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Diverse structural assemblies of U-shaped hydrazinyl-sulfonamides: experimental and theoretical analysis of non-covalent interactions stabilizing the solid state conformations

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Table S1. Bond lengths [Å] and angles [°] for compound **5a**.

S(1)-O(2)	1.434(2)	N(1)-H(1)	0.79(4)
S(1)-O(1)	1.436(2)	C(7)-C(8)	1.536(3)
S(1)-N(1)	1.610(2)	C(7)-C(71)	1.542(4)
S(1)-C(1)	1.772(3)	C(7)-H(7)	0.9800
C(1)-C(6)	1.380(4)	C(71)-C(72)	1.521(4)
C(1)-C(2)	1.385(4)	C(71)-C(73)	1.522(4)
C(2)-C(3)	1.387(4)	C(71)-H(71)	0.9800
C(2)-H(2)	0.9300	C(72)-H(72A)	0.9600
C(3)-C(4)	1.389(6)	C(72)-H(72B)	0.9600
C(3)-H(3)	0.9300	C(72)-H(72C)	0.9600
C(4)-C(5)	1.389(5)	C(73)-H(73A)	0.9600
C(4)-C(41)	1.509(5)	C(73)-H(73B)	0.9600
C(41)-H(41A)	0.9600	C(73)-H(73C)	0.9600
C(41)-H(41B)	0.9600	C(8)-O(8)	1.227(3)
C(41)-H(41C)	0.9600	C(8)-N(2)	1.320(3)
C(5)-C(6)	1.378(5)	N(2)-N(3)	1.412(3)
C(5)-H(5)	0.9300	N(2)-H(2A)	0.80(4)
C(6)-H(6)	0.9300	N(3)-H(3A)	0.83(4)
N(1)-C(7)	1.460(3)	N(3)-H(3B)	0.74(5)
O(2)-S(1)-O(1)	119.65(14)	C(4)-C(3)-H(3)	119.5
O(2)-S(1)-N(1)	107.75(14)	C(5)-C(4)-C(3)	118.0(3)
O(1)-S(1)-N(1)	105.93(15)	C(5)-C(4)-C(41)	120.5(4)
O(2)-S(1)-C(1)	106.30(14)	C(3)-C(4)-C(41)	121.5(4)
O(1)-S(1)-C(1)	108.83(14)	C(4)-C(41)-H(41A)	109.5
N(1)-S(1)-C(1)	107.92(12)	C(4)-C(41)-H(41B)	109.5
C(6)-C(1)-C(2)	120.1(3)	H(41A)-C(41)-H(41B)	109.5
C(6)-C(1)-S(1)	120.2(2)	C(4)-C(41)-H(41C)	109.5
C(2)-C(1)-S(1)	119.6(2)	H(41A)-C(41)-H(41C)	109.5
C(1)-C(2)-C(3)	119.5(3)	H(41B)-C(41)-H(41C)	109.5
C(1)-C(2)-H(2)	120.2	C(6)-C(5)-C(4)	121.5(3)
C(3)-C(2)-H(2)	120.2	C(6)-C(5)-H(5)	119.2
C(2)-C(3)-C(4)	121.1(3)	C(4)-C(5)-H(5)	119.2
C(2)-C(3)-H(3)	119.5	C(5)-C(6)-C(1)	119.7(3)

C(5)-C(6)-H(6)	120.2	H(72A)-C(72)-H(72B)	109.5
C(1)-C(6)-H(6)	120.2	C(71)-C(72)-H(72C)	109.5
C(7)-N(1)-S(1)	122.22(19)	H(72A)-C(72)-H(72C)	109.5
C(7)-N(1)-H(1)	114(2)	H(72B)-C(72)-H(72C)	109.5
S(1)-N(1)-H(1)	116(2)	C(71)-C(73)-H(73A)	109.5
N(1)-C(7)-C(8)	109.7(2)	C(71)-C(73)-H(73B)	109.5
N(1)-C(7)-C(71)	109.5(2)	H(73A)-C(73)-H(73B)	109.5
C(8)-C(7)-C(71)	109.6(2)	C(71)-C(73)-H(73C)	109.5
N(1)-C(7)-H(7)	109.3	H(73A)-C(73)-H(73C)	109.5
C(8)-C(7)-H(7)	109.3	H(73B)-C(73)-H(73C)	109.5
C(71)-C(7)-H(7)	109.3	O(8)-C(8)-N(2)	122.1(2)
C(72)-C(71)-C(73)	109.8(3)	O(8)-C(8)-C(7)	121.4(2)
C(72)-C(71)-C(7)	111.7(2)	N(2)-C(8)-C(7)	116.5(2)
C(73)-C(71)-C(7)	110.8(3)	C(8)-N(2)-N(3)	121.8(2)
C(72)-C(71)-H(71)	108.2	C(8)-N(2)-H(2A)	121(3)
C(73)-C(71)-H(71)	108.2	N(3)-N(2)-H(2A)	117(3)
C(7)-C(71)-H(71)	108.2	N(2)-N(3)-H(3A)	110(3)
C(71)-C(72)-H(72A)	109.5	N(2)-N(3)-H(3B)	102(4)
C(71)-C(72)-H(72B)	109.5	H(3A)-N(3)-H(3B)	120(5)

Table S2. Bond lengths [Å] and angles [°] for compound **5b**.

S(1)-O(1)	1.4352(19)	C(7)-C(71)	1.531(3)
S(1)-O(2)	1.4363(18)	C(7)-H(7)	0.9800
S(1)-N(1)	1.599(2)	C(71)-C(72)	1.526(5)
S(1)-C(1)	1.766(2)	C(71)-H(71A)	0.9700
C(1)-C(6)	1.372(3)	C(71)-H(71B)	0.9700
C(1)-C(2)	1.391(4)	C(72)-C(73)	1.503(6)
C(2)-C(3)	1.379(4)	C(72)-C(74)	1.524(7)
C(2)-H(2)	0.9300	C(72)-H(72)	0.9800
C(3)-C(4)	1.383(5)	C(73)-H(73A)	0.9600
C(3)-H(3)	0.9300	C(73)-H(73B)	0.9600
C(4)-C(5)	1.389(4)	C(73)-H(73C)	0.9600
C(4)-C(41)	1.512(4)	C(74)-H(74A)	0.9600
C(41)-H(41A)	0.9600	C(74)-H(74B)	0.9600
C(41)-H(41B)	0.9600	C(74)-H(74C)	0.9600
C(41)-H(41C)	0.9600	C(8)-O(8)	1.225(3)
C(5)-C(6)	1.386(4)	C(8)-N(2)	1.337(3)
C(5)-H(5)	0.9300	N(2)-N(3)	1.411(3)
C(6)-H(6)	0.9300	N(2)-H(2N)	0.81(3)
N(1)-C(7)	1.464(3)	N(3)-H(3N1)	0.91(3)
N(1)-H(1N)	0.82(3)	N(3)-H(3N2)	0.94(3)
C(7)-C(8)	1.530(3)		

O(1)-S(1)-O(2)	119.15(12)	C(2)-C(3)-C(4)	121.7(3)
O(1)-S(1)-N(1)	106.20(12)	C(2)-C(3)-H(3)	119.1
O(2)-S(1)-N(1)	108.00(11)	C(4)-C(3)-H(3)	119.1
O(1)-S(1)-C(1)	107.09(11)	C(3)-C(4)-C(5)	117.9(3)
O(2)-S(1)-C(1)	107.18(12)	C(3)-C(4)-C(41)	121.1(3)
N(1)-S(1)-C(1)	108.94(10)	C(5)-C(4)-C(41)	121.0(3)
C(6)-C(1)-C(2)	120.1(2)	C(4)-C(41)-H(41A)	109.5
C(6)-C(1)-S(1)	121.43(19)	C(4)-C(41)-H(41B)	109.5
C(2)-C(1)-S(1)	118.5(2)	H(41A)-C(41)-H(41B)	109.5
C(3)-C(2)-C(1)	119.3(3)	C(4)-C(41)-H(41C)	109.5
C(3)-C(2)-H(2)	120.3	H(41A)-C(41)-H(41C)	109.5
C(1)-C(2)-H(2)	120.3	H(41B)-C(41)-H(41C)	109.5

C(6)-C(5)-C(4)	121.2(3)	C(73)-C(72)-H(72)	108.1
C(6)-C(5)-H(5)	119.4	C(74)-C(72)-H(72)	108.1
C(4)-C(5)-H(5)	119.4	C(71)-C(72)-H(72)	108.1
C(1)-C(6)-C(5)	119.8(2)	C(72)-C(73)-H(73A)	109.5
C(1)-C(6)-H(6)	120.1	C(72)-C(73)-H(73B)	109.5
C(5)-C(6)-H(6)	120.1	H(73A)-C(73)-H(73B)	109.5
C(7)-N(1)-S(1)	123.53(16)	C(72)-C(73)-H(73C)	109.5
C(7)-N(1)-H(1N)	119(2)	H(73A)-C(73)-H(73C)	109.5
S(1)-N(1)-H(1N)	109.8(19)	H(73B)-C(73)-H(73C)	109.5
N(1)-C(7)-C(8)	109.33(17)	C(72)-C(74)-H(74A)	109.5
N(1)-C(7)-C(71)	107.5(2)	C(72)-C(74)-H(74B)	109.5
C(8)-C(7)-C(71)	113.00(19)	H(74A)-C(74)-H(74B)	109.5
N(1)-C(7)-H(7)	109.0	C(72)-C(74)-H(74C)	109.5
C(8)-C(7)-H(7)	109.0	H(74A)-C(74)-H(74C)	109.5
C(71)-C(7)-H(7)	109.0	H(74B)-C(74)-H(74C)	109.5
C(72)-C(71)-C(7)	116.1(3)	O(8)-C(8)-N(2)	122.5(2)
C(72)-C(71)-H(71A)	108.3	O(8)-C(8)-C(7)	121.7(2)
C(7)-C(71)-H(71A)	108.3	N(2)-C(8)-C(7)	115.76(19)
C(72)-C(71)-H(71B)	108.3	C(8)-N(2)-N(3)	121.4(2)
C(7)-C(71)-H(71B)	108.3	C(8)-N(2)-H(2N)	120(3)
H(71A)-C(71)-H(71B)	107.4	N(3)-N(2)-H(2N)	119(3)
C(73)-C(72)-C(74)	109.7(4)	N(2)-N(3)-H(3N1)	110(2)
C(73)-C(72)-C(71)	113.5(3)	N(2)-N(3)-H(3N2)	108(2)
C(74)-C(72)-C(71)	109.3(4)	H(3N1)-N(3)-H(3N2)	103(3)

Table S3. Bond lengths [Å] and angles [°] for compound **5c**.

