Supporting information

Antitubercular and Antiparasitic 2-Nitroimidazopyrazinones with Improved Potency and Solubility

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LC/MS/MS detection and analysis parameters for plasma protein binding, microsomal and plasma stability

LC/MS/MS analysis was performed using AB Sciex 4000 QTRAP System and Shimadzu Nexara UPLC System equipped with Waters Atlantis T3, 2.1 × 50 mm, 5 µm, with guard column and column temperature was set to 40 °C. Injection volume was 3–5 µL and the autosampler cooler was set to 12 °C. The flow rate was 0.2 mL/min with gradient: 5% B for 1 minute then 5–100% B for 5 minutes (A: 0.1% (v/v) formic acid in water and B: 0.1% (v/v) formic acid in acetonitrile). Mass spectrometer parameters in Selected Reaction Monitoring (SRM) mode are tabulated below:

Table S1. Mass spectrometer parameters of analogs tested for their plasma protein binding, microsomal and plasma stability.

Compound	Ionization Mode	Declustering Potential	Collision Energy	*m/z*
pretomanid 2	positive	70	32	360.1→174.8 360.1→200.9
verapamil	positive	70	35	455.3→165.3 455.3→303.3
eucatropine	positive	70	30	292.3→109.4
carbutamide	positive	70	25	272.1→155.8
sulfamethoxazole	positive	60	17	254.3→155.9
17k	positive	70	35	329.2→105.1
26j	positive	70	35	322.1→143.2
34e	positive	70	35	348.2→168.1
34g	positive	70	40	432.0→252.2
34j	positive	70	35	432.1→252.2
34k	positive	70	40	432.2→252.2
34p	positive	70	40	354.2→174.2

HEK293 mammalian cytotoxicity assay (assay B) for *T. b. brucei* selectivity

Compounds were tested for activity against human embryonic kidney cells (HEK293), as described in Sykes et al (2012), with a slight modification, by using resazurin as a viability indicator. Briefly, 7.27×10^4 HEK cells/ml were added in 55 uL of DMEM, high glucose medium to 384-well plates. Following 24 h incubation at 37˚C / 5% CO_2, compounds were added following pre-dilution in DMEM on a Minitrak compound handling system (PerkinElmer). Cells were grown for 72 h before the addition of 10 µL of a final concentration of 49 µM of resazurin, prepared in DMEM. Following 4 h incubation, plates were read on an Envision plate reader (PerkinElmer).

IC_{50} values were calculated from two independent experiments in GraphPad Prism 6 (GraphPad Software).

Table S2. Additional cytotoxicity data to determine selectivity indices of compounds 17a–k, 26a–k, and 34a–p.

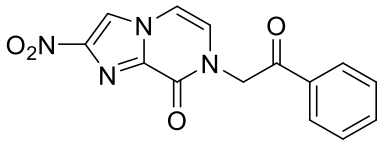
Compound	HEK293 (Assay A)[a] CC_{50} (µM)	HEK293 (Assay B)[b] CC_{50} (µM)	3T3[c] CC_{50} (µM)
17a	>100	>79.4	>73.3
17b	>100	>79.4	>73.3
17c	>100	>79.4	>73.3
17d	>100	>79.4	>73.3
17e	>100	>79.4	>73.3
17f	>100	>79.4	>73.3
17g	>100	>79.4	ND
17h	>100	ND	ND
17i	>100	>79.4	>73.3
17j	>100	>79.4	>73.3
17k	>100	>79.4	>73.3
26a	>100	>73.3	ND
26b	>100	>73.3	ND
26c	>100	>73.3	ND
26d	>100	>73.3	ND
26e	>100	>73.3	ND
26f	>25	>18.3	ND
26g	>118	ND	ND
26h	>94	>79.4	>36.6
26i	>100	>73.3	ND
26j	>100	>79.4	>73.3
26k	>100	>36.6	ND

Compound	HEK293 (Assay A)[a] CC_{50} (µM)	HEK293 (Assay B)[b] CC_{50} (µM)	3T3[c] CC_{50} (µM)
34a	>100	>73.3	>36.6
34b	>100	>79.4	>73.3
34c	>50	>36.6	>36.6
34d	>100	>73.3	>73.3
34e	>92	>79.4	>36.6
34f	>50	>36.6	>18.3
34g	>50	>39.7	>36.6
34h	>50	>36.6	>18.3
34i	>50	>36.6	>36.6
34j	>74	>79.4	>36.6
34k	>100	>79.4	>36.6
34l	>94	>79.4	>36.6
34m	>100	>79.4	>36.6
34n	>50	>36.6	>18.3
34o	>50	>39.7	>18.3
34p	>100	>73.3	>36.6

[a] Assay A was performed based on 20 h of incubation. [b] Assay B was performed based on 72 h of incubation, following a procedure as described in S3. [c] Assay was performed based on 48 h of incubation, to determine the selectivity to *T. cruzi* amastigotes over 3T3 host cells. ND – not determined.

^{1}H and ^{13}C NMR spectra

2-Nitro-7-(2-oxo-2-phenylethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17a)



^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
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5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
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14	Presaturation Frequency	
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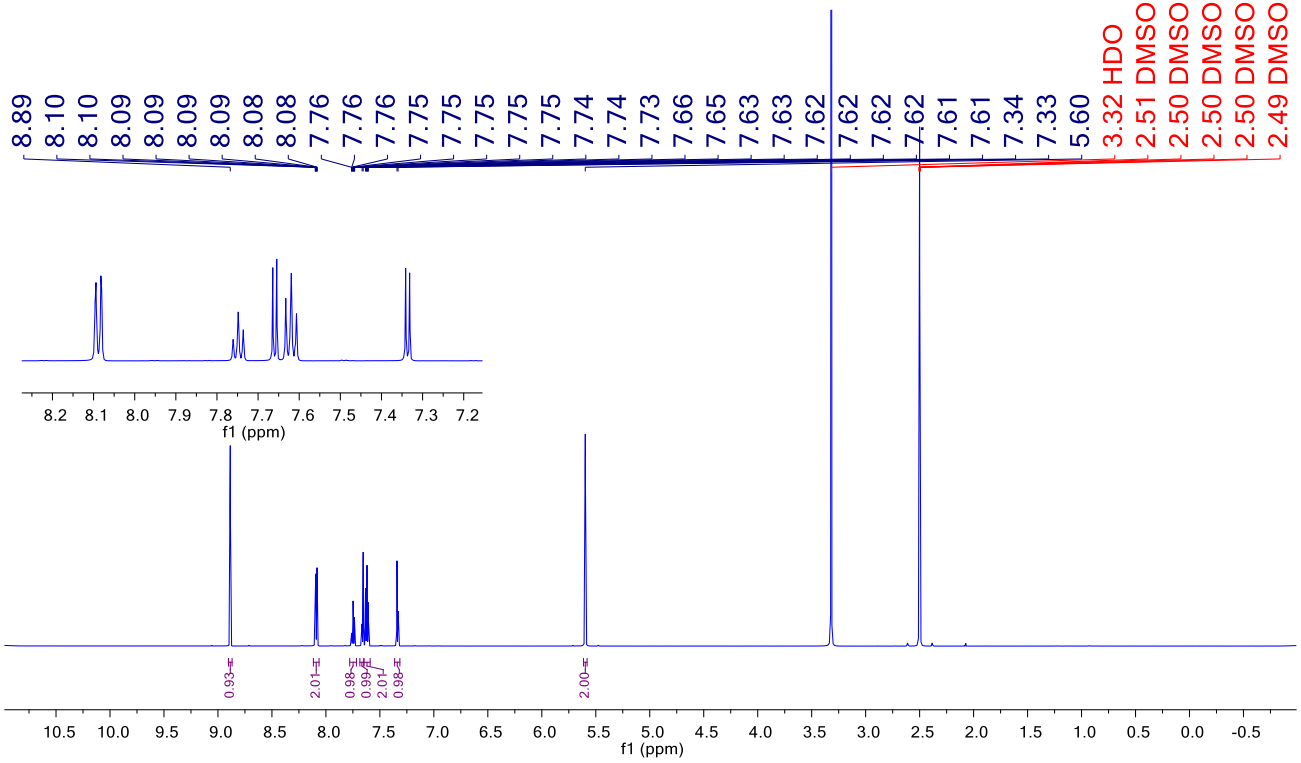
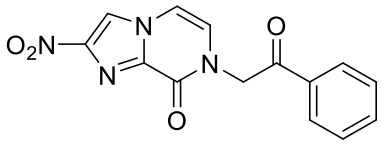
17	Modification Date	2017-10-08T13:27:40
18	Spectrometer Frequency	600.13
19	Spectral Width	7183.9
20	Lowest Frequency	-591.3
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536



2-Nitro-7-(2-oxo-2-phenylethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17a)



^{13}C NMR (150 MHz, DMSO-d_6)

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3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-10-10T07:39:28
17	Modification Date	2017-10-10T07:39:28
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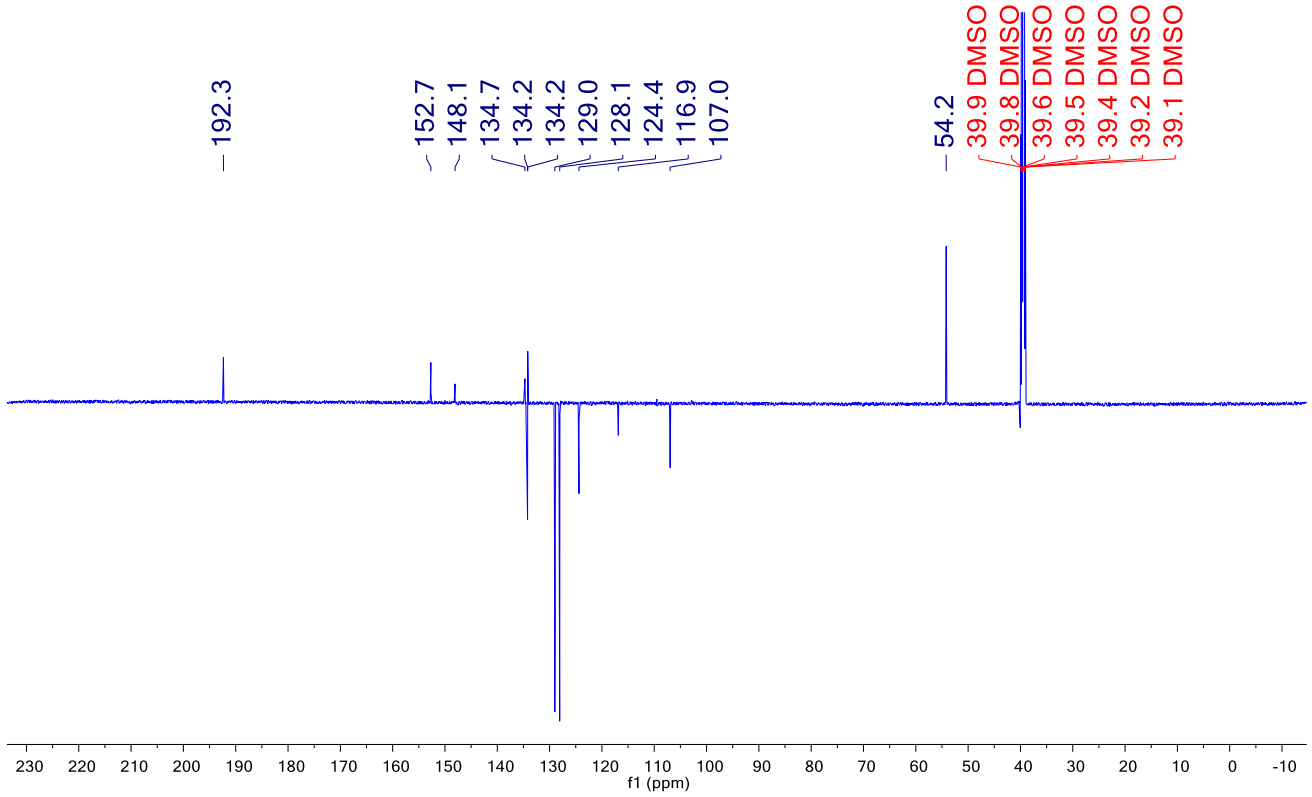
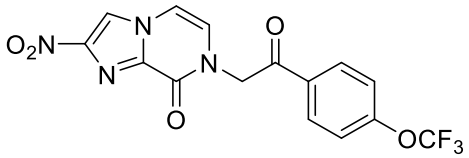
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



2-Nitro-7-(2-oxo-2-(4-(trifluoromethoxy)phenyl)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17b)



^{1}H NMR (600 MHz, DMSO-d_6)

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3	Owner	nmr
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5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
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10	Number of Scans	16
11	Receiver Gain	155.2
12	Relaxation Delay	5.0000
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21	Nucleus	1H
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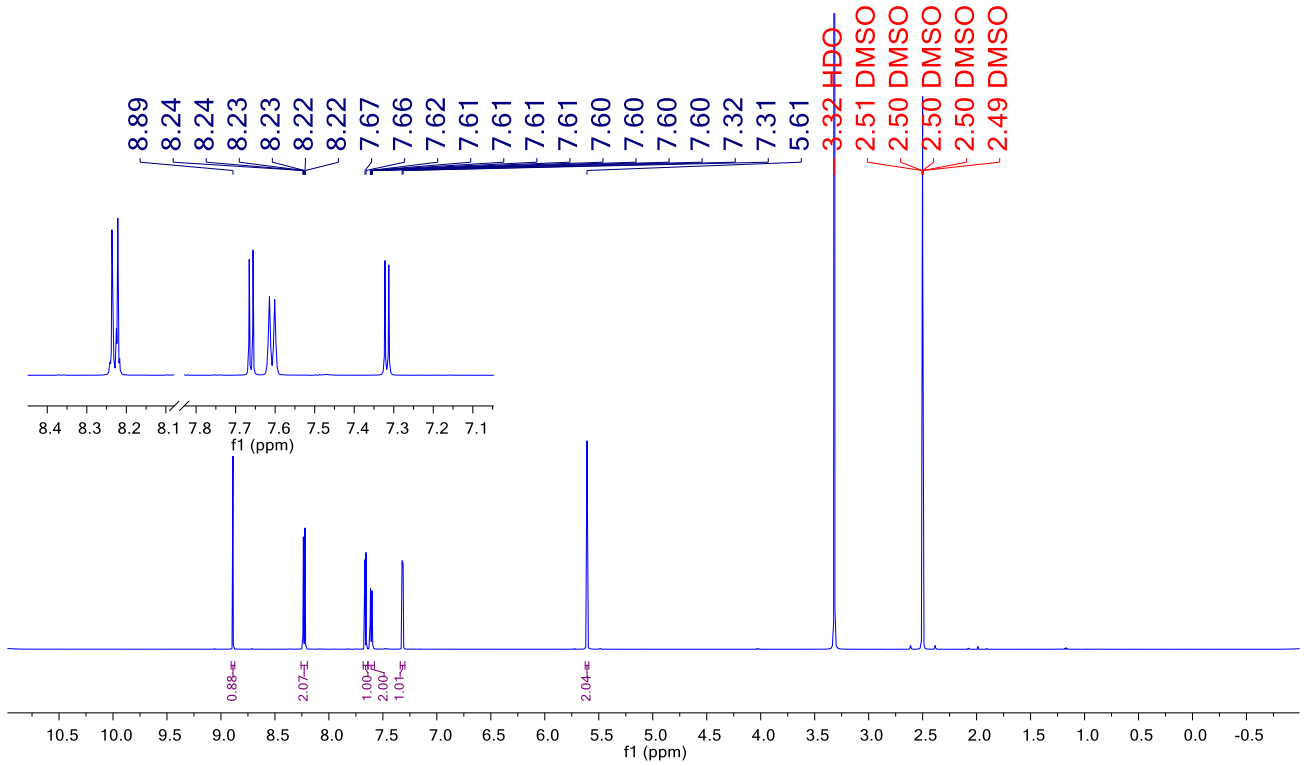
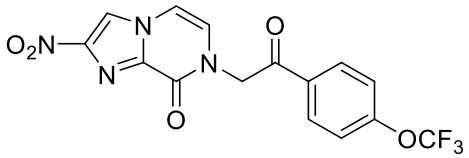


2-Nitro-7-(2-oxo-2-(4-(trifluoromethoxy)phenyl)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17b)



^{13}C NMR (150 MHz, DMSO-*d*$_6$)

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3	Owner	nmr
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6	Temperature	298.0
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8	Experiment	JMOD
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11	Receiver Gain	191.6
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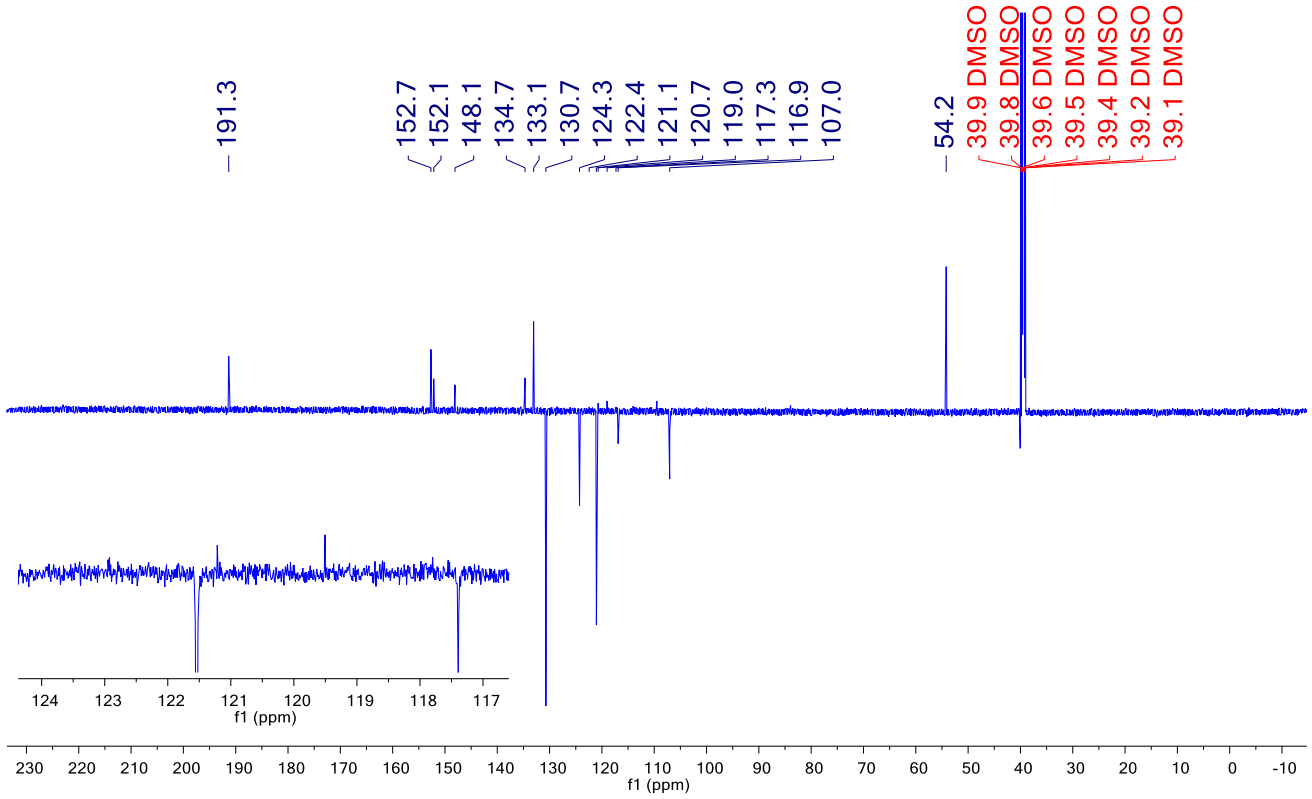
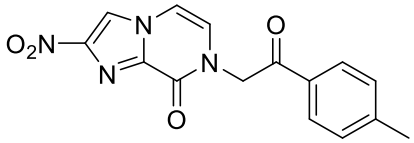
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



2-Nitro-7-(2-oxo-2-(*p*-tolyl)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17c)



^{1}H NMR (600 MHz, DMSO-d_6)

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3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	172.8
12	Relaxation Delay	5.0000
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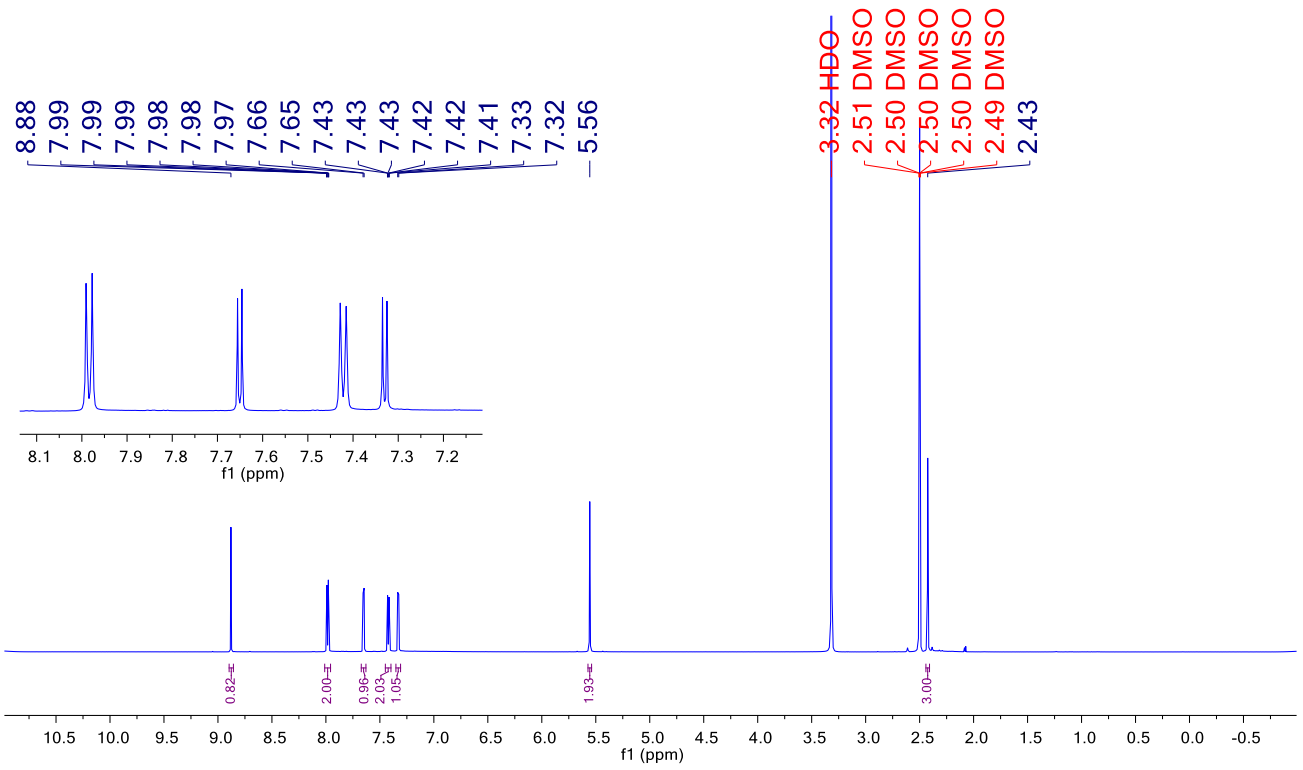
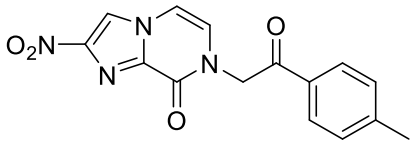
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536



2-Nitro-7-(2-oxo-2-(*p*-tolyl)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17c)



^{13}C NMR (150 MHz, DMSO-d_6)

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7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
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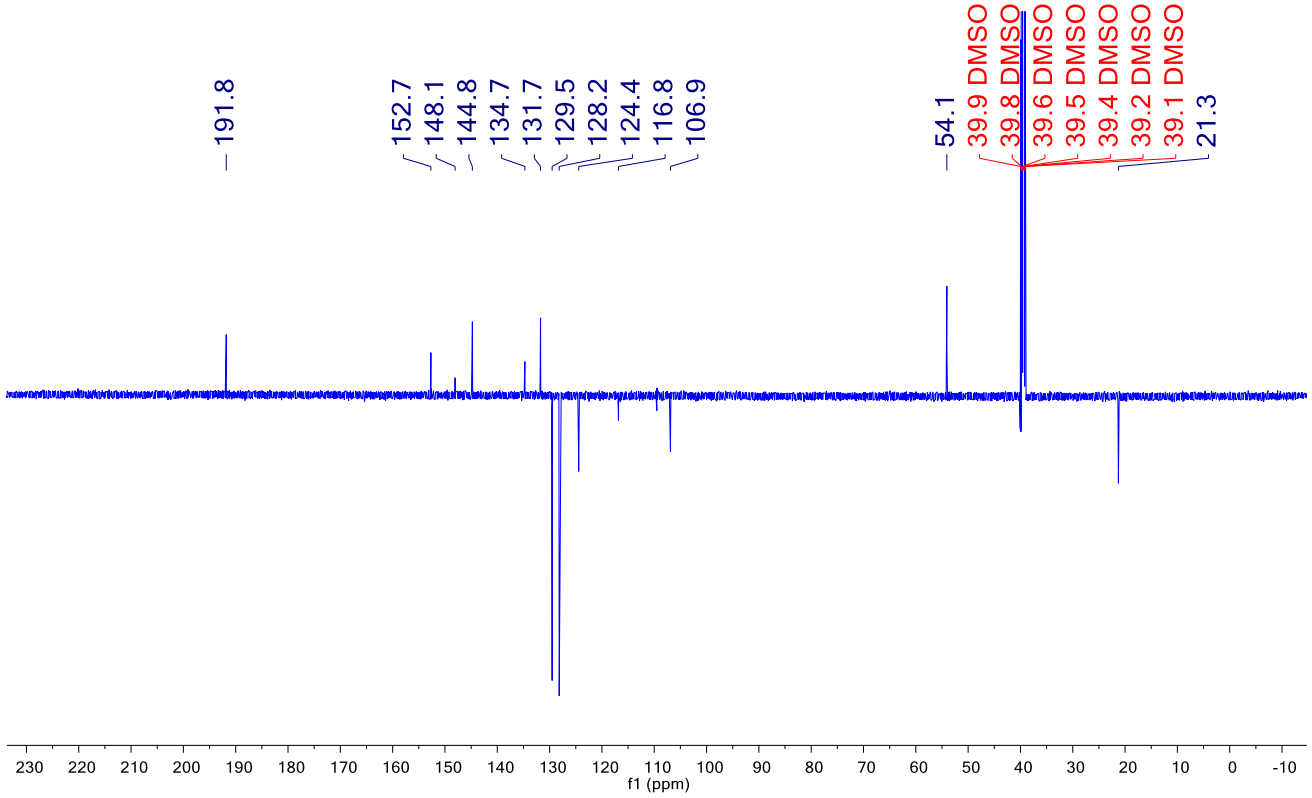
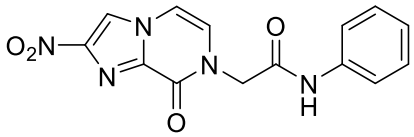
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)-*N*-phenylacetamide (17d)



^{1}H NMR (600 MHz, DMSO-d_6)

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5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
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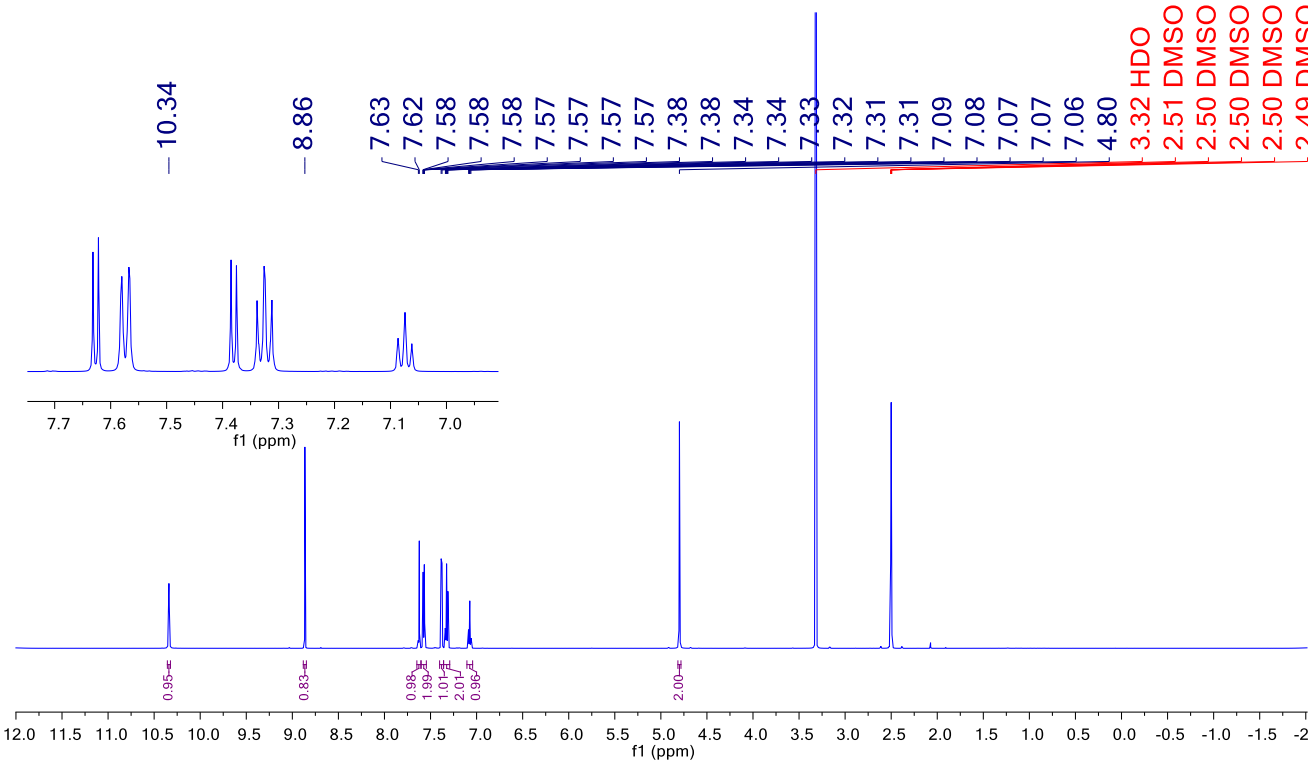
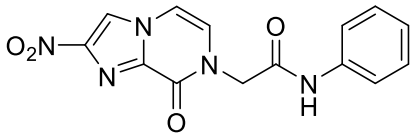
22	Acquired Size	16384
23	Spectral Size	65536



2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)-*N*-phenylacetamide (17d)



^{13}C NMR (150 MHz, DMSO-d_6)

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3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	7500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
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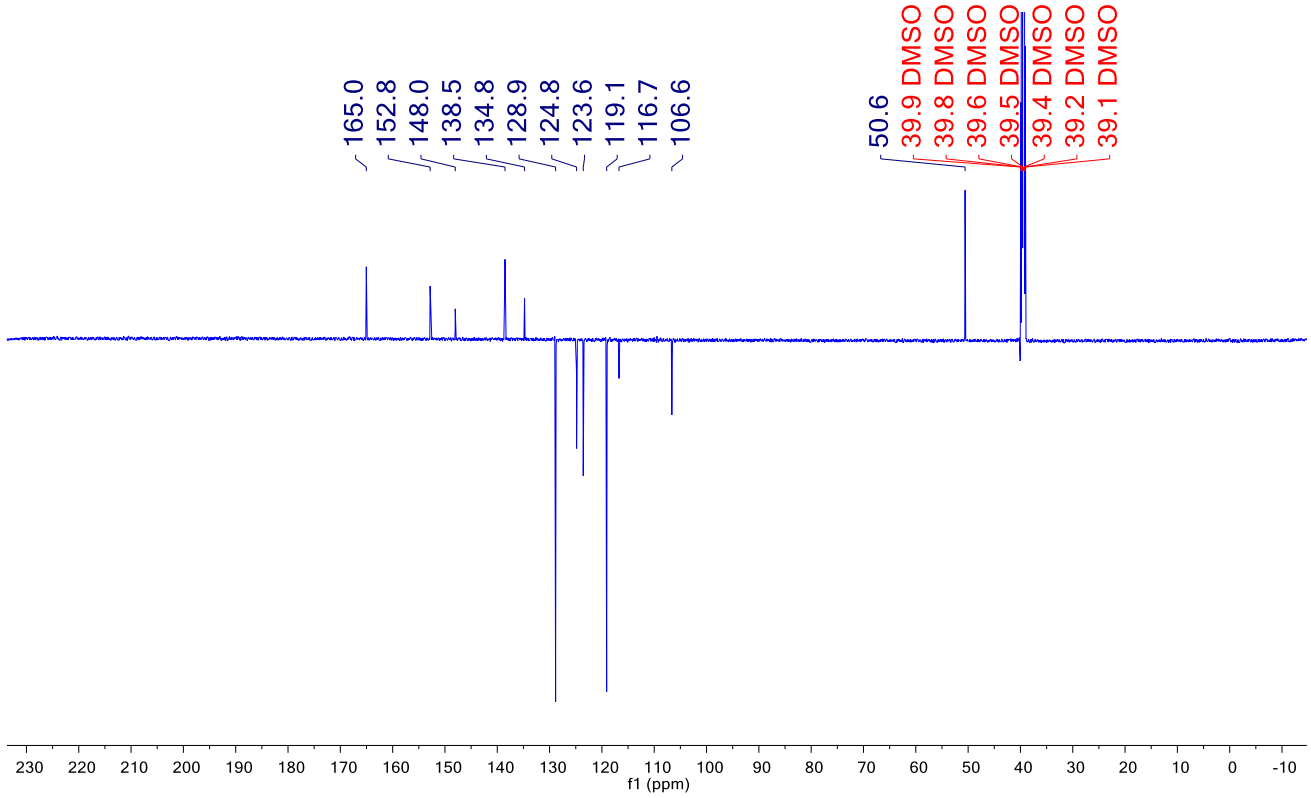
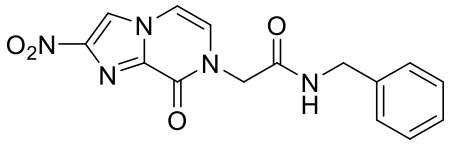
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



N-Benzyl-2-(2-nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)acetamide (17e)



^{1}H NMR (600 MHz, DMSO-d_6)

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6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	140.4
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
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17	Modification Date	2017-09-17T13:21:29
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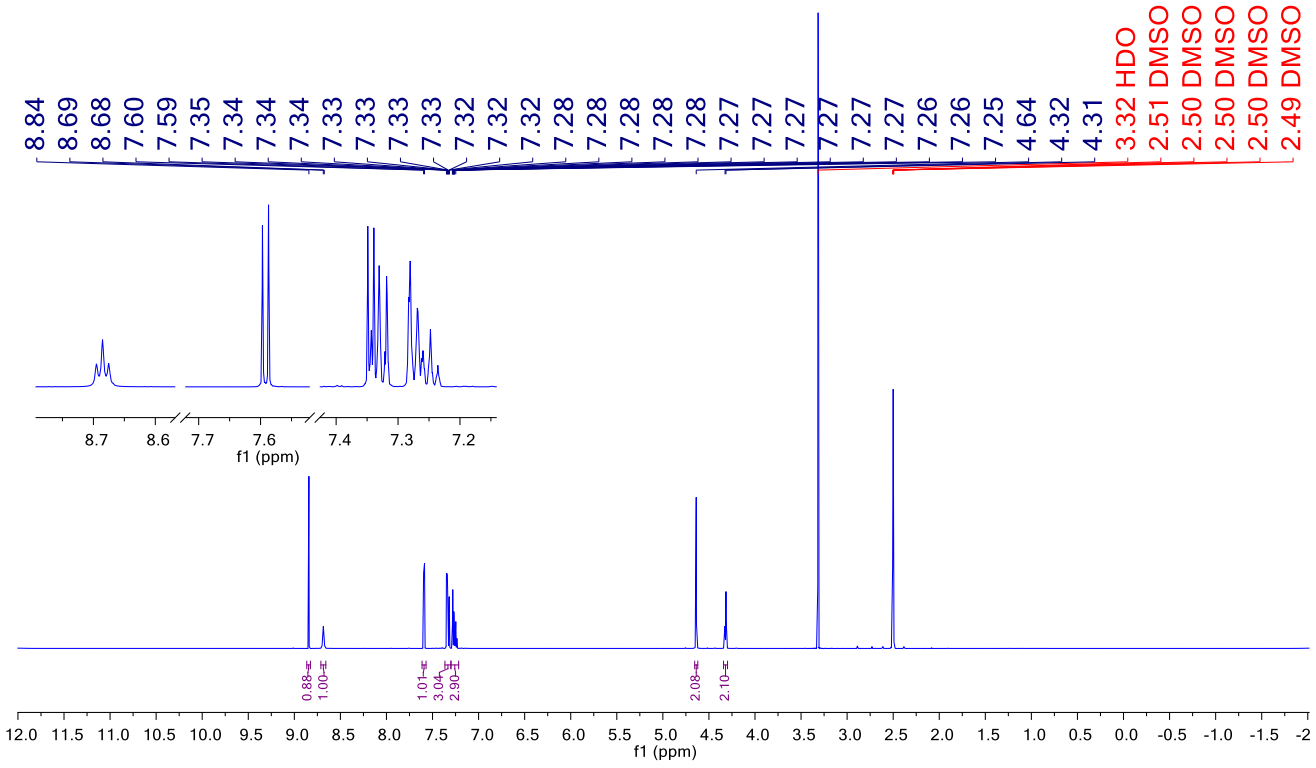
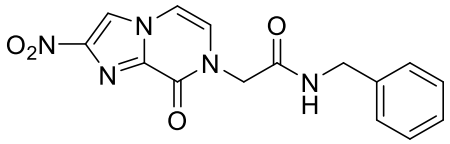
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536



