

Supporting information

2,3-Di-*O*-picolinyl building blocks as glycosyl donors with switchable stereoselectivity

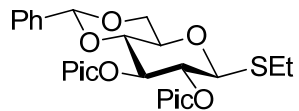
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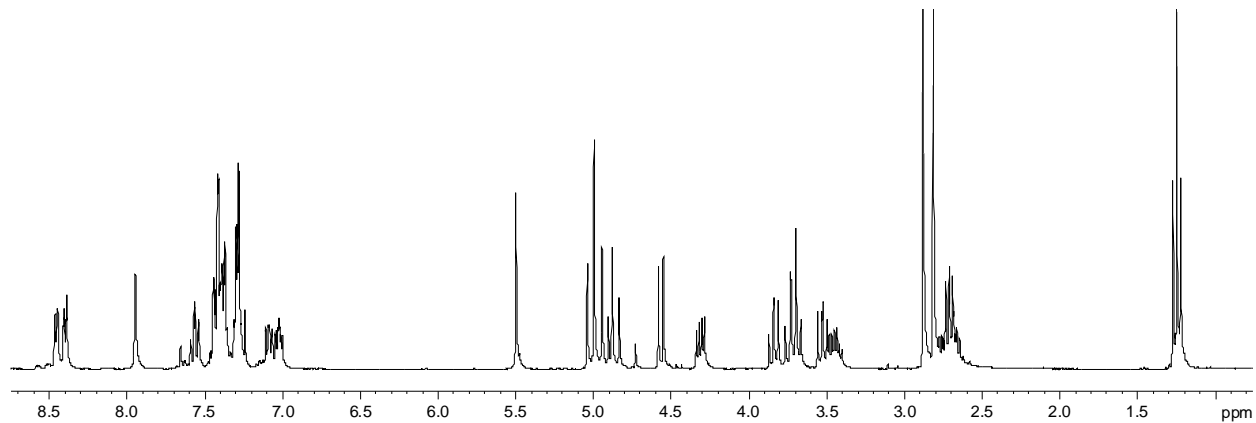
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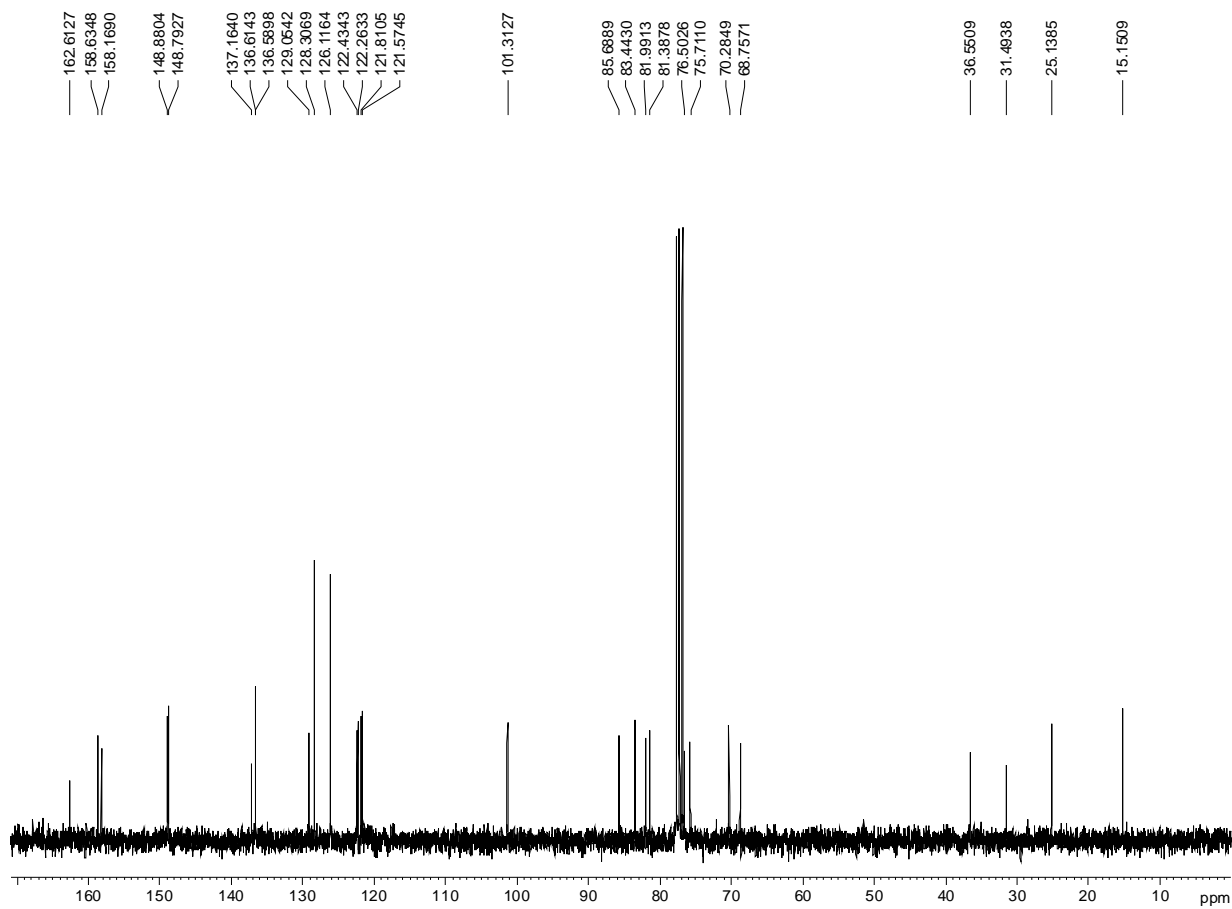
NMR spectra