S(1)-O(2)	1.433(2)	C(5)-H(5)	0.9300
S(1)-O(1)	1.4352(19)	C(6)-H(6)	0.9300
S(1)-N(1)	1.604(2)	C(7)-C(8)	1.519(4)
S(1)-C(1)	1.762(3)	C(7)-C(71)	1.537(3)
O(8)-C(8)	1.223(3)	C(7)-H(7)	0.9800
N(1)-C(7)	1.463(3)	C(8)-N(2)	1.327(4)
N(1)-H(1N)	0.80(3)	C(71)-C(72)	1.512(4)
C(1)-C(6)	1.376(4)	C(71)-C(73)	1.520(5)
C(1)-C(2)	1.387(4)	C(71)-H(71)	0.9800
C(2)-C(3)	1.371(4)	C(72)-H(72A)	0.9600
C(2)-H(2)	0.9300	C(72)-H(72B)	0.9600
C(3)-C(4)	1.395(4)	C(72)-H(72C)	0.9600
C(3)-H(3)	0.9300	C(73)-H(73A)	0.9600
C(4)-O(4)	1.353(3)	C(73)-H(73B)	0.9600
C(4)-C(5)	1.379(4)	C(73)-H(73C)	0.9600
O(4)-C(41)	1.413(4)	N(2)-N(3)	1.417(4)
C(41)-H(41A)	0.9600	N(2)-H(2N)	0.79(3)
C(41)-H(41B)	0.9600	N(3)-H(3N1)	0.91(3)
C(41)-H(41C)	0.9600	N(3)-H(3N2)	0.79(3)
C(5)-C(6)	1.384(4)		

O(2)-S(1)-O(1)	119.59(13)	C(3)-C(2)-H(2)	120.1
O(2)-S(1)-N(1)	107.57(12)	C(1)-C(2)-H(2)	120.1
O(1)-S(1)-N(1)	106.42(12)	C(2)-C(3)-C(4)	120.3(3)
O(2)-S(1)-C(1)	107.14(12)	C(2)-C(3)-H(3)	119.8
O(1)-S(1)-C(1)	106.81(13)	C(4)-C(3)-H(3)	119.8
N(1)-S(1)-C(1)	109.00(12)	O(4)-C(4)-C(5)	125.4(3)
C(7)-N(1)-S(1)	122.74(18)	O(4)-C(4)-C(3)	114.9(3)
C(7)-N(1)-H(1N)	119(2)	C(5)-C(4)-C(3)	119.7(3)
S(1)-N(1)-H(1N)	112(2)	C(4)-O(4)-C(41)	118.0(3)
C(6)-C(1)-C(2)	120.1(3)	O(4)-C(41)-H(41A)	109.5
C(6)-C(1)-S(1)	121.0(2)	O(4)-C(41)-H(41B)	109.5
C(2)-C(1)-S(1)	118.9(2)	H(41A)-C(41)-H(41B)	109.5
C(3)-C(2)-C(1)	119.7(3)	O(4)-C(41)-H(41C)	109.5

H(41A)-C(41)-H(41C)	109.5	C(73)-C(71)-H(71)	108.4
H(41B)-C(41)-H(41C)	109.5	C(7)-C(71)-H(71)	108.4
C(4)-C(5)-C(6)	119.7(2)	C(71)-C(72)-H(72A)	109.5
C(4)-C(5)-H(5)	120.2	C(71)-C(72)-H(72B)	109.5
C(6)-C(5)-H(5)	120.2	H(72A)-C(72)-H(72B)	109.5
C(1)-C(6)-C(5)	120.4(3)	C(71)-C(72)-H(72C)	109.5
C(1)-C(6)-H(6)	119.8	H(72A)-C(72)-H(72C)	109.5
C(5)-C(6)-H(6)	119.8	H(72B)-C(72)-H(72C)	109.5
N(1)-C(7)-C(8)	111.6(2)	C(71)-C(73)-H(73A)	109.5
N(1)-C(7)-C(71)	109.3(2)	C(71)-C(73)-H(73B)	109.5
C(8)-C(7)-C(71)	109.3(2)	H(73A)-C(73)-H(73B)	109.5
N(1)-C(7)-H(7)	108.9	C(71)-C(73)-H(73C)	109.5
C(8)-C(7)-H(7)	108.9	H(73A)-C(73)-H(73C)	109.5
C(71)-C(7)-H(7)	108.9	H(73B)-C(73)-H(73C)	109.5
O(8)-C(8)-N(2)	122.6(3)	C(8)-N(2)-N(3)	123.3(2)
O(8)-C(8)-C(7)	121.4(2)	C(8)-N(2)-H(2N)	123(2)
N(2)-C(8)-C(7)	115.9(2)	N(3)-N(2)-H(2N)	114(2)
C(72)-C(71)-C(73)	110.3(3)	N(2)-N(3)-H(3N1)	107(2)
C(72)-C(71)-C(7)	111.3(2)	N(2)-N(3)-H(3N2)	105(3)
C(73)-C(71)-C(7)	110.0(3)	H(3N1)-N(3)-H(3N2)	114(4)
C(72)-C(71)-H(71)	108.4		

Table S4. Bond lengths [Å] and angles [°] for compound **5d**.

Cl(14)-C(14)	1.730(4)	Cl(24)-C(24)	1.744(4)
S(1)-O(11)	1.427(3)	S(2)-O(21)	1.431(3)
S(1)-O(12)	1.436(3)	S(2)-O(22)	1.431(3)
S(1)-N(11)	1.604(3)	S(2)-N(21)	1.600(3)
S(1)-C(11)	1.765(3)	S(2)-C(21)	1.772(3)
O(18)-C(18)	1.213(4)	O(28)-C(28)	1.216(4)
N(11)-C(17)	1.454(4)	N(21)-C(27)	1.461(4)
N(11)-HN11	0.77(4)	N(21)-HN21	0.78(4)
N(12)-C(18)	1.332(4)	N(22)-C(28)	1.332(4)
N(12)-N(13)	1.414(4)	N(22)-N(23)	1.418(4)
N(12)-HN12	0.79(4)	N(22)-HN22	0.83(4)
N(13)-H(131)	0.89(5)	N(23)-H(231)	0.95(4)
N(13)-H(132)	0.92(5)	N(23)-H(232)	1.04(4)
C(11)-C(16)	1.383(5)	C(21)-C(22)	1.374(5)
C(11)-C(12)	1.385(5)	C(21)-C(26)	1.382(5)
C(12)-C(13)	1.377(6)	C(22)-C(23)	1.395(5)
C(12)-H(12)	0.9300	C(22)-H(22)	0.9300
C(13)-C(14)	1.385(7)	C(23)-C(24)	1.365(6)
C(13)-H(13)	0.9300	C(23)-H(23)	0.9300
C(14)-C(15)	1.361(6)	C(24)-C(25)	1.374(6)
C(15)-C(16)	1.385(5)	C(25)-C(26)	1.379(6)
C(15)-H(15)	0.9300	C(25)-H(25)	0.9300
C(16)-H(16)	0.9300	C(26)-H(26)	0.9300
C(17)-C(171)	1.509(6)	C(27)-C(271)	1.520(5)
C(17)-C(18)	1.536(4)	C(27)-C(28)	1.532(4)
C(17)-H(17)	0.9800	C(27)-H(27)	0.9800
C(171)-H(171)	0.9600	C(271)-H(271)	0.9600
C(171)-H(172)	0.9600	C(271)-H(272)	0.9600
C(171)-H(173)	0.9600	C(271)-H(273)	0.9600
O(11)-S(1)-O(12)	119.84(18)	O(12)-S(1)-C(11)	107.09(17)
O(11)-S(1)-N(11)	105.83(17)	N(11)-S(1)-C(11)	108.61(15)
O(12)-S(1)-N(11)	107.35(17)	C(17)-N(11)-S(1)	122.4(3)
O(11)-S(1)-C(11)	107.75(17)	C(17)-N(11)-HN11	115(3)

