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Data Article

HPLC, quantitative NMR and HRMS spectroscopic data of nusbiarylins as a new class of antimicrobial agents

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ABSTRACT

Bacterial transcription is a valid but underutilized target for antimicrobial agent discovery [1]. Nusbiarylins are the first-in-class bacterial ribosomal RNA synthesis inhibitors that possess potent activity against various types of multidrug-resistant bacteria with a novel mode of action by targeting the interaction of bacterial transcription factors NusB and NusE [2]. To facilitate the characterization of nusbiarylin derivatives produced by other researchers, high-performance liquid chromatography (HPLC) profiles, quantitative nuclear magnetic resonance (qNMR) and high-resolution mass spectrometry (HRMS) spectroscopic data were presented for the quick determination of purity and characterization of 95 nusbiarylin compounds. The data presented in this article supplement the ^{1}H and ^{13}C NMR data provided previously [3,4], and assist the reproduction of nusbiarylins for chemical, biological and drug discovery research.

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Specifications Table

Subject	Chemistry
Specific subject area	Organic chemistry Analytical chemistry
Type of data	Table Figure
How data were acquired	Agilent 1100 series and 1260 infinity system Bruker ultrashield™ NMR spectrometer 600 MHz Agilent Technologies 6520 Accurate-Mass Q-TOF LC/MS spectrometer
Data format	Raw (as supplementary file) Analyzed
Parameters for data collection	The purified compounds were subjected to HPLC and qNMR analysis. The mobile phase for HPLC analysis were acetonitrile and water. The ratio was specified in the "Experimental Design, Materials, and Methods" section. The flow rate was set as 1.000 mL/min. Compounds were dissolved in *d*-DMSO prior to qNMR analysis. The parameters for qNMR analysis were adjusted according to the literature [5].
Description of data collection	HPLC profiles of 95 novel compounds were recorded on and exported from an Agilent 1100 series and 1260 infinity system. Area% and RetTime stands for purity and retention time, respectively. qNMR spectra data of 95 novel compounds were recorded on and exported form a Bruker ultrashield™ NMR spectroscope 600 MHz spectrometer using standard Bruker pulse programs. Chemical shifts were shown as δ-values. Positive- and negative-ion HRESI-TOF-MS of 95 novel compounds were recorded on and exported from an Agilent Technologies 6520 Accurate-Mass Q-TOF LC/MS spectrometer.
Data source location	Department of Applied Biology and Chemical Technology, the Hong Kong Polytechnic University, Hong Kong SAR
Data accessibility	Data are available with the article

Value of the Data

- Nusbiarylins are the first-in-class bacterial ribosomal RNA synthesis inhibitors that possess potent activity against various types of multidrug-resistant bacteria with a novel mode of action
- Spectral data of nusbiarylins are useful for elucidating their purity
- The HPLC profiles, qNMR and HRMS spectroscopic data are of 95 unreported compounds and could be useful for the characterization by other researchers

1. Data

Bacterial transcription is a valid but underutilized target for antimicrobial agent discovery [1]. NusB and NusE are bacteria-specific transcription factors essential for cell viability [1,2]. Inhibitors of the NusB-NusE interaction were discovered and named nusbiarylins. The name was derived from the target protein NusB and their biaryl structure [2–4]. The dataset contains high-performance liquid chromatography (HPLC) profiles of 90 compounds, quantitative nuclear magnetic resonance (qNMR) spectroscopic data of 5 compounds and high-resolution mass spectrometry (HRMS) profiles of all 95 compounds [3,4]. The data file (HPLC, qNMR and HRMS spectra) is available publicly within this data article as a supplementary file. The compound structures were presented in Table 1, purities in Table 2 and HRMS data in Table 3. The testing methods and parameters of different compounds by HPLC, HRMS and qNMR were also described.

