

2,3-Dihydroquinazolin-4(1*H*)-ones and Quinazolin-4(3*H*)-ones as Broad-Spectrum Cytotoxic Agents and Impact on Tubulin Polymerisation

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Supplementary Data

Contents

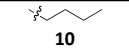
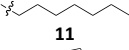
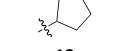
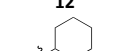
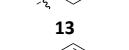
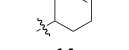
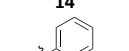
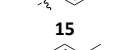
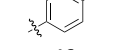
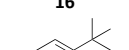
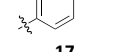
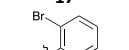
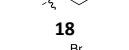
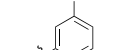
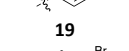
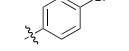
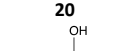
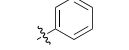
Initial toxicity screening data at 25µM compound concentration




















Table S1 – Library 1, compounds **10-46**

Table S2 – Library 2, compounds **47-57** and **60-66**

NMR and compound analysis data

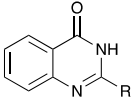



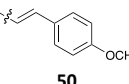







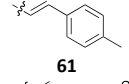






Table S1. Growth inhibition of a panel of cancer cell lines (glioblastoma (U87 and SJ-G2), ovarian (A2780), lung (H460), skin (A431), prostate (Du145), neuroblastoma (BE2-C), pancreas (MIA) and normal breast (MCF10A)) by *Library 1* quinazolin-4(1*H*)-ones (**10-17**). Data is presented as percentage growth inhibition relative to untreated control at 25 μ M compound concentration (MTT assay, 72 h), higher number indicate higher potency.

	HT29 ^a	U87 ^b	MC-7 ^c	A2780 ^d	H460 ^e	A431 ^f	Du145 ^g	BE2-C ^h	SJ-G2 ^b	MIA ⁱ	MCF10A ⁱ
 10	32±3	9±4	25±6	59±4	<10	30± 14	25±4	38±29	<10	16±10	13±6
 11	93±3	39±3	>100	96±2	61±6	91± 5	53±5	85±4	77±3	75±4	80±3
 12	22±5	11±6	35±3	39±6	<10	15±15	22±2	20±18	<10	19±10	12±7
 13	23±3	10±5	18±6	41±3	<10	22±11	18±2	32 ± 26	<10	12±11	8±7
 14	>100	67±5	72±8	99±1	91±3	>100	67±5	97±3	87±11	82±3	89±2
 15	>100	91±4	94±3	97±1	95±2	>100	>100	94±6	>100	87±2	97±0
 16	>100	>100	90±7	>100	>100	>100	>100	87±13	>100	95±3	100±1
 17	79 ± 6	40±6	>100	63±3	44±5	32±9	47±5	47±10	46± 10	60±4	53±5
 18	>100	80±3	82±4	96±1	95±1	>100	100±3	>100	>100	89±2	94±1
 19	>100	98±3	104 ± 4	99±1	101±1	>100	>100	>100	>100	90 ± 2	99±1
 20	>100	88±5	89 ± 7	99±1	97±2	>100	>100	>100	>100	90 ± 3	95±2
 21	>100	65±1	66±8	95±1	94±1	>100	72±3	97±3	>100	86±2	92±1
 22	>100	72±3	55±6	95±1	88±3	108 ± 1	90±5	100±3	>100	84±3	91±1
 23	37 ± 2	<10	49±11	48±1	43±8	22 ± 2	20±5	19±15	49±8	20±10	20±8
 24	24 ± 14	10±1	43±5	10±8	12±0	<10	31±3	12	12±4	13±5	22±6
 25	18 ± 0	13±7	41±8	<10	<10	<10	36±2	12	10±5	14±3	8±6
 26	28 ± 12	16±1	16±7	33±8	35±6	36 ± 2	27±2	<10	33±22	21±10	16±8
 27	78 ± 4	20±5	>100	69±3	59±3	67 ± 5	33±4	58±10	61±3	56±3	54±6

 28	70 ± 4	22±4	>100	65±3	61±3	57 ± 3	50±2	53±5	56±6	52±4	58±7
 29	>100	99±3	85±8	100±1	100±1	>100	>100	>100	>100	94±4	>100
 30	>100z	>100	83±7	100±0	100±2	>100	>100	>100	>100	95±4	>100
 31	31 ± 10	19±2	60±27	54±4	17±10	34±3	26±8	20±5	18±12	14±4	12±4
 32	16 ± 5	<10	40±19	18±0	11±8	<10	10±1	<10	14±4	11±8	10±3
 33	49±3	29±3	56±7	36±23	19±11	21±12	40±4	27	10±6	34±7	51±3
 34	<10	<10	21±8	<10	<10	<10	<10	<10	<10	11±4	<10
 35	90±10	56±5	91±16	98±1	88±2	>100	57±5	91±4	60±10	74±4	84±4
 36	<10	<10	13±3	37±4	<10	<10	<10	20±22	12±14	<10	<10
 37	>100	>100	>100	>100	>100	>100	>100	92±12	>100	>100	98±1
 38	>100	94±5	135±9	>100	100±1	>100	>100	98±5	>100	>100	99±2
 39	>100	93±3	>100	>100	>100	>100	>100	>100	>100	94±3	>100
 40	>100	95±5	74±3	>100	91±2	>100	>100	95±2	>100	80±3	97±2
 41	>100	70±3	78±6	99±1	96±2	>100	77±5	97±2	>100	79±5	90±1
 42	35±18	<10	49±11	60±1	21±4	25±8	22±12	64±0	29±46	22±8	41±12
 43	29±4	<10	38±2	29±10	<10	14±4	27±1	19	16±1	27±1	23±2
 44	>100	95±11	>100	94±4	97±7	>100	>100	87±11	>100	81±9	99±4
 45	37±12	24±18	55±7	69±32	35±6	40±31	66±15	53±6	81±40	32±7	13±9
 46	90±13	99±4	83±18	>100	93±2	>100	100±3	100±2	100±5	93±2	100±1

^a Colon, ^b Glioblastoma, ^c Breast, ^d Ovarian, ^e Lung, ^f Skin, ^g Prostate, ^h Neuroblastoma, ⁱ Pancreas, ^j Breast (normal)

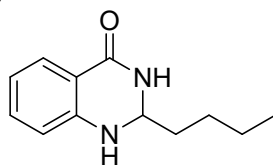
Table S2. Growth inhibition of a panel of cancer cell lines (glioblastoma (U87 and SJ-G2), ovarian (A2780), lung (H460), skin (A431), prostate (Du145), neuroblastoma (BE2-C), pancreas (MIA) and normal breast (MCF10A)) by *Library 4* 2,3-dihydroquinazolin-4(1*H*)-ones (**47-52**). Data is presented as percentage growth inhibition relative to untreated control at 25 μ M compound concentration (MTT assay, 72 h), higher number indicate higher potency.

											
	HT29 ^a	U87 ^b	MC-7 ^c	A2780 ^d	H460 ^e	A431 ^f	Du145 ^g	BE2-C ^h	SJ-G2 ^b	MIA ⁱ	MCF10A ^j
 40	92±2	47±2	63±6	57±6	77±2	75±1	28±7	66±6	71±19	76±3	76±2
 41	84±2	91±3	116±7	94±2	87±3	79±5	>100	89±2	>100	90±2	95±1
 49	11±2	<10	<10	<10	15±3	<10	<10	<10	<10	10±4	<10
 50	78±2	24±9	>100	66±4	60±4	45±4	41±7	66±3	89±10	67±4	60±5
 51	>100	>100	>100	>100	>100	>100	>100	>100	>100	96±3	>100
 52	94±2	83±4	>100	93±1	70±5	78±5	77±3	78±1	76±13	68±5	86±6
 53	<10	25±2	16±11	43±6	33±5	22±7	26±9	<10	16±28	18±3	11±7
 54	28±2	12±2	21±4	15±10	12±6	<10	23±8	<10	<10	23±5	15±2
 55	15±11	14±0	10±1	13±10	20±1	12±6	25±2	23	11±3	24±3	17±3
 56	91±3	91±6	99±4	83±5	68±5	88±3	98±5	77±2	66±7	71±2	91±3
 57	-	-	-	-	-	-	-	-	-	-	-
 60	40±4	11±3	77±2	16±1	34±2	8±2	32±4	47±1	43±1	39±2	48±7
 61	>100	51±1 2	>100	97±2	69±5	93±3	61±4	82±4	57±7	85 ± 4	86±5
 62	>100	73±6	>100	>100	>100	>100	>100	>100	>100	>100	97±1
 63	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100
 64	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100
 65	>100	75±11	>100	>100	>100	>100	78±2	99±1	100±3	93±2	95±2
 66	50±2	21±4	85±4	62±4	35±3	11±2	34±4	61±2	47±5	89±2	57±5

^a Colon, ^b Glioblastoma, ^c Breast, ^d Ovarian, ^e Lung, ^f Skin, ^g Prostate, ^h Neuroblastoma, ⁱ Pancreas, ^j Breast (normal); ‘-’
Not Tested: Compound INSOLUBLE at 2.5 mM.

Spectra and Characterisation

2-Butyl-2,3-dihydroquinazolin-4(1H)-one (**10**)



Chemical Formula: C₁₂H₁₆N₂O

Exact Mass: 204.13

Molecular Weight: 204.27

IR (neat): ν_{\max} = 3340 (NH), 3178 (NH), 2926 (CH₂), 1643 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 7.87 (s, 1H), 7.58 (dd, J = 7.7, 1.2 Hz, 1H), 7.24 – 7.20 (m, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.65 (dd, J = 11.0, 3.9 Hz, 1H), 6.55 (s, 1H), 4.68 (t, J = 5.3 Hz, 1H), 1.64 – 1.61 (m, 2H), 1.40 – 1.28 (m, 4H), 0.88 (t, J = 7.2 Hz, 3H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.9, 148.5, 133.0, 127.3, 116.9, 115.0, 114.4, 64.4, 34.7, 25.4, 22.1, 13.9.

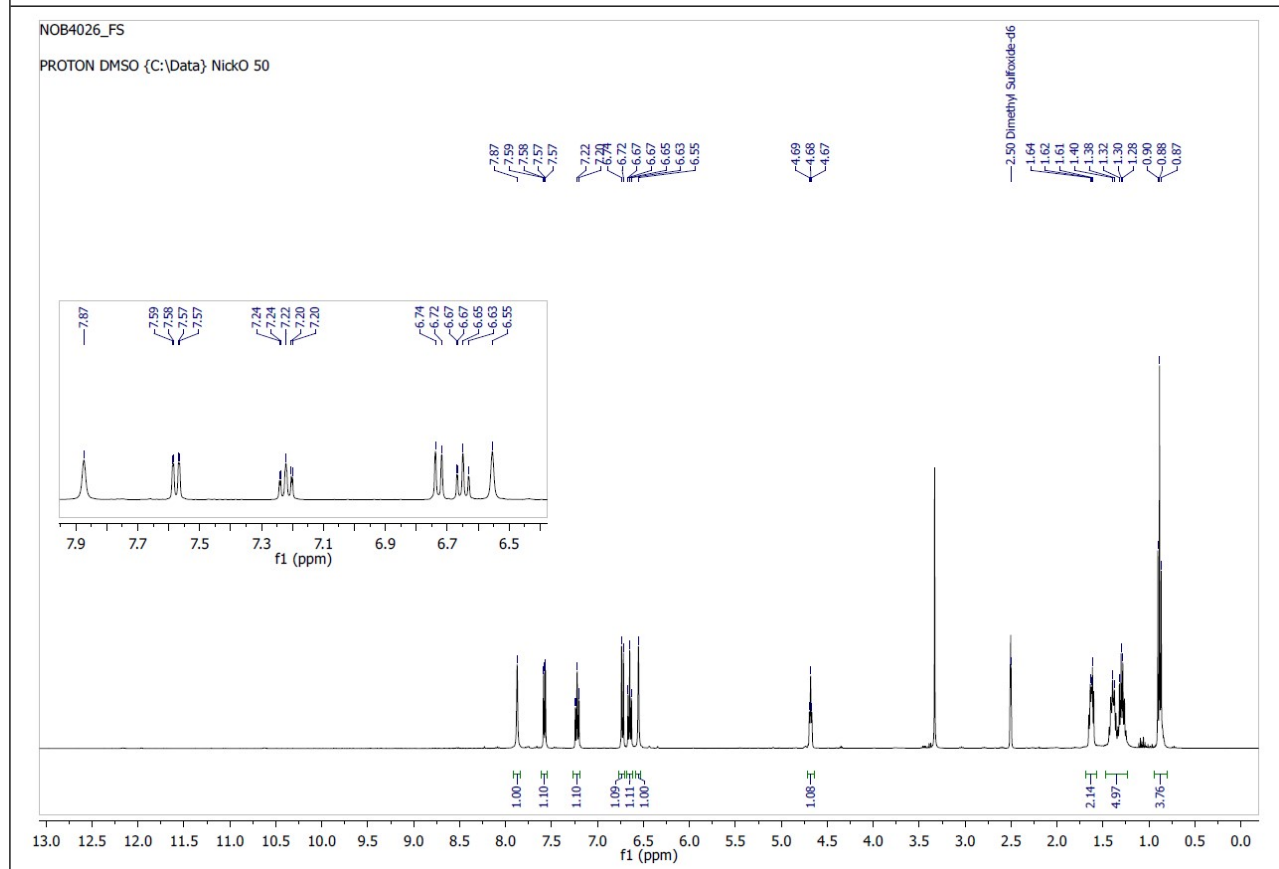
LRMS (ESI+): 205.2 (M+H, C₁₂H₁₇N₂O, 100%).

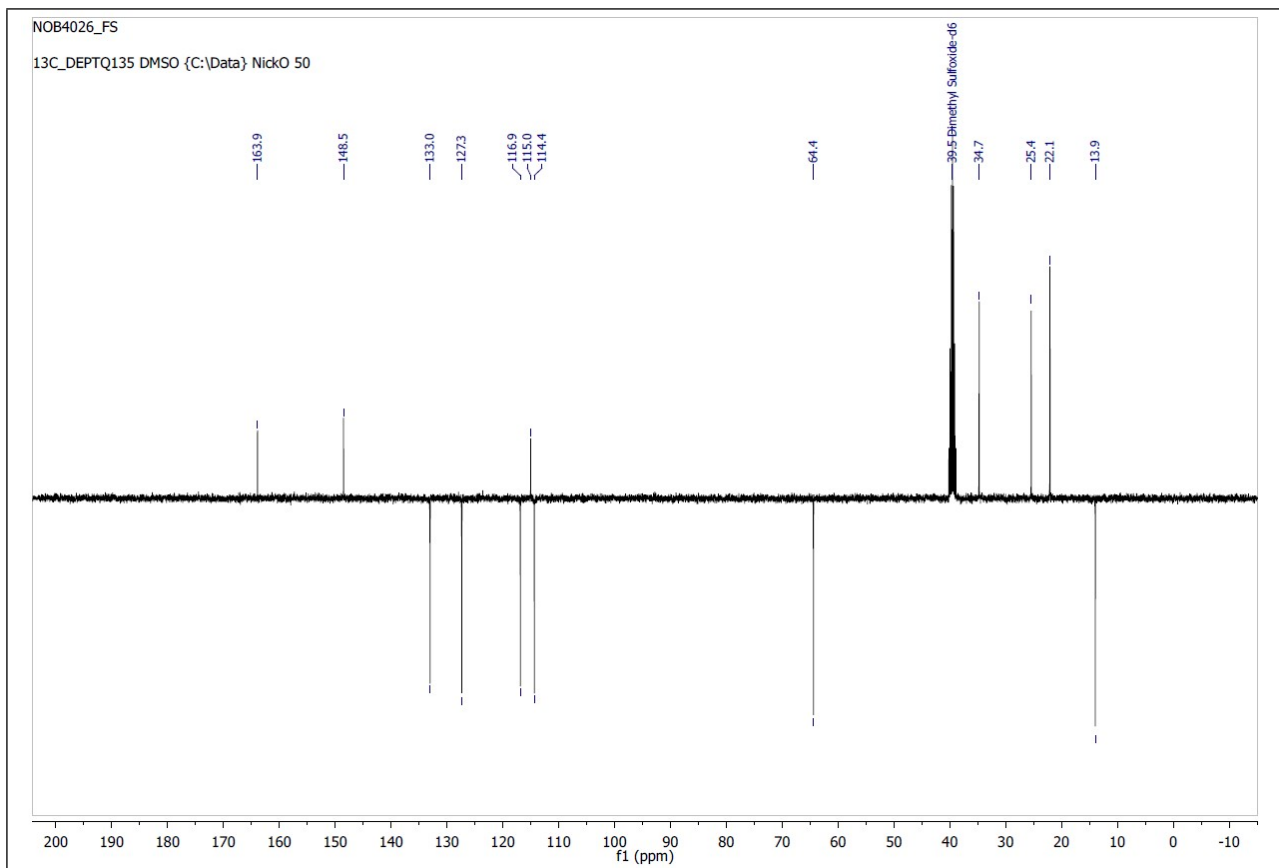
Mass 136 mg

m.p. 137 – 143 °C

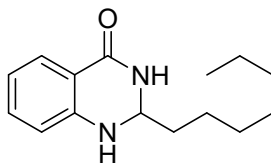
yield: 34 %

white solid





2-Heptyl-2,3-dihydroquinazolin-4(1H)-one (**11**)



Chemical Formula: C₁₅H₂₂N₂O

Exact Mass: 246.17

Molecular Weight: 246.35

IR (neat): ν_{\max} = 3333 (NH), 3185 (NH), 22925 (CH₂), 1641 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 7.87 (s, 1H), 7.58 (dd, J = 7.7, 1.5 Hz, 1H), 7.22 (ddd, J = 8.3, 7.2, 1.6 Hz, 1H), 6.73 (d, 1H), 6.65 (d, 1H), 6.55 (s, 1H), 4.68 (t, J = 5.2 Hz, 1H), 1.68 – 1.55 (m, 2H), 1.44 - 1.39 (m, 2H), 1.31-1.25 (m, 8H), 0.87 (t, J = 6.8 Hz, 3H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.91, 148.50, 133.00, 127.33, 116.84, 115.01, 114.34, 64.42, 35.02, 31.18, 28.90, 28.65, 23.22, 22.08, 13.95.

LRMS (ESI⁺): 247.2 (M+H, C₁₅H₂₃N₂O, 100%); LRMS (ESI⁻): 291.2 (M+FA-H, C₁₆H₂₅N₂O₃, 100%).

Mass 113.3 mg

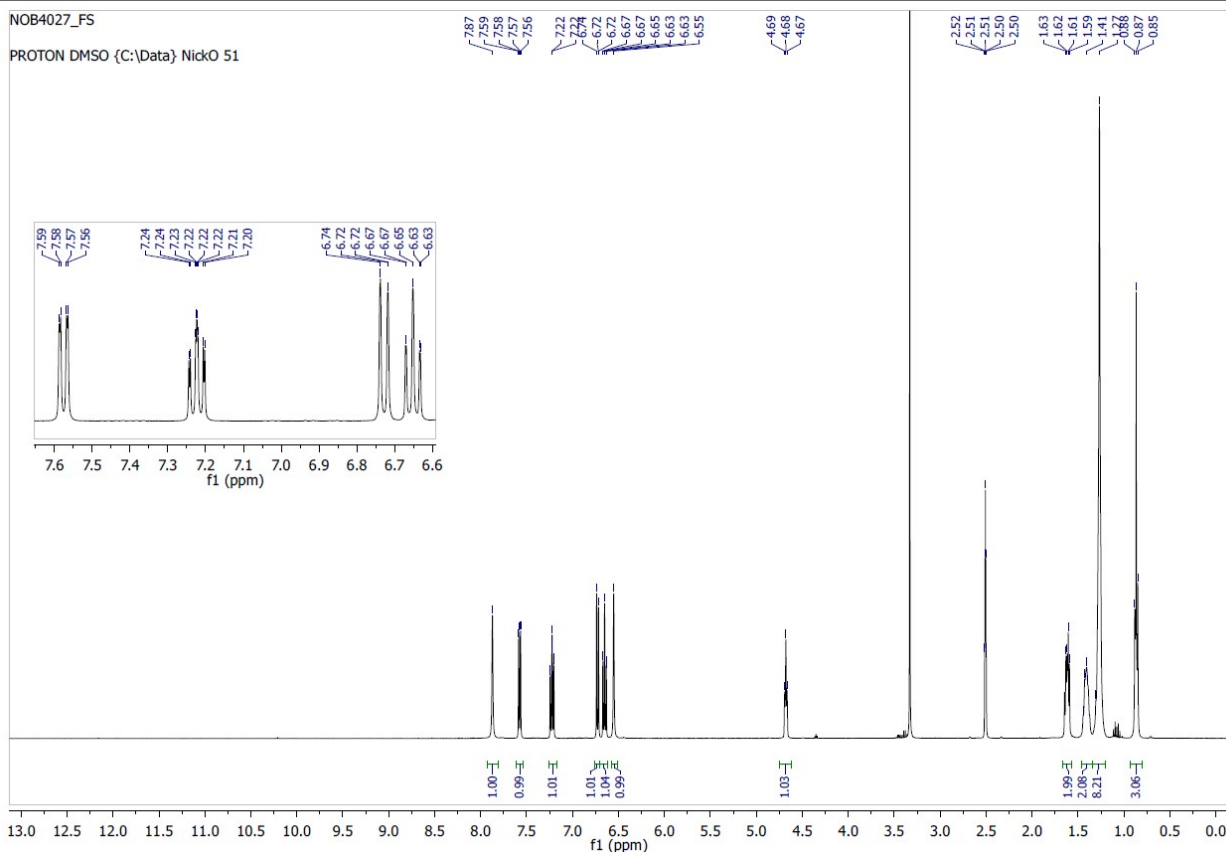
m.p. 160 – 163 °C

yield 35 %

colour white solid

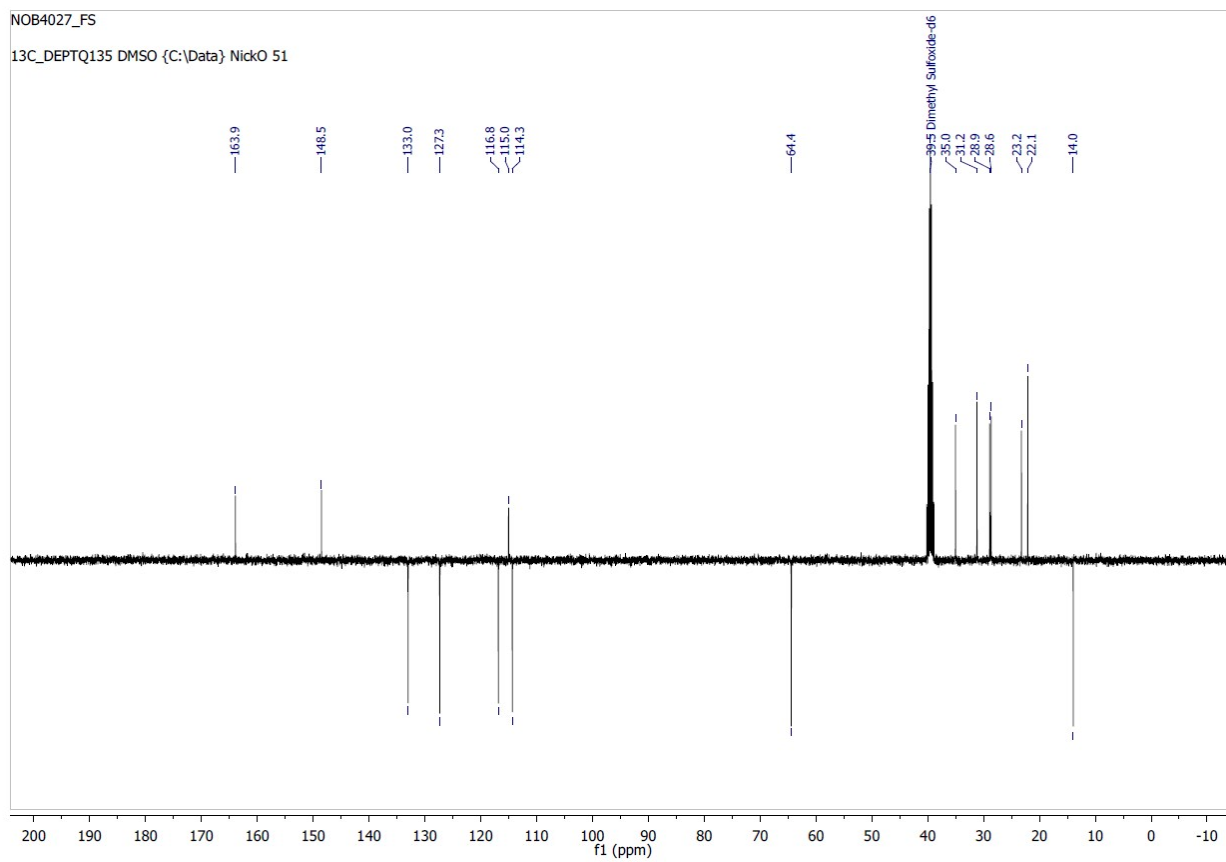
NOB4027_FS

PROTON DMSO (C:\Data) NickO 51

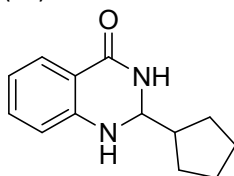


NOB4027_FS

13C DEPTQ135 DMSO (C:\Data) NickO 51



2-cyclopentyl-2,3-dihydroquinazolin-4(1H)-one (**12**)



Chemical Formula: C₁₃H₁₆N₂O

Exact Mass: 216.13

Molecular Weight: 216.28

IR (neat): ν_{\max} = 3329 (NH), 3185 (NH), 2964 (CH₂), 1635 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 7.91 (s, 1H), 7.56 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.23 – 7.19 (m, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 6.64 – 6.60 (m, 1H), 6.53 (s, 1H), 4.48 (d, *J* = 6.6 Hz, 1H), 2.25 – 2.10 (m, 1H), 1.65 – 1.43 (m, 8H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.6, 148.2, 133.0, 127.2, 116.6, 115.1, 114.3, 67.7, 44.9, 27.3, 27.2, 25.1, 25.0.

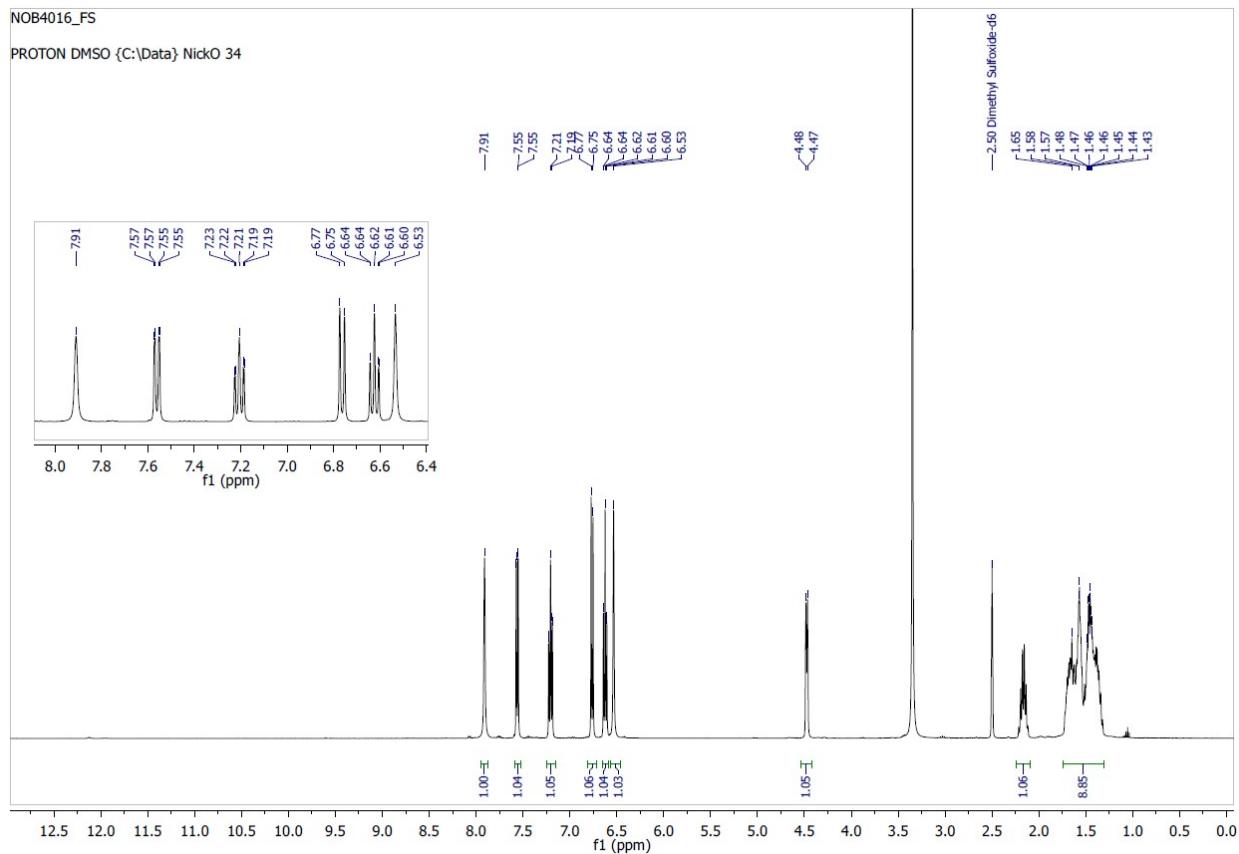
LRMS (ESI+): 217.1 (M+H, C₁₃H₁₇N₂O, 100%)

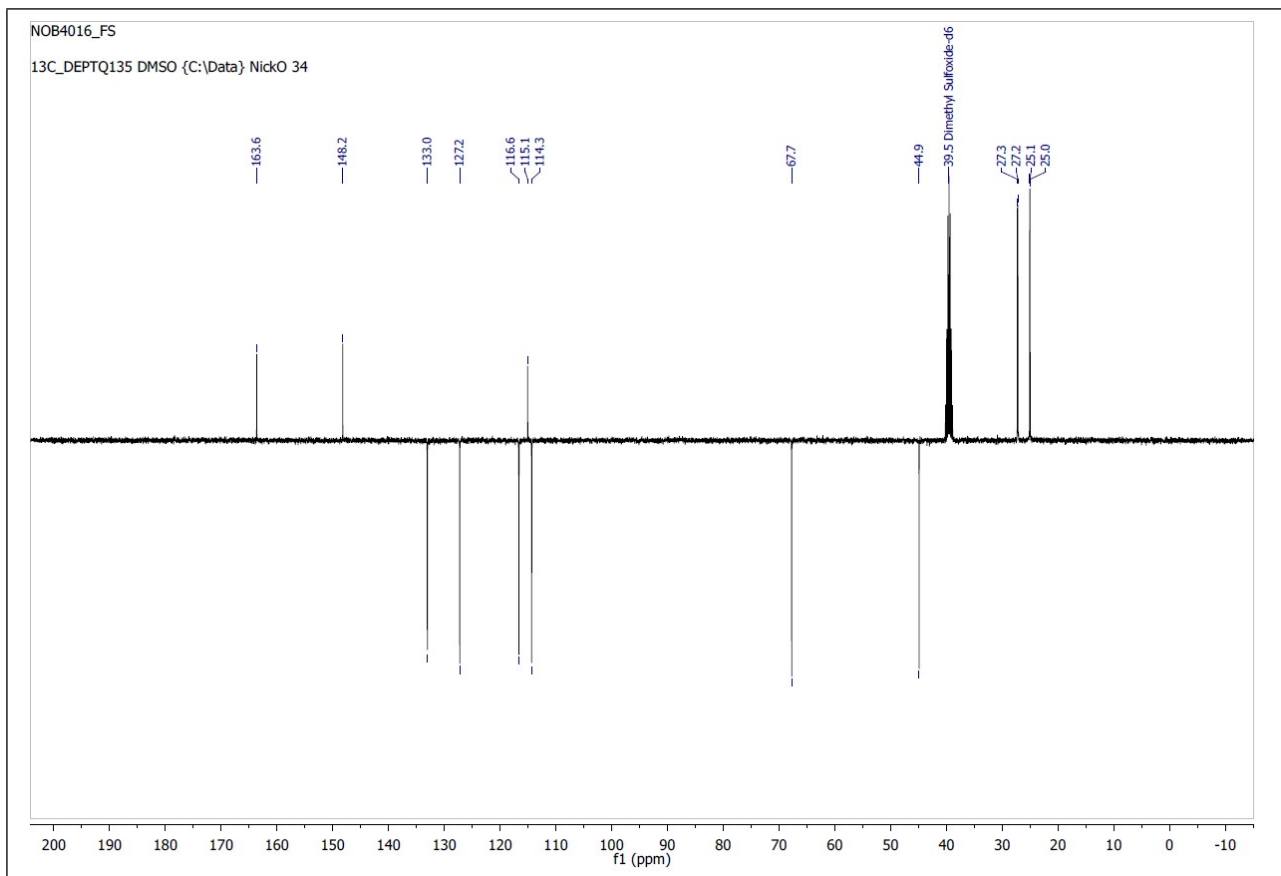
Mass 303.8

m.p. 166 – 167°C

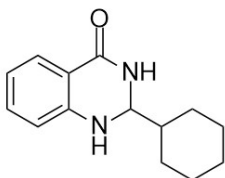
yield: 87 %

colour white solid





2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one (**13**)



2-cyclohexyl-2,3-dihydroquinazolin-4(1H)-one

Chemical Formula: $C_{14}H_{18}N_2O$

Exact Mass: 230.14

Molecular Weight: 230.31

IR (neat): ν_{\max} = 3336 (NH), 3172 (NH), 2921 (CH₂), 1642 (C=O) cm^{-1}

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.86 (s, 1H), 7.55 (dd, J = 7.7, 1.5 Hz, 1H), 7.19 (ddd, J = 8.7, 7.2, 1.6 Hz, 1H), 6.74 (d, J = 7.7 Hz, 1H), 6.62 – 6.58 (m, 1H), 6.54 (s, 1H), 4.45 – 4.43 (m, 1H), 1.71 – 1.55 (m, 6H), 1.16 – 1.07 (m, 4H).

¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.7, 148.3, 133.0, 127.2, 116.4, 114.8, 114.1, 68.6, 42.8, 27.0, 26.7, 25.9, 25.6, 25.5.

LRMS (ESI+) 231.2 (M+H, $C_{15}H_{19}N_2O$, 100%).

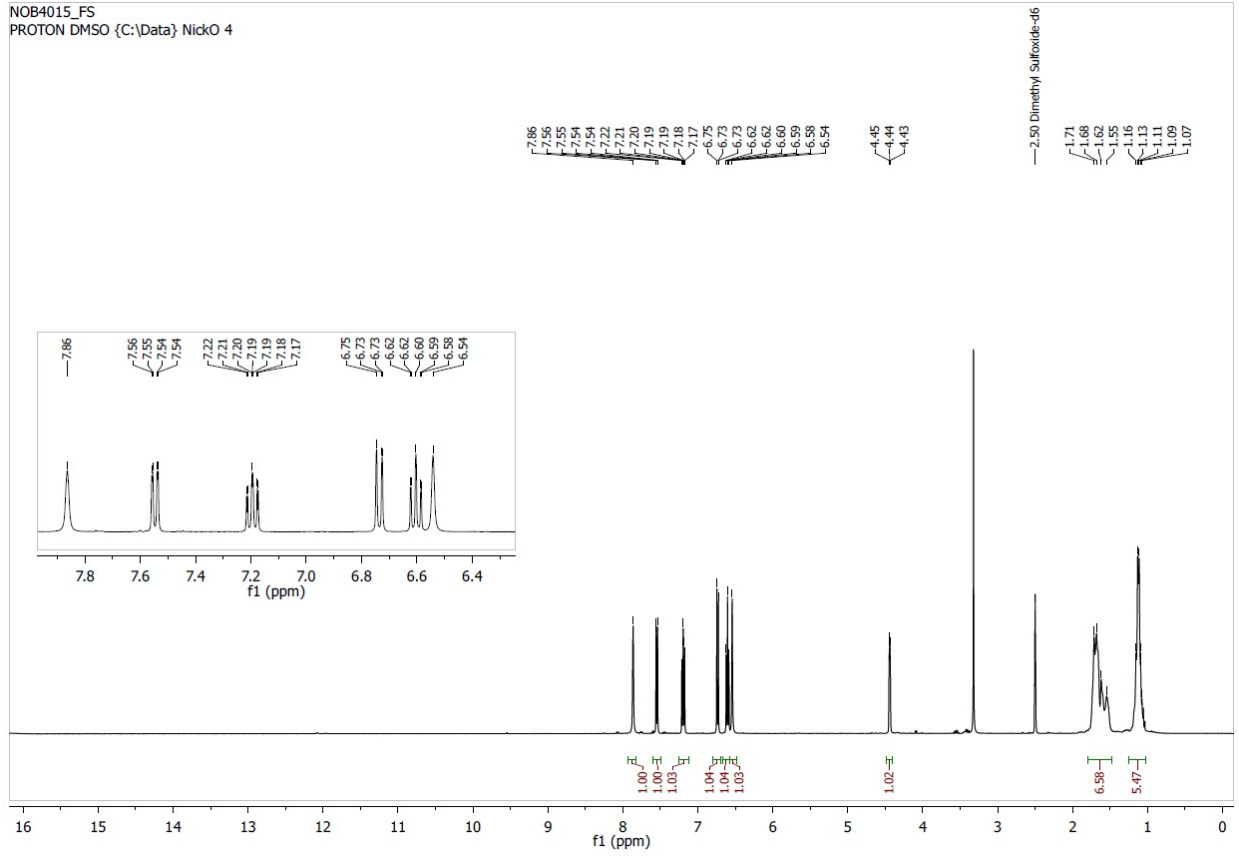
Mass: 223.4 mg

m.p. 176 – 184°C

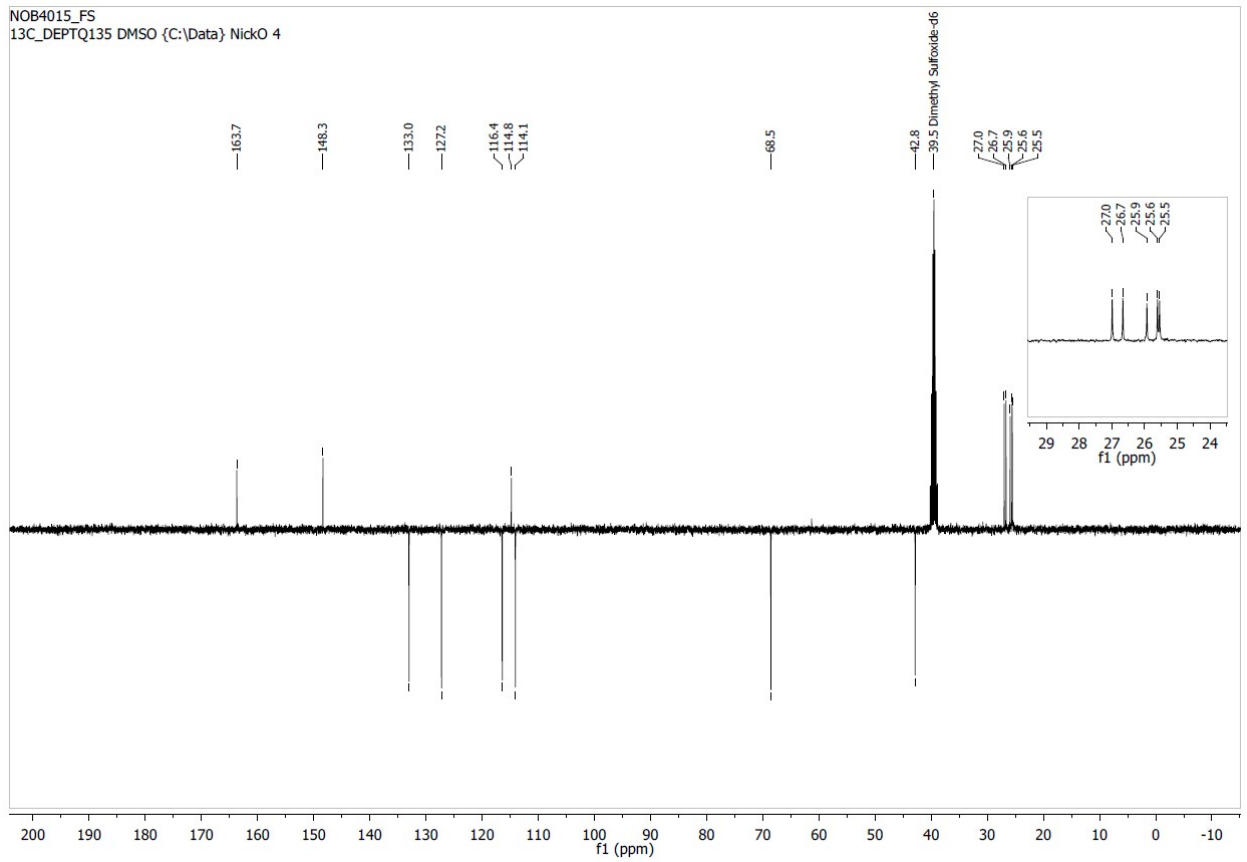
yield: 89 %

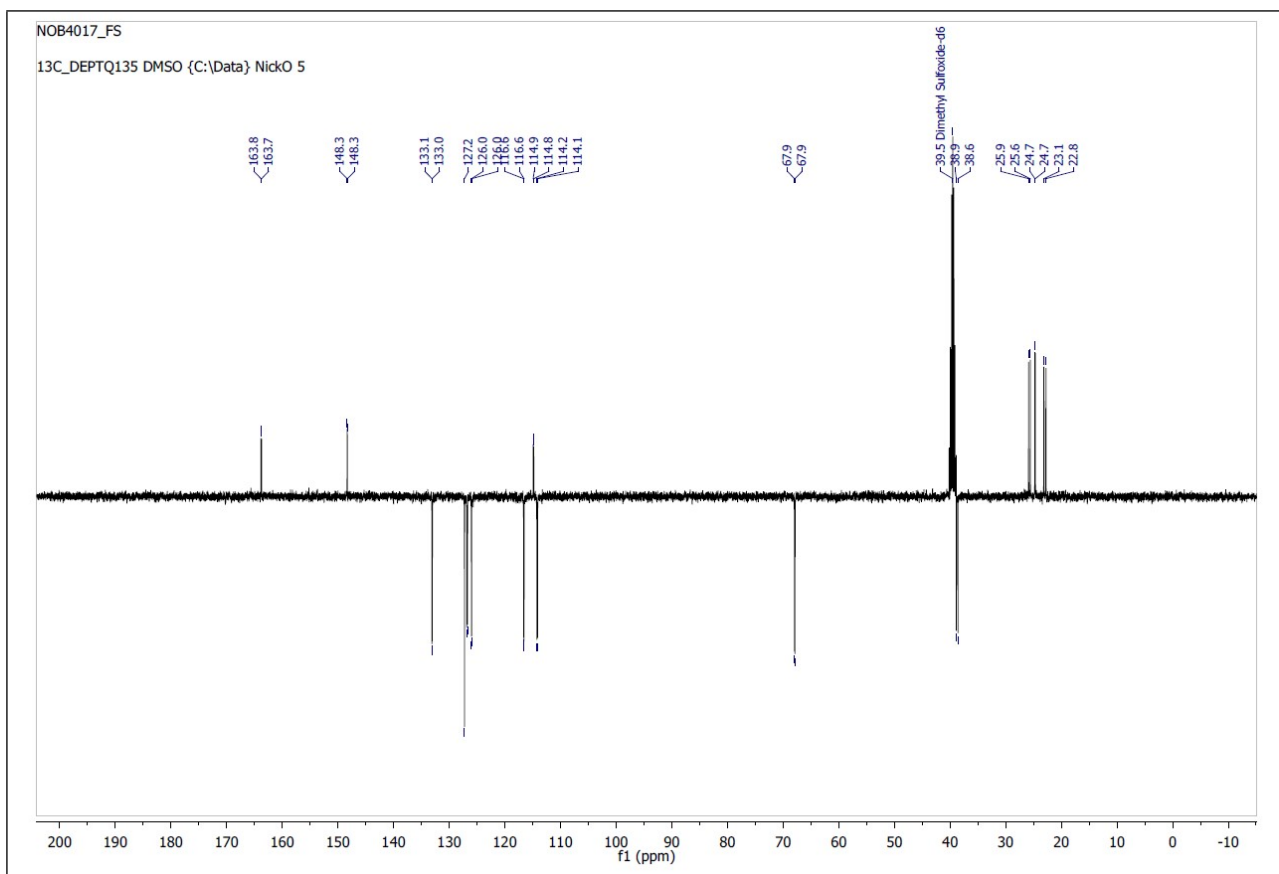
white solid

NOB4015_FS
PROTON DMSO {C:\Data} NickO 4

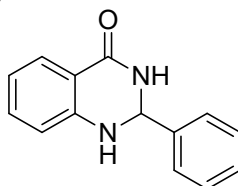


NOB4015_FS
13C_DEPTQ135 DMSO {C:\Data} NickO 4





2-phenyl-2,3-dihydroquinazolin-4(1H)-one (**15**)



Chemical Formula: C₁₄H₁₂N₂O

Exact Mass: 224.09

Molecular Weight: 224.26

IR (neat): ν_{\max} = 3308 (NH), 3169 (NH), 3061 (CH), 1649 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.27 (s, 1H), 7.61 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.49 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.43 – 7.31 (m, 3H), 7.24 (ddd, *J* = 8.2, 7.2, 1.6 Hz, 1H), 7.10 (s, 1H), 6.75 – 6.73 (m, 1H), 6.69 – 6.65 (m, 1H), 5.75 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.6, 147.9, 141.6, 133.3, 128.4, 128.3 (2C), 127.3, 126.8 (2C), 117.1, 114.9, 114.4, 66.5.

LRMS (ESI+): 225 (M+H, C₁₄H₁₃N₂O, 100%); (ESI-): 223 (M-H C₁₄H₁₁N₂O, 100%).

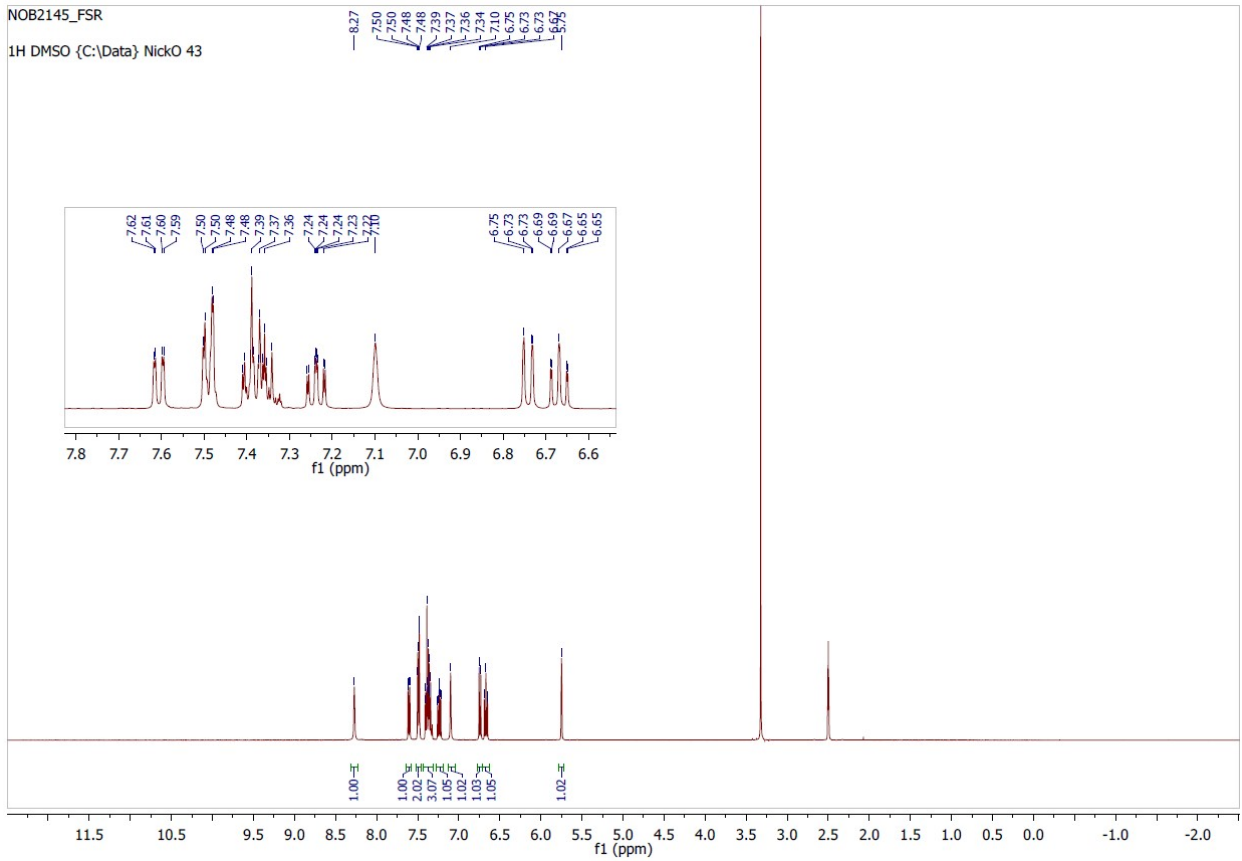
m.p. : >225.6°C (decomp.)

Yield 80%

White crystalline solid

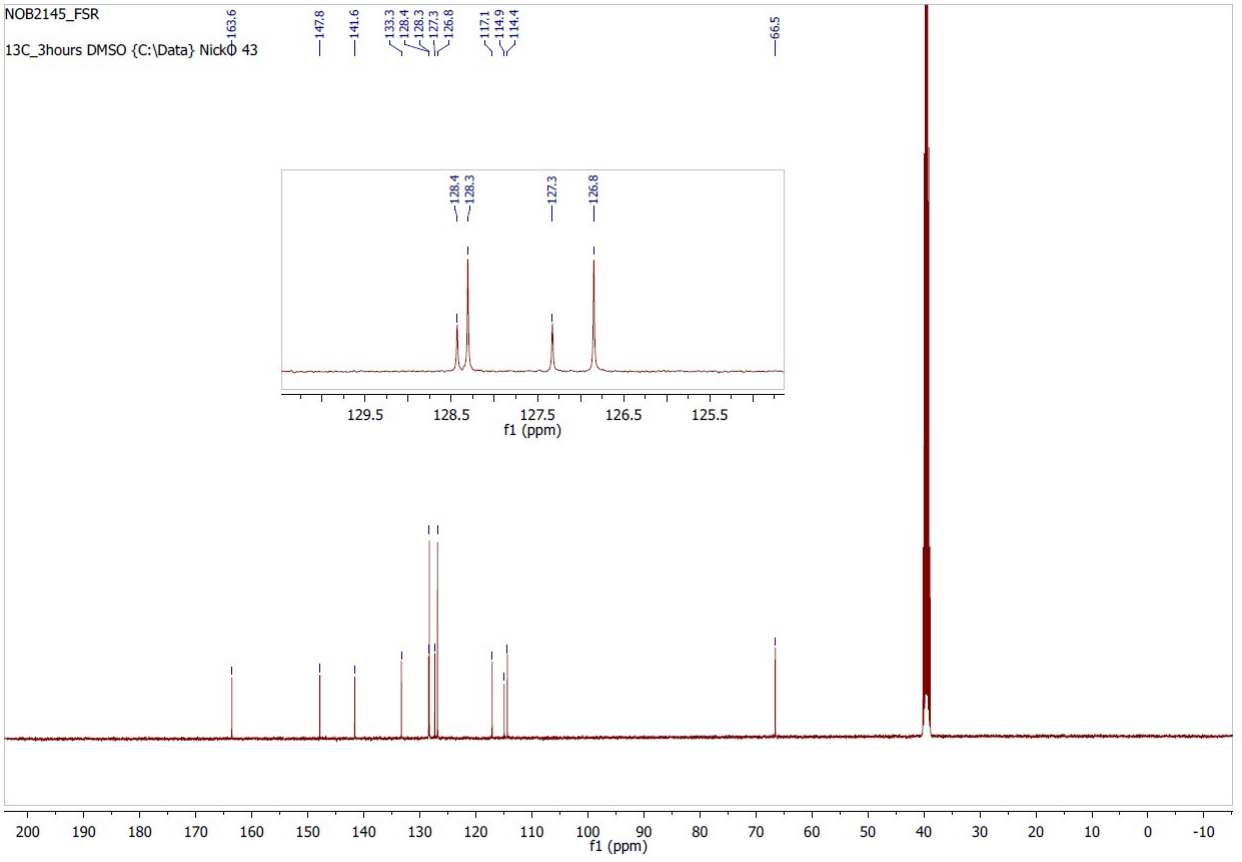
NOB2145_FSR

1H DMSO {C:\Data} NickO 43

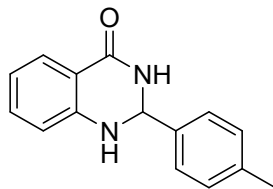


NOB2145_FSR

13C_3hours DMSO {C:\Data} NickO 43



2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (16)



Chemical Formula: C₁₅H₁₄N₂O

Exact Mass: 238.11

Molecular Weight: 238.28

IR (neat): ν_{\max} = 3312 (NH), 2918 (CH), 1655 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.22 (s, 1H), 7.60 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.23 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.04 (s, 1H), 6.73 (d, *J* = 8.1 Hz, 1H), 6.68 – 6.64 (m, 1H), 5.70 (s, 1H), 2.29 (s, 3H).

