

Supplementary Information

Anverenes B-E, New polyhalogenated monoterpenes from the Antarctic red alga *Plocamium cartilagineum*

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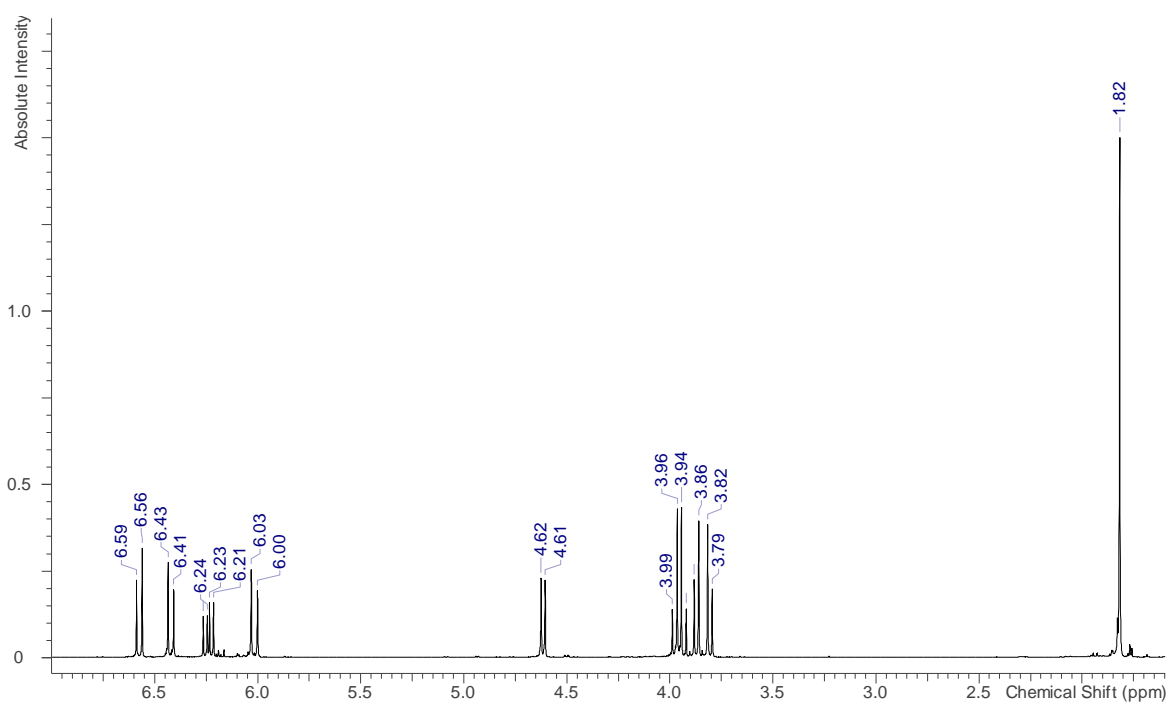
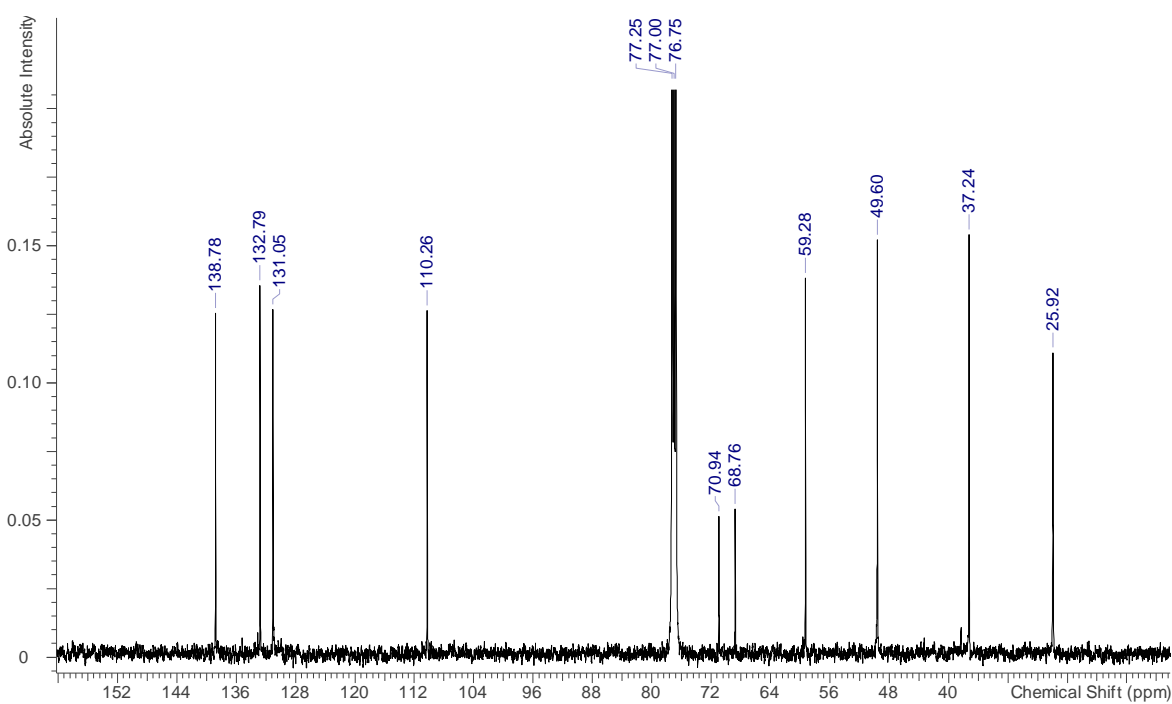
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Table S1: Reported and predicted ^{13}C NMR shifts of relevant compounds or theoretical alternate regio-isomers

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Figure S1: Anverene B ^1H NMR spectrum (500 MHz, CDCl_3).Figure S2: Anverene B ^{13}C NMR spectrum (125 MHz, CDCl_3).

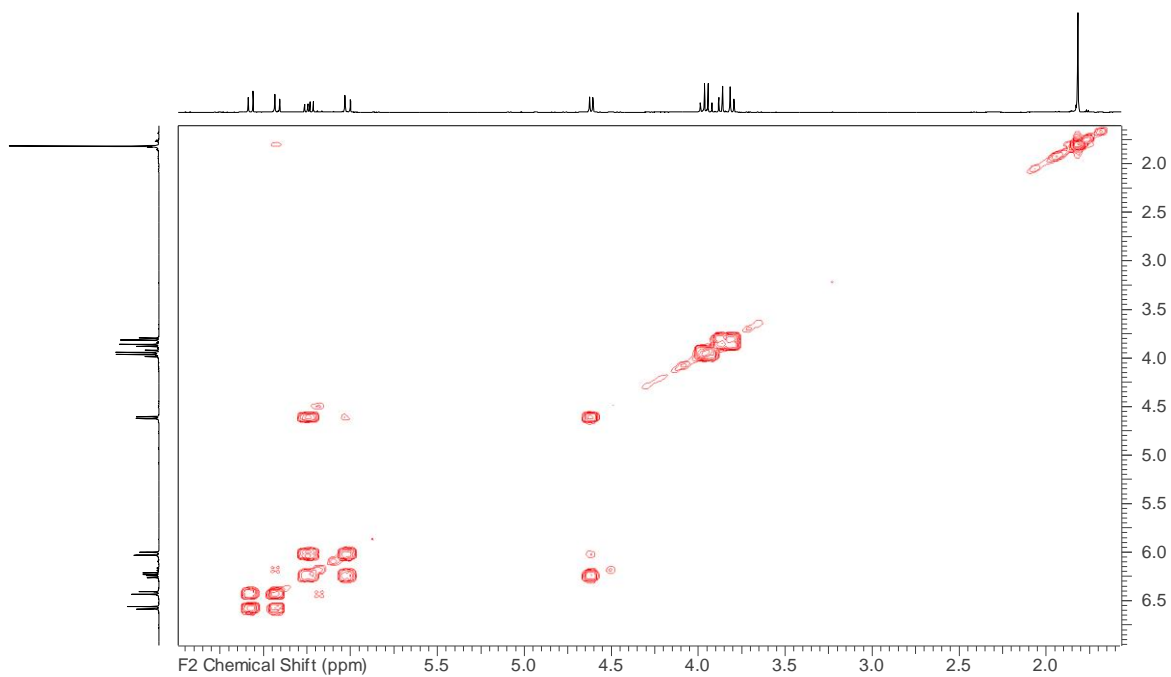


Figure S3: Anverene B COSY spectrum (500 MHz, CDCl₃).

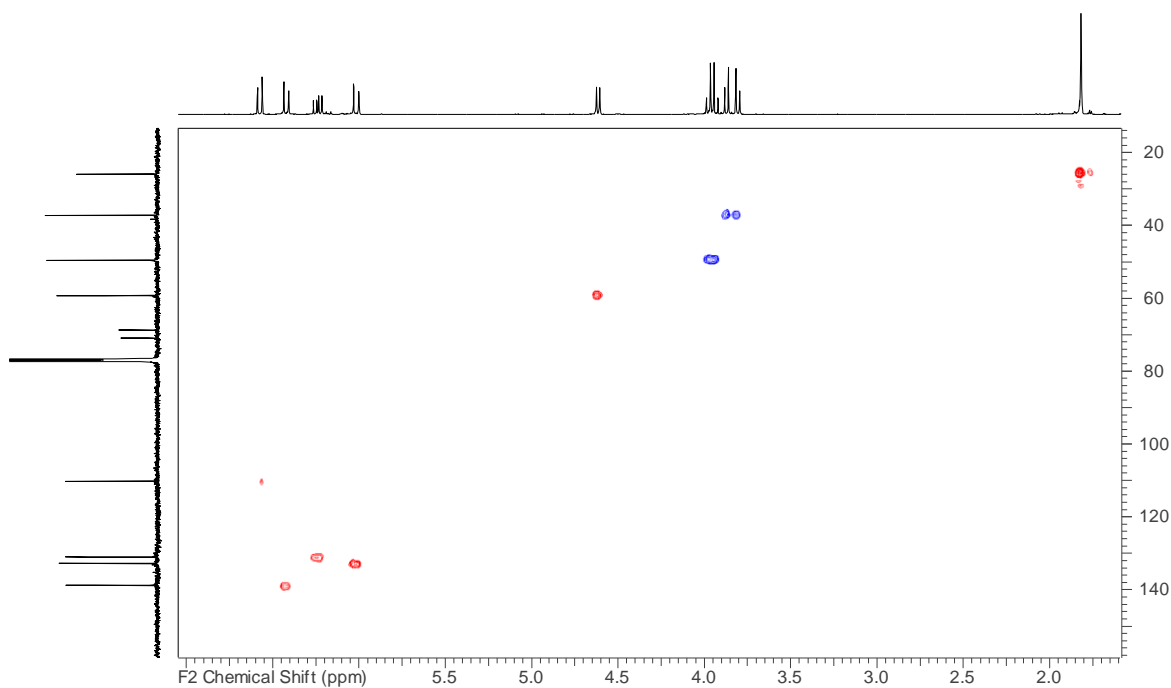


Figure S4: Anverene B HSQC spectrum (500 MHz, CDCl₃).