2. Experimental design, materials, and methods

2.1. HPLC analysis

2.1.1. Sample preparation and HPLC analysis

Approximately 0.1 mg of derivatives were dissolved in 1 mL of HPLC grade acetonitrile. 20 μL of supernatant was manually loaded onto the sample loop. The analysis was carried out on Agilent 1100

series and 1260 infinity system consisting of G1322A degasser, G1311A quat pump and G1365B multi-wavelength detector (MWD). The chromatographic parameters were set as follows:

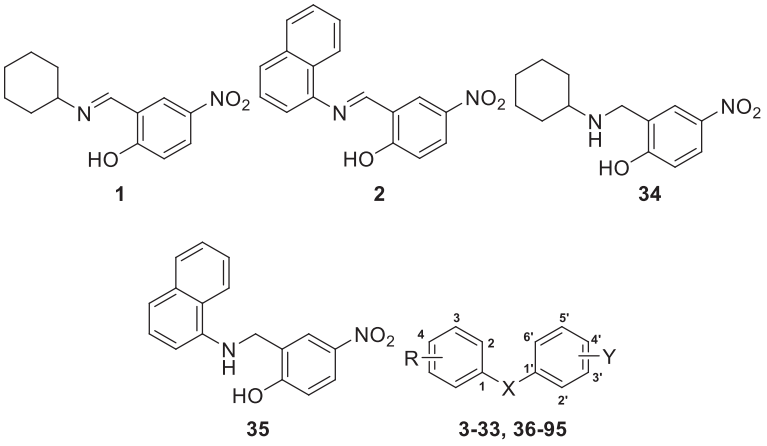
Mobile phase: Mobile phase A: MeCN, Mobile phase B: H_2O
Detector: MWD at 254 nm
Column: Agilent ZORBAX Eclipse Plus C18 (4.6 × 100 mm, 5 μm)
Flow rate: 1.000 mL/min
Gradient programme:
For compound **29, 60, 76, 87, 88**

t/min	Mobile phase A	Mobile phase B
0	30%	70%
2	40%	60%
3	50%	50%
9	80%	20%
14	90%	10%
15	100%	0%
16.5	80%	20%
17	60%	40%
20	30%	70%

For compound **34, 62, 94**

t/min	Mobile phase A	Mobile phase B
0	10%	90%
8	30%	70%
14	50%	50%
24	100%	0%
25	80%	20%
27	40%	60%
28	10%	90%

Table 1
Chemical structures of 95 nusbiarylin compounds as NusB-NusE inhibitors.



(*continued on next page*)

Table 1 (*continued*)

No.	R	X	Y	Cpd	R	X	Y
3	H	-N=CH-	2′-OH 5′-NO_2	**51**	2-OCH_3	-NH-CH_2-	2′-OH 5′-NO_2
4	2-F			**52**	3-OCH_3		
5	3-F			**53**	4-OCH_3		
6	4-F			**54**	2-$COOCH_3$		
7	2-CH_3			**55**	3-$COOCH_3$		
8	3-CH_3			**56**	4-$COOCH_3$		
9	4-CH_3			**57**	2-CF_3		
10	2-$C(CH_3)_3$			**58**	3-CF_3		
11	3-$C(CH_3)_3$			**59**	4-CF_3		
12	4-$C(CH_3)_3$			**60**	3-ethynyl		
13	2-OH			**61**	3-CH_2OH		
14	3-OH			**62**	3-COOH		
15	4-OH			**63**	3-ethynyl	-N=CH-	2′-OH, 5′-$COOCH_3$
16	2-Cl			**64**			2′-OH, 5′-F
17	3-Cl	-N=CH-	2′-OH 5′-NO_2	**65**	3-ethynyl	-N=CH-	2′-OH, 5′-CN
18	4-Cl			**66**			2′-OH, 5′-CH_2CN
19	2-OCH_3			**67**			2′-OH, 5′-OCH_3
20	3-OCH_3			**68**			2′-OH
21	4-OCH_3			**69**			5′-NO_2
22	2-$COOCH_3$			**70**			2′-OCH3, 5′-NO_2
23	3-$COOCH_3$			**71**			2′-OH, 4′-NO_2
24	4-$COOCH_3$			**72**			2′-OH, 3′-NO_2
25	2-CF_3			**73**			3′-OH, 6′-NO_2
26	3-CF_3			**74**			2′-OH, 3′-Br, 5′-
27	4-CF_3			**75**			2′-OH, 3′-Cl, 5′-Cl
28	2-ethynyl			**76**		-NH-CH_2-	2′-OH, 5′-$COOCH_3$
29	3-ethynyl			**77**			2′-OH, 5′-F
30	4-ethynyl			**78**			2′-OH, 5′-CN
31	3-CH_2OH			**79**			2′-OH, 5′-CH_2CN
32	4-CH_2OH			**80**			2′-OH, 5′-OCH_3
33	3-COOH			**81**			2′-OH
36	H	-NH-CH_2-		**82**			5′-NO_2
37	2-F			**83**			2′-OCH_3
38	3-F			**84**			2′-OH, 4′-NO_2
39	4-F			**85**			2′-OH, 3′-NO_2
40	2-CH_3			**86**			2′-OH, 3′-Br, 5′-
41	3-CH_3			**87**			2′-OH, 3′-Cl, 5′-Cl
42	4-CH_3			**88**	H	(*E*)-CH=CH-	2′-OH, 5′-NO_2
43	2-$C(CH_3)_3$			**89**	2-OCH_3		
44	3-$C(CH_3)_3$			**90**	3-OCH_3		
45	4-$C(CH_3)_3$			**91**	2-CN		
46	2-OH			**92**	3-$COOCH_3$		
47	3-OH			**93**	4-$COOCH_3$		
48	2-Cl			**94**	3-ethynyl	-NHCO-	
49	3-Cl			**95**	H	-CO-	
50	4-Cl						

