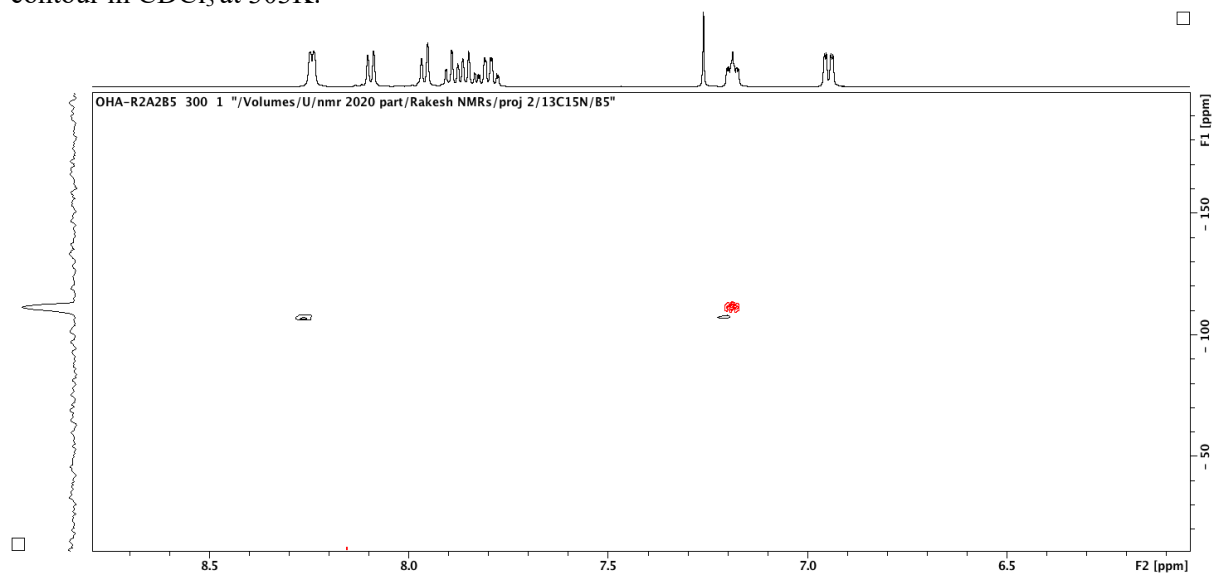


Figure S39. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NBSac-2 in red contour in CDCl_3 at 303K.

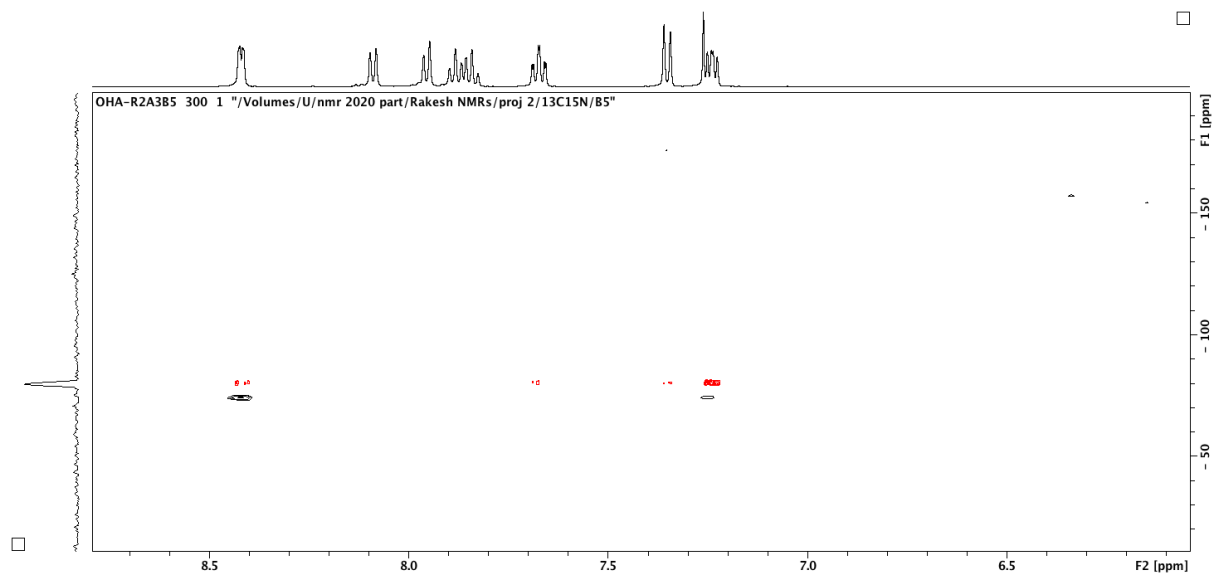


Figure S40. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NBSac-**3** in red contour in CDCl_3 at 303K.

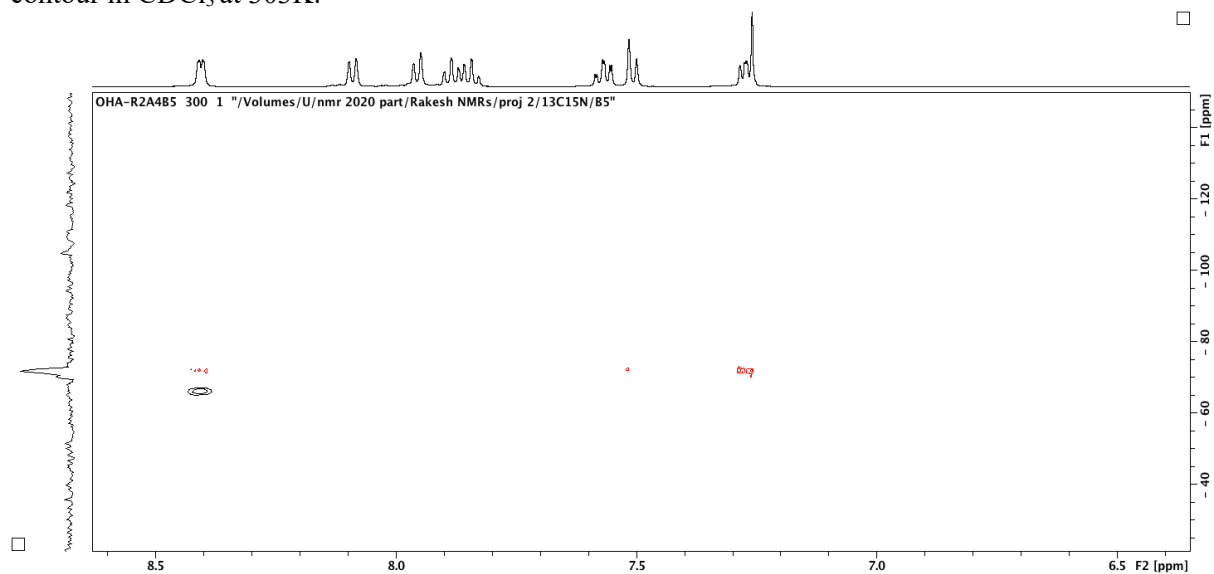


Figure S41. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NBSac-**4** in red contour in CDCl_3 at 303K.

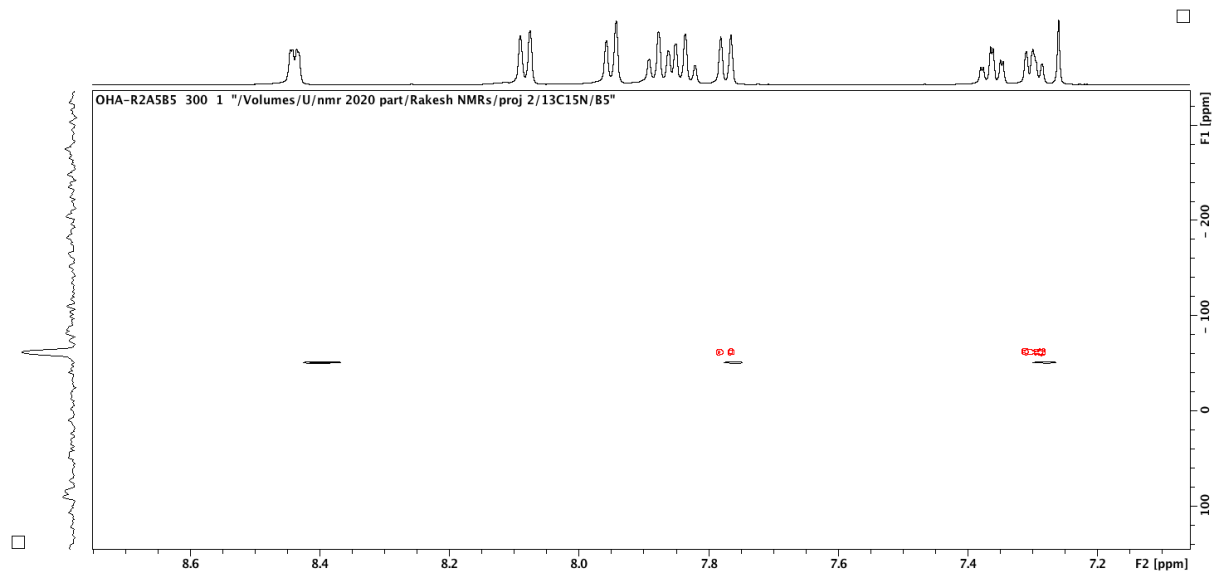


Figure S42. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex NBSac-**5** in red contour in CDCl_3 at 303K.

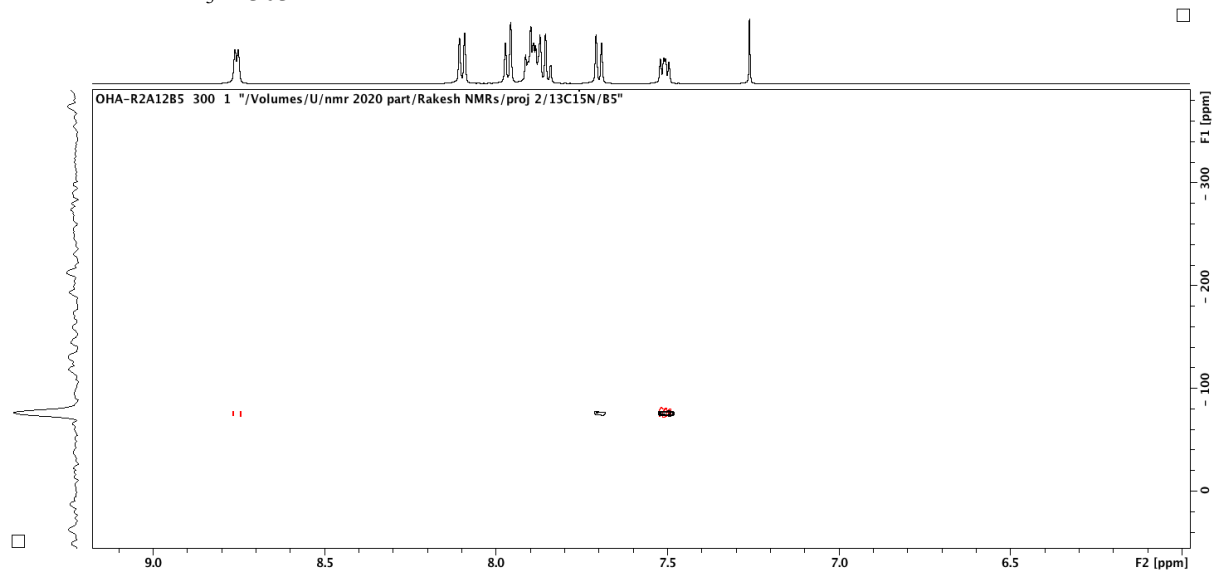


Figure S43. ^1H - ^{15}N HMBC-NMR Spectra of **6** in black contour and 1:1 complex NBSac-**6** in red contour in CDCl_3 at 303K.

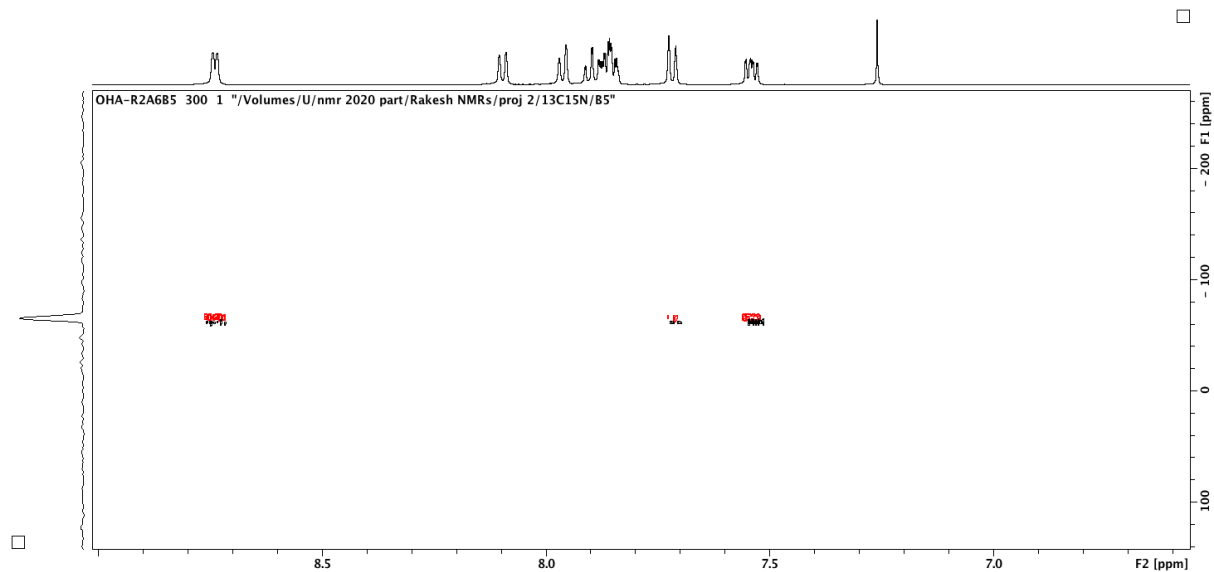


Figure S44. ^1H - ^{15}N HMBC-NMR Spectra of **7** in black contour and 1:1 complex NBSac-**7** in red contour in CDCl_3 at 303K.

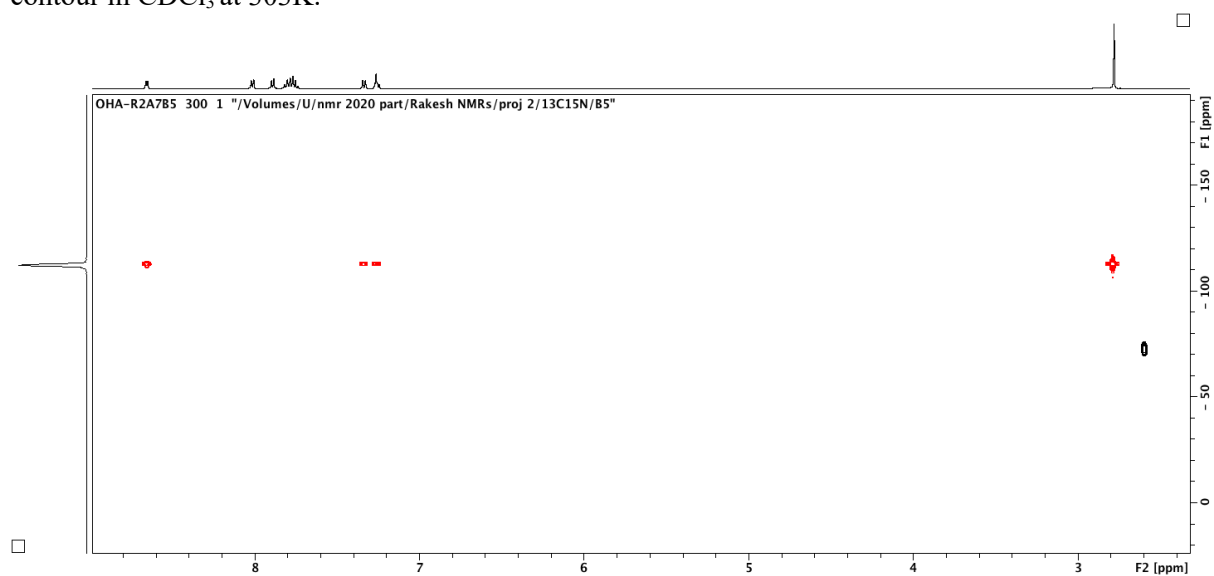


Figure S45. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NBSac-**8** in red contour in CDCl_3 at 303K.

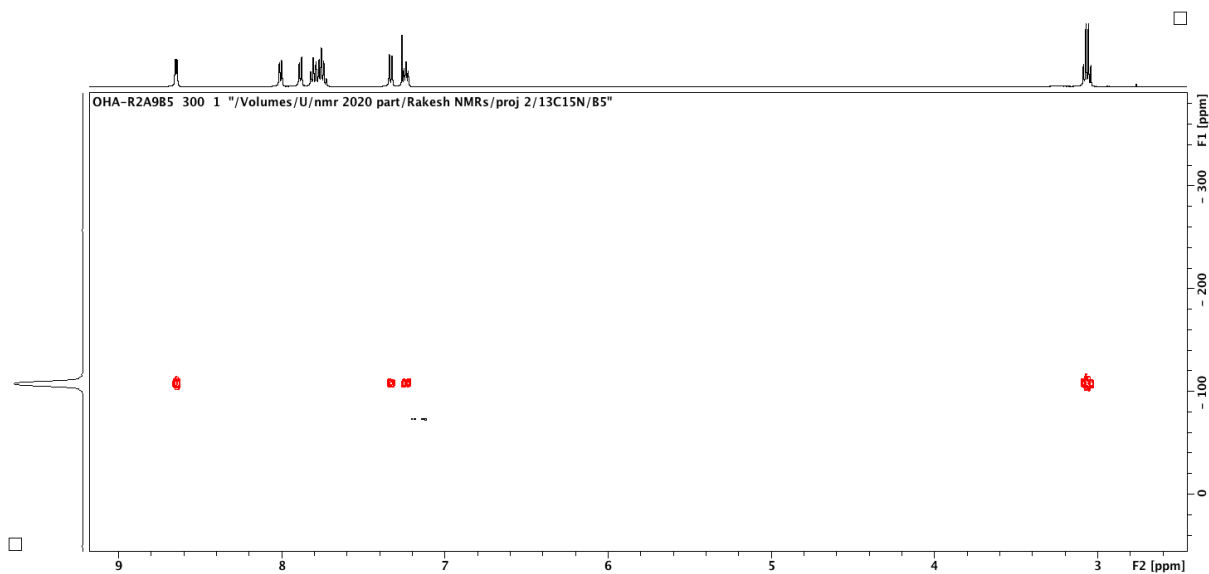


Figure S46. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NBSac-**9** in red contour in CDCl_3 at 303K.

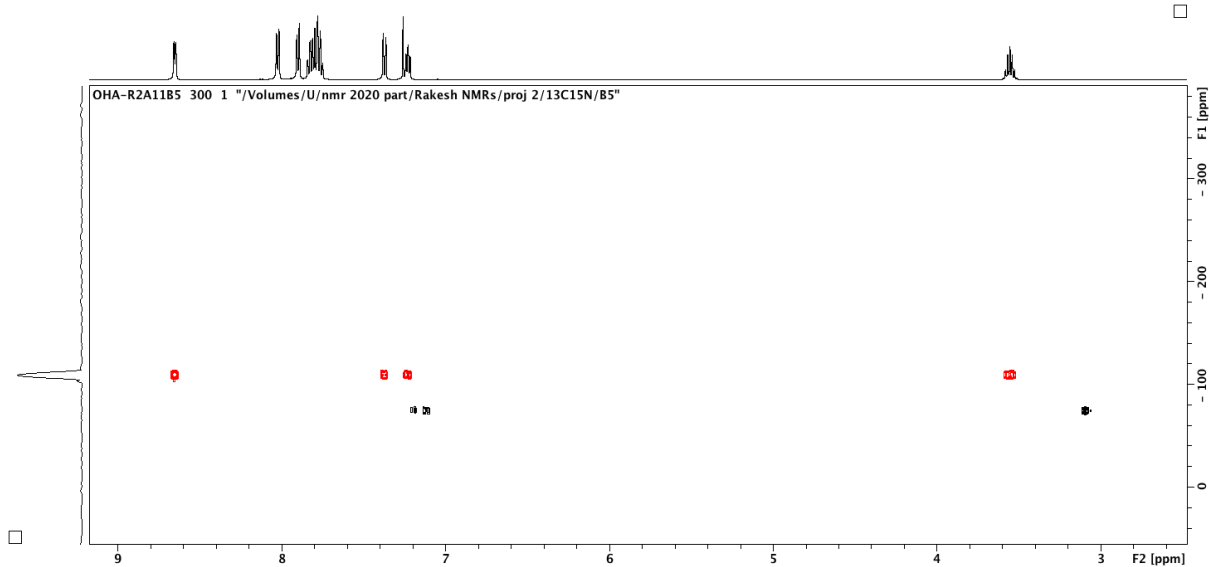


Figure S47. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NBSac-**10** in red contour in CDCl_3 at 303K.

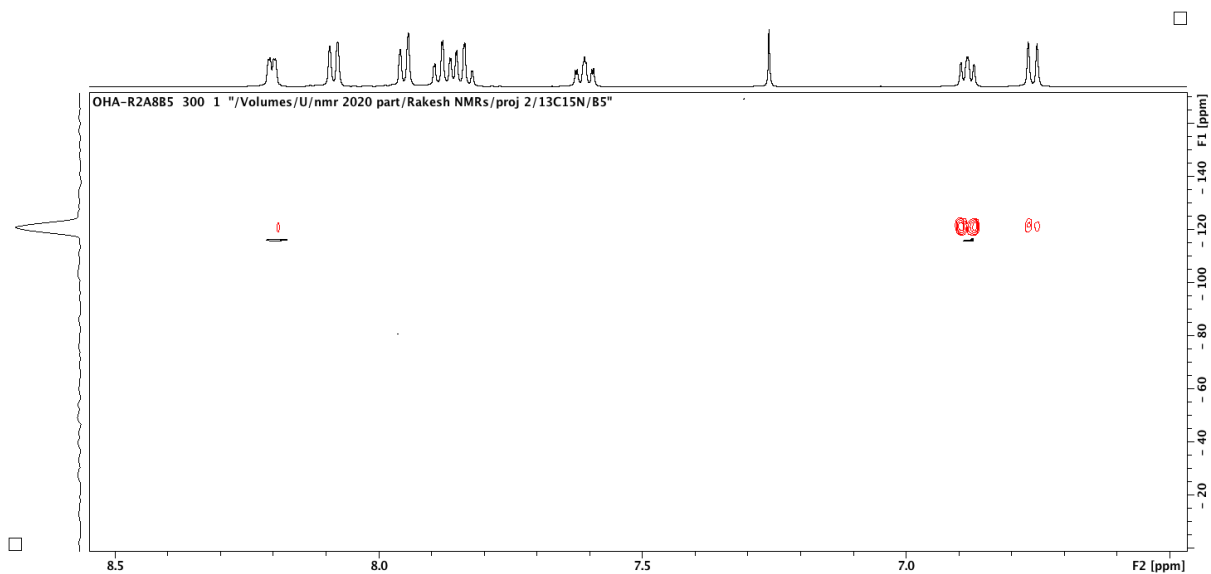


Figure S48. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NBSac-**11** in red contour in CDCl_3 at 303K.

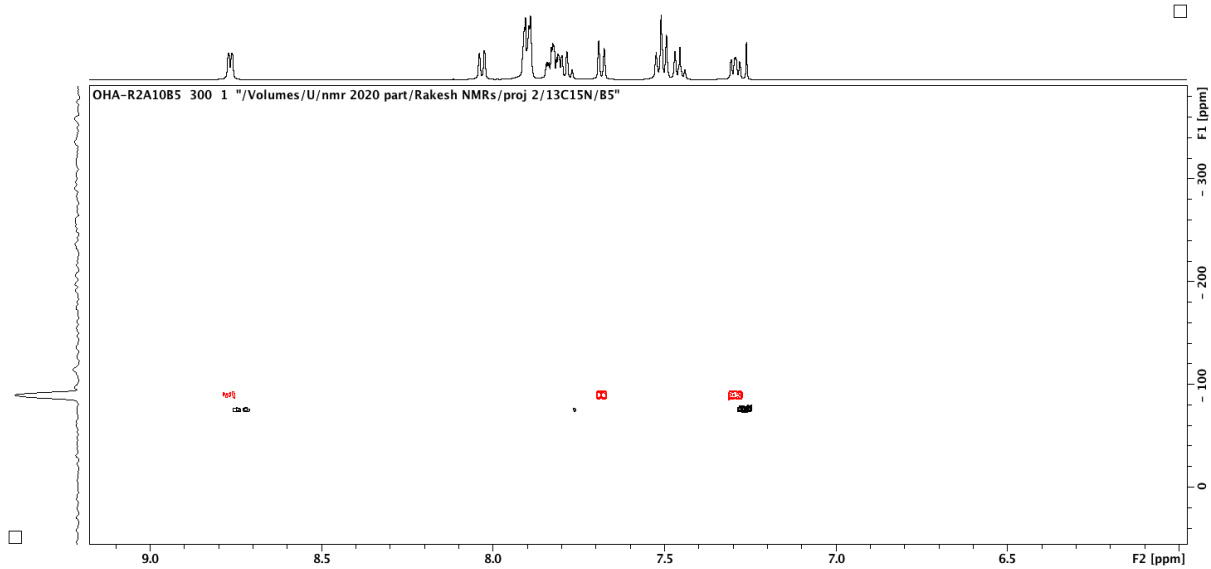


Figure S49. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour and 1:1 complex NBSac-**12** in red contour in CDCl_3 at 303K.

