Electronic Supplementary Material (ESI) for MedChemComm.

Supplementary Information

3-Aminooxazolidinone AHL analogs as hydrolytically-stable quorum sensing agonists in Gram-negative bacteria

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1. Supplementary figures.

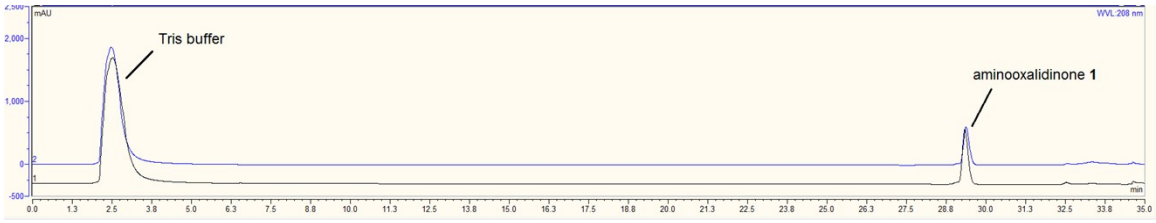


Figure S1. Stability studies of 3-oxo-C12-3-aminooxazolidinone (**1**) in 250 mM Tris-buffer (pH=8.0). HPLC analysis at time = 0 and 3 h. (Time = 0 min is the blue trace on top, and time = 3 h is the black trace on bottom). No new peak appeared, implying that 3-oxo-C12-3-aminooxazolidinone is stable at pH=8.0.

HPLC conditions: Detector: UV/Vis detector at 208 nM; Column: Cosmosil 5C_{18}-MS-II; Column temperature 25 °C; Flow rate: 1.0 mL/min; Injection volumn: 200 µL; Mobile phase: water, acetonitrile; Gradient: 50% acetonitrile to 100% acetonitrile in 35 min.

