

Supporting Information

Nucleophile-Induced Transformation of Phenoxathiin-Based Thiacalixarenes

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1. Spectral characterization of compounds

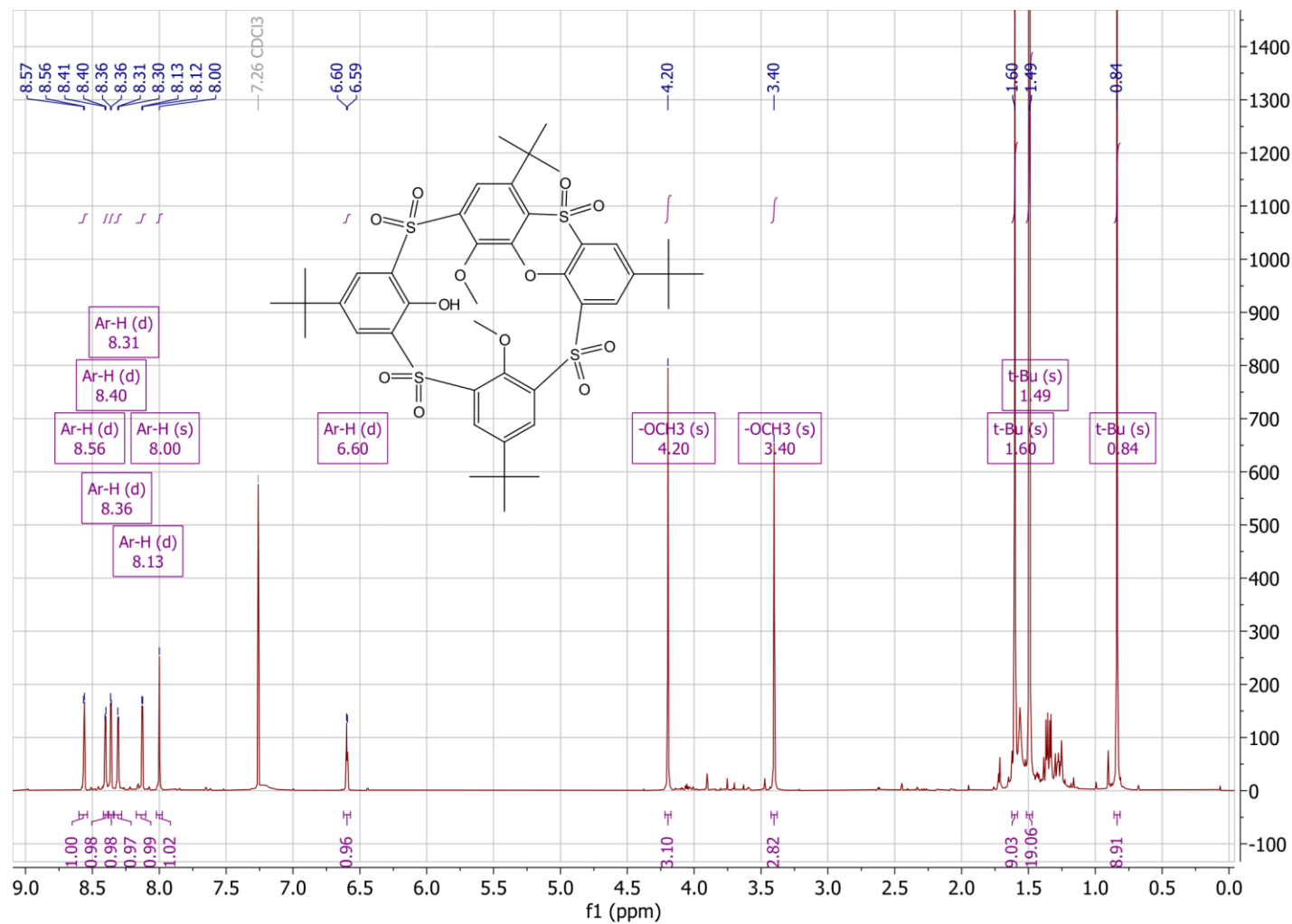


Figure S1: ¹H NMR (400 MHz, CDCl₃, 298 K) spectrum of compound **7**

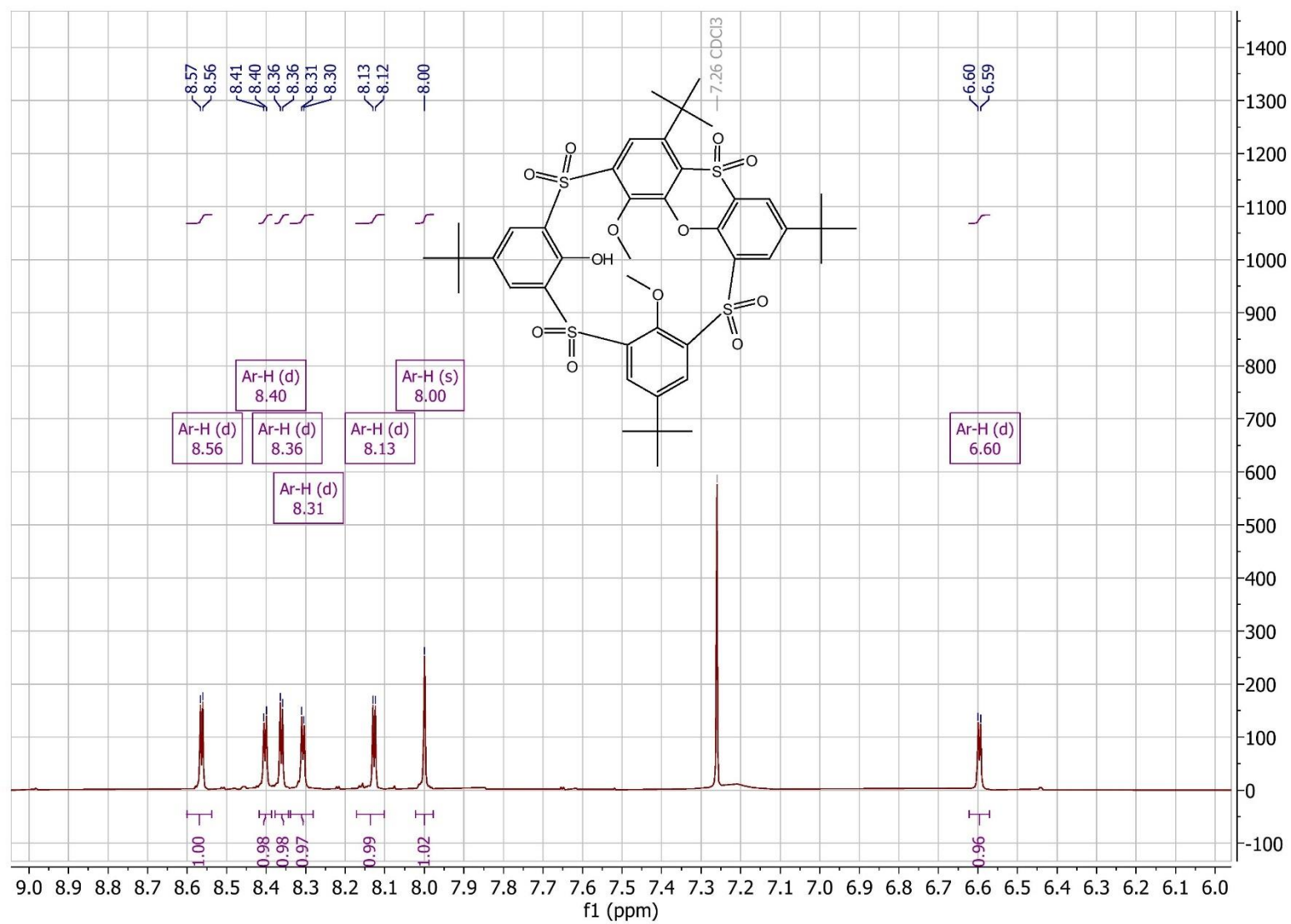


Figure S2: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **7** (aromatic region)

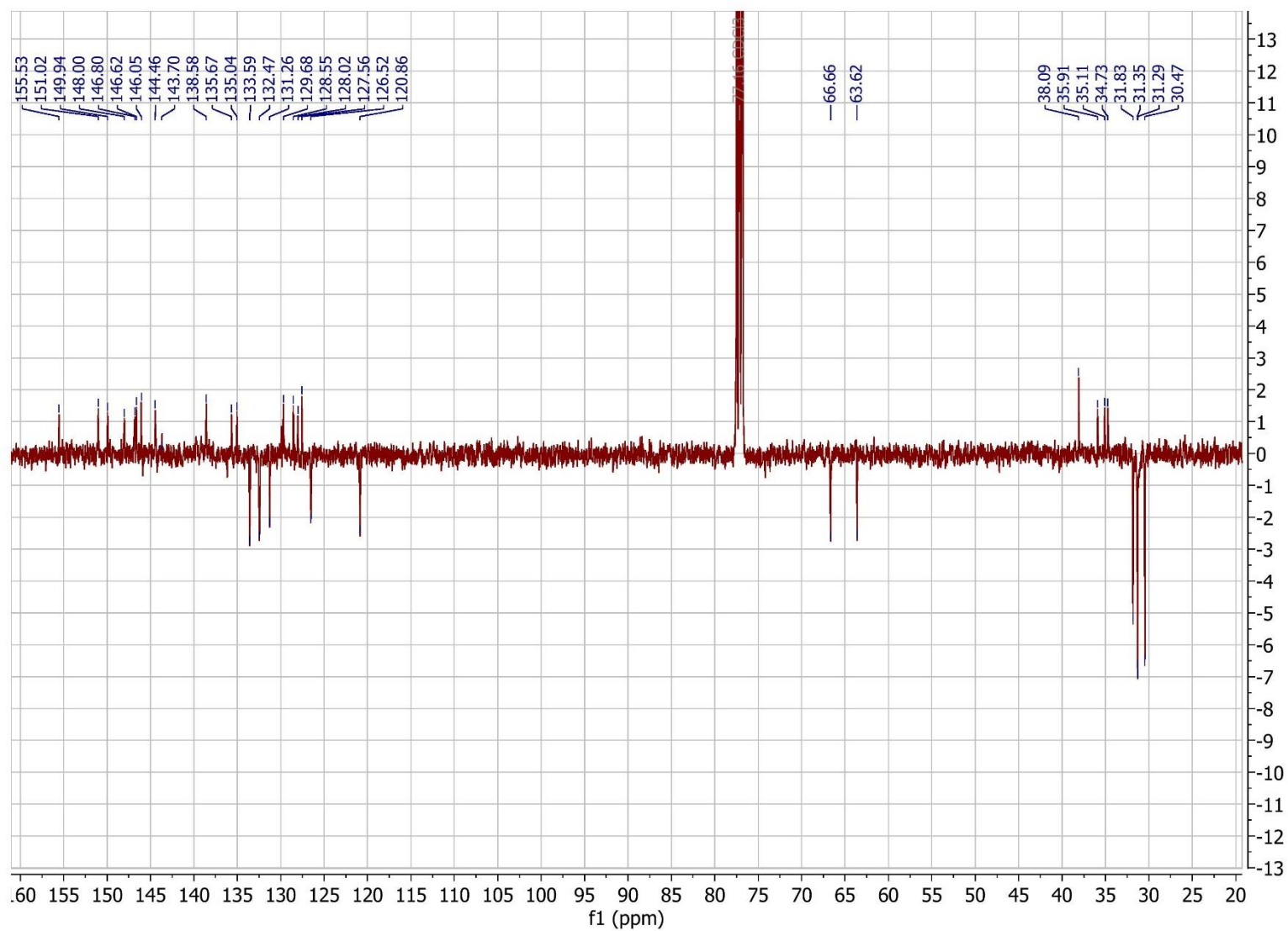


Figure S3: ^{13}C NMR (APT, 101 MHz, CDCl_3 , 298 K) spectrum of compound **7**

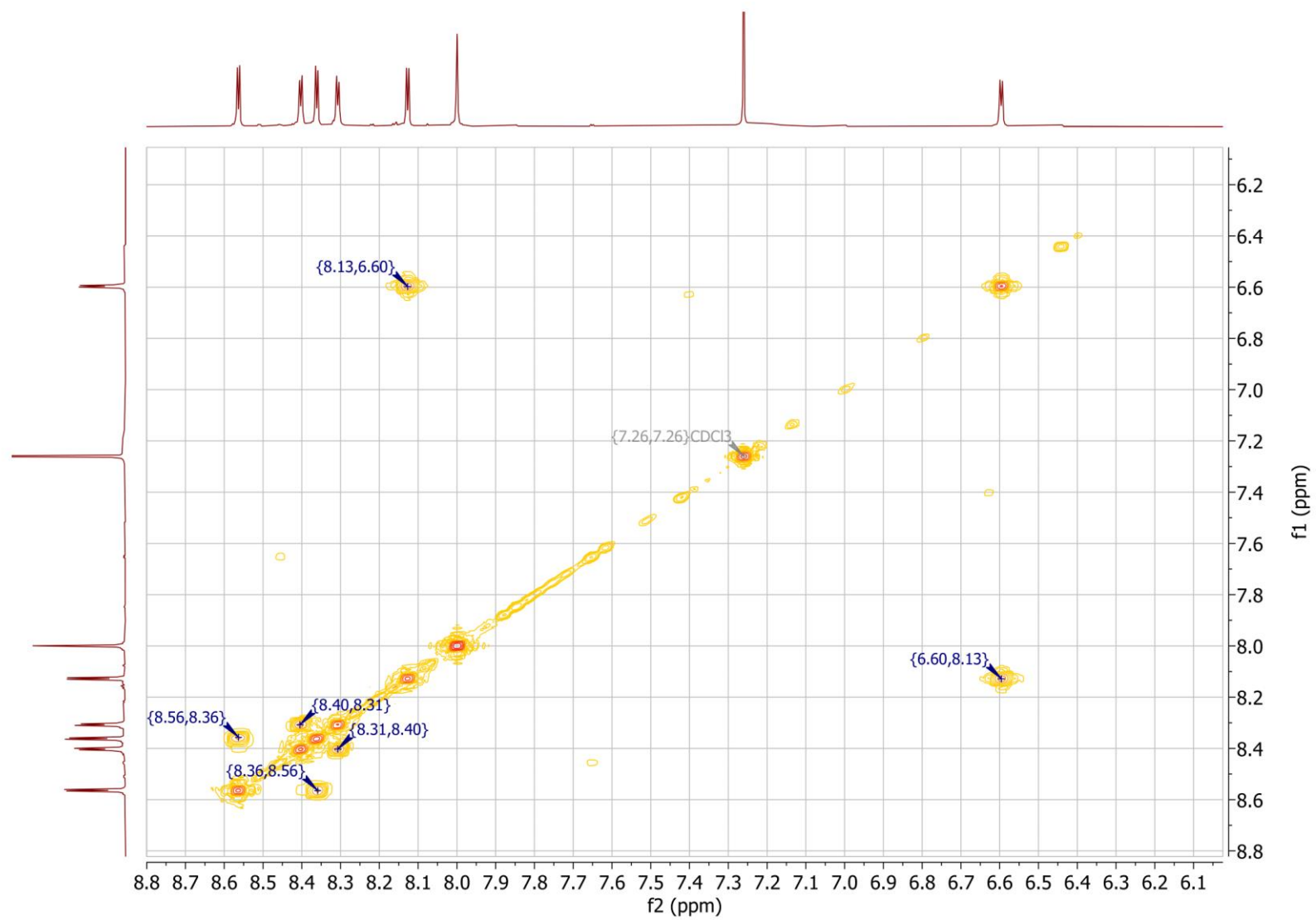


Figure S4: COSY spectrum of compound **7**

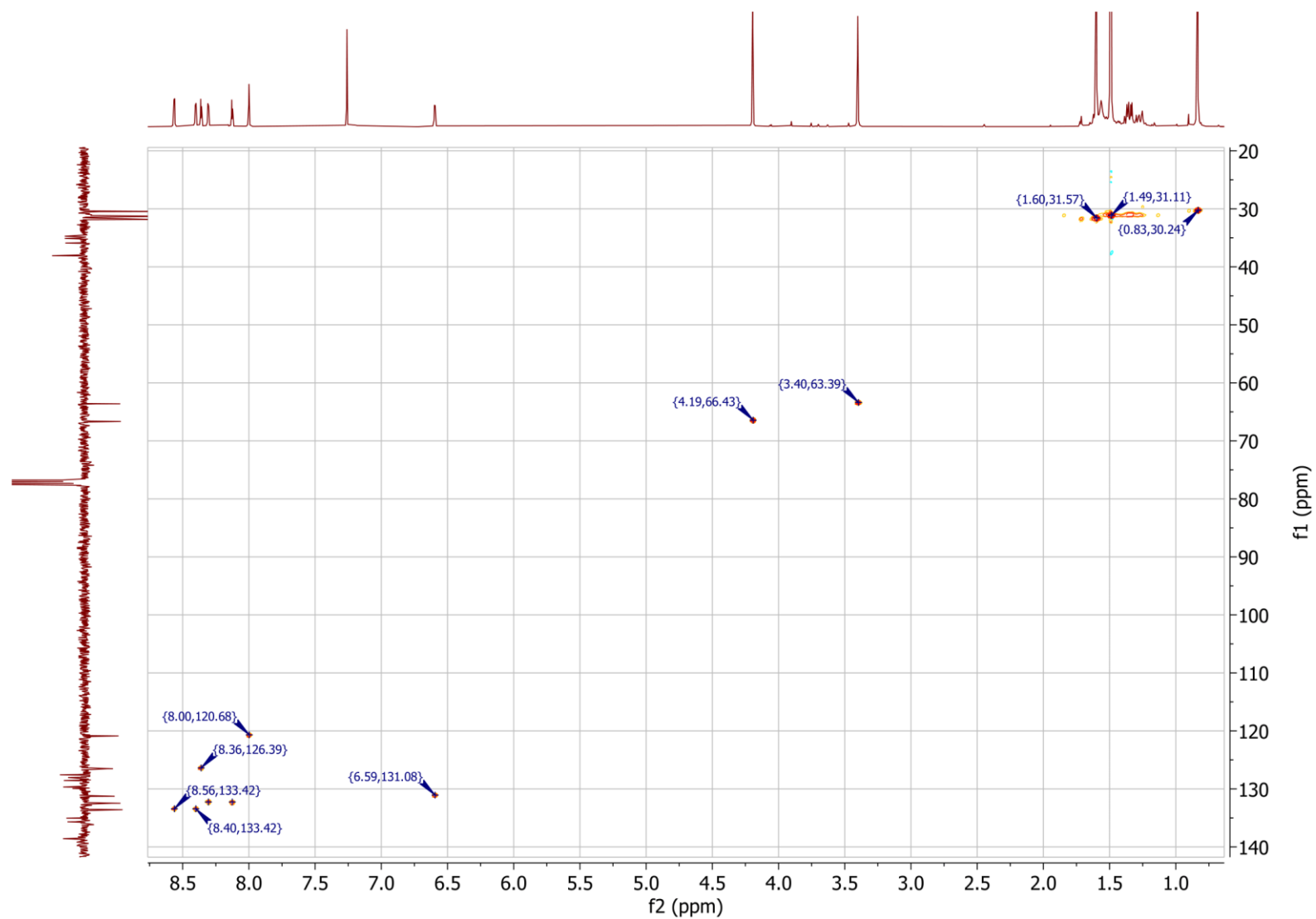


Figure S5: HMQC spectrum of compound **7**

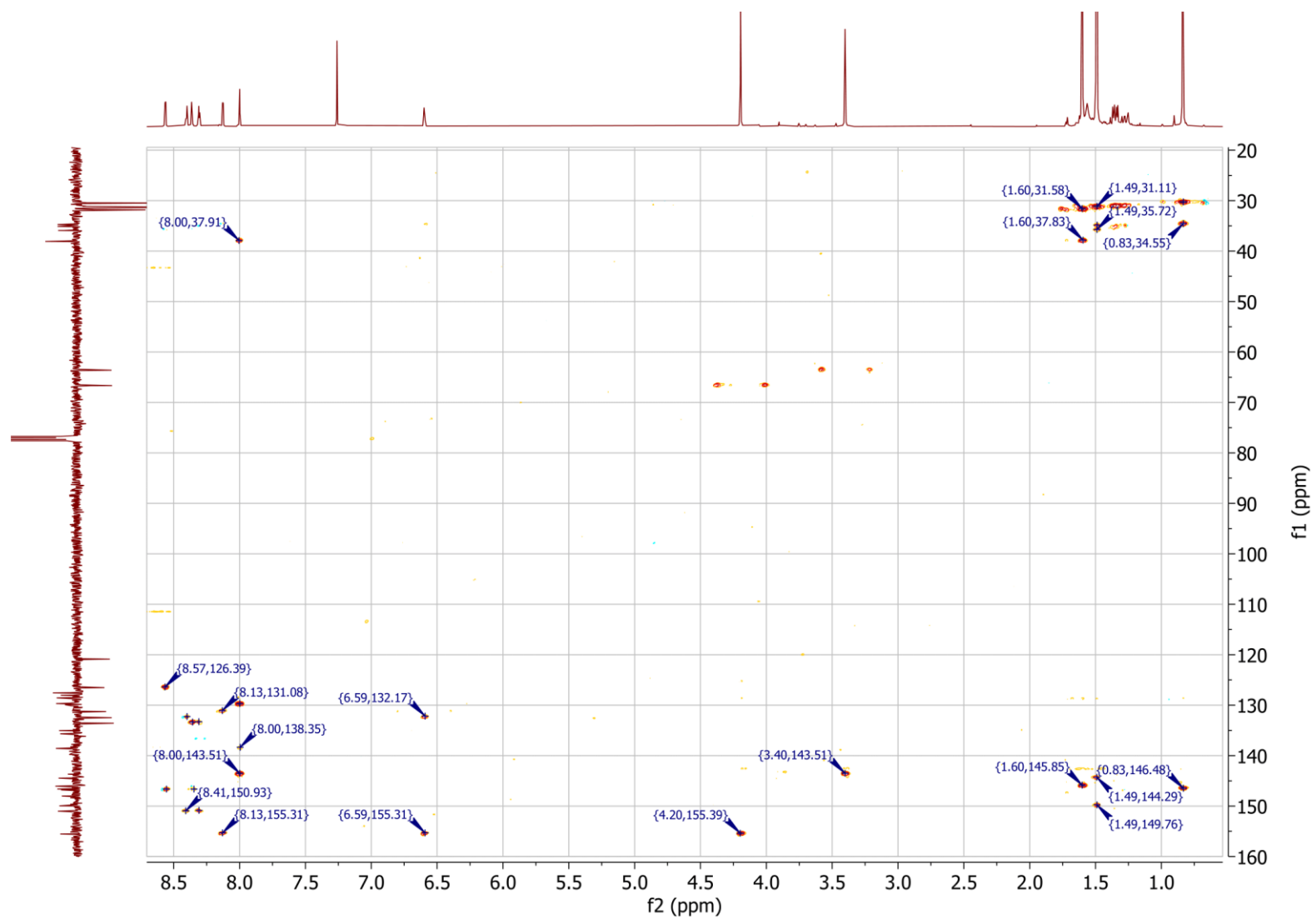


Figure S6: HMBC spectrum of compound 7

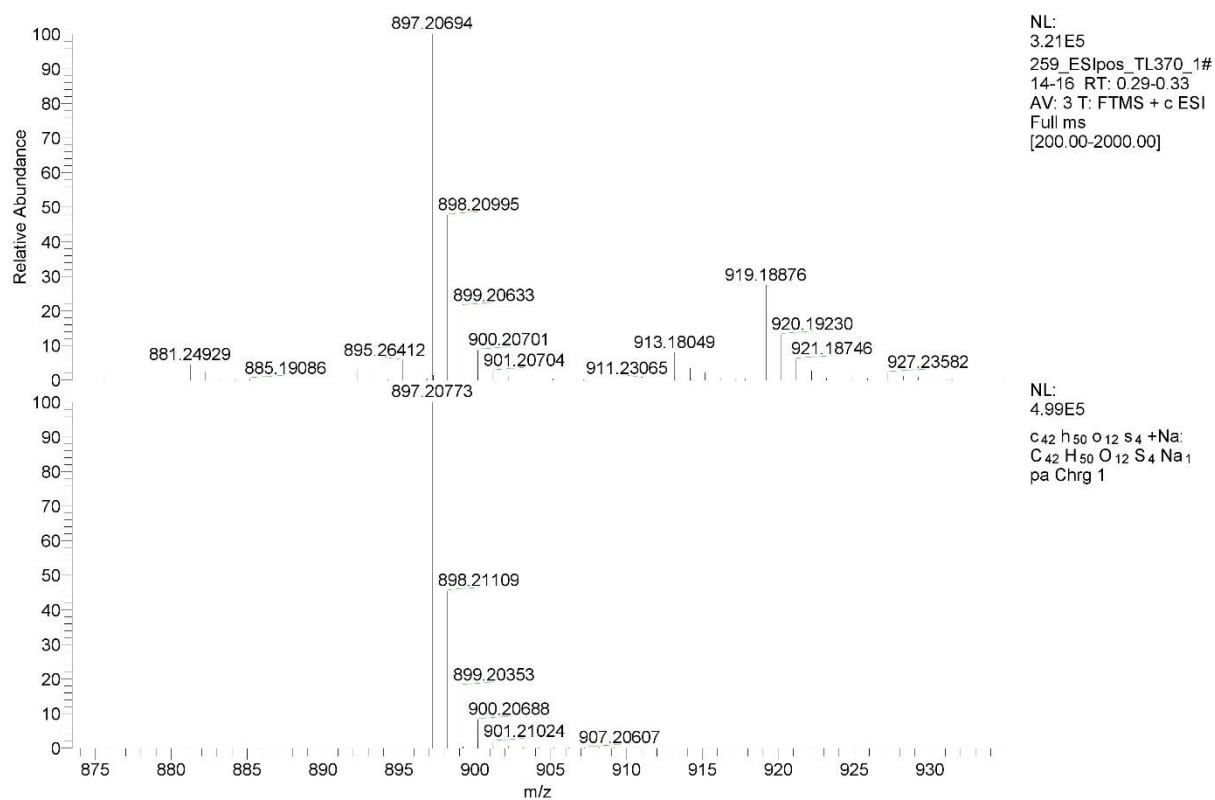


Figure S7: HRMS spectrum of compound 7

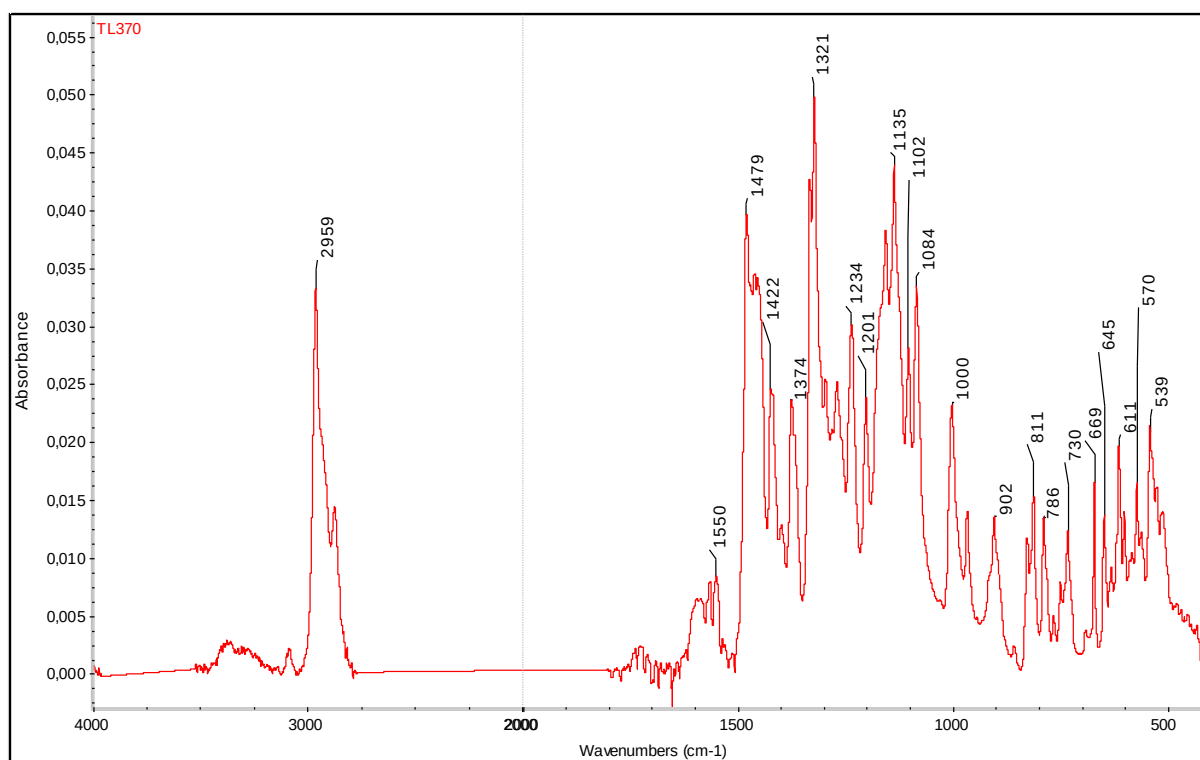


Figure S8: IR spectrum of compound 7

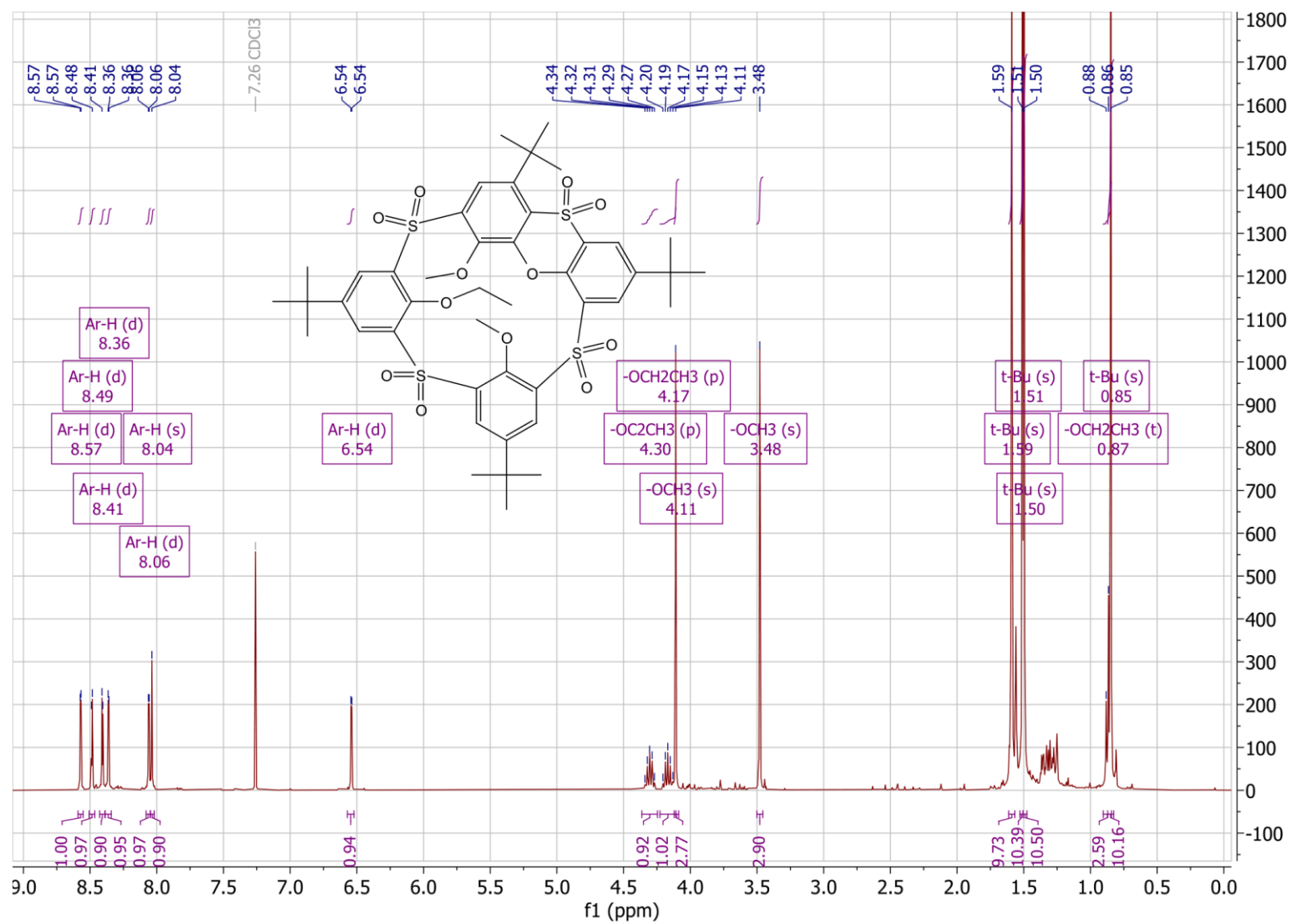


Figure S9: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **8**

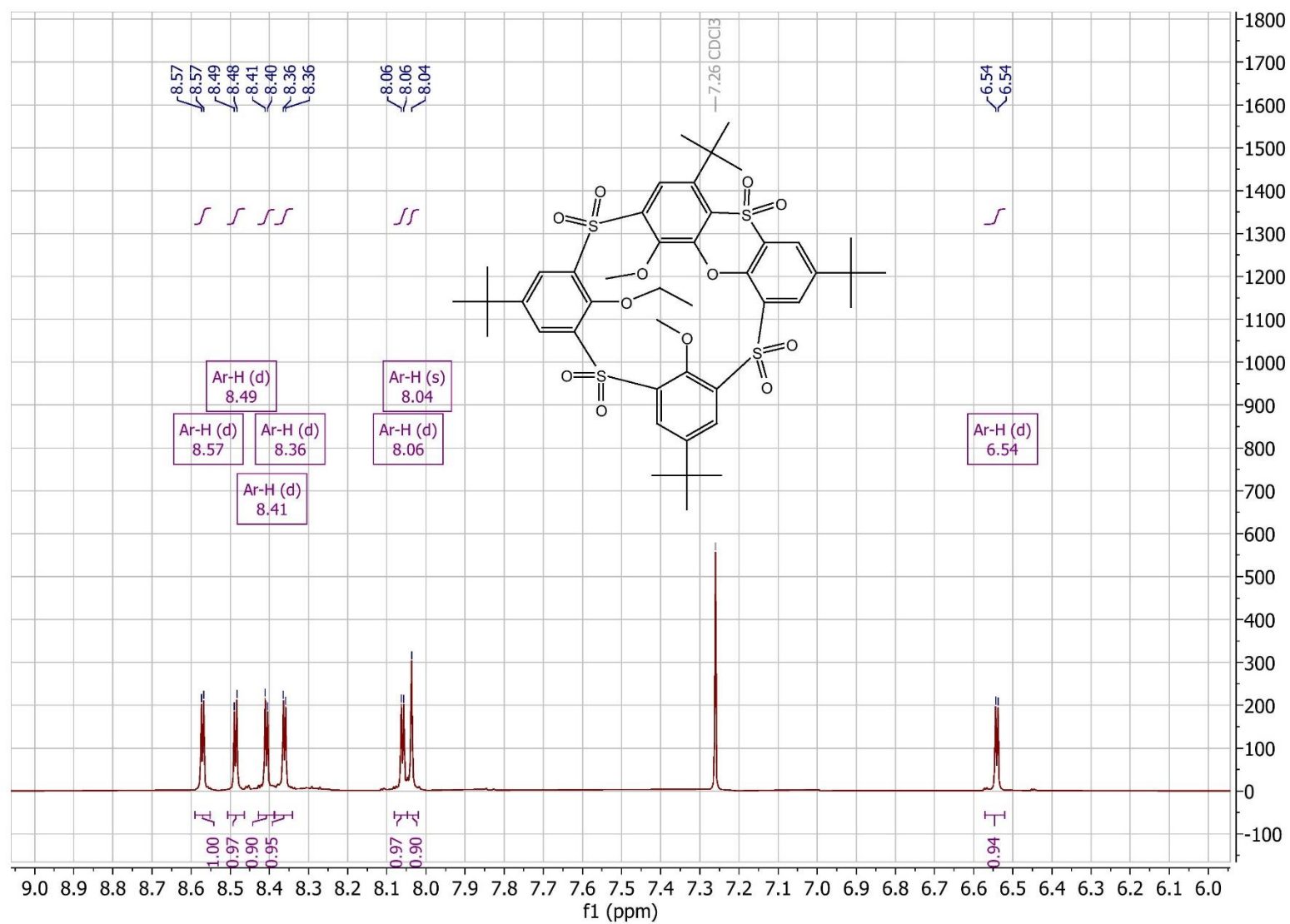


Figure S10: ¹H NMR (400 MHz, CDCl₃, 298 K) spectrum of compound **8** (aromatic region)

