

Supplementary Materials

Developing novel indanone-chalcone hybrids bearing ester group with potential anti-Alzheimer effects by combining molecular hybridization and bioisosteric replacement drug design approaches

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¹HNMR , ¹³CNMR, IR spectra, Mass and HPTLC analysis of target compounds 8a-n.

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¹H NMR spectra

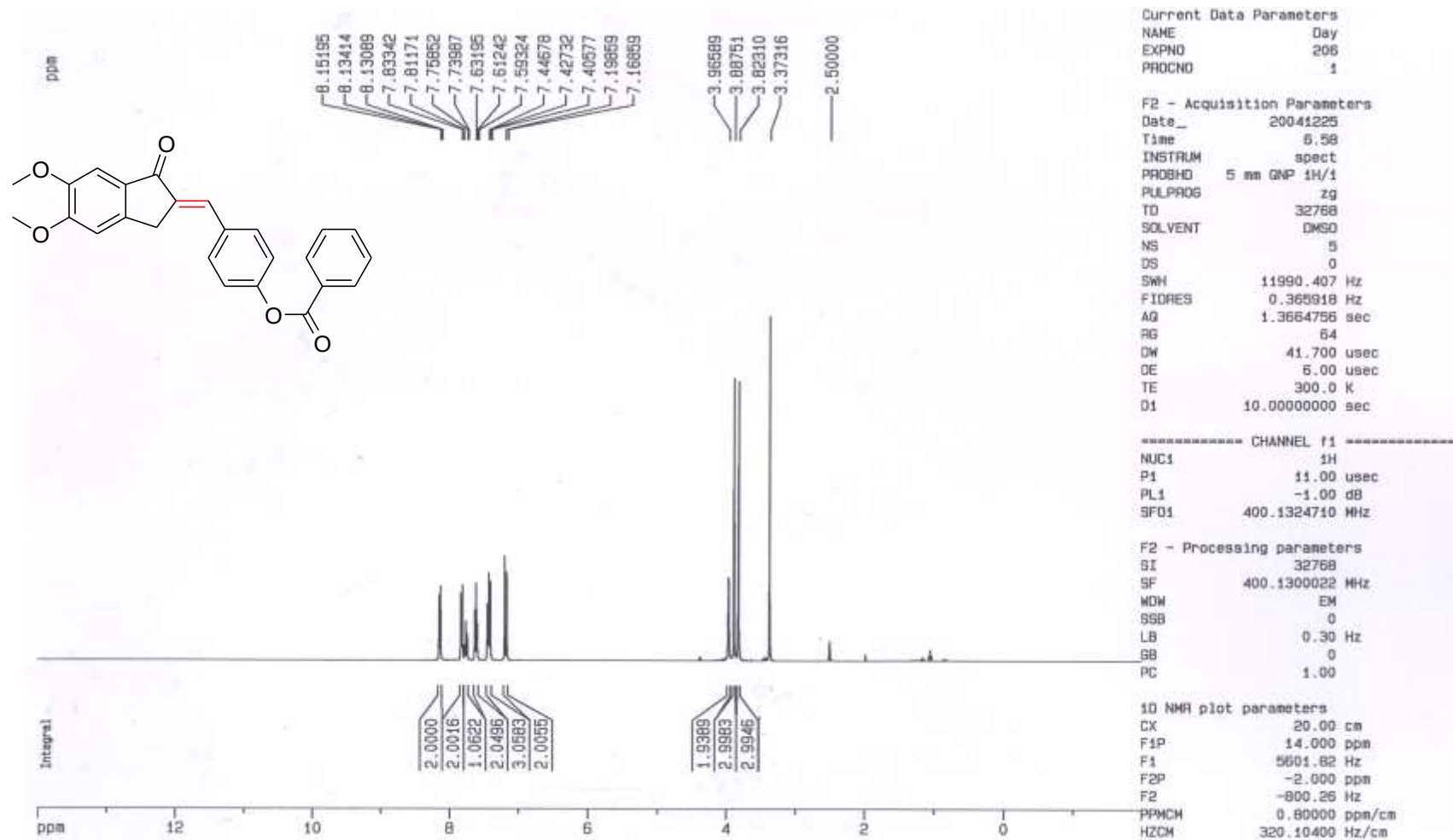


Fig.S1. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8a).

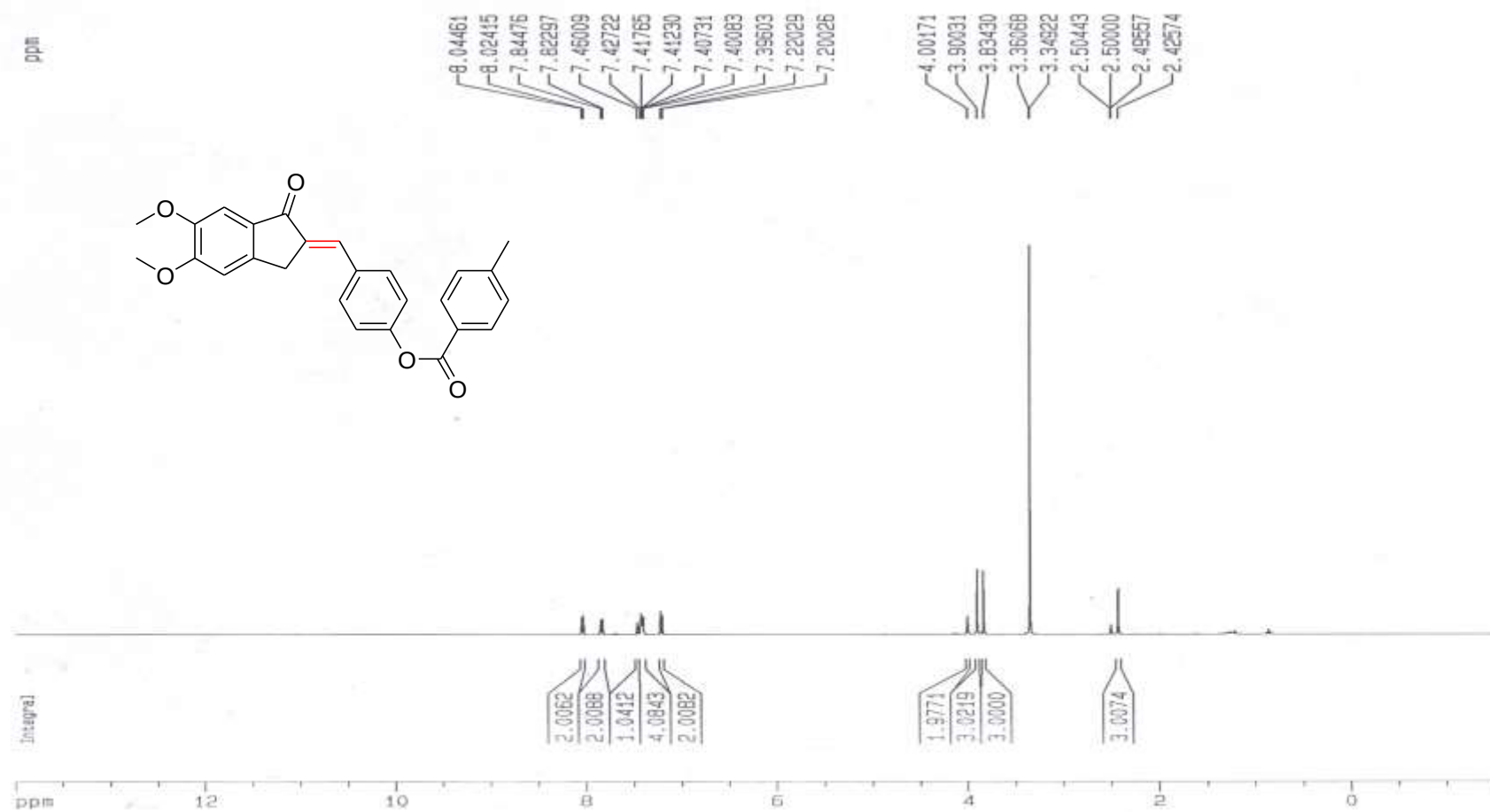


Fig.S2.4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (8b)

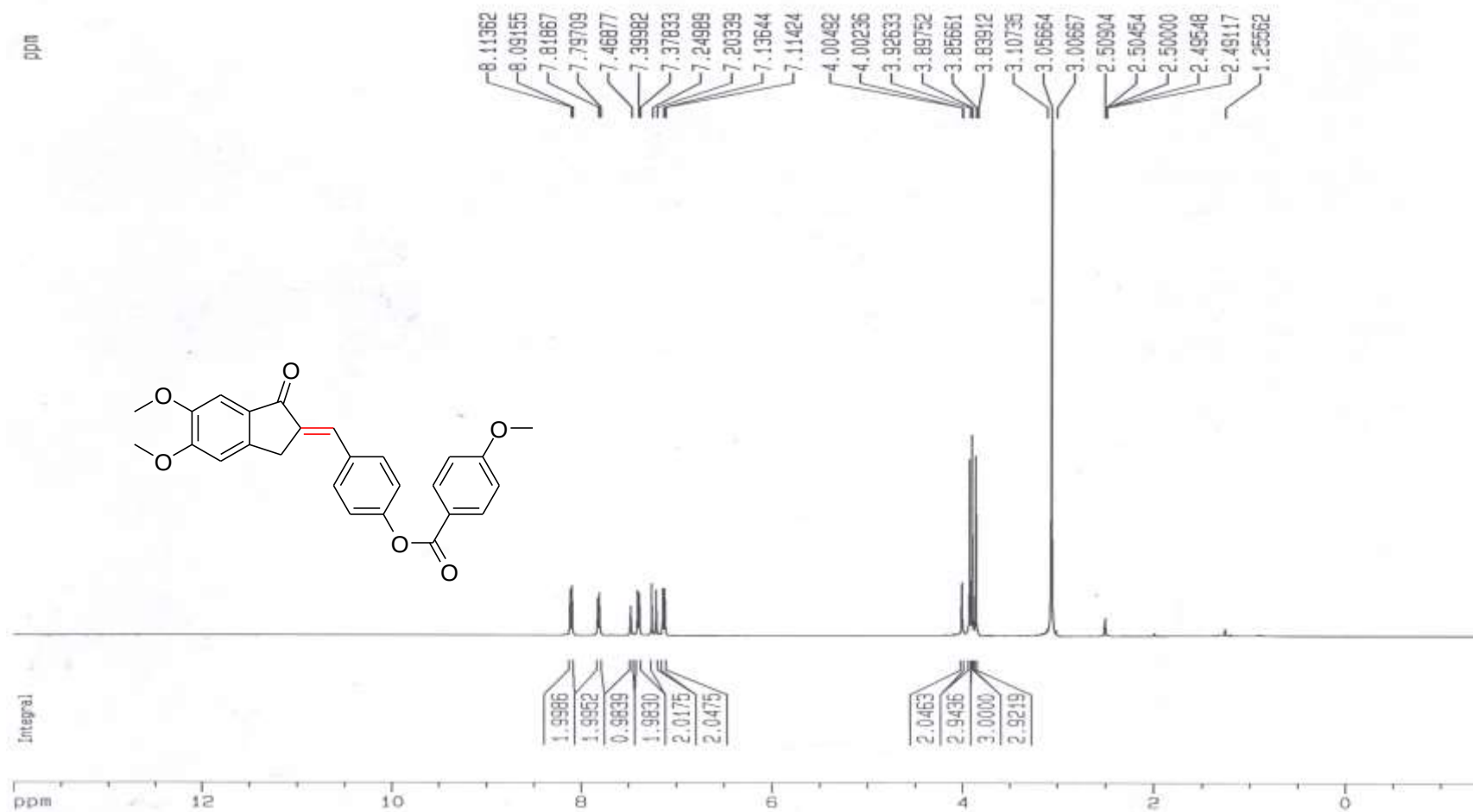


Fig.S3. 4-((E)-(8,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8c)

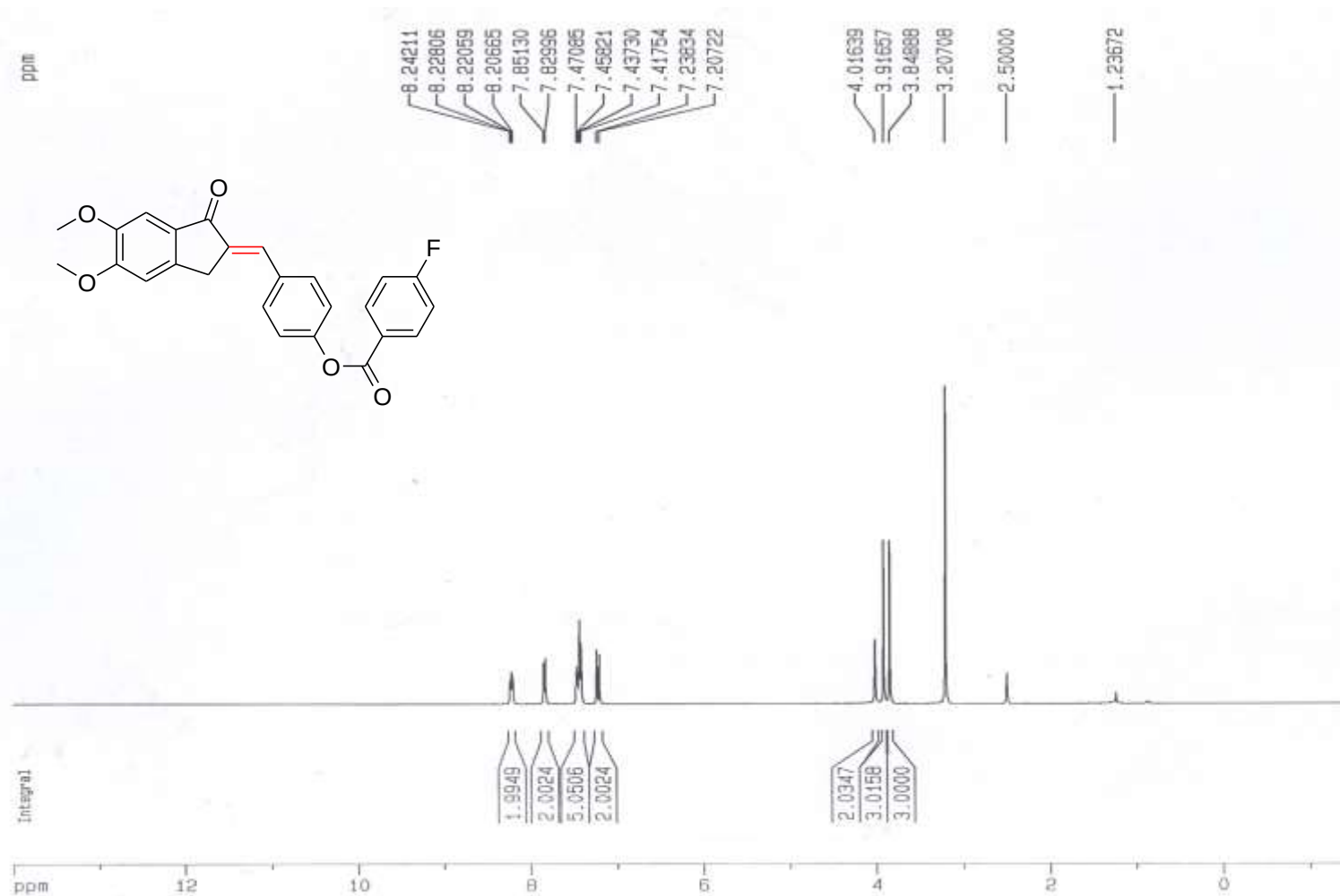


Fig. S4. 4-((E)-(8,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8d)

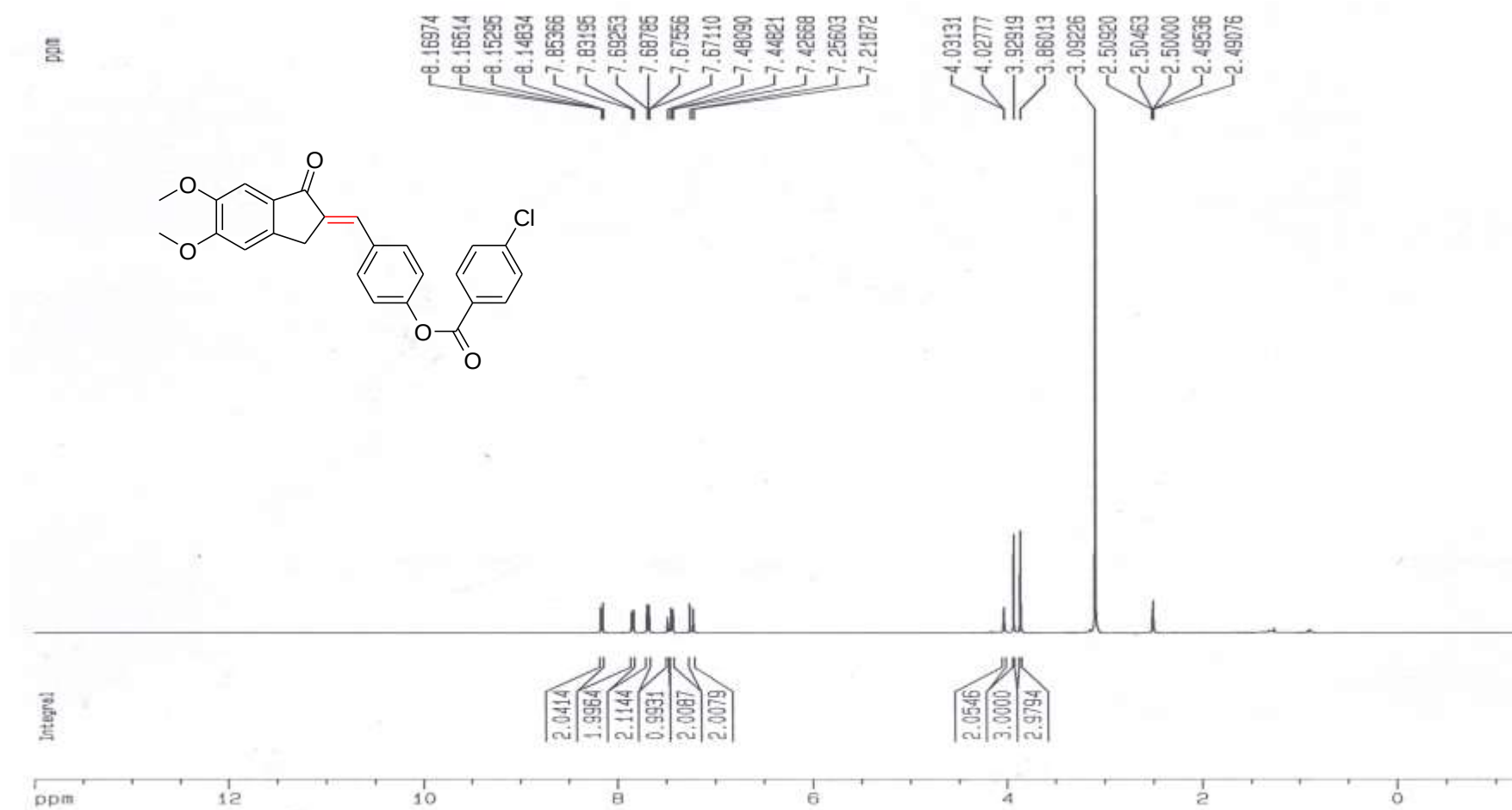


Fig. S8. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-chlorobenzoate (8e)

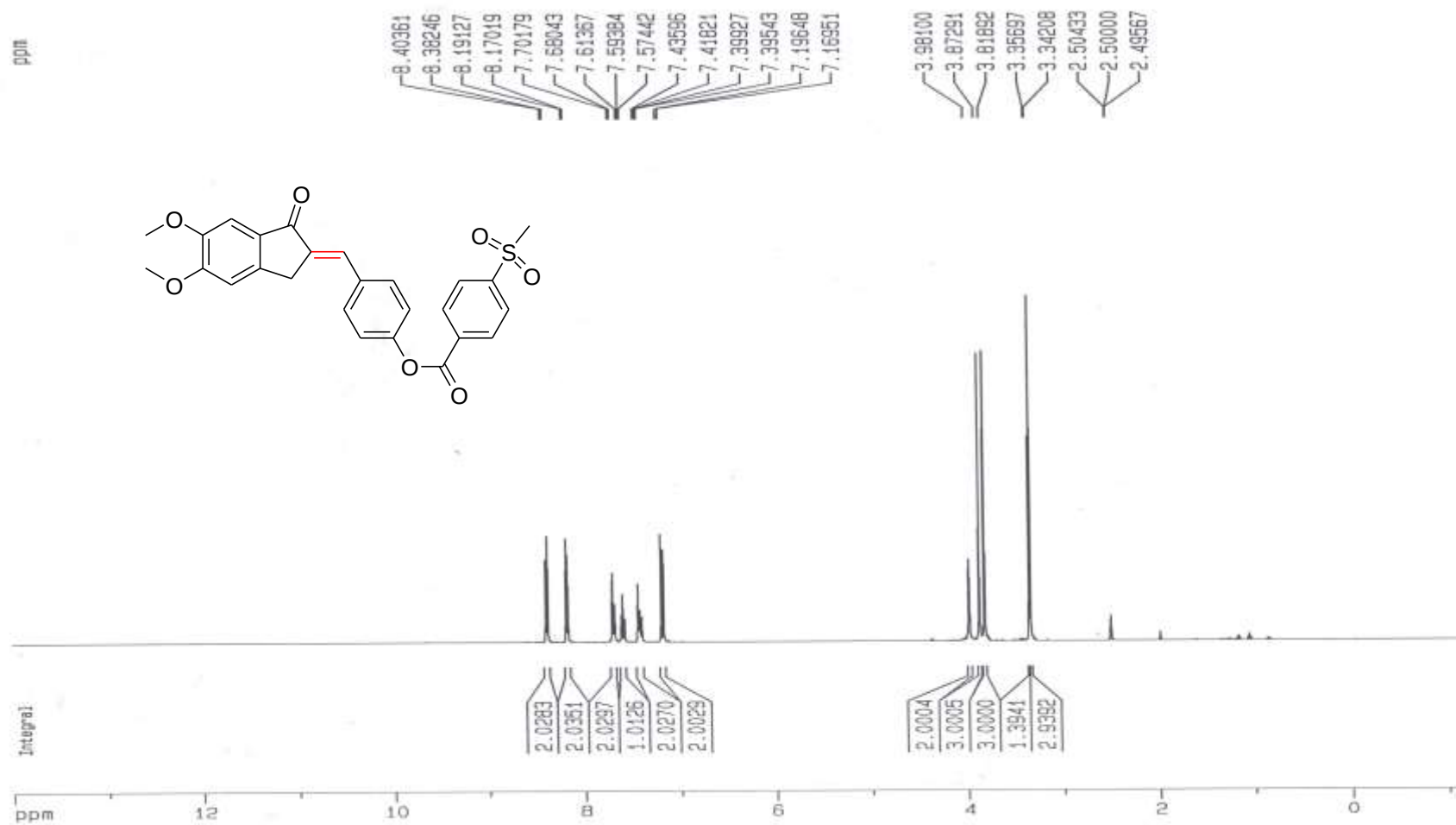


Fig.S6. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-(methylsulfonyl)benzoate (8f)

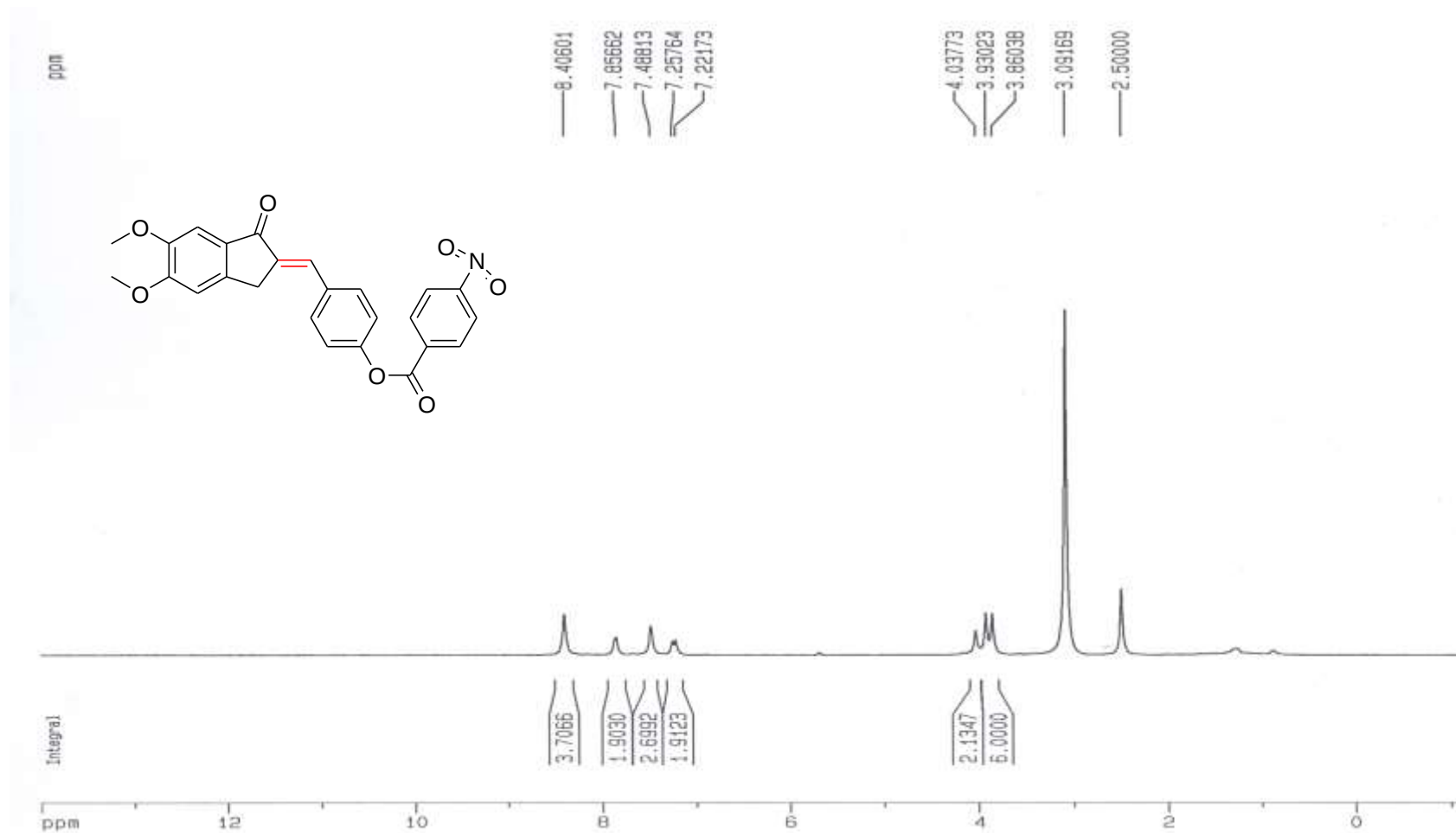


Fig.S7. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-nitrobenzoate (8g)

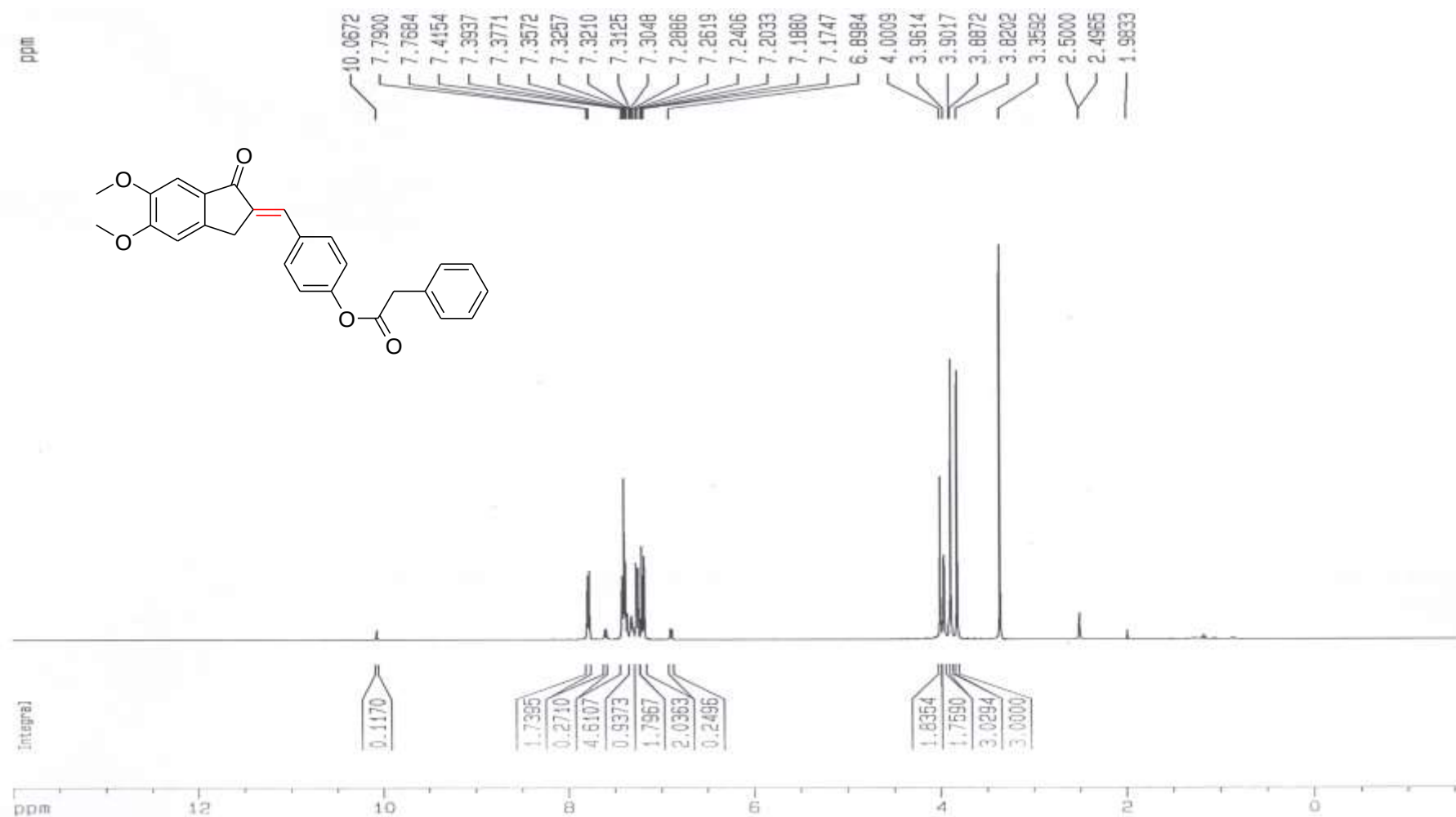


Fig. S8. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 2-phenylacetate(8h)