¹³C NMR (100 MHz, DMSO-d₆) δ 164.1, 148.3, 139.1, 138.2, 133.7, 129.3 (2C), 127.8, 127.2 (2C), 117.54, 115.4, 114.9, 66.8, 21.2.

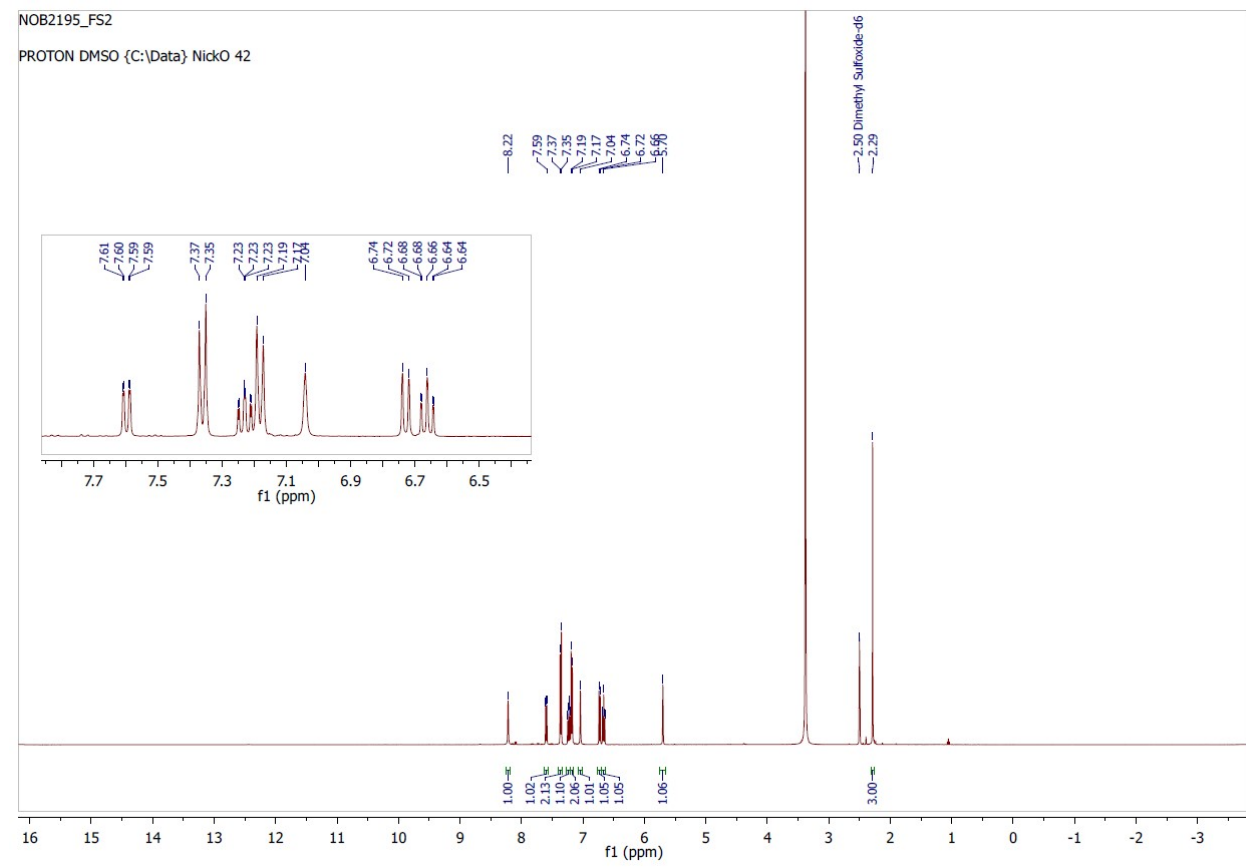
LRMS (ESI⁺): 239.1 (M+H, C₁₅H₁₅N₂O, 100%); LRMS (ESI⁻): 237.2 (M-H, C₁₅H₁₃N₂O₃, 100%).

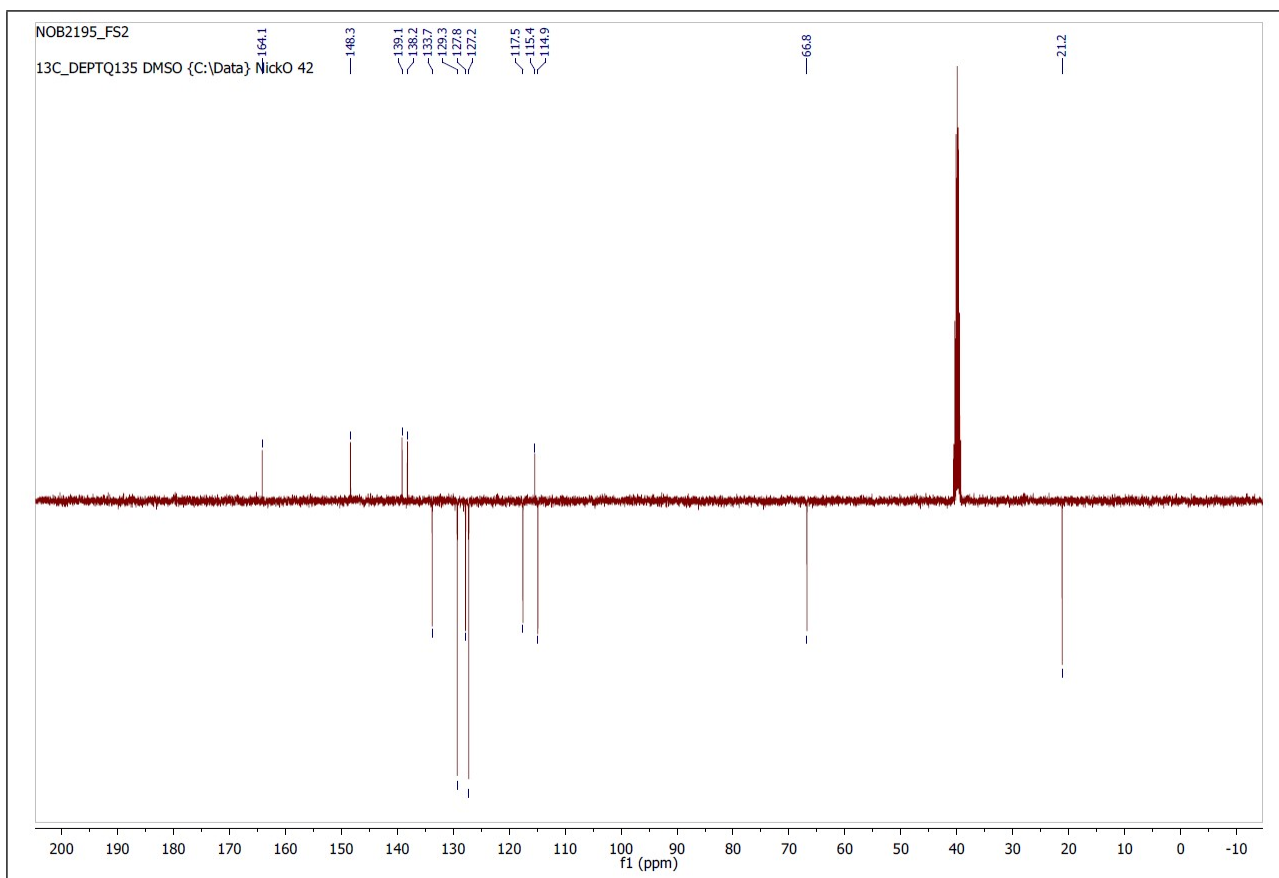
Mass: 141 mg

m.p. >207.6 °C

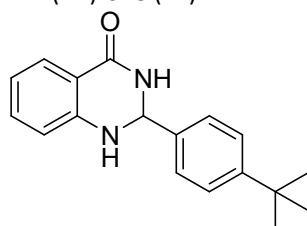
yield 60%

off white solid





2-(4-(tert-Butyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (**17**)



Chemical Formula: C₁₈H₂₀N₂O

Exact Mass: 280.16

Molecular Weight: 280.36

IR (neat): ν_{\max} = 3270 (NH), 1959 (CH), 1651 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.22 (s, 1H), 7.61 (dd, J = 7.7, 1.4 Hz, 1H), 7.42 (s, 4H), 7.24 (ddd, J = 8.6, 7.3, 1.6 Hz, 1H), 7.06 (s, 1H), 6.73 (d, J = 7.8 Hz, 1H), 6.69 – 6.65 (m, 1H), 5.72 (s, 1H), 1.28 (s, 9H).

¹³C NMR (100 MHz, DMSO-d₆) δ 164.1, 151.5, 148.4, 139.1, 133.7, 127.8, 127.1, 125.6, 117.5, 115.4, 114.8, 66.9, 31.6.

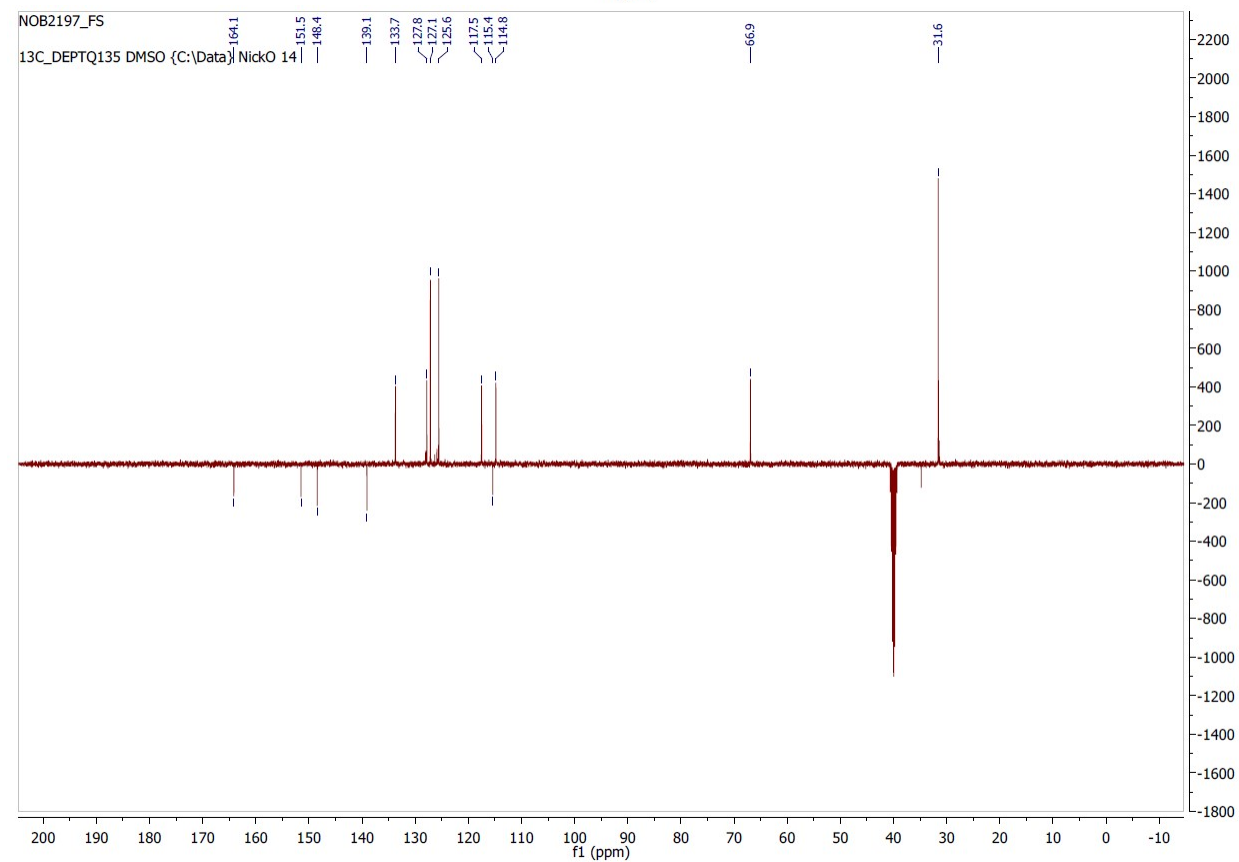
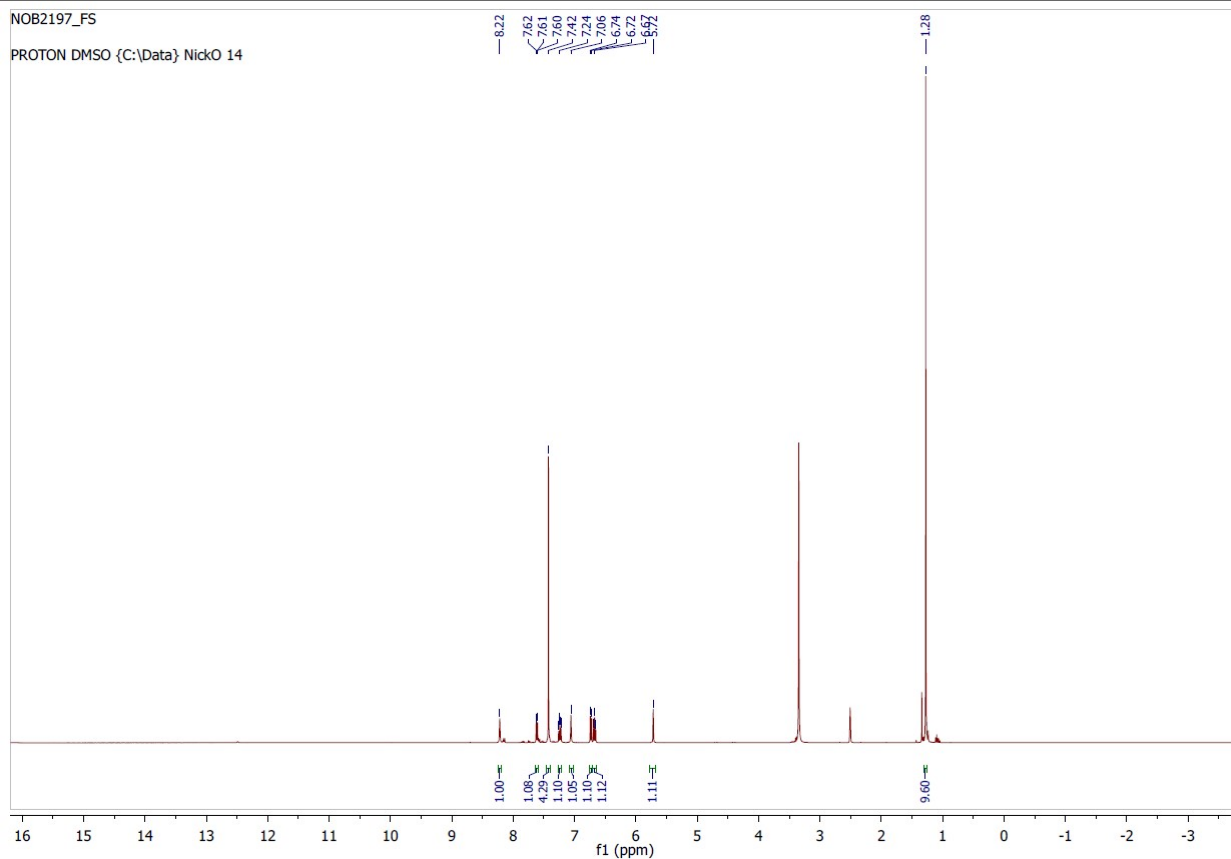
LRMS (ESI) m/z (%): non-ionisable

Mass: 175 mg

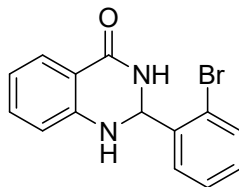
m.p. >200°C (dec.)

yield 38%

off white solid



2-(2-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (**18**)



Chemical Formula: C₁₄H₁₁BrN₂O

Exact Mass: 302.01

Molecular Weight: 303.15

IR (neat): ν_{\max} = 3365 (NH), 1646 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.19 (s, 1H, NH), 7.69-7.64 (m, 3H), 7.45 (td, J = 7.5, 1.1 Hz, 1H), 7.33 (ddd, J = 7.9, 7.4, 1.8 Hz, 1H), 7.26 (ddd, J = 8.2, 7.2, 1.6 Hz, 1H), 6.98 (s, 1H, NH, H₁), 6.77-6.70 (m, 2H), 6.09 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.6, 147.7, 139.1, 133.4, 132.8, 130.7, 129.1, 128.1, 127.4, 122.2, 117.5, 114.7, 114.6, 66.4.

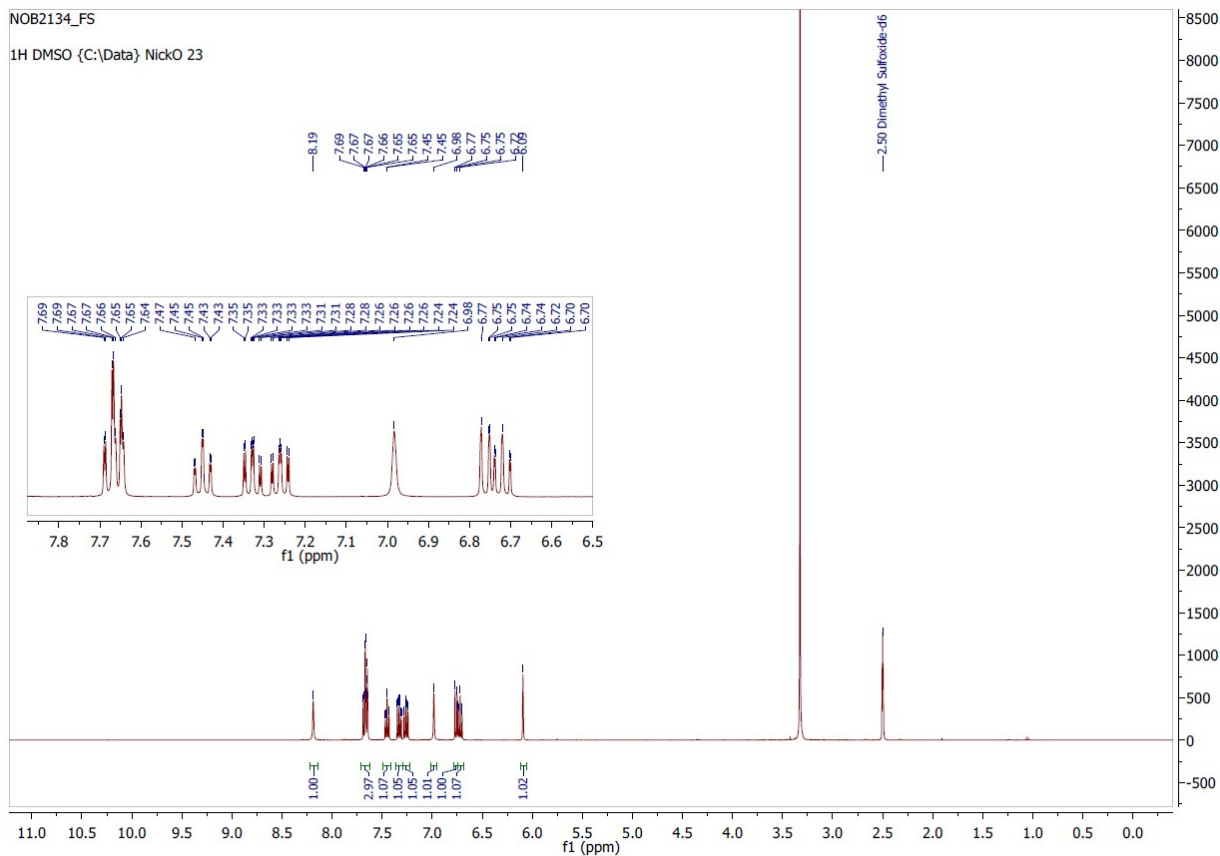
LRMS (ESI +) m/z : 303 (M+H, C₁₄H₁₂⁷⁹BrN₂O, 100%), 305 (M+H, C₁₄H₁₂⁸¹BrN₂O, 95%); (ESI-) m/z : 301 (M-H, C₁₄H₉⁷⁹BrN₂O, 100%), 303 (M-H, C₁₄H₉⁸¹BrN₂O, 95%).

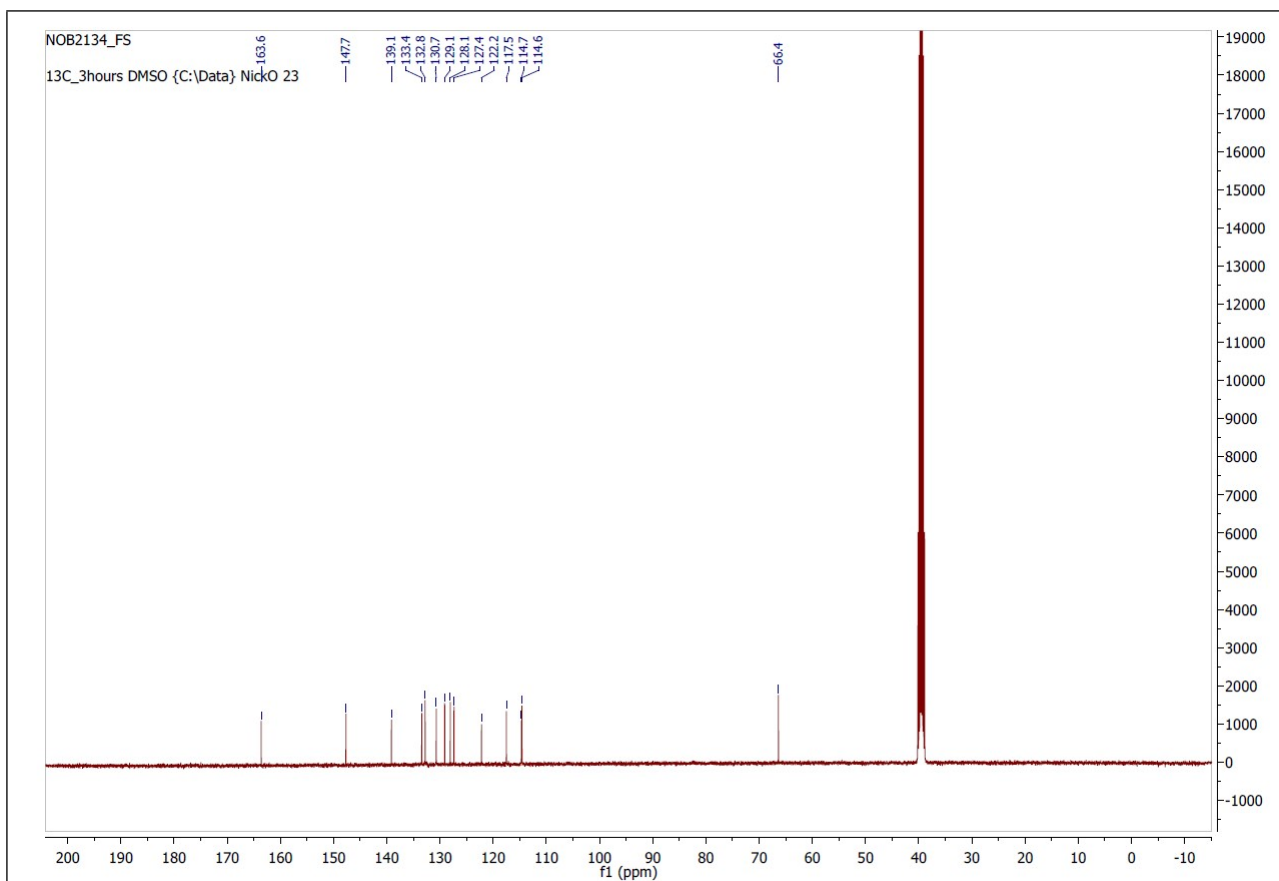
Mass: 187 mg

m.p. >173°C (decomp.)

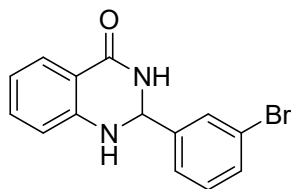
Yield: 40 %

White crystalline solid





2-(3-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (**19**)



Chemical Formula: $C_{14}H_{11}BrN_2O$

Exact Mass: 302.01

Molecular Weight: 303.15

IR (neat): ν_{max} = 3282 (NH), 3172 (NH), 3062 (CH), 1645 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.39 (s, 1H), 7.65 (t, J = 1.7 Hz, 1H), 7.60 (dd, J = 7.7, 1.4 Hz, 1H), 7.52 (ddd, J = 7.9, 1.8, 1.0 Hz, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.34 (t, J = 7.8 Hz, 1H), 7.25 (ddd, J = 8.6, 7.3, 1.6 Hz, 1H), 7.20 (s, 1H), 6.75 (d, J = 7.8 Hz, 1H), 6.72 – 6.64 (m, 1H), 5.76 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.60, 147.54, 144.75, 133.68, 131.29, 130.74, 129.67, 127.50, 125.84, 121.72, 117.51, 114.93, 114.60, 65.54.

LRMS (ESI +) m/z : 303 (M+H, $C_{14}H_{12}^{79}BrN_2O$, 100%), 305 (M+H, $C_{14}H_{12}^{81}BrN_2O$, 90%); (ESI-) m/z : 301 (M-H, $C_{14}H_{10}^{79}BrN_2O$, 100%), 303 (M-H, $C_{14}H_{10}^{81}BrN_2O$, 90%).

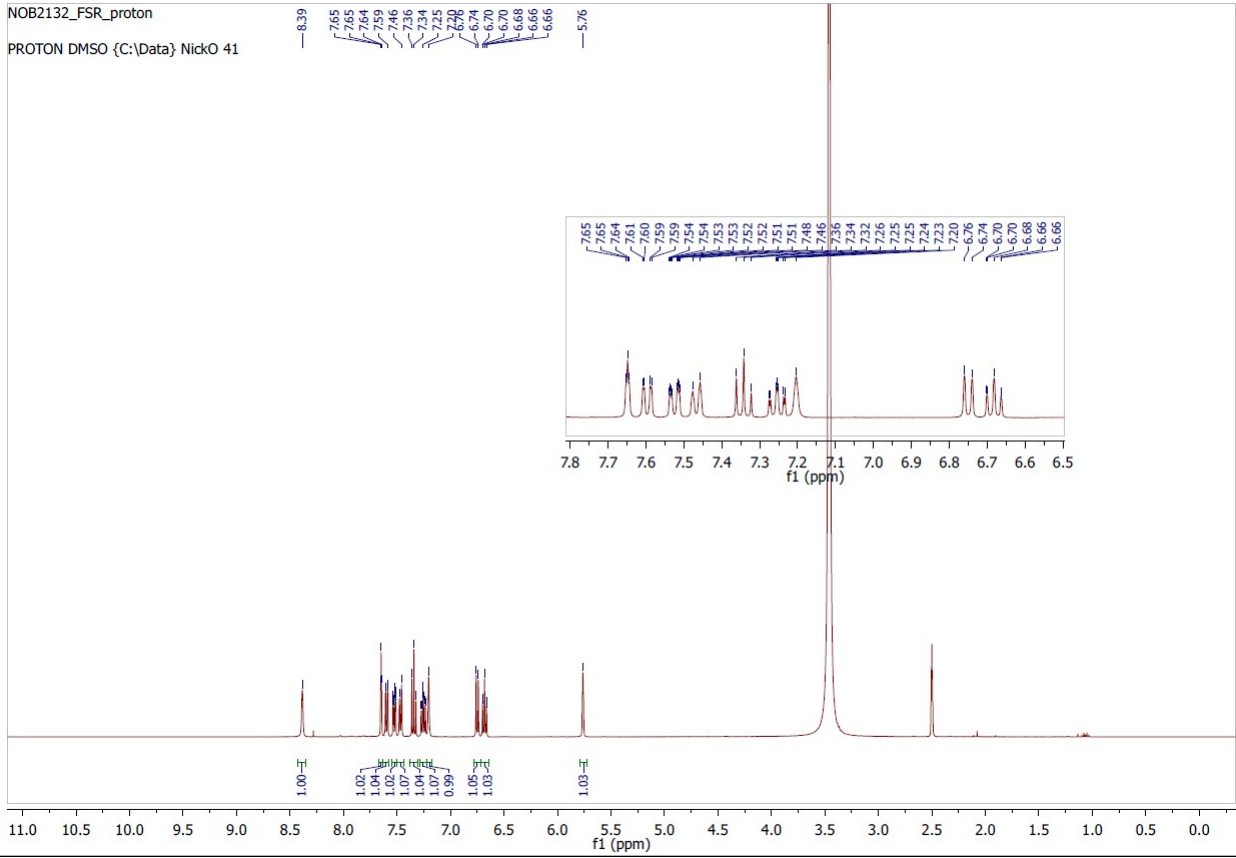
Mass: 491 mg

M.p. >174°C (decomp.)

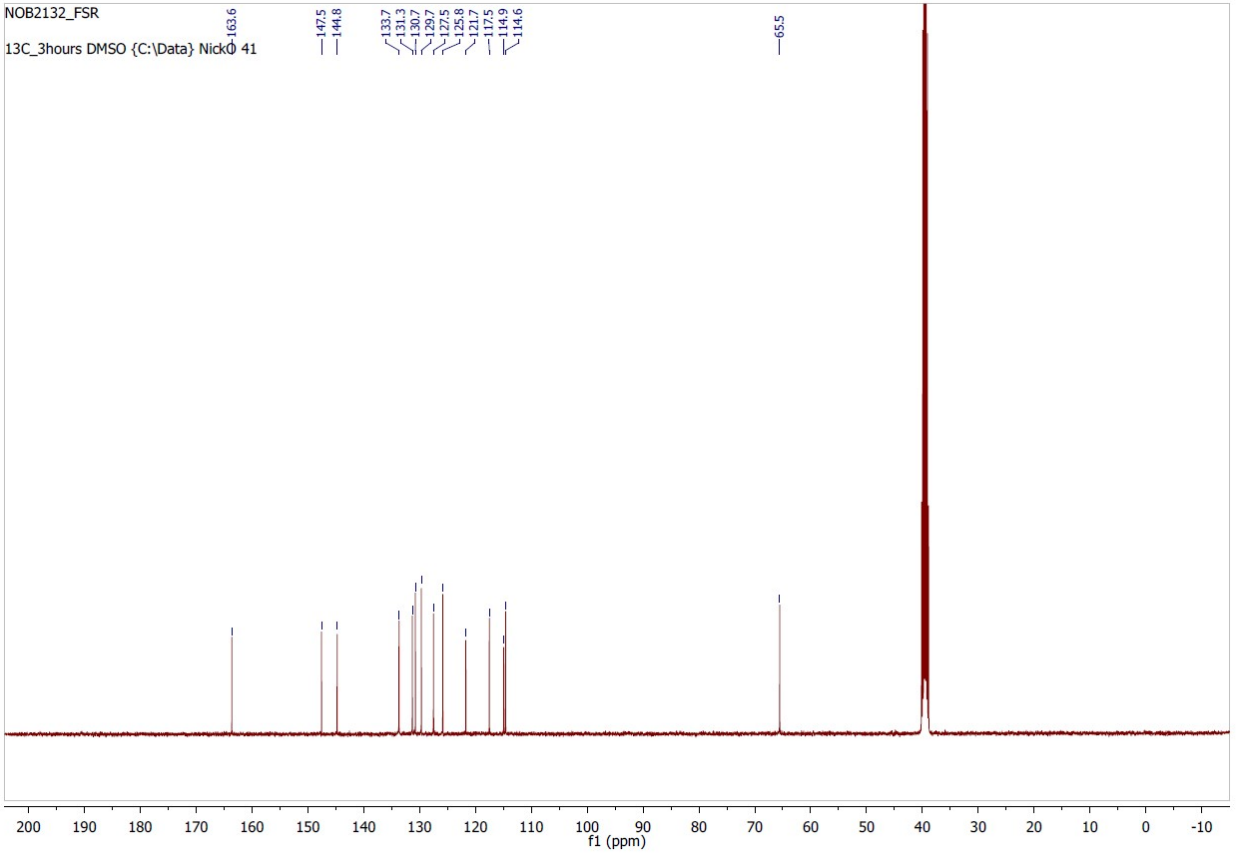
Yield: 96%

White crystalline solid

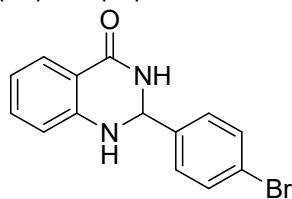
NOB2132_FSR_proton
PROTON DMSO {C:\Data} NickO 41



NOB2132_FSR
13C_3hours DMSO {C:\Data} NickO 41



2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (**20**)



Chemical Formula: C₁₄H₁₁BrN₂O

Exact Mass: 302.01

Molecular Weight: 303.15

IR (neat): ν_{\max} = (3308, N-H), 1652 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.32 (s, 1H, NH), 7.61-7.57 (m, 3H), 7.44 – 7.42 (m, 2H), 7.25 (ddd, *J* = 8.2, 7.2, 1.6 Hz, 1H), 7.13 (s, 1H, NH), 6.74 (dd, *J* = 8.1, 0.5 Hz), 6.70 – 6.66 (m, 1H), 5.75 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.5, 147.6, 141.1, 133.4, 131.2 (2C), 129.1 (2C), 127.4, 121.6, 117.3, 114.9, 114.5, 65.8.

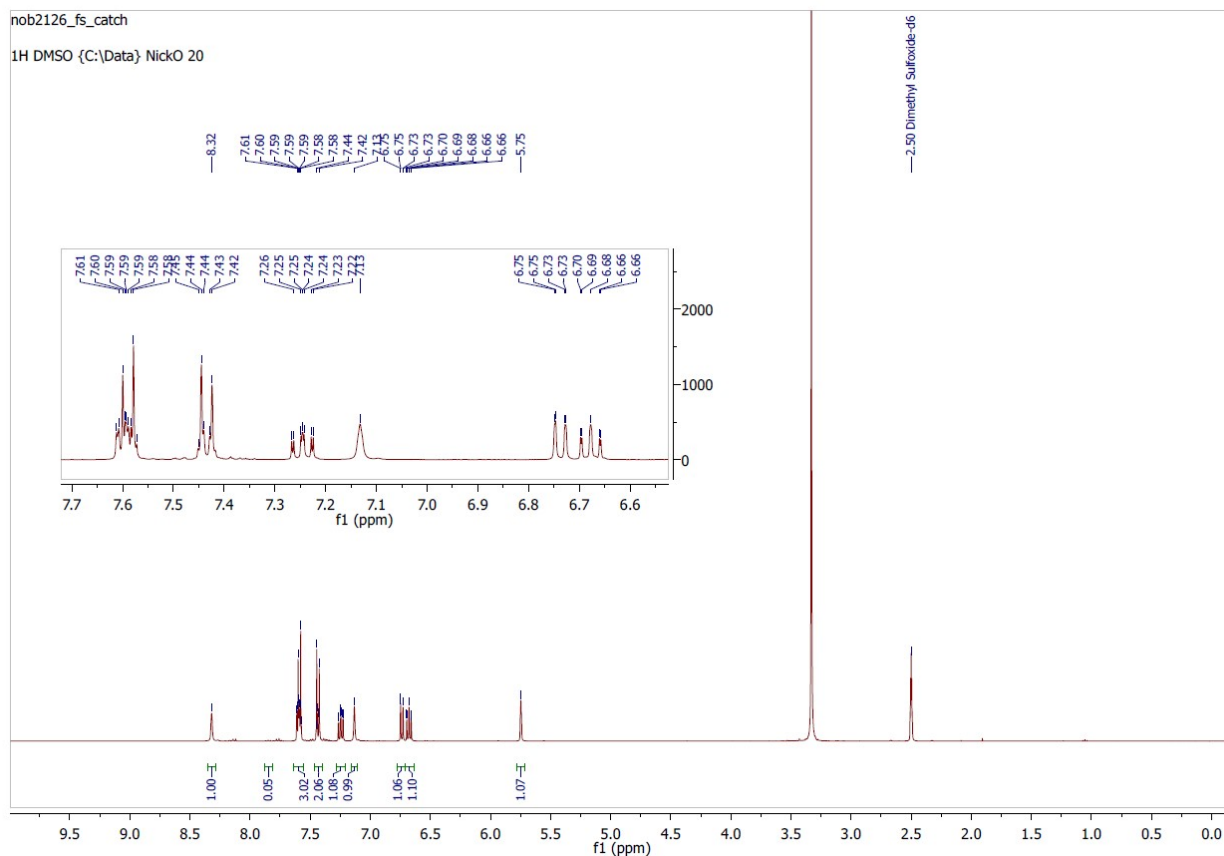
LRMS (ESI +) *m/z*: 303 (M+H, C₁₄H₁₂⁷⁹BrN₂O, 100%), 305 (M+H, C₁₄H₁₂⁸¹BrN₂O, 95%), 347 (M+FA-H, C₁₄H₁₂⁷⁹BrN₂O, 100%), 349 (M+FA-H, C₁₄H₁₂⁸¹BrN₂O, 95%); (ESI-) *m/z*: 301 (M-H, C₁₄H₁₀⁷⁹BrN₂O, 100%), 303 (M-H, C₁₄H₁₀⁸¹BrN₂O, 95%).

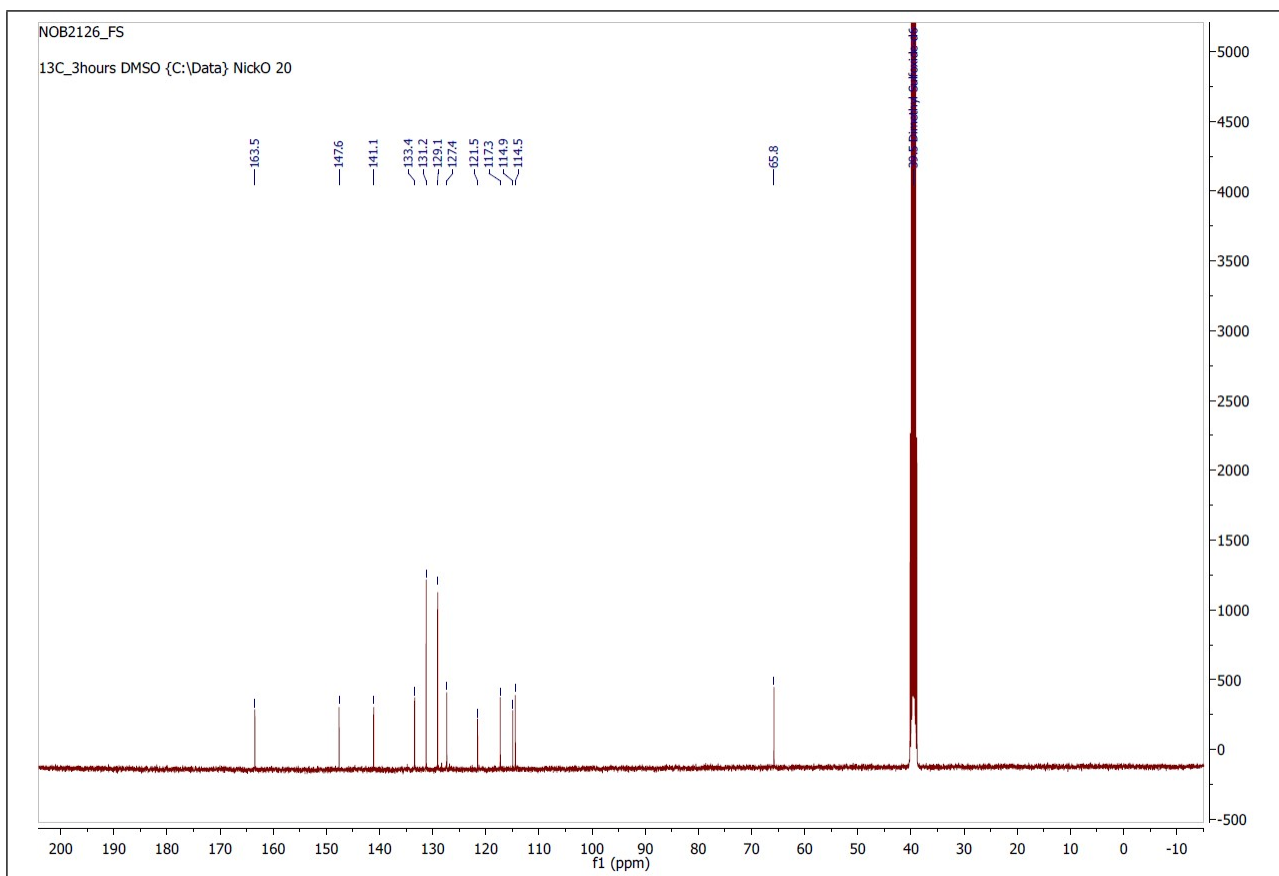
Mass: 418 mg

m.p.: >191°C (decomp.)

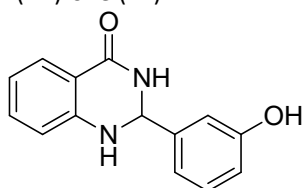
Yield: 94 %

White crystalline solid





2-(3-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (**21**)



Chemical Formula: $C_{14}H_{12}N_2O_2$

Exact Mass: 240.09

Molecular Weight: 240.26

IR (neat): ν_{\max} = 3282 (NH), 3100 (OH) 1650 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 9.52 (d, J = 1.7 Hz, 1H), 8.22 (s, 1H), 7.59 (dd, J = 7.7, 1.4 Hz, 1H), 7.27 – 7.19 (m, 1H), 7.16 (t, J = 8.1 Hz, 1H), 7.06 (s, 1H), 6.88 (t, J = 4.0 Hz, 2H), 6.72 (ddd, J = 7.1, 3.1, 1.8 Hz, 2H), 6.69 – 6.62 (m, 1H), 5.64 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.7, 157.4, 147.9, 143.3, 133.4, 129.4, 127.4, 117.5, 117.1, 115.4, 114.9, 114.4, 113.7, 66.5.

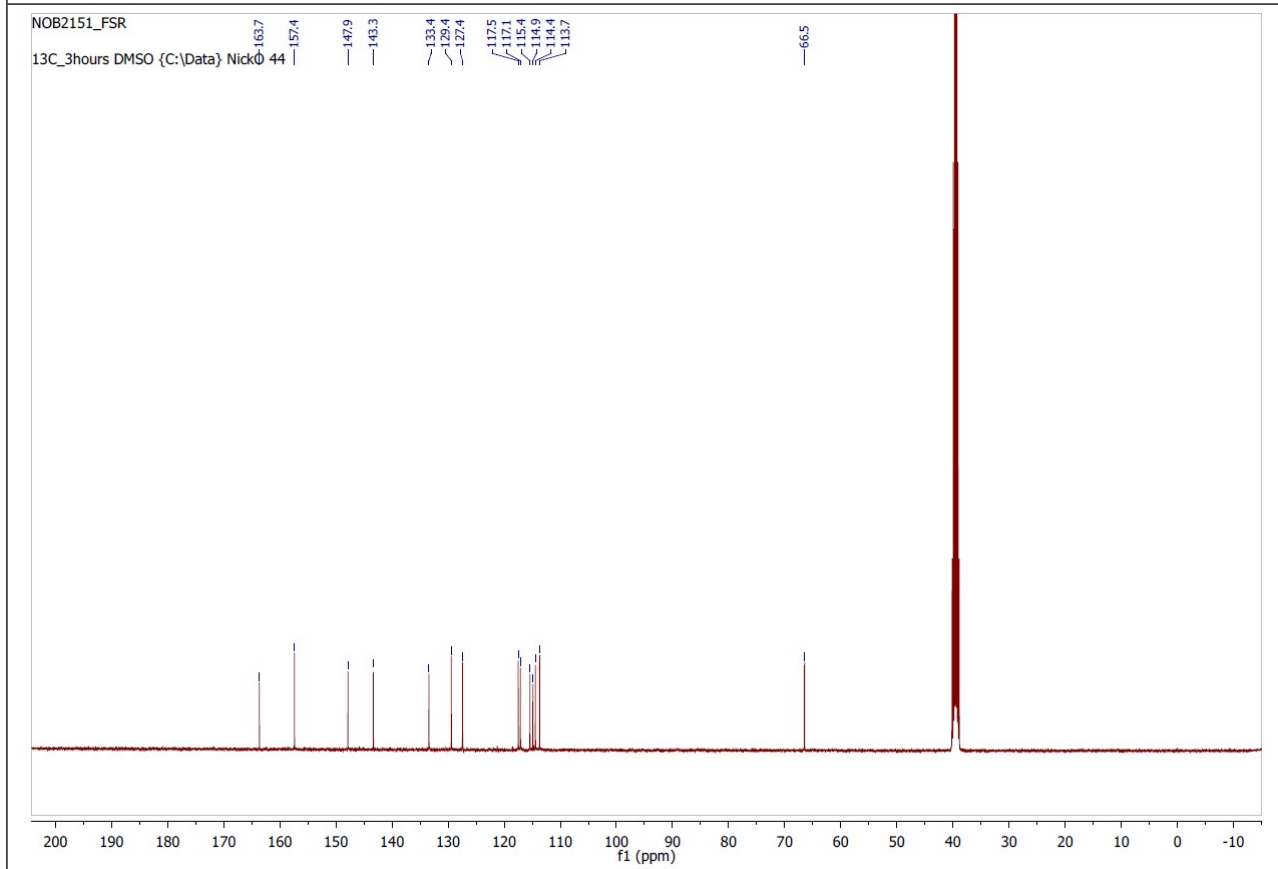
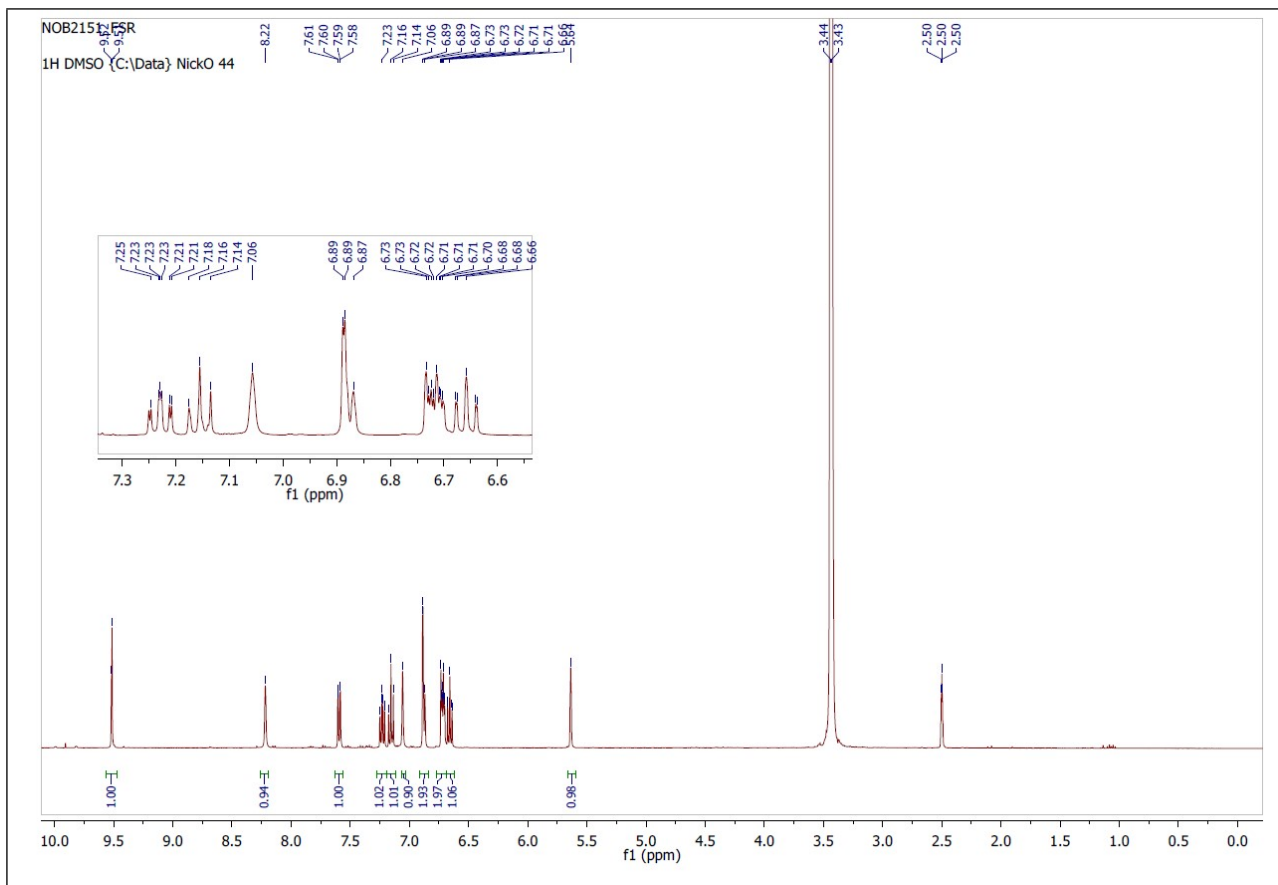
LRMS (ESI+): 241.1 (M+H, $C_{14}H_{13}N_2O_2$, 100%), 481.2 (2M+H, $C_{14}H_{13}N_2O_2$, 10%); (ESI-) 239.1 (M-H, $C_{14}H_{11}N_2O_2$, 100%), 479.2 (2M+H, $C_{14}H_{11}N_2O_2$, 50%).

Mass 260.3 mg

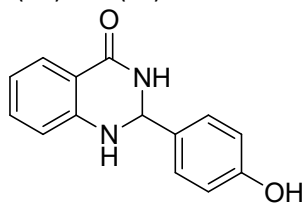
m.p. 206 – 209 °C

Yield: 67%

White solid



2-(4-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (22)



Chemical Formula: C₁₄H₁₂N₂O₂

Exact Mass: 240.09

Molecular Weight: 240.26

IR (neat): ν_{\max} = 3346 (NH), 3175 (NH), 1229 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 9.53 (s, 1H), 8.09 (d, J = 4.3 Hz, 1H), 7.61 (dd, J = 7.7, 1.5 Hz, 1H), 7.32 – 7.29 (m, 2H), 7.24 (ddd, J = 8.3, 7.2, 1.6 Hz, 1H), 6.94 (s, 1H), 6.79 – 6.66 (m, 4H), 5.66 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 164.2, 158.1, 148.6, 133.7, 132.1, 128.7 (2C), 127.8, 117.5, 115.4 (2C), 114.8, 67.1.

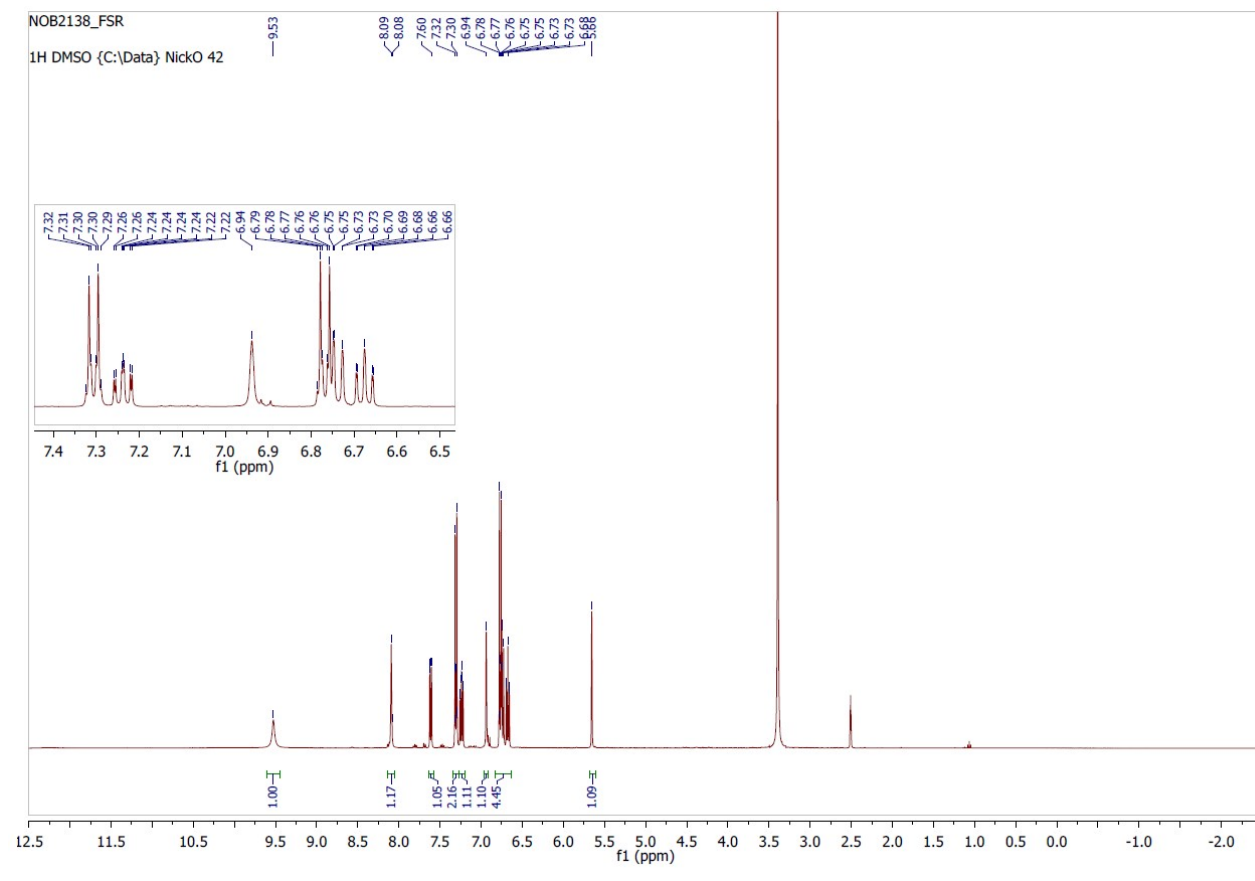
LRMS (ESI+): 241.1 (M+H, C₁₄H₁₃N₂O₂, 100%); (ESI-) 239.1 (M-H, C₁₄H₁₂N₂O₂, 100%).

