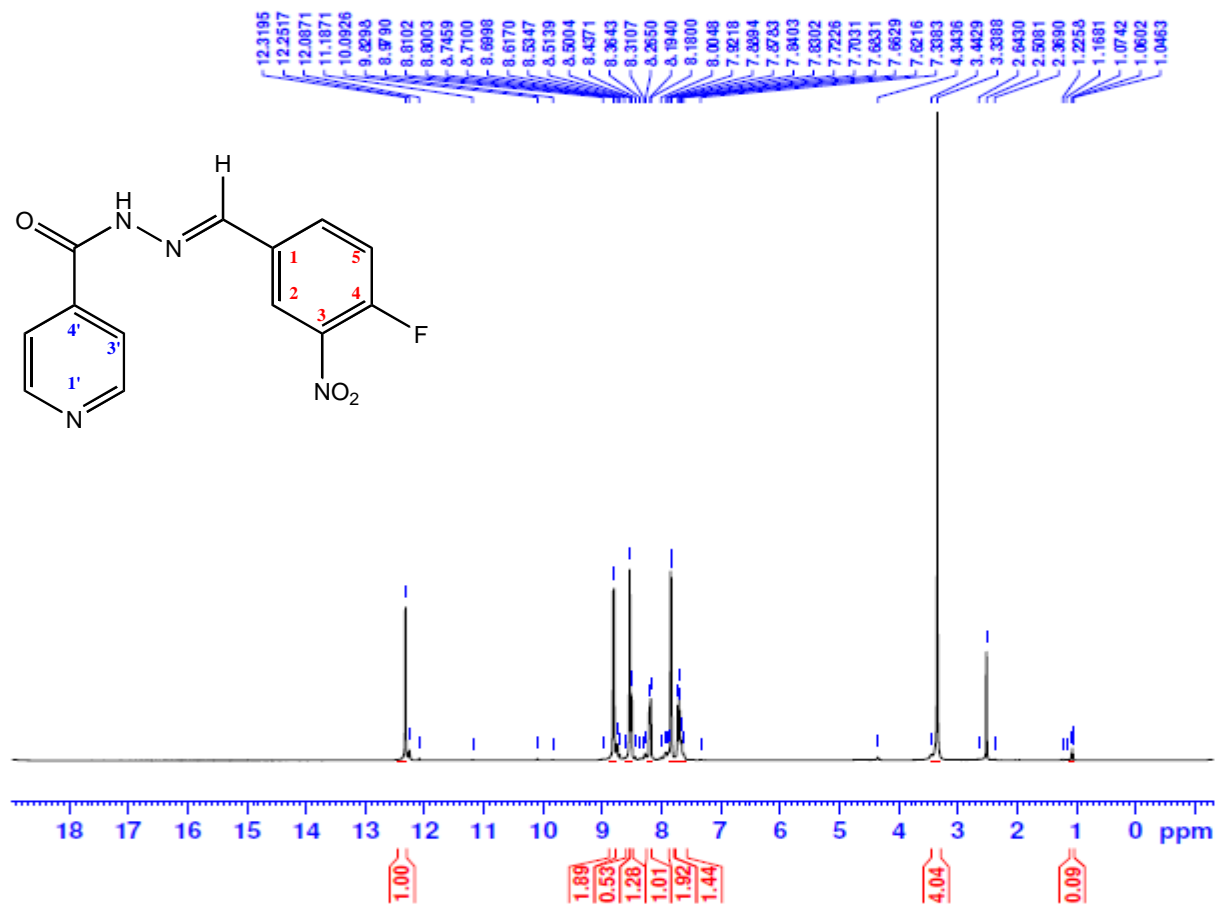


Figure S1: Representative  $^1\text{H}$ NMR of (E)-N'-((5-(2-nitrophenyl)furan-2-yl)methylene)isonicotinohydrazide

3N4FB14  
1H1 NMR



The University of Jordan  
Faculty of Science  
Department of Chemistry

Instrument Model:  
Bruker 500 MHz-Avance III

Operator: Rola Hassouneh  
nmr500@ju.edu.jo

Current Data Parameters  
NAME 17jan01jalal  
EXPNO 101  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170105  
Time 9.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 0  
SWH 10135.135 Hz  
FIDRES 0.154650 Hz  
AQ 3.2331092 sec  
RG 49.66  
DW 49.333 usec  
DE 6.50 usec  
TE 300.4 K  
D1 2.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
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NUC1 1H  
P1 10.60 usec  
PLW1 17.39999962 W

F2 - Processing parameters  
SI 131072  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
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PC 1.00

Figure S2: Representative <sup>1</sup>H NMR of (E)-N'-(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide