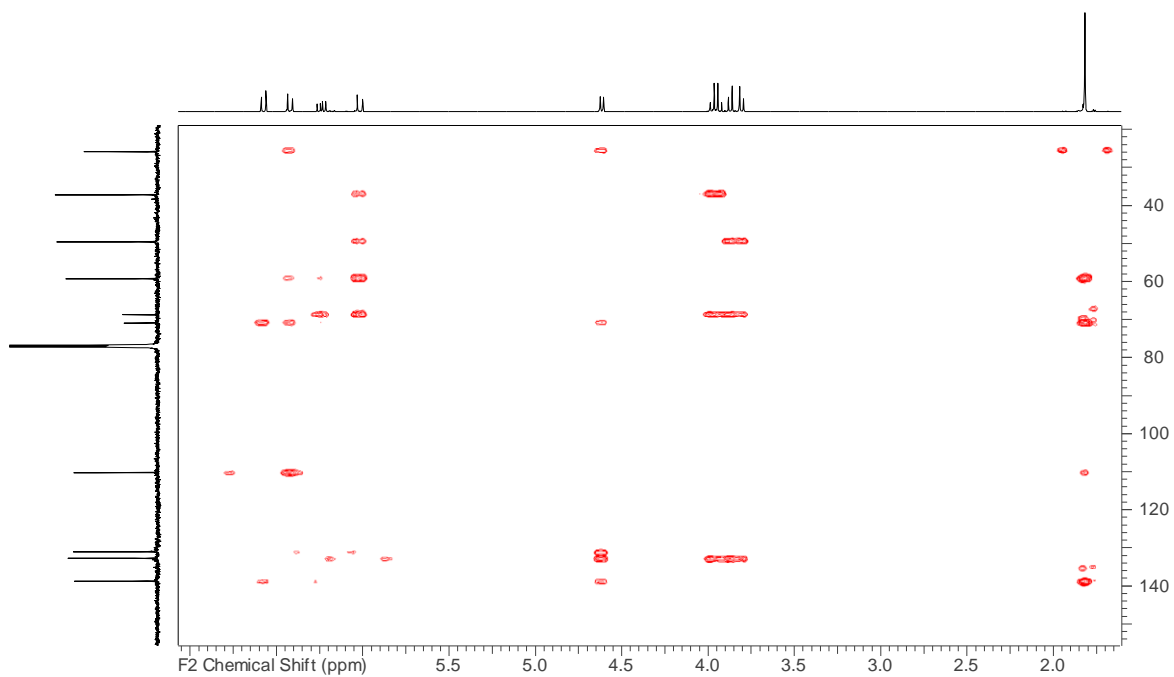
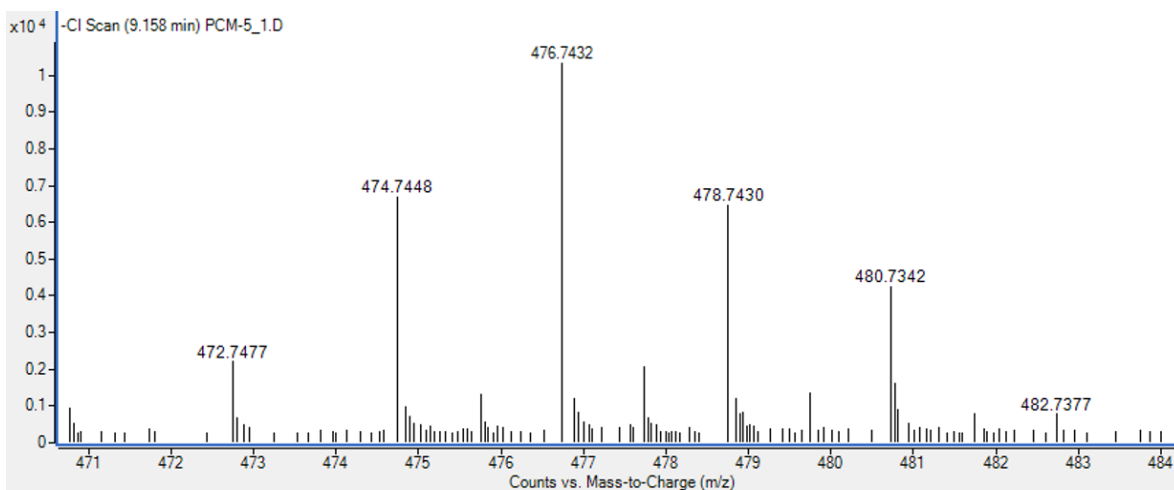
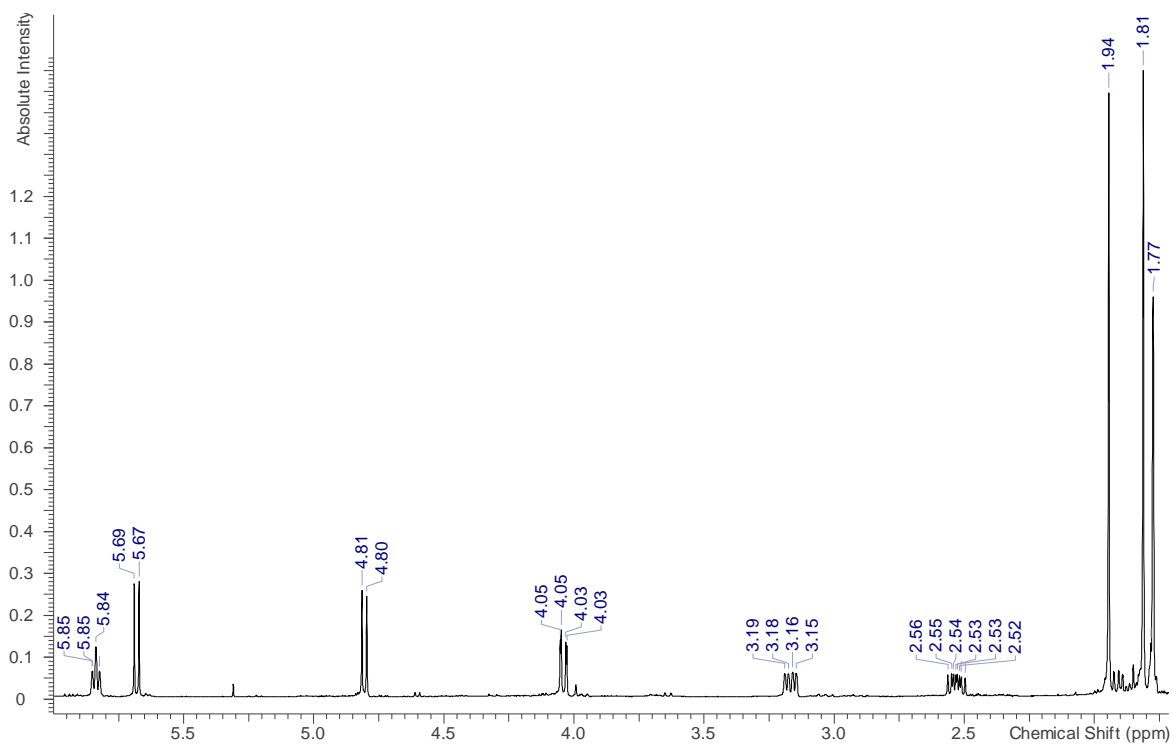
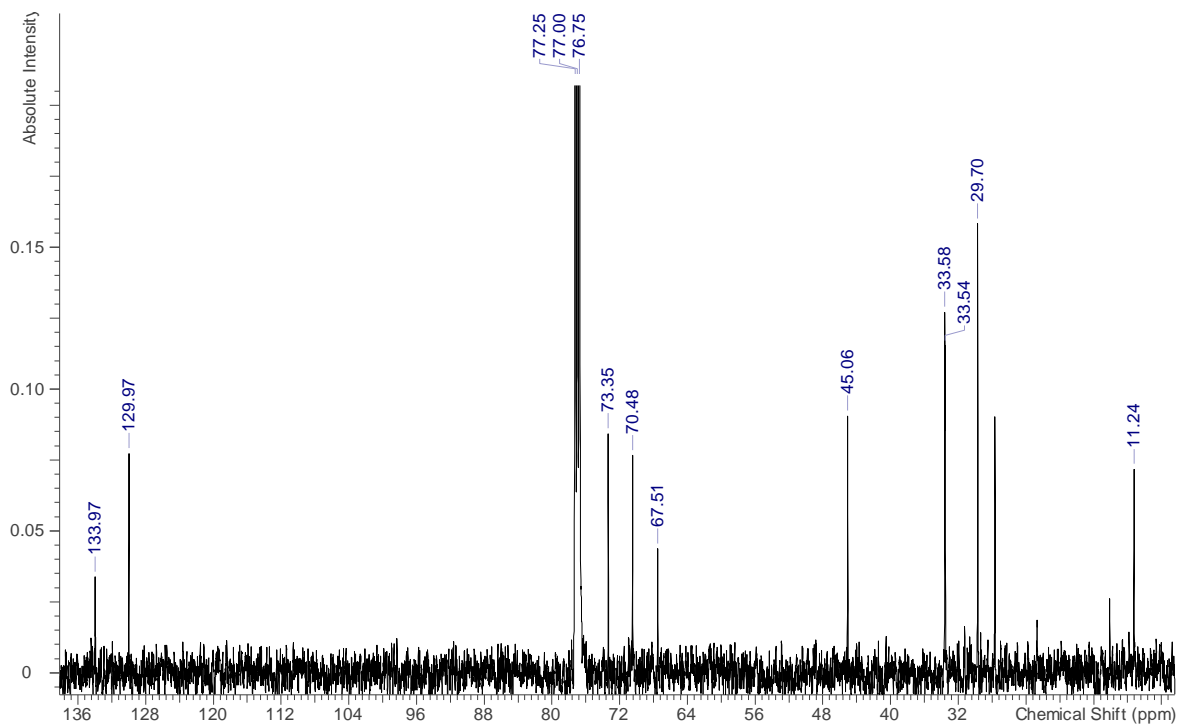