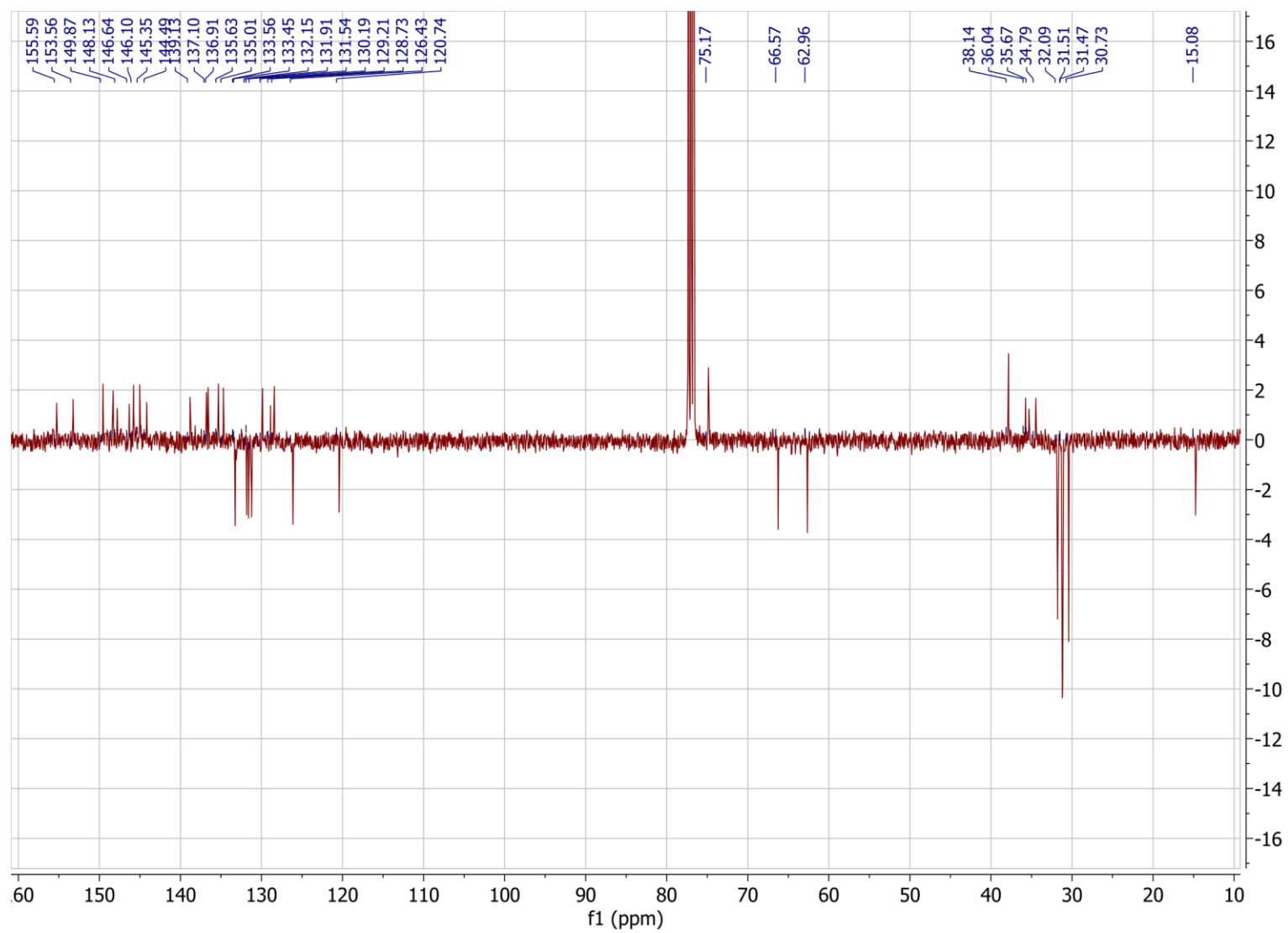


Figure S11: ¹³C NMR (APT, 101 MHz, CDCl₃, 298 K) spectrum of compound **8**

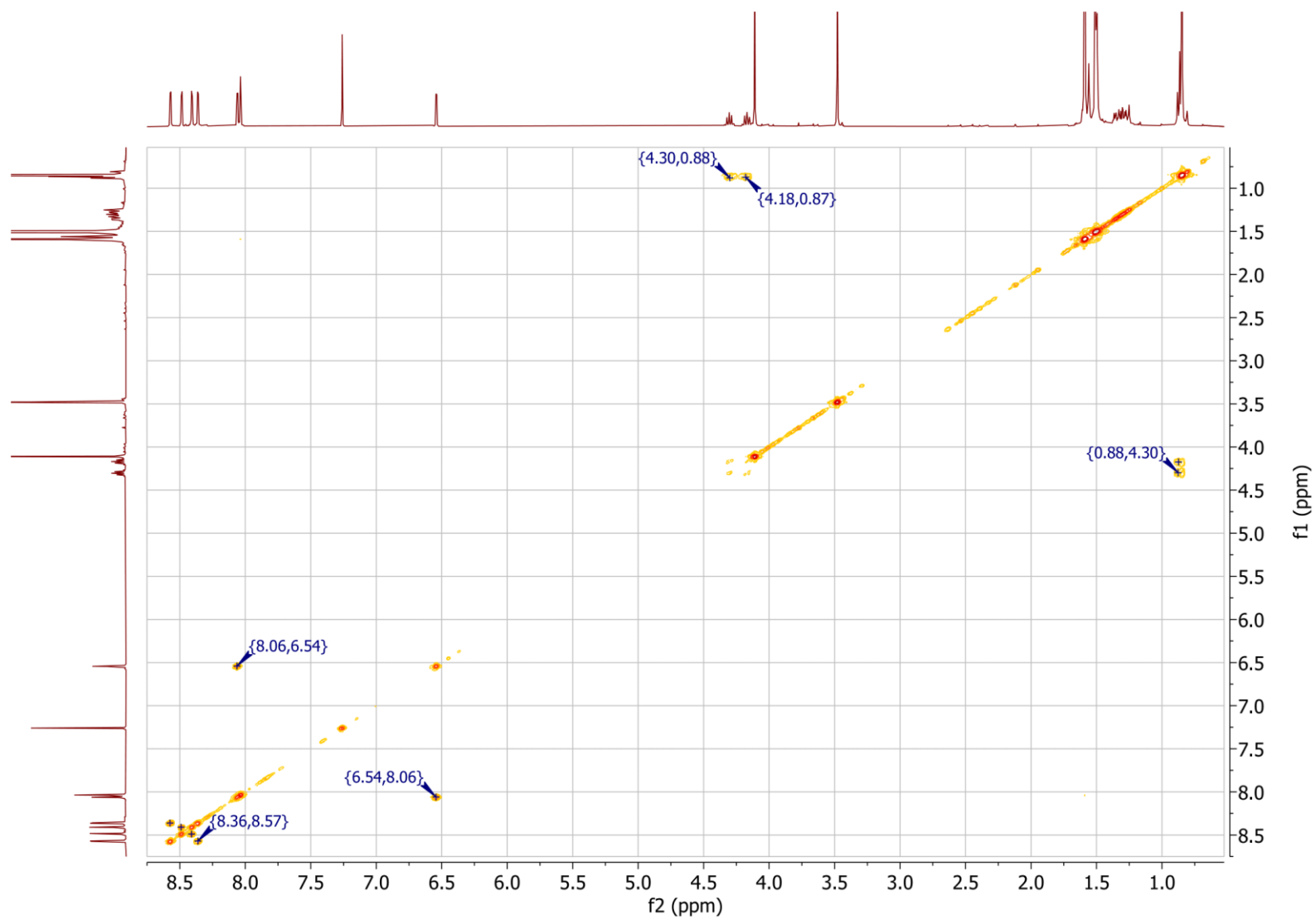


Figure S12: COSY spectrum of compound **8**

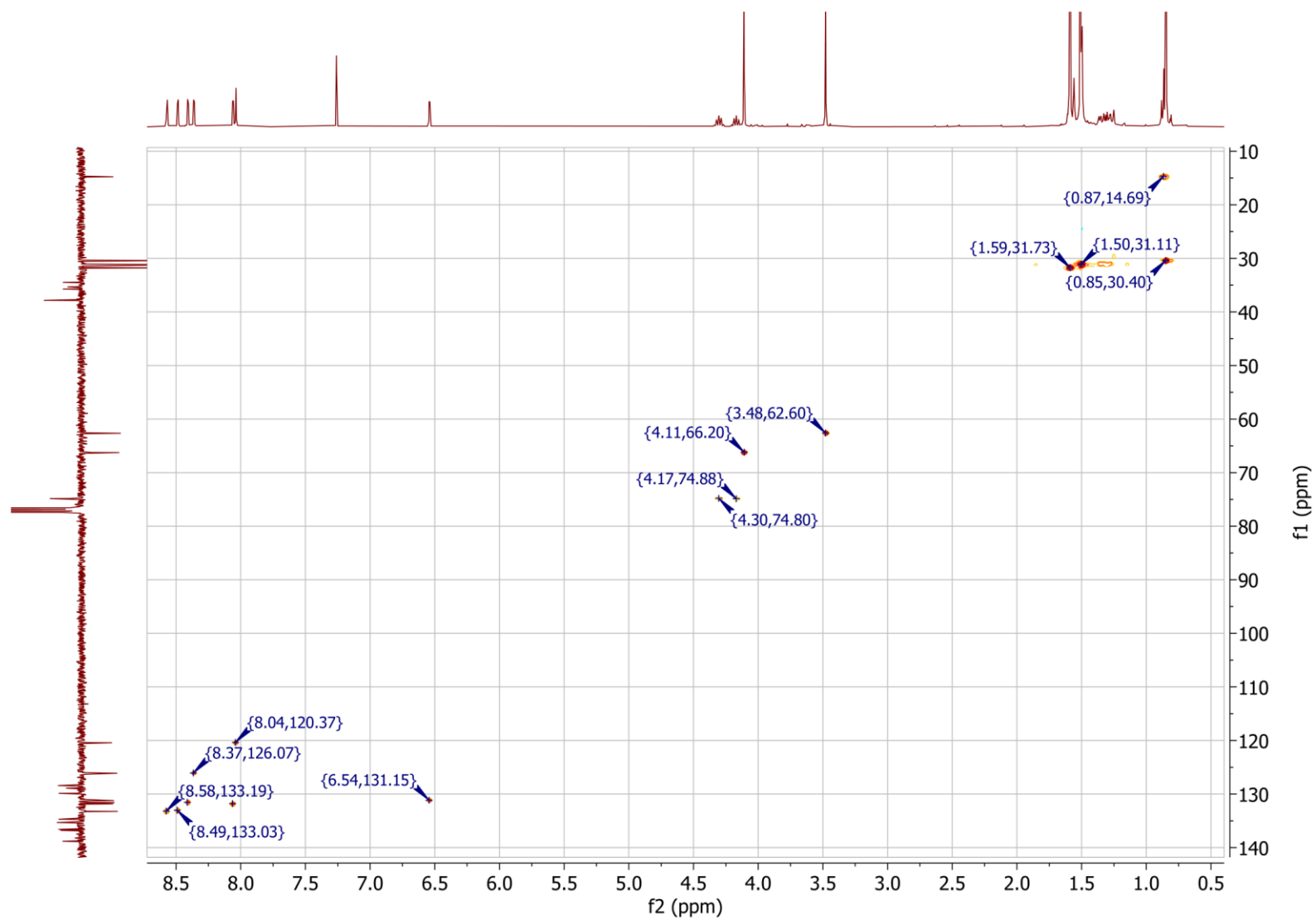


Figure S13: HMQC spectrum of compound **8**

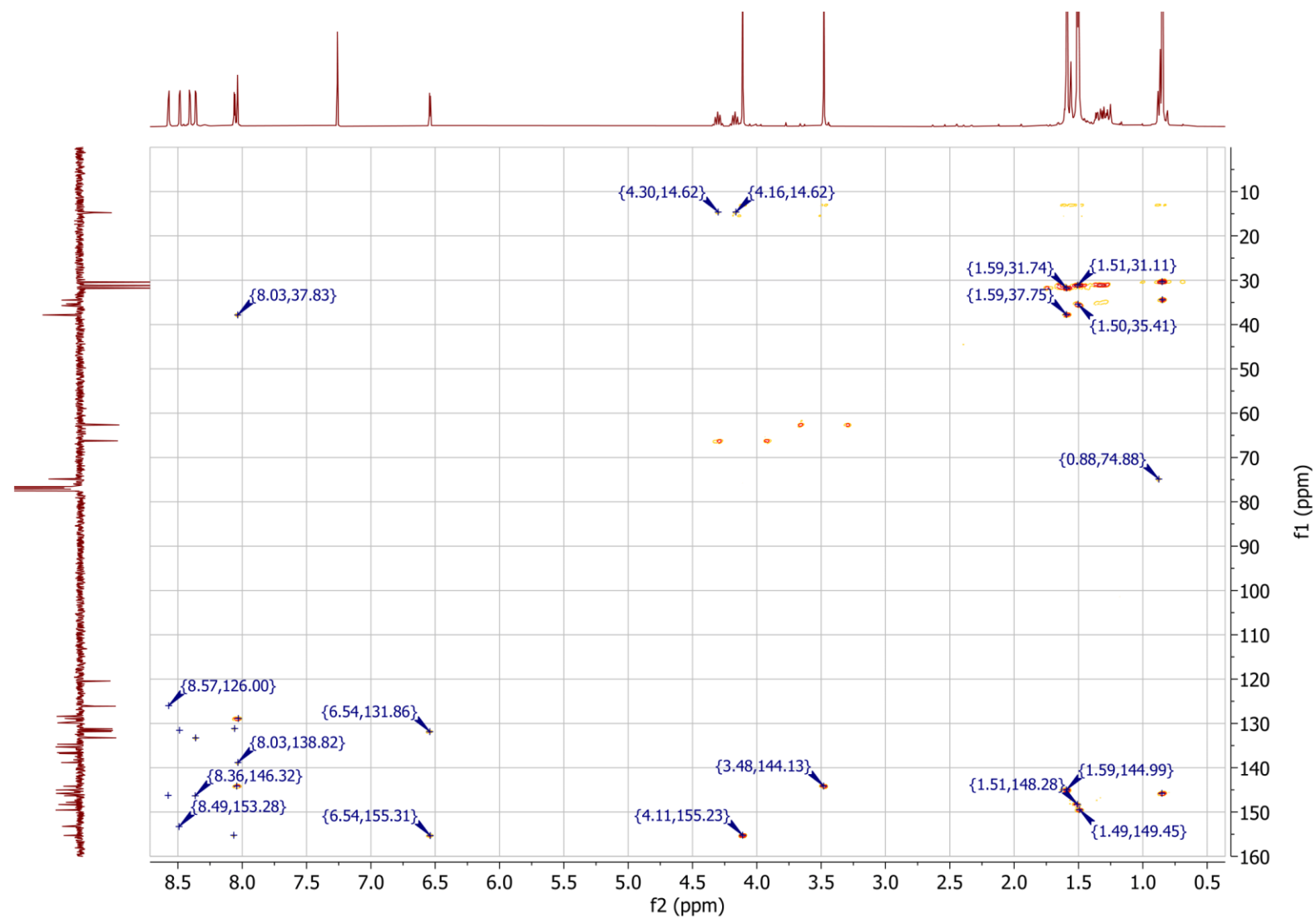


Figure S14: HMBC spectrum of compound 8

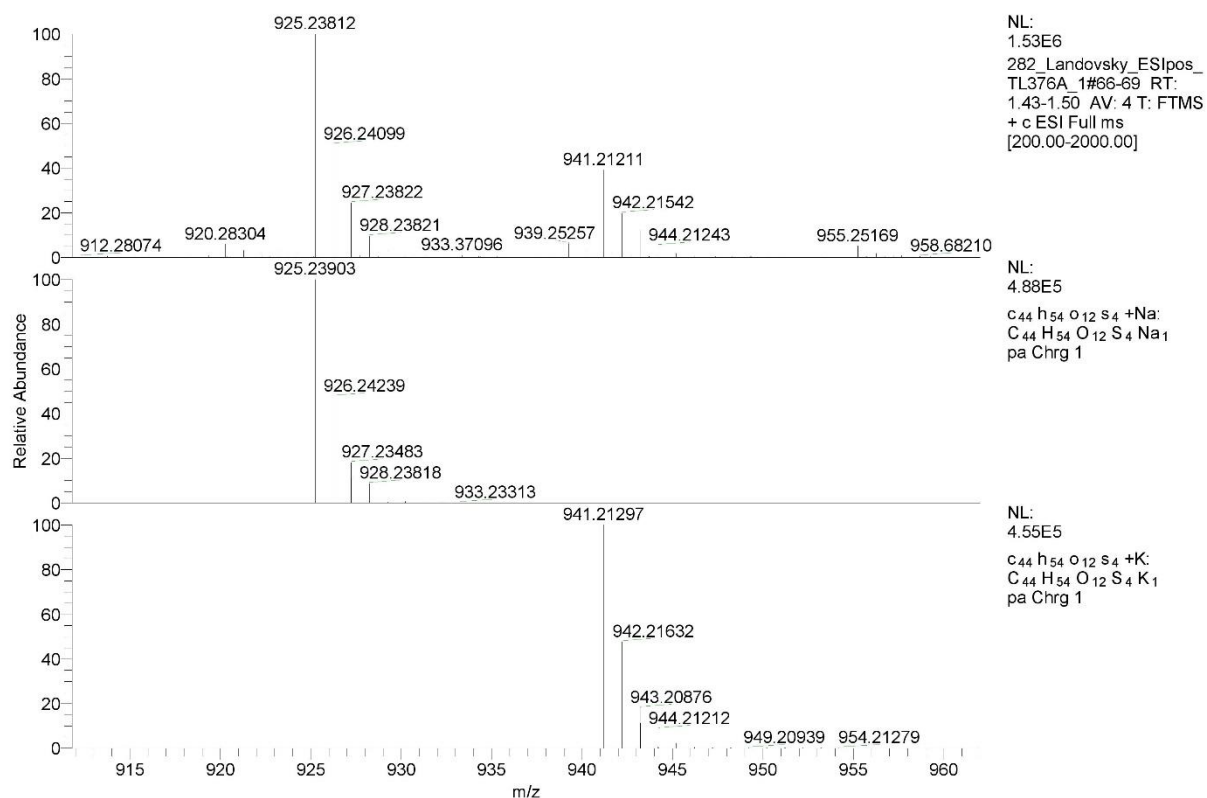


Figure S15: HRMS spectrum of compound 8

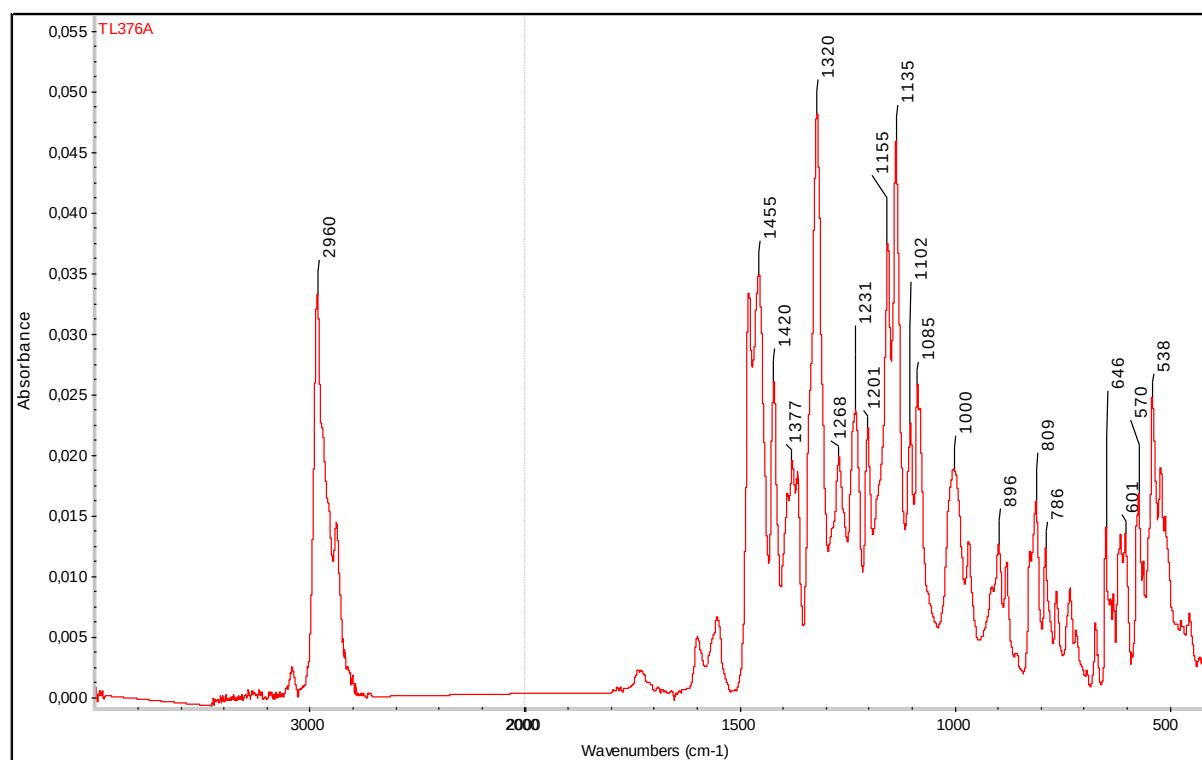


Figure S16: IR spectrum of compound 8

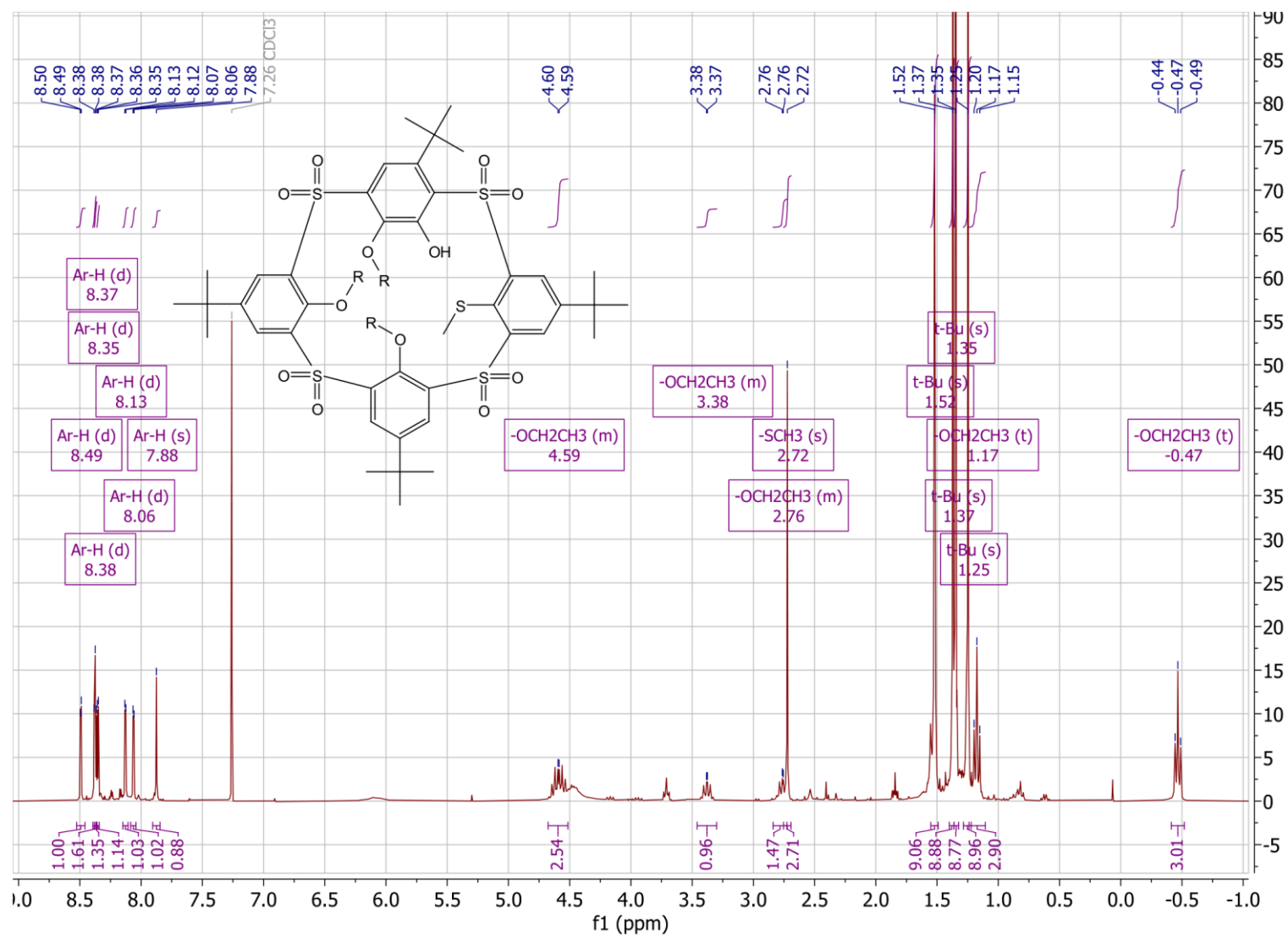


Figure S17: ¹H NMR (300 MHz, CDCl₃, 298 K) spectrum of compound **9**

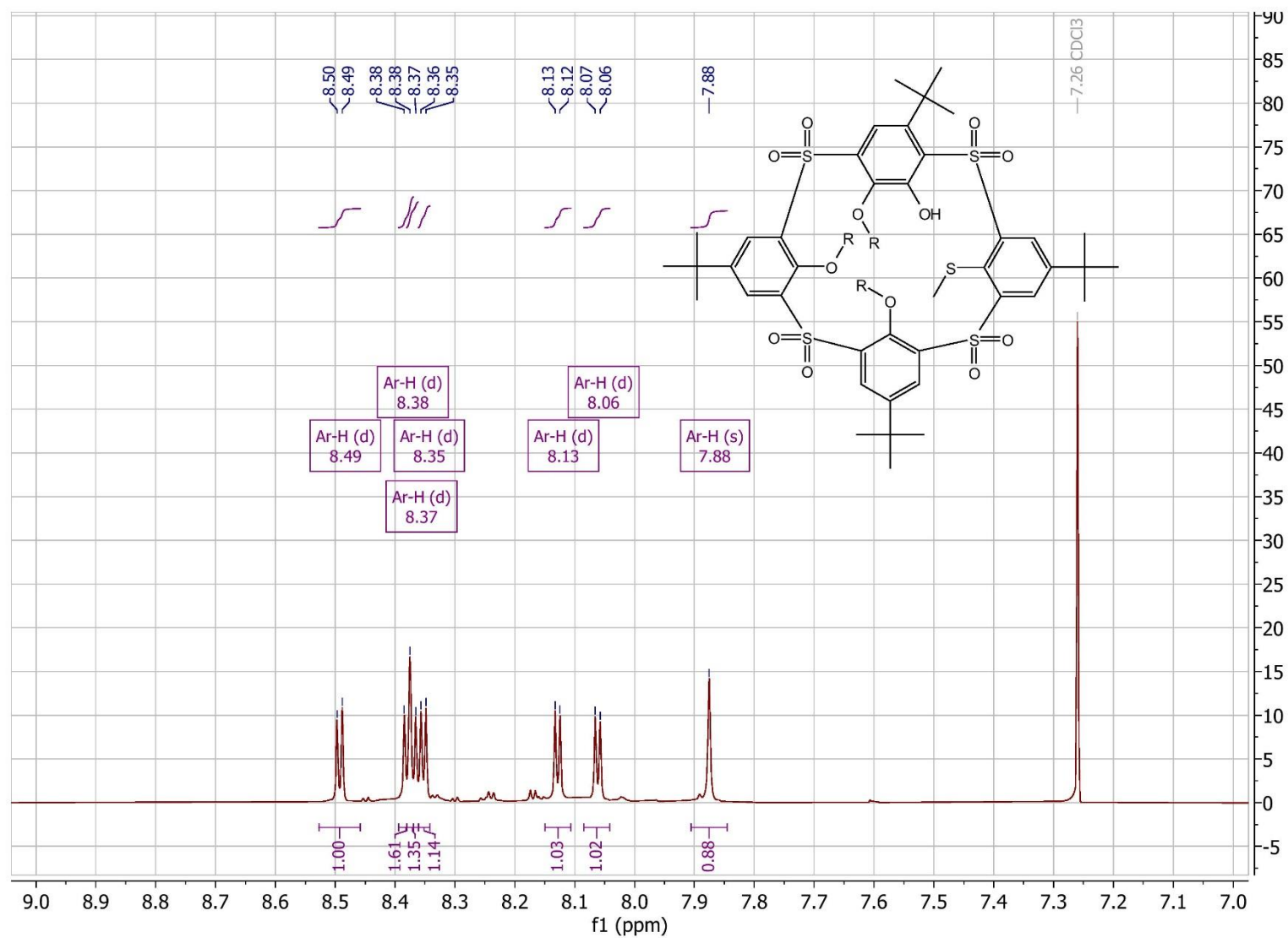


Figure S18: ^1H NMR (300 MHz, CDCl_3 , 298 K) spectrum of compound **9** (aromatic region)

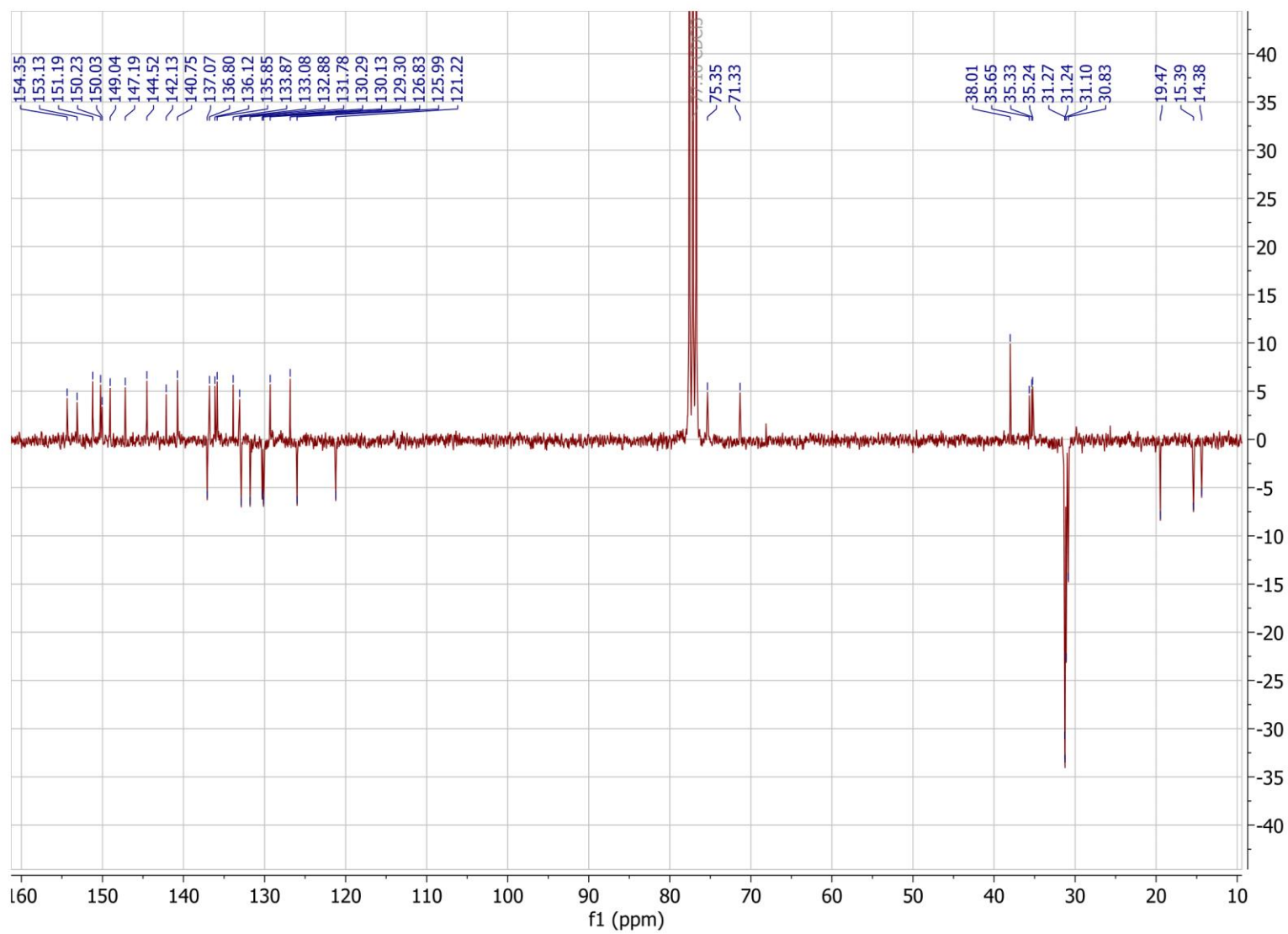


Figure S19: ^{13}C NMR (APT, 75 MHz, CDCl_3 , 298 K) spectrum of compound **9**

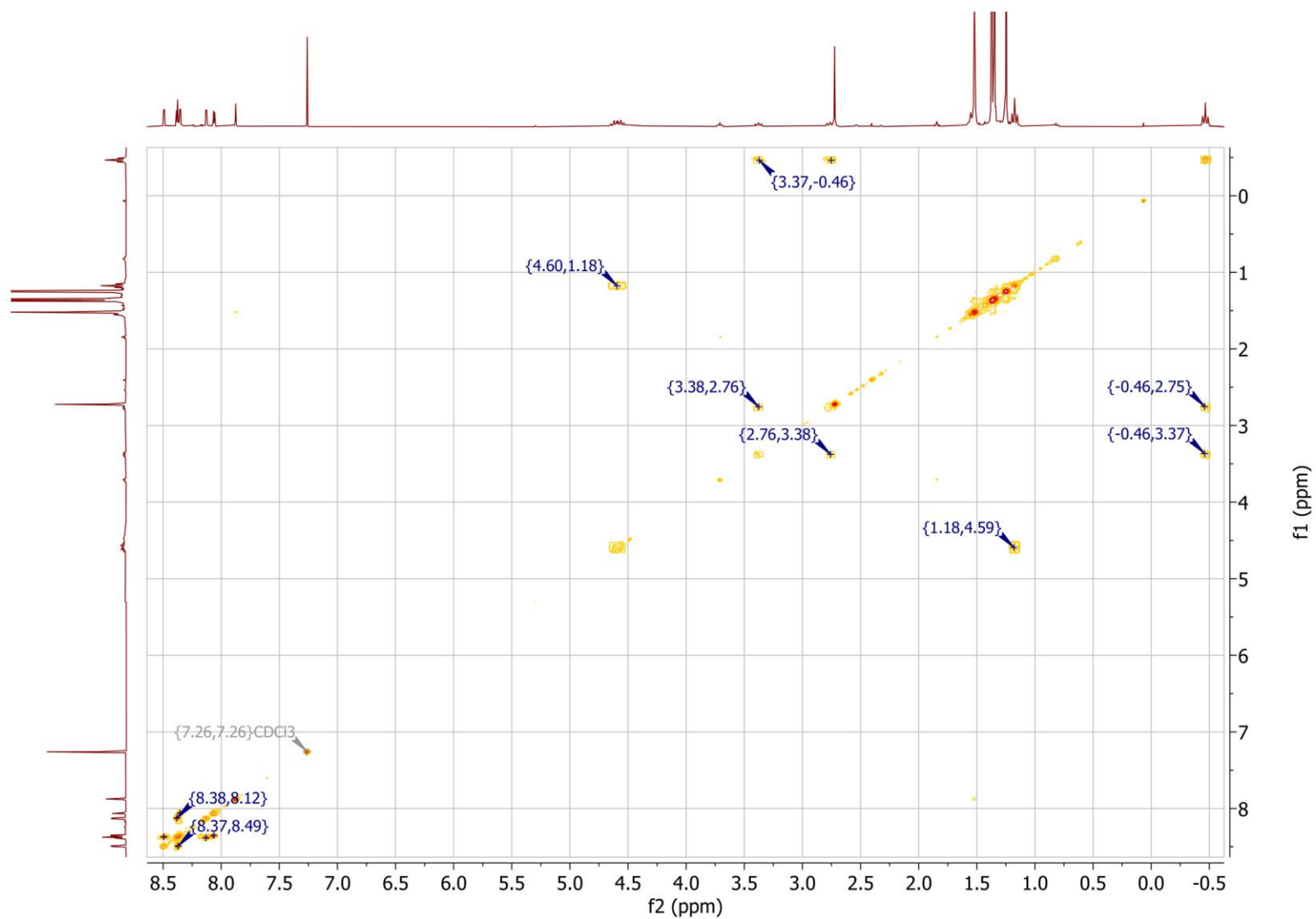


Figure S20: COSY spectrum of compound **9**

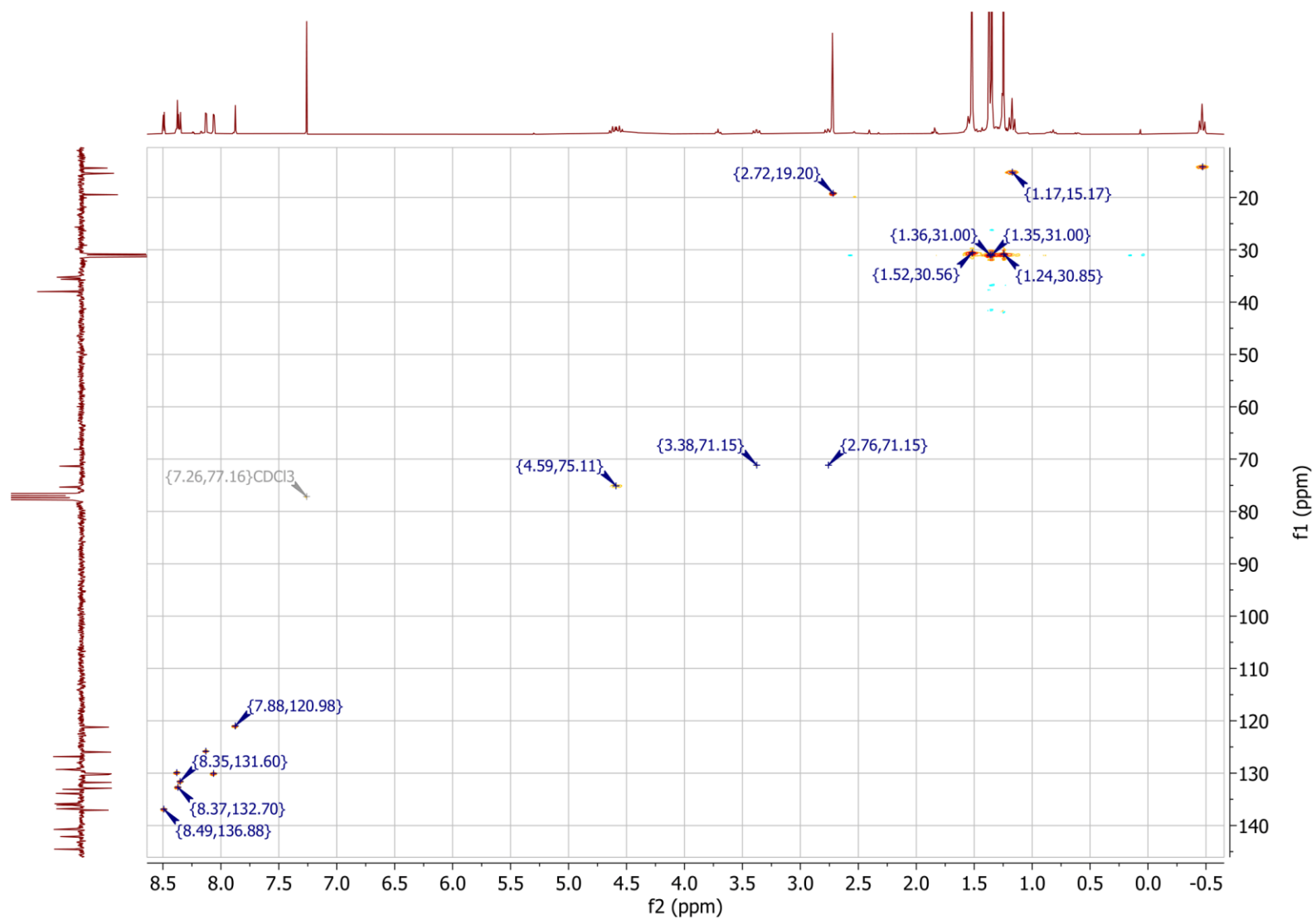


Figure S21: HMQC spectrum of compound 9

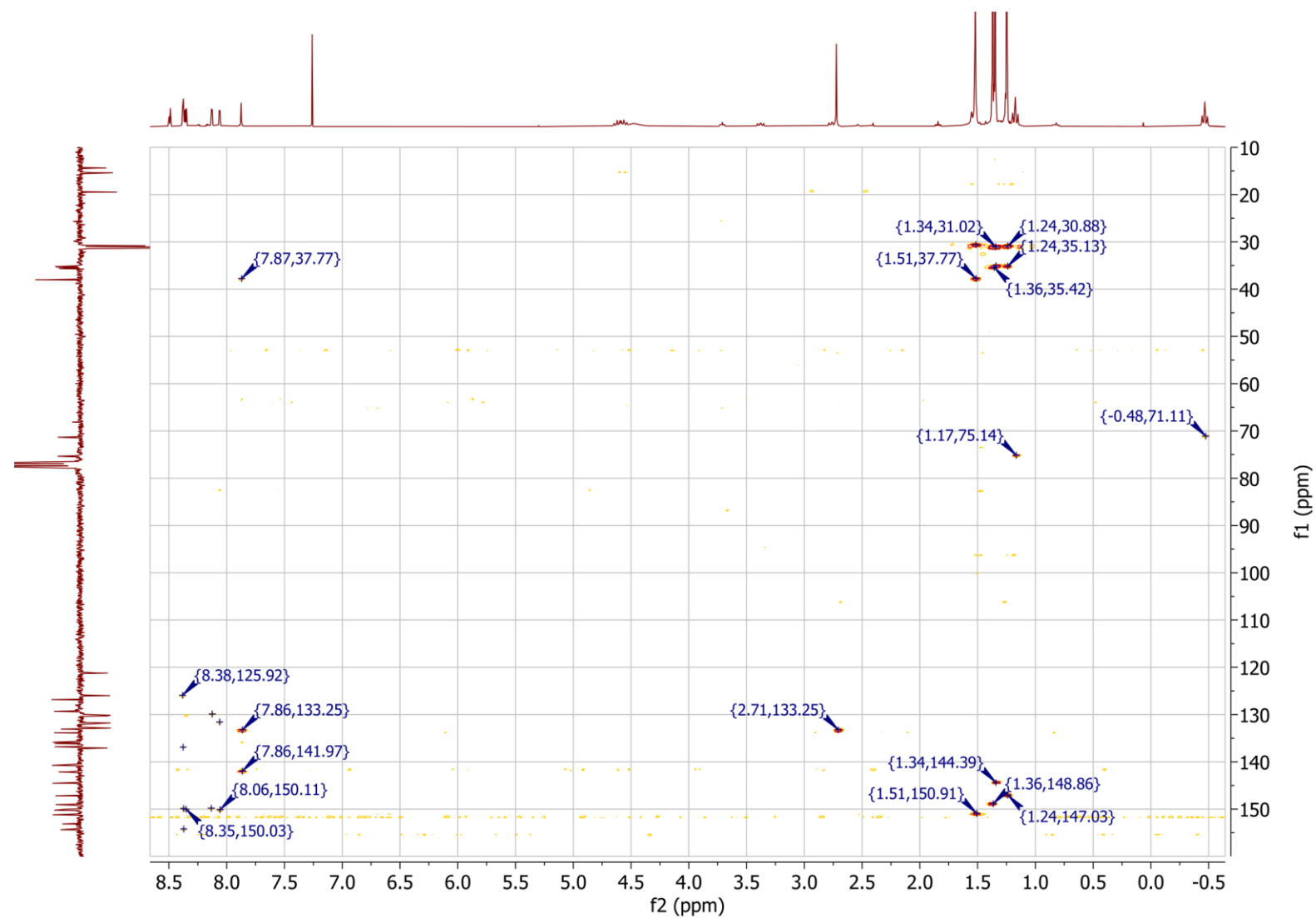


Figure S22: HMBC spectrum of compound 9

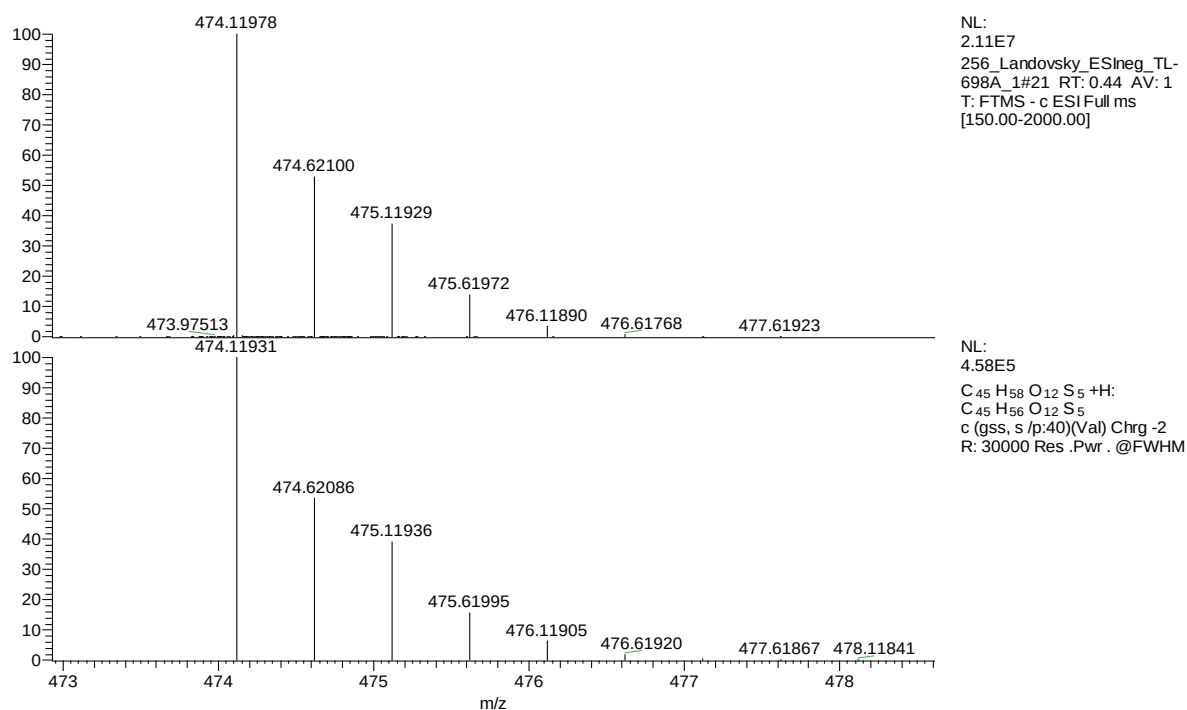


Figure S23: HRMS spectrum of compound 9

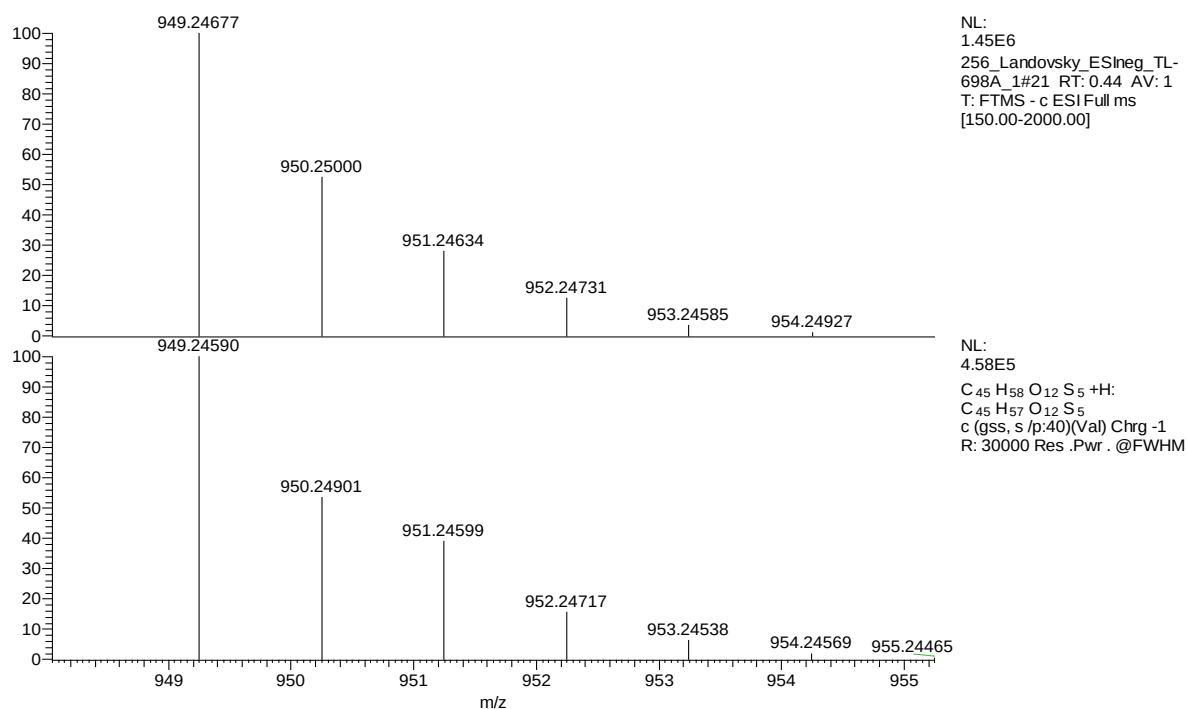


Figure S24: HRMS spectrum of compound 9

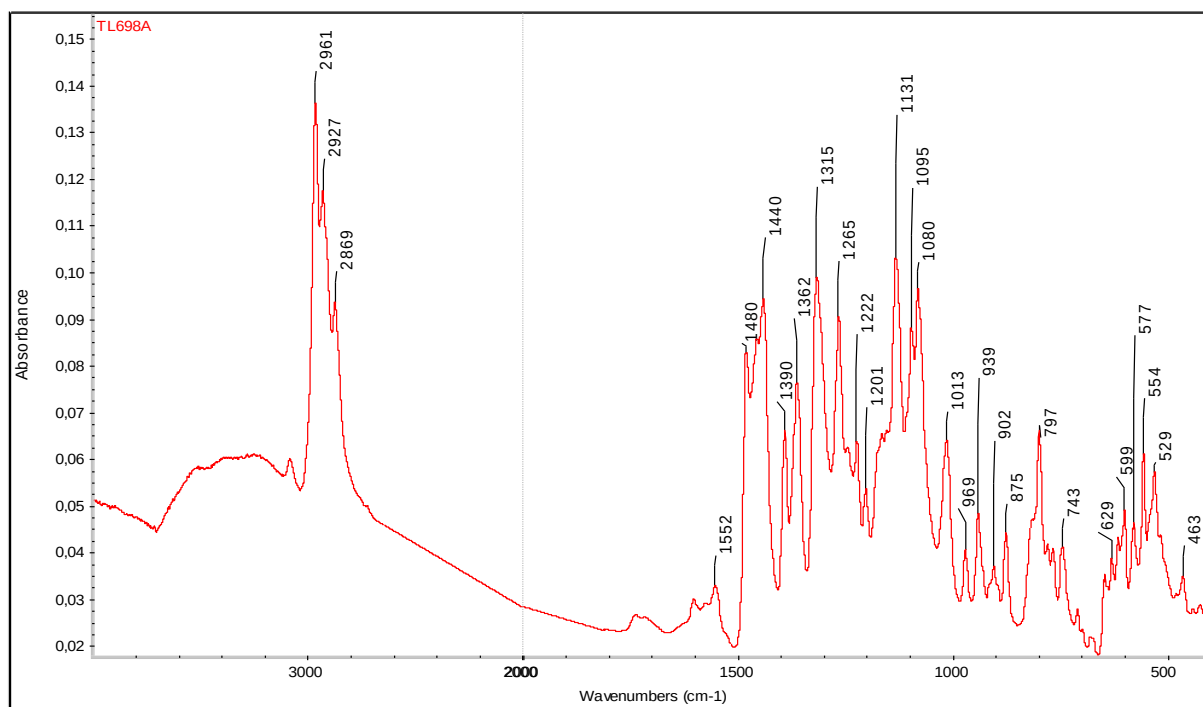


Figure S25: IR spectrum of compound **9**

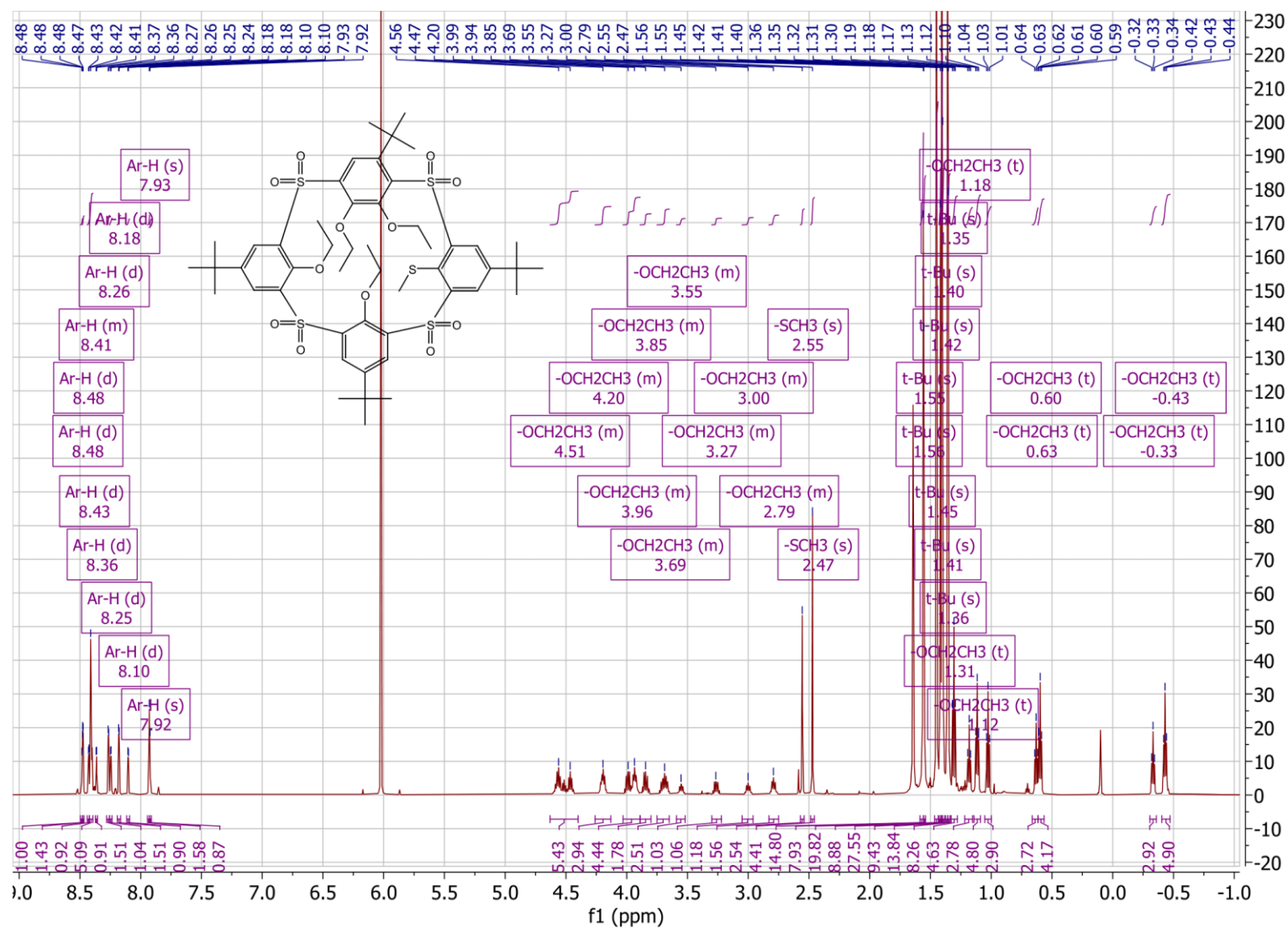


Figure S26: ^1H NMR (600 MHz, CDCl_3 , 298 K) spectrum of compound **10**

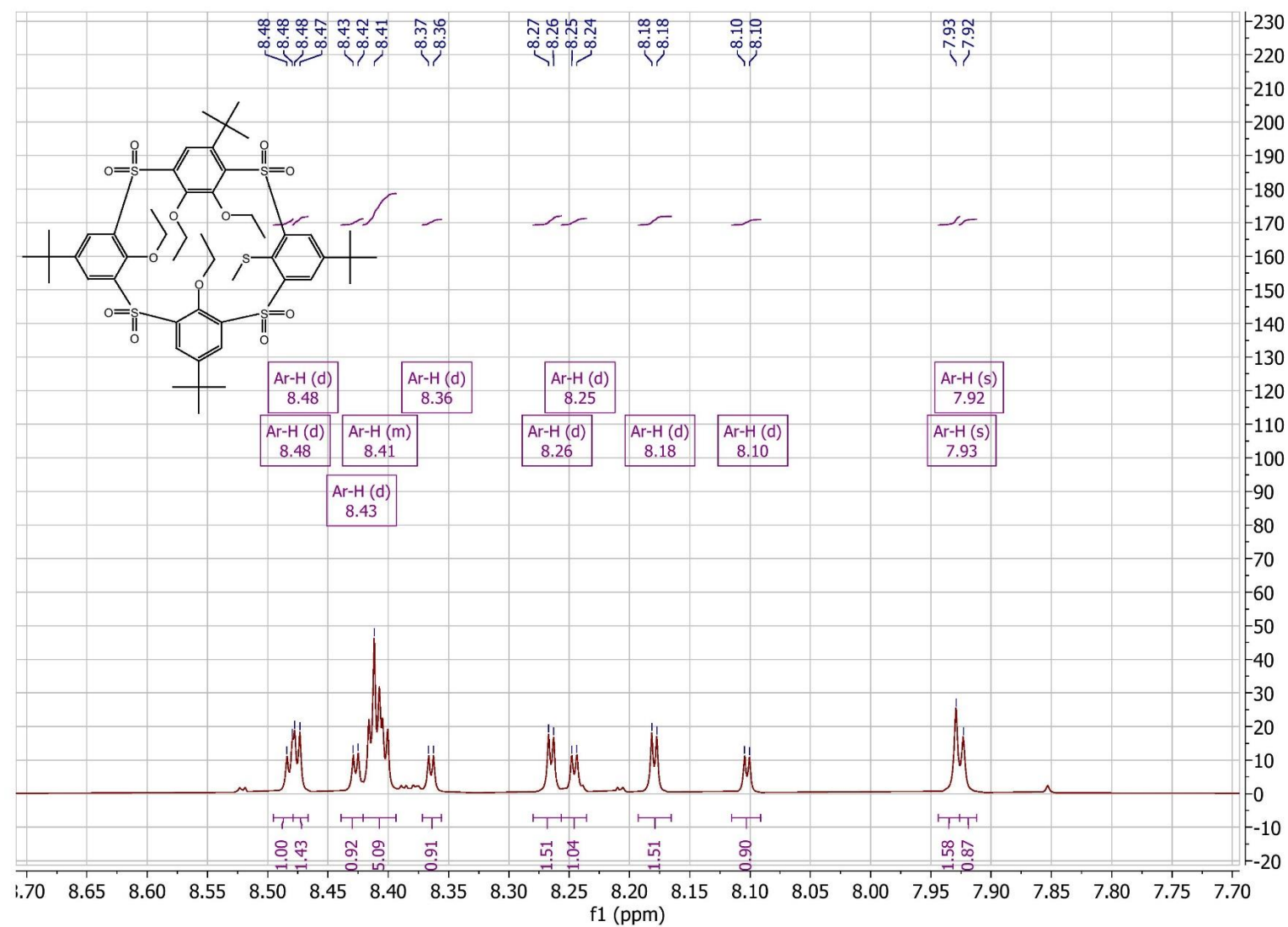


Figure S27: ^1H NMR (600 MHz, CDCl_3 , 298 K) spectrum of compound **10** (zoom 1)

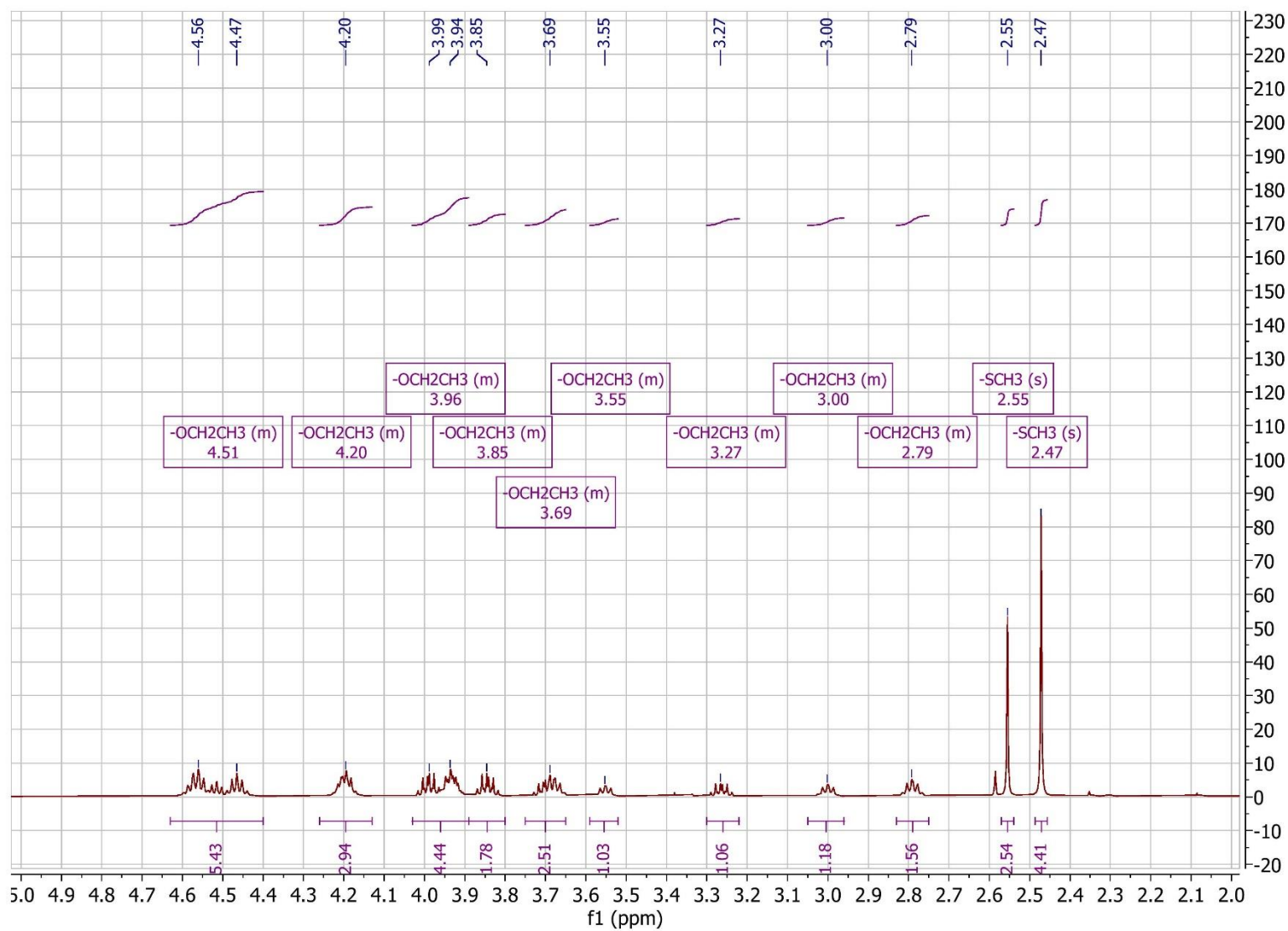


Figure S28: ^1H NMR (600 MHz, CDCl_3 , 298 K) spectrum of compound **10** (zoom 2)

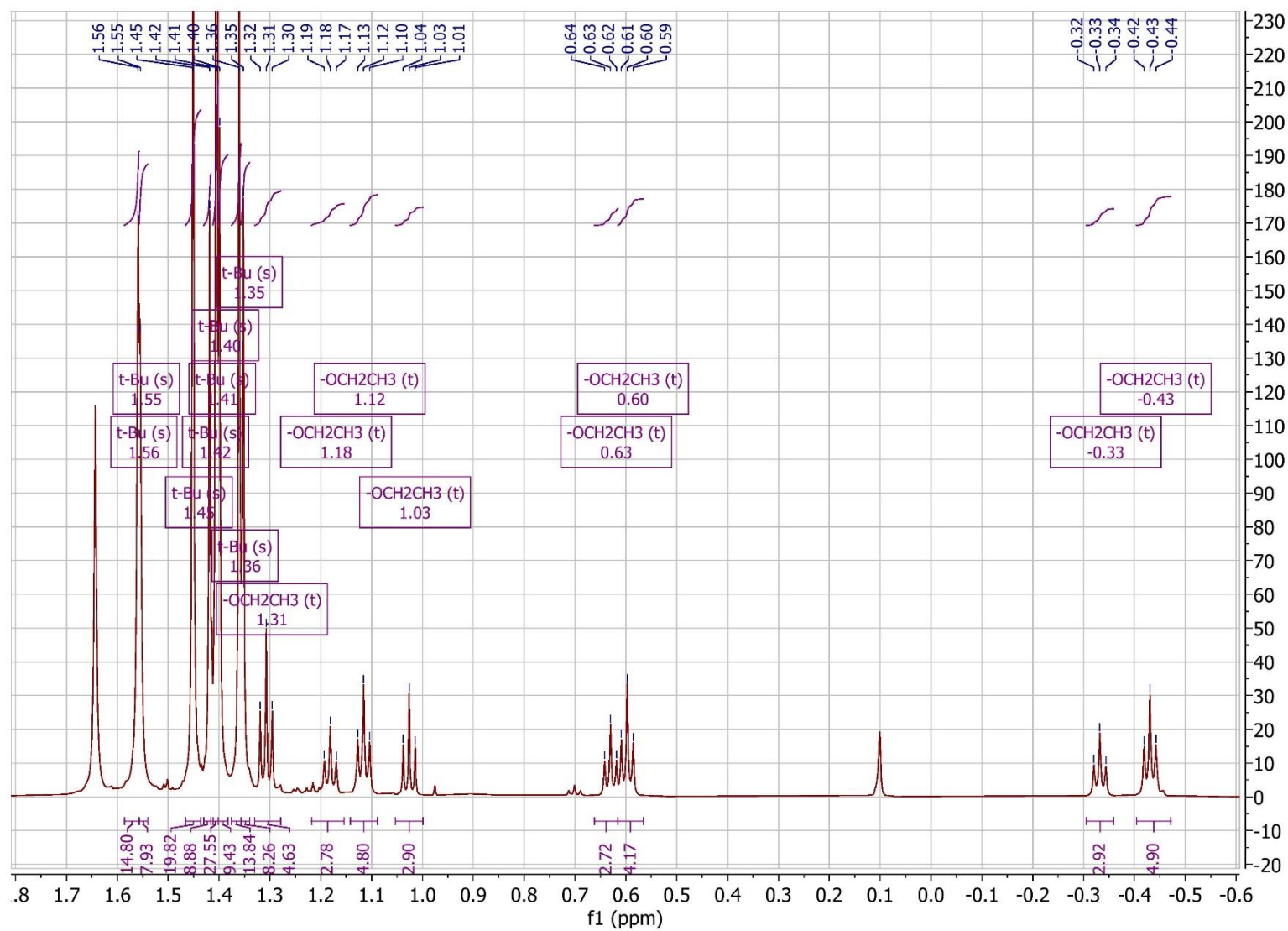


Figure S29: ^1H NMR (600 MHz, CDCl_3 , 298 K) spectrum of compound **10** (zoom 3)

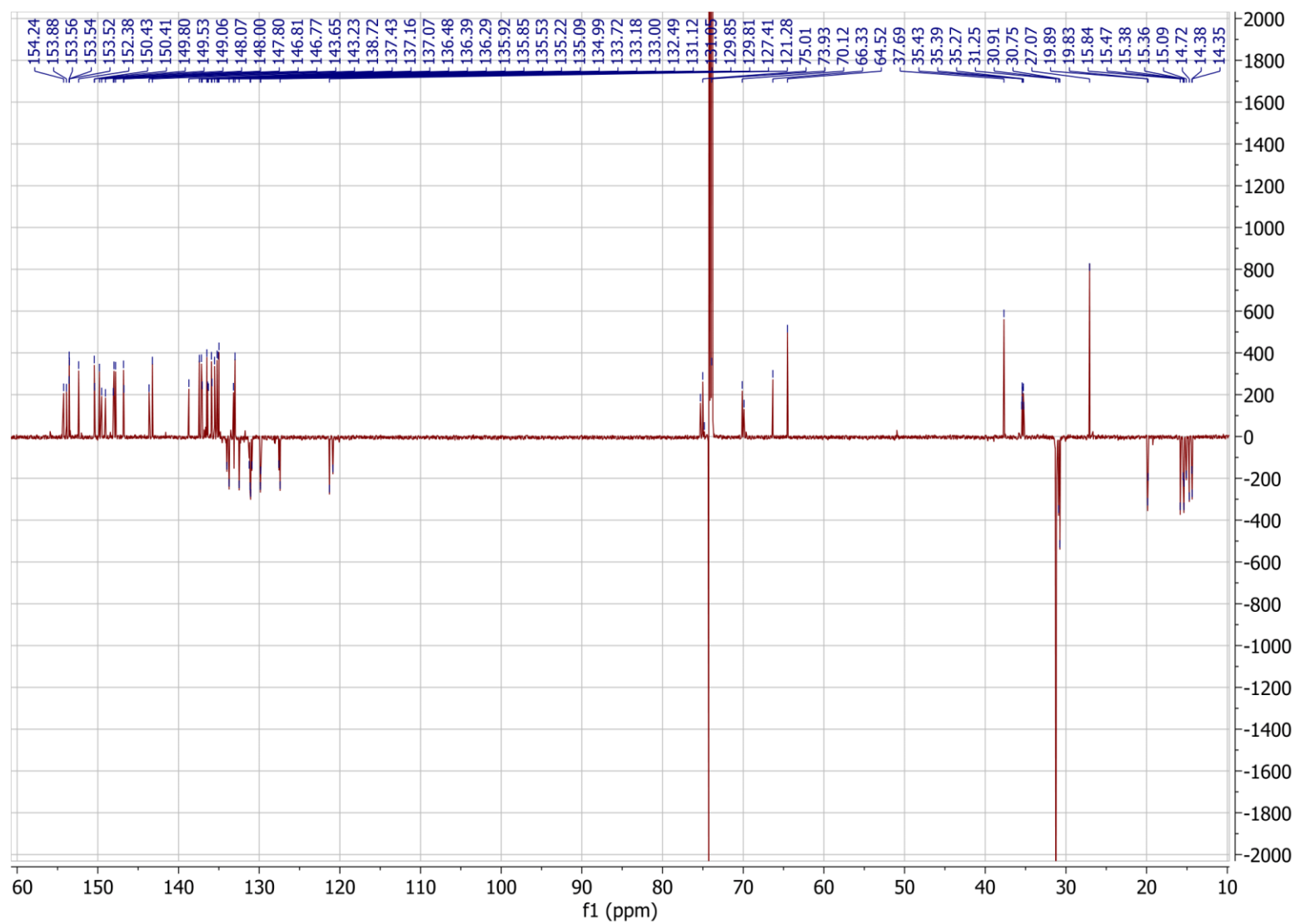


Figure S30: ^{13}C NMR (APT, 150 MHz, CDCl_3 , 298 K) spectrum of compound **10**