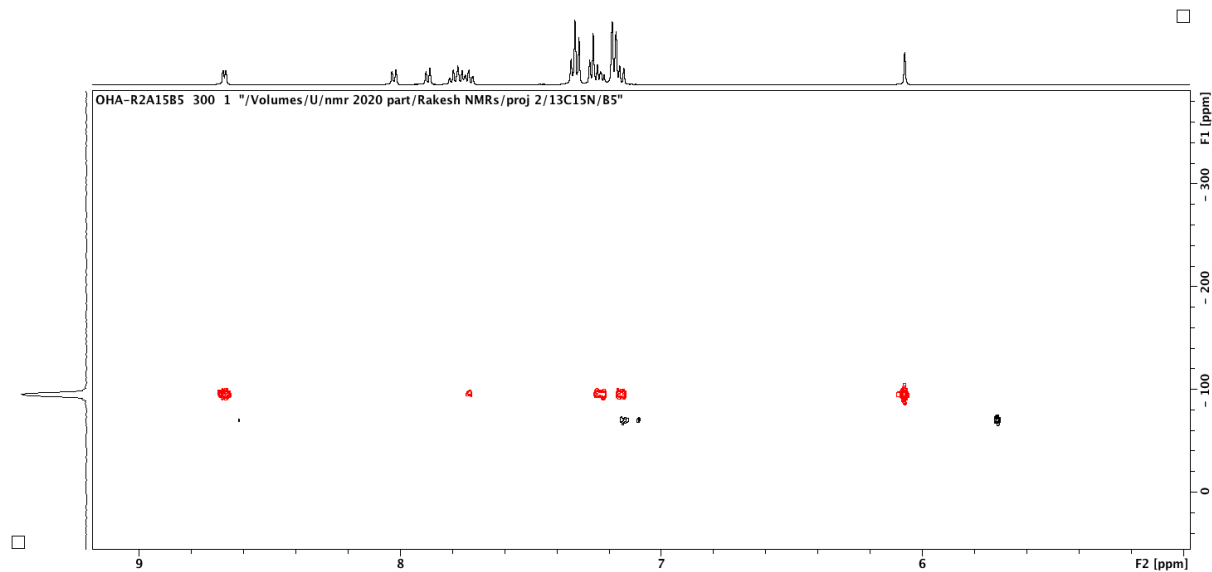


Figure S50. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NBSac-**13** in red contour in CDCl_3 at 303K.

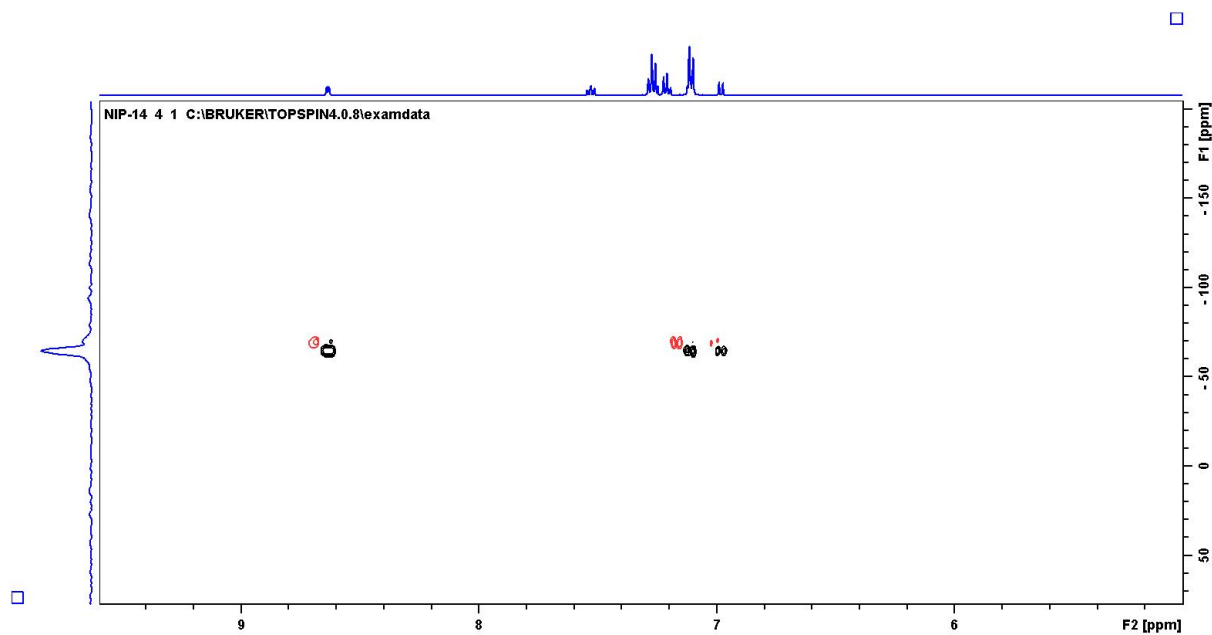


Figure S51. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NBSac-**14** in red contour in CDCl_3 at 303K.

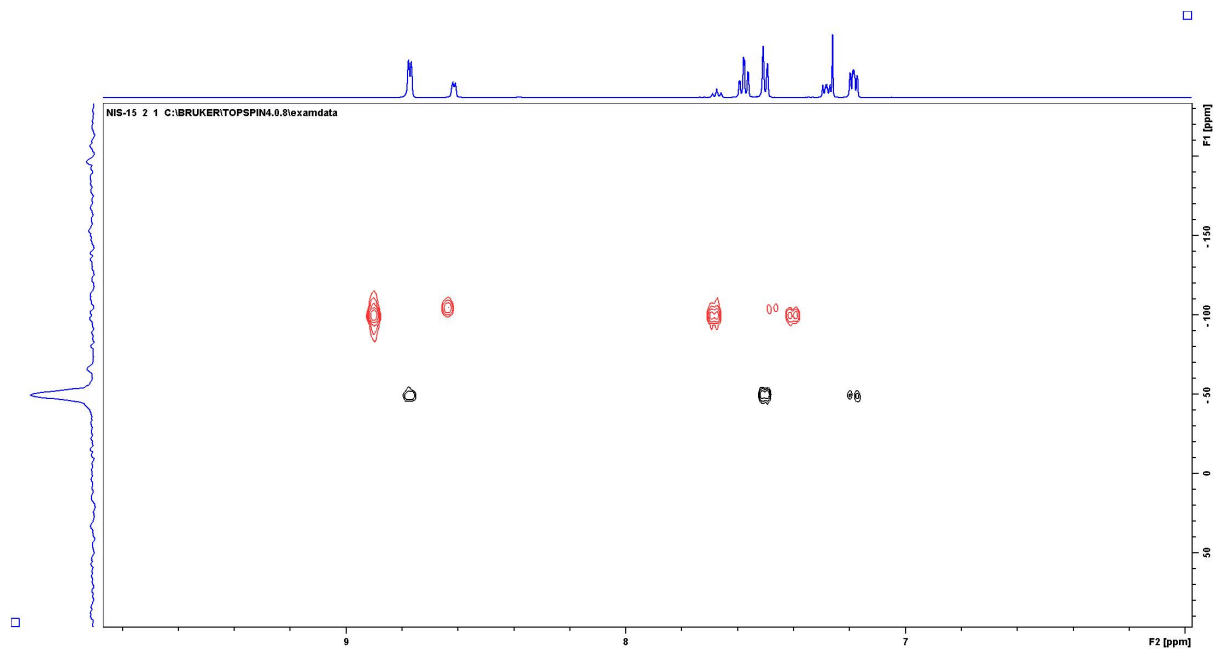


Figure S52. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NBSac-**15** in red contour in CDCl_3 at 303K.

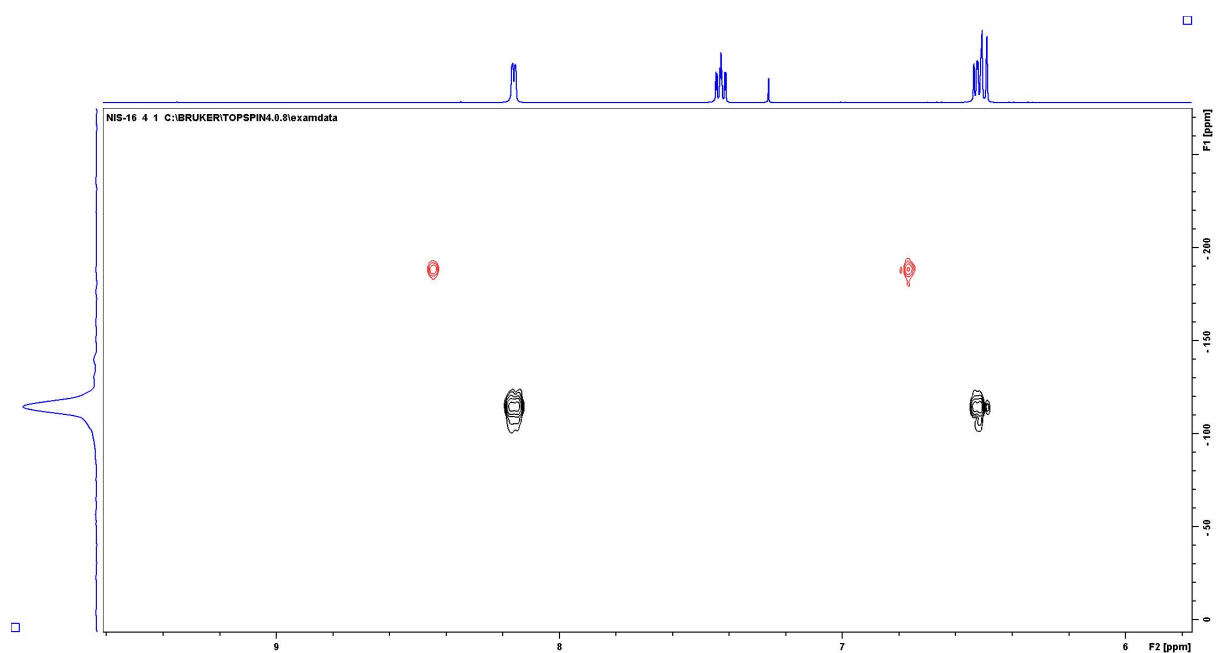


Figure S53. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NBSac-**16** in red contour in CDCl_3 at 303K.

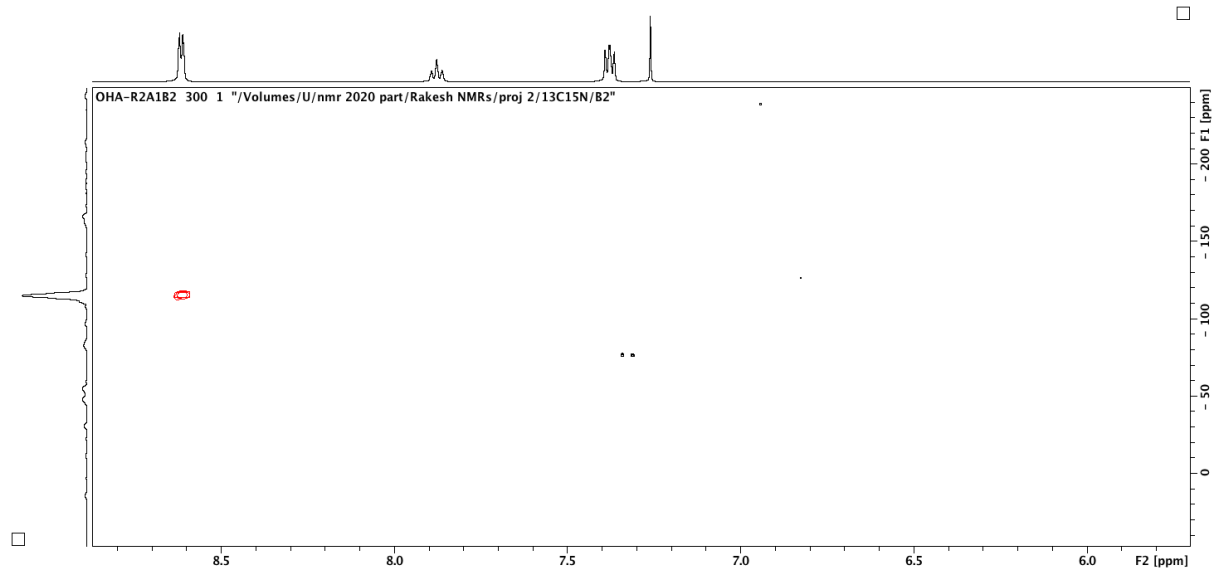


Figure S54. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NIS-1 in red contour in CDCl_3 at 303K.

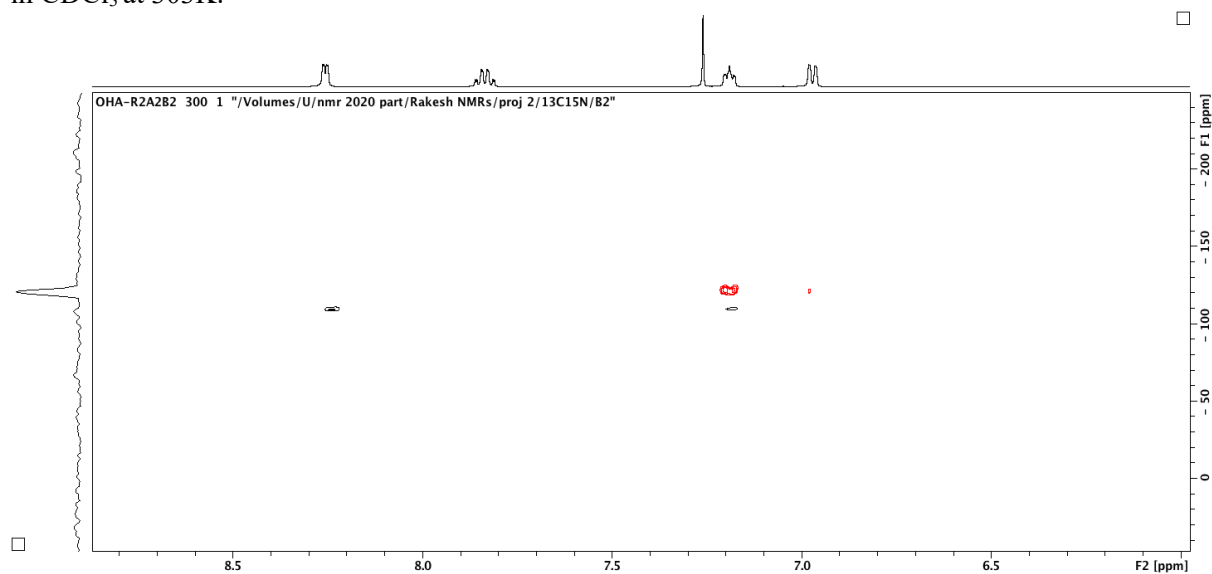


Figure S55. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NIS-2 in red contour in CDCl_3 at 303K.

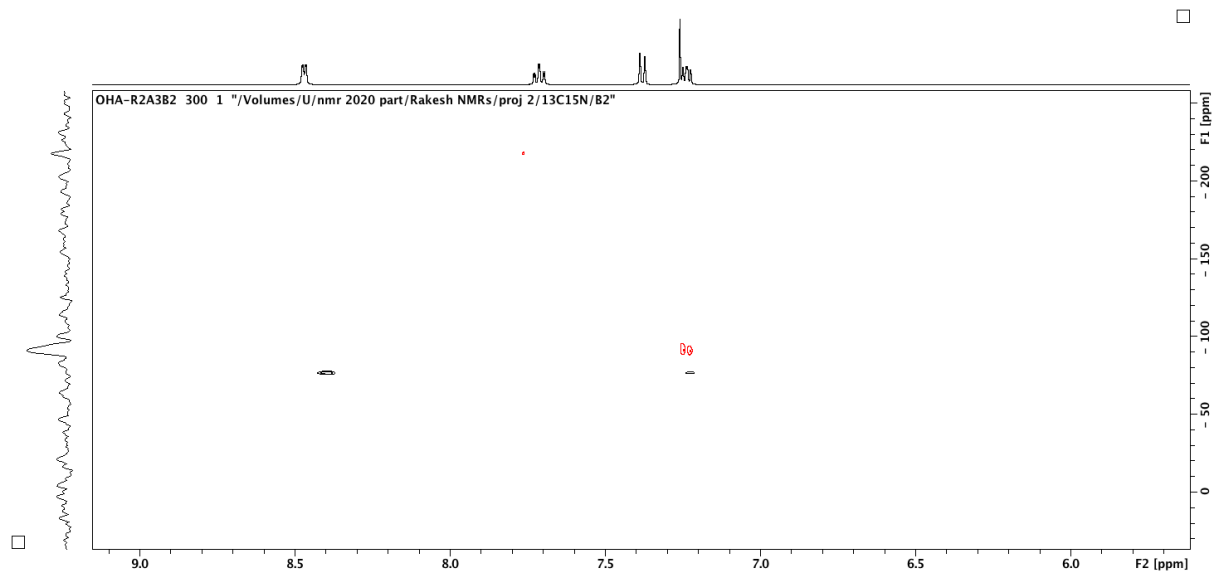


Figure S56. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NIS-**3** in red contour in CDCl_3 at 303K.

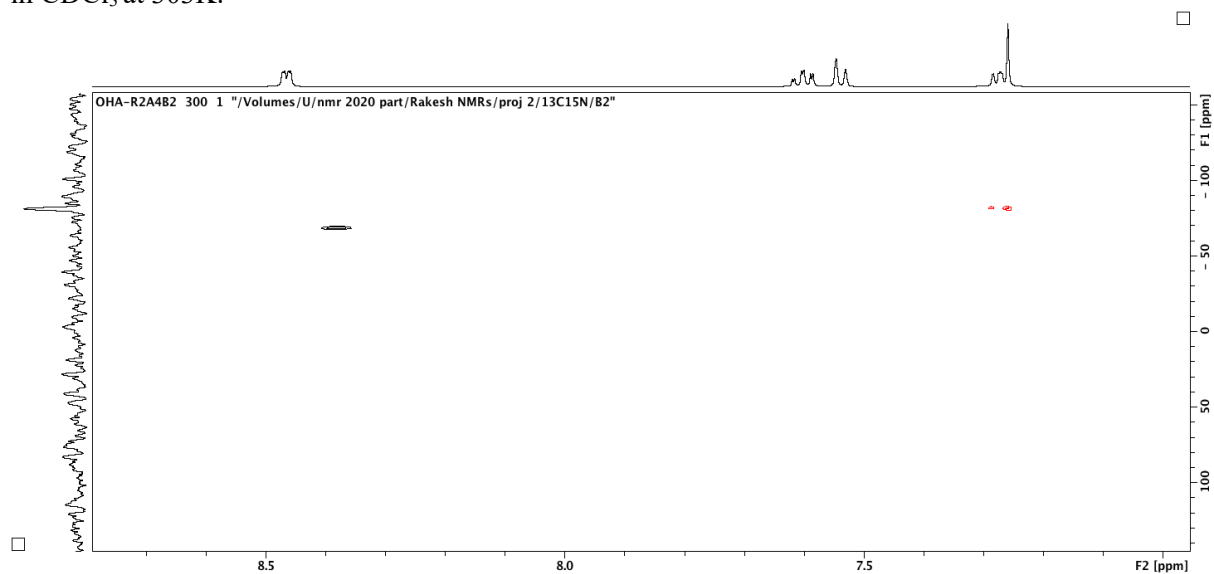


Figure S57. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NIS-**4** in red contour in CDCl_3 at 303K.

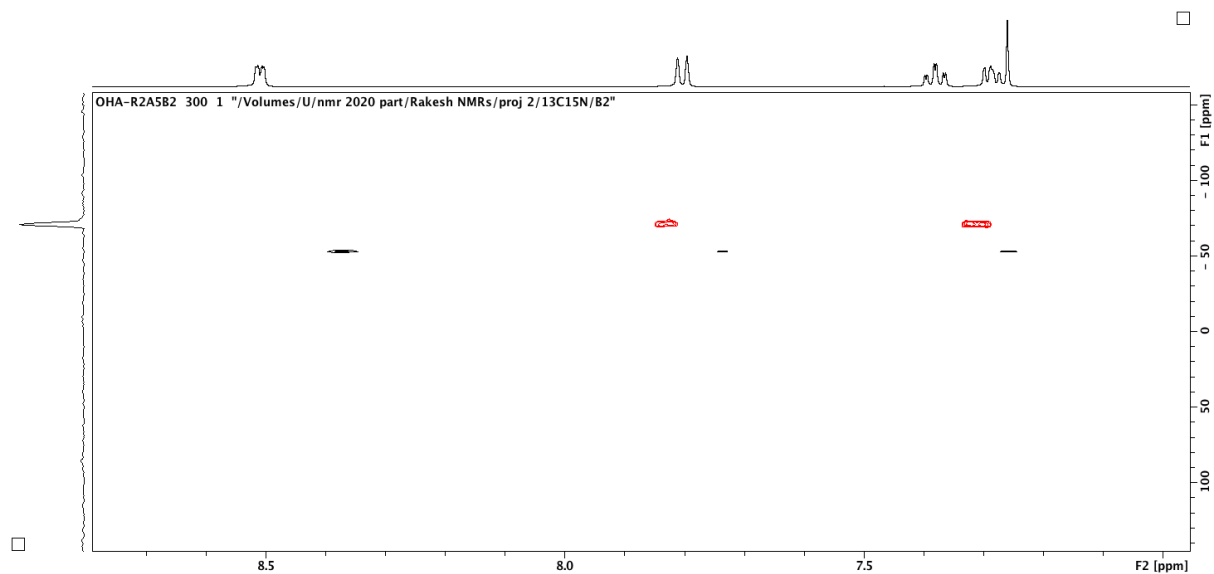


Figure S58. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex NIS-**5** in red contour in CDCl_3 at 303K.

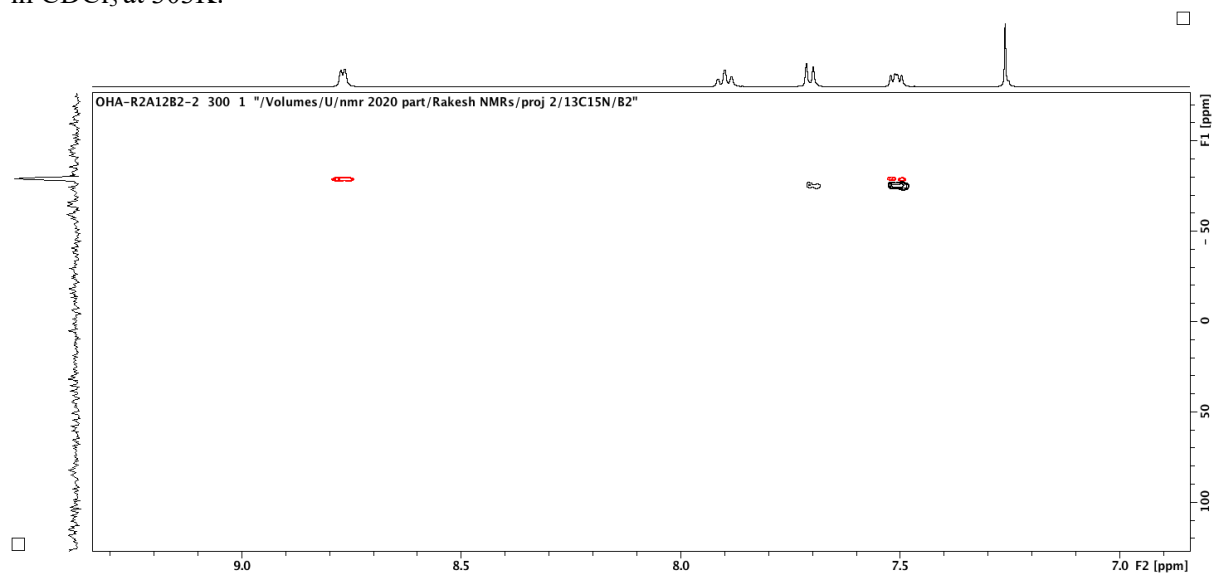


Figure S59. ^1H - ^{15}N HMBC-NMR Spectra of **6** in black contour and 1:1 complex NIS-**6** in red contour in CDCl_3 at 303K.

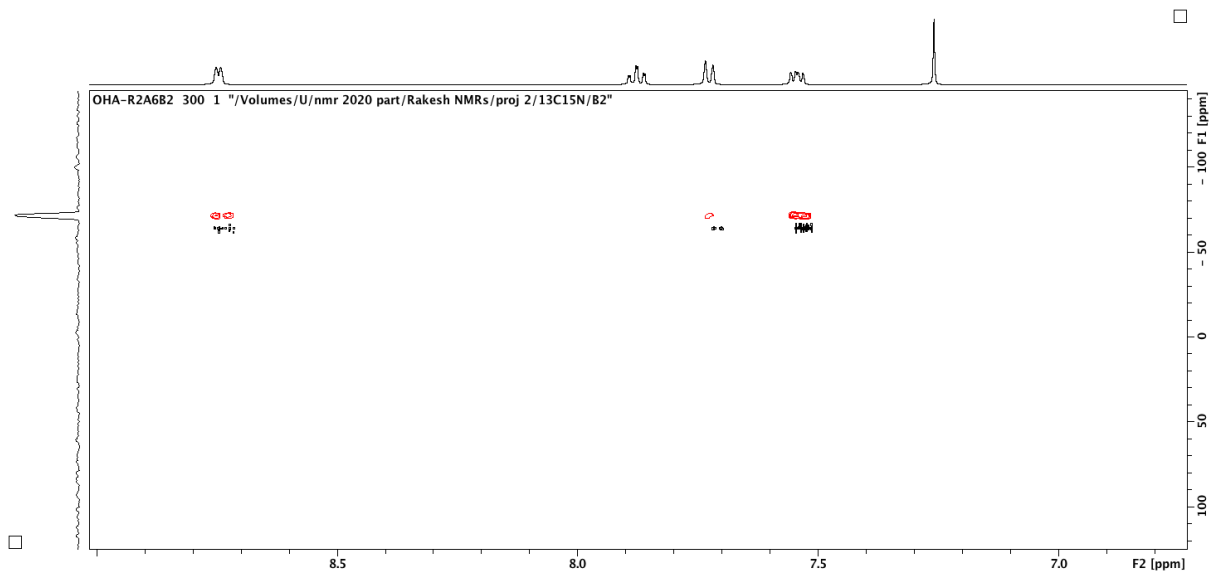


Figure S60. ^1H - ^{15}N HMBC-NMR Spectra of **7** in black contour and 1:1 complex NIS-**7** in red contour in CDCl_3 at 303K.

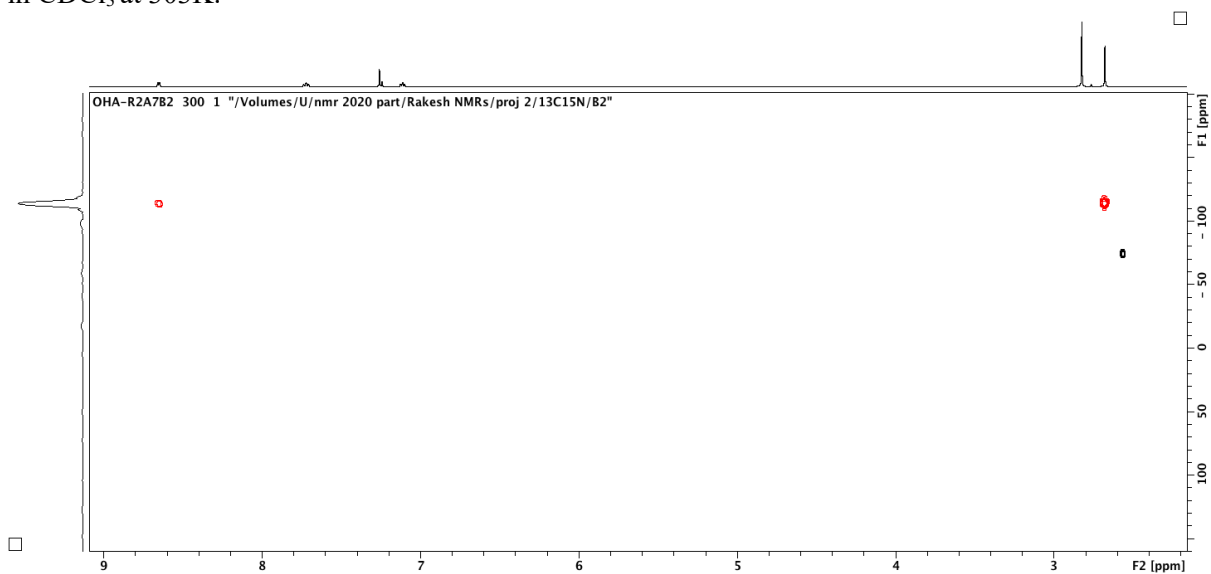


Figure S61. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NIS-**8** in red contour in CDCl_3 at 303K.

