

Supplementary Material

High temperature bromination Part XXIII: Bromination of octahydro-1*H*-indene and octahydro-1*H*-4,7-methanoindene

Melek Sermin Ozer^a, Benan Kilbas^{a,b}, Metin Balci*^a

^a Department of Chemistry, Middle East Technical University, 06531 Ankara, Turkey

^b Department of Chemistry, Faculty of Sciences, Duzce University, 81620 Duzce,
Turkey

E-mail: mbalci@metu.edu.tr

Table of Contents

| | |
|--|-----|
| 1. ¹ H-NMR Spectrum of compound 12 | S3 |
| 2. ¹³ C-NMR Spectrum of compound 12 | S4 |
| 3. DEPT-135 Spectrum of compound 12 | S4 |
| 4. COSY Spectrum of compound 12 | S5 |
| 5. HSQC Spectrum of compound 12 | S6 |
| 6. HMBC Spectrum of compound 12 | S6 |
| 7. ¹ H-NMR Spectrum of compound 13 | S7 |
| 8. ¹³ C-NMR Spectrum of compound 13 | S7 |
| 9. ¹ H-NMR Spectrum of compound 14 | S8 |
| 10. ¹³ C-NMR Spectrum of compound 14 SError! Bookmark not defined. | S9 |
| 11. DEPT-135 Spectrum of compound 14 | S9 |
| 12. HSQC Spectrum of compound 14 SError! Bookmark not defined. | S10 |
| 13. COSY Spectrum of compound 14 | S10 |
| 14. HMBC Spectrum of compound 14 | S10 |
| 15. ¹ H-NMR Spectrum of compound 15 | S11 |
| 16. ¹³ C-NMR Spectrum of compound 15 | S11 |
| 17. DEPT-135 Spectrum of compound 15 | S12 |
| 18. HSQC Spectrum of compound 15 | S12 |
| 19. COSY Spectrum of compound 15 | S13 |
| 20. HMBC Spectrum of compound 15 | S13 |
| 21. ¹ H-NMR Spectrum of compound 16 | S14 |
| 22. ¹³ C-NMR Spectrum of compound 16 | S14 |
| 23. DEPT-135 Spectrum of compound 16 | S14 |
| 24. HSQC Spectrum of compound 16 | S15 |
| 25. COSY Spectrum of compound 16 | S15 |
| 26. HMBC Spectrum of compound 16 | S16 |

| | |
|---|-----|
| 27. ^1H -NMR Spectrum of compound 23 | S16 |
| 28. ^{13}C -NMR Spectrum of compound 23 | S17 |
| 29. DEPT-135 Spectrum of compound 23 | S17 |
| 30. HSQC Spectrum of compound 23 | S18 |
| 31. COSY Spectrum of compound 23 | S18 |
| 32. HMQC Spectrum of compound 23 | S19 |
| 33. ^1H -NMR Spectrum of compound 25 | S19 |
| 34. ^{13}C -NMR Spectrum of compound 25 | S20 |
| 35. DEPT-135 Spectrum of compound 25 | S20 |
| 36. COSY Spectrum of compound 25 | S21 |
| 37. HSQC Spectrum of compound 25 | S21 |
| 38. HMBC Spectrum of compound 25 | S22 |
| 39. ^1H -NMR Spectrum of compound 24 | S22 |
| 40. ^{13}C -NMR Spectrum of compound 24 | S23 |
| 41. DEPT-135 Spectrum of compound 24 | S23 |
| 42. HSQC Spectrum of compound 24 | S24 |
| 43. COSY Spectrum of compound 24 | S24 |
| 44. HMBC Spectrum of compound 24 | S25 |
| 45. ^1H -NMR Spectrum of compound 38 | S25 |
| 46. ^{13}C -NMR Spectrum of compound 38 | S26 |
| 47. DEPT-135 Spectrum of compound 38 | S26 |
| 48. HSQC Spectrum of compound 38 | S27 |
| 49. COSY Spectrum of compound 38 | S27 |
| 50. HMBC Spectrum of compound 38 | S28 |
| Atom coordinates for 12 | S28 |
| Atom coordinates for 13 | S29 |
| Atom coordinates for 14 | S30 |
| Atom coordinates for 12 | S31 |
| Atom coordinates for 18 | S32 |
| Atom coordinates for 19 | S33 |
| Atom coordinates for 17 | S34 |
| Atom coordinates for 29 | S35 |
| Atom coordinates for 30 | S36 |

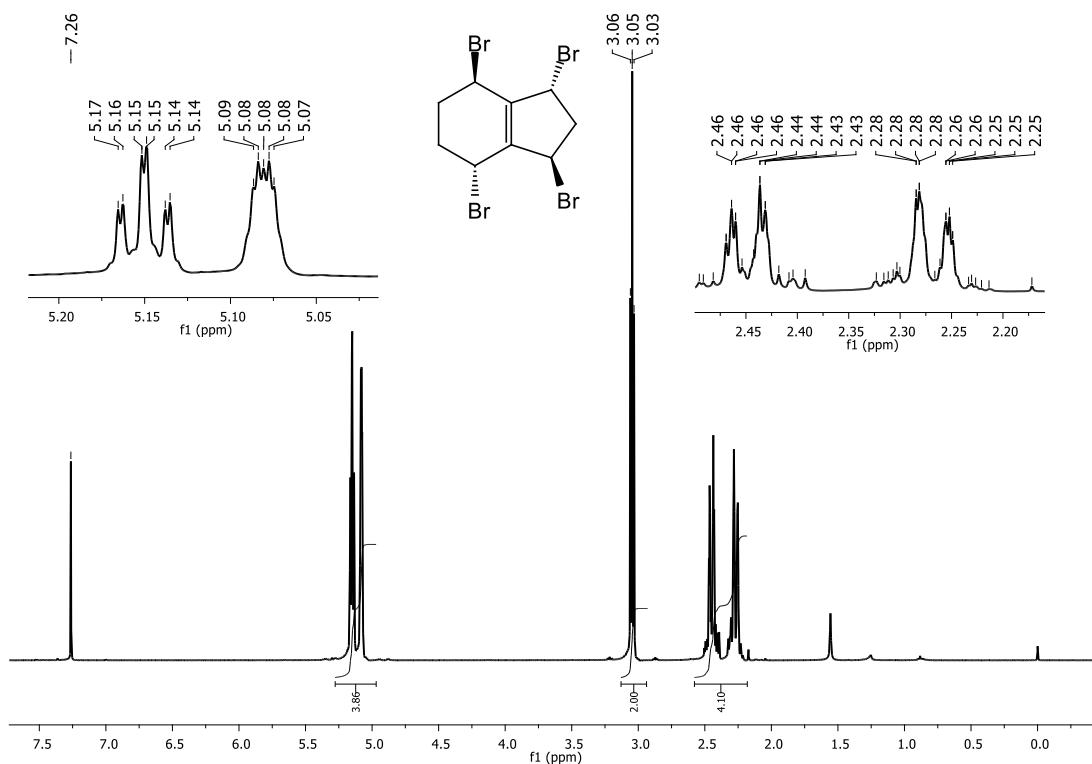


Figure S1. ¹H-NMR Spectrum of compound 12.

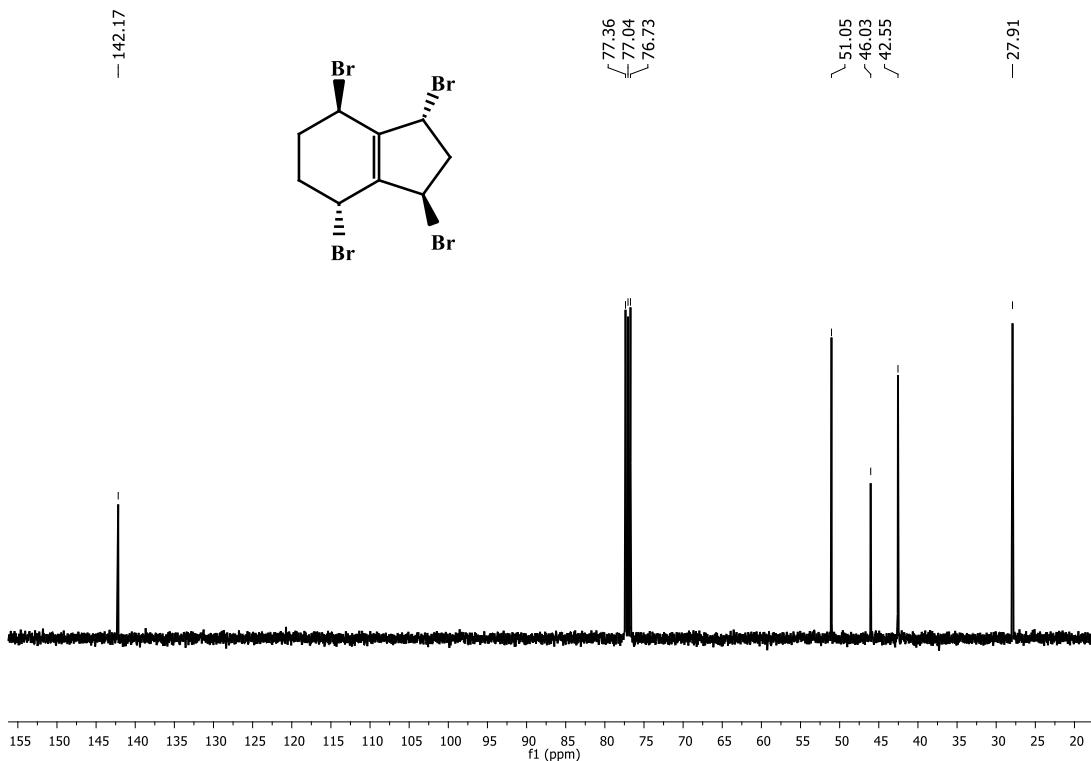


Figure S2. ^{13}C -NMR Spectrum of compound 12.

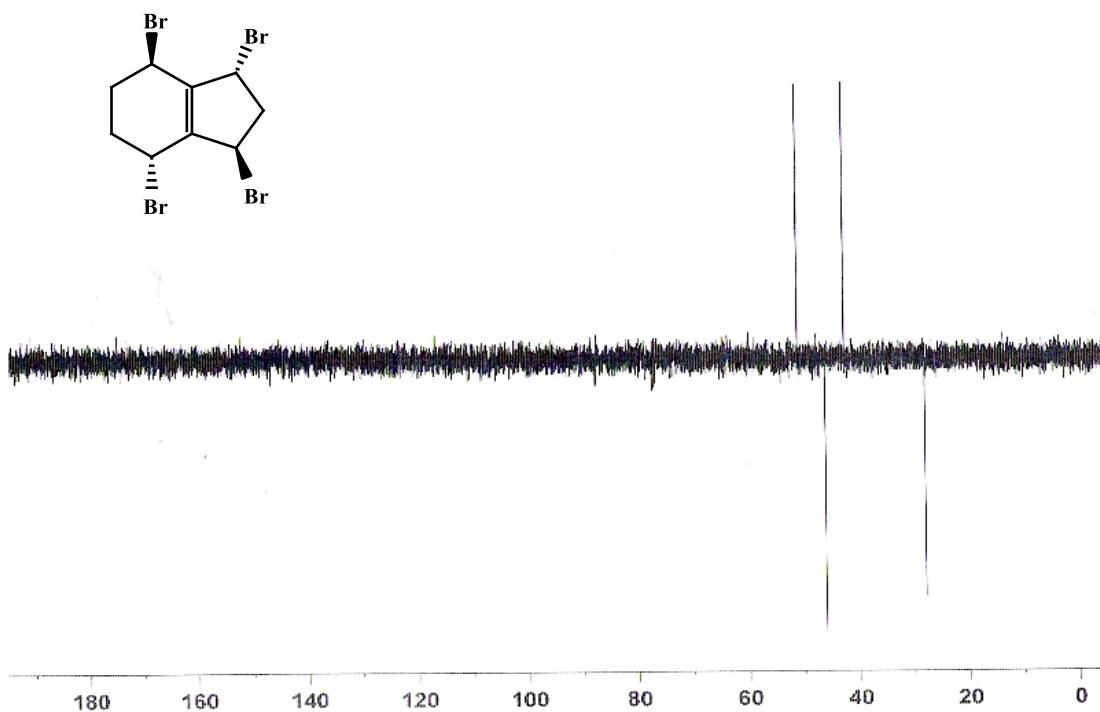


Figure S3. DEPT-135 Spectrum of compound 12.

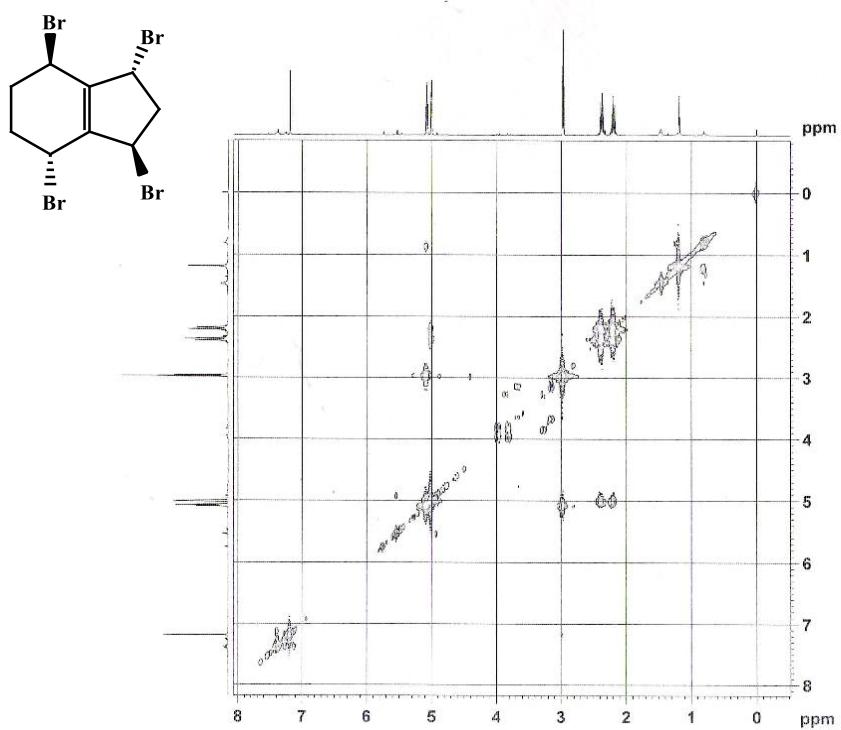


Figure S4. COSY Spectrum of compound 12.

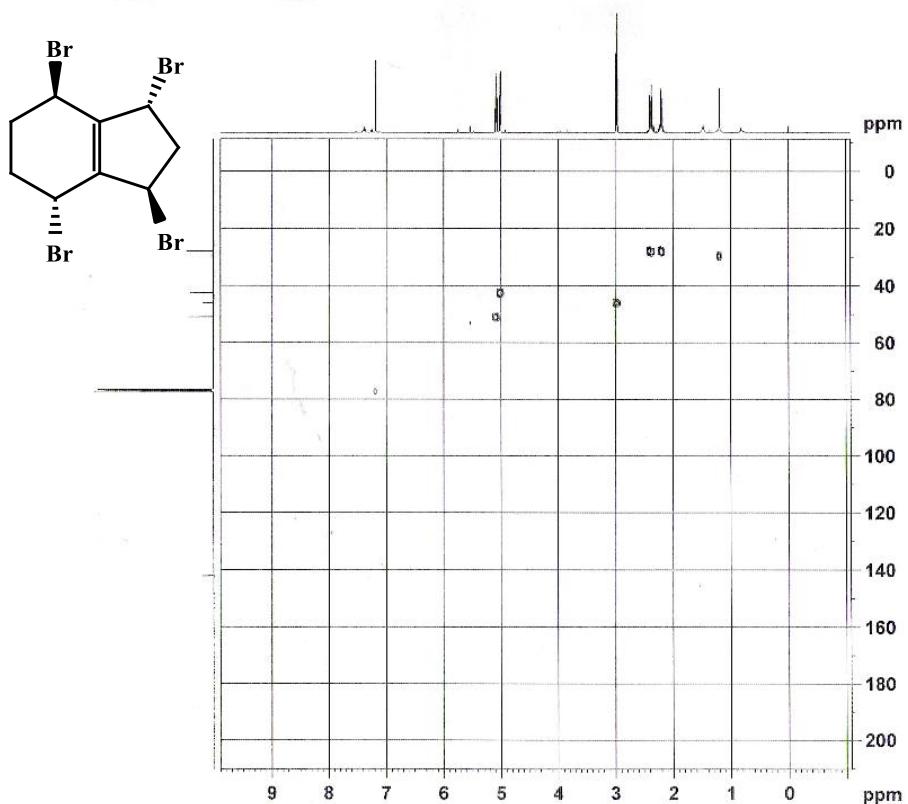


Figure S5. HSQC Spectrum of compound 12.

