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SUPPORTING INFORMATION

Butterflyene: An entry into an aesthetically pleasing carbocycle *via* Diels–Alder Reaction on a Tetrasubstituted olefin

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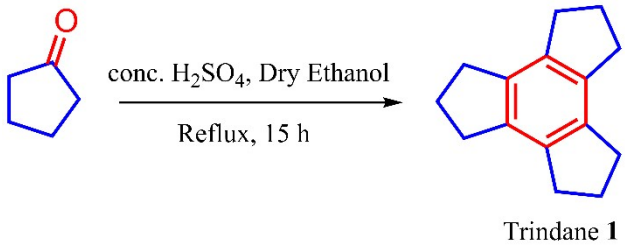
Experimental Procedures:

General Information

All the chemicals were purchased from Sigma Aldrich, Spectrochem and SD Fine-Chem Limited. All solvents were dried and distilled prior to use and stored on oven dried molecular sieves. All the compounds were purified by column chromatography using Acme silica gel (60-120 mesh). Thin Layer Chromatography was performed on silica gel aluminium plates. The spots were visualized under UV light or with iodine vapour. The melting points of all synthesized compounds were recorded under optical Polarized Light Microscope attached with Nikon camera and Linkam heating stage. IR spectra were recorded on a SHIMADZU FTIR-245068 spectrophotometer over KBr pellets. Bruker Avance 400 MHz & 600 MHz NMR was used to record ^{1}H & ^{13}C NMR spectra. HRMS data of final compounds were recorded in XEVO G2-XS QTOF Mass Spectrometer from IIT Ropar.

Typical procedure for synthesis of trindane 1



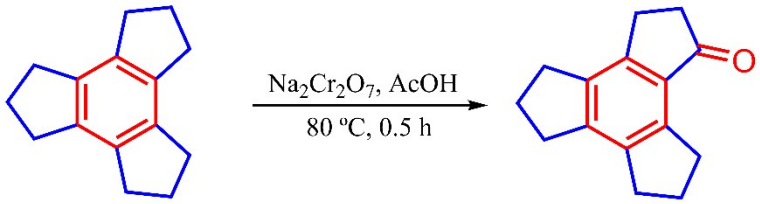
Trindane **1**

Scheme S1

Cyclopentanone (16 ml, 180 mmol) and dry ethanol (18 ml) was taken in two-neck round-bottomed flask (100 mL) equipped with a condenser. A dropwise addition of concentrated sulfuric acid (8 ml, 150 mmol) into reaction mixture followed by refluxed for 15 h. After completion of reaction, mixture was poured on to ice, neutralized with sodium carbonate and extracted with ethyl acetate (3 x 30 ml). Organic layer was washed with water, brine and dried over Na_2SO_4. Removal of solvent under reduced pressure furnished a dark brown liquid which was chromatographed on

a column of silica gel using light petroleum to furnished trindane as white solid (3.8 g, 32 %Yield); mp 90 °C (lit 95–97 °C)[1]

General procedure for synthesis of trindan-1-one 6



Trindane **1** Trindan-1-one **6**

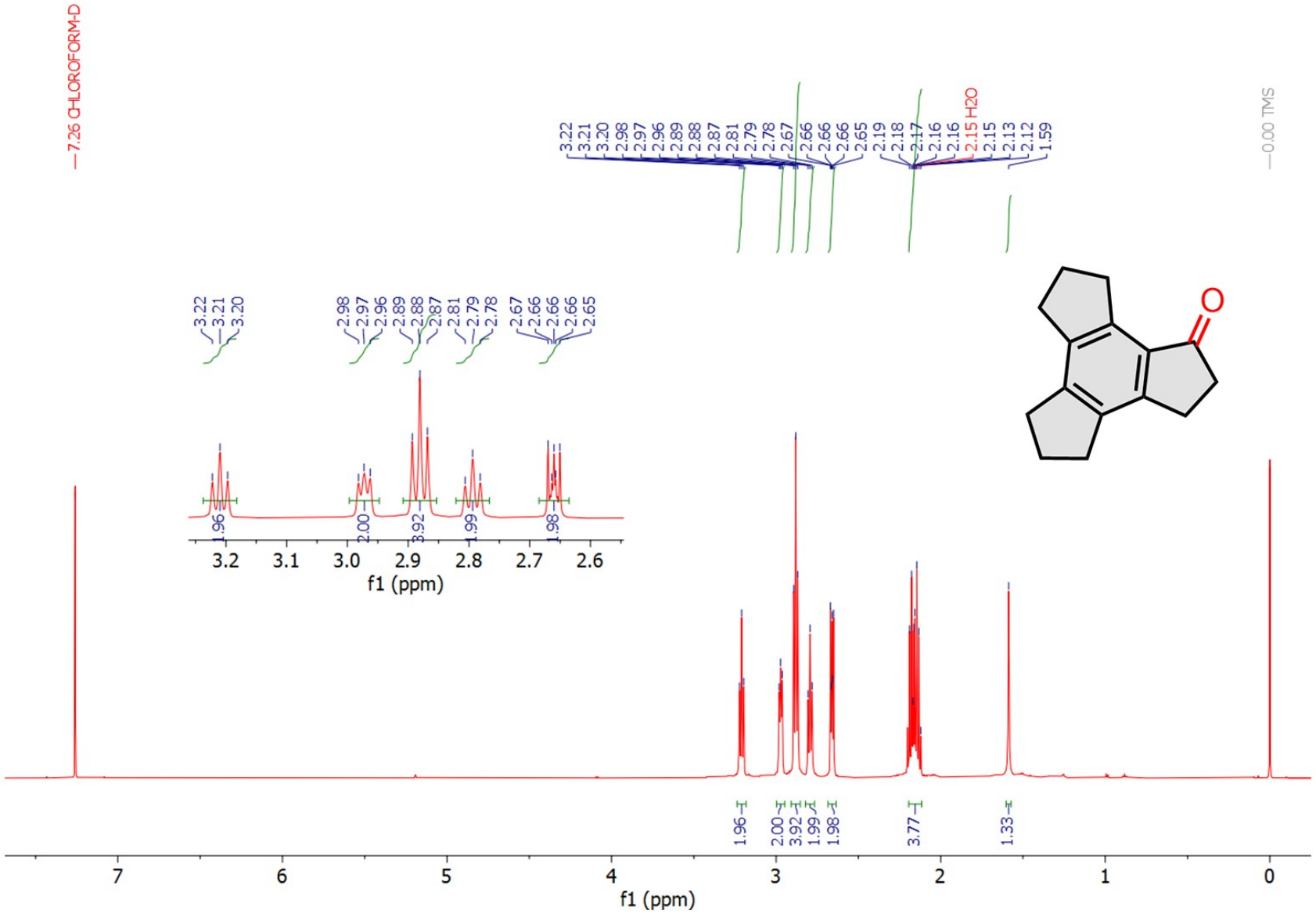
Scheme S2

Trindane (2.50 g, 12.62 mmol) was dissolved in glacial acetic acid (25 mL) and the stirred solution was maintained at 80 ºC. Sodium dichromate dihydrate (4.50 g, 15.14 mmol, 1.2 equiv.) in glacial acetic acid (20 mL) was added dropwise at 80 ºC. After 30 min reaction mixture was poured into ice water and the precipitate which formed was separated, washed with water (2 × 10 mL) and dried under vacuum. Resulted light yellow solid was then chromatographed on a column of silica gel using light petroleum and ethyl acetate (98:2) to furnished trindan-1-one as white solid (1.5 g, 56 %Yield); mp 115 ºC (lit 115 °C)[2]; IR (KBr cm^{-1}): 2953, 1703, ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.21 (t, J = 7.5 Hz, 2H), 3.00 – 2.95 (m, 2H), 2.88 (t, J = 7.5 Hz, 4H), 2.79 (t, J = 7.5 Hz, 2H), 2.68 – 2.64 (m, 2H), 2.19 – 2.12 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 207.71, 149.53, 147.05, 141.39, 139.96, 139.18, 131.49, 36.89, 31.96, 30.97, 30.39, 30.00, 25.55, 25.16, 24.59.

References

[1] S. Ranganathan, K. M. Muraleedharan, P. Bharadwaj and K. P. Madhusudanan, *Chem. Commun.* **1998**, 2239–2240.