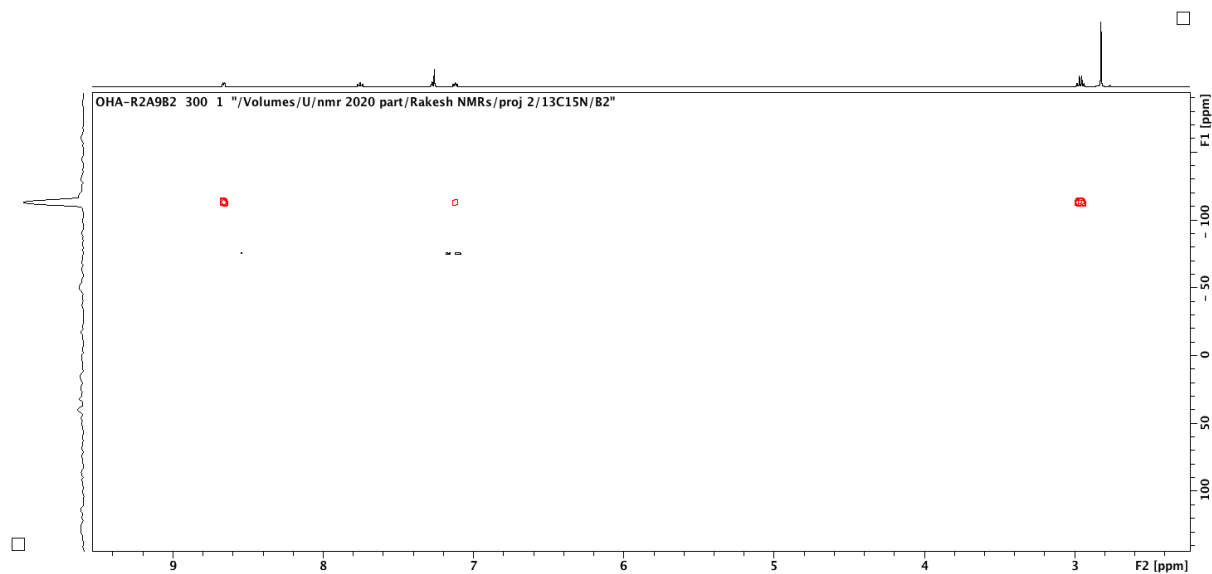


Figure S62. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NIS-**9** in red contour in CDCl_3 at 303K.

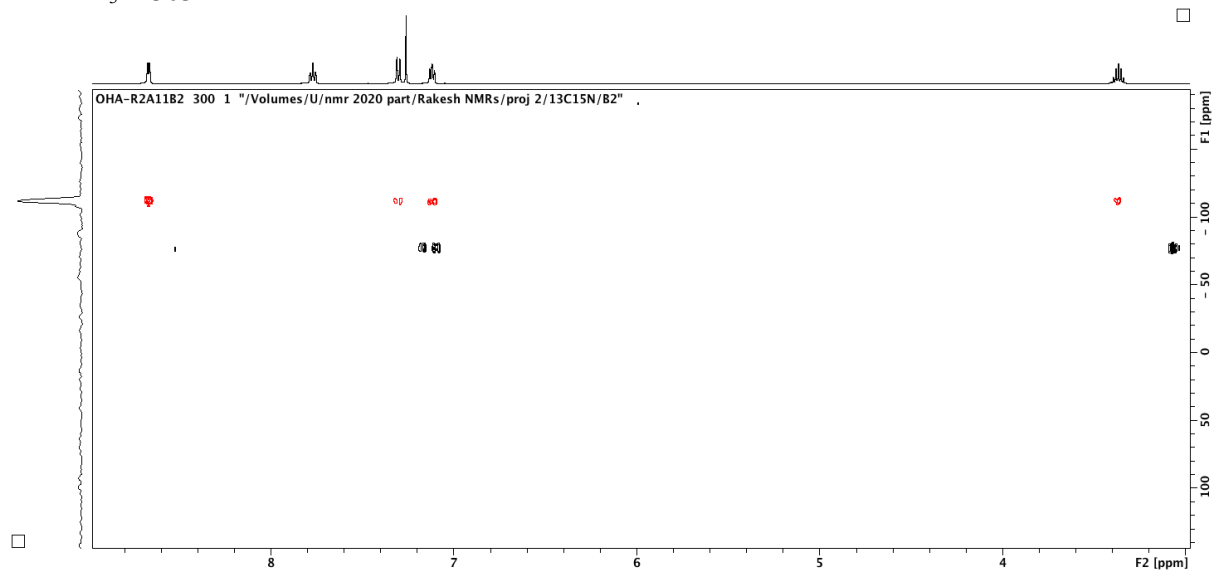


Figure S63. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NIS-**10** in red contour in CDCl_3 at 303K.

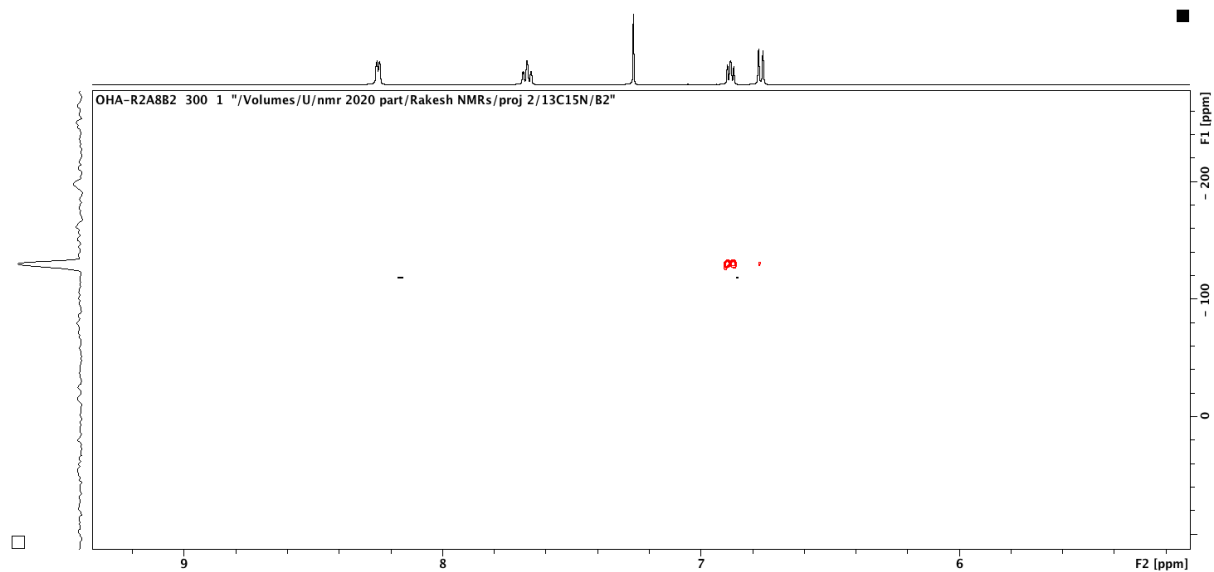


Figure S64. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NIS-**11** in red contour in CDCl_3 at 303K.

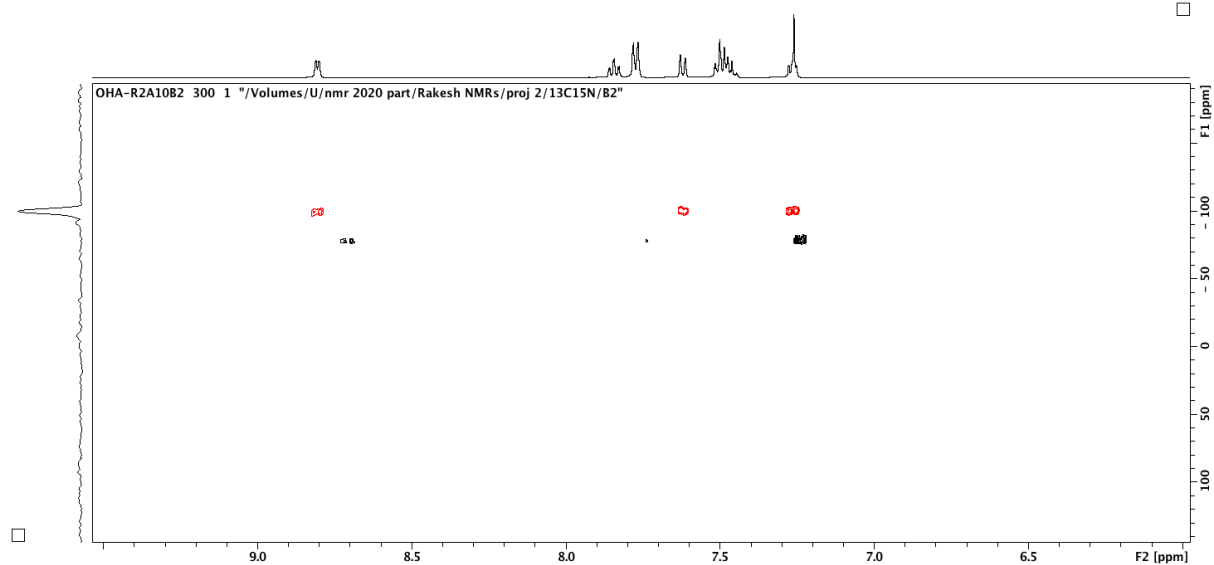


Figure S65. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour and 1:1 complex NIS-**12** in red contour in CDCl_3 at 303K.

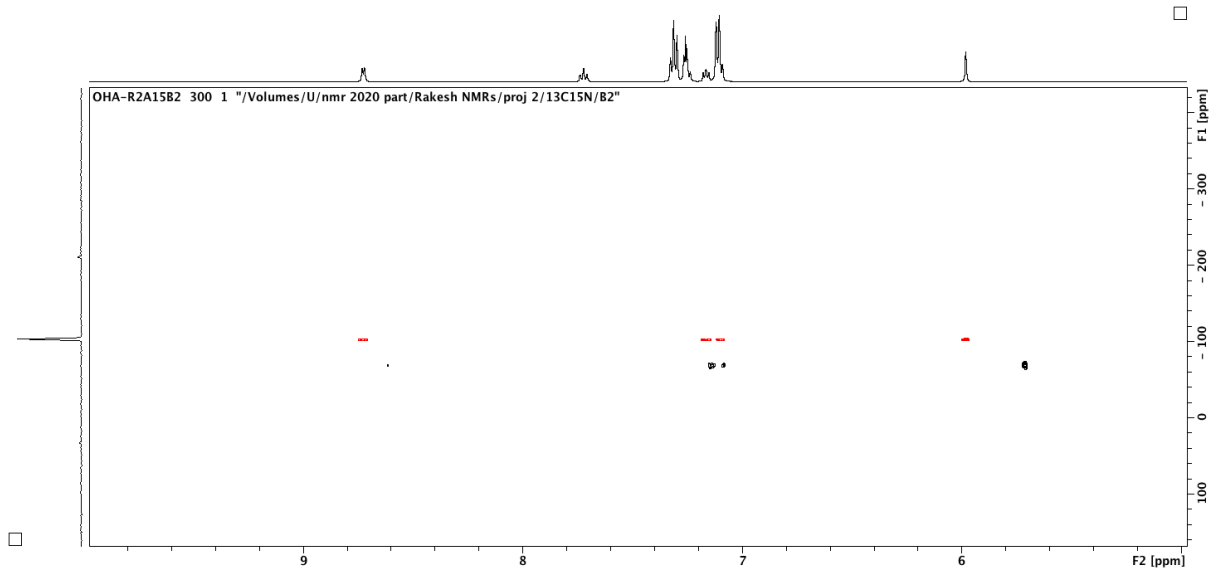


Figure S66. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NIS-**13** in red contour in CDCl_3 at 303K.

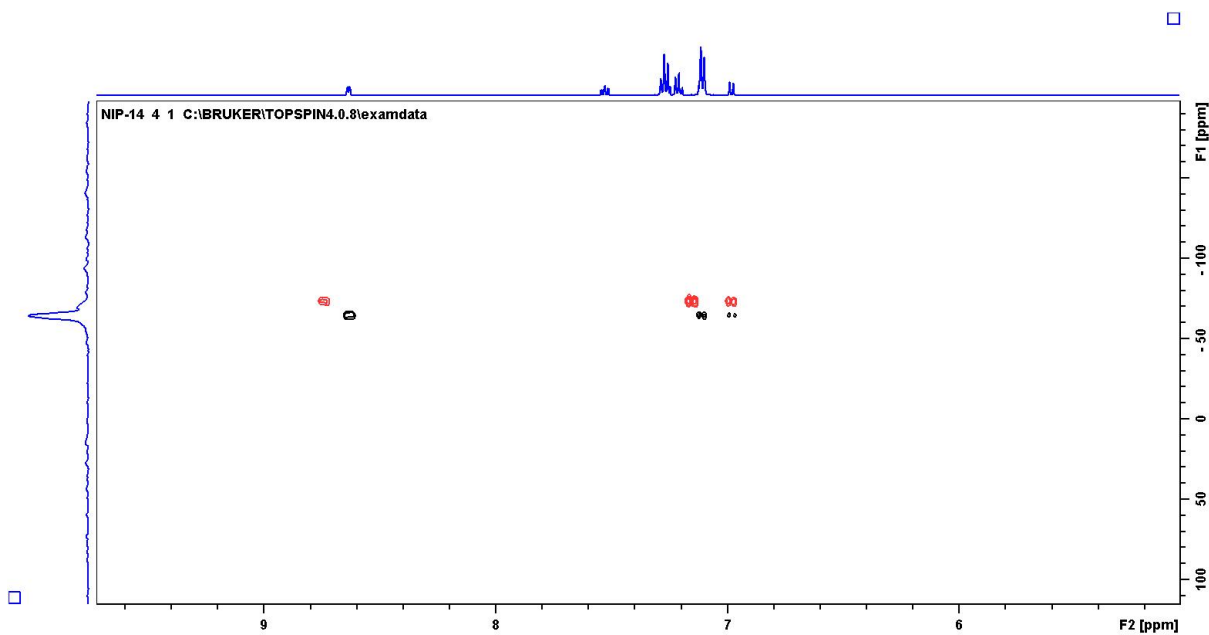


Figure S67. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NIS-**14** in red contour in CDCl_3 at 303K.

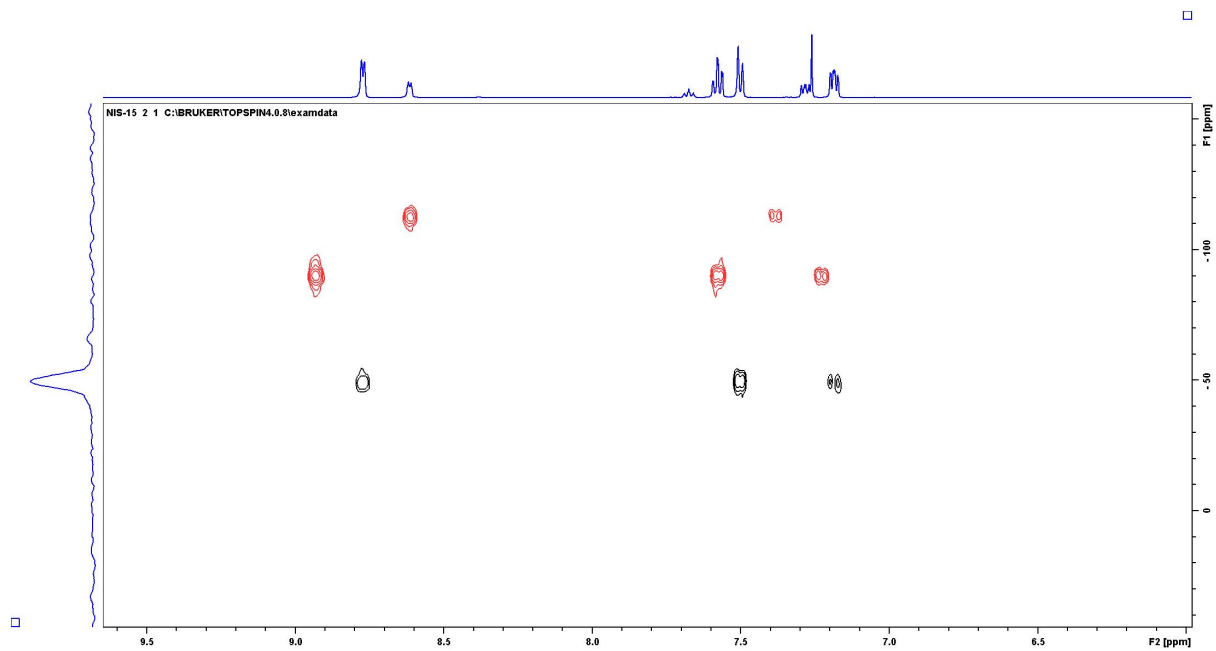


Figure S68. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NIS-**15** in red contour in CDCl_3 at 303K.

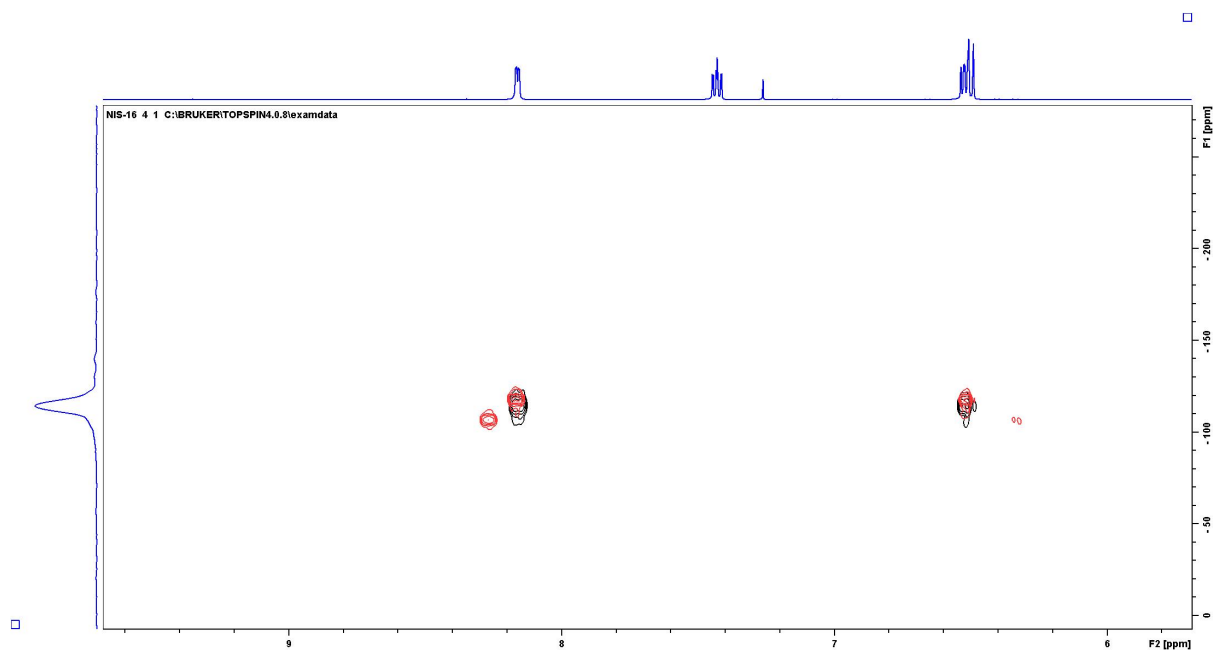


Figure S69. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NIS-**16** in red contour in CDCl_3 at 303K.

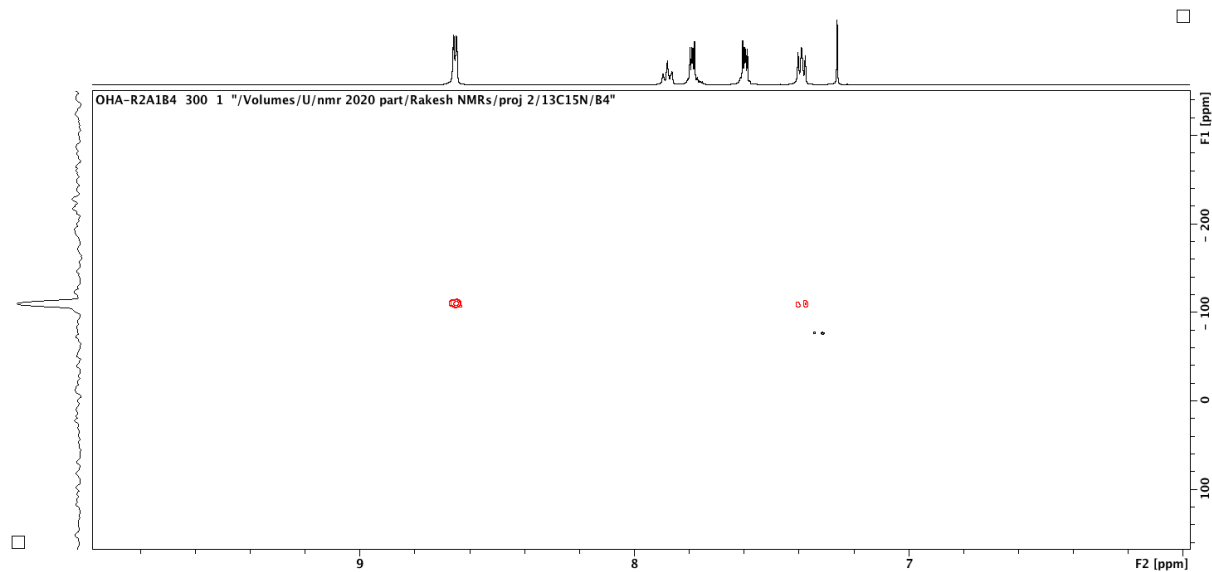


Figure S70. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NIP-1 in red contour in CDCl_3 at 303K.

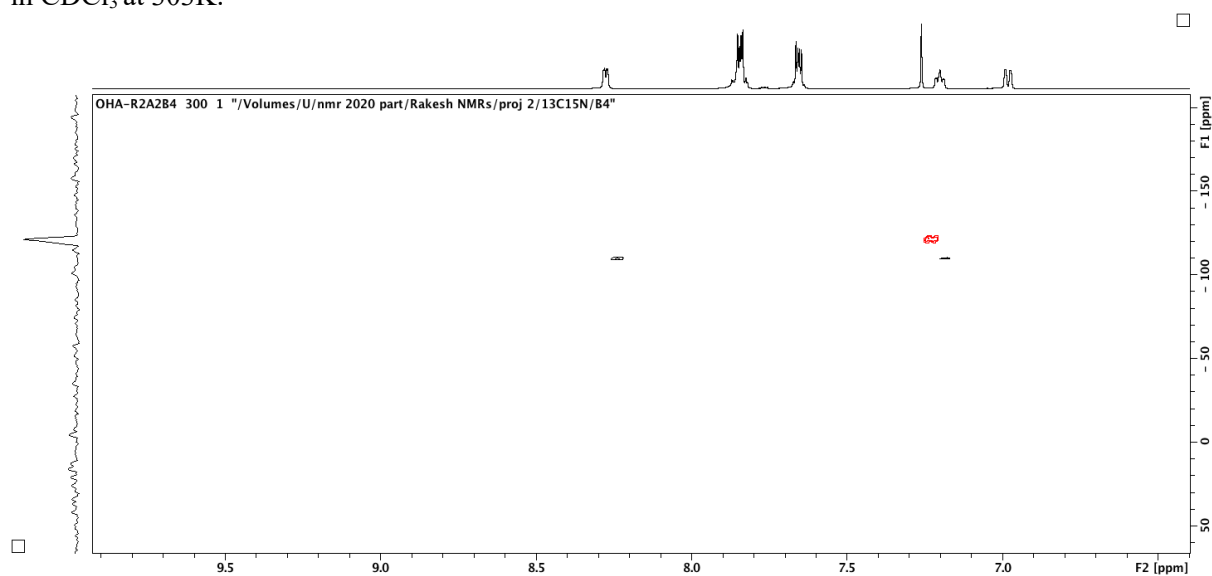


Figure S71. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NIP-2 in red contour in CDCl_3 at 303K.

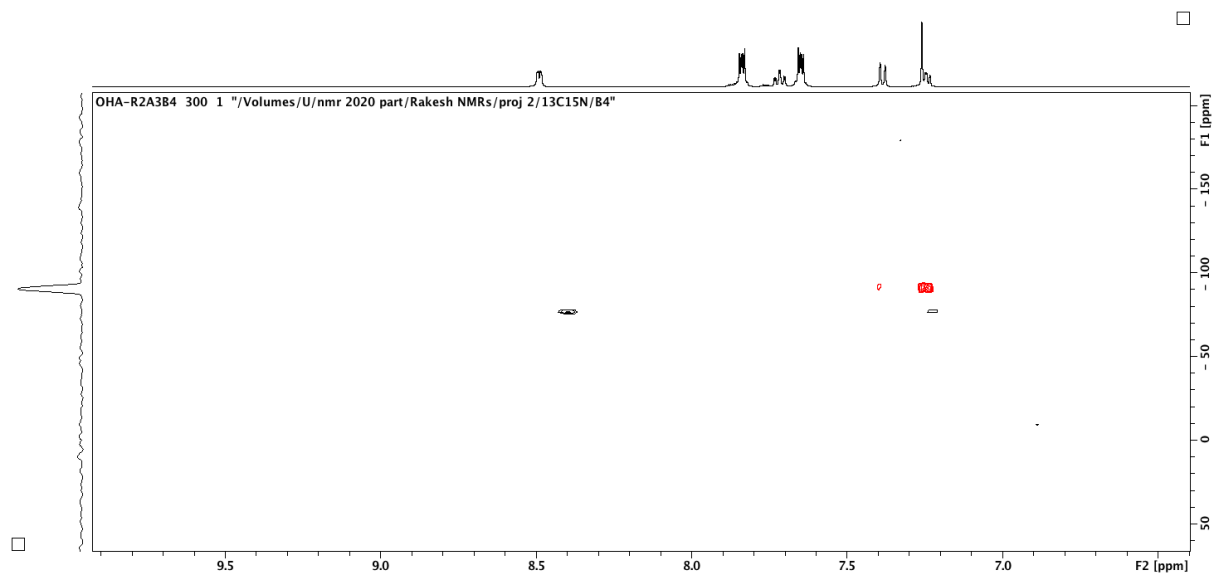


Figure S72. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NIP-**3** in red contour in CDCl_3 at 303K.