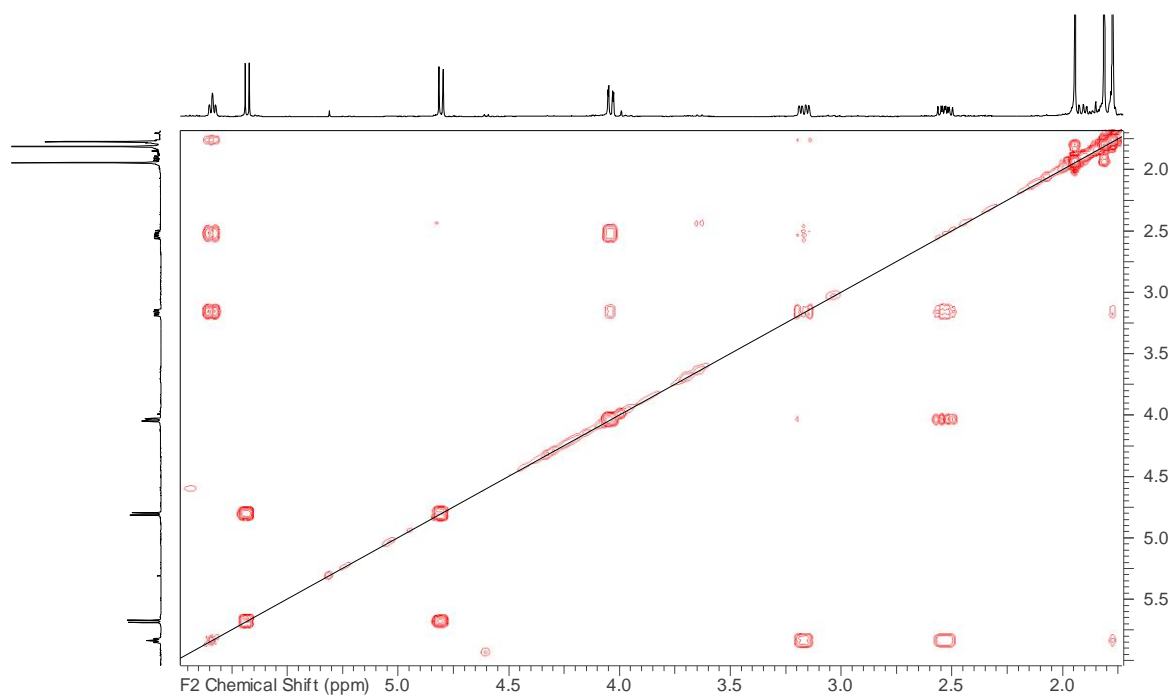
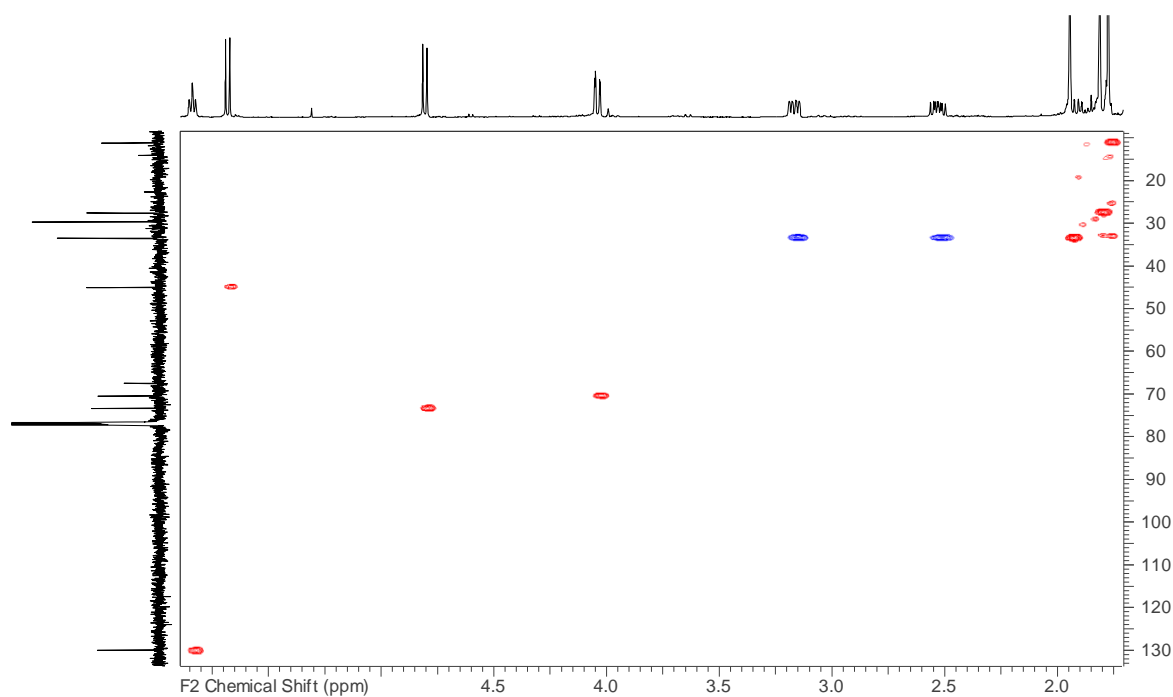
Figure S5: Anverene B HMBC spectrum (500 MHz, CDCl₃).



| Formula | Species | Abundance (counts) | Ion Mass | Measured Mass | Error (ppm) | Error (mDa) |
|---|--------------------|--------------------|----------|---------------|-------------|-------------|
| C ₁₀ H ₁₂ Br ₃ Cl ₃ | [M-H] ⁻ | 2231.10 | 472.7482 | 472.7477 | -1.058 | -0.5 |

Figure S6: Anverene B HRNCIMS (-).

Figure S7: Anverene C ¹H NMR spectrum (500 MHz, CDCl₃).Figure S8: Anverene C ¹³C NMR spectrum (125 MHz, CDCl₃).

Figure S9: Anverene C COSY spectrum (500 MHz, CDCl₃).Figure S10 Anverene C HSQC spectrum (500 MHz, CDCl₃).

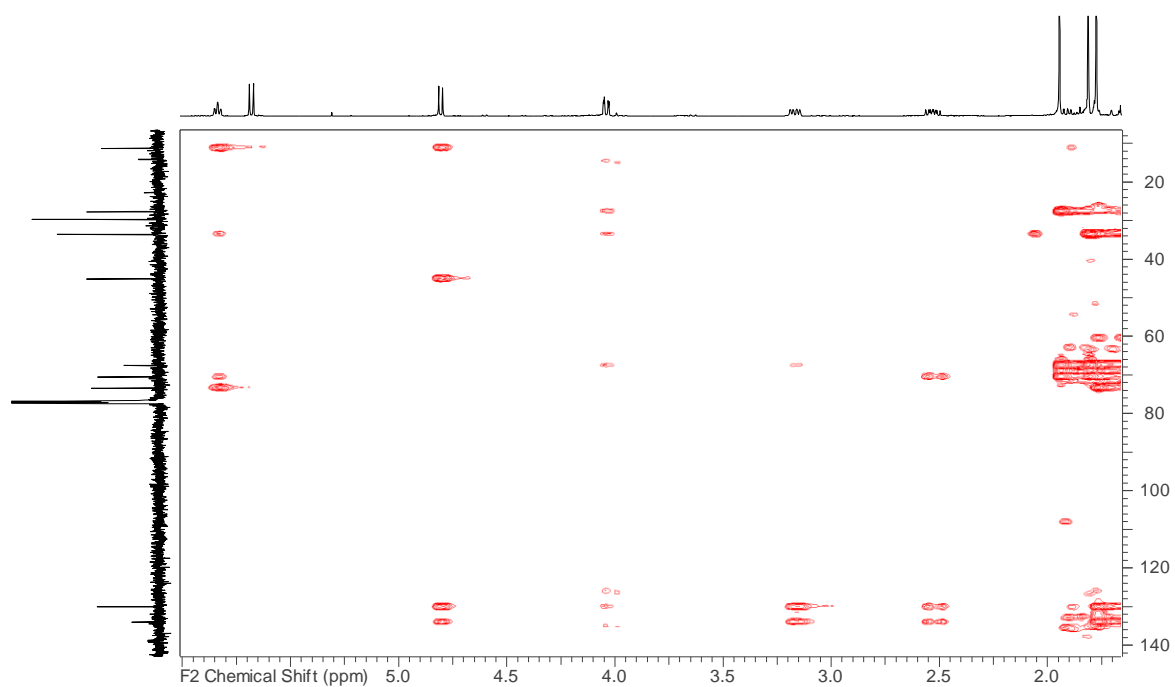


Figure S11: Anverene C HMBC spectrum (500 MHz, CDCl₃).

