

## Some bis (3-(4-nitrophenyl)acrylamide derivatives: Synthesis, characterization, DFT, antioxidant, antimicrobial properties, molecular docking and molecular dynamics simulation studies

Şükriye Çakmak<sup>1\*</sup> & Taner Erdoğan<sup>2</sup>

<sup>1</sup>Department of Medical Services and Techniques, Vocational School of Health Services, Sinop University, Sinop, Turkey

<sup>2</sup>Department of Chemistry and Chemical Processing Technologies, Kocaeli Vocational School, Kocaeli University, Kocaeli, Turkey

Received 23 May 2022; revised 14 December 2022

### Supplementary data

Table S1 — Calculated geometric parameters of 1

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(1,2)	1.390	A(2,1,6)	121.92	D(6,1,2,3)	0.00
R(1,6)	1.387	A(2,1,36)	119.01	D(6,1,2,42)	179.95
R(1,36)	1.456	A(6,1,36)	119.07	D(36,1,2,3)	-179.93
R(2,3)	1.380	A(1,2,3)	118.88	D(36,1,2,42)	0.03
R(2,42)	1.082	A(1,2,42)	119.96	D(2,1,6,5)	-0.02
R(3,4)	1.403	A(3,2,42)	121.16	D(2,1,6,45)	-179.98
R(3,43)	1.084	A(2,3,4)	120.83	D(36,1,6,5)	179.90
R(4,5)	1.401	A(2,3,43)	118.81	D(36,1,6,45)	-0.06
R(4,7)	1.456	A(4,3,43)	120.37	D(2,1,36,37)	179.84
R(5,6)	1.383	A(3,4,5)	118.67	D(2,1,36,38)	-0.15
R(5,44)	1.085	A(3,4,7)	123.09	D(6,1,36,37)	-0.08
R(6,45)	1.082	A(5,4,7)	118.24	D(6,1,36,38)	179.93
R(7,8)	1.337	A(4,5,6)	121.17	D(1,2,3,4)	0.01
R(7,46)	1.088	A(4,5,44)	119.40	D(1,2,3,43)	179.95
R(8,9)	1.481	A(6,5,44)	119.43	D(42,2,3,4)	-179.94
R(8,47)	1.086	A(1,6,5)	118.52	D(42,2,3,43)	0.00
R(9,10)	1.365	A(1,6,45)	120.16	D(2,3,4,5)	0.01
R(9,11)	1.227	A(5,6,45)	121.32	D(2,3,4,7)	-180.00
R(10,12)	1.400	A(4,7,8)	126.89	D(43,3,4,5)	-179.93
R(10,48)	1.010	A(4,7,46)	116.31	D(43,3,4,7)	0.07
R(12,13)	1.400	A(8,7,46)	116.79	D(3,4,5,6)	-0.03
R(12,17)	1.395	A(7,8,9)	119.89	D(3,4,5,44)	179.99
R(13,14)	1.382	A(7,8,47)	121.83	D(7,4,5,6)	179.97
R(13,49)	1.086	A(9,8,47)	118.28	D(7,4,5,44)	-0.01
R(14,15)	1.396	A(8,9,10)	113.01	D(3,4,7,8)	0.92
R(14,50)	1.086	A(8,9,11)	122.82	D(3,4,7,46)	-179.17
R(15,16)	1.390	A(10,9,11)	124.18	D(5,4,7,8)	-179.08
R(15,18)	1.508	A(9,10,12)	129.28	D(5,4,7,46)	0.83
R(16,17)	1.391	A(9,10,48)	115.78	D(4,5,6,1)	0.04

(Contd.)

Table S1 — Calculated geometric parameters of 1 (Contd.)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(16,51)	1.086	A(12,10,48)	114.93	D(4,5,6,45)	-180.00
R(17,52)	1.080	A(10,12,13)	116.99	D(44,5,6,1)	-179.98
R(18,19)	1.508	A(10,12,17)	123.96	D(44,5,6,45)	-0.02
R(18,53)	1.094	A(13,12,17)	119.06	D(4,7,8,9)	179.94
R(18,54)	1.094	A(12,13,14)	120.51	D(4,7,8,47)	0.03
R(19,20)	1.396	A(12,13,49)	119.74	D(46,7,8,9)	0.03
R(19,24)	1.390	A(14,13,49)	119.75	D(46,7,8,47)	-179.88
R(20,21)	1.382	A(13,14,15)	121.08	D(7,8,9,10)	179.93
R(20,55)	1.086	A(13,14,50)	119.29	D(7,8,9,11)	-0.08
R(21,22)	1.400	A(15,14,50)	119.63	D(47,8,9,10)	-0.15
R(21,56)	1.086	A(14,15,16)	117.91	D(47,8,9,11)	179.83
R(22,23)	1.395	A(14,15,18)	120.49	D(8,9,10,12)	-180.00
R(22,25)	1.400	A(16,15,18)	121.58	D(8,9,10,48)	-0.28
R(23,24)	1.391	A(15,16,17)	121.93	D(11,9,10,12)	0.02
R(23,57)	1.080	A(15,16,51)	119.40	D(11,9,10,48)	179.74
R(24,58)	1.086	A(17,16,51)	118.67	D(9,10,12,13)	179.47
R(25,26)	1.365	A(12,17,16)	119.51	D(9,10,12,17)	-0.65
R(25,59)	1.010	A(12,17,52)	119.83	D(48,10,12,13)	-0.25
R(26,27)	1.481	A(16,17,52)	120.65	D(48,10,12,17)	179.63
R(26,28)	1.227	A(15,18,19)	111.99	D(10,12,13,14)	-179.93
R(27,29)	1.337	A(15,18,53)	109.75	D(10,12,13,49)	0.06
R(27,60)	1.086	A(15,18,54)	109.22	D(17,12,13,14)	0.19
R(29,30)	1.456	A(19,18,53)	109.22	D(17,12,13,49)	-179.82
R(29,61)	1.088	A(19,18,54)	109.75	D(10,12,17,16)	-179.96
R(30,31)	1.403	A(53,18,54)	106.76	D(10,12,17,52)	-0.03
R(30,35)	1.401	A(18,19,20)	120.49	D(13,12,17,16)	-0.08
R(31,32)	1.380	A(18,19,24)	121.58	D(13,12,17,52)	179.85
R(31,62)	1.084	A(20,19,24)	117.91	D(12,13,14,15)	-0.20
R(32,33)	1.390	A(19,20,21)	121.08	D(12,13,14,50)	179.58
R(32,63)	1.082	A(19,20,55)	119.63	D(49,13,14,15)	179.81
R(33,34)	1.387	A(21,20,55)	119.29	D(49,13,14,50)	-0.41
R(33,39)	1.456	A(20,21,22)	120.51	D(13,14,15,16)	0.10
R(34,35)	1.383	A(20,21,56)	119.75	D(13,14,15,18)	178.60
R(34,64)	1.082	A(22,21,56)	119.74	D(50,14,15,16)	-179.68
R(35,65)	1.085	A(21,22,23)	119.06	D(50,14,15,18)	-1.18
R(36,37)	1.222	A(21,22,25)	116.99	D(14,15,16,17)	0.01
R(36,38)	1.222	A(23,22,25)	123.96	D(14,15,16,51)	-179.93
R(39,40)	1.222	A(22,23,24)	119.51	D(18,15,16,17)	-178.47
R(39,41)	1.222	A(22,23,57)	119.83	D(18,15,16,51)	1.59
		A(24,23,57)	120.65	D(14,15,18,19)	-68.37
		A(19,24,23)	121.93	D(14,15,18,53)	53.12
		A(19,24,58)	119.40	D(14,15,18,54)	169.84
		A(23,24,58)	118.67	D(16,15,18,19)	110.07
		A(22,25,26)	129.28	D(16,15,18,53)	-128.44
		A(22,25,59)	114.93	D(16,15,18,54)	-11.72
		A(26,25,59)	115.78	D(15,16,17,12)	-0.02
		A(25,26,27)	113.01	D(15,16,17,52)	-179.94
		A(25,26,28)	124.18	D(51,16,17,12)	179.92

(Contd.)