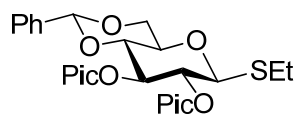
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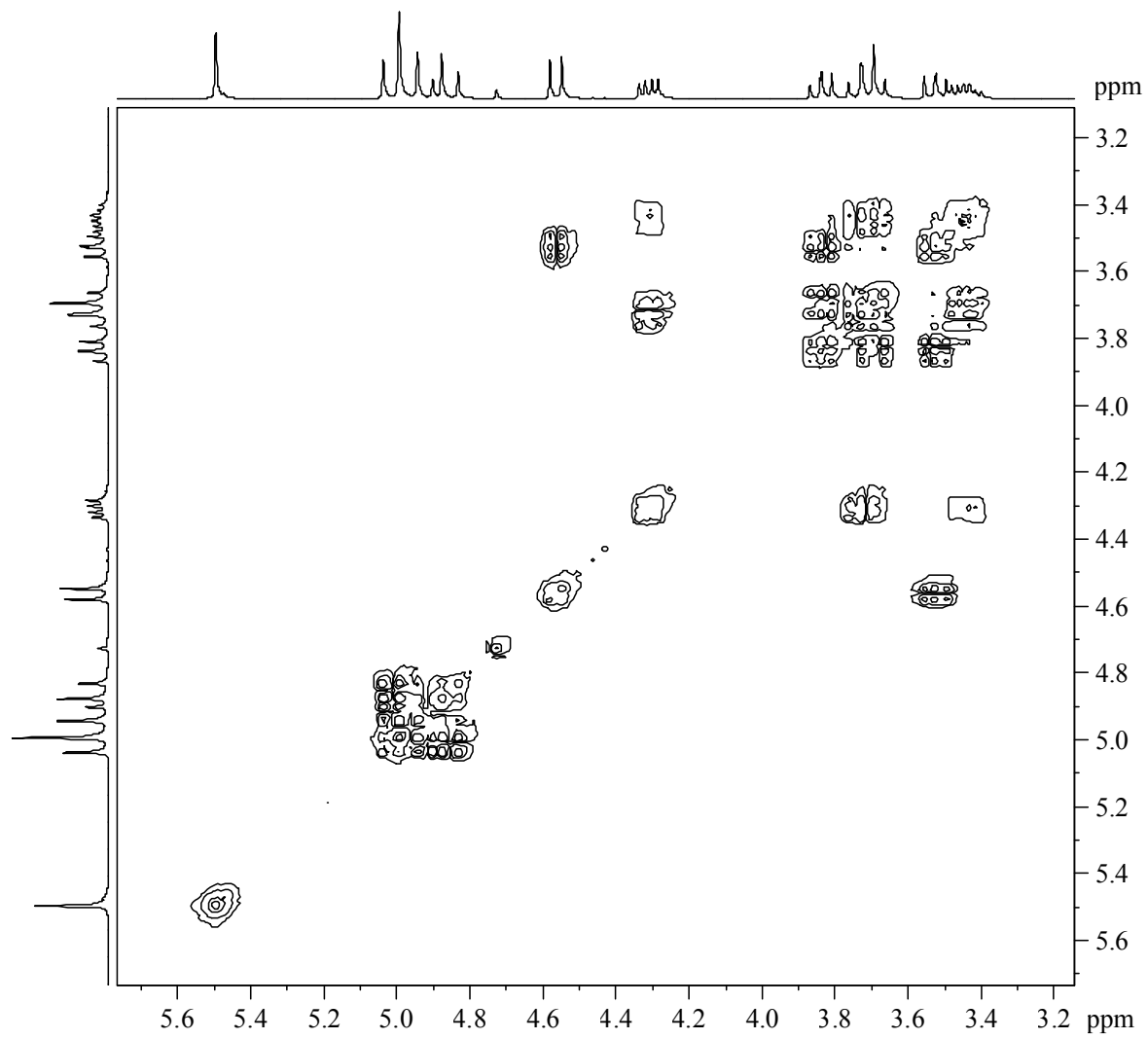
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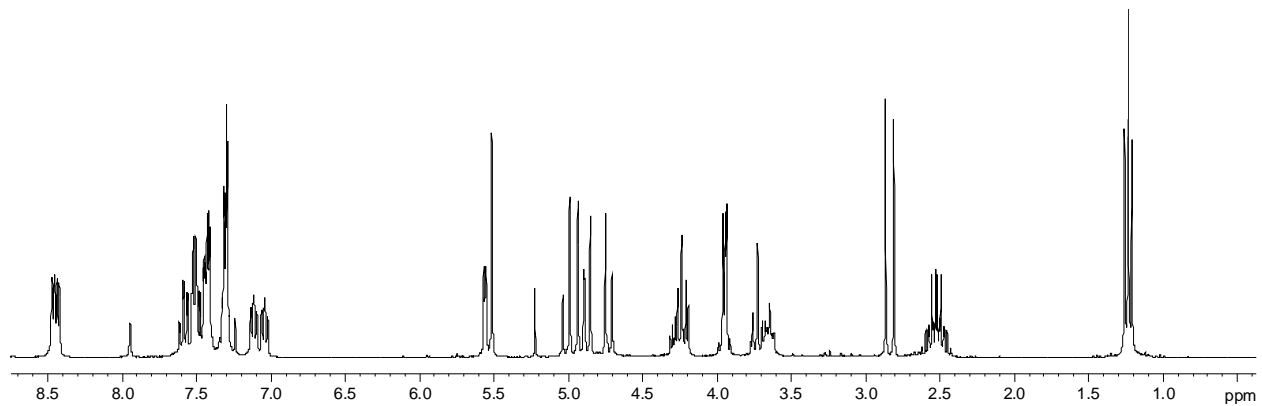
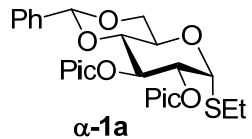
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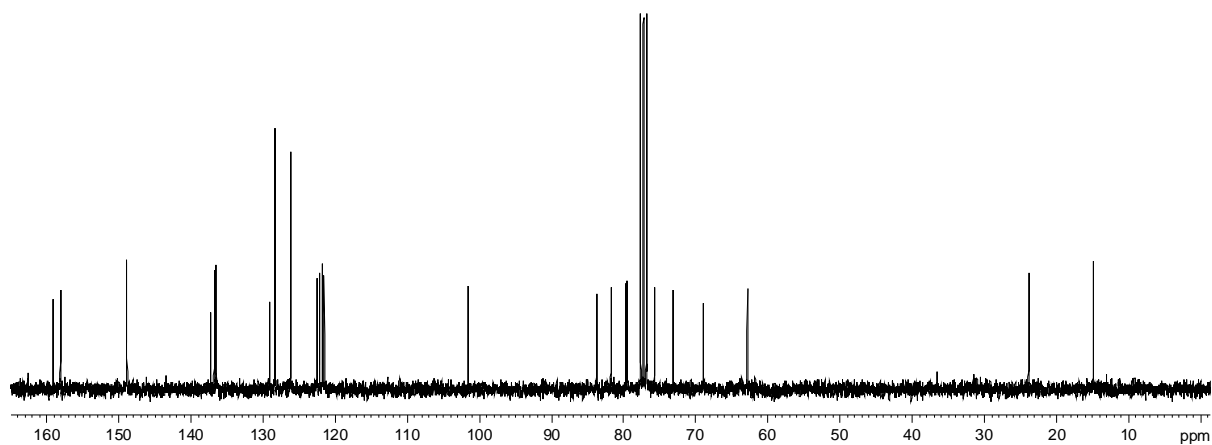
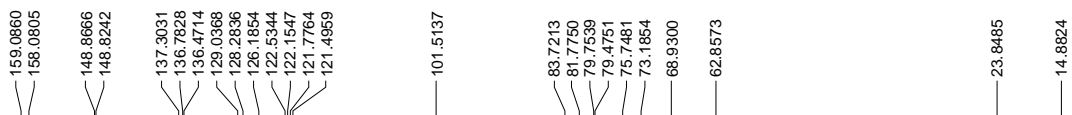
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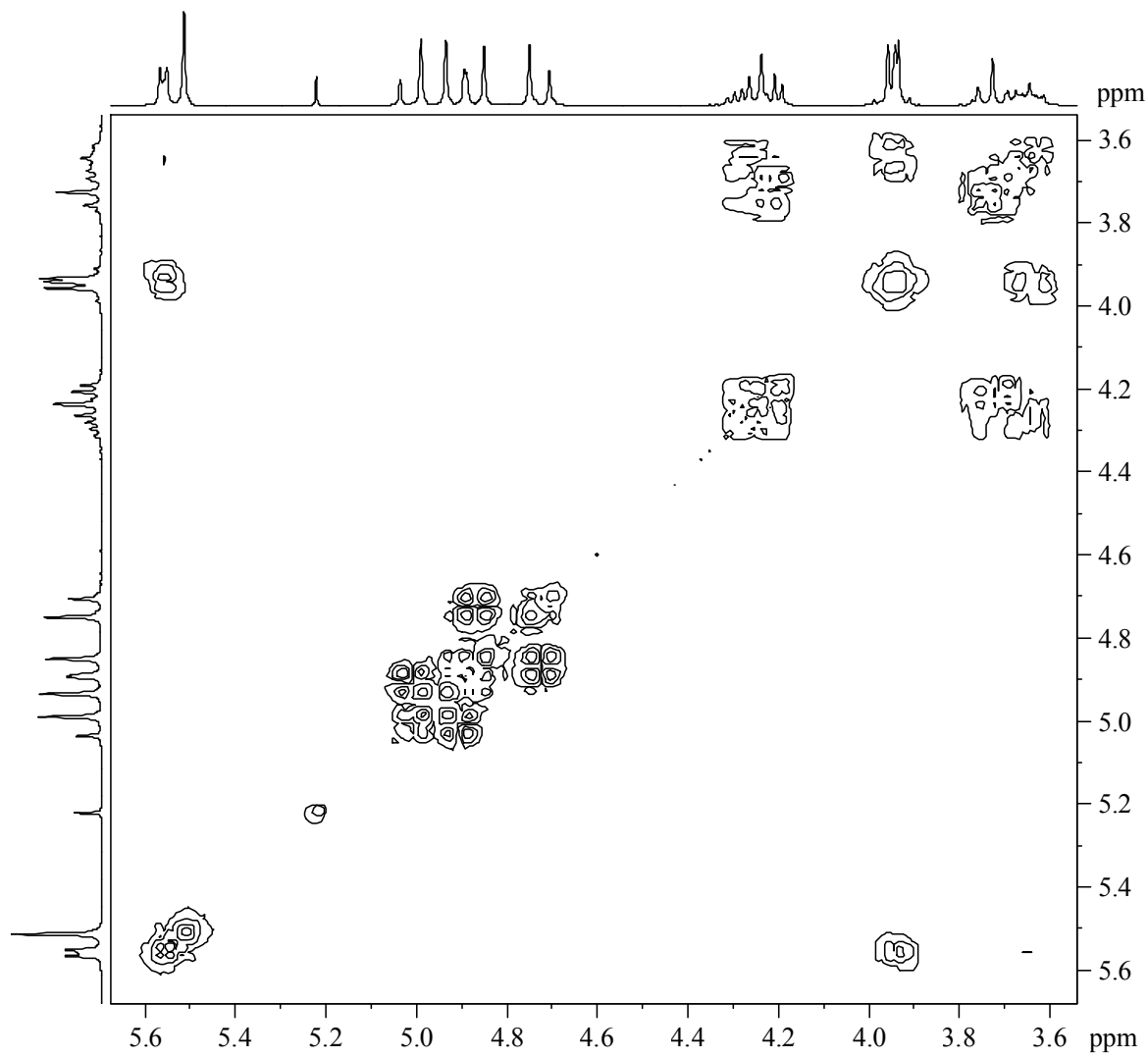
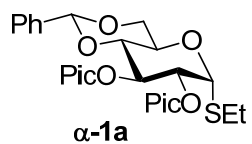
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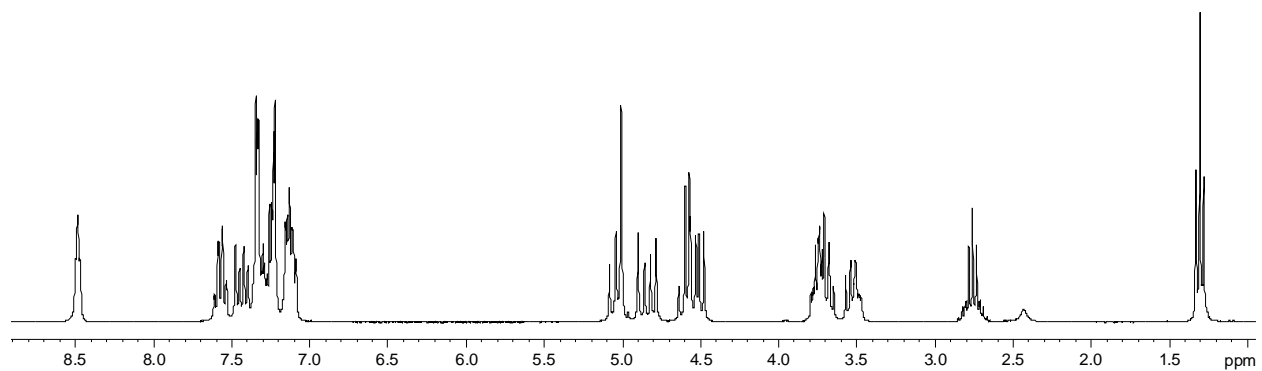
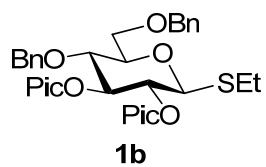
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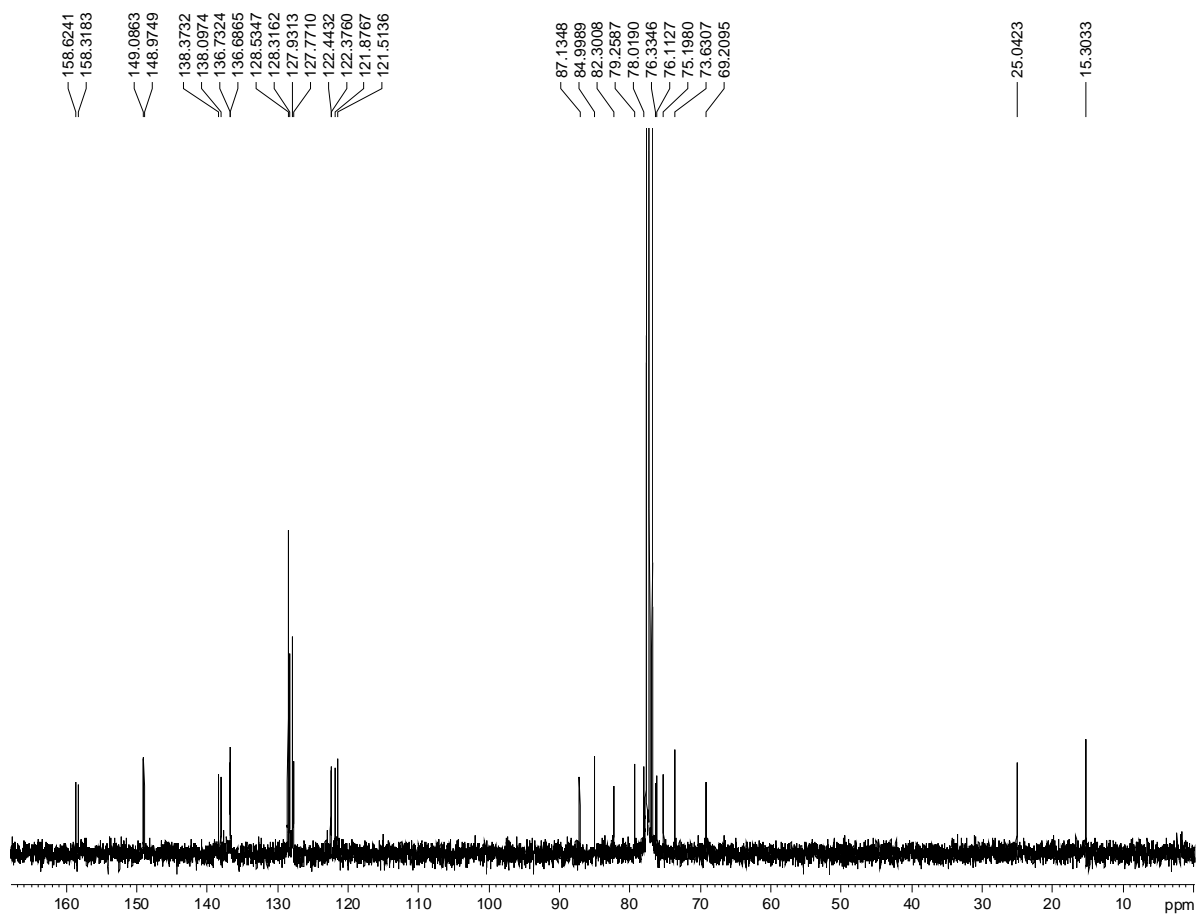
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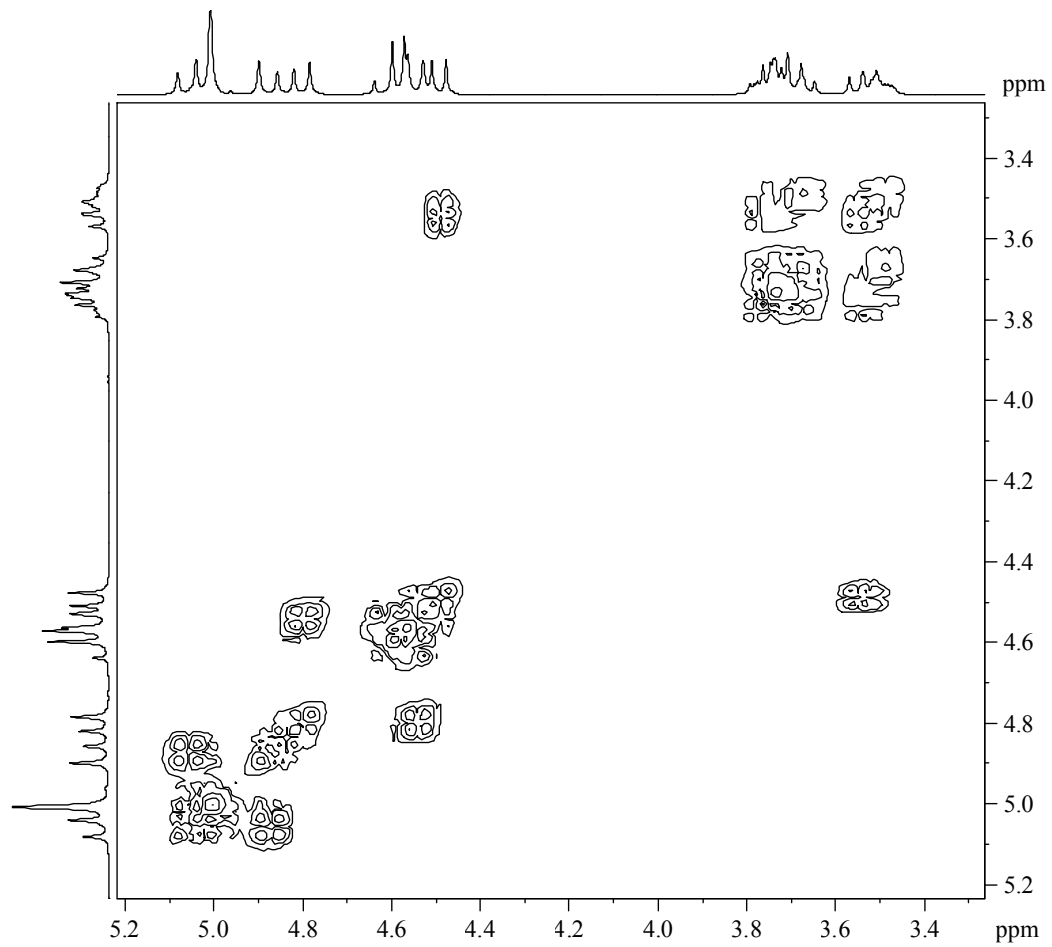
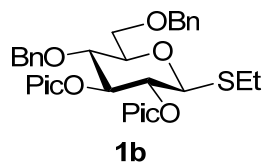
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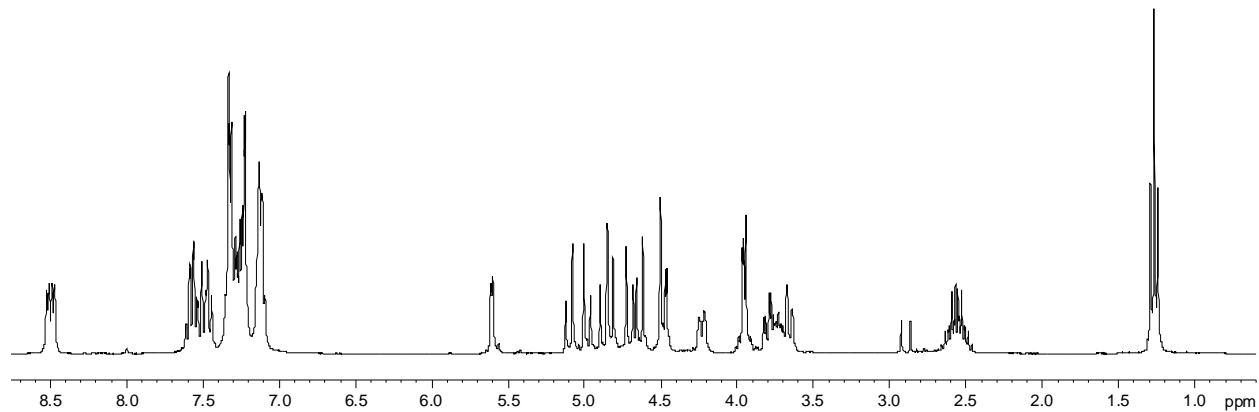
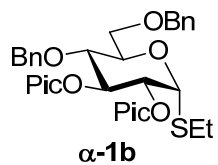
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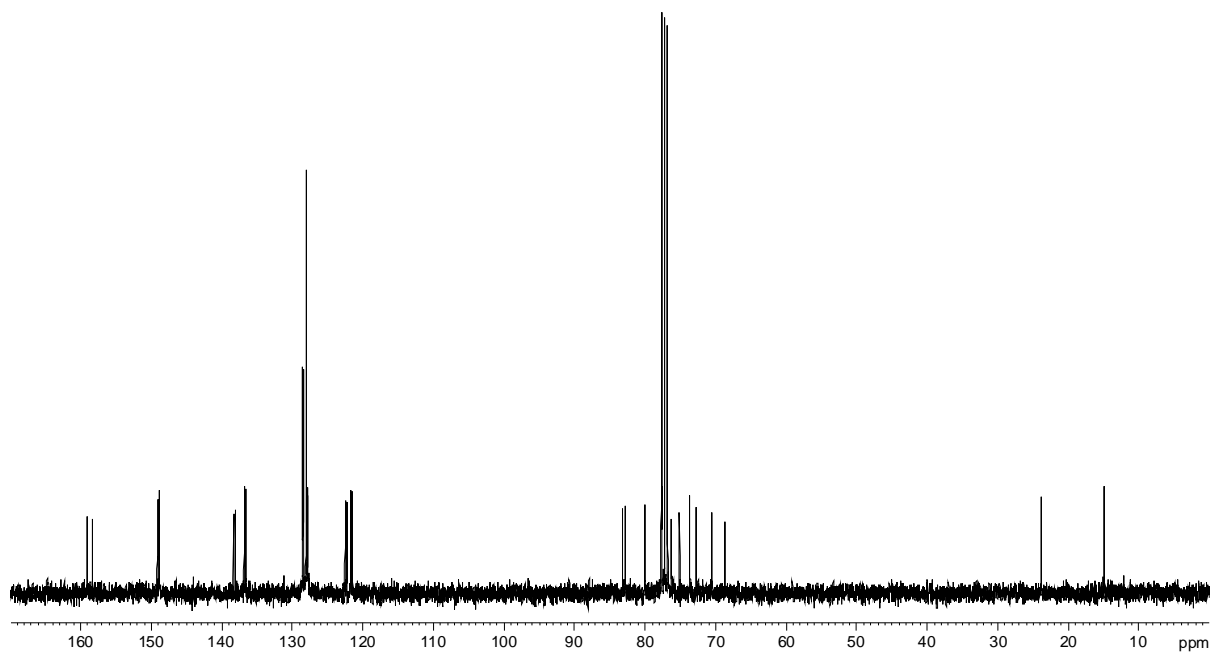
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136.7792
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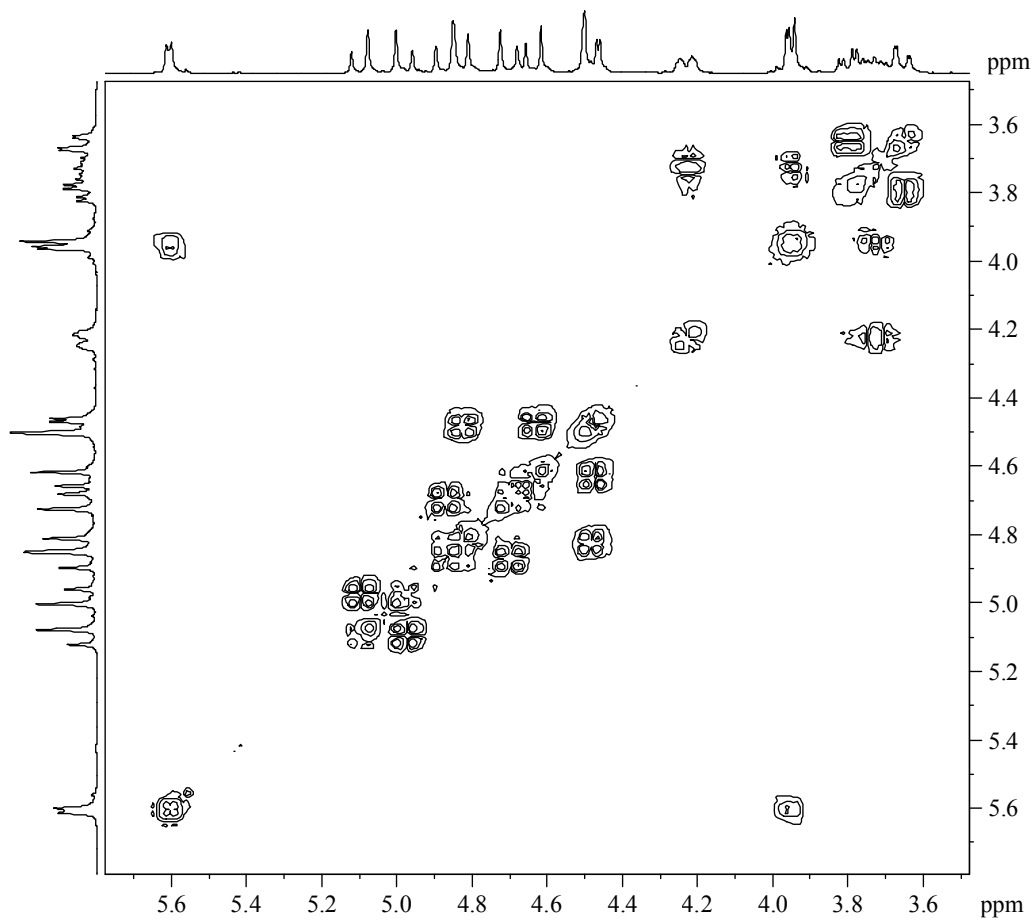
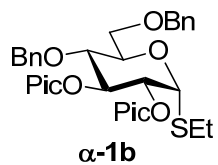
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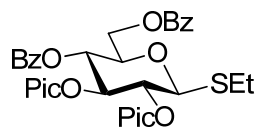
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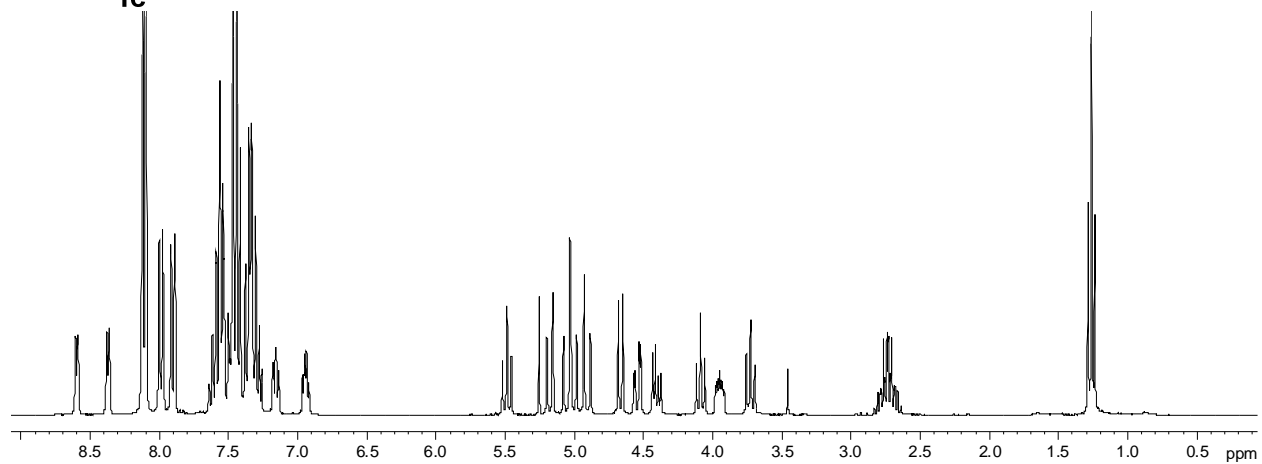
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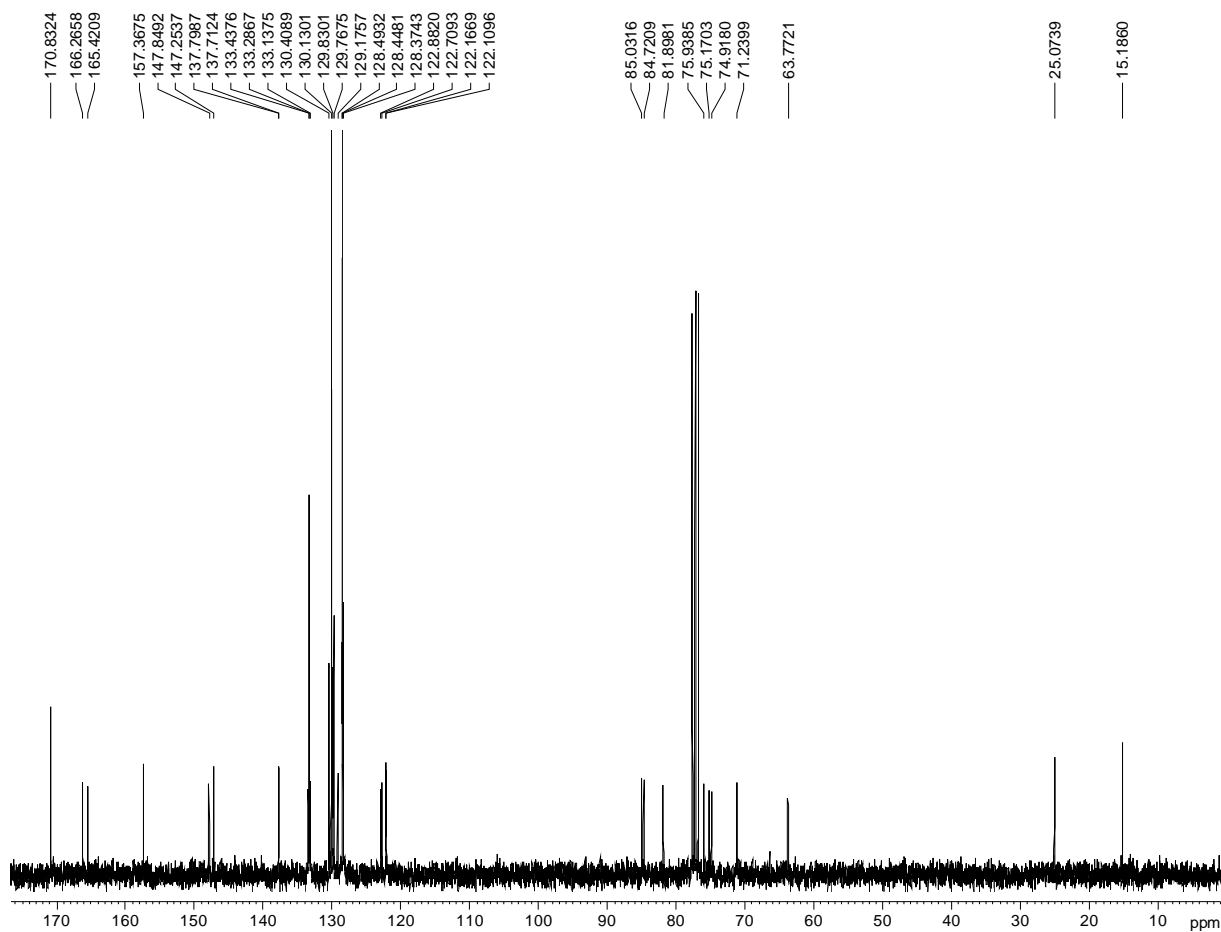
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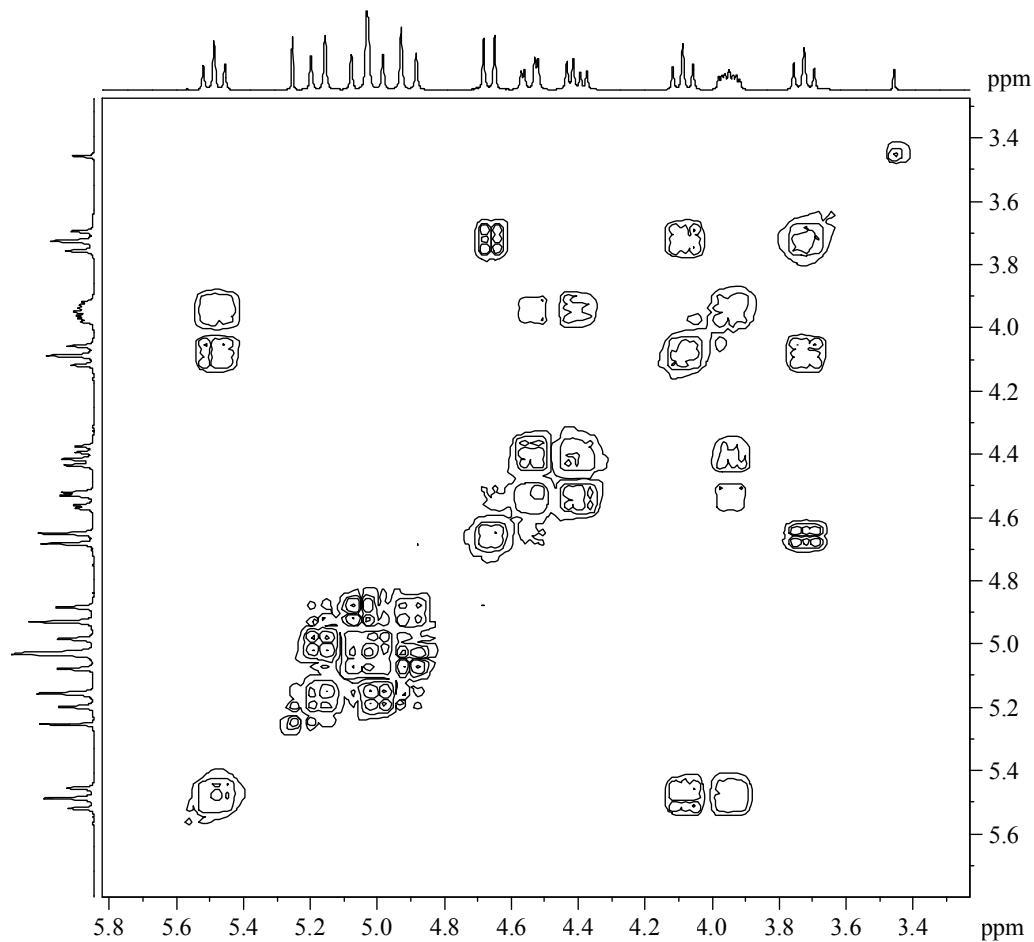
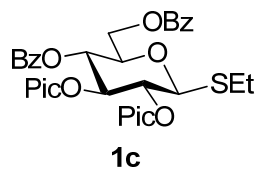
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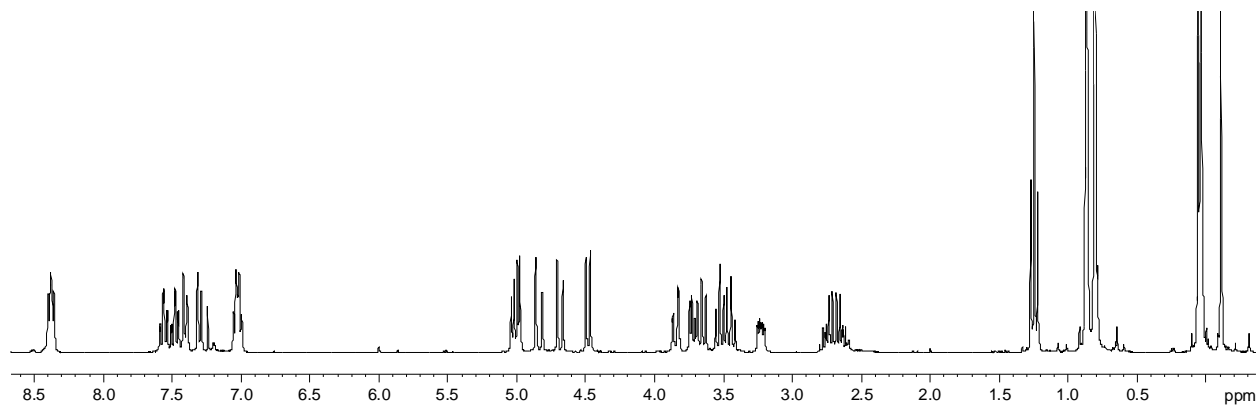
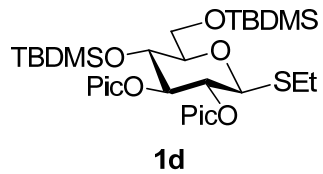
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CDCl₃ 75 MHz