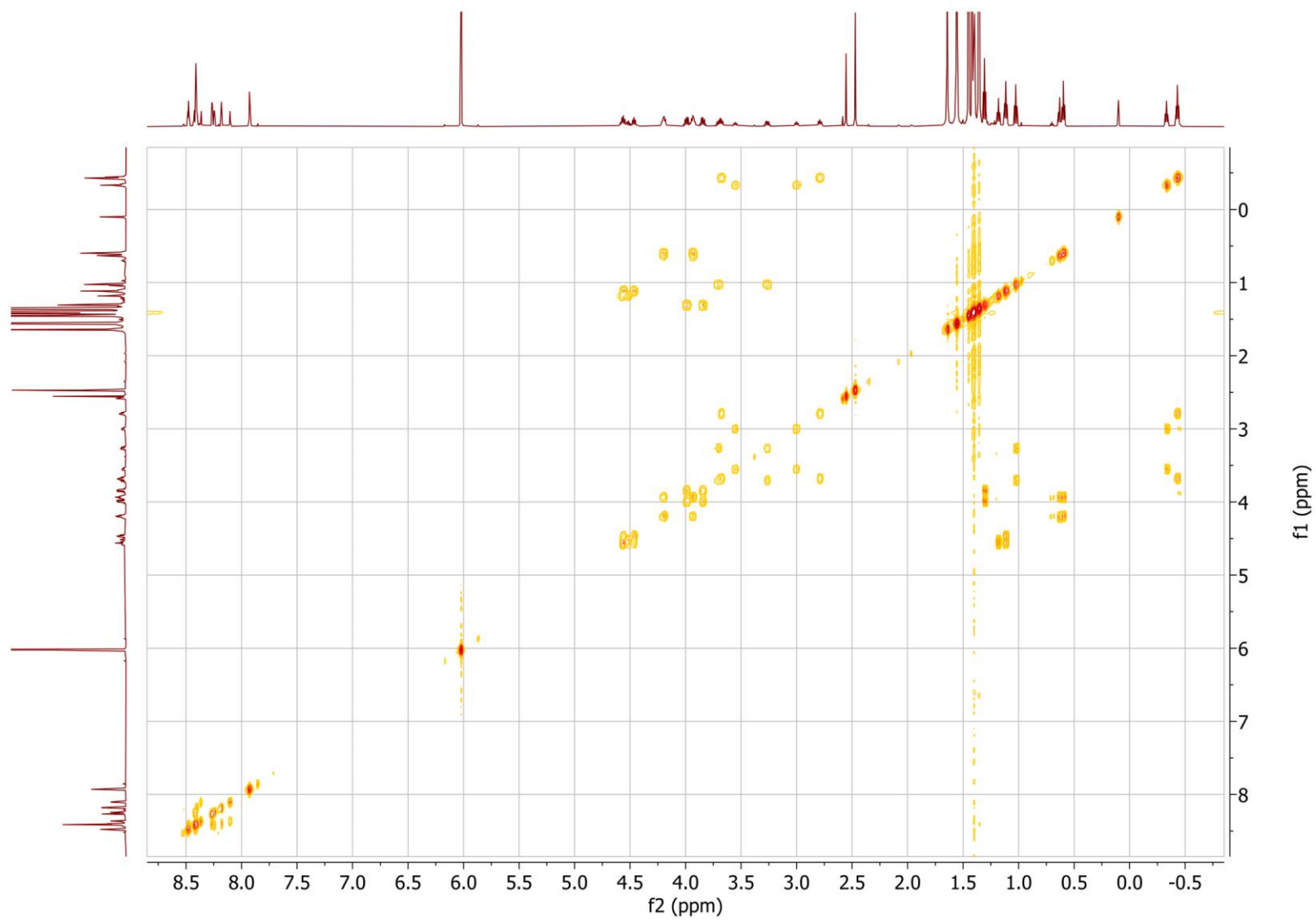


Figure S31: COSY spectrum of compound **10**



Figure S32: HMQC spectrum of compound **10**



Figure S33: HMBC spectrum of compound **10**

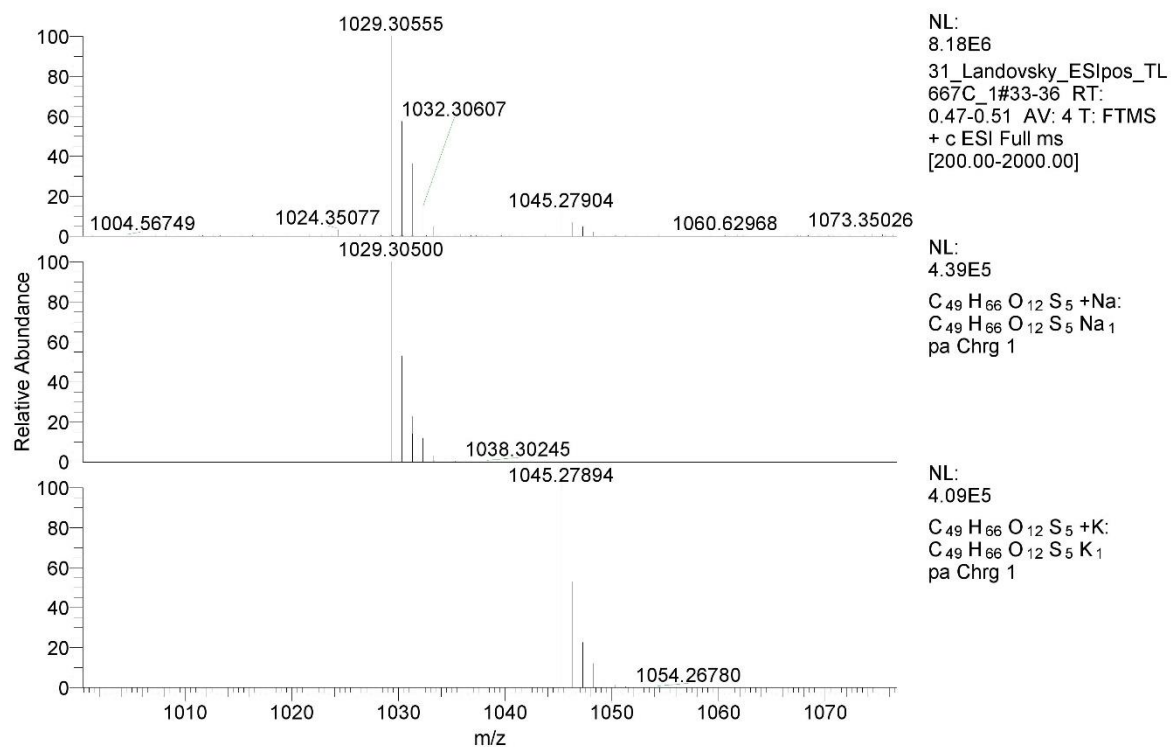


Figure S34: HRMS spectrum of compound **10**

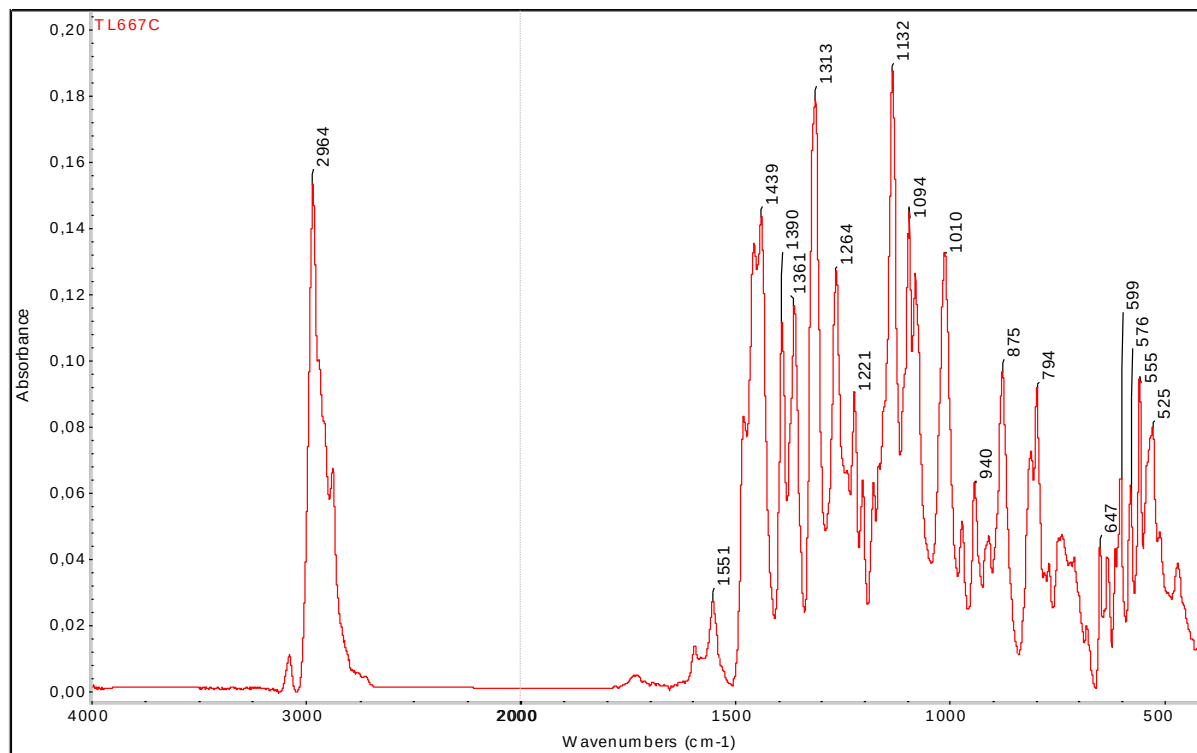


Figure S35: IR spectrum of compound **10**

$[\text{C}_{46}\text{H}_{58}\text{O}_{12}\text{S}_5]^{2-}$ 481.1276 $[\text{M}-2\text{Na}]^{2-}$

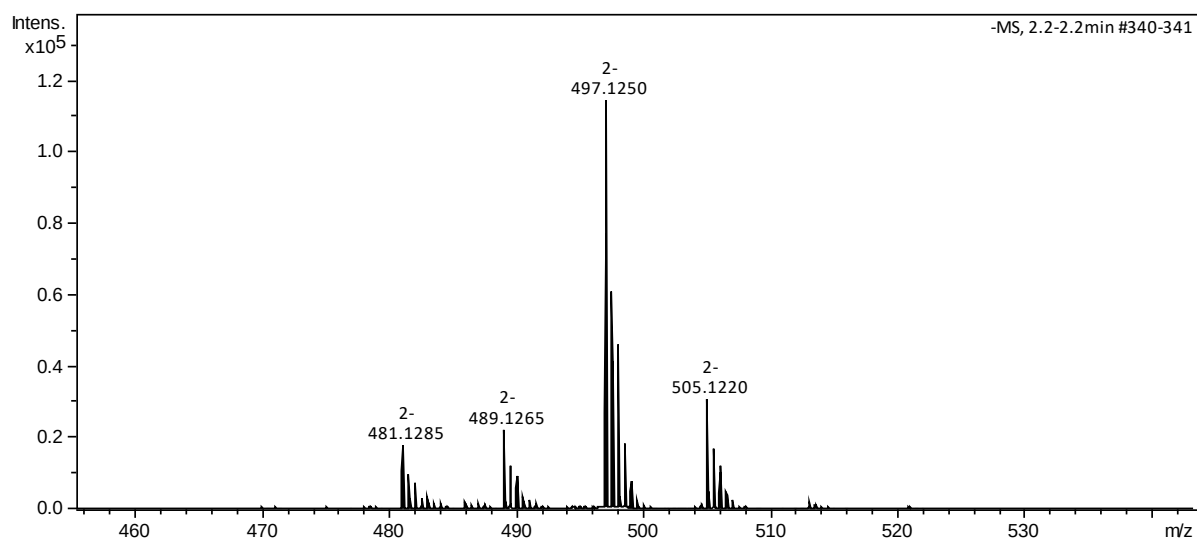


Figure S37: HRMS spectrum of compound **11a**

$[\text{C}_{49}\text{H}_{64}\text{O}_{12}\text{S}_5]^{2-}$ 502.1506 $[\text{M}-2\text{Na}]^{2-}$

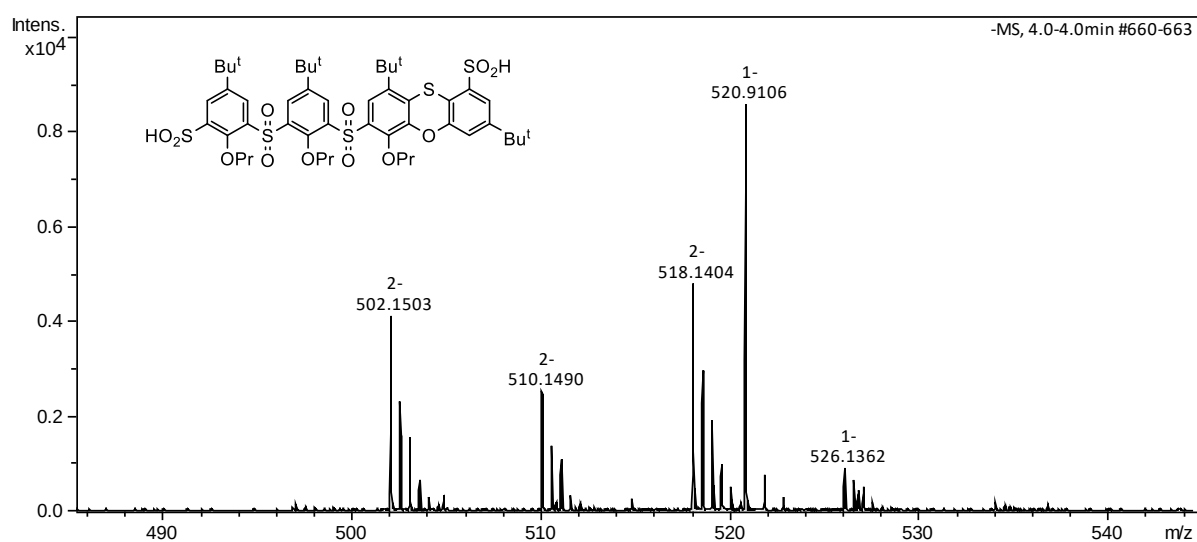


Figure S38: HRMS spectrum of compound **11b**

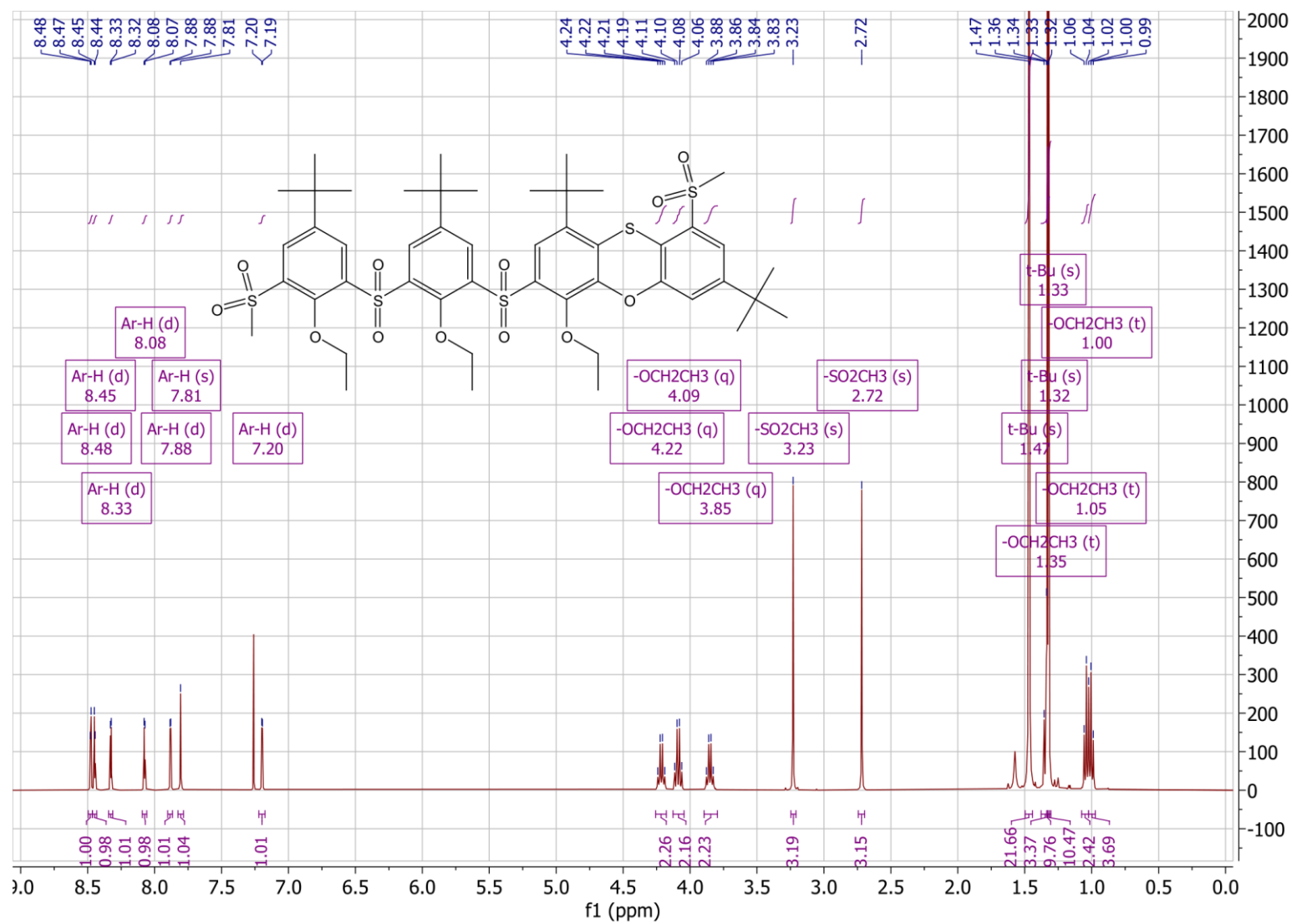


Figure S39: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **12a**

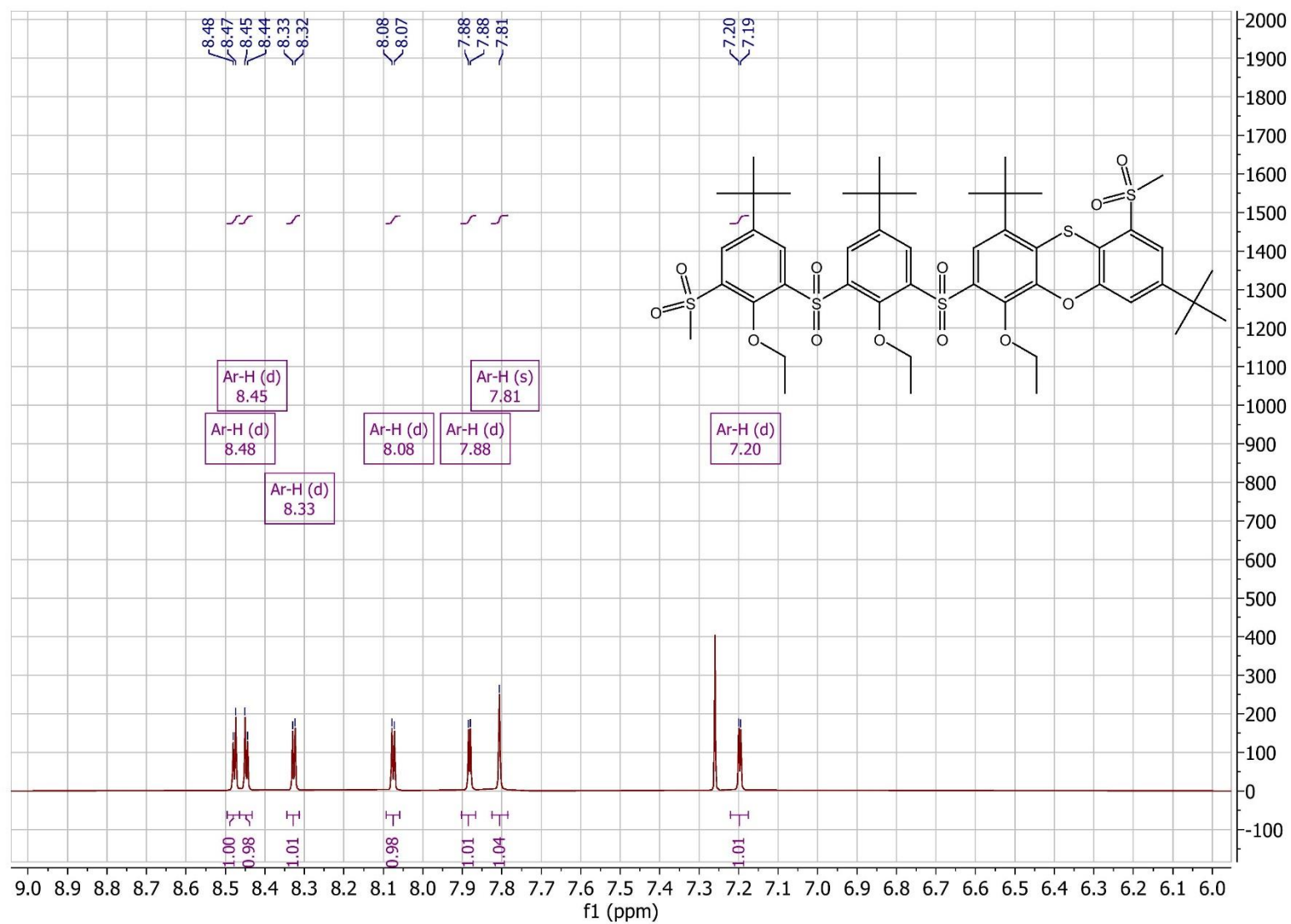


Figure S40: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **12a** (aromatic region)

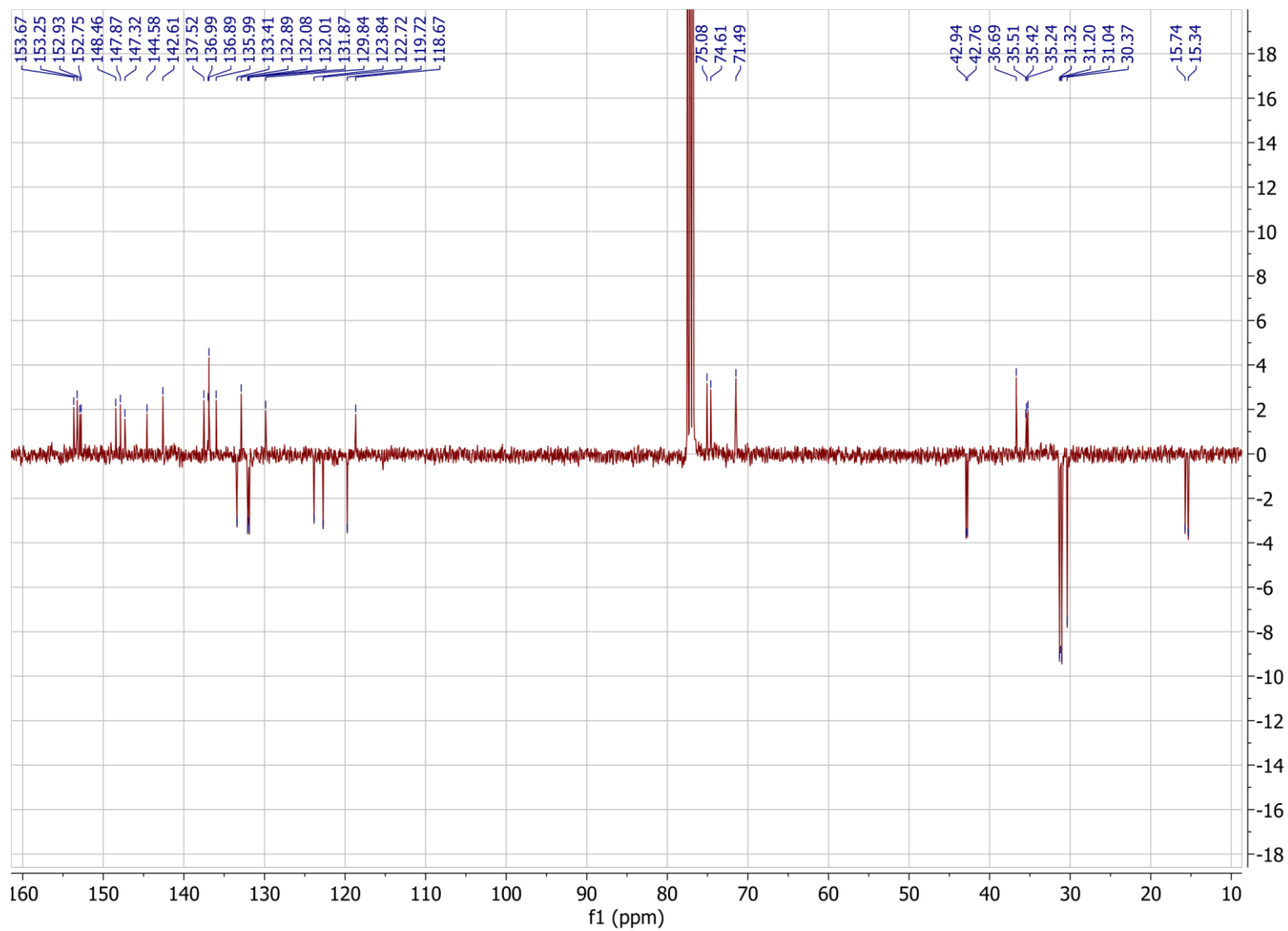


Figure S41: ¹³C NMR (APT, 101 MHz, CDCl₃, 298 K) spectrum of compound **12a**

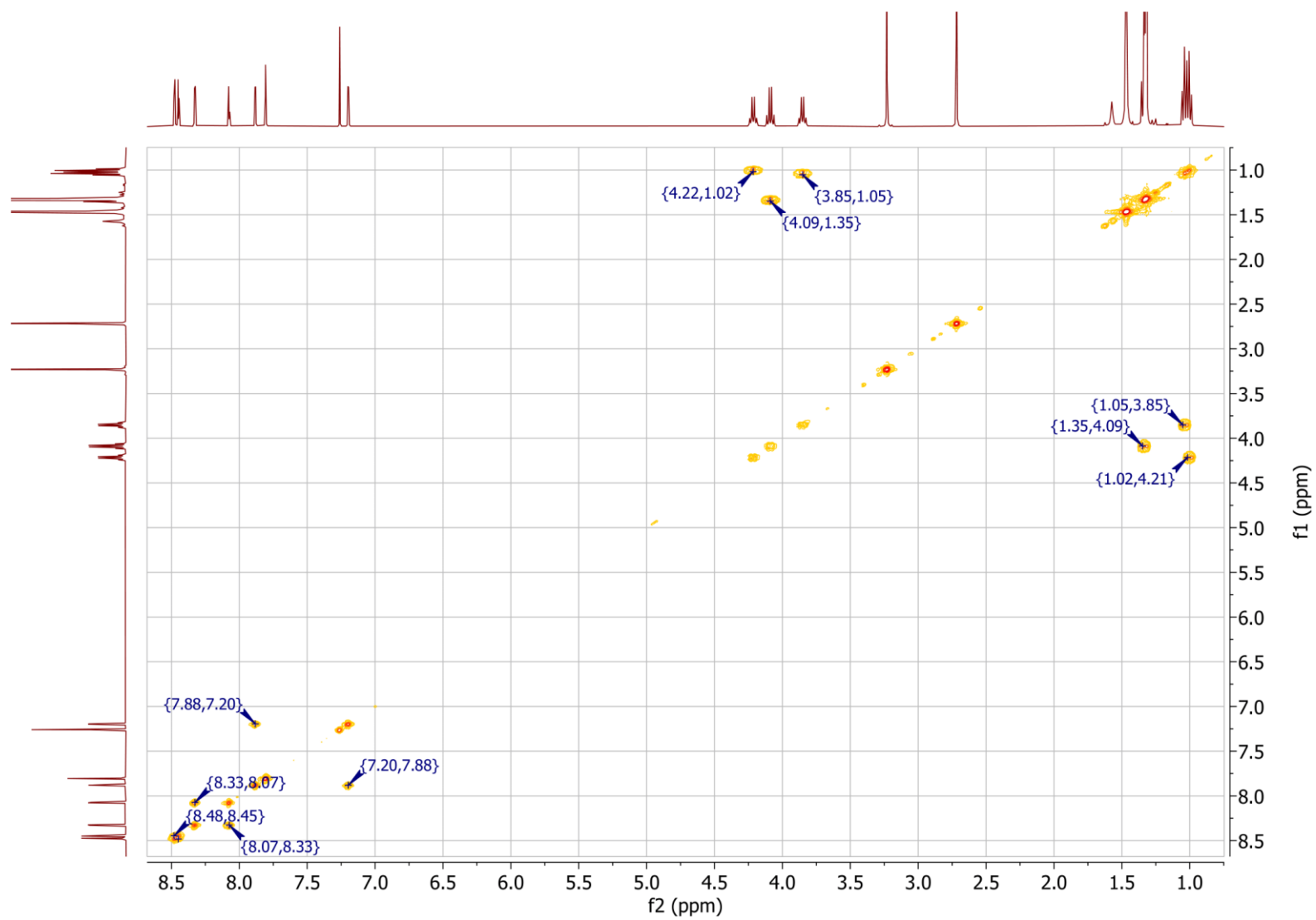


Figure S42: COSY spectrum of compound **12a**

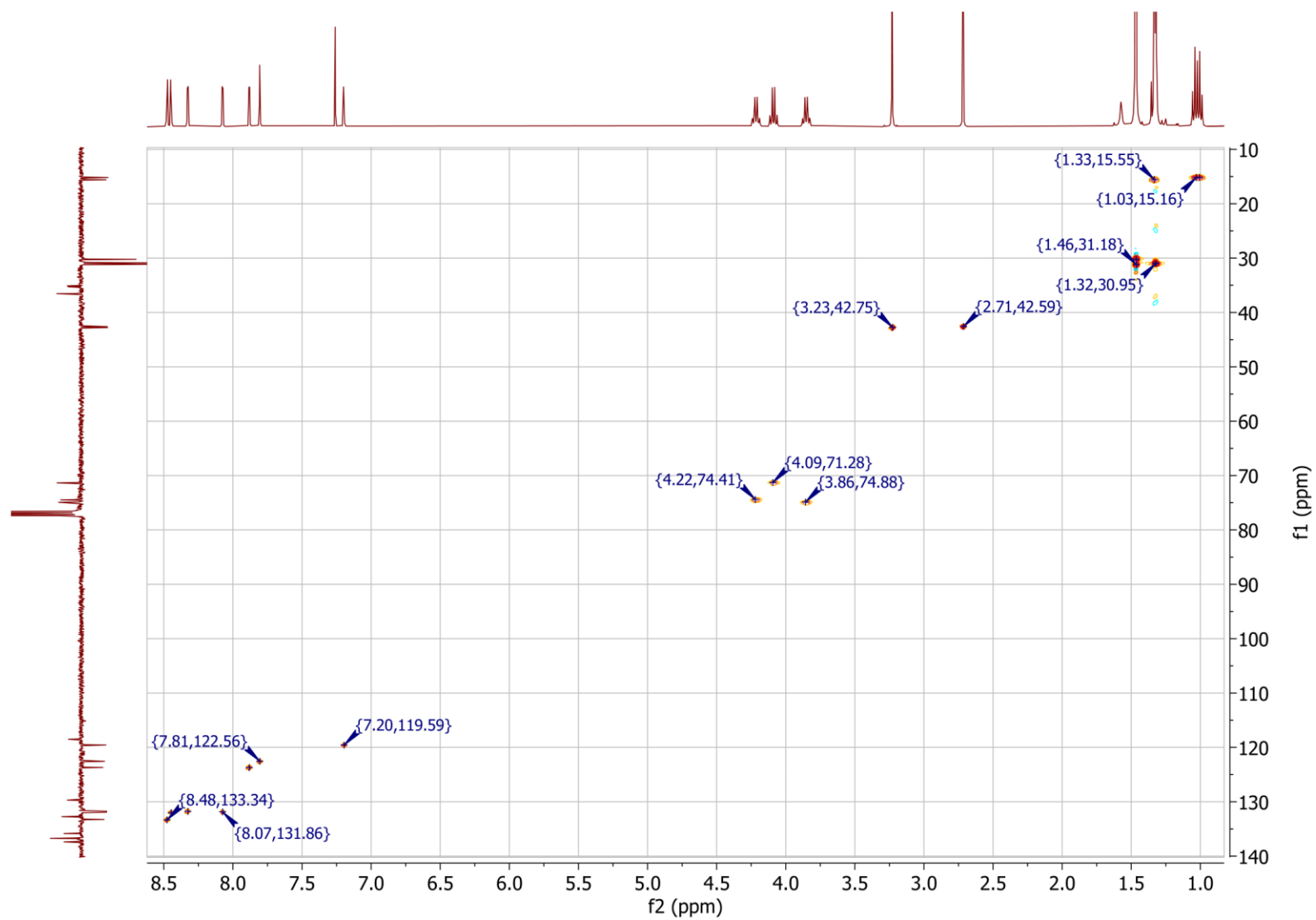


Figure S43: HMQC spectrum of compound **12a**

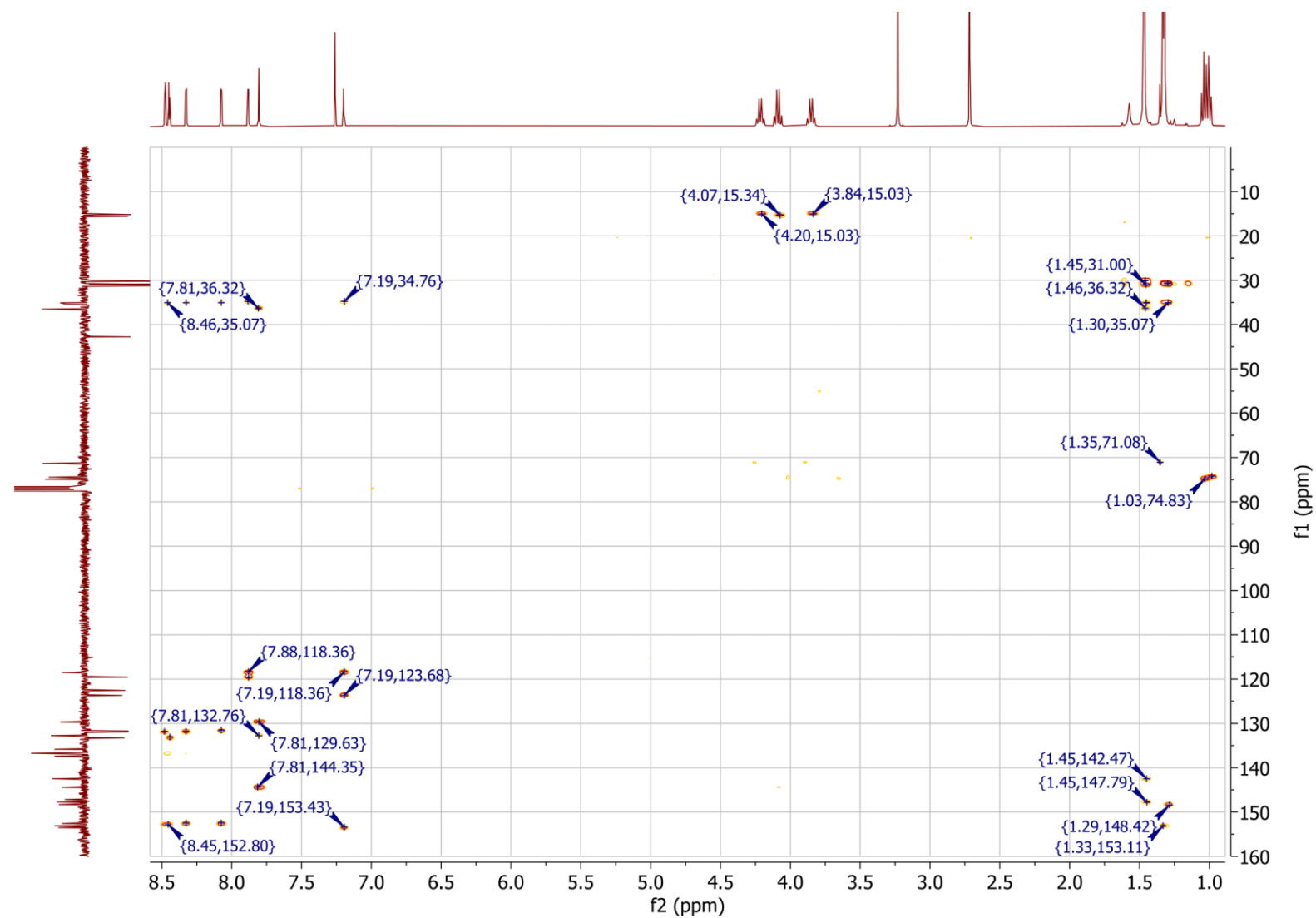


Figure S44: HMBC spectrum of compound 12a

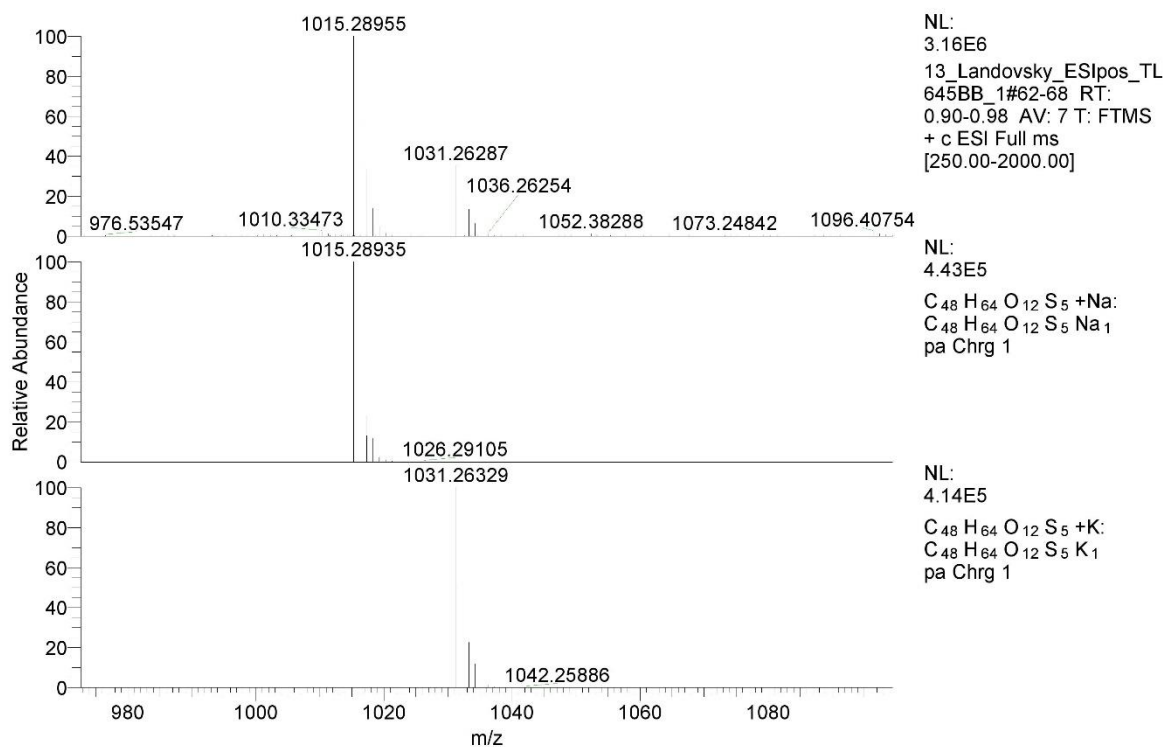


Figure S45: HRMS spectrum of compound 12a

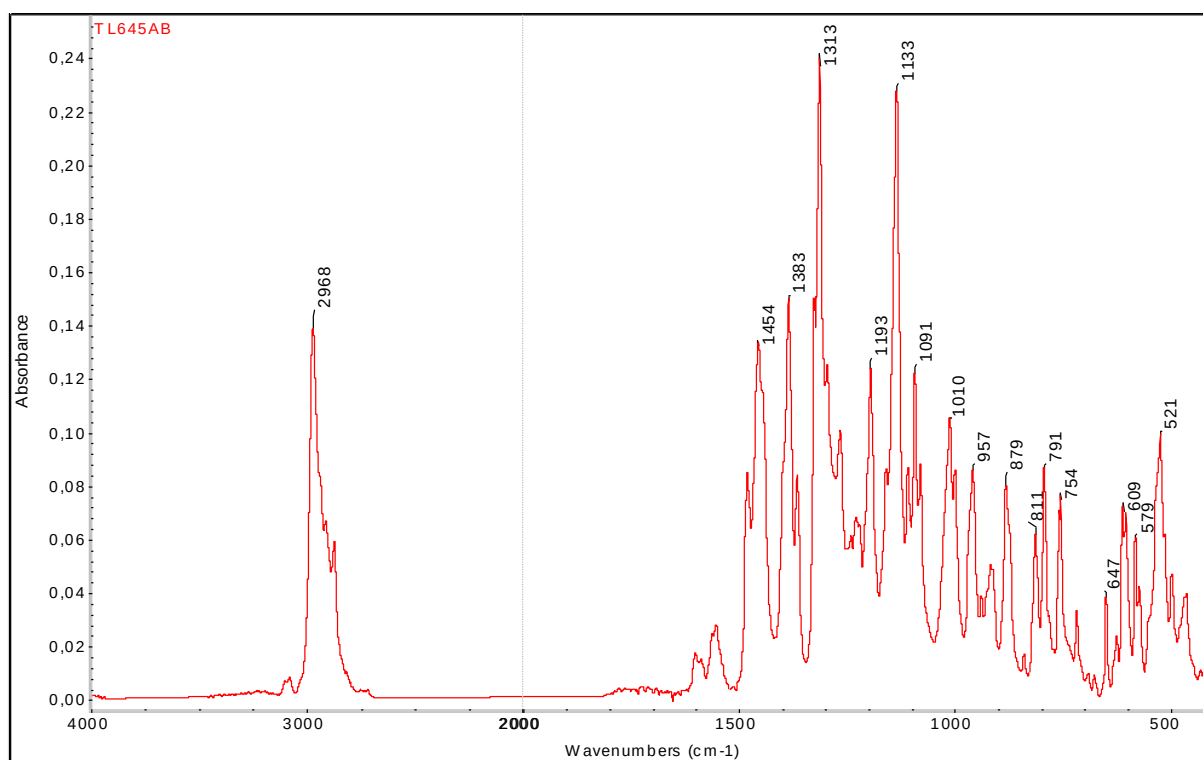


Figure S46: IR spectrum of compound 12a

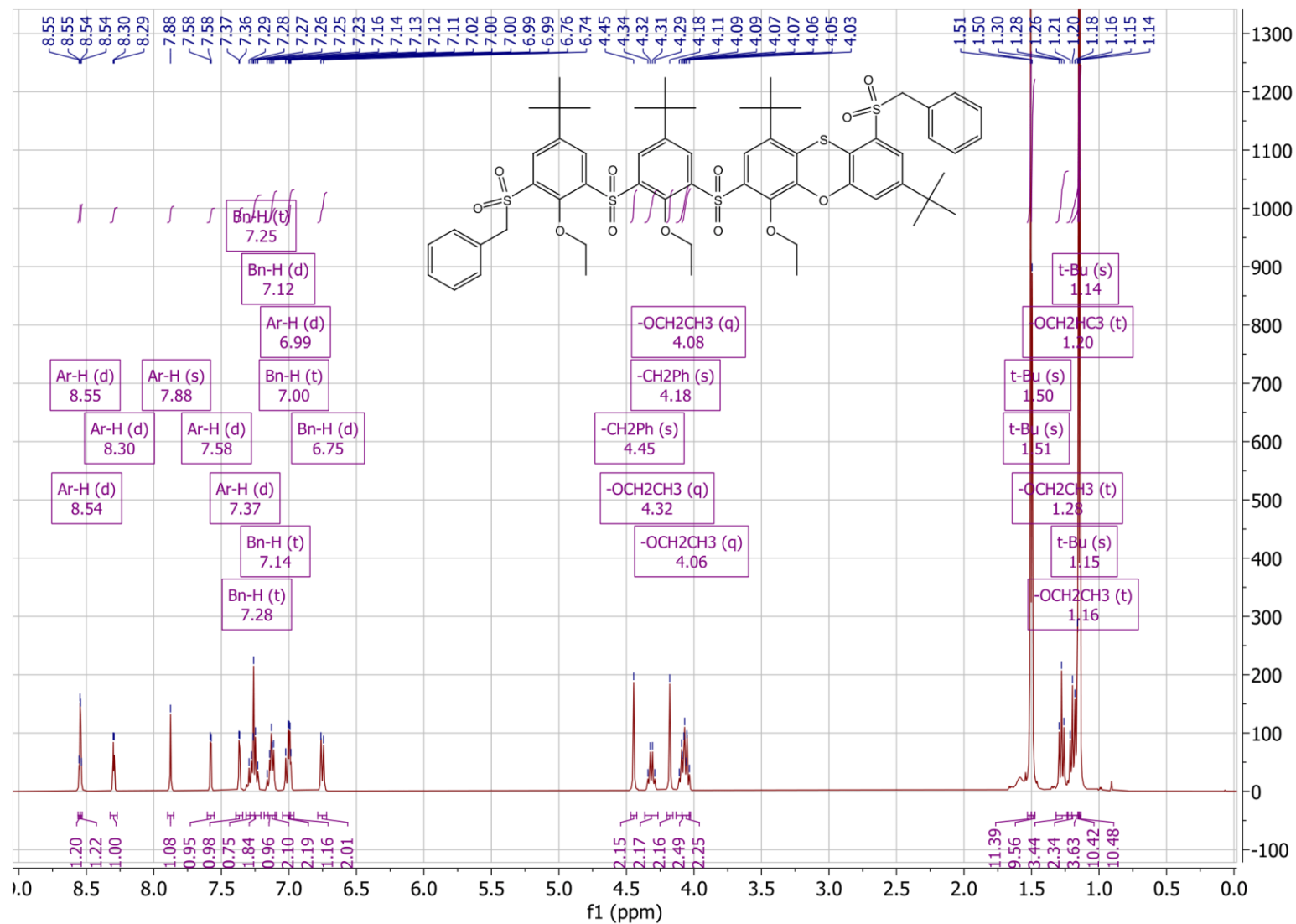


Figure S47: ¹H NMR (400 MHz, CDCl₃, 298 K) spectrum of compound **12b**

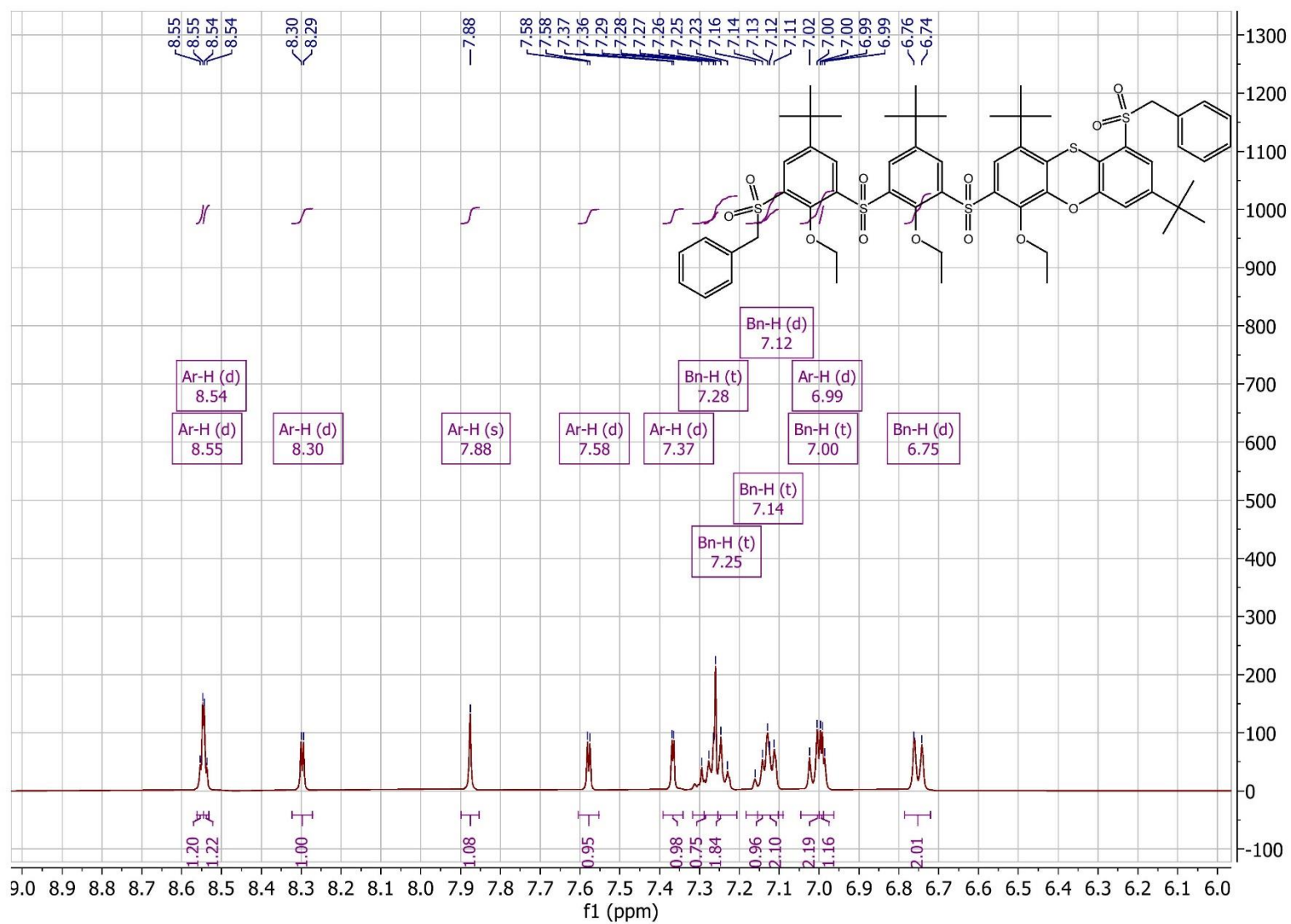


Figure S48: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **12b** (aromatic region)