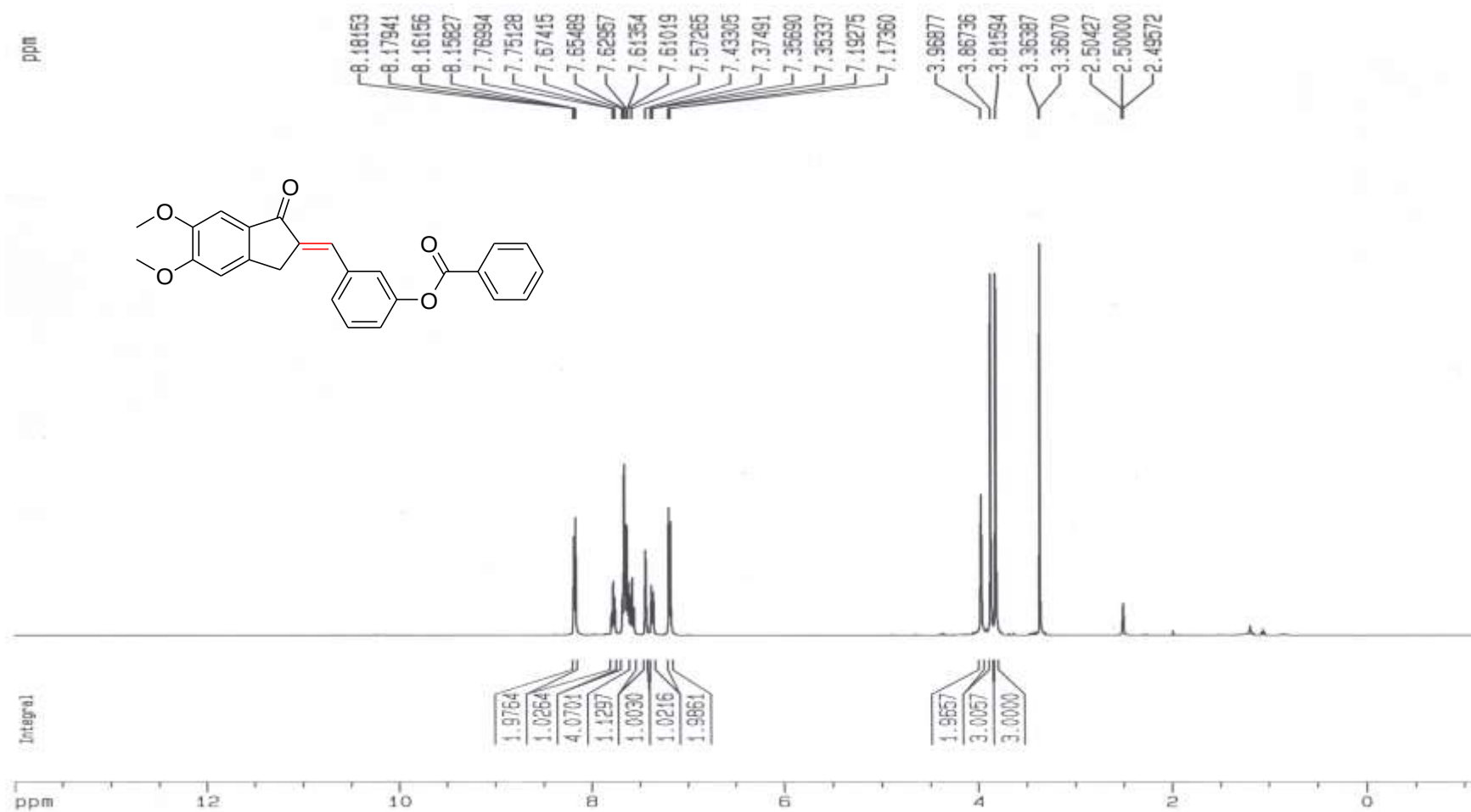


Fig.S9. 3-((E)-((5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8i)

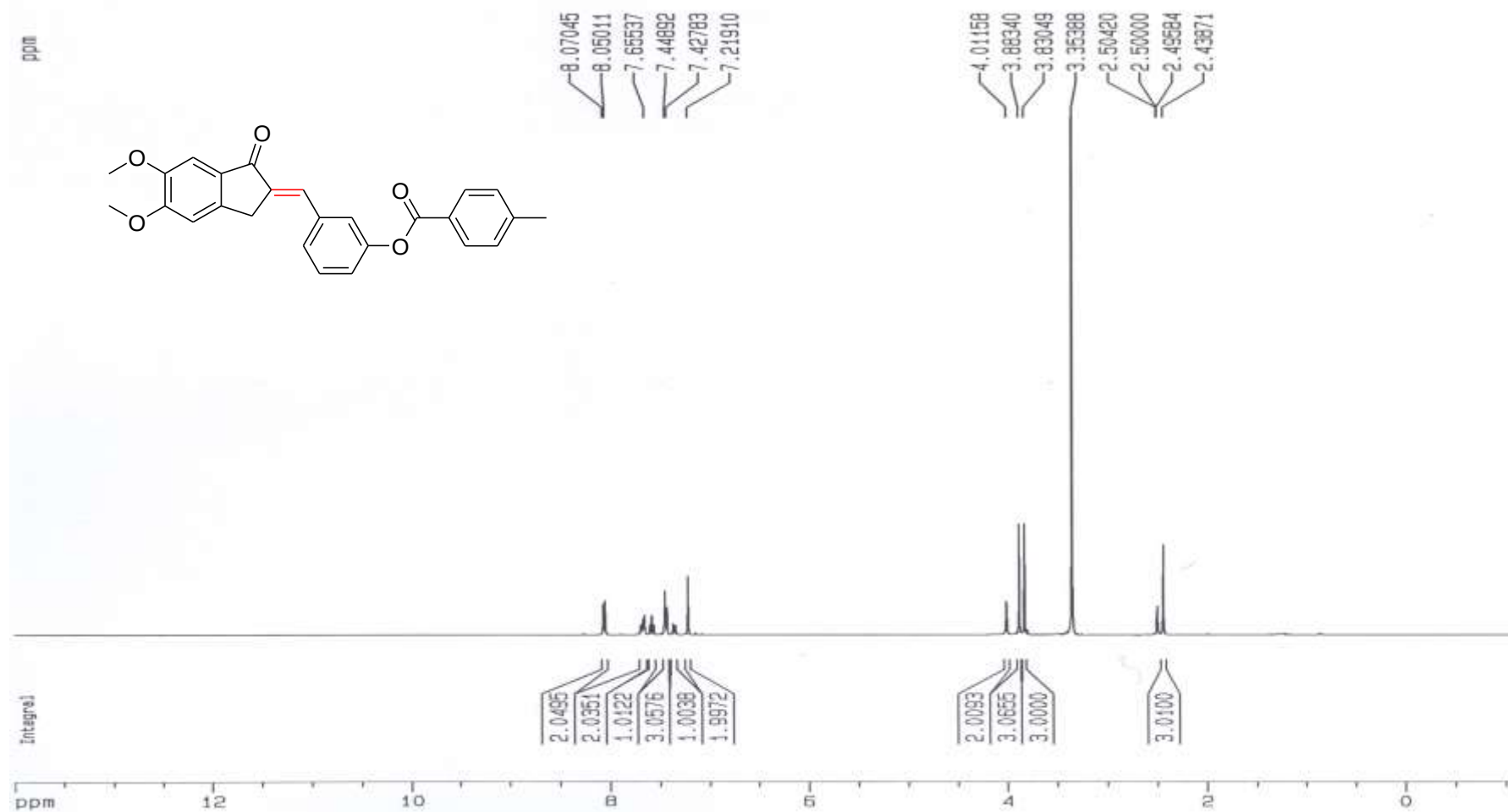


Fig.S10.3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (8j)

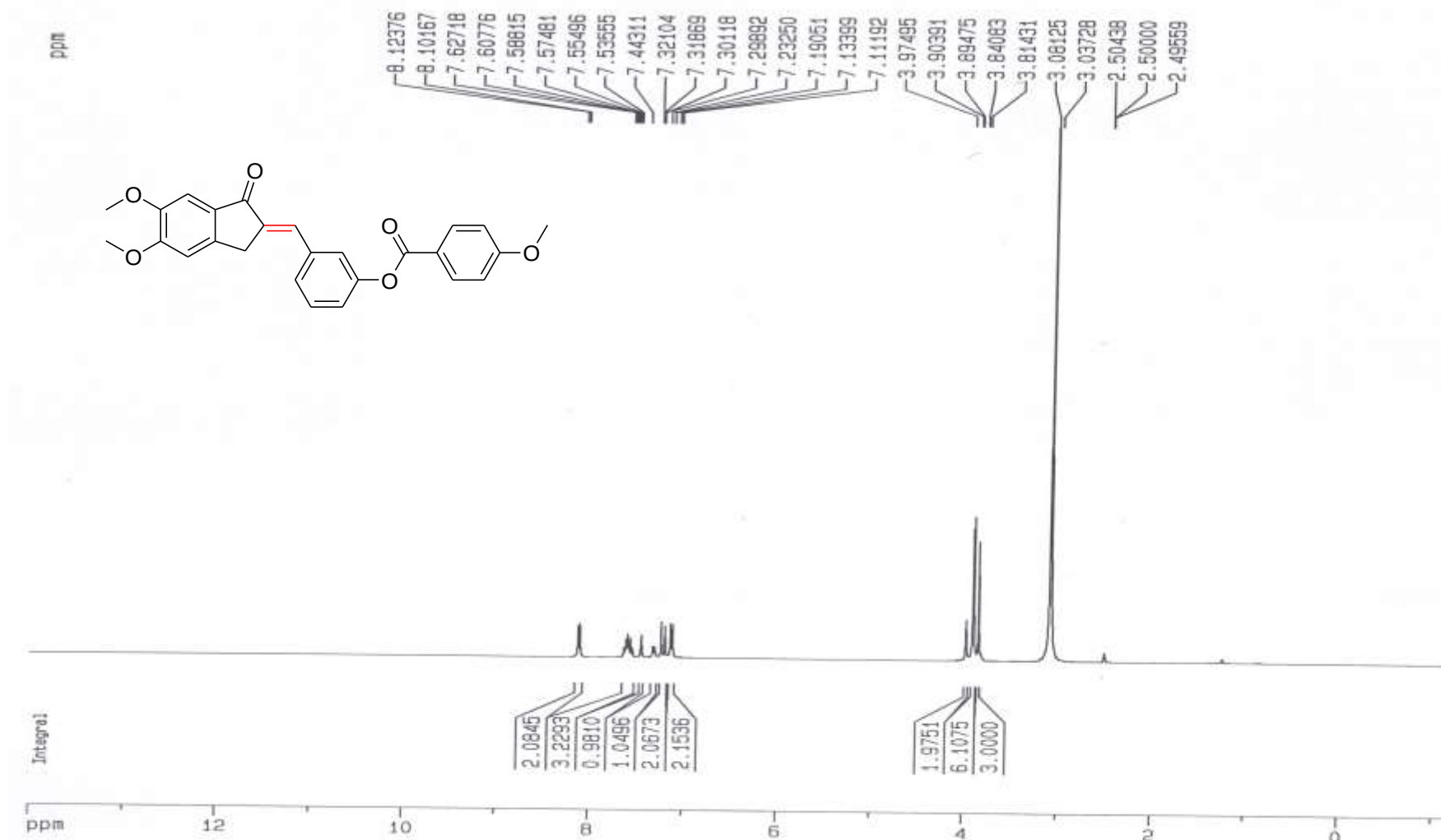


Fig.S11. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8k)

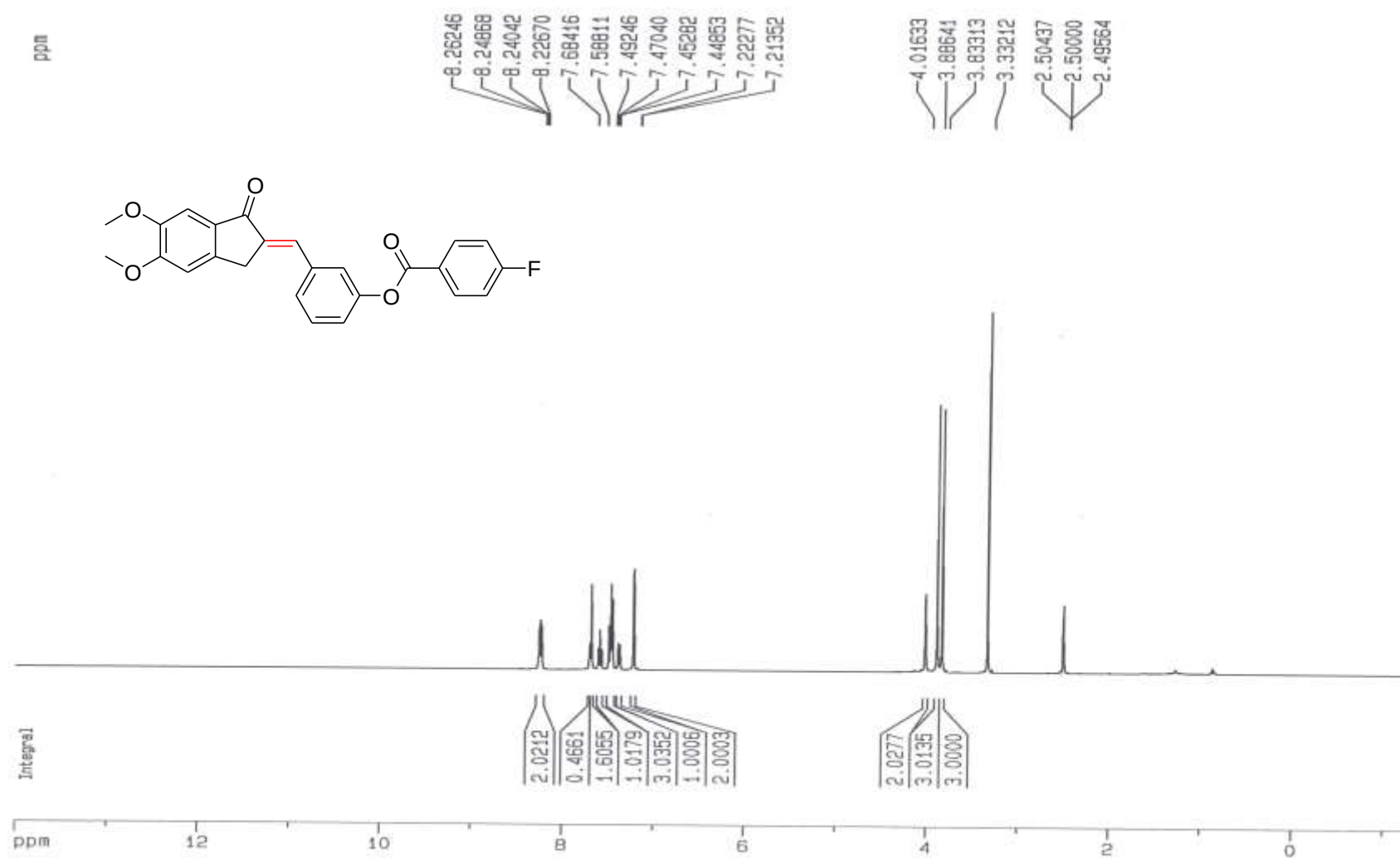


Fig.S12. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8l)

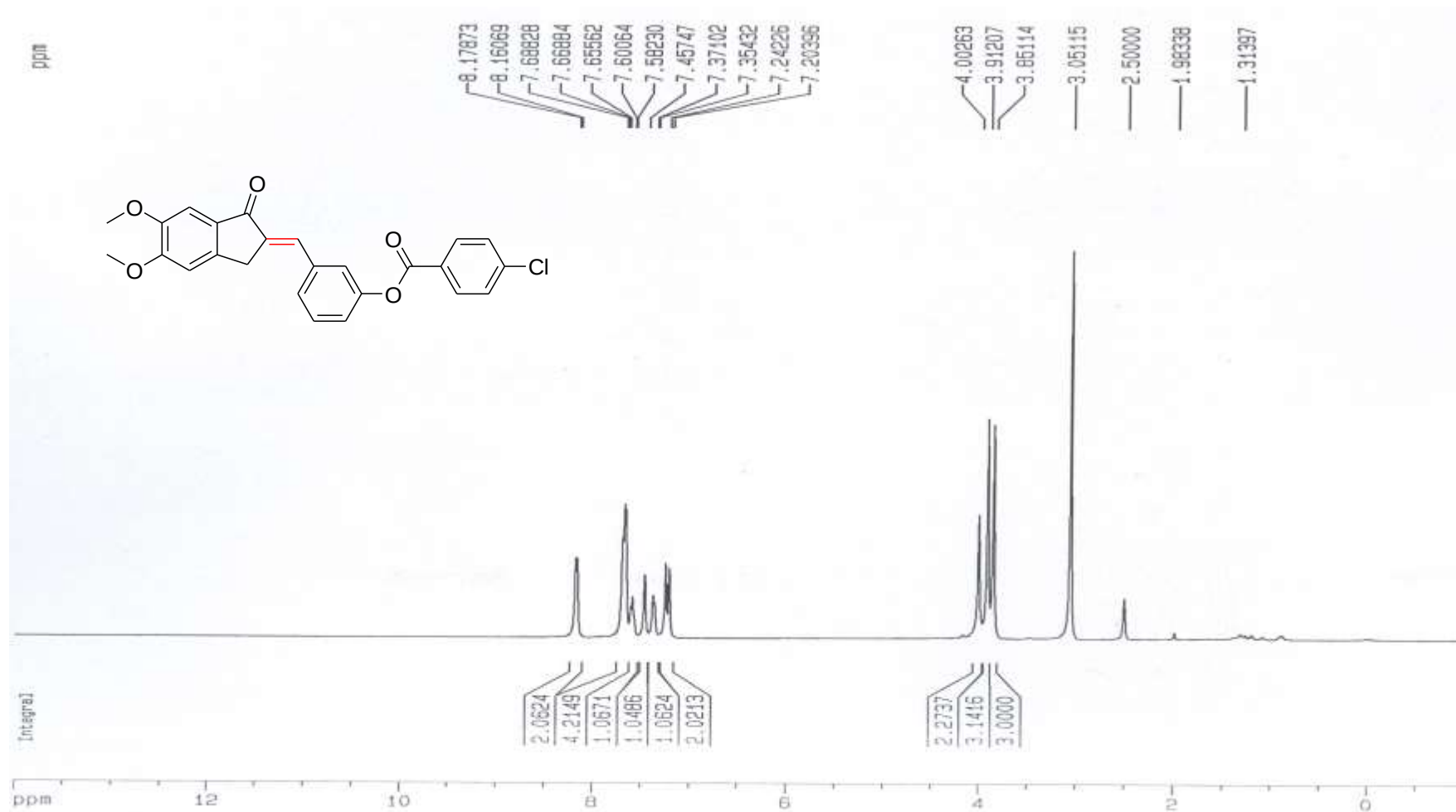


Fig.S13. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-chlorobenzoate (8m)

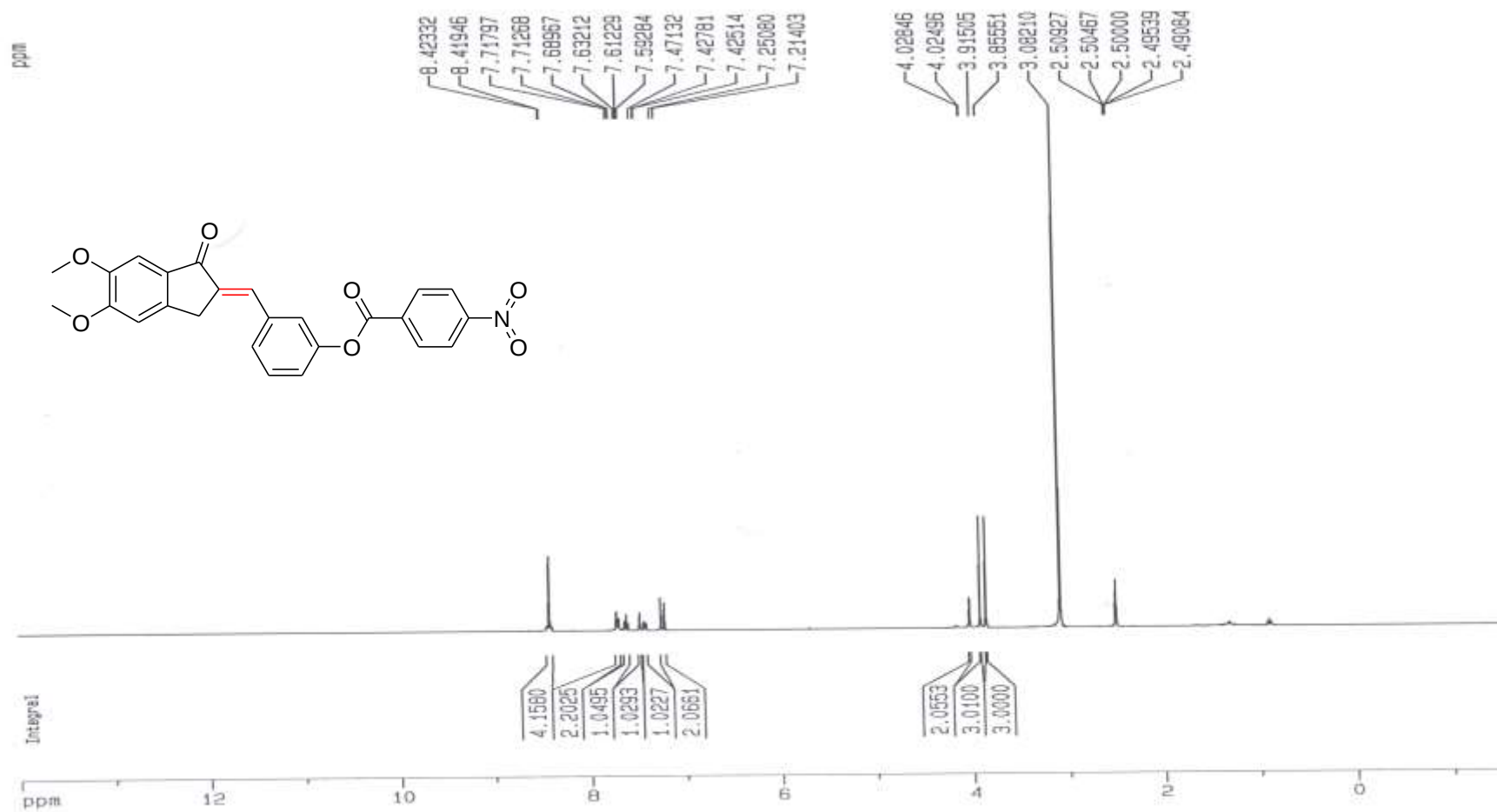


Fig.S14. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-nitrobenzoate (8n)

¹³CNMR spectra

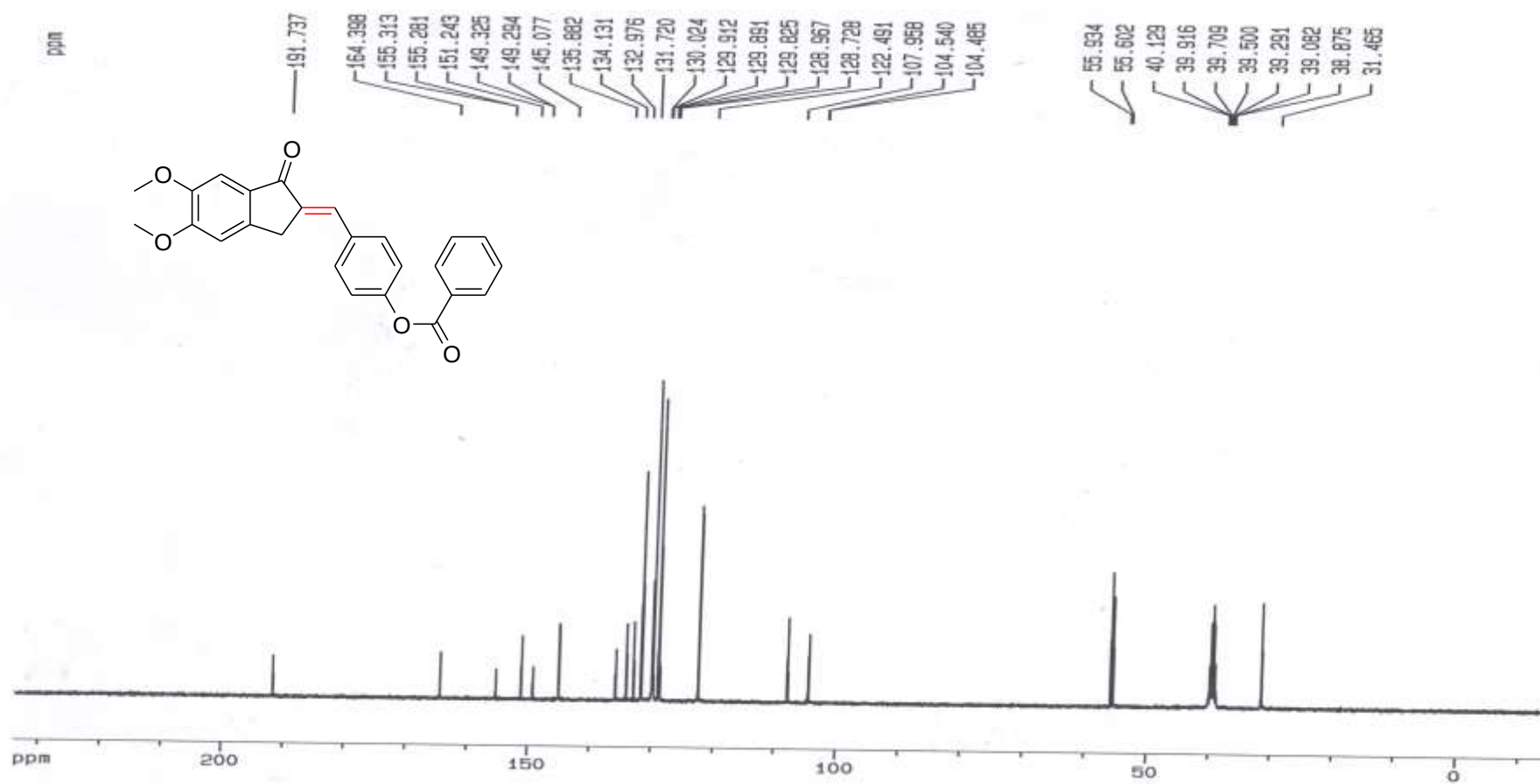


Fig.S15. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8a).