N-Benzyl-2-(2-nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)acetamide (17e)



^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
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3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	7000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-09-17T17:15:58
17	Modification Date	2017-09-17T17:15:58
18	Spectrometer Frequency	150.92
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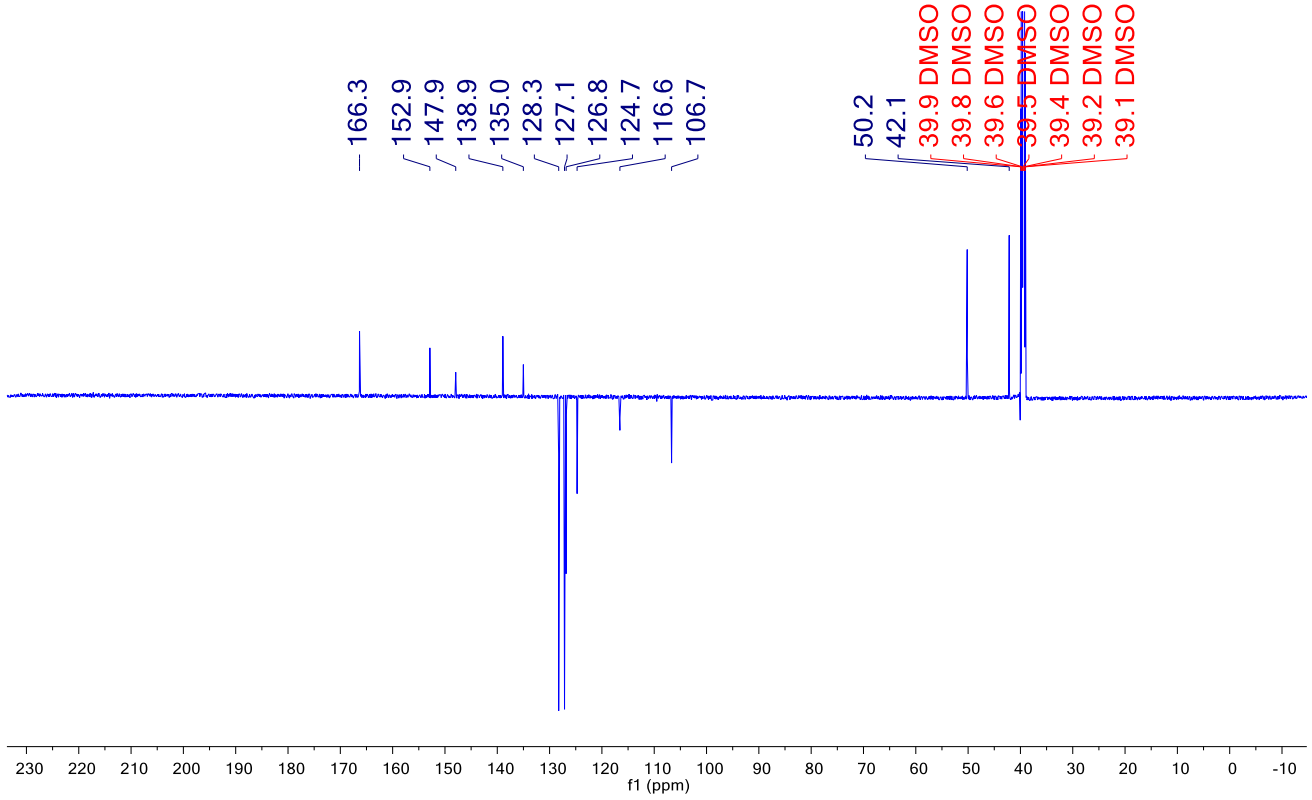
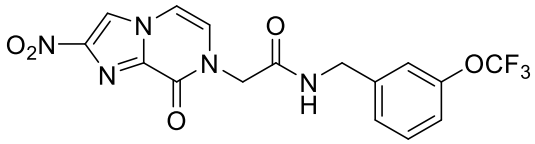
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

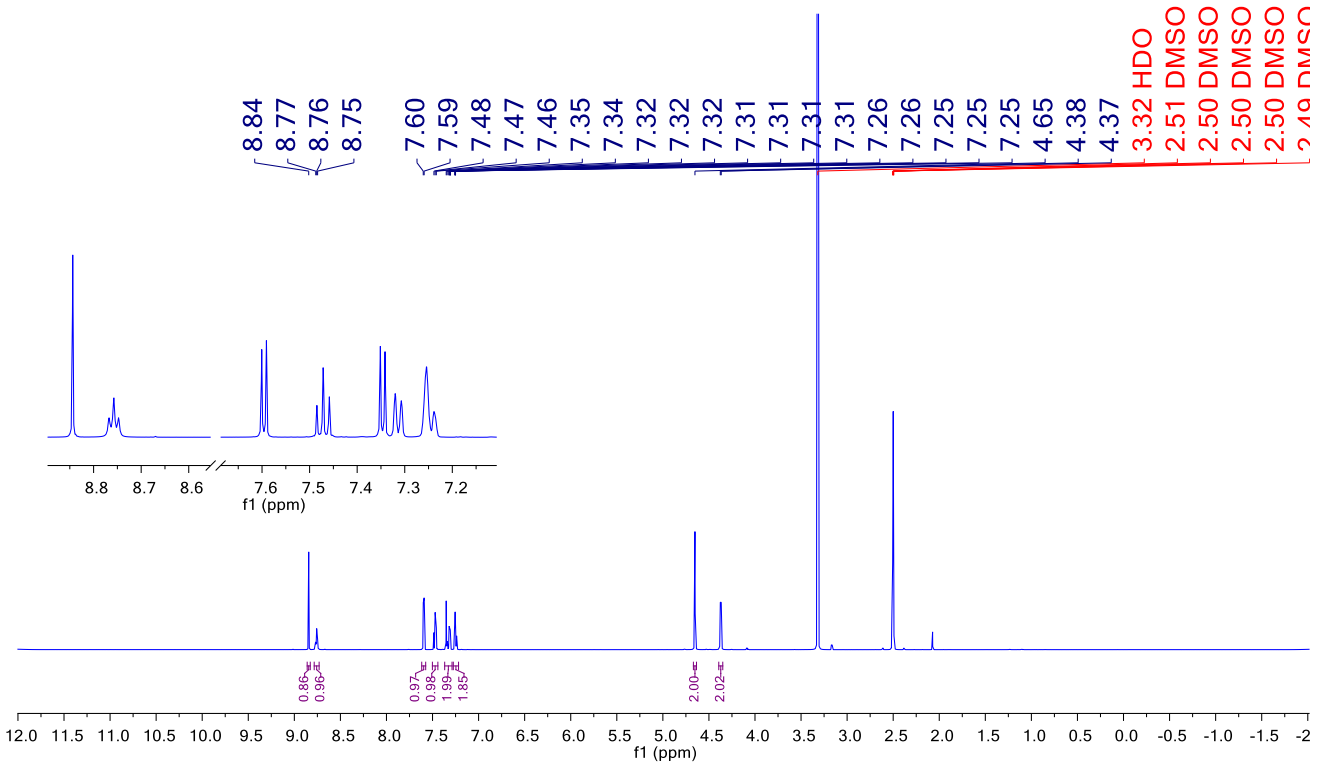


2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)-*N*-(3-(trifluoromethoxy)benzyl)acetamide (17f)

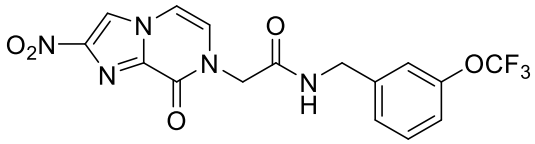


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_111_ppt_ACN.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	116.1
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2017-10-14T16:29:47
17	Modification Date	2017-10-14T16:29:47
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

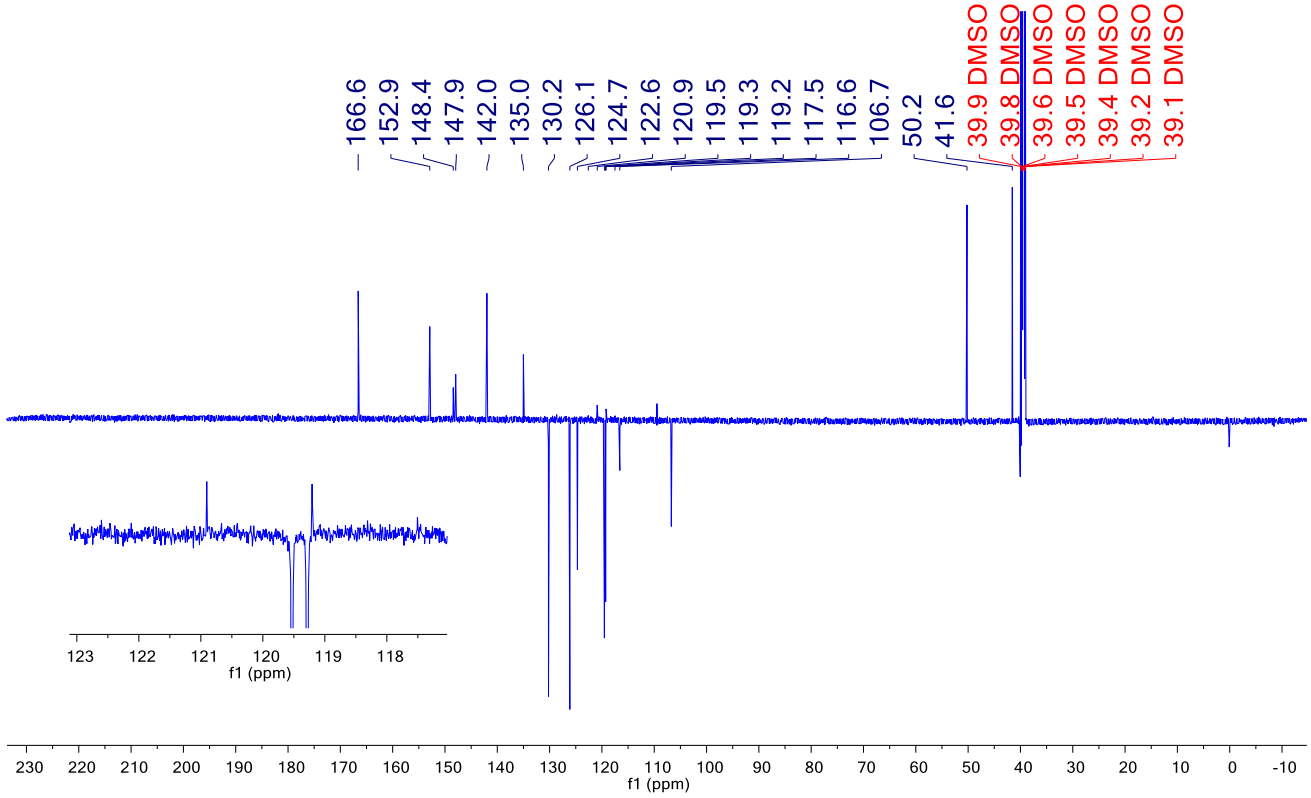


2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)-*N*-(3-(trifluoromethoxy)benzyl)acetamide (17f)

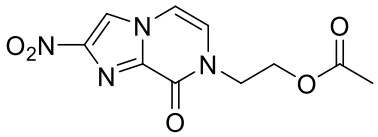


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_111_ppt_ACN.3.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-10-18T22:58:00
17	Modification Date	2017-10-18T22:58:00
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

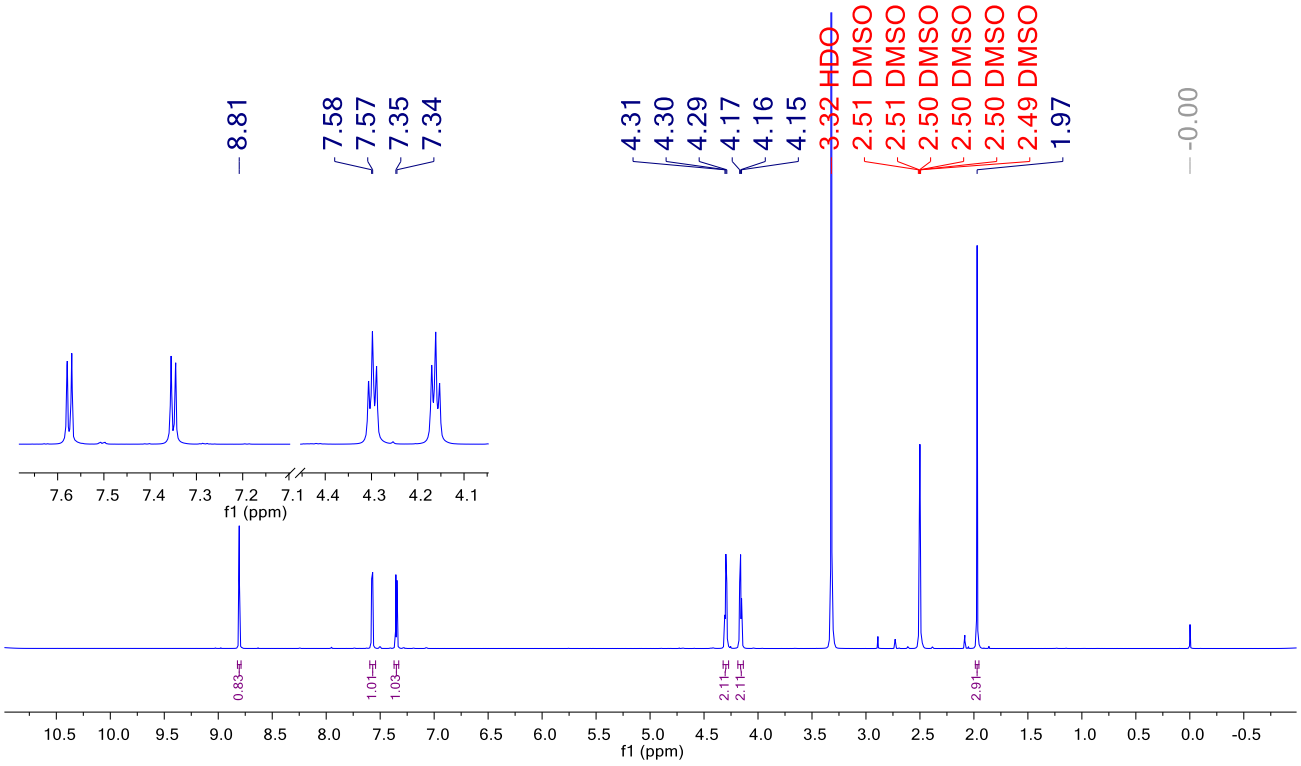


2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)ethyl acetate (17g)

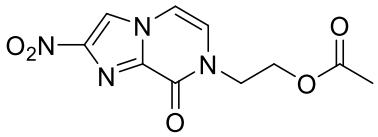


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_082_crude.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	109.3
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	2.2807
16	Acquisition Date	2017-06-01T10:13:19
17	Modification Date	2017-06-01T10:13:19
18	Spectrometer Frequency	600.13
19	Spectral Width	7183.9
20	Lowest Frequency	-592.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

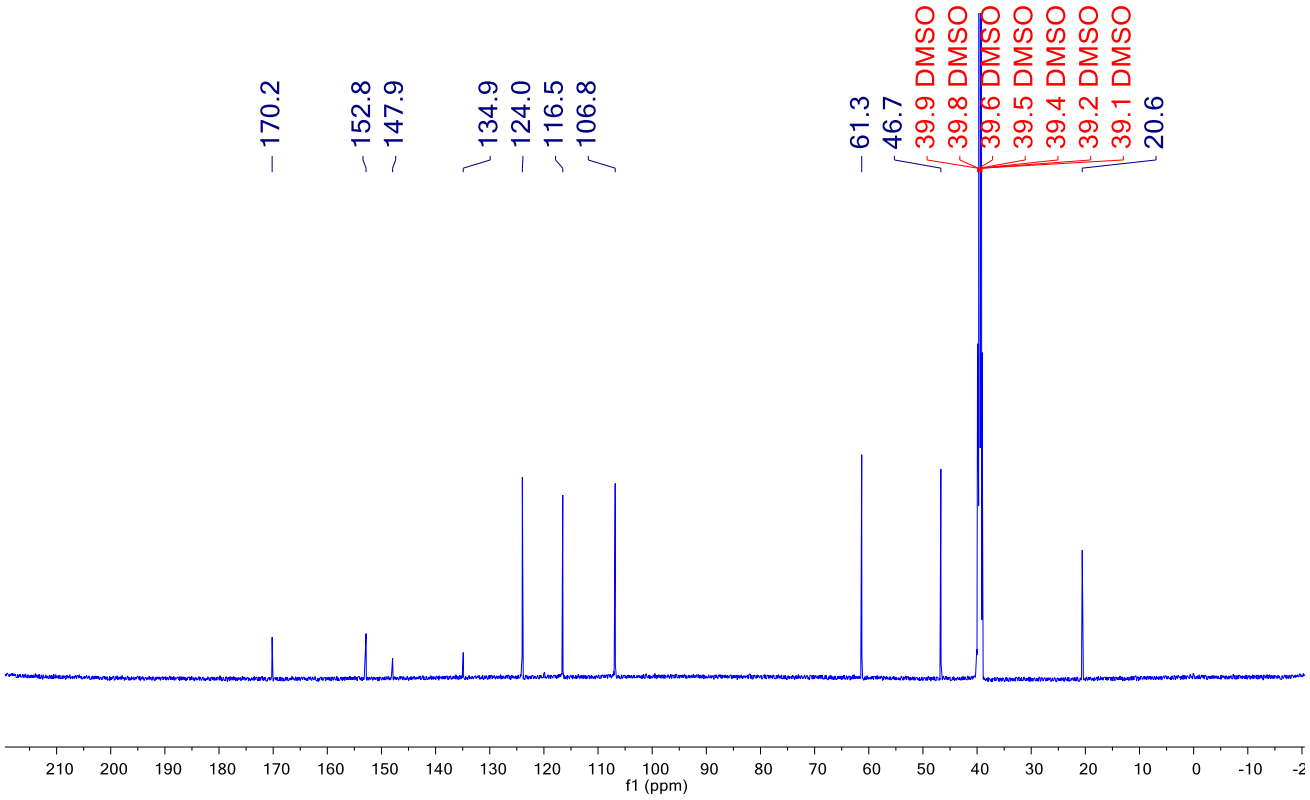


2-(2-Nitro-8-oxoimidazo[1,2-*a*]pyrazin-7(8*H*)-yl)ethyl acetate (17g)

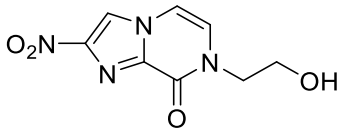


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_082_crude.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zgpg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	2560
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.9044
16	Acquisition Date	2017-06-01T11:38:16
17	Modification Date	2017-06-01T11:38:16
18	Spectrometer Frequency	150.92
19	Spectral Width	36231.9
20	Lowest Frequency	-3025.7
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

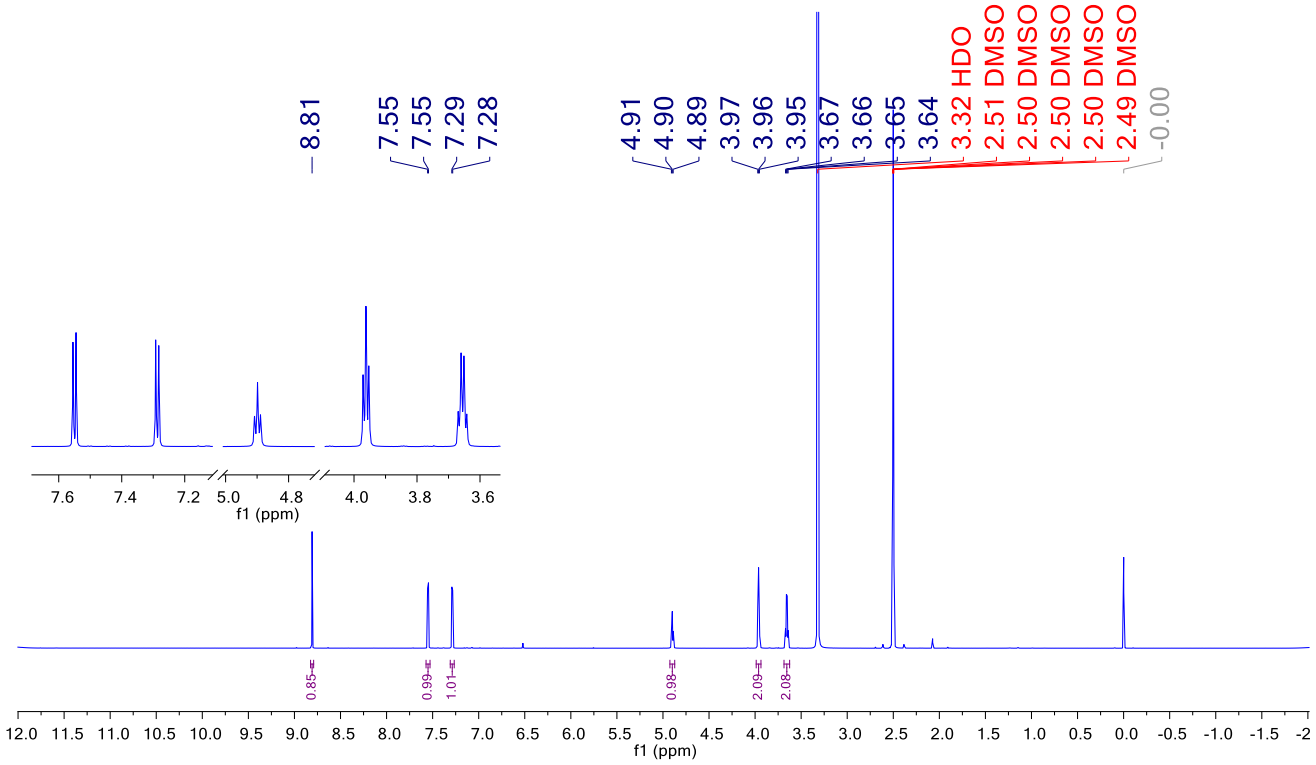


7-(2-Hydroxyethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17h)

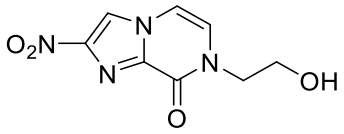


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_083_purified.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	116.1
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2017-06-06T18:17:20
17	Modification Date	2017-06-06T18:17:20
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1211.0
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

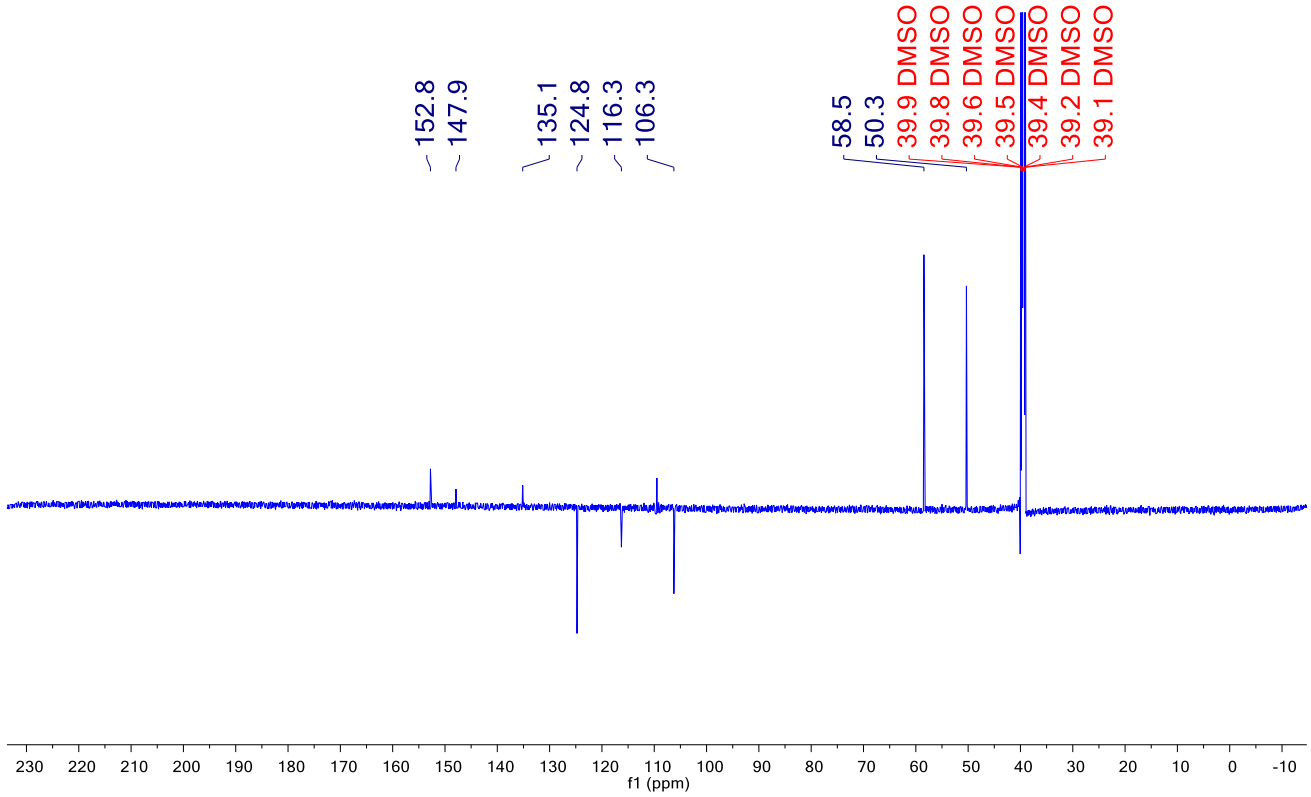


7-(2-Hydroxyethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17h)

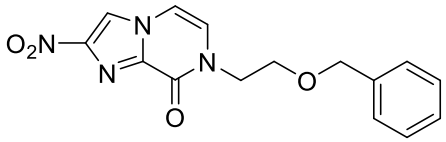


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_083_purified.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	8000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-06-06T22:34:17
17	Modification Date	2017-06-06T22:34:17
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

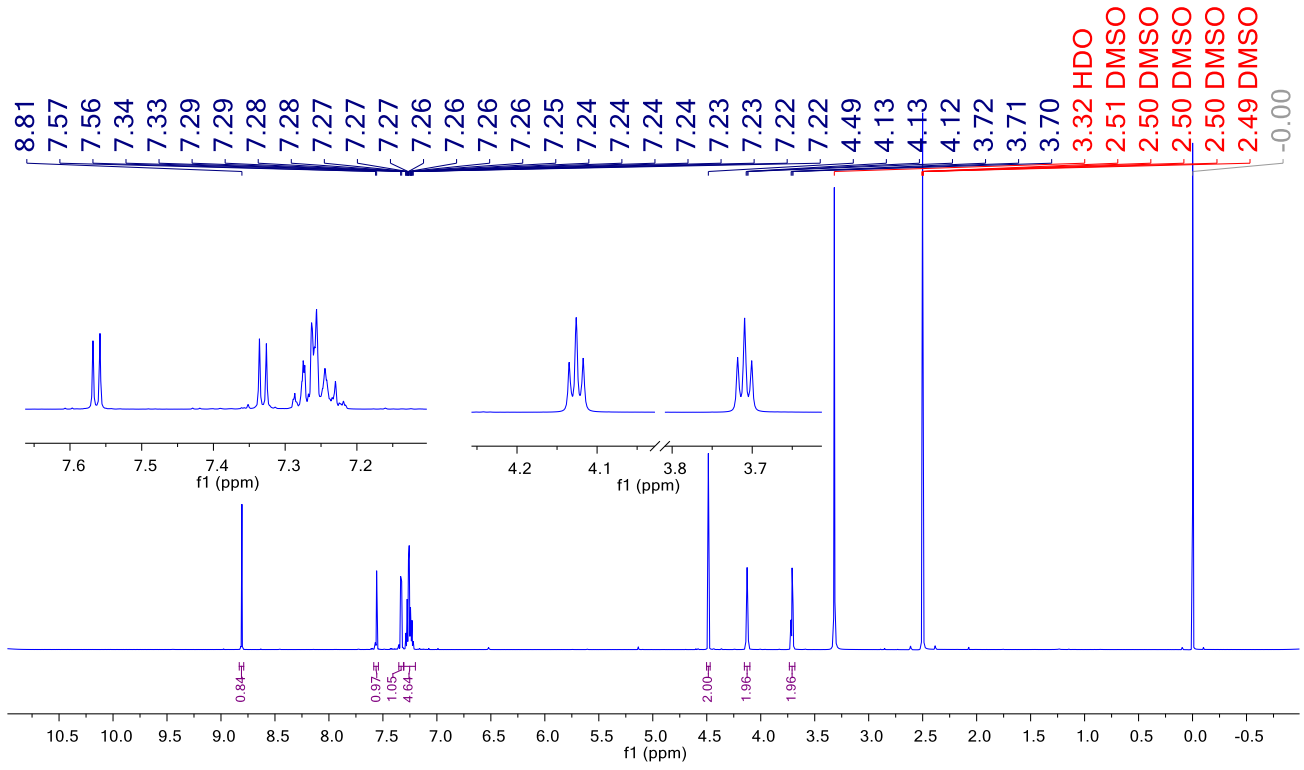


7-(2-(Benzyloxy)ethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17i)

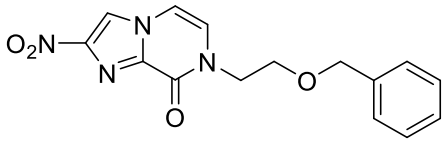


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_112IIA_f16-17+2f13-14.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	140.4
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	2.2807
16	Acquisition Date	2017-07-27T11:58:39
17	Modification Date	2017-07-27T11:58:39
18	Spectrometer Frequency	600.13
19	Spectral Width	7183.9
20	Lowest Frequency	-594.7
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

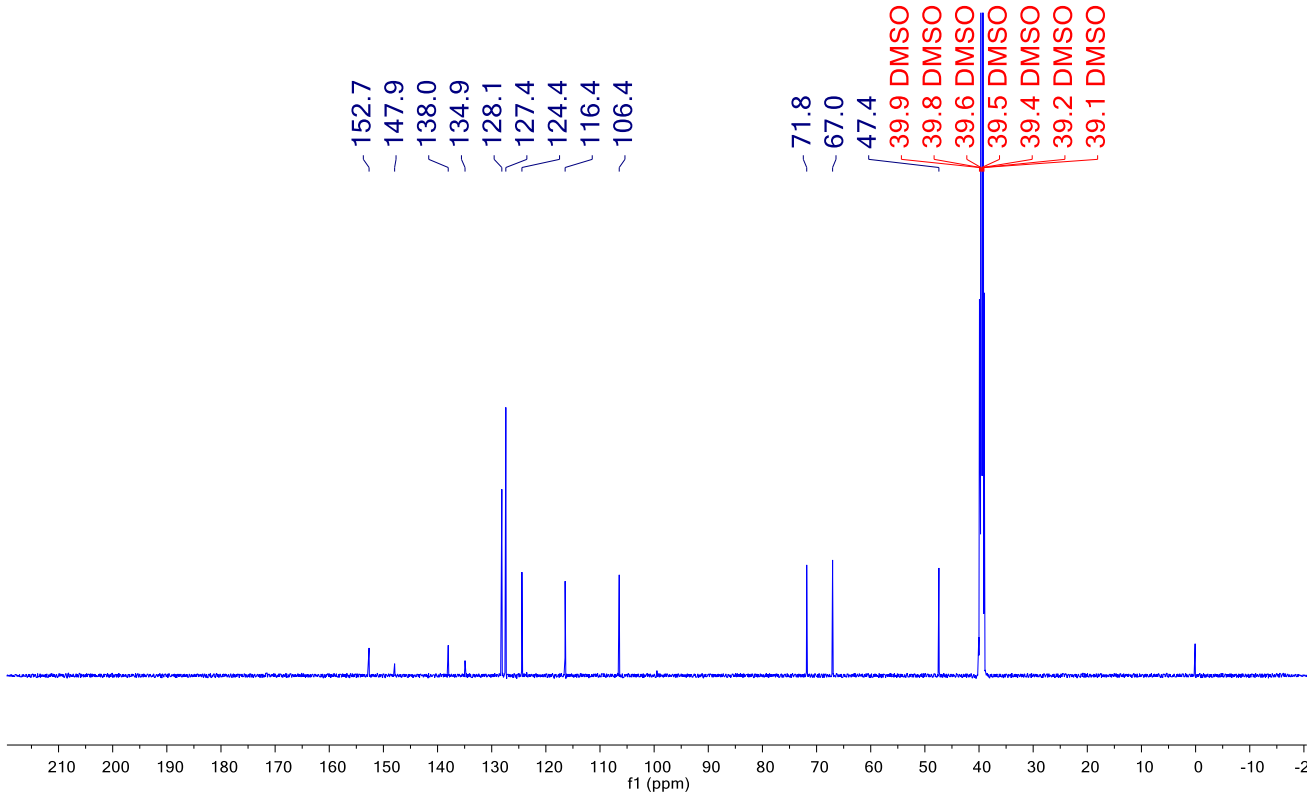


7-(2-(Benzyloxy)ethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17i)

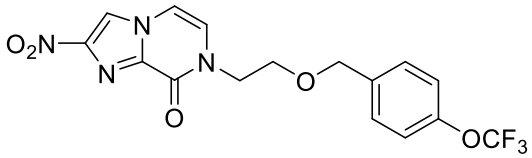


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8412_112IIA_f16-17+2f13-14.3.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zgpg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	3000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.9044
16	Acquisition Date	2017-07-27T13:49:29
17	Modification Date	2017-07-27T13:49:29
18	Spectrometer Frequency	150.92
19	Spectral Width	36231.9
20	Lowest Frequency	-3188.5
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

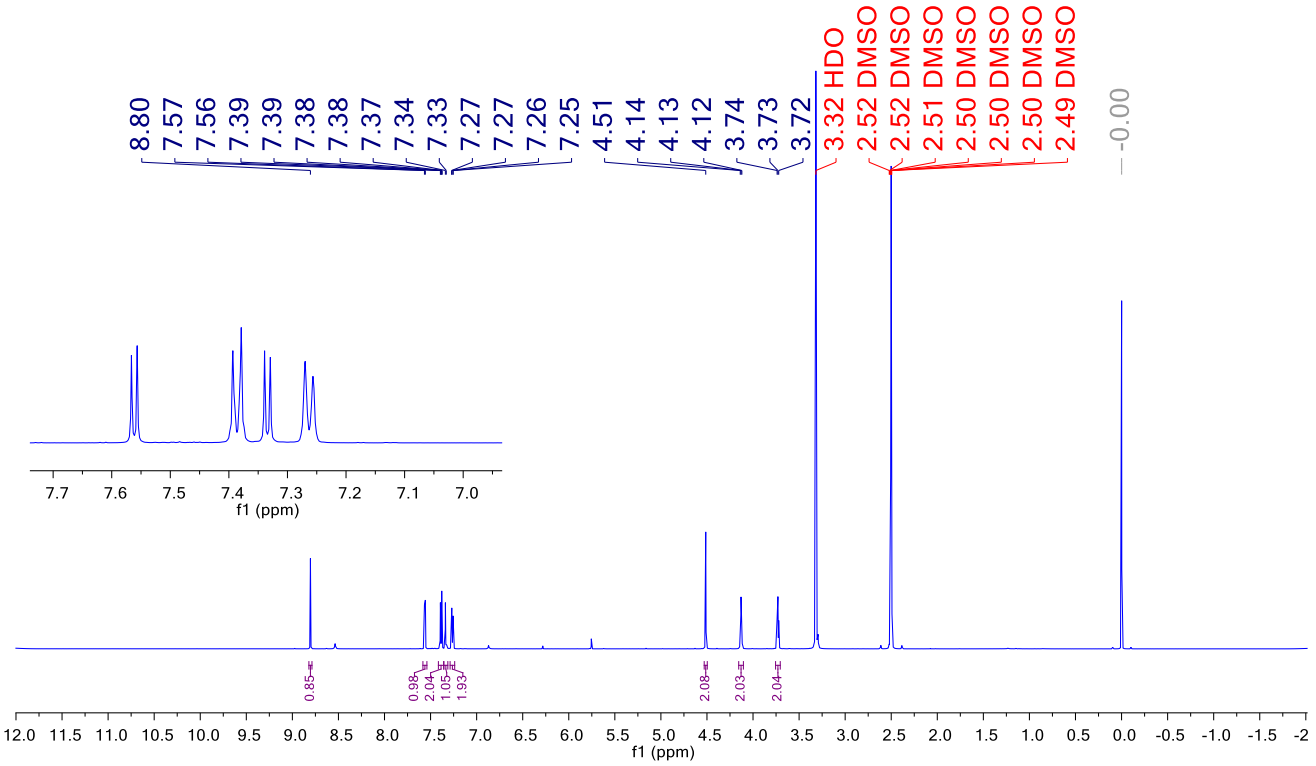


2-Nitro-7-(2-((4-(trifluoromethoxy)benzyl)oxy)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17j)