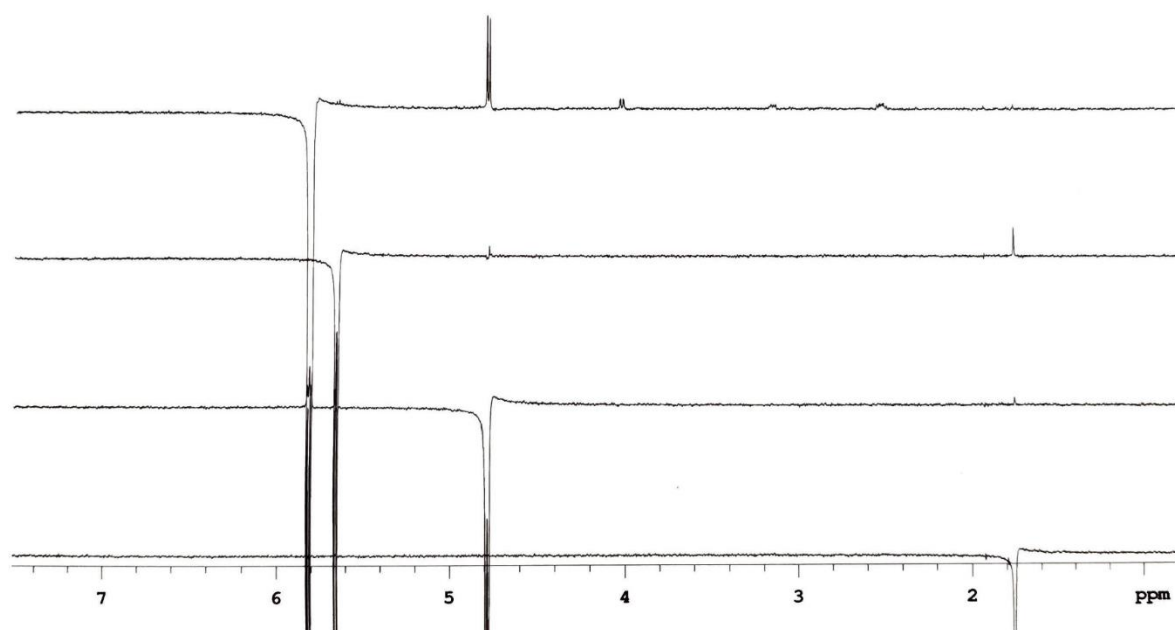
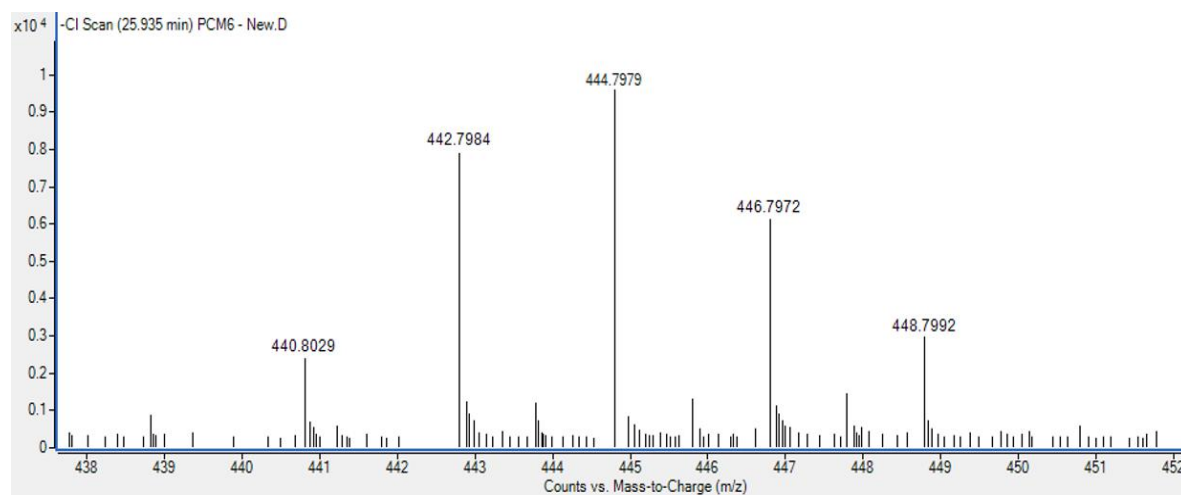
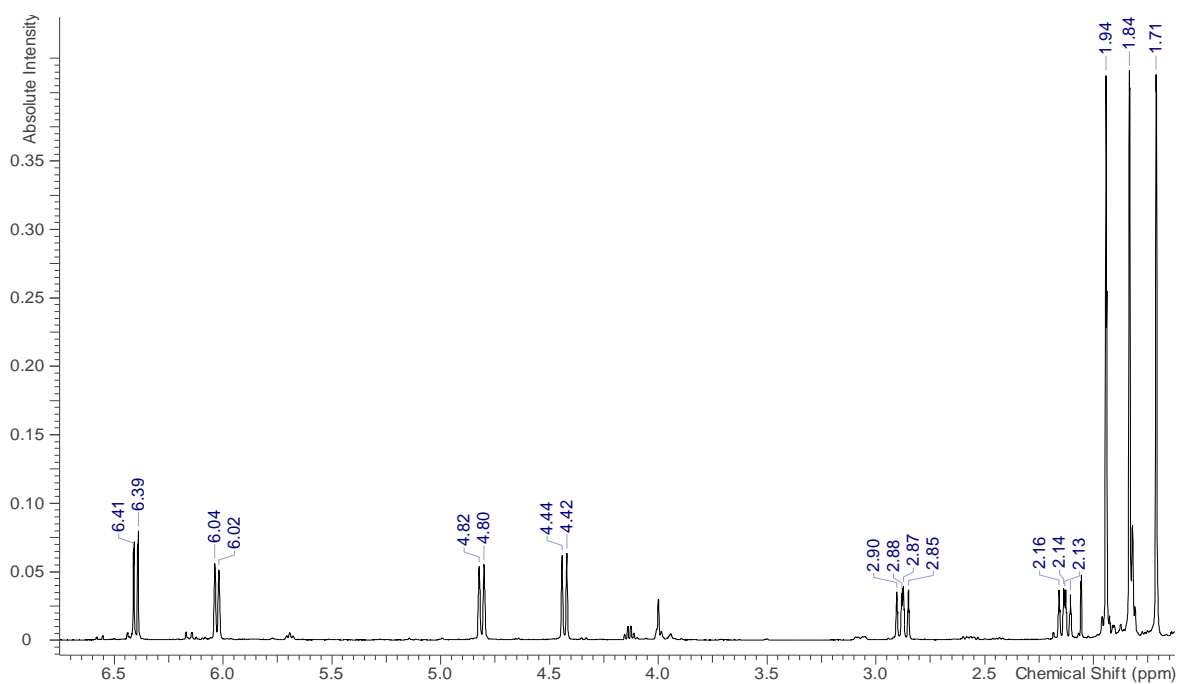