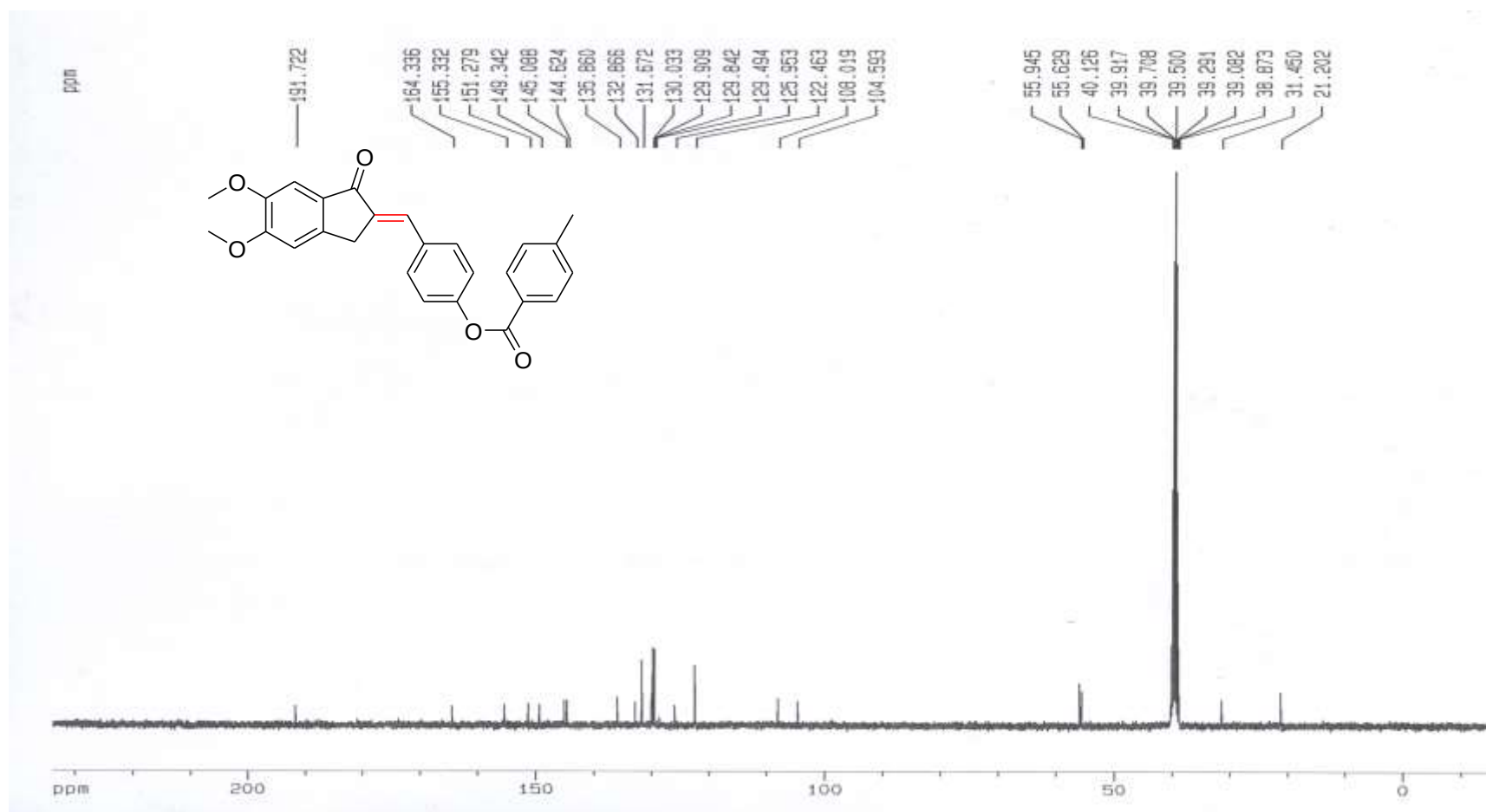


Fig.S16.4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (8b)

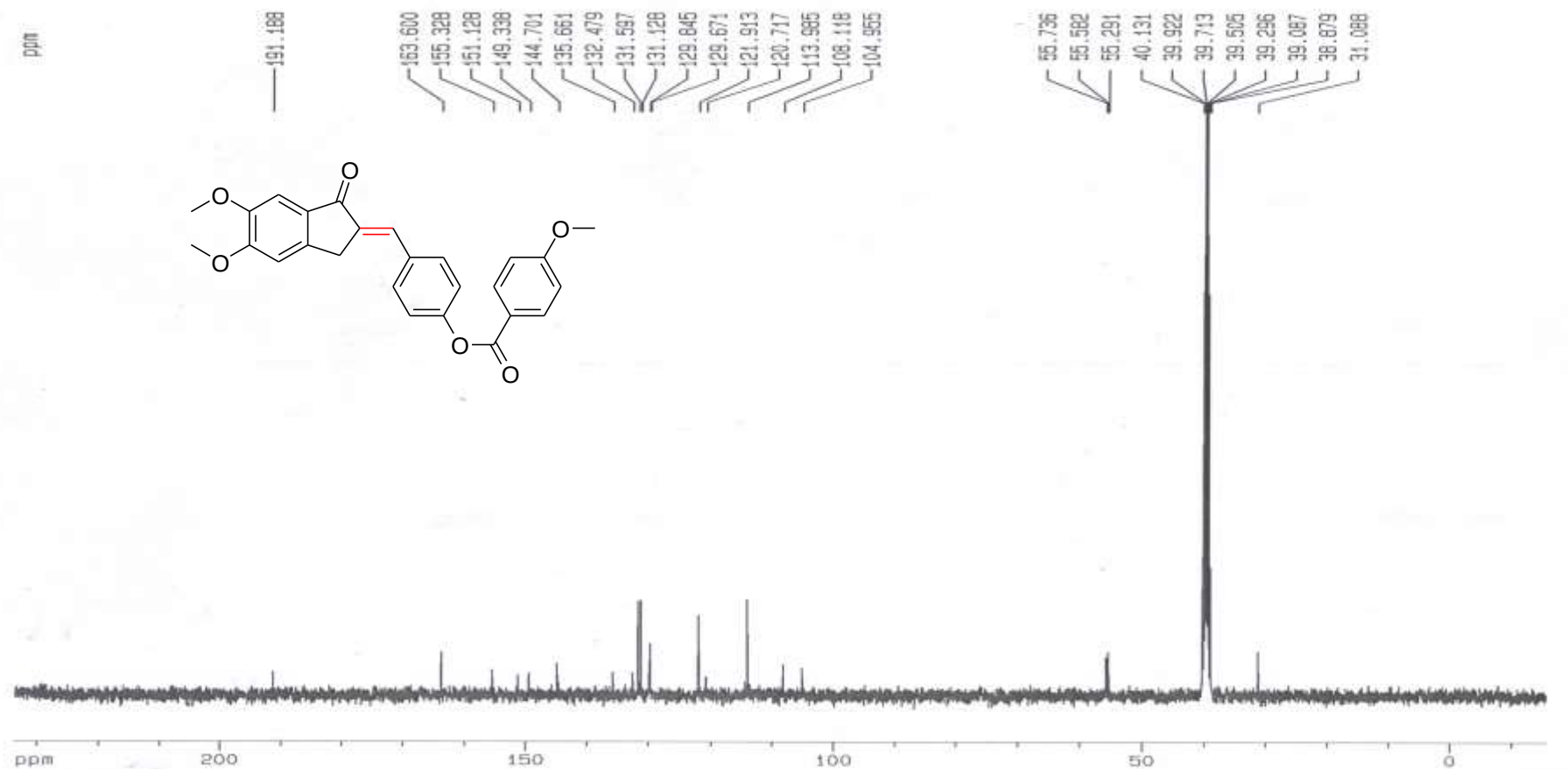


Fig.S17. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8c)

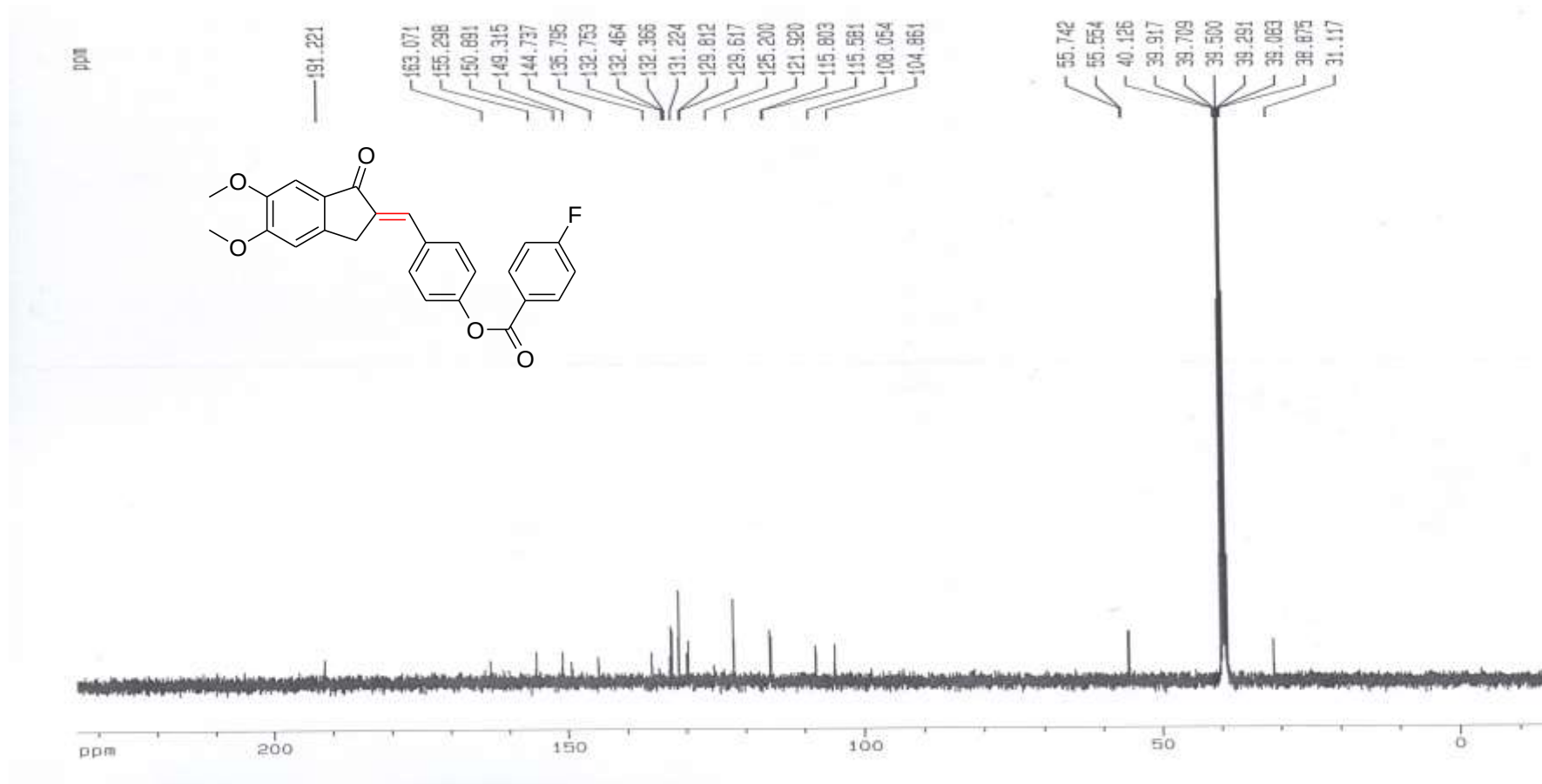


Fig. S17. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8d)

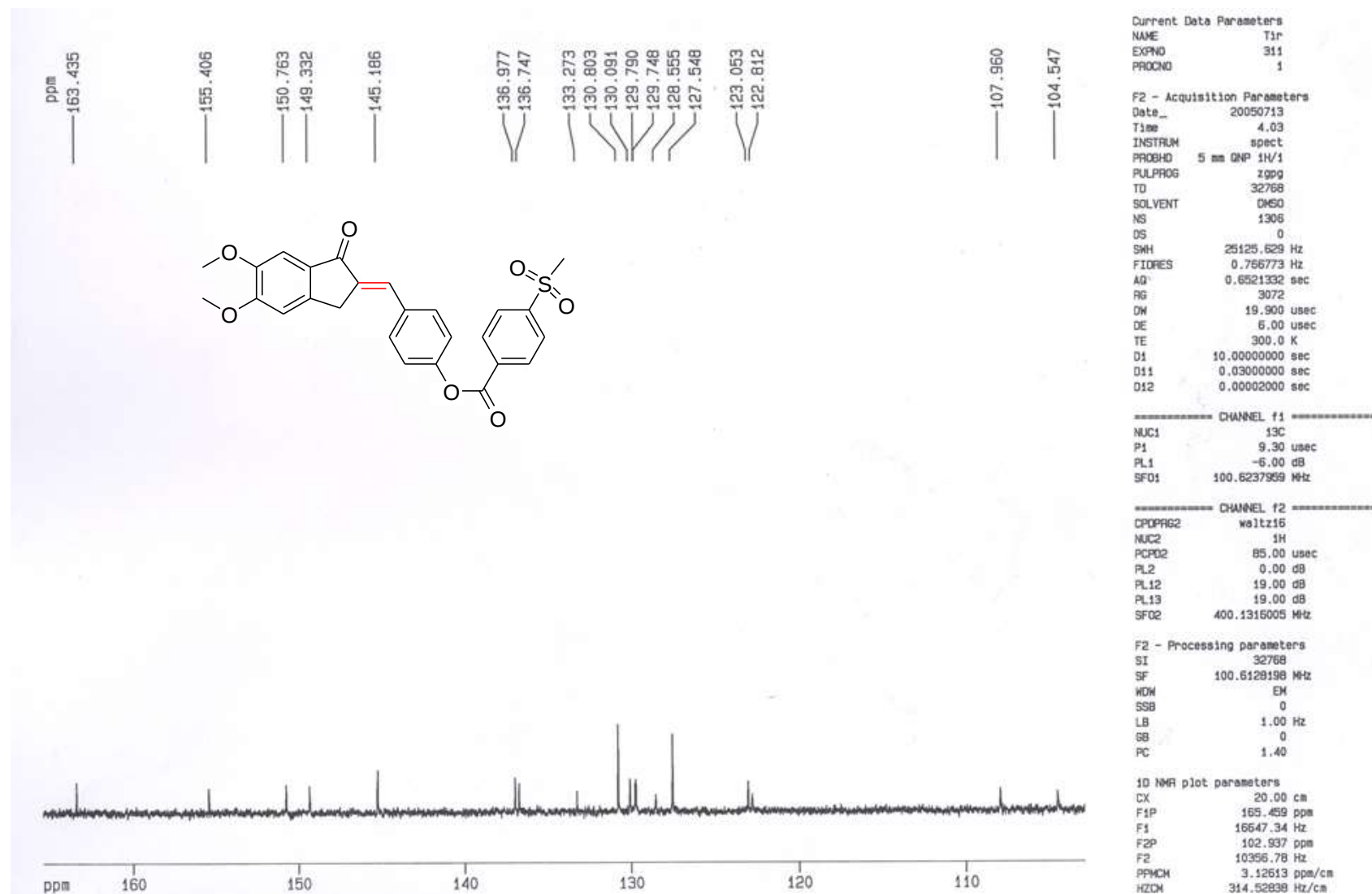


Fig.S18. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-(methylsulfonyl)benzoate (8f)

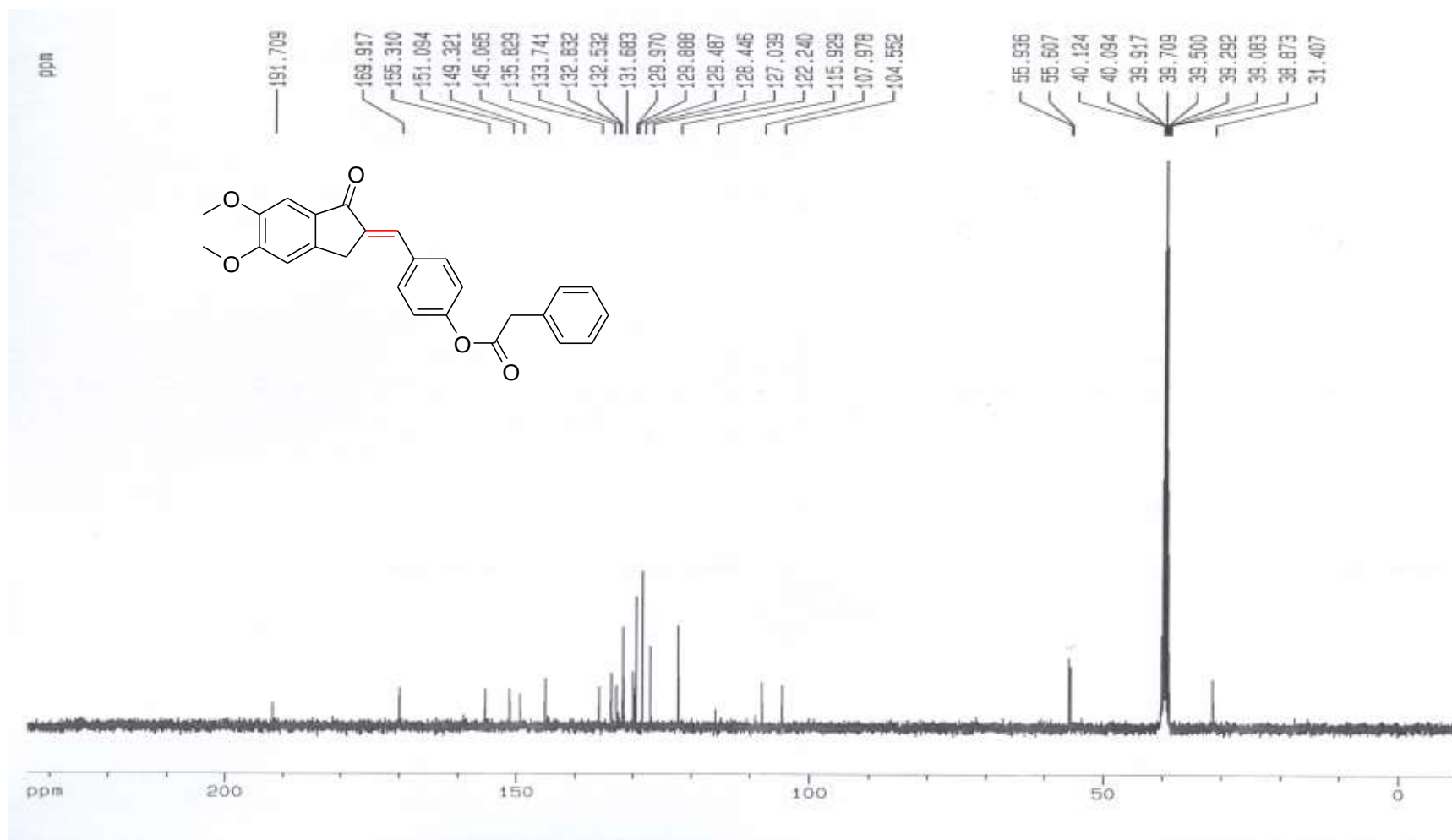


Fig. S19. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 2-phenylacetate(8h)

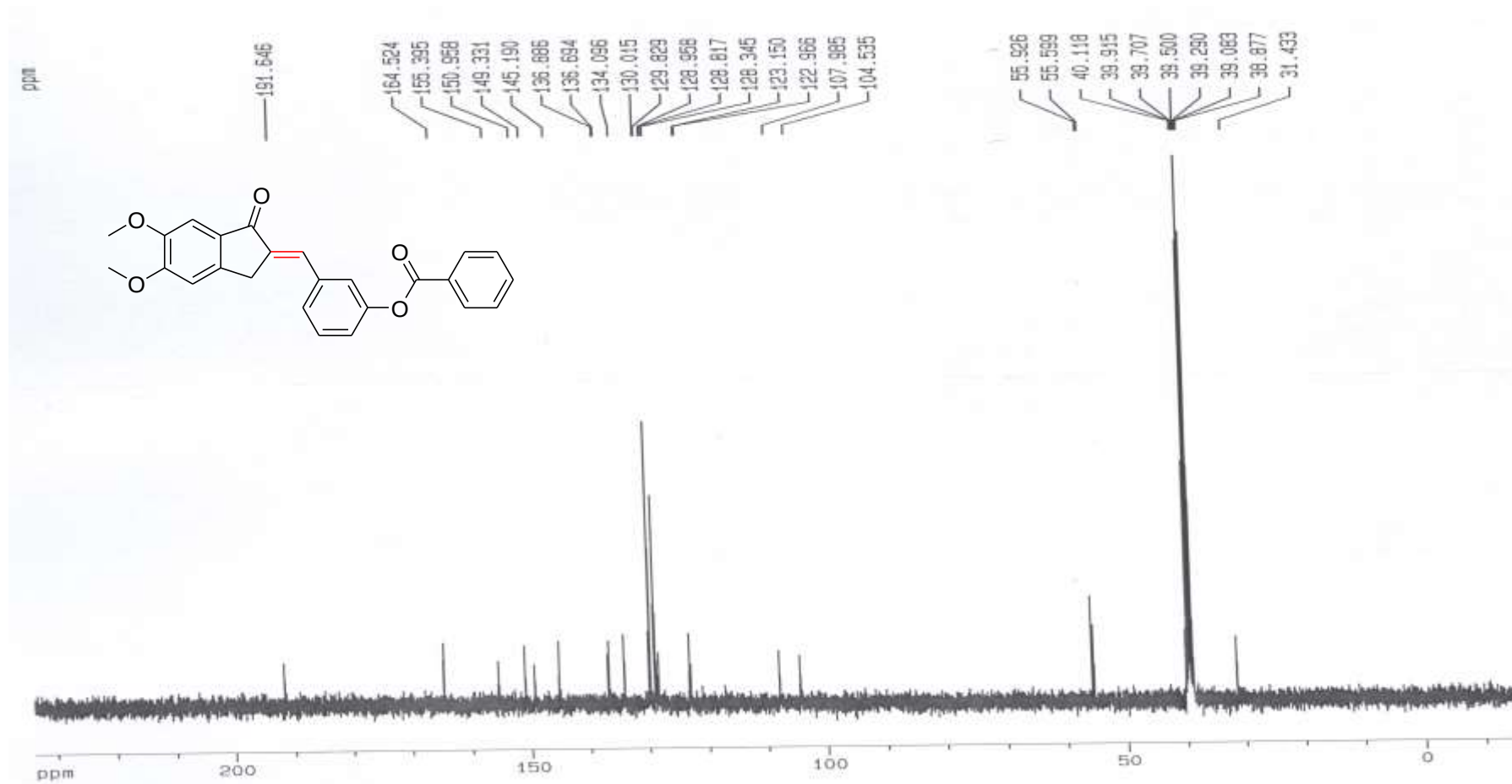


Fig.S20. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8i)

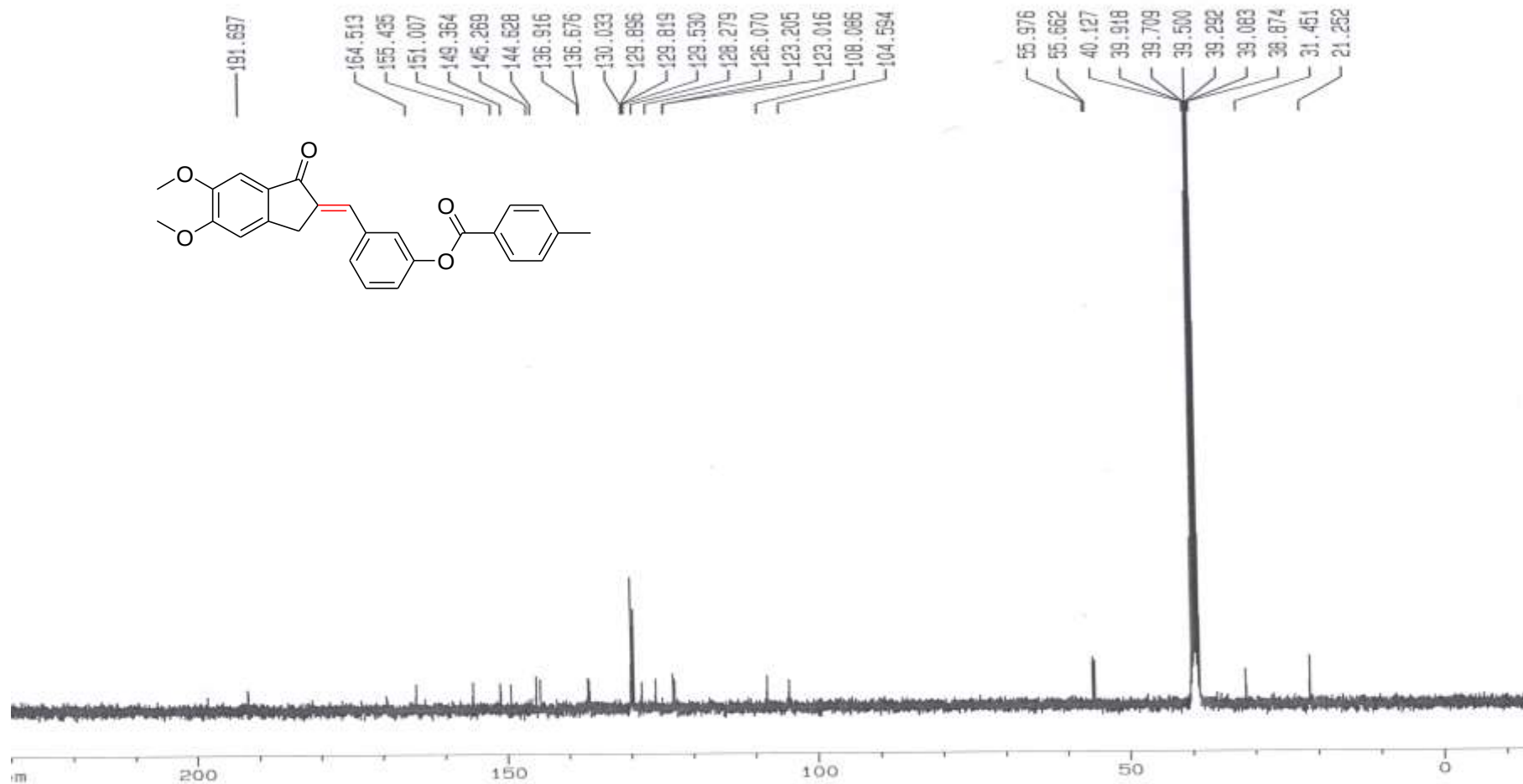


Fig.S21.3-((E)-((5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (8j)

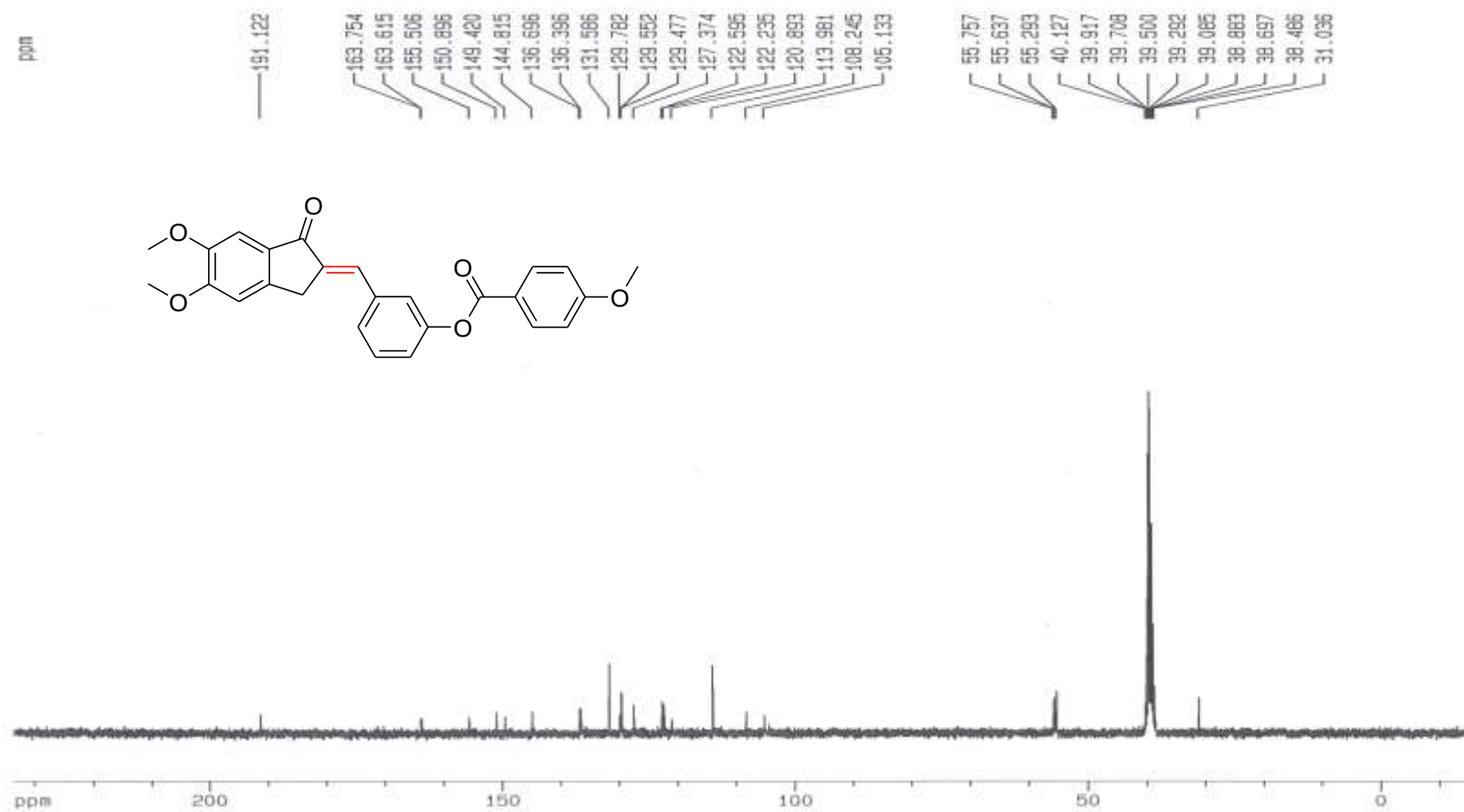


Fig.S22. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8k)

