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MDPI

Supplementary Information

Toward an Understanding of the Formation and Desolvation of Methanol Solvate, and Structure of Methanolysis Product: A Case Study of Nicosulfuron

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Table S1. Crystallographic data of II, S1, S3, Hydrate, and DMF solvate based on NS.

Parameters	II [a]	S1 [a]	S3 [a]	Hydrate [b]	DMF Solvate [b]
Formula	$C_{15}H_{18}N_6O_6S\cdot H_2O$	$C_{15}H_{18}N_6O_6S\cdot CH_4O$	$C_{15}H_{18}N_6O_6S\cdot CH_3CN$	$C_{15}H_{18}N_6O_6S\cdot H_2O$	$C_{15}H_{18}N_6O_6S\cdot C_3H_7ON$
Crystal system	triclinic	triclinic	monoclinic	triclinic	monoclinic
Space group	P−1	P−1	C2/c	P−1	$P2_1/c$
Temperature /K	113(2)	113(2)	113(2)	293(2)	113(2)
Radiation type	Mo Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα
Wavelength/ Å	0.71073	0.71073	0.71073	0.71073	0.71073
a/ Å	14.141(3)	7.85333(16)	23.197(5)	14.360(3)	7.3627(15)
b/ Å	15.307(3)	20.401(4)	14.331(3)	15.312(3)	22.736(5)
c/ Å	19.905(3)	25.859(5)	13.596(3)	19.927(4)	13.769(3)
α/ °	67.42(3)	85.55(3)	90	112.54(3)	90
β/ °	77.79(3)	83.76(3)	112.54(3)	97.82(3)	99.90(3)
γ/ °	83.87(3)	85.07(3)	90	97.12(3)	90
Volume/ $Å^3$	3886.9(16)	4093.5(15)	4174.6(17)	3934.3(14)	2270.5(8)
Z	8	8	8	8	4
Density/g·cm^{-3}	1.464	1.436	1.437	1.44	1.414
R_{int}	0.0762	0.0655	0.0599	0.0595	0.0472
$R_1[I > 2\sigma(I)]$	0.0873	0.0684	0.0595	0.0595	0.0472
ωR_2	0.2068	0.1560	0.1225	0.1429	0.1075
goodness-of-fit	1.125	0.988	1.142	0.903	1.057
CCDC No.	1863680	1863688	1863687	1875784	1875778

[a] Crystal structure was retrieved from the literature [18].

[b] Crystal structure was retrieved from the literature [19].

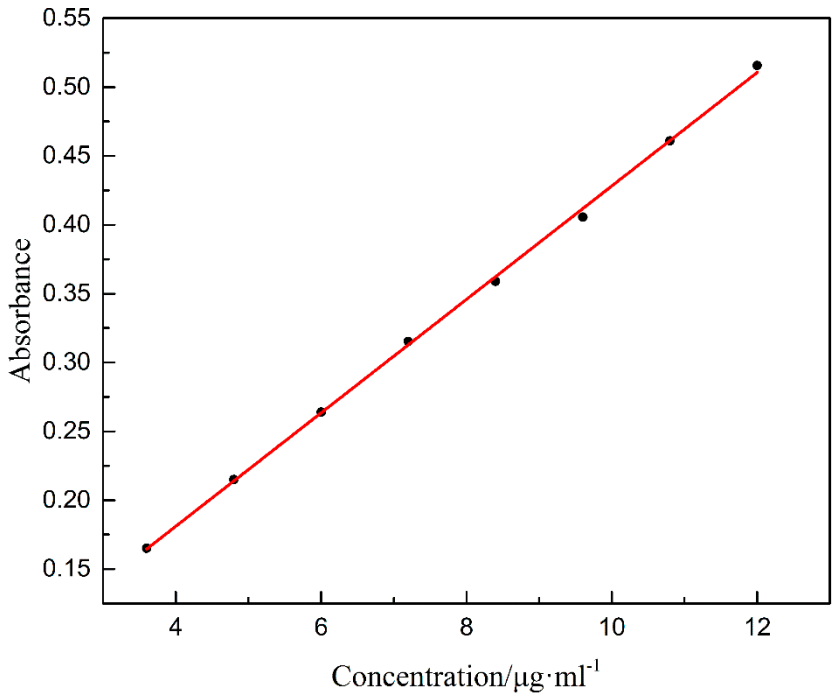

Figure S1. Plot of UV standard curve for NS in aqueous.