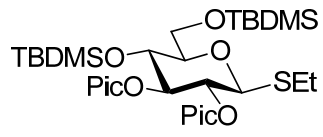
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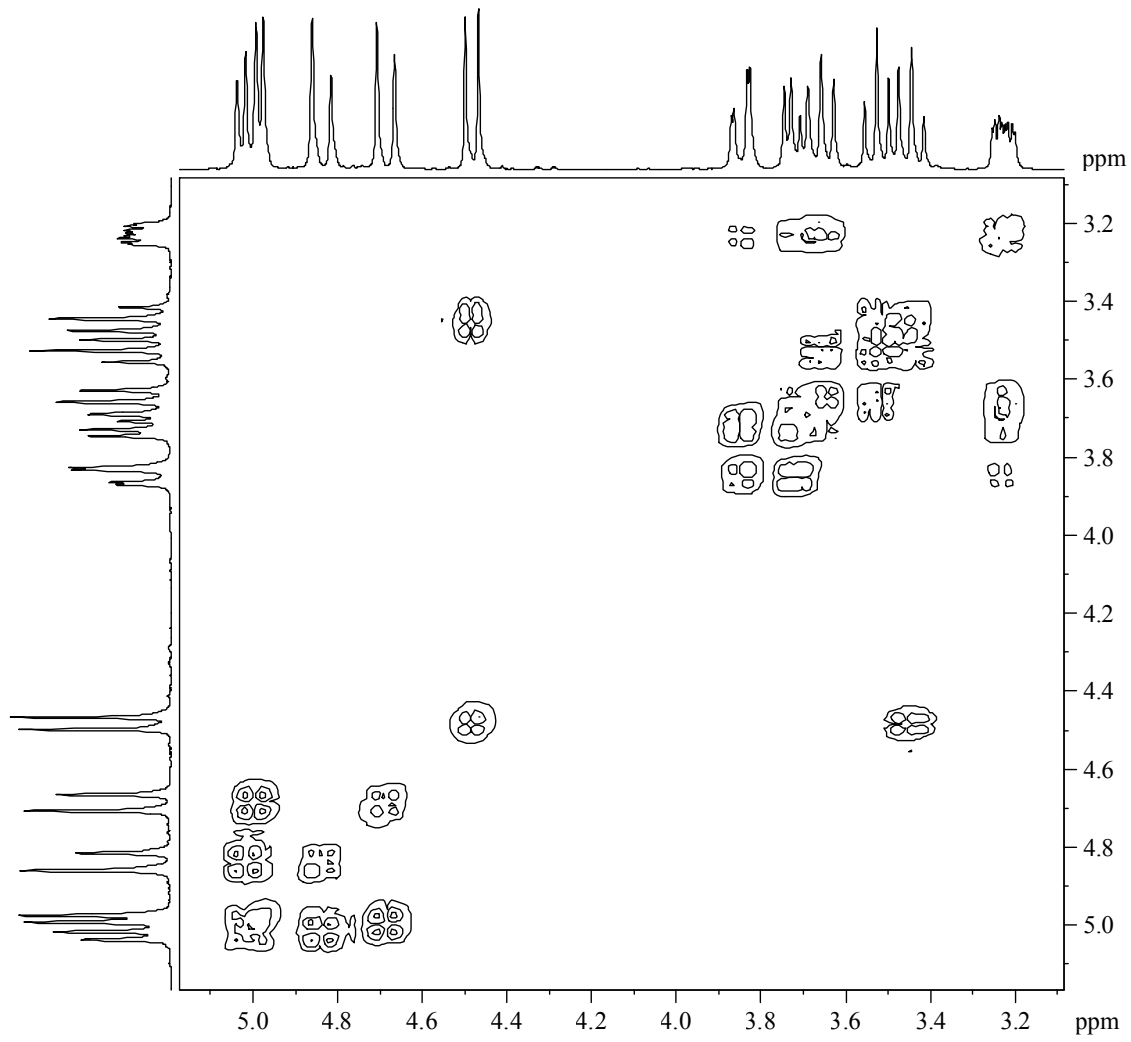
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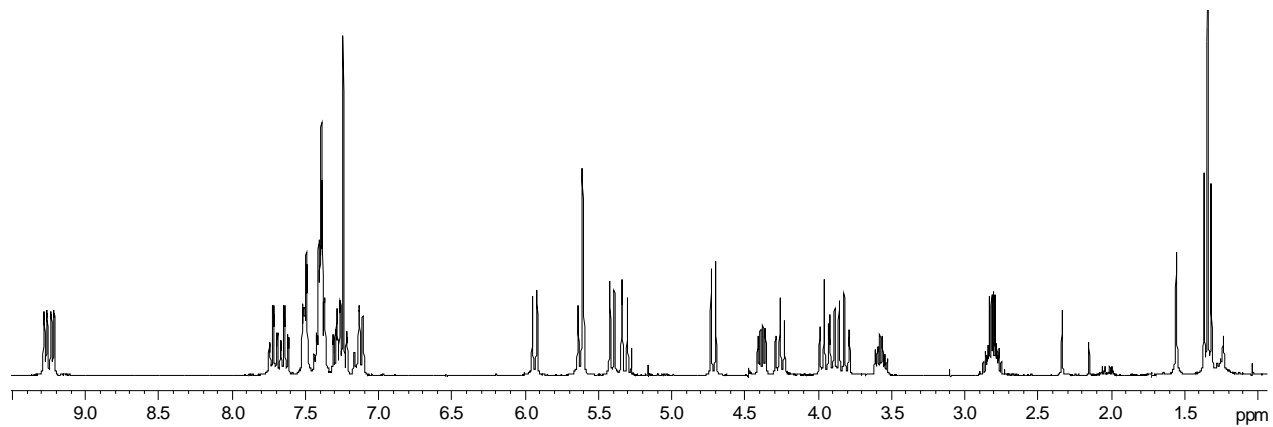
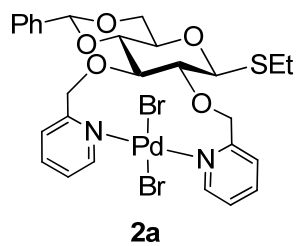
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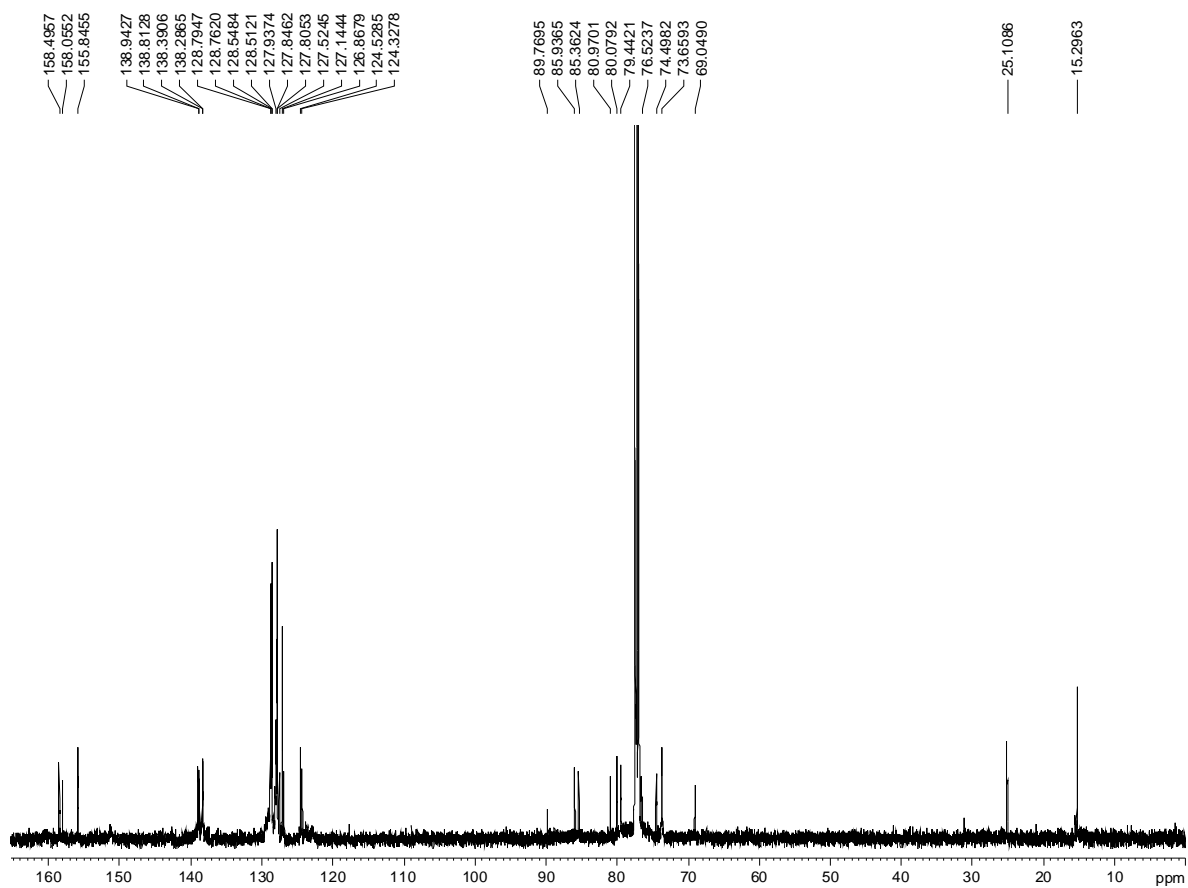
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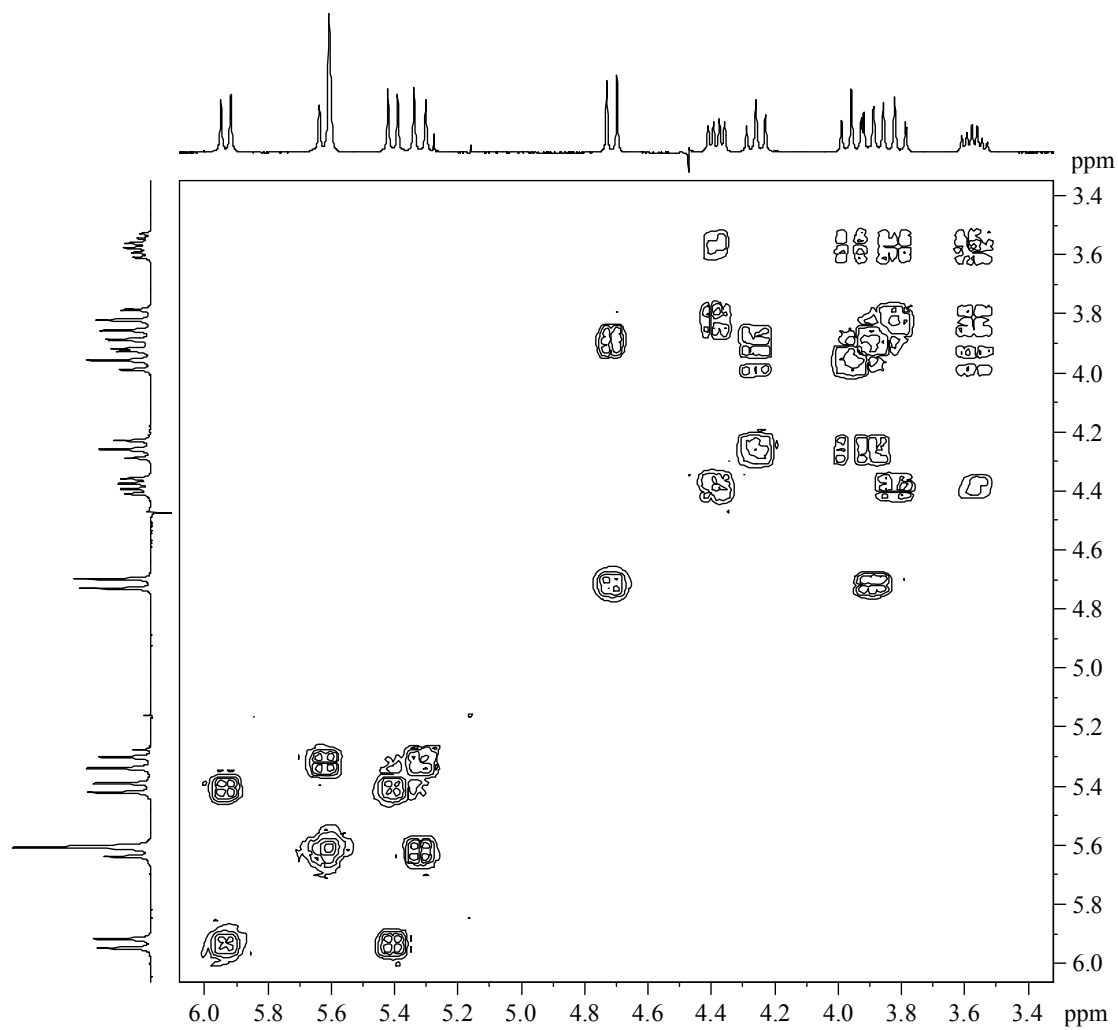
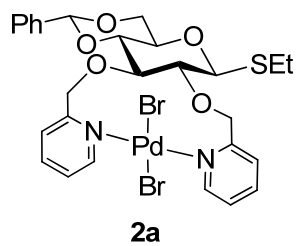
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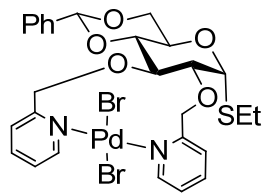
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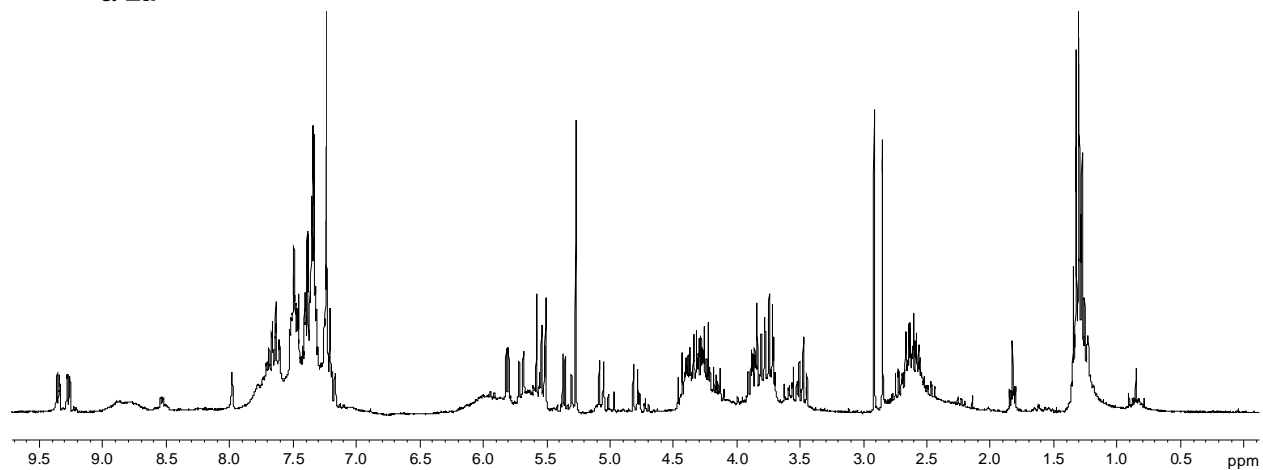
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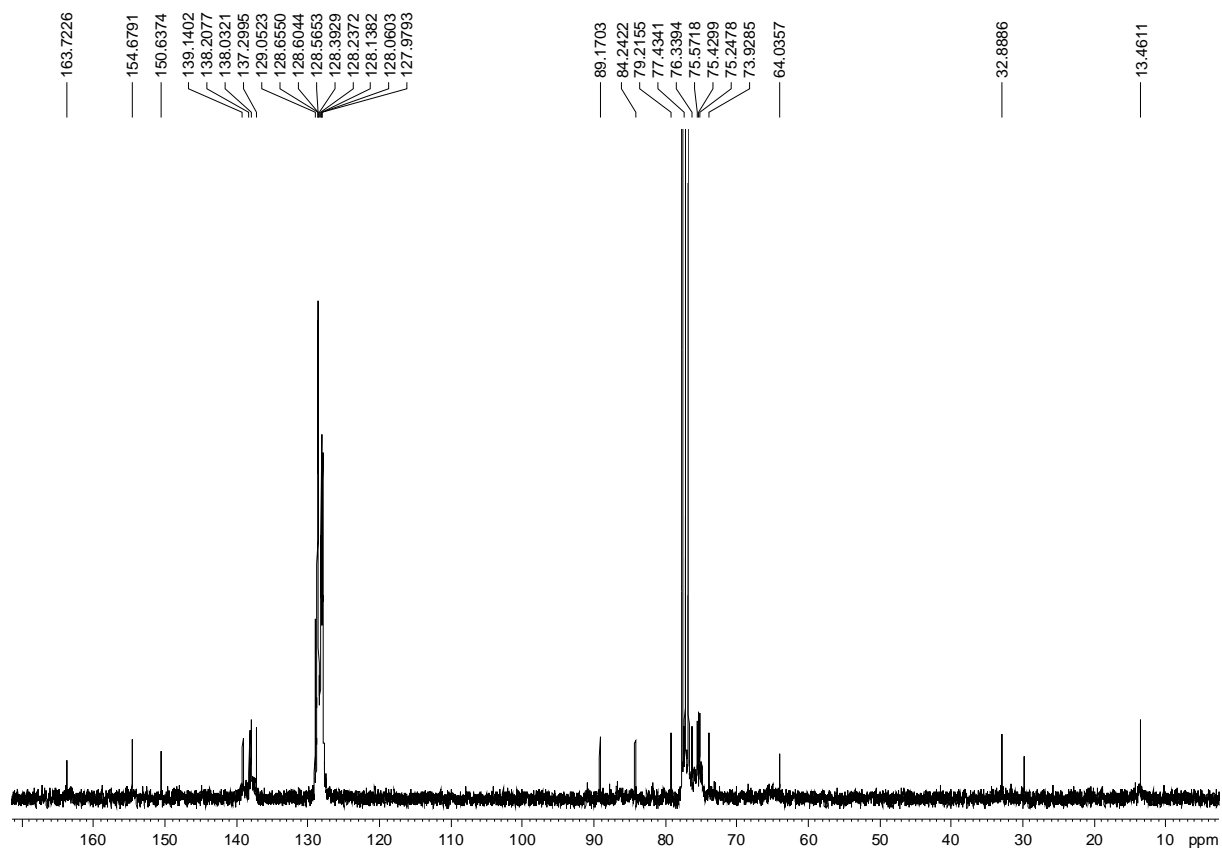
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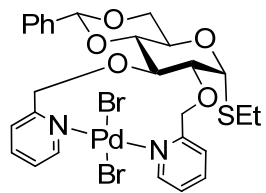
α -2a