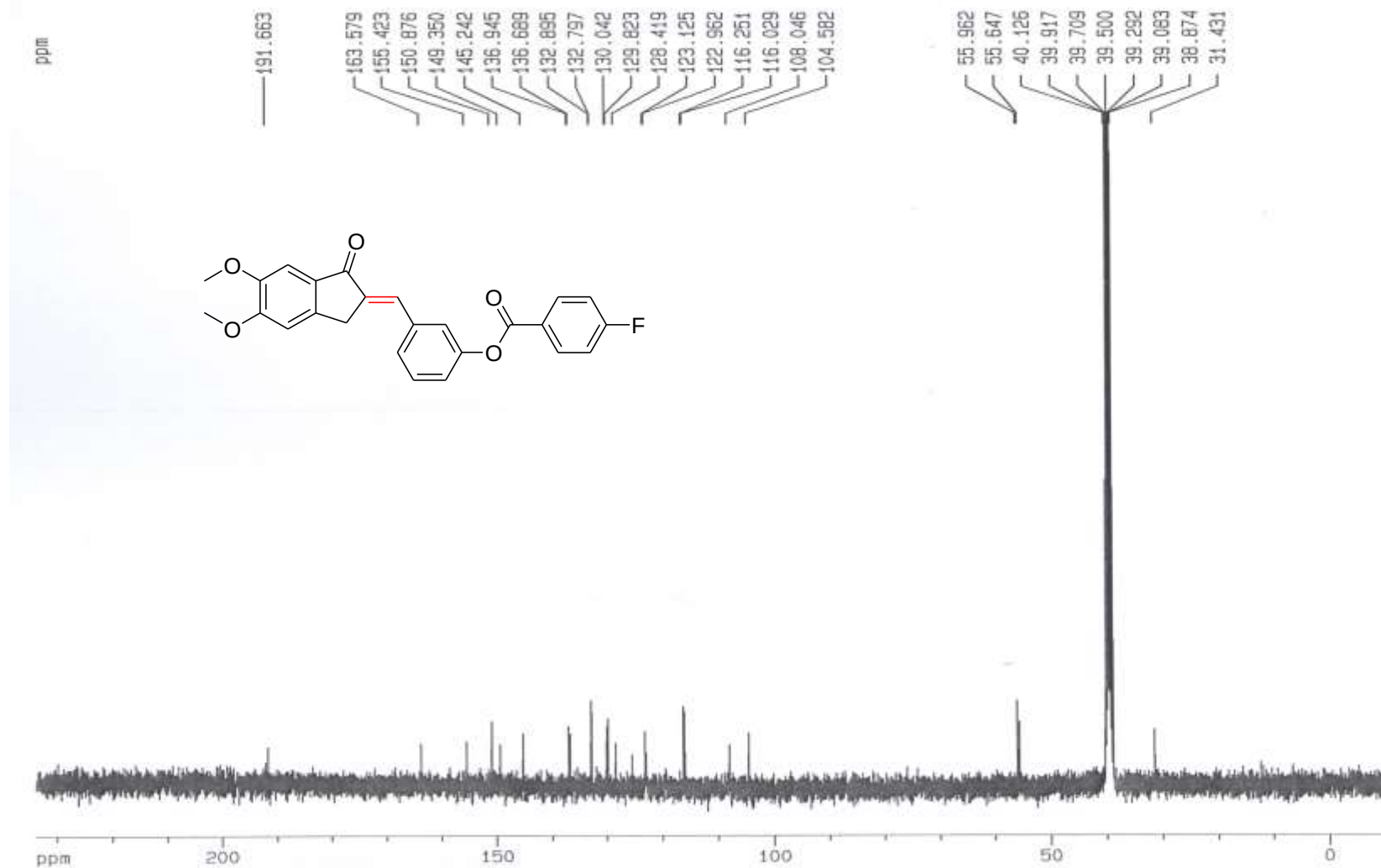


Fig.S23. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8l)

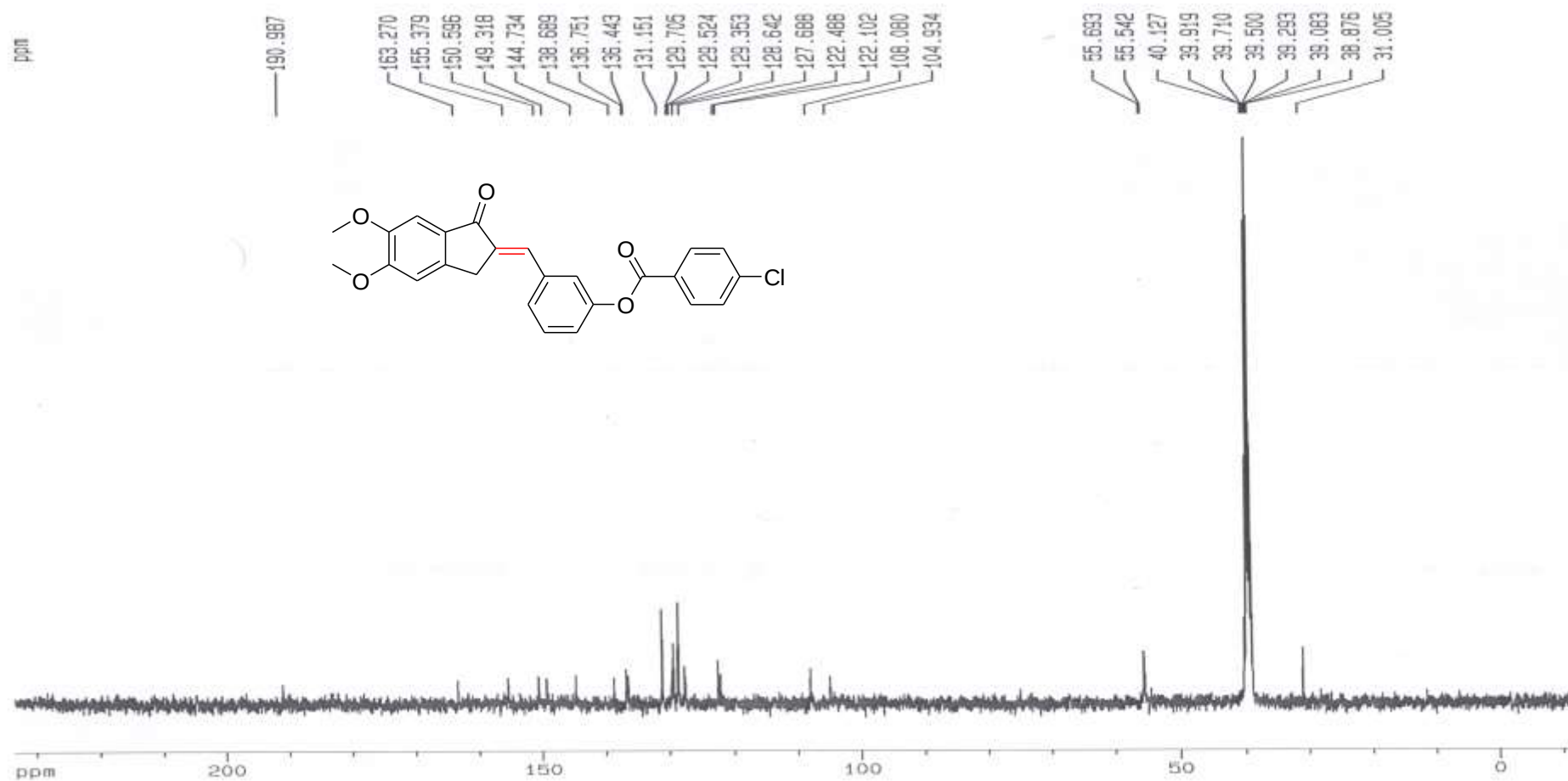


Fig.S24. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-chlorobenzoate (8m)

Mass spectra

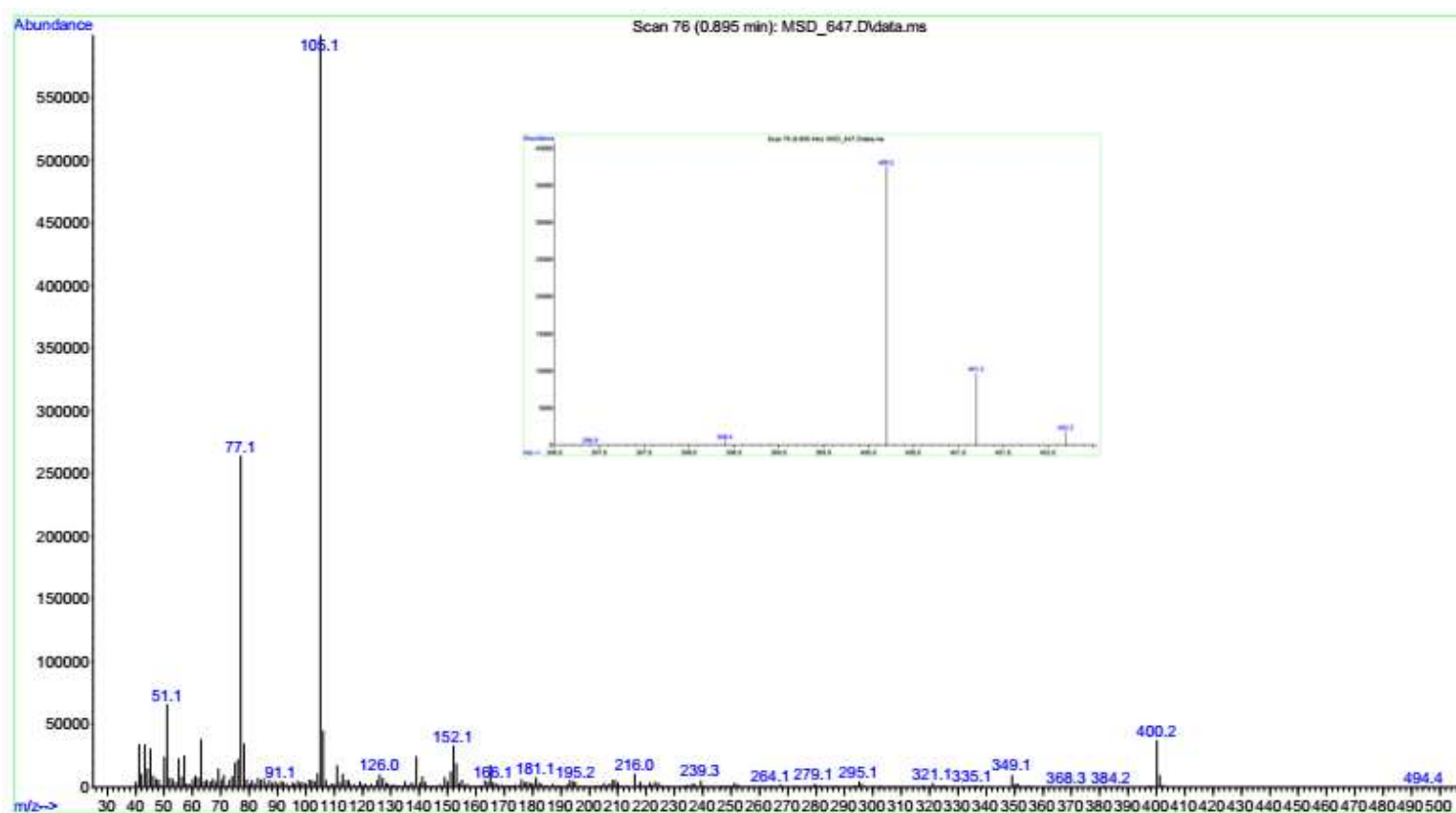


Fig.S25. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl benzoate (**8a**).

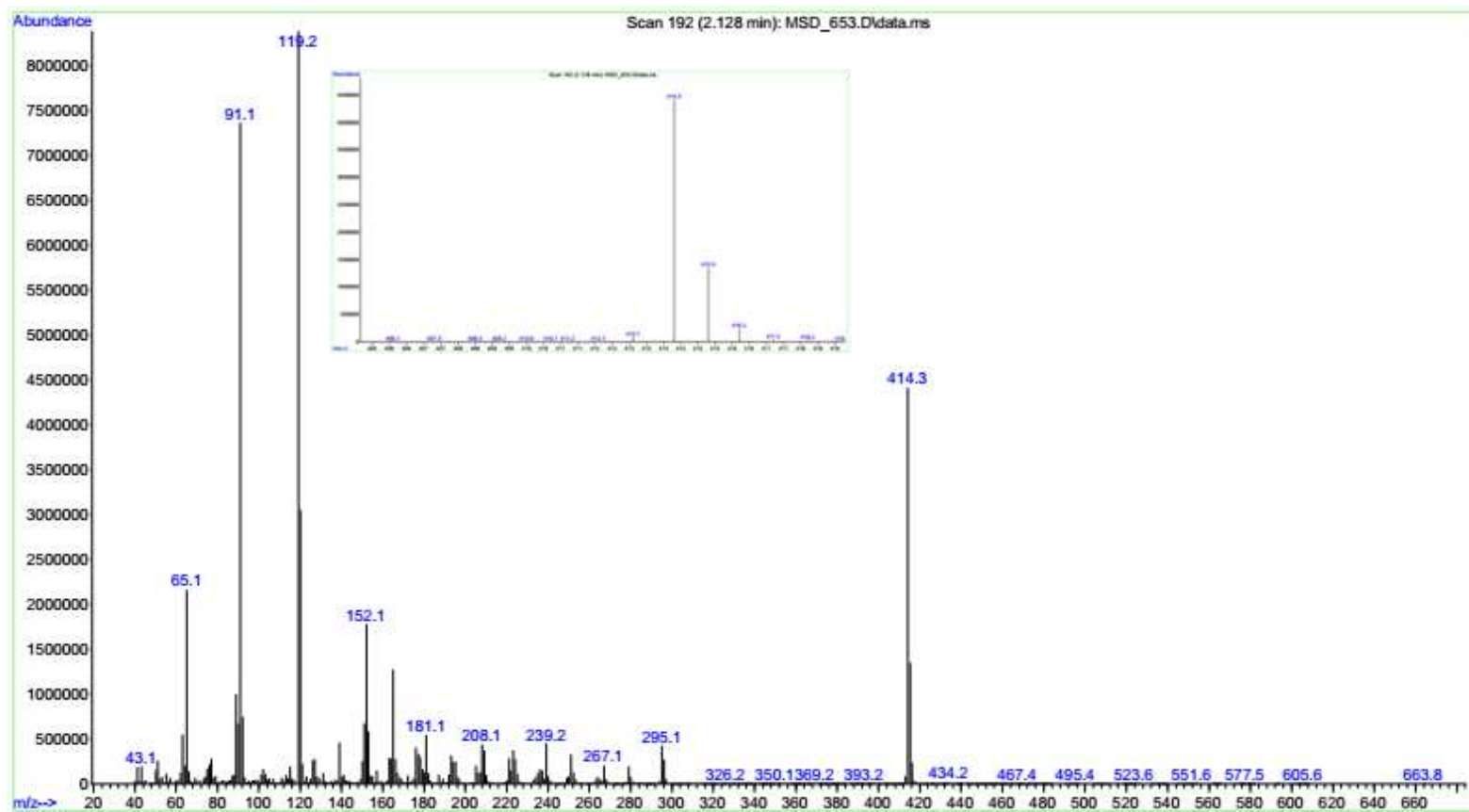


Fig.S26.4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (8b)

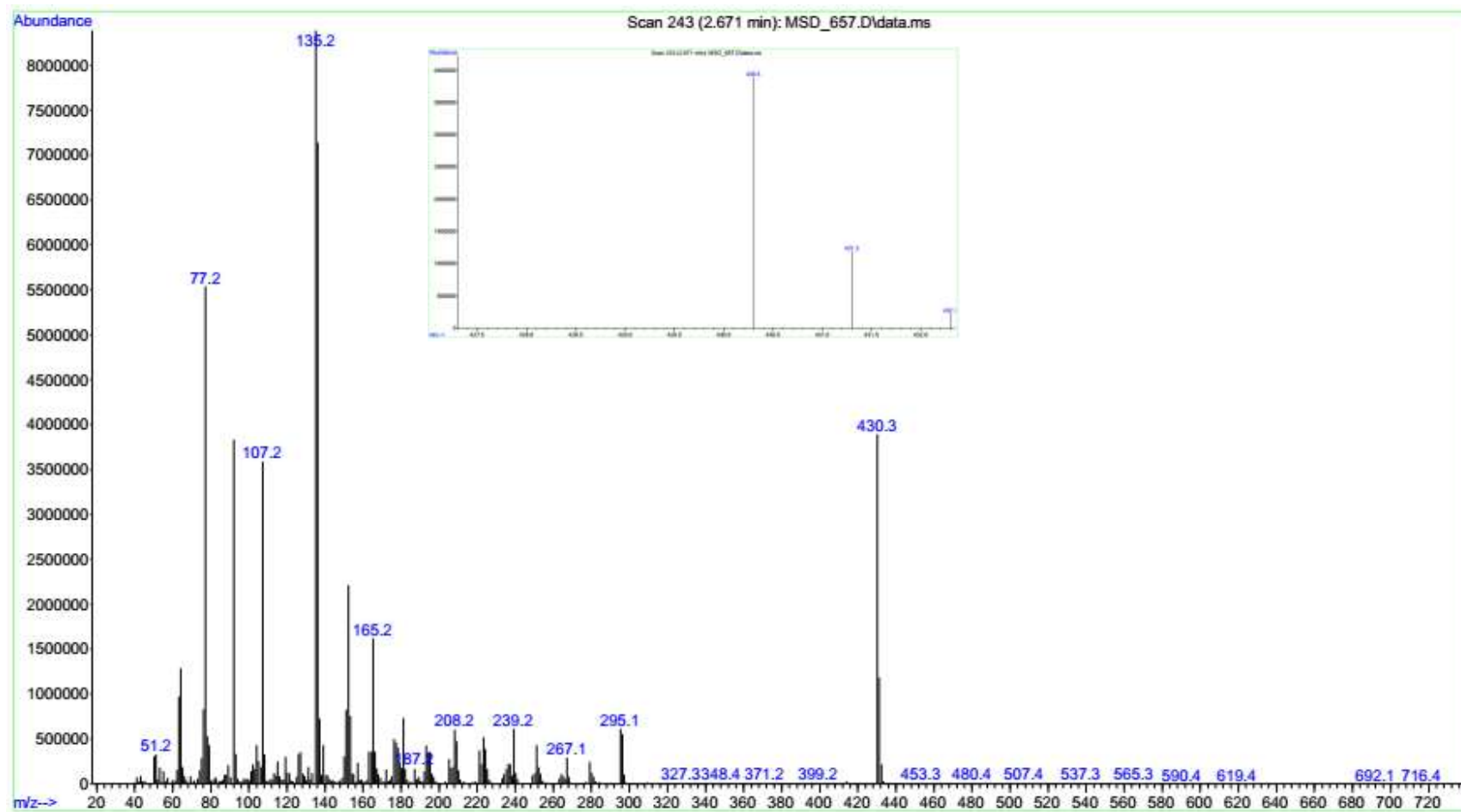


Fig.S27. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8c)

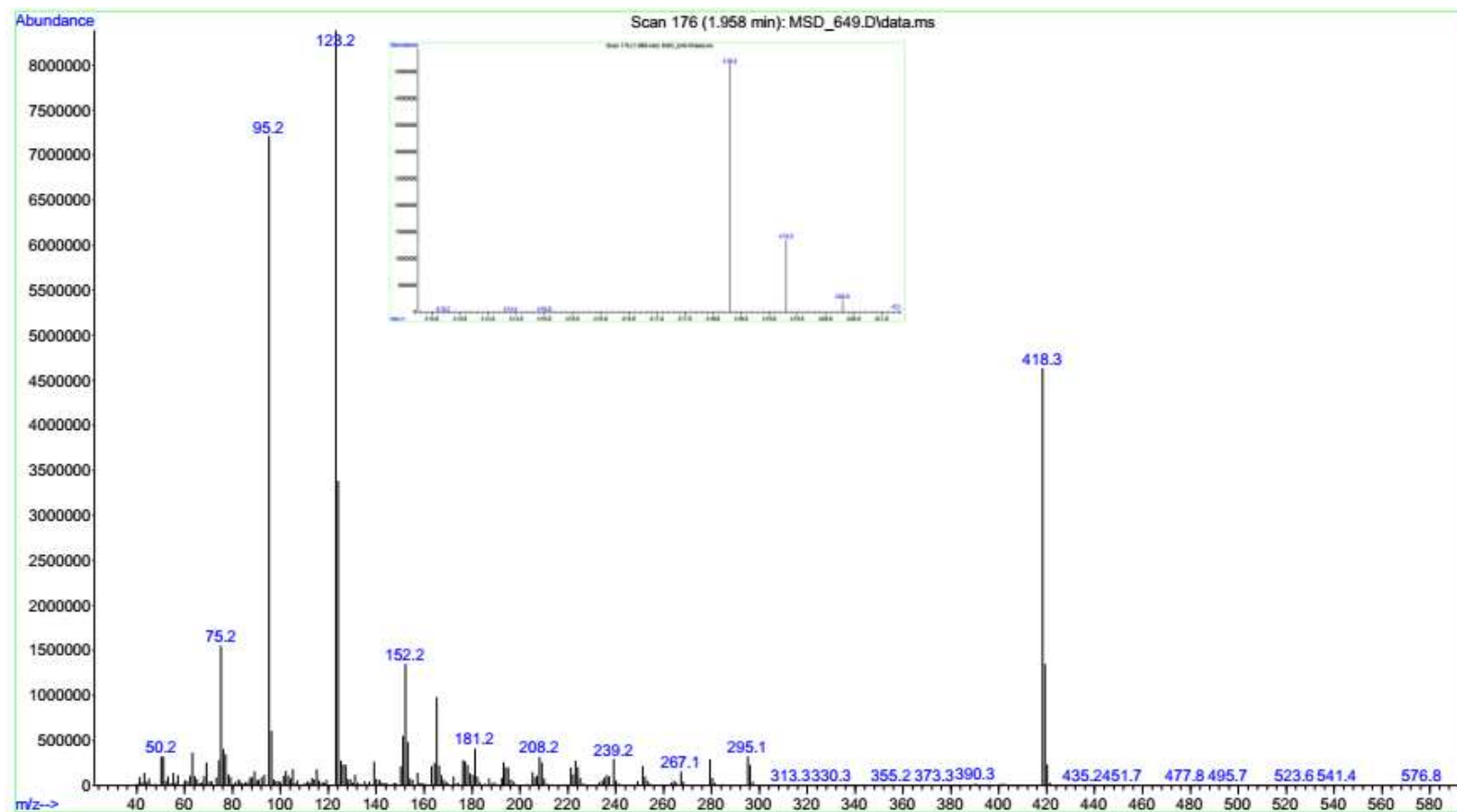


Fig. S28. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-fluorobenzoate (8d)

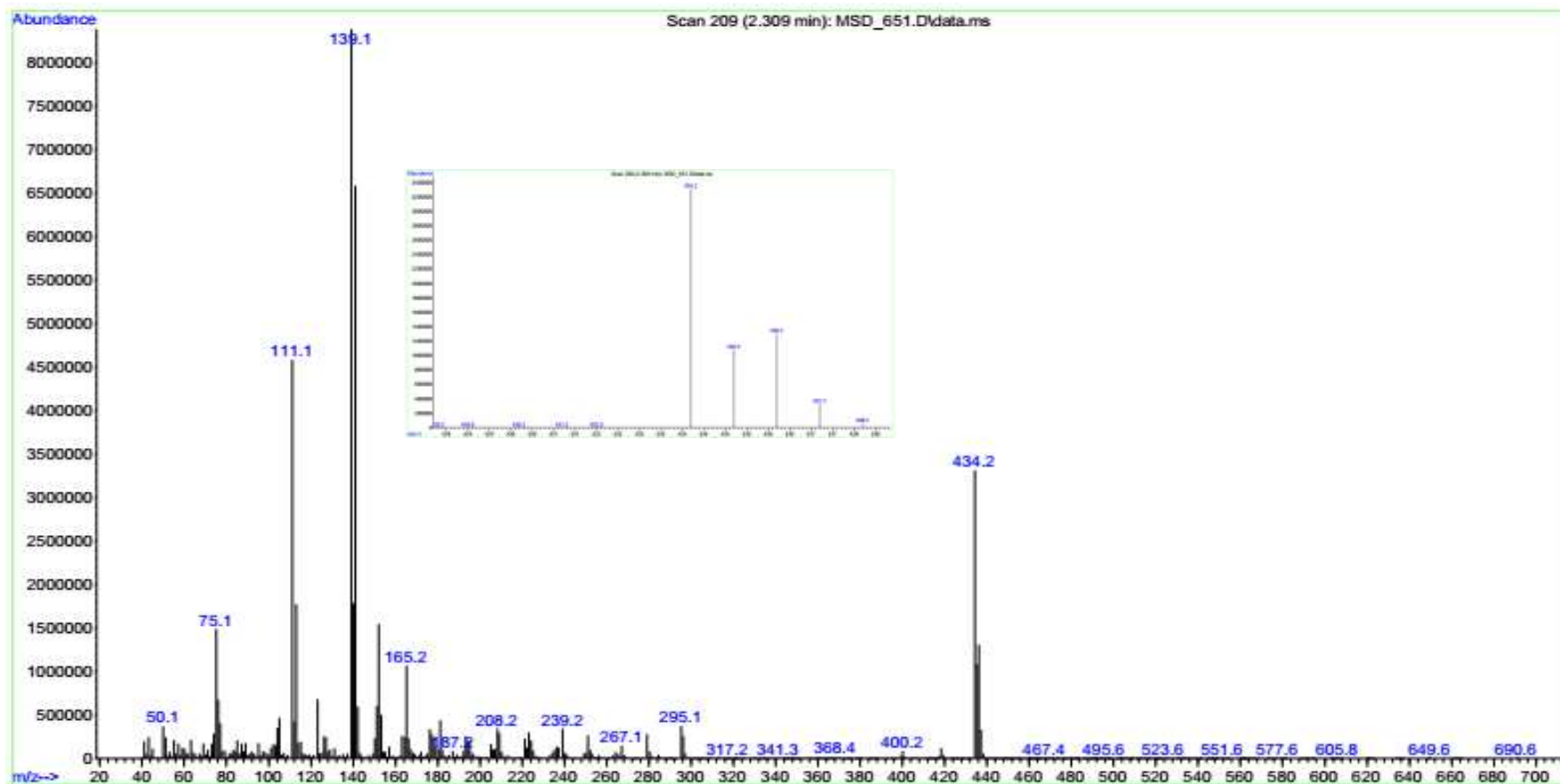


Fig. S29. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-chlorobenzoate (**8e**)

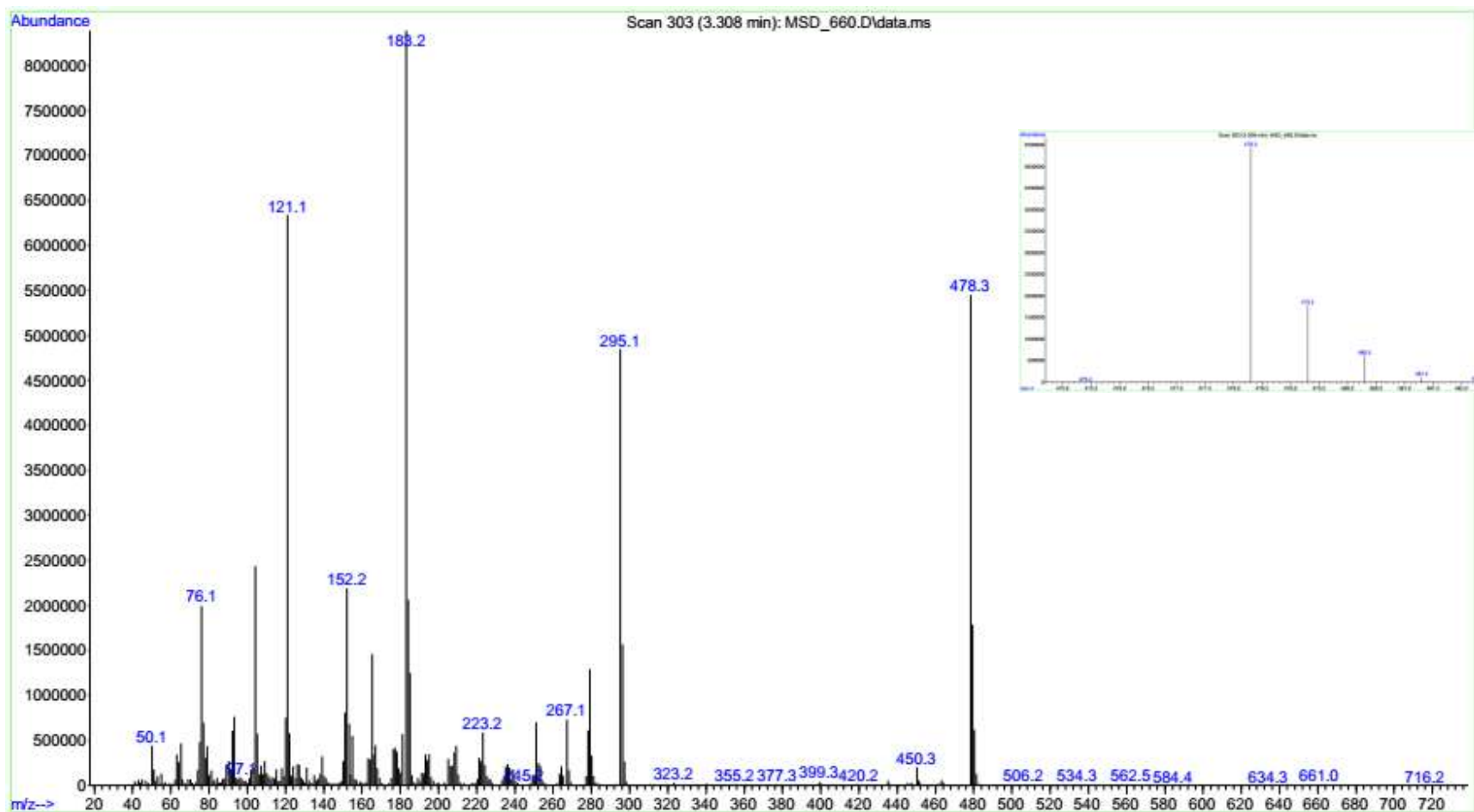


Fig.S30. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-(methylsulfonyl)benzoate (8f)