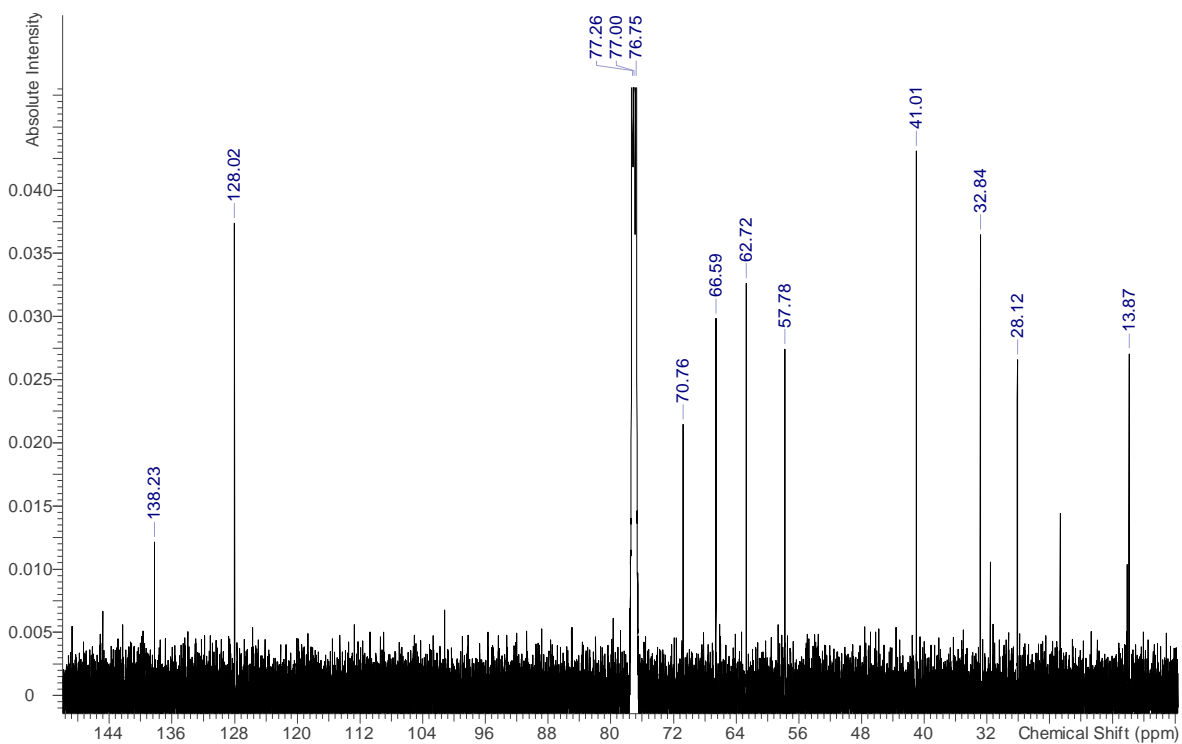
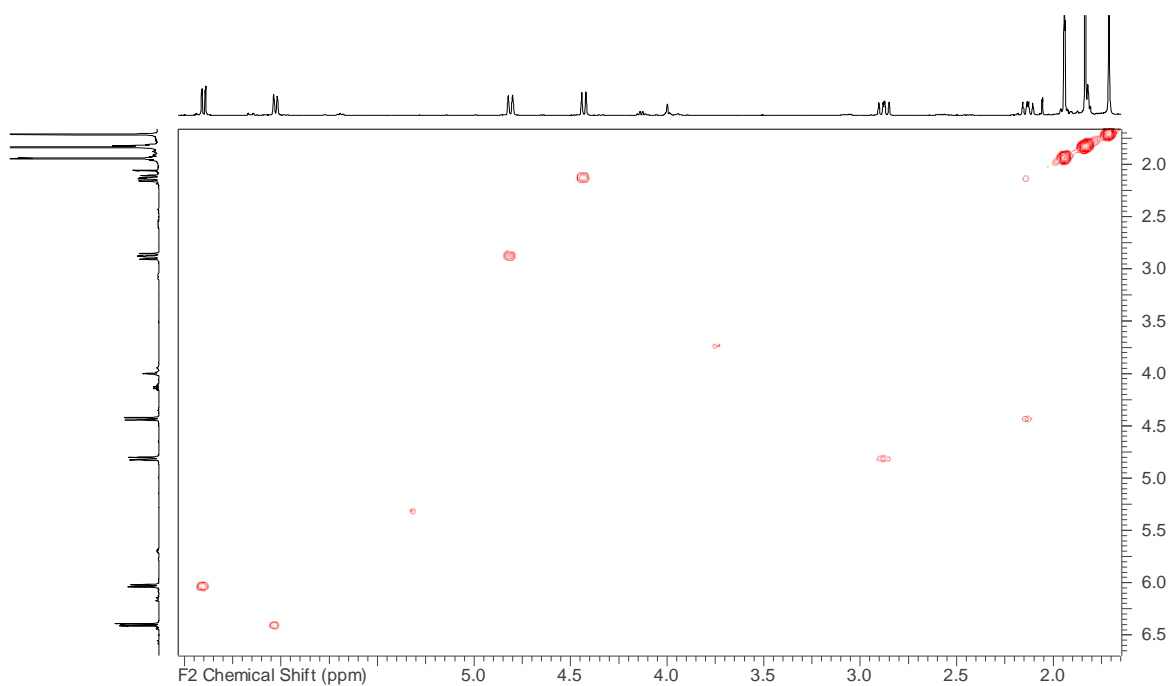
Figure S12: Anverene C 1D NOESY spectrum (600 MHz, CDCl₃).

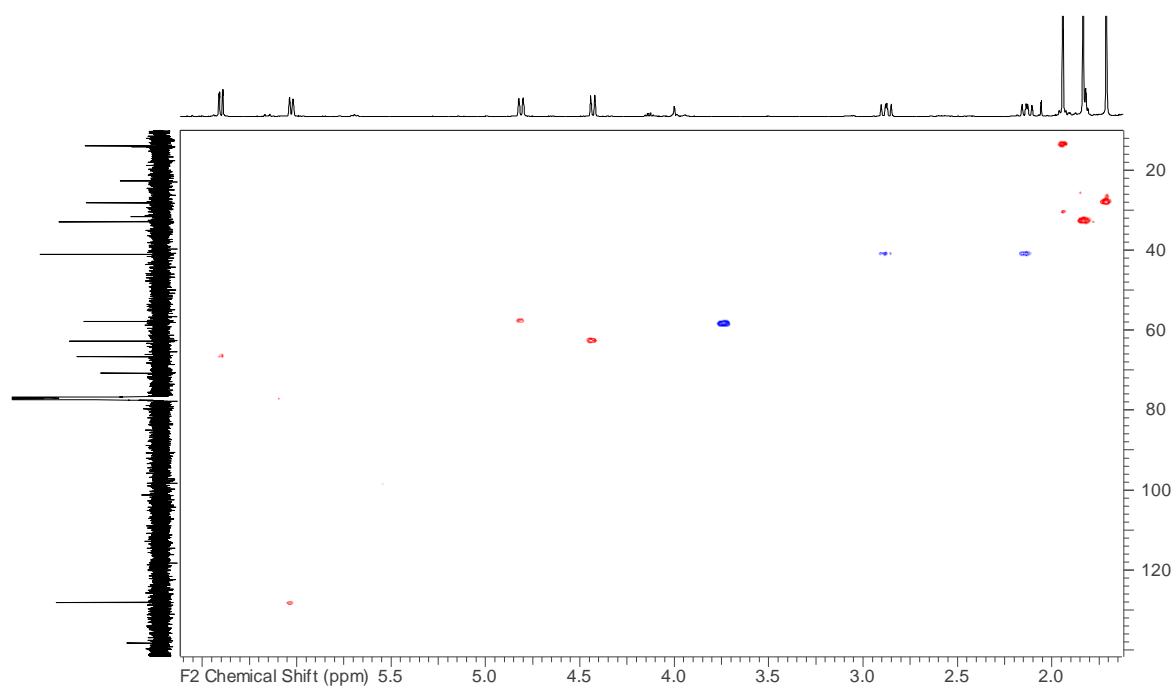
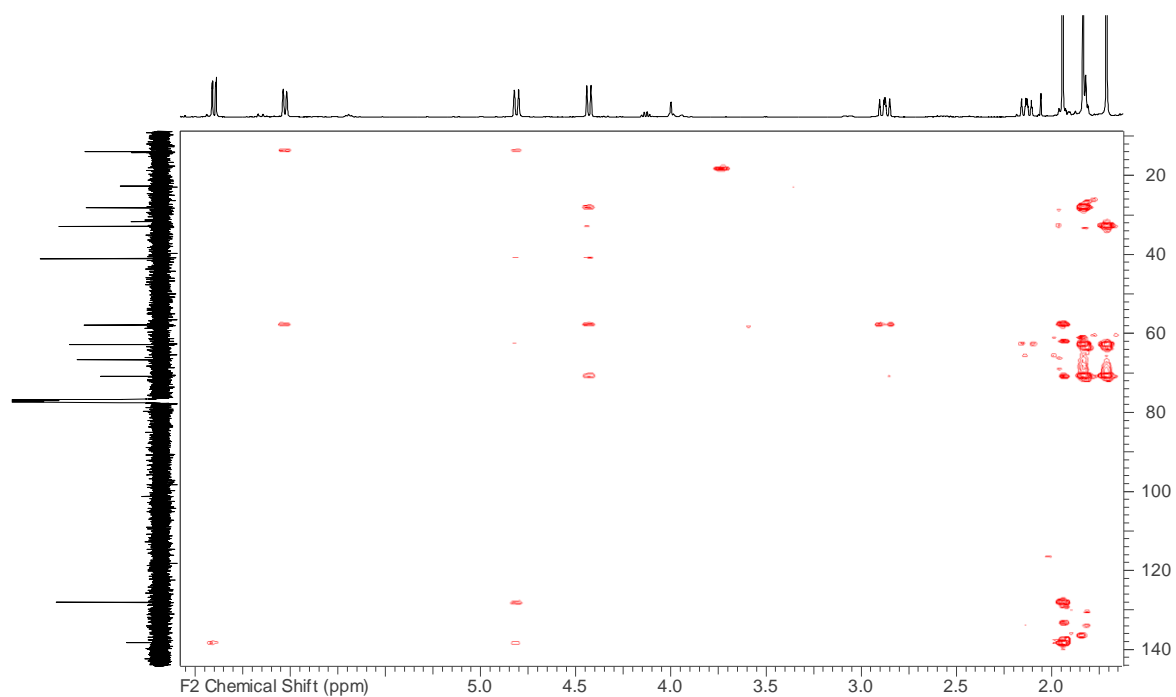


| Formula | Species | Abundance (counts) | Ion Mass | Measured Mass | Error (ppm) | Error (mDa) |
|---|--------------------|--------------------|----------|---------------|-------------|-------------|
| C ₁₀ H ₁₅ Br ₃ Cl ₂ | [M-H] ⁻ | 2403.53 | 440.8028 | 440.8029 | 0.227 | 0.1 |

Figure S13: Anverene C HRNCIMS (-).

Figure S14: Anverene D ¹H NMR spectrum (500 MHz, CDCl₃).

Figure S15: Anverene D ^{13}C NMR spectrum (125 MHz, CDCl_3).Figure S16: Anverene D COSY spectrum (500 MHz, CDCl_3).

Figure S17: Anverene D HSQC spectrum (500 MHz, CDCl₃).Figure S18: Anverene D HMBC spectrum (500 MHz, CDCl₃).