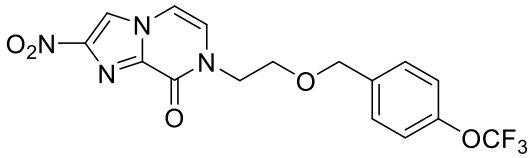


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_042_f9-11_C18_combined1.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	140.4
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2017-09-01T16:44:02
17	Modification Date	2017-09-01T16:44:02
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1211.4
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

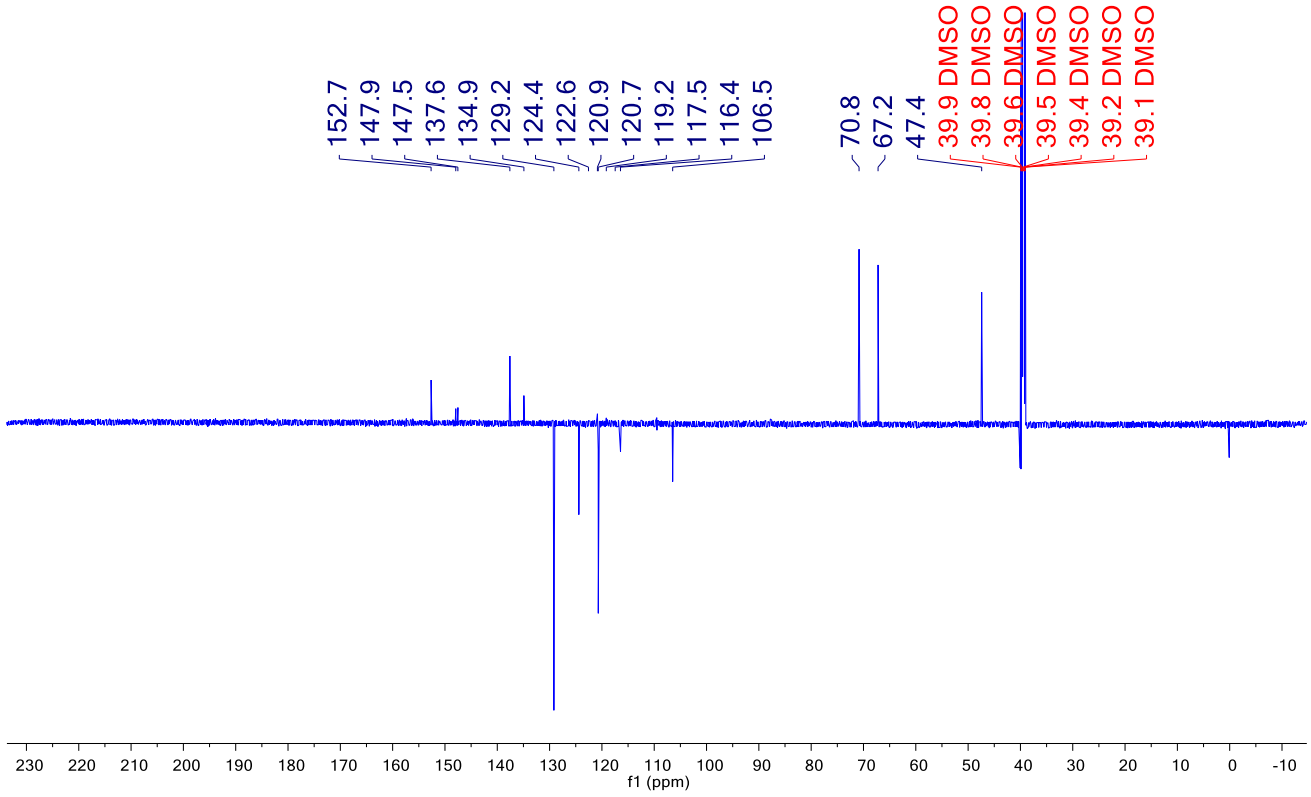


2-Nitro-7-(2-((4-(trifluoromethoxy)benzyl)oxy)ethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (17j)

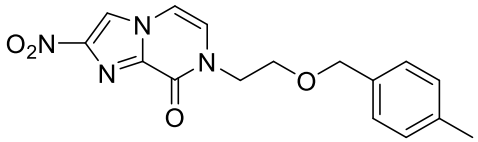


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_042_f9-11_C18_combined1.4.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-09-01T22:33:15
17	Modification Date	2017-09-01T22:33:15
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2313.9
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

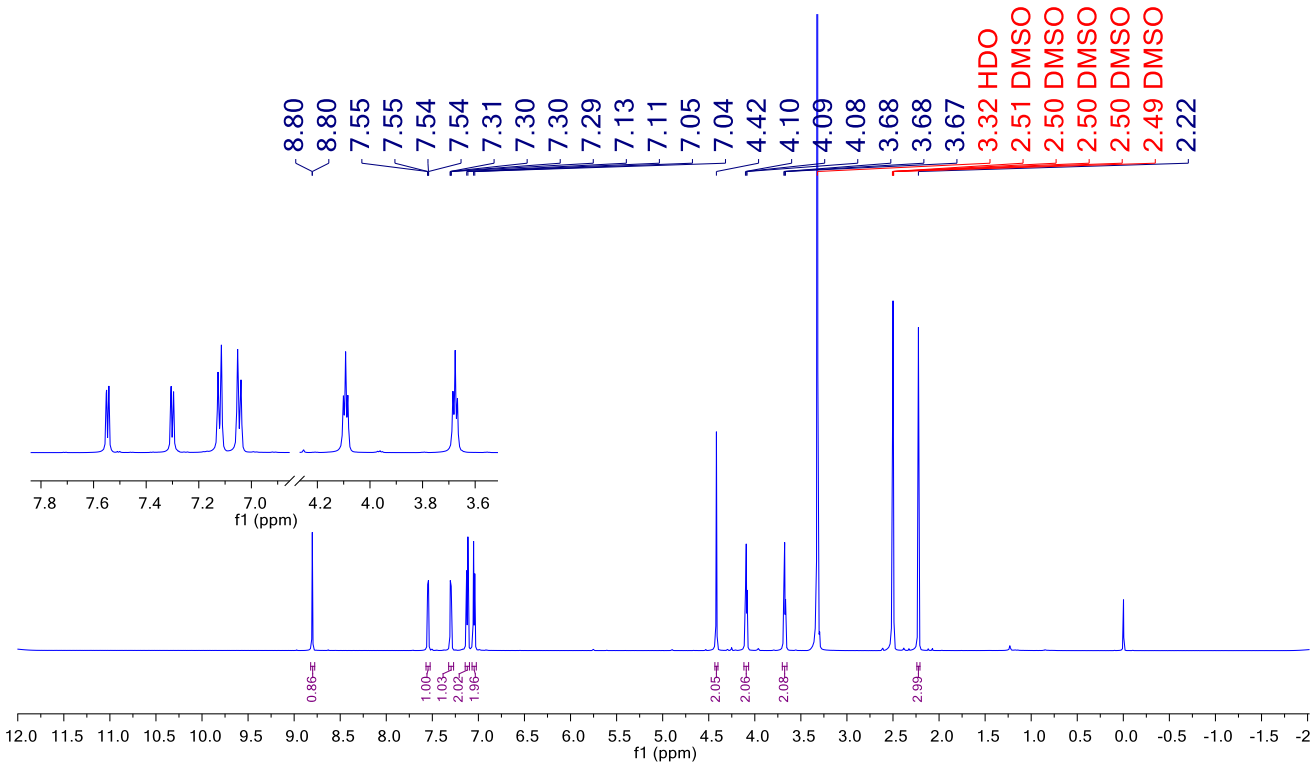


7-(2-((4-Methylbenzyl)oxy)ethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17k)

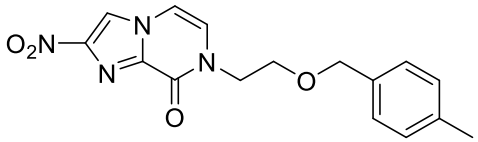


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_045_ppt.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2017-09-04T16:42:44
17	Modification Date	2017-09-04T16:42:44
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1212.4
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

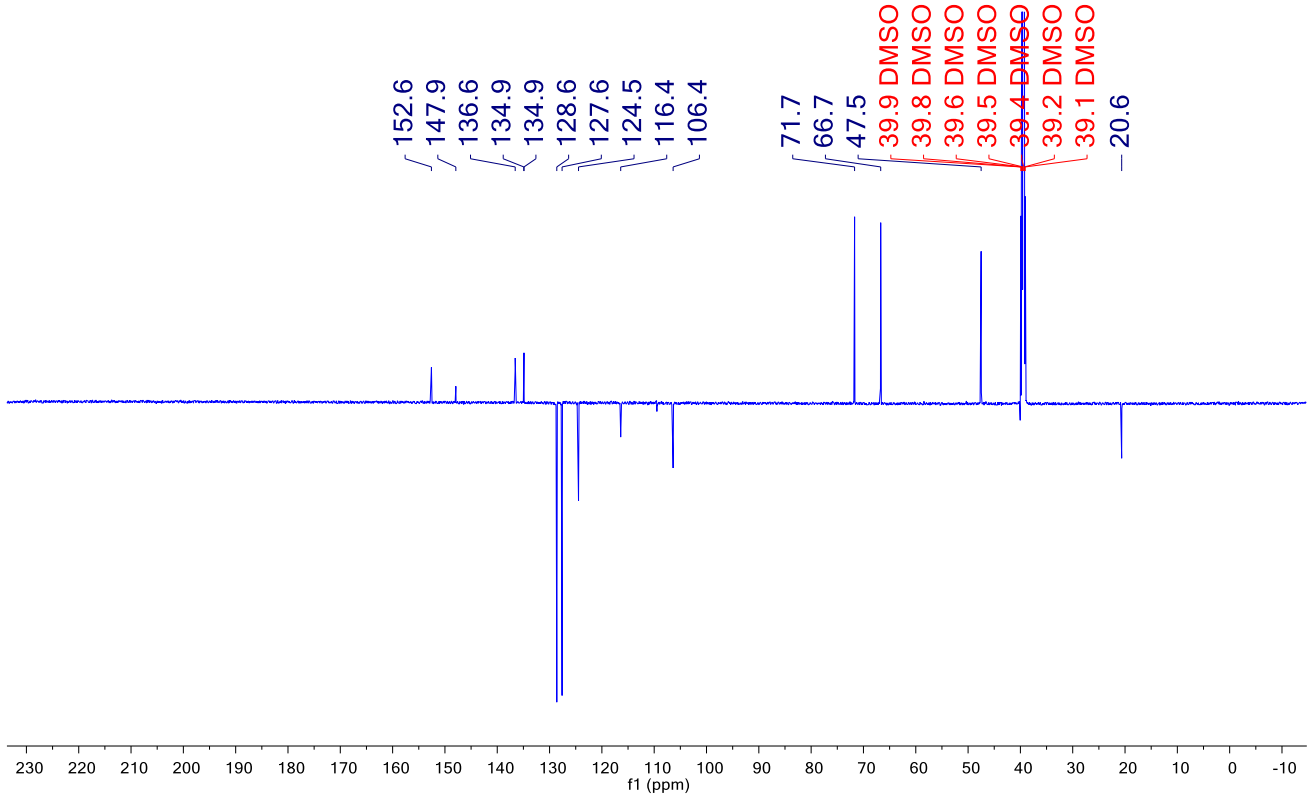


7-(2-((4-Methylbenzyl)oxy)ethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (17k)

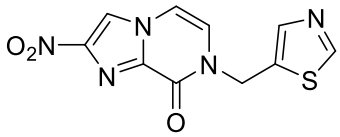


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_045_ppt.3.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2017-09-04T22:11:13
17	Modification Date	2017-09-04T22:11:13
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

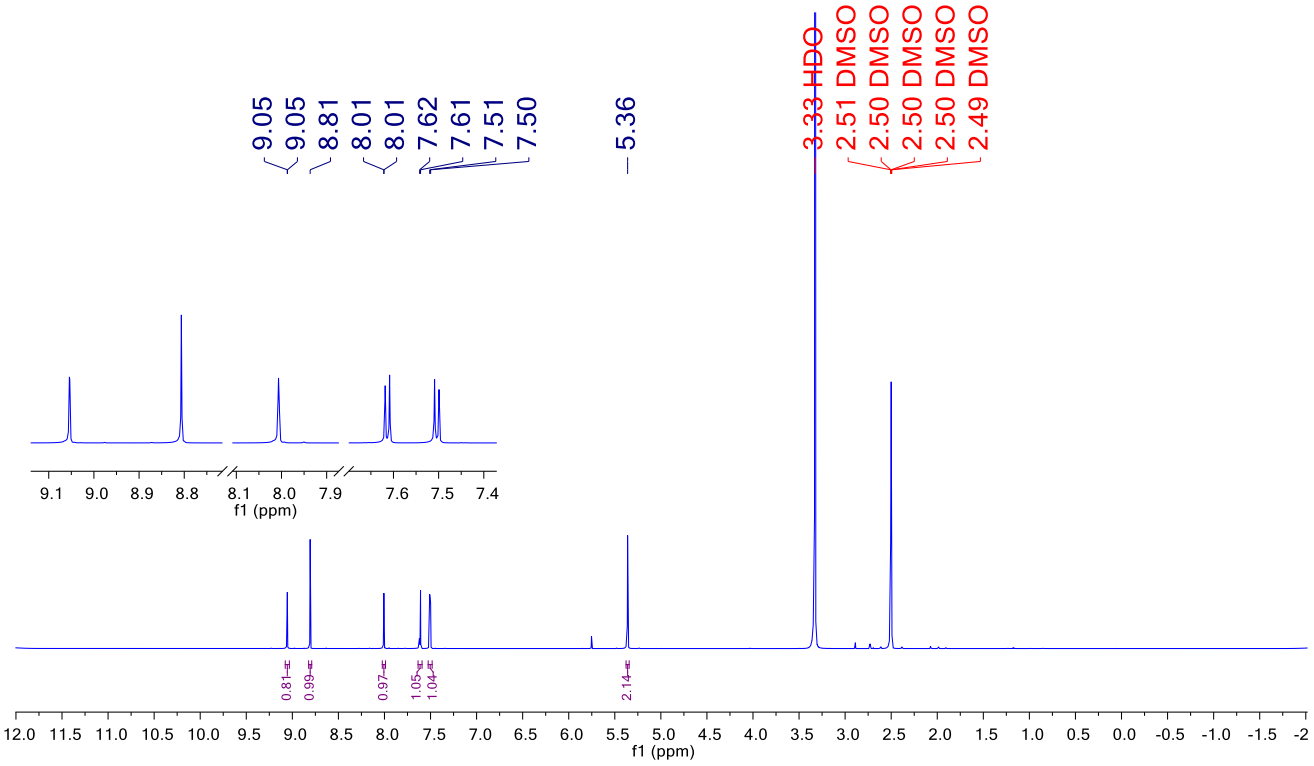


2-Nitro-7-(thiazol-5-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26a)

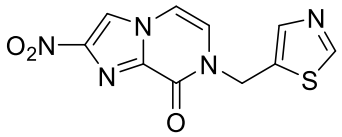


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_023_ppt_DCM_MeOH.6.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	10.0000
13	Pulse Width	7.0100
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-04-12T16:23:02
17	Modification Date	2018-04-12T16:23:02
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

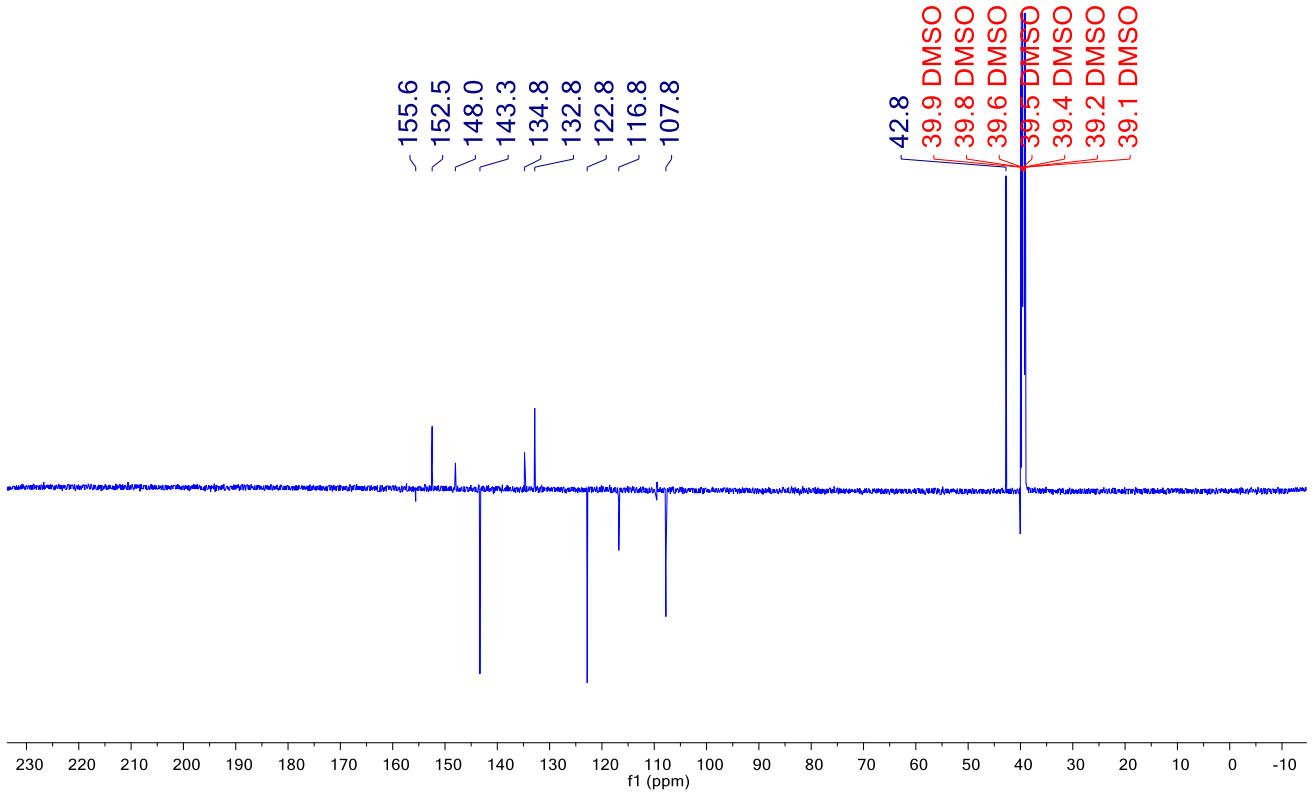


2-Nitro-7-(thiazol-5-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26a)

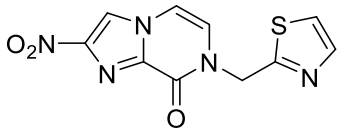


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_023_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	9500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-04-10T23:00:22
17	Modification Date	2018-04-10T23:00:22
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

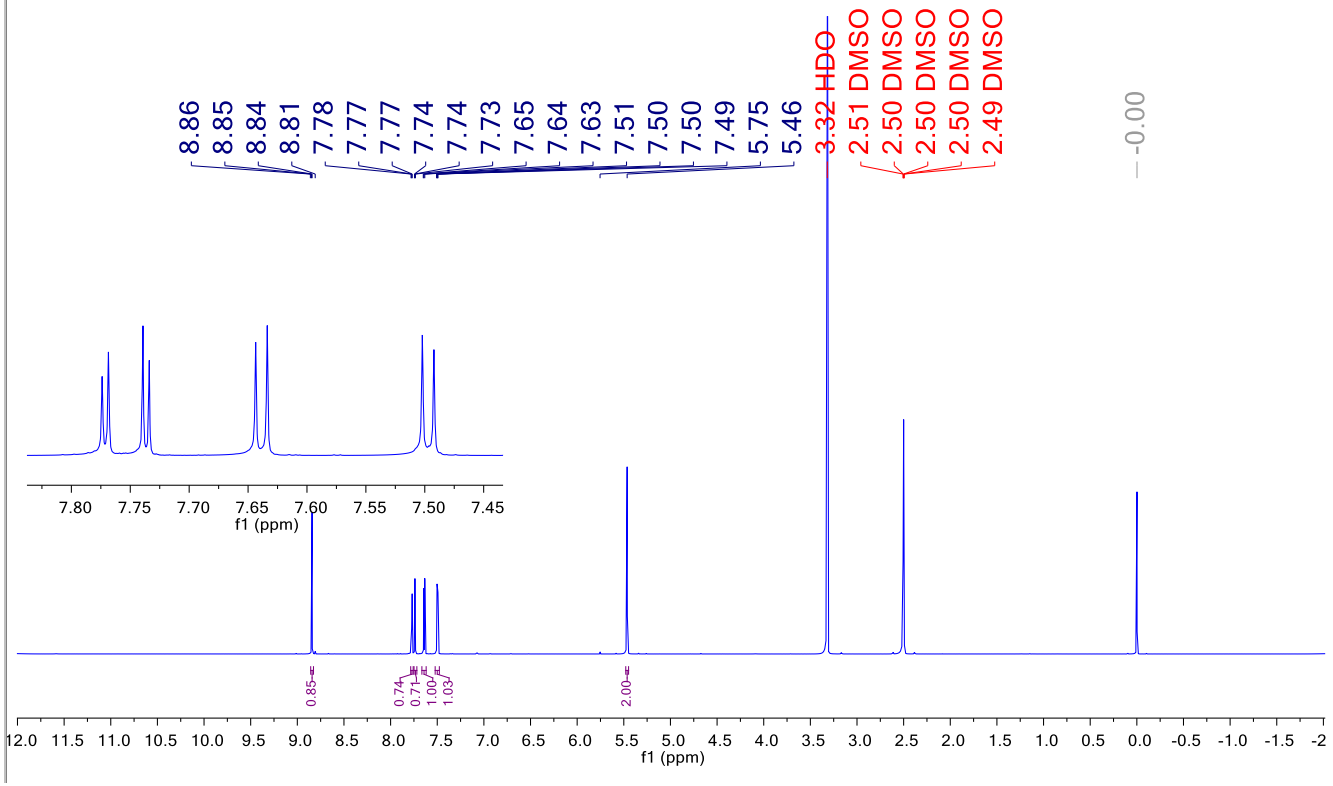


2-Nitro-7-(thiazol-2-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26b)

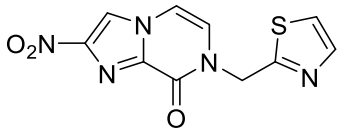


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_066/ NMR/ CWA8805_066_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8805_066_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8805_066_ppt_DCM_MeOH 1.7mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	16
15	Receiver Gain	116.1
16	Relaxation Delay	5.0000
17	Pulse Width	7.0100
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-01-25T16:46:34
21	Modification Date	2018-01-25T16:46:34
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest Frequency	-1208.1
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536

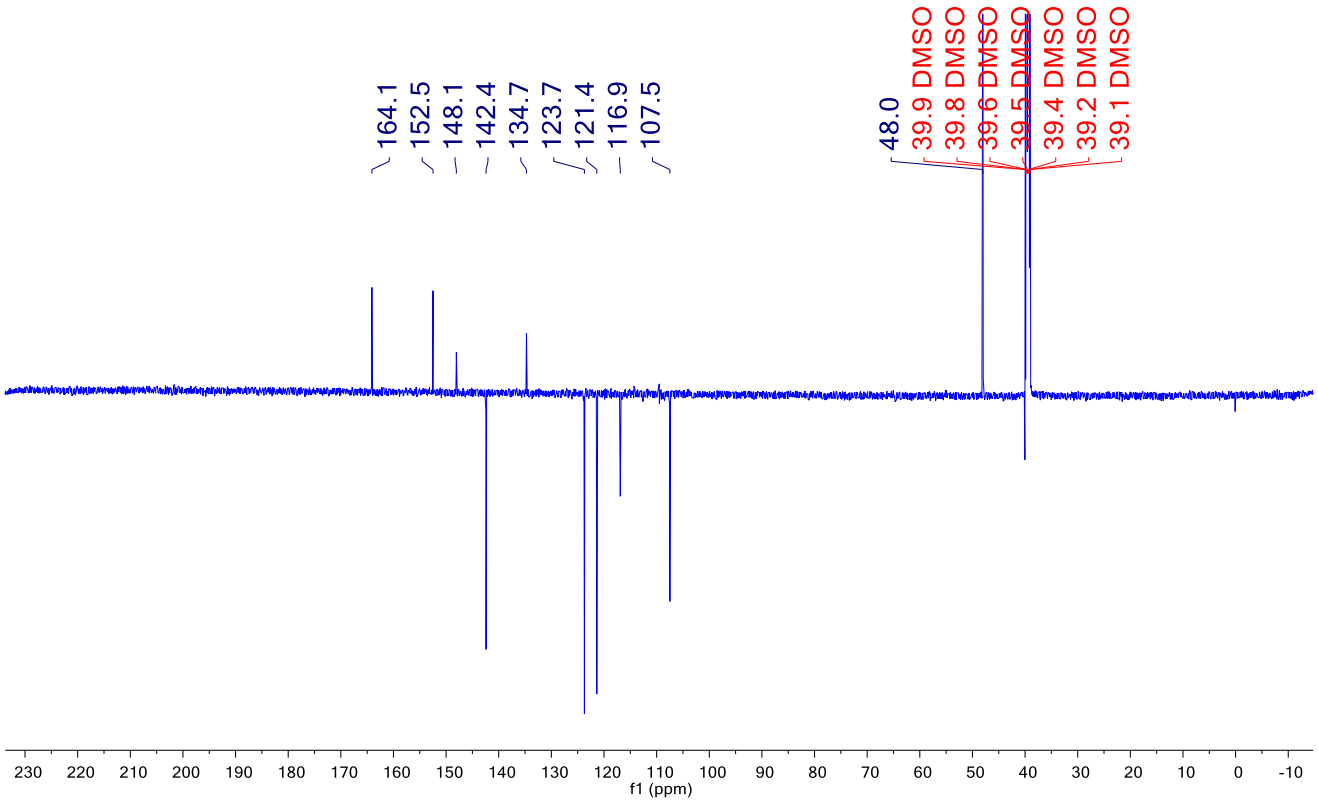


2-Nitro-7-(thiazol-2-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26b)

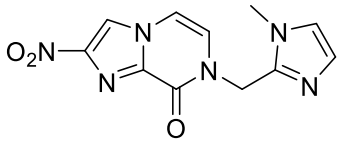


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_066/ NMR/ CWA8805_066_ppt_DCM_MeOH/ 2/ fid
2	Title	CWA8805_066_ppt_DCM_MeOH.2.fid
3	Comment	13C JMOD NMR of CWA8805_066_ppt_DCM_MeOH 1.7mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Experiment	JMOD
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	9000
15	Receiver Gain	191.6
16	Relaxation Delay	1.0000
17	Pulse Width	11.5000
18	Presaturation Frequency	
19	Acquisition Time	0.8738
20	Acquisition Date	2018-01-27T13:55:32
21	Modification Date	2018-01-27T13:55:32
22	Class	
23	Spectrometer Frequency	150.92
24	Spectral Width	37500.0
25	Lowest Frequency	-2151.2
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

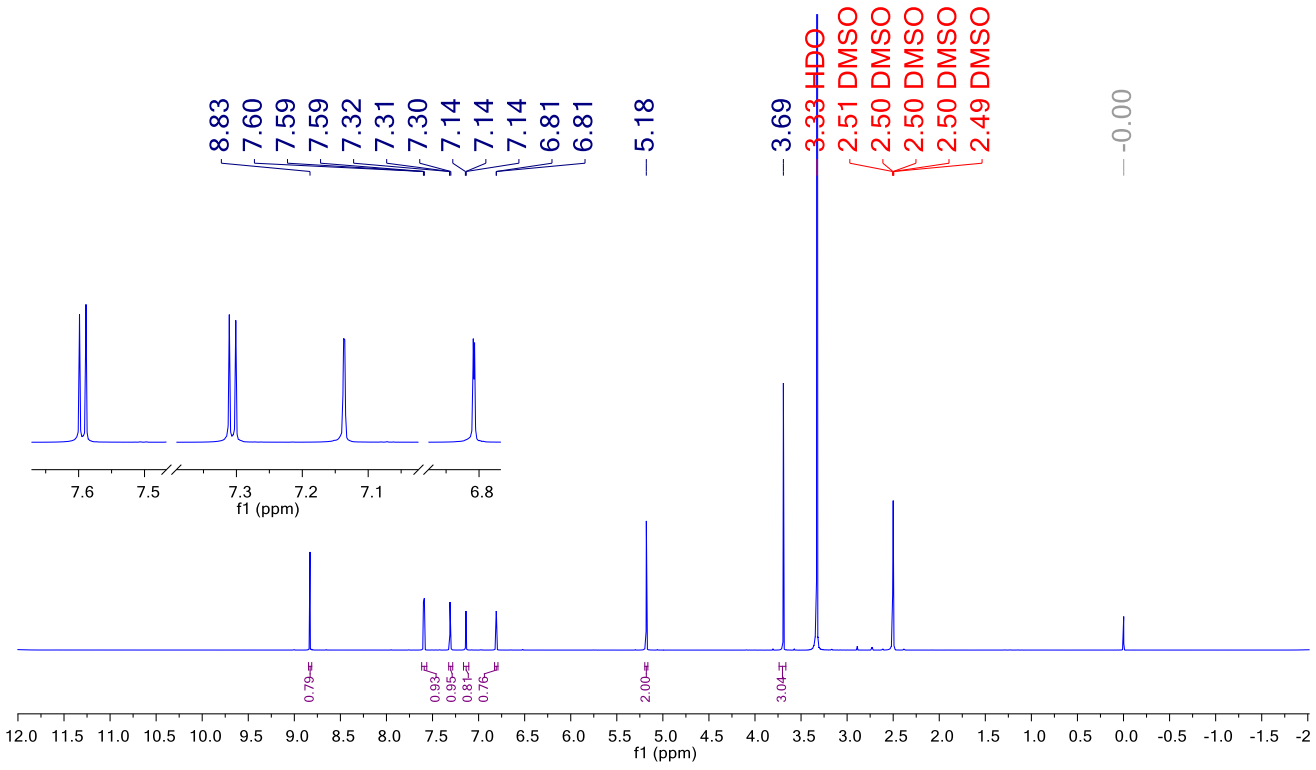


7-((1-Methyl-1*H*-imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26c)

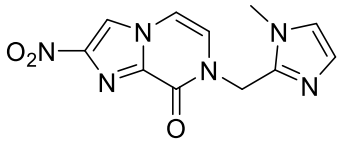


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_059_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-07-04T13:44:59
17	Modification Date	2018-07-04T13:44:59
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

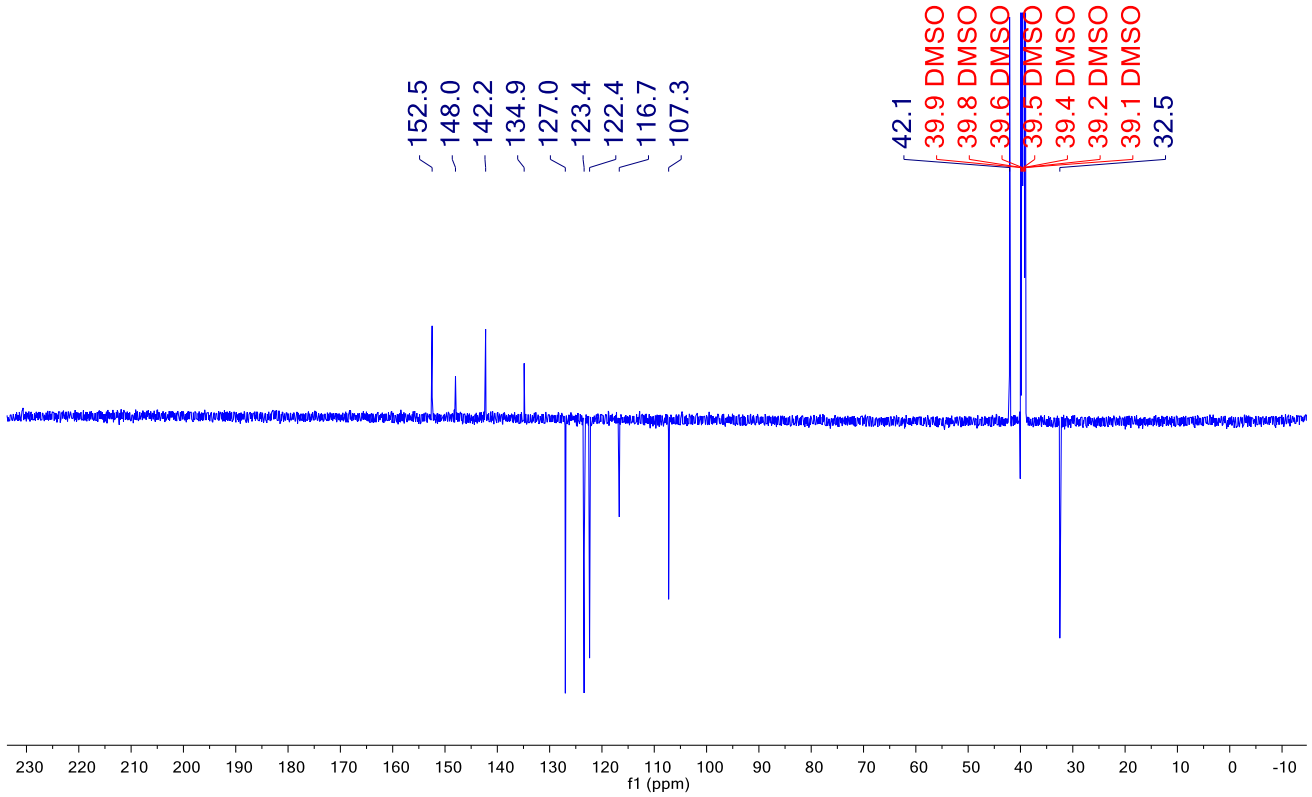


7-((1-Methyl-1*H*-imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26c)

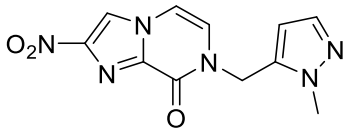


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_059_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	4096
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-07-04T16:01:59
17	Modification Date	2018-07-04T16:01:59
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

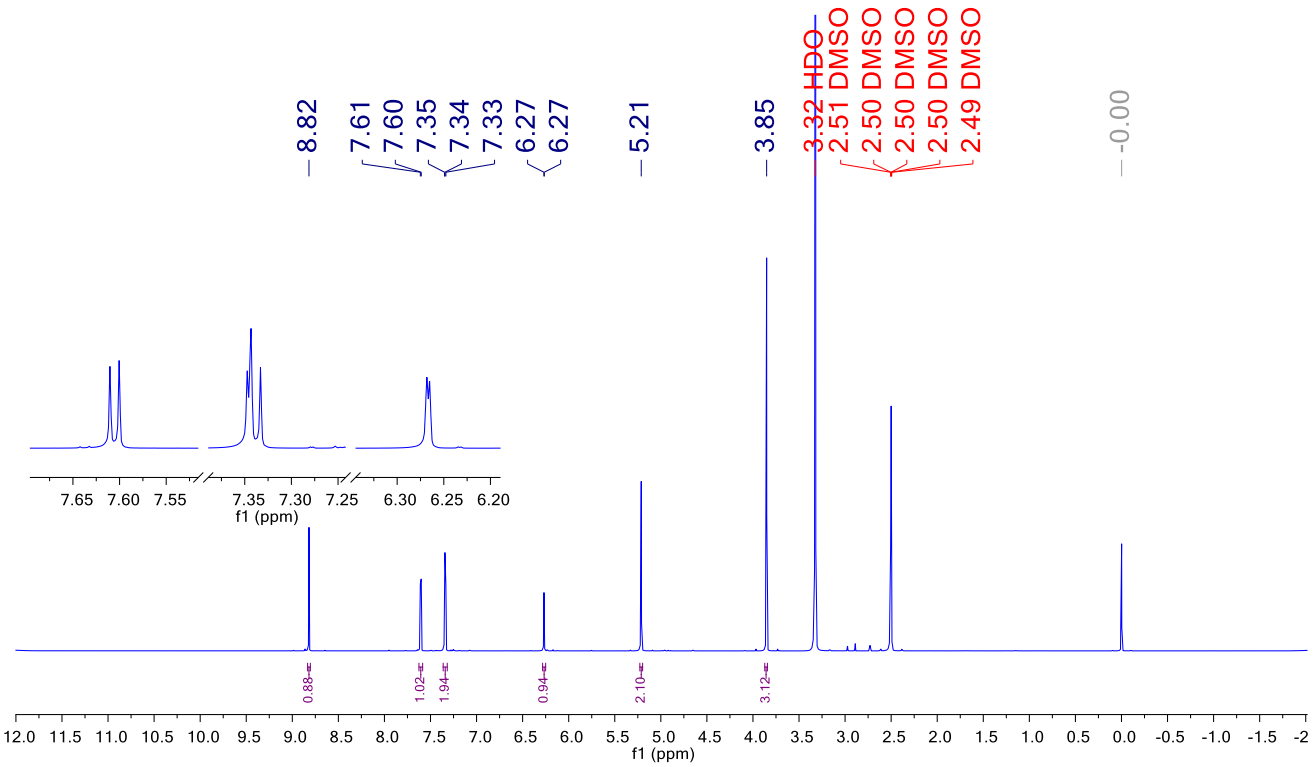


7-((1-Methyl-1*H*-pyrazol-5-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26d)