Table S1 — Calculated geometric parameters of 1 (Contd.)

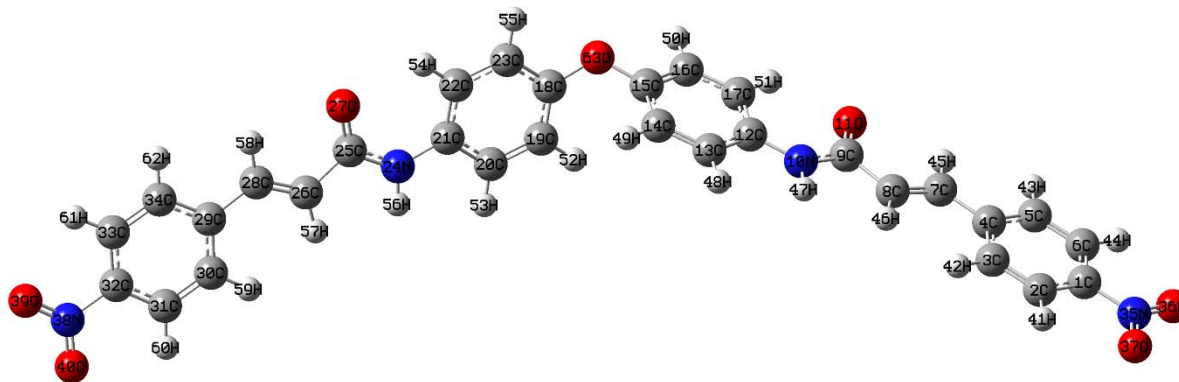
Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
		A(27,26,28)	122.82	D(51,16,17,52)	0.00
		A(26,27,29)	119.89	D(15,18,19,20)	-68.38
		A(26,27,60)	118.28	D(15,18,19,24)	110.06
		A(29,27,60)	121.83	D(53,18,19,20)	169.83
		A(27,29,30)	126.89	D(53,18,19,24)	-11.73
		A(27,29,61)	116.79	D(54,18,19,20)	53.11
		A(30,29,61)	116.32	D(54,18,19,24)	-128.45
		A(29,30,31)	123.09	D(18,19,20,21)	178.60
		A(29,30,35)	118.24	D(18,19,20,55)	-1.19
		A(31,30,35)	118.67	D(24,19,20,21)	0.10
		A(30,31,32)	120.83	D(24,19,20,55)	-179.68
		A(30,31,62)	120.37	D(18,19,24,23)	-178.47
		A(32,31,62)	118.81	D(18,19,24,58)	1.59
		A(31,32,33)	118.88	D(20,19,24,23)	0.01
		A(31,32,63)	121.16	D(20,19,24,58)	-179.93
		A(33,32,63)	119.96	D(19,20,21,22)	-0.20
		A(32,33,34)	121.92	D(19,20,21,56)	179.81
		A(32,33,39)	119.01	D(55,20,21,22)	179.58
		A(34,33,39)	119.07	D(55,20,21,56)	-0.41
		A(33,34,35)	118.52	D(20,21,22,23)	0.19
		A(33,34,64)	120.16	D(20,21,22,25)	-179.93
		A(35,34,64)	121.32	D(56,21,22,23)	-179.83
		A(30,35,34)	121.17	D(56,21,22,25)	0.06
		A(30,35,65)	119.40	D(21,22,23,24)	-0.08
		A(34,35,65)	119.43	D(21,22,23,57)	179.85
		A(1,36,37)	117.97	D(25,22,23,24)	-179.96
		A(1,36,38)	117.94	D(25,22,23,57)	-0.03
		A(37,36,38)	124.09	D(21,22,25,26)	179.50
		A(33,39,40)	117.97	D(21,22,25,59)	-0.24
		A(33,39,41)	117.93	D(23,22,25,26)	-0.61
		A(40,39,41)	124.10	D(23,22,25,59)	179.64
				D(22,23,24,19)	-0.02
				D(22,23,24,58)	179.92
				D(57,23,24,19)	-179.94
				D(57,23,24,58)	0.00
				D(22,25,26,27)	-180.01
				D(22,25,26,28)	0.01
				D(59,25,26,27)	-0.26
				D(59,25,26,28)	179.75
				D(25,26,27,29)	179.93
				D(25,26,27,60)	-0.16
				D(28,26,27,29)	-0.08
				D(28,26,27,60)	179.83
				D(26,27,29,30)	179.94
				D(26,27,29,61)	0.03
				D(60,27,29,30)	0.03
				D(60,27,29,61)	-179.88
				D(27,29,30,31)	0.91

(Contd.)

Table S1 — Calculated geometric parameters of 1 (*Contd.*)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
				D(27,29,30,35)	-179.09
				D(61,29,30,31)	-179.18
				D(61,29,30,35)	0.82
				D(29,30,31,32)	-180.00
				D(29,30,31,62)	0.06
				D(35,30,31,32)	0.01
				D(35,30,31,62)	-179.94
				D(29,30,35,34)	179.97
				D(29,30,35,65)	-0.01
				D(31,30,35,34)	-0.03
				D(31,30,35,65)	179.99
				D(30,31,32,33)	0.01
				D(30,31,32,63)	-179.94
				D(62,31,32,33)	179.95
				D(62,31,32,63)	0.00
				D(31,32,33,34)	0.00
				D(31,32,33,39)	-179.92
				D(63,32,33,34)	179.95
				D(63,32,33,39)	0.03
				D(32,33,34,35)	-0.02
				D(32,33,34,64)	-179.98
				D(39,33,34,35)	179.90
				D(39,33,34,64)	-0.06
				D(32,33,39,40)	179.83
				D(32,33,39,41)	-0.16
				D(34,33,39,40)	-0.10
				D(34,33,39,41)	179.91
				D(33,34,35,30)	0.04
				D(33,34,35,65)	-179.98
				D(64,34,35,30)	-180.00
				D(64,34,35,65)	-0.02