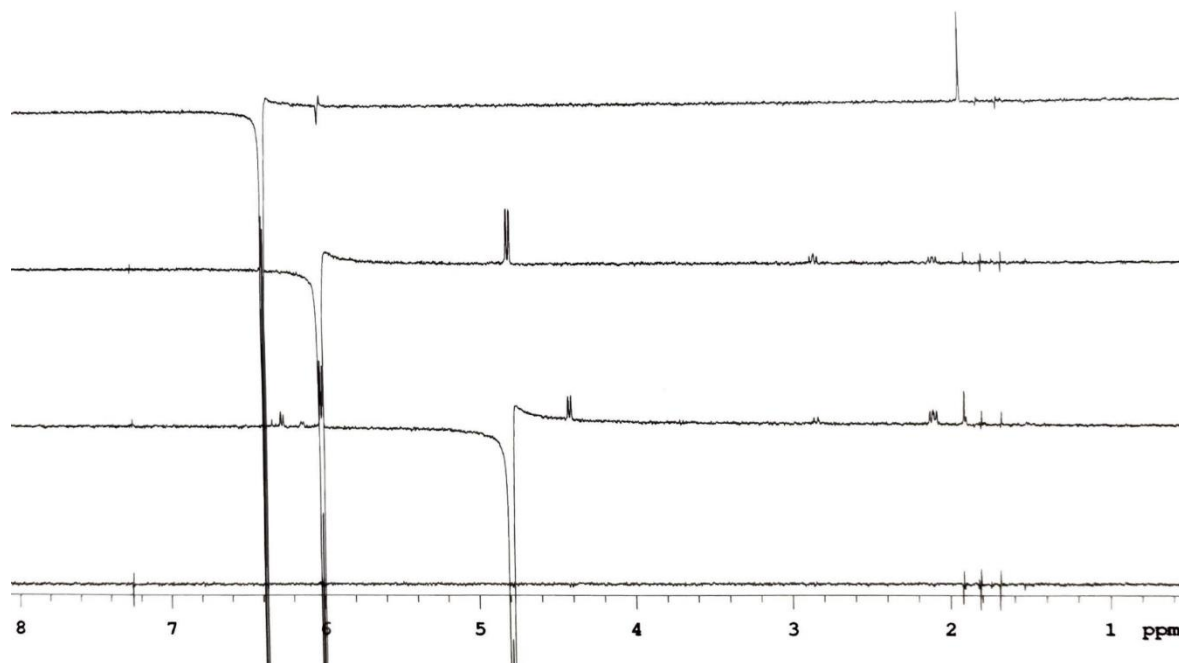
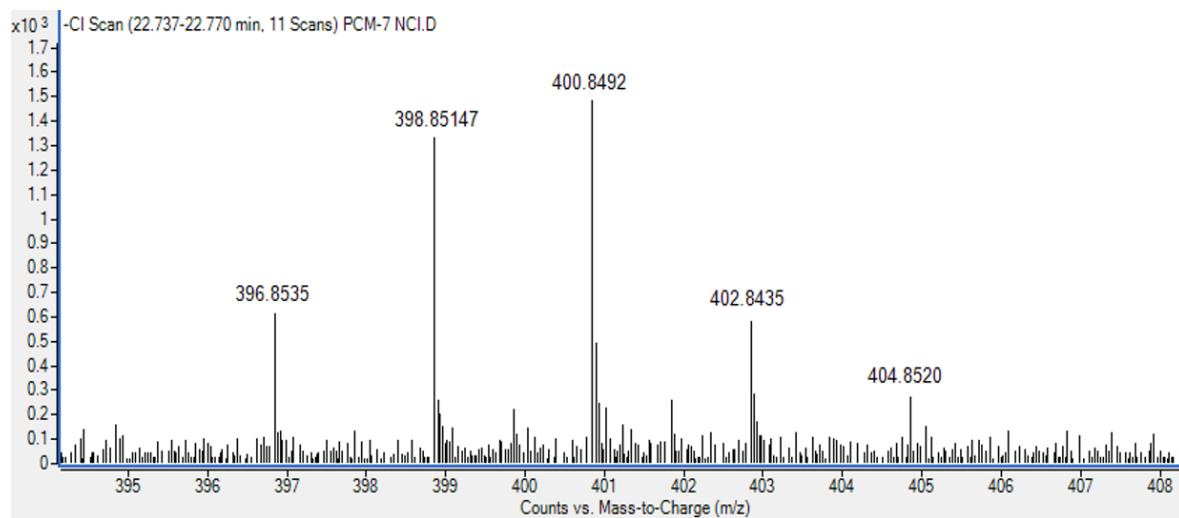
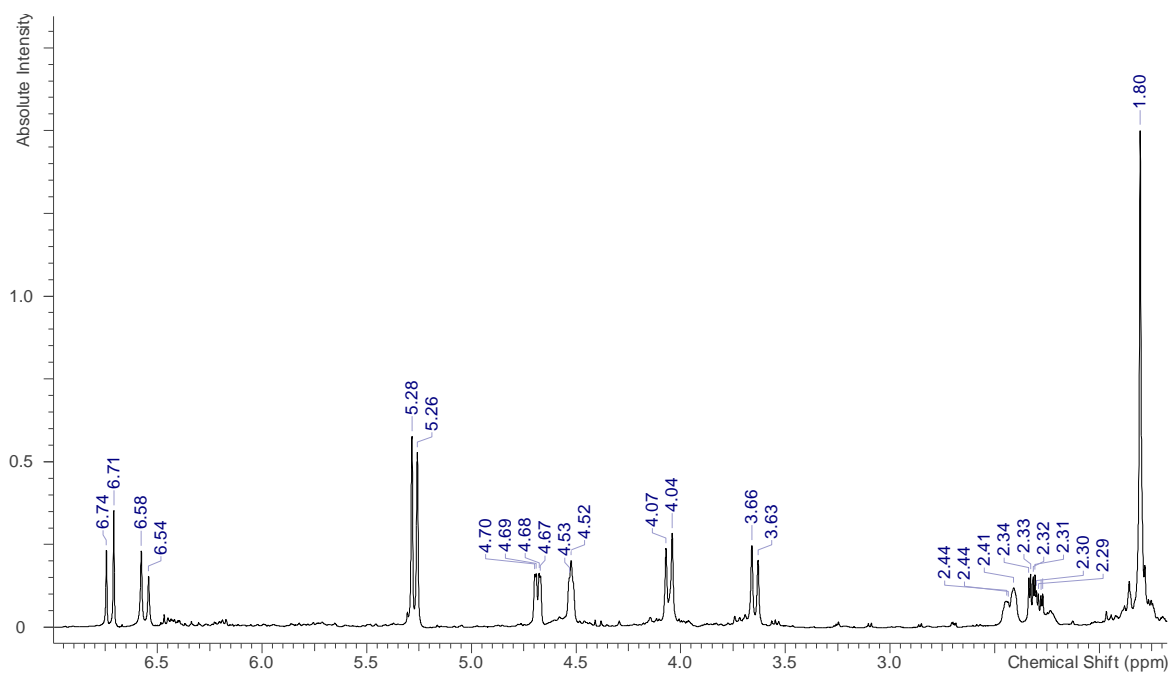
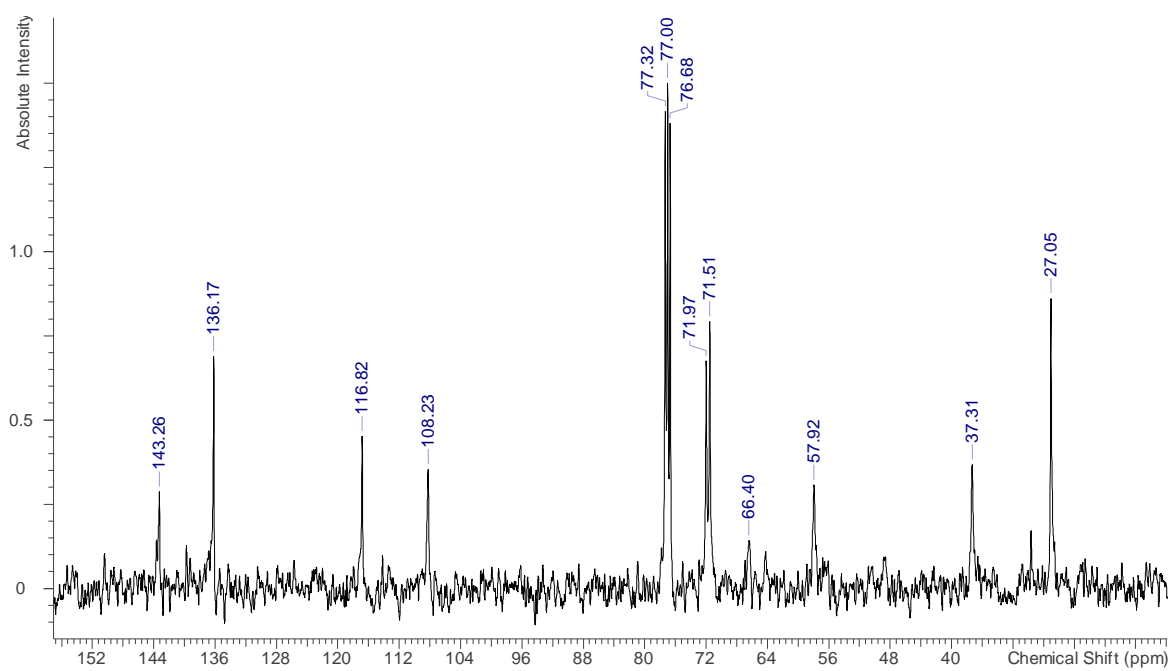


