

Supporting Information for

Study of β -Oxygen effect in the Barton–McCombie Reaction for the Total synthesis of (4*R*,5*R*)-4-hydroxy- γ -decalactone (Japanese orange fly lactone): A Carbohydrate based Approach

Janardana Reddi Desireddi, * ^{a,b} Mallikarjuna Rao Mora, ^c Kiran Kumar Murahari, ^a Rajasekhar Reddy Nimma Reddy, ^a Thirupathi Mothe, ^b Arun Kumar Lingala, ^b Bhimcharan Maiti, ^a and Ravinder Manchal, * ^b

^a Aragen life sciences Private Limited (formerly known as GVK Biosciences Private Limited) Medicinal Chemistry Division, 28A, IDA Nacharam, Hyderabad - 500076, Telangana, India.

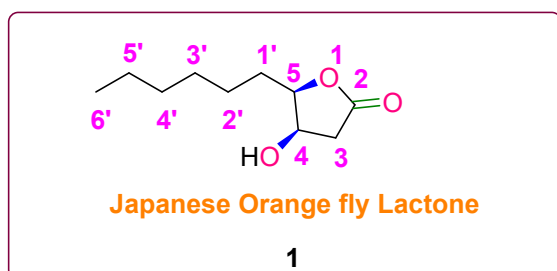
^b Department of Chemistry Chaitanya (Deemed to be University) Warangal-506001, Telangana, India.

^c Accrete Pharmaceuticals Private Limited, Tangadpalli Village, Choutuppal Mandal, Yadadri Bhuvanagiri District-508252, Telangana, India

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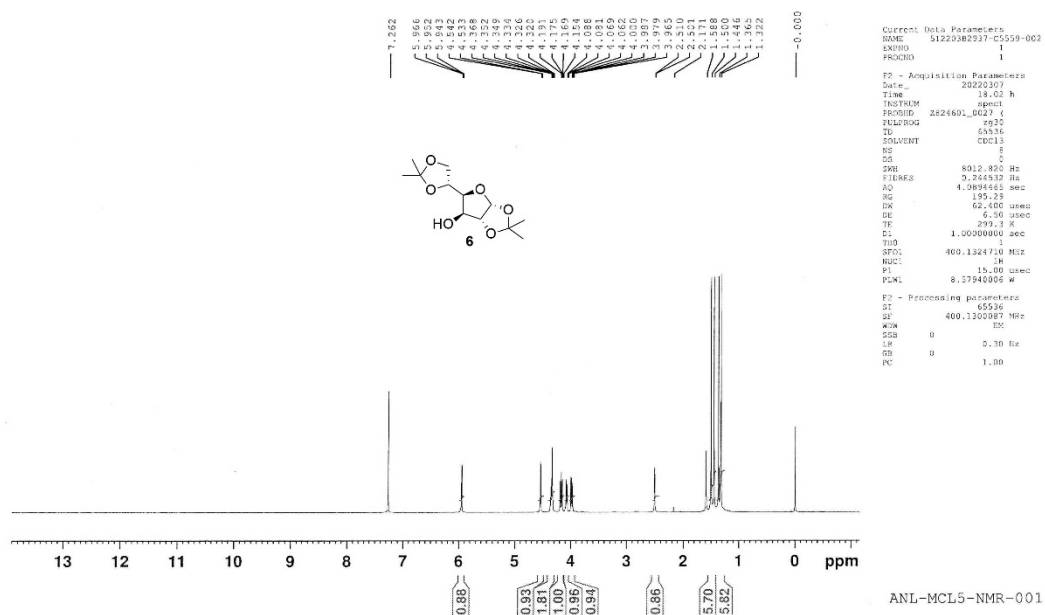
Table1: NMR chemical shift values of Japanese orange fly lactone in comparison to the isolated compound.



Position	Natural Japanese Orange Fly Lactone 1HNMR data in ppm (multiplicity, J in Hz)	Synthetic Japanese Orange Fly Lactone 1HNMR data in ppm (multiplicity, J in Hz)	Natural Japanese Orange Fly Lactone ¹³ CNMR data in ppm (multiplicity, J in Hz)	Synthetic Japanese Orange Fly Lactone ¹³ CNMR data in ppm (multiplicity, J in Hz)
2			175.3	176.1
3	2.80 (dd, 17.6, 5.6) 2.56 (dd, 17.6, 1.0)	2.81 (dd, 17.6, 5.6) 2.56 (dd, 17.6, 0.8)	39.6	39.5
4	4.49 (m)	4.47 (m)	69.3	68.9
5	4.37 (m)	4.39, (m)	84.7	85.1
1'	1.88 (m)	1.89-1.82 (m)	28.4	28.2
2'	1.71 (m)	1.77-1.68 (m)	25.7	25.5
3'	1.55-1.25 (m)	1.54-1.25 (m)	29.3	29.1
4'	1.55-1.25 (m)	1.54-1.25 (m)	22.7	22.5
5'	1.55-1.25 (m)	1.54-1.25 (m)	31.8	31.6
6'	0.90, t (7.0)	0.88, t (7.2)	14.2	14.0

Spectral data:

C5559-002



Chemical structure of compound **7** is shown above the spectrum. The structure is a substituted furanose derivative with a benzyloxy group (BnO) and a tert-butyl group.

¹H NMR spectrum (CDCl₃) of compound **7** is shown below. The x-axis represents the chemical shift in ppm, ranging from 0 to 8. The spectrum displays several peaks corresponding to the protons in the molecule.

Peak list (ppm): 7.352, 7.331, 7.315, 7.306, 7.282, 7.260, 5.992, 5.993, 5.970, 5.958, 5.939, 5.920, 4.581, 4.569, 4.548, 4.529, 4.510, 4.494, 4.474, 4.452, 4.432, 4.412, 4.096, 4.027, 4.007, 4.002, 4.000, 3.985, 1.548, 1.493, 1.428, 1.412, 1.391, 1.371, -0.000.

Integration values (from left to right): 4.91, 0.95, 1.80, 1.28, 1.00, 1.96, 1.98, 12.45.

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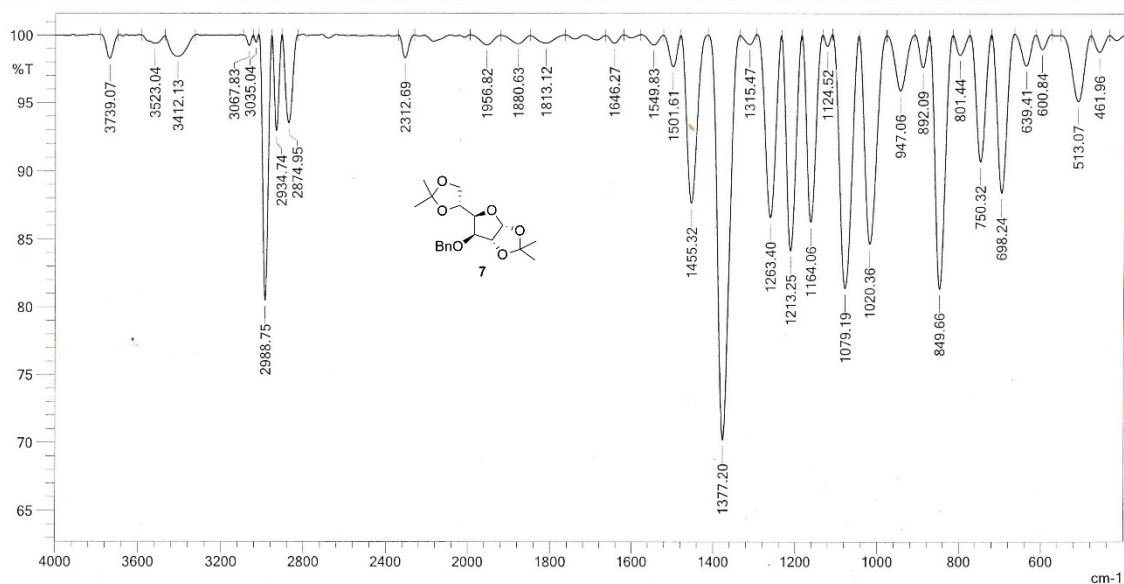
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ANL-MCL5-NMR-007