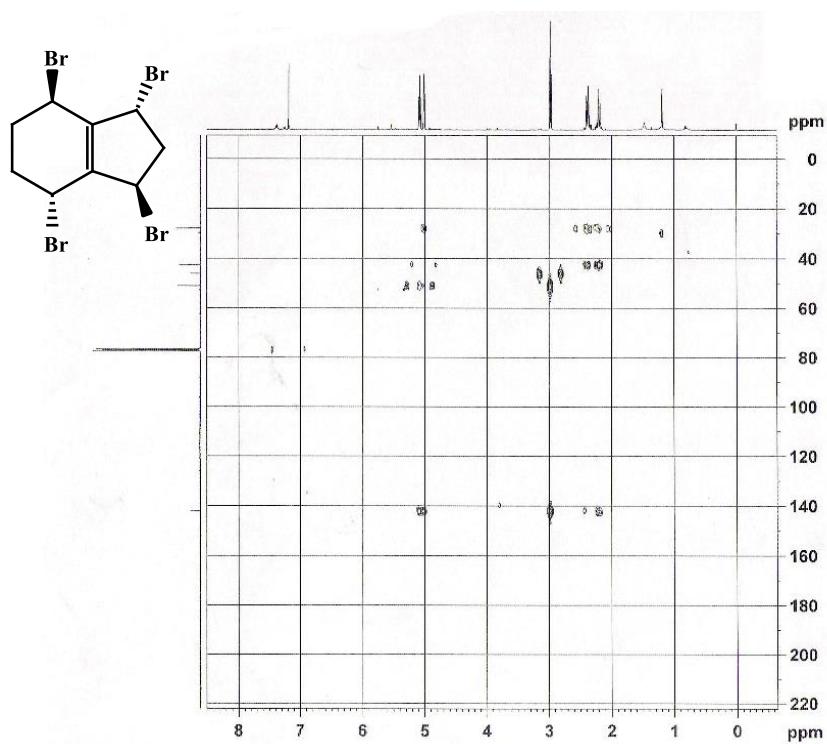


Figure S6. HMBC Spectrum of compound 12.

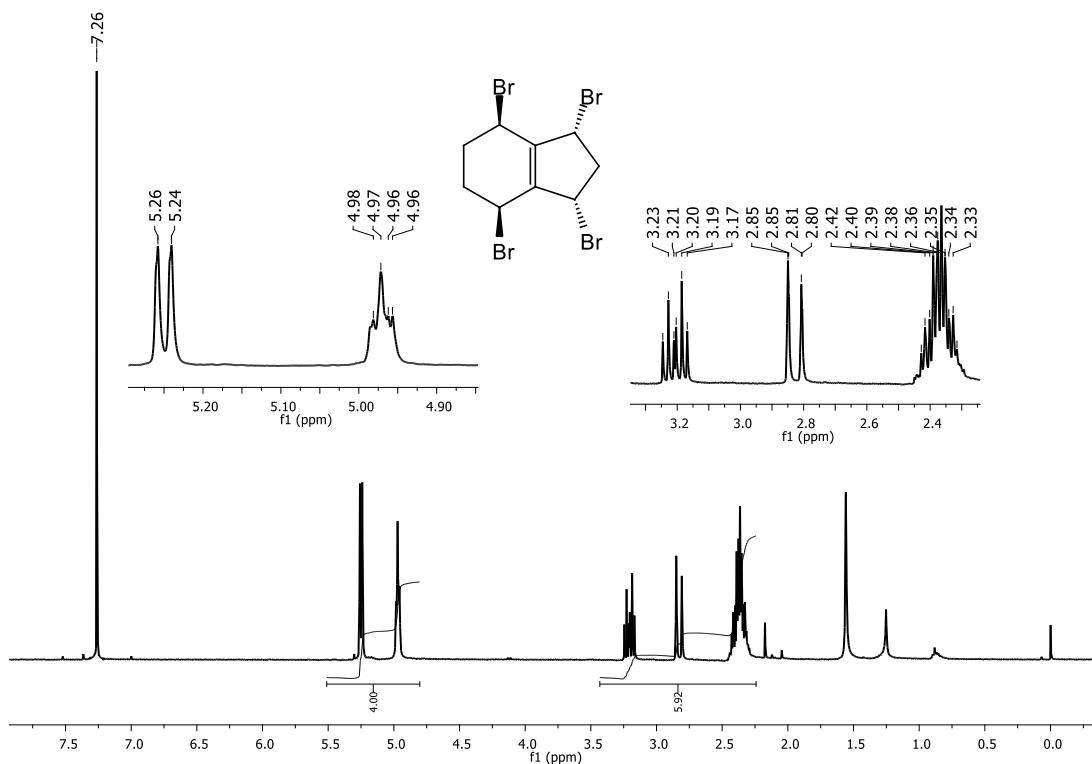


Figure S7. ¹H-NMR Spectrum of compound 13.

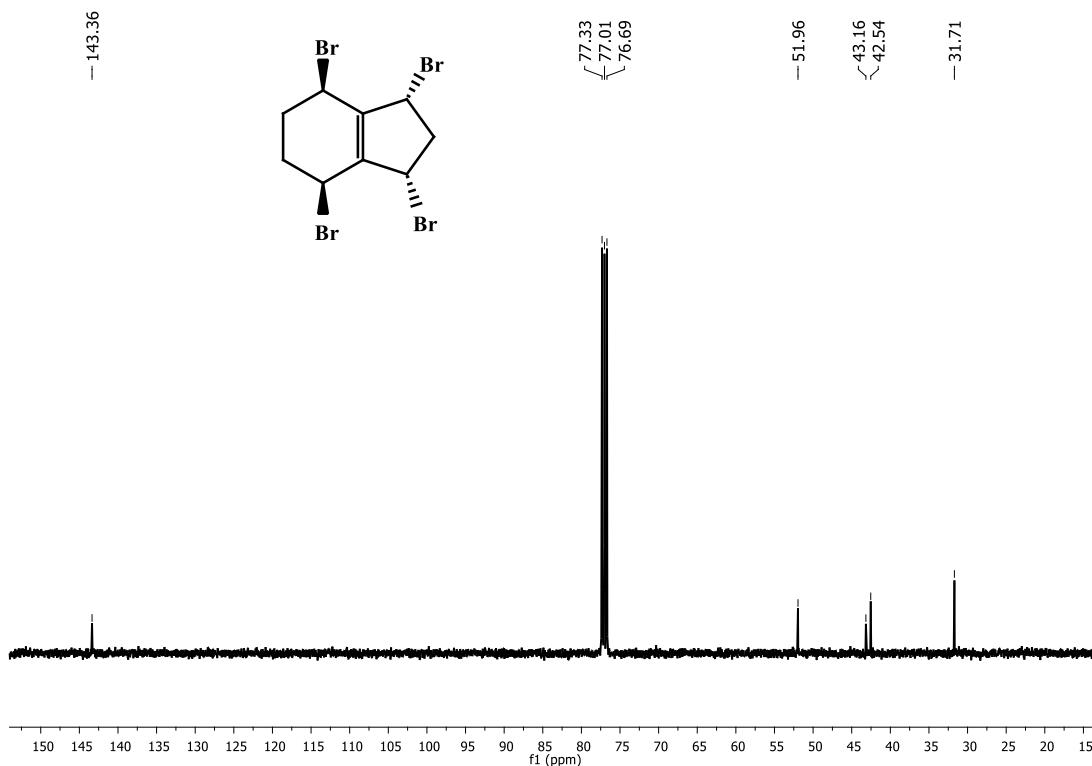


Figure S8. ¹³C-NMR Spectrum of compound 13.

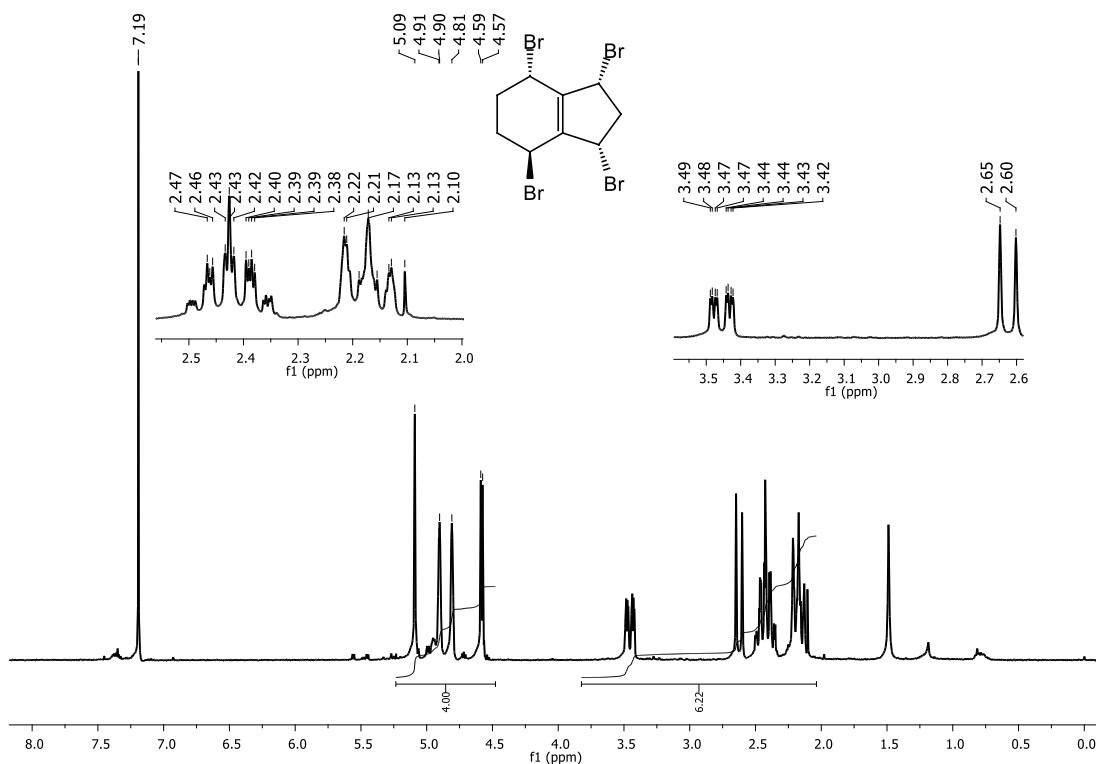


Figure S9. ¹H-NMR Spectrum of compound 14.

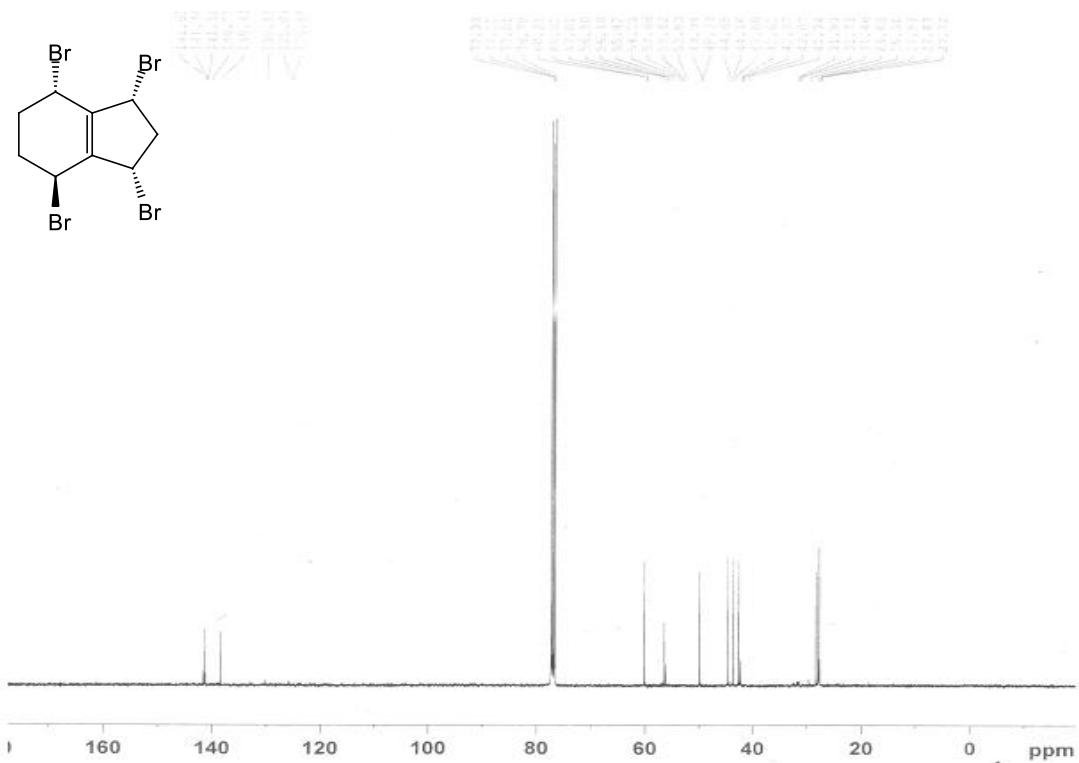


Figure S10. ¹³C-NMR Spectrum of compound 14.

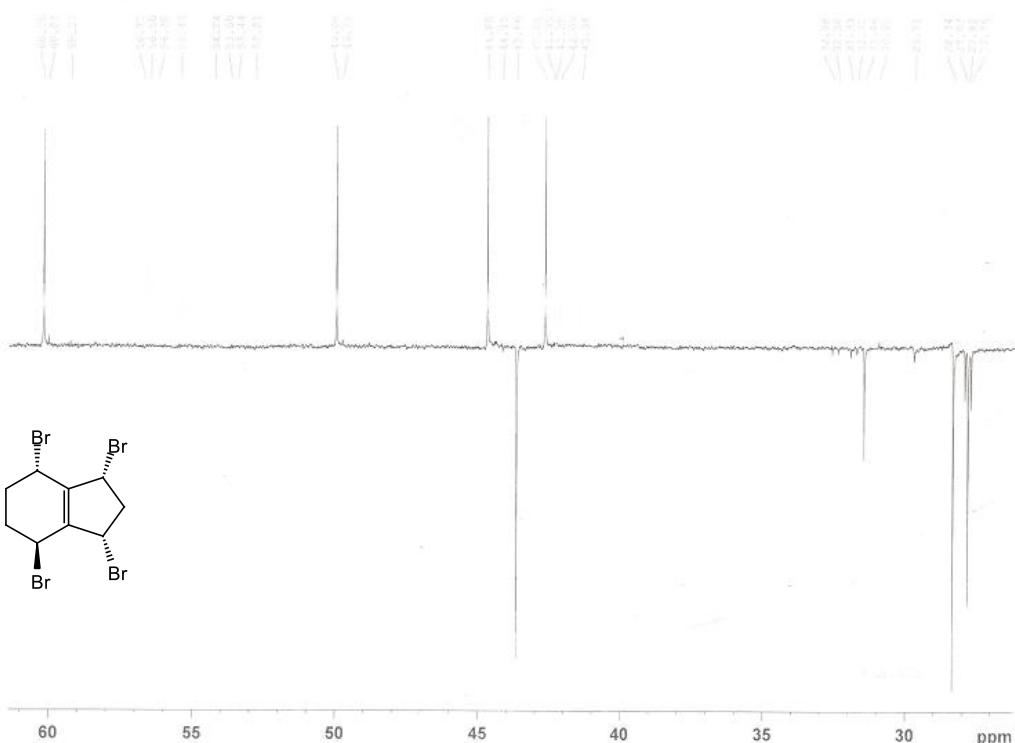


Figure S11. DEPT-135 Spectrum of compound 14.

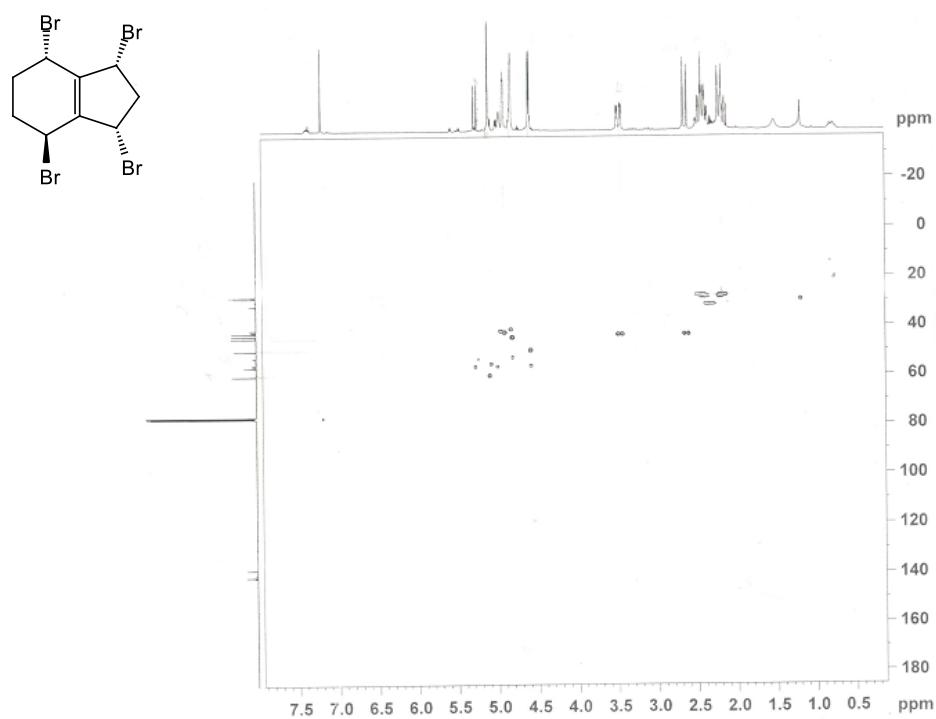


Figure S12. HSQC Spectrum of compound 14.