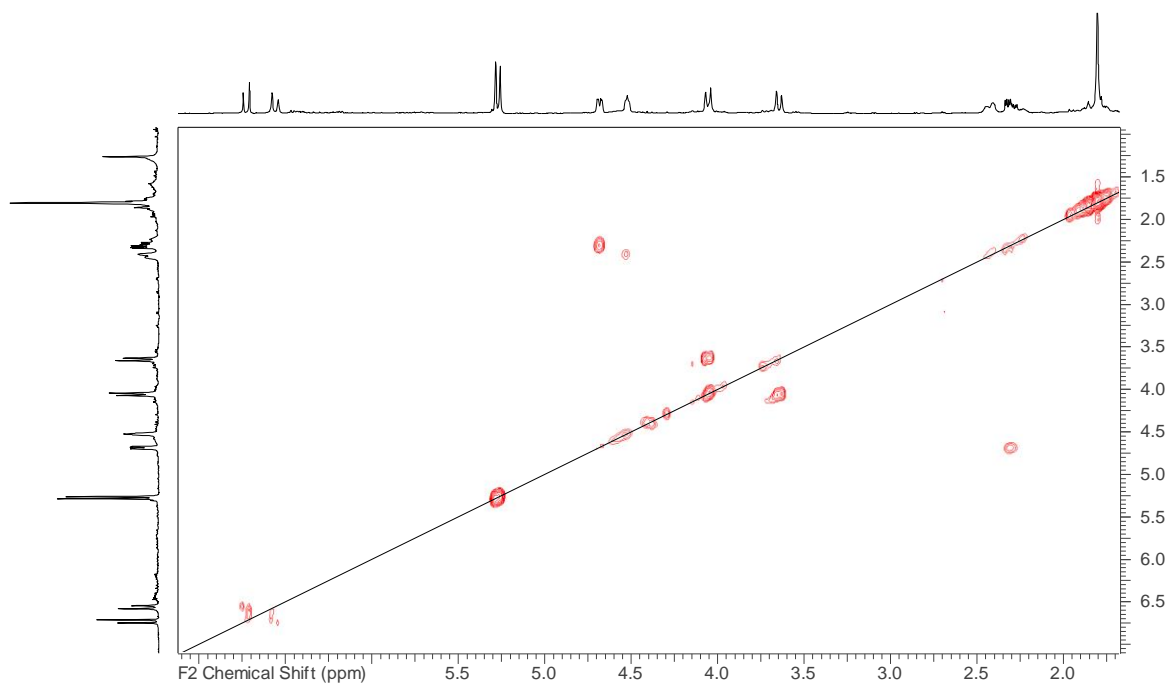
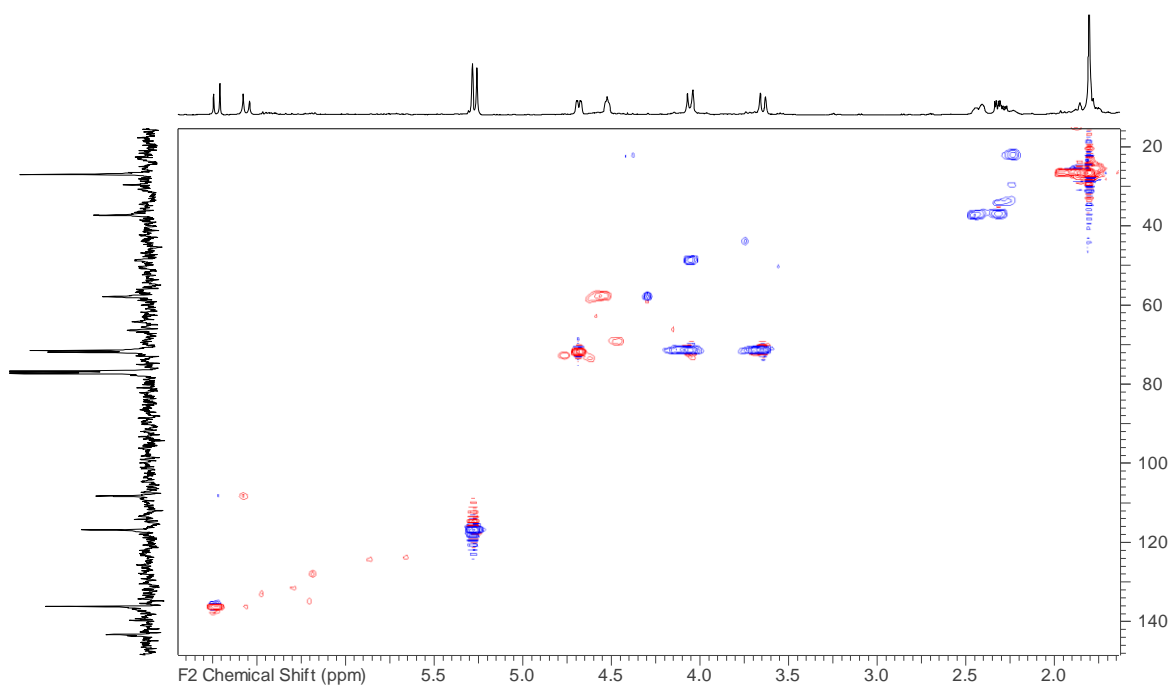
Figure S19: Anverene C 1D NOESY spectrum (600 MHz, CDCl₃).

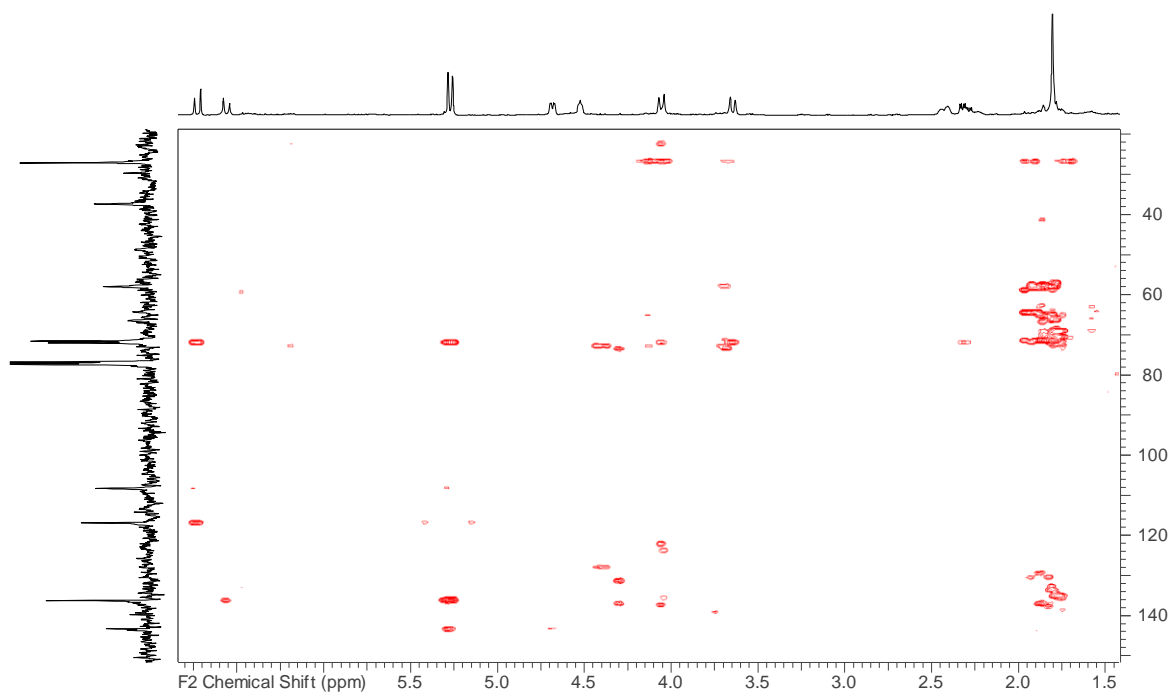
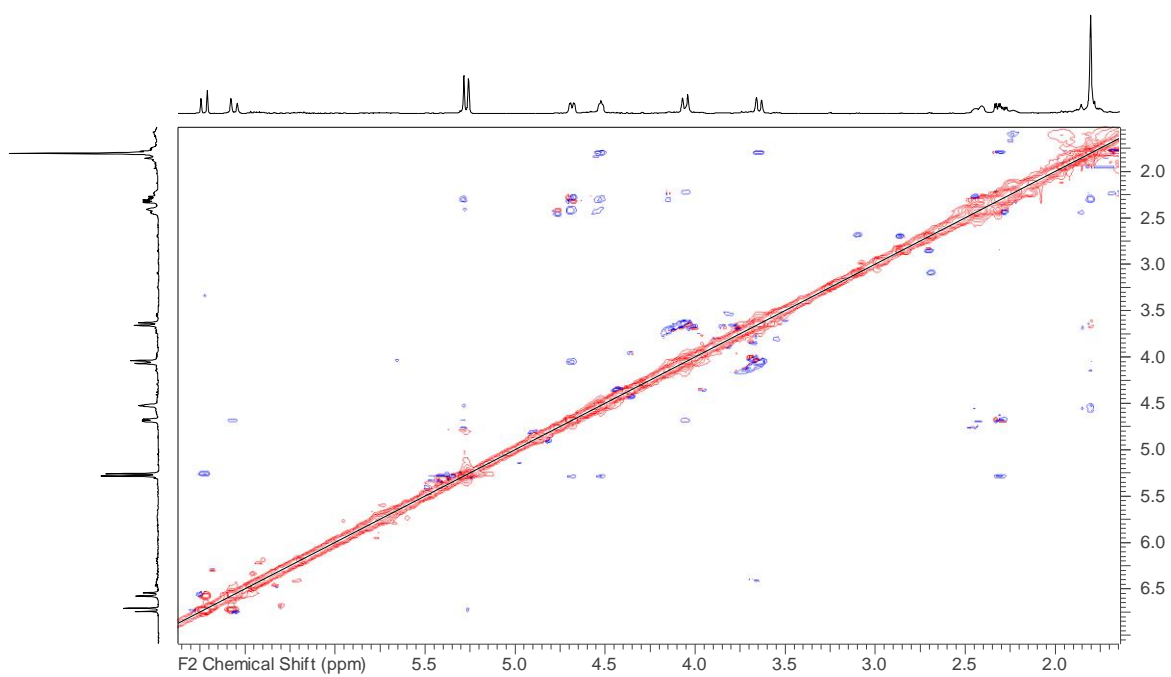