For the remaining compounds **except** compounds **22, 24, 27, 33, 74**

t/min	Mobile phase A	Mobile phase B
0	30%	70%
2	40%	60%
3	50%	50%
13	100%	0%
16.5	30%	70%

2.1.2. Data processing

The automated integration software ChemStation for LC systems B.03.02 [341] was used to acquire the *area under the curve* (mAU). The obtained spectra were then exported as images.

2.2. qNMR analysis

2.2.1. Sample preparation and qNMR analysis

Samples were weighed into 5 mm standard NMR tubes using OHAUS® analytical plus balance, followed by addition of 500 μL of DMSO-d_6 and indicated volume of internal reference 1,3,5-trioxane (99.66% pure, 9.98 mg/mL in DMSO-d_6) purchased from Dieckmann (Hong Kong) Chemical Industry co., LTD. qNMR analysis were carried out *via* Bruker ultrashield™ NMR spectrometer 600 MHz. NMR instrument controlled parameters were adjusted as follows [5]:

Sample Temperature: 25 °C (298 K, regulated ± 0.1 K)
Data Points (acquired): 64 K
Zero-Filling (SI or FN): to 256 K
Dummy Scans: 4
Relaxation delay (D1): 60 s
Scans (NS or NT): 16

2.2.2. Data processing

The software Bruker topspin 3.2 was used to acquire the integrals of the signals of sample and internal reference. The normalized integrals values per proton equivalent by dividing each integral by the corresponding number of protons were calculated, so as the integral of the analyte ($\boldsymbol{Int_t}$ and $\boldsymbol{Int_{IC}}$) as the average of all normalized integrals. The total number of protons ($\boldsymbol{n_t}$ and $\boldsymbol{n_{IC}}$) was set to one [5]. Purities was then calculated according to the equation as below:

$$P\,[\%] = \frac{n_{IC} * Int_t * MW_t * m_{IC}}{n_t * Int_{IC} * MW_{IC} * m_s} * P_{IC}$$

where: $\boldsymbol{P}$ = purity of tested compound

$\boldsymbol{m_{IC}}$ = weight of the internal calibrant (IC)
$\boldsymbol{m_s}$ = weight of the sample
$\boldsymbol{Int_{IC}}$ = integral of the IC resonance signal being used for quantification
$\boldsymbol{Int_t}$ = integral of the target analyte (t) resonance signal being used for quantification
$\boldsymbol{n_{IC}}$ = number of protons that give rise to $\boldsymbol{Int_{IC}}$
$\boldsymbol{n_t}$ = number of protons of the target analyte that give rise to $\boldsymbol{Int_t}$
$\boldsymbol{MW_{IC}}$ = molecular weight of the internal calibrant

Table 2
Data on purities by HPLC or qNMR and retention time (HPLC) of nusbiarylin compounds.