[2] R. J. Ferrier, S. G. Holden and O. Gladkikh, *J. Chem. Soc., Perkin Trans. 1*, **2000**, 3505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2.66
2.66
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2.65
2.19
2.18
2.17
2.16
2.16
2.15 H2O
2.15
2.13
2.12
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1.98
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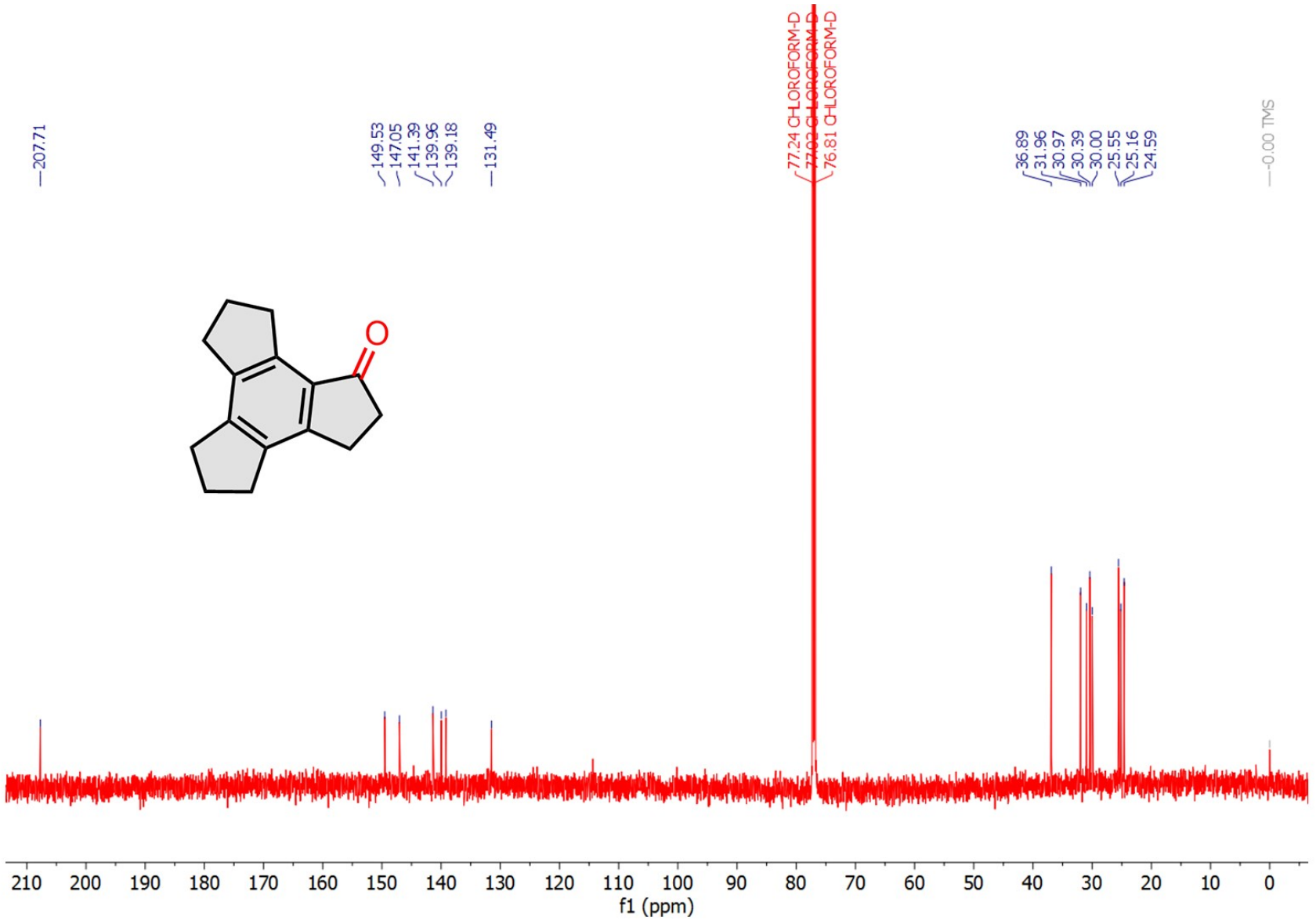
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77.03 CHLOROFORM-D
76.81 CHLOROFORM-D
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31.96
30.97
30.39
30.00
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24.59
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O
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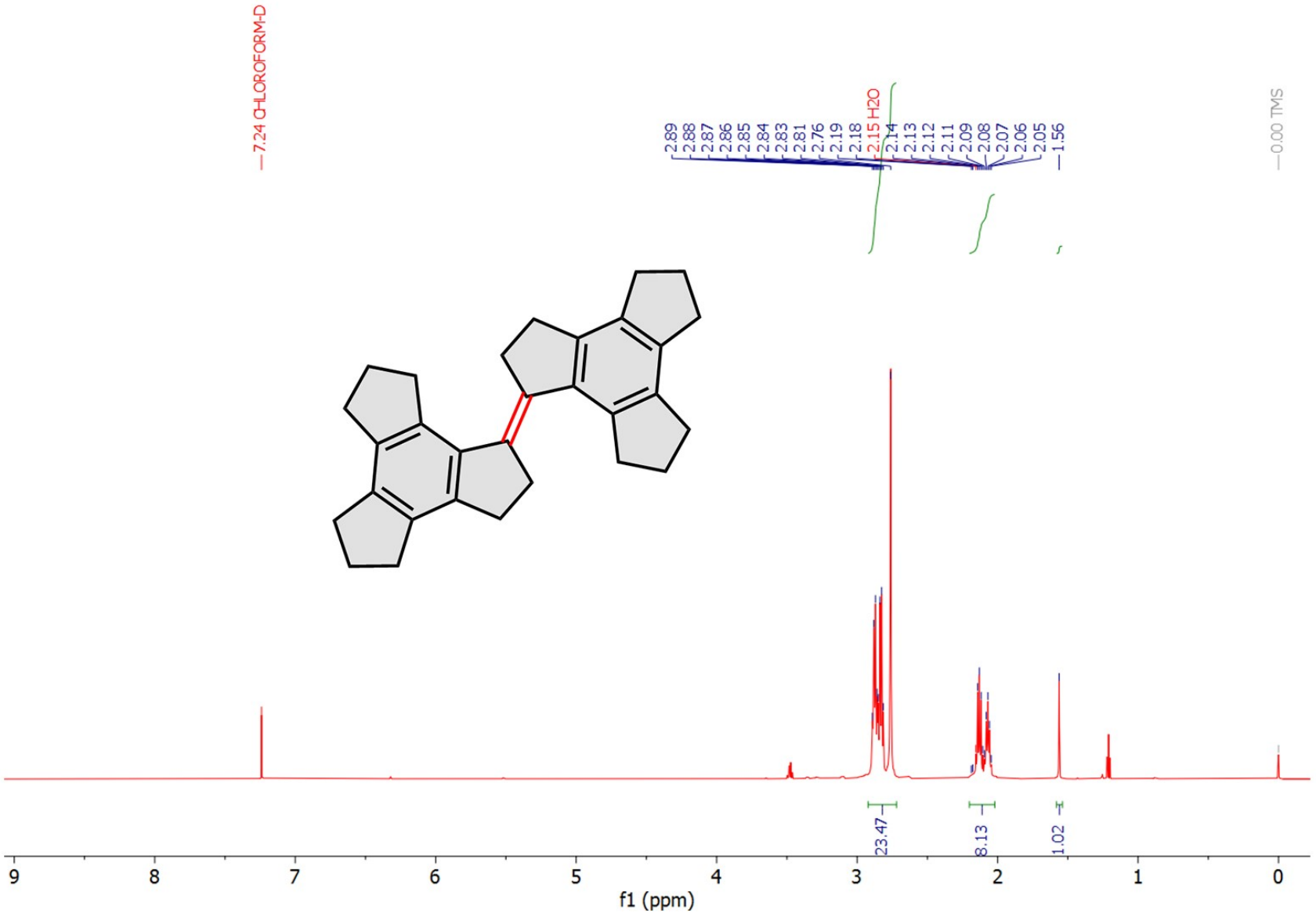
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2.07
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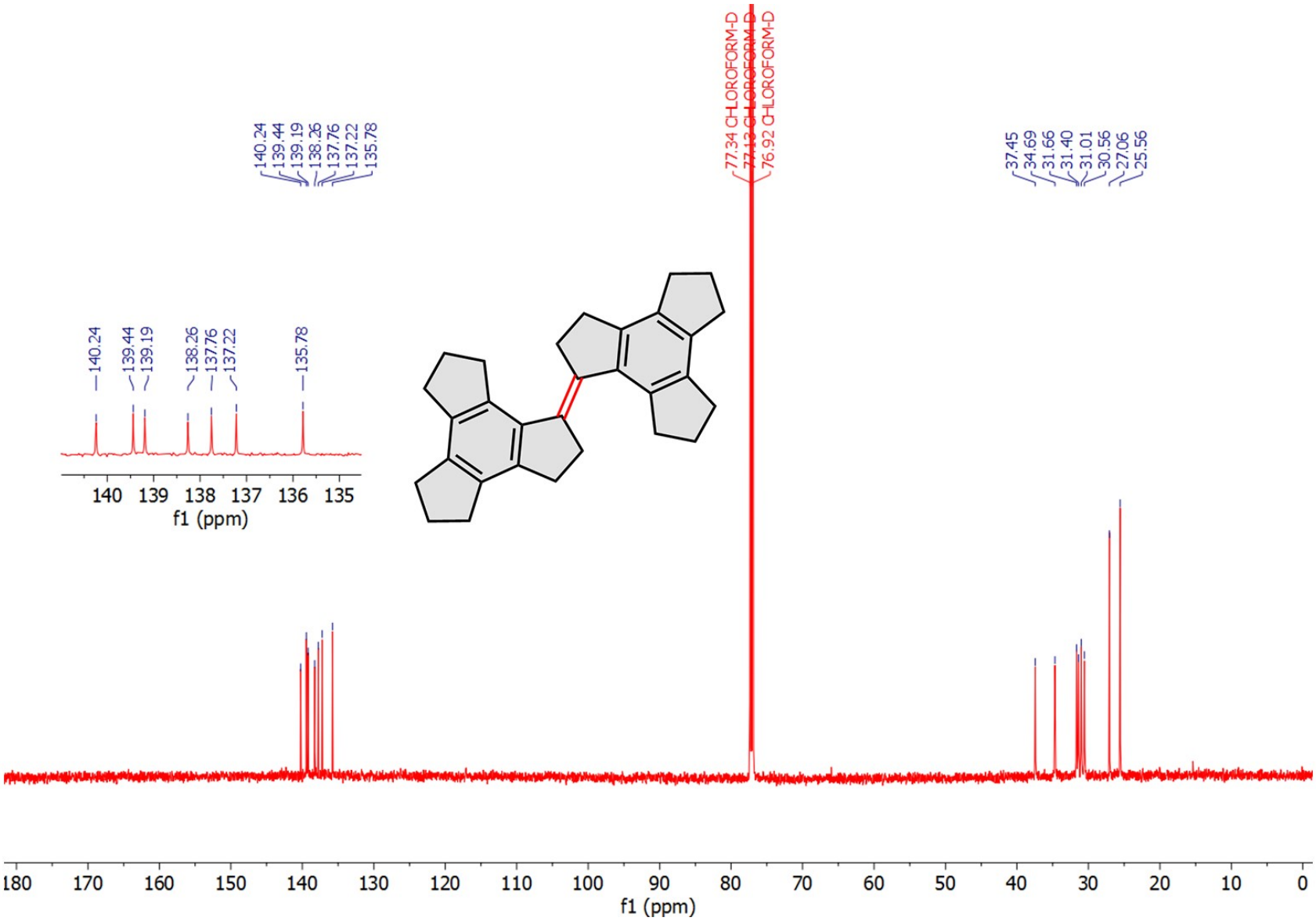
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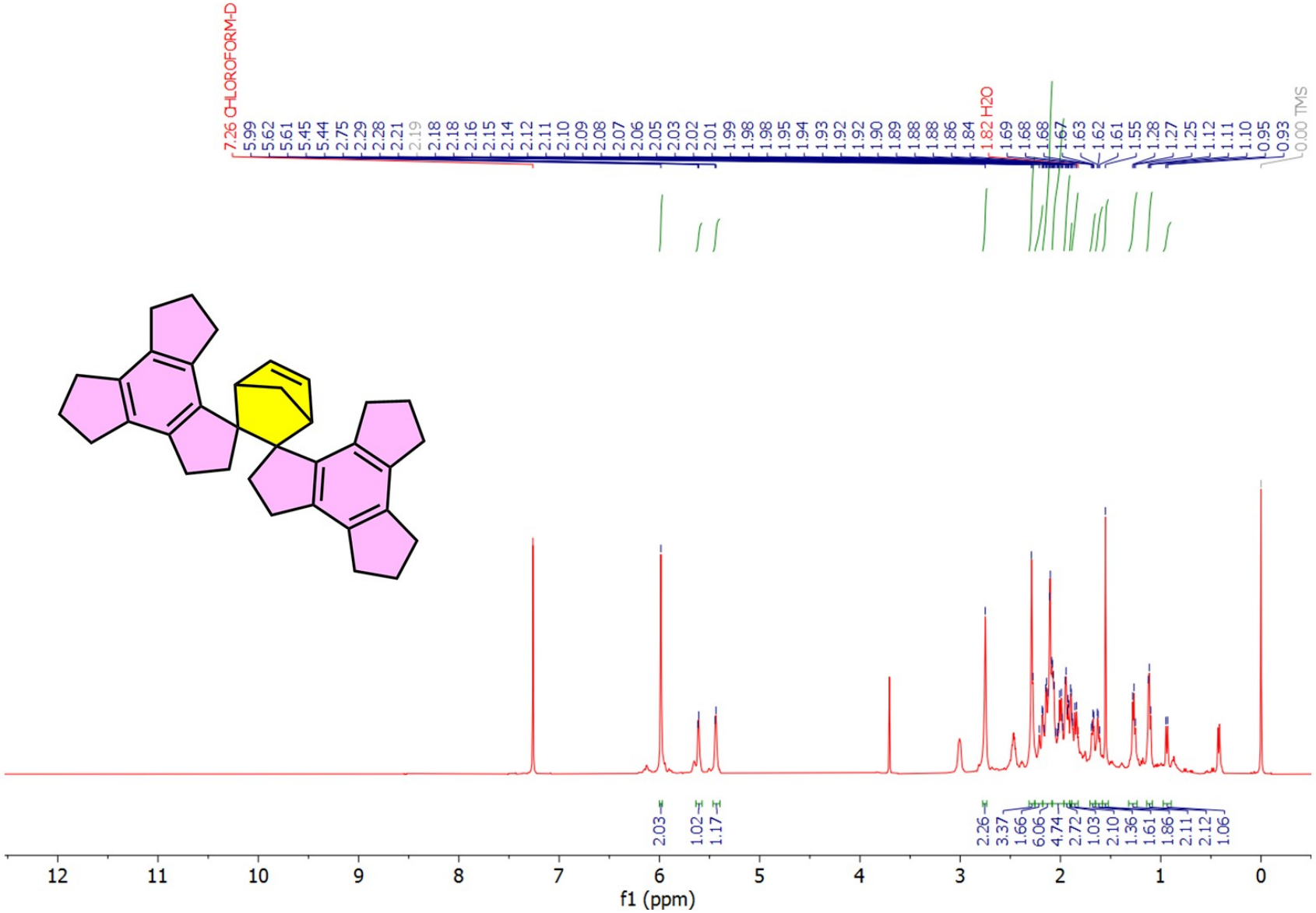
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6.06
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1.03
2.10
1.36
1.61
1.86
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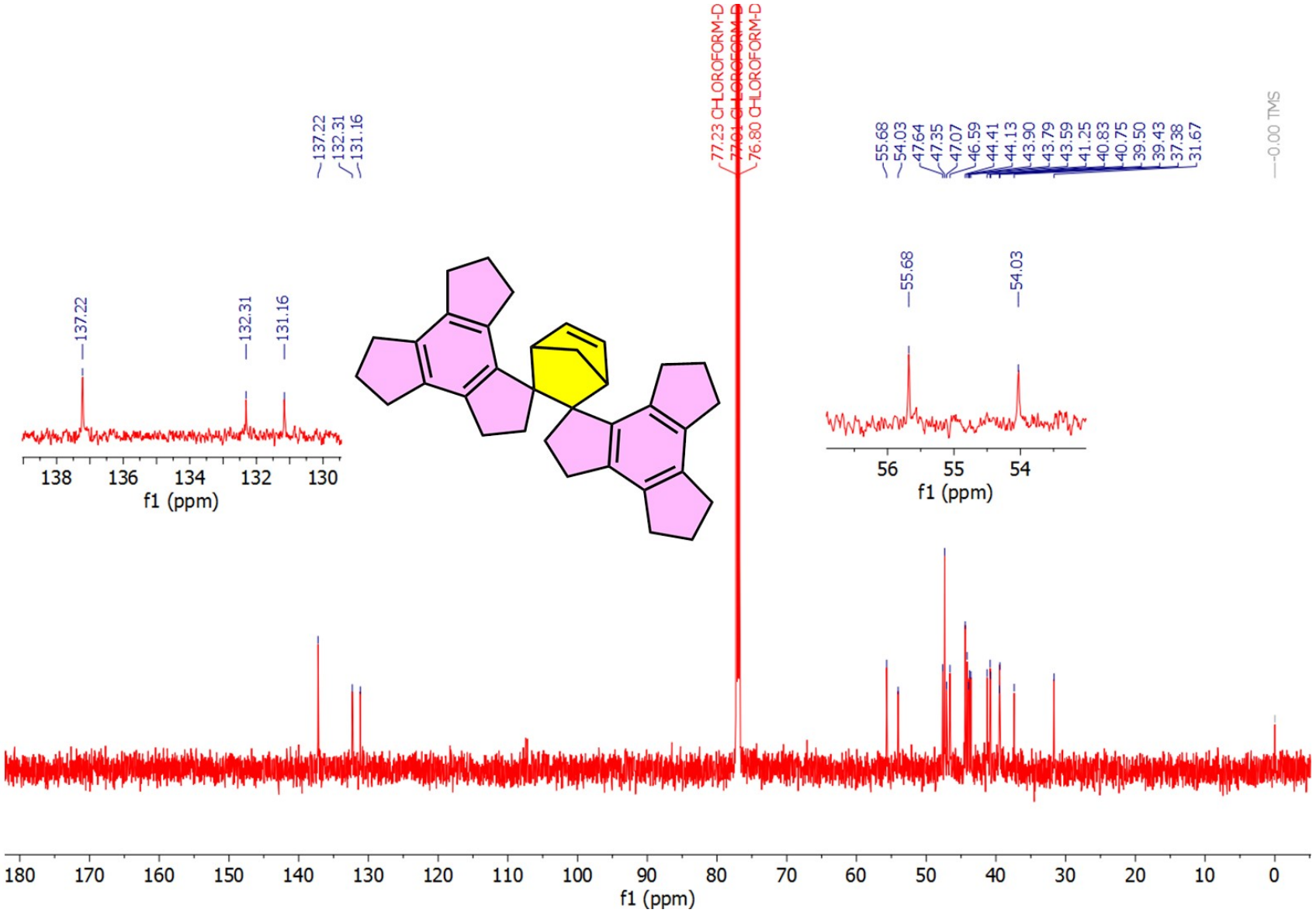
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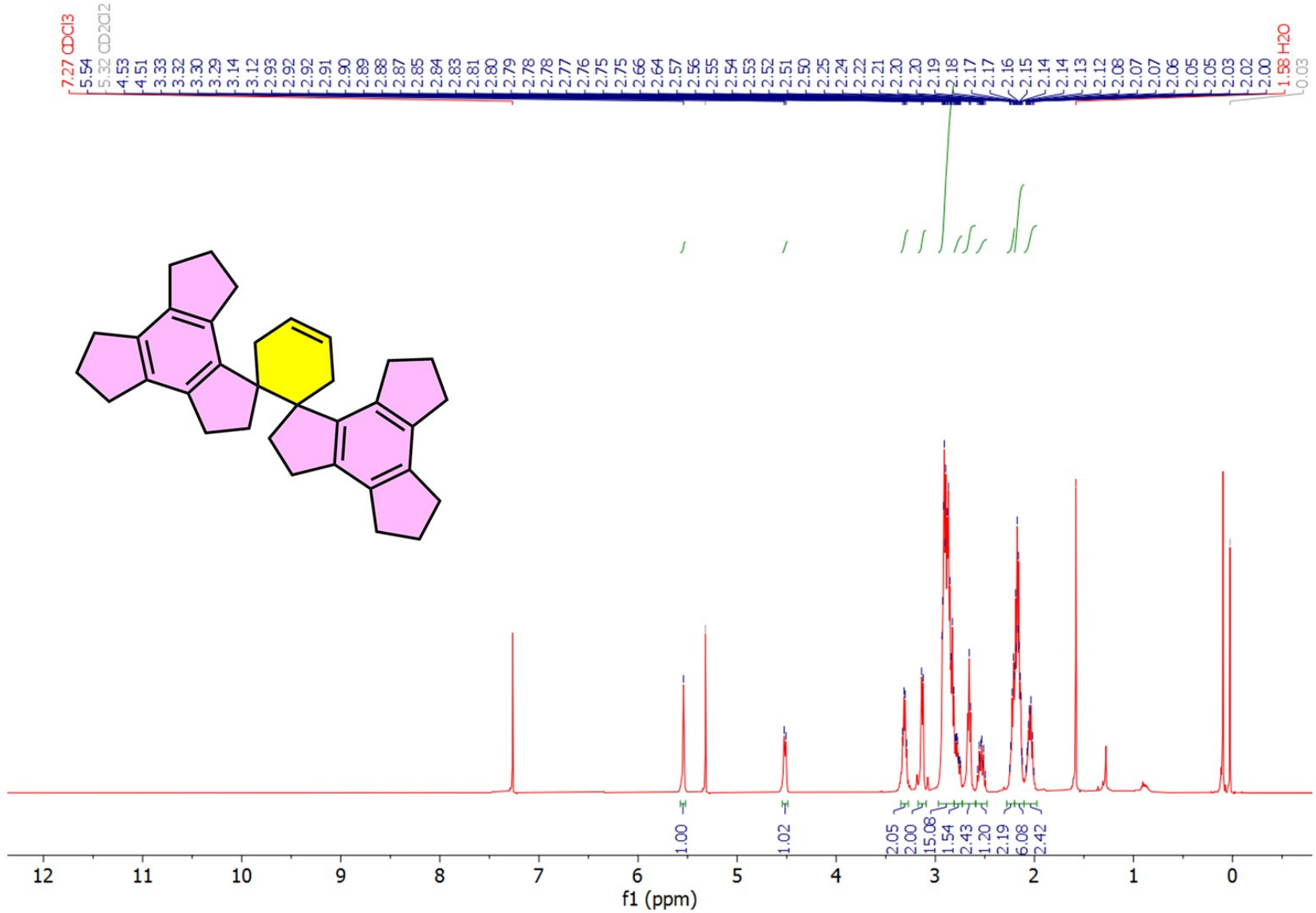
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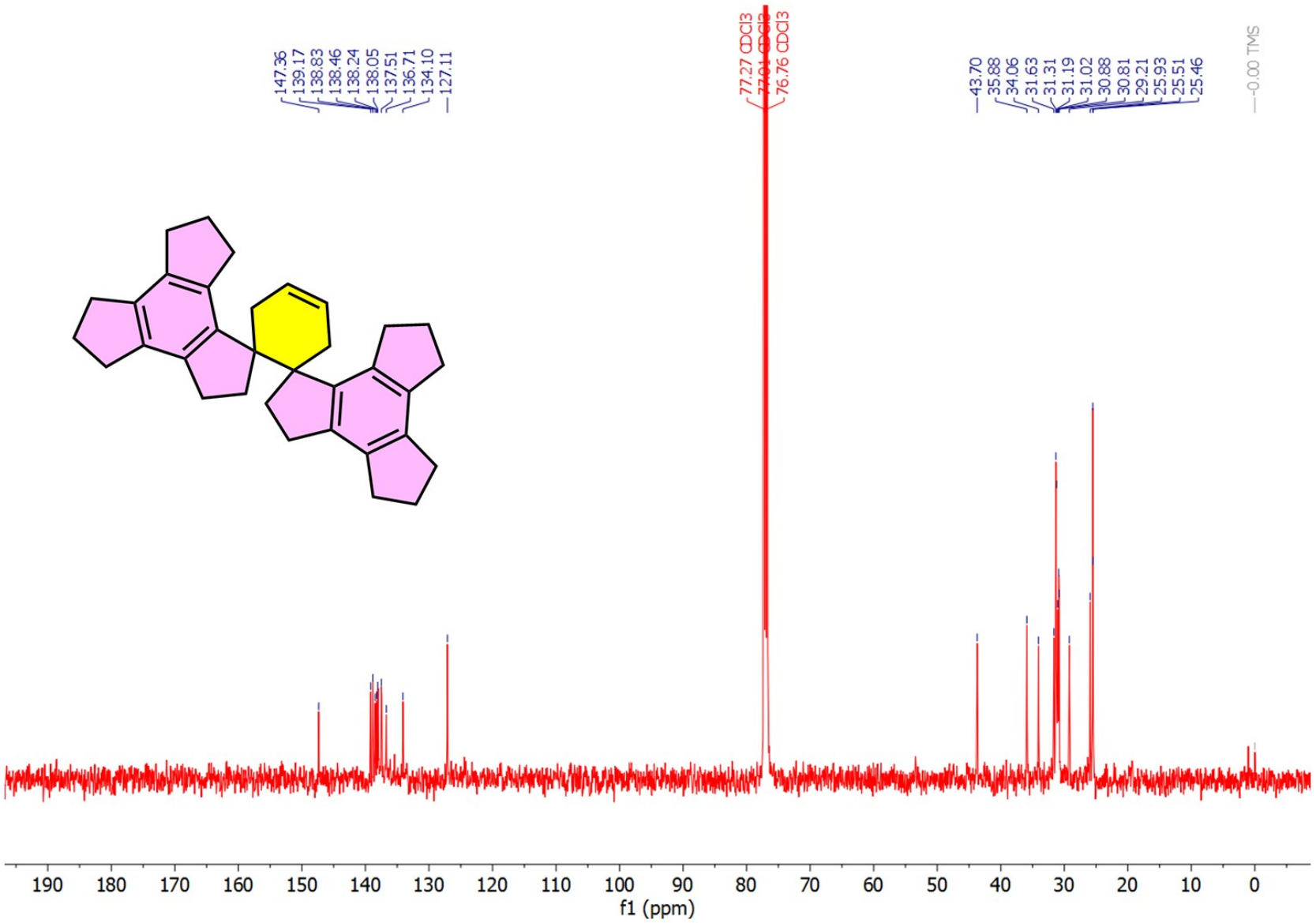
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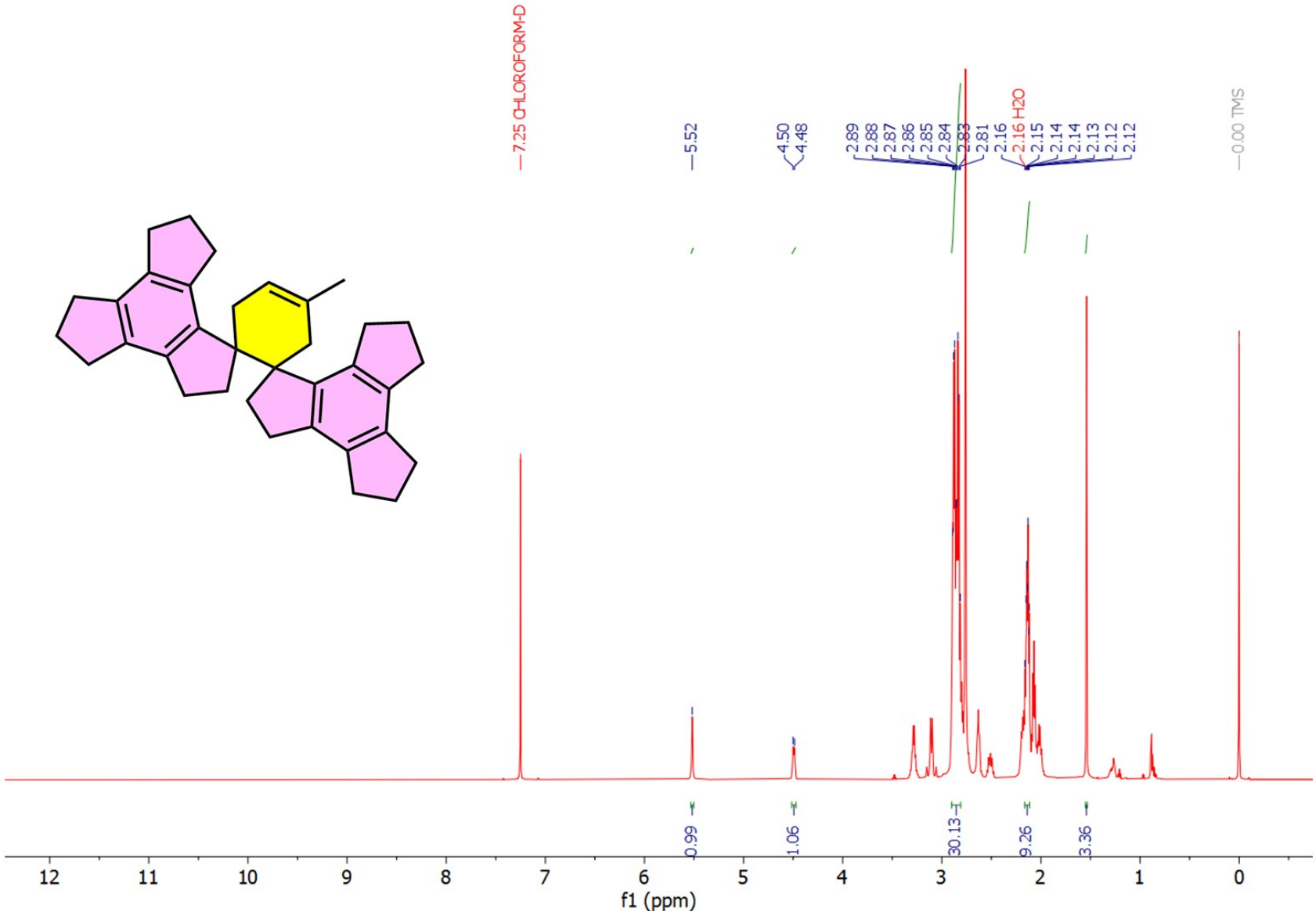
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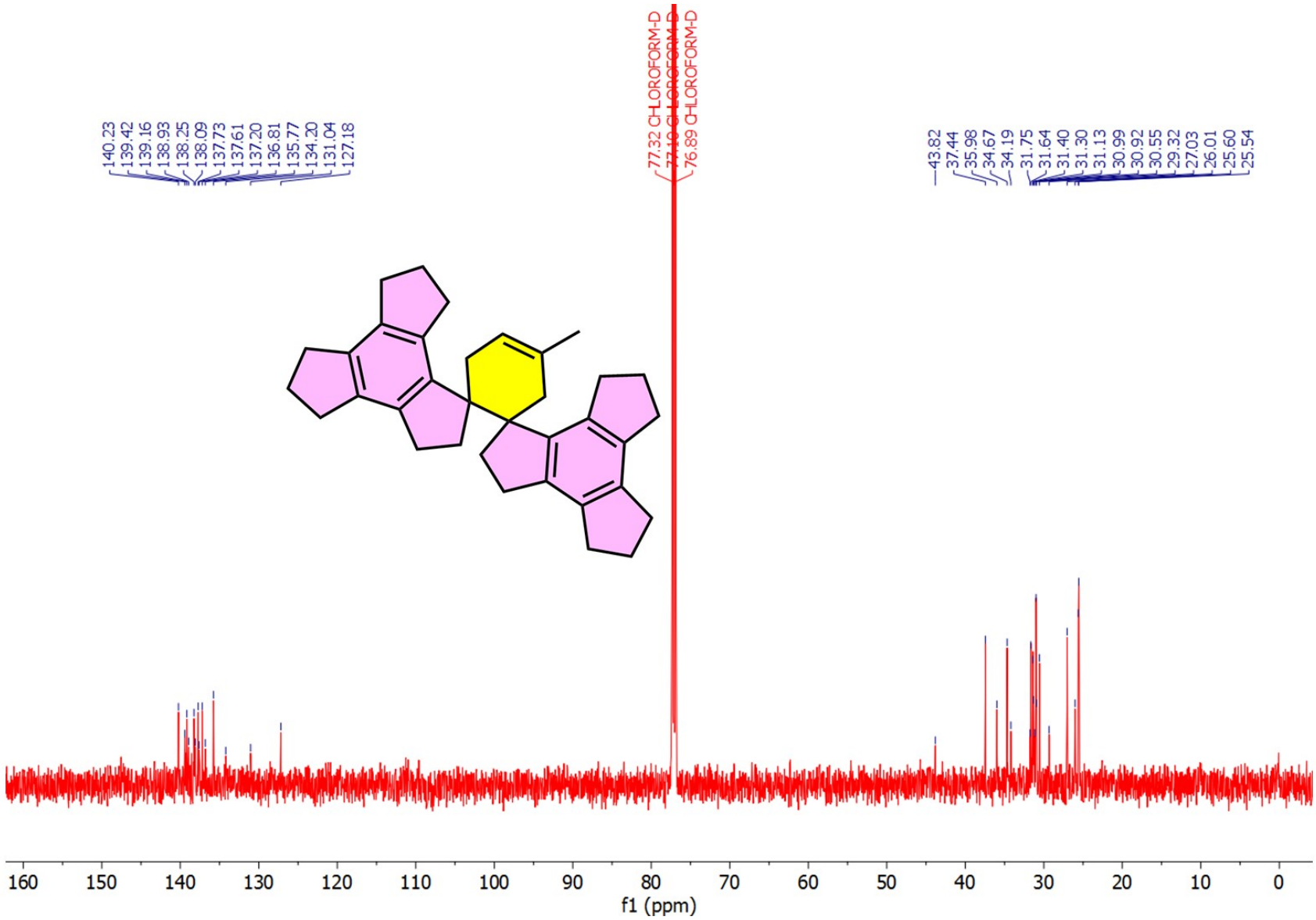
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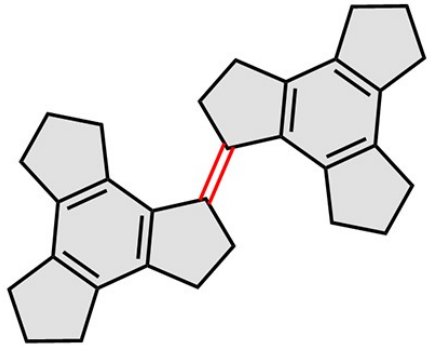

