

Supplementary Material

Simple, practical and efficient synthesis of triarylmethanes

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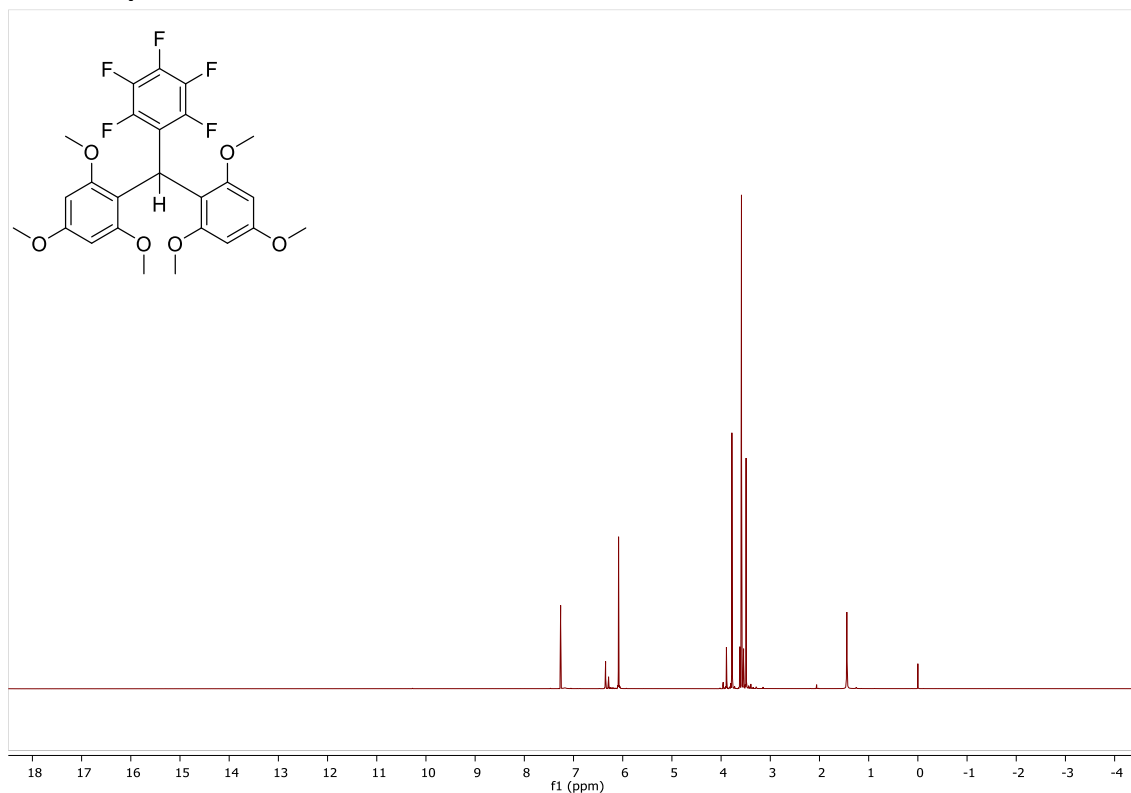
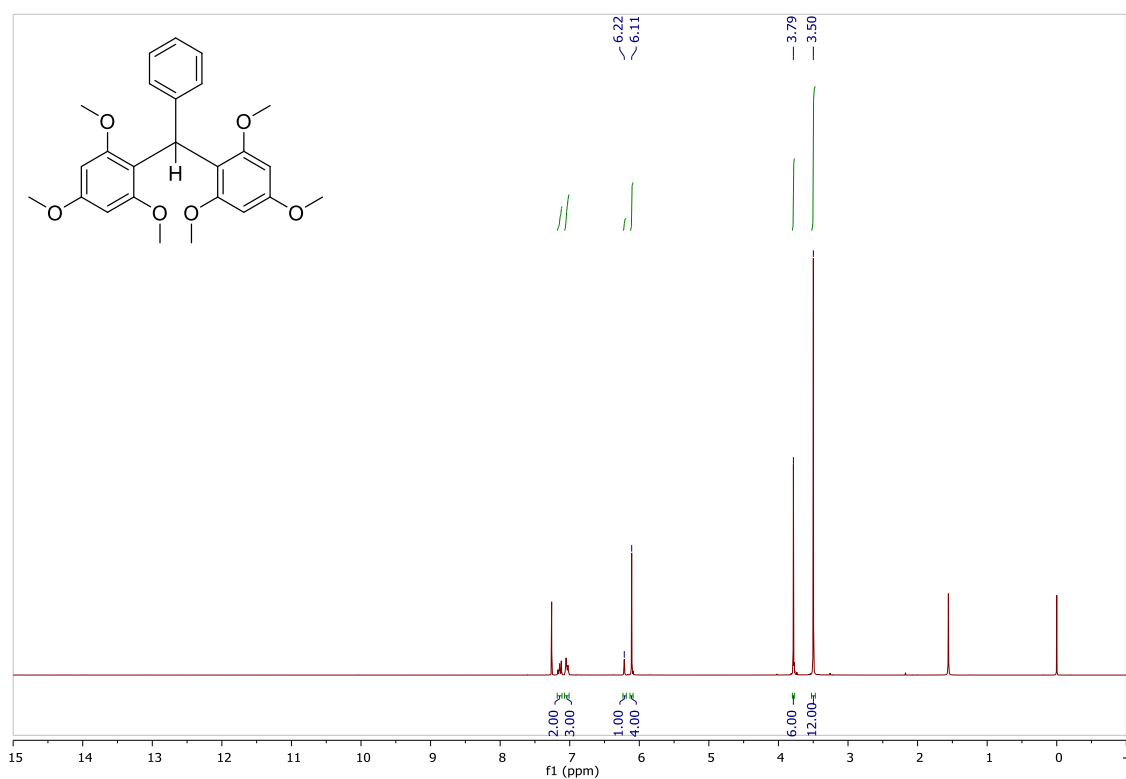