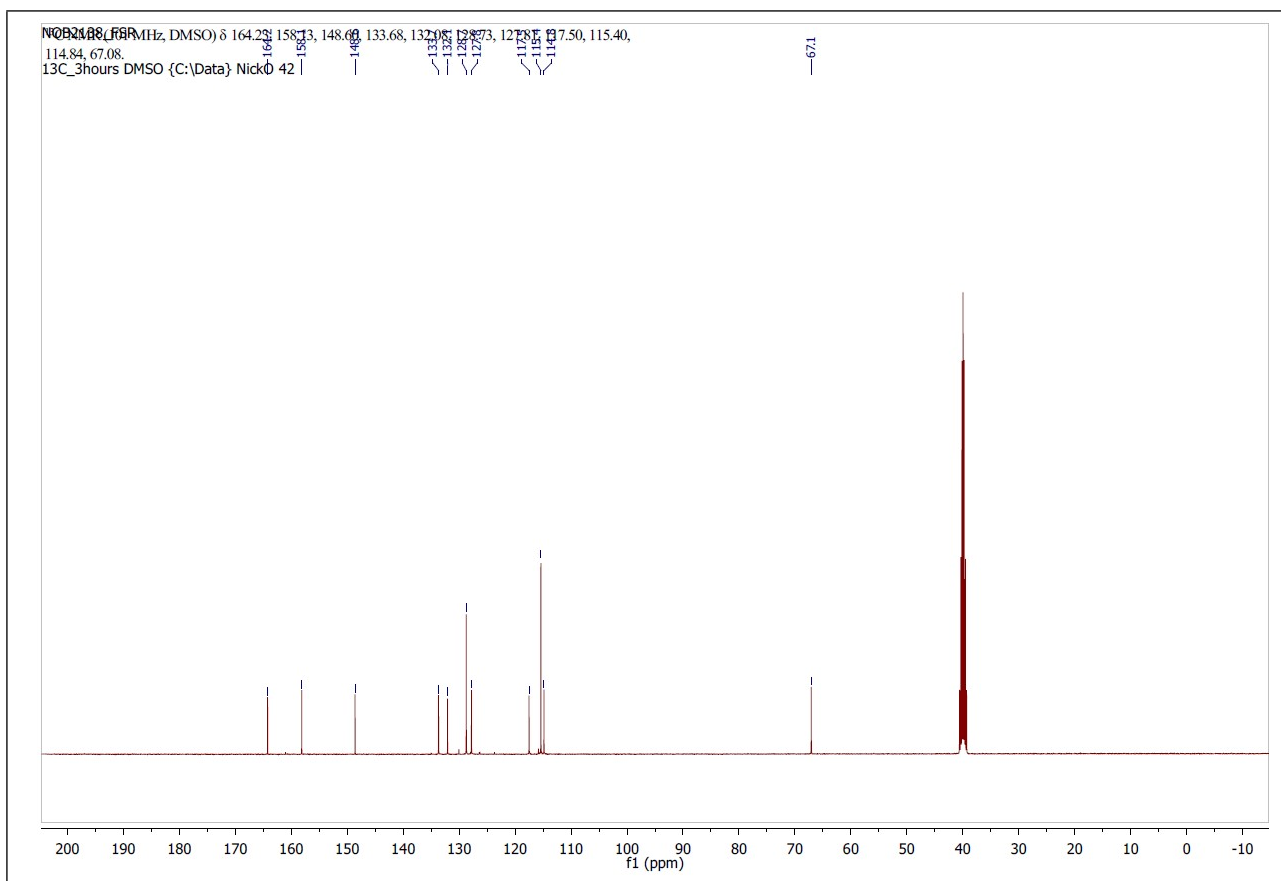
Mass 163 mg

m.p. >200°C (decomp.)

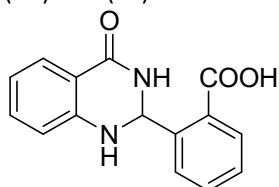
Yield: 39%

White solid





2-(2-Carboxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (**23**)



Chemical Formula: $C_{15}H_{12}N_2O_3$

Exact Mass: 268.08

Molecular Weight: 268.27

IR (neat): ν_{max} = 3282 (NH), 3036 (NH), 1726 (C=O), 1674 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 9.48 (s, 1H), 8.22 (s, 1H), 7.60 (dd, J = 7.7, 1.5 Hz, 1H), 7.23 (ddd, J = 8.2, 7.2, 1.6 Hz, 1H), 7.16 (t, J = 7.9 Hz, 1H), 7.06 (s, 1H), 6.89 (t, J = 4.3 Hz, 2H), 6.76 – 6.69 (m, 2H), 6.69 – 6.63 (m, 1H), 5.64 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.50, 157.34, 147.81, 143.22, 133.27, 129.31, 127.33, 117.43, 116.98, 115.33, 114.86, 114.33, 113.65, 66.45, 39.52.

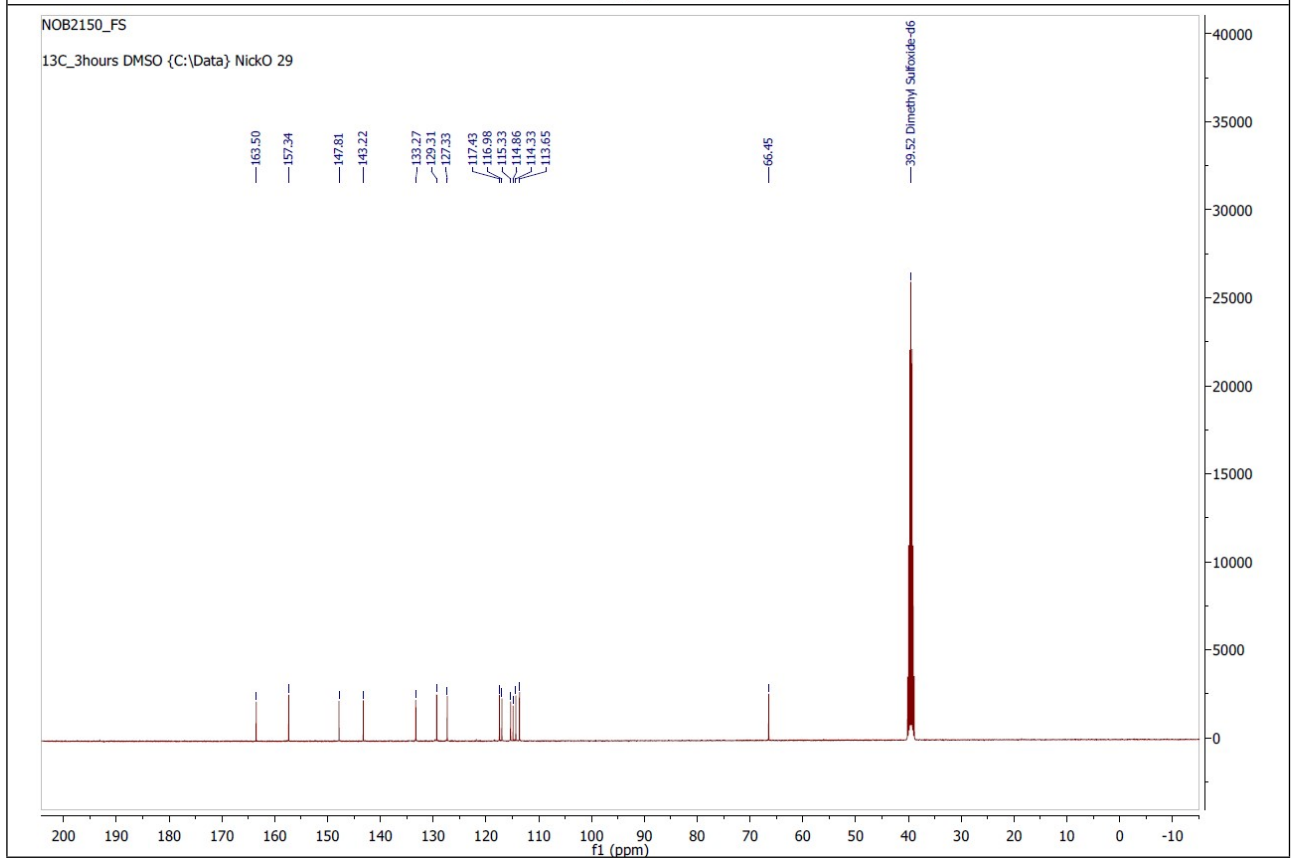
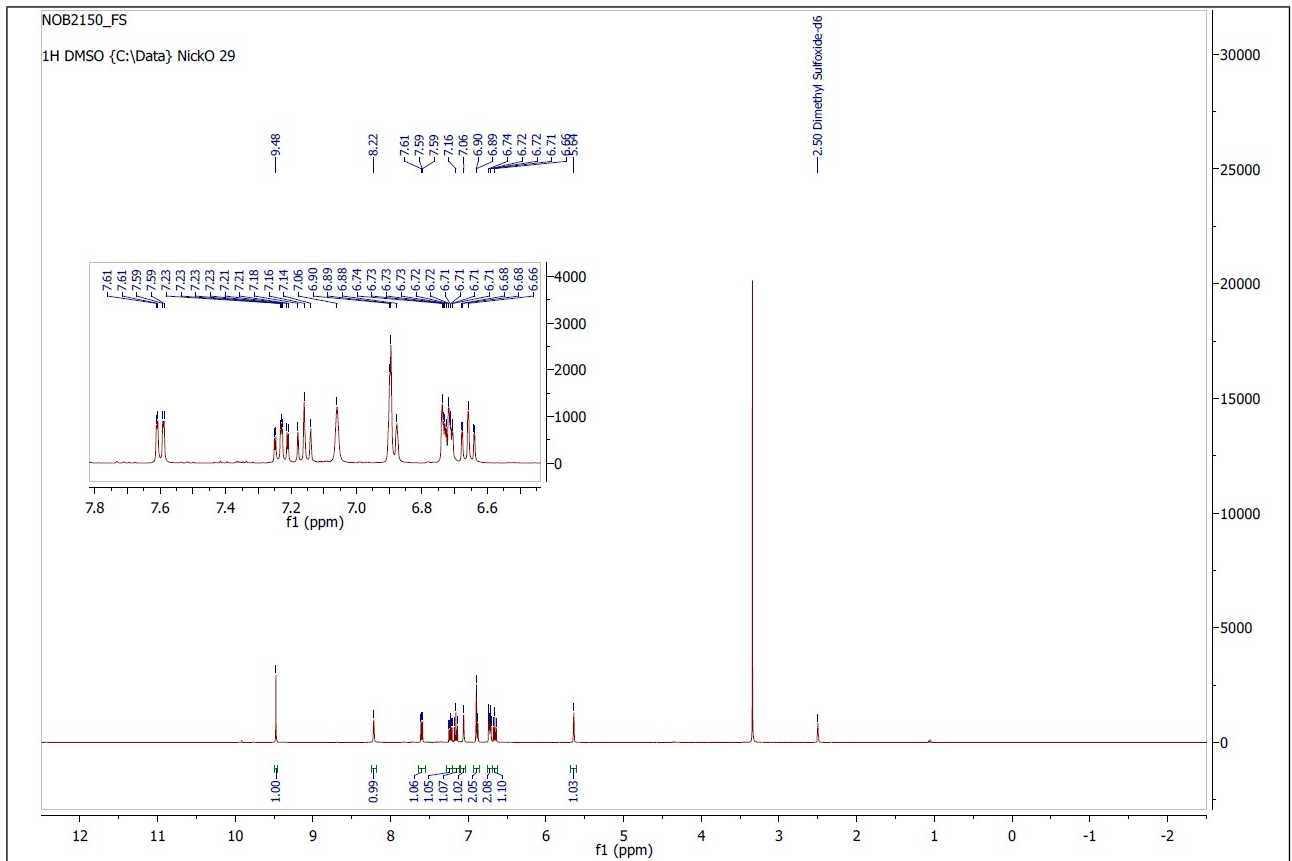
LRMS (ESI+): 251.1 (M+H- H_2O , $C_{15}H_{11}N_2O_2$, 100%); (ESI-): 249.1 (M-H- H_2O , $C_{15}H_9N_2O_2$, 100%)

Mass: 251.8 mg

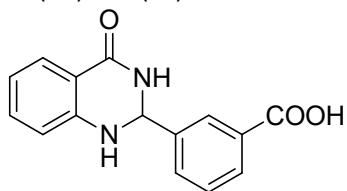
m.p. >240 °C (decomp.)

Yield: 58%

Amorphous yellow solid



2-(3-Carboxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (**24**)



Chemical Formula: C₁₅H₁₂N₂O₃

Exact Mass: 268.08

Molecular Weight: 268.27

IR (neat): ν_{\max} = 3334 (NH), 3200 (NH), 1666 (C=O), 750.5 (C=C) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.38 (s, 1H), 8.08 (s, 1H), 7.90 (dt, 1H), 7.71 (dt, 1H), 7.60 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.51 (t, *J* = 9.6, 1H), 7.25 (ddd, *J* = 8.2, 7.2, 1.6 Hz, 1H), 7.19 (s, 1H), 6.74 (d, 1H), 6.71 – 6.65 (m, 1H), 5.83 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 167.4, 163.8, 147.8, 142.5, 133.8, 131.5, 131.1, 129.5, 129.0, 127.9, 127.6, 117.6, 115.0, 114.7, 66.1.

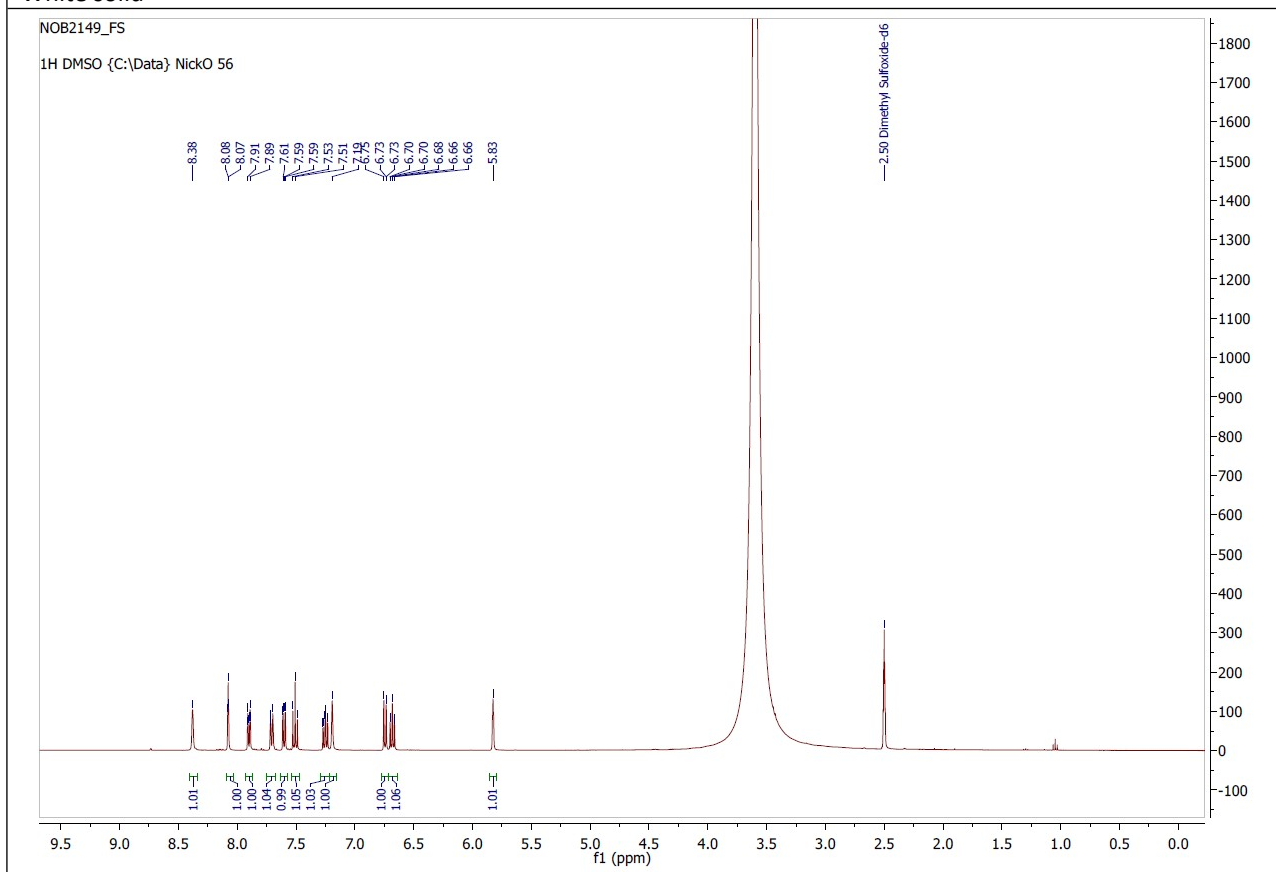
LRMS (ESI+): 269.2 (M+H, C₁₅H₁₃N₂O₃, 100%); (ESI-): 267.1 (M-H, C₁₅H₁₅N₂O₃, 100%), 535.2 (2M-H, C₁₅H₁₅N₂O₃, 100%).

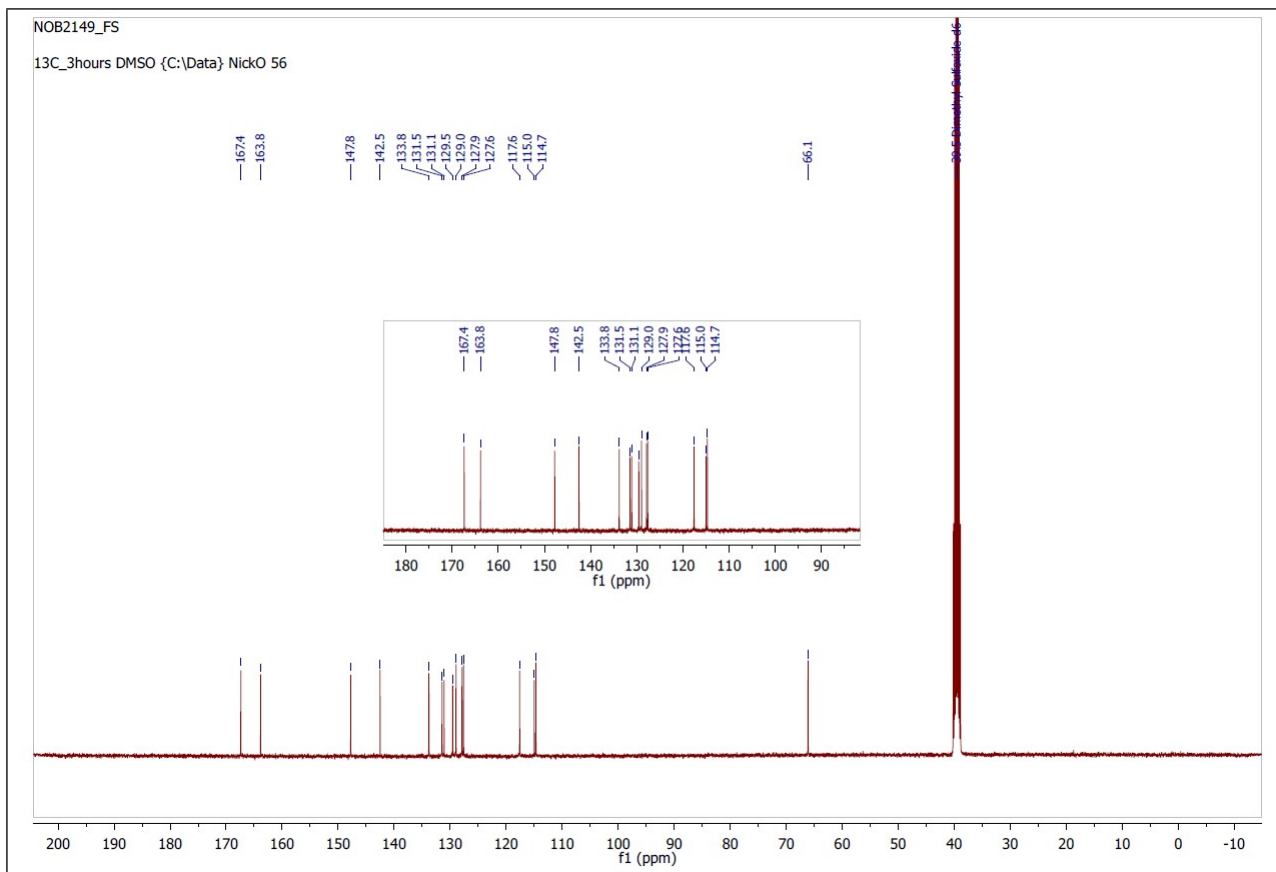
Mass: 398 mg

m.p. >300 °C

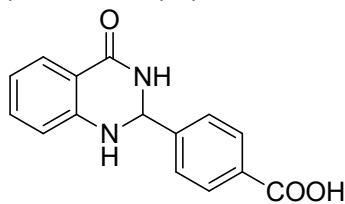
Yield: 86%

White solid





4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzoic acid (**25**)



Chemical Formula: $C_{15}H_{12}N_2O_3$

Exact Mass: 268.08

Molecular Weight: 268.27

IR (neat): ν_{\max} = 3289 (NH), 2800 (OH), 1695 (C=O), 725 (C=C) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.38 (s, 1H), 7.94 – 7.92 (m, 2H), 7.60 (dd, J = 12.0, 4.9 Hz, 3H), 7.25 (ddd, J = 8.7, 7.3, 1.6 Hz, 1H), 7.20 (s, 1H), 6.74 (d, J = 7.7 Hz, 1H), 6.70 – 6.68 (m, 1H), 5.82 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 167.3, 163.8, 147.7, 146.7, 133.8, 131.0 (2C), 129.6, 127.6, 127.1 (2C), 117.6, 115.0, 114.7, 66.1.

MS Analysis (low res): LRMS (ESI+): 269.2 (M+H, $C_{15}H_{13}N_2O_3$, 100%); (ESI-): 267.1 (M-H, $C_{15}H_{11}N_2O_3$, 100%).

Mass: 341.0 mg

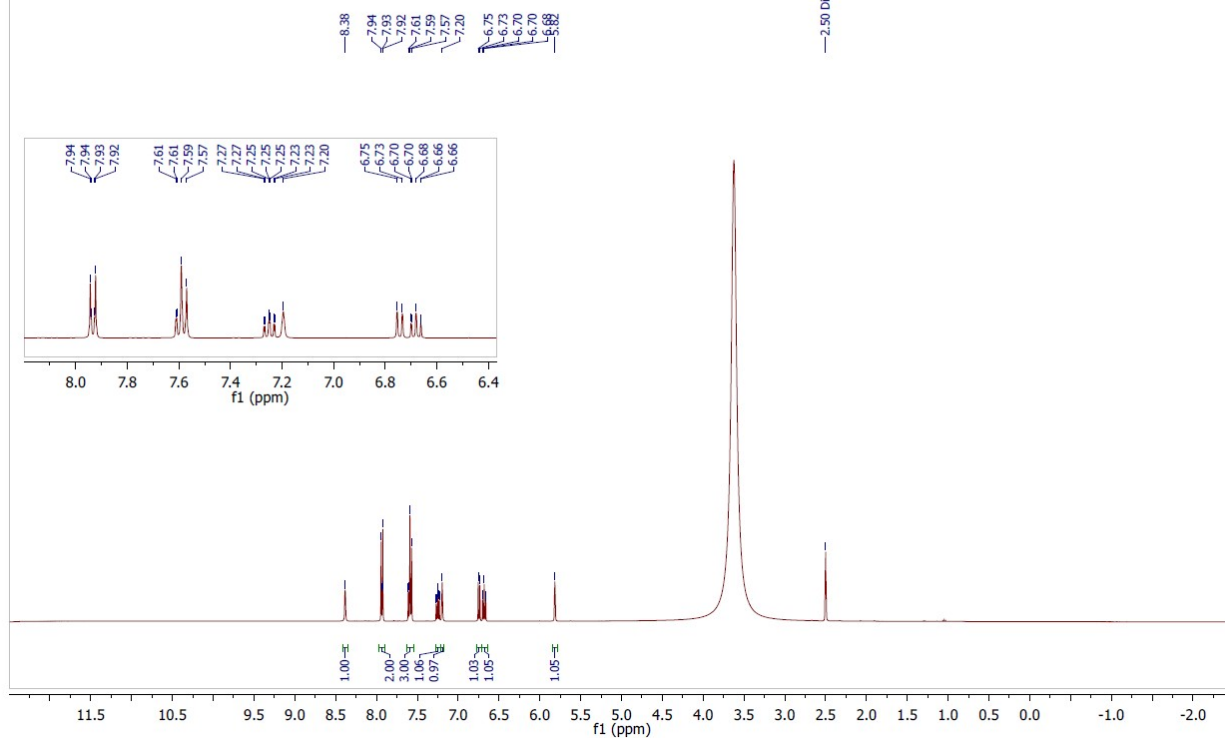
m.p. >300°C

Yield 75 %

White solid

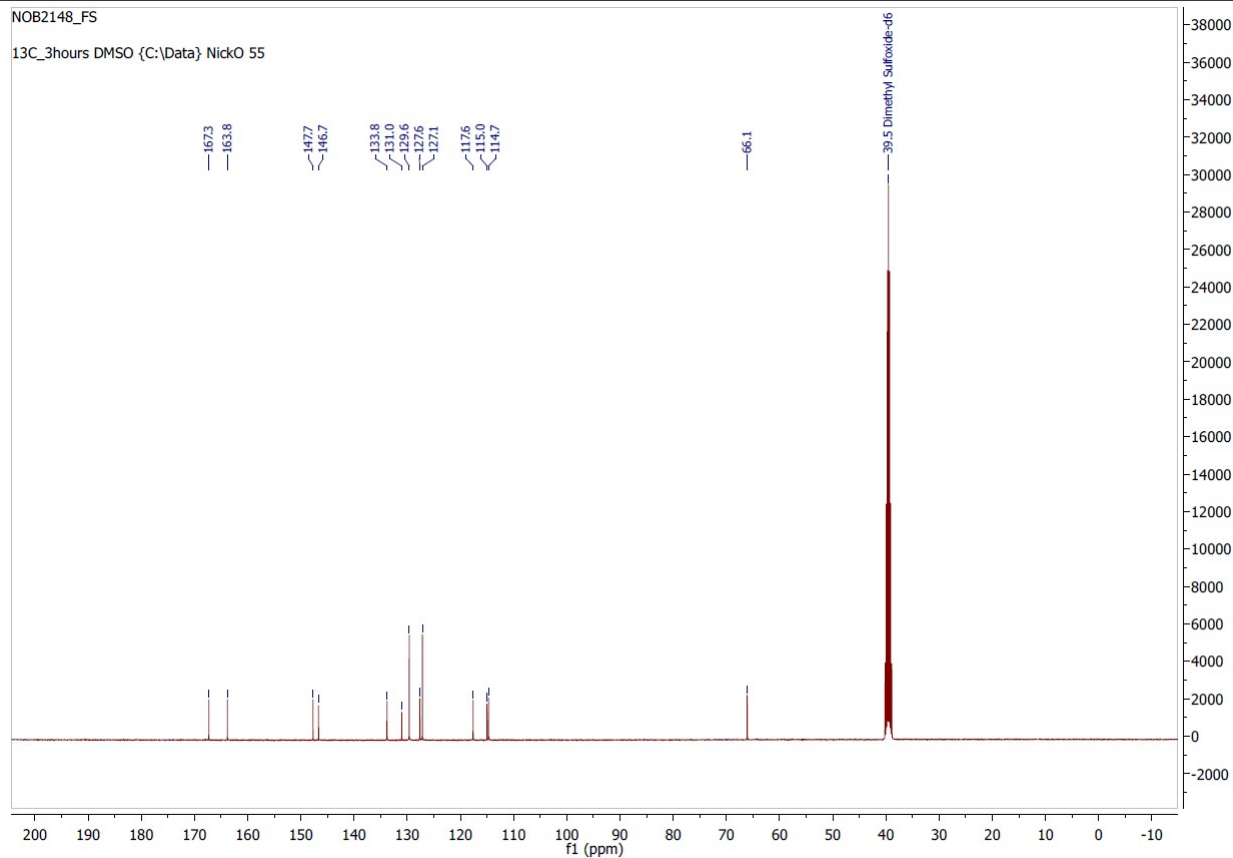
NOB2148_FS

1H DMSO (C:\Data) NickO 55

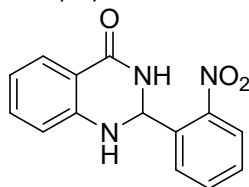


NOB2148_FS

13C_3hours DMSO (C:\Data) NickO 55



2-(2-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (26)



Chemical Formula: C₁₅H₁₂N₂O₃

Exact Mass: 268.08

Molecular Weight: 268.27

IR (neat): ν_{\max} = 3409 (NH), 3182 (NO), 1654 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.21 (s, 1H), 8.06 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.85 - 7.84 (m, 1H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.66 - 7.61 (m, 2H), 7.28 - 7.24 (m, 1H), 7.00 (s, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 6.72 (t, *J* = 7.5 Hz, 1H), 6.33 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.3, 147.7, 147.1, 135.9, 133.9, 133.5, 129.9, 128.9, 127.3, 124.7, 117.7, 114.9, 114.5, 62.2.

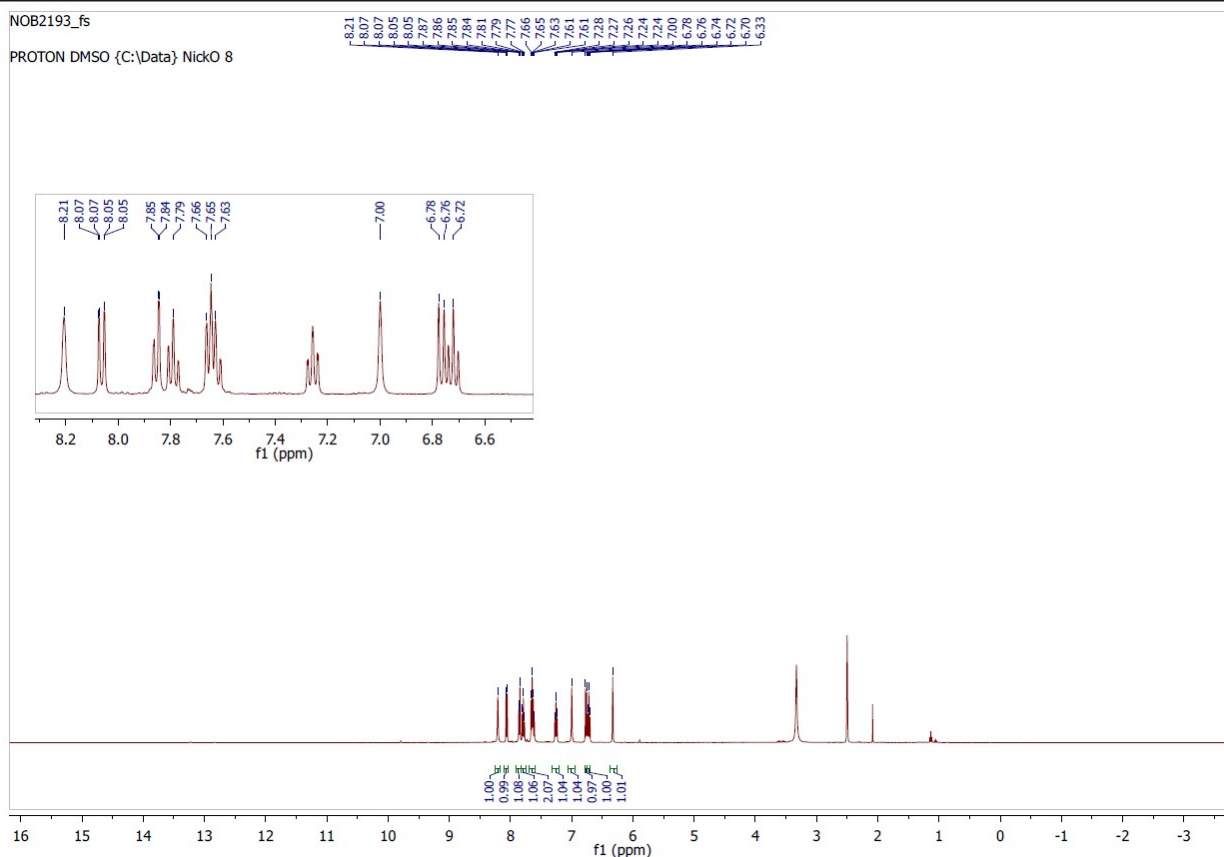
LRMS (ESI+): 270.1 (M+H, C₁₄H₁₁N₃O₃, 100%)

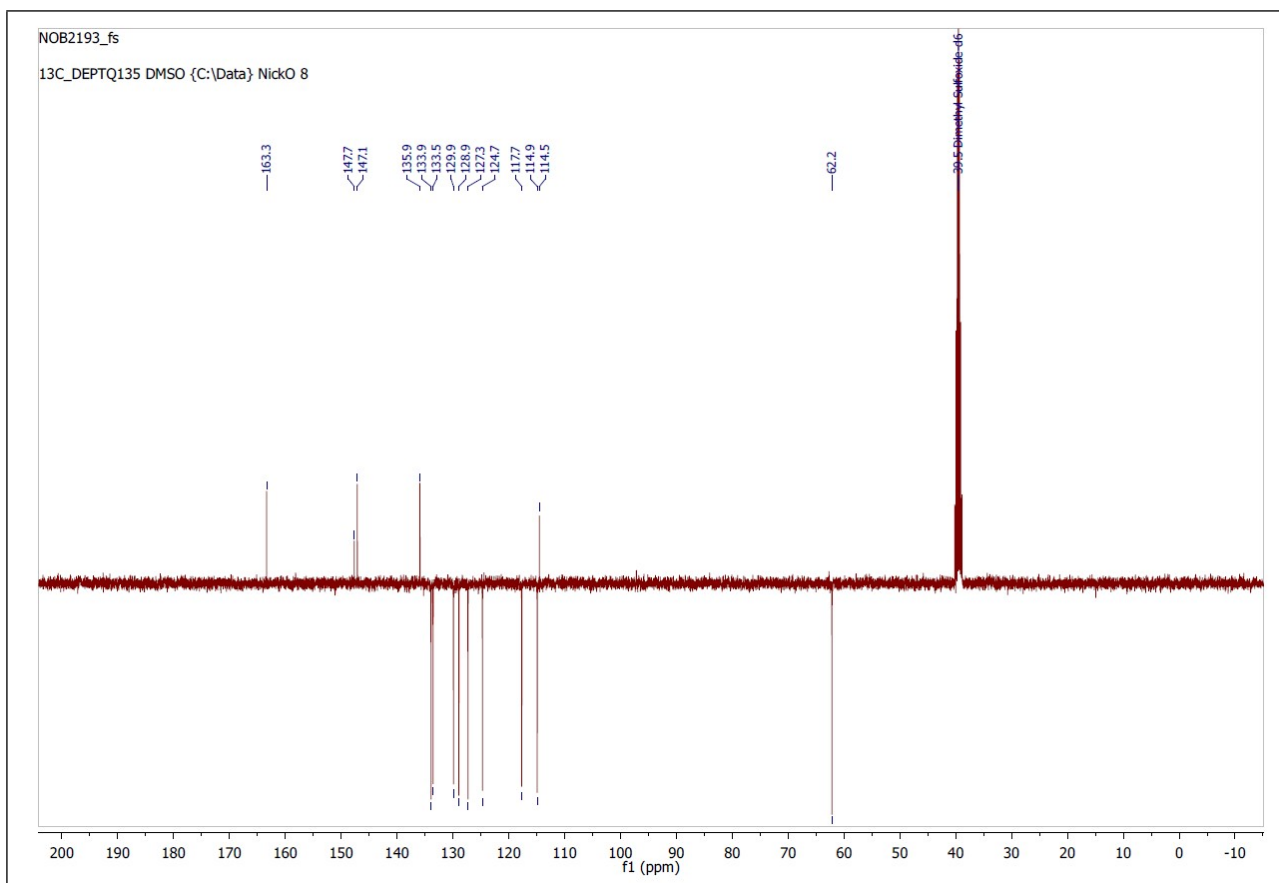
Mass 414 mg

m.p. >195°C (decomp)

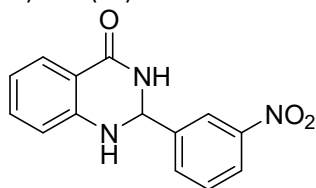
Yield: 90%

Orange solid





2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (**27**)



Chemical Formula: $C_{14}H_{11}N_3O_3$

Exact Mass: 269.08

Molecular Weight: 269.26

IR (neat): ν_{\max} = 3289 (NH), 3179 (NH), 3072 (CH), 1650 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.52 (s, 1H), 8.36 (s, 1H), 8.13 – 8.19 (m, 1H), 7.94 (d, J = 7.7 Hz, 1H), 7.70 (t, J = 7.9 Hz, 1H), 7.62 (d, J = 7.3 Hz, 1H), 7.34 (s, 1H), 7.27 (t, 1H), 6.79 (d, J = 8.1 Hz, 1H), 6.70 (t, J = 7.4 Hz, 1H), 5.95 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.3, 147.7, 147.3, 144.3, 133.6, 133.4, 130.0, 127.4, 123.3, 121.6, 117.5, 114.9, 114.6, 65.2.

LRMS (ESI+): 270.1 (M+H, $C_{14}H_{11}N_3O_3$, 100%); LRMS (ESI-): 268.1 (M-H, $C_{14}H_{11}N_3O_3$, 100%).

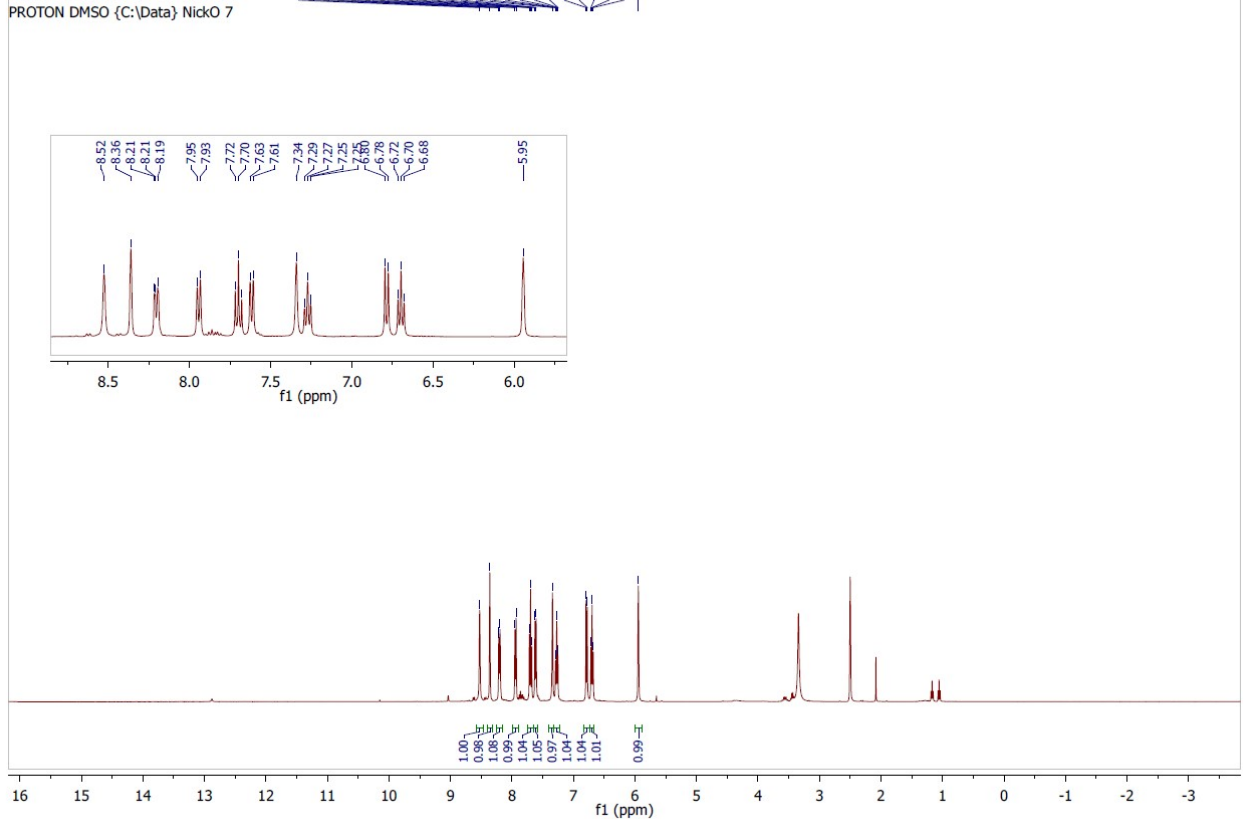
Mass: 356.2 mg

m.p. >194 °C (decomp)

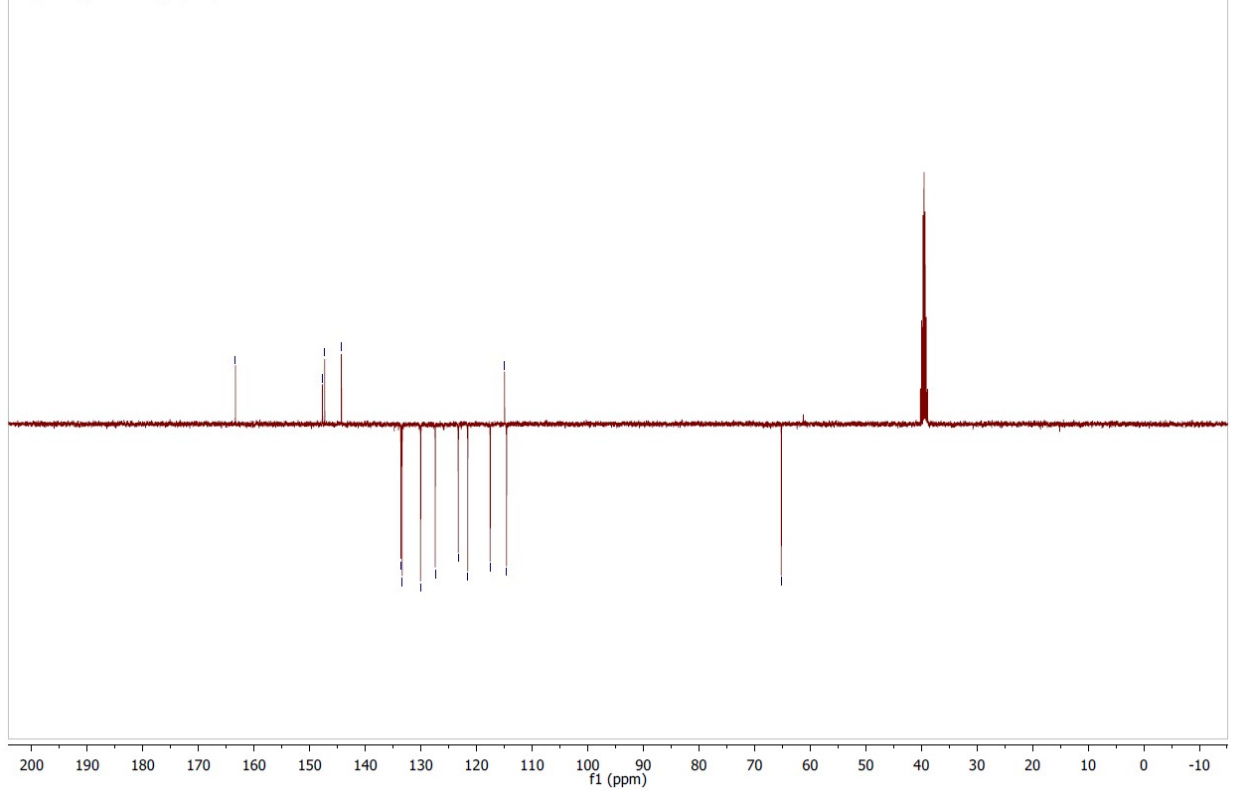
Yield: 78 %

Yellow/orange solid

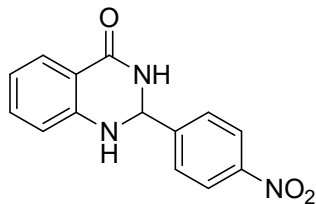
NOB2192_fs
PROTON DMSO {C:\Data} NickO 7



NOB2192_fs
13C_DEPTQ135 DMSO {C:\Data} NickO 7



2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (**28**)



Chemical Formula: $C_{14}H_{11}N_3O_3$

Exact Mass: 269.08

Molecular Weight: 269.26

IR (neat): ν_{\max} = 3279 (NH), 3173 (NH), 3100 (CH), 1644 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.51 (s, 1H), 8.25 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 8.7 Hz, 2H), 7.62 – 7.60 (m, 1H), 7.32 (s, 1H), 7.28 – 7.24 (m, 1H), 6.76 (d, J = 8.0 Hz, 1H), 6.69 (t, J = 7.4 Hz, 1H), 5.91 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.3, 149.3, 147.2, 133.6, 128.0, 127.4, 123.6, 117.5, 114.9, 114.5, 65.3.

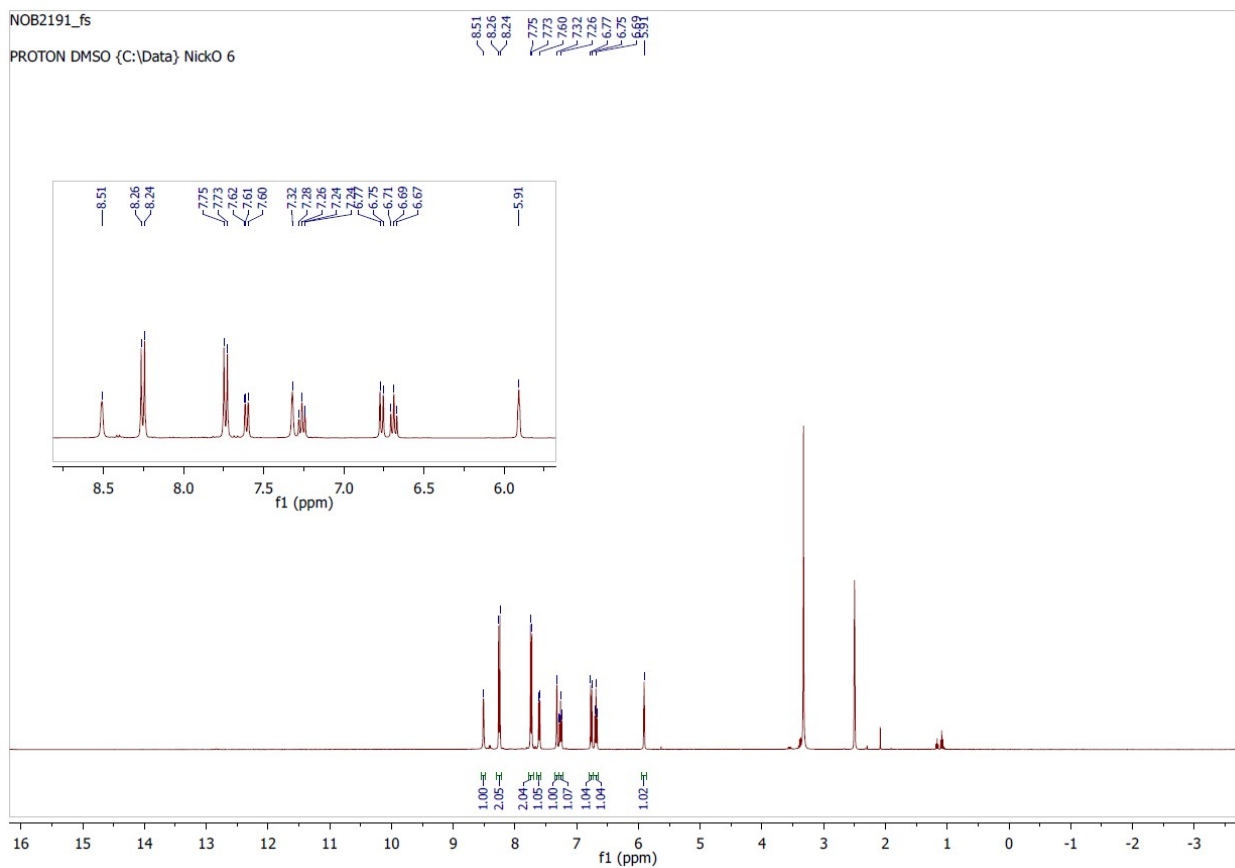
LRMS (ESI+): 270.1 (M+H, $C_{14}H_{11}N_3O_3$, 100%); LRMS (ESI-): 268.1 (M-H, $C_{14}H_{11}N_3O_3$, 100%).

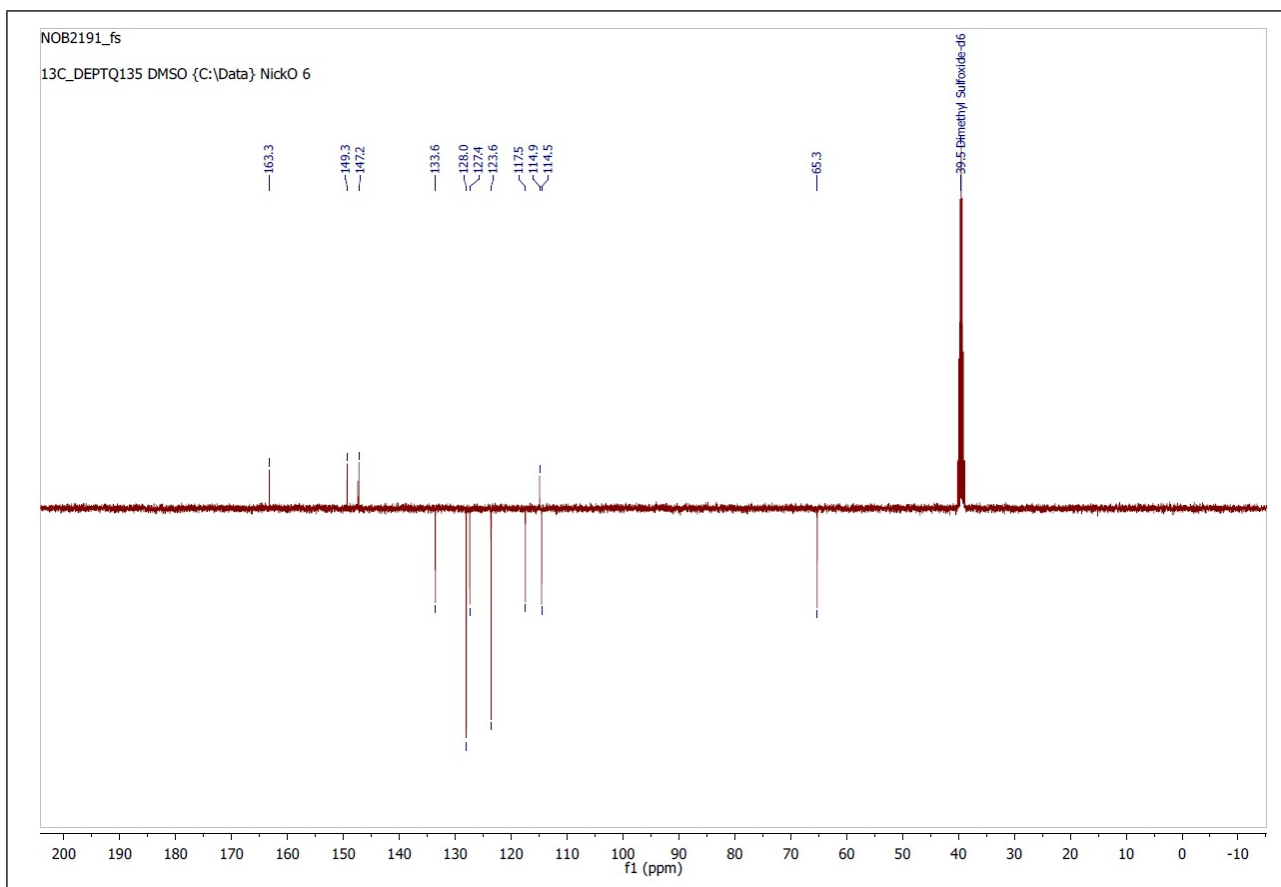
Mass: 424.6 mg

m.p. >197 °C (decomp)

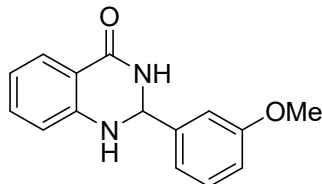
Yield: 91 %

Yellow solid





2-(3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (**29**)



Chemical Formula: $C_{15}H_{14}N_2O_2$

Exact Mass: 254.11

Molecular Weight: 254.28

IR (neat): ν_{\max} = 3288 (NH), 3053 (NH), 2916 (CH), 1645 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.29 (s, 1H), 7.61 (dd, J = 7.7, 1.5 Hz, 1H), 7.30 (t, J = 8.1 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.12 (s, 1H), 7.09 – 7.04 (m, 2H), 6.91 (ddd, J = 8.2, 2.5, 0.8 Hz, 1H), 6.78 – 6.74 (m, 1H), 6.70 – 6.64 (m, 1H), 5.72 (s, 1H), 3.75 (s, 3H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 164.0, 159.7, 148.3, 143.8, 133.8, 129.9, 127.8, 119.4, 117.6, 115.4, 114.90, 114.1, 113.0, 66.5, 55.6.