Compound	Purity/%	Retention time/min
1	99.9	6.51
2	99.0	11.23
3	99.8	9.06
4	98.2	9.35
5	98.0	9.47
6	100.0	9.32
7	99.5	9.90
8	99.8	10.12
9	99.9	10.12
10	99.4	12.10
11	100.0	12.35
12	99.2	12.50
13	96.0	5.66
14	97.8	6.59
15	96.1	6.35
16	98.5	10.17
17	96.6	10.51
18	95.5	10.50
19	97.8	7.80
20	98.7	9.04
21	99.9	9.02
22	98.4	qNMR
23	97.2	9.15
24	98.9	qNMR
25	100.0	10.09
26	98.3	10.55
27	97.3	qNMR
28	97.4	8.98
29	97.0	9.76
30	95.5	9.69
31	95.3	5.95
32	97.2	5.77
33	91.0	qNMR
34	99.2	9.21
35	100.0	7.86
36	99.4	6.48
37	99.7	6.81
38	97.7	6.70
39	99.8	6.58
40	99.8	7.14
41	100.0	7.11
42	98.0	7.17
43	99.4	8.67
44	98.6	8.92
45	99.6	9.15
46	96.3	5.25
47	99.3	4.70
48	99.5	7.45
49	99.3	7.35
50	99.7	7.32
51	98.9	6.82
52	99.7	6.27
53	97.6	6.05
54	99.6	7.44
55	98.0	6.21
56	99.6	5.80
57	99.4	7.84
58	99.0	7.72
59	97.6	7.68
60	98.7	6.79
61	99.4	4.33

Table 2 (*continued*)

Compound	Purity/%	Retention time/min
62	98.9	12.92
63	98.1	9.85
64	97.1	9.87
65	99.4	9.02
66	97.7	8.46
67	97.6	9.46
68	99.8	9.68
69	99.9	9.32
70	99.8	9.62
71	97.2	9.73
72	98.0	8.46
73	95.1	7.03
74	97.7	qNMR
75	99.4	12.08
76	98.3	6.52
77	99.2	6.98
78	99.1	6.33
79	99.7	6.19
80	98.7	6.54
81	99.6	6.94
82	99.4	8.25
83	99.9	8.43
84	99.6	7.23
85	99.5	8.45
86	99.7	7.93
87	100.0	8.96
88	95.5	8.02
89	97.2	8.05
90	97.4	7.91
91	96.8	7.20
92	97.6	7.79
93	97.7	7.76
94	98.9	17.74
95	99.7	7.46

$\boldsymbol{MW_t}$ = molecular weight of the target analyte
$\boldsymbol{P_{IC}}$ = purity of the internal calibrant, as percent value

2.3. HRMS analysis for all compounds

2.3.1. Sample preparation and HRMS analysis

Approximately 0.1 mg of derivatives were dissolved in 1 mL of HPLC grade acetonitrile. After sonication and filtration *via* 0.22 μm PTFE syringe filter, 10 μL of the upper layer was injected using an autosampler onto Agilent Technologies 6520 Accurate-Mass Q-TOF LC/MS spectrometer. The spectrometer was calibrated before each chromatographic run for optimal mass accuracy. The mobile phase gradient was 100% acetonitrile, at a flow rate of 0.5 ml/min. The mass spectra were acquired in positive- or negative-ion mode with source temperature at 300 °C. Ion spray voltage and fragmentor voltage were adjusted to 3.5 kV and 175 V, respectively. The range of mass detected was between 100 m/z and 1000 m/z.

2.3.2. Data processing

HRMS profiles were acquired and processed using MassHunter B.07 software. The obtained spectra were then exported as images.

Table 3
HRMS data of nusbiarylin compounds.