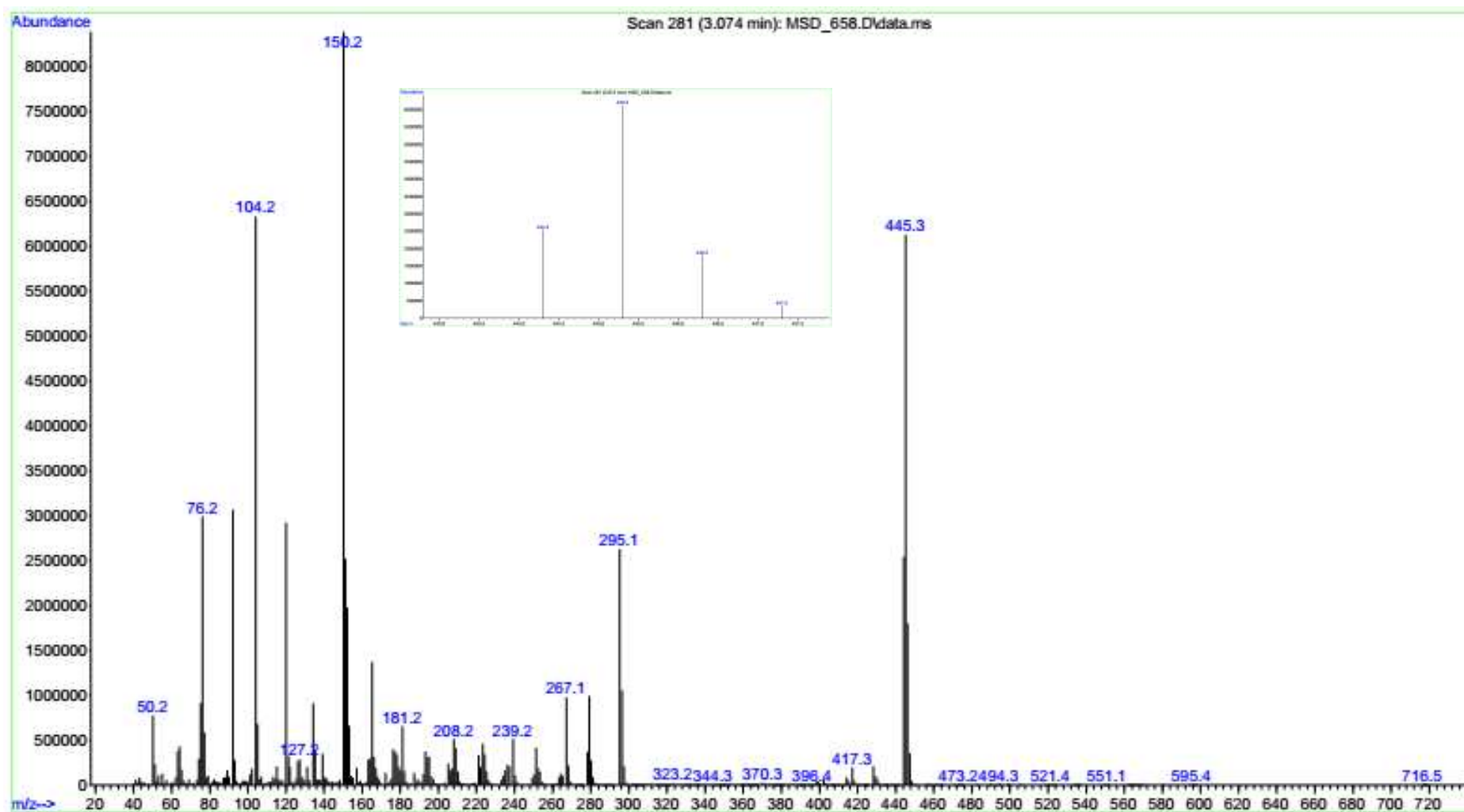


Fig.S31. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-nitrobenzoate (8*g*)

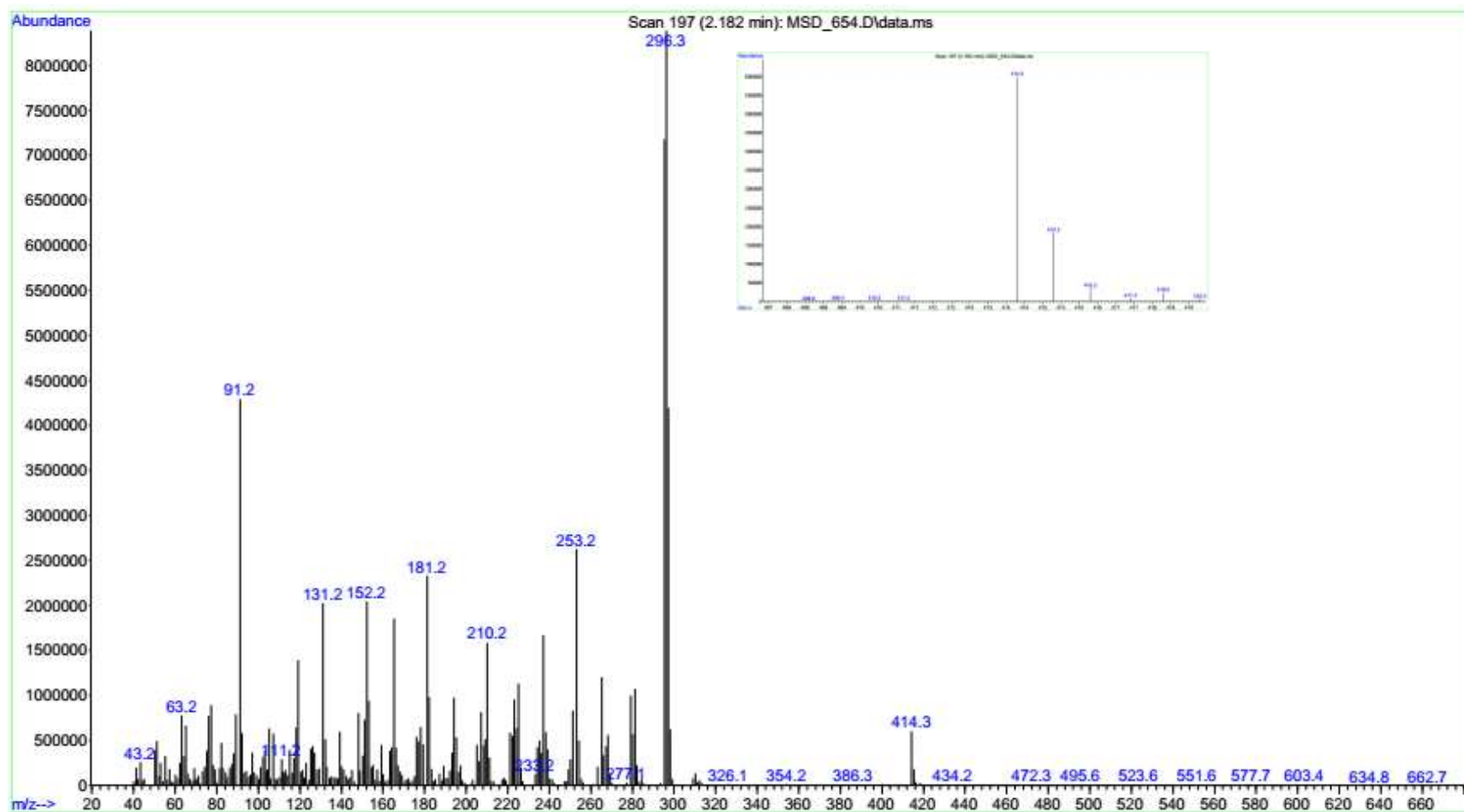


Fig. S32. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 2-phenylacetate(8*h*)

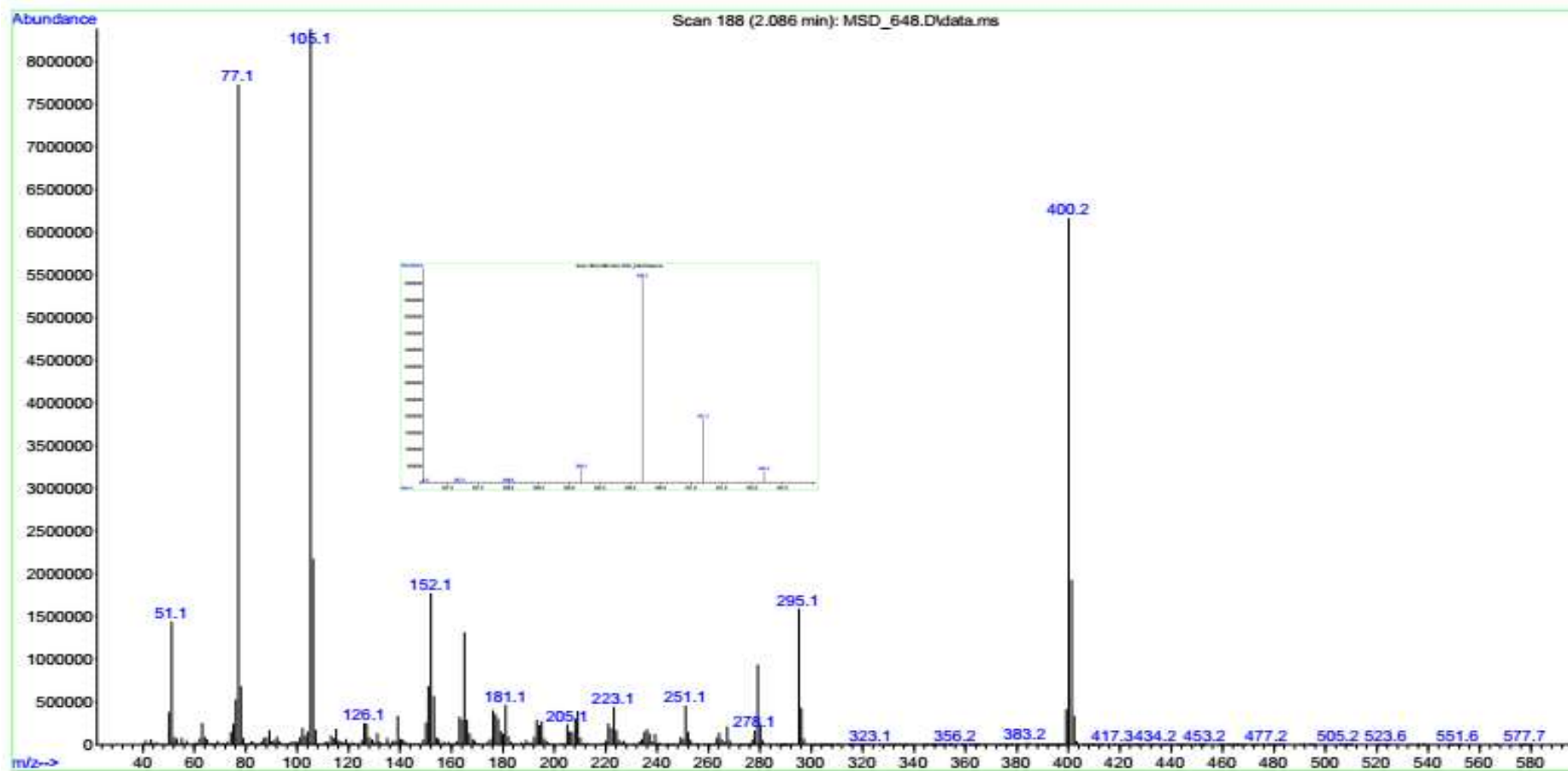


Fig.S33. 3-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl benzoate (8i)

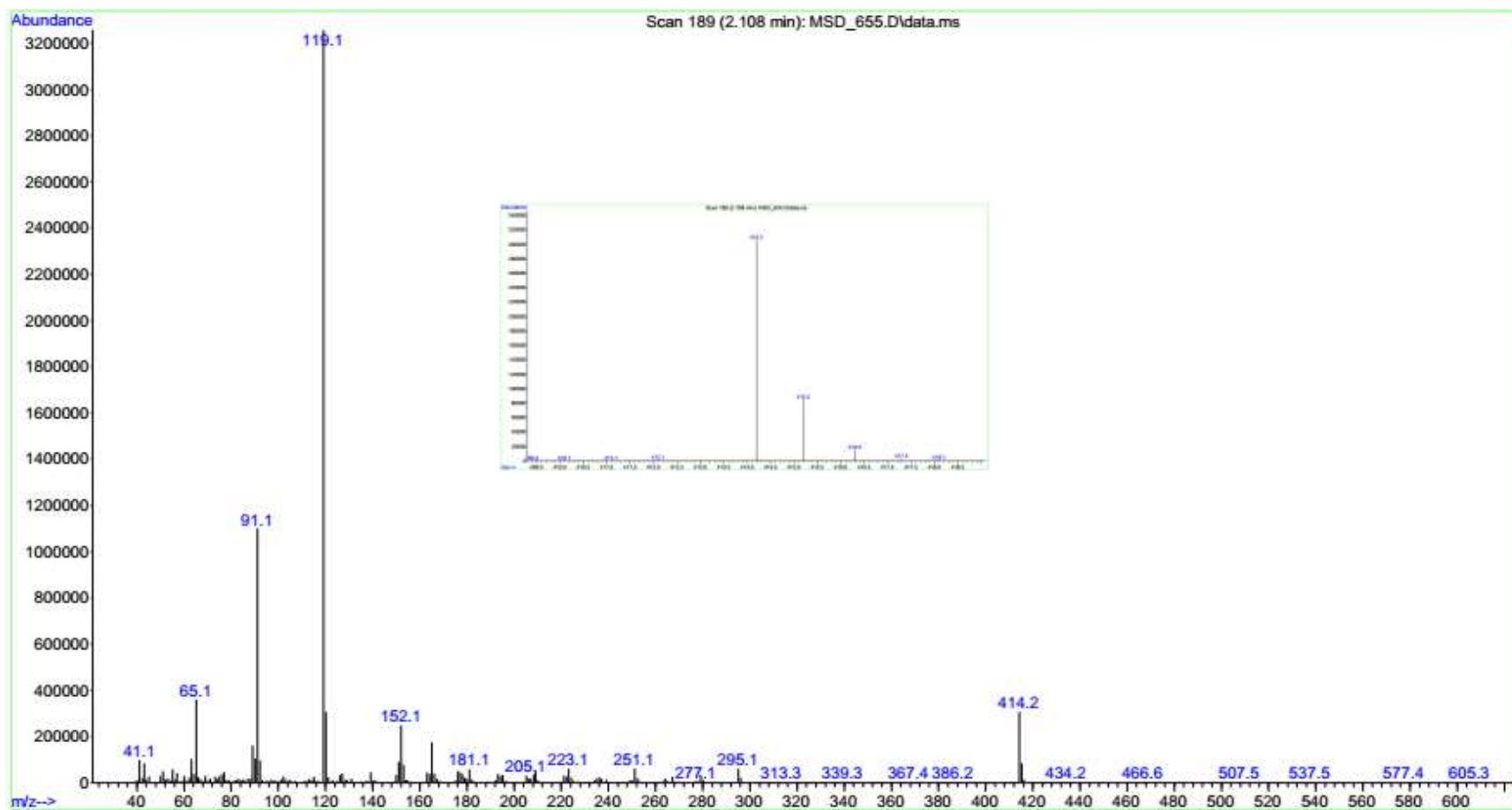


Fig.S34.3-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-methylbenzoate (8j)

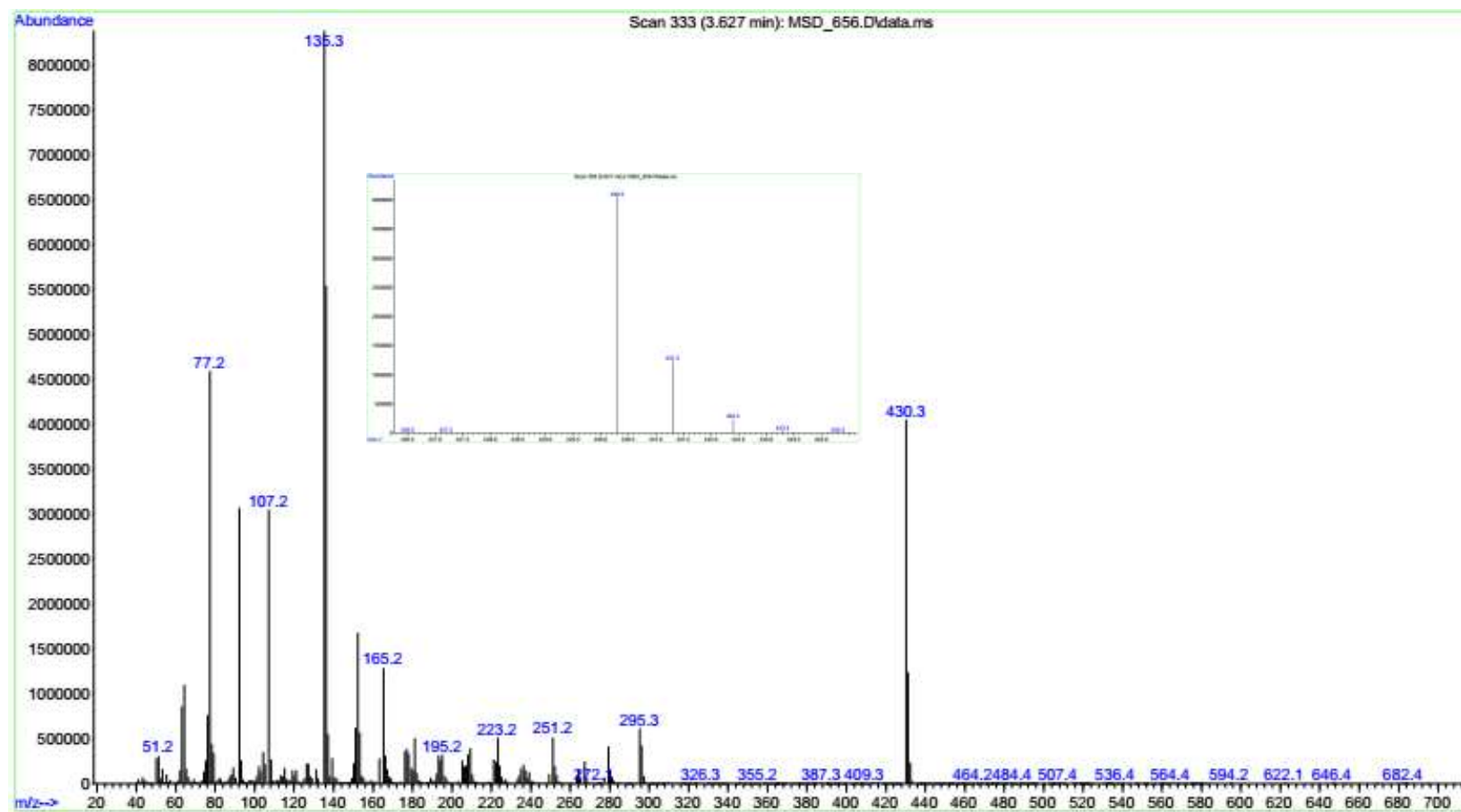


Fig.S35. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8k)

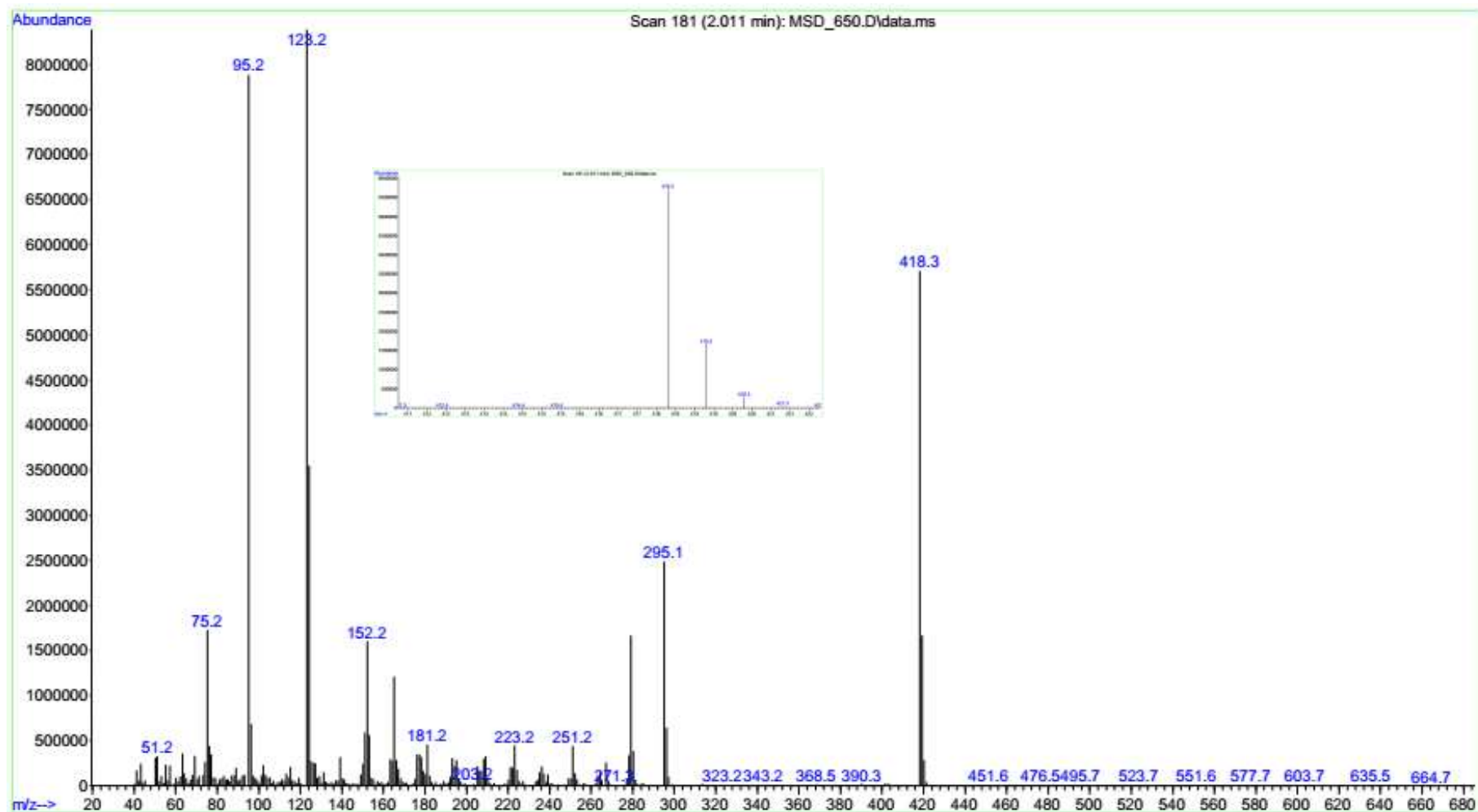


Fig.S36. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8l)

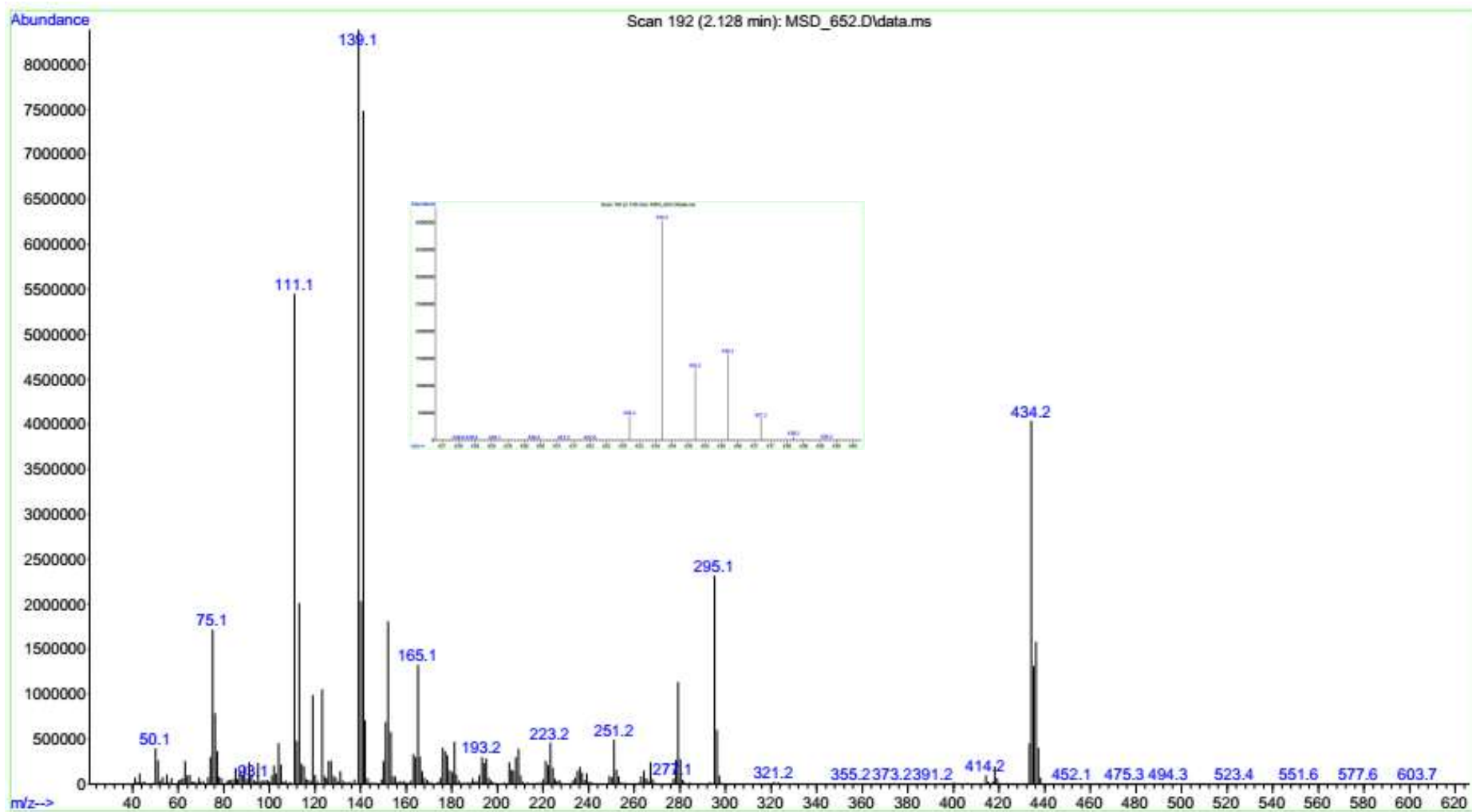


Fig.S37. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-chlorobenzoate (8m)

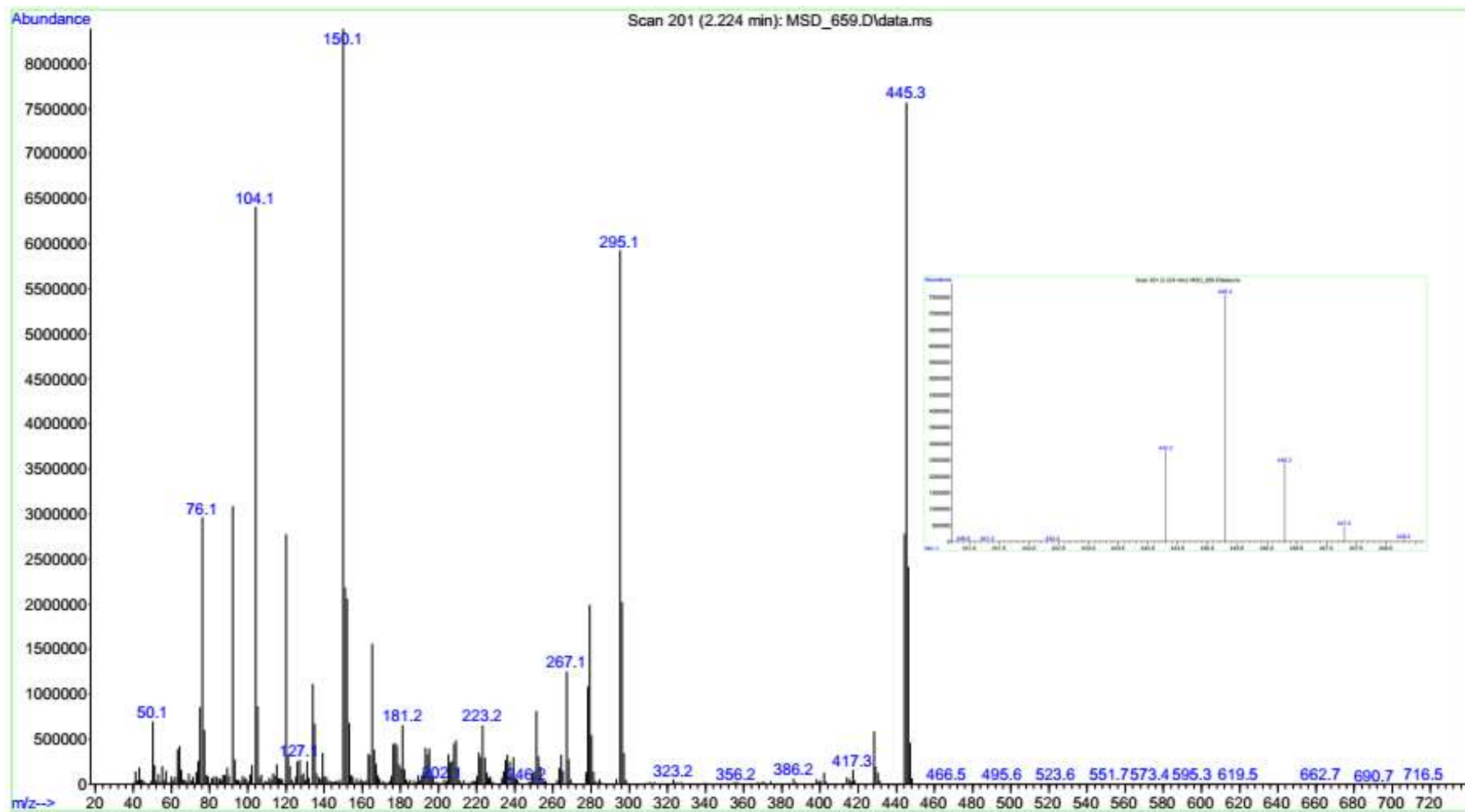


Fig.S38. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-nitrobenzoate (8n)

FT-IR spectra

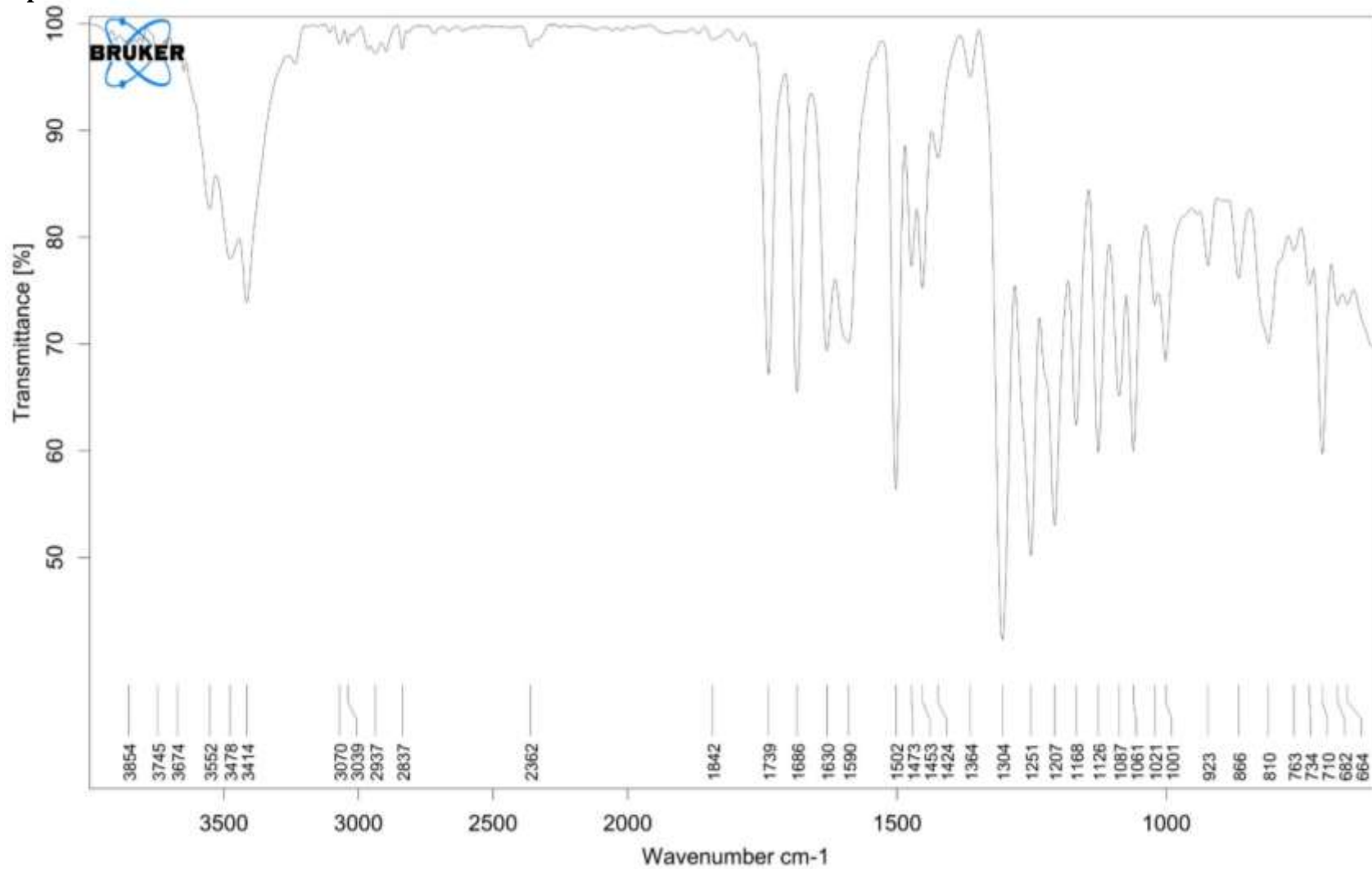


Fig.S39. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8a).