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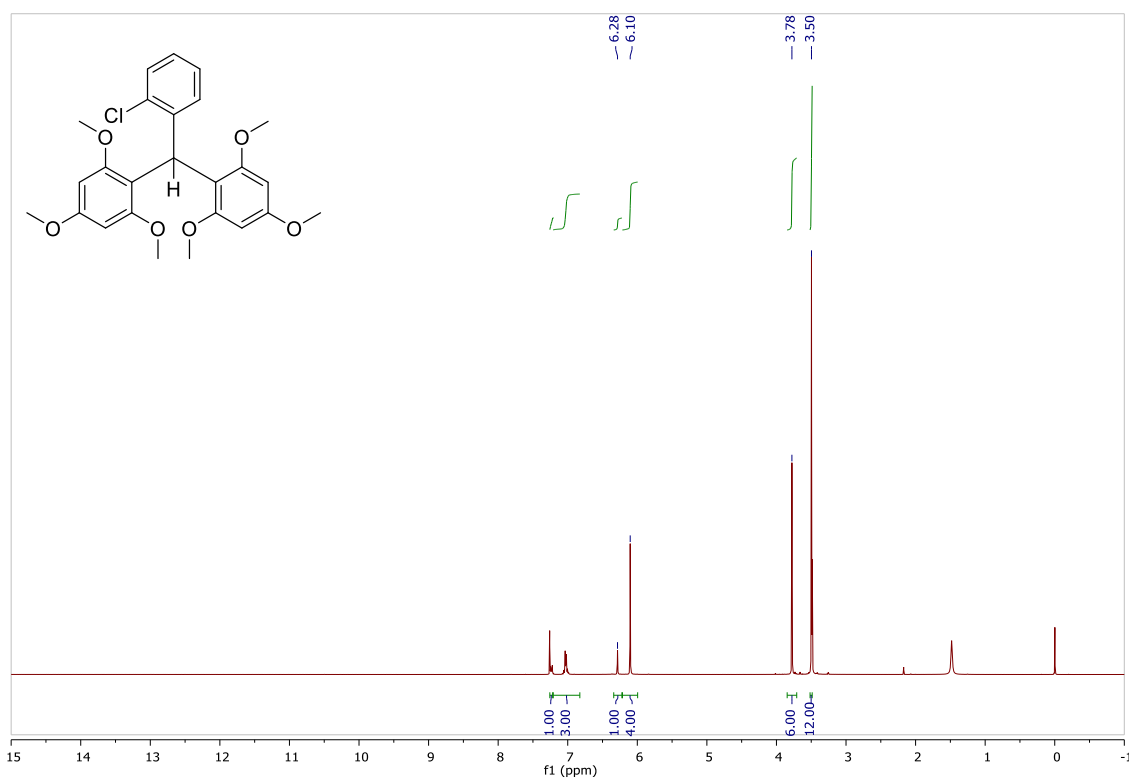
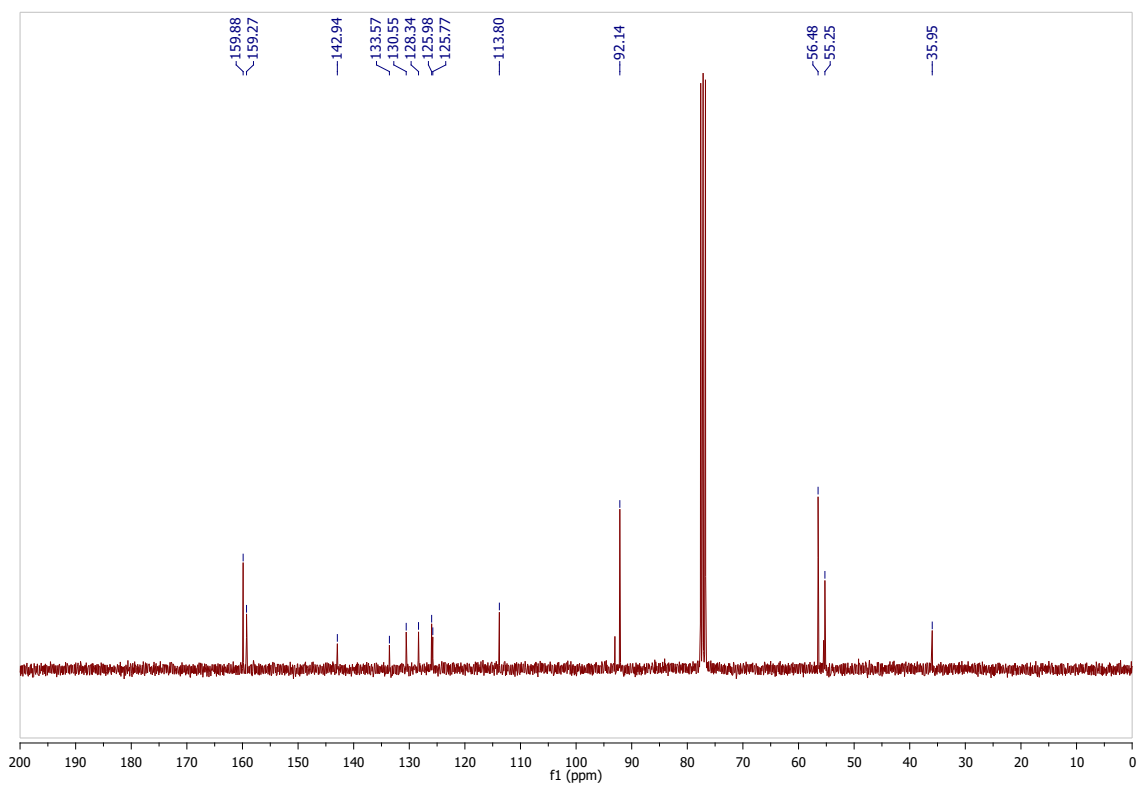
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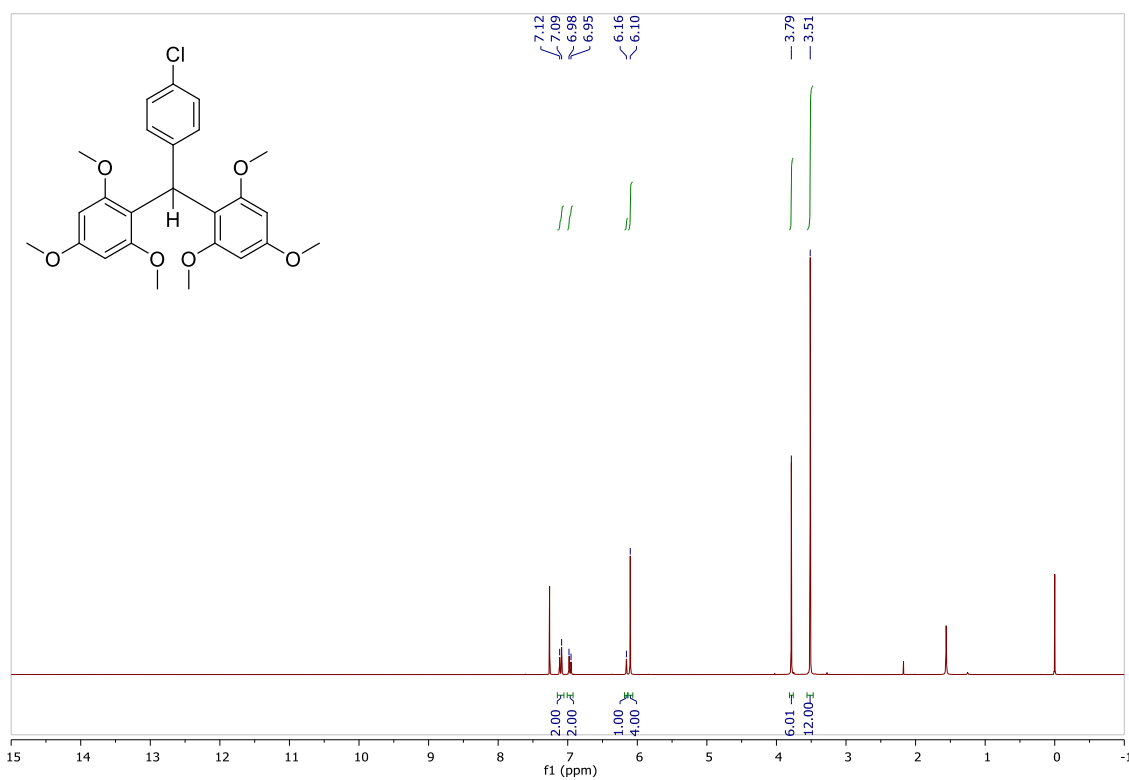
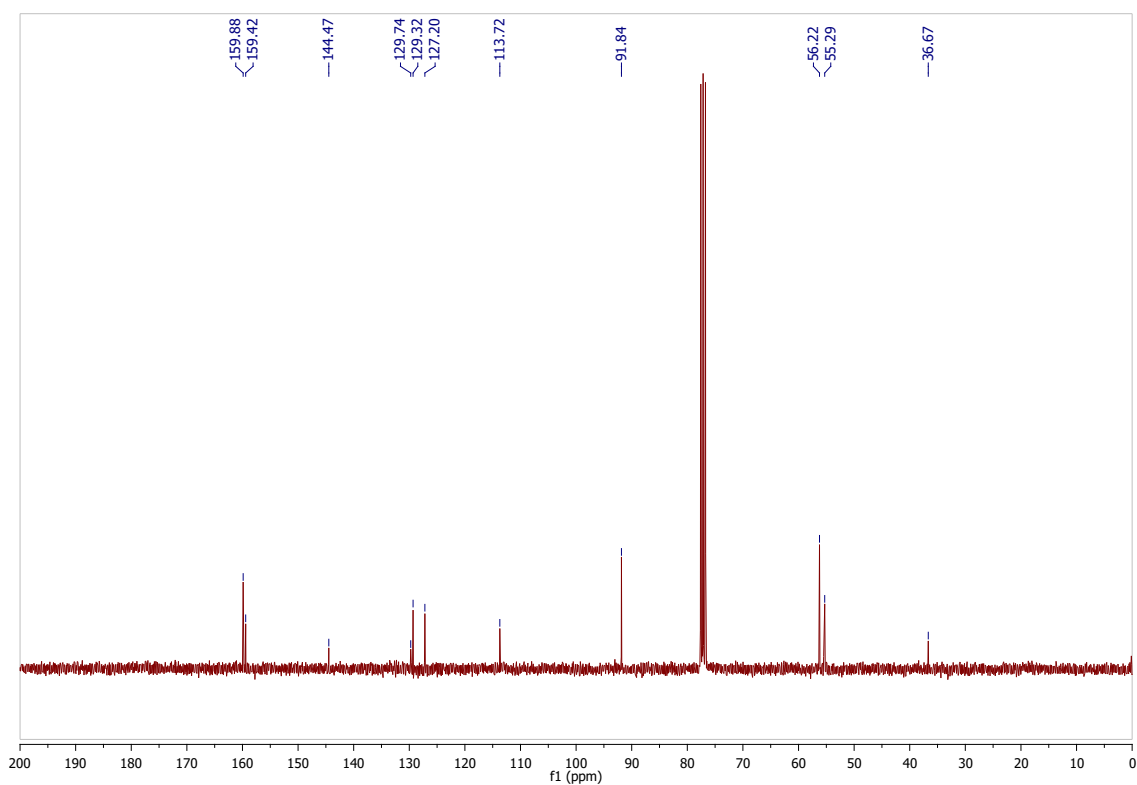
