Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Impact of aliphatic side chain length on photovoltaic properties of fullerenes functionalized with 3-(1-indenyl)propionic acid esters.

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Wojciech Mech and Piotr Piotrowski have contributed equally to this work

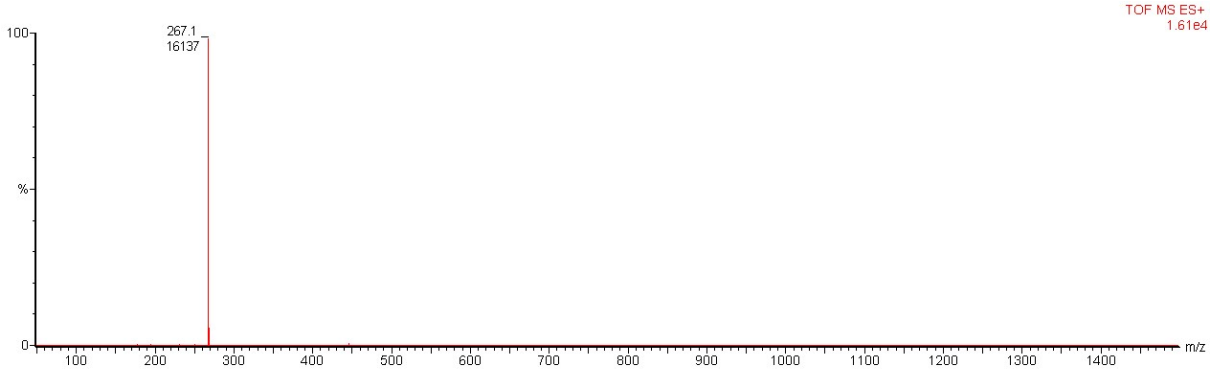


Figure S1. ESI-MS spectrum of butyl 3-(1*H*-inden-3-yl)propanoate (IB).

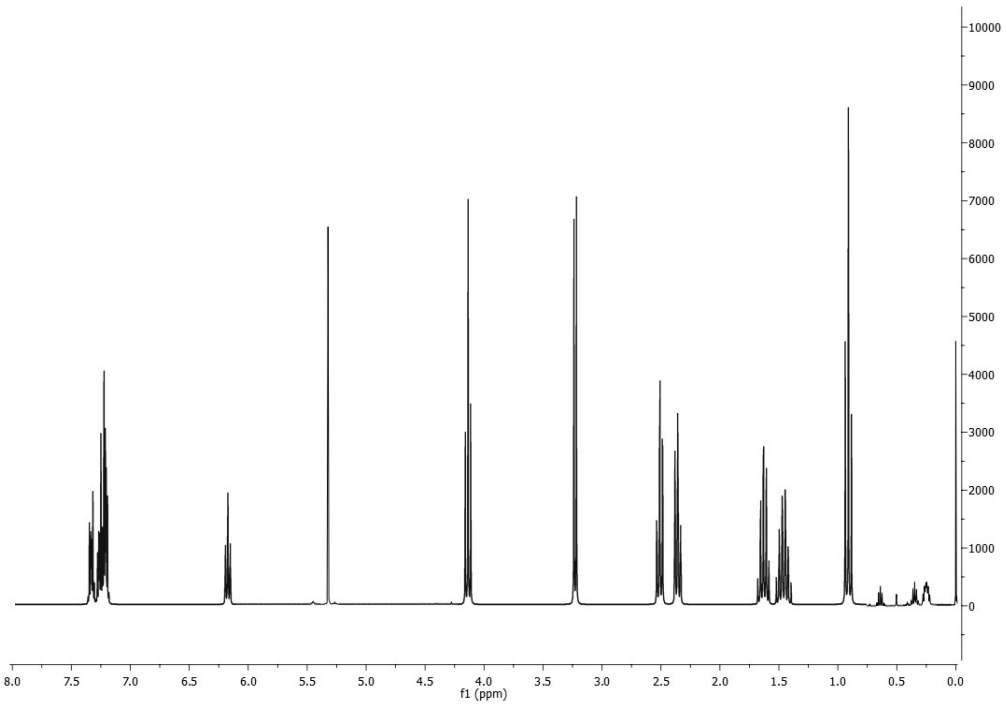


Figure S2. [1]H NMR spectrum of butyl 3-(1*H*-inden-3-yl)propanoate (IB).

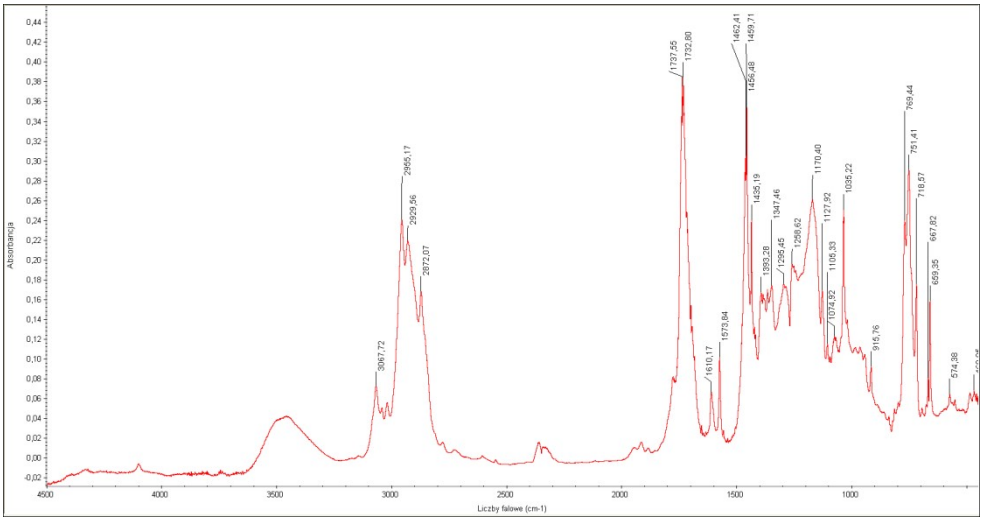


Figure S3. FT-IR spectrum of butyl 3-(1*H*-inden-3-yl)propanoate (IB).

Figure S4. ESI-MS spectrum of hexyl 3-(1*H*-inden-3-yl)propanoate (IH).

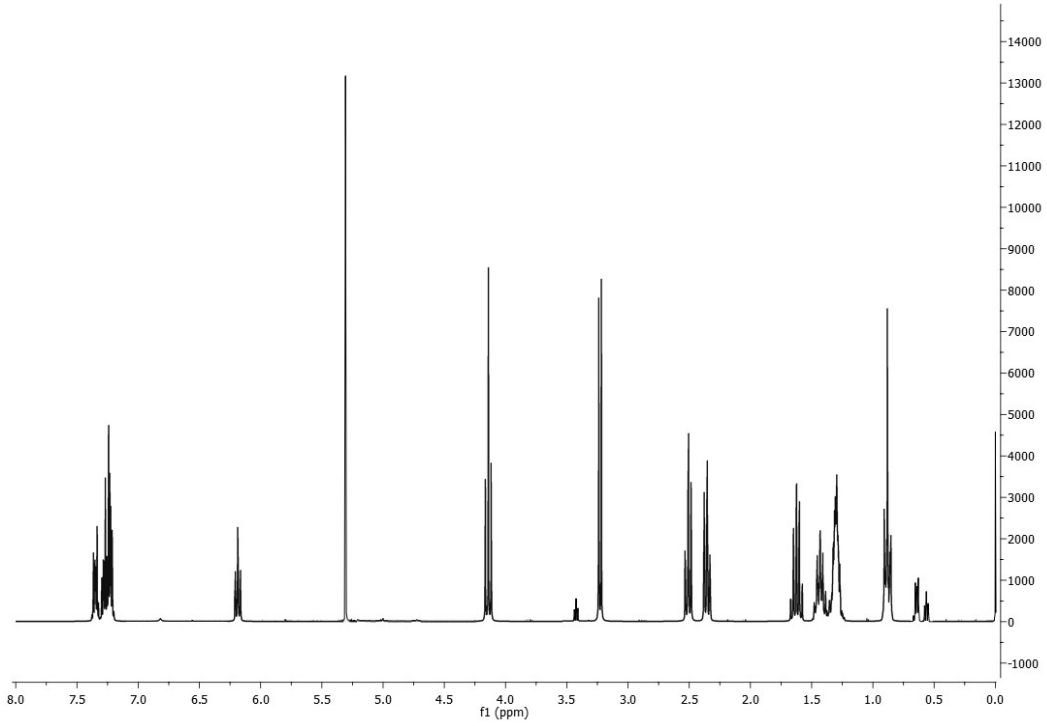


Figure S5. [1]H NMR spectrum of hexyl 3-(1*H*-inden-3-yl)propanoate (IH).

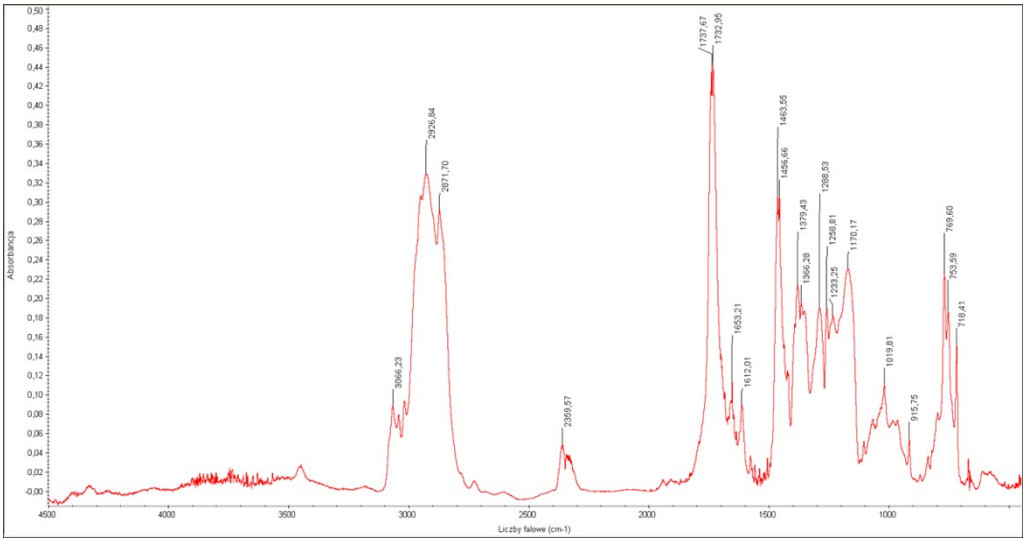


Figure S6. FT-IR spectrum of hexyl 3-(1*H*-inden-3-yl)propanoate (IH).

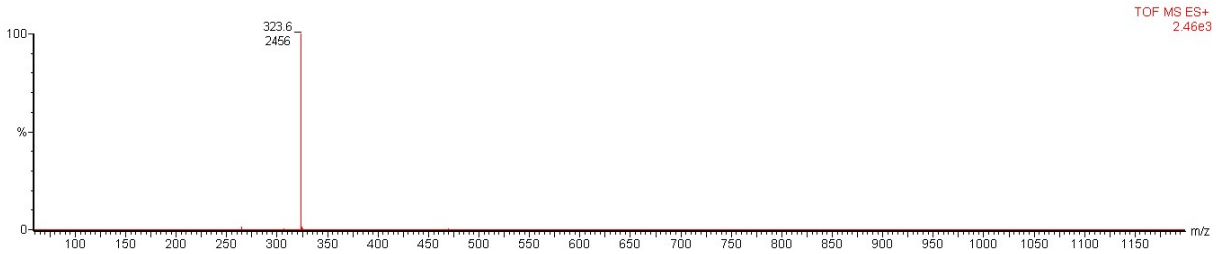


Figure S7. ESI-MS spectrum of octyl 3-(1*H*-inden-3-yl)propanoate (IO).

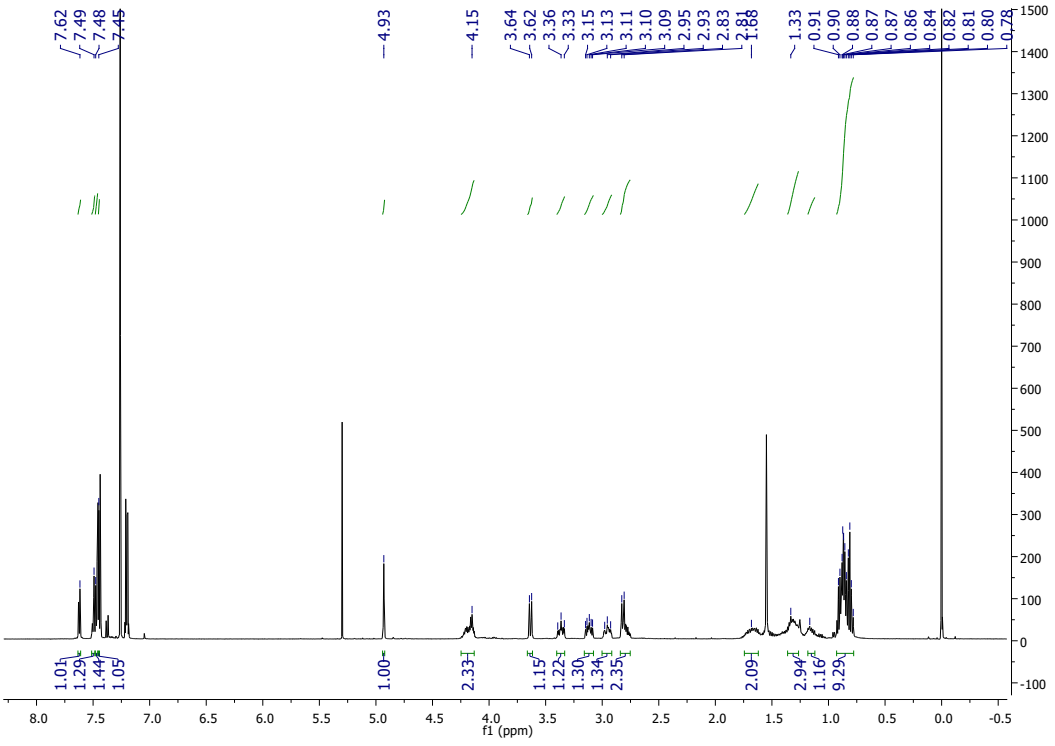


Figure S8. [1]H NMR spectrum of octyl 3-(1*H*-inden-3-yl)propanoate (IO).

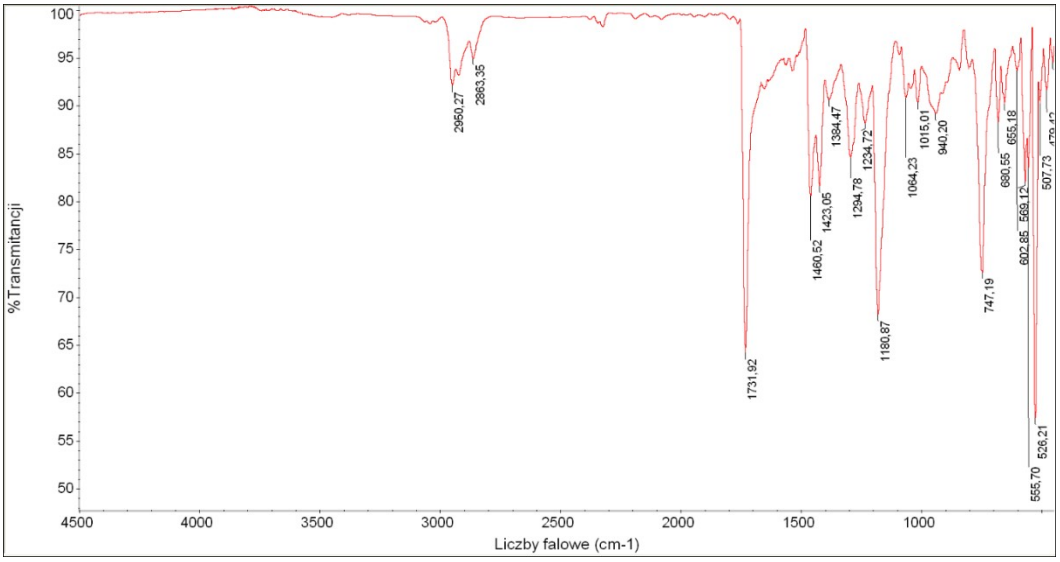


Figure S9. FT-IR spectrum of octyl 3-(1*H*-inden-3-yl)propanoate (IO).

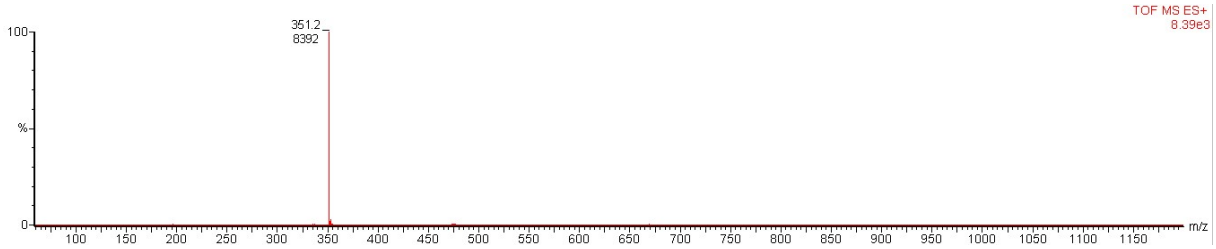


Figure S10. ESI-MS spectrum of decyl 3-(1*H*-inden-3-yl)propanoate (ID).