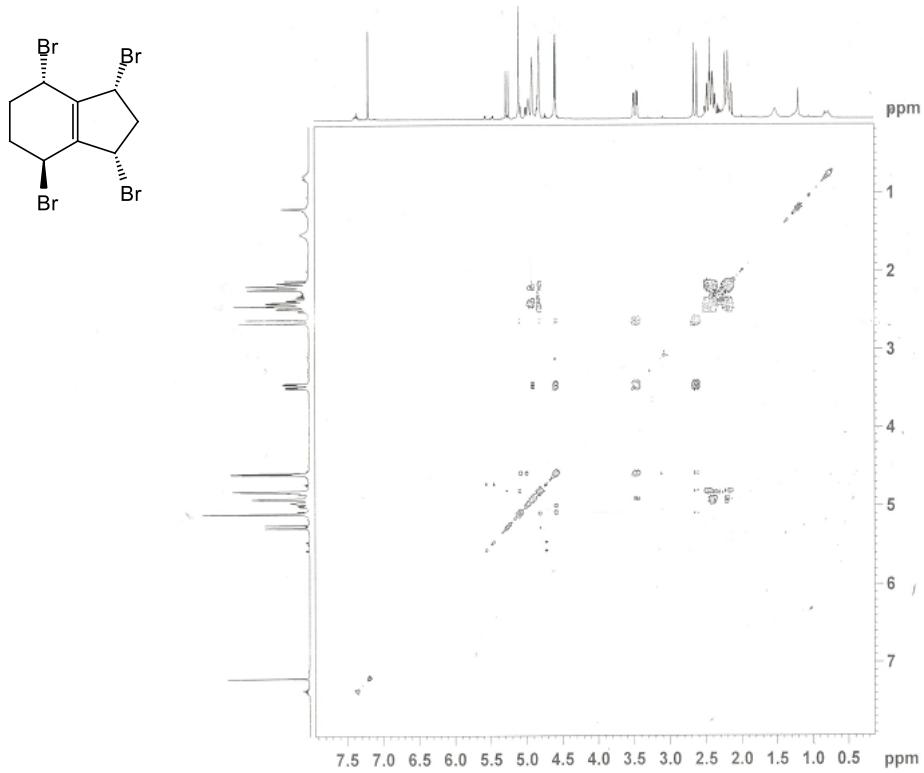


Figure S13. COSY Spectrum of compound **14**.

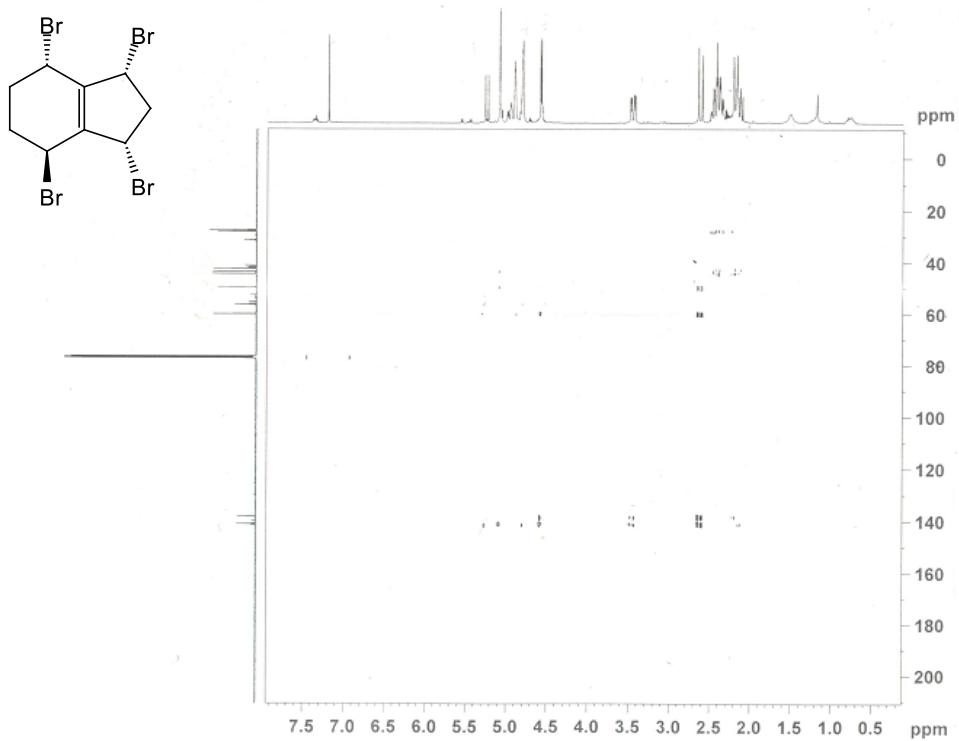
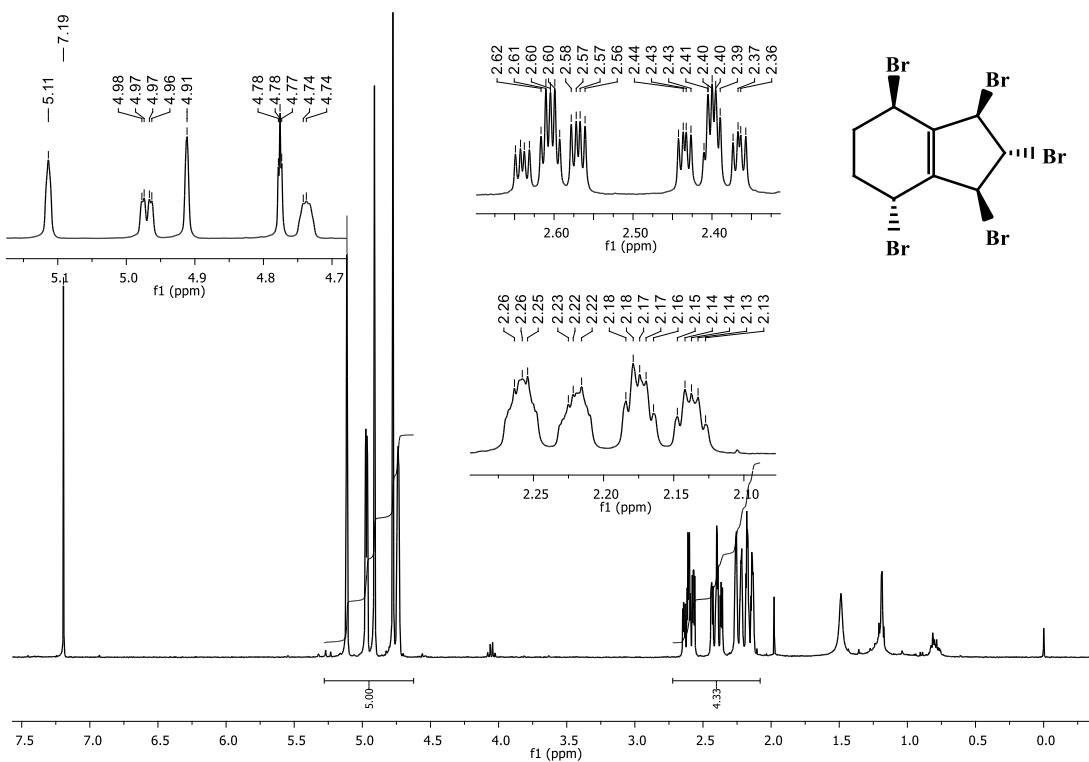


Figure S14. HMBC Spectrum of compound **14**.

**Figure S15.** ¹H-NMR Spectrum of compound 15.**Figure S16.** ¹³C-NMR Spectrum of compound 15.

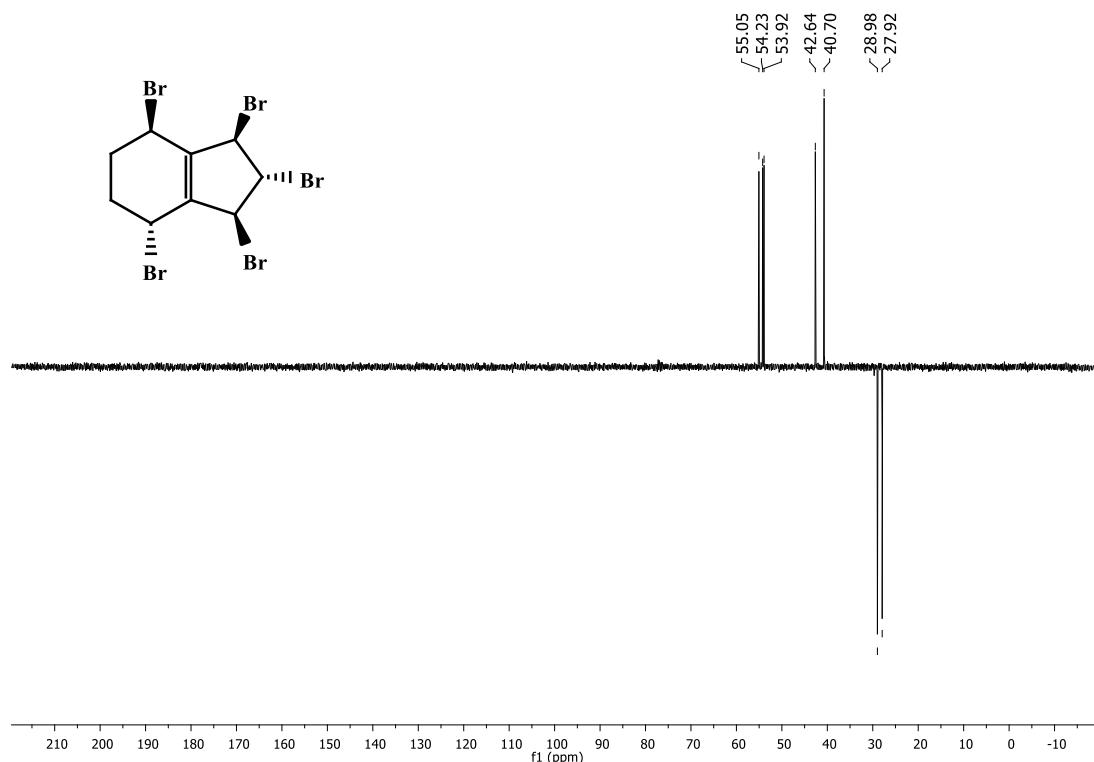


Figure S17. DEPT-135 Spectrum of compound 15.

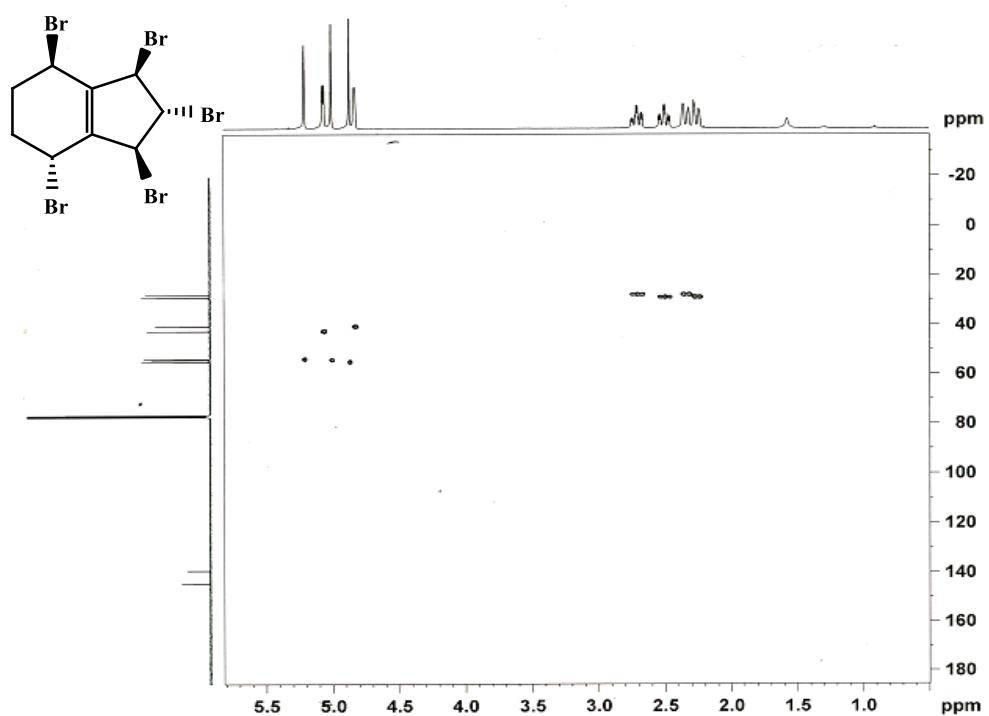


Figure S18. HSQC Spectrum of compound 15.

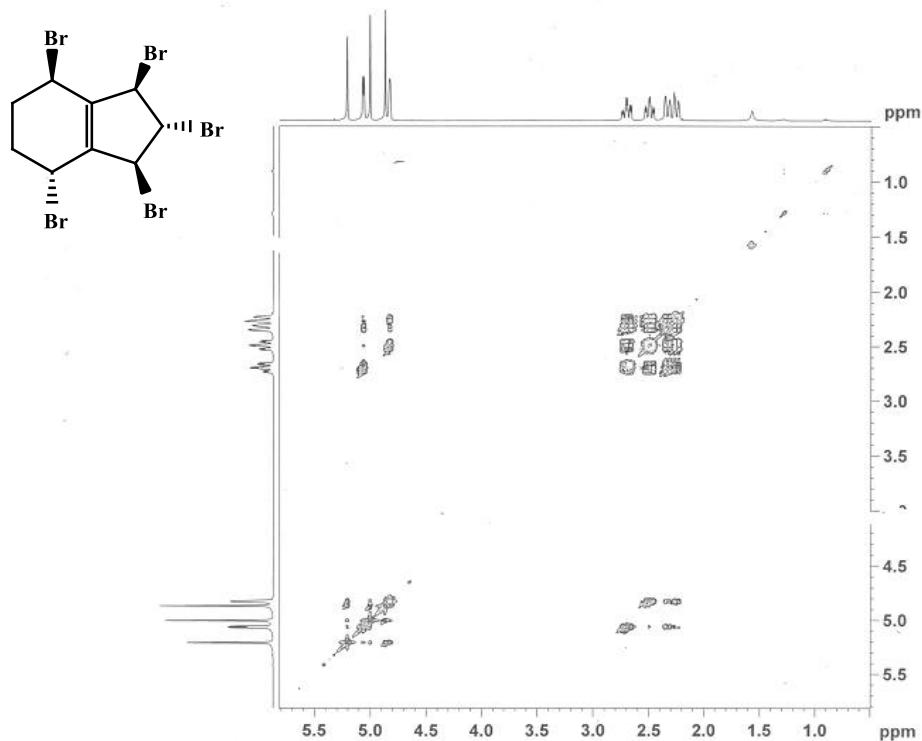


Figure S19. COSY Spectrum of compound 15.

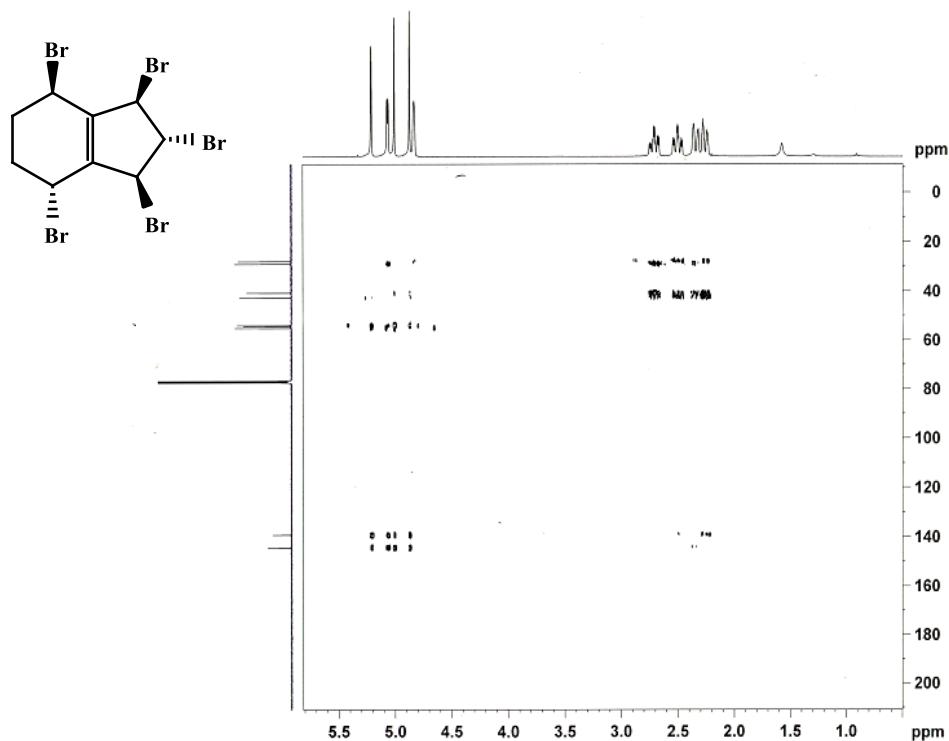


Figure S20. HMBC Spectrum of compound 15.