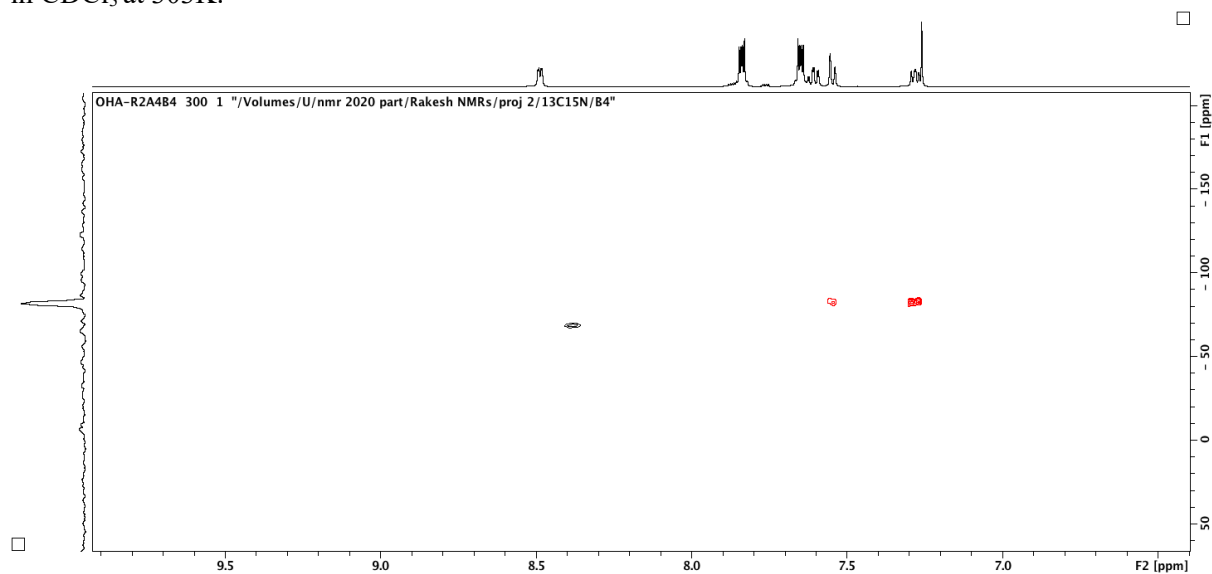


Figure S73. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NIP-**4** in red contour in CDCl_3 at 303K.

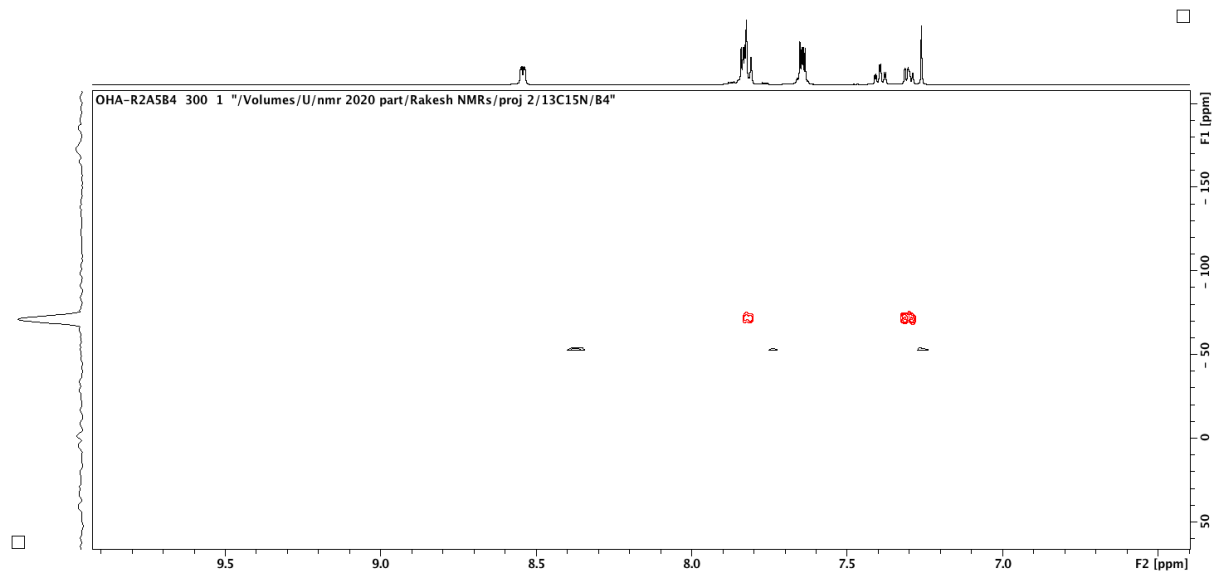


Figure S74. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex NIP-**5** in red contour in CDCl_3 at 303K.

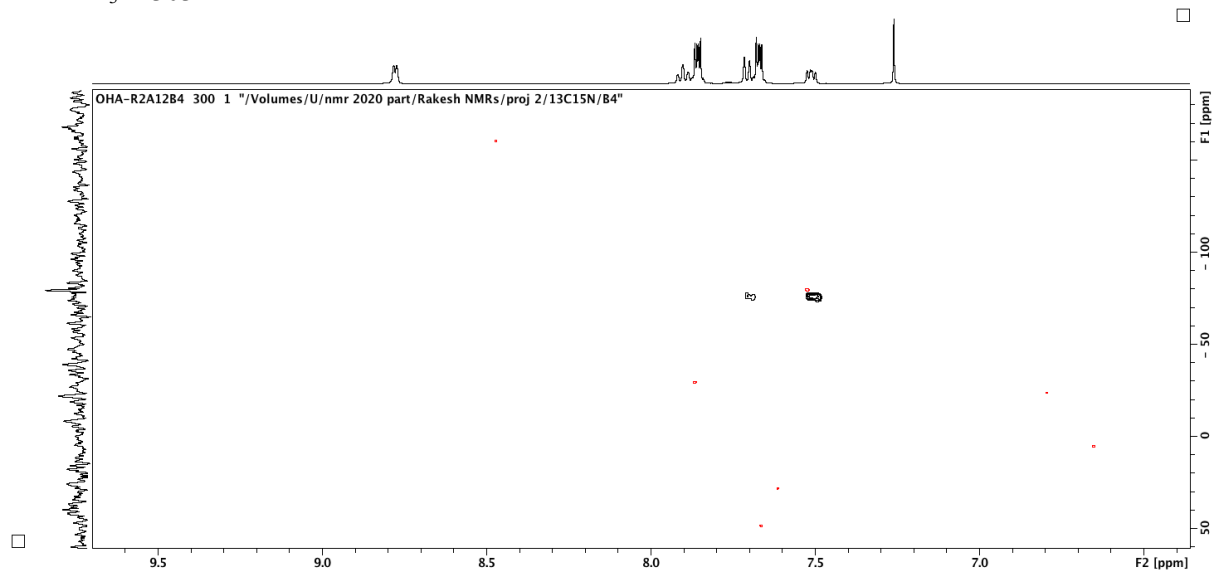


Figure S75. ^1H - ^{15}N HMBC-NMR Spectra of Compound **6** in black contour and 1:1 complex NIP-**6** in red contour in CDCl_3 at 303K.

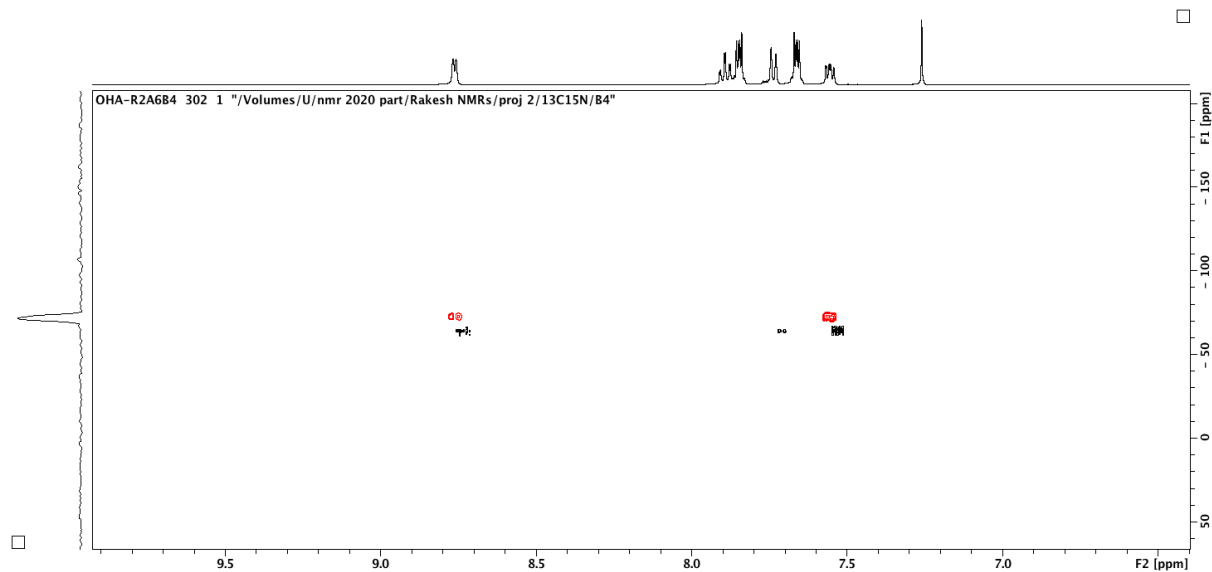


Figure S76. ^1H - ^{15}N HMBC-NMR Spectra of Compound **7** in black contour and 1:1 complex NIP-**7** in red contour in CDCl_3 at 303K.

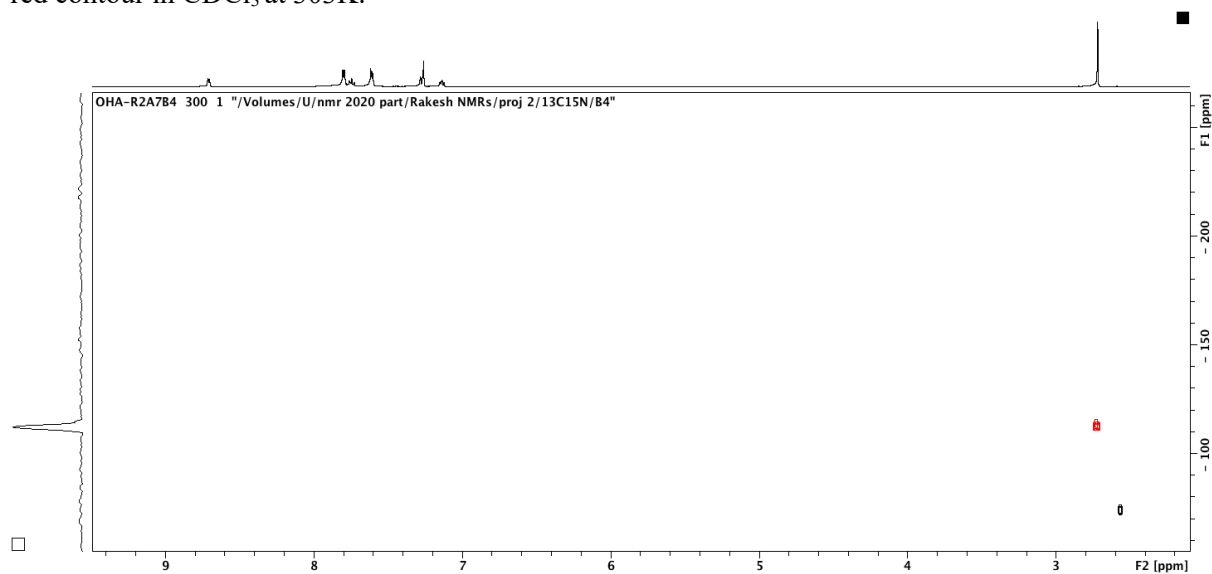


Figure S77. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NIP-**8** in red contour in CDCl_3 at 303K.

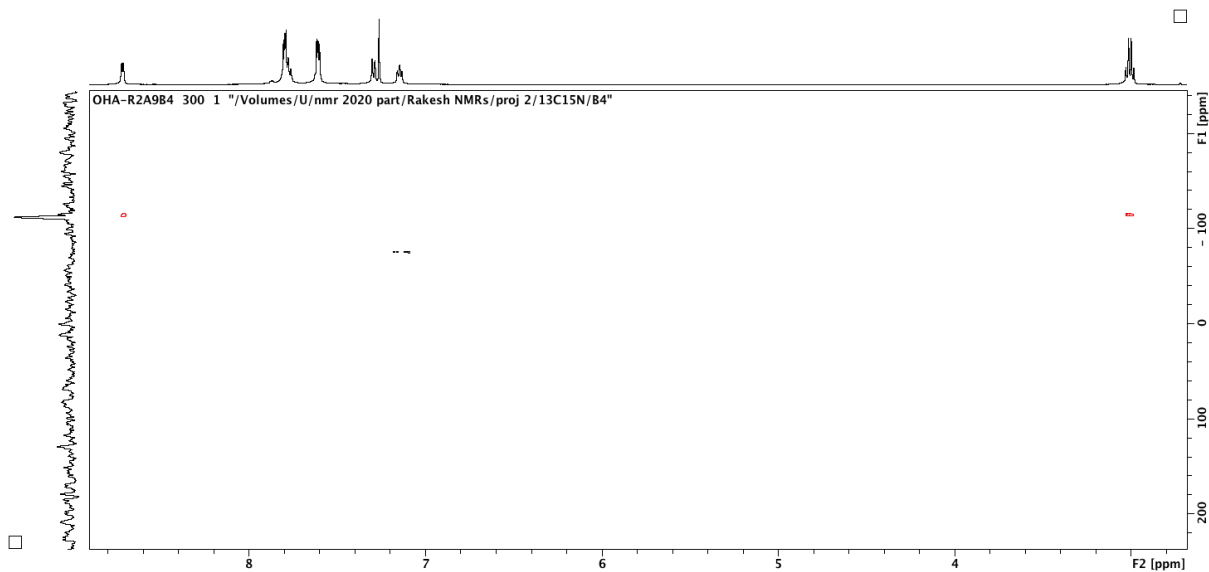


Figure S78. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NIP-**9** in red contour in CDCl_3 at 303K.

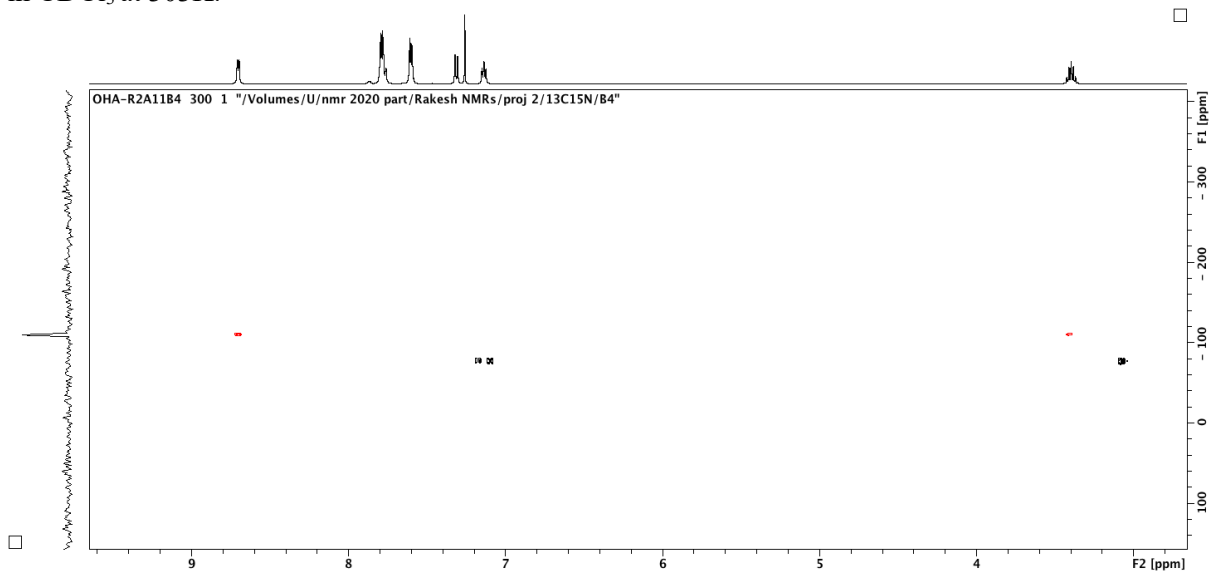


Figure S79. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NIP-**10** in red contour in CDCl_3 at 303K.

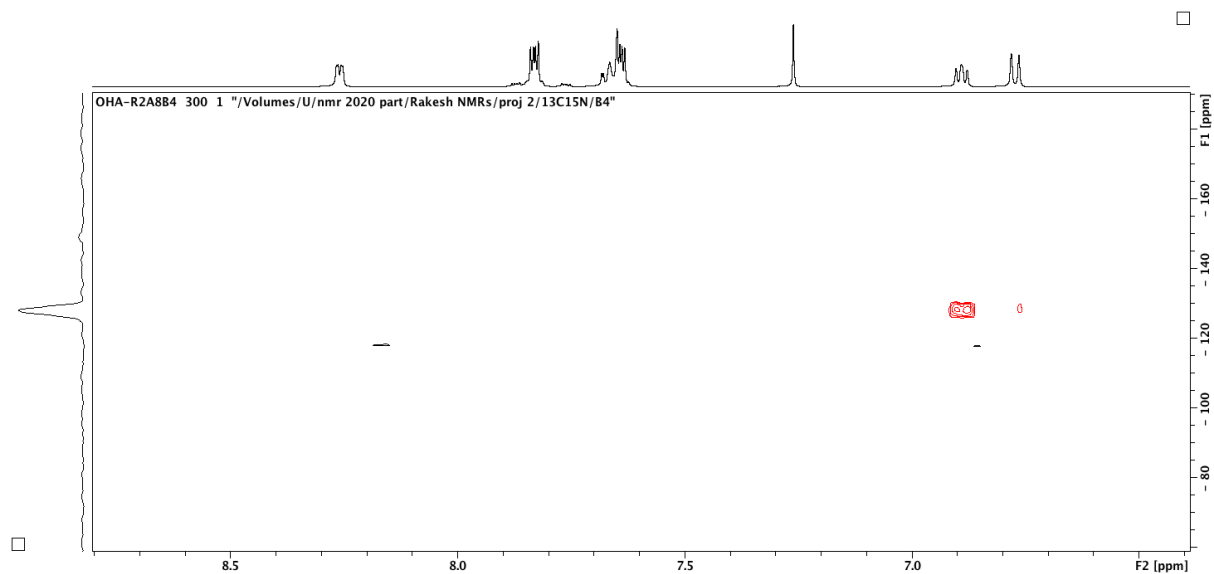


Figure S80. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NIP-**11** in red contour in CDCl_3 at 303K.

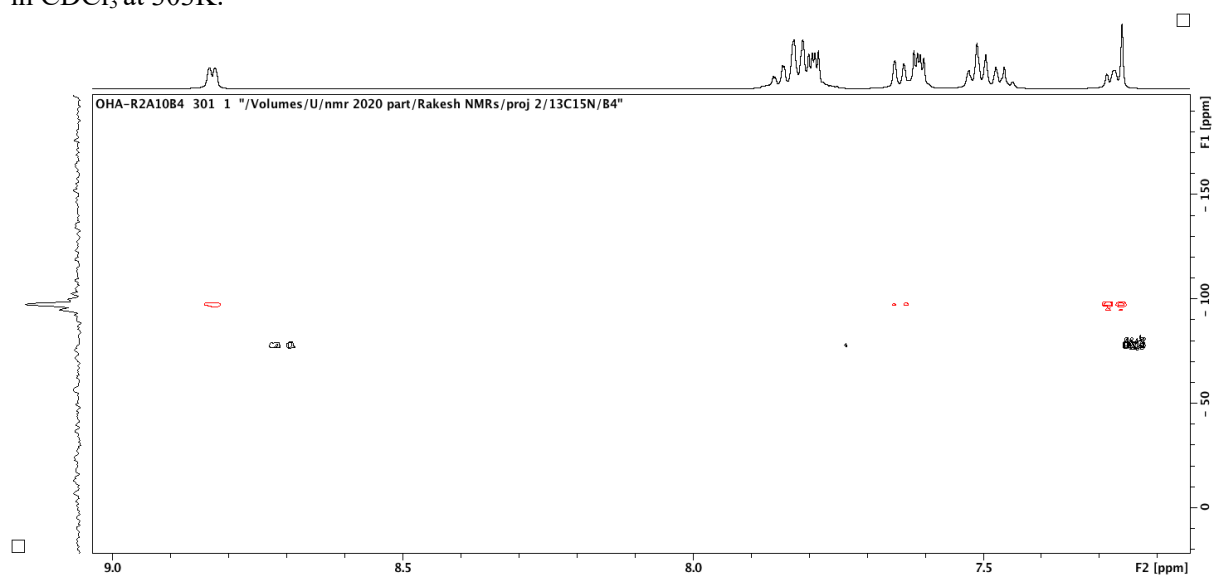


Figure S81. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour and 1:1 complex NIP-**12** in red contour in CDCl_3 at 303K.

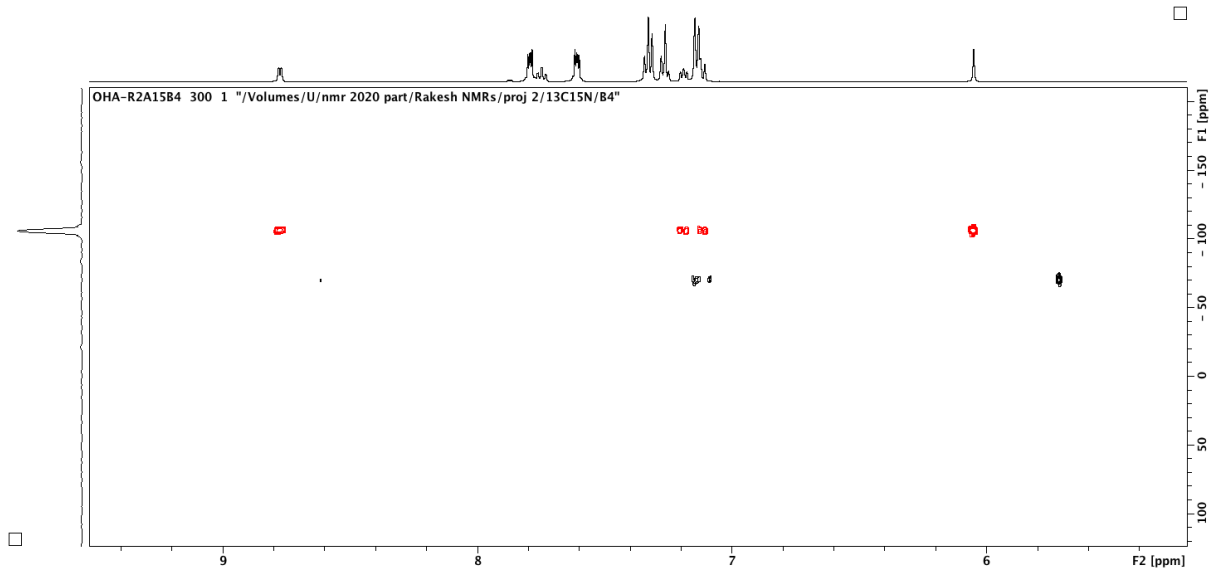


Figure S82. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NIP-**13** in red contour in CDCl_3 at 303K.

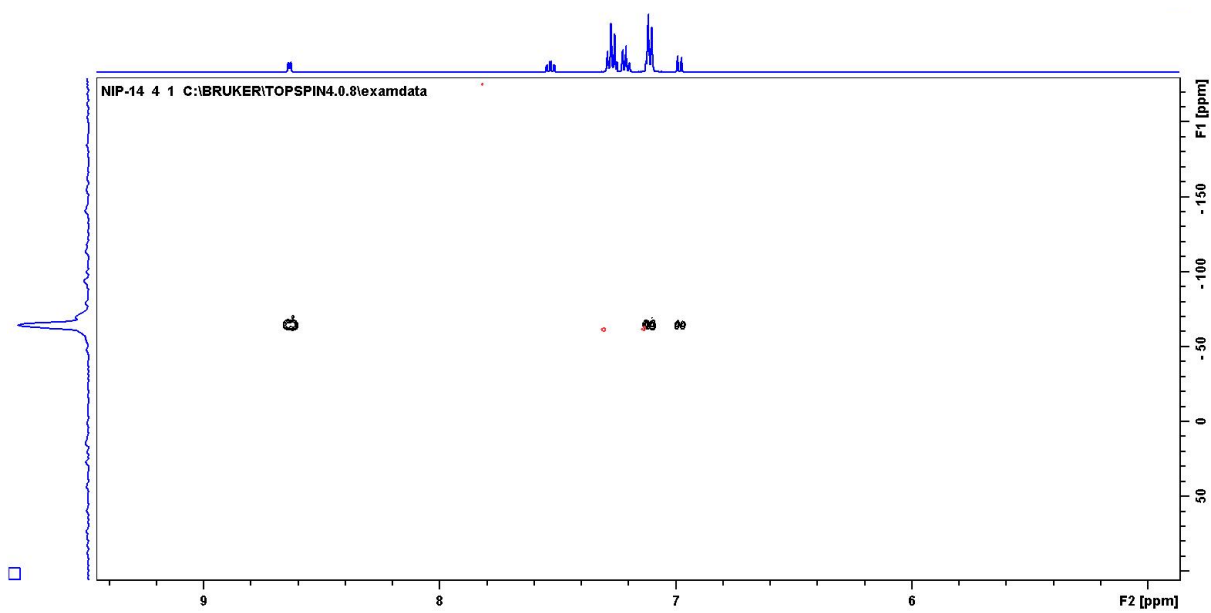


Figure S83. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NIP-**14** in red contour in CDCl_3 at 303K.