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Monoisotopic Mass, Even Electron Ions
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Elements Used:
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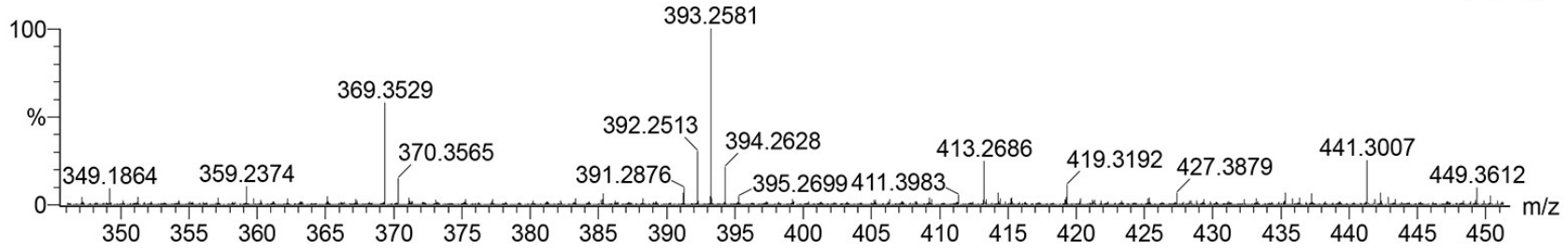

