

SUPPLEMENTARY MATERIALS

Synthesis and Structure of Novel Hybrid Compounds Containing Phthalazin-1(2*H*)-imine and 4,5-Dihydro-1*H*-imidazole Cores and their Sulfonyl Derivatives with Potential Biological Activities

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Figure S24. CheckCIF/PLATON report for 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).

Figure S25. Crystal packing in **6e** and **6c**.

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Spectra of 2-(4,5-dihydro-1H-imidazol-2-yl)phthalazin-1(2H)-imine (5)

Figure S1. IR spectrum of 2-(4,5-dihydro-1H-imidazol-2-yl)phthalazin-1(2H)-imine (5).

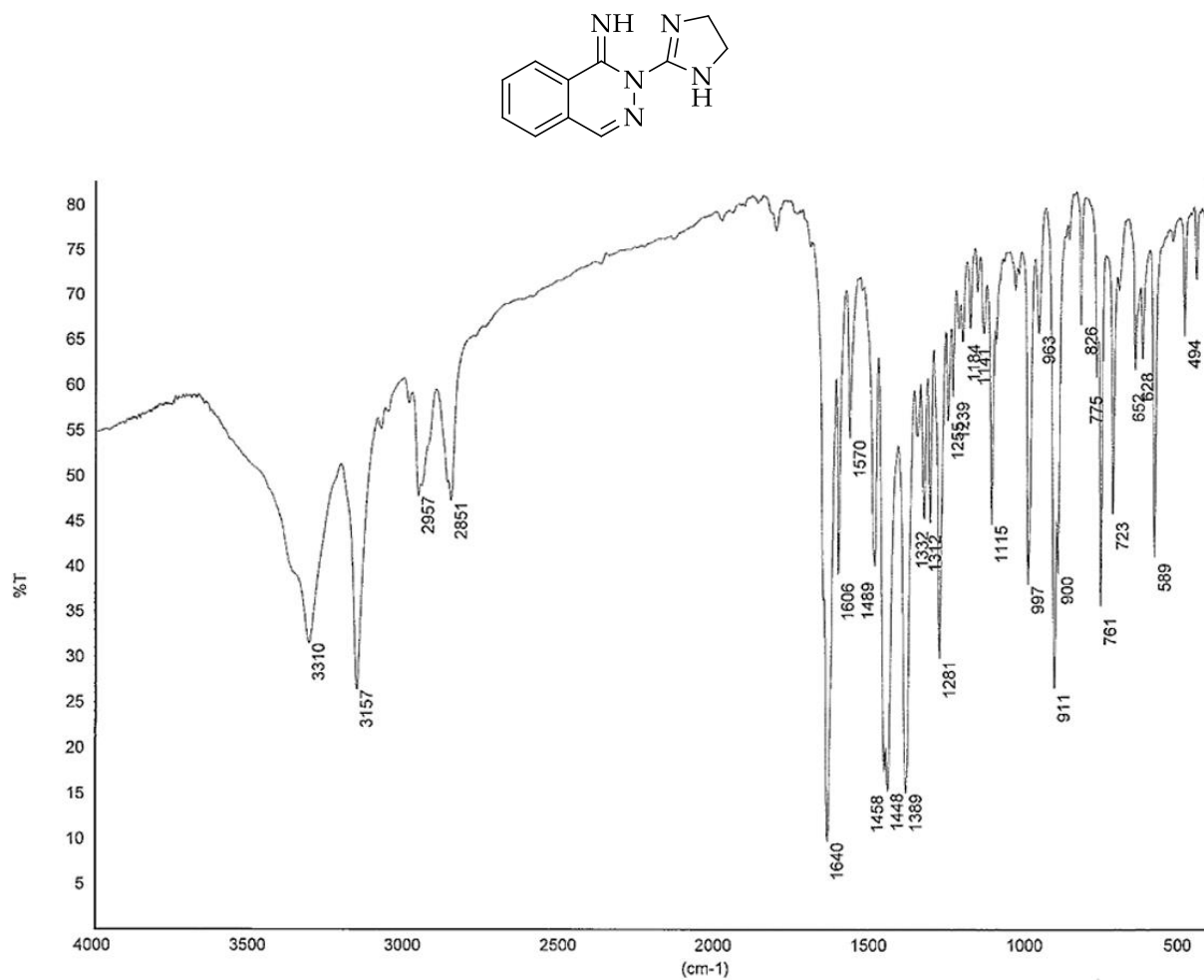
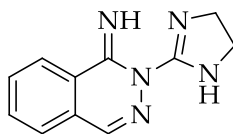


Figure S2. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (5).



INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	5434.9	10.874	5.4	17	1938.6	3.879	8.2
2	4175.7	8.355	7.8	18	1680.5	3.362	49.2
3	4173.5	8.350	9.7	19	1662.4	3.326	8.1
4	4170.2	8.344	5.0	20	1248.9	2.499	5.2
5	4165.8	8.335	11.6	21	1247.2	2.495	6.4
6	4054.4	8.112	37.0	22	1245.0	2.491	4.9
7	3861.1	7.725	8.6				
8	3856.7	7.716	26.2				
9	3854.5	7.712	47.2				
10	3852.3	7.708	22.3				
11	3850.6	7.704	12.7				
12	3848.4	7.700	15.7				
13	3846.8	7.697	10.1				
14	3844.6	7.692	5.2				
15	3842.4	7.688	4.4				
16	3470.1	6.943	5.1				

Solvent: dmsc
Ambient temperature
File: TCA_172_1H
INNOVA-500
Total time 15 min

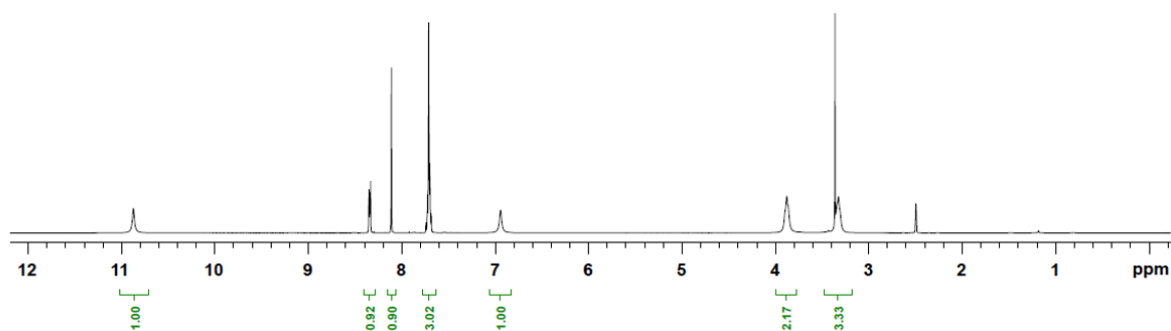
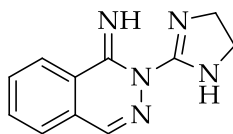


Figure S3. ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (5).



INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	20315.2	161.648	16.1	17	4981.2	39.635	25.5
2	18588.2	147.907	15.7	18	4960.1	39.467	8.4
3	17383.8	138.323	49.3				
4	16677.1	132.700	41.2				
5	16650.3	132.486	38.7				
6	16320.4	129.961	15.4				
7	15998.2	127.298	49.8				
8	15804.5	125.756	53.1				
9	15729.7	125.161	23.0				
10	6808.9	54.178	5.7				
11	5385.8	42.855	5.9				
12	5085.7	40.467	9.8				
13	5064.6	40.299	28.0				
14	5043.5	40.131	54.5				
15	5022.4	39.963	62.5				
16	5001.3	39.795	51.7				

Solvent: dmsd
 Ambient temperature
 File: TCA_172_13C
 INOVA-500
 Total time 15 min

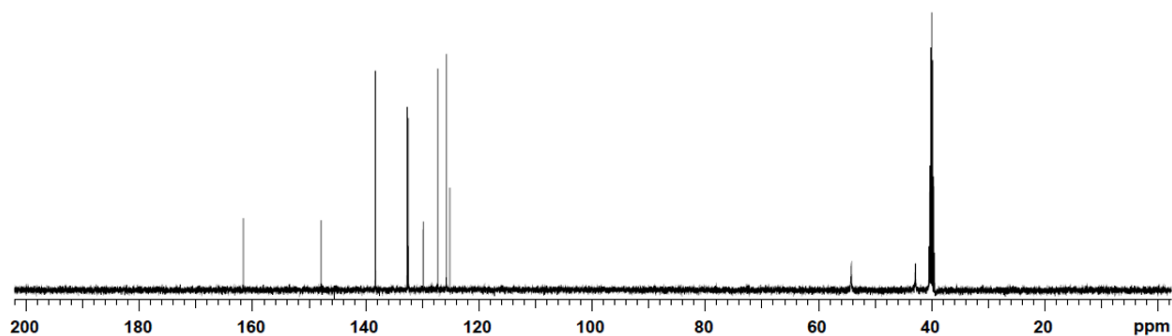


Figure S4. Heteronuclear single quantum coherence (HSQC) of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (**5**).