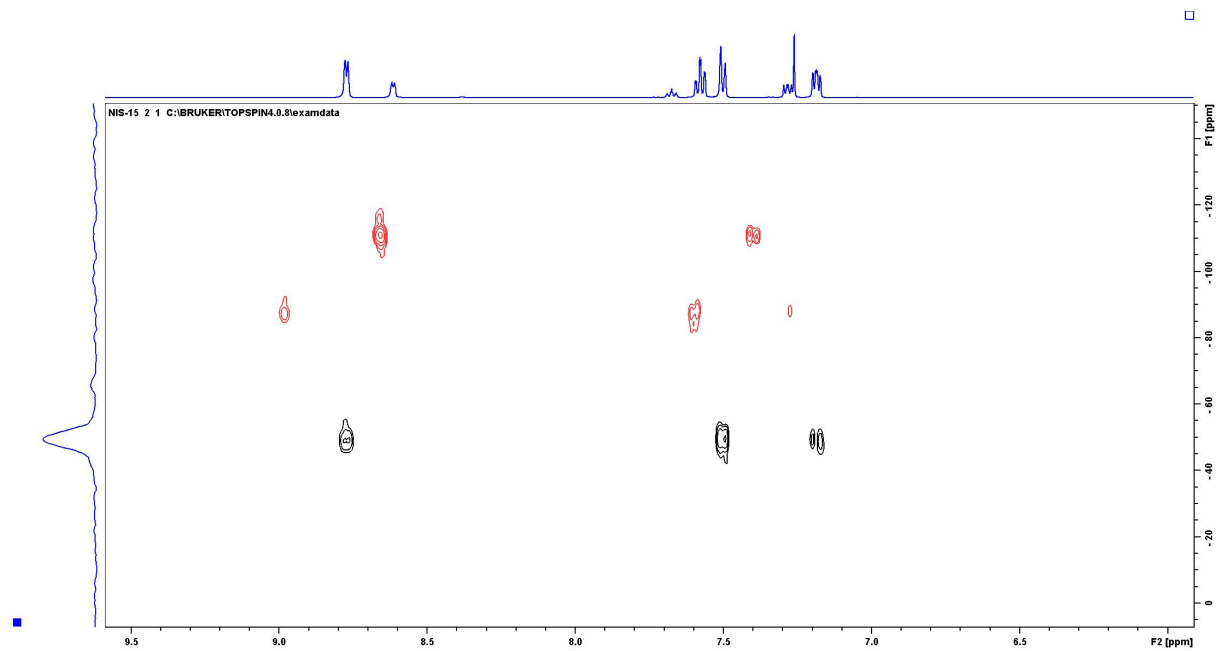


Figure S84. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NIP-**15** in red contour in CDCl_3 at 303K.

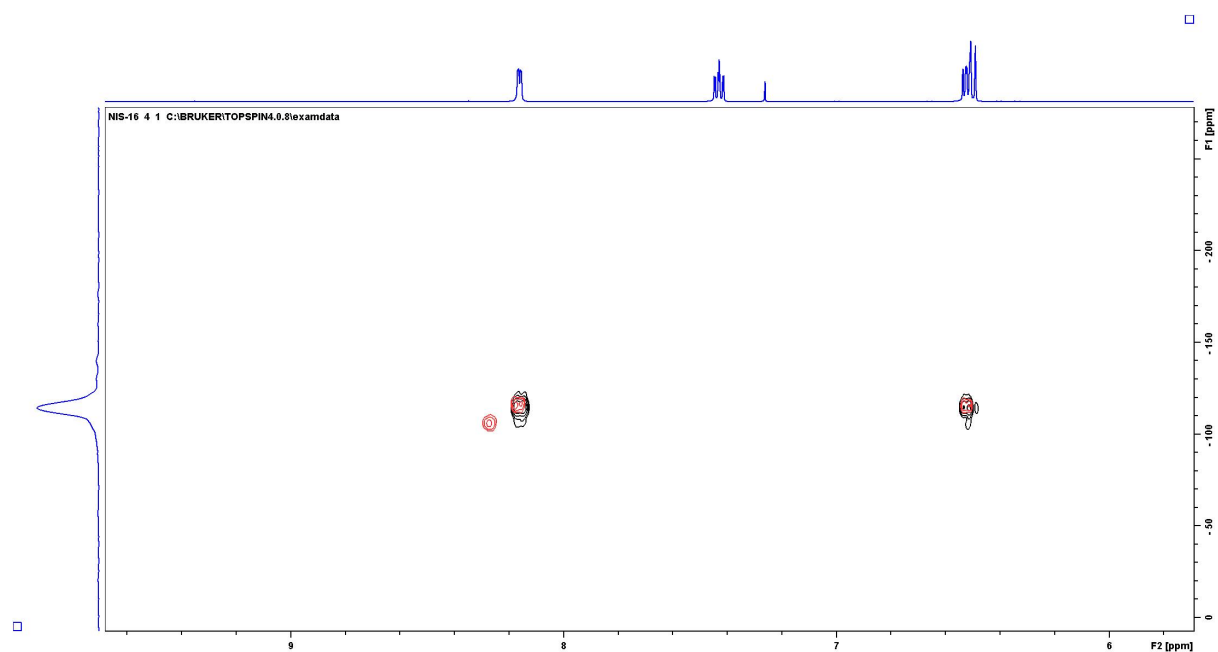


Figure S85. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NIP-**16** in red contour in CDCl_3 at 303K.

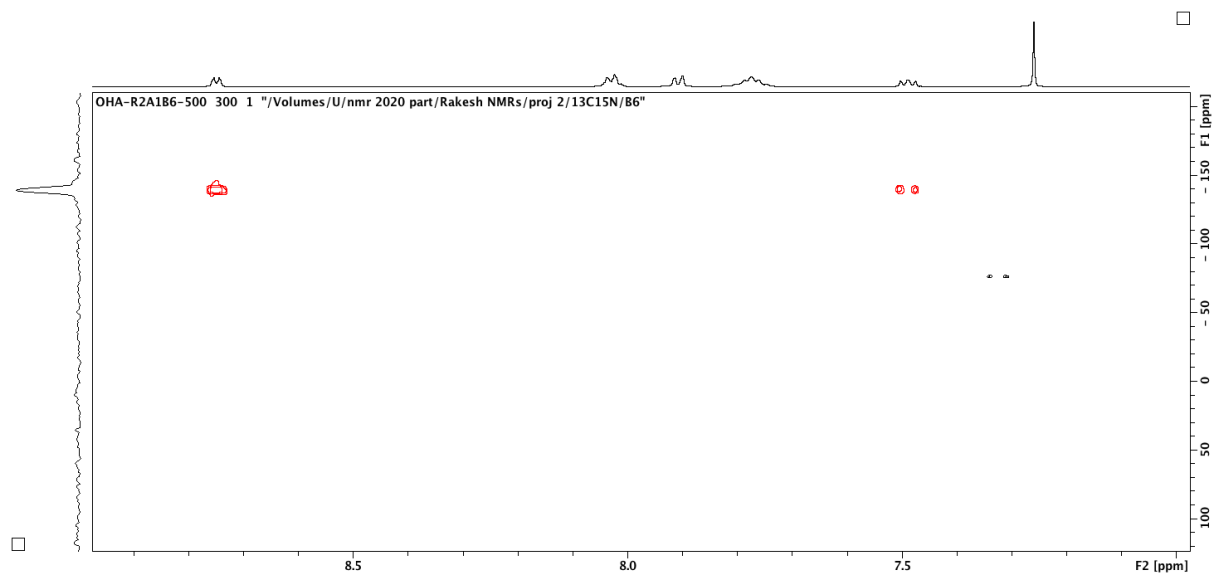


Figure S86. ^1H - ^{15}N HMBC-NMR Spectra of **1** in black contour and 1:1 complex NISac-1 in red contour in CDCl_3 at 303K.

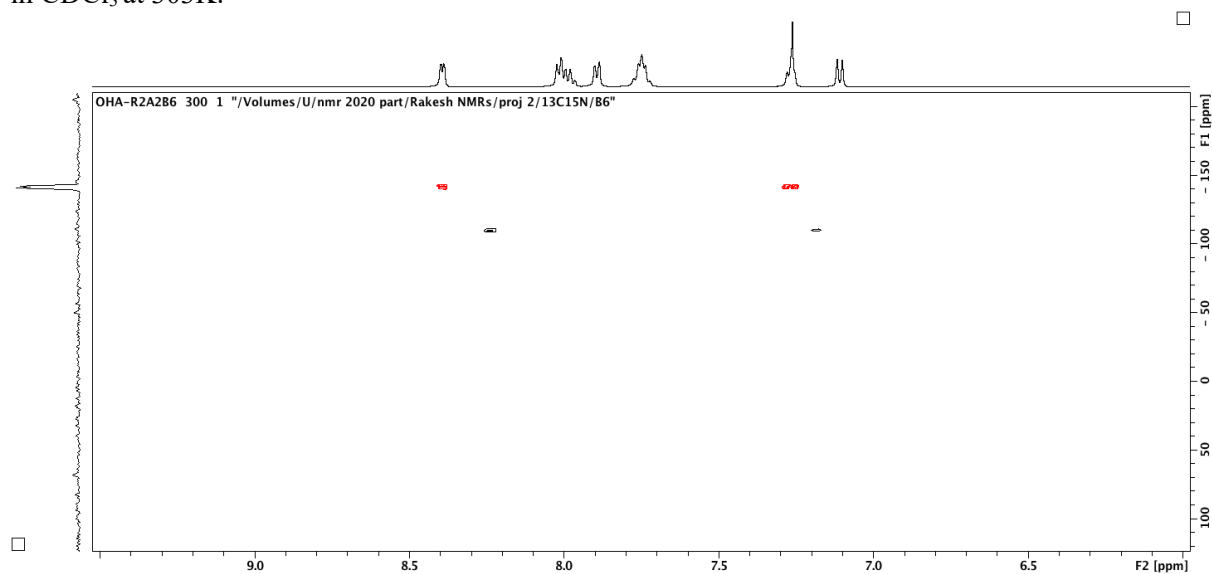


Figure S87. ^1H - ^{15}N HMBC-NMR Spectra of **2** in black contour and 1:1 complex NISac-2 in red contour in CDCl_3 at 303K.

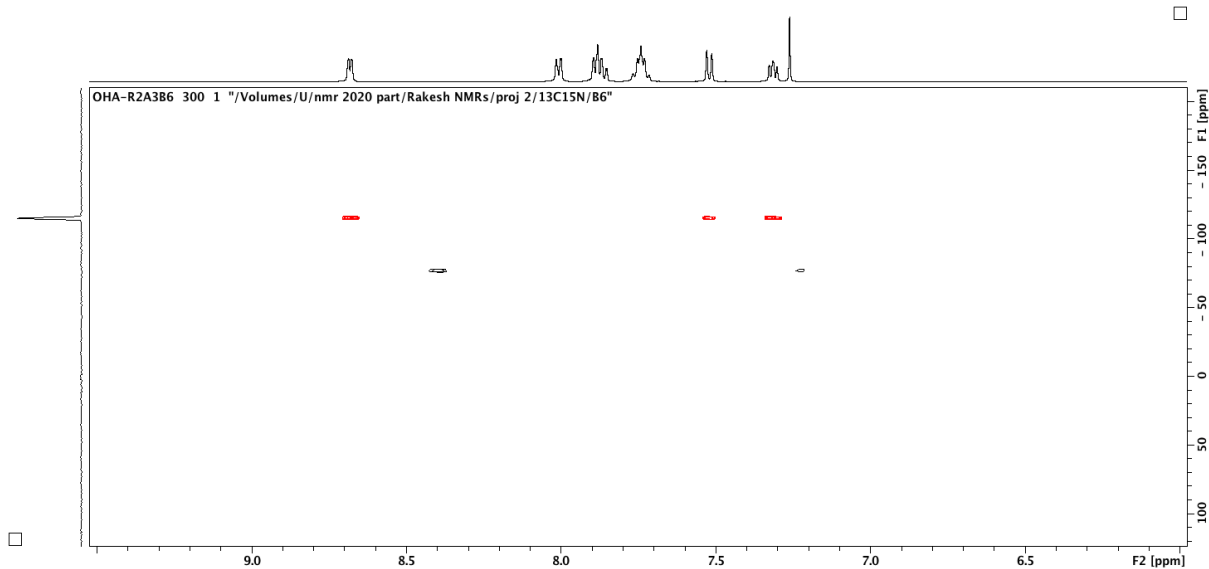


Figure S88. ^1H - ^{15}N HMBC-NMR Spectra of **3** in black contour and 1:1 complex NISac-**3** in red contour in CDCl_3 at 303K.

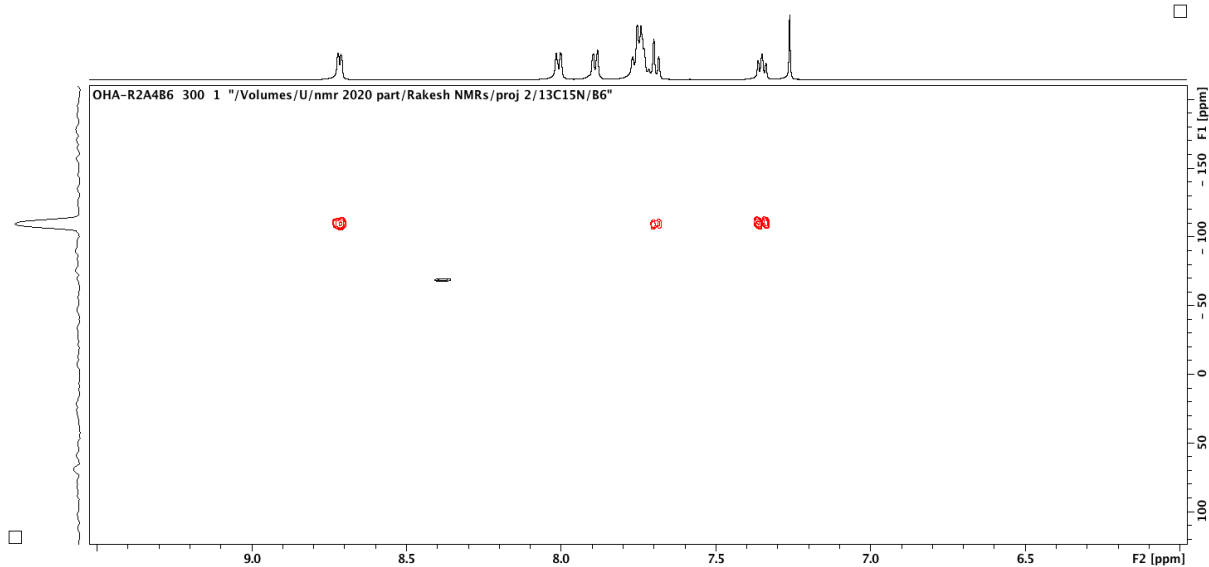


Figure S89. ^1H - ^{15}N HMBC-NMR Spectra of **4** in black contour and 1:1 complex NISac-**4** in red contour in CDCl_3 at 303K.

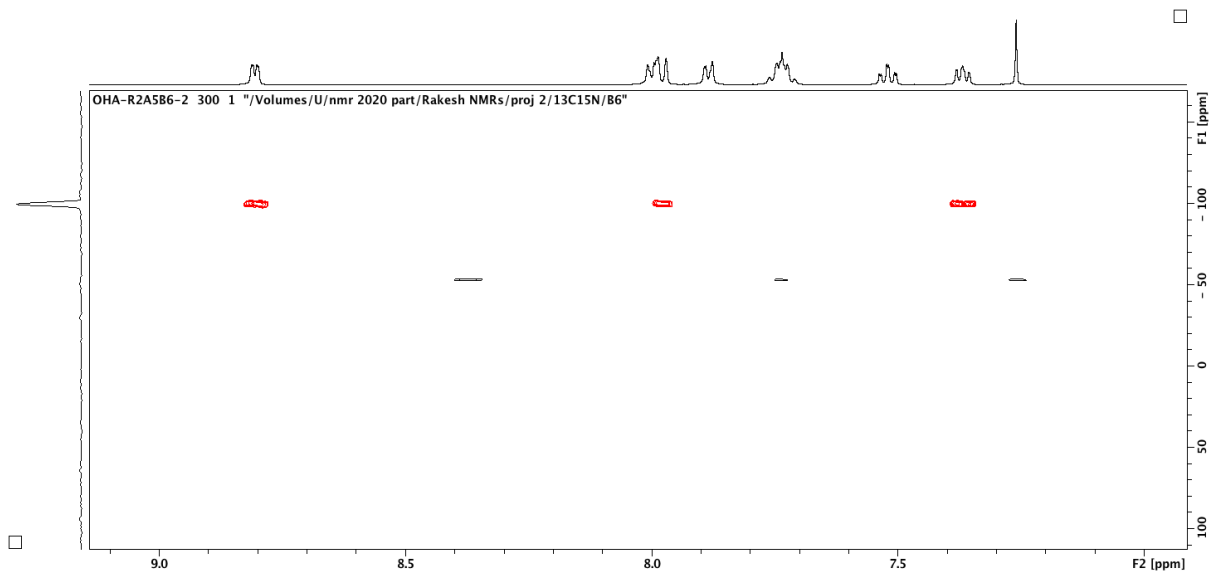


Figure S90. ^1H - ^{15}N HMBC-NMR Spectra of **5** in black contour and 1:1 complex **NISac-5** in red contour in CDCl_3 at 303K.

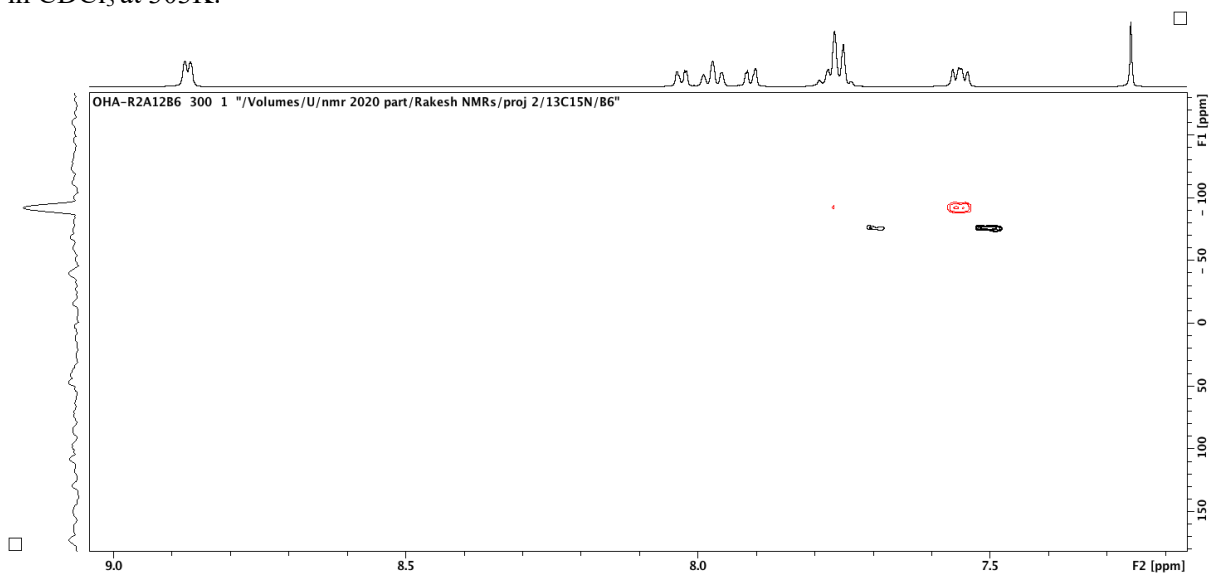


Figure S91. ^1H - ^{15}N HMBC-NMR Spectra of **6** in black contour and 1:1 complex **NISac-6** in red contour in CDCl_3 at 303K.

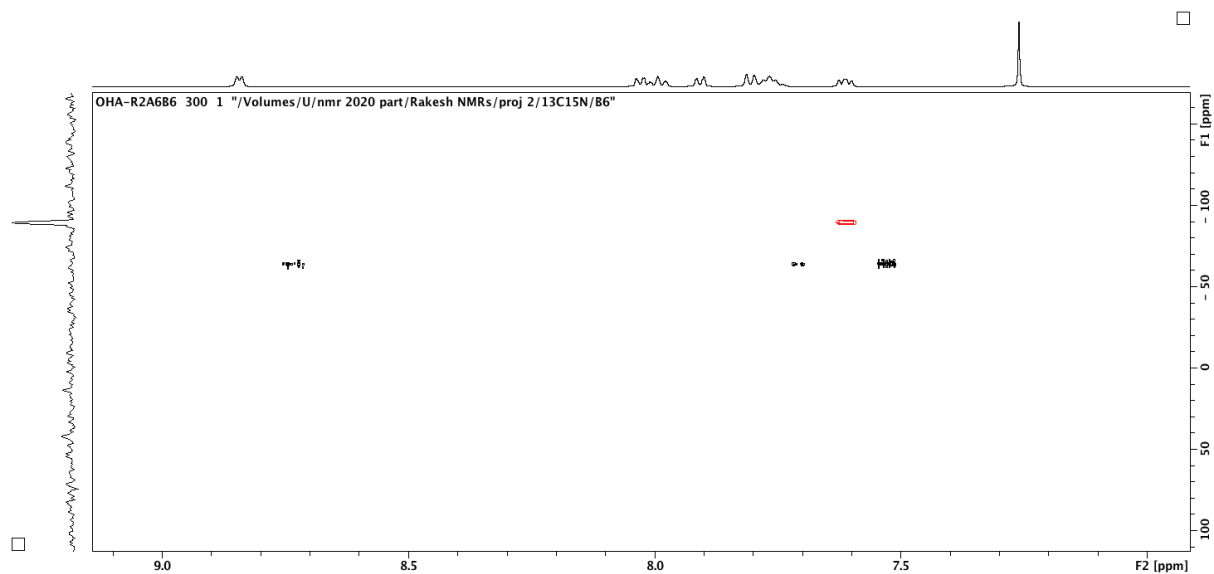


Figure S92. ^1H - ^{15}N HMBC-NMR Spectra of **7** in black contour and 1:1 complex NISac-**7** in red contour in CDCl_3 at 303K.

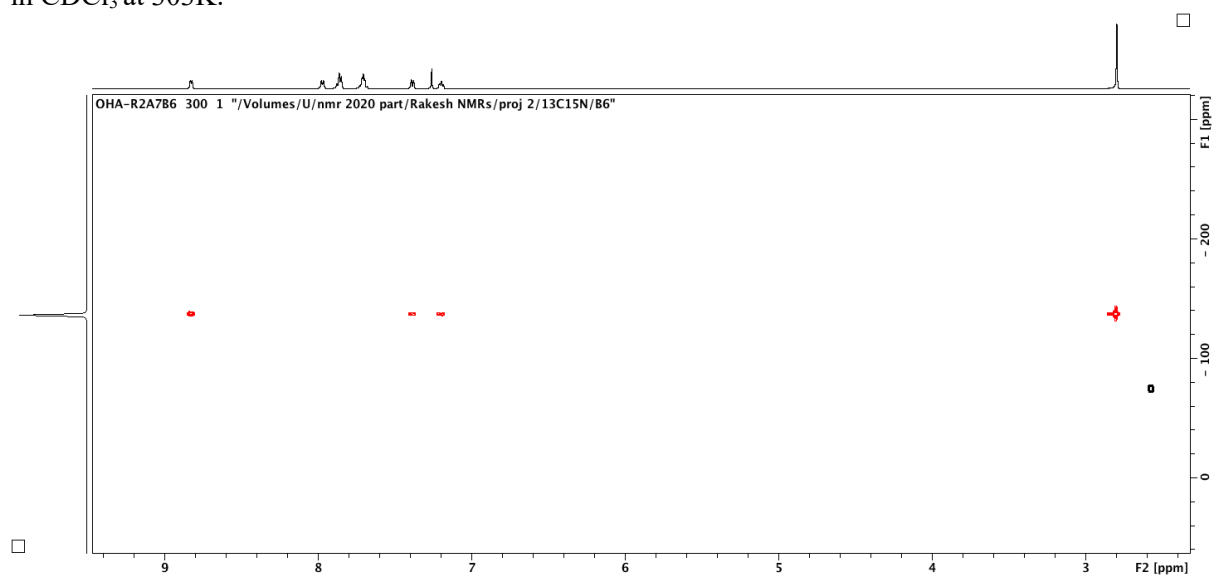


Figure S93. ^1H - ^{15}N HMBC-NMR Spectra of **8** in black contour and 1:1 complex NISac-**8** in red contour in CDCl_3 at 303K.

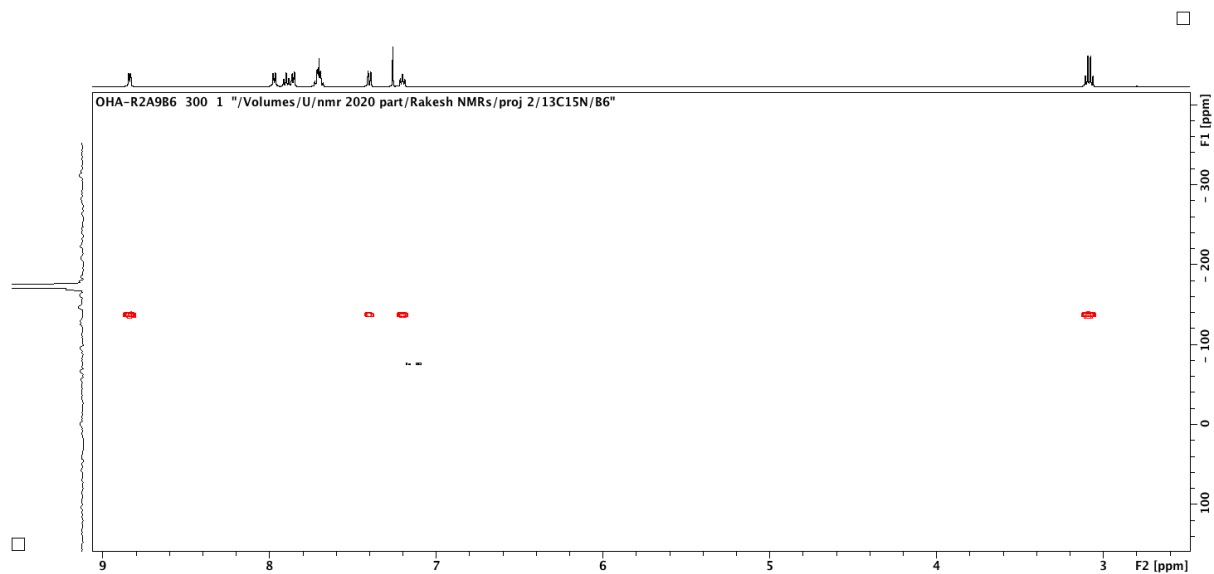


Figure S94. ^1H - ^{15}N HMBC-NMR Spectra of **9** in black contour and 1:1 complex NISac-**9** in red contour in CDCl_3 at 303K.