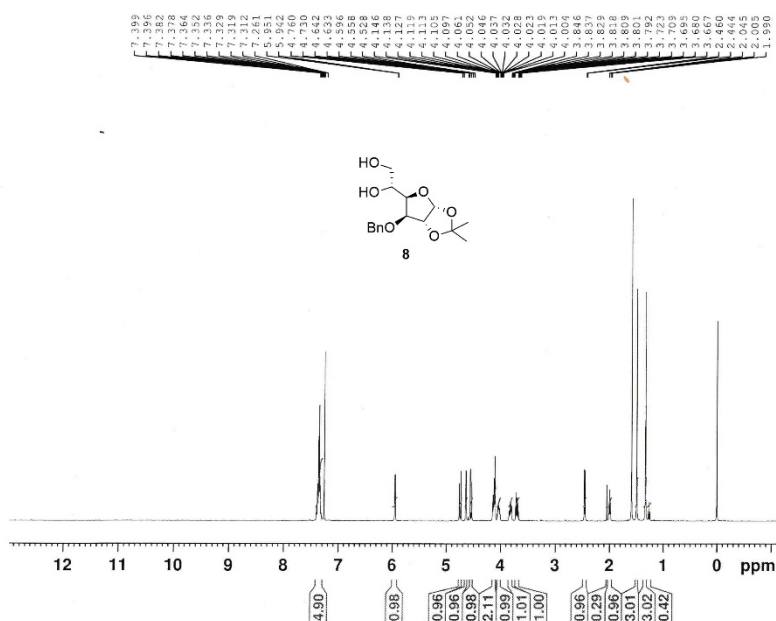
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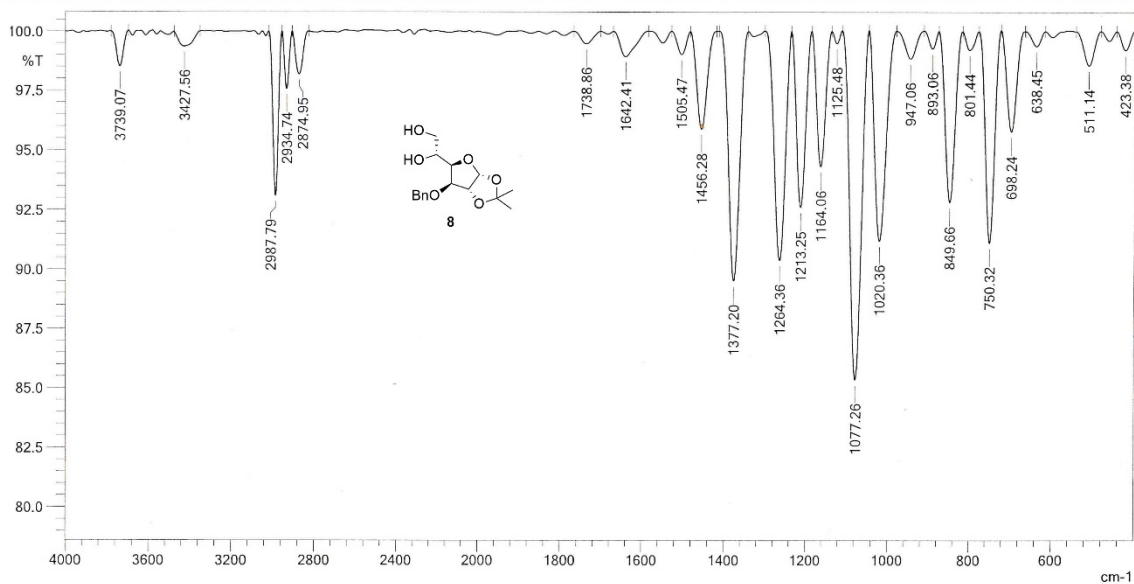
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ANL-MCL5-NMR-007



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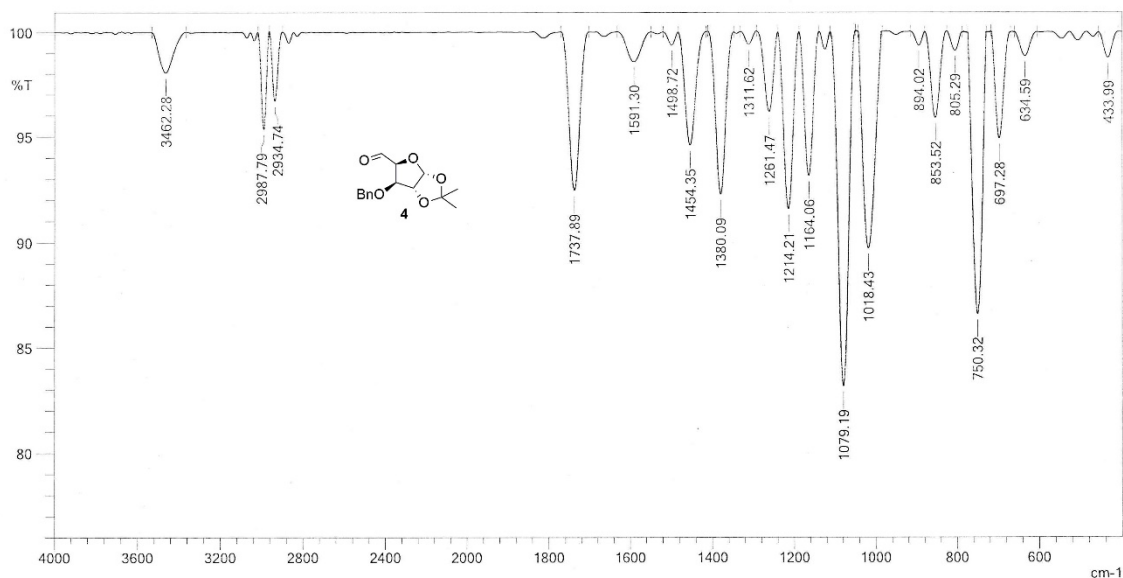


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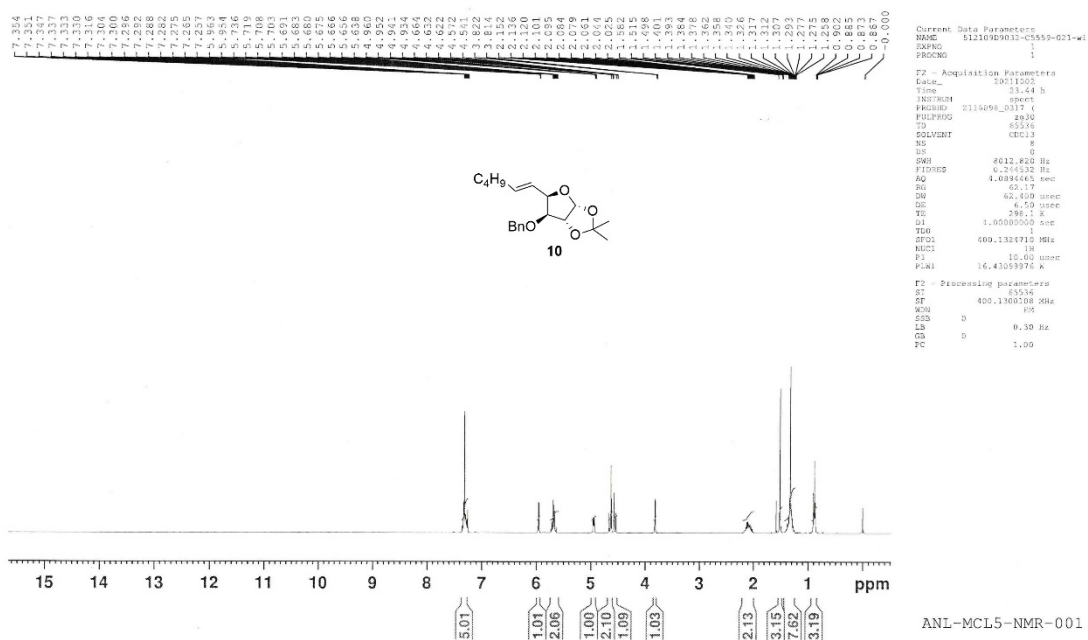
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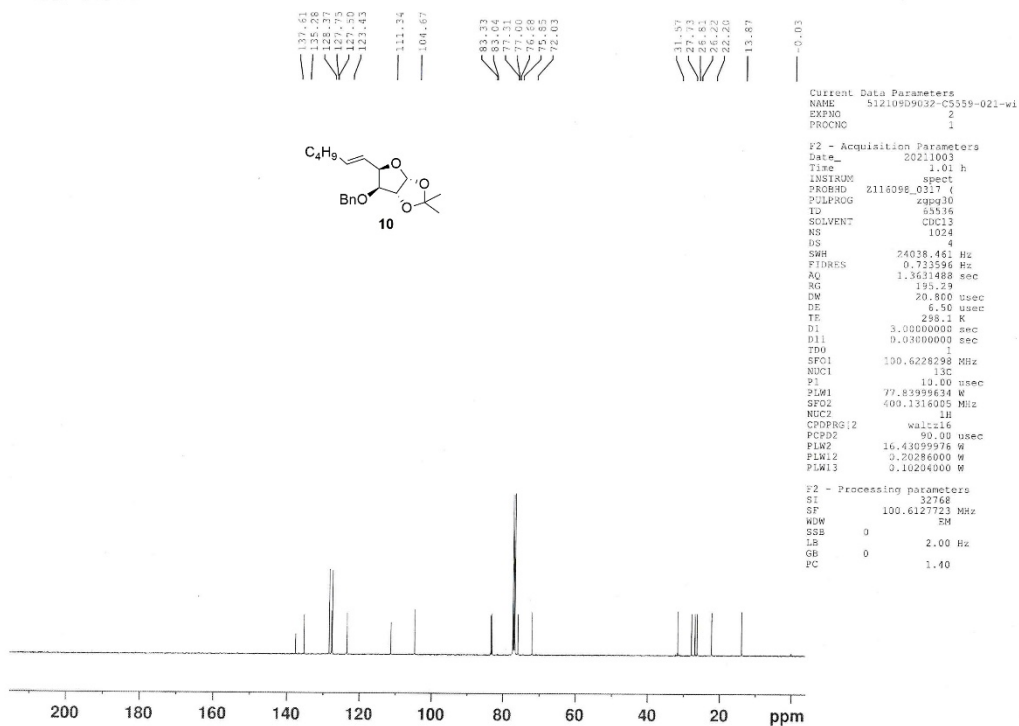
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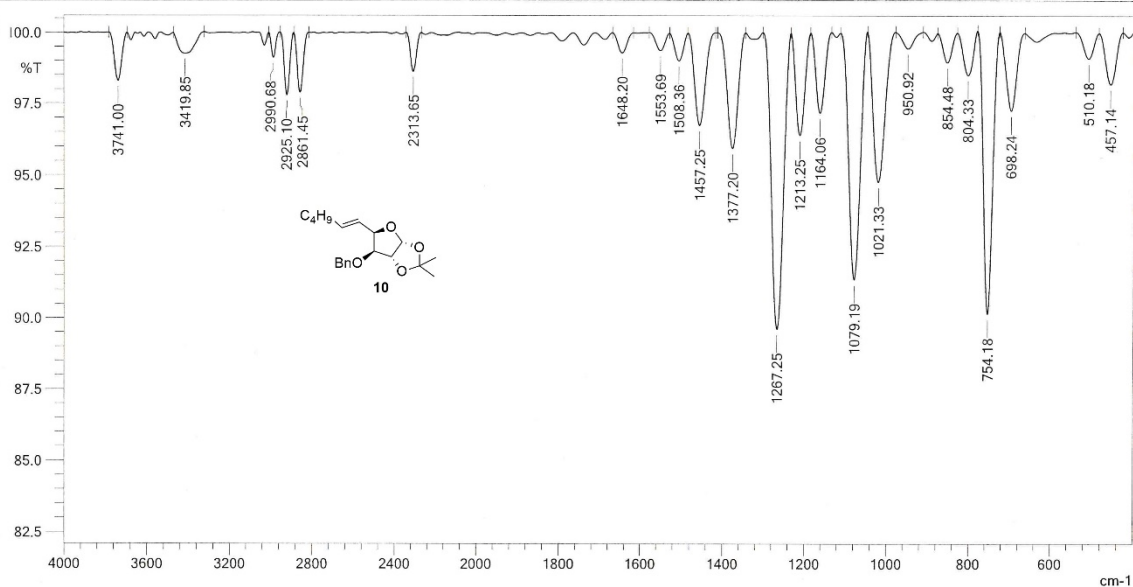
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C5559-021-wi