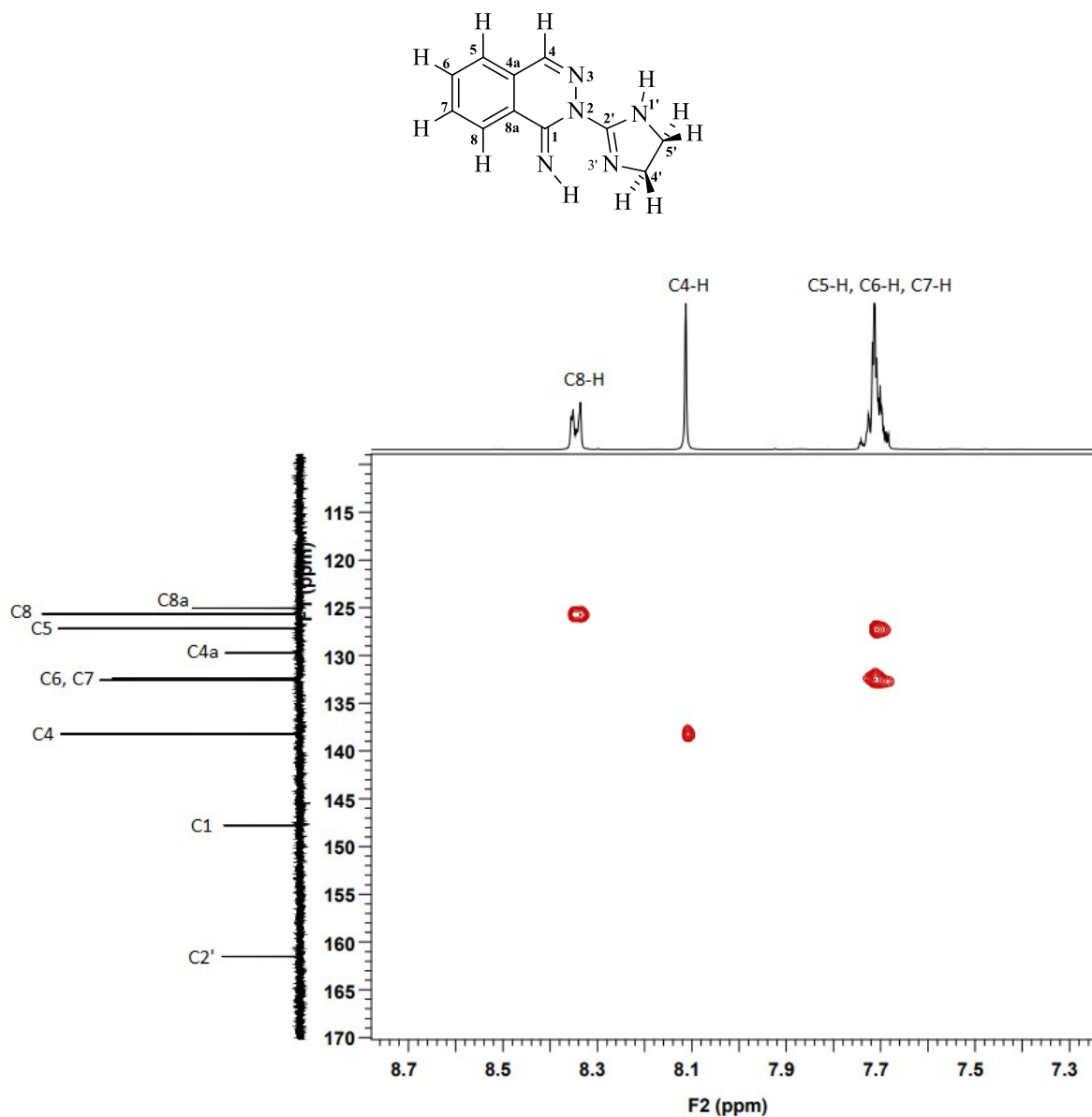


Figure S5. Heteronuclear multiple bond correlation (HMBC) spectrum of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (**5**).

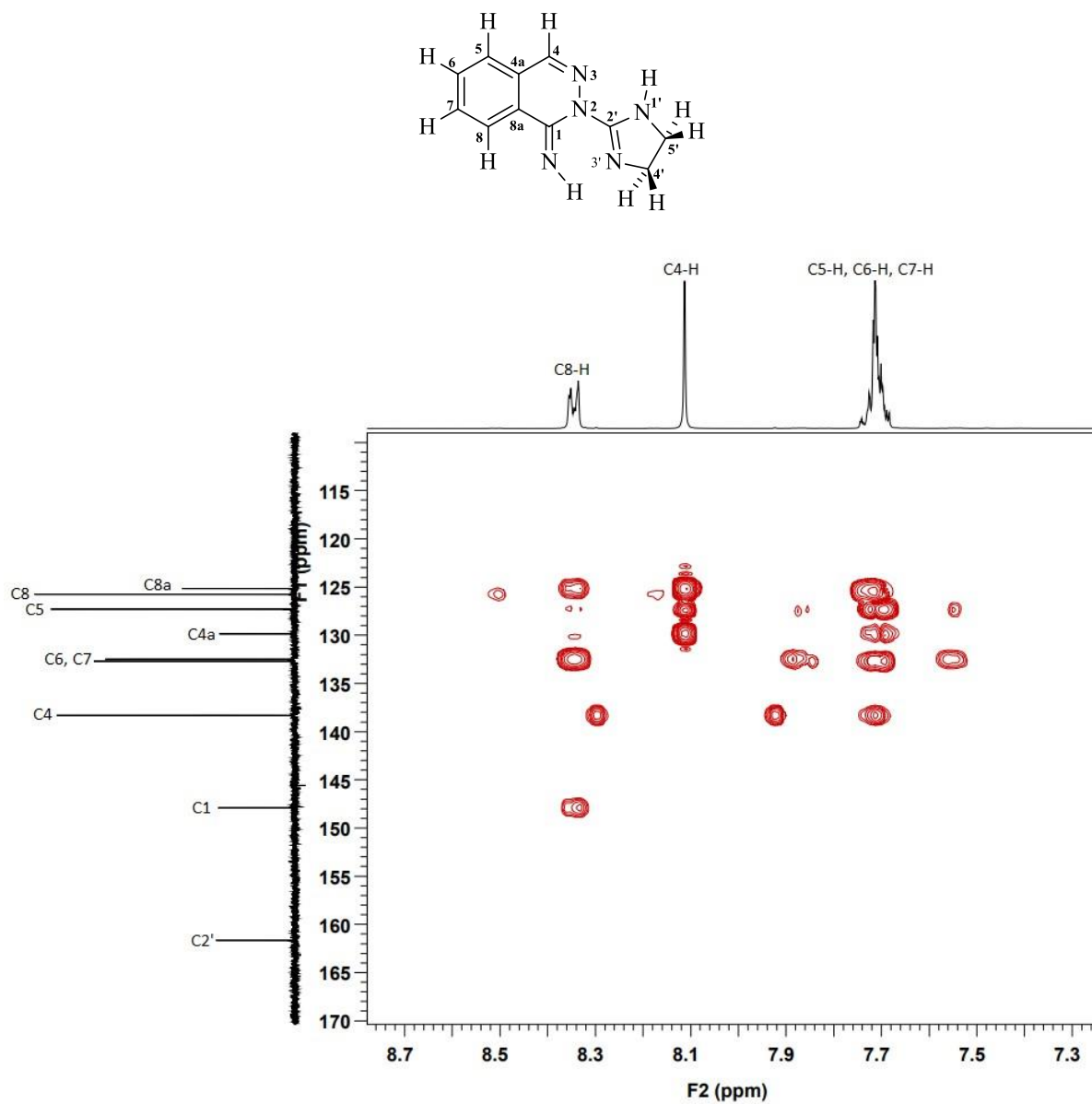


Figure S6. ^1H - ^1H ROESY (Rotating-Frame Overhauser Enhancement Spectroscopy) spectrum of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (**5**).