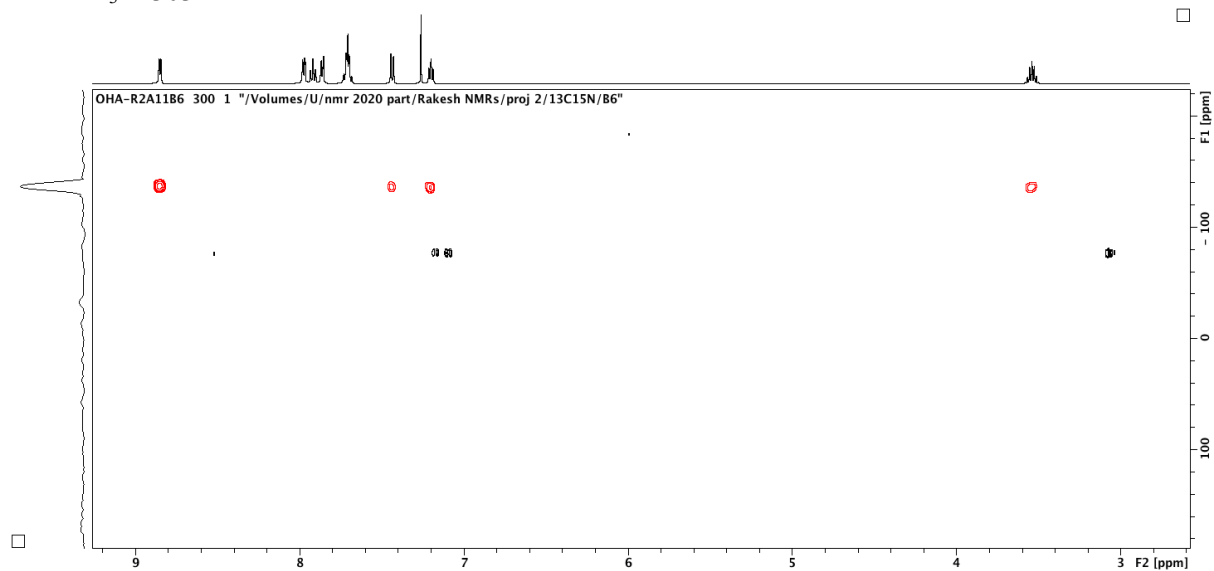


Figure S95. ^1H - ^{15}N HMBC-NMR Spectra of **10** in black contour and 1:1 complex NISac-**10** in red contour in CDCl_3 at 303K.

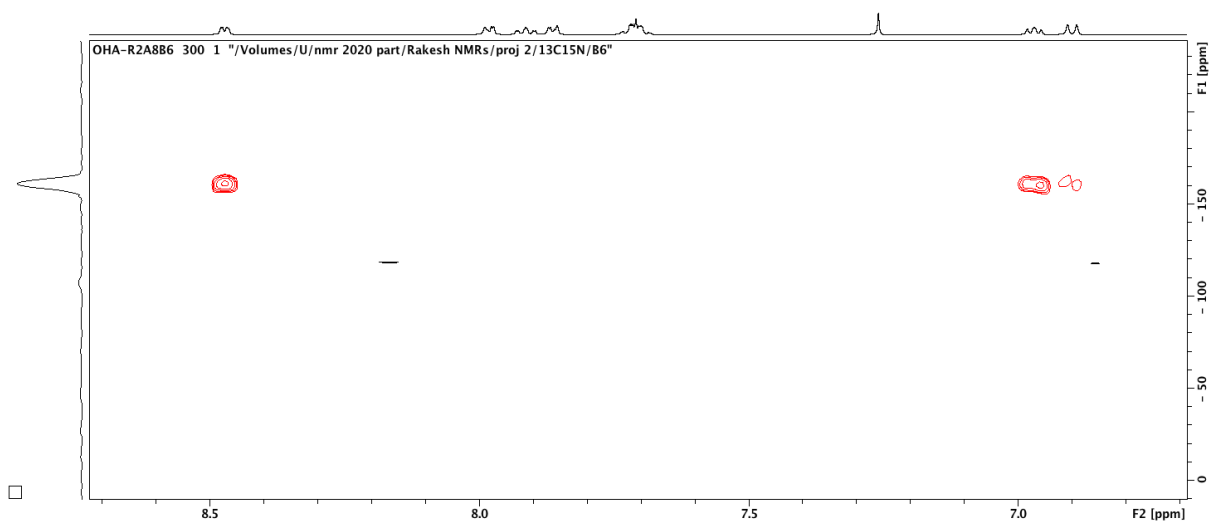


Figure S96. ^1H - ^{15}N HMBC-NMR Spectra of **11** in black contour and 1:1 complex NISac-**11** in red contour in CDCl_3 at 303K.

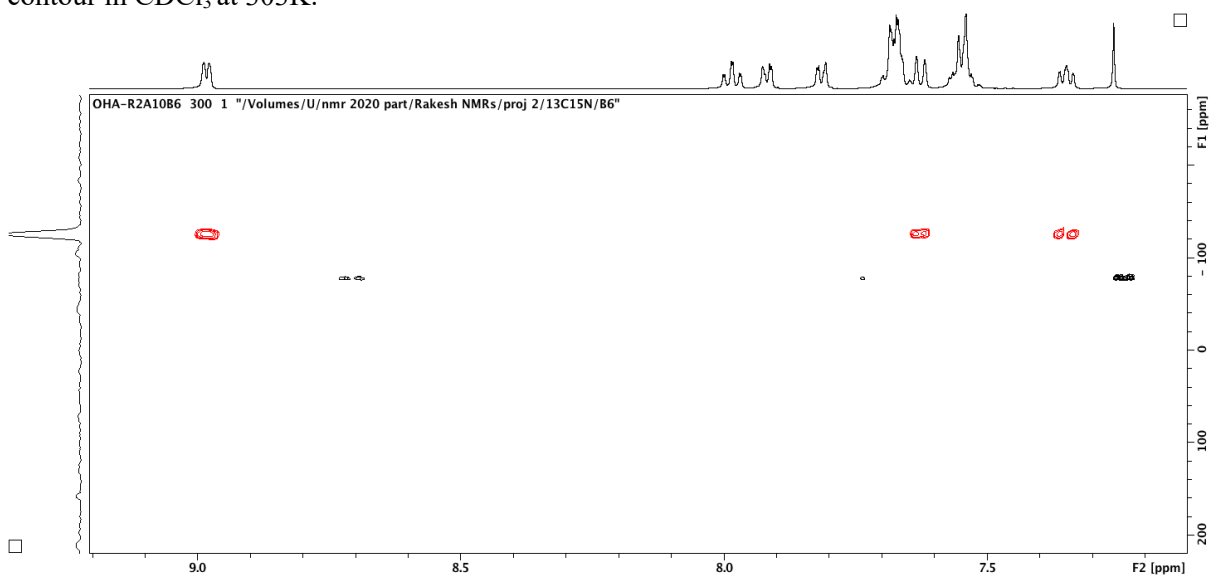


Figure S97. ^1H - ^{15}N HMBC-NMR Spectra of **12** in black contour 1:1 complex NISac-**12** in red contour in CDCl_3 at 303K.

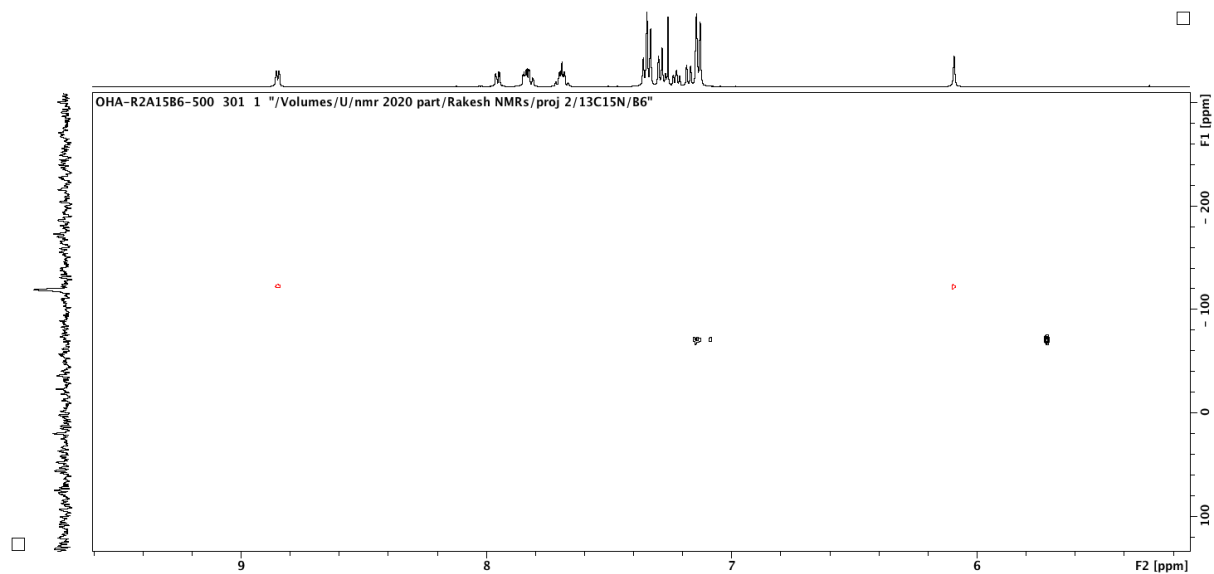


Figure S98. ^1H - ^{15}N HMBC-NMR Spectra of **13** in black contour and 1:1 complex NISac-**13** in red contour in CDCl_3 at 303K.

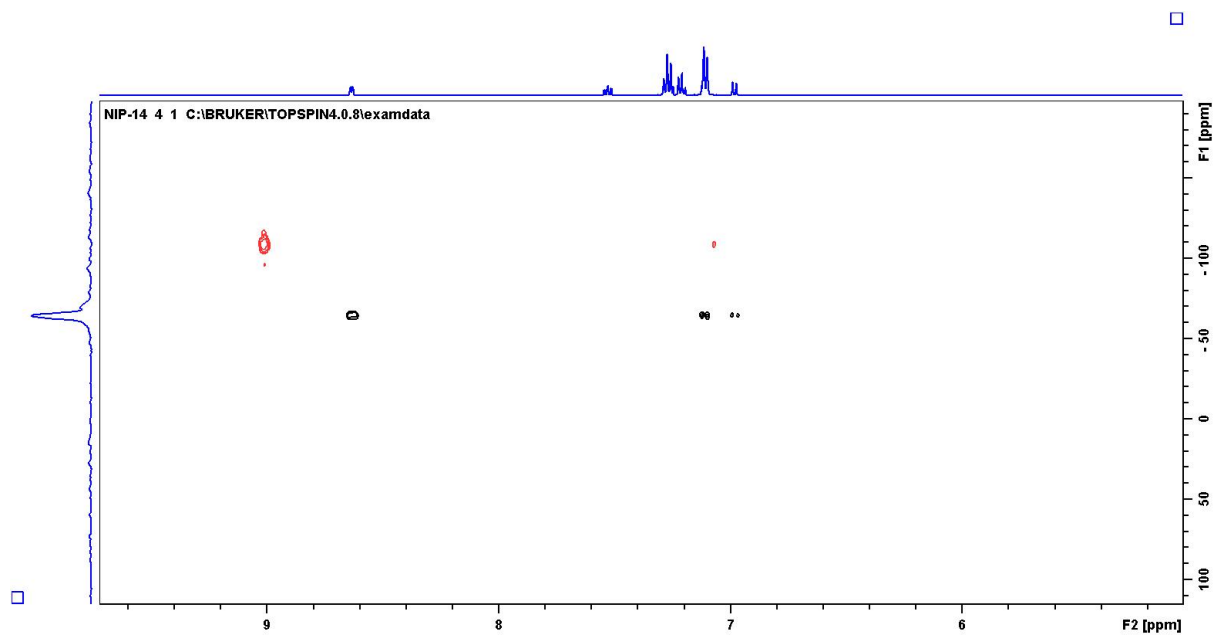


Figure S99. ^1H - ^{15}N HMBC-NMR Spectra of **14** in black contour and 1:1 complex NISac-**14** in red contour in CDCl_3 at 303K.

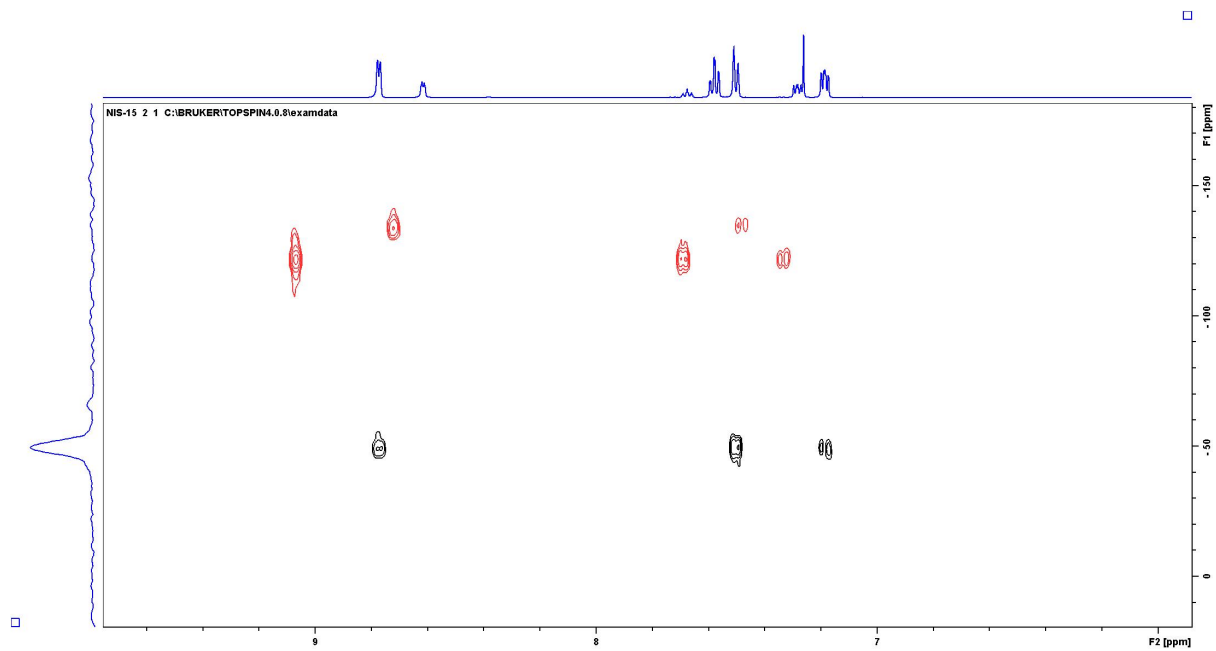


Figure S100. ^1H - ^{15}N HMBC-NMR Spectra of **15** in black contour and 1:1 complex NISac-**15** in red contour in CDCl_3 at 303K.

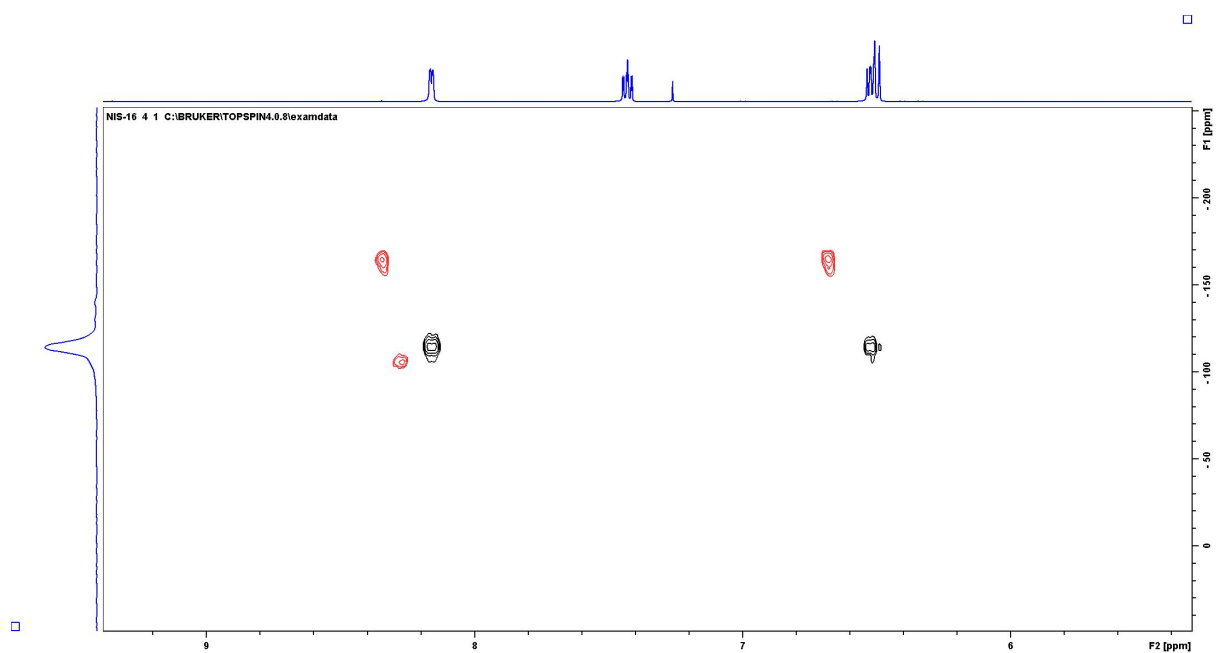
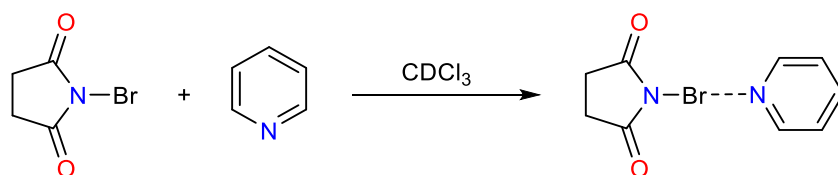


Figure S101. ^1H - ^{15}N HMBC-NMR Spectra of **16** in black contour and 1:1 complex NISac-**16** in red contour in CDCl_3 at 303K.

6. Solution ¹H NMR association constants in CDCl₃

6.1. ¹H Titration experiments for NBS-Z

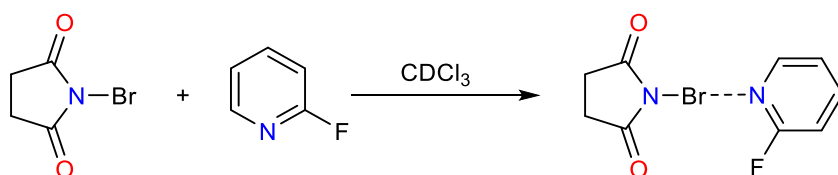
6.1.1. ¹H Titration experiments for NBS-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 4.02 M ⁻¹ | ± 1.0153% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

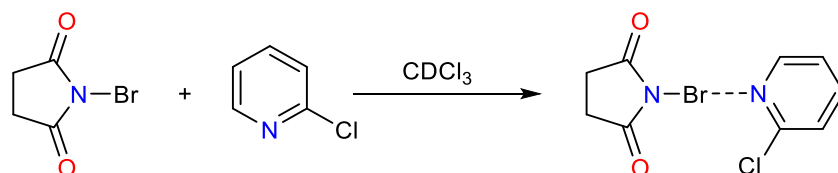
6.1.2. ¹H Titration experiments for NBS-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.14 M ⁻¹ | ± 1.7155% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

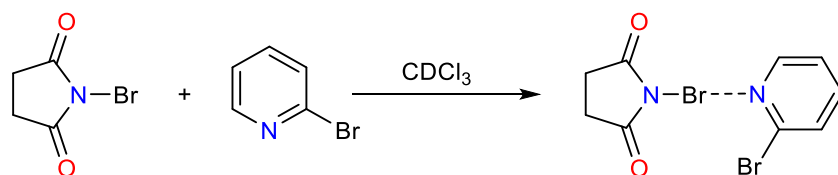
6.1.3. ¹H Titration experiments for NBS-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.93 M ⁻¹ | ± 4.2996% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

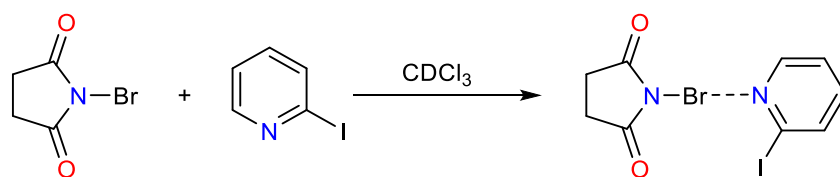
6.1.4. ¹H Titration experiments for NBS-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|-----------|----------------------|
| K (0 → ∞) | 9.31 e-5 M ⁻¹ | ± 0.6538% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

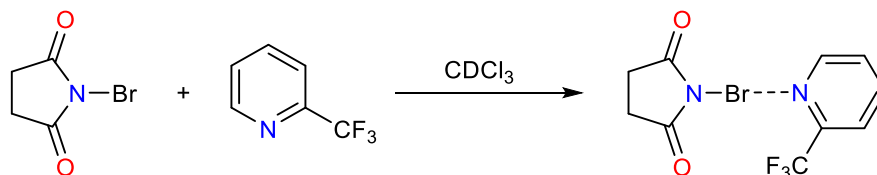
6.1.5. ¹H Titration experiments for NBS-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|--------------|----------------------|
| K (0 → ∞) | 1.85 e-5 M ⁻¹ | ± 3.8367e-3% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

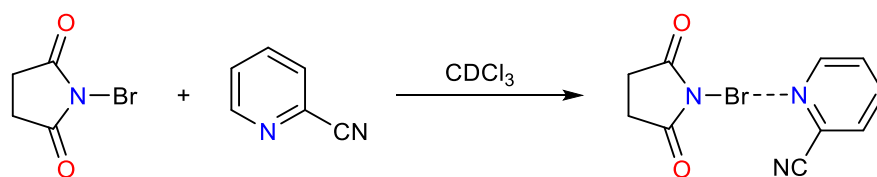
6.1.6. ¹H Titration experiments for NBS-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.02 M ⁻¹ | ± 2.8176% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

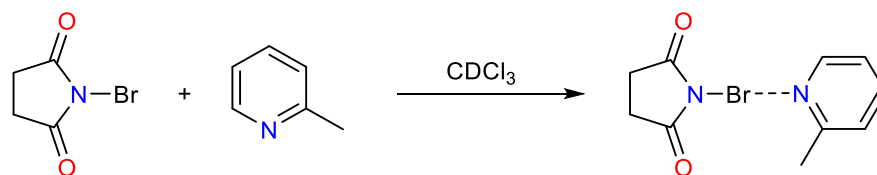
6.1.7. ¹H Titration experiments for NBS-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.29 M ⁻¹ | ± 3.0793% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

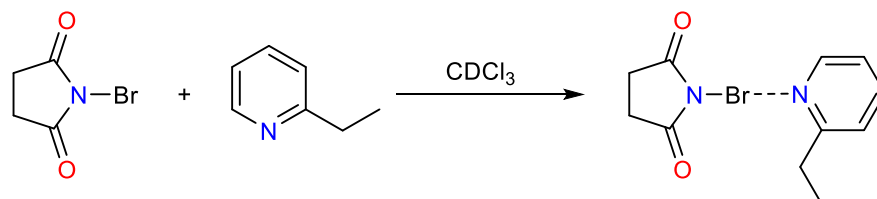
6.1.8. ¹H Titration experiments for NBS-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 5.40 M ⁻¹ | ± 0.3821% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

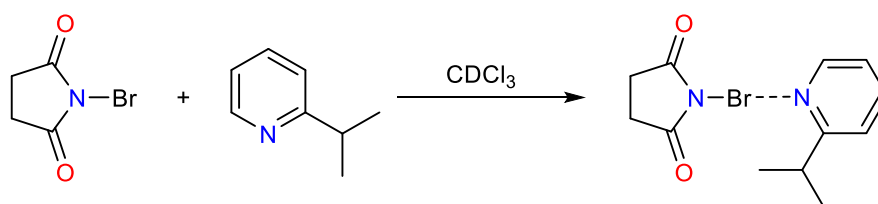
6.1.9. ¹H Titration experiments for NBS-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 4.26 M ⁻¹ | ± 0.7283% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

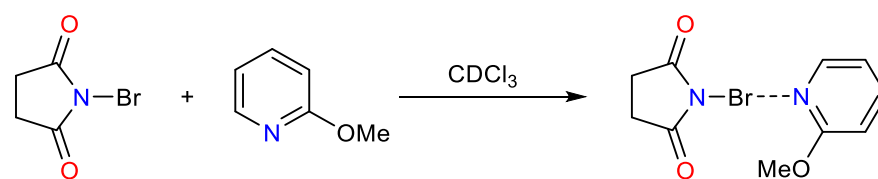
6.1.10. ¹H Titration experiments for NBS-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.16 M ⁻¹ | ± 0.3106% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

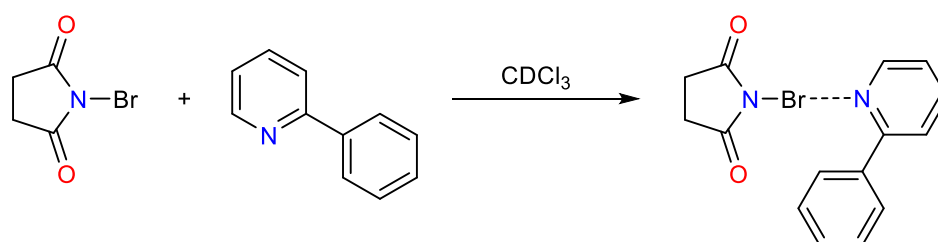
6.1.11. ¹H Titration experiments for NBS-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.54 M ⁻¹ | ± 1.9841% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

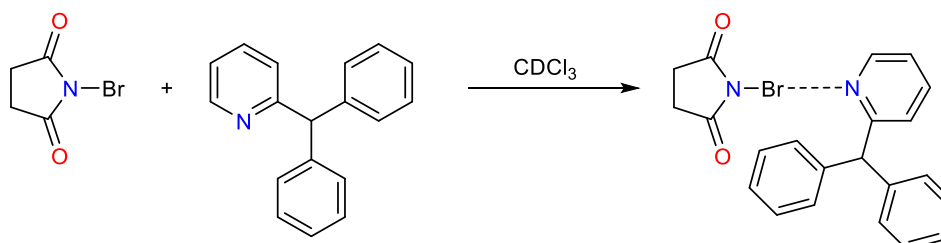
6.1.12. ¹H Titration experiments for NBS-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 3.60e-2 M ⁻¹ | ± 0.6035% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