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Maximum:		2.0	10.0	50.0				
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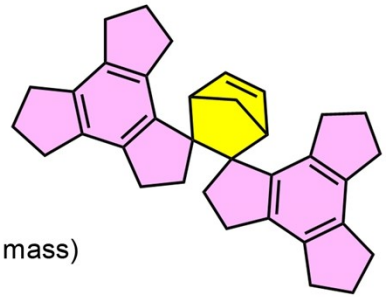
Elemental Composition Report



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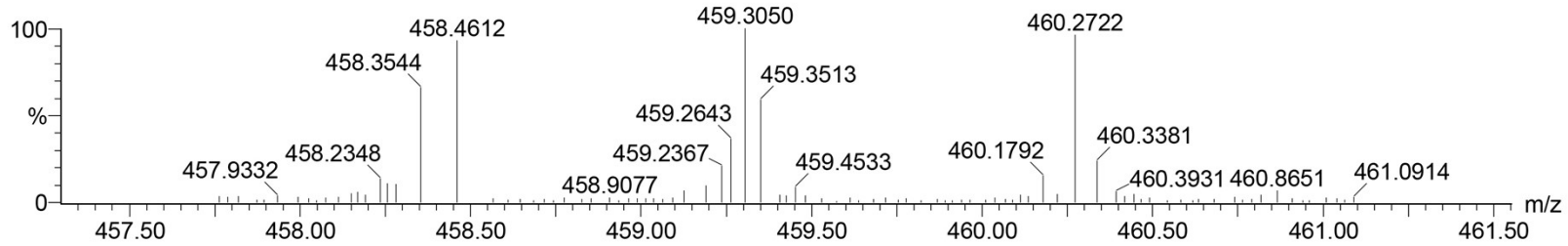

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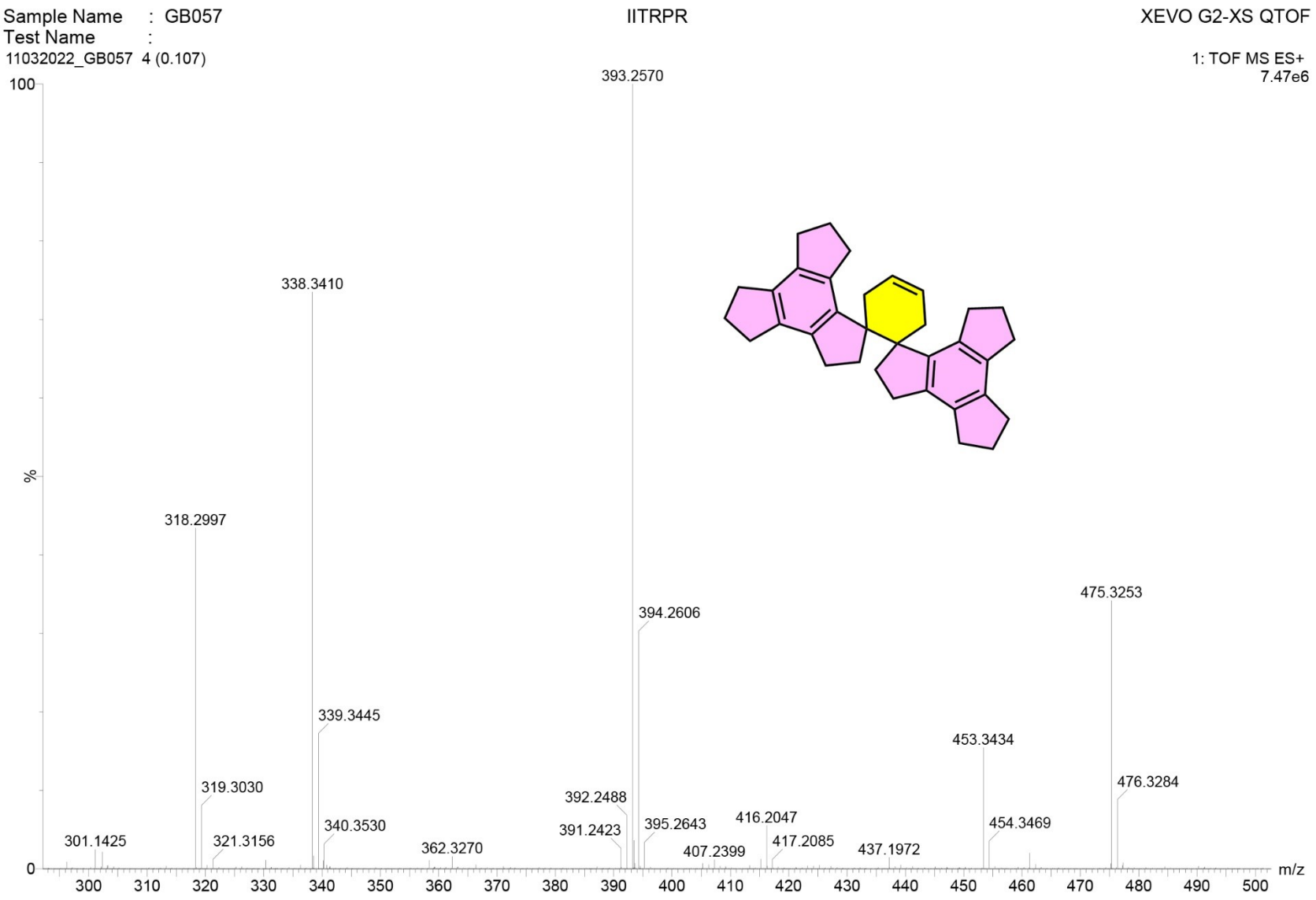
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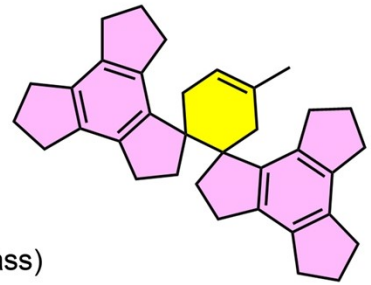

Single Mass Analysis

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Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
517 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)
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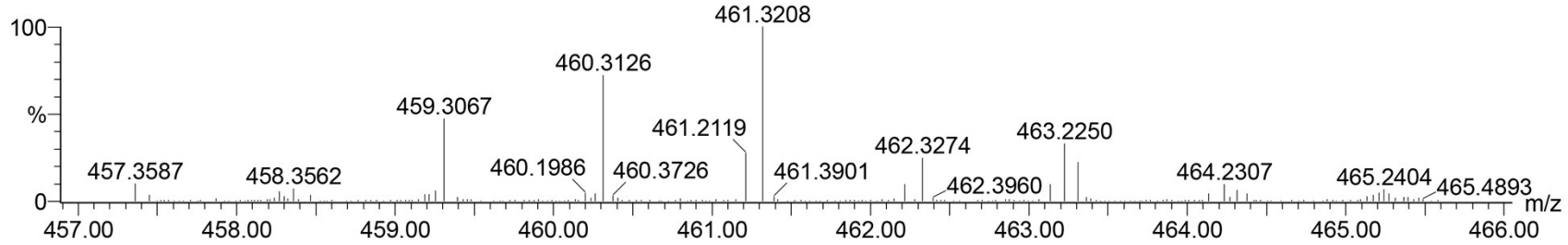