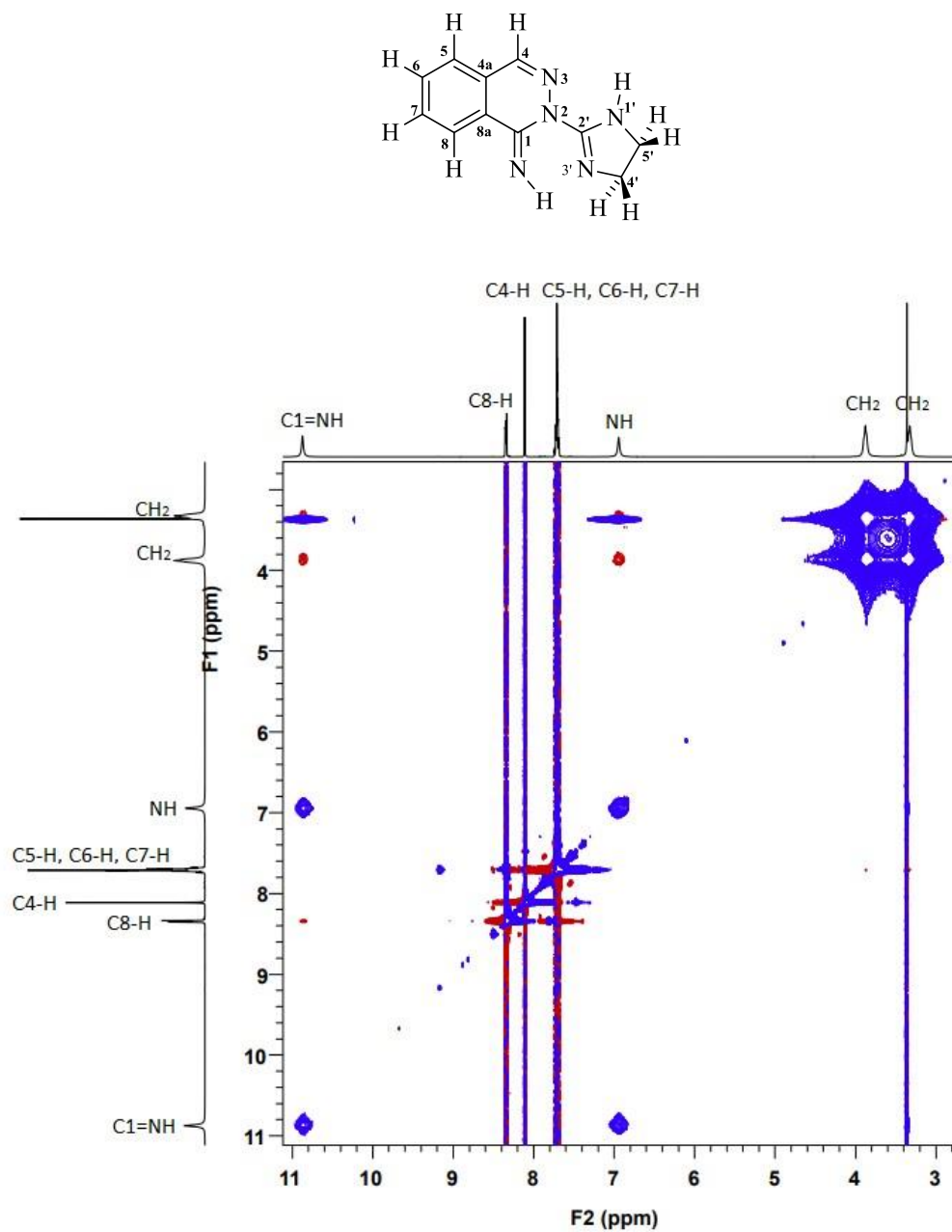
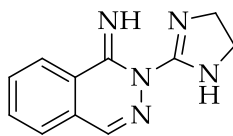
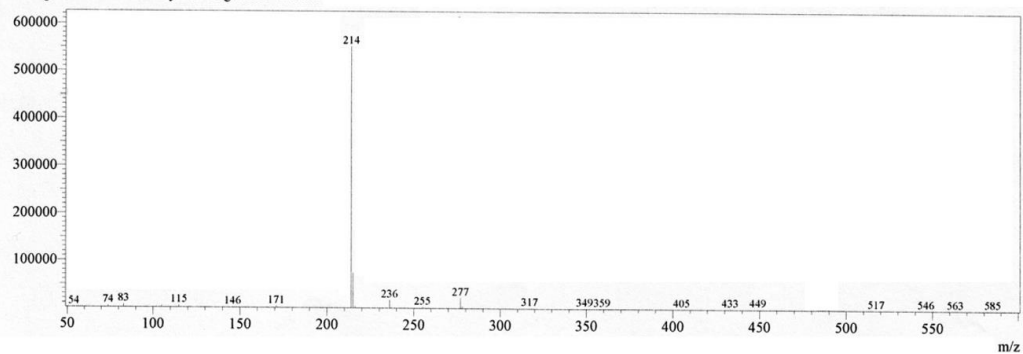


Figure S7. MS spectrum of of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (**5**).



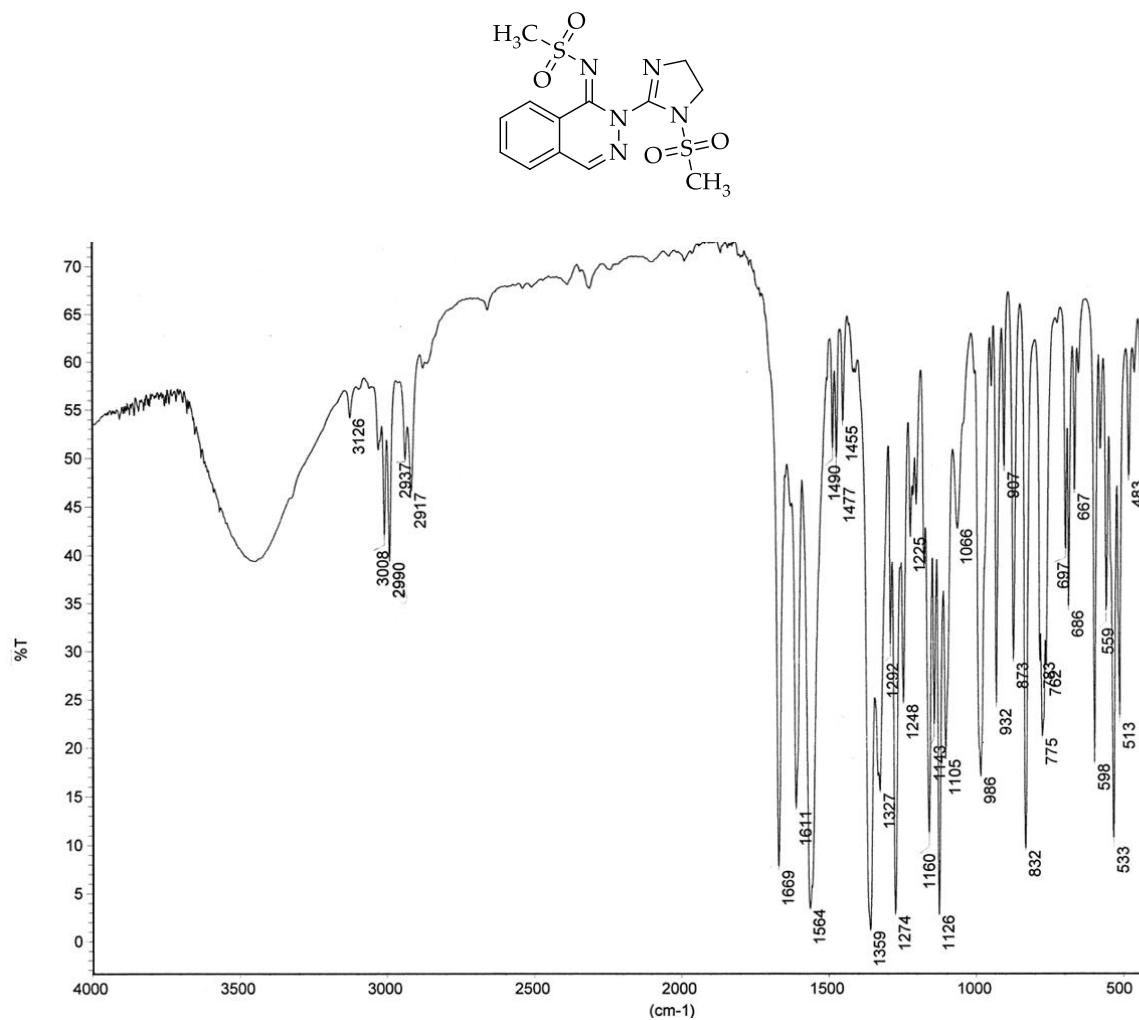
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Max Peak:546 Base Peak:213.95(551933)
Spectrum:Single 1.883(227)
Background:None Polarity:Pos Segment1 - Event1



Spectra of Representative Compounds 6a, 7a, and 7k

Figure S8. IR spectrum of *N*-(2-(1-(methylsulfonyl)-4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-ylidene)methanesulfonamide (**6a**).



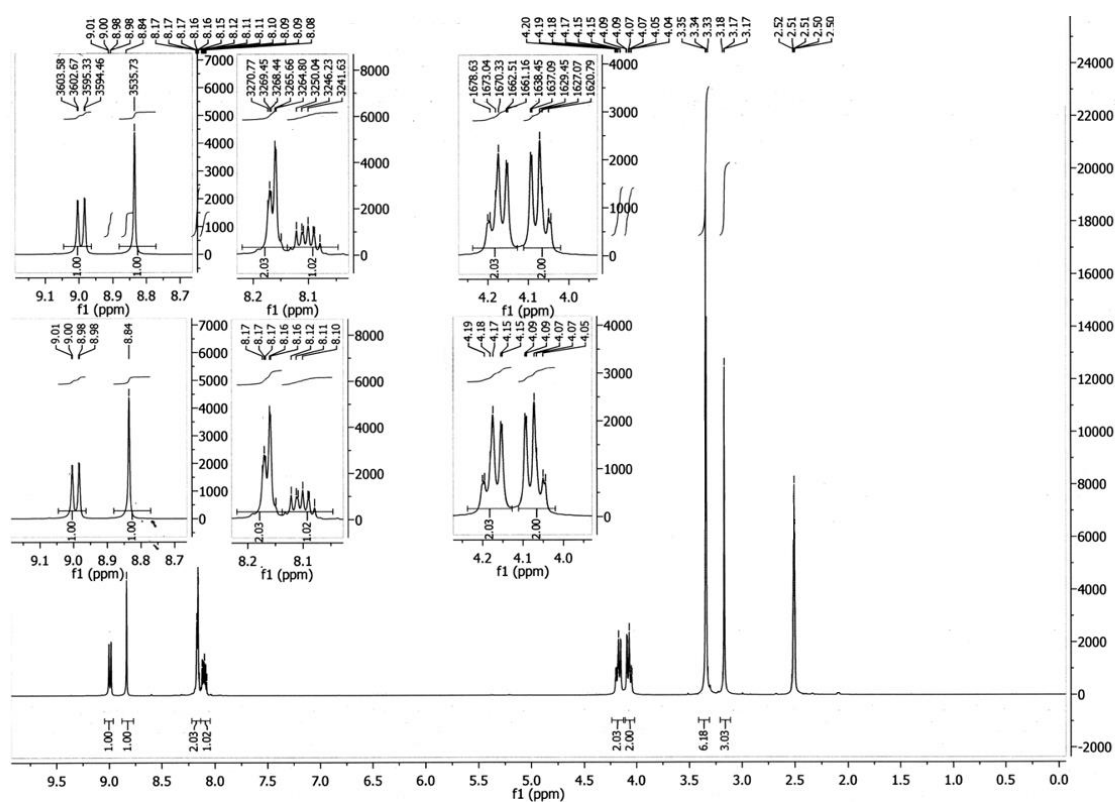
Cs1nnc2c3c(ccccc3n2)S(=O)(=O)c4ccccc41

Figure S10. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of *N*-(2-(1-(methylsulfonyl)-4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-ylidene)methanesulfonamide (**6a**).