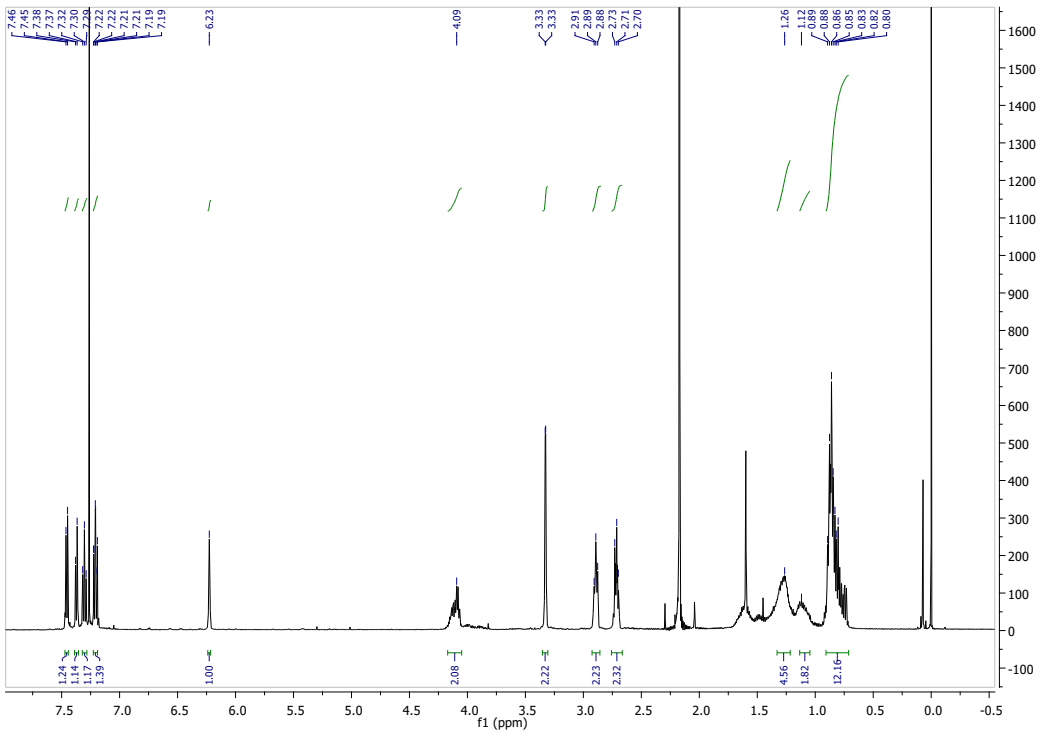


Figure S11. [1]H NMR spectrum of decyl 3-(1*H*-inden-3-yl)propanoate (ID).

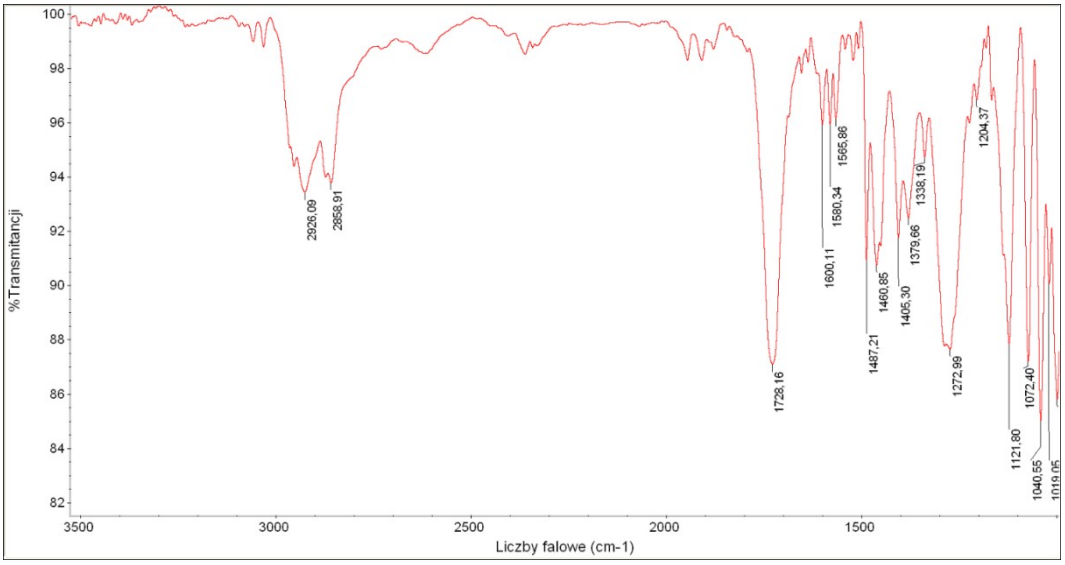


Figure S12. FT-IR spectrum of decyl 3-(1*H*-inden-3-yl)propanoate (ID).

Figure S13. ESI-MS spectrum of lauryl 3-(1*H*-inden-3-yl)propanoate (IL)

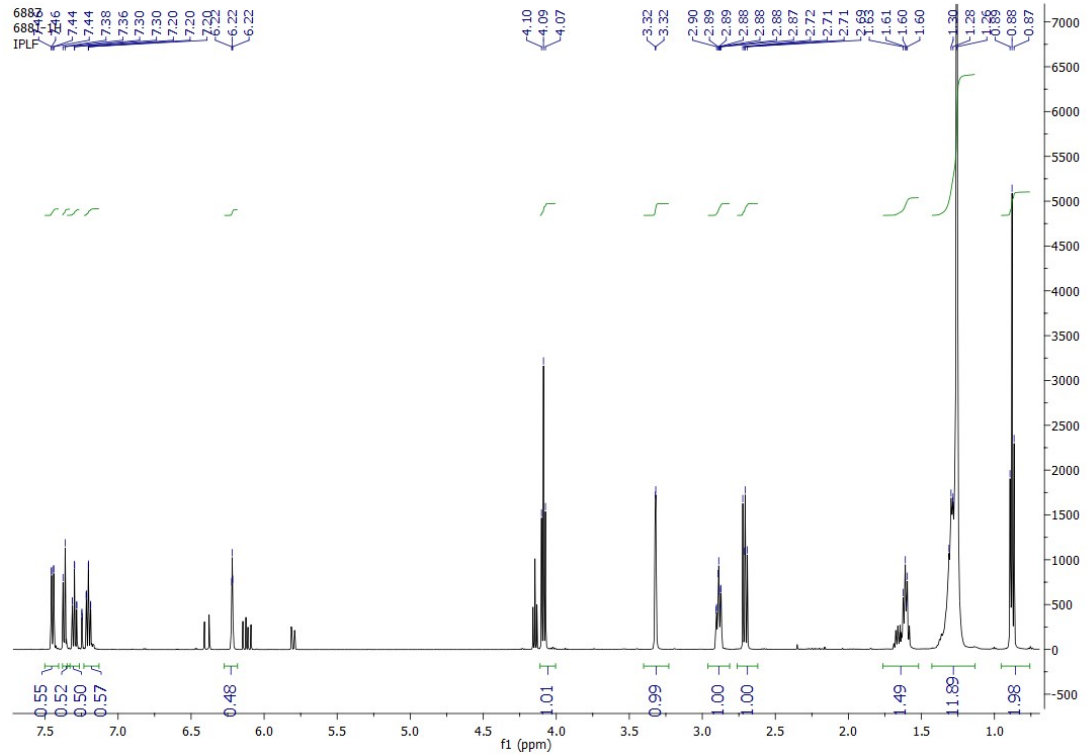


Figure S14. [1]H NMR spectrum of lauryl 3-(1*H*-inden-3-yl)propanoate (IL).

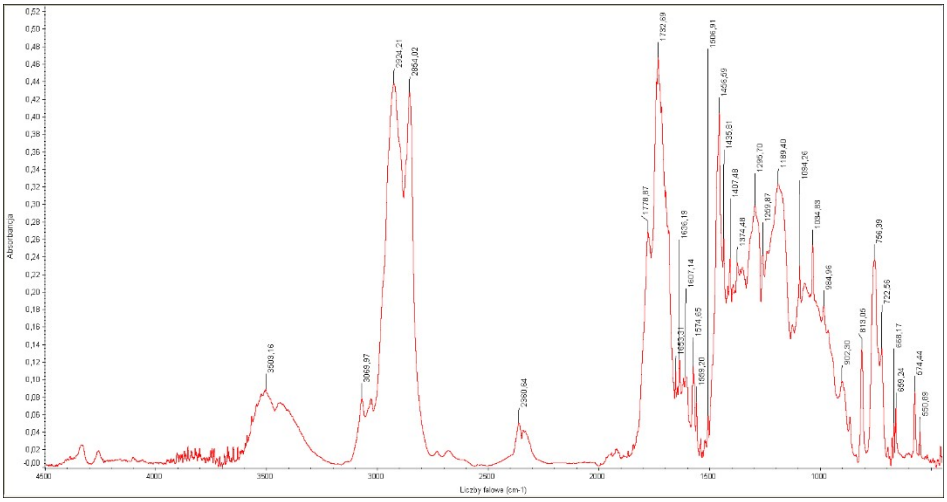


Figure S15. FT-IR spectrum of lauryl 3-(1*H*-inden-3-yl)propanoate (IL).

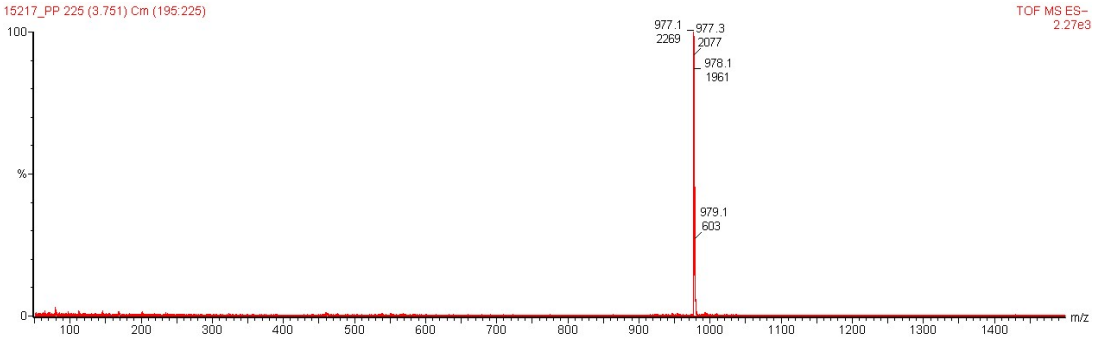


Figure S16. ESI-MS spectrum of **60IPB** fullerene derivative.

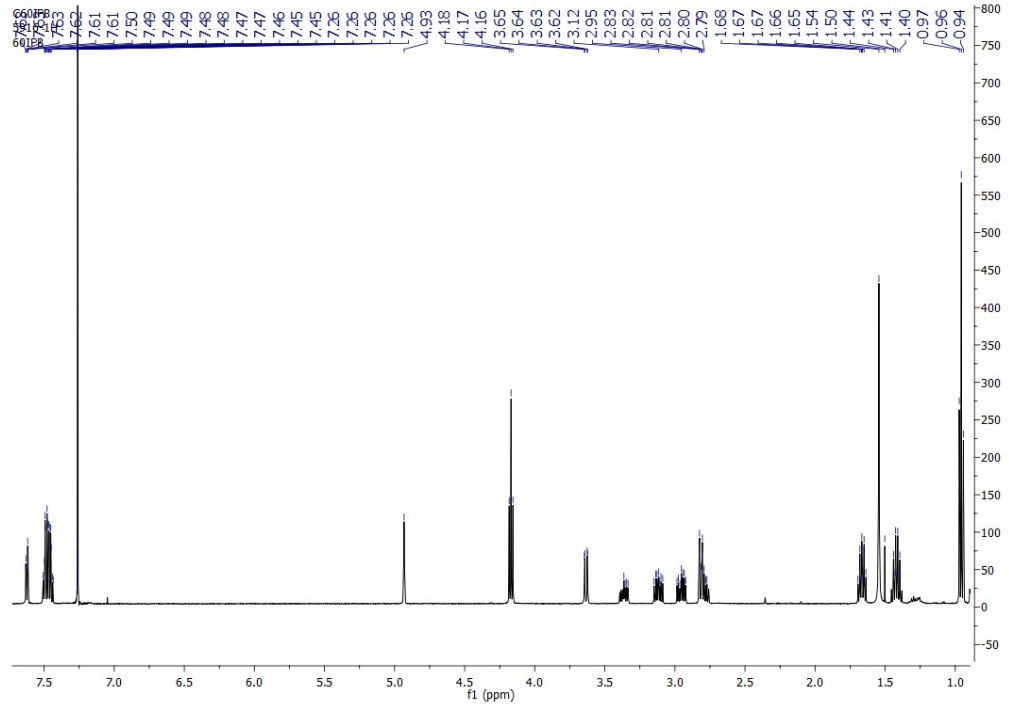


Figure S17. [1]H NMR spectrum of **60IPB** fullerene derivative.

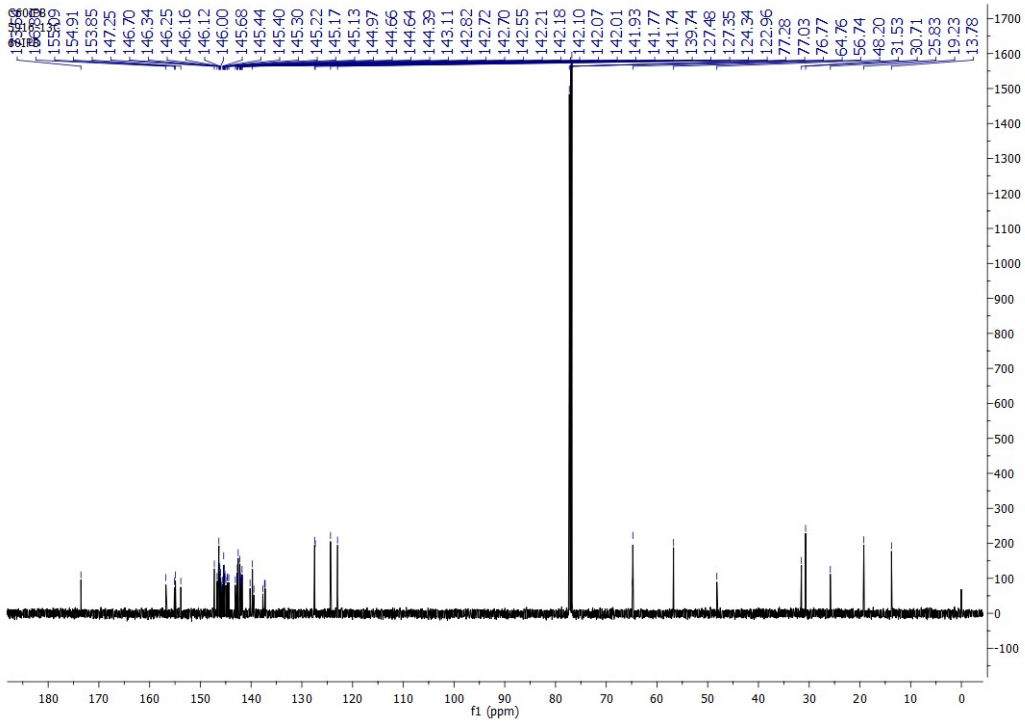


Figure S18. [13]C NMR spectrum of **60IPB** fullerene derivative.

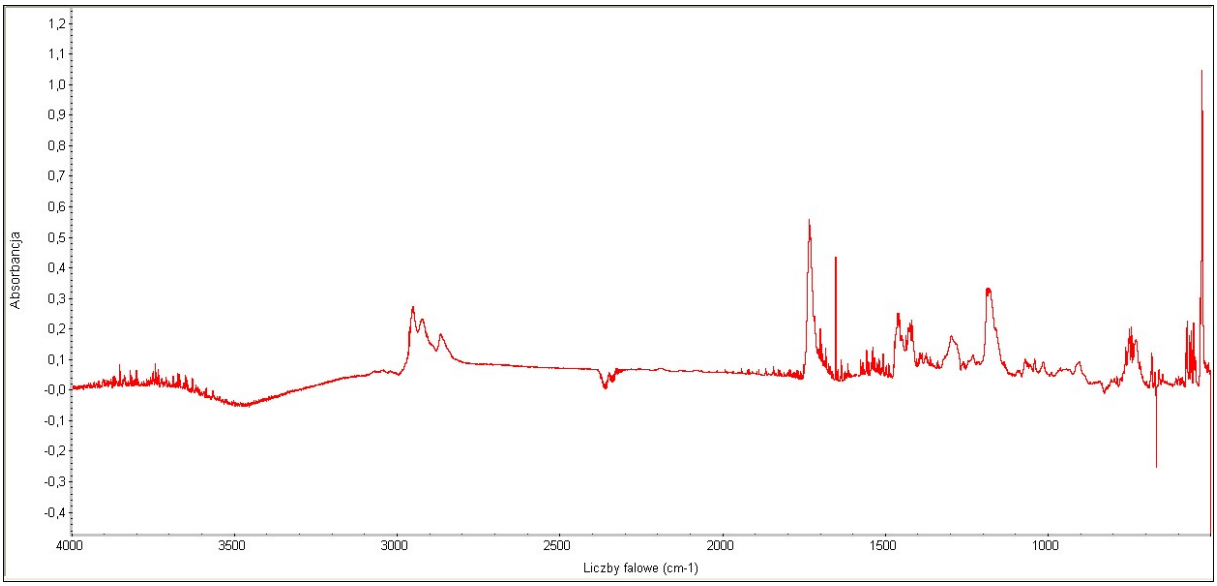


Figure S19. FT-IR spectrum of **60IPB** fullerene derivative.