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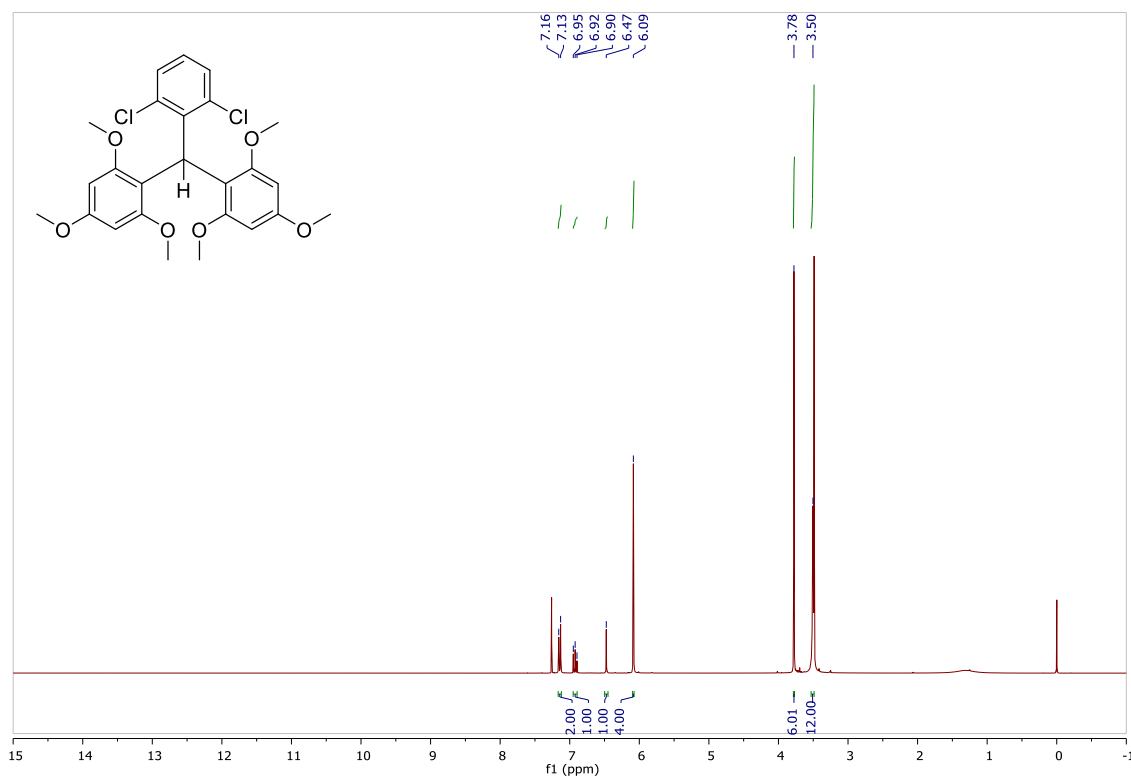
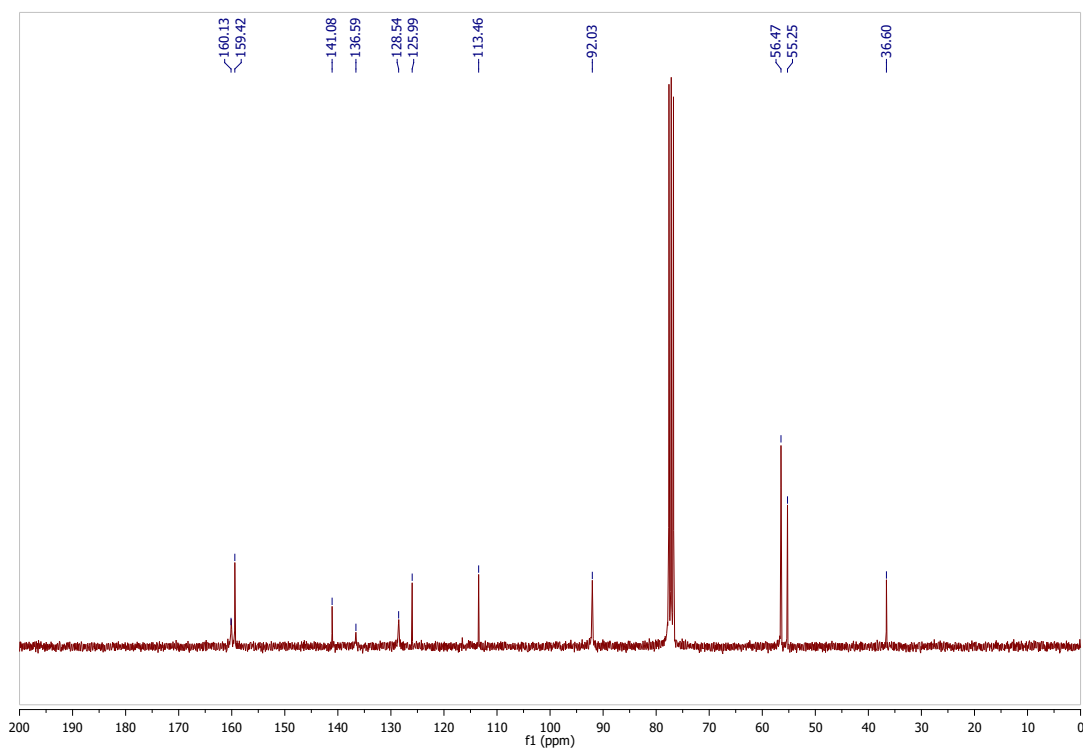
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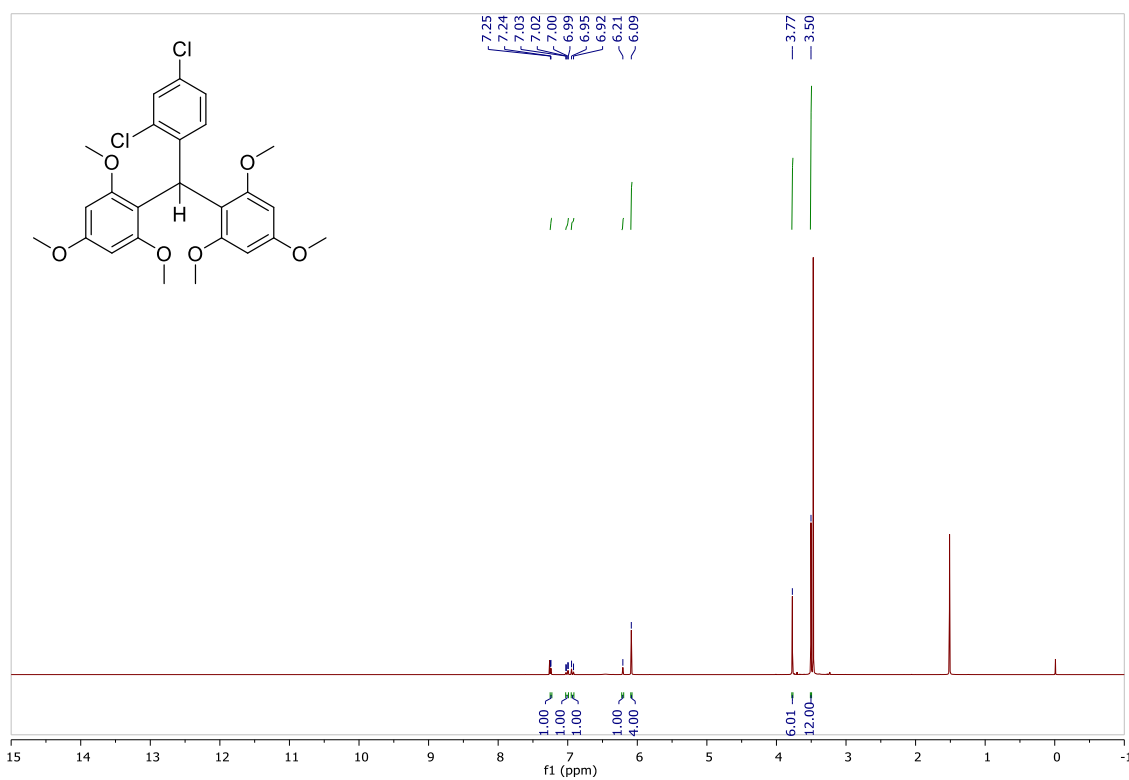
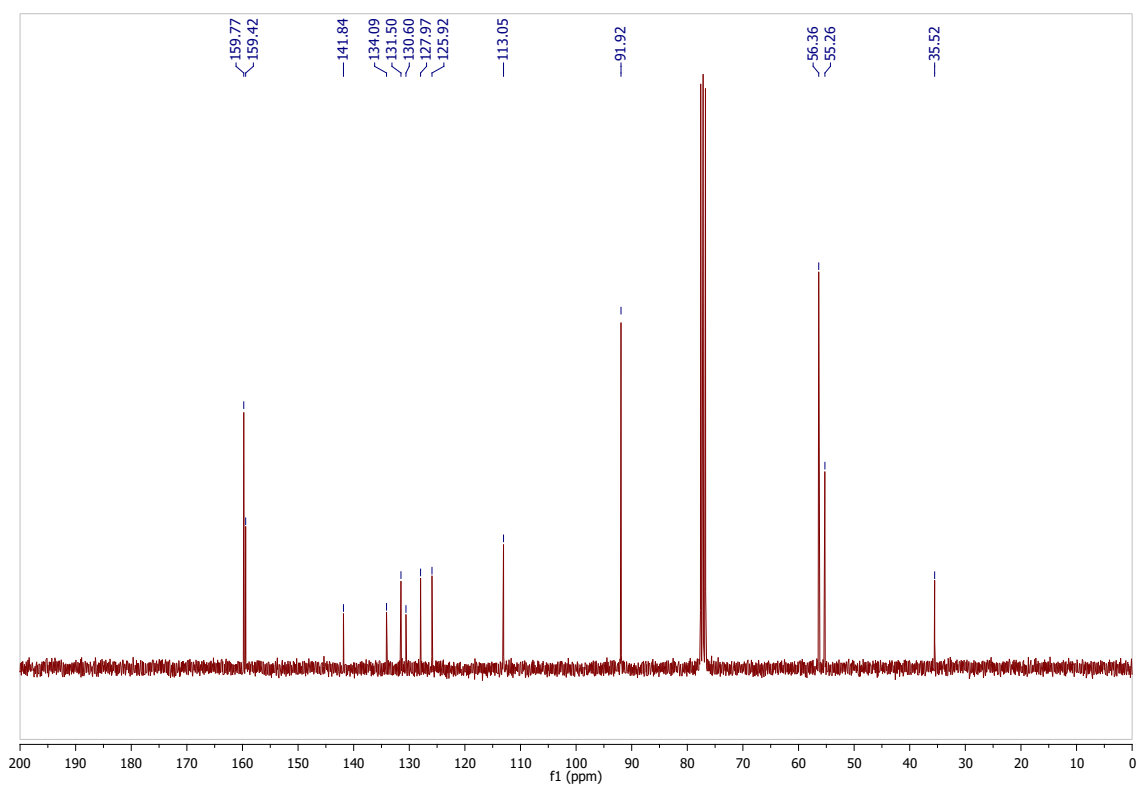
1. NMR spectra