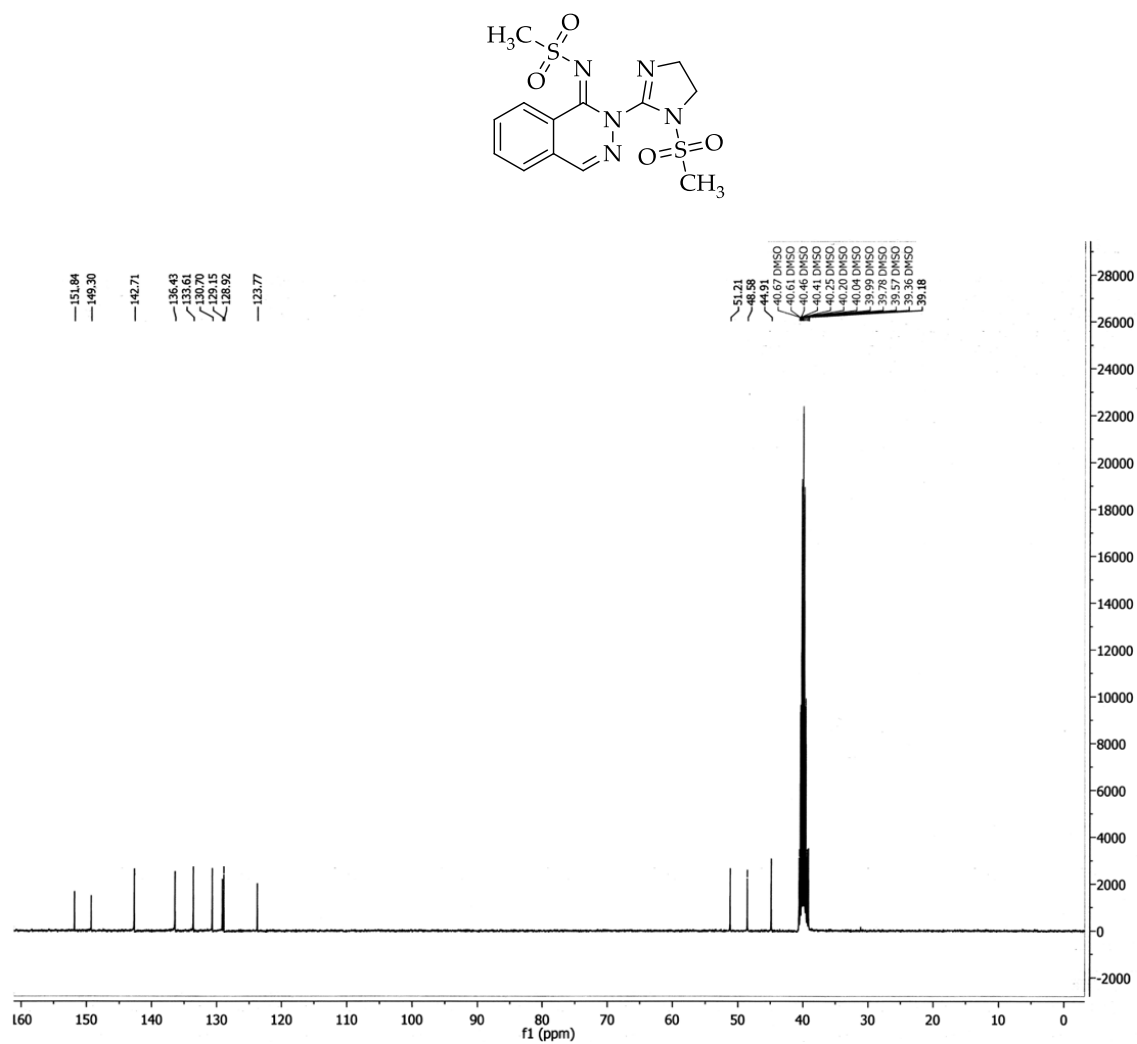
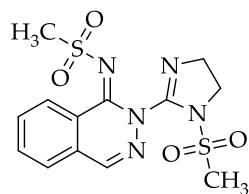


Figure S11. MS spectrum of *N*-(2-(1-(methylsulfonyl)-4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-ylidene)methanesulfonamide (**6a**).



<Spectrum>

Retention Time: 4.475(Scan#: 538)
 Max Peak: 445 Base Peak: 392.00(683612)
 Spectrum: Single 4.475(538)
 Background: None Polarity: Pos Segment1 - Event1

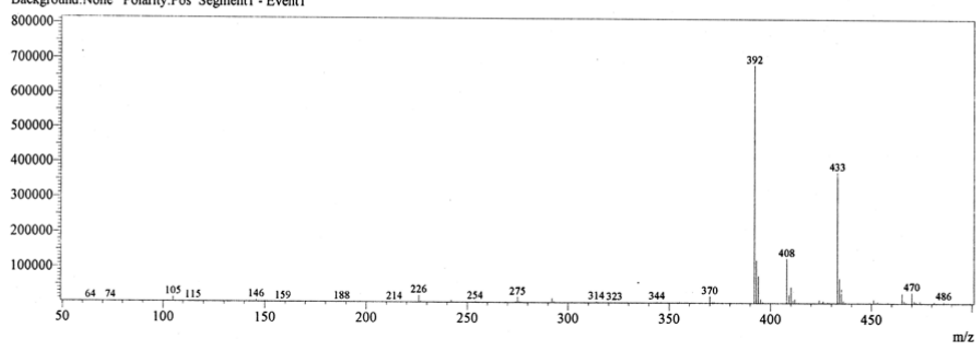


Figure S12. IR spectrum of 2-(((1-(methylsulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7a**).

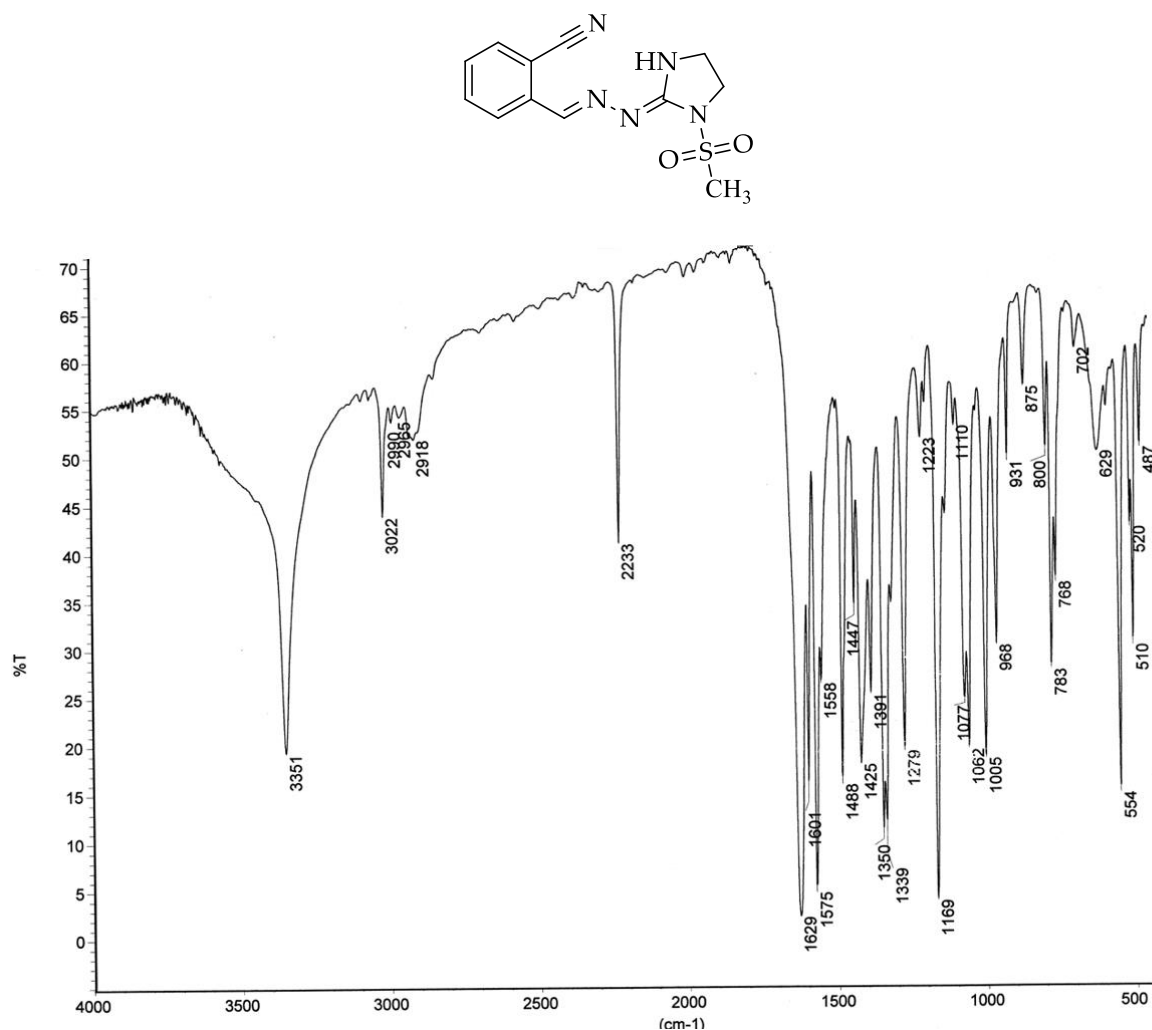


Figure S13. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of 2-(((1-(methylsulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7a**).