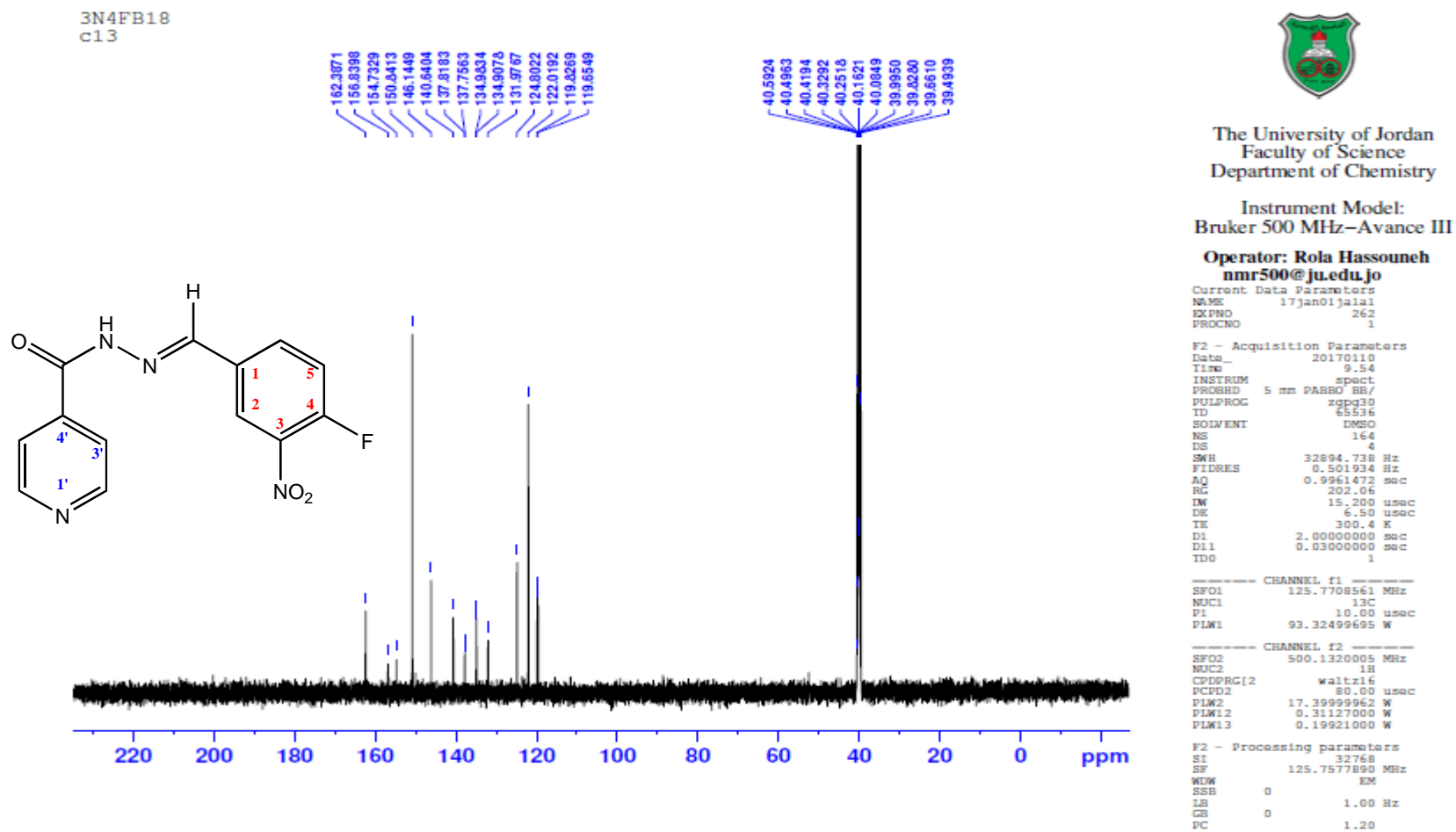
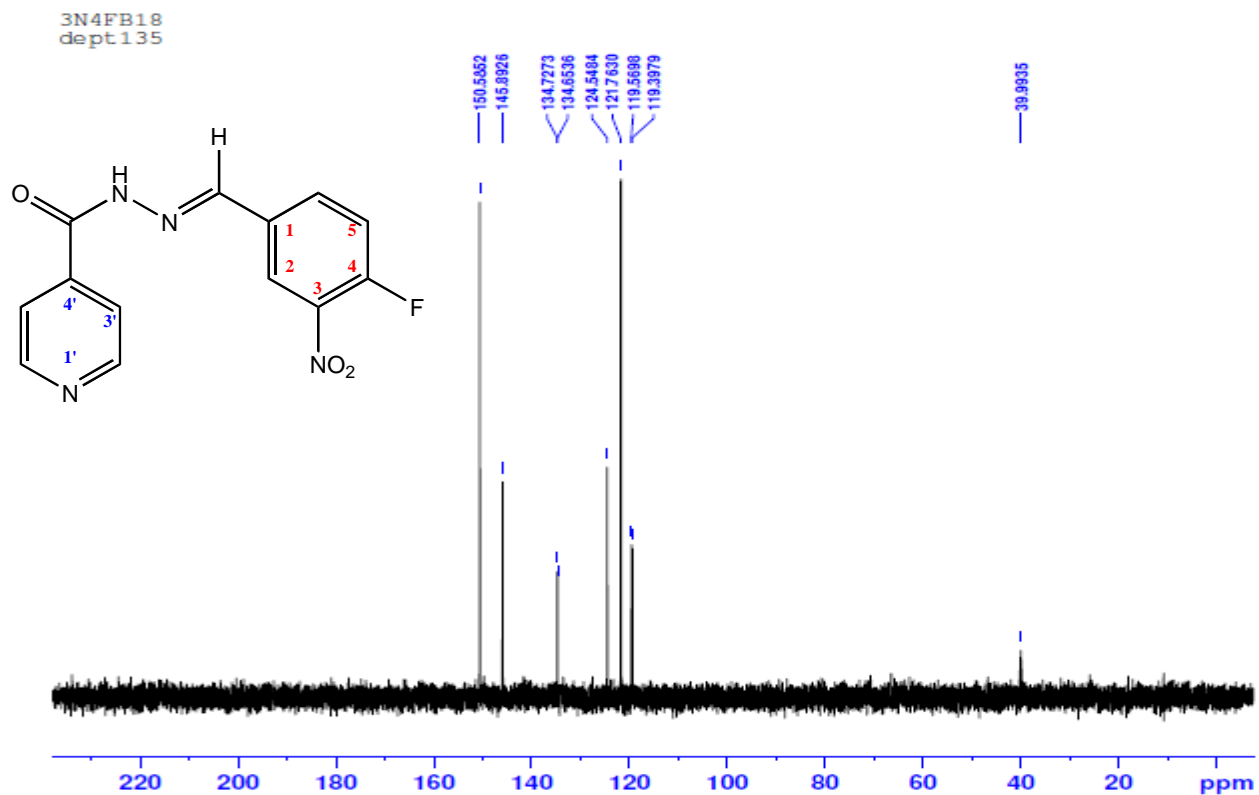