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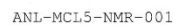


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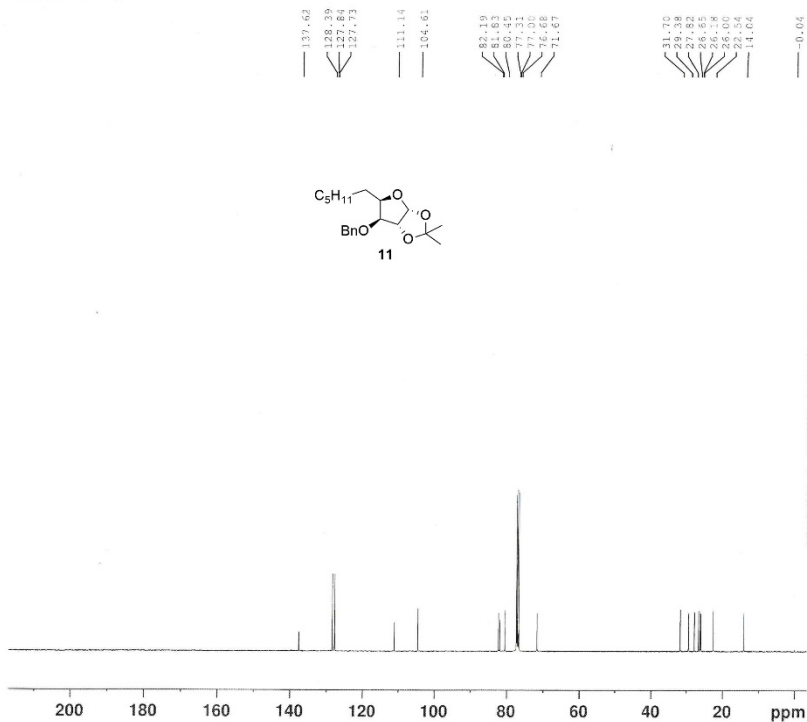
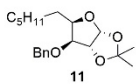
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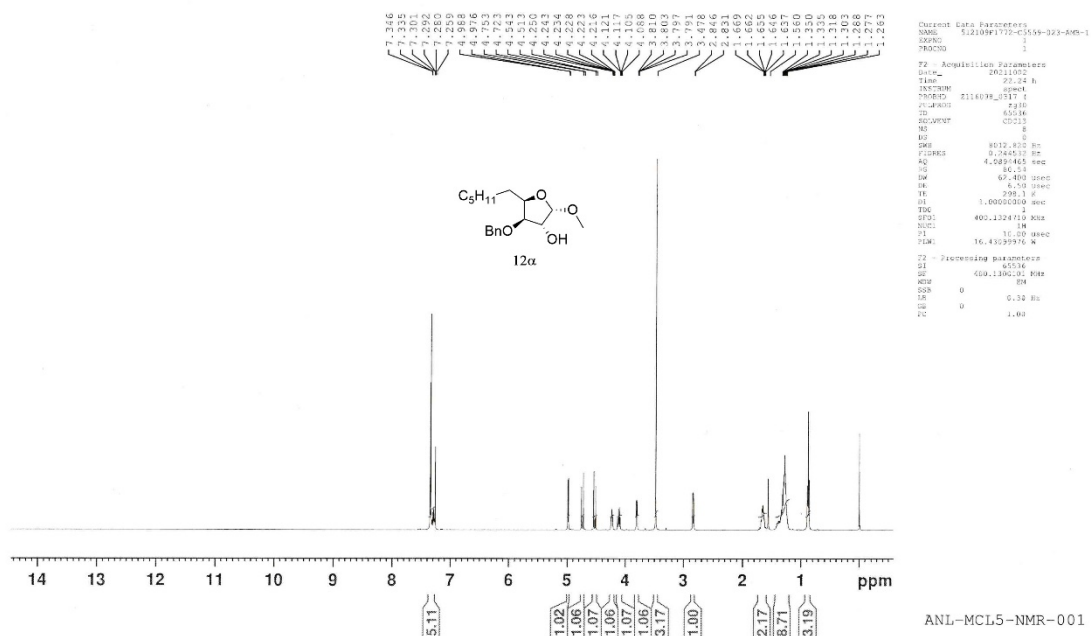
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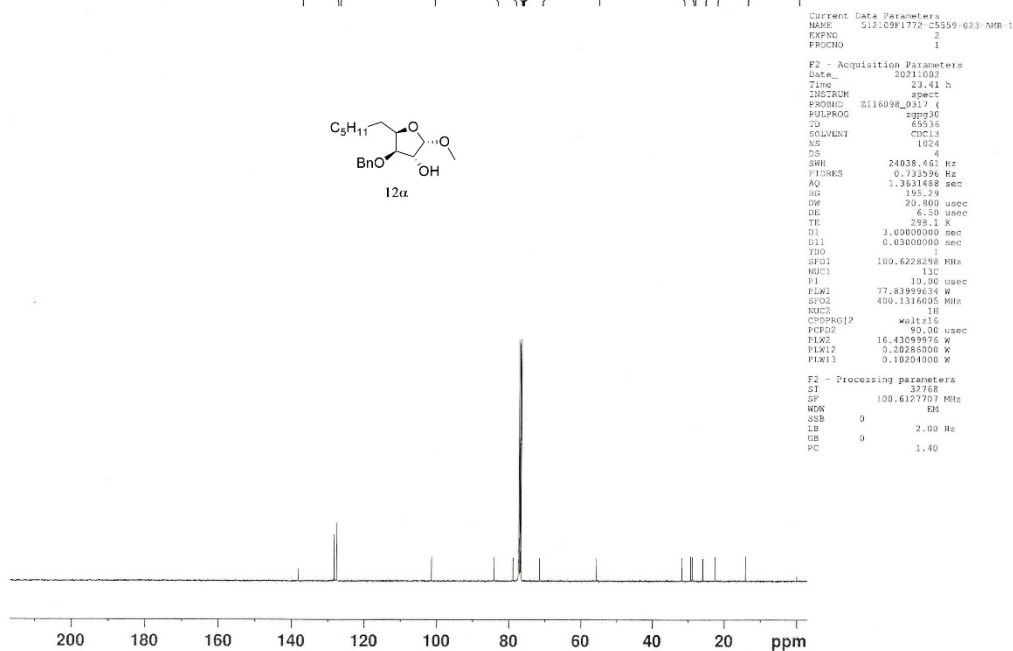
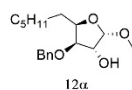
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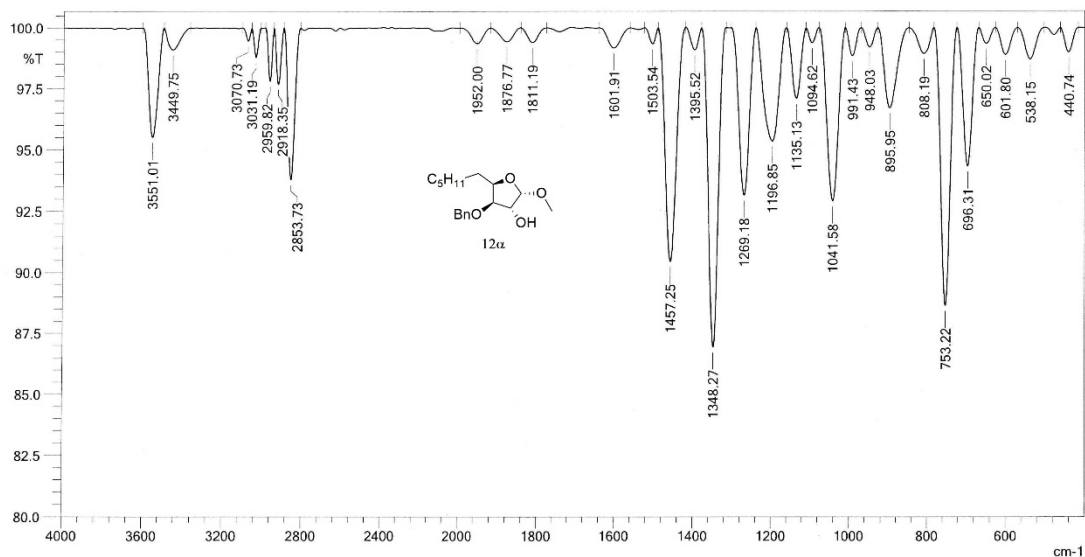
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12 α