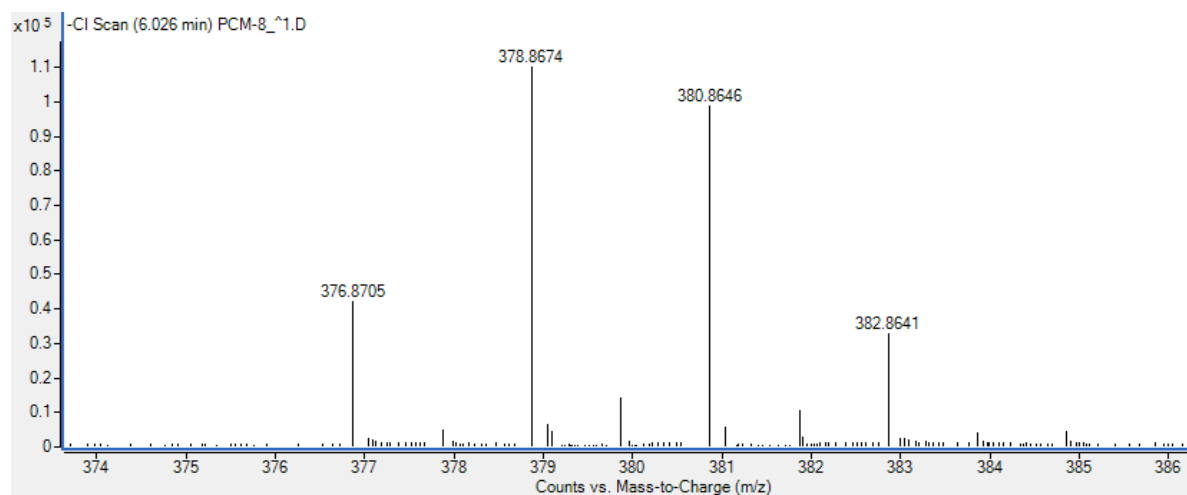
| Formula | Species | Abundance (counts) | Ion Mass | Measured Mass | Error (ppm) | Error (mDa) |
|---|--------------------|--------------------|----------|---------------|-------------|-------------|
| C ₁₀ H ₁₅ Br ₂ Cl ₃ | [M-H] ⁻ | 610.34 | 396.8533 | 396.8535 | 0.504 | 0.2 |

Figure S20: Anverene D HRNCIMS (-).

Figure S21: Anverene E ¹H NMR spectrum (500 MHz, CDCl₃).Figure S22: Anverene E ¹³C NMR spectrum (125 MHz, CDCl₃).

Figure S23: Anverene E COSY spectrum (500 MHz, CDCl₃).Figure S24: Anverene E HSQC spectrum (500 MHz, CDCl₃).

Figure S25: Anverene E HMBC spectrum (500 MHz, CDCl₃).Figure S26: Anverene E NOESY spectrum (500 MHz, CDCl₃).



| Formula | Species | Abundance (counts) | Ion Mass | Measured Mass | Error (ppm) | Error (mDa) |
|---|---------------------|--------------------|----------|---------------|-------------|-------------|
| C ₁₀ H ₁₃ BrCl ₂ O | [M+Br] ⁻ | 42070.74 | 376.8716 | 376.8705 | -2.918 | -1.1 |

Figure S27: Anverene E HRNCIMS (-).

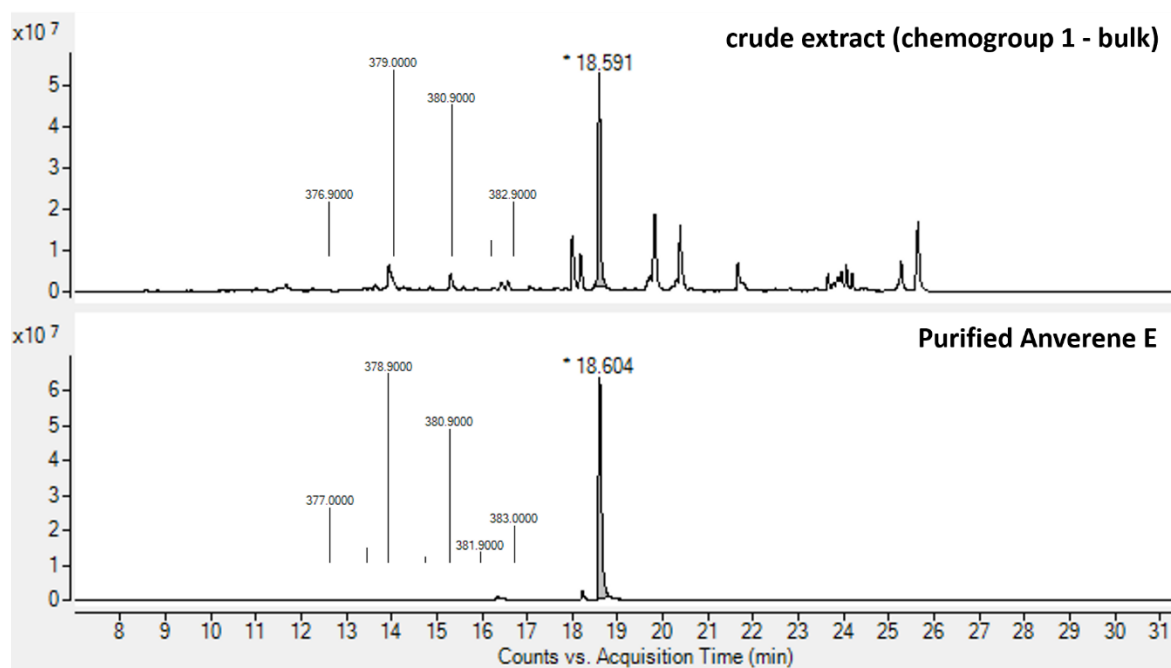
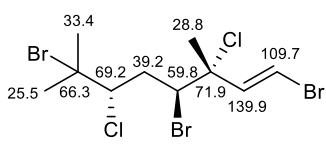
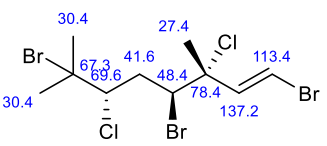
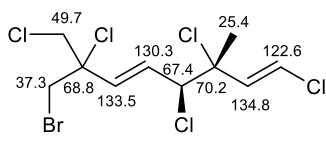
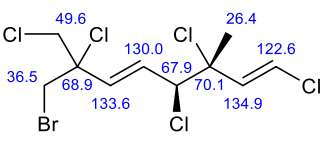
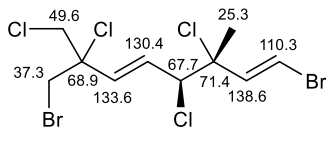
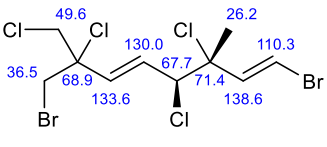
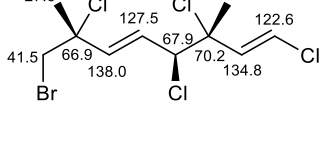
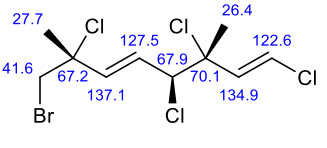
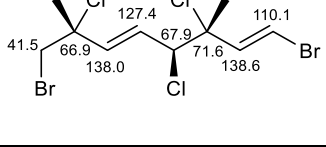
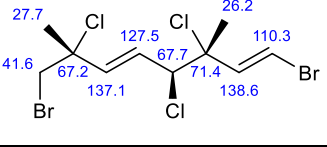
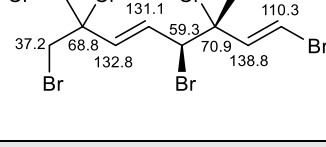
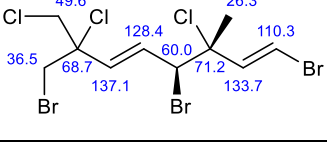
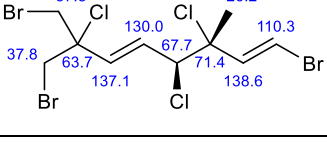
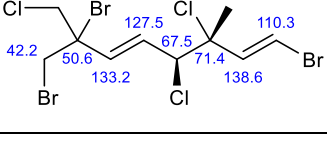
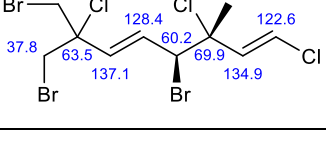


Figure S28: GC/MS identification of Anverene E in crude extract

Table S1: Reported and predicted ^{13}C NMR shifts of relevant compounds or possible regio-isomers

| Compound | Reported ^{13}C Shifts | ChemDraw Chem NMR ^{13}C Estimations |
|--|---|--|
| (1) Anverene |  |  |
| (2) |  |  |
| (3) Oregonene A |  |  |
| (4) |  |  |
| (5) |  |  |
| (6) Anverene B |  |  |
| Theoretical Regio-Isomer Of Anverene B | |  |
| Theoretical Regio-Isomer Of Anverene B | |  |
| Theoretical Regio-Isomer Of Anverene B | |  |

| | | |
|--|--|--|
| Theoretical Regio-Isomer Of Anverene B | | |
| Theoretical Regio-Isomer Of Anverene B | | |
| (7) Anverene C | | |
| (10) | | |
| Theoretical Regio-Isomer Of Anverene C | | |
| Theoretical Regio-Isomer Of Anverene C | | |
| Theoretical Regio-Isomer Of Anverene C | | |
| Theoretical Regio-Isomer Of Anverene C | | |
| Theoretical Regio-Isomer Of Anverene C | | |
| (8) Anverene D | | |

| | | |
|--|--|--|
| (11) Plocoralide B | | |
| Theoretical Regio-Isomer Of Anverene D | | |
| Theoretical Regio-Isomer Of Anverene D | | |
| Theoretical Regio-Isomer Of Anverene D | | |
| Theoretical Regio-Isomer Of Anverene D | | |
| Theoretical Regio-Isomer Of Anverene D | | |
| (9) Anverene E | | |
| Theoretical Regio-Isomer Of Anverene E | | |
| Theoretical Regio-Isomer Of Anverene E | | |