Electronic supplementary information

for the manuscript

When Cl substitution goes rogue: highly selective templated synthesis of cis bis(dihydrofurano)fullerenes from $C_{60}Cl_6$

Valeria S. Bolshakova,[a] Alexander S. Peregudov,[b] Nikita A. Slesarenko,[a] Ivan A. Godovikov,[b] Olga A. Kraevaya,[a] Alexander F. Shestakov[*a] and Pavel A. Troshin[*c,a]

[a] *Federal Research Center for Problems of Chemical Physics and Medicinal Chemistry of Russian Academy of Sciences, Semenov av., 1, 142432 Chernogolovka, Russian Federation*

[b] *A. N. Nesmeyanov Institute of Organometallic Compounds of RAS, Vavilova str., 28, Moscow, 119334, Russia*

[c] *Zhengzhou Research Institute of HIT, Longyuan East 7th, 26, Jinshui District, 450003, Zhengzhou, China*

*Corresponding author: troshin2003@inbox.ru, a_shestakov@list.ru

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General information

Reagents and solvents were purchased from Macklin, Acros, Chimmed and used without purification unless noted otherwise. Reactions were monitored by analytical HPLC (Shimadzu, Japan) using Nacalai Tesque COSMOSIL 5PYE column and toluene/acetonitrile mixtures as eluent. Preparative HPLC (Shimadzu, Japan) was performed using Phenomenex Luna 10u Silica(2) 100A, AXIA packed, Dr. Maisch Reprosil-Pur Basic C18 and Nacalai Tesque COSMOSIL 5PBB columns and toluene/heptane, toluene/ acetonitrile mixtures as eluent. ^{1}H NMR, {^{1}H} decoupled ^{13}C NMR and ^{19}F NMR, ^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC,^{1}H-^{1}H ROESY spectra were recorded on Bruker AVANCE-III 500 [500 MHz (^{1}H), 126 MHz (^{13}C), 471 MHz (^{19}F)] spectrometers. ^{1}H-^{19}F HOESY spectra were recorded using Bruker AVANCE 400. MALDI mass spectra (negative ion mode) were acquired using a Bruker Autoflex Speed TOF/TOF device (SmartBeam II laser, 355 nm). Trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB, ≥98%, Macklin) was used as a matrix, the matrix-to-analyte molar ratio being 700–3000. Thermogravimetric analysis was performed using a TGA/DSC3+ Star system from Mettler Toledo. Measurements were carried out in aluminum oxide crucibles with a heating rate of 10°C/min and a nitrogen flow rate of 20 mL/min. The CV curves were registered at the scan rate of 50 mV s^{-1} at ambient temperature in a three-electrode electrochemical cell with glassy carbon disc working electrode (WE), a platinum wire counter electrode (CE), and an $Ag/AgNO_3$ reference electrode (RE) in dimethyl formamide:o-dichlorobenzene (20/80 v/v) using 0.1M $Bu4NPF_6$ as the supporting electrolyte. Ferrocene was used as an internal standard. The electrolyte solution was purged with argon before the measurements were performed.

HPLC profiles and MALDI ToF mass spectra of reaction mixture with ethyl 3-oxobutanoate

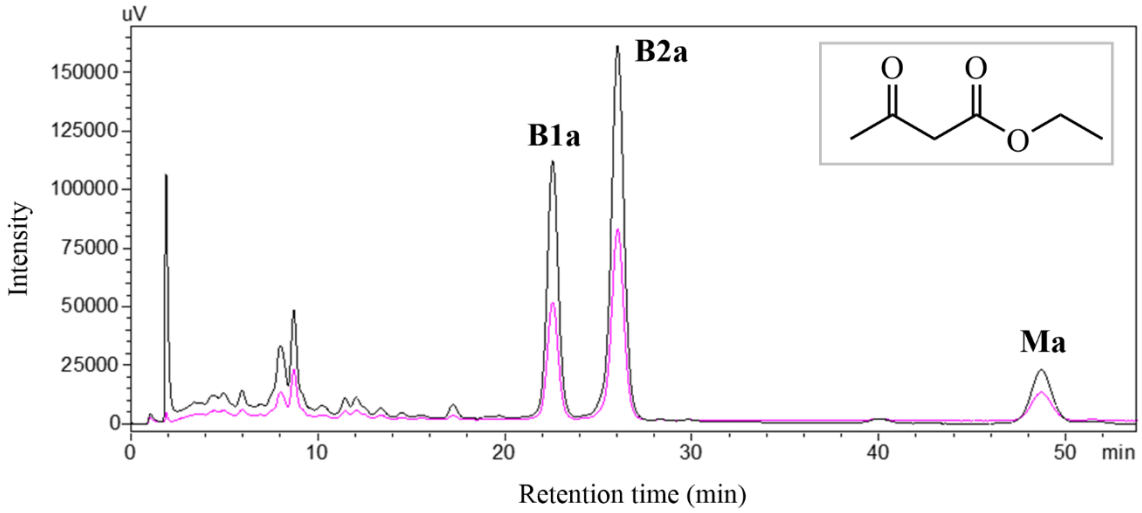


Figure S1. HPLC profile of the reaction mixture with ethyl 3-oxobutanoate.

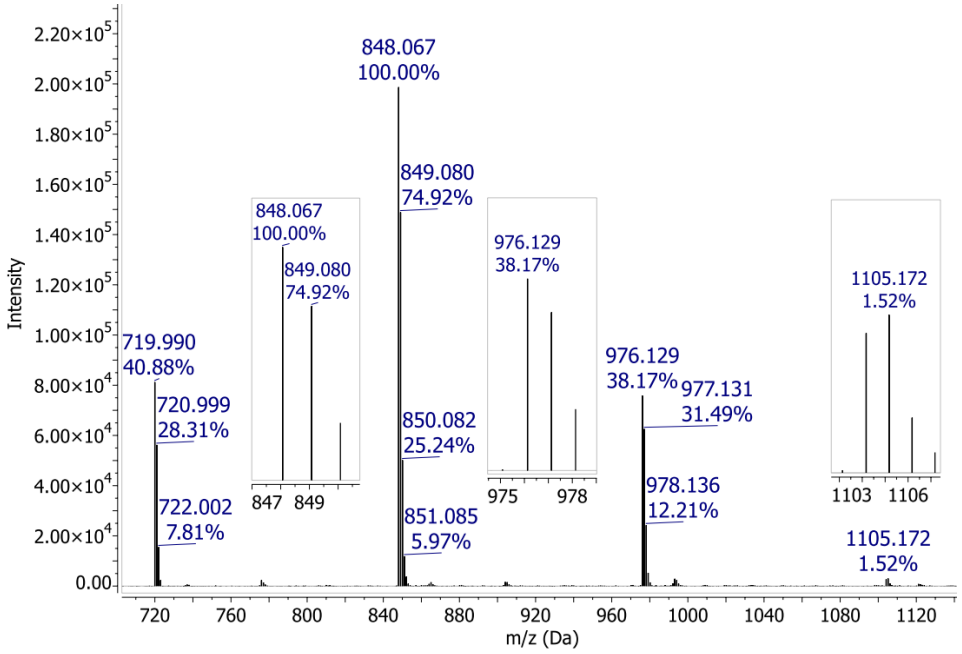
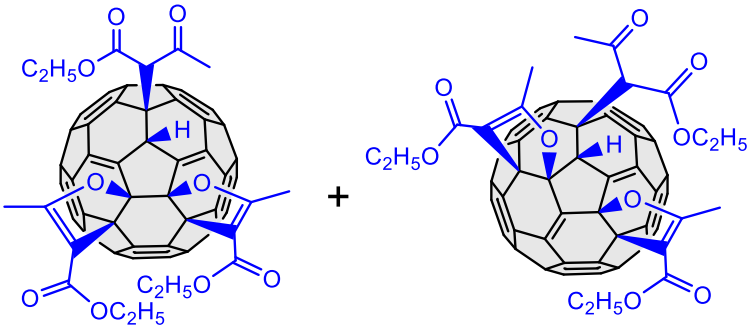


Figure S2. Negative ion MALDI mass spectrum of the reaction mixture with ethyl 3-oxobutanoate.

NMR and MALDI ToF mass spectra of a mixture of isomers tris-1a and tris-2a

Mixture of isomers **tris-1a** and **tris-2a**



tris-1a + ***tris-2a***

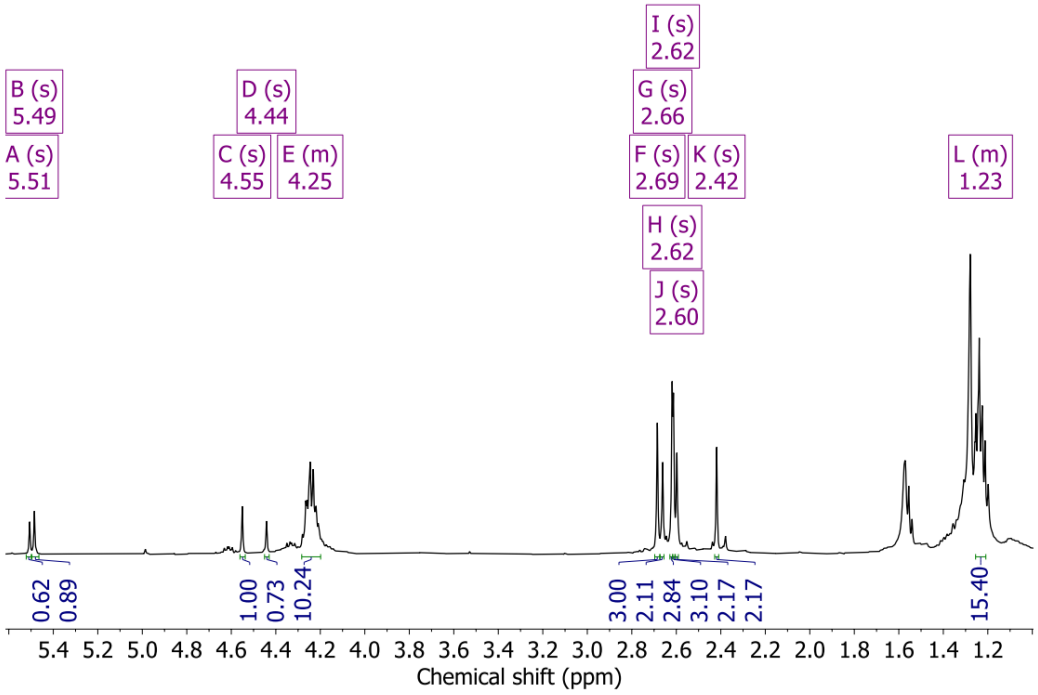


Figure S3. ^{1}H NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

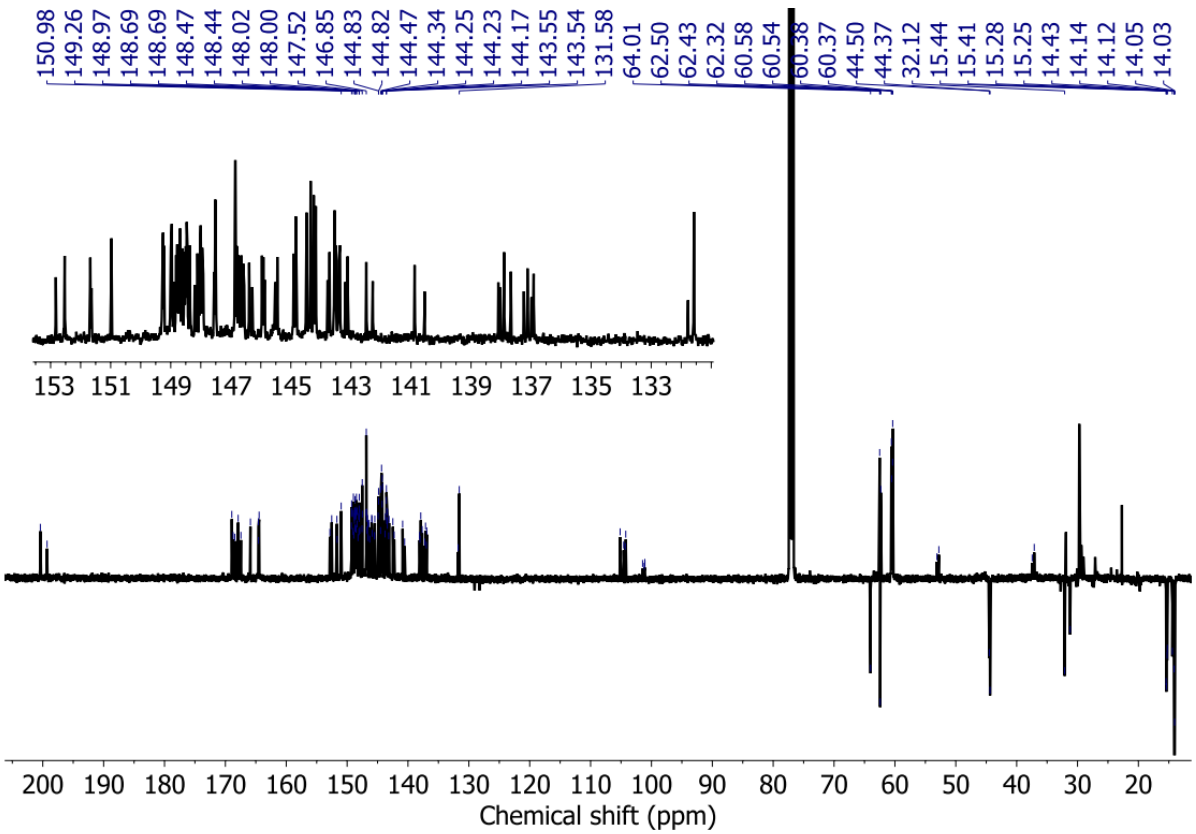


Figure S4. ^{13}C NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

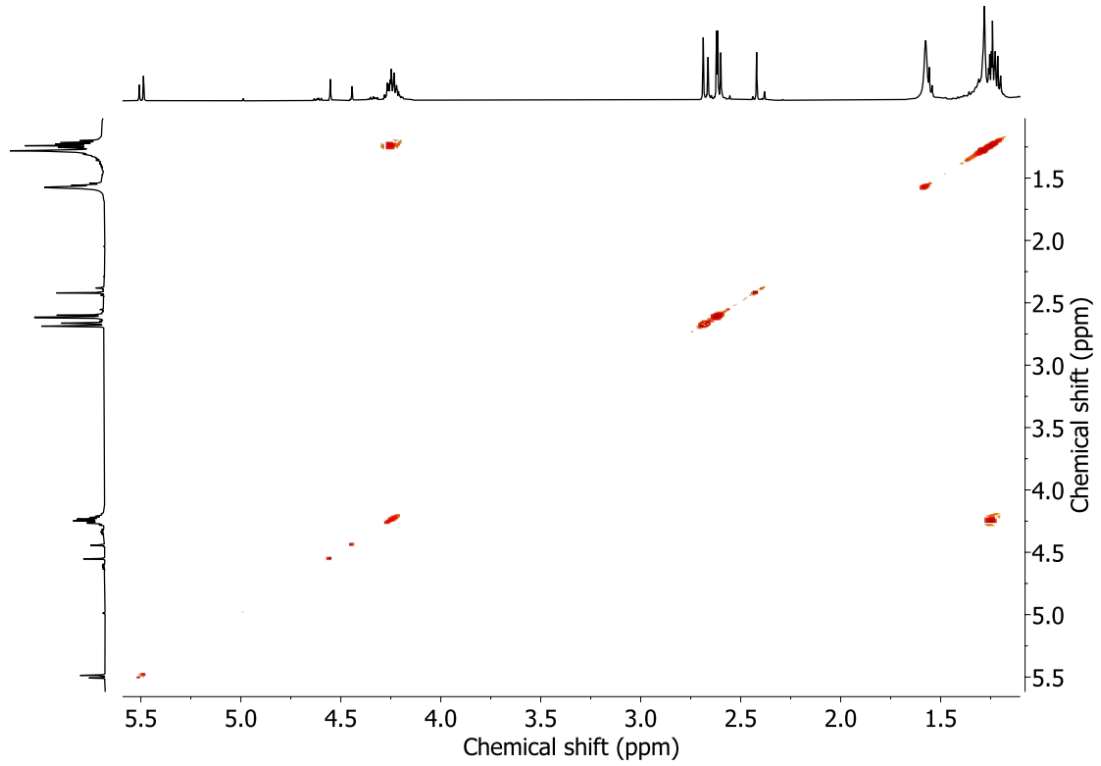


Figure S5. ^{1}H-^{1}H COSY NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

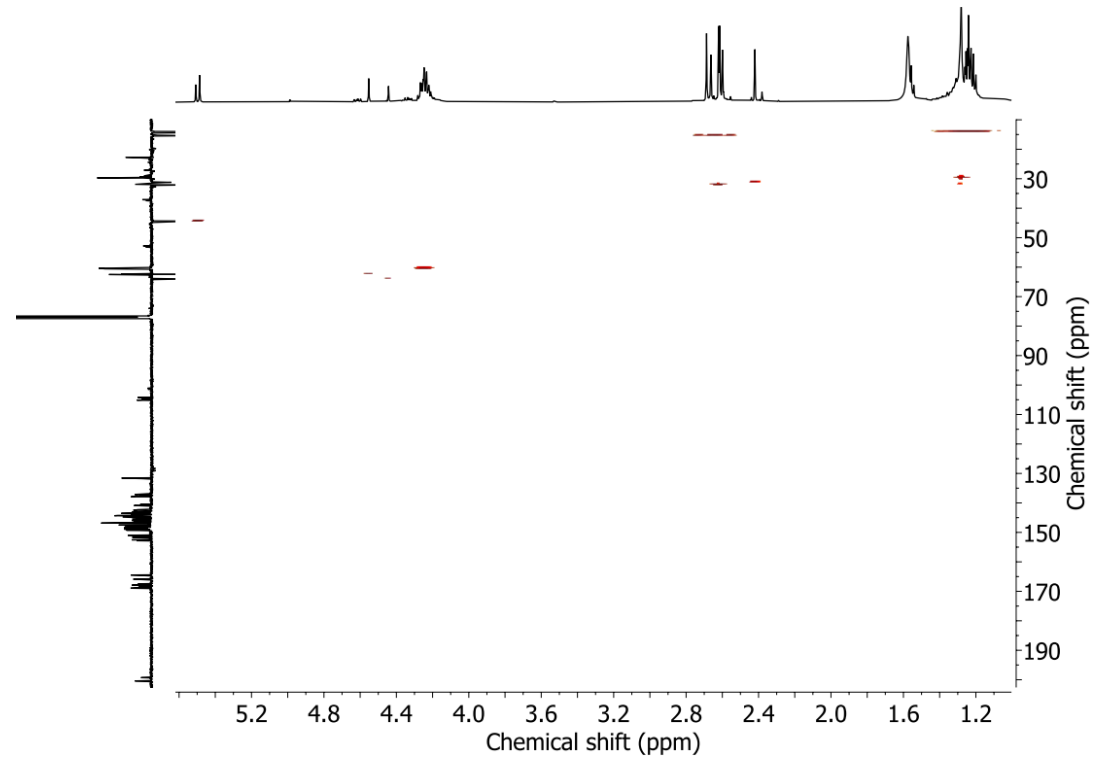


Figure S6. ^{1}H-^{13}C HSQC NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

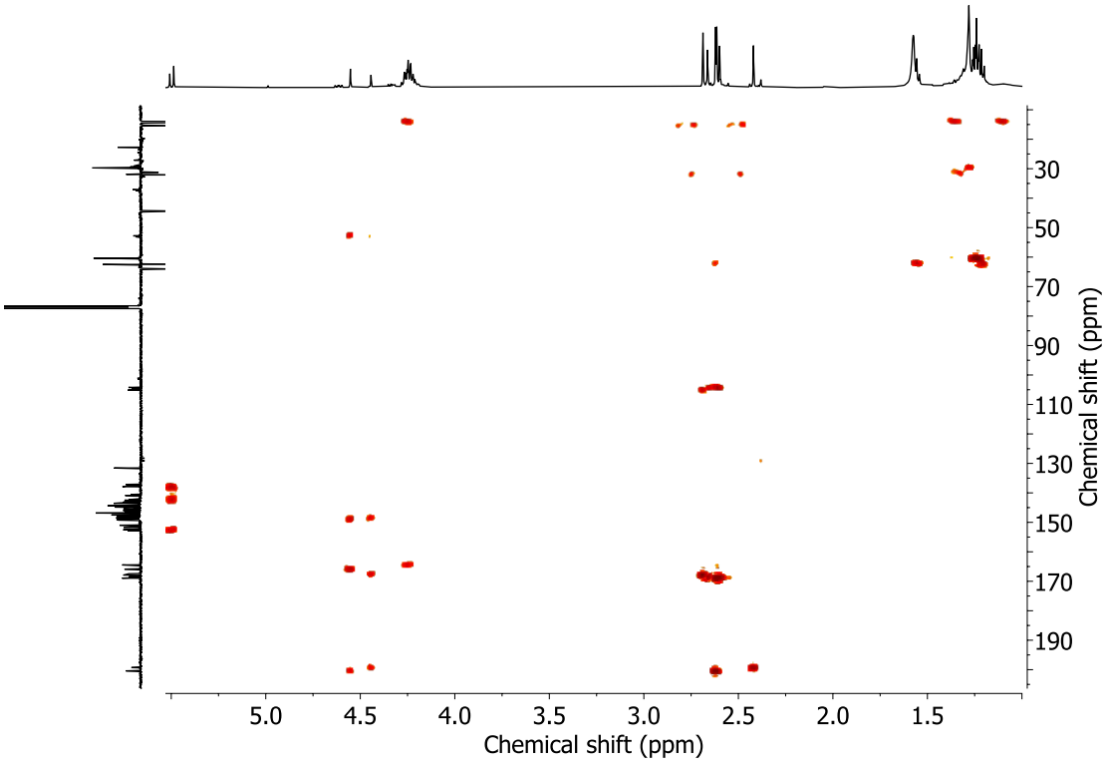


Figure S7. ^{1}H-^{13}C HMBC NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

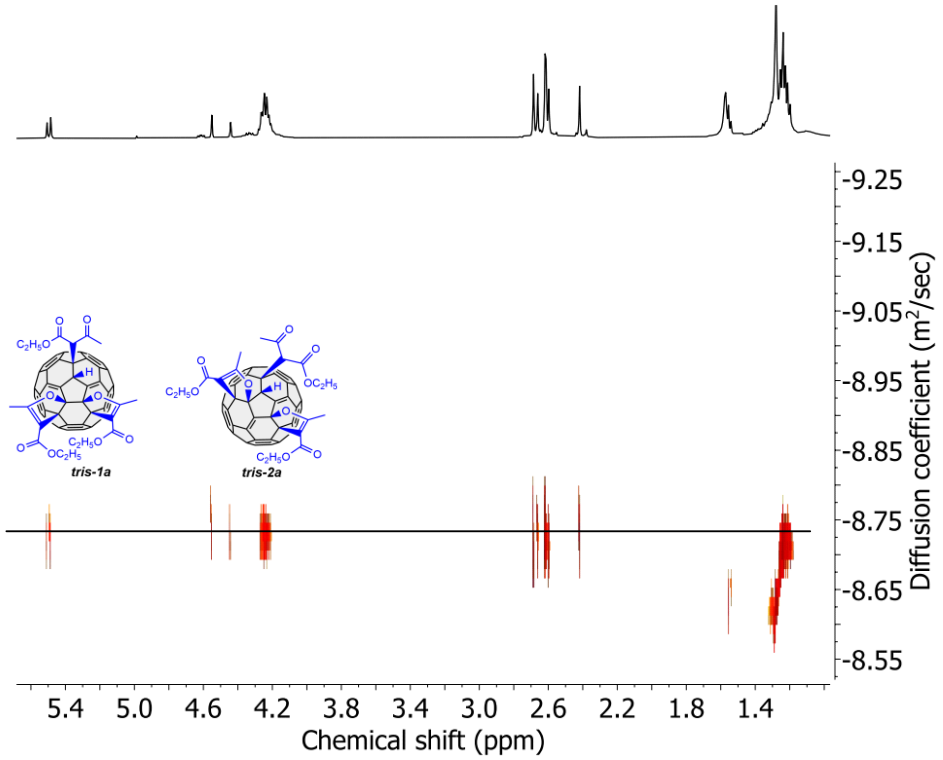


Figure S8. ^{1}H DOSY NMR spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

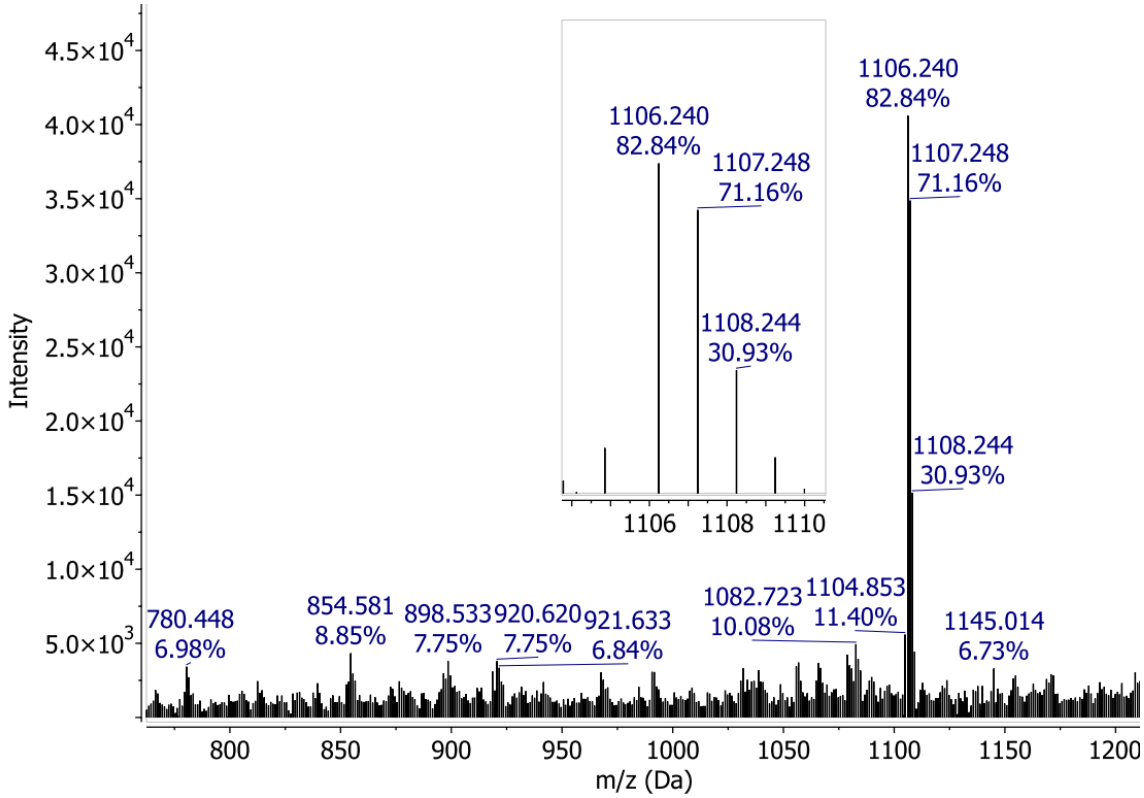
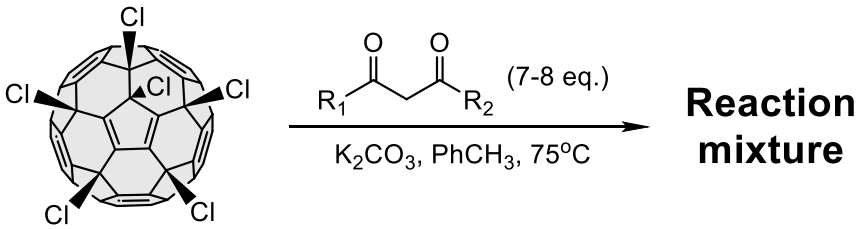


Figure S9. Negative ion MALDI mass spectrum of a mixture of isomers **tris-1a** and **tris-2a**.

HPLC profiles and MALDI ToF mass spectra of reaction mixtures with acetylacetone, 1-phenylbutane-1,3-dione, 1,3-diphenylpropane-1,3-dione, 4,4,4-trifluoro-1-(naphthalen-2-yl)butane-1,3-dione, dimethyl malonate, dimethyl 2-bromomalonate



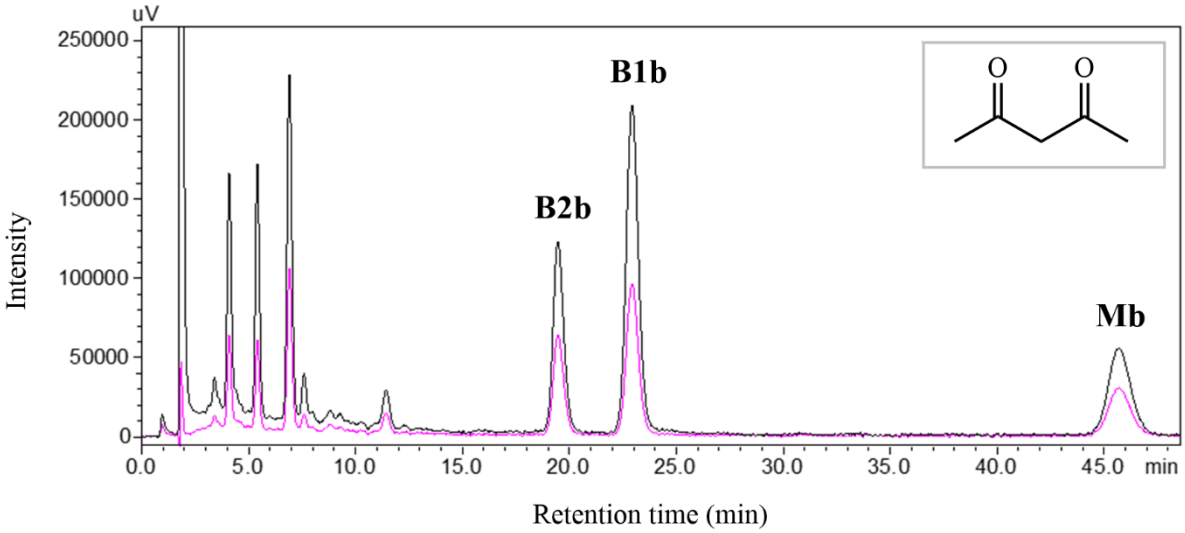


Figure S10. HPLC profile of the reaction mixture with acetylacetone.

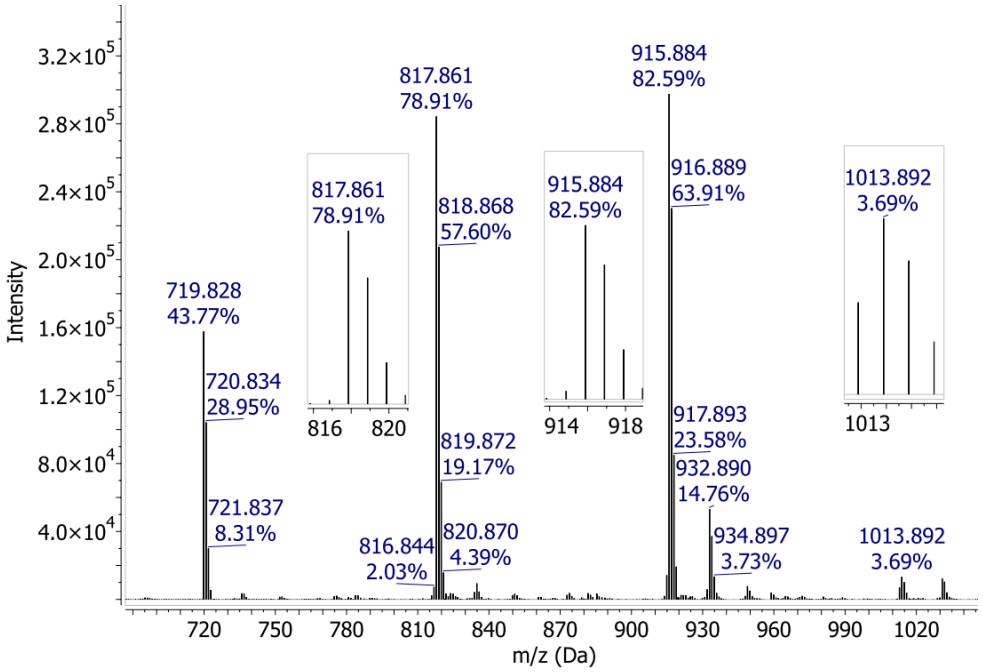


Figure S11. Negative ion MALDI mass spectrum of the reaction mixture with acetylacetone.

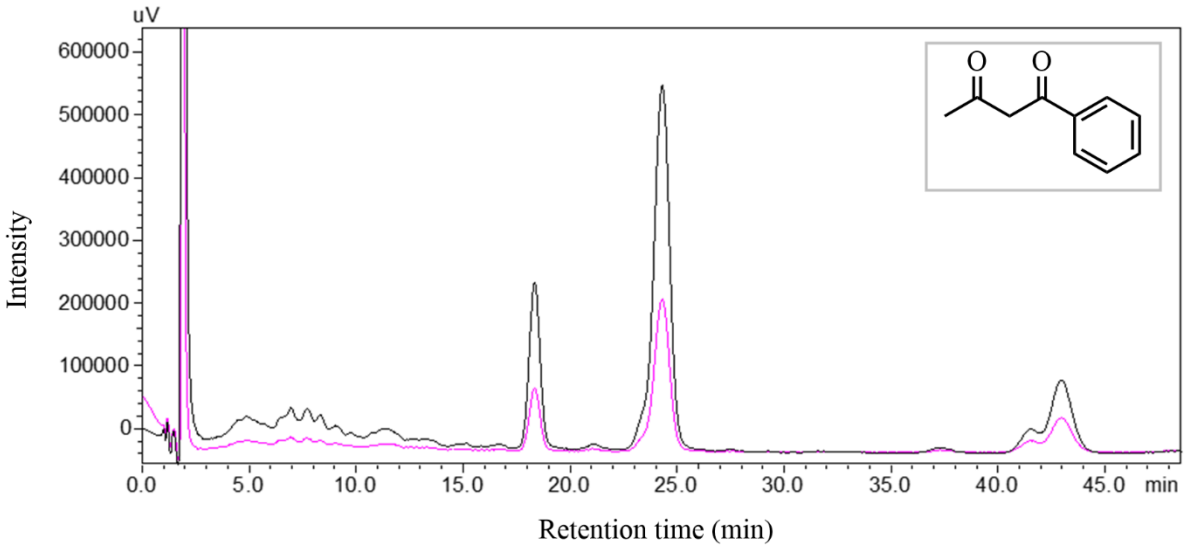


Figure S12. HPLC profile of the reaction mixture with 1-phenylbutane-1,3-dione.

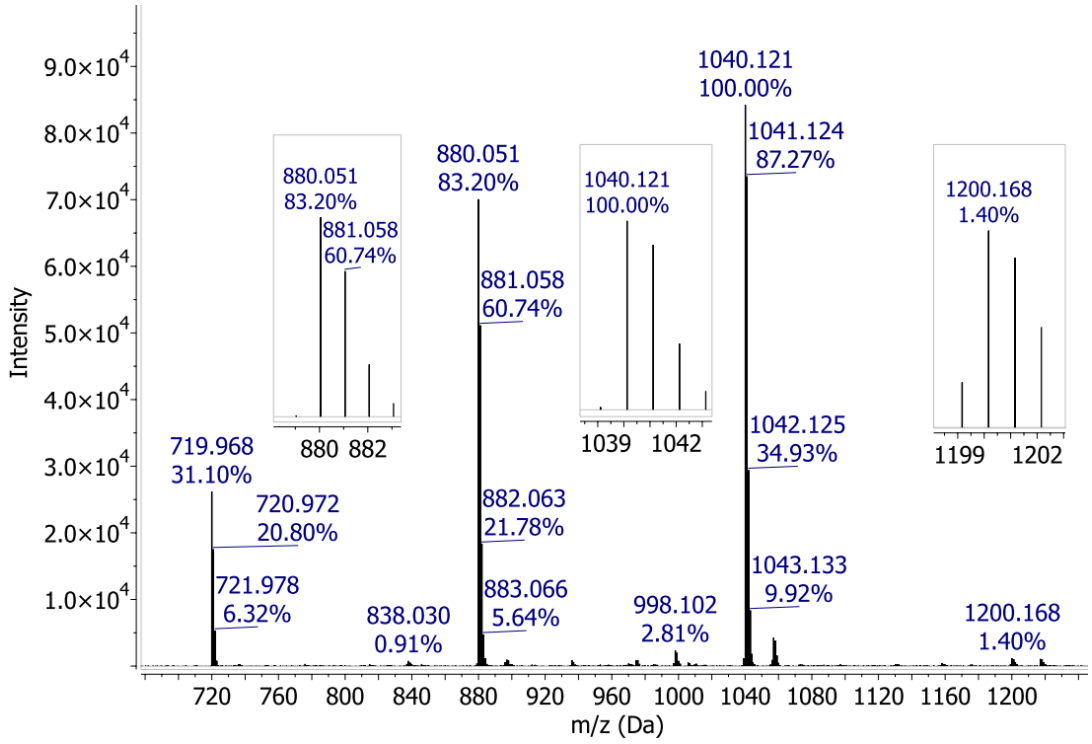


Figure S13. Negative ion MALDI mass spectrum of the reaction mixture with 1-phenylbutane-1,3-dione.

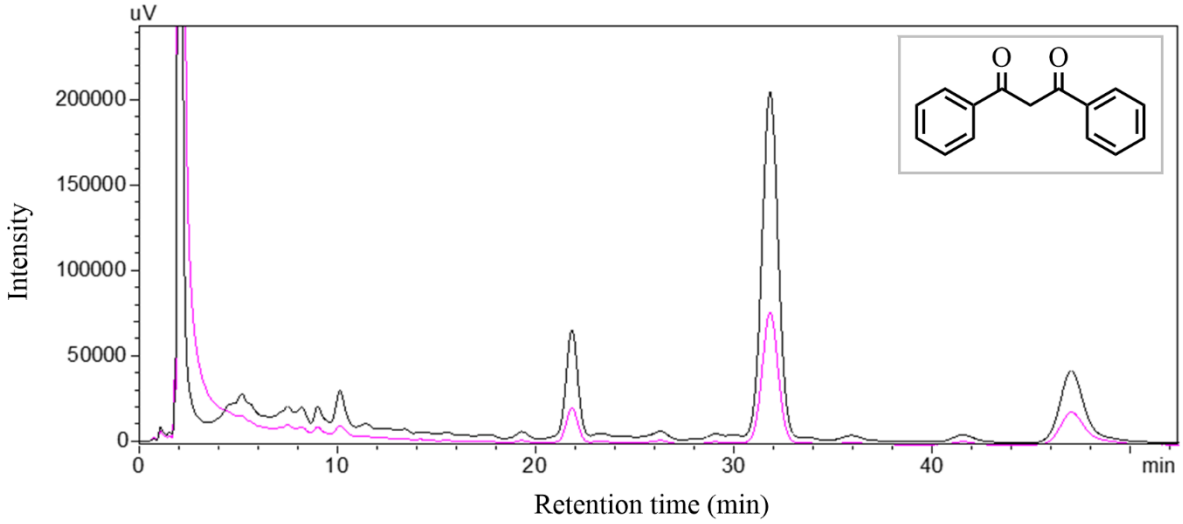


Figure S14. HPLC profile of the reaction mixture with 1,3-diphenylpropane-1,3-dione.

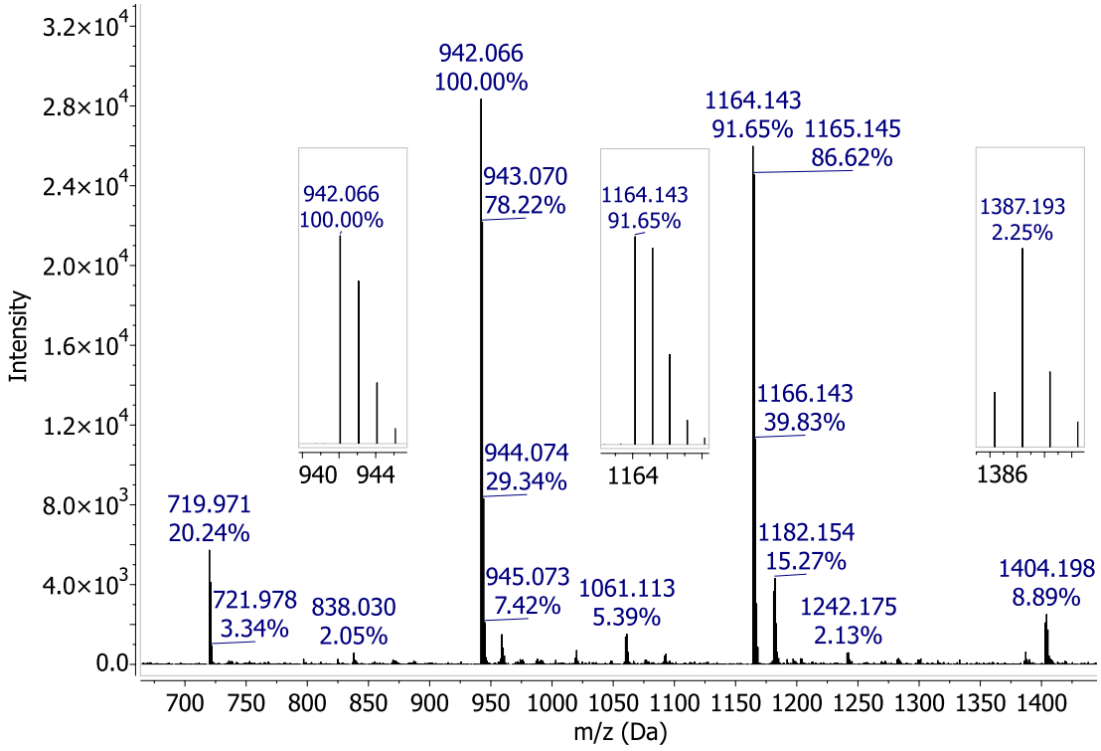


Figure S15. Negative ion MALDI mass spectrum of the reaction mixture with 1,3-diphenylpropane-1,3-dione.

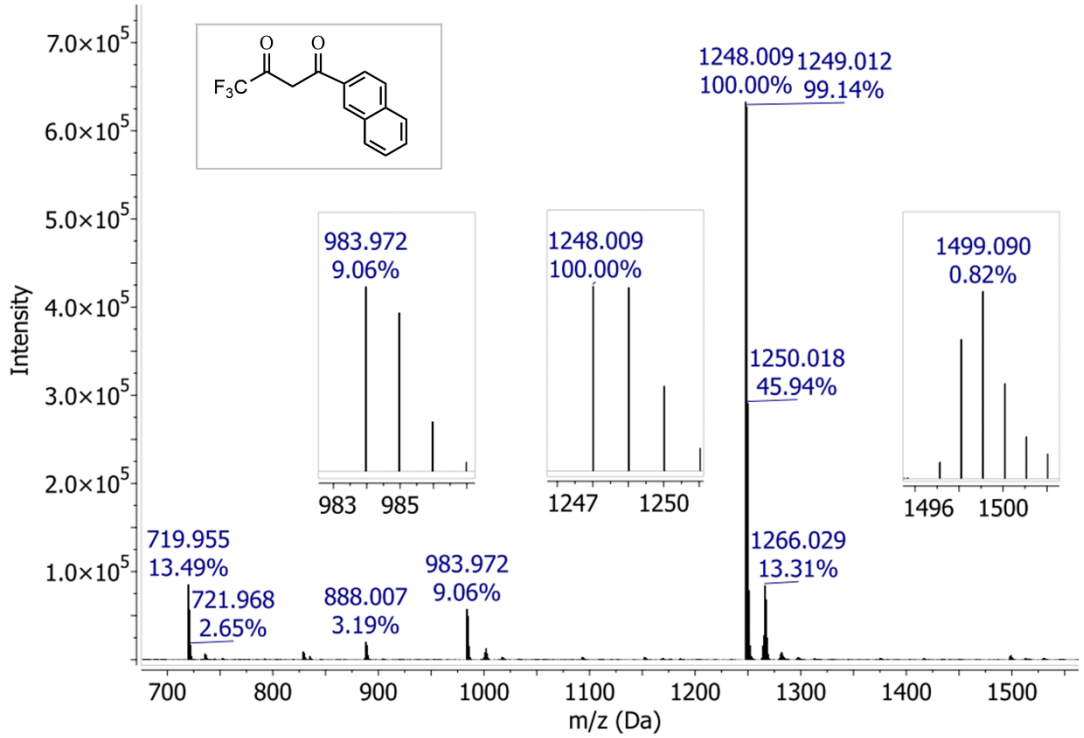


Figure S16. Negative ion MALDI mass spectrum of the reaction mixture with 4,4,4-trifluoro-1-(naphthalen-2-yl)butane-1,3-dione.

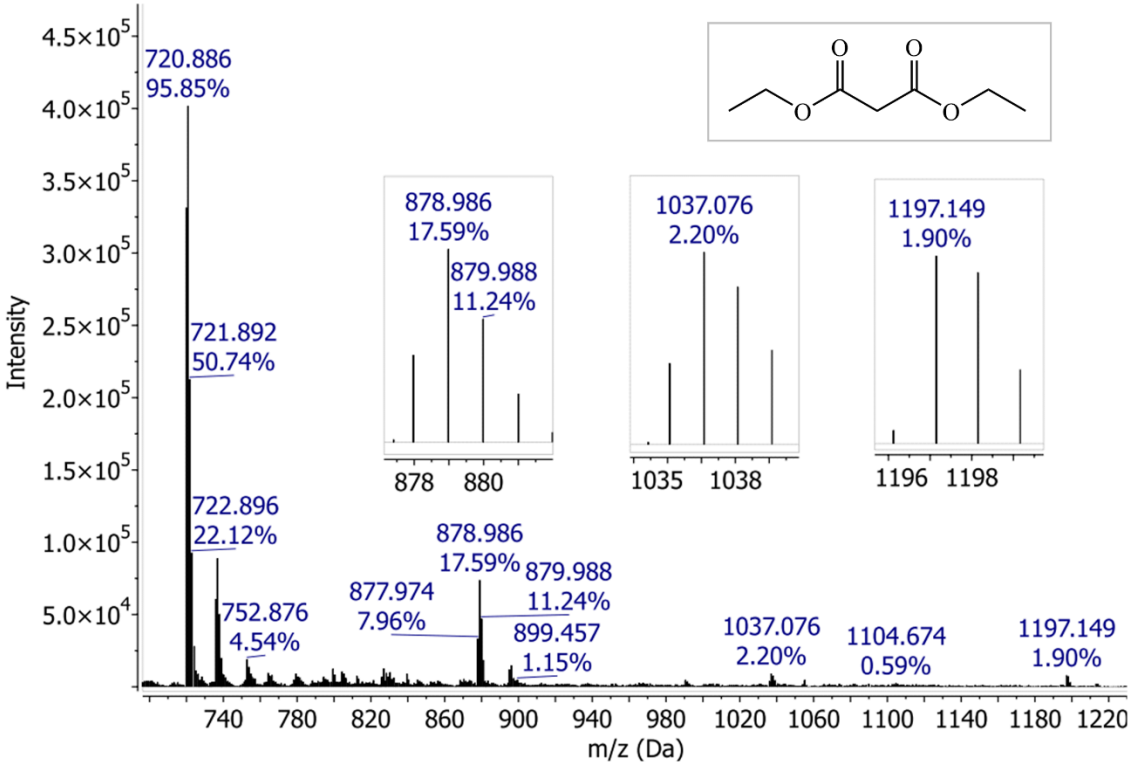


Figure S17. Negative ion MALDI mass spectrum of the reaction mixture with dimethyl malonate.