Compound	Ion formula	m/z (calculated)	m/z (found)
1	$C_{13}H_{15}N_2O_3$ $[M-H]^-$	247.1088	247.1089
2	$C_{17}H_{11}N_2O_3$ $[M-H]^-$	291.0775	291.0773
3	$C_{13}H_9N_2O_3$ $[M-H]^-$	241.0619	241.0620
4	$C_{13}H_8FN_2O_3$ $[M-H]^-$	259.0524	259.0523
5	$C_{13}H_8FN_2O_3$ $[M-H]^-$	259.0524	259.0528
6	$C_{13}H_8FN_2O_3$ $[M-H]^-$	259.0524	259.0522
7	$C_{14}H_{11}N_2O_3$ $[M-H]^-$	255.0775	255.0771
8	$C_{14}H_{11}N_2O_3$ $[M-H]^-$	255.0775	255.0772
9	$C_{14}H_{11}N_2O_3$ $[M-H]^-$	255.0775	255.0772
10	$C_{17}H_{17}N_2O_3$ $[M-H]^-$	297.1245	297.1247
11	$C_{17}H_{17}N_2O_3$ $[M-H]^-$	297.1245	297.1242
12	$C_{17}H_{17}N_2O_3$ $[M-H]^-$	297.1245	297.1243
13	$C_{13}H_9N_2O_4$ $[M-H]^-$	257.0568	257.0565
14	$C_{13}H_9N_2O_4$ $[M-H]^-$	257.0568	257.0568
15	$C_{13}H_9N_2O_4$ $[M-H]^-$	257.0568	257.0567
16	$C_{13}H_8ClN_2O_3$ $[M-H]^-$	275.0229	275.0227
17	$C_{13}H_8ClN_2O_3$ $[M-H]^-$	275.0229	275.0226
18	$C_{13}H_8ClN_2O_3$ $[M-H]^-$	275.0229	275.0226
19	$C_{14}H_{11}N_2O_4$ $[M-H]^-$	271.0724	271.0719
20	$C_{14}H_{11}N_2O_4$ $[M-H]^-$	271.0724	271.0721
21	$C_{14}H_{11}N_2O_4$ $[M-H]^-$	271.0724	271.0727
22	$C_{15}H_{11}N_2O_5$ $[M-H]^-$	299.0673	299.0672
23	$C_{15}H_{11}N_2O_5$ $[M-H]^-$	299.0673	299.0669
24	$C_{15}H_{11}N_2O_5$ $[M-H]^-$	299.0673	299.0672
25	$C_{14}H_8F_3N_2O_3$ $[M-H]^-$	309.0493	309.0492
26	$C_{14}H_8F_3N_2O_3$ $[M-H]^-$	309.0493	309.0491
27	$C_{14}H_8F_3N_2O_3$ $[M-H]^-$	309.0493	309.0490
28	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0618
29	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0620
30	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0615
31	$C_{14}H_{11}N_2O_4$ $[M-H]^-$	271.0724	271.0721
32	$C_{14}H_{11}N_2O_4$ $[M-H]^-$	271.0724	271.0722
33	$C_{14}H_9N_2O_5$ $[M-H]^-$	285.0517	285.0513
34	$C_{13}H_{17}N_2O_3$ $[M-H]^-$	249.1245	249.1245
35	$C_{17}H_{13}N_2O_3$ $[M-H]^-$	293.0932	293.0929
36	$C_{13}H_{11}N_2O_3$ $[M-H]^-$	243.0775	243.0775
37	$C_{13}H_{10}FN_2O_3$ $[M-H]^-$	261.0681	261.0683
38	$C_{13}H_{10}FN_2O_3$ $[M-H]^-$	261.0681	261.0679
39	$C_{13}H_{10}FN_2O_3$ $[M-H]^-$	261.0681	261.0682
40	$C_{14}H_{13}N_2O_3$ $[M-H]^-$	257.0932	257.0928
41	$C_{14}H_{13}N_2O_3$ $[M-H]^-$	257.0932	257.0928
42	$C_{14}H_{13}N_2O_3$ $[M-H]^-$	257.0932	257.0927
43	$C_{17}H_{19}N_2O_3$ $[M-H]^-$	299.1401	299.1401
44	$C_{17}H_{19}N_2O_3$ $[M-H]^-$	299.1401	299.1399
45	$C_{17}H_{19}N_2O_3$ $[M-H]^-$	299.1401	299.1404
46	$C_{13}H_{11}N_2O_4$ $[M-H]^-$	259.0724	259.0723
47	$C_{13}H_{11}N_2O_4$ $[M-H]^-$	259.0724	259.0723
48	$C_{13}H_{10}ClN_2O_3$ $[M-H]^-$	277.0385	277.0384
49	$C_{13}H_{10}ClN_2O_3$ $[M-H]^-$	277.0385	277.0387
50	$C_{13}H_{10}ClN_2O_3$ $[M-H]^-$	277.0385	277.0386
51	$C_{14}H_{13}N_2O_4$ $[M-H]^-$	273.0881	273.0878
52	$C_{14}H_{13}N_2O_4$ $[M-H]^-$	273.0881	273.0876
53	$C_{14}H_{13}N_2O_4$ $[M-H]^-$	273.0881	273.0881
54	$C_{15}H_{13}N_2O_5$ $[M-H]^-$	301.0830	301.0833
55	$C_{15}H_{13}N_2O_5$ $[M-H]^-$	301.0830	301.0831
56	$C_{15}H_{13}N_2O_5$ $[M-H]^-$	301.0830	301.0826
57	$C_{14}H_{10}F_3N_2O_3$ $[M-H]^-$	311.0649	311.0651
58	$C_{14}H_{10}F_3N_2O_3$ $[M-H]^-$	311.0649	311.0650
59	$C_{14}H_{10}F_3N_2O_3$ $[M-H]^-$	311.0649	311.0654
60	$C_{15}H_{11}N_2O_3$ $[M-H]^-$	267.0775	267.0773
61	$C_{14}H_{13}N_2O_4$ $[M-H]^-$	273.0881	273.0879