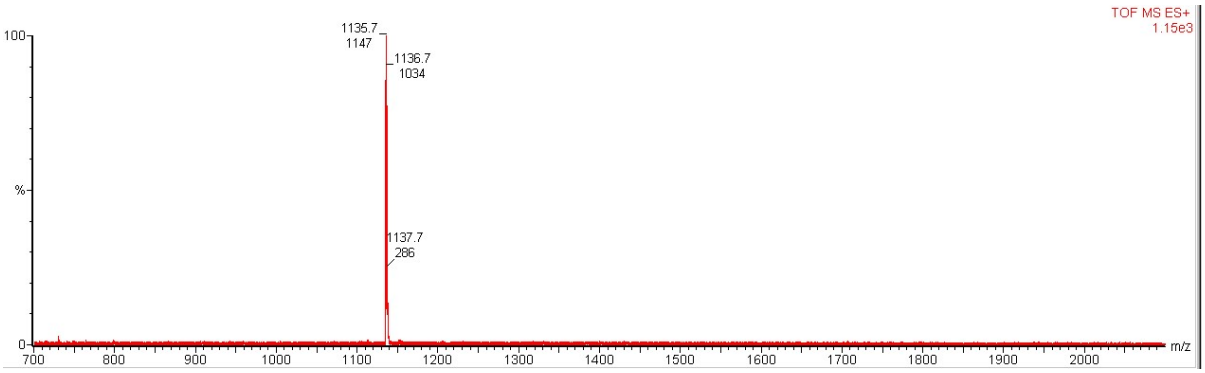


Figure S20. ESI-MS spectrum of **70IPB** fullerene derivative.

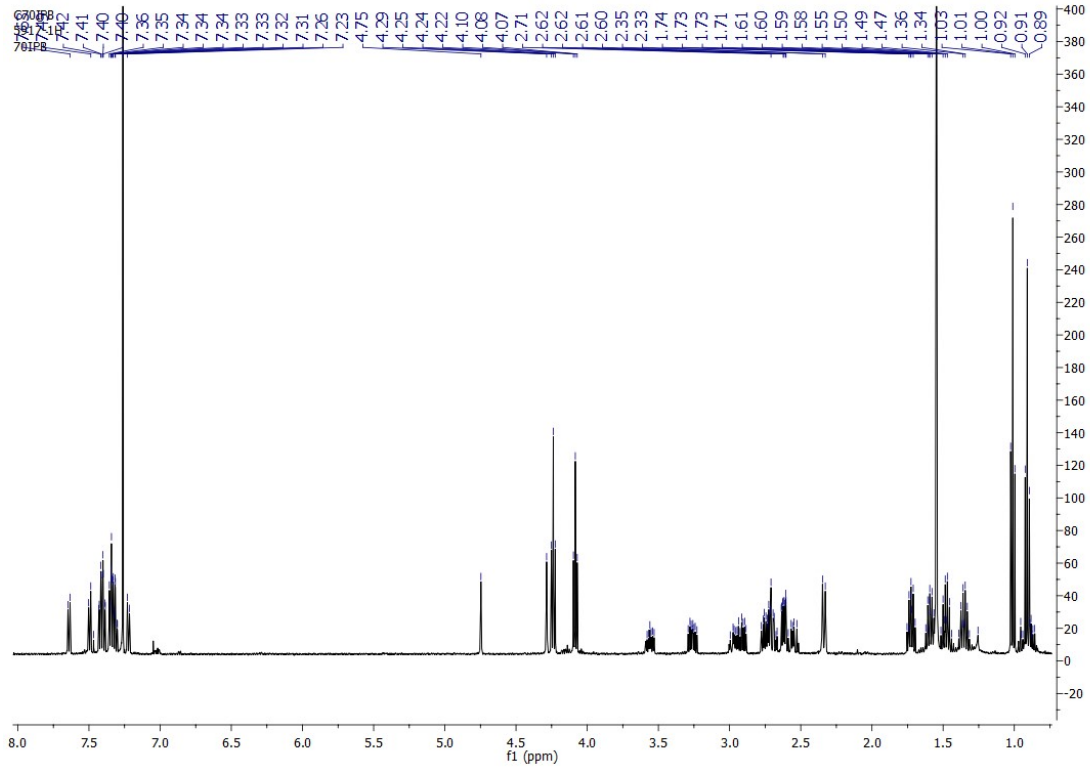


Figure S21. ^{1}H NMR spectrum of **70IPB** fullerene derivative.

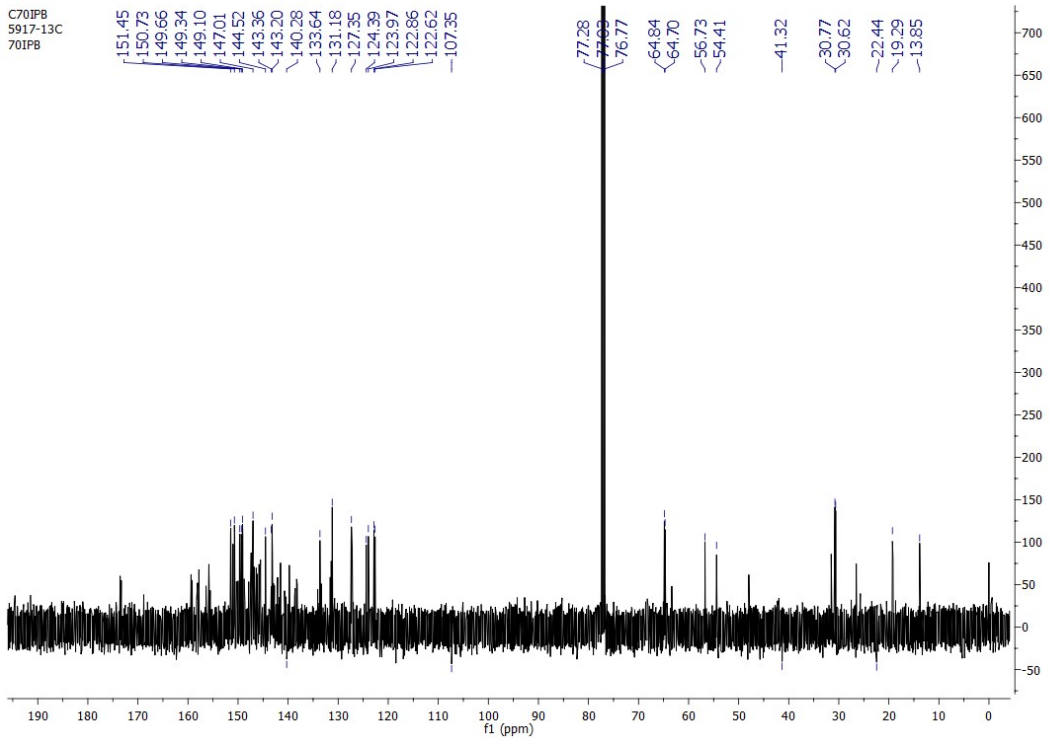


Figure S22. ^{13}C NMR spectrum of **70IPB** fullerene derivative.

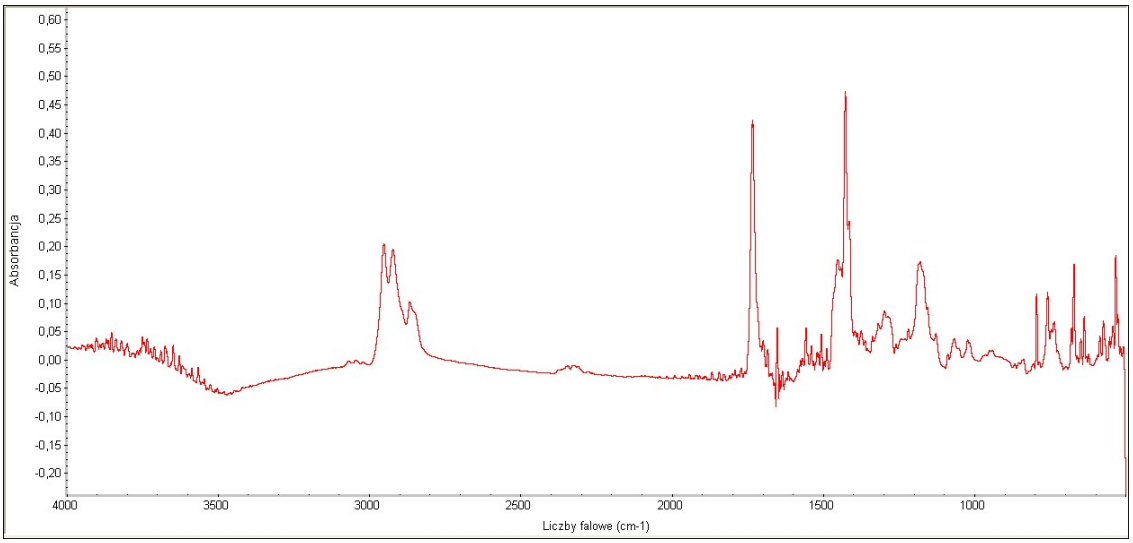


Figure S23. FT-IR spectrum of **70IPB** fullerene derivative.

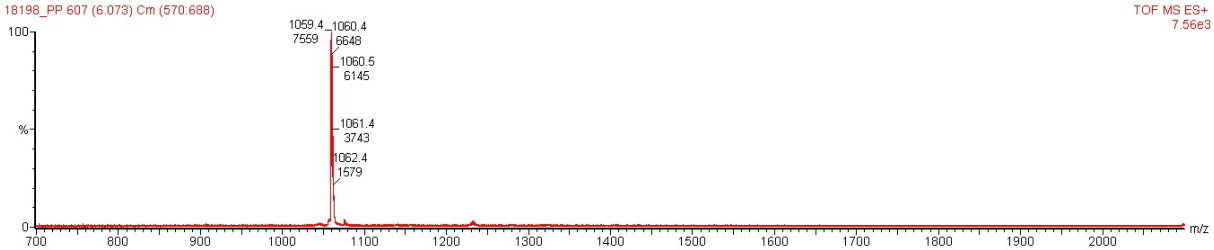


Figure S24. ESI-MS spectrum of **60IPH** fullerene derivative.

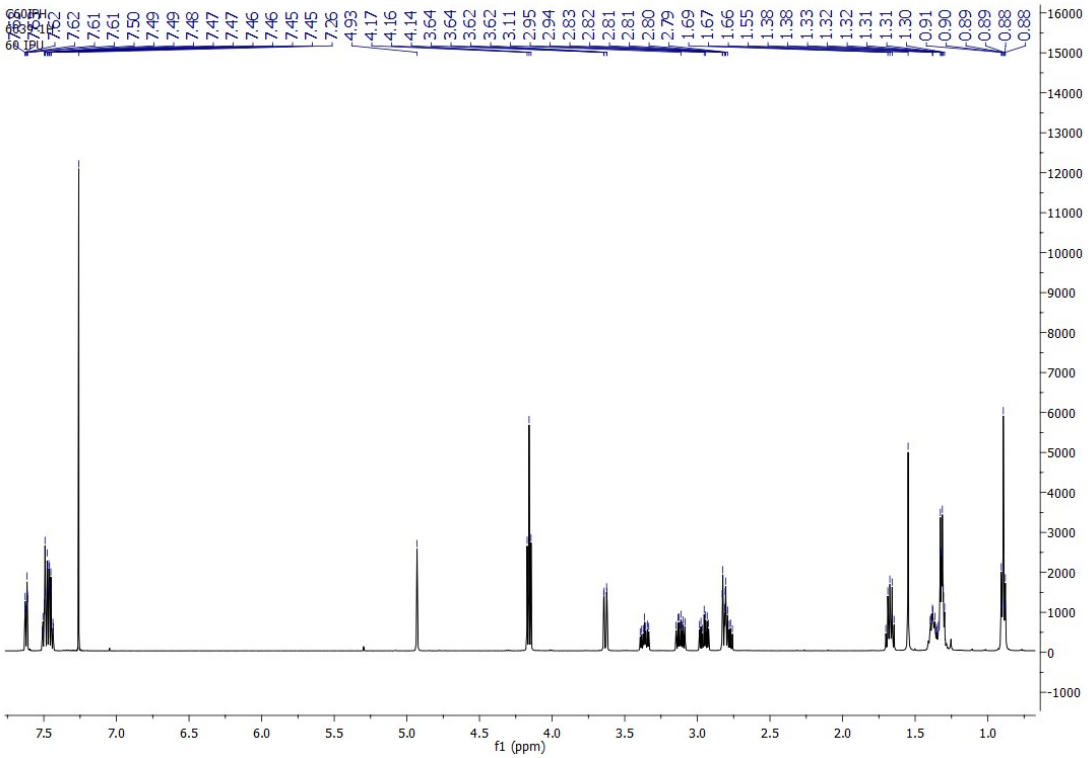


Figure S25. ^{1}H NMR spectrum of **60IPH** fullerene derivative.

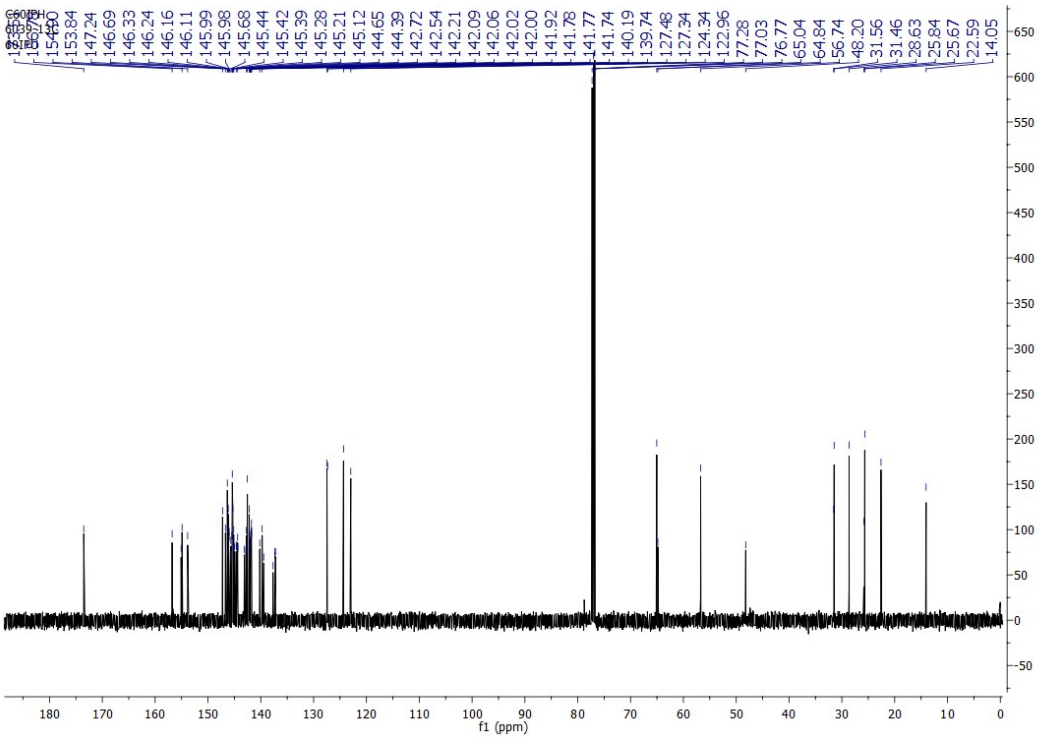


Figure S26. ^{13}C NMR spectrum of **60IPH** fullerene derivative.

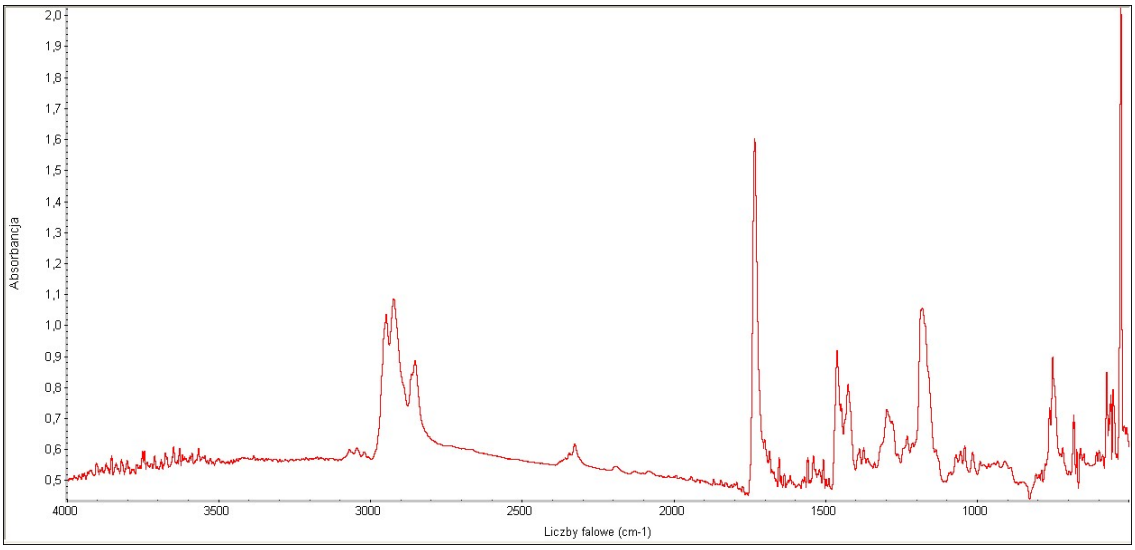


Figure S27. FT-IR spectrum of **60IPH** fullerene derivative.