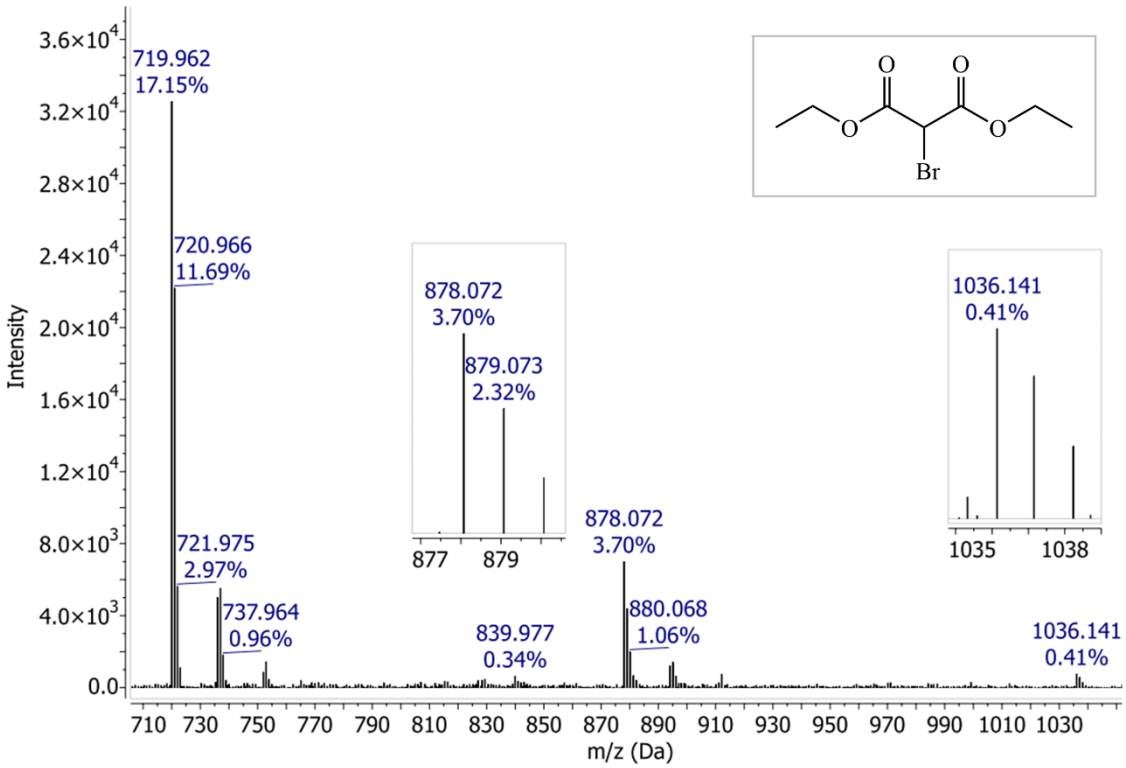
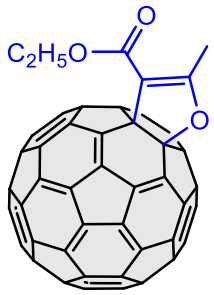


Figure S18. Negative ion MALDI mass spectrum of the reaction mixture with dimethyl 2-bromomalonate.

NMR and MALDI ToF mass spectra of compounds M, B1 and B2

Compound **Ma**



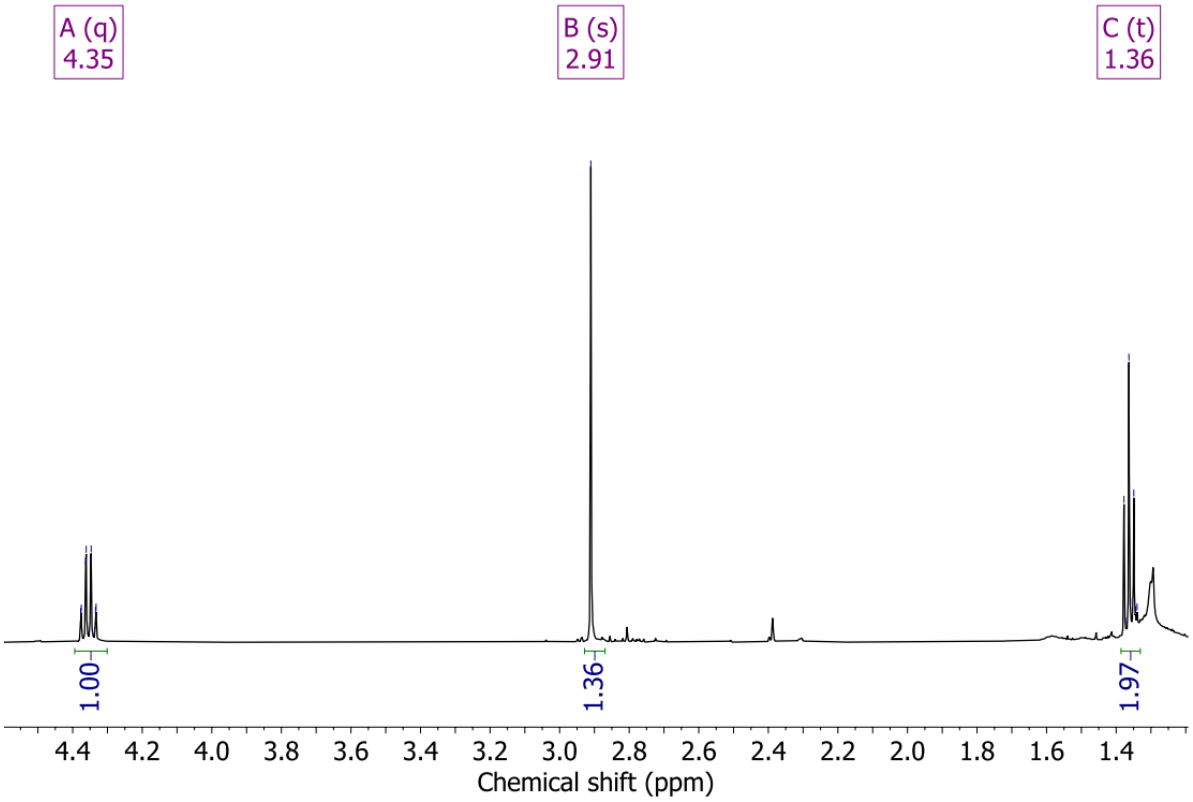


Figure S19. ^{1}H NMR spectrum of compound **Ma**.

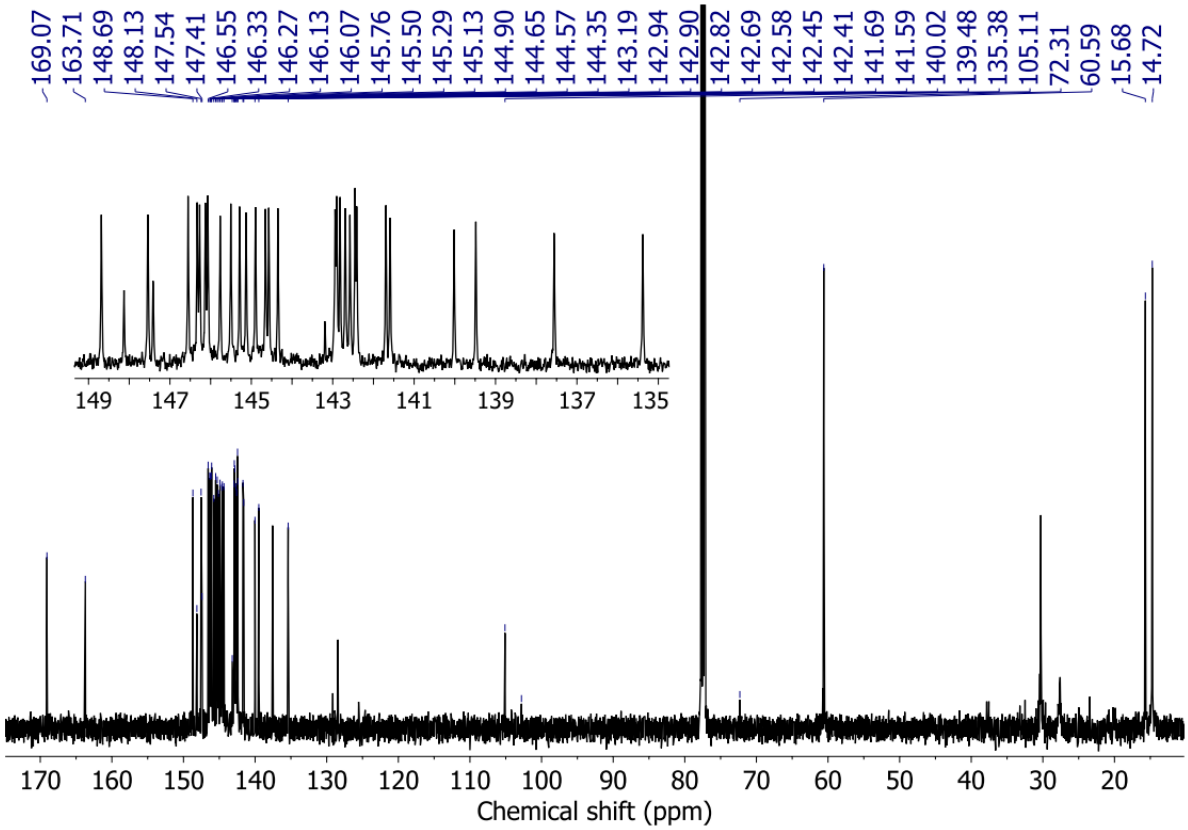


Figure S20. ^{13}C NMR spectrum of compound **Ma**.

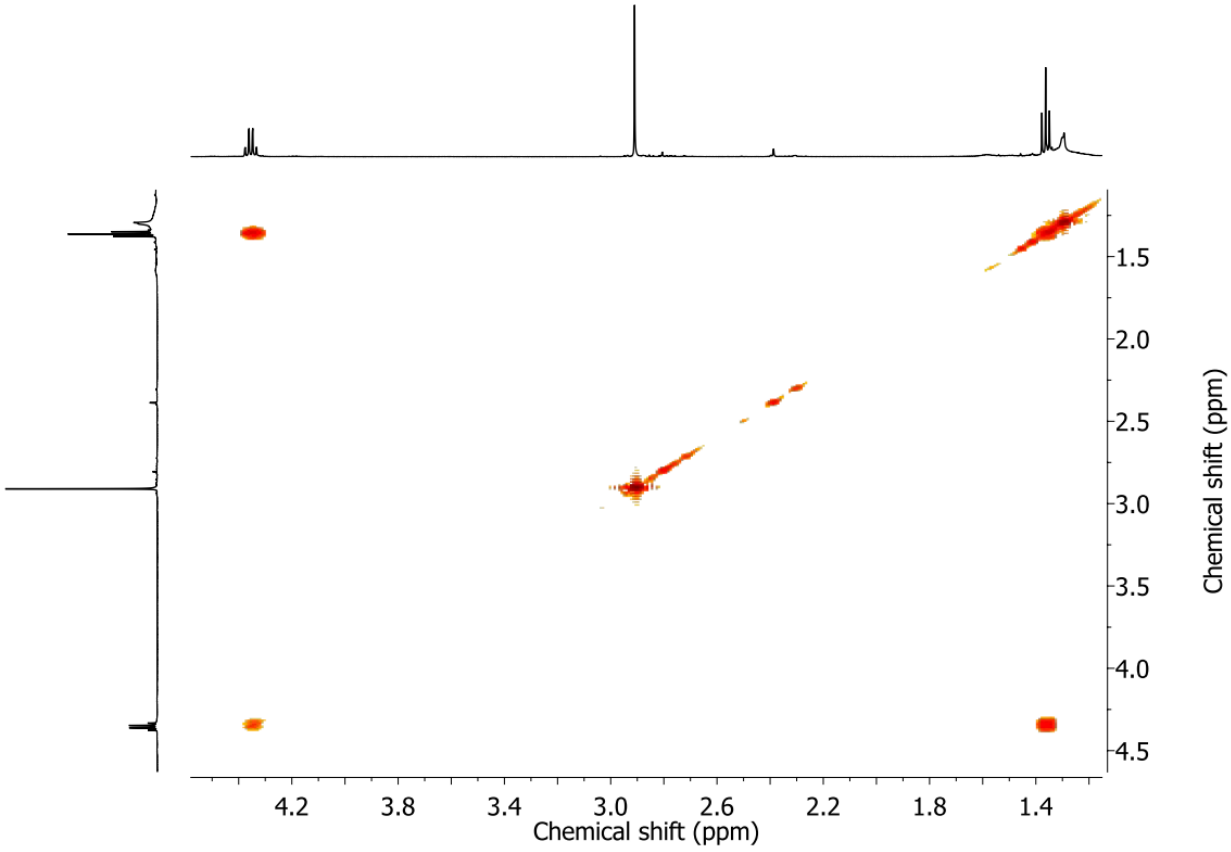


Figure S21. ^{1}H-^{1}H COSY NMR spectrum of compound **Ma**.

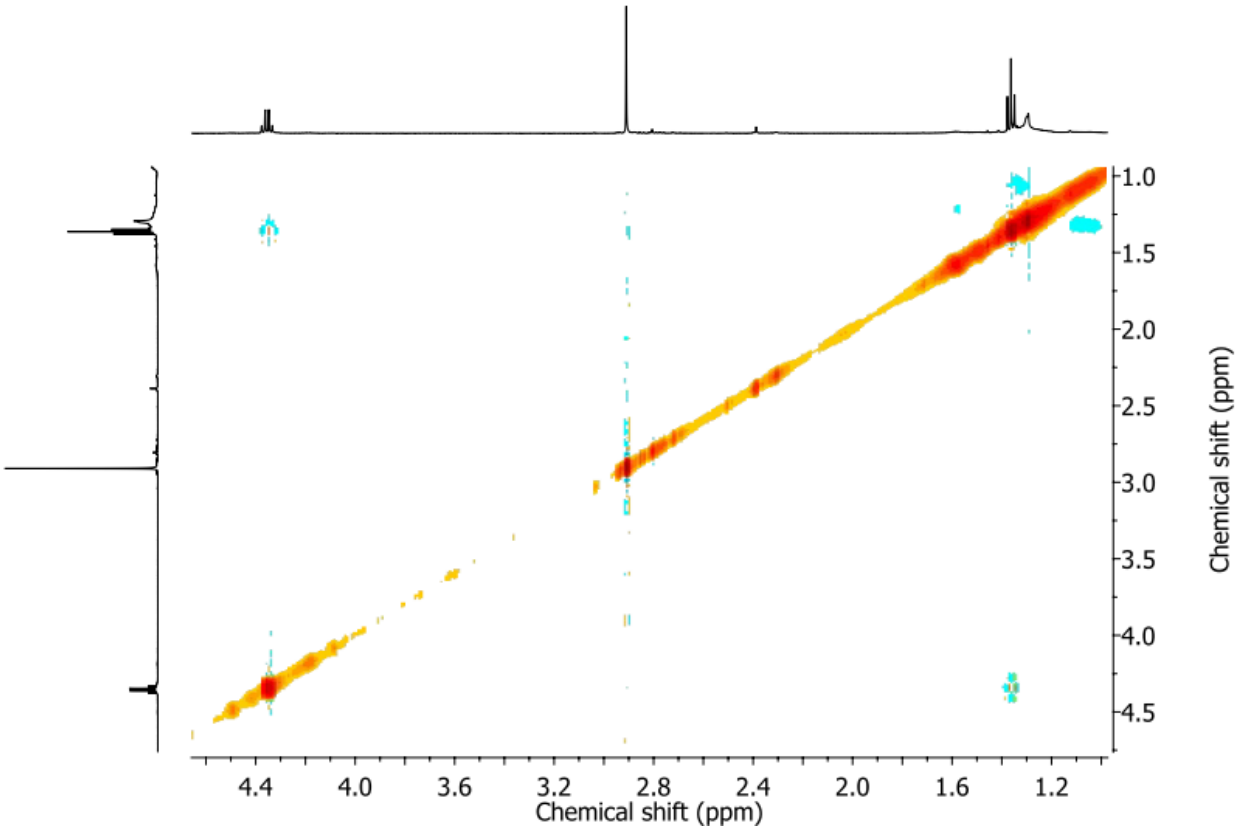


Figure S22. ^{1}H-^{1}H NOESY NMR spectrum of compound **Ma**.

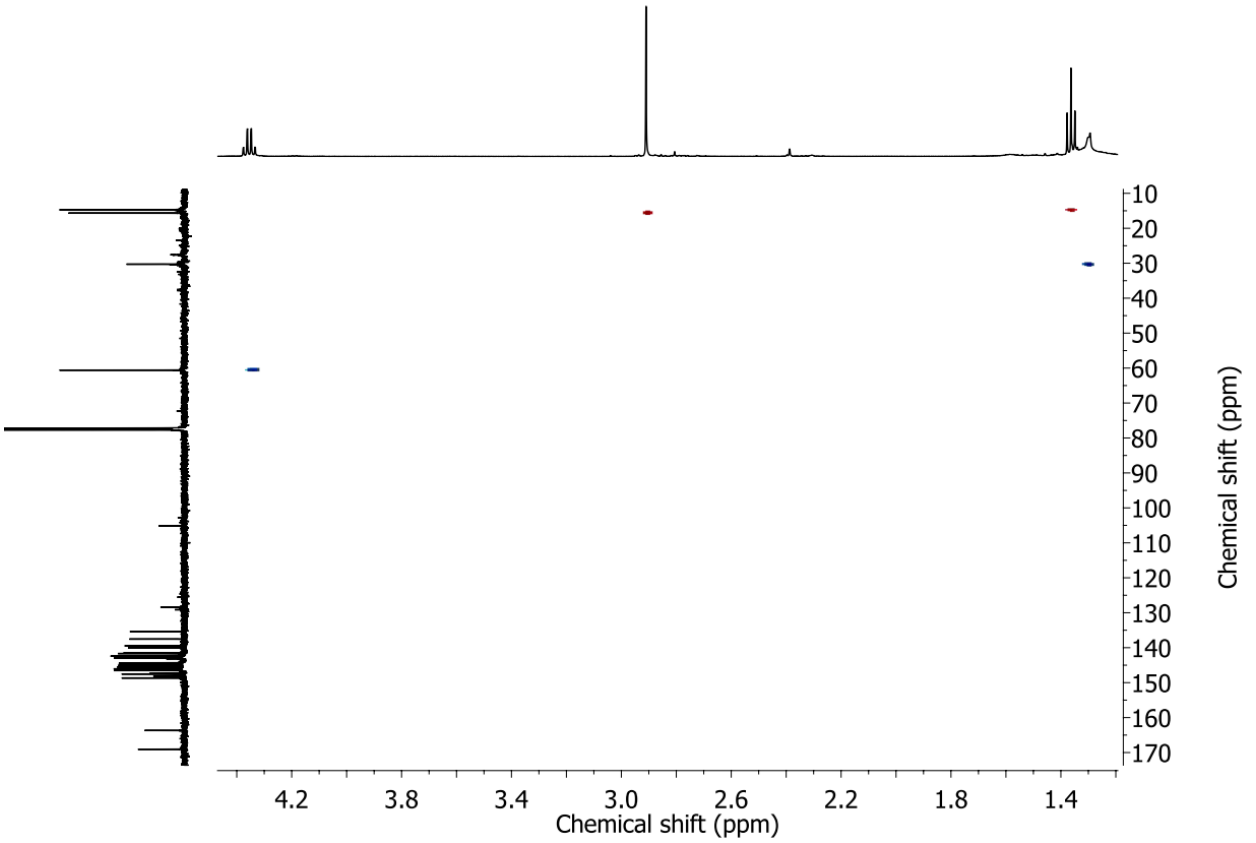


Figure S23. ^{1}H-^{13}C HSQC NMR spectrum of compound **Ma**.

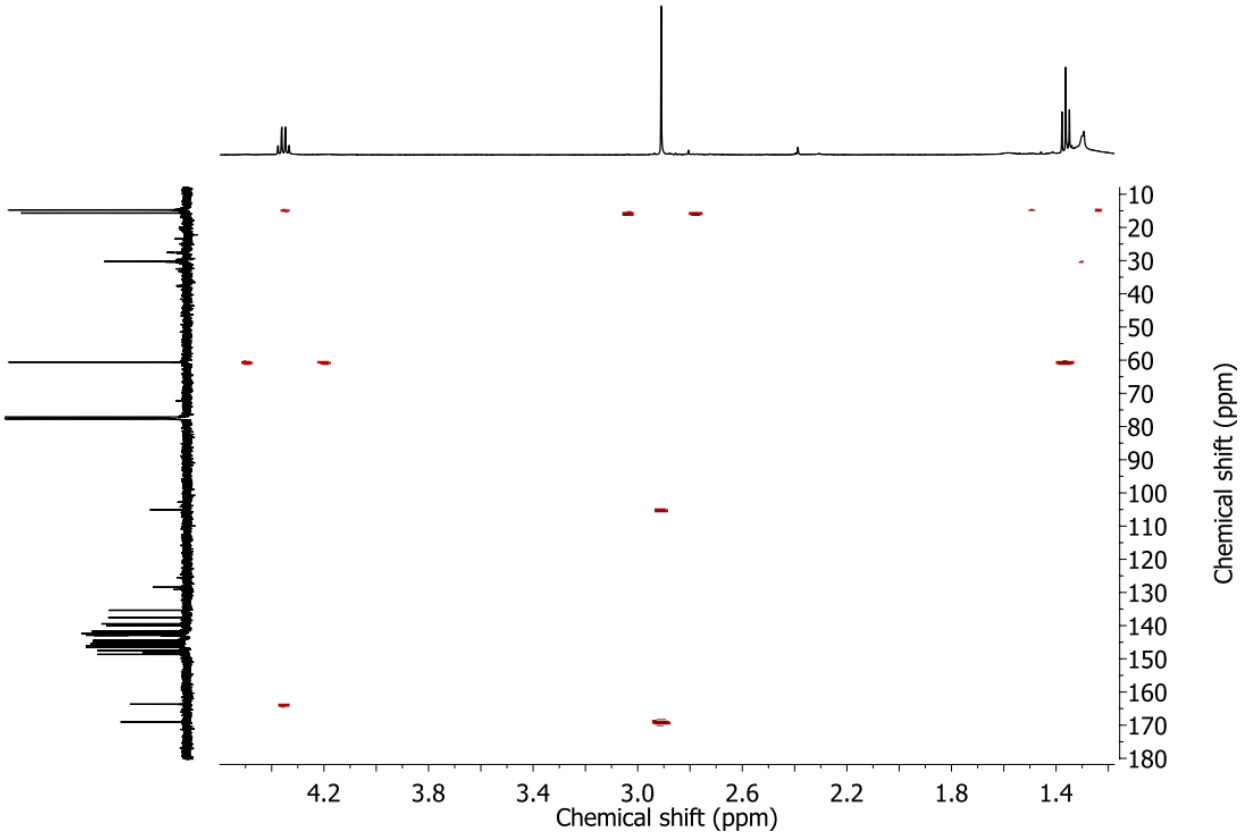


Figure S24. ^{1}H-^{13}C HMBC NMR spectrum of compound **Ma**.

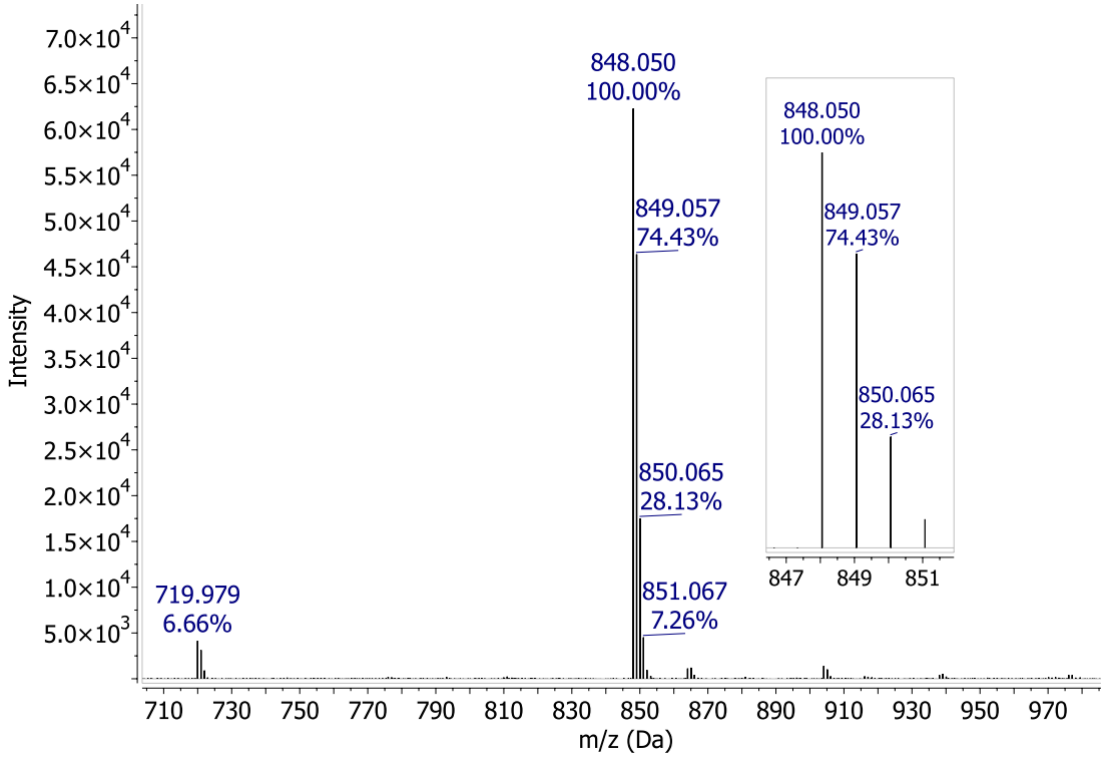
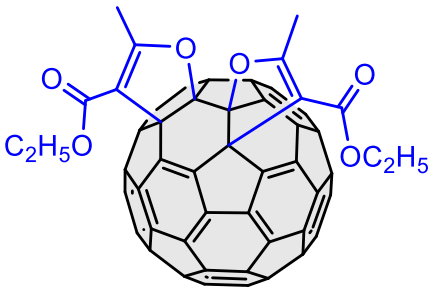


Figure S25. Negative ion MALDI mass spectrum of compound **Ma**.

Compound **B1a**



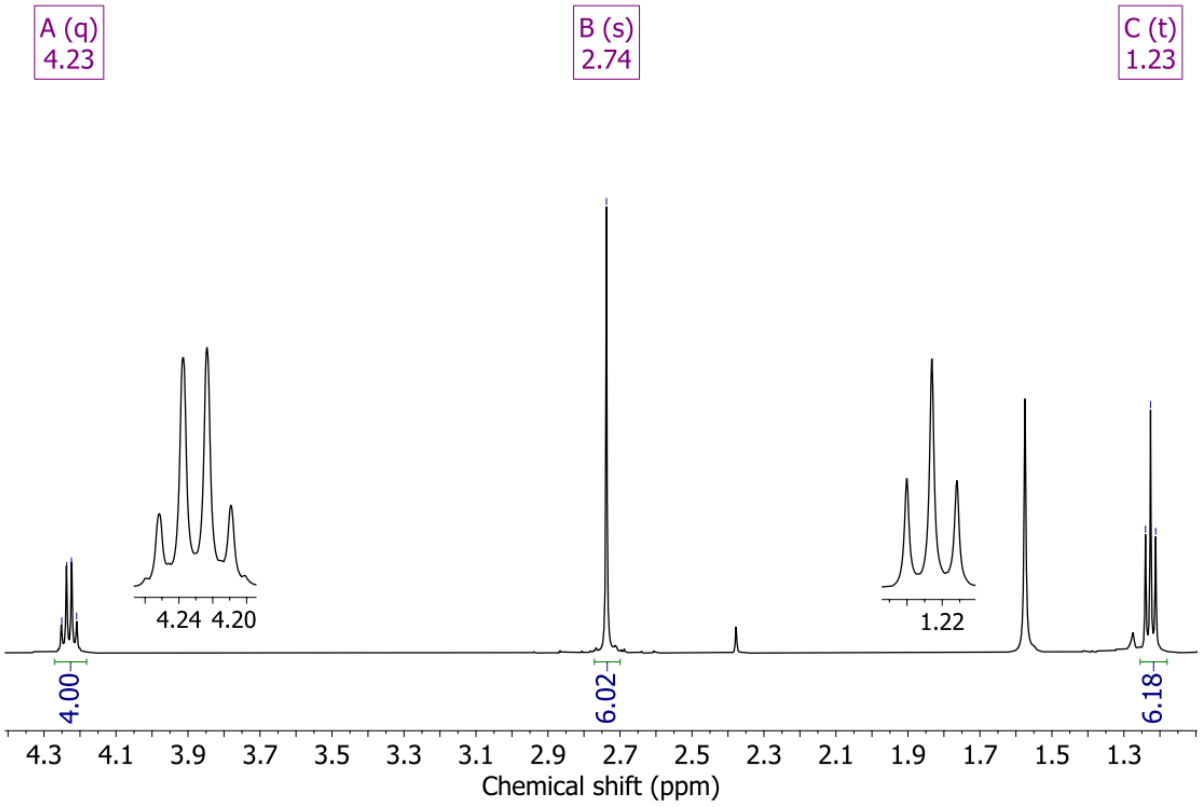


Figure S26. ^{1}H NMR spectrum of compound **B1a**.

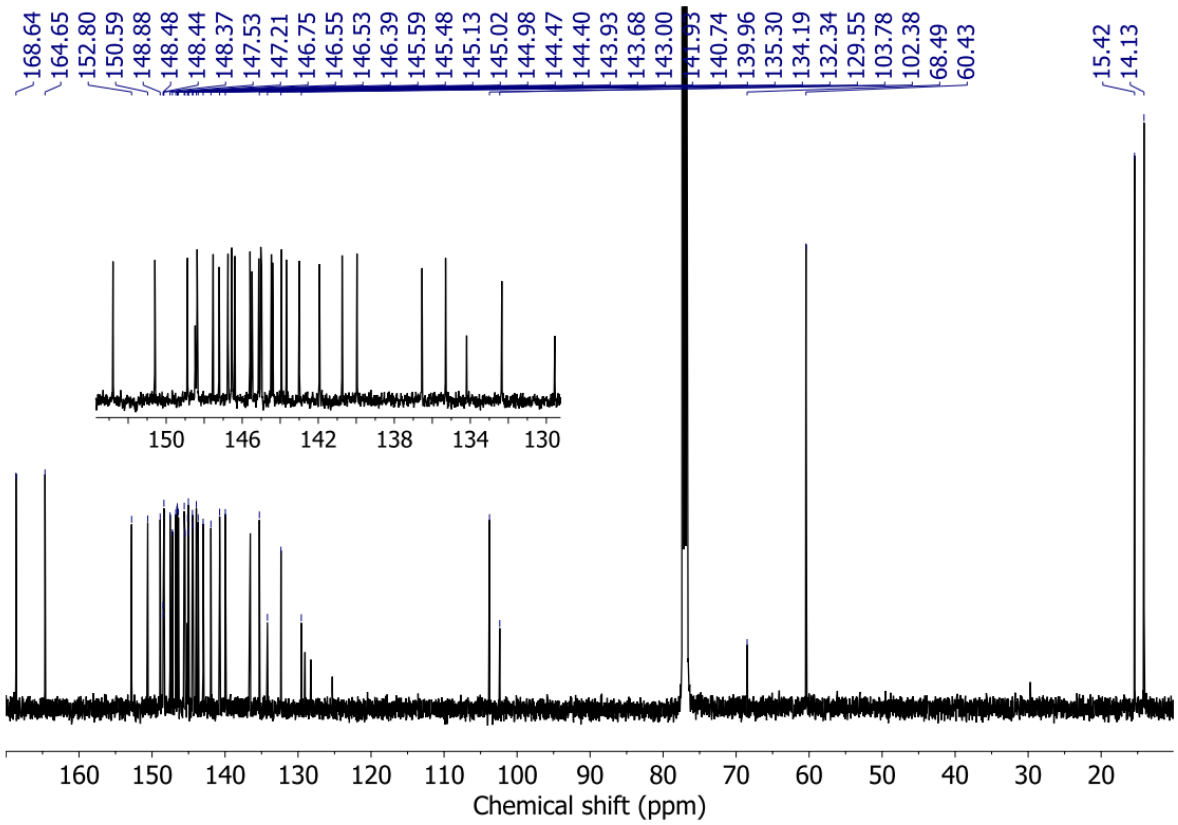


Figure S27. ^{13}C NMR spectrum of compound **B1a**.

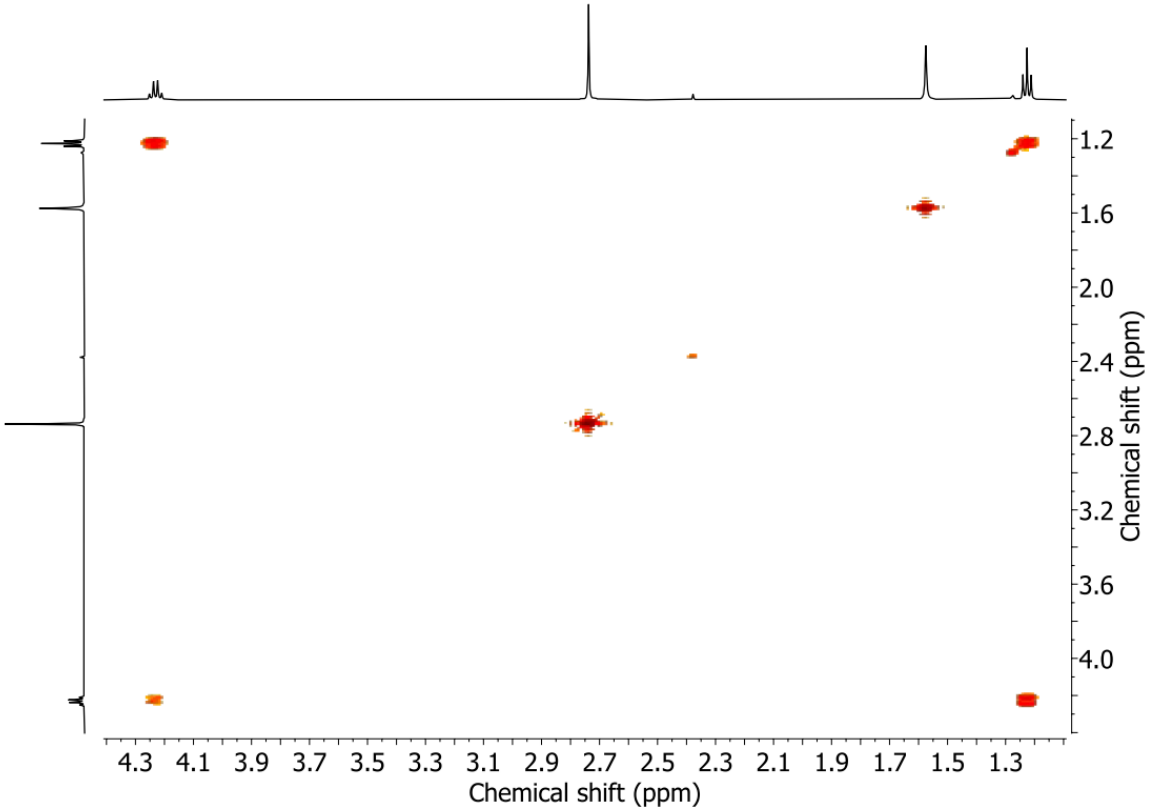


Figure S28. ^{1}H-^{1}H COSY NMR spectrum of compound **B1a**.

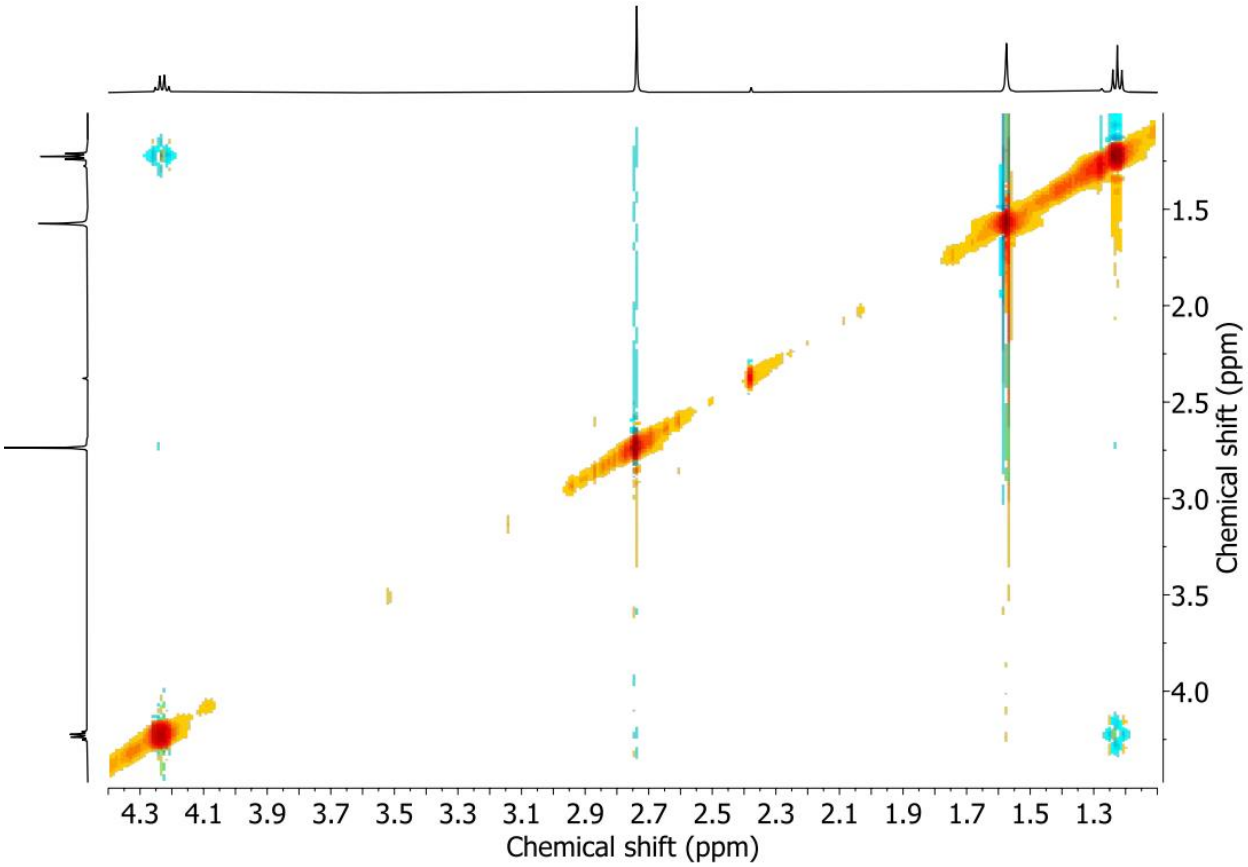


Figure S29. ^{1}H-^{1}H NOESY NMR spectrum of compound **B1a**.

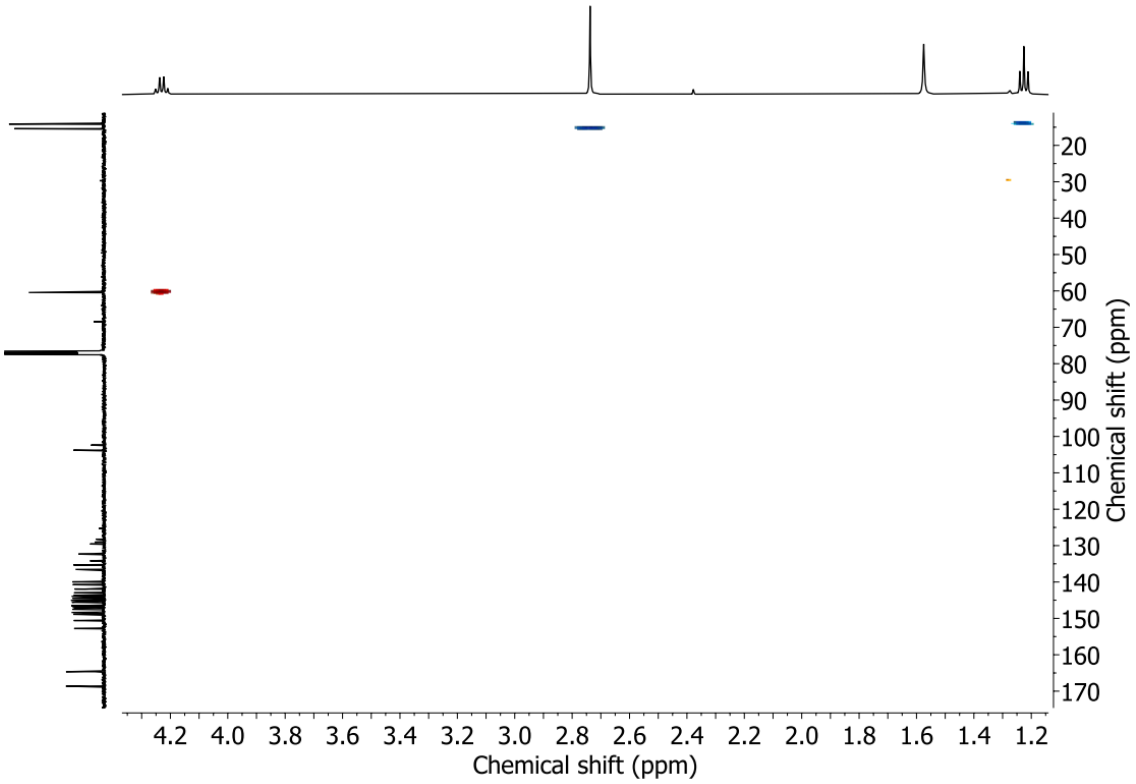


Figure S30. ^{1}H-^{13}C HSQC NMR spectrum of compound **B1a**.

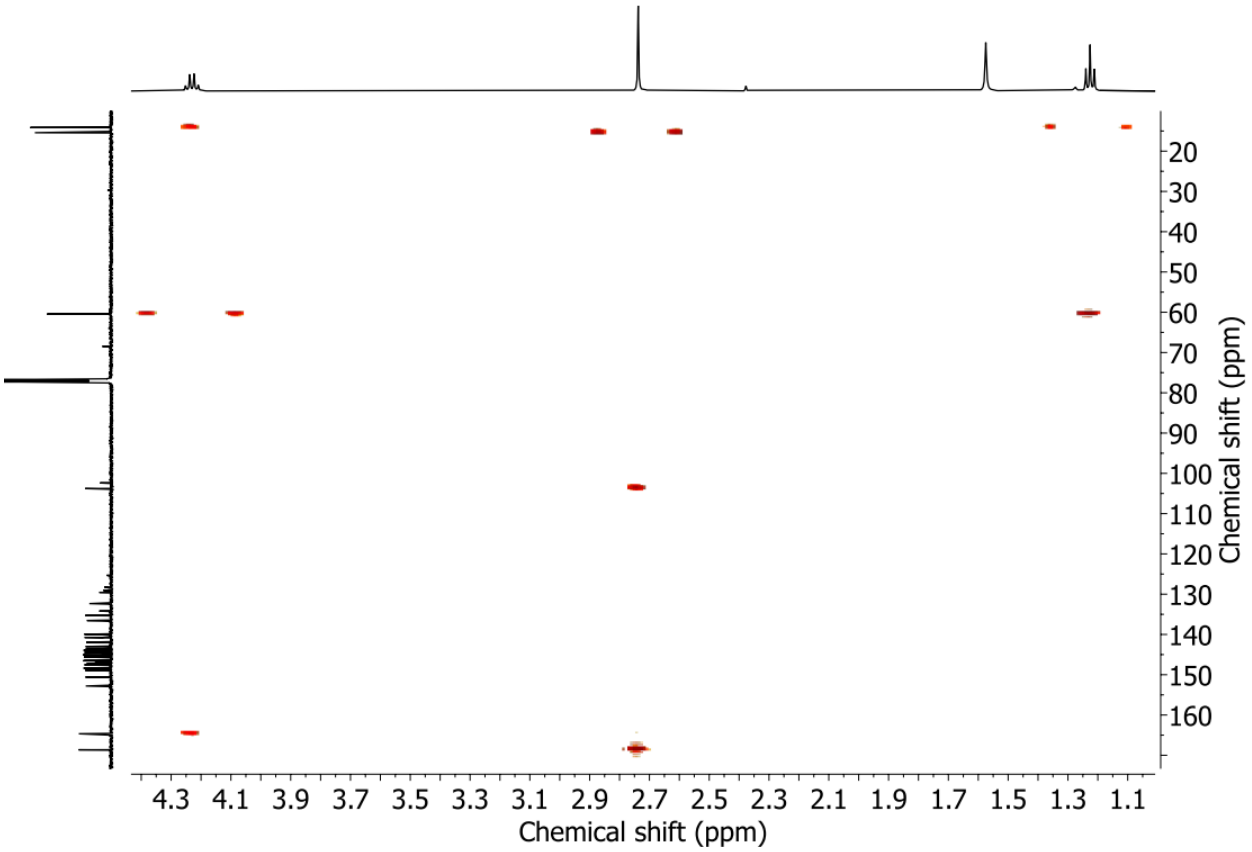


Figure S31. ^{1}H-^{13}C HMBC NMR spectrum of compound **B1a**.