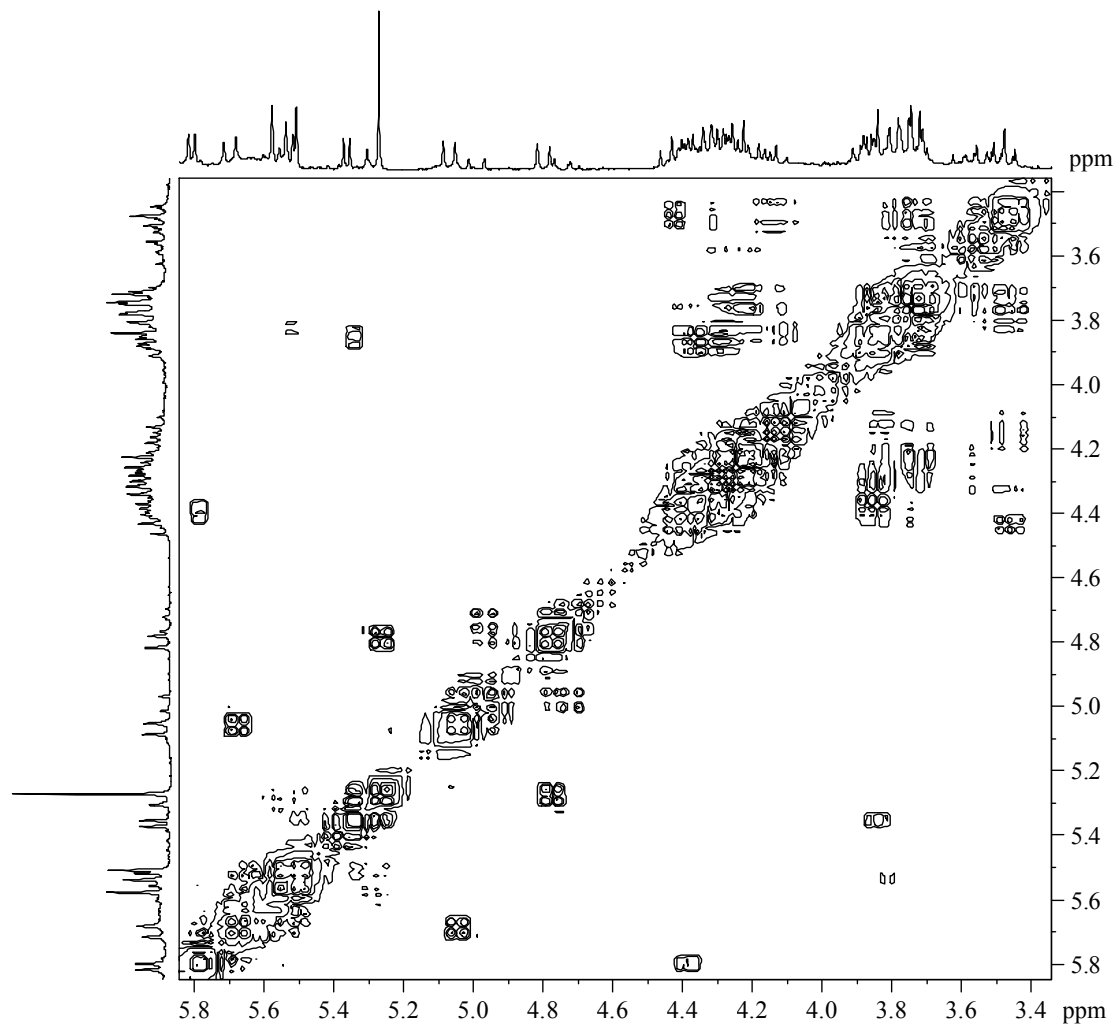
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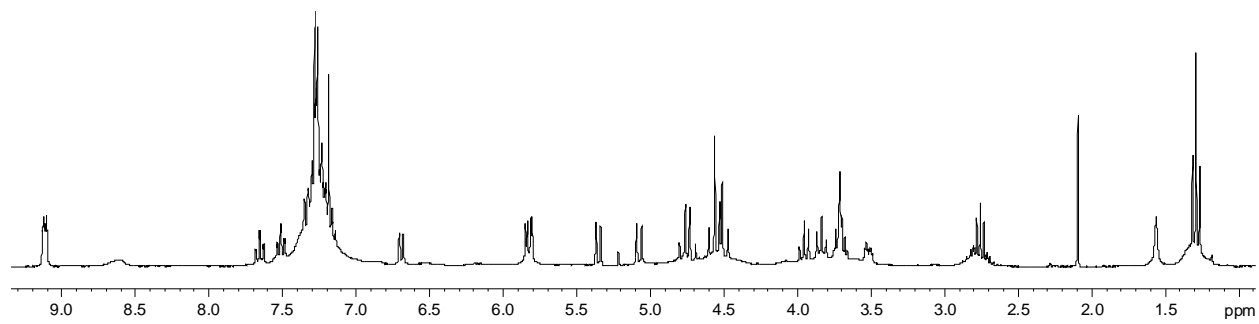
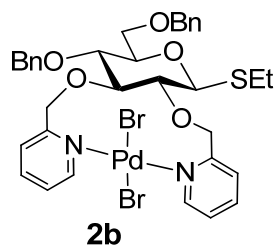
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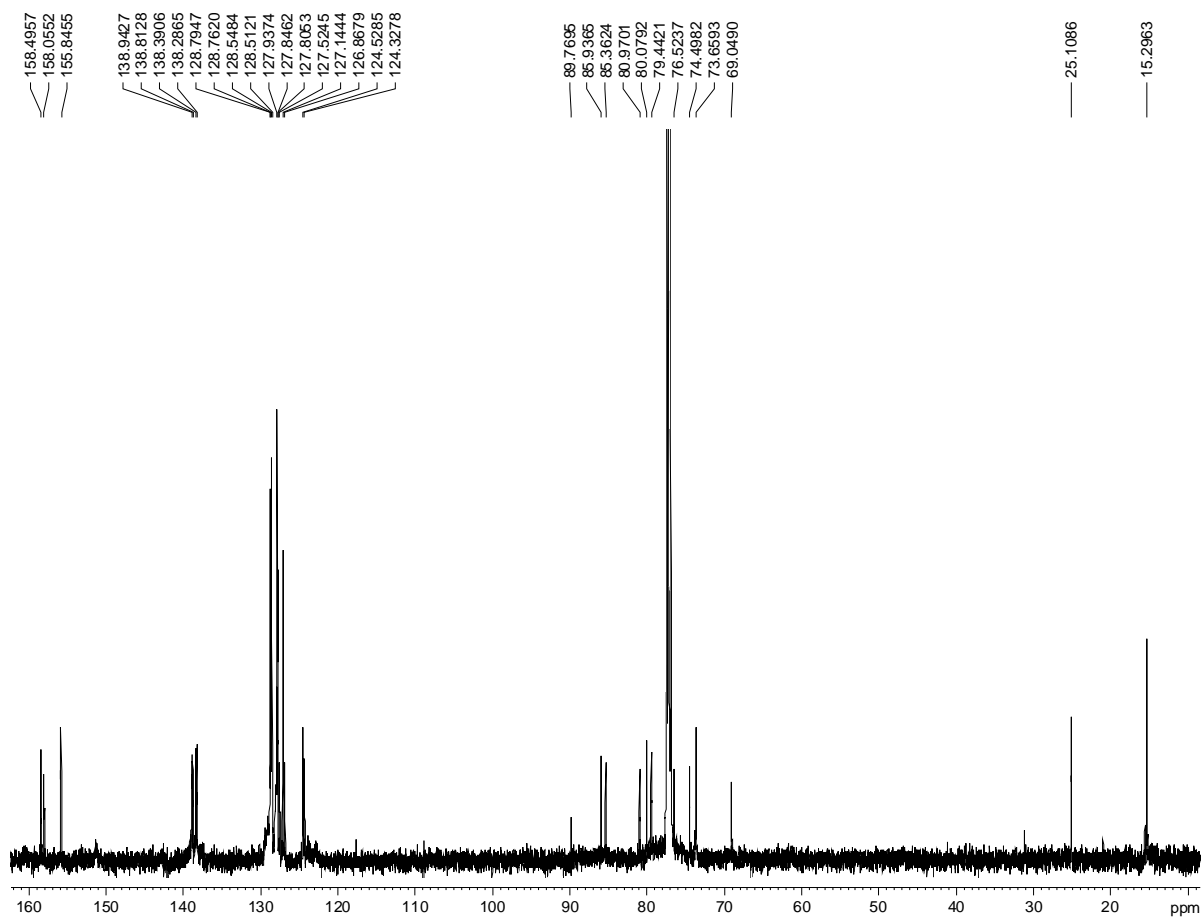
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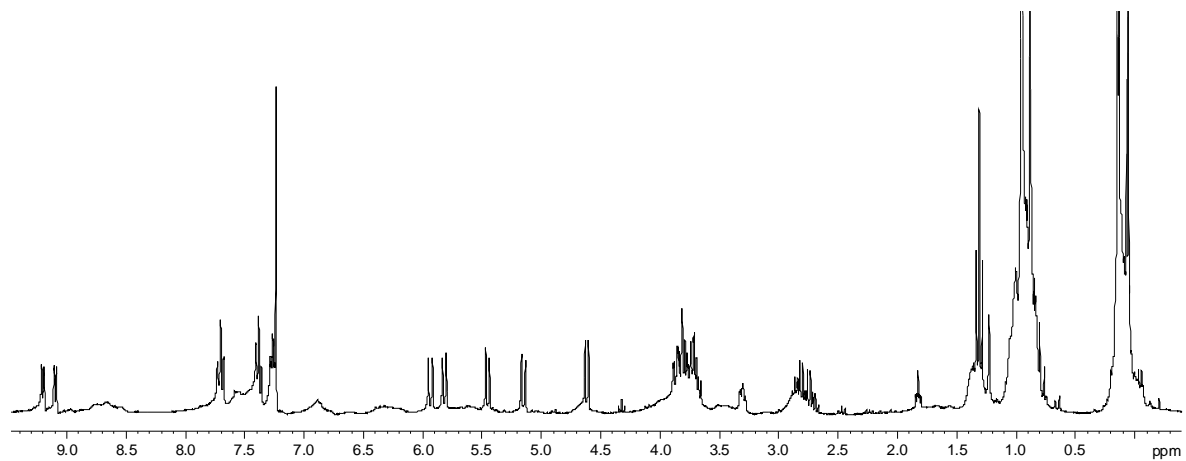
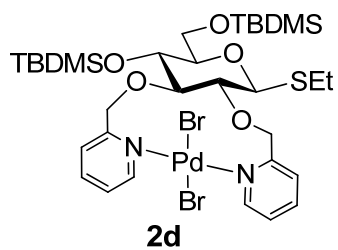
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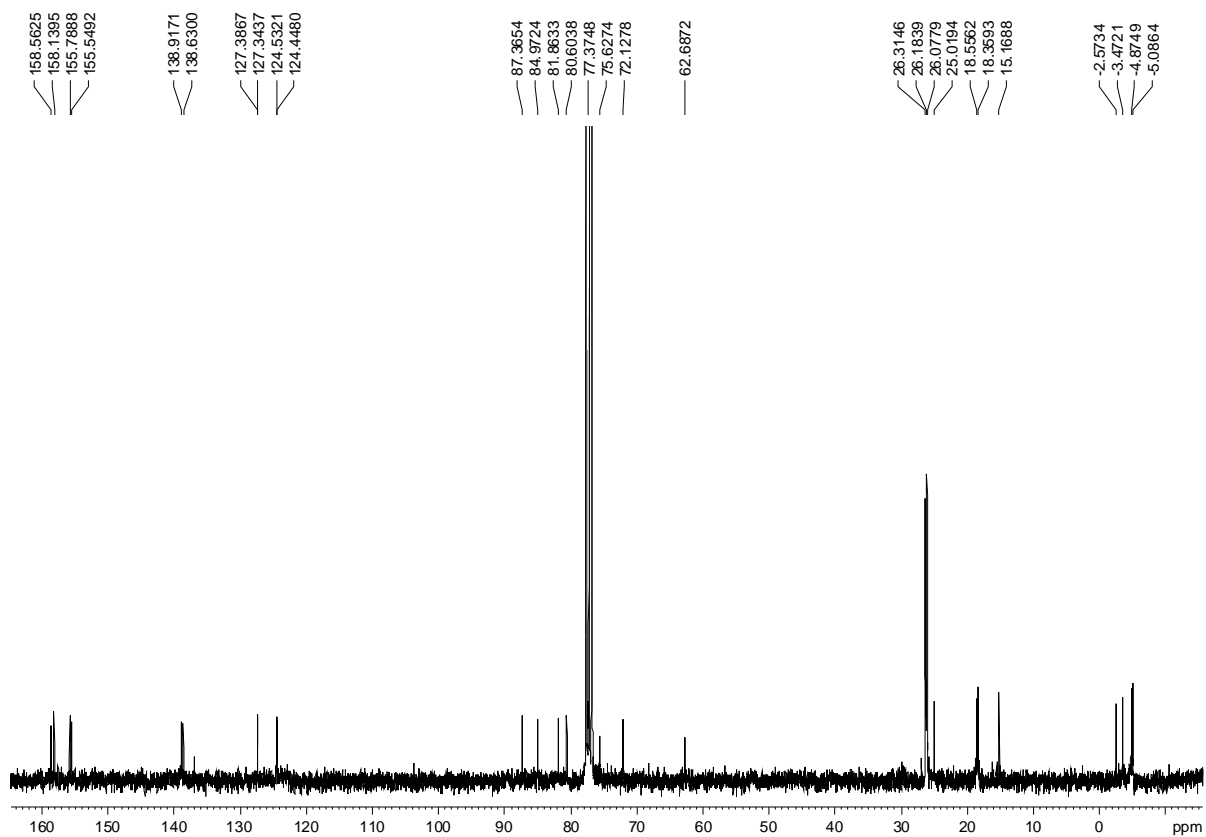
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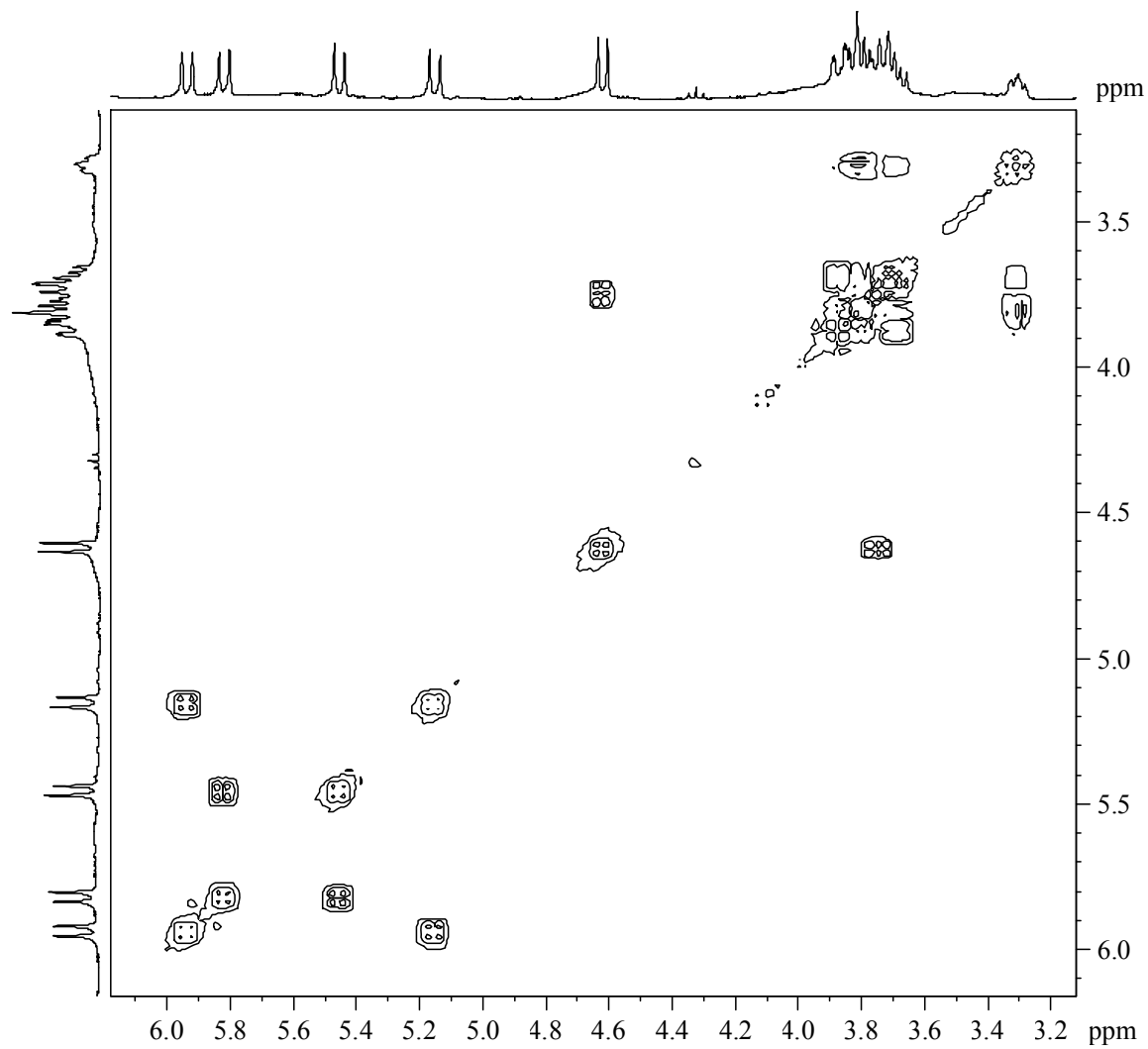
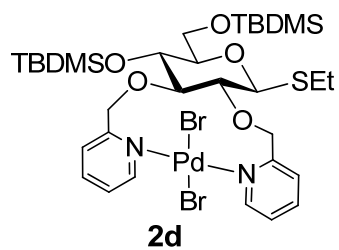
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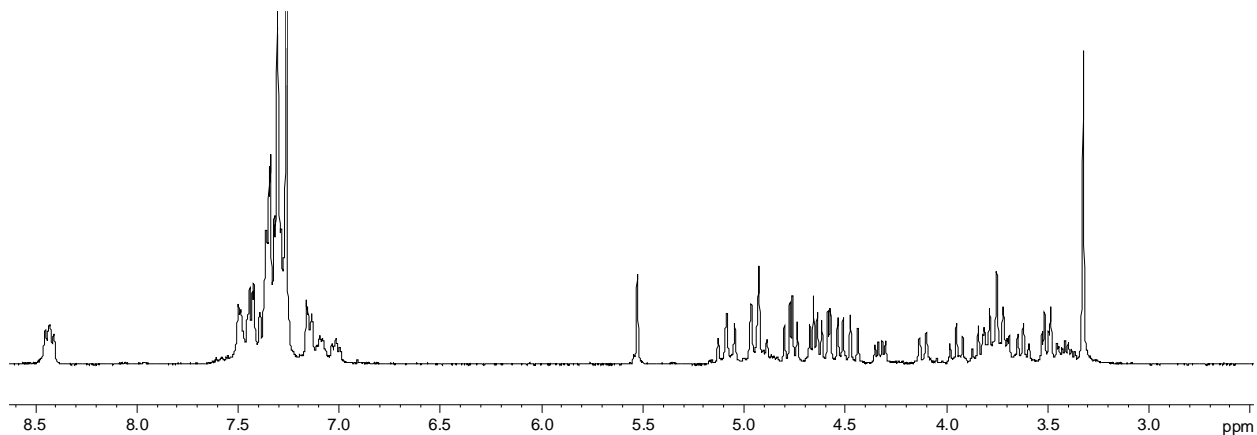
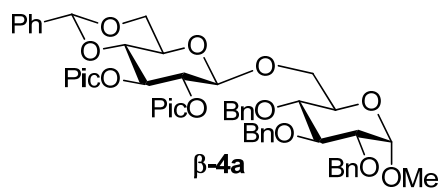
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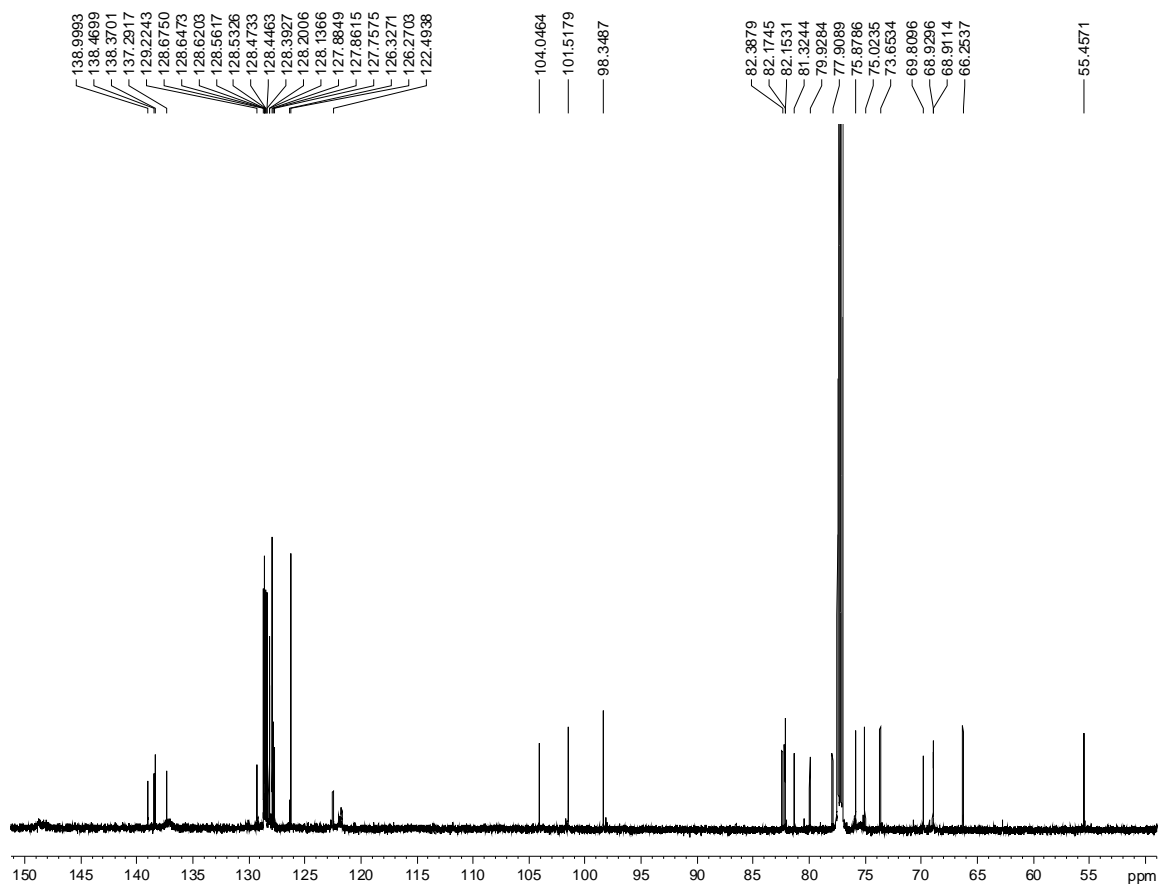
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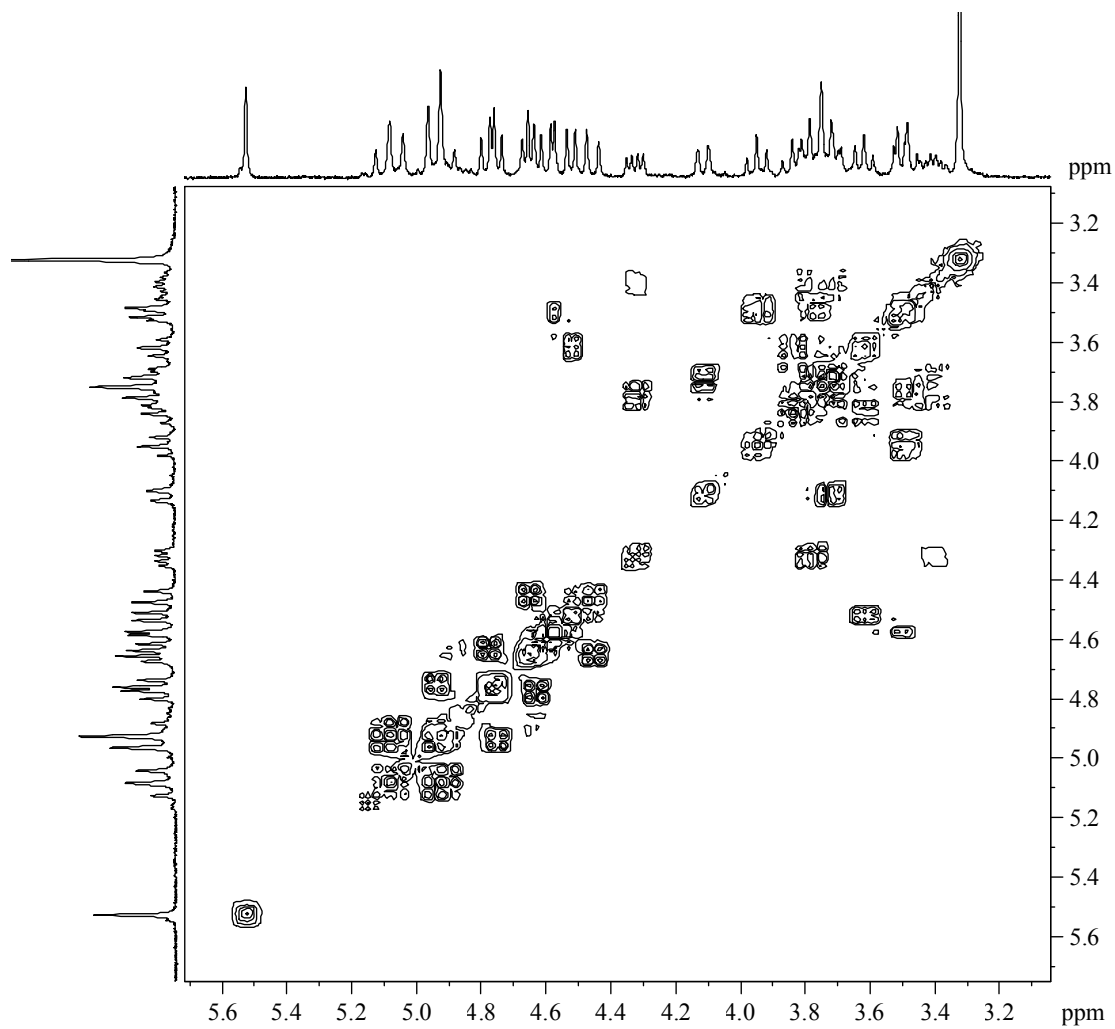
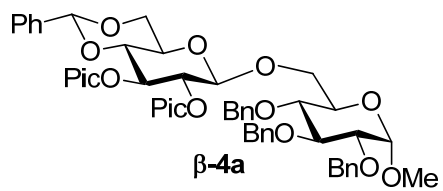