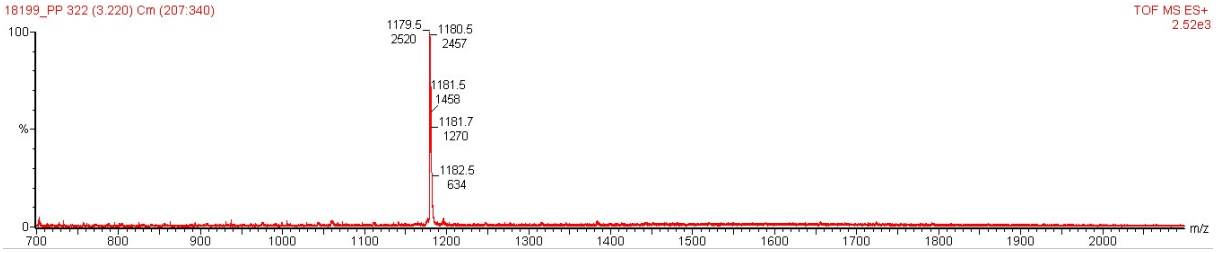


Figure S28. ESI-MS spectrum of **70IPH** fullerene derivative.

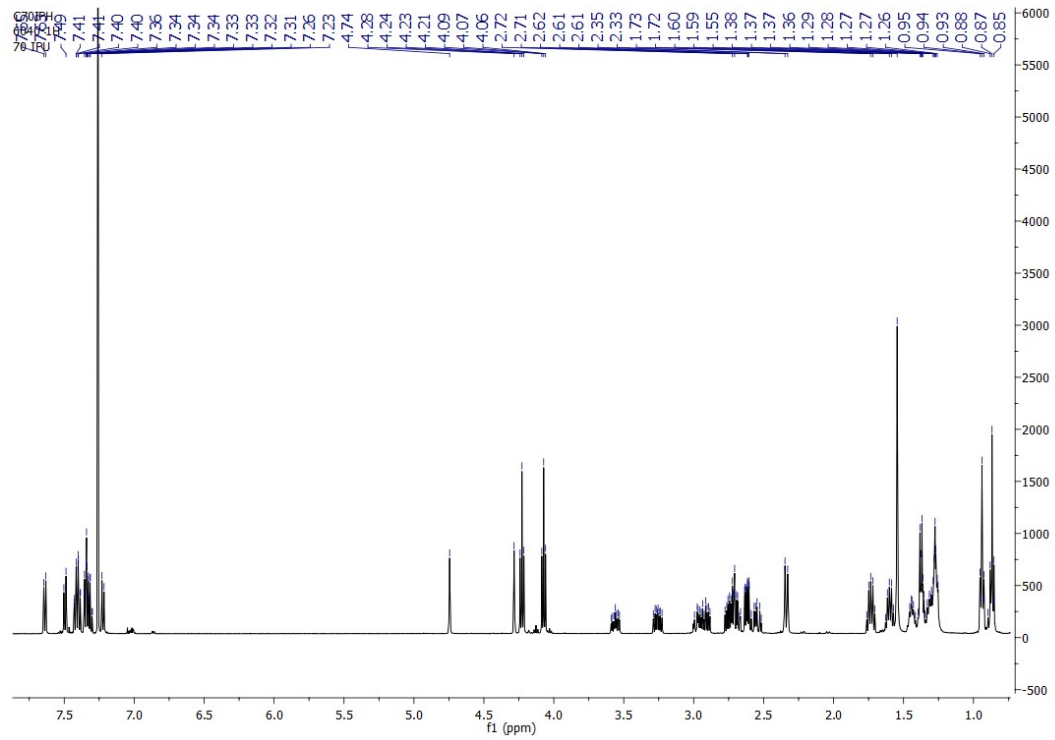


Figure S29. ^{1}H NMR spectrum of **70IPH** fullerene derivative.

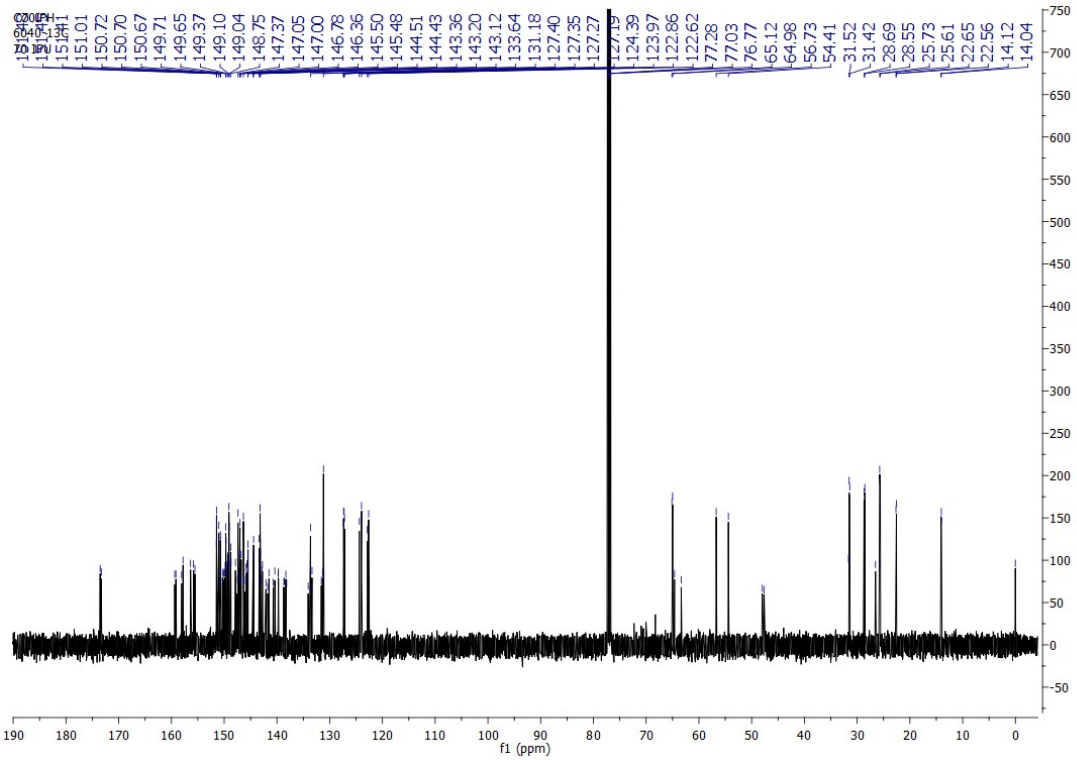


Figure S30. ^{13}C NMR spectrum of **70IPH** fullerene derivative.

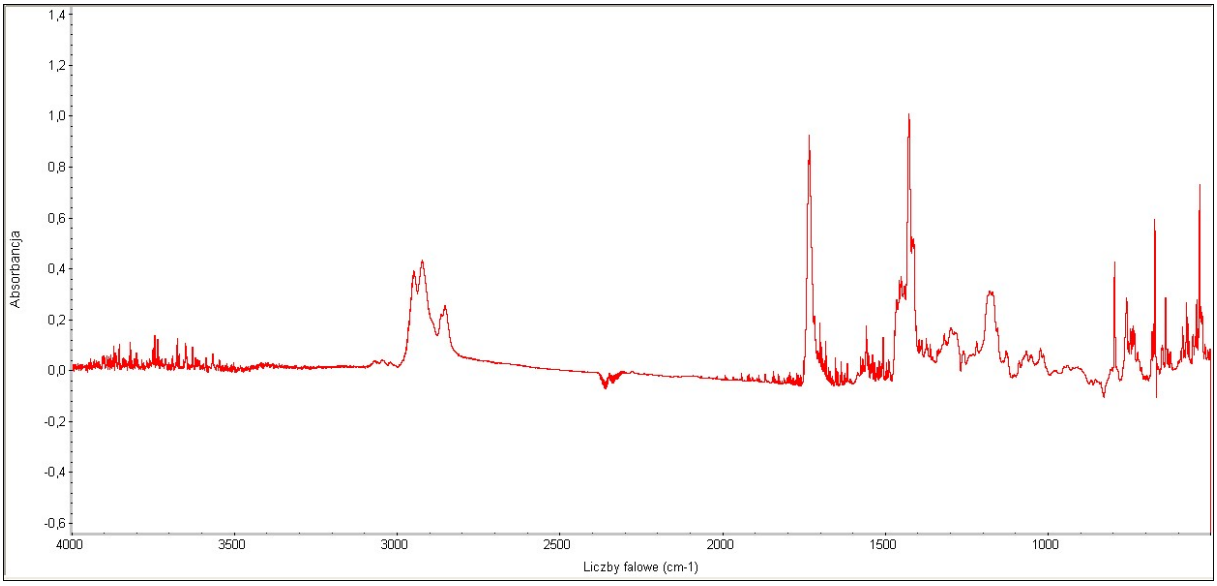


Figure S31. FT-IR spectrum of **70IPH** fullerene derivative.

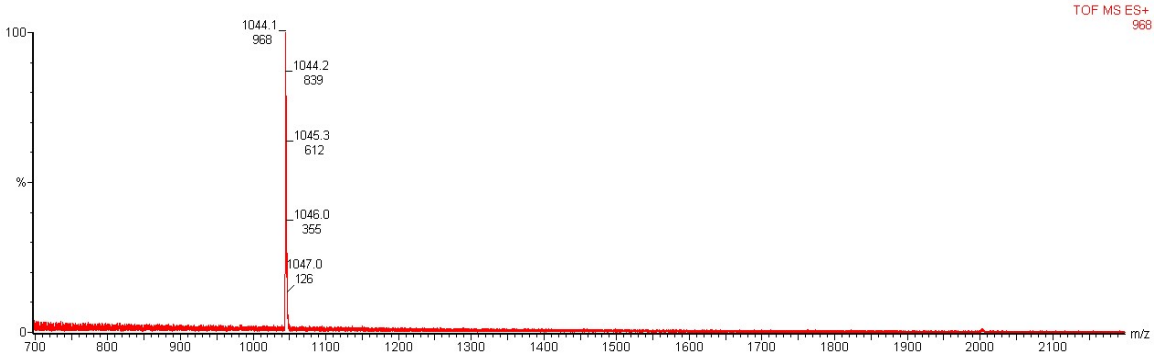


Figure S32. ESI-MS spectrum of **60IPO** fullerene derivative.

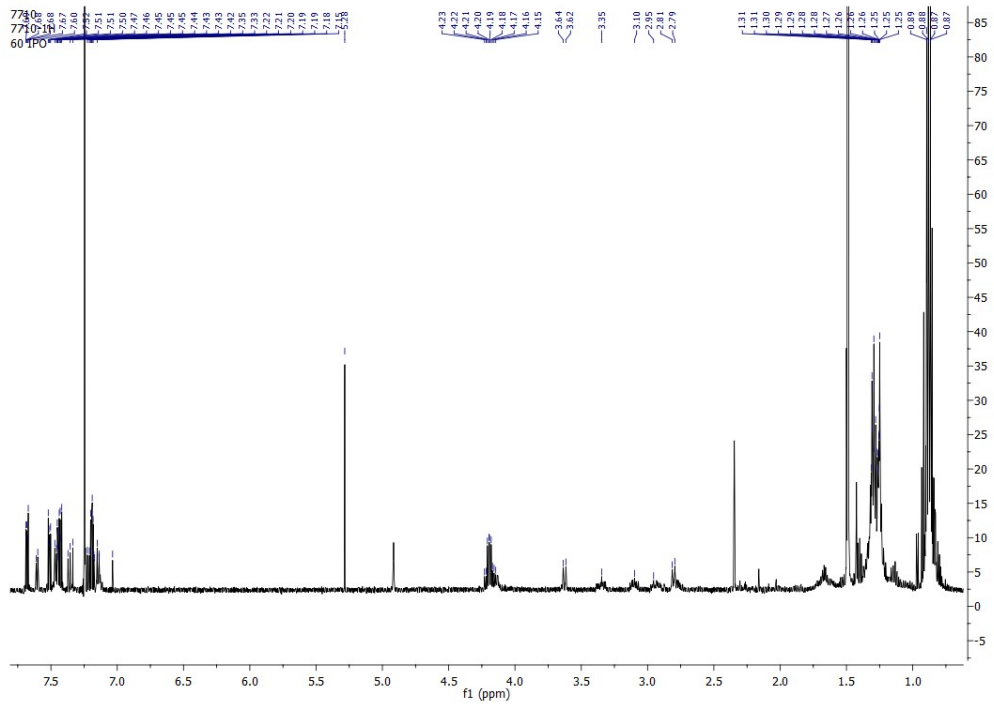


Figure S33. ^{1}H NMR spectrum of **60IPO** fullerene derivative.

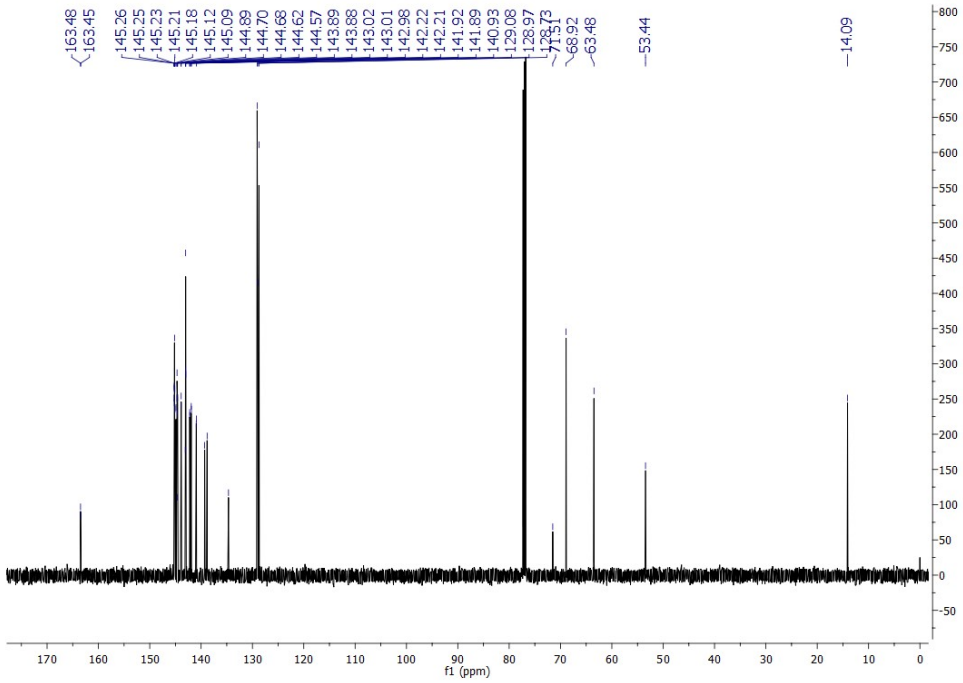


Figure S34. ^{13}C NMR spectrum of **60IPO** fullerene derivative.

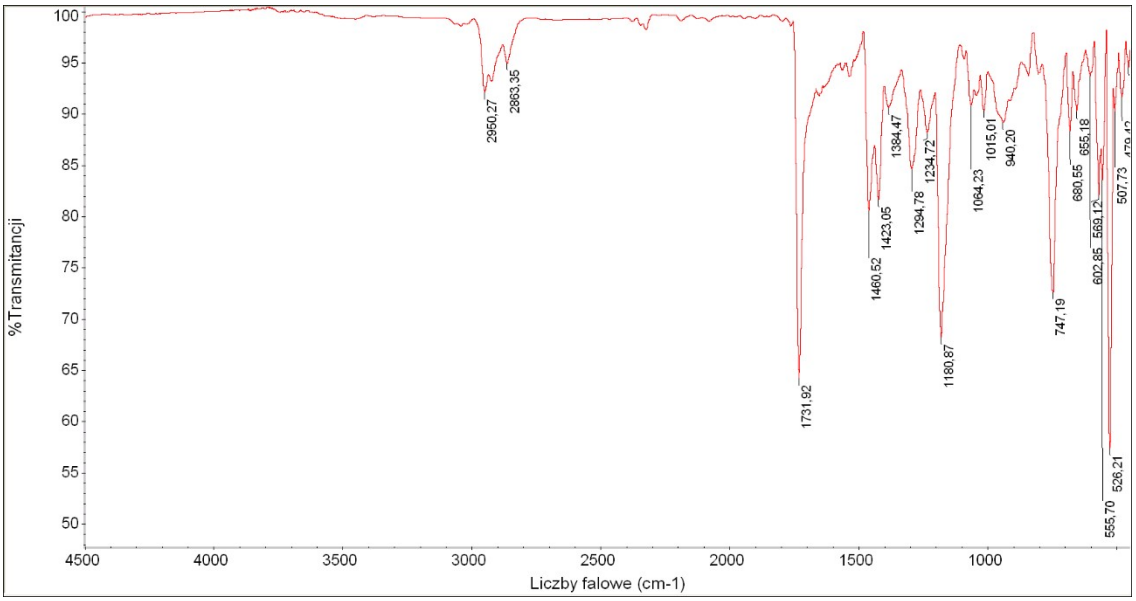


Figure S35. FT-IR spectrum of **60IPO** fullerene derivative.