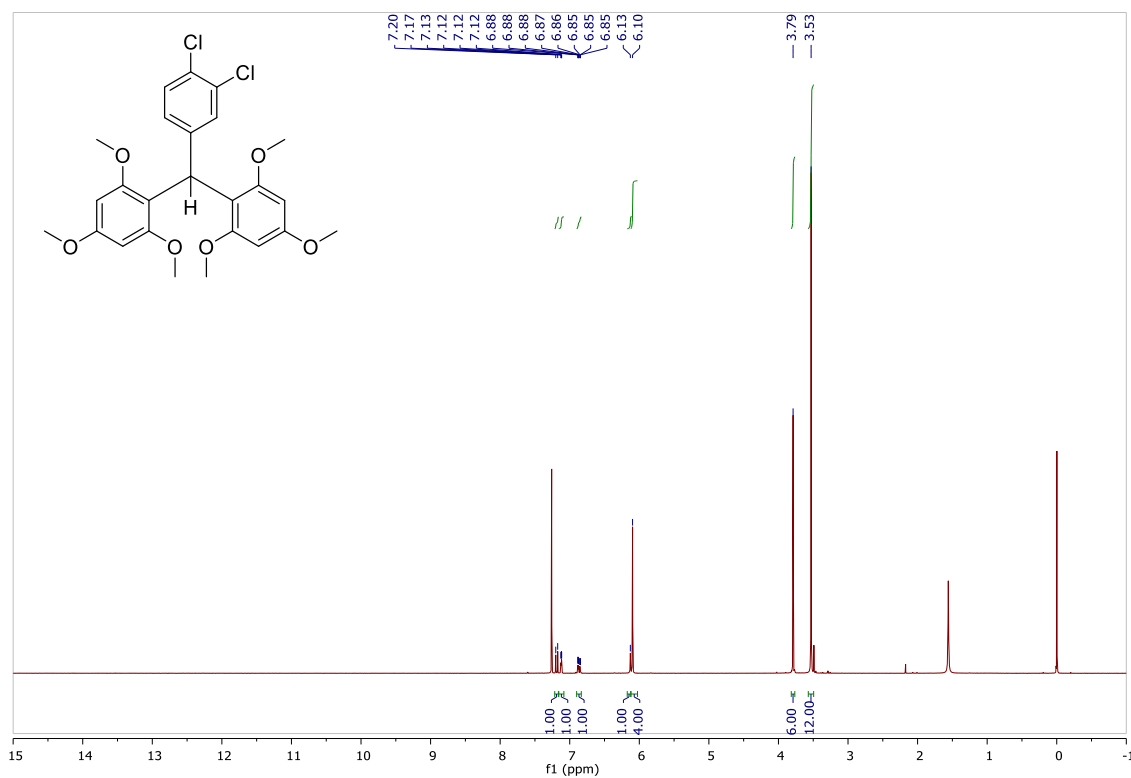
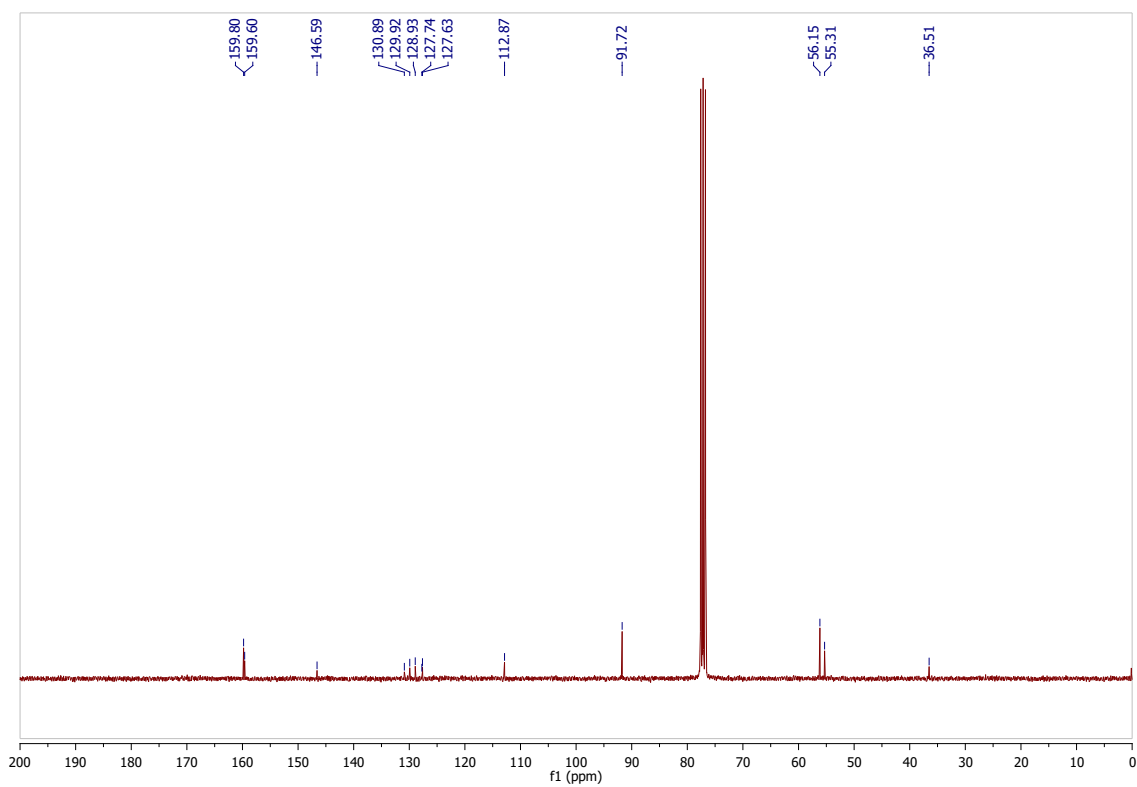
Figure S01. ¹H NMR spectrum (300 MHz, CDCl₃) of **3a**.Figure S02. ¹H NMR spectrum (300 MHz, CDCl₃) of **3b**.