S(1)-N(11)-HN11	114(3)	H(171)-C(171)-H(172)	109.5
C(18)-N(12)-N(13)	121.8(3)	C(17)-C(171)-H(173)	109.5
C(18)-N(12)-HN12	121(3)	H(171)-C(171)-H(173)	109.5
N(13)-N(12)-HN12	117(3)	H(172)-C(171)-H(173)	109.5
N(12)-N(13)-H(131)	110(3)	O(21)-S(2)-O(22)	120.06(16)
N(12)-N(13)-H(132)	110(3)	O(21)-S(2)-N(21)	107.44(15)
H(131)-N(13)-H(132)	112(4)	O(22)-S(2)-N(21)	106.06(16)
C(16)-C(11)-C(12)	120.8(3)	O(21)-S(2)-C(21)	106.72(16)
C(16)-C(11)-S(1)	120.3(3)	O(22)-S(2)-C(21)	107.58(17)
C(12)-C(11)-S(1)	118.8(3)	N(21)-S(2)-C(21)	108.58(14)
C(13)-C(12)-C(11)	119.2(4)	C(27)-N(21)-S(2)	121.9(2)
C(13)-C(12)-H(12)	120.4	C(27)-N(21)-HN21	118(3)
C(11)-C(12)-H(12)	120.4	S(2)-N(21)-HN21	115(3)
C(12)-C(13)-C(14)	119.4(4)	C(28)-N(22)-N(23)	122.2(3)
C(12)-C(13)-H(13)	120.3	C(28)-N(22)-HN22	122(3)
C(14)-C(13)-H(13)	120.3	N(23)-N(22)-HN22	115(3)
C(15)-C(14)-C(13)	121.7(4)	N(22)-N(23)-H(231)	112(3)
C(15)-C(14)-Cl(14)	119.5(4)	N(22)-N(23)-H(232)	105(2)
C(13)-C(14)-Cl(14)	118.9(3)	H(231)-N(23)-H(232)	104(3)
C(14)-C(15)-C(16)	119.3(4)	C(22)-C(21)-C(26)	120.9(3)
C(14)-C(15)-H(15)	120.3	C(22)-C(21)-S(2)	120.1(3)
C(16)-C(15)-H(15)	120.3	C(26)-C(21)-S(2)	119.0(3)
C(11)-C(16)-C(15)	119.5(4)	C(21)-C(22)-C(23)	119.3(4)
C(11)-C(16)-H(16)	120.2	C(21)-C(22)-H(22)	120.4
C(15)-C(16)-H(16)	120.2	C(23)-C(22)-H(22)	120.4
N(11)-C(17)-C(171)	109.1(3)	C(24)-C(23)-C(22)	119.2(4)
N(11)-C(17)-C(18)	111.1(3)	C(24)-C(23)-H(23)	120.4
C(171)-C(17)-C(18)	109.4(3)	C(22)-C(23)-H(23)	120.4
N(11)-C(17)-H(17)	109.1	C(23)-C(24)-C(25)	121.8(4)
C(171)-C(17)-H(17)	109.1	C(23)-C(24)-Cl(24)	118.8(3)
C(18)-C(17)-H(17)	109.1	C(25)-C(24)-Cl(24)	119.5(3)
O(18)-C(18)-N(12)	122.9(3)	C(24)-C(25)-C(26)	119.2(4)
O(18)-C(18)-C(17)	121.6(3)	C(24)-C(25)-H(25)	120.4
N(12)-C(18)-C(17)	115.6(3)	C(26)-C(25)-H(25)	120.4
C(17)-C(171)-H(171)	109.5	C(25)-C(26)-C(21)	119.7(4)
C(17)-C(171)-H(172)	109.5	C(25)-C(26)-H(26)	120.1

C(21)-C(26)-H(26)	120.1	C(27)-C(271)-H(272)	109.5
N(21)-C(27)-C(271)	109.1(3)	H(271)-C(271)-H(272)	109.5
N(21)-C(27)-C(28)	111.1(3)	C(27)-C(271)-H(273)	109.5
C(271)-C(27)-C(28)	109.5(3)	H(271)-C(271)-H(273)	109.5
N(21)-C(27)-H(27)	109.0	H(272)-C(271)-H(273)	109.5
C(271)-C(27)-H(27)	109.0	O(28)-C(28)-N(22)	122.7(3)
C(28)-C(27)-H(27)	109.0	O(28)-C(28)-C(27)	122.5(3)
C(27)-C(271)-H(271)	109.5	N(22)-C(28)-C(27)	114.8(3)

Table S5. Bond lengths [Å] and angles [°] for compound **5e**.

S(1)-O(1)	1.432(2)	C(7)-C(71)	1.550(4)
S(1)-O(2)	1.433(2)	C(7)-H(7)	0.9800
S(1)-N(1)	1.596(2)	C(71)-C(72)	1.502(5)
S(1)-C(1)	1.775(3)	C(71)-C(73)	1.521(6)
C(1)-C(6)	1.371(4)	C(71)-H(71)	0.9800
C(1)-C(2)	1.380(4)	C(72)-H(72A)	0.9600
C(2)-C(3)	1.391(5)	C(72)-H(72B)	0.9600
C(2)-H(2)	0.9300	C(72)-H(72C)	0.9600
C(3)-C(4)	1.384(6)	C(73)-H(73A)	0.9600
C(3)-H(3)	0.9300	C(73)-H(73B)	0.9600
C(4)-C(5)	1.361(5)	C(73)-H(73C)	0.9600
C(4)-Cl(4)	1.735(4)	C(8)-O(8)	1.224(4)
C(5)-C(6)	1.394(4)	C(8)-N(2)	1.324(4)
C(5)-H(5)	0.9300	N(2)-N(3)	1.412(4)
C(6)-H(6)	0.9300	N(2)-H(2N)	0.80(4)
N(1)-C(7)	1.466(4)	N(3)-H(3N2)	0.84(4)
N(1)-H(1N)	0.74(4)	N(3)-H(3N1)	0.72(4)
C(7)-C(8)	1.512(4)		

O(1)-S(1)-O(2)	119.79(15)	C(5)-C(4)-C(3)	121.4(3)
O(1)-S(1)-N(1)	106.45(15)	C(5)-C(4)-Cl(4)	119.0(3)
O(2)-S(1)-N(1)	108.04(14)	C(3)-C(4)-Cl(4)	119.6(3)
O(1)-S(1)-C(1)	106.62(15)	C(4)-C(5)-C(6)	119.0(3)
O(2)-S(1)-C(1)	106.59(14)	C(4)-C(5)-H(5)	120.5
N(1)-S(1)-C(1)	109.04(14)	C(6)-C(5)-H(5)	120.5
C(6)-C(1)-C(2)	120.6(3)	C(1)-C(6)-C(5)	120.3(3)
C(6)-C(1)-S(1)	119.8(2)	C(1)-C(6)-H(6)	119.8
C(2)-C(1)-S(1)	119.7(2)	C(5)-C(6)-H(6)	119.8
C(1)-C(2)-C(3)	119.3(3)	C(7)-N(1)-S(1)	123.4(2)
C(1)-C(2)-H(2)	120.4	C(7)-N(1)-H(1N)	116(3)
C(3)-C(2)-H(2)	120.4	S(1)-N(1)-H(1N)	112(3)
C(4)-C(3)-C(2)	119.4(3)	N(1)-C(7)-C(8)	111.3(2)
C(4)-C(3)-H(3)	120.3	N(1)-C(7)-C(71)	108.6(2)
C(2)-C(3)-H(3)	120.3	C(8)-C(7)-C(71)	109.5(2)

N(1)-C(7)-H(7)	109.1
C(8)-C(7)-H(7)	109.1
C(71)-C(7)-H(7)	109.1
C(72)-C(71)-C(73)	110.5(4)
C(72)-C(71)-C(7)	111.2(3)
C(73)-C(71)-C(7)	109.7(3)
C(72)-C(71)-H(71)	108.4
C(73)-C(71)-H(71)	108.4
C(7)-C(71)-H(71)	108.4
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(71)-C(73)-H(73A)	109.5
C(71)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(71)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
O(8)-C(8)-N(2)	122.5(3)
O(8)-C(8)-C(7)	121.4(3)
N(2)-C(8)-C(7)	116.0(2)
C(8)-N(2)-N(3)	122.8(2)
C(8)-N(2)-H(2N)	120(3)
N(3)-N(2)-H(2N)	117(3)
N(2)-N(3)-H(3N2)	111(3)
N(2)-N(3)-H(3N1)	103(4)
H(3N2)-N(3)-H(3N1)	104(5)

Table S6. Torsion angles [°] for compound **5a**.

O(2)-S(1)-C(1)-C(6)	-0.2(3)
O(1)-S(1)-C(1)-C(6)	130.0(2)
N(1)-S(1)-C(1)-C(6)	-115.5(2)
O(2)-S(1)-C(1)-C(2)	177.3(2)
O(1)-S(1)-C(1)-C(2)	-52.5(3)
N(1)-S(1)-C(1)-C(2)	62.0(3)
C(6)-C(1)-C(2)-C(3)	-1.2(4)
S(1)-C(1)-C(2)-C(3)	-178.7(2)
C(1)-C(2)-C(3)-C(4)	0.0(5)
C(2)-C(3)-C(4)-C(5)	0.7(5)
C(2)-C(3)-C(4)-C(41)	-179.4(3)
C(3)-C(4)-C(5)-C(6)	-0.2(5)
C(41)-C(4)-C(5)-C(6)	179.9(3)
C(4)-C(5)-C(6)-C(1)	-1.0(5)
C(2)-C(1)-C(6)-C(5)	1.7(4)
S(1)-C(1)-C(6)-C(5)	179.2(2)
O(2)-S(1)-N(1)-C(7)	-54.4(2)
O(1)-S(1)-N(1)-C(7)	176.4(2)
C(1)-S(1)-N(1)-C(7)	60.0(2)
S(1)-N(1)-C(7)-C(8)	-87.1(2)
S(1)-N(1)-C(7)-C(71)	152.6(2)
N(1)-C(7)-C(71)-C(72)	-58.4(3)
C(8)-C(7)-C(71)-C(72)	-178.7(3)
N(1)-C(7)-C(71)-C(73)	178.9(3)
C(8)-C(7)-C(71)-C(73)	58.5(3)
N(1)-C(7)-C(8)-O(8)	-58.8(4)
C(71)-C(7)-C(8)-O(8)	61.5(4)
N(1)-C(7)-C(8)-N(2)	121.9(3)
C(71)-C(7)-C(8)-N(2)	-117.9(3)
O(8)-C(8)-N(2)-N(3)	-0.6(5)
C(7)-C(8)-N(2)-N(3)	178.8(3)

Table S7. Torsion angles [°] for compound **5b**.