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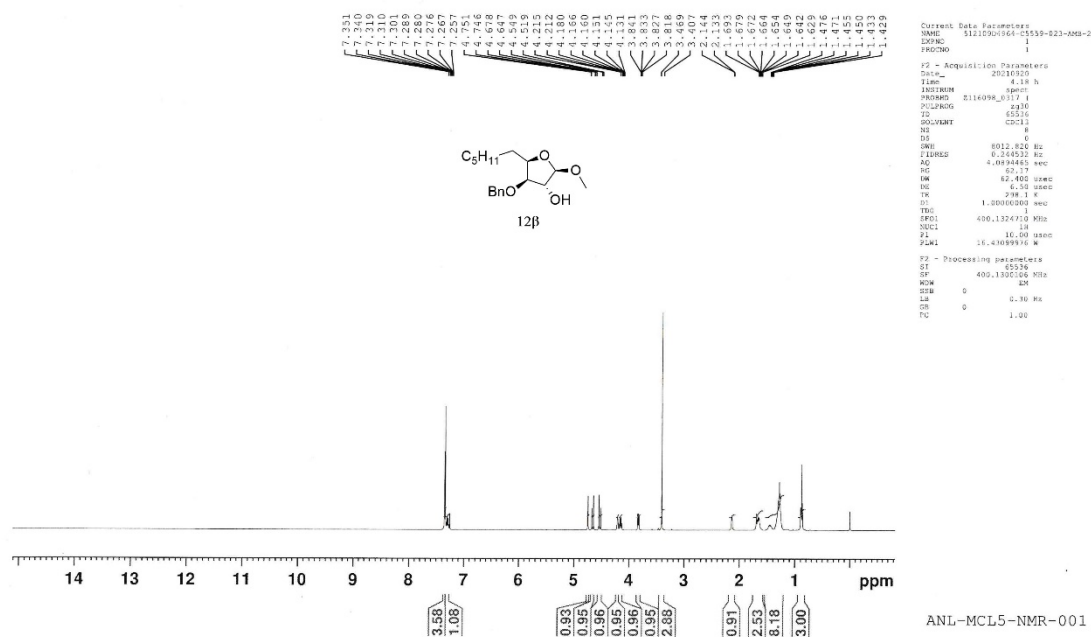
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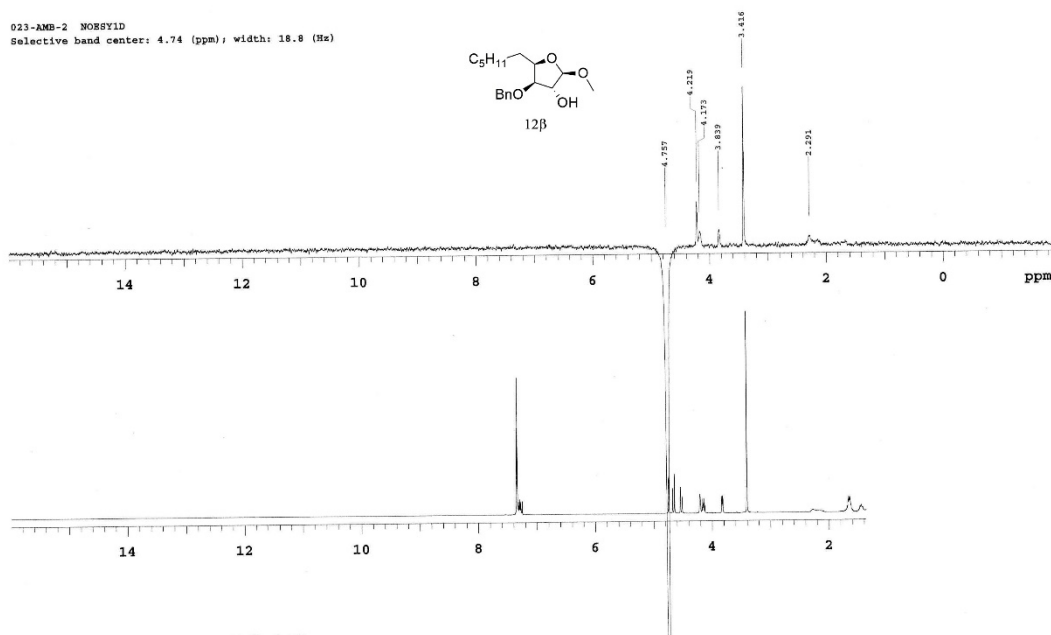
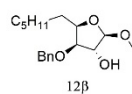
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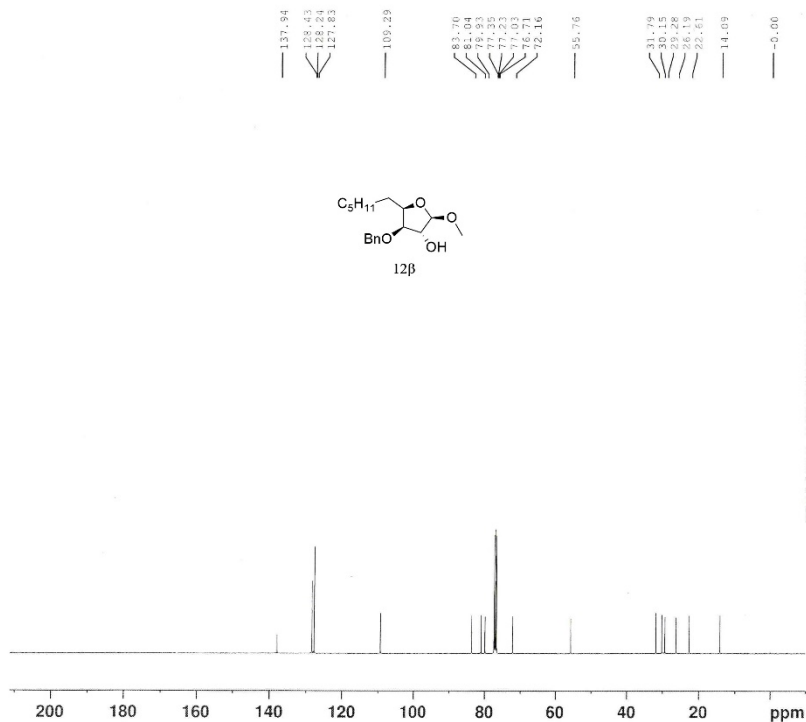


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C5559-023-AMB-2



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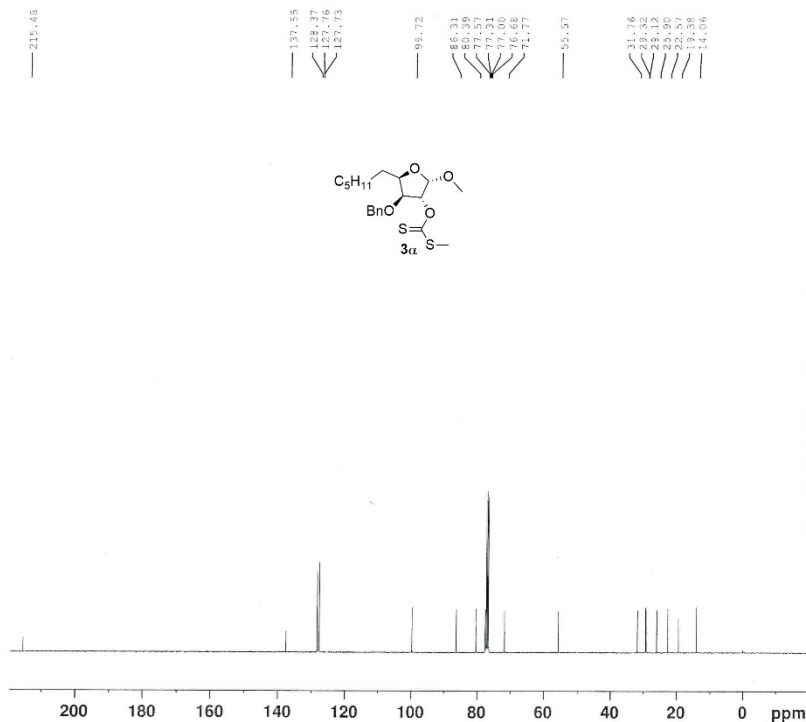
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ANL-MCL5-NMR-001