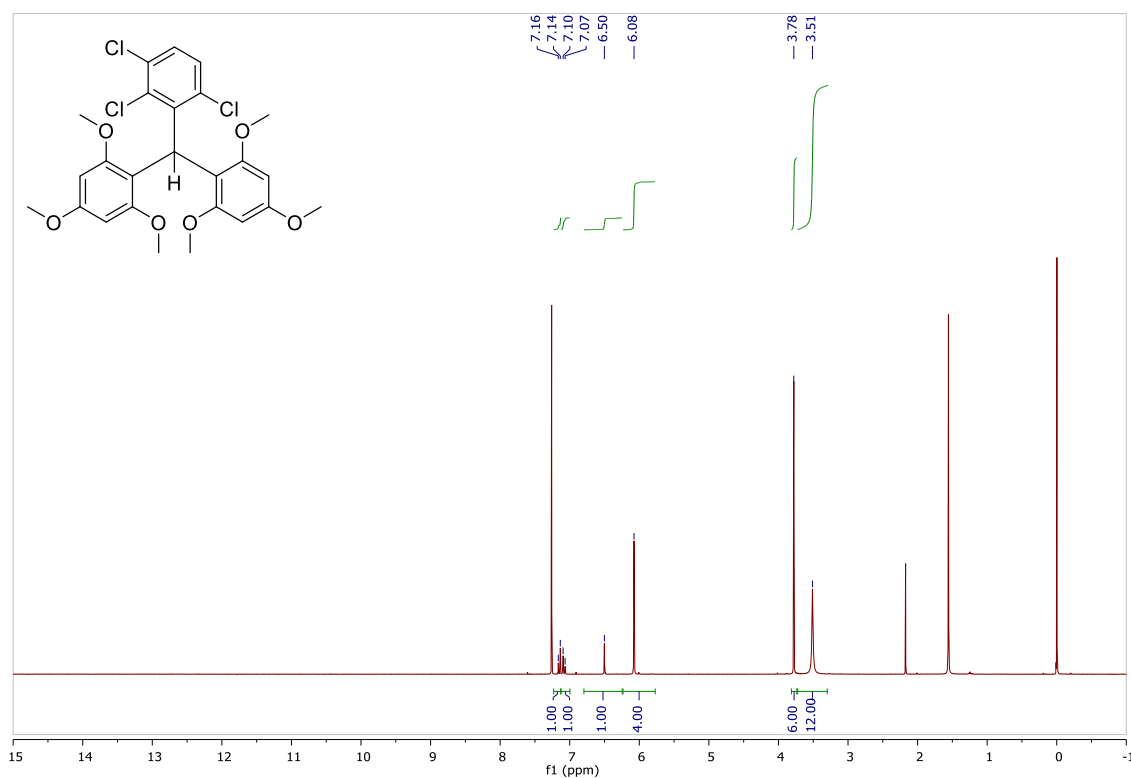
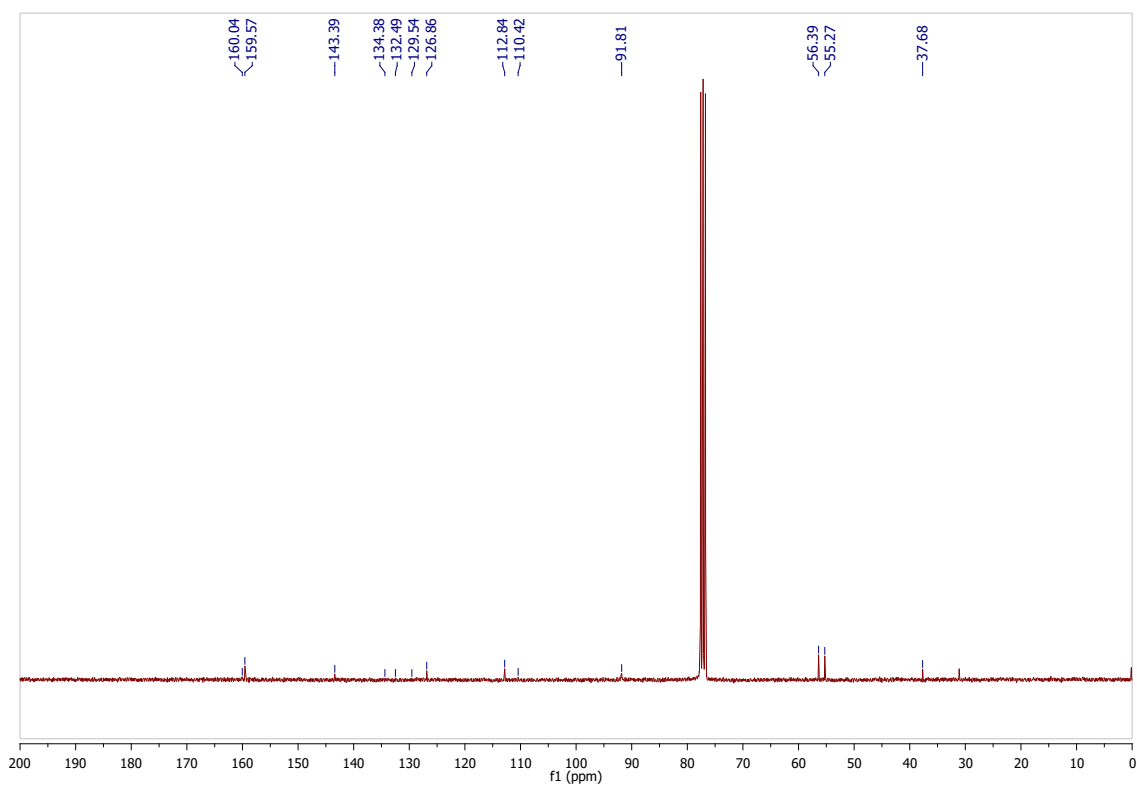
Figure S03. ¹H NMR spectrum (300 MHz, CDCl₃) of **3c**.Figure S04. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3c**.

