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The first synthesis of *N*-substituted *cis*/*trans*-perhydropentaazapyrenes

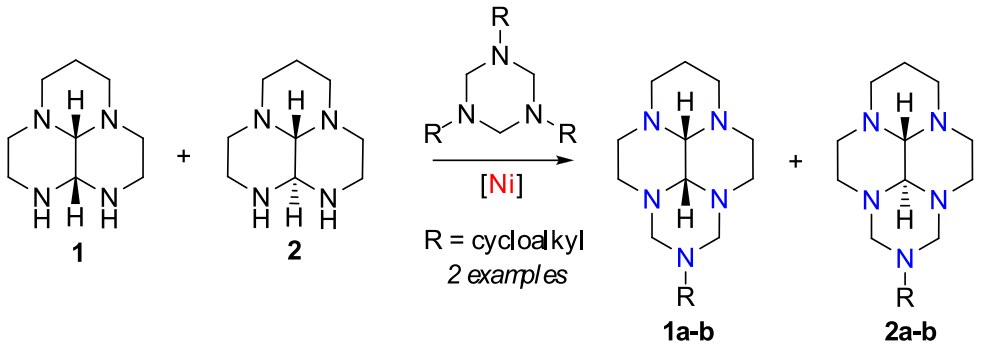
Elena B. Rakhimova, Victor Yu. Kirsanov, Yulia S. Blokhina and Tatyana V. Tyumkina

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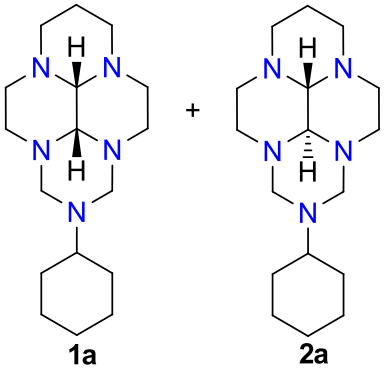
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General information. The ^{1}H and ^{13}C NMR spectra, including two dimensional homo- (COSY, NOESY) and heteronuclear (HSQC, HMBC) spectra, were recorded on a Bruker Avance 500 spectrometer (500.17 MHz for ^{1}H and 125.78 MHz for ^{13}C) according to standard Bruker protocols using $CDCl_3$ as solvent and TMS as internal standard. The high-resolution mass spectra were recorded on a Bruker MaXis Impact instrument (TOF mass analyzer, electrospray ionization). Elemental analysis of the samples was performed using an EMA 502 microanalyzer (VELP SCIENTIFICA, Italy). Sulfanilic acid was used as the standard. The melting points were measured on a PHMK 80/2617 melting point apparatus. Commercially available reagents used in this work were purchased from Sigma–Aldrich and Acros Organics. Quantum-chemical calculations were performed in the Priroda-20 program [S1, S2] at the DFT level using the Perdew–Burke–Ernzerhof (PBE) functional [S3] and the 3ζ basis set, the data of which were in good agreement with PBE-0 [S4]. The optimization of the geometry of the complexes, analysis of vibrational frequencies, calculation of entropic and thermodynamic corrections to the total energy of the compounds were performed.

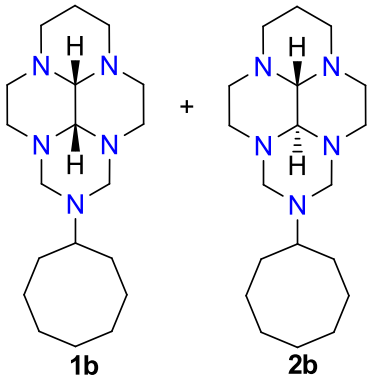
Heterocyclization of a stereoisomeric mixture of perhydrotetraazaphenalenes (1, 2) with 1,3,5-trisubstituted 1,3,5-triazinanes (General procedure). A round-bottomed flask equipped with a magnetic stirrer bar was charged with CH_3CN (15 mL), $NiCl_2 \cdot 6H_2O$ (0.012 g, 0.05 mmol), and the appropriate 1,3,5-trisubstituted 1,3,5-triazinane (1.00 mmol), prepared *in situ* by the reported procedure [S5]. Then a stereoisomeric mixture of perhydrotetraazaphenalenes **1**, **2** (0.18 g, 1.00 mmol), obtained by the method [S6], in CH_3CN (10 mL) was added, and the mixture was stirred at 40 °C for 7 days. The reaction mass was concentrated, washed twice with acetone (2×10 ml) and a mixture of the corresponding *cis*/*trans*-2,3a,5a,8a,10a-pentaazapyrenes **1a–b/2a–b** were obtained as white powders.



Analytical data for compounds 1a–b/2a–b

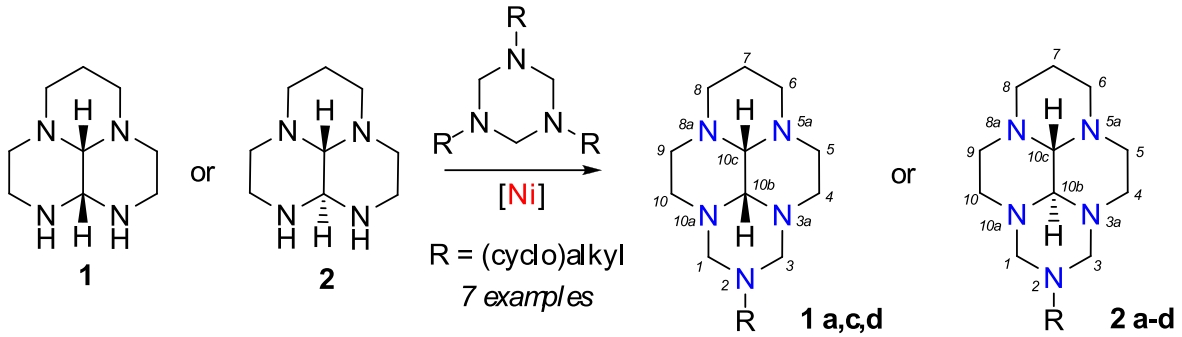


A mixture of *cis*/*trans*-2-cyclohexyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrenes (1a/2a). White powder; yield 0.16 g (53%); R_f 0.15 (MeOH). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 19.7, 25.4, 26.1, 29.2, 29.8, 44.5, 45.6, 50.6, 52.5, 54.1, 55.8, 59.1, 71.5, 74.3, 76.7, 76.9 (*cis* isomer); 24.3, 25.3, 26.0, 30.6, 48.5, 52.4, 53.9, 57.0, 71.6, 82.3, 84.1 (*trans* isomer).

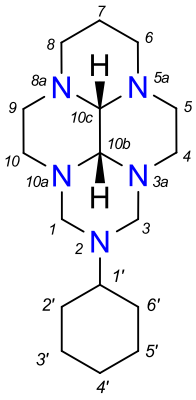


A mixture of *cis*/*trans*-2-cyclooctyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrenes (1b/2b). White powder; yield 0.14 g (42%); R_f 0.15 (MeOH). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 19.7, 24.7, 26.0, 26.8, 29.2, 29.3, 44.5, 45.5, 50.6, 54.0, 55.8, 60.0, 71.4, 74.5, 76.6, 76.8 (*cis* isomer); 24.3, 24.4, 24.8, 27.2, 29.1, 48.6, 52.4, 53.8, 58.3, 72.1, 82.3, 83.8 (*trans* isomer).

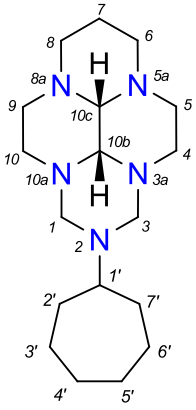
Heterocyclization of *cis*-perhydrotetraazaphenalene 1 or *trans*-perhydrotetraazaphenalene 2 with 1,3,5-trisubstituted 1,3,5-triazinanes (General procedure). A round-bottomed flask equipped with a magnetic stirrer bar was charged with CH_3CN (15 mL), $NiCl_2 \cdot 6H_2O$ (0.012 g, 0.05 mmol), and the appropriate 1,3,5-trisubstituted 1,3,5-triazinane (1.00 mmol), prepared *in situ* by the reported procedure [S5]. Then *cis*-perhydrotetraazaphenalene **1** (0.18 g, 1.00 mmol) or *trans*-perhydrotetraazaphenalene **2** (0.18 g, 1.00 mmol), obtained by the method [S7], in CH_3CN (10 mL) was added, and the mixture was stirred at 40 °C for 7 days. The reaction mass was passed through a SiO_2 layer, concentrated, and washed twice with acetone (2×10 ml). As a result, individual stereoisomerically pure *cis*-2,3a,5a,8a,10a-pentaazapyrenes (**1a**,**c**,**d**) and stereoisomerically pure *trans*-2,3a,5a,8a,10a-pentaazapyrenes (**2a–d**) were obtained as white powders.



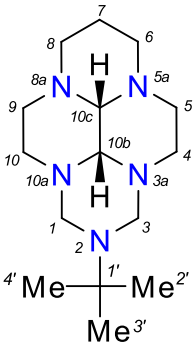
Analytical data for compounds 1a,c,d and 2a-d



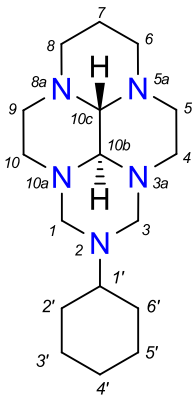
***cis*-2-Cyclohexyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (1a).** White powder; yield 0.17 g (56%); mp 100–102 °C; R_f 0.45 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.12–1.16 (m, 1H, CH_2, H_a-4′), 1.19–1.24 (m, 5H, CH_2, H_a-2′,3′,5′,6′, H_a-7), 1.59 (d, 1H, CH_2, H_b-4′; J_{ba} = 12), 1.76–1.82 (m, 4H, CH_2, H_b-2′,3′,5′,6′), 2.07–2.13 (m, 1H, CH_2, H_a-8), 2.18–2.29 (m, 3H, CH_2, H_a-4,9, H_b-7; 1H, CH, H-1′), 2.35–2.42 (m, 2H, CH_2, H_a-5,10), 2.67 (d, 1H, CH_2, H_b-9; J_{ba} = 12), 2.73 (d, 1H, CH_2, H_b-4; J_{ba} = 11.5), 2.77 (d, 1H, CH_2, H_a-3; $^2J_{ab}$ = 7.5), 2.94–2.98 (m, 2H, CH_2, H-6; 1H, CH_2, H_b-8), 3.04 (d, 1H, CH, H-10b, ^3J = 2.5), 3.08 (d, 1H, CH, H-10c, ^3J = 2.5), 3.54–3.58 (m, 2H, CH_2, H_a-1, H_b-5), 3.75–3.79 (m, 2H, CH_2, H_b-1, H_b-10), 3.84–3.88 (m, 1H, CH_2, H_b-3). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 19.7 (C-7), 25.4 (C-3′,5′), 26.2 (C-4′), 29.2 (C-2′), 29.8 (C-6′), 44.6 (C-5), 45.6 (C-10), 50.6 (C-4), 52.5 (C-6), 54.1 (C-9), 55.9 (C-8), 59.2 (C-1′), 71.5 (C-1), 74.3 (C-3), 76.7 (C-10c), 76.9 (C-10b). Mass-spectrum: Found *m/z* 306.2652 [*M* + H]$^+$, Calculated for $C_{17}H_{32}N_5^+$ 306.2658. Anal. Calcd for $C_{17}H_{31}N_5$: C, 66.84; H, 10.23; N, 22.93. Found: C, 65.11; H, 10.01; N, 23.59.



***cis*-2-Cycloheptyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (1c).** White powder; yield 0.17 g (53%); mp 103–105 °C; R_f 0.50 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.22 (d, 1H, CH_2, H_a-7; J_{ab} = 13), 1.35–1.41 (m, 2H, CH_2, H_a-3′,6′), 1.48–1.58 (m, 6H, CH_2, H_a-2′,7′, H-4′,5′), 1.61–1.67 (m, 2H, CH_2, H_b-3′,6′), 1.72–1.78 (m, 2H, CH_2, H_b-2′,7′), 2.12 (t, 1H, CH_2, H_a-8; J_{ab} = 11), 2.18–2.28 (m, 3H, CH_2, H_a-4,9, H_b-7), 2.34–2.41 (m, 2H, CH_2, H_a-5,10), 2.47 (sept, 1H, CH, H-1′; J = 3.5), 2.66 (d, 1H, CH_2, H_b-4; J_{ba} = 10), 2.71–2.76 (m, 2H, CH_2, H_b-9, H_a-3), 2.91–2.98 (m, 2H, CH_2, H-6; 1H, CH_2, H_b-8), 3.01 (d, 1H, CH, H-10b, ^{3}J = 2.5), 3.08 (d, 1H, CH, H-10c, ^{3}J = 2.5), 3.52–3.57 (m, 2H, CH_2, H_a-1, H_b-5), 3.68 (d, 1H, CH_2, H_b-1; $^2J_{ba}$ = 11), 3.76–3.80 (m, 2H, CH_2, H_b-3; H_b-10). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 19.7 (C-7), 25.1 (C-3′,6′), 28.0 (C-4′,5′), 30.6 (C-2′), 30.7 (C-7′), 44.5 (C-5), 45.5 (C-10), 50.6 (C-4), 52.5 (C-6), 54.1 (C-9), 55.8 (C-8), 61.2 (C-1′), 71.5 (C-1), 74.4 (C-3), 76.7 (C-10c), 76.9 (C-10b). Anal. Calcd for $C_{18}H_{33}N_5$: C, 67.67; H, 10.41; N, 21.92. Found: C, 67.58; H, 10.37; N, 21.80.

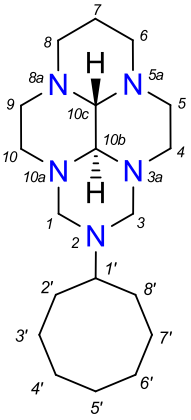


***cis*-2-*tert*-Butyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (1d).** White powder; yield 0.13 g (46%); mp 108–110 °C; R_f 0.55 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.06 (br. s, 9H, CH_3, H-2′,3′,4′), 1.23 (d, 1H, CH_2, H_a-7, J_{ab} = 13.5), 2.09–2.15 (m, 1H, CH_2, H_a-8), 2.22–2.28 (m, 2H, CH_2, H_a-4,9; 1H, CH_2, H_b-7), 2.35 (t, 2H, CH_2, H_a-5,10, J_{ab} = 14), 2.65–2.80 (m, 2H, CH_2, H_b-4,9; 1H, CH_2, H_a-3), 2.94–2.98 (m, 2H, CH_2, H-6; 1H, CH_2, H_b-8), 3.02 (d, 1H, CH, H-10b, ^{3}J = 2.5), 3.09 (d, 1H, CH, H-10c, ^{3}J = 2.5), 3.48 (d, 1H, CH_2, H_a-1, $^2J_{ab}$ = 10.5), 3.55 (t, 1H, CH_2, H_b-5, J_{ba} = 10.5), 3.77 (t, 1H, CH_2, H_b-10, J_{ba} = 10.5), 3.90 (d, 1H, CH_2, H_b-1, $^2J_{ba}$ = 10.5), 3.98 (d, 1H, CH_2, H_b-3, $^2J_{ba}$ = 7.5). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 19.7 (C-7), 26.4 (C-2′,3′,4′), 44.6 (C-5), 45.2 (C-10), 50.6 (C-4), 51.6 (C-1′), 52.5 (C-6), 54.0 (C-9), 55.8 (C-8), 68.9 (C-1), 72.0 (C-3), 76.7 (C-10c), 76.9 (C-10b). Anal. Calcd for $C_{15}H_{29}N_5$: C, 64.48; H, 10.46; N, 25.06. Found: C, 64.37; H, 10.40; N, 25.01.

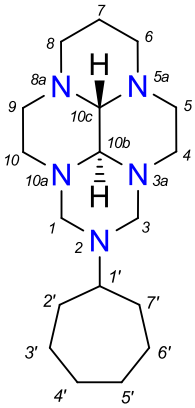


***trans*-2-Cyclohexyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (2a).** White powder; yield 0.15 g (49%); mp 160–162 °C; R_f 0.50 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.11–1.17 (m, 3H, CH_2, H_a-2′,4′,6′), 1.23–1.29 (m, 2H, CH_2, H_a-3′,5′), 1.53–1.62 (m, 1H, CH_2, H_a-7; 1H, CH_2, H_b-4′), 1.73–1.77 (m, 2H, CH_2, H_b-3′,5′), 1.96–1.99 (m, 1H, CH_2, H_b-7; 2H, CH_2, H_b-2′,6′), 2.07 (t, 2H, CH_2, H_a-6,8, J_{ab} = 12), 2.17 (d, 1H, CH, H-10b, ^{3}J = 7.2), 2.19 (d, 1H, CH, H-10c, ^{3}J = 6.8), 2.25–2.31 (m, 2H, CH_2, H_a-4,10), 2.43 (t, 2H, CH_2, H_a-5,9, J_{ab}

= 11.2), 2.52 (d, 2H, CH_2, H_b-4,10, J_{ba} = 10.8), 2.69 (d, 2H, CH_2, H_b-5,9, J_{ba} = 10.8), 2.77–2.80 (m, 1H, CH, H-1′), 2.85 (d, 2H, CH_2, H_b-6,8, J_{ba} = 10.8), 2.95 (d, 2H, CH_2, H_a-1,3, $^2J_{ab}$ = 10), 3.84 (d, 2H, CH_2, H_b-1,3, $^2J_{ba}$ = 10). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 24.3 (C-7), 25.3 (C-3′,5′), 26.0 (C-4′), 30.6 (C-2′,6′), 48.5 (C-4,10), 52.4 (C-5,9), 53.9 (C-6,8), 57.1 (C-1′), 71.5 (C-1,3), 82.2 (C-10c), 84.1 (C-10b). Mass-spectrum: Found *m/z* 306.2650 [*M* + H]$^+$, Calculated for $C_{17}H_{32}N_5^+$ 306.2658. Anal. Calcd for $C_{17}H_{31}N_5$: C, 66.84; H, 10.23; N, 22.93. Found: C, 64.97; H, 9.80; N, 23.99.

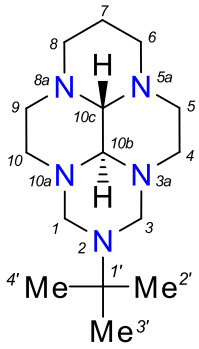


***trans*-2-Cyclooctyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (2b).** White powder; yield 0.12 g (36%); mp 151–153 °C; R_f 0.55 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.42–1.49 (m, 5H, CH_2, H_a-3′,4′,5′,6′,7′), 1.52–1.63 (m, 6H, CH_2, H_a-7, H_a-2′,8′, H_b-4′,5′,6′), 1.68–1.75 (m, 2H, CH_2, H_b-3′,7′), 1.80–1.87 (m, 2H, CH_2, H_b-2′,8′), 1.95–2.02 (m, 1H, CH_2, H_b-7), 2.08 (t, 2H, CH_2, H_a-6,8, J_{ab} = 12), 2.17 (d, 1H, CH, H-10b, ^{3}J = 6.5), 2.23 (d, 1H, CH, H-10c, ^{3}J = 7), 2.33 (td, 2H, CH_2, H_a-4,10; J_{ab} = 11 и 2.5), 2.45 (td, 2H, CH_2, H_a-5,9, J_{ab} = 11.5 и 3), 2.56 (d, 2H, CH_2, H_b-4,10, J_{ba} = 10.5), 2.70 (d, 2H, CH_2, H_b-5,9, J_{ba} = 10.5), 2.87 (d, 2H, CH_2, H_b-6,8, J_{ba} = 11), 2.92 (d, 2H, CH_2, H_a-1,3, $^2J_{ab}$ = 10), 2.97–3.02 (m, 1H, CH, H-1′), 3.78 (d, 2H, CH_2, H_b-1,3, $^2J_{ba}$ = 9.5). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 24.3 (C-7), 24.4 (C-3′,7′), 26.1 (C-5′), 27.2 (C-4′,6′), 29.2 (C-2′,8′), 48.7 (C-4,10), 52.5 (C-5,9), 53.9 (C-6,8), 58.4 (C-1′), 72.1 (C-1,3), 82.4 (C-10c), 83.9 (C-10b). Mass-spectrum: Found *m/z* 332.2868 [*M* – H]$^+$, Calculated for $C_{19}H_{34}N_5^+$ 332.2814. Anal. Calcd for $C_{19}H_{35}N_5$: C, 68.42; H, 10.58; N, 21.00. Found: C, 66.48; H, 9.93; N, 22.09.



***trans*-2-Cycloheptyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (2c).** White powder; yield 0.14 g (44%); mp 157–159 °C; R_f 0.55 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.38–1.45 (m, 2H, CH_2, H_a-3′,6′), 1.48–1.57 (m, 7H, CH_2, H_a-7; H_a-2′,7′; H-4′,5′), 1.62–1.68 (m, 2H, CH_2, H_b-3′,6′), 1.86–1.93 (m, 2H, CH_2, H_b-2′,7′), 1.96–2.02 (m, 1H, CH_2, H_b-7), 2.08 (t, 2H, CH_2, H_a-6,8, J_{ab} = 11.5), 2.15 (d, 1H, CH, H-10b, ^{3}J = 6.5), 2.23 (d, 1H, CH, H-10c, ^{3}J = 6.5), 2.32 (td, 2H, CH_2, H_a-4,10; J_{ab} = 11 и 2.5), 2.45 (td, 2H, CH_2, H_a-5,9, J_{ab} = 11 и 2.5), 2.56 (d, 2H, CH_2, H_b-4,10, J_{ba} = 10.5), 2.70 (d, 2H, CH_2, H_b-5,9, J_{ba} = 11), 2.86 (d, 2H, CH_2, H_b-6,8, J_{ba} = 11), 2.92 (d, 2H, CH_2, H_a-1,3, $^2J_{ab}$ = 9), 2.93–2.97 (m, 1H, CH, H-1′), 3.77 (d, 2H, CH_2, H_b-1,3, $^2J_{ba}$ = 9.5). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 24.3 (C-7), 24.7 (C-3′,6′), 28.4 (C-4′,5′), 31.3 (C-2′,7′), 48.7 (C-4,10), 52.5 (C-5,9), 53.9 (C-6,8), 60.1 (C-1′), 72.1 (C-1,3), 82.4 (C-10c), 83.9

(C-10b). Mass-spectrum: Found *m/z* 321.2839 [*M* + 2H]$^+$, Calculated for $C_{18}H_{35}N_5^+$ 321.2892. Anal. Calcd for $C_{18}H_{33}N_5$: C, 67.67; H, 10.41; N, 21.92. Found: C, 66.99; H, 10.01; N, 22.15.



***trans*-2-*tert*-Butyl-decahydro-1*H*,6*H*-2,3a,5a,8a,10a-pentaazapyrene (2d).** White powder; yield 0.12 g (43%); mp 154–156 ºC; R_f 0.60 (MeOH). ^{1}H NMR (500.17 MHz, $CDCl_3$): δ = 1.12 (br. s, 9H, CH_3, H-2′,3′,4′), 1.50–1.57 (m, 1H, CH_2, H_a-7), 1.92–1.98 (m, 1H, CH_2, H_b-7), 2.01–2.06 (m, 2H, CH_2, H_a-6,8), 2.08 (d, 1H, CH, H-10b, ^3J = 7), 2.23 (d, 1H, CH, H-10c, ^3J = 6.5), 2.34 (td, 2H, CH_2, H_a-4,10; J_{ab} = 11 и 2.5), 2.43 (td, 2H, CH_2, H_a-5,9, J_{ab} = 11 и 2.5), 2.59 (d, 2H, CH_2, H_b-4,10, J_{ba} = 10.5), 2.68 (dd, 2H, CH_2, H_b-5,9, J_{ba} = 9 и 2.5), 2.70 (d, 2H, CH_2, H_a-1,3, $^2J_{ab}$ = 9), 2.84 (d, 2H, CH_2, H_b-6,8, J_{ba} = 11), 3.89 (d, 2H, CH_2, H_b-1,3, $^2J_{ba}$ = 9). ^{13}C NMR (125.78 MHz, $CDCl_3$): δ = 24.3 (C-7), 26.9 (C-2′,3′,4′), 49.0 (C-4,10), 52.5 (C-5,9), 52.7 (C-1′), 53.8 (C-6,8), 70.2 (C-1,3), 82.5 (C-10c), 83.3 (C-10b). Mass-spectrum: Found *m/z* 281.2526 [*M* + 2H]$^+$, Calculated for $C_{15}H_{31}N_5^+$ 281.2579. Anal. Calcd for $C_{15}H_{29}N_5$: C, 64.48; H, 10.46; N, 25.06. Found: C, 64.40; H, 10.35; N, 25.06.

References

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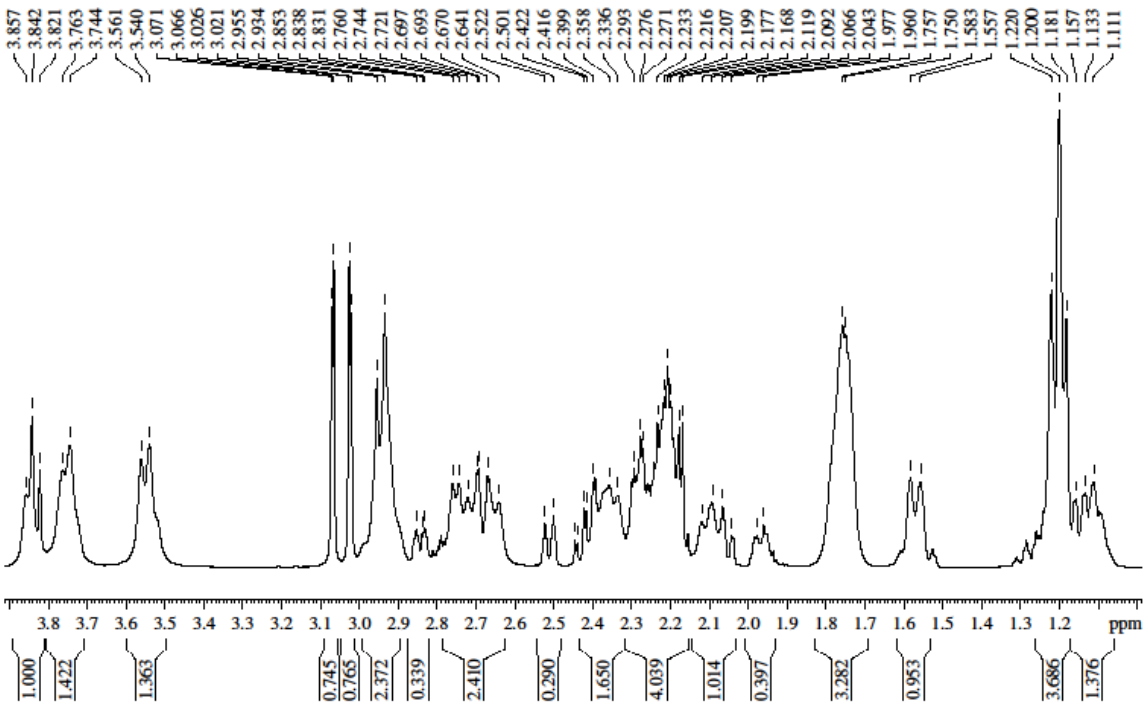
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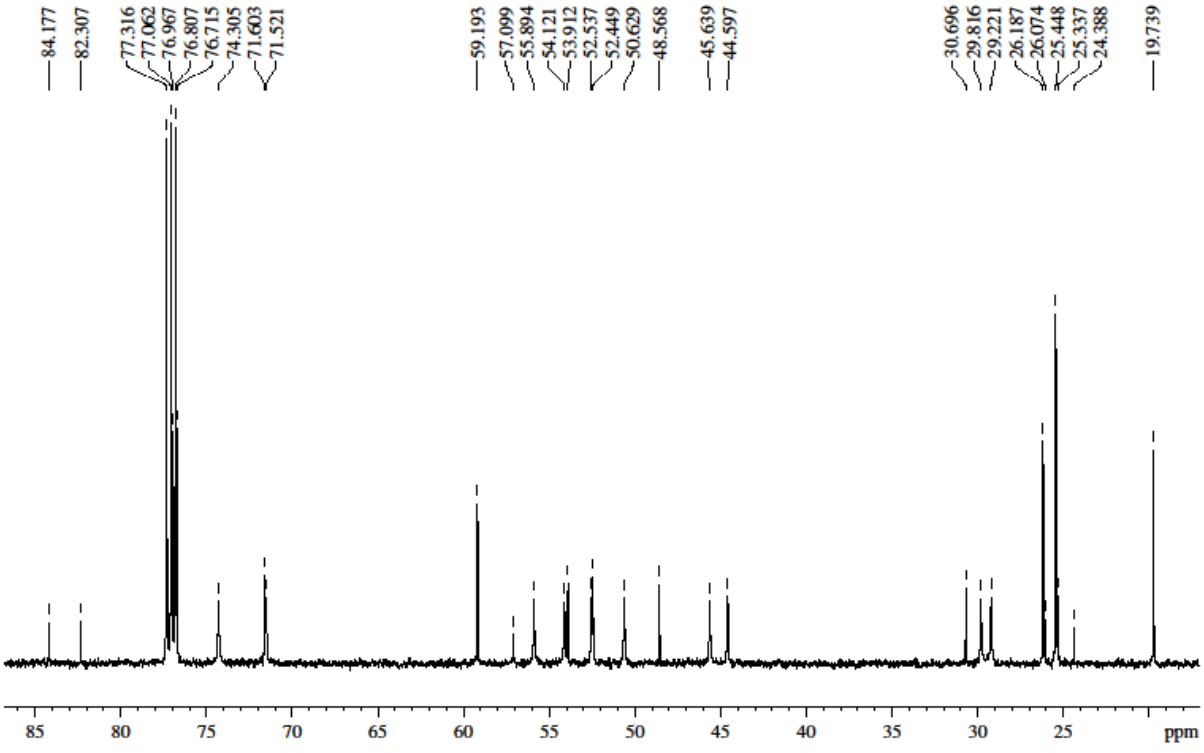
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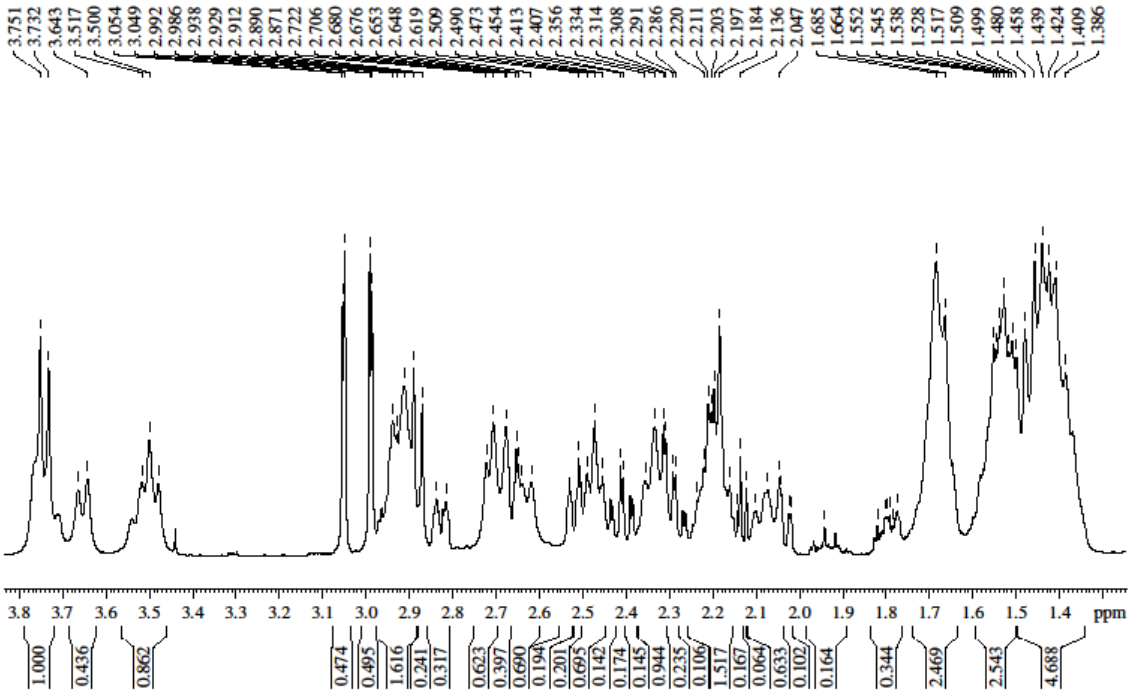
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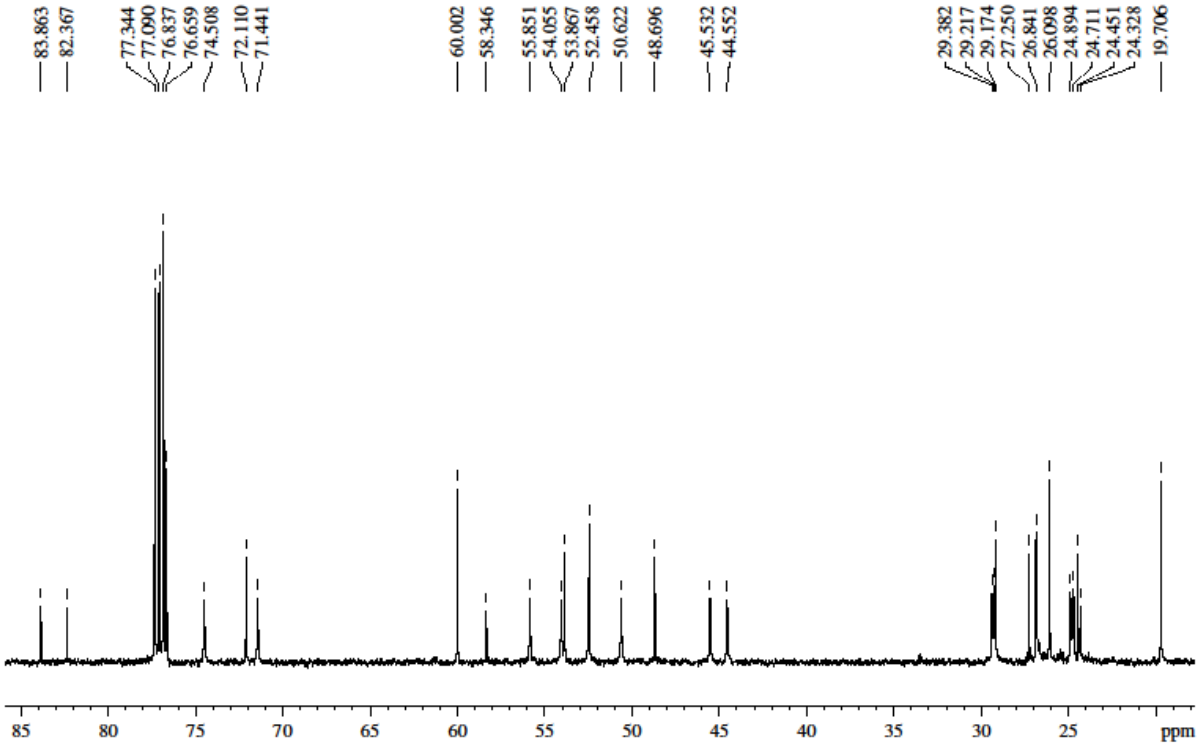
FigureS1. ^{1}H NMR spectrum of compounds **1a/2a**