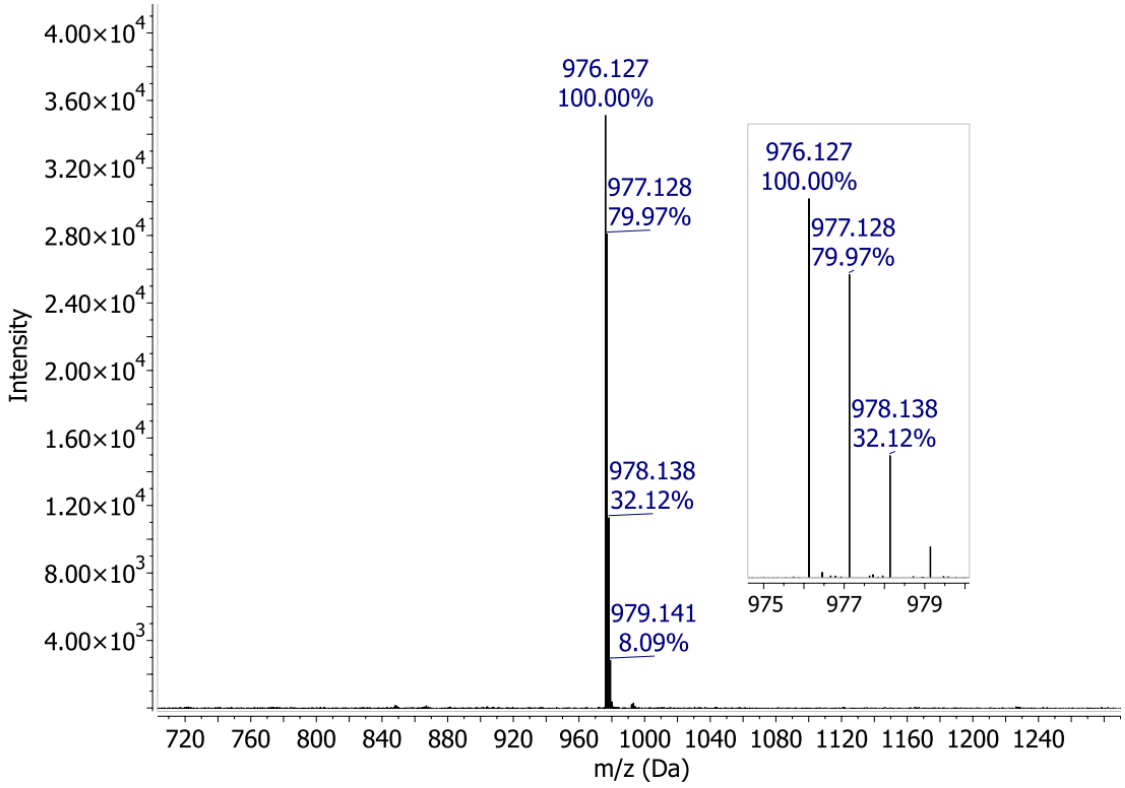
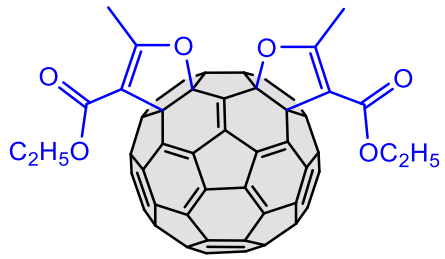


Figure S32. Negative ion MALDI mass spectrum of compound **B1a**.

Compound **B2a**



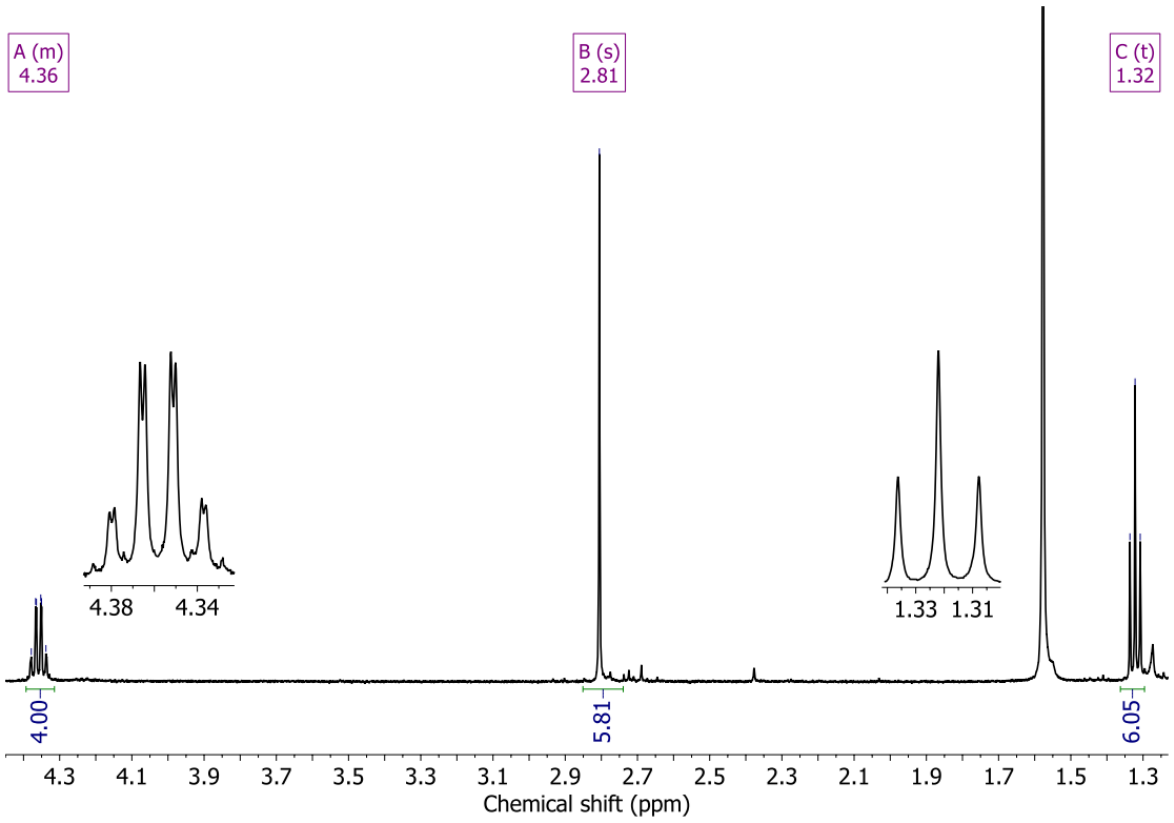


Figure S33. ^{1}H NMR spectrum of compound **B2a**.

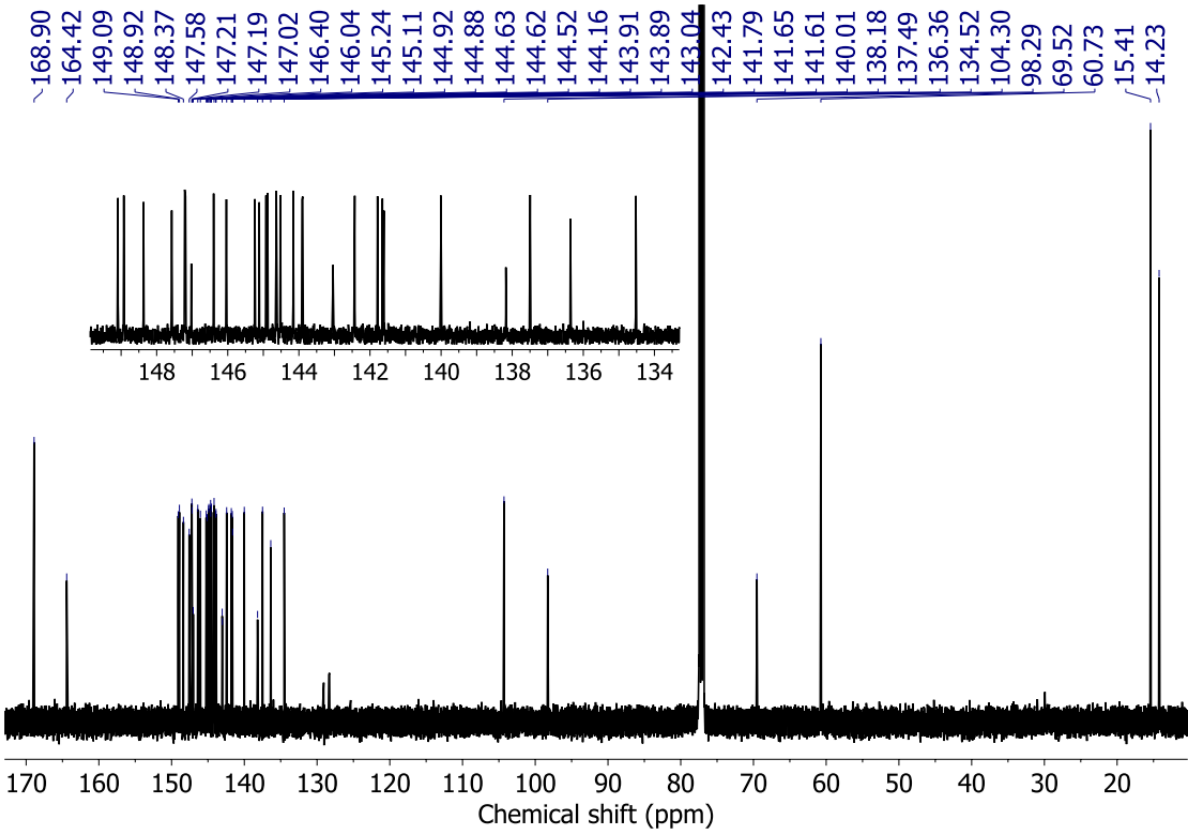


Figure S34. ^{13}C NMR spectrum of compound **B2a**.

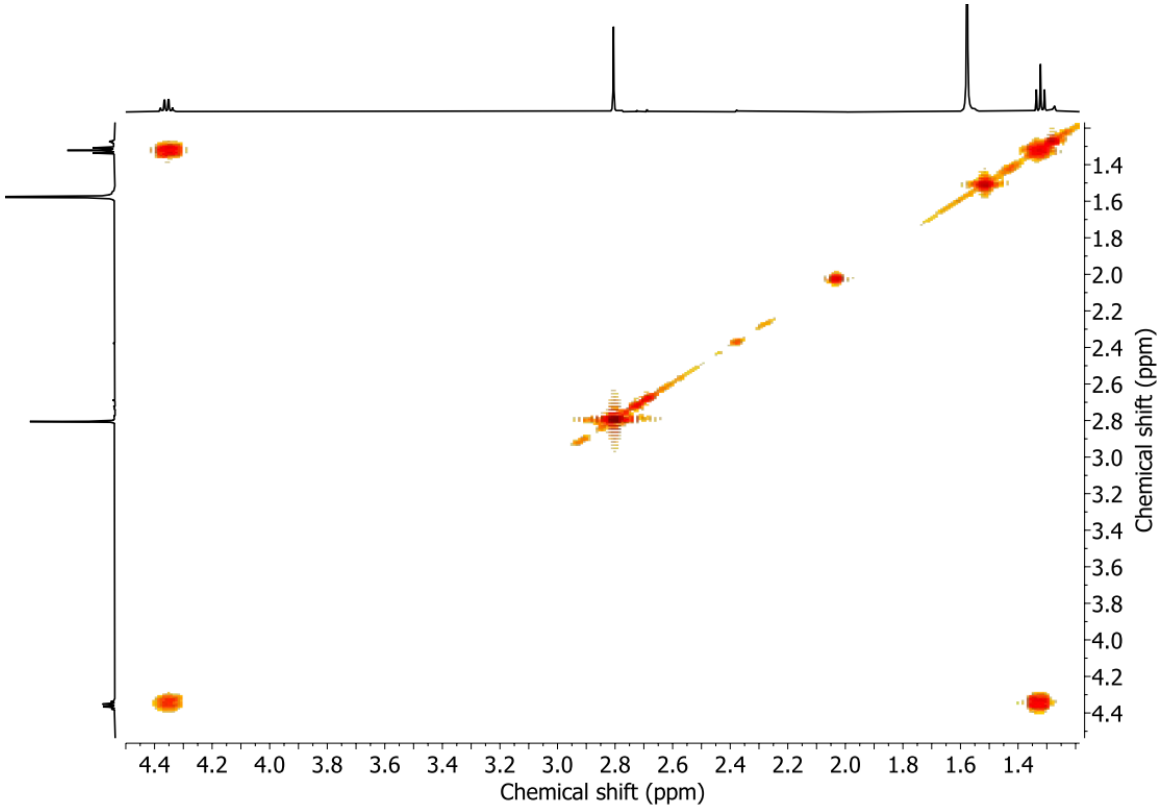


Figure S35. ^{1}H-^{1}H COSY NMR spectrum of compound **B2a**.

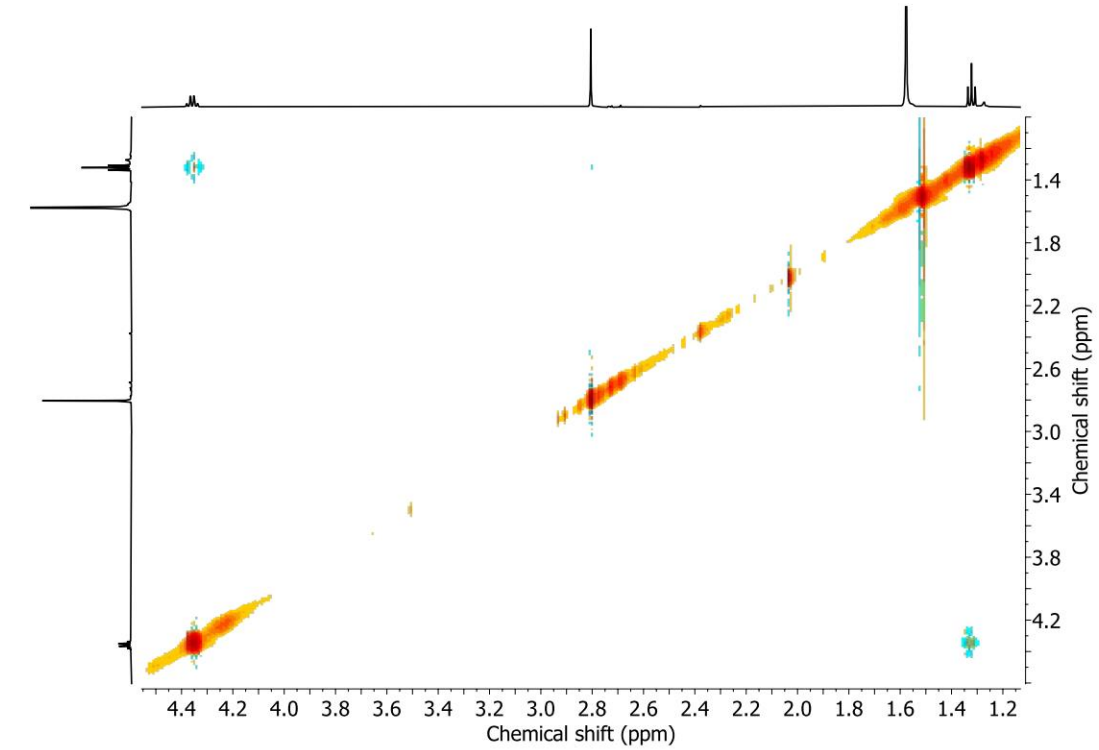


Figure S36. ^{1}H-^{1}H NOESY NMR spectrum of compound **B2a**.

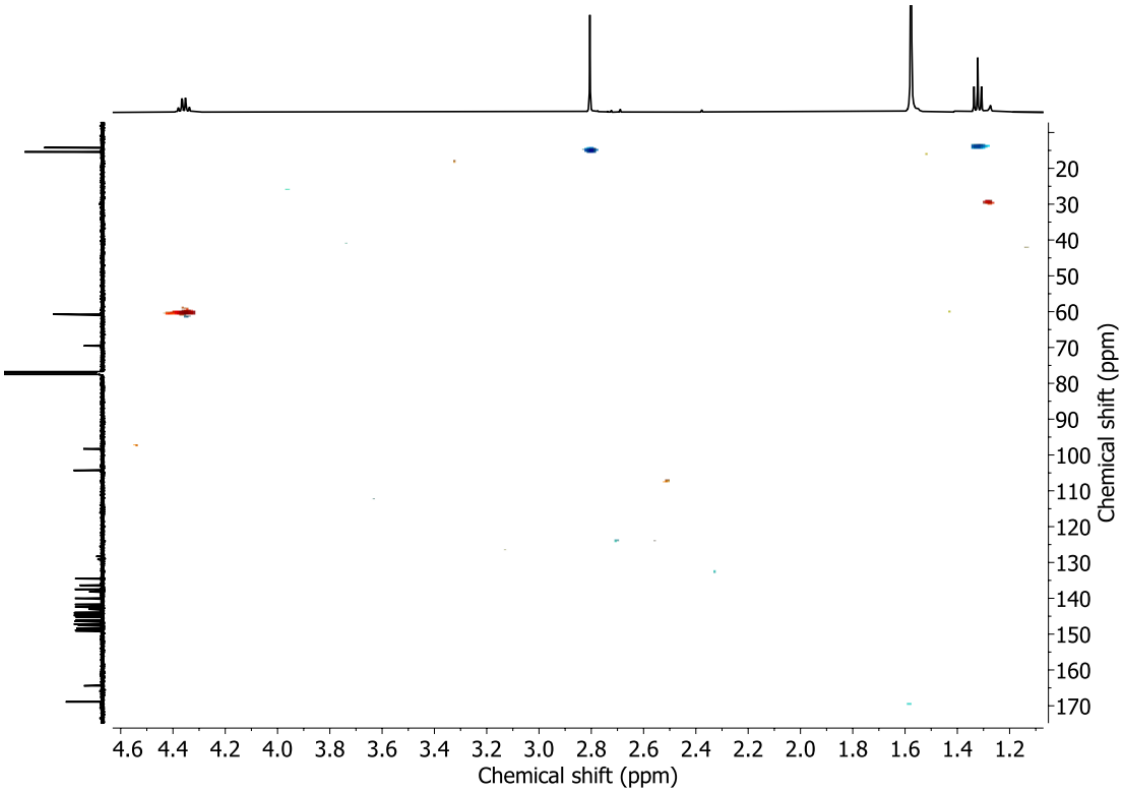


Figure S37. ^{1}H-^{13}C HSQC NMR spectrum of compound **B2a**.

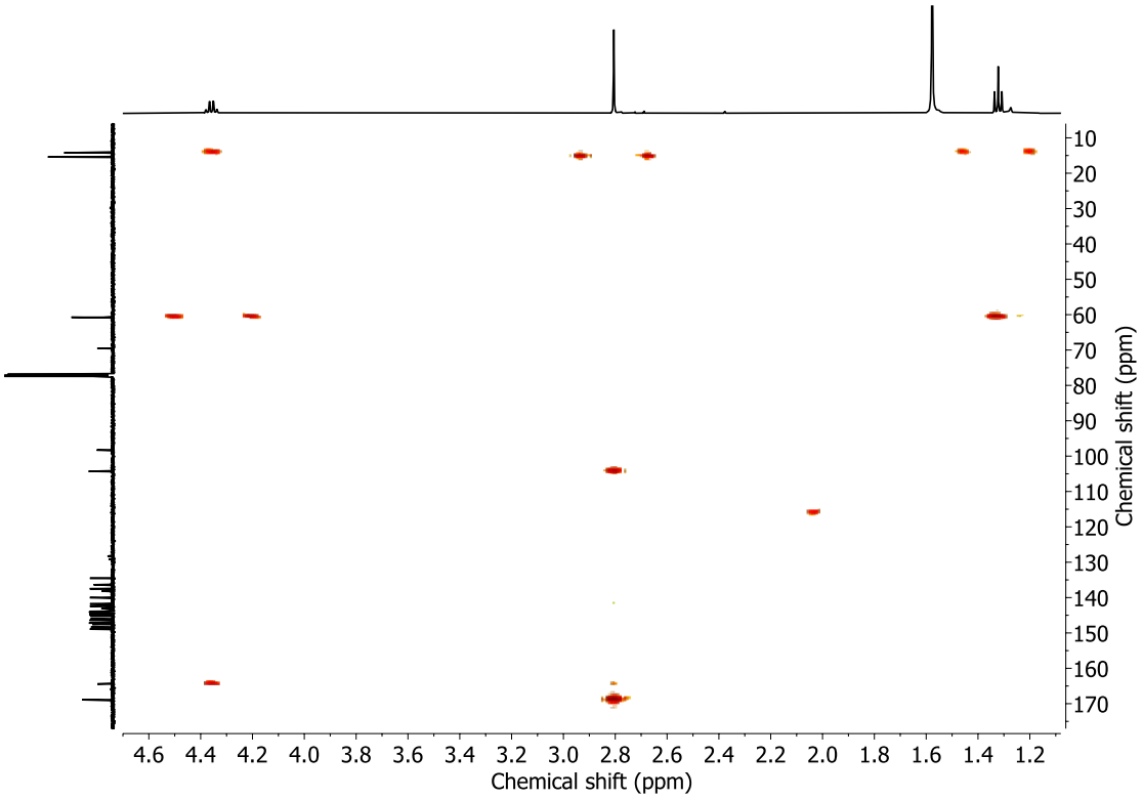


Figure S38. ^{1}H-^{13}C HMBC NMR spectrum of compound **B2a**.

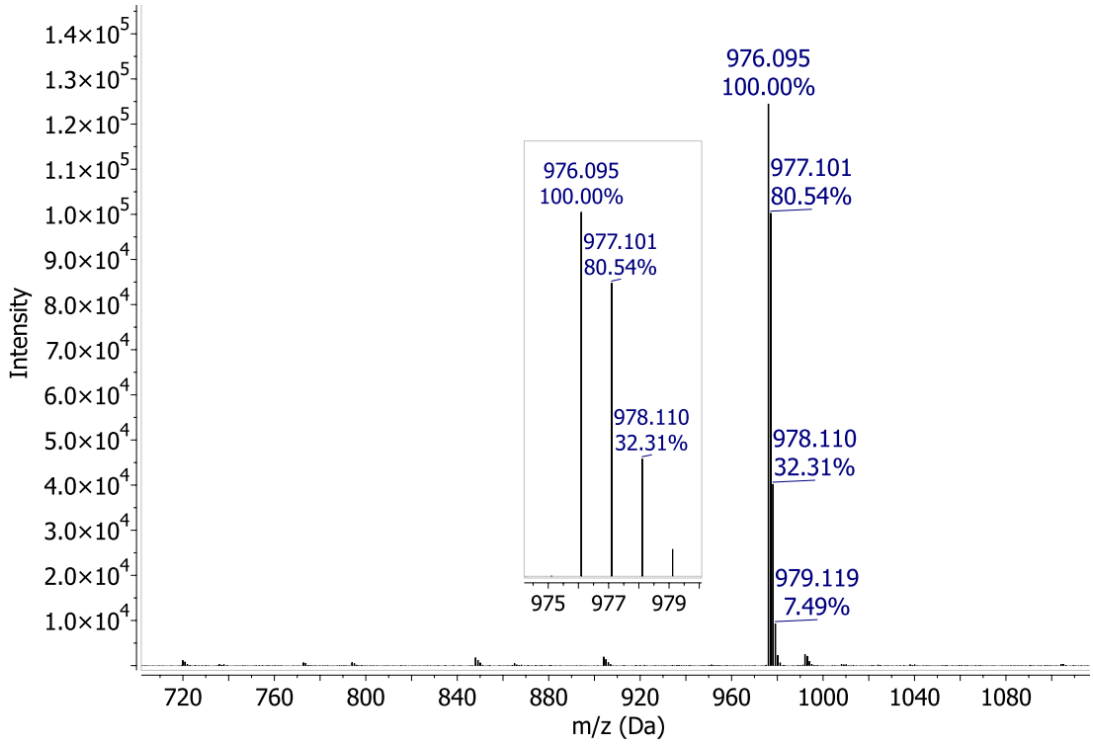
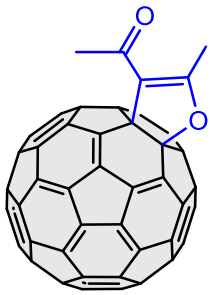


Figure S39. Negative ion MALDI mass spectrum of compound **B2a**.

Compound **Mb**



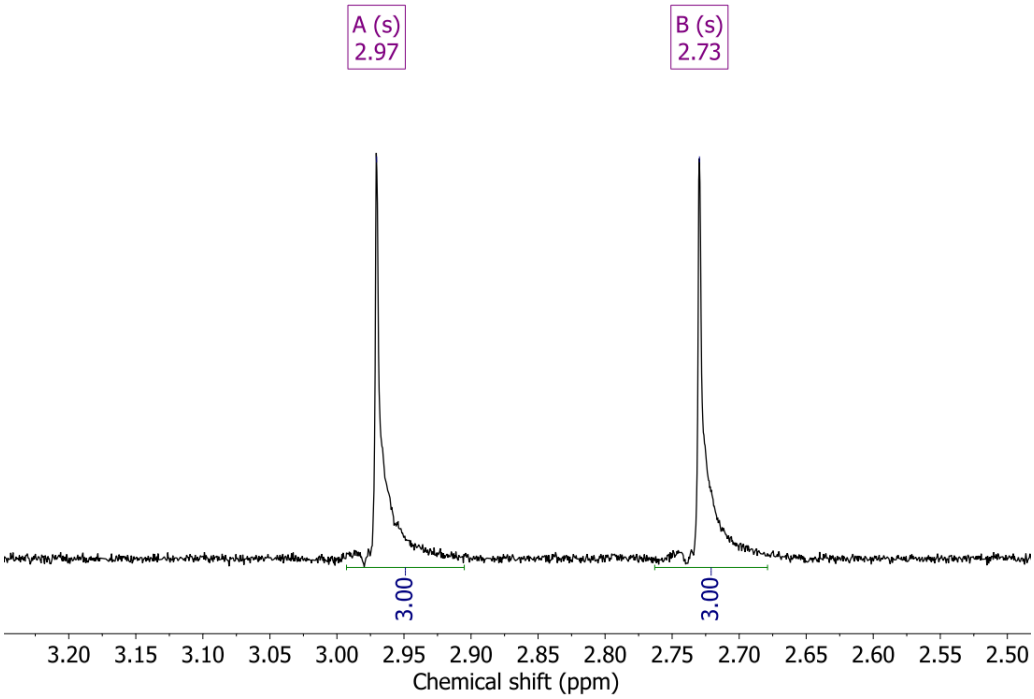


Figure S40. ^{1}H NMR spectrum of compound **Mb**.

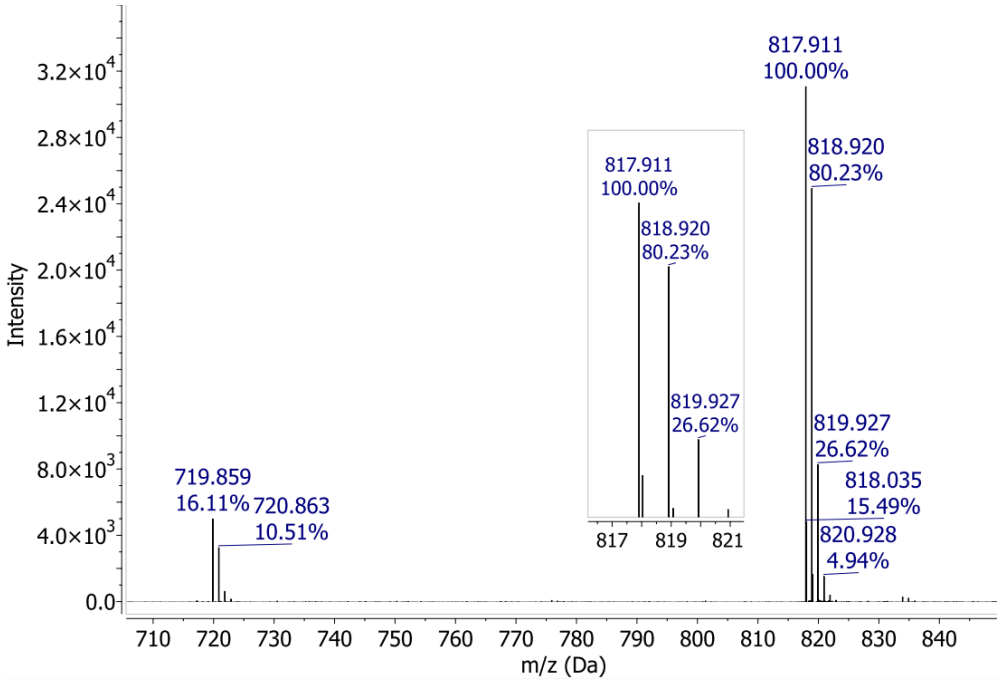
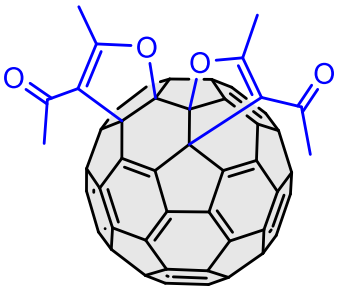


Figure S41. Negative ion MALDI mass spectrum of compound **Mb**.

Compound **B1b**



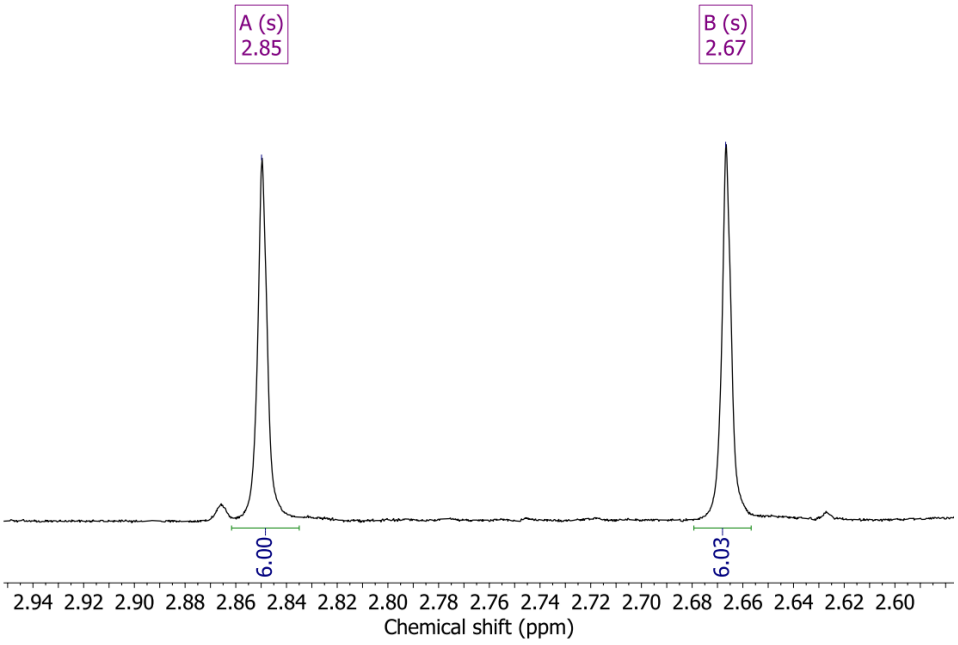


Figure S42. ^{1}H NMR spectrum of compound **B1b**.

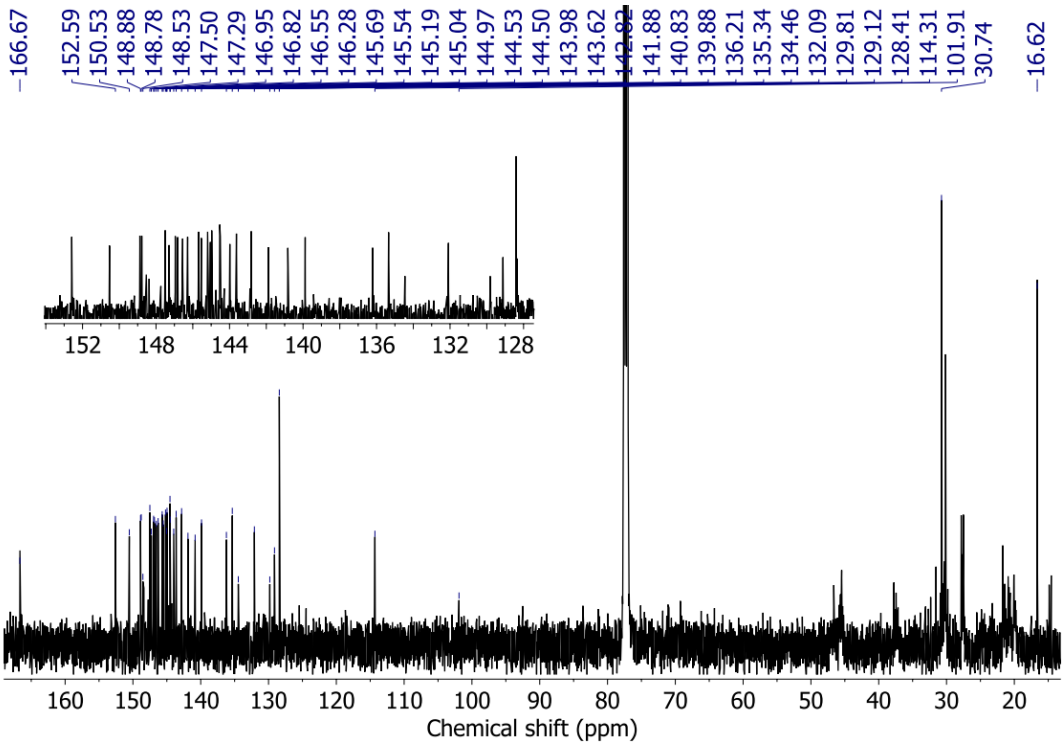


Figure S43. ^{13}C NMR spectrum of compound **B1b**.

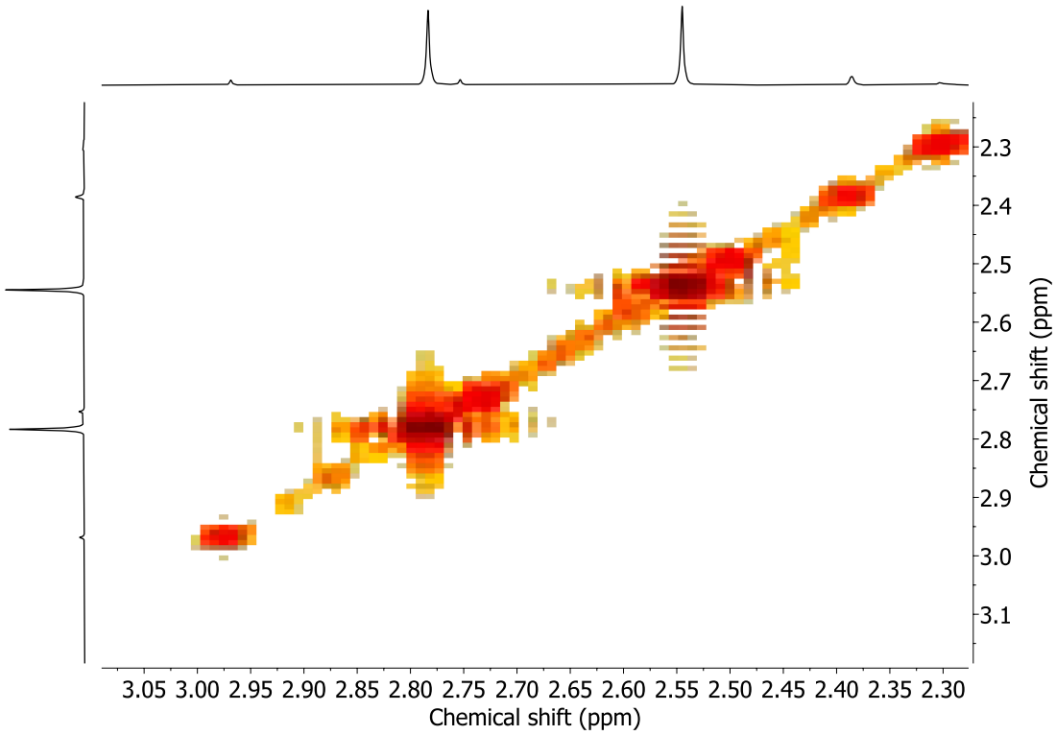


Figure S44. ^{1}H-^{1}H COSY NMR spectrum of compound **B1b**.

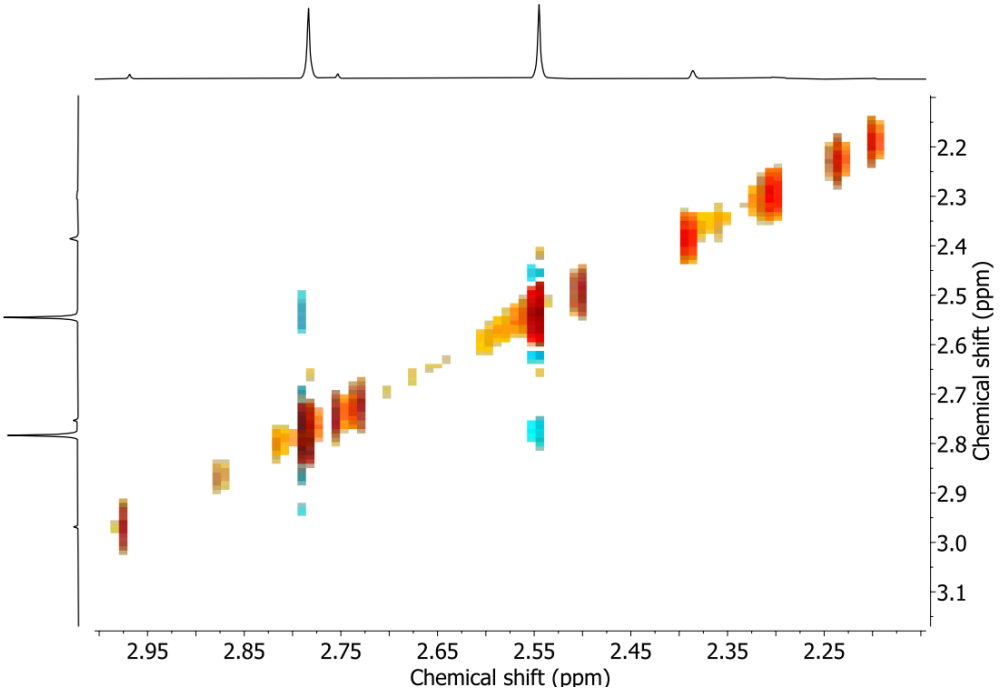


Figure S45. ^{1}H-^{1}H NOESY NMR spectrum of compound **B1b**.

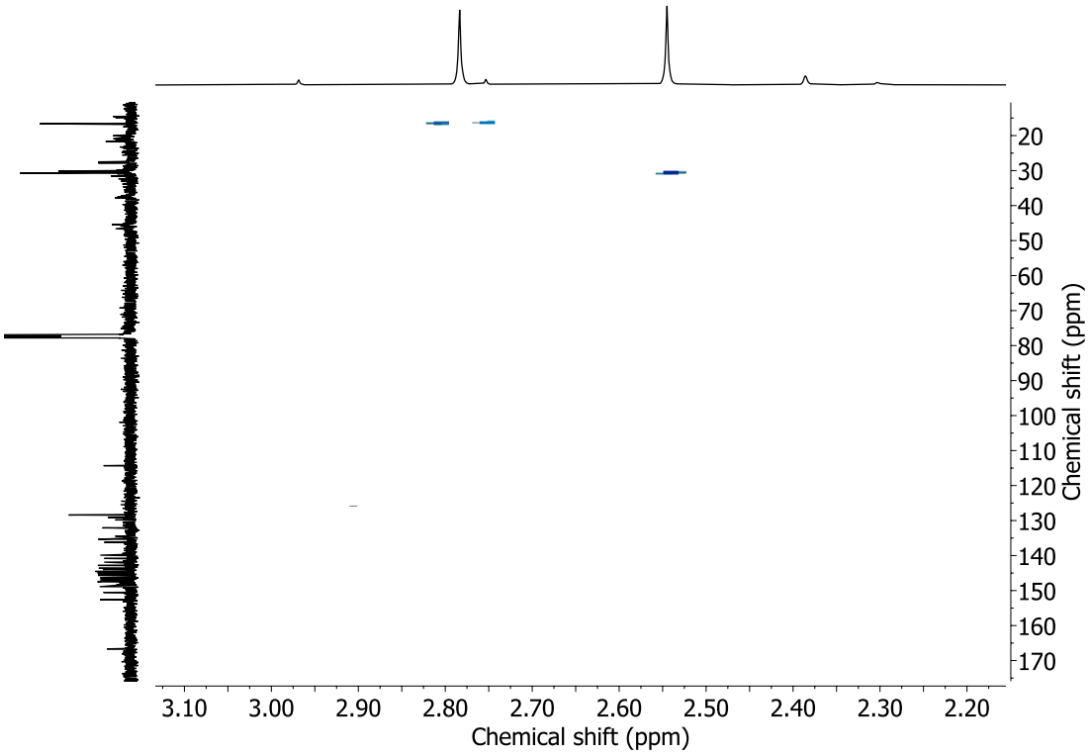


Figure S46. ^{1}H-^{13}C HSQC NMR spectrum of compound **B1b**.

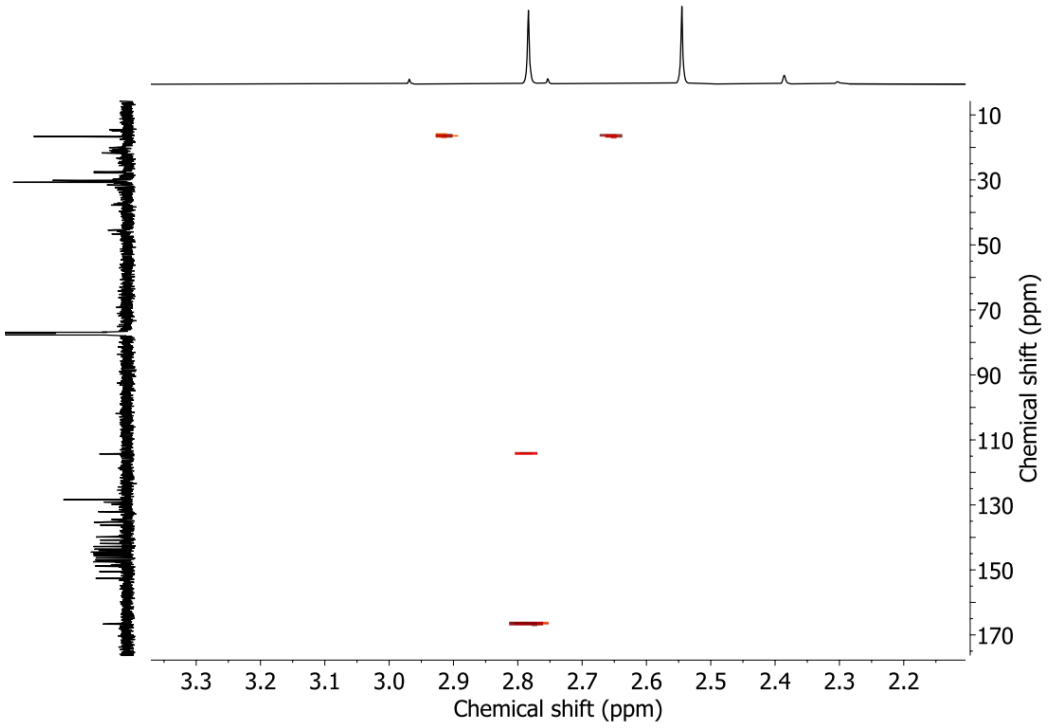


Figure S47. ^{1}H-^{13}C HMBC NMR spectrum of compound **B1b**.

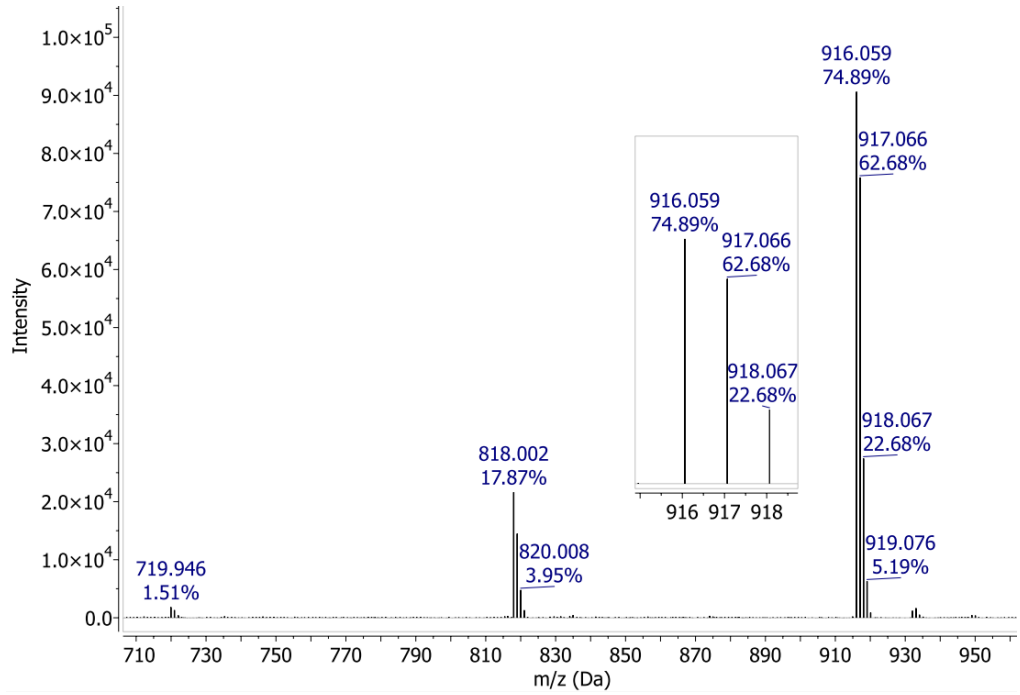
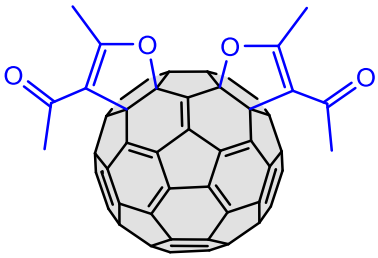


Figure S48. Negative ion MALDI mass spectrum of compound **B1b**.