O(1)-S(1)-C(1)-C(6)	133.2(2)
O(2)-S(1)-C(1)-C(6)	4.3(2)
N(1)-S(1)-C(1)-C(6)	-112.4(2)
O(1)-S(1)-C(1)-C(2)	-45.9(2)
O(2)-S(1)-C(1)-C(2)	-174.8(2)
N(1)-S(1)-C(1)-C(2)	68.5(2)
C(6)-C(1)-C(2)-C(3)	-0.7(4)
S(1)-C(1)-C(2)-C(3)	178.4(2)
C(1)-C(2)-C(3)-C(4)	-0.4(5)
C(2)-C(3)-C(4)-C(5)	1.2(5)
C(2)-C(3)-C(4)-C(41)	-179.0(3)
C(3)-C(4)-C(5)-C(6)	-0.9(4)
C(41)-C(4)-C(5)-C(6)	179.3(3)
C(2)-C(1)-C(6)-C(5)	1.0(4)
S(1)-C(1)-C(6)-C(5)	-178.1(2)
C(4)-C(5)-C(6)-C(1)	-0.1(4)
O(1)-S(1)-N(1)-C(7)	-172.12(18)
O(2)-S(1)-N(1)-C(7)	-43.2(2)
C(1)-S(1)-N(1)-C(7)	72.8(2)
S(1)-N(1)-C(7)-C(8)	-74.4(2)
S(1)-N(1)-C(7)-C(71)	162.53(16)
N(1)-C(7)-C(71)-C(72)	-163.8(2)
C(8)-C(7)-C(71)-C(72)	75.5(3)
C(7)-C(71)-C(72)-C(73)	-76.5(4)
C(7)-C(71)-C(72)-C(74)	160.7(3)
N(1)-C(7)-C(8)-O(8)	-58.1(3)
C(71)-C(7)-C(8)-O(8)	61.6(3)
N(1)-C(7)-C(8)-N(2)	119.3(2)
C(71)-C(7)-C(8)-N(2)	-121.0(2)
O(8)-C(8)-N(2)-N(3)	1.8(4)
C(7)-C(8)-N(2)-N(3)	-175.6(2)

Table S8. Torsion angles [°] for compound **5c**.

O(2)-S(1)-N(1)-C(7)	-43.0(2)
O(1)-S(1)-N(1)-C(7)	-172.3(2)
C(1)-S(1)-N(1)-C(7)	72.8(2)
O(2)-S(1)-C(1)-C(6)	28.1(2)
O(1)-S(1)-C(1)-C(6)	157.4(2)
N(1)-S(1)-C(1)-C(6)	-88.0(2)
O(2)-S(1)-C(1)-C(2)	-153.2(2)
O(1)-S(1)-C(1)-C(2)	-24.0(3)
N(1)-S(1)-C(1)-C(2)	90.6(2)
C(6)-C(1)-C(2)-C(3)	-2.4(4)
S(1)-C(1)-C(2)-C(3)	179.0(2)
C(1)-C(2)-C(3)-C(4)	1.9(5)
C(2)-C(3)-C(4)-O(4)	-179.5(3)
C(2)-C(3)-C(4)-C(5)	-0.7(5)
C(5)-C(4)-O(4)-C(41)	3.5(5)
C(3)-C(4)-O(4)-C(41)	-177.8(3)
O(4)-C(4)-C(5)-C(6)	178.6(3)
C(3)-C(4)-C(5)-C(6)	0.0(4)
C(2)-C(1)-C(6)-C(5)	1.6(4)
S(1)-C(1)-C(6)-C(5)	-179.7(2)
C(4)-C(5)-C(6)-C(1)	-0.4(4)
S(1)-N(1)-C(7)-C(8)	-85.8(3)
S(1)-N(1)-C(7)-C(71)	153.19(19)
N(1)-C(7)-C(8)-O(8)	-53.6(3)
C(71)-C(7)-C(8)-O(8)	67.4(3)
N(1)-C(7)-C(8)-N(2)	129.4(2)
C(71)-C(7)-C(8)-N(2)	-109.6(3)
N(1)-C(7)-C(71)-C(72)	-59.4(3)
C(8)-C(7)-C(71)-C(72)	178.3(3)
N(1)-C(7)-C(71)-C(73)	178.1(3)
C(8)-C(7)-C(71)-C(73)	55.8(3)
O(8)-C(8)-N(2)-N(3)	-1.8(5)
C(7)-C(8)-N(2)-N(3)	175.1(2)

Table S9. Torsion angles [°] for compound **5d**.

O(11)-S(1)-N(11)-C(17)	-174.2(2)
O(12)-S(1)-N(11)-C(17)	-45.1(3)
C(11)-S(1)-N(11)-C(17)	70.3(3)
O(11)-S(1)-C(11)-C(16)	139.4(3)
O(12)-S(1)-C(11)-C(16)	9.2(4)
N(11)-S(1)-C(11)-C(16)	-106.4(3)
O(11)-S(1)-C(11)-C(12)	-43.6(3)
O(12)-S(1)-C(11)-C(12)	-173.8(3)
N(11)-S(1)-C(11)-C(12)	70.6(3)
C(16)-C(11)-C(12)-C(13)	0.2(6)
S(1)-C(11)-C(12)-C(13)	-176.8(3)
C(11)-C(12)-C(13)-C(14)	0.2(6)
C(12)-C(13)-C(14)-C(15)	-0.3(6)
C(12)-C(13)-C(14)-Cl(14)	178.0(3)
C(13)-C(14)-C(15)-C(16)	-0.1(6)
Cl(14)-C(14)-C(15)-C(16)	-178.3(3)
C(12)-C(11)-C(16)-C(15)	-0.5(6)
S(1)-C(11)-C(16)-C(15)	176.4(3)
C(14)-C(15)-C(16)-C(11)	0.4(6)
S(1)-N(11)-C(17)-C(171)	165.2(3)
S(1)-N(11)-C(17)-C(18)	-74.2(3)
N(13)-N(12)-C(18)-O(18)	-0.4(6)
N(13)-N(12)-C(18)-C(17)	179.3(3)
N(11)-C(17)-C(18)-O(18)	-46.5(5)
C(171)-C(17)-C(18)-O(18)	73.9(5)
N(11)-C(17)-C(18)-N(12)	133.8(3)
C(171)-C(17)-C(18)-N(12)	-105.8(4)
O(21)-S(2)-N(21)-C(27)	-42.2(3)
O(22)-S(2)-N(21)-C(27)	-171.8(2)
C(21)-S(2)-N(21)-C(27)	72.8(3)
O(21)-S(2)-C(21)-C(22)	7.3(3)
O(22)-S(2)-C(21)-C(22)	137.4(3)
N(21)-S(2)-C(21)-C(22)	-108.3(3)
O(21)-S(2)-C(21)-C(26)	-173.3(3)

O(22)-S(2)-C(21)-C(26)	-43.2(3)
N(21)-S(2)-C(21)-C(26)	71.1(3)
C(26)-C(21)-C(22)-C(23)	-0.6(6)
S(2)-C(21)-C(22)-C(23)	178.8(3)
C(21)-C(22)-C(23)-C(24)	0.1(6)
C(22)-C(23)-C(24)-C(25)	0.2(6)
C(22)-C(23)-C(24)-Cl(24)	-179.3(3)
C(23)-C(24)-C(25)-C(26)	0.1(6)
Cl(24)-C(24)-C(25)-C(26)	179.5(3)
C(24)-C(25)-C(26)-C(21)	-0.5(6)
C(22)-C(21)-C(26)-C(25)	0.8(6)
S(2)-C(21)-C(26)-C(25)	-178.6(3)
S(2)-N(21)-C(27)-C(271)	158.0(2)
S(2)-N(21)-C(27)-C(28)	-81.2(3)
N(23)-N(22)-C(28)-O(28)	3.3(5)
N(23)-N(22)-C(28)-C(27)	-177.8(3)
N(21)-C(27)-C(28)-O(28)	-49.0(4)
C(271)-C(27)-C(28)-O(28)	71.6(4)
N(21)-C(27)-C(28)-N(22)	132.2(3)
C(271)-C(27)-C(28)-N(22)	-107.3(3)

Table S10. Torsion angles [°] for compound **5e**.