C5559-024-XN-1



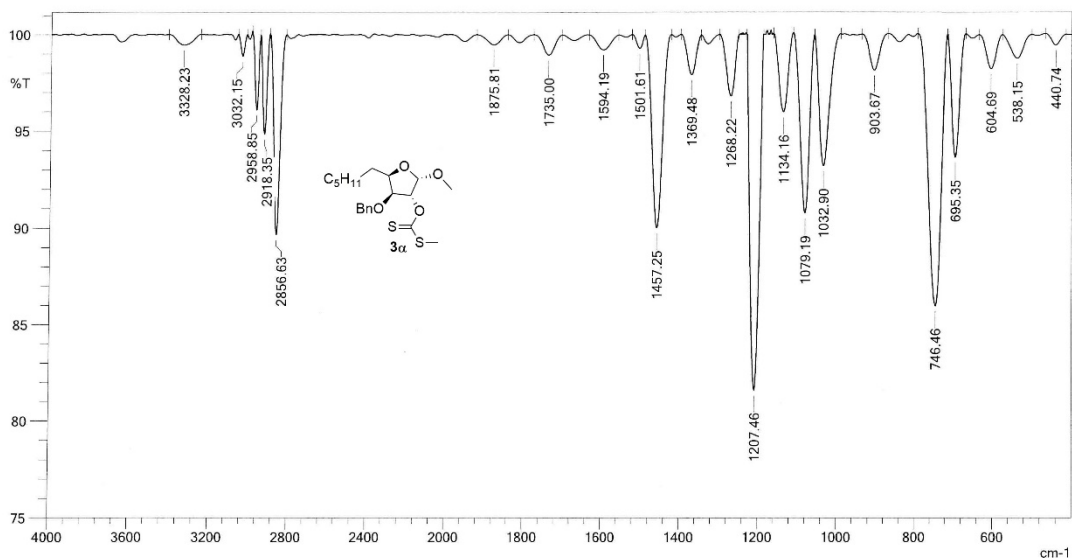
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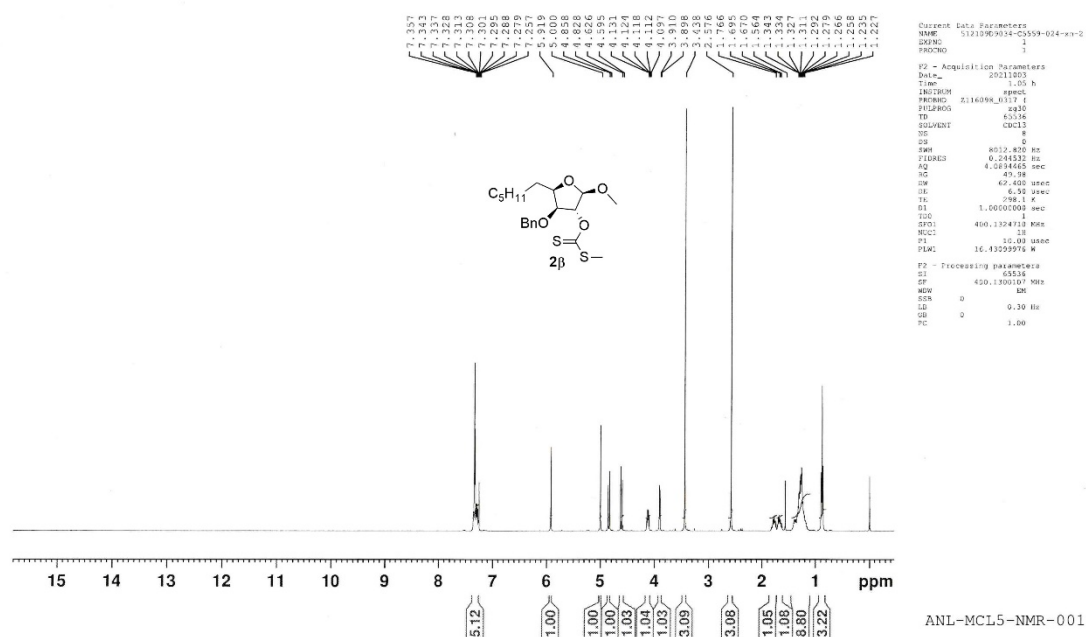
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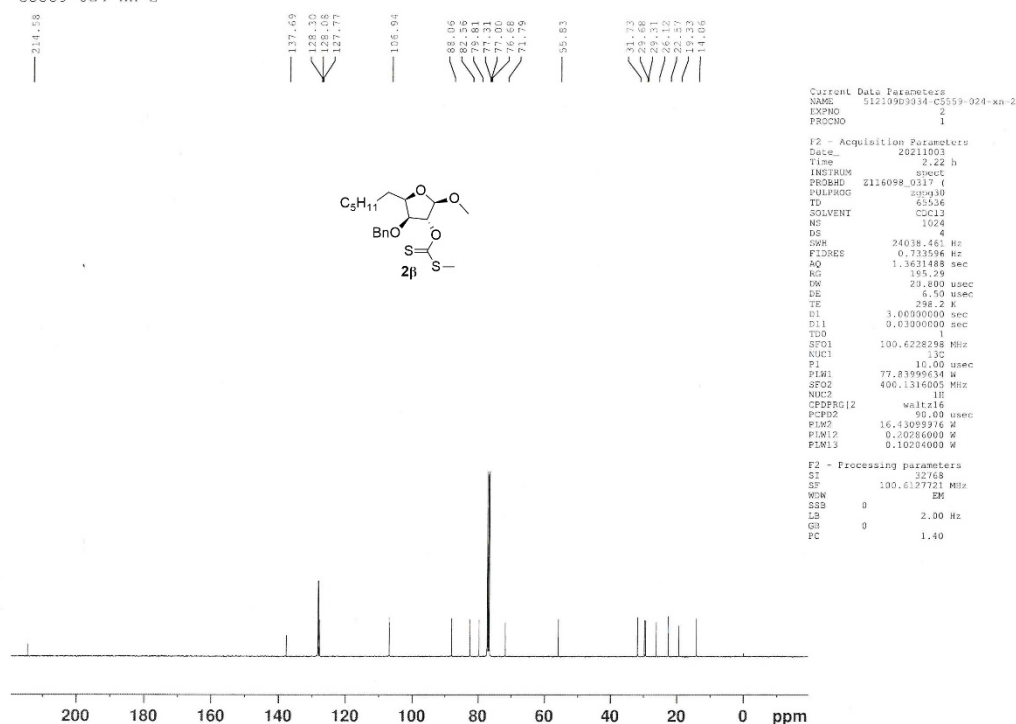
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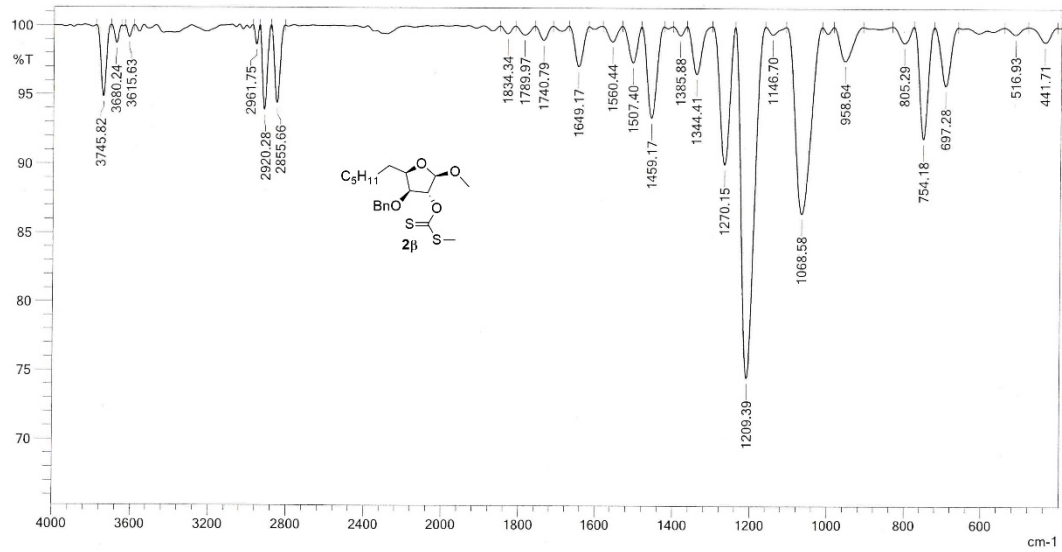
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C5559-024-xn-2





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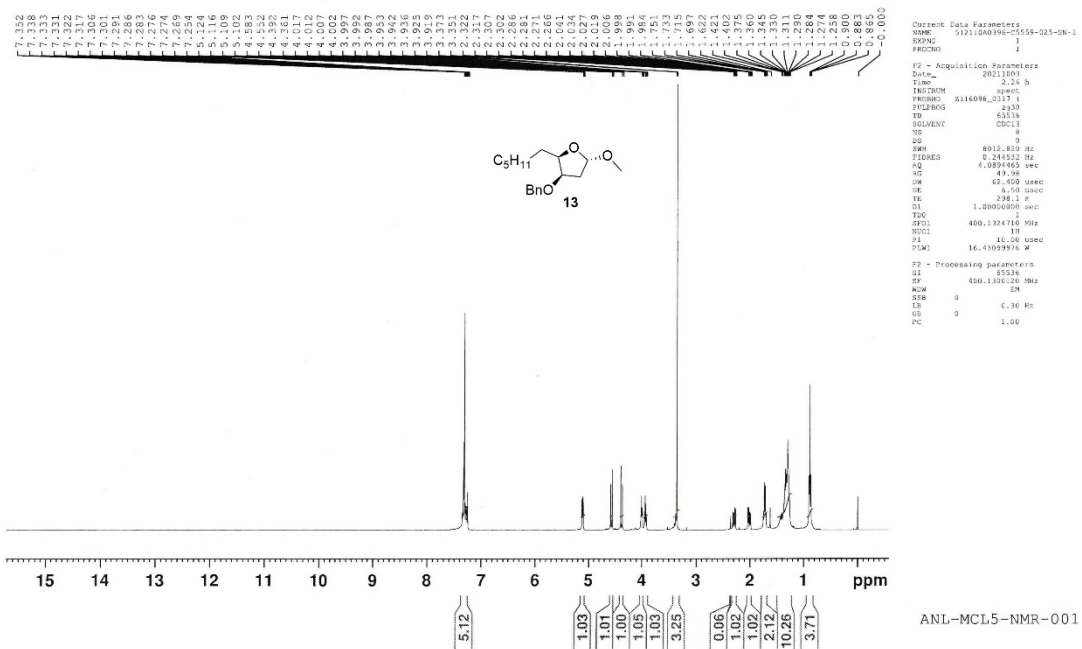
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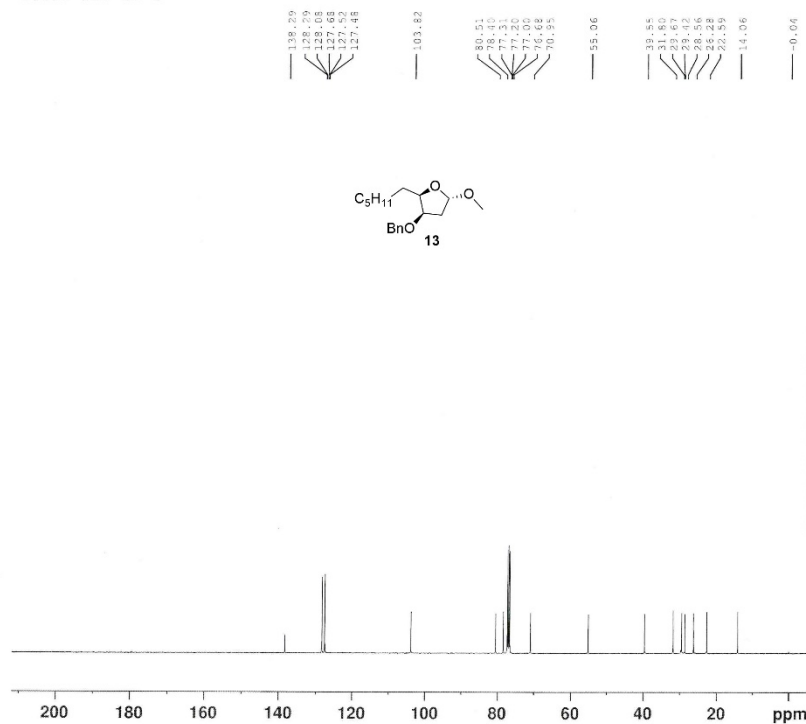
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C5559-025-SN-1