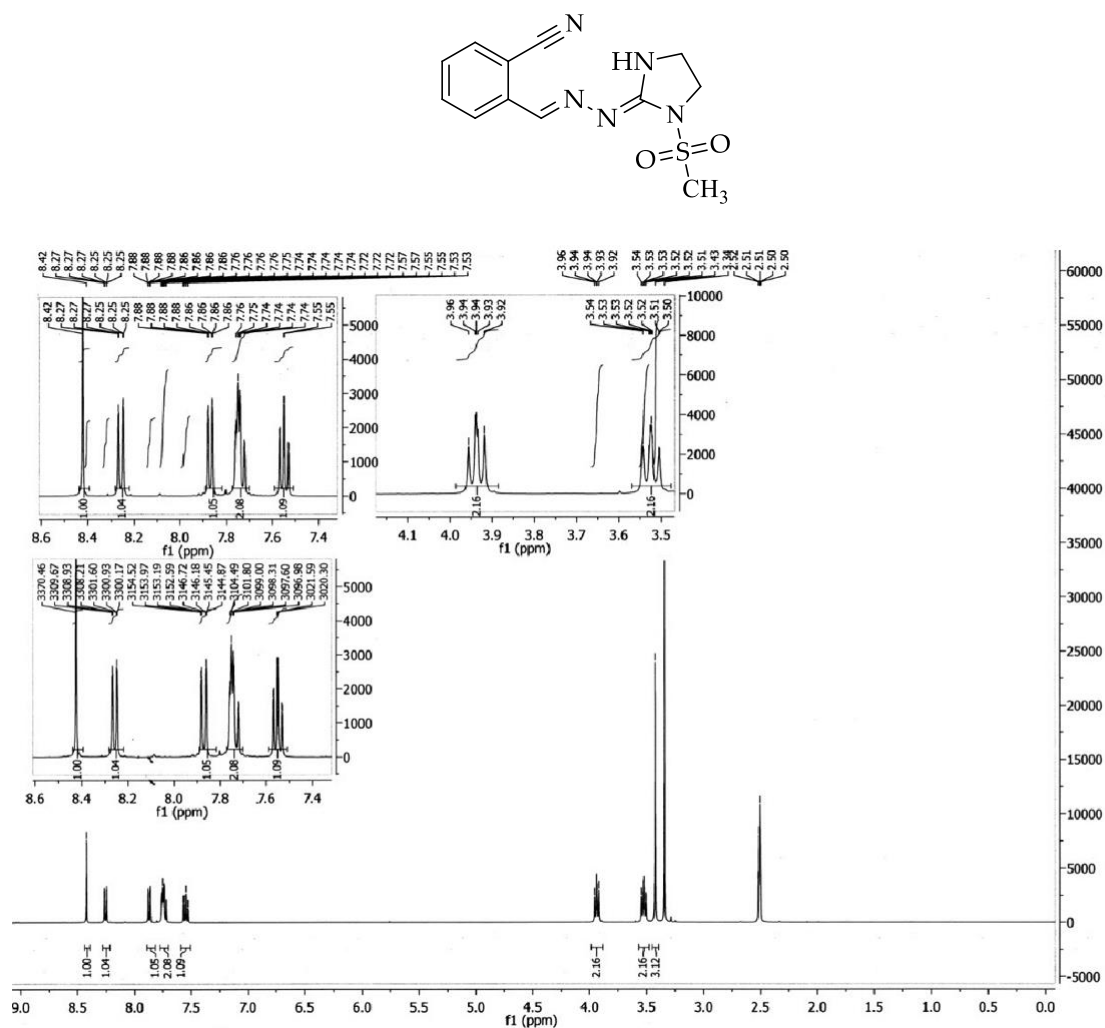


Figure S14. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of 2-(((1-(methylsulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7a**).

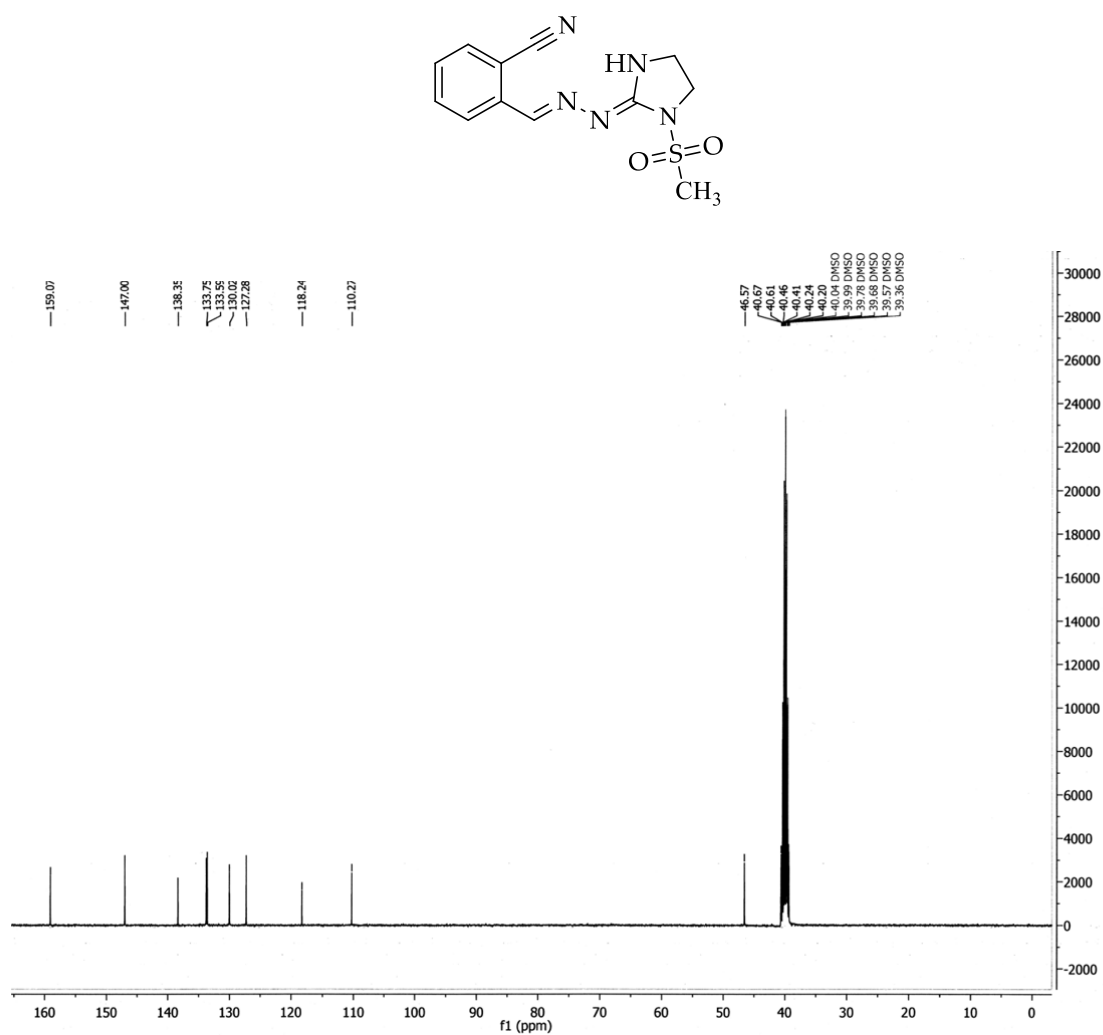
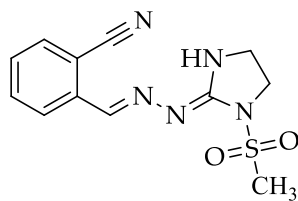


Figure S15. MS spectrum of 2-(((1-(methylsulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7a**).



<Spectrum>

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 Max Peak: 638 Base Peak: 291.95 (97369)
 Spectrum: Single 0.125 (16)
 Background: None Polarity: Pos Segment: 1 - Event: 1

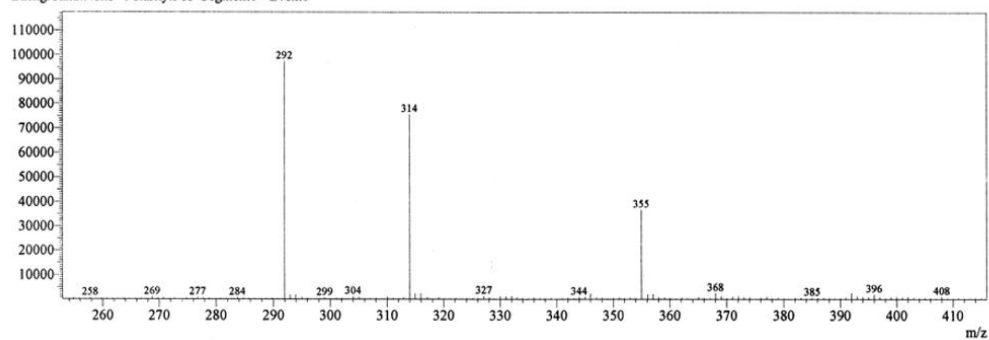


Figure S16. IR spectrum of 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).