O(1)-S(1)-C(1)-C(6)	153.7(3)
O(2)-S(1)-C(1)-C(6)	24.7(3)
N(1)-S(1)-C(1)-C(6)	-91.7(3)
O(1)-S(1)-C(1)-C(2)	-26.7(3)
O(2)-S(1)-C(1)-C(2)	-155.7(3)
N(1)-S(1)-C(1)-C(2)	87.9(3)
C(6)-C(1)-C(2)-C(3)	-2.2(5)
S(1)-C(1)-C(2)-C(3)	178.2(3)
C(1)-C(2)-C(3)-C(4)	0.7(5)
C(2)-C(3)-C(4)-C(5)	0.2(6)
C(2)-C(3)-C(4)-Cl(4)	-178.9(3)
C(3)-C(4)-C(5)-C(6)	0.2(5)
Cl(4)-C(4)-C(5)-C(6)	179.3(3)
C(2)-C(1)-C(6)-C(5)	2.7(5)
S(1)-C(1)-C(6)-C(5)	-177.7(2)
C(4)-C(5)-C(6)-C(1)	-1.7(5)
O(1)-S(1)-N(1)-C(7)	-172.4(2)
O(2)-S(1)-N(1)-C(7)	-42.6(3)
C(1)-S(1)-N(1)-C(7)	72.9(2)
S(1)-N(1)-C(7)-C(8)	-85.1(3)
S(1)-N(1)-C(7)-C(71)	154.3(2)
N(1)-C(7)-C(71)-C(72)	-63.2(4)
C(8)-C(7)-C(71)-C(72)	175.1(3)
N(1)-C(7)-C(71)-C(73)	174.3(3)
C(8)-C(7)-C(71)-C(73)	52.5(4)
N(1)-C(7)-C(8)-O(8)	-54.4(4)
C(71)-C(7)-C(8)-O(8)	65.7(4)
N(1)-C(7)-C(8)-N(2)	128.9(3)
C(71)-C(7)-C(8)-N(2)	-111.0(3)
O(8)-C(8)-N(2)-N(3)	-1.3(5)
C(7)-C(8)-N(2)-N(3)	175.3(3)

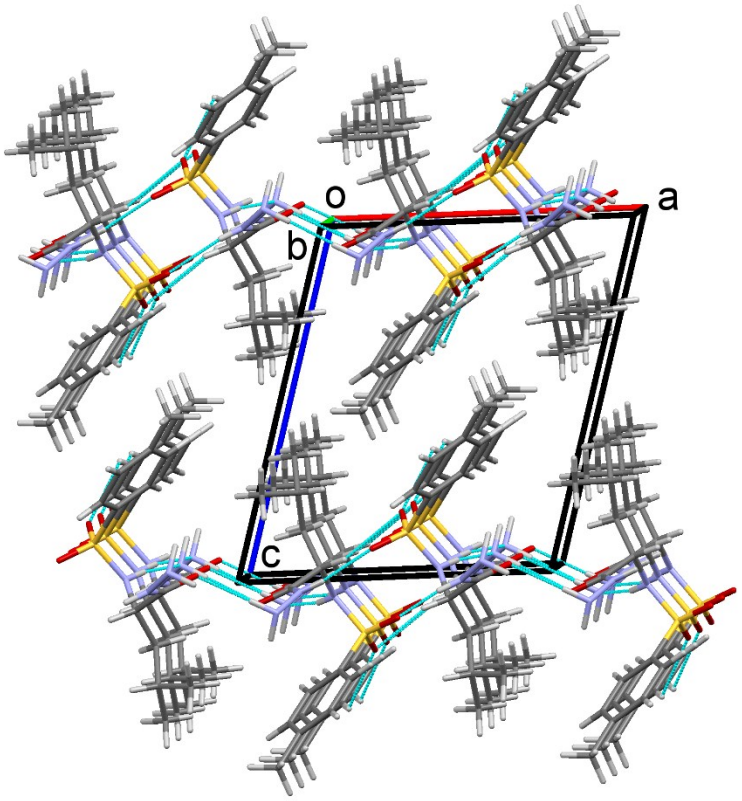


Fig. S1 Overall packing for **5b** viewed along the *b* axis direction.

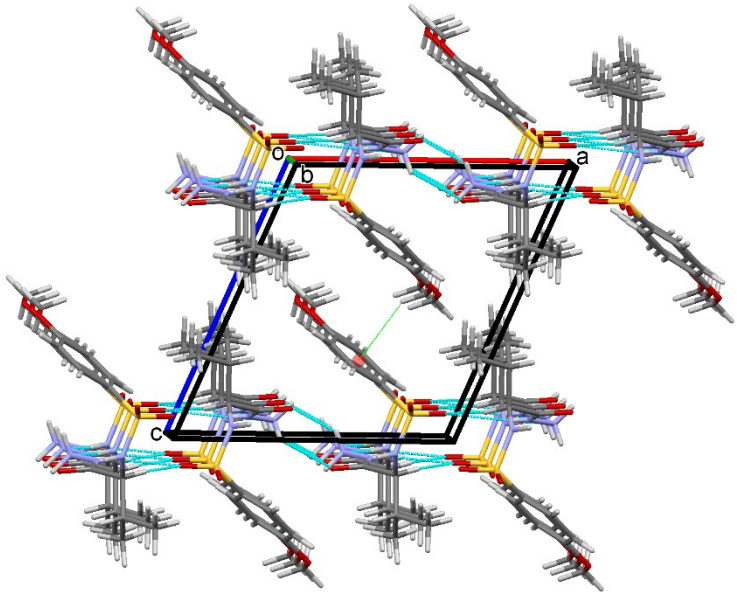


Fig. S2 Overall packing for **5c** viewed along the *b* axis direction.

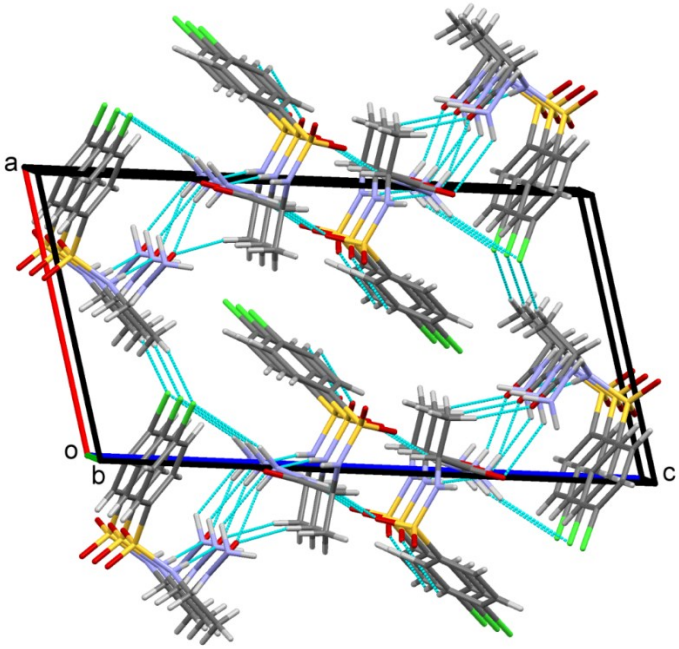
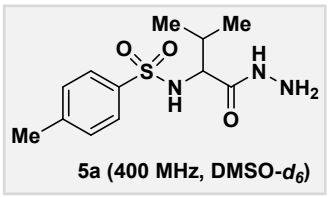
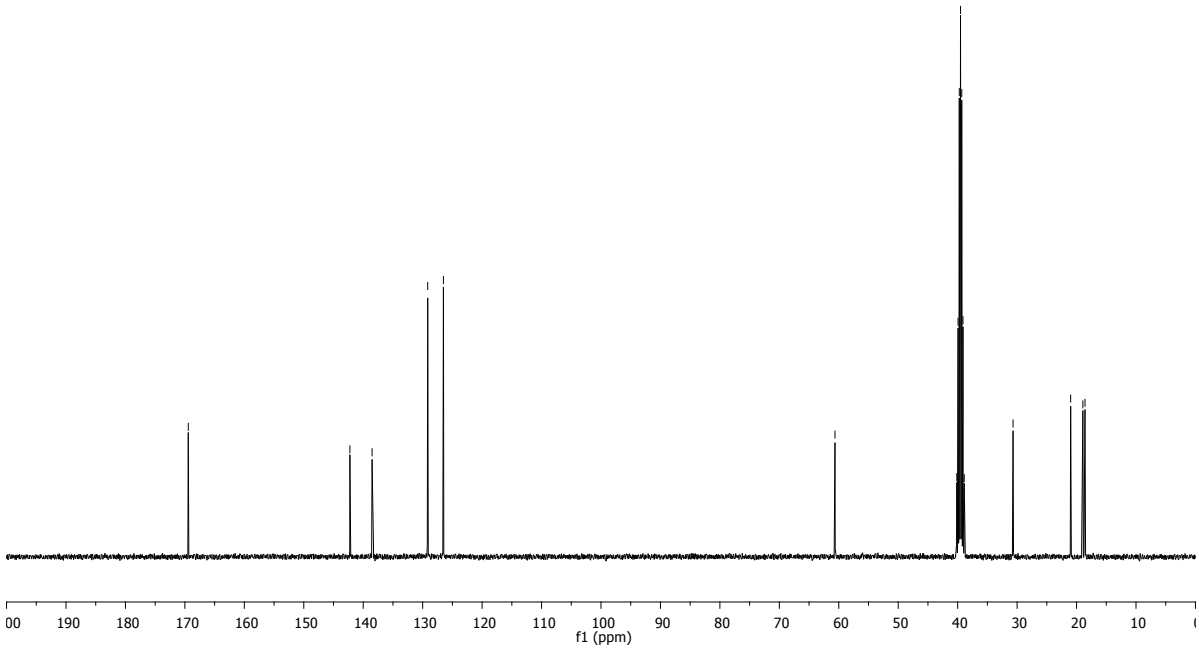
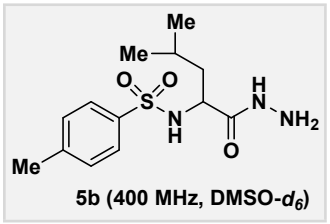


Fig. S3 Overall packing for **5d** viewed along the *b* axis direction.