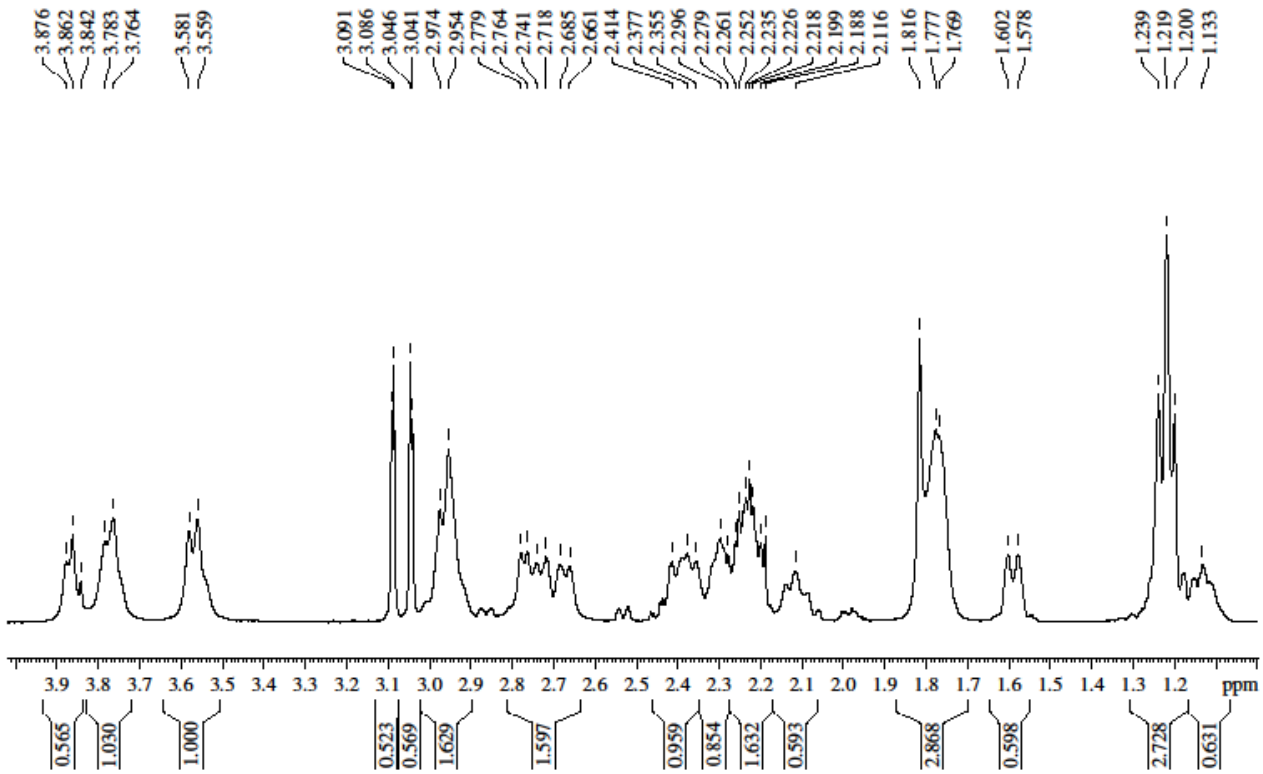
FigureS2. ^{13}C NMR spectrum of compounds **1a/2a**



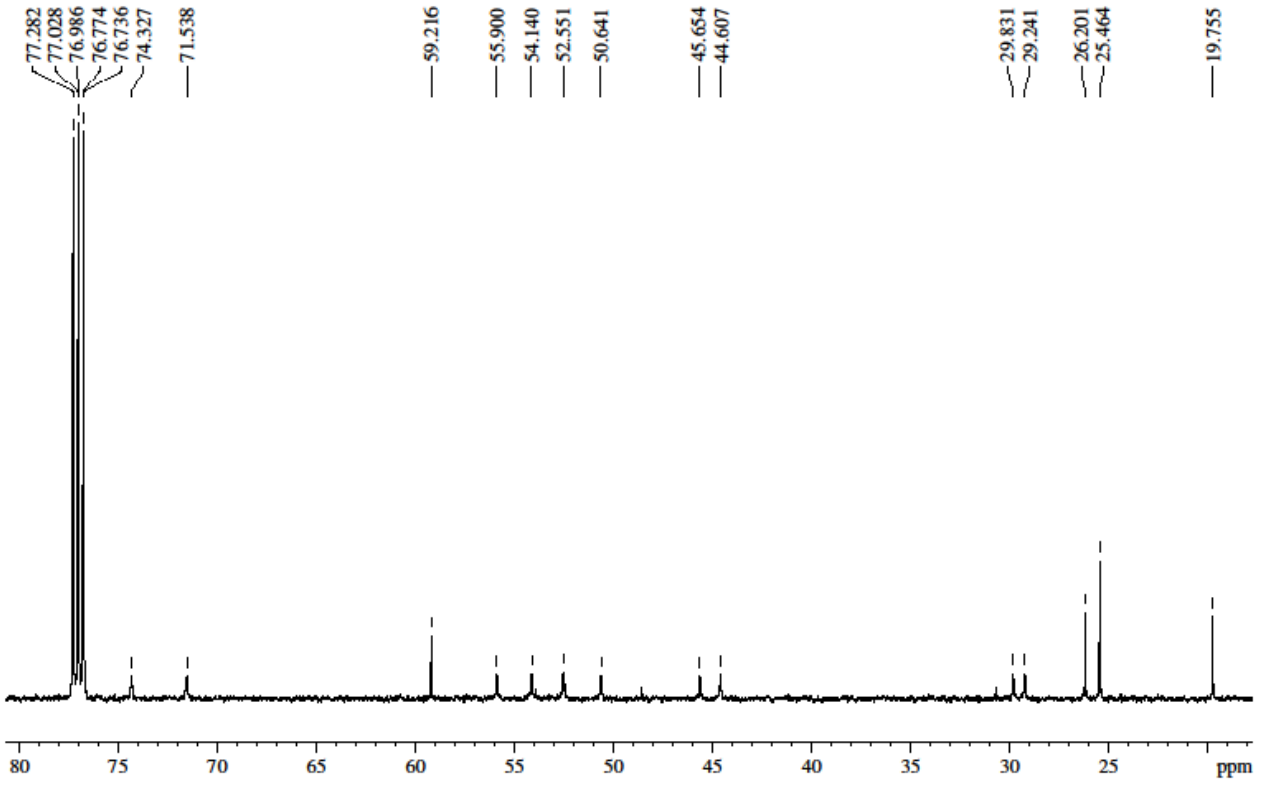
FigureS3. ^{1}H NMR spectrum of compounds **1b/2b**



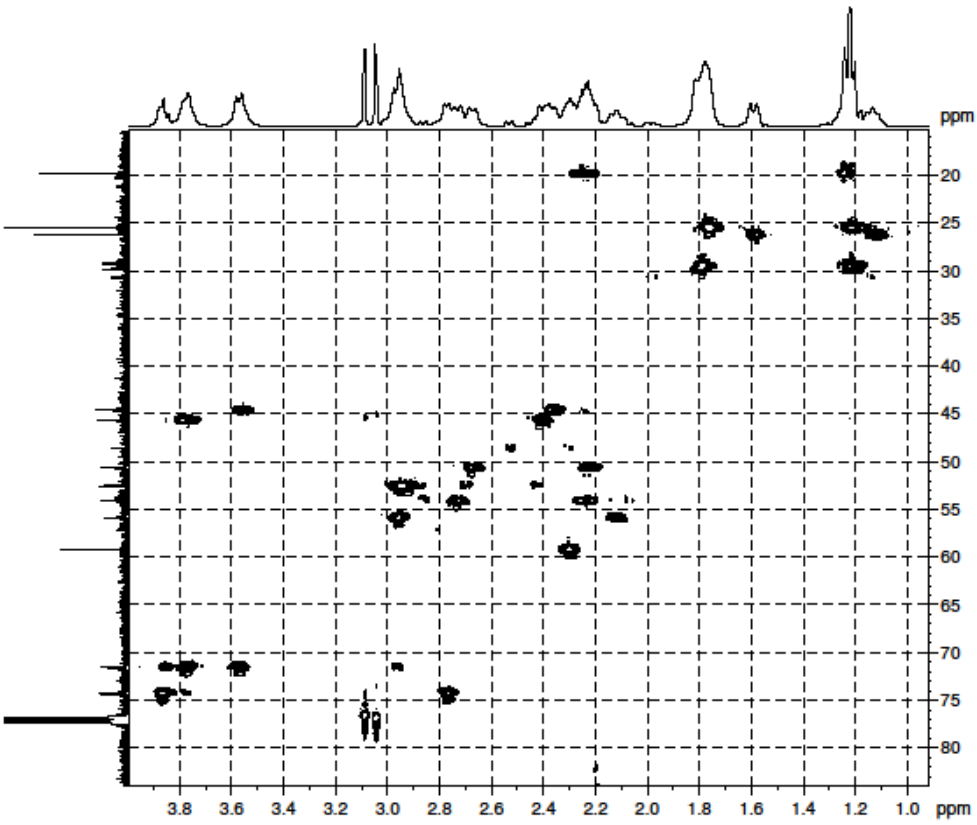
FigureS4. ^{13}C NMR spectrum of compounds **1b/2b**



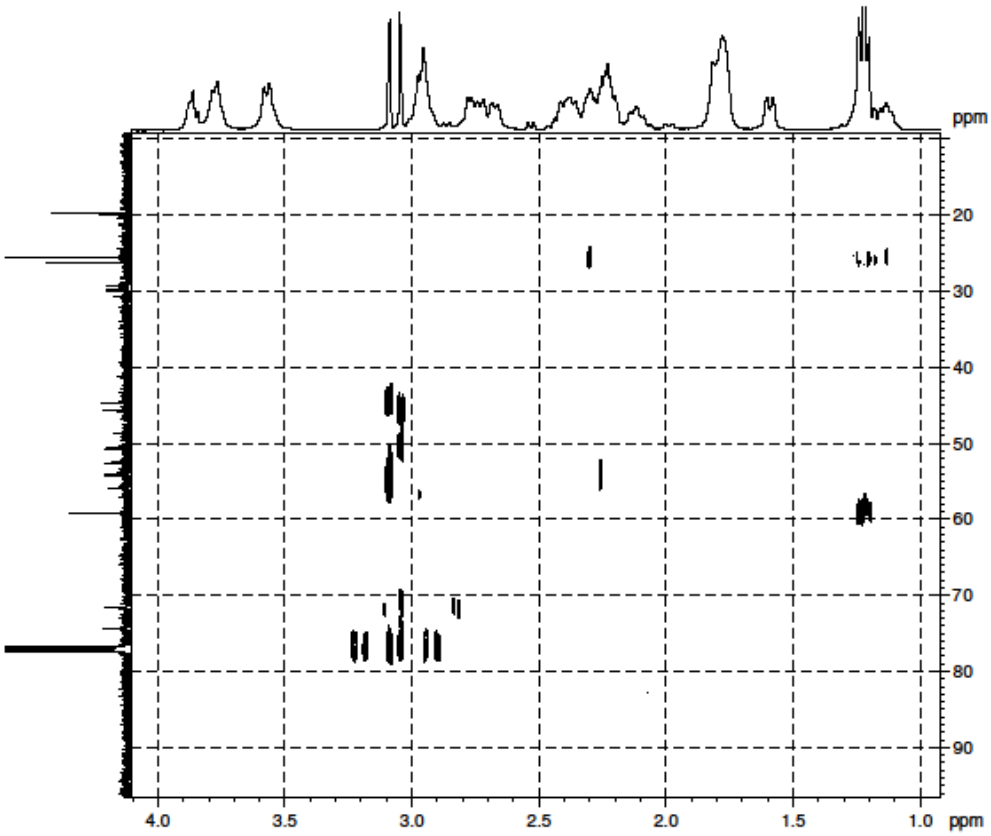
FigureS5. ^{1}H NMR spectrum of compound **1a**



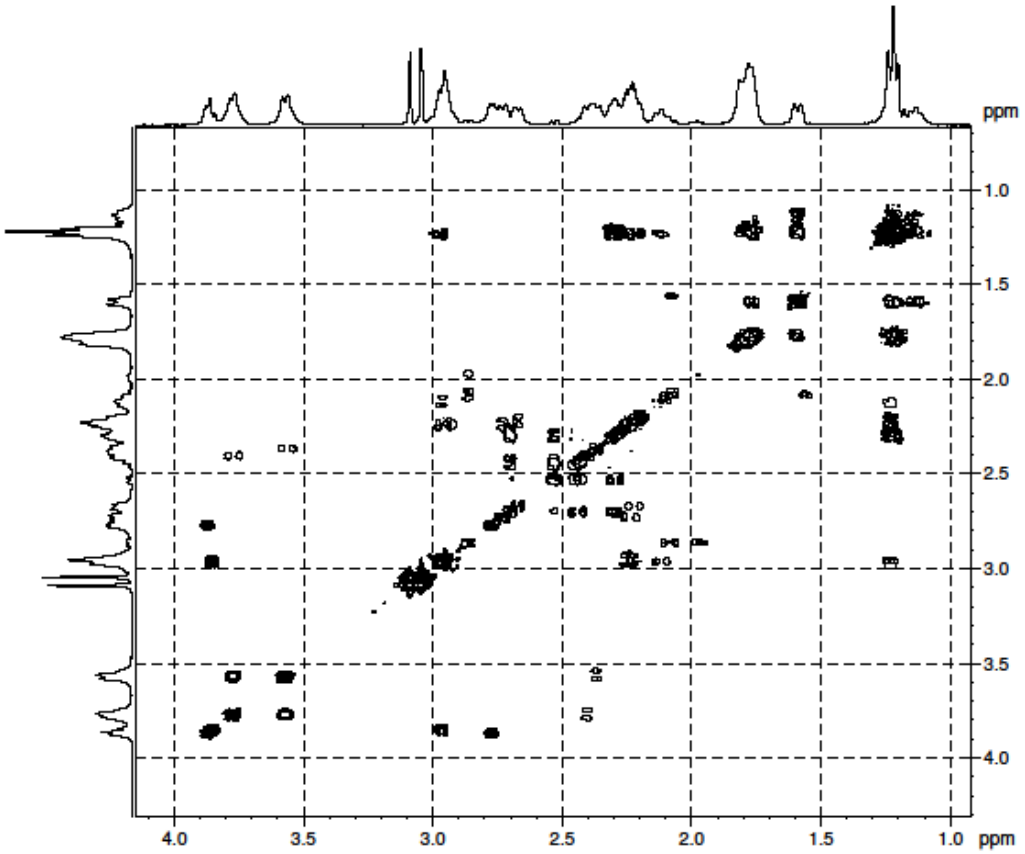
FigureS6. ^{13}C NMR spectrum of compound **1a**



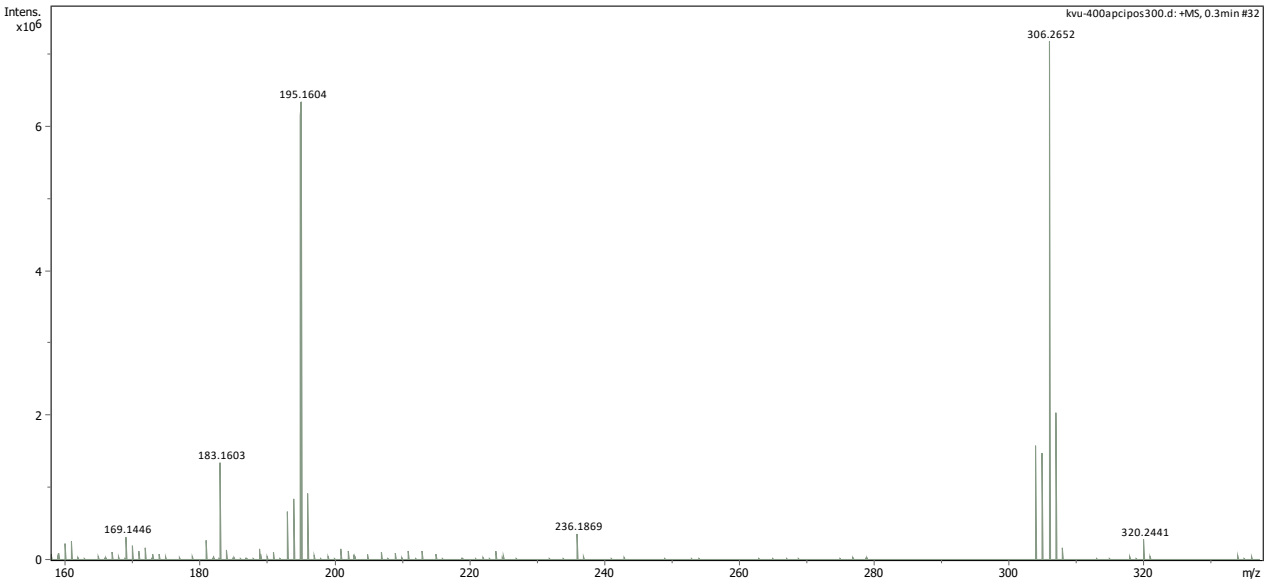
FigureS7. HSQC spectrum of compound **1a**



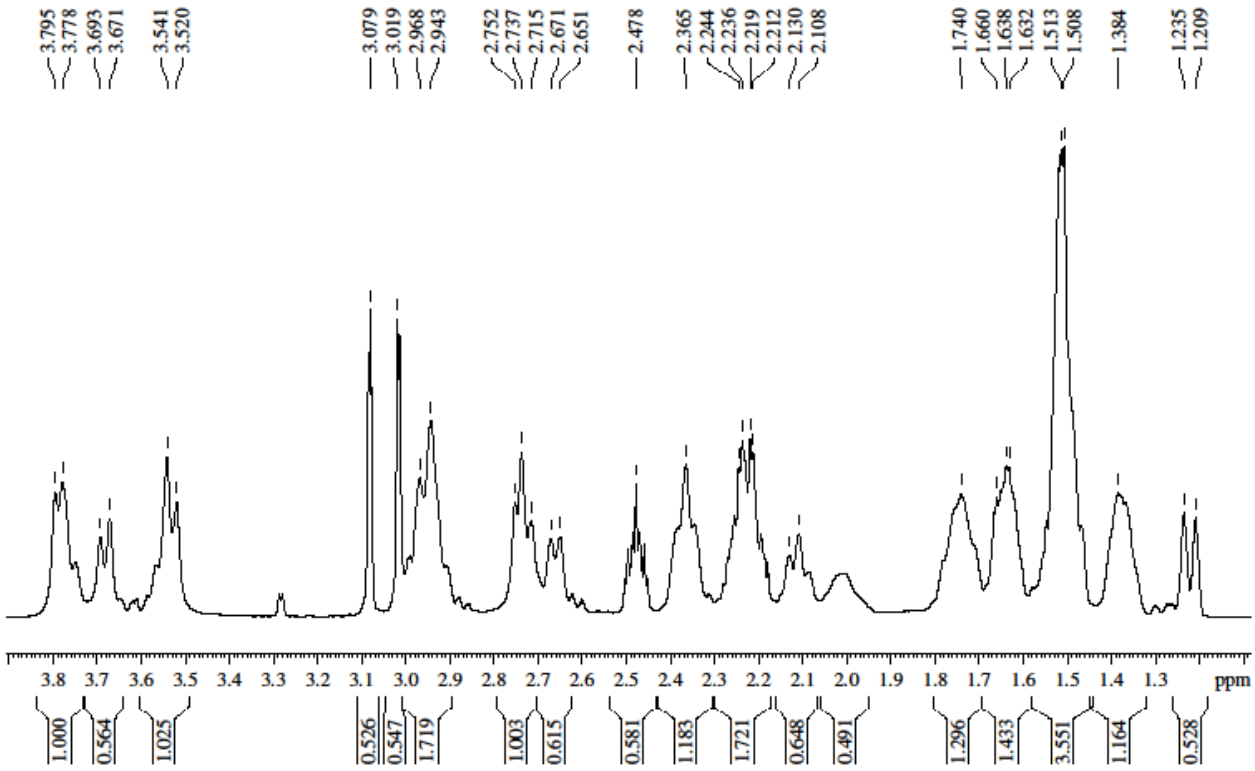
FigureS8. HMBC spectrum of compound **1a**



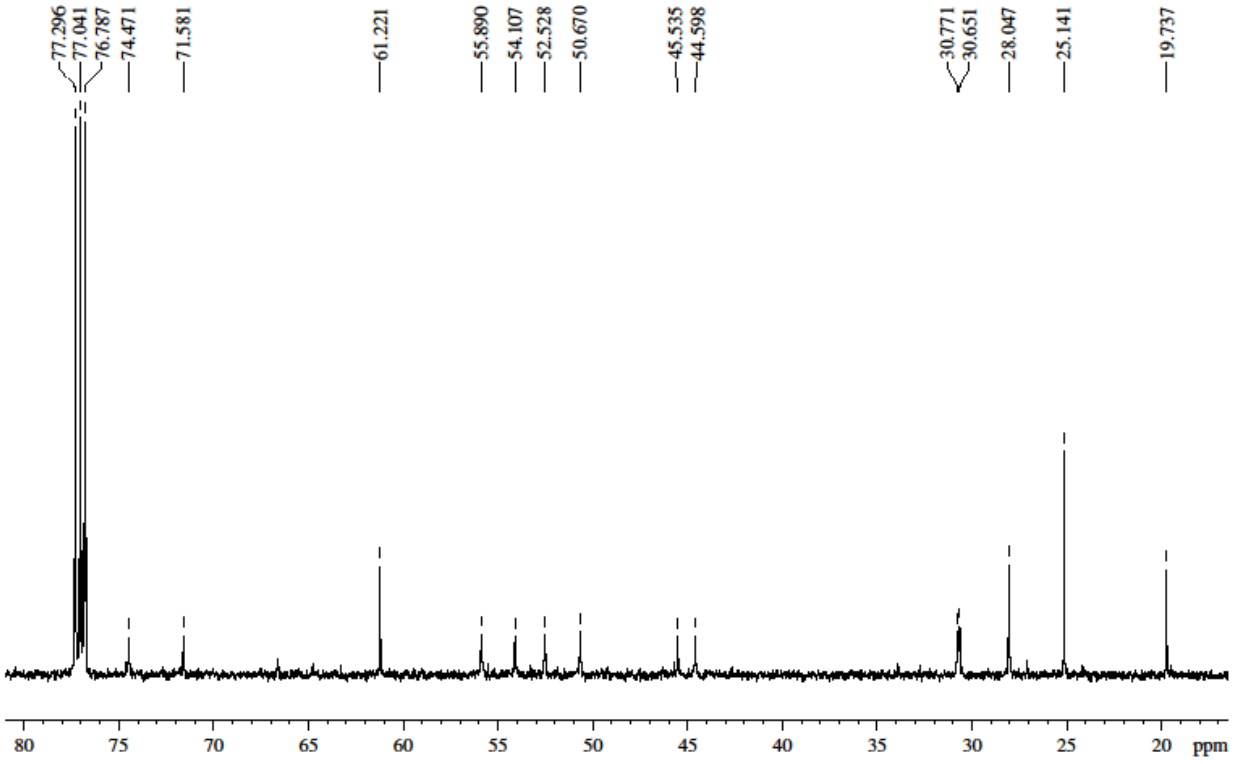
FigureS9. COSY spectrum of compound **1a**



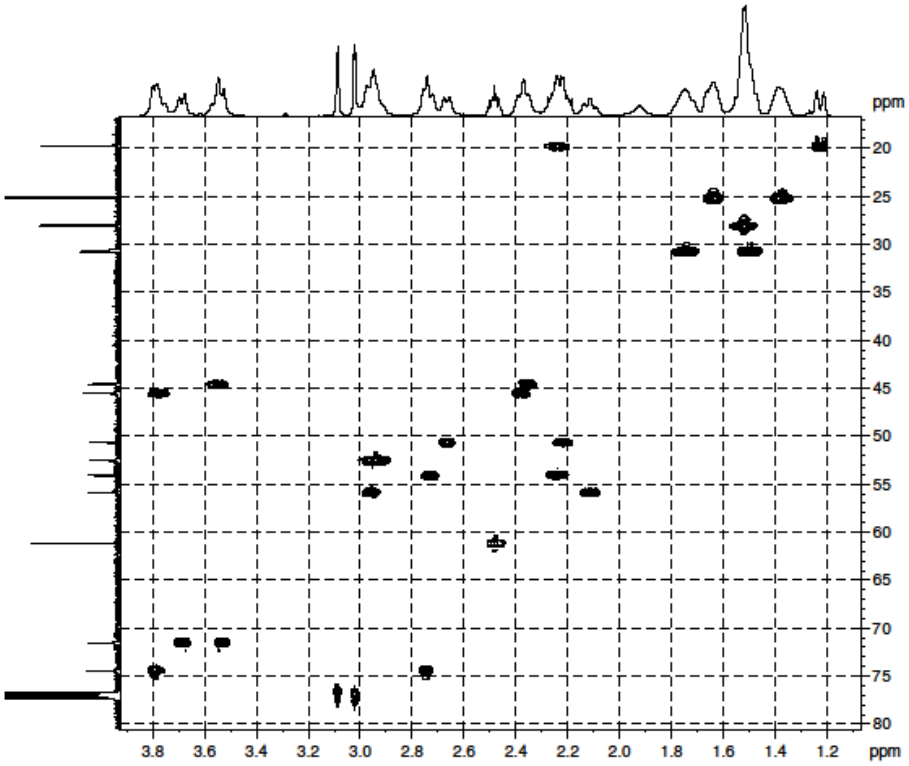
FigureS10. Mass spectrum of compound **1a**



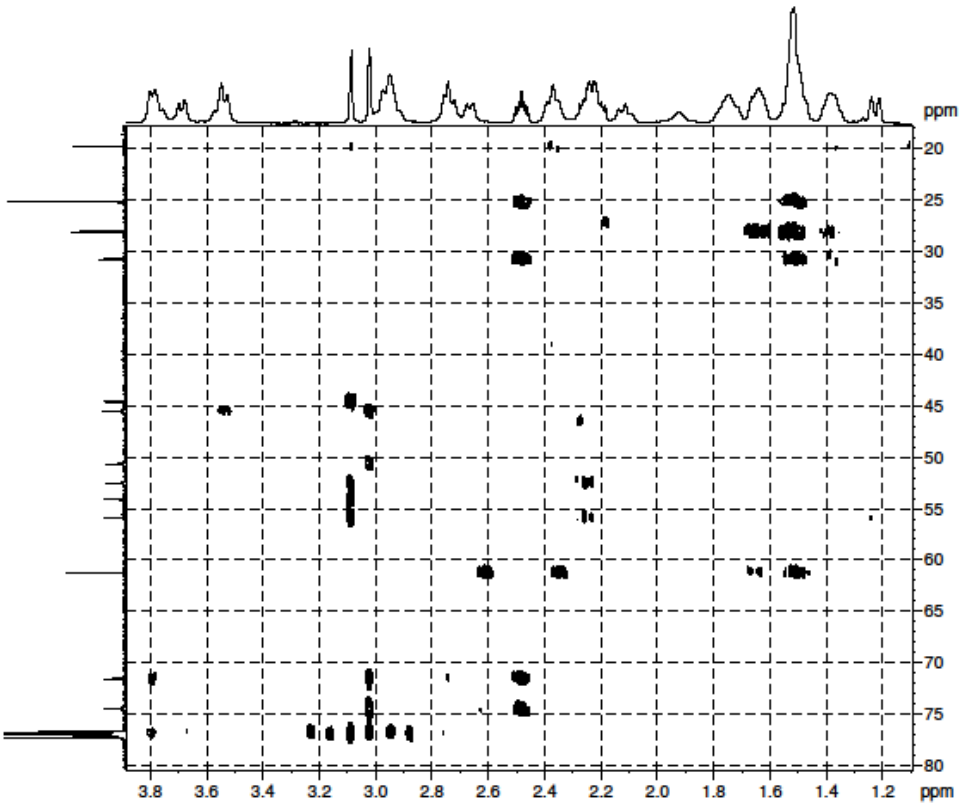
FigureS11. ^{1}H NMR spectrum of compound **1c**