Figure S3: Representative  $^{13}\text{C}$ NMR of (E)-N'-(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide



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Bruker 500 MHz-Avance III

Operator: Rola Hassouneh  
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Current Data Parameters  
NAME 17jan01.je1a1  
EXPNO 263  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170115  
Time 13.58  
INSTRUM spect  
PROBHD 5 mm PABBO HX/  
PULPROG dept135  
TD 65536  
SOLVENT DMSO  
NS 179  
DS 4  
SWH 30864.197 Hz  
FIDRES 0.470950 Hz  
AQ 1.0616832 sec  
RG 202.56  
DW 16.200 usec  
DE 6.50 usec  
TE 300.5 K  
CRST2 145.0000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD 1

----- CHANNEL f1 -----

SFO1 125.7722923 MHz  
NUC1 13C  
P1 10.00 usec  
P13 2000.00 usec  
PLM0 0 W  
PLM1 93.32499695 W  
SFO1S1 Cmp60comp.4  
SFO1S 0.500  
SFOFFS5 0 Hz  
SFO5 13.69400024 W

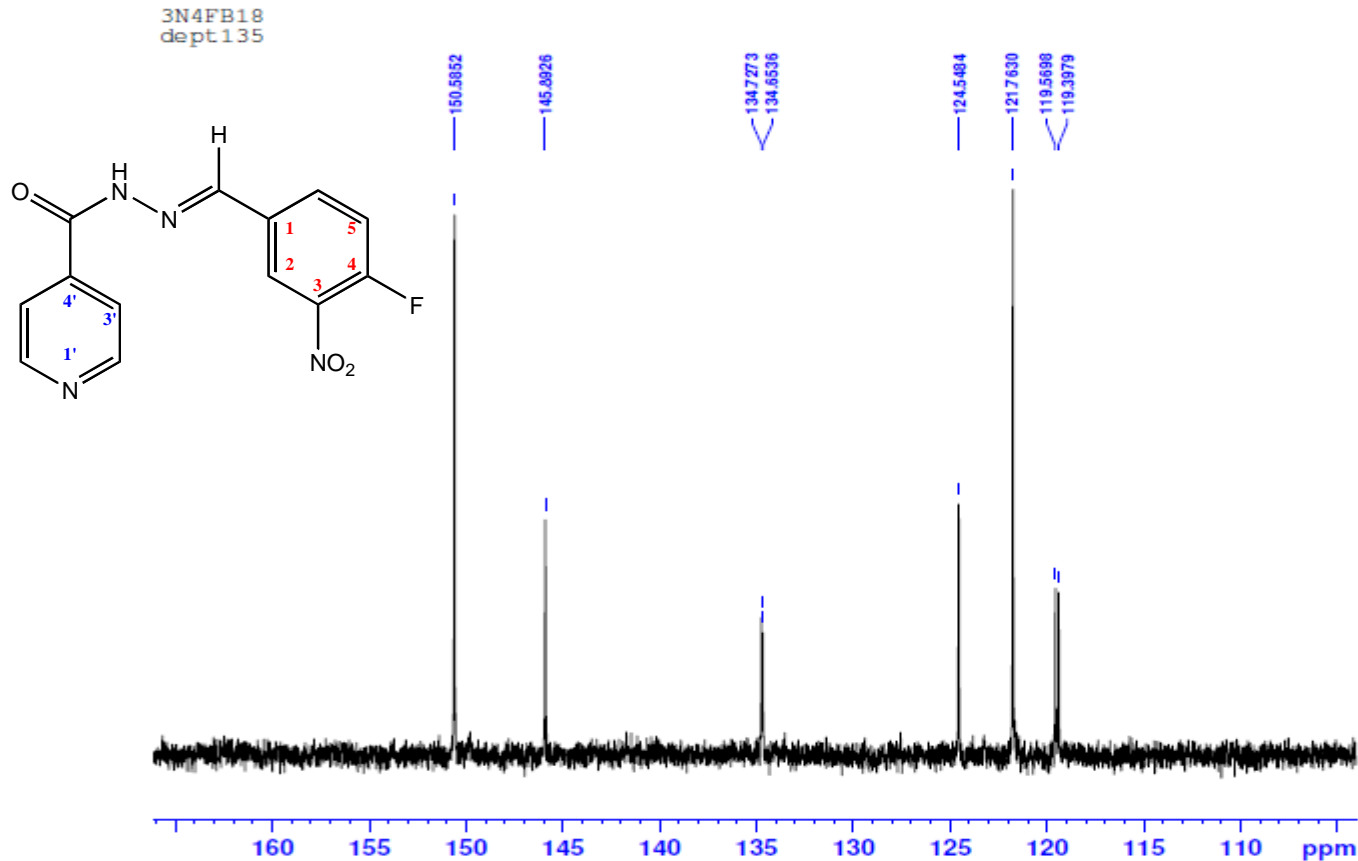
----- CHANNEL f2 -----

SFO2 500.1315995 MHz  
NUC2 1H  
CPCPRG2 waltz16  
P3 11.50 usec  
P4 23.00 usec  
PCPD2 80.00 usec  
PLM2 17.37800026 W  
PLM12 0.36307999 W

F2 - Processing parameters

SF 32768  
CF 125.7578211 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 2.00

Figure S4: Representative DEPT-<sup>13</sup>CNMR of (E)-N'-(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide



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Instrument Model:  
Bruker 500 MHz-Avance III

Operator: Rola Hassouneh  
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Current Data Parameters  
NAME 17jan01je1a1  
EXPNO 26.3  
PROCNO 1

