Supporting Information

Schroeder, *et al.* 10.1073/pnas.0806840105

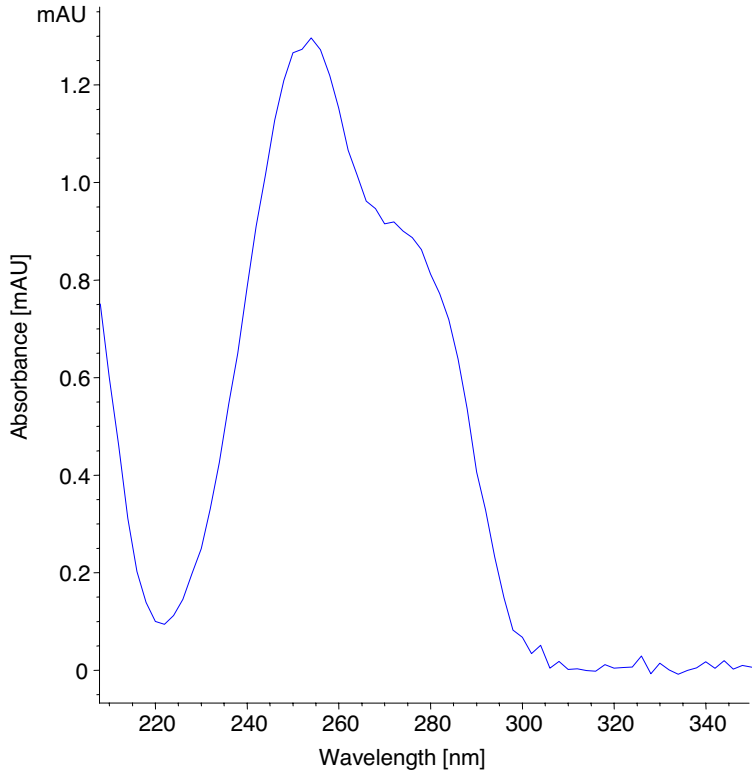


Fig. S1. UV spectrum of compound **3**.

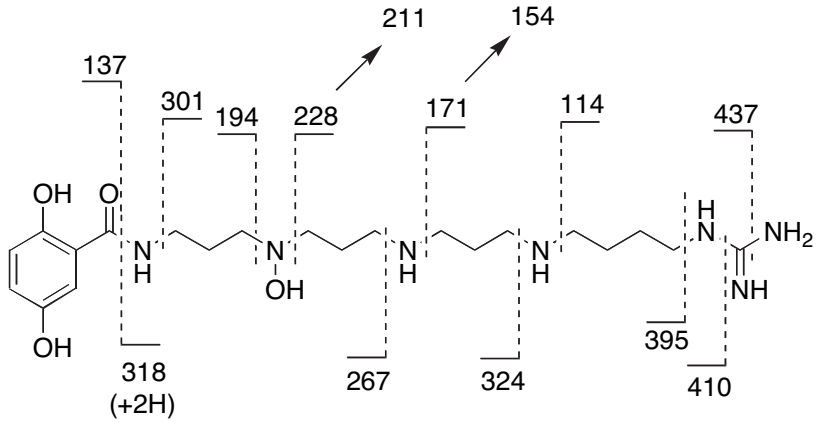


Fig. S2. Electrospray-MS fragmentation pattern of compound **5** [(M + 1)/*z* = 454.3 AMU] (see ref. 1 for a discussion of the fragmentation pattern).

1. Chesnov S, Bigler L, Hesse M (2000) The spider *Paracoelotes birulai*: Detection and structure elucidation of new acylpolyamines by on-line coupled HPLC-APCI-MS andHPLC-APCI-MS/MS. *Helv Chim Acta* 83:3295–3305.