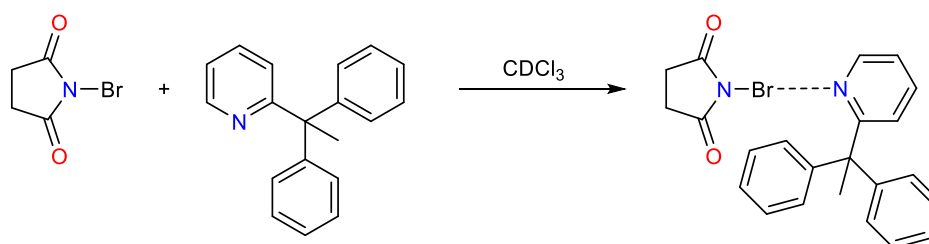
6.1.13. ¹H Titration experiments for NBS-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.56 M ⁻¹ | ± 0.5826% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

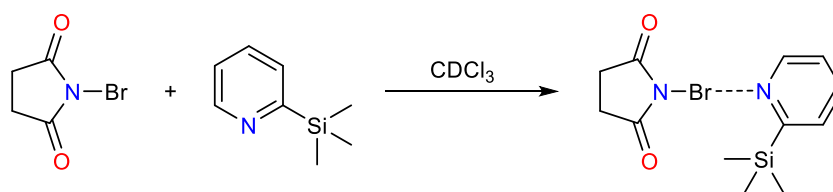
6.1.14. ¹H Titration experiments for NBS-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.56 M ⁻¹ | ± 0.5826% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.1.15. ¹H Titration experiments for NBS-15^a

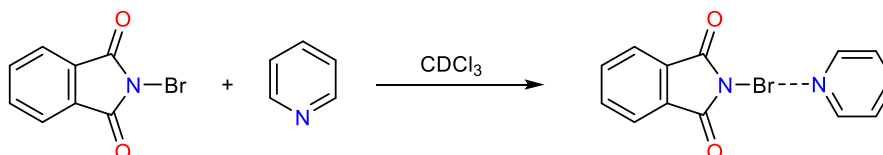


| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.51 M ⁻¹ | ± 0.3821% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.2. ¹H Titration experiments for NBP-Z

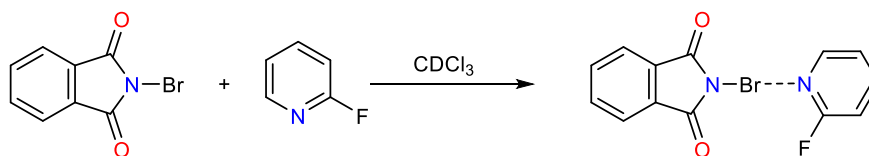
6.2.1. ¹H Titration experiments for NBP-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.34 M ⁻¹ | ± 0.3782% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

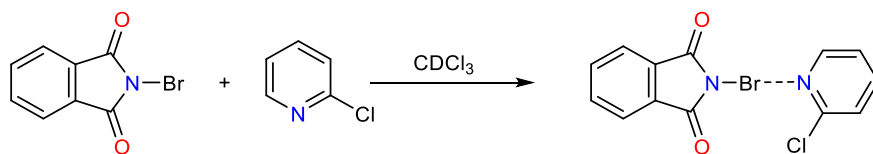
6.2.2. ¹H Titration experiments for NBP-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 1.59e-4 M ⁻¹ | ± 0.7428% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

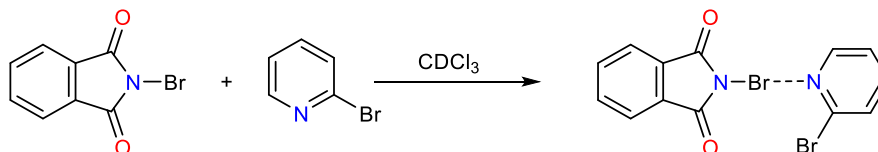
6.2.3. ¹H Titration experiments for NBP-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 1.22e-4 M ⁻¹ | ± 0.2997% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

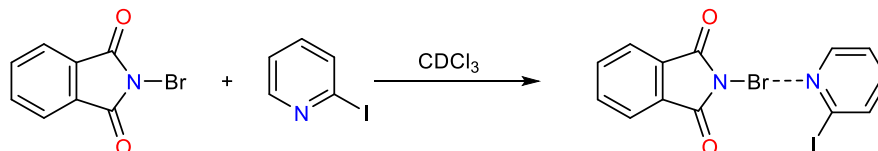
6.2.4. ¹H Titration experiments for NBP-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.25 M ⁻¹ | ± 0.6637% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

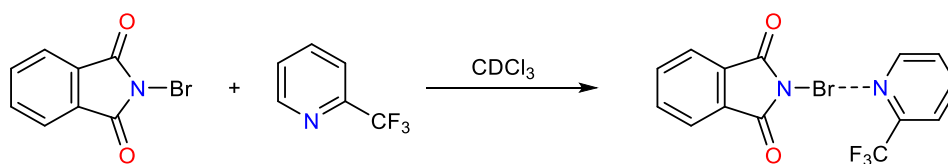
6.2.5. ¹H Titration experiments for NBP-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1.10e-4 M ⁻¹ | ± 0.0873% | 1.00e-4 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.2.6. ¹H Titration experiments for NBP-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1.02e-4 M ⁻¹ | ± 0.1388% | 1.00e-4 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.2.7. ¹H Titration experiments for NBP-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 1.71e-4 M ⁻¹ | ± 1.2154% | 0.10 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

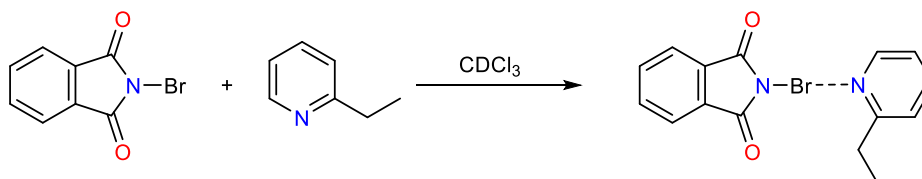
6.2.8. ¹H Titration experiments for NBP-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 3.98 M ⁻¹ | ± 0.1659% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

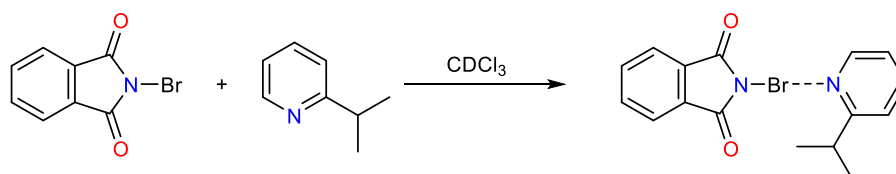
6.2.9. ¹H Titration experiments for NBP-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.76 M ⁻¹ | ± 0.3071% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

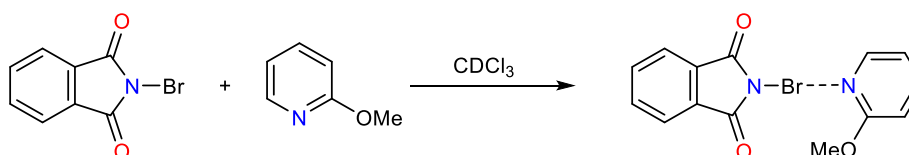
6.2.10. ¹H Titration experiments for NBP-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.44 M ⁻¹ | ± 0.1446% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

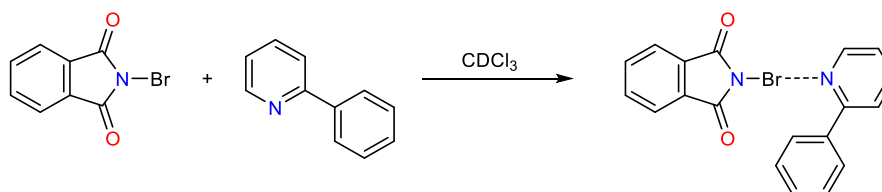
6.2.11. ¹H Titration experiments for NBP-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 9.80e-5 M ⁻¹ | ± 0.0838% | 0.10 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

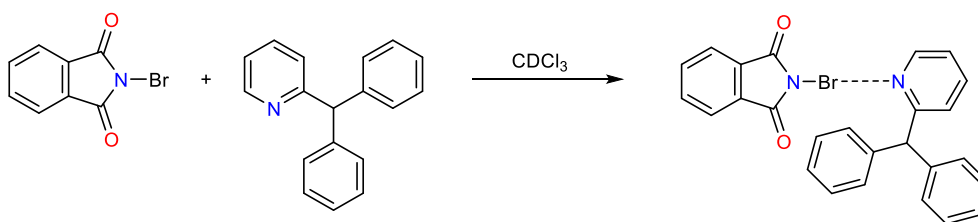
6.2.12. ¹H Titration experiments for NBP-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 7.63e-5 M ⁻¹ | ± 0.1360% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

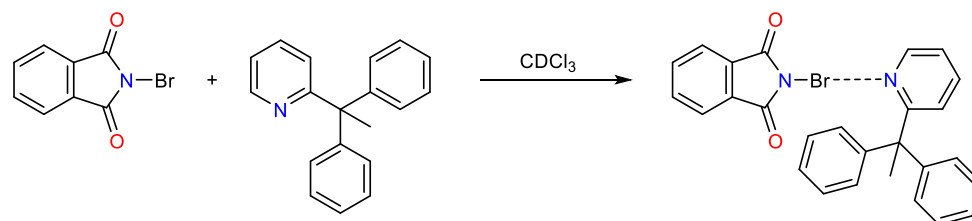
6.2.13. ¹H Titration experiments for NBP-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.73 M ⁻¹ | ± 0.5241% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

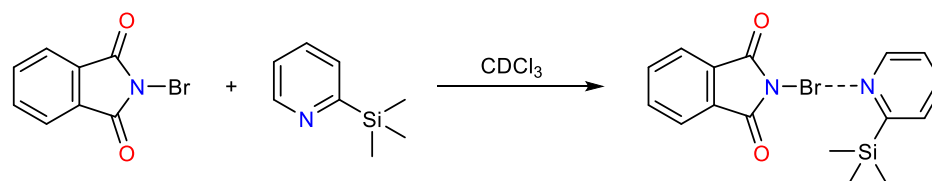
6.2.14. ¹H Titration experiments for NBP-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.73 M ⁻¹ | ± 0.5241% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.2.15. ¹H Titration experiments for NBP-15^a

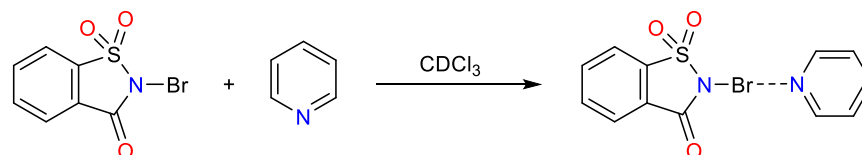


| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.86 M ⁻¹ | ± 0.2434% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.3. ¹H Titration experiments for NBSac-Z (1-15)

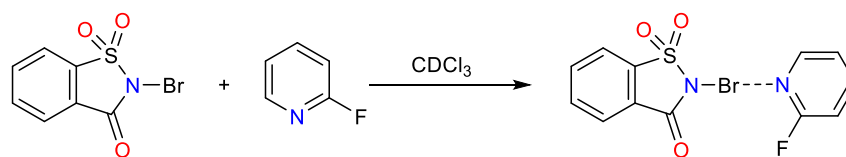
6.3.1. ¹H Titration experiments for NBSac-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 423.78 M ⁻¹ | ± 4.3343% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

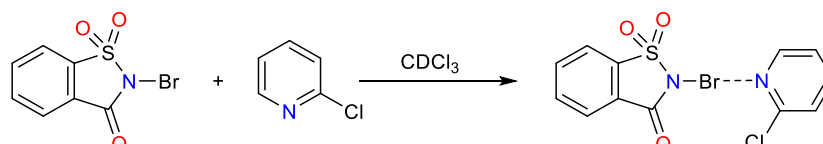
6.3.2. ¹H Titration experiments for NBSac-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 1.17 M ⁻¹ | ± 0.8769% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

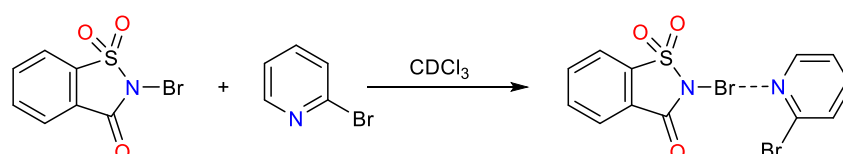
6.3.3. ¹H Titration experiments for NBSac-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 5.31 M ⁻¹ | ± 0.3510% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

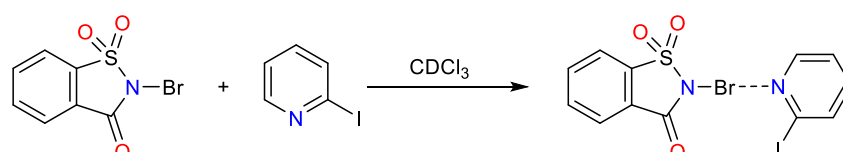
6.3.4. ¹H Titration experiments for NBSac-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 5.03 M ⁻¹ | ± 0.3709% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

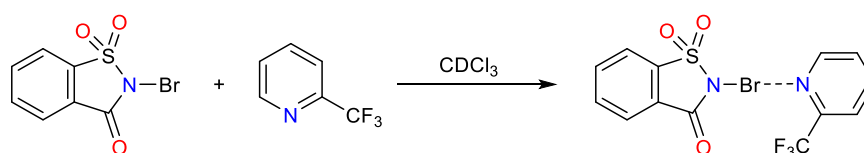
6.3.5. ¹H Titration experiments for NBSac-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 14.29 M ⁻¹ | ± 0.5387% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.3.6. ¹H Titration experiments for NBSac-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.72 M ⁻¹ | ± 1.6387% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

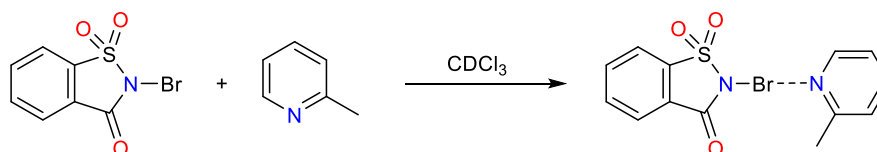
6.3.7. ¹H Titration experiments for NBSac-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.40 M ⁻¹ | ± 0.3756% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

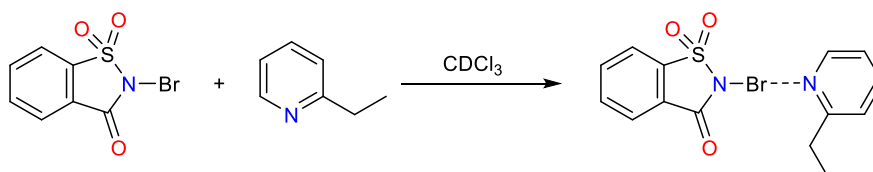
6.3.8. ¹H Titration experiments for NBSac-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 330.50 M ⁻¹ | ± 2.5802% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

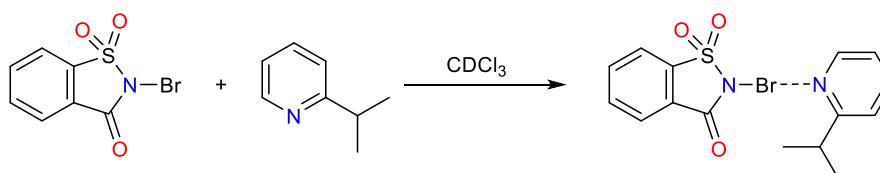
6.3.9. ¹H Titration experiments for NBSac-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 455.41 M ⁻¹ | ± 1.9234% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

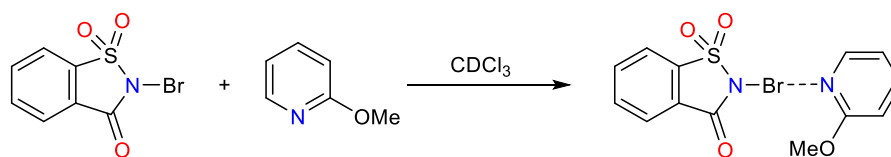
6.3.10. ¹H Titration experiments for NBSac-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|----------------------|
| K (0 → ∞) | 209.79 M ⁻¹ | ± 2.1042% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

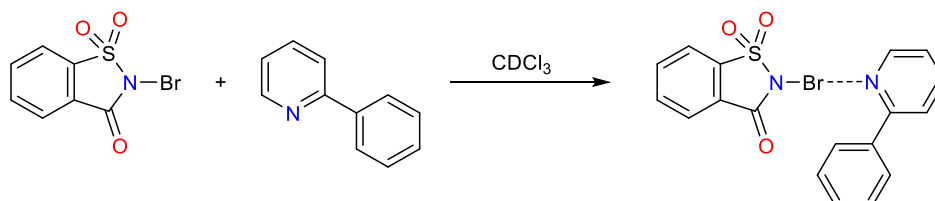
6.3.11. ¹H Titration experiments for NBSac-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 3.67 M ⁻¹ | ± 0.4597% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

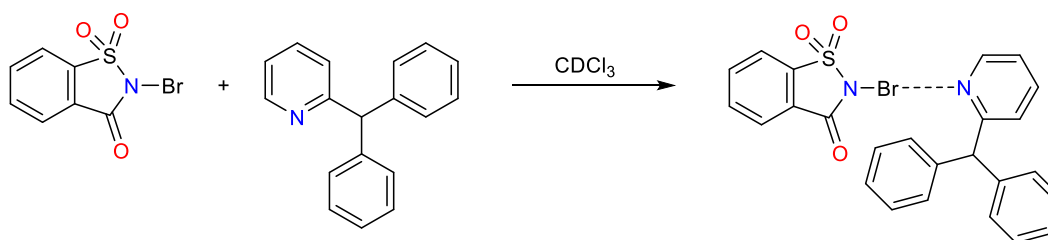
6.3.12. ¹H Titration experiments for NBSac-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|------------------------|
| K (0 → ∞) | 21.29 M ⁻¹ | ± 0.9460% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

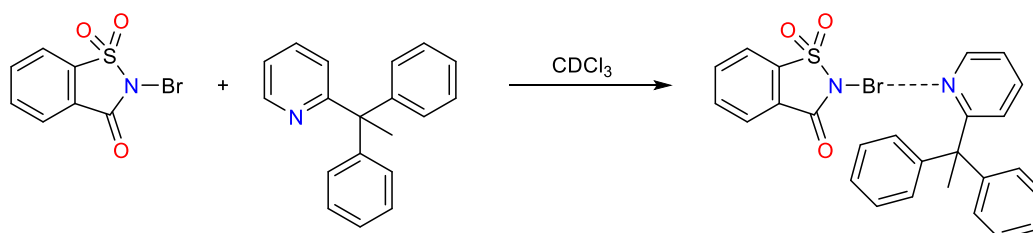
6.3.13. ¹H Titration experiments for NBSac-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 147.07 M ⁻¹ | ± 0.9839% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

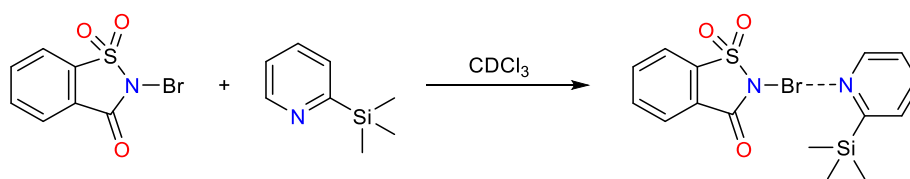
6.3.14. ¹H Titration experiments for NBSac-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 147.07 M ⁻¹ | ± 0.9839% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.3.15. ¹H Titration experiments for NBSac-15^a

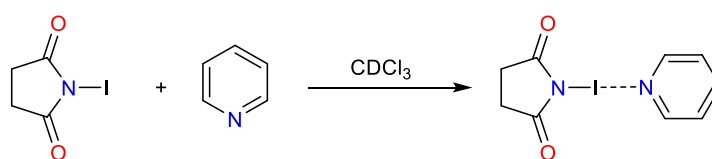


| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 394.09 M ⁻¹ | ± 2.9606% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.4. ¹H Titration experiments for NIS-Z (1-15)

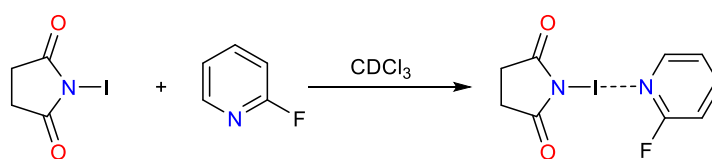
6.4.1. ¹H Titration experiments for NIS-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 1470.69 M ⁻¹ | ± 48.7749% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

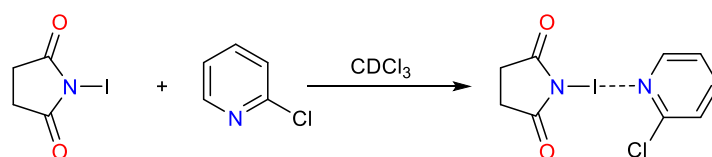
6.4.2. ¹H Titration experiments for NIS-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.14 M ⁻¹ | ± 1.7155% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

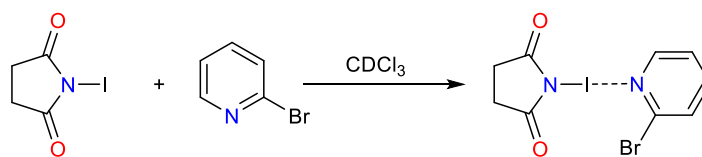
6.4.3. ¹H Titration experiments for NIS-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.93 M ⁻¹ | ± 4.2996% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

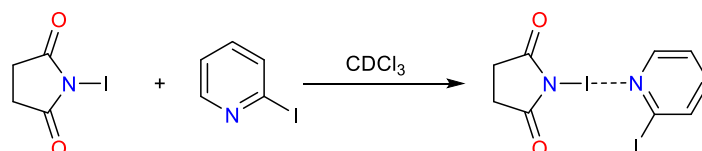
6.4.4. ¹H Titration experiments for NIS-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|-----------|----------------------|
| K (0 → ∞) | 9.31 e-5 M ⁻¹ | ± 0.6538% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

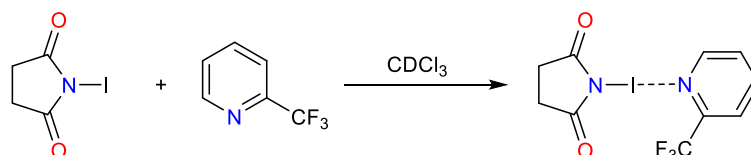
6.4.5. ¹H Titration experiments for NIS-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|--------------|----------------------|
| K (0 → ∞) | 1.85 e-5 M ⁻¹ | ± 3.8367e-3% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

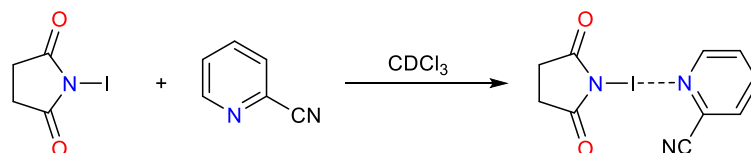
6.4.6. ¹H Titration experiments for NIS-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 2.02 M ⁻¹ | ± 2.8176% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

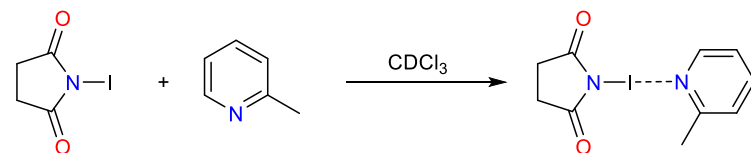
6.4.7. ¹H Titration experiments for NIS-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|----------------------|
| K (0 → ∞) | 11.92 M ⁻¹ | ± 0.6619% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

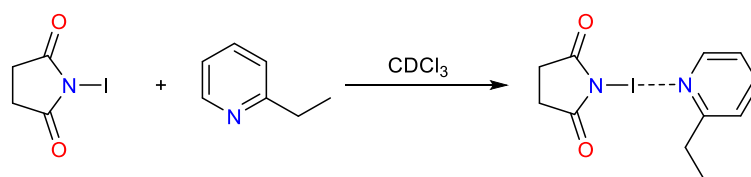
6.4.8. ¹H Titration experiments for NIS-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 3493.51 M ⁻¹ | ± 44.4667% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

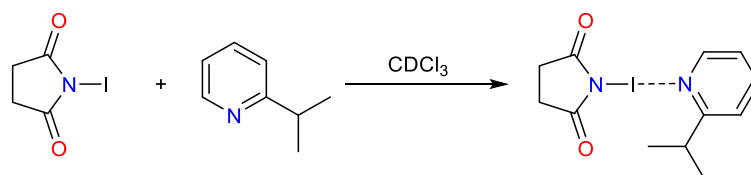
6.4.9. ¹H Titration experiments for NIS-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 3397.65 M ⁻¹ | ± 47.4420% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

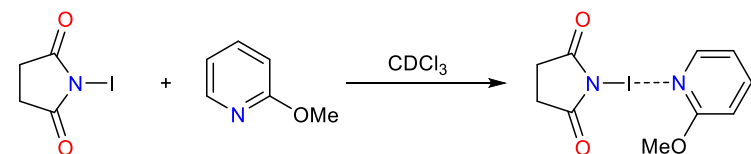
6.4.10. ¹H Titration experiments for NIS-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|------------|------------------------|
| K (0 → ∞) | 588.41 M ⁻¹ | ± 27.2024% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

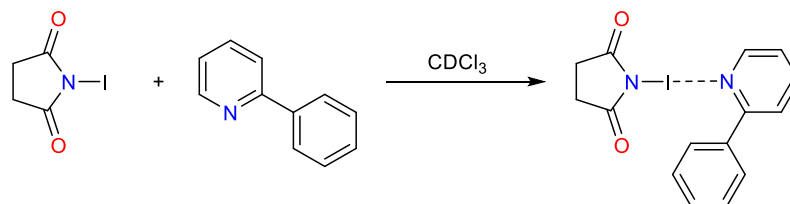
6.4.11. ¹H Titration experiments for NIS-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|----------------------|
| K (0 → ∞) | 0.54 M ⁻¹ | ± 1.9841% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

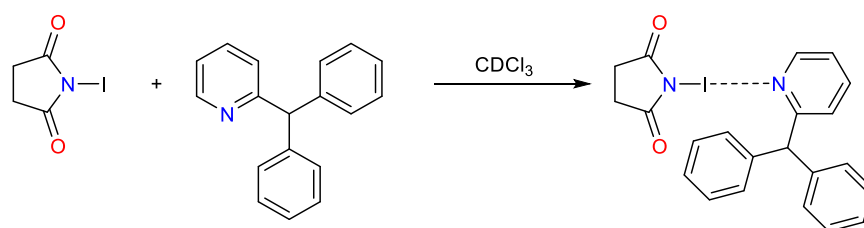
6.4.12. ¹H Titration experiments for NIS-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|----------------------|
| K (0 → ∞) | 3.60e-2 M ⁻¹ | ± 0.6035% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