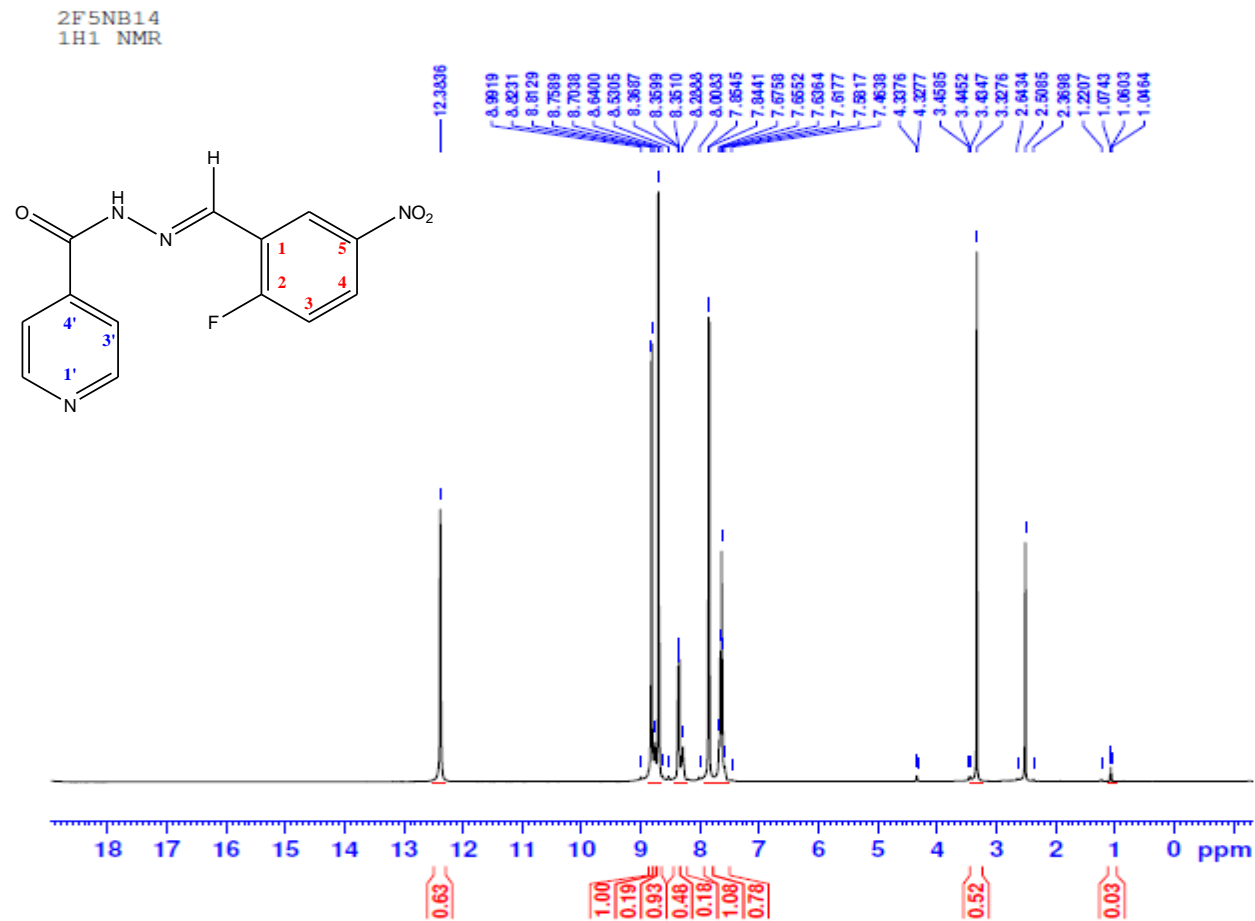
F2 - Acquisition Parameters  
Date\_ 20170115  
Time 13.58  
INSTRUM spect  
PROBHD 5 mm PASAD 8B/  
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 179  
DS 4  
SWH 30864.197 Hz  
FIDRES 0.470950 Hz  
AQ 1.0616832 sec  
RG 202.04  
EW 16.200 usec  
DE 6.50 usec  
TE 300.2  
CNS2 145.000000  
D1 2.0000000 sec  
D2 0.00044028 sec  
D12 0.0002000 sec  
TD 1

----- CHANNEL f1 -----  
SFO1 125.7722923 MHz  
NUC1 13C  
P1 10.00 usec  
PL1 2000.00 usec  
PLNG 0 W  
PLM1 93.32499695 W  
SFO1S1 Crp60comp.4  
SFO1S2 0.500  
SFOFFS1 0 Hz  
SFOFFS2 13.69400024 W

----- CHANNEL f2 -----  
SFO2 500.1315995 MHz  
NUC2 1H  
CFOFFS12 waitz16  
P2 11.50 usec  
PL2 23.00 usec  
PCPD2 80.00 usec  
PLM2 17.37800026 W  
PLNG2 0.36307999 W

F2 - Processing parameters  
SI 32768  
SF 125.7578211 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 2.00

Figure S5: Representative DEPT-<sup>13</sup>CNMR of (E)-N'-(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide (enlarged View)



The University of Jordan  
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Department of Chemistry

Instrument Model:  
Bruker 500 MHz-Avance III

Operator: Rola Hassouneh  
nmr500@ju.edu.jo

Current Data Parameters  
NAME 17jan01jalal  
EXPNO 91  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170105  
Time 9.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 0  
SWH 10135.135 Hz  
FIDRES 0.154650 Hz  
AQ 3.2331092 sec  
RG 71.89  
DW 49.333 usec  
DE 6.50 usec  
TE 300.5 K  
D1 2.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 500.1344108 MHz  
NUC1 1H  
P1 10.60 usec  
PLW1 17.39999962 W

F2 - Processing parameters  
SI 131072  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00

Figure S6: Representative <sup>1</sup>HNMR of (E)-N'-(2-fluoro-5-nitrobenzylidene)isonicotinohydrazide