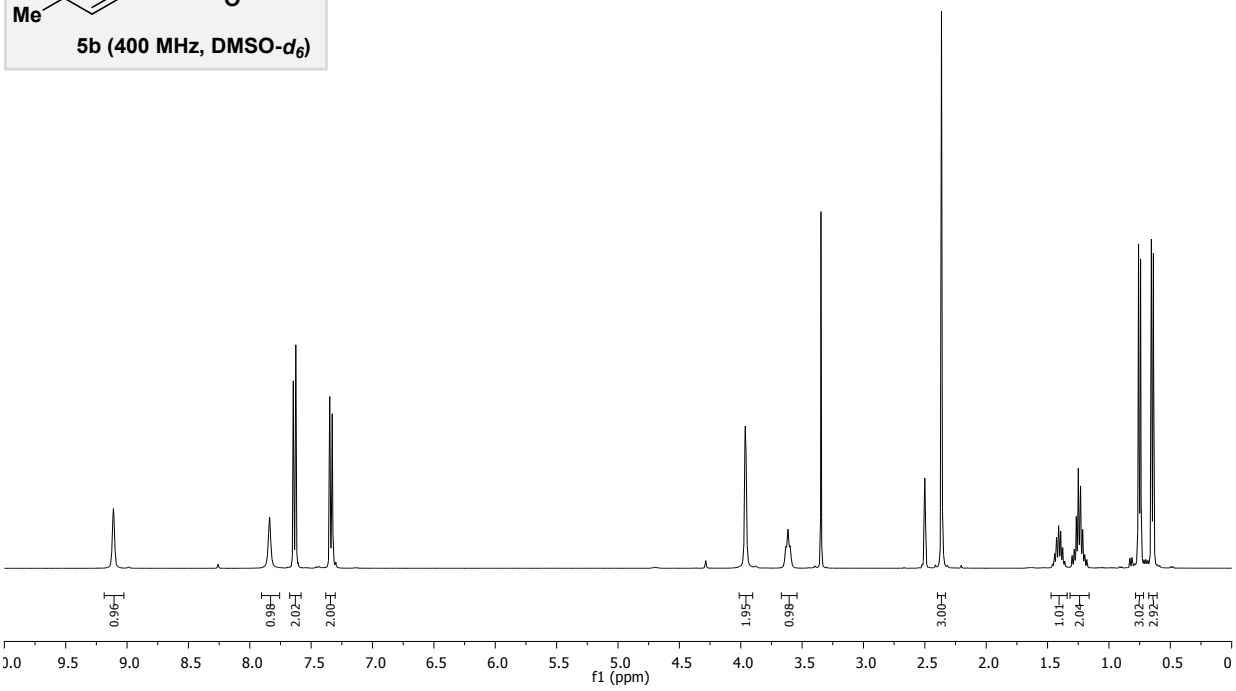


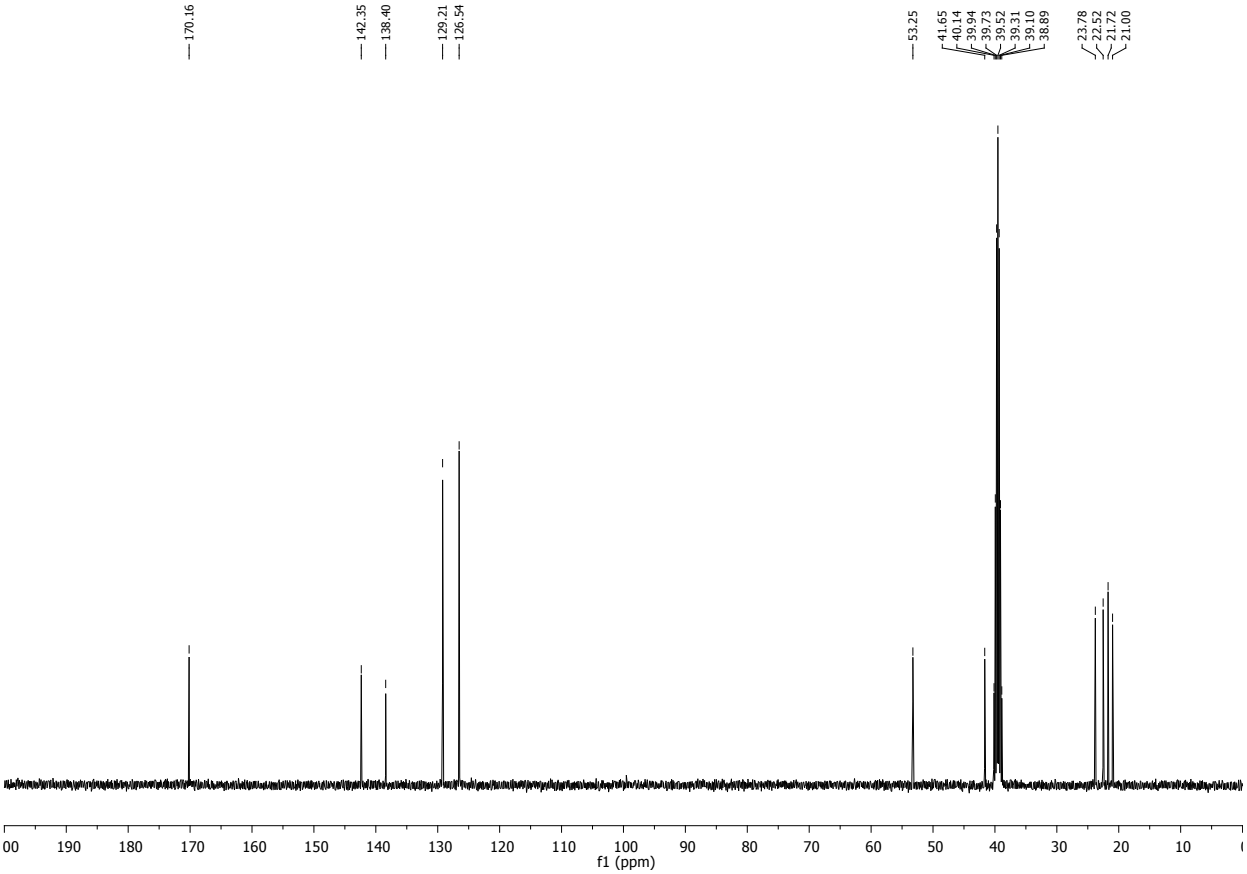
5a (400 MHz, DMSO-d_6)