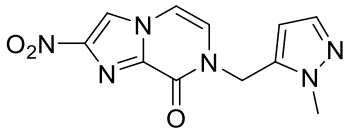


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_005/ NMR/ CWA8967_005_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8967_005_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8967_005_ppt_DCM_MeOH 1.5mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	32
15	Receiver Gain	96.4
16	Relaxation Delay	5.0000
17	Pulse Width	7.0100
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-03-16T17:02:24
21	Modification Date	2018-03-16T17:02:24
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest	-1208.1

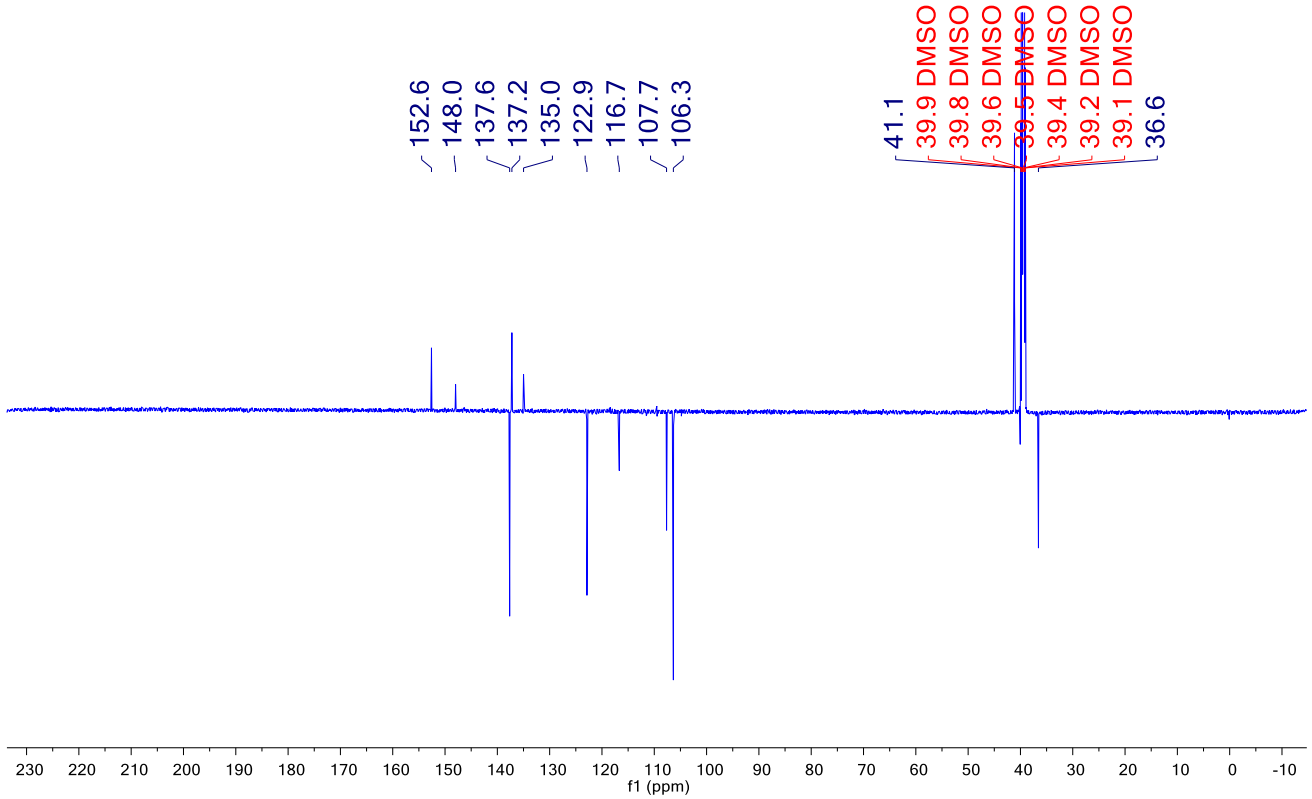


7-((1-Methyl-1*H*-pyrazol-5-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26d)

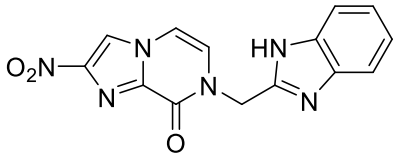


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_005/ NMR/ CWA8967_005_ppt_DCM_MeOH/ 2/ fid
2	Title	CWA8967_005_ppt_DCM_MeOH.2.fid
3	Comment	13C JMOD NMR of CWA8967_005_ppt_DCM_MeOH 1.5mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Experiment	JMOD
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	9500
15	Receiver Gain	191.6
16	Relaxation Delay	1.0000
17	Pulse Width	11.5000
18	Presaturation Frequency	
19	Acquisition Time	0.8738
20	Acquisition Date	2018-03-16T22:13:59
21	Modification Date	2018-03-16T22:13:59
22	Class	
23	Spectrometer Frequency	150.92
24	Spectral Width	37500.0
25	Lowest Frequency	-2151.2
26	Nucleus	13C
27	Acquired Size	32768

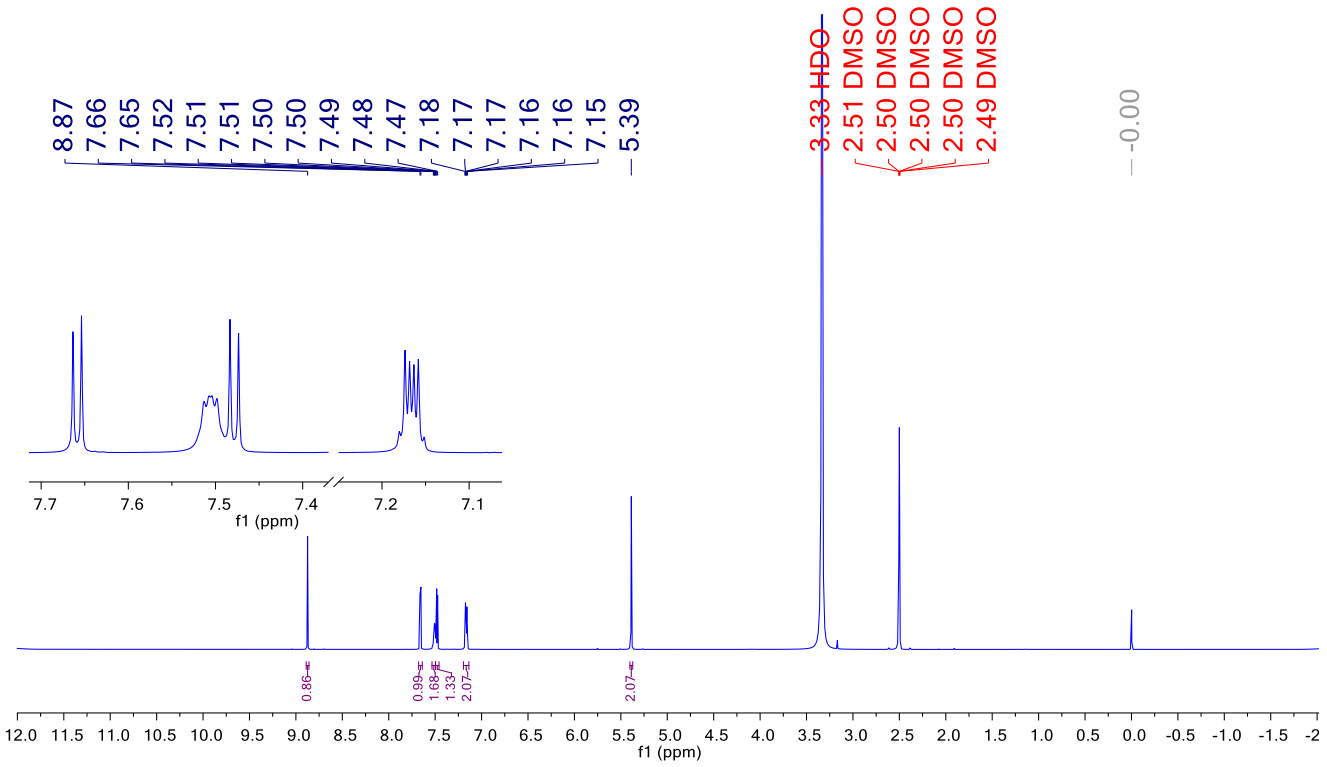


7-((1*H*-benzo[*d*]imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26e)

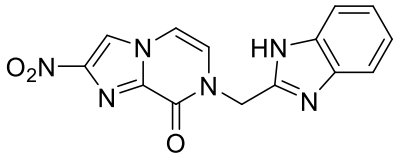


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_007/ NMR/ CWA8967_007_f7-9_ppt_DCM _MeOH/ 1/ fid
2	Title	CWA8967_007_f7-9_ppt_DCM _MeOH.1.fid
3	Comment	1H NMR of CWA8967_007_f7-9_ppt_DCM _MeOH 1.5mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	16
15	Receiver Gain	59.7
16	Relaxation Delay	5.0000
17	Pulse Width	7.0100
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-04-03T16:07:29
21	Modification Date	2018-04-03T16:07:29
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest Frequency	-1208.1
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536

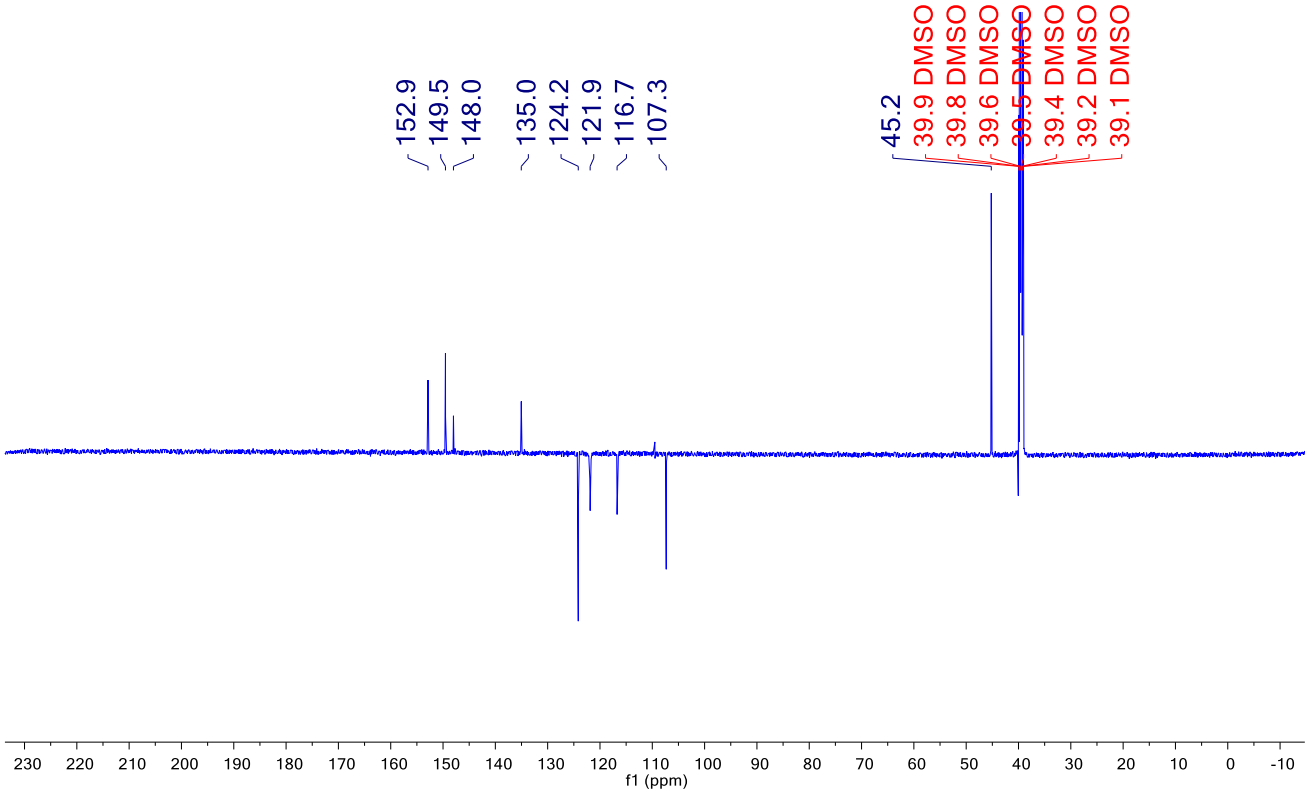


7-((1*H*-benzo[*d*]imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26e)

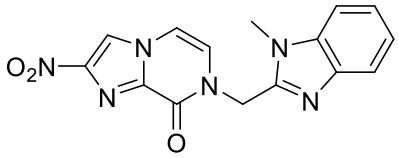


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_007_f7-9_ppt_DCM_MeOH.4.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	9000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	11.5000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-04-03T22:50:43
17	Modification Date	2018-04-03T22:50:43
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

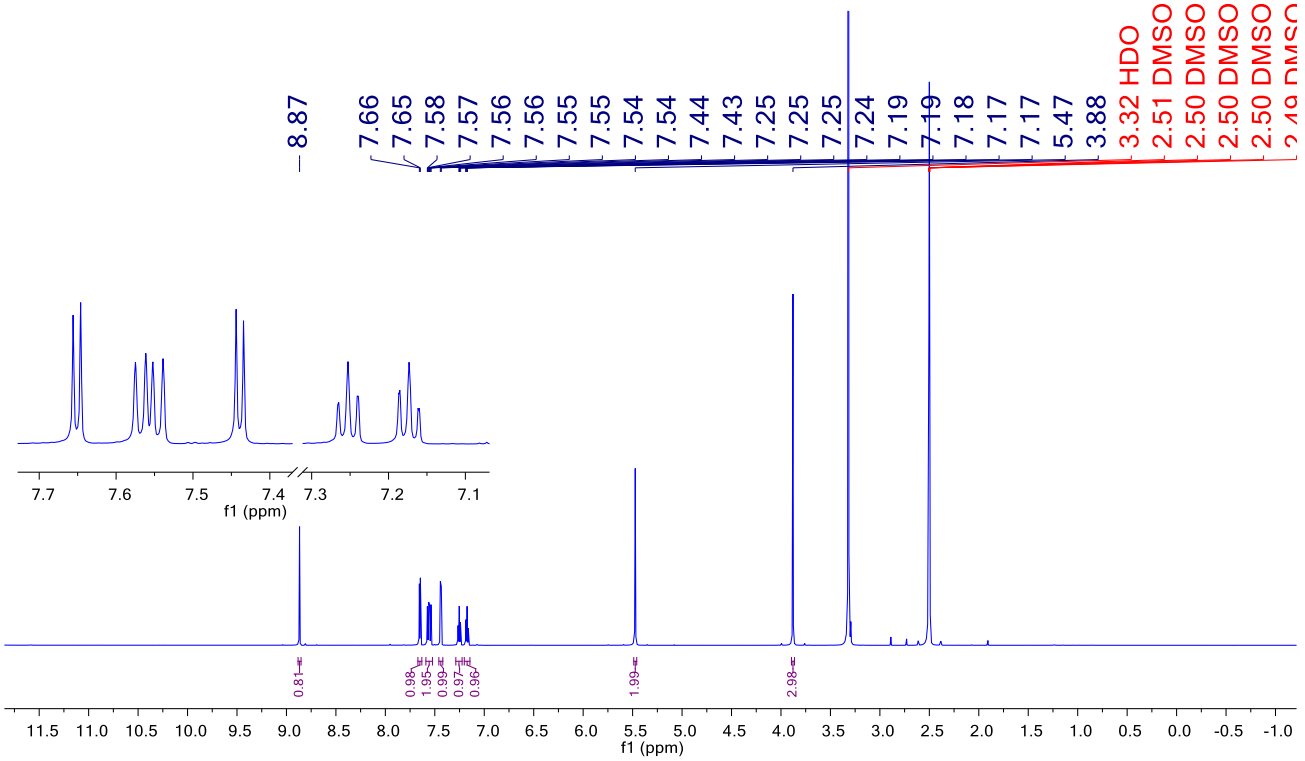


7-((1-Methyl-1*H*-benzo[*d*]imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26f)

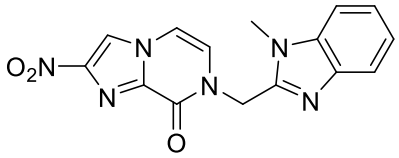


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_046/ NMR/ CWA8967_046_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8967_046_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8967_046_ppt_DCM_MeOH 1mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	64
15	Receiver Gain	109.3
16	Relaxation Delay	5.0000
17	Pulse Width	8.0000
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-05-09T12:07:23
21	Modification Date	2018-05-09T12:07:24
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest Frequency	-1208.1

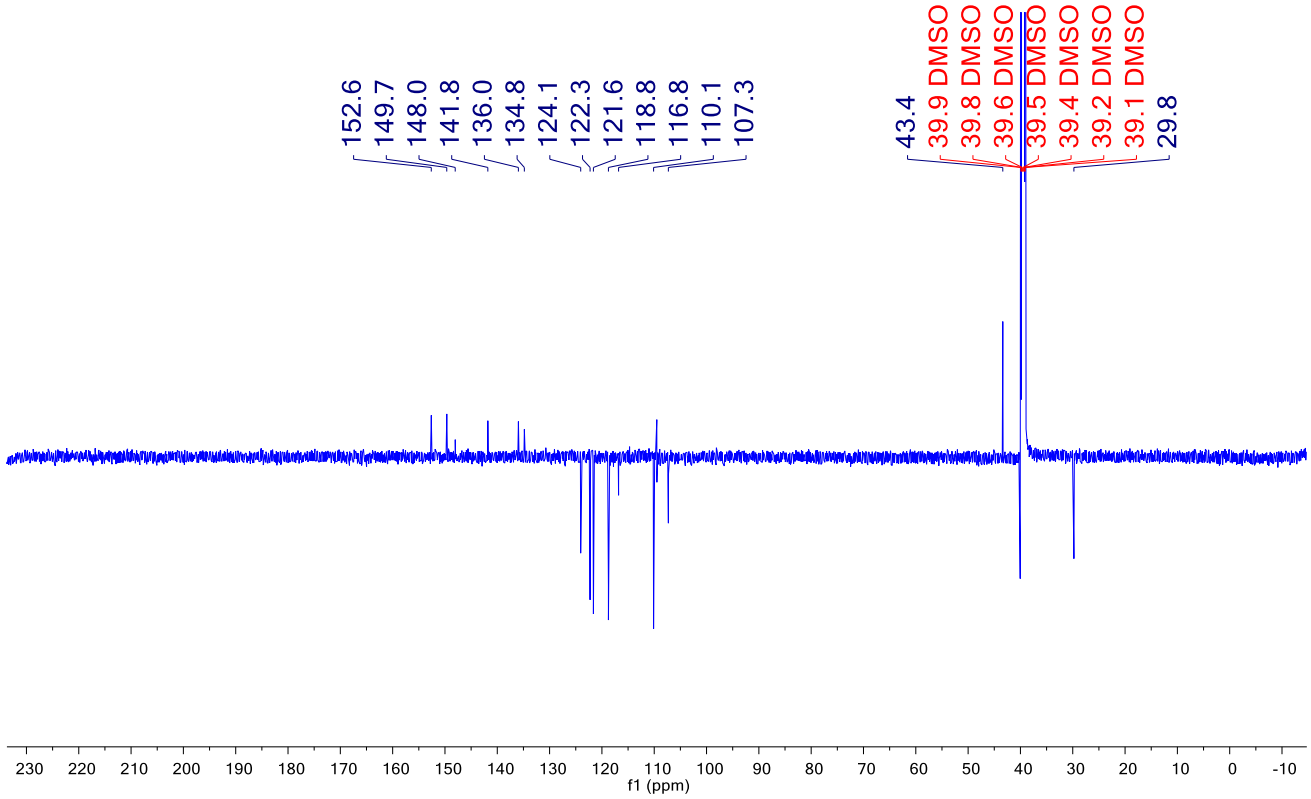


7-((1-Methyl-1*H*-benzo[*d*]imidazol-2-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26f)

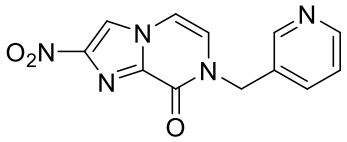


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_046_ppt_DCM_MeOH.4.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	11000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-05-10T00:31:53
17	Modification Date	2018-05-10T00:31:53
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

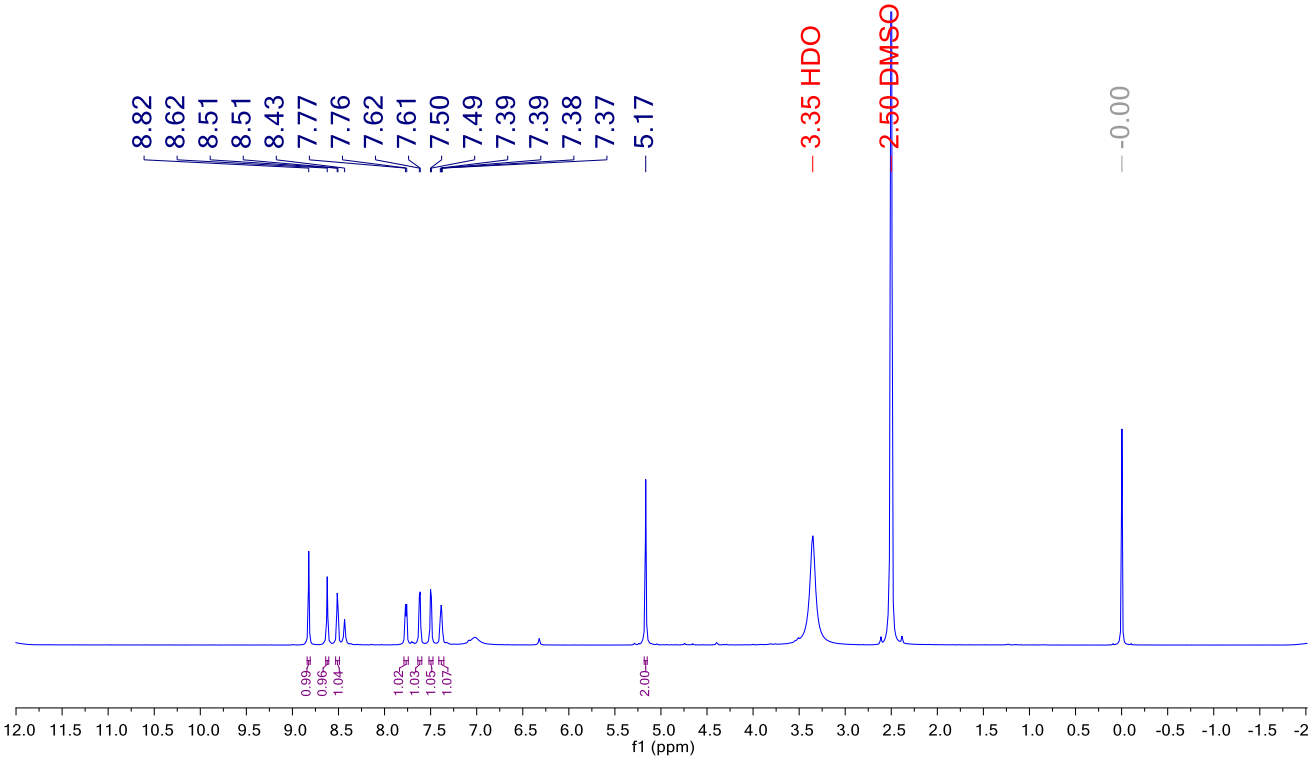


2-Nitro-7-(pyridin-3-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26g)

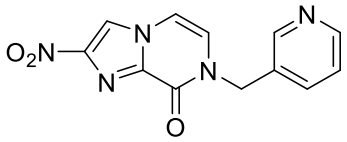


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_064_repurified_combined1.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	291.7
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	155.2
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2019-06-19T17:14:50
17	Modification Date	2019-06-19T17:14:50
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

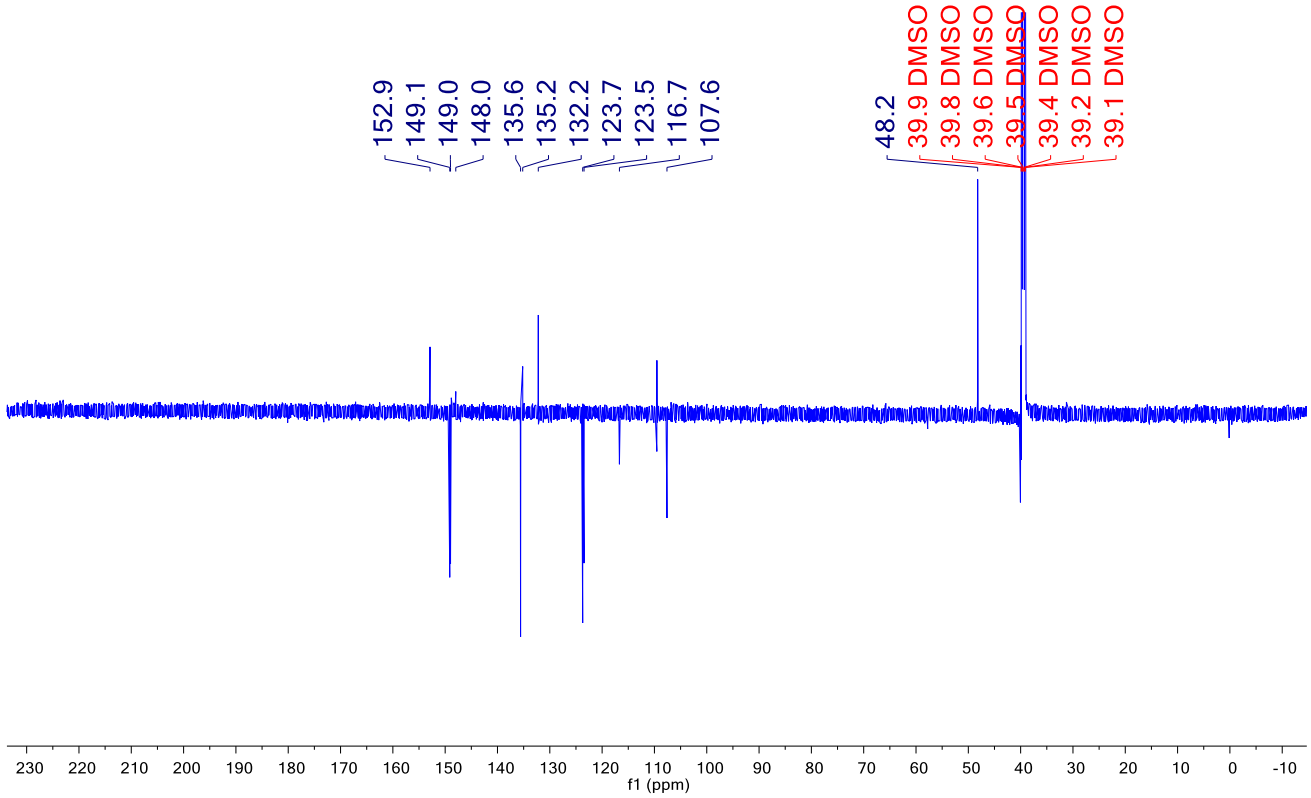


2-Nitro-7-(pyridin-3-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26g)

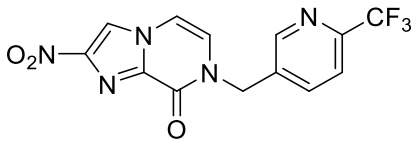


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8692_064_repurified_combined1.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	291.7
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2019-06-19T22:47:09
17	Modification Date	2019-06-19T22:47:09
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

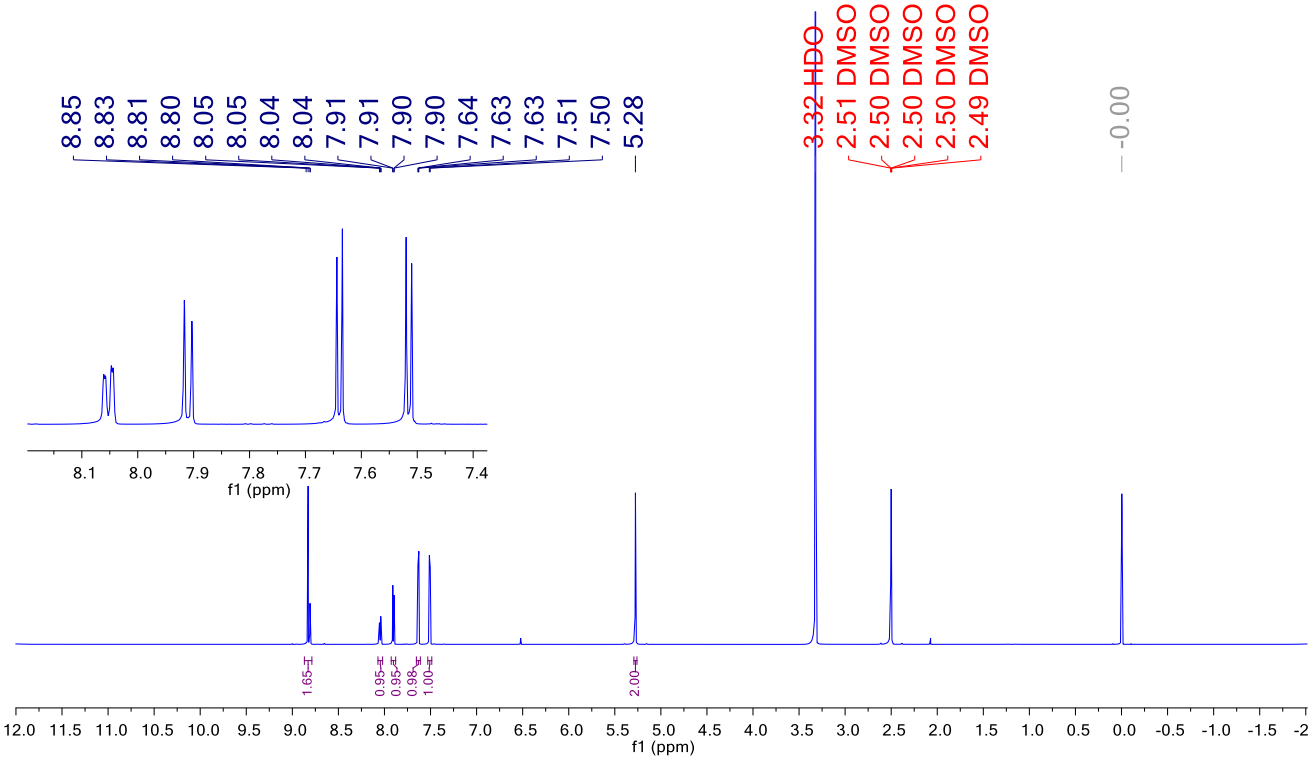


2-Nitro-7-((6-(trifluoromethyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26h)

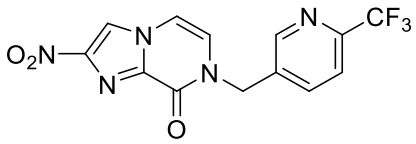


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_103_filtrate_f3_cryoprobe.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2019-05-01T17:17:49
17	Modification Date	2019-05-01T17:17:49
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

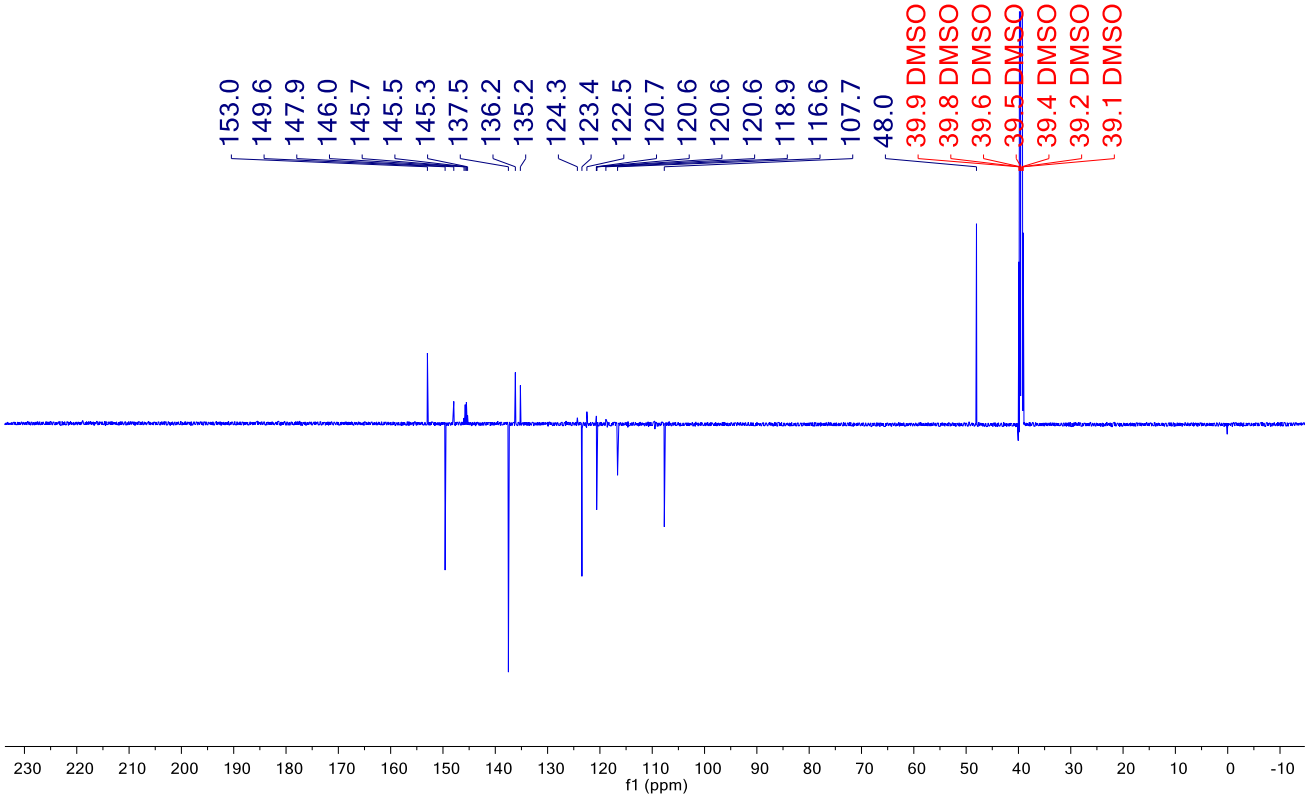


2-Nitro-7-((6-(trifluoromethyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26h)

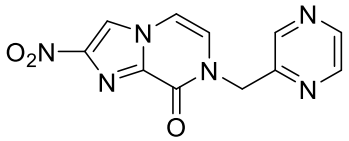


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_103_filtrate_f3_cryoprobe.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	7500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2019-05-01T21:18:17
17	Modification Date	2019-05-01T21:18:17
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