LRMS (ESI+): 255.1 (M+H, $C_{15}H_{15}N_2O_2$, 100%); LRMS (ESI-): 253.1 (M-H, $C_{15}H_{13}N_2O_2$, 100%).

Mass: 71.6 mg

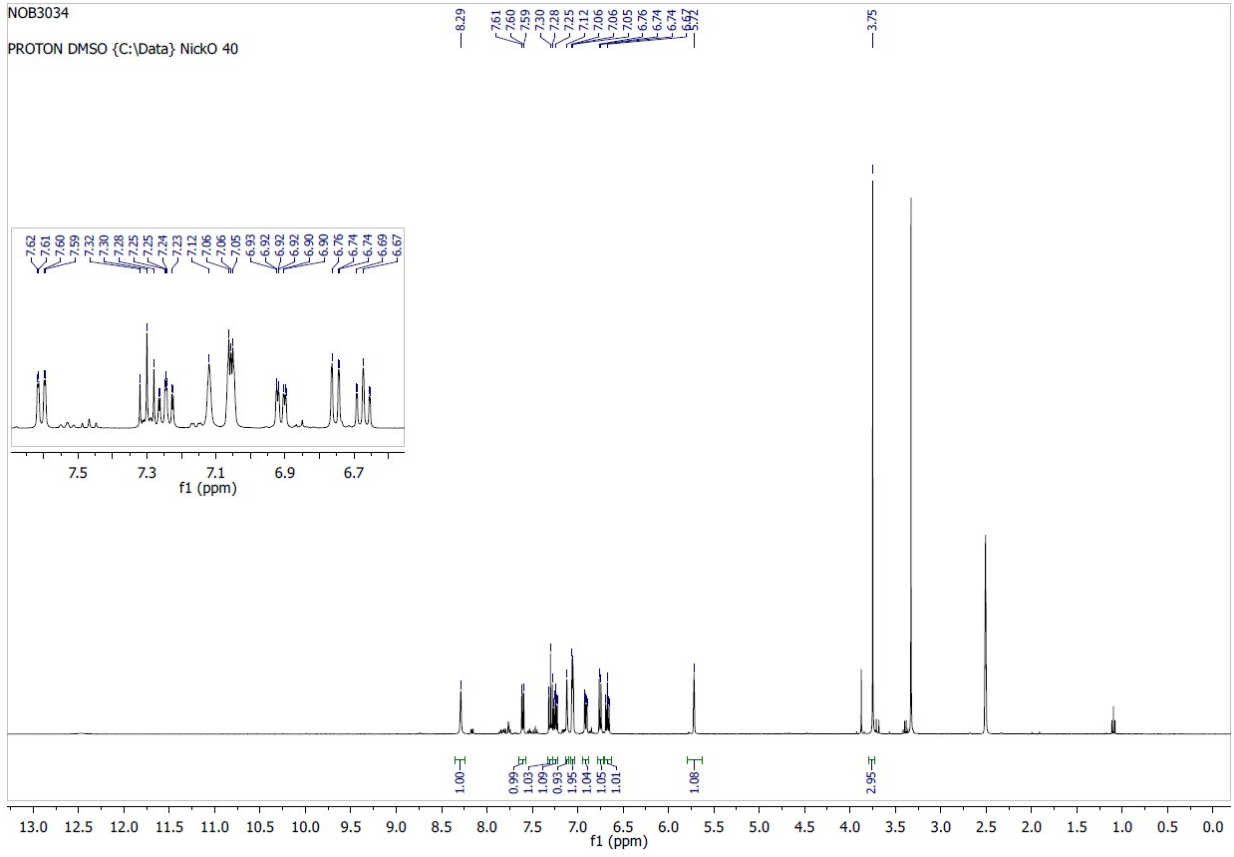
m.p. 139.7 – 146.5 °C

yield: 18 %

colour: off white solid

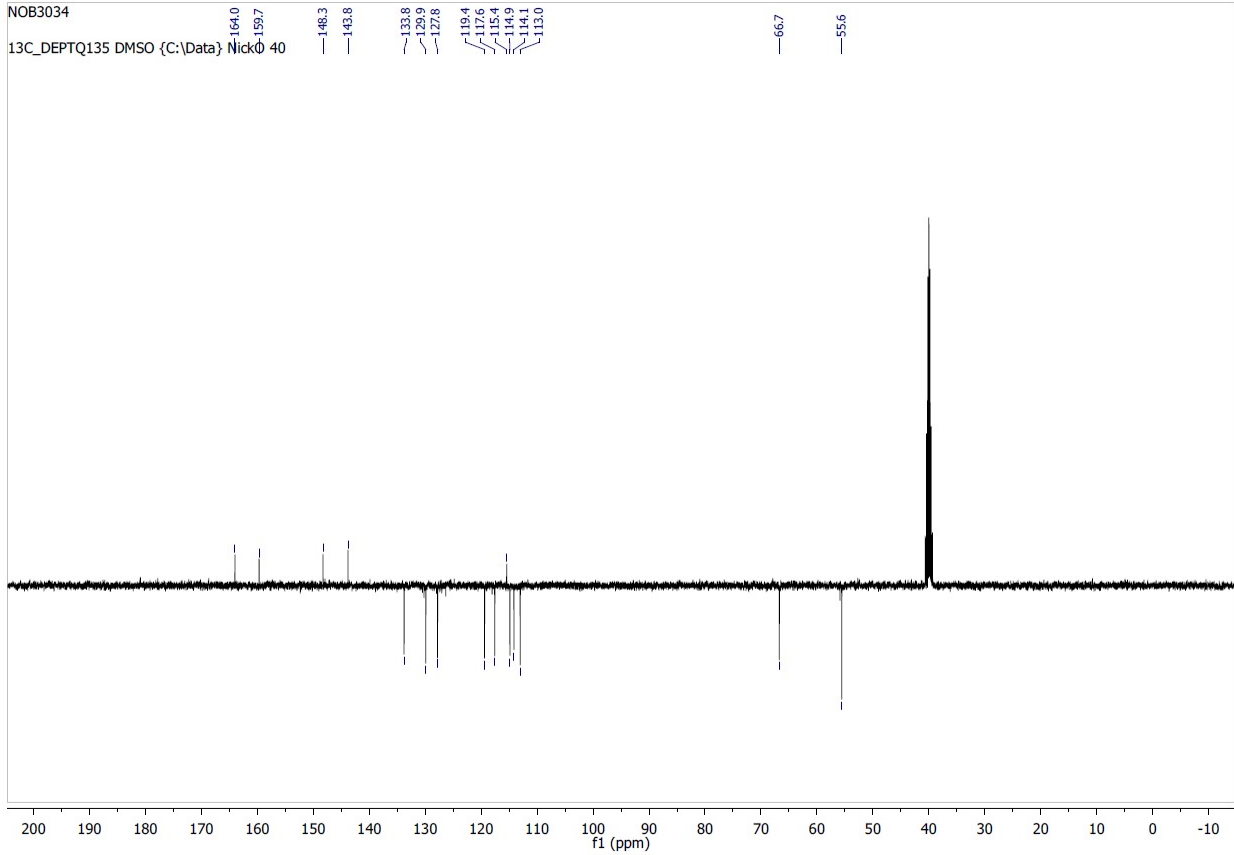
NOB3034

PROTON DMSO {C:\Data} NickO 40

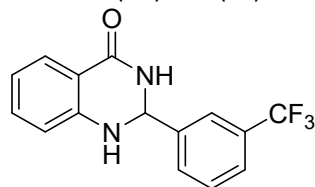


NOB3034

13C_DEPTQ135 DMSO {C:\Data} NickO 40



2-(3-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (**30**)



Chemical Formula: C₁₅H₁₁F₃N₂O

Exact Mass: 292.08

Molecular Weight: 292.26

IR (neat): ν_{\max} = 3275 (NH), 3211 (NH), 1645 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.42 (s, 1H), 7.85 (s, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.64 – 7.610 (m, 2H), 7.29 – 7.23 (m, 2H), 6.78 – 6.76 (m, 1H), 6.72 – 6.68 (m, 1H), 5.89 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.5, 147.6, 143.1, 133.5, 131.0, 129.5, 127.4, 125.20, 125.16, 123.64, 123.60, 117.4, 114.9, 114.5, 65.7.

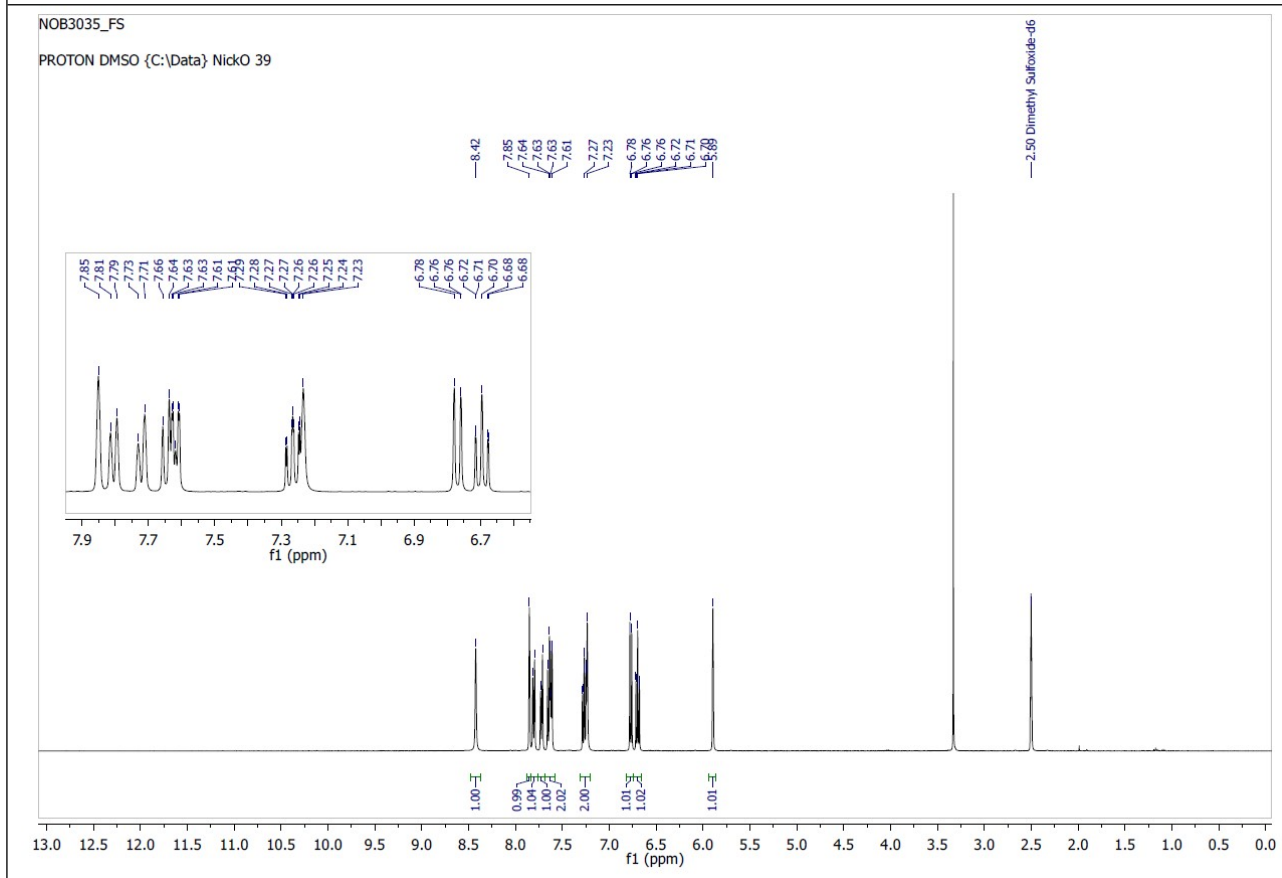
LRMS (ESI+): 293.1 (M+H, C₁₅H₁₂F₃N₂O, 100%); LRMS (ESI-): 291.1 (M-H, C₁₅H₁₀F₃N₂O, 100%).

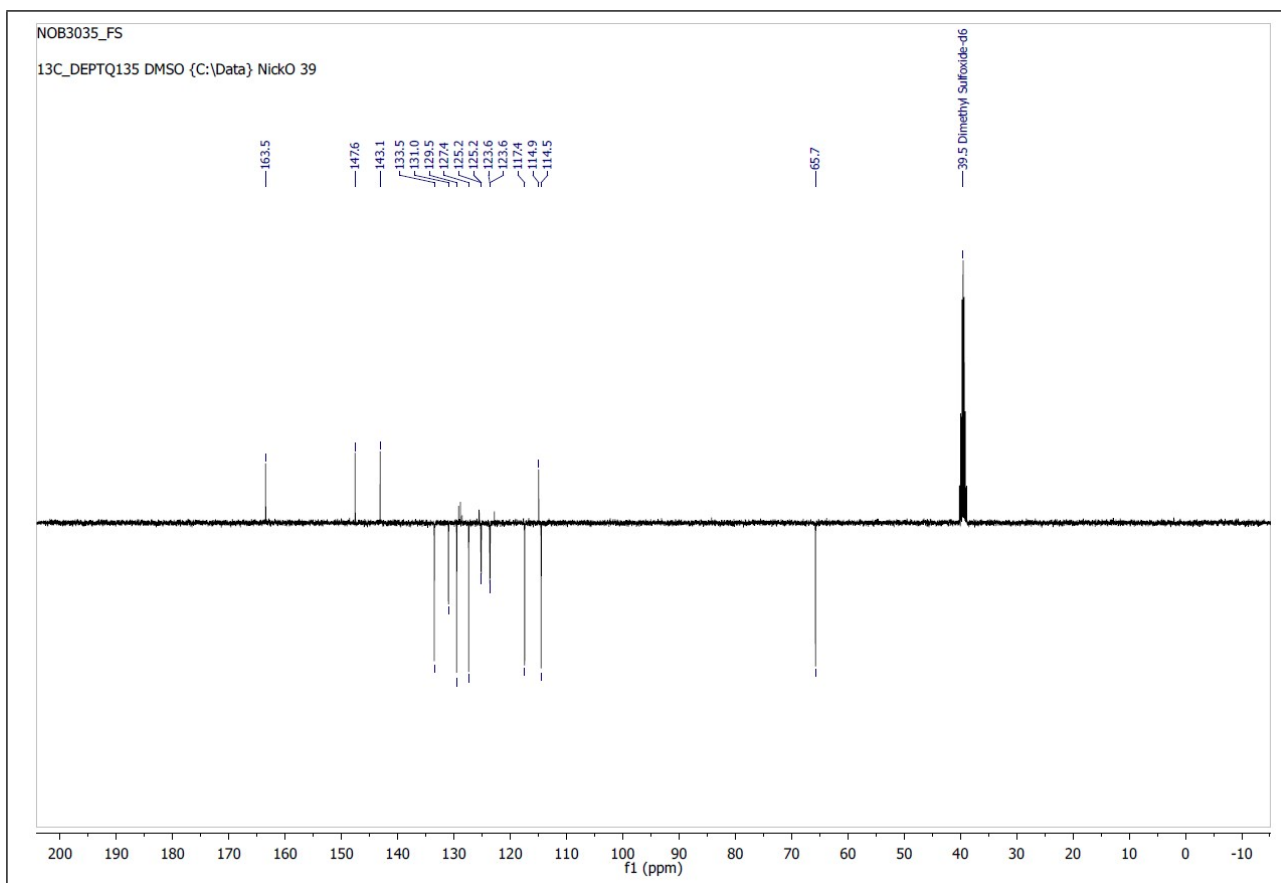
Mass: 138.3

m.p. 137 – 141 °C

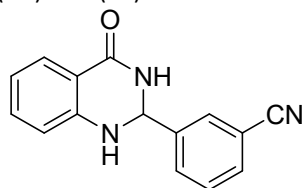
yield: 29 %

colour white solid





2-(3-Cyanophenyl)-2,3-dihydroquinazolin-4(1H)-one (**31**)



Chemical Formula: C₁₅H₁₁N₃O

Exact Mass: 249.09

Molecular Weight: 249.27

IR (neat): ν_{\max} = 3372 (NH), 3178 (NH), 2232 (CN), 1659 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO) δ 8.42 (s, 1H), 7.91 (s, 1H), 7.85 – 7.82 (m, 2H), 7.62 (ddd, J = 7.8, 4.6, 3.3 Hz, 2H), 7.33 – 7.20 (m, 2H), 6.77 (d, J = 8.0 Hz, 1H), 6.73 – 6.68 (m, 1H), 5.85 (s, 1H).

¹³C NMR (100 MHz, DMSO) δ 163.4, 147.5, 143.3, 133.5, 132.2, 131.7, 130.6, 129.7, 127.4, 118.7, 117.5, 115.0, 114.6, 111.2, 65.5.

LRMS (ESI⁺): 250.1 (M+H, C₁₅H₁₂N₃O, 100%); LRMS (ESI⁻): 248.1 (M-H, C₁₅H₁₀N₃O, 100%).

Mass 308.2 mg

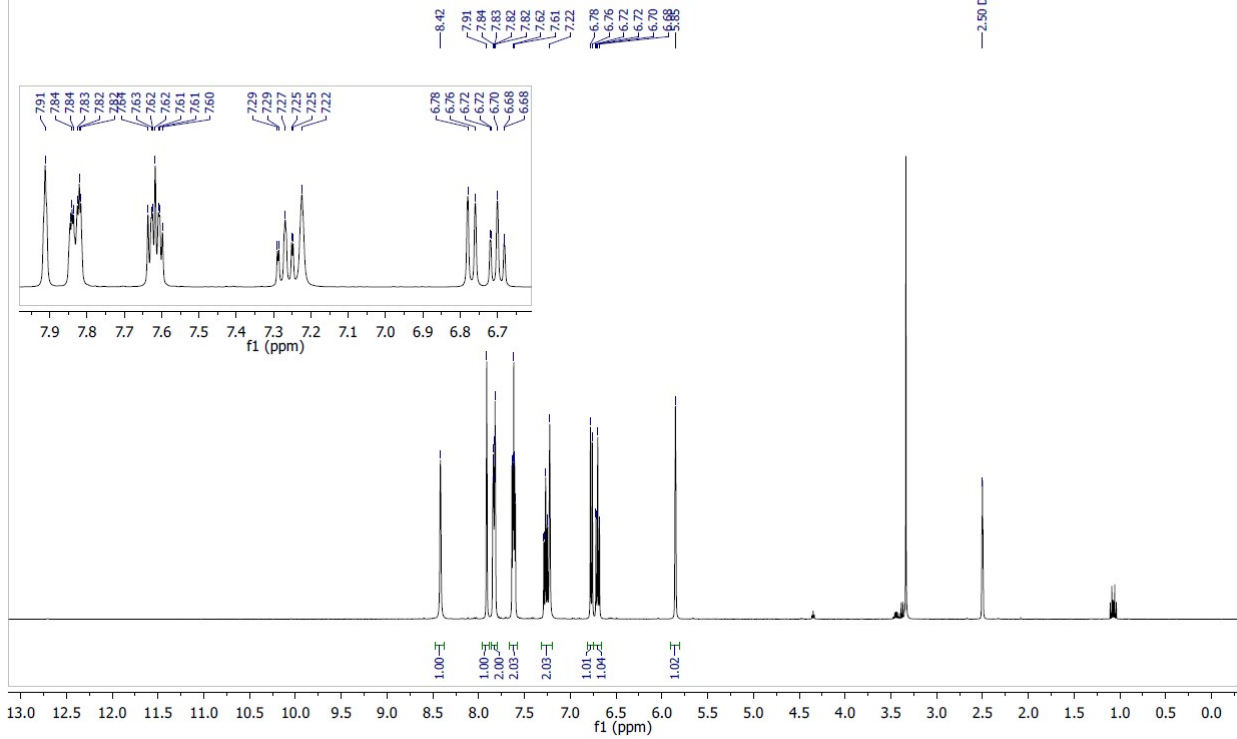
m.p. 224 – 230 °C

yield: 72 %

colour white solid

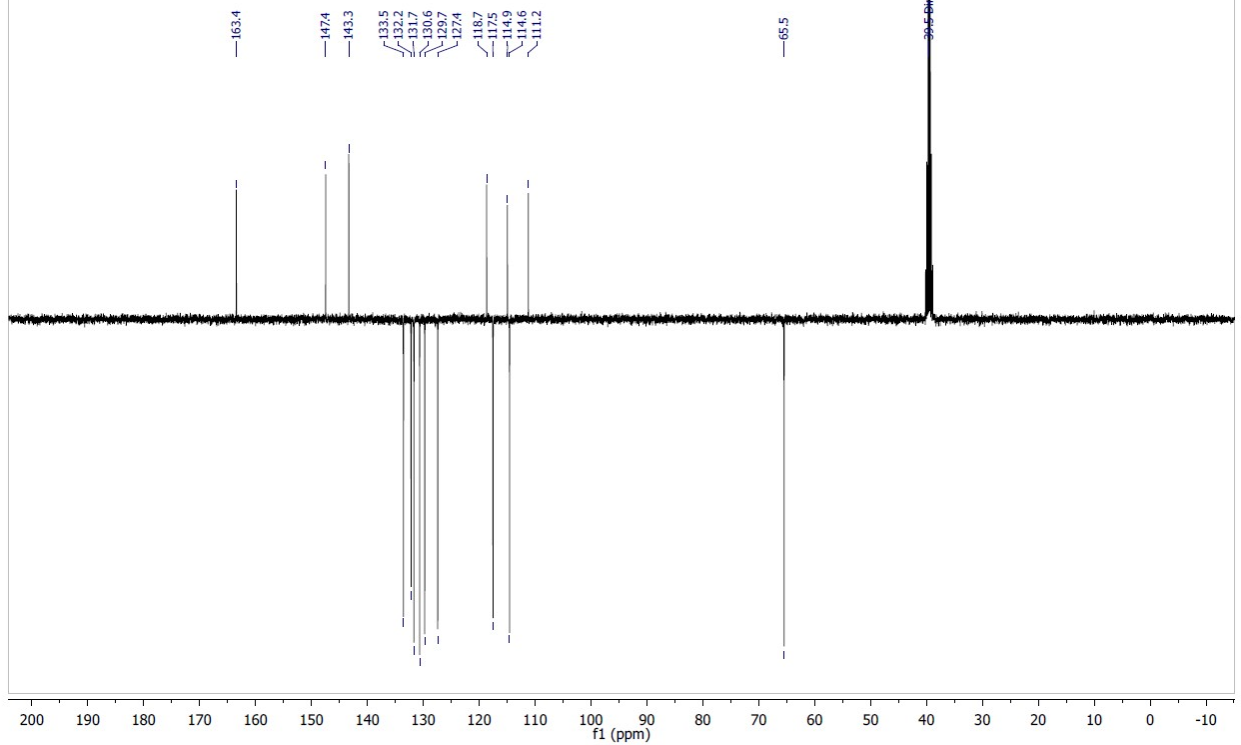
NOB4040_FS

PROTON DMSO {C:\Data} NickO 12

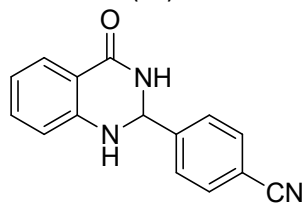


NOB4040_FS

13C_DEPTQ135 DMSO {C:\Data} NickO 12



4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzotrile (32)



Chemical Formula: C₁₅H₁₁N₃O

Exact Mass: 249.09

Molecular Weight: 249.27

IR (neat): ν_{\max} = 3346 (NH), 2227 (CN), 1664 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.47 (s, 1H), 7.90 – 7.84 (m, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.61 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.31 – 7.22 (m, 2H), 6.76 (d, *J* = 8.1 Hz, 1H), 6.71 – 6.65 (m, 1H), 5.85 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.8, 147.81, 147.79, 134.0, 132.9, 128.1, 127.9, 119.1, 117.9, 115.4, 115.0, 111.5, 66.0.

LRMS (ESI+): 250.1 (M+H, C₁₅H₁₂N₃O, 100%); LRMS (ESI-): 248.1 (M-H, C₁₅H₁₀N₃O, 100%).

Mass 346.7 mg

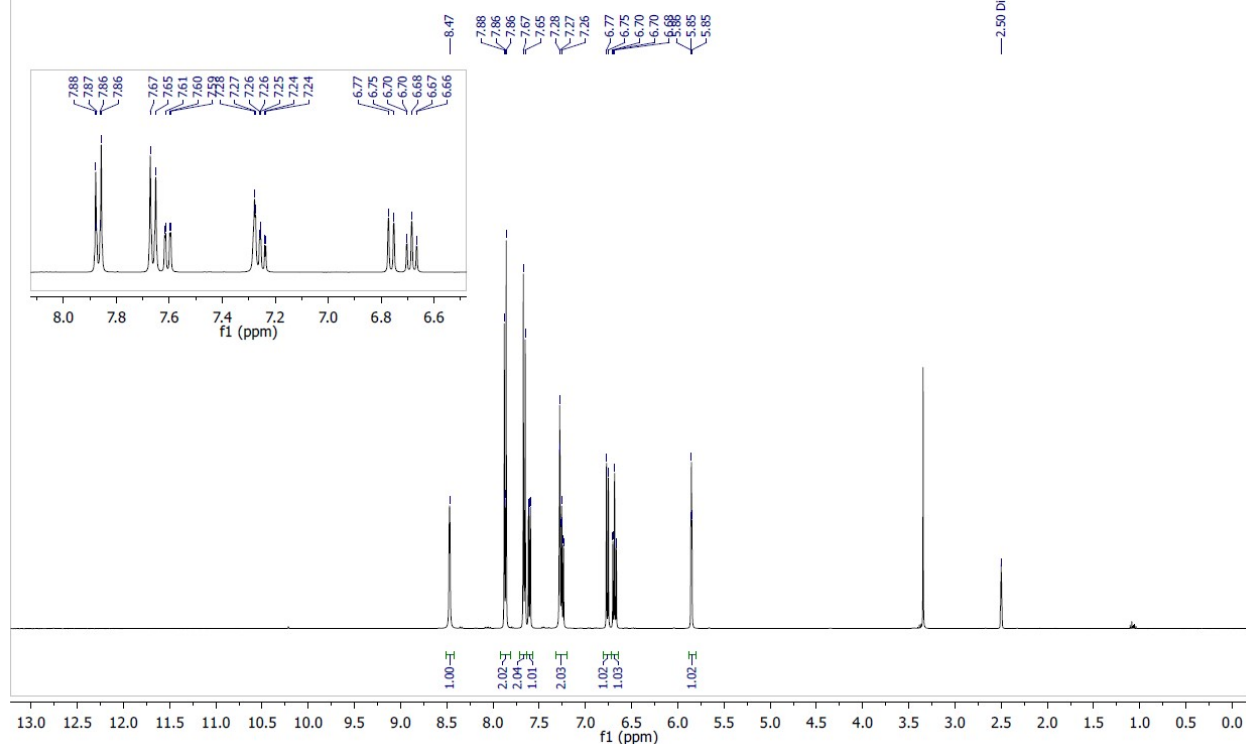
m.p. 240 – 247 °C

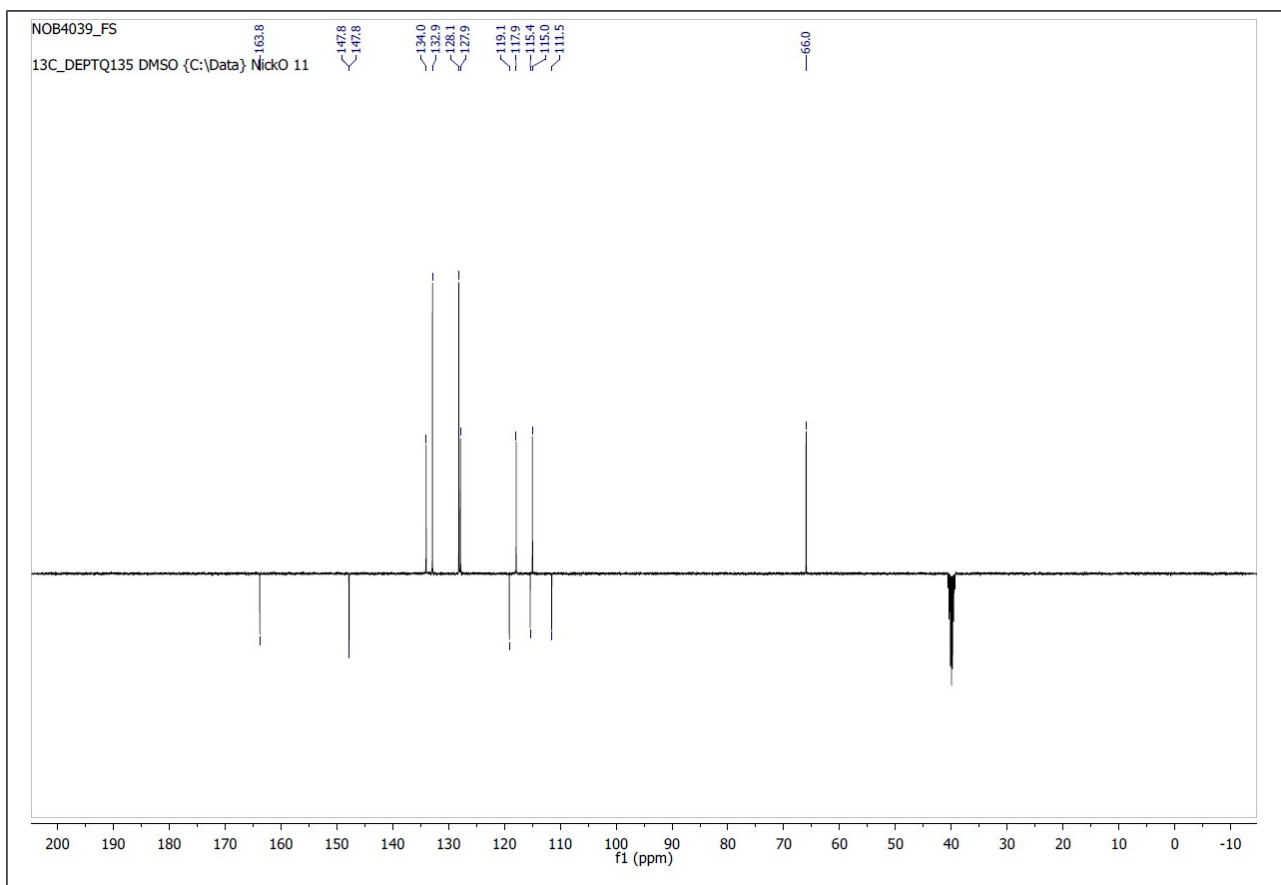
yield 86 %

colour white solid

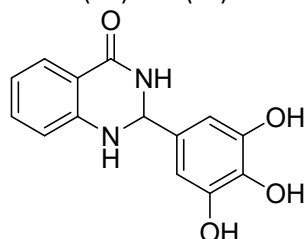
NOB4039_FS

PROTON DMSO {C:\Data} NickO 11





2-(3,4,5-trihydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (**33**)



Chemical Formula: $C_{14}H_{12}N_2O_4$

Exact Mass: 272.08

Molecular Weight: 272.26

IR (neat): ν_{\max} = 3448 (NH), 3308 (OH), 1639 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.93 (s, 2H), 8.02 (d, J = 1.8 Hz, 1H), 7.60 (dd, J = 7.8, 1.4 Hz, 1H), 7.22 (ddd, J = 8.2, 7.2, 1.6 Hz, 1H), 6.75 – 6.69 (m, 1H), 6.69 – 6.60 (m, 1H), 6.41 (s, 2H), 5.47 (d, J = 1.9 Hz, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 164.1, 148.4, 146.2 (2C), 133.7, 132.1, 127.8, 117.3, 115.2, 114.7, 106.2 (2C), 67.2.

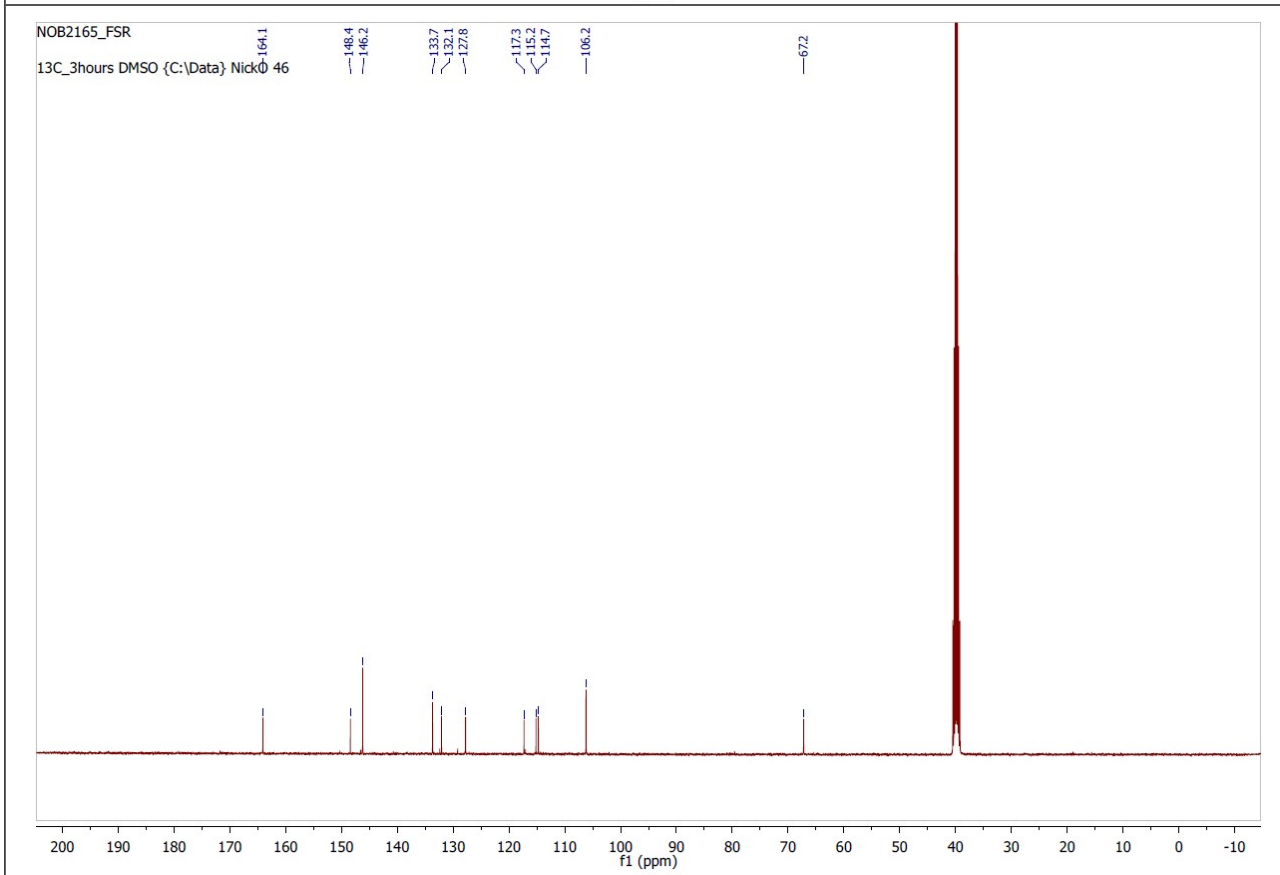
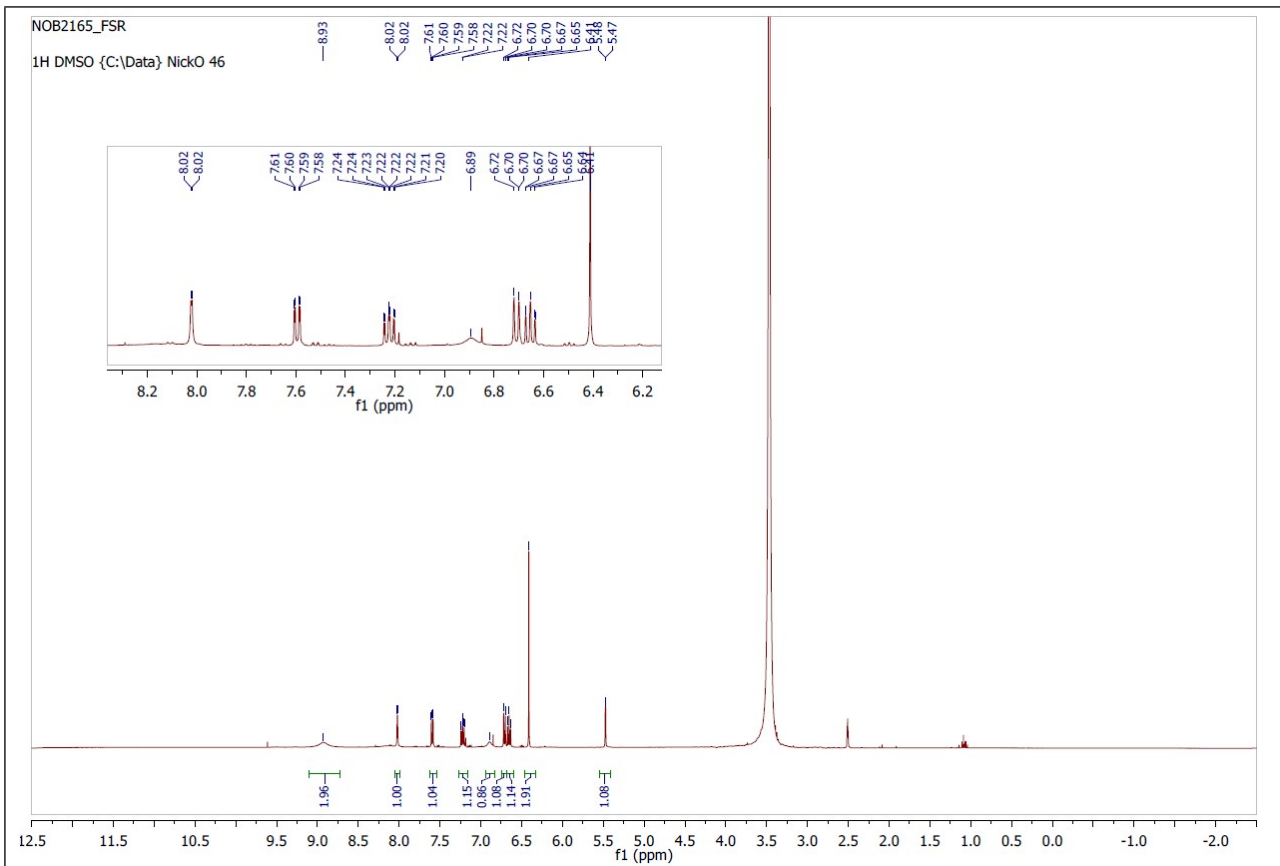
LRMS (ESI+): 273.1 (M+H, $C_{14}H_{13}N_2O_4$, 70%); (ESI-): 271.1 (M-H, $C_{14}H_{12}N_2O_4$, 100%), 269.1 (M-2H, $C_{14}H_{11}N_2O_4$, 70%)

Mass: 193.3 mg

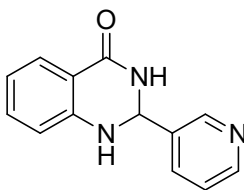
m.p. >164 °C

Yield: 40 %

Amorphous Red solid



2-(pyridin-3-yl)-2,3-dihydroquinazolin-4(1H)-one (**34**)



Chemical Formula: C₁₃H₁₁N₃O

Exact Mass: 225.09

Molecular Weight: 225.25

IR (neat): ν_{\max} = 3256 (NH), 2978 (CH), 1652 (C=O)

¹H NMR (400 MHz, DMSO-d₆) δ 8.67 (d, J = 2.1 Hz, 1H), 8.56 (dd, J = 4.8, 1.6 Hz, 1H), 8.38 (s, 1H), 7.90 (dt, J = 7.9, 1.9 Hz, 1H), 7.63 (dd, J = 7.7, 1.5 Hz, 1H), 7.43 (ddd, J = 7.9, 4.8, 0.5 Hz, 1H), 7.27 (ddd, J = 8.2, 7.3, 1.6 Hz, 1H), 7.17 (s, 1H), 6.73 (ddd, J = 15.0, 8.1, 4.3 Hz, 2H), 5.86 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) 164.0, 150.1, 148.8, 148.2, 137.3, 135.1, 133.9, 127.9, 124.0, 118.0, 115.5, 115.0, 65.1.

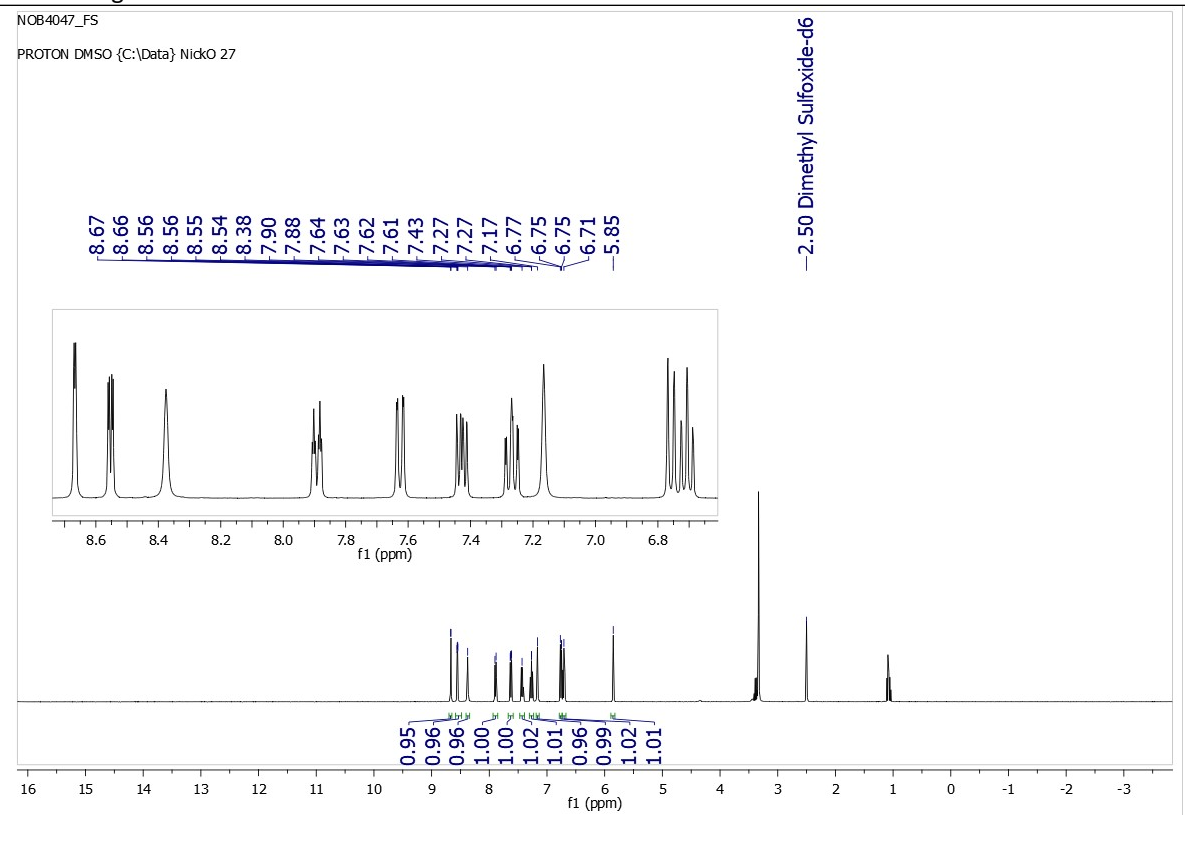
LRMS (ESI+) 226.1 (C₁₃H₁₂N₃O, 100%); LRMS (ESI-) 224.1 (C₁₃H₁₀N₃O, 100%).

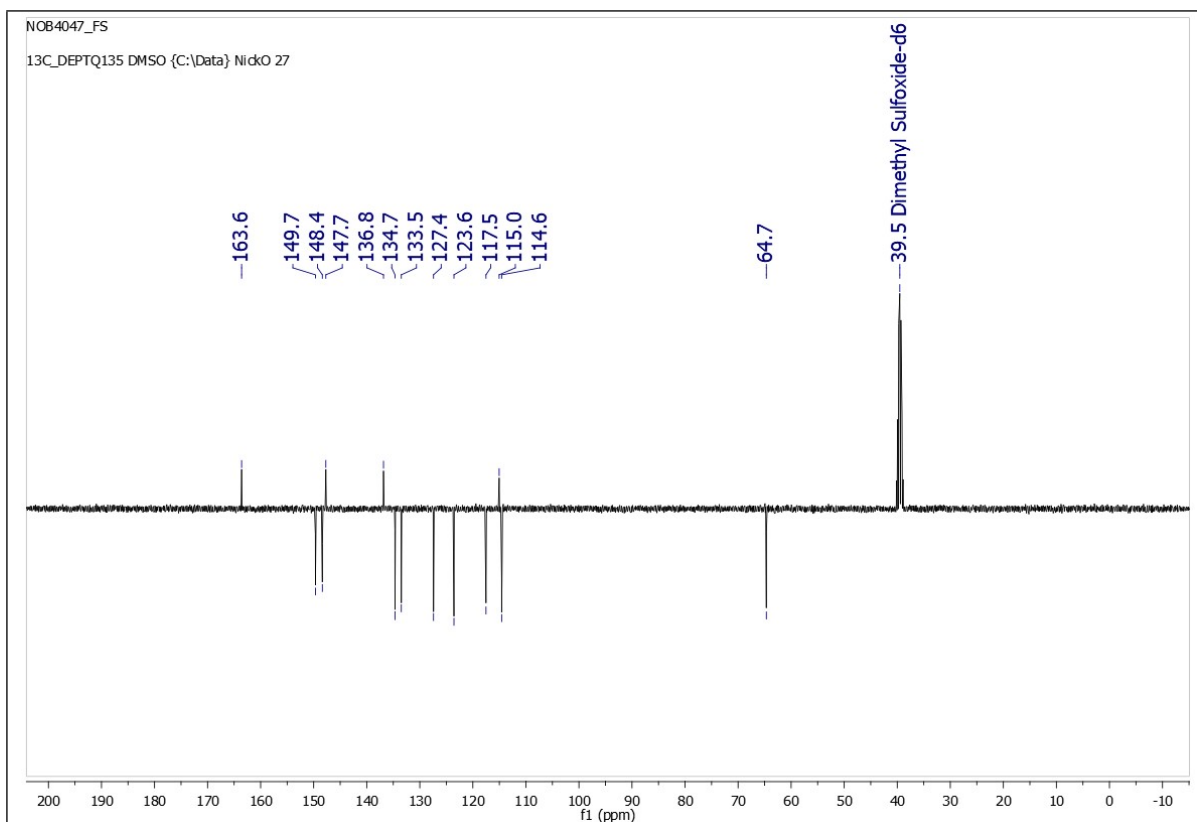
Mass: 298 mg

m.p. >250 °C

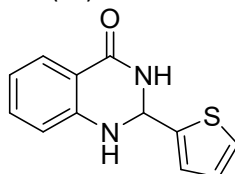
Yield: 84 %

Pale orange solid





2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (**35**)



Chemical Formula: C₁₂H₁₀N₂OS

Exact Mass: 230.05

Molecular Weight: 230.29

IR (neat): ν_{\max} = 3295 (NH), 3172 (NH), 1649 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.44 (s, 1H), 7.62 (dd, J = 7.7, 1.3 Hz, 1H), 7.45 (dd, J = 5.0, 1.2 Hz, 1H), 7.26 – 7.24 (m, 2H), 7.12 (d, J = 3.0 Hz, 1H), 6.98 (dd, J = 5.0, 3.5 Hz, 1H), 6.76 (d, J = 7.8 Hz, 1H), 6.70 (t, 1H), 6.02 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.1, 147.2, 146.4, 133.4, 127.3, 126.5, 125.9, 125.7, 117.5, 115.1, 114.7, 62.6.

LRMS (ESI⁺): 231.1 (M+H, C₁₂H₁₁N₂OS, 100%); **LRMS** (ESI⁻): 229.1 (M-H, C₁₂H₁₁N₂OS, 100%).