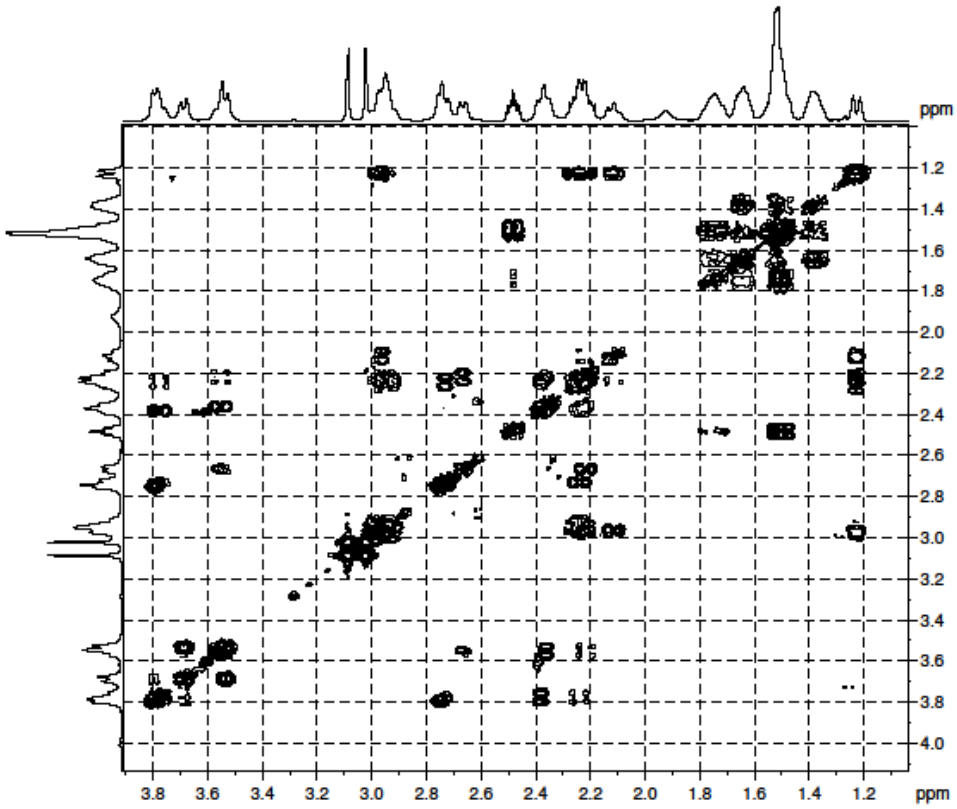
FigureS12. ^{13}C NMR spectrum of compound **1c**



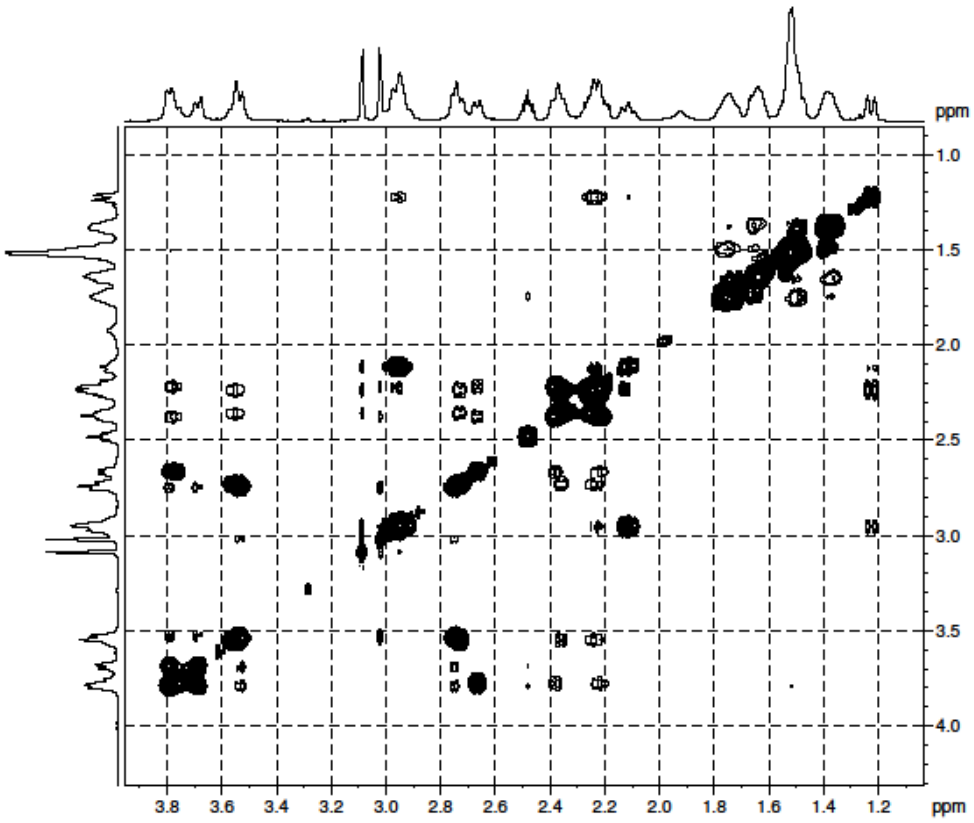
FigureS13. HSQC spectrum of compound **1c**



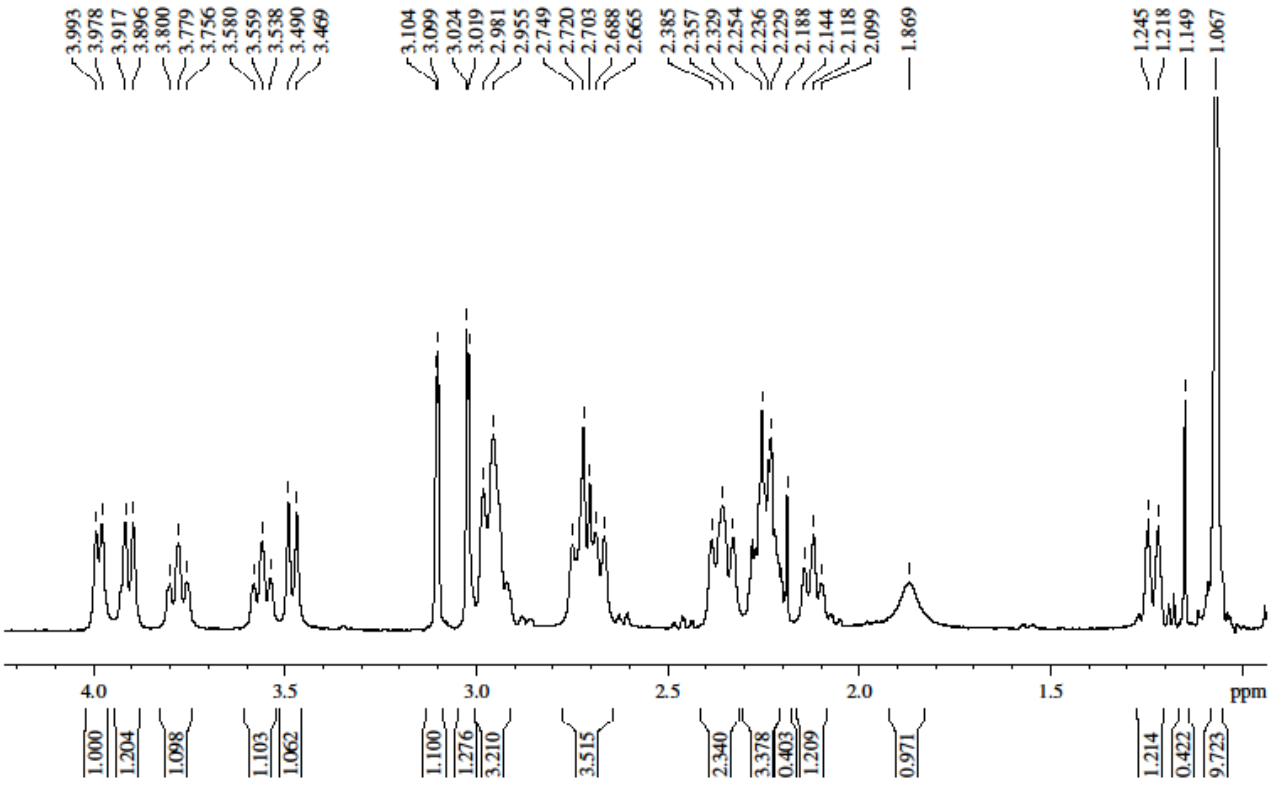
FigureS14. HMBC spectrum of compound **1c**



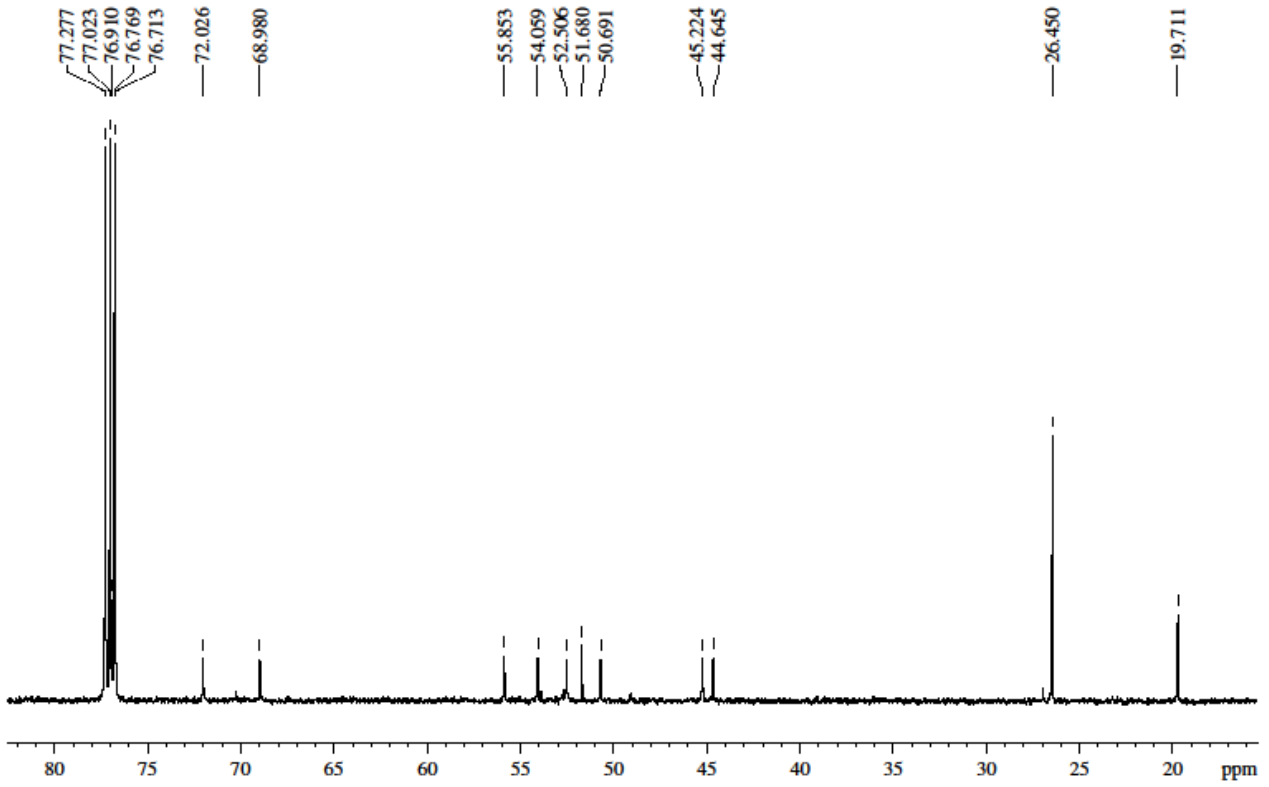
FigureS15. COSY spectrum of compound **1c**



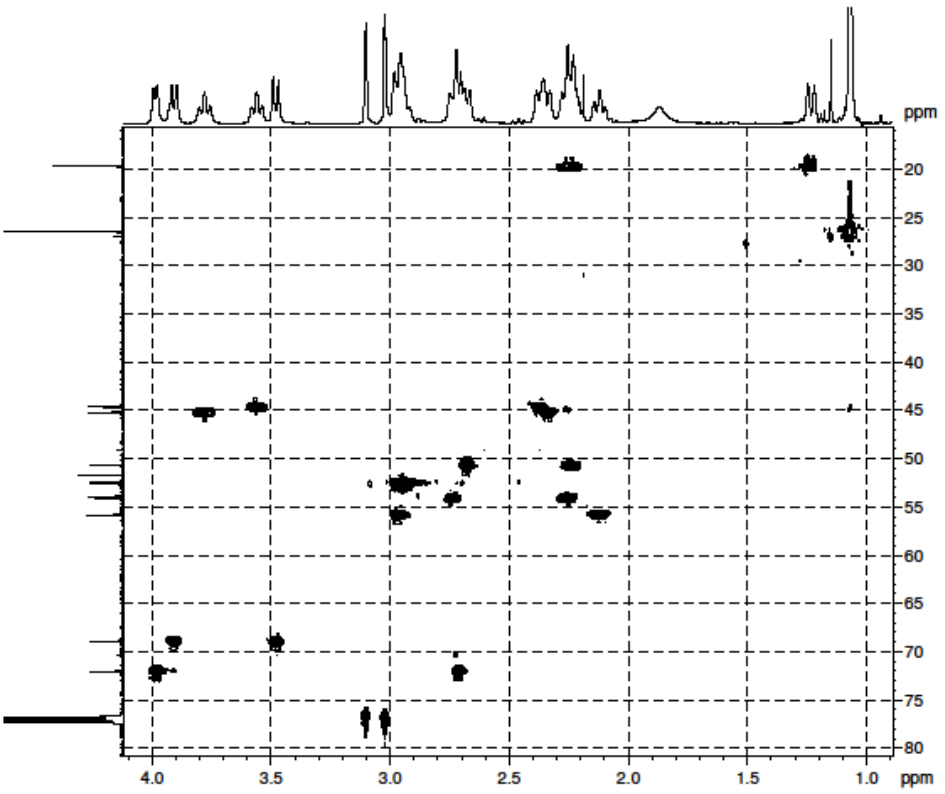
FigureS16. NOESY spectrum of compound **1c**



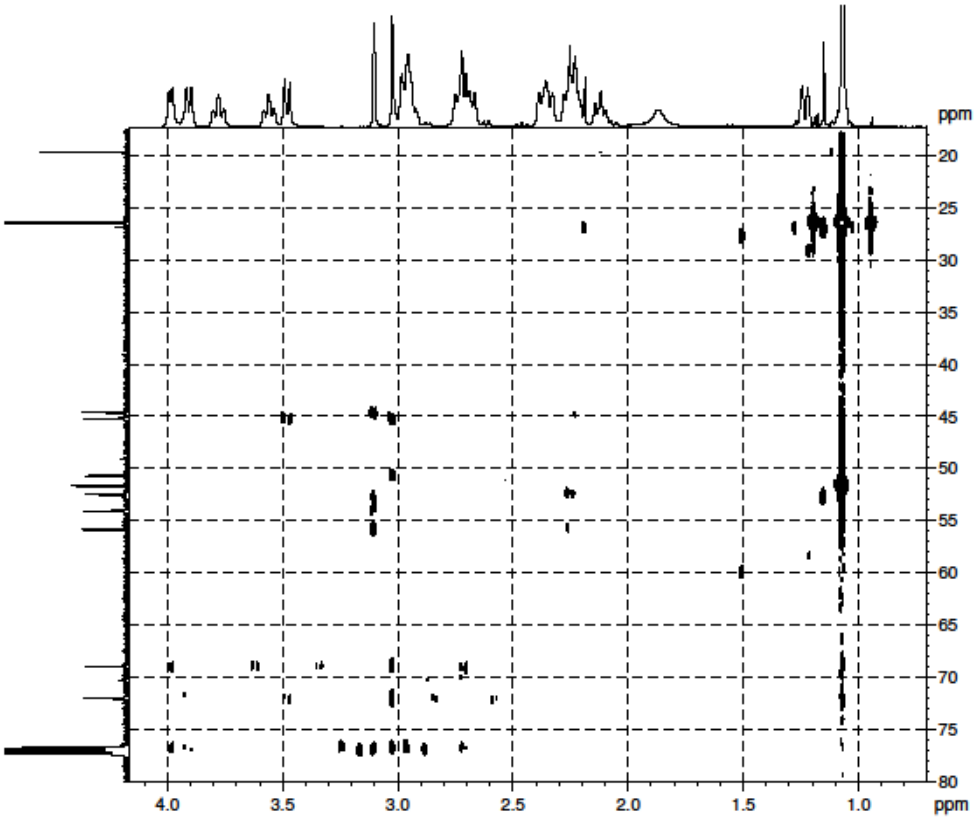
FigureS17. ^{1}H NMR spectrum of compound **1d**



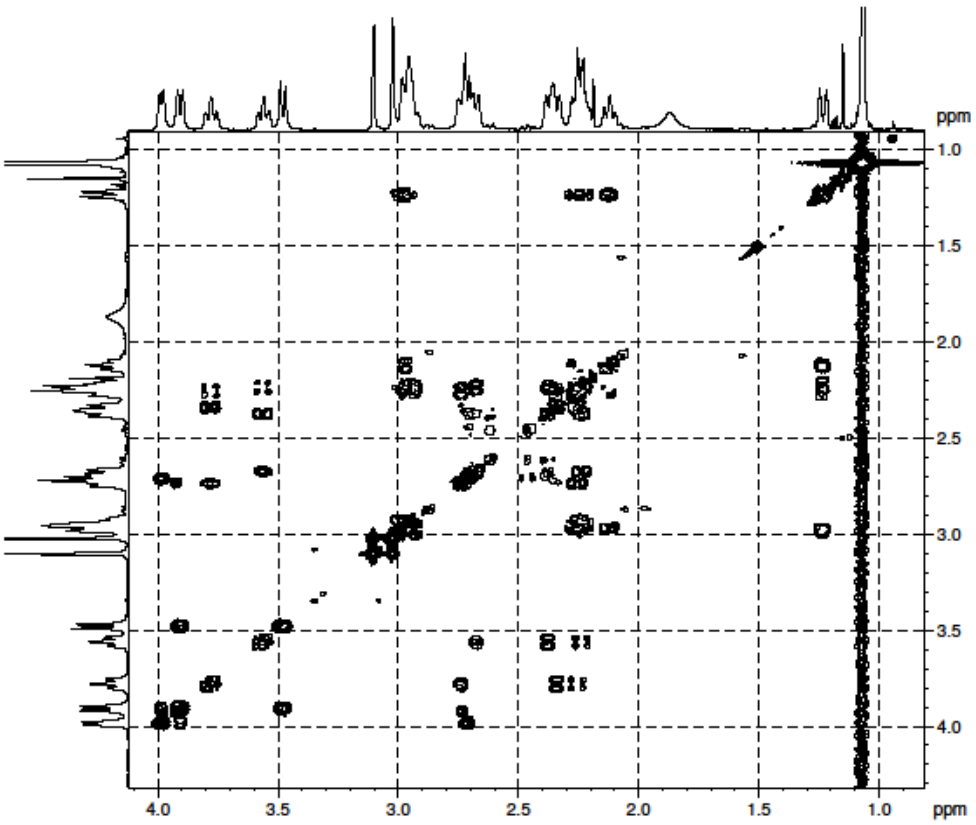
FigureS18. ^{13}C NMR spectrum of compound **1d**



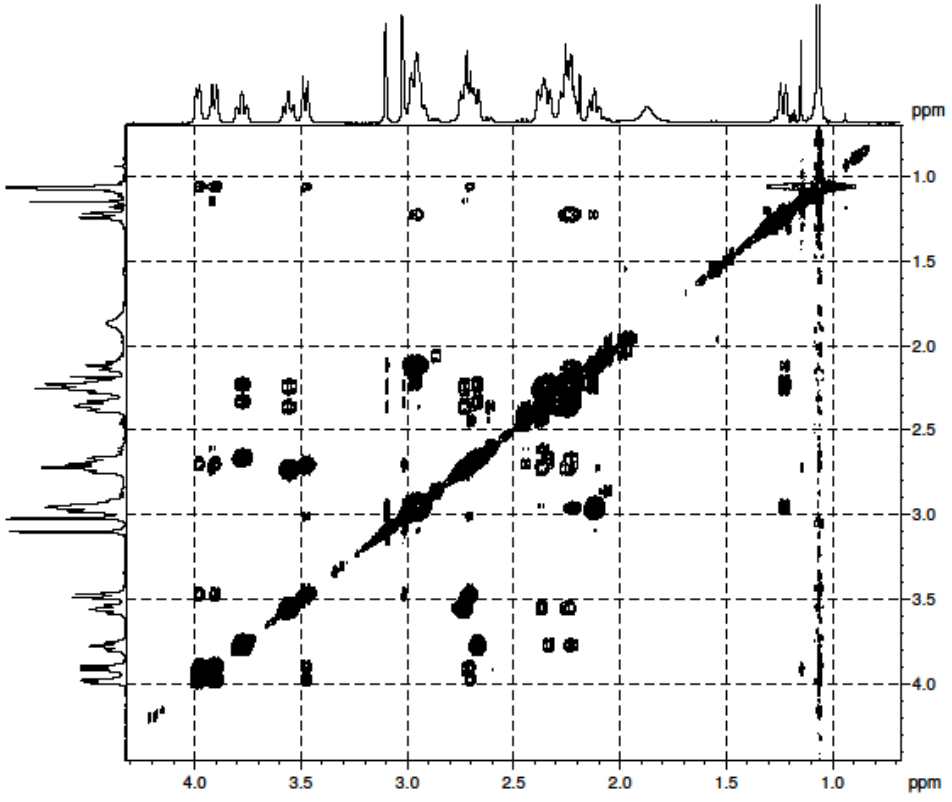
FigureS19. HSQC spectrum of compound **1d**



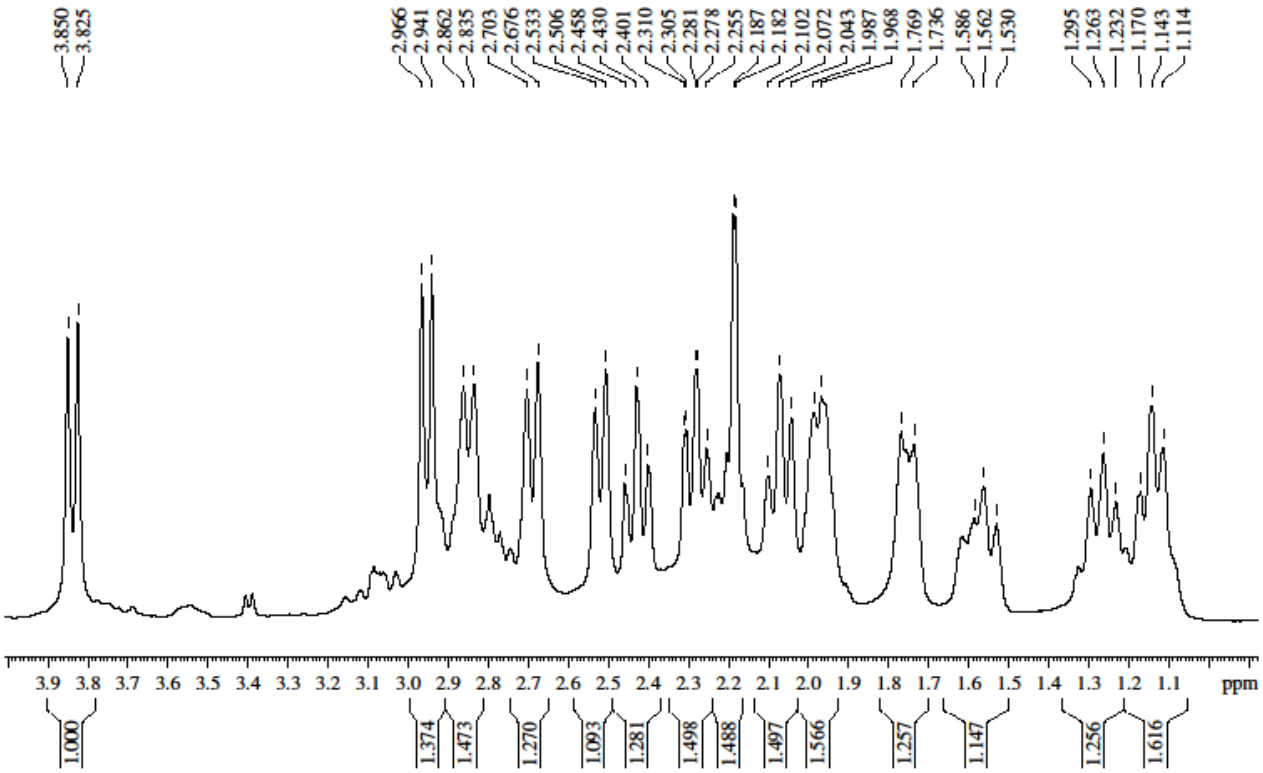
FigureS20. HMBC spectrum of compound **1d**



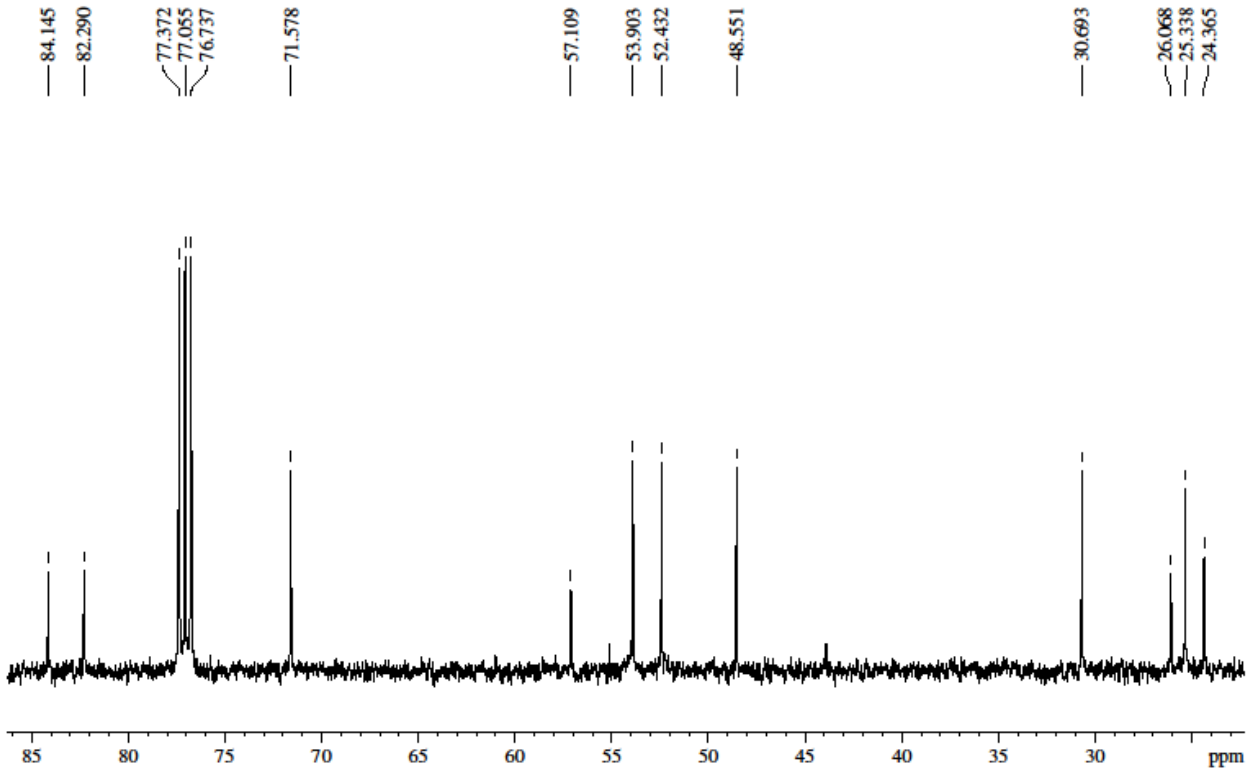
FigureS21. COSY spectrum of compound **1d**



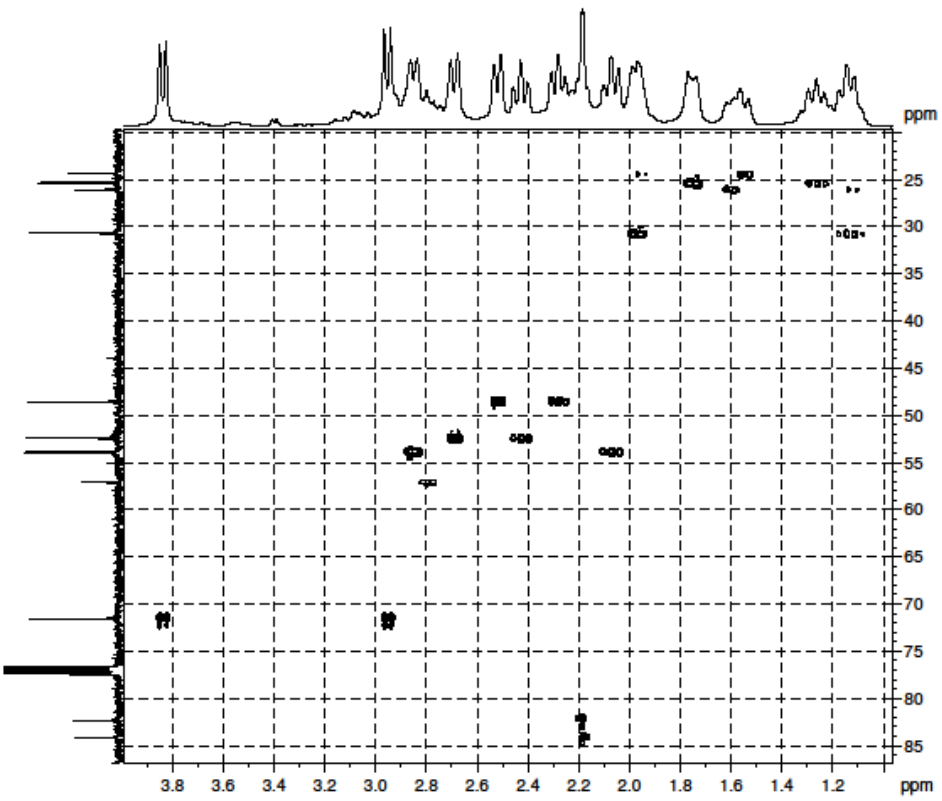
FigureS22. NOESY spectrum of compound **1d**



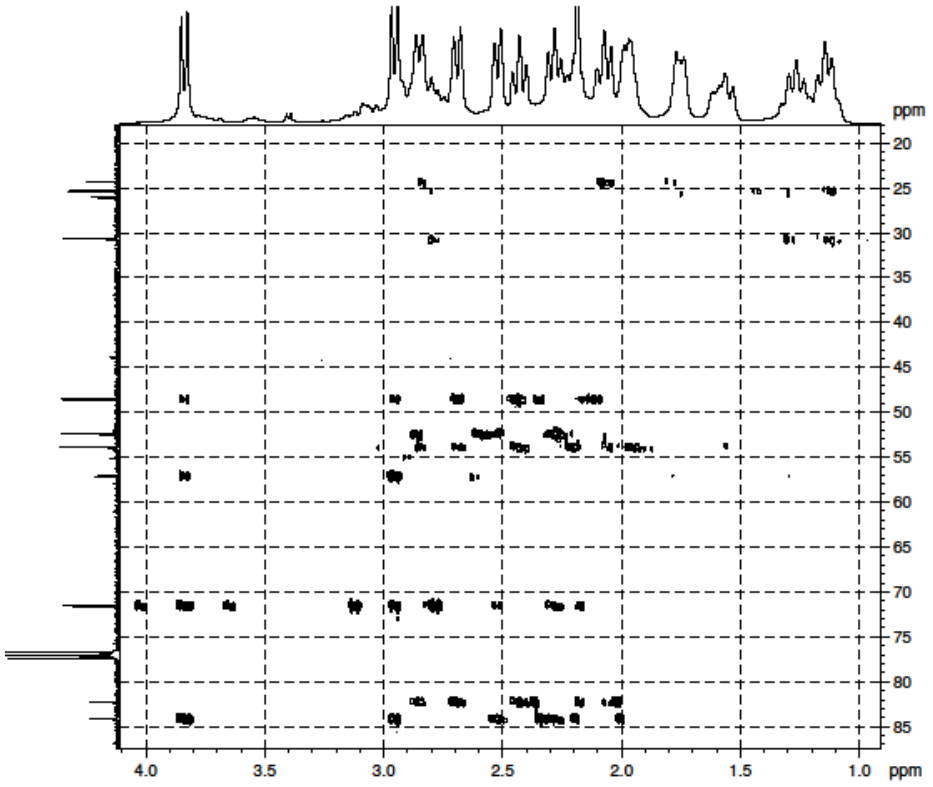
FigureS23. ^{1}H NMR spectrum of compound **2a**