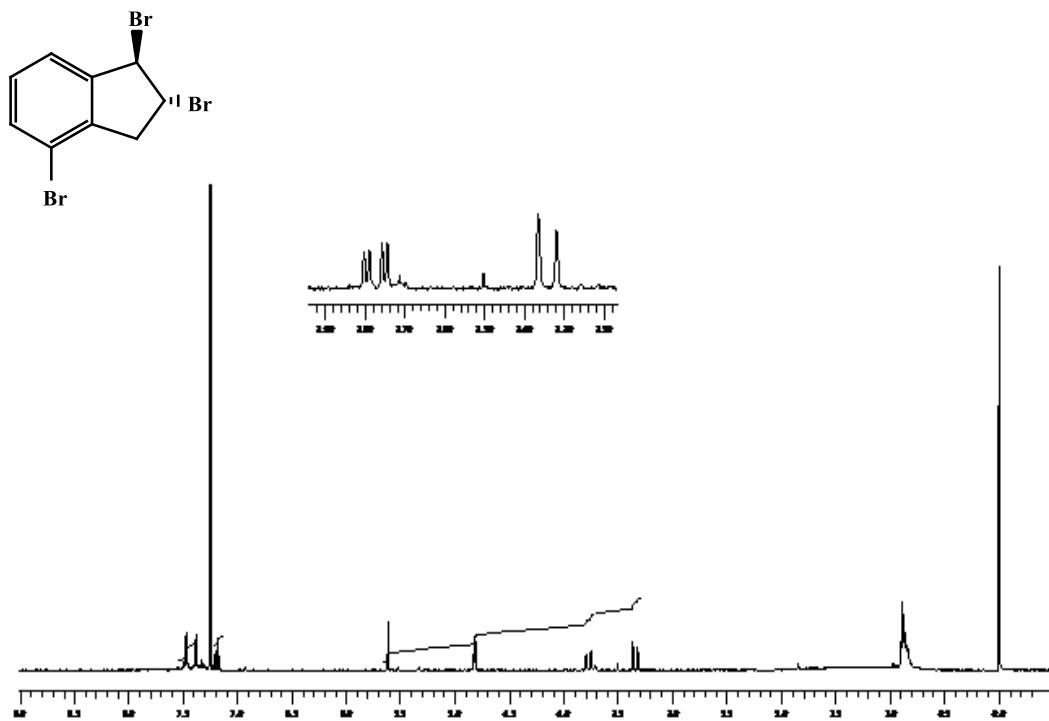


Figure S21. ¹H-NMR Spectrum of compound 16.

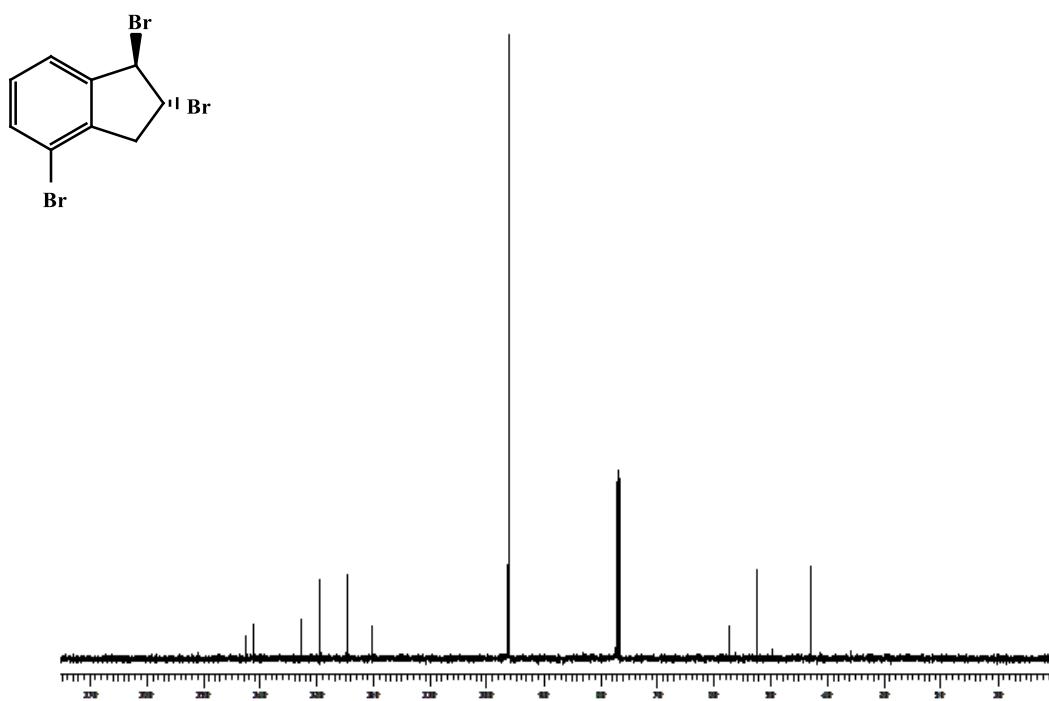


Figure S22. ¹³C-NMR Spectrum of compound 16.

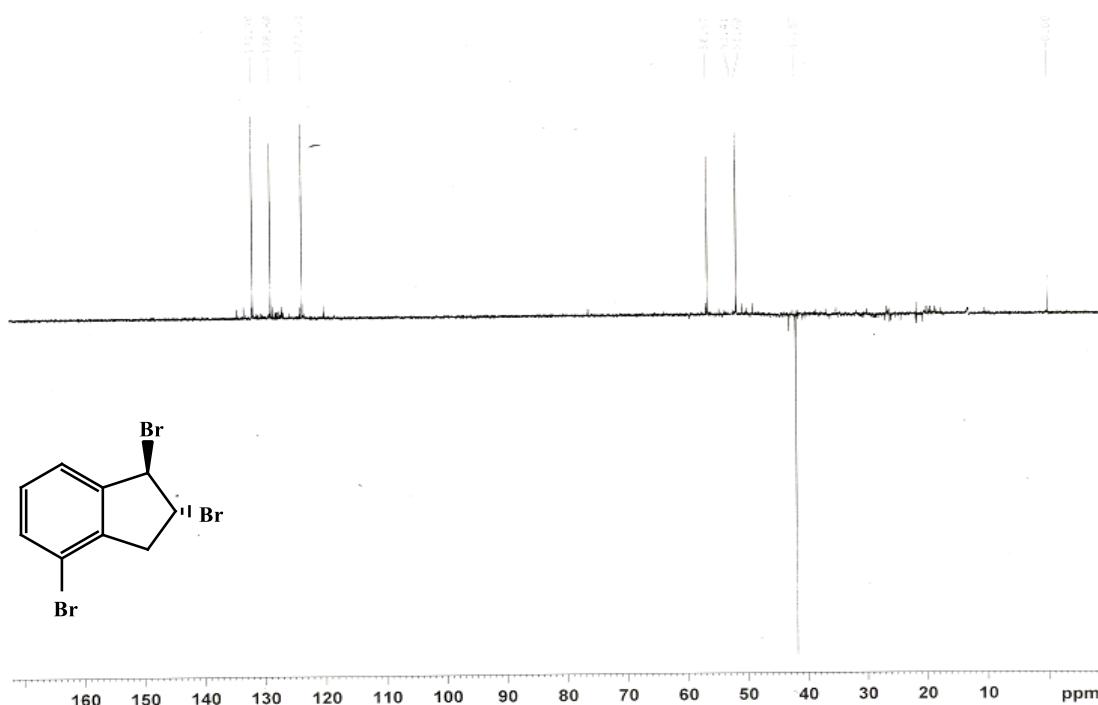


Figure S23. DEPT-135 Spectrum of compound **16**.

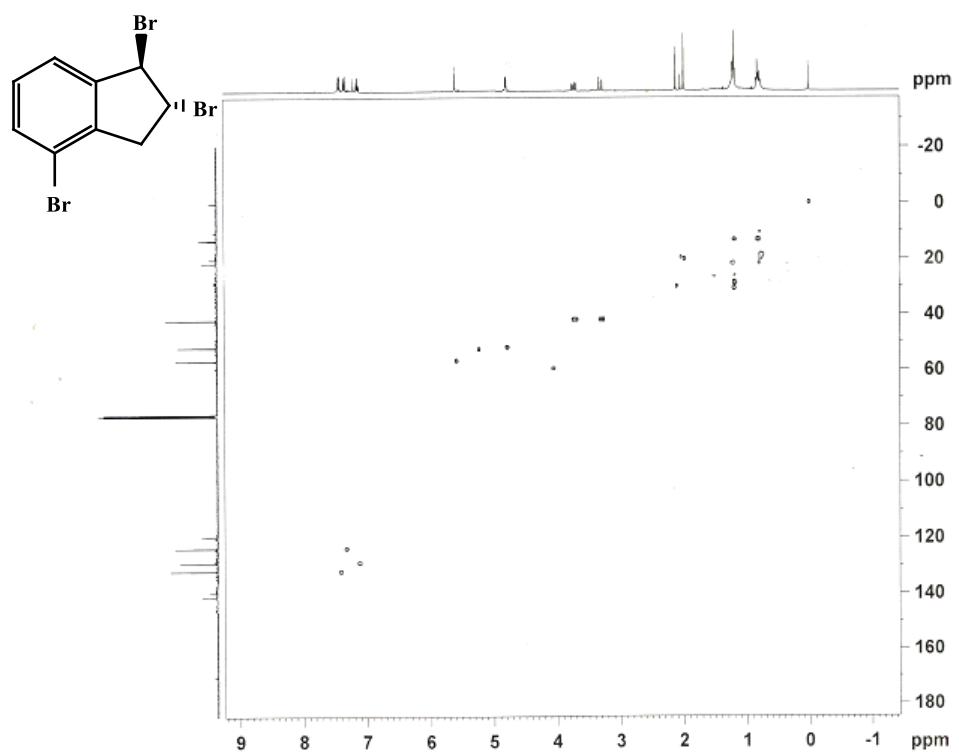


Figure S24. HSQC Spectrum of compound **16**.

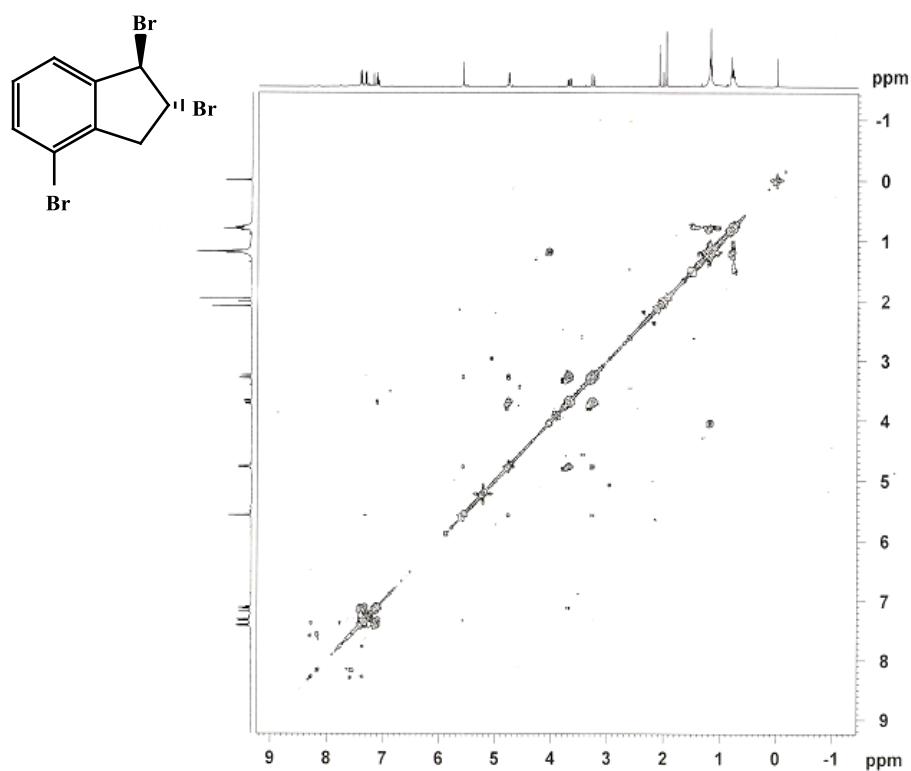


Figure S25. COSY Spectrum of compound 16.

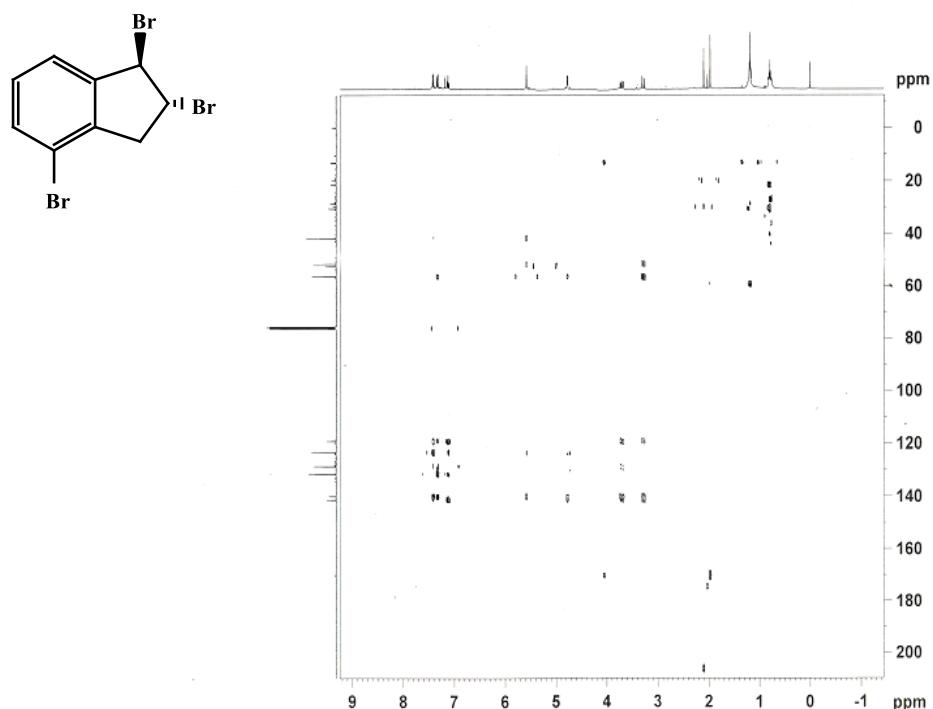


Figure S26. HMBC Spectrum of compound 16.

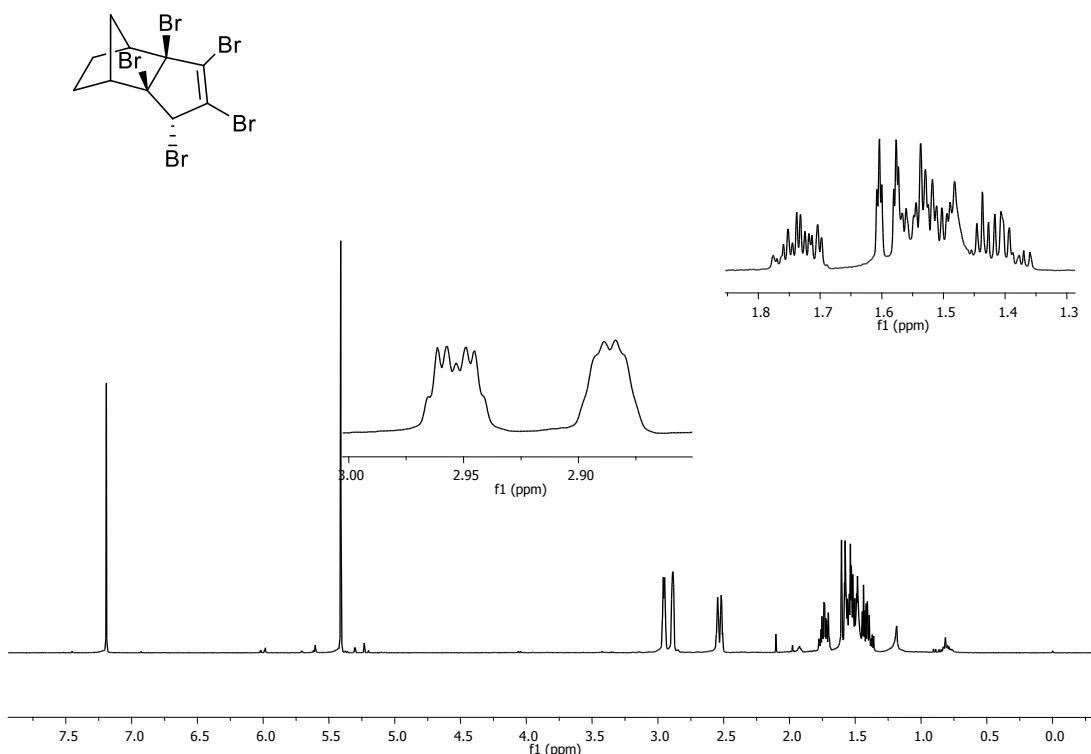


Figure S27. ¹H-NMR Spectrum of compound 23.