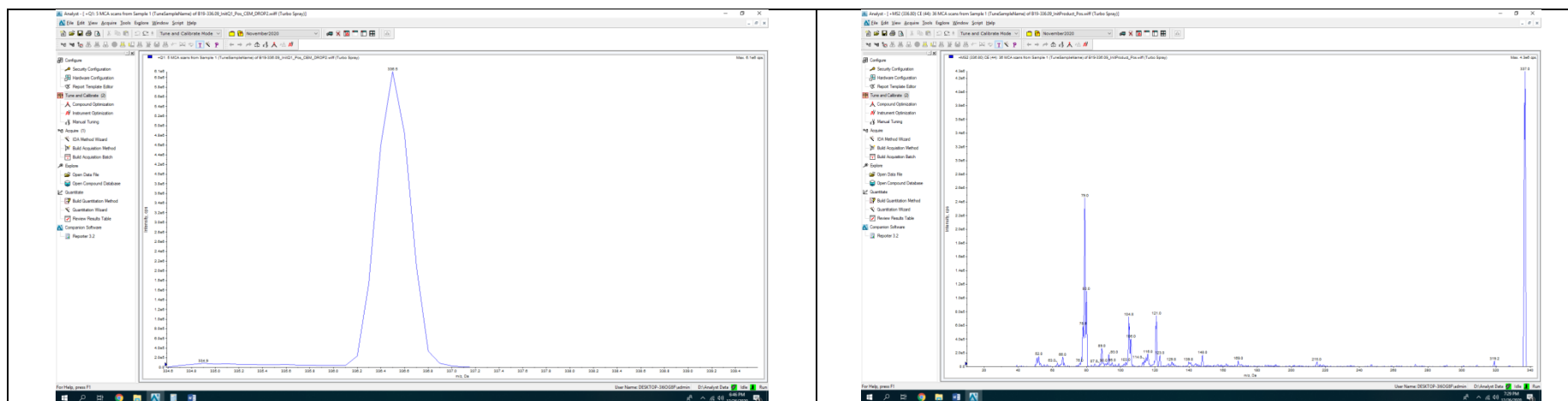


Figure S7: ESI-LC-MS-MS spectrum and fragmentation pattern of (E)-N'-((5-(2-nitrophenyl)furan-2-yl)methylene)isonicotinohydrazide in KBr (19)

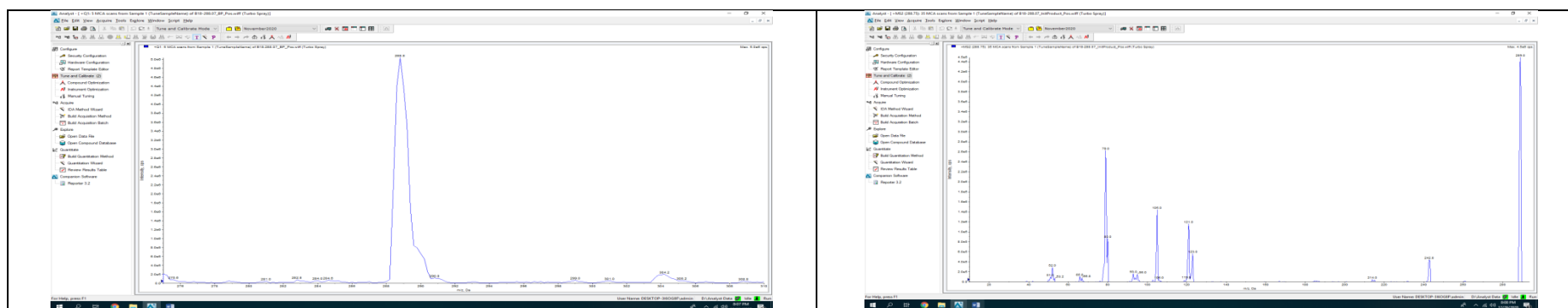


Figure S8: ESI-LC-MS-MS spectrum and fragmentation pattern of (E)-N'--(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide in KBr