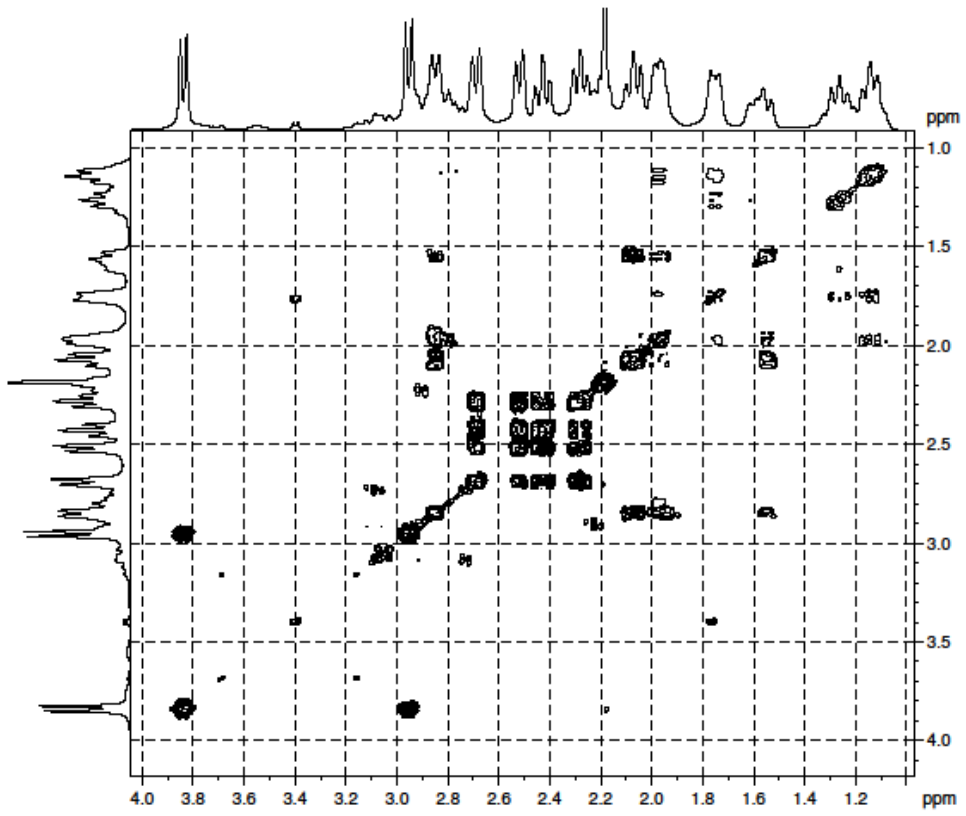
FigureS24. ^{13}C NMR spectrum of compound **2a**



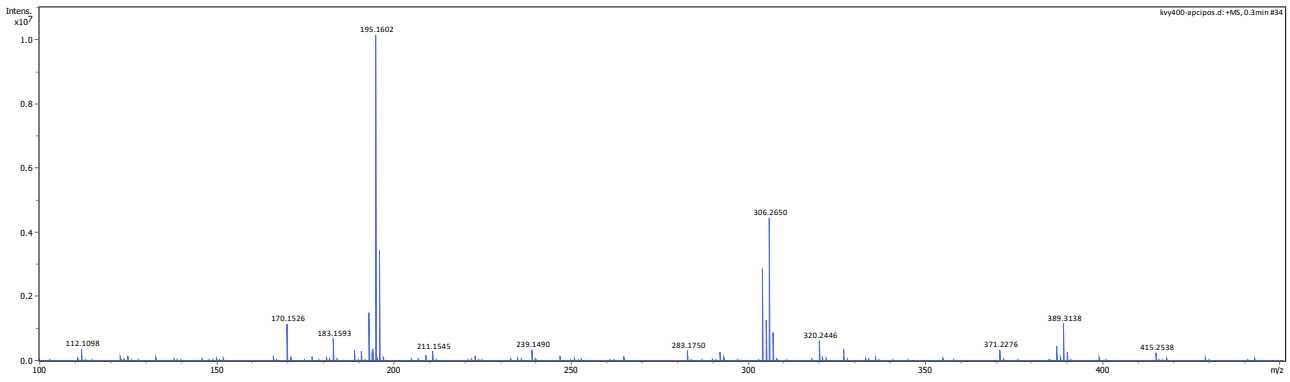
FigureS25. HSQC spectrum of compound **2a**



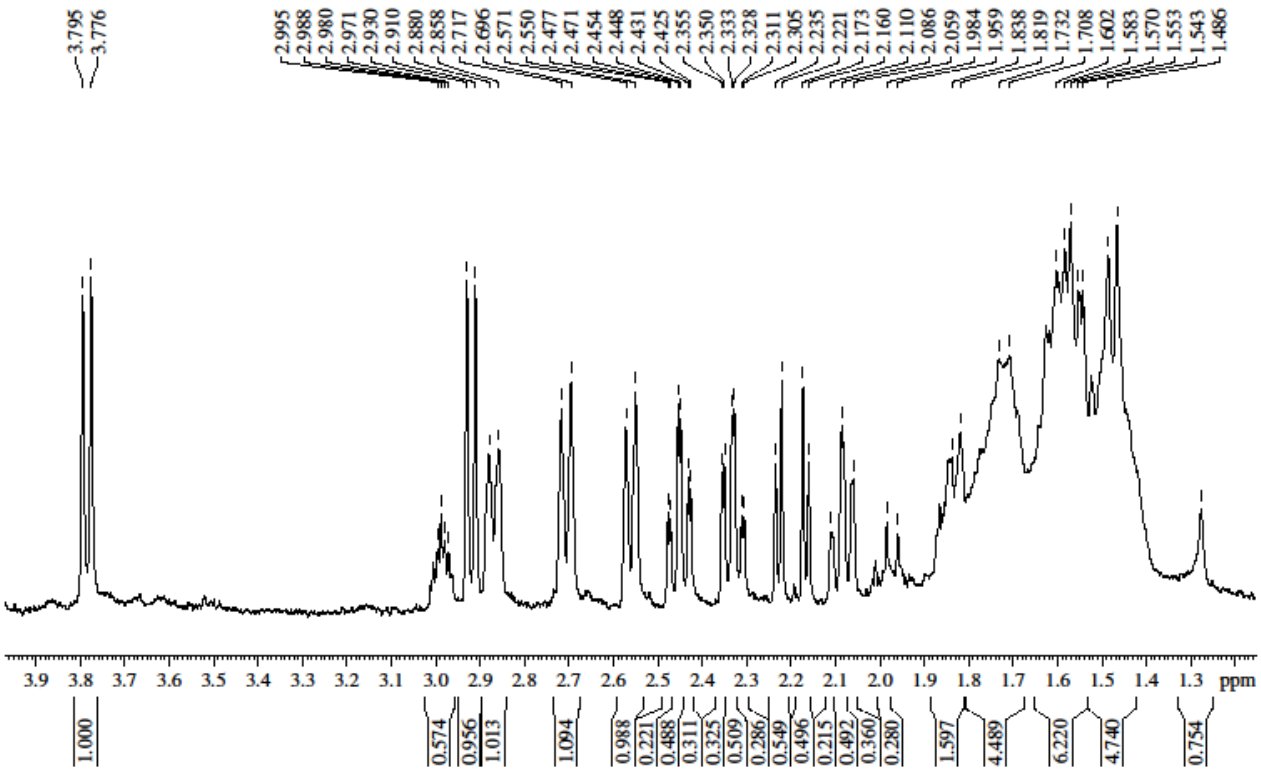
FigureS26. HMBC spectrum of compound **2a**



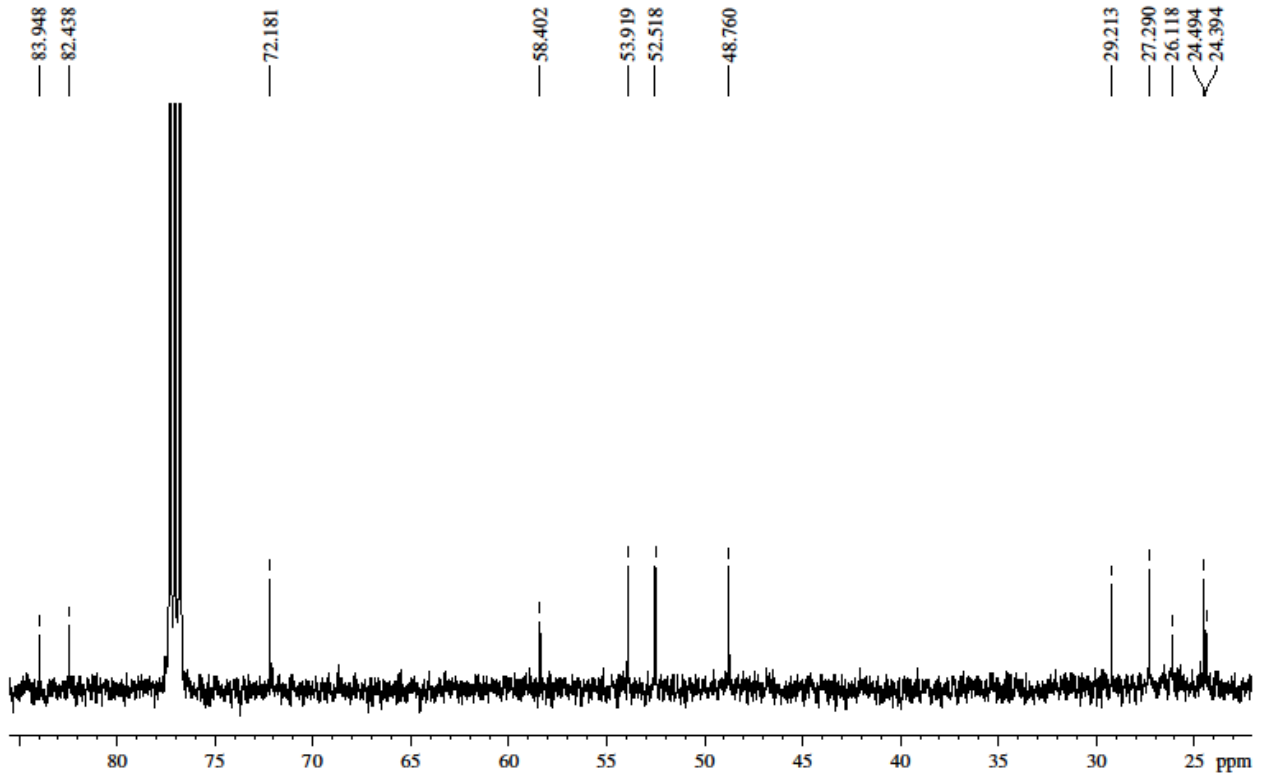
FigureS27. COSY spectrum of compound **2a**



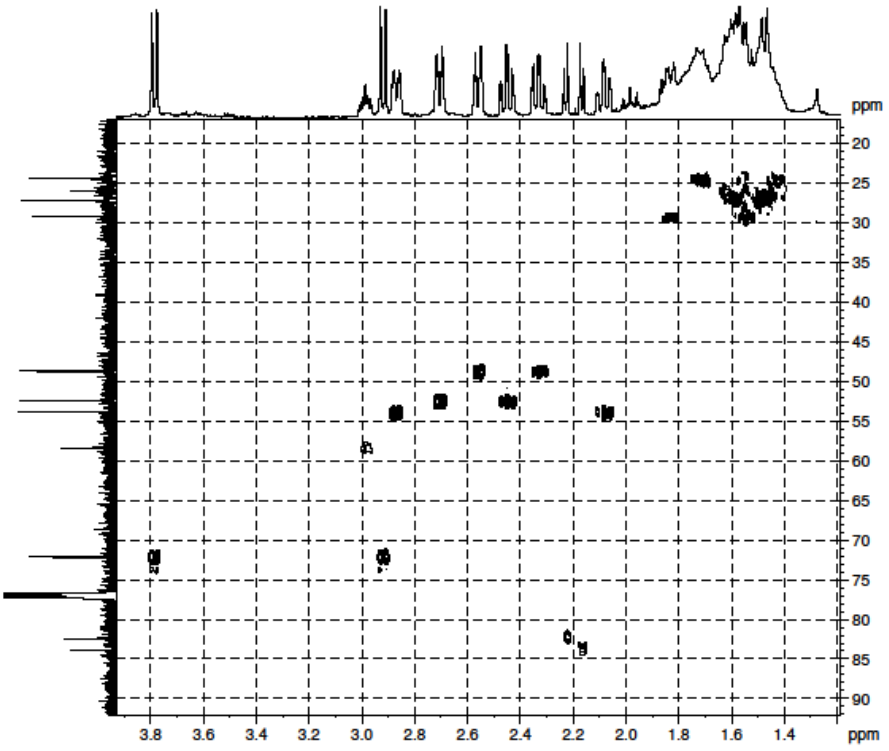
FigureS28. Mass spectrum of compound **2a**



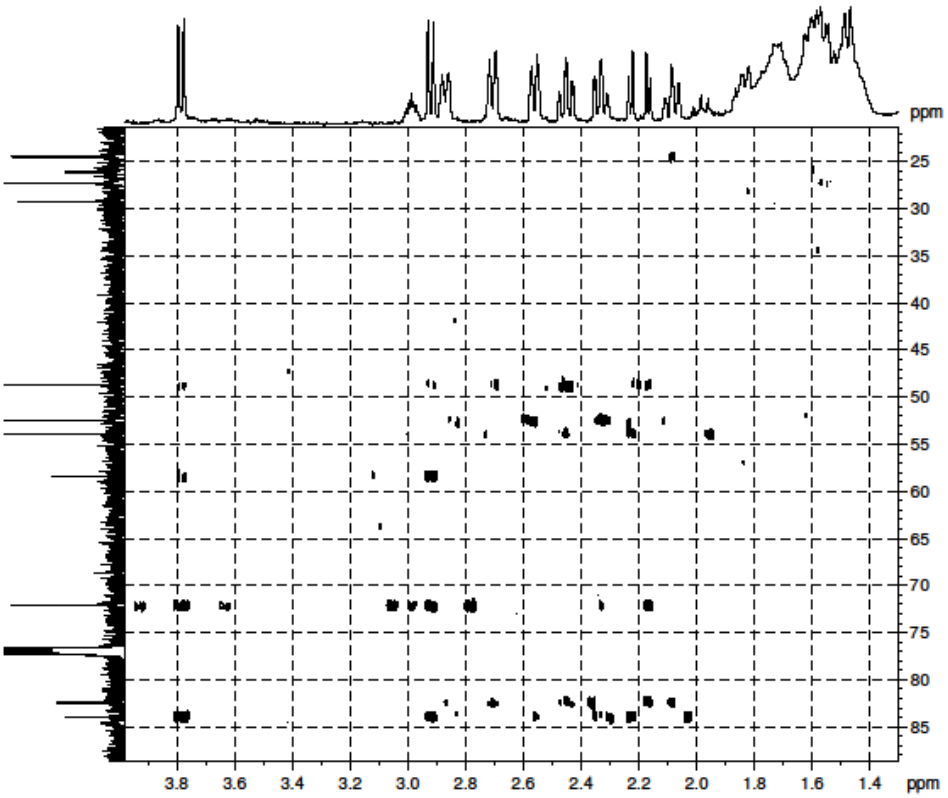
FigureS29. ^{1}H NMR spectrum of compound **2b**



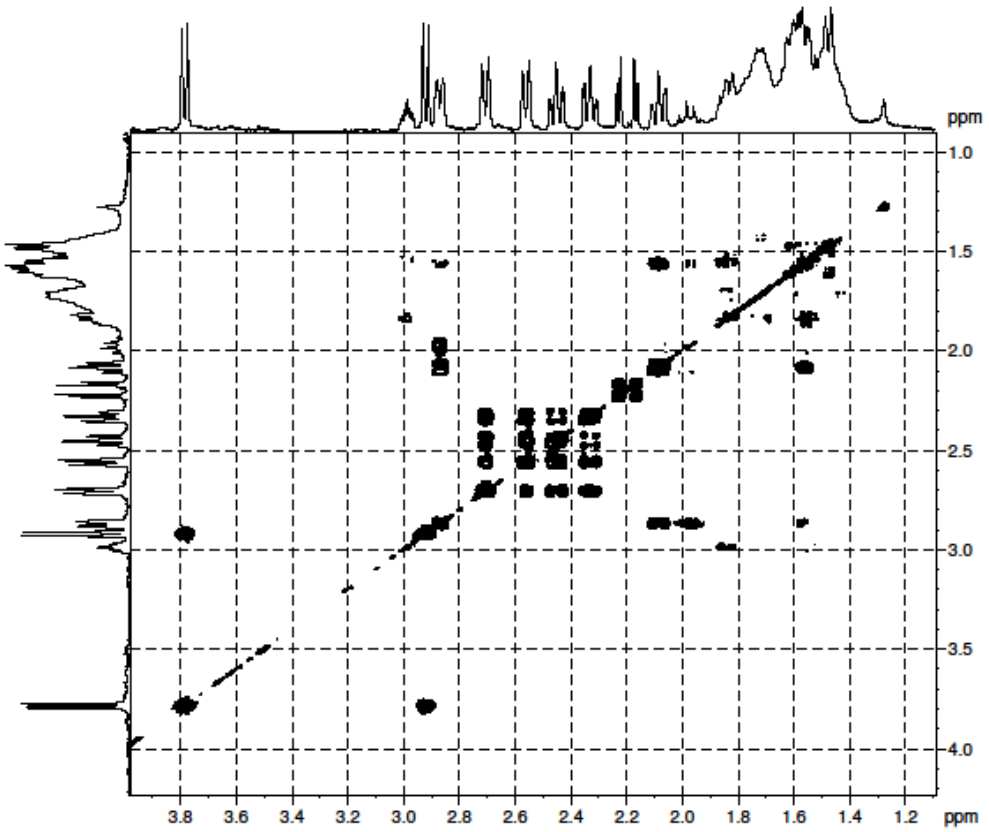
FigureS30. ^{13}C NMR spectrum of compound **2b**



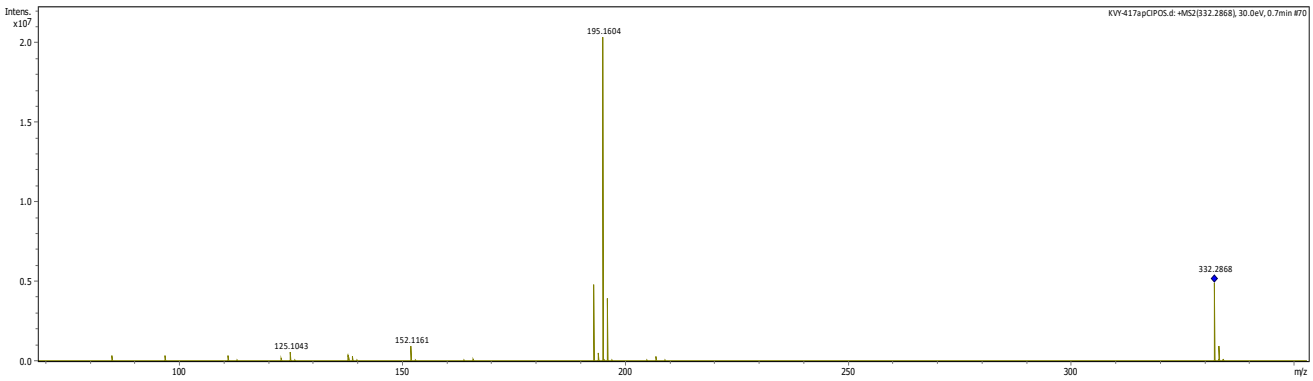
FigureS31. HSQC spectrum of compound **2b**



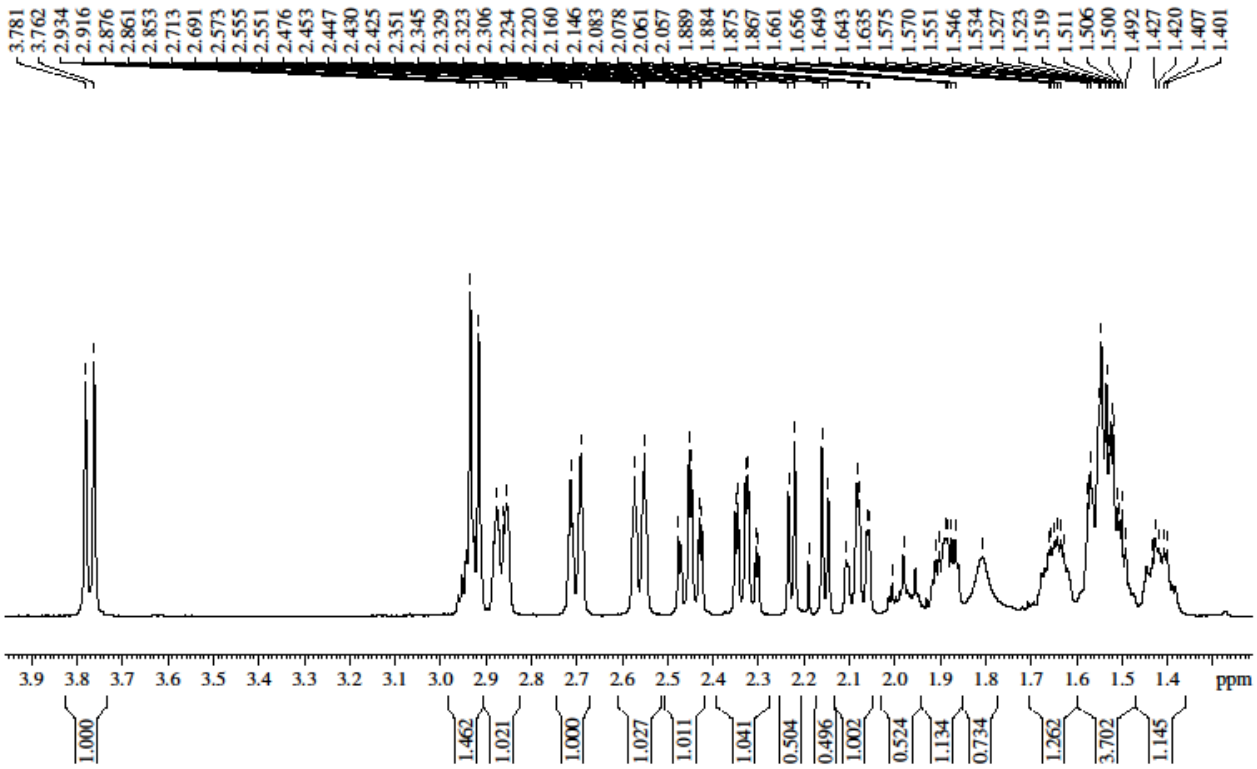
FigureS32. HMBC spectrum of compound **2b**



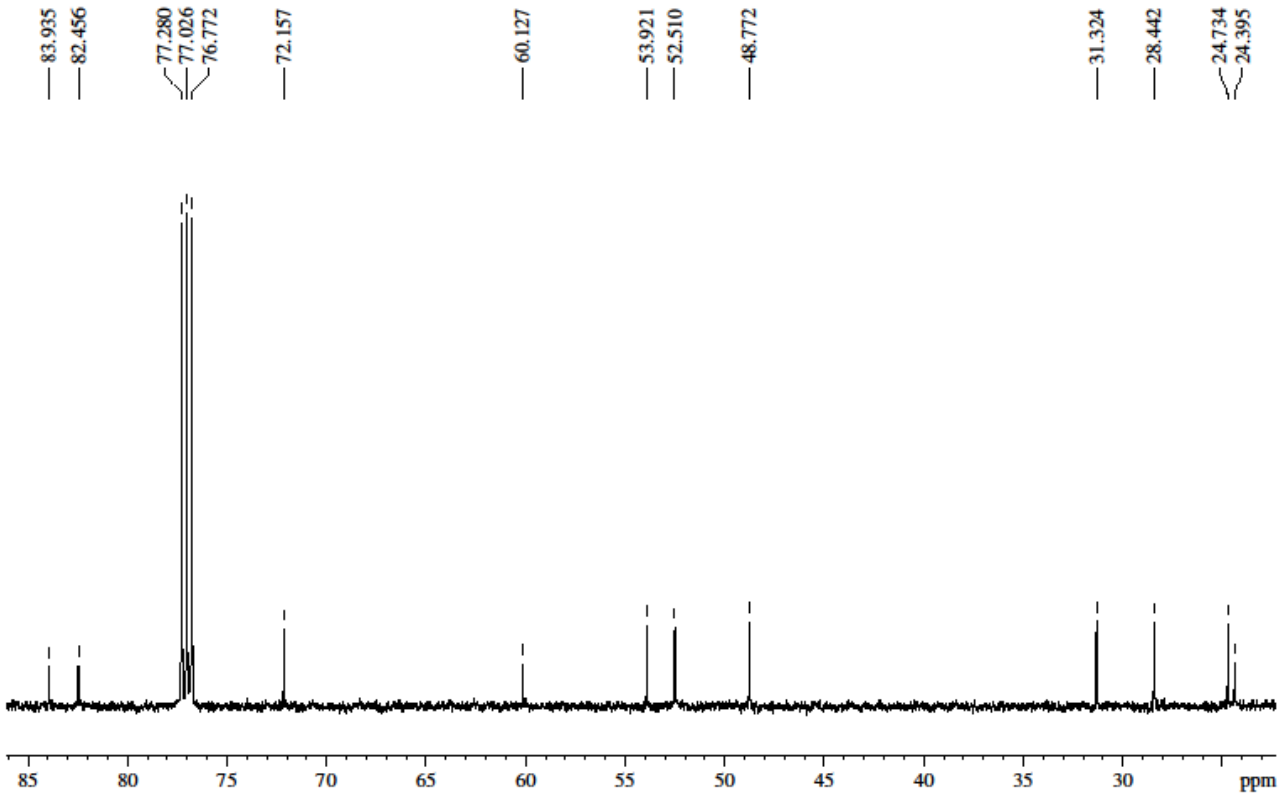
FigureS33. COSY spectrum of compound **2b**



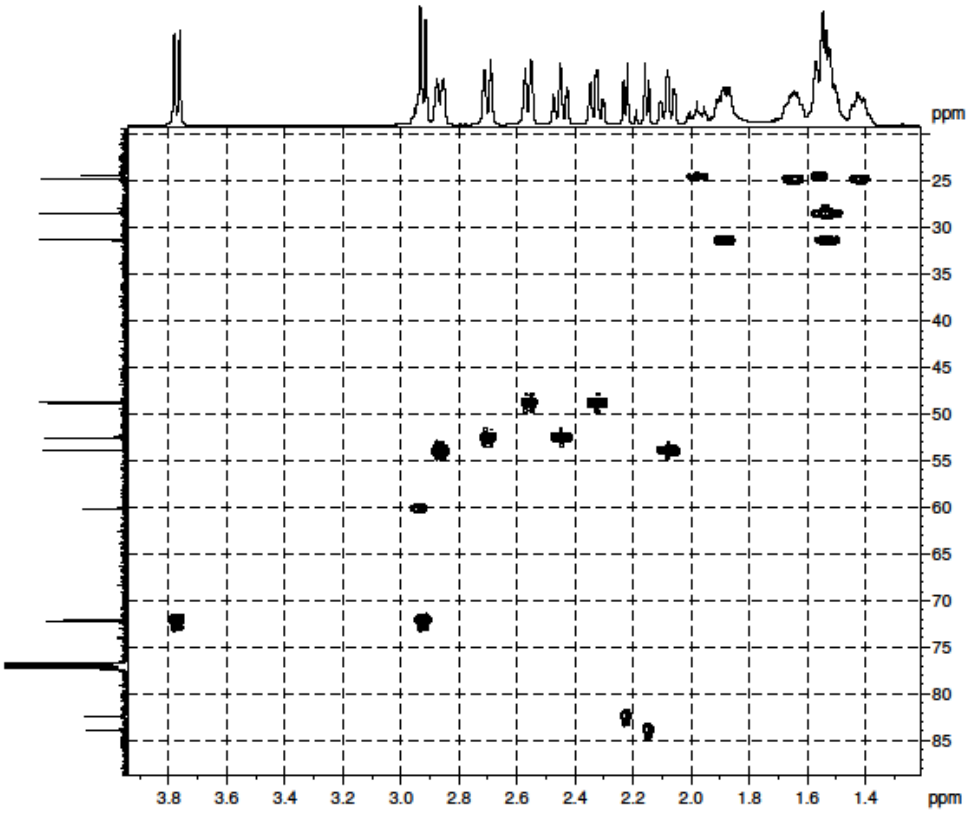
FigureS34. Mass spectrum of compound **2b**



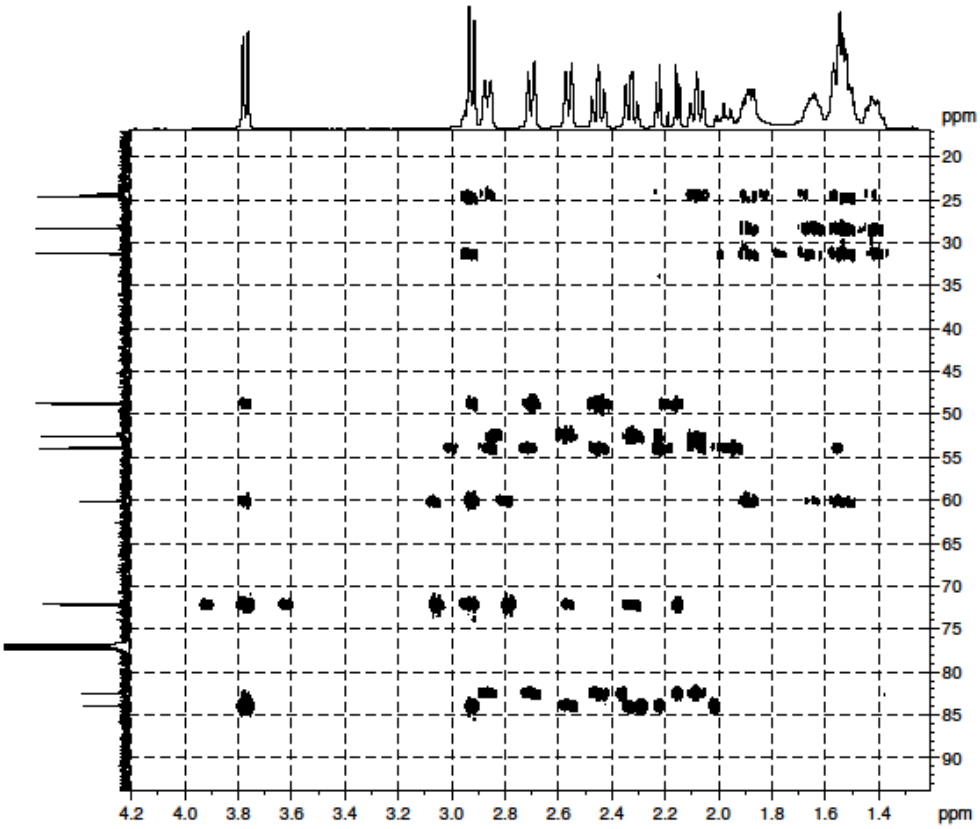
FigureS35. ^{1}H NMR spectrum of compound **2c**