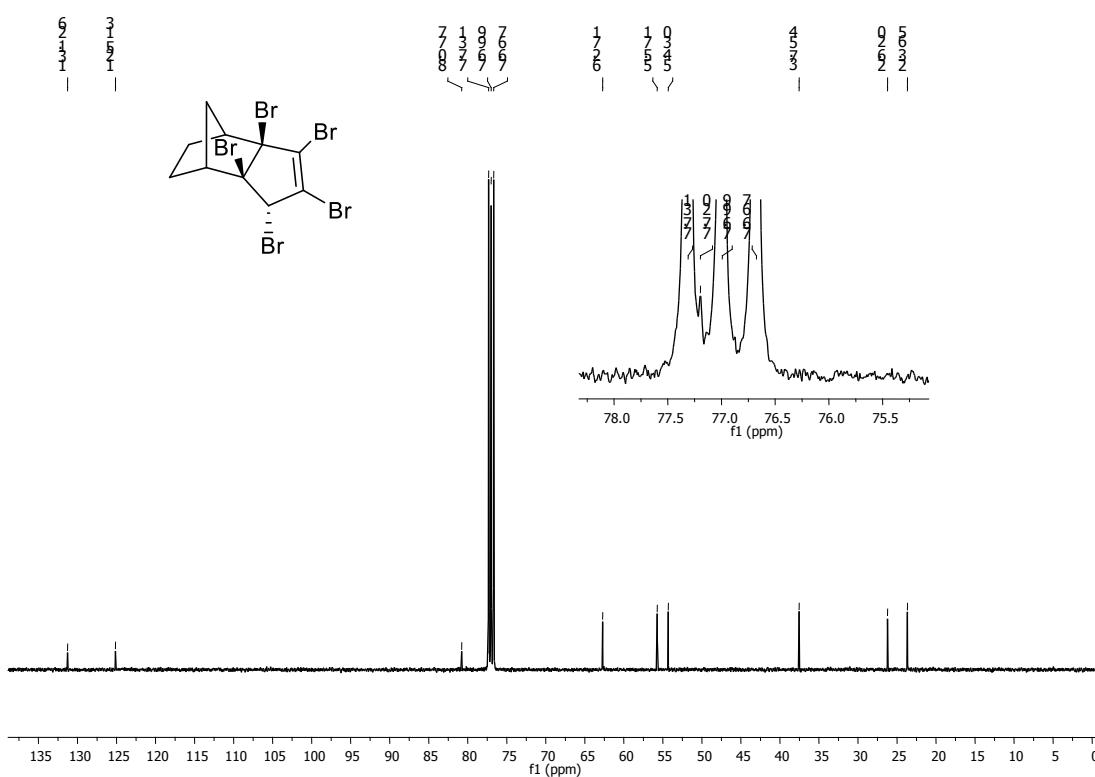


Figure S28. ¹³C-NMR Spectrum of compound 23.

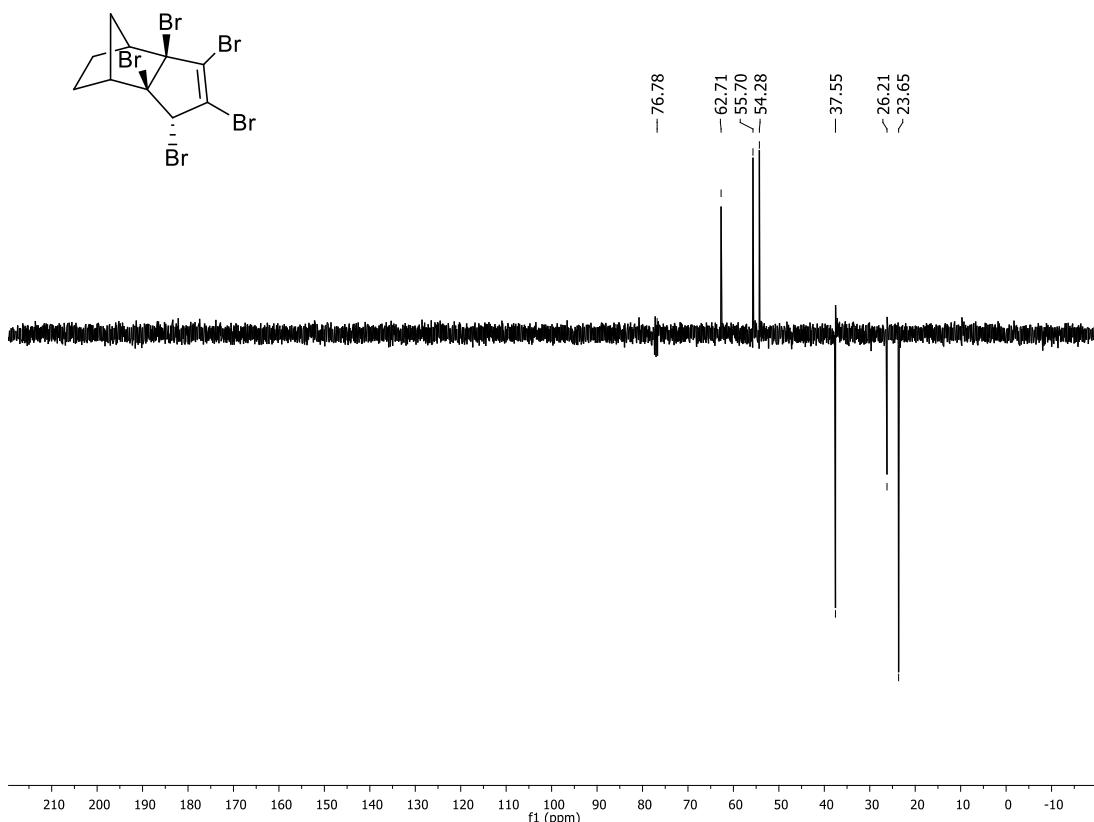


Figure S29. DEPT-135 Spectrum of compound 23.

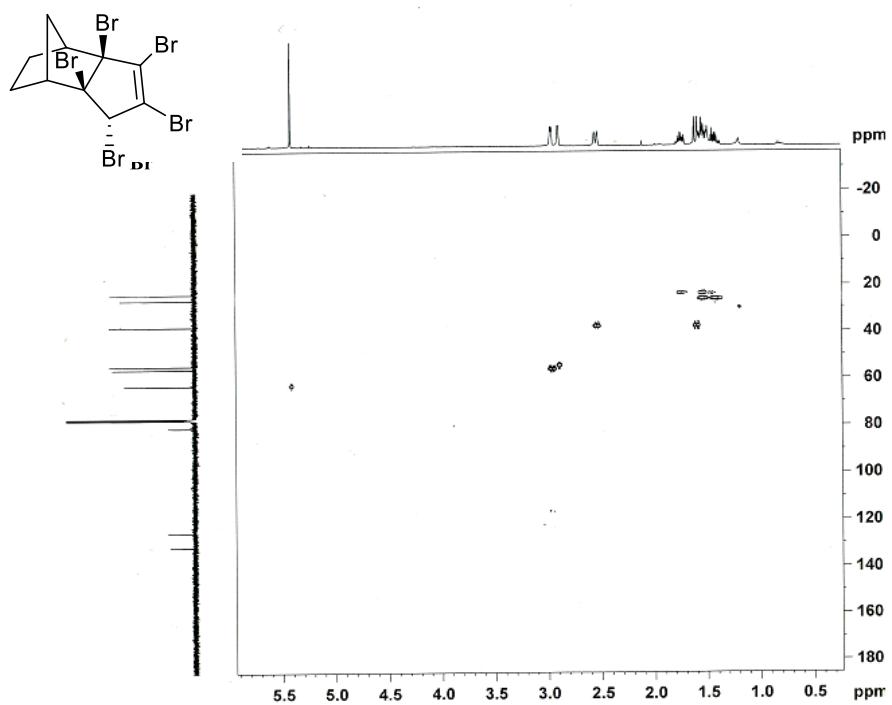


Figure S30. HSQC Spectrum of compound 23.

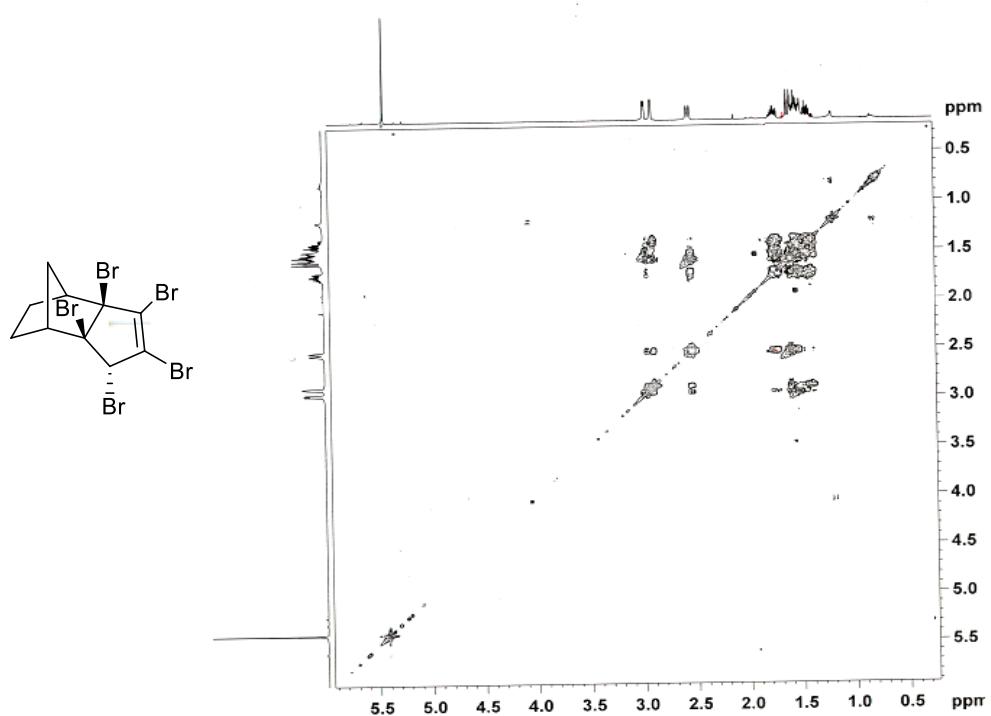


Figure S31. COSY Spectrum of compound 23.

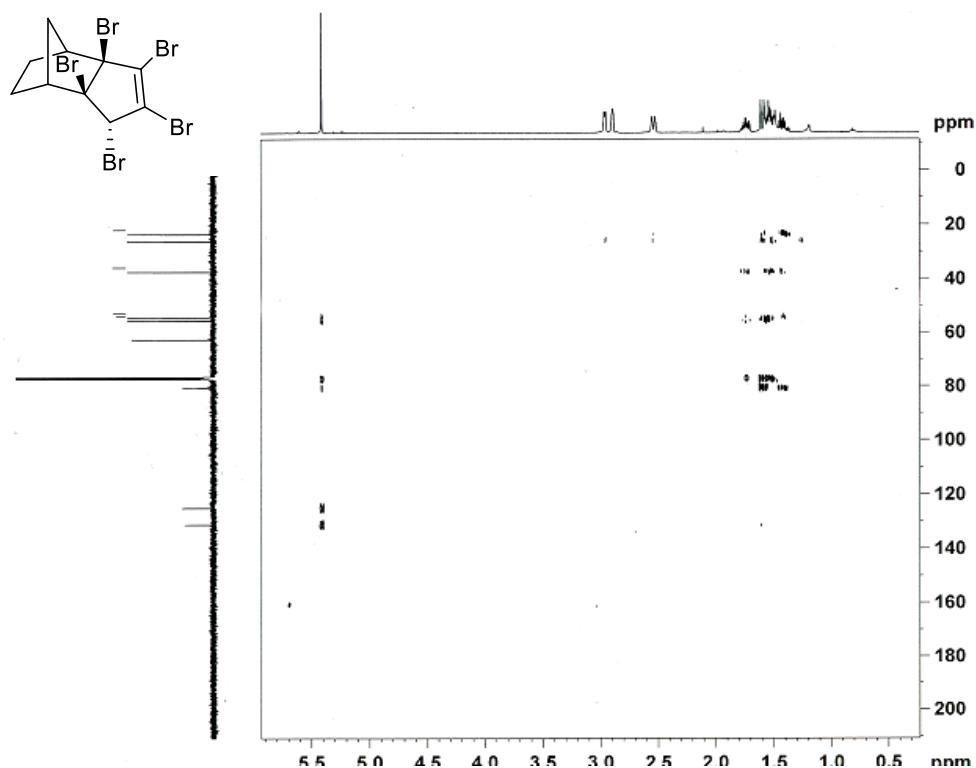


Figure S32. HMQC Spectrum of compound 23.

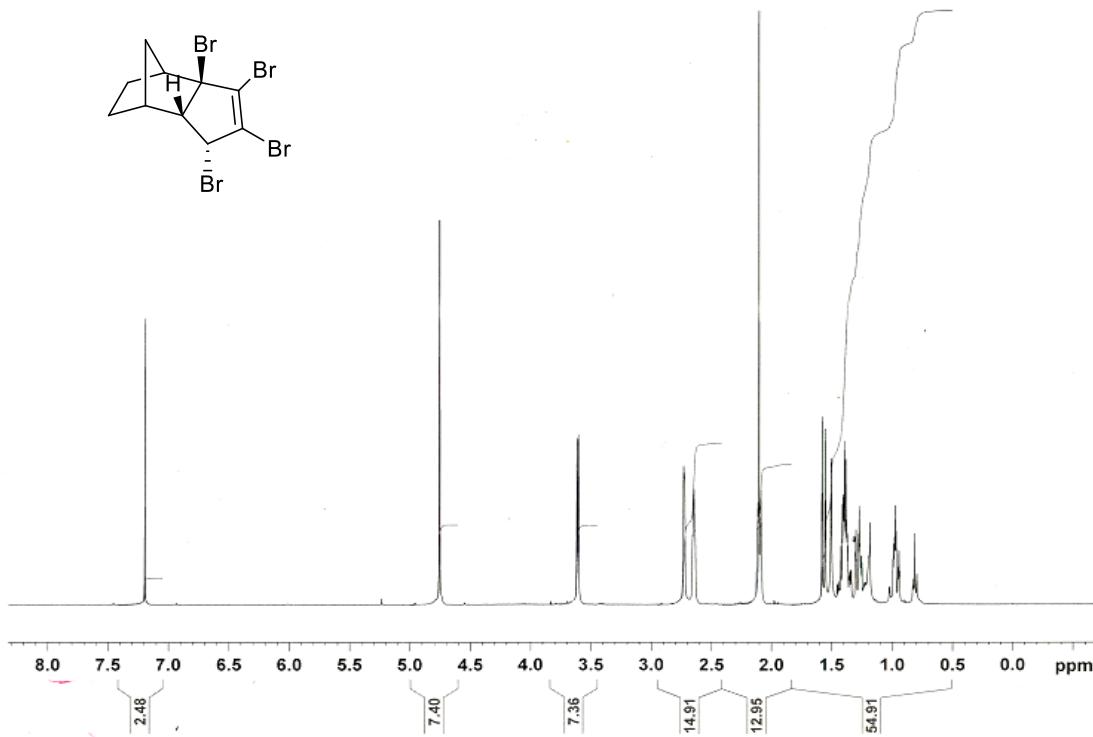


Figure S33. ¹H-NMR Spectrum of compound 25.

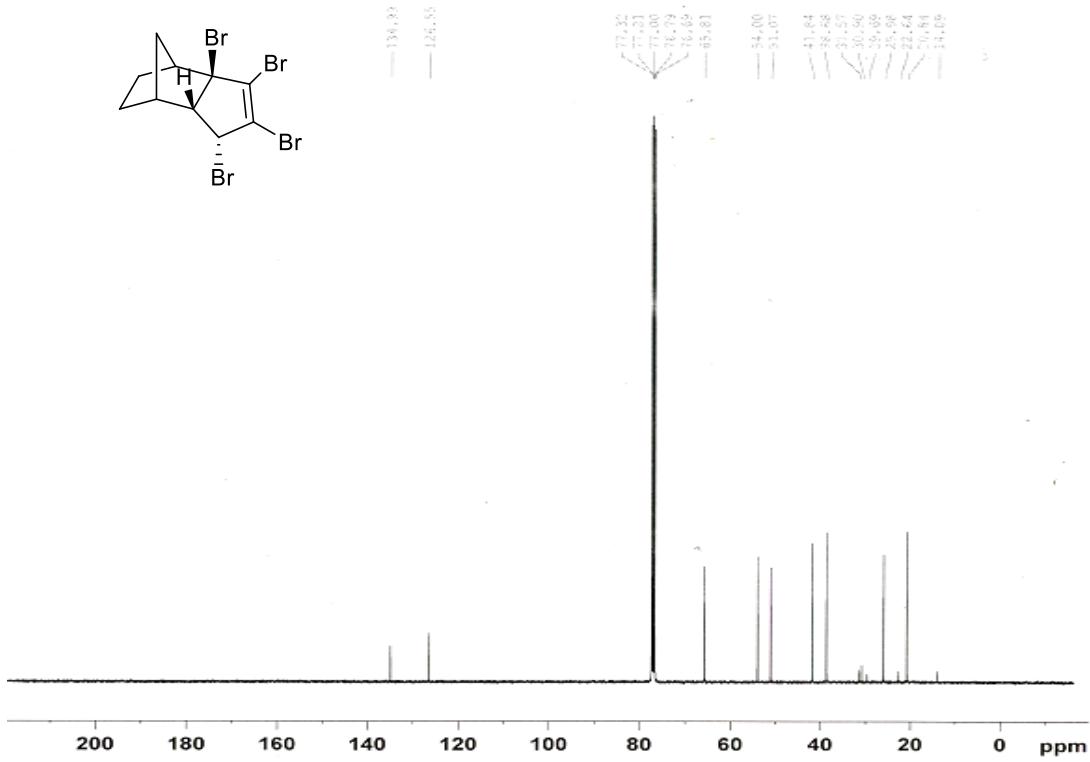


Figure S34. ¹³C-NMR Spectrum of compound 25.