Table S2 — Calculated geometric parameters of 2



Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(1,2)	1.390	A(2,1,6)	121.92	D(6,1,2,3)	0.04
R(1,6)	1.387	A(2,1,35)	119.01	D(6,1,2,41)	-179.94
R(1,35)	1.456	A(6,1,35)	119.07	D(35,1,2,3)	-179.94
R(2,3)	1.379	A(1,2,3)	118.88	D(35,1,2,41)	0.08
R(2,41)	1.082	A(1,2,41)	119.97	D(2,1,6,5)	-0.04
R(3,4)	1.403	A(3,2,41)	121.16	D(2,1,6,44)	179.97
R(3,42)	1.084	A(2,3,4)	120.83	D(35,1,6,5)	179.95
R(4,5)	1.401	A(2,3,42)	118.79	D(35,1,6,44)	-0.05
R(4,7)	1.456	A(4,3,42)	120.37	D(2,1,35,36)	-179.79
R(5,6)	1.383	A(3,4,5)	118.68	D(2,1,35,37)	0.23
R(5,43)	1.085	A(3,4,7)	123.05	D(6,1,35,36)	0.23
R(6,44)	1.082	A(5,4,7)	118.27	D(6,1,35,37)	-179.76
R(7,8)	1.337	A(4,5,6)	121.16	D(1,2,3,4)	0.03
R(7,45)	1.088	A(4,5,43)	119.41	D(1,2,3,42)	-179.85
R(8,9)	1.480	A(6,5,43)	119.44	D(41,2,3,4)	-179.99
R(8,46)	1.086	A(1,6,5)	118.53	D(41,2,3,42)	0.12
R(9,10)	1.365	A(1,6,44)	120.16	D(2,3,4,5)	-0.10
R(9,11)	1.227	A(5,6,44)	121.31	D(2,3,4,7)	179.94
R(10,12)	1.400	A(4,7,8)	126.85	D(42,3,4,5)	179.78
R(10,47)	1.010	A(4,7,45)	116.32	D(42,3,4,7)	-0.18
R(12,13)	1.399	A(8,7,45)	116.83	D(3,4,5,6)	0.11
R(12,17)	1.396	A(7,8,9)	119.95	D(3,4,5,43)	-179.93
R(13,14)	1.382	A(7,8,46)	121.85	D(7,4,5,6)	-179.94
R(13,48)	1.086	A(9,8,46)	118.20	D(7,4,5,43)	0.02
R(14,15)	1.392	A(8,9,10)	113.00	D(3,4,7,8)	-1.43
R(14,49)	1.084	A(8,9,11)	122.86	D(3,4,7,45)	178.68
R(15,16)	1.385	A(10,9,11)	124.14	D(5,4,7,8)	178.61
R(15,63)	1.376	A(9,10,12)	129.10	D(5,4,7,45)	-1.27
R(16,17)	1.388	A(9,10,47)	115.81	D(4,5,6,1)	-0.04
R(16,50)	1.085	A(12,10,47)	115.09	D(4,5,6,44)	179.96
R(17,51)	1.080	A(10,12,13)	117.15	D(43,5,6,1)	-180.00
R(18,19)	1.392	A(10,12,17)	123.77	D(43,5,6,44)	0.00
R(18,23)	1.386	A(13,12,17)	119.08	D(4,7,8,9)	-179.91
R(18,63)	1.375	A(12,13,14)	120.95	D(4,7,8,46)	-0.05
R(19,20)	1.383	A(12,13,48)	119.86	D(45,7,8,9)	-0.02

(Contd.)

Table S2 — Calculated geometric parameters of 2 (Contd.)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(19,52)	1.084	A(14,13,48)	119.19	D(45,7,8,46)	179.83
R(20,21)	1.398	A(13,14,15)	119.51	D(7,8,9,10)	-179.82
R(20,53)	1.086	A(13,14,49)	120.27	D(7,8,9,11)	0.21
R(21,22)	1.397	A(15,14,49)	120.22	D(46,8,9,10)	0.32
R(21,24)	1.400	A(14,15,16)	120.05	D(46,8,9,11)	-179.65
R(22,23)	1.387	A(14,15,63)	122.52	D(8,9,10,12)	-179.77
R(22,54)	1.080	A(16,15,63)	117.33	D(8,9,10,47)	-0.12
R(23,55)	1.085	A(15,16,17)	120.58	D(11,9,10,12)	0.20
R(24,25)	1.364	A(15,16,50)	119.18	D(11,9,10,47)	179.84
R(24,56)	1.010	A(17,16,50)	120.24	D(9,10,12,13)	178.19
R(25,26)	1.481	A(12,17,16)	119.84	D(9,10,12,17)	-2.01
R(25,27)	1.227	A(12,17,51)	119.81	D(47,10,12,13)	-1.46
R(26,28)	1.337	A(16,17,51)	120.36	D(47,10,12,17)	178.35
R(26,57)	1.086	A(19,18,23)	119.97	D(10,12,13,14)	179.83
R(28,29)	1.456	A(19,18,63)	122.89	D(10,12,13,48)	0.27
R(28,58)	1.088	A(23,18,63)	117.05	D(17,12,13,14)	0.01
R(29,30)	1.403	A(18,19,20)	119.52	D(17,12,13,48)	-179.55
R(29,34)	1.401	A(18,19,52)	120.28	D(10,12,17,16)	179.73
R(30,31)	1.380	A(20,19,52)	120.19	D(10,12,17,51)	0.18
R(30,59)	1.084	A(19,20,21)	121.00	D(13,12,17,16)	-0.47
R(31,32)	1.390	A(19,20,53)	119.11	D(13,12,17,51)	179.99
R(31,60)	1.082	A(21,20,53)	119.89	D(12,13,14,15)	0.49
R(32,33)	1.387	A(20,21,22)	119.01	D(12,13,14,49)	-179.67
R(32,38)	1.456	A(20,21,24)	117.21	D(48,13,14,15)	-179.95
R(33,34)	1.383	A(22,21,24)	123.78	D(48,13,14,49)	-0.11
R(33,61)	1.082	A(21,22,23)	119.88	D(13,14,15,16)	-0.53
R(34,62)	1.085	A(21,22,54)	119.79	D(13,14,15,63)	-176.72
R(35,36)	1.222	A(23,22,54)	120.32	D(49,14,15,16)	179.63
R(35,37)	1.222	A(18,23,22)	120.61	D(49,14,15,63)	3.44
R(38,39)	1.222	A(18,23,55)	119.16	D(14,15,16,17)	0.07
R(38,40)	1.222	A(22,23,55)	120.22	D(14,15,16,50)	-179.81
		A(21,24,25)	129.09	D(63,15,16,17)	176.45
		A(21,24,56)	115.11	D(63,15,16,50)	-3.42
		A(25,24,56)	115.80	D(14,15,63,18)	-43.92
		A(24,25,26)	113.05	D(16,15,63,18)	139.80
		A(24,25,27)	124.14	D(15,16,17,12)	0.43
		A(26,25,27)	122.81	D(15,16,17,51)	179.97
		A(25,26,28)	119.89	D(50,16,17,12)	-179.69
		A(25,26,57)	118.28	D(50,16,17,51)	-0.15
		A(28,26,57)	121.83	D(23,18,19,20)	-0.41
		A(26,28,29)	126.86	D(23,18,19,52)	179.64
		A(26,28,58)	116.81	D(63,18,19,20)	-176.76
		A(29,28,58)	116.33	D(63,18,19,52)	3.28
		A(28,29,30)	123.07	D(19,18,23,22)	-0.02
		A(28,29,34)	118.26	D(19,18,23,55)	-179.91
		A(30,29,34)	118.67	D(63,18,23,22)	176.55
		A(29,30,31)	120.83	D(63,18,23,55)	-3.34
		A(29,30,59)	120.34	D(19,18,63,15)	-37.70

(Contd.)