Compound **B2b**



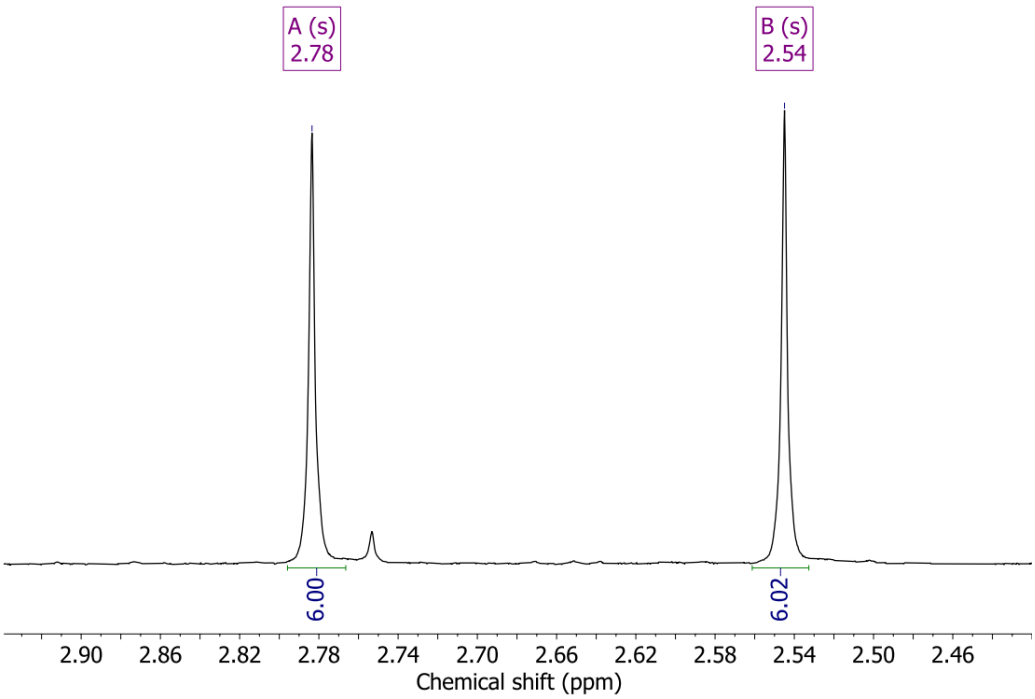


Figure S49. ^{1}H NMR spectrum of compound **B2b**.

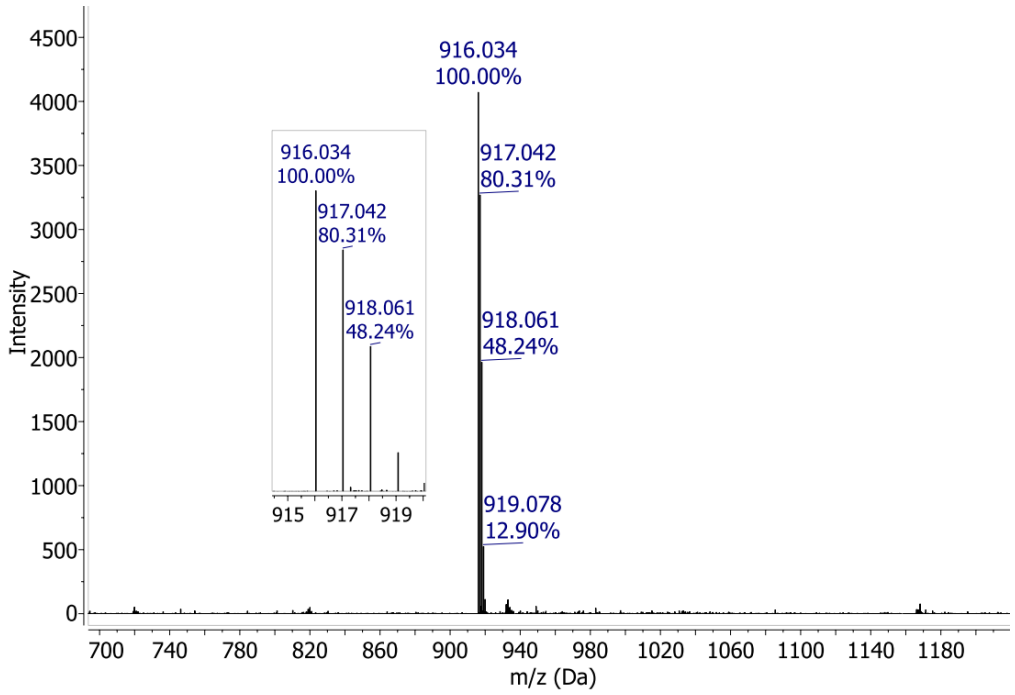


Figure S50. Negative ion MALDI mass spectrum of compound **B2b**.

UV-vis spectra of compounds M, B1 and B2

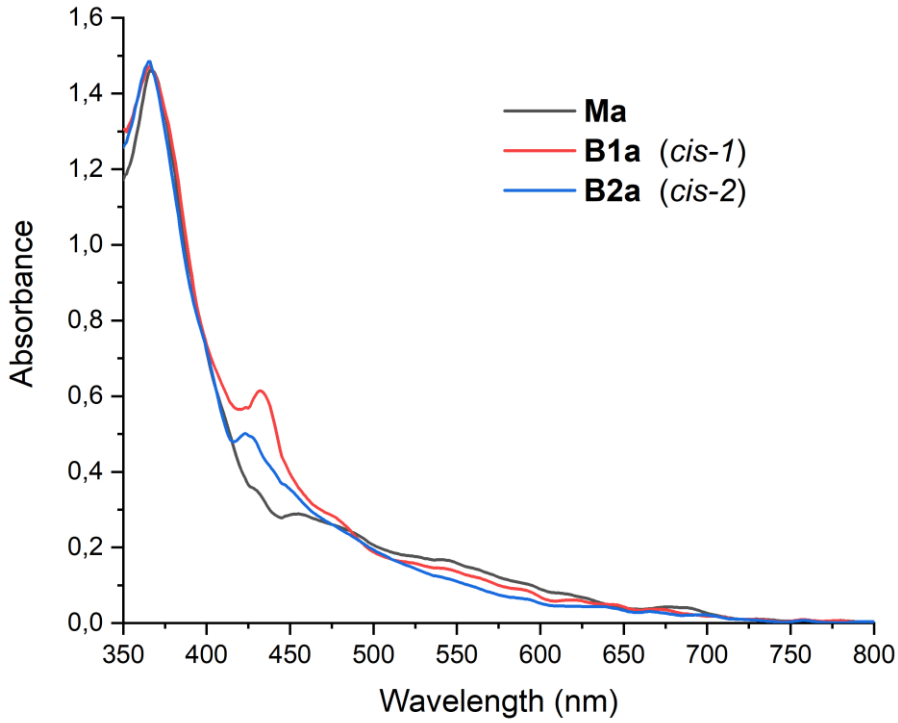


Figure S51. Comparison of the UV-vis spectra of the compounds **Ma, B1a** and **B2a**.

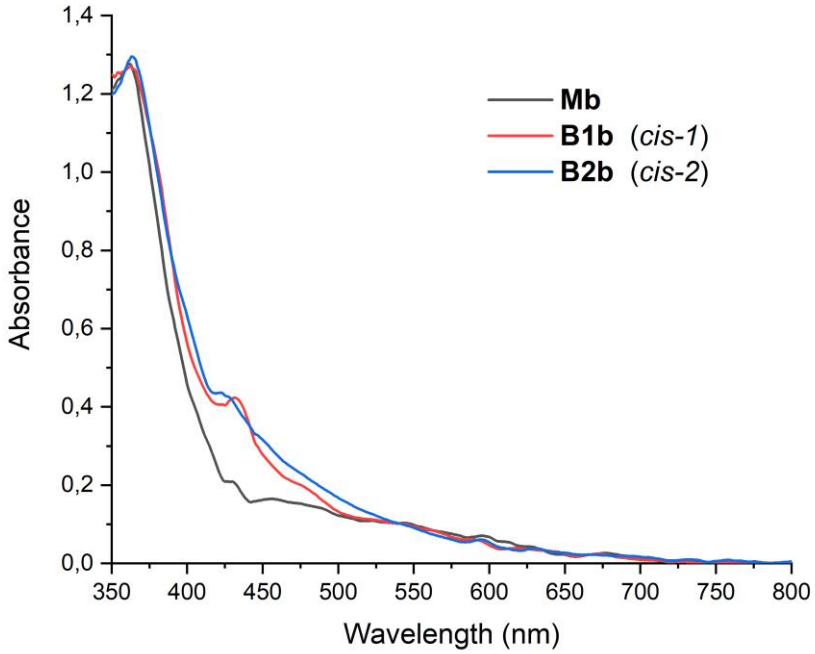


Figure S52. Comparison of the UV-vis spectra of the compounds **Mb**, **B1b** and **B2b**.

Thermogravimetric analysis of compounds M, B1 and B2

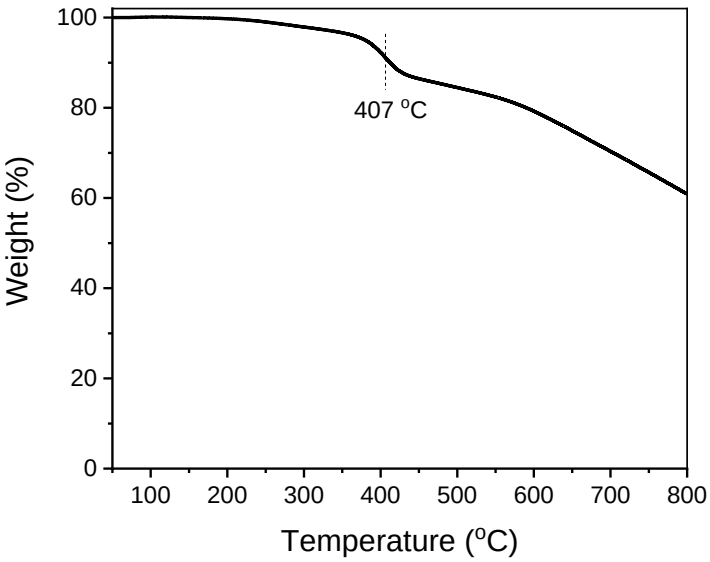


Figure S53. TGA profile of compound **Ma**.

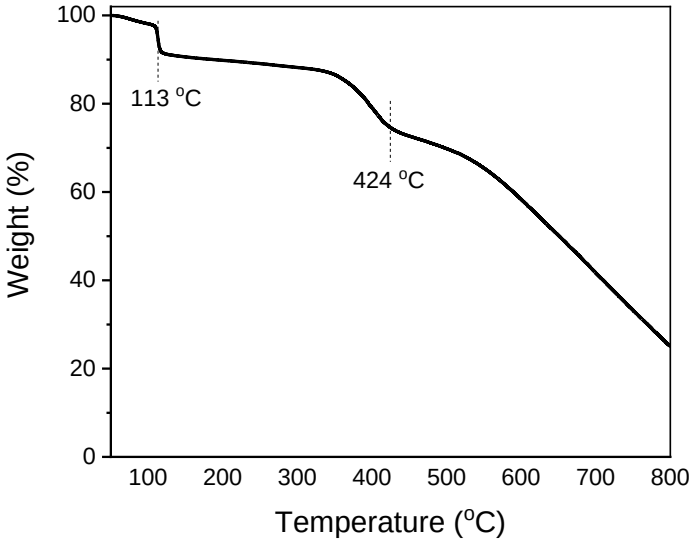


Figure S54. TGA profile of compound **B1a**.

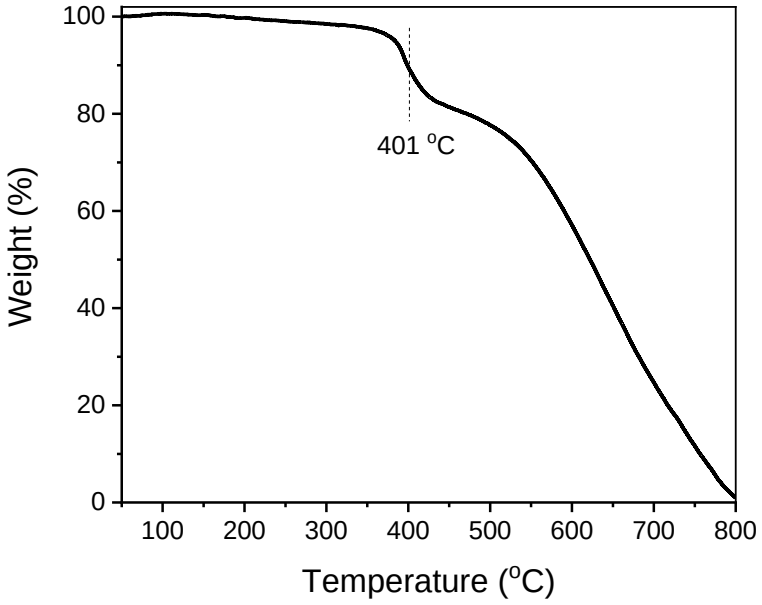


Figure S55. TGA profile of compound **B2a**.

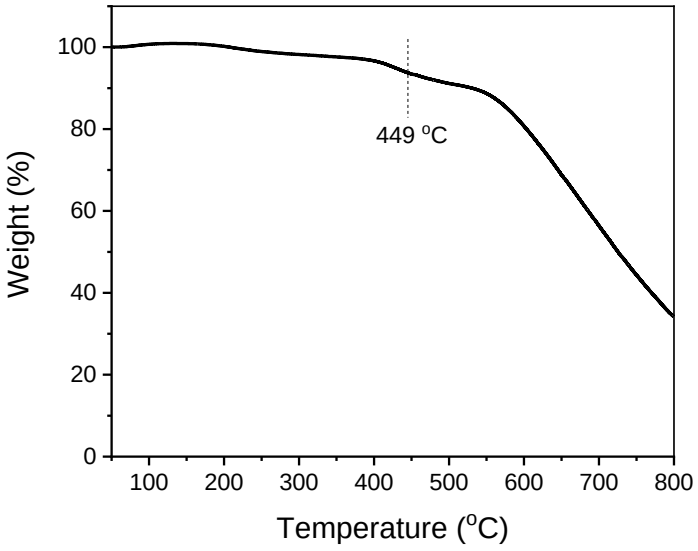


Figure S56. TGA profile of compound **Mb**.

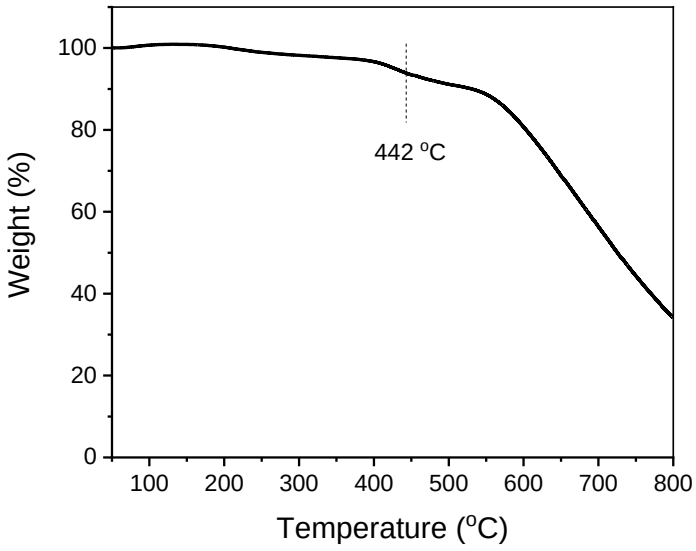


Figure S57. TGA profile of compound **B1b**.

NMR spectra of ethyl 4,4,4-trifluoro-3-oxobutanoate

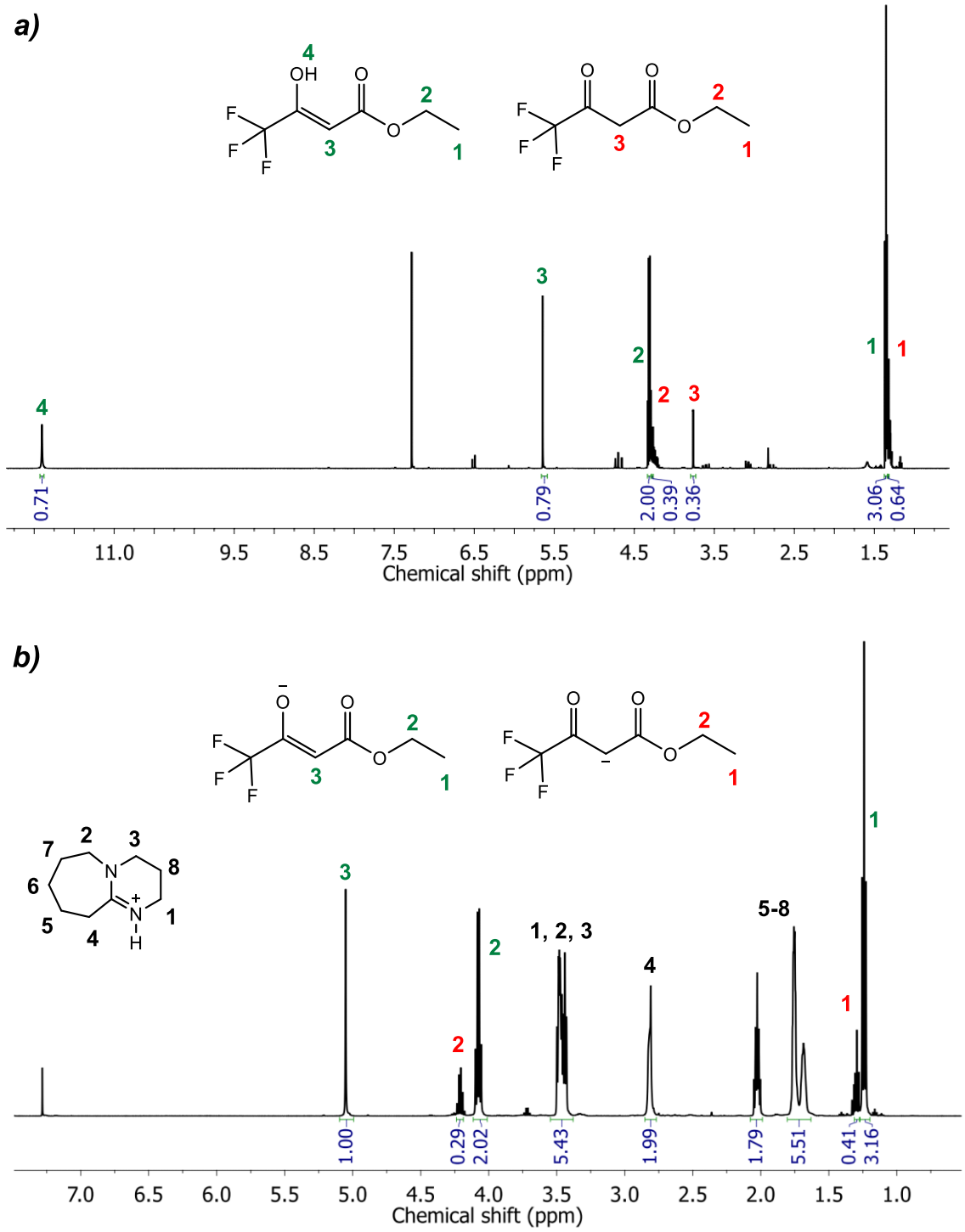


Figure S58. ^{1}H NMR spectrum of ethyl 4,4,4-trifluoro-3-oxobutanoate (a) and its 1:1 mol mixture with 1,8-diazabicyclo(5.4.0)undec-7-ene (b) (recorded in $CDCl_3$).

HPLC profile, NMR and MALDI ToF mass spectra of compounds 1-6

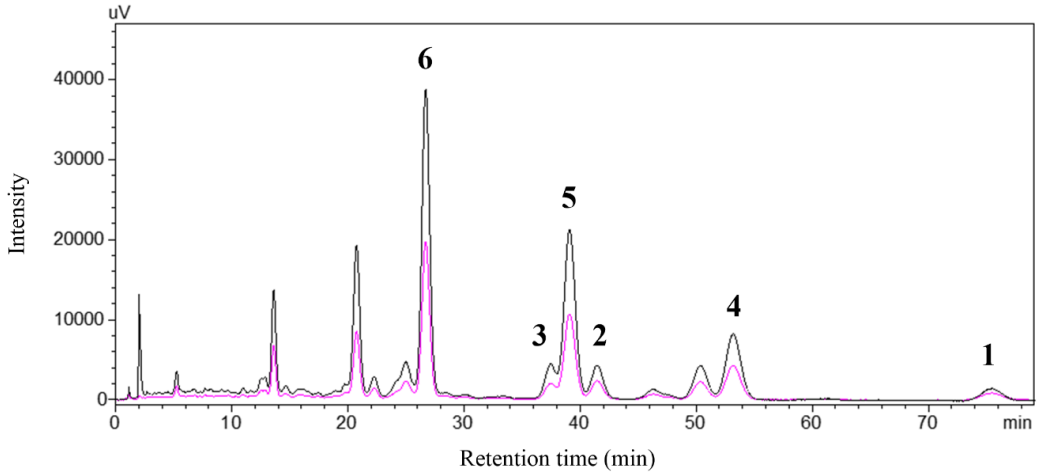
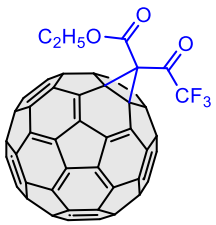


Figure S59. HPLC profile of the reaction mixture with ethyl 4,4,4-trifluoro-3-oxobutanoate.

Compound **1**



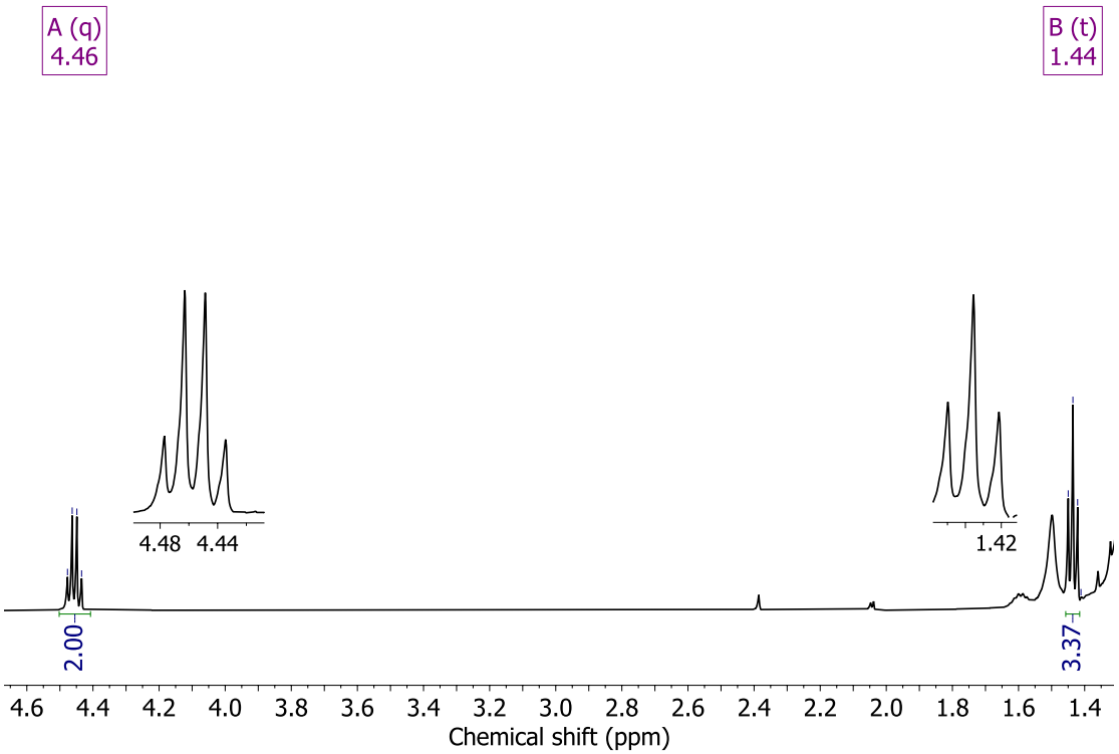


Figure S60. ^{1}H NMR spectrum of compound **1**.

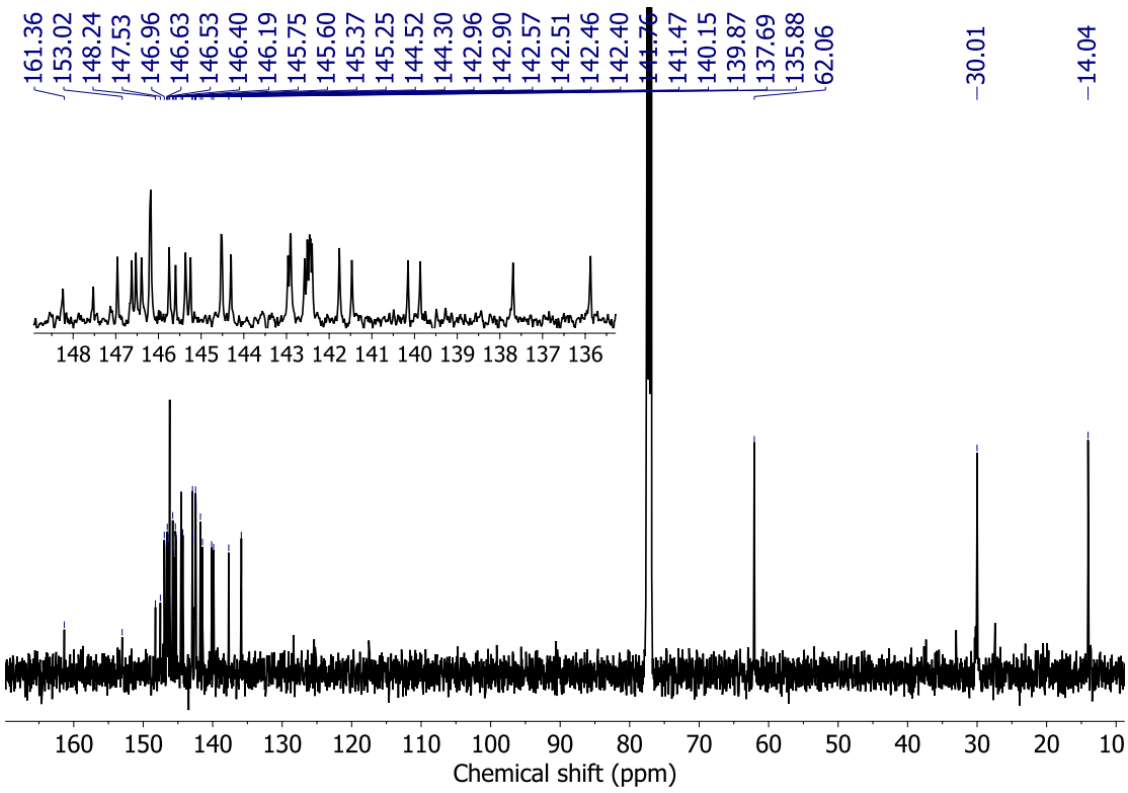


Figure S61. ^{13}C NMR spectrum of compound **1**.

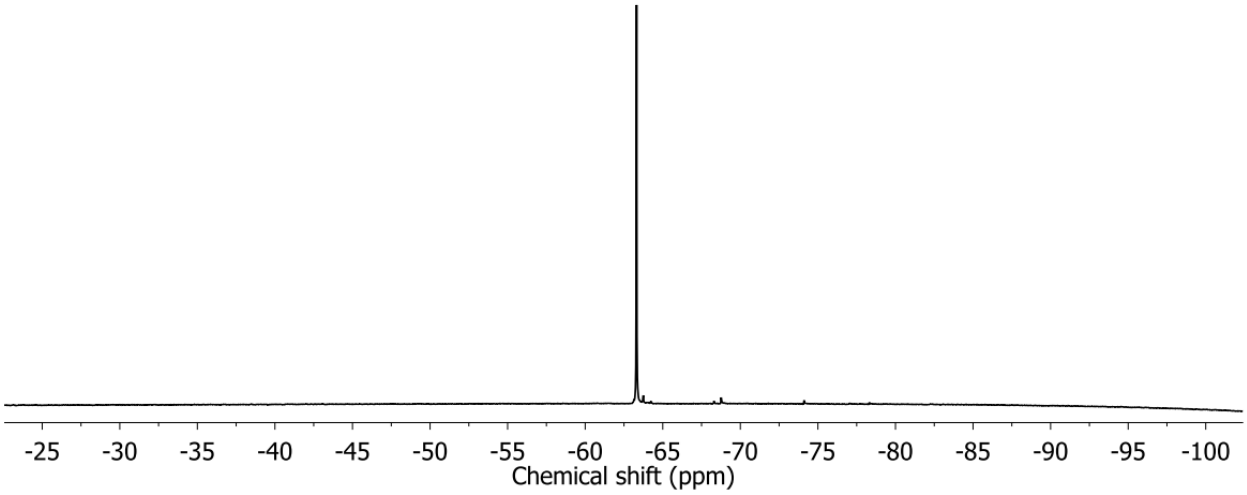


Figure S62. ^{19}F NMR spectrum of compound **1**.

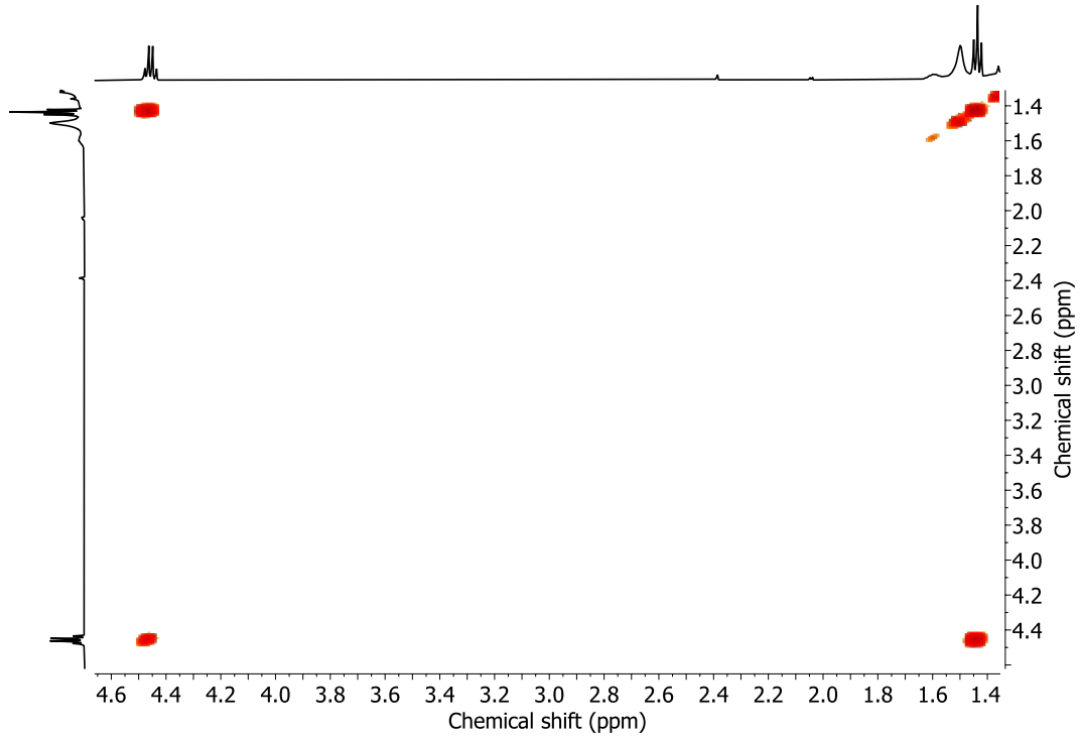


Figure S63. ^{1}H-^{1}H COSY NMR spectrum of compound **1**.

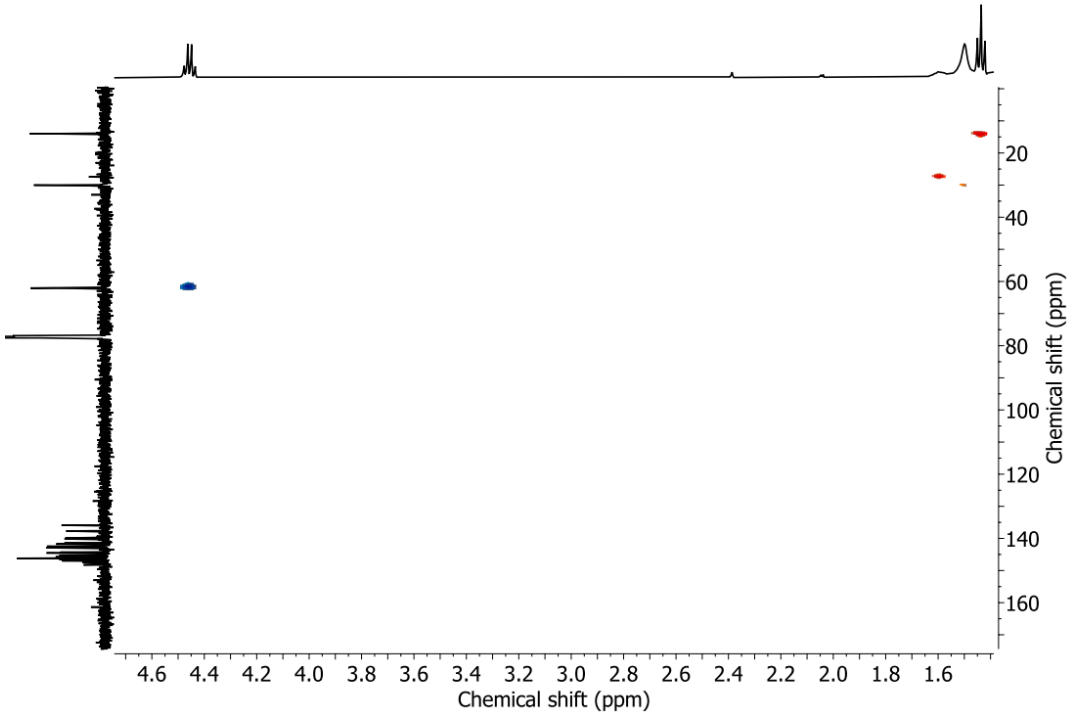


Figure S64. ^{1}H-^{13}C HSQC NMR spectrum of compound **1**.

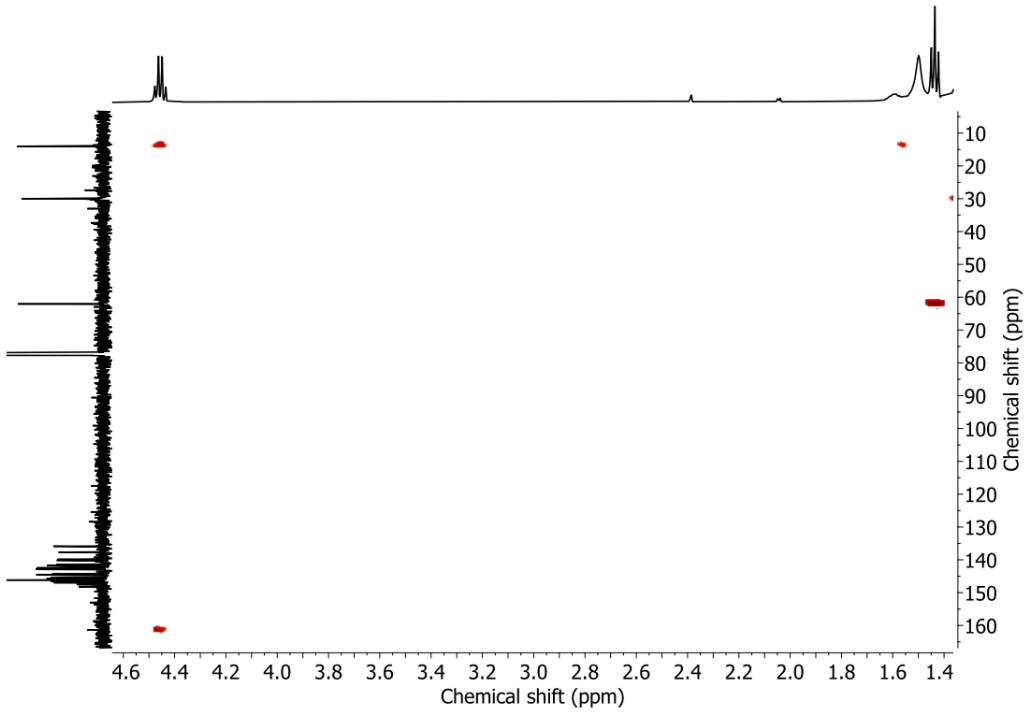


Figure S65. ^{1}H-^{13}C HMBC NMR spectrum of compound **1**.

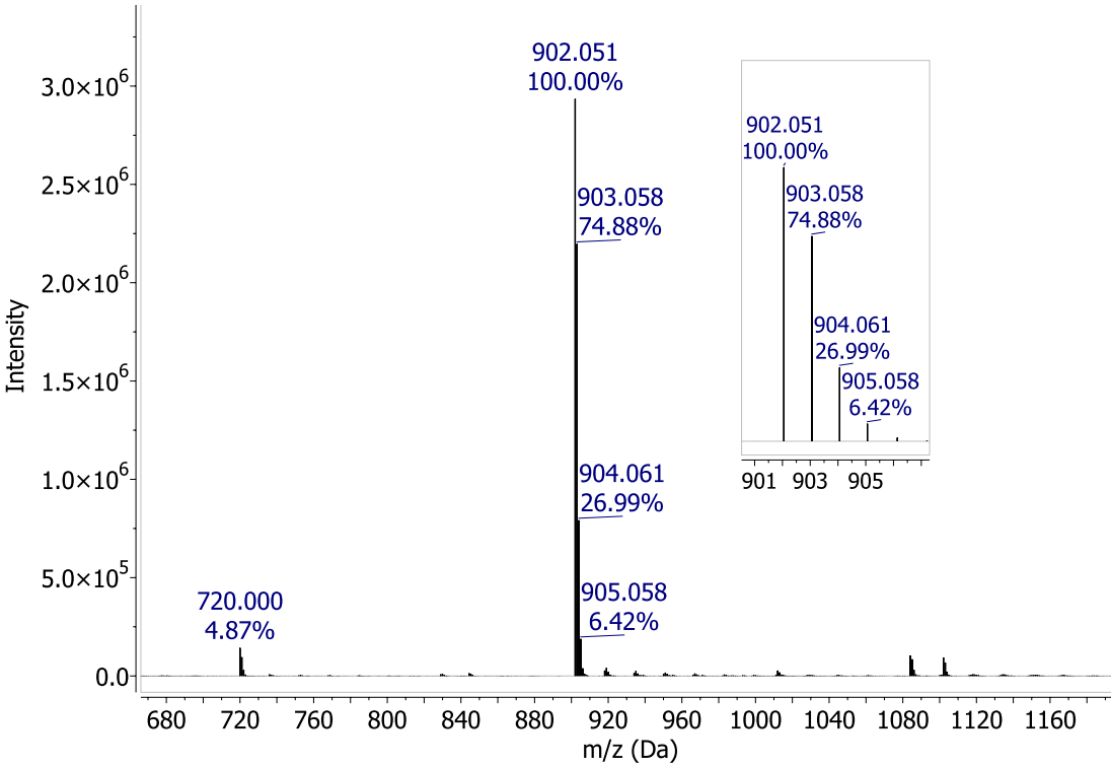
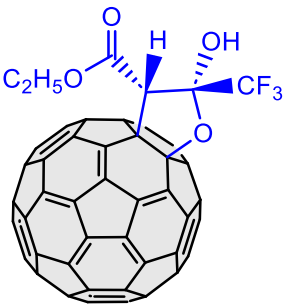


Figure S66. Negative ion MALDI mass spectrum of compound **1**.

Compound **2**



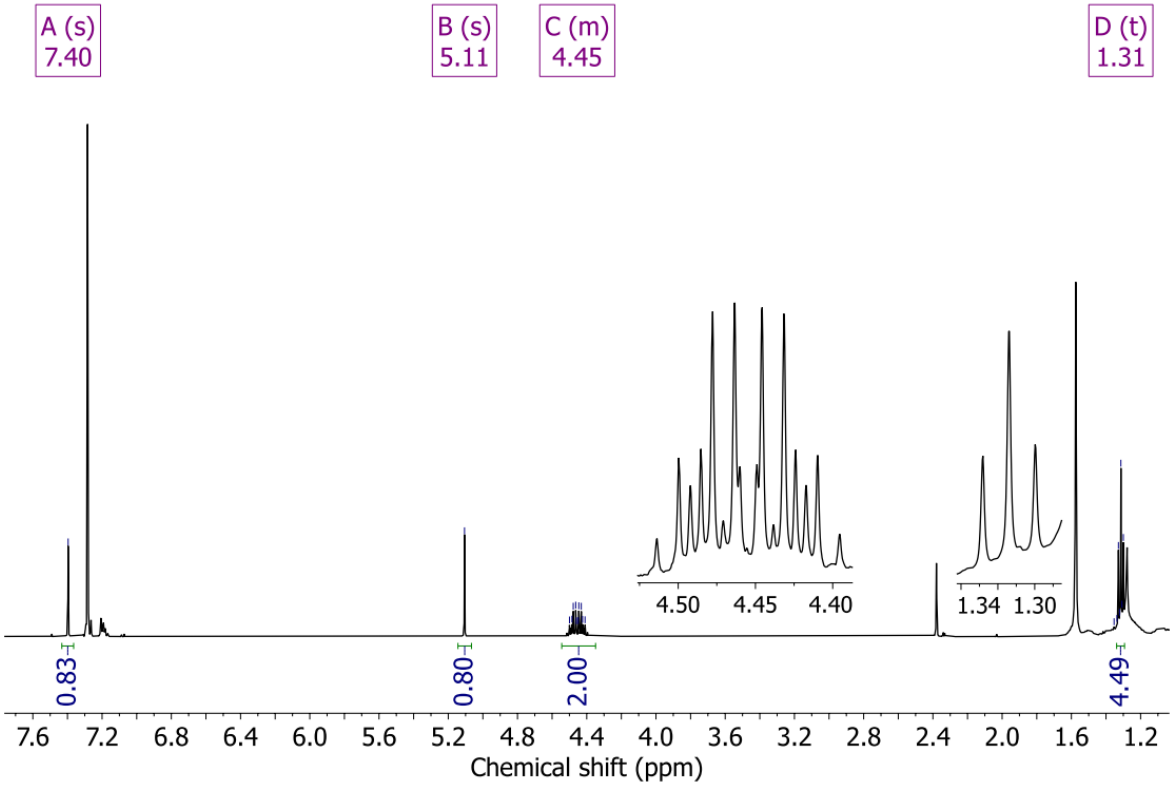


Figure S67. ^{1}H NMR spectrum of compound **2**.

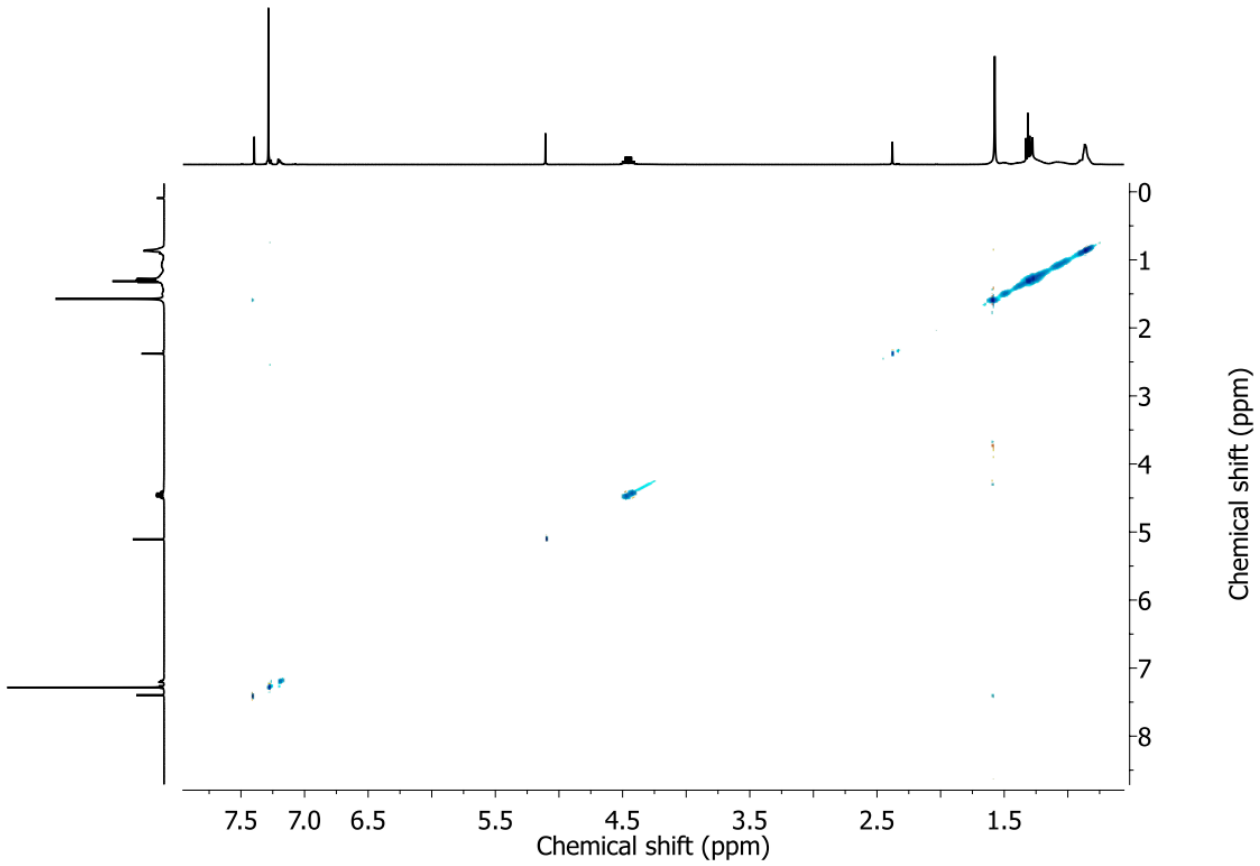


Figure S68. ^{1}H-^{1}H NOESY NMR spectrum of compound **2**.