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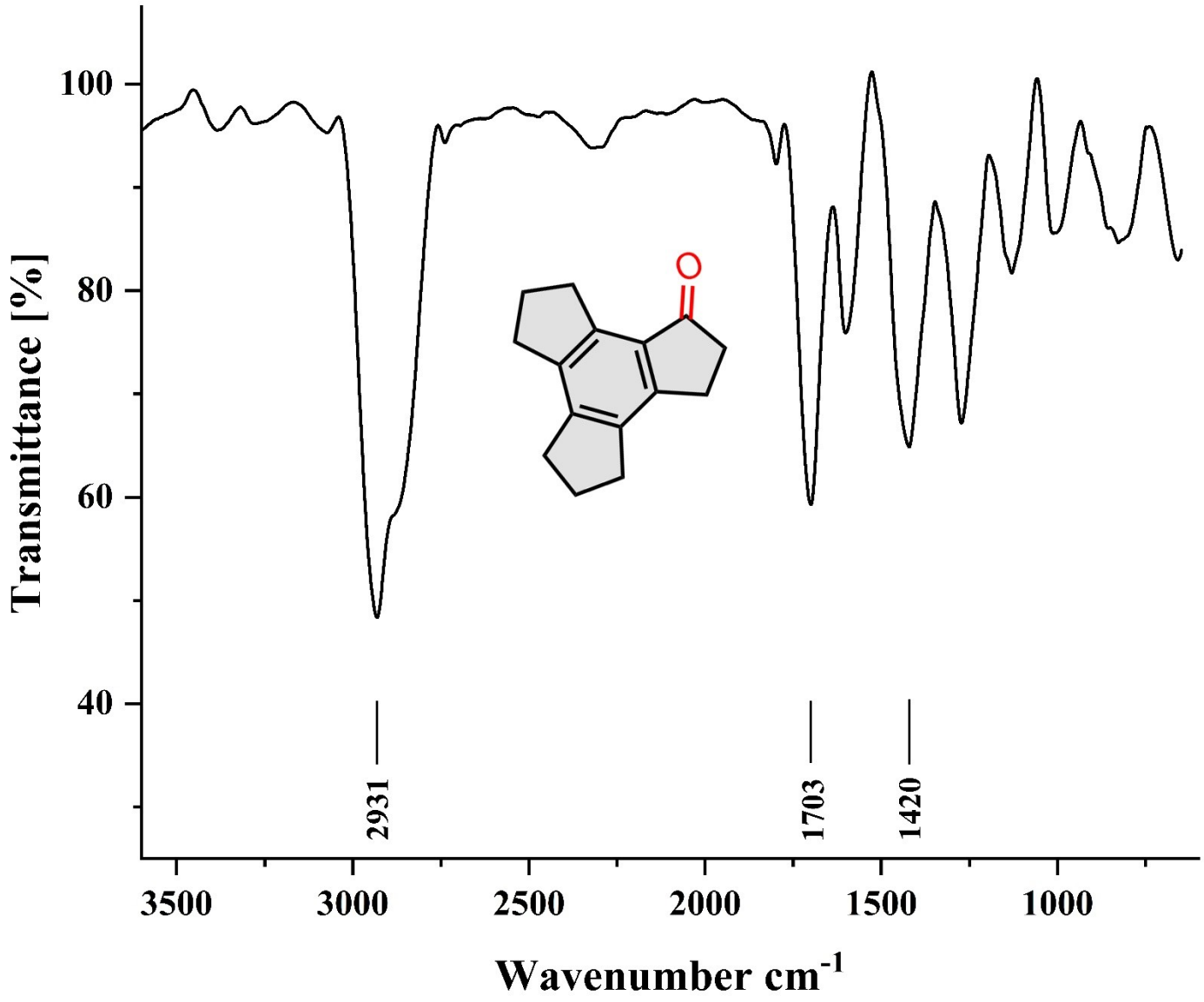
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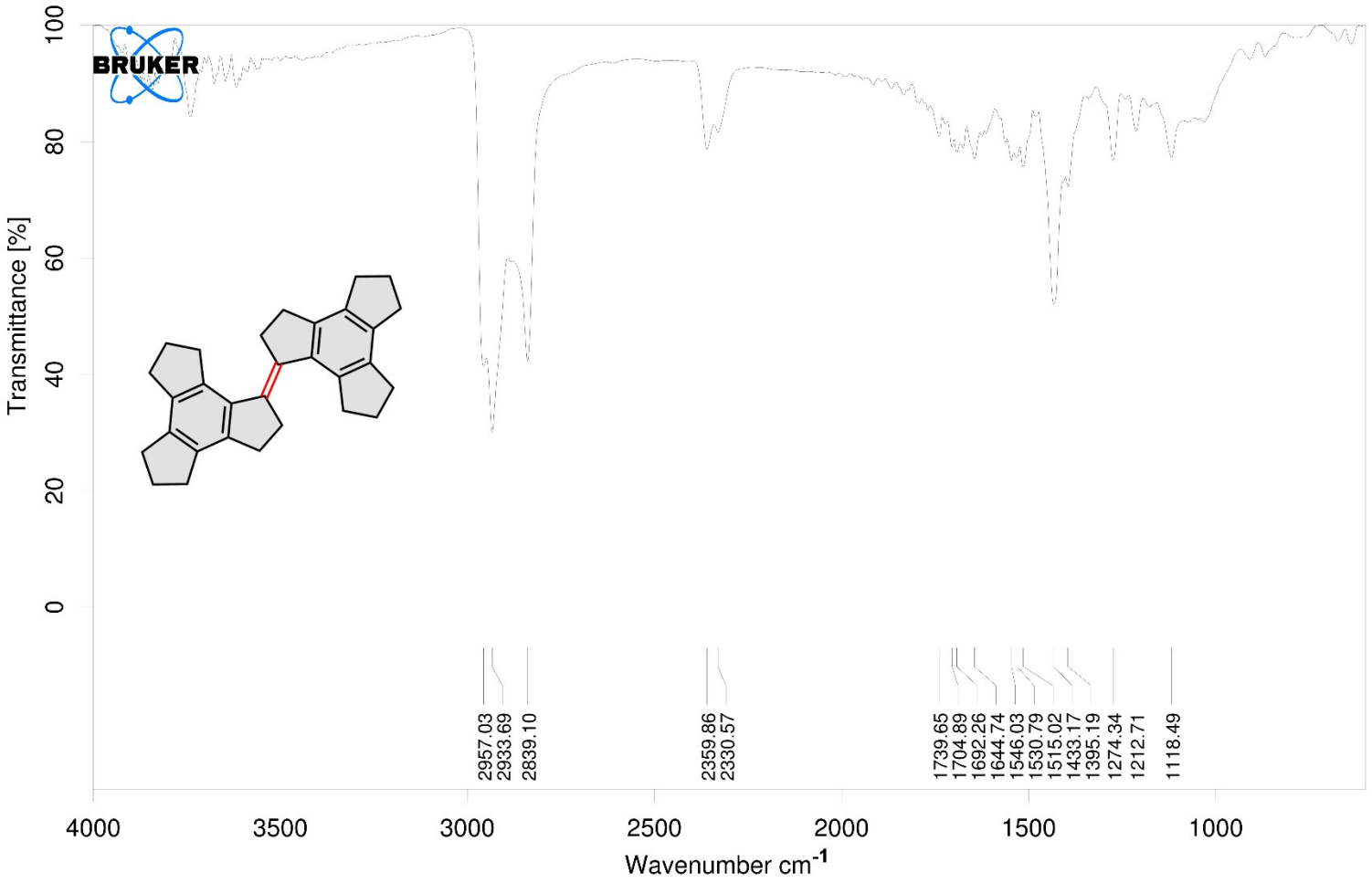
1000
Wavenumber cm-1



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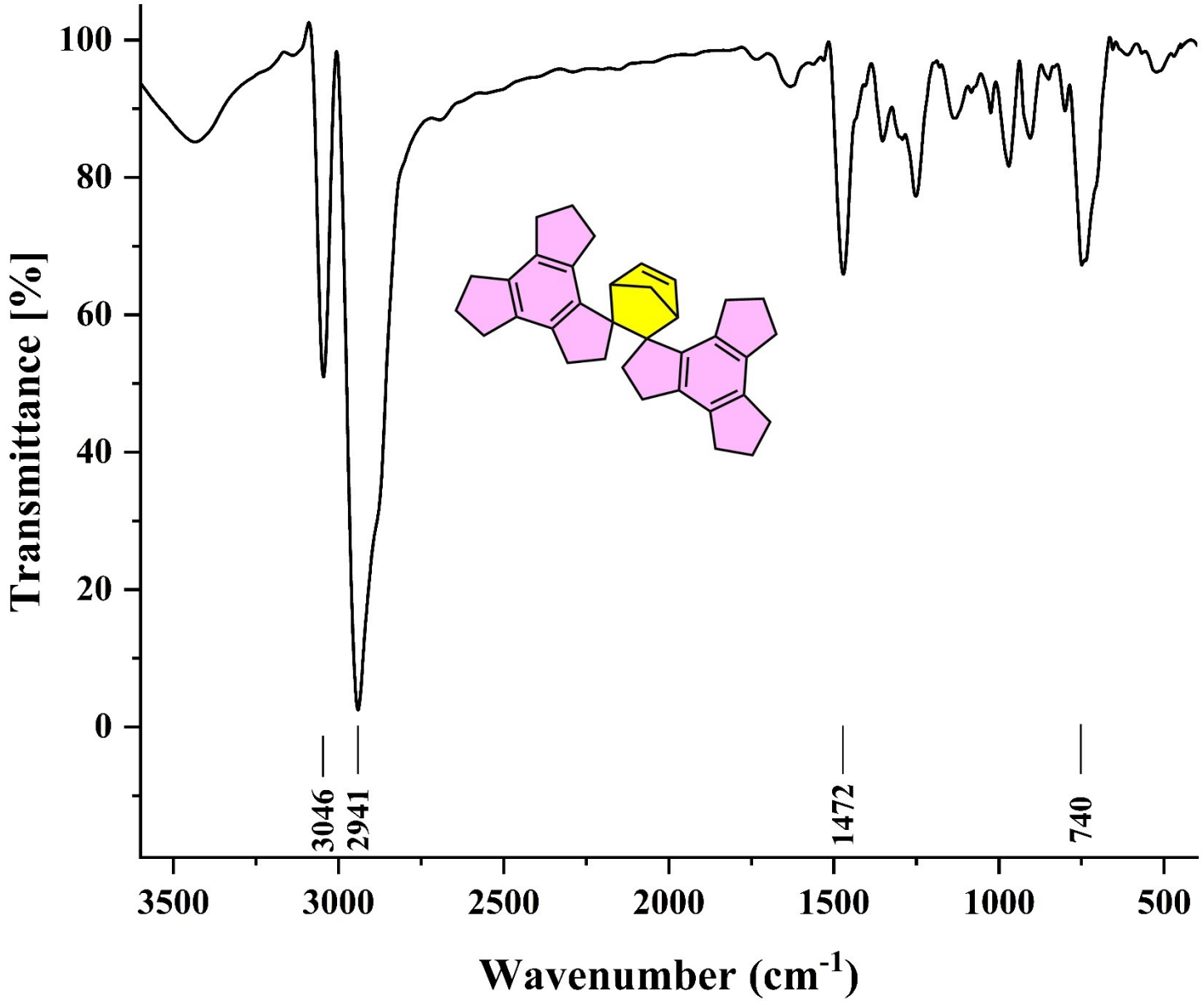
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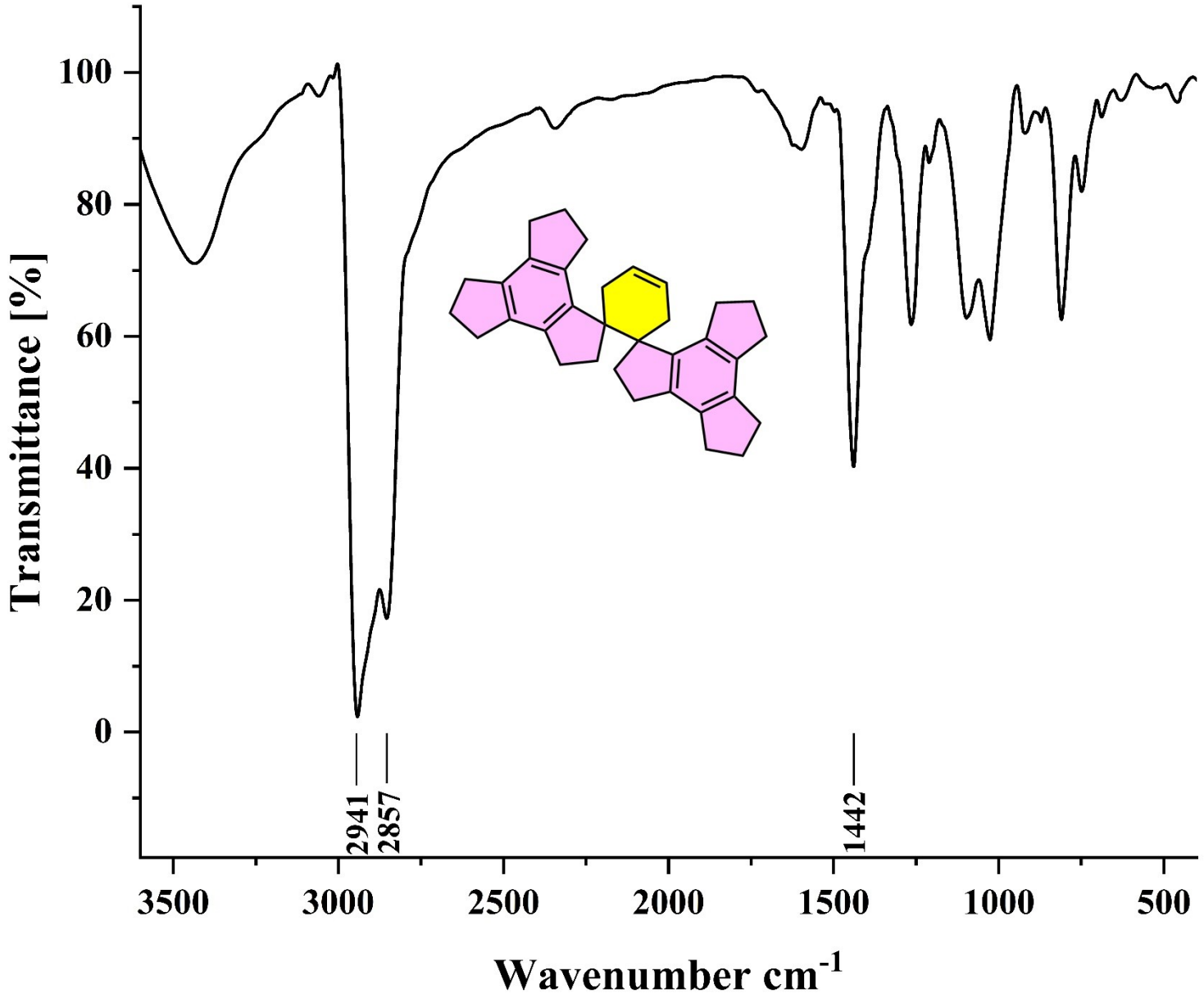
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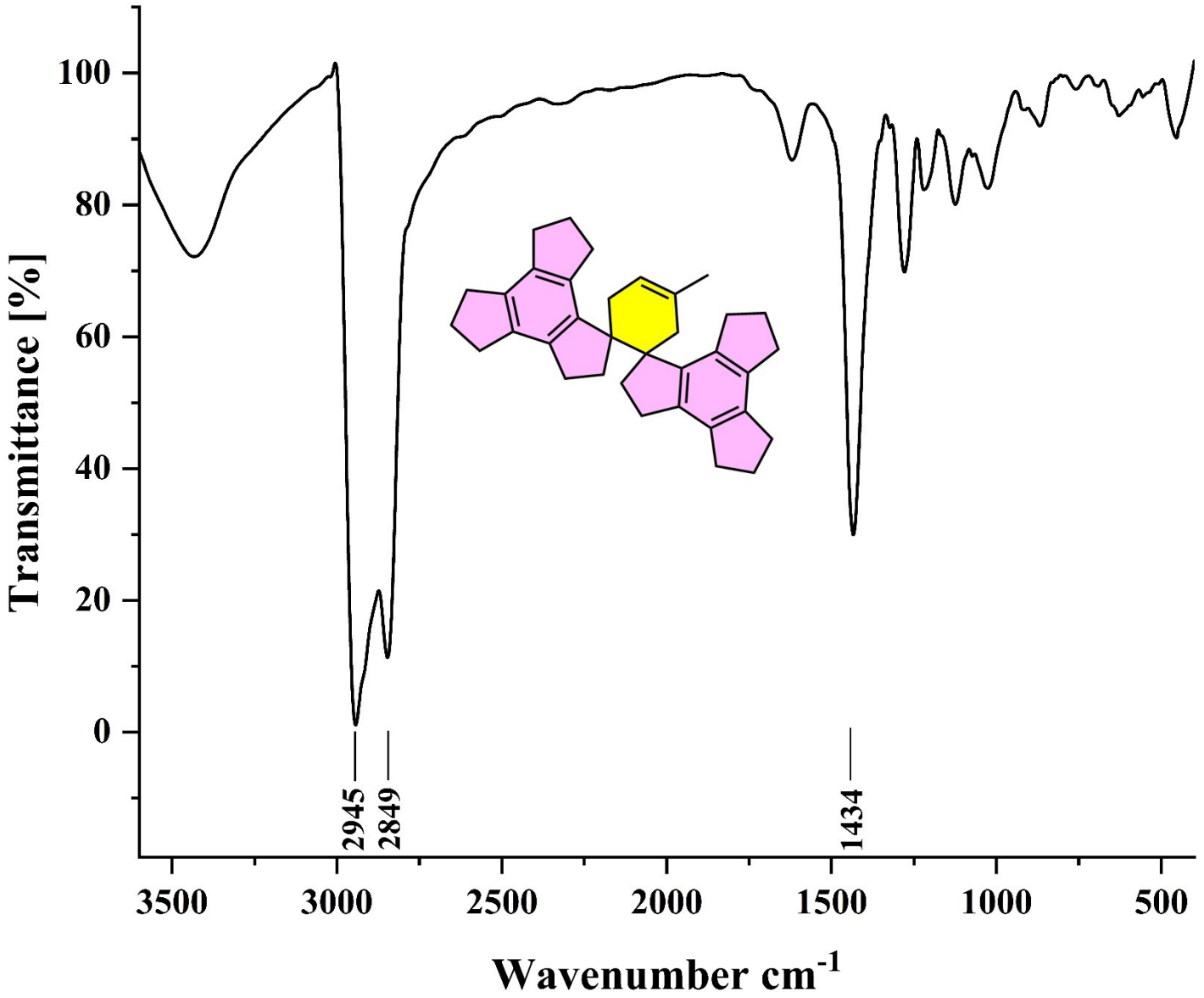
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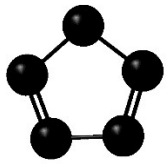
Optimized Atomic Coordinates of Compounds in Angstrom (Å) using DFT calculations