Table S2 — Calculated geometric parameters of 2 (Contd.)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
		A(31,30,59)	118.83	D(23,18,63,15)	145.85
		A(30,31,32)	118.89	D(18,19,20,21)	0.45
		A(30,31,60)	121.16	D(18,19,20,53)	-179.99
		A(32,31,60)	119.95	D(52,19,20,21)	-179.59
		A(31,32,33)	121.92	D(52,19,20,53)	-0.03
		A(31,32,38)	119.02	D(19,20,21,22)	-0.07
		A(33,32,38)	119.06	D(19,20,21,24)	179.93
		A(32,33,34)	118.52	D(53,20,21,22)	-179.63
		A(32,33,61)	120.17	D(53,20,21,24)	0.37
		A(34,33,61)	121.31	D(20,21,22,23)	-0.36
		A(29,34,33)	121.17	D(20,21,22,54)	-179.93
		A(29,34,62)	119.40	D(24,21,22,23)	179.65
		A(33,34,62)	119.42	D(24,21,22,54)	0.08
		A(1,35,36)	117.97	D(20,21,24,25)	-179.61
		A(1,35,37)	117.94	D(20,21,24,56)	0.08
		A(36,35,37)	124.09	D(22,21,24,25)	0.38
		A(32,38,39)	117.97	D(22,21,24,56)	-179.92
		A(32,38,40)	117.95	D(21,22,23,18)	0.40
		A(39,38,40)	124.09	D(21,22,23,55)	-179.71
		A(15,63,18)	119.15	D(54,22,23,18)	179.97
				D(54,22,23,55)	-0.15
				D(21,24,25,26)	-180.00
				D(21,24,25,27)	-0.02
				D(56,24,25,26)	0.31
				D(56,24,25,27)	-179.72
				D(24,25,26,28)	-179.26
				D(24,25,26,57)	0.53
				D(27,25,26,28)	0.76
				D(27,25,26,57)	-179.45
				D(25,26,28,29)	180.00
				D(25,26,28,58)	0.37
				D(57,26,28,29)	0.21
				D(57,26,28,58)	-179.41
				D(26,28,29,30)	3.94
				D(26,28,29,34)	-176.21
				D(58,28,29,30)	-176.44
				D(58,28,29,34)	3.41
				D(28,29,30,31)	-179.97
				D(28,29,30,59)	0.34
				D(34,29,30,31)	0.18
				D(34,29,30,59)	-179.51
				D(28,29,34,33)	179.86
				D(28,29,34,62)	-0.06
				D(30,29,34,33)	-0.28
				D(30,29,34,62)	179.80
				D(29,30,31,32)	0.00
				D(29,30,31,60)	-179.90
				D(59,30,31,32)	179.70

(Contd.)

Table S2 — Calculated geometric parameters of 2 (*Contd.*)

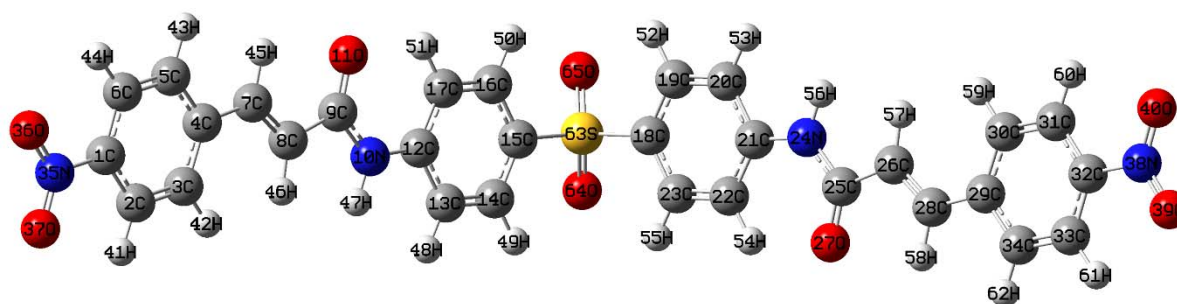
---

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
				D(59,30,31,60)	-0.20
				D(30,31,32,33)	-0.10
				D(30,31,32,38)	-179.95
				D(60,31,32,33)	179.80
				D(60,31,32,38)	-0.05
				D(31,32,33,34)	0.01
				D(31,32,33,61)	-179.89
				D(38,32,33,34)	179.86
				D(38,32,33,61)	-0.03
				D(31,32,38,39)	-179.84
				D(31,32,38,40)	0.16
				D(33,32,38,39)	0.30
				D(33,32,38,40)	-179.70
				D(32,33,34,29)	0.18
				D(32,33,34,62)	-179.90
				D(61,33,34,29)	-179.92
				D(61,33,34,62)	0.00

---



Table S3 — Calculated geometric parameters of 3



Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(1,2)	1.390	A(2,1,6)	121.98	D(6,1,2,3)	0.06
R(1,6)	1.386	A(2,1,35)	119.00	D(6,1,2,41)	-179.95
R(1,35)	1.457	A(6,1,35)	119.03	D(35,1,2,3)	-179.98
R(2,3)	1.380	A(1,2,3)	118.85	D(35,1,2,41)	0.01
R(2,41)	1.082	A(1,2,41)	119.97	D(2,1,6,5)	-0.01
R(3,4)	1.403	A(3,2,41)	121.18	D(2,1,6,44)	179.96
R(3,42)	1.083	A(2,3,4)	120.80	D(35,1,6,5)	-179.97
R(4,5)	1.401	A(2,3,42)	118.81	D(35,1,6,44)	0.00
R(4,7)	1.456	A(4,3,42)	120.39	D(2,1,35,36)	179.61
R(5,6)	1.383	A(3,4,5)	118.75	D(2,1,35,37)	-0.37
R(5,43)	1.085	A(3,4,7)	123.00	D(6,1,35,36)	-0.42
R(6,44)	1.082	A(5,4,7)	118.26	D(6,1,35,37)	179.59
R(7,8)	1.337	A(4,5,6)	121.12	D(1,2,3,4)	-0.04
R(7,45)	1.088	A(4,5,43)	119.43	D(1,2,3,42)	-179.99
R(8,9)	1.479	A(6,5,43)	119.45	D(41,2,3,4)	179.96
R(8,46)	1.085	A(1,6,5)	118.51	D(41,2,3,42)	0.02
R(9,10)	1.372	A(1,6,44)	120.17	D(2,3,4,5)	-0.02
R(9,11)	1.223	A(5,6,44)	121.32	D(2,3,4,7)	179.97
R(10,12)	1.391	A(4,7,8)	126.78	D(42,3,4,5)	179.93
R(10,47)	1.010	A(4,7,45)	116.28	D(42,3,4,7)	-0.08
R(12,13)	1.402	A(8,7,45)	116.94	D(3,4,5,6)	0.07
R(12,17)	1.400	A(7,8,9)	119.88	D(3,4,5,43)	-179.98
R(13,14)	1.380	A(7,8,46)	121.90	D(7,4,5,6)	-179.93
R(13,48)	1.086	A(9,8,46)	118.22	D(7,4,5,43)	0.03
R(14,15)	1.390	A(8,9,10)	112.87	D(3,4,7,8)	-0.86
R(14,49)	1.084	A(8,9,11)	123.20	D(3,4,7,45)	179.24
R(15,16)	1.387	A(10,9,11)	123.93	D(5,4,7,8)	179.13
R(15,63)	1.766	A(9,10,12)	129.17	D(5,4,7,45)	-0.76
R(16,17)	1.385	A(9,10,47)	115.68	D(4,5,6,1)	-0.05
R(16,50)	1.084	A(12,10,47)	115.15	D(4,5,6,44)	179.98
R(17,51)	1.079	A(10,12,13)	116.90	D(43,5,6,1)	179.99
R(18,19)	1.390	A(10,12,17)	123.49	D(43,5,6,44)	0.02
R(18,23)	1.387	A(13,12,17)	119.61	D(4,7,8,9)	-179.96
R(18,63)	1.766	A(12,13,14)	120.58	D(4,7,8,46)	0.01
R(19,20)	1.380	A(12,13,48)	119.84	D(45,7,8,9)	-0.06
R(19,52)	1.084	A(14,13,48)	119.58	D(45,7,8,46)	179.90
R(20,21)	1.402	A(13,14,15)	119.23	D(7,8,9,10)	179.86
R(20,53)	1.086	A(13,14,49)	120.43	D(7,8,9,11)	-0.12

(Contd.)