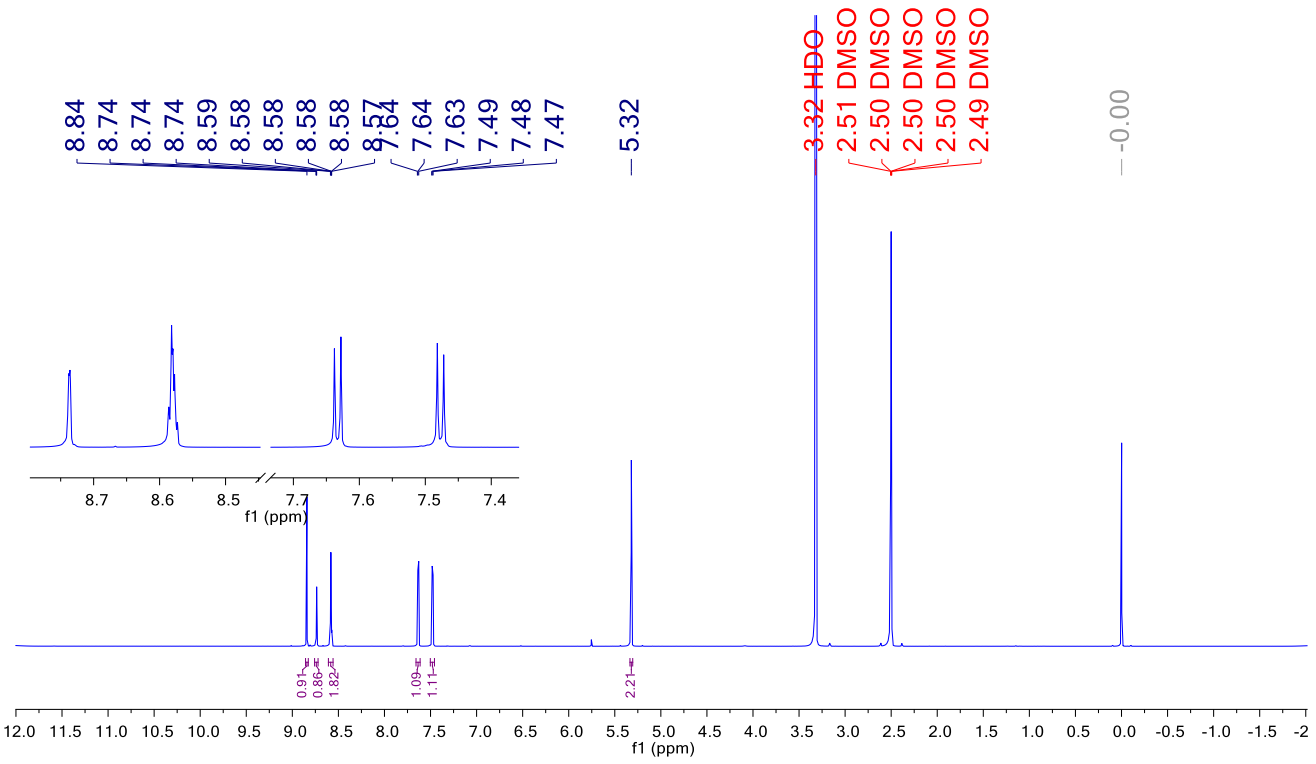


2-Nitro-7-(pyrazin-2-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26i)

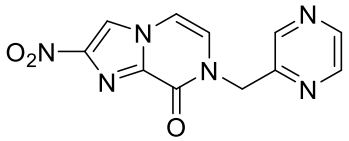


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_111/ NMR/ CWA8805_111_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8805_111_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8805_111_ppt_DCM_MeOH 1mg in 480uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	32
15	Receiver Gain	116.1
16	Relaxation Delay	5.0000
17	Pulse Width	7.0100
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-03-09T15:03:45
21	Modification Date	2018-03-09T15:03:45
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest Frequency	-1208.1
26	Nucleus	1H
27	Acquired Size	16384

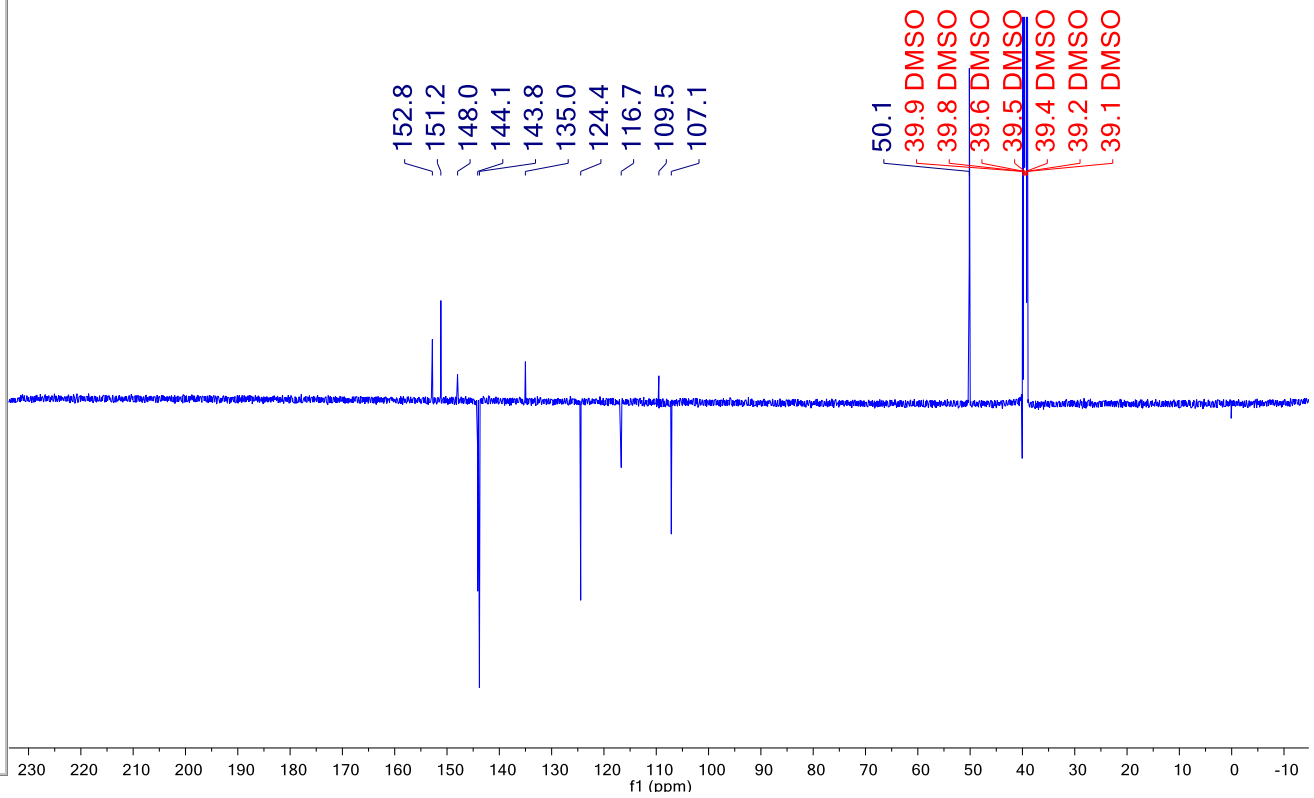


2-Nitro-7-(pyrazin-2-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26i)

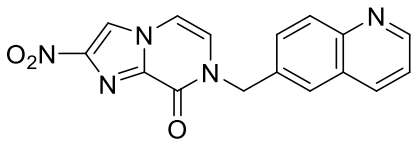


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_111/ NMR/ CWA8805_111_ppt_DCM_MeOH/ 2/ fid
2	Title	CWA8805_111_ppt_DCM_MeOH.2.fid
3	Comment	13C JMOD NMR of CWA8805_111_ppt_DCM_MeOH 1mg in 480uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Experiment	JMOD
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	9000
15	Receiver Gain	191.6
16	Relaxation Delay	1.0000
17	Pulse Width	11.5000
18	Presaturation Frequency	
19	Acquisition Time	0.8738
20	Acquisition Date	2018-03-09T21:58:02
21	Modification Date	2018-03-09T21:58:02
22	Class	
23	Spectrometer Frequency	150.92
24	Spectral Width	37500.0
25	Lowest Frequency	-2151.2
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

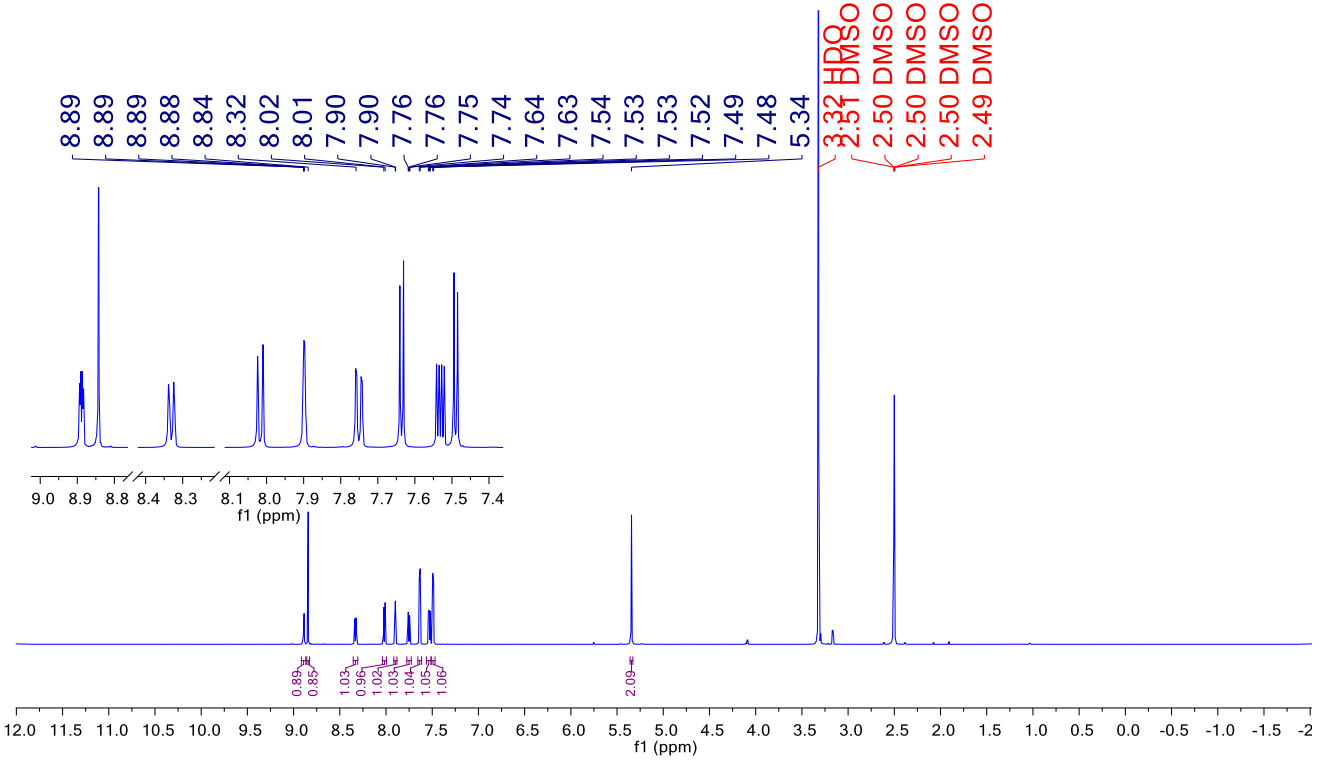


2-Nitro-7-(quinolin-6-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26j)

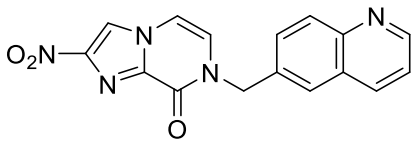


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_044/ NMR/ CWA8967_044_f16-40_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8967_044_f16-40_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8967_044_f16-40_ppt_DCM_MeOH 1.7mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	32
15	Receiver Gain	140.4
16	Relaxation Delay	5.0000
17	Pulse Width	8.0000
18	Presaturation Frequency	
19	Acquisition Time	1.9464
20	Acquisition Date	2018-05-11T11:21:13
21	Modification Date	2018-05-11T11:21:13
22	Class	
23	Spectrometer Frequency	600.13
24	Spectral Width	8417.5
25	Lowest Frequency	-1208.1
26	Nucleus	1H
27	Acquired Size	16384

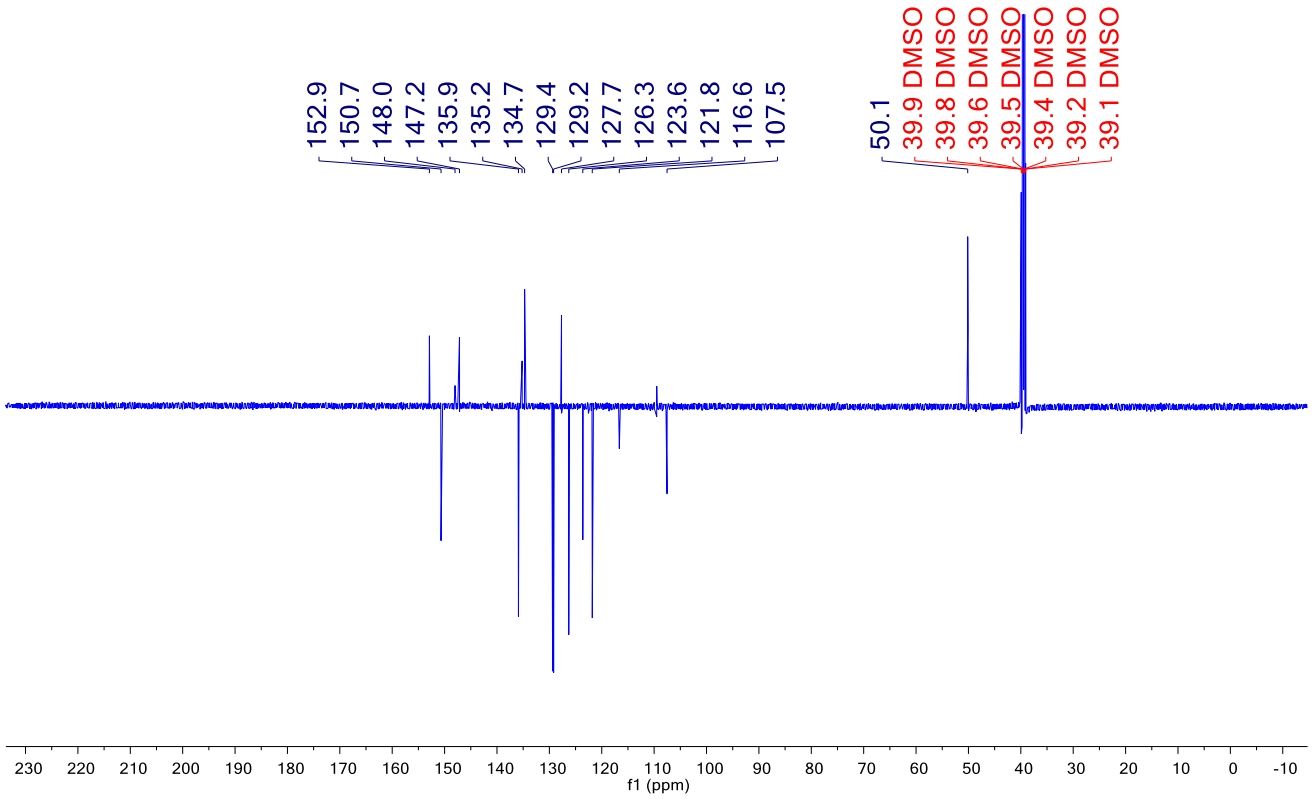


2-Nitro-7-(quinolin-6-ylmethyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (26j)

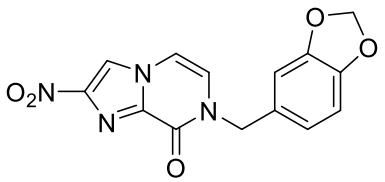


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8967/ CWA8967_044/ NMR/ CWA8967_044_f16-40_ppt_DCM_MeOH/ 2/ fid
2	Title	CWA8967_044_f16-40_ppt_DCM_MeOH.2.fid
3	Comment	13C JMOD NMR of CWA8967_044_f16-40_ppt_DCM_MeOH 1.7mg in 500uL DMSO-d6; cryoprobe
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Experiment	JMOD
13	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
14	Number of Scans	7500
15	Receiver Gain	191.6
16	Relaxation Delay	1.0000
17	Pulse Width	12.0000
18	Presaturation Frequency	
19	Acquisition Time	0.8738
20	Acquisition Date	2018-05-15T20:10:48
21	Modification Date	2018-05-15T20:10:49
22	Class	
23	Spectrometer Frequency	150.92
24	Spectral Width	37500.0
25	Lowest Frequency	-2151.2
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

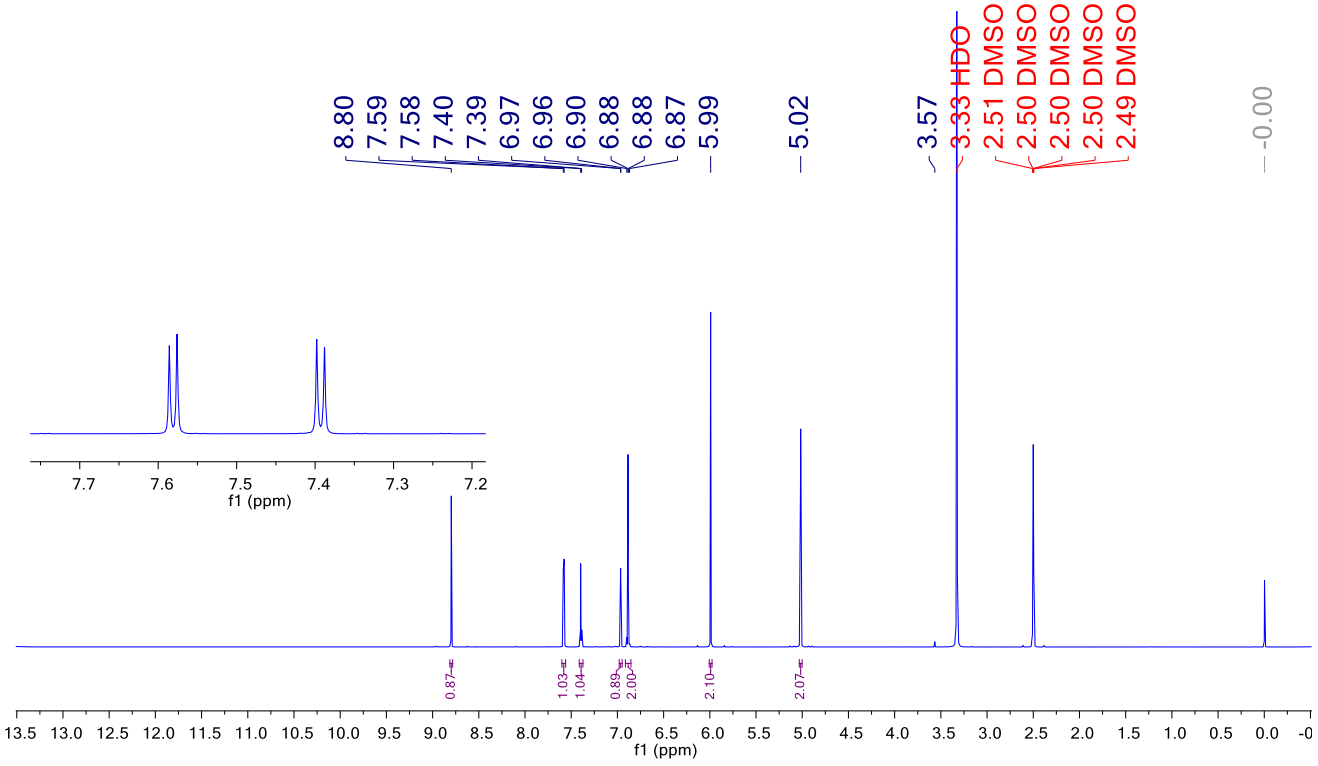


7-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26k)

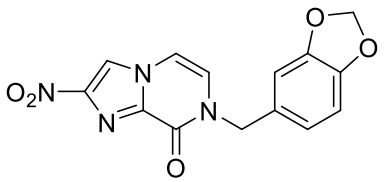


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_073/ NMR/ CWA8805_073_ppt_DCM_MeOH/ 1/ fid
2	Title	CWA8805_073_ppt_DCM_MeOH.1.fid
3	Comment	1H NMR of CWA8805_073_ppt_DCM_MeOH 2.2mg in 500uL DMSO-d6; LC-NMR AA_1H DMSO C:\ \ c.ang 10
4	Origin	Bruker BioSpin GmbH
5	Owner	biodiversity
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm PASEI 1H/ D-13C Z-GRD Z866801/ 0003
14	Number of Scans	16
15	Receiver Gain	287.0
16	Relaxation Delay	5.0000
17	Pulse Width	9.8000
18	Presaturation Frequency	
19	Acquisition Time	1.9465
20	Acquisition Date	2018-01-31T17:24:00
21	Modification Date	2018-01-31T17:25:06
22	Class	
23	Spectrometer Frequency	600.08

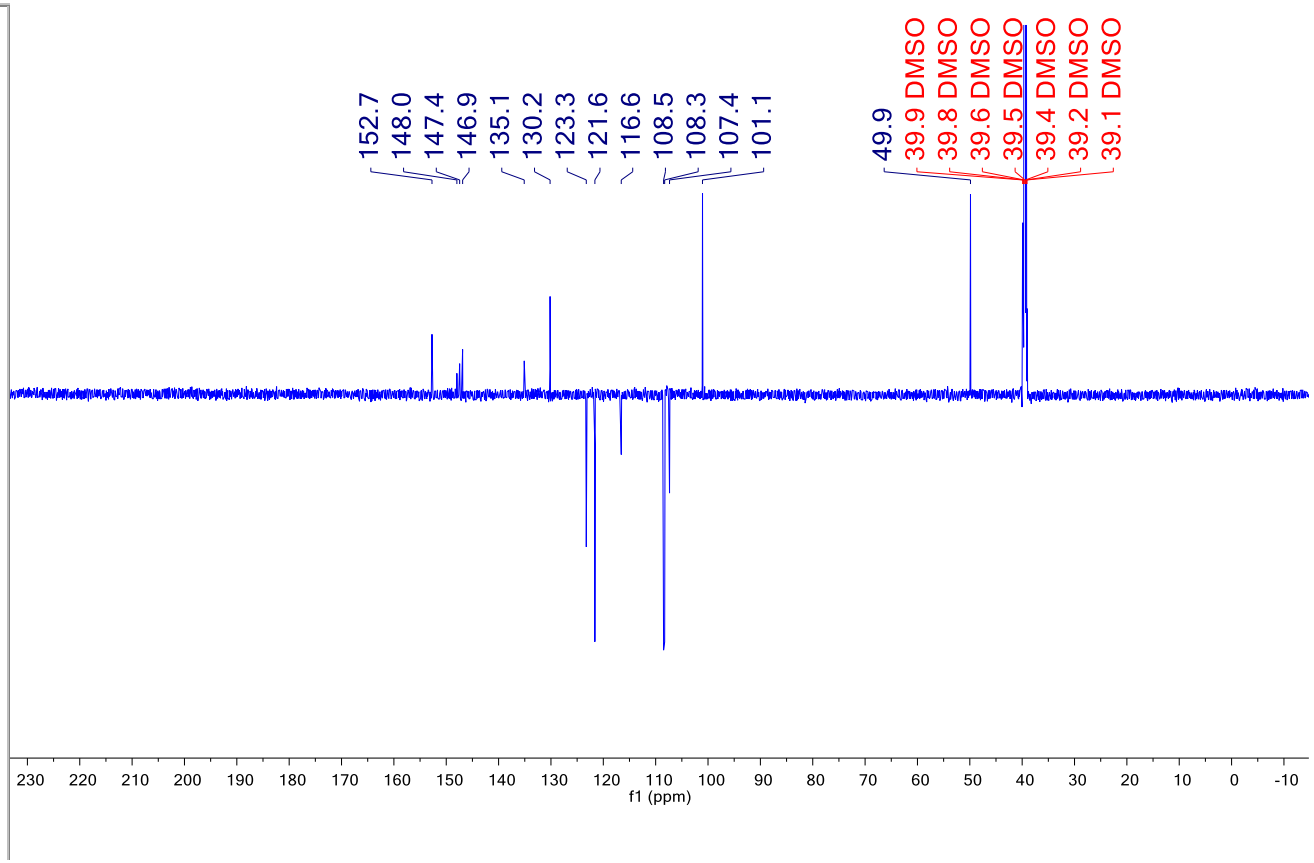


7-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (26k)

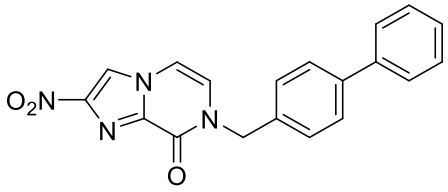


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Data File Name	Z:/ Projects/ 029_Anaerobic/ 029E_Chemistry/ LaboratoryNoteBooks/ CWA8805/ CWA8805_073/ NMR/ CWA8805_073_ppt_DCM_MeOH/ 2/ fid
2	Title	CWA8805_073_ppt_DCM_MeOH.2.fid
3	Comment	13C JMOD NMR of CWA8805_073_ppt_DCM_MeOH 2.2mg in 500uL DMSO-d6; LC-NMR A_13C_JMOD DMSO C:\ \ c.ang 10
4	Origin	Bruker BioSpin GmbH
5	Owner	biodiversity
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Experiment	JMOD
13	Probe	5 mm PASEI 1H/ D-13C Z-GRD Z866801/ 0003
14	Number of Scans	10000
15	Receiver Gain	2050.0
16	Relaxation Delay	1.0000
17	Pulse Width	14.0000
18	Presaturation Frequency	
19	Acquisition Time	0.8739
20	Acquisition Date	2018-01-31T22:30:00
21	Modification Date	2018-01-31T22:47:51
22	Class	
23	Spectrometer Frequency	150.91
24	Spectral Width	37500.0
25	Lowest Frequency	-2227.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

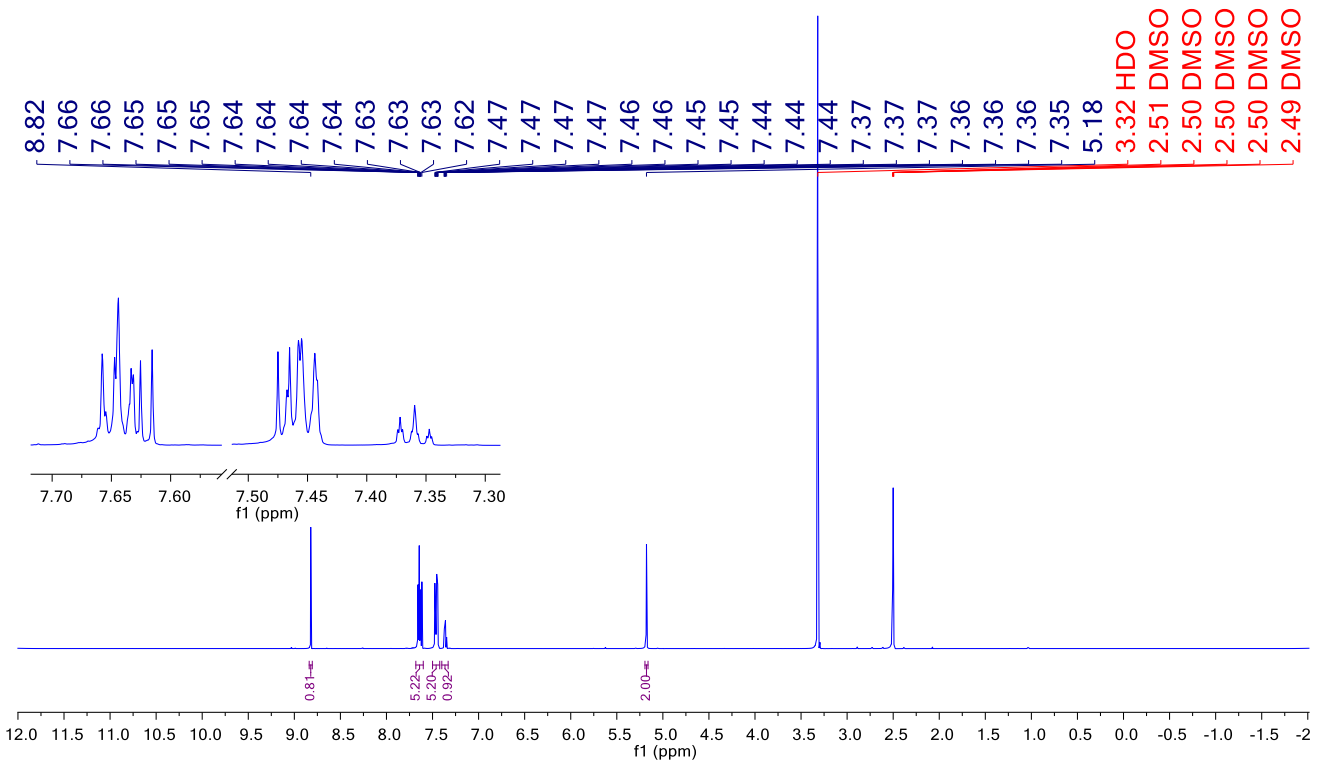


7-([1,1'-Biphenyl]-4-ylmethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (34a)

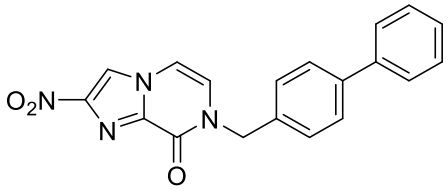


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_048_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-05-11T11:27:49
17	Modification Date	2018-05-11T11:27:49
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

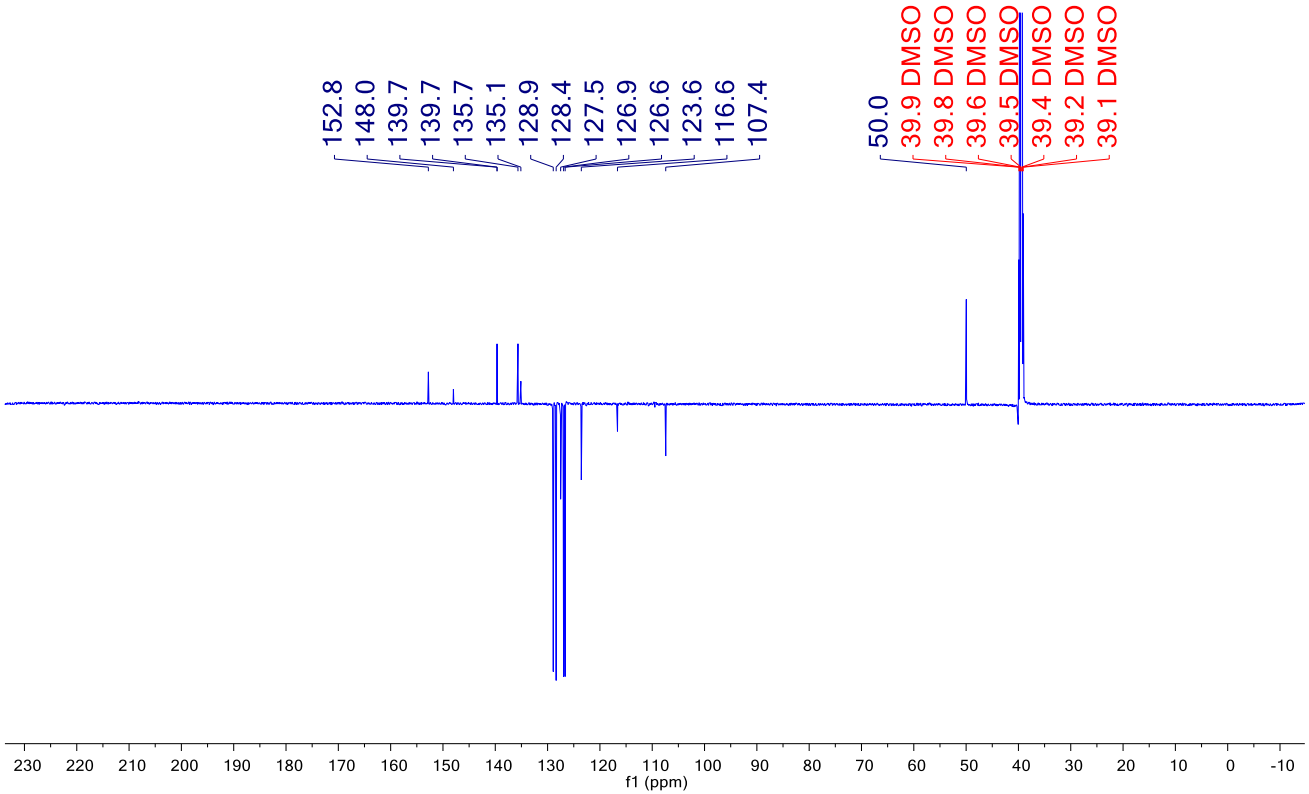


7-([1,1'-Biphenyl]-4-ylmethyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (34a)

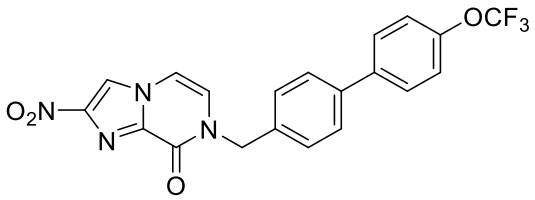


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_048_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	6000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-05-11T14:54:55
17	Modification Date	2018-05-11T14:54:55
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

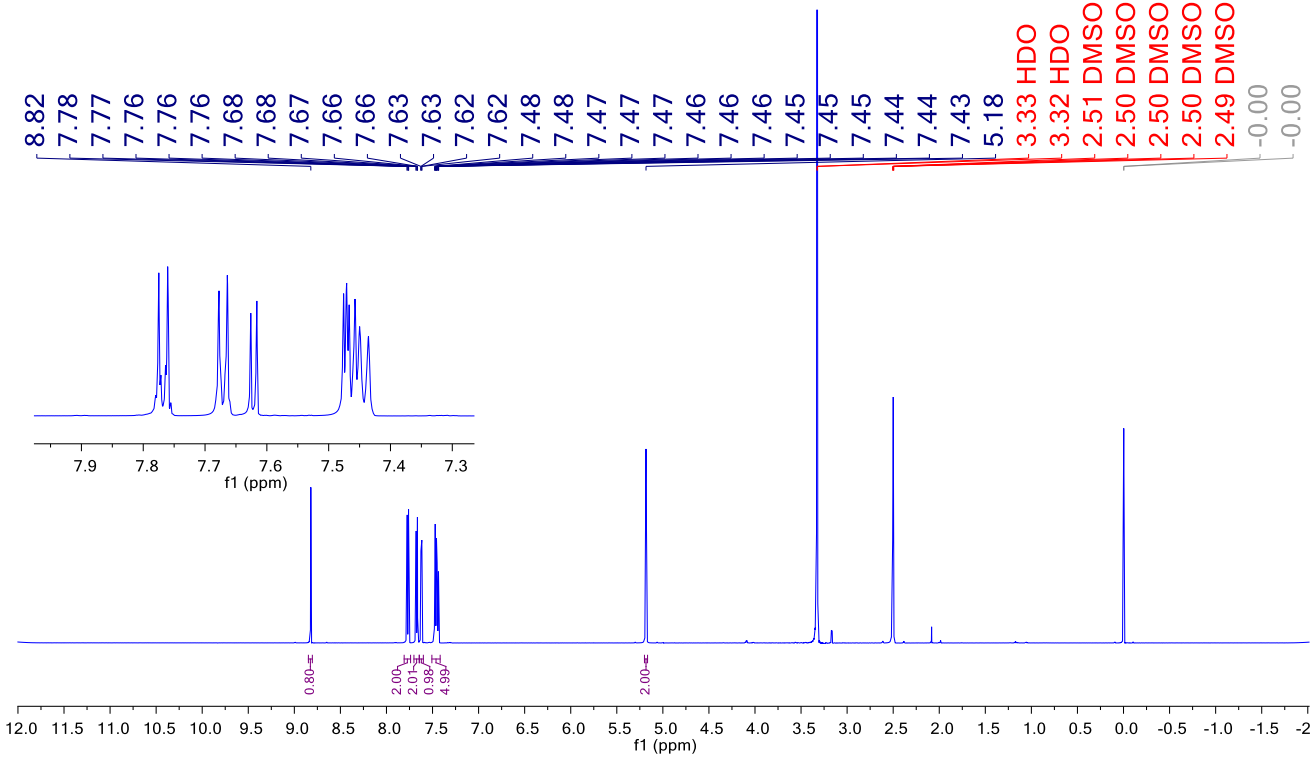


2-Nitro-7-((4′-(trifluoromethoxy)-[1,1′-biphenyl]-4-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34b)

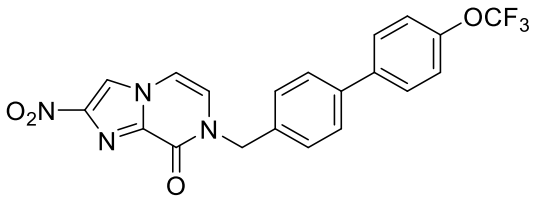


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_089_ppt_MeOH_acetone.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9465
16	Acquisition Date	2018-07-27T11:20:00
17	Modification Date	2018-07-28T12:13:16
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