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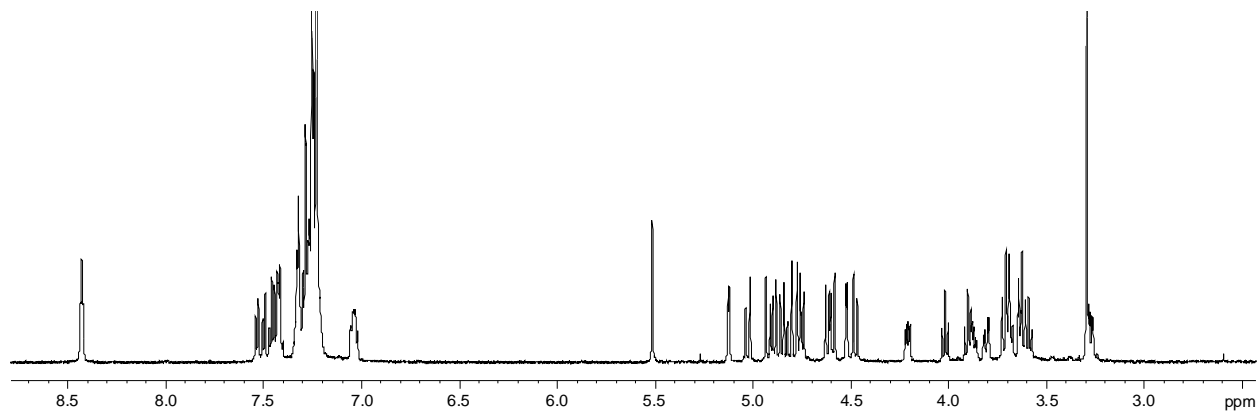
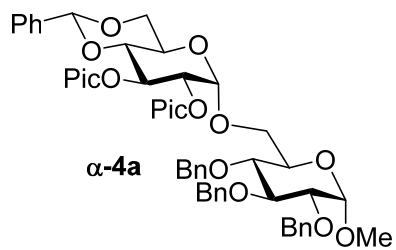
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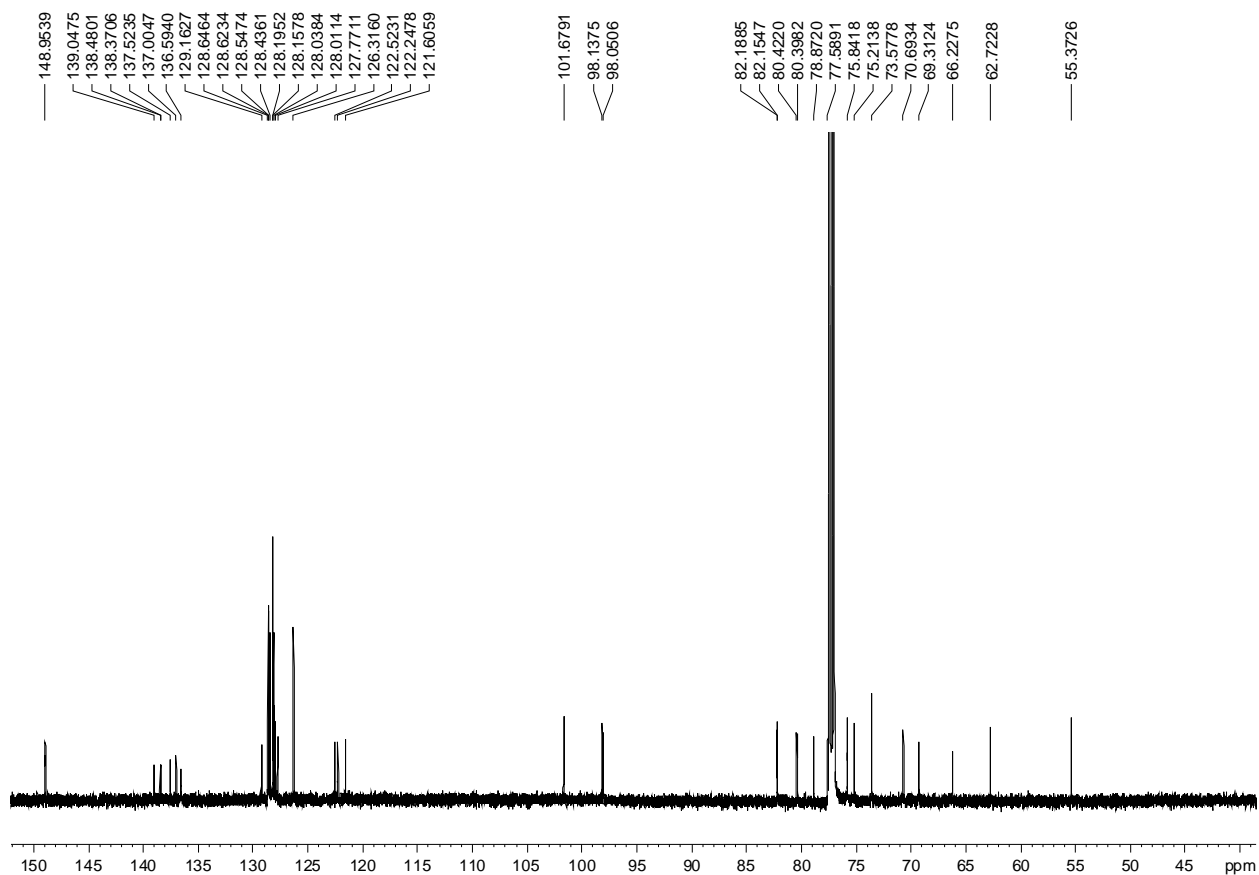
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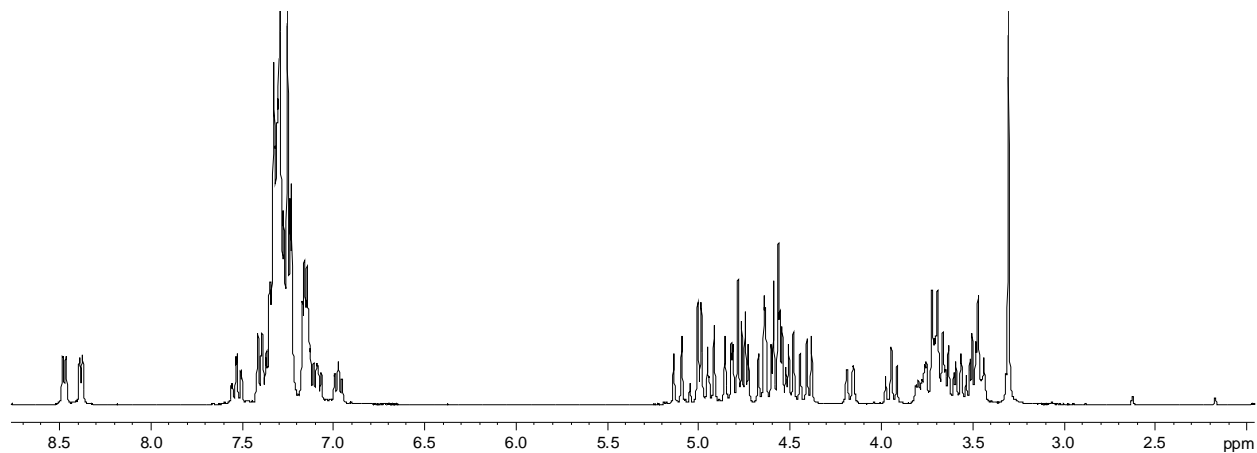
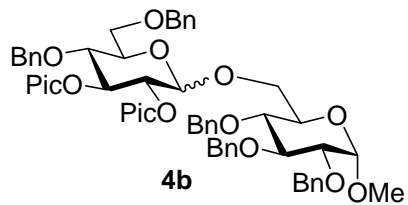
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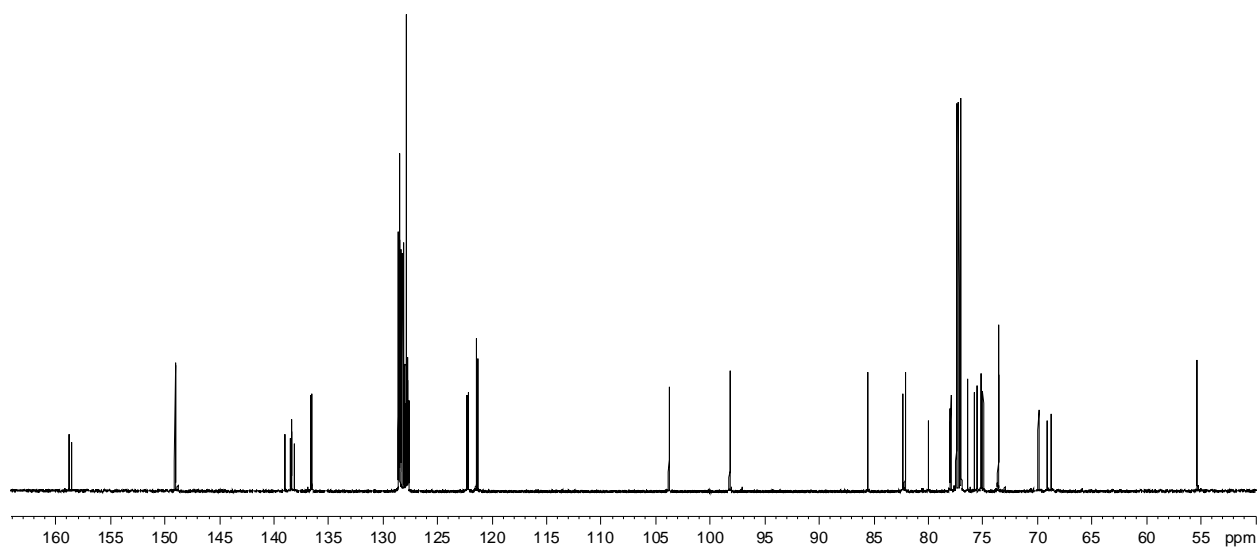
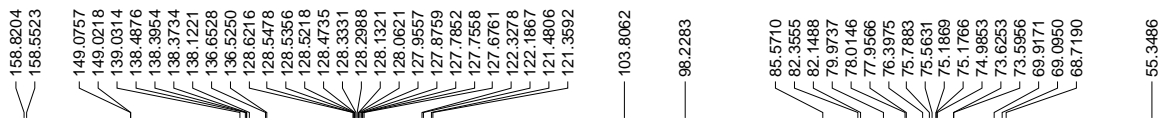
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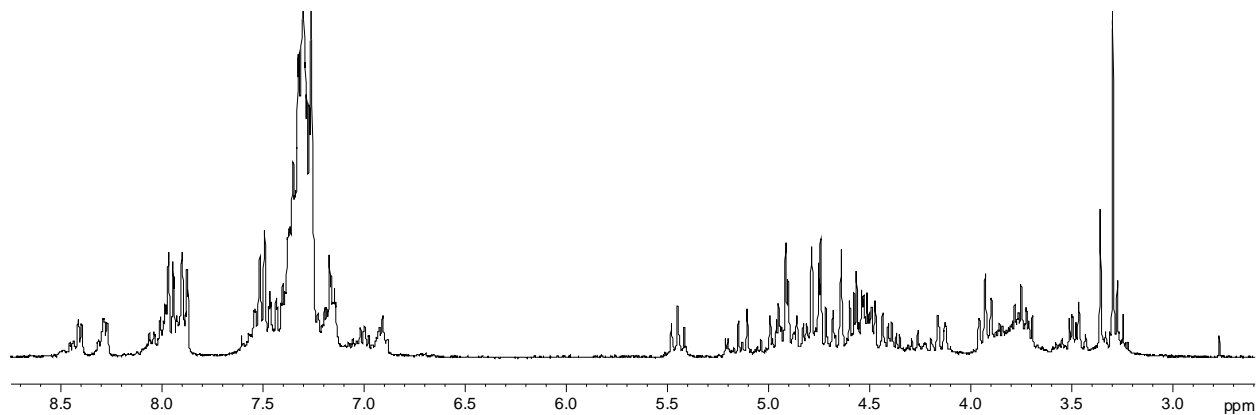
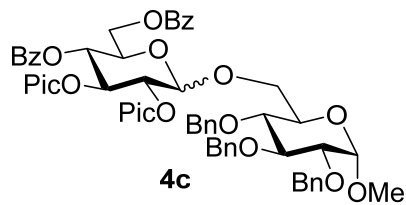
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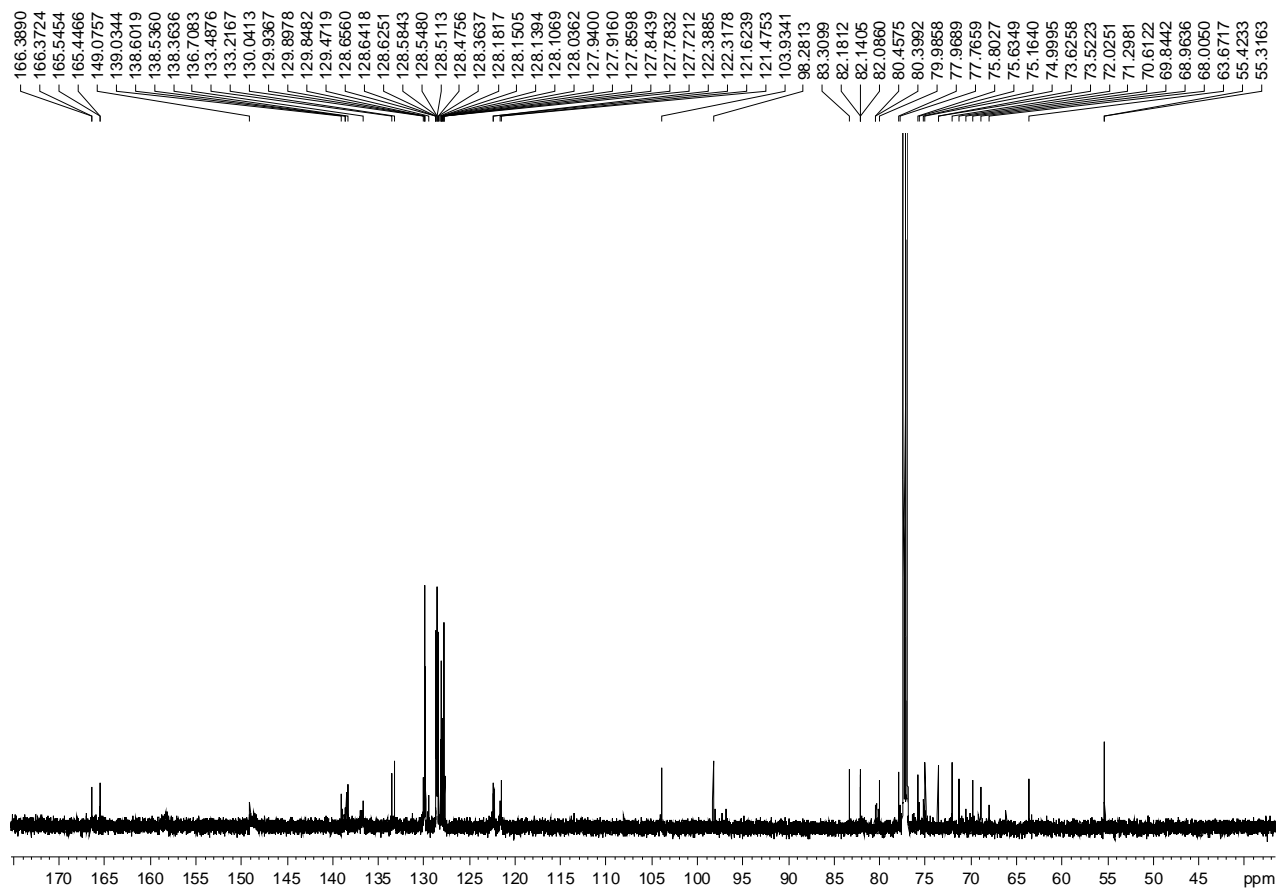
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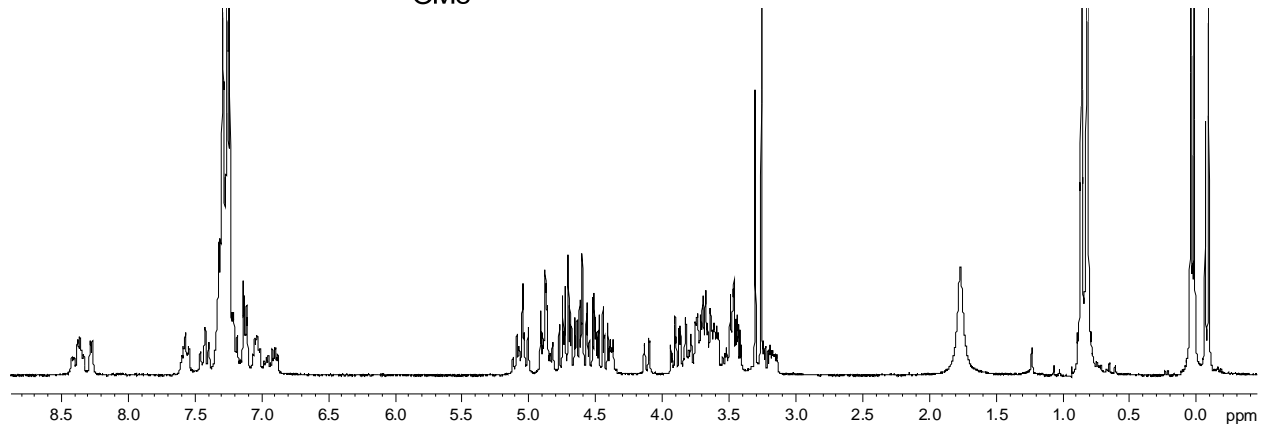
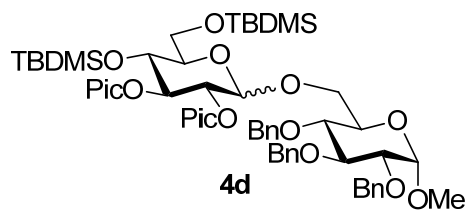
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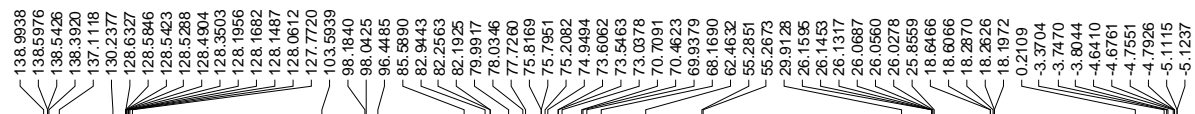
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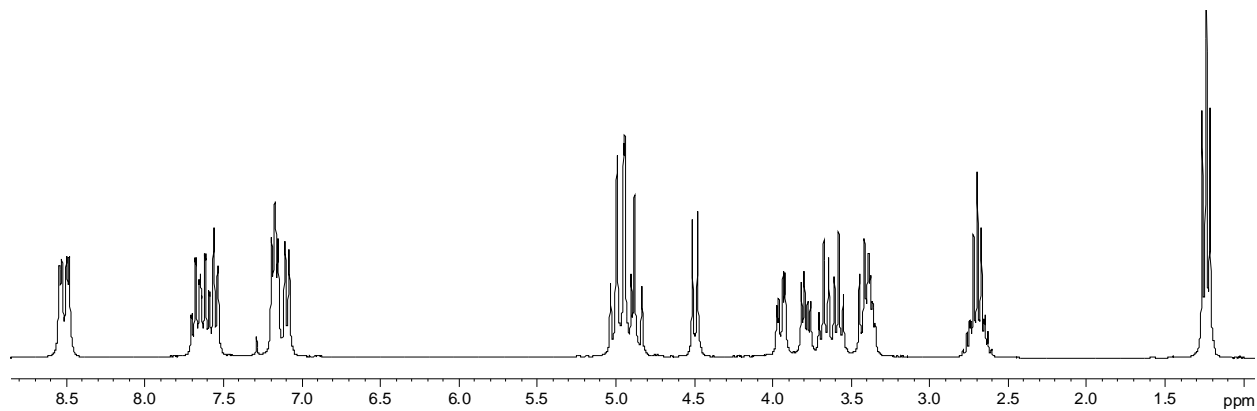
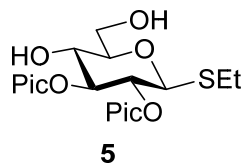