Table S3 — Calculated geometric parameters of 3 (Contd.)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
R(21,22)	1.400	A(15,14,49)	120.33	D(46,8,9,10)	-0.11
R(21,24)	1.391	A(14,15,16)	120.90	D(46,8,9,11)	179.92
R(22,23)	1.385	A(14,15,63)	119.47	D(8,9,10,12)	-179.81
R(22,54)	1.079	A(16,15,63)	119.60	D(8,9,10,47)	-0.60
R(23,55)	1.084	A(15,16,17)	120.09	D(11,9,10,12)	0.16
R(24,25)	1.372	A(15,16,50)	120.01	D(11,9,10,47)	179.37
R(24,56)	1.010	A(17,16,50)	119.89	D(9,10,12,13)	177.52
R(25,26)	1.479	A(12,17,16)	119.59	D(9,10,12,17)	-2.87
R(25,27)	1.223	A(12,17,51)	119.85	D(47,10,12,13)	-1.69
R(26,28)	1.337	A(16,17,51)	120.56	D(47,10,12,17)	177.92
R(26,57)	1.085	A(19,18,23)	120.90	D(10,12,13,14)	179.89
R(28,29)	1.456	A(19,18,63)	119.47	D(10,12,13,48)	0.05
R(28,58)	1.088	A(23,18,63)	119.60	D(17,12,13,14)	0.27
R(29,30)	1.403	A(18,19,20)	119.23	D(17,12,13,48)	-179.58
R(29,34)	1.401	A(18,19,52)	120.33	D(10,12,17,16)	-179.87
R(30,31)	1.380	A(20,19,52)	120.43	D(10,12,17,51)	-0.07
R(30,59)	1.083	A(19,20,21)	120.58	D(13,12,17,16)	-0.27
R(31,32)	1.390	A(19,20,53)	119.58	D(13,12,17,51)	179.53
R(31,60)	1.082	A(21,20,53)	119.84	D(12,13,14,15)	-0.16
R(32,33)	1.386	A(20,21,22)	119.61	D(12,13,14,49)	-179.59
R(32,38)	1.457	A(20,21,24)	116.90	D(48,13,14,15)	179.68
R(33,34)	1.383	A(22,21,24)	123.49	D(48,13,14,49)	0.25
R(33,61)	1.082	A(21,22,23)	119.59	D(13,14,15,16)	0.06
R(34,62)	1.085	A(21,22,54)	119.85	D(13,14,15,63)	178.24
R(35,36)	1.222	A(23,22,54)	120.56	D(49,14,15,16)	179.49
R(35,37)	1.222	A(18,23,22)	120.09	D(49,14,15,63)	-2.33
R(38,39)	1.222	A(18,23,55)	120.01	D(14,15,16,17)	-0.07
R(38,40)	1.222	A(22,23,55)	119.89	D(14,15,16,50)	-179.47
R(63,64)	1.454	A(21,24,25)	129.17	D(63,15,16,17)	-178.24
R(63,65)	1.454	A(21,24,56)	115.15	D(63,15,16,50)	2.36
		A(25,24,56)	115.68	D(14,15,63,18)	-89.62
		A(24,25,26)	112.87	D(14,15,63,64)	25.05
		A(24,25,27)	123.93	D(14,15,63,65)	155.76
		A(26,25,27)	123.20	D(16,15,63,18)	88.57
		A(25,26,28)	119.88	D(16,15,63,64)	-156.75
		A(25,26,57)	118.22	D(16,15,63,65)	-26.05
		A(28,26,57)	121.90	D(15,16,17,12)	0.17
		A(26,28,29)	126.78	D(15,16,17,51)	-179.63
		A(26,28,58)	116.94	D(50,16,17,12)	179.57
		A(29,28,58)	116.28	D(50,16,17,51)	-0.23
		A(28,29,30)	123.00	D(23,18,19,20)	0.06
		A(28,29,34)	118.26	D(23,18,19,52)	179.49
		A(30,29,34)	118.74	D(63,18,19,20)	178.24
		A(29,30,31)	120.80	D(63,18,19,52)	-2.33
		A(29,30,59)	120.39	D(19,18,23,22)	-0.07
		A(31,30,59)	118.81	D(19,18,23,55)	-179.47
		A(30,31,32)	118.85	D(63,18,23,22)	-178.24
		A(30,31,60)	121.18	D(63,18,23,55)	2.36

(Contd.)

Table S3 — Calculated geometric parameters of 3 (Contd.)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
		A(32,31,60)	119.97	D(19,18,63,15)	-89.62
		A(31,32,33)	121.98	D(19,18,63,64)	155.75
		A(31,32,38)	119.00	D(19,18,63,65)	25.05
		A(33,32,38)	119.03	D(23,18,63,15)	88.57
		A(32,33,34)	118.51	D(23,18,63,64)	-26.05
		A(32,33,61)	120.17	D(23,18,63,65)	-156.75
		A(34,33,61)	121.32	D(18,19,20,21)	-0.16
		A(29,34,33)	121.12	D(18,19,20,53)	179.68
		A(29,34,62)	119.43	D(52,19,20,21)	-179.59
		A(33,34,62)	119.45	D(52,19,20,53)	0.25
		A(1,35,36)	117.94	D(19,20,21,22)	0.27
		A(1,35,37)	117.91	D(19,20,21,24)	179.89
		A(36,35,37)	124.14	D(53,20,21,22)	-179.58
		A(32,38,39)	117.94	D(53,20,21,24)	0.05
		A(32,38,40)	117.91	D(20,21,22,23)	-0.27
		A(39,38,40)	124.14	D(20,21,22,54)	179.53
		A(15,63,18)	104.38	D(24,21,22,23)	-179.87
		A(15,63,64)	107.90	D(24,21,22,54)	-0.07
		A(15,63,65)	107.97	D(20,21,24,25)	177.53
		A(18,63,64)	107.97	D(20,21,24,56)	-1.69
		A(18,63,65)	107.90	D(22,21,24,25)	-2.86
		A(64,63,65)	119.71	D(22,21,24,56)	177.92
				D(21,22,23,18)	0.17
				D(21,22,23,55)	179.57
				D(54,22,23,18)	-179.63
				D(54,22,23,55)	-0.23
				D(21,24,25,26)	-179.81
				D(21,24,25,27)	0.16
				D(56,24,25,26)	-0.60
				D(56,24,25,27)	179.37
				D(24,25,26,28)	179.86
				D(24,25,26,57)	-0.11
				D(27,25,26,28)	-0.12
				D(27,25,26,57)	179.92
				D(25,26,28,29)	-179.96
				D(25,26,28,58)	-0.06
				D(57,26,28,29)	0.01
				D(57,26,28,58)	179.90
				D(26,28,29,30)	-0.86
				D(26,28,29,34)	179.13
				D(58,28,29,30)	179.24
				D(58,28,29,34)	-0.77
				D(28,29,30,31)	179.97
				D(28,29,30,59)	-0.08
				D(34,29,30,31)	-0.02
				D(34,29,30,59)	179.93
				D(28,29,34,33)	-179.93
				D(28,29,34,62)	0.03

(Contd.)