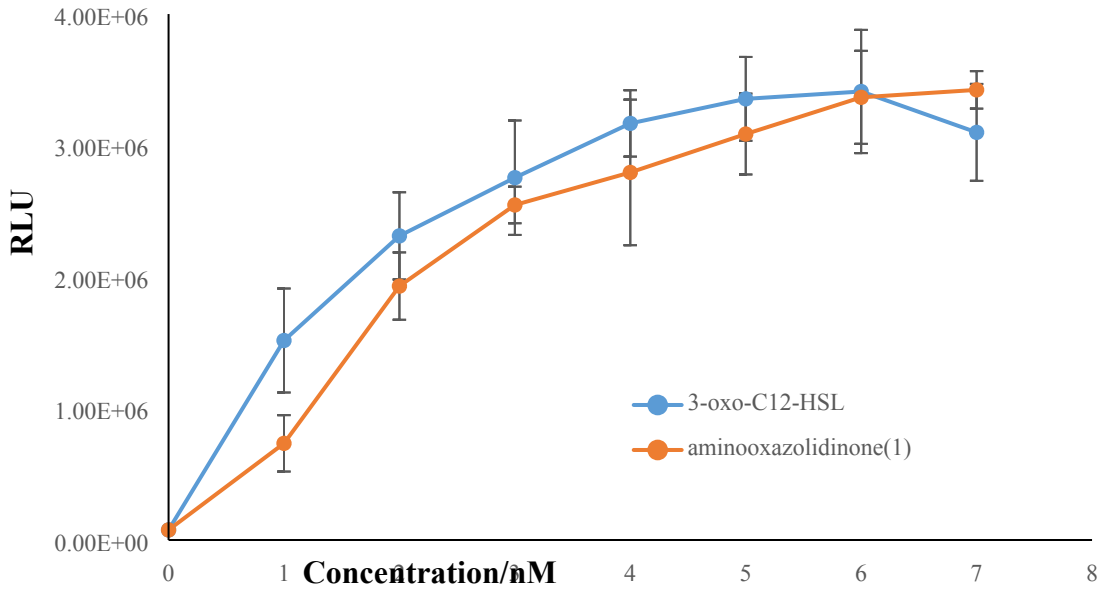
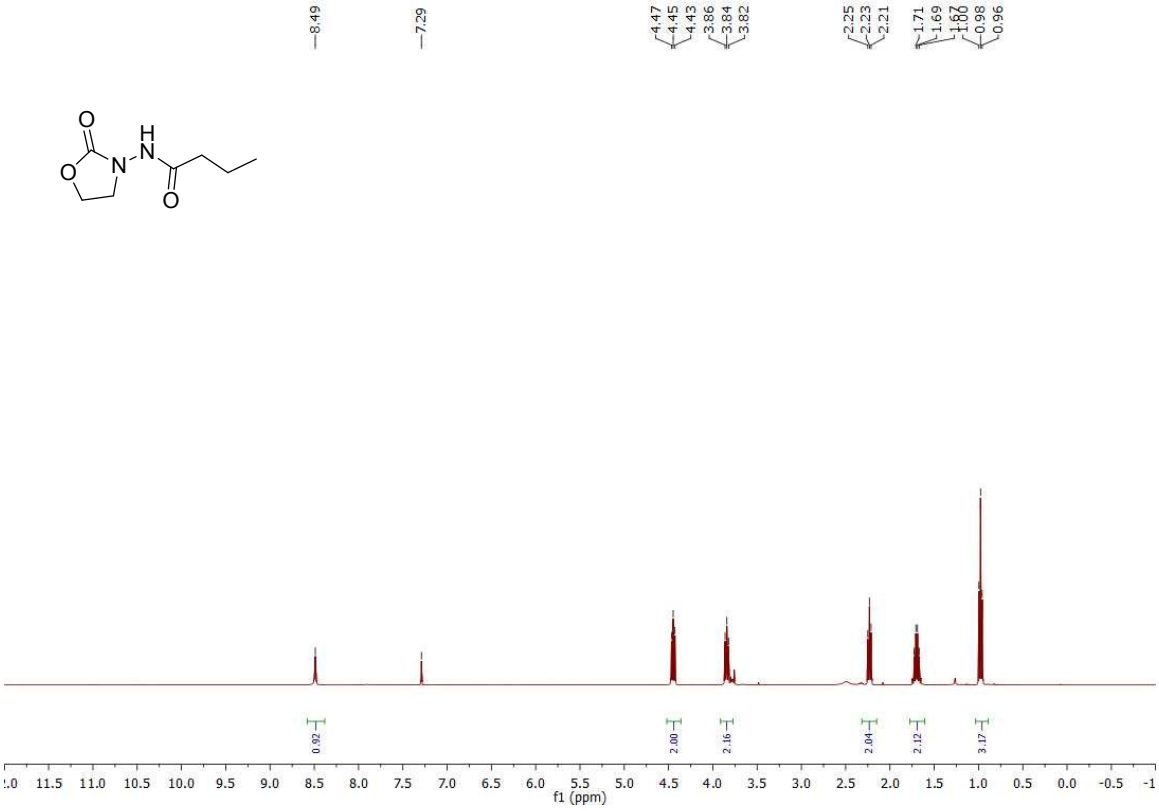