Figure S05. ¹H NMR spectrum (300 MHz, CDCl₃) of **3d**.Figure S06. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3d**.

Figure S07. ¹H NMR spectrum (300 MHz, CDCl₃) of **3e**.Figure S08. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3e**.

Figure S09. ¹H NMR spectrum (300 MHz, CDCl₃) of **3f**.Figure S10. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3f**.

Figure S11. ¹H NMR spectrum (300 MHz, CDCl₃) of **3g**.Figure S12. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3g**.

Figure S13. ¹H NMR spectrum (300 MHz, CDCl₃) of **3h**.Figure S14. ¹³C NMR spectrum (75 MHz, CDCl₃) of **3h**.

2. Single Crystal X-ray Diffraction

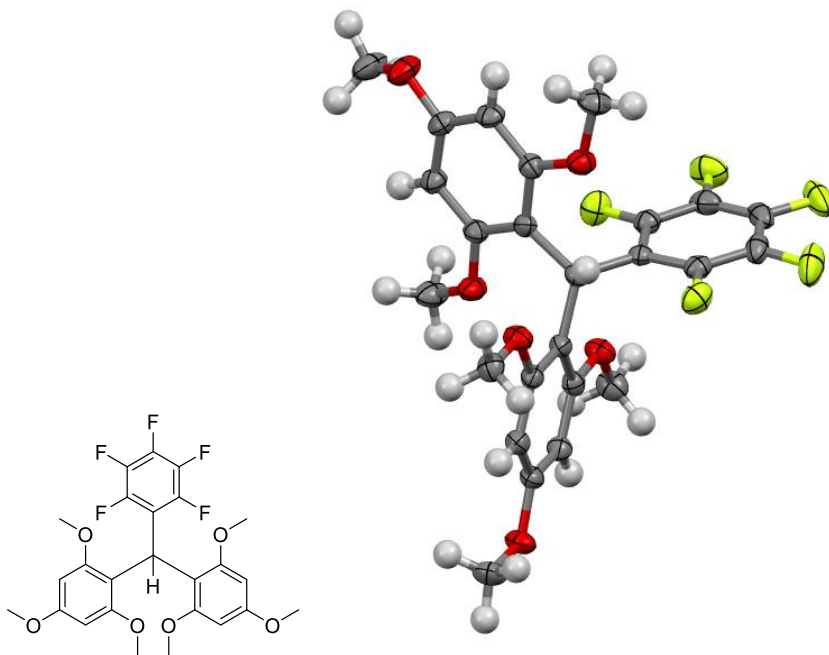
Single-crystals of compounds **3a-h** were manually selected from the crystallization vial. A suitable single-crystal was mounted on a glass fiber with the help of silicon grease.

Data were collected at 150(2) K or at room temperature on a RIGAKU XtaLAB Synergy-i instrument equipped with a Mo K α ($\lambda = 0.71073 \text{ \AA}$) PhotonJet-i micro source and a HyPix3000 detector. The data was controlled by the CrysAlisPro software (Y. Oxford Diffraction Ltd, England, 2022, CrysAlis PRO, Rigaku V1.171.142.173a) and an Oxford Cryosystems Series 800 cryostream was used. The diffraction images were processed using CrysAlisPro software (Y. Oxford Diffraction Ltd, England, 2022, CrysAlis PRO, Rigaku V1.171.142.173a.). The data was corrected for absorption using the multi-scan absorption correction with spherical harmonics implemented in the SCALE3 ABSPACK scaling algorithm. The structures were solved using direct methods with SHELXT 2014/5 and refined using the weighted full-matrix least-squares method on F^2 with SHELXL 2018/3. Anisotropic thermal parameters were used to refine all non-hydrogen atoms. Molecular diagrams were created using Mercury software.

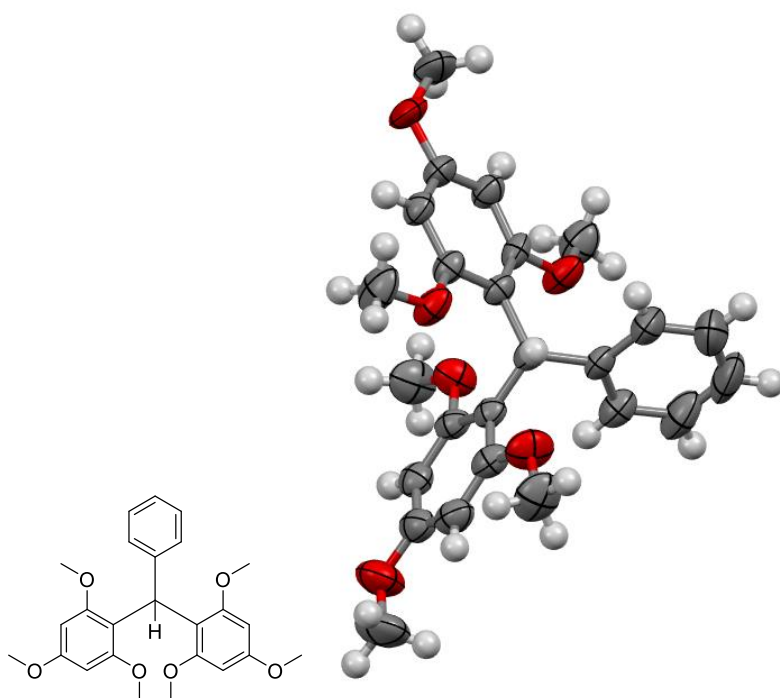
Hydrogen atoms bound to carbon were located at their idealized positions using appropriate *HFIX* instructions in SHELXL (43 for the aromatic and vinylic, 23 for the –CH₂– moieties and 13 for the chiral tertiary carbon atoms) and included in subsequent refinement cycles in riding-motion approximation with isotropic thermal displacements parameters (U_{iso}) fixed at 1.2 times U_{eq} of the atom to which they are attached.

Crystallographic data for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC 2541525-2541532. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 2EZ, U.K. Fax: (+44) 1223 336033. E-mail: deposit@ccdc.cam.ac.uk.