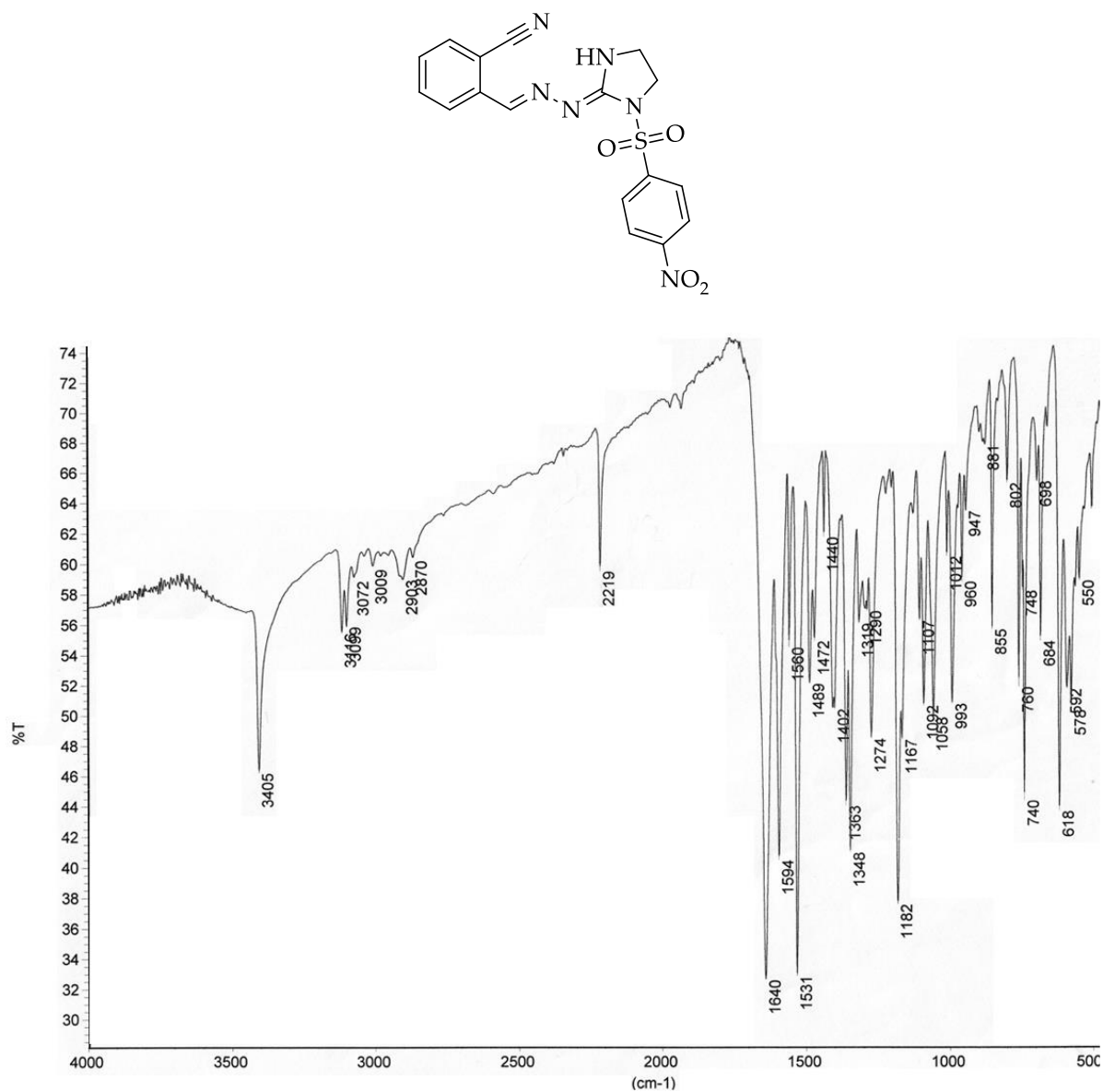


Figure S17. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).

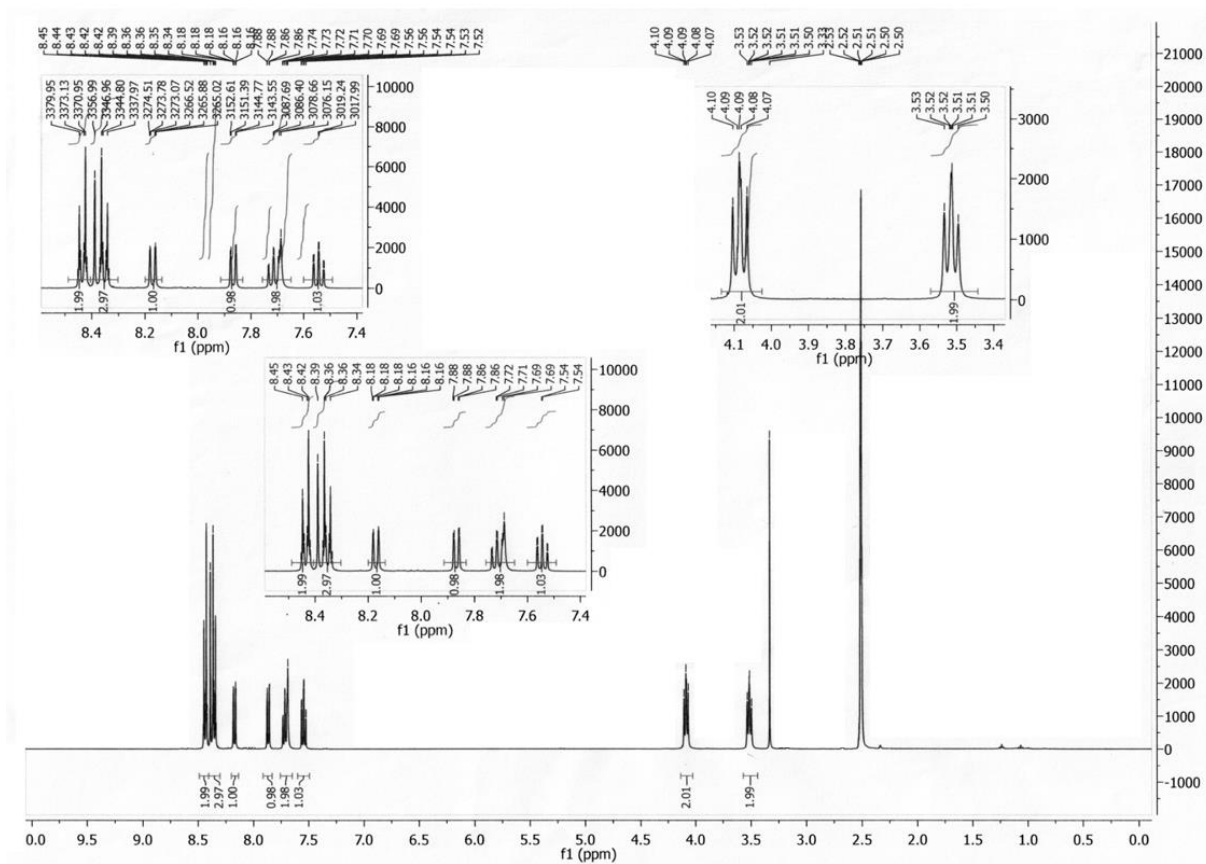
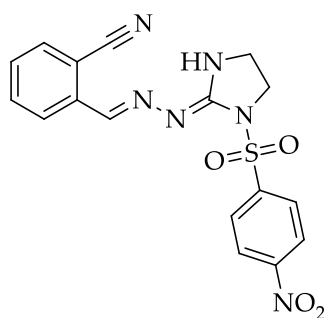


Figure S18. ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).