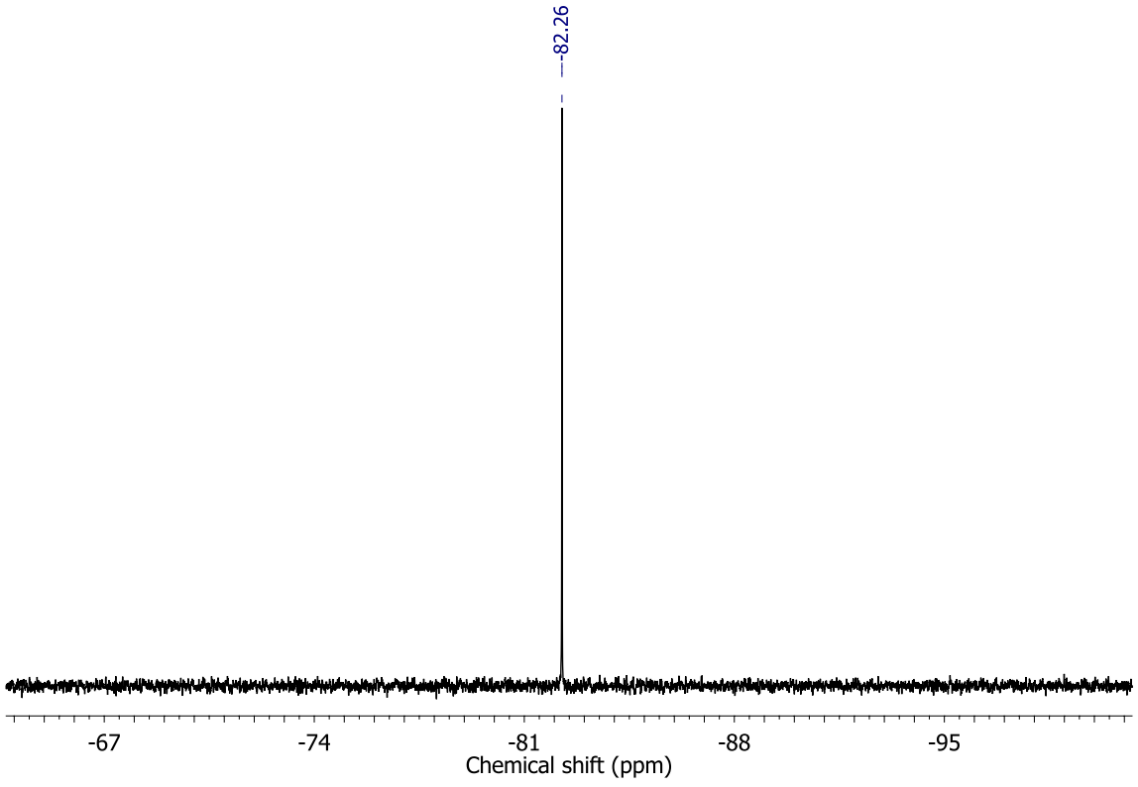


Figure S69. ^{19}F NMR spectrum of compound **2**.

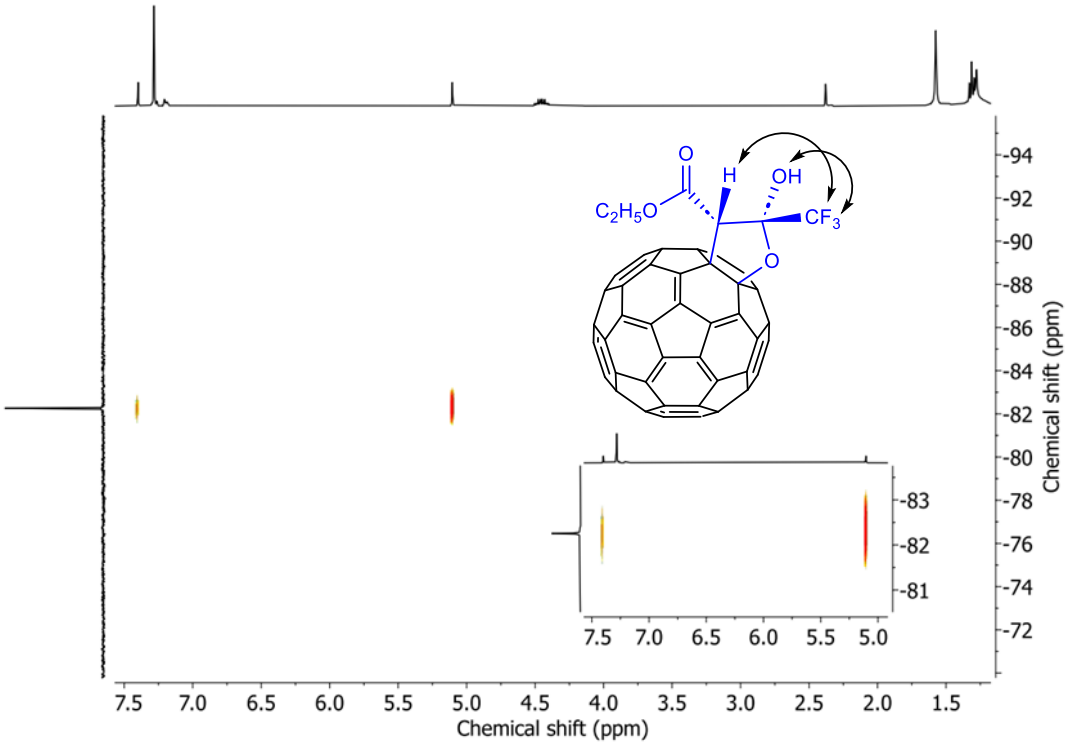


Figure S70. ^{1}H-^{19}F HOESY NMR spectrum of compound **2**.

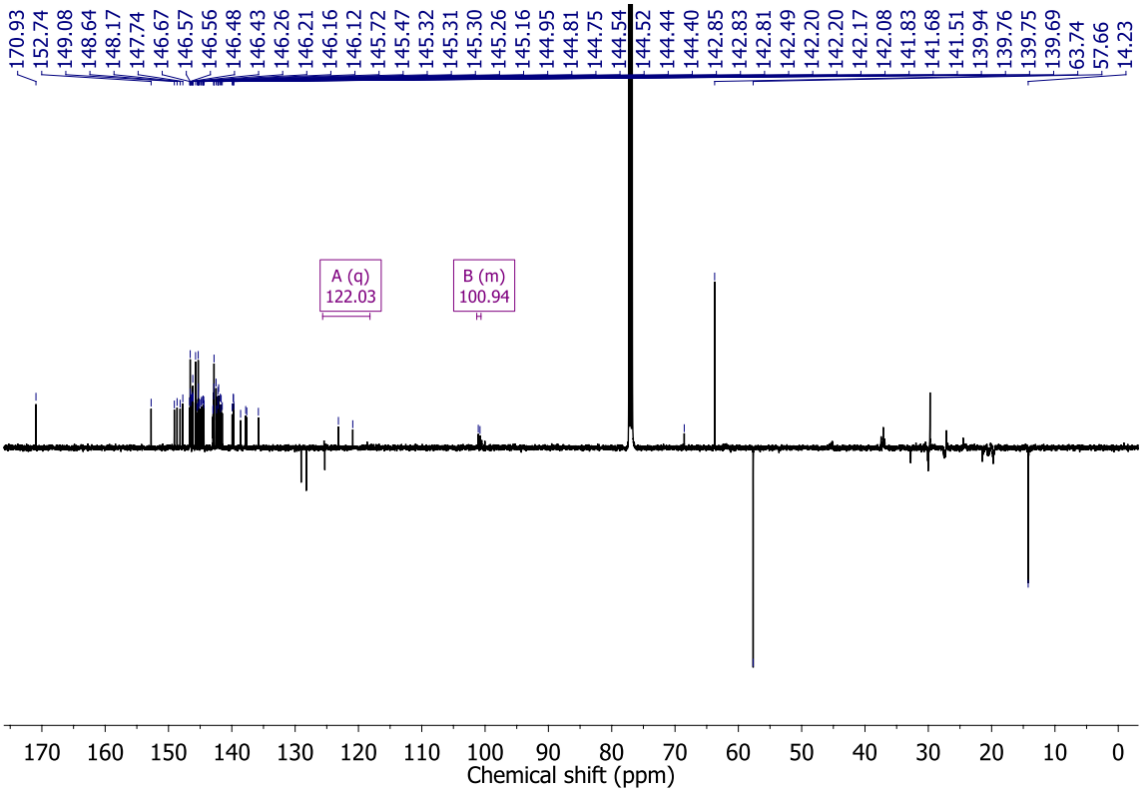


Figure S71. ^{13}C NMR spectrum of compound **2**.

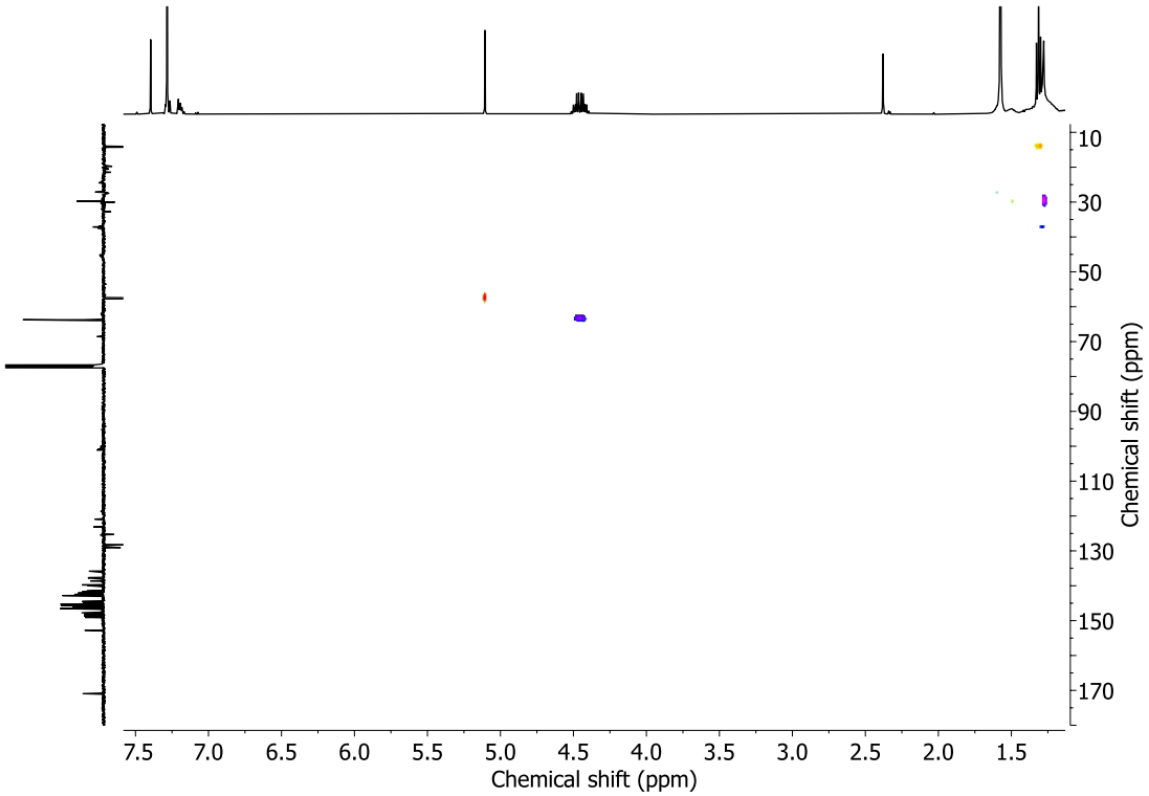


Figure S72. ^{1}H-^{13}C HSQC NMR spectrum of compound **2**.

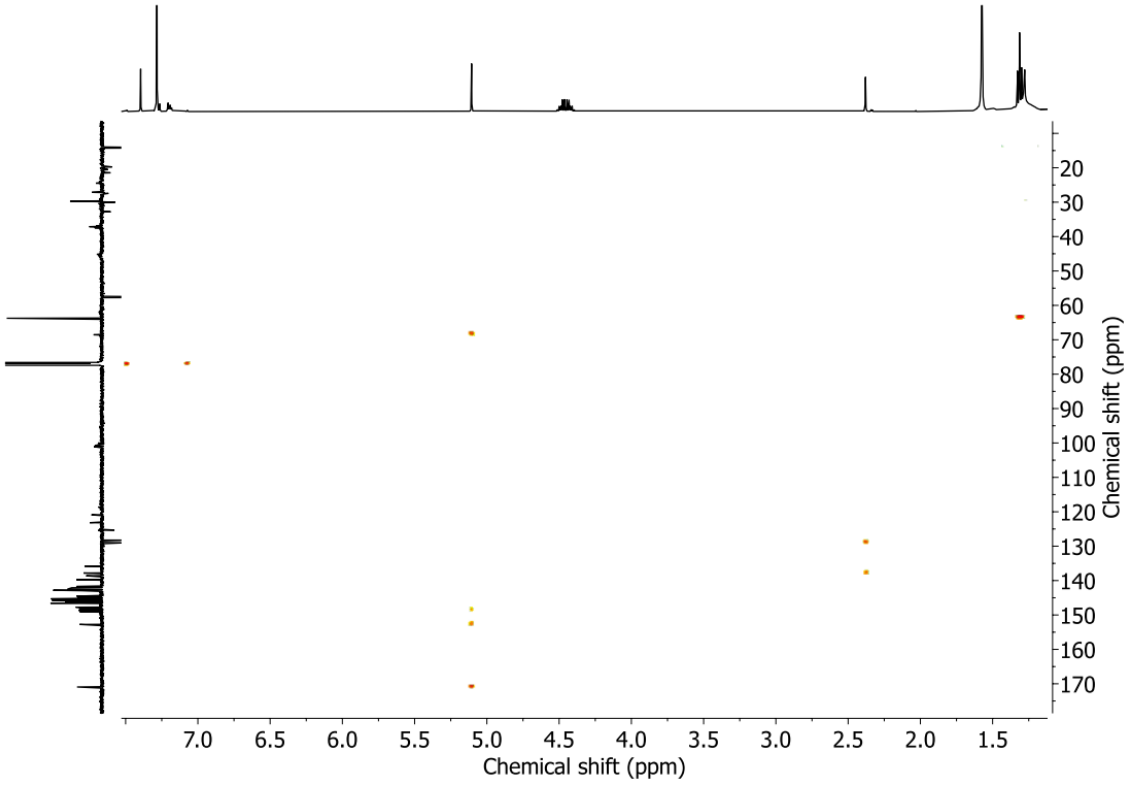


Figure S73. ^{1}H-^{13}C HMBC NMR spectrum of compound **2**.

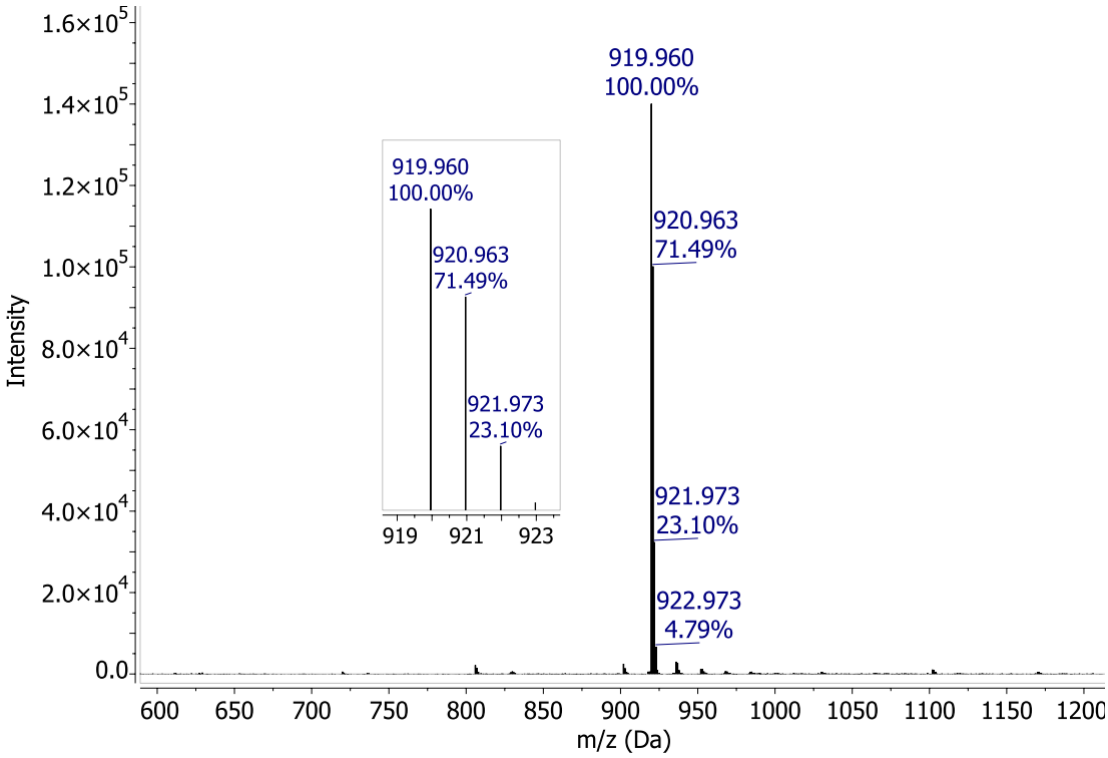
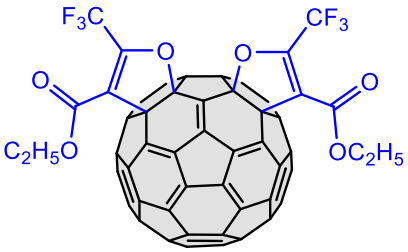


Figure S74. Negative ion MALDI mass spectrum of compound **2**.

Compound **3**



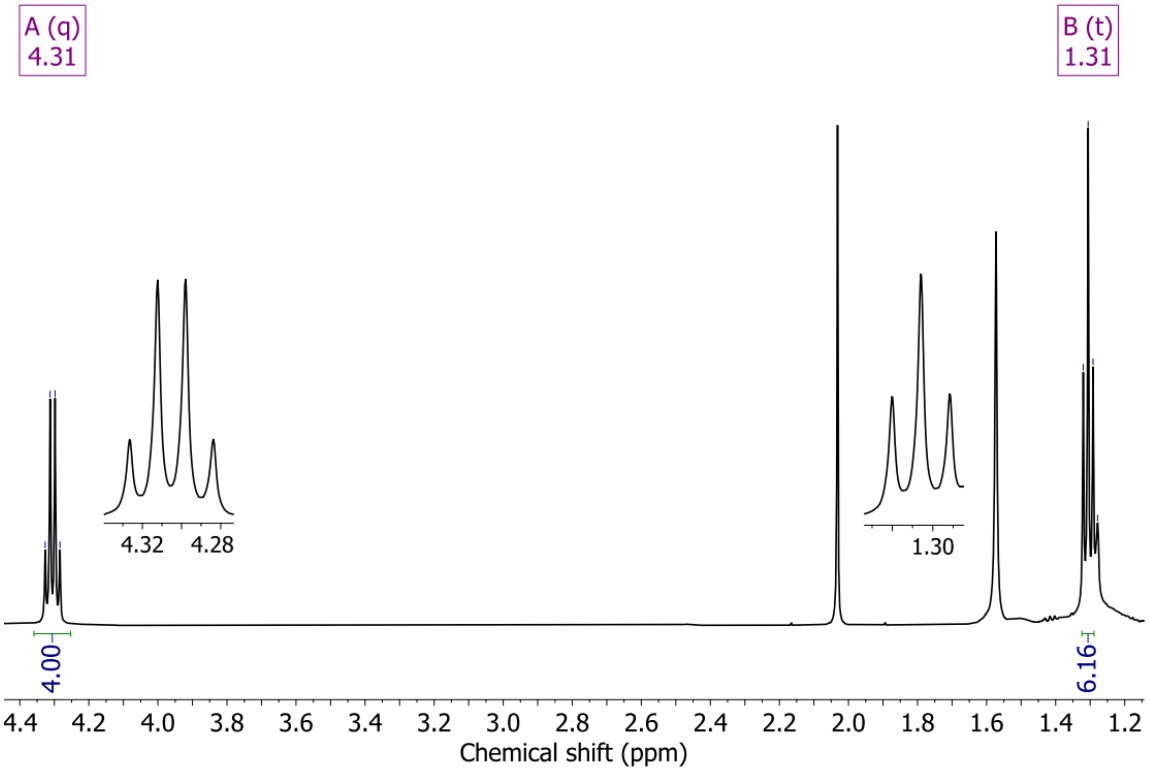


Figure S75. ^{1}H NMR spectrum of compound **3**.

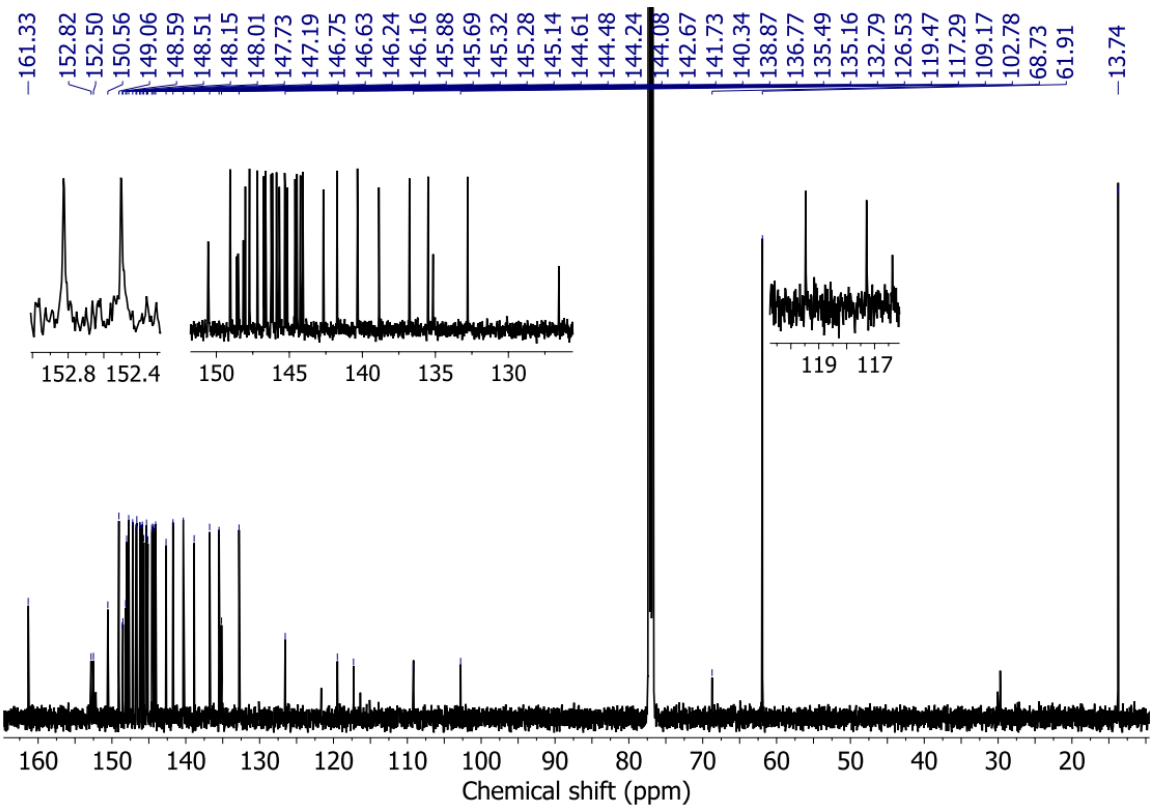


Figure S76. ^{13}C NMR spectrum of compound **3**.

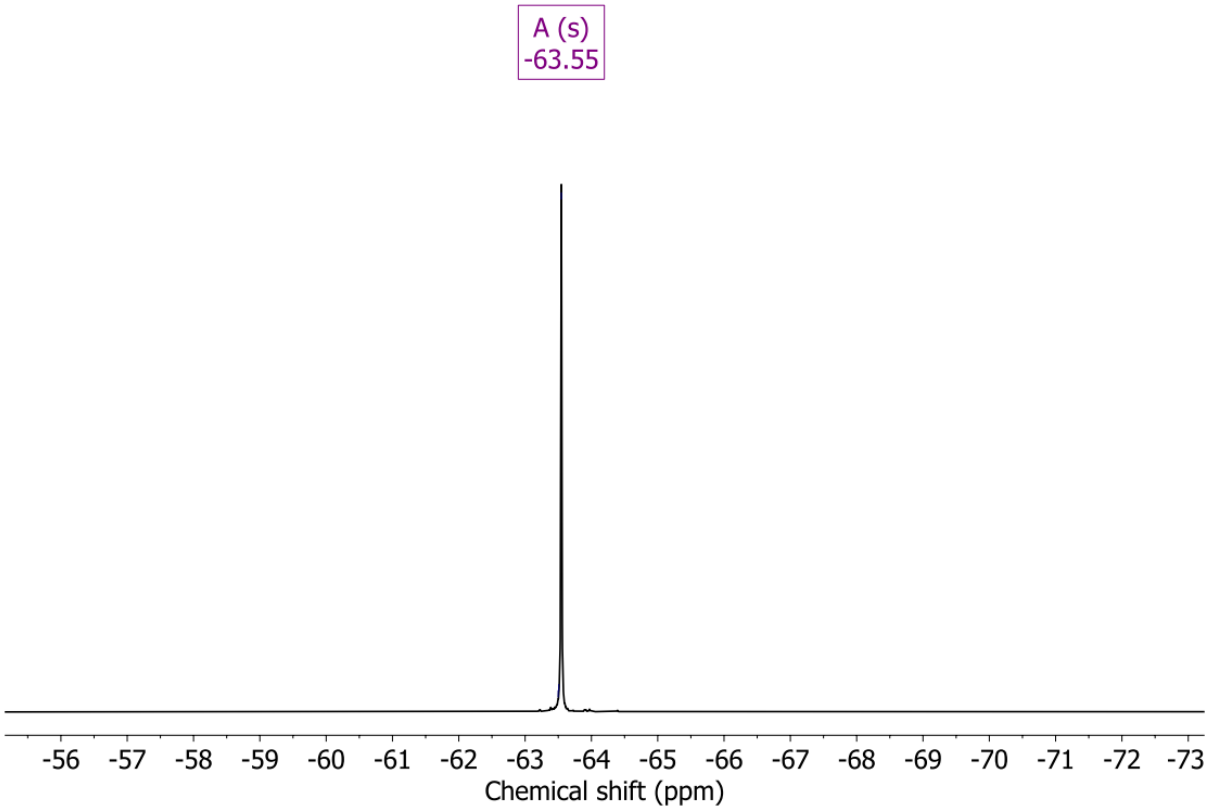


Figure S77. ^{19}F NMR spectrum of compound **3**.

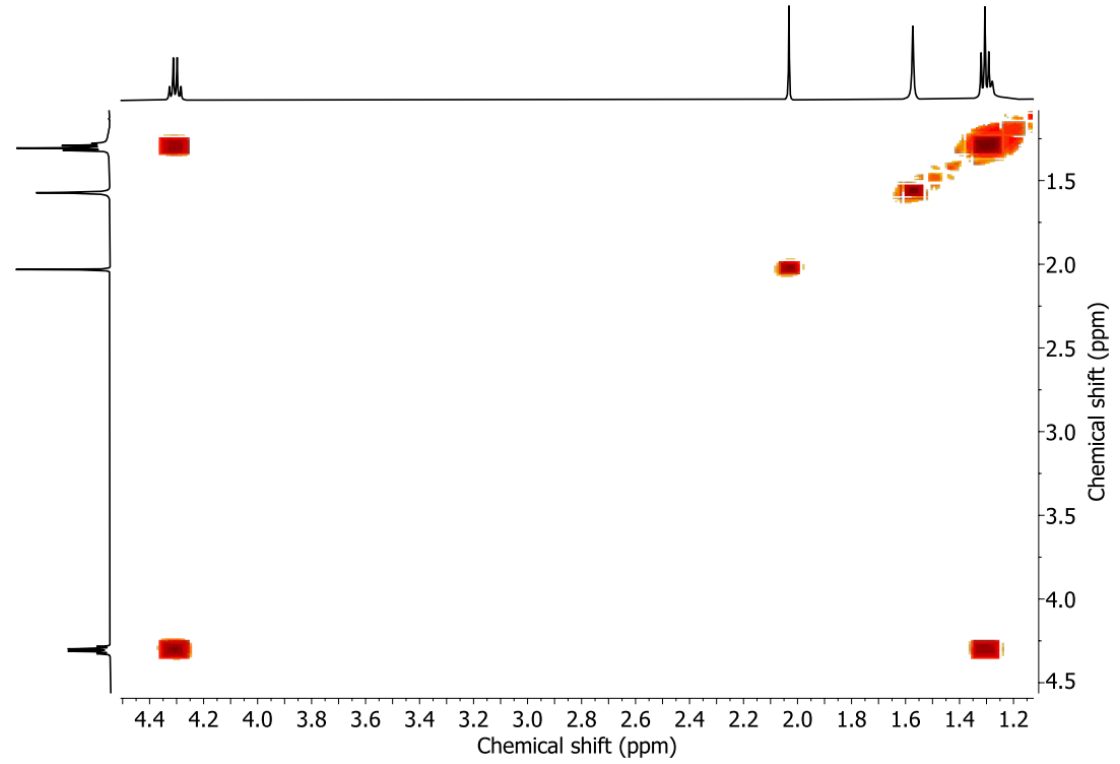


Figure S78. ^{1}H-^{1}H COSY NMR spectrum of compound **3**.

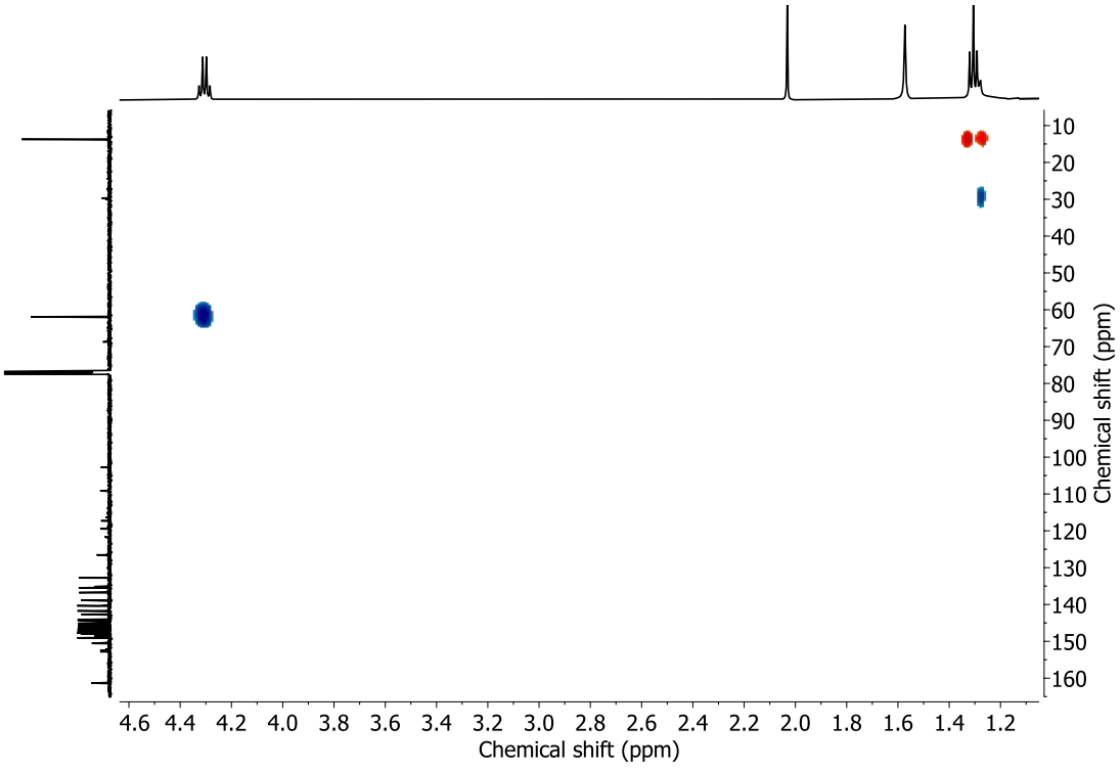


Figure S79. ^{1}H-^{13}C HSQC NMR spectrum of compound **3**.

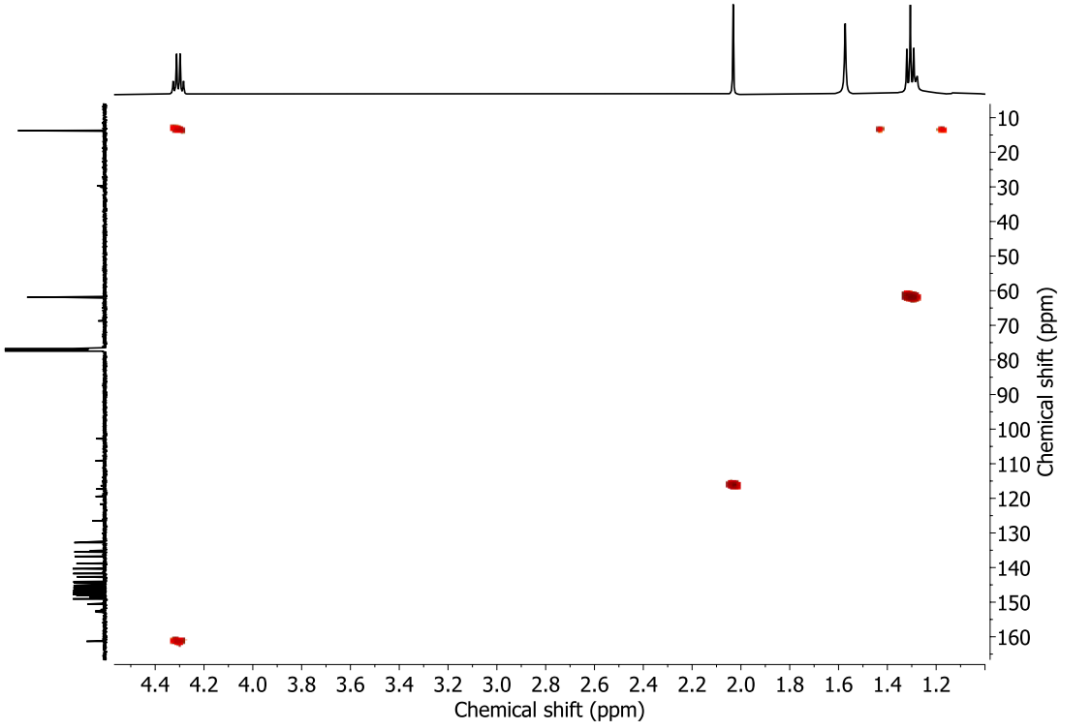


Figure S80. ^{1}H-^{13}C HMBC NMR spectrum of compound **3**.

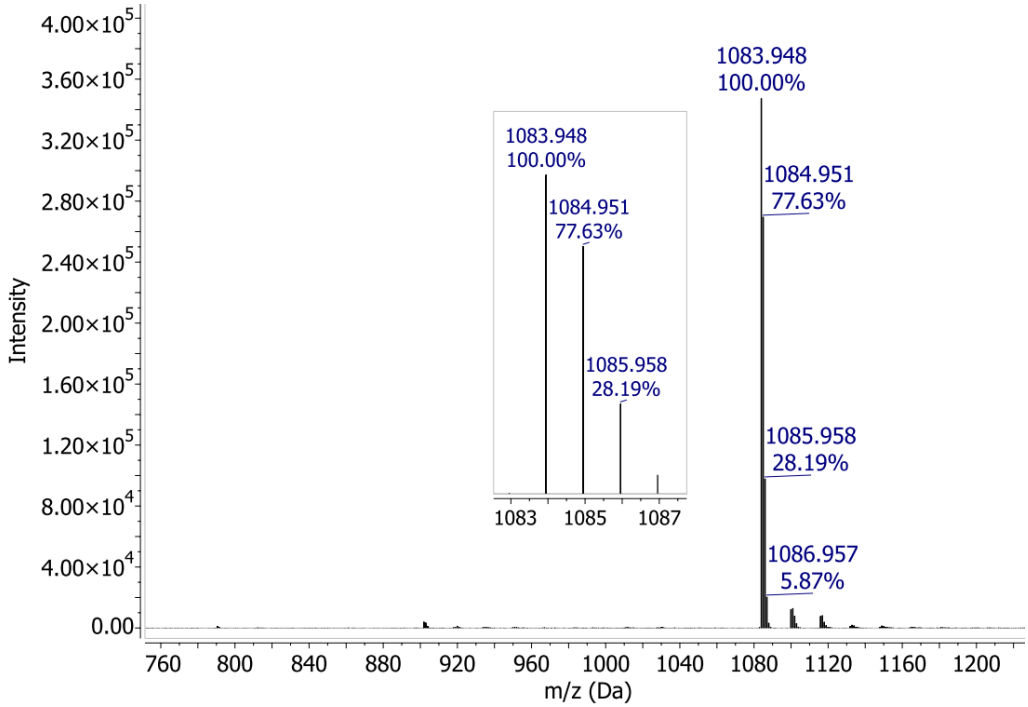
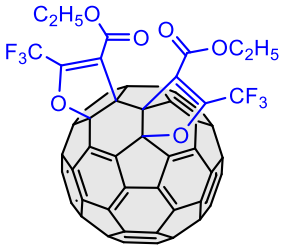


Figure S81. Negative ion MALDI mass spectrum of compound **3**.

Compound **4**



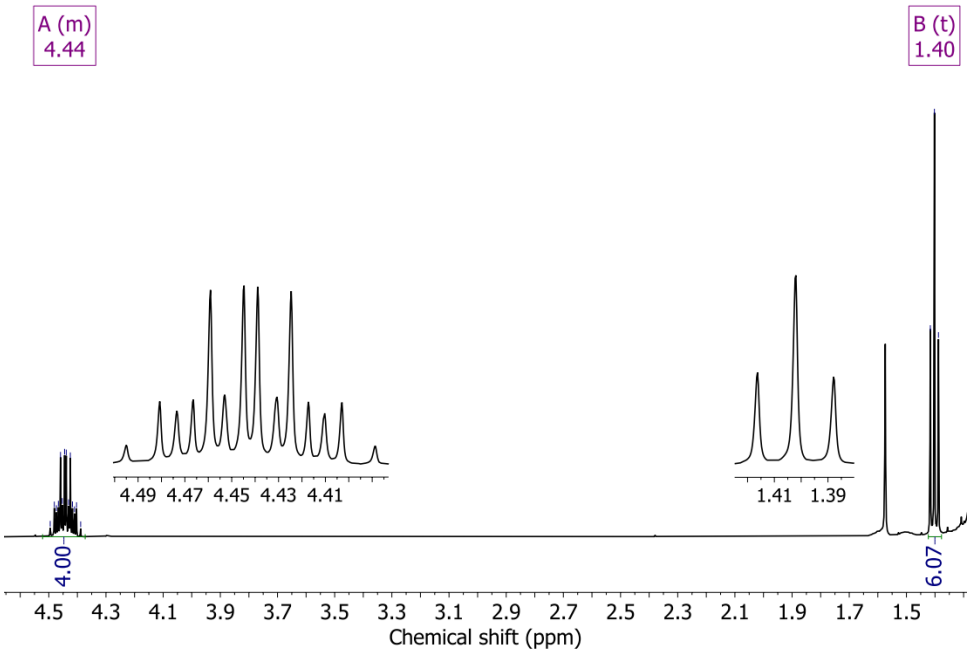


Figure S82. ^{1}H NMR spectrum of compound **4**.

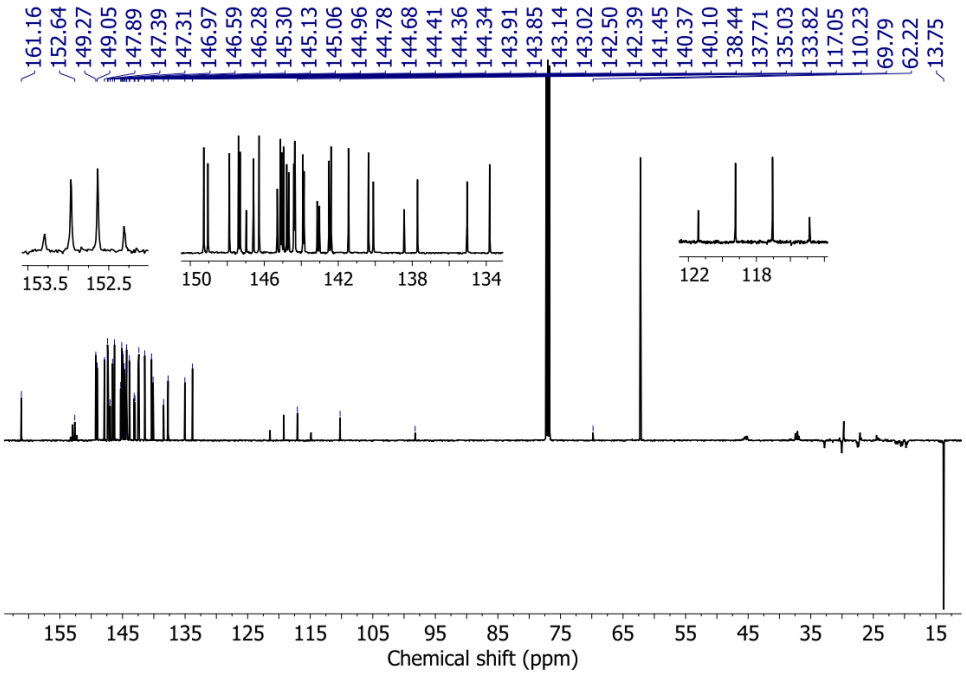


Figure S83. ^{13}C JMOD NMR spectrum of compound **4**.

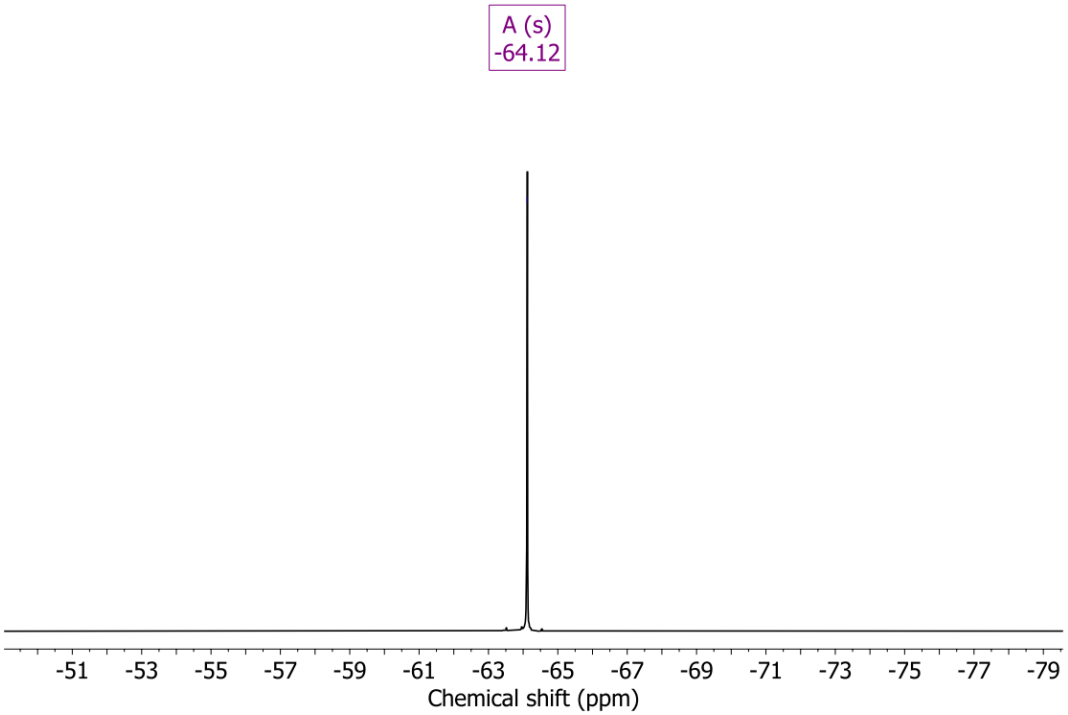


Figure S84. ^{19}F NMR spectrum of compound **4**.

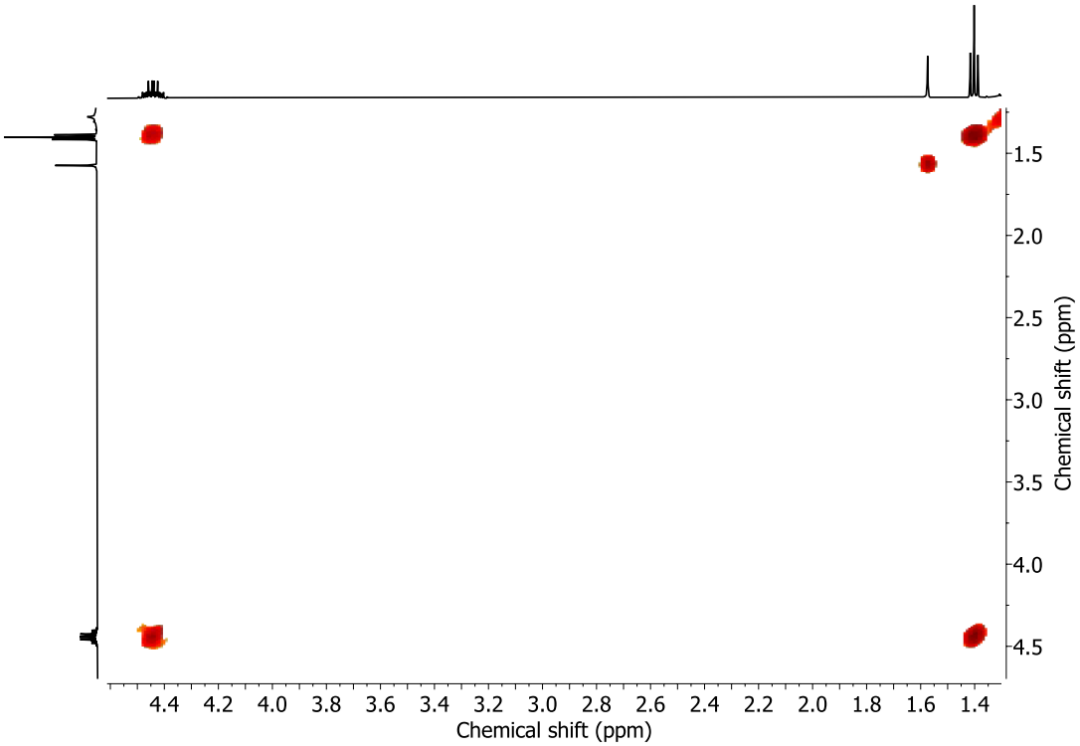


Figure S85. ^{1}H-^{1}H COSY NMR spectrum of compound **4**.