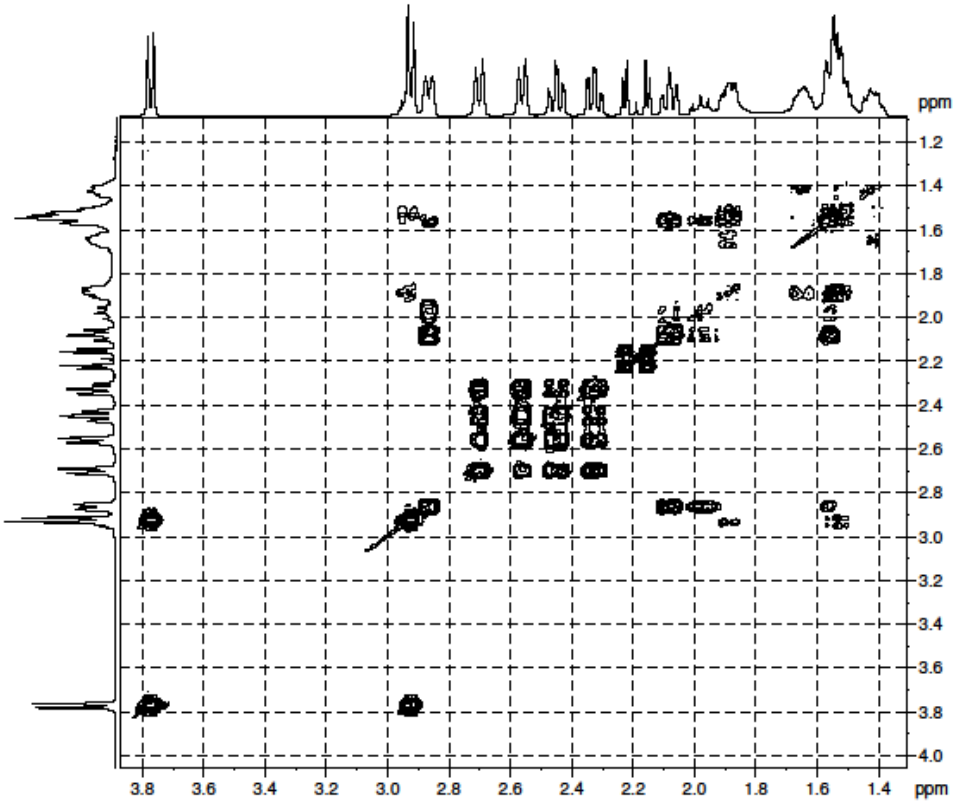
FigureS36. ^{13}C NMR spectrum of compound **2c**



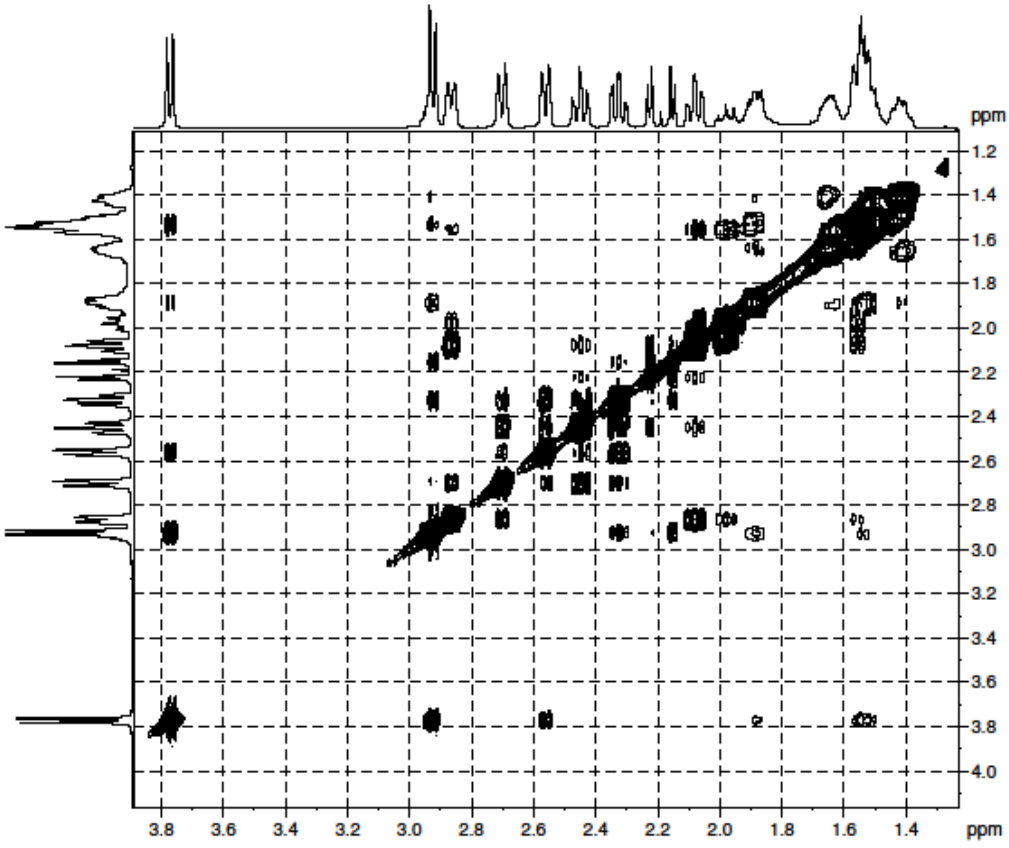
FigureS37. HSQC spectrum of compound **2c**



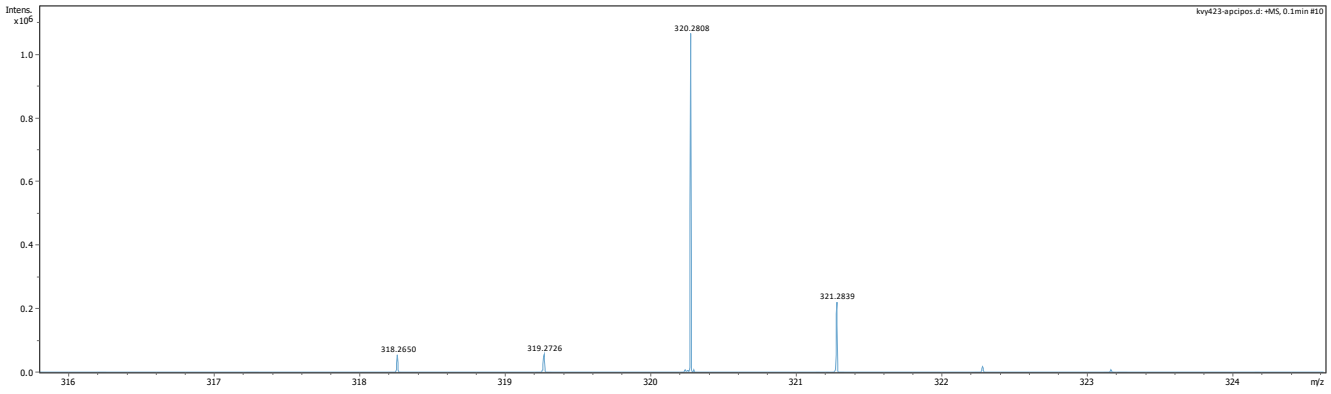
FigureS38. HMBC spectrum of compound **2c**



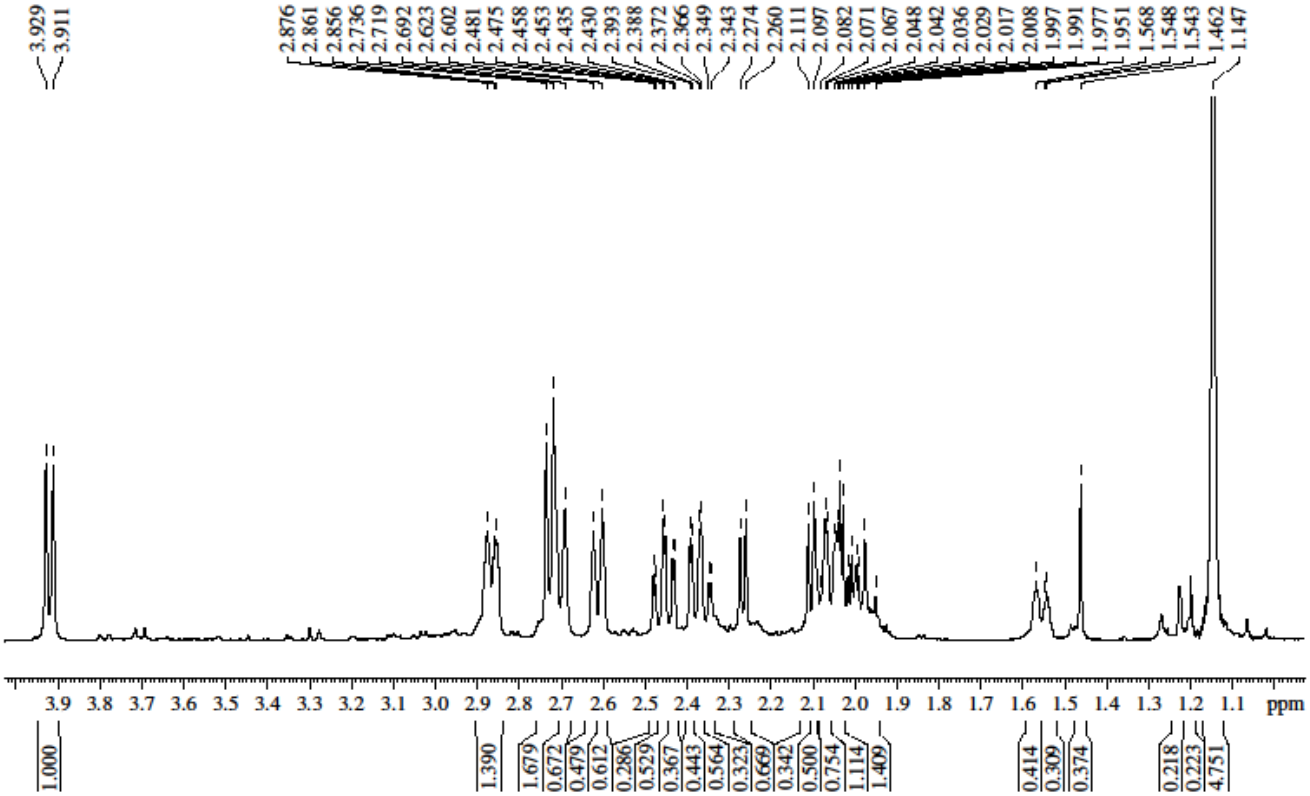
FigureS39. COSY spectrum of compound **2c**



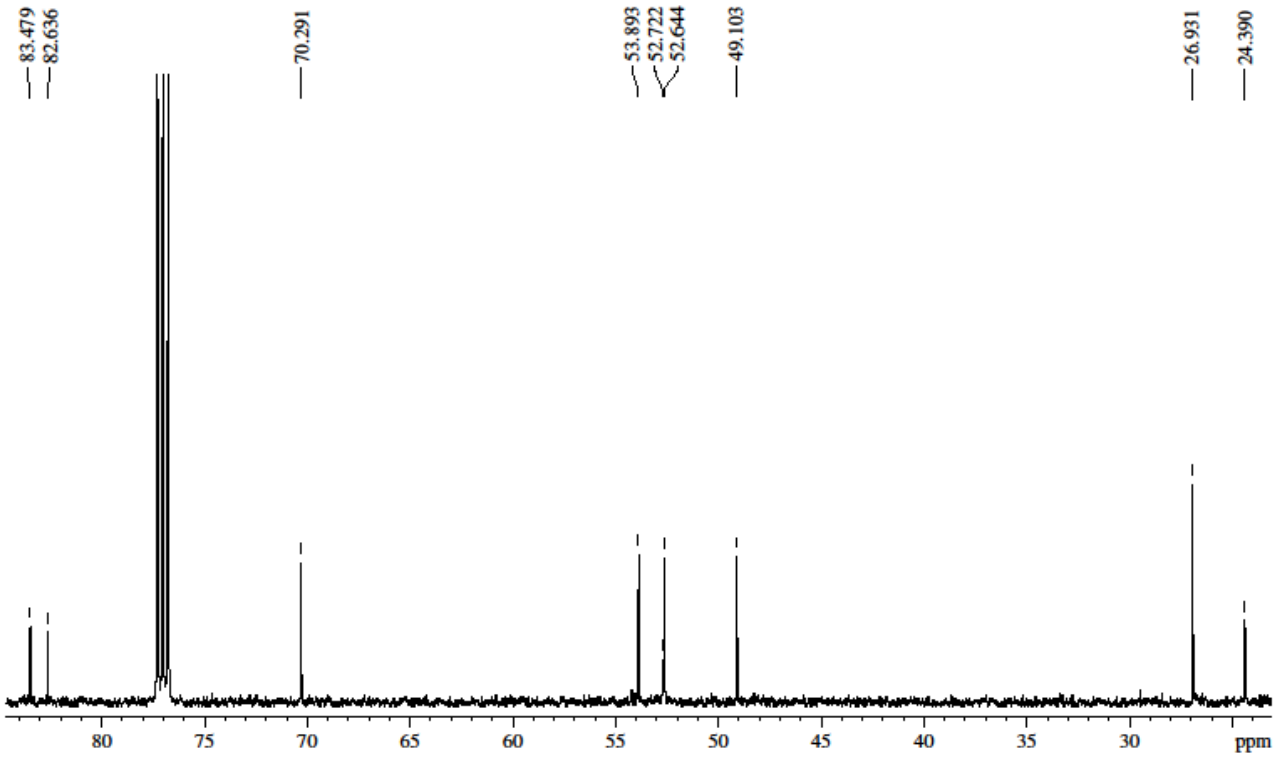
FigureS40. NOESY spectrum of compound **2c**



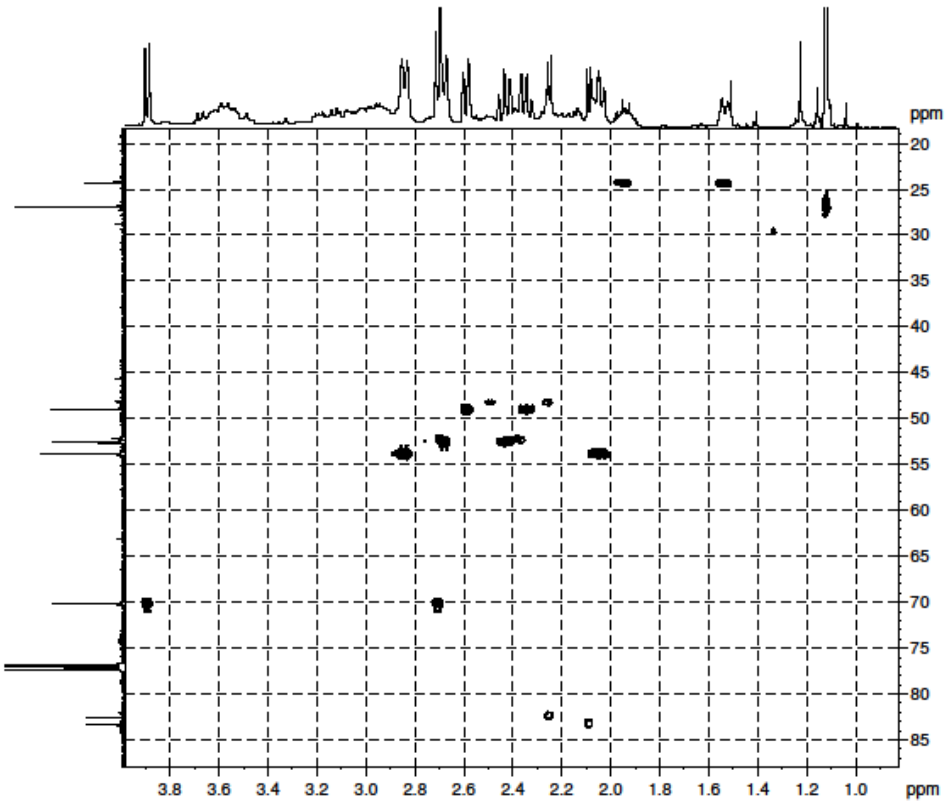
FigureS41. Mass spectrum of compound **2c**



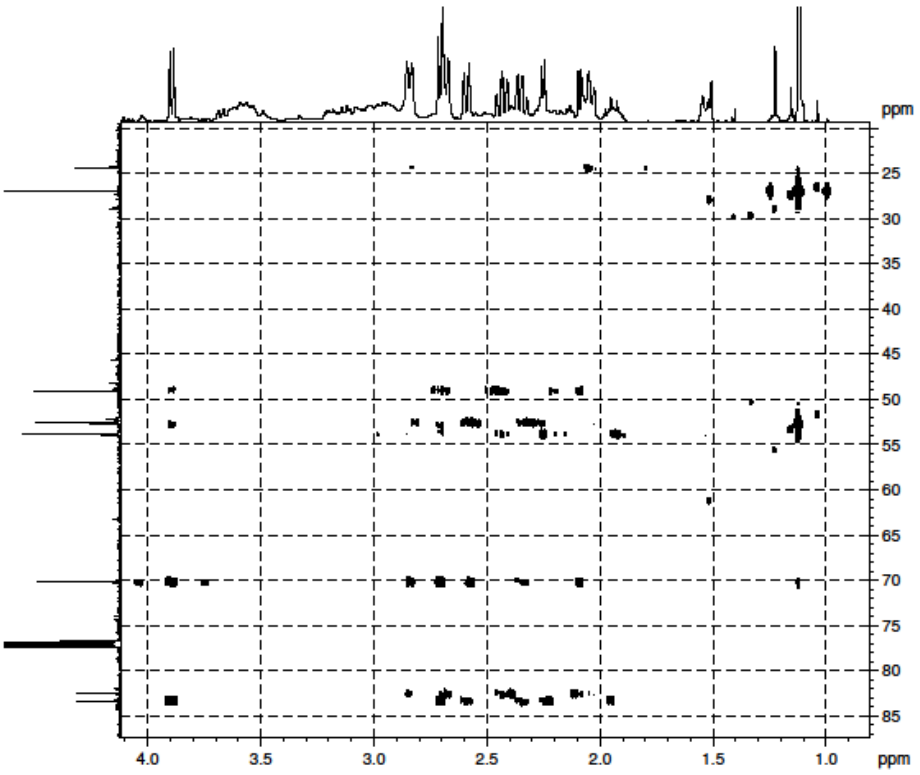
FigureS42. ^{1}H NMR spectrum of compound **2d**



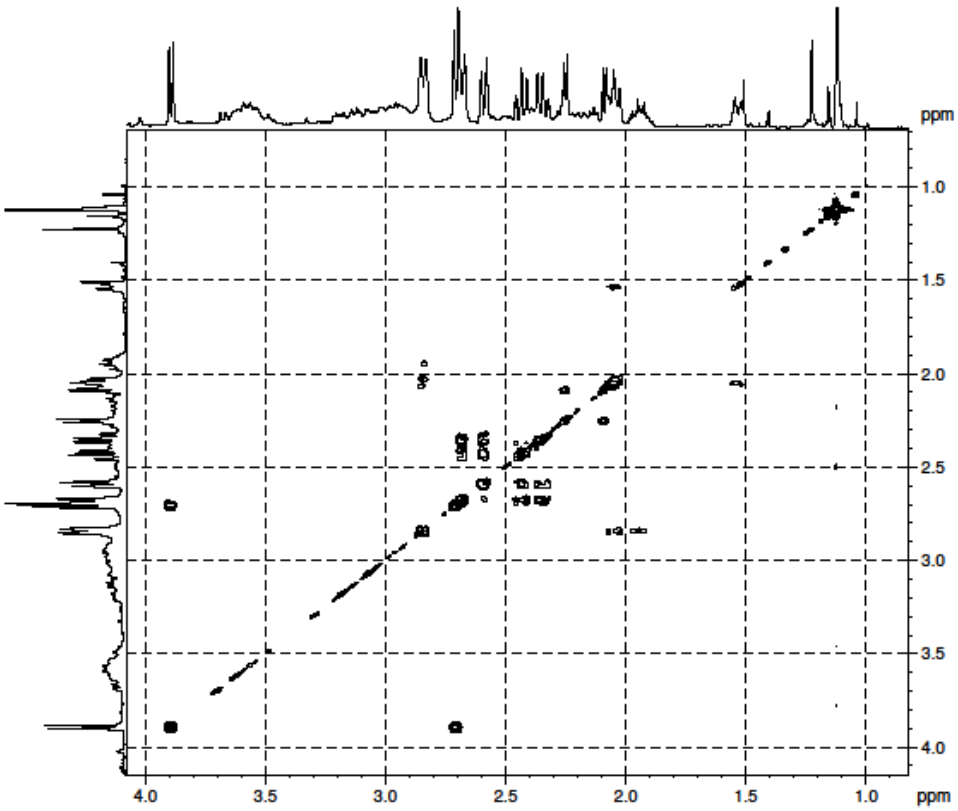
FigureS43. ^{13}C NMR spectrum of compound **2d**



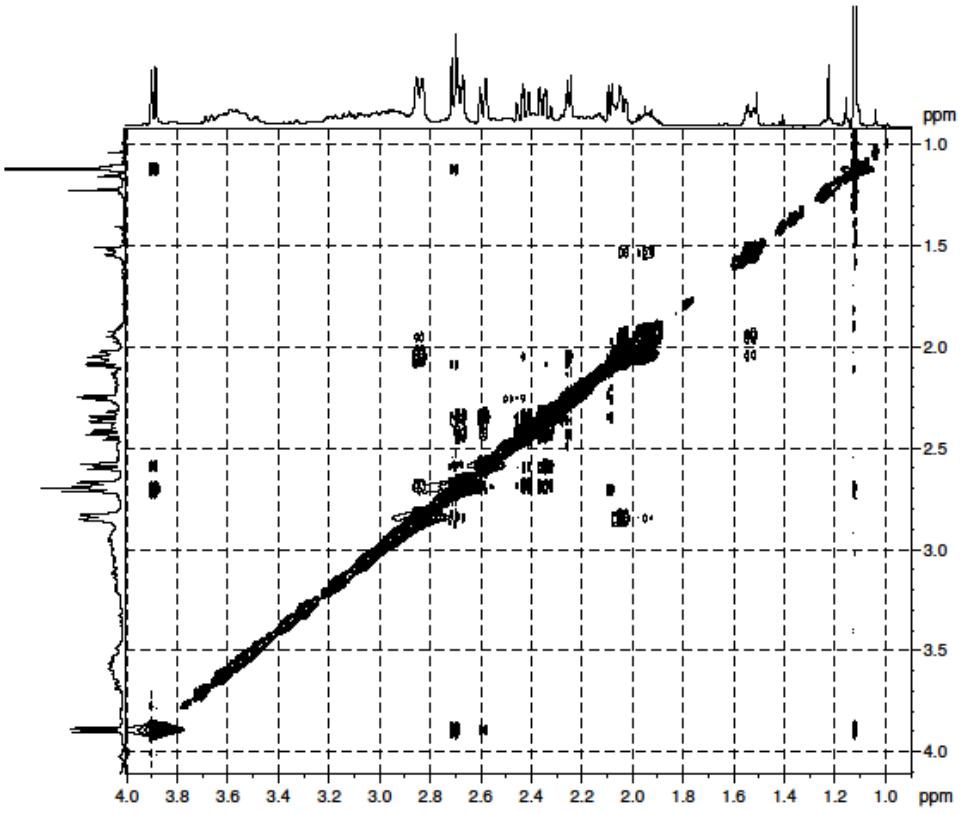
FigureS44. HSQC spectrum of compound **2d**



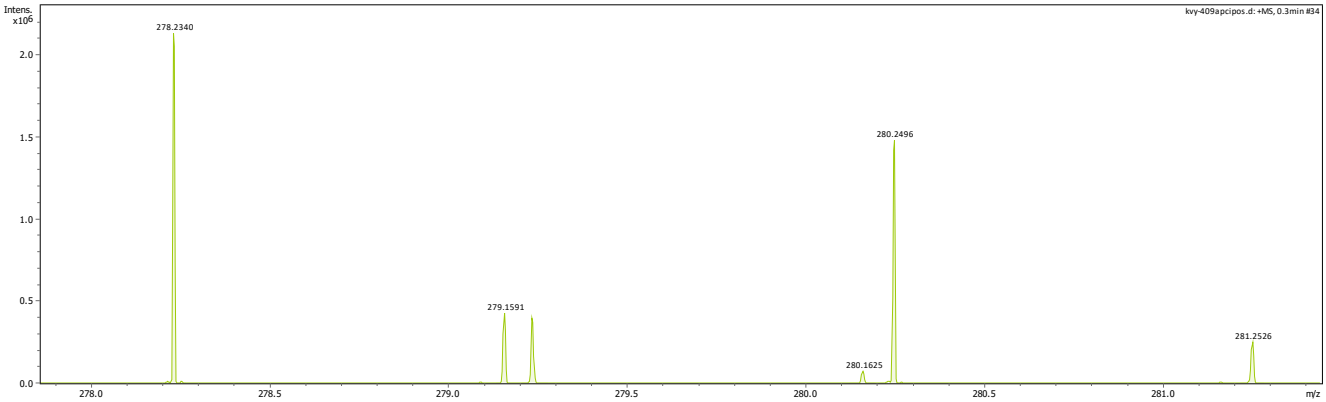
FigureS45. HMBC spectrum of compound **2d**



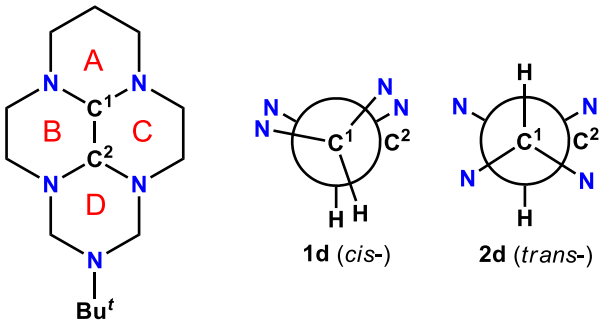
FigureS46. COSY spectrum of compound **2d**



FigureS47. NOESY spectrum of compound **2d**



FigureS48. Mass spectrum of compound **2d**



Compound	Ring A conformation	Ring B conformation	Ring C conformation	Ring D conformation	Bu^t position
1d-K1	twist boat	twist boat	twist boat	twist boat	eq
1d-K2	twist boat	twist boat	twist boat	twist boat	ax
1d-K3	twist boat	twist boat	twist boat	chair	eq
1d-K4	twist boat	twist boat	twist boat	chair	ax
1d-K5	twist boat	twist boat	chair	boat	eq
1d-K6	twist boat	twist boat	chair	boat	ax
1d-K7	twist boat	twist boat	chair	chair	eq
1d-K8	twist boat	twist boat	chair	chair	ax
1d-K9	chair	twist boat	chair	twist boat	eq
1d-K10	chair	twist boat	chair	twist boat	ax
1d-K11	chair	twist boat	chair	chair	eq
1d-K12	chair	twist boat	chair	chair	ax
1d-K13	chair	twist boat	twist boat	twist boat	eq
1d-K14	chair	twist boat	twist boat	twist boat	ax
1d-K15	chair	boat	boat	chair	eq
1d-K16	chair	boat	boat	chair	ax
2d-K1	twist	twist	chair	twist boat	eq
2d-K2	twist	twist	chair	twist boat	ax
2d-K3	twist	twist	chair	chair	eq
2d-K4	twist	twist	chair	chair	ax
2d-K5	twist boat	chair	chair	twist boat	eq
2d-K6	twist boat	chair	chair	twist boat	ax
2d-K7	twist boat	chair	chair	chair	eq
2d-K8	twist boat	chair	chair	chair	ax
2d-K9	chair	twist	chair	twist boat	eq
2d-K10	chair	twist	chair	twist boat	ax
2d-K11	chair	twist	chair	chair	eq
2d-K12	chair	twist	chair	chair	ax
2d-K13	chair	chair	chair	twist boat	eq
2d-K14	chair	chair	chair	twist boat	ax
2d-K15	chair	chair	chair	chair	eq
2d-K16	chair	chair	chair	chair	ax
2d-K17	twist boat	chair	twist	twist boat	eq
2d-K18	twist boat	chair	twist	twist boat	ax
2d-K19	twist boat	chair	twist	chair	eq
2d-K20	twist boat	chair	twist	chair	ax

Calculated (PBE/3ζ) thermodynamic parameters for all optimized compounds at 298.15 K and 1 atm (table 1)

Compound	H, kcal mol^{-1}	G, kcal mol^{-1}	S, calmol^{-1}K^{-1}
1d-K1	-540588.854815056	-540630.159115056	138.5353
1d-K2	-540586.229095882	-540627.547495882	138.5827
1d-K3	-540591.363427784	-540633.028127784	139.7440
1d-K4	-540593.992244050	-540634.983044050	137.4838
1d-K5	-540591.575964811	-540632.851464811	138.4386
1d-K6	-540587.095861517	-540628.511061517	138.9072
1d-K7	-540597.097842626	-540638.303342626	138.2042
1d-K8	-540595.003621561	-540635.443421561	135.6357
1d-K9	-540598.972291887	-540639.658091887	136.4608
1d-K10	-540596.015782587	-540636.575482587	136.0379
1d-K11	-540604.093638270	-540645.019738270	137.2666
1d-K12	-540601.983234292	-540642.122834292	134.6289
1d-K13	-540595.300574358	-540636.287074358	137.4694
1d-K14	-540592.551610889	-540633.672310890	137.9194
1d-K15	-540598.792934783	-540641.773334783	144.1570
1d-K16	-540601.810766848	-540643.812966848	140.8759
2d-K1	-540595.523795834	-540636.484395834	137.3827
2d-K2	-540591.799023369	-540633.347823369	139.3552
2d-K3	-540599.621380341	-540641.226280341	139.5437
2d-K4	-540602.031394989	-540643.717194989	139.8149
2d-K5	-540598.005635688	-540639.117735688	137.8905
2d-K6	-540595.636480201	-540636.747980201	137.8886
2d-K7	-540604.268317508	-540645.407417508	137.9810
2d-K8	-540606.680970088	-540647.712870088	137.6219
2d-K9	-540598.252060592	-540639.092560592	136.9799
2d-K10	-540595.915906257	-540636.680206257	136.7242
2d-K11	-540602.120393672	-540643.254093672	137.9633
2d-K12	-540604.441039505	-540645.171039505	136.6094
2d-K13	-540607.395499381	-540647.758699381	135.3789
2d-K14	-540604.963104810	-540645.372504810	135.5340
2d-K15	-540613.310701113	-540653.955201113	136.3220
2d-K16	-540615.717703117	-540656.677403117	137.3795
2d-K17	-540590.651373971	-540631.960473971	138.5513
2d-K18	-540588.340660174	-540629.587360174	138.3422

2d-K19	-540594.935239251	-540636.577639251	139.6693
2d-K20	-540597.297397728	-540638.469697728	138.0924

Calculated (PBE/3ζ) relative thermodynamic parameters for all optimized compounds at 298.15 K and 1 atm (table 2)

Compound	ΔH, kcal/mol	ΔG, kcal/mol	ΔS, cal/(mol·K)
1d-K1	26.9	26.5	3.9
1d-K2	29.5	29.1	4.0
1d-K3	24.4	23.6	5.1
1d-K4	21.7	21.7	2.9
1d-K5	24.1	23.8	3.8
1d-K6	28.6	28.2	4.3
1d-K7	18.6	18.4	3.6
1d-K8	20.7	21.2	1.0
1d-K9	16.7	17.0	1.8
1d-K10	19.7	20.1	1.4
1d-K11	11.6	11.7	2.6
1d-K12	13.7	14.6	0.0
1d-K13	20.4	20.4	2.8
1d-K14	23.2	23.0	3.3
1d-K15	16.9	14.9	9.5
1d-K16	13.9	12.9	6.2
2d-K1	20.2	20.2	2.8
2d-K2	23.9	23.3	4.7
2d-K3	16.1	15.5	4.9
2d-K4	13.7	13.0	5.2
2d-K5	17.7	17.6	3.3
2d-K6	20.1	19.9	3.3
2d-K7	11.4	11.3	3.4
2d-K8	9.0	9.0	3.0
2d-K9	17.5	17.6	2.4
2d-K10	19.8	20.0	2.1
2d-K11	13.6	13.4	3.3
2d-K12	11.3	11.5	2.0
2d-K13	8.3	8.9	0.8
2d-K14	10.8	11.3	0.9
2d-K15	2.4	2.7	1.7
2d-K16	0.0	0.0	2.8
2d-K17	25.1	24.7	3.9
2d-K18	27.4	27.1	3.7
2d-K19	20.8	20.1	5.0
2d-K20	18.4	18.2	3.5