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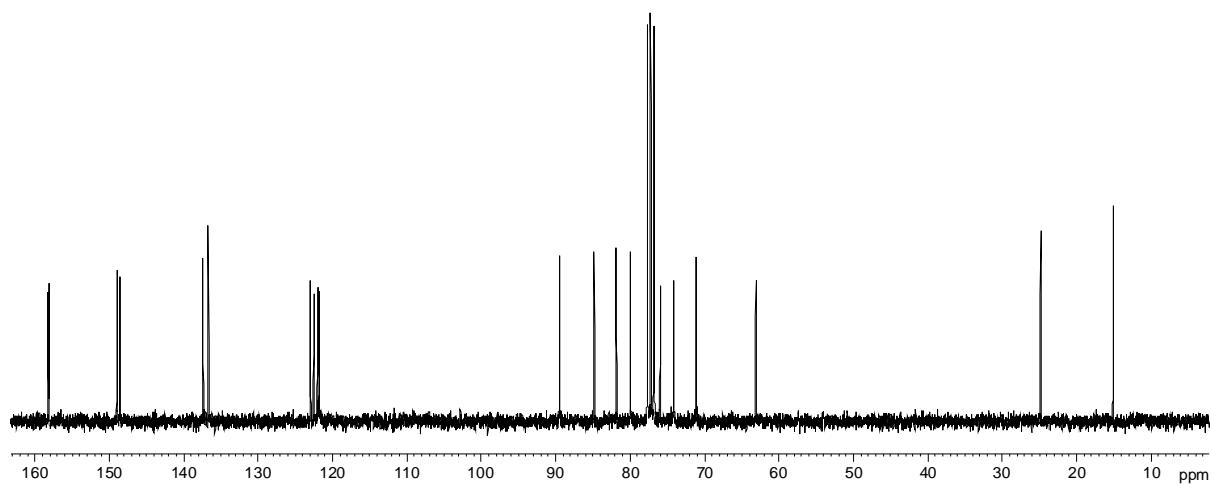
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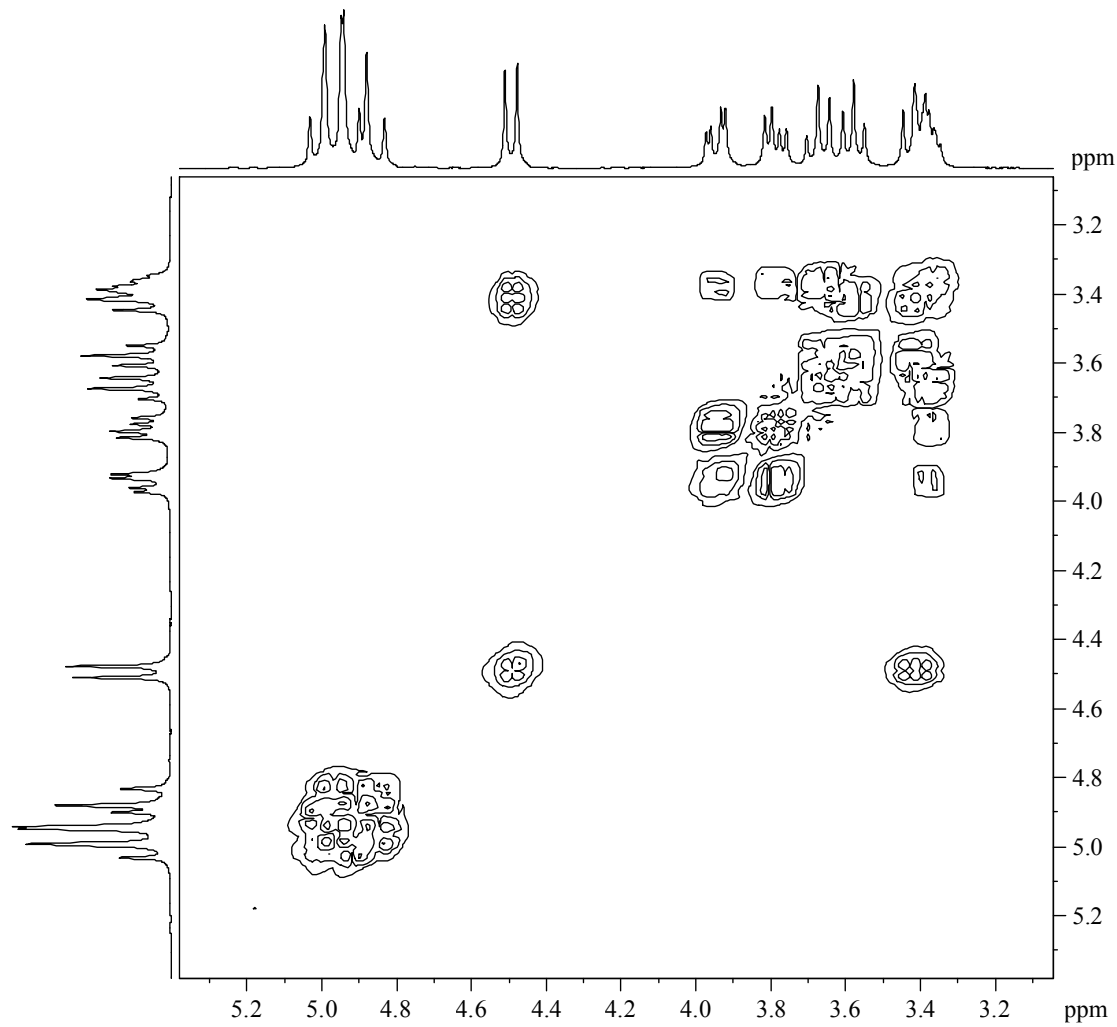
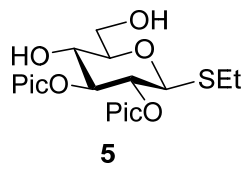
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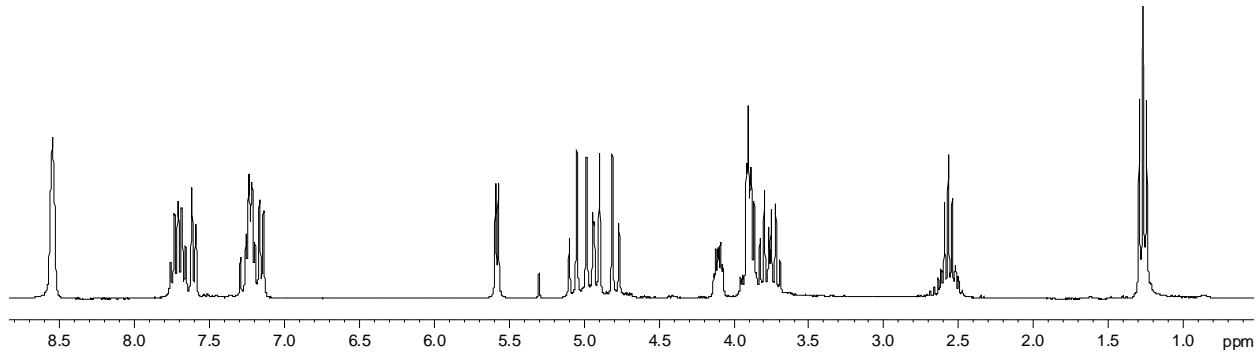
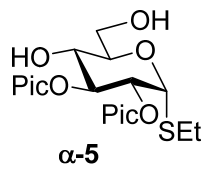
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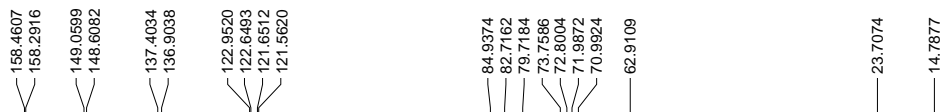
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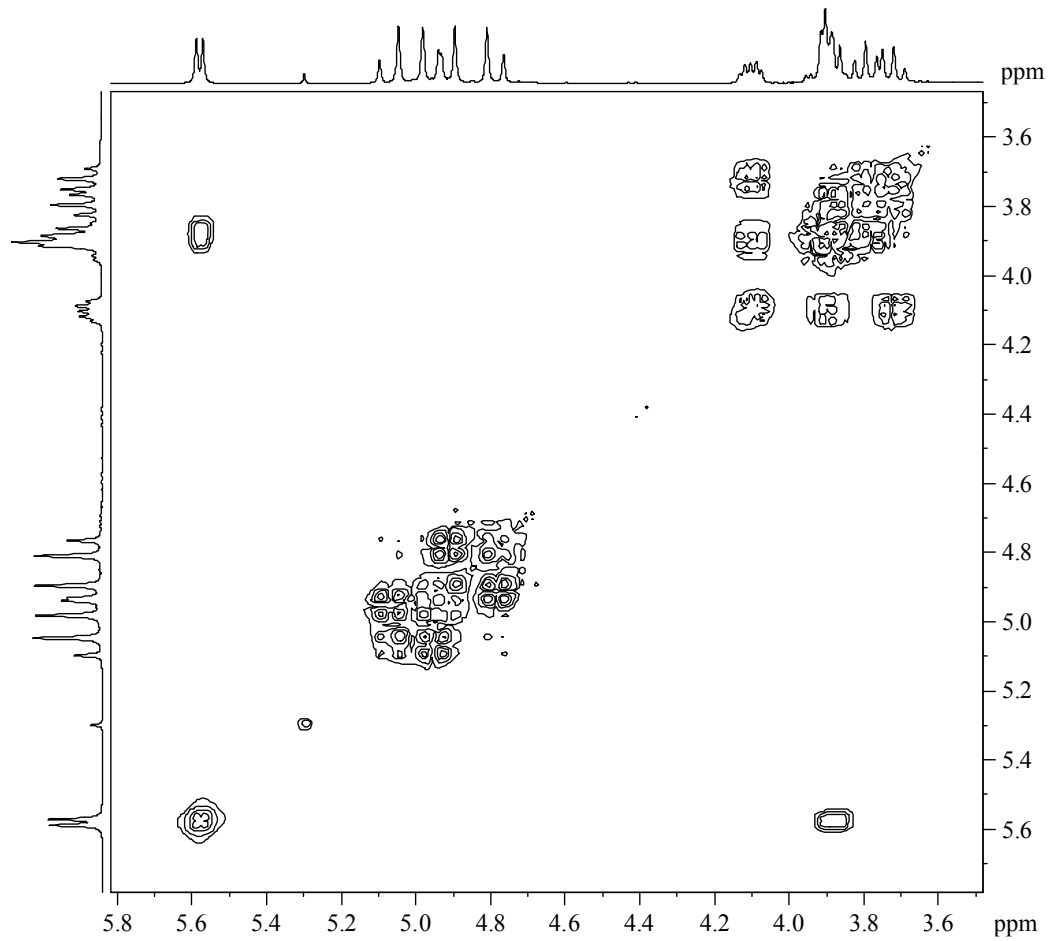
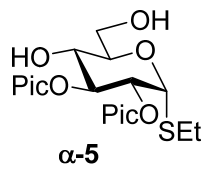
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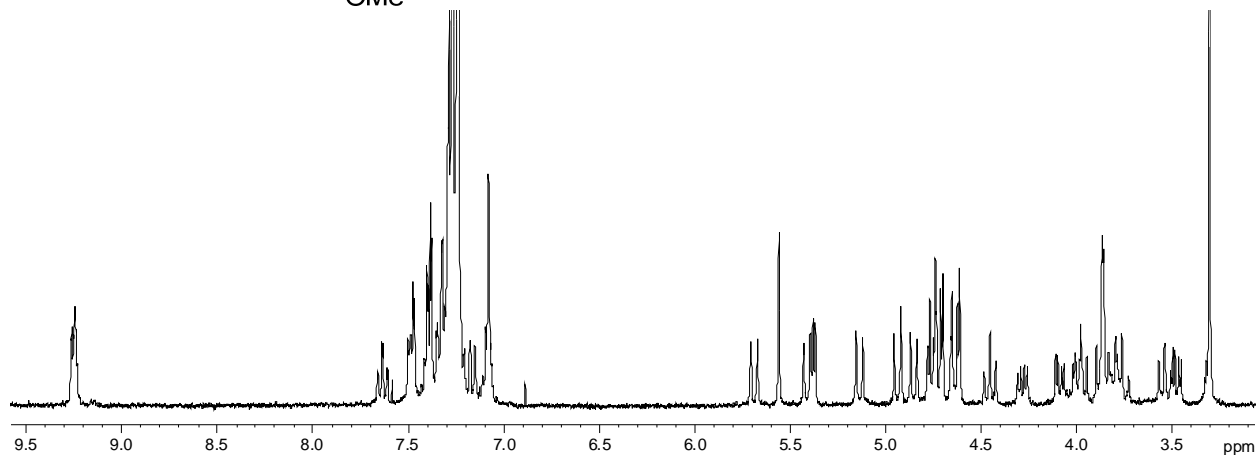
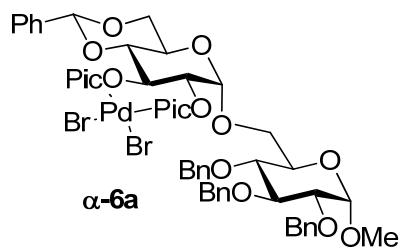
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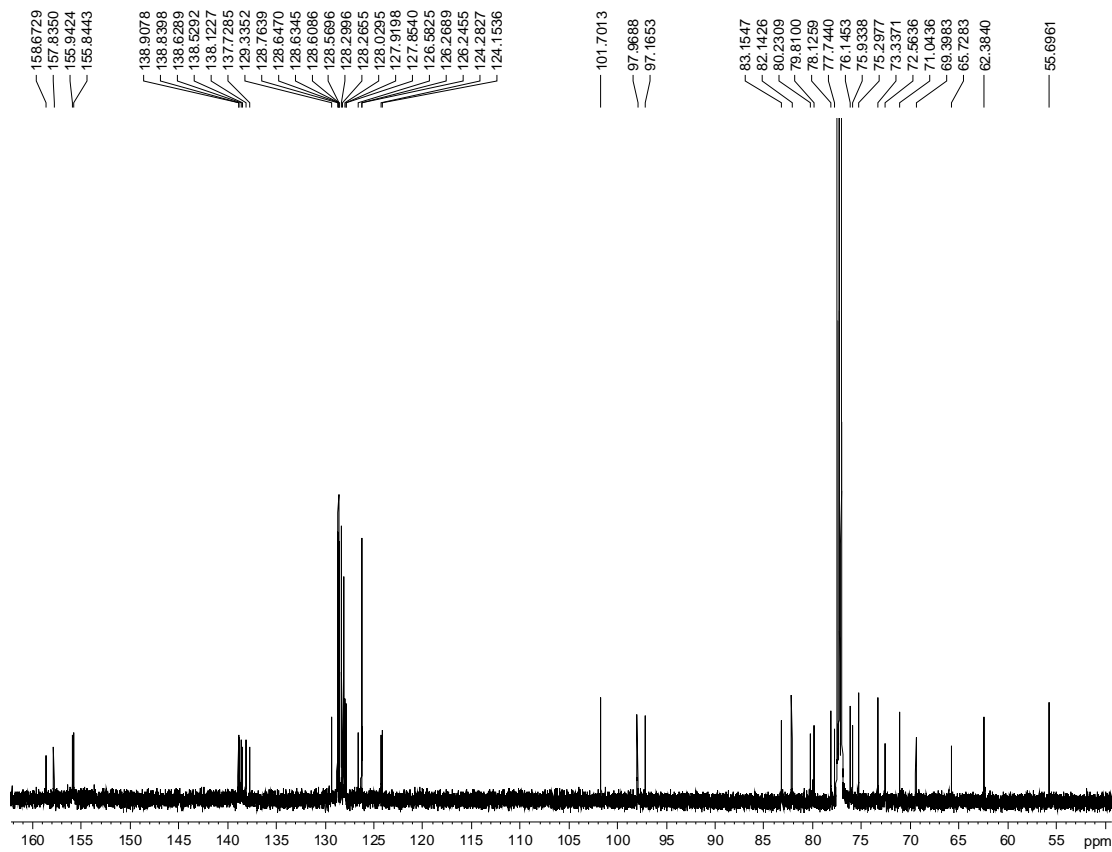
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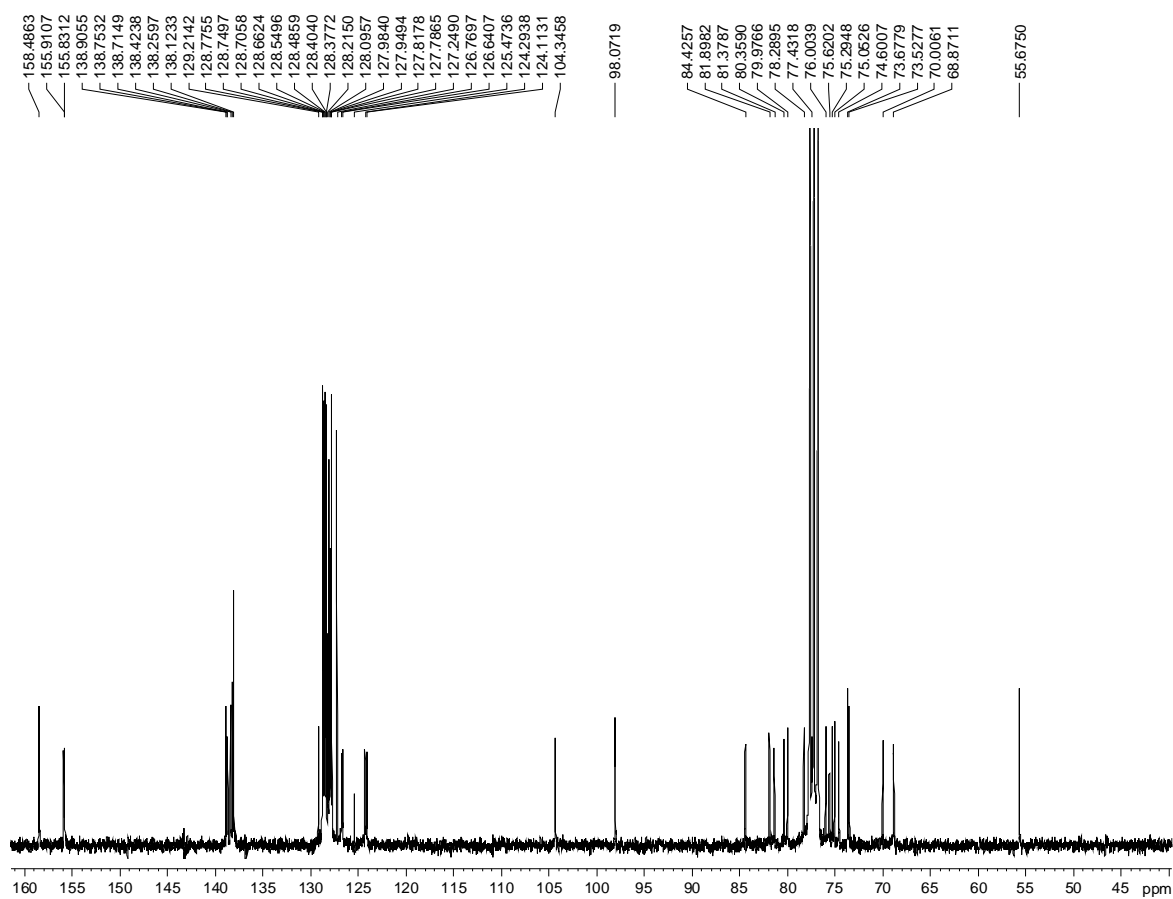
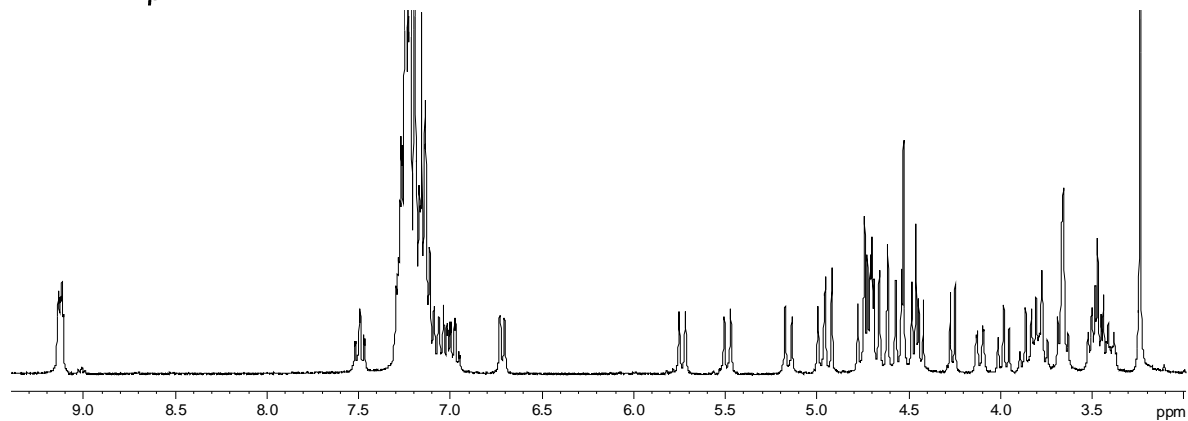
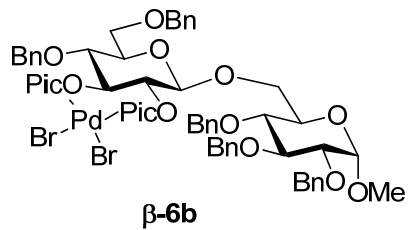
CDCl₃ 300 MHz