Compound 3a

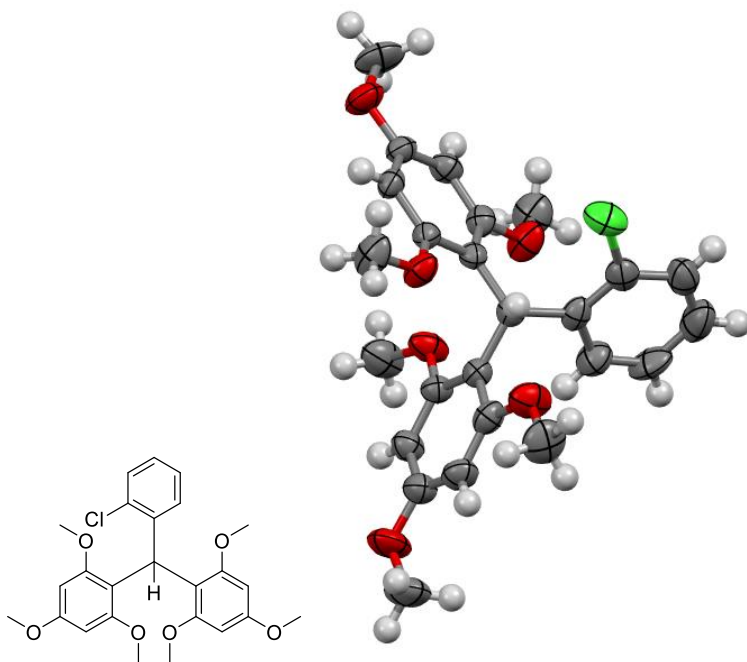


Deposition Number CCDC 2541525
Cell: a=8.1370(5) b=20.2509(12) c=14.0663(9)
alpha=90 beta=95.415(6) gamma=90
Temperature: 150 K
Volume 2307.5(2)
Space group P 21/n
Hall group -P 2yn
Moiety formula C₂₅ H₂₃ F₅ O₆
Sum formula C₂₅ H₂₃ F₅ O₆
Mr 514.43
Z 4
Mu (mm⁻¹) 0.131
F000 1064.0
F000' 1064.81
h,k,lmax 10,26,18
Nref 5351
Tmin,Tmax 0.969,0.987
Data completeness= 0.961 Theta(max)= 27.976
R(reflections)= 0.0544(3433)
wR2(reflections)= 0.1461(5351)
S = 1.037
Npar= 331

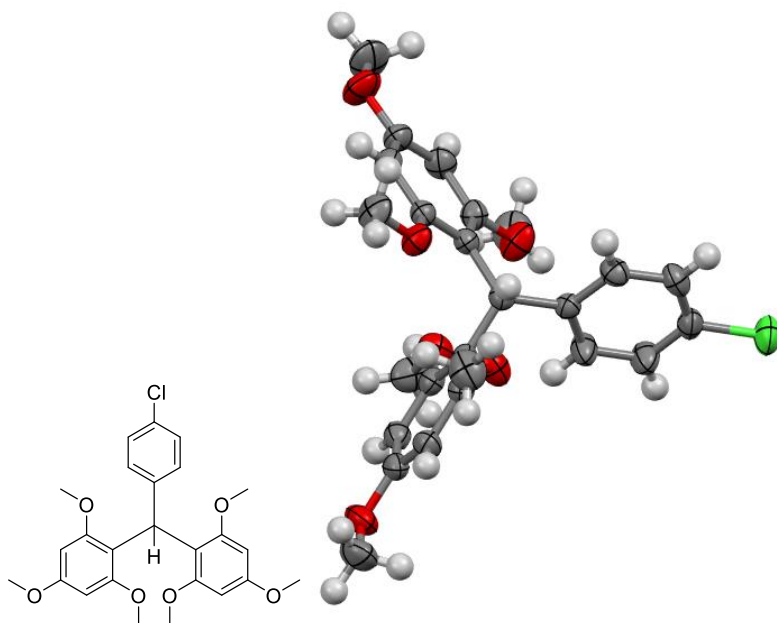
Compound **3b**

Deposition Number CCDC 2541526
Cell: a=12.440(4) b=8.0078(18) c=22.595(8)
alpha=90 beta=93.586(7) gamma=90
Temperature: 297 K
Volume 2246.4(12)
Space group P 21/c
Hall group -P 2ybc
Moiety formula C₂₅ H₂₈ O₆
Sum formula C₂₅ H₂₈ O₆
Mr 424.47
Z 4
Mu (mm⁻¹) 0.089
F000 904.0
F000' 904.48
h,k,lmax 15,9,28
Nref 4439
Tmin,Tmax 0.984,0.996
Tmin' 0.974
Data completeness= 0.965 Theta(max)= 26.397
R(reflections)= 0.0762 (1589)
wR2(reflections)= 0.2031 (4439)
S = 0.979
Npar= 286

Compound 3c

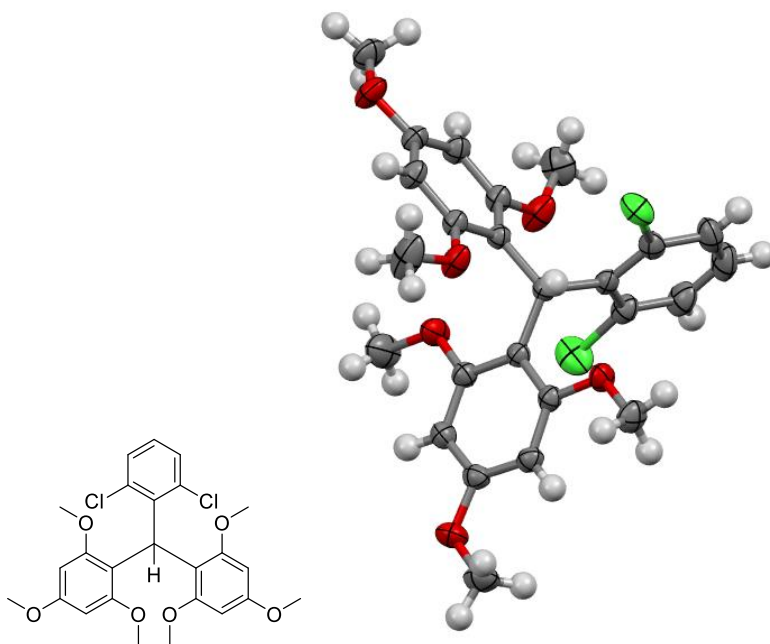


Deposition Number CCDC 2541527
Cell: a=13.825(4) b=21.123(7) c=8.112(3)
alpha=90 beta=97.955(14) gamma=90
Temperature: 293 K
Volume 2346.1(13)
Space group C c
Hall group C -2yc
Moiety formula C₂₅ H₂₇ Cl O₆
Sum formula C₂₅ H₂₇ Cl O₆
Mr 458.94
Z 4
Mu (mm⁻¹) 0.201
F₀₀₀ 968.0
F₀₀₀' 969.08
h,k,lmax 17,26,10
N_{ref} 4231
T_{min},T_{max} 0.981,0.990
T_{min}' 0.904
Data completeness= 1.72/0.86 Theta(max)= 26.599
R(reflections)= 0.0561 (3267)
wR₂(reflections)=0.1403 (4231)
S = 1.066
N_{par}= 295

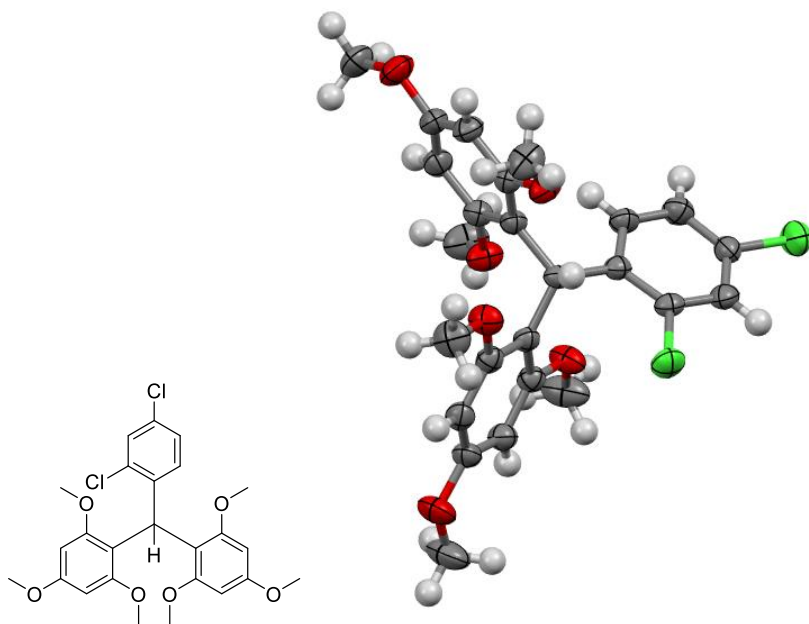
Compound **3d**

Deposition Number CCDC 2541529
Cell: a=8.1392(16) b=12.639(3) c=12.663(3)
alpha=111.322(7) beta=100.789(8) gamma=94.907(8)
Temperature: 297 K
Volume 1175.1(4)
Space group P -1
Hall group -P 1
Moiety formula C₂₅ H₂₇ Cl O₆
Sum formula C₂₅ H₂₇ Cl O₆
Mr 458.91
Z 2
Mu (mm⁻¹) 0.200
F₀₀₀ 484.0
F₀₀₀' 484.54
h,k,lmax 10,15,15
Nref 4784
Tmin,Tmax 0.942,0.990
Tmin' 0.942
Data completeness= 0.982 Theta(max)= 26.504
R(reflections)= 0.0434 (3589)
wR2(reflections)=0.1283 (4784)
S = 1.045
Npar= 295