Table 3 (*continued*)

Compound	Ion formula	m/z (calculated)	m/z (found)
62	$C_{14}H_{11}N_2O_5$ $[M-H]^-$	287.0673	287.0673
63	$C_{17}H_{12}NO_3$ $[M-H]^-$	278.0823	278.0822
64	$C_{15}H_9FNO$ $[M-H]^-$	238.0674	238.0672
65	$C_{16}H_9N_2O$ $[M-H]^-$	245.0720	245.0719
66	$C_{17}H_{11}N_2O$ $[M-H]^-$	259.0877	259.0876
67	$C_{16}H_{12}NO_2$ $[M-H]^-$	258.0874	258.0875
68	$C_{15}H_{10}NO$ $[M-H]^-$	220.0768	220.0772
69	$C_{15}H_{11}N_2O_2$ $[M+H]^+$	251.0815	251.0818
70	$C_{16}H_{13}N_2O_3$ $[M+H]^+$	281.0921	281.0922
71	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0620
72	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0616
73	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0621
74	$C_{15}H_8BrN_2O_3$ $[M-H]^-$	342.9724	342.9727
75	$C_{15}H_8Cl_2NO$ $[M-H]^-$	287.9988	287.9987
76	$C_{17}H_{14}NO_3$ $[M-H]^-$	280.0979	280.0974
77	$C_{15}H_{11}FNO$ $[M-H]^-$	240.0830	240.0829
78	$C_{16}H_{11}N_2O$ $[M-H]^-$	247.0877	247.0876
79	$C_{17}H_{13}N_2O$ $[M-H]^-$	261.1033	261.1032
80	$C_{16}H_{14}NO_2$ $[M-H]^-$	252.1030	252.1023
81	$C_{15}H_{12}NO$ $[M-H]^-$	222.0924	222.0923
82	$C_{15}H_{13}N_2O_2$ $[M+H]^+$	253.0972	253.0974
83	$C_{16}H_{15}N_2O_3$ $[M+H]^+$	283.1077	283.1080
84	$C_{15}H_{11}N_2O_3$ $[M-H]^-$	267.0775	267.0773
85	$C_{15}H_{11}N_2O_3$ $[M-H]^-$	267.0775	267.0770
86	$C_{15}H_{10}BrN_2O_3$ $[M-H]^-$	344.9880	344.9878
87	$C_{15}H_{10}Cl_2NO$ $[M-H]^-$	290.0145	290.0141
88	$C_{14}H_{10}NO_3$ $[M-H]^-$	240.0666	240.0662
89	$C_{15}H_{12}NO_4$ $[M-H]^-$	270.0772	270.0769
90	$C_{15}H_{12}NO_4$ $[M-H]^-$	270.0772	270.0771
91	$C_{15}H_9N_2O_3$ $[M-H]^-$	265.0619	265.0617
92	$C_{16}H_{12}NO_5$ $[M-H]^-$	298.0721	298.0717
93	$C_{16}H_{12}NO_5$ $[M-H]^-$	298.0721	298.0719
94	$C_{15}H_9N_2O_4$ $[M-H]^-$	281.0568	281.0571
95	$C_{13}H_8NO_4$ $[M-H]^-$	242.0459	242.0454

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.dib.2020.105313.

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