ANL-MCL5-NMR-001

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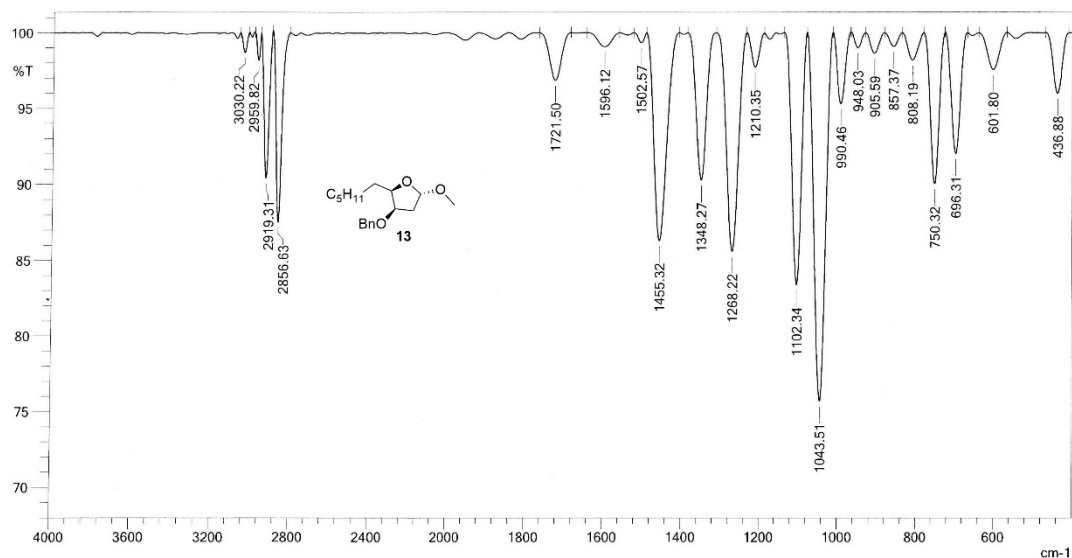
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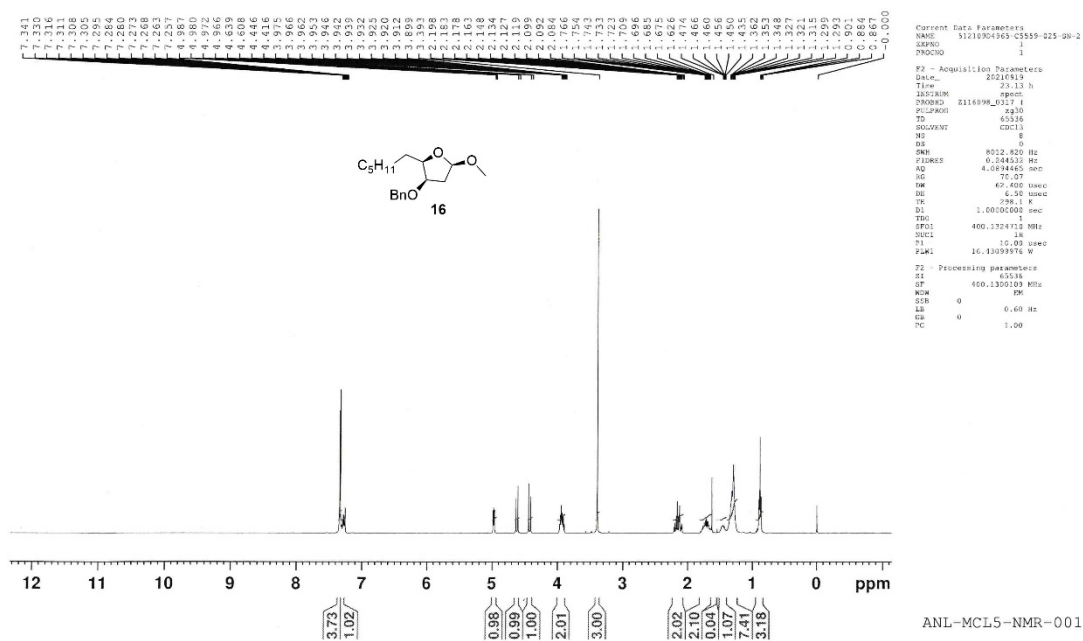
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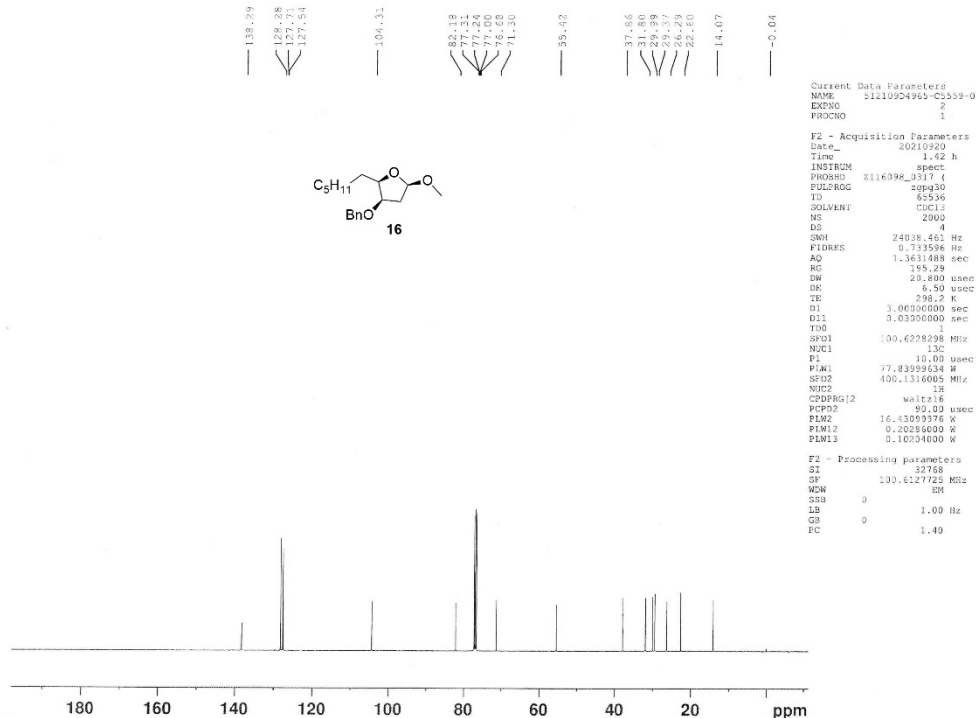
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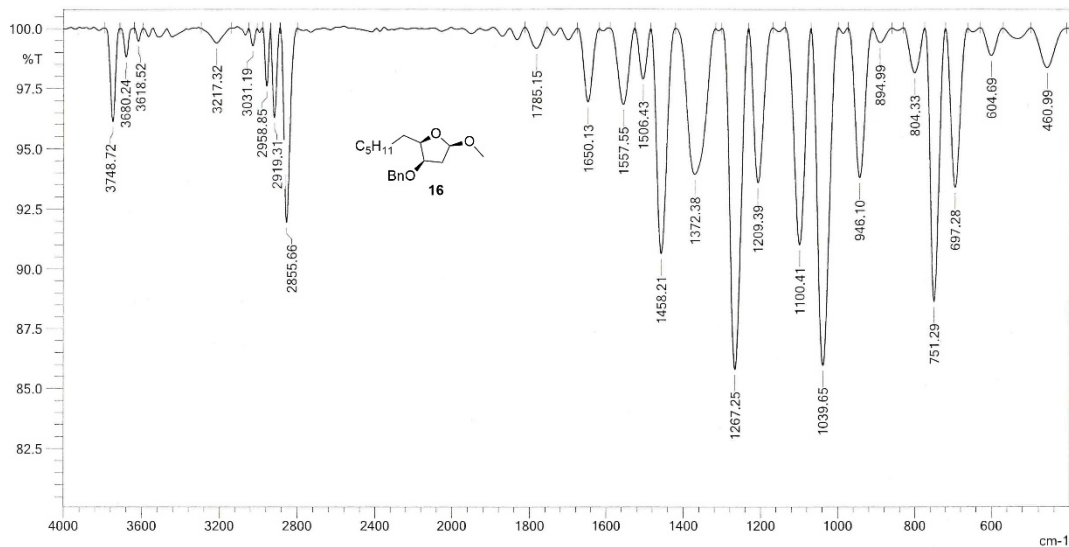
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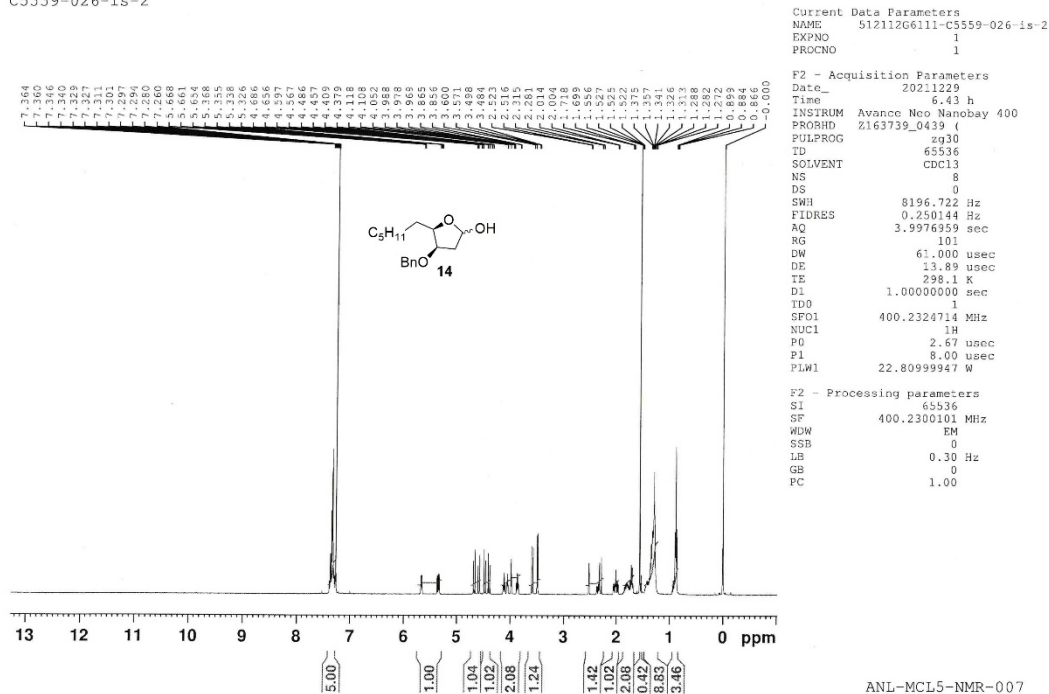
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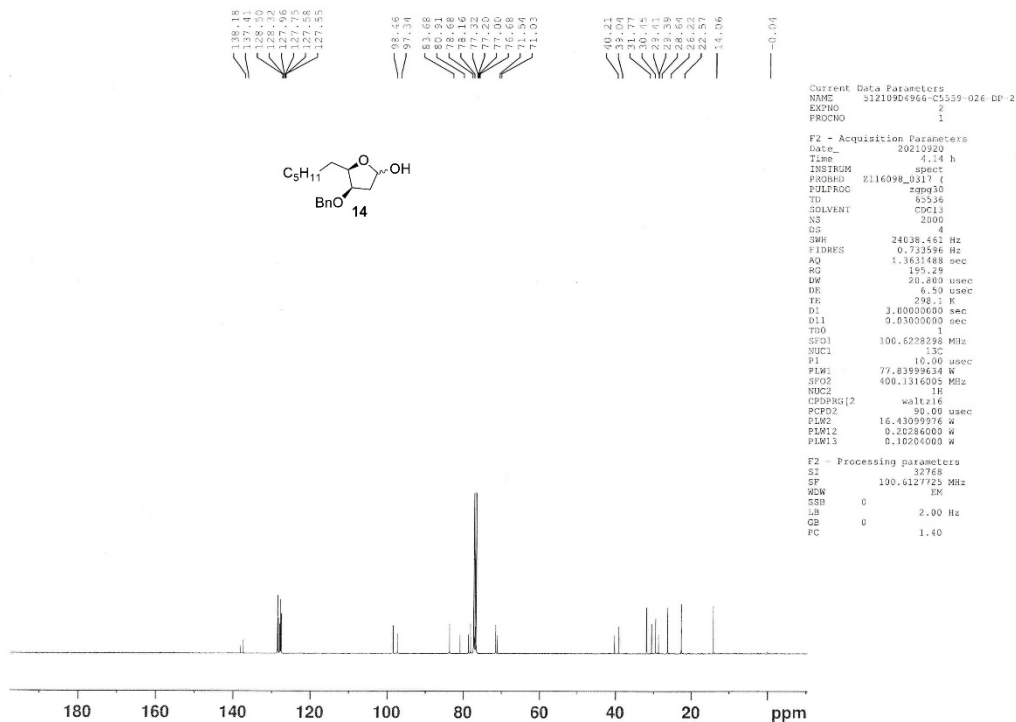