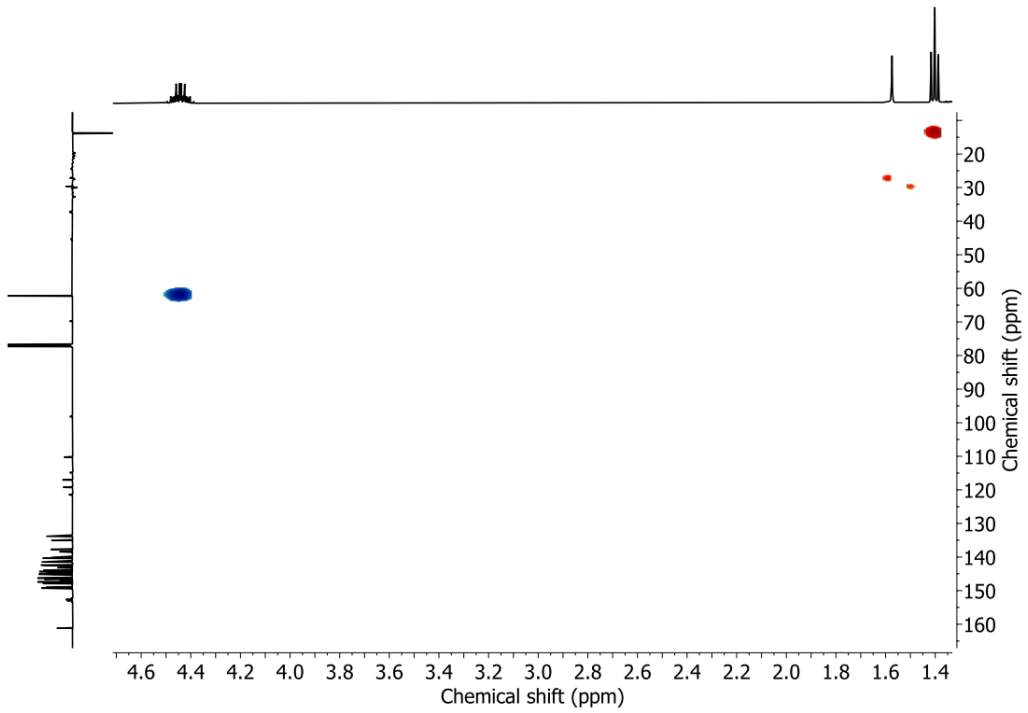


Figure S86. ^{1}H-^{13}C HSQC NMR spectrum of compound **4**.

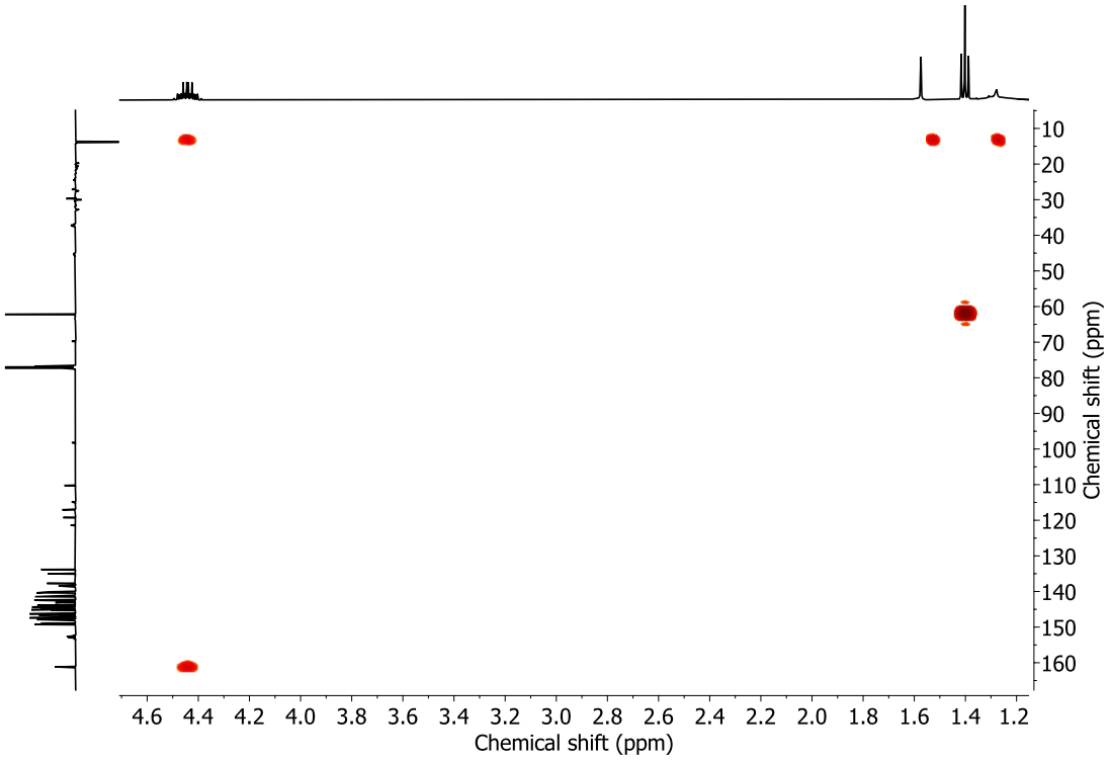


Figure S87. ^{1}H-^{13}C HMBC NMR spectrum of compound **4**.

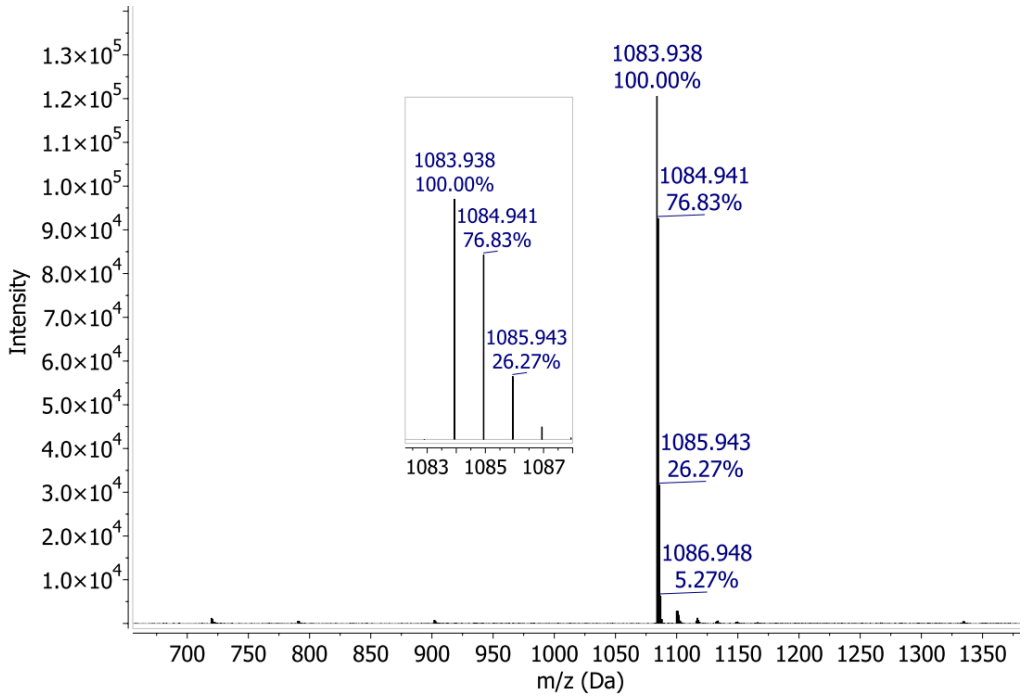
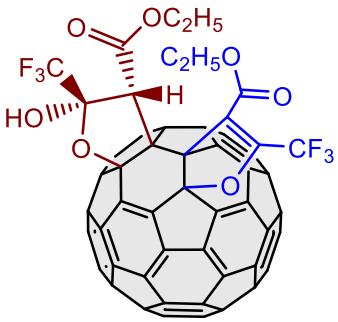


Figure S88. Negative ion MALDI mass spectrum of compound **4**.

Compound **5**



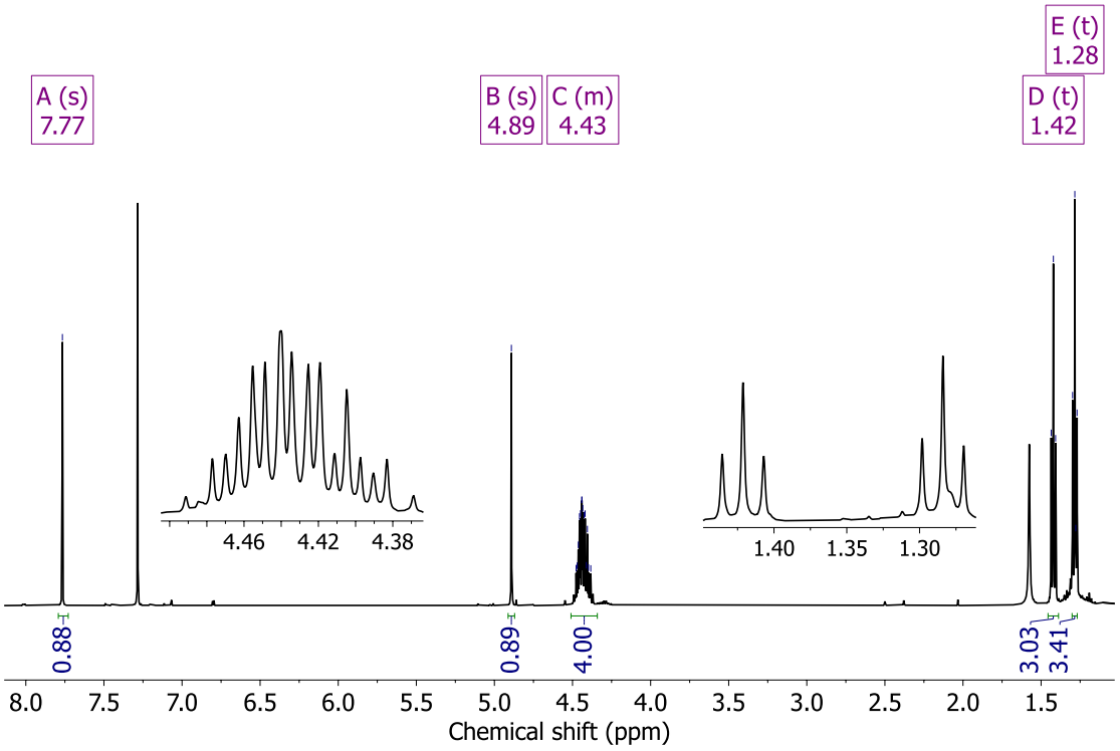


Figure S89. ^{1}H NMR spectrum of compound **5**.

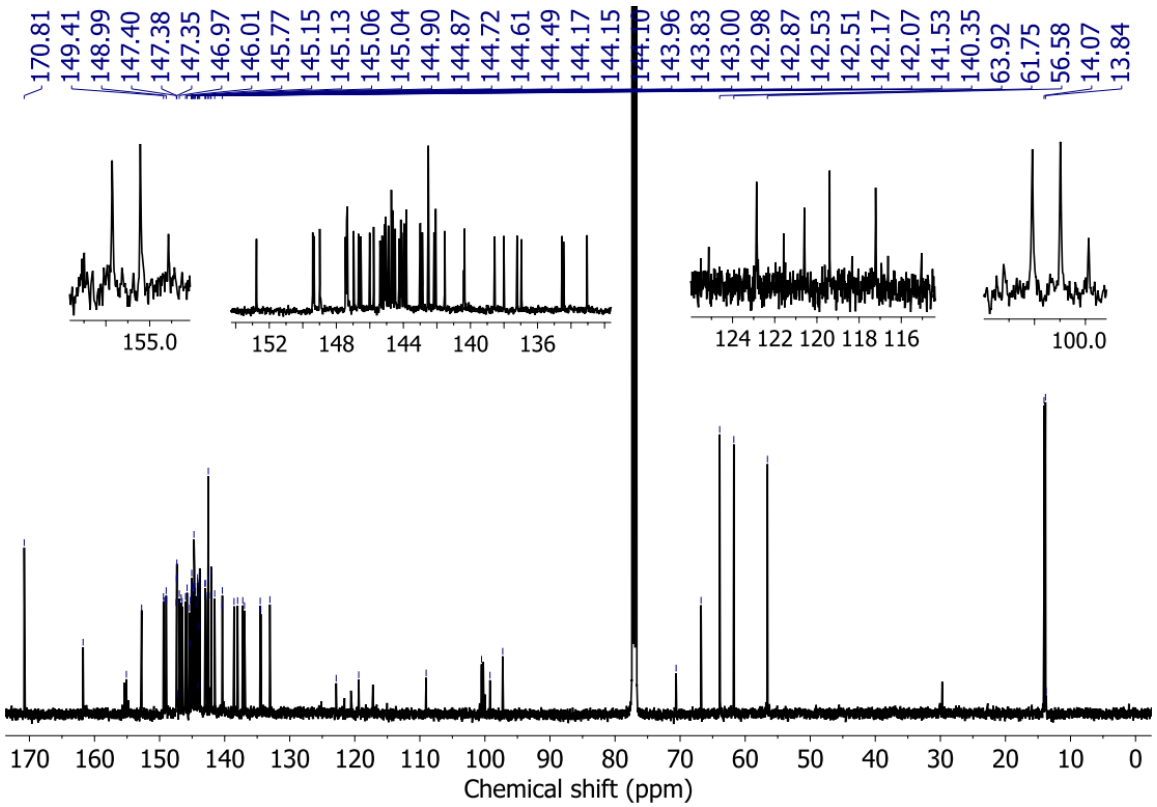


Figure S90. ^{13}C NMR spectrum of compound **5**.

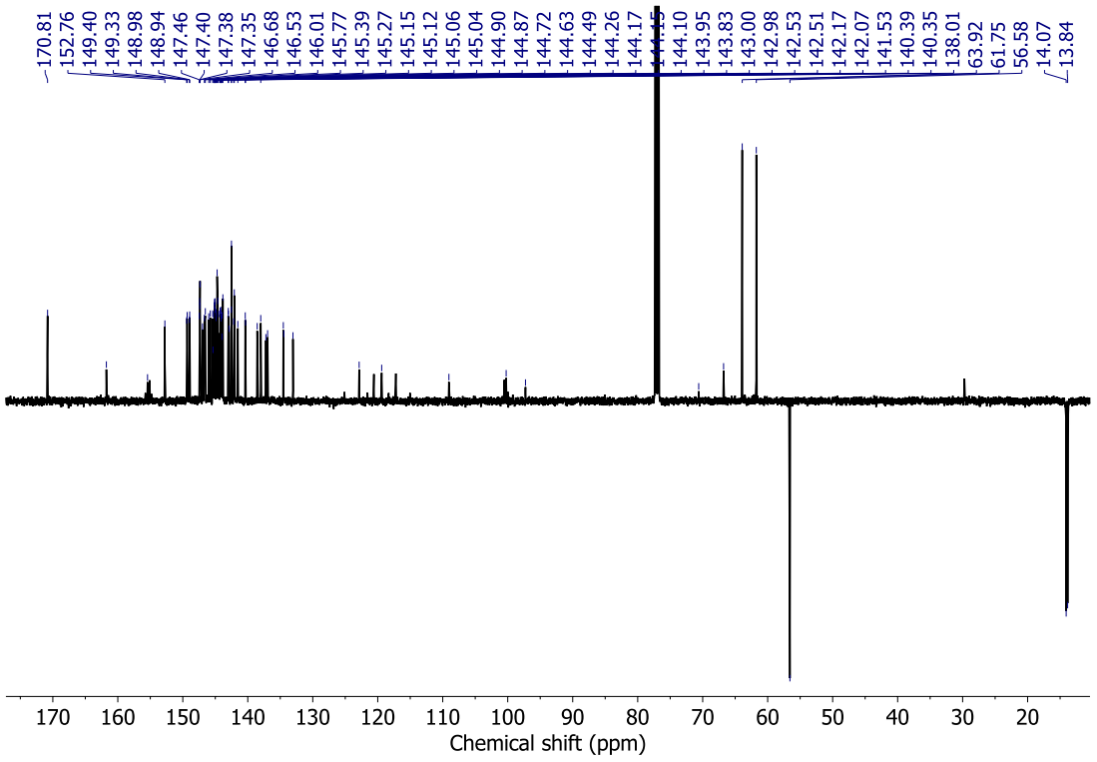


Figure S91. ^{13}C JMOD NMR spectrum of compound **5**.

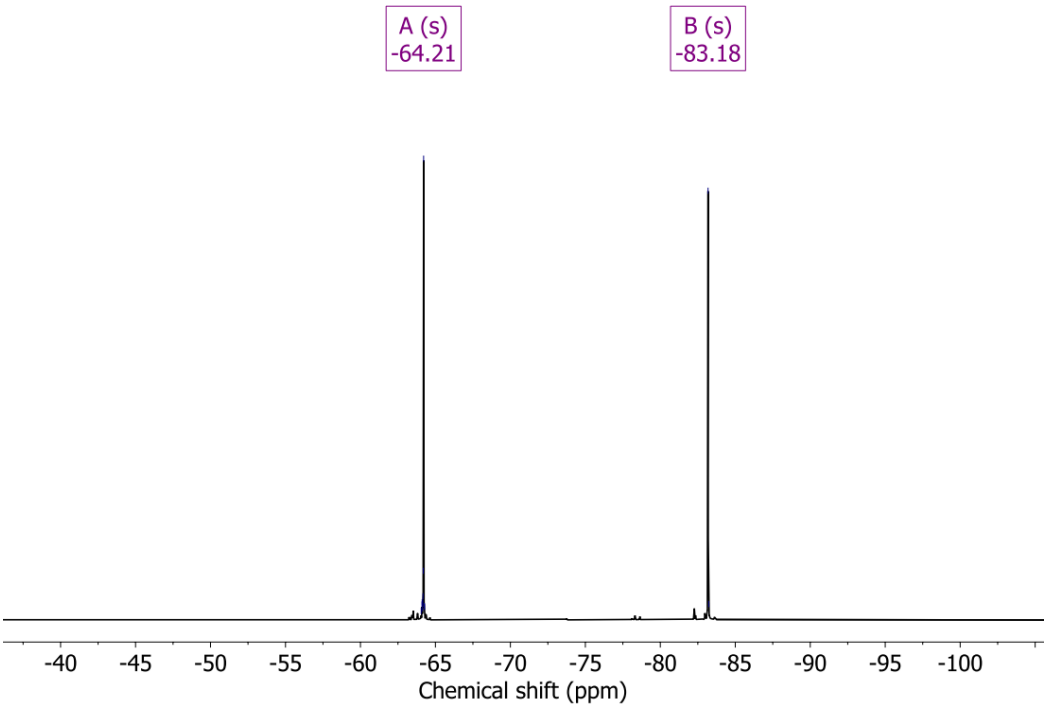


Figure S92. ^{19}F NMR spectrum of compound **5**.

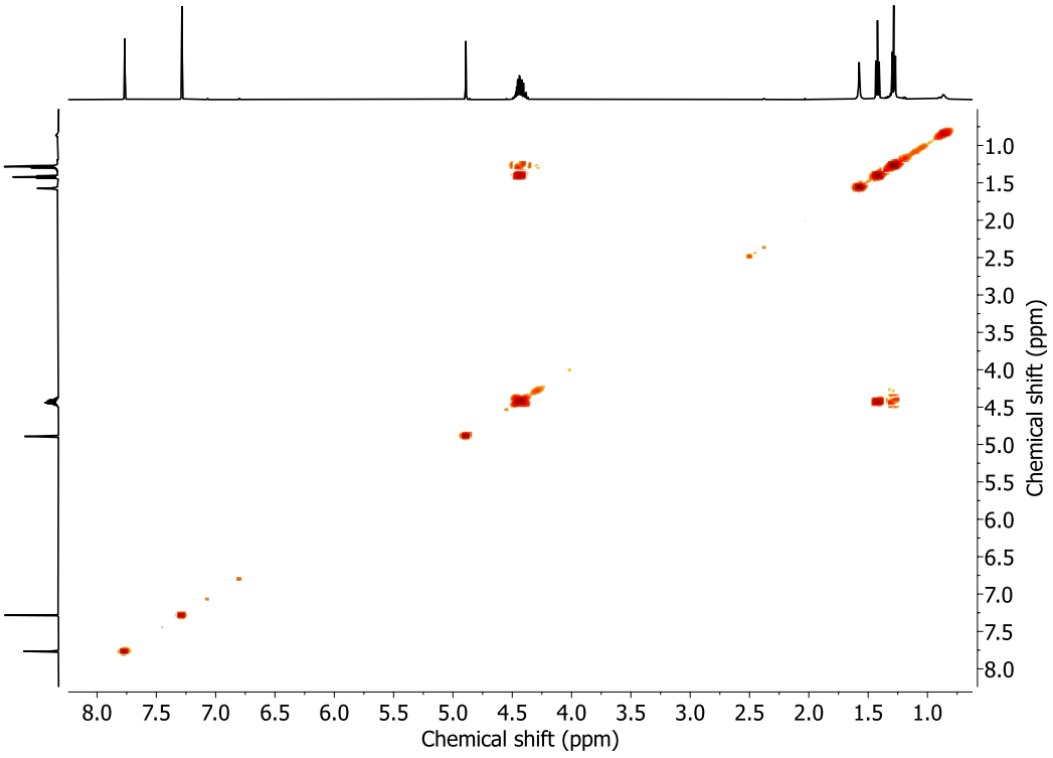


Figure S93. ^{1}H-^{1}H COSY NMR spectrum of compound **5**.

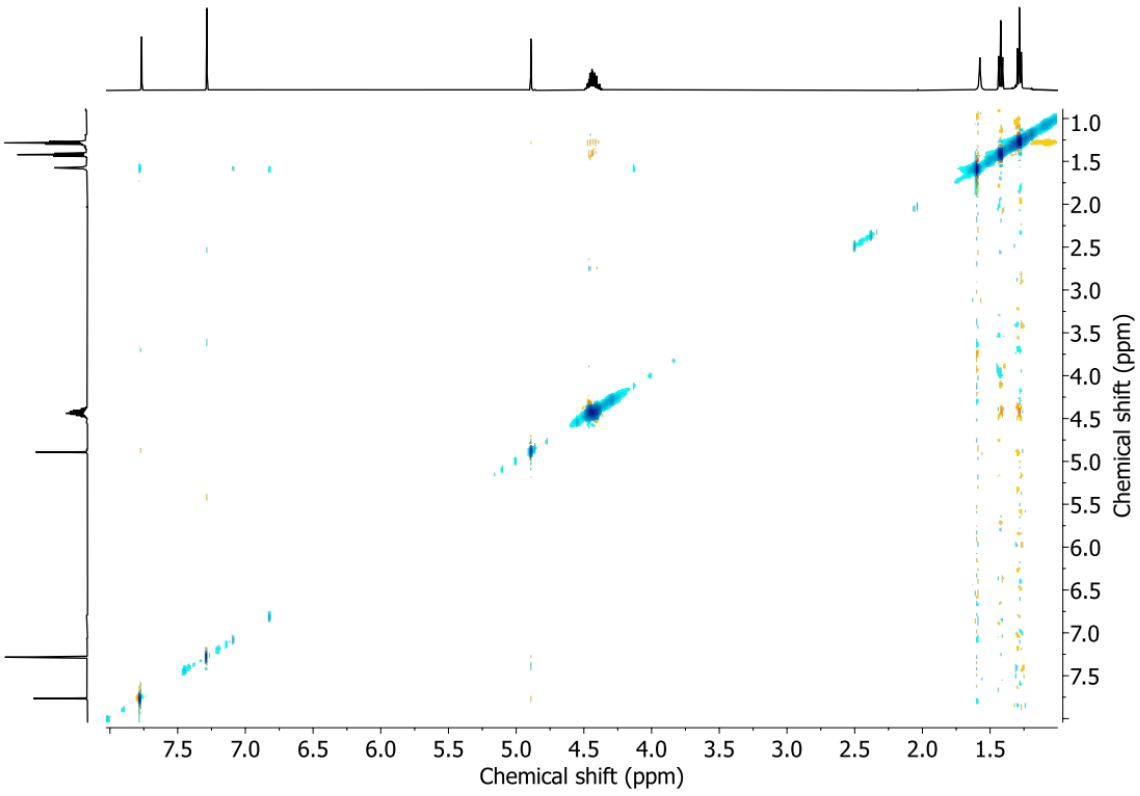


Figure S94. ^{1}H-^{1}H NOESY NMR spectrum of compound **5**.

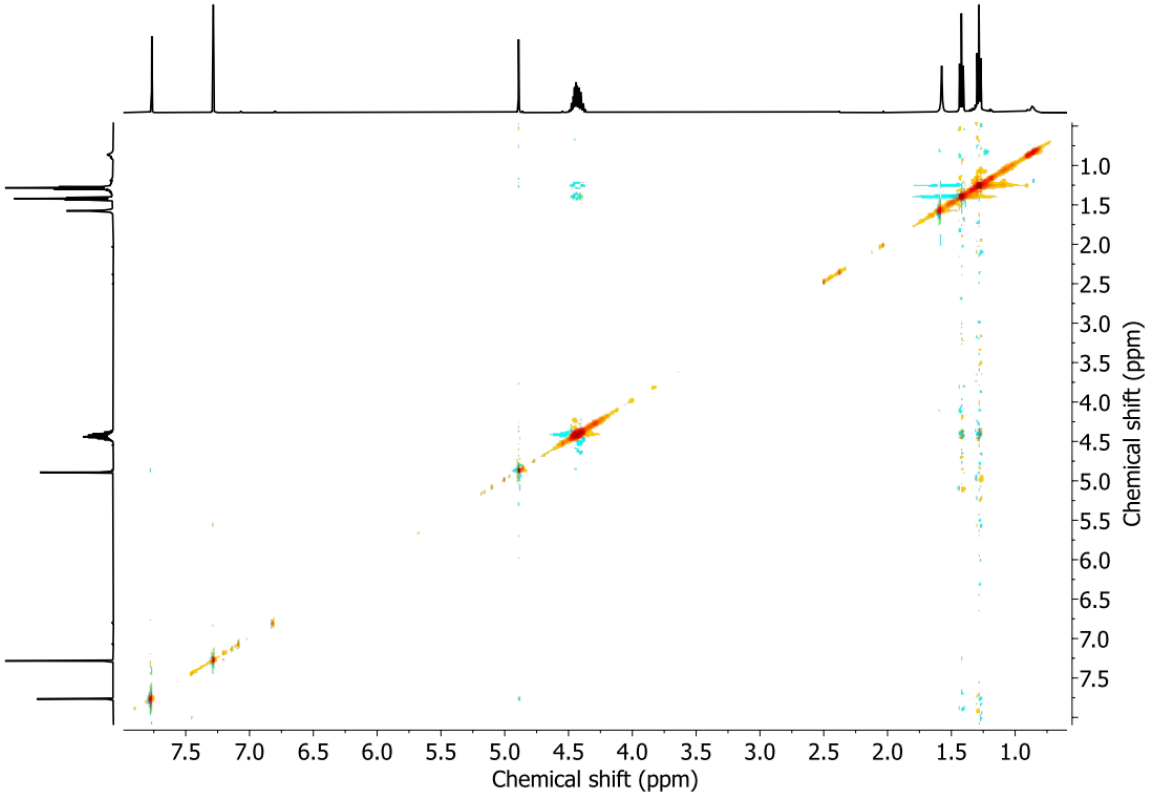


Figure S95. ^{1}H-^{1}H ROESY NMR spectrum of compound **5**.

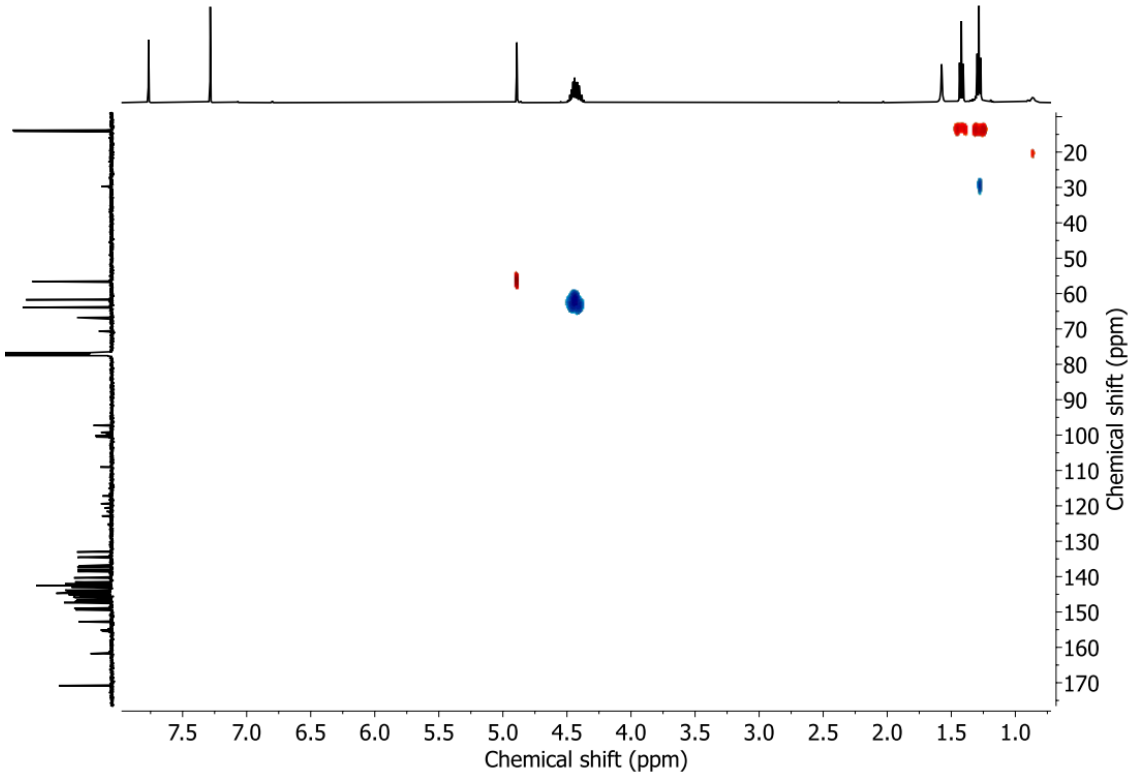


Figure S96. ^{1}H-^{13}C HSQC NMR spectrum of compound **5**.

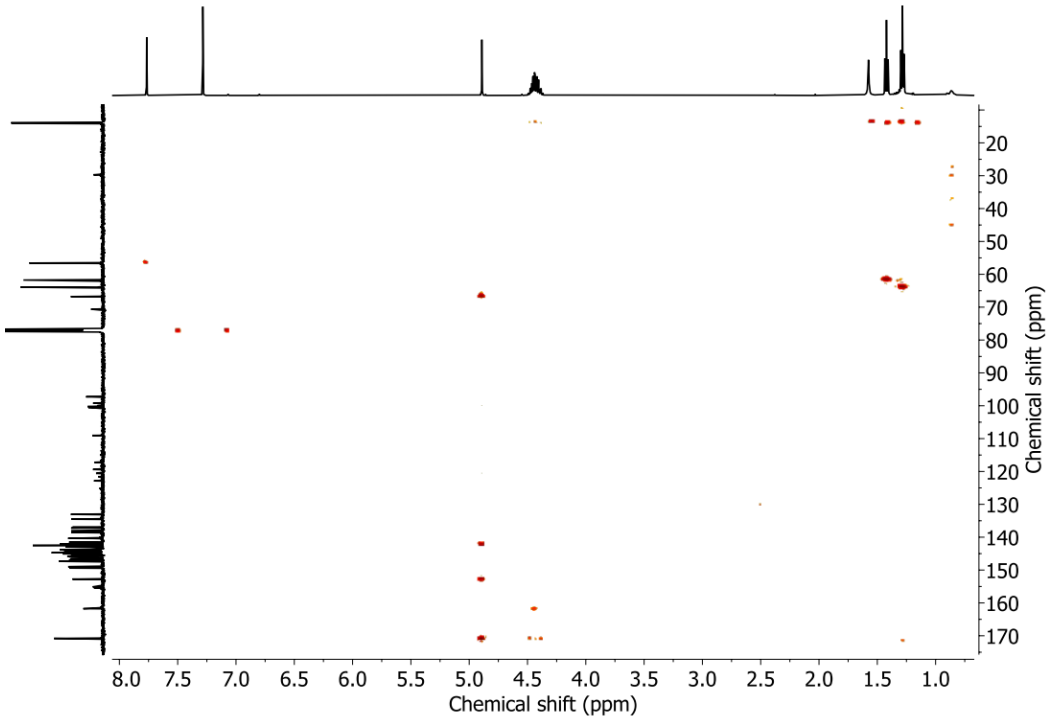


Figure S97. ^{1}H-^{13}C HMBC NMR spectrum of compound **5**.

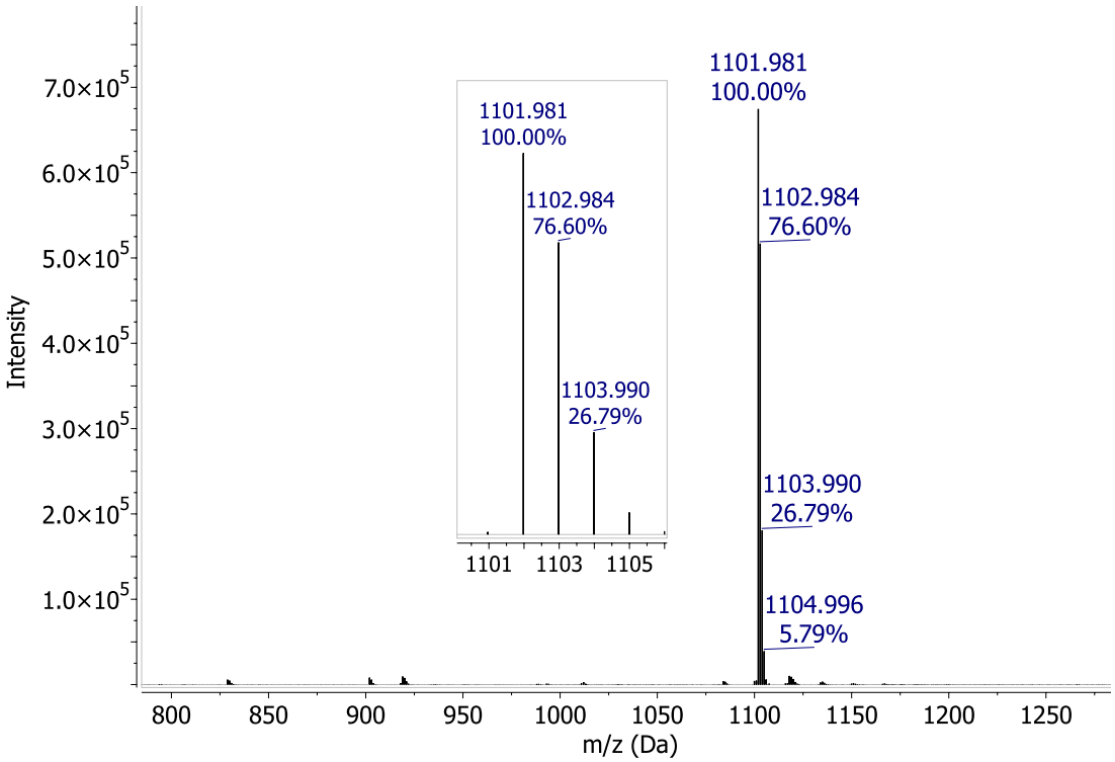
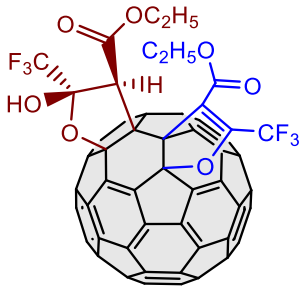


Figure S98. Negative ion MALDI mass spectrum of compound **5**.

Compound **6**



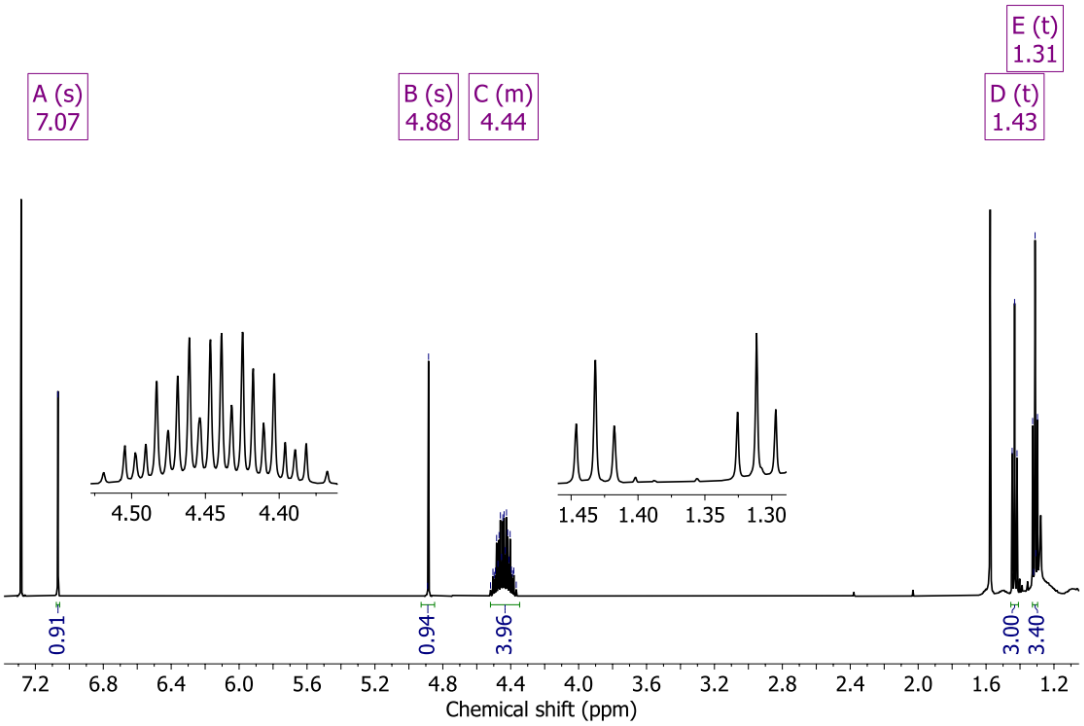


Figure S99. ^{1}H NMR spectrum of compound **6**.

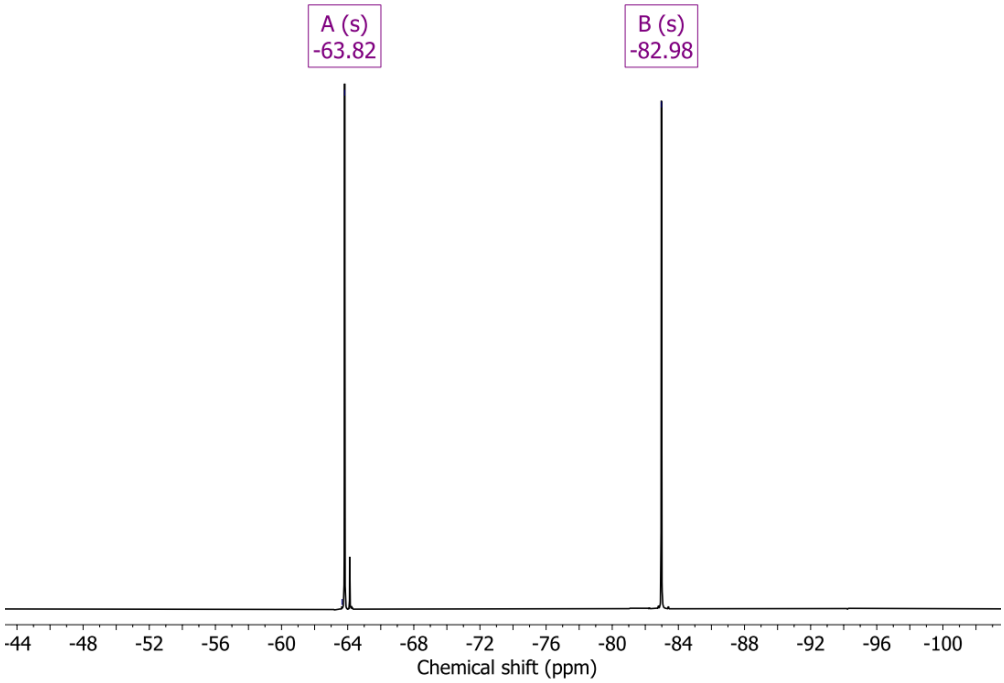


Figure S100. ^{19}F NMR spectrum of compound **6**.

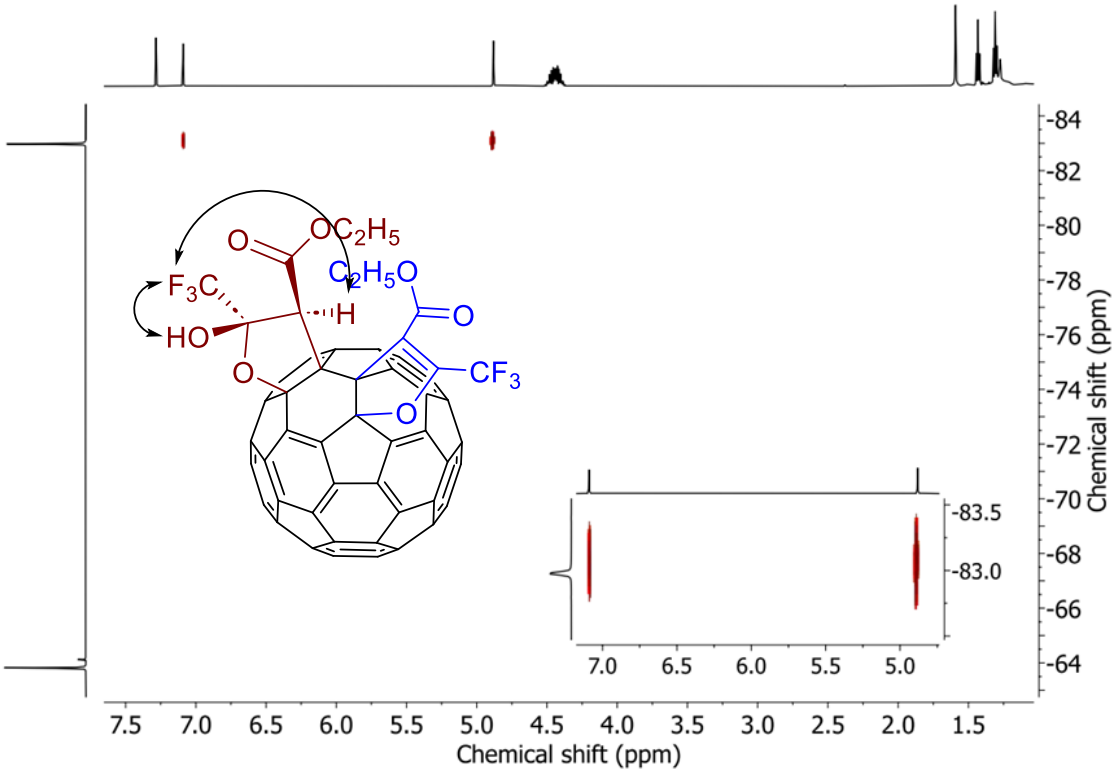


Figure S101. ^{1}H-^{19}F HOESY NMR spectrum of compound **6**.

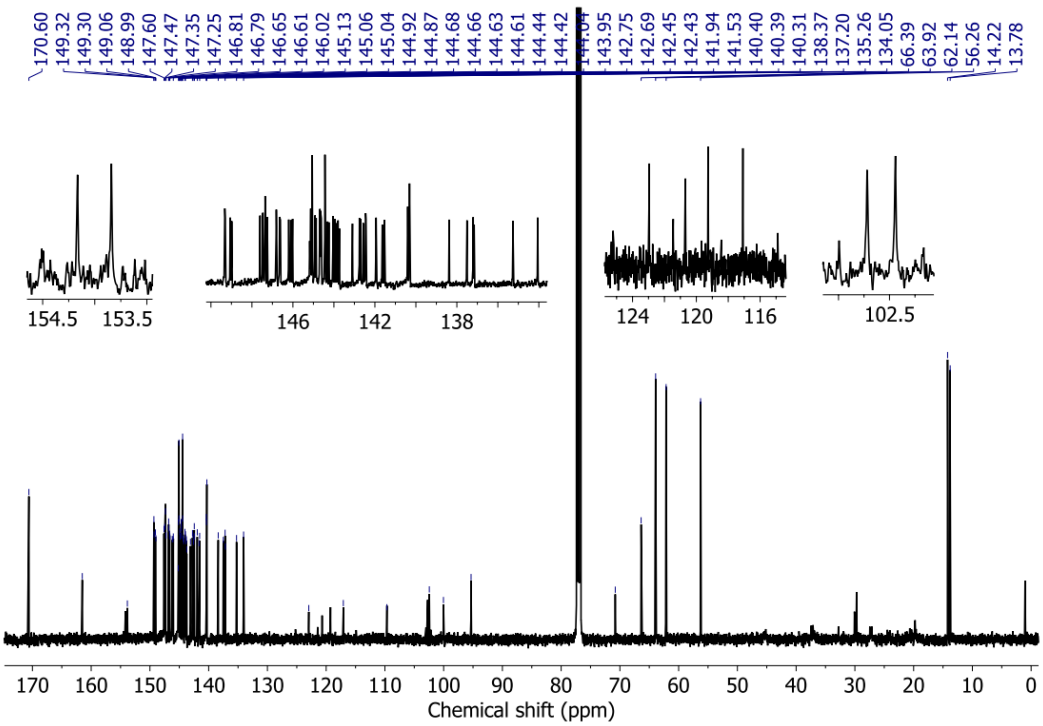


Figure S102. ^{13}C NMR spectrum of compound **6**.

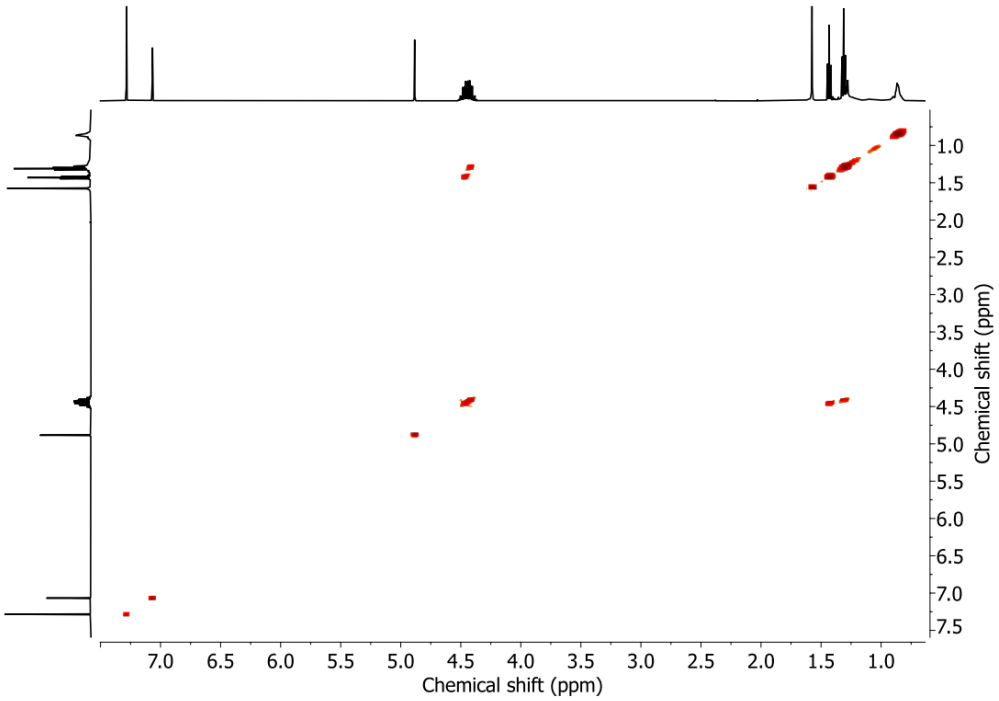


Figure S103. ^{1}H-^{1}H COSY NMR spectrum of compound **6**.