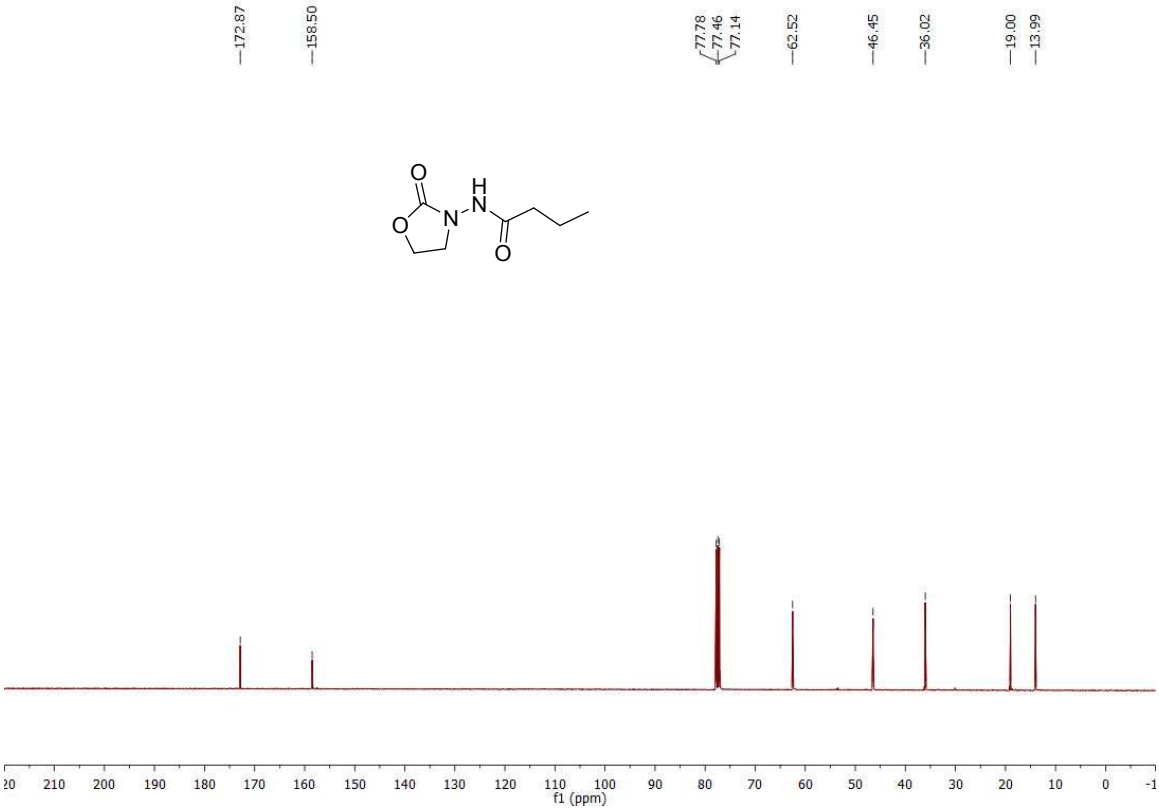
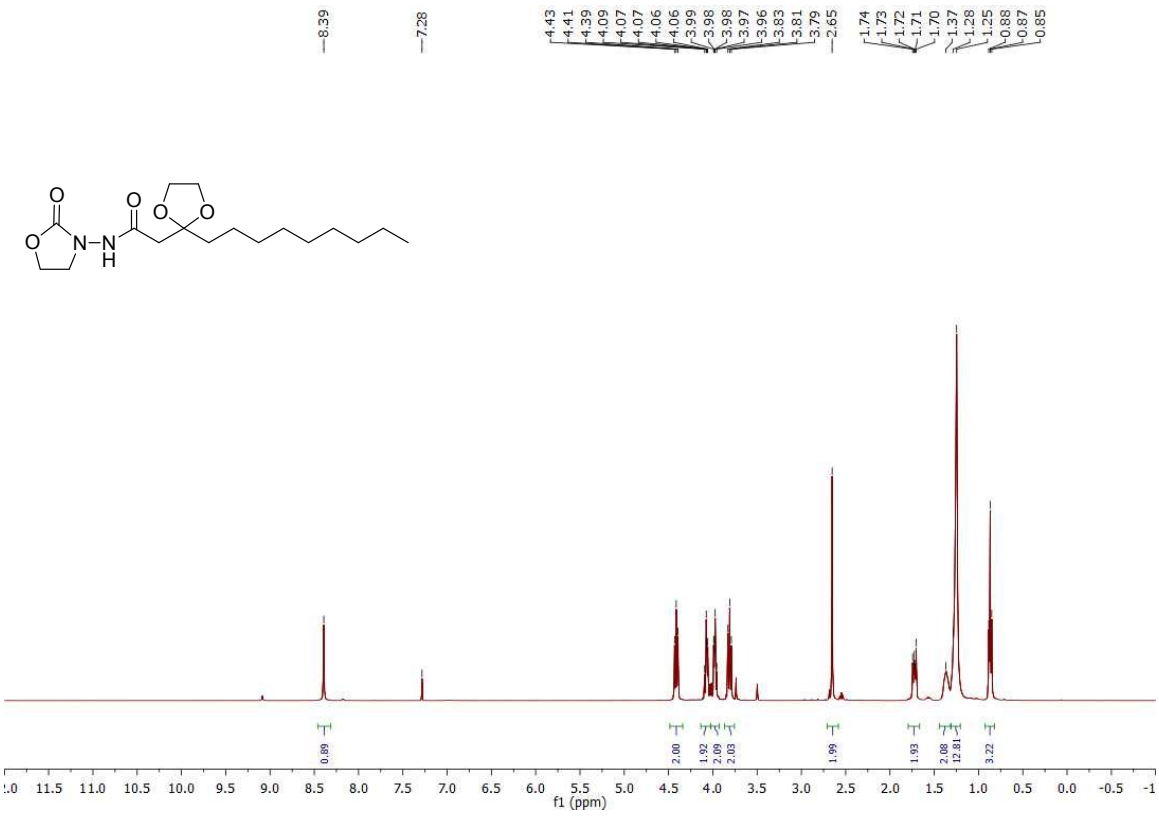