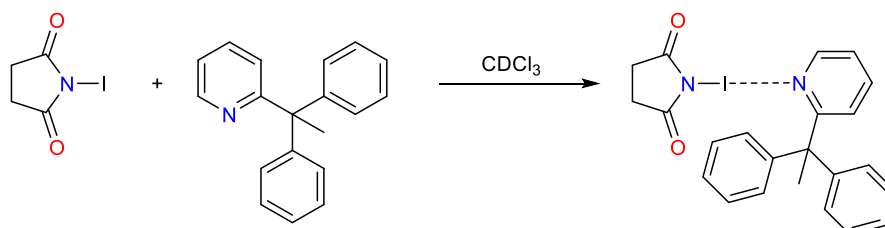
6.4.13. ¹H Titration experiments for NIS-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|------------|------------------------|
| K (0 → ∞) | 489.16 M ⁻¹ | ± 12.0930% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

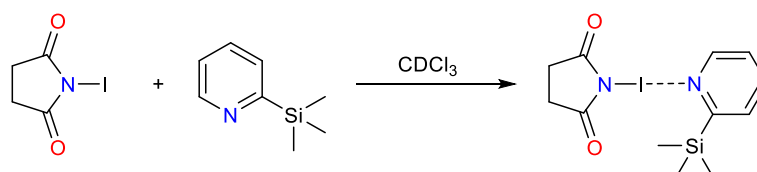
6.4.14. ¹H Titration experiments for NIS-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|------------|------------------------|
| K (0 → ∞) | 489.16 M ⁻¹ | ± 12.0930% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.4.15. ¹H Titration experiments for NIS-15^a

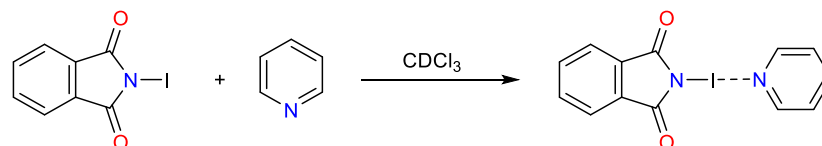


| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|------------|------------------------|
| K (0 → ∞) | 521.76 M ⁻¹ | ± 16.7211% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.5. ¹H Titration experiments for NIP-Z

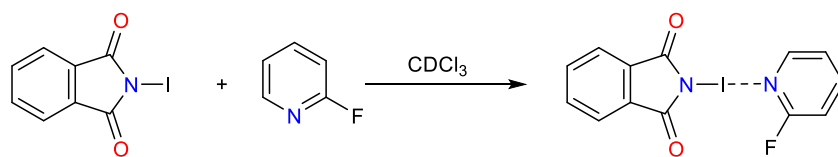
6.5.1. ¹H Titration experiments for NIP-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 1123.54 M ⁻¹ | ± 13.8345% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

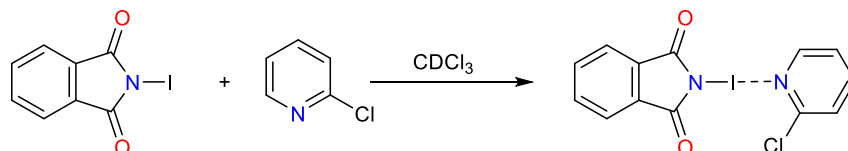
6.5.2. ¹H Titration experiments for NIP-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|----------------------|
| K (0 → ∞) | 11.28 M ⁻¹ | ± 0.1680% | 1.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

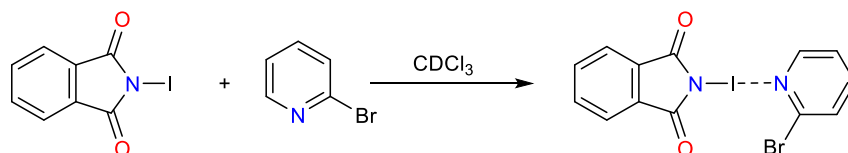
6.5.3. ¹H Titration experiments for NIP-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 23.09 M ⁻¹ | ± 0.2044% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

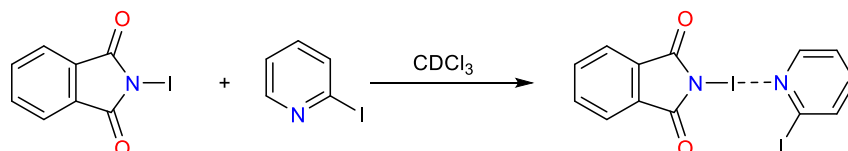
6.5.4. ¹H Titration experiments for NIP-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 17.86 M ⁻¹ | ± 0.2676% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

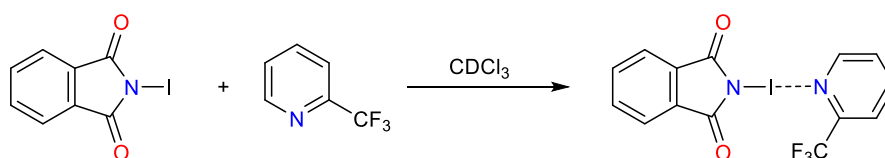
6.5.5. ¹H Titration experiments for NIP-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 56.17 M ⁻¹ | ± 0.2821% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.5.6. ¹H Titration experiments for NIP-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|-----------------------|
| K (0 → ∞) | 6.45 M ⁻¹ | ± 0.7056% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

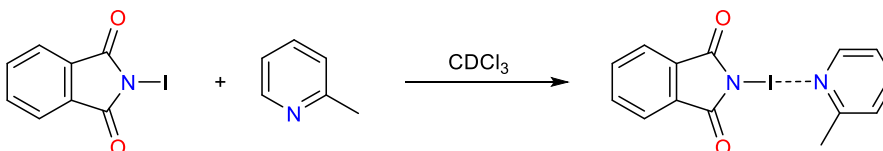
6.5.7. ¹H Titration experiments for NIP-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 14.90 M ⁻¹ | ± 0.6524% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

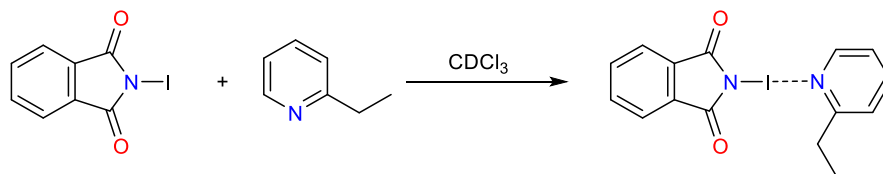
6.5.8. ¹H Titration experiments for NIP-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 2790.09 M ⁻¹ | ± 14.2909% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

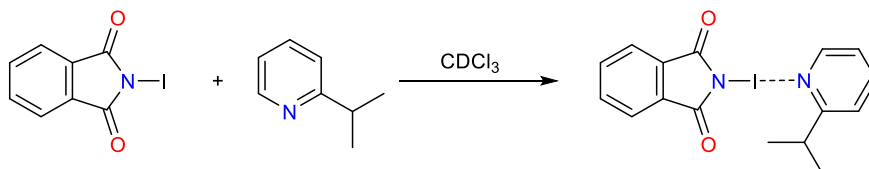
6.5.9. ¹H Titration experiments for NIP-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 506.03 M ⁻¹ | ± 7.4095% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

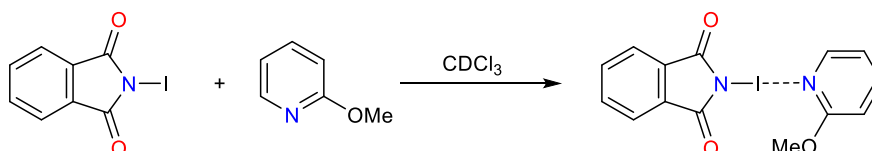
6.5.10. ¹H Titration experiments for NIP-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 617.11 M ⁻¹ | ± 5.5849% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

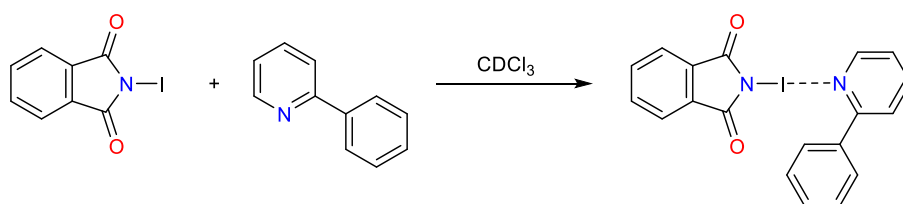
6.5.11. ¹H Titration experiments for NIP-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|------------|-----------------------|
| K (0 → ∞) | 21.78 M ⁻¹ | ± 0.47188% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

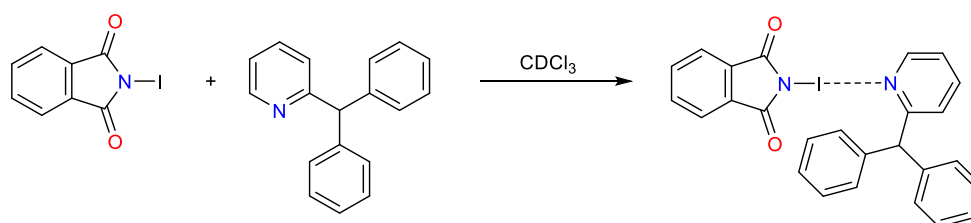
6.5.12. ¹H Titration experiments for NIP-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|-----------------------|
| K (0 → ∞) | 59.22 M ⁻¹ | ± 1.6816% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

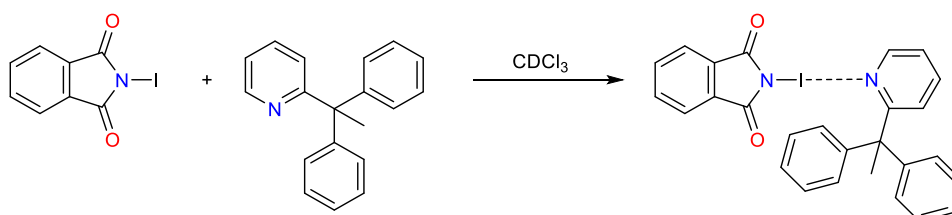
6.5.13. ¹H Titration experiments for NIP-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 374.71 M ⁻¹ | ± 2.9105% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

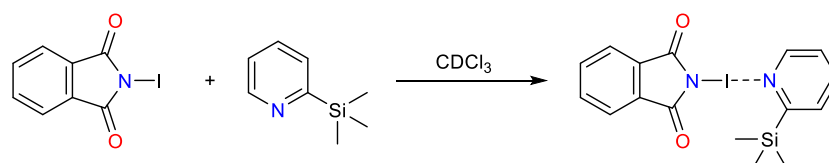
6.5.14. ¹H Titration experiments for NIP-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 374.71 M ⁻¹ | ± 2.9105% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.5.15. ¹H Titration experiments for NIP-15^a

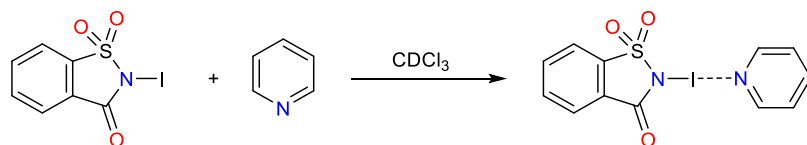


| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|-----------------------|
| K (0 → ∞) | 290.94 M ⁻¹ | ± 5.4769% | 10.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

6.6. ¹H Titration experiments for NISac-Z

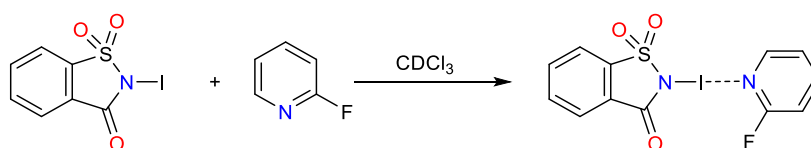
6.6.1. ¹H Titration experiments for NISac-1^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 2610.15 M ⁻¹ | ± 11.8584% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

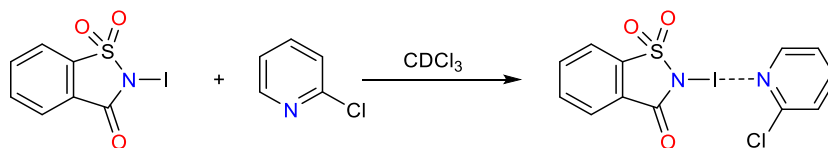
6.6.2. ¹H Titration experiments for NISac-2^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1099.59 M ⁻¹ | ± 1.8770% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

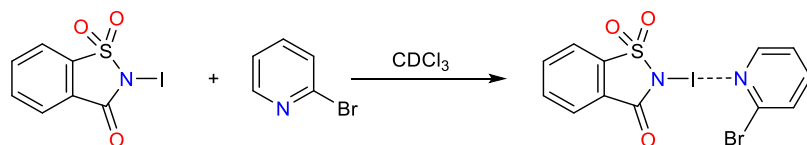
6.6.3. ¹H Titration experiments for NISac-3^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1423.90 M ⁻¹ | ± 3.3000% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

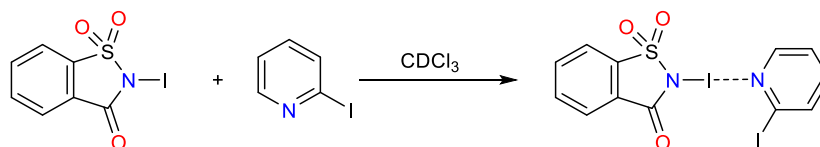
6.6.4. ¹H Titration experiments for NISac-4^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1472.40 M ⁻¹ | ± 2.6246% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

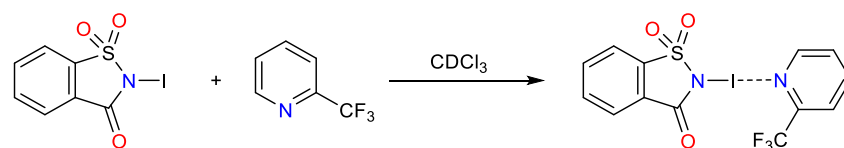
6.6.5. ¹H Titration experiments for NISac-5^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|-------------|-------------------------|
| K (0 → ∞) | 44271.80 M ⁻¹ | ± 175.1732% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

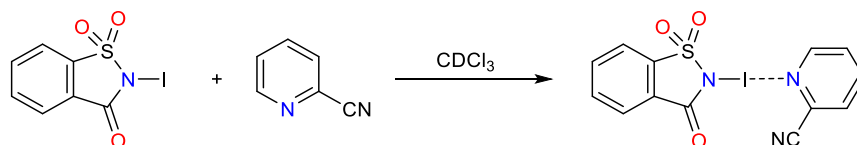
6.6.6. ¹H Titration experiments for NISac-6^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|------------------------|
| K (0 → ∞) | 81.72 M ⁻¹ | ± 1.4025% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

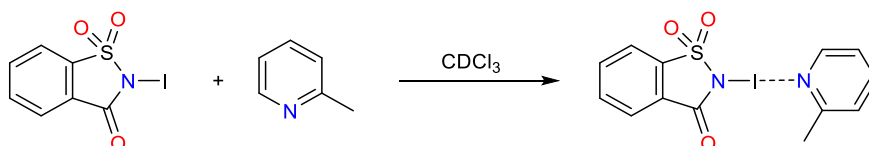
6.6.7. ¹H Titration experiments for NISac-7^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|-----------|------------------------|
| K (0 → ∞) | 388.55 M ⁻¹ | ± 1.7069% | 100.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

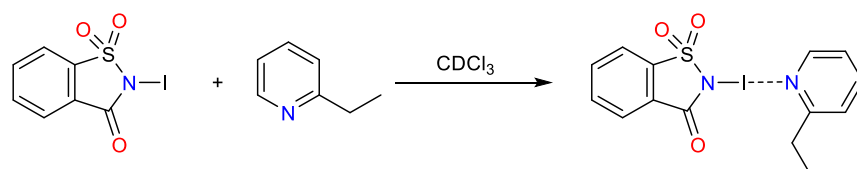
6.6.8. ¹H Titration experiments for NISac-8^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|------------|-------------------------|
| K (0 → ∞) | 14521.51 M ⁻¹ | ± 26.1383% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

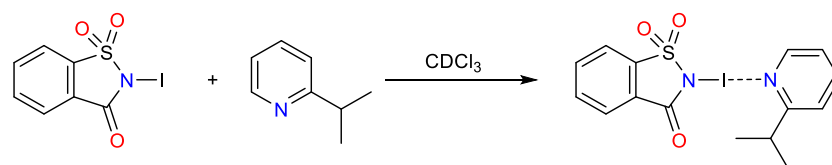
6.6.9. ¹H Titration experiments for NISac-9^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 2535.49 M ⁻¹ | ± 5.7089% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

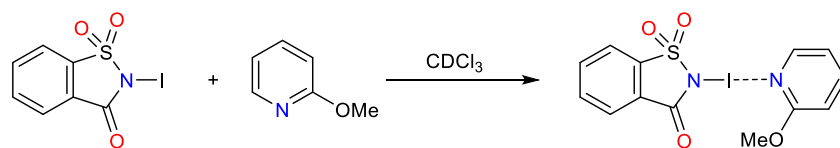
6.6.10. ¹H Titration experiments for NISac-10^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|------------|-------------------------|
| K (0 → ∞) | 3249.64 M ⁻¹ | ± 11.4627% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

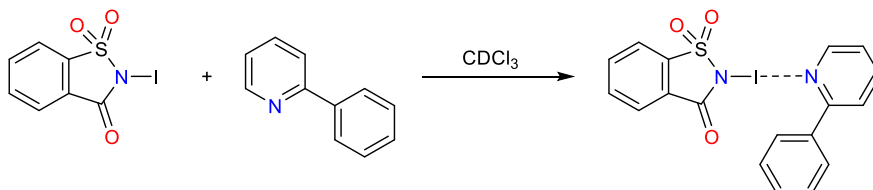
6.6.11. ¹H Titration experiments for NISac-11^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-------------------------|-----------|-------------------------|
| K (0 → ∞) | 1545.32 M ⁻¹ | ± 9.2064% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

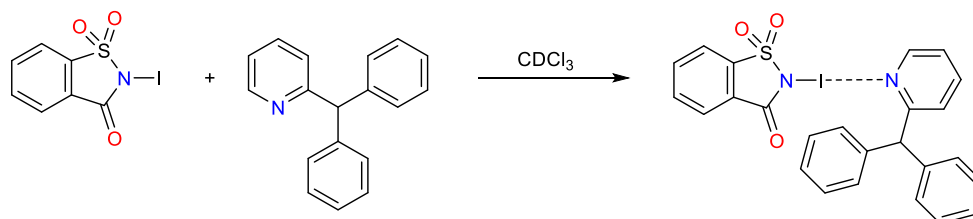
6.6.12. ¹H Titration experiments for NISac-12^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|---------------------------|-------------|-------------------------|
| K (0 → ∞) | 125281.27 M ⁻¹ | ± 375.2407% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

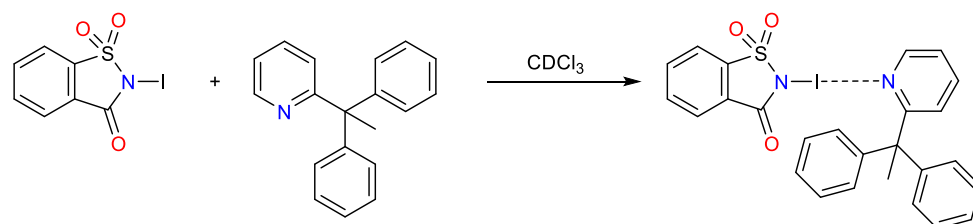
6.6.13. ¹H Titration experiments for NISac-13^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|-------------|-------------------------|
| K (0 → ∞) | 25495.07 M ⁻¹ | ± 168.4289% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

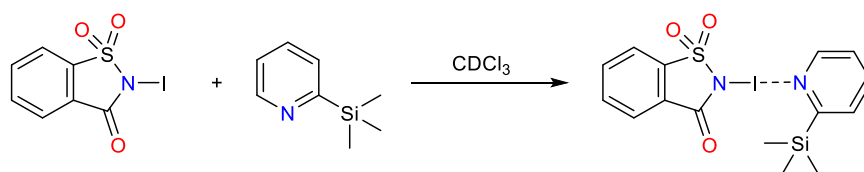
6.6.14. ¹H Titration experiments for NISac-14^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|--------------------------|-------------|-------------------------|
| K (0 → ∞) | 25495.07 M ⁻¹ | ± 168.4289% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

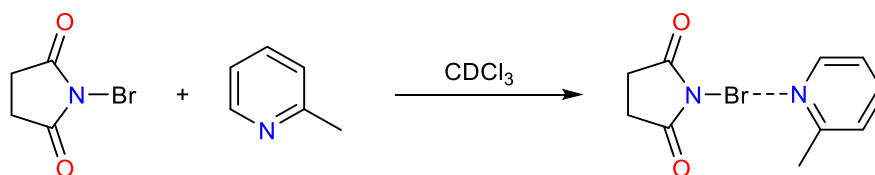
6.6.15. ¹H Titration experiments for NISac-15^a



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|---------------------------|-------------|-------------------------|
| K (0 → ∞) | 144459.18 M ⁻¹ | ± 297.3053% | 1000.00 M ⁻¹ |

^a See: [link](#) for BindFit v0.5 results.

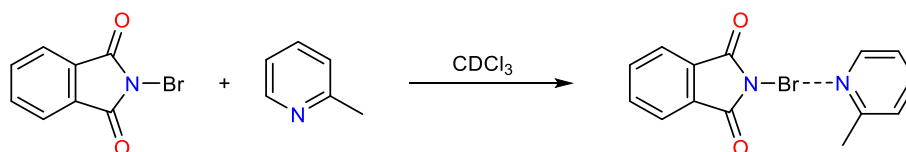
6.6.16. ¹H Titration experiments for NBS-8^{a,b}



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|-----------------------|-----------|---------------------|
| K (0 → ∞) | 21.14 M ⁻¹ | ± 1.7549% | 100 M ⁻¹ |

^aFor BindFit v0.5 results, see: <http://app.supramolecular.org/bindfit/view/30cf3404-e228-4974-b77d-7eddbbc81e331>; ^bStock solution concentration of ligand **8** is 1M

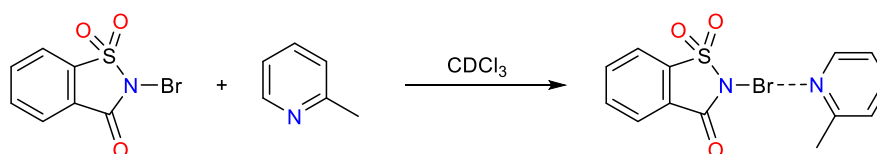
6.2.17. ¹H Titration experiments for NBP-8^{a,b}



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|----------------------|-----------|---------------------|
| K (0 → ∞) | 19.2 M ⁻¹ | ± 1.0611% | 100 M ⁻¹ |

^aFor BindFit v0.5 results, see <http://app.supramolecular.org/bindfit/view/013f1a8d-359f-447e-aff3-68676f8ce7fe>; ^bStock solution concentration of ligand **8** is 1M

6.3.18. ¹H Titration experiments for NBSac-8^{a,b}



| Parameter (bounds) | Optimized | Error | Initial |
|--------------------|------------------------|------------|------------------------|
| K (0 → ∞) | 422.99 M ⁻¹ | ± 10.6095% | 100.00 M ⁻¹ |

^aFor BindFit v0.5 results, see <http://app.supramolecular.org/bindfit/view/974090c2-14da-492a-b36f-c1175cd943bc>; ^bStock solution concentration of ligand **8** is 1M

7. ^{15}N NMR of halogenation reaction of NISac-16 in acetone- d_6

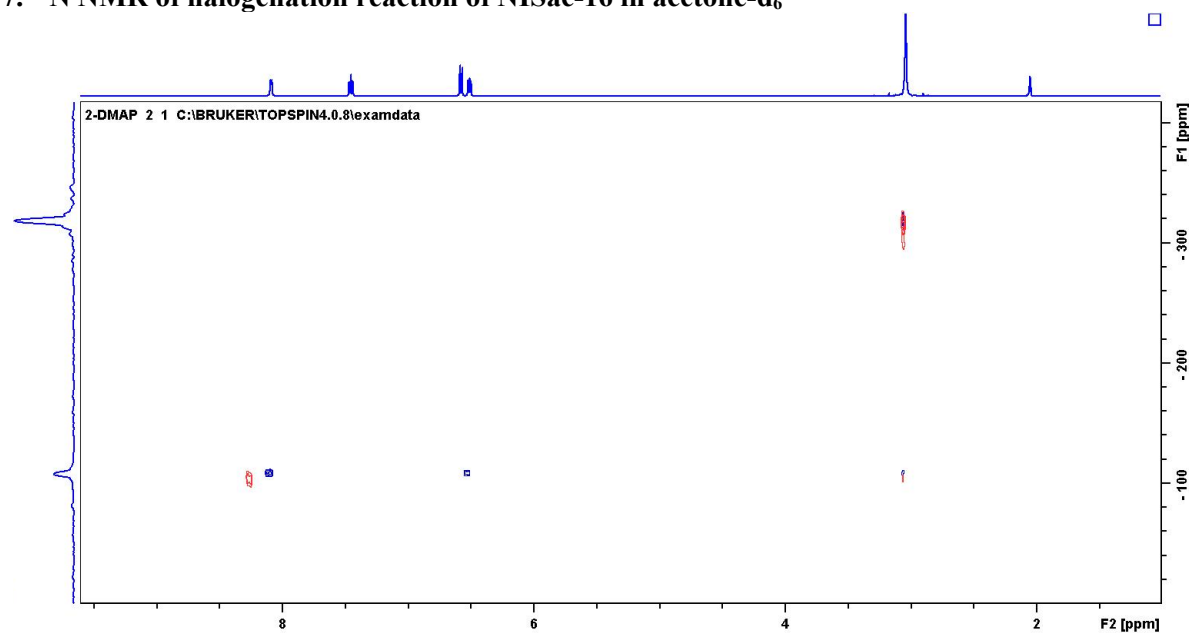


Figure S102. ^1H - ^{15}N HMBC-NMR Spectra of **16** in blue contour and 1:1 equivalent mixture of NISac-**16** in red contour measured in acetone- d_6 at 303K.

10). References

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