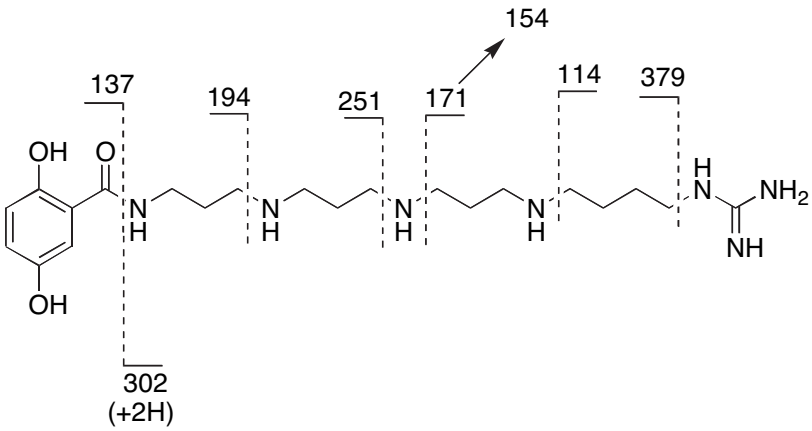
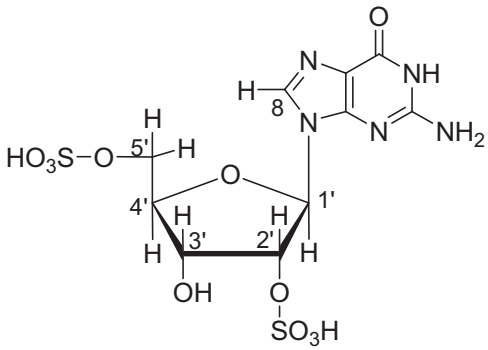


Fig. S3. Electrospray-MS fragmentation pattern of compound 6 [$(M + 1)/z = 438.3$ AMU] (see ref. 1 for a discussion of the fragmentation pattern).

1. Chesnov S, Bigler L, Hesse M (2000) The spider *Paracoelotes birulai*: Detection and structure elucidation of new acylpolyamines by on-line coupled HPLC-APCI-MS andHPLC-APCI-MS/MS. *Helv Chim Acta* 83:3295–3305.

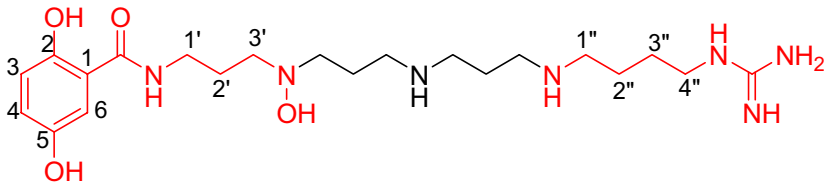
Table S1. NMR spectroscopic and MS data of compound 3



Position	δ ^{13}C, ppm	δ ^{1}H, ppm	Relevant HMBC correlations
2	156.1*		
4	154.1		
5	118.6		
6	161.5*		
8	140.3	8.02 (s)	C-4, C-5
1′	88.1	6.17 ($J_{1'\text{-}2'}$ = 5.7)	C-8, C-4
2′	80.2	5.41 ($J_{2'\text{-}3'}$ = 5.5)	
3′	71.6	4.76 ($J_{3'\text{-}4'}$ = 3.4)	
4′	84.5	4.43 ($J_{4'\text{-}5'ab}$ = 3.2)	
5′ab	69.4	4.37	
ESI-MS (negative ion): (M-1)/z = 442.00 AMU			

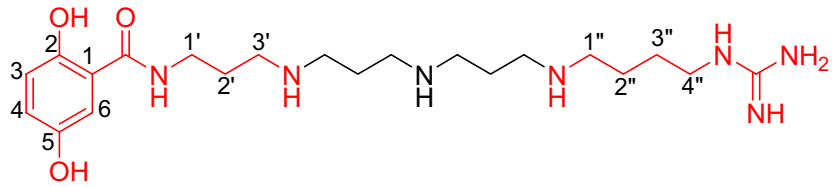
*These ^{13}C chemical shift values were determined from HMBC spectra of a synthetic sample acquired by using a delay of 120 ms.