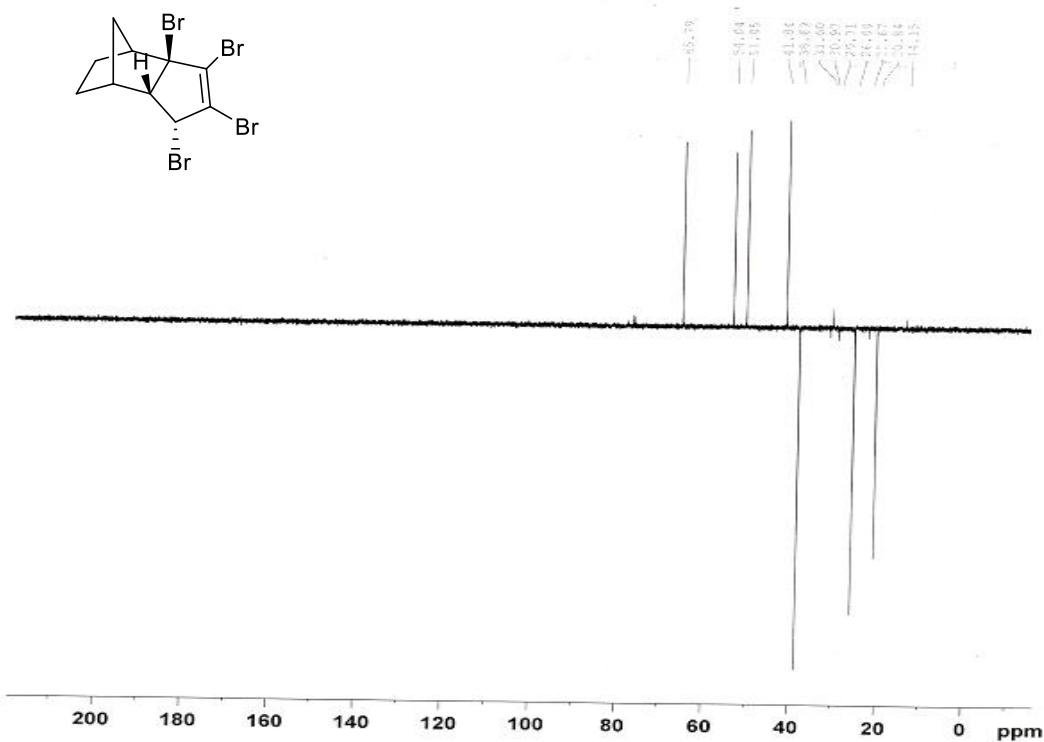


Figure S35. DEPT-135 Spectrum of compound 25.

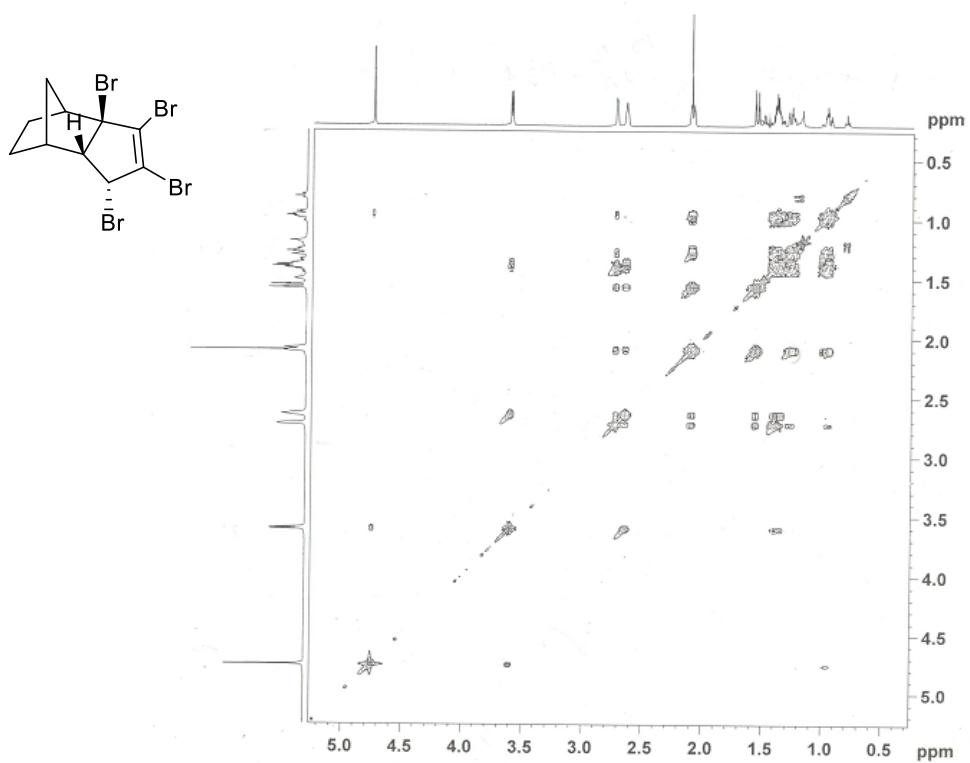


Figure S36. COSY Spectrum of compound 25.

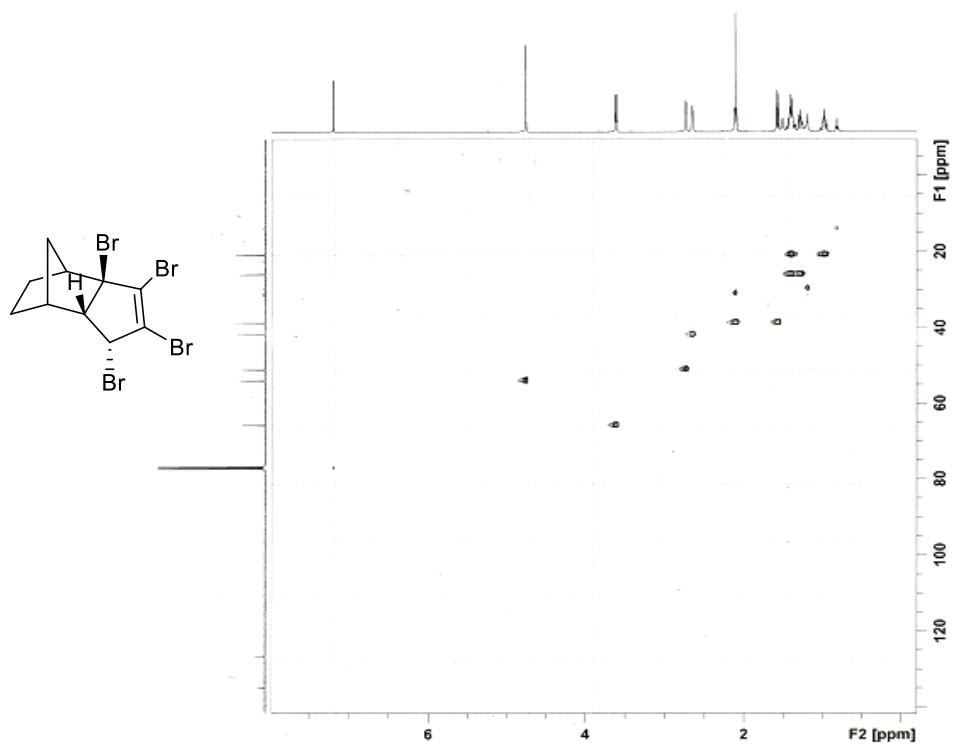


Figure S37. HSQC Spectrum of compound 25.

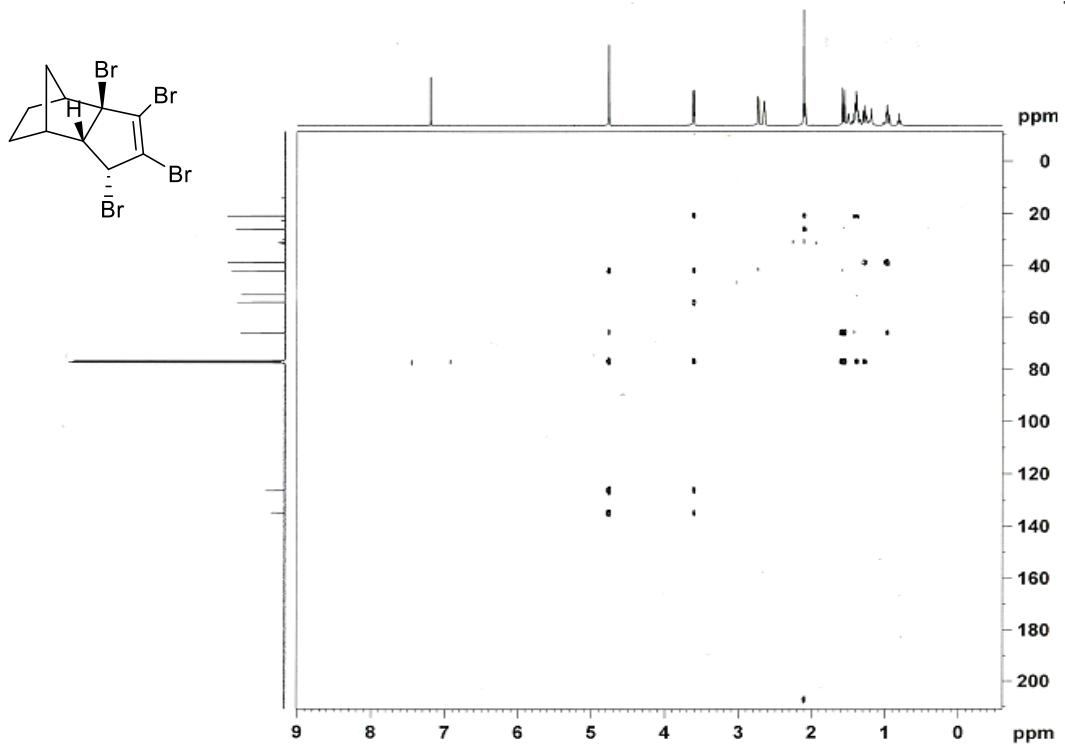


Figure S38. HMBC Spectrum of compound 25.

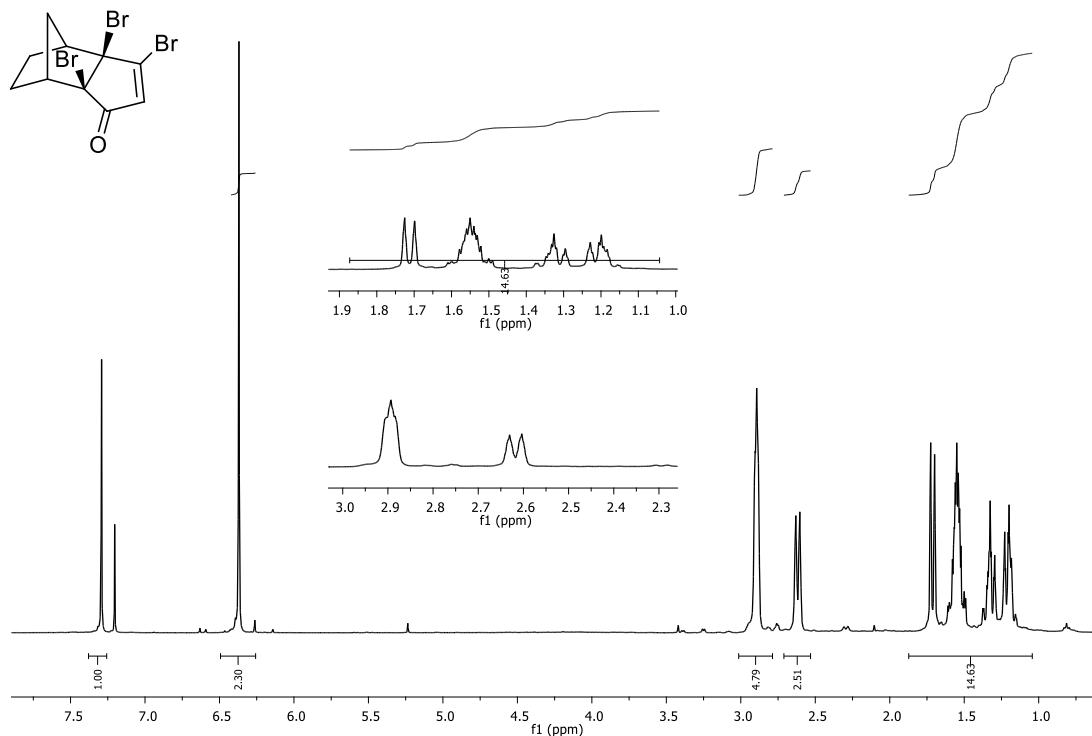


Figure S39. ¹H-NMR Spectrum of compound 24.

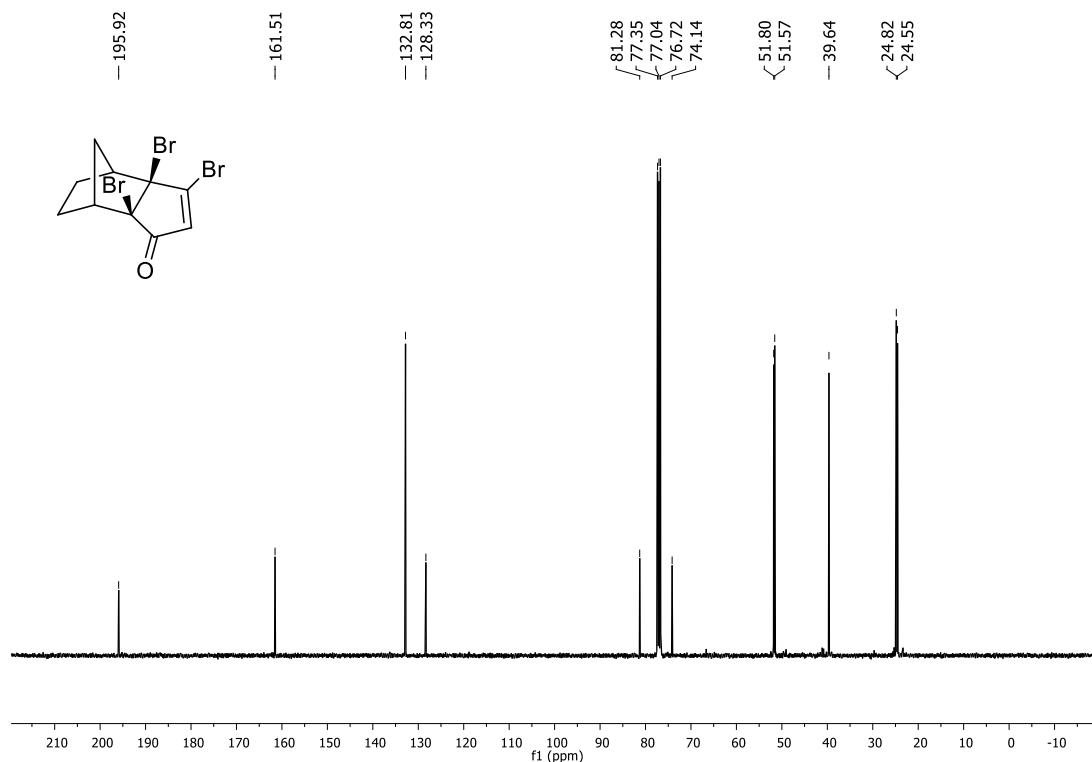


Figure S40. ¹³C-NMR Spectrum of compound 24.

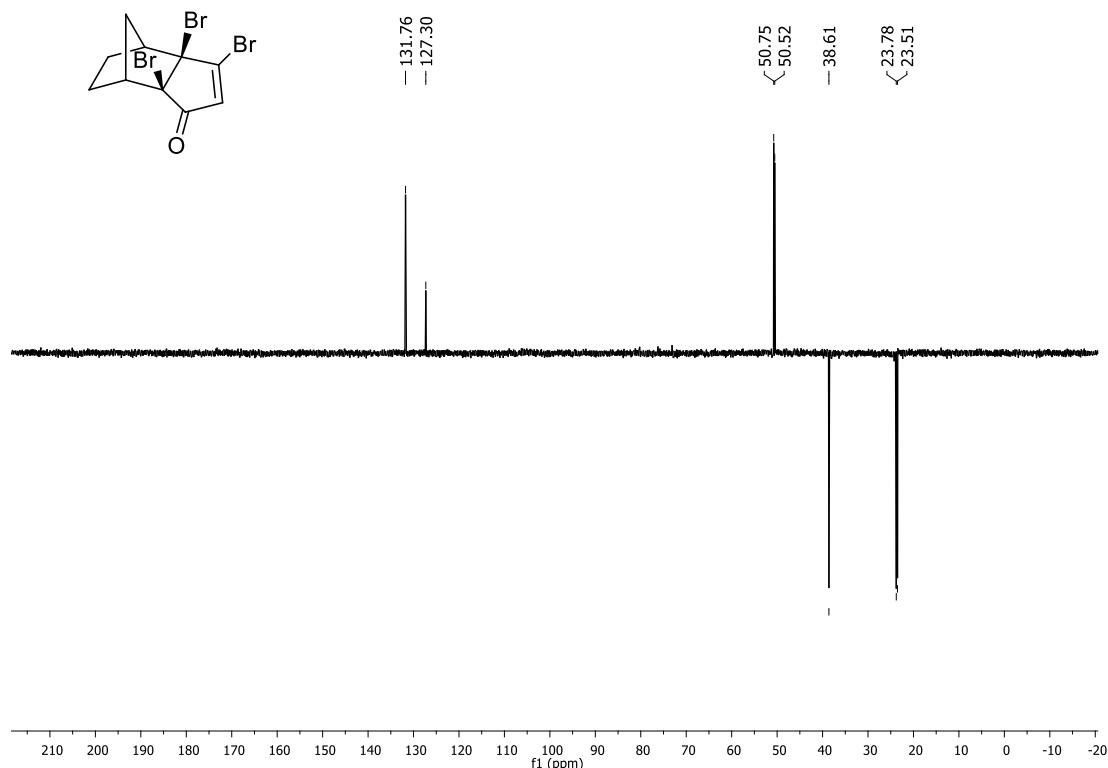


Figure S41. DEPT-135 Spectrum of compound 24.