Table S3 — Calculated geometric parameters of 3 (*Contd.*)

Atoms	Bond Length (Å)	Atoms	Bond Angle (°)	Atoms	Dihedral Angle (°)
				D(30,29,34,33)	0.07
				D(30,29,34,62)	-179.98
				D(29,30,31,32)	-0.04
				D(29,30,31,60)	179.96
				D(59,30,31,32)	-179.99
				D(59,30,31,60)	0.02
				D(30,31,32,33)	0.06
				D(30,31,32,38)	-179.98
				D(60,31,32,33)	-179.95
				D(60,31,32,38)	0.01
				D(31,32,33,34)	-0.01
				D(31,32,33,61)	179.96
				D(38,32,33,34)	-179.97
				D(38,32,33,61)	0.00
				D(31,32,38,39)	179.61
				D(31,32,38,40)	-0.37
				D(33,32,38,39)	-0.42
				D(33,32,38,40)	179.59
				D(32,33,34,29)	-0.05
				D(32,33,34,62)	179.99
				D(61,33,34,29)	179.98
				D(61,33,34,62)	0.02

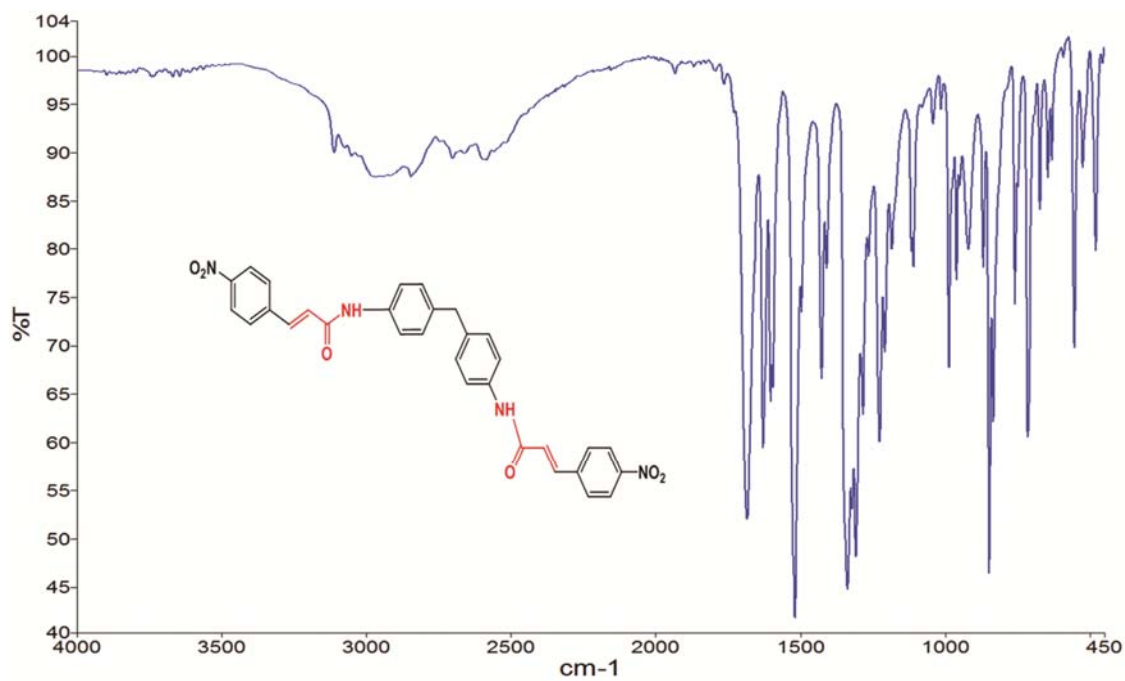


Fig S1 — IR spectrum of compound 1

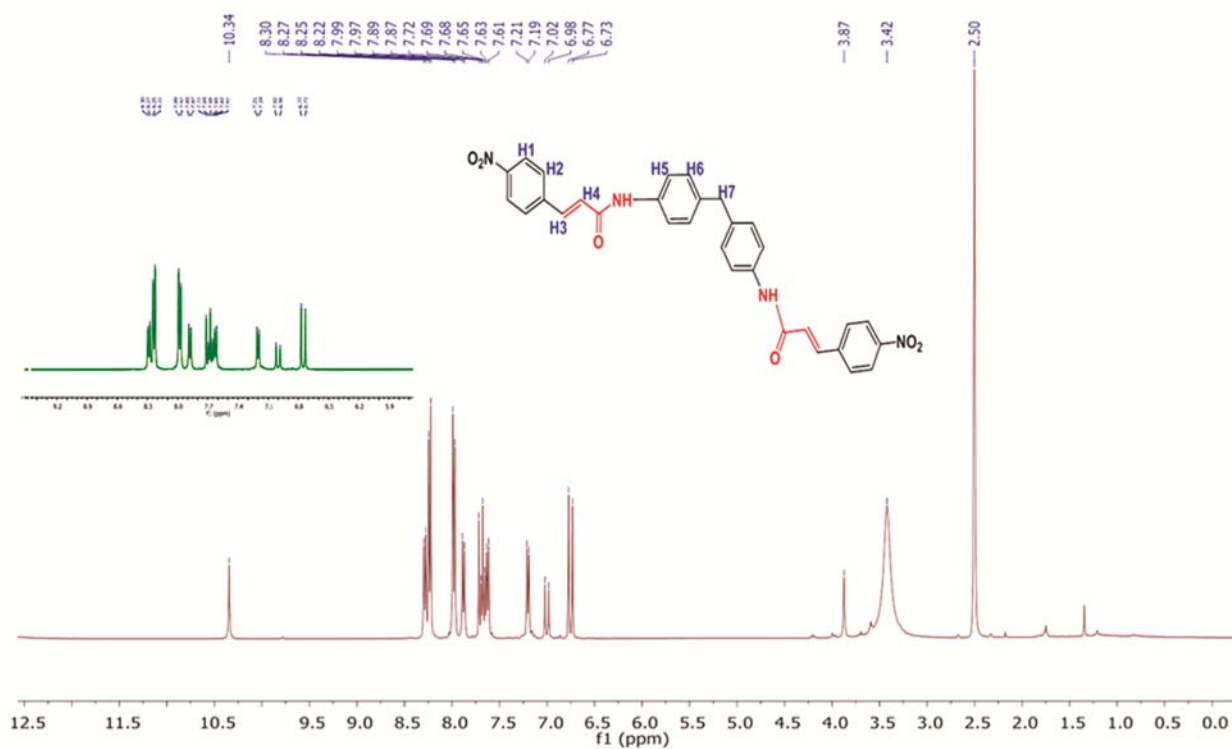


Fig S2 — <sup>1</sup>H NMR spectrum of compound 1

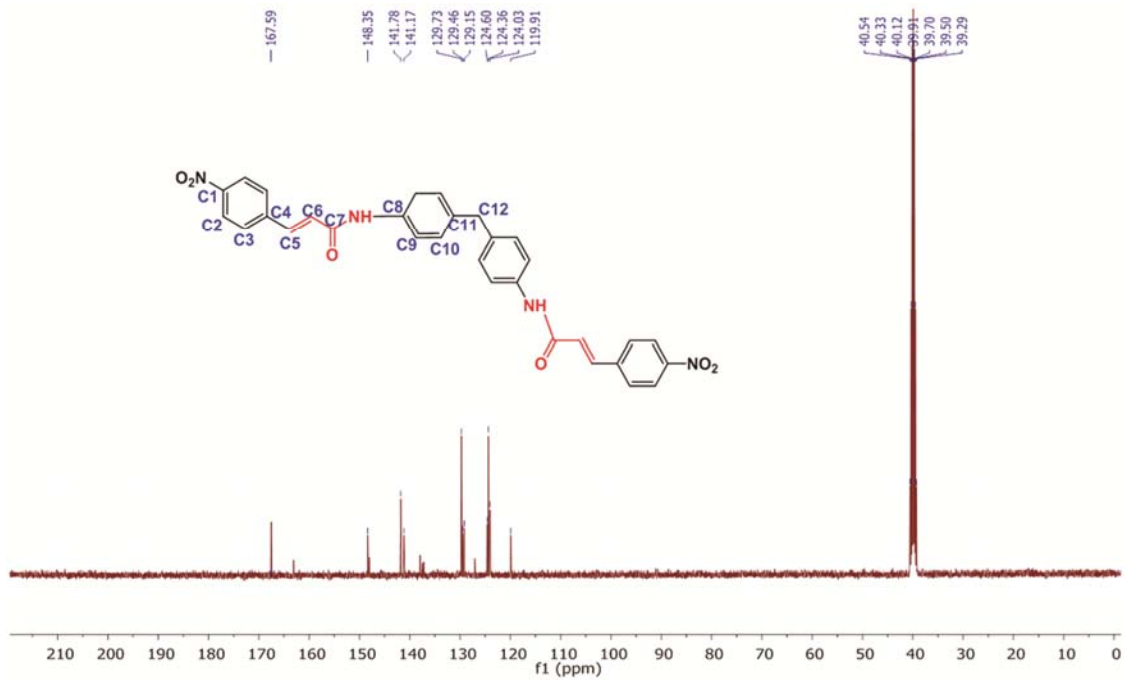
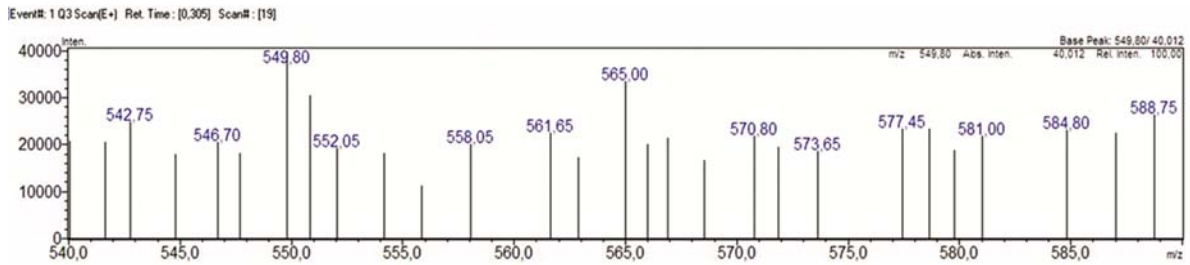
Fig S3 —  $^{13}\text{C}$  NMR spectrum of compound 1