Table S2. Partial NMR spectroscopic data of compound 5



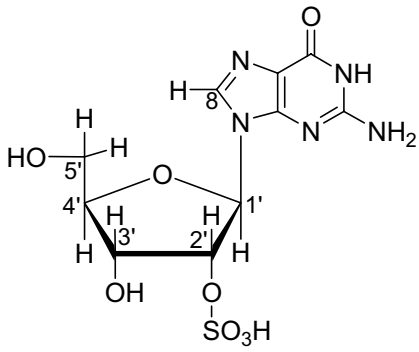
Position	δ ^{13}C, ppm	δ ^{1}H, ppm	Relevant HMBC correlations
1	117.1		
2	147.9		
3	117.8	6.902	C = O
4	120.8	6.99	
5	150.0		
6	113.7	7.18	C = O
C	168.6		
=			
O			
1′	37.0	3.46	C = O
2′	25.4	1.91	
3′	57.2	2.83	
1″		3.08	
2″		1.75	
3″		1.66	
4″		3.23	C = N
C	156.1		
=			
N			

Table S3. Partial NMR spectroscopic data of compound 6



Position	δ ^{13}C, ppm	δ ^{1}H, ppm	Relevant HMBC correlations
1			
2	147.9		
3	117.8	6.905	C = O
4	120.8	7.00	
5			
6	113.7	7.20	C = O
C	169.0		
=			
O			
1′	35.8	3.51	C = O
2′	25.1	2.03	
3′	44.8	3.14	
1″		3.05	
2″		1.73	
3″		1.63	
4″		3.20	C = N
C	156.1		
=			
N			

Table S4. NMR spectroscopic and MS data of compound 4



Position	δ ^{1}H, ppm
8	8.00 (s)
1′	6.14 ($J_{1'\text{-}2'}$ = 5.5)
2′	5.40 ($J_{2'\text{-}3'}$ = 5.5)
3′	4.66 ($J_{3'\text{-}4'}$ = 3.4)
4′	4.28 ($J_{4'\text{-}5'a}$ = 3.7) ($J_{4'\text{-}5'a}$ = 3.2)
5′a 5′b	3.87 ($J_{5'a\text{-}5'b}$ = 12.0) 3.93
ESI-MS (negative ion): (M-1)/*z* = 362.05 AMU	

Table S5. NMR-spectroscopic data of 2′,3′,5′-trisulfated guanosine

Position	δ ^{13}C, ppm	δ ^{1}H, ppm
2	156.1	
4	154.2	
5	118.1	
6	161.4	
8	140.5	8.01 (s)
1′	87.9	6.17 ($J_{1'\text{-}2'}$ = 5.7)
2′	78.0	5.58 ($J_{2'\text{-}3'}$ = 5.6)
3′	77.2	5.30 ($J_{3'\text{-}4'}$ = 3.3)
4′	83.2	4.72 ($J_{4'\text{-}5'ab}$ = 3.2)
5′ab	69.4	4.38

Table S6. NMR-spectroscopic data of 3′,5′-disulfated guanosine

Position	δ ^{13}C, ppm	δ ^{1}H, ppm
2	156.1	
4	154.2	
5	118.1	
6	161.4	
8	139.8	8.04 (s)
1′	88.8	5.96 ($J_{1'\text{-}2'} = 5.8$)
2′	74.3	4.97 ($J_{2'\text{-}3'} = 5.6$)
3′	78.9	5.07 ($J_{3'\text{-}4'} = 3.4$)
4′	83.5	4.70 ($J_{4'\text{-}5'\text{ab}} = 3.3$)
5′ab	69.6	4.34

Table S7. NMR-spectroscopic data of 5′-sulfated guanosine

Position	δ ^{13}C, ppm	δ ^{1}H ppm
2	156.1	
4	154.0	
5	118.1	
6	161.4	
8	139.6	8.03 (s)
1′	89.3	5.94 ($J_{1'\text{-}2'} = 5.7$)
2′	75.7	4.75 ($J_{2'\text{-}3'} = 5.5$)
3′	72.6	4.49 ($J_{3'\text{-}4'} = 3.4$)
4′	84.9	4.40 ($J_{4'\text{-}5'\text{ab}} = 3.2$)
5′ab	69.6	4.29–4.38