Calculated (PBE/3ζ) relative thermodynamic parameters for 1d (table 3)

Compound	ΔH, kcal/mol	ΔG, kcal/mol	ΔS, cal/(mol·K)
1d-K1	15.2	14.9	3.9
1d-K2	17.9	17.5	4.0
1d-K3	12.7	12.0	5.1
1d-K4	10.1	10.0	2.9
1d-K5	12.5	12.2	3.8
1d-K6	17.0	16.5	4.3
1d-K7	7.0	6.7	3.6
1d-K8	9.1	9.6	1.0
1d-K9	5.1	5.4	1.8
1d-K10	8.1	8.4	1.4
1d-K11	0.0	0.0	2.6
1d-K12	2.1	2.9	0.0
1d-K13	8.8	8.7	2.8
1d-K14	11.5	11.3	3.3
1d-K15	5.3	3.2	9.5
1d-K16	2.3	1.2	6.2

Calculated (PBE/3ζ) relative thermodynamic parameters for 2d (table 4)

Compound	ΔH, kcal/mol	ΔG, kcal/mol	ΔS, cal/(mol·K)
2d-K1	20.2	20.2	2.0
2d-K2	23.9	23.3	4.0
2d-K3	16.1	15.5	4.2
2d-K4	13.7	13.0	4.4
2d-K5	17.7	17.6	2.5
2d-K6	20.1	19.9	2.5
2d-K7	11.4	11.3	2.6
2d-K8	9.0	9.0	2.2
2d-K9	17.5	17.6	1.6
2d-K10	19.8	20.0	1.3
2d-K11	13.6	13.4	2.6
2d-K12	11.3	11.5	1.2
2d-K13	8.3	8.9	0.0
2d-K14	10.8	11.3	0.2
2d-K15	2.4	2.7	0.9
2d-K16	0.0	0.0	2.0
2d-K17	25.1	24.7	3.2
2d-K18	27.4	27.1	3.0
2d-K19	20.8	20.1	4.3
2d-K20	18.4	18.2	2.7

Cartesian coordinates (PBE/3ζ)

1d-K1

6	-0.98420700	-1.40740338	-2.72109500
7	-0.48313131	-2.21443766	-1.61547333
6	-1.03228010	0.09086244	-2.31189493
6	-1.03888018	-1.76954425	-0.34993952
7	-0.11098420	0.35200958	-1.21514907
6	-0.49066828	-0.36801835	-0.01095456
1	-0.30820885	-1.54484370	-3.57893625
6	-0.53974903	-3.67523607	-1.78046164
7	-0.65810513	-2.71636689	0.68859944
7	0.70178630	-0.49446901	0.80674309
6	-1.45529054	-3.94175375	0.57451927
6	-1.64528239	-4.30602829	-0.91644341
1	-0.71307368	-3.90618415	-2.84294153
6	-0.69874737	-2.10868011	2.01497923
1	-0.92385067	-4.74348512	1.11199721
1	-1.64683854	-5.39844660	-1.04186214
1	-2.07322320	0.38075060	-2.04304166
6	0.33916260	-0.95583797	2.14174567
1	-0.47855106	-2.89072899	2.75638982
1	-0.10426786	-0.15280642	2.77198053
1	-2.16361460	-1.68296650	-0.39755278
1	-1.29822189	0.19112968	0.53538519
1	-1.71890581	-1.72908595	2.25165901
1	1.25000197	-1.31546284	2.64344583
1	-0.74395711	0.71751617	-3.16908387
1	-2.00631117	-1.70556628	-3.05314197
1	-2.45352262	-3.82653349	1.05610156
1	-2.62449055	-3.94675113	-1.26668748
1	0.43464604	-4.11384759	-1.50812279
6	0.06878263	1.77186701	-0.91235775
1	0.69065956	2.20524452	-1.72719329
1	-0.90348677	2.31284628	-0.90212201
6	1.52299972	0.71241333	0.69892701
1	2.05544345	0.86167976	1.64616977
1	2.27591484	0.55407623	-0.09708329
7	0.67757677	1.89181235	0.42351371
6	1.27575425	3.22320895	0.72757347
6	1.51363578	3.32483249	2.24647408
6	0.26609005	4.32135005	0.34381161
1	0.11031399	4.38403316	-0.74173174
1	-0.70452626	4.14096713	0.82695130
1	0.64258155	5.29777852	0.67828570
1	0.58735411	3.09962787	2.79271525
1	1.83405057	4.34390424	2.50442535
1	2.29839499	2.64131088	2.59707166
6	2.60817251	3.47205198	-0.01790451
1	3.37608311	2.74501800	0.28193759
1	2.48068563	3.40081840	-1.10762793
1	2.99228572	4.47737485	0.20740012

1d-K2

6	0.11434848	-1.10676529	-3.07817600
7	0.65394807	-1.87296216	-1.96222951
6	-0.39485122	0.27181278	-2.57640905
6	-0.18078683	-1.73680311	-0.78231856
7	0.26228353	0.63639701	-1.32890537
6	-0.09673374	-0.28301175	-0.25621735
1	0.91672006	-0.96914808	-3.81906238
6	1.03254451	-3.26776378	-2.23615234
7	0.29104838	-2.67002451	0.23178112
7	0.92577317	-0.18400621	0.75969087
6	-0.12047993	-4.03611194	-0.10849364
6	0.02778961	-4.26333162	-1.63119627
1	1.09637930	-3.40982216	-3.32599100
6	-0.10294947	-2.25196093	1.57198297
1	0.51753321	-4.73261524	0.45867382
1	0.35078584	-5.29524407	-1.83072053
1	-1.50233476	0.24914766	-2.45794225
6	0.58790205	-0.91789012	1.96633723
1	0.18684501	-3.04167725	2.28046052
1	-0.09650693	-0.37056042	2.65535092
1	-1.26638615	-1.94253258	-1.01509882
1	-1.11473706	-0.01529430	0.14456408
1	-1.20926661	-2.14701050	1.65246703
1	1.51640682	-1.12295381	2.52146911
1	-0.17504614	1.04575460	-3.32667712
1	-0.73064802	-1.61975854	-3.59446732
1	-1.17478739	-4.23250104	0.19348507
1	-0.94715339	-4.13620325	-2.12494858
1	2.03644088	-3.46340813	-1.82423383
6	0.00343807	2.01599532	-0.90901886
1	0.44162833	2.67873000	-1.68194672
1	-1.09181288	2.22361445	-0.88101539
6	1.48425487	1.17532814	0.82684333
1	1.85663750	1.35931290	1.84023127
1	2.34740864	1.20760041	0.14410688
7	0.58252256	2.25524280	0.41855126
6	-0.23711837	3.02721189	1.39103109
6	-0.55534404	4.39443944	0.74661338
6	0.58831088	3.29849325	2.66038913
1	0.73861219	2.39366045	3.26518758
1	1.57085118	3.72107269	2.40697102
1	0.05451697	4.02331510	3.28996508
1	0.37504858	4.91245553	0.47590430
1	-1.11847755	5.02497249	1.44941636
1	-1.16530854	4.28695127	-0.16093805
6	-1.56435193	2.34795347	1.80685604
1	-2.21072409	2.14961680	0.94042920
1	-1.37825777	1.39333482	2.31819893
1	-2.12591587	2.99694751	2.49520136

1d-K3

6	-1.20386389	-1.32658707	-2.60326888
7	-0.42266093	-2.09693495	-1.64599861
6	-1.41631289	0.11369634	-2.05258873
6	-0.92688725	-1.89562094	-0.29879843
7	-0.41312310	0.38830218	-1.03573884
6	-0.66088165	-0.42611908	0.14499968
1	-0.64625830	-1.29315582	-3.55115141
6	-0.18672104	-3.51013509	-1.97037256
7	-0.29588958	-2.85770251	0.59230311
7	0.48814261	-0.31291641	1.02930266
6	-0.86411307	-4.19694369	0.36694505
6	-1.08225522	-4.44409634	-1.14185294
1	-0.36866667	-3.65889869	-3.04543854
6	-0.43738202	-2.42586290	1.97574521
1	-0.16307039	-4.93252811	0.79124493
1	-0.87085977	-5.49449985	-1.38887662
1	-2.45281755	0.22253104	-1.65961357
6	0.35579294	-1.13407734	2.23908267
1	-0.06272467	-3.22415003	2.63303595
1	-0.15785033	-0.58045367	3.05650861
1	-2.04803420	-2.03469941	-0.25984642
1	-1.59155750	-0.05013119	0.66389927
1	-1.51186027	-2.28020970	2.23611799
1	1.37127582	-1.37310855	2.59241473
1	-1.30528848	0.84581838	-2.86508283
1	-2.20273694	-1.77500207	-2.81626480
1	-1.83232638	-4.31165658	0.90496603
1	-2.13521536	-4.26234746	-1.40395000
1	0.87142063	-3.75668058	-1.78272466
6	-0.26185135	1.78548450	-0.66729898
1	-0.10840806	2.36399124	-1.58629672
1	-1.19304775	2.16826089	-0.16399819
6	0.70293254	1.08946839	1.39045288
1	-0.17549977	1.45126396	1.99670868
1	1.59183200	1.13443482	2.03206686
7	0.90907922	1.91220322	0.20269573
6	1.36768441	3.31077175	0.46420001
6	1.70954543	3.97206922	-0.88567549
6	2.66861165	3.25558788	1.28911478
1	2.49628961	2.95712958	2.33175932
1	3.38082355	2.55272615	0.83513602
1	3.12936529	4.25245153	1.31184518
1	2.38685851	3.32980207	-1.46507113
1	2.20637891	4.93542849	-0.70721516
1	0.81810314	4.17876700	-1.49281492
6	0.33123728	4.18575837	1.20928830
1	-0.59794820	4.29246102	0.63192558
1	0.07488846	3.76172685	2.19033629
1	0.73585058	5.19438315	1.37784293

1d-K4

6	-1.81769735	-0.69876303	-2.15083360
7	-1.09075415	-1.56182907	-1.22853470
6	-1.74358431	0.77150717	-1.64013702
6	-1.44610073	-1.23629856	0.14180210
7	-0.62056675	0.90679535	-0.72342269
6	-0.89067149	0.16780993	0.50572973
1	-1.34851950	-0.78346878	-3.14233579
6	-1.11944297	-3.00561513	-1.49745728
7	-0.94815579	-2.28188105	1.02421725
7	0.33357644	0.09568412	1.29033836
6	-1.83662891	-3.44939503	0.90013607
6	-2.11762163	-3.75078757	-0.59320447
1	-1.37590501	-3.15973947	-2.55637494
6	-0.88993580	-1.78339299	2.39315849
1	-1.35738329	-4.30088595	1.40506563
1	-2.06034545	-4.83197265	-0.78530163
1	-2.70873419	1.05722656	-1.16418727
6	0.15675479	-0.66377471	2.53467053
1	-0.62695630	-2.61755501	3.06012120
1	-0.16508622	-0.00439876	3.37148432
1	-2.56867169	-1.16882704	0.26125181
1	-1.69245925	0.71364847	1.08593763
1	-1.89103836	-1.41847481	2.72146857
1	1.13521025	-1.08759468	2.81186226
1	-1.59270266	1.45686604	-2.48677821
1	-2.89079339	-0.98090299	-2.26007660
1	-2.80118460	-3.23335623	1.41346134
1	-3.14093980	-3.43872688	-0.84873525
1	-0.11019979	-3.41984119	-1.34367817
6	-0.22978163	2.27602787	-0.37410615
1	-0.12340395	2.86111781	-1.29425071
1	-1.01956766	2.76307113	0.24705127
6	0.80755421	1.46851854	1.58201118
1	0.05895820	1.97888665	2.23535837
1	1.74091779	1.38909335	2.15414863
7	0.99537689	2.29982542	0.40778635
6	2.31331348	2.19258830	-0.30531104
6	3.39296342	2.76164576	0.63849024
6	2.28036607	3.09047003	-1.55458897
1	1.65410916	2.66923224	-2.35255397
1	1.91854131	4.09962643	-1.30887384
1	3.29802177	3.18245719	-1.95712921
1	3.13902727	3.78736000	0.93960916
1	4.36581982	2.77442472	0.12765919
1	3.51422982	2.15464099	1.54589087
6	2.70346151	0.75998798	-0.72791881
1	3.67608885	0.77766736	-1.24443587
1	2.78847239	0.09455672	0.14072869
1	1.95206919	0.32674544	-1.39921305

1d-K5

6	-0.28101886	-1.13731816	-2.68697386
7	0.06139015	-2.24249365	-1.80949203
6	0.41257718	0.17096273	-2.21567060
6	-0.37251627	-2.05462852	-0.42823195
7	0.68724243	0.10508718	-0.77514897
6	-0.44252630	-0.55643717	-0.10494836
1	0.05989049	-1.38617115	-3.70310537
6	-0.29148316	-3.57786017	-2.28637415
7	0.59667508	-2.74464727	0.40697195
7	-0.48618584	-0.30807594	1.31806814
6	0.89765740	-4.10043510	-0.08977416
6	-0.13384062	-4.58663980	-1.12443064
1	-1.33541675	-3.62512654	-2.67453831
6	0.32612787	-2.55954615	1.81980470
1	1.90241769	-4.11045229	-0.54714800
1	0.17043867	-5.56776967	-1.51631838
1	-0.25088555	1.02461388	-2.47609057
6	0.46595265	-1.06898831	2.13189339
1	1.06931446	-3.12177871	2.40403423
1	0.22194192	-0.89041130	3.19069302
1	-1.41219539	-2.45463662	-0.27047913
1	-1.40046738	-0.17034512	-0.51509277
1	-0.68944487	-2.90492568	2.12793749
1	1.52130911	-0.77019470	1.96415941
1	1.36700462	0.30731690	-2.74699914
1	-1.38203967	-0.98324859	-2.75640029
1	0.92364582	-4.80151914	0.76024308
1	-1.10319717	-4.73308421	-0.62637593
1	0.37846690	-3.83435796	-3.12363647
6	-0.60869045	1.12680157	1.63161855
1	-1.65007195	1.36245144	1.90089611
1	0.02728641	1.32256678	2.52373430
6	0.98394636	1.37868789	-0.12469595
1	1.40200520	2.06797684	-0.86877098
1	1.76681356	1.20896277	0.64595403
7	-0.23139152	1.95625503	0.47447246
6	-0.21829807	3.43013819	0.71165004
6	-1.52174072	3.84235046	1.42164565
6	-0.19041989	4.14446538	-0.65335303
1	0.74286798	3.96374115	-1.20317843
1	-1.02937892	3.80497861	-1.27603644
1	-0.27656751	5.23043080	-0.50821091
1	-2.39744373	3.45453032	0.88213535
1	-1.59072647	4.93848333	1.44685483
1	-1.56433196	3.48678782	2.45983838
6	0.98894850	3.89518279	1.55955574
1	1.00435931	3.40693966	2.54452099
1	1.94206035	3.68079938	1.05576133
1	0.93993892	4.98058099	1.72903163

1d-K6

6	0.30258562	-1.13990407	-2.36926523
7	0.63563480	-2.15373197	-1.39122677
6	1.06940453	0.14902761	-2.03445016
6	0.22745338	-1.82017413	-0.03365999
7	1.05485734	0.45252836	-0.59298443
6	0.03317251	-0.30095411	0.15224552
1	0.61983033	-1.49225948	-3.36256942
6	0.27452014	-3.53284358	-1.71172111
7	1.23576656	-2.38857404	0.85097240
7	-0.04608887	0.02734910	1.57230822
6	1.59599698	-3.76330430	0.44441940
6	0.53619877	-4.41228717	-0.46581504
1	-0.79173830	-3.62887253	-2.02098982
6	0.87639111	-2.16310549	2.23908629
1	2.56204396	-3.74217330	-0.08678873
1	0.87016359	-5.41444745	-0.77074286
1	0.62571673	0.97884794	-2.62410854
6	0.89340246	-0.65652046	2.46505641
1	1.62652948	-2.63615752	2.88961726
1	0.58625190	-0.43345046	3.50047324
1	-0.78460112	-2.25790930	0.19370690
1	-0.97474841	-0.08670355	-0.25719880
1	-0.12549185	-2.57383949	2.50865342
1	1.93473888	-0.29233050	2.33581097
1	2.11364079	0.03575170	-2.37211341
1	-0.79298092	-0.94803852	-2.43593308
1	1.73807666	-4.37419561	1.34935740
1	-0.39686365	-4.54903768	0.09975073
1	0.89360673	-3.86109310	-2.56229216
6	-0.02087387	1.50420034	1.81447510
1	-0.83691987	1.78090219	2.49305510
1	0.93681960	1.72992856	2.33621353
6	1.03503735	1.90012928	-0.25905173
1	1.00429377	2.48743773	-1.19026457
1	1.98299038	2.15049855	0.25765113
7	-0.05793166	2.28929884	0.61256188
6	-1.25462012	2.99721014	0.08157366
6	-0.81085759	4.41121999	-0.35790839
6	-2.31336140	3.15371915	1.18300639
1	-2.71655868	2.18429764	1.50726769
1	-1.91157550	3.68234217	2.05878434
1	-3.14924603	3.74635077	0.78765869
1	-0.38468595	4.95728321	0.49450381
1	-1.66455532	4.98109378	-0.75254504
1	-0.04995930	4.36682793	-1.14986880
6	-1.91491638	2.29214887	-1.12504840
1	-1.19994038	2.14681050	-1.94704152
1	-2.32373267	1.31260713	-0.84226445
1	-2.74287650	2.90409635	-1.51235702

1d-K7

6	-0.42798693	-1.15542177	-2.92404906
7	-0.15099746	-2.23729665	-2.00422475
6	0.31627060	0.11212433	-2.46727868
6	-0.62531637	-1.98835947	-0.64901086
7	0.33108127	0.26285127	-0.99547560
6	-0.77109380	-0.48001602	-0.36799611
1	-0.06357719	-1.44061975	-3.92253215
6	-0.51013068	-3.58532748	-2.43887398
7	0.32845935	-2.63764108	0.23861378
7	-0.89508897	-0.23500035	1.06391630
6	0.66301272	-4.00058607	-0.22189463
6	-0.35477310	-4.54890000	-1.23932551
1	-1.55265777	-3.63925657	-2.82881542
6	-0.02355365	-2.45242173	1.63419819
1	1.66597779	-3.99532844	-0.68164781
1	-0.03368434	-5.54073908	-1.58834962
1	-0.17680429	0.98378251	-2.94853157
6	0.05425375	-0.95745660	1.92408605
1	0.70735368	-2.98286966	2.26184214
1	-0.24158216	-0.76008916	2.96734064
1	-1.65998730	-2.40623978	-0.50374519
1	-1.74543193	-0.15294182	-0.80394787
1	-1.04092189	-2.83371157	1.88919893
1	1.09618129	-0.61857575	1.78423802
1	1.35836034	0.08098400	-2.82294413
1	-1.51856526	-0.95475075	-3.03367801
1	0.71189032	-4.67031364	0.65118208
1	-1.32625795	-4.68815076	-0.74340468
1	0.16296369	-3.87141431	-3.26348389
6	-0.92804494	1.19579574	1.31707834
1	-1.84546034	1.59287775	0.82788237
1	-1.01289953	1.35620691	2.39812497
6	0.27909512	1.68485527	-0.64465860
1	-0.63609982	2.15195327	-1.11000002
1	1.15913850	2.16567829	-1.09060300
7	0.28113284	1.86289788	0.80230741
6	0.51662317	3.25741479	1.28761843
6	1.82825303	3.78665865	0.67707220
6	0.70806874	3.21064367	2.81682606
1	-0.21996922	2.96846578	3.35132932
1	1.46908040	2.46382427	3.08189314
1	1.03995164	4.19385923	3.17739835
1	2.63727506	3.05474347	0.81027330
1	2.11567592	4.71915592	1.18152068
1	1.73365437	4.01412666	-0.39304694
6	-0.63323917	4.23528458	0.94746763
1	-0.79102327	4.31274994	-0.13749729
1	-1.58006425	3.92404866	1.41128341
1	-0.39854196	5.24244540	1.32232363

1d-K8

6	-0.78126735	-0.73293832	-2.97275103
7	-0.65811207	-1.84770914	-2.05753184
6	0.12518155	0.41481550	-2.50068122
6	-1.11595261	-1.54067386	-0.70991139
7	0.11872838	0.59938047	-1.02977942
6	-1.06314154	-0.02980842	-0.40916586
1	-0.45103682	-1.05882536	-3.97085749
6	-1.20759048	-3.12679286	-2.50612688
7	-0.28837398	-2.32786379	0.19575818
7	-1.17104886	0.21508875	1.02552140
6	-0.12823529	-3.71606008	-0.28626816
6	-1.20067086	-4.11482965	-1.31636785
1	-2.24442087	-3.02210998	-2.90001521
6	-0.70796763	-2.13138951	1.57130843
1	0.86902806	-3.82774351	-0.74326296
1	-1.01293105	-5.13784205	-1.67248694
1	-0.21256051	1.34116828	-3.01061122
6	-0.42694651	-0.67264958	1.91902891
1	-0.11376954	-2.78257377	2.22871225
1	-0.76486343	-0.47456685	2.95354157
1	-2.20141791	-1.81298341	-0.58703136
1	-1.98746564	0.42142689	-0.84565419
1	-1.78772199	-2.35720595	1.74001213
1	0.66861419	-0.52579692	1.88239928
1	1.16109826	0.21911706	-2.82045693
1	-1.83445571	-0.38791974	-3.08678942
1	-0.16595316	-4.39712243	0.57800274
1	-2.18746683	-4.12555083	-0.83131279
1	-0.57896059	-3.49931343	-3.33097055
6	-1.04039421	1.65031374	1.29914855
1	-1.94712608	2.12449047	0.87747164
1	-1.05084727	1.80012959	2.38324832
6	0.11334793	2.04915828	-0.71898288
1	-0.79265188	2.51578143	-1.18123972
1	0.99061720	2.50159319	-1.20157254
7	0.09696116	2.34044923	0.69223259
6	1.40561972	2.57741250	1.37159808
6	1.21159584	2.61454875	2.89422657
6	1.89641496	3.97585523	0.93034061
1	2.03462821	4.02996367	-0.15862082
1	1.16776893	4.74466334	1.22059212
1	2.86460944	4.21106433	1.39587169
1	0.43082736	3.33442528	3.17942246
1	2.15059640	2.93415382	3.36569005
1	0.95443208	1.62933489	3.30667887
6	2.50156805	1.54499244	1.02497194
1	3.44081641	1.81594333	1.53021799
1	2.22327046	0.53118495	1.33723658
1	2.69762611	1.51381401	-0.05478425

1d-K9

6	-0.23360807	-1.10736643	-2.69726883
7	0.03297419	-2.21919013	-1.80103649
6	0.51020110	0.15970652	-2.18919103
6	-0.53815292	-2.02140224	-0.46988350
7	0.72288191	0.05357003	-0.74046365
6	-0.49353504	-0.51794871	-0.13494359
1	0.13385767	-1.37445350	-3.69829791
6	-0.25567844	-3.55905264	-2.28589580
7	0.20311453	-2.86850482	0.46740688
7	-0.59807436	-0.25075775	1.27858641
6	-0.05219005	-4.27062403	0.13440162
6	0.36552504	-4.56778724	-1.31060038
1	-1.35300971	-3.74516436	-2.37519480
6	-0.09738169	-2.54954804	1.85792500
1	-1.13338789	-4.51695103	0.26630528
1	1.46045301	-4.50401445	-1.38770942
1	-0.09578635	1.05275161	-2.45712637
6	0.24616720	-1.08969241	2.12875365
1	0.51561440	-3.20391585	2.49767685
1	0.01826670	-0.85175301	3.17847050
1	-1.62344648	-2.32550258	-0.46233641
1	-1.38859976	-0.05530922	-0.60315244
1	-1.16759178	-2.72410025	2.11568622
1	1.33248530	-0.93357777	1.96646741
1	1.49077924	0.24941905	-2.68120915
1	-1.32111553	-0.89486083	-2.80534504
1	0.51428367	-4.90529800	0.83335458
1	0.05925462	-5.59081933	-1.57871661
1	0.18097115	-3.67864539	-3.28902759
6	1.08765784	1.29619570	-0.06512482
1	1.80144113	1.05813221	0.75288737
1	1.61400119	1.94305743	-0.77785069
6	-0.63224230	1.18987888	1.58016801
1	-1.67009276	1.50612562	1.76874758
1	-0.05406237	1.34059273	2.51879315
7	-0.10647436	1.98159608	0.45509177
6	0.01922101	3.44893853	0.69846690
6	-1.28939595	3.97338571	1.31926488
6	0.20289964	4.15607503	-0.65788341
1	1.14980528	3.88975345	-1.14629367
1	-0.62089008	3.89613524	-1.33655799
1	0.20819189	5.24546277	-0.51284542
1	-2.15569402	3.66763889	0.71561750
1	-1.26237070	5.07119608	1.35068218
1	-1.43719419	3.61959994	2.34841299
6	1.20140380	3.80745230	1.62898894
1	1.10997613	3.31467302	2.60773603
1	2.16435440	3.51279038	1.18818717
1	1.23419274	4.89211279	1.80587612

1d-K10

6	0.21501207	-1.29888392	-2.28899646
7	0.60996215	-2.23894931	-1.25690706
6	0.81032686	0.09562258	-1.96299906
6	0.01122625	-1.94957226	0.04441712
7	0.91301656	0.25806610	-0.51232558
6	-0.18901935	-0.42383881	0.17550670
1	0.61582789	-1.65120526	-3.24990396
6	0.52822480	-3.65919016	-1.55450774
7	0.87764649	-2.53623641	1.07014422
7	-0.33690760	-0.00005738	1.54974938
6	0.84106666	-3.99299966	0.93545689
6	1.29541654	-4.42102135	-0.46532671
1	-0.52769502	-4.01916530	-1.59632452
6	0.54831328	-2.07930912	2.41493846
1	-0.18856487	-4.38099657	1.12606467
1	2.36819896	-4.20702108	-0.57546498
1	0.16954333	0.86536441	-2.44809006
6	0.65397212	-0.56048945	2.46855655
1	1.26937806	-2.53290470	3.11313340
1	0.41226835	-0.20991380	3.48281458
1	-1.01167048	-2.41741084	0.11509629
1	-1.15687192	-0.19162933	-0.32053405
1	-0.47520151	-2.38366761	2.73372027
1	1.69698734	-0.26146193	2.23706447
1	1.81769664	0.18207006	-2.40051433
1	-0.88952898	-1.22814728	-2.41241581
1	1.50074287	-4.43174996	1.70002343
1	1.14536501	-5.50526706	-0.58465700
1	0.97903604	-3.84567969	-2.54098423
6	1.13539871	1.60618298	0.03034608
1	1.88353913	1.51597573	0.83931454
1	1.58875459	2.23128443	-0.74720800
6	-0.62819235	1.43944367	1.66548187
1	-1.72042803	1.58479976	1.64219360
1	-0.28148427	1.74666004	2.66989478
7	-0.02325475	2.27313549	0.61487718
6	-0.91945518	3.17875271	-0.15560623
6	-0.09144724	3.99129764	-1.16419633
6	-1.53863395	4.18027860	0.84543812
1	-2.16218909	3.67559342	1.59613183
1	-0.74538524	4.72793551	1.37247608
1	-2.17767962	4.90334770	0.31836411
1	0.76026224	4.48066440	-0.67080292
1	-0.72598576	4.77214282	-1.60485104
1	0.28692395	3.37430417	-1.99083082
6	-2.06382542	2.46632310	-0.91656680
1	-1.67113688	1.79407614	-1.69184258
1	-2.69831277	1.87657577	-0.23994996
1	-2.71123660	3.20687102	-1.40939836

1d-K11

6	-0.27830583	-1.12565999	-2.95034577
7	0.01890577	-2.18496972	-2.00859272
6	0.39297004	0.16792053	-2.46025908
6	-0.63785996	-1.98277497	-0.71920233
7	0.36953594	0.27631532	-0.98519842
6	-0.77274748	-0.46511944	-0.42061240
1	0.13654005	-1.39836881	-3.93128019
6	-0.15679169	-3.55488773	-2.46696405
7	0.11242718	-2.75411252	0.27785980
7	-0.97525598	-0.21375632	0.99893213
6	-0.02722155	-4.17938242	-0.02875705
6	0.48489100	-4.49118982	-1.43790001
1	-1.23450592	-3.81462449	-2.59633233
6	-0.28592137	-2.44474782	1.64477186
1	-1.09484188	-4.49597698	0.05572035
1	1.57532171	-4.35336254	-1.46500883
1	-0.13222875	1.02832004	-2.92916563
6	-0.08251467	-0.96094017	1.89210765
1	0.35000520	-3.03268017	2.32486895
1	-0.37069664	-0.71365298	2.92581197
1	-1.69336816	-2.37648894	-0.76091108
1	-1.71355298	-0.12427557	-0.91436193
1	-1.34752254	-2.71404201	1.85169093
1	0.98189937	-0.69993592	1.75558627
1	1.44315490	0.19566651	-2.79075310
1	-1.37125429	-0.97121711	-3.09928387
1	0.54170696	-4.75142505	0.72011861
1	0.26253549	-5.54016356	-1.68744277
1	0.33060747	-3.66713759	-3.44710112
6	0.31576939	1.69547381	-0.61806564
1	1.22016760	2.17120972	-1.01910098
1	-0.57103346	2.17678764	-1.12153014
6	-1.00084883	1.21477838	1.26263823
1	-1.88176309	1.63258646	0.72557705
1	-1.14681542	1.36415762	2.33855131
7	0.24744074	1.86276751	0.82719545
6	0.48386270	3.24982230	1.33246146
6	1.86294901	3.73018298	0.84145987
6	0.53678790	3.20228400	2.87238147
1	-0.44355130	3.00092679	3.32426359
1	1.24244138	2.42918771	3.20667637
1	0.87481064	4.17371277	3.25835357
1	2.63209243	2.97650977	1.06045713
1	2.13104734	4.66247411	1.35701186
1	1.87772508	3.94211083	-0.23586081
6	-0.59679923	4.26489393	0.89146320
1	-0.64694267	4.35173076	-0.20313385
1	-1.59336021	3.97839035	1.25687411
1	-0.36989136	5.26268278	1.29433089