Mass 309.3

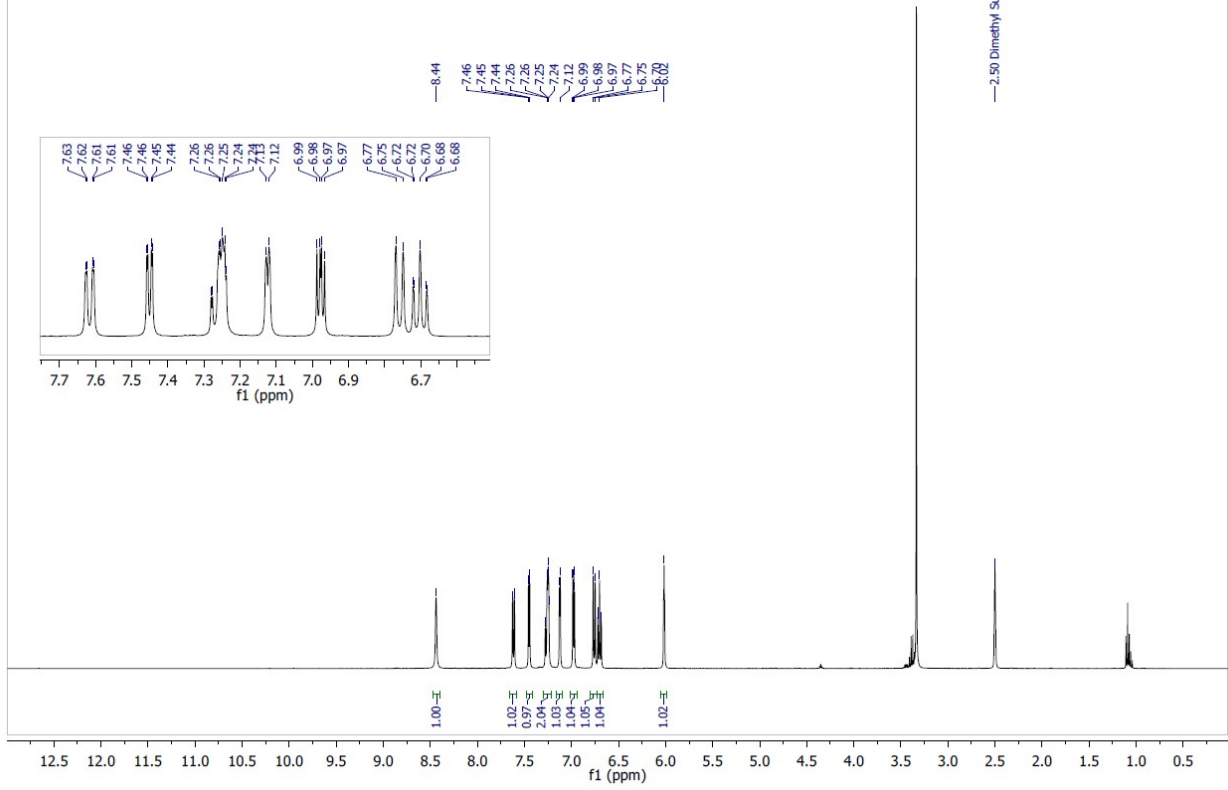
m.p. 206 – 207 °C

yield 80 %

colour white solid

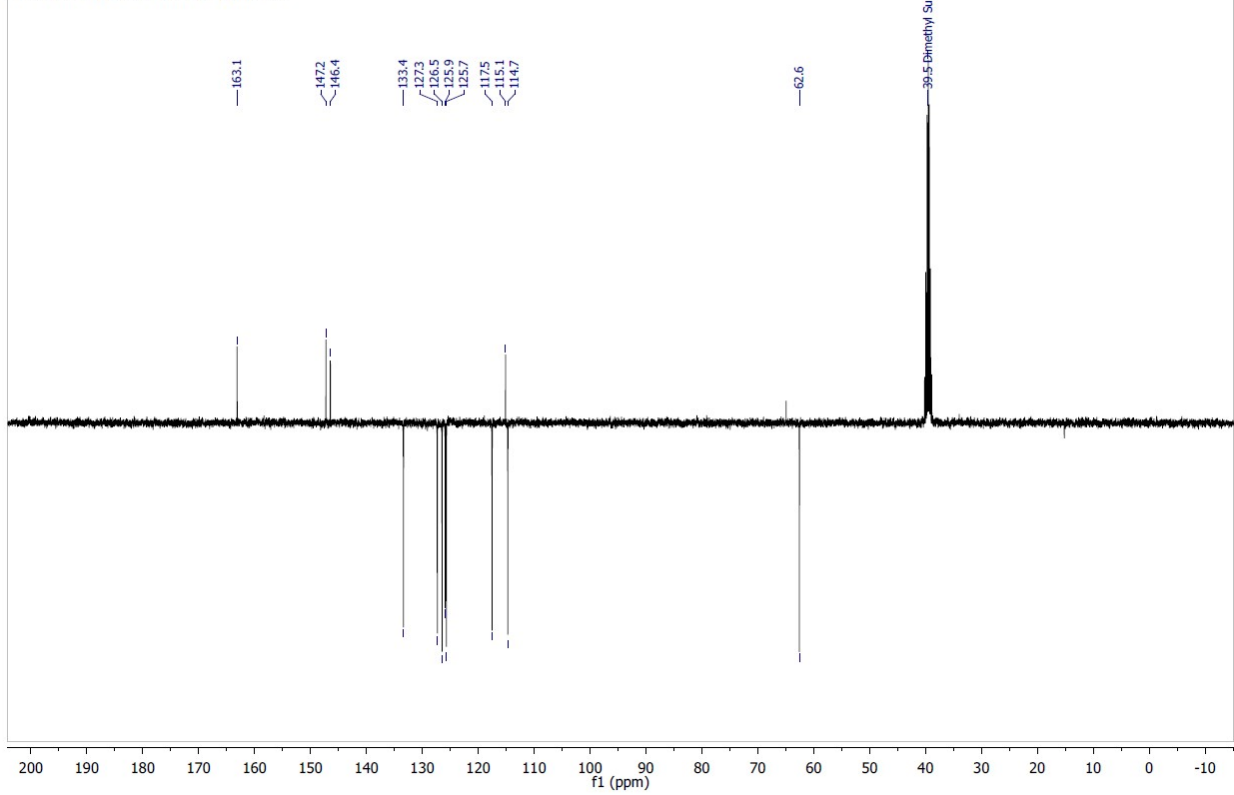
NOB4045_FS

PROTON DMSO {C:\Data} NickO 25

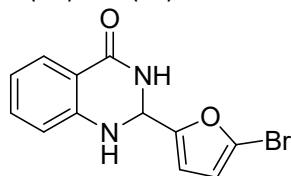


NOB4045_FS

13C_DEPTQ135 DMSO {C:\Data} NickO 25



2-(5-bromofuran-2-yl)-2,3-dihydroquinazolin-4(1H)-one (36)



Chemical Formula: $C_{12}H_9BrN_2O_2$

Exact Mass: 291.98

Molecular Weight: 293.12

IR neat): ν_{\max} = 3270 (NH), 3165 (NH), 1651 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.44 (s, 1H), 7.61 (s, 1H), 7.27 (s, 2H), 6.73 (d, J = 30.9 Hz, 2H), 6.56 – 6.21 (m, 2H), 5.75 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.1, 156.6, 146.9, 133.4, 127.3, 121.0, 117.5, 114.9, 114.6, 112.3, 110.2, 60.0.

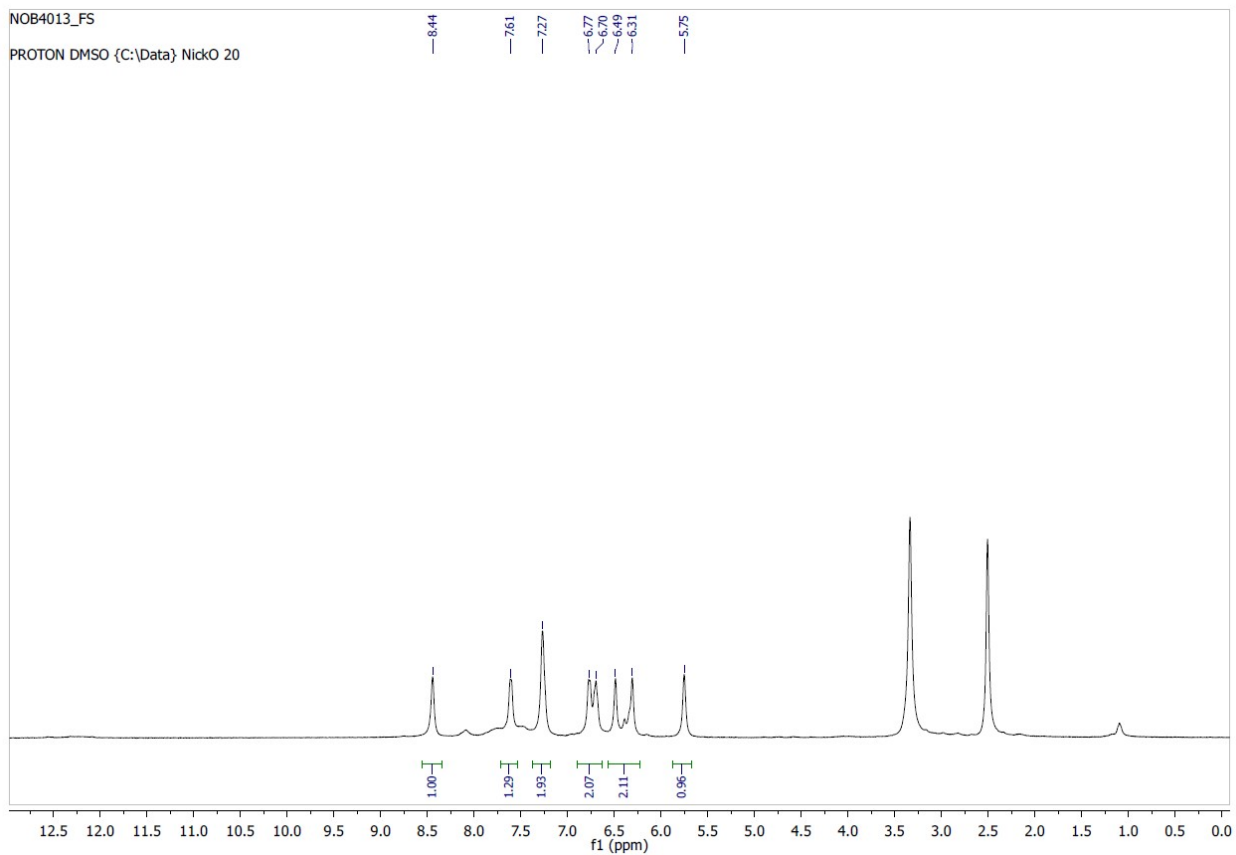
LRMS (ESI+): 293.1 (M+H, $C_{12}H_{10}^{79}BrN_2O_2$, 100%), 295.1 (M+H, $C_{12}H_{10}^{81}BrN_2O_2$, 100%); LRMS (ESI-): 291.1 (M-H, $C_{12}H_8^{79}BrN_2O_2$, 100%), 293.1 (M-H, $C_{12}H_8^{81}BrN_2O_2$, 100%).

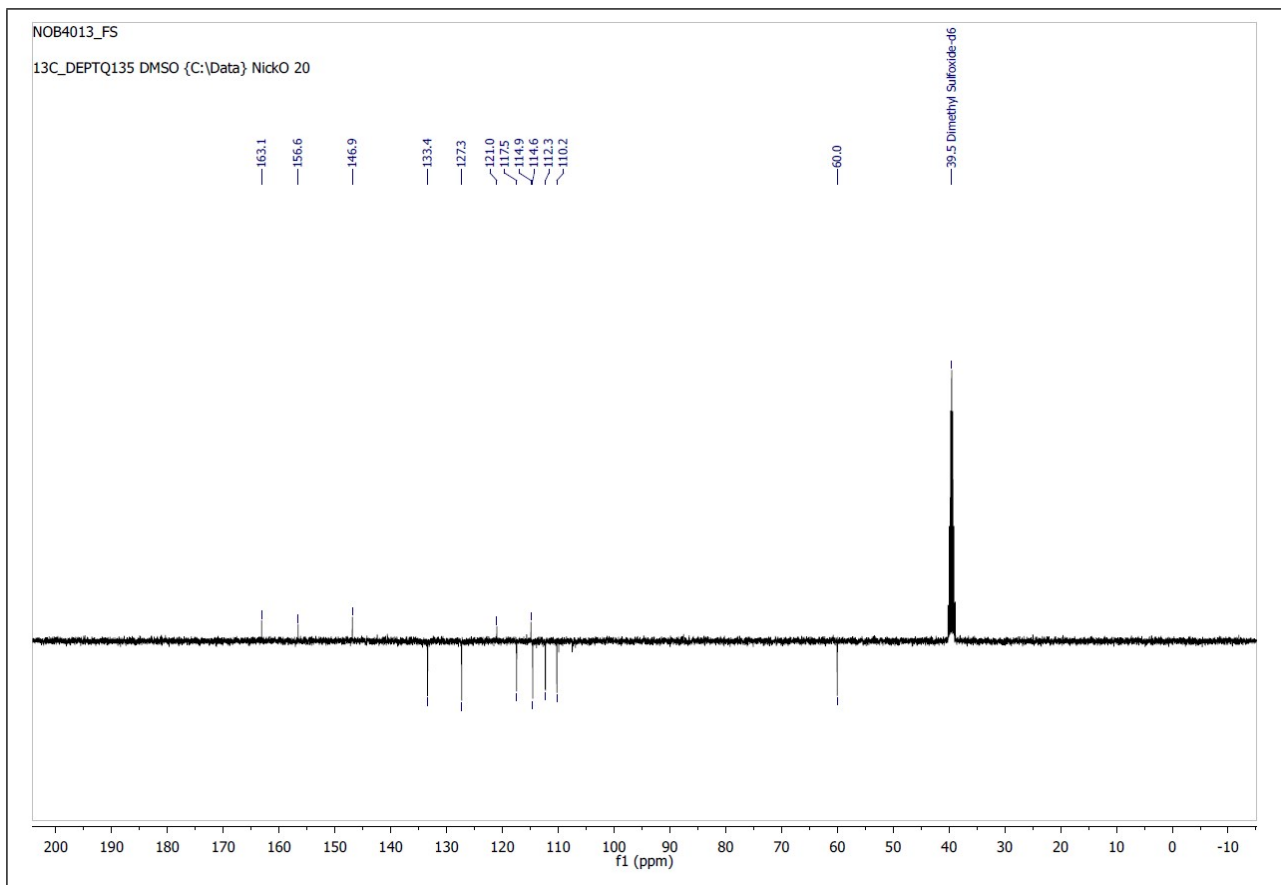
Mass 123 mg

m.p. >150 °C (dec.)

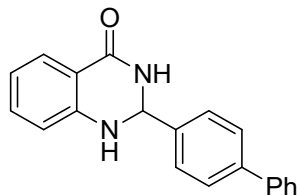
yield 26 %

colour off white solid





2-([1,1'-biphenyl]-4-yl)-2,3-dihydroquinazolin-4(1H)-one (**37**)



Chemical Formula: C₂₀H₁₆N₂O

Exact Mass: 300.13

Molecular Weight: 300.35

IR (neat): ν_{\max} = 3295 (NH), 3178 (NH), 2971 (CH), 1652 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.35 (s, 1H), 7.70 – 7.67 (m, 5H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 10.4, 4.8 Hz, 2H), 7.39 – 7.37 (m, 1H), 7.26 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.17 (s, 1H), 6.77 (d, *J* = 7.8 Hz, 1H), 6.71 – 6.67 (m, 1H), 5.81 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.6, 147.8, 140.9, 140.3, 139.7, 133.4, 129.0 (2C), 127.5 (2C), 127.4, 126.7 (2C), 126.65 (2C), 117.2, 115.0, 114.4, 66.2. Quaternary carbon not observed.

LRMS (ESI⁺): 301.2 (M+H, C₂₀H₁₇N₂O, 100%); LRMS (ESI⁻): 299.1 (M-H, C₂₀H₁₅N₂O, 100%).

Mass 372.1 mg

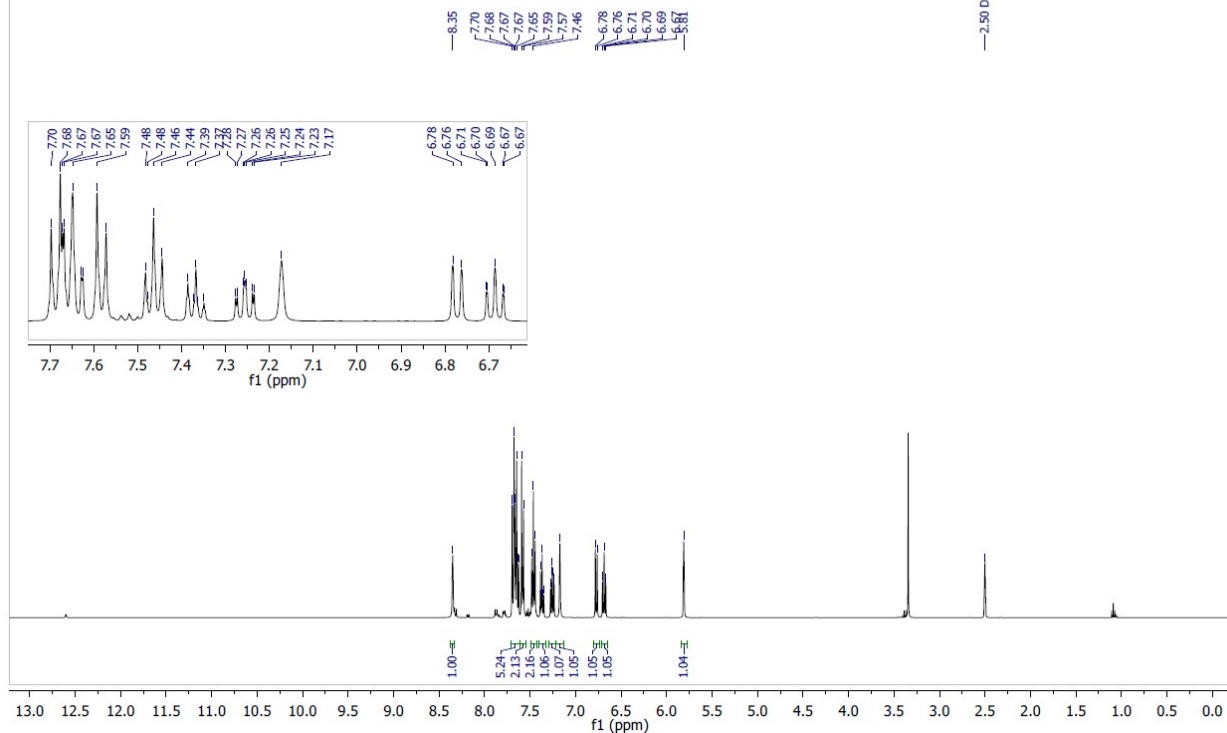
m.p. 217 – 221 °C

yield 74 %

colour white solid

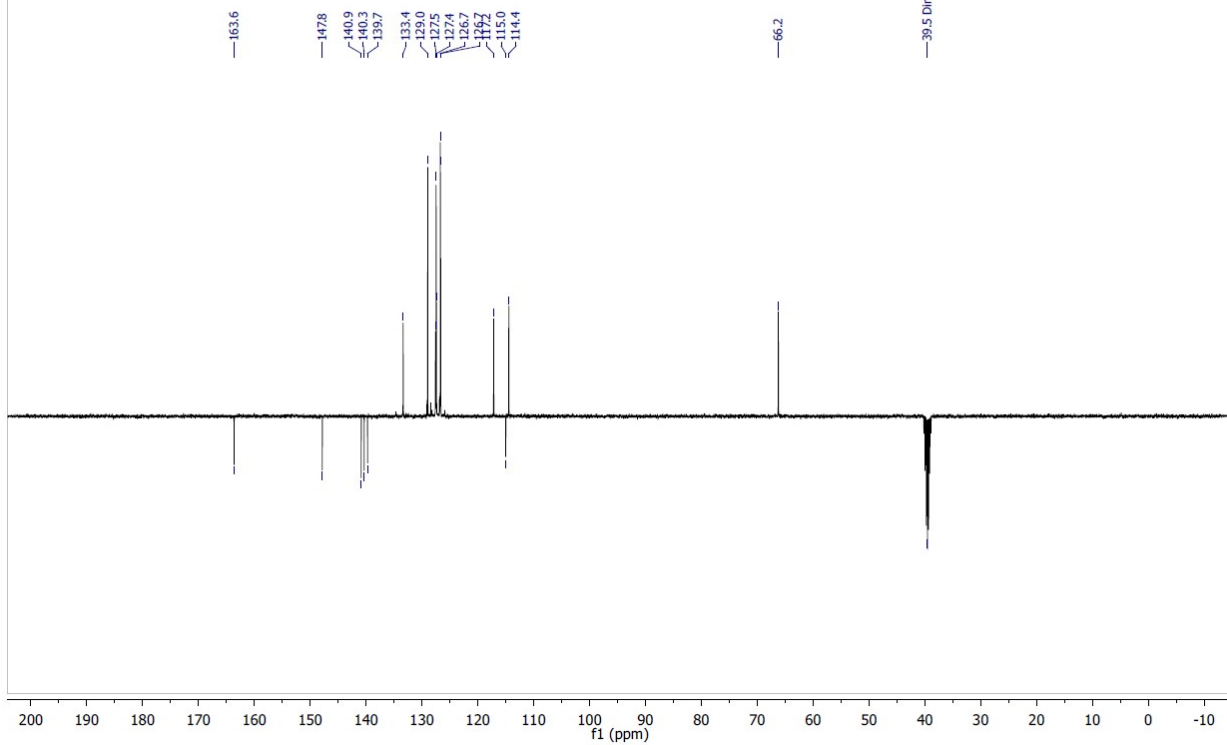
NOB4048_FS

PROTON DMSO (C:\Data) NickO 28

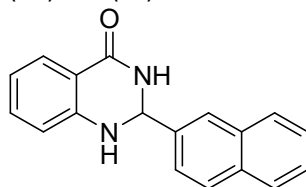


NOB4048_FS

13C_DEPTQ135 DMSO (C:\Data) NickO 28



2-(naphthalen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (38)



Chemical Formula: C₁₈H₁₄N₂O

Exact Mass: 274.11

Molecular Weight: 274.32

IR (neat): ν_{\max} = 3275 (NH), 8978 (CH), 1646 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.37 (s, 1H), 7.96 – 7.90 (m, 4H), 7.70 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.64 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.53 (dd, *J* = 6.2, 3.3 Hz, 2H), 7.25 (ddd, *J* = 8.3, 7.3, 1.6 Hz, 1H), 7.19 (s, 1H), 6.77 (d, *J* = 7.7 Hz, 1H), 6.71 – 6.67 (m, 1H), 5.94 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.6, 147.9, 138.9, 133.4, 133.0, 132.5, 128.1, 128.0, 127.6, 127.4, 126.43, 126.38, 125.9, 124.8, 117.2, 114.9, 114.4, 66.8.

LRMS (ESI+): 275.1 (M+H, C₁₈H₁₅N₂O, 100%); LRMS (ESI-): 273.1 (M-H, C₁₈H₁₃N₂O, 100%).

Mass: 374.3 mg

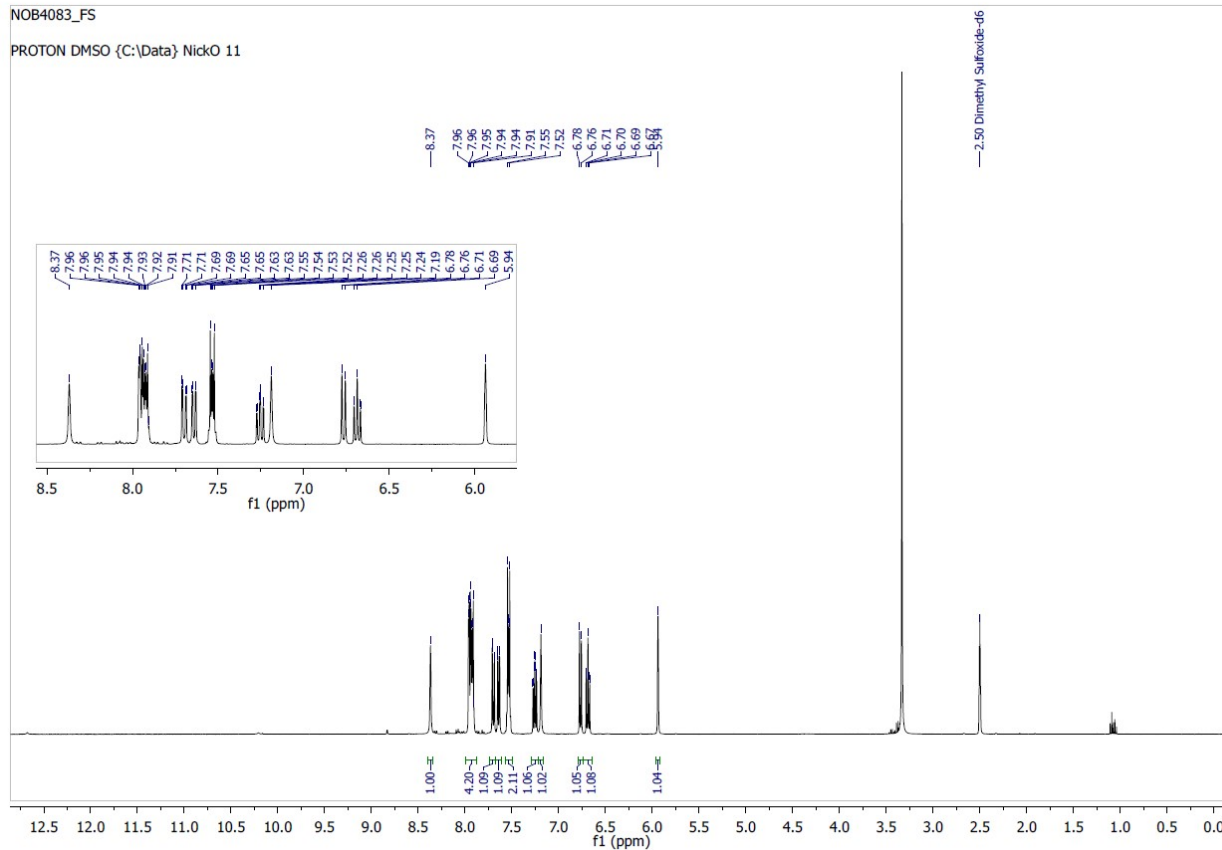
m.p. 202 – 206 °C

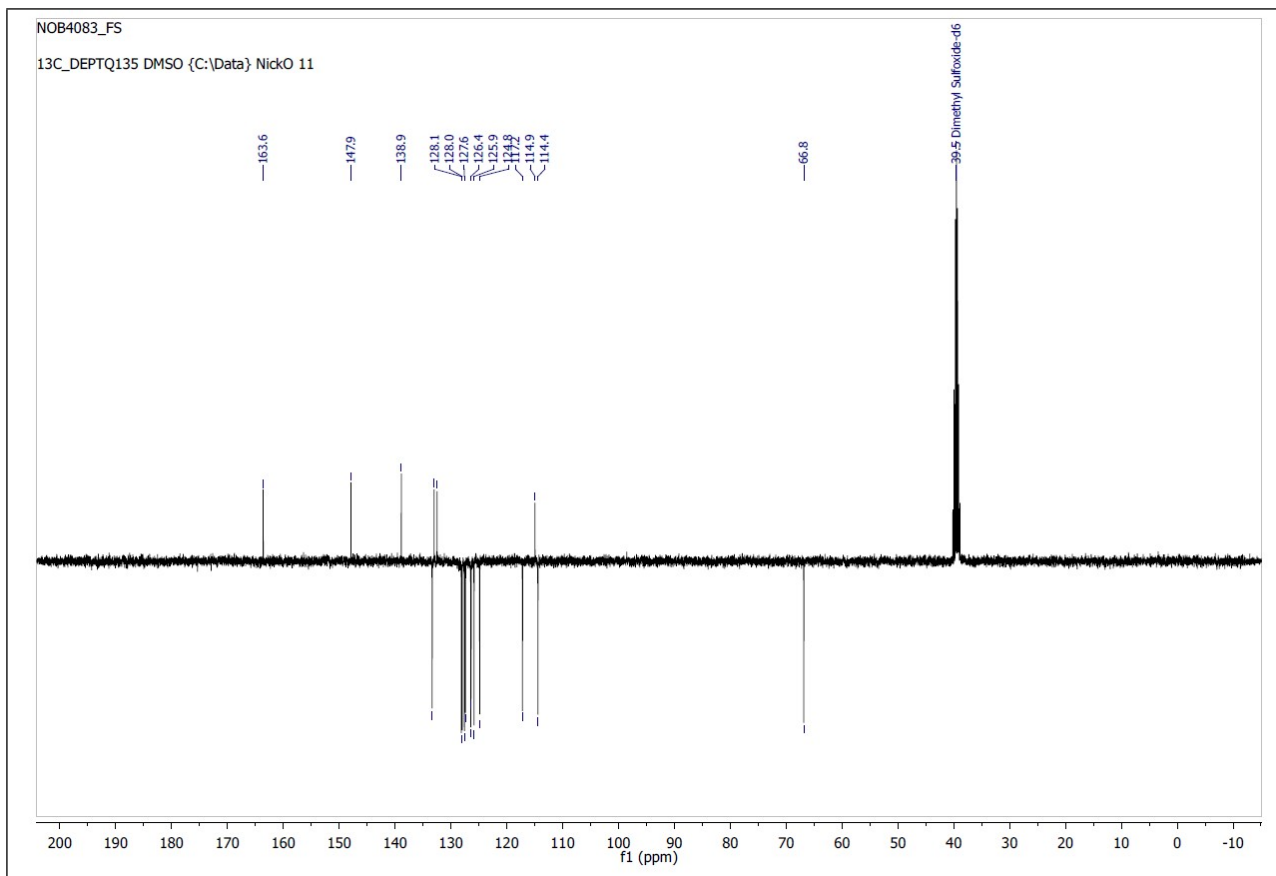
yield: 87 %

colour: white solid

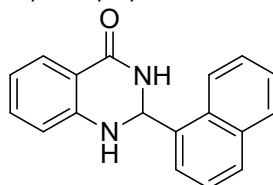
NOB4083_FS

PROTON DMSO {C:\Data} NickO 11





2-(naphthalen-1-yl)-2,3-dihydroquinazolin-4(1H)-one (**39**)



Chemical Formula: C₁₈H₁₄N₂O

Exact Mass: 274.11

Molecular Weight: 274.32

IR (neat): ν_{\max} = 3359, 3217 (NH), 3004, 1649 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.57 – 8.54 (m, 1H), 8.27 (s, 1H), 8.01 – 7.96 (m, 2H), 7.72 – 7.69 (m, 2H), 7.59 – 7.51 (m, 3H), 7.28 – 7.24 (m, 1H), 7.08 (s, 1H), 6.76 – 6.71 (m, 2H), 6.49 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 164.5, 148.9, 135.6, 134.2, 133.7, 131.0, 129.8, 129.1, 128.0, 126.51, 126.50, 126.3, 125.7, 125.1, 117.7, 115.4, 115.0, 66.4.

LRMS (ESI+) 275.2 (M+H, C₁₈H₁₅N₂O, 100%).

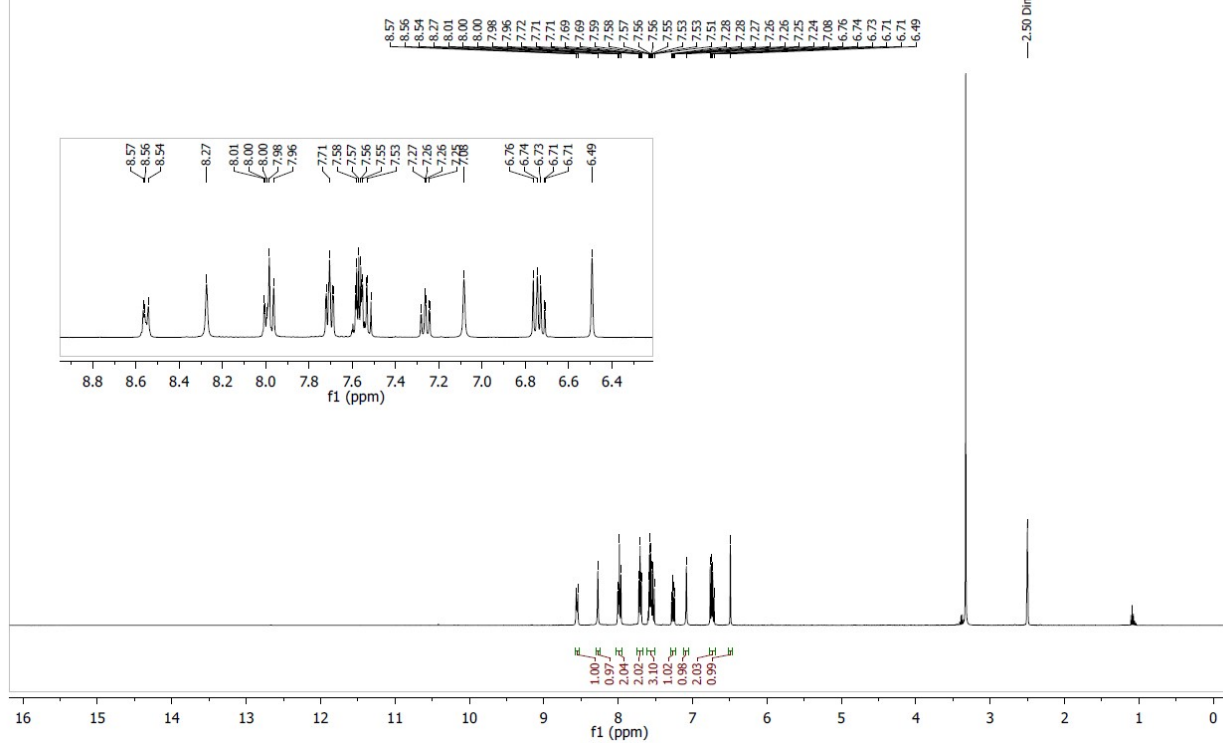
Mass: 129.9 mg

m.p. 182 – 186 °C

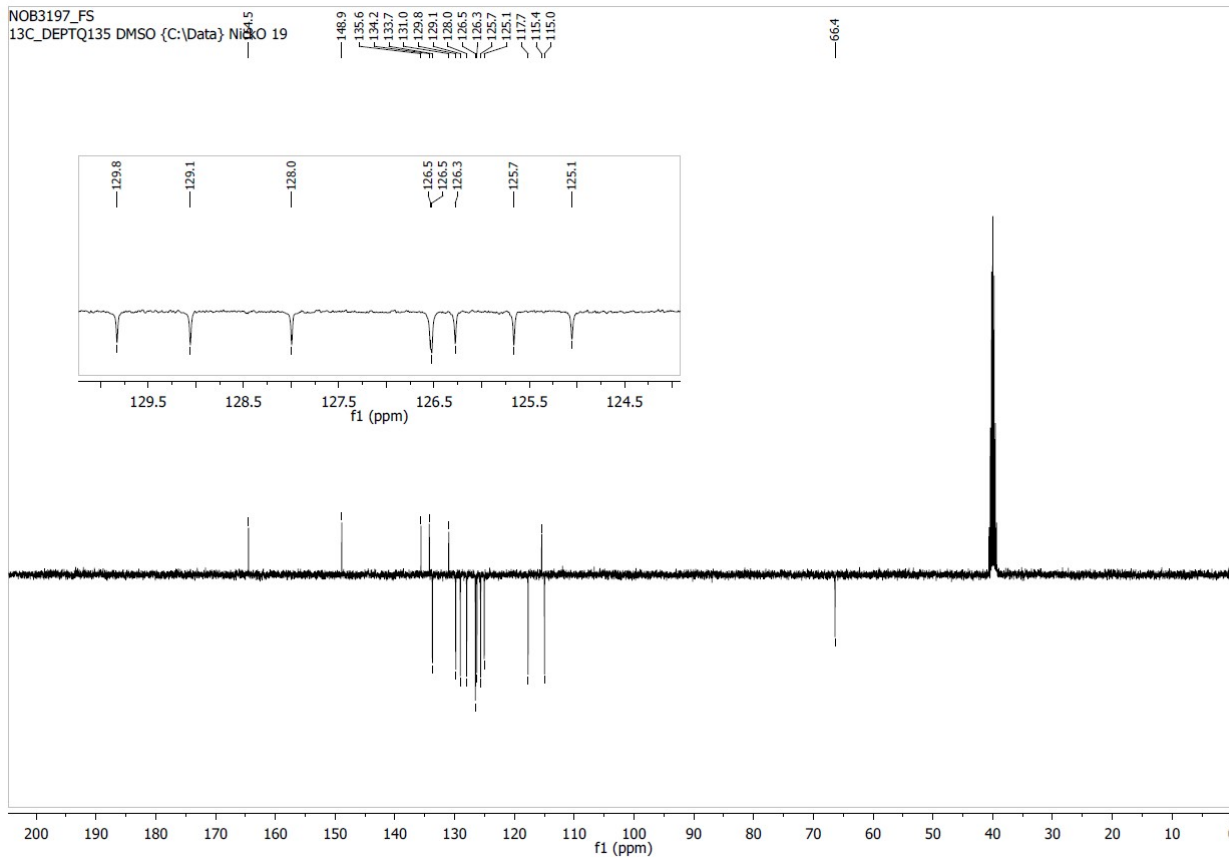
yield: 30 %

colour: off white solid

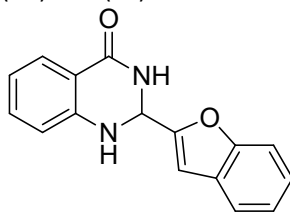
NOB3197_FS
PROTON DMSO {C:\Data} NickO 19



NOB3197_FS
13C DEPTQ135 DMSO {C:\Data} NickO 19



2-(benzofuran-2-yl)-2,3-dihydroquinazolin-4(1H)-one (40)



Chemical Formula: $C_{16}H_{12}N_2O_2$

Exact Mass: 264.09

Molecular Weight: 264.28

IR (neat): ν_{\max} = 3269 (NH), 3178 (NH), 3010, 1662 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.59 (d, J = 2.9 Hz, 1H), 7.61 (ddd, J = 8.3, 7.7, 1.1 Hz, 2H), 7.52 (dd, J = 8.2, 0.6 Hz, 1H), 7.42 (s, 1H), 7.30 – 7.19 (m, 3H), 6.79 (d, J = 7.7 Hz, 1H), 6.72 – 6.67 (m, 2H), 5.93 (t, J = 2.9 Hz, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 163.2, 157.3, 154.2, 146.9, 133.4, 127.5, 127.3, 124.6, 123.0, 121.4, 117.4, 115.0, 114.6, 111.2, 104.0, 60.4.

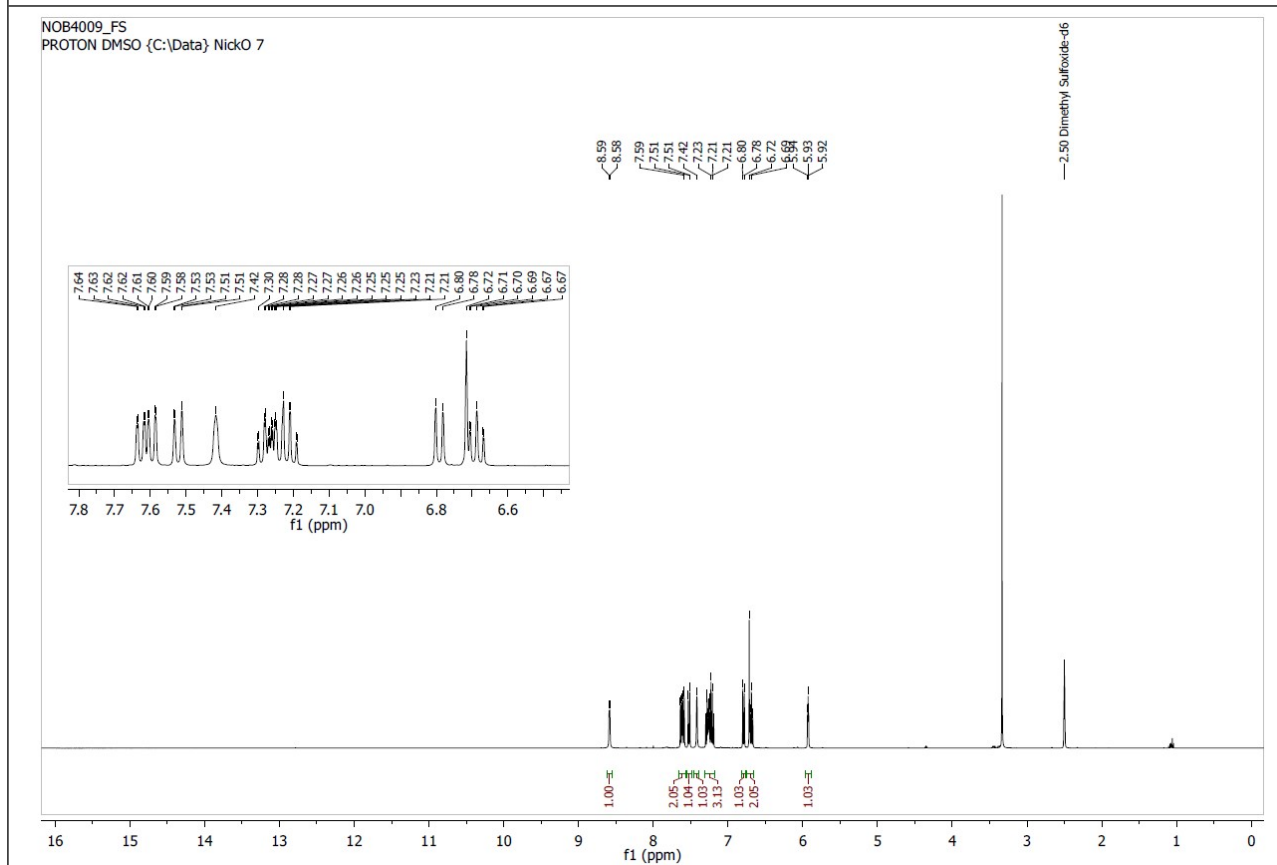
LRMS (ESI+) 265.1 (M+H, $C_{16}H_{13}N_2O_2$, 100%); (ESI-): 263.1 (M-H, $C_{16}H_{11}N_2O_2$, 100%).

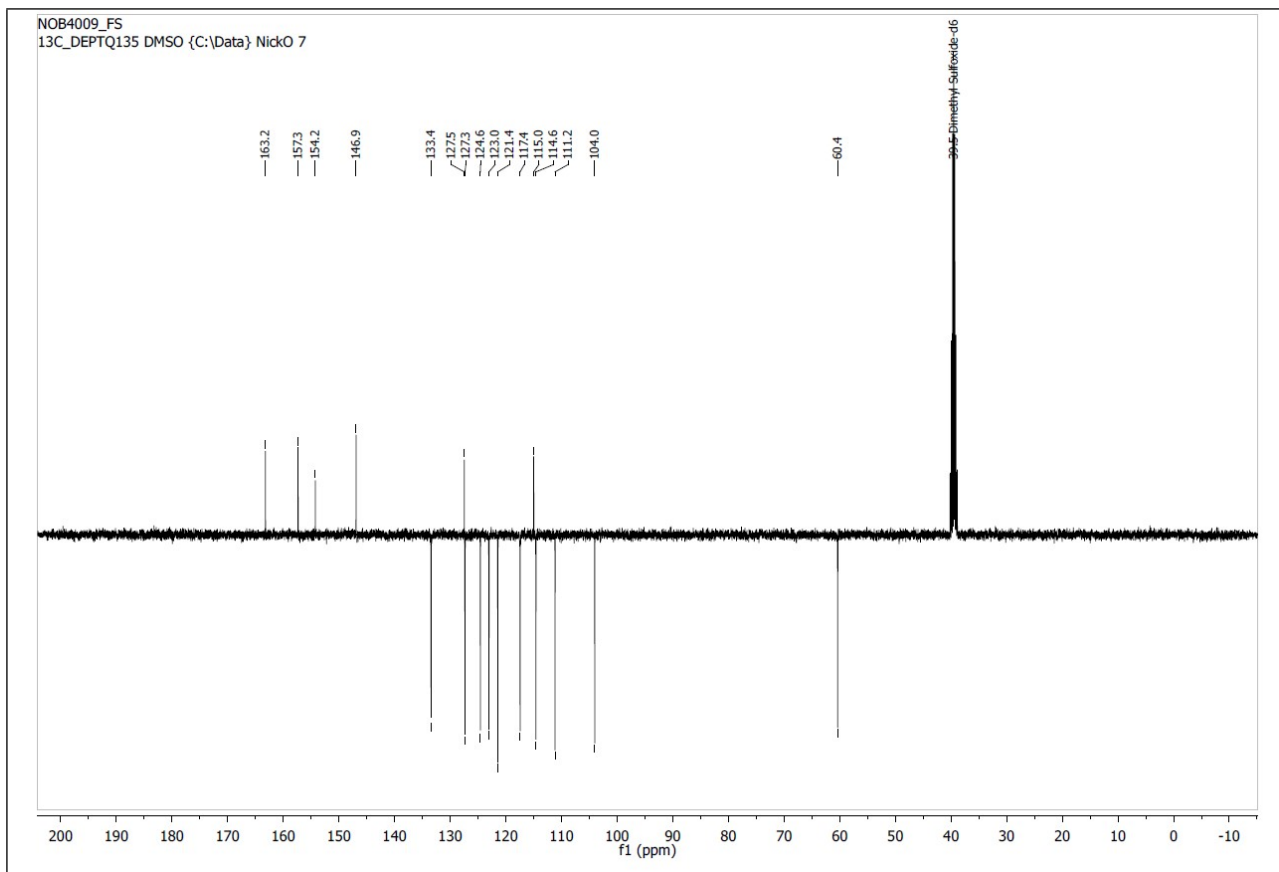
Mass: 171.4 mg

m.p. 192 – 198 °C

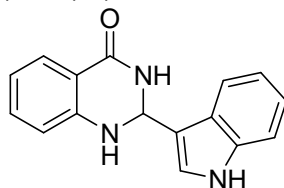
yield: 71%

colour: white solid





2-(1H-indol-3-yl)-2,3-dihydroquinazolin-4(1H)-one (**41**)



Chemical Formula: C₁₆H₁₃N₃O

Exact Mass: 263.11

Molecular Weight: 263.29

IR (neat): ν_{\max} = 3579, 3398, 3185 (NH), 2991, 1641 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 11.09 (s, 1H), 8.09 (s, 1H), 7.78 – 7.76 (m, 1H), 7.66 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.41 – 7.39 (m, 2H), 7.24 (dt, 1H), 7.11 – 7.10 (m, 1H), 7.01 – 6.98 (m, 1H), 6.92 (s, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 6.71 – 6.68 (m, 1H), 6.04 (s, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 164.2, 148.8, 136.6, 133.0, 127.5, 125.4, 124.7, 121.4, 120.0, 118.8, 117.0, 115.3, 114.40, 114.41, 111.7, 61.7.

LRMS (ESI+) 264.1 (M+H, C₁₆H₁₄N₃O, 100%); (ESI-): 262 (M-H, C₁₆H₁₂N₃O, 100%).

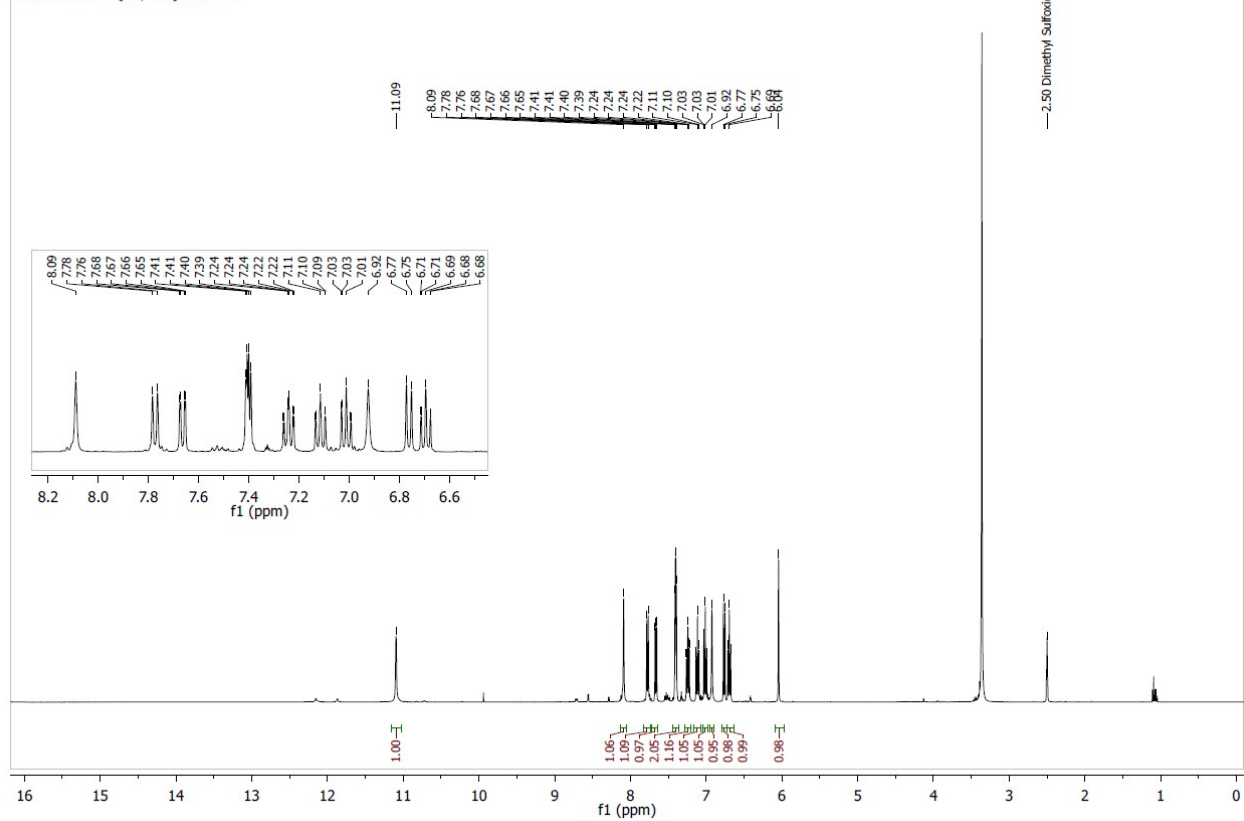
Mass 219.5 mg

m.p. 196 – 216°C

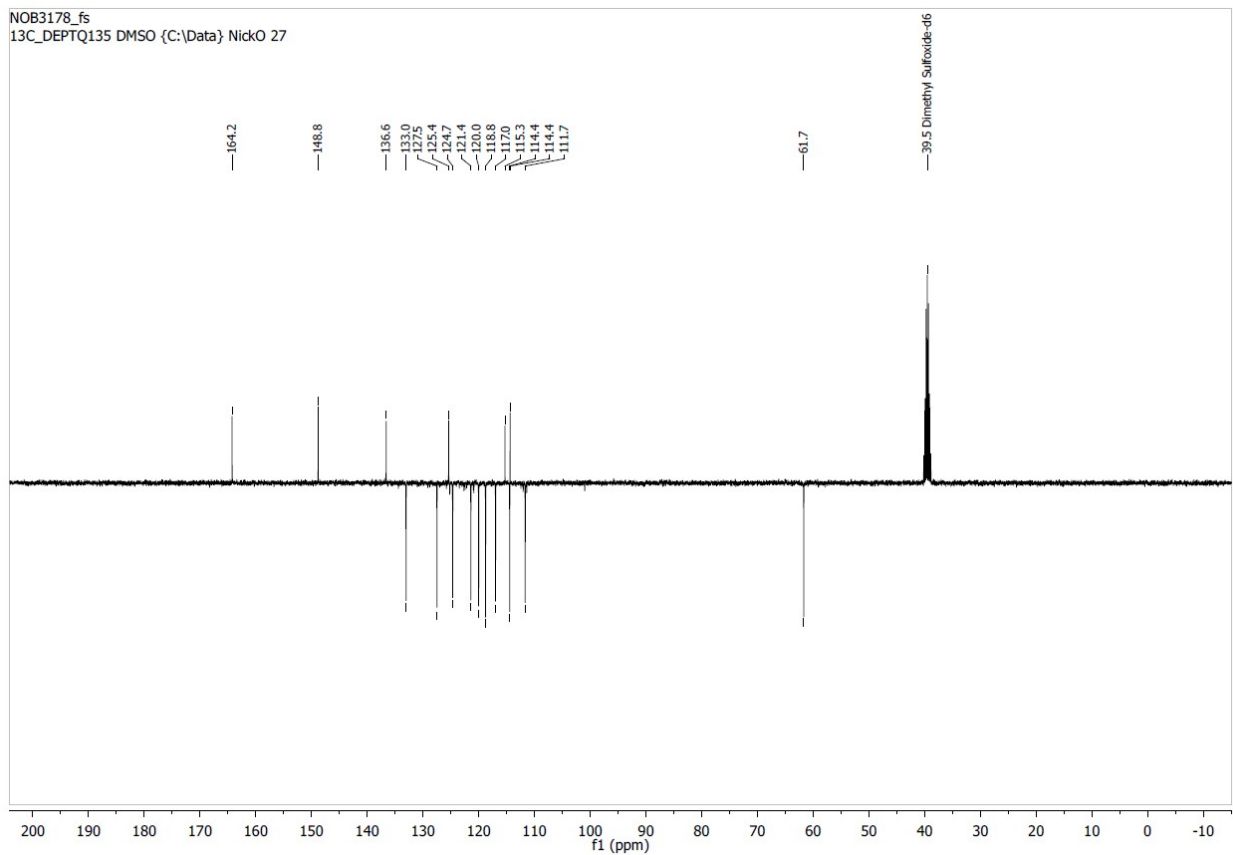
yield 53 %

colour Light orange solid

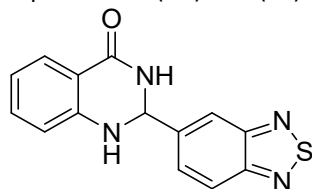
NOB3178_fs
PROTON DMSO {C:\Data} NickO 27



NOB3178_fs
13C_DEPTQ135 DMSO {C:\Data} NickO 27



2-(benzo[c][1,2,5]thiadiazol-5-yl)-2,3-dihydroquinazolin-4(1H)-one (**42**)



Chemical Formula: C₁₄H₁₀N₄OS

Exact Mass: 282.06

Molecular Weight: 282.32

IR (neat): ν_{\max} = 3243 (NH), 3029.1654 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.54 (s, 1H), 8.13 (d, *J* = 9.2 Hz, 1H), 8.04 (s, 1H), 7.92 (dd, *J* = 9.1, 1.6 Hz, 1H), 7.63 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.35 (s, 1H), 7.29 – 7.25 (m, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.72 – 6.65 (m, 1H), 6.01 (s, 1H).

¹³C NMR (10 MHz, DMSO-d₆) δ 163.4, 154.2, 154.0, 147.4, 143.6, 133.6, 129.2, 127.4, 121.5, 118.5, 117.4, 114.9, 114.5, 65.8.