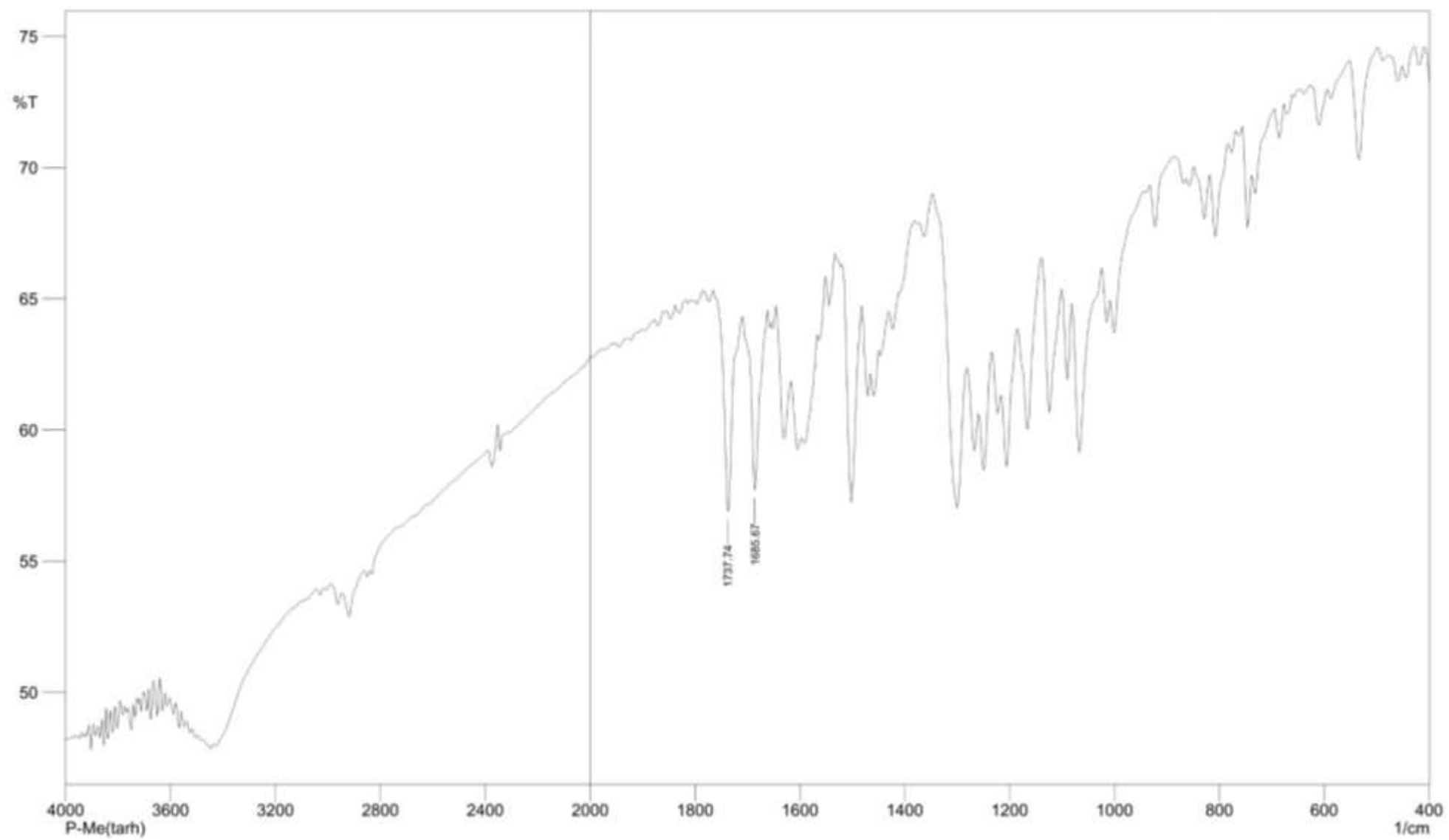


Fig.S40.4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-methylbenzoate (**8b**)

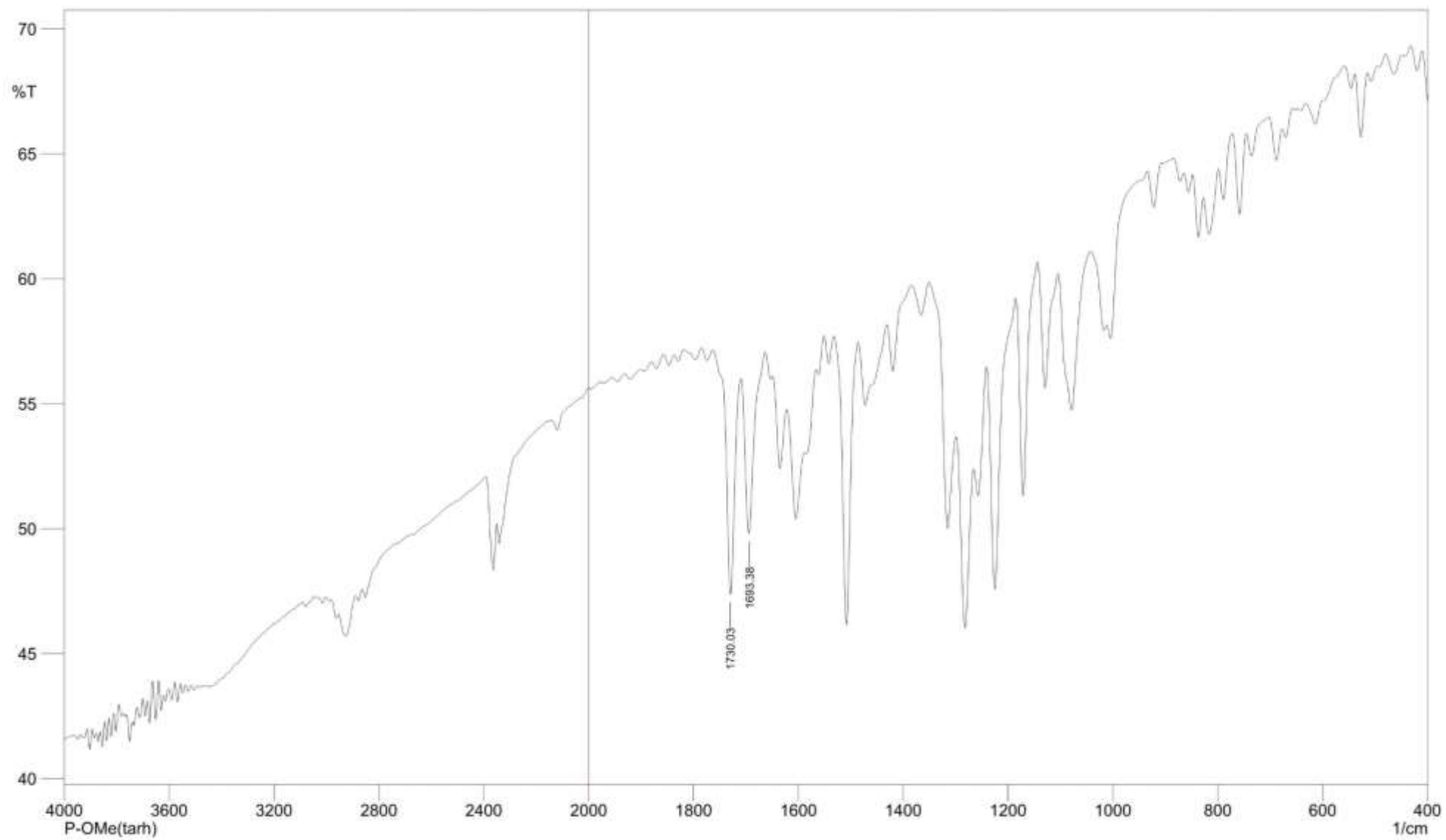


Fig.S41. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8c)

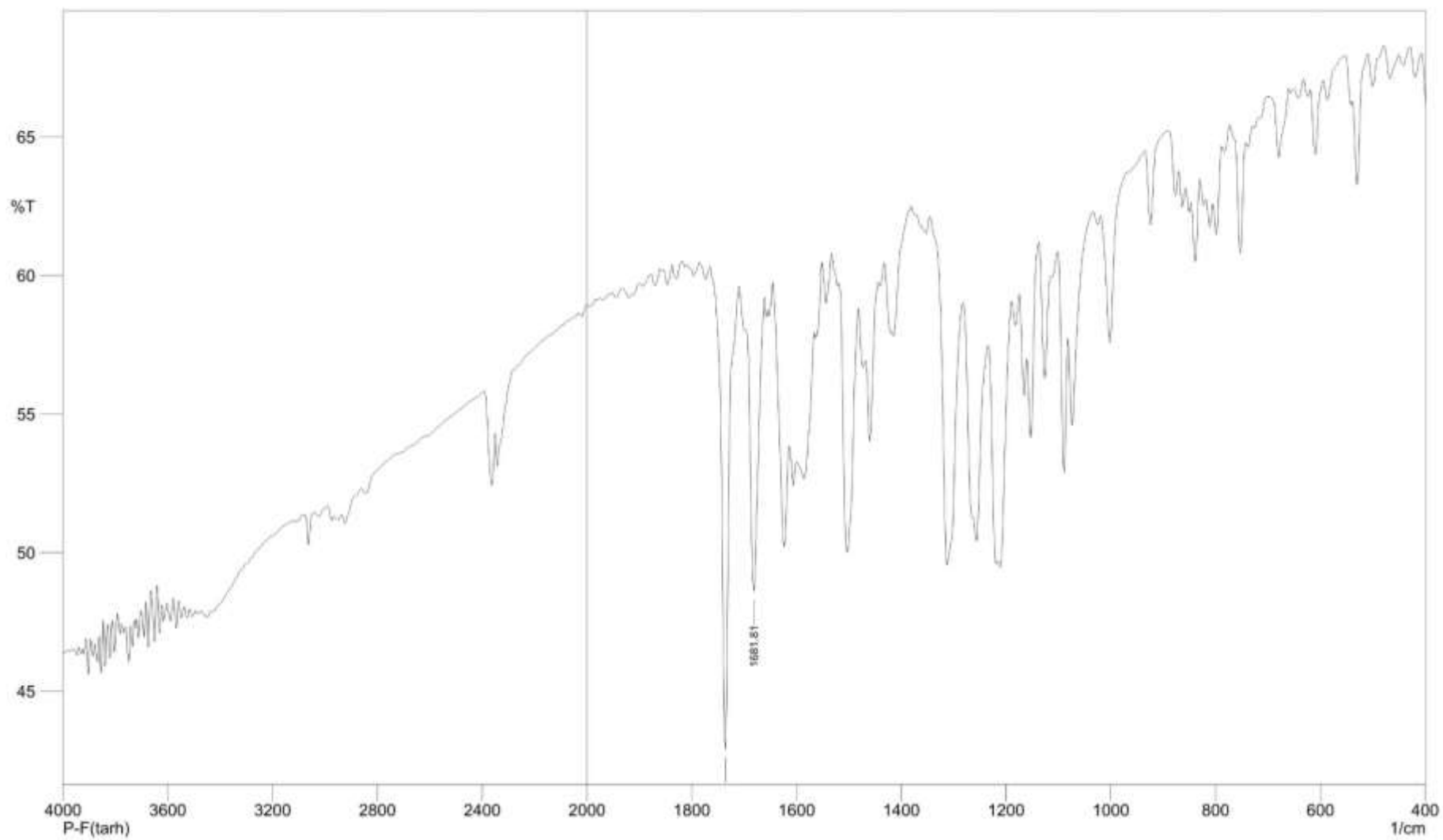


Fig. S42. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-fluorobenzoate (**8d**)

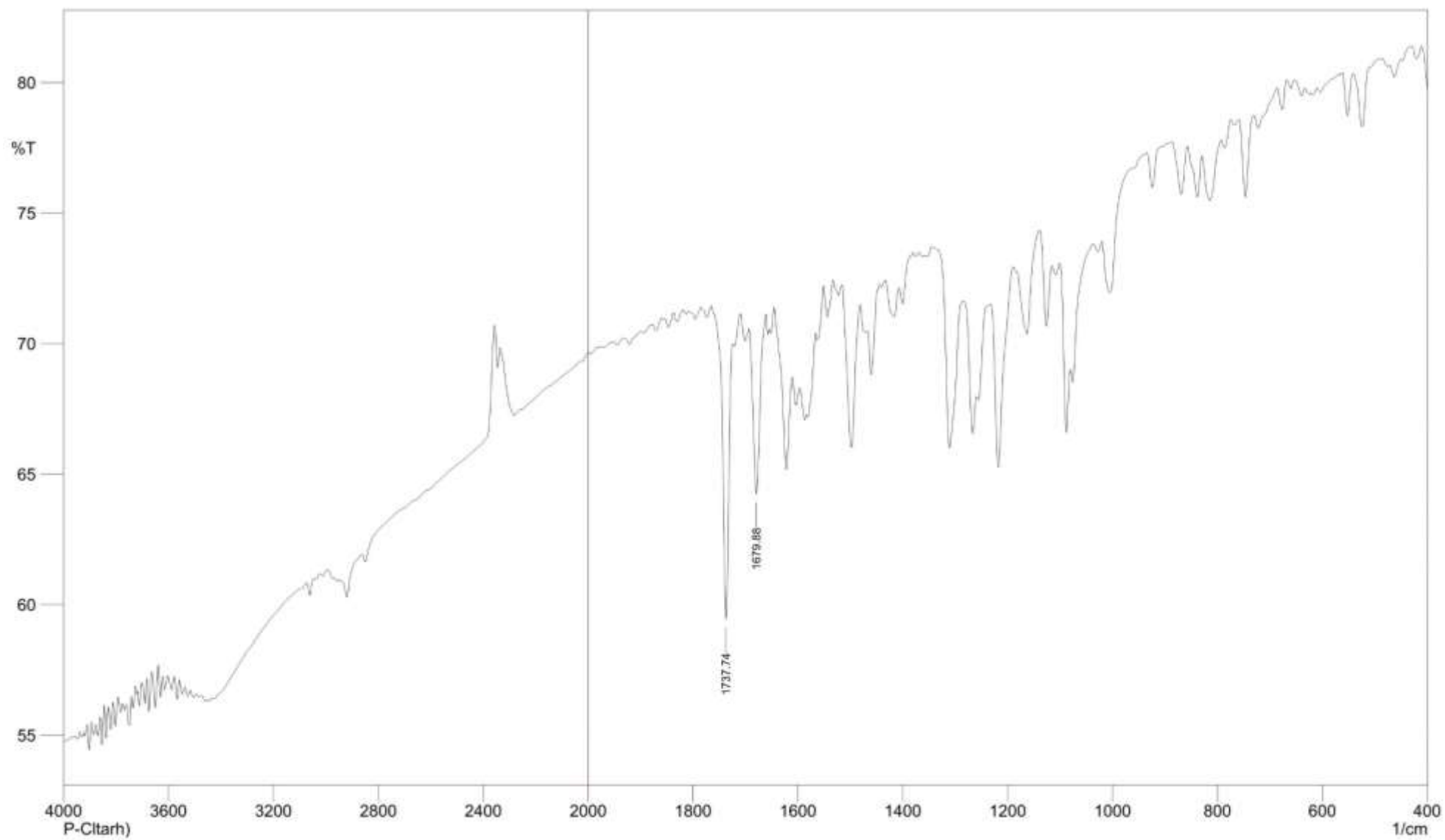


Fig. S43. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-chlorobenzoate (**8e**)

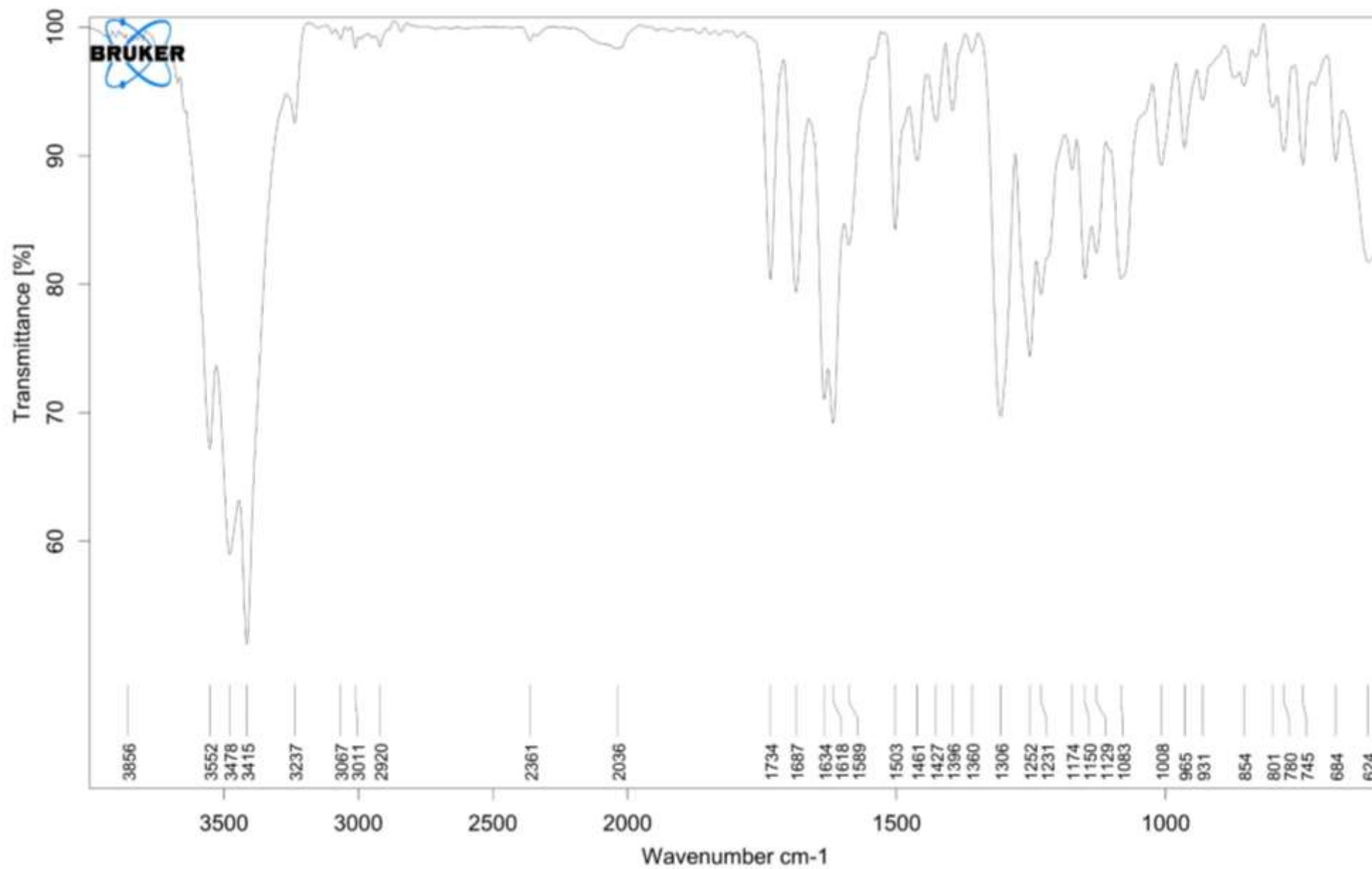


Fig.S44. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-(methylsulfonyl)benzoate (**8f**)

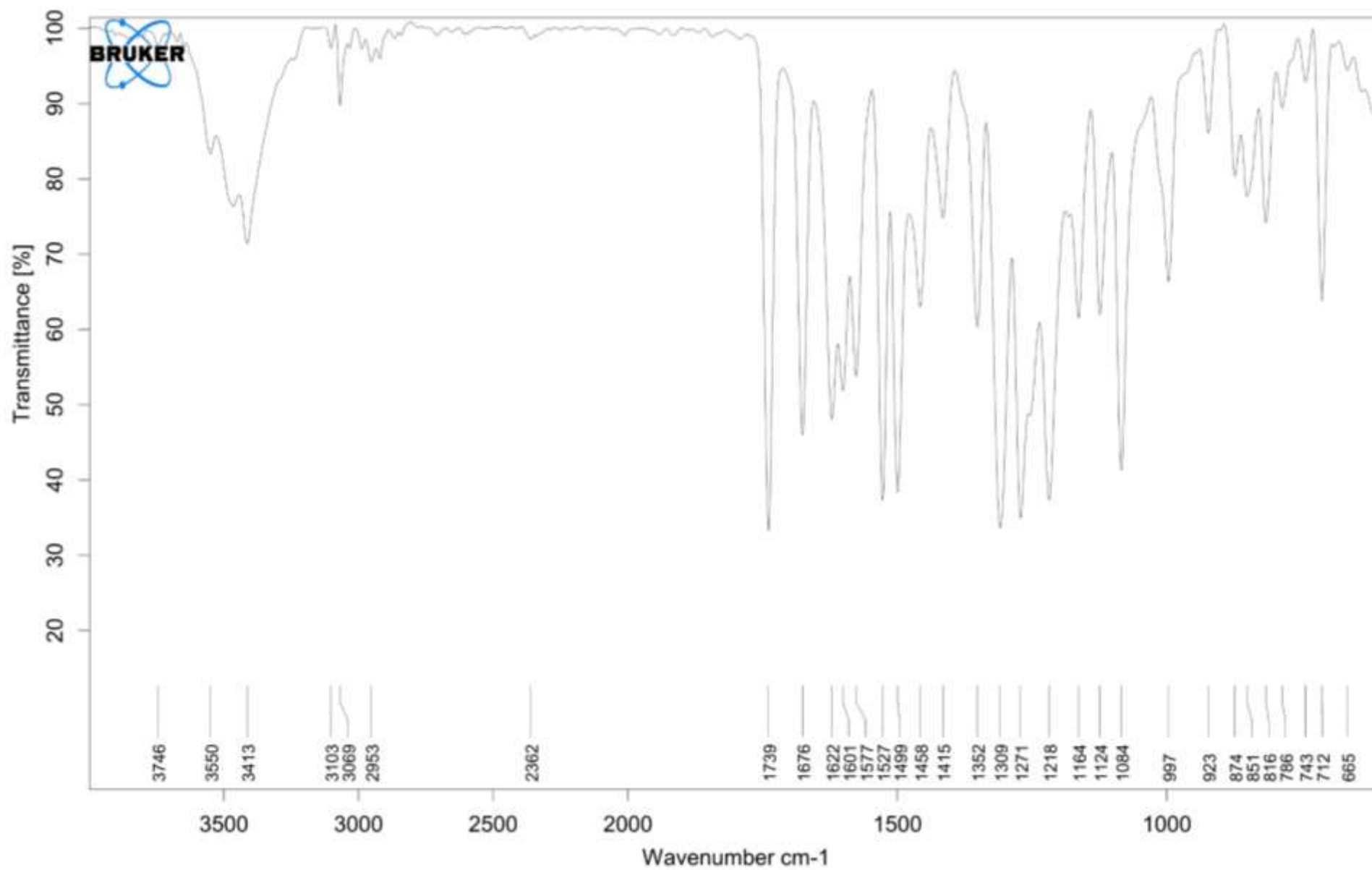


Fig.S45. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-nitrobenzoate (8g)

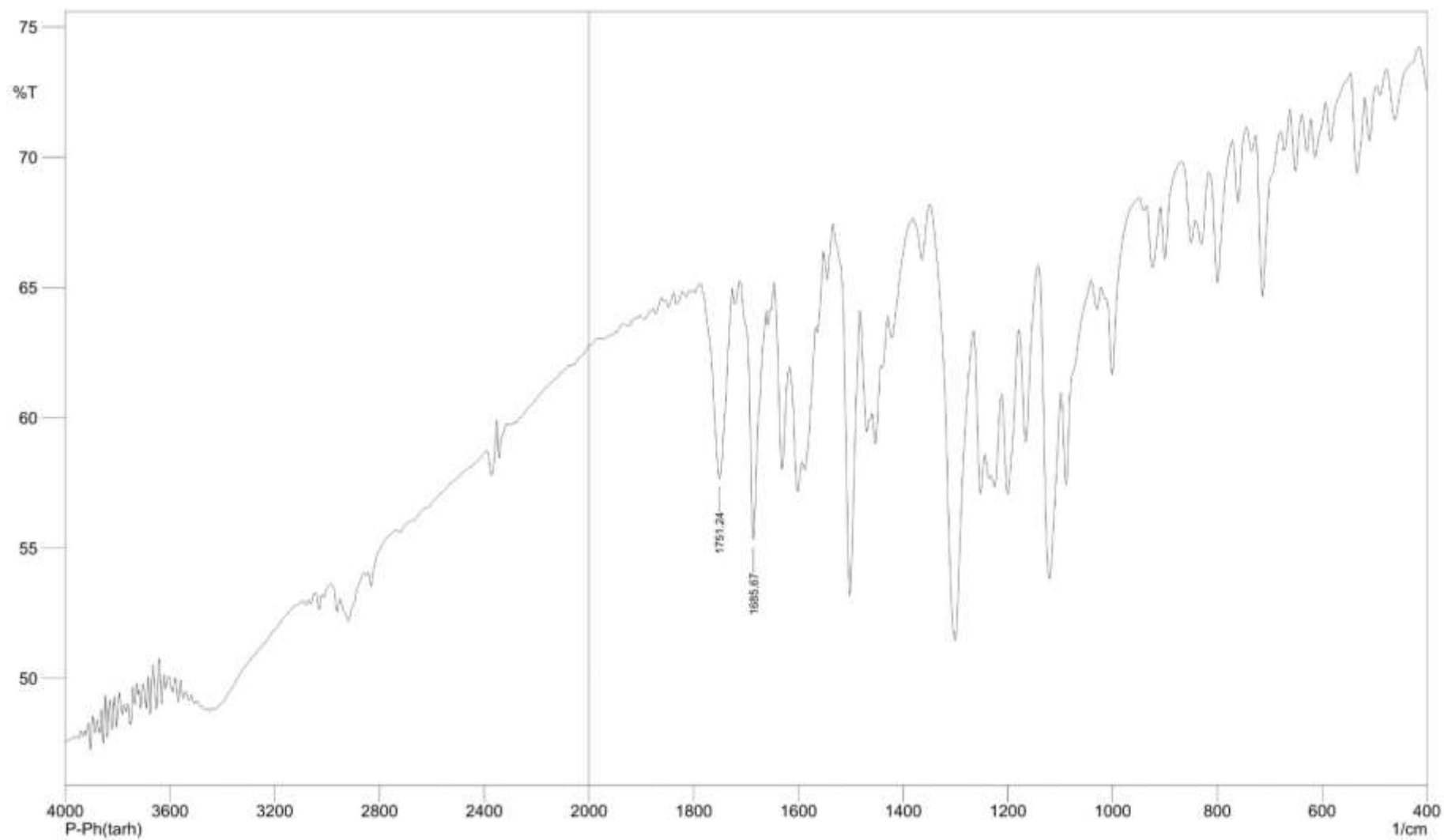


Fig. S46. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 2-phenylacetate(8*h*)