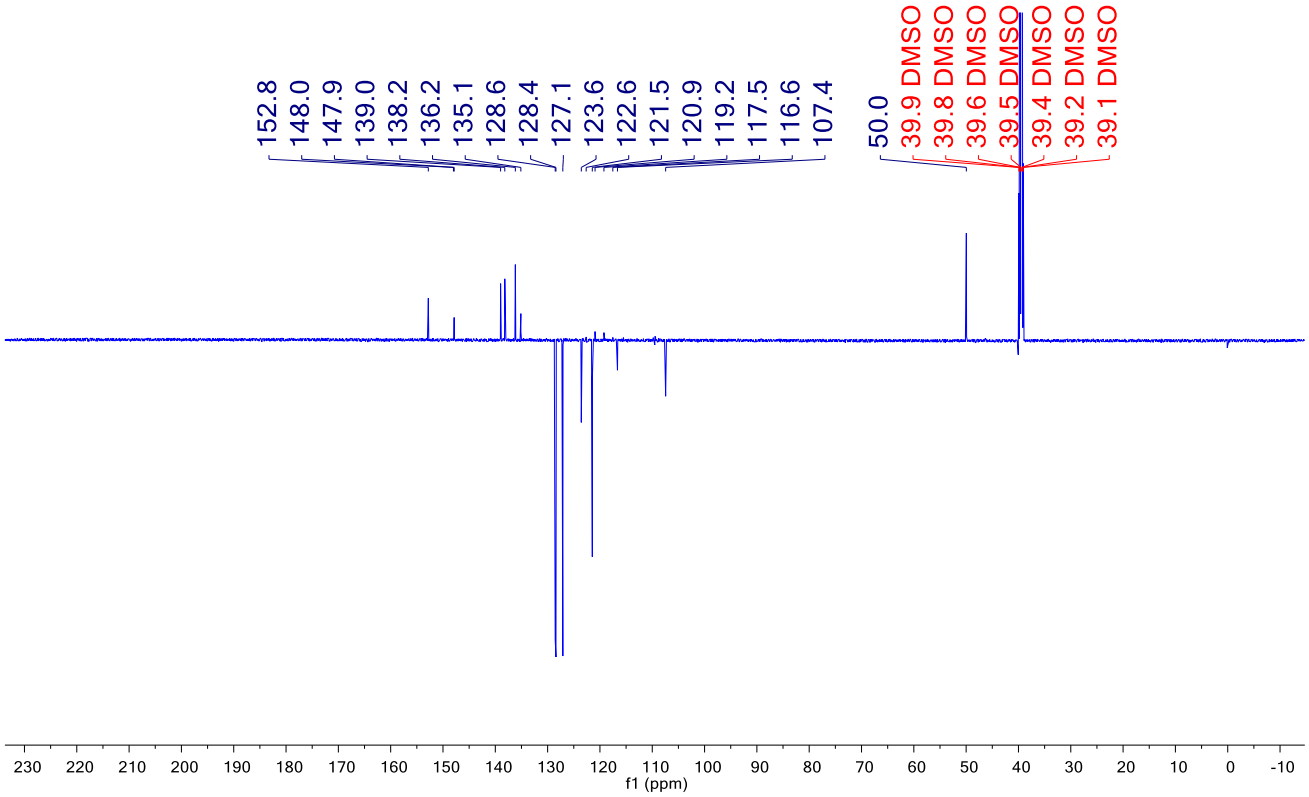


2-Nitro-7-((4′-(trifluoromethoxy)-[1,1′-biphenyl]-4-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34b)

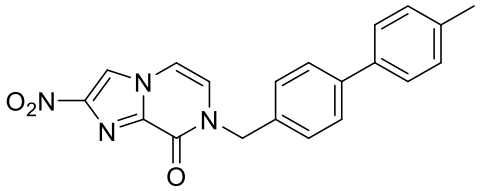


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_089_ppt_MeOH_acetone.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	10240
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-07-28T17:41:24
17	Modification Date	2018-07-28T17:41:25
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

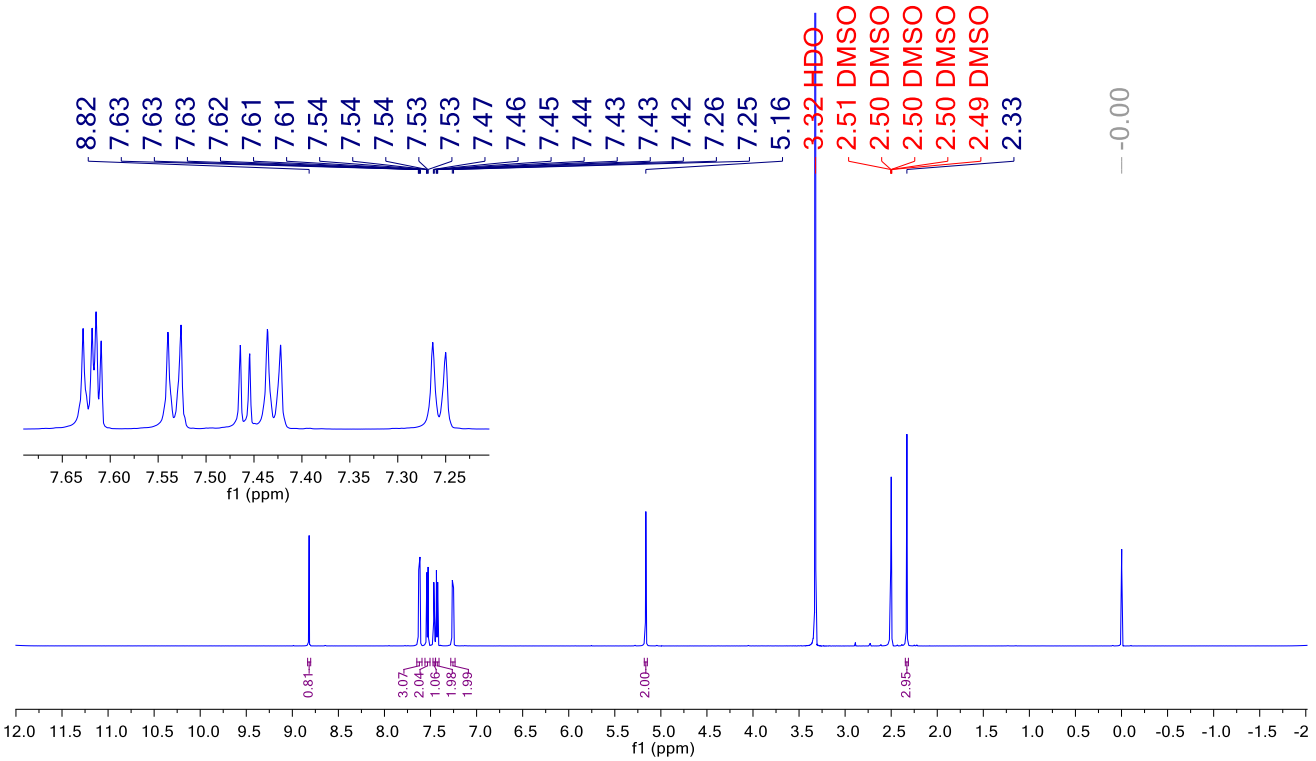


7-((4'-Methyl-[1,1'-biphenyl]-4-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (34c)

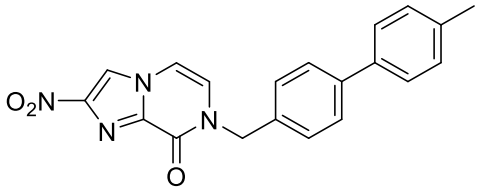


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_033_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-09-07T15:10:38
17	Modification Date	2018-09-07T15:10:38
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

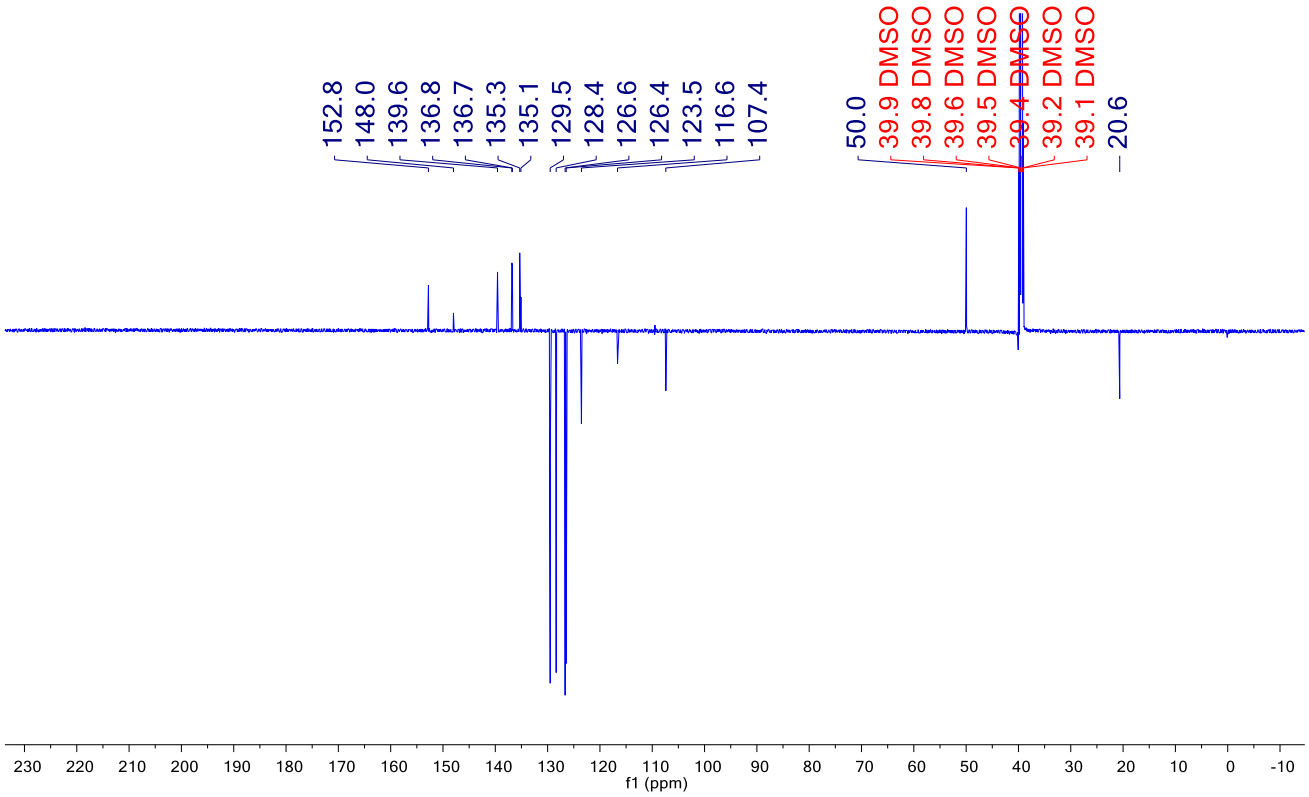


7-((4'-Methyl-[1,1'-biphenyl]-4-yl)methyl)-2-nitroimidazo[1,2-*a*]pyrazin-8(7*H*)-one (34c)

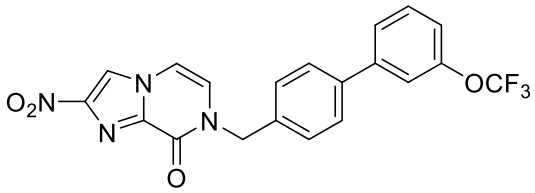


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_033_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	5120
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-09-07T19:54:41
17	Modification Date	2018-09-07T19:54:41
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

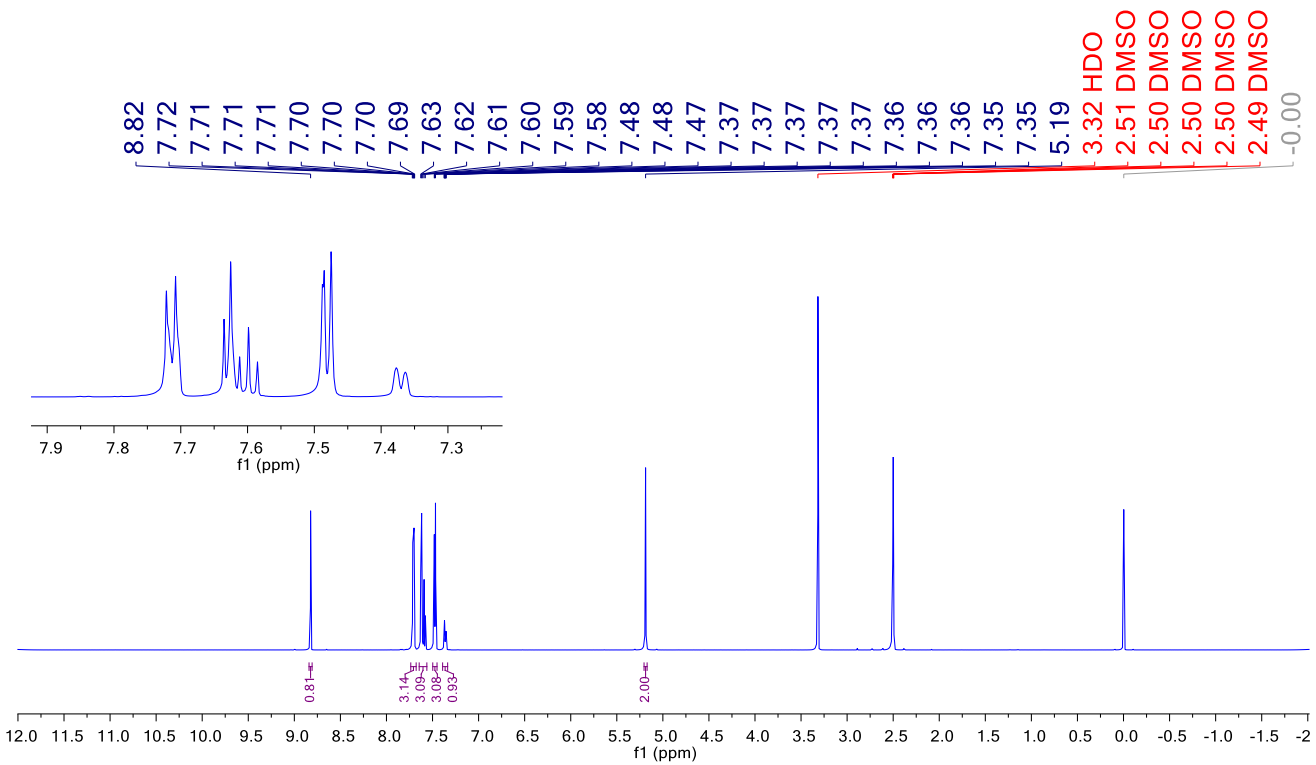


2-Nitro-7-((3'-(trifluoromethoxy)-[1,1'-biphenyl]-4-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34d)

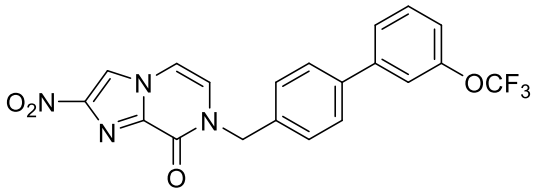


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_106_ppt_MeOH_DCM.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	109.3
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-08-16T18:02:27
17	Modification Date	2018-08-16T18:02:27
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

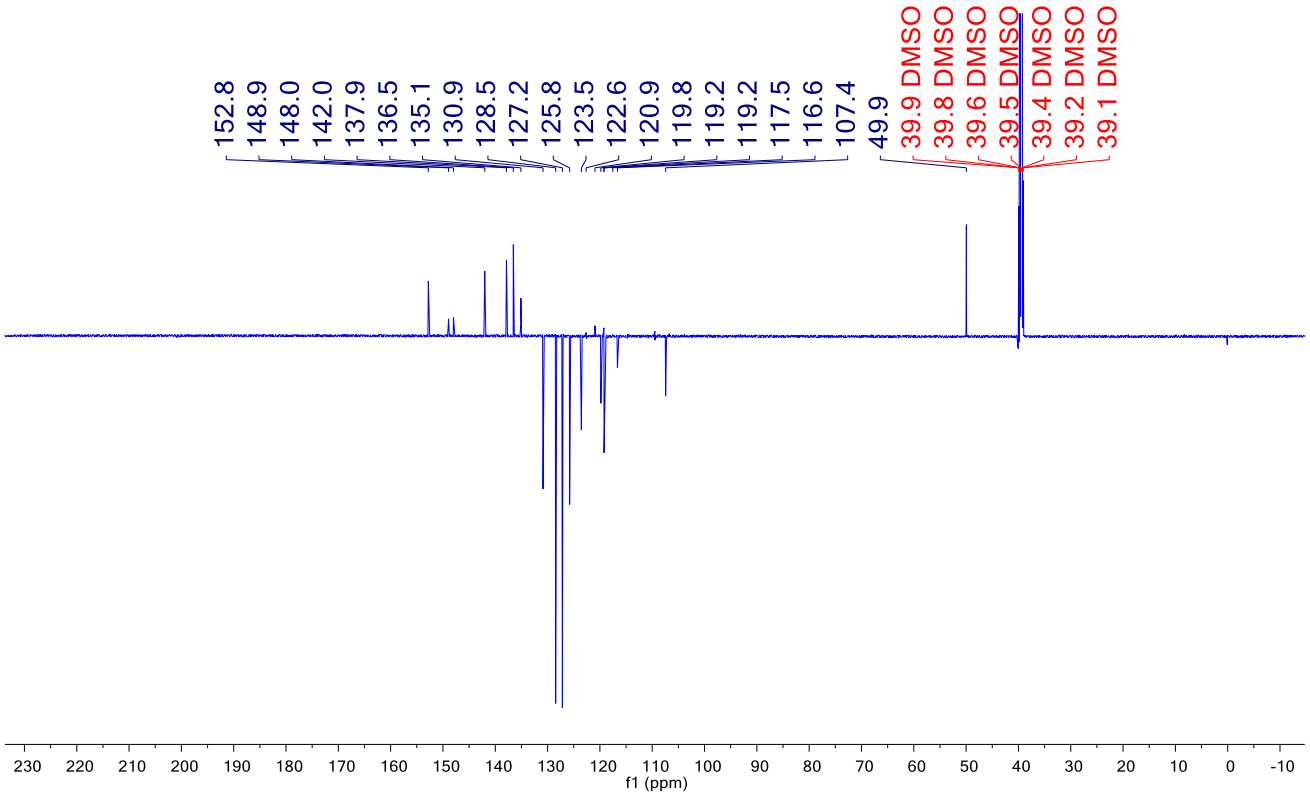


2-Nitro-7-((3'-(trifluoromethoxy)-[1,1'-biphenyl]-4-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34d)

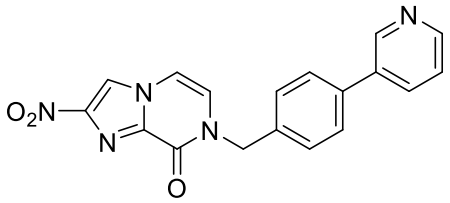


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_106_ppt_MeOH_DCM.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	9000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-08-16T22:51:47
17	Modification Date	2018-08-16T22:51:47
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

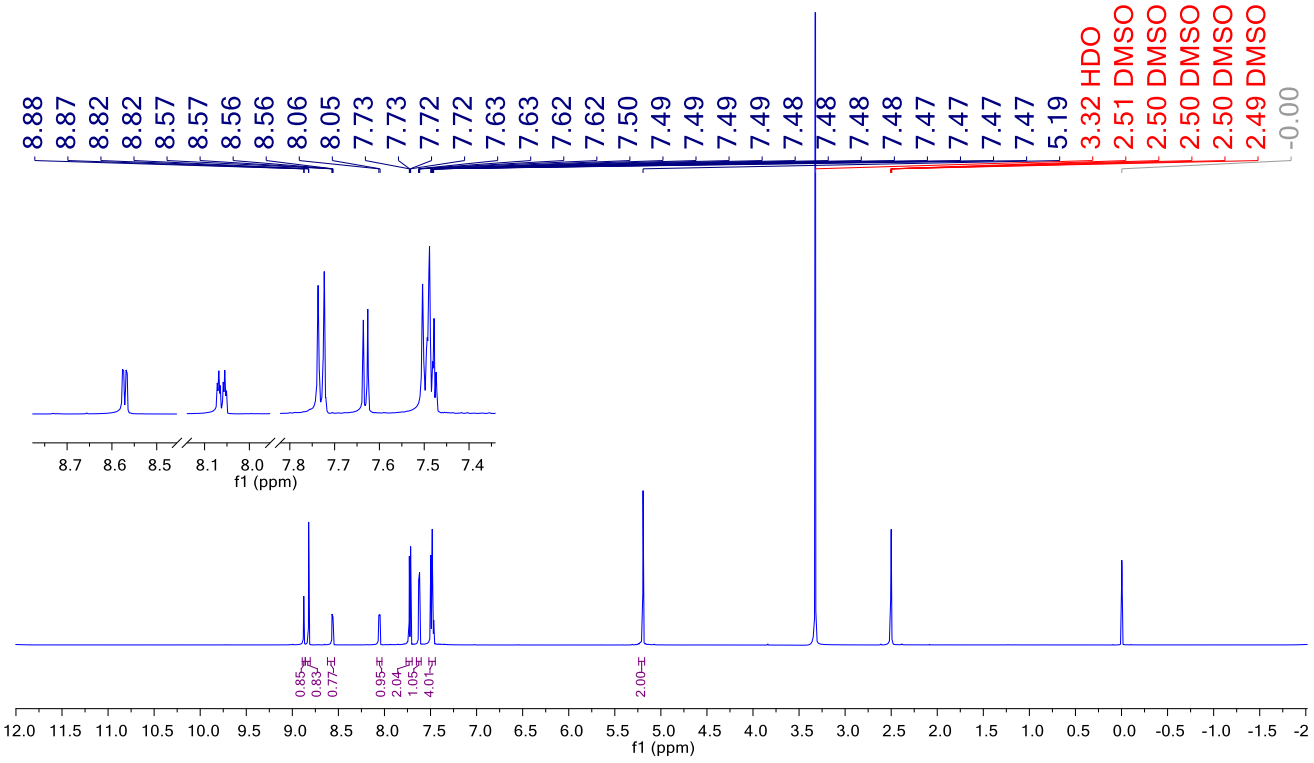


2-Nitro-7-(4-(pyridin-3-yl)benzyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34e)

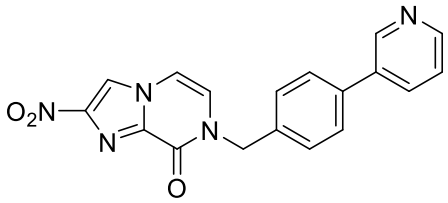


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_097_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2019-04-24T17:07:32
17	Modification Date	2019-04-24T17:07:32
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

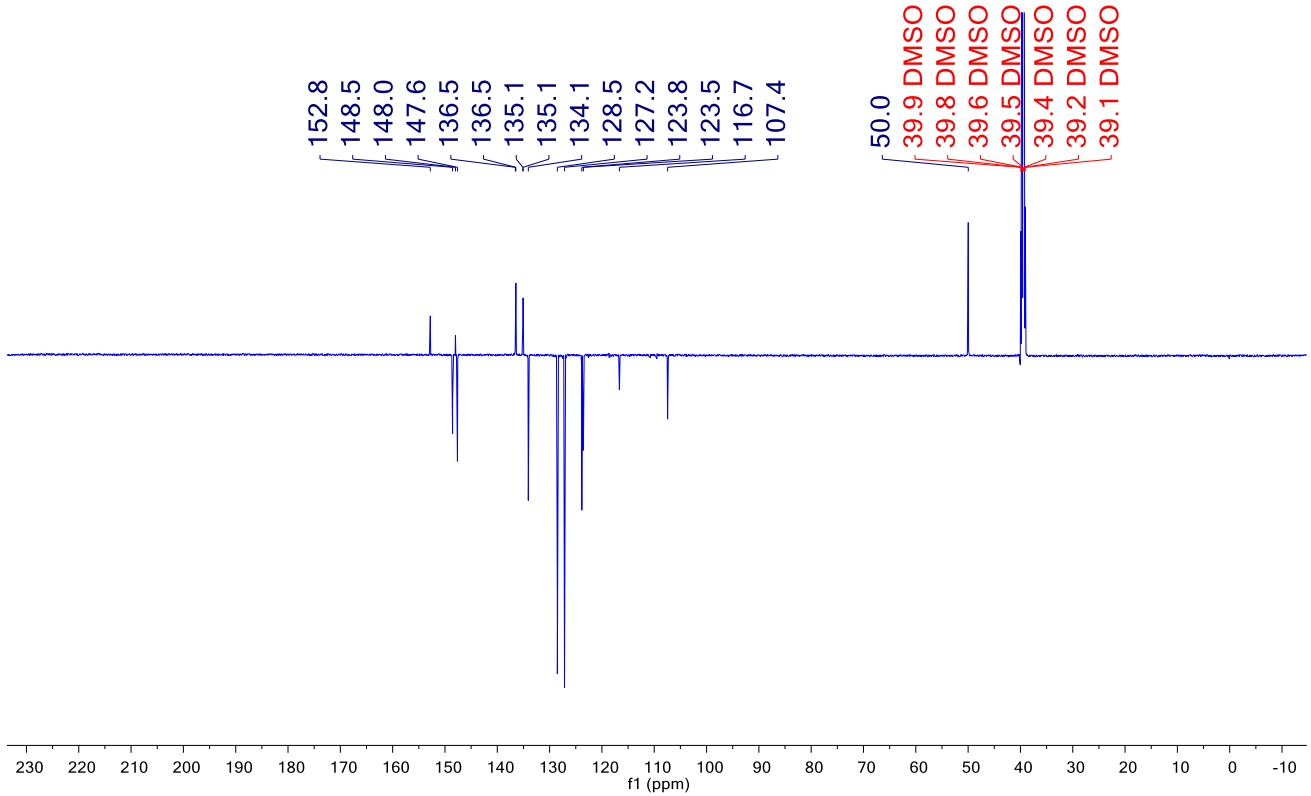


2-Nitro-7-(4-(pyridin-3-yl)benzyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34e)

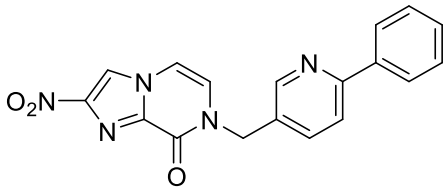


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_097_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	7500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2019-04-24T21:08:24
17	Modification Date	2019-04-24T21:08:24
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

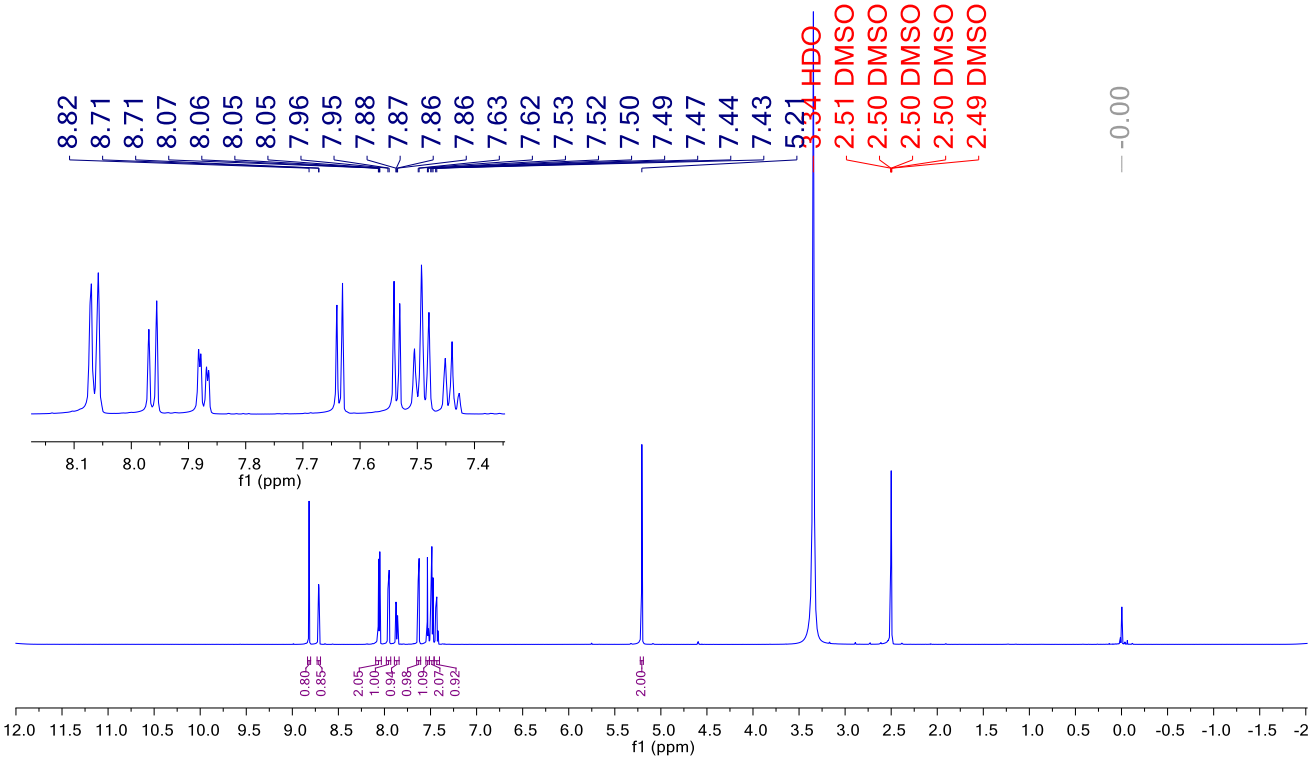


2-Nitro-7-((6-phenylpyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34f)

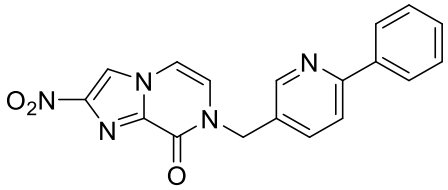


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_042_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-09-10T17:16:22
17	Modification Date	2018-09-10T17:16:22
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

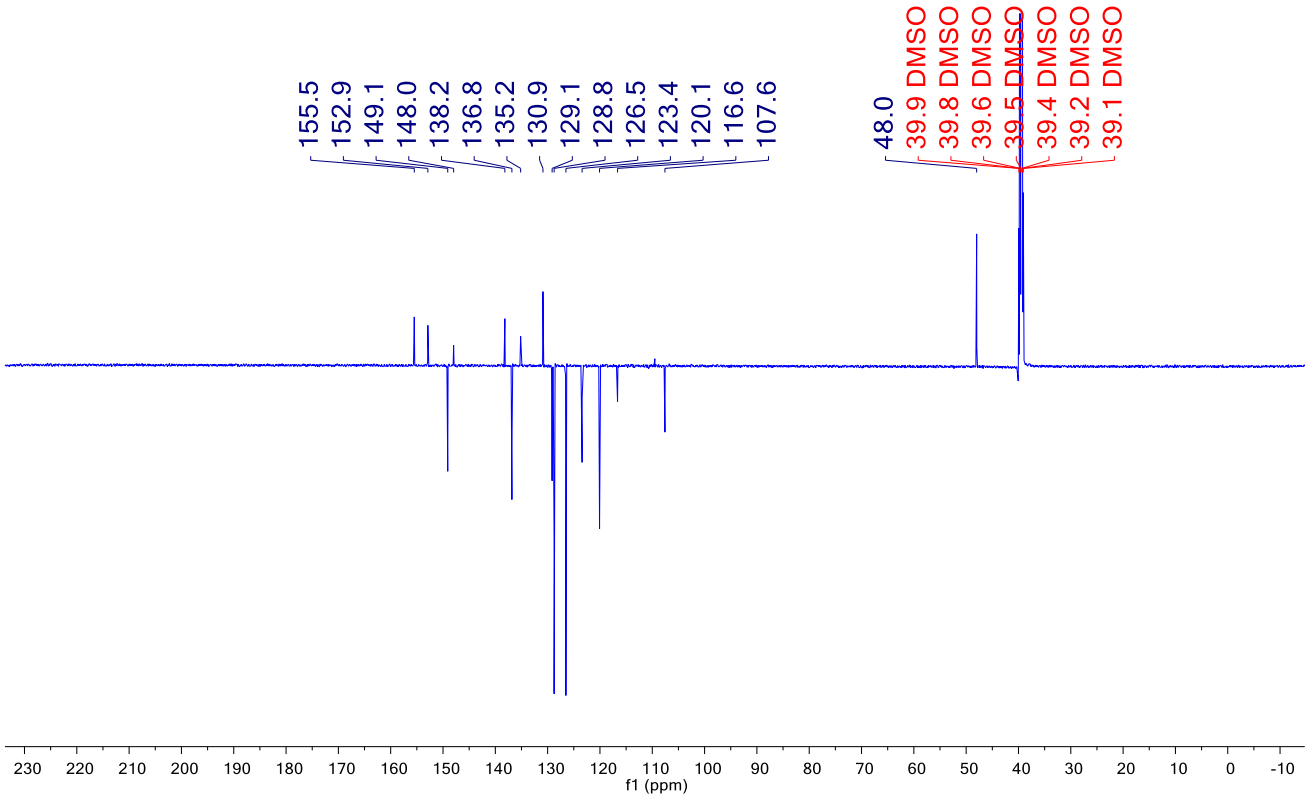


2-Nitro-7-((6-phenylpyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34f)

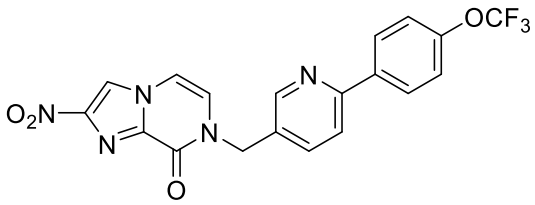


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_042_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	6500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-09-10T21:01:32
17	Modification Date	2018-09-10T21:01:32
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

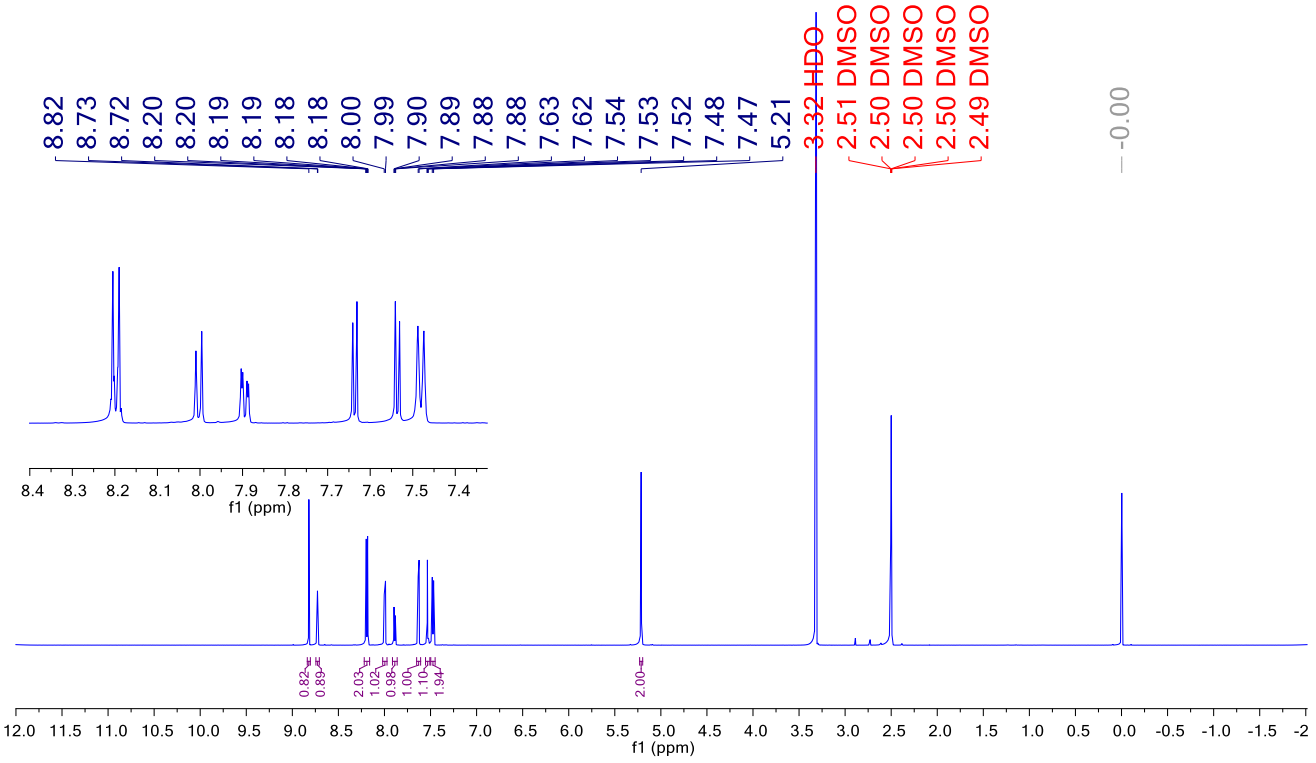


2-Nitro-7-((6-(4-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-a]pyrazin-8(7*H*)-one (34g)

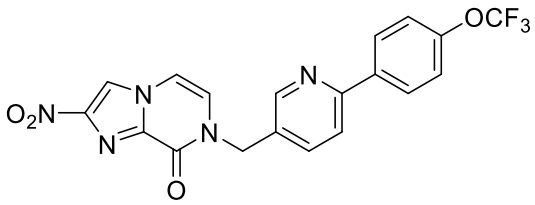


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_058_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	155.2
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-09-12T13:08:02
17	Modification Date	2018-09-12T13:08:02
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