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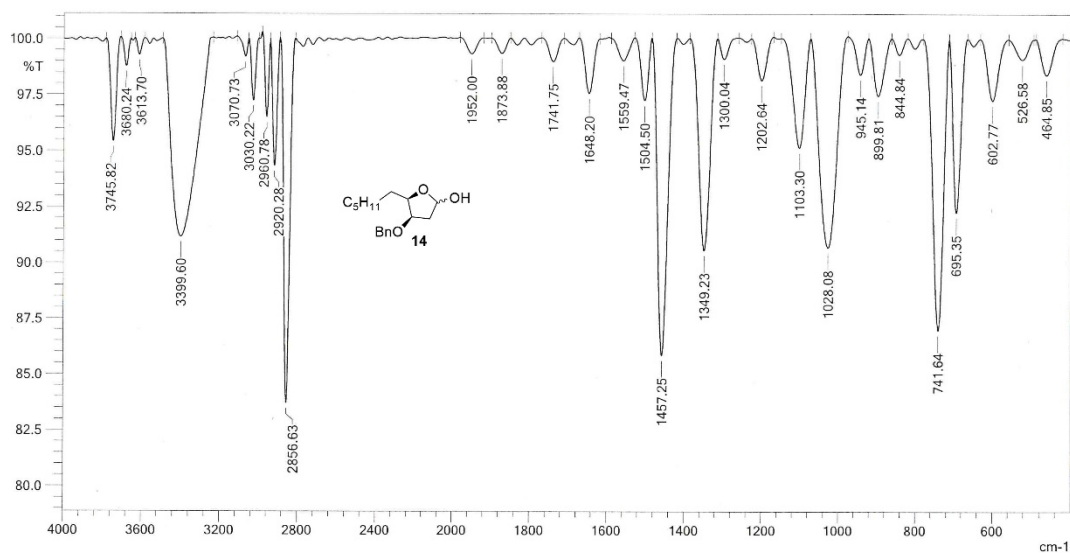
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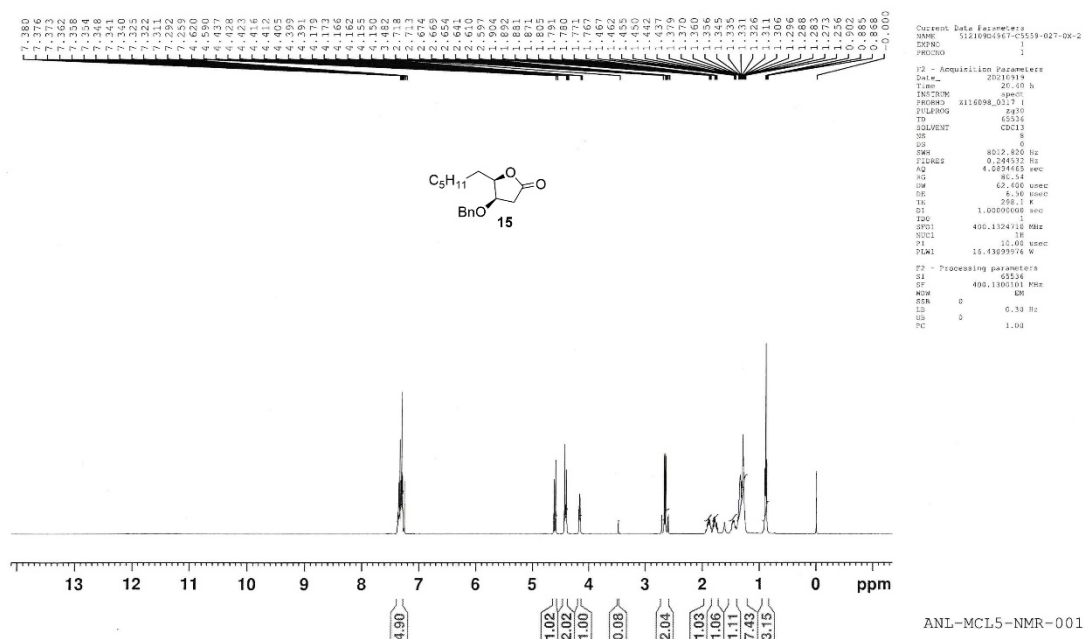
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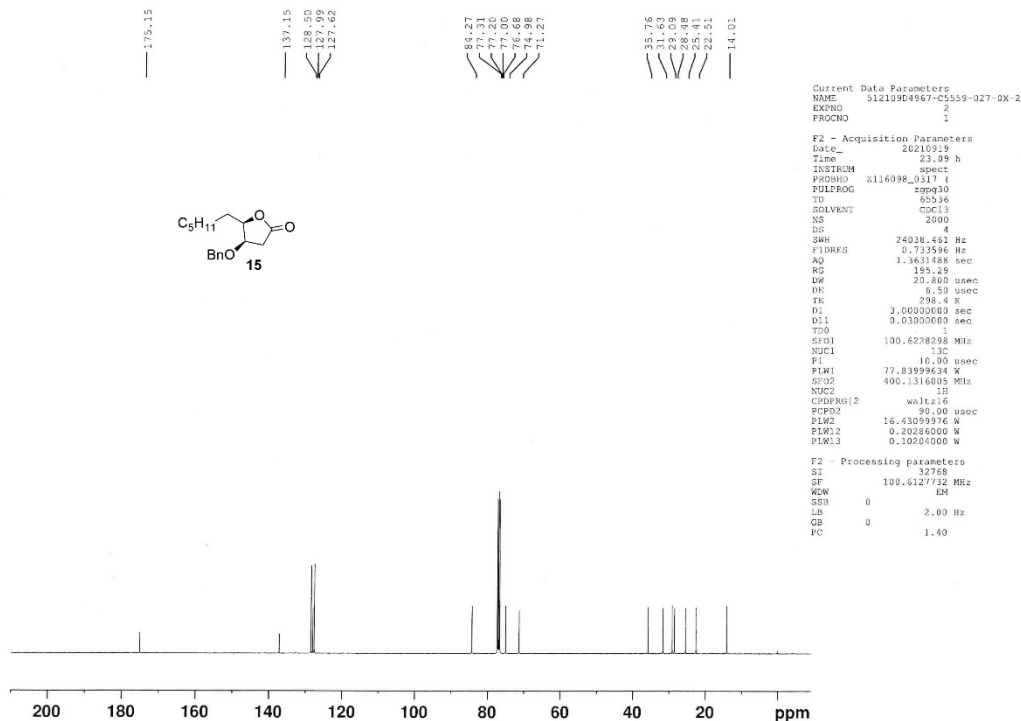
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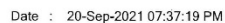
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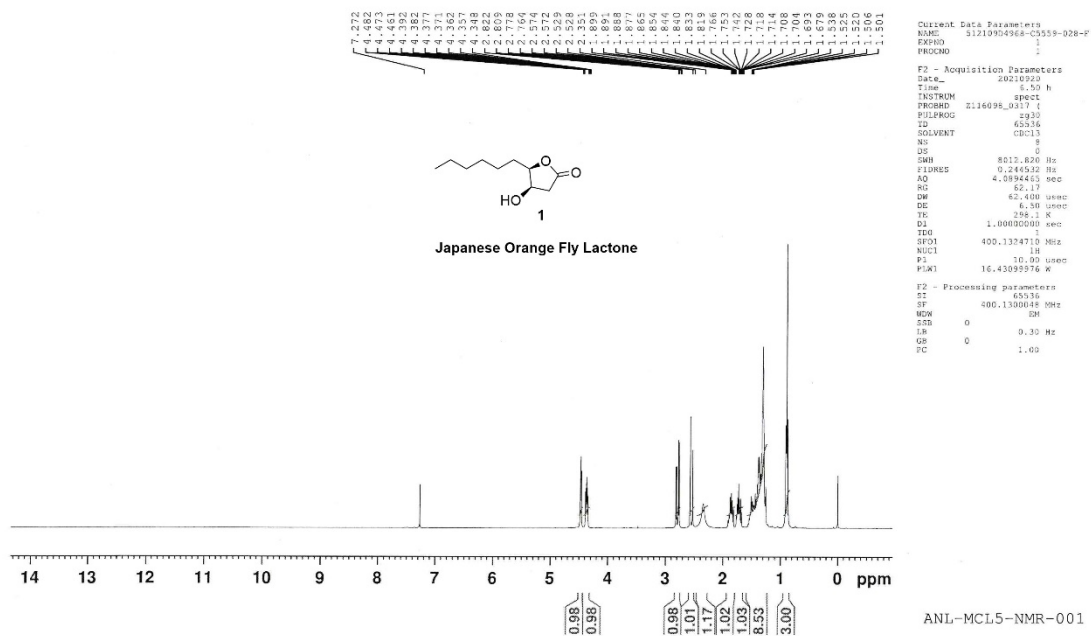
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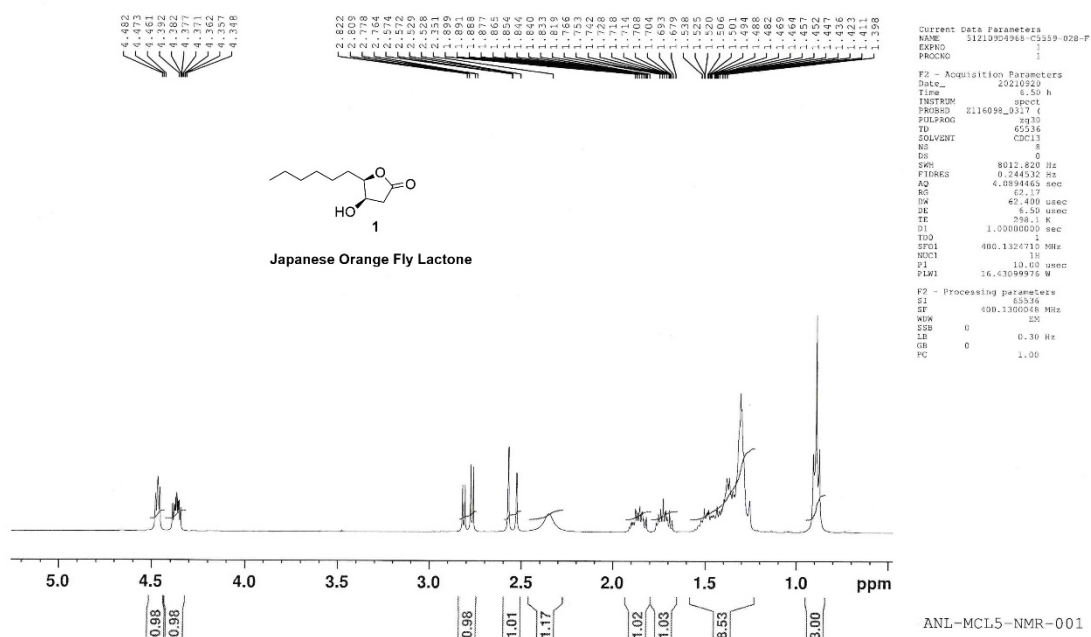