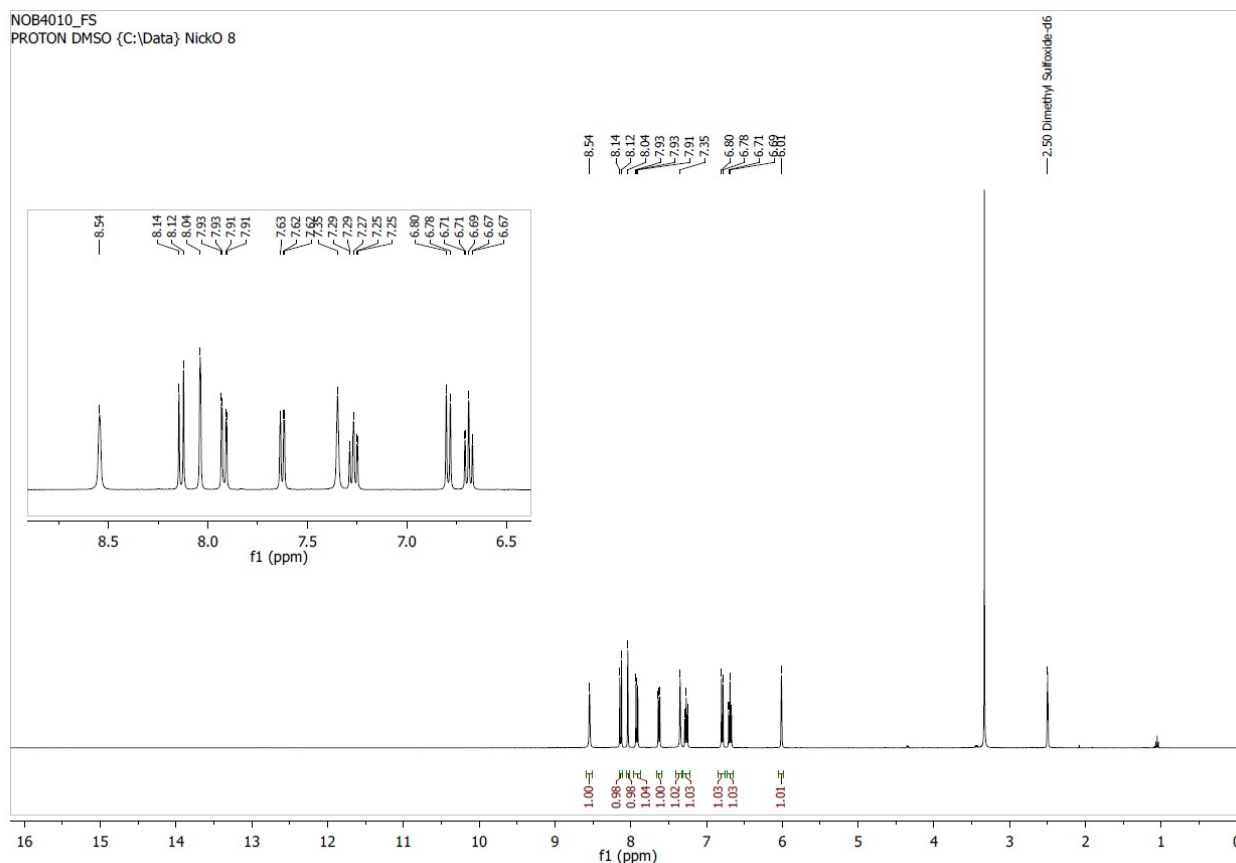
LRMS (ESI+) 283.1 (M+H, C₁₄H₁₁N₄OS, 100%); (ESI-): 281.1 (M-H, C₁₄H₉N₄OS, 100%).

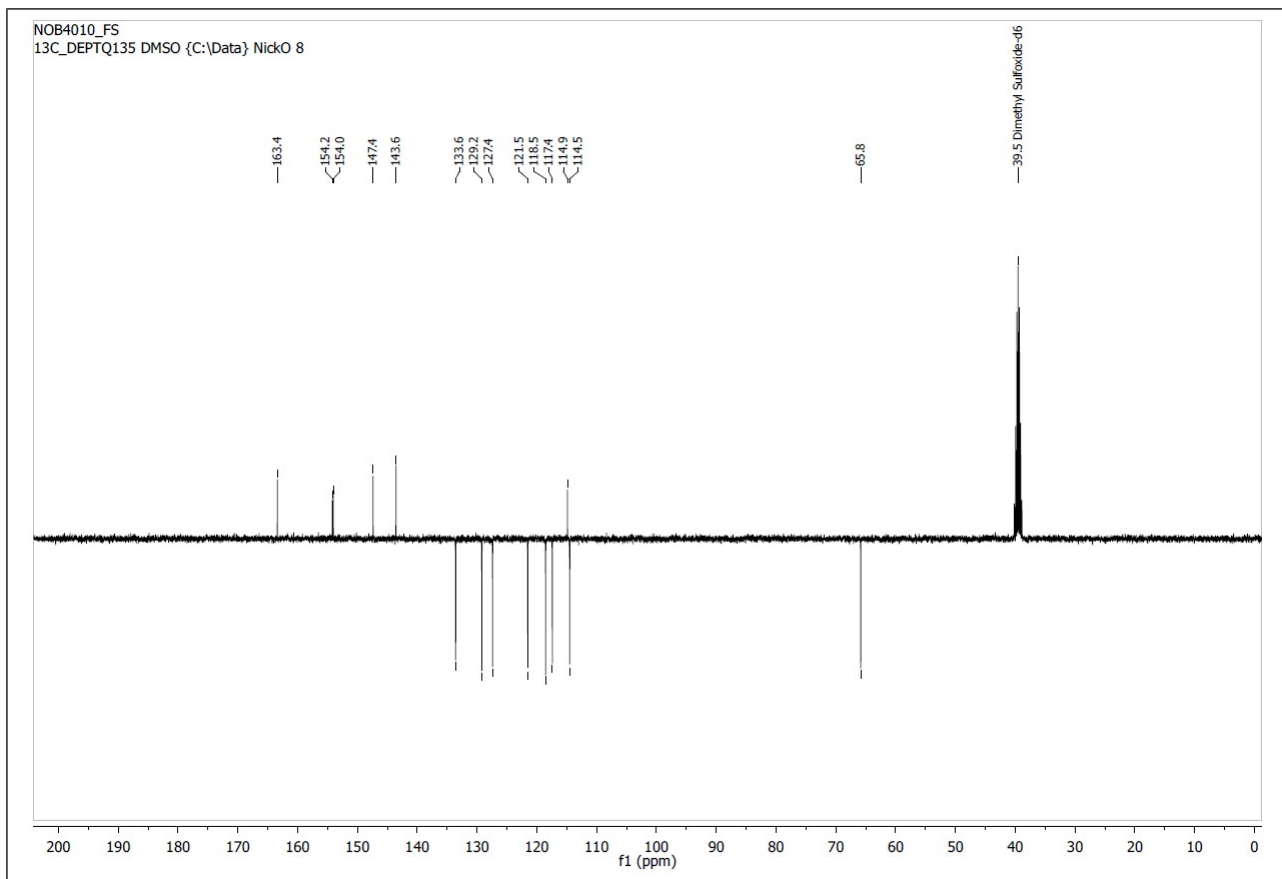
Mass: 112.4 mg

m.p. 216-218 °C

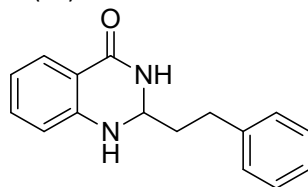
yield: 48 %

colour: fine brown solid





2-phenethyl-2,3-dihydroquinazolin-4(1H)-one (**43**)



Chemical Formula: $C_{16}H_{16}N_2O$

Exact Mass: 252.13

Molecular Weight: 252.31

IR (neat): ν_{max} = 3302 (NH), 3175 (NH), 3000 (CH_2), 1647 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.02 (s, 1H, NH, H₃), 7.60 (dd, J = 7.7, 1.5 Hz, 1H), 7.32 – 7.15 (m, 6H), 6.77 – 6.73 (m, 1H), 6.71 – 6.65 (m, 2H), 4.74 (t, J = 5.0 Hz, 1H, H₂), 2.79 – 2.72 (m, 2H), 1.97 – 1.89 (m, 2H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 164.1, 148.6, 141.6, 133.1, 128.4 (2C), 128.3 (2C), 127.4, 125.8, 117.1, 115.1, 114.4, 64.0, 36.7, 29.3.

LRMS (ESI+) m/z : 253.2 (M+H, $C_{16}H_{17}N_2O$, 100%); (ESI-), 251.1 (M-H, $C_{16}H_{15}N_2O$, 100%), 297.2 (M+FA-H, $C_{16}H_{15}N_2O$, 100%).

Mass: 158.5 mg

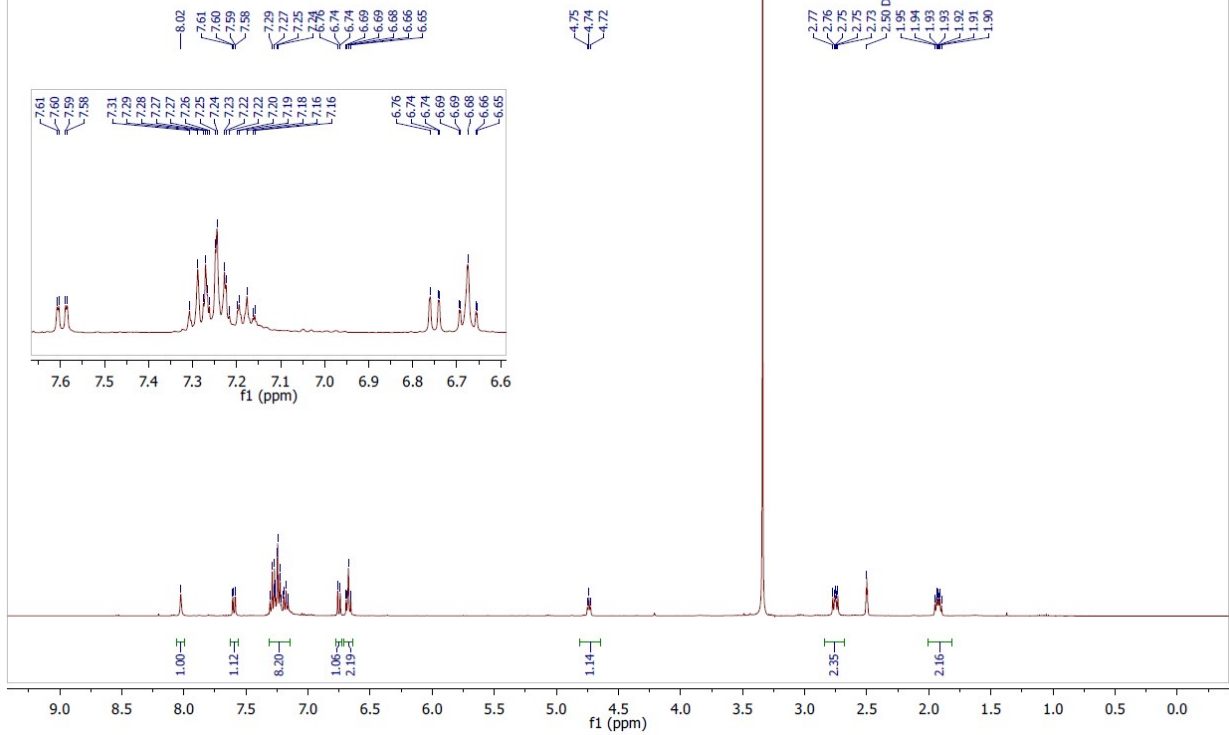
m.p. >128°C (decomp.)

Yield: 39 %

Yellow solid

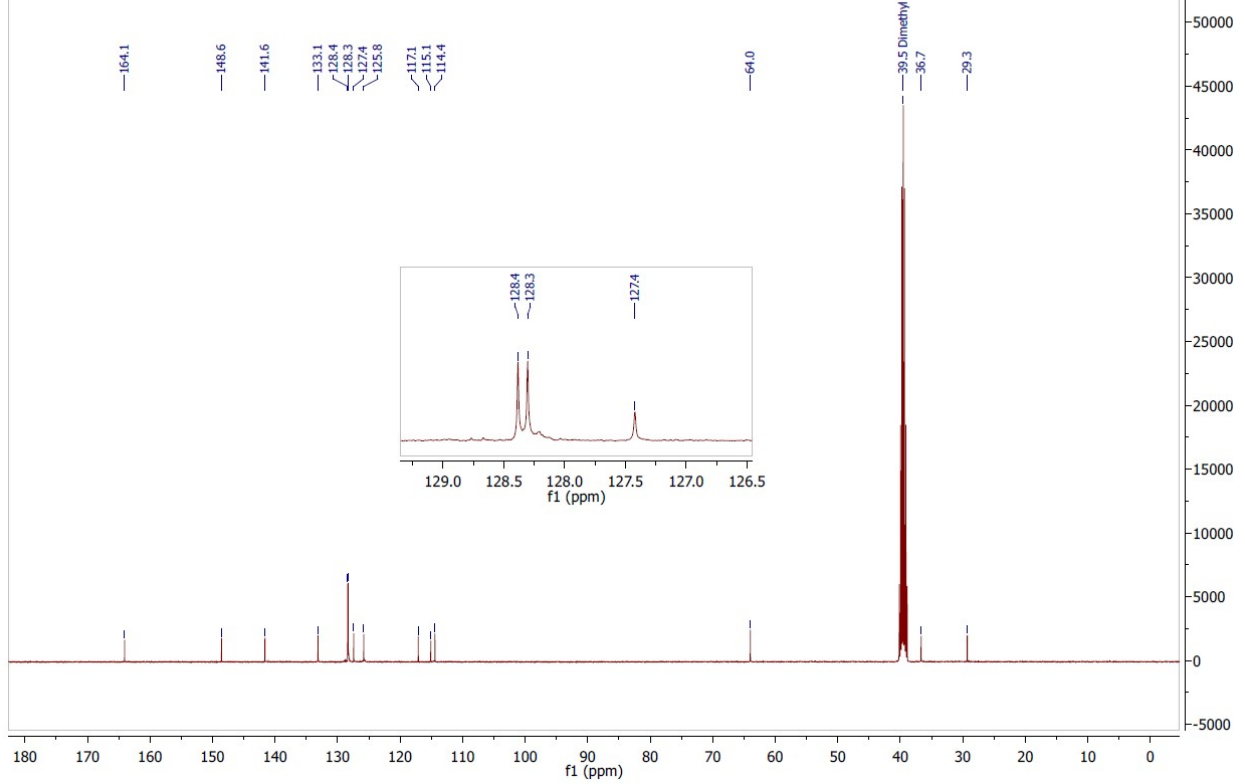
NOB2138_FS

1H DMSO {C:\Data} NickO 25

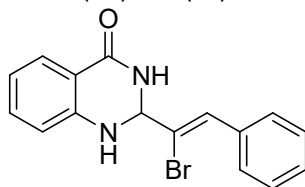


NOB2138_FS

13C_3hours DMSO {C:\Data} NickO 25



2-(1-bromo-2-phenylvinyl)-2,3-dihydroquinazolin-4(1H)-one (**44**)



Chemical Formula: $C_{16}H_{13}BrN_2O$

Exact Mass: 328.02

Molecular Weight: 329.19

IR (neat): ν_{max} = 3263 (NH), 3178 (NH), 3053 (CH), 1646 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.30 (d, J = 1.3 Hz, 1H), 7.64 – 7.63 (m, 2H), 7.58 (dd, J = 7.7, 1.4 Hz, 1H), 7.43 – 7.39 (m, 2H), 7.37 (dd, J = 4.9, 3.6 Hz, 1H), 7.25 – 7.19 (m, 3H), 6.72 (d, J = 8.0 Hz, 1H), 6.62 (t, 1H), 5.64 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.6, 146.9, 134.3, 133.4, 129.6, 129.0 (2C), 128.6, 128.5, 128.5, 128.4 (2C), 127.0, 116.6, 113.6, 113.4, 70.6,

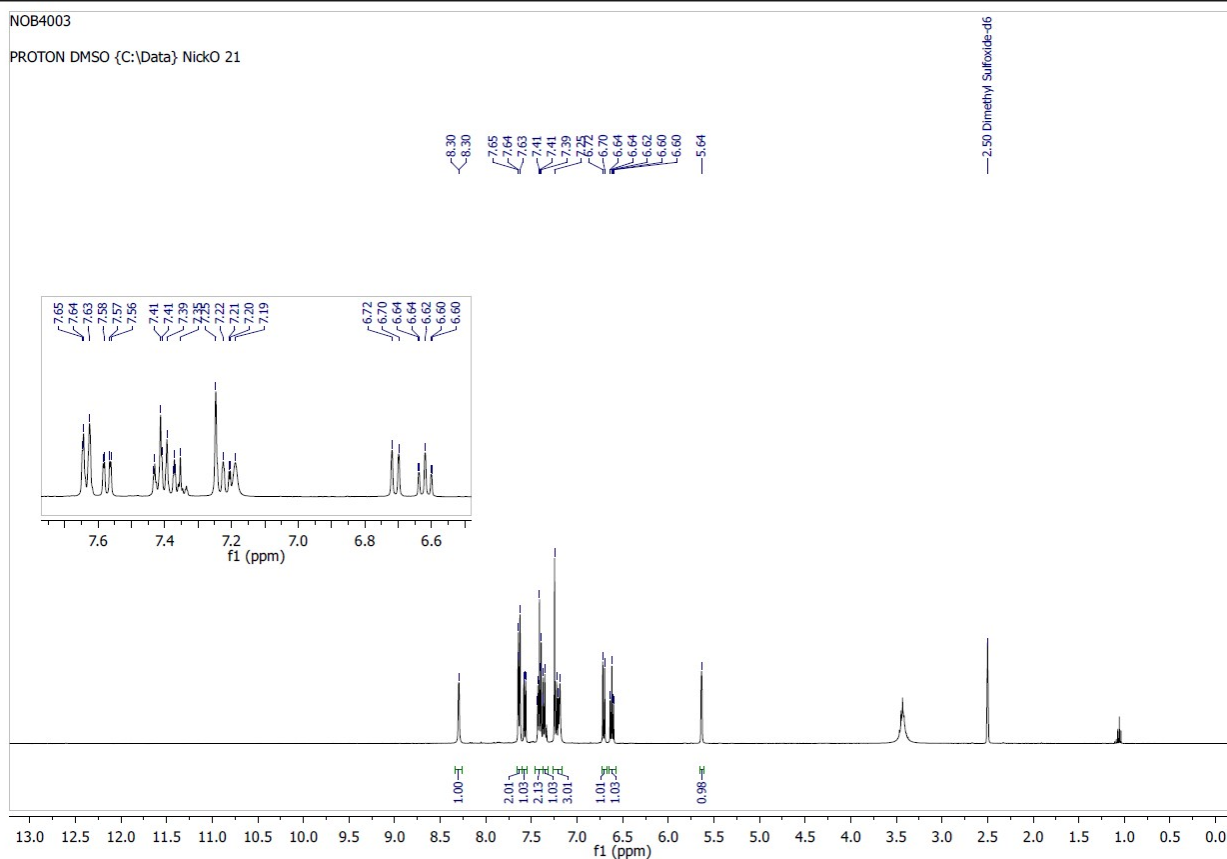
LRMS (ESI+): 329.1 (M+H, $C_{16}H_{13}^{79}BrN_2O$, 100%) 331.1 (M+H, $C_{16}H_{13}^{81}BrN_2O$, 95%).

Mass 211.8 mg

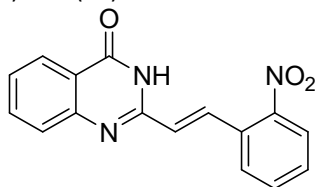
m.p. 180 – 183 °C

yield 40 %

colour light yellow solid



2-(2-nitrostyryl)-2,3-dihydroquinazolin-4(1H)-one (45)



Chemical Formula: C₁₆H₁₁N₃O₃

Exact Mass: 293.08

Molecular Weight: 293.28

IR (neat): ν_{\max} = 3249 (NH), 2971 (NH), 1668 (C=O), 1519 (NO), 1349 (NO) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.50 (d, *J* = 8.9 Hz, 1H), 8.35 (s, 1H), 8.09 (d, *J* = 7.0 Hz, 1H), 8.05 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.94 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.81 – 7.76 (m, 1H), 7.74 (d, *J* = 15.8 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.53 (td, *J* = 7.7, 1.6 Hz, 1H), 7.37 – 7.31 (m, 2H), 7.23 – 7.21 (m, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 167.1, 163.2, 149.0, 148.2, 139.3, 133.6, 132.4, 131.9, 130.6, 129.9, 129.7, 128.7, 128.1, 126.3, 124.6, 118.9.

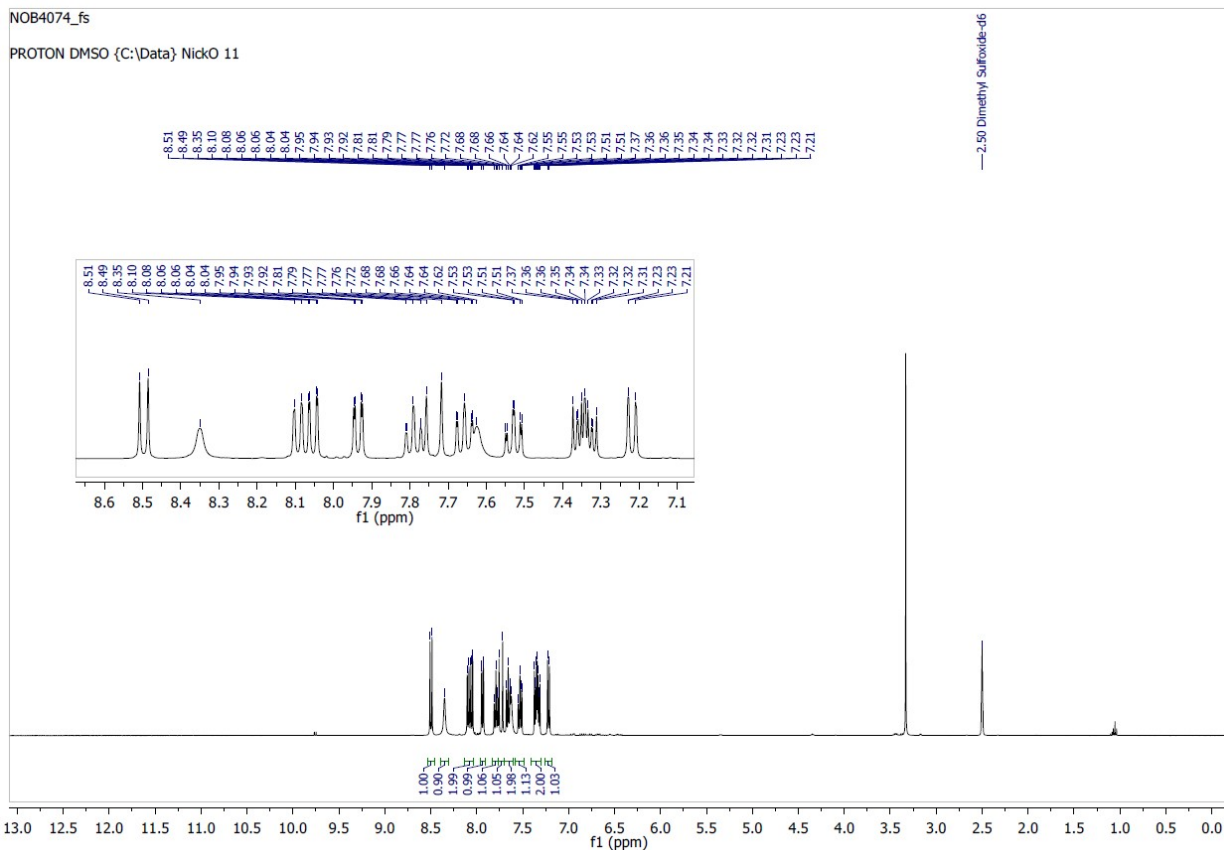
LRMS (ESI⁺): 296.1 (M+H, C₁₆H₁₄N₃O₃, 100%).

Mass 289 mg

m.p. 127 - 134 °C

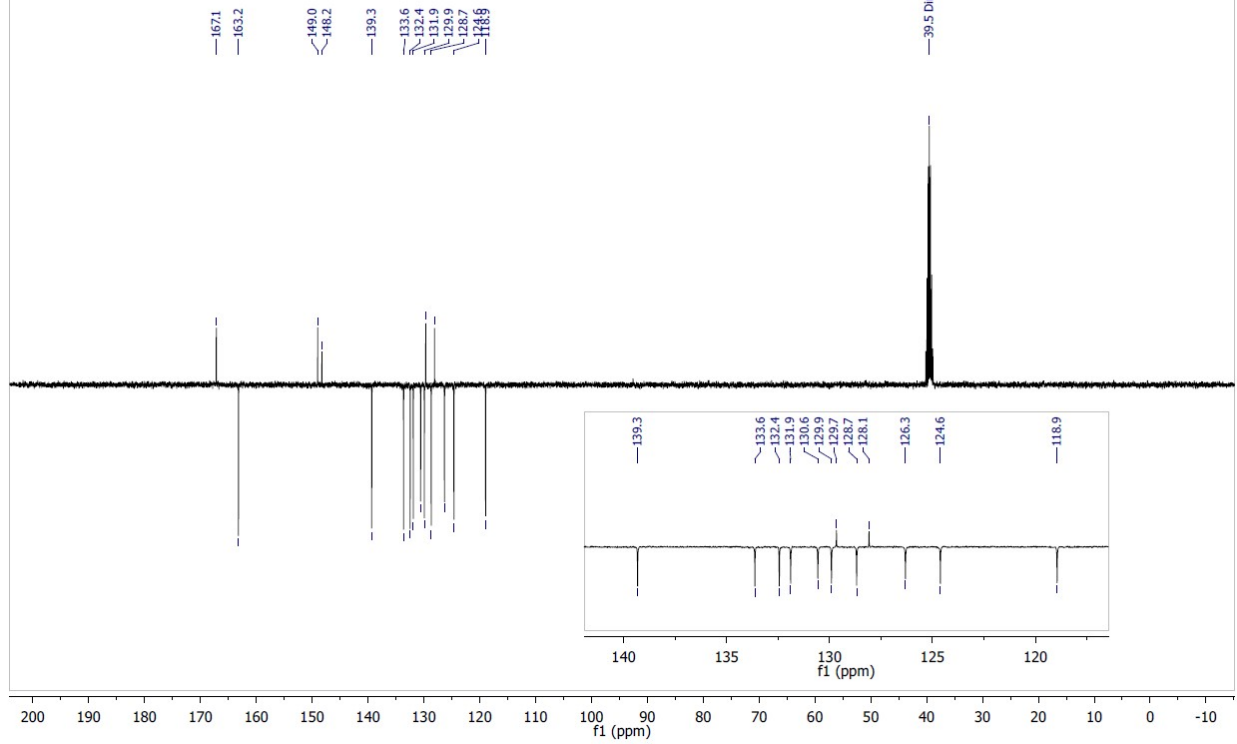
yield 59 %

yellow solid



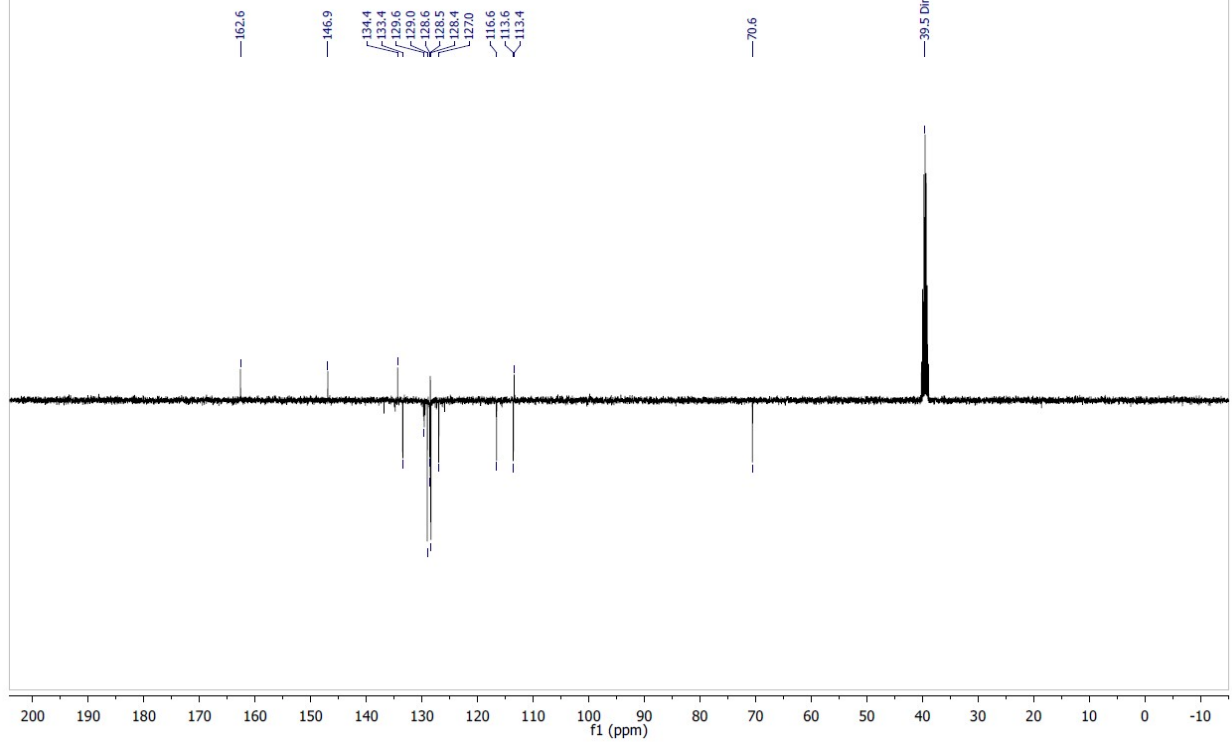
NOB4074_fs

13C_DEPTQ135 DMSO (C:\Data) NickO 11

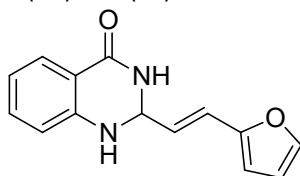


NOB4003_FS

13C_DEPTQ135 DMSO (C:\Data) NickO 21



2-(2-(furan-2-yl)vinyl)-2,3-dihydroquinazolin-4(1H)-one (**46**)



Chemical Formula: C₁₄H₁₂N₂O₂

Exact Mass: 240.09

Molecular Weight: 240.26

IR (neat): ν_{\max} = 3236 (NH), 2971 (NH), 1634 (C=O). cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.13 (s, 1H), 7.63 – 7.59 (m, 2H), 7.27 – 7.22 (m, 1H), 6.87 (s, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.71 – 6.65 (m, 1H), 6.54 – 6.48 (m, 3H), 6.12 (dd, *J* = 15.8, 6.5 Hz, 1H), 5.26 (d, *J* = 6.5 Hz, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 163.3, 151.1, 147.6, 143.2, 133.3, 127.3, 126.7, 119.9, 117.2, 114.9, 114.6, 111.8, 109.6, 65.0.

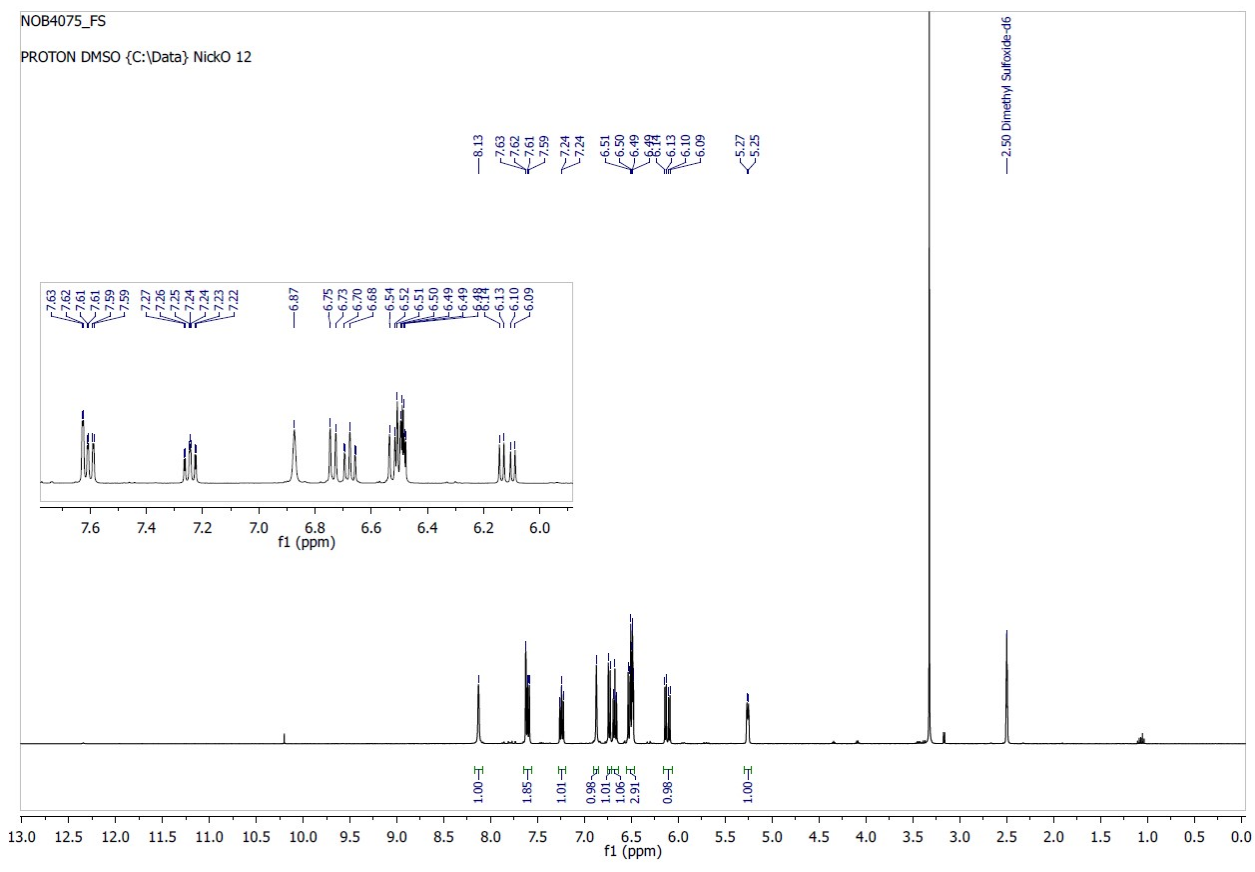
LRMS (ESI+): 241.1 (M+H, C₁₄H₁₃N₂O₂, 100%).

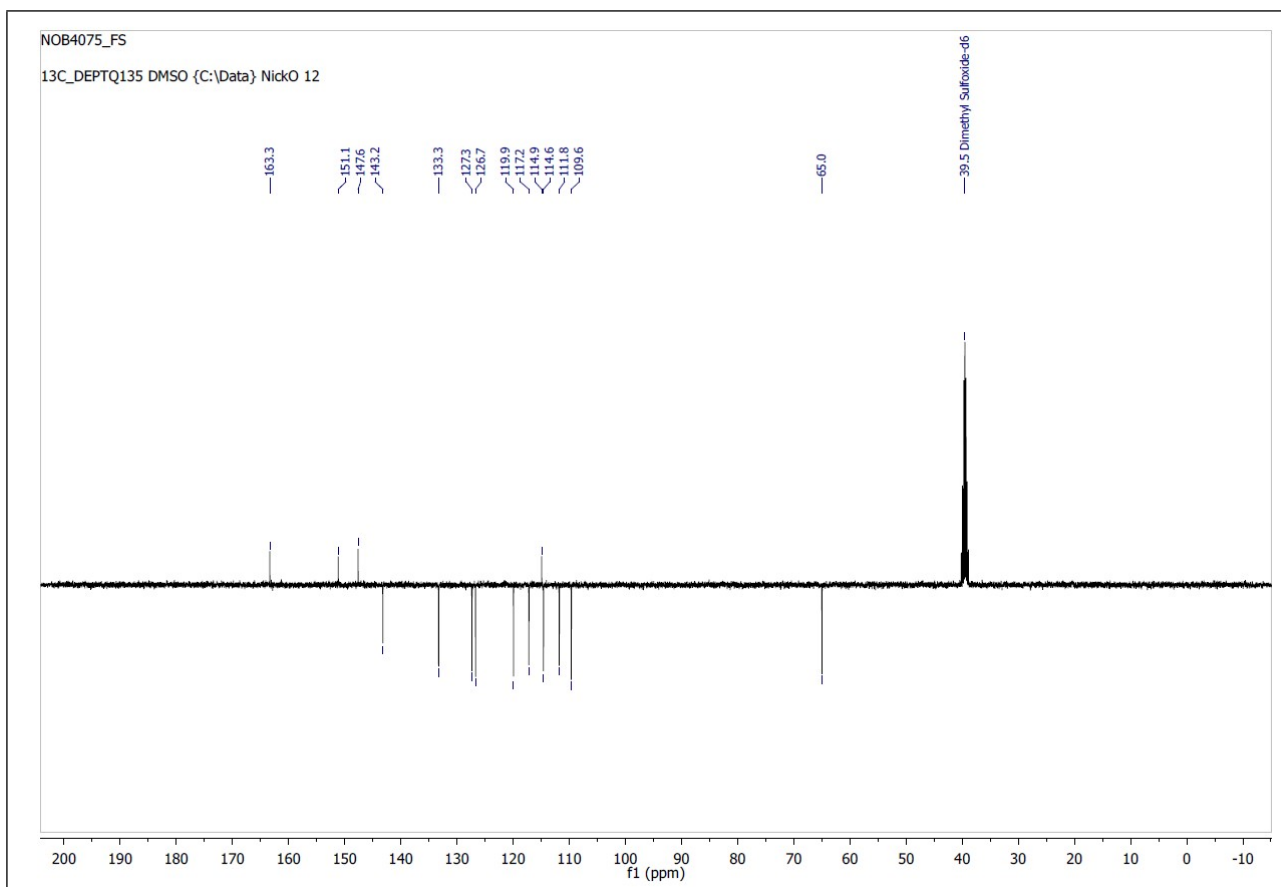
Mass 109 mg

m.p. 148 - 151 °C

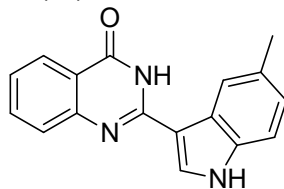
yield 28 %

white solid





2-(5-methyl-1H-indol-3-yl)quinazolin-4(3H)-one (**47**)



Chemical Formula: C₁₇H₁₃N₃O

Exact Mass: 275.11

Molecular Weight: 275.30

IR (neat): ν_{\max} = 3385 (NH), 3114 (NH), 2965, 1663 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.09 (s, 1H), 11.74 (s, 1H), 8.50 - 8.49 (m, 2H), 8.10 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.79–7.75 (m, 2H), 7.41 – 7.35 (m, 2H), 7.06 (dd, *J* = 8.3, 1.4 Hz, 1H), 2.47 (s, 3H).

¹³C NMR (100 MHz, DMSO-d₆) δ 162.1, 150.4, 149.8, 135.2, 134.3, 129.6, 129.1, 127.0, 125.81, 125.80, 125.1, 124.1, 122.1, 120.4, 111.6, 108.1, 21.5.

LRMS (ESI+) 276.2 (M+H, C₁₇H₁₄N₃O, 100%); (ESI-) 274.1 (M-H, C₁₇H₁₂N₃O, 100%)

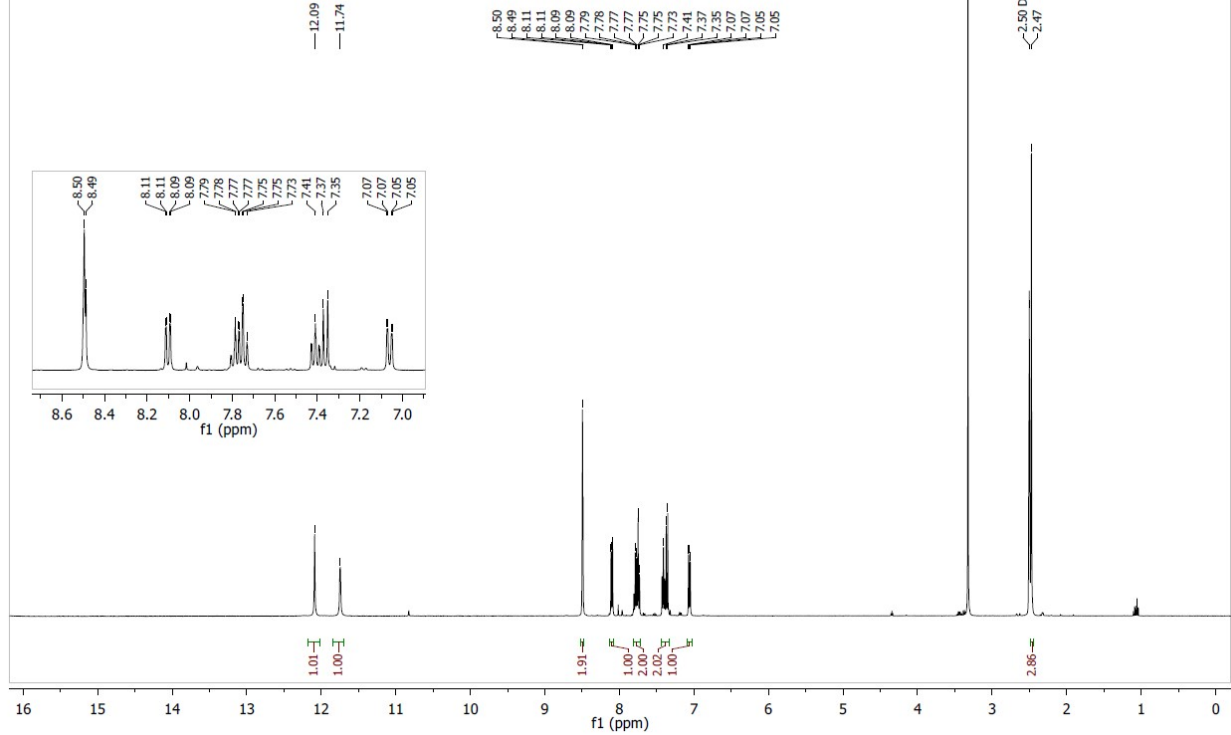
Mass 73.4 mg

m.p. >155 °C (decomp).

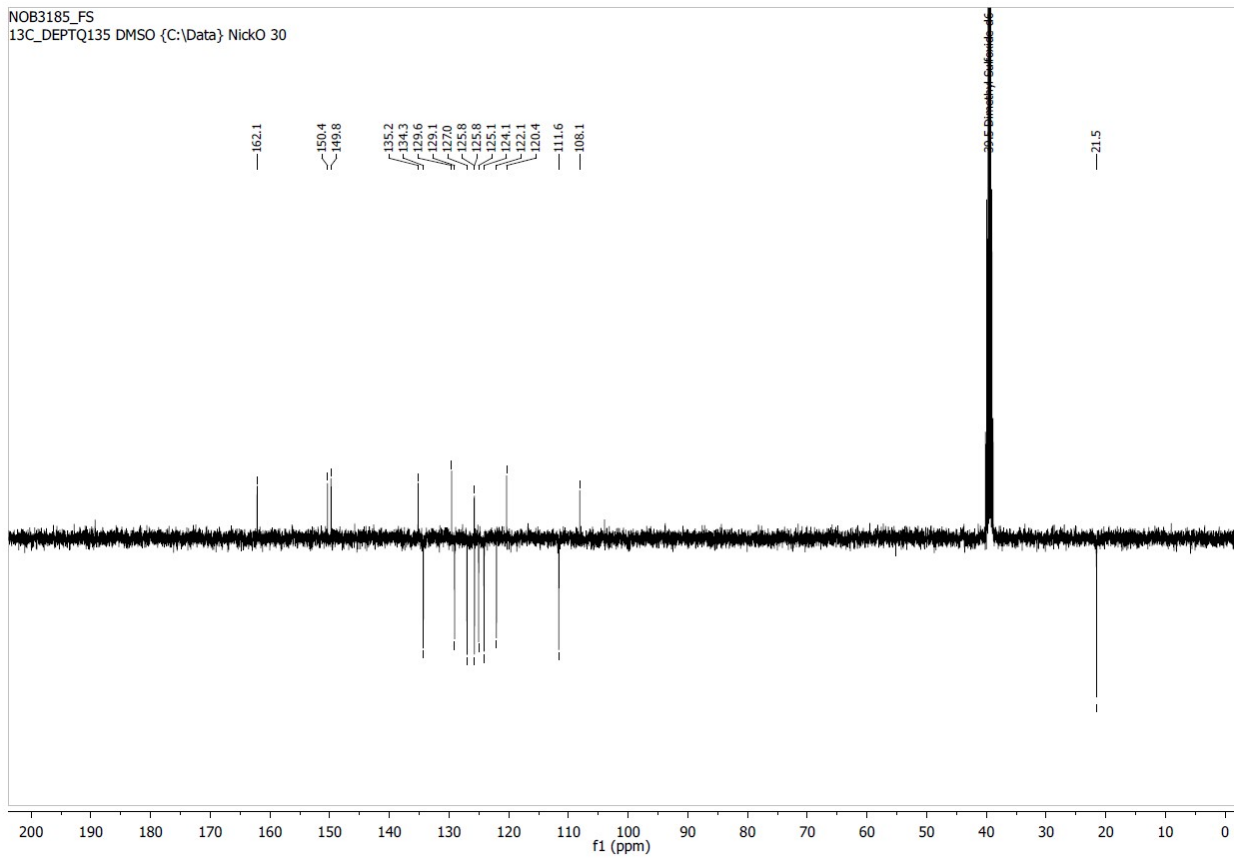
Yield 17 %

Colour pale pink solid

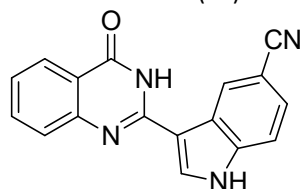
NOB3185_FS
PROTON DMSO {C:\Data} NickO 30



NOB3185_FS
13C_DEPTQ135 DMSO {C:\Data} NickO 30



3-(4-oxo-3,4-dihydroquinazolin-2-yl)-1H-indole-5-carbonitrile (**48**)



Chemical Formula: C₁₇H₁₀N₄O

Exact Mass: 286.09

Molecular Weight: 286.29

IR (neat): ν_{\max} = 3282 (NH), 3120 (NH), 2227 (CN), 1679 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.35 (s, 1H), 12.30 (s, 1H), 9.10 (s, 1H), 8.71 (d, *J* = 2.5 Hz, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 7.80 (dt, *J* = 14.9, 7.5 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.44 (dd, *J* = 15.9, 9.2 Hz, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 162.0, 149.4, 149.3, 138.7, 134.5, 131.4, 127.6, 127.3, 125.8, 125.6, 125.5, 125.3, 120.6, 120.5, 113.6, 109.3, 103.2.

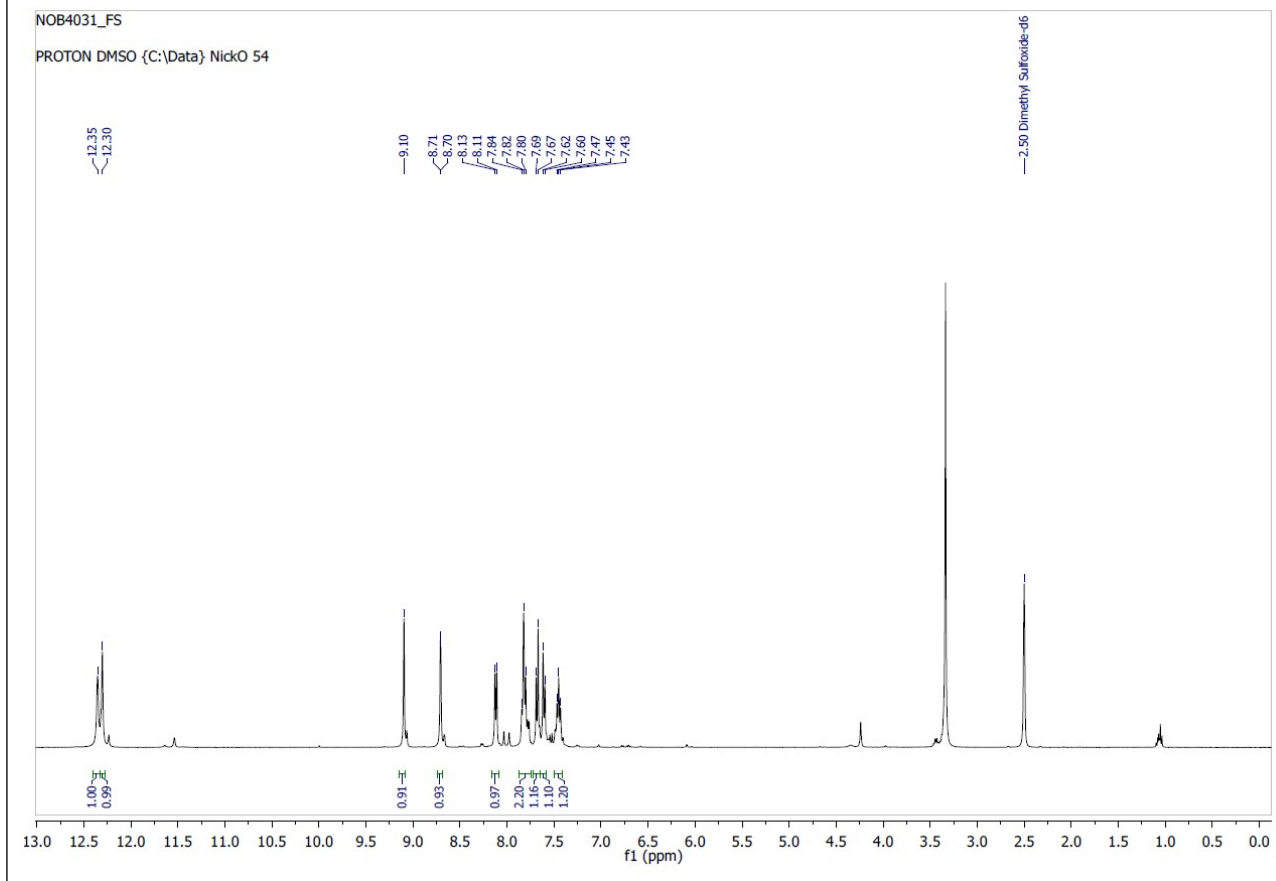
LRMS (ESI+): 287.1 (M+H, C₁₇H₁₁N₄O, 100%); LRMS (ESI-): 285.1 (M-H, C₁₇H₉N₄O, 100%).

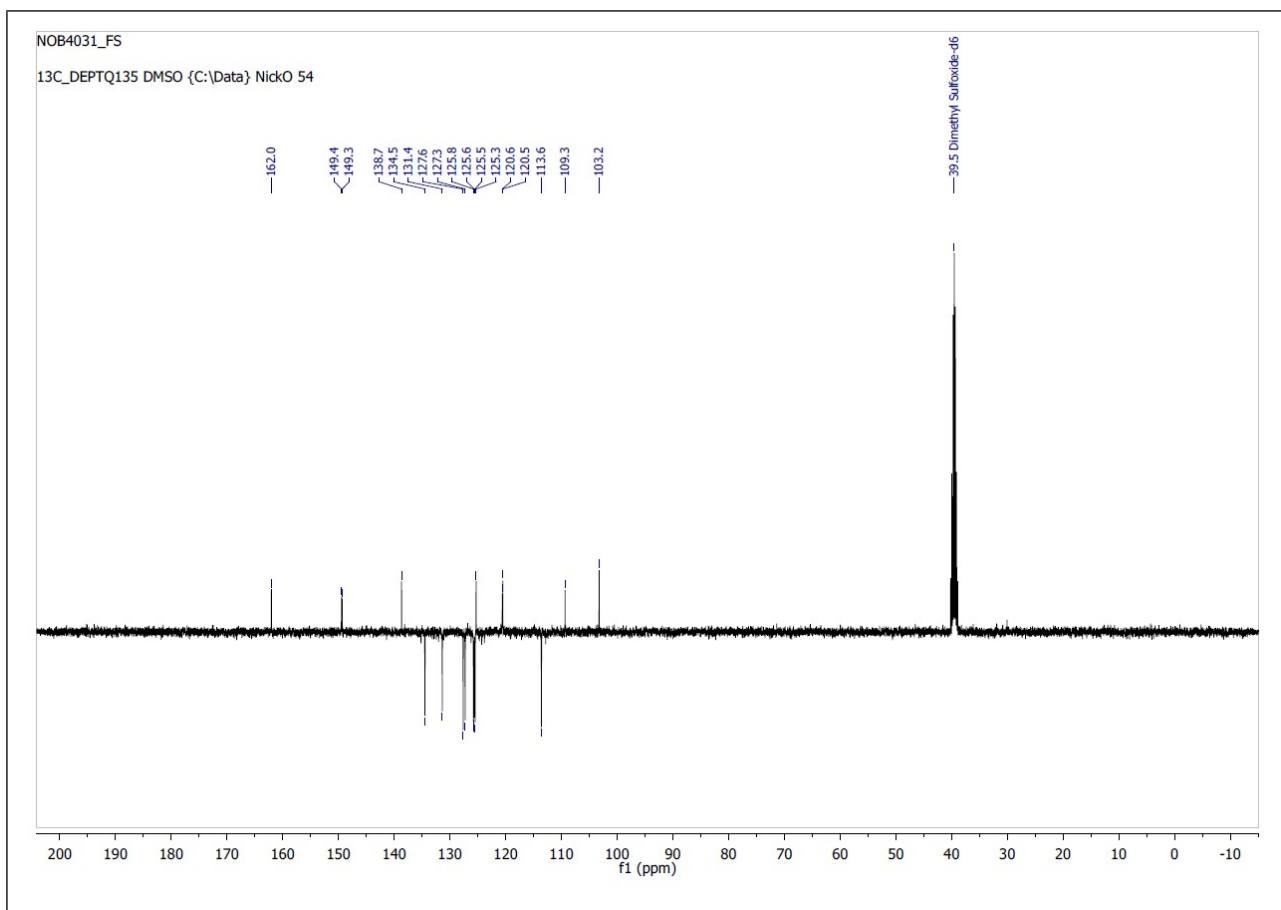
Mass 102.6 mg

m.p. >250°C (decomp.)