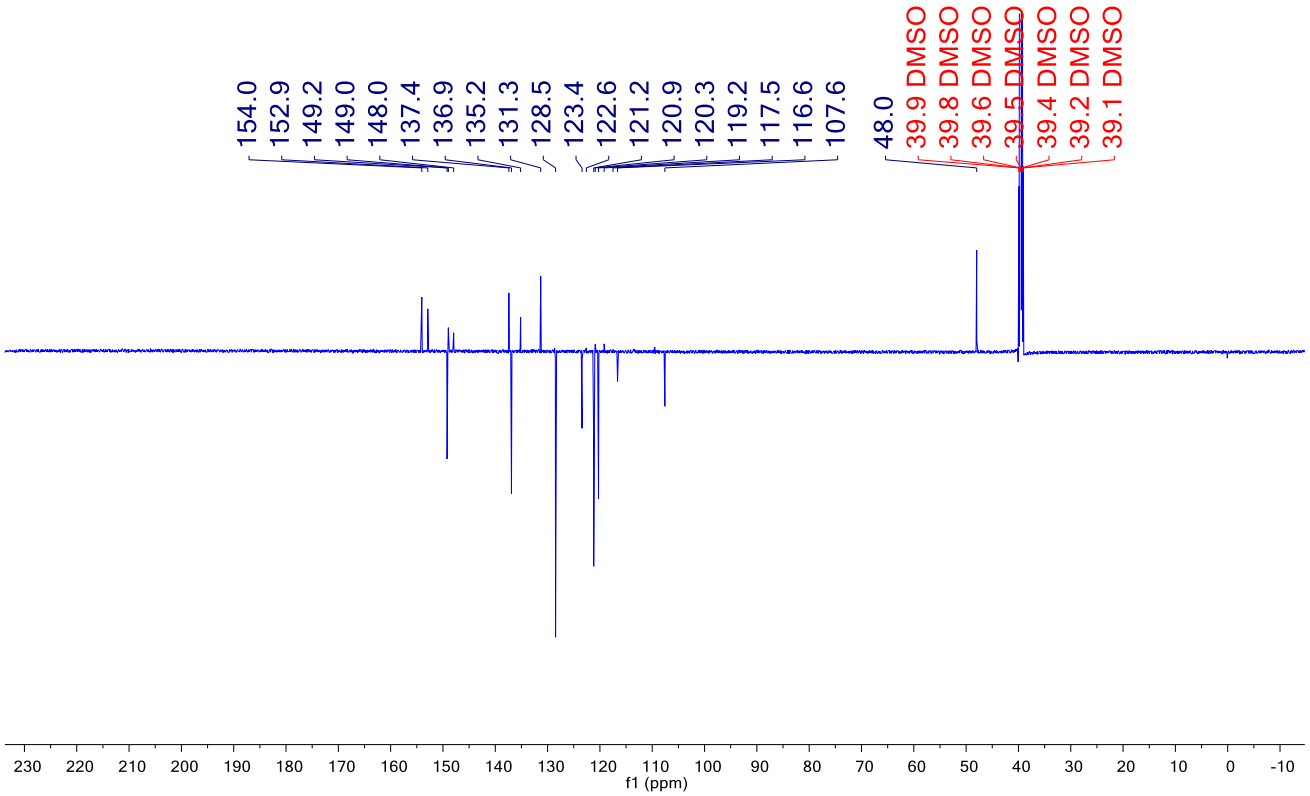


2-Nitro-7-((6-(4-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-a]pyrazin-8(7*H*)-one (34g)

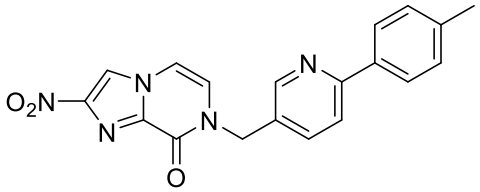


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_058_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	6500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-09-14T20:27:30
17	Modification Date	2018-09-14T20:27:30
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

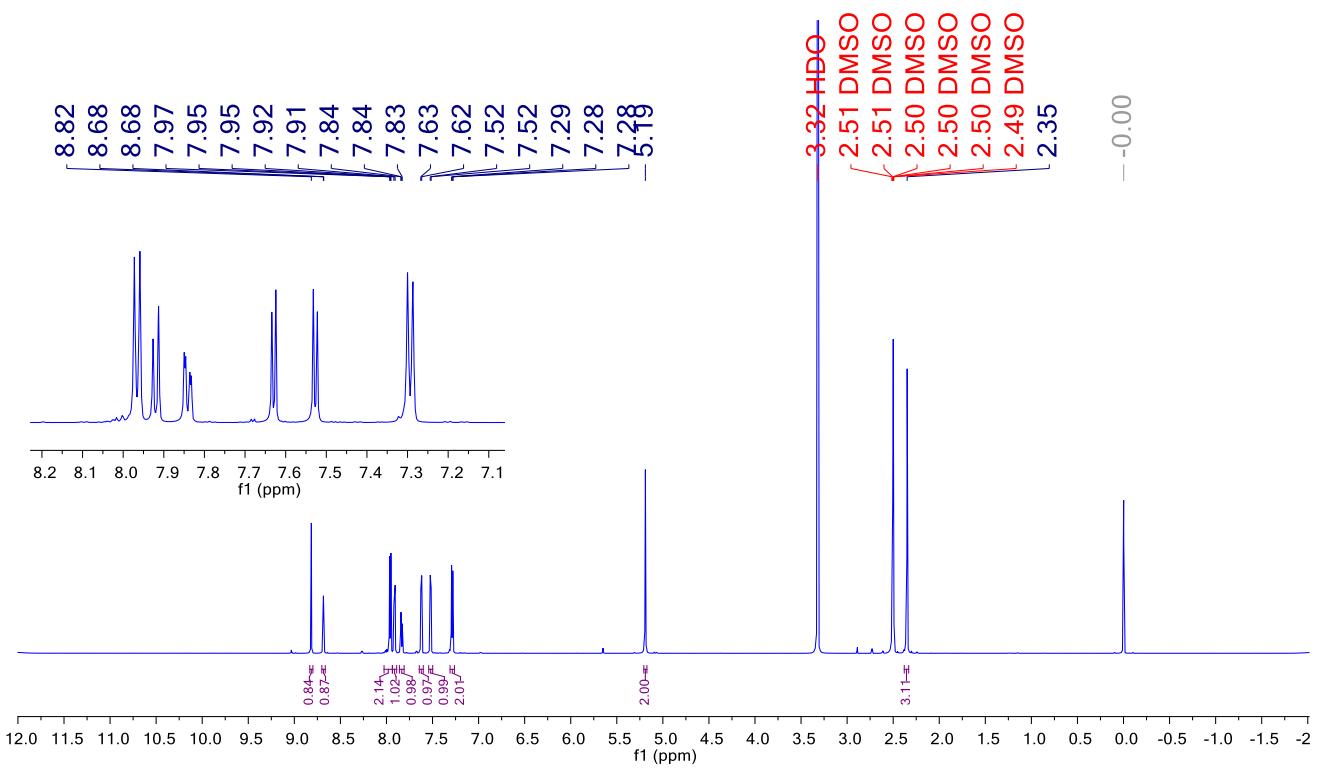


2-Nitro-7-((6-(*p*-tolyl)pyridin-3-yl)methyl)imidazo[1,2-a]pyrazin-8(7*H*)-one (34h)

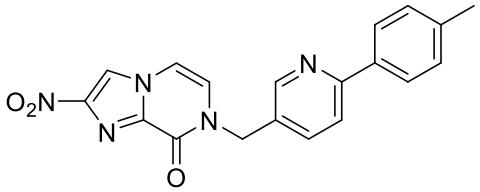


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_023_ppt_MeOH_DCM.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	155.2
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-09-03T11:12:58
17	Modification Date	2018-09-03T11:12:58
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

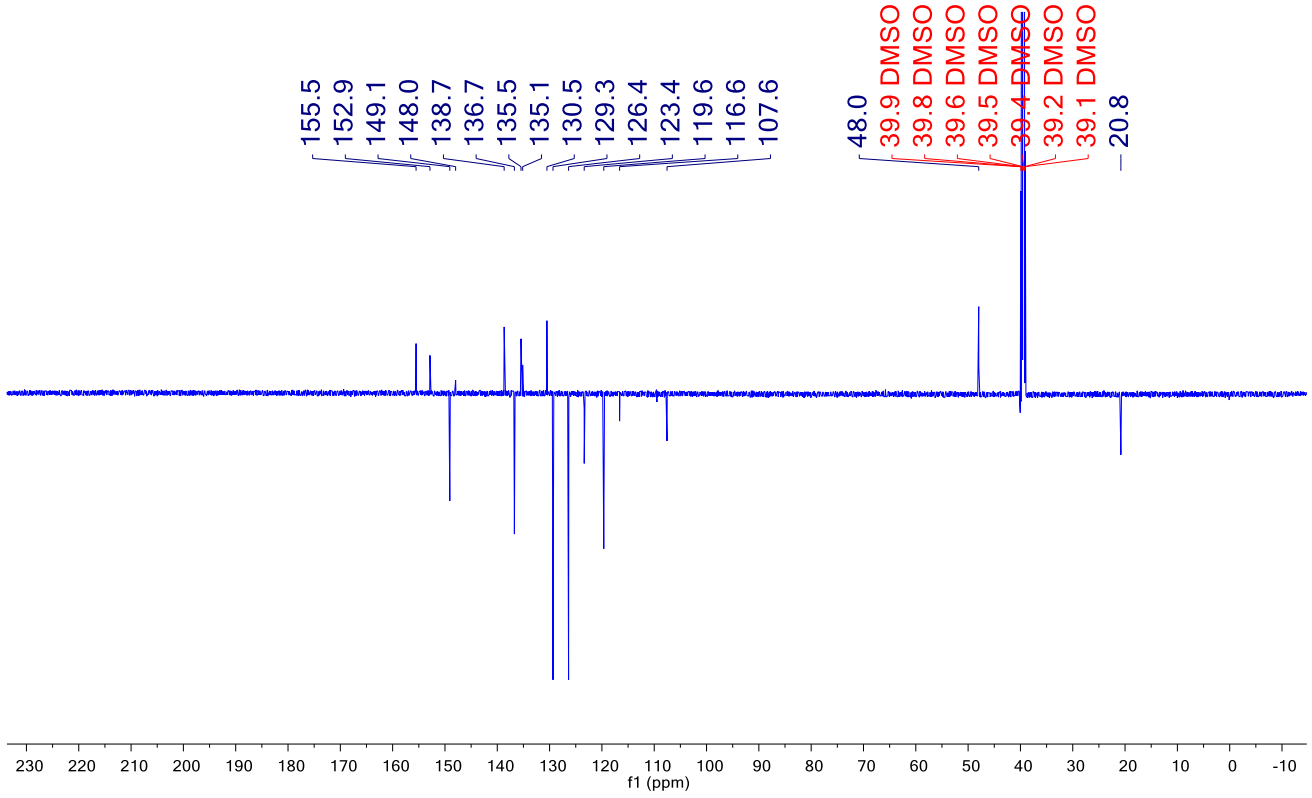


2-Nitro-7-((6-(*p*-tolyl)pyridin-3-yl)methyl)imidazo[1,2-a]pyrazin-8(7*H*)-one (34h)

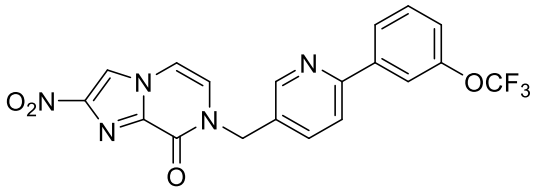


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_023_ppt_MeOH_DCM.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	4600
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-09-03T14:00:53
17	Modification Date	2018-09-03T14:00:53
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

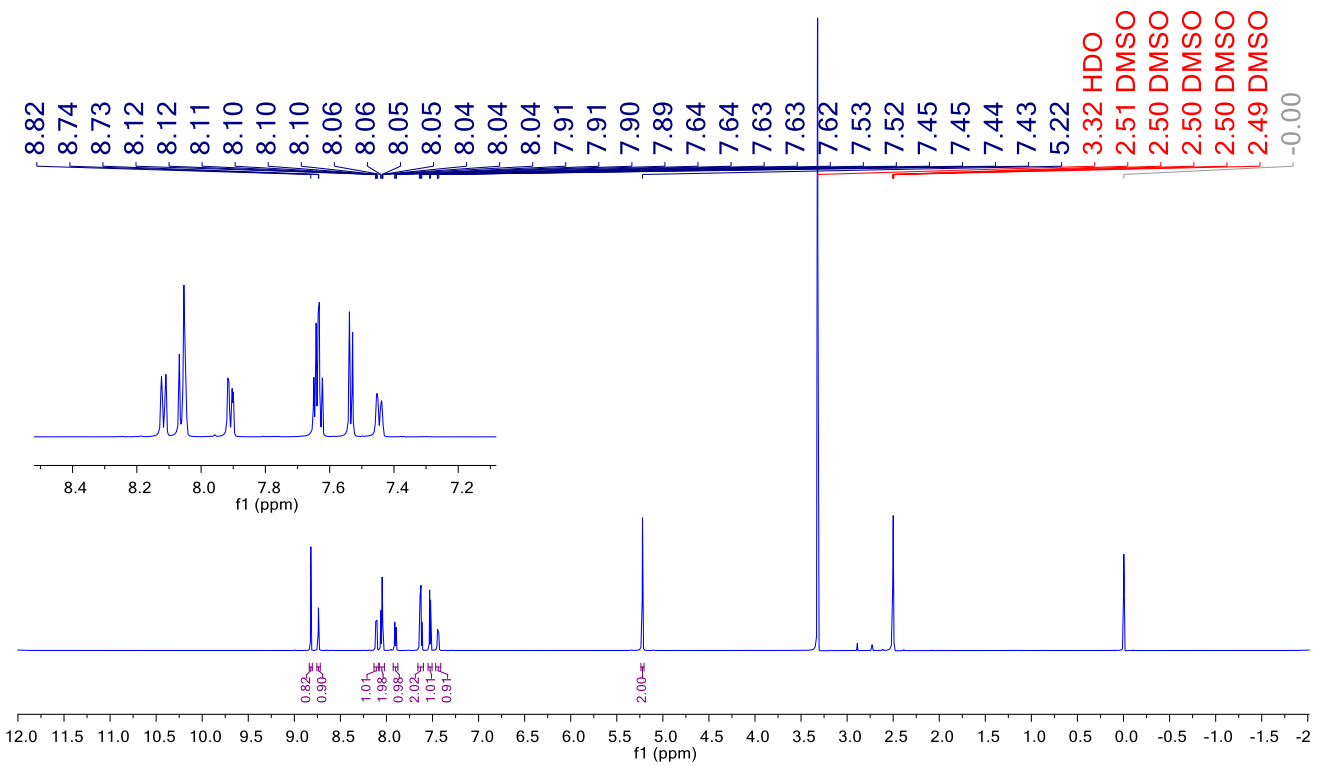


2-Nitro-7-((6-(3-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34i)

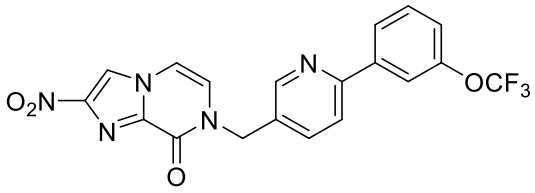


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_114_ppt_MeOH_DCM.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	116.1
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-08-16T17:57:51
17	Modification Date	2018-08-16T17:57:51
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

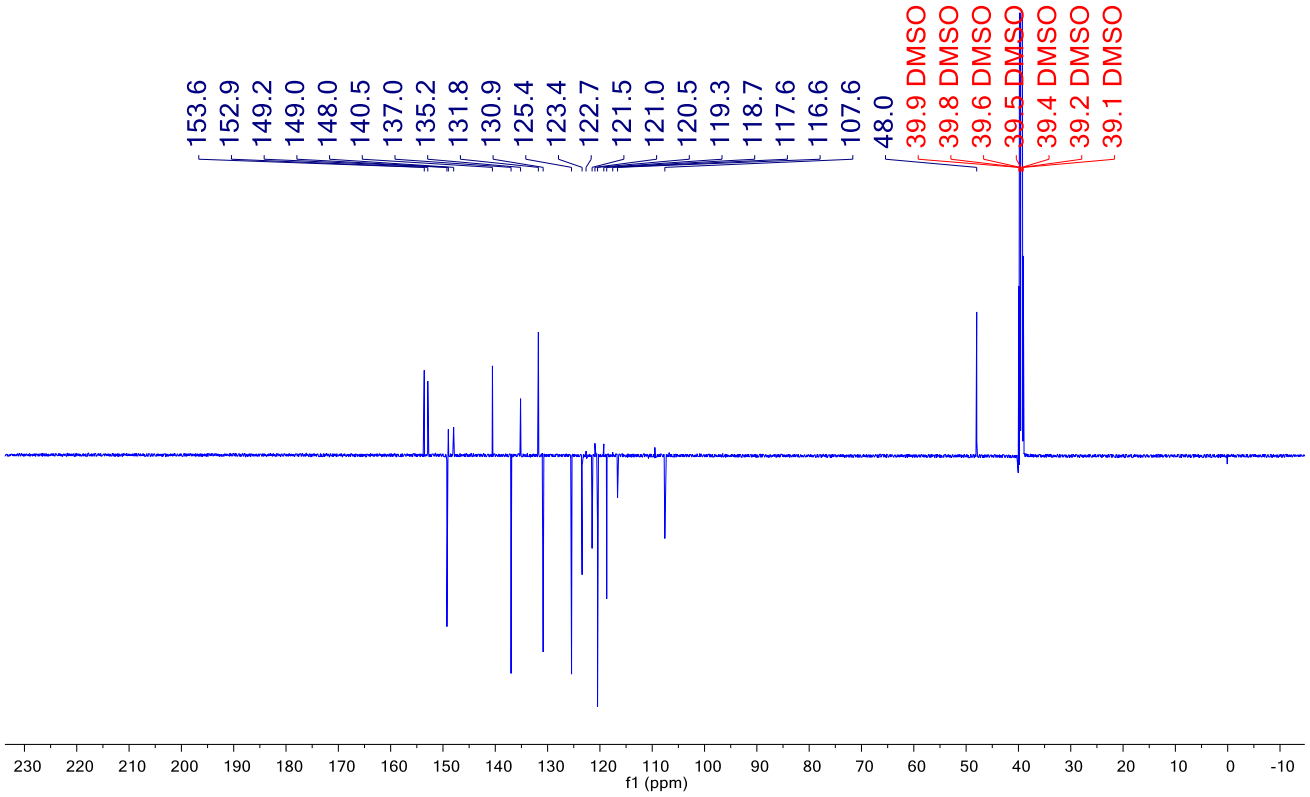


2-Nitro-7-((6-(3-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34i)

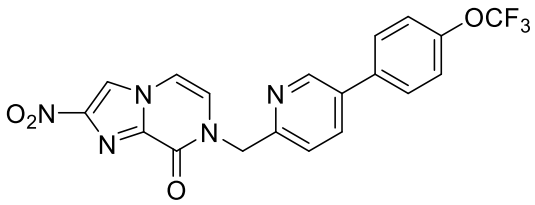


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_114_ppt_MeOH_DCM.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	9500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-08-17T05:55:30
17	Modification Date	2018-08-17T05:55:30
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

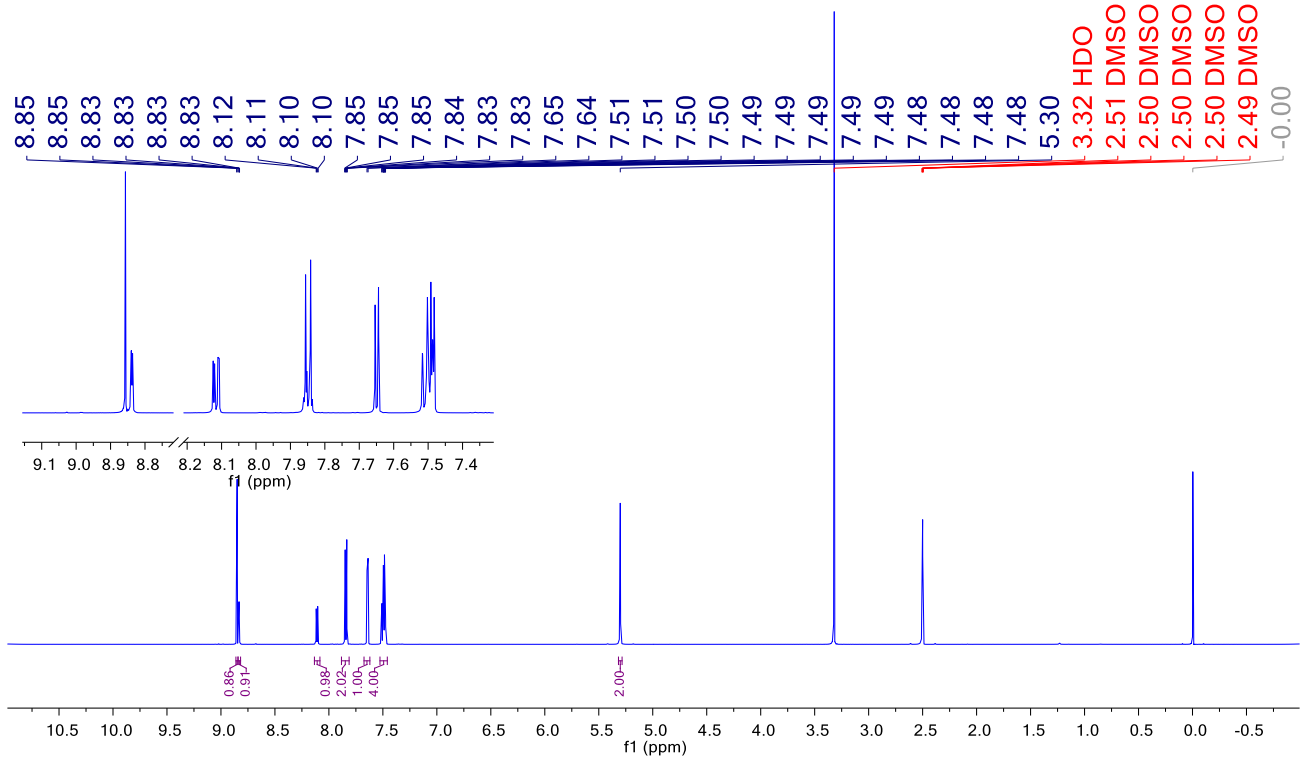


2-Nitro-7-((5-(4-(trifluoromethoxy)phenyl)pyridin-2-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34j)

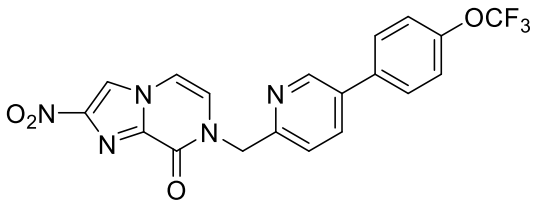


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_091_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	116.1
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	2.2807
16	Acquisition Date	2019-04-17T17:00:51
17	Modification Date	2019-04-17T17:00:51
18	Spectrometer Frequency	600.13
19	Spectral Width	7183.9
20	Lowest Frequency	-591.3
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

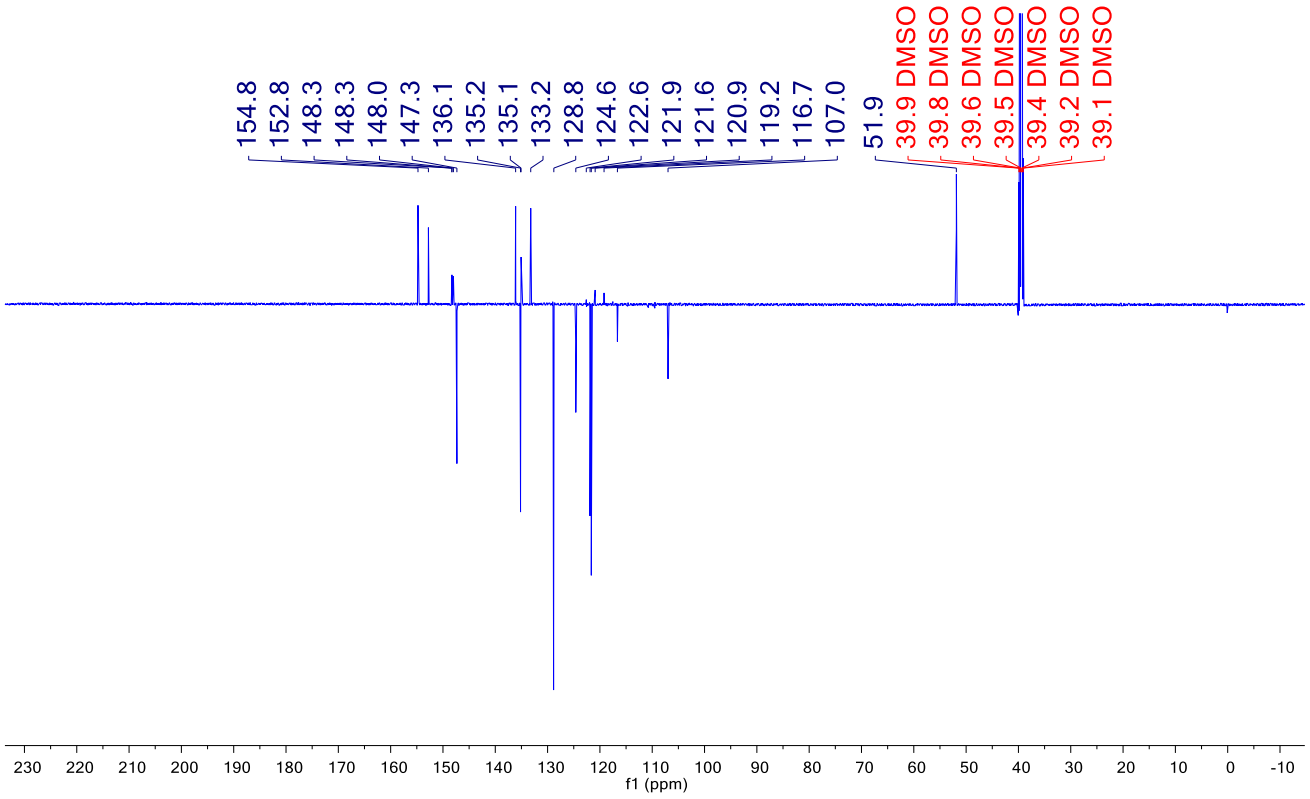


2-Nitro-7-((5-(4-(trifluoromethoxy)phenyl)pyridin-2-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34j)

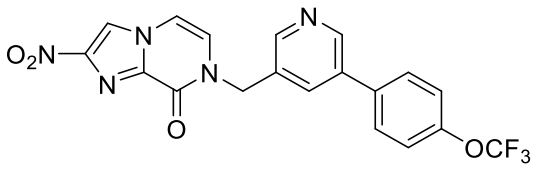


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_091_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	9000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2019-04-18T03:42:49
17	Modification Date	2019-04-18T03:42:49
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

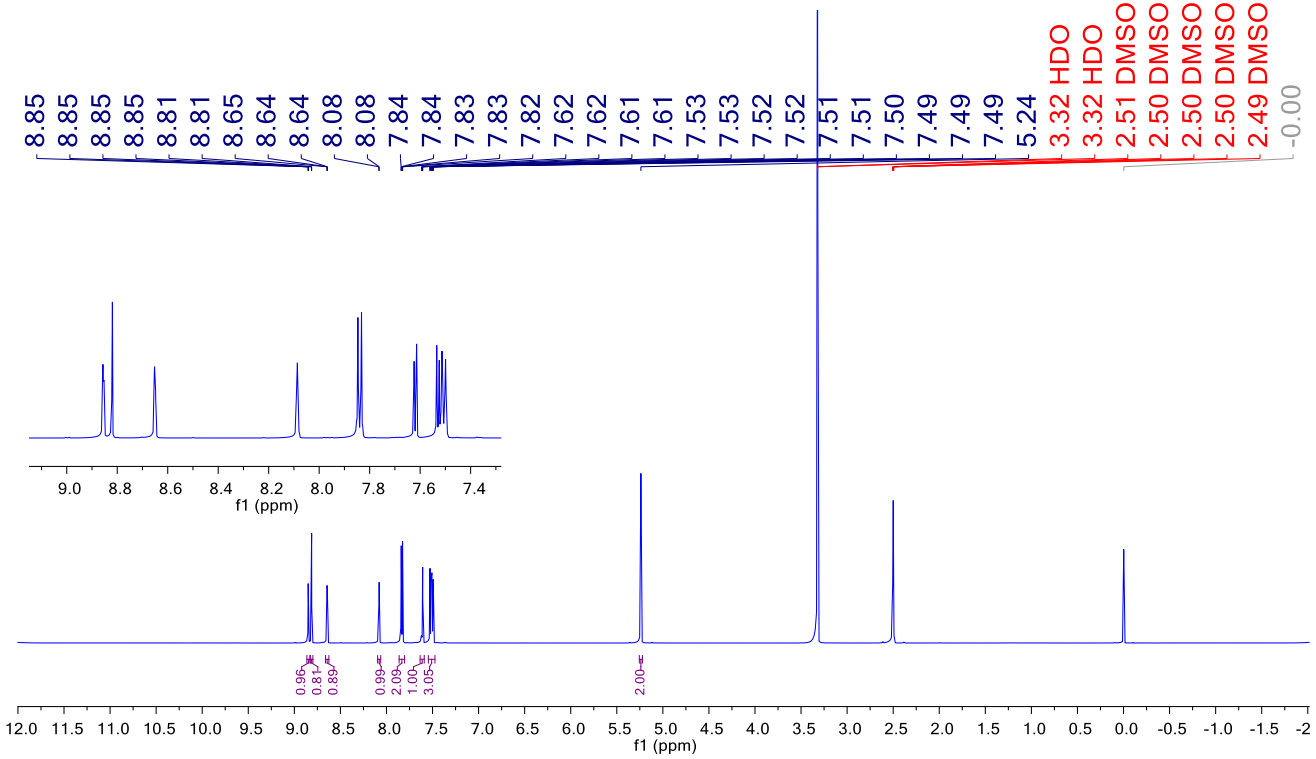


2-Nitro-7-((5-(4-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34k)

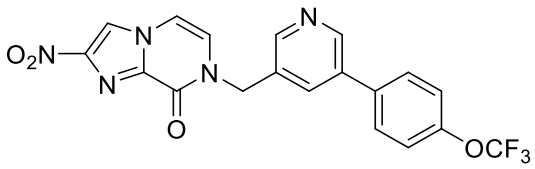


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_099_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	140.4
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-10-07T11:53:36
17	Modification Date	2018-10-07T11:53:36
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

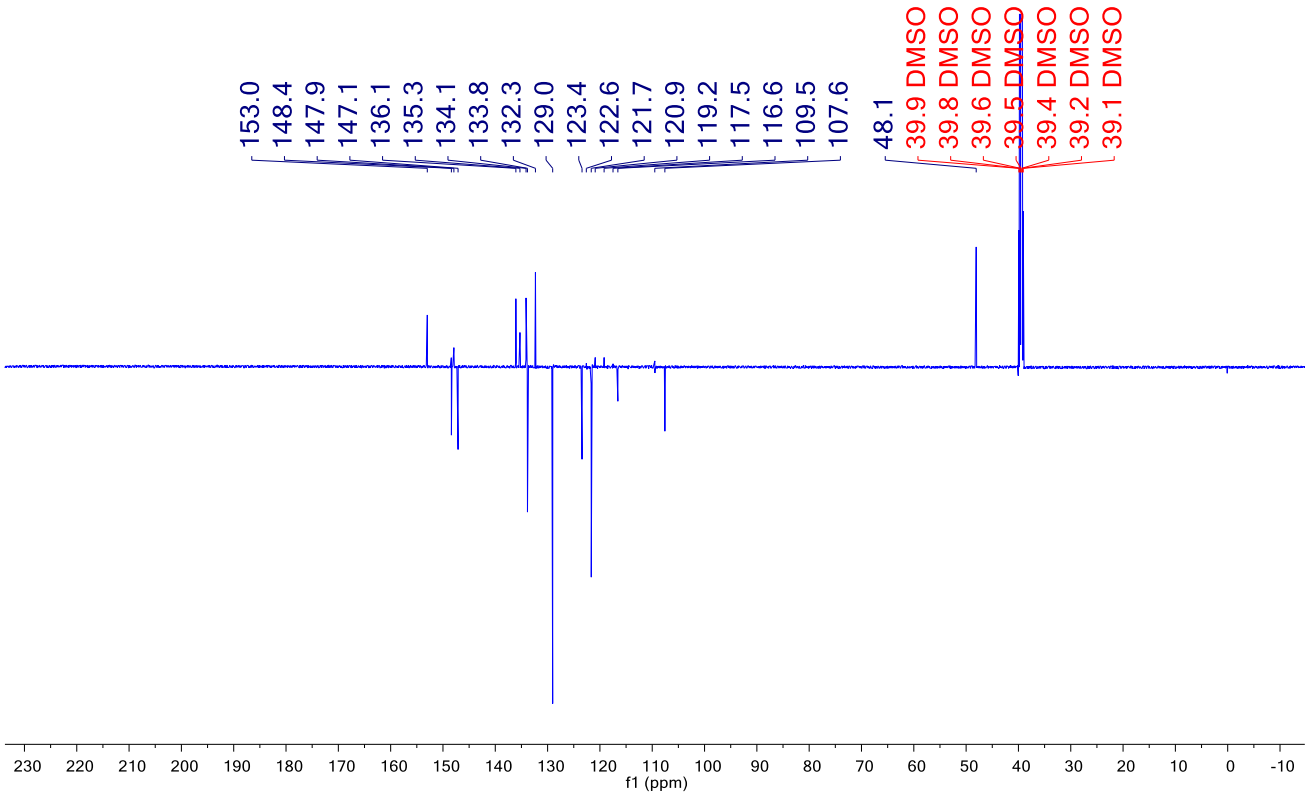


2-Nitro-7-((5-(4-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34k)

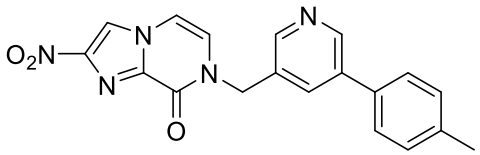


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_099_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	9500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-10-07T17:18:52
17	Modification Date	2018-10-07T17:18:52
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

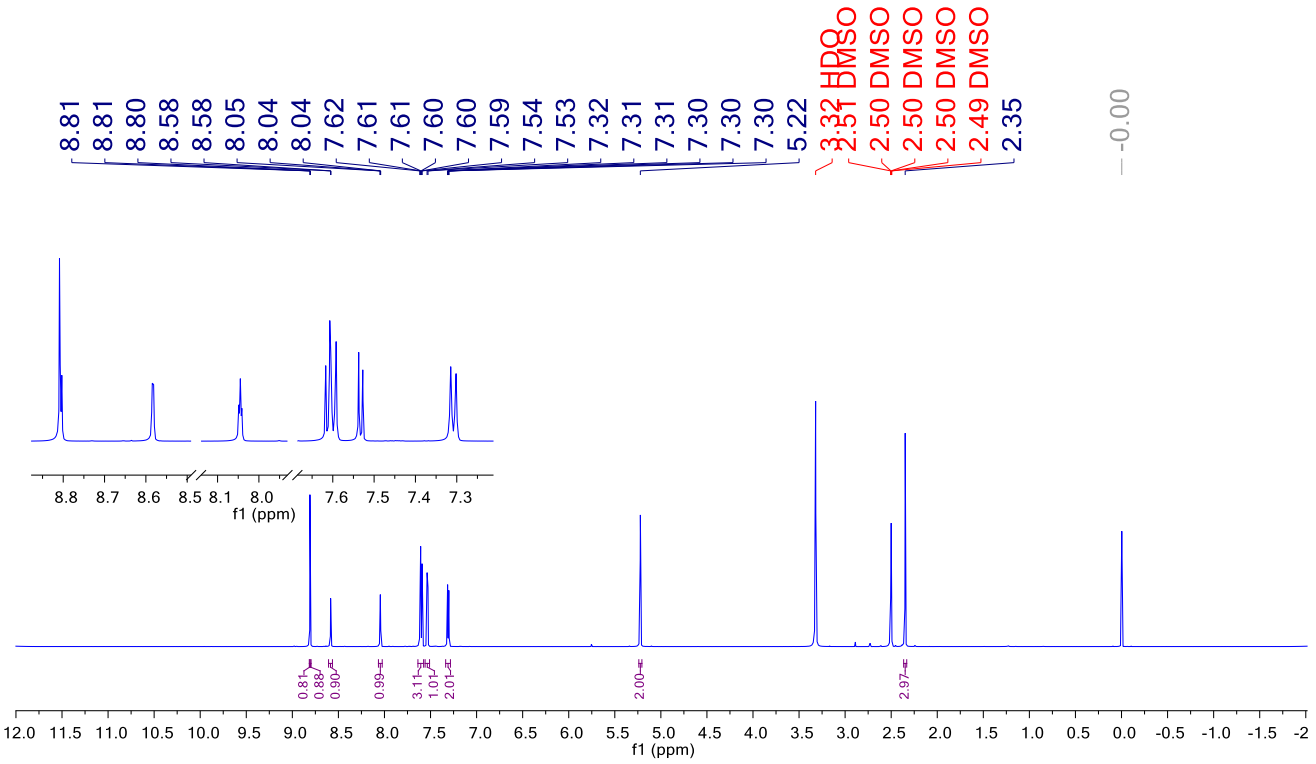


2-Nitro-7-((5-(*p*-tolyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34l)