1d-K12

6	-0.39106621	-0.69253135	-3.05530480
7	-0.25694357	-1.78710806	-2.11439901
6	0.34356587	0.53081362	-2.48989381
6	-1.02187653	-1.54499705	-0.89297582
7	0.20942535	0.64089335	-1.02000167
6	-1.02422512	-0.02696133	-0.54693598
1	0.07317461	-0.98601449	-4.00777418
6	-0.52542971	-3.12087524	-2.63497435
7	-0.48571985	-2.42880632	0.14911791
7	-1.30150317	0.20839887	0.86283854
6	-0.74106307	-3.82072042	-0.23144288
6	-0.10083272	-4.14702459	-1.58190524
1	-1.60493689	-3.25765972	-2.88349901
6	-1.02932343	-2.12160642	1.46569835
1	-1.83900296	-4.01612797	-0.28632643
1	0.99367208	-4.12247807	-1.48088774
1	-0.06222546	1.43668706	-2.99018289
6	-0.66203837	-0.69198420	1.81689472
1	-0.57930550	-2.81785661	2.19046391
1	-1.05026648	-0.44347374	2.81742451
1	-2.10418337	-1.81240753	-1.06387588
1	-1.89520958	0.41450664	-1.08917447
1	-2.13566681	-2.24605613	1.51111963
1	0.44134835	-0.61314438	1.84502079
1	1.41592041	0.46858040	-2.73350290
1	-1.45409607	-0.44859677	-3.28116573
1	-0.33318284	-4.47299428	0.55579550
1	-0.39667206	-5.15962869	-1.89635644
1	0.04800441	-3.25906465	-3.56388057
6	0.15521349	2.08355097	-0.67174118
1	1.07718889	2.55116804	-1.04475976
1	-0.69681377	2.55404113	-1.22383701
6	-1.22531497	1.63863575	1.17290431
1	-2.07282419	2.11043631	0.63992661
1	-1.38624878	1.77243732	2.24774284
7	-0.02685893	2.34630678	0.73148458
6	1.18741615	2.57000681	1.57126306
6	0.81022513	2.56187412	3.05975989
6	1.71585034	3.98261088	1.23055789
1	1.98018173	4.06850327	0.16721853
1	0.95218590	4.73945298	1.45476665
1	2.62066601	4.20857225	1.81340686
1	-0.00657554	3.26728586	3.27014611
1	1.68228222	2.87326864	3.65023406
1	0.51562637	1.56305466	3.40990638
6	2.32468853	1.55248568	1.33168485
1	3.19714844	1.81871028	1.94707313
1	2.02178619	0.53074863	1.59101309
1	2.64383551	1.54508775	0.28133503

1d-K13

6	-1.09228837	-1.52793109	-2.33251794
7	-0.14210606	-2.35558060	-1.59774826
6	-0.66746544	-0.03183614	-2.25630188
6	-0.24120509	-2.09057465	-0.16410799
7	0.24367621	0.12645019	-1.12969640
6	-0.30699556	-0.54866559	0.03342732
1	-1.10297556	-1.86288240	-3.37911381
6	-0.20940442	-3.78209826	-1.87636006
7	0.89218495	-2.68002890	0.53920967
7	0.44339197	-0.09470692	1.19206076
6	0.95413847	-4.12475624	0.31692661
6	0.96621198	-4.46328573	-1.17346836
1	-1.17054560	-4.23405931	-1.52977042
6	0.88596439	-2.38265502	1.97918373
1	1.86018030	-4.51158448	0.80970568
1	1.90499636	-4.11290412	-1.62564219
1	-1.58074281	0.59735831	-2.16528963
6	0.26462834	-1.01312018	2.30483936
1	1.92954390	-2.42111484	2.32946032
1	-0.81463869	-1.12695916	2.55784665
1	-1.20823996	-2.52759627	0.22254300
1	-1.39305735	-0.28712904	0.16450522
1	0.32105572	-3.15501129	2.54651913
1	0.75380024	-0.59289342	3.19637227
1	-0.13889128	0.26420699	-3.17458951
1	-2.12976670	-1.64949609	-1.94666512
1	0.08211041	-4.63173265	0.79828007
1	0.90578297	-5.55503458	-1.30023214
1	-0.15080802	-3.92954071	-2.96548701
6	0.66653733	1.48322431	-0.78902209
1	0.57355902	2.11230361	-1.68245880
1	1.73424367	1.45586857	-0.49791838
6	0.05288873	1.27934691	1.52961690
1	-0.88543217	1.29061586	2.12732148
1	0.86519314	1.70026921	2.16217805
7	-0.17906008	2.03286539	0.28825131
6	-0.18176712	3.51600740	0.44259894
6	-1.08701372	3.88838004	1.63176917
6	-0.79704219	4.14416060	-0.82237505
1	-0.16435182	4.01067199	-1.70997606
1	-1.78131741	3.70107172	-1.02708626
1	-0.92308787	5.22586959	-0.67532782
1	-2.08554736	3.44492344	1.51186725
1	-1.19705581	4.98036912	1.68089950
1	-0.67040703	3.55674525	2.59256202
6	1.23079182	4.10334666	0.67162665
1	1.70776064	3.67384721	1.56427188
1	1.88780582	3.91337658	-0.18882835
1	1.17476714	5.19189875	0.81614061

1d-K14

6	-0.55583799	-1.48624137	-2.25424094
7	0.57931081	-2.09197076	-1.56923680
6	-0.45134197	0.06300932	-2.18016899
6	0.46427214	-1.88507486	-0.12651187
7	0.37706153	0.40795552	-1.04199041
6	0.07273951	-0.39203005	0.12352409
1	-0.54495941	-1.81251568	-3.30350500
6	0.82080012	-3.49247407	-1.88526552
7	1.71775144	-2.23088537	0.53371690
7	0.78527962	0.18942823	1.25399335
6	2.09056625	-3.62048607	0.26749513
6	2.13793356	-3.91162045	-1.23153382
1	-0.00560507	-4.15326098	-1.52728129
6	1.68289165	-1.98386419	1.98141178
1	3.07190435	-3.80838841	0.73128358
1	2.96213994	-3.34921076	-1.69305478
1	-1.48392820	0.48071114	-2.13806388
6	0.82589527	-0.76182521	2.35343320
1	2.72215913	-1.83960677	2.31632081
1	-0.20329565	-1.08405223	2.63655110
1	-0.37444825	-2.53048307	0.26812801
1	-1.03251870	-0.38962984	0.34712914
1	1.28069604	-2.86409229	2.53063242
1	1.25461366	-0.26507443	3.23646331
1	0.02743170	0.45512114	-3.09057014
1	-1.52546772	-1.82437895	-1.82308611
1	1.36480675	-4.31923583	0.75117041
1	2.31833505	-4.98580651	-1.38995571
1	0.87653850	-3.59881662	-2.97929929
6	0.64299342	1.80885789	-0.69350494
1	0.42756664	2.43849836	-1.56308333
1	1.71975620	1.89392923	-0.47954612
6	0.14463780	1.45258984	1.64998753
1	-0.83398543	1.24916124	2.14446331
1	0.80365333	1.91975965	2.40840156
7	-0.05942235	2.31812336	0.48591790
6	-1.35400184	3.04661777	0.39999558
6	-1.32902253	3.99481221	-0.81079500
6	-1.47886451	3.91708970	1.66958323
1	-1.51965701	3.30564730	2.58175684
1	-0.61981146	4.59730732	1.75019318
1	-2.40054973	4.51521047	1.63270626
1	-0.41726267	4.60863849	-0.81061149
1	-2.19643607	4.66701784	-0.76190929
1	-1.39108272	3.45592967	-1.76628123
6	-2.60522681	2.14252356	0.28811117
1	-2.58101853	1.54305495	-0.63227728
1	-2.68995014	1.45388903	1.14048243
1	-3.51803969	2.75614154	0.26892103

1d-K15

6	-1.20892458	-1.61236759	-2.47865625
7	-0.29974392	-2.32865704	-1.59149832
6	-1.07245689	-0.08304024	-2.29663579
6	-0.67170244	-2.04935556	-0.20587866
7	-0.24216038	0.23096425	-1.13752370
6	-0.69194022	-0.49809248	0.04061740
1	-0.96542644	-1.89443125	-3.51270924
6	-0.30961858	-3.76336397	-1.86656663
7	0.24274136	-2.70311377	0.72589132
7	0.16026564	-0.14499267	1.16938148
6	0.27833323	-4.14961802	0.51766488
6	0.65413259	-4.47572137	-0.92367035
1	-1.33428195	-4.19212358	-1.74380515
6	-0.13415465	-2.40510662	2.10646473
1	1.00850153	-4.57647255	1.22266184
1	1.68154751	-4.14075661	-1.12529223
1	-2.08857822	0.36614321	-2.20947837
6	-0.27000612	-0.88281758	2.34867890
1	0.64507436	-2.83067598	2.75576974
1	-1.32242999	-0.63746251	2.62217620
1	-1.72026171	-2.43435400	-0.02919208
1	-1.75754705	-0.20507061	0.28080813
1	-1.09101254	-2.90802639	2.37733535
1	0.36104671	-0.57254388	3.19421671
1	-0.59313190	0.37089644	-3.17714941
1	-2.26457454	-1.92327638	-2.30061800
1	-0.71231388	-4.61098854	0.75225159
1	0.60496958	-5.56310419	-1.08506430
1	-0.01732419	-3.91145543	-2.91739610
6	-0.25710289	1.67126904	-0.88798533
1	-1.31507316	2.00858363	-0.69627049
1	0.09447113	2.16683298	-1.80143148
6	0.12412856	1.29546320	1.40651108
1	-0.92487821	1.61310014	1.66752092
1	0.76655137	1.50483477	2.27042855
7	0.61845350	1.99838134	0.22943906
6	0.91468321	3.45094956	0.41856113
6	1.53870458	3.99620637	-0.88106331
6	1.97185009	3.59164395	1.53150147
1	1.56683902	3.37163262	2.52834793
1	2.81883408	2.91839415	1.34098717
1	2.34336648	4.62499942	1.55643868
1	2.35322948	3.34091594	-1.21847048
1	1.94845549	4.99860058	-0.69829493
1	0.80512469	4.09205048	-1.69260984
6	-0.32537205	4.30174150	0.78312982
1	-1.09418687	4.25342623	-0.00081082
1	-0.77826755	3.97294754	1.72907970
1	-0.03883329	5.35701146	0.90220749

1d-K16

6	-1.54592974	-1.13474858	-2.40525109
7	-0.74725220	-1.88537701	-1.44111883
6	-1.37079980	0.39032716	-2.21094423
6	-1.18001789	-1.54728106	-0.08656710
7	-0.54527284	0.67445084	-1.04309349
6	-1.08672418	0.00530063	0.13456870
1	-1.21966070	-1.43207881	-3.41208891
6	-0.84271048	-3.32207537	-1.69027249
7	-0.37657534	-2.24883113	0.91184039
7	-0.25588866	0.31852791	1.29462576
6	-0.44365318	-3.69828389	0.73390644
6	-0.00011078	-4.08366333	-0.67299087
1	-1.90201861	-3.67264654	-1.63090244
6	-0.81168029	-1.88520842	2.25938902
1	0.20258390	-4.16417887	1.49393373
1	1.06115216	-3.83141087	-0.81001866
1	-2.37390118	0.86921881	-2.12631449
6	-0.79842429	-0.35214083	2.46876920
1	-0.12792152	-2.37716504	2.96658488
1	-1.82939857	0.00469636	2.69721898
1	-2.26386675	-1.84487751	0.03447454
1	-2.13452407	0.38538583	0.32845856
1	-1.83229413	-2.27972873	2.46980704
1	-0.17101440	-0.08683715	3.33253246
1	-0.87562974	0.83817328	-3.08587257
1	-2.62431112	-1.40416001	-2.32384926
1	-1.48087817	-4.07527634	0.90911056
1	-0.12166213	-5.16740518	-0.81963408
1	-0.49333755	-3.51378869	-2.71644914
6	-0.47301959	2.13072575	-0.81013197
1	-1.50269176	2.53479577	-0.65382022
1	-0.07089628	2.59461170	-1.71982372
6	-0.22519655	1.78039675	1.48816210
1	-1.26435535	2.15778046	1.64989717
1	0.34846163	1.99176431	2.39794012
7	0.31317893	2.49421433	0.35048975
6	1.80333363	2.58622584	0.18640975
6	2.42099825	2.99176919	1.53688978
6	2.09004210	3.72742237	-0.81051549
1	1.74328607	3.49085206	-1.82555937
1	1.60450145	4.65770660	-0.48451841
1	3.17322297	3.89912440	-0.87499579
1	1.89740346	3.85773514	1.96732015
1	3.47276023	3.26804675	1.38378511
1	2.40710572	2.16836672	2.26358534
6	2.48269858	1.29097550	-0.30788120
1	2.30107249	0.46021068	0.38515097
1	2.10064016	0.98724051	-1.29050095
1	3.56917608	1.45111768	-0.39173570

2d-K1

6	-1.18237152	-1.00628596	-2.52355952
7	-1.49428363	-2.08765024	-1.58421502
6	-1.71173022	0.32630039	-1.99311990
6	-1.29271206	-1.70529617	-0.16108025
7	-1.07155817	0.71280782	-0.72352949
6	-0.48296369	-0.41416399	-0.01864127
1	-0.09008829	-0.92046758	-2.72301961
6	-0.83318154	-3.33861411	-1.95186411
7	-0.55723835	-2.75330604	0.55973799
7	-0.41337835	-0.04737939	1.39349170
6	-1.26429459	-4.03028167	0.44060776
6	-1.30855552	-4.47295447	-1.04143088
1	-1.09972941	-3.56121466	-2.99739284
6	-0.33461923	-2.38598715	1.96346983
1	-0.73117456	-4.76939877	1.05693554
1	-0.66699423	-5.35125161	-1.20444171
1	-2.80214779	0.24439368	-1.84895931
6	0.39251245	-1.04370645	2.08958118
1	0.26602554	-3.18478366	2.42565234
1	0.46626939	-0.77562676	3.15381864
1	-2.28975994	-1.54302394	0.31060085
1	0.54251166	-0.64125016	-0.40445078
1	-1.29616068	-2.31387199	2.51854703
1	1.42132155	-1.13192589	1.67639264
1	-1.53862420	1.11666714	-2.73911403
1	-1.66562776	-1.23850684	-3.48662629
1	-2.29494712	-3.94771069	0.85288538
1	-2.33405578	-4.75767894	-1.31554355
1	0.27307273	-3.25516802	-1.90828796
6	-0.07101602	1.77846555	-0.85791087
1	0.59685124	1.60796924	-1.72976656
1	-0.62262726	2.72874416	-1.03389386
6	-0.03379160	1.36683257	1.51934184
1	-0.96016843	1.96319775	1.62964992
1	0.55948171	1.48984796	2.43366777
7	0.76095441	1.80021894	0.35714813
6	1.57913498	3.03406333	0.54164801
6	2.28976240	3.36351364	-0.78440289
6	2.67010826	2.75187983	1.59248526
1	2.25611621	2.58504808	2.59589137
1	3.25390392	1.86648327	1.30615794
1	3.34916582	3.61307035	1.66283728
1	2.85615912	2.49445366	-1.14748647
1	2.99364072	4.19175179	-0.62474275
1	1.58696927	3.67661976	-1.56839539
6	0.73989147	4.25440019	0.98718804
1	-0.05732152	4.48112154	0.26479314
1	0.27126471	4.08258808	1.96649932
1	1.37600391	5.14706641	1.07284641

2d-K2

6	-0.80396206	-0.98329862	-2.24529652
7	-1.68397968	-1.69431846	-1.30908423
6	-0.88542612	0.54342460	-2.10023081
6	-1.57678732	-1.21541604	0.09947701
7	-0.84147507	0.91149837	-0.69167924
6	-0.46590654	-0.16301757	0.20503703
1	0.25408998	-1.30806648	-2.13737610
6	-1.49132496	-3.14099291	-1.42611955
7	-1.33863867	-2.31060334	1.04223368
7	-0.36361235	0.38037547	1.55486508
6	-2.41452081	-3.30137713	0.92596855
6	-2.45326222	-3.89023092	-0.50366590
1	-1.68443397	-3.42126651	-2.47375218
6	-1.29859541	-1.74326754	2.39387994
1	-2.23397105	-4.08613389	1.67570394
1	-2.17581040	-4.95417643	-0.49453003
1	-1.82386605	0.90688409	-2.55603858
6	-0.18779768	-0.70735598	2.51914411
1	-1.11594070	-2.56048150	3.10807854
1	-0.19456924	-0.27845956	3.53344015
1	-2.52869269	-0.69865308	0.36572932
1	0.50423824	-0.65503807	-0.06752376
1	-2.27216845	-1.27178552	2.65707270
1	0.79287115	-1.21518931	2.37428670
1	-0.04983101	0.98078745	-2.68836800
1	-1.10961881	-1.25702453	-3.26692751
1	-3.39387750	-2.83345721	1.17352568
1	-3.47328141	-3.81984833	-0.90648794
1	-0.44499358	-3.43732192	-1.19835241
6	-0.42307270	2.23609929	-0.23747877
1	-0.34869288	2.90183787	-1.10494927
1	-1.20877797	2.64333126	0.42067173
6	0.77450296	1.31863015	1.65110906
1	0.67264049	1.83726457	2.62412400
1	1.72605206	0.74428825	1.68481636
7	0.81827825	2.27008816	0.53405305
6	2.13604109	2.44038013	-0.14477755
6	3.14965940	2.91226273	0.91989243
6	2.02469980	3.56038206	-1.19435060
1	1.44774098	3.25465508	-2.07780848
1	1.55843263	4.45621113	-0.76069312
1	3.03041330	3.83042120	-1.54388732
1	2.79629030	3.83691658	1.39664496
1	4.12536011	3.10711876	0.45268454
1	3.30610004	2.15946631	1.70445468
6	2.68217017	1.16902212	-0.83681712
1	3.66683572	1.37210807	-1.28353304
1	2.80900764	0.33933099	-0.12724948
1	2.01146300	0.83399616	-1.63991572

2d-K3

6	-0.52221318	-1.30954906	-2.67682143
7	-1.13158836	-2.24909585	-1.73592374
6	-0.92887569	0.12826884	-2.36473727
6	-1.00189310	-1.81970811	-0.31529113
7	-0.65239628	0.50315808	-0.96211652
6	-0.08952862	-0.58936631	-0.18185855
1	0.58725542	-1.39333341	-2.69314733
6	-0.65704507	-3.61216159	-1.97687726
7	-0.48543821	-2.91343627	0.51545221
7	-0.00736526	-0.17034312	1.21678346
6	-1.37304708	-4.07546749	0.39669182
6	-1.37250189	-4.60104295	-1.05640369
1	-0.87198390	-3.85595035	-3.02936925
6	-0.37960695	-2.47718366	1.90918637
1	-1.01556635	-4.84400779	1.09722896
1	-0.86328276	-5.57371022	-1.11922628
1	-2.00560648	0.25519064	-2.56911006
6	0.53094905	-1.26240655	2.02539953
1	0.03374113	-3.31056177	2.49758788
1	0.57118524	-0.93078275	3.07434242
1	-2.00838830	-1.51188562	0.05227889
1	0.94109772	-0.86822074	-0.53499694
1	-1.37735722	-2.22118740	2.33028750
1	1.56253269	-1.54550609	1.71588047
1	-0.37930223	0.79397592	-3.05326173
1	-0.87204125	-1.56565995	-3.68960008
1	-2.40596474	-3.80406680	0.71021024
1	-2.40554673	-4.74658396	-1.40179910
1	0.44183453	-3.69823296	-1.84153237
6	0.16506813	1.70741270	-0.84371176
1	1.18913473	1.52530940	-1.27570196
1	-0.31645625	2.49482418	-1.43473558
6	0.82561723	1.02814584	1.32620934
1	0.87429992	1.30248190	2.38711245
1	1.86984230	0.79335951	0.97913129
7	0.23695938	2.11802427	0.55522021
6	0.82933748	3.46854116	0.80464903
6	0.63129124	3.82008839	2.29252785
6	0.04614655	4.50863717	-0.02009618
1	0.26302878	4.44522708	-1.09482766
1	-1.03507572	4.38174791	0.12921243
1	0.32703216	5.51916823	0.30572095
1	-0.41925294	3.67958445	2.58139594
1	0.90476375	4.87049575	2.46171108
1	1.26065991	3.21386606	2.95756859
6	2.33262191	3.57112713	0.45313733
1	2.94011717	2.88868537	1.06388723
1	2.51714745	3.33933140	-0.60525640
1	2.69566068	4.59279939	0.63758876

2d-K4

6	0.30521400	-0.95932960	-2.84307912
7	-0.12040843	-2.05183497	-1.96830014
6	-0.39114750	0.34611070	-2.46948359
6	-0.10332806	-1.68755276	-0.52369814
7	-0.21426287	0.69941670	-1.04450408
6	0.53726128	-0.30733637	-0.30089398
1	1.40877043	-0.81697909	-2.83153988
6	0.61692259	-3.28017111	-2.26682784
7	0.61315870	-2.70029131	0.25958224
7	0.51868518	0.03885433	1.12267056
6	-0.01415114	-4.01145419	0.06170219
6	0.08862907	-4.43746848	-1.42056541
1	0.47362216	-3.50027302	-3.33652369
6	0.61926492	-2.33470920	1.67719542
1	0.49932500	-4.73001385	0.71760643
1	0.76360076	-5.29809447	-1.53389486
1	-1.46809044	0.26006084	-2.69321859
6	1.25904966	-0.96813561	1.87898540
1	1.19043630	-3.10053380	2.22407927
1	1.22348178	-0.69804759	2.94599723
1	-1.15760908	-1.61276257	-0.16674392
1	1.60803061	-0.35421806	-0.64244423
1	-0.41244926	-2.31484147	2.09462959
1	2.32975558	-1.01416398	1.57573058
1	0.01688356	1.14743191	-3.11023388
1	0.03409414	-1.22573081	-3.87718789
1	-1.07953330	-3.98214453	0.38295055
1	-0.89991122	-4.74202974	-1.79180971
1	1.70844361	-3.15957145	-2.10263742
6	0.40187542	2.02246071	-0.83683094
1	1.46161427	2.01204120	-1.18776211
1	-0.14029406	2.75628808	-1.44241367
6	1.10573559	1.38385790	1.30855996
1	1.09830849	1.60788614	2.38257235
1	2.16995097	1.37343449	0.97278610
7	0.42706411	2.42171957	0.55747441
6	-0.80564056	3.03089367	1.16048470
6	-1.31980232	4.13204036	0.21382548
6	-0.39263977	3.71650188	2.47847500
1	-0.09232092	2.99398046	3.24926065
1	0.44023351	4.41285418	2.30865861
1	-1.24417375	4.27991218	2.88404299
1	-0.50416734	4.80469636	-0.08823383
1	-2.08258324	4.72749499	0.73297138
1	-1.79354568	3.71914329	-0.68695248
6	-1.95360795	2.03632126	1.44062442
1	-2.26742964	1.52978747	0.51934245
1	-1.64477480	1.26096013	2.15293183
1	-2.81754037	2.57353922	1.86263963

2d-K5

6	-0.72527980	-1.26421167	-2.68956728
7	-0.11664486	-2.20288796	-1.74733925
6	-0.38712661	0.18240715	-2.29389888
6	-0.58856531	-1.93484957	-0.38377773
7	-0.80312187	0.39243870	-0.90911882
6	-0.05907838	-0.52957249	-0.05012433
1	-0.32264274	-1.46841310	-3.69279670
6	-0.16862490	-3.62621877	-2.12424361
7	-0.08540528	-2.94545651	0.53590100
7	-0.25836703	-0.14576956	1.33817196
6	-0.67485884	-4.27552165	0.26251273
6	-1.10176310	-4.41982954	-1.20758652
1	-0.50295530	-3.70888507	-3.17019913
6	-0.34647808	-2.53818187	1.91780377
1	0.07401700	-5.04112709	0.52430188
1	-1.10104458	-5.48302043	-1.48918111
1	-0.94485087	0.87278167	-2.94424299
6	0.27295352	-1.18208591	2.22645341
1	0.08989329	-3.29367074	2.58973708
1	0.04165279	-0.90491486	3.26724626
1	-1.70702160	-1.87163150	-0.33925226
1	1.02758701	-0.53276005	-0.31027742
1	-1.43986698	-2.49751074	2.12575833
1	1.37932826	-1.25912994	2.13499529
1	0.70095658	0.35608320	-2.44186400
1	-1.83391862	-1.36464404	-2.73307688
1	-1.55929358	-4.44737137	0.91122424
1	-2.13184492	-4.05532551	-1.33688221
1	0.84689148	-4.05767340	-2.07550435
6	0.39671153	1.15046985	1.62063613
1	-0.17189037	1.62950447	2.44962869
1	1.43415740	0.98384134	1.97293738
6	-0.76673795	1.75613083	-0.38141145
1	-0.79487417	2.45966335	-1.22256891
1	-1.67747830	1.92047971	0.23009967
7	0.45543209	1.97152323	0.40564836
6	0.85049326	3.39480046	0.62531619
6	1.25594773	4.00377333	-0.73047711
6	2.08892421	3.43757565	1.53945097
1	1.86034181	3.12812756	2.56827500
1	2.88430307	2.78879058	1.14632333
1	2.47333228	4.46570696	1.58335847
1	2.04815324	3.40157484	-1.19570876
1	1.63209806	5.02552943	-0.58124734
1	0.41360909	4.06880570	-1.43208808
6	-0.27638373	4.24676800	1.25568625
1	-1.15152788	4.31001291	0.59376052
1	-0.60669615	3.83229651	2.21878383
1	0.07755808	5.27157790	1.43842439

2d-K6

6	-1.02048592	-0.98025811	-2.50259277
7	-0.49043155	-1.95949355	-1.55284351
6	-0.54765921	0.43243411	-2.11913052
6	-0.94911811	-1.64904145	-0.19316114
7	-0.92429144	0.68418595	-0.73749810
6	-0.30364445	-0.29273609	0.14823038
1	-0.64394462	-1.23079770	-3.50557464
6	-0.65676046	-3.37576253	-1.92596693
7	-0.54822307	-2.69480173	0.73654011
7	-0.51335467	0.11446474	1.53033450
6	-1.22849840	-3.97924827	0.45409615
6	-1.66180376	-4.08419765	-1.01643950
1	-0.98543851	-3.43330299	-2.97525920
6	-0.80675817	-2.26284125	2.11204647
1	-0.53472954	-4.79729022	0.70970026
1	-1.75545858	-5.14304044	-1.29881673
1	-1.04174273	1.17045873	-2.76886503
6	-0.09004858	-0.95823701	2.43234759
1	-0.44624769	-3.04810370	2.79469198
1	-0.32086137	-0.65740381	3.46664276
1	-2.05771876	-1.48355559	-0.16183390
1	0.78897594	-0.40936910	-0.06896270
1	-1.89780212	-2.13594970	2.29493732
1	1.00902535	-1.12571791	2.36635983
1	0.55044757	0.48948487	-2.29466364
1	-2.13377781	-0.98136277	-2.53686036
1	-2.12271711	-4.09423353	1.10125324
1	-2.65450734	-3.62854740	-1.14980823
1	0.31865645	-3.89011210	-1.86501973
6	0.25099747	1.34812464	1.83401297
1	-0.16463461	1.74954088	2.77947967
1	1.31329354	1.08757992	2.02778328
6	-0.90406497	2.04069704	-0.16742346
1	-0.92585696	2.77012243	-0.98428067
1	-1.83643115	2.16139082	0.40830779
7	0.18802474	2.33024902	0.75092960
6	1.47407068	2.93459639	0.30084037
6	2.09115032	3.66436567	1.51418954
6	1.19097614	3.99357459	-0.77782435
1	0.88392453	3.54758822	-1.73384832
1	0.41128163	4.69405844	-0.44686543
1	2.10813646	4.56729759	-0.96788352
1	1.39061027	4.41690747	1.90164047
1	3.02465611	4.16659674	1.22289998
1	2.33252322	2.96914505	2.33015863
6	2.50750082	1.92876839	-0.25821566
1	3.43314188	2.45334083	-0.53762324
1	2.77509432	1.16210808	0.48206876
1	2.12452426	1.41832399	-1.15223037

2d-K7

6	-0.28718834	-1.31898234	-2.85212062
7	0.57933126	-2.11763087	-1.99298885
6	-0.14096833	0.15482041	-2.47164316
6	0.14765694	-1.95991224	-0.60062143
7	-0.44133879	0.35862495	-1.05103010
6	0.41315331	-0.49284846	-0.22299506
1	0.02945709	-1.44881637	-3.89717744
6	0.79469110	-3.51812265	-2.39684614
7	0.89236192	-2.87946322	0.25199503
7	0.12652920	-0.26290826	1.18806969
6	0.53072813	-4.28834144	-0.01692806
6	0.06773986	-4.49131834	-1.46822735
1	0.45037615	-3.64477221	-3.43473034
6	0.71550501	-2.57619702	1.67281437
1	1.41524427	-4.91082620	0.19687070
1	0.25482002	-5.53051169	-1.77567141
1	-0.84486364	0.76492490	-3.05955932
6	1.01171450	-1.11509166	1.98171921
1	1.39786178	-3.22274117	2.24760184
1	0.81886166	-0.92466888	3.04857431
1	-0.95858130	-2.11219673	-0.49768293
1	1.49672474	-0.28335613	-0.43550480
1	-0.32197415	-2.80395548	2.00533196
1	2.08588212	-0.90032022	1.78241961
1	0.89324465	0.48024905	-2.72264247
1	-1.35881950	-1.61309884	-2.77523608
1	-0.27625017	-4.61946142	0.67080839
1	-1.01728560	-4.32505346	-1.54493700
1	1.87588752	-3.74037463	-2.38589681
6	0.30560410	1.15048310	1.52262654
1	0.07569943	1.26899480	2.58819449
1	1.37990116	1.44603650	1.36197297
6	-0.25974503	1.76415097	-0.68518512
1	0.79931932	2.07662937	-0.90042963
1	-0.92370249	2.36056816	-1.32301433
7	-0.60018217	1.96310491	0.71916283
6	-0.75015152	3.38786806	1.14687631
6	-1.16574296	3.41627927	2.63077726
6	-1.89949462	4.02043927	0.33737991
1	-1.64562400	4.15533881	-0.72236838
1	-2.80099651	3.39626107	0.40362681
1	-2.12999490	5.01562209	0.74153897
1	-1.99906435	2.72264682	2.80959855
1	-1.49334658	4.42975405	2.89865665
1	-0.33962798	3.15593679	3.30598115
6	0.53109148	4.23500143	0.96278723
1	0.36253939	5.26112035	1.32087943
1	1.37516756	3.81879927	1.53077003
1	0.82784926	4.29731555	-0.09359744

2d-K8

6	0.21079937	-0.87223009	-2.86564449
7	1.14608704	-1.59717811	-2.01320621
6	0.21892140	0.60355889	-2.46619034
6	0.70270980	-1.49704894	-0.61918341
7	-0.09843018	0.76602439	-1.04489359
6	0.82990361	-0.01608357	-0.22306792
1	0.54090302	-0.96077550	-3.91087986
6	1.49147493	-2.96643556	-2.43459351
7	1.53239356	-2.35276836	0.22105435
7	0.53232976	0.17272587	1.19577824
6	1.30651845	-3.78624474	-0.06456720
6	0.86104043	-4.01457937	-1.51734402
1	1.15821898	-3.11226070	-3.47355848
6	1.33677227	-2.08535074	1.64642986
1	2.24735497	-4.32354826	0.13956966
1	1.14353352	-5.02799888	-1.83764263
1	-0.53515246	1.15483899	-3.05062721
6	1.49576122	-0.60716835	1.97262248
1	2.07963503	-2.67337374	2.20895495
1	1.29470875	-0.44759753	3.04334285
1	-0.38492274	-1.75482787	-0.51773419
1	1.89005109	0.29361916	-0.43240744
1	0.32741094	-2.41449260	1.98192215
1	2.54312987	-0.28823879	1.77074985
1	1.21916407	1.02658185	-2.71045914
1	-0.82925762	-1.26590985	-2.79679126
1	0.53730152	-4.20199376	0.62061554
1	-0.23501612	-3.94999316	-1.59095416
1	2.58877659	-3.08604867	-2.42758176
6	0.61740775	1.61156538	1.51827789
1	0.44747195	1.73252671	2.59447955
1	1.64647614	1.98173259	1.29523914
6	-0.03070208	2.19110045	-0.65795957
1	0.99134439	2.58628644	-0.86839166
1	-0.73572792	2.74479300	-1.29065503
7	-0.30044598	2.42401004	0.74722057
6	-1.73251691	2.52201646	1.18494612
6	-2.36199101	3.72839840	0.45934510
6	-1.76215116	2.82813911	2.69366451
1	-1.47294400	1.95986169	3.30075072
1	-1.09896966	3.67058862	2.93752474
1	-2.78510818	3.09943887	2.98732104
1	-1.75716192	4.63253084	0.61479926
1	-3.37171757	3.90978532	0.85237137
1	-2.46546869	3.55874229	-0.62084046
6	-2.58407991	1.26237970	0.91225703
1	-2.17310223	0.39093008	1.43736582
1	-3.61690214	1.42849449	1.25652645
1	-2.60583199	1.02147751	-0.15795566