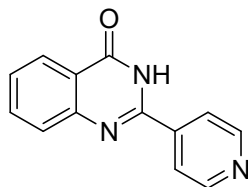
yield 21 %

colour yellow solid





2-(Pyridin-4-yl)quinazolin-4(3H)-one (**49**)



Chemical Formula: $C_{13}H_9N_3O$

Exact Mass: 223.07

Molecular Weight: 223.23

IR (neat): ν_{\max} = 2965 (CH), 1674 (C=O)

1H NMR (400 MHz, DMSO- d_6) δ 12.77 (s, 1H), 8.80 (dd, J = 4.6, 1.5 Hz, 2H), 8.19 (dd, J = 7.9, 1.1 Hz, 1H), 8.12 (dd, J = 4.6, 1.6 Hz, 2H), 7.92 – 7.84 (m, 1H), 7.80 (d, J = 7.9 Hz, 1H), 7.66 – 7.53 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.5, 151.0, 150.7, 148.7, 140.4, 135.3, 128.3, 127.9, 126.4, 122.1, 122.0.

224 (M+H, $C_{13}H_{10}N_3O$, 100%);

LRMS (ESI-): 222 (M-H, $C_{13}H_8N_3O$, 100%)

Mass: 110 mg

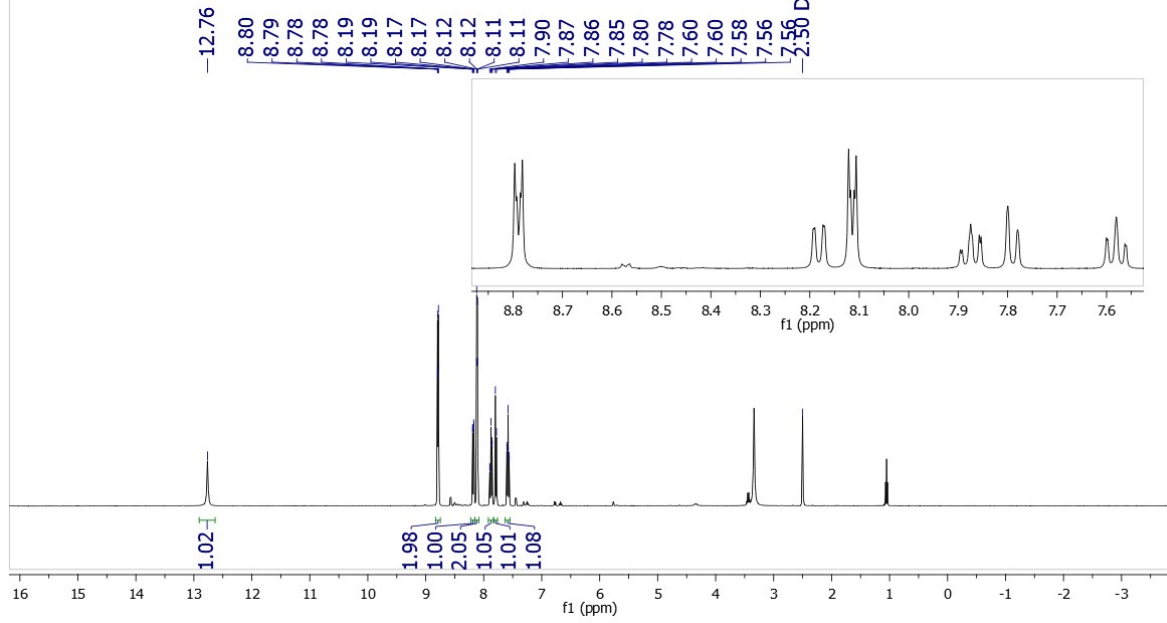
m.p. >250 °C

yield: 43 %

pale brown solid

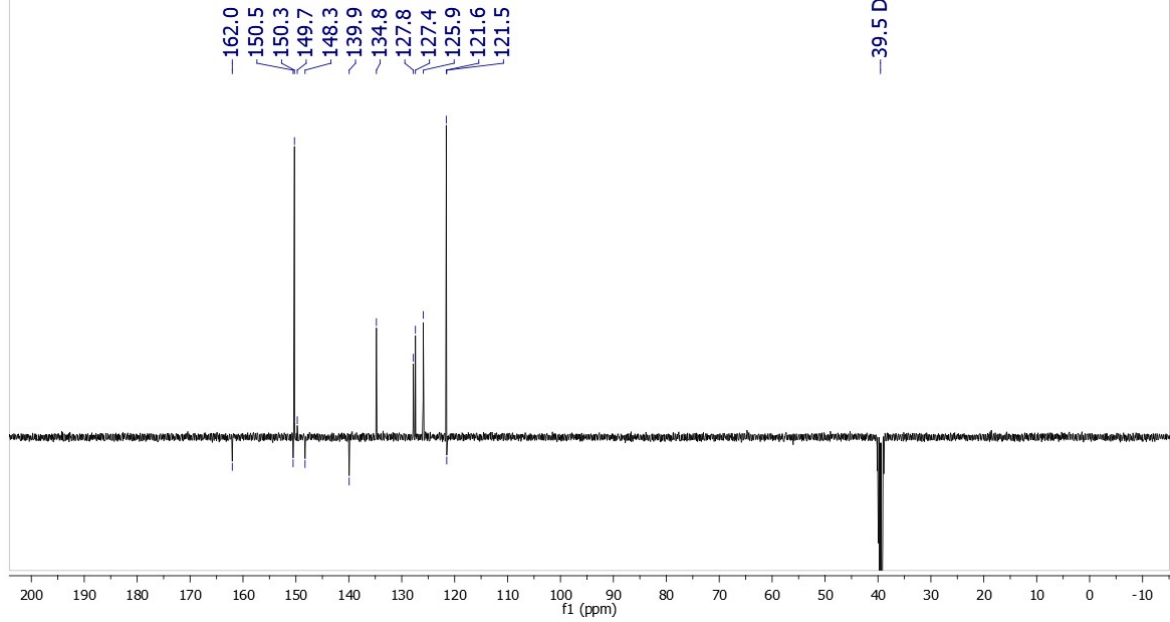
NOB4062_FS

PROTON DMSO {C:\Data} NickO 33

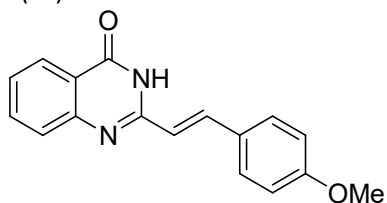


NOB4062_FS

¹³C DEPTQ135 DMSO {C:\Data} NickO 33



2-(4-methoxystyryl)quinazolin-4(3H)-one (50)



Chemical Formula: C₁₇H₁₄N₂O₂

Exact Mass: 278.11

Molecular Weight: 278.31

IR (neat): ν_{\max} = 3100 (NH), 3049, 1668 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.25 (s, 1H), 8.10 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.91 (d, *J* = 16.1 Hz, 1H), 7.81 – 7.77 (m, 1H), 7.66 – 7.60 (m 3H), 7.47 – 7.43 (m, 1H), 7.02 (d, *J* = 8.7 Hz, 2H), 6.85 (d, *J* = 16.1 Hz, 1H), 3.81 (s, 3H).

¹³C NMR (100 MHz, DMSO-d₆) δ 161.8, 160.6, 151.7, 149.2, 138.0, 134.5, 129.3 (2C), 127.6, 127.0, 125.9, 125.8, 121.0, 118.5, 114.6 (2C), 55.3.

LRMS (ESI+) 279.1 (M+H, C₁₇H₁₅N₂O₂, 100%); (ESI-) 277.1 (M-H, C₁₇H₁₃N₂O₂, 100%).

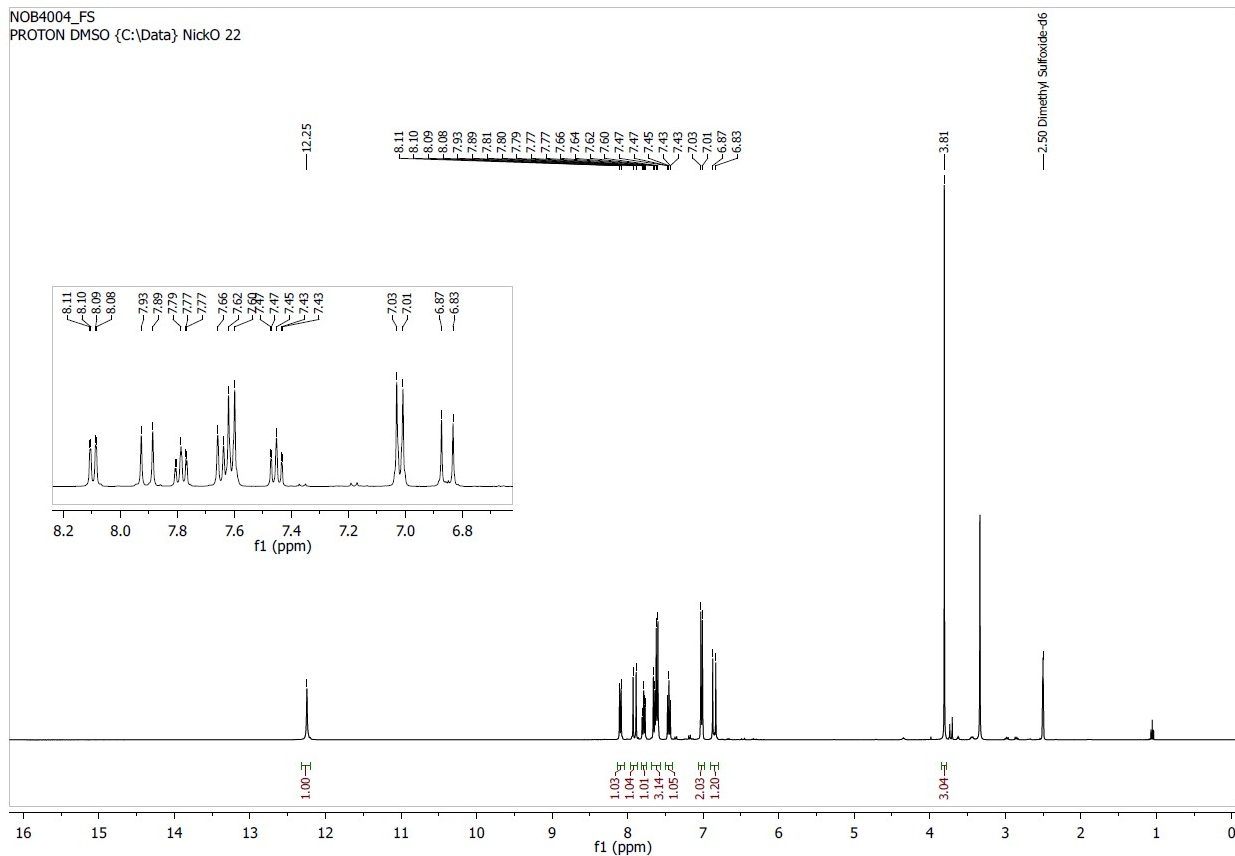
Mass 165 mg

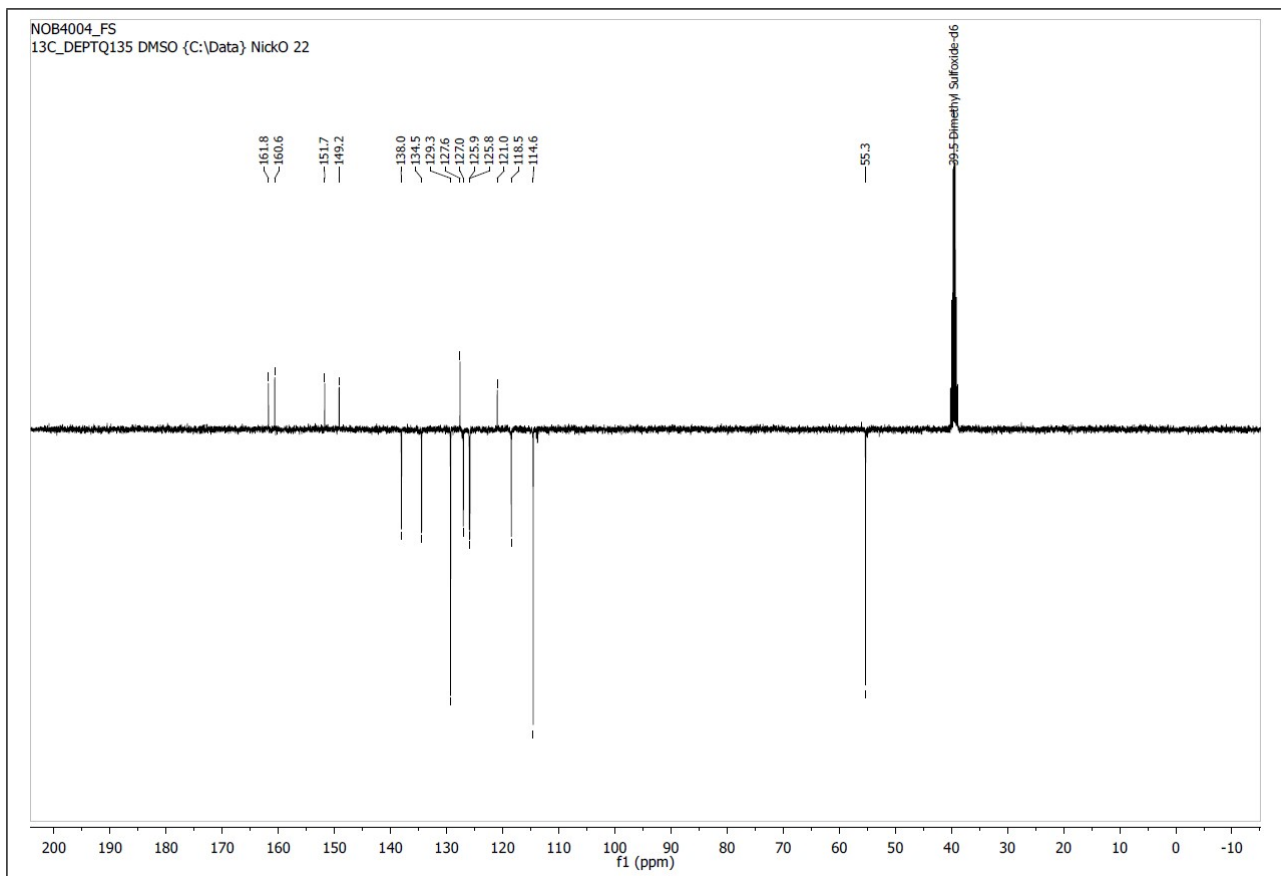
m.p. >210 °C (dec.)

yield 37 %

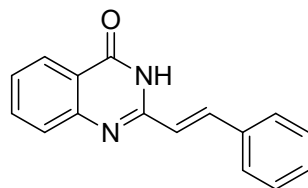
pale yellow solid

NOB4004_FS
PROTON DMSO {C:\Data} NickO 22





2-styrylquinazolin-4(3H)-one (**51**)



Chemical Formula: C₁₆H₁₂N₂O

Exact Mass: 248.09

Molecular Weight: 248.28

IR (neat): ν_{\max} = 3105 (NH), 3042 (CH), 1668 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.33 (s, 1H), 8.11 (d, J = 7.4 Hz, 1H), 7.95 (d, J = 16.2 Hz, 1H), 7.81 (t, J = 7.1 Hz, 1H), 7.72 – 7.63 (m, 3H), 7.50 – 7.40 (m, 4H), 7.01 (d, J = 16.2 Hz, 1H).

¹³C NMR (100 MHz, DMSO-d₆) δ 161.7, 151.4, 149.0, 138.3, 135.0, 134.5, 129.8, 129.1 (2C), 127.6 (2C), 127.1, 126.2, 125.9, 121.1. Quaternary carbon not observed.

LRMS (ESI⁺): 249.1 (M+H, C₁₆H₁₃N₂O, 100%); **LRMS** (ESI⁻): 247.2 (M-H, C₁₆H₁₁N₂O, 100%).

Mass: 248 mg

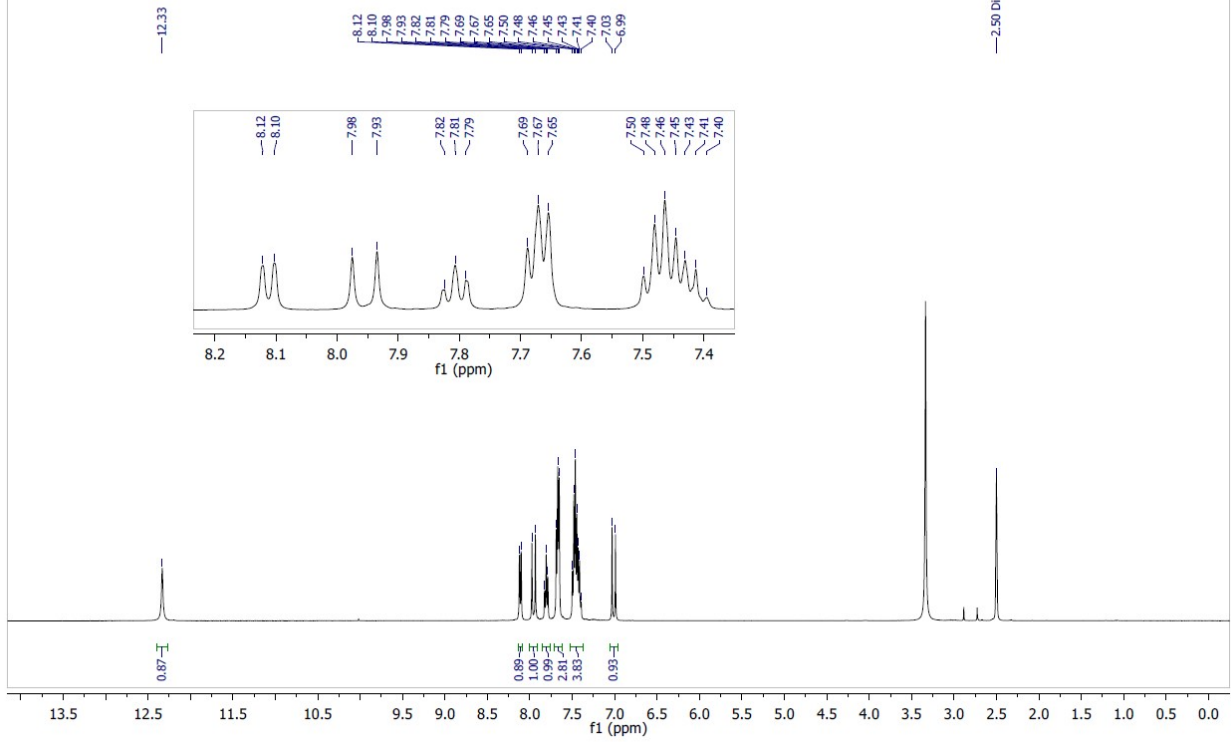
m.p. 243 – 256 °C

yield 59 %

colour off white solid

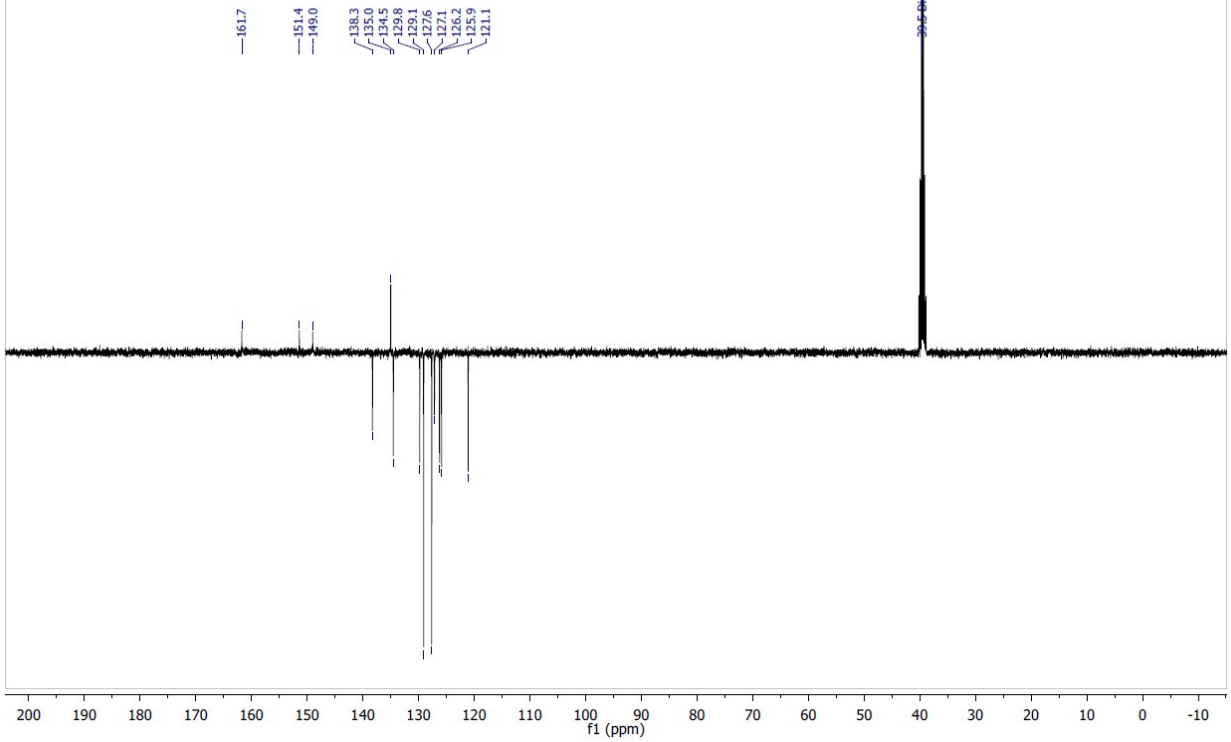
NOB4049_FS

PROTON DMSO {C:\Data} NickO 60

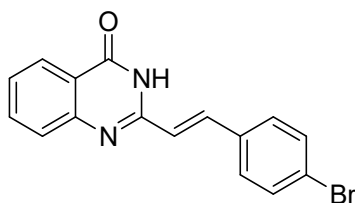


NOB4049_FS

13C_DEPTQ135 DMSO {C:\Data} NickO 60



4-(bromostyryl)quinazolin-4(3H)-one (52)



Chemical Formula: $C_{16}H_{11}BrN_2O$

Exact Mass: 326.01

Molecular Weight: 327.18

IR (neat): $\nu_{\max} = 3004, 1665$ (C=O), 770 (C-Br) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 12.34 (s, 1H), 8.12 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.92 (d, $J = 16.2$ Hz, 1H), 7.84 – 7.80 (m, 1H), 7.67 (dd, $J = 8.1, 6.1$ Hz, 3H), 7.62 (d, $J = 8.6$ Hz, 2H), 7.49 (t, $J = 7.5$ Hz, 1H), 7.03 (d, $J = 16.2$ Hz, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.2, 151.7, 149.4, 137.4, 135.0, 134.8, 132.5 (2C), 130.0 (2C), 127.6, 126.8, 126.3, 123.4, 122.4, 121.6. 2D confirms 2C assignment

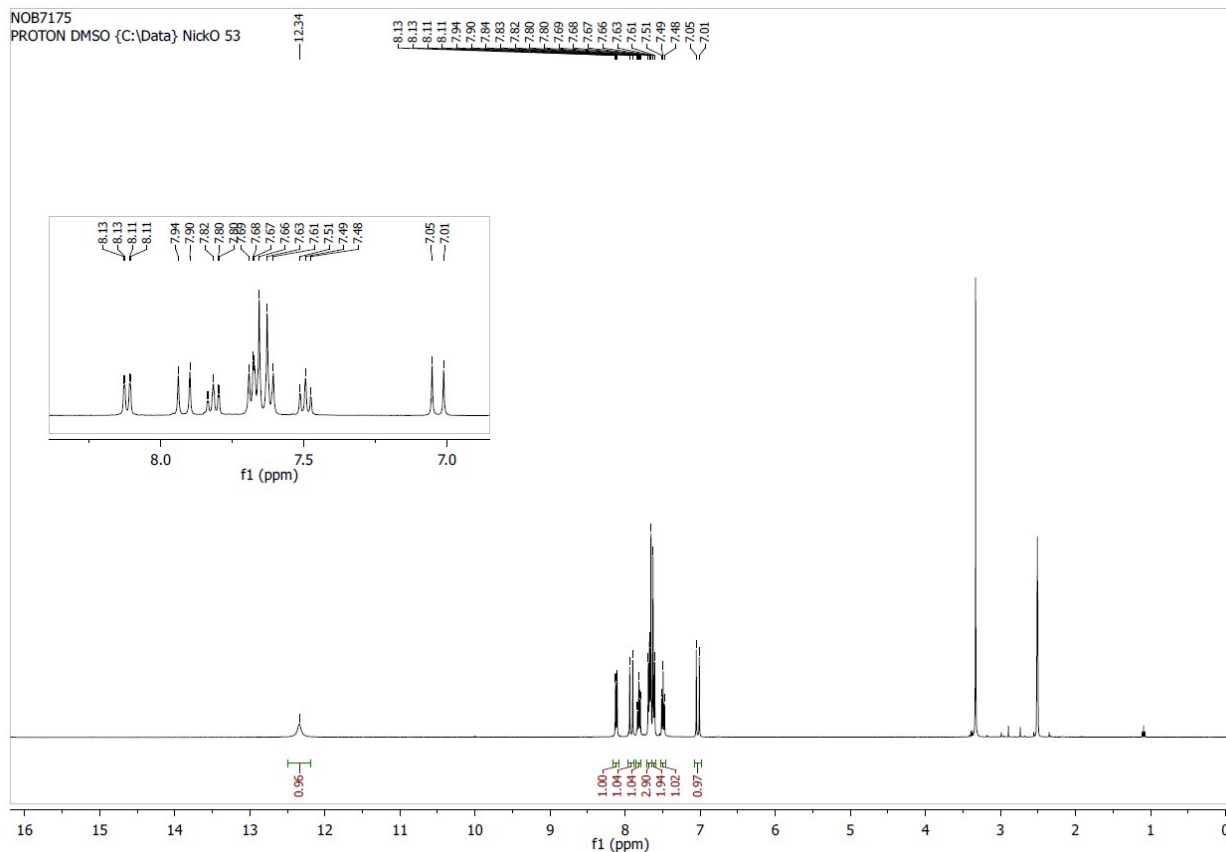
LRMS (ESI+) 327 (M+H, $C_{16}H_{12}Br^{79}N_2O$, 100%) 329 (M+H, $C_{16}H_{12}Br^{81}N_2O$, 85%); (ESI-): 325 (M-H, $C_{16}H_{10}Br^{79}N_2O$, 100%), 327 (M-H, $C_{16}H_{10}Br^{81}N_2O$, 95%)

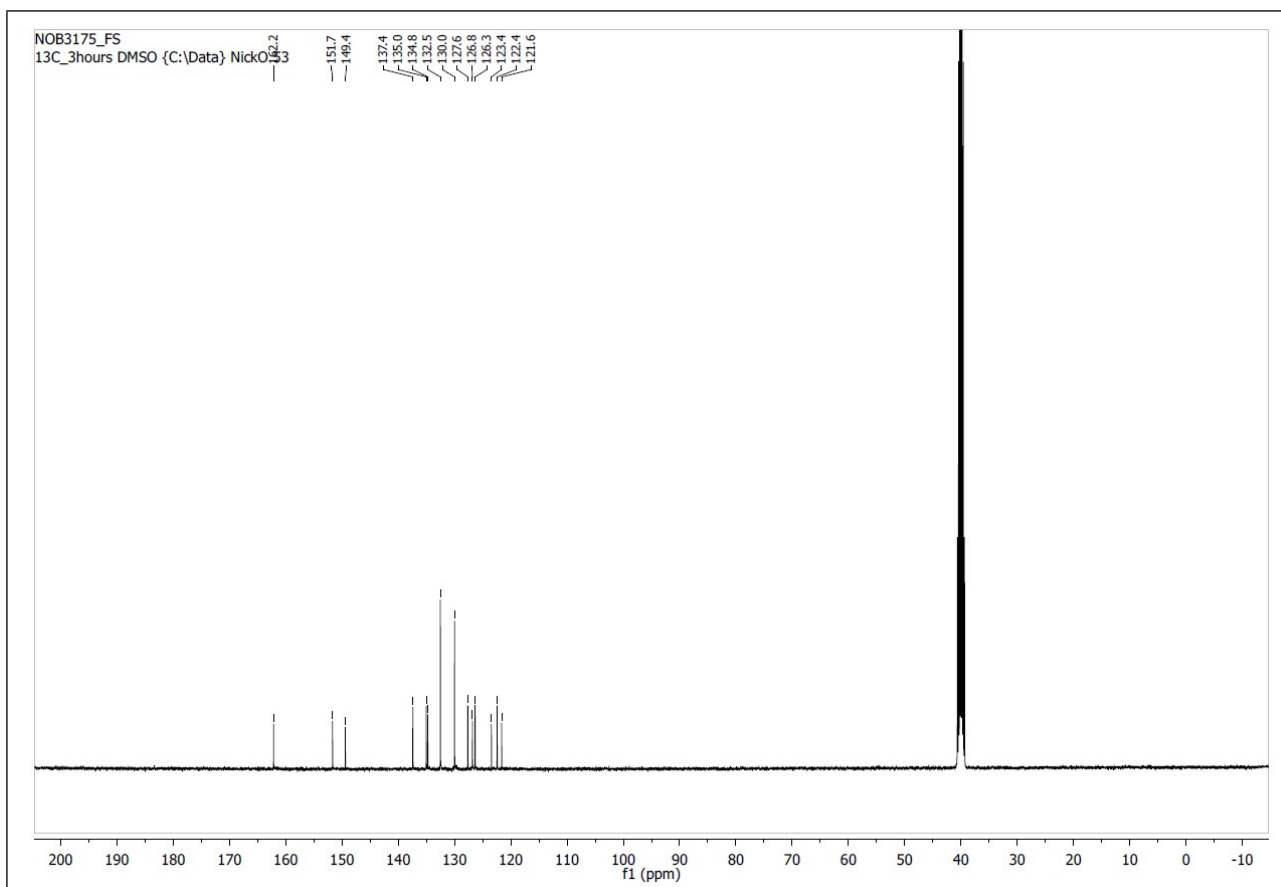
Mass 81.7 mg

m.p. 296 – 310°C

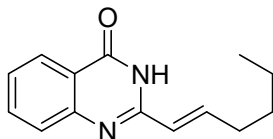
yield 39 %

colour Off-white solid





2-(hex-1-en-yl)quinazolin-4(3H)-one (**53**)



Chemical Formula: C₁₄H₁₆N₂O

Exact Mass: 228.13

Molecular Weight: 228.29

IR (neat): ν_{\max} = 2908 (CH), 1708 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 8.14 (s, 1H), 7.94-7.88 (m, 2H), 7.64 (s, 1H), 2.85 (s, 1H), 2.64 (s, 1H), 1.79 (s, 1H), 1.36-1.28 (m, 4H), 0.89 (m, 4H).

¹³C NMR (100 MHz, DMSO-d₆) δ 160.8, 135.9, 128.1, 126.8, 120.4, 32.9, 31.2, 29.6, 28.5, 27.5, 22.3, 22.1, 14.4.

LRMS (ESI⁺): 229.1 (M+H, C₁₄H₁₇N₂O, 100%); **LRMS** (ESI⁻): 227.1 (M-H, C₁₄H₁₅N₂O, 100%).

Mass 109 mg

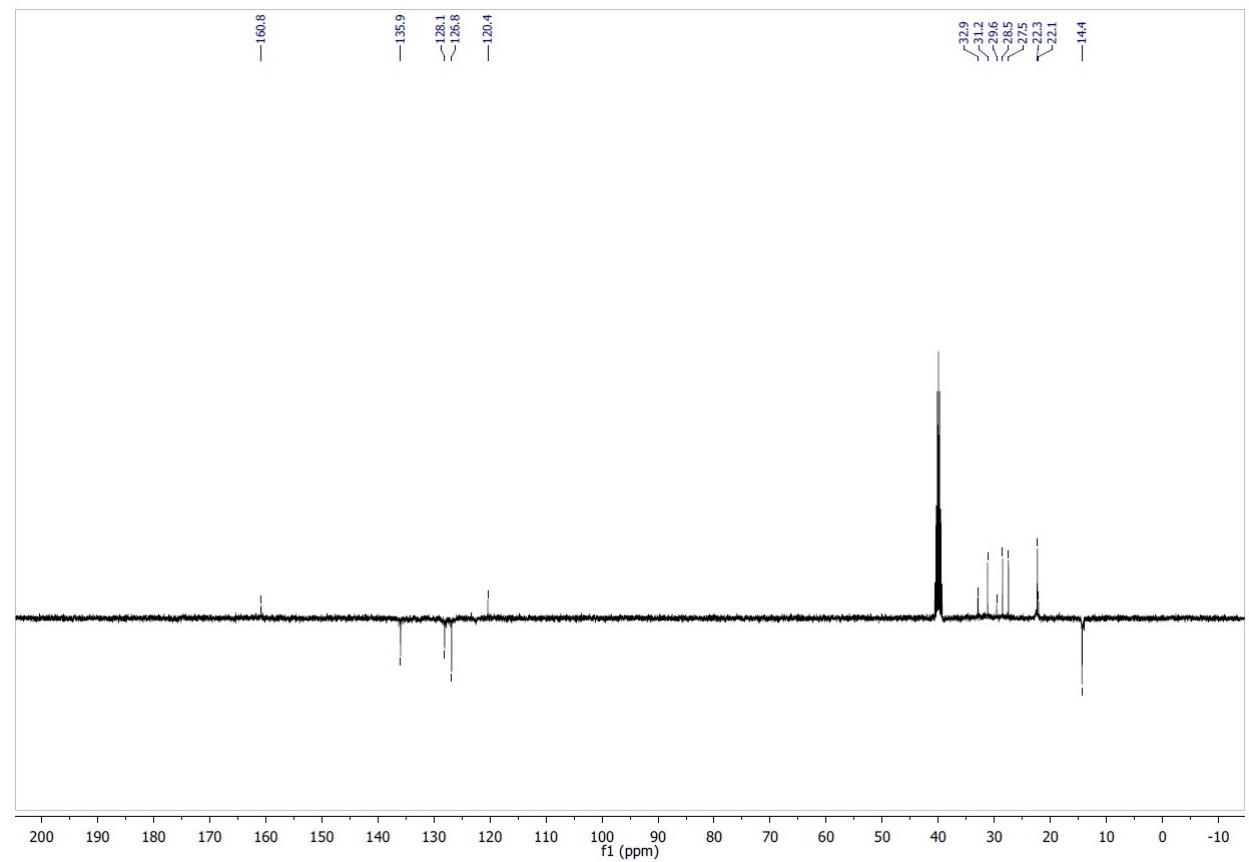
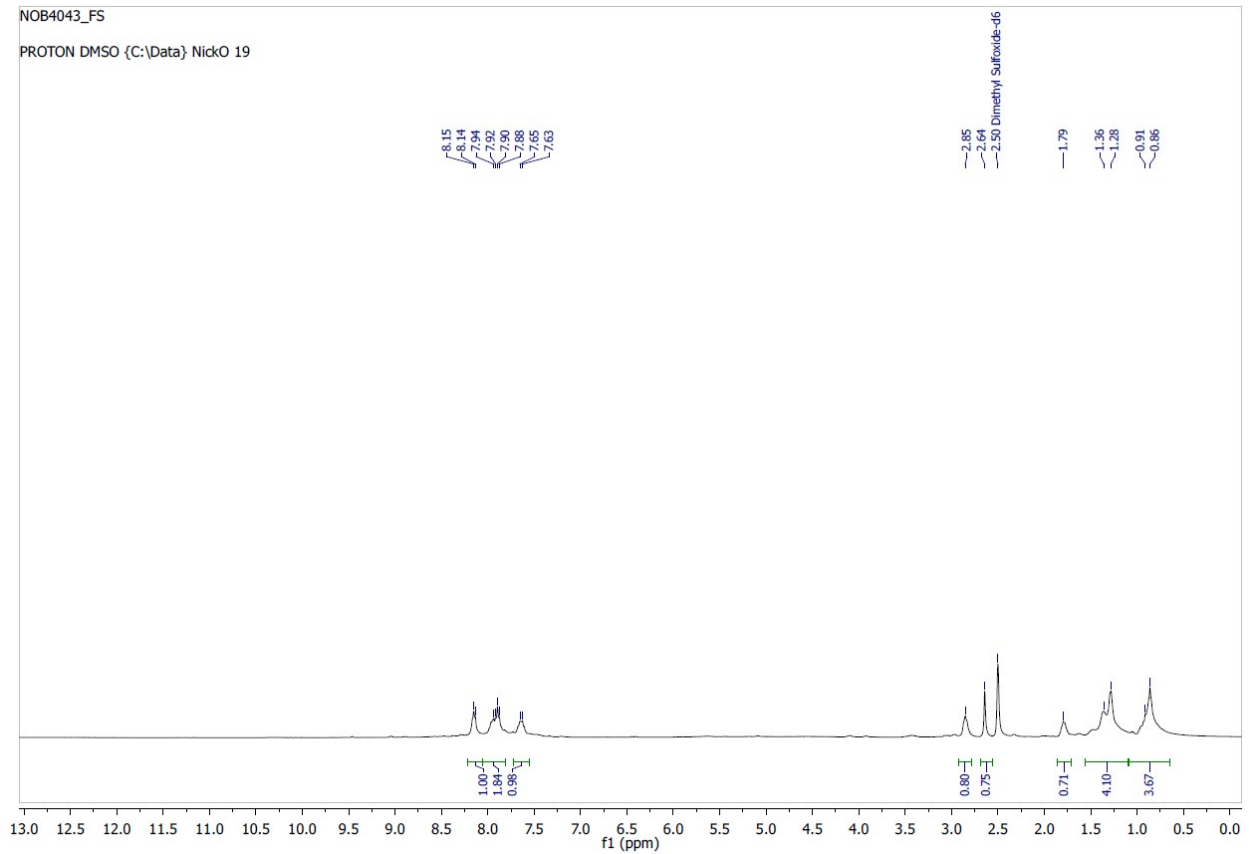
m.p. 148 - 151 °C

yield 28 %

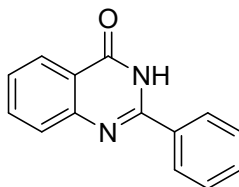
white solid

NOB4043_FS

PROTON DMSO (C:\Data) NickO 19



2-phenylquinazolin-4(3H)-one (54)



Chemical Formula: C₁₄H₁₀N₂O

Exact Mass: 222.08

Molecular Weight: 222.24

IR (neat): ν_{\max} = 3060 (N-H stretch), 1661 (C=O), 766.5 (C=C) cm⁻¹

¹H NMR (400 MHz, CDCl₃) δ 8.34 (dd, J = 7.9, 0.9 Hz, 1H), 8.27 (m, 2H), 7.87 – 7.77 (m, 2H), 7.64 – 7.55 (m, 3H), 7.51 (dt, 1H). NH proton not observed.

¹³C NMR (100 MHz, CDCl₃) δ 164.0, 151.9, 149.7, 135.0, 133.0, 131.8, 129.2 (2C), 128.2, 127.6 (2C), 126.9, 126.5, 121.0.

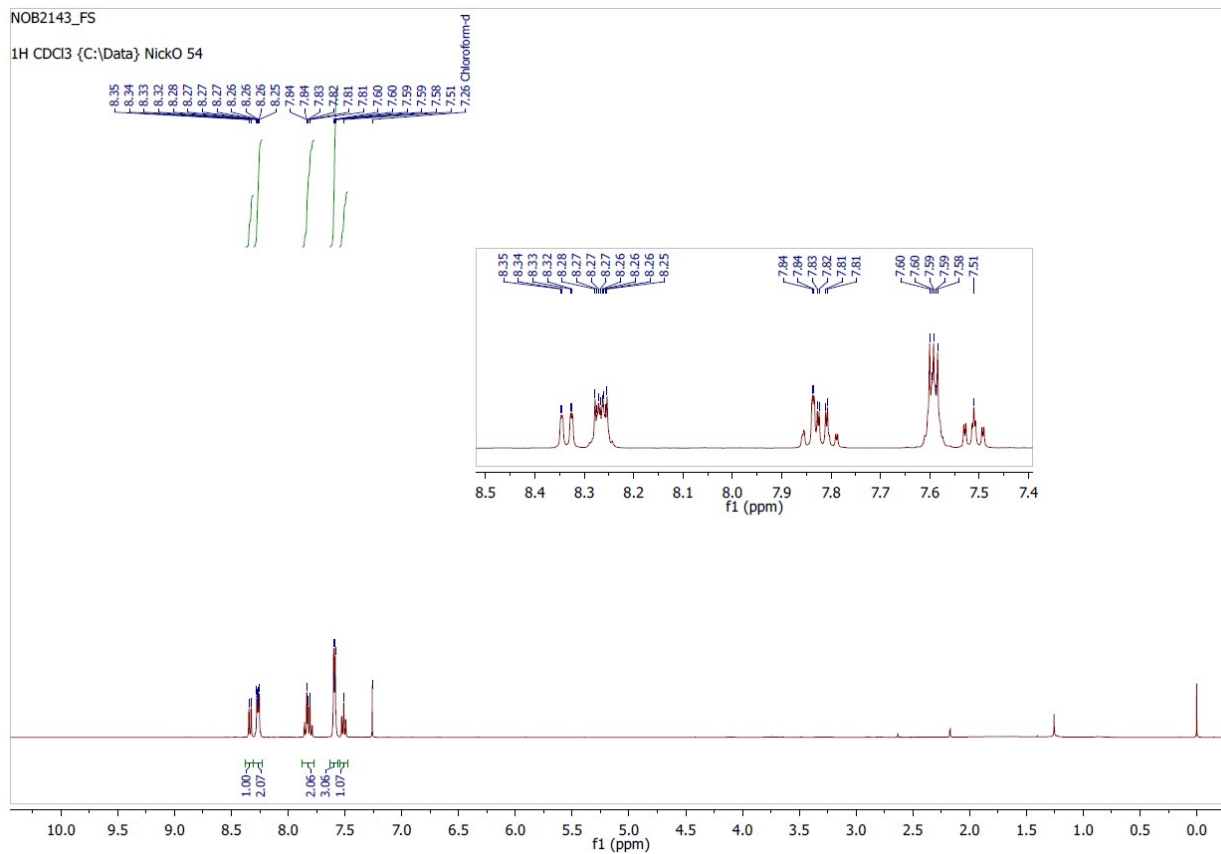
LRMS (ESI+): 223.2 (M+H, C₁₄H₁₁N₂O, 100%); (ESI-): 221.1 (M-H, C₁₄H₉N₂O, 100%).

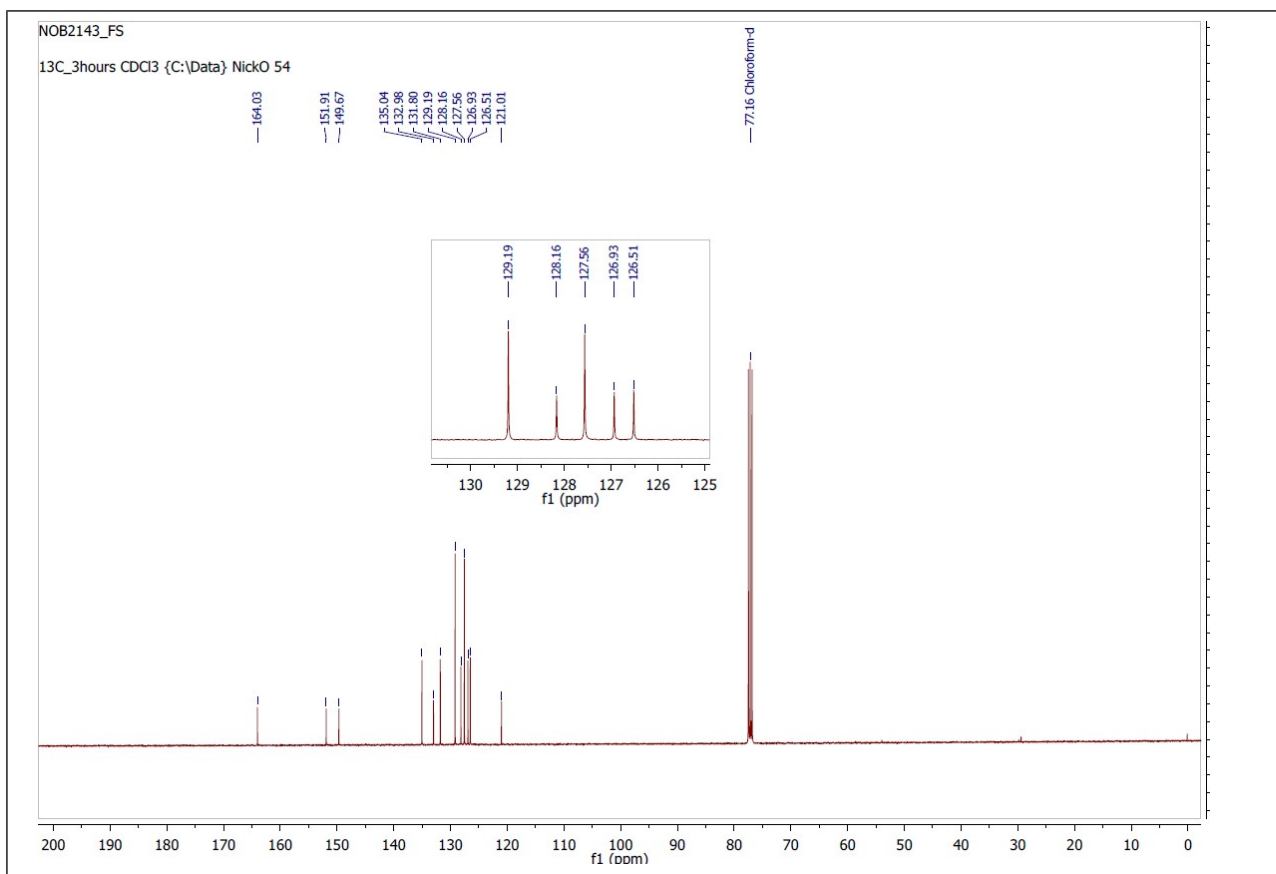
Mass 115.5 mg

m.p. >223 °C (dec.)

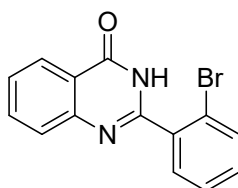
yield 81 %

white crystals





2-(2-bromophenyl)quinazolin-4(1H)-one (**55**)



Chemical Formula: $C_{14}H_9BrN_2O$

Exact Mass: 299.99

Molecular Weight: 301.14

IR (neat): ν_{max} = 3282 (NH), 3159 (NNH), 1666 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.27 (s, 1H), 8.17 (dd, J = 8.0, 1.1 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.76 (dd, J = 7.9, 1.1 Hz, 1H), 7.70 (dd, J = 8.1, 0.5 Hz, 1H), 7.65 – 7.45 (m, 3H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.0, 153.9, 148.9, 136.3, 135.1, 133.1, 132.2, 131.2, 128.2, 127.9, 127.6, 126.3, 121.6, 121.4.

LRMS (ESI +) m/z : 301 (M+H, $C_{14}H_{10}^{79}BrN_2O$, 100%), 303 (M+H, $C_{14}H_{10}^{81}BrN_2O$, 95%); (ESI-) m/z : 199 (M-H, $C_{14}H_8^{79}BrN_2O$, 100%), 301 (M-H, $C_{14}H_8^{81}BrN_2O$, 95%).

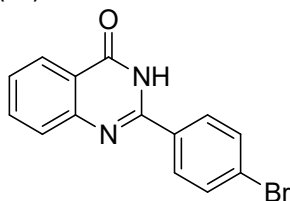
Mass 93 mg

m.p. >165 °C (dec.)

yield 65 %

white crystals

2-(4-bromophenyl)quinazolin-4(1H)-one (56)



Chemical Formula: $C_{14}H_9BrN_2O$

Exact Mass: 299.99

Molecular Weight: 301.14

IR (neat): $\nu_{\max} = 2928$ (CH), 1670 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 8.19 – 8.10 (m, 3H), 7.85-7.83 (m, 1H), 7.78-7.74 (m, 3H), 7.58 – 7.50 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.1, 151.5, 148.6, 134.7, 131.9, 131.6 (2C), 129.8 (2C), 127.5, 126.9, 125.8, 125.3, 121.0.

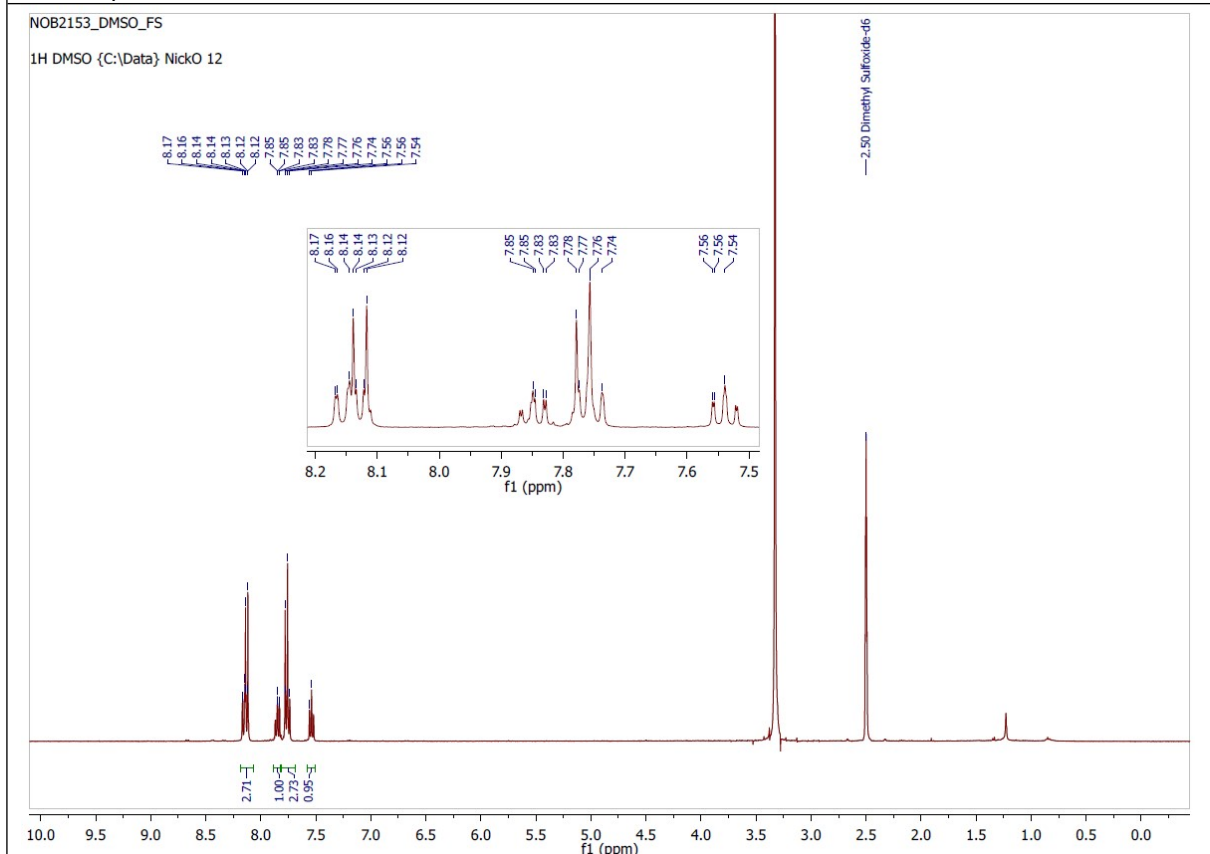
LRMS (ESI+): 301 (M+H, $C_{14}H_9^{79}BrN_2O$, 100%), 303.1 (M+H, $C_{14}H_9^{81}BrN_2O$, 100%); (ESI-): 299 (M-H, $C_{14}H_8^{79}BrN_2O$, 95%), 301 (M-H, $C_{14}H_8^{81}BrN_2O$, 95%).