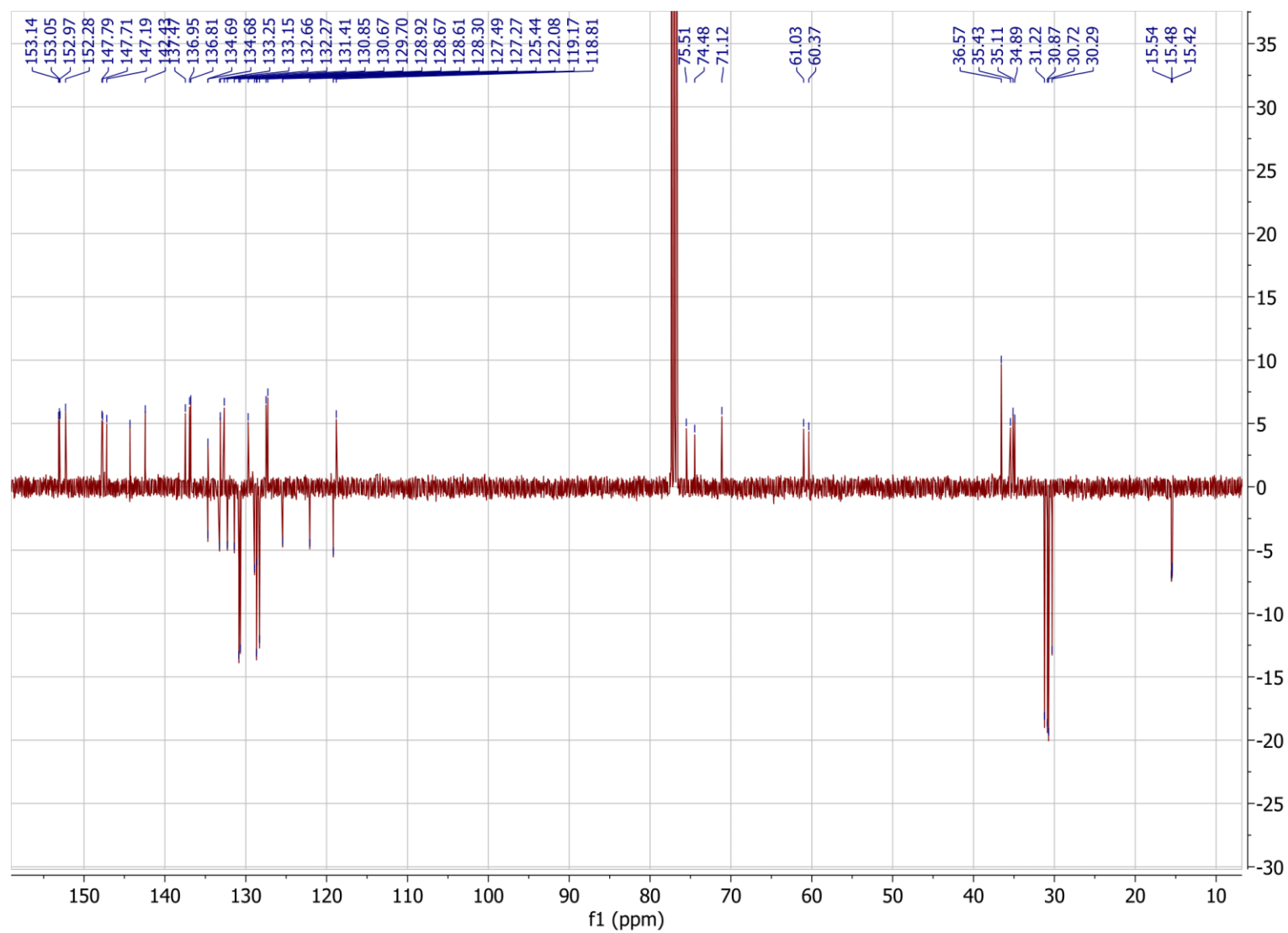


Figure S49: ¹³C NMR (APT, 101 MHz, CDCl₃, 298 K) spectrum of compound **12b**

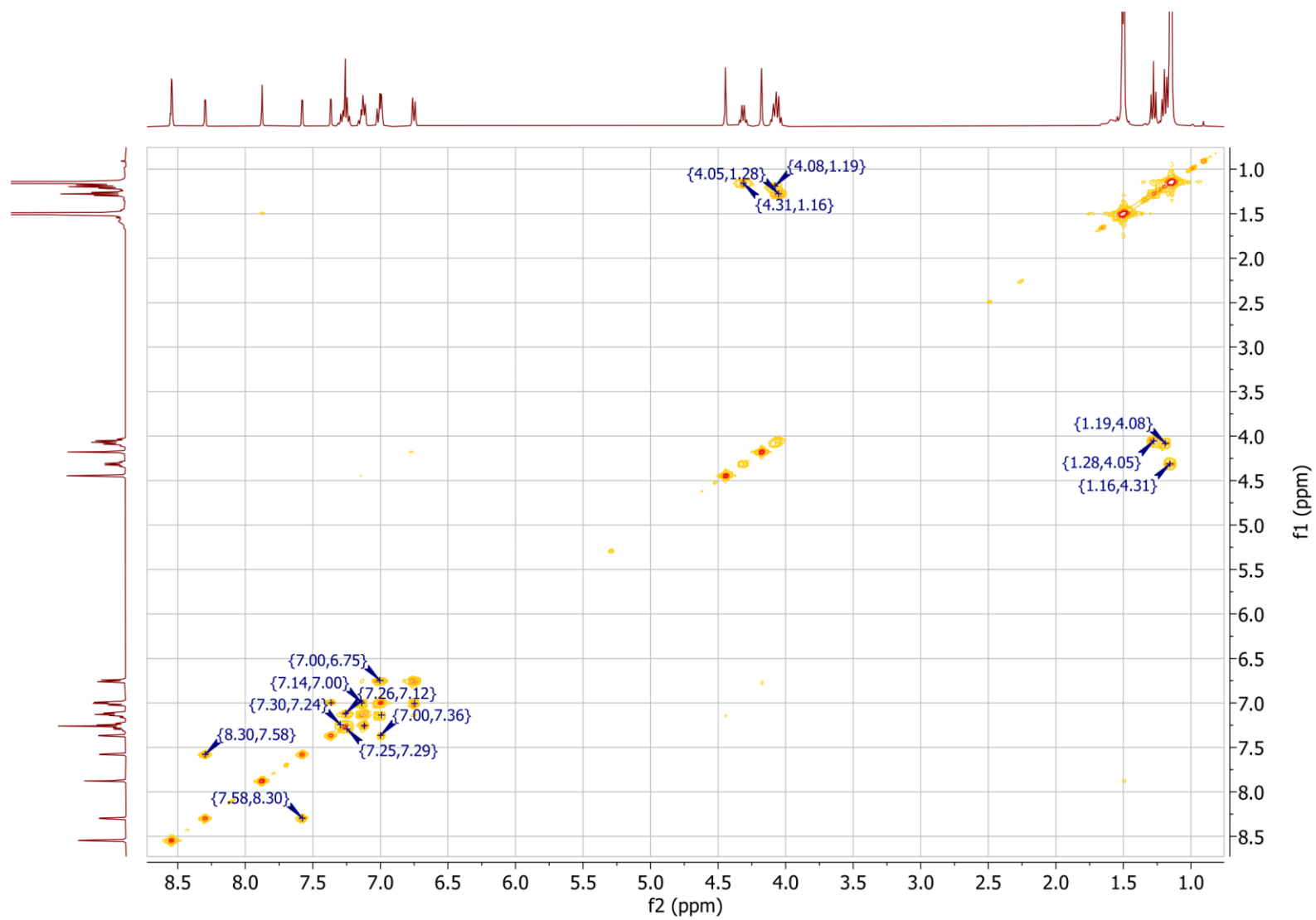


Figure S50: COSY spectrum of compound **12b**

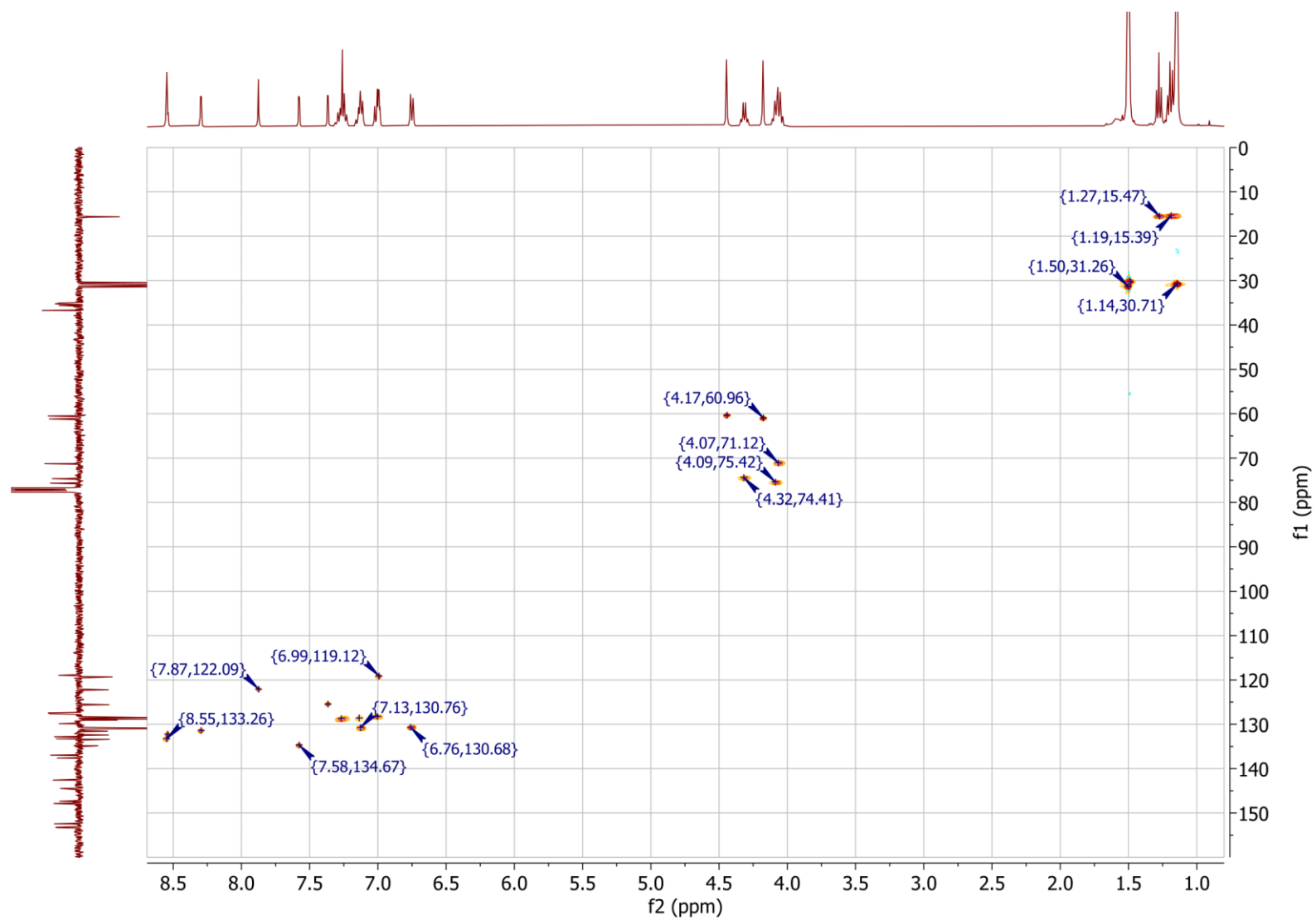


Figure S51: HMQC spectrum of compound **12b**

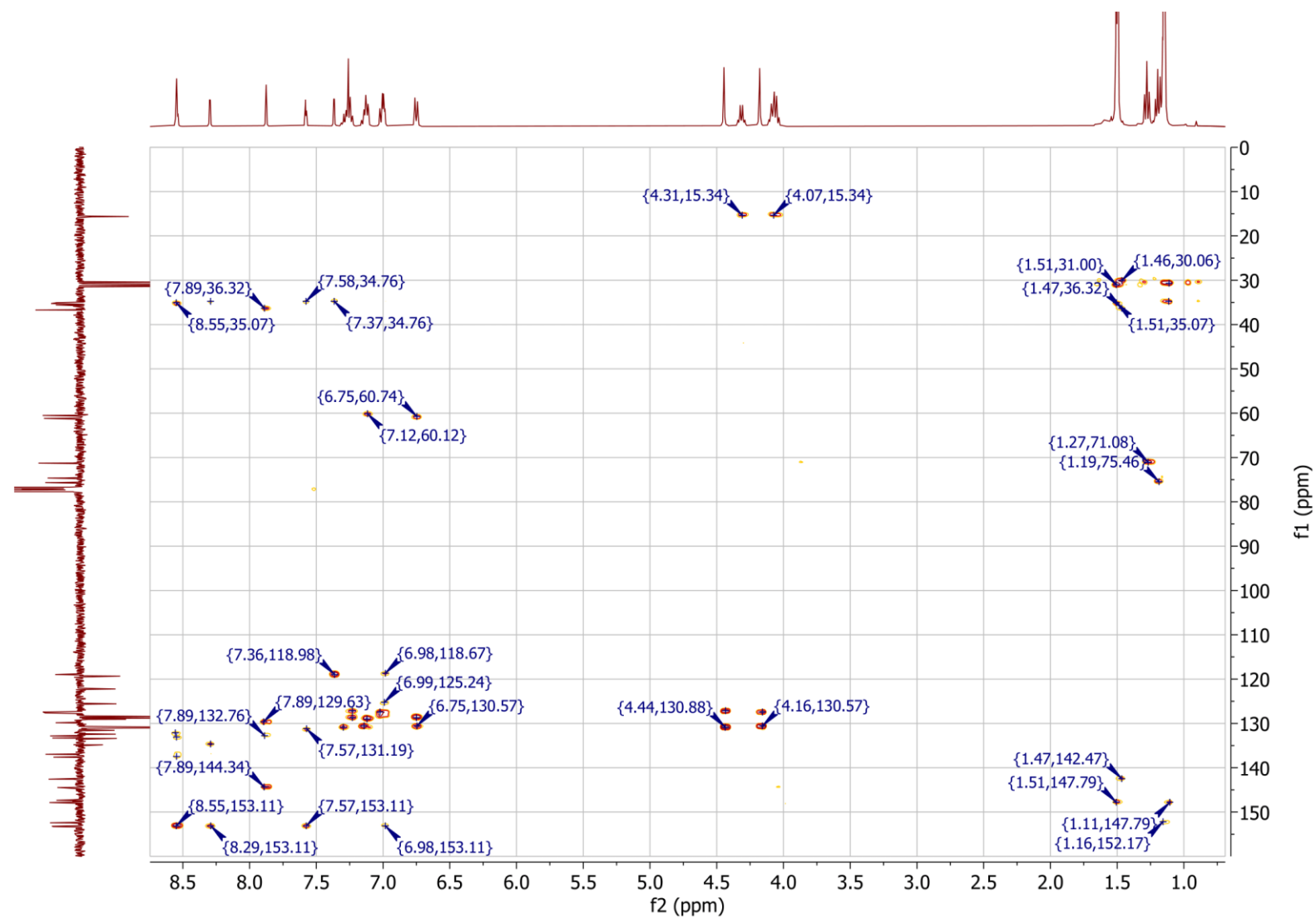


Figure S52: HMBC spectrum of compound 12b

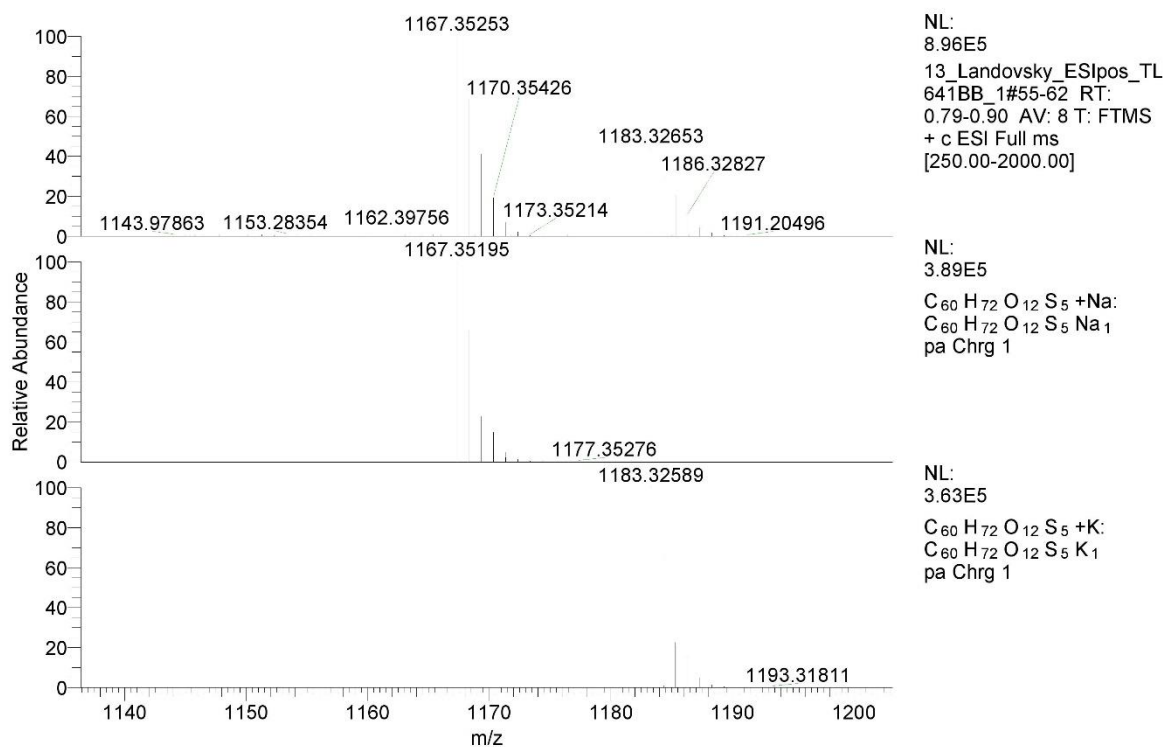


Figure S53: HRMS spectrum of compound **12b**

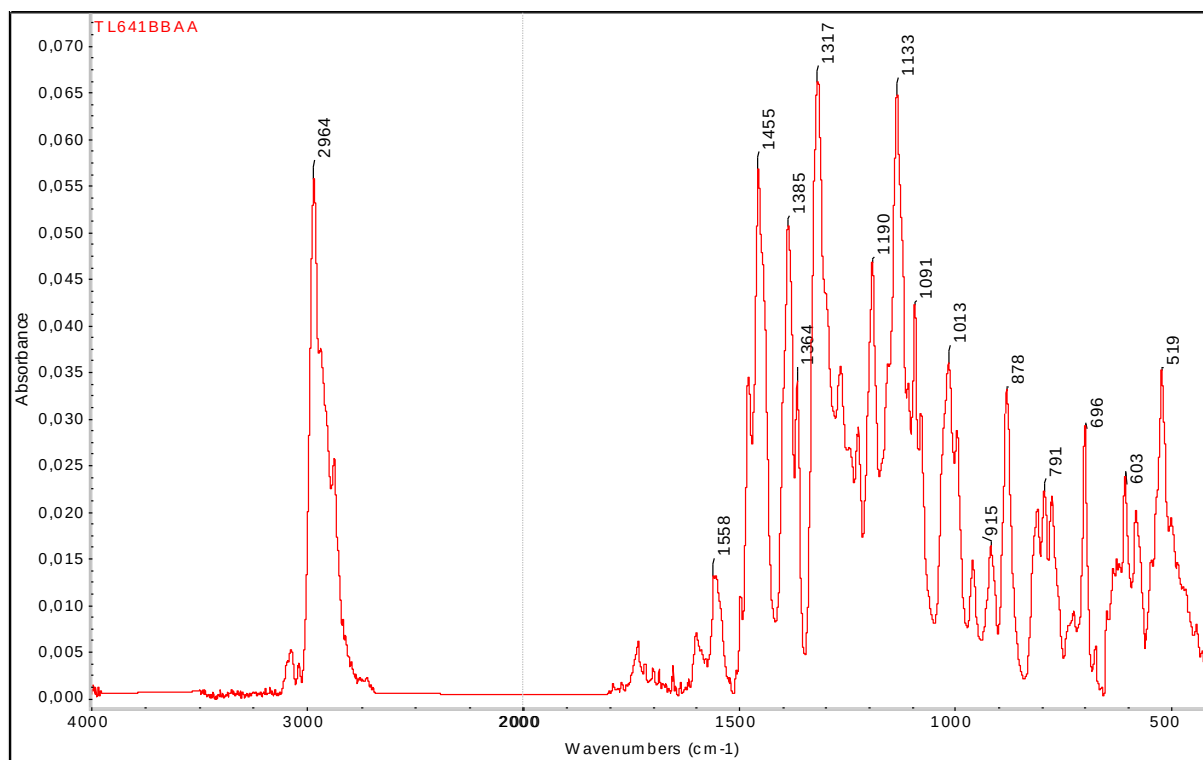


Figure S54: IR spectrum of compound **12b**

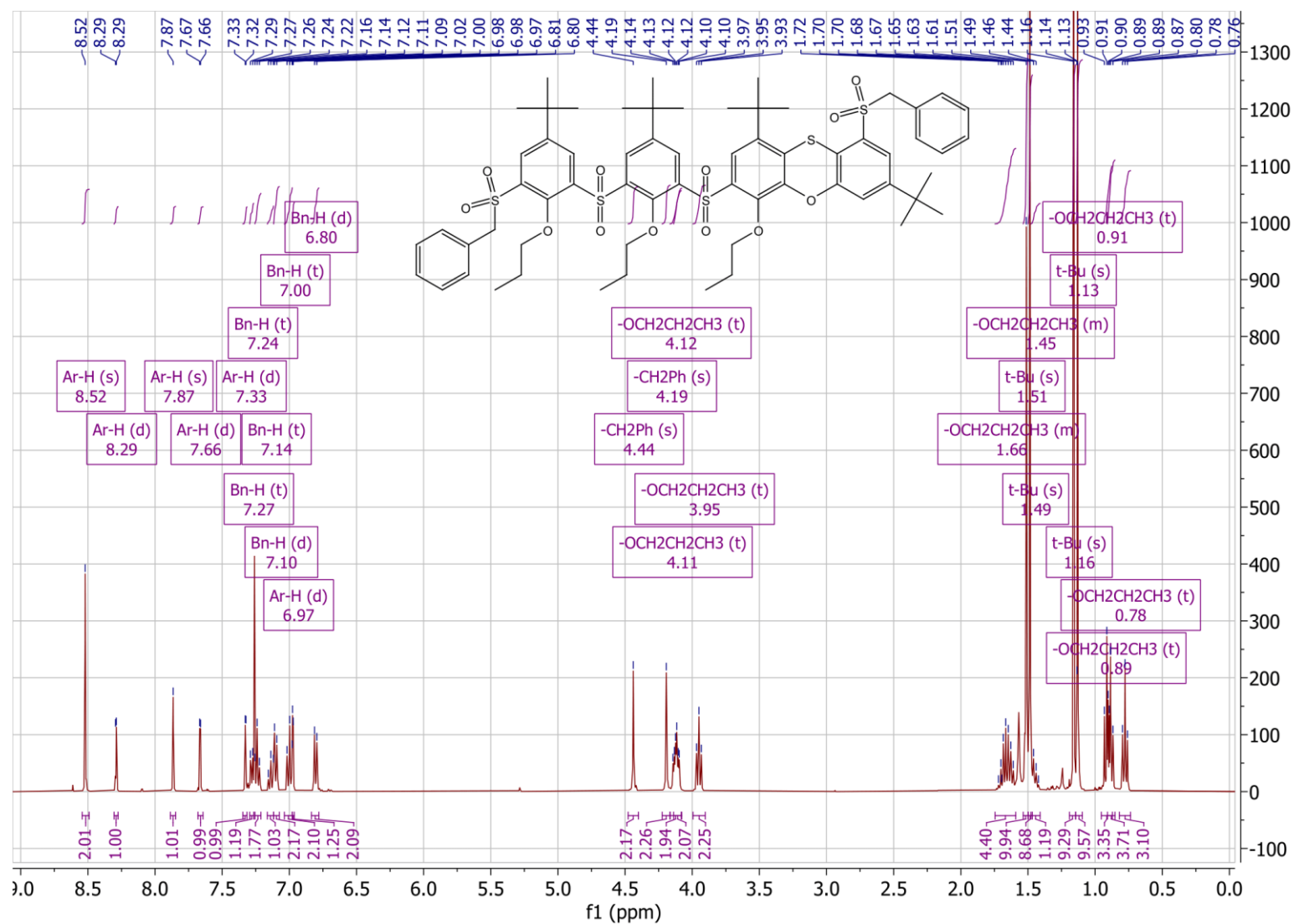


Figure S55: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **12c**

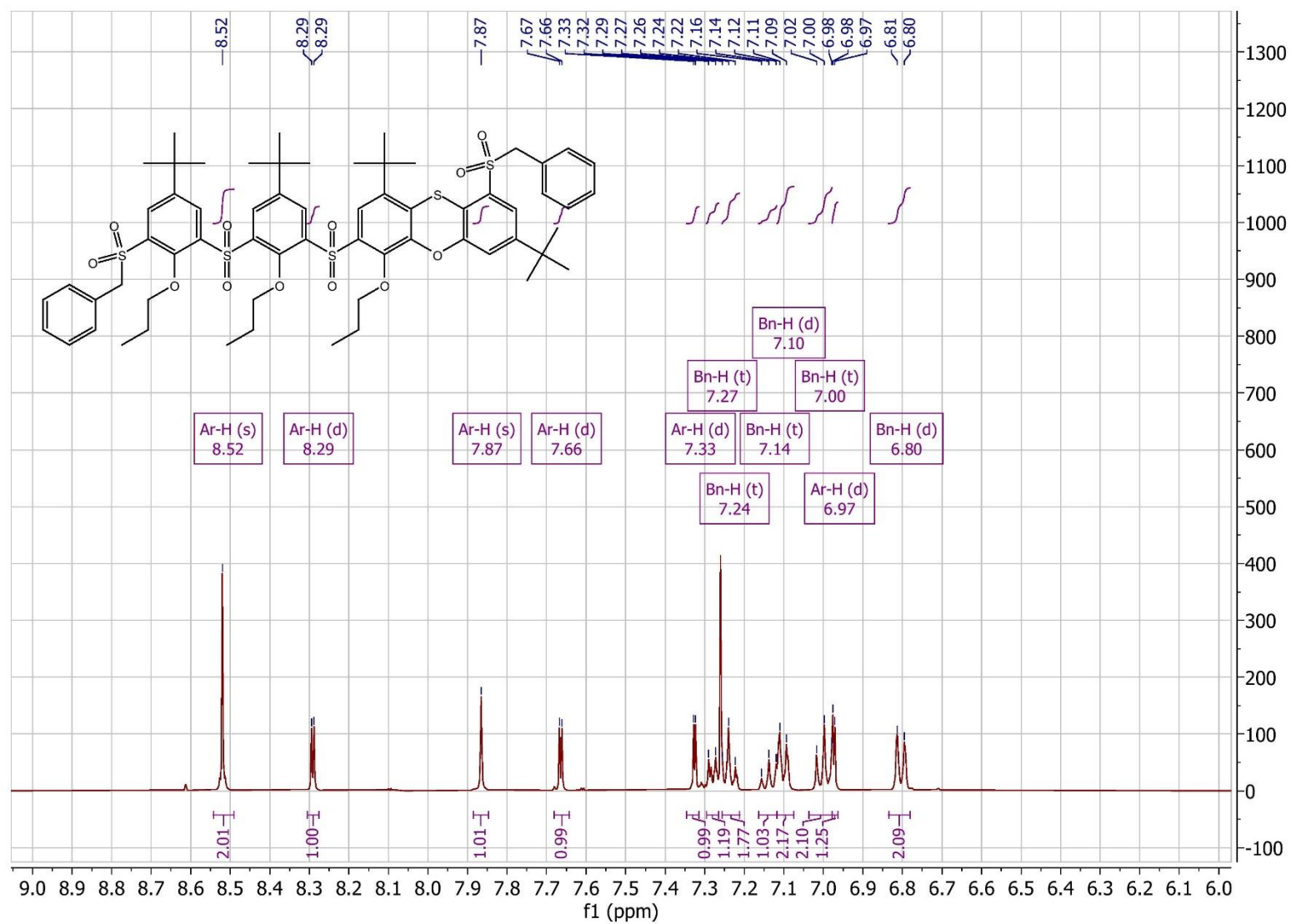


Figure S56: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **12c** (aromatic region)

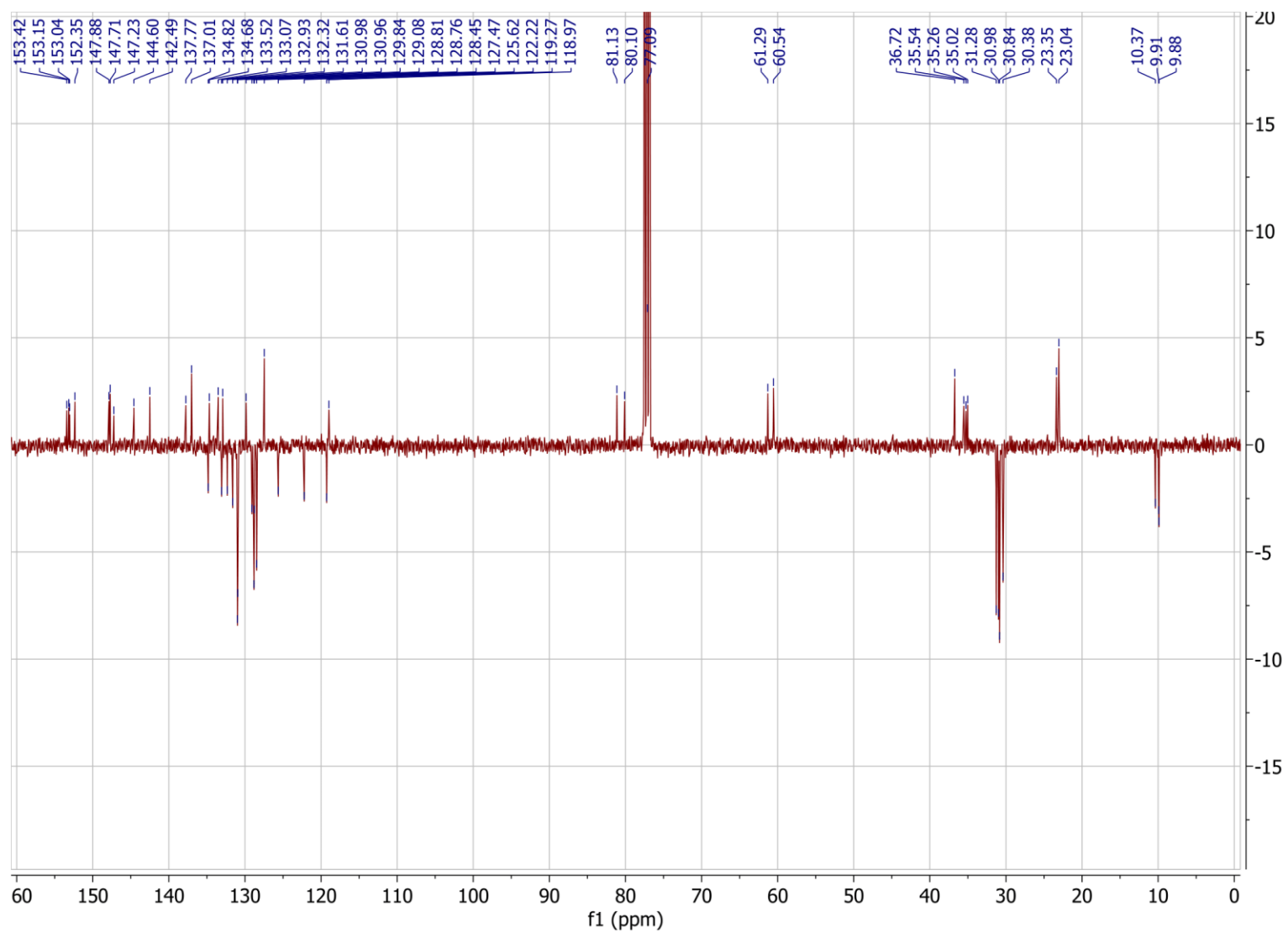


Figure S57: ^{13}C NMR (APT, 101 MHz, CDCl_3 , 298 K) spectrum of compound **12c**

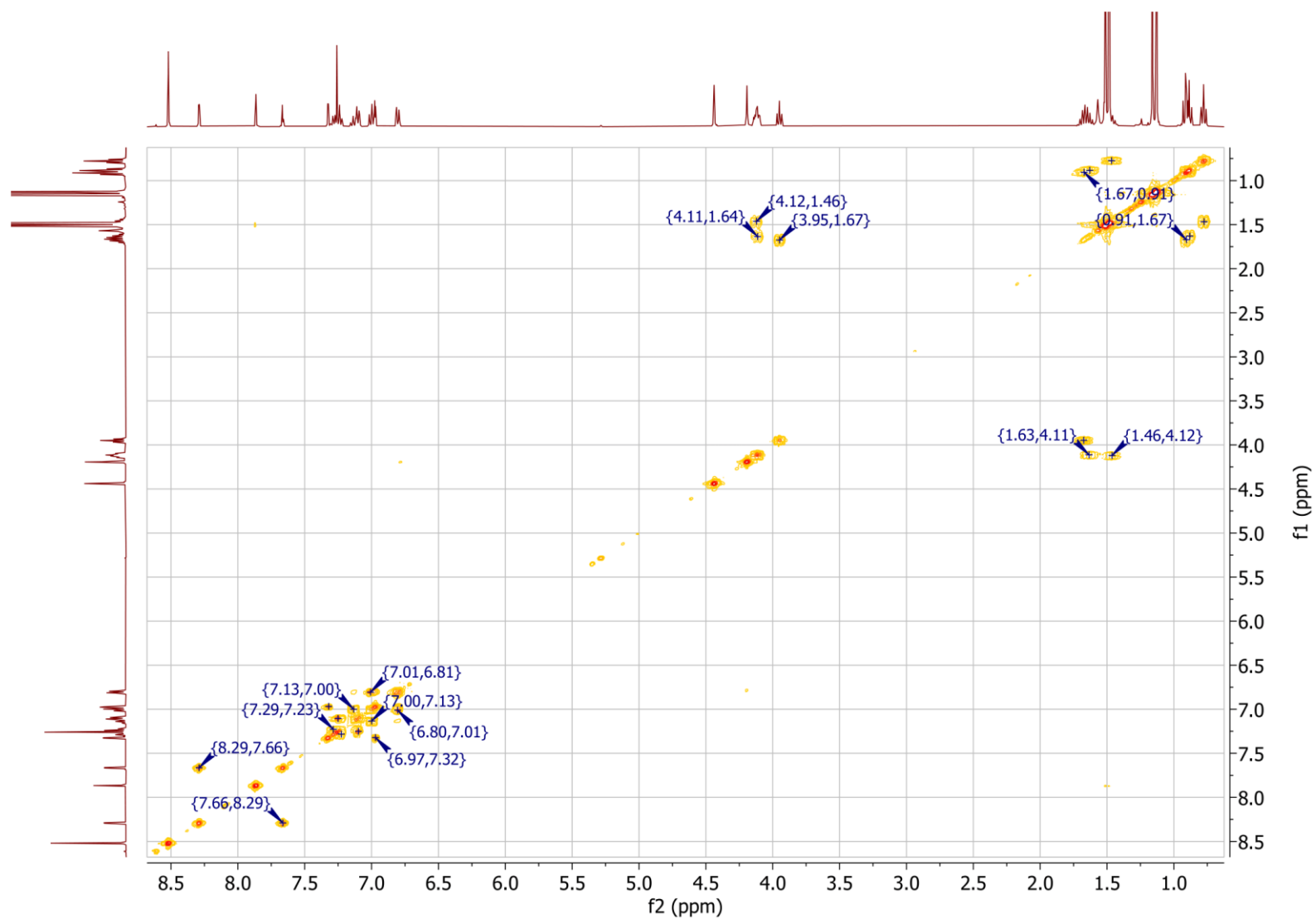


Figure S58: COSY spectrum of compound **12c**

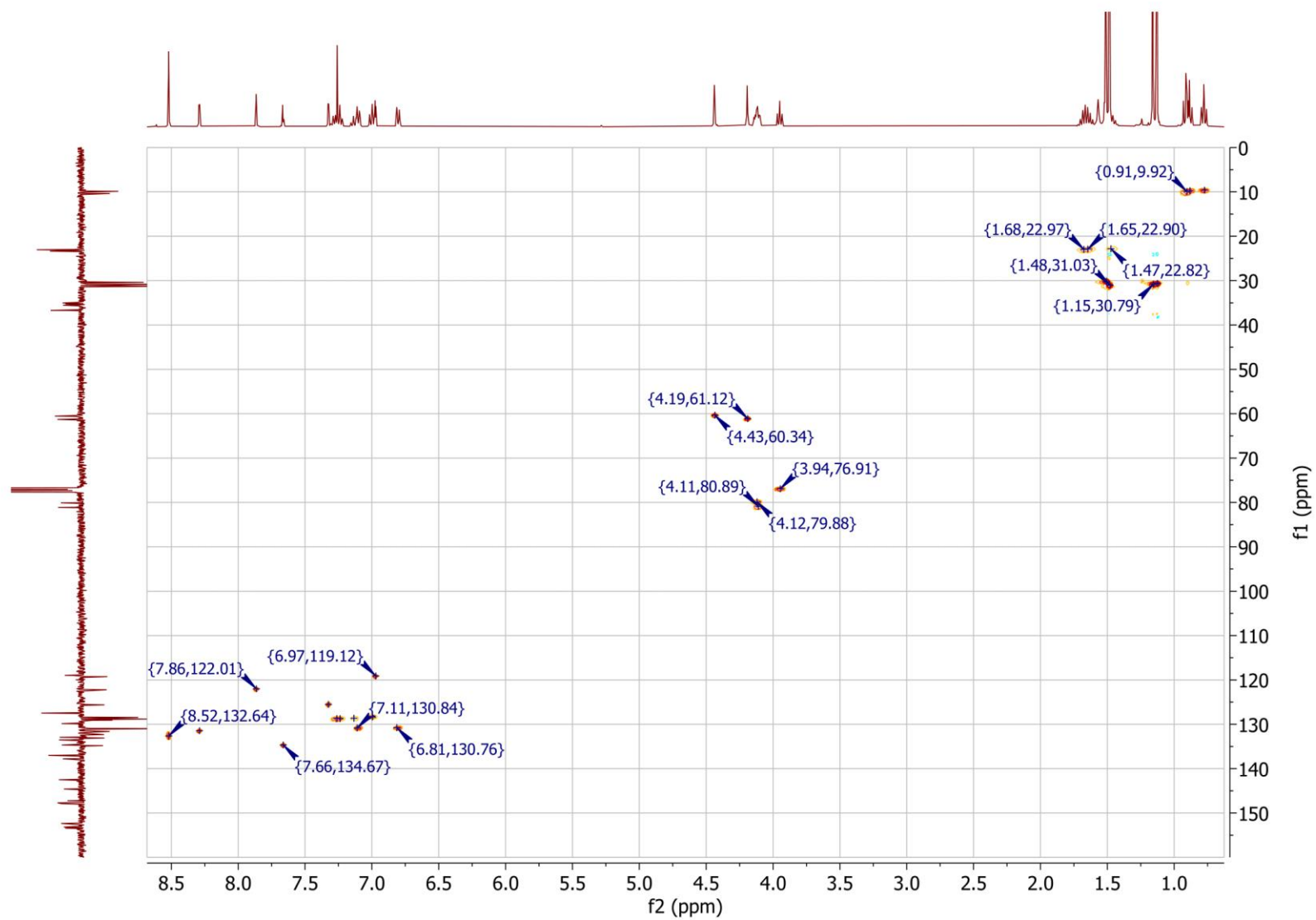


Figure S59: HMQC spectrum of compound **12c**

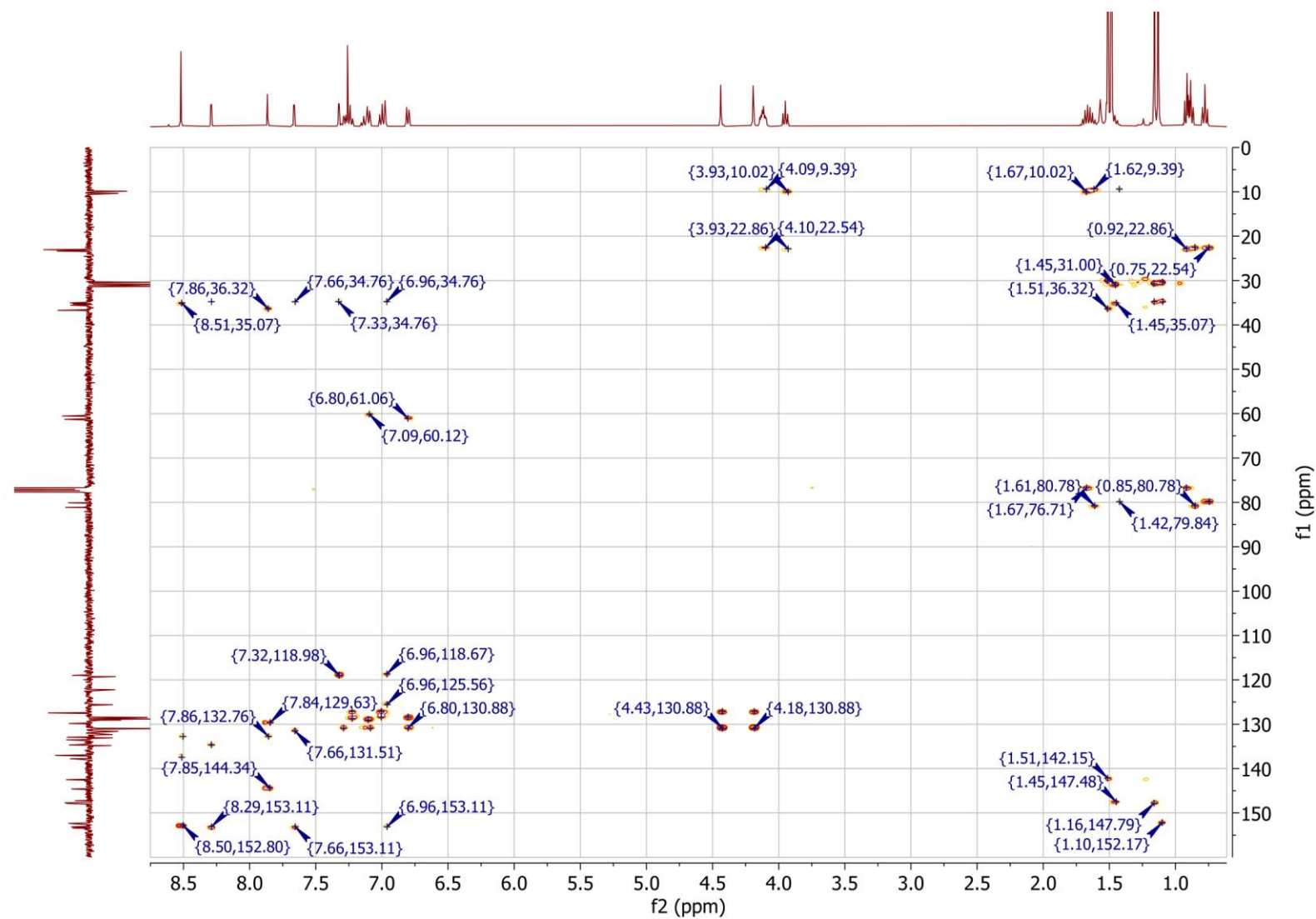


Figure S60: HMBC spectrum of compound 12c

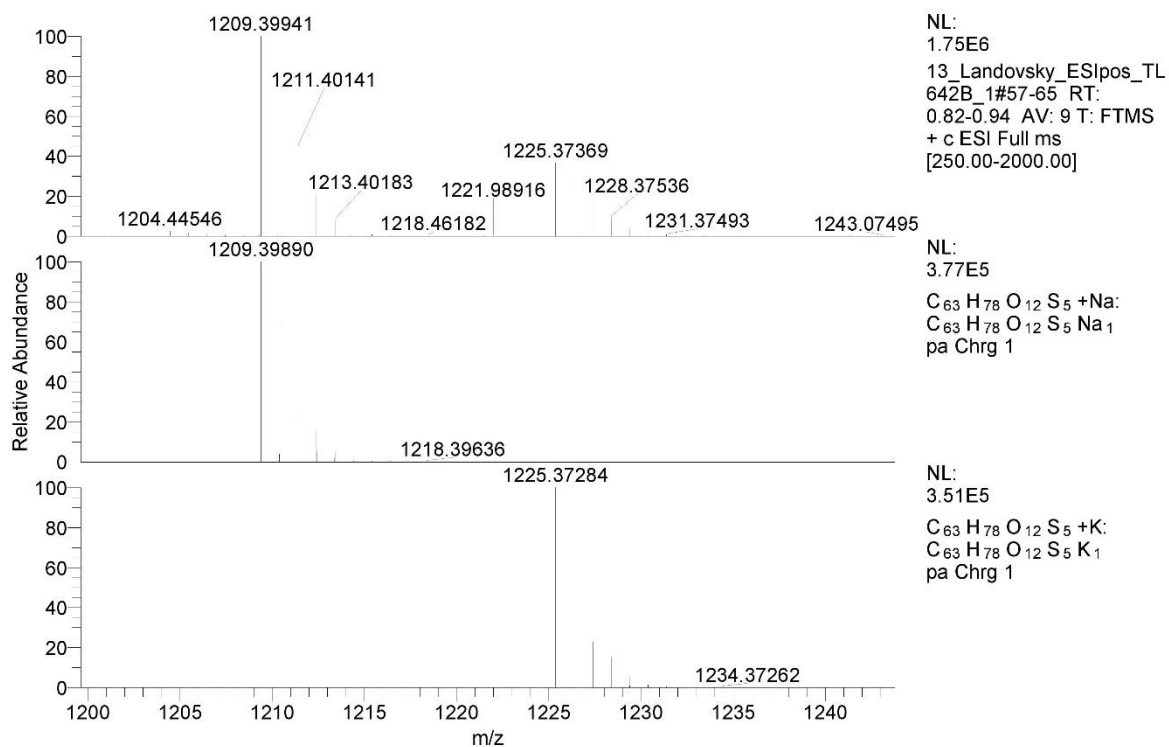


Figure S61: HRMS spectrum of compound 12c

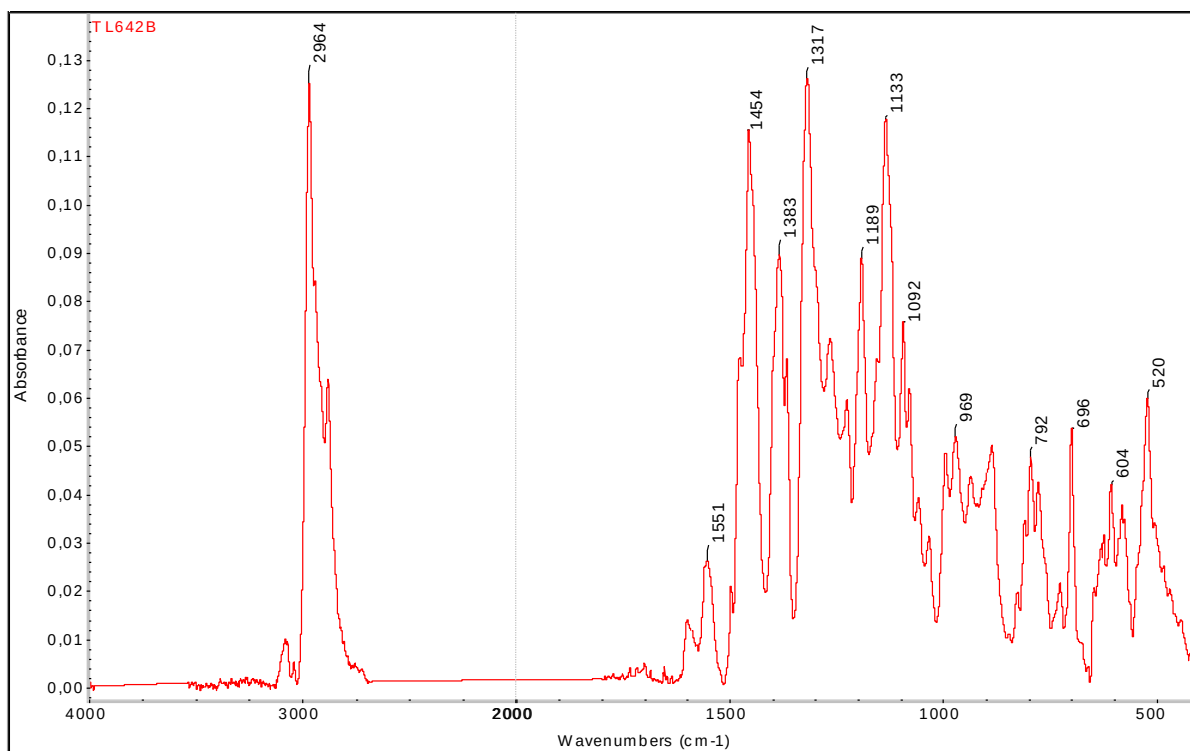


Figure S62: IR spectrum of compound 12c

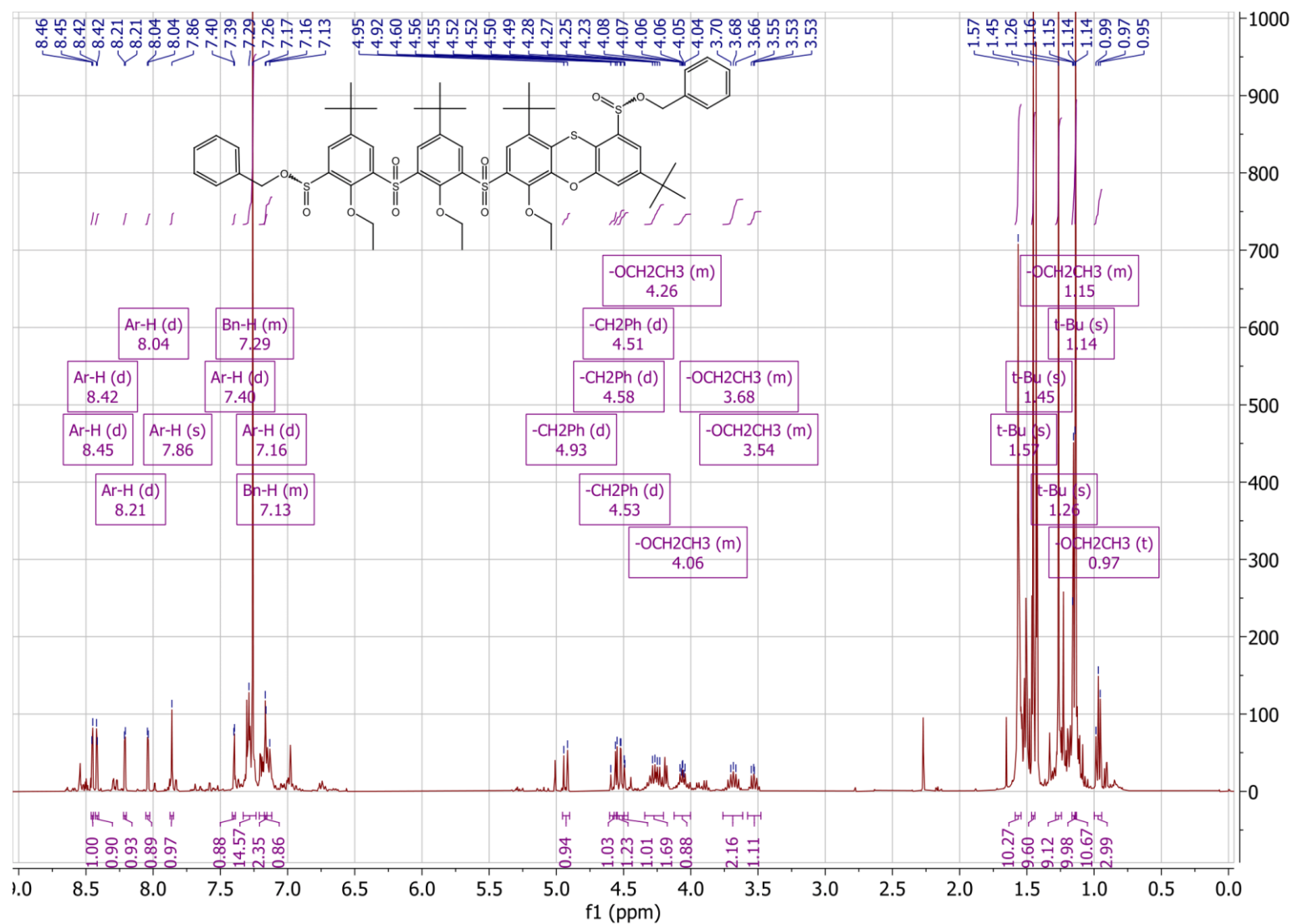


Figure S63: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **13b**

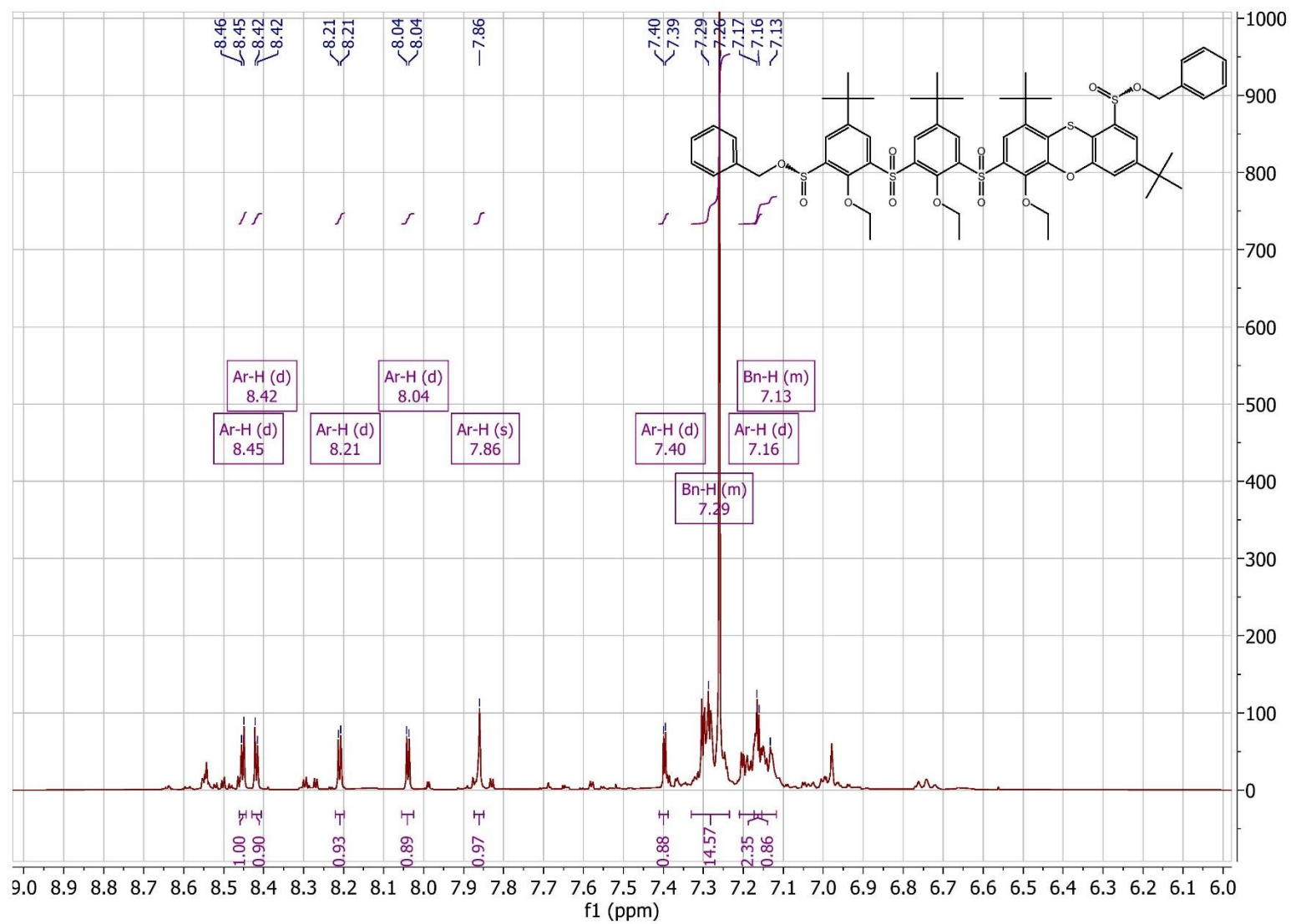


Figure S64: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **13b** (aromatic region)

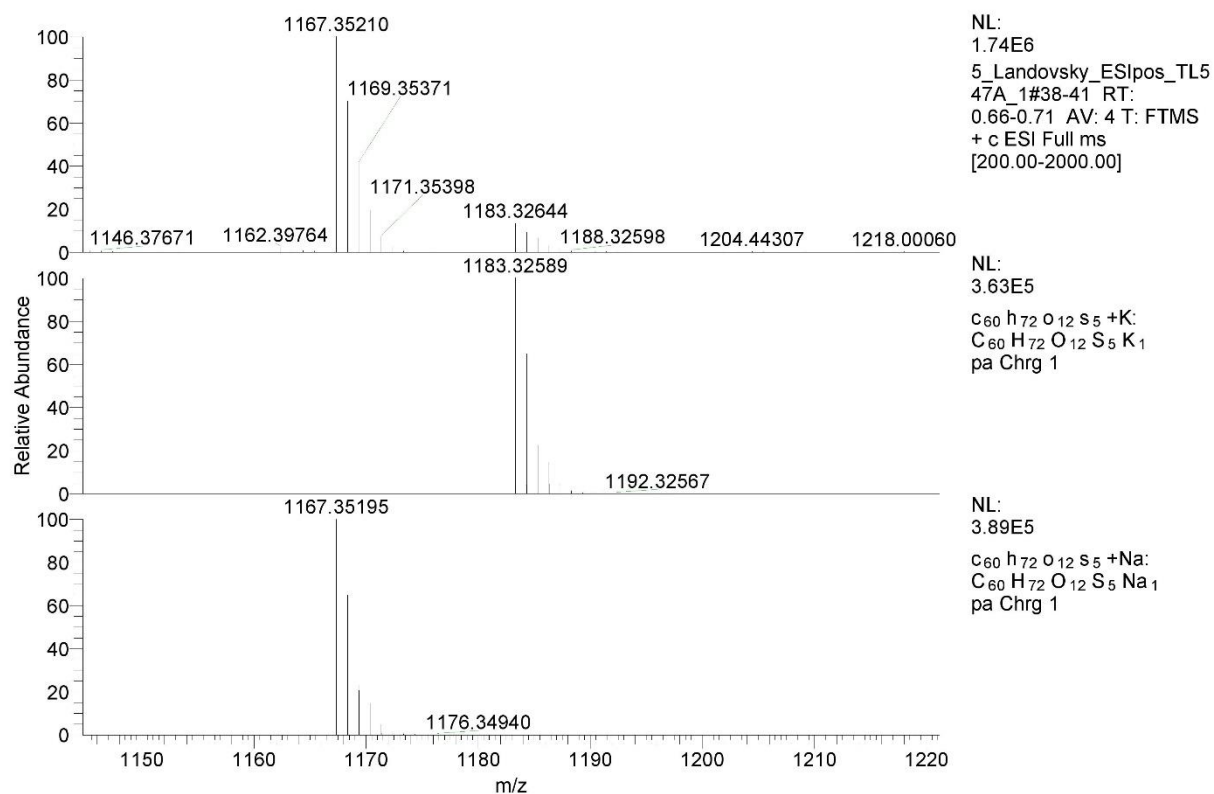


Figure S65: HRMS spectrum of compound **13b**

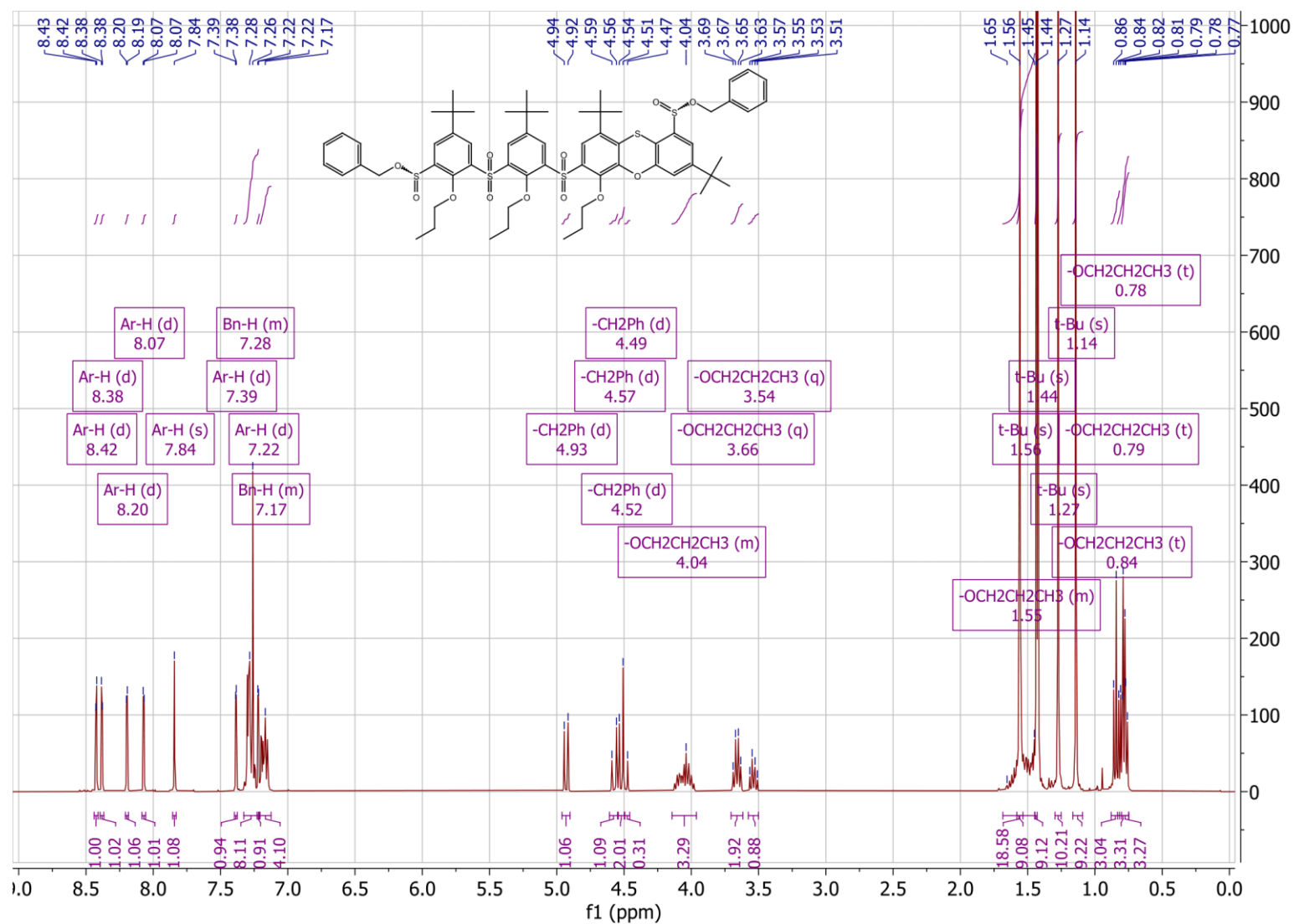


Figure S66: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **13c**

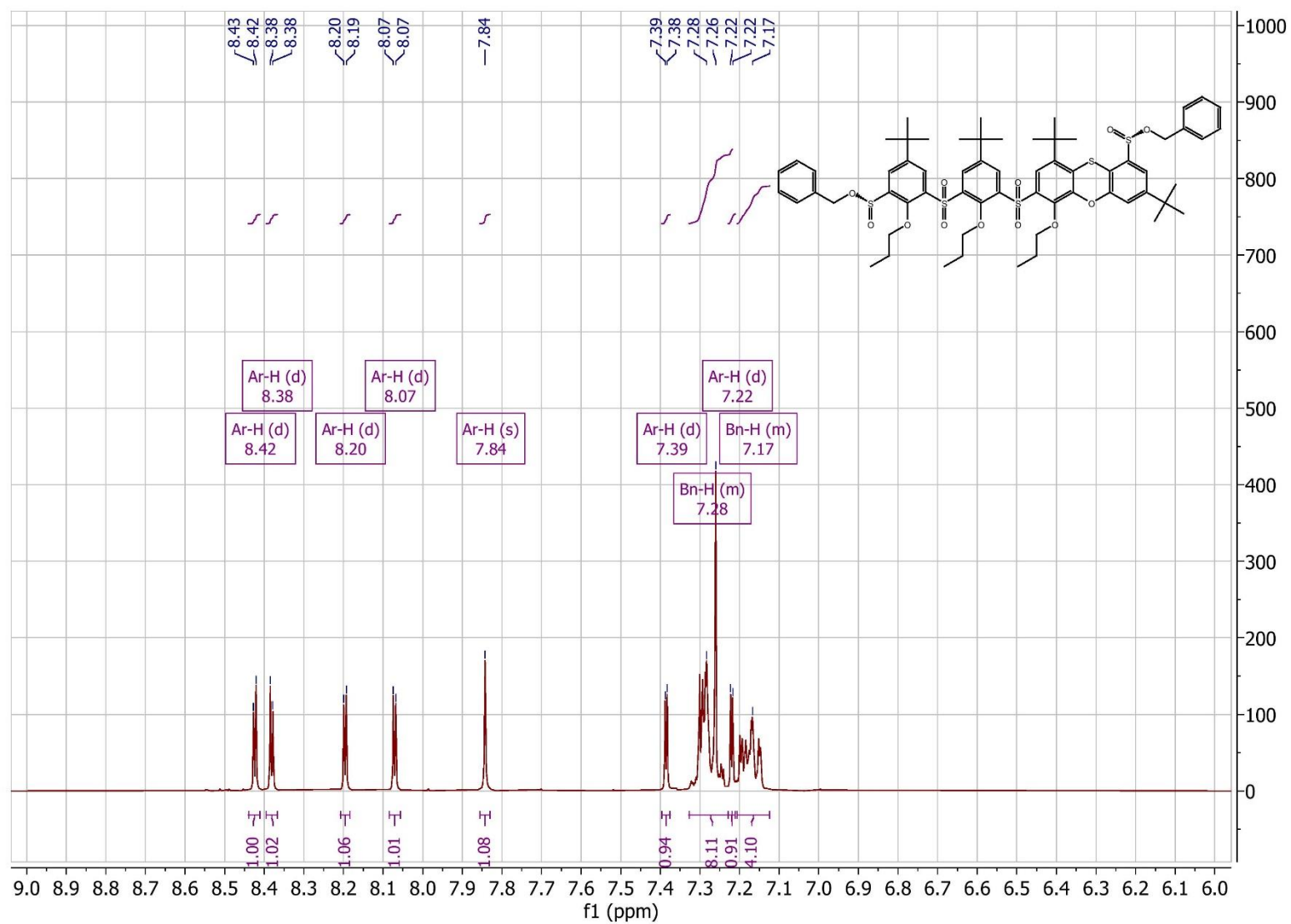


Figure S67: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **13c** (aromatic region)