CDCl₃ 300 MHz



CDCl₃ 150 MHz



X-Ray data

Table 1S. Crystal data and structure refinement for avd13811.

| | |
|-----------------------------------|---|
| Identification code | d13811/lt/Ning/dipic-Pd |
| Empirical formula | C ₂₇ H ₃₀ Br ₂ N ₂ O ₅ Pd S |
| Formula weight | 760.81 |
| Temperature | 100(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | P2 ₁ |
| Unit cell dimensions | a = 8.3369(4) Å α = 90°. b = 20.8048(10) Å β = 112.222(3)°. c = 8.5721(4) Å γ = 90°. |
| Volume | 1376.38(12) Å ³ |
| Z | 2 |
| Density (calculated) | 1.836 Mg/m ³ |
| Absorption coefficient | 3.694 mm ⁻¹ |
| F(000) | 756 |
| Crystal size | 0.266 x 0.179 x 0.157 mm ³ |
| Theta range for data collection | 1.958 to 27.634°. |
| Index ranges | -10 ≤ h ≤ 10, -26 ≤ k ≤ 27, -11 ≤ l ≤ 11 |
| Reflections collected | 47319 |
| Independent reflections | 6319 [R(int) = 0.0407] |
| Completeness to theta = 25.242° | 100.0 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.4305 and 0.3967 |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 6319 / 151 / 363 |
| Goodness-of-fit on F ² | 1.025 |
| Final R indices [I > 2σ(I)] | R1 = 0.0262, wR2 = 0.0574 |
| R indices (all data) | R1 = 0.0308, wR2 = 0.0592 |
| Absolute structure parameter | -0.002(4) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.553 and -0.457 e.Å ⁻³ |

Table 2S. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for avd13811. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|----------|----------|-----------|----------------|
| Pd(1) | 6432(1) | 2268(1) | 9362(1) | 21(1) |
| Br(1) | 8669(1) | 2997(1) | 9215(1) | 28(1) |
| Br(2) | 3983(1) | 1654(1) | 9479(1) | 34(1) |
| S(1) | 12357(1) | 329(1) | 12879(1) | 21(1) |
| O(1) | 11398(4) | -164(2) | 9872(4) | 22(1) |
| O(2) | 9658(4) | -880(2) | 5743(4) | 31(1) |
| O(3) | 8135(4) | 69(2) | 5664(4) | 22(1) |
| O(4) | 7779(4) | 1256(2) | 7422(4) | 24(1) |
| C(1) | 10675(6) | 199(2) | 10858(6) | 20(1) |
| C(2) | 9934(7) | 823(2) | 9959(6) | 24(1) |
| C(3) | 8482(6) | 672(2) | 8241(6) | 21(1) |
| C(4) | 9323(6) | 262(2) | 7286(5) | 22(1) |
| C(5) | 10082(6) | -338(2) | 8312(6) | 22(1) |
| C(6) | 10921(6) | -756(3) | 7385(6) | 31(1) |
| C(7) | 9026(6) | -308(3) | 4868(6) | 28(1) |
| C(8) | 7815(6) | -479(3) | 3106(6) | 30(1) |
| C(9) | 8099(7) | -1051(3) | 2397(6) | 29(1) |
| C(10) | 7060(8) | -1205(3) | 747(7) | 36(1) |
| C(11) | 5762(7) | -793(3) | -190(7) | 39(2) |
| C(12) | 5484(7) | -223(4) | 499(7) | 53(2) |
| C(13) | 6519(7) | -68(4) | 2164(7) | 49(2) |
| C(14) | 5965(6) | 1199(2) | 6421(6) | 24(1) |
| N(1) | 5229(4) | 2313(1) | 6849(3) | 24(1) |
| C(15) | 5186(5) | 1823(1) | 5734(4) | 27(1) |
| C(16) | 4252(6) | 1902(2) | 4017(3) | 46(2) |
| C(17) | 3360(6) | 2471(2) | 3416(3) | 68(3) |
| C(18) | 3403(6) | 2962(1) | 4532(4) | 50(2) |
| C(19) | 4337(5) | 2883(1) | 6249(4) | 34(1) |
| N(2) | 7689(9) | 2300(4) | 11909(7) | 19(3) |
| C(20) | 6902(8) | 2668(4) | 12774(10) | 19(1) |
| C(21) | 7633(9) | 2701(4) | 14523(10) | 19(1) |

| | | | | |
|--------|-----------|---------|-----------|-------|
| C(22) | 9150(9) | 2367(4) | 15407(7) | 21(3) |
| C(23) | 9937(8) | 2000(4) | 14542(7) | 22(2) |
| C(24) | 9206(9) | 1966(3) | 12793(7) | 18(2) |
| C(25) | 10060(11) | 1645(5) | 11813(12) | 18(2) |
| O(5) | 8981(10) | 1126(4) | 10877(9) | 17(2) |
| N(2') | 7479(9) | 2227(4) | 11891(7) | 19(3) |
| C(20') | 7391(10) | 2777(3) | 12777(11) | 19(1) |
| C(21') | 8234(11) | 2795(3) | 14519(11) | 19(1) |
| C(22') | 9166(10) | 2264(4) | 15376(7) | 29(4) |
| C(23') | 9254(10) | 1715(4) | 14490(7) | 24(2) |
| C(24') | 8410(10) | 1696(3) | 12747(7) | 20(2) |
| C(25') | 8497(12) | 1147(5) | 11711(13) | 22(2) |
| O(5') | 9649(12) | 1330(4) | 10963(10) | 21(2) |
| C(26) | 12828(7) | -503(2) | 13501(7) | 26(1) |
| C(27) | 14190(6) | -533(2) | 15252(6) | 24(1) |

Table 3S. Bond lengths [Å] and angles [°] for avd13811.

| | |
|-------------|-----------|
| Pd(1)-N(1) | 2.005(2) |
| Pd(1)-N(2') | 2.010(6) |
| Pd(1)-N(2) | 2.035(5) |
| Pd(1)-Br(2) | 2.4426(6) |
| Pd(1)-Br(1) | 2.4432(6) |
| S(1)-C(1) | 1.790(5) |
| S(1)-C(26) | 1.809(5) |
| O(1)-C(5) | 1.419(5) |
| O(1)-C(1) | 1.426(5) |
| O(2)-C(7) | 1.401(7) |
| O(2)-C(6) | 1.426(6) |
| O(3)-C(7) | 1.420(6) |
| O(3)-C(4) | 1.427(5) |
| O(4)-C(3) | 1.415(6) |
| O(4)-C(14) | 1.434(6) |
| C(1)-C(2) | 1.518(7) |
| C(1)-H(1) | 1.0000 |
| C(2)-O(5') | 1.436(9) |
| C(2)-O(5) | 1.456(8) |
| C(2)-C(3) | 1.544(6) |
| C(2)-H(2) | 1.0000 |
| C(3)-C(4) | 1.523(6) |
| C(3)-H(3) | 1.0000 |
| C(4)-C(5) | 1.521(7) |
| C(4)-H(4) | 1.0000 |
| C(5)-C(6) | 1.516(7) |
| C(5)-H(5) | 1.0000 |
| C(6)-H(6A) | 0.9900 |
| C(6)-H(6B) | 0.9900 |
| C(7)-C(8) | 1.508(6) |
| C(7)-H(7) | 1.0000 |
| C(8)-C(13) | 1.375(9) |
| C(8)-C(9) | 1.397(8) |
| C(9)-C(10) | 1.388(7) |

| | |
|--------------|-----------|
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.376(9) |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.383(9) |
| C(11)-H(11) | 0.9500 |
| C(12)-C(13) | 1.398(8) |
| C(12)-H(12) | 0.9500 |
| C(13)-H(13) | 0.9500 |
| C(14)-C(15) | 1.470(5) |
| C(14)-H(14A) | 0.9900 |
| C(14)-H(14B) | 0.9900 |
| N(1)-C(15) | 1.3900 |
| N(1)-C(19) | 1.3900 |
| C(15)-C(16) | 1.3900 |
| C(16)-C(17) | 1.3900 |
| C(16)-H(16) | 0.9500 |
| C(17)-C(18) | 1.3900 |
| C(17)-H(17) | 0.9500 |
| C(18)-C(19) | 1.3900 |
| C(18)-H(18) | 0.9500 |
| C(19)-H(19) | 0.9500 |
| N(2)-C(20) | 1.3900 |
| N(2)-C(24) | 1.3900 |
| C(20)-C(21) | 1.3900 |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.3900 |
| C(21)-H(21) | 0.9500 |
| C(22)-C(23) | 1.3900 |
| C(22)-H(22) | 0.9500 |
| C(23)-C(24) | 1.3900 |
| C(23)-H(23) | 0.9500 |
| C(24)-C(25) | 1.453(10) |
| C(25)-O(5) | 1.439(12) |
| C(25)-H(25A) | 0.9900 |
| C(25)-H(25B) | 0.9900 |
| N(2')-C(20') | 1.3900 |

| | |
|-------------------|-----------|
| N(2')-C(24') | 1.3900 |
| C(20')-C(21') | 1.3900 |
| C(20')-H(20') | 0.9500 |
| C(21')-C(22') | 1.3900 |
| C(21')-H(21') | 0.9500 |
| C(22')-C(23') | 1.3900 |
| C(22')-H(22') | 0.9500 |
| C(23')-C(24') | 1.3900 |
| C(23')-H(23') | 0.9500 |
| C(24')-C(25') | 1.466(11) |
| C(25')-O(5') | 1.394(12) |
| C(25')-H(25C) | 0.9900 |
| C(25')-H(25D) | 0.9900 |
| C(26)-C(27) | 1.503(7) |
| C(26)-H(26A) | 0.9900 |
| C(26)-H(26B) | 0.9900 |
| C(27)-H(27A) | 0.9800 |
| C(27)-H(27B) | 0.9800 |
| C(27)-H(27C) | 0.9800 |
| | |
| N(1)-Pd(1)-N(2') | 176.1(2) |
| N(1)-Pd(1)-N(2) | 175.4(2) |
| N(1)-Pd(1)-Br(2) | 88.98(10) |
| N(2')-Pd(1)-Br(2) | 87.8(2) |
| N(2)-Pd(1)-Br(2) | 94.1(2) |
| N(1)-Pd(1)-Br(1) | 89.85(9) |
| N(2')-Pd(1)-Br(1) | 93.1(2) |
| N(2)-Pd(1)-Br(1) | 86.7(2) |
| Br(2)-Pd(1)-Br(1) | 173.19(2) |
| C(1)-S(1)-C(26) | 98.3(2) |
| C(5)-O(1)-C(1) | 110.2(3) |
| C(7)-O(2)-C(6) | 111.2(4) |
| C(7)-O(3)-C(4) | 109.1(3) |
| C(3)-O(4)-C(14) | 111.8(3) |
| O(1)-C(1)-C(2) | 109.5(4) |
| O(1)-C(1)-S(1) | 107.6(3) |

| | |
|------------------|----------|
| C(2)-C(1)-S(1) | 112.4(3) |
| O(1)-C(1)-H(1) | 109.1 |
| C(2)-C(1)-H(1) | 109.1 |
| S(1)-C(1)-H(1) | 109.1 |
| O(5')-C(2)-C(1) | 116.8(5) |
| O(5)-C(2)-C(1) | 107.3(5) |
| O(5')-C(2)-C(3) | 118.3(5) |
| O(5)-C(2)-C(3) | 102.3(5) |
| C(1)-C(2)-C(3) | 109.4(4) |
| O(5)-C(2)-H(2) | 112.4 |
| C(1)-C(2)-H(2) | 112.4 |
| C(3)-C(2)-H(2) | 112.4 |
| O(4)-C(3)-C(4) | 113.8(4) |
| O(4)-C(3)-C(2) | 109.0(4) |
| C(4)-C(3)-C(2) | 105.8(4) |
| O(4)-C(3)-H(3) | 109.4 |
| C(4)-C(3)-H(3) | 109.4 |
| C(2)-C(3)-H(3) | 109.4 |
| O(3)-C(4)-C(5) | 108.4(4) |
| O(3)-C(4)-C(3) | 113.0(4) |
| C(5)-C(4)-C(3) | 108.9(4) |
| O(3)-C(4)-H(4) | 108.8 |
| C(5)-C(4)-H(4) | 108.8 |
| C(3)-C(4)-H(4) | 108.8 |
| O(1)-C(5)-C(6) | 107.2(4) |
| O(1)-C(5)-C(4) | 109.8(4) |
| C(6)-C(5)-C(4) | 110.0(4) |
| O(1)-C(5)-H(5) | 110.0 |
| C(6)-C(5)-H(5) | 110.0 |
| C(4)-C(5)-H(5) | 110.0 |
| O(2)-C(6)-C(5) | 107.8(4) |
| O(2)-C(6)-H(6A) | 110.1 |
| C(5)-C(6)-H(6A) | 110.1 |
| O(2)-C(6)-H(6B) | 110.1 |
| C(5)-C(6)-H(6B) | 110.1 |
| H(6A)-C(6)-H(6B) | 108.5 |

| | |
|---------------------|------------|
| O(2)-C(7)-O(3) | 111.8(4) |
| O(2)-C(7)-C(8) | 108.1(4) |
| O(3)-C(7)-C(8) | 109.7(4) |
| O(2)-C(7)-H(7) | 109.1 |
| O(3)-C(7)-H(7) | 109.1 |
| C(8)-C(7)-H(7) | 109.1 |
| C(13)-C(8)-C(9) | 120.0(5) |
| C(13)-C(8)-C(7) | 121.4(5) |
| C(9)-C(8)-C(7) | 118.5(5) |
| C(10)-C(9)-C(8) | 119.8(5) |
| C(10)-C(9)-H(9) | 120.1 |
| C(8)-C(9)-H(9) | 120.1 |
| C(11)-C(10)-C(9) | 120.0(6) |
| C(11)-C(10)-H(10) | 120.0 |
| C(9)-C(10)-H(10) | 120.0 |
| C(10)-C(11)-C(12) | 120.5(5) |
| C(10)-C(11)-H(11) | 119.8 |
| C(12)-C(11)-H(11) | 119.8 |
| C(11)-C(12)-C(13) | 119.7(6) |
| C(11)-C(12)-H(12) | 120.1 |
| C(13)-C(12)-H(12) | 120.1 |
| C(8)-C(13)-C(12) | 120.0(6) |
| C(8)-C(13)-H(13) | 120.0 |
| C(12)-C(13)-H(13) | 120.0 |
| O(4)-C(14)-C(15) | 111.9(4) |
| O(4)-C(14)-H(14A) | 109.2 |
| C(15)-C(14)-H(14A) | 109.2 |
| O(4)-C(14)-H(14B) | 109.2 |
| C(15)-C(14)-H(14B) | 109.2 |
| H(14A)-C(14)-H(14B) | 107.9 |
| C(15)-N(1)-C(19) | 120.0 |
| C(15)-N(1)-Pd(1) | 125.26(16) |
| C(19)-N(1)-Pd(1) | 114.70(16) |
| N(1)-C(15)-C(16) | 120.0 |
| N(1)-C(15)-C(14) | 118.6(3) |
| C(16)-C(15)-C(14) | 121.0(3) |

| | |
|---------------------|----------|
| C(15)-C(16)-C(17) | 120.0 |
| C(15)-C(16)-H(16) | 120.0 |
| C(17)-C(16)-H(16) | 120.0 |
| C(18)-C(17)-C(16) | 120.0 |
| C(18)-C(17)-H(17) | 120.0 |
| C(16)-C(17)-H(17) | 120.0 |
| C(17)-C(18)-C(19) | 120.0 |
| C(17)-C(18)-H(18) | 120.0 |
| C(19)-C(18)-H(18) | 120.0 |
| C(18)-C(19)-N(1) | 120.0 |
| C(18)-C(19)-H(19) | 120.0 |
| N(1)-C(19)-H(19) | 120.0 |
| C(20)-N(2)-C(24) | 120.0 |
| C(20)-N(2)-Pd(1) | 115.8(4) |
| C(24)-N(2)-Pd(1) | 124.2(4) |
| N(2)-C(20)-C(21) | 120.0 |
| N(2)-C(20)-H(20) | 120.0 |
| C(21)-C(20)-H(20) | 120.0 |
| C(22)-C(21)-C(20) | 120.0 |
| C(22)-C(21)-H(21) | 120.0 |
| C(20)-C(21)-H(21) | 120.0 |
| C(23)-C(22)-C(21) | 120.0 |
| C(23)-C(22)-H(22) | 120.0 |
| C(21)-C(22)-H(22) | 120.0 |
| C(22)-C(23)-C(24) | 120.0 |
| C(22)-C(23)-H(23) | 120.0 |
| C(24)-C(23)-H(23) | 120.0 |
| C(23)-C(24)-N(2) | 120.0 |
| C(23)-C(24)-C(25) | 122.4(5) |
| N(2)-C(24)-C(25) | 117.3(5) |
| O(5)-C(25)-C(24) | 109.1(7) |
| O(5)-C(25)-H(25A) | 109.9 |
| C(24)-C(25)-H(25A) | 109.9 |
| O(5)-C(25)-H(25B) | 109.9 |
| C(24)-C(25)-H(25B) | 109.9 |
| H(25A)-C(25)-H(25B) | 108.3 |

| | |
|----------------------|----------|
| C(25)-O(5)-C(2) | 105.8(7) |
| C(20')-N(2')-C(24') | 120.0 |
| C(20')-N(2')-Pd(1) | 117.6(4) |
| C(24')-N(2')-Pd(1) | 122.1(4) |
| C(21')-C(20')-N(2') | 120.0 |
| C(21')-C(20')-H(20') | 120.0 |
| N(2')-C(20')-H(20') | 120.0 |
| C(22')-C(21')-C(20') | 120.0 |
| C(22')-C(21')-H(21') | 120.0 |
| C(20')-C(21')-H(21') | 120.0 |
| C(21')-C(22')-C(23') | 120.0 |
| C(21')-C(22')-H(22') | 120.0 |
| C(23')-C(22')-H(22') | 120.0 |
| C(24')-C(23')-C(22') | 120.0 |
| C(24')-C(23')-H(23') | 120.0 |
| C(22')-C(23')-H(23') | 120.0 |
| C(23')-C(24')-N(2') | 120.0 |
| C(23')-C(24')-C(25') | 123.5(6) |
| N(2')-C(24')-C(25') | 116.5(6) |
| O(5')-C(25')-C(24') | 105.5(8) |
| O(5')-C(25')-H(25C) | 110.6 |
| C(24')-C(25')-H(25C) | 110.6 |
| O(5')-C(25')-H(25D) | 110.6 |
| C(24')-C(25')-H(25D) | 110.6 |
| H(25C)-C(25')-H(25D) | 108.8 |
| C(25')-O(5')-C(2) | 112.0(8) |
| C(27)-C(26)-S(1) | 109.4(3) |
| C(27)-C(26)-H(26A) | 109.8 |
| S(1)-C(26)-H(26A) | 109.8 |
| C(27)-C(26)-H(26B) | 109.8 |
| S(1)-C(26)-H(26B) | 109.8 |
| H(26A)-C(26)-H(26B) | 108.2 |
| C(26)-C(27)-H(27A) | 109.5 |
| C(26)-C(27)-H(27B) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 |
| C(26)-C(27)-H(27C) | 109.5 |