Figure S2. Bioluminescence induction after 8-hour incubation with native 3-oxo-C12-HSL and 3-aminooxazolidinone analogs **1** at different concentrations in *E. coli* pSB1075.

2. NMR spectra.



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4.43
4.41
4.39
4.09
4.07
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4.06
4.06
3.99
3.98
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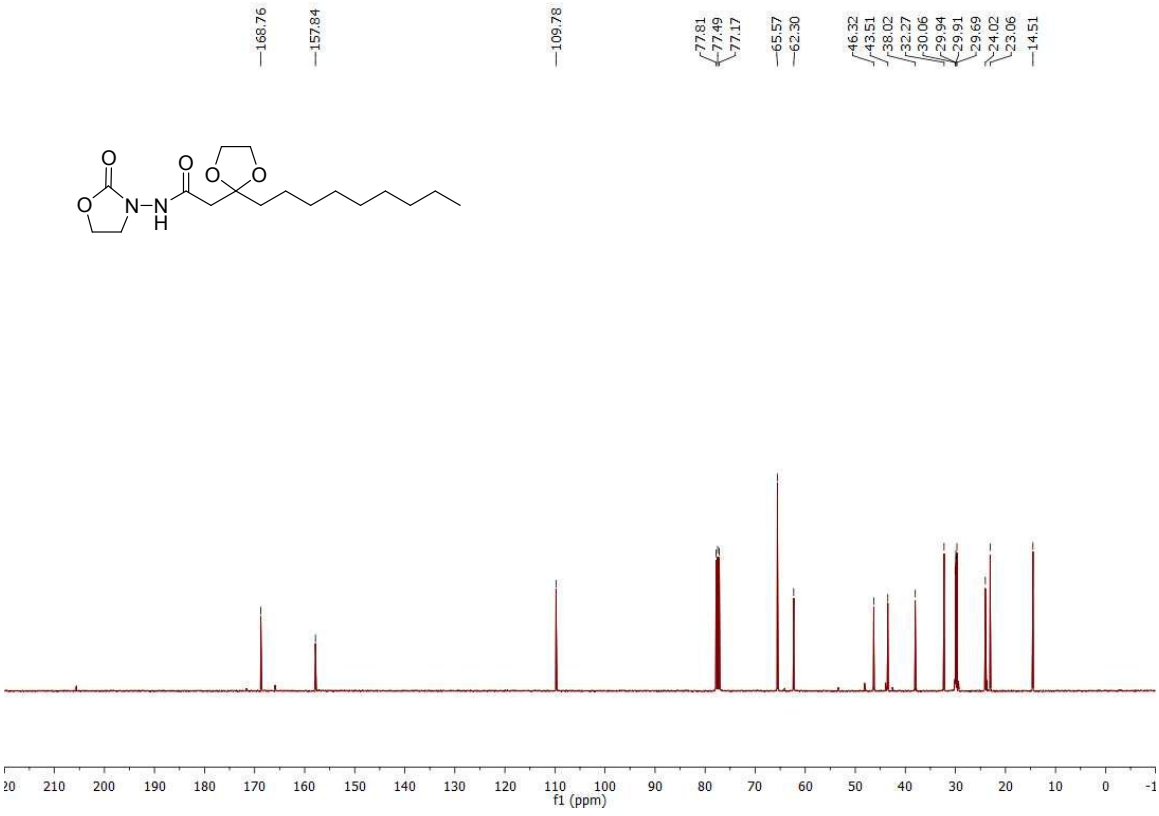
3.97
3.96
3.83
3.81
3.79
2.65
1.74
1.73
1.72
1.71
1.70
1.37
1.28
1.25
0.88
0.87
0.85
0.89
2.00
1.92
2.09
2.03
1.99
1.93
2.08
12.81
3.22