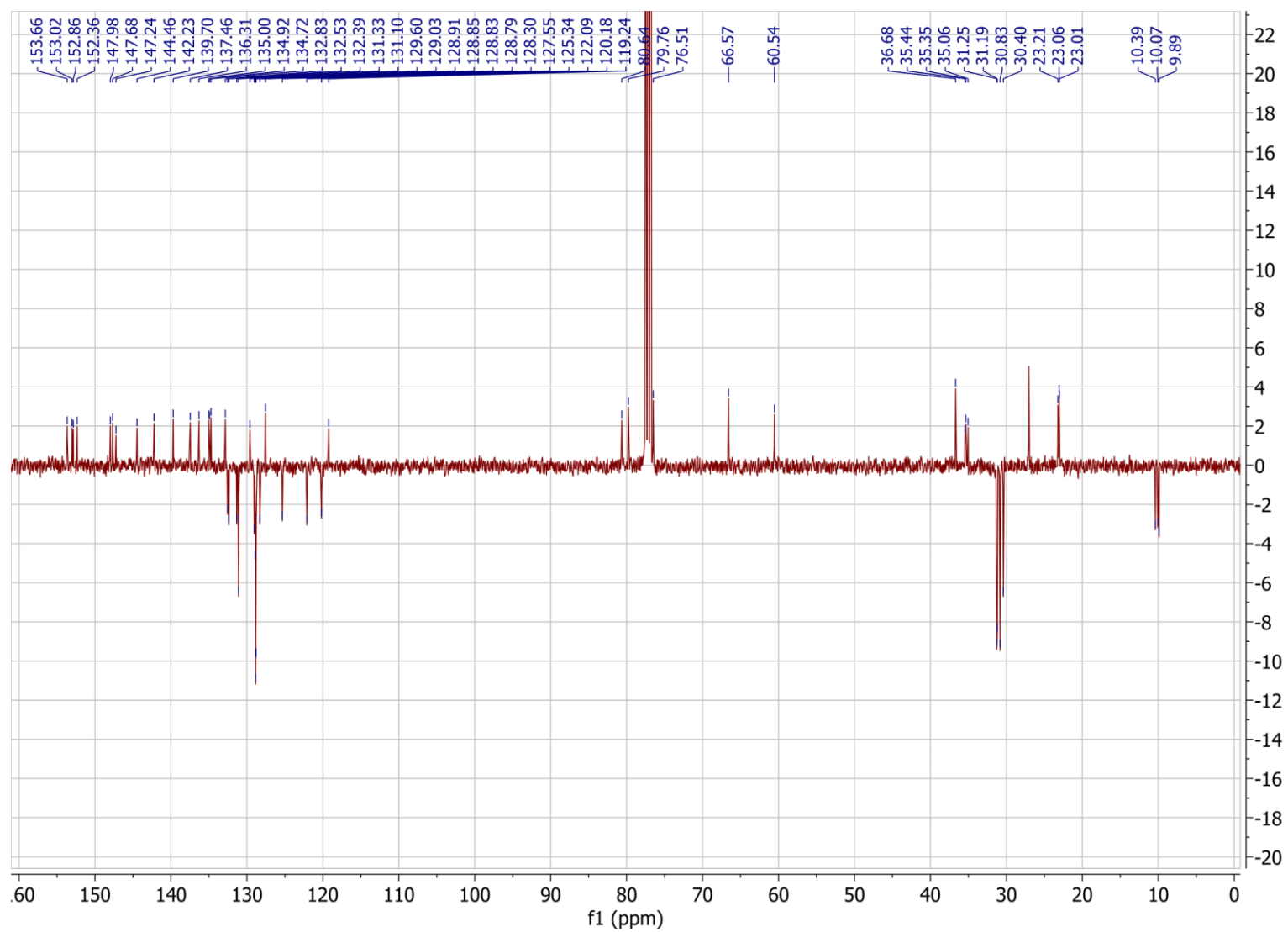


Figure S68: ^{13}C NMR (APT, 101 MHz, CDCl_3 , 298 K) spectrum of compound **13c**

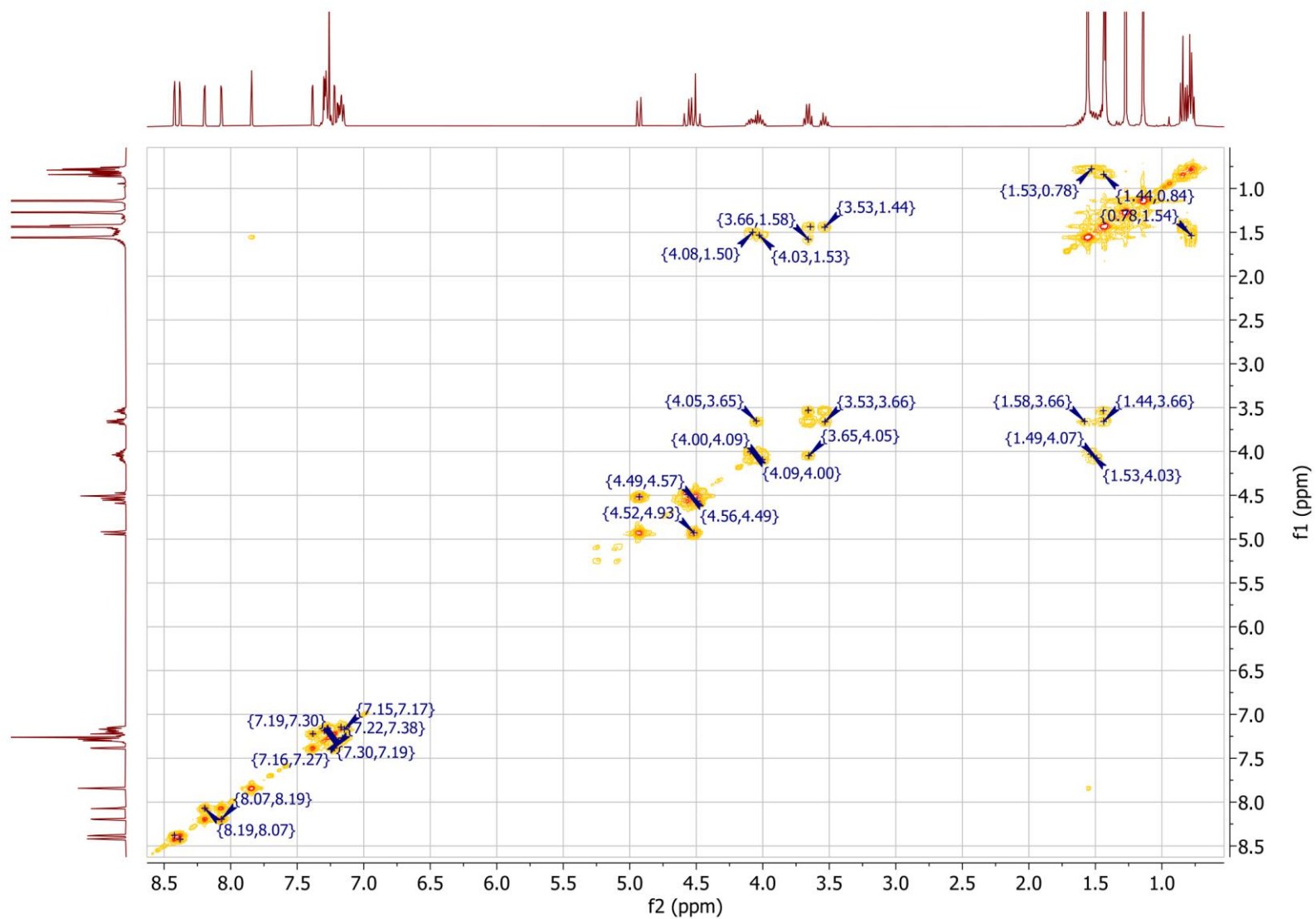


Figure S69: COSY spectrum of compound **13c**

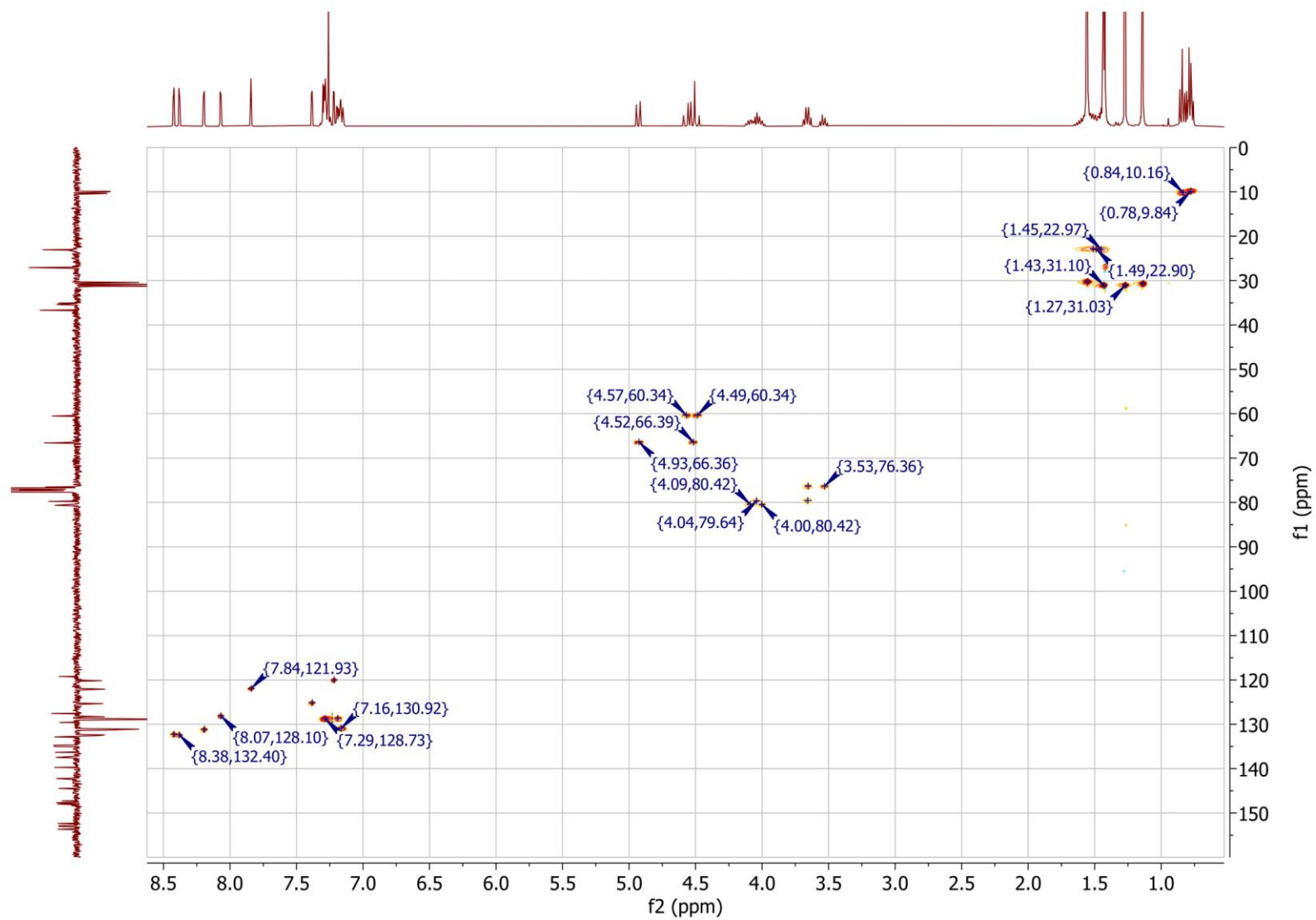


Figure S70: HMQC spectrum of compound **13c**

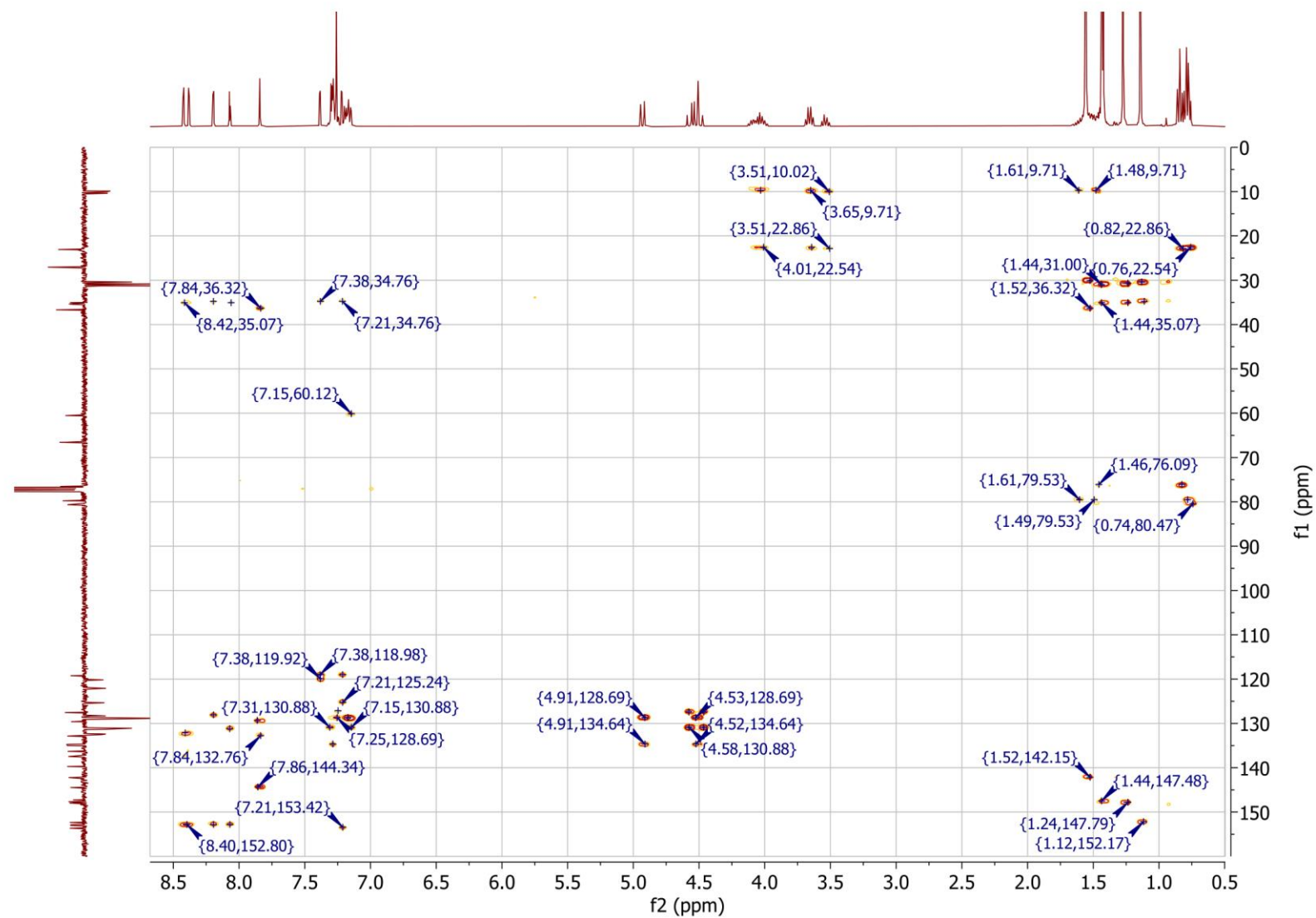


Figure S71: HMBC spectrum of compound **13c**

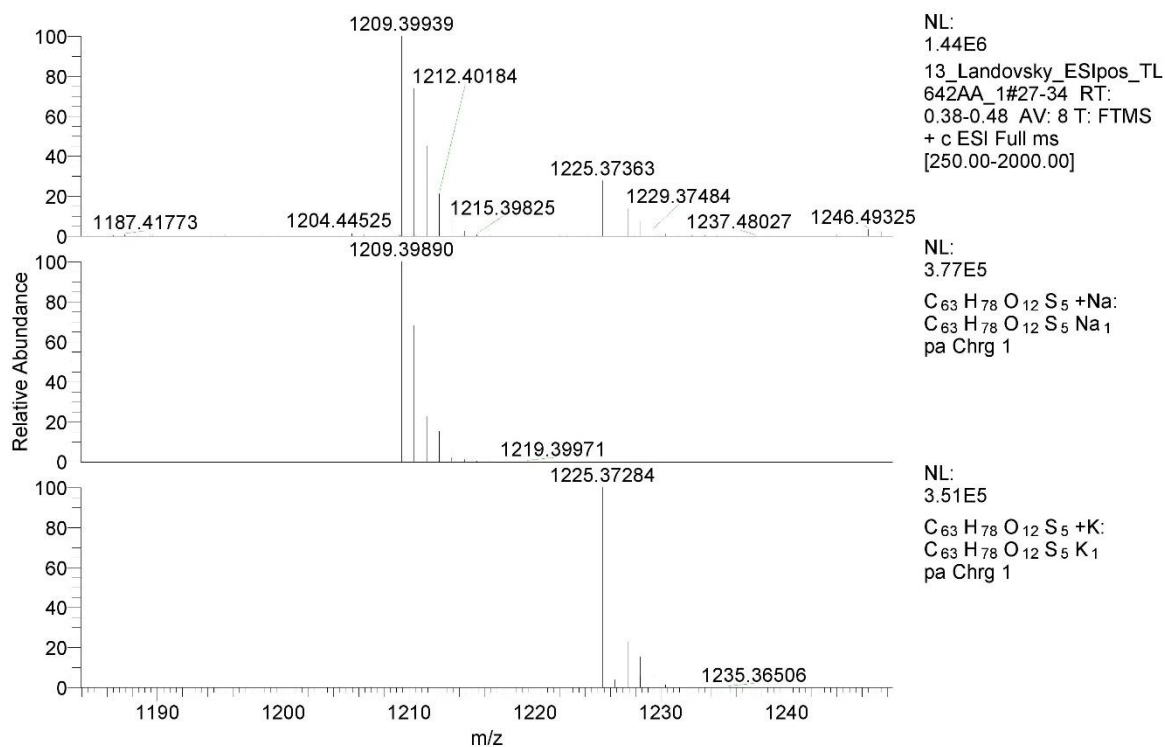


Figure S72: HRMS spectrum of compound **13c**

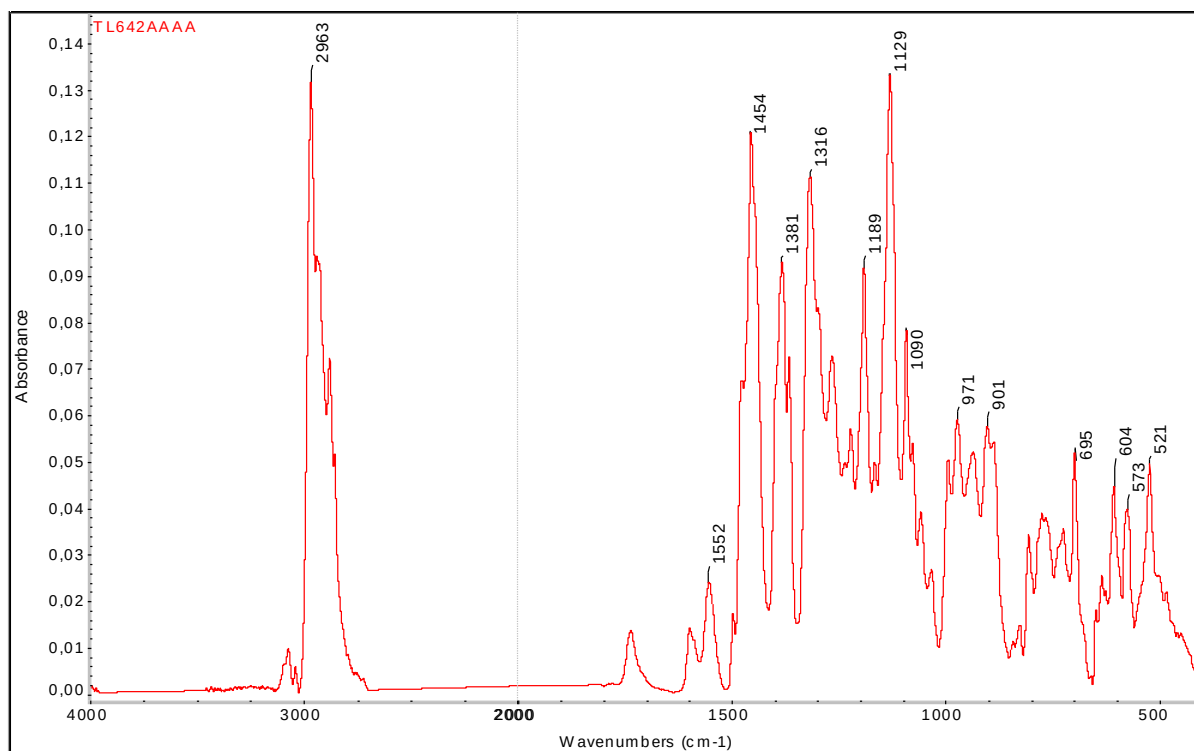


Figure S73: IR spectrum of compound **13c**

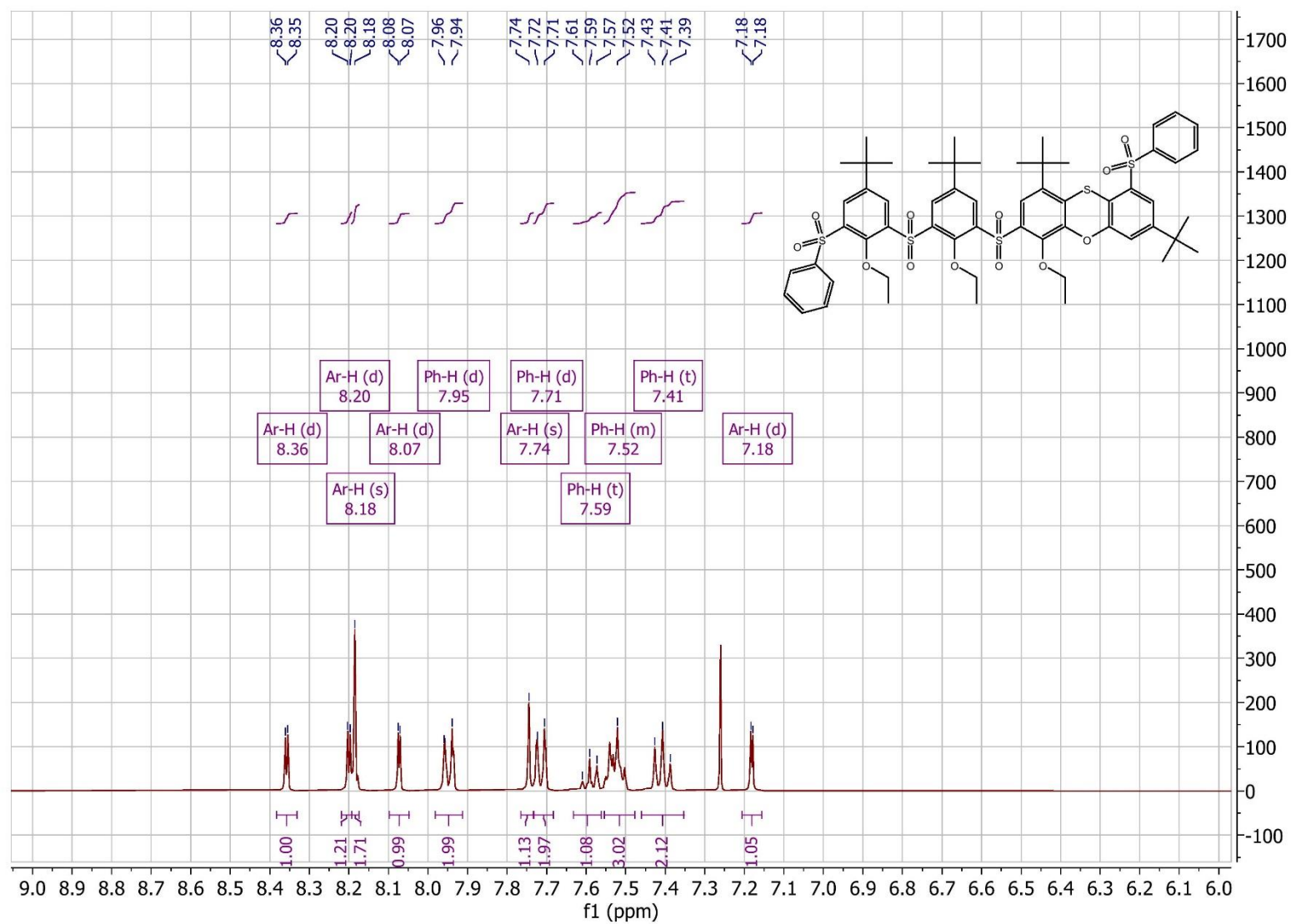


Figure S75: ^1H NMR (400 MHz, CDCl_3 , 298 K) spectrum of compound **14** (aromatic region)

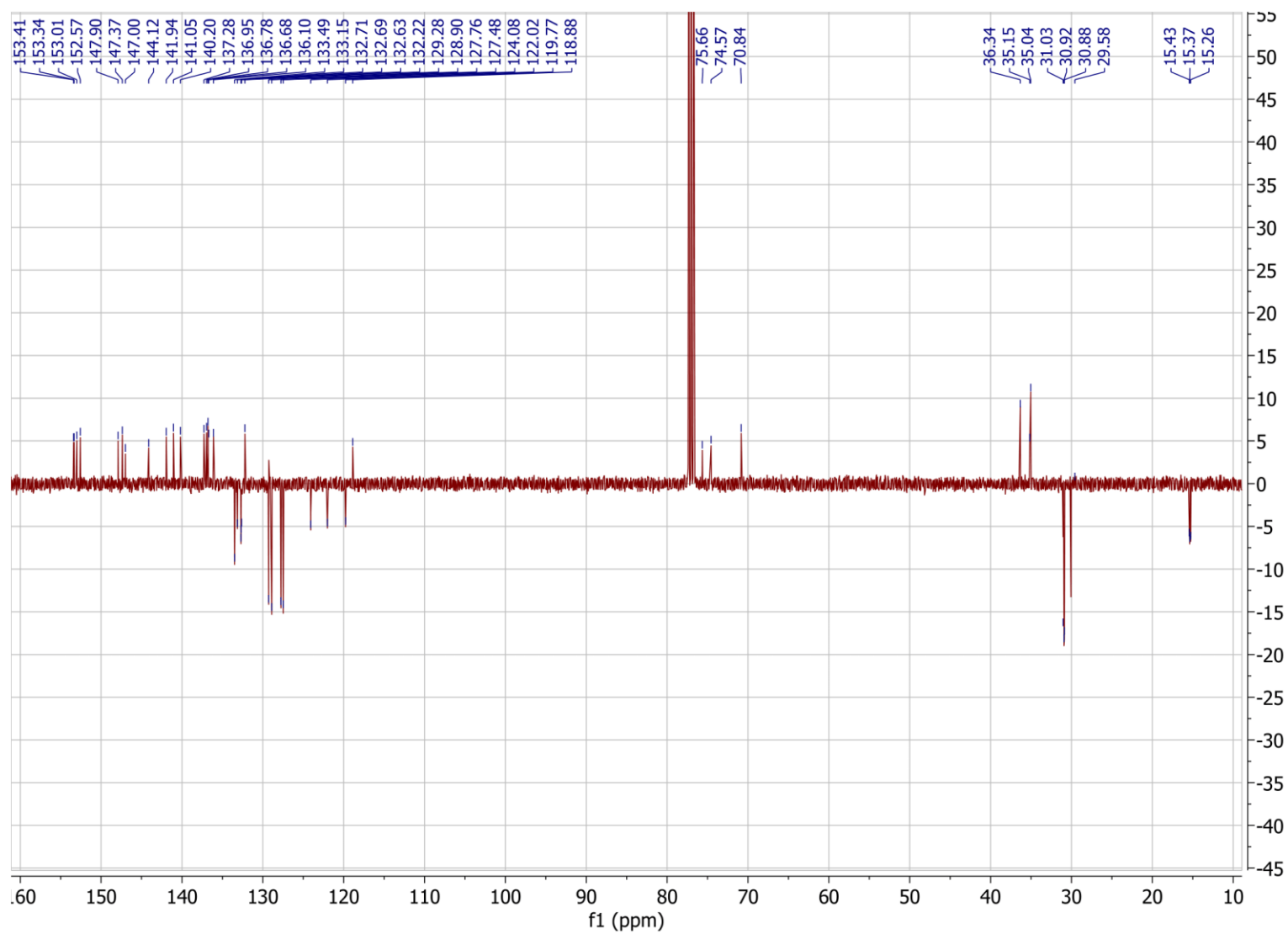


Figure S76: ¹³C NMR (APT, 101 MHz, CDCl₃, 298 K) spectrum of compound **14**

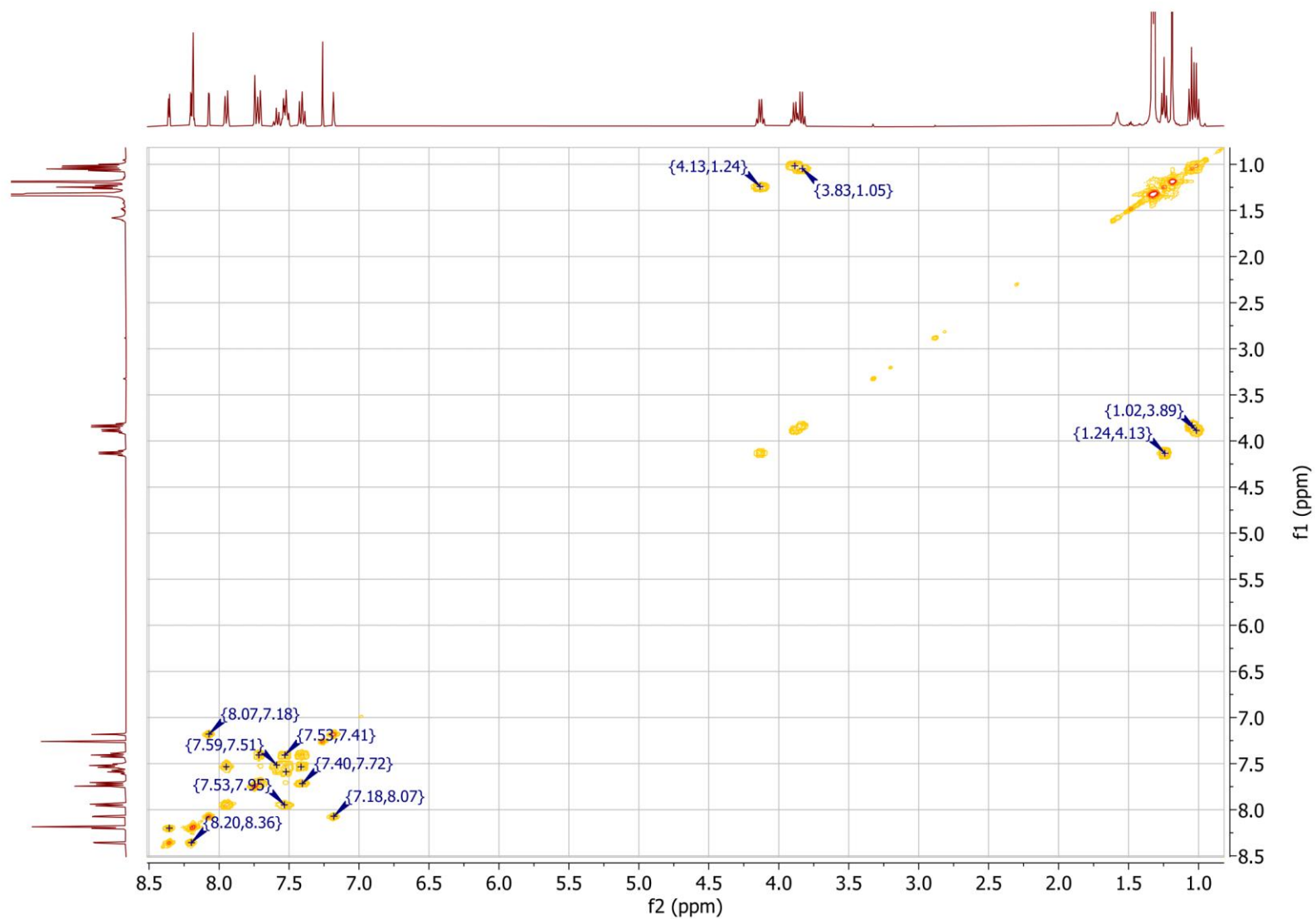


Figure S77: COSY spectrum of compound **14**

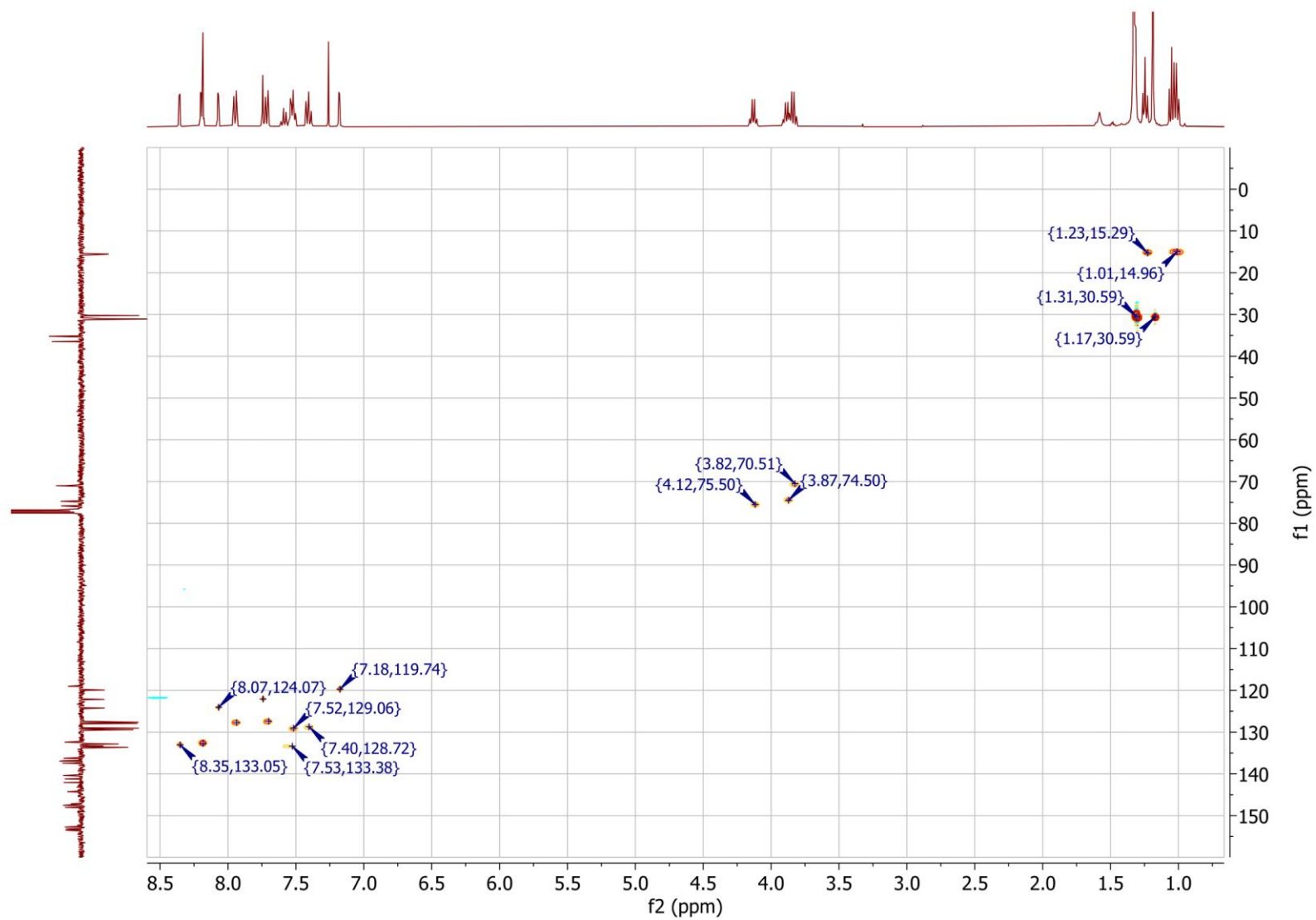


Figure S78: HMQC spectrum of compound **14**

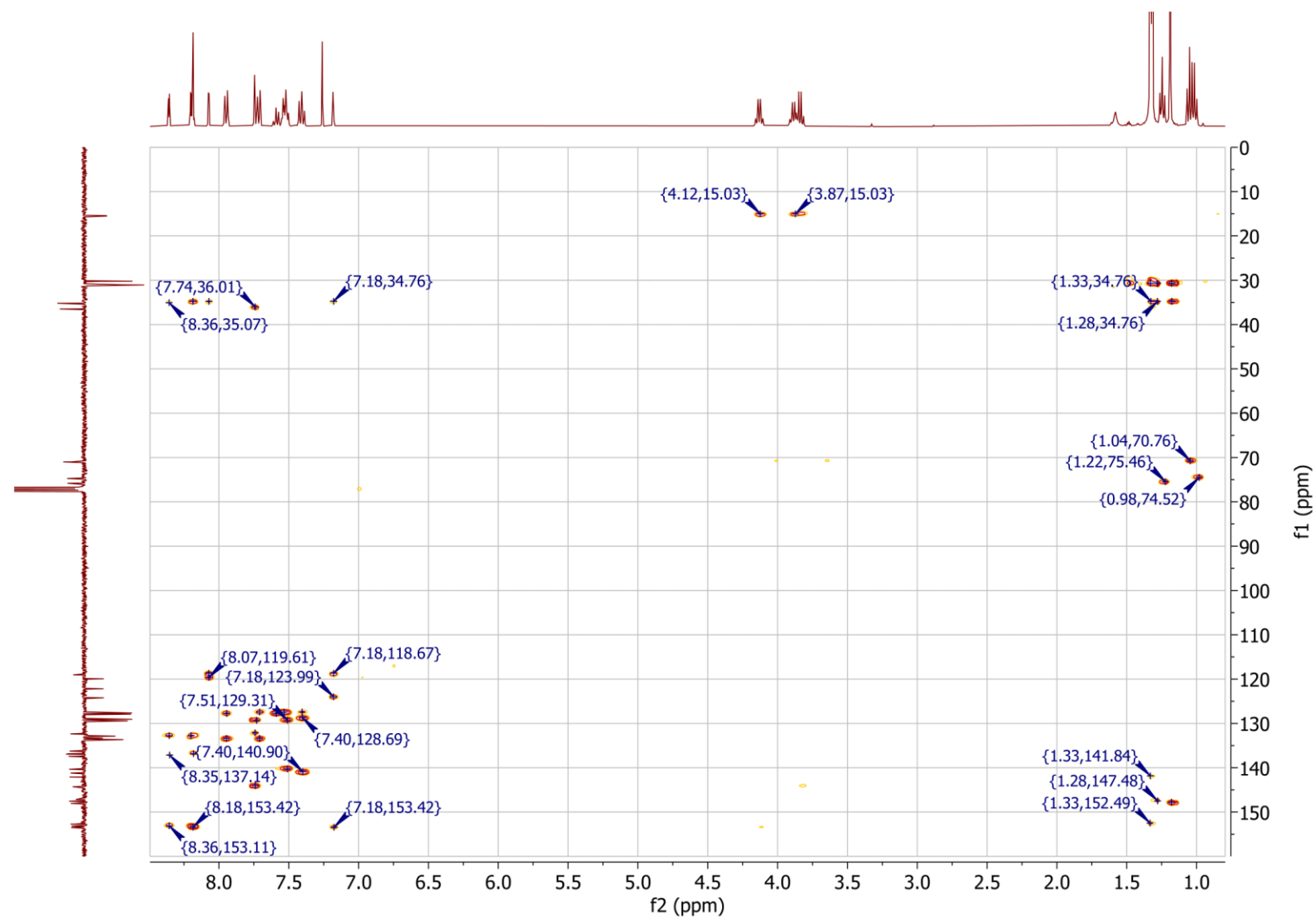
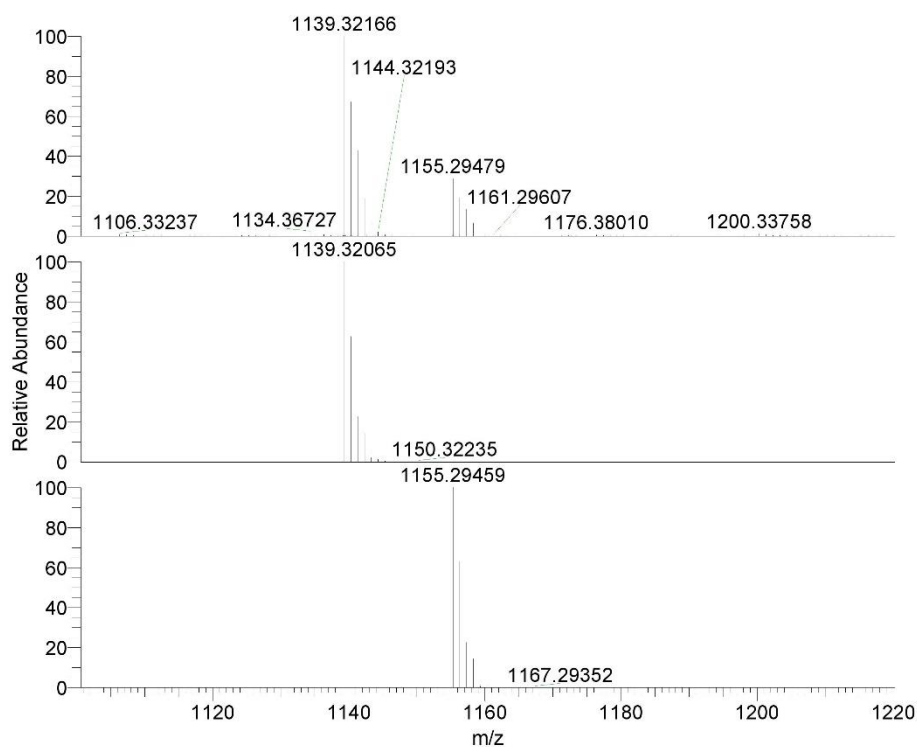


Figure S79: HMBC spectrum of compound 14



NL:
4.79E6
13_Landovsky_ESIpos_TL
646A_1#56-63 RT:
0.81-0.91 AV: 8 T: FTMS
+ c ESI Full ms
[250.00-2000.00]

NL:
3.98E5
C₅₈H₆₈O₁₂S₅+Na:
C₅₈H₆₈O₁₂S₅Na₁
pa Chrg 1

NL:
3.71E5
C₅₈H₆₈O₁₂S₅+K:
C₅₈H₆₈O₁₂S₅K₁
pa Chrg 1

Figure S80: HRMS spectrum of compound 14

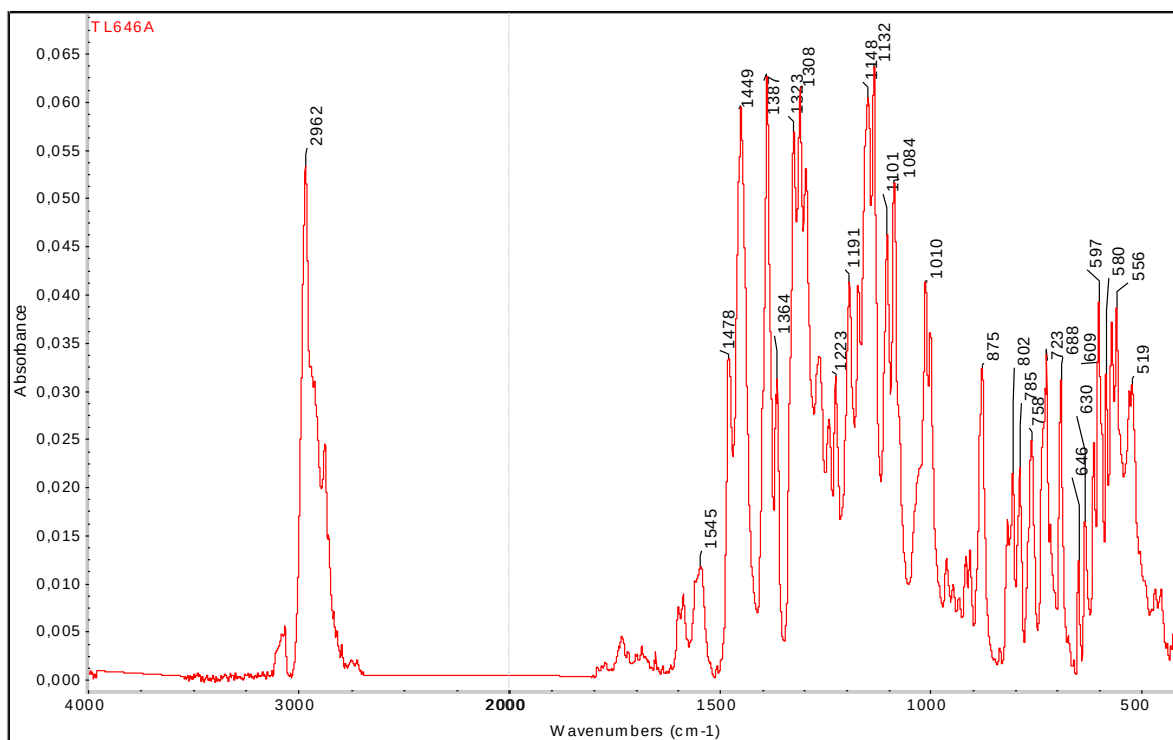


Figure S81: IR spectrum of compound 14

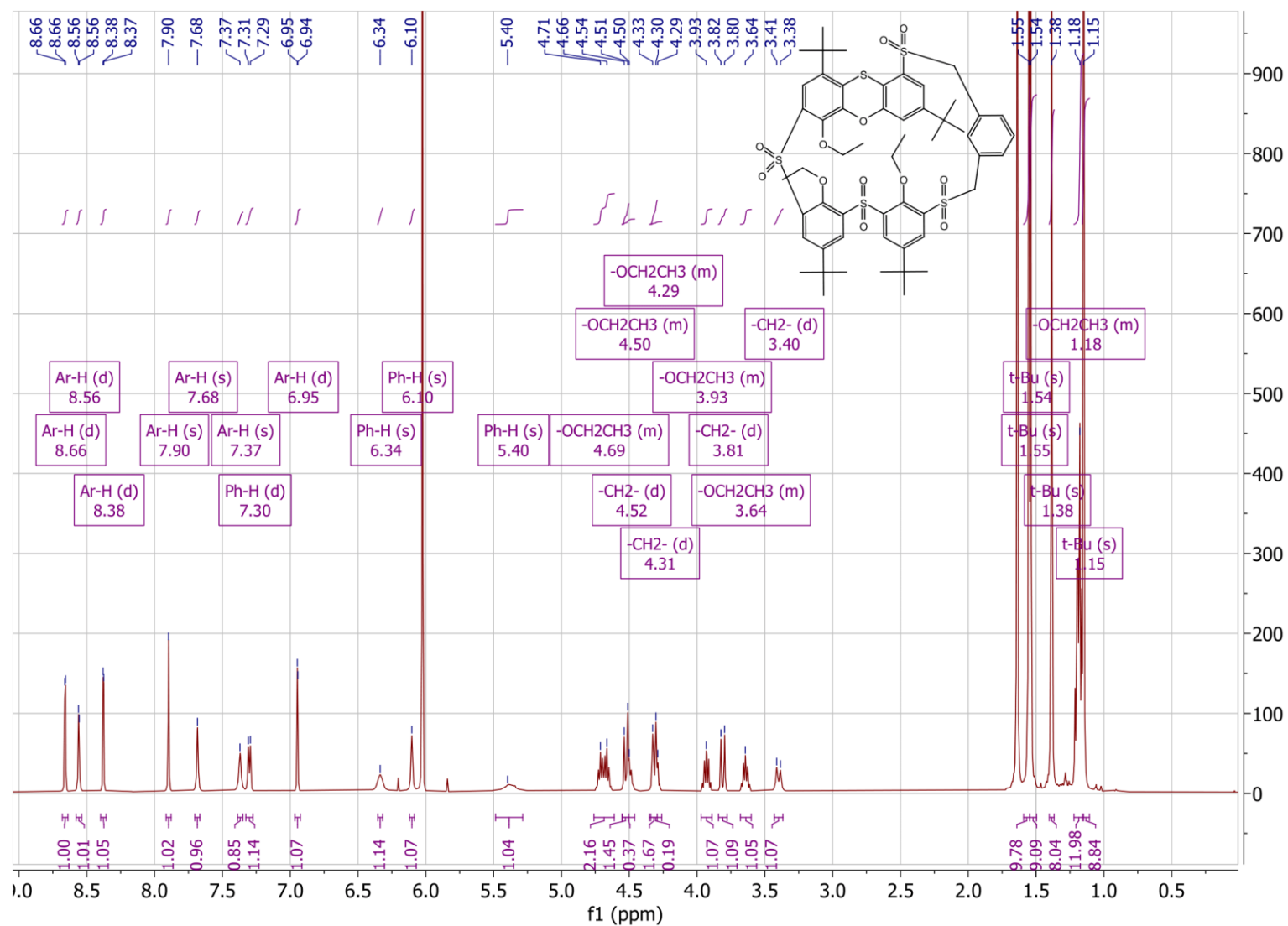


Figure S82: ^1H NMR (500 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$, 298 K) spectrum of compound **15**

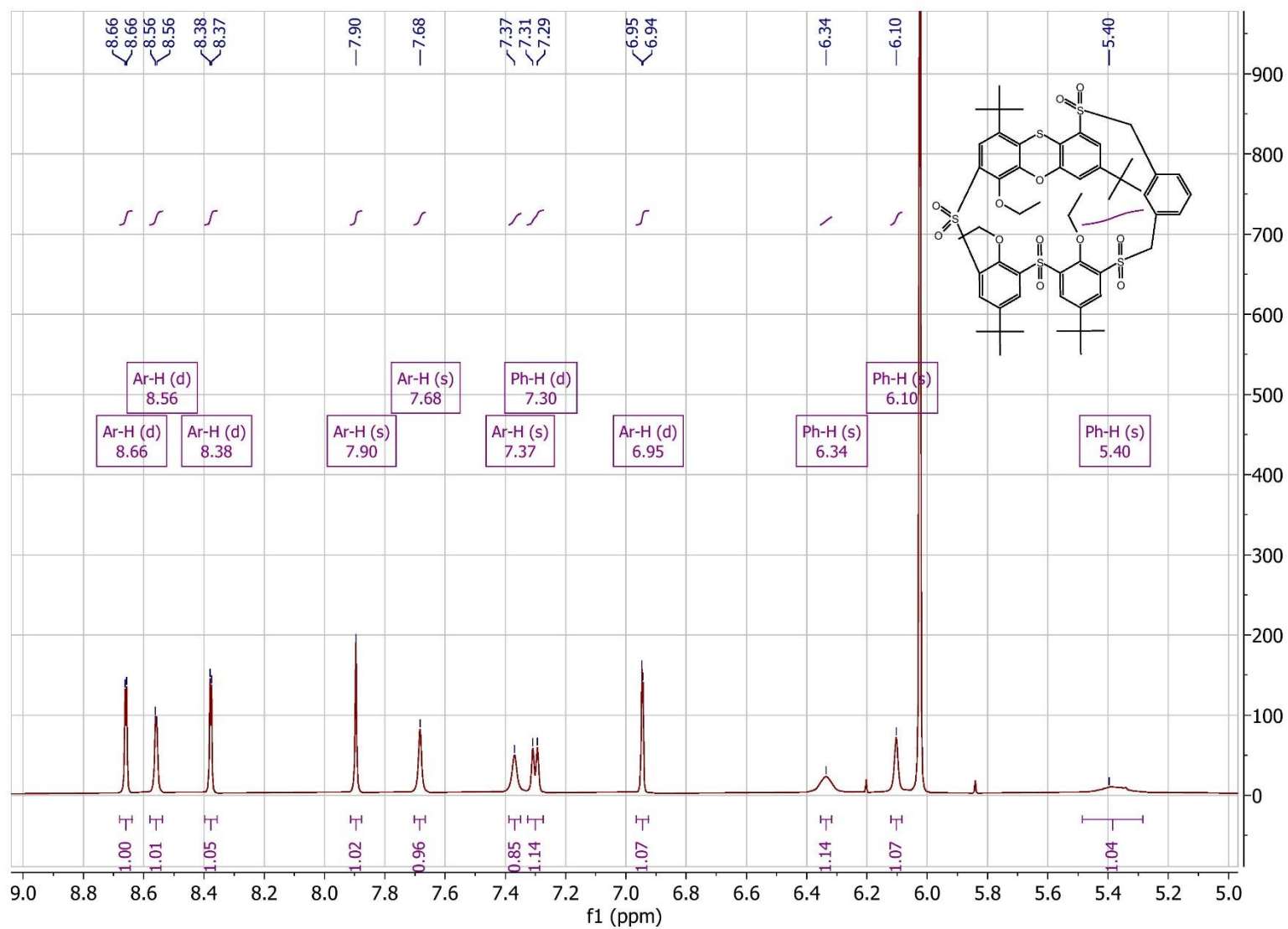


Figure S83: ^1H NMR (500 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$, 298 K) spectrum of compound **15** (aromatic region)

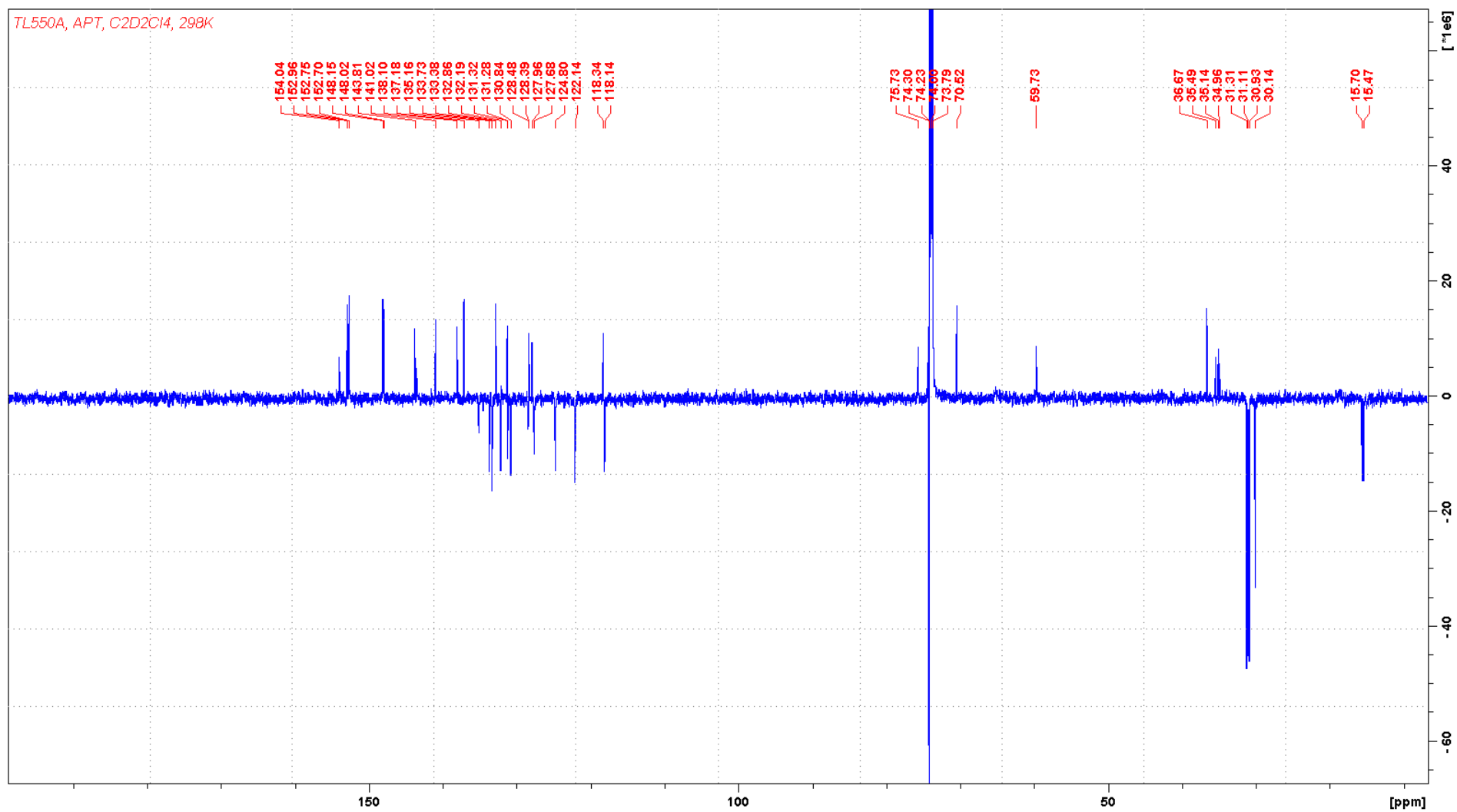


Figure S84: ^{13}C NMR (APT, 125 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$, 298 K) spectrum of compound **15**