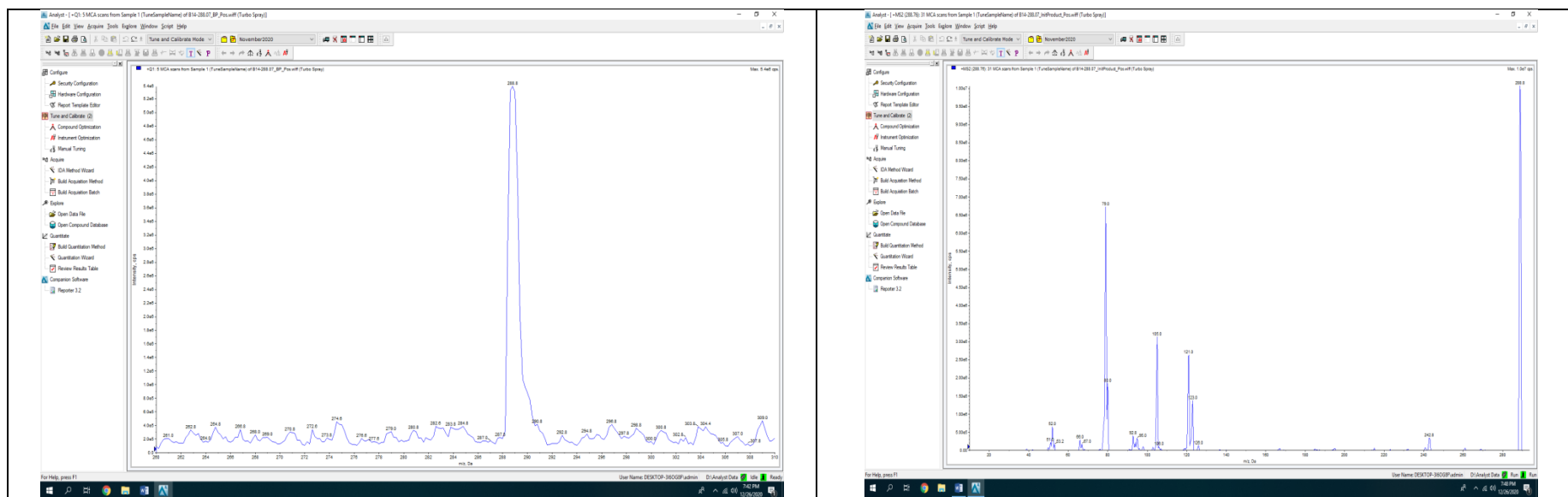
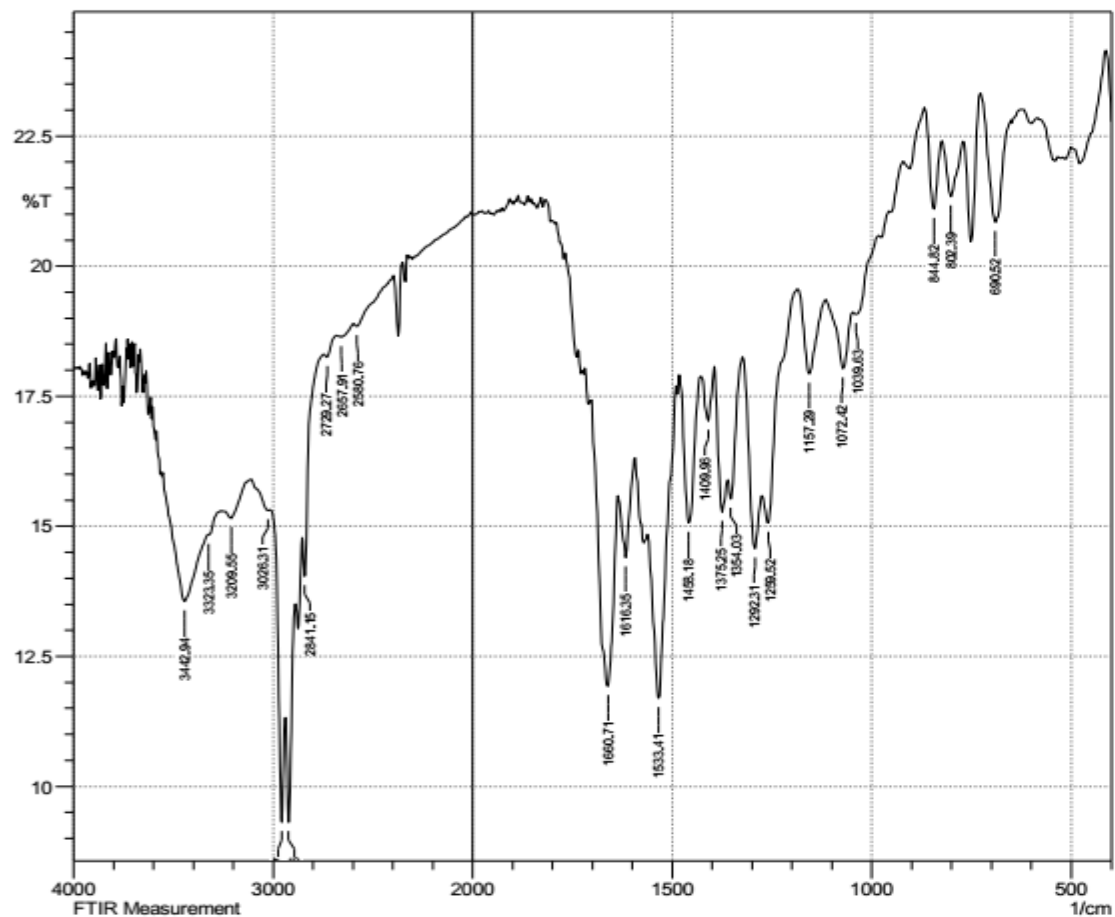


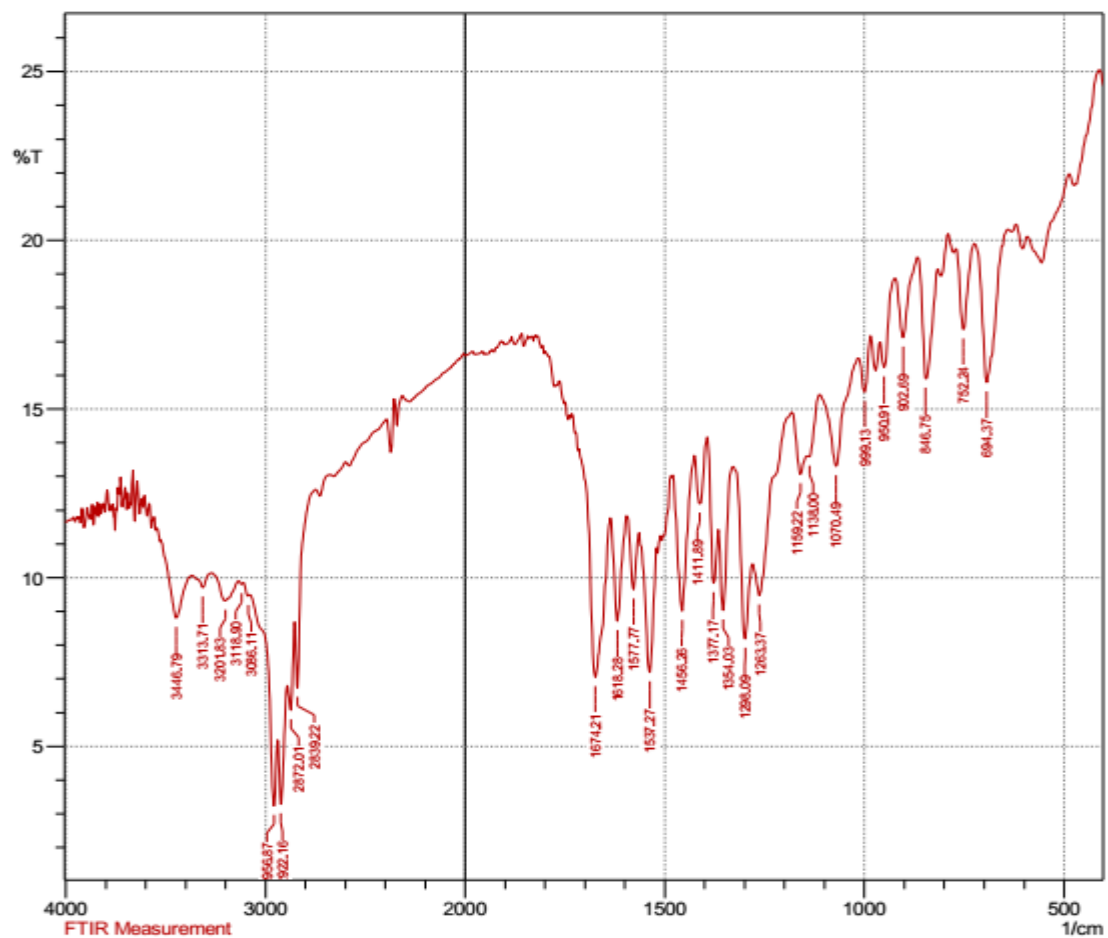
Figure S9: ESI-LC-MS-MS spectrum and fragmentation pattern (E)-N<sup>1</sup>-(2-fluoro-5-nitrobenzylidene)isonicotinohydrazide





