Diastereoselective Synthesis of Novel Spiro Indanone Fused Pyrano[3,2-c]Chromene Derivatives following Hetero-Diels-Alder reaction and In Vitro Anticancer Studies

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**Experimental Section**

**General remarks:**

$^1$H NMR spectra were recorded on 400 MHz (100 MHz for $^{13}$C NMR) JEOL NMR spectrometer with CDCl$_3$ as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl$_3$ at 7.26 ppm (for $^1$H NMR) or 77.0 ppm (for $^{13}$C NMR). Melting points are uncorrected and were determined with SMP10 digital melting point apparatus using open capillary tubes. All reagents and solvents used in this study were commercially available (from Sigma-Aldrich) and were used without further purification.
FIGURE 1: Structure of all products
% Transmittance

Wavenumbers (cm⁻¹)

4000 3500 3000 2500 2000 1500 1000 500

3048 2820 2707 1670 1570 1457 1216 996 612 520
8a

8b

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Analysis Info
Analysis Name  D:\Data\SEPT-2016\INN-SP-SLB-CA 1.d
Method         Tune_pos_NAICS-L500A.m
Sample Name    INN-SP-SLB-CA 1
Comment        C18H12O2

Acquisition Parameter
Source Type    ESI
Focus          Active
Scan Begin     50 m/z
Scan End       700 m/z
Ion Polarity   Positive
Ion Capillary  3700 V
Set End Plate  Offset -500 V
Set Collision  Cell RF 900 8 Vpp
Set Nebulizer  0.3 Bar
Set Dry Heater 180 °C
Set Divert Valve Source

Intens x10^4

Meas. m/z # Ion Formula m/z err [ppm] mSigma # Sigma Score rdb e-conf N-Rule
250.0730  1 C16H12NaO2  250.0730  -0.0  26.8  1 100.00 10.5 even ok

261.0652
256.0652
264.1368
262.1216
263.1127
271.1093
268.5882
273.0553
MeO

8c

CHO
**DEPARTMENT OF CHEMISTRY, I.T.T.(B)**

**Analysis Info**
- Analysis Name: D:\Data\SEPT-2016\INN-SP-SLB-CAT.d
- Sample Name: INN-SP-SLB-CAT.7
- Instrument: maXis impact 282001.00081
- Operator: SIG IN
- Acquisition Date: 9/10/2016 9:49:27 PM

**Acquisition Parameter**
- Source Type: ESI
- Focus: Active
- Scan Begin: 50 m/z
- Scan End: 1000 m/z
- Ion Polarity: Positive
- Set Capillary: 3700 V
- Set End Plate Offset: -500 V
- Set Collision Cell RF: 900.0 Vpp
- Set Nebulizer: 0.3 Bar
- Set Dry Heater: 180 °C
- Set Dry Gas: 4.0 l/min
- Set Divert Valve: Source

**Chemical Structures**

1. **8c**
   - Chemical formula: MeO
   - Molecular structure:

2. **8d**
   - Chemical formula: OEt
   - Molecular structure:

**Measured m/z**
- 285.0837: C17H14NaO3
- 285.0830: 0.7

**Chart and Graphs**

- Mass spectrum with peaks at 285.0837 and 286.0709
- 3D chemical structure images of 8c and 8d
Generic Display Report

Analysis Info
Analysis Name: D:\Data\AUG-2016\CSP\31082016_CSP_SDPSNT_01.d
Method: Pos_tune_low m
Sample Name: Bruker micro TOF-Q II
Comment:

Acquisition Date: 8/31/2016 7:39:12 PM
Operator: Amit S. Sahu
Instrument: micrOTOF-Q II

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Diagram:

- TIC +All MS

- MS, 0.1-0.4min #5-21

- MS, 0.1-0.4min #5-21

Bruker Compass DataAnalysis 4.0
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10d

Br-\[\text{CHO}\]

10d

Br-\[\text{CHO}\]
Display Report

Analysis Info
Analysis Name: D:\Data\DEC-2016\NKS\GC\11102017_NKS_GC-PRA-169.d
Method: pos tune_wide.m
Sample Name: ESI-MS
Comment:
Acquistion Date: 10/13/2017 8:26:43 PM
Operator: G.CREDDY
Instrument: microTOF-Q II 10337

Acquisition Parameter
- Source Type: ESI
- Ion Polarity: Positive
- Focus: Not active
- Set Capillary: 4500 V
- Set Ultrasound: 0.4 Bar
- Set End Plate Offset: -500 V
- Set Dry Heater: 180 °C
- Scan Begin: 50 m/z
- Scan End: 3000 m/z
- Set Collision Cell RF: 690.6 Vpp
- Set Divert Valve: Waste
- Mobile Phase: H2O:4.5%
- Flow: 3.5 mL/min

Graphs and spectra showing mass spectrometry data.
Display Report

Analysis Info
Analysis Name: D:\Data\DEC-2016\NKS\GCT1102017_NKS_GC-PRA_165.d
Method: Wash_pos_tune_low_22692017.m
Sample Name: ESI-MS
Comment:

Acquisition Date: 10/12/2017 7:52:56 PM
Operator: Amit S. Sahu
Instrument: microTOF-Q II 10337

Acquisition Parameter
Source Type: ESI
Focus: Active
Ion Polarity: Positive
Set Nebulizer: 0.4 Bar
Set Capillary: 4000 V
Set End Plate Offset: -500 V
Set Dry Heater: 180 °C
Set Collison Cell RF: 200.0 Vpp
Set Divert Valve: Source
Set Dry Gas: 4.0 l/min

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## Display Report

### Analysis Info
- **Analysis Name**: D:\Data\DEC-2016\NKS\GC\11102017\NKS_GC-PRA_73.d
- **Method**: Wash pos tune_low_22092017.m
- **Sample Name**: ESI-MS
- **Operator**: G. CREDDY
- **Instrument**: microTOF-Q II 10337
- **Acquisition Date**: 10/12/2017 8:00:41 PM

### Acquisition Parameter
- **Source Type**: ESI
- **Focus**: Active
- **Scan Begin**: 50 m/z
- **Scan End**: 3000 m/z
- **Ion Polarity**: Positive
- **Set Capillary**: 4000 V
- **Set End Plate Offset**: -500 V
- **Set Collision Cell RF**: 200.0 Vpp
- **Set Dry Gas**: 4.0 l/min
- **Set Nebulizer**: 0.4 Bar
- **Set Dry Heater**: 180 °C
- **Set Diver Valve**: Source

### Chromatogram

The chromatogram shows the elution profiles of various compounds with peaks at different retention times.

### Mass Spectrum

The mass spectrum displays the molecular ion peaks and fragment ions for the compounds of interest.

### Structural Diagram

The structural diagram illustrates the molecular structure of the compound, highlighting key functional groups and substituents (e.g., OMe, 3'b).

### Peaks at m/z

- 188.0865
- 211.0735
- 226.0777
- 288.0770
- 321.1016
- 349.1124
- 371.0652
- 387.0606

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