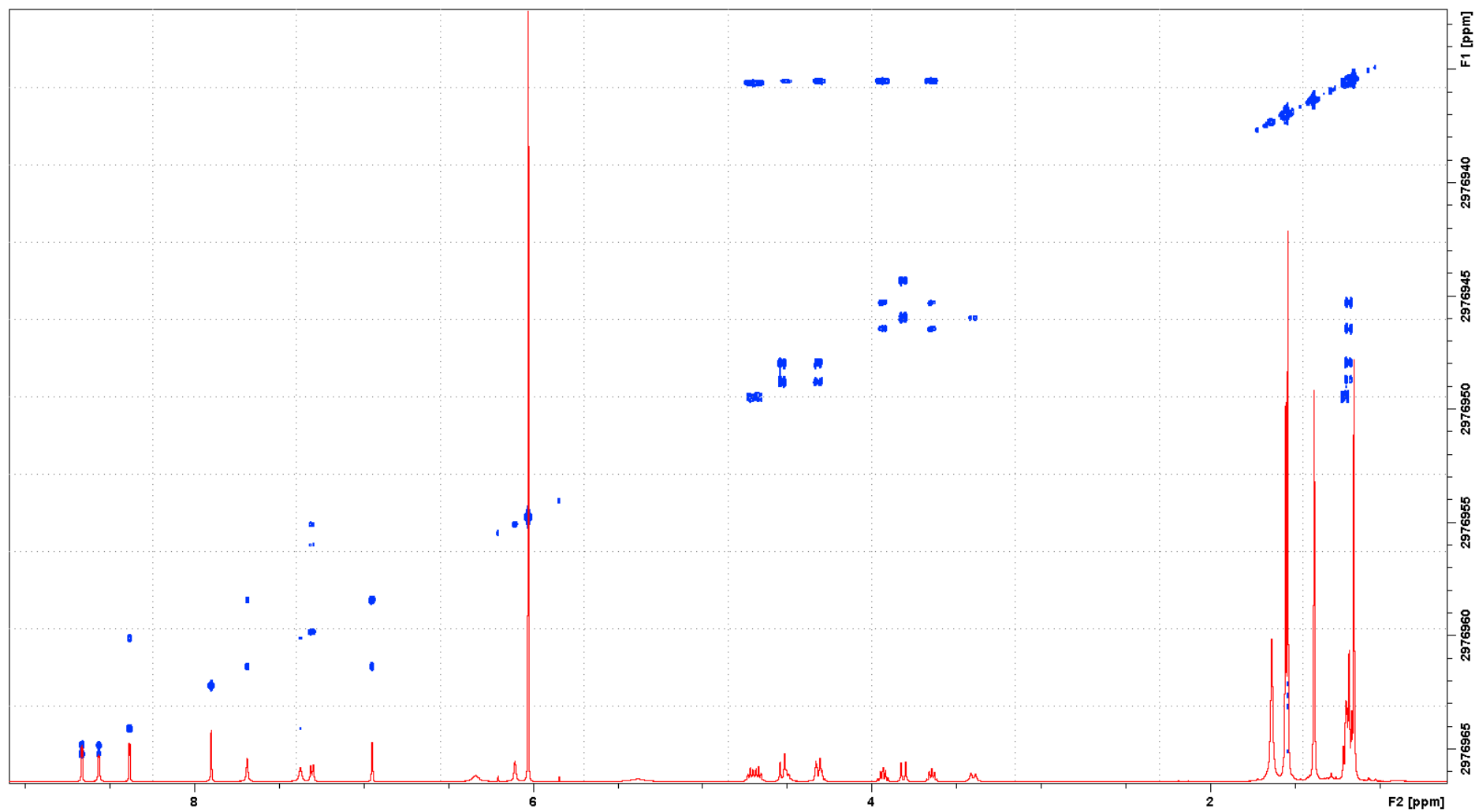


Figure S85: COSY spectrum of compound 15

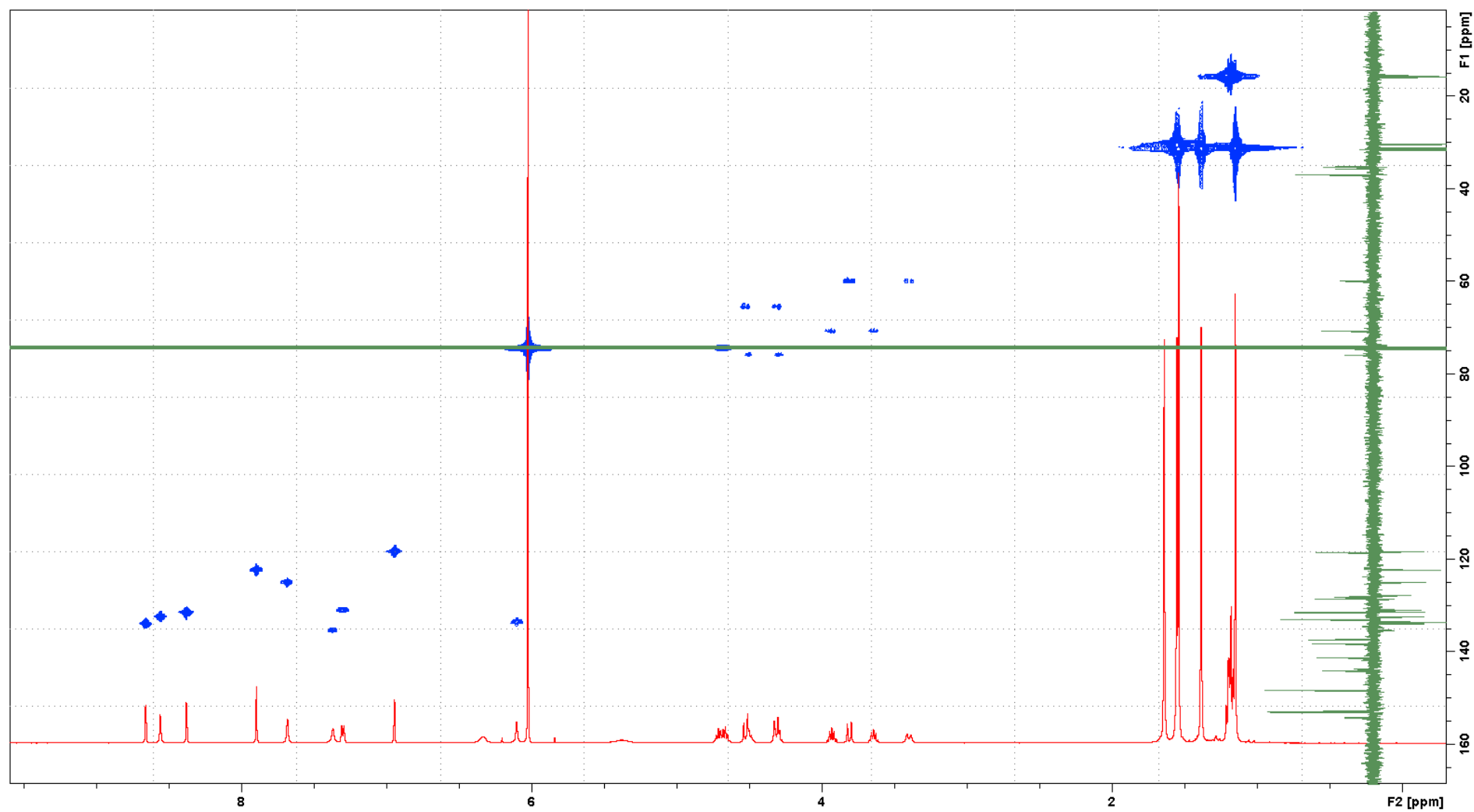


Figure S86: HMQC spectrum of compound 15

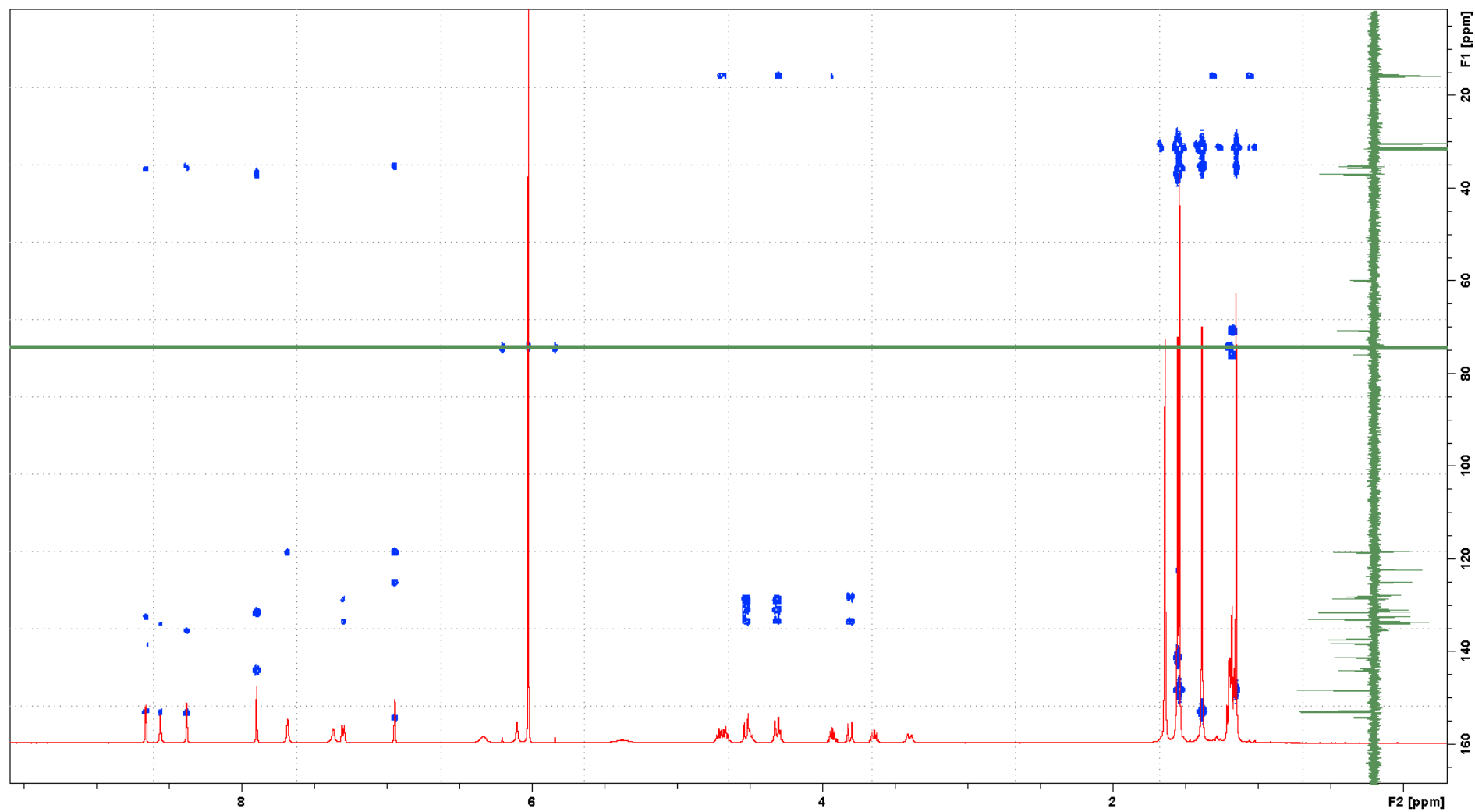


Figure S87: HMBC spectrum of compound 15

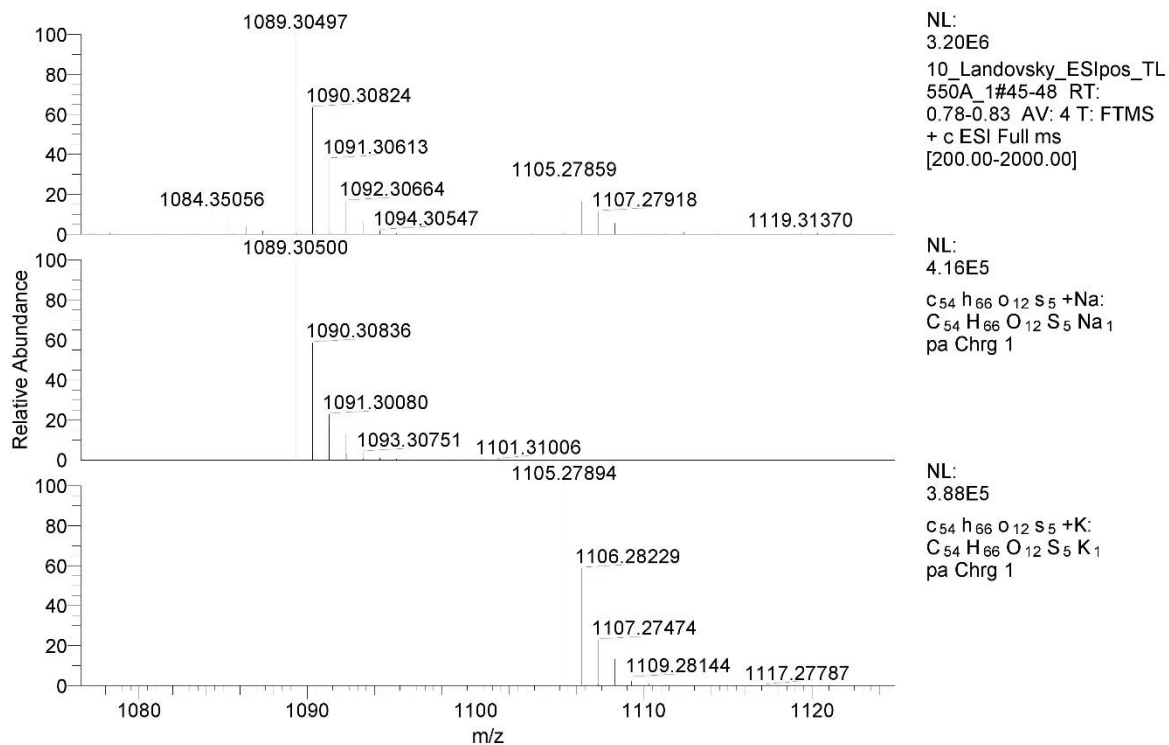


Figure S88: HRMS spectrum of compound 15

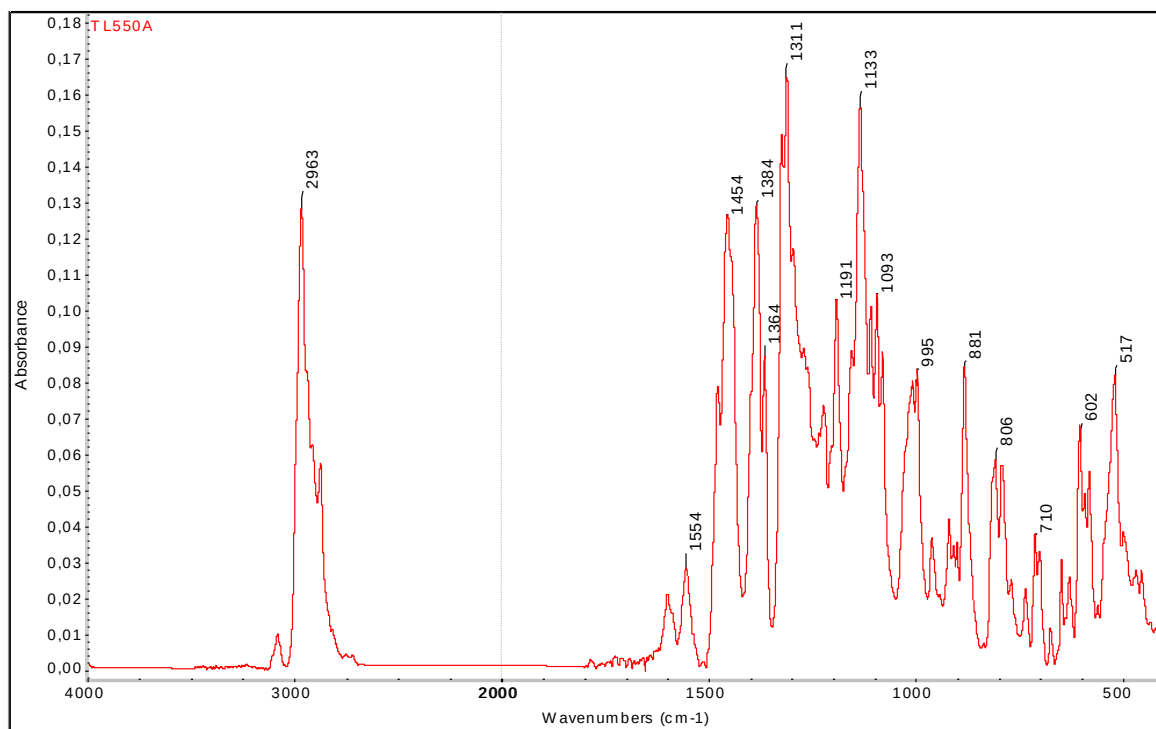


Figure S89: IR spectrum of compound 15

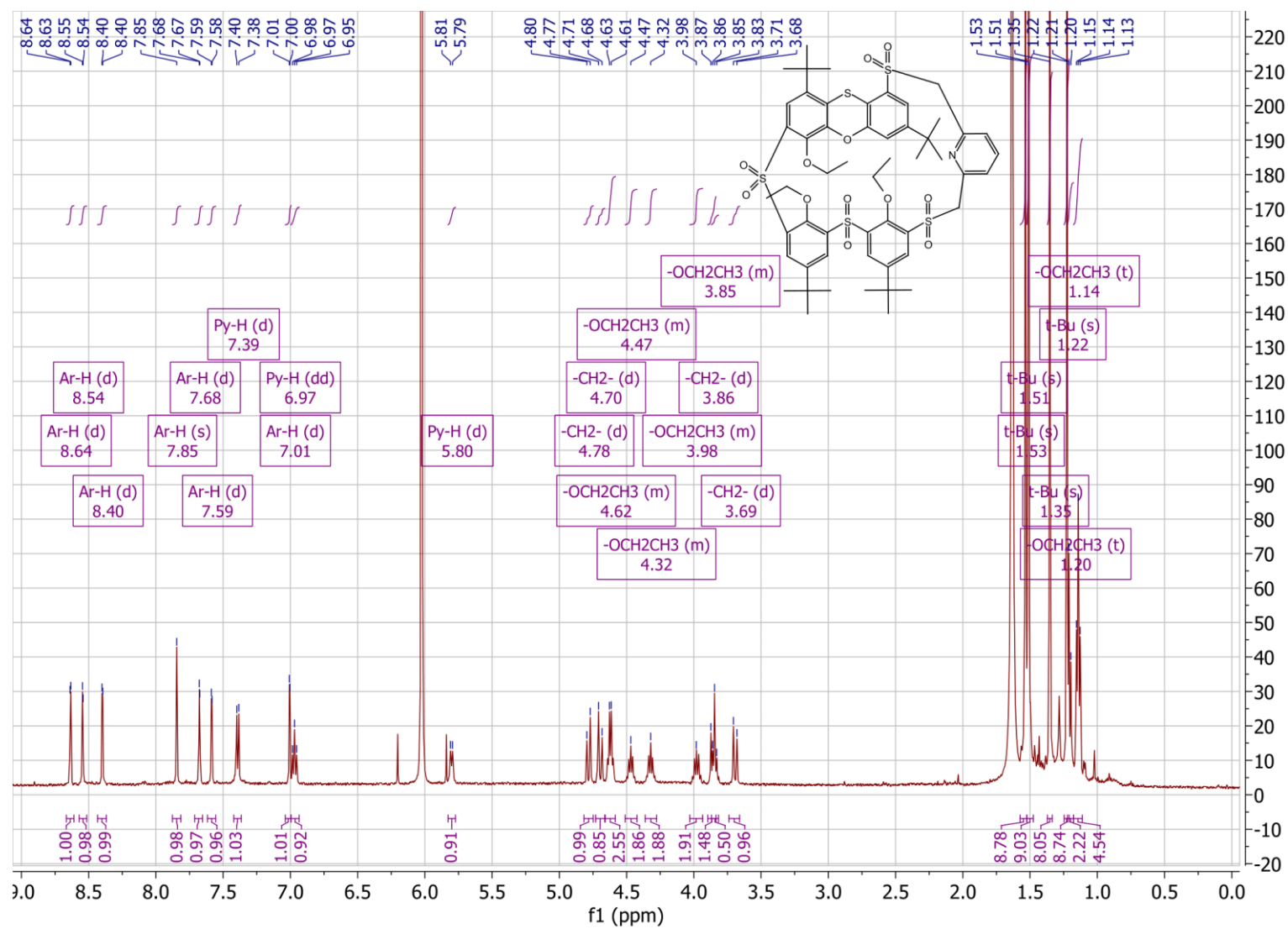


Figure S90: ^1H NMR (600 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$, 298 K) spectrum of compound **16**

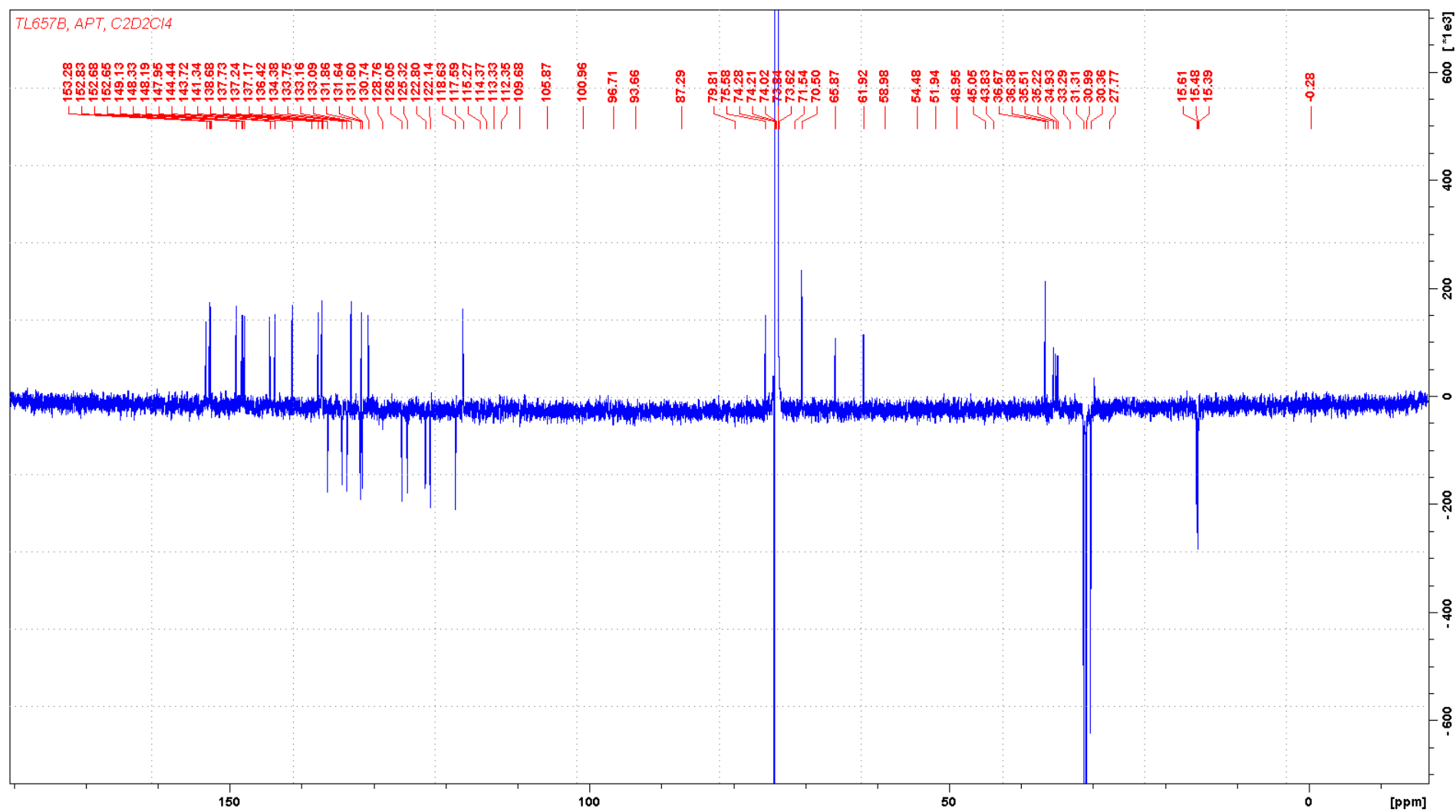


Figure S92: ^{13}C NMR (APT, 150 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$, 298 K) spectrum of compound **16**

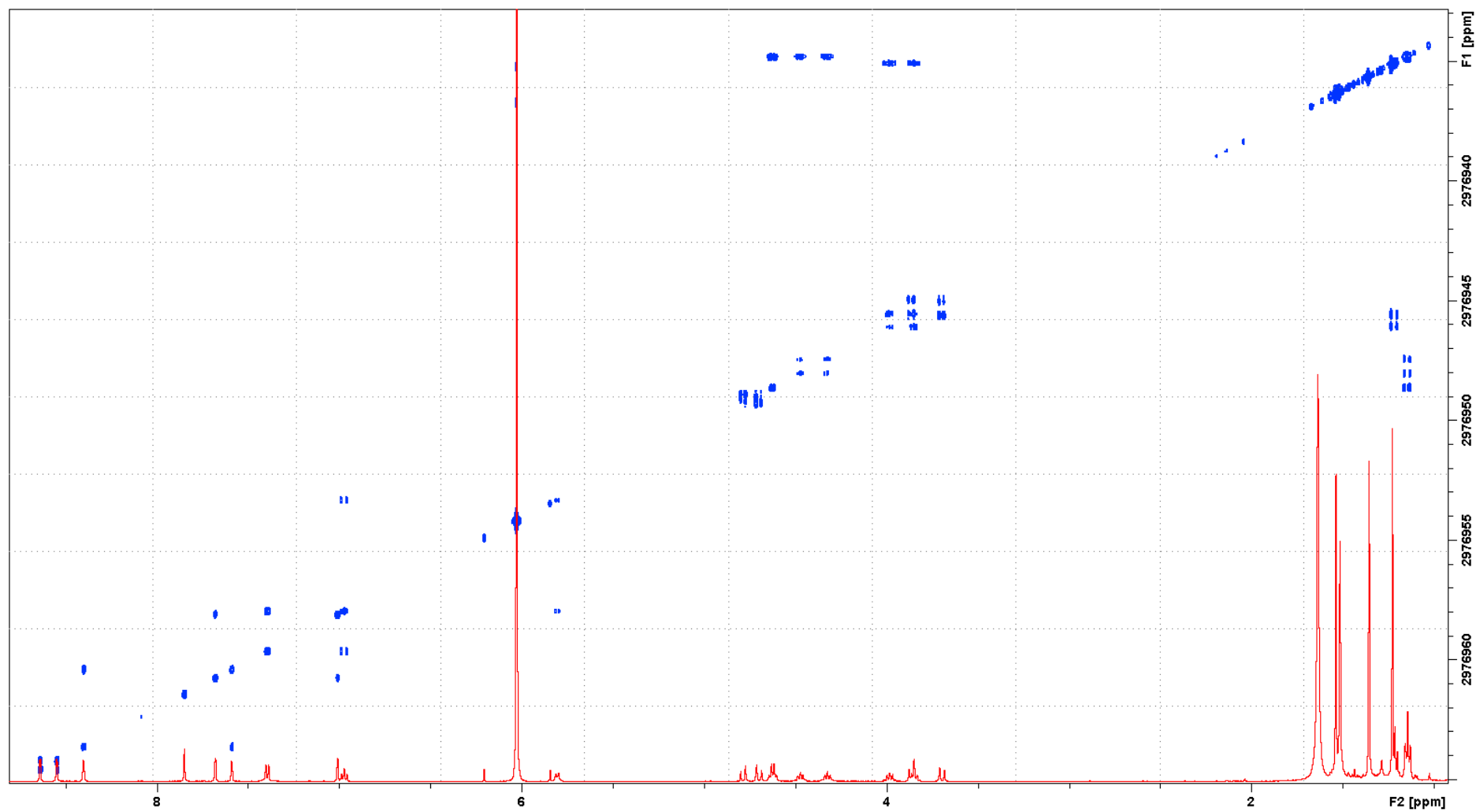


Figure S93: COSY spectrum of compound 16

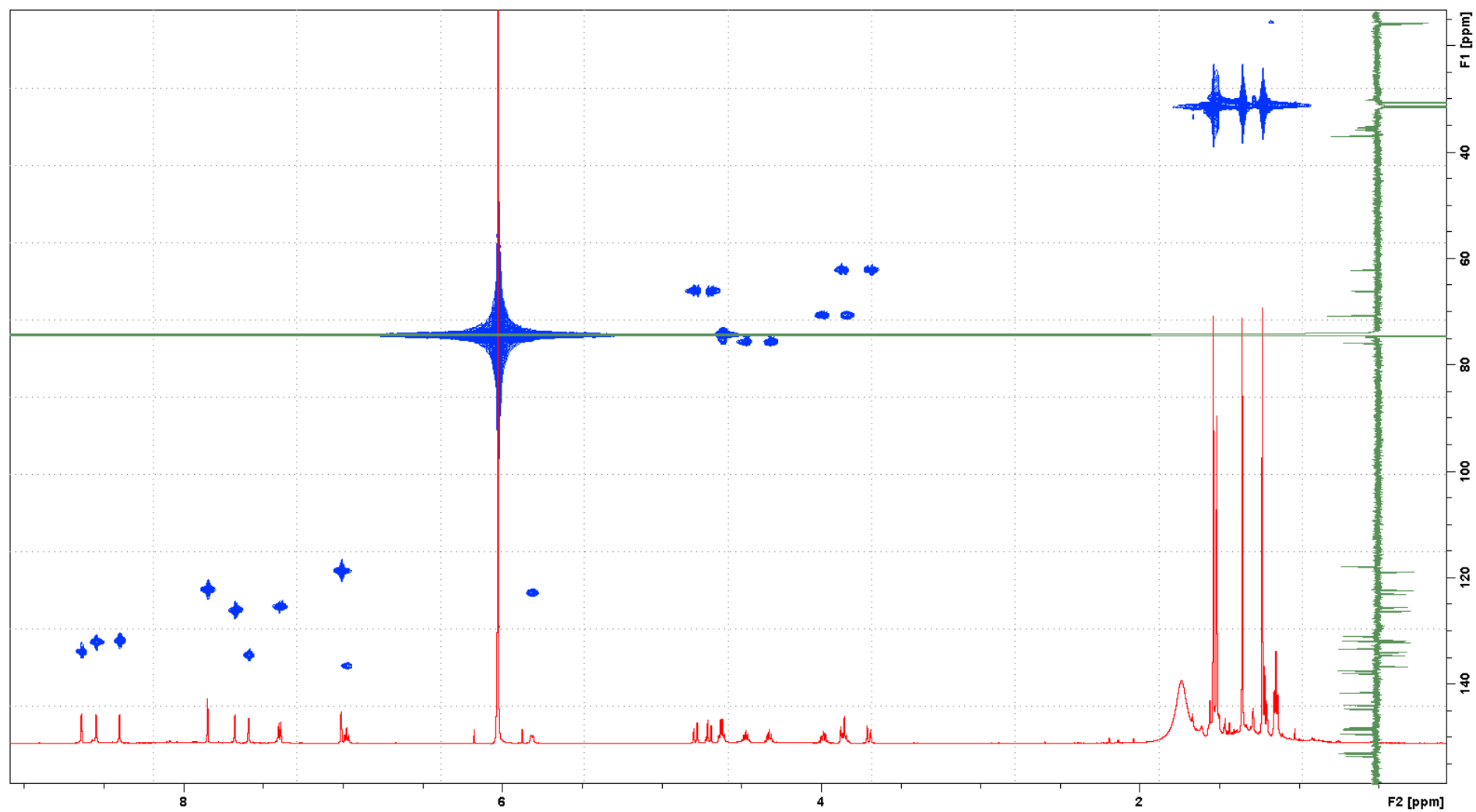


Figure S94: HMQC spectrum of compound 16

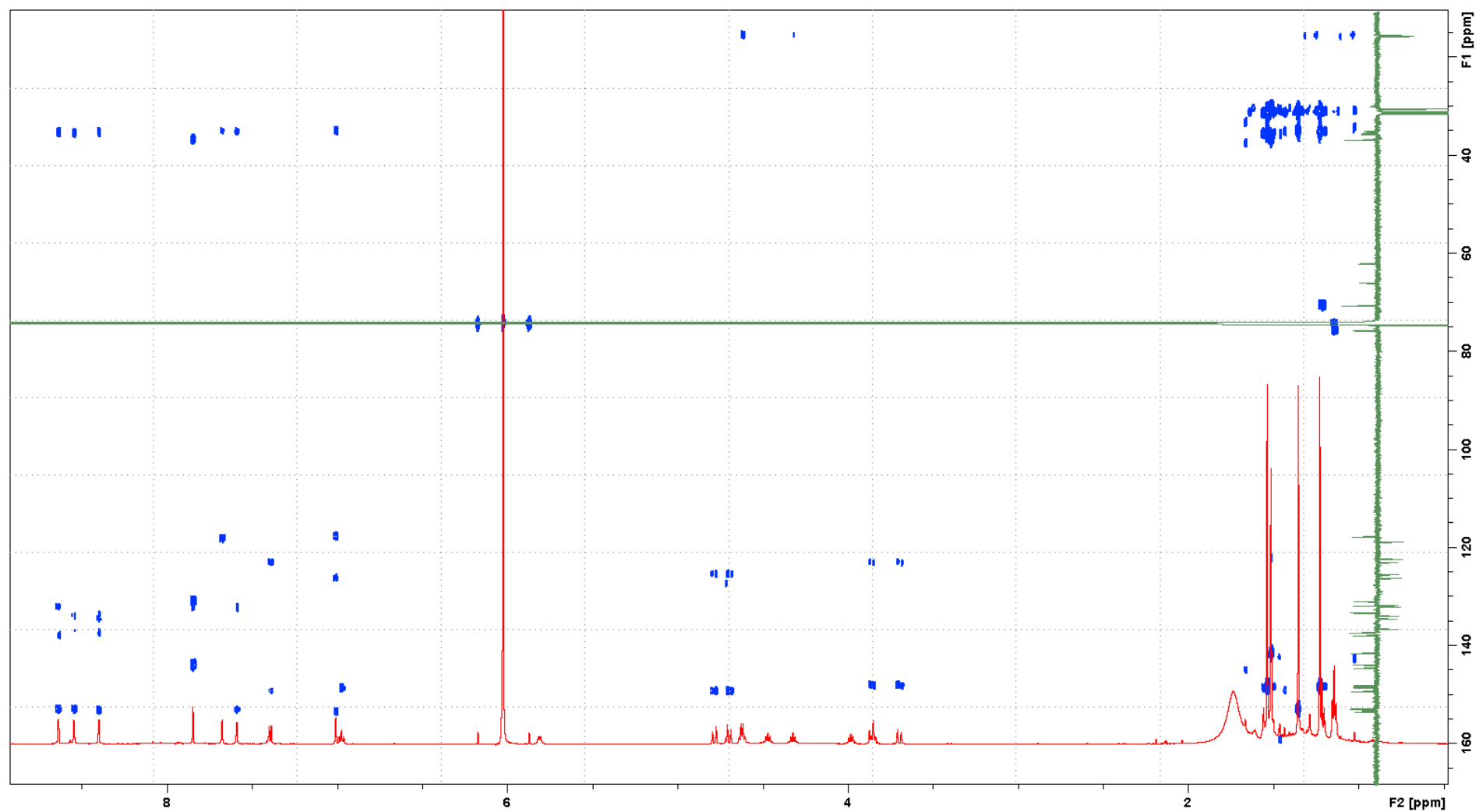


Figure S95: HMBC spectrum of compound 16

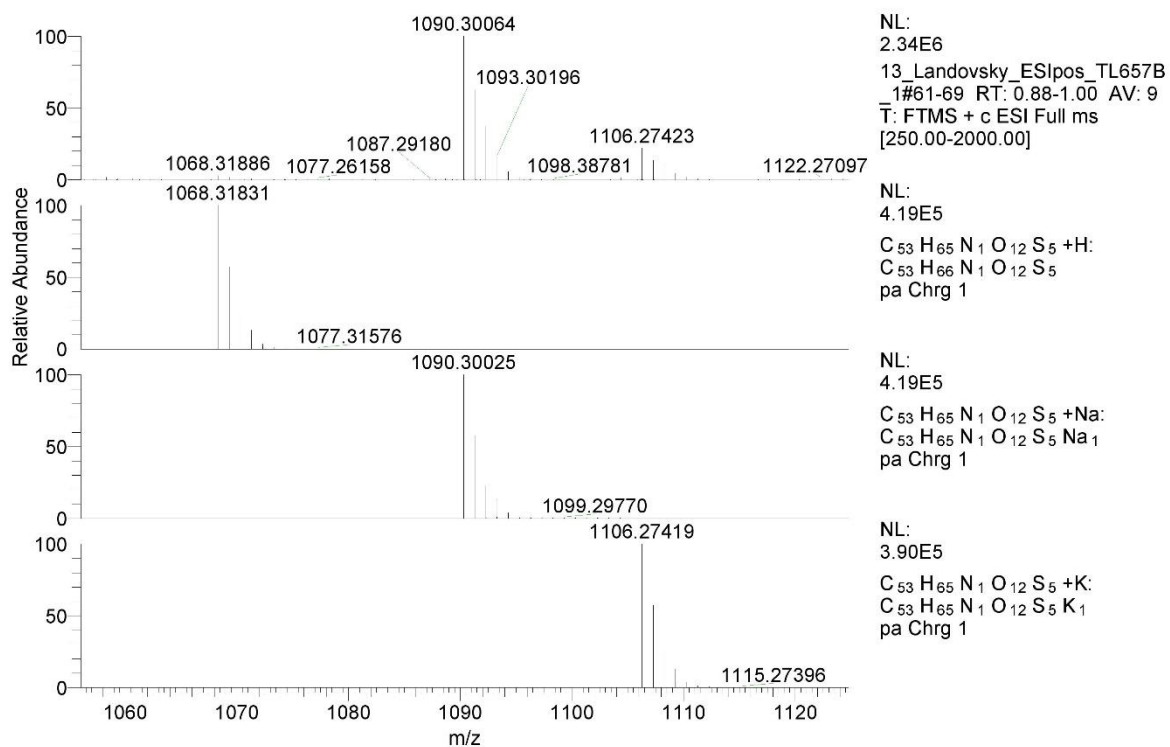


Figure S96: HRMS spectrum of compound 16

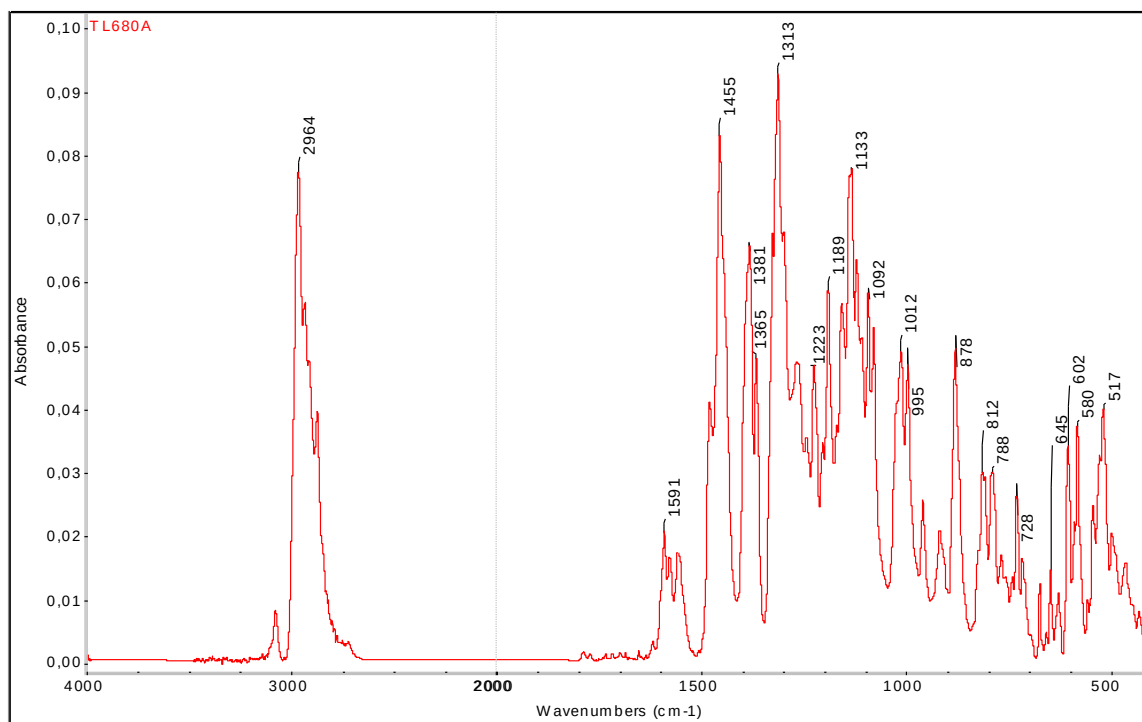


Figure S97: IR spectrum of compound 16

2. Comparison between compounds **5b**, **9** and **10**

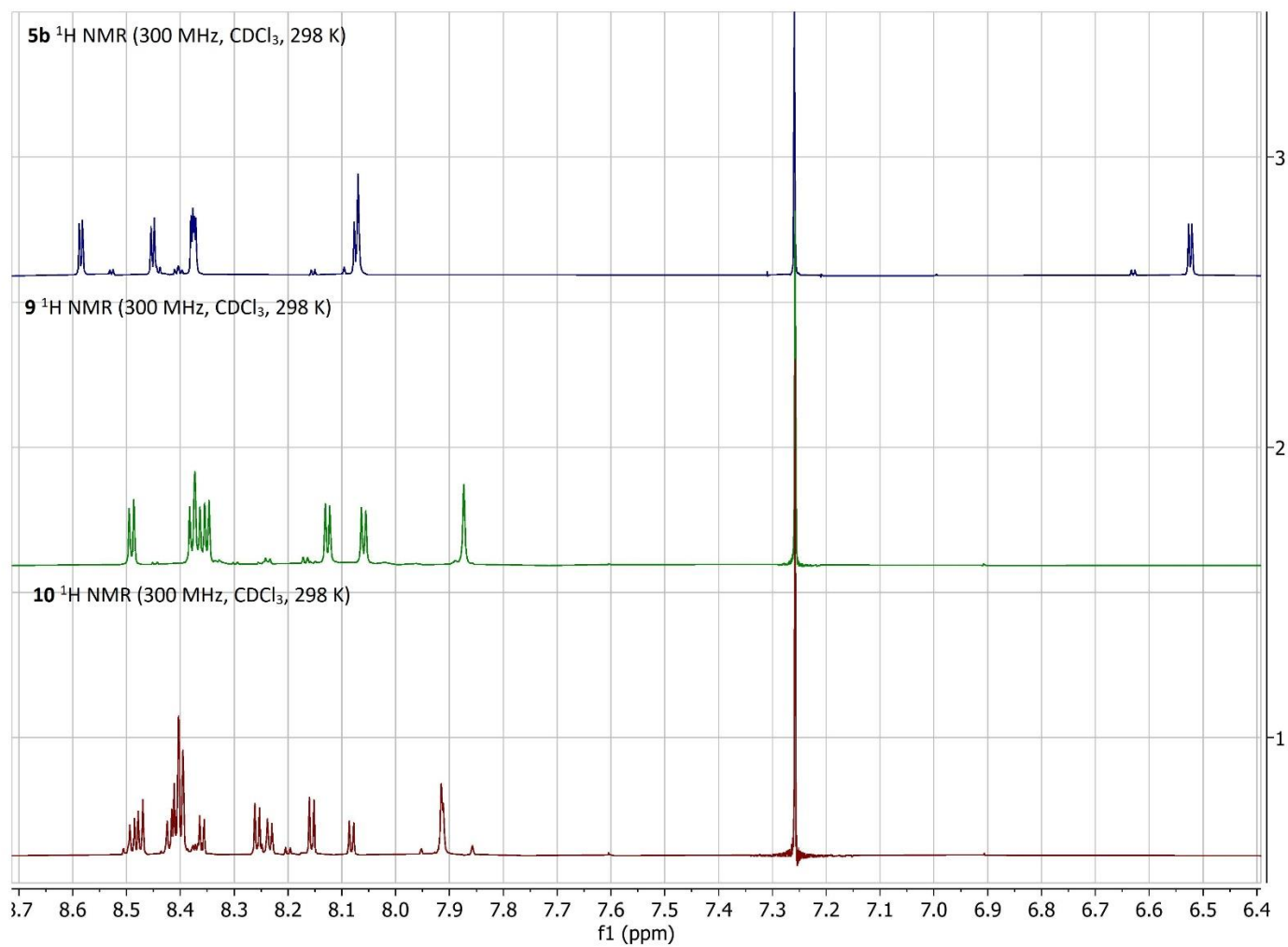


Figure S98: Comparison between compounds **5b**, **9** and **10** (^1H NMR spectra, aromatic region)

3. Variable temperature NMR spectra

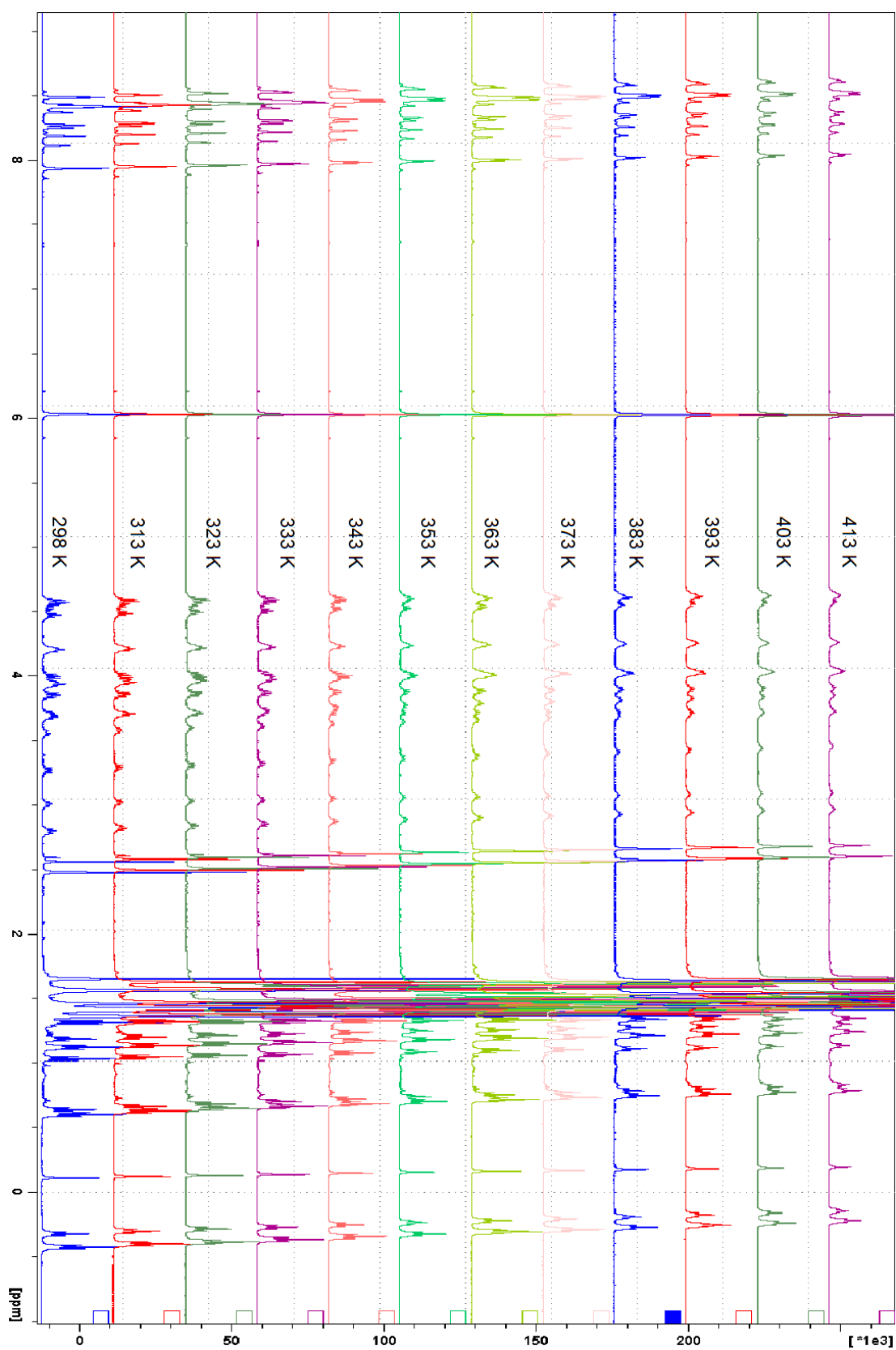


Figure S99: VT NMR spectrum (heating) of compound **10** (600 MHz, C₂D₂Cl₄)

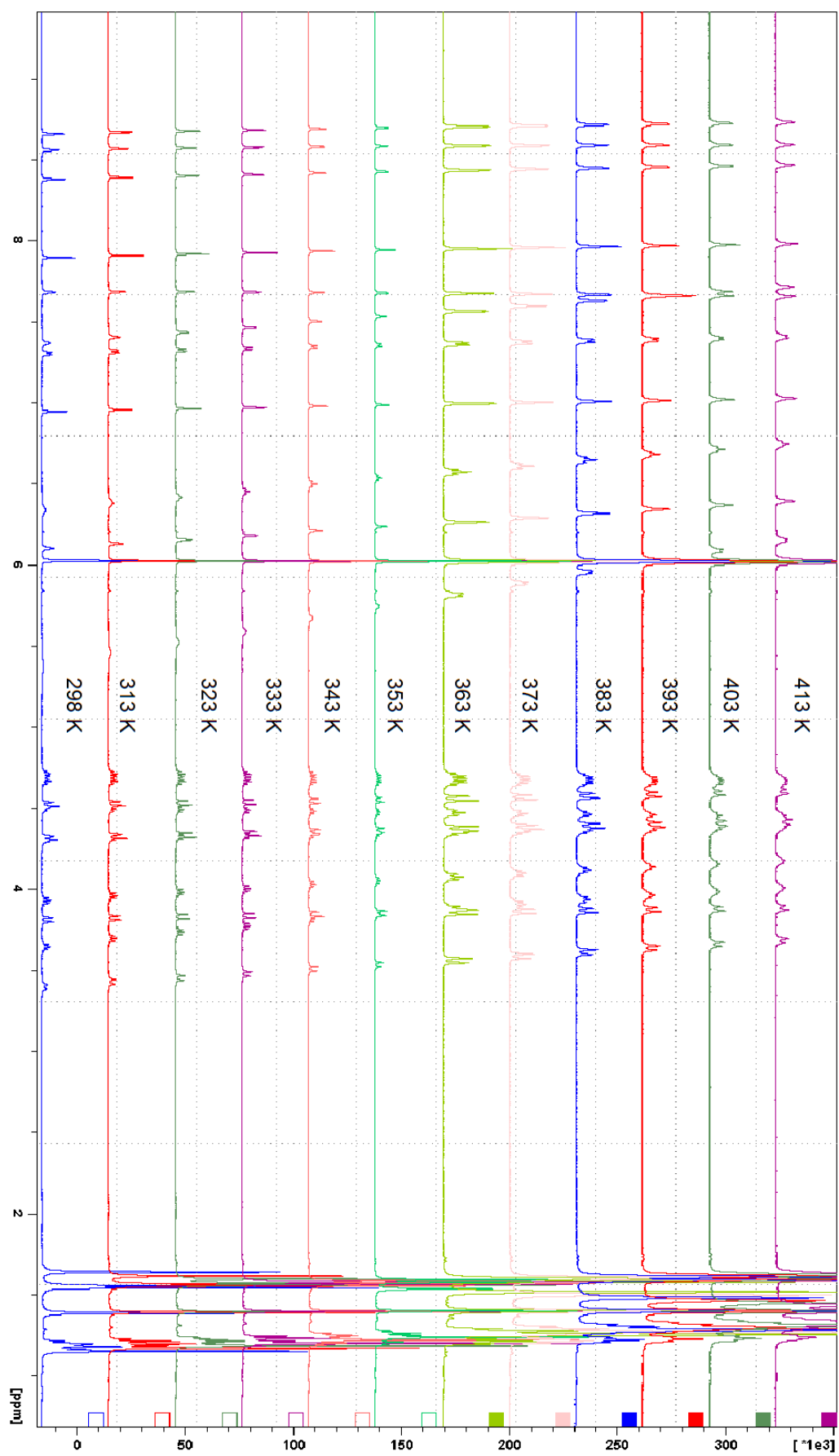


Figure S100: VT NMR spectrum (heating) of compound **15** (600 MHz, $C_2D_2Cl_4$)

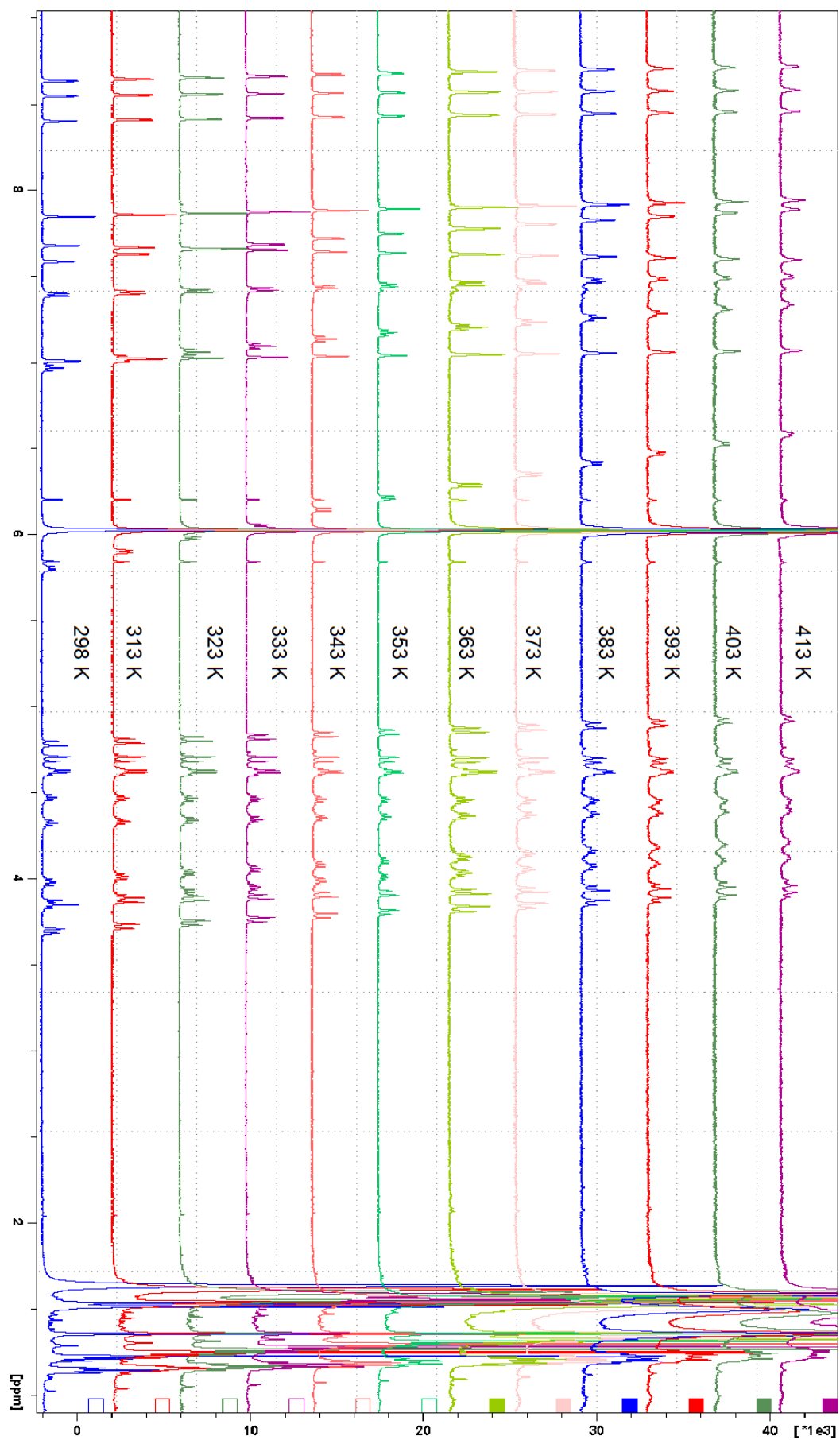


Figure S101: VT NMR spectrum (heating) of compound **16** (600 MHz, C₂D₂Cl₄)

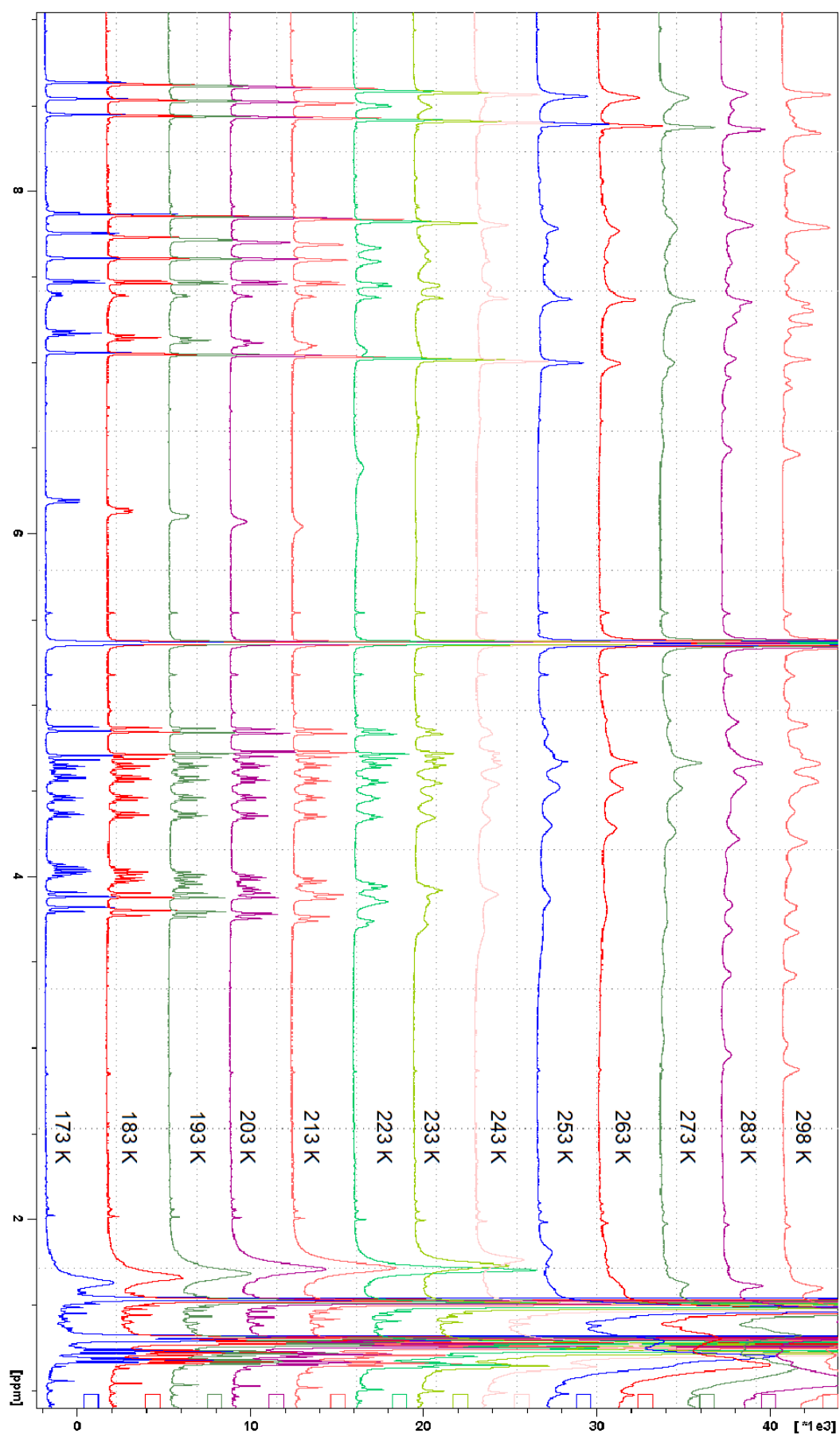


Figure S102: VT NMR spectrum (cooling) of compound **16** (600 MHz, CD₂Cl₂)

4. Crystallographic data

Compound 7

The structure of **7** was measured using D8 VENTURE equipped with Photon CMOS detector with Cu-K α ($\lambda=1.54178$ Å) radiation at 180 K. The structure was in monoclinic system, $P 2_1/c$ space group with lattice parameters $a=15.8648(5)$ Å, $b=13.9916(3)$ Å, $c=19.6709(6)$ Å, $\alpha=90^\circ$ $\beta=95.999(3)^\circ$ $\gamma=90^\circ$, $Z=4$, $V=4342.5(2)$ Å³, $D_c=1.339$ g/cm³, $\mu(\text{Cu-K } \alpha)=2.518$ mm⁻¹. The data reduction and absorption correction were done with Apex3 software. The structure was solved by charge-flipping methods using Superflip^{S3} software and refined by full matrix least squares on F squared value using Crystals^{S4} software to final values $R=0.0392$ and $wR=0.0942$ using 8608 independent reflections ($\theta_{\max}=72.490^\circ$), 552 parameters and 48 restraints. MCE^{S5} software was used for visualization of residual electron density maps. According to common practice, the hydrogen atoms attached to carbon atoms were placed geometrically with $U_{\text{iso}}(\text{H})$ in range 1.2–1.5 U_{eq} of parent atom (C). The disordered functional groups were refined with restrained geometry and occupancy constrained to full for each atomic position. The structure was deposited into Cambridge Structural Database under number CCDC 2069227.