Fig S4 — LS-MS/MS spectrum of compound 1

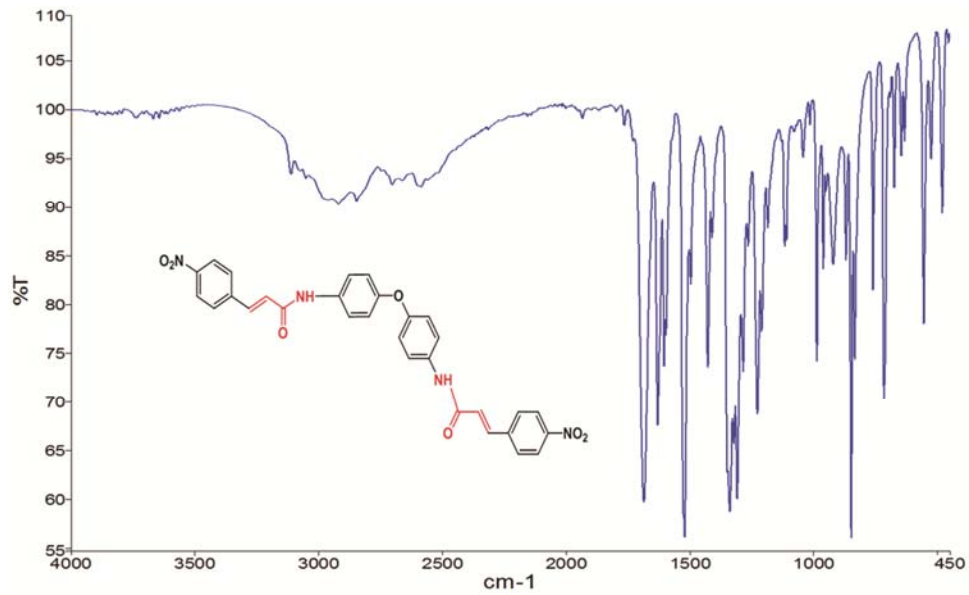


Fig S5 — IR spectrum of compound 2

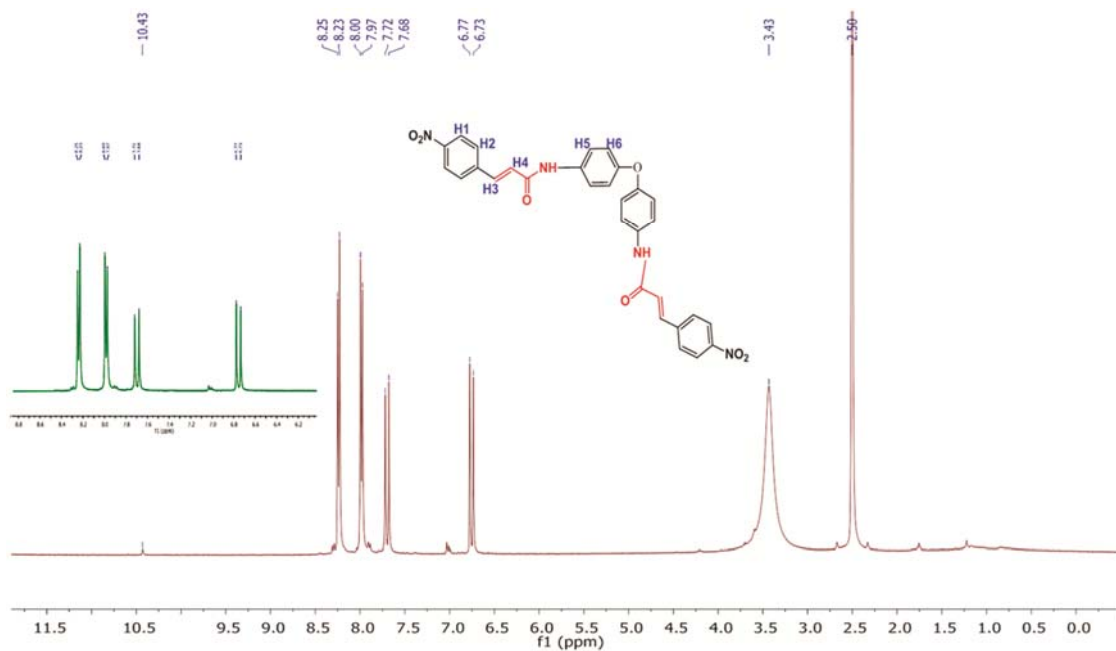


Fig S6 — <sup>1</sup>H NMR spectrum of compound 2

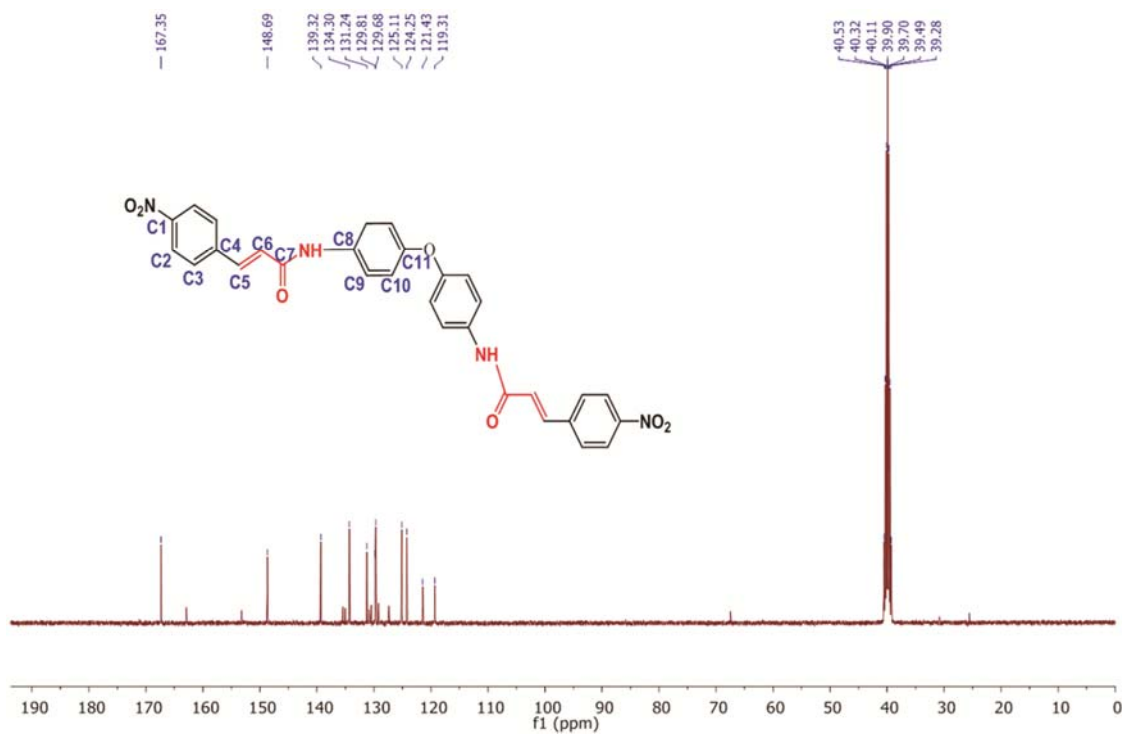


Fig S7 — <sup>13</sup>C NMR spectrum of compound 2

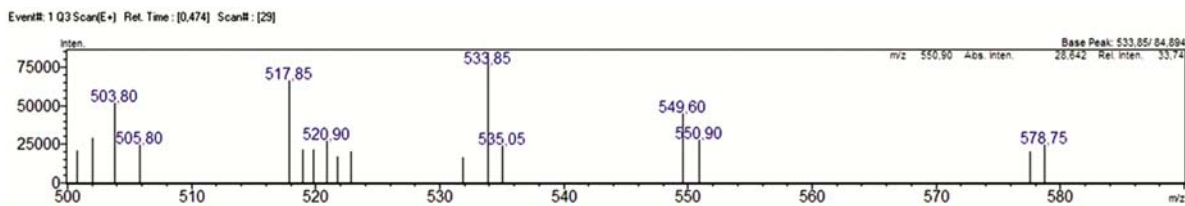