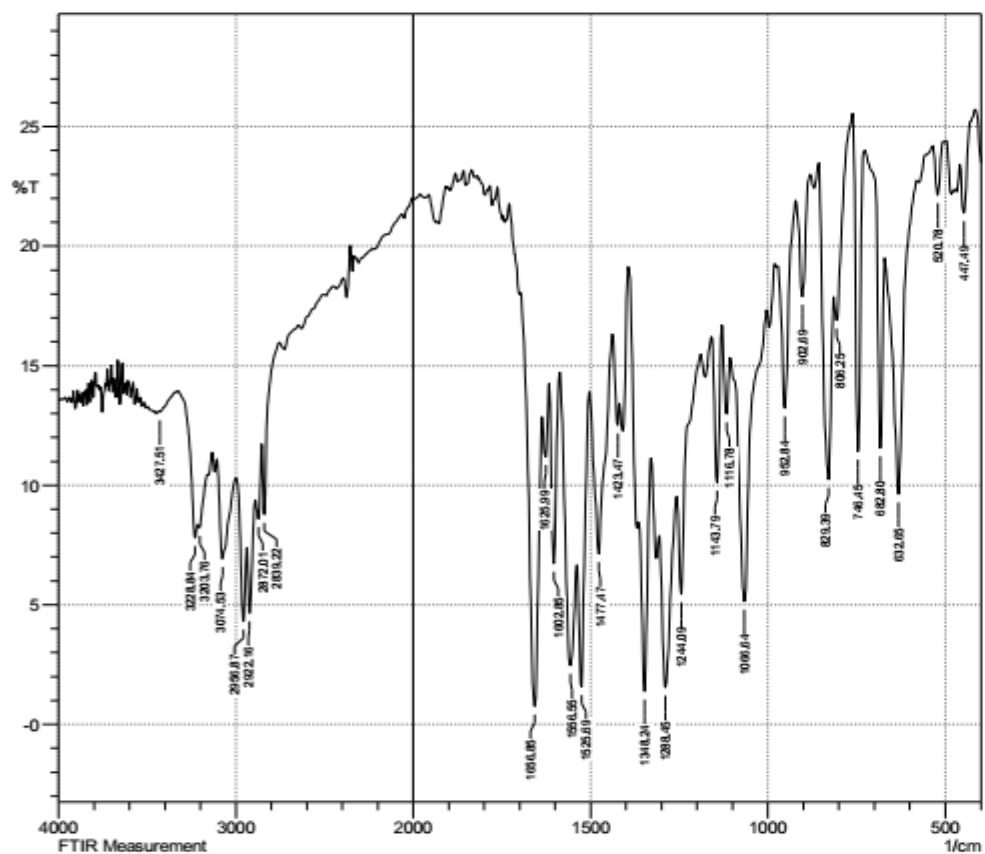
No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	690.52	20.846	0.312	729.09	686.66	27.89	0.07
2	802.39	21.339	1.061	823.6	771.53	34.41	0.572
3	844.82	21.099	1.612	867.97	823.6	29.22	0.671
4	1039.63	19.075	0.216	1047.35	983.7	44.801	0.155
5	1072.42	18.036	1.158	1114.86	1049.28	47.729	0.768
6	1157.29	17.935	1.537	1184.29	1116.78	49.14	1.133
7	1259.52	15.063	1.215	1274.95	1186.22	67.195	0.571
8	1292.31	14.568	1.897	1323.17	1276.88	37.044	1.193
9	1354.03	15.524	0.842	1361.74	1323.17	29.928	0.275
10	1375.25	15.278	1.511	1394.53	1361.74	25.989	0.71
11	1409.96	17.023	0.956	1427.32	1394.53	24.836	0.395
12	1458.18	15.069	2.824	1481.33	1429.25	40.856	1.935
13	1533.41	11.7	4.252	1560.41	1490.97	59.139	4.337
14	1616.35	14.403	1.514	1635.64	1595.13	33.128	0.832
15	1660.71	11.923	4.252	1701.22	1637.56	54.893	4.875
16	2580.76	18.842	0.111	2594.26	2397.52	140.469	0.142
17	2657.91	18.639	0.085	2681.05	2596.19	61.752	0.109
18	2729.27	18.248	0.146	2744.71	2682.98	45.315	0.08
19	2841.15	14.038	1.128	2852.72	2746.63	81.766	0.473
20	2922.16	9.31	2.71	2937.59	2889.37	46.051	2.356
21	2956.87	9.315	2.932	3014.74	2939.52	67.864	2.255
22	3026.31	15.301	0.078	3109.25	3016.67	74.783	0.09
23	3209.55	15.153	0.302	3246.2	3111.18	109.37	0.45
24	3323.35	14.836	0.017	3325.28	3261.63	52.255	0.026
25	3442.94	13.559	1.494	3520.09	3327.21	163.278	4.437