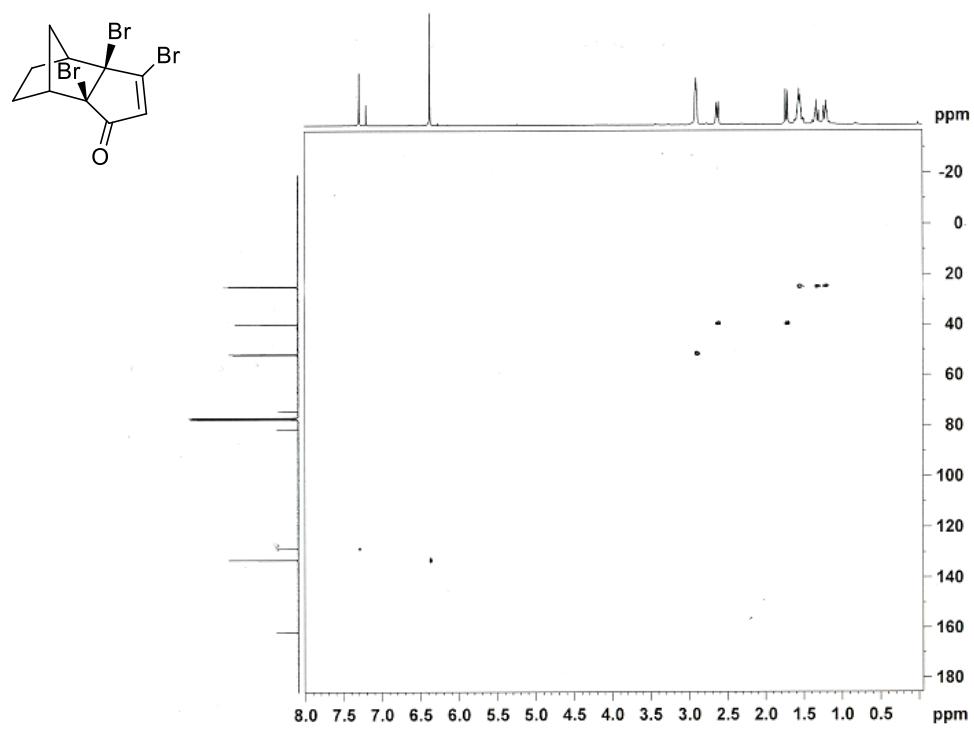


Figure S42. HSQC Spectrum of compound 24.

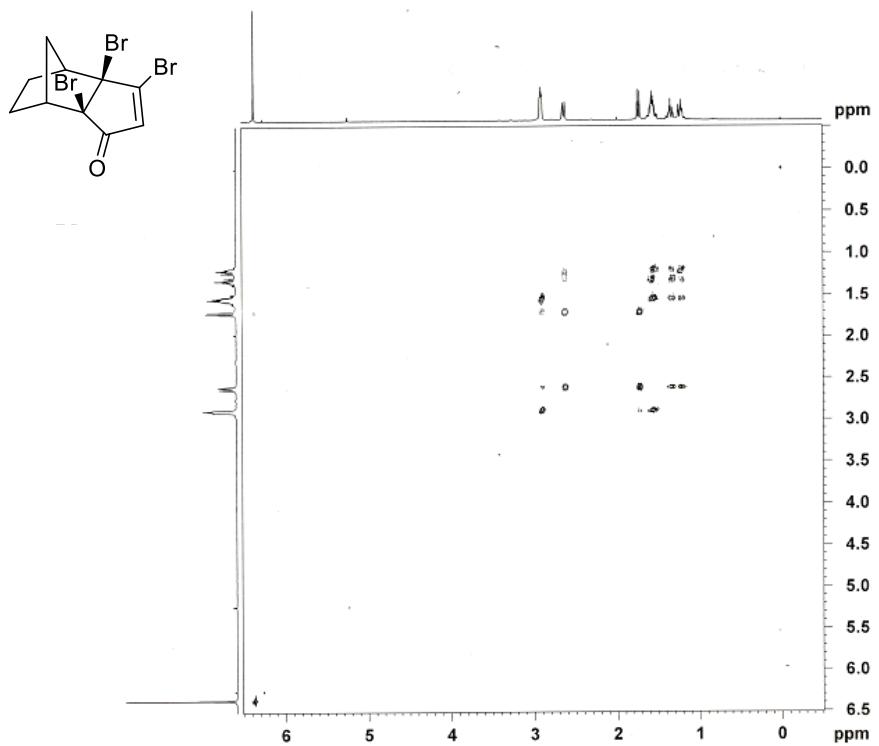


Figure S43. COSY Spectrum of compound 24.

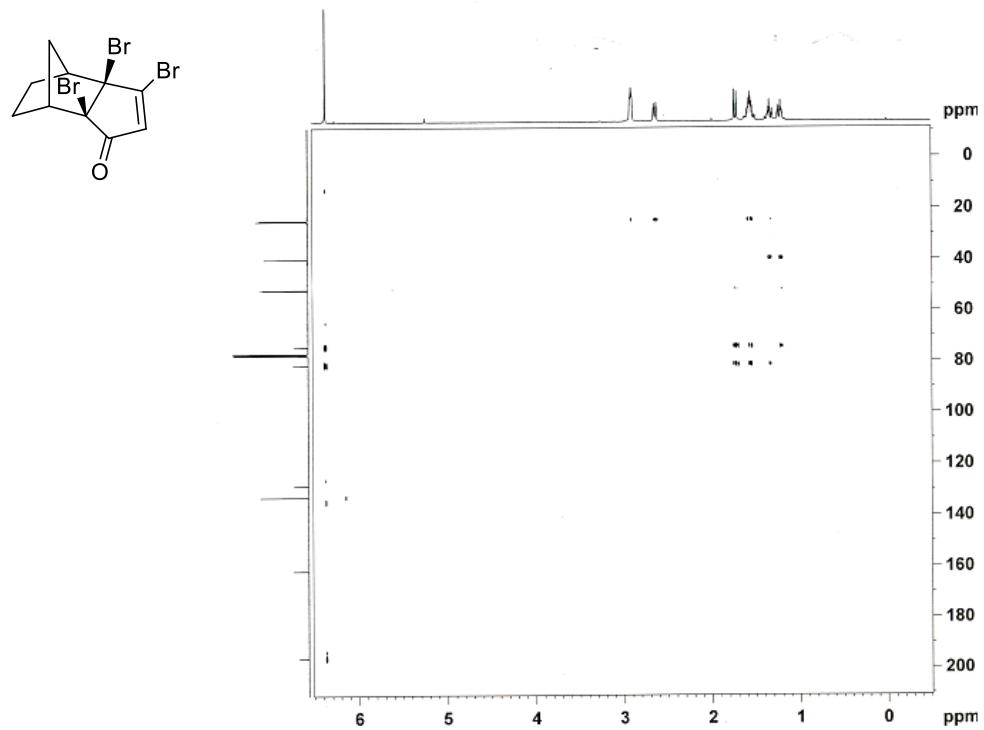


Figure S44. HMBC Spectrum of compound 24.

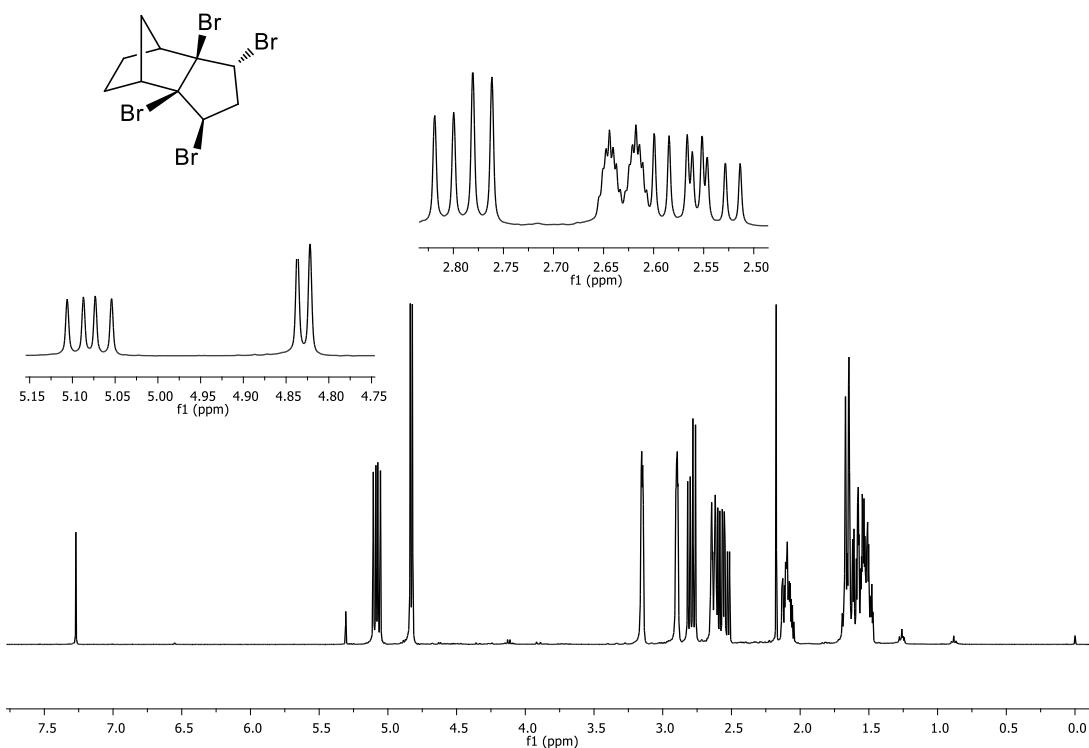


Figure S45. ¹H-NMR Spectrum of compound 38.

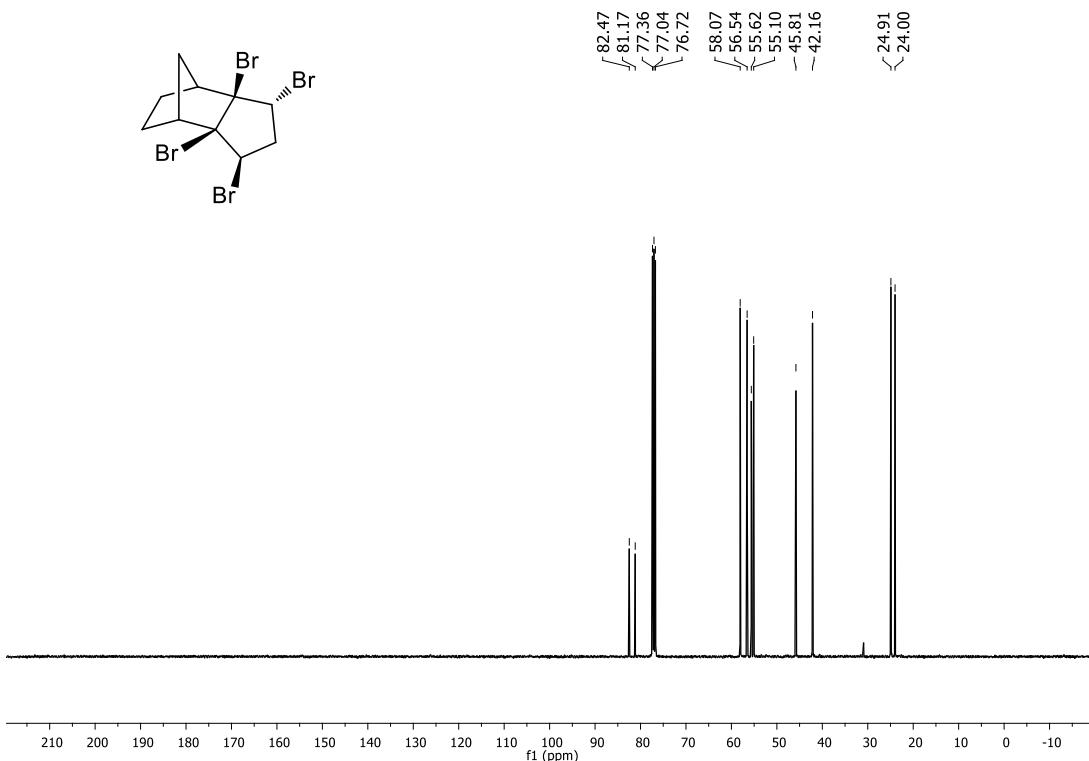
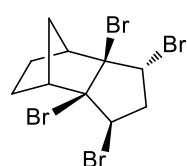


Figure S46. ¹³C-NMR Spectrum of compound 38.



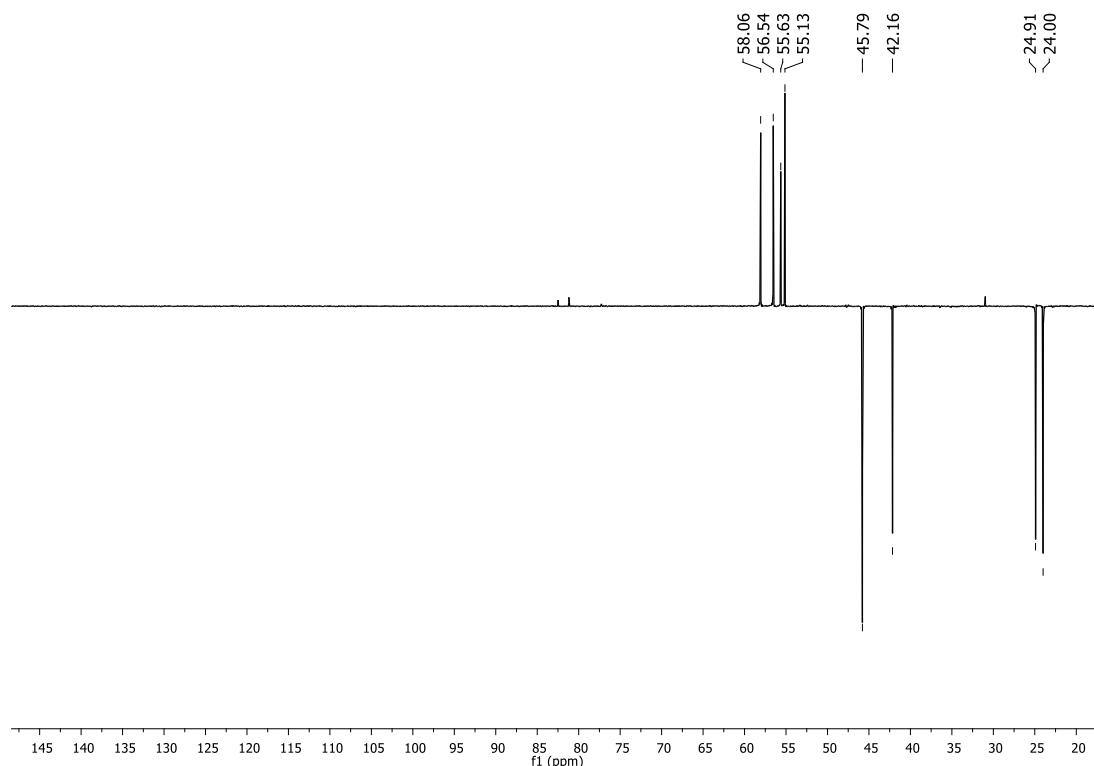


Figure S47. DEPT-135 Spectrum of compound **38**.

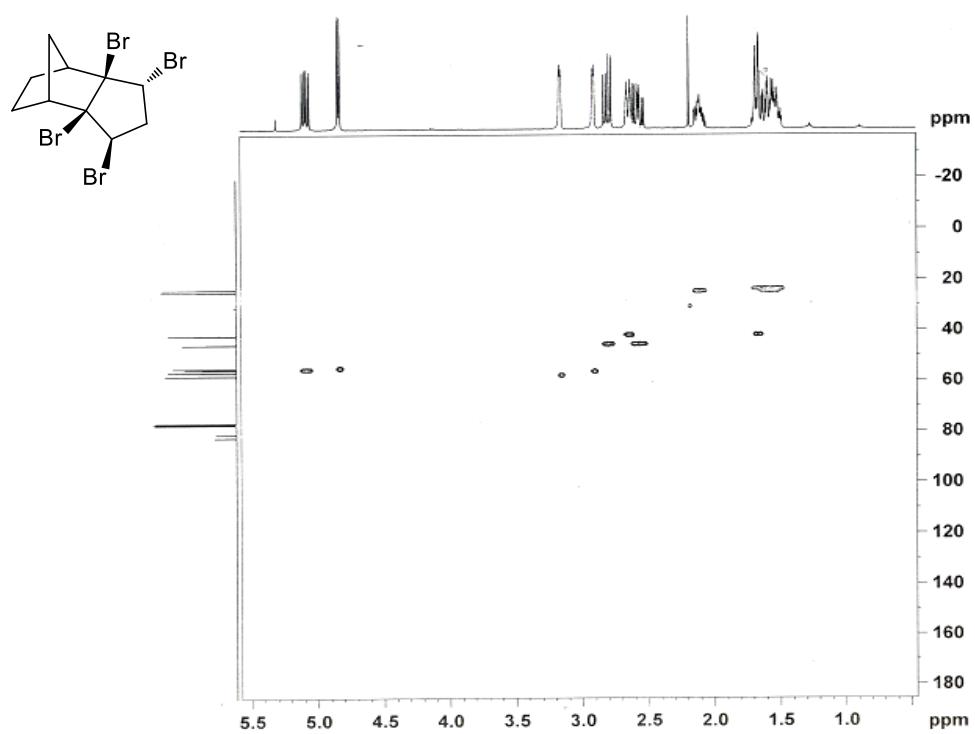


Figure S48. HSQC Spectrum of compound **38**.