Compound 12a

The structure of **12a** was measured using D8 VENTURE equipped with Photon CMOS detector with Cu-K α ($\lambda=1.54178$ Å) radiation at 180 K. The structure was in triclinic system, $P -1$ space group with lattice parameters $a=13.7779(4)$ Å, $b=14.4703(4)$ Å, $c=14.6125(4)$ Å, $\alpha=81.1803(12)^\circ$ $\beta=76.6391(10)^\circ$ $\gamma=63.6398(10)^\circ$, $Z=2$, $V=2535.42(12)$ Å³, $D_c=1.301$ g/cm³, $\mu(\text{Cu-K } \alpha)=2.592$ mm⁻¹. The data reduction and absorption correction were done with Apex3 software. The structure was solved by charge-flipping methods using Superflip^{S3} software and refined by full matrix least squares on F squared value using Crystals^{S4} software to final values $R=0.0604$ and $wR=0.1406$ using 9618 independent reflections ($\theta_{\max}=70.067^\circ$), 653 parameters and 36 restraints. MCE^{S5} software was used for visualization of residual electron density maps. According to common practice, the hydrogen atoms attached to carbon atoms were placed geometrically with $U_{\text{iso}}(\text{H})$ in range 1.2–1.5 U_{eq} of parent atom (C). The disordered functional groups were refined with restrained geometry and occupancy constrained to full for each atomic position. The residual electron density map contains one peak. This peak was probably caused due to the deformation of electron density nearby the sulphur atom. It is not in a reasonable position to be occupied by an atom or by caused by a disorder. The structure was deposited into Cambridge Structural Database under number CCDC 2069369.

Compound 14

$M = 1178.54$ g.mol⁻¹, triclinic system, space group $P-1$, $a = 13.1197(4)$ Å, $b = 15.7488(5)$ Å, $c = 16.2572(5)$ Å, $\alpha = 103.3475(9)^\circ$, $\beta = 99.6156(9)^\circ$, $\gamma = 105.3475(9)^\circ$, $Z = 2$, $V = 3054.01(17)$ Å³, $D_c = 1.282$ g.cm⁻³, $\mu(\text{Cu-K}\alpha) = 2.27$ mm⁻¹, crystal dimensions of $0.40 \times 0.35 \times 0.33$ mm. Data were collected at 200 (2) K on a D8 Venture Photon CMOS diffractometer with Incoatec microfocus sealed tube Cu-K α radiation. The structure was solved by charge flipping methods^{S3} and anisotropically refined by full matrix least squares on F squared using CRYSTALS^{S6} to final value $R = 0.038$ and $wR = 0.104$ using 11988 independent reflections ($\theta_{\max} = 72.2^\circ$), 771 parameters and 98 restrains. The hydrogen atoms bonded to carbon atoms were placed in calculated positions refined with a riding constrains. The positions of disordered *tert*-butyl groups found in difference electron density maps, refined with restrained geometry and occupancy constrained to full for each position. The resulting occupancy ratios were 837:163 and 736:264. MCE^{S5} was used for visualization of electron density maps. The structure was deposited into Cambridge Structural Database under number CCDC 2069939.

Compound 15

The structure of **15** was measured using D8 VENTURE equipped with Photon CMOS detector with Mo-K α ($\lambda = 0.71073 \text{ \AA}$) radiation at 180 K. The structure was in triclinic system, $P-1$ space group with lattice parameters $a = 15.2602(10) \text{ \AA}$, $b = 15.3461(10) \text{ \AA}$, $c = 15.8961(10) \text{ \AA}$, $\alpha = 111.084(2)^\circ$, $\beta = 108.289(2)^\circ$, $\gamma = 93.047(2)^\circ$, $Z = 2$, $V = 3239.5(4) \text{ \AA}^3$, $D_c = 1.345 \text{ g/cm}^3$, $\mu(\text{Mo-K}\alpha) = 0.253 \text{ mm}^{-1}$. The data reduction and absorption correction were done with Apex3 software. The structure was solved by charge-flipping methods using Sir92^{S7} software and refined by full matrix least squares on F squared value using Crystals^{S4} software to final values $R = 0.0408$ and $wR = 0.1083$ using 13209 independent reflections ($\theta_{\max} = 26.372^\circ$), 784 parameters and 0 restraints. According to common practice, the hydrogen atoms attached to carbon atoms were placed geometrically with $U_{\text{iso}}(\text{H})$ in range 1.2–1.5 U_{eq} of parent atom (C). The crystal was solvated with four molecules of nitromethane. The structure was deposited into Cambridge Structural Database under number CCDC 2068963.

Compound 16

$M = 1208.96 \text{ g.mol}^{-1}$, triclinic system, space group $P-1$, $a = 13.12948(15) \text{ \AA}$, $b = 14.11541(19) \text{ \AA}$, $c = 19.1344(2) \text{ \AA}$, $\alpha = 94.9881(10)^\circ$, $\beta = 105.9354(10)^\circ$, $\gamma = 114.8298(12)^\circ$, $Z = 2$, $V = 3010.41(8) \text{ \AA}^3$, $D_c = 1.334 \text{ g.cm}^{-3}$, $\mu(\text{Cu-K}\alpha) = 2.36 \text{ mm}^{-1}$, crystal dimensions of $0.16 \times 0.14 \times 0.09 \text{ mm}$. Data were collected at 95 (2) K on a Rigaku OD Supernova diffractometer with Atlas S2 CCD detector and microfocus sealed tube Cu-K α radiation. The structure was solved by charge flipping methods^{S3} and anisotropically refined by full matrix least squares on F squared using CRYSTALS^{S6} to final value $R = 0.028$ and $wR = 0.076$ using 12048 independent reflections ($\theta_{\max} = 74.2^\circ$), 786 parameters and 73 restraints. The hydrogen atoms were placed in calculated positions and refined with a riding constraints. The positions of disordered solvent were found in difference electron density maps and refined with restrained geometry. MCE^{S5} was used for visualization of electron density maps. The structure was deposited into Cambridge Structural Database under number CCDC 2069940.

(S3) L. Palatinus, G. Chapuis, *J. Appl. Cryst.* 2007, **40**, 786-790.

(S4) R. I. Cooper, A. L. Thompson, D. J. Watkin, *J. Appl. Cryst.* 2010, **43**, 1100-1107.

(S5) J. Rohlíček, M. Husák, *J. Appl. Cryst.* 2007, **40**, 600-601.

(S6) P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, D. J. Watkin, *J. Appl. Cryst.* 2003, **36**, 1487.

(S7) A. Altomare, G. Cascarano, G. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori, M. Camalli, *J. Appl. Cryst.* 1994, **27**, 435-436.

5. Single crystal X-ray structures

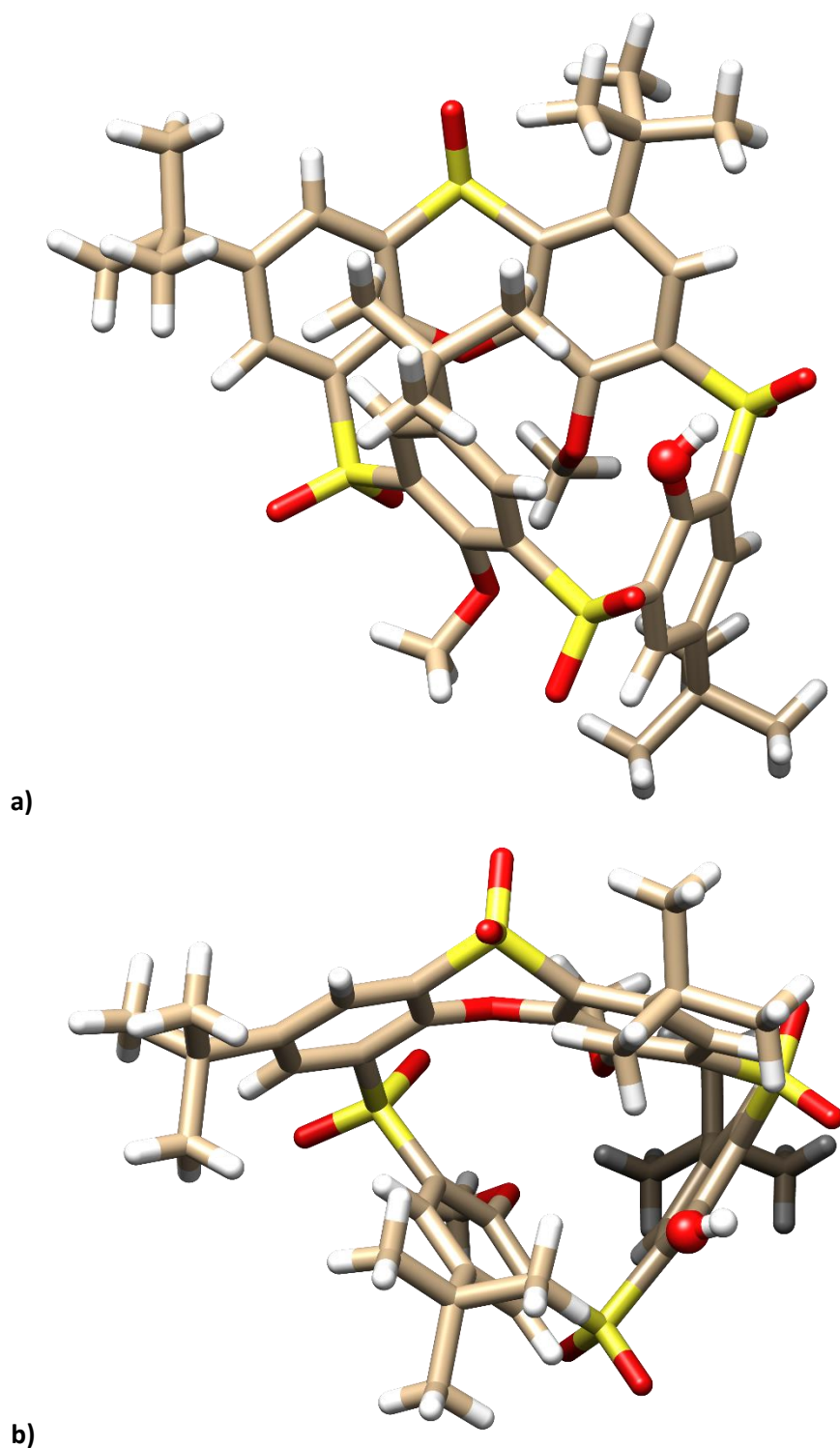


Figure S103: Single X-ray structure of compound **7**: (a) side view, (b) top view; free -OH group is shown as balls for better clarity.

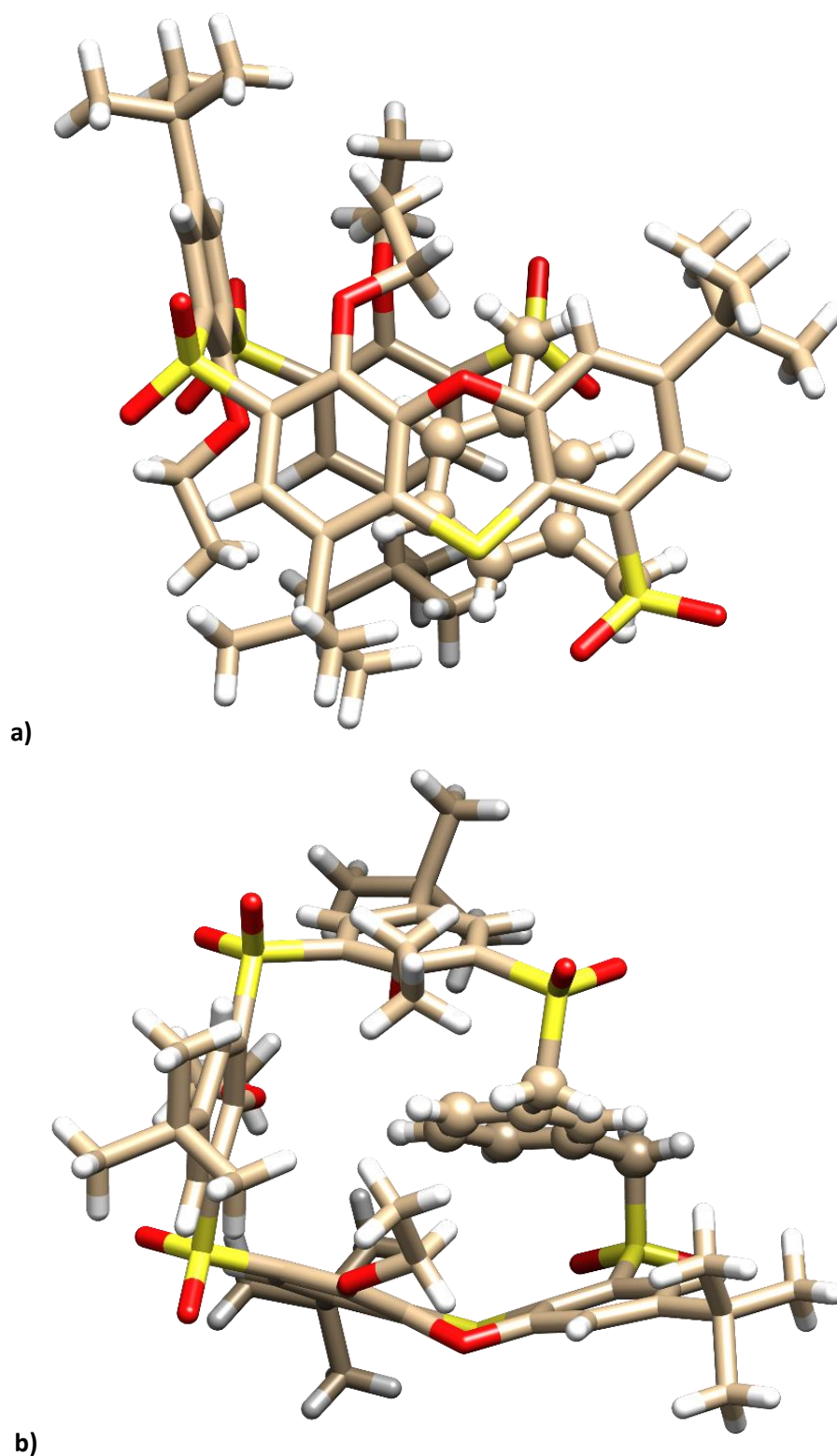


Figure S104: Single X-ray structure of compound **15**: (a) side view, (b) top view; xylene bridging moiety is shown as balls for better clarity.

6. Theoretical calculations – energies and geometries

Structure 5

120

energy: -189.968017788841 gnrm: 0.000334545330 xtb: 6.4.0 (d4b70c2)

C	1.32014916041750	-2.22370944320028	0.80742791942661
C	2.33938426019666	-2.49696799316915	-0.08766444522933
C	2.11750689485437	-2.77869589878764	-1.43071737631354
C	0.79180187438943	-2.77427642320818	-1.85044011159822
C	-0.22469000403951	-2.53030939079946	-0.95329428496328
C	-0.00972322581944	-2.25959019941386	0.39528825223890
C	4.49743519132655	1.33764364261715	0.20588245894182
C	5.16329173134867	0.36233407913409	0.94217733654657
C	4.36816761954707	-0.50264476065365	1.69592637209418
C	3.00220227630882	-0.33752729173635	1.78005559779118
C	2.35456895214904	0.71871328837050	1.14257551628132
C	3.12939336653449	1.51507944476277	0.31316490796287
C	-3.93611440861230	0.46060120763424	-0.18772403695636
C	-2.93425374008440	-0.29634210030584	-0.76111899594536
C	-3.05865040962438	-1.67941286232307	-0.68964995243623
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S	-1.90179456848066	-2.73294935730928	-1.56230400350931
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O	2.88709164569494	-2.72946132939957	2.86306976294156
O	1.00160272047971	-1.25963387931154	3.34361244173845
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H	3.34221050141695	-2.48688713209151	0.30680850106947
H	0.50274870723509	-2.97174383279764	-2.86908361268727
H	5.01630944084351	1.99448242004501	-0.47164474104137
H	4.78847921985831	-1.34041780906723	2.23074795557851
H	-4.15691037960394	-3.33472792244426	-0.03603665411842
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H	0.47349156737762	4.62700434159374	0.15862949133754
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H	-7.97938368885216	-1.73381707598666	2.51649613357959
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H	-6.46875808903413	-3.60063701331667	2.94099422842331
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H	-5.09232279566501	-2.51248702397815	3.12622162699931
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H	-0.54315326681812	6.14093000347489	1.17546357270897
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H	-3.82471457721407	6.28107956196741	-0.36685257120224
H	-4.06068236773717	4.59460121183965	-0.78402810467669
H	6.73289791569325	-1.40682940880810	-0.49048655342026
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H	6.62597626131112	-1.96288581780431	1.18310351293643
H	7.04593114241896	1.05034080508203	-1.01413501890886
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H	6.88524985430800	1.47111914750540	2.70350868631436
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H	8.24145551112669	0.37500520417947	2.43411006298989
H	3.72689937084425	-3.53418605830422	-4.40225333374581
H	2.21343134768846	-4.21966570754561	-3.82174061172127
H	2.31591972019632	-2.49927222595960	-4.22365638522485
H	3.61143049902029	-0.90925137015329	-2.66838426101400
H	5.00749319903689	-1.91992414749139	-3.05426736673609

H	4.58396306314100	-1.58418570469496	-1.37218942188072
H	4.45403089678131	-4.06928529271124	-0.82220340884502
H	3.46707564567994	-5.12995322179237	-1.82457874442991
H	4.94691290747679	-4.42387470785384	-2.47668311019085
H	-1.97832477470824	4.51229165240810	2.40539631976986
H	-3.21154377033660	5.73651357671399	2.08885094015239
H	-3.54779611127983	4.04593704397619	1.73315524941695
H	1.34857318020259	-0.48043465648662	-3.27605291390948
H	-0.41718093734390	-0.29225648613278	-3.14026665259616
H	-0.41973641880864	1.94132552284265	2.22919550872074
H	0.51194614220812	0.84064045513430	3.28164140731750
H	-0.64901933428846	-2.61228939514055	3.10109185287484
H	-2.35802644466264	-2.59797439488425	2.59125198627430
H	-1.65600532438014	-4.93343297649330	2.77416353180883
H	-1.82300760548021	-4.56279885569125	1.04589549294710
H	-0.22083578539489	-4.64582617226485	1.78595992231724
H	1.52757470833403	1.97751335040500	-3.82075566000118
H	0.60934416755132	1.06056779419372	-5.03341056807112
H	-0.24002377465305	2.07448344836173	-3.86218638670652
H	0.97900943939210	3.29200168338548	3.70435251651284
H	2.42688026854079	2.37329170572555	3.28846147516462
H	1.67339633895674	3.41631732904707	2.07926263093481

Structure SH⁻

2

energy: -4.035322688237 gnorm: 0.000655600275 xtb: 6.4.0 (d4b70c2)

S	0.0000000000000000	0.0000000000000000	-0.19234031182841
H	0.0000000000000000	0.0000000000000000	1.13934031182841

Structure A

122

energy: -194.016262300523 gnorm: 0.000555225424 xtb: 6.4.0 (d4b70c2)

C	1.40527151175736	2.15536811334727	1.15107983449600
C	2.40380826363471	2.68290247963182	0.33963510143128
C	2.18467904560392	3.23355104311907	-0.91148842126800
C	0.86877174247125	3.20375617269880	-1.35971561383815
C	-0.13570261350629	2.71286653477495	-0.56155151659616
C	0.07276833512966	2.20497427163384	0.72839867801322
C	4.56362382526229	-1.46569413995749	-0.11016111821287
C	5.28805701431652	-0.46397521915775	0.53376859531757
C	4.56746236510045	0.37238484696293	1.37957913328342
C	3.22708046486945	0.14932282648993	1.62829861128397
C	2.53365419173018	-0.92219362701715	1.07414975672051
C	3.22617323820355	-1.69418745284355	0.14393314945716
C	-3.71296046364830	-0.26536762368842	0.24919414323653
C	-2.79085493273287	0.42084708378293	-0.56843649748885
C	-3.00205881818058	1.82476676842222	-0.59074157338249
C	-4.16489191410632	2.38988560283131	-0.13252319135914
C	-5.17433714440968	1.64114801717593	0.47710081409076
C	-4.89435945170827	0.28989023327302	0.67770771276215
C	-6.45581242927622	2.31658399896475	0.93490108640876
C	3.33873796379223	3.81576085585841	-1.70847555455499
C	6.78247639002905	-0.33116757323289	0.29444847419481

S	2.50003187541881	-2.99375002702349	-0.88016581691850
S	-1.77749828802695	2.89214175527379	-1.29759553001122
S	2.27298570976600	1.37381267688749	2.54692283806988
O	3.20840589601028	2.36209204684865	3.04517613215564
O	1.48535812649048	0.74900789812193	3.57749594563855
O	2.73613256019247	-4.25967103733265	-0.21591513453219
O	3.10121581710212	-2.87352696624139	-2.18875374487201
O	-1.60369253645124	2.58553626098221	-2.70653054483879
O	-2.17266295311997	4.26340279031108	-1.02996966881010
O	-1.47819001879916	0.01528611674723	-0.66613868763058
C	-0.09690372292292	-3.85680556344208	-0.76770055511740
C	0.72659019672689	-2.76742905139978	-0.96060604399667
C	0.22700855426334	-1.48867760371237	-1.06700547800924
C	-1.12994586334161	-1.29360566138158	-0.72813257060810
C	-1.94482932126210	-2.39181060736379	-0.44292887088267
C	-1.46304901989579	-3.70853887139830	-0.57176489126708
C	-2.34212413511469	-4.94991608768394	-0.50542327832411
S	-3.31539096767312	-1.92750875846705	0.64500262291123
O	-2.65444768700405	-1.95496731777206	1.94128592050279
O	-4.52663824073390	-2.71216690688357	0.58416546747591
C	-6.11780779386740	3.37123801786410	1.99882780497829
C	-7.11923586287132	2.99452832553485	-0.27267568175171
C	-7.44875389374539	1.31824254449808	1.53637277645924
C	-1.60413189609873	-6.19231481224122	-1.03009089297248
C	-2.75582226922701	-5.23537278525174	0.94387805511365
C	7.45955347204809	-1.60149754277259	0.83168117155567
C	7.05925782358733	-0.19399915567185	-1.20911817922466
C	7.37858311200944	0.88330619097317	1.01136269645662
C	3.89624650485864	5.02696484359413	-0.94635904099402
C	4.43174735745783	2.74836936347639	-1.86122043733033
C	2.90020149930123	4.27221716193937	-3.10232049824474
C	-3.56446665767612	-4.74035136327321	-1.40969279073439
O	1.08186017503348	-0.46044314282686	-1.36053012544052
C	0.86491130652885	0.16030600954473	-2.63733127403118
O	1.23226117063054	-1.10579815358865	1.43345309709941
C	0.93145136897113	-2.34258954919192	2.09874607884645
O	-1.05520301374085	1.88888714352767	1.38083173544163
C	-1.06492338495749	1.50640546719396	2.75257416611299
C	-2.49559232312314	1.63358043882414	3.24899603928344
C	0.96658660786704	-0.83349388634878	-3.78645364300566
C	1.56982083065281	-2.41689026068573	3.48020716709395
S	-3.36168969431708	-0.36521216850266	-2.75158325422835
H	3.39918867229770	2.66667976967098	0.74954926977345
H	0.57415596973864	3.56160127033202	-2.33208862901917
H	5.02121885115352	-2.10349858265324	-0.84941026889774
H	5.01915269198119	1.21129975917096	1.88360445793173
H	-4.24011580019521	3.46093780834614	-0.23825244242960
H	-5.55913587946658	-0.36433376106026	1.21749423484159
H	0.38064759744578	-4.82030618507412	-0.73477291319251
H	-5.44017552654330	4.12089884838628	1.60045488230464
H	-7.02598902561814	3.86758294548199	2.33331561555095
H	-5.64182825751949	2.89768277053859	2.85426335690361

H	-6.46592125692332	3.74677731016393	-0.70557071274146
H	-8.04805682235014	3.47382884837976	0.02908838065713
H	-7.33981729778013	2.25616162563755	-1.04026958896723
H	-7.69393954213959	0.53943617523512	0.81878480512033
H	-7.04159912408697	0.85703154158953	2.43242335473742
H	-8.36568426589321	1.83740660981153	1.80675373793175
H	-0.80630870688026	-6.50052864570358	-0.35991358266407
H	-2.31402077587544	-7.01302164002965	-1.09918967942005
H	-1.19381224121112	-6.01180247505215	-2.02030366600540
H	-3.33512723151015	-4.41874456209079	1.35710429183748
H	-1.87121656787887	-5.37653588665906	1.56131089166392
H	-3.35988034885512	-6.13868242636918	0.97860162567716
H	7.07719489775595	-2.48713279232861	0.33233309729807
H	8.53281679154574	-1.54634902235235	0.66786465125845
H	7.27541228044757	-1.70397093147874	1.89850927930127
H	8.12615312264671	-0.06687355276639	-1.37456365363755
H	6.53918748755860	0.67129126651084	-1.61057437113141
H	6.73196988913266	-1.07275701555943	-1.75579288675389
H	8.44661944944380	0.92851548173862	0.81284220624784
H	6.92928366647299	1.80554511623537	0.65330228090511
H	7.23764719702300	0.81229137739988	2.08636198364787
H	3.13043633185761	5.79326577991398	-0.85395513981274
H	4.21733218369898	4.74575281116305	0.05234160236804
H	4.74462209015514	5.44529665043709	-1.48252081446004
H	4.02192715284095	1.85085159039011	-2.31977658847570
H	4.84767902133664	2.47441458391387	-0.89640832956190
H	5.23237070842910	3.12817258264527	-2.49151346832630
H	2.49700945022383	3.44066120131471	-3.67488434531879
H	2.14477183873042	5.05077756219575	-3.03705709942572
H	3.75679337617514	4.67381442396688	-3.63873585081949
H	-3.24370189091833	-4.50202175215548	-2.42192634722688
H	-4.16372973377464	-5.64715140090757	-1.43703920604386
H	-4.18809965282590	-3.93113883595037	-1.04996061228207
H	-0.10140958378939	0.67563209978855	-2.65334480181399
H	1.66155312863756	0.90511893235319	-2.68822770050587
H	-0.16016526438922	-2.34521122525072	2.16755563425091
H	1.25913396539731	-3.18946413113283	1.48497733485132
H	-0.71567743752994	0.47384032867895	2.84948785058881
H	-0.39236457639317	2.15945913812413	3.32030642540742
H	-3.13247322184007	0.93334722472903	2.71431197502617
H	-2.52698184416962	1.40696306928084	4.31007657729330
H	-2.86120490151332	2.64250299925252	3.07548343458073
H	0.09008755121110	-1.47885879921881	-3.80439993319825
H	1.01556015116079	-0.29064132335822	-4.72561617250784
H	1.85580414414336	-1.45073624127190	-3.66942779302179
H	2.64806520147732	-2.53772914407975	3.39361855279870
H	1.36064486796358	-1.50220359919110	4.02945783861511
H	1.15726960785348	-3.26555897534700	4.01682817424214
H	-2.79017640314485	0.71185495071054	-3.26694482866401

Structure B

energy: -194.038057866849 gnrm: 0.000369995383 xtb: 6.4.0 (d4b70c2)

C	1.21239596794500	2.59794356332519	0.62374044922427
C	1.12421422977557	2.62485198752790	-0.75473066679687
C	-0.09989816538962	2.72719348758909	-1.40271728634629
C	-1.22851328674539	2.74360123865989	-0.58969571863658
C	-1.14420377431286	2.67539002928345	0.78570820382577
C	0.08695913055809	2.63119988449482	1.44041898589895
C	4.76607236716678	-0.99592921217934	-0.76764188303200
C	5.35242284534341	0.24379750401967	-1.01225624761797
C	4.75540631720483	1.34076939924666	-0.40180199646619
C	3.65755057808567	1.17529506725106	0.41642776376942
C	3.07385468353025	-0.06323748500551	0.67341143008503
C	3.66068830359933	-1.16047902758154	0.04362687046304
C	-3.54160700530535	-0.89571657704660	-0.35702565481679
C	-3.06256202204525	-0.03286734263120	0.62172649522743
C	-3.52157312128507	1.28000629646982	0.57714874362926
C	-4.46844001959071	1.68332681904102	-0.34572445593114
C	-4.98428542128824	0.80611463526207	-1.29570727819184
C	-4.47833176994214	-0.49047960215286	-1.28610613633615
C	-6.06224836402257	1.27819589027550	-2.25767877335451
C	-0.25375659818602	2.84434636248664	-2.90701045464079
C	6.56448683659448	0.34443688189113	-1.92317342477818
S	3.04041611619217	-2.85604940637029	0.13568317908797
S	-2.75934836662116	2.55716069985093	1.57626035503030
S	2.91154737649258	2.60019857153309	1.21207687539015
O	3.51830692286009	3.78300824135964	0.63118810506460
O	3.05215363805142	2.49455858515592	2.64036693572261
O	3.53862697641720	-3.54190775144322	-1.03981516833798
O	3.49894444113418	-3.42772807147885	1.39027940348738
O	-3.44941232246895	3.80932273949647	1.35960105161160
O	-2.67230109049282	2.13717063168317	2.96116635084625
O	-1.46618655601533	-1.23975790574085	-1.56092650457206
C	0.57938347313431	-3.74668273600958	0.92785730581792
C	1.25649600242963	-2.86300248087266	0.10519981261350
C	0.63585563608904	-2.03230823410431	-0.78730255710443
C	-0.79612235571923	-2.02270905751606	-0.82074390313818
C	-1.45510701018807	-2.94953023831301	0.03181047202482
C	-0.80717050740820	-3.84945711039105	0.87936947924659
C	-1.50521343854399	-4.92593429793462	1.70199712092248
S	-3.20341084163681	-2.66537621849683	-0.27760201556787
O	-4.08306456854118	-3.06810682025710	0.81132051743957
O	-3.55736250751341	-3.26852627138836	-1.54677602734313
C	-6.45104422680866	0.19416329835032	-3.26601274188835
C	-7.30499150203115	1.65801690630740	-1.43844383010097
C	-5.55815202893950	2.50330349875504	-3.03362896593516
C	-2.45647634064871	-5.71904933290854	0.79632514613698
C	-0.51110692014495	-5.93399945980185	2.29902231342513
C	7.08765929950400	1.77932828650163	-2.03284165839339
C	7.68536444786842	-0.54225565533361	-1.36207691714919
C	6.16809886935360	-0.14444369826097	-3.32382007173153
C	1.05881882534669	2.54882102217855	-3.63582731568971
C	-1.32957147053662	1.85593269951230	-3.38281220458701

C	-0.68905890451349	4.28210016443919	-3.23181235746338
C	-2.26042242711805	-4.27587940991710	2.86825620575833
O	1.42251910619685	-1.22177544563120	-1.58182659375067
C	1.20276937035009	-1.35003060178168	-2.98828650361823
O	1.94506854352189	-0.05098154225254	1.41694104495015
C	1.78560470006944	-0.96345761763141	2.51221709172247
O	0.20483837969705	2.59637590778834	2.79085979794678
C	-0.19277786180859	3.78345600962818	3.48525807749858
C	0.78287538913841	4.92900598546423	3.24884296271406
C	1.43251416489037	-2.76982274993919	-3.49124223712313
C	2.08221573669343	-0.25548426202639	3.82744399811788
S	-1.92132517643180	-0.62083626330845	1.82000258136409
H	2.05279892644155	2.59460644643387	-1.29961904002917
H	-2.21350643712136	2.80410493772686	-1.02216832217386
H	5.14096655965050	-1.89428774240661	-1.23249291521423
H	5.11216509953709	2.34931579704257	-0.53140117075636
H	-4.78445151196035	2.71338593878079	-0.28792909161686
H	-4.78932258486650	-1.24093400391485	-1.99328303381815
H	1.18290394160717	-4.35274014807680	1.57787172846751
H	-6.86509310251301	-0.67548018848016	-2.76232406064701
H	-7.20407835715521	0.58549950667473	-3.94645804975491
H	-5.58908534596220	-0.11772961453932	-3.85023183797255
H	-7.65209458512185	0.79960784271215	-0.86796574787284
H	-8.10280300775622	1.98078162645003	-2.10299224501260
H	-7.08396583594958	2.46297300171785	-0.74330282460282
H	-5.31610095125776	3.32400521792955	-2.36472456423227
H	-4.66870852217574	2.24183448212489	-3.60193478797937
H	-6.32433077865977	2.84135739705028	-3.72697452840395
H	-3.20956707530336	-5.07790205841619	0.35365751083932
H	-1.89543055231423	-6.19322690821682	-0.00725169906329
H	-2.96184321347026	-6.48986063582052	1.37413233516099
H	-1.07227886324749	-6.73237697034843	2.77992907895565
H	0.12130804613343	-5.46949987655248	3.05083656901838
H	0.11493494528038	-6.37428593387288	1.52684137895771
H	6.33869210985296	2.43608888186954	-2.46646604229371
H	7.37381668457978	2.16323072370249	-1.05734044261756
H	7.96461630611704	1.79395211948652	-2.67574496780836
H	8.56324766887738	-0.47694607153524	-2.00030680624864
H	7.37522686355469	-1.58155654534313	-1.30931837987948
H	7.95727737693905	-0.21533147512512	-0.36130669727677
H	7.02161674207676	-0.08146503244988	-3.99430657635568
H	5.82467038629561	-1.17424119151130	-3.29580766654062
H	5.36600525373259	0.47133567751008	-3.72300533865786
H	1.42582770061403	1.56322353512627	-3.36309202485843
H	0.89156977013134	2.56978172982505	-4.71002915943090
H	1.81364664995791	3.29305813952435	-3.39570392275044
H	-2.32543672967363	2.20078286581586	-3.11931795114501
H	-1.19032016284595	0.87811987832553	-2.92597447379690
H	-1.28457083894756	1.74526464392719	-4.46331324206437
H	0.08059758036741	4.98614654025536	-2.92453367829546
H	-0.85157863613868	4.38438341875089	-4.30170147898889
H	-1.60994772985553	4.53332010612148	-2.71288154777434

H	-1.58225818838346	-3.65643418328658	3.45148298440067
H	-3.06850482187046	-3.65514549245678	2.49852551863139
H	-2.67904536010959	-5.04538454986140	3.51284415542762
H	0.18813620200257	-1.01695247270370	-3.23416851447099
H	1.93577129805952	-0.66509593905494	-3.42249113891412
H	0.73848448020530	-1.27982023848966	2.47619648574310
H	2.43007743906181	-1.83590242662336	2.38768386621830
H	-1.21103588606625	4.06776597822369	3.19354449190187
H	-0.19496400169995	3.48163469889321	4.53382378516829
H	0.53949965710954	5.75548571185790	3.90973997901234
H	1.79647692141413	4.58753725370819	3.44552386453269
H	0.73089148103671	5.26962824235758	2.21628870133591
H	1.48043952514894	-2.76882201208773	-4.57632056992251
H	2.36096877737270	-3.16093644170919	-3.07948197533195
H	0.61600682614319	-3.41568223695748	-3.17260912628620
H	3.12816918568663	0.03652149243345	3.87558556453468
H	1.47745487203714	0.64446446308645	3.89949136132569
H	1.85162558153849	-0.92288917861510	4.65233248369247
H	-2.08711952162532	0.41400037109154	2.66146680221264

Structure C

122

energy: -194.037082548473 gnorn: 0.000702278279 xtb: 6.4.0 (d4b70c2)

C	-1.47028928619378	-2.67713687384335	-1.09095712270807
C	-1.13021419458146	-2.27113656249161	-2.36087557018919
C	0.20513770046480	-2.13949171145564	-2.74084687732100
C	1.15757249527741	-2.37578610699083	-1.75854938265498
C	0.80903996885470	-2.71271691445507	-0.46038904988169
C	-0.51840419766086	-2.92981590799185	-0.10579657057356
C	-3.41674524392317	0.59248668478580	2.40730967639367
C	-3.55911206411113	-0.71920536322218	2.85155395471122
C	-3.49445954895596	-1.71015894992491	1.88061222318958
C	-3.35505799014451	-1.38165705060325	0.54925068917090
C	-3.24380722394181	-0.06675712157707	0.09436392232807
C	-3.25862081760566	0.92904800191863	1.07569629327333
C	3.60388304068479	0.90569692743897	-0.23757601885737
C	2.67910226449460	-0.10810200478867	0.05776876898066
C	3.26242334019431	-1.37523038783840	0.24707164548859
C	4.61238101187570	-1.60865824534243	0.18930958495450
C	5.51701751833812	-0.57623420924897	-0.06934921180737
C	4.96397672870001	0.68039331803328	-0.29583399989754
C	7.00952953119093	-0.86000028900011	-0.09108434848270
C	0.55021973941163	-1.71024497432290	-4.15625737981798
C	-3.77631058452666	-1.00494226895339	4.32767152334672
S	-2.96866514108118	2.70514020595133	0.81286617515102
S	2.17953081136307	-2.71799872989561	0.71174848795190
S	-3.19604565154165	-2.73668232855647	-0.62312277555654
O	-4.00044644904909	-2.52496970950267	-1.80594671273140
O	-3.50601312141950	-3.96774403838324	0.07102380310437
O	-3.90257935905772	3.26485985943062	-0.13920478350824
O	-3.04981475455759	3.31910991188645	2.12332441743911
O	2.90179727854009	-3.96529218141686	0.50873081937003

O	1.74061891972542	-2.50417207888783	2.07231741969189
O	0.75942225654473	2.74615093646613	-2.66967692577615
C	-0.32952229023739	3.10763870472455	1.25933964251527
C	-1.26889081418352	2.89579409075121	0.26852083704701
C	-0.91043239956273	2.85436848328936	-1.06097503337482
C	0.47391467444634	2.86550120442830	-1.36396445470071
C	1.42252053833858	2.98356162803774	-0.33986585937946
C	1.02850989438984	3.20589884623321	0.99741748537836
C	1.96550411200168	3.60493399954004	2.13603004668576
S	3.13218649604844	2.54096346449850	-0.81288156733172
O	4.10409997828515	3.50993240025806	-0.35239992718351
O	3.18574333369478	2.41171314808923	-2.27363268776386
C	7.42582654140962	-1.41427657961263	1.27965929187237
C	7.30575005004313	-1.89883277326735	-1.18253195240321
C	7.83509519697214	0.39724817779523	-0.37747084283136
C	1.21858243472934	3.77093390294498	3.46870460974066
C	3.06411253620025	2.56036382466422	2.37523225101171
C	-5.10747887150444	-0.36928452144938	4.75579247151147
C	-3.82948589270918	-2.50712117022064	4.61694444760034
C	-2.62503933919988	-0.39319749075879	5.13839891940359
C	-0.15569415119422	-0.37901624239533	-4.45015130588379
C	2.05554122199868	-1.51102735060583	-4.35268865359638
C	0.05987133736586	-2.78957026421807	-5.13287653891481
C	2.57350334557070	4.97396676742400	1.78988210247737
O	-1.85794596713497	2.69429861600947	-2.01945759151151
C	-1.93751110849122	3.68328983861508	-3.05206299594467
O	-3.08551346415034	0.12035324234496	-1.23779519097861
C	-4.12196711489999	0.83030804383087	-1.94086824580900
O	-0.94833349354679	-3.30365904833433	1.12671417530337
C	-0.44581700441652	-4.54558611651972	1.63318149887457
C	-0.91307564558612	-5.73031713714587	0.79670013766426
C	-2.30871218365507	5.05312180016737	-2.49715214892160
C	-5.49935556134458	0.20921927571569	-1.75155067726954
S	1.00011051464349	0.08821882658766	0.21047042430878
H	-1.94399771287590	-2.06402591620273	-3.03646739461071
H	2.21059758967933	-2.24260593547034	-1.95105449402116
H	-3.41994392263691	1.41624956260337	3.10358387509676
H	-3.55539010587802	-2.76027980526148	2.11020211466479
H	4.93375740809571	-2.62582282619868	0.35421941276597
H	5.57707553324525	1.53658573928551	-0.52679929265511
H	-0.72081978300263	3.19202522190417	2.25611603639036
H	6.89568579473638	-2.33503513178854	1.50661188608209
H	8.49418476985337	-1.61773706312698	1.29217570482236
H	7.19839458466623	-0.69131568497908	2.05995623471892
H	6.99296963507532	-1.52020789146322	-2.15313951193675
H	6.77536066906074	-2.82753765434294	-0.99156273281008
H	8.37200284977361	-2.11070792639661	-1.21730874715560
H	8.89296794591789	0.14377398195991	-0.37293475837066
H	7.58781434807006	0.81109353592563	-1.35185152222417
H	7.66254456750897	1.15595319287237	0.38180046153137
H	1.92957564576651	4.09420786423940	4.22614044507819
H	0.43823643847320	4.52389339864169	3.40089422087056

H	0.78775136712547	2.82746514755074	3.79278620813221
H	3.84258377424598	2.62420449404983	1.62603064298407
H	2.64144135549130	1.55742862153297	2.36250695542234
H	3.52217818913432	2.72485284514629	3.34797671527782
H	-5.27896234003094	-0.54809486001857	5.81426702446320
H	-5.09972551777932	0.70286851292291	4.58157692533625
H	-5.92864271961709	-0.80360747748745	4.19075558538048
H	-2.89861835244124	-2.98516472687970	4.32265875502351
H	-4.65302467104317	-2.97837760201899	4.08713884300586
H	-3.97439195021395	-2.66615804097102	5.68310255395058
H	-2.61201001739045	0.68898639140052	5.05004930023865
H	-2.73461315225705	-0.65065791343200	6.18917567011620
H	-1.67165521538465	-0.77783107711205	4.78400504487870
H	-1.23530917086639	-0.48797107852747	-4.41557971307379
H	0.12832507027396	0.37019128041433	-3.71420092056131
H	0.12511406489361	-0.01891700591403	-5.43711714937066
H	2.24785593599835	-1.19408011999255	-5.37521092807404
H	2.60164547534272	-2.43433629057082	-4.17395825365727
H	2.43104145834877	-0.73882852052681	-3.68431694317801
H	-1.01188461831588	-2.93867600499384	-5.03873865834238
H	0.28152821649850	-2.49192635516433	-6.15484540576861
H	0.55734040996116	-3.73506713031501	-4.92860076931412
H	3.17987104408444	4.91342294837564	0.89330764641810
H	1.78095182900563	5.70292602317615	1.63375306054329
H	3.20304268354744	5.31109499394715	2.60961226424490
H	-0.99864535784153	3.72681816991969	-3.61147053894716
H	-2.73038556004394	3.30472400084339	-3.70011157203893
H	-4.13094387222081	1.87778289957383	-1.63437377224991
H	-3.80124962673651	0.75639451864566	-2.98080243459944
H	0.64629357551863	-4.52210356466516	1.69812889238421
H	-0.85935495050543	-4.59375888437700	2.64237872271880
H	-0.40519201321529	-5.73501531486253	-0.16607046503276
H	-0.68644767609645	-6.65405915967290	1.32059876241904
H	-1.98472634602947	-5.65241272567876	0.62673132608769
H	-1.48737272682118	5.46188596871344	-1.91148187352259
H	-2.53363451182305	5.73020307833806	-3.31596189009275
H	-3.17889382621876	4.95669221574287	-1.85143858629041
H	-6.19942455111220	0.69412181622602	-2.42549097044323
H	-5.45976569700662	-0.85556522637263	-1.96762769197983
H	-5.84073055664686	0.35185419779926	-0.72763066846849
H	1.74114207479870	2.63704318283353	-2.78374385955090

Structure D

122

energy: -193.993476090727 xtb: 6.4.0 (d4b70c2)

C	1.38096907875965	-2.32238050926644	-1.29164390362628
C	1.11731642885096	-2.72736785469786	-0.00208101958040
C	-0.18535019820215	-2.94065149219900	0.42529462952353
C	-1.17869839495466	-2.69072685357284	-0.51241925113726
C	-0.93096142628005	-2.21613901210028	-1.78976734266790
C	0.38644306891805	-2.03405716284355	-2.23173615779546
C	4.81282573553335	0.64555880887821	1.31372890439767

C	5.29711329474354	-0.65865051569789	1.35595833660471
C	4.76570808148699	-1.54685511475675	0.42838036614064
C	3.83660672829155	-1.12633296856443	-0.49930781582667
C	3.35899337885923	0.17856711776451	-0.55354242813806
C	3.87498688950324	1.06430918696198	0.39285944991274
C	-3.78184155936720	0.70102024207487	0.09616990791970
C	-3.06238619550520	0.10025601648123	-0.93285141344300
C	-3.50890934344624	-1.14617576170857	-1.36051132627400
C	-4.62931666969428	-1.74243451663726	-0.82812329434400
C	-5.35157563882164	-1.13145168858990	0.19616604288567
C	-4.87743432531023	0.09255615188109	0.66214552953279
C	-6.58548281734665	-1.80796900831651	0.76080957726493
C	-0.53779989769639	-3.47129363932510	1.80154784084998
C	6.32261432372461	-1.04639829721852	2.40677627539212
S	3.24352033022253	2.73366006069343	0.64410222237385
S	-2.54178752619582	-1.98622717384519	-2.60796668873272
S	3.14079402670840	-2.31486380912713	-1.65535843181192
O	3.48205313888239	-1.95965575931083	-3.00932518422377
O	3.62187306662130	-3.62195181661530	-1.24507087119232
O	3.57756604002961	3.11457959613321	2.00272860237902
O	3.78225718034674	3.61745785418470	-0.37414234109282
O	-2.52642957631660	-1.19676057825770	-3.81823186694761
O	-3.09243742612719	-3.31751741856099	-2.77506590078343
O	-1.12371427123960	0.38337774117287	1.53972938325847
C	0.80604076538473	3.49990963095368	-0.35579536962221
C	1.49586352734752	2.61827014668689	0.44275188796469
C	0.84713580454351	1.59360258850676	1.11647964348308
C	-0.51349436501817	1.42616043564500	0.89153224372886
C	-1.18968310300210	2.25926489823178	-0.02984703196362
C	-0.54994804513829	3.37490835914479	-0.60501597149155
C	-1.17261187248913	4.43566453313329	-1.51068168907182
S	-3.24942159649945	2.27383887952159	0.85440879317892
O	-4.43374826663229	3.14604221698627	0.78049152322085
O	-2.99509763494616	1.87389858084645	2.26711549594494
C	-7.25184415938267	-0.97659043993381	1.86121083436970
C	-7.59247101383214	-2.01050290043828	-0.38052925345888
C	-6.17468642436752	-3.16326894277163	1.35791939879035
C	-1.22421857375891	5.77634817209593	-0.76541717729529
C	-0.32402626925413	4.68174979089748	-2.76603458494461
C	6.78580071003050	-2.49726623970688	2.25280018849415
C	7.54551336009207	-0.12662313330329	2.27742339780259
C	5.68153415813989	-0.87355605502881	3.79167870874464
C	-0.97019132542421	-4.93811696488902	1.65530291579134
C	0.65860919537502	-3.39493421664470	2.75349007837726
C	-1.69185538426504	-2.64530777840891	2.38936020144156
C	-2.57518397624881	4.02548198191603	-1.95107242005658
O	1.60861079355148	0.74767505550099	1.88003789264494
C	1.21769970135418	0.55777729890530	3.24224228374460
O	2.36277113083420	0.42228196247992	-1.44153915533387
C	2.51525148229946	1.47967160171521	-2.39556141553173
O	0.82794693622577	-1.57435775654300	-3.41373443152196
C	0.23373946538244	-1.98067712335638	-4.64744625117446

C	0.33109458683256	-3.48830028743425	-4.83975277558193
C	1.18789931856461	1.87556326098511	4.00415136066817
C	3.57132323343370	1.14688484180514	-3.44140153752494
S	-1.70995603795323	0.84794678694952	-1.66987023040475
H	1.96793331923226	-2.90773129544980	0.63269265378343
H	-2.21196488856739	-2.86108784458062	-0.25601370585960
H	5.12754427002147	1.38723282393997	2.03071339609058
H	5.04558327847656	-2.58670346945411	0.38842414071873
H	-4.90522522693768	-2.70258647122468	-1.23762901266670
H	-5.34765753898759	0.61856246292099	1.47729906182260
H	-1.91858090136401	0.76840900940695	2.00327820935719
H	1.37792774124590	4.29129099409502	-0.80926727435765
H	-6.57907486713131	-0.83471871417285	2.70392436105157
H	-7.55459956860857	-0.00276753951257	1.48342543188439
H	-8.13804524731555	-1.49515983237599	2.22040798311920
H	-7.86096874017329	-1.04955765421881	-0.81565453918920
H	-8.49149288816034	-2.48968545679759	0.00041894565949
H	-7.17359490194935	-2.63097391516652	-1.16779723402008
H	-7.04429165321238	-3.66674377609317	1.77317068541285
H	-5.73139137793560	-3.80659005487854	0.60303564575182
H	-5.44470825983560	-3.01828848207891	2.15318489902130
H	-1.71235897374757	6.51442749329070	-1.39871046435544
H	-1.77807839017645	5.68975832507383	0.16380888806075
H	-0.22589856662055	6.13144756601310	-0.52697262608376
H	-0.83407287949583	5.41143270444333	-3.39126698791011
H	-0.18956815006568	3.76379904902267	-3.32870833231974
H	0.65693668248921	5.07859521579967	-2.52731630894742
H	7.22887649287478	-2.65963710437161	1.27378116727708
H	7.53555860457789	-2.71816633062569	3.00889452909553
H	5.95663011928178	-3.18744497300603	2.38318839913581
H	8.29505307279687	-0.40133937760734	3.01564390221114
H	7.27585596705342	0.91362568657949	2.43297559220522
H	7.98223764089905	-0.22204407146315	1.28622393639703
H	6.39533129689476	-1.13607378238869	4.56854956927101
H	5.36026412425740	0.15226685402820	3.94693225946834
H	4.81157536639538	-1.52009592320532	3.88351333550636
H	-1.81495551149348	-5.02342890889576	0.97685777770021
H	-0.15088355289346	-5.53349801919891	1.25811573989998
H	-1.26080371547577	-5.33580301237596	2.62495097801811
H	1.45300463022737	-4.06350239050381	2.43272117004570
H	0.34876157422406	-3.69010850383597	3.75327752341715
H	1.04087352530673	-2.37859543164066	2.79486975112150
H	-1.84211120704003	-2.90480826556949	3.43463601752140
H	-1.45968012757144	-1.58854378116195	2.31689786106053
H	-2.62256836451484	-2.82449101825280	1.85841491865660
H	-2.52596924448790	3.05642661861172	-2.44010035632885
H	-3.23833270189513	3.97889353490952	-1.08928133961785
H	-2.97553196539885	4.74006353617107	-2.66665937532909
H	0.25025457550452	0.04926613012956	3.29332792316312
H	1.99814217565027	-0.09961431316348	3.63401583162003
H	1.52229438182649	1.55041049080514	-2.84524992979130
H	2.75861137089006	2.42086634103701	-1.89738693583563