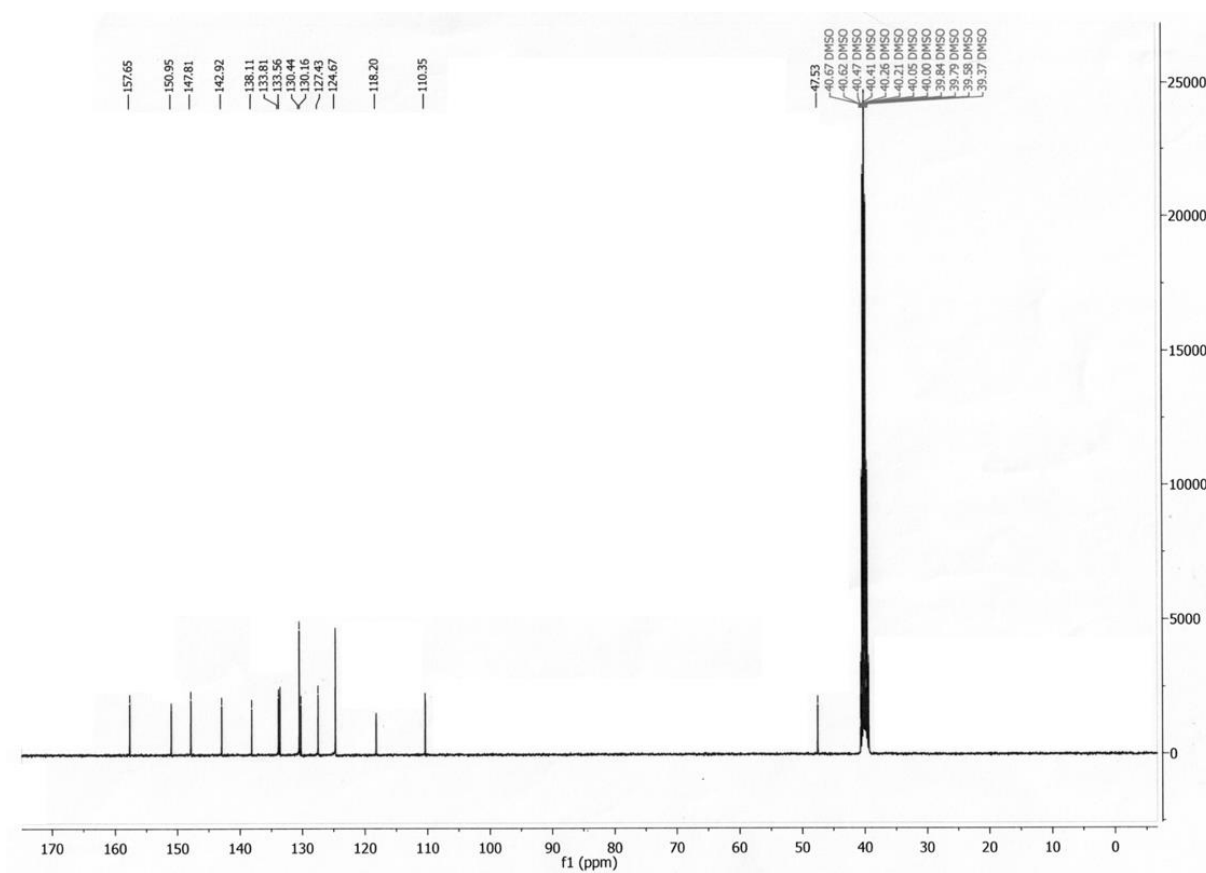
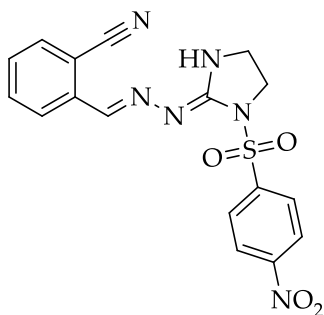
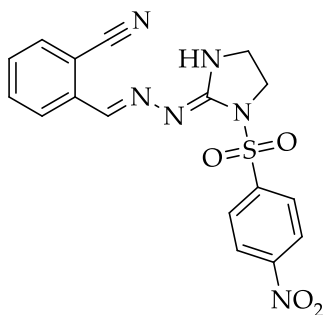
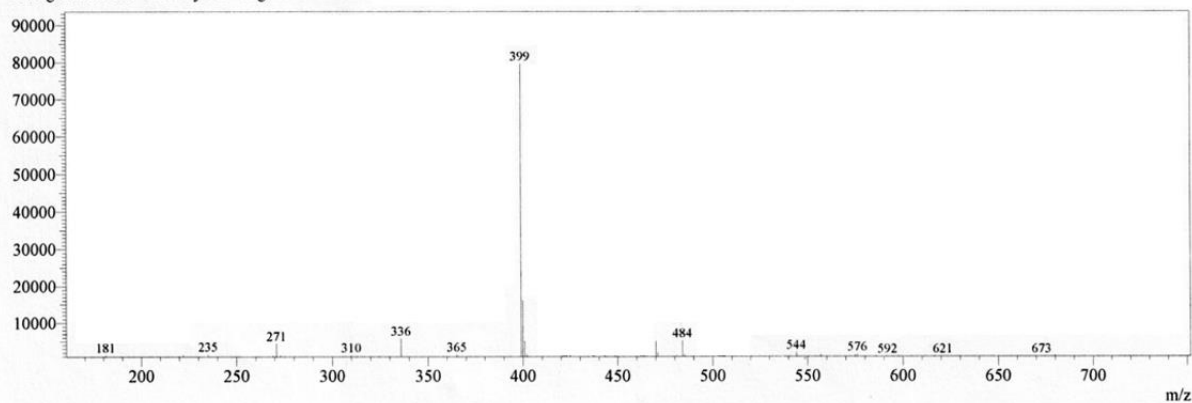


Figure S19. MS spectrum of 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).



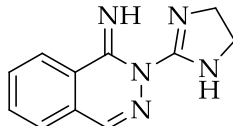
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 Spectrum: Single 3.067 (369)
 Background: None Polarity: Pos Segment: 1 - Event: 1



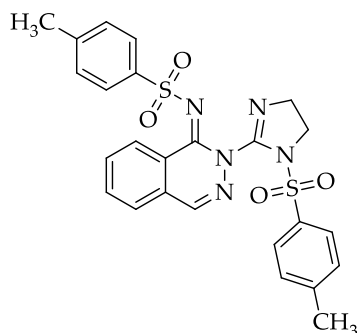
X-ray Crystallographic Studies

Figure S20. CheckCIF/PLATON report for 2-(4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-imine (5).



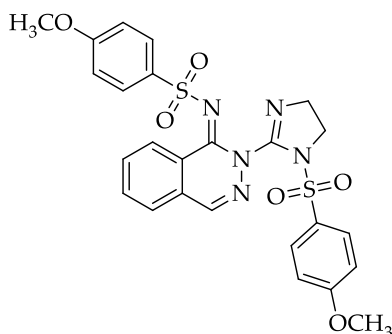
Bond precision: C-C = 0.0017 Å		Wavelength=1.54184	
Cell:	a=6.81358(7)	b=12.04885(14)	c=12.51063(14)
	alpha=90	beta=96.2273(10)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1021.01(2)	1021.01(2)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C11 H11 N5	C11 H11 N5	
Sum formula	C11 H11 N5	C11 H11 N5	
Mr	213.25	213.25	
Dx, g cm-3	1.387	1.387	
Z	4	4	
Mu (mm-1)	0.729	0.729	
F000	448.0	448.0	
F000'	449.27		
h, k, lmax	8, 15, 15	8, 15, 15	
Nref	2154	2111	
Tmin, Tmax	0.804, 0.896	0.889, 1.000	
Tmin'	0.804		
Correction method= # Reported T Limits: Tmin=0.889 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness= 0.980		Theta(max)= 76.628	
R(reflections)= 0.0340(1903)		wR2(reflections)= 0.1025(2111)	
S = 1.047		Npar= 153	
Alert level C			
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=		0.600	3 Report
Alert level G			
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF			Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature		(K) 293	Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature		(K) 293	Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=		0.600	41 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF			3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.			7 Info
0 ALERT level A = Most likely a serious problem - resolve or explain			
0 ALERT level B = A potentially serious problem, consider carefully			
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight			
6 ALERT level G = General information/check it is not something unexpected			
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data			
1 ALERT type 2 Indicator that the structure model may be wrong or deficient			
2 ALERT type 3 Indicator that the structure quality may be low			
1 ALERT type 4 Improvement, methodology, query or suggestion			
0 ALERT type 5 Informative message, check			

Figure S21. CheckCIF/PLATON report for 4-methyl-*N*-(2-(1-tosyl-4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-ylidene)benzenesulfonamide (**6c**).



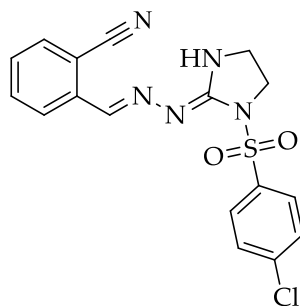
Bond precision:	C-C = 0.0037 Å	Wavelength=0.71073
Cell:	a=9.8874(3) alpha=90	b=10.3839(3) beta=97.633(3) c=23.6423(8) gamma=90
Temperature:	293 K	
Volume	Calculated 2405.84(13)	Reported 2405.83(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H23 N5 O4 S2	C25 H23 N5 O4 S2
Sum formula	C25 H23 N5 O4 S2	C25 H23 N5 O4 S2
Mr	521.60	521.60
Dx, g cm ⁻³	1.440	1.440
Z	4	4
Mu (mm ⁻¹)	0.265	0.265
F000	1088.0	1088.0
F000'	1089.42	
h, k, lmax	12, 12, 29	12, 12, 29
Nref	4911	4904
Tmin, Tmax	0.909, 0.948	0.991, 1.000
Tmin'	0.899	
Correction method=	# Reported T Limits: Tmin=0.991 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.999	Theta(max)= 26.372
R(reflections)=	0.0469(3447)	wR2(reflections)= 0.1163(4904)
S =	1.021	Npar= 327
Alert level B		
PLAT230_ALERT_2_B	Hirshfeld Test Diff for S26	--028 . 7.3 s.u.
Alert level C		
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.668 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6 Note
Alert level G		
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K) 293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K) 293 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info
0 Alert level A = Most likely a serious problem - resolve or explain 1 Alert level B = A potentially serious problem, consider carefully 3 Alert level C = Check. Ensure it is not caused by an omission or oversight 5 Alert level G = General information/check it is not something unexpected 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 2 ALERT type 2 Indicator that the structure model may be wrong or deficient 2 ALERT type 3 Indicator that the structure quality may be low 2 ALERT type 4 Improvement, methodology, query or suggestion 0 ALERT type 5 Informative message, check		

Figure S22. CheckCIF/PLATON report for 4-methoxy-*N*-(2-(1-((4-methoxyphenyl)sulfonyl)-4,5-dihydro-1*H*-imidazol-2-yl)phthalazin-1(2*H*)-ylidene)benzenesulfonamide (**6e**).