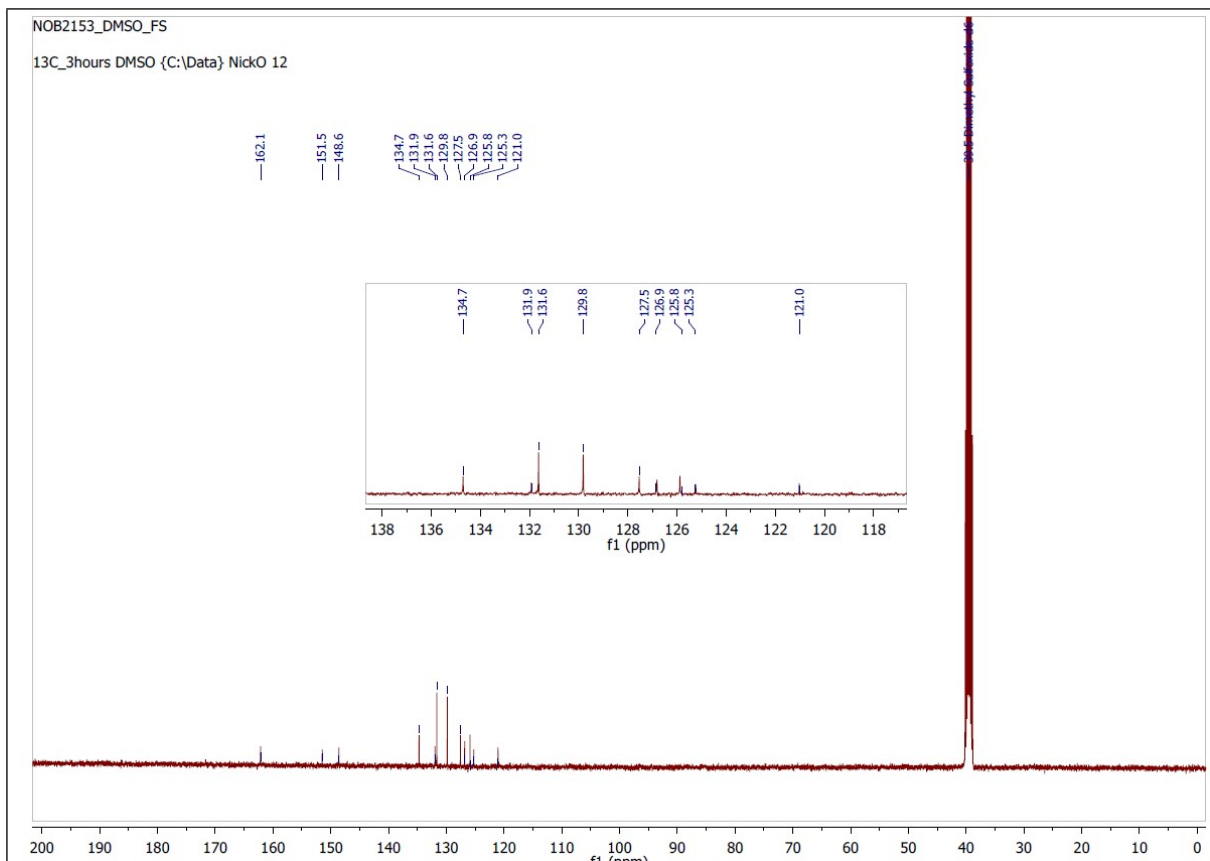
Mass 147 mg

m.p. >300 °C

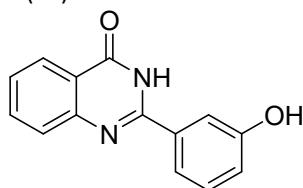
yield 84 %

white crystals





2-(3-hydroxyphenyl)quinazolin-4(3H)-one (**57**)



Chemical Formula: $C_{14}H_{10}N_2O_2$

Exact Mass: 238.07

Molecular Weight: 238.24

IR (neat): ν_{\max} = 3228 (OH) 1657 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 12.43 (s, 1H), 9.79 (s, 1H), 8.15 (d, J = 7.7 Hz, 1H), 7.84 (t, J = 7.3 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.60 (m, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.34 (t, J = 8.1 Hz, 1H), 6.99 (d, J = 7.3 Hz, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 157.97, 135.05, 134.50, 130.14, 127.91, 126.99, 126.32, 121.44, 118.98, 118.82, 115.03.

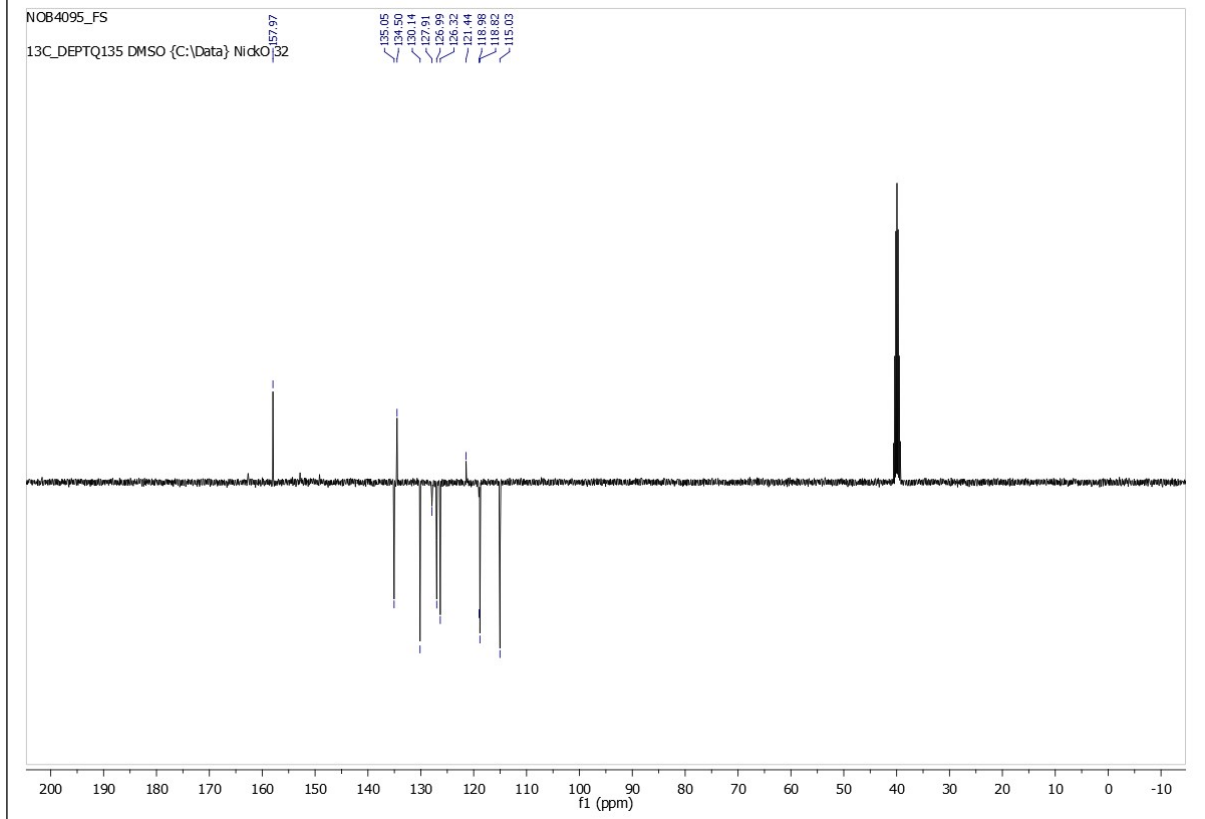
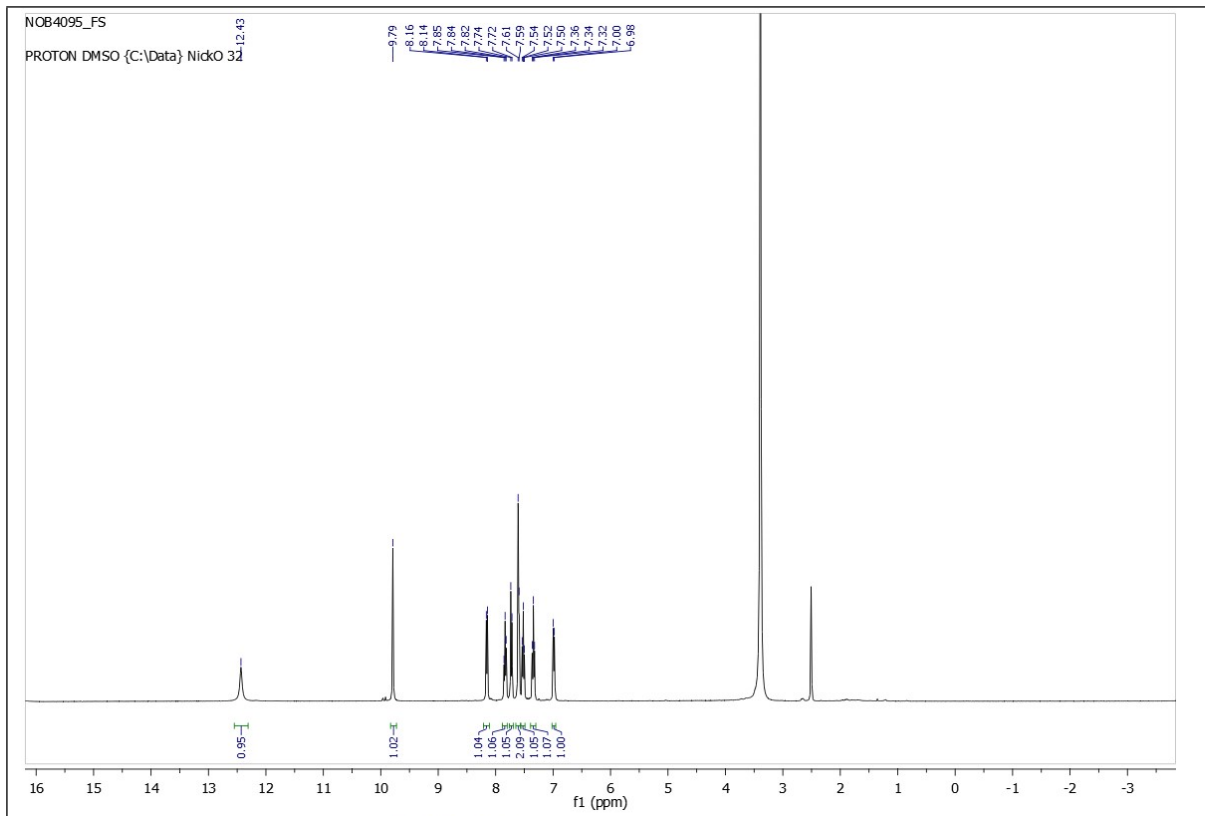
LRMS (ESI-): 237.1 (M-H, $C_{14}H_{10}N_2O_2$, 100%).

Mass 225 mg

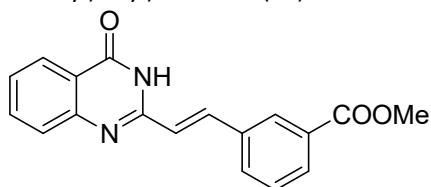
m.p. >250 °C

yield 71 %

white solid



methyl 3-(2-(4-oxo-3,4-dihydroquinazolin-2-yl)vinyl)benzoate (**60**)



Chemical Formula: C₁₈H₁₄N₂O₃

Exact Mass: 306.10

Molecular Weight: 306.32

IR (neat): ν_{\max} = 2990 (CH), 1725 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.33 (s, 1H), 8.22 (s, 1H), 8.15 – 8.07 (m, 1H), 8.04 – 7.95 (m, 3H), 7.86 – 7.78 (m, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.64 – 7.58 (m, 2H), 7.52 – 7.47 (m, 1H), 7.12 (d, J = 16.2 Hz, 1H), 3.90 (s, 3H).

¹³C NMR (101 MHz, DMSO-d₆) δ 165.9, 137.1, 135.6, 134.6, 132.4, 130.5, 130.1, 129.7, 127.8, 126.5, 125.9, 122.4, 121.2, 52.4, 39.5.

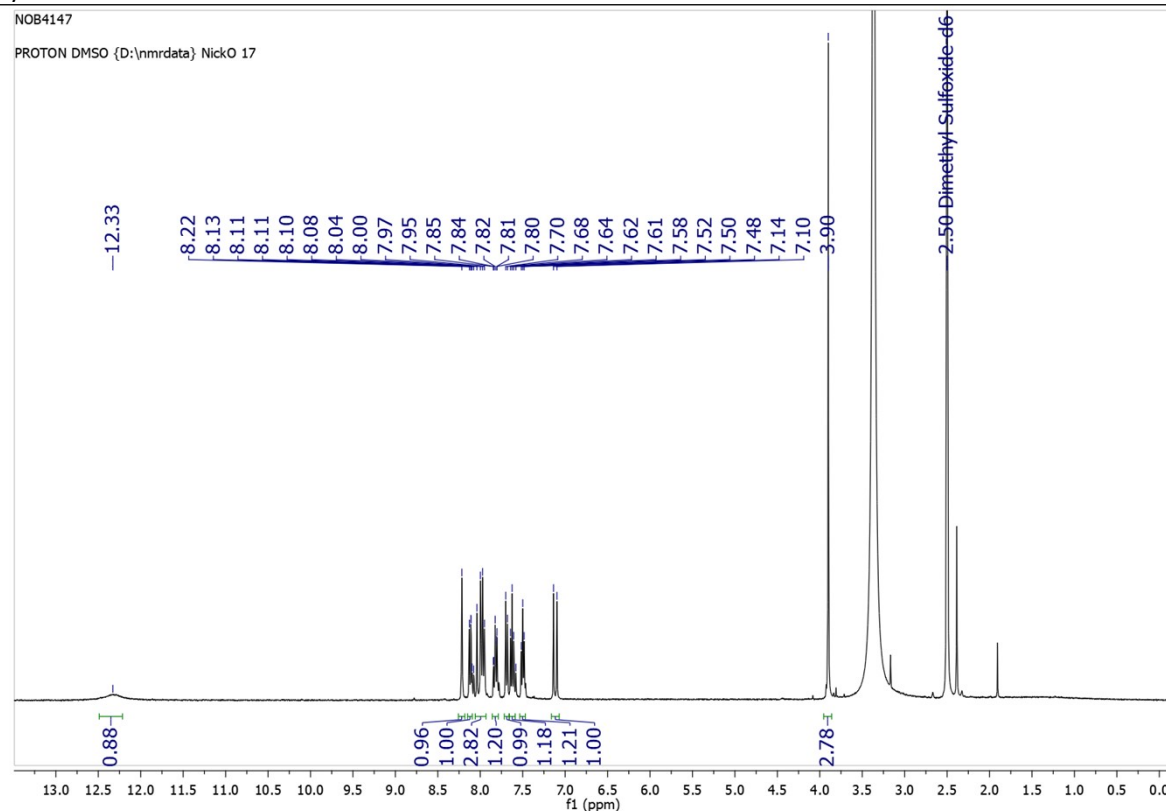
LRMS (ESI+): 307.1 (M+H, C₁₈H₁₅N₂O₃, 100%), (ESI-): 305.1 (M-H, C₁₈H₁₃N₂O₃, 100%),

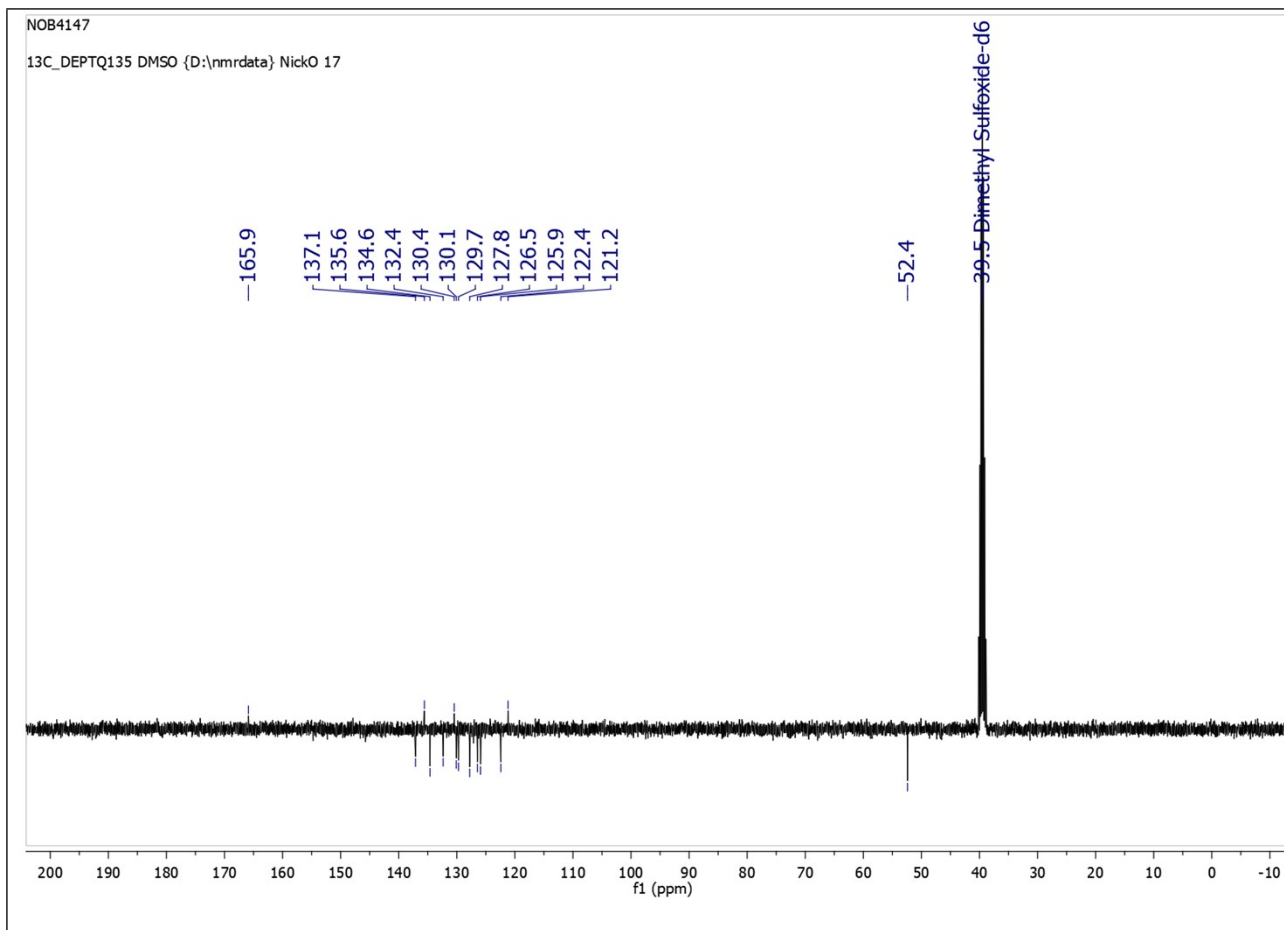
Mass 88 mg

m.p. >183 °C (dec.)

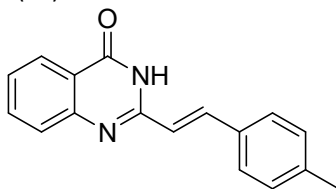
yield 31 %

yellow solid





2-(4-methylstyryl)quinazolin-4(3H)-one (**61**)



Chemical Formula: $C_{17}H_{14}N_2O$

Exact Mass: 262.11

Molecular Weight: 262.31

IR (neat): ν_{\max} 3049 (CH), 1674 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 12.29 (s, 1H), 8.11 (dd, $J = 7.9, 1.3$ Hz, 1H), 7.92 (d, $J = 16.2$ Hz, 1H), 7.85 – 7.78 (m, 1H), 7.67 (d, $J = 7.9$ Hz, 1H), 7.56 (d, $J = 8.1$ Hz, 2H), 7.51 – 7.44 (m, 1H), 7.28 (d, $J = 8.0$ Hz, 2H), 6.95 (d, $J = 16.2$ Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 140.15, 138.76, 134.98, 132.72, 130.15, 128.09, 127.54, 126.59, 126.32, 121.49, 120.43, 21.47.

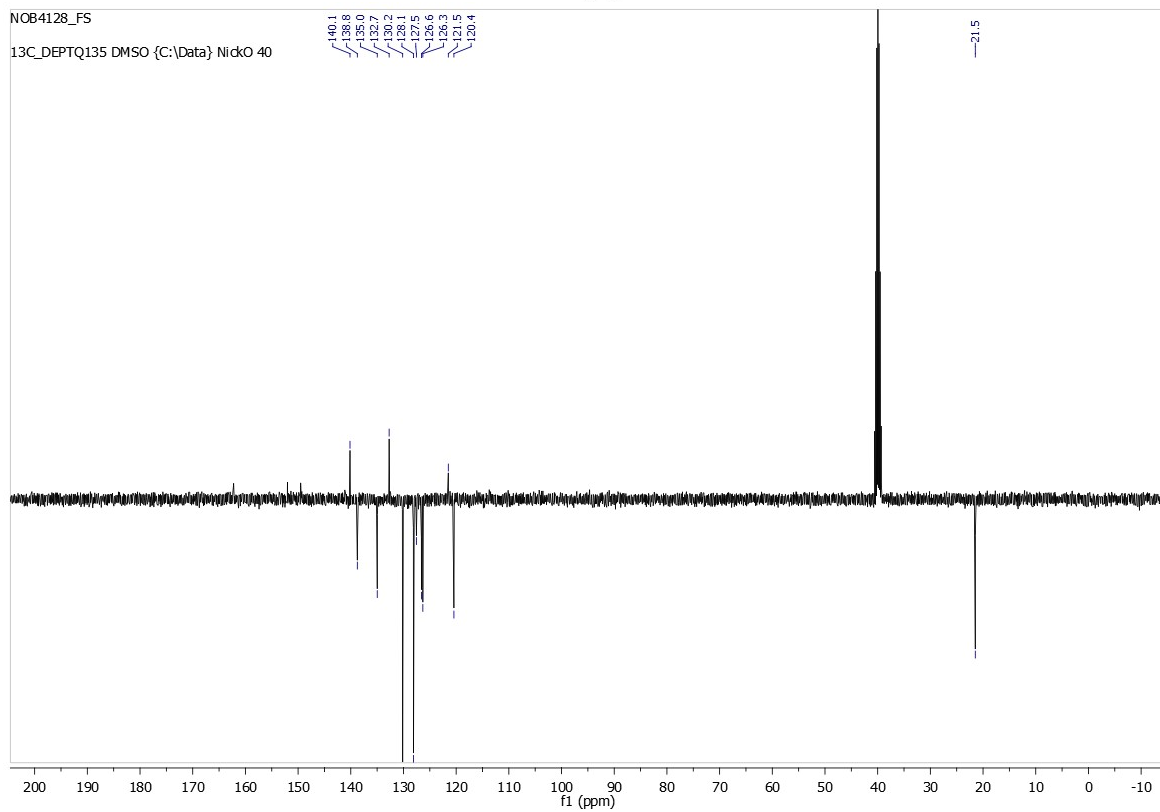
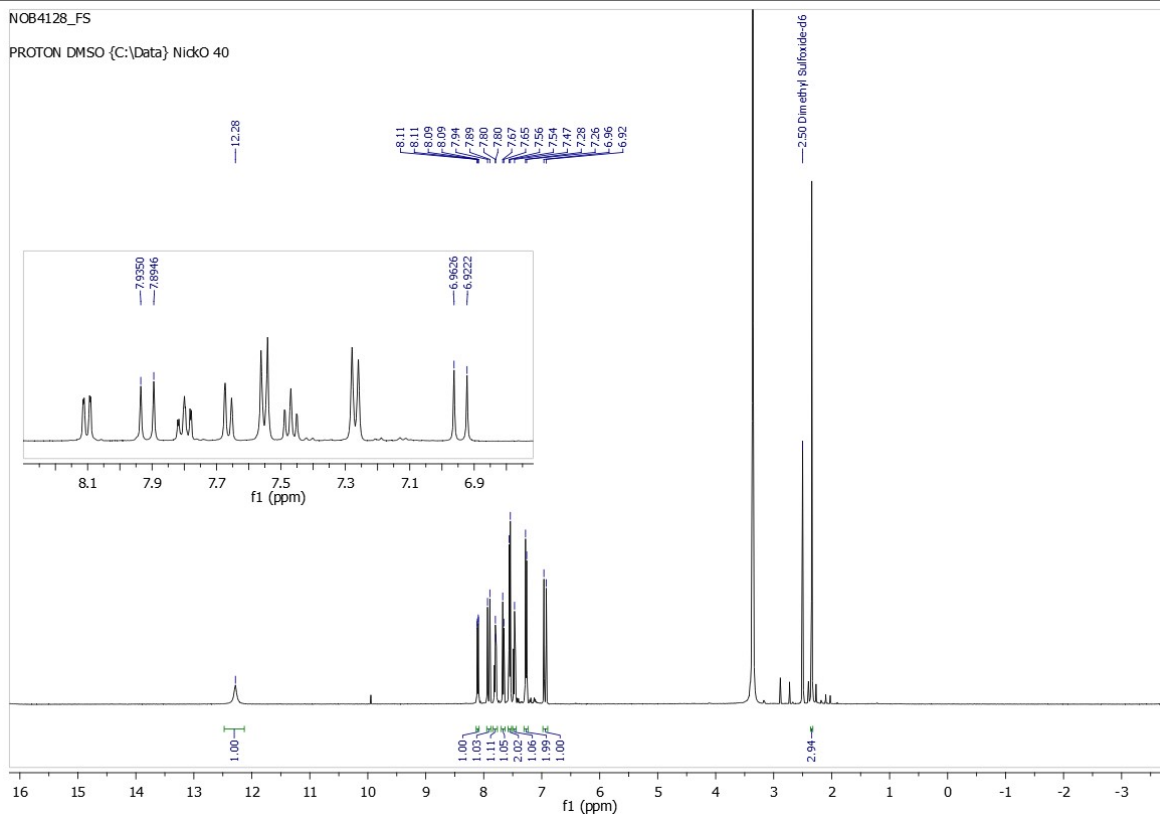
LRMS (ESI+): 263.1 (M+H, $C_{17}H_{15}N_2O$, 100%); LRMS (ESI-): 261.1 (M-H, $C_{17}H_{13}N_2O$, 100%).

Mass: 49.8 mg

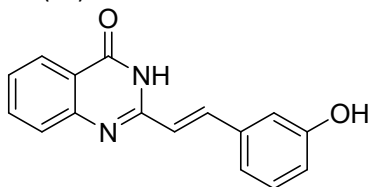
m.p. >250 °C

yield 20 %

white solid



2-(3-hydroxystyryl)quinazolin-4(3H)-one (**62**)



Chemical Formula: C₁₆H₁₂N₂O₂

Exact Mass: 264.09

Molecular Weight: 264.28

IR (neat): ν_{\max} = 3053 (OH), 1680 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.32 (s, 1H), 9.67 (s, 1H), 8.11 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.87 (d, *J* = 16.1 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.1 Hz, 1H), 7.26 (t, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 7.03 (s, 1H), 6.92 (d, *J* = 16.1 Hz, 1H), 6.83 (dd, *J* = 8.0, 1.8 Hz, 1H).

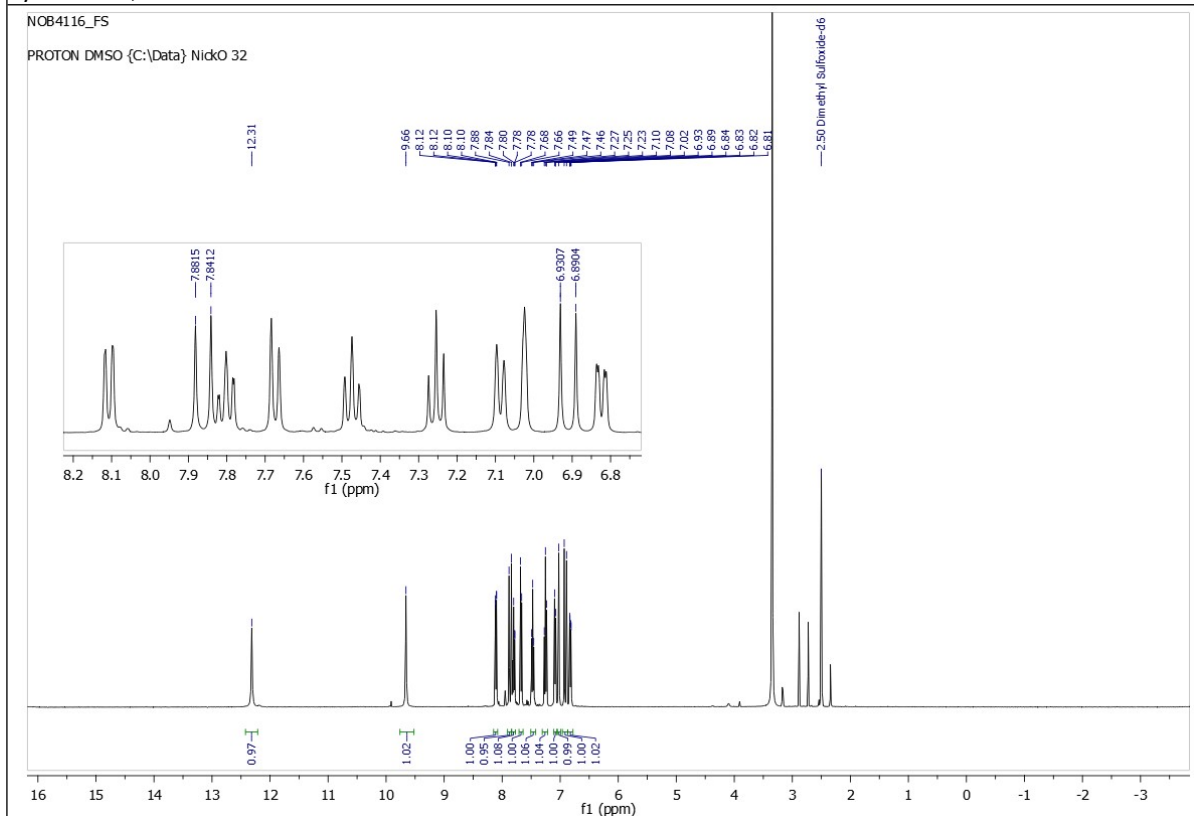
¹³C NMR (100 MHz, DMSO-d₆) δ 162.20, 158.25, 151.86, 149.48, 138.95, 136.71, 134.98, 130.55, 127.60, 126.66, 126.32, 121.56, 121.24, 119.32, 117.53, 114.21.

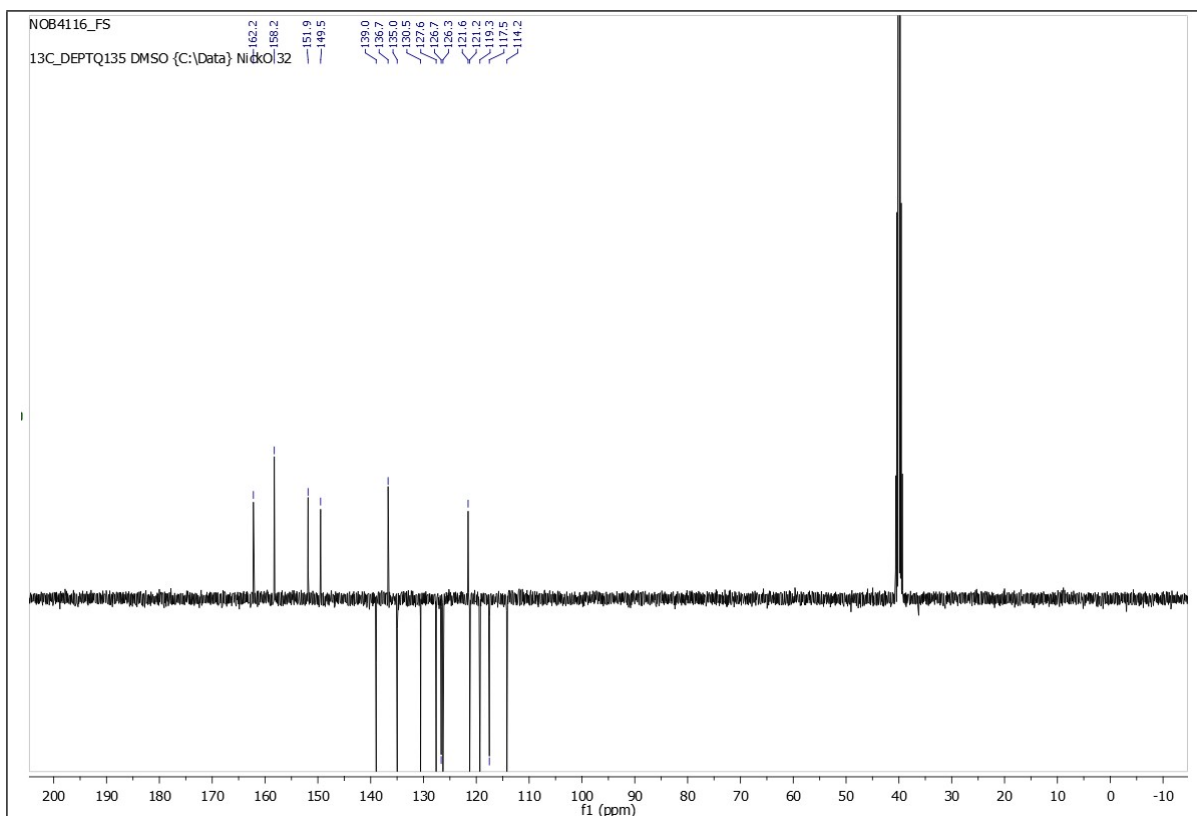
LRMS (ESI⁺): 265.1 (M+H, C₁₆H₁₃N₂O₂, 100%); LRMS (ESI⁻): 263.1 (M-H, C₁₆H₁₁N₂O₂, 100%).

Mass 67.1 mg

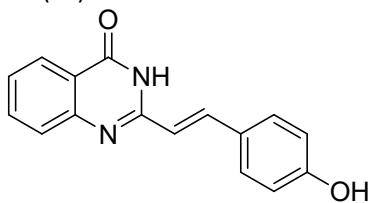
m.p. >250 °C

yield 28 %; brown solid





2-(4-hydroxystyryl)quinazolin-4(3H)-one (**63**)



Chemical Formula: $C_{16}H_{12}N_2O_2$

Exact Mass: 264.09

Molecular Weight: 264.28

IR (neat): $\nu_{\max} = 3064$ (OH), 1674 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 12.22 (s, 1H), 9.99 (s, 1H), 8.09 (dd, $J = 7.9, 1.2$ Hz, 1H), 7.87 (d, $J = 16.1$ Hz, 1H), 7.83 – 7.73 (m, 1H), 7.64 (d, $J = 7.8$ Hz, 1H), 7.51 (d, $J = 8.6$ Hz, 2H), 7.45 (ddd, $J = 8.1, 7.2, 1.1$ Hz, 1H), 6.85 (dd, $J = 9.1, 2.2$ Hz, 2H), 6.78 (d, $J = 16.1$ Hz, 1H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.27, 159.74, 152.36, 149.67, 138.99, 134.93, 129.95, 127.41, 126.52, 126.30, 121.34, 117.77, 116.41.

LRMS (ESI+): 265.1 (M+H, $C_{16}H_{13}N_2O_2$, 100%); LRMS (ESI-): 263.1 (M-H, $C_{16}H_{11}N_2O_2$, 100%).

Mass 92.9 mg

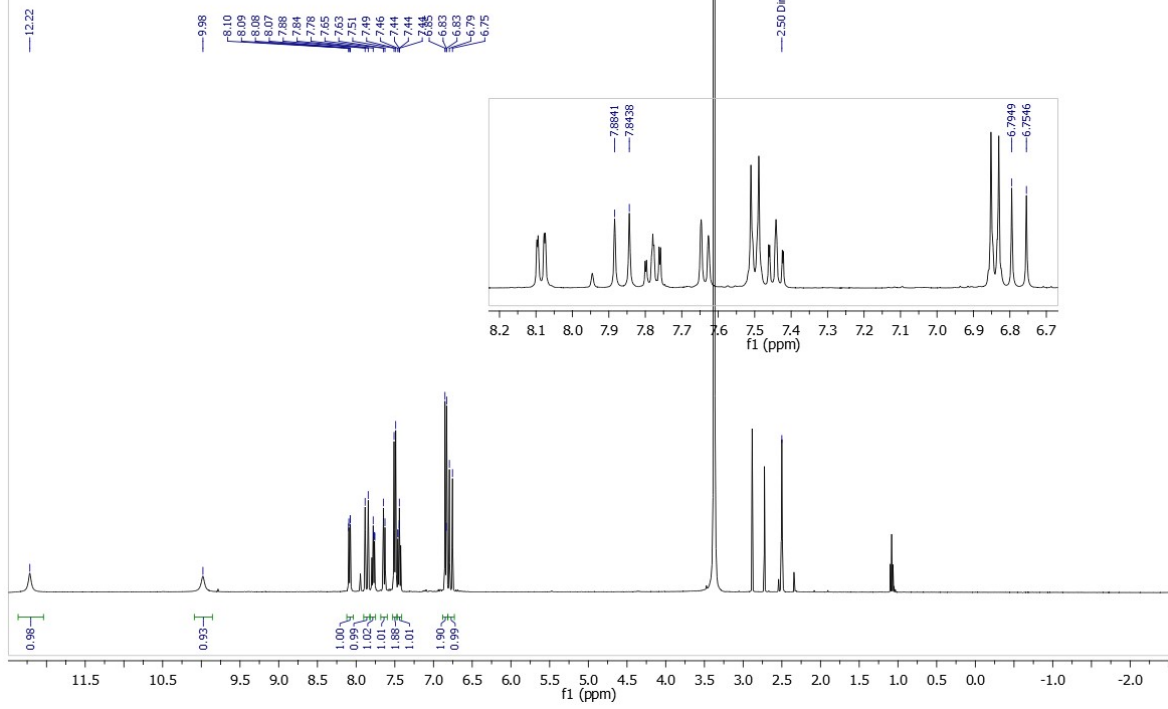
m.p. >250 °C

yield 43 %

white solid

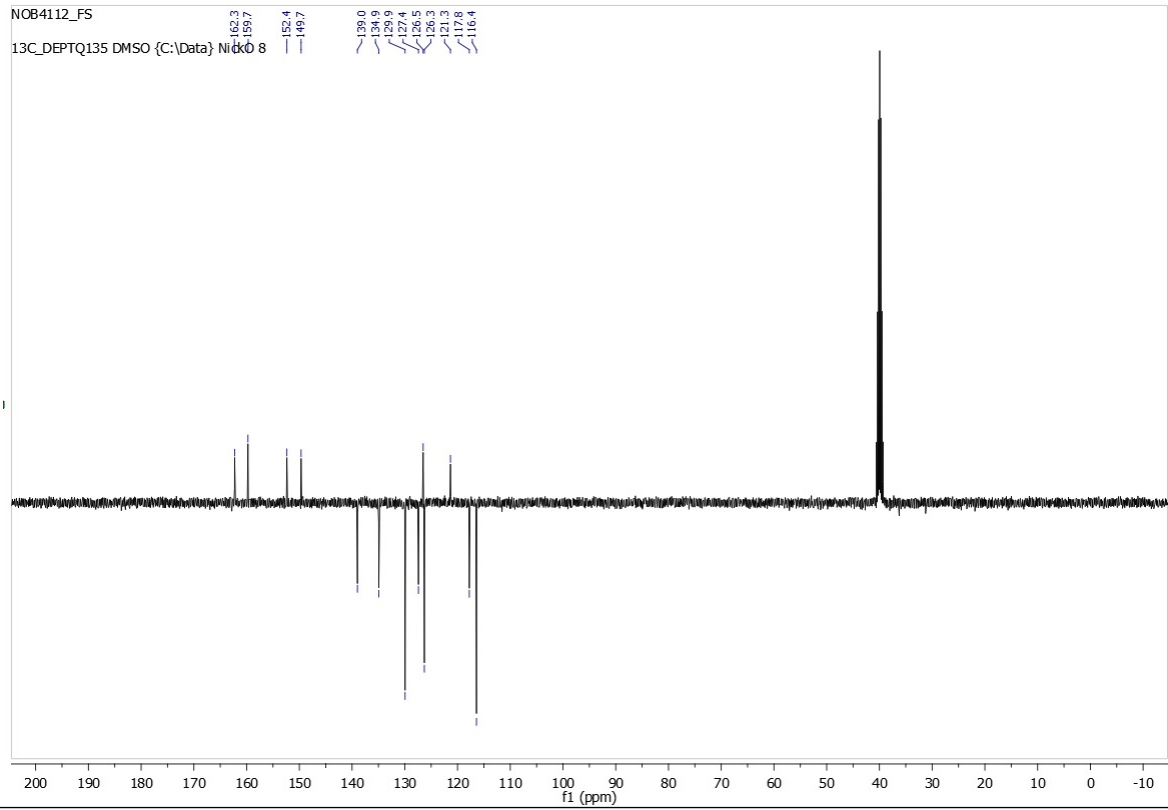
NOB4112_FS

1H DMSO {C:\Data} NickO 8

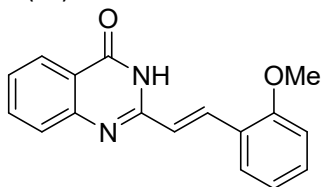


NOB4112_FS

13C DEPTQ135 DMSO {C:\Data} NickO 8



2-(2-methoxystyryl)quinazolin-4(3H)-one (**64**)



Chemical Formula: C₁₇H₁₄N₂O₂

Exact Mass: 278.11

Molecular Weight: 278.31

IR (neat): ν_{\max} = 3087 (NH), 1677 (C=O) cm⁻¹

¹H NMR (400 MHz, DMSO-d₆) δ 12.35 (s, 1H), 8.17 (d, *J* = 16.2 Hz, 1H), 8.11 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.85 – 7.75 (m, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.62 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.44 – 7.37 (m, 1H), 7.16 –

¹³C NMR (100 MHz, DMSO-d₆) δ 162.24, 158.23, 152.27, 149.56, 134.94, 134.08, 131.68, 128.65, 127.60, 126.49, 126.29, 123.88, 121.85, 121.51, 121.31, 112.30, 56.09.

LRMS (ESI+): 279.1 (M+H, C₁₇H₁₅N₂O₂, 100%);

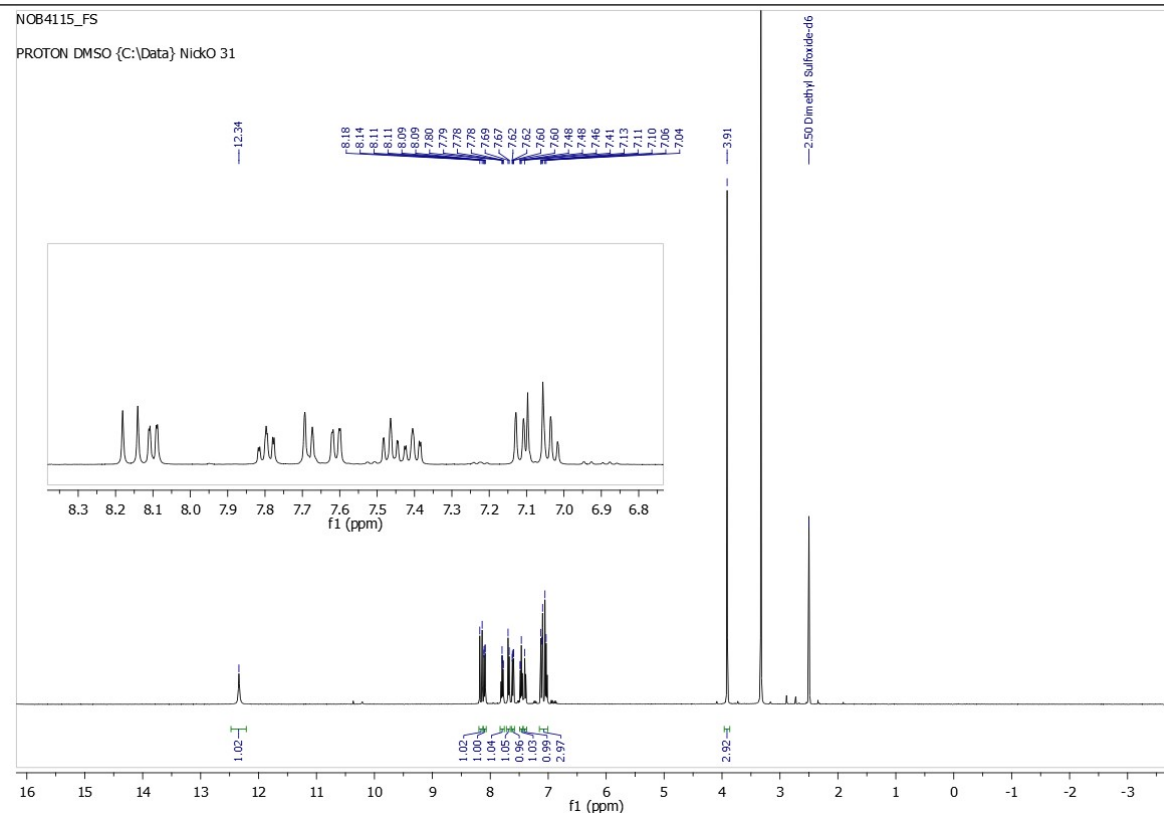
LRMS (ESI-): 277.1 (M-H, C₁₇H₁₃N₂O₂, 100%).

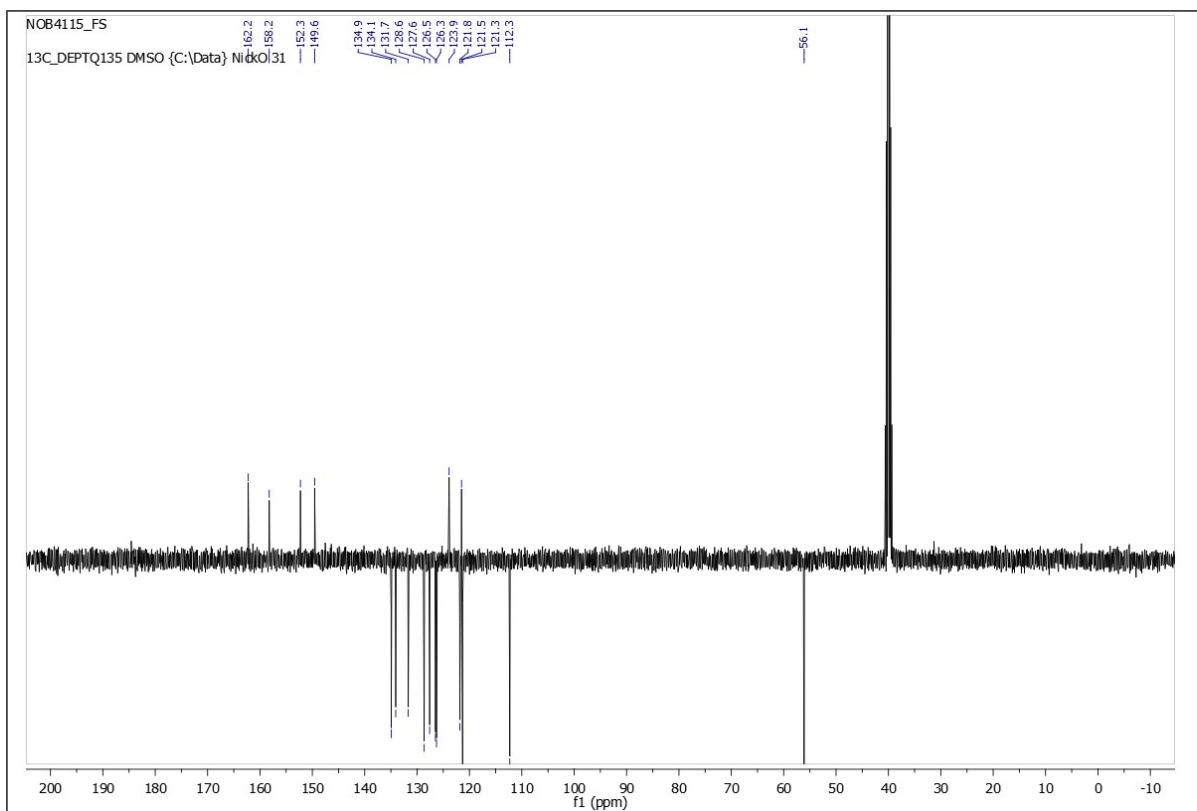
Mass 88.7 mg

m.p. >225 °C (dec.)

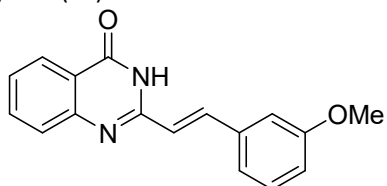
yield 34 %

white solid





2-(3-methoxystyryl)quinazolin-4(3H)-one (**65**)



Chemical Formula: $C_{17}H_{14}N_2O_2$

Exact Mass: 278.11

Molecular Weight: 278.31

IR (neat): ν_{\max} = 3022 (CH), 1674 (C=O) cm^{-1}

1H NMR (400 MHz, DMSO- d_6) δ 12.30 (s, 1H), 8.12 (d, J = 7.1 Hz, 1H), 7.92 (d, J = 16.2 Hz, 1H), 7.85 – 7.76 (m, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.48 (t, J = 7.4 Hz, 1H), 7.38 (t, J = 7.9 Hz, 1H), 7.24 (m, 2H), 7.01 (m, 2H), 3.82 (s, 3H).

^{13}C NMR (100 MHz, DMSO- d_6) δ 162.36, 160.14, 152.05, 149.45, 138.59, 136.92, 134.92, 130.57, 127.51, 126.65, 126.34, 122.08, 121.60, 120.48, 116.08, 113.08, 55.64.

LRMS (ESI+): 279.1 (M+H, $C_{17}H_{15}N_2O_2$, 100%); **LRMS** (ESI-): 277.1 (M-H, $C_{17}H_{13}N_2O_2$, 100%).

Mass 54 mg

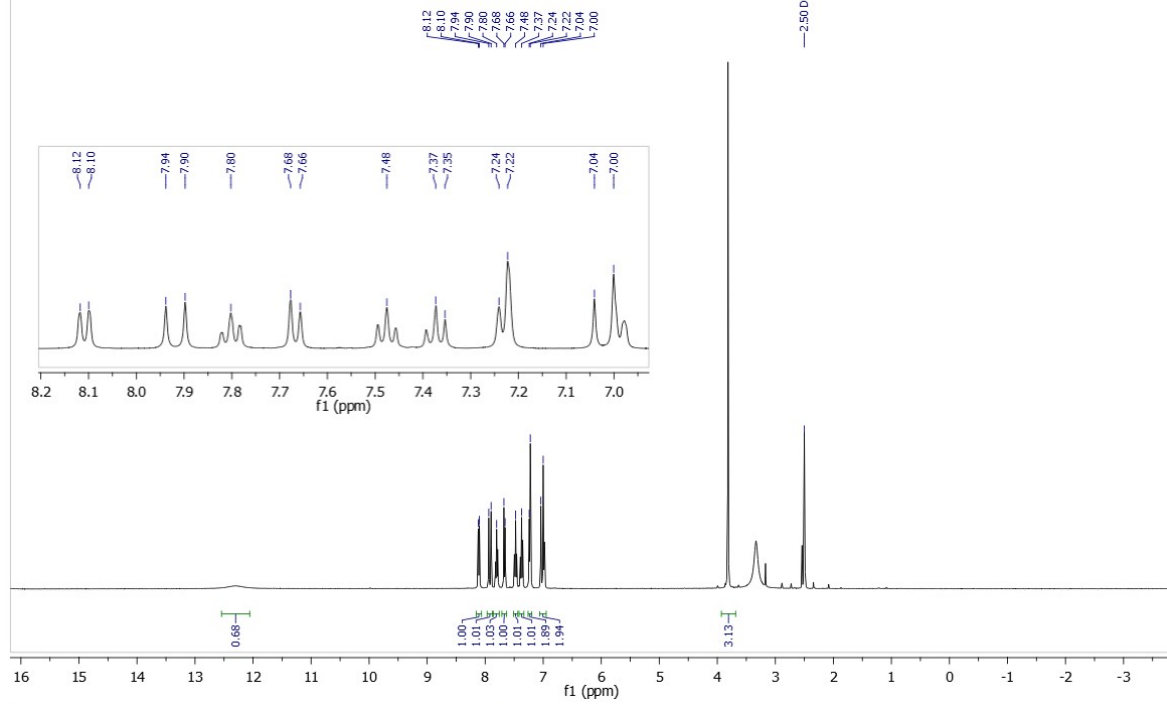
m.p. >250 °C

yield 31 %

white solid

NOB4114_FS

PROTON DMSO {C:\Data} NickO 30



NOB4114_FS

13C_DEPTQ135 DMSO {C:\Data} NickO 30