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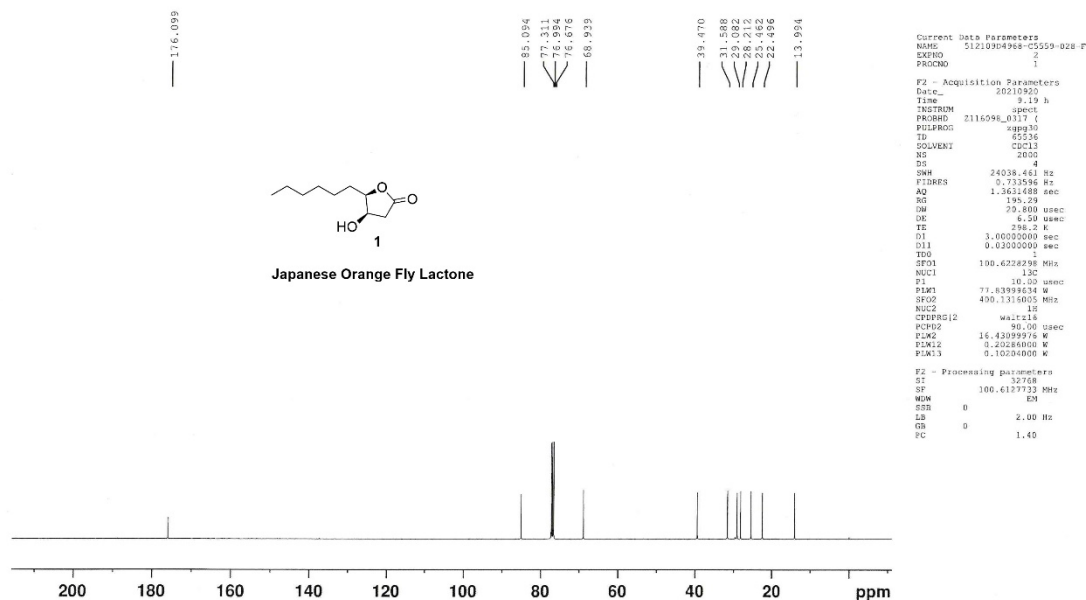
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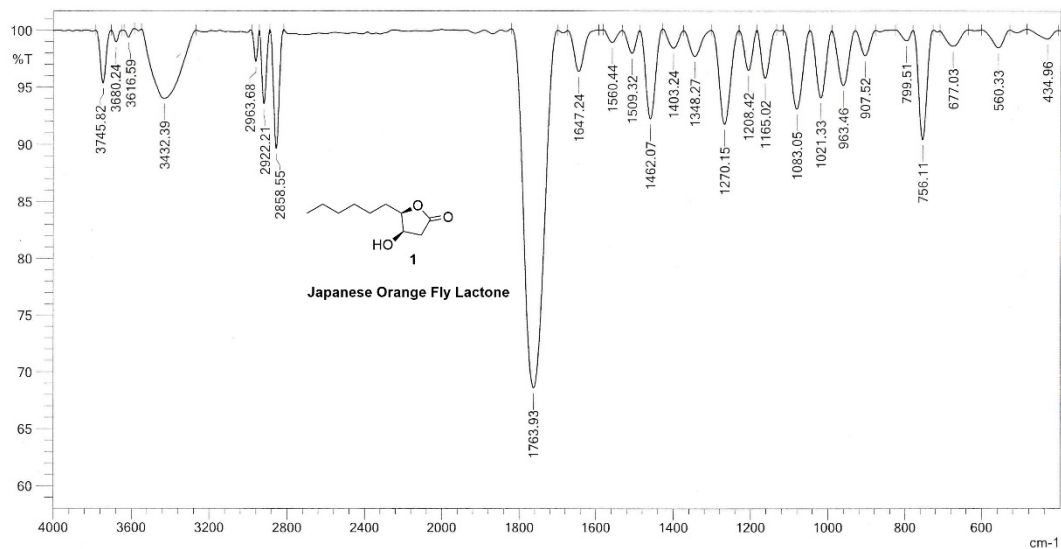


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C5559-028-F





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