Bond precision:	C-C = 0.0034 Å	Wavelength=0.71073
Cell:	a=7.5517 (2) alpha=90	b=17.1382 (6) beta=94.443 (3)
Temperature:	293 K	c=19.2240 (6) gamma=90
Volume	Calculated 2480.54 (13)	Reported 2480.54 (13)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H23 N5 O6 S2	C25 H23 N5 O6 S2
Sum formula	C25 H23 N5 O6 S2	C25 H23 N5 O6 S2
Mr	553.60	553.60
Dx, g cm ⁻³	1.482	1.482
Z	4	4
Mu (mm ⁻¹)	0.267	0.267
F000	1152.0	1152.0
F000'	1153.50	
h, k, lmax	9, 21, 24	9, 21, 24
Nref	5080	5074
Tmin, Tmax	0.899, 0.948	0.987, 1.000
Tmin'	0.899	
Correction method= # Reported T Limits: Tmin=0.987 Tmax=1.000		
AbsCorr = MULTI-SCAN		
Data completeness=	0.999	Theta(max)= 26.371
R(reflections)=	0.0479 (3545)	wR2(reflections)= 0.1074 (5074)
S =	1.037	Npar= 345
Alert level C		
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C13 Check
PLAT411_ALERT_2_C	Short Inter H...H Contact H5 ..H5	2.10 Ang.
	-x, l-y, l-z =	3.566 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.044 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6 Note
Alert level G		
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary.	Please Do !
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2 Check
0 Alert level A = Most likely a serious problem - resolve or explain		
0 Alert level B = A potentially serious problem, consider carefully		
4 Alert level C = Check. Ensure it is not caused by an omission or oversight		
6 Alert level G = General information/check it is not something unexpected		
4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data		
3 ALERT type 2 Indicator that the structure model may be wrong or deficient		
2 ALERT type 3 Indicator that the structure quality may be low		
0 ALERT type 4 Improvement, methodology, query or suggestion		
1 ALERT type 5 Informative message, check		

Figure S23. CheckCIF/PLATON report for 2-(((1-((4-chlorophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7g**).



Bond precision: C-C = 0.0081 Å		Wavelength=0.71073	
Cell:	a=7.6338(8)	b=10.1714(8)	c=11.6609(8)
	alpha=82.556(6)	beta=88.506(7)	gamma=80.477(8)
Temperature:	293 K		
	Calculated	Reported	
Volume	885.41(13)	885.41(13)	
Space group	P 1	P 1	
Hall group	P 1	P 1	
Moiety formula	C17 H14 Cl N5 O2 S	C17 H14 Cl N5 O2 S	
Sum formula	C17 H14 Cl N5 O2 S	C17 H14 Cl N5 O2 S	
Mr	387.84	387.84	
Dx, g cm-3	1.455	1.455	
Z	2	2	
Mu (mm-1)	0.356	0.356	
F000	400.0	400.0	
F000'	400.68		
h, k, lmax	9, 12, 14	9, 12, 14	
Nref	7272[3636]	7192	
Tmin, Tmax	0.918, 0.931	0.979, 1.000	
Tmin'	0.837		
Correction method= # Reported T Limits: Tmin=0.979 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness= 1.98/0.99		Theta(max)= 26.372	
R(reflections)= 0.0486(5086)		wR2(reflections)= 0.0899(7192)	
S = 0.995		Npar= 477	

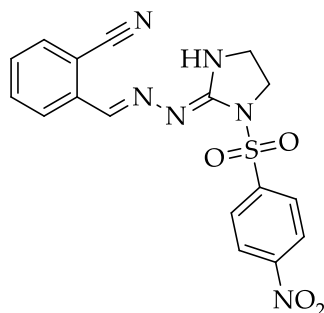
Alert level C			
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C23A Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C23B Check
PLAT245_ALERT_2_C	U(iso) H16B	Smaller than U(eq) N16B by	0.012 Ang**2
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C20A -C25A	1.37 Ang.
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C20B -C25B	1.37 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00807 Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N16A --H16A	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report

Alert level G			
PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	Please Check
PLAT153_ALERT_1_G	The s.u.'s on the Cell Axes	are Equal .. (Note)	0.0008 Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	 (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	 (K)	293 Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C2A --C7A	5.2 s.u.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s)	Below Theta(Min).	4 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

4 **ALERT** type 1 CIF construction/syntax error, inconsistent or missing data
8 **ALERT** type 2 Indicator that the structure model may be wrong or deficient
3 **ALERT** type 3 Indicator that the structure quality may be low
0 **ALERT** type 4 Improvement, methodology, query or suggestion
0 **ALERT** type 5 Informative message, check

Figure S24. CheckCIF/PLATON report for 2-(((1-((4-nitrophenyl)sulfonyl)imidazolidin-2-ylidene)hydrazono)methyl)benzonitrile (**7k**).



Bond precision:	C-C = 0.0052 Å	Wavelength=0.71073	
Cell:	a=7.2342 (11)	b=14.748 (3)	c=16.643 (2)
	alpha=90	beta=91.217 (14)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1775.2 (5)	1775.2 (5)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C17 H14 N6 O4 S	C17 H14 N6 O4 S	
Sum formula	C17 H14 N6 O4 S	C17 H14 N6 O4 S	
Mr	398.40	398.40	
Dx, g cm-3	1.491	1.491	
Z	4	4	
Mu (mm-1)	0.222	0.222	
F000	824.0	824.0	
F000'	824.84		
h, k, lmax	8, 17, 19	8, 17, 19	
Nref	3143	4958	
Tmin, Tmax	0.961, 0.985	0.979, 1.000	
Tmin'	0.915		
Correction method= # Reported T Limits: Tmin=0.979 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness= 1.577	Theta(max)= 25.026		
R(reflections)= 0.0432 (2608)	wR2(reflections)= 0.0790 (4958)		
S = 0.831	Npar= 258		

Alert level C

PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C20 -C25	1.37 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.0052 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		4.737 Check

Alert level G

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 (K)	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 (K)	Check
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed		! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)		2 Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1)	Est.d BASF	0.38 Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (1 0 0)	Est.d BASF	0.31 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

The crystal packing of molecules in **6e** and **6c** is shown in **Figure S25**. In **6e** the molecules are arranged into centrosymmetric dimers via π - π stacking interactions between phthalazinimine fragments. Those dimers are further assembled into 1D chains along [010] via stacking interactions between 4-methoxyphenyl groups of the sulfonyl substituent at the imidazolidine ring. Stacking interactions between 1-phthalazinimine fragments are absent in **6e** where 4-methyl groups are already involved in π - π intramolecular stacking. Here intermolecular stacking interactions between one of the 4-methylphenyl groups and 1-phthalazinimine fragment of inversion center related molecule result in compact dimers shown in **Figure S26**.

Figure S25. Crystal packing in **6e** (left) and **6c** (right).

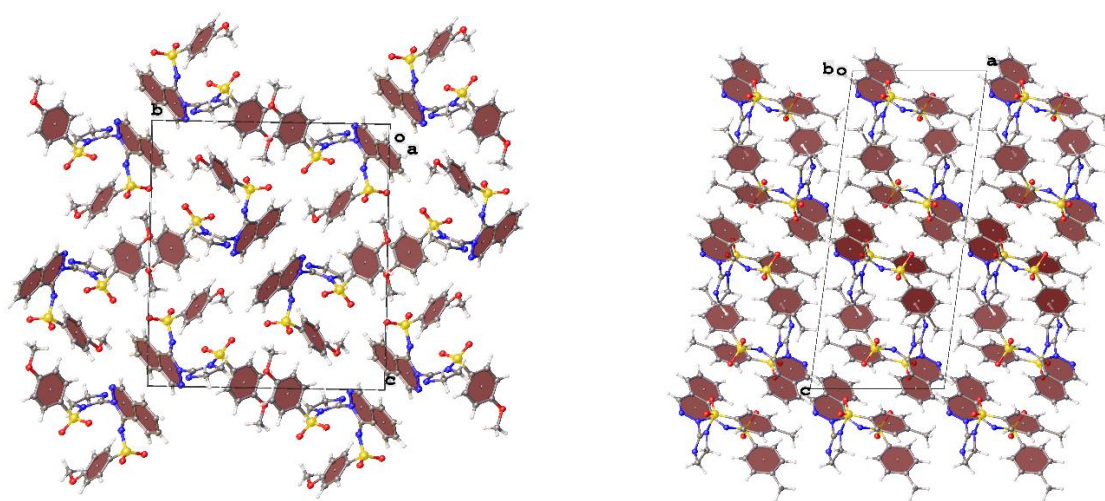
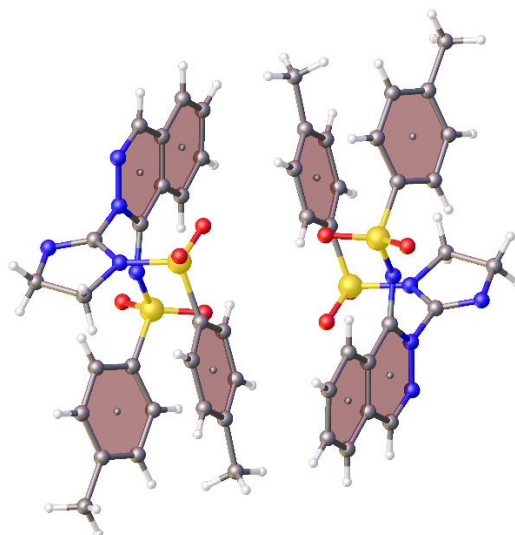


Figure S26. Centrosymmetric dimer via π - π stacking interactions in **6c**.



The crystal packing of molecules in **7g** and **7k** as shown in **Figure S27** is mostly driven by weak intermolecular forces. Among specific interactions the main role is played by stacking

interactions between aromatic rings, or aromatic ring and extended π -systems, as well as weak N-H $\cdots$ N (**7g**) or N-H $\cdots$ O (**7k**) hydrogen bonds.

Figure S27. Crystal packing in **7g** and **7k**. Hydrogen bonds are shown with dashed lines.