H	-0.79994596502694	-1.63656901583039	-4.71195219411256
H	0.83135242286045	-1.45119779113384	-5.39297179649344
H	-0.30675875435154	-4.00033897909936	-4.12051356918778
H	0.00431138196066	-3.74778743881486	-5.84218481164245
H	1.35867545514743	-3.81510819997163	-4.69502053457983
H	2.08682371719122	2.44408944905469	3.76675347764457
H	0.31666008183769	2.45844049143223	3.70927683066531
H	1.14493505793420	1.68487361407310	5.07196119098814
H	3.49334803127106	1.84735109562499	-4.26719076046708
H	4.56628835388465	1.21988818338934	-3.00579276731995
H	3.42057153147427	0.13220112542151	-3.80214758443282

Structure E

122

energy: -194.053980695099 gnrm: 0.000417325677 xtb: 6.4.0 (d4b70c2)

C	1.20107317230441	-2.38519977273646	-0.86261878836488
C	0.85642432737478	-2.83264991725883	0.39725267517901
C	-0.42770220964555	-2.66644520077393	0.90021454376474
C	-1.31733848812571	-1.94814823443358	0.10523118929107
C	-0.96810424697981	-1.47556404185653	-1.14339213148760
C	0.29344408901522	-1.72340533443389	-1.68694901723203
C	4.90656028553794	0.62593840973503	1.15239499055534
C	5.38843367517420	-0.67127033253595	1.29621874780754
C	4.76199838264238	-1.65712128385253	0.53506120358125
C	3.78175195188253	-1.33613217763931	-0.37747020110538
C	3.35645083966139	-0.02659663920520	-0.58043243974389
C	3.91220568305141	0.94275537223445	0.24579444745365
C	-4.53204421356087	0.90682349757966	0.96875974632069
C	-3.58900736652286	1.00465037709554	-0.05612375339841
C	-3.45993070117681	-0.10395846966732	-0.88324033045718
C	-4.30710789855671	-1.19190044174279	-0.73840011410706
C	-5.31542055399924	-1.24230118879085	0.21869779687347
C	-5.36341546854472	-0.17810642119622	1.11807894997549
C	-6.26994776363188	-2.42350966368119	0.25770641380527
C	-0.86704537760622	-3.28474285692400	2.21722684693475
C	6.51666375306879	-1.04365328682147	2.24456358194119
S	3.24007747992928	2.61467315348013	0.31665259663913
S	-2.12258678613850	-0.40687584749896	-2.03548770987810
S	2.93058265514109	-2.63460269348610	-1.27862025297642
O	3.21648414549537	-2.54658388698054	-2.68912842183488
O	3.32588371240715	-3.89174014099052	-0.67075048946833
O	3.47979036386335	3.08862064791471	1.66582105722560
O	3.88315390309835	3.41584076586446	-0.71140501672668
O	-1.42853162677287	0.79206390371560	-2.42840414981630
O	-2.70733930172575	-1.17058542013516	-3.12511828827523
O	-1.42454776189072	0.75970879216205	1.11676385225754
C	0.92969380253333	3.50324864309558	-0.83364547050393
C	1.48618911233779	2.56492035797384	0.01006695416864
C	0.74280446457505	1.61985643437219	0.68029109840625
C	-0.66308560321393	1.61267318467264	0.51744050889533
C	-1.20106613007718	2.61435799192220	-0.33359457847956
C	-0.44636410648314	3.56179312785132	-1.02470808725781

C	-1.05503546592158	4.64143169963810	-1.91761437898282
S	-4.43695144670076	2.19509255542056	2.28295638077299
O	-5.51121283821660	1.85480317736452	3.20736068724727
O	-3.06887998660925	1.59381411641830	2.94410053938113
C	-7.31982650982095	-2.27862590173960	1.36269333031490
C	-6.99227616957697	-2.50866632240626	-1.09496737612339
C	-5.47539126430629	-3.71392814282557	0.50328498018054
C	0.02582525006588	5.45827533073853	-2.63861574237640
C	-1.95142868667616	4.01024493231769	-2.99722719293002
C	7.63457274073320	-1.71642519440460	1.43382020017690
C	7.10188463639170	0.17830650105334	2.95799419432360
C	5.98138096922432	-2.01978232565849	3.30181547317600
C	-1.34264942604451	-4.71370628240449	1.90767852683887
C	0.29267061879614	-3.34757120921484	3.21771525588119
C	-2.01857688874327	-2.49141960655288	2.84763951780876
C	-1.86575800102864	5.61609303855011	-1.05031015255530
O	1.43198897479553	0.70419375729974	1.45559567027098
C	0.99527911011508	0.55276814733522	2.80494743918890
O	2.37006303444648	0.18929660327515	-1.48567514479229
C	2.62563263203707	1.09864060518126	-2.56326472690622
O	0.66894094608785	-1.31556473448960	-2.92444722832242
C	0.10295425188225	-2.00444006077642	-4.04921309692751
C	0.45033152728345	-3.48815945329693	-4.06151999749964
C	1.04750840056702	1.85480231188416	3.59412418342038
C	3.65958946528802	0.53885053993590	-3.53163437808589
S	-2.97512294480262	2.64224693648137	-0.34863621234192
H	1.62538177689772	-3.34278876329037	0.95321529858601
H	-2.30564487955083	-1.73254753978123	0.47014748521104
H	5.26199314328367	1.43933516067052	1.76306763858503
H	5.01338553708879	-2.70199675846451	0.62773732839057
H	-4.14918610943334	-2.00311907058362	-1.43179874501993
H	-6.04072080095085	-0.15439567190862	1.95776309746237
H	-2.40313760777287	1.31641698196763	2.24742909206432
H	1.61171318147035	4.18130455774820	-1.31367105696924
H	-6.85339121479702	-2.25599191595787	2.34415334685126
H	-7.90139894652855	-1.37061266151470	1.22722404805237
H	-7.99879853371752	-3.12748555003727	1.32906142334226
H	-7.54775465320615	-1.59234398384267	-1.28080782911746
H	-7.68866417633243	-3.34383762337156	-1.09236308887265
H	-6.28658059675525	-2.64934500656864	-1.90871146865355
H	-6.14964097378960	-4.56680245844948	0.52342661702845
H	-4.73790038834410	-3.87706313496694	-0.27810817574733
H	-4.95956657626225	-3.66028688351785	1.45965442236654
H	-0.45625747046447	6.20602622849308	-3.26501775850522
H	0.66856223557722	5.97900499060958	-1.93311492251521
H	0.63508839740798	4.81981056451670	-3.27364935779957
H	-2.04895607478517	4.68611021293688	-3.84348329897679
H	-2.94489531926808	3.80090600371405	-2.61439120463583
H	-1.52077385787599	3.07289866805740	-3.34217017503475
H	8.00214566470243	-1.03698883293968	0.66829983807192
H	8.46021410034983	-1.97974214439342	2.09031115137716
H	7.27865136136479	-2.61956264083949	0.94706941369321

H	7.92066388307819	-0.13730533928008	3.60039550001671
H	6.35322701031812	0.66517466718535	3.57736297386836
H	7.48836201884458	0.89818871247027	2.24113870866706
H	6.77558160824351	-2.28579402086702	3.99512123570246
H	5.17254539866828	-1.55664687523137	3.86171237024612
H	5.60536244459111	-2.92856047979486	2.84164195751904
H	-2.16694287791052	-4.69270272413389	1.19909469260107
H	-0.53238767670391	-5.29600751897024	1.47599271404019
H	-1.67776629242286	-5.19834570679065	2.82118178996446
H	1.06285802812847	-4.03870408733790	2.88860116501161
H	-0.07531299559044	-3.68898831259658	4.18218981189201
H	0.73205615246297	-2.36202317187055	3.34410842973506
H	-2.18179132645217	-2.82148337538595	3.87056402876346
H	-1.79339728403086	-1.42768878746197	2.86023751675898
H	-2.94552248961540	-2.63324041006513	2.29831334231164
H	-2.66518322750147	5.10057420575722	-0.52619666616432
H	-1.21796929640311	6.08681537084211	-0.31362312037477
H	-2.30476638121554	6.38794176199536	-1.67773194313542
H	-0.01760724673340	0.13423438586461	2.82113686745683
H	1.70084255777335	-0.17639508305707	3.21317869301328
H	1.64713524001148	1.19730273720164	-3.03852484041996
H	2.94769849674334	2.07189793392793	-2.18272457495872
H	-0.98112075882593	-1.85803323599919	-4.07596149438592
H	0.55629429717870	-1.49731119590702	-4.90322208374302
H	-0.05128760637166	-4.00474559997586	-3.24491804858116
H	0.13009138652976	-3.92113970892270	-5.00466526428066
H	1.52465002435988	-3.61298251453380	-3.94683620234807
H	1.99989250624407	2.35227502027727	3.42004923368170
H	0.24748878579317	2.51976543352835	3.27410963795536
H	0.92608375056707	1.64381498025568	4.65263598390179
H	3.66724102246602	1.13939951793635	-4.43606798975925
H	4.64951422930767	0.56324570270281	-3.07931713818896
H	3.41069256620023	-0.49157409365932	-3.77368979019654

Structure F

121

energy: -193.820045928569 gnrm: 0.000655408961 xtb: 6.4.0 (d4b70c2)

C	-1.17352195309838	1.71842417665937	-1.83801829821260
C	-1.09521995206886	2.67965799552805	-0.84880135340929
C	0.12547120220807	3.19228144946132	-0.43159564014213
C	1.25709424266615	2.63386223665047	-1.01410420714398
C	1.18681321072148	1.64142859695635	-1.97031048601577
C	-0.04173489540566	1.19042478321341	-2.45396905897887
C	-4.43318502930563	-0.02611620235317	1.73600805757887
C	-4.85121735532941	1.21351146306372	1.25302494207363
C	-4.37228453055059	1.58720447792207	0.00402282408149
C	-3.59317128158025	0.72794392323199	-0.74788951667101
C	-3.25009207550704	-0.54198049280272	-0.29933090142118
C	-3.65482620132882	-0.88619521024145	0.99163115558160
C	3.88770258439444	-0.79314570415054	0.92174396198024
C	3.34917219643000	-0.57527241948170	-0.34126340114223
C	3.65657366896750	0.61317111805801	-0.98620764781156

C	4.46474456402618	1.56331639454932	-0.38427818461238
C	5.00545186702037	1.36159224287601	0.87837951461098
C	4.67194083204507	0.16640936328337	1.51743538880761
C	5.91289421388780	2.36749810827000	1.57031371633950
C	0.24642751557565	4.35431353315025	0.54049920097409
C	-5.72896162697422	2.10828122767720	2.11293622335344
S	-2.90772249128518	-2.28895829325569	1.86749607943880
S	2.83715364582069	1.11558139743255	-2.50112482950445
S	-2.87391793162299	1.33155545851954	-2.28551063303622
O	-3.02798103054521	0.36398537547559	-3.34148767712192
O	-3.50818130665140	2.61058942059870	-2.55691700771868
O	-2.99210446827883	-1.97538078498624	3.28006525587058
O	-3.61116544622763	-3.51296032940387	1.50877240249434
O	2.81455196084905	0.06464311891646	-3.49035863648424
O	3.48058975849331	2.33940897729077	-2.95994037530179
O	1.13143310417091	0.12889645299859	0.23518210338642
C	-0.73238943013927	-3.48850557858766	0.67555652505607
C	-1.24560649630469	-2.34317970519914	1.25034911398915
C	-0.61140084713340	-1.12787493307305	1.18118019511253
C	0.58806951336578	-1.00503089788228	0.43788825699400
C	1.09635633286540	-2.21143789510515	-0.13046872215090
C	0.47761011207168	-3.45474955900059	-0.01525887772886
C	1.02463076570993	-4.73316041616881	-0.64952919855385
S	3.46802335581090	-2.36801643109429	1.87352734788382
O	4.66858367719036	-2.47892283290438	2.76389038944251
O	2.27737606134283	-1.90215809357053	2.65636663087837
C	6.15770085897044	3.61783929271530	0.72060606521407
C	5.26076325295830	2.79758487982698	2.89209882981468
C	7.26588040341375	1.69886450352157	1.85270241128504
C	2.45184193910205	-5.00284309039277	-0.15543223596938
C	0.18298149700478	-5.96558556227884	-0.28970002609329
C	-6.14557158622830	3.38697982237782	1.38049209563104
C	-6.99737331091343	1.33815600393383	2.50659635637557
C	-4.94134380965326	2.49638394590283	3.37250586480923
C	1.40016194415322	4.11157131297050	1.52252124235609
C	0.53621927441772	5.61694386432775	-0.28688640628524
C	-1.04436312444803	4.56411977219767	1.33813468249976
C	1.00763392378363	-4.59456172464208	-2.17764175824059
O	-1.26043580884214	-0.01745529271375	1.70825548960991
C	-0.52350668807220	0.71687812462017	2.67876533521796
O	-2.49080416810103	-1.32399884428378	-1.10995034981532
C	-3.03661940222904	-2.60151907133879	-1.47393629100311
O	-0.17770162399557	0.39871254589875	-3.55101078829372
C	-0.04729123965740	-1.02020760476465	-3.38700684148128
C	-0.72744685104619	-1.67040300103710	-4.57802460436629
C	-0.24796266095224	-0.09084448915100	3.93990165790729
C	-4.27065925197266	-2.45355046022300	-2.35567355799418
S	2.51345745403064	-1.90571463526972	-1.16491841600938
H	-2.02743106528377	3.03220019119842	-0.44023525652527
H	2.24564710423214	2.95734645787458	-0.73218865833060
H	-4.66460506463736	-0.35048248437631	2.73862044747118
H	-4.58647437616037	2.54643236892792	-0.43789209242277

H	4.65493859008652	2.45659847052102	-0.95735064100621
H	5.04227700293850	-0.07321011599280	2.50611743079991
H	-1.31627120622393	-4.38510997336350	0.77905881453260
H	5.22425422998225	4.13689853076276	0.51778150134107
H	6.81661396660607	4.29612328383408	1.25860878608844
H	6.62698900573573	3.35795945721068	-0.22478298311406
H	4.28542805404608	3.24027872945799	2.70077215027795
H	5.88657252712244	3.52734637038597	3.40151011174110
H	5.11619599312282	1.94460668376757	3.54969448808769
H	7.92860672526231	2.39345543831199	2.36466079386548
H	7.13885541006088	0.81643293719398	2.47384740067092
H	7.73080828833864	1.38976427759215	0.91911544794798
H	2.47842688238937	-4.99974925906671	0.93183872596226
H	2.79402590122708	-5.96965592567867	-0.51774086338874
H	3.13850381143706	-4.23957370753156	-0.50297476995790
H	-0.83015235236706	-5.88190325955546	-0.67483463493101
H	0.14623577560996	-6.10593562798883	0.78758094597289
H	0.64353039509877	-6.84544254663231	-0.73398963311790
H	-6.80591364924409	3.96826248208037	2.01969434243964
H	-5.27949782783304	3.99814171684974	1.14248288398929
H	-6.67476903427088	3.15098871611384	0.46123016310447
H	-7.63926243470290	1.97006378119908	3.11561757432973
H	-6.75323605400021	0.44522772711218	3.07387665002247
H	-7.54377189820881	1.03906575158300	1.61545824684344
H	-5.54427615171286	3.14260481926212	4.00599147020360
H	-4.65593032201882	1.61633056383694	3.94160491728939
H	-4.03263627494851	3.02624690402762	3.09591081780053
H	1.32219066543795	3.11842476831209	1.95969030459475
H	2.36323430987761	4.18189148972707	1.02459003888371
H	1.37506860497245	4.84935858233436	2.32135819623674
H	-0.28486729262396	5.81228823759962	-0.97237843628791
H	1.44315723821176	5.48562147845775	-0.87131763176249
H	0.66108907606719	6.47214736672961	0.37292141669668
H	-1.85410988614994	4.88743013004849	0.68983762244678
H	-1.33328778656668	3.64032304526124	1.83399554301093
H	-0.88637070978356	5.32975030608393	2.09422918586176
H	-0.01016919706055	-4.42296751146136	-2.52251469558317
H	1.62225816997509	-3.75894362410608	-2.49757801354927
H	1.38902980030390	-5.50373933587869	-2.63610259771020
H	0.41638510545986	1.06833523119782	2.23509520451800
H	-1.17063688441782	1.57373856612497	2.89548655404692
H	-2.21941540069213	-3.07761205130369	-2.01960972751941
H	-3.26460241754903	-3.18847720081748	-0.57980160341735
H	1.01620413786620	-1.28105055667057	-3.34462950410206
H	-0.52222408183853	-1.31942996873855	-2.44414346783465
H	-0.23263221456632	-1.35220802054146	-5.49095591442664
H	-0.66140823183677	-2.74997705854295	-4.48478221456032
H	-1.76749074988306	-1.35674244576224	-4.60481361627147
H	-1.15770619682937	-0.59894421372565	4.25440338075176
H	0.51611221563110	-0.83914916348901	3.73359591691457
H	0.10571422077621	0.56730142665748	4.72920442980498
H	-4.51601010176095	-3.41667761850195	-2.79240353764074

H	-5.11465031657085	-2.10230359128218	-1.76550353259231
H	-4.06649908614753	-1.73046102975679	-3.14202690893103

Structure G

121

energy: -193.761949106820 xtb: 6.4.0 (d4b70c2)

C	-2.33857112232953	-1.50688914328105	1.51771178268288
C	-2.80428524617183	-2.64491658381161	0.89479345189194
C	-1.93121566969427	-3.65795187044211	0.52708521342726
C	-0.59333689379330	-3.43522529852032	0.82088736620183
C	-0.11059039749604	-2.30181138455205	1.44765068822442
C	-0.98444841339573	-1.26411495218683	1.78877835196688
C	-3.94284639844354	1.57012431852672	-2.07928857337346
C	-4.84331755801754	0.59163077019049	-1.67644211386889
C	-4.71781988132234	0.13477286765203	-0.36895607444448
C	-3.80803465340353	0.66421327971182	0.52950217123762
C	-2.95653615547202	1.69805035449451	0.14451414476321
C	-3.03446073059833	2.09694562501210	-1.18852907131110
C	4.46919738836364	-0.30974051725575	-0.77053517591552
C	3.58654366011133	-0.39114368092892	0.28450182496156
C	2.94469114136346	-1.61315390892720	0.50545943853226
C	3.31414390541515	-2.69166233200140	-0.25108494361871
C	4.31553355806681	-2.65477580550109	-1.22406207908899
C	4.84885140980736	-1.41478117865416	-1.51462264898619
C	4.81121066754892	-3.98611365425030	-1.76203328834245
C	-2.43148058628952	-4.95215119335333	-0.09366995152145
C	-5.89120288804274	-0.01376668849820	-2.59377585595018
S	-1.76644257533152	3.22325009180801	-1.79584354725180
S	1.67149617144685	-2.53993579173885	1.88346831951403
S	-3.60563546158777	-0.33877013493021	2.01086629684006
O	-3.26543846180038	0.40491864424140	3.19957639649961
O	-4.83730154211968	-1.09970925986046	2.14750225090842
O	-1.78249620856868	3.12345214854407	-3.24563668063281
O	-2.06109498827549	4.55925804515778	-1.30492588022445
O	1.68398007998896	-2.44045037488116	3.35457334253812
O	1.90542487309093	-3.95086425419793	1.56014848778783
O	1.10351035090561	-0.44834170613923	-0.00740998461066
C	0.58682158599237	3.57810367154582	-0.48557616041179
C	-0.23342325651105	2.66317011806601	-1.10211963359604
C	-0.00588414795584	1.31408979755508	-1.05307802625583
C	1.05724695817345	0.81234499429820	-0.25035990440760
C	1.95457059695882	1.80277749842746	0.28100608654562
C	1.74363377696868	3.18676090519561	0.17595355498974
C	2.62158538061713	4.28515051454581	0.78920077280126
S	5.04422711373571	1.41137303568106	-1.31611425197236
O	6.36133277240459	1.11732356428720	-1.96366975382807
O	3.99214740659154	1.66853224400916	-2.34728665919620
C	3.66079363872667	-4.79058783260090	-2.37941040671724
C	5.90775184691605	-3.80148568095222	-2.81161612607022
C	5.39115811840544	-4.75821726683006	-0.56433035124658
C	2.65542871335090	4.10022267376113	2.31266914958460
C	4.03645891076696	4.22334405170279	0.20356946656214

C	-5.86764333719515	0.61385541215855	-3.99003755172314
C	-5.61062811189749	-1.51775102107459	-2.72825699927798
C	-7.27774840174108	0.21938648223944	-1.97439603480678
C	-3.18147646230081	-4.63109881285147	-1.39242140598289
C	-1.28163003057444	-5.91053473742928	-0.41984046852875
C	-3.37275144089503	-5.64115039197239	0.90670383401847
C	2.09091608687223	5.70690622941183	0.51326185561309
O	-0.96057969938042	0.48400463029317	-1.63459890333237
C	-0.48704999601471	-0.38444003997432	-2.65532864198313
O	-2.01390913852509	2.29198651555383	0.91928394491569
C	-2.43753362617706	3.05809590406410	2.05561222661875
O	-0.73332043920261	-0.03677108262535	2.28065963070741
C	0.26042977818294	0.21150464877497	3.26844650336080
C	-0.06998954969447	-0.49848376840121	4.57152183593739
C	0.09592550865758	0.36608804351663	-3.84886856882224
C	-3.42921877577375	4.15227970117833	1.68122336081674
S	3.30354721351663	1.10663191998544	1.21176437000856
H	-3.86782853242021	-2.71777557004271	0.74370325062374
H	0.14489570389565	-4.18346152294976	0.59323886655260
H	-3.89785375026349	1.94929511331089	-3.08695541079617
H	-5.33604260697481	-0.66560597660178	0.00477010607362
H	2.88082357535759	-3.64674009009476	-0.01696869608401
H	5.58115801341180	-1.24528523880687	-2.28986866647893
H	0.26246523235600	4.59833756410383	-0.54217720394272
H	2.90260571929915	-5.01587297823899	-1.63516936086231
H	3.19321175607817	-4.22770967187963	-3.18403816332703
H	4.03987274415299	-5.72691480588718	-2.78160758778989
H	5.52506490961343	-3.24418686772494	-3.66388025746406
H	6.25451297200535	-4.77224748240328	-3.16042633331916
H	6.75069734909724	-3.26346339844918	-2.38351240265422
H	6.19296053027639	-4.18546191767237	-0.10239969101435
H	4.63420855451908	-4.93502595250863	0.19421884857293
H	5.77743962265093	-5.71968584600756	-0.88874298933805
H	3.25673721655537	4.88008498889740	2.77352872357186
H	1.64306506920978	4.15236941099328	2.70957274055794
H	3.07557855184913	3.13384205747221	2.57430722080008
H	3.99606427416471	4.31252823690920	-0.88109858024321
H	4.52247643909076	3.28355140883095	0.44042918362549
H	4.64161091779205	5.03513700859724	0.60178935814203
H	-6.64097586955905	0.15860963612299	-4.60454581935865
H	-6.05619541167734	1.68308655340525	-3.93761821644912
H	-4.90716334761382	0.44911882486618	-4.47169289205421
H	-6.31358436316862	-1.96784307852563	-3.42491764965372
H	-5.70215195191791	-2.01980177607995	-1.76993918692158
H	-4.59902543098649	-1.67697086916754	-3.09724400134926
H	-8.04571547374003	-0.21070806538928	-2.61249468763249
H	-7.34821326163490	-0.23156305369689	-0.98904751874013
H	-7.46413233249201	1.28630292508851	-1.87187395080058
H	-2.52554442341911	-4.09225196618477	-2.07384825637414
H	-3.50632872531213	-5.55137187773954	-1.87215609174429
H	-4.05293837608828	-4.01456754761060	-1.19599817945948
H	-0.56487402679167	-5.43988521528352	-1.08808215223373

H	-1.66960787609723	-6.79750267548691	-0.91436088541102
H	-0.76590666437285	-6.21922283873285	0.48614633499659
H	-2.83877006571617	-5.84960643287114	1.83090974497791
H	-4.22699389634031	-5.01337576608168	1.14460871206167
H	-3.73088197377474	-6.57913371190208	0.48939002456141
H	2.80872934215478	6.42142183308764	0.91139865065141
H	1.98750542846030	5.88994375071032	-0.55332936728722
H	1.13475504426102	5.88173791218809	1.00128906566881
H	0.25302603802615	-1.07890092848813	-2.23459434142059
H	-1.38374960322107	-0.94144639603212	-2.94730457040299
H	-2.84480998685599	2.39396385207618	2.82346424911234
H	-1.50009559922939	3.49001606254135	2.41367837561411
H	1.25805732114991	-0.06532861132364	2.91274902538129
H	0.21391070761230	1.29728570797684	3.40078803492696
H	-1.10072286504137	-0.28695883974919	4.84331576518883
H	0.07029782797563	-1.56927754258289	4.44666983089881
H	0.60458061103685	-0.15007038033782	5.34654643639639
H	-0.57132315130592	1.17772650582544	-4.13426451857077
H	1.06256649347515	0.79528684172586	-3.58534937038144
H	0.22822456982136	-0.31693109271551	-4.68388208520076
H	-3.54533559548205	4.83209013266189	2.52014171453418
H	-3.06073443683421	4.69848544045255	0.81466296055555
H	-4.39709300478933	3.71895586033508	1.43614271736215

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energy: -194.043635192030 gnrm: 0.000901489831 xtb: 6.4.0 (d4b70c2)

C	-1.08944466843779	-2.06063700866693	1.71575879034672
C	-0.81037405725034	-2.81759241197271	0.58759934536377
C	0.39431704210018	-2.73000986914751	-0.09036874589688
C	1.29034390240885	-1.75937086130126	0.36016598082741
C	1.03711982145163	-1.02841713740743	1.49699721811755
C	-0.13881691014138	-1.18367436220636	2.23724851622603
C	-4.65337834997534	0.07350065594615	-1.32190219342709
C	-5.09759899865975	-1.23113063541513	-1.11139115769820
C	-4.51466863680284	-1.92529684674241	-0.05588050443591
C	-3.60192463174176	-1.30509225766842	0.77179289609436
C	-3.20869841991000	0.01872136050197	0.60262402018677
C	-3.73167926482972	0.68866538104813	-0.49960908381208
C	4.13222175832154	0.44512493099132	-1.29624033379953
C	3.50950158913291	0.88370630713110	-0.13353334832276
C	3.55765999616137	0.05426653663135	0.97049873702343
C	4.39954767026539	-1.05551794873241	0.96708430802832
C	5.18926439682268	-1.37515213454860	-0.12866239341311
C	4.93824727594670	-0.66109189992672	-1.31191858578125
C	6.27622039464143	-2.43689377593543	-0.09619612066236
C	0.76455704431985	-3.62228795274310	-1.26213873506219
C	-6.17325180586189	-1.81995868564142	-2.00961742331449
S	-3.20385526062987	2.34719125465815	-0.97898856686468
S	2.27264795396008	0.08228164599774	2.21451196881704
S	-2.83637260364762	-2.20102691151611	2.12928927754974
O	-3.23119618578522	-1.60677102948050	3.38301442799931

O	-3.20165248876573	-3.59657618506402	1.99402184378603
O	-3.54127690029817	2.50374257174023	-2.37826777786210
O	-3.86853071627255	3.30269425991338	-0.10894885058517
O	1.73077285685708	1.40388558311167	2.39513653951180
O	2.77518711386624	-0.57220327959643	3.40637315544063
O	1.54933953609132	0.67542992710263	-1.60243477609309
C	-0.93899802869367	3.48790464322719	0.03661176068623
C	-1.44629350836092	2.45944875669731	-0.72342220617534
C	-0.64880594709606	1.49292570019144	-1.29692415175468
C	0.75151645597497	1.55423098111141	-1.09461515418353
C	1.23463315118648	2.62026226320954	-0.27917861000776
C	0.42870797487874	3.60591166225300	0.28327342488675
C	0.83176331393860	4.79411335320865	1.15807160303645
S	3.38340228165146	1.25231129546106	-2.76208706037774
O	4.86245886964052	1.91131908119096	-3.31891250157518
O	3.20589555501790	0.15471899933041	-3.69434729767037
C	6.38628400747379	-3.11312849716197	1.27294237732318
C	6.01686385851496	-3.51913657203015	-1.15238967690531
C	7.60749227813926	-1.73160367989441	-0.40209200104998
C	2.32852531415401	4.95748489595938	1.41881506227814
C	0.34324722888784	6.09015714050876	0.48901364434544
C	-6.53892504132720	-3.25309224005742	-1.61344820273761
C	-7.43139659403634	-0.94626092103924	-1.89154497132624
C	-5.68050515785928	-1.82170418120026	-3.46321141858921
C	-0.23059279802692	-4.77177483467621	-1.44853126424853
C	0.79533022196487	-2.77488466436183	-2.53883545886645
C	2.15394512094845	-4.22370759594996	-1.00944556468398
C	0.15646921122795	4.60651110669783	2.52657373687413
O	-1.26823575031572	0.50288966790446	-2.03448043278514
C	-0.80945911032903	0.36568136991577	-3.38389320936142
O	-2.29320779150078	0.50604201312825	1.48221594296798
C	-2.63577830214118	1.66132197687346	2.26329208128435
O	-0.23248606311739	-0.46499326123899	3.36889952936410
C	-0.71468693328293	-1.09394239049125	4.56412638853314
C	0.30076018690830	-0.86438055525418	5.67484010071778
C	-1.00732587363310	1.63369158025947	-4.20511187601989
C	-3.90029843347920	1.45764691424669	3.08727596296805
S	3.00160226662023	2.58771643424133	-0.12644155023596
H	-1.58610996543583	-3.49462227289231	0.27057126938672
H	2.20324595071904	-1.58346468342326	-0.18233892409662
H	-5.00302776494558	0.66080036434982	-2.15663815641725
H	-4.74955186700216	-2.95314197983354	0.16644760331447
H	4.39858195757177	-1.64584086547464	1.86820992228196
H	5.36434679448854	-0.95697319837411	-2.25828700645910
H	-1.64662885757765	4.19876402174579	0.42832780314757
H	5.46876009466009	-3.64063713651701	1.52161107554761
H	7.19905671057232	-3.83568676215939	1.25362723971200
H	6.59529123484574	-2.38349450193401	2.05100715614381
H	6.84822819339253	-4.22011216276617	-1.17109927790472
H	5.90895720865256	-3.08994043194058	-2.14405691919687
H	5.10935042087254	-4.06791663109114	-0.91503735843765
H	7.79795748339473	-0.95375349465083	0.33406726232319

H	8.42483111546447	-2.44823195072159	-0.37175492644578
H	7.58505307852842	-1.27094611511006	-1.38575403098247
H	2.48591367135663	5.85844138244854	2.00919322211397
H	2.71340961796586	4.11038848401403	1.97710946056898
H	2.88514394354495	5.05390646639087	0.49075389840437
H	-0.73283093762017	6.09478922743040	0.34521524699689
H	0.81766984315602	6.20532713165210	-0.48312635635619
H	0.60799877368720	6.94388255848664	1.10861869173766
H	-5.68157098466284	-3.91416305202209	-1.70449178450125
H	-6.90966070643618	-3.29102708345958	-0.59267929578771
H	-7.32114083637089	-3.61952850468232	-2.27399370907176
H	-8.22447608858398	-1.35442926234620	-2.51326323688033
H	-7.23243076834415	0.07260916402770	-2.21056142975962
H	-7.77531162290687	-0.92089374475724	-0.86027075520112
H	-5.43356078832160	-0.81822362761101	-3.79636492938860
H	-4.79208347340947	-2.44046316635300	-3.55945907398456
H	-6.45398772025802	-2.22138030824019	-4.11443003044669
H	0.11393398117409	-5.41684432427601	-2.25324030311417
H	-0.31166538366384	-5.36380623075905	-0.54045918448524
H	-1.21384505174541	-4.39699140254865	-1.71674043495996
H	-0.19683992585597	-2.38401429680225	-2.74954369518886
H	1.12313669546856	-3.37568772793683	-3.38387898037688
H	1.46911489261552	-1.92694324298678	-2.43904868100879
H	2.40172784046402	-4.92386497405824	-1.80360930114357
H	2.91208440503750	-3.44667104522673	-0.99350812844671
H	2.17141286150083	-4.75104274058639	-0.05803206025117
H	-0.92685568650374	4.62680487716253	2.44984926952280
H	0.45567634318070	3.64445552730319	2.93807313616065
H	0.47051575753537	5.39412170961180	3.20796579154939
H	0.24535702684888	0.06993638676323	-3.39164518791835
H	-1.42288036925844	-0.44776882266488	-3.77938024965906
H	-1.75568672491717	1.78913460716957	2.89737141282500
H	-2.75212614729963	2.53543832169480	1.62022920439298
H	-1.68248476308504	-0.65426649109489	4.81927778979144
H	-0.86259880475044	-2.16367279108148	4.38149923909668
H	-0.00655778130181	-1.40530165090200	6.56494428596781
H	1.28216165685767	-1.20320649657852	5.35231597809131
H	0.36901284042974	0.19572943714241	5.89858135022384
H	-0.30457858787446	2.40031012009483	-3.88327515081512
H	-0.83097754247249	1.41348651659102	-5.25372569444125
H	-2.01914842499511	2.00941478530227	-4.06736408104283
H	-4.77428137924840	1.48336396835040	2.43862891017327
H	-3.86528844118786	0.49850191841719	3.59829226321239
H	-3.98045789894732	2.25786064229067	3.81656112972326
H	4.97098650982412	2.80226504769141	-2.97705875344107

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energy: -194.017370889878 xtb: 6.4.0 (d4b70c2)

C	-2.33936778028641	-1.42440119460727	-0.33762580658847
C	-2.88828394728867	-2.14810085362147	0.69336630810986
C	-2.06920394094232	-2.90086018867016	1.53246905136792

C	-0.71018417296420	-2.87088824580816	1.25808019070428
C	-0.15519432408778	-2.15532575762271	0.21258497465176
C	-0.97148855507778	-1.39821704372820	-0.62738707132696
C	-1.86090377263977	3.63619553014314	-2.26721243361938
C	-2.32128014146352	2.86714853698988	-3.33182932947509
C	-2.80090884628993	1.59531116557258	-3.02560276643044
C	-2.87773598139209	1.13161549150385	-1.72962080326250
C	-2.47985015374721	1.92695335199781	-0.65990700596634
C	-1.93988193671229	3.17265603612052	-0.96908679818107
C	4.55960294989540	-0.49318753729491	1.82803769200410
C	3.27311773707759	-0.85270984929332	1.56022339189247
C	2.86498409296038	-1.03920993717709	0.21378997053278
C	3.89049783778206	-1.10058590723281	-0.77880204585657
C	5.20890592888737	-0.84744839662155	-0.47723825705260
C	5.54529594211262	-0.53877128509668	0.84408797148767
C	6.24318854610407	-0.88194124393543	-1.59802853816144
C	-2.66358827050833	-3.79170590305103	2.60903388946157
C	-2.28882454649116	3.32507470139380	-4.78088009440570
S	-1.12672538817183	4.09512797938259	0.35579458908142
S	1.65708723854817	-2.49789520251805	0.06134245031101
S	-3.40286032922391	-0.57931188500224	-1.51114056109155
O	-3.28818323001968	-1.22755656801574	-2.79783832016504
O	-4.74973849198847	-0.59381932650188	-0.96918353887134
O	-0.34300082726915	5.15064206258810	-0.24773892621677
O	-2.10908339925892	4.56459292900565	1.31171240506471
O	1.82914200806224	-3.06016560952043	-1.26979132836695
O	1.97650364522751	-3.47750519800251	1.08788345300323
O	1.81160508205785	0.10282258996647	-0.18153125286465
C	-0.30610020277047	2.49159589400605	2.44735946975987
C	-0.10627813099929	2.85013740013751	1.13077481611900
C	0.67397836740463	2.10237709021752	0.26720146058719
C	1.25332528376028	0.90990395954526	0.74719529513285
C	1.11762789791928	0.61517153610914	2.11642214763013
C	0.31775553389840	1.37575171082491	2.98285050550643
C	0.04827204218926	0.93799255246721	4.42059771049533
S	5.26642304966321	0.23829697802151	3.34334461089685
O	4.96990966398172	-0.94218779894094	4.46086632431456
O	4.40388707744472	1.37656201501991	3.64994784321639
C	6.23334680720176	-2.28386763829702	-2.23829333252430
C	5.87818810507737	0.18776987997623	-2.63710126390517
C	7.66311460364717	-0.59003772146805	-1.09944603362569
C	-0.84597619531474	1.94276996961420	5.15597788964755
C	-0.70674610417092	-0.39889549468123	4.37979881913279
C	-1.71542993243042	4.73784459672366	-4.92962461591344
C	-1.41444740398703	2.36500643990153	-5.59874947671321
C	-3.72760799866036	3.29028082952532	-5.32714176583456
C	-3.39633947978593	-4.94300586965054	1.89479481294776
C	-1.58539366552891	-4.37341582770976	3.52961838516268
C	-3.67332072025635	-3.01355364029937	3.46377471247023
C	1.34938463571335	0.79122889513837	5.23202797084386
O	0.72647855107323	2.52152114288499	-1.03537872216887
C	2.01045545689203	2.59871359080466	-1.66068666621555

O	-2.49665448083233	1.50831504883086	0.63781480728067
C	-3.77999942170994	1.32638084278188	1.26459346941105
O	-0.67395187608550	-0.57027438824498	-1.65605180791711
C	0.32508647118365	-0.87024566115675	-2.63107829908343
C	-0.08498514692698	-2.04509290652334	-3.51205579325170
C	1.87302140444308	3.52031823493143	-2.86059881767574
C	-4.59624606830858	2.61154287827513	1.33620189215573
S	1.96804931398495	-0.81437360919665	2.72579048490316
H	-3.96169248923863	-2.12856734387149	0.79536945743691
H	-0.00941598432684	-3.44195565036606	1.84503192751923
H	-1.40041049472372	4.60185039716254	-2.40183672147128
H	-3.11115275015564	0.90974619397299	-3.79582966044759
H	3.56774326899352	-1.33444004673009	-1.78048363693330
H	6.56556866780172	-0.36118383772732	1.13752585655038
H	-0.98451449017776	3.10722814452519	3.01144827923038
H	7.01056467028963	-2.36994727917616	-2.99605627304358
H	6.41275293469842	-3.04200797751609	-1.47753187491421
H	5.27409401715727	-2.49864782974535	-2.70329183792362
H	6.62115919411225	0.21863273732961	-3.43095777723977
H	5.85232913616906	1.16102322757773	-2.15299511354171
H	4.91121262584223	-0.00180228908198	-3.08630266096126
H	7.97815493842346	-1.33685227176634	-0.37348742949193
H	8.35512656861576	-0.62426040722189	-1.93900667245103
H	7.72015582033841	0.40027902505649	-0.65358503435854
H	-1.02475663146889	1.58032268697765	6.16591753030487
H	-0.35891035450885	2.91244935359619	5.21842873765689
H	-1.80955515171515	2.04576396503199	4.66314865220987
H	-0.93786441421421	-0.72013945406584	5.39232169559226
H	-0.12116863186745	-1.17578687236114	3.89806339533838
H	-1.63088400420869	-0.28244518861421	3.81627096412360
H	-1.73603168440651	5.02552291127365	-5.97875247370363
H	-2.31460571024853	5.45518603562214	-4.37272458313233
H	-0.68496346364023	4.77565763827696	-4.58327143506637
H	-1.35977128736651	2.70874645136944	-6.62885369536292
H	-1.81291155779585	1.35619878799444	-5.59737127359817
H	-0.40809292824499	2.33468653690388	-5.18845132566639
H	-4.36332261157816	3.94956193996064	-4.73914501288600
H	-3.74726161881801	3.62245399710997	-6.36244866303503
H	-4.13396875772319	2.28228511661966	-5.28615379870382
H	-3.87952501904173	-5.59053522774477	2.62271163380494
H	-4.15406582812323	-4.56001920954259	1.21526972752700
H	-2.68975248283133	-5.53100614297145	1.31440091969243
H	-2.05829905229574	-4.94482848535803	4.32492448449717
H	-0.99760360007735	-3.58098067194486	3.98329784326377
H	-0.92187112367423	-5.04122337787015	2.98784541189017
H	-3.19954426480986	-2.15380114436938	3.92801014618422
H	-4.51440451324373	-2.67101760430772	2.86702945074562
H	-4.06140072980313	-3.66154777981403	4.24667442068270
H	1.74410326960700	-0.21535229383213	5.16551240597783
H	2.11214873559618	1.47715298947225	4.87100100867235
H	1.15883003488046	1.00297411835330	6.28011895333862
H	2.73585325259557	2.99980037629573	-0.94206619245995

H	2.35202422545265	1.60437933333912	-1.96342349747758
H	-4.34294208667246	0.54266429590455	0.75014676673797
H	-3.50658188874386	0.99054493774879	2.26697178989574
H	0.37312214232353	0.05392741121644	-3.21485613036153
H	1.28400841986931	-1.05048964691982	-2.13480537116807
H	0.50777418103647	-2.05477174862520	-4.42319065673933
H	0.08381539131631	-2.97430150158461	-2.97037023878681
H	-1.13940002319333	-1.95315671559517	-3.77568770128120
H	2.82698897986452	3.64461300872007	-3.36176966859309
H	1.13787506063280	3.11985215596349	-3.55208943334281
H	1.53311635516505	4.49289923680765	-2.52321127474887
H	-5.40362936852444	2.47562554011360	2.05039144877720
H	-3.96116729691983	3.44123492968192	1.64781317665378
H	-5.02280802681361	2.84998823218069	0.36401202195974
H	4.05086956362947	-1.20673031064041	4.54636717476972

Structure K

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energy: -194.090309635312 gnorm: 0.000687252437 xtb: 6.4.0 (d4b70c2)

C	-1.57299327507168	-2.17067039472361	2.01581423013384
C	-1.39381450091064	-3.53770143607087	1.97900948727214
C	-0.16122965512384	-4.07284937416758	1.62264141822532
C	0.83563616262842	-3.16073412820889	1.28179278234149
C	0.66441441501723	-1.79222757167371	1.31419978081377
C	-0.55997703657637	-1.26559907175114	1.71109640789807
C	-4.18057921416882	1.90219645858234	-0.41848362216998
C	-4.52442188810540	2.01846467254850	0.92757884676937
C	-4.19058892134992	0.95183261608186	1.75716487353328
C	-3.56719914826740	-0.18097889735350	1.26967872160802
C	-3.23792494467957	-0.29993035896971	-0.07393239501620
C	-3.55751621337026	0.77206884489274	-0.89843515263133
C	4.39692359448349	0.89713588828116	0.12066114822982
C	3.38833314114132	1.12723122563984	-0.79256159400193
C	2.58165381795590	2.24214998455416	-0.63062686758357
C	2.84459221794479	3.15264087417563	0.37728302494837
C	3.91714470311641	2.97516376311442	1.25039700422831
C	4.66584688143854	1.81185576565045	1.11841541246228
C	4.19008612724429	4.02304424735443	2.31757753088807
C	0.12928977572202	-5.56515751377078	1.59722071869664
C	-5.22778510196100	3.27138870248765	1.42259744351328
S	-3.08217093118858	0.65711404766189	-2.62468749515970
S	2.15432370754756	-0.76725425151093	0.82112127885913
S	-3.16082994295585	-1.48506107948126	2.44969476333741
O	-3.10229087807776	-0.88144726688342	3.76312834399732
O	-4.16502097860097	-2.52656035258460	2.31248473033221
O	-3.65900259627647	-0.53756151661405	-3.19898553287212
O	-3.47006262635693	1.88540057060410	-3.28381335041277
O	2.99632057236013	-1.78735154358817	0.13988806975642
O	2.74253086288263	-0.49187729731572	2.18915746705292
O	1.48686579941813	2.46659967299794	-1.43637993917864
C	-0.68568309687319	-0.60281832163314	-3.15811790962224
C	-1.30286722190005	0.49954859224994	-2.61282310033443

C	-0.58387760724816	1.52168224997655	-2.01799793121759
C	0.81200410008656	1.38568680664908	-1.96897156640370
C	1.43324720189828	0.23159377328658	-2.45857323177978
C	0.69200031814394	-0.77154892053677	-3.11568872818282
C	1.32549642816236	-1.99540387229262	-3.77058436561198
S	5.27814704229005	-0.71332372306054	0.05638003278025
O	6.67055598128324	-0.32691072829514	-0.20860398492645
O	5.23962920484671	-0.98650837217643	1.65204547024545
C	4.47035281995106	5.37165213612931	1.63829087983522
C	2.95548224022642	4.13794429825150	3.22411476415880
C	5.39584409350036	3.66153987225980	3.18882297399235
C	2.44742652462402	-1.57215963422323	-4.72944103960125
C	1.85322525602370	-2.93559401241830	-2.67984748686015
C	-6.56960361818224	3.40002078803199	0.68604030738068
C	-5.49860850866567	3.22966084569727	2.92865757909462
C	-4.34686777687469	4.49131548090299	1.11765084051783
C	1.24065913380619	-5.85836385953938	2.61608770923523
C	-1.10069349631486	-6.40186529371439	1.96040759427642
C	0.59863286052171	-5.97265364721927	0.19347111597875
C	0.31309274326805	-2.78684249845068	-4.61178966101678
O	-1.28961192400636	2.53963503488776	-1.45075903692759
C	-0.98222184620661	3.89062859816406	-1.81664429465380
O	-2.57093983231340	-1.37403049143017	-0.59159038060966
C	-3.38845263623853	-2.53547727750002	-0.82691910350515
O	-0.92002111826548	0.03580653262963	1.83685298362903
C	0.01239534839520	1.06863242572178	1.56216211444275
C	-0.67769907375159	2.38997095412471	1.85331133132661
C	-1.09680765012405	4.12295732801712	-3.31642023448632
C	-2.49179280707084	-3.63335073664911	-1.36576623469699
S	3.19031987577417	0.07632279805201	-2.19120136229493
H	-2.24753182739911	-4.14635414895013	2.22680534944115
H	1.81070685629212	-3.49742799888641	0.95846528445232
H	-4.37902765404537	2.68345254933085	-1.13477650577454
H	-4.38182871076482	0.96596059336579	2.81722724115208
H	2.19342945934359	4.00798357019319	0.45612917034928
H	5.47282703418831	1.57129315312594	1.79064742132759
H	-1.33571579674822	-1.32370962654792	-3.61997816056472
H	3.62072850120541	5.69871000201020	1.04620465920514
H	4.67916111697857	6.12904451635456	2.39021031717600
H	5.33293495859226	5.28561755834849	0.98140761124818
H	3.16186028344673	4.81181430865346	4.05229795023231
H	2.69787559308403	3.16005354127477	3.62564602517246
H	2.09779121131627	4.51919405528797	2.67754694031340
H	6.29626564877224	3.56459902377891	2.58698166439126
H	5.56035870687868	4.44547847475158	3.92511974404026
H	5.22379770365120	2.72824792840313	3.71975074723110
H	2.06822528344102	-0.85075460960277	-5.44936167386538
H	3.28623840647042	-1.13032750505258	-4.20477775887276
H	2.81194056224621	-2.44341681263076	-5.26735143072747
H	1.02701231161718	-3.28517055313603	-2.06297958874766
H	2.56793924988092	-2.44827999536967	-2.02510858628393
H	2.33793783517473	-3.79506521339819	-3.13598789277887

H	-6.42155357457369	3.48802075522498	-0.38611439121598
H	-7.18621835071742	2.52456196281624	0.87567844249268
H	-7.10099111993120	4.28160383100443	1.03611319326194
H	-6.14386620752305	2.39381493527264	3.18607494340753
H	-5.99586563160985	4.14843906918215	3.23065175374008
H	-4.57105573674089	3.14501410906451	3.48854630630669
H	-4.17680223088797	4.59438211874724	0.05026753013817
H	-4.83019279214095	5.39553469116136	1.47908267554857
H	-3.38391742195512	4.38978248694563	1.61235861931641
H	2.14710832744397	-5.31149561565839	2.37093419638020
H	0.92491926782964	-5.56093721065324	3.61411625611314
H	1.47031813181312	-6.92151781986435	2.62532600002175
H	-1.44392769642348	-6.17320869601856	2.96635282162176
H	-0.84268262712248	-7.45781382351421	1.92088880288208
H	-1.91245923547157	-6.22205193630924	1.26030713487180
H	1.48721194211327	-5.42051792709307	-0.09807828758560
H	0.83219241147344	-7.03462740841023	0.17438990734083
H	-0.18209898333332	-5.77553770418981	-0.53748928877748
H	-0.13695022255272	-2.16081878730340	-5.37824513277284
H	0.83368106136464	-3.60607900790478	-5.10200790763451
H	-0.46880221858360	-3.21960327895796	-3.99423650676875
H	-1.73472058165018	4.46771179050224	-1.27520524628907
H	0.01381304697576	4.16419862784887	-1.45691496766812
H	-3.86993167684193	-2.84008269998388	0.10931784693739
H	-4.15517318631025	-2.26988710098524	-1.56560575271781
H	0.90914035598350	0.94551998444475	2.17985260621809
H	0.31014978520522	1.01090720175554	0.50925022922674
H	0.03374651437434	3.19838011040408	1.72090134000569
H	-1.51306865641627	2.52237512914112	1.17054431633988
H	-1.04497424647272	2.38990611627433	2.87559927462069
H	-0.28156425252504	3.62655046500425	-3.83895474520933
H	-2.03933849644000	3.71454250905017	-3.67472053289794
H	-1.05482221145601	5.18781781630888	-3.52483311360602
H	-3.07276025941385	-4.54190571356086	-1.49316720587933
H	-2.08073629712243	-3.33055956919888	-2.32397426474791
H	-1.67401256414927	-3.81354844344080	-0.67276292601170
H	4.28620450474089	-0.92036153276317	1.94461043553868

Structure L

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energy: -193.819040873572 gnorm: 0.000870307756 xtb: 6.4.0 (d4b70c2)

C	1.15376025145538	2.50873344689105	1.05166436349003
C	1.15866207931066	2.62562057348280	-0.32374119138599
C	-0.02562970742686	2.77256952828298	-1.02717925790088
C	-1.18468703656727	2.75284003021239	-0.26429840229635
C	-1.21598515616000	2.59112189828015	1.11262393453425
C	-0.01325931714674	2.50414165947656	1.82599046388395
C	4.72349459255381	-0.64675455309076	-1.11807858022403
C	5.08162758170670	0.69803311101220	-1.15436395157463
C	4.46838971037471	1.52016372053486	-0.21902094264607
C	3.57172729106814	1.07050305471090	0.74099752646484
C	3.25504949248940	-0.28844852475362	0.80787742295560

C	3.84756709898820	-1.10341037705053	-0.16503379630332
C	-3.45611972730292	-0.86569868004207	-0.50287285643265
C	-3.02363801805857	0.04688287975571	0.47004127465244
C	-3.60701180123754	1.31627089316546	0.38938206832250
C	-4.55221476295457	1.65946129459675	-0.55707839578409
C	-4.97748273528142	0.73813595508433	-1.50425405459761
C	-4.39343551933969	-0.53429166063408	-1.44448525901973
C	-6.01825816526751	1.04283138469161	-2.57033959921087
C	-0.09763907593038	2.98481817579180	-2.52755391331461
C	6.05584426278098	1.28589787314163	-2.16237861625674
S	3.28981218917196	-2.81297499195485	-0.19076052874743
S	-2.99854610918317	2.54853767264969	1.52527650214138
S	2.82711028563623	2.41494500920948	1.70588193220450
O	3.48323299136648	3.63879546806798	1.28118209940599
O	2.94809723979801	2.16348810311491	3.12342749389114
O	3.74033270482923	-3.38147293666992	-1.45225914522829
O	3.81803848850203	-3.50762971669693	0.96781638120857
O	-3.48307356591892	3.85273545092011	1.08648336754864
O	-3.37747057513406	2.25641843490497	2.88982789630953
O	-1.27073913949396	-1.14602301645972	-1.69309090623504
C	0.84841453630728	-3.68399482930371	0.69660130750375
C	1.50369981269591	-2.80279085466749	-0.14226575347399
C	0.84712852357403	-1.93806409421464	-0.97742517442906
C	-0.58351795101721	-1.92135953978829	-0.96037431646473
C	-1.22043458266088	-2.84575857452748	-0.08815749539911
C	-0.54455907520767	-3.75361272471020	0.72441046694226
C	-1.21809953998167	-4.81781288724077	1.58573231751863
S	-2.98070191404491	-2.59307061140268	-0.40776971585900
O	-3.86801357631577	-3.08971597112876	0.64294781300863
O	-3.26228592416278	-3.23132871463451	-1.68889080936779
C	-6.57515843938794	2.46460157617548	-2.44953131382718
C	-5.37213349558457	0.88661517036174	-3.95423119787283
C	-7.18488659365619	0.05409656881979	-2.43017150433279
C	-1.99642656495407	-4.14857018302482	2.72435214273189
C	-2.14367049472304	-5.66327038250580	0.70046422752028
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C	7.23092021886027	1.92192109568657	-1.40627868304165
C	6.60512467898951	0.22255679212579	-3.11685590454728
C	-0.45421675274127	4.45695958617907	-2.78567811264631
C	1.24054074018134	2.66865371376671	-3.20015621935441
C	-1.18243351226033	2.07640859665858	-3.12351305445230
C	-0.20846480234243	-5.78221892101695	2.22760889439879
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C	1.32821335874366	-1.20129330131381	-3.18627168318277
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C	1.53396051493716	-0.44016087566862	2.55188042688398
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C	-0.83929674198134	2.24961003114753	4.09216902559982
C	-0.17728442992906	2.14882447537094	5.45675631181089
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S	-1.86638561293584	-0.31082276540072	1.65026029002081

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H	-4.92410137447812	2.67171674996333	-0.51738001657536
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H	-6.10446473224086	1.07502745740380	-4.73672071313807
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H	0.32263221283747	5.10535148644542	-2.38708792647308
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Structure M

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energy: -193.677944371173 xtb: 6.4.0 (d4b70c2)

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C	4.92779157094238	-1.50627330759572	-1.01389605466323
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S	1.80871511853715	-2.21872059848204	2.51321771291149
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O	-3.42714288988745	0.73970987533786	3.28800237170854
O	-2.08084998797773	2.71259838456951	-3.41058321418697
O	-2.26285916444589	4.37325166108641	-1.63192074450544
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O	1.81678957449102	-1.84654139927094	3.96143721366114
O	1.25507134460191	-0.47339891447285	-0.78492061021006
C	0.59235837165467	3.52966690894219	-1.12559370408383
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C	6.36761742224038	-3.91414395074510	-1.77235064533422

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C	3.47702445116311	4.94354157042314	-1.44933874872175
C	1.94184931971780	5.58483019076362	0.38291638713074
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C	-7.51111789502287	0.18850981798292	-1.57702224765341
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C	-0.75796877494549	-0.83147810220729	-2.57706298522603
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