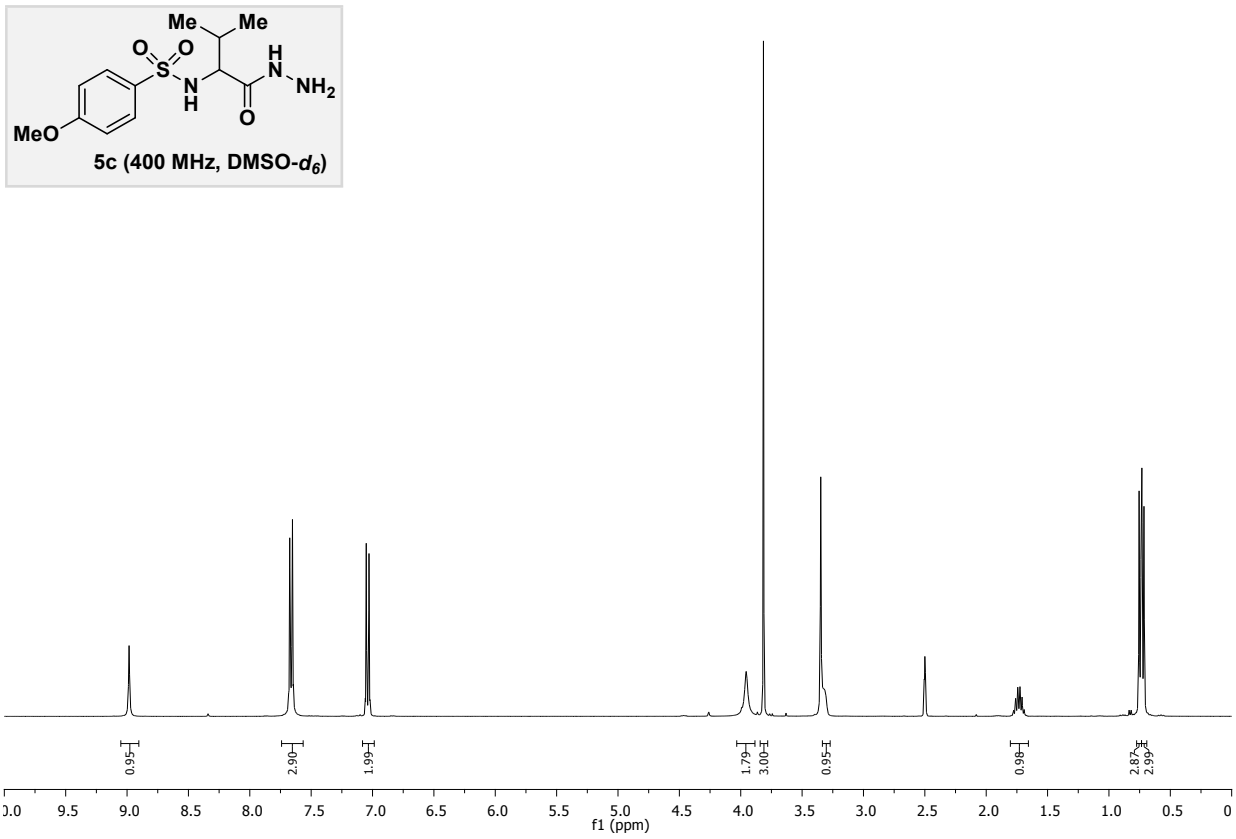


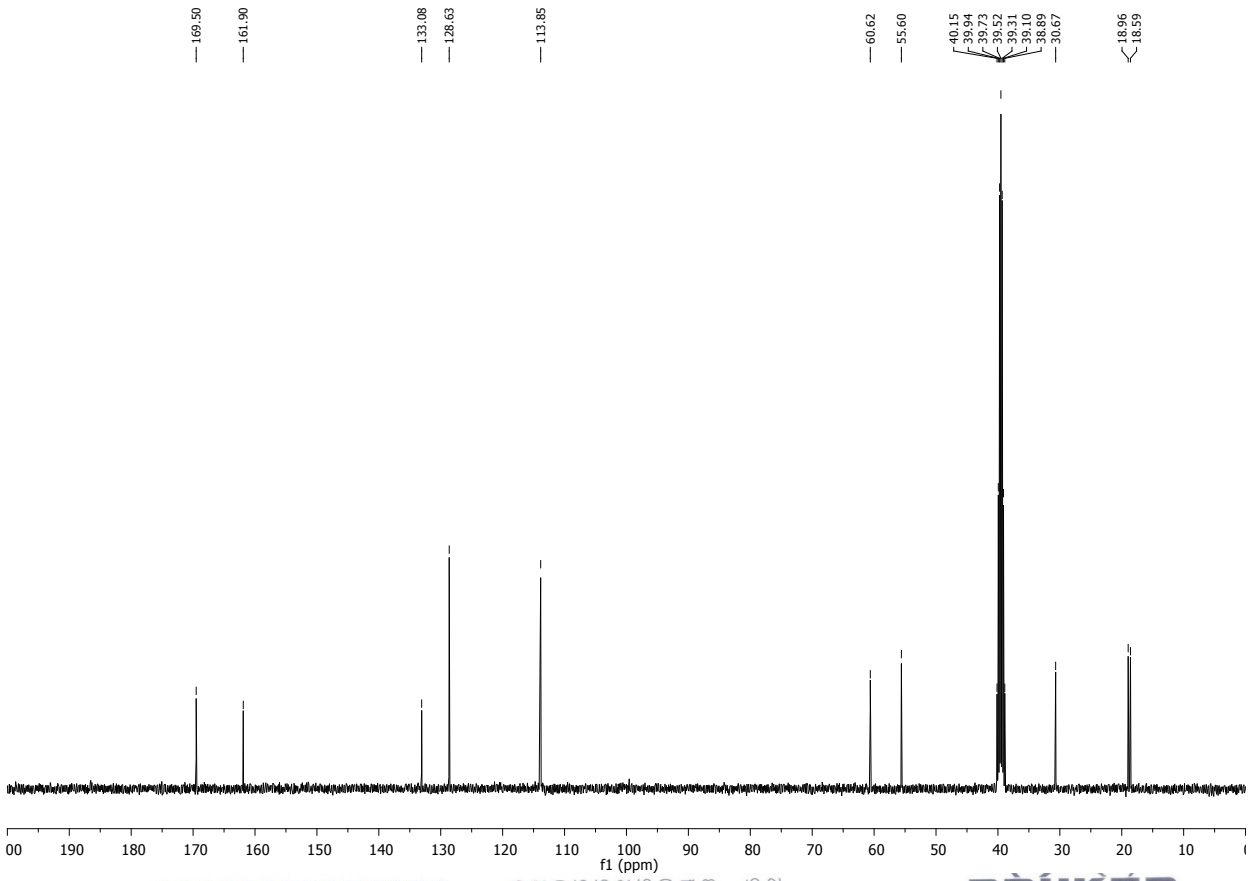


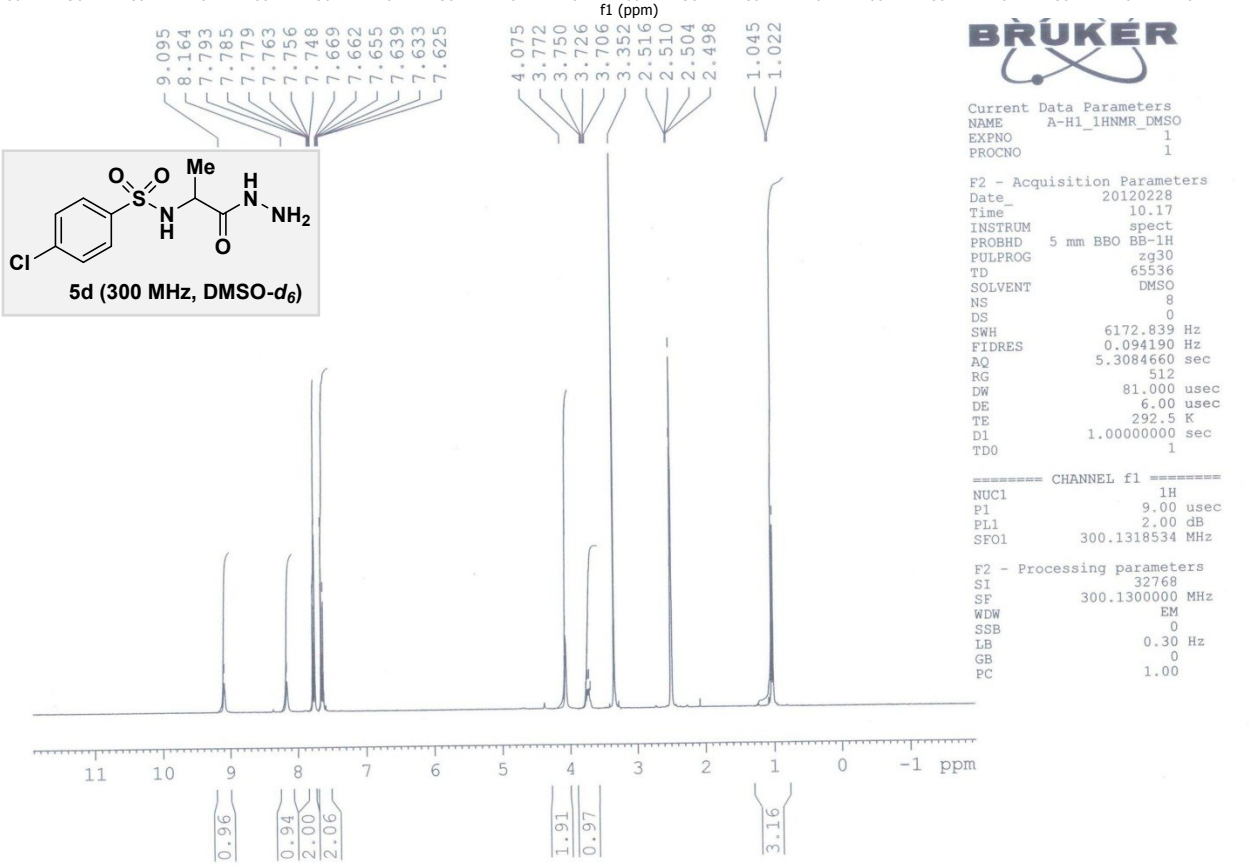
5b (400 MHz, DMSO-d_6)



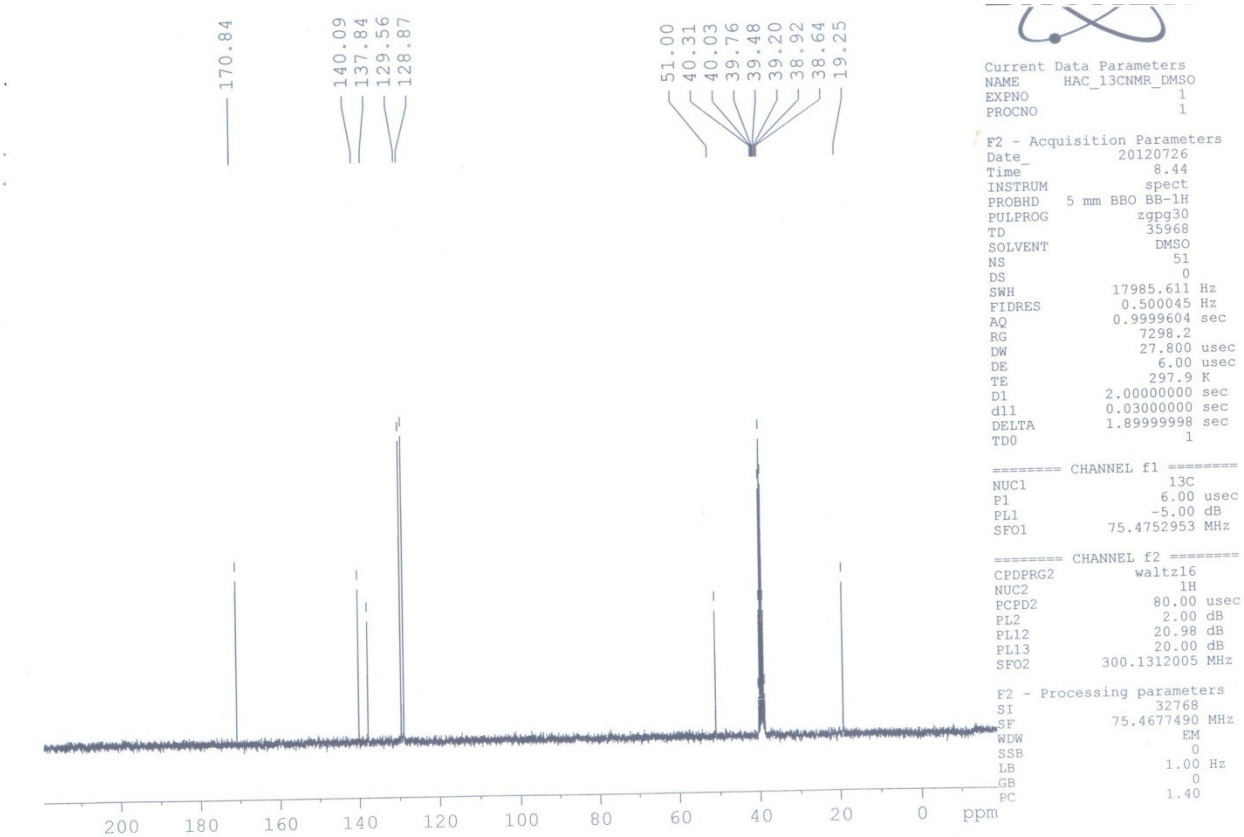

170.16
142.35
138.40
129.21
126.54
53.25
41.65
40.14
39.94
39.73
39.52
39.31
39.10
38.89
23.78
22.52
21.72
21.00
f1 (ppm)