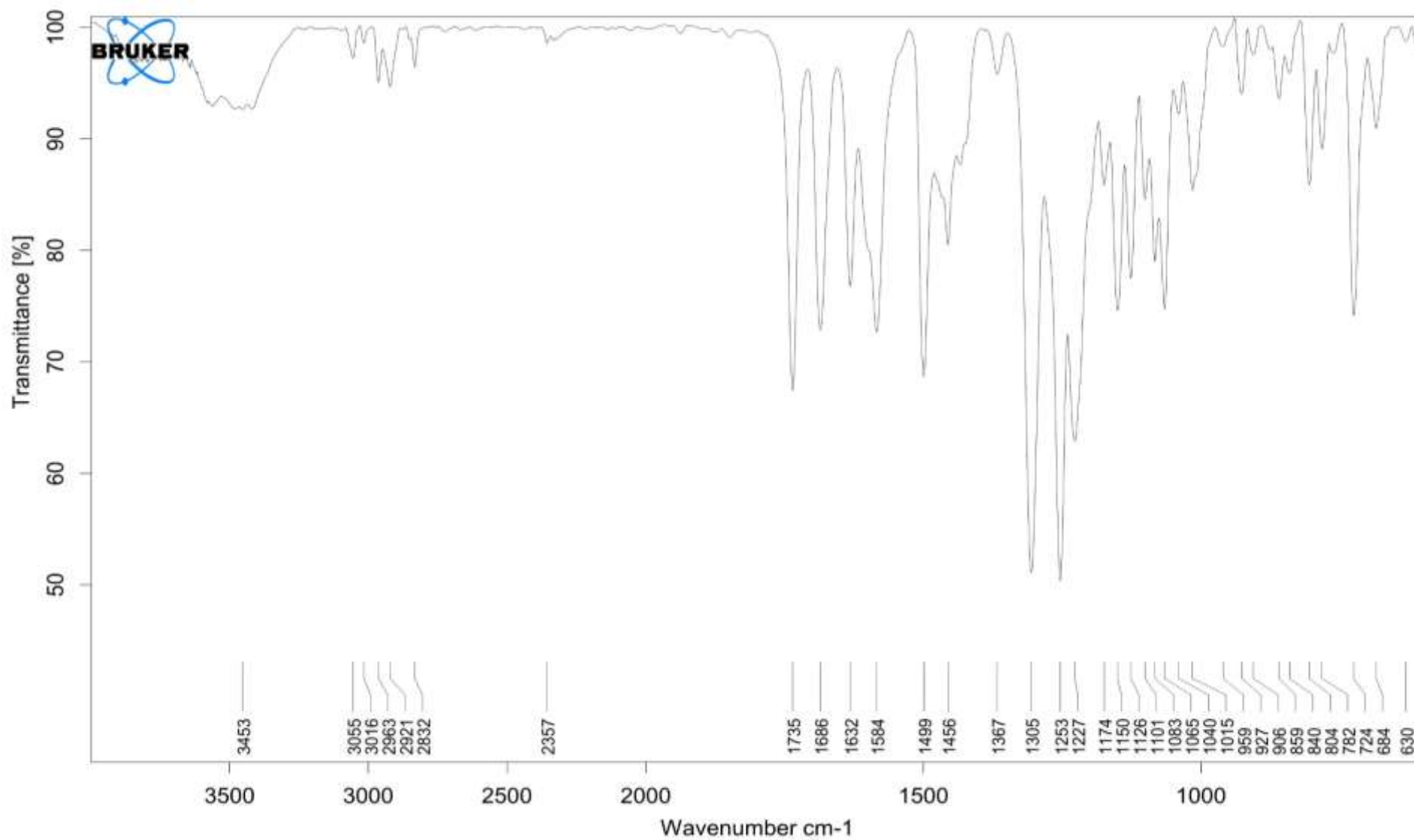


Fig.S47. 3-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl benzoate (**8i**)

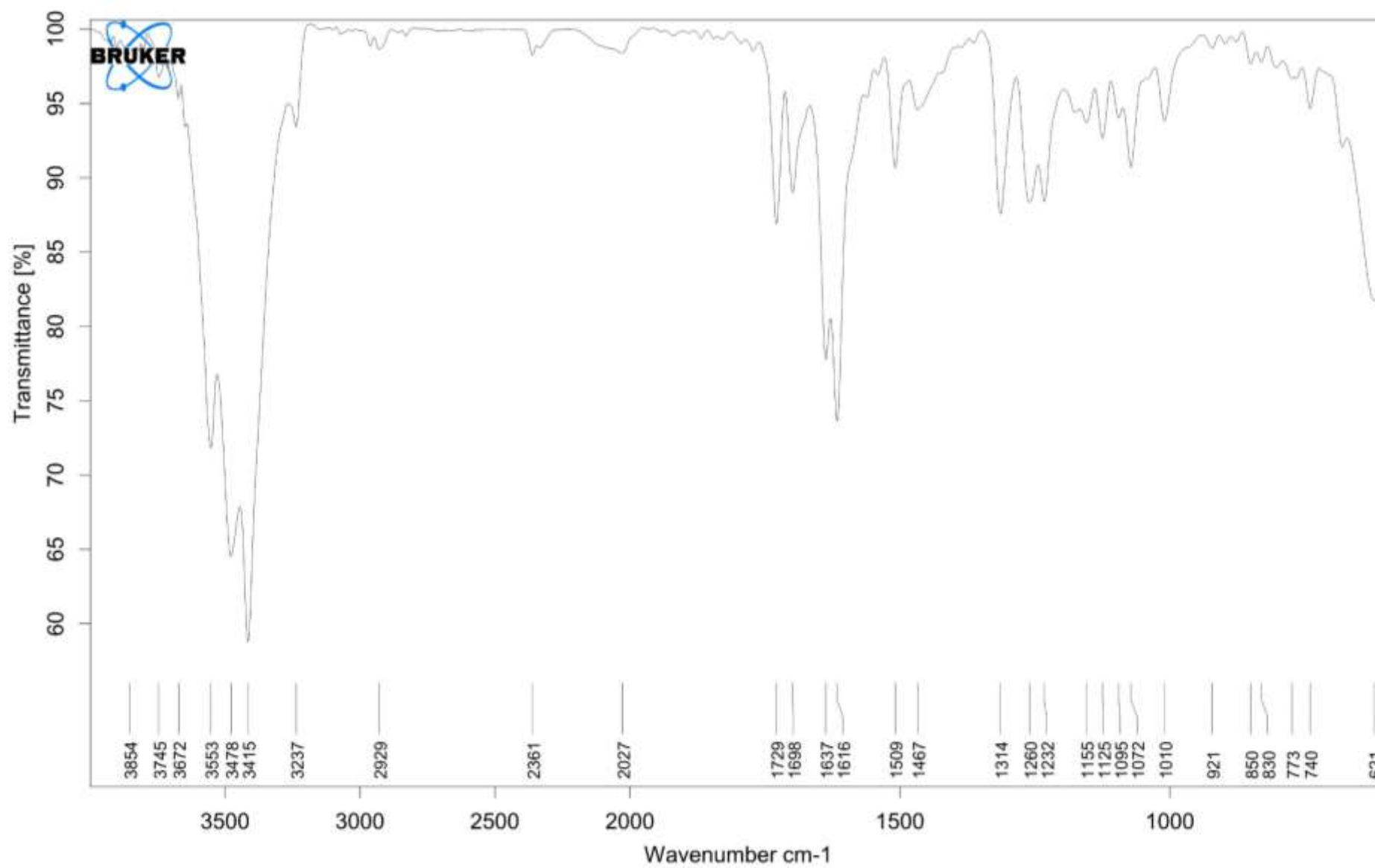


Fig.S48. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl benzoate (8i)

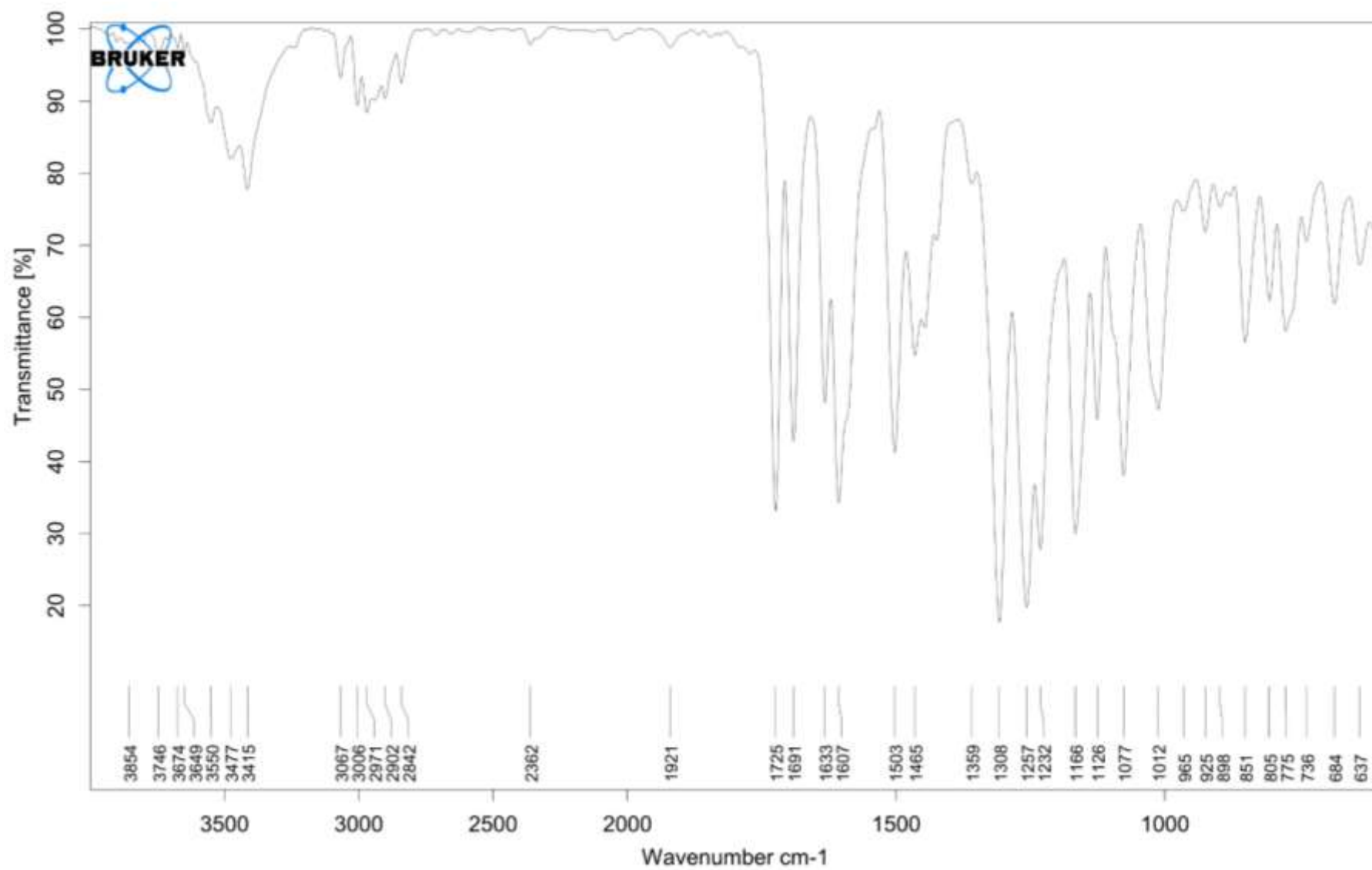


Fig.S49. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8k)

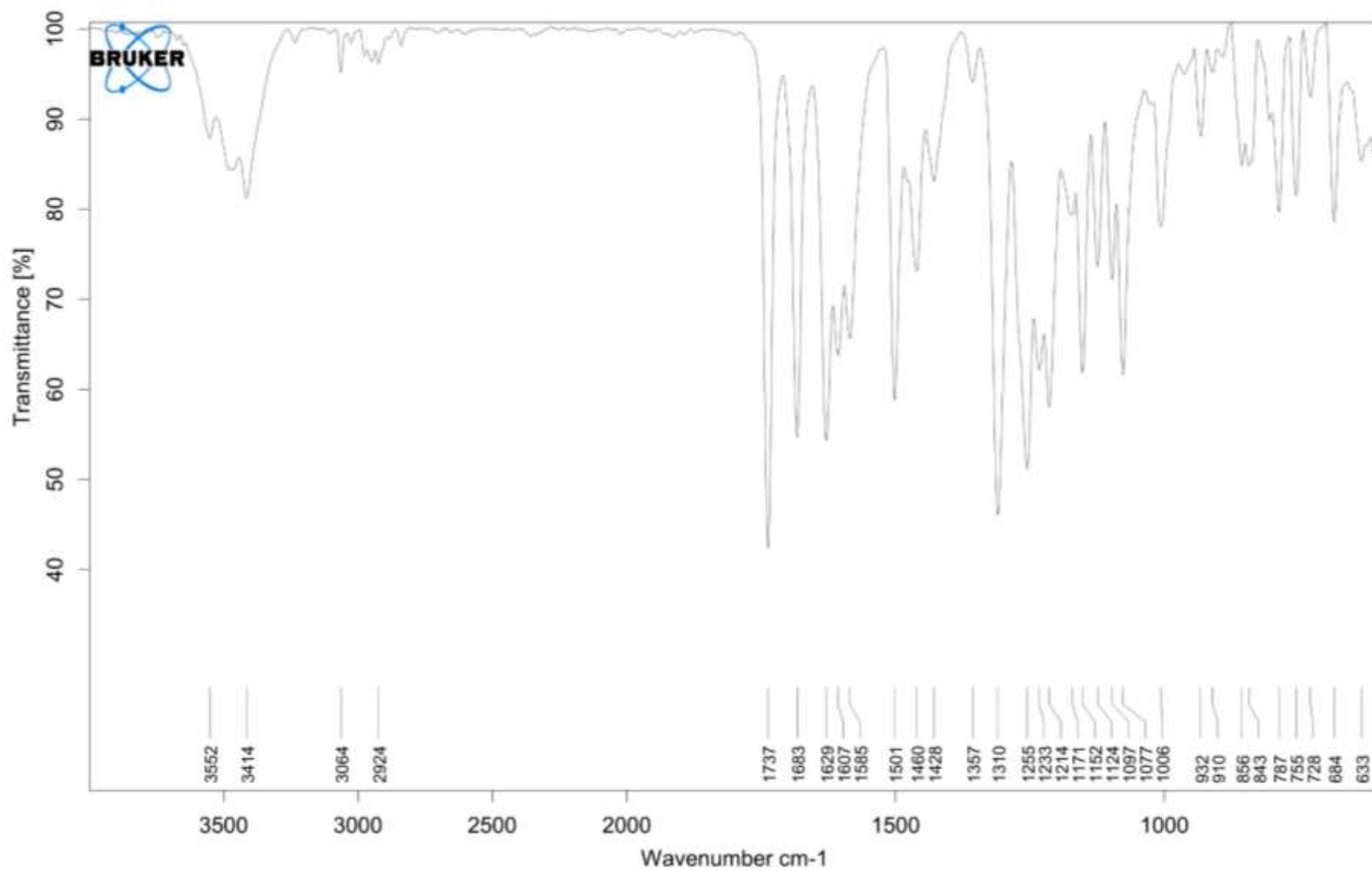


Fig.S50. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8l)

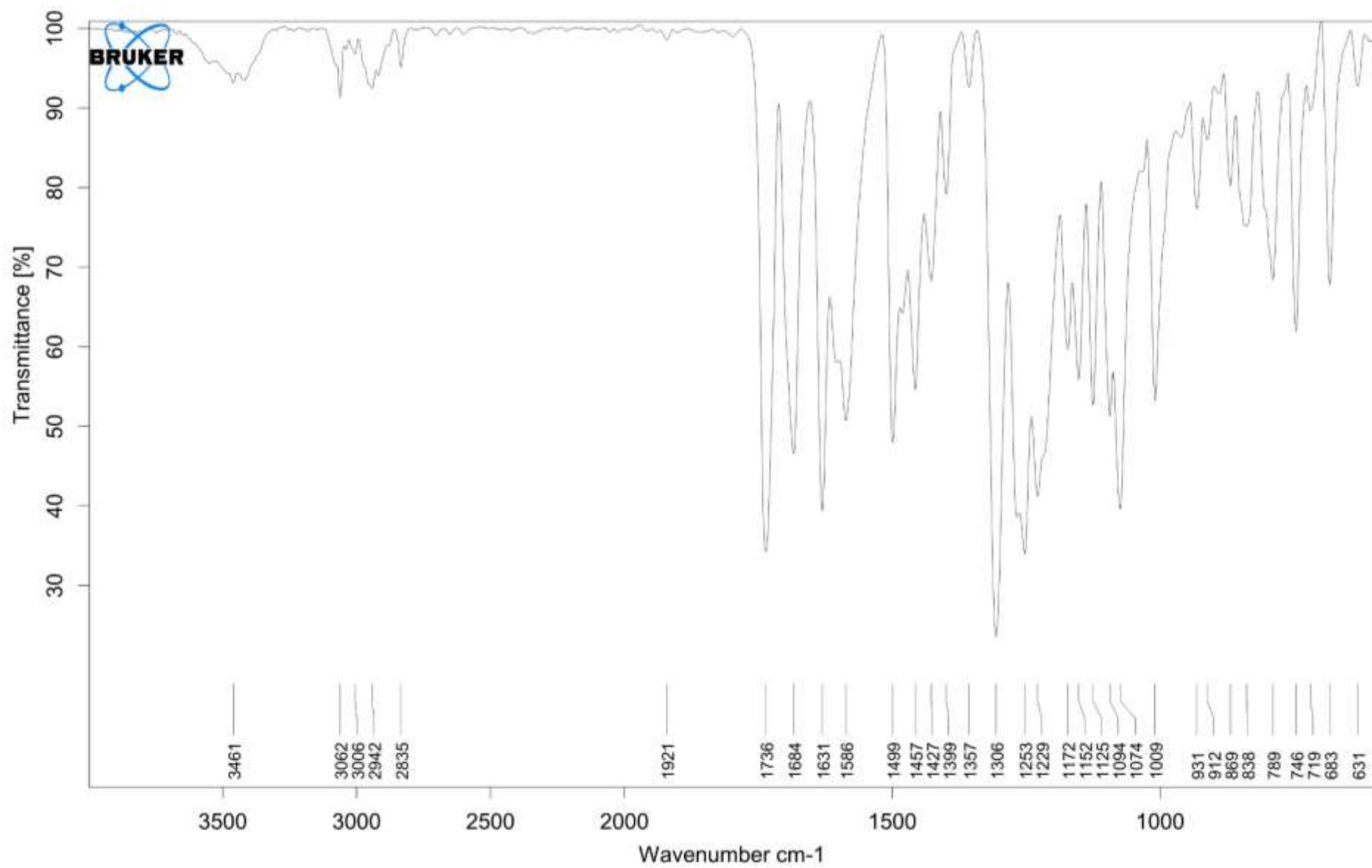


Fig.S51. 3-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-chlorobenzoate (*8m*)

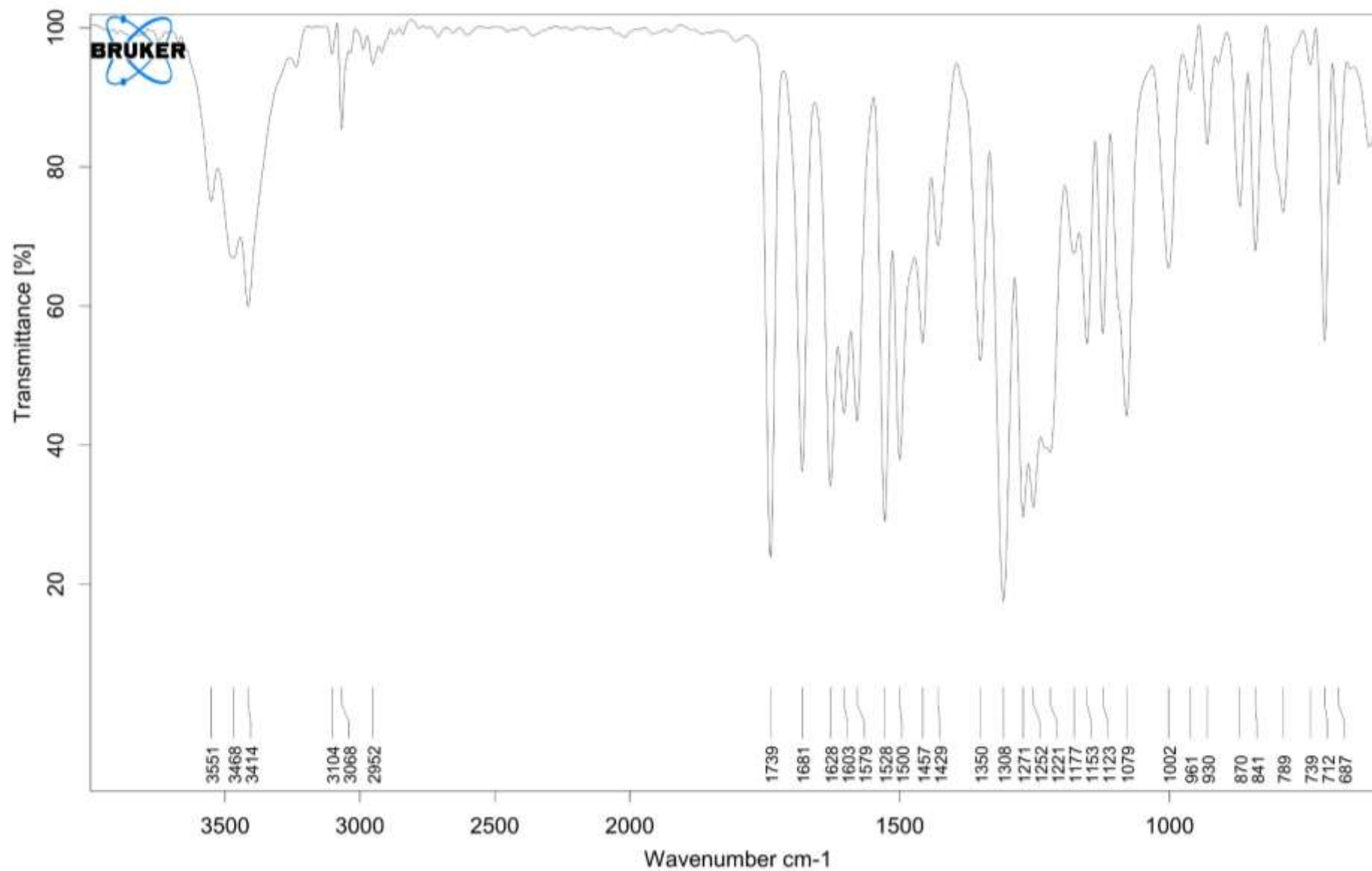
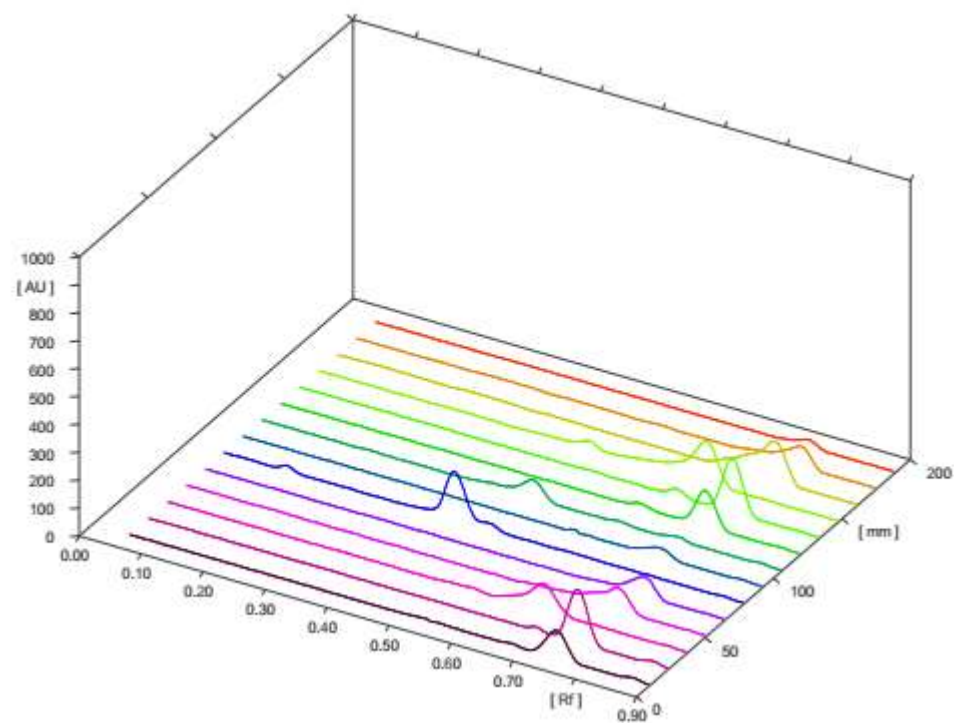


Fig.S52. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-nitrobenzoate (8n)

HPTLC chromatograms



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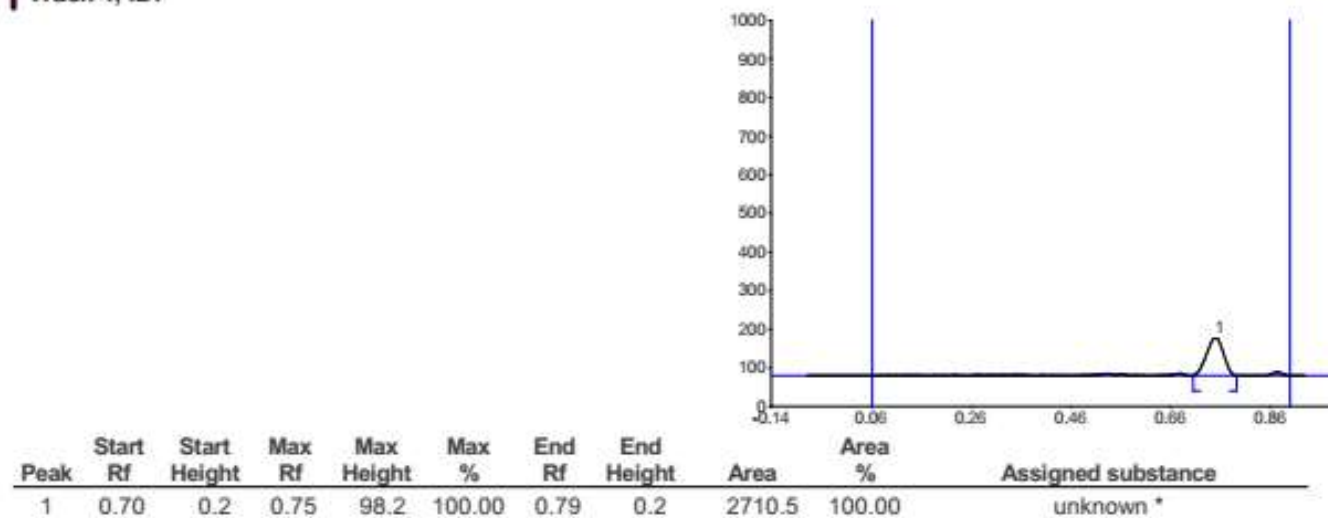


Fig.S53. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl benzoate (8a).