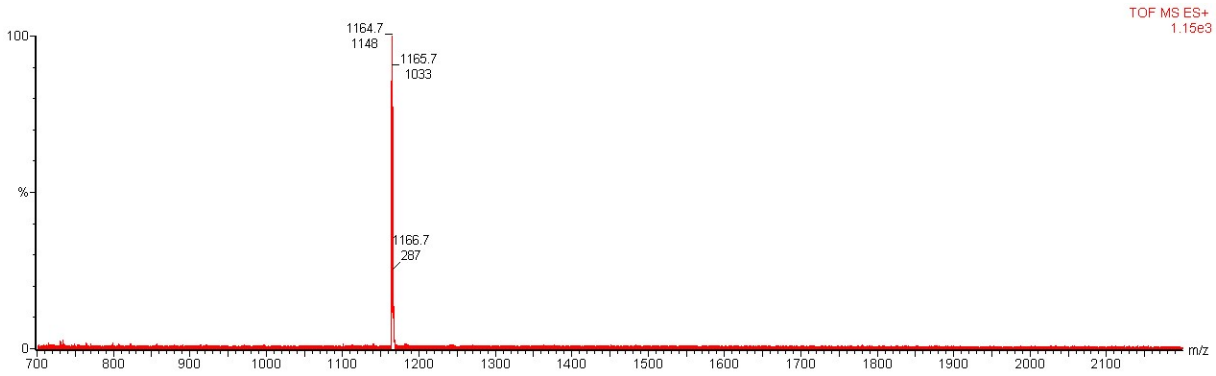


Figure S36. ESI-MS spectrum of **70IPO** fullerene derivative.

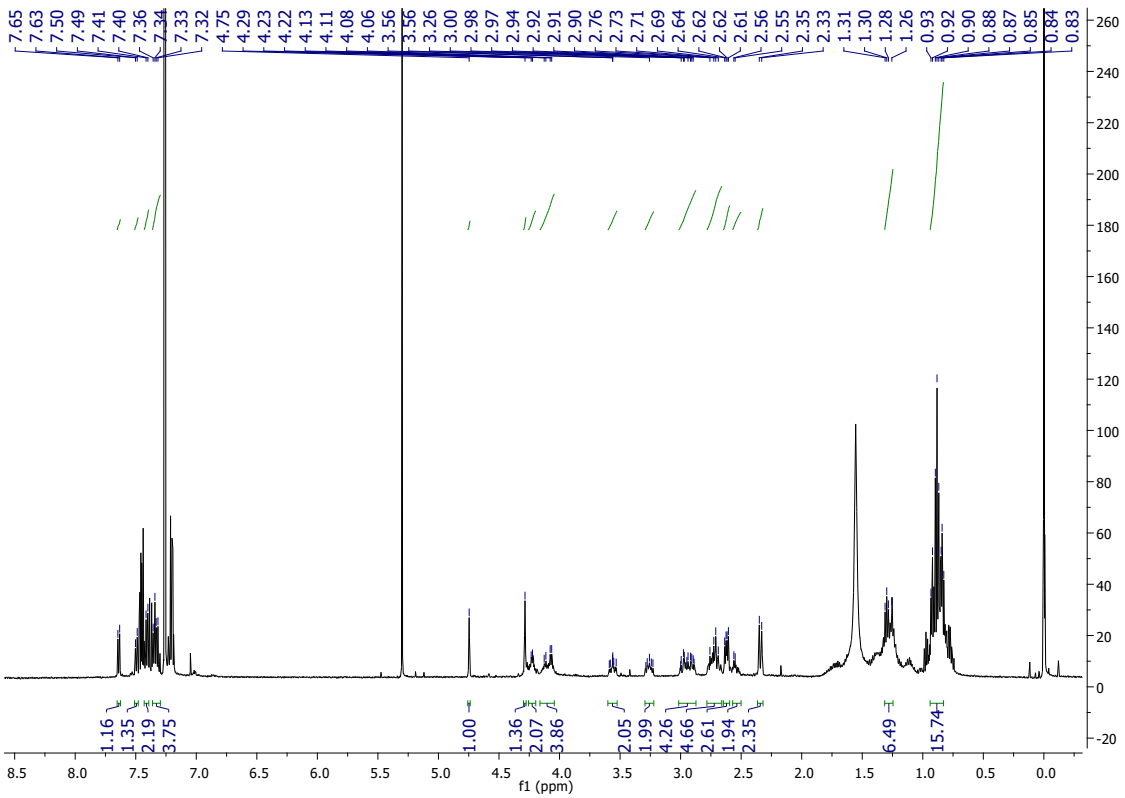


Figure S37. ^{1}H NMR spectrum of **70IPO** fullerene derivative.

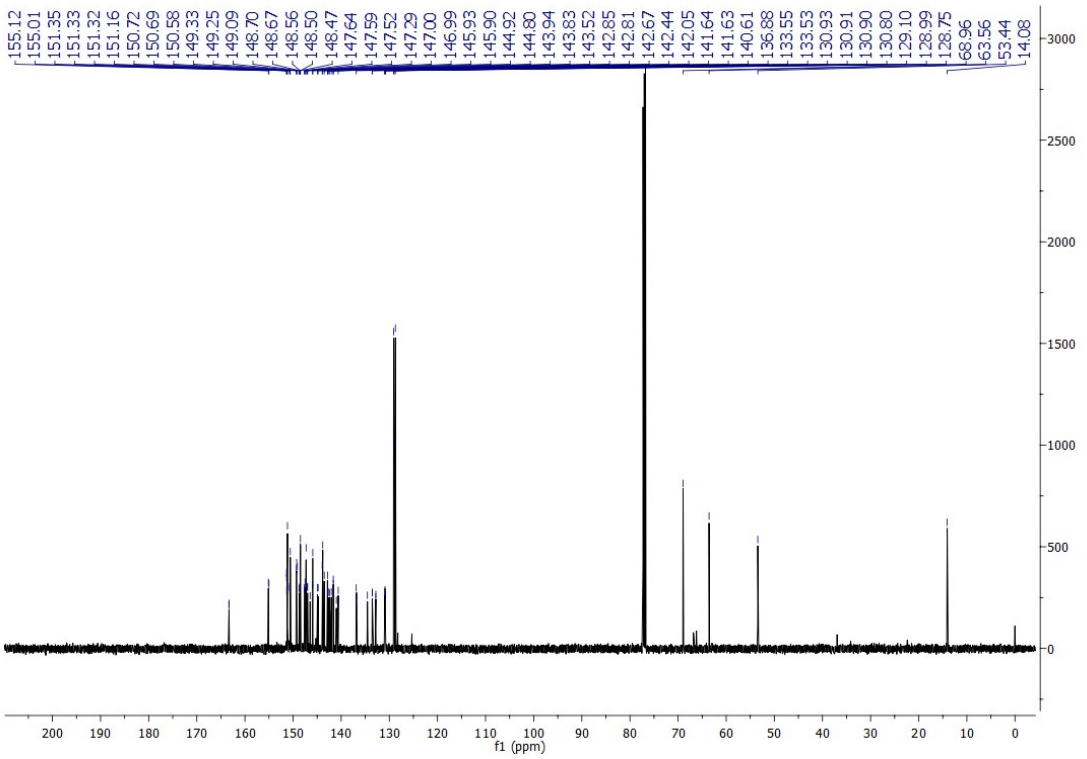


Figure S38. ^{13}C NMR spectrum of **70IPO** fullerene derivative.

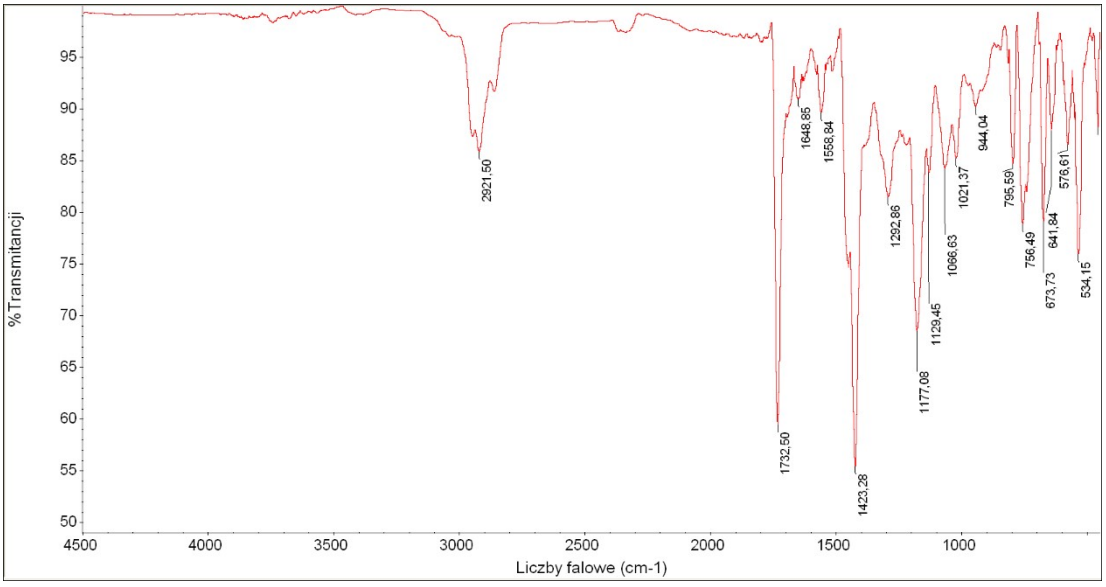


Figure S39. FT-IR spectrum of **70IPO** fullerene derivative.

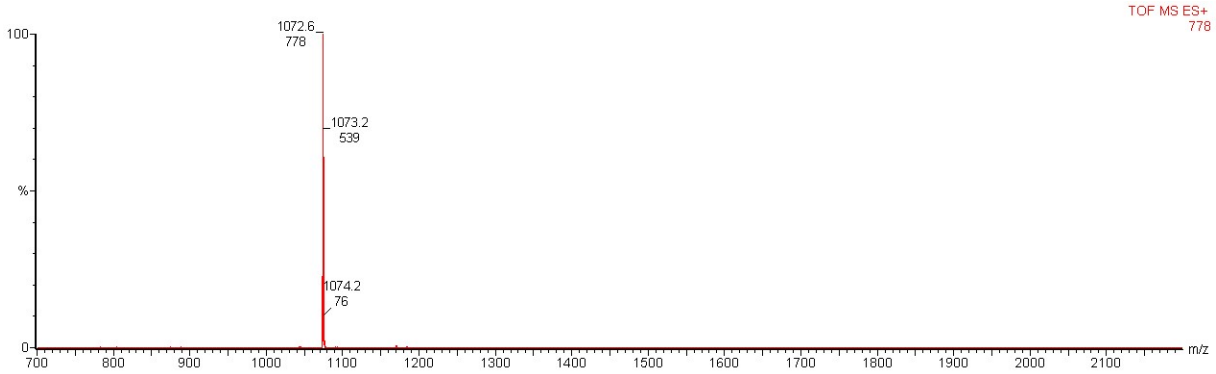


Figure S40. ESI-MS spectrum of **60IPD** fullerene derivative.

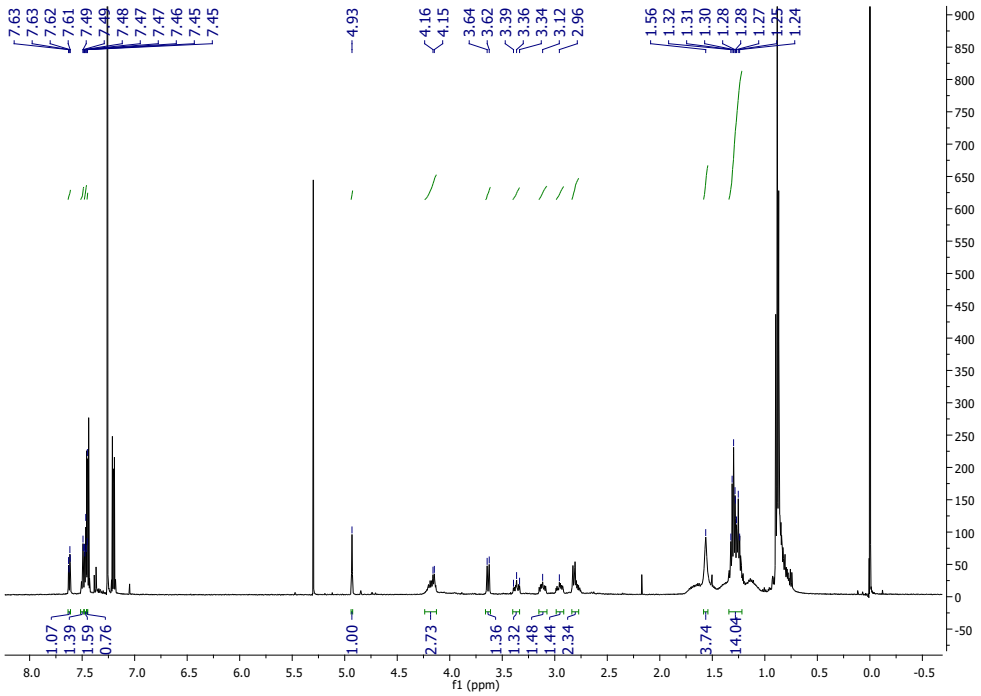


Figure S41. ^{1}H NMR spectrum of **60IPD** fullerene derivative.

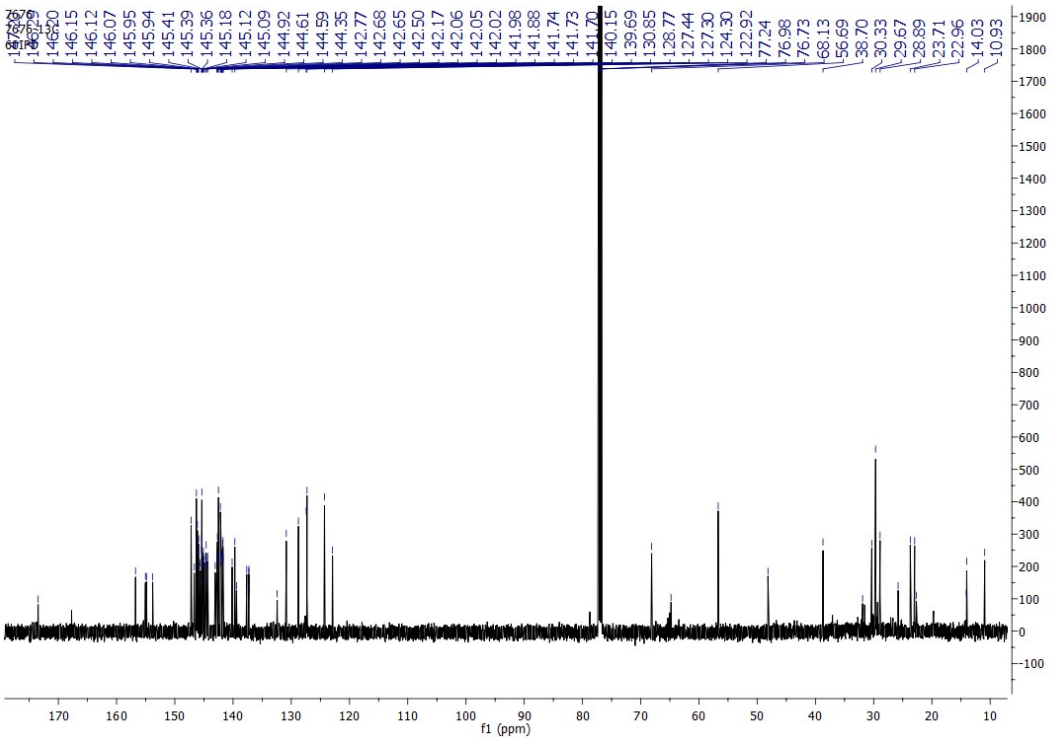


Figure S42. ^{13}C NMR spectrum of **60IPD** fullerene derivative.

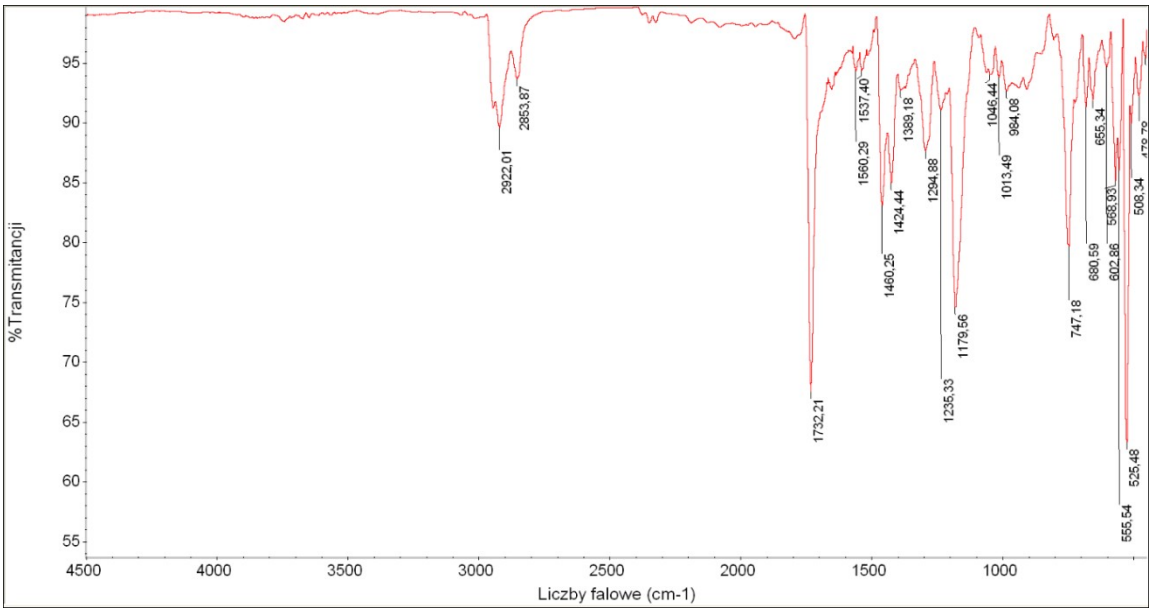


Figure S43. FT-IR spectrum of **60IPD** fullerene derivative.