Figure S10: IR of (E)-N'-((5-(2-nitrophenyl)furan-2-yl)methylene)isonicotinohydrazide in KBr (19)



No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	399.26	24.504	0	412.77	399.26	8.171	-0.009
2	694.37	15.79	4.253	723.31	642.3	59.977	3.54
3	752.24	17.362	2.44	769.6	725.23	32.327	1.149
4	846.75	15.903	3.443	866.04	817.82	36.511	2.068
5	902.69	17.116	1.97	921.97	867.97	39.794	1.07
6	950.91	16.237	1.236	960.55	923.9	27.756	0.458
7	999.13	15.51	1.349	1014.56	985.62	22.916	0.544
8	1070.49	13.31	2.572	1111	1016.49	78.016	2.697
9	1138	13.586	0.263	1141.86	1112.93	24.31	0.123
10	1159.22	13.063	1.086	1180.44	1143.79	31.676	0.614
11	1263.37	9.479	1.628	1278.81	1182.36	88.006	1.502
12	1298.09	8.191	3.294	1327.03	1280.73	45.638	2.575
13	1354.03	9.03	2.984	1365.6	1328.95	34.982	1.758
14	1377.17	9.839	2.551	1392.61	1367.53	23.896	1.279
15	1411.89	12.193	1.662	1425.4	1394.53	27.383	0.938
16	1456.26	9.023	4.239	1479.4	1427.32	49.627	3.994
17	1537.27	7.192	3.778	1564.27	1521.84	44.208	3.581
18	1577.77	9.651	1.829	1593.2	1566.2	26.387	1.019
19	1618.28	8.723	2.977	1633.71	1595.13	38.217	2.309
20	1674.21	7.055	5.713	1714.72	1635.64	79.162	8.364
21	2839.22	6.742	2.461	2852.72	2750.49	99.495	1.9
22	2872.01	6.072	1.646	2889.37	2854.65	40.492	1.861
23	2922.16	3.29	2.432	2937.59	2891.3	61.731	5.072
24	2956.87	3.232	2.475	3078.39	2939.52	160.602	4.842
25	3086.11	9.465	0.099	3109.25	3080.32	29.464	0.099
26	3118.9	9.807	0.063	3134.33	3111.18	23.306	0.035
27	3201.83	9.314	0.71	3267.41	3136.25	133.117	2.076
28	3313.71	9.708	0.401	3365.78	3269.34	96.644	0.65
29	3446.79	8.805	1.788	3523.95	3367.71	158.023	5.53

Figure S11: IR spectrum of (E)-N'-(4-fluoro-3-nitrobenzylidene)isonicotinohydrazide in KBr



No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	447.49	21.387	2.755	459.06	430.13	18.532	0.759
2	520.78	22.139	2.151	536.21	505.35	19.523	0.557
3	632.65	9.628	11.133	669.3	580.57	69.228	9.136
4	682.8	11.563	8.902	725.23	671.23	38.601	2.957
5	746.45	11.412	13.459	761.88	727.16	25.52	4.48
6	806.25	16.894	2.121	813.96	761.88	34.906	0.609
7	829.39	10.232	9.465	856.39	815.89	34.159	6.119
8	902.69	17.886	4.527	921.97	879.54	29.189	1.663
9	952.84	13.223	6.867	970.19	923.9	35.272	3.352
10	1066.64	5.146	10.921	1105.21	1004.91	93.104	14.054
11	1116.78	12.977	2.927	1130.29	1107.14	19.494	1.074
12	1143.79	10.126	6.351	1159.22	1130.29	25.56	2.89
13	1244.09	5.455	5.256	1257.59	1190.08	64.52	3.385
14	1288.45	1.542	6.907	1305.81	1259.52	63.058	13.815
15	1348.24	1.377	8.271	1363.67	1330.88	43.328	10.125
16	1423.47	12.509	1.686	1438.9	1417.68	18.104	0.489
17	1477.47	7.124	7.731	1502.55	1438.9	61.238	8.976
18	1525.69	1.562	7.515	1537.27	1504.48	41.344	8.107
19	1556.55	2.459	7.162	1585.49	1539.2	58.449	11.516
20	1602.85	6.736	7.743	1616.35	1587.42	28.626	4.356
21	1625.99	11.204	2.35	1635.64	1616.35	17.637	0.885
22	1656.85	0.749	13.789	1695.43	1637.56	70.626	23.103
23	2839.22	8.782	3.522	2852.72	2754.35	85.755	2.179
24	2872.01	8.599	1.935	2889.37	2854.65	35.604	1.671
25	2922.16	4.646	3.396	2937.59	2891.3	54.977	5.077
26	2956.87	4.318	3.899	2997.38	2939.52	67.607	6.153
27	3074.53	6.934	3.904	3105.39	2999.31	112.87	9.767
28	3203.76	8.223	0.521	3213.41	3161.33	53.921	0.451
29	3228.84	7.798	1.247	3325.28	3215.34	104.142	1.021
30	3427.51	13.071	0.105	3435.22	3344.57	79.005	0.169

Figure S12: IR spectrum of (E)-N'-(2-fluoro-5-nitrobenzylidene)isonicotinohydrazide