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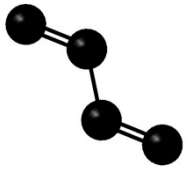

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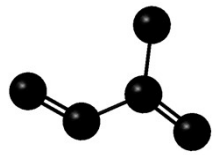
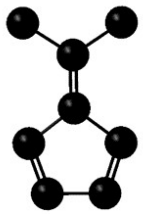
C	0.328641000000	1.811865000000	0.000000000000
C	-0.328641000000	-1.811865000000	0.000000000000
H	-1.416076000000	0.645607000000	0.000000000000
H	1.416076000000	-0.645607000000	0.000000000000
H	-0.192325000000	2.761054000000	0.000000000000
H	1.413499000000	1.840834000000	0.000000000000
H	0.192325000000	-2.761054000000	0.000000000000

H	-1.413499000000	-1.840834000000	0.000000000000



D_3 C_5H_8

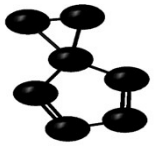
C	0.505402000000	-0.107646000000	-0.000032000000
C	-0.865234000000	-0.640579000000	-0.000038000000
C	1.532114000000	-0.964641000000	0.000025000000
C	0.748411000000	1.385098000000	-0.000009000000
C	-2.001536000000	0.057385000000	0.000023000000
H	-0.927078000000	-1.726486000000	-0.000075000000
H	2.559575000000	-0.617225000000	0.000022000000
H	1.370308000000	-2.036706000000	0.000081000000
H	-0.174300000000	1.961520000000	-0.001235000000
H	1.320273000000	1.676093000000	0.883113000000
H	1.322409000000	1.675765000000	-0.881845000000
H	-2.958073000000	-0.450636000000	0.000021000000
H	-2.028061000000	1.139973000000	0.000096000000



D_4 C_8H_{10}

C	-0.000024000000	-0.732879000000	-2.246106000000
C	0.000024000000	0.732879000000	-2.246106000000
C	0.000000000000	-1.172334000000	-0.969074000000
C	0.000000000000	1.172334000000	-0.969074000000

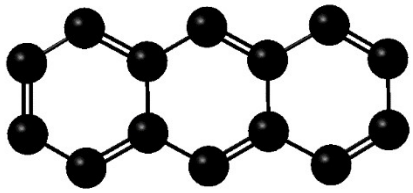
C	0.000000000000	0.000000000000	-0.079190000000
H	-0.000126000000	-1.350458000000	-3.133637000000
H	0.000126000000	1.350458000000	-3.133637000000
H	-0.000149000000	-2.203766000000	-0.651567000000
H	0.000149000000	2.203766000000	-0.651567000000
C	-0.000222000000	1.258430000000	2.088702000000
C	0.000000000000	0.000000000000	1.271390000000
H	-0.001091000000	2.161193000000	1.483253000000
H	0.878115000000	1.276793000000	2.741621000000
C	0.000222000000	-1.258430000000	2.088702000000
H	-0.878115000000	-1.276793000000	2.741621000000
H	0.001091000000	-2.161193000000	1.483253000000
H	0.877849000000	-1.275797000000	2.742600000000
H	-0.877849000000	1.275797000000	2.742600000000



D_5 C_7H_8

C	-1.736932000000	-0.733279000000	0.000034000000
C	-1.736957000000	0.733244000000	0.000211000000
C	-0.462526000000	-1.172466000000	-0.000564000000
C	-0.462569000000	1.172479000000	-0.000299000000
C	0.433245000000	0.000024000000	-0.000797000000
H	-2.625068000000	-1.350138000000	0.000798000000
H	-2.625113000000	1.350075000000	0.000660000000
H	-0.118381000000	-2.198107000000	-0.000749000000
H	-0.118470000000	2.198135000000	-0.000478000000
C	1.766040000000	0.000226000000	-0.740929000000
H	2.024756000000	-0.913656000000	-1.258483000000

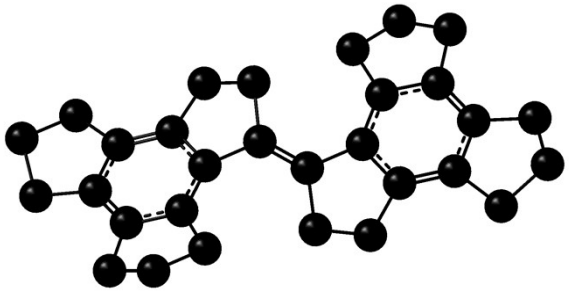
C	1.765073000000	-0.000231000000	0.741882000000
H	2.022788000000	0.913764000000	1.259688000000
H	2.022609000000	-0.914517000000	1.259245000000
H	2.024641000000	0.914461000000	-1.257906000000



D_6 $C_{14}H_{10}$

C	3.645678000000	-0.713831000000	0.000013000000
C	2.472522000000	-1.403838000000	-0.000039000000
C	1.217274000000	-0.717130000000	-0.000037000000
C	1.217274000000	0.717129000000	-0.000013000000
C	2.472522000000	1.403838000000	0.000024000000
C	3.645679000000	0.713831000000	0.000046000000
C	0.000001000000	-1.398991000000	-0.000025000000
C	0.000001000000	1.398991000000	-0.000012000000
C	-1.217274000000	0.717130000000	-0.000021000000
C	-1.217274000000	-0.717129000000	-0.000003000000
C	-2.472521000000	-1.403838000000	0.000037000000
H	-2.468009000000	-2.488574000000	0.000085000000
C	-3.645679000000	-0.713830000000	0.000040000000
C	-3.645679000000	0.713830000000	0.000000000000
C	-2.472521000000	1.403838000000	-0.000030000000
H	-0.000004000000	-2.484936000000	-0.000024000000
H	4.590233000000	-1.244646000000	0.000031000000
H	2.468008000000	-2.488574000000	-0.000076000000
H	2.468005000000	2.488574000000	0.000034000000

H	4.590230000000	1.244651000000	0.000084000000
H	-0.000004000000	2.484936000000	-0.000017000000
H	-4.590230000000	-1.244651000000	0.000055000000
H	-4.590231000000	1.244650000000	0.000010000000
H	-2.468009000000	2.488574000000	-0.000069000000

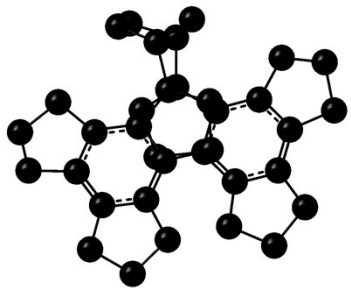


Bitrindanylidine 7 $C_{30}H_{32}$

C	-4.733312000000	-0.085079000000	-0.298577000000
C	-4.061045000000	-1.059157000000	0.420424000000
C	-2.666293000000	-1.000654000000	0.567500000000
C	-1.955049000000	0.048545000000	-0.013468000000
C	-2.654603000000	1.066911000000	-0.692770000000
C	-4.024875000000	0.991522000000	-0.851357000000
C	-0.522545000000	0.404015000000	0.027959000000
C	-0.454489000000	1.895843000000	-0.249328000000
C	-1.702722000000	2.154771000000	-1.125733000000
C	-4.621050000000	-2.230133000000	1.193620000000
C	-3.501302000000	-2.514400000000	2.214455000000
C	-2.204554000000	-2.112704000000	1.483797000000
C	-4.970871000000	1.941195000000	-1.548116000000
C	-6.344396000000	1.548821000000	-0.961585000000
C	-6.209605000000	0.057934000000	-0.582989000000
C	2.657486000000	0.982239000000	0.611976000000
C	1.960302000000	-0.082153000000	0.039874000000

C	2.676391000000	-1.115060000000	-0.597242000000
C	4.048393000000	-1.034482000000	-0.739206000000
C	4.742421000000	0.055264000000	-0.196822000000
C	4.054411000000	1.037392000000	0.496154000000
C	5.013535000000	-2.014947000000	-1.364406000000
C	6.295714000000	-1.170959000000	-1.532770000000
C	6.228375000000	-0.106787000000	-0.415812000000
C	0.527130000000	-0.437048000000	0.052062000000
C	0.466580000000	-1.935737000000	-0.188205000000
C	1.738352000000	-2.217759000000	-1.022968000000
C	4.599681000000	2.223683000000	1.256482000000
C	3.453381000000	2.537950000000	2.238702000000
C	2.174861000000	2.119849000000	1.485111000000
H	-0.542448000000	2.471693000000	0.677949000000
H	0.476562000000	2.175925000000	-0.742111000000
H	-1.450400000000	2.039590000000	-2.185740000000
H	-2.116812000000	3.156238000000	-0.992571000000
H	-4.768555000000	-3.089718000000	0.528708000000
H	-5.582692000000	-2.012122000000	1.662830000000
H	-3.640784000000	-1.865643000000	3.083218000000
H	-3.489625000000	-3.548244000000	2.562278000000
H	-1.825316000000	-2.961557000000	0.904742000000
H	-1.404336000000	-1.795431000000	2.156371000000
H	-4.943754000000	1.769355000000	-2.630575000000
H	-4.724552000000	2.992154000000	-1.381512000000
H	-6.520470000000	2.130194000000	-0.052904000000
H	-7.170638000000	1.740797000000	-1.647082000000
H	-6.839625000000	-0.222637000000	0.263997000000
H	-6.491646000000	-0.586596000000	-1.424023000000
H	5.185283000000	-2.857498000000	-0.683793000000

H	4.653660000000	-2.429013000000	-2.308709000000
H	6.263489000000	-0.668153000000	-2.502688000000
H	7.206905000000	-1.769007000000	-1.496302000000
H	6.704052000000	-0.471546000000	0.502741000000
H	6.726189000000	0.825813000000	-0.689828000000
H	-0.450703000000	-2.229164000000	-0.698765000000
H	0.528728000000	-2.487038000000	0.755896000000
H	1.514827000000	-2.134643000000	-2.092527000000
H	2.150797000000	-3.213532000000	-0.848339000000
H	4.771092000000	3.066182000000	0.575423000000
H	5.546251000000	2.010800000000	1.757753000000
H	3.567355000000	1.912592000000	3.128076000000
H	3.435723000000	3.580784000000	2.558230000000
H	1.813083000000	2.953516000000	0.873697000000
H	1.356552000000	1.822651000000	2.145000000000



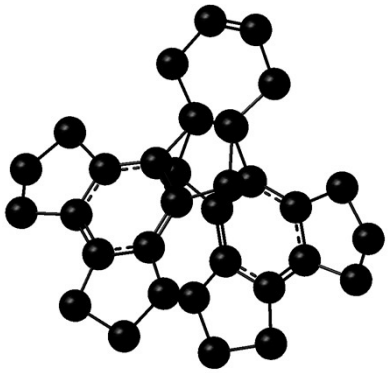
Butterflyene adducts 8 $C_{35}H_{38}$

C	3.416552000000	1.644578000000	0.492350000000
C	3.795715000000	0.474250000000	-0.141176000000
C	2.936849000000	-0.639215000000	-0.171539000000
C	1.686428000000	-0.566889000000	0.447774000000
C	1.355541000000	0.597692000000	1.165970000000
C	2.194978000000	1.697274000000	1.167830000000

C	0.517078000000	-1.555141000000	0.520421000000
C	-0.155645000000	-1.085641000000	1.836489000000
C	0.053003000000	0.433691000000	1.904627000000
C	5.093614000000	0.177593000000	-0.853005000000
C	5.116726000000	-1.360446000000	-0.867245000000
C	3.632045000000	-1.768303000000	-0.916914000000
C	2.031346000000	3.029413000000	1.861050000000
C	3.073076000000	3.914958000000	1.142527000000
C	4.173339000000	2.940618000000	0.666813000000
C	-2.887058000000	-0.682874000000	0.083073000000
C	-1.669975000000	-0.566543000000	-0.604219000000
C	-1.392327000000	0.655755000000	-1.250736000000
C	-2.259911000000	1.730207000000	-1.180383000000
C	-3.463583000000	1.609768000000	-0.488066000000
C	-3.776321000000	0.408578000000	0.122544000000
C	-2.133972000000	3.105226000000	-1.792990000000
C	-3.192333000000	3.920282000000	-1.016967000000
C	-4.258551000000	2.890487000000	-0.581456000000
C	-0.457916000000	-1.503242000000	-0.762403000000
C	0.227257000000	-0.873312000000	-2.013129000000
C	-0.078899000000	0.623978000000	-1.979263000000
C	-5.043533000000	0.063048000000	0.864333000000
C	-4.629647000000	-1.177349000000	1.668937000000
C	-3.535757000000	-1.846495000000	0.818236000000
C	0.800348000000	-3.514258000000	-0.919396000000
C	-0.664668000000	-3.037805000000	-1.055173000000
C	-1.254711000000	-3.777878000000	0.130424000000
C	-0.329723000000	-3.812143000000	1.090443000000
C	0.894211000000	-3.080138000000	0.559107000000
H	0.386225000000	-1.554602000000	2.665927000000