Track 2, ID:

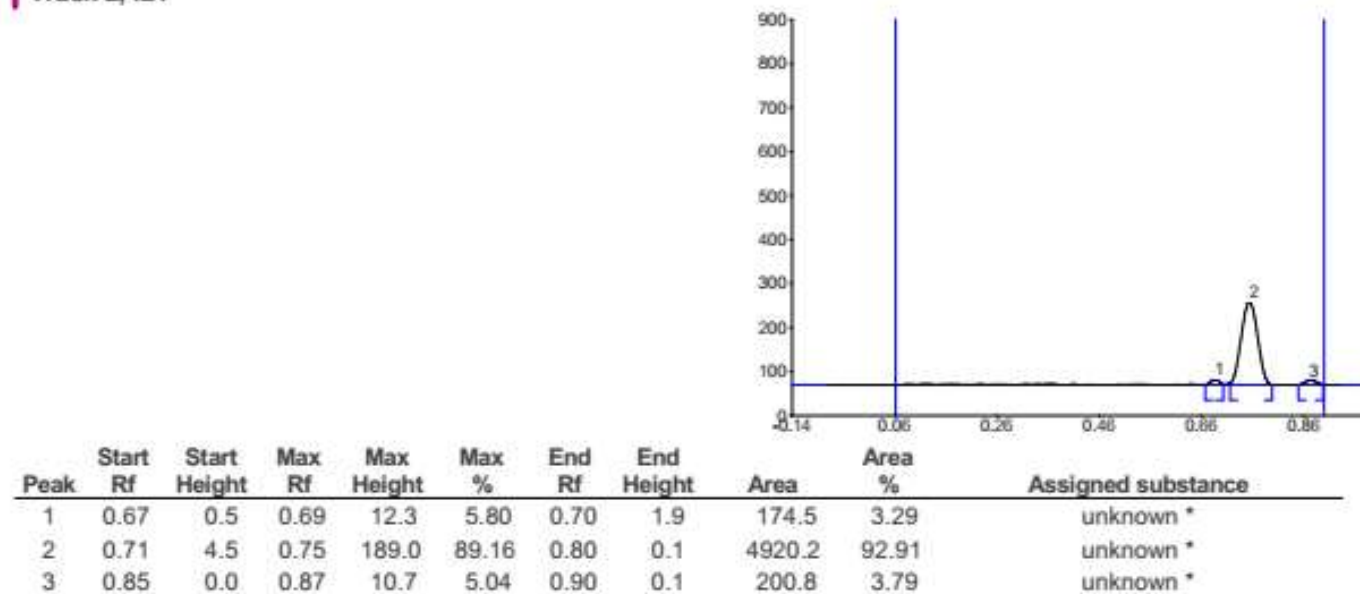


Fig.S54.4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl4-methylbenzoate (8b)

Track 3, ID:

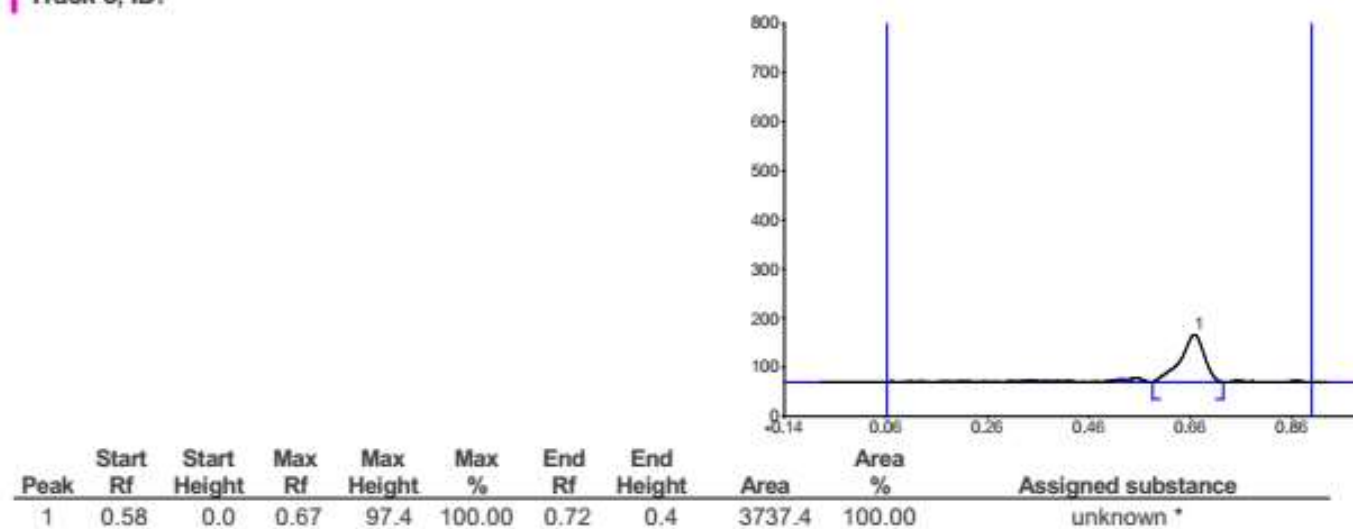


Fig.S55. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8c)

Track 4, ID:

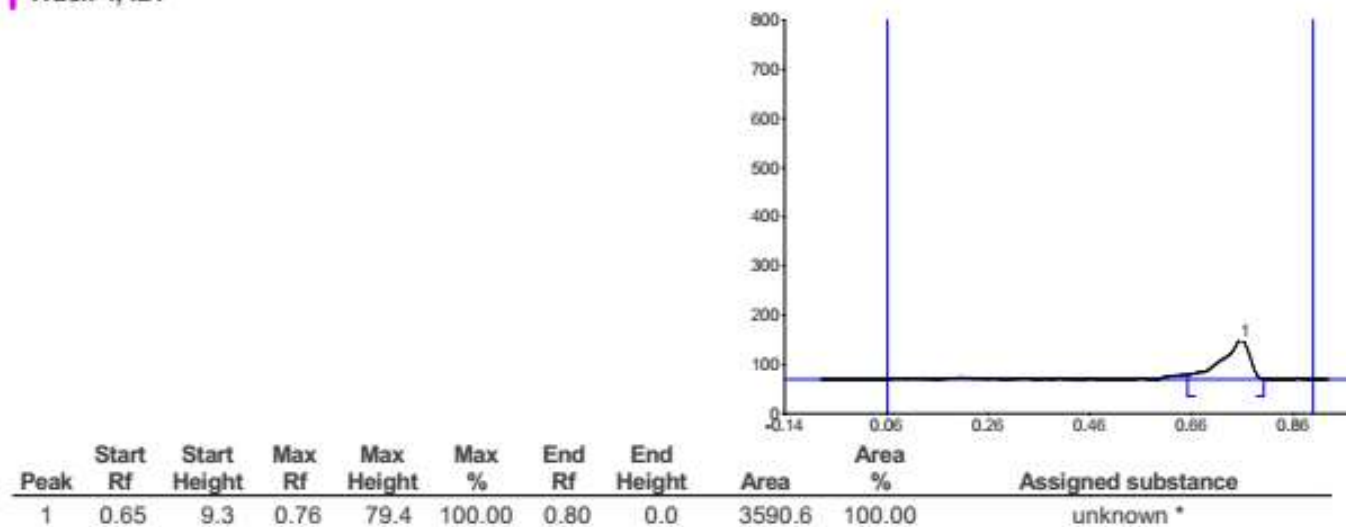


Fig. S56. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8d)

Track 5, ID:

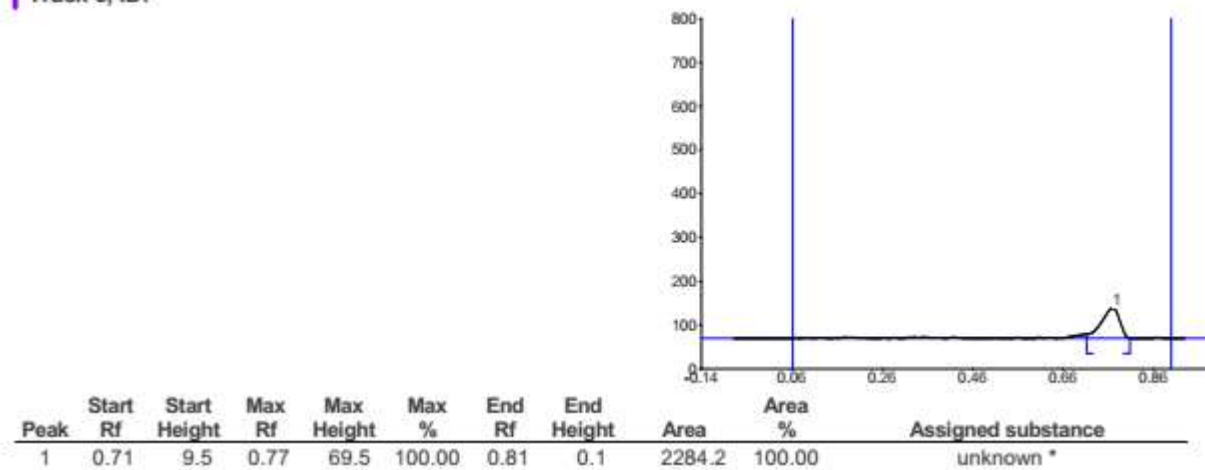


Fig. S57. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-chlorobenzoate (*8e*)

Track 6, ID:

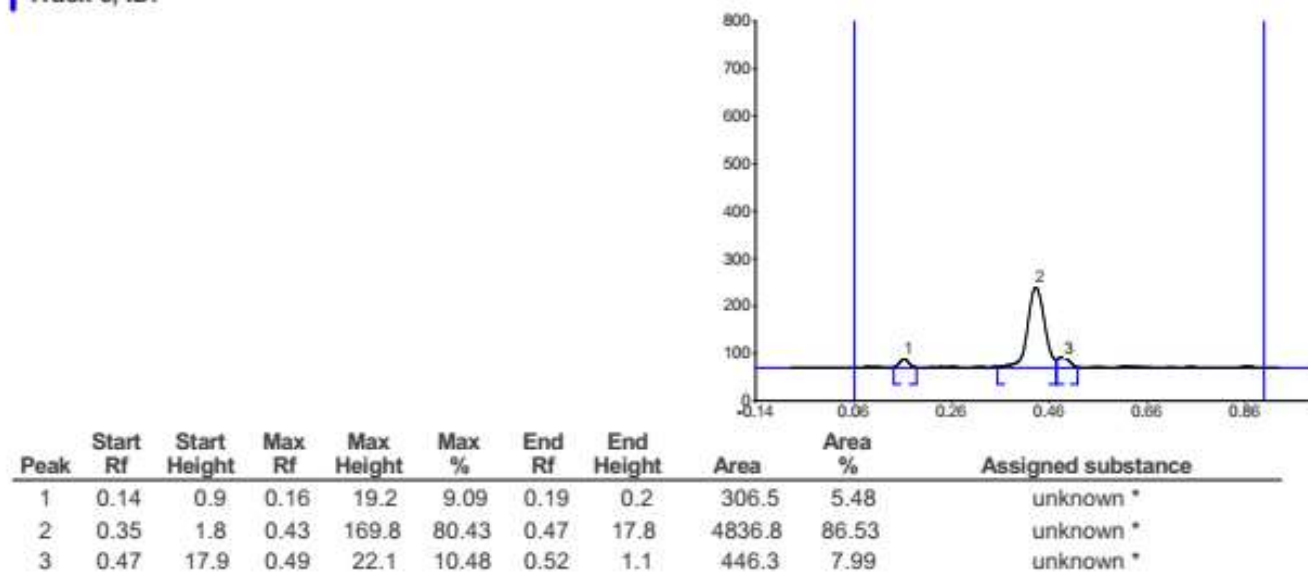


Fig.S58. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-(methylsulfonyl)benzoate (8f)

Track 7, ID:

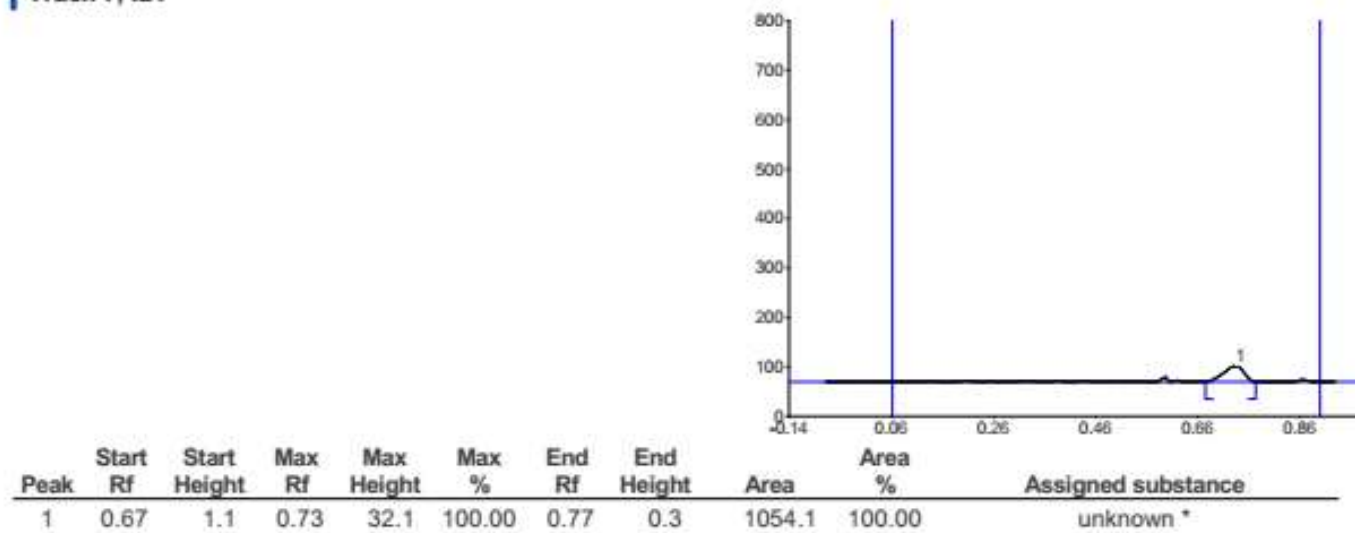


Fig.S59. 4-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl 4-nitrobenzoate (8g)

Track 8, ID:

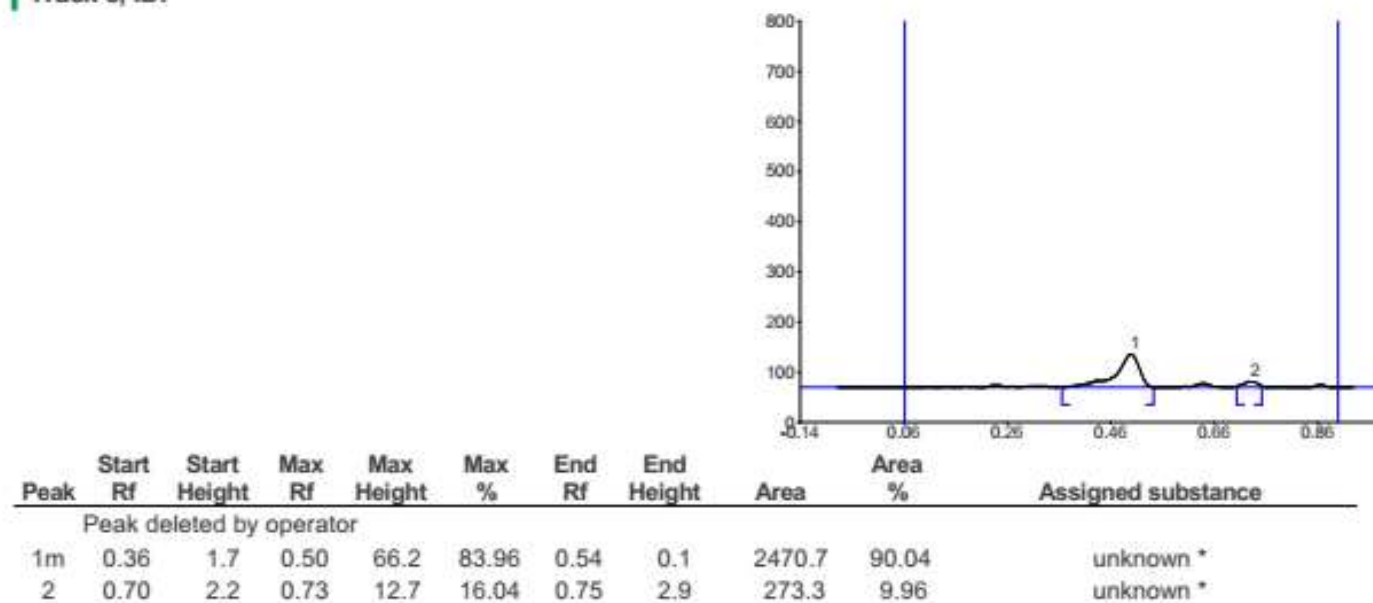


Fig. S60. 4-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 2-phenylacetate(8h)

Track 9, ID:

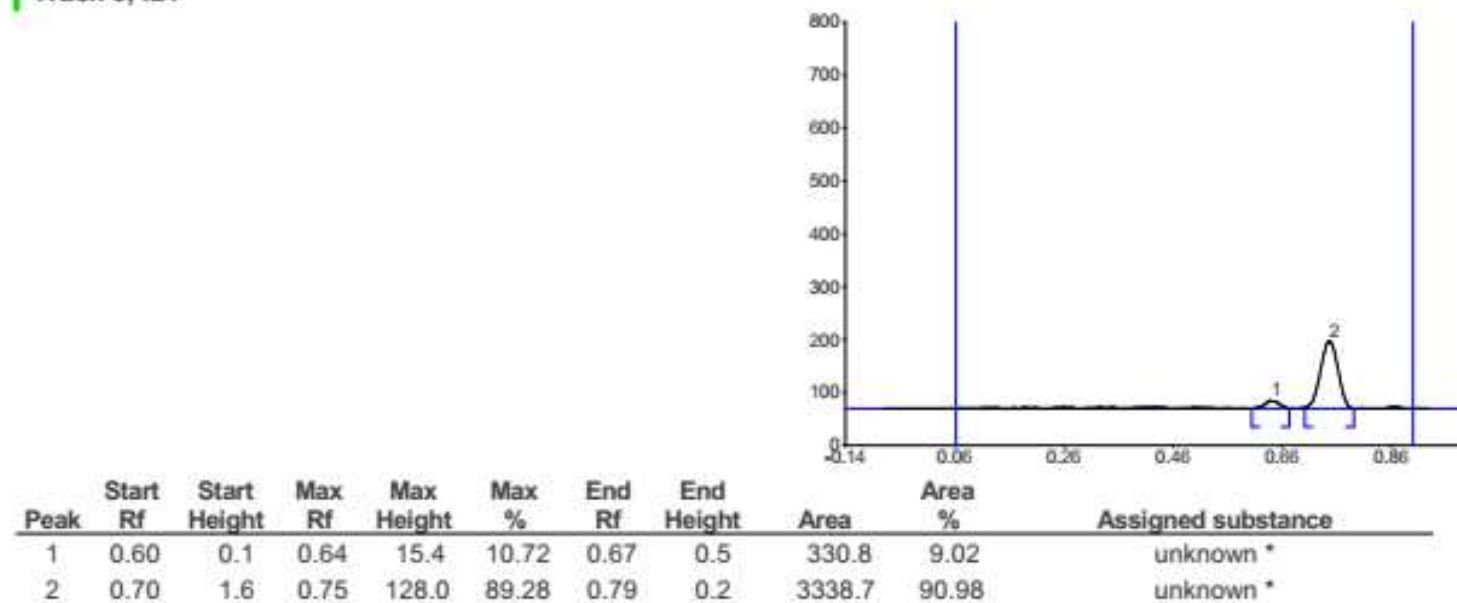
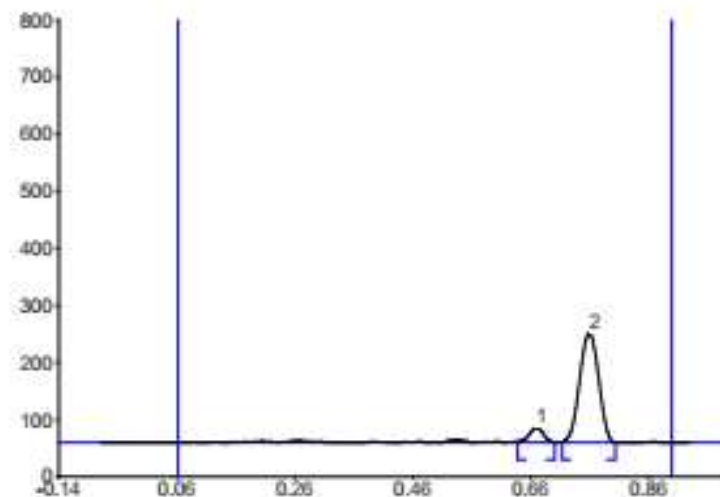


Fig.S61. 3-((*E*)-(5,6-dimethoxy-1-oxo-1*H*-inden-2(3*H*)-ylidene)methyl)phenyl benzoate (8i)

Track 10, ID:



Peak	Start Rf	Start Height	Max Rf	Max Height	Max %	End Rf	End Height	Area	Area %	Assigned substance
1	0.64	1.8	0.67	26.4	12.09	0.70	0.2	528.8	9.49	unknown *
2	0.71	0.7	0.76	191.8	87.91	0.80	0.1	5045.3	90.51	unknown *

Fig.S62.3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methylbenzoate (5j)

Track 11, ID:

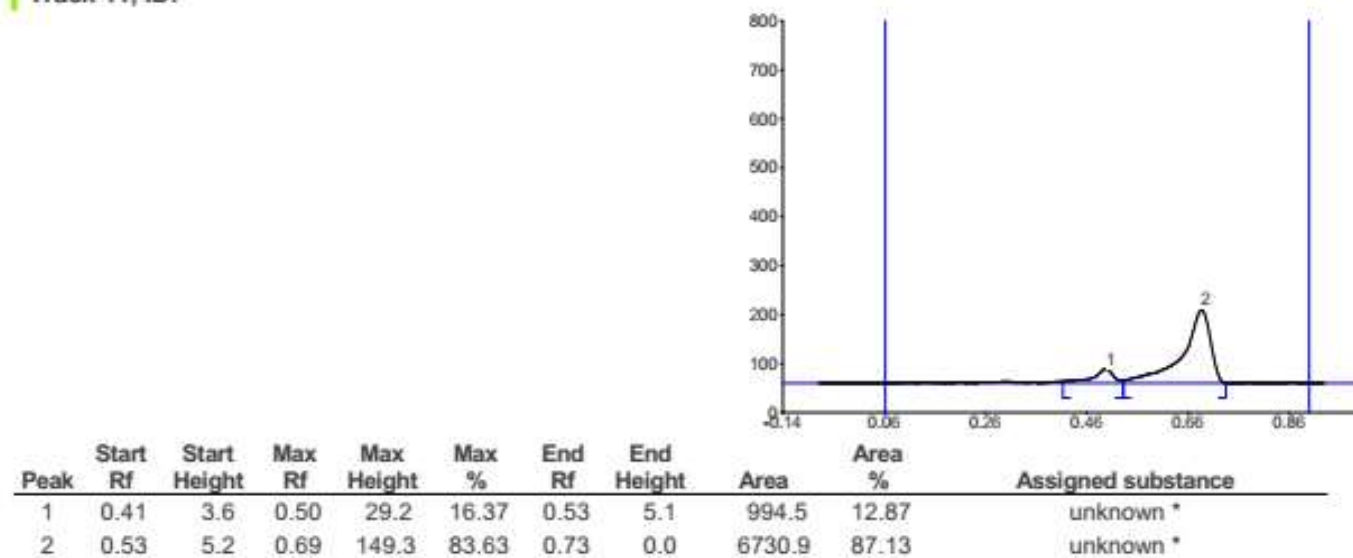


Fig.S63. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-methoxybenzoate (8k)

Track 13, ID:

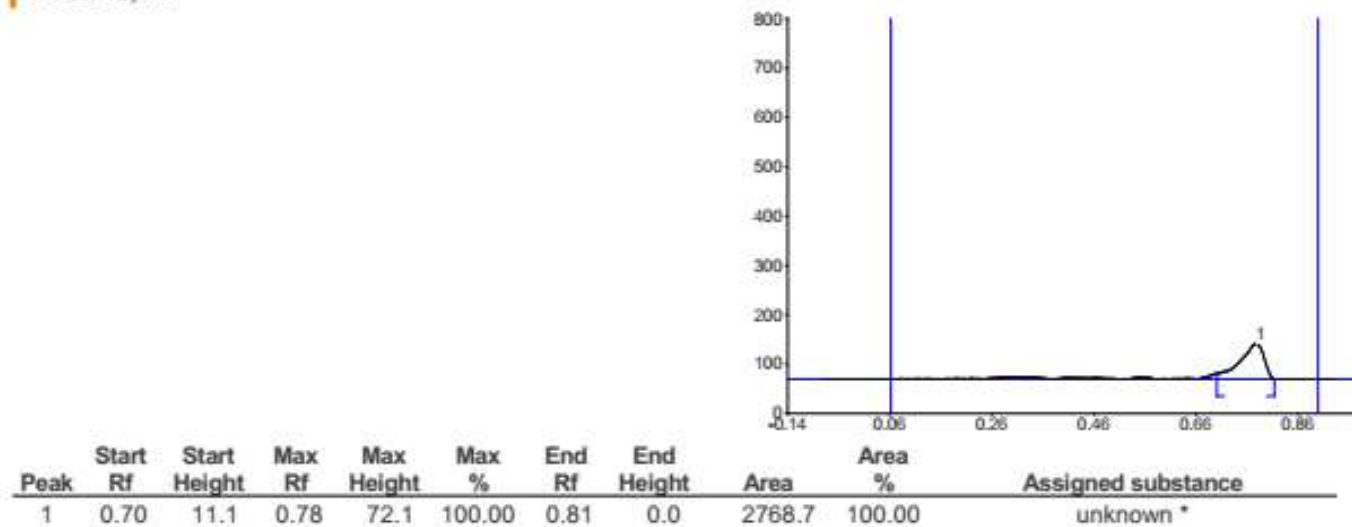


Fig.S64. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-fluorobenzoate (8l)

Track 14, ID:

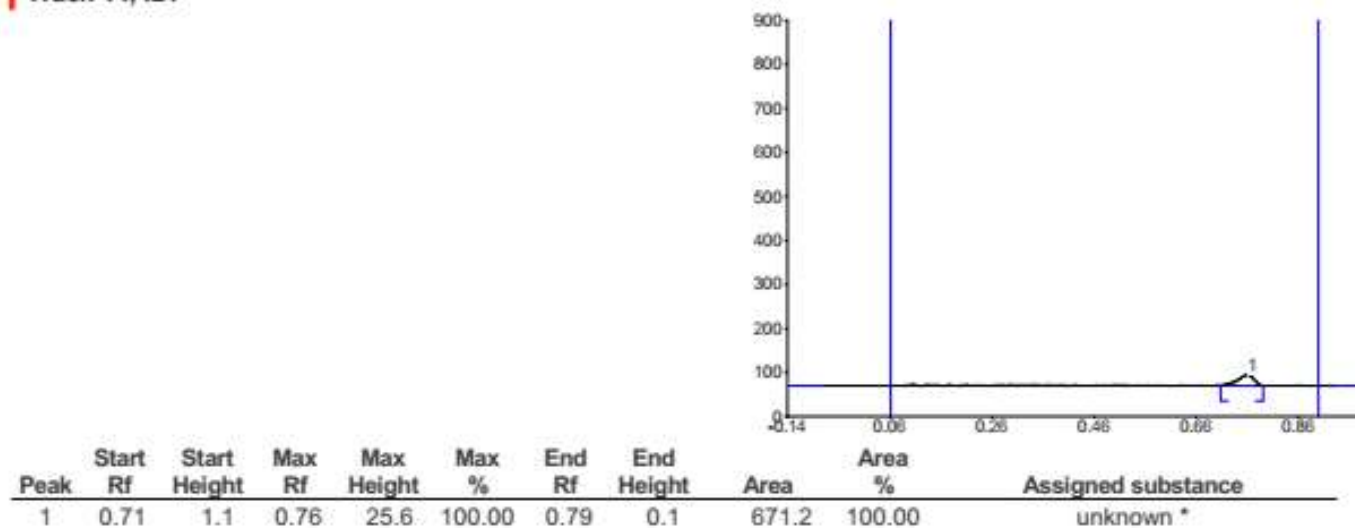


Fig.S65. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-chlorobenzoate (8m)

Track 12, ID:

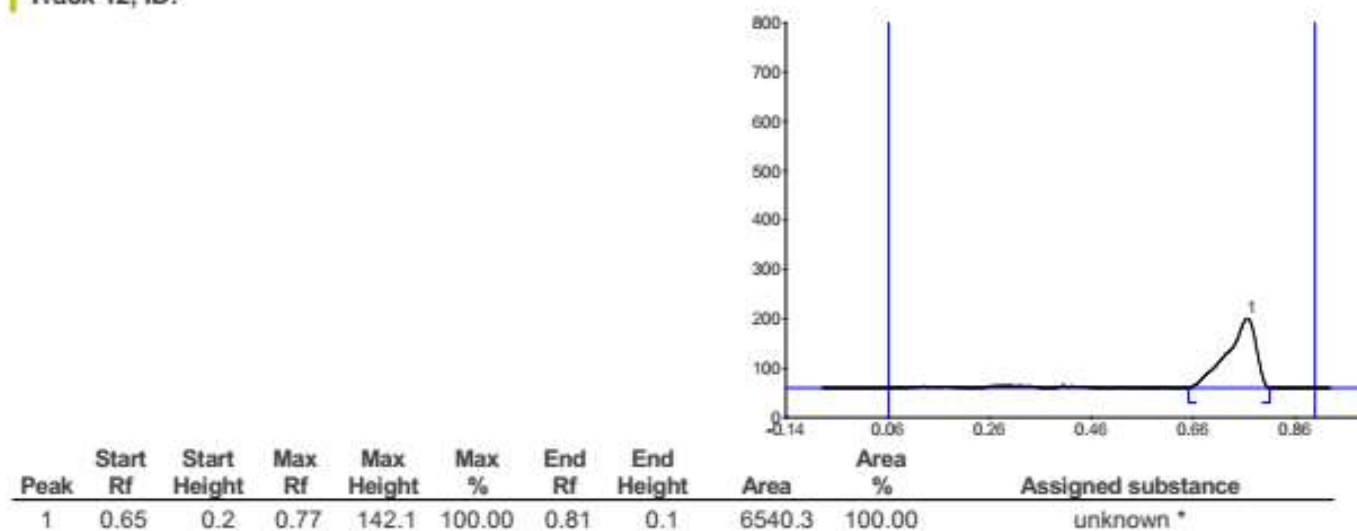


Fig.S66. 3-((E)-(5,6-dimethoxy-1-oxo-1H-inden-2(3H)-ylidene)methyl)phenyl 4-nitrobenzoate (8n)

Table S1-Substituent constants.

Substitutions	σ_p	π	Es
CH ₃	-0.17	0.56	-1.24
NO ₂	0.78	-0.28	-2.52
H	0	0	0
F	0.06	0.14	-0.46
Cl	0.23	0.71	-0.97
OCH ₃	-0.27	-	-