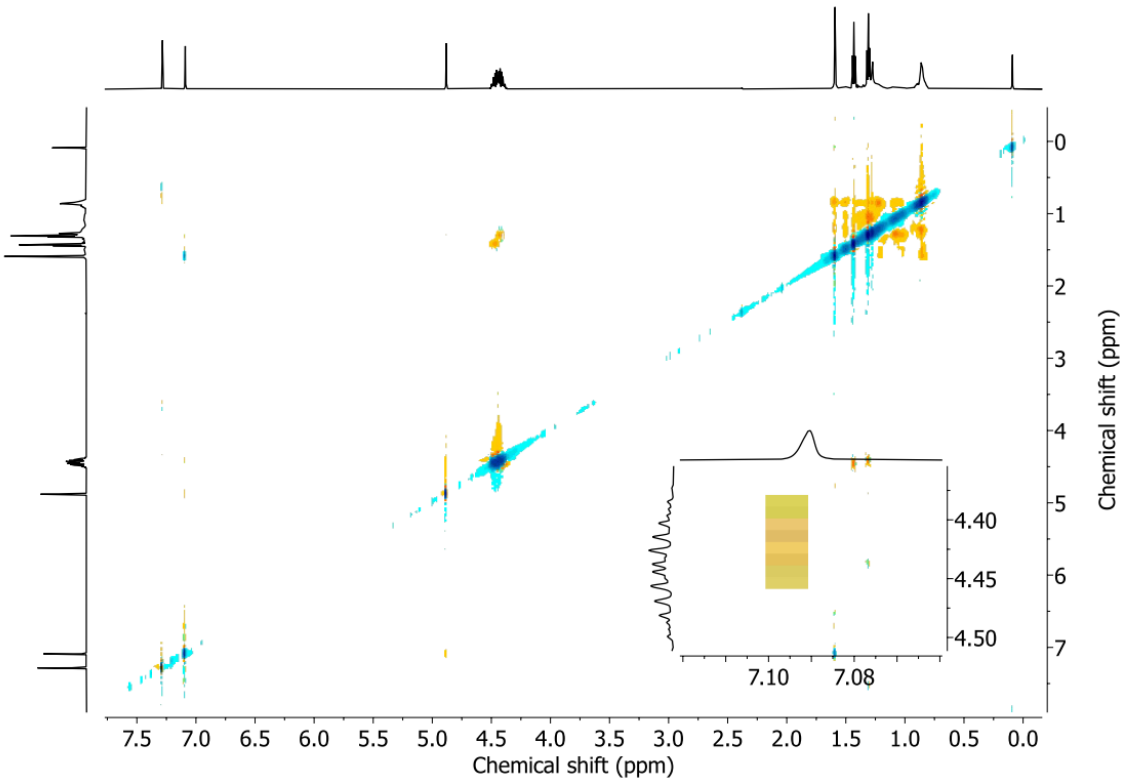


Figure S104. ^{1}H-^{1}H NOESY NMR spectrum of compound **6**.

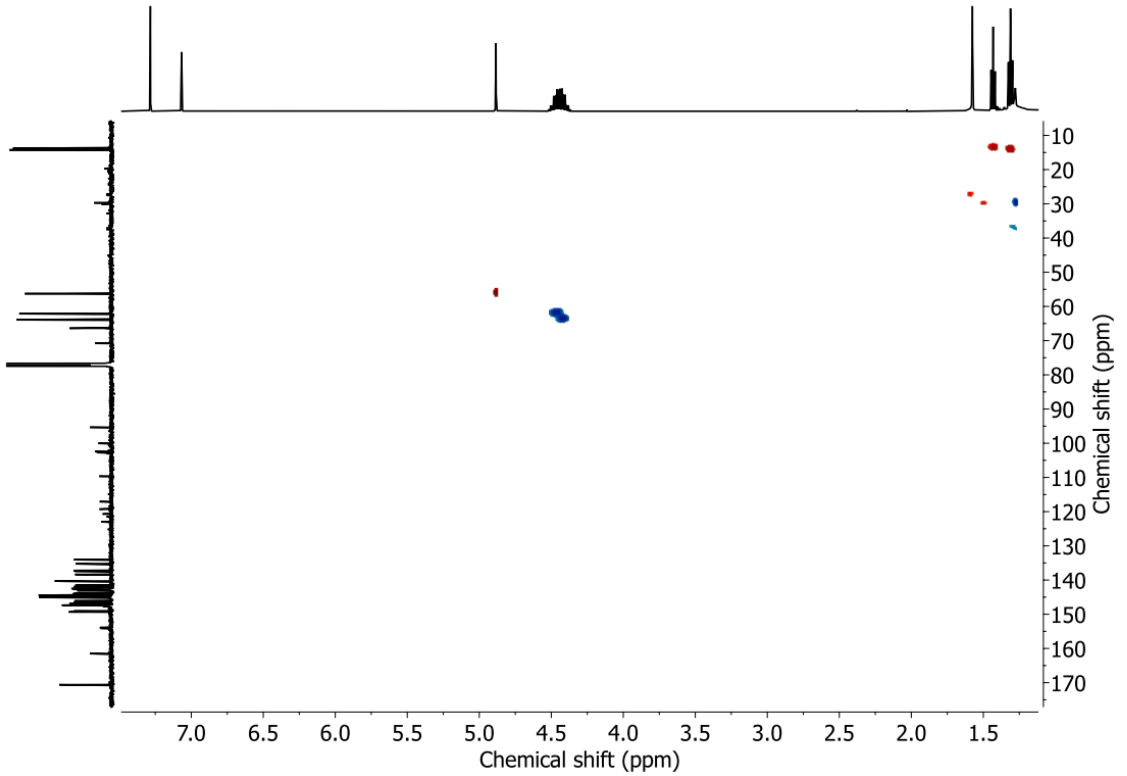


Figure S105. ^{1}H-^{13}C HSQC NMR spectrum of compound **6**.

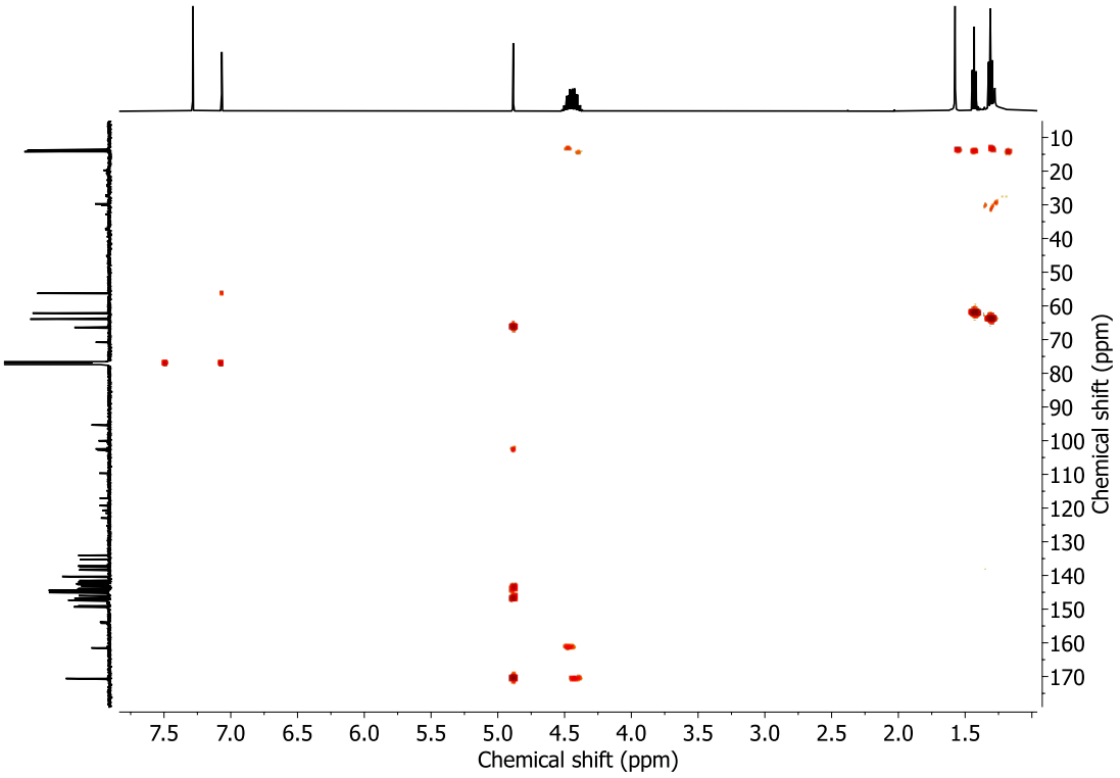


Figure S106. ^{1}H-^{13}C HMBC NMR spectrum of compound **6**.

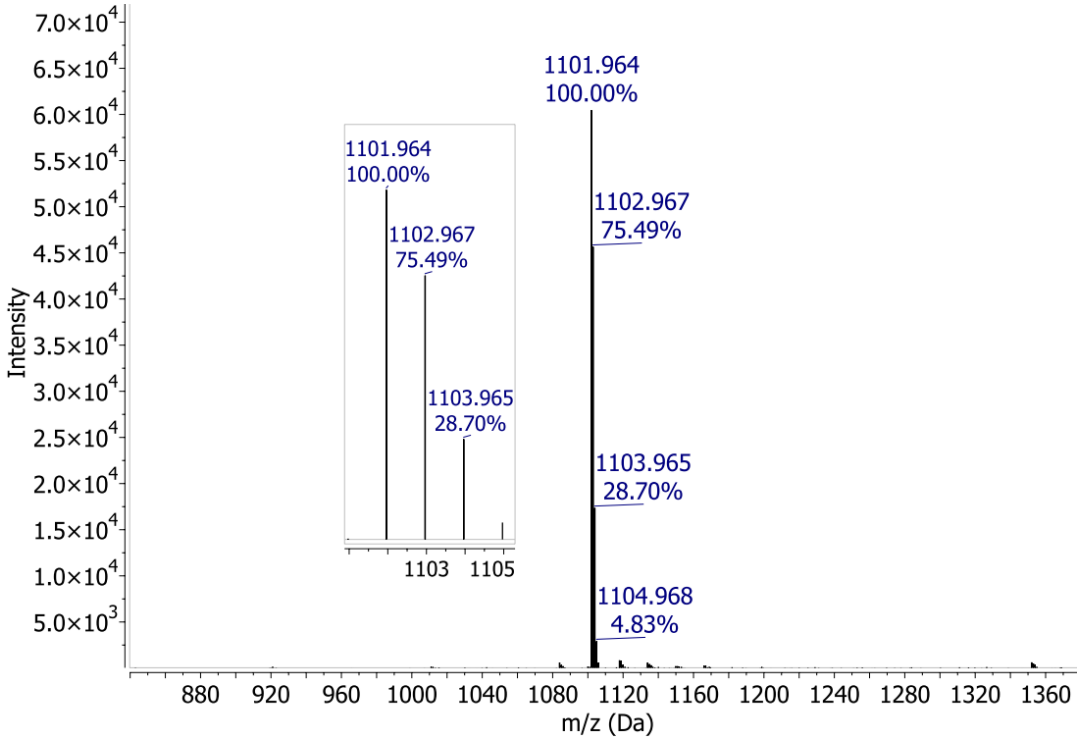


Figure S107. Negative ion MALDI mass spectrum of compound **6**.

UV-vis spectra of compounds 1-6

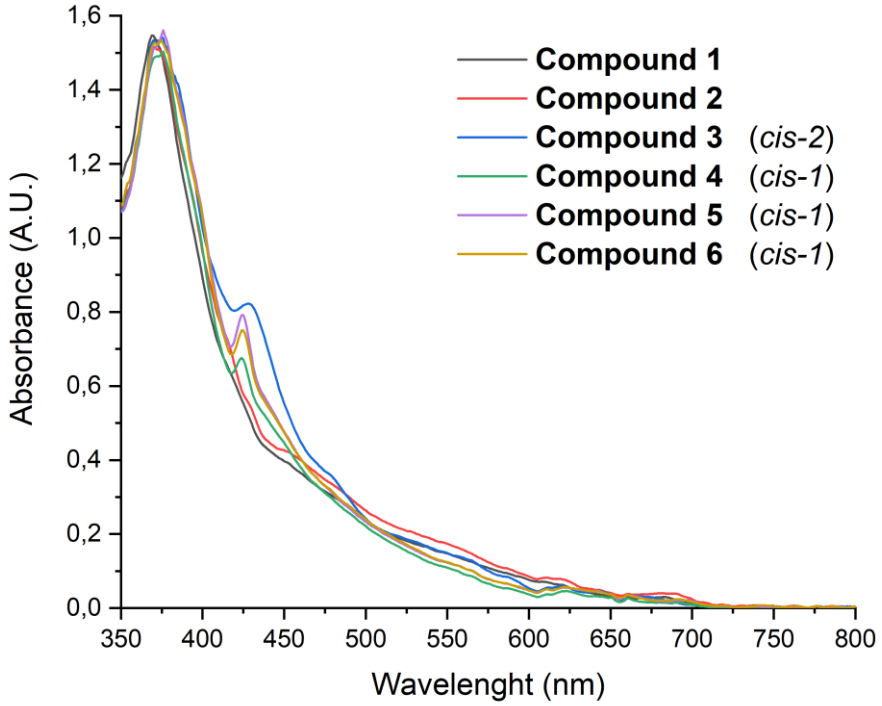


Figure S108. Comparison of the UV-vis spectra of compounds **1-6**.

Quantum-chemical calculations

The structure of isomers of C_{60} with different addends was optimized using the non-empirical Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional (*Phys. Rev. Lett.,* 1996, **77**, 3865–3868) using the extended basis H [5s1p/2s1p], C, O, F Cl [5s5p2d/3s3p2d] for valence electrons and SBK pseudopotential (*J. Chem. Phys.,* 1984, **81**, 6026-6033). All calculations were carried out at the Joint Supercomputer Center using Priroda package (*Chem. Phys. Lett*., 1997, **281**, 151–156).

The primary reaction product between acacH (acac=CH(COMe)$_2$) and $C_{60}Cl_6$ exhibits strong steric hindrance, resulting in short contacts about 2.4 Å between the H atoms of the methyl groups and the O atoms of the carbonyl groups of adjacent addends. Therefore, elimination of acacCl from $C_{60}(acac)_5Cl$ proceeds with an energy gain of 14 kcal/mol, which is higher than the 10 kcal/mol required for elimination of acacCl from $C_{60}(acac)_5Cl$.

In methanofullerene (**1**), the addition of H_2O to form (**2**) proceeds with an energy gain of 20.8 kcal/mol. It is important that a hydrogen bond of 1.78 Å is possible only in the structure with a trans- arrangement of C-H and C-OH as in (**2**). In the case of an isomeric cis- structure, its energy increases by 9.9 kcal/mol due to the disappearance of the strong intramolecular hydrogen bond. The coordinates for all structures consistent with the observed NMR data are provided below.

Note that isomeric structures in which a five-membered ring is formed with the participation of the O atom of the ester group have a higher energy.

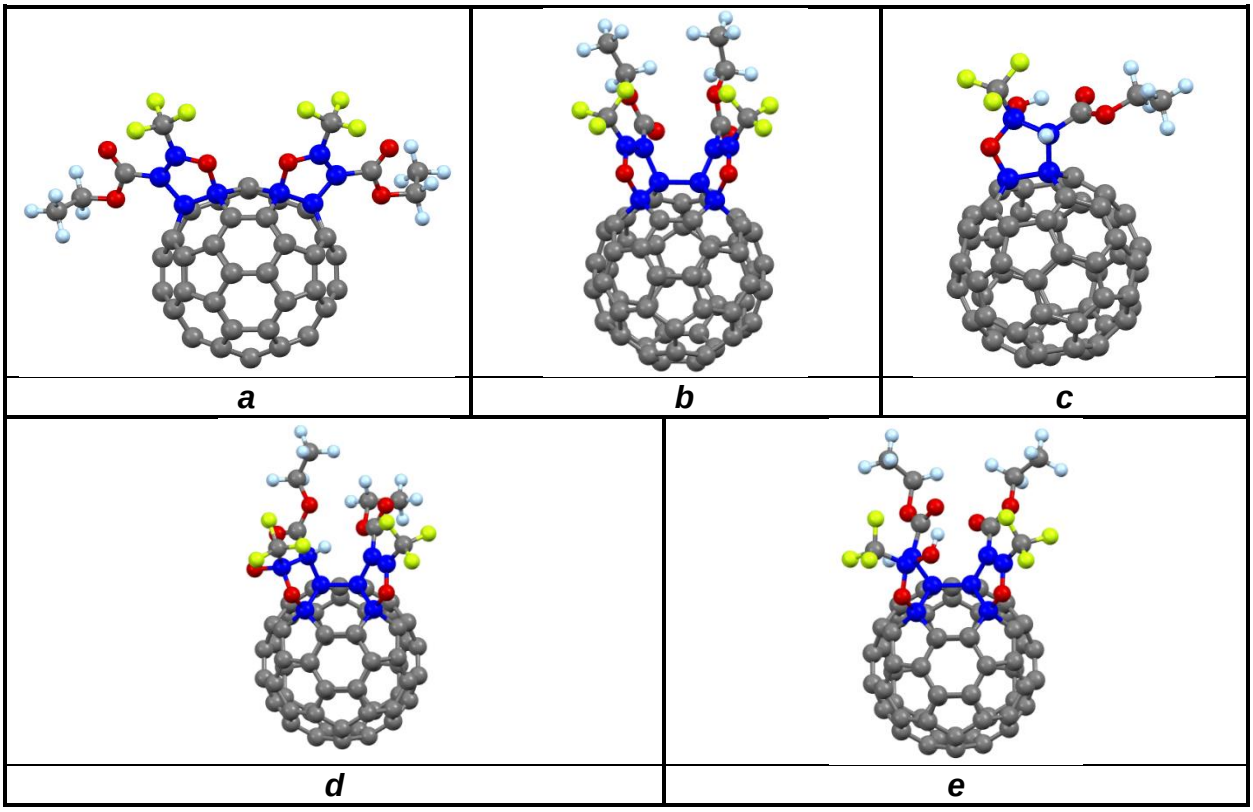


Figure S109. 3D structures of compounds **3** (a), **4** (b), **2** (c), **5** (d) and **6** (e) optimized by DFT calculations.

Cyclic voltammetry data

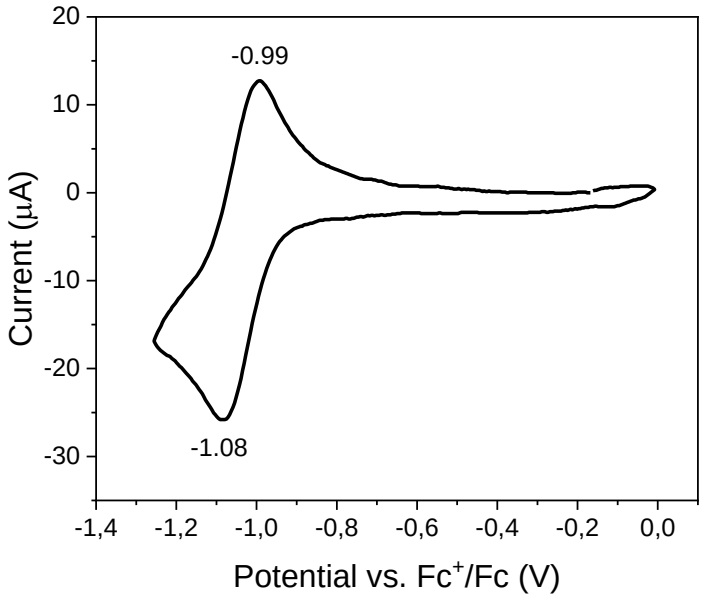


Figure S110. Cyclic voltammogram of compound **Ma**.

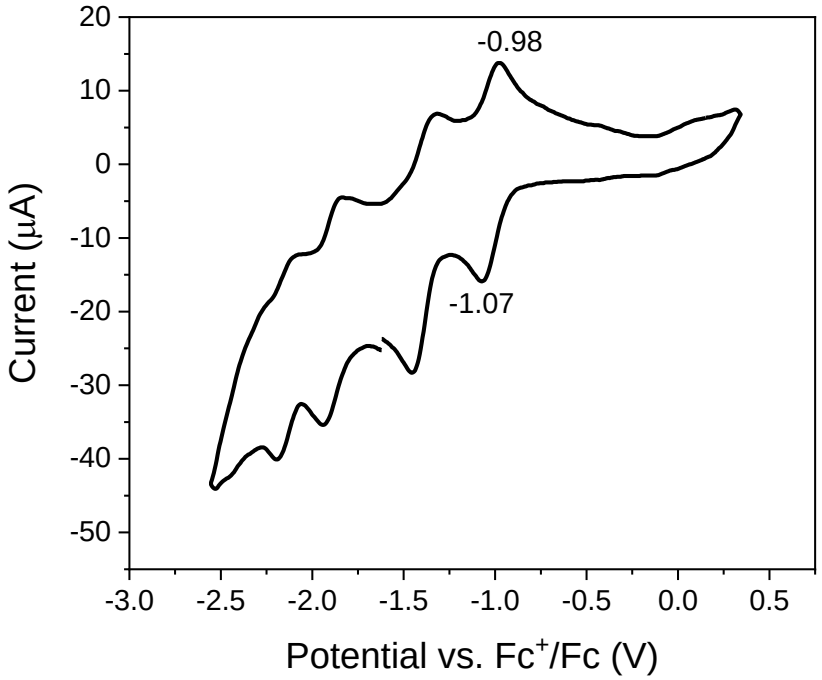


Figure S111. Cyclic voltammogram of compound **Ma** revealing multiple reduction processes.

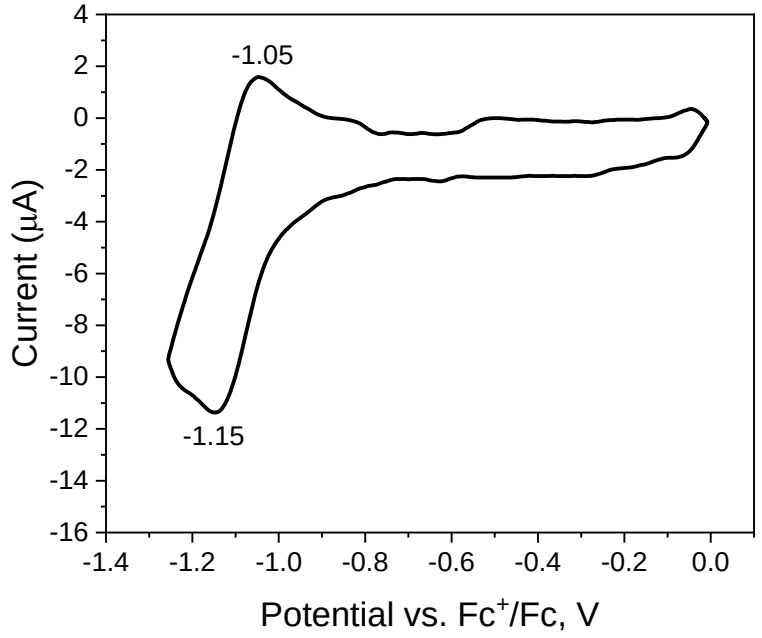


Figure S112. Cyclic voltammogram of compound **B1a**.

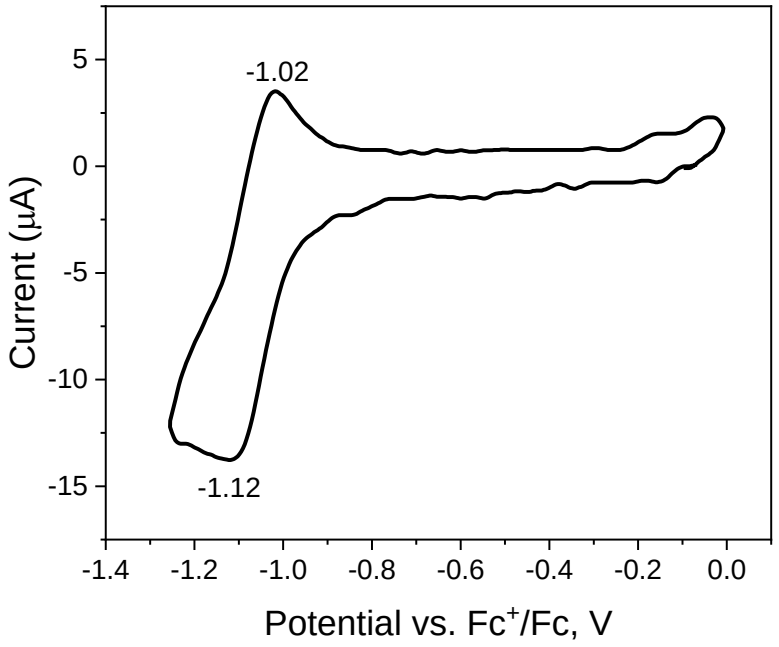


Figure S113. Cyclic voltammogram of compound **B2a**.

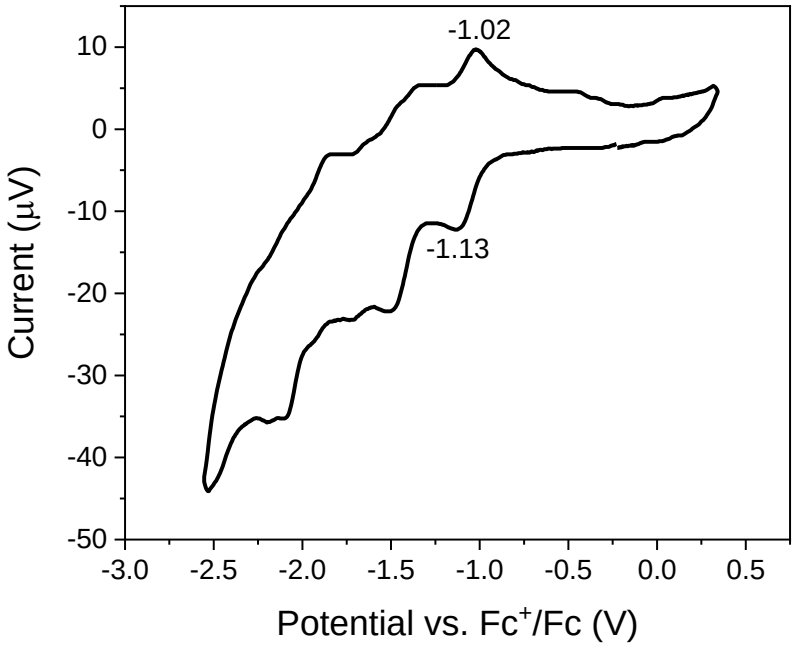


Figure S114. Cyclic voltammogram of compound **B2a** revealing multiple reduction processes.

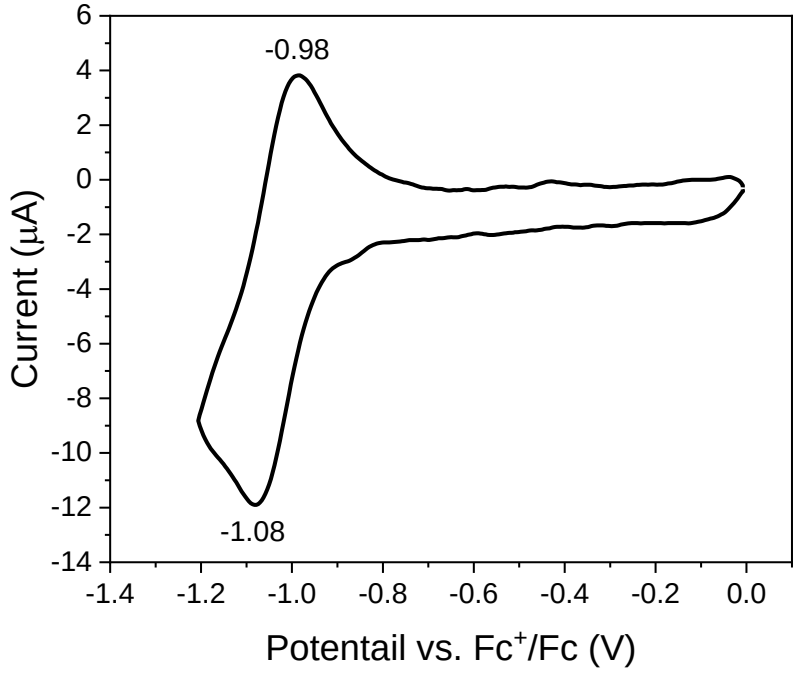


Figure S115. Cyclic voltammogram of compound **Mb**.

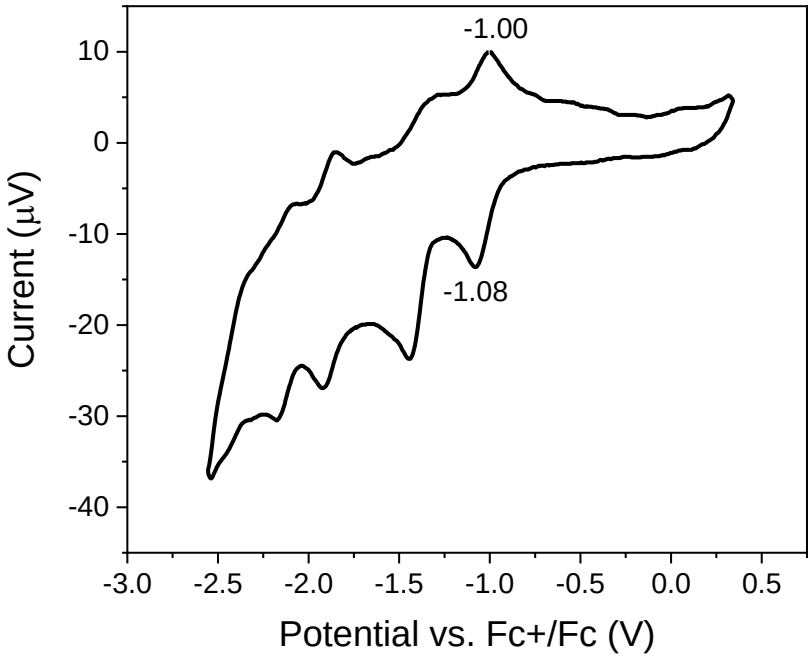


Figure S116. Cyclic voltammogram of compound **Mb** revealing multiple reduction processes.

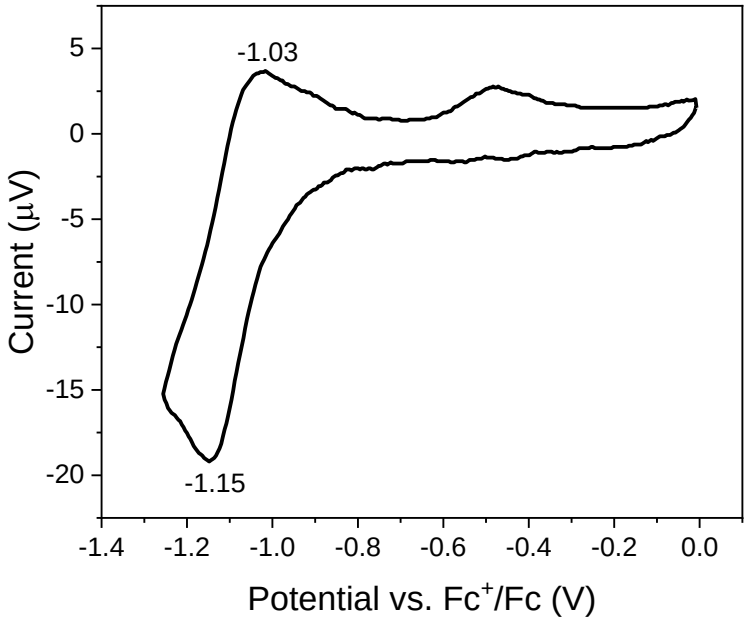


Figure S117. Cyclic voltammogram of compound **B1b**.

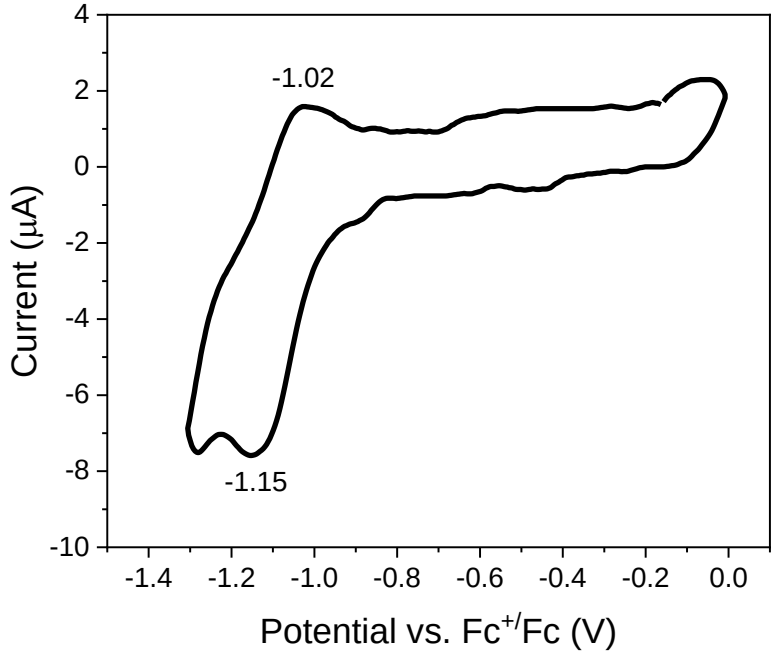


Figure S118. Cyclic voltammogram of compound **B2b**.

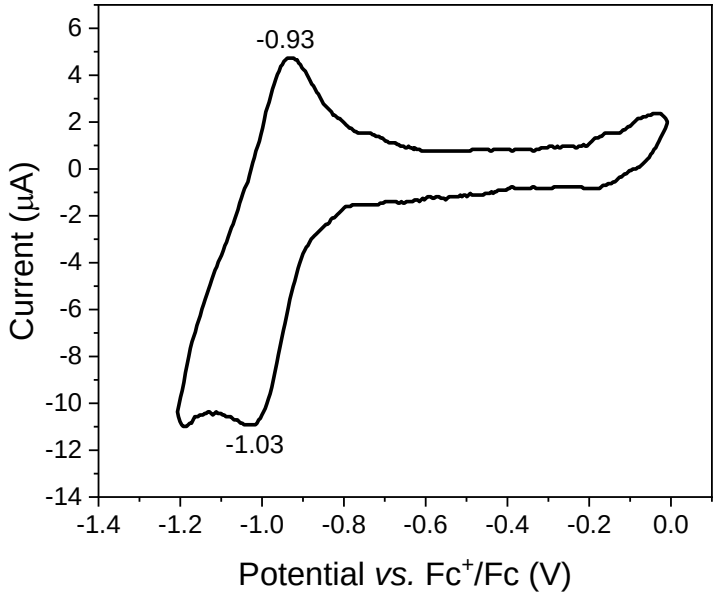


Figure S119. Cyclic voltammogram of compound **1**.

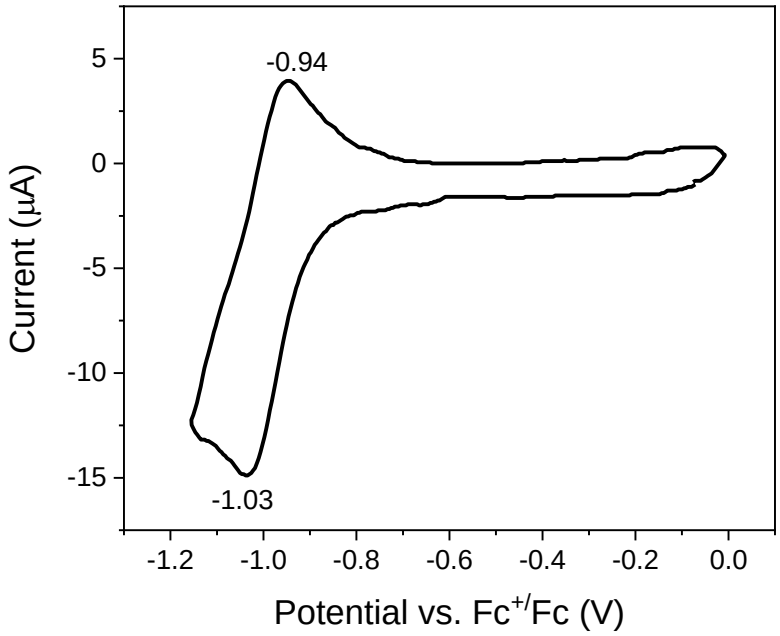


Figure S120. Cyclic voltammogram of compound **2**.

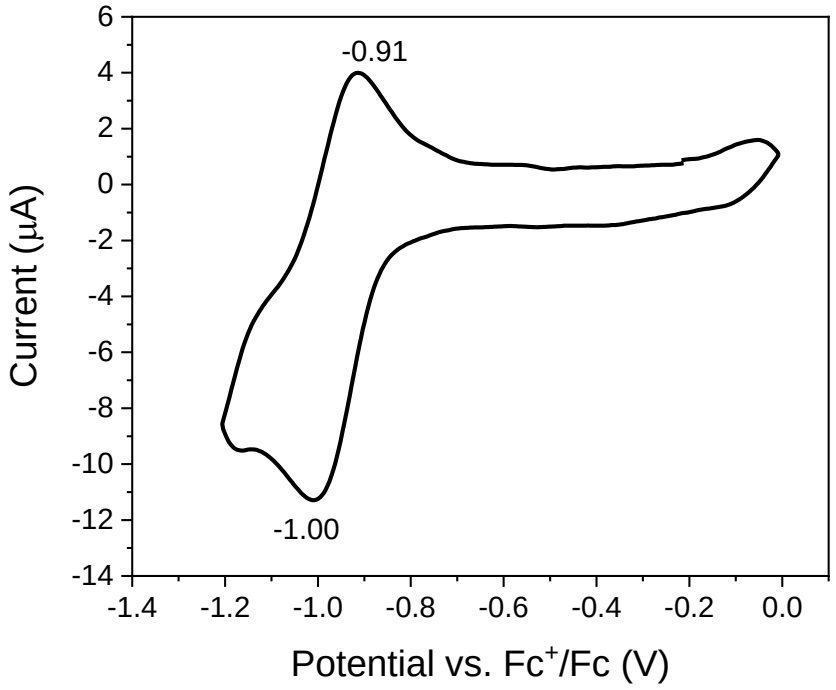


Figure S121. Cyclic voltammogram of compound **3**.

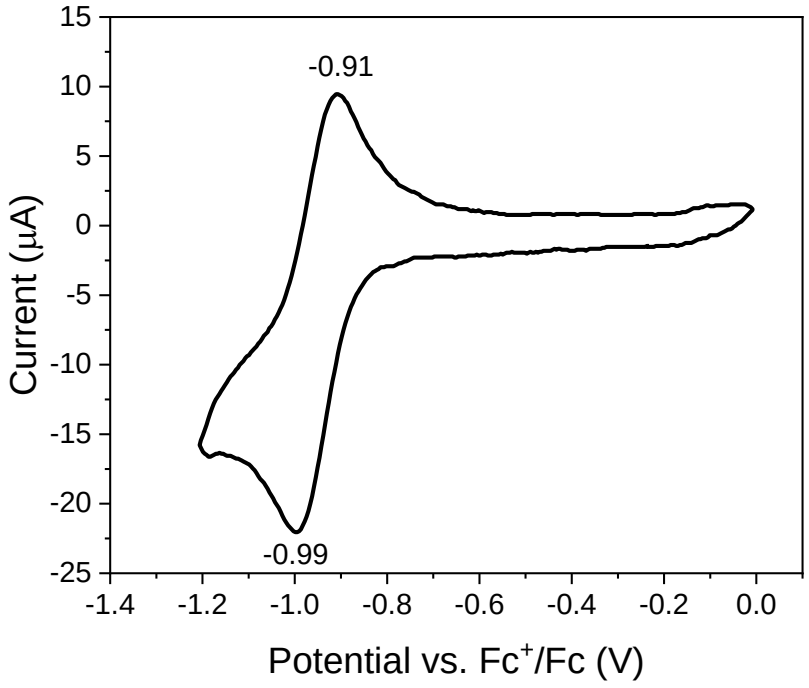


Figure S122. Cyclic voltammogram of compound **4**.

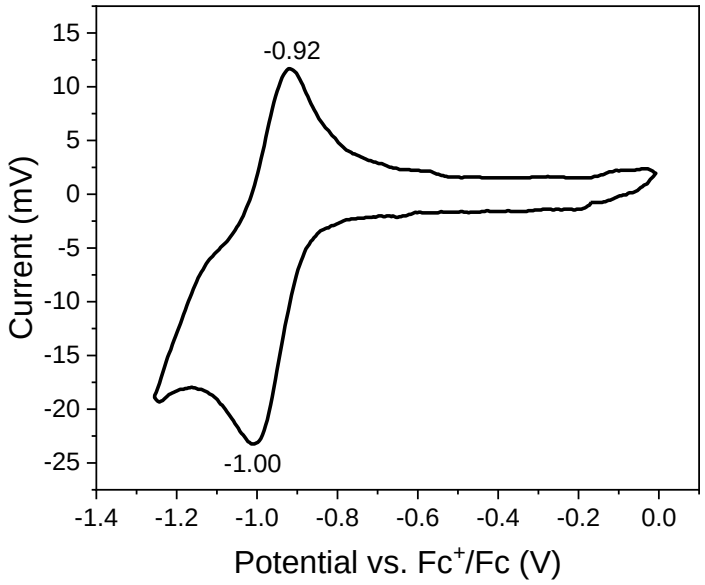


Figure S123. Cyclic voltammogram of compound **5**.

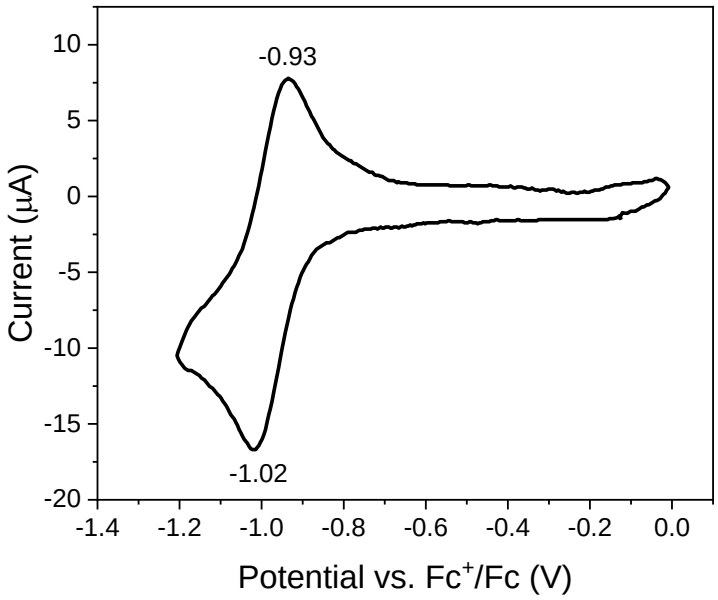


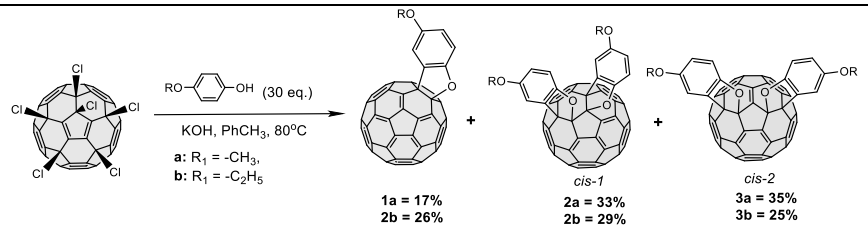
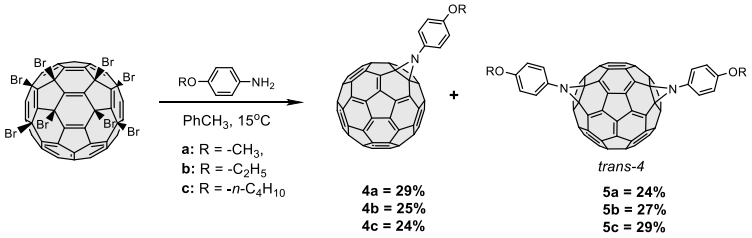
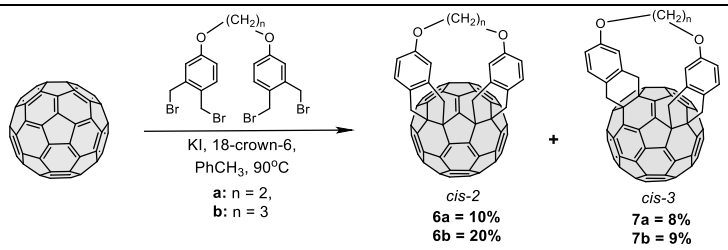
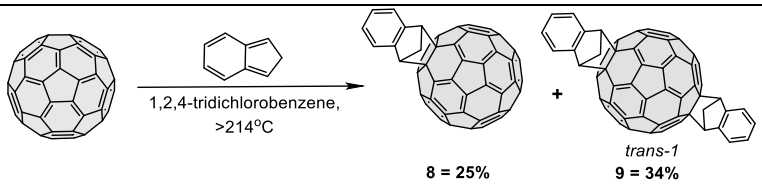
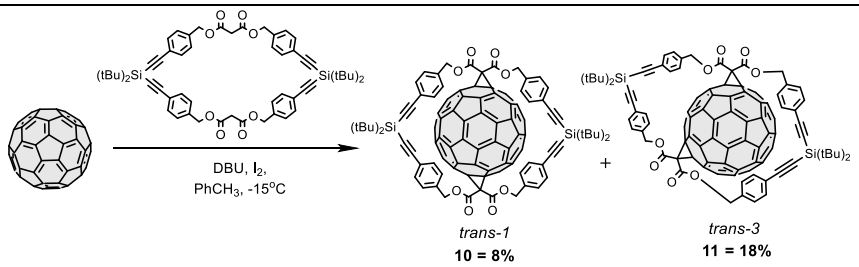
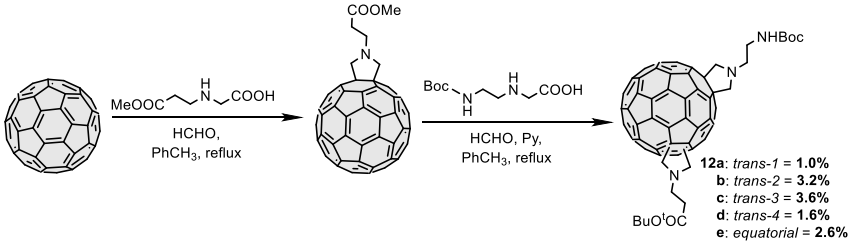
Figure S124. Cyclic voltammogram of compound **6**.