Fig S8 — LS-MS/MS spectrum of compound 2

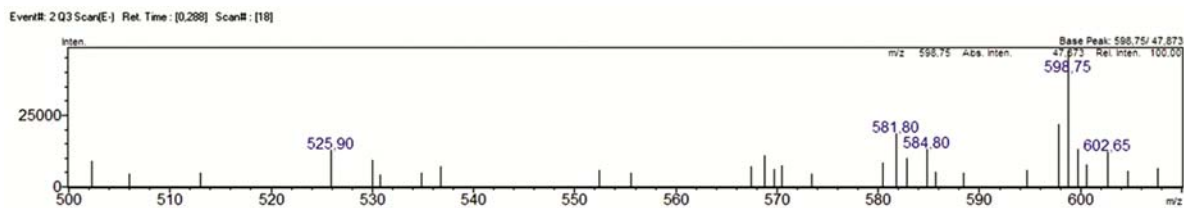


Fig S9: LS-MS/MS spectrum of compound 3

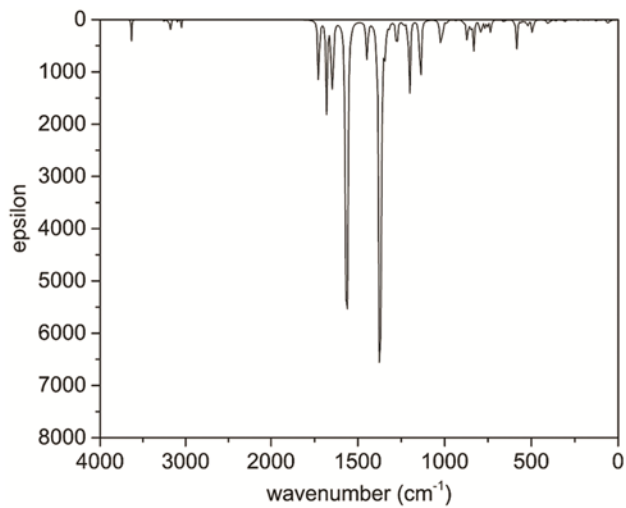


Fig S10 — Calculated IR spectra of 1

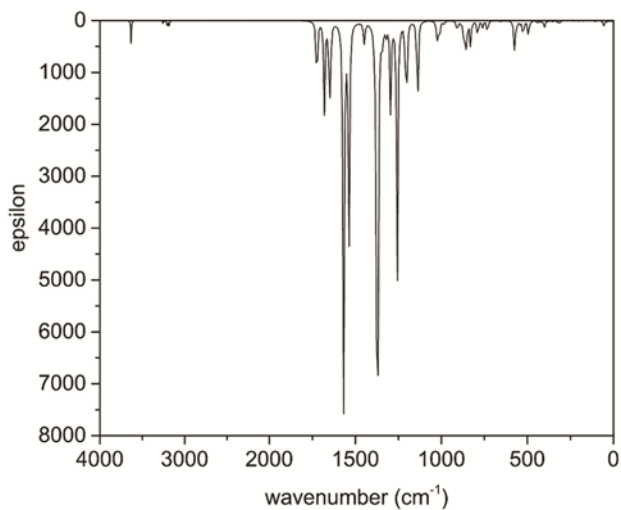


Fig S11 — Calculated IR spectra of 2



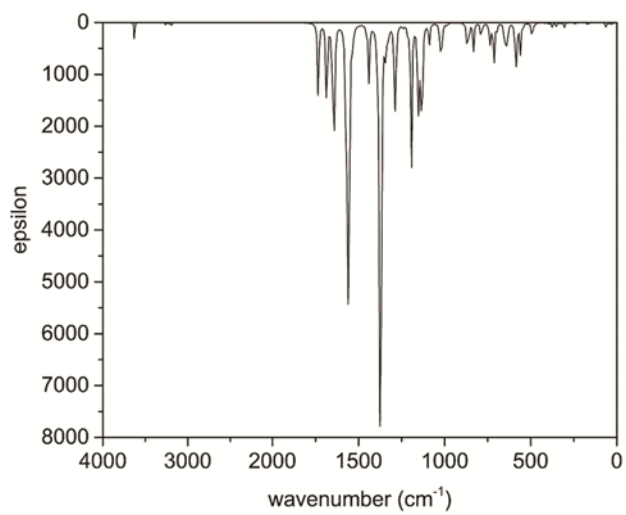


Fig S12 — Calculated IR spectra of 3