H	-1.199782000000	-1.373624000000	1.914951000000
H	-0.761169000000	0.973013000000	1.409005000000
H	0.117020000000	0.802668000000	2.931656000000
H	5.961952000000	0.614753000000	-0.355321000000
H	5.065903000000	0.577424000000	-1.874095000000
H	5.553732000000	-1.718407000000	0.068739000000
H	5.696977000000	-1.776272000000	-1.692005000000
H	3.296010000000	-1.807416000000	-1.960699000000
H	3.456048000000	-2.752278000000	-0.482857000000
H	2.268835000000	2.929803000000	2.927136000000
H	1.016241000000	3.426550000000	1.790930000000
H	3.458419000000	4.717255000000	1.772742000000
H	2.604208000000	4.372417000000	0.267274000000
H	4.669290000000	3.276065000000	-0.246629000000
H	4.949218000000	2.820761000000	1.432673000000
H	-2.375281000000	3.063722000000	-2.862045000000
H	-1.128722000000	3.523422000000	-1.704237000000
H	-3.608198000000	4.742932000000	-1.599770000000
H	-2.726319000000	4.344725000000	-0.123807000000
H	-4.751413000000	3.161708000000	0.354777000000
H	-5.041630000000	2.790047000000	-1.342473000000
H	-0.242828000000	-1.314034000000	-2.898785000000
H	1.293460000000	-1.067317000000	-2.070419000000
H	0.690696000000	1.178959000000	-1.431629000000
H	-0.152437000000	1.059953000000	-2.979098000000
H	-5.839630000000	-0.180344000000	0.149922000000
H	-5.408237000000	0.880803000000	1.489879000000
H	-5.461155000000	-1.846782000000	1.893353000000
H	-4.189511000000	-0.855939000000	2.617518000000
H	-2.850615000000	-2.428957000000	1.427910000000

H	-3.981502000000	-2.533804000000	0.088218000000
H	1.490911000000	-3.017248000000	-1.593728000000
H	0.892745000000	-4.595181000000	-1.029694000000
H	-1.158557000000	-3.210047000000	-2.011321000000
H	-2.260785000000	-4.168720000000	0.177710000000
H	-0.438119000000	-4.201917000000	2.094558000000
H	1.826525000000	-3.272430000000	1.090405000000

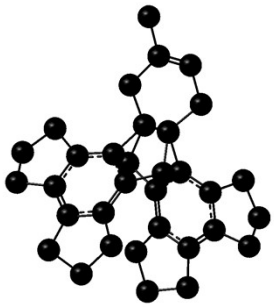


Butadiene adducts 9 $C_{34}H_{38}$

C	-2.509692000000	-1.770671000000	0.969627000000
C	-3.049616000000	-0.910333000000	0.028249000000
C	-2.500014000000	0.366544000000	-0.176911000000
C	-1.400602000000	0.778513000000	0.582187000000
C	-0.919378000000	-0.074300000000	1.588749000000
C	-1.442342000000	-1.344147000000	1.760273000000
C	-0.573299000000	2.071010000000	0.552150000000
C	0.025540000000	2.063075000000	1.990324000000
C	0.141153000000	0.590828000000	2.424325000000
C	-4.253644000000	-1.137893000000	-0.853298000000
C	-4.099863000000	-0.045230000000	-1.924945000000
C	-3.335623000000	1.092642000000	-1.221541000000
C	-1.058497000000	-2.412846000000	2.755944000000

C	-1.716756000000	-3.678255000000	2.163311000000
C	-2.936193000000	-3.164461000000	1.366436000000
C	2.499797000000	0.367959000000	0.176988000000
C	1.400165000000	0.779325000000	-0.582134000000
C	0.919446000000	-0.073762000000	-1.588709000000
C	1.443190000000	-1.343277000000	-1.760300000000
C	2.510808000000	-1.769181000000	-0.969686000000
C	3.050185000000	-0.908572000000	-0.028247000000
C	1.059996000000	-2.412164000000	-2.756021000000
C	1.719056000000	-3.677193000000	-2.163473000000
C	2.938177000000	-3.162683000000	-1.366577000000
C	0.572072000000	2.071336000000	-0.552083000000
C	-0.026862000000	2.063015000000	-1.990206000000
C	-0.141557000000	0.590702000000	-2.424210000000
C	4.254352000000	-1.135460000000	0.853285000000
C	4.099863000000	-0.043018000000	1.925047000000
C	3.334886000000	1.094438000000	1.221774000000
C	1.444634000000	3.324905000000	-0.364302000000
C	0.643069000000	4.580426000000	-0.165080000000
C	-0.645922000000	4.580016000000	0.164868000000
C	-1.446666000000	3.323988000000	0.364206000000
H	0.953047000000	2.626298000000	2.072617000000
H	-0.695856000000	2.554346000000	2.649469000000
H	-0.056422000000	0.465204000000	3.492645000000
H	1.123863000000	0.159445000000	2.224613000000
H	-5.174021000000	-0.993931000000	-0.274311000000
H	-4.291000000000	-2.145425000000	-1.273779000000
H	-3.484939000000	-0.432282000000	-2.742945000000
H	-5.050363000000	0.282084000000	-2.348140000000
H	-4.034601000000	1.771645000000	-0.718322000000

H	-2.759634000000	1.686445000000	-1.929419000000
H	-1.475818000000	-2.177518000000	3.742689000000
H	0.022396000000	-2.515471000000	2.875644000000
H	-1.014570000000	-4.147943000000	1.469502000000
H	-1.983260000000	-4.415756000000	2.921307000000
H	-3.181070000000	-3.799453000000	0.511976000000
H	-3.829070000000	-3.117436000000	2.001397000000
H	1.477152000000	-2.176519000000	-3.742761000000
H	-0.020835000000	-2.515461000000	-2.875708000000
H	1.017174000000	-4.147367000000	-1.469687000000
H	1.986016000000	-4.414479000000	-2.921518000000
H	3.831023000000	-3.115065000000	-2.001536000000
H	3.183452000000	-3.797572000000	-0.512154000000
H	-0.954748000000	2.625635000000	-2.072410000000
H	0.694164000000	2.554769000000	-2.649397000000
H	0.056032000000	0.465215000000	-3.492543000000
H	-1.123977000000	0.158688000000	-2.224438000000
H	5.174645000000	-0.990851000000	0.274323000000
H	4.292344000000	-2.143012000000	1.273661000000
H	3.485184000000	-0.430561000000	2.742999000000
H	5.050149000000	0.284861000000	2.348287000000
H	4.033431000000	1.773983000000	0.718685000000
H	2.758484000000	1.687743000000	1.929731000000
H	2.089248000000	3.431200000000	-1.243409000000
H	2.130506000000	3.208365000000	0.479054000000
H	1.163474000000	5.526207000000	-0.287483000000
H	-1.166957000000	5.525464000000	0.287159000000
H	-2.091389000000	3.429951000000	1.243272000000
H	-2.132427000000	3.206895000000	-0.479175000000

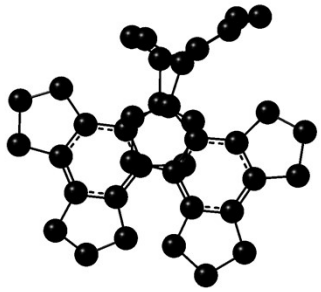


Isoprene adduct 10 $C_{35}H_{40}$

C	-0.832611000000	3.037643000000	0.978256000000
C	0.149966000000	3.200205000000	0.015983000000
C	1.106758000000	2.196357000000	-0.210288000000
C	1.073839000000	1.022748000000	0.548787000000
C	0.122637000000	0.911408000000	1.575955000000
C	-0.838892000000	1.888006000000	1.768651000000
C	1.940878000000	-0.242921000000	0.499215000000
C	1.731132000000	-0.791498000000	1.941889000000
C	0.339497000000	-0.325530000000	2.405808000000
C	0.390947000000	4.398231000000	-0.870274000000
C	1.312818000000	3.830605000000	-1.962895000000
C	2.077755000000	2.682853000000	-1.276520000000
C	-1.950408000000	1.951166000000	2.789213000000
C	-2.871840000000	3.050813000000	2.217019000000
C	-1.941040000000	3.973488000000	1.399516000000
C	-0.823063000000	-2.421293000000	0.182062000000
C	-0.036297000000	-1.564146000000	-0.593372000000
C	-0.659968000000	-0.793272000000	-1.587898000000
C	-2.036266000000	-0.791631000000	-1.733747000000
C	-2.823305000000	-1.614431000000	-0.927513000000
C	-2.216911000000	-2.440686000000	0.003787000000
C	-2.895652000000	-0.031561000000	-2.715956000000
C	-4.305639000000	-0.156180000000	-2.097763000000

C	-4.281376000000	-1.477589000000	-1.298187000000
C	1.475316000000	-1.296792000000	-0.595547000000
C	1.666470000000	-0.741062000000	-2.038329000000
C	0.343598000000	-0.066381000000	-2.442192000000
C	-2.870799000000	-3.464687000000	0.899684000000
C	-1.782418000000	-3.737414000000	1.951590000000
C	-0.452668000000	-3.470188000000	1.221208000000
C	2.302089000000	-2.582144000000	-0.423547000000
C	3.773397000000	-2.326642000000	-0.253974000000
C	4.294730000000	-1.143413000000	0.069506000000
C	3.429491000000	0.072483000000	0.280507000000
C	5.774263000000	-0.924082000000	0.218470000000
H	1.891432000000	-1.864886000000	2.019736000000
H	2.478037000000	-0.317563000000	2.585370000000
H	0.322645000000	-0.096087000000	3.475019000000
H	-0.444296000000	-1.062683000000	2.221069000000
H	0.895943000000	5.188733000000	-0.301781000000
H	-0.531090000000	4.826532000000	-1.269883000000
H	0.698473000000	3.415424000000	-2.767411000000
H	1.975386000000	4.578226000000	-2.400825000000
H	2.986703000000	3.061250000000	-0.793292000000
H	2.383507000000	1.920972000000	-1.991642000000
H	-1.549010000000	2.243725000000	3.767227000000
H	-2.463311000000	0.995746000000	2.920376000000
H	-3.593407000000	2.587476000000	1.539019000000
H	-3.430123000000	3.583682000000	2.987655000000
H	-1.536056000000	4.777585000000	2.025666000000
H	-2.449039000000	4.446397000000	0.555954000000
H	-2.854810000000	-0.509908000000	-3.702246000000
H	-2.580766000000	1.006461000000	-2.844550000000

H	-4.459780000000	0.673692000000	-1.403093000000
H	-5.102427000000	-0.123112000000	-2.841766000000
H	-4.590099000000	-2.322229000000	-1.925821000000
H	-4.946153000000	-1.459830000000	-0.431555000000
H	2.541969000000	-0.103122000000	-2.141248000000
H	1.825873000000	-1.596848000000	-2.700482000000
H	0.129140000000	-0.195337000000	-3.506846000000
H	0.327523000000	1.005728000000	-2.236391000000
H	-3.099620000000	-4.371579000000	0.326711000000
H	-3.808431000000	-3.113615000000	1.336612000000
H	-1.888454000000	-3.017845000000	2.768935000000
H	-1.836001000000	-4.739221000000	2.379666000000
H	-0.104784000000	-4.377144000000	0.712020000000
H	0.330990000000	-3.166102000000	1.913059000000
H	1.944317000000	-3.170719000000	0.425560000000
H	2.135191000000	-3.217306000000	-1.300231000000
H	4.439627000000	-3.174770000000	-0.395096000000
H	3.794995000000	0.631654000000	1.150241000000
H	3.575180000000	0.746291000000	-0.569125000000
H	6.339385000000	-1.829765000000	-0.005788000000
H	6.115335000000	-0.128766000000	-0.452539000000
H	6.017437000000	-0.605888000000	1.237093000000

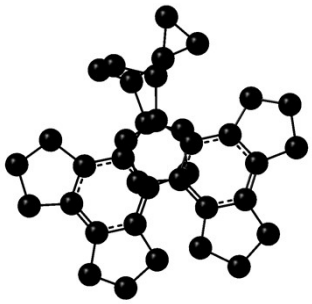


6,6-dimethylfulvene adduct $C_{38}H_{42}$

C	-3.852200000000	0.380108000000	0.546593000000
C	-3.772415000000	-0.844851000000	-0.095355000000
C	-2.565852000000	-1.564911000000	-0.123398000000
C	-1.417858000000	-1.021791000000	0.460178000000
C	-1.541208000000	0.175951000000	1.192396000000
C	-2.735507000000	0.874195000000	1.223111000000
C	0.059844000000	-1.410949000000	0.399590000000
C	0.582966000000	-0.727965000000	1.694453000000
C	-0.260904000000	0.537088000000	1.897744000000
C	-4.864399000000	-1.588312000000	-0.824864000000
C	-4.336026000000	-3.033017000000	-0.834640000000
C	-2.798254000000	-2.903508000000	-0.800192000000
C	-3.054315000000	2.194028000000	1.883700000000
C	-4.598992000000	2.217024000000	1.878214000000
C	-5.016218000000	1.333441000000	0.681151000000
C	2.509077000000	1.035699000000	-0.177284000000
C	1.339443000000	0.549263000000	-0.764865000000
C	0.404971000000	1.470609000000	-1.271967000000
C	0.569954000000	2.830574000000	-1.074499000000
C	1.701330000000	3.309089000000	-0.409869000000
C	2.680042000000	2.418352000000	-0.000644000000
C	-0.312100000000	3.976727000000	-1.509837000000
C	0.187209000000	5.140671000000	-0.625933000000
C	1.669108000000	4.817673000000	-0.332494000000
C	0.793351000000	-0.868253000000	-0.932369000000
C	-0.172652000000	-0.655819000000	-2.130319000000
C	-0.706560000000	0.779740000000	-2.016003000000
C	4.005212000000	2.717794000000	0.658119000000
C	4.805854000000	1.429678000000	0.392542000000
C	3.745807000000	0.311613000000	0.317701000000