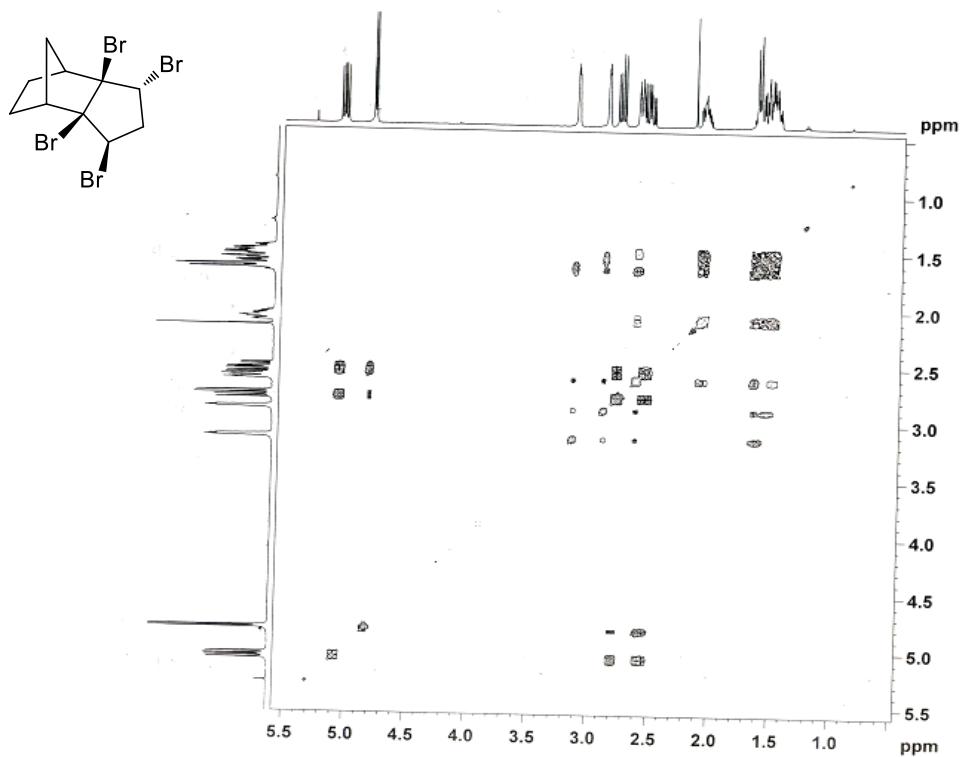


Figure S49. COSY Spectrum of compound 38.

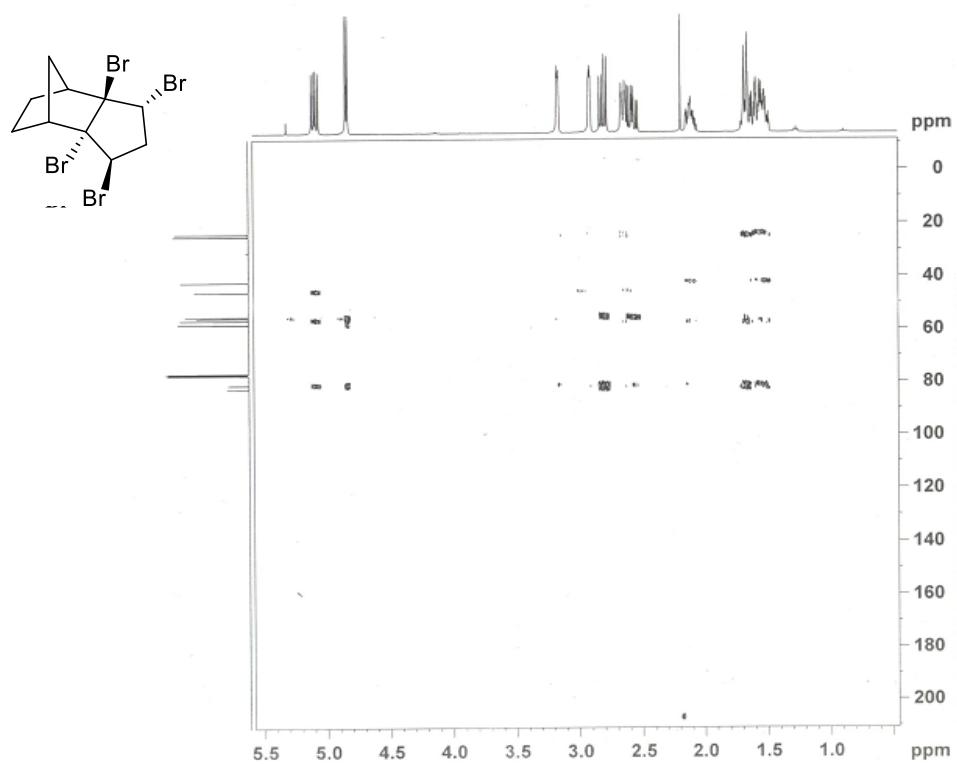
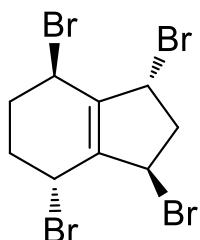
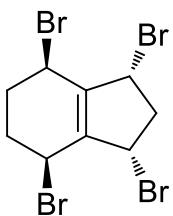


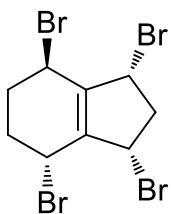
Figure S50. HMBC Spectrum of compound 38.

**12**

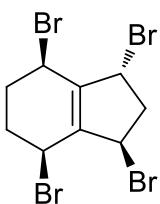
| | | | |
|----|-----------|-----------|-----------|
| H | 1.913956 | 1.682391 | -0.692075 |
| C | 1.112811 | 1.501561 | 0.022885 |
| C | -1.189011 | 2.220561 | 0.804021 |
| C | -0.793941 | -0.113683 | -0.022131 |
| C | -1.813624 | 0.915722 | 0.315316 |
| C | 0.526804 | 0.146664 | -0.143188 |
| C | 0.054628 | 2.601442 | -0.003712 |
| H | -0.905636 | 2.064463 | 1.853624 |
| H | -0.223333 | 2.754330 | -1.055325 |
| H | -1.929031 | 3.023580 | 0.786705 |
| H | -2.553616 | 0.529985 | 1.015939 |
| H | 0.479291 | 3.541050 | 0.356184 |
| C | 1.302034 | -1.110786 | -0.411412 |
| H | 1.949035 | -1.382402 | 0.423661 |
| C | 0.225384 | -2.161702 | -0.745693 |
| H | 0.133873 | -2.260530 | -1.831126 |
| H | 0.452220 | -3.146309 | -0.337183 |
| C | -1.087736 | -1.565975 | -0.212806 |
| H | -1.961216 | -1.776510 | -0.827240 |
| Br | 2.129625 | 1.530312 | 1.791346 |
| Br | -2.944616 | 1.236619 | -1.342712 |
| Br | -1.622803 | -2.380346 | 1.570729 |
| Br | 2.607933 | -0.893012 | -1.919013 |

**13**

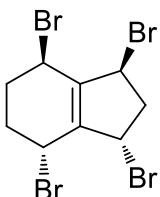
| | | | |
|----|-----------|-----------|-----------|
| C | -0.389743 | -0.449553 | -0.035551 |
| C | -2.206591 | 0.608767 | 1.344118 |
| C | -0.089959 | 1.893630 | 0.797351 |
| C | -1.098417 | 1.524486 | 1.882720 |
| C | 0.285718 | 0.722473 | -0.036656 |
| C | -1.617121 | -0.687171 | 0.780657 |
| H | -2.746875 | 1.134803 | 0.551459 |
| H | -0.535636 | 1.013466 | 2.676612 |
| H | -1.410556 | -1.424077 | 1.560450 |
| H | -2.928559 | 0.373883 | 2.130070 |
| H | 0.793457 | 2.382314 | 1.207555 |
| H | -1.529652 | 2.425375 | 2.325508 |
| C | 0.298197 | -1.470321 | -0.883875 |
| H | -0.374945 | -2.053280 | -1.508042 |
| C | 1.349432 | -0.670727 | -1.668424 |
| H | 0.937546 | -0.457890 | -2.662756 |
| H | 2.290565 | -1.200711 | -1.803927 |
| C | 1.491749 | 0.662893 | -0.917391 |
| H | 1.607278 | 1.528675 | -1.567864 |
| Br | -3.024290 | -1.625592 | -0.316334 |
| Br | 1.119523 | -2.898223 | 0.295924 |
| Br | 3.173937 | 0.755167 | 0.206385 |
| Br | -0.833730 | 3.347450 | -0.417354 |

**14**

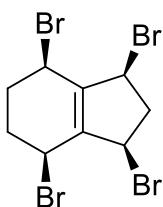
| | | | |
|----|-----------|-----------|-----------|
| H | -2.161636 | -0.087771 | 1.516362 |
| C | -1.887122 | 0.491939 | 0.635212 |
| C | -0.881412 | 2.645304 | -0.214318 |
| C | 0.250148 | 0.462836 | -0.682220 |
| C | 0.419362 | 1.945264 | -0.613039 |
| C | -0.817351 | -0.178278 | -0.149121 |
| C | -1.556824 | 1.943048 | 0.966069 |
| H | -1.551663 | 2.618850 | -1.084015 |
| H | -0.871751 | 1.933156 | 1.824102 |
| H | -0.686136 | 3.694746 | 0.015689 |
| H | 0.816475 | 2.336618 | -1.550229 |
| H | -2.457286 | 2.475964 | 1.277524 |
| C | -0.811976 | -1.636096 | -0.481867 |
| H | -1.786213 | -2.016010 | -0.783318 |
| C | 0.263796 | -1.767643 | -1.569476 |
| H | 0.848312 | -2.683677 | -1.502942 |
| H | -0.245531 | -1.762188 | -2.541312 |
| C | 1.112214 | -0.485978 | -1.465852 |
| Br | -3.612378 | 0.400799 | -0.461785 |
| Br | 1.877243 | 2.468921 | 0.694917 |
| Br | -0.422261 | -2.721450 | 1.167791 |
| H | 1.411354 | -0.087744 | -2.435345 |
| Br | 2.897466 | -0.858210 | -0.607599 |

**18**

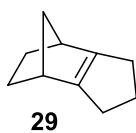
| | | | |
|----|-----------|-----------|-----------|
| H | 2.342224 | 1.499725 | -0.824571 |
| C | 1.318355 | 1.502134 | -0.453688 |
| C | -1.061933 | 2.266768 | -0.925036 |
| C | -0.531467 | -0.176704 | -0.701885 |
| C | -1.476873 | 0.838779 | -1.278957 |
| C | 0.752500 | 0.129819 | -0.399090 |
| C | 0.429459 | 2.473235 | -1.226952 |
| H | -1.253274 | 2.446184 | 0.137546 |
| H | 0.619758 | 2.297718 | -2.295774 |
| H | -1.667618 | 2.976970 | -1.493230 |
| H | 0.725047 | 3.504155 | -1.018204 |
| C | 1.510978 | -1.103469 | 0.015633 |
| H | 1.718455 | -1.122619 | 1.086887 |
| C | 0.616792 | -2.256284 | -0.465023 |
| H | 0.891211 | -2.517989 | -1.492354 |
| H | 0.690946 | -3.152463 | 0.150520 |
| C | -0.787731 | -1.639941 | -0.494177 |
| H | -1.483249 | -2.101221 | -1.192536 |
| Br | 1.588618 | 2.149664 | 1.459353 |
| Br | -1.679940 | -1.950993 | 1.303478 |
| Br | 3.332507 | -1.210606 | -0.798845 |
| H | -1.505200 | 0.704688 | -2.364825 |
| Br | -3.393221 | 0.551454 | -0.795728 |

**19**

| | | | |
|----|-----------|-----------|-----------|
| H | -1.704029 | 1.401169 | 1.805836 |
| C | -1.356188 | 1.373057 | 0.772264 |
| C | 0.227608 | 2.413115 | -0.899543 |
| C | 0.528940 | 0.032127 | -0.204447 |
| C | 1.181808 | 1.224034 | -0.815745 |
| C | -0.637329 | 0.096253 | 0.485978 |
| C | -0.520977 | 2.604263 | 0.422108 |
| H | -0.492422 | 2.207063 | -1.702547 |
| H | 0.207988 | 2.752771 | 1.228850 |
| H | 0.775975 | 3.316838 | -1.173047 |
| H | -1.156060 | 3.491537 | 0.390894 |
| C | -1.034363 | -1.264699 | 0.987534 |
| C | 0.253526 | -2.087456 | 0.844700 |
| H | 0.859700 | -1.940545 | 1.745660 |
| H | 0.084086 | -3.154799 | 0.704968 |
| C | 0.958012 | -1.413475 | -0.338660 |
| Br | -3.123100 | 1.475480 | -0.236155 |
| H | -1.476972 | -1.269698 | 1.982532 |
| H | 0.612890 | -1.814551 | -1.295653 |
| H | 1.650979 | 0.986271 | -1.770402 |
| Br | -2.483898 | -2.137154 | -0.136636 |
| Br | 2.897525 | -1.807153 | -0.380806 |
| Br | 2.788909 | 1.778605 | 0.312270 |

**17**

| | | | |
|----|-----------|-----------|-----------|
| H | 2.284929 | 1.605074 | -1.600361 |
| C | 1.408595 | 1.607524 | -0.951601 |
| C | -0.867655 | 2.626756 | -0.529635 |
| C | -0.635780 | 0.146277 | -0.918970 |
| C | -1.569220 | 1.322044 | -0.907469 |
| C | 0.711459 | 0.287738 | -0.985294 |
| C | 0.457519 | 2.755576 | -1.290171 |
| H | -0.670175 | 2.635570 | 0.546321 |
| H | 0.272701 | 2.719548 | -2.373708 |
| H | -1.524462 | 3.471841 | -0.750098 |
| H | 0.931475 | 3.716540 | -1.077197 |
| C | 1.383104 | -1.014343 | -1.311901 |
| C | 0.221370 | -1.939390 | -1.714063 |
| H | 0.131486 | -1.911414 | -2.807999 |
| H | 0.362207 | -2.976255 | -1.413833 |
| C | -1.036185 | -1.287019 | -1.121208 |
| H | -1.932068 | -1.415979 | -1.727321 |
| Br | 2.244453 | 1.950307 | 0.863972 |
| Br | -1.553198 | -2.178106 | 0.615019 |
| H | 2.134516 | -0.909294 | -2.094383 |
| H | -2.020817 | 1.401468 | -1.901680 |
| Br | 2.479168 | -1.772744 | 0.198575 |
| Br | -3.187008 | 1.086762 | 0.237966 |



| | | | |
|---|-----------|-----------|-----------|
| H | -2.717736 | -1.004975 | -1.176354 |
| C | -1.698500 | -0.970254 | -0.781033 |
| C | -1.017153 | 0.399394 | -1.138524 |
| H | -1.189369 | 0.734020 | -2.161910 |
| C | -1.585323 | 1.287711 | 0.000000 |
| H | -1.166006 | 2.295854 | 0.000000 |
| H | -2.679046 | 1.341493 | 0.000000 |
| C | -1.017153 | 0.399394 | 1.138524 |
| H | -1.189369 | 0.734020 | 2.161910 |
| C | 0.418612 | 0.280656 | -0.669580 |
| C | 0.418612 | 0.280656 | 0.669580 |
| H | -1.152596 | -1.816740 | -1.202871 |
| C | -1.698500 | -0.970254 | 0.781033 |
| H | -2.717736 | -1.004975 | 1.176354 |
| H | -1.152596 | -1.816740 | 1.202871 |
| C | 1.738004 | -0.150439 | -1.248025 |
| H | 2.093472 | 0.474954 | -2.073451 |
| H | 1.679014 | -1.176940 | -1.638249 |
| C | 1.738004 | -0.150439 | 1.248025 |
| H | 1.679014 | -1.176940 | 1.638249 |
| H | 2.093472 | 0.474954 | 2.073451 |
| C | 2.670303 | -0.066683 | 0.000000 |
| H | 3.443417 | -0.838508 | 0.000000 |
| H | 3.177492 | 0.901740 | 0.000000 |



| | | | |
|---|-----------|-----------|-----------|
| H | 1.398768 | -0.151373 | 2.221206 |
| C | 1.682137 | -0.094780 | 1.166965 |
| C | 0.976527 | -1.168477 | 0.290744 |
| C | 1.407677 | -0.732984 | -1.133743 |
| C | 1.564387 | 0.820803 | -1.024109 |
| C | 1.063547 | 1.118986 | 0.420572 |
| H | 2.772856 | -0.121170 | 1.091137 |
| H | 1.215106 | -2.205741 | 0.532093 |
| H | 2.352895 | -1.207768 | -1.407870 |
| H | 0.674988 | -1.018029 | -1.891774 |
| H | 0.985768 | 1.358889 | -1.776232 |
| H | 2.612826 | 1.119630 | -1.123115 |
| H | 1.318661 | 2.113215 | 0.788009 |
| C | -0.492943 | -0.758316 | 0.569002 |
| H | -0.694918 | -0.994512 | 1.625785 |
| C | -0.401511 | 0.749714 | 0.398711 |
| C | -1.562328 | 1.274625 | 0.006712 |
| H | -1.761761 | 2.318225 | -0.209236 |
| C | -1.736825 | -1.116392 | -0.260612 |
| H | -2.255893 | -2.009598 | 0.095964 |
| H | -1.465952 | -1.282112 | -1.308537 |
| C | -2.605668 | 0.175817 | -0.156001 |
| H | -3.240197 | 0.326050 | -1.035158 |
| H | -3.280948 | 0.127366 | 0.710187 |