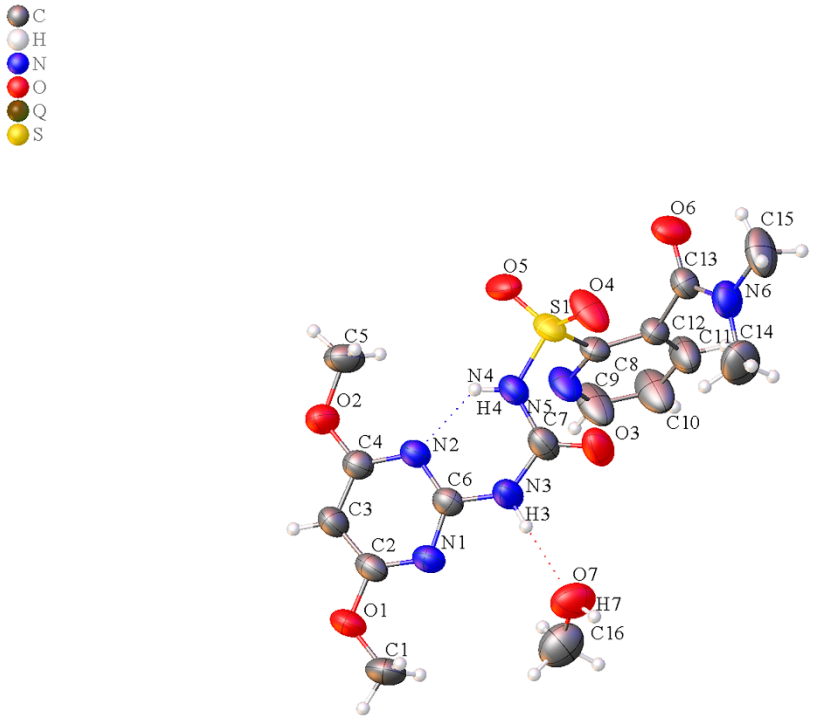

Figure S2. ORTEP view of NS-MeOH with an atom labelling scheme.

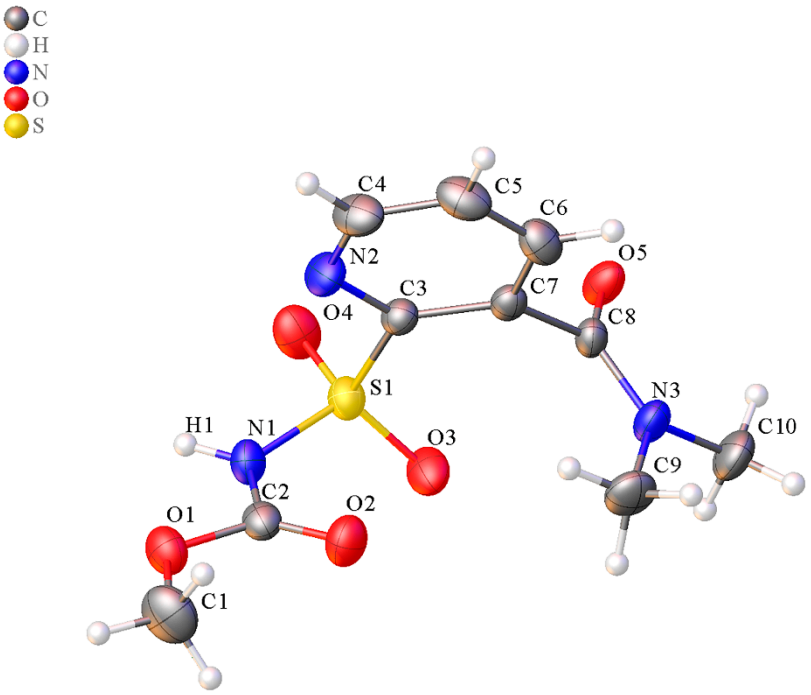

Figure S3. ORTEP view of PCM with an atom labelling scheme.

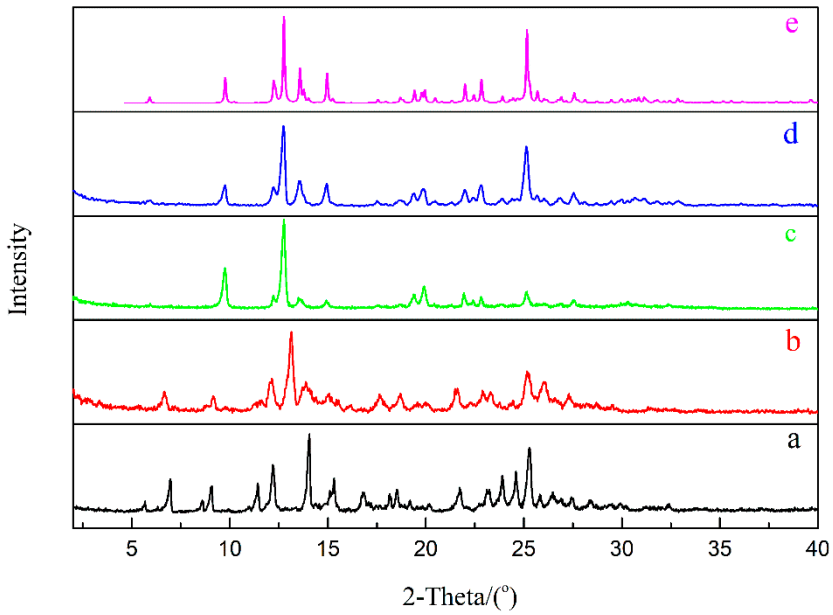

Figure S4. PXRD patterns of (**a**) NS, (**b**) desolvation product of NS-MeOH, (**c**) undissolved powders of NS after dissolution experiment, and (**d**) undissolved powders of NS-MeOH after the dissolution experiment. (**e**) Simulated pattern of NS hydrate.