H	0.389699000000	-1.420760000000	2.521114000000
H	1.650924000000	-0.537989000000	1.671426000000
H	0.207288000000	1.423876000000	1.459328000000
H	-0.435668000000	0.749733000000	2.956270000000
H	-4.967461000000	-1.198815000000	-1.844615000000
H	-5.840037000000	-1.495453000000	-0.342624000000
H	-4.669831000000	-3.537181000000	0.075815000000
H	-4.690356000000	-3.614309000000	-1.686757000000
H	-2.374555000000	-2.927515000000	-1.810195000000
H	-2.345493000000	-3.722741000000	-0.242590000000
H	-2.641841000000	3.016994000000	1.286946000000
H	-2.633475000000	2.284029000000	2.887670000000
H	-4.962129000000	1.756045000000	2.800315000000
H	-5.010335000000	3.225731000000	1.825432000000
H	-5.971028000000	0.827852000000	0.842060000000
H	-5.116890000000	1.931196000000	-0.232559000000
H	-0.150558000000	4.193378000000	-2.572812000000
H	-1.376917000000	3.769609000000	-1.379785000000
H	-0.368326000000	5.132305000000	0.315799000000
H	0.047659000000	6.118539000000	-1.088212000000
H	2.323565000000	5.246226000000	-1.101252000000
H	2.004316000000	5.206541000000	0.631464000000
H	-0.962765000000	-1.399260000000	-2.179161000000
H	0.422896000000	-0.741450000000	-3.046445000000
H	-1.650421000000	0.821465000000	-1.462701000000
H	-0.880127000000	1.235589000000	-2.994795000000
H	3.864244000000	2.877924000000	1.733916000000
H	4.488821000000	3.611128000000	0.256735000000
H	5.302904000000	1.515892000000	-0.577286000000
H	5.571252000000	1.236605000000	1.145487000000

H	3.585466000000	-0.137652000000	1.304476000000
H	4.046855000000	-0.494877000000	-0.346884000000
C	0.227986000000	-3.657734000000	-0.860930000000
C	0.998143000000	-3.162364000000	-1.830069000000
C	0.541358000000	-2.903552000000	0.426791000000
C	1.821789000000	-2.034834000000	-1.218039000000
C	2.028404000000	-2.670144000000	0.151381000000
H	-0.494232000000	-4.454966000000	-0.955465000000
H	1.003574000000	-3.443846000000	-2.874982000000
H	0.265409000000	-3.416242000000	1.346315000000
H	2.692746000000	-1.714811000000	-1.787096000000
C	4.508453000000	-2.942750000000	0.271269000000
C	3.110317000000	-3.059314000000	0.819048000000
H	4.527869000000	-2.586930000000	-0.758399000000
H	4.989472000000	-3.926190000000	0.293066000000
C	3.036093000000	-3.703443000000	2.179127000000
H	3.663840000000	-3.153387000000	2.888616000000
H	2.022783000000	-3.729172000000	2.576952000000
H	3.420534000000	-4.728277000000	2.144573000000
H	5.122829000000	-2.273659000000	0.883617000000



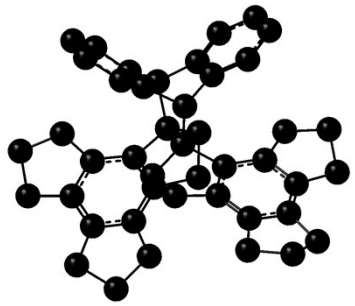
Spiro[2.4]hepta-4,6-diene adduct $C_{37}H_{40}$

C	-3.406002000000	1.493178000000	0.457881000000

C	-3.719830000000	0.281329000000	-0.134963000000
C	-2.821008000000	-0.798374000000	-0.086664000000
C	-1.573858000000	-0.638850000000	0.525121000000
C	-1.316108000000	0.564486000000	1.210411000000
C	-2.208941000000	1.620488000000	1.164314000000
C	-0.308826000000	-1.500330000000	0.545346000000
C	0.378947000000	-0.965224000000	1.833942000000
C	-0.013526000000	0.513384000000	1.960845000000
C	-4.977322000000	-0.092492000000	-0.880664000000
C	-4.961395000000	-1.628655000000	-0.810616000000
C	-3.469309000000	-2.013408000000	-0.725724000000
C	-2.089128000000	3.000842000000	1.764431000000
C	-3.536928000000	3.534970000000	1.690512000000
C	-4.189898000000	2.783424000000	0.508647000000
C	2.838833000000	0.058563000000	-0.058948000000
C	1.575514000000	-0.090511000000	-0.636208000000
C	0.978572000000	1.041296000000	-1.226100000000
C	1.549571000000	2.295717000000	-1.110557000000
C	2.775246000000	2.450082000000	-0.460476000000
C	3.432426000000	1.330954000000	0.019434000000
C	1.062673000000	3.622120000000	-1.644089000000
C	1.900299000000	4.637517000000	-0.835996000000
C	3.211285000000	3.896285000000	-0.491367000000
C	0.619991000000	-1.285463000000	-0.756082000000
C	-0.193168000000	-0.849435000000	-2.011382000000
C	-0.268959000000	0.682318000000	-1.983482000000
C	4.799394000000	1.252016000000	0.655616000000
C	5.155665000000	-0.233858000000	0.477813000000
C	3.797367000000	-0.957824000000	0.531201000000
H	-0.032445000000	-1.522057000000	2.683091000000

H	1.453807000000	-1.113174000000	1.832188000000
H	0.734409000000	1.178167000000	1.517100000000
H	-0.141913000000	0.816986000000	3.003771000000
H	-4.915908000000	0.255425000000	-1.918724000000
H	-5.878416000000	0.344764000000	-0.444997000000
H	-5.462511000000	-1.945716000000	0.107533000000
H	-5.471054000000	-2.102811000000	-1.650286000000
H	-3.057143000000	-2.216608000000	-1.720166000000
H	-3.325605000000	-2.912141000000	-0.126787000000
H	-1.408216000000	3.611201000000	1.158325000000
H	-1.692466000000	2.993434000000	2.782182000000
H	-4.059989000000	3.265817000000	2.611707000000
H	-3.586548000000	4.619225000000	1.583682000000
H	-5.262684000000	2.630720000000	0.646557000000
H	-4.060140000000	3.336515000000	-0.429204000000
H	1.279047000000	3.699265000000	-2.716570000000
H	-0.013634000000	3.763064000000	-1.519925000000
H	1.372812000000	4.870763000000	0.092885000000
H	2.068010000000	5.573713000000	-1.369624000000
H	3.963386000000	4.044111000000	-1.275855000000
H	3.653388000000	4.233243000000	0.448716000000
H	-1.171098000000	-1.316413000000	-2.067952000000
H	0.376702000000	-1.160809000000	-2.894291000000
H	-1.171093000000	1.040183000000	-1.477391000000
H	-0.264322000000	1.114481000000	-2.988206000000
H	4.739875000000	1.513866000000	1.719205000000
H	5.523765000000	1.926093000000	0.193331000000
H	5.600300000000	-0.377894000000	-0.510540000000
H	5.861329000000	-0.601742000000	1.223969000000
H	3.535389000000	-1.172131000000	1.573077000000

H	3.804084000000	-1.904840000000	-0.008152000000
C	-0.860882000000	-3.696127000000	-0.692925000000
C	0.101670000000	-3.533013000000	-1.599823000000
C	-0.383785000000	-3.068503000000	0.613753000000
C	1.221936000000	-2.738757000000	-0.930639000000
C	1.106981000000	-3.400642000000	0.455690000000
H	-1.810295000000	-4.186450000000	-0.846548000000
H	0.075135000000	-3.819977000000	-2.642874000000
H	-0.867868000000	-3.429637000000	1.523189000000
H	2.189606000000	-2.763153000000	-1.431899000000
C	1.613772000000	-4.772963000000	0.754216000000
C	2.074723000000	-3.595613000000	1.577868000000
H	3.103876000000	-3.290073000000	1.464562000000
H	1.687240000000	-3.501549000000	2.586010000000
H	2.329623000000	-5.206801000000	0.065922000000
H	0.925623000000	-5.480618000000	1.200974000000



Anthracene adduct $C_{44}H_{42}$

C	3.870676000000	-2.095730000000	0.857121000000
C	3.775260000000	-1.402591000000	-0.333240000000
C	2.644732000000	-0.614167000000	-0.648433000000
C	1.569611000000	-0.546457000000	0.260322000000
C	1.726625000000	-1.222224000000	1.494227000000
C	2.840556000000	-1.985039000000	1.786450000000

C	0.260556000000	0.310094000000	0.369129000000
C	-0.478222000000	-0.424904000000	1.518809000000
C	0.606685000000	-0.936394000000	2.453979000000
C	4.819970000000	-1.336725000000	-1.419831000000
C	4.438297000000	-0.044389000000	-2.149534000000
C	2.910946000000	0.001738000000	-2.021278000000
C	3.159588000000	-2.775771000000	3.033700000000
C	4.679346000000	-3.021864000000	2.901636000000
C	4.967916000000	-2.989259000000	1.383950000000
C	-3.204632000000	-0.185909000000	-0.033425000000
C	-2.008751000000	-0.296181000000	-0.752082000000
C	-1.758482000000	-1.500502000000	-1.440935000000
C	-2.616289000000	-2.581375000000	-1.347978000000
C	-3.769445000000	-2.487470000000	-0.570360000000
C	-4.066077000000	-1.293639000000	0.062475000000
C	-2.523503000000	-3.942345000000	-1.996701000000
C	-3.503258000000	-4.786747000000	-1.151726000000
C	-4.546469000000	-3.781831000000	-0.613929000000
C	-0.738487000000	0.588371000000	-0.869844000000
C	-0.229167000000	0.073870000000	-2.235714000000
C	-0.476246000000	-1.431544000000	-2.225175000000
C	-5.247370000000	-1.001197000000	0.953725000000
C	-5.256691000000	0.534958000000	1.019764000000
C	-3.804884000000	0.975598000000	0.733596000000
H	-1.221160000000	0.212162000000	2.000092000000
H	-0.995372000000	-1.292772000000	1.108957000000
H	0.295421000000	-1.816868000000	3.020260000000
H	0.918914000000	-0.176979000000	3.182449000000
H	4.727241000000	-2.201142000000	-2.089427000000
H	5.838965000000	-1.335393000000	-1.027036000000

H	4.865395000000	0.813136000000	-1.620445000000
H	4.774738000000	-0.009564000000	-3.186809000000
H	2.469640000000	-0.639994000000	-2.794608000000
H	2.526620000000	1.009620000000	-2.153528000000
H	2.605024000000	-3.721744000000	3.030151000000
H	2.896612000000	-2.251093000000	3.954999000000
H	5.213988000000	-2.197404000000	3.380255000000
H	5.002735000000	-3.949012000000	3.376170000000
H	5.970901000000	-2.624028000000	1.152689000000
H	4.878797000000	-3.989971000000	0.945185000000
H	-2.854765000000	-3.883684000000	-3.040521000000
H	-1.509726000000	-4.348478000000	-2.000346000000
H	-2.959584000000	-5.217487000000	-0.306990000000
H	-3.952318000000	-5.606754000000	-1.713198000000
H	-5.393478000000	-3.686514000000	-1.303987000000
H	-4.952239000000	-4.072653000000	0.357553000000
H	0.781242000000	0.368795000000	-2.456375000000
H	-0.872537000000	0.522932000000	-3.001757000000
H	0.330600000000	-1.966452000000	-1.710342000000
H	-0.574643000000	-1.856747000000	-3.227034000000
H	-5.080895000000	-1.441804000000	1.943915000000
H	-6.182615000000	-1.415529000000	0.569965000000
H	-5.905311000000	0.919674000000	0.228781000000
H	-5.630927000000	0.919844000000	1.968903000000
H	-3.248159000000	1.185018000000	1.654808000000
H	-3.791847000000	1.890012000000	0.149264000000
C	2.235682000000	3.775576000000	-2.533128000000
C	0.911070000000	3.338723000000	-2.443609000000
C	0.486687000000	2.685721000000	-1.297215000000
C	1.384123000000	2.451045000000	-0.248386000000

C	2.697181000000	2.885904000000	-0.334577000000
C	3.121626000000	3.556216000000	-1.483497000000
C	-0.908503000000	2.151715000000	-1.006418000000
C	0.756250000000	1.712465000000	0.911229000000
C	-0.424021000000	2.546804000000	1.339275000000
C	-1.298889000000	2.828394000000	0.289301000000
C	-2.319438000000	3.750836000000	0.468425000000
H	-2.965912000000	4.016549000000	-0.362235000000
C	-2.524172000000	4.317274000000	1.725172000000
C	-1.699498000000	3.971985000000	2.792131000000
C	-0.633321000000	3.094056000000	2.597352000000
H	-1.610512000000	2.374978000000	-1.812983000000
H	2.571765000000	4.293062000000	-3.424032000000
H	0.219720000000	3.511660000000	-3.261936000000
H	3.387026000000	2.696280000000	0.481293000000
H	4.145519000000	3.903339000000	-1.559698000000
H	1.467270000000	1.562890000000	1.725555000000
H	-3.327476000000	5.029682000000	1.871683000000
H	-1.867910000000	4.409567000000	3.769130000000
H	0.043857000000	2.860329000000	3.412699000000