2d-K9

6	-0.43221109	-1.16557672	-2.71320794
7	-0.17012626	-2.24937035	-1.74987685
6	-1.38027033	-0.08551667	-2.16548964
6	-0.53592628	-1.94166443	-0.37094391
7	-0.94968433	0.44084528	-0.86610559
6	-0.17331031	-0.49633363	-0.07066780
1	0.52356654	-0.69380034	-3.00509938
6	-0.61894903	-3.58686142	-2.11210231
7	0.21313658	-2.82464779	0.53572588
7	-0.45374803	-0.18147988	1.32445851
6	-0.18424281	-4.21306325	0.29412238
6	0.04720461	-4.59724807	-1.17085069
1	-1.72868591	-3.69129637	-2.04378974
6	0.04484798	-2.44898722	1.94474618
1	-1.25994910	-4.36622037	0.55015340
1	1.12727992	-4.61625499	-1.37595314
1	-2.39676372	-0.50381387	-2.06989730
6	0.41652808	-0.98092138	2.17866064
1	0.69656070	-3.10515572	2.54296392
1	0.22944147	-0.72570635	3.23202302
1	-1.63751626	-2.07899408	-0.19835808
1	0.92056303	-0.40081067	-0.28181990
1	-1.00217514	-2.60059340	2.28997094
1	1.49699062	-0.82707590	1.96437783
1	-1.44417918	0.74506596	-2.88552165
1	-0.87056316	-1.59290380	-3.62949649
1	0.40355546	-4.86454290	0.95919250
1	-0.35878847	-5.60425765	-1.35363505
1	-0.33146147	-3.79203688	-3.15377471
6	-0.47777321	1.28057966	1.49377010
1	-1.53408583	1.61268292	1.47203500
1	-0.06451771	1.52722537	2.47949851
6	-0.28820243	1.74520899	-0.87542128
1	0.51755962	1.80525559	-1.63859577
1	-1.05740468	2.50813897	-1.13107899
7	0.32437777	1.94854275	0.45062235
6	0.74808563	3.34784962	0.74553403
6	1.52421486	3.90098645	-0.46432216
6	1.71432824	3.33132726	1.94580095
1	1.21811736	3.04528656	2.88276201
1	2.53888815	2.62952770	1.76044488
1	2.13481723	4.33533283	2.09693211
1	2.34922914	3.22815216	-0.73763002
1	1.94879490	4.88102791	-0.20728289
1	0.88119372	4.04216033	-1.34347454
6	-0.44205115	4.28604609	1.05702943
1	-1.15814580	4.32013589	0.22347701
1	-0.98293383	3.96243511	1.95749304
1	-0.08561609	5.31132071	1.23260126

2d-K10

6	-1.12890055	-0.90306255	-2.53430433
7	-0.96852238	-1.96132776	-1.52013911
6	-1.81441201	0.35837138	-1.98402588
6	-1.14778464	-1.51413372	-0.14214394
7	-1.16775761	0.87674072	-0.77323242
6	-0.50213779	-0.14551192	0.02308053
1	-0.13833527	-0.63146099	-2.94251872
6	-1.67882337	-3.21231367	-1.75136763
7	-0.49545459	-2.46992117	0.76612887
7	-0.56771000	0.28794678	1.40843975
6	-1.15466697	-3.77293341	0.65219757
6	-1.12296016	-4.27264307	-0.79492037
1	-2.77901142	-3.10630801	-1.59315678
6	-0.47609103	-1.99353989	2.15483581
1	-2.21365913	-3.71088816	0.99914710
1	-0.08413251	-4.49561200	-1.07856579
1	-2.87107993	0.13224771	-1.76207897
6	0.19078873	-0.61764617	2.25605384
1	0.08401055	-2.73240641	2.74968184
1	0.14524048	-0.26853015	3.29828501
1	-2.23545246	-1.43018485	0.12578095
1	0.56132708	-0.27489274	-0.30325132
1	-1.50142764	-1.91691989	2.58009591
1	1.26184831	-0.71069008	1.96504257
1	-1.81237761	1.14607471	-2.75334228
1	-1.72352196	-1.29401419	-3.37566432
1	-0.63713804	-4.48370750	1.31490032
1	-1.71070955	-5.20011026	-0.87611978
1	-1.52394690	-3.52452223	-2.79459980
6	-0.36197608	1.75601850	1.46958163
1	-1.36387735	2.21122243	1.49747375
1	0.14071204	2.00749327	2.40946543
6	-0.25359477	2.00923506	-0.95406990
1	0.55716620	1.77439119	-1.68066139
1	-0.84312839	2.84712219	-1.37712042
7	0.34972236	2.35013494	0.34058341
6	1.80390713	2.66239445	0.36953919
6	2.20205395	3.15113351	1.77259426
6	2.05179749	3.82944321	-0.61170101
1	1.80827840	3.55263709	-1.64670549
1	1.43741490	4.69727897	-0.33437948
1	3.11026638	4.12583959	-0.59057618
1	1.53302390	3.95323693	2.11480279
1	3.22533382	3.54879046	1.73698577
1	2.19445188	2.34226197	2.51607231
6	2.72434502	1.47932814	-0.01422472
1	3.77795524	1.79535511	0.00466398
1	2.60859549	0.64273904	0.68869298
1	2.51035076	1.10584345	-1.02525555

2d-K11

6	0.01388455	-1.36650810	-2.70178337
7	0.04828342	-2.43423149	-1.69156529
6	-0.89303650	-0.18867373	-2.31374251
6	-0.33610755	-2.01072365	-0.34805493
7	-0.60997274	0.32224227	-0.96465832
6	0.16101113	-0.58464860	-0.12742349
1	1.03829254	-0.99052807	-2.87271896
6	-0.58295845	-3.70387758	-2.02686695
7	0.23367024	-2.94523880	0.62874831
7	-0.00003433	-0.14966529	1.25857676
6	-0.35700825	-4.27046526	0.42060679
6	-0.11833271	-4.75498237	-1.01222290
1	-1.69709419	-3.63865250	-2.01343847
6	0.02801530	-2.46719056	1.99635377
1	-1.45434916	-4.24570497	0.62262490
1	0.95580745	-4.93867503	-1.15951864
1	-1.95007766	-0.50407617	-2.37187575
6	0.65484211	-1.08836096	2.16829424
1	0.50687193	-3.18364056	2.68148699
1	0.49996295	-0.73475886	3.19926964
1	-1.45400725	-1.99638786	-0.23306210
1	1.25415168	-0.56214617	-0.39364390
1	-1.05117025	-2.40929743	2.26196801
1	1.75108245	-1.16001642	1.98919340
1	-0.75910856	0.62002102	-3.05020507
1	-0.33431915	-1.78989012	-3.65650525
1	0.09146236	-4.96815934	1.14473368
1	-0.65731526	-5.70139092	-1.17354807
1	-0.27994706	-3.99681295	-3.04267102
6	0.54463877	1.20369676	1.38648779
1	0.42918098	1.51399870	2.43202681
1	1.64369280	1.18610033	1.14740036
6	-0.07205887	1.67067568	-0.87361181
1	0.99296914	1.70160511	-1.23504428
1	-0.67123489	2.32235947	-1.51939623
7	-0.17951661	2.12962573	0.51498084
6	0.12579141	3.57662725	0.73843892
6	-0.22457096	3.93002961	2.19758340
6	-0.79325394	4.41703217	-0.17017451
1	-0.50532539	4.36160836	-1.22861768
1	-1.83644027	4.08588596	-0.07155794
1	-0.73353871	5.47343679	0.12438984
1	-1.23470247	3.57553384	2.44497414
1	-0.19287664	5.01993202	2.33045132
1	0.48286473	3.49842965	2.91824610
6	1.59881707	3.96292586	0.46252646
1	2.29103713	3.41844350	1.11991145
1	1.88353199	3.75670462	-0.57877164
1	1.74849571	5.03778908	0.64140516

2d-K12

6	0.73600338	-0.95589153	-2.79277608
7	0.85247897	-2.03865804	-1.80608674
6	-0.30213816	0.10920847	-2.40990348
6	0.40250900	-1.69147719	-0.46195879
7	-0.11715573	0.61400912	-1.04110696
6	0.72932545	-0.22369067	-0.19992564
1	1.71907720	-0.46877607	-2.92023569
6	0.36642014	-3.35939681	-2.18193107
7	1.05986718	-2.57987442	0.50380691
7	0.49737728	0.15642870	1.19621566
6	0.62322131	-3.95731202	0.25651619
6	0.92890747	-4.37837434	-1.18403519
1	-0.74829521	-3.41511411	-2.18421713
6	0.78649214	-2.16240020	1.87947020
1	-0.47178148	-4.06026704	0.44572953
1	2.01821694	-4.44227814	-1.32016909
1	-1.31816123	-0.31325949	-2.51274231
6	1.24721044	-0.72456050	2.09010672
1	1.33719323	-2.83642733	2.55366949
1	1.04783320	-0.41587700	3.12813854
1	-0.71200220	-1.80756298	-0.36657462
1	1.81935001	-0.07385105	-0.43674303
1	-0.29508093	-2.23618975	2.13271768
1	2.34551712	-0.66405200	1.91980841
1	-0.23033836	0.94690945	-3.12322596
1	0.46766452	-1.39051800	-3.76791836
1	1.14031427	-4.61899955	0.96823654
1	0.49715295	-5.37332936	-1.37350714
1	0.71274220	-3.59294908	-3.19923035
6	0.90152786	1.57261886	1.34028854
1	0.80158599	1.85462275	2.39425996
1	1.97769850	1.67541270	1.06359970
6	0.27860931	2.02133994	-0.89179829
1	1.34327760	2.16845776	-1.19016718
1	-0.34368781	2.63138290	-1.55699179
7	0.15740331	2.48029583	0.48583608
6	-1.19563828	2.95351387	0.93319938
6	-1.52219137	4.23564189	0.13970476
6	-1.12015777	3.34538146	2.41995040
1	-1.05488726	2.46852606	3.07811496
1	-0.25998870	4.00257864	2.61317279
1	-2.03417413	3.88834196	2.69541205
1	-0.72454318	4.98055373	0.26574520
1	-2.46686989	4.66623572	0.49975217
1	-1.64797141	4.04162279	-0.93423793
6	-2.33975157	1.93241452	0.74714299
1	-2.47893366	1.67215087	-0.30981892
1	-2.12877273	1.00354069	1.29137735
1	-3.28245591	2.35989802	1.12332955

2d-K13

6	-0.97775261	-1.47934695	-2.65968085
7	-0.09159134	-2.31157176	-1.84381208
6	-0.64758473	-0.00692726	-2.45960992
6	-0.32715052	-1.99593273	-0.43494899
7	-0.78671876	0.38191258	-1.05574863
6	-0.04645127	-0.50811486	-0.17281020
1	-0.82153823	-1.74231403	-3.71680012
6	-0.29623156	-3.73655150	-2.10679293
7	0.56807277	-2.76195268	0.44247129
7	-0.45444046	-0.23176641	1.20499969
6	0.40061606	-4.20207572	0.24234131
6	0.63110930	-4.56485902	-1.22220290
1	-1.35478399	-4.03236088	-1.91277812
6	0.35687498	-2.40831053	1.85320696
1	1.11984529	-4.72366414	0.89264550
1	1.67688203	-4.35897336	-1.49332290
1	-1.33052007	0.61314504	-3.06251814
6	0.48652909	-0.90238554	2.09528775
1	1.10760693	-2.95119656	2.44882103
1	0.21655630	-0.68623993	3.13948369
1	-1.40009216	-2.19746304	-0.17195799
1	1.05614329	-0.36988663	-0.29620664
1	-0.65110006	-2.72895294	2.19914932
1	1.53729697	-0.57995019	1.92824966
1	0.38711422	0.17544215	-2.82580113
1	-2.04921903	-1.66176567	-2.41856421
1	-0.62036054	-4.53331773	0.54875049
1	0.43849570	-5.63723375	-1.37658456
1	-0.09424544	-3.92233989	-3.17300044
6	-0.69993621	1.19532617	1.41382955
1	-1.78185074	1.38881567	1.26694896
1	-0.45102157	1.44465198	2.45253026
6	-0.34706995	1.78144137	-0.87592053
1	0.48972208	2.01073148	-1.56626570
1	-1.20777460	2.42998099	-1.15667687
7	0.12077916	1.99753226	0.49743465
6	0.32786460	3.42643983	0.87785815
6	1.12983833	4.13004398	-0.23235796
6	1.17832569	3.47061244	2.16169335
1	0.65597576	3.04312229	3.02801355
1	2.11609891	2.91762964	2.01505530
1	1.42000247	4.51302573	2.41203101
1	2.04844238	3.57147127	-0.46063408
1	1.41309171	5.13633607	0.10512253
1	0.55002450	4.24490497	-1.15818604
6	-0.99738265	4.18930210	1.11092979
1	-1.64279980	4.16009503	0.22149412
1	-1.56115764	3.76805894	1.95520275
1	-0.79453457	5.24543173	1.33963125

2d-K14

6	-1.67483645	-1.16229047	-2.46491474
7	-0.87559534	-2.08832729	-1.65935239
6	-1.09860157	0.24393419	-2.37954927
6	-0.94381746	-1.66152785	-0.26214064
7	-1.06396195	0.72293349	-0.99746949
6	-0.39405699	-0.23062366	-0.12107057
1	-1.64516395	-1.50161608	-3.51139384
6	-1.33335002	-3.46933770	-1.81722520
7	-0.13284647	-2.52591424	0.60622389
7	-0.60633894	0.17982149	1.26069853
6	-0.55424408	-3.92445140	0.50582198
6	-0.49343436	-4.39634235	-0.94404811
1	-2.40864617	-3.57022025	-1.53586225
6	-0.18758338	-2.07226071	2.00341997
1	0.11113703	-4.52772852	1.14263451
1	0.54946958	-4.38533325	-1.29300878
1	-1.71572182	0.93814510	-2.97217737
6	0.23836120	-0.60803822	2.14081450
1	0.48503243	-2.71857375	2.58923555
1	0.08467017	-0.28575994	3.18139842
1	-2.01202353	-1.65165103	0.08442987
1	0.69801989	-0.29745234	-0.36280717
1	-1.21428469	-2.17769131	2.41916839
1	1.32359898	-0.52409670	1.90598945
1	-0.07847946	0.23331618	-2.82567381
1	-2.73972541	-1.15234407	-2.14067661
1	-1.59203166	-4.05856062	0.89410106
1	-0.87157329	-5.42708041	-1.01764705
1	-1.24624852	-3.74126955	-2.88052248
6	-0.70586631	1.64214902	1.40037171
1	-1.77297959	1.90111794	1.30475135
1	-0.38861347	1.92268235	2.41054185
6	-0.39201852	2.04335008	-0.95286254
1	0.50788210	2.02588831	-1.60416656
1	-1.10194427	2.76918105	-1.39732505
7	0.00320659	2.42670927	0.40135337
6	1.39718781	2.91511912	0.59924338
6	1.58771710	3.33560155	2.06608393
6	1.57158981	4.17901987	-0.27123458
1	1.45465939	3.95733596	-1.34107194
1	0.82513161	4.93631437	0.00514113
1	2.57584365	4.60369349	-0.13076408
1	0.78455253	4.01275865	2.38964501
1	2.54396110	3.86639854	2.16655946
1	1.62181636	2.47501670	2.74841164
6	2.50285599	1.89763144	0.23291175
1	3.49532937	2.34829573	0.38123859
1	2.44270039	0.99845422	0.86090020
1	2.43926460	1.58362359	-0.81812497

2d-K15

6	-0.34404195	-1.41244869	-2.78551474
7	0.35338256	-2.31423053	-1.86716941
6	-0.00373554	0.03746692	-2.47533348
6	-0.01756611	-2.00667667	-0.48140231
7	-0.38150707	0.34767708	-1.09738774
6	0.33554843	-0.53656306	-0.18020251
1	-0.02405217	-1.65646445	-3.81012056
6	0.07046616	-3.71188510	-2.19916231
7	0.70729580	-2.87472925	0.45307541
7	-0.03137455	-0.20554621	1.19577373
6	0.43506267	-4.28916859	0.19097009
6	0.81085151	-4.64111235	-1.24393789
1	-1.02424365	-3.92233545	-2.14591580
6	0.36064274	-2.52747300	1.83226126
1	1.01829831	-4.88597272	0.90902412
1	1.89574575	-4.52426850	-1.38117442
1	-0.56913307	0.70148813	-3.14741179
6	0.69786293	-1.07225677	2.12044399
1	0.93950068	-3.18094820	2.50283978
1	0.39164532	-0.82006088	3.14750197
1	-1.12538307	-2.12354302	-0.34077957
1	1.44518229	-0.42616093	-0.32310229
1	-0.71975844	-2.69826769	2.03777173
1	1.79923148	-0.93011899	2.04422519
1	1.08142056	0.20575754	-2.65776496
1	-1.44755868	-1.54672494	-2.73152392
1	-0.64187273	-4.52785423	0.36064413
1	0.54580363	-5.68776827	-1.45631514
1	0.38537283	-3.88404751	-3.23989082
6	0.25176867	1.20331558	1.47620313
1	-0.03606222	1.39549073	2.51667111
1	1.35651803	1.39332967	1.37799102
6	-0.09703827	1.74973202	-0.78687490
1	0.99980428	1.95439502	-0.93395640
1	-0.65642582	2.36503685	-1.50177538
7	-0.51827695	2.05134732	0.57524207
6	-0.56747256	3.50249820	0.93201018
6	-1.15796863	3.63892324	2.34885622
6	-1.53294858	4.21190081	-0.03729792
1	-1.12436475	4.29843501	-1.05292900
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1	-1.72545234	5.23274386	0.31949959
1	-2.09540887	3.07156757	2.42948457
1	-1.36954770	4.69659345	2.55649139
1	-0.46876459	3.29026855	3.12942540
6	0.80986044	4.20589136	0.88469806
1	1.51945025	3.75364564	1.59191575
1	1.25338516	4.15948788	-0.11992202
1	0.70450961	5.26729844	1.15258617

2d-K16

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6	0.43689215	0.50023481	-2.44354125
6	0.62513742	-1.57815715	-0.49356248
7	0.00351918	0.73817864	-1.06778016
6	0.79987636	-0.08452076	-0.15340754
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6	0.93640916	-3.22085197	-2.24609925
7	1.43089329	-2.37986301	0.43368930
7	0.38011177	0.17017622	1.22642121
6	1.32729856	-3.80975559	0.13601228
6	1.76445156	-4.08159749	-1.29866820
1	-0.12718341	-3.55750431	-2.21540564
6	1.02737580	-2.11002874	1.81455026
1	1.96419612	-4.35154219	0.85206133
1	2.83065118	-3.83757936	-1.41310164
1	-0.18549124	1.11287936	-3.11451101
6	1.18807218	-0.63324639	2.14168514
1	1.66842513	-2.70992856	2.47858117
1	0.84154465	-0.44218685	3.16953450
1	-0.46435319	-1.82659665	-0.37549646
1	1.89165702	0.15571951	-0.27481468
1	-0.02833914	-2.41216263	1.99713311
1	2.26651870	-0.36180619	2.08864847
1	1.49921709	0.79460853	-2.59883116
1	-0.81145065	-1.23217018	-2.76277176
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1	1.62518070	-5.14620648	-1.53932798
1	1.28391536	-3.33091833	-3.28483322
6	0.51532901	1.60952988	1.53559158
1	0.21320674	1.75759169	2.57978276
1	1.58619493	1.91024192	1.44782915
6	0.16236368	2.16300432	-0.70868607
1	1.23689641	2.45042399	-0.79954880
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7	-0.24438390	2.46507232	0.64713433
6	-1.70096384	2.67609187	0.94090916
6	-2.26342585	3.67799588	-0.08472323
6	-1.80666265	3.33554636	2.33087360
1	-1.51627870	2.65257941	3.14056774
1	-1.17250135	4.23138266	2.38407967
1	-2.84756944	3.63101680	2.52053666
1	-1.62330236	4.56900884	-0.15620168
1	-3.26487810	3.99759807	0.23320529
1	-2.37045848	3.23568490	-1.08428044
6	-2.56407305	1.39562058	0.91804902
1	-2.51864543	0.90824172	-0.06405803
1	-2.21677444	0.66862890	1.66285083
1	-3.61279435	1.64903724	1.13911864

2d-K17

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6	-0.52532584	-0.00512939	-2.37630370
6	-0.58077174	-1.93732506	-0.25768696
7	-0.86821988	0.34496335	-1.00093205
6	-0.12955599	-0.50048968	-0.06848683
1	-0.63014188	-1.78137713	-3.61673688
6	-0.38055336	-3.78688772	-1.82227689
7	0.13245734	-2.83515044	0.63773429
7	-0.42045274	-0.00200773	1.26637942
6	-0.53557440	-4.13755205	0.70447660
6	-1.15161191	-4.46611158	-0.67616382
1	-0.88900783	-3.99131951	-2.77823099
6	0.53433418	-2.22626342	1.91366444
1	0.21133005	-4.89874656	0.98382523
1	-1.16055025	-5.55483863	-0.83044569
1	-1.08873329	0.64471676	-3.06246612
6	-0.34844190	-1.02939439	2.31669809
1	1.58586396	-1.89436413	1.85061139
1	-1.36630306	-1.38664589	2.55050618
1	-1.68610656	-1.95409713	-0.07135838
1	0.96535166	-0.47383212	-0.29012967
1	0.48893972	-2.99301298	2.70270676
1	0.04970186	-0.57550360	3.23818644
1	0.55973317	0.10455318	-2.59421949
1	-2.04933048	-1.53310732	-2.54944910
1	-1.33757162	-4.16674019	1.47632322
1	-2.19998105	-4.13553021	-0.70344619
1	0.62899457	-4.22688432	-1.89362028
6	0.34715818	1.21982831	1.51287640
1	1.37955514	1.00140480	1.86175226
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6	-0.76641517	1.74817759	-0.57285436
1	-0.71885224	2.38799263	-1.46279531
1	-1.68688486	2.00847120	-0.01369874
7	0.44344525	1.96383535	0.24385123
6	0.90289050	3.37700491	0.37164439
6	1.35223309	3.87933107	-1.01435940
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1	1.88092999	3.18048550	2.33927360
1	2.90591521	2.72232334	0.95156117
1	2.55694179	4.43594208	1.28978701
1	2.10137867	3.19846327	-1.44090020
1	1.79844125	4.87919122	-0.92016655
1	0.51776584	3.96400800	-1.72322817
6	-0.18853573	4.31990199	0.93061001
1	-1.05604936	4.37310467	0.25786365
1	-0.54287729	3.98673830	1.91667184
1	0.20813399	5.33887945	1.04608003

2d-K18

6	-1.48650669	-1.05539743	-2.34380209
7	-0.99664325	-1.98679446	-1.32958853
6	-0.74216131	0.28428677	-2.20521012
6	-1.19108806	-1.46697520	0.02565390
7	-0.95008565	0.77470833	-0.85036912
6	-0.42469017	-0.15911564	0.13427979
1	-1.28687659	-1.48665298	-3.33641647
6	-1.43695936	-3.39417009	-1.43840062
7	-0.68067021	-2.45240425	0.96565379
7	-0.57151904	0.46452168	1.44248680
6	-1.61003494	-3.57702098	1.10206055
6	-2.31593870	-3.82426273	-0.25105981
1	-1.99761412	-3.52724713	-2.37754836
6	-0.13870804	-1.88402920	2.20850026
1	-1.03679030	-4.46885488	1.40489213
1	-2.57416135	-4.88882540	-0.34702988
1	-1.15911744	1.01057894	-2.91910907
6	-0.72934948	-0.50095629	2.54181168
1	0.96044955	-1.80297944	2.13229879
1	-1.80144108	-0.61119426	2.77955879
1	-2.26846975	-1.22298414	0.21612448
1	0.64612630	-0.40723953	-0.07735060
1	-0.34878008	-2.57804747	3.03720669
1	-0.24268620	-0.09801008	3.44414426
1	0.32933620	0.11752603	-2.45934067
1	-2.58015867	-0.86040005	-2.26281783
1	-2.37964234	-3.40117467	1.88710347
1	-3.26266715	-3.26589816	-0.28404524
1	-0.55257711	-4.05185086	-1.49505817
6	0.49254968	1.46056581	1.61450565
1	1.47818590	0.97773588	1.80435214
1	0.24161819	2.06278143	2.51045910
6	-0.57843227	2.15680990	-0.46471693
1	-0.44385082	2.75751333	-1.37048688
1	-1.43625618	2.57259468	0.08631372
7	0.59056422	2.28382517	0.40224762
6	1.95052197	2.60002821	-0.11253520
6	2.72923192	3.30108793	1.02214300
6	1.84513565	3.59601749	-1.27978167
1	1.42888374	3.13697212	-2.18697030
1	1.22730817	4.46271498	-1.00515142
1	2.85065155	3.95829025	-1.53364973
1	2.19594588	4.20499233	1.34782992
1	3.73159204	3.58912735	0.67425248
1	2.85920394	2.64606847	1.89457932
6	2.75784457	1.37058839	-0.59318692
1	2.25369073	0.86867376	-1.43054517
1	3.75684608	1.68049297	-0.93437386
1	2.89819009	0.63398312	0.21008635

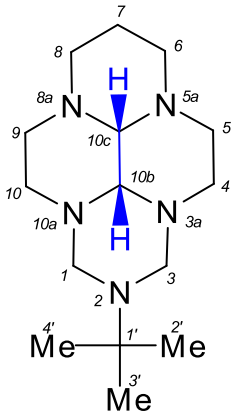
2d-K19

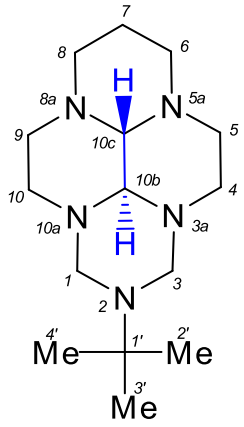
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6	-0.39617200	-3.89697347	-1.87569712
7	0.41467141	-2.95189485	0.47493679
7	-0.01273898	-0.14297473	1.16262588
6	-0.37184653	-4.17285111	0.66170196
6	-1.12752575	-4.48407119	-0.65360470
1	-0.98361547	-4.08812063	-2.78748905
6	1.04889116	-2.36037980	1.65524140
1	0.31842208	-4.99416442	0.91378735
1	-1.23709740	-5.57139731	-0.77508471
1	-0.92405603	0.55331940	-3.12699301
6	0.30707730	-1.13094729	2.20934023
1	2.08404841	-2.07049352	1.40477830
1	-0.62763497	-1.44801089	2.70555507
1	-1.38420617	-1.94215780	-0.07485302
1	1.33911318	-0.60471213	-0.43932908
1	1.11638418	-3.12770129	2.44111447
1	0.94051634	-0.66653813	2.98480773
1	0.70382809	-0.14877638	-2.86129228
1	-2.00461753	-1.53908867	-2.40316514
1	-1.10571477	-4.09001851	1.49458118
1	-2.14439555	-4.06855241	-0.60626448
1	0.57138091	-4.41078535	-2.00110840
6	0.52989689	1.19244725	1.36322376
1	1.64696120	1.19112308	1.22520178
1	0.31493954	1.49612472	2.39397626
6	0.08763911	1.66172477	-0.93640540
1	1.17834108	1.66700505	-1.21074466
1	-0.43963378	2.32538644	-1.63263461
7	-0.12462183	2.12055031	0.43707029
6	0.16350398	3.56963201	0.67006694
6	-0.20182643	3.91567965	2.12700918
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1	-0.47536667	4.33774426	-1.30187516
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1	-0.69564942	5.46257575	0.04117360
1	-1.20812744	3.54586732	2.36827662
1	-0.19023071	5.00609369	2.25807689
1	0.50978894	3.49728162	2.85139653
6	1.63500605	3.97221524	0.40969908
1	1.77562072	5.04404899	0.61264046
1	2.32737874	3.41763244	1.05853447
1	1.92648888	3.79201461	-0.63442807

2d-K20

6	-0.13103740	-1.14075810	-2.77640598
7	0.74752667	-1.94370222	-1.93437121
6	0.19318006	0.33654433	-2.53485487
6	0.51963001	-1.63521197	-0.52489049
7	-0.00822450	0.67736794	-1.12413179
6	0.81756048	-0.16767355	-0.25349027
1	0.06144490	-1.38720755	-3.83092888
6	0.75964199	-3.40689303	-2.15923807
7	1.37815702	-2.50107216	0.26412149
7	0.48923345	0.14429676	1.13170115
6	0.81390982	-3.84878045	0.35308164
6	0.12819699	-4.18975844	-0.99264719
1	0.22041461	-3.63094991	-3.09305574
6	1.90651751	-1.89451443	1.48755885
1	1.63472323	-4.55543422	0.55707803
1	0.20126687	-5.26930604	-1.18817366
1	-0.47518942	0.97270685	-3.13668016
6	0.97031644	-0.84488986	2.11276991
1	2.87982675	-1.42185652	1.26924763
1	0.10477869	-1.35013122	2.57904753
1	-0.56077202	-1.77226885	-0.25454150
1	1.90245202	0.02193165	-0.48018380
1	2.09968643	-2.69179272	2.22103483
1	1.51774457	-0.33392593	2.92428246
1	1.23848829	0.52516641	-2.86646841
1	-1.21256649	-1.31437664	-2.57194259
1	0.07404656	-3.95450224	1.17816754
1	-0.94392133	-3.95240980	-0.93522836
1	1.80083403	-3.74209046	-2.29917842
6	0.80542050	1.55131527	1.41551831
1	1.89388446	1.74822553	1.26920148
1	0.56880399	1.75641061	2.46632790
6	0.33305580	2.08587688	-0.83570243
1	1.42007411	2.24923964	-1.02775345
1	-0.22525667	2.72668204	-1.52719251
7	0.08559799	2.46900565	0.54312696
6	-1.30938753	2.84631515	0.95214517
6	-1.91418727	3.76638566	-0.12324957
6	-1.20115437	3.67220496	2.25094930
1	-0.82375318	3.07717446	3.09379448
1	-0.53158554	4.53107682	2.10609201
1	-2.19401687	4.04379485	2.54044905
1	-1.22220058	4.58095826	-0.38188716
1	-2.83848733	4.21429292	0.26562978
1	-2.17956567	3.21901970	-1.03770895
6	-2.26634293	1.65577068	1.18246109
1	-2.35118407	1.04009303	0.27847646
1	-1.91208410	1.00655358	1.99332153
1	-3.26549695	2.03109668	1.45432084

Correlation of calculated and experimental data of skeleton chemical shifts in the ^{13}C NMR spectrum using the example of model compounds 1d and 2d

Compound 1d	Calculated data	Experimental data
	31.9 (C-7)	19.7 (C-7)
	51.0 (C-5)	44.6 (C-5)
	53.3 (C-10)	45.2 (C-10)
	56.4 (C-4)	50.6 (C-4)
	58.4 (C-9)	52.5 (C-6)
	60.8 (C-6)	54.0 (C-9)
	62.6 (C-8)	55.8 (C-8)
	80.0 (C-10b)	68.9 (C-1)
	76.9 (C-1)	72.0 (C-3)
	80.6 (C-3)	76.7 (C-10c)
	91.9 (C-10c)	76.9 (C-10b)

Compound 2d	Calculated data	Experimental data
	30.2 (C-7)	24.3 (C-7)
	54.3 (C-4)	49.0 (C-4,10)
	54.4 (C-10)	
	59.4 (C-9)	52.5 (C-5,9)
	59.5 (C-5)	
	61.1 (C-6)	53.8 (C-6,8)
	60.9 (C-8)	
	76.6 (C-3)	70.2 (C-1,3)
	77.1 (C-1)	
	91.2 (C-10c)	82.5 (C-10c)
	94.0 (C-10b)	83.3 (C-10b)