f1 (ppm)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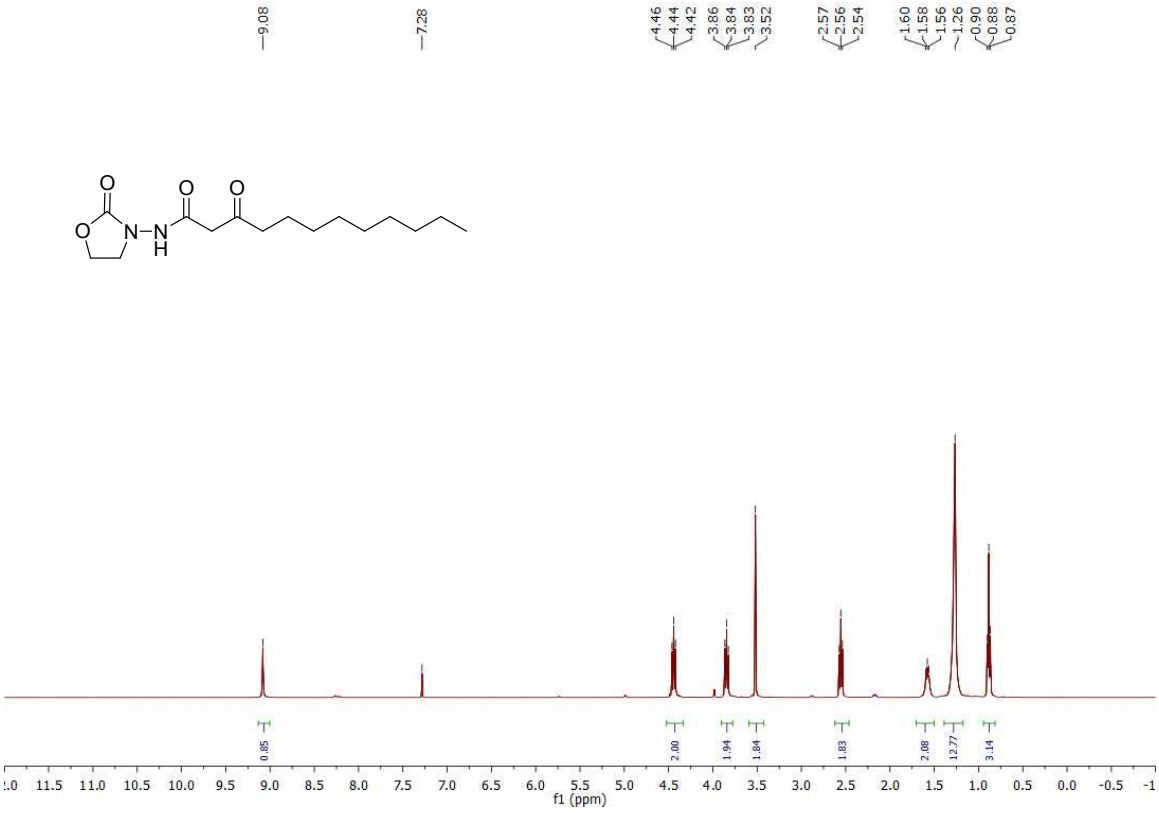
109.78
77.81
77.49
77.17
65.57
62.30
46.32
43.51
38.02
32.27
30.06
29.94
29.91
29.69
24.02
23.06
14.51
f1 (ppm)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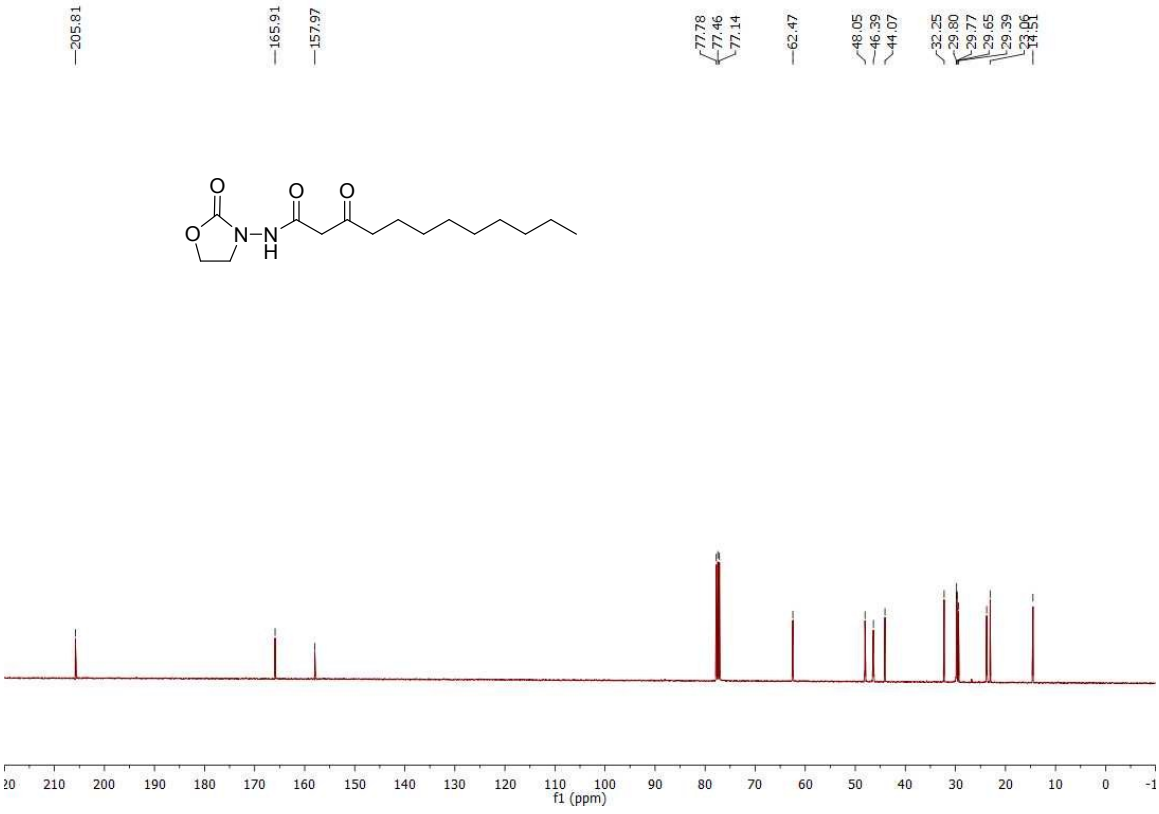
4.46
4.44
4.42
3.86
3.84
3.83
3.52
2.57
2.56
2.54
1.60
1.58
1.56
1.26
0.90
0.88
0.87
0.85
2.00
1.94
1.84
1.83
2.08
12.77
3.14
f1 (ppm)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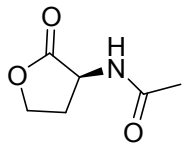
77.78
77.46
77.14
62.47
48.05
46.39
44.07
32.25
29.80
29.77
29.65
29.39
23.06
14.51
f1 (ppm)