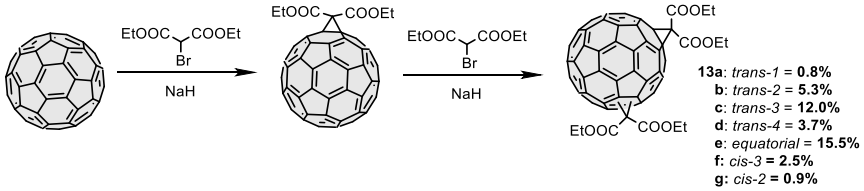
Table S1. First half-wave reduction potentials ($E^1_{1/2}$) for all synthesized compounds.

$E^1_{1/2}$, V					
Ma	**B1a**	**B2a**	**Mb**	**B1b**	**B2b**
-1.04	-1.10	-1.07	-1.03	-1.09	-1.09
1	**2**	**3**	**4**	**5**	**6**
-0.98	-0.99	-0.96	-0.95	-0.96	-0.98

Comparison of the proposed approach with the traditional methods for the synthesis of fullerene bis-adducts

Table S2. Comparison of the proposed approach with the traditional methods for the synthesis of fullerene bis-adducts.

Ref.	Synthesis scheme	Yield of the bis-adducts
[1]		*cis-1*: 29-33% *cis-2*: 25-35%
[2]		*trans-4*: 24-29%
[3]		*cis-2*: 10-20% *cis-3*: 8-9%
[4]		*trans-1*: 34%
[5]		*trans-1*: 8% *trans-3*: 18%
[6]		*trans-1:* 1.0% *trans-2:* 3.2% *trans-3:* 3.6% *trans-4:* 1.6% *e:* 2.6%

[7]		*trans-1:* 0.8% *trans-2:* 5.3% *trans-3:* 12.0% *trans-4:* 3.7% *e:* 15.5% *cis-3:* 2.5% *cis-2:* 0.9%

References:

[1] L. Ding, B. Jin, Z. Guo, Y. Zhao, J. Chen, and R. Peng, *Org. Lett.*, 2019, **21**, 9924-9928.

[2] M. Taki, S. Sugita, Y. Nakamura, E. Kasashima, E. Yashima, Y. Okamoto and J. Nishimura, *J. Am. Chem. Soc.*, 1997, **119**, 926–932.

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Cartesian coordinates of the calculated molecular structures

Structure 1

6	1.79218018	-0.16210508	1.95814944
6	0.47412232	-0.01227402	2.59708650
6	-1.55759049	-1.62082931	-1.19226864
6	0.31831275	1.38311509	2.96377229
6	1.96952839	-1.03614504	0.89074291
6	-1.89963029	-0.07946345	1.99499881
6	1.43676824	4.69606239	0.10375361
6	2.42224409	1.14280450	1.93821288
6	1.42989887	3.40481465	2.06791938
6	-1.68009281	-1.57813933	0.19304220
6	-0.62672703	-0.74090703	2.15336774
6	-2.87033877	3.70813442	-0.85046897
6	-1.90803129	3.22621721	-3.07773287
6	2.23817660	3.80972600	0.92773566
6	2.73191107	-0.61089776	-0.25715625
6	-2.55060660	1.92510919	-3.05850476
6	-0.93290590	2.01191218	2.85813397
6	-2.54255995	-0.59051878	0.79796297
6	-0.23949093	-1.77361464	-1.83098802
6	3.36678592	0.64156824	-0.27847001
6	-0.44360713	1.68305418	-4.08265423
6	1.51850053	2.09562951	2.55938222
6	-2.06818783	1.26432954	2.36587724
6	-1.02870898	3.36692586	2.34201981
6	-2.06350595	4.10218571	-1.99302499
6	1.53296756	4.63310123	-1.29430179
6	-3.49372158	2.45183985	-0.83327056
6	-0.92245970	4.85643666	-1.49939018
6	0.13401731	4.84520799	0.73729354
6	-1.54080662	-0.32982375	-3.15773798
6	-3.23039396	0.19254572	-1.43099785
6	-2.34686178	-0.72891887	-2.01678352
6	3.21006074	1.53787386	0.84475654
6	0.81112153	1.06692653	-3.97238728
6	0.92091786	-1.87913069	-1.06806672
6	3.11271194	2.89231227	0.32776531
6	0.13152066	4.05122281	1.95238466
6	-3.33039193	1.54320943	-1.95744837
6	1.95094289	1.82598204	-3.48182161
6	0.33147423	4.71289561	-2.10957304
6	-3.32930091	0.26466534	0.00864639
6	-1.64357535	0.96787392	-3.67483244
6	-0.24271646	-0.97203421	-3.04011128
6	0.91210481	-0.28379095	-3.44525182
6	3.37343664	1.43325289	-1.49768890
6	1.79437209	3.17208693	-3.11972560
6	3.21456014	2.82837032	-1.12227117
6	-0.60521927	3.07658091	-3.71110949
6	2.43761985	3.68243579	-1.91842370
6	-2.87450674	2.15019374	1.54156888

6	-3.49475763	1.65937594	0.38548117
6	2.09015975	-1.12231335	-1.45438103
6	-2.23066466	3.45314198	1.52682578
6	0.49337364	3.80884836	-3.23718370
6	-1.02369218	4.92685143	-0.05044696
6	2.75345398	0.94141755	-2.65335742
6	-2.22703361	4.21777180	0.35100983
6	2.10578586	-0.36061849	-2.63432427
6	-0.52736109	-1.81687301	1.11502348
6	0.90675547	-1.98003713	0.42667742
6	0.29702975	-3.09557922	1.27360572
6	-0.15668665	-4.37396389	0.58348351
8	-0.83790735	-4.44604037	-0.41533528
6	0.91504114	-3.36190153	2.64217912
8	2.08860534	-3.25345848	2.90708860
6	-0.07020973	-3.81138412	3.78731008
9	0.33941680	-4.97635617	4.33060579
9	-1.34512308	-3.97340246	3.34434702
9	-0.08381707	-2.87224522	4.76218596
8	0.34293715	-5.43163262	1.26442702
6	-0.01487531	-6.75750750	0.74998763
1	-1.11141632	-6.82038106	0.71094182
1	0.37204518	-6.83542359	-0.27578039
6	0.59426639	-7.78787261	1.68008849
1	1.68904553	-7.70396090	1.70627445
1	0.20619820	-7.68081969	2.70189703
1	0.33511156	-8.79364528	1.31925819

Structure 2

6	0.90411378	1.71592810	1.52398328
6	0.90702992	0.65846922	2.55613721
6	1.14485834	-2.52660859	-0.71614532
6	-0.30099280	0.80519854	3.34030078
6	1.40437987	1.46771731	0.25688690
6	0.68828121	-1.76180363	2.71781089
6	-4.29488358	1.52570141	1.36716392
6	-0.30825767	2.48875674	1.69517947
6	-2.45198529	1.89001885	2.77691598
6	1.53061767	-2.24707017	0.58311787
6	1.40397196	-0.59840856	2.26930621
6	-3.84279177	-2.96958681	1.53184438
6	-4.05120886	-2.73623865	-0.92188836
6	-3.16231958	2.39718993	1.61232454
6	0.67319144	1.94310110	-0.88935658
6	-2.83998803	-3.51634729	-1.08518739
6	-0.98151365	-0.32816984	3.81628500
6	0.76252204	-2.77560790	1.67754056
6	1.14082242	-1.46824288	-1.74811153
6	-0.49440187	2.71413867	-0.74467445
6	-2.84824047	-1.82899212	-2.72947942
6	-1.05218994	1.92977597	2.81153915
6	-0.47455272	-1.64345851	3.49734221

6	-2.43097194	-0.37918411	3.76757435
6	-4.54402571	-2.46546213	0.36345072
6	-4.67570805	1.22150745	0.05152747
6	-2.67290734	-3.72729402	1.37474310
6	-5.05383208	-1.14152213	0.68138853
6	-4.29026292	0.48180170	2.38418128
6	-0.69359376	-2.88659766	-2.13640659
6	-0.71199062	-3.94765942	0.09651412
6	0.01184405	-3.39260932	-0.97202520
6	-0.99652868	2.99439012	0.57998722
6	-2.17749076	-0.68689376	-3.19284950
6	1.51603806	-0.17387440	-1.42840446
6	-2.44694877	2.94141232	0.53488400
6	-3.15467807	0.70945982	3.25655858
6	-2.16116934	-4.00626007	0.04123950
6	-2.69414023	0.63600236	-2.87548866
6	-5.05858933	-0.13686538	-0.29715311
6	-0.32674610	-3.63352319	1.45400346
6	-2.09157647	-2.95311999	-2.19879066
6	0.00386203	-1.70418831	-2.61346869
6	-0.72782351	-0.62582319	-3.13911840
6	-1.63149139	2.48518115	-1.62280011
6	-3.86046825	0.76765422	-2.10782574
6	-2.84125292	2.62609867	-0.82962931
6	-4.05596614	-1.69210385	-1.93863123
6	-3.93553112	1.78125050	-1.06644887
6	-1.60874099	-2.52139205	3.25267515
6	-1.53645475	-3.49724853	2.25055916
6	0.74242090	0.92932596	-1.92742707
6	-2.82110169	-1.73737290	3.41907606
6	-4.55397653	-0.41696507	-1.63156063
6	-4.66618362	-0.82706305	2.04673515
6	-1.56011077	1.51005983	-2.62572638
6	-3.91820221	-1.95616188	2.57301698
6	-0.34819876	0.72357876	-2.79002179
6	2.20906567	-0.93748071	1.00233617
6	2.21381443	0.21413802	-0.12000894
6	3.76373821	0.44712286	-0.34116861
6	4.12835606	1.88117903	-0.69265444
8	4.32811718	2.76438065	0.13597484
6	4.37826543	-0.06942385	0.98681120
8	3.60198523	-1.20214321	1.29917432
6	5.83592132	-0.60594921	0.79828907
9	6.32472692	-1.12538549	1.93761531
9	6.64813669	0.42061909	0.41615927
9	5.90802067	-1.55886642	-0.16863928
8	4.19523301	2.06418248	-2.01775129
6	4.52825582	3.42296882	-2.46512918
1	3.76168573	4.10706144	-2.07515246
1	5.49332921	3.69640551	-2.01638004
6	4.57631468	3.40261311	-3.97986520
1	5.33736143	2.69852373	-4.34265862

1	3.60386504	3.12202352	-4.40656314
1	4.83370254	4.40642443	-4.34706277
1	4.09046285	-0.21048682	-1.15646126
8	4.35503273	0.86572097	2.02015265
1	4.40064454	1.76237272	1.59980865

Structure 3

6	-2.16912044	-1.86217848	1.14439523
6	-1.81536178	-3.10073148	0.57074431
6	2.58481991	-1.92450226	0.57198261
6	-2.13501846	-3.10943076	-0.88834435
6	-1.21783140	-1.16245663	1.90586554
6	-0.01911421	-4.05249522	-0.48357260
6	-2.85390410	0.58669457	-3.52162954
6	-2.99202777	-1.15695910	0.16732198
6	-3.46895172	-1.28675933	-2.25226576
6	1.71184078	-2.99194211	0.66983548
6	-0.53373329	-3.61370256	0.78987848
6	0.79635792	-1.65620694	-4.69513756
6	1.93390634	0.45385737	-4.09973848
6	-3.44566882	0.16728085	-2.27075815
6	-1.24898100	0.34727750	2.06950346
6	2.84750070	-0.30182742	-3.25363513
6	1.37421482	-3.74997657	-0.53480372
6	2.49004515	-0.65956989	1.45810214
6	-2.31013513	1.12909328	1.16045540
6	2.34513347	1.70326545	-2.15689485
6	-3.01369056	-1.94803337	-1.07536337
6	-0.92448415	-3.74299250	-1.53831956
6	-2.53307759	-3.01093450	-3.64844280
6	0.93862813	-0.21399647	-4.83007792
6	-1.96165682	1.66889504	-3.54130620
6	1.63987253	-2.37391655	-3.84471775
6	-0.39480102	0.34483772	-4.93810653
6	-2.58866053	-0.61104781	-4.29263789
6	3.25512370	-0.14733529	-0.80848132
6	2.88959746	-2.34176074	-1.86000064
6	3.16685285	-1.58896790	-0.70416663
6	-3.05669343	0.21861525	0.15455820
6	1.73087954	2.20648534	-0.99877029
6	1.08726270	-0.51243193	2.23815590
6	-3.19837674	0.89112878	-1.10469442
6	-3.10887207	-1.76656298	-3.56500559
6	2.71745584	-1.69351497	-3.14689764
6	0.38144713	2.73186712	-1.06906791
6	-0.70107720	1.54201887	-4.26619134
6	1.92809706	-3.40524262	-1.77270819
6	3.10827135	0.48355994	-2.06238576
6	2.70301857	0.42302109	0.38473747
6	1.91187857	1.55367611	0.27882777
6	-1.65605038	2.09623693	0.14728336

6	-0.30331575	2.76215525	-2.29566812
6	-2.33472761	2.04459037	-1.11642315
6	1.62052674	1.69353532	-3.41987765
6	-1.69967178	2.41203324	-2.32328236
6	-0.32225603	-3.57943968	-2.86825230
6	1.08873063	-3.37924341	-2.94317512
6	0.21929983	0.67794708	1.86098119
6	-1.14673685	-3.01223371	-3.91614925
6	0.32238988	2.22350220	-3.49430049
6	-1.35080060	-0.75852836	-4.93632446
6	-0.30693151	2.40203368	0.16054845
6	-0.60345083	-1.98569864	-4.74620647
6	0.63607706	1.65349916	1.01513789
6	0.47066839	-2.88430748	1.47669241
6	0.10535022	-1.65560451	2.04620961
8	1.44944486	-0.41727216	3.67383659
6	2.78492497	-0.48793448	3.79139561
6	3.48697638	-0.61918920	2.63513695
6	3.26725086	-0.40565236	5.24831469
9	2.20740420	-0.25808344	6.07955264
8	5.37828925	-0.82130549	1.26321769
6	6.82224546	-0.92334556	1.07228989
1	7.23445012	-1.54938280	1.87491225
6	7.48226006	0.44755292	1.04394476
1	7.04837911	1.08243862	0.25888730
1	7.38095457	0.95313903	2.01300038
1	8.55532889	0.32868947	0.83134927
9	4.08154264	0.65463602	5.43648891
1	6.92600991	-1.44405453	0.11141444
9	3.91636327	-1.53137131	5.61432530
6	4.95714509	-0.71983233	2.55606731
8	5.70607817	-0.71850317	3.51848460
6	-3.19222516	1.79848243	2.23474566
8	-1.62461159	0.66600771	3.47205673
6	-2.70635579	1.45964536	3.45880190
6	-3.19360788	1.83786327	4.86692855
9	-3.12954700	3.17142723	5.06670615
9	-2.40967167	1.24789695	5.80148751
8	-5.01362433	3.19364174	2.90487521
9	-4.45988786	1.41953186	5.07695617
8	-4.63976821	2.80766833	0.68821832
6	-5.79101578	3.64480418	0.36281633
1	-5.57184067	4.01574299	-0.64699964
1	-5.81625691	4.48827678	1.06546327
6	-4.36650025	2.66495302	2.01677118
1	-7.30129209	2.49375283	1.41689611
6	-7.08883832	2.85115163	0.40095275
1	-7.05026486	1.99191051	-0.28298534
1	-7.91980714	3.50013864	0.08625495

Structre 4

6	0.46572413	-2.88674061	-2.13039498

6	1.77075426	-3.37187236	-1.74588729
6	2.09096364	-3.46201915	-0.38075163
6	1.11517120	-3.09896291	0.62841676
6	-0.14672049	-2.65981450	0.26598620
6	-0.44546992	-2.50500825	-1.13020286
6	0.61845929	-2.06899060	-3.32434114
6	2.02595923	-2.04398959	-3.67135924
6	2.74178967	-2.85093112	-2.69052820
6	4.00763210	-2.44509726	-2.24442864
6	3.40374919	-3.03953473	0.07653747
6	1.84479176	-2.42546927	1.71875884
6	1.27642225	-1.34931673	2.37708961
6	-1.41497310	-0.69200563	0.00057981
6	-1.23421916	-1.30389608	-1.29379571
6	-1.11578791	-0.53940522	-2.46053679
6	-0.16404304	-0.91819027	-3.48991754
6	2.60477595	-0.86666885	-4.17037882
6	1.79339879	0.32631464	-4.34812887
6	0.43041729	0.30067526	-4.01377430
6	-0.16481901	1.42676233	-3.31296033
6	-1.11634438	0.89718918	-2.35217772
6	-1.23523978	1.47770313	-1.08385013
6	-1.41587258	0.67839774	0.10391555
6	3.24955265	-2.40625432	1.37425946
6	3.24818050	2.16929626	1.71999474
6	4.05176087	1.03032071	1.89411961
6	5.02687202	0.66262588	0.88398354
6	5.16710541	1.45141299	-0.26724957
6	4.34708978	2.64265188	-0.44231543
6	2.08879058	3.47516083	0.14296894
6	1.11345843	2.96472763	1.08656981
6	1.84338592	2.13553527	2.06349289
6	1.27561602	0.97226064	2.55246542
6	2.07465664	-0.20467971	2.68283119
6	3.45671338	-0.18275553	2.39867743
6	5.02722093	-0.79001851	0.77420576
6	5.16785722	-1.39681697	-0.48243189
6	5.32084252	-0.57951931	-1.67017898
6	5.32048820	0.82186630	-1.56431716
6	4.60445495	1.62402666	-2.54388858
6	4.00606739	2.75162891	-1.85188345
6	2.73999253	3.21902559	-2.23214399
6	1.76869459	3.59145167	-1.22008109
6	-0.14803756	2.58414264	0.66201894
6	-0.44686051	2.64076823	-0.74155978
6	0.46389985	3.16902939	-1.67307785
6	0.61698998	2.54011752	-2.97642119
6	2.02454844	2.56824600	-3.32309247
6	2.60406272	1.47958072	-3.99323630
6	3.91662642	0.99859206	-3.59504312
6	3.91705242	-0.45008970	-3.70444803
6	4.60526569	-1.22592308	-2.75915341

6	4.05244126	-1.30588851	1.71760185
6	4.34871685	-2.54883995	-0.83450552
6	3.40195725	2.99060294	0.53215327
6	-0.19780200	0.63542069	2.43892467
6	-1.00053861	1.48315736	1.34493281
6	-2.17042062	2.02759619	2.19379267
6	-3.34753805	2.79362275	1.73421148
8	-4.30231601	3.07732622	2.43705934
6	-1.93491154	1.69960643	3.48872613
8	-0.81822406	0.97950647	3.71576396
6	-2.71211535	2.02832432	4.77157348
9	-2.01373170	1.60622020	5.85438633
9	-3.91020574	1.40895977	4.79069304
9	-2.89998432	3.35870852	4.90442969
8	-3.24289583	3.15148444	0.42482380
6	-4.37549041	3.91338300	-0.09226300
1	-5.28512003	3.30880178	0.03512827
1	-4.48771274	4.82096890	0.51844654
6	-4.09819953	4.23450478	-1.54912511
1	-3.99908633	3.32023361	-2.15051219
1	-4.93945717	4.81577988	-1.95390223
1	-3.18610842	4.83708038	-1.65970925
6	-0.19711789	-1.00037958	2.31520319
6	-0.99936307	-1.67377208	1.10623789
6	-2.17106649	-2.33712162	1.86279233
6	-3.35557322	-3.01186961	1.29191550
8	-4.32204460	-3.37243335	1.94163532
6	-1.93508459	-2.20968398	3.19226281
8	-0.81676670	-1.53441801	3.52549374
6	-2.71372947	-2.72669441	4.41007962
9	-2.92969084	-4.05682232	4.32746329
9	-3.89878199	-2.09421001	4.53625935
9	-2.00333283	-2.50000121	5.54232426
8	-3.24477894	-3.18471349	-0.05369175
6	-4.38848242	-3.83994360	-0.68099812
1	-4.51757361	-4.82763506	-0.21548326
1	-5.28811920	-3.24650190	-0.46277165
6	-4.11398022	-3.93948556	-2.16981378
1	-3.21307612	-4.53490237	-2.37261327
1	-4.96515633	-4.43582015	-2.65825482
1	-3.99640571	-2.94569166	-2.62360617

Structure 5

6	0.35661035	-1.24342005	2.13812879
6	-0.29547748	-0.29661793	3.05827728
6	-1.62633539	2.15516092	-0.55095531
6	0.71875539	0.22714075	3.95028708
6	-0.05080629	-1.33065446	0.81286186
6	-1.31290964	1.90396789	2.96638166
6	4.75395759	1.51849165	2.39523685
6	1.75763636	-1.29400804	2.49057275

6	3.17547749	0.34669114	3.68153967
6	-1.95510328	1.77617801	0.72089810
6	-1.30595938	0.51655918	2.59004324
6	2.12462051	5.18097787	2.04649086
6	2.72811052	4.96880821	-0.34547743
6	4.18484708	0.20783148	2.64057905
6	0.95930925	-1.40339172	-0.19708745
6	1.32104189	5.02298061	-0.69149847
6	0.68475847	1.57127806	4.35869054
6	-1.72842232	2.68261666	1.81821481
6	-1.23792069	1.19953565	-1.65934491
6	2.33207734	-1.50436526	0.12333308
6	2.36137291	3.49483903	-2.14133874
6	1.98566299	-0.38959446	3.60546172
6	-0.36156577	2.43208351	3.85653646
6	1.91181443	2.34221759	4.42018349
6	3.12298476	5.04211084	0.99939310
6	5.09210588	1.90584224	1.08742816
6	0.76287848	5.23773488	1.71194652
6	4.17414543	4.16910968	1.49598221
6	4.10715665	2.46699351	3.28884175
6	-0.07416752	3.33352890	-1.84916176
6	-0.85724140	4.36158463	0.25812676
6	-1.05729668	3.45814008	-0.79271410
6	2.74225736	-1.44284610	1.50187790
6	2.38897173	2.14234598	-2.52069380
6	-0.95440724	-0.33148133	-1.28277564
6	3.97376178	-0.67680679	1.57271535
6	3.13556096	1.74254267	4.08835102
6	0.35674438	5.15449967	0.31812903
6	3.43938762	1.27536519	-2.01716812
6	4.79424379	3.25459687	0.63079492
6	-1.20386628	3.96302957	1.60225305
6	1.09708788	4.10863086	-1.80211180
6	-0.05617315	1.96366160	-2.29228454
6	1.15999893	1.37435517	-2.58488021
6	3.30446058	-0.79763857	-0.67477200
6	4.42733644	1.78110365	-1.16183106
6	4.32295396	-0.27458896	0.21664458
6	3.37361203	4.01972697	-1.24400182
6	4.87174038	0.99513178	-0.01900988
6	0.21057744	3.74814166	3.61189016
6	-0.20868018	4.50557282	2.50854195
6	0.53005922	-0.66771030	-1.34005508
6	1.61746958	3.69404017	3.96022767
6	4.38637905	3.17869944	-0.76043372
6	3.82574806	3.76932199	2.84790057
6	2.86341766	-0.03455195	-1.76610003
6	2.55826922	4.39391118	3.18924676
6	1.45985867	0.01413400	-2.10500113
6	-2.00753305	0.34039691	1.21873487
6	-1.37990984	-0.80566600	0.26048158

8	-2.36954292	1.15784977	-2.62159265
6	-2.49731972	-0.10227530	-3.05653724
6	-1.72124313	-1.02837796	-2.42625023
6	-3.50092557	-0.24588646	-4.21227539
9	-4.12971367	0.93534374	-4.42635804
8	-0.49679250	-3.03049752	-2.31043347
6	-0.13031561	-4.34019344	-2.83670169
1	0.36760742	-4.83538704	-1.99247675
6	0.79628659	-4.21947870	-4.03840082
1	0.28873580	-3.72570317	-4.87727171
1	1.70574238	-3.65785984	-3.78473646
1	1.09687719	-5.22601710	-4.36562478
9	-4.44638402	-1.16609546	-3.93897539
1	-1.04911547	-4.88222428	-3.09780176
9	-2.87113135	-0.58505777	-5.35996681
8	-3.39890566	-0.00354483	1.37329297
6	-3.50723690	-1.40647074	1.39620920
8	-3.19118442	-1.93955011	2.64420853
1	-2.53188802	-2.66407970	2.51971264
6	-2.56072849	-1.85884853	0.23378340
1	-3.11493160	-1.72336639	-0.70333462
6	-2.23970786	-3.33692274	0.39675773
8	-1.67491366	-3.80120676	1.38392735
8	-2.76684083	-4.07454080	-0.58780695
1	-3.05124723	-5.75573690	0.61380549
6	-2.72203261	-5.52907057	-0.40954438
1	-1.67545199	-5.85094300	-0.51083076
1	-3.30862704	-5.86687626	-2.47557761
6	-3.62685817	-6.14174753	-1.46078305
1	-3.59450500	-7.23706130	-1.37024936
1	-4.66614875	-5.81581800	-1.32172126
9	-5.41147983	-1.18729854	-0.08829899
6	-5.01335645	-1.70810884	1.10021985
9	-5.20850924	-3.05458493	1.04438634
9	-5.80901634	-1.21050733	2.06489104
6	-1.54240888	-2.40945373	-2.92932746
8	-2.20823136	-2.92067116	-3.81284511

Structure 6

6	1.78083854	-1.47822288	-1.28343970
6	1.06005005	-1.59733856	-2.56242433
6	-2.20188046	1.12538444	-0.90396500
6	0.78210249	-3.00533755	-2.77972561
6	1.52146195	-0.40541531	-0.44195577
6	-1.12184173	-1.05452452	-3.47670147
6	-0.75572593	-5.62295903	0.56273780
6	1.94087384	-2.80932080	-0.74322230
6	0.65250593	-4.87709043	-1.16396778
6	-1.53959585	0.73074676	-2.02923962
6	0.14195937	-0.63127794	-2.93003185
6	-4.45167183	-3.84266238	-1.34061934
6	-4.79410836	-2.96422560	0.94875114

6	0.56380455	-5.09585984	0.27347622
6	1.39203556	-0.63952119	0.95673986
6	-4.95843435	-1.63231592	0.39928975
6	-0.42963723	-3.41026598	-3.36357742
6	-2.15777134	-0.19581417	-2.94143233
6	-1.52120112	1.57729837	0.36642107
6	1.59988584	-1.92028527	1.51338236
6	-3.78991787	-1.43615807	2.42838761
6	1.32690586	-3.75341434	-1.66143037
6	-1.40632372	-2.40786211	-3.72621075
6	-1.13953729	-4.56278357	-2.84107702
6	-4.54195943	-4.04961571	0.09521952
6	-1.43200822	-5.22556186	1.72873046
6	-4.61470579	-2.55487740	-1.87368648
6	-3.55506199	-5.05062176	0.46601288
6	-1.48143728	-5.73962055	-0.69264685
6	-3.61649412	0.40964920	0.81480103
6	-4.14006256	-0.28744153	-1.49937186
6	-3.51334255	0.60092859	-0.61695828
6	1.87197262	-3.03372997	0.64079560
6	-2.56335908	-1.04005745	2.98738322
6	0.06636805	1.37935759	0.50760460
6	1.16808877	-4.19237998	1.15977761
6	-0.60993462	-5.28321729	-1.76058890
6	-4.87008516	-1.43157638	-0.98590563
6	-1.58084127	-2.04487896	3.35144267
6	-2.85614001	-4.93257144	1.67715729
6	-3.44245452	-0.69666414	-2.69624147
6	-4.33422909	-0.68928777	1.31668684
6	-2.38598308	0.85052101	1.42094200
6	-1.85739812	0.11533931	2.46543871
6	0.74587317	-2.37254947	2.58288115
6	-1.85168005	-3.40592980	3.15395937
6	0.46696506	-3.78033761	2.36902029
6	-4.06835792	-2.84275875	2.20707527
6	-0.81126783	-4.28841310	2.64459532
6	-2.73078985	-2.93870029	-3.43592323
6	-3.73586572	-2.09673534	-2.93800989
6	0.40880944	0.24829942	1.47941755
6	-2.56701127	-4.27145140	-2.88858016
6	-3.11672616	-3.81034100	2.56062248
6	-2.85616757	-5.46142275	-0.73901394
6	-0.26098078	-1.51579293	3.05348978
6	-3.40908539	-4.71439871	-1.85672121
6	-0.41658669	-0.18819131	2.50209314
6	-0.03071243	0.72602128	-2.20259598
6	0.87703196	0.90714706	-0.88153340
8	-1.73935159	3.03988275	0.47932648
6	-0.63845973	3.57564460	1.02366984
6	0.42431564	2.73346848	1.15048038
6	-0.82274736	5.05591260	1.38484362
9	0.22423640	5.80749811	0.98349336

8	1.65123608	4.09250481	2.62620351
6	2.82105249	4.35049024	3.45361411
1	2.93301956	3.52291317	4.16890427
6	2.60648092	5.68451170	4.14448804
1	2.49120515	6.49597960	3.41343546
1	1.71560439	5.65936458	4.78647583
1	3.47839268	5.91021212	4.77552921
9	-0.98198245	5.21410181	2.72365016
1	3.70829086	4.36300813	2.80321435
9	-1.93075666	5.54589352	0.78516154
8	0.29836782	1.82121450	-3.10130195
6	1.28005360	2.66771604	-2.56711372
8	0.70626765	3.81651153	-2.01198352
1	1.37100522	4.16096378	-1.36518440
6	2.02222013	1.78990651	-1.53959771
1	2.60883516	1.06026264	-2.11652475
6	3.04294382	2.56916746	-0.71714086
8	2.91854971	3.75129079	-0.41174859
8	4.12425563	1.82137101	-0.47502272
1	5.72408354	1.61532517	0.75264596
6	5.22940726	2.45593053	0.25137527
1	4.80182424	3.12580698	1.00654056
1	5.65389716	4.02114594	-1.19672175
6	6.16207863	3.18094818	-0.70580475
1	7.01697420	3.58130315	-0.14062718
1	6.55014292	2.49772660	-1.47346383
9	2.74835559	1.97727515	-4.37155944
6	2.17216678	3.06814126	-3.79542181
9	1.44871358	3.70426940	-4.73410240
9	3.18053609	3.89707934	-3.40695524
6	1.63666231	2.91424904	1.96603477
8	2.51296514	2.06209587	2.07365324

Structue of $C_{60}(acac)_5Cl$

6	-0.52489788	-4.41587120	-1.47659523
6	-0.70711431	-3.73549291	-2.73141354
6	0.05209001	-2.58114418	-2.98590445
6	1.07323677	-2.12006694	-2.07874788
6	1.25768029	-2.77727946	-0.87641351
6	0.41038025	-3.90194550	-0.55958875
6	-1.82660988	-4.87516760	-1.01999244
6	-2.81556701	-4.47642639	-2.00653675
6	-2.12120671	-3.77053727	-3.06787515
6	-2.72514515	-2.66476428	-3.68159688
6	-0.58413606	-1.43489170	-3.59817075
6	1.28642619	-0.59940004	-2.27060700
6	1.11512741	0.02127496	-0.88801127
6	1.36815649	-0.60364330	0.29943618
6	1.70695246	-2.08246560	0.43658624
6	0.66715824	-2.66818806	1.40952060
6	0.06168968	-3.84189387	0.84282664
6	-1.17598450	-4.32407639	1.29258120

6	-2.14688984	-4.83551091	0.34323500
6	-4.09261273	-4.05350644	-1.59611337
6	-4.42181112	-4.01149531	-0.18208093
6	-3.46463583	-4.39726642	0.77149320
6	-3.30067261	-3.61872489	1.98715463
6	-1.88342014	-3.57544276	2.29926416
6	-1.30721236	-2.39544305	2.79359566
6	-0.00276290	-1.95112388	2.37246075
6	0.14329237	-0.44156913	2.66776830
6	0.84716943	0.29514397	1.45227588
6	0.00867027	-0.24500444	-3.06401564
6	-2.26448765	2.17953548	0.11896009
6	-1.95515444	2.09864271	-1.21998128
6	-2.89763476	1.56282766	-2.15986889
6	-4.17618209	1.14784042	-1.75612460
6	-4.50242210	1.19354891	-0.35417799
6	-3.34784288	0.96997102	1.80928306
6	-1.95001926	1.03271126	2.14947318
6	-1.21467903	2.06044913	1.25881976
6	-0.00301194	1.33851921	0.68676233
6	0.25855442	1.21875693	-0.64572895
6	-0.52233526	1.92257584	-1.75347498
6	-2.17272297	0.81884360	-3.16950875
6	-2.75604816	-0.32267799	-3.74401135
6	-4.06462017	-0.77413303	-3.30324563
6	-4.76302553	-0.05256050	-2.32539829
6	-5.45782470	-0.75565490	-1.26222330
6	-5.29526900	0.01603744	-0.04147754
6	-5.12010521	-0.64215287	1.18269582
6	-4.13603102	-0.14656686	2.12852947
6	-1.35125393	-0.05708130	2.74175318
6	-2.13423168	-1.23235021	3.02269277
6	-3.51073290	-1.28198100	2.75705898
6	-4.10255799	-2.49059894	2.21336026
6	-5.09798115	-2.09450530	1.23260232
6	-5.25216828	-2.84177702	0.05221655
6	-5.43613090	-2.16076992	-1.21684208
6	-4.71854638	-2.90914874	-2.23494973
6	-4.04514650	-2.22643019	-3.26244937
6	-0.76469065	0.88559681	-2.86901562
6	-1.93535793	-1.48233661	-3.97241242
6	-3.53897880	1.66479987	0.55676351
17	2.36520240	1.24086567	2.04208522
6	0.01422357	3.36341846	-2.14351937
1	0.01414312	3.92759636	-1.20369886
6	1.40583270	3.48130941	-2.76365554
8	1.79450954	2.74538412	-3.66219869
6	-0.99969522	4.12367289	-3.06142679
8	-1.77994002	4.90654236	-2.54232033
6	-0.95517662	3.90292959	-4.55496740
1	-1.90645396	4.21375885	-5.00161855
1	-0.15346111	4.53521380	-4.97366422

1	-0.69897269	2.87079428	-4.82523100
6	2.24228232	4.63263194	-2.24919751
1	2.47008386	4.47353344	-1.18344958
1	3.16274541	4.72730779	-2.83618990
1	1.66222389	5.56898278	-2.28971157
6	2.52798417	-0.18329532	-3.19888711
1	2.18844921	0.74852514	-3.68411520
6	3.92450105	0.25170714	-2.71411004
8	4.88044619	0.00982327	-3.43686638
6	2.63839249	-1.19616816	-4.37655012
8	2.00424791	-0.97635215	-5.39751909
6	3.49922011	-2.43319514	-4.23464885
1	3.03501458	-3.25935757	-4.78873903
1	4.47116324	-2.20865398	-4.69873339
1	3.69412298	-2.70237590	-3.19074714
6	4.07963568	1.19434418	-1.53926916
1	3.40738571	0.98652878	-0.70049729
1	5.12591018	1.17754804	-1.21153011
1	3.85820223	2.20865781	-1.90711203
6	-0.97469274	3.38229133	2.12176188
1	-0.87511940	3.06668417	3.16698742
6	0.25037156	4.24002237	1.81335350
8	0.75216546	4.33220201	0.70039012
6	-2.26543756	4.27111817	2.12453378
8	-3.09029526	4.10143262	3.00612756
6	-2.41852342	5.33270579	1.05964755
1	-3.45856592	5.67642853	1.02933172
1	-1.77829786	6.18931886	1.33522753
1	-2.08689991	5.00749254	0.06355797
6	0.79151487	5.01599312	2.99606812
1	-0.01899998	5.53693312	3.53020426
1	1.22346341	4.30414883	3.71591445
1	1.55138604	5.73098077	2.66248458
6	3.15295889	-2.44950352	0.97556783
1	3.18953490	-2.10269906	2.01488546
6	3.32827605	-4.00506610	1.09183038
8	2.95560029	-4.55991159	2.11001850
6	4.30887472	-1.85253492	0.19138998
8	4.32894660	-1.85305048	-1.03269383
6	5.45912301	-1.31398051	1.01685773
1	6.30838585	-1.06414869	0.37146470
1	5.11812314	-0.41534529	1.55675001
1	5.75605353	-2.04081939	1.78943503
6	3.97141237	-4.76292124	-0.04823850
1	3.59807751	-4.43415904	-1.02716910
1	5.05548732	-4.55812196	-0.05033068
1	3.81565721	-5.83748667	0.09733917
6	0.69464735	-0.27804050	4.16034270
1	0.23796156	-1.14275018	4.67428846
6	2.21013181	-0.54036168	4.41516587
8	2.74853910	-1.50900448	3.90808565
6	0.17722699	0.96721547	4.90665393

8	0.45883431	2.10331267	4.55060007
6	-0.67480644	0.70457928	6.13120317
1	-0.89223845	1.64297119	6.65254407
1	-1.61949305	0.22735585	5.82181698
1	-0.17887347	-0.00939211	6.80843342
6	2.93510679	0.33723538	5.41239602
1	2.93965255	1.38214872	5.07309607
1	2.41568391	0.31940770	6.38461859
1	3.95811146	-0.03236690	5.54153149

Structue of $C_{60}(acac)_4$

6	0.50522627	3.10583325	3.24238963
6	1.38180288	2.01852869	3.58864510
6	2.04193655	1.32747900	2.55852091
6	1.94746838	1.73381561	1.18078603
6	1.09530509	2.77682681	0.85209173
6	0.34540690	3.44077263	1.88682403
6	-0.64877512	3.05640372	4.12523496
6	-0.47560610	1.93070396	5.02657009
6	0.78303507	1.28733407	4.69330110
6	0.89286100	-0.10804132	4.75528574
6	2.13530271	-0.11690620	2.61731137
6	2.22390374	0.51535250	0.26423520
6	1.05539475	0.40607521	-0.70144117
6	0.22679553	1.45657309	-1.04104552
6	0.32364436	2.87269047	-0.48909530
6	-1.06643493	3.31249538	0.02700280
6	-0.97570713	3.77044754	1.37808746
6	-2.09165623	3.74169294	2.24115011
6	-1.92395842	3.36731808	3.63238106
6	-1.58392748	1.15557436	5.41016763
6	-2.90502043	1.47951571	4.90079400
6	-3.07175636	2.56735356	4.02692125
6	-3.94815734	2.44822584	2.87531790
6	-3.33627641	3.17808459	1.77485119
6	-3.40115154	2.66139469	0.47245065
6	-2.25400750	2.73007364	-0.40226787
6	-2.23212234	1.49321397	-1.19110343
6	-1.03878380	0.87428257	-1.48241746
6	2.07529023	-0.63893325	1.28084627
6	-1.87952484	-2.49403887	-0.21305625
6	-0.61981704	-2.77209495	0.28250719
6	-0.45087295	-3.09638515	1.66990080
6	-1.55208515	-3.18608622	2.53986222
6	-2.86342921	-2.87074174	2.03460303
6	-3.89589586	-1.40548146	0.33359165
6	-3.31930889	-0.69974996	-0.76818654
6	-2.13243715	-1.49522779	-1.36639351
6	-0.92064619	-0.58090649	-1.44521986
6	0.33653562	-0.86498803	-0.95376327
6	0.69430428	-2.17981188	-0.28879650
6	0.79853942	-2.52187610	2.13032854

6	0.90211683	-2.05725628	3.45243549
6	-0.24365448	-2.12208355	4.34373603
6	-1.45047058	-2.67557258	3.89623367
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6	-3.58446235	-2.15209301	3.07335545
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6	-4.60547466	-0.71737504	1.34120814
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6	-4.10528848	1.41054534	0.22303258
6	-4.72115756	0.72193037	1.27898902
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6	-4.45387666	0.11904412	3.53285887
6	-3.60740058	0.23391893	4.64874011
6	-2.72041704	-0.86088688	5.00117687
6	-1.47047201	-0.29090085	5.47260431
6	-0.25189756	-0.91165648	5.14822923
6	1.42824159	-1.83547868	1.03051356
6	1.59676905	-0.82184520	3.70563748
6	-3.00608324	-2.50186711	0.68513314
6	1.34801404	-3.28085048	-1.23476432
1	0.52397019	-3.90823833	-1.60059678
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6	1.98540997	-3.65034791	-3.70418552
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1	2.74436275	-3.36295936	-4.44042191
1	2.07474290	-4.71666891	-3.44884393
6	3.64871779	0.38493549	-0.40411476
1	3.65925792	-0.59224754	-0.90199789
6	4.01231002	1.44492533	-1.44823301
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6	4.78222225	0.39494636	0.66872178
8	4.94568316	1.35259205	1.40289033
6	5.64939931	-0.84390070	0.71526204
1	6.38579308	-0.76121594	1.52227869
1	5.02743823	-1.74447620	0.83867630
1	6.16595787	-0.96925304	-0.25088563
6	4.72413645	0.93609036	-2.68213930
1	4.05046970	0.26163263	-3.23397466
1	5.03739476	1.77586517	-3.31248092
1	5.59806274	0.32698722	-2.40059148
6	-2.63752735	-2.15208365	-2.74712438
1	-3.70795614	-1.91723962	-2.83984478
6	-1.92371241	-1.49229959	-3.96872831
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6	-2.48160857	-3.67190268	-2.87089820

8	-1.47061694	-4.26168512	-2.52393987
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1	-3.40621278	-5.45015920	-3.66473055
1	-4.53785228	-4.31269147	-2.85226790
1	-3.92630098	-3.92235814	-4.46321974
6	-2.66435173	-0.34702785	-4.62198124
1	-3.58778537	-0.73407513	-5.08485516
1	-2.97898316	0.39950935	-3.87721797
1	-2.03565317	0.12530044	-5.38438894
6	0.99294542	3.90149635	-1.47872189
1	1.99575626	3.51094817	-1.70466382
6	0.27232945	4.08430474	-2.82472593
8	-0.80340274	3.57178794	-3.08097624
6	1.17972878	5.28938371	-0.80422479
8	0.21145390	5.99567187	-0.56941681
6	2.59650902	5.69722284	-0.47515970
1	2.60357294	6.65251961	0.06123530
1	3.09927698	4.90851195	0.10503129
1	3.17598780	5.78512262	-1.40954303
6	1.00230354	4.95690182	-3.83352760
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6	0.78210249	-3.00533755	-2.77972561
6	1.52146195	-0.40541531	-0.44195577
6	-1.12184173	-1.05452452	-3.47670147
6	-0.75572593	-5.62295903	0.56273780
6	1.94087384	-2.80932080	-0.74322230
6	0.65250593	-4.87709043	-1.16396778
6	-1.53959585	0.73074676	-2.02923962
6	0.14195937	-0.63127794	-2.93003185
6	-4.45167183	-3.84266238	-1.34061934
6	-4.79410836	-2.96422560	0.94875114
6	0.56380455	-5.09585984	0.27347622
6	1.39203556	-0.63952119	0.95673986
6	-4.95843435	-1.63231592	0.39928975
6	-0.42963723	-3.41026598	-3.36357742
6	-2.15777134	-0.19581417	-2.94143233
6	-1.52120112	1.57729837	0.36642107
6	1.59988584	-1.92028527	1.51338236
6	-3.78991787	-1.43615807	2.42838761
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6	-1.40632372	-2.40786211	-3.72621075

6	-1.13953729	-4.56278357	-2.84107702
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6	-4.61470579	-2.55487740	-1.87368648
6	-3.55506199	-5.05062176	0.46601288
6	-1.48143728	-5.73962055	-0.69264685
6	-3.61649412	0.40964920	0.81480103
6	-4.14006256	-0.28744153	-1.49937186
6	-3.51334255	0.60092859	-0.61695828
6	1.87197262	-3.03372997	0.64079560
6	-2.56335908	-1.04005745	2.98738322
6	0.06636805	1.37935759	0.50760460
6	1.16808877	-4.19237998	1.15977761
6	-0.60993462	-5.28321729	-1.76058890
6	-4.87008516	-1.43157638	-0.98590563
6	-1.58084127	-2.04487896	3.35144267
6	-2.85614001	-4.93257144	1.67715729
6	-3.44245452	-0.69666414	-2.69624147
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6	-2.38598308	0.85052101	1.42094200
6	-1.85739812	0.11533931	2.46543871
6	0.74587317	-2.37254947	2.58288115
6	-1.85168005	-3.40592980	3.15395937
6	0.46696506	-3.78033761	2.36902029
6	-4.06835792	-2.84275875	2.20707527
6	-0.81126783	-4.28841310	2.64459532
6	-2.73078985	-2.93870029	-3.43592323
6	-3.73586572	-2.09673534	-2.93800989
6	0.40880944	0.24829942	1.47941755
6	-2.56701127	-4.27145140	-2.88858016
6	-3.11672616	-3.81034100	2.56062248
6	-2.85616757	-5.46142275	-0.73901394
6	-0.26098078	-1.51579293	3.05348978
6	-3.40908539	-4.71439871	-1.85672121
6	-0.41658669	-0.18819131	2.50209314
6	-0.03071243	0.72602128	-2.20259598
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6	-0.63845973	3.57564460	1.02366984
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6	-0.82274736	5.05591260	1.38484362
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   6    5.22940726   2.45593053   0.25137527
   1    4.80182424   3.12580698   1.00654056
   1    5.65389716   4.02114594  -1.19672175
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   1    6.55014292   2.49772660  -1.47346383
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   6   -2.57565934  -0.54432014  -0.91125081
   6    1.90538201   1.71414313  -2.98678764
   6    0.85708162   1.17042587   0.39103401
   6   -0.88033993   1.45884679  -3.28781429
   6    3.89834157  -2.33737878  -3.06676028
   6    2.90854077   1.05461448  -0.96541226
   6    3.69352781   0.00351432  -3.06168903
   6   -2.16570574   0.59575183  -1.53777488
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   6   -0.07123265  -2.93173851  -5.15024360
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6	3.38388682	-0.03998741	-0.22660433
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