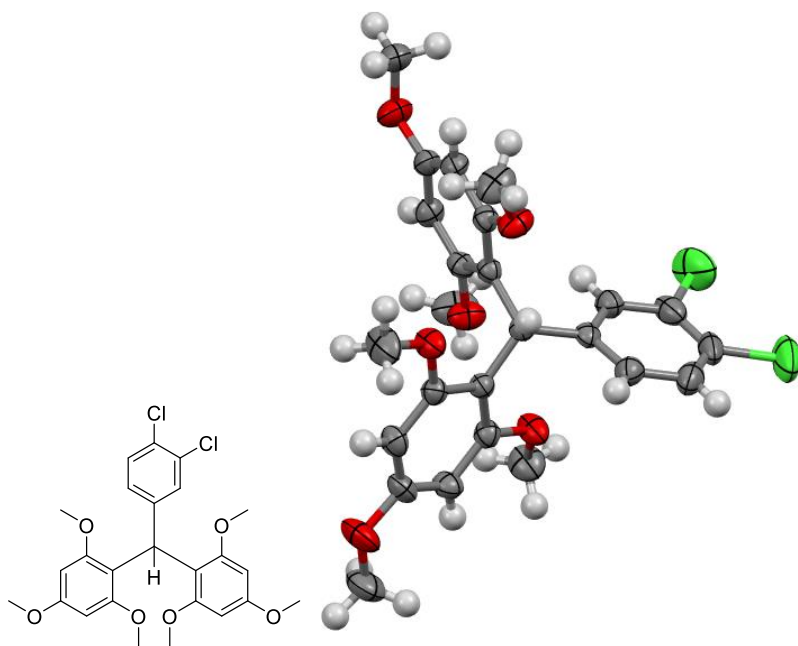
Compound 3e



Deposition Number CCDC 2541531
Cell: a=8.8554(7) b=9.6183(8) c=14.8884(11)
alpha=96.842(3) beta=105.880(3) gamma=98.200(3)
Temperature: 298 K
Volume 1190.46(16)
Space group P -1
Hall group -P 1
Moiety formula C₂₅ H₂₆ Cl₂ O₆
Sum formula C₂₅ H₂₆ Cl₂ O₆
Mr 493.36
Z 2
Mu (mm⁻¹) 0.312
F000 516.0
F000' 516.84
h,k,lmax 12,13,21
Nref 7139
Tmin,Tmax 0.861,0.969
Tmin' 0.829
Data completeness= 0.976 Theta(max)= 30.563
R(reflections)= 0.0445 (5822)
wR2(reflections)= 0.1331 (7139)
S = 1.060
Npar= 304

Compound **3f**

Deposition Number CCDC 2541532
Cell: a=7.5624(19) b=22.248(6) c=14.569(4)
alpha=90 beta=99.658(8) gamma=90
Temperature: 293 K
Volume 2416.4(11)
Space group P 21/c
Hall group -P 2ybc
Moiety formula C₂₅ H₂₆ Cl₂ O₆
Sum formula C₂₅ H₂₆ Cl₂ O₆
Mr 493.38
Z 4
Mu (mm⁻¹) 0.307
F₀₀₀ 1032.0
F₀₀₀' 1033.68
h,k,lmax 9,27,18
Nref 4919
Tmin,Tmax 0.912,0.946
Tmin' 0.912
Data completeness= 0.981 Theta(max)= 26.500
R(reflections)= 0.0792 (3222)
wR2(reflections)= 0.2510 (4919)
S = 1.095
Npar= 304

Compound **3g**

Deposition Number CCDC 2541530

Cell: a=7.882(2) b=12.414(4) c=13.181(5)

alpha=92.149(14) beta=98.590(13) gamma=106.594(12)

Temperature: 297 K

Volume 1217.8(7)

Space group P -1

Hall group -P 1

Moiety formula C₂₅ H₂₆ Cl₂ O₆

Sum formula C₂₅ H₂₆ Cl₂ O₆

Mr 493.36

Z 2

Mu (mm⁻¹) 0.305

F₀₀₀ 516.0

F₀₀₀' 516.84

h,k,lmax 9,15,16

N_{ref} 4888

T_{min},T_{max} 0.947,0.985

T_{min}' 0.913

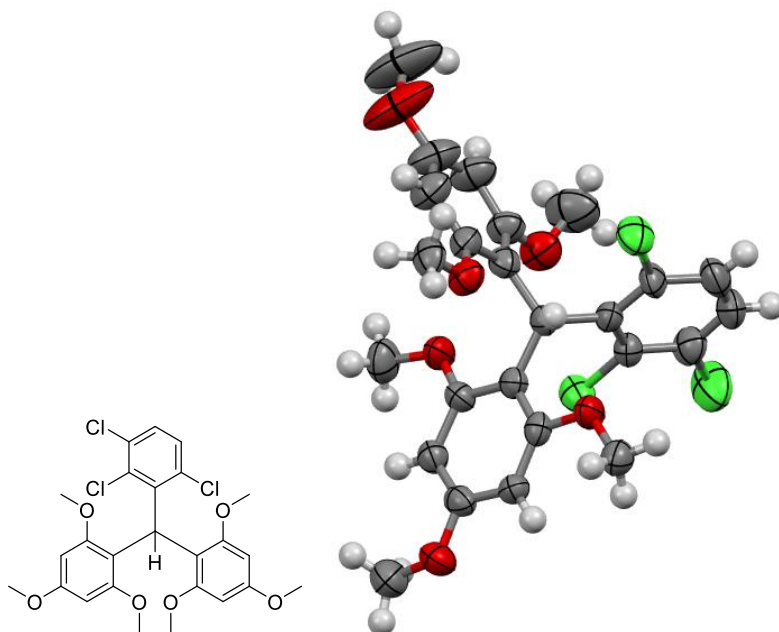
Data completeness= 0.965 Theta(max)= 26.544

R(reflections)= 0.0533 (2723)

wR₂(reflections)= 0.1282 (4888)

S = 1.014

N_{par}= 304

Compound **3h**

Deposition Number CCDC 2541528
Cell: a=8.508(3) b=10.642(4) c=14.830(6)
alpha=79.077(13) beta=75.941(13) gamma=75.447(11)
Temperature: 297 K
Volume 1248.8(8)
Space group P -1
Hall group -P 1
Moiety formula C₂₅ H₂₅ Cl₃ O₆
Sum formula C₂₅ H₂₅ Cl₃ O₆
Mr 527.80
Z 2
Mu (mm⁻¹) 0.406
F000 548.0
F000' 549.14
h,k,lmax 10,13,18
Nref 5174
Tmin,Tmax 0.850,0.980
Tmin' 0.850
Data completeness= 0.994 Theta(max)= 26.555
R(reflections)= 0.1252 (2210)
wR2(reflections)= 0.4150 (5174)
S = 1.201
Npar= 313