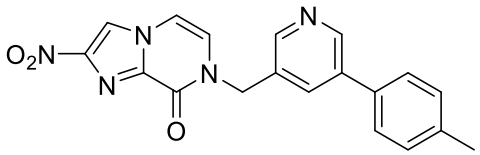


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_090_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2019-04-17T17:05:39
17	Modification Date	2019-04-17T17:05:39
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

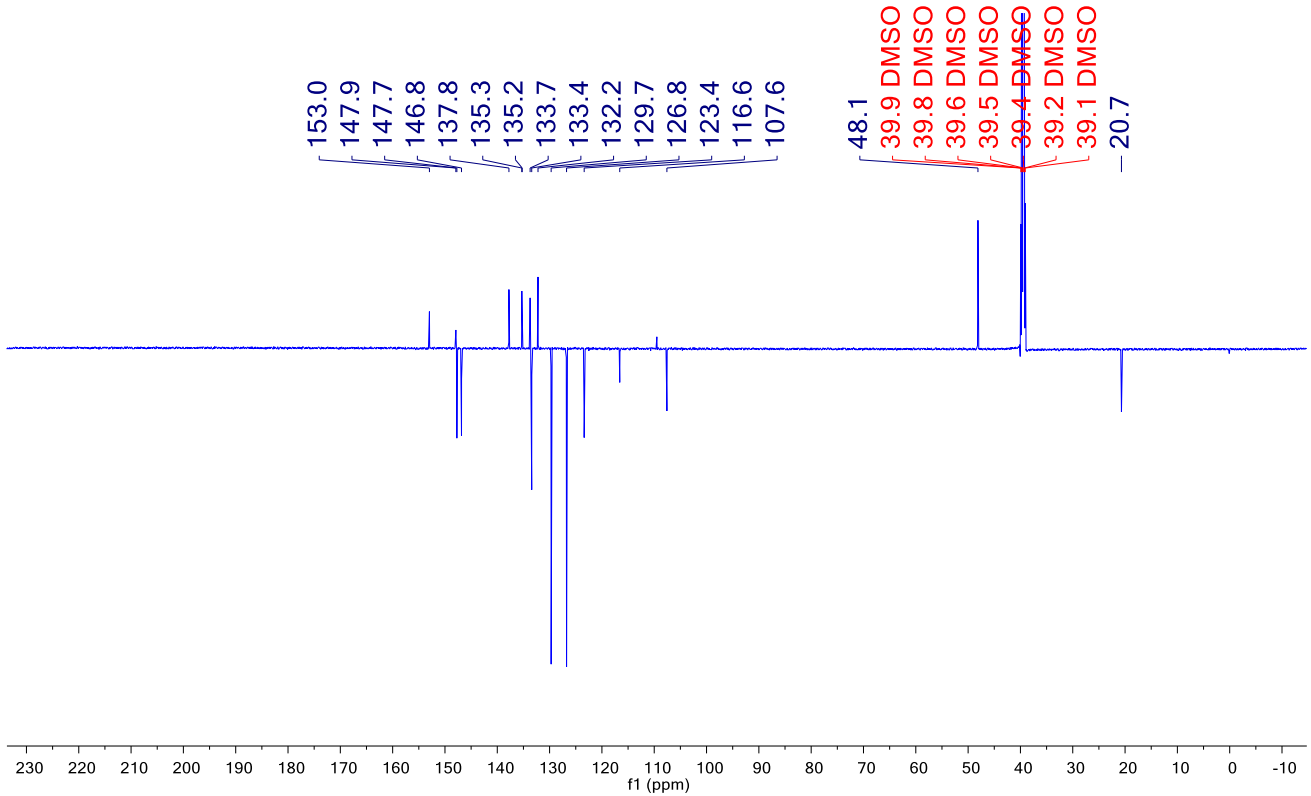


2-Nitro-7-((5-(*p*-tolyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34l)

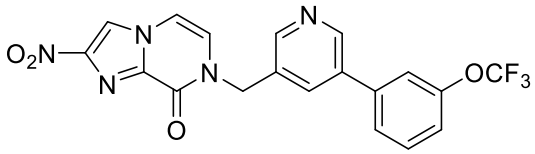


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9171_090_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	6500
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2019-04-17T20:34:03
17	Modification Date	2019-04-17T20:34:04
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

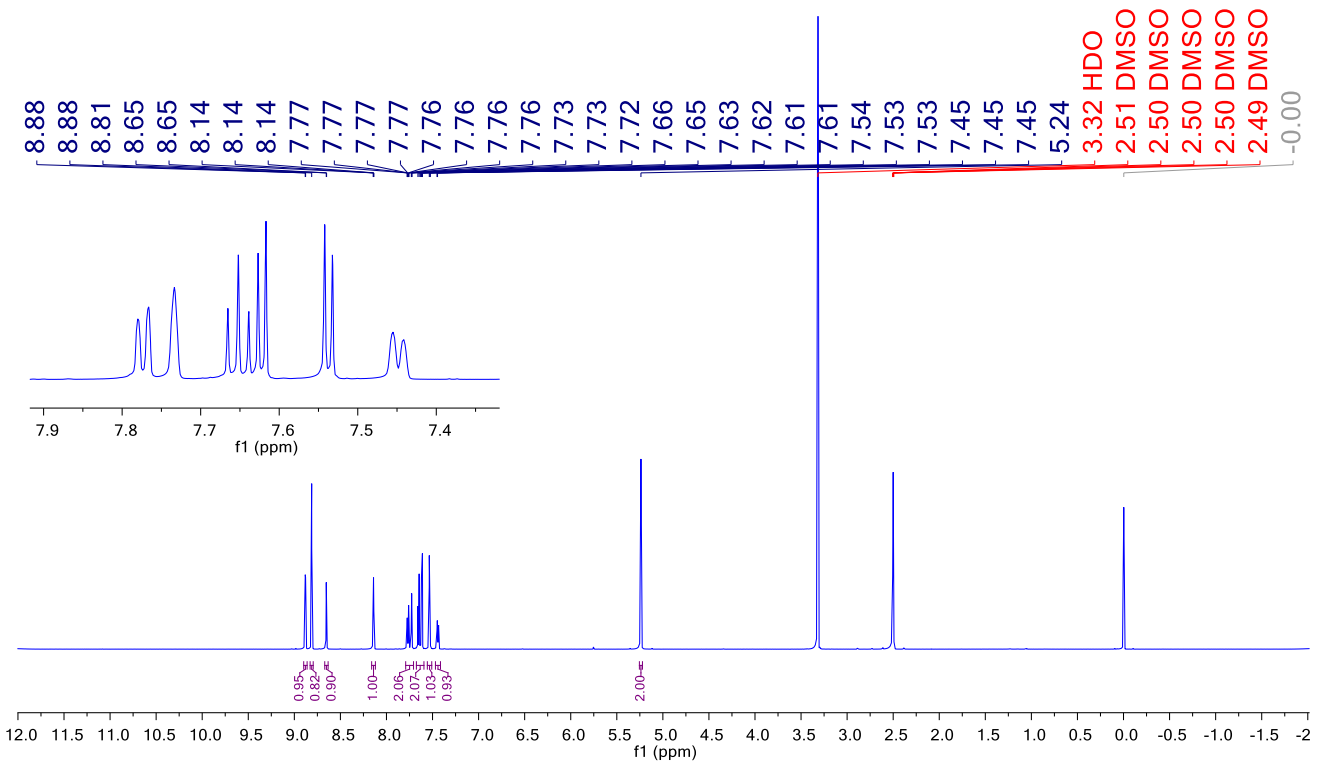


2-Nitro-7-((5-(3-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34m)

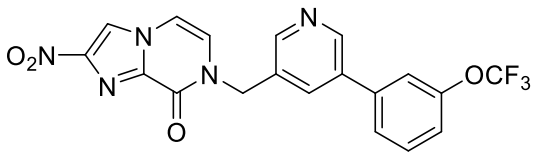


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_115_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	155.2
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-10-16T17:18:51
17	Modification Date	2018-10-16T17:18:51
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

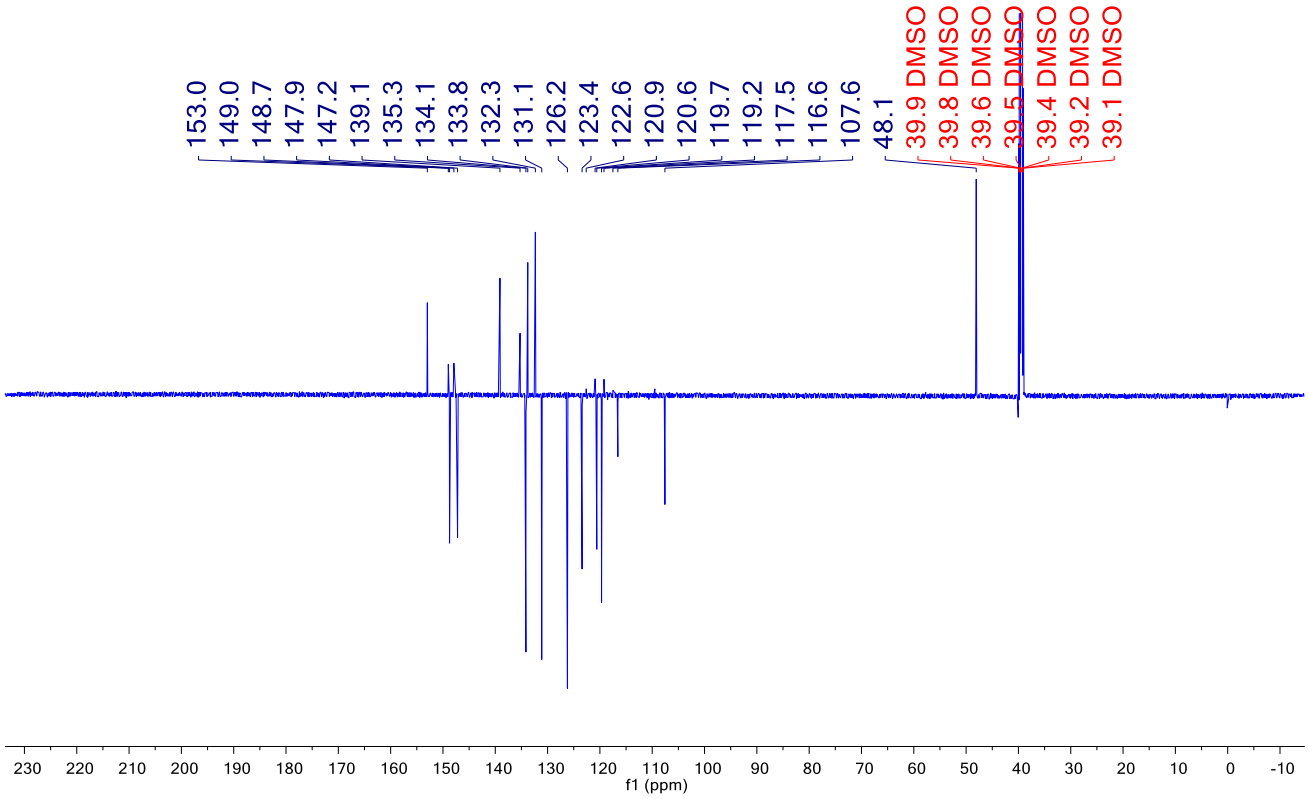


2-Nitro-7-((5-(3-(trifluoromethoxy)phenyl)pyridin-3-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34m)

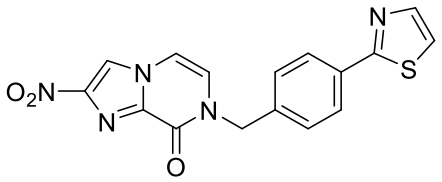


^{13}C NMR (150 MHz, DMSO-*d*$_6$)

	Parameter	Value
1	Title	CWA9117_115_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	10000
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-10-16T22:39:45
17	Modification Date	2018-10-16T22:39:45
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

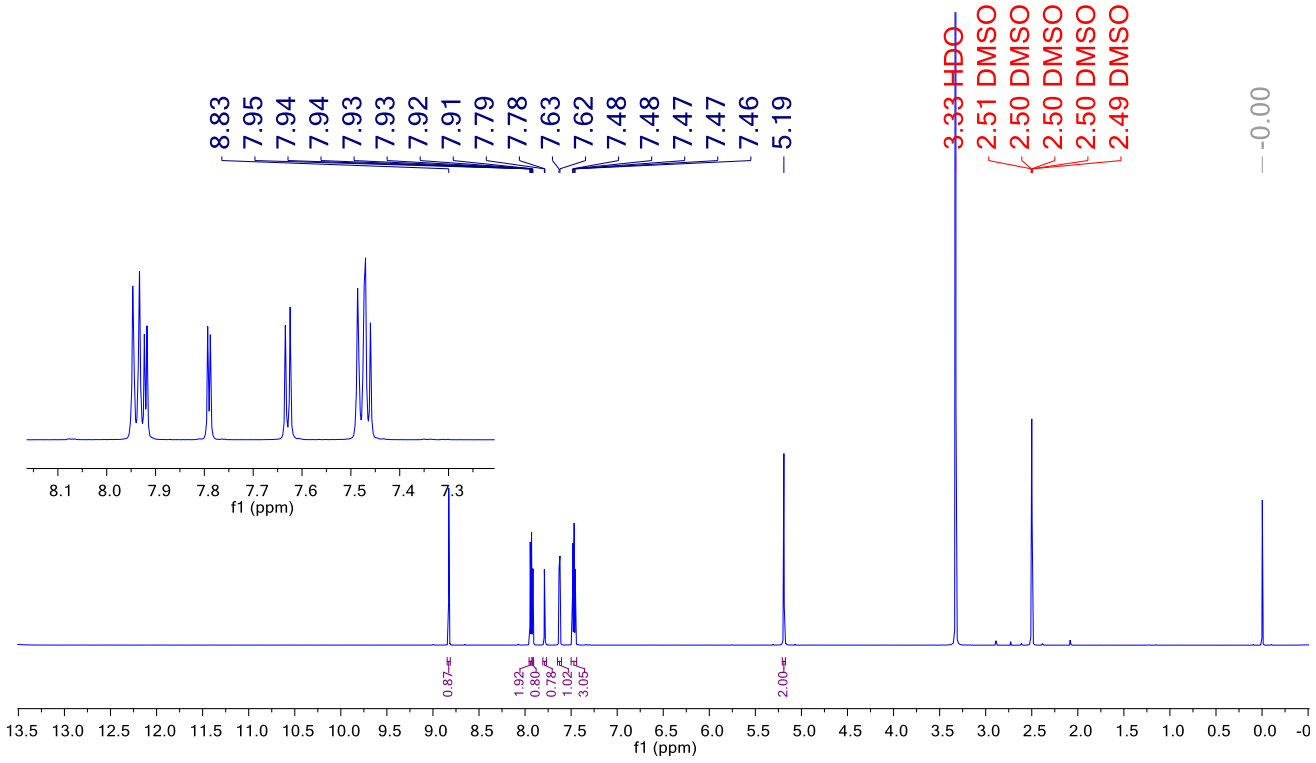


2-Nitro-7-(4-(thiazol-2-yl)benzyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34n)

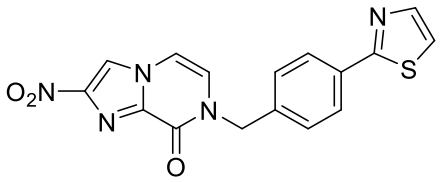


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_072_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	biodiversity
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	5 mm PASEI 1H/ D-13C Z-GRD Z866801/ 0003
10	Number of Scans	16
11	Receiver Gain	287.0
12	Relaxation Delay	5.0000
13	Pulse Width	9.8000
14	Presaturation Frequency	
15	Acquisition Time	1.9465
16	Acquisition Date	2018-09-18T14:53:00
17	Modification Date	2018-09-18T14:53:58
18	Spectrometer Frequency	600.08
19	Spectral Width	8417.5
20	Lowest Frequency	-308.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

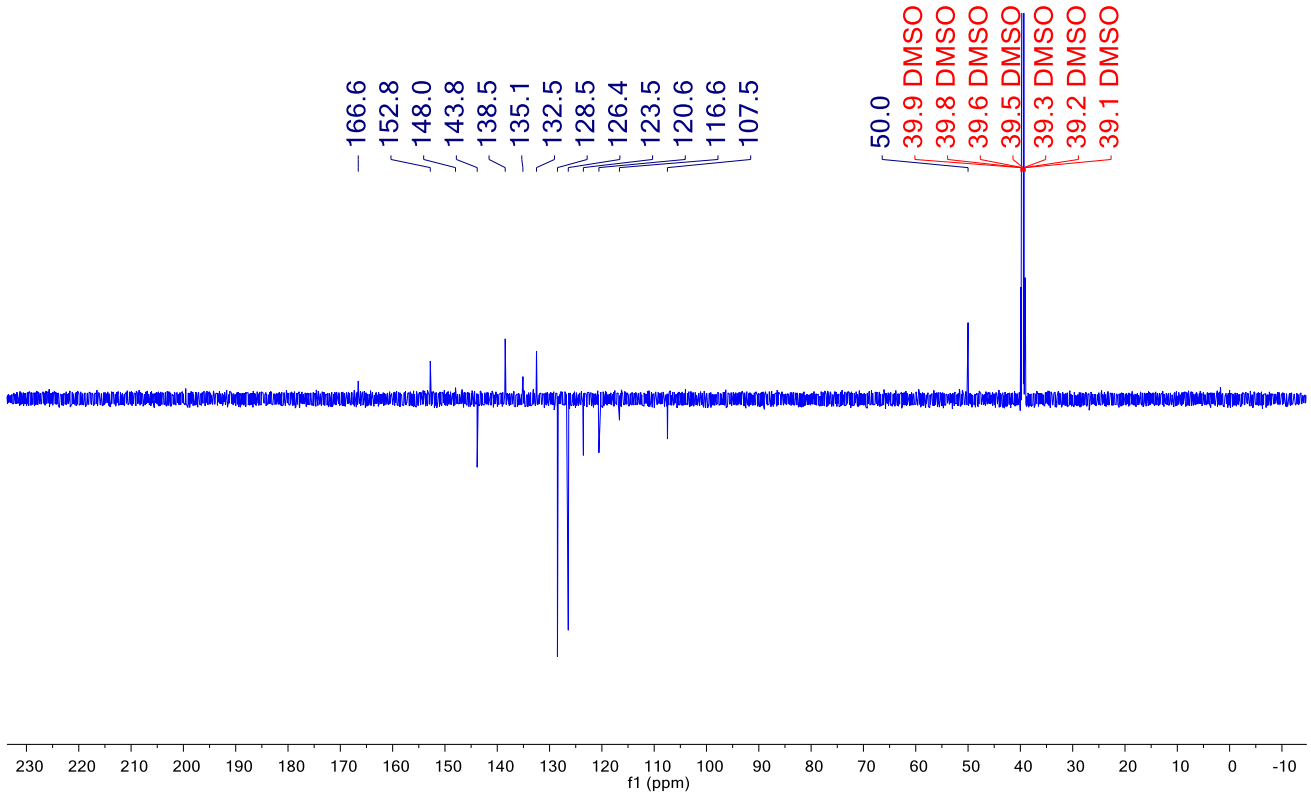


2-Nitro-7-(4-(thiazol-2-yl)benzyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34n)

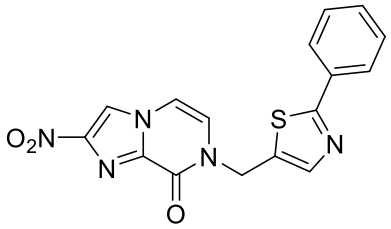


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_072_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	biodiversity
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	297.9
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	5 mm PASEI 1H/ D-13C Z-GRD Z866801/ 0003
10	Number of Scans	7500
11	Receiver Gain	2050.0
12	Relaxation Delay	1.0000
13	Pulse Width	14.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8739
16	Acquisition Date	2018-09-18T21:45:00
17	Modification Date	2018-09-18T21:45:36
18	Spectrometer Frequency	150.91
19	Spectral Width	37500.0
20	Lowest Frequency	-2227.5
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

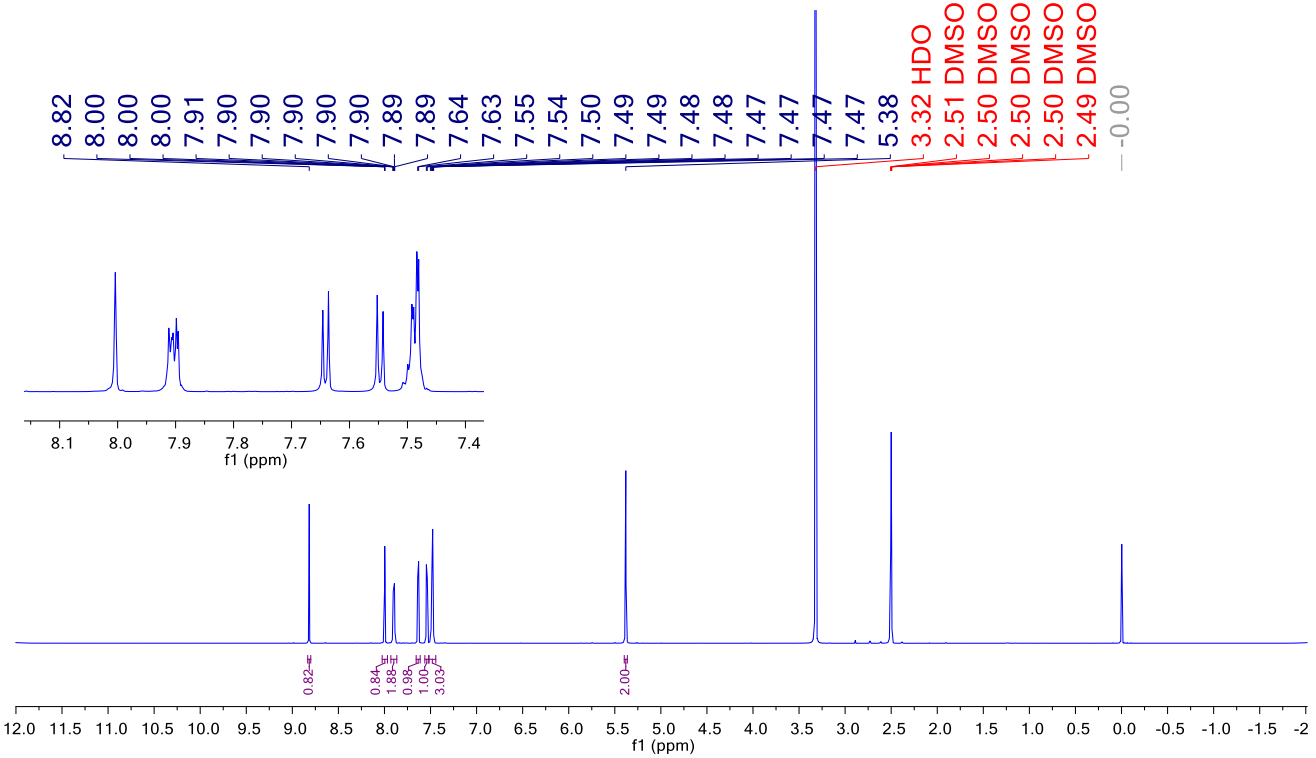


2-Nitro-7-((2-phenylthiazol-5-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34o)

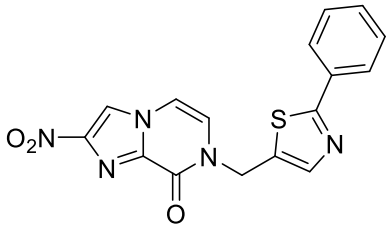


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_100_ppt_DCM_MeOH.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	16
11	Receiver Gain	109.3
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-10-23T12:59:20
17	Modification Date	2018-10-23T12:59:20
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

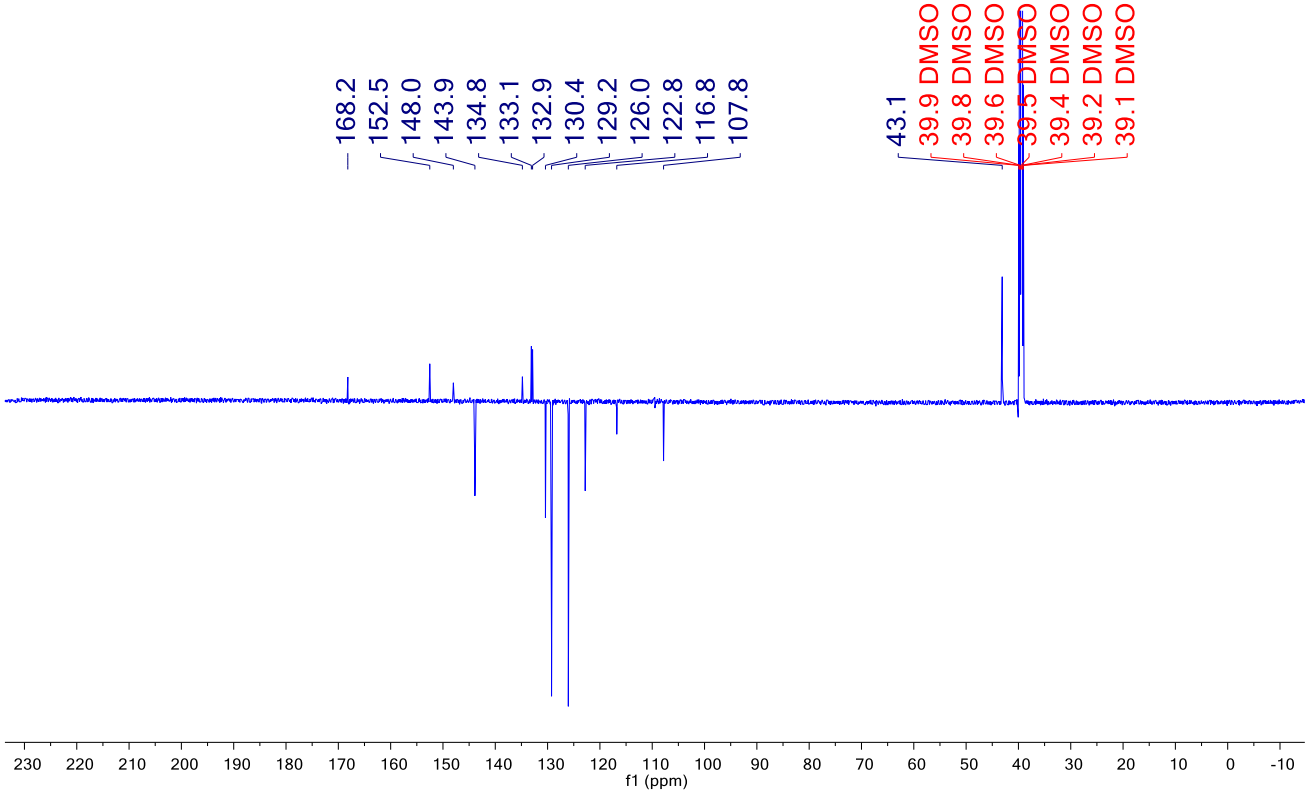


2-Nitro-7-((2-phenylthiazol-5-yl)methyl)imidazo[1,2-*a*]pyrazin-8(7*H*)-one (34o)

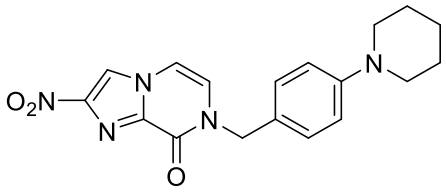


^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA9117_100_ppt_DCM_MeOH.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	jmod
8	Experiment	JMOD
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/N-D-05 Z)
10	Number of Scans	5200
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.8738
16	Acquisition Date	2018-10-23T15:46:56
17	Modification Date	2018-10-23T15:46:56
18	Spectrometer Frequency	150.92
19	Spectral Width	37500.0
20	Lowest Frequency	-2151.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

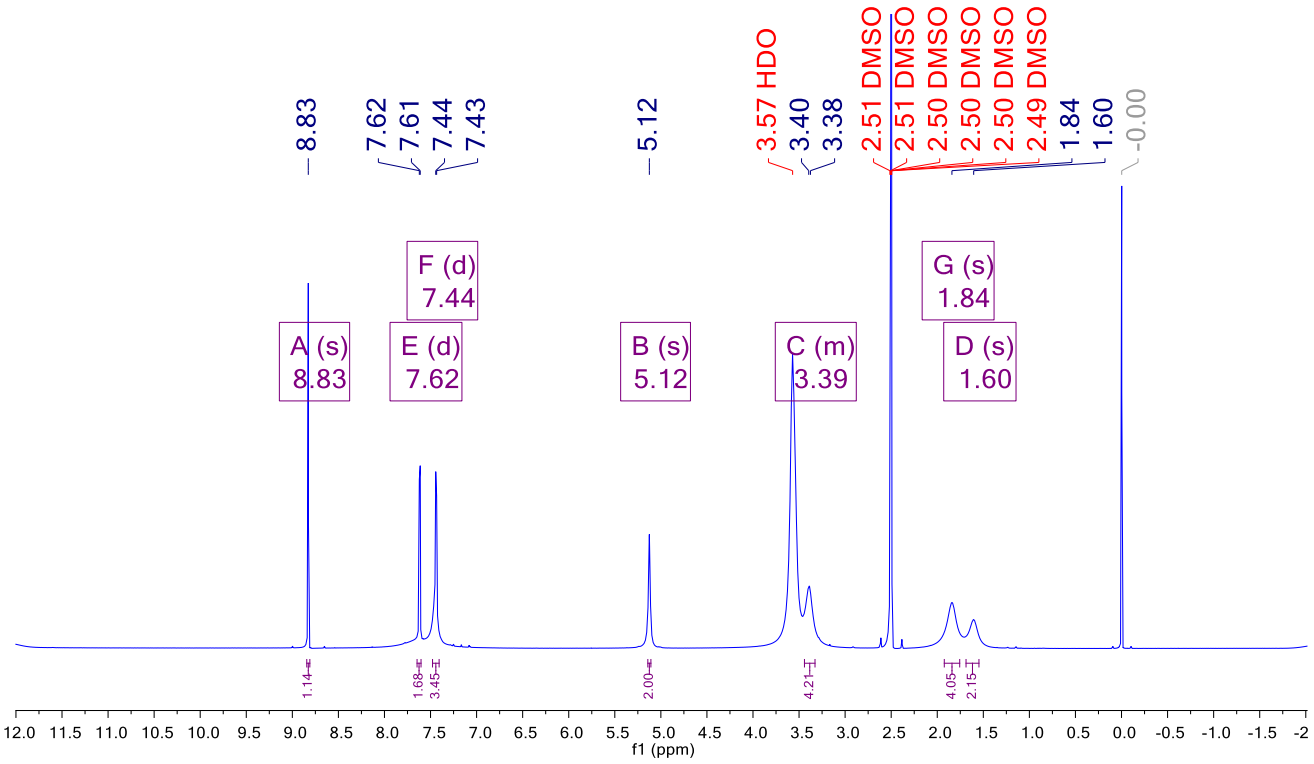


2-Nitro-7-(4-(piperidin-1-yl)benzyl)imidazo[1,2 *a*]pyrazin-8(7*H*)-one (34p)

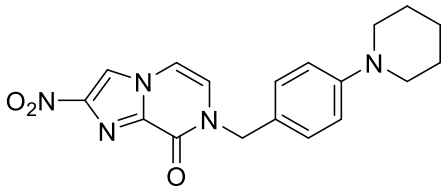


^{1}H NMR (600 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_055_ppt_DCM_MeOH_cryoprobe.1.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	32
11	Receiver Gain	59.7
12	Relaxation Delay	5.0000
13	Pulse Width	8.0000
14	Presaturation Frequency	
15	Acquisition Time	1.9464
16	Acquisition Date	2018-05-16T02:12:37
17	Modification Date	2018-05-16T02:12:37
18	Spectrometer Frequency	600.13
19	Spectral Width	8417.5
20	Lowest Frequency	-1208.1
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	65536

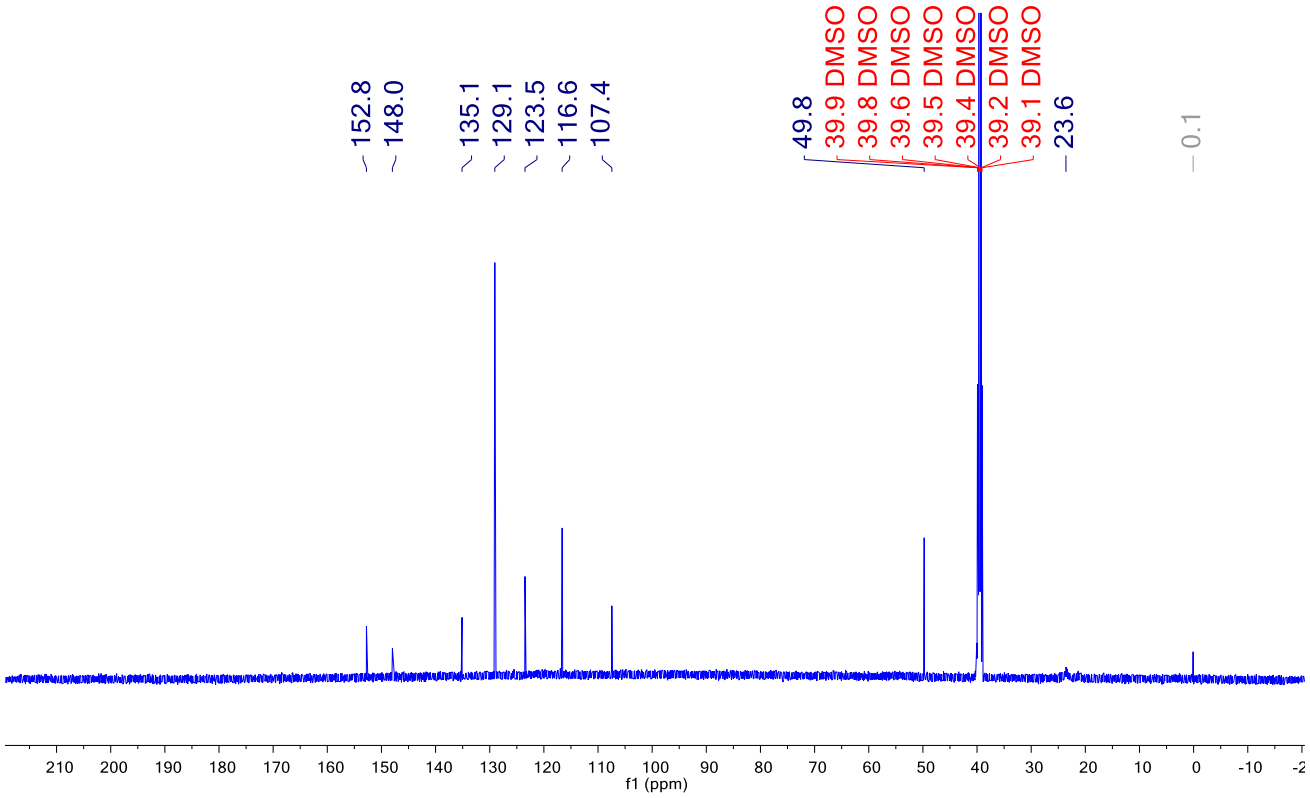


2-Nitro-7-(4-(piperidin-1-yl)benzyl)imidazo[1,2 *a*]pyrazin-8(7*H*)-one (34p)



^{13}C NMR (150 MHz, DMSO-d_6)

	Parameter	Value
1	Title	CWA8967_055_ppt_DCM_MeOH_cryoprobe.2.fid
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Spectrometer	spect
5	Solvent	DMSO
6	Temperature	298.0
7	Pulse Sequence	zgpg
8	Experiment	1D
9	Probe	Z129649_0009 (CP TCI 600S3 H&F-C/ N-D-05 Z)
10	Number of Scans	2560
11	Receiver Gain	191.6
12	Relaxation Delay	1.0000
13	Pulse Width	12.0000
14	Presaturation Frequency	
15	Acquisition Time	0.9044
16	Acquisition Date	2018-05-16T03:36:59
17	Modification Date	2018-05-16T03:36:59
18	Spectrometer Frequency	150.92
19	Spectral Width	36231.9
20	Lowest Frequency	-3025.7
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



References

1. Sykes, M. L.; Baell, J. B.; Kaiser, M.; Chatelain, E.; Moawad, S. R.; Ganame, D.; Ioset, J.-R.; Avery, V. M. Identification of compounds with anti-proliferative activity against *Trypanosoma brucei brucei* strain 427 by a whole cell viability based HTS campaign. *PLoS Negl. Trop. Dis.* **2012,** 6, e1896-e1896.