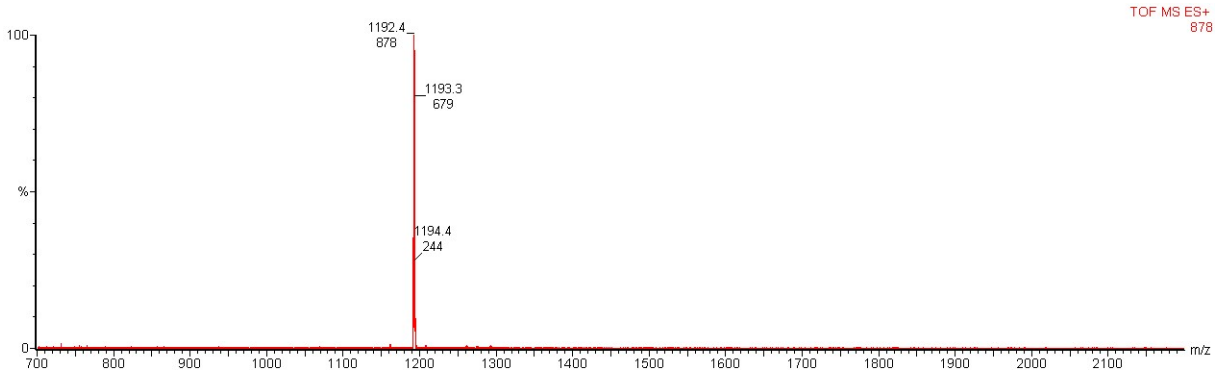


Figure S44. ESI-MS spectrum of **70IPD** fullerene derivative.

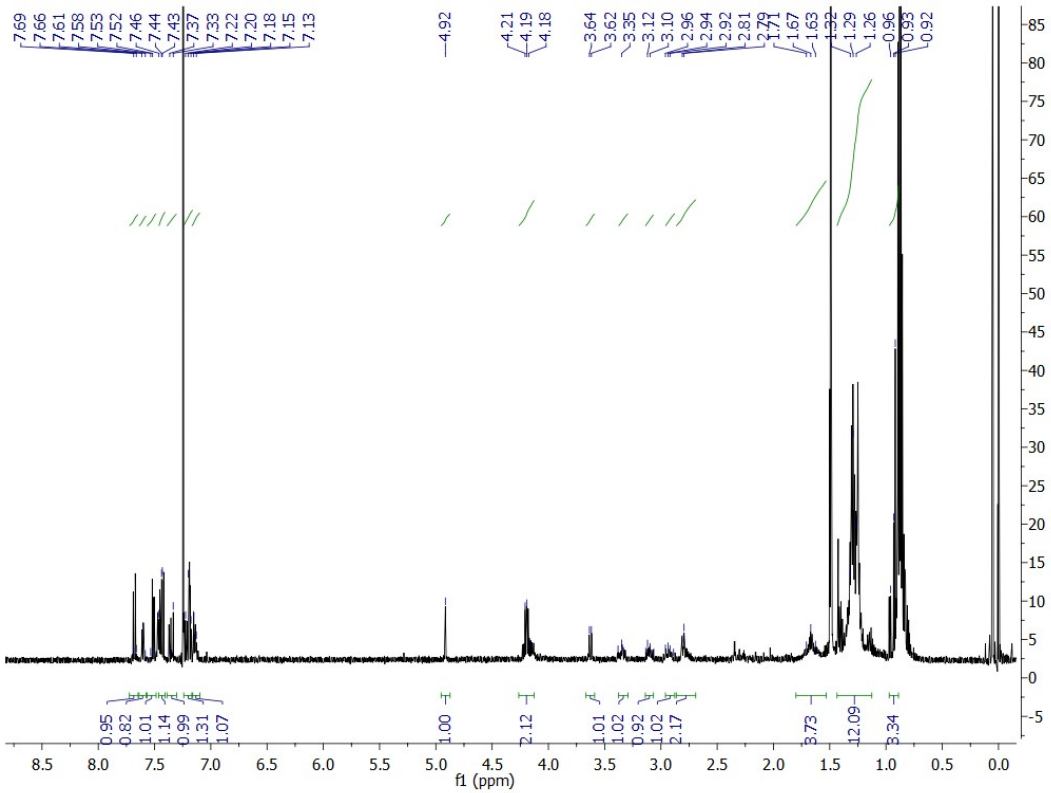


Figure S45. ^{1}H NMR spectrum of **70IPD** fullerene derivative.

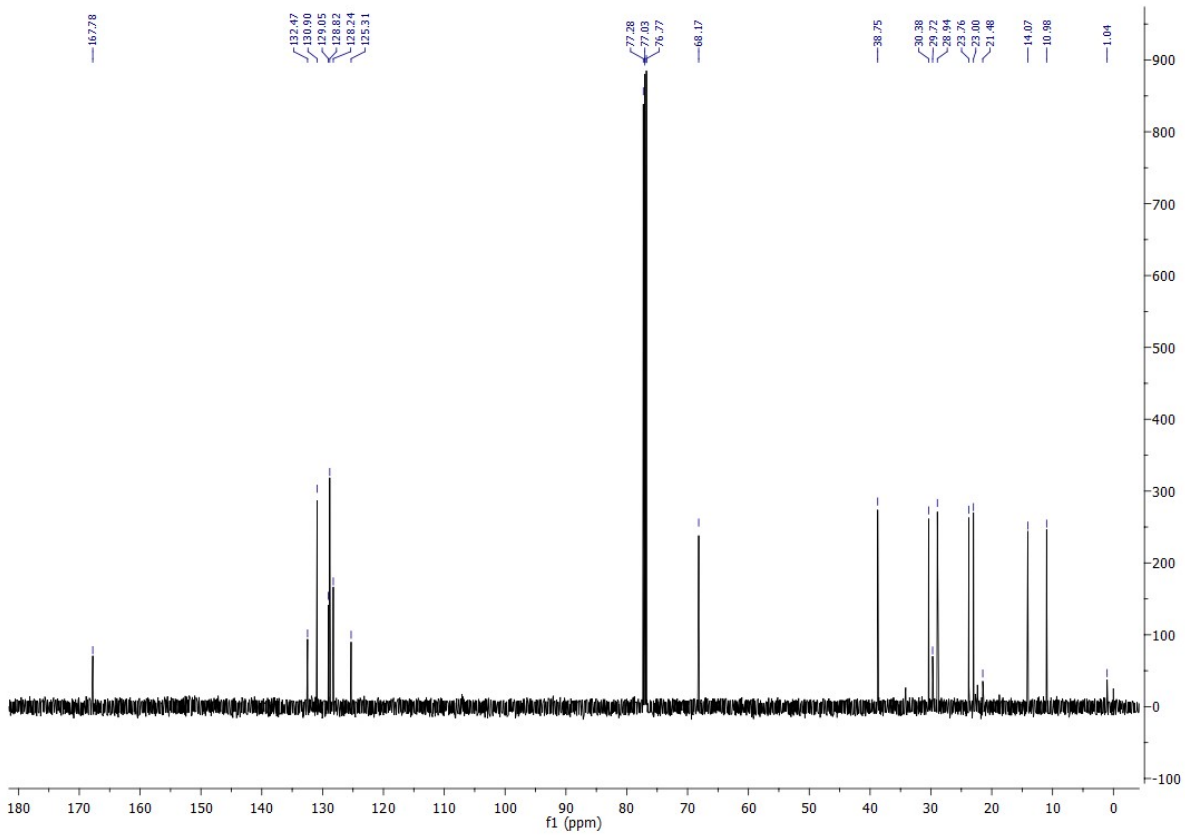


Figure S46. ^{13}C NMR spectrum of **70IPD** fullerene derivative.

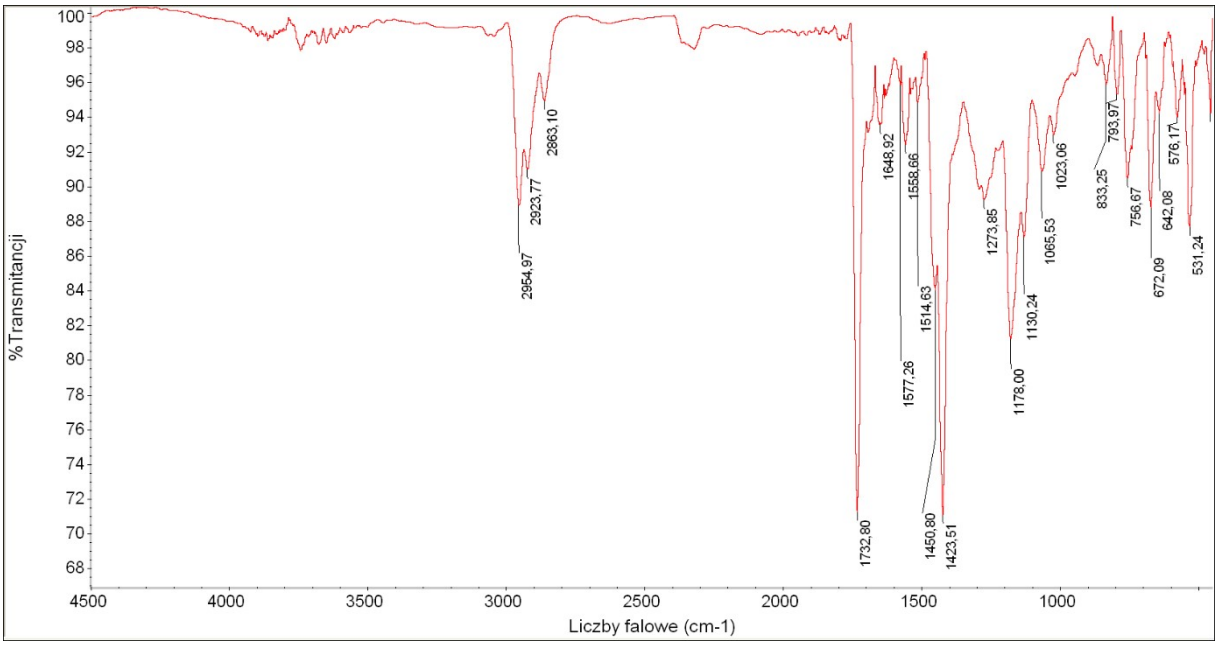


Figure S47. FT-IR spectrum of **70IPD** fullerene derivative.

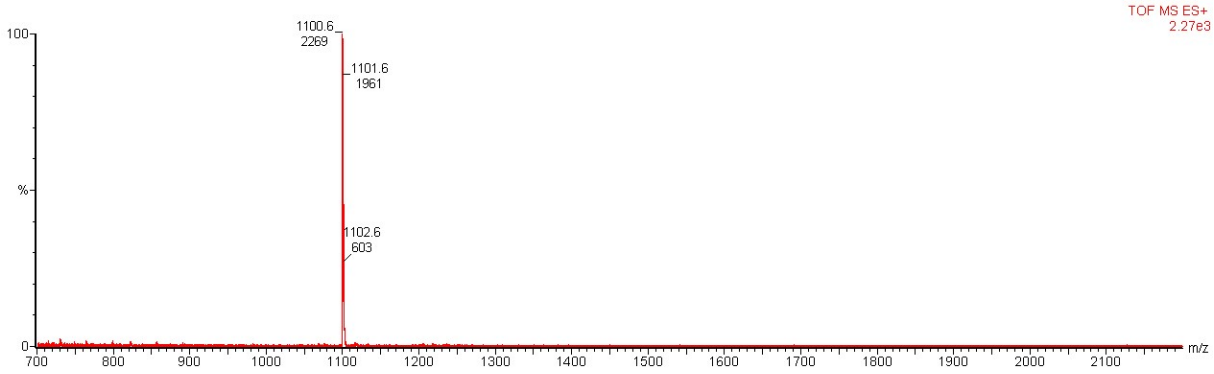


Figure S48. ESI-MS spectrum of **60IPL** fullerene derivative.

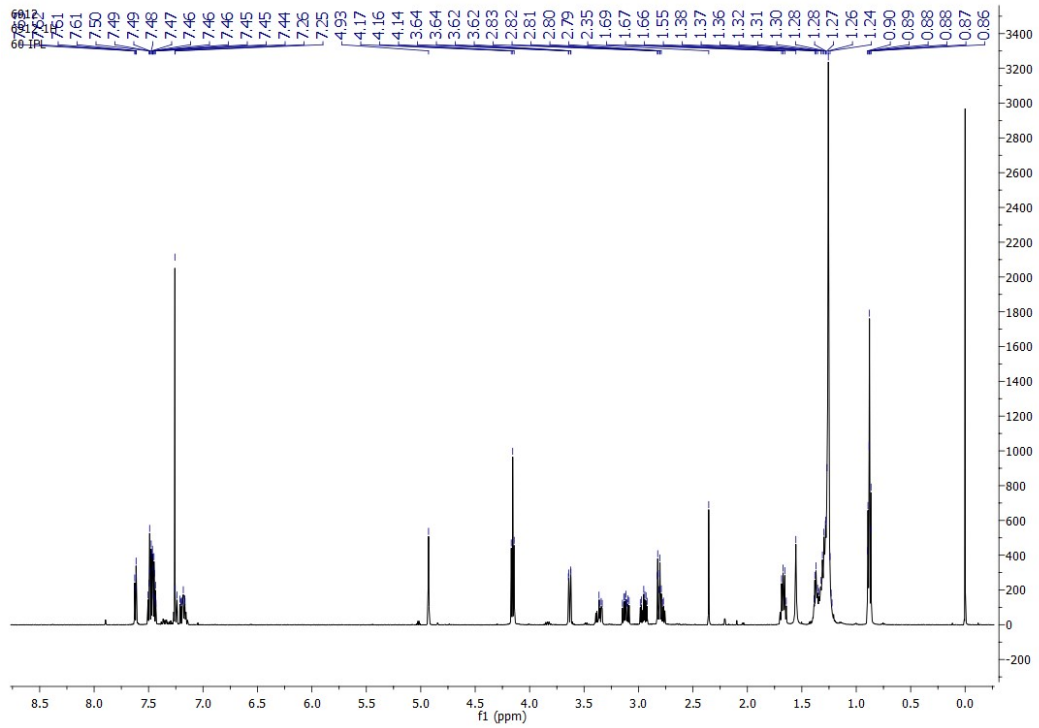


Figure S49. ^{1}H NMR spectrum of **60IPL** fullerene derivative.

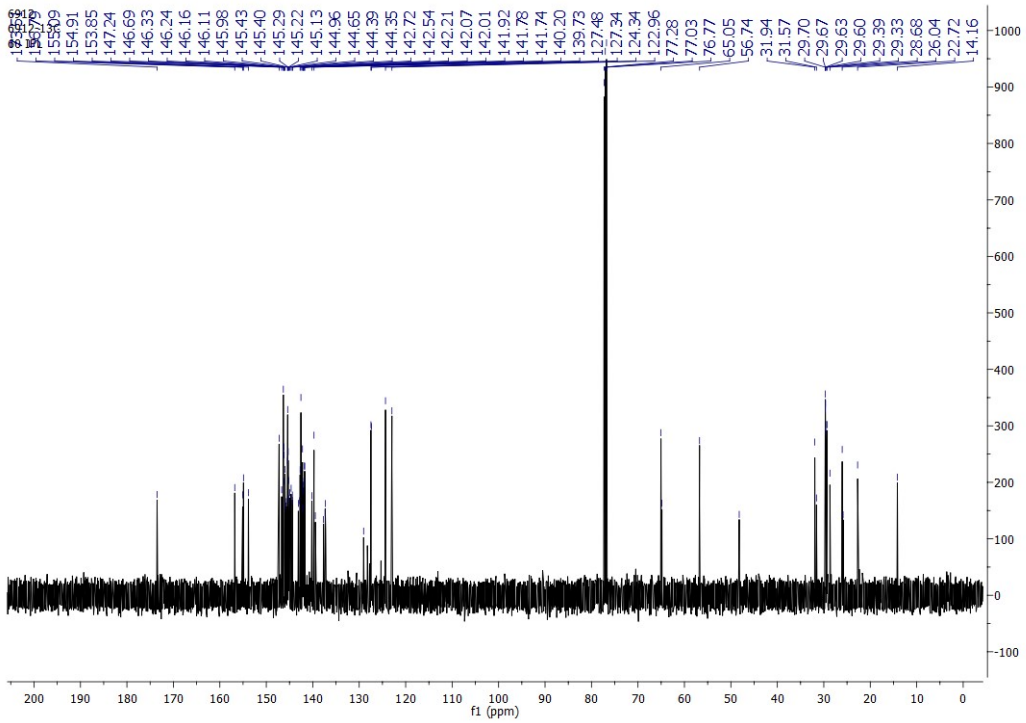


Figure S50. ^{13}C NMR spectrum of **60IPL** fullerene derivative.