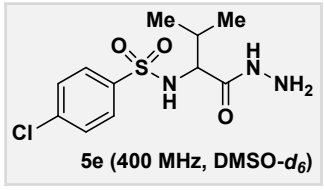

Me
Me
O
O
S
N
H
H
N
NH2
O
MeO
5c (400 MHz, DMSO-d6)
0.95
2.90
1.99
1.79
3.00
0.95
0.98
2.87
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)



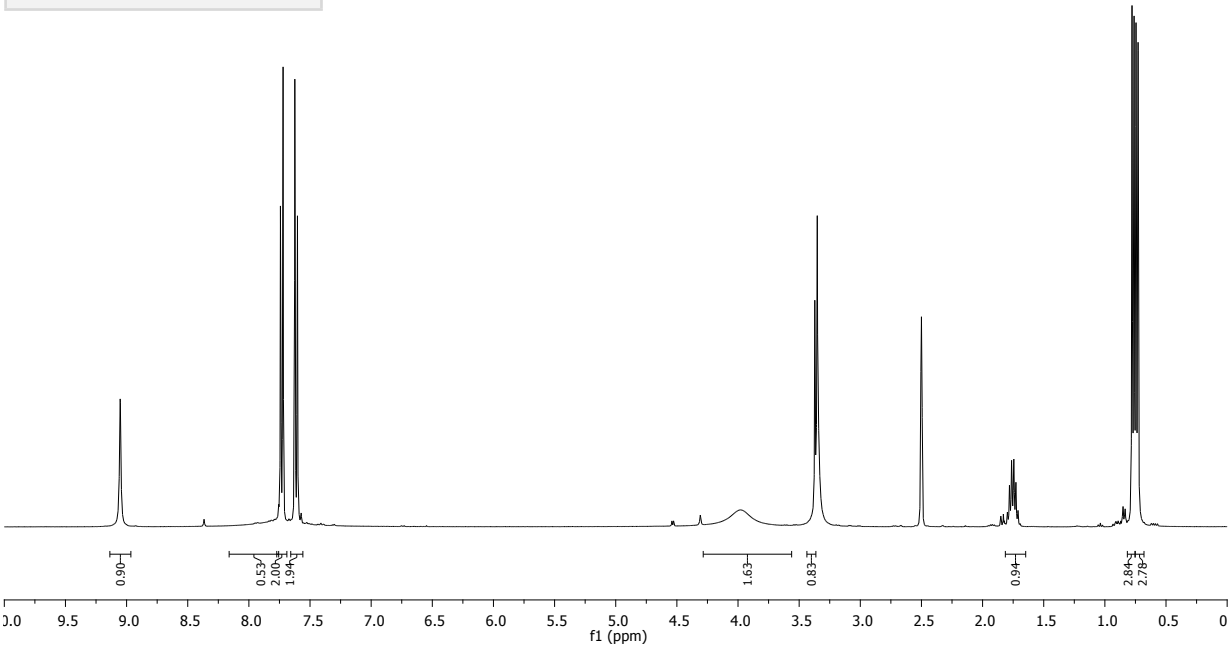


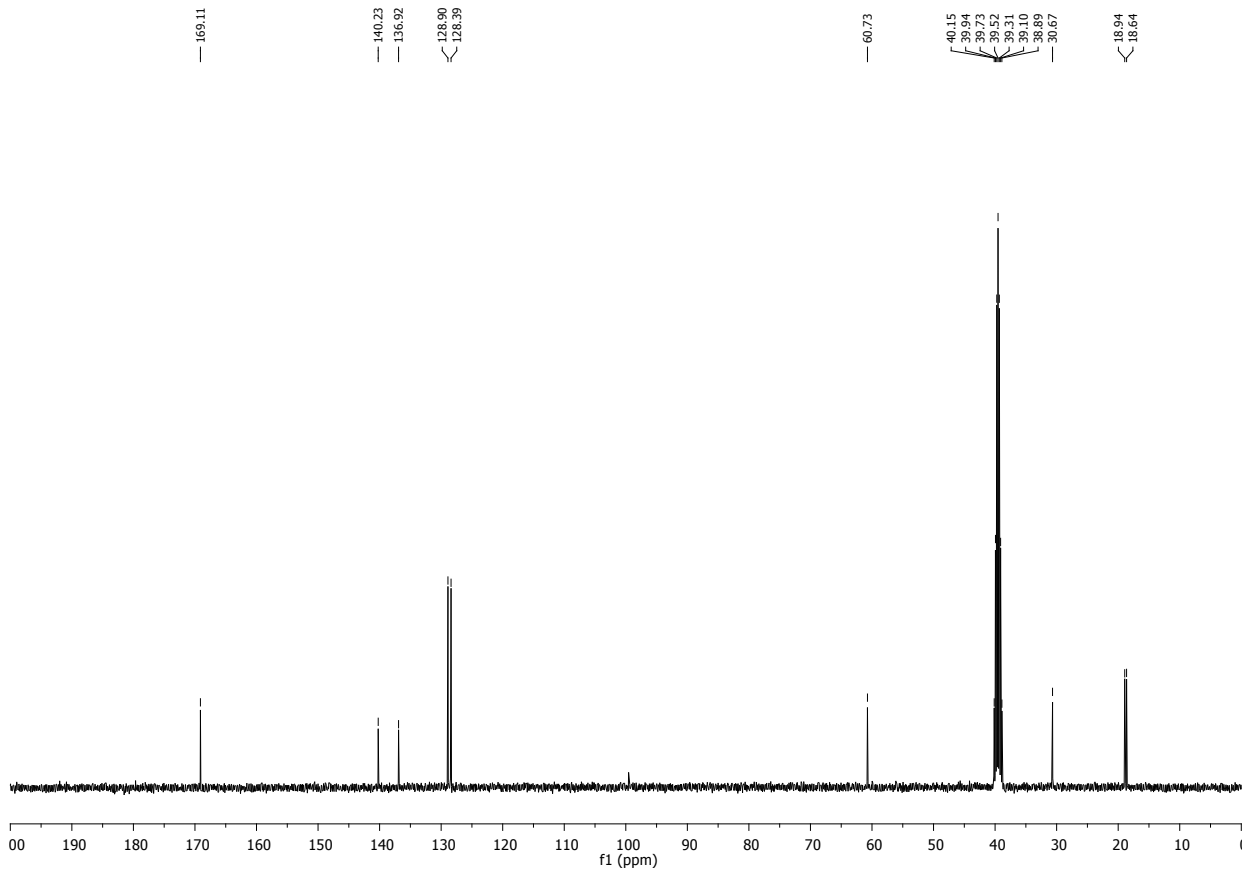
5d (300 MHz, DMSO-d_6)





5e (400 MHz, DMSO-d_6)





Conformational analysis compound 5d (denoted as I)

In Fig. S4a we show the three dihedral angles used for the conformational analysis in compound **IA** (steps of 60º, 216 calculations). We have used the M06-2X/6-31G* level of theory and the Spartan program[1] for the initial conformational analysis. Subsequently the five more stable conformation were fully optimized at the M06-2X/def2-TZVP level of theory using Gaussian-09 program.[2] As a final result, conformations denoted as **IA** and **IB** where found the most stable. It should be noted that the stability of compound **IB** is due to the formation of an intramolecular H-bond that is established between the sulfonamide NH group (excellent H-bond donor) and the hydrazido CO group (excellent H-bond acceptor). In fact, the intramolecular distance is quite short (2.09 Å) taking into consideration the restriction of the five-membered supramolecular ring. In addition, a C–H···O interaction involving the methyl group and the O-atom of the sulfonamide is also present in this conformation. These H-bonds reduce significantly the number of stable (local minimum) conformations in this particular hydrazinyl-sulfonamide combination.

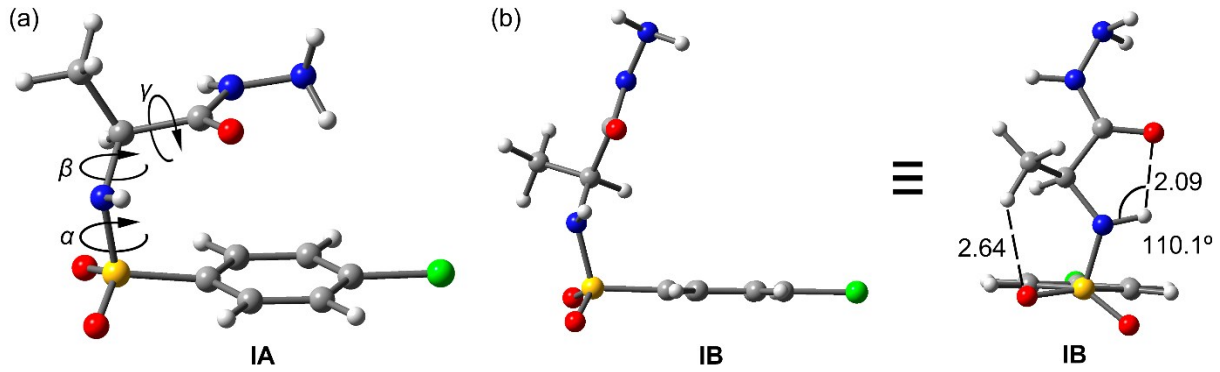


Fig. S4. (a) Indication of the α, β, γ dihedral angles used in the conformational search. (b) conformation **IB** and the geometric details of the H-bond.

References

1. Spartan'10 v. 1.1.0, Wavefunction Inc., Irvine, CA

2. Gaussian 09, Revision C.01 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09 (Gaussian, Inc., Wallingford CT, 2009).