3. Gaussian calculation results.

All the structures interested were optimized at B3LYP/6-311+G(d,2p) level using Gaussian 09.[1]



C2-HSL

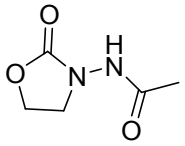
Total energy of the optimized structure: -530.6919083 a.u.

Number of imaginary frequencies: 0

Cartesian Coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.207400	0.597804	0.417294
2	6	0	-2.488988	-0.789922	0.126249
3	6	0	-1.135221	-1.405660	-0.243829
4	7	0	-0.426173	-0.199802	-0.663400
5	6	0	-0.986195	0.933748	-0.067118
6	8	0	-0.509517	2.030586	-0.019531
7	7	0	0.938859	-0.227980	-0.868638
8	6	0	1.806973	-0.233053	0.212484
9	6	0	3.253739	0.026629	-0.139456
10	8	0	1.418354	-0.456282	1.338508
11	1	0	-2.938874	-1.233962	1.011189
12	1	0	-3.197045	-0.822955	-0.703787
13	1	0	-1.215010	-2.123624	-1.060265
14	1	0	-0.641145	-1.869584	0.612245
15	1	0	1.241964	0.170495	-1.744742

16	1	0	3.463705	-0.079523	-1.204685
17	1	0	3.501542	1.045191	0.167576
18	1	0	3.882720	-0.658875	0.426597



C2-3-aminooxazolidinone

Total energy of the optimized structure: -514.6702856 a.u.

Number of imaginary frequencies: 0

Cartesian Coordinates:

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1	8	0	2.134690	0.578829	-0.515899
2	6	0	2.415670	-0.823569	-0.282464
3	6	0	1.119685	-1.442440	0.254461
4	6	0	0.421095	-0.234184	0.887613
5	6	0	1.001203	0.962826	0.109672
6	8	0	0.575851	2.079839	0.082757
7	7	0	-1.024813	-0.253123	0.923912
8	6	0	-1.777717	-0.220358	-0.223210
9	6	0	-3.262048	0.005887	-0.029387
10	8	0	-1.277448	-0.368928	-1.324122
11	1	0	2.740697	-1.248342	-1.229975
12	1	0	3.237967	-0.880390	0.434742
13	1	0	1.312689	-2.244081	0.967066
14	1	0	0.511857	-1.825909	-0.561280
15	1	0	0.760761	-0.105998	1.919653

16	1	0	-1.465837	0.048584	1.777201
17	1	0	-3.594605	-0.155548	0.997147
18	1	0	-3.492810	1.034358	-0.316175
19	1	0	-3.809104	-0.657712	-0.697768

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4. Reference

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford, CT, USA, 2009.