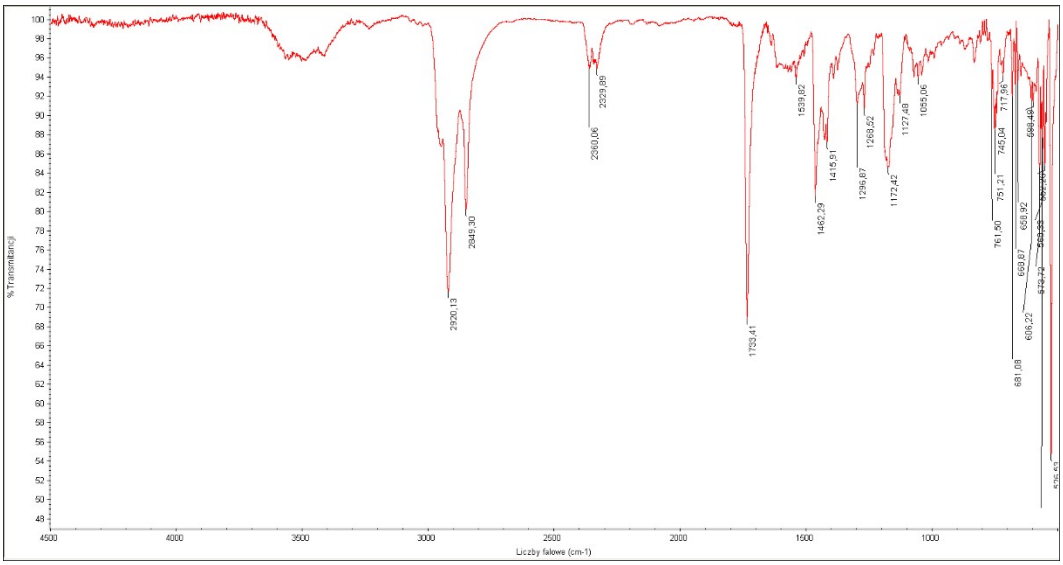


Figure S51. FT-IR spectrum of **60IPL** fullerene derivative.

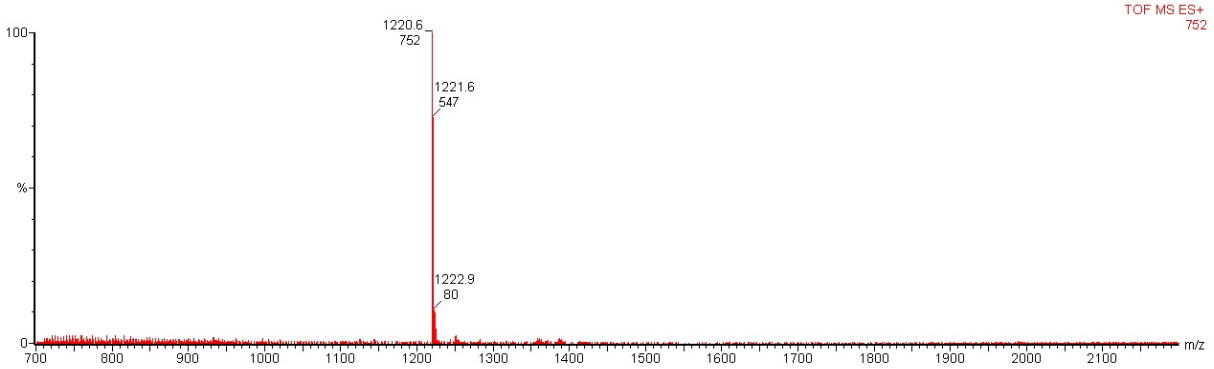


Figure S52. ESI-MS spectrum of **70IPL** fullerene derivative.

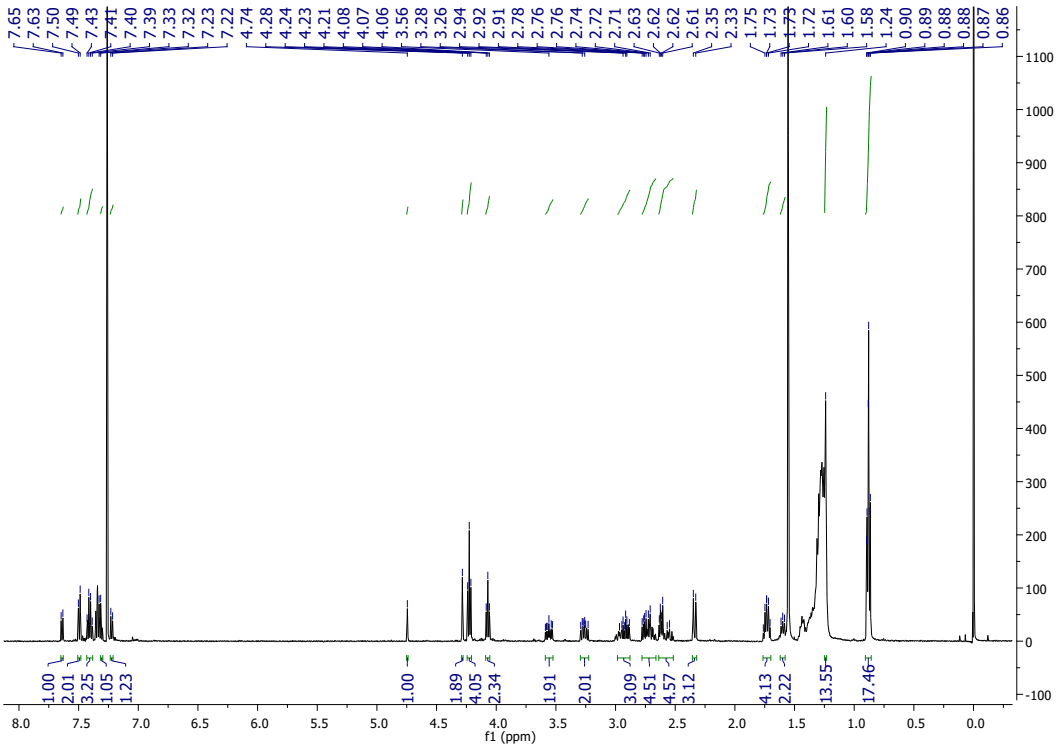


Figure S53. ^{1}H NMR spectrum of **70IPL** fullerene derivative.

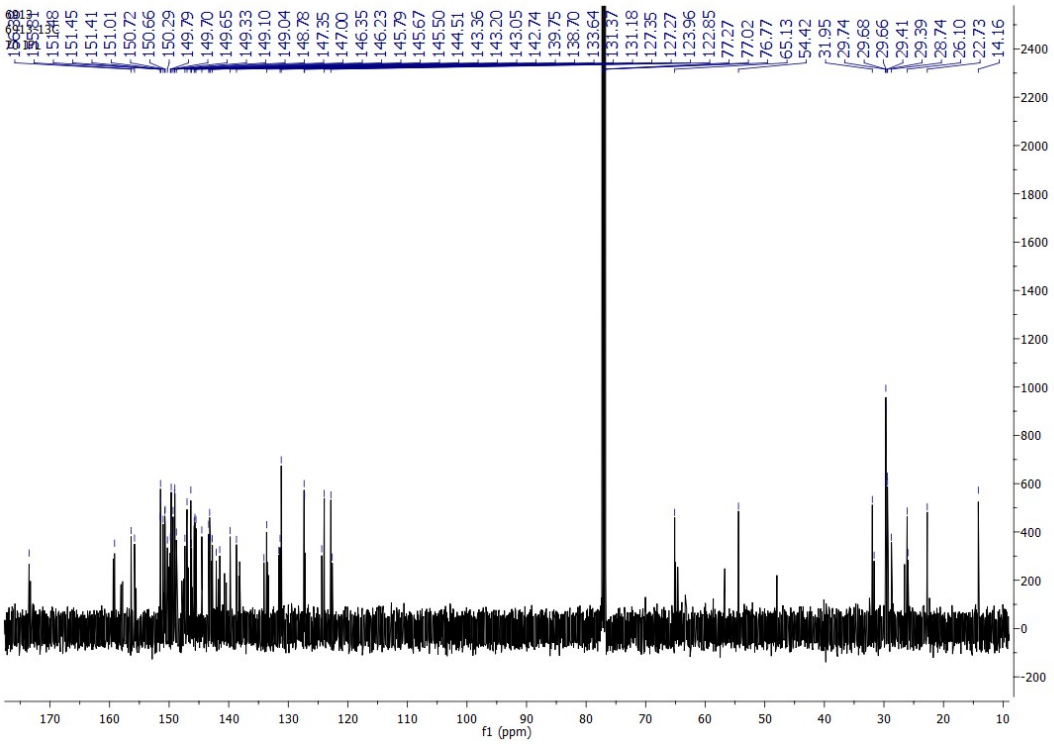


Figure S54. ^{13}C NMR spectrum of **70IPL** fullerene derivative.

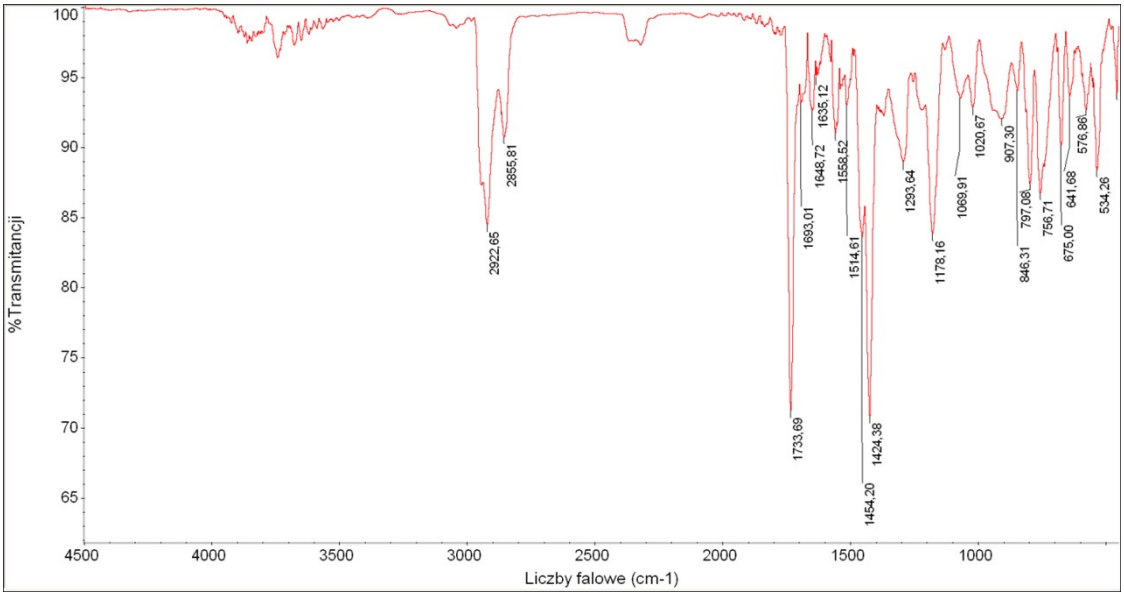
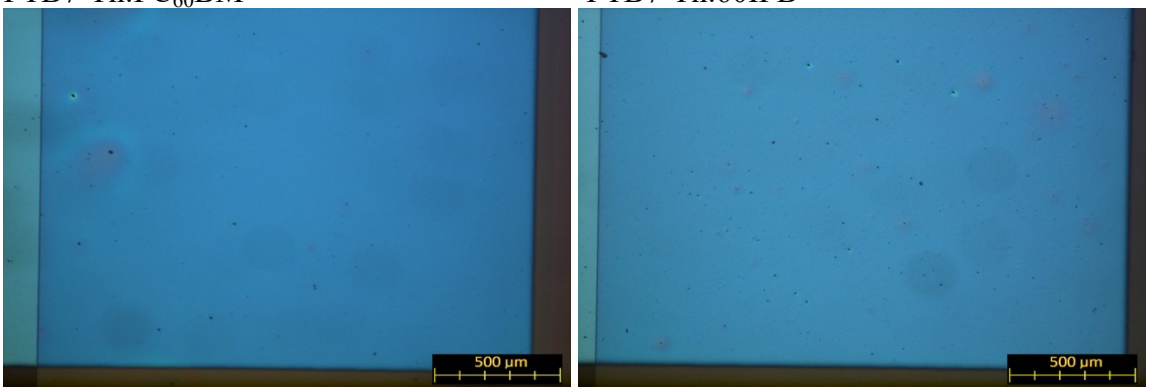
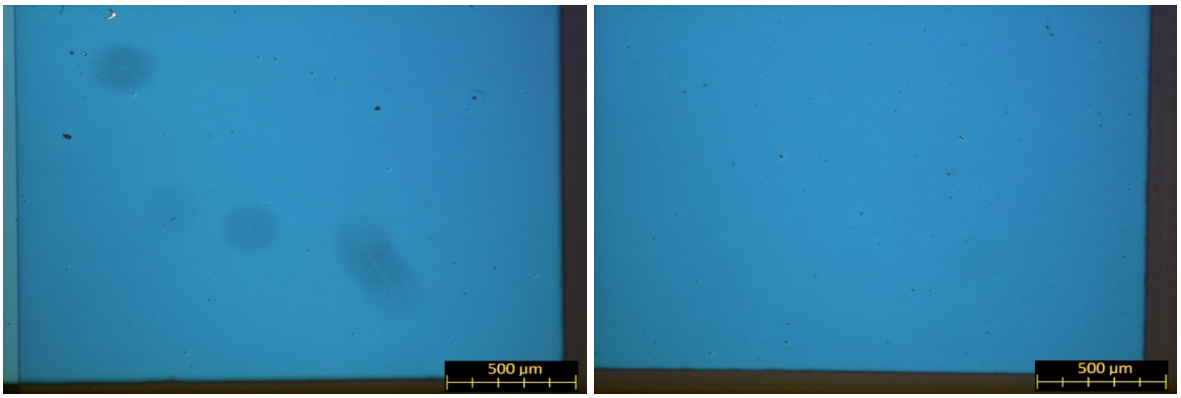


Figure S55. FT-IR spectrum of **70IPL** fullerene derivative.

PTB7-Th:$PC_{60}BM$ PTB7-Th:60IPB



PTB7-Th:60IPH PTB7-Th:60IPO



PTB7-Th:60IPD PTB7-Th:60IPL

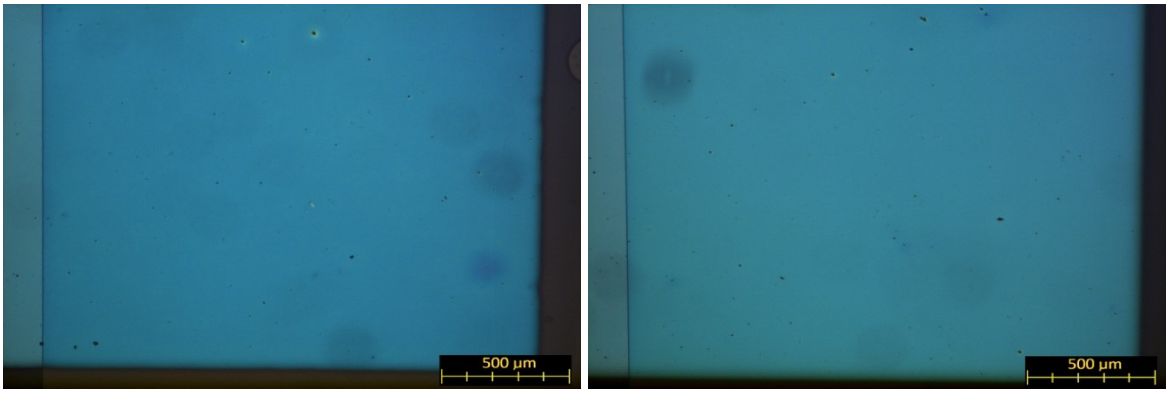
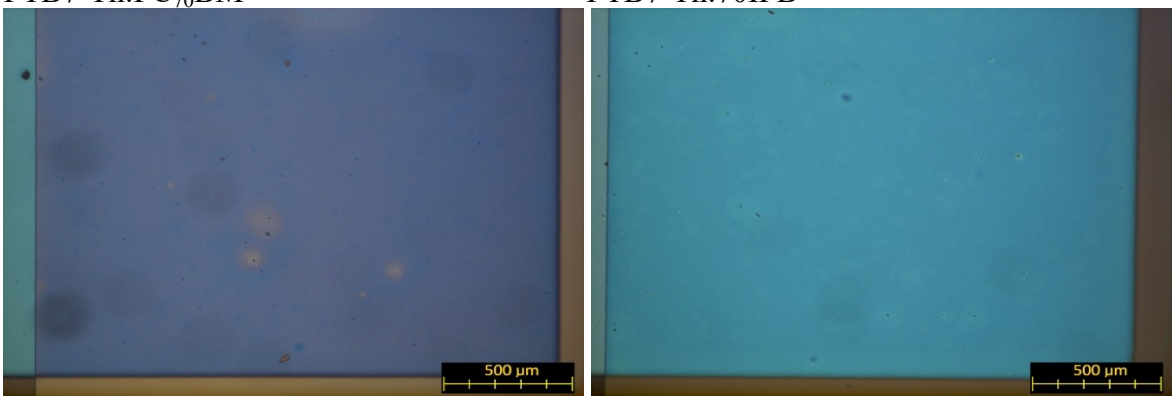
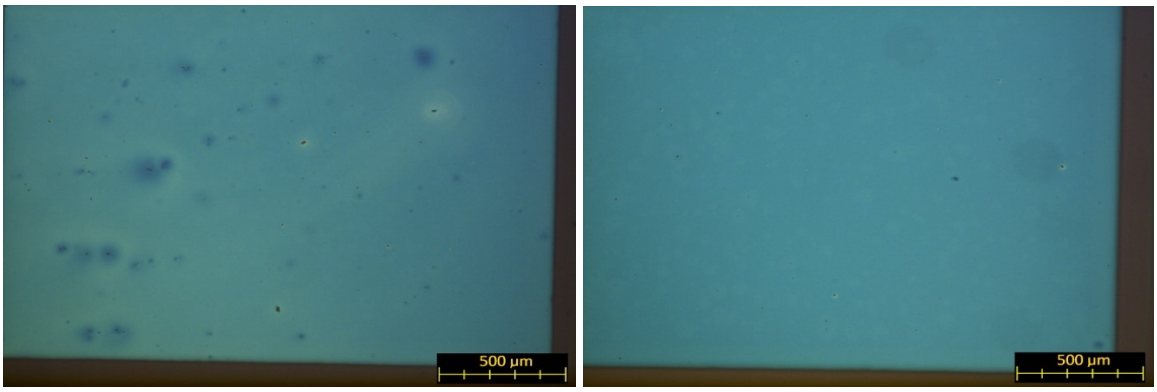


Figure S56. Morphology of PTB7-Th_C_{60} solar cells active layers as observed by microscope with differential interference contrast (5X magnification).