H(27A)-C(27)-H(27C) 109.5
H(27B)-C(27)-H(27C) 109.5

Table 4S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for avd13811. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U ¹¹ | U ²² | U ³³ | U ²³ | U ¹³ | U ¹² |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Pd(1) | 29(1) | 17(1) | 15(1) | 1(1) | 7(1) | 0(1) |
| Br(1) | 40(1) | 18(1) | 23(1) | -3(1) | 8(1) | -8(1) |
| Br(2) | 28(1) | 44(1) | 31(1) | 9(1) | 13(1) | 0(1) |
| S(1) | 22(1) | 21(1) | 16(1) | -2(1) | 5(1) | -2(1) |
| O(1) | 19(2) | 32(2) | 14(2) | -9(1) | 5(1) | 0(1) |
| O(2) | 25(2) | 47(2) | 18(2) | -12(2) | 4(1) | 5(2) |
| O(3) | 17(2) | 35(2) | 13(2) | -7(1) | 5(1) | -6(1) |
| O(4) | 24(2) | 25(2) | 18(2) | 2(1) | 4(1) | -7(1) |
| C(1) | 18(2) | 28(2) | 14(2) | -3(2) | 8(2) | -1(2) |
| C(2) | 28(2) | 29(3) | 13(2) | -5(2) | 7(2) | 2(2) |
| C(3) | 21(2) | 27(2) | 14(2) | 0(2) | 7(2) | -7(2) |
| C(4) | 17(2) | 36(3) | 12(2) | -4(2) | 4(2) | -7(2) |
| C(5) | 17(2) | 32(3) | 19(2) | -6(2) | 7(2) | -1(2) |
| C(6) | 21(2) | 54(4) | 17(2) | -13(2) | 7(2) | 3(2) |
| C(7) | 18(2) | 51(3) | 15(2) | -10(2) | 8(2) | -6(2) |
| C(8) | 18(2) | 59(4) | 14(2) | -13(2) | 9(2) | -12(2) |
| C(9) | 30(3) | 39(3) | 19(2) | -1(2) | 9(2) | -12(2) |
| C(10) | 43(3) | 45(3) | 20(3) | -9(2) | 14(2) | -19(3) |
| C(11) | 24(3) | 78(5) | 14(2) | -13(3) | 3(2) | -13(3) |
| C(12) | 20(3) | 109(6) | 22(3) | -21(3) | -2(2) | 15(3) |
| C(13) | 18(3) | 94(5) | 29(3) | -28(3) | 4(2) | 15(3) |
| C(14) | 27(2) | 17(2) | 22(2) | -1(2) | 3(2) | -4(2) |
| N(1) | 32(2) | 14(2) | 21(2) | 4(2) | 5(2) | 0(2) |
| C(15) | 37(3) | 18(2) | 19(2) | 0(2) | 3(2) | -6(2) |
| C(16) | 86(5) | 18(3) | 19(3) | 1(2) | 1(3) | 0(3) |
| C(17) | 129(7) | 20(3) | 20(3) | 5(2) | -12(3) | 9(3) |
| C(18) | 82(5) | 19(3) | 29(3) | 7(2) | -3(3) | 8(3) |

| | | | | | | |
|--------|-------|-------|-------|-------|-------|--------|
| C(19) | 47(3) | 20(3) | 27(3) | 7(2) | 3(2) | 3(2) |
| N(2) | 23(4) | 17(5) | 18(5) | -4(4) | 9(4) | -6(4) |
| C(20) | 23(4) | 17(2) | 24(2) | -5(2) | 14(3) | -12(2) |
| C(21) | 23(4) | 17(2) | 24(2) | -5(2) | 14(3) | -12(2) |
| C(22) | 30(7) | 20(5) | 19(6) | -7(4) | 16(5) | -13(4) |
| C(23) | 29(5) | 22(5) | 14(4) | -2(3) | 6(3) | -3(4) |
| C(24) | 25(4) | 15(4) | 18(4) | -2(3) | 11(3) | -6(3) |
| C(25) | 18(4) | 15(4) | 17(4) | -4(4) | 4(3) | -6(3) |
| O(5) | 17(4) | 23(4) | 18(4) | -7(3) | 12(3) | -7(3) |
| N(2') | 23(5) | 21(5) | 14(5) | 0(3) | 8(4) | -3(4) |
| C(20') | 23(4) | 17(2) | 24(2) | -5(2) | 14(3) | -12(2) |
| C(21') | 23(4) | 17(2) | 24(2) | -5(2) | 14(3) | -12(2) |
| C(22') | 33(8) | 33(6) | 20(6) | -2(4) | 10(5) | -4(5) |
| C(23') | 30(5) | 29(5) | 14(4) | 2(3) | 10(4) | -1(4) |
| C(24') | 26(5) | 24(4) | 15(4) | 0(3) | 13(3) | -5(4) |
| C(25') | 21(4) | 23(5) | 19(4) | 0(3) | 6(4) | -4(3) |
| O(5') | 25(5) | 22(5) | 17(4) | 0(3) | 10(4) | -4(3) |
| C(26) | 28(3) | 19(2) | 29(3) | -3(2) | 7(2) | 2(2) |
| C(27) | 25(2) | 19(2) | 26(3) | 1(2) | 8(2) | -1(2) |

Table 5S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for avd13811.

| | x | y | z | U(eq) |
|-------|-------|-------|-------|-------|
| H(1) | 9724 | -56 | 11005 | 24 |
| H(2) | 10846 | 1111 | 9849 | 28 |
| H(3) | 7551 | 418 | 8426 | 25 |
| H(4) | 10282 | 514 | 7147 | 26 |
| H(5) | 9150 | -585 | 8516 | 27 |
| H(6A) | 11933 | -532 | 7300 | 37 |
| H(6B) | 11324 | -1165 | 8000 | 37 |
| H(7) | 10018 | -54 | 4807 | 33 |
| H(9) | 9002 | -1333 | 3041 | 35 |

| | | | | |
|--------|-------|-------|-------|----|
| H(10) | 7245 | -1595 | 264 | 43 |
| H(11) | 5052 | -901 | -1317 | 47 |
| H(12) | 4592 | 61 | -156 | 64 |
| H(13) | 6328 | 322 | 2645 | 58 |
| H(14A) | 5364 | 1019 | 7122 | 28 |
| H(14B) | 5801 | 897 | 5481 | 28 |
| H(16) | 4223 | 1566 | 3254 | 56 |
| H(17) | 2722 | 2525 | 2243 | 82 |
| H(18) | 2793 | 3351 | 4121 | 60 |
| H(19) | 4366 | 3218 | 7011 | 41 |
| H(20) | 5865 | 2896 | 12170 | 23 |
| H(21) | 7095 | 2952 | 15114 | 23 |
| H(22) | 9650 | 2390 | 16602 | 25 |
| H(23) | 10974 | 1771 | 15146 | 26 |
| H(25A) | 10262 | 1954 | 11029 | 21 |
| H(25B) | 11196 | 1475 | 12574 | 21 |
| H(20') | 6754 | 3140 | 12192 | 23 |
| H(21') | 8174 | 3171 | 15125 | 23 |
| H(22') | 9743 | 2277 | 16566 | 35 |
| H(23') | 9891 | 1352 | 15075 | 29 |
| H(25C) | 8924 | 760 | 12417 | 26 |
| H(25D) | 7340 | 1053 | 10842 | 26 |
| H(26A) | 11762 | -721 | 13471 | 32 |
| H(26B) | 13246 | -725 | 12706 | 32 |
| H(27A) | 15285 | -364 | 15247 | 35 |
| H(27B) | 14352 | -980 | 15640 | 35 |
| H(27C) | 13821 | -274 | 16013 | 35 |

Table 6. Torsion angles [°] for avd13811.

| | |
|----------------------|-----------|
| C(5)-O(1)-C(1)-C(2) | -63.4(5) |
| C(5)-O(1)-C(1)-S(1) | 174.1(3) |
| C(26)-S(1)-C(1)-O(1) | -60.2(3) |
| C(26)-S(1)-C(1)-C(2) | 179.1(3) |
| O(1)-C(1)-C(2)-O(5') | -161.1(6) |
| S(1)-C(1)-C(2)-O(5') | -41.6(7) |
| O(1)-C(1)-C(2)-O(5) | 171.3(5) |
| S(1)-C(1)-C(2)-O(5) | -69.1(5) |
| O(1)-C(1)-C(2)-C(3) | 61.1(5) |
| S(1)-C(1)-C(2)-C(3) | -179.4(3) |
| C(14)-O(4)-C(3)-C(4) | 95.2(4) |
| C(14)-O(4)-C(3)-C(2) | -146.9(4) |
| O(5')-C(2)-C(3)-O(4) | 41.9(7) |
| O(5)-C(2)-C(3)-O(4) | 65.6(5) |
| C(1)-C(2)-C(3)-O(4) | 179.1(4) |
| O(5')-C(2)-C(3)-C(4) | 164.7(5) |
| O(5)-C(2)-C(3)-C(4) | -171.7(5) |
| C(1)-C(2)-C(3)-C(4) | -58.2(5) |
| C(7)-O(3)-C(4)-C(5) | -59.2(4) |
| C(7)-O(3)-C(4)-C(3) | 179.9(4) |
| O(4)-C(3)-C(4)-O(3) | -61.4(5) |
| C(2)-C(3)-C(4)-O(3) | 179.0(4) |
| O(4)-C(3)-C(4)-C(5) | 178.1(4) |
| C(2)-C(3)-C(4)-C(5) | 58.4(5) |
| C(1)-O(1)-C(5)-C(6) | -176.5(4) |
| C(1)-O(1)-C(5)-C(4) | 64.1(5) |
| O(3)-C(4)-C(5)-O(1) | 174.1(3) |
| C(3)-C(4)-C(5)-O(1) | -62.5(5) |
| O(3)-C(4)-C(5)-C(6) | 56.5(5) |
| C(3)-C(4)-C(5)-C(6) | 179.8(4) |
| C(7)-O(2)-C(6)-C(5) | 57.8(5) |
| O(1)-C(5)-C(6)-O(2) | -174.1(4) |
| C(4)-C(5)-C(6)-O(2) | -54.8(5) |
| C(6)-O(2)-C(7)-O(3) | -63.7(5) |

| | |
|-------------------------|-----------|
| C(6)-O(2)-C(7)-C(8) | 175.4(4) |
| C(4)-O(3)-C(7)-O(2) | 63.8(5) |
| C(4)-O(3)-C(7)-C(8) | -176.3(4) |
| O(2)-C(7)-C(8)-C(13) | 155.0(5) |
| O(3)-C(7)-C(8)-C(13) | 32.8(7) |
| O(2)-C(7)-C(8)-C(9) | -29.0(6) |
| O(3)-C(7)-C(8)-C(9) | -151.2(4) |
| C(13)-C(8)-C(9)-C(10) | -0.7(8) |
| C(7)-C(8)-C(9)-C(10) | -176.8(5) |
| C(8)-C(9)-C(10)-C(11) | 0.5(8) |
| C(9)-C(10)-C(11)-C(12) | 0.1(8) |
| C(10)-C(11)-C(12)-C(13) | -0.6(10) |
| C(9)-C(8)-C(13)-C(12) | 0.2(9) |
| C(7)-C(8)-C(13)-C(12) | 176.2(6) |
| C(11)-C(12)-C(13)-C(8) | 0.4(11) |
| C(3)-O(4)-C(14)-C(15) | 173.2(4) |
| C(19)-N(1)-C(15)-C(16) | 0.0 |
| Pd(1)-N(1)-C(15)-C(16) | 177.6(3) |
| C(19)-N(1)-C(15)-C(14) | -172.8(4) |
| Pd(1)-N(1)-C(15)-C(14) | 4.8(4) |
| O(4)-C(14)-C(15)-N(1) | -60.7(5) |
| O(4)-C(14)-C(15)-C(16) | 126.6(3) |
| N(1)-C(15)-C(16)-C(17) | 0.0 |
| C(14)-C(15)-C(16)-C(17) | 172.6(4) |
| C(15)-C(16)-C(17)-C(18) | 0.0 |
| C(16)-C(17)-C(18)-C(19) | 0.0 |
| C(17)-C(18)-C(19)-N(1) | 0.0 |
| C(15)-N(1)-C(19)-C(18) | 0.0 |
| Pd(1)-N(1)-C(19)-C(18) | -177.8(2) |
| C(24)-N(2)-C(20)-C(21) | 0.0 |
| Pd(1)-N(2)-C(20)-C(21) | 177.8(5) |
| N(2)-C(20)-C(21)-C(22) | 0.0 |
| C(20)-C(21)-C(22)-C(23) | 0.0 |
| C(21)-C(22)-C(23)-C(24) | 0.0 |
| C(22)-C(23)-C(24)-N(2) | 0.0 |
| C(22)-C(23)-C(24)-C(25) | 173.5(8) |

| | |
|-----------------------------|-----------|
| C(20)-N(2)-C(24)-C(23) | 0.0 |
| Pd(1)-N(2)-C(24)-C(23) | -177.7(6) |
| C(20)-N(2)-C(24)-C(25) | -173.9(7) |
| Pd(1)-N(2)-C(24)-C(25) | 8.5(7) |
| C(23)-C(24)-C(25)-O(5) | 119.3(7) |
| N(2)-C(24)-C(25)-O(5) | -67.0(8) |
| C(24)-C(25)-O(5)-C(2) | -179.0(6) |
| O(5')-C(2)-O(5)-C(25) | -11.0(8) |
| C(1)-C(2)-O(5)-C(25) | 104.4(6) |
| C(3)-C(2)-O(5)-C(25) | -140.5(6) |
| C(24')-N(2')-C(20')-C(21') | 0.0 |
| Pd(1)-N(2')-C(20')-C(21') | -173.9(5) |
| N(2')-C(20')-C(21')-C(22') | 0.0 |
| C(20')-C(21')-C(22')-C(23') | 0.0 |
| C(21')-C(22')-C(23')-C(24') | 0.0 |
| C(22')-C(23')-C(24')-N(2') | 0.0 |
| C(22')-C(23')-C(24')-C(25') | 177.3(8) |
| C(20')-N(2')-C(24')-C(23') | 0.0 |
| Pd(1)-N(2')-C(24')-C(23') | 173.7(6) |
| C(20')-N(2')-C(24')-C(25') | -177.5(7) |
| Pd(1)-N(2')-C(24')-C(25') | -3.8(7) |
| C(23')-C(24')-C(25')-O(5') | -103.1(8) |
| N(2')-C(24')-C(25')-O(5') | 74.3(8) |
| C(24')-C(25')-O(5')-C(2) | 177.3(6) |
| O(5)-C(2)-O(5')-C(25') | 15.4(9) |
| C(1)-C(2)-O(5')-C(25') | -59.8(9) |
| C(3)-C(2)-O(5')-C(25') | 74.2(8) |
| C(1)-S(1)-C(26)-C(27) | -177.3(4) |

Table 7. Hydrogen bonds for avd13811 [\AA and $^\circ$].

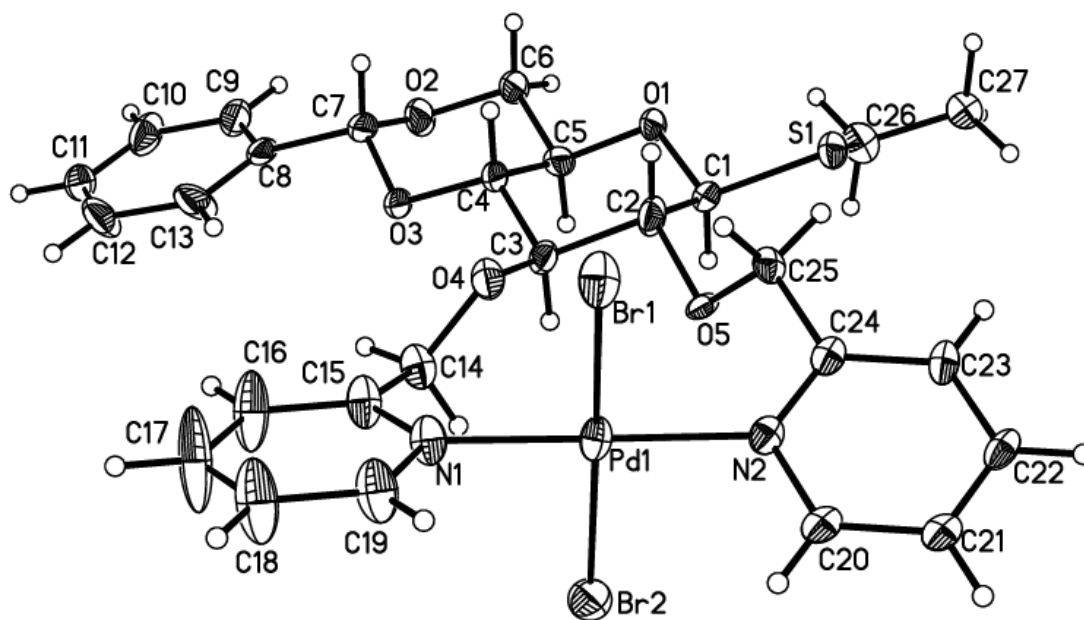
| D-H...A | d(D-H) | d(H...A) | d(D...A) | $\angle(\text{DHA})$ |
|-----------------------|--------|----------|-----------|----------------------|
| C(2)-H(2)...Br(2)#1 | 1.00 | 2.97 | 3.950(5) | 165.6 |
| C(6)-H(6B)...Br(1)#2 | 0.99 | 2.96 | 3.820(6) | 146.5 |
| C(14)-H(14A)...Br(2) | 0.99 | 2.99 | 3.711(5) | 131.0 |
| C(14)-H(14B)...O(3) | 0.99 | 2.56 | 3.180(6) | 120.7 |
| C(16)-H(16)...S(1)#3 | 0.95 | 2.96 | 3.604(4) | 126.1 |
| C(18)-H(18)...O(2)#4 | 0.95 | 2.63 | 3.452(5) | 144.8 |
| C(25)-H(25A)...Br(1) | 0.99 | 2.71 | 3.502(9) | 137.6 |
| C(25)-H(25B)...S(1) | 0.99 | 2.55 | 3.267(9) | 129.3 |
| C(25')-H(25C)...S(1) | 0.99 | 2.88 | 3.437(10) | 116.5 |
| C(25')-H(25D)...Br(2) | 0.99 | 2.88 | 3.673(10) | 137.8 |
| C(27)-H(27A)...O(3)#5 | 0.98 | 2.44 | 3.411(6) | 171.9 |

Symmetry transformations used to generate equivalent atoms:

#1 $x+1, y, z$ #2 $-x+2, y-1/2, -z+2$ #3 $x-1, y, z-1$

#4 $-x+1, y+1/2, -z+1$ #5 $x+1, y, z+1$

Projection view with 50% probability ellipsoids- disorder atoms omitted for clarity:



Projection view with 50% probability ellipsoids