PTB7-Th:$PC_{70}BM$ PTB7-Th:70IPB



PTB7-Th:70IPH PTB7-Th:70IPO



PTB7-Th:70IPD PTB7-Th:70IPL

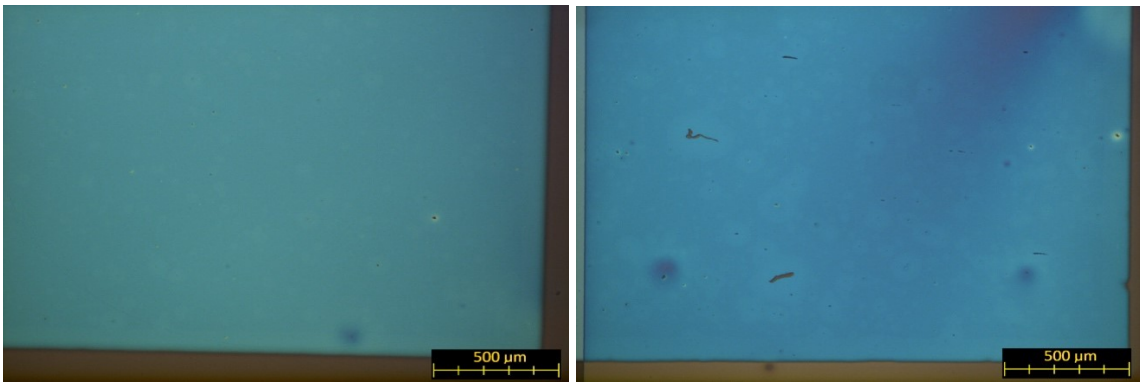


Figure S57. Morphology of PTB7-Th_C_{70} solar cells active layers as observed by microscope with differential interference contrast (5X magnification).

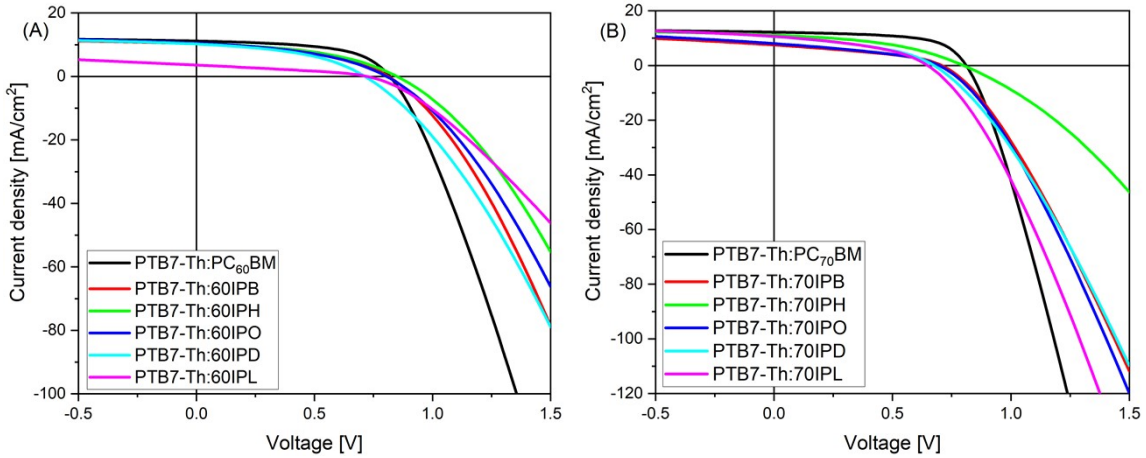


Figure S58. J-V characteristics of solar cells with A) PTB7-Th:C_{60} and b) PTB7-Th:C_{70} active layers.

Table S1. Electrical parameters of solar cells with PTB7-Th:C_{60} active layers.

Sample	Voc [V]	J_{SC} [mA/cm^2]	FF [%]	Rs [Ω*cm^2]	Rsh [Ω*cm^2]	PCE [%]	3 cells Av. PCE [%]	8 cells Av. PCE [%]
PTB7-Th:PC_{60}BM	0.820	11.2	55.5	4.18	620	5.078	5.043 ±0.041	4.957 ±0.078
PTB7-Th:60IPB	0.814	10.3	46.4	6.52	396	3.885	3.801 ±0.066	3.556 ±0.237
PTB7-Th:60IPH	0.850	10.4	43.9	8.85	346	3.876	3.870 ±0.005	3.679 ±0.173
PTB7-Th:60IPO	0.805	10.5	42.3	7.82	279	3.568	3.537 ±0.025	3.2876 ±0.230
PTB7-Th:60IPD	0.714	10.2	43.6	7.45	271	3.179	3.080 ±0.070	2.919 ±0.193
PTB7-Th:60IPL	0.723	3.59	32.5	12.9	276	0.844	0.823 ±0.015	0.743 ±0.139

Table S2. Electrical parameters of solar cells with PTB7-Th:C_{70} active layers.

Sample	Voc [V]	J_{SC} [mA/cm^2]	FF [%]	Rs [Ω*cm^2]	Rsh [Ω*cm^2]	PCE [%]	3 cells Av. PCE [%]	8 cells Av. PCE [%]
PTB7-Th:PC_{70}BM	0.811	12.2	61.3	2.66	663	6.076	6.060 ±0.013	5.856 ±0.275
PTB7-Th:70IPB	0.708	7.51	37.4	5.54	172	1.988	1.960 ±0.021	1.897 ±0.055
PTB7-Th:70IPH	0.800	11.1	42.4	11.7	276	3.772	3.722 ±0.048	3.373 ±0.273
PTB7-Th:70IPO	0.675	10.6	39.9	5.78	156	2.844	2.771 ±0.058	2.338 ±0.398
PTB7-Th:70IPD	0.696	8.03	37.2	5.09	159	2.078	2.068 ±0.008	1.815 ±0.223
PTB7-Th:70IPL	0.648	10.7	40.5	4.27	158	2.796	2.774 ±0.027	2.493 ±0.248

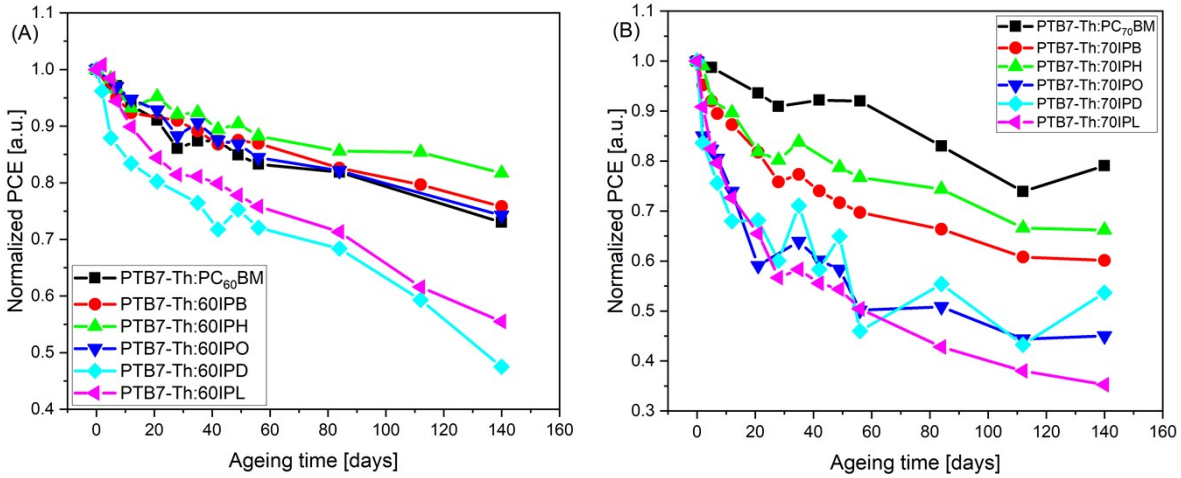


Figure S59. Normalized PCE of solar cells with different fullerenes derivatives in function of ageing time: A) C_{60}, B) C_{70}.

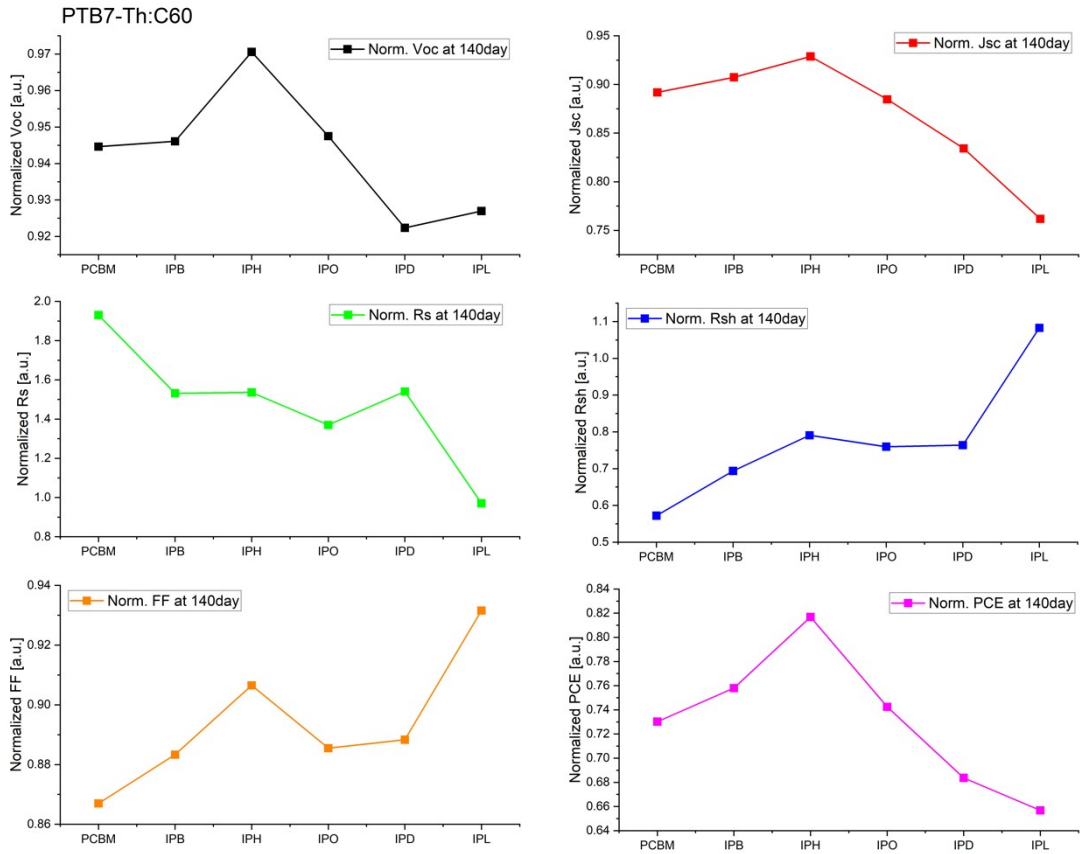


Figure S60. Normalized electrical parameters of solar cells with different C60 fullerenes derivatives after 140 days' degradation

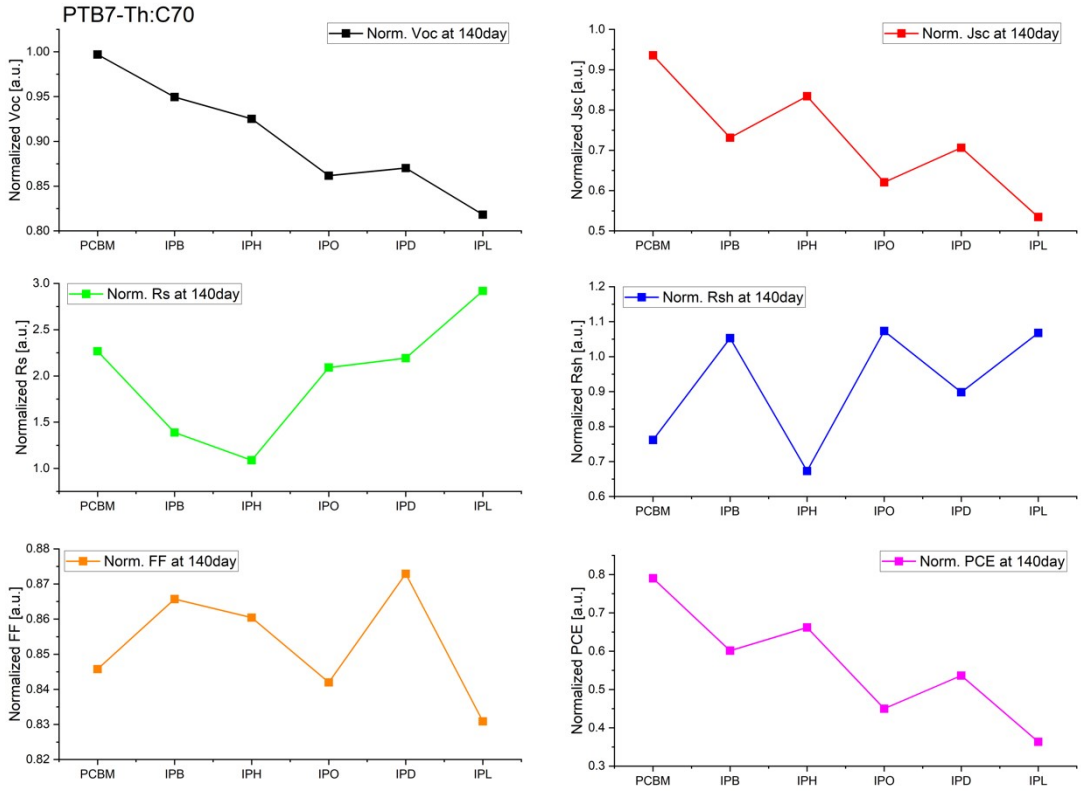


Figure S61. Normalized electrical parameters of solar cells with different C70 fullerenes derivatives after 140 days' degradation

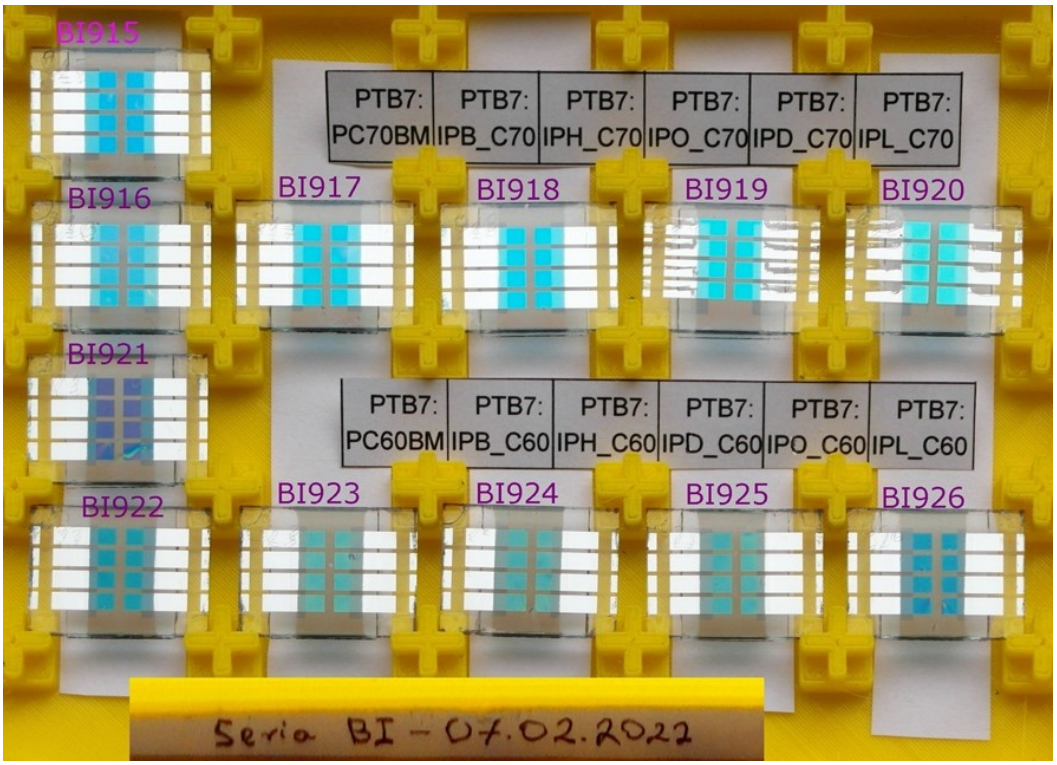


Figure S62. Photo of solar cells samples form one production series after encapsulation process