Arabinose based gelators: Rheological characterization of the gels and phase selective organogelation of crude-oil

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1. **Gelation Tests**

Gelation test were carried out by adding exact weights of compounds **3a-3g** individually to 1 ml of appropriate solvent in a vial. The vial was sealed and suspension was heated to dissolve the compound to get a clear solution. The solution was allowed to cool after which gelation was tested by inverting the sample vial. If the inverted vial was able to hold the system, it was considered as a gel. Apart from **3a** and **3g** the other triazoylarabinoside derivatives **3b, 3c-f** were also tested in the same manner but they were not able to form gels in any solvent.

2. **Determination of Minimum Gelation Concentration (MGC)**

1 ml of solvent was taken in 5 ml of sample vial, 1 mg of gelator **3a** and **3g** was added to the solvent which was then heated till a clear solution was obtained. Then the solution was cooled and the vial inverted to confirm gelation. If partial or no gelation was observed, the cycle was repeated adding 1 mg of **3a** or **3g** at the beginning of each heating cooling cycle till complete gelation of the solvent was observed by inversion of the vial.

3. **Gel characterization**

3.1 **Optical Microscopy**

An optical microscope (Olympus - CH20i) equipped with a digital camera (Nikon - Eclipse E200 MV Pole) for digital imaging was used for analyzing the microstructure of the organogels. The experiments were carried out by placing a small amount of the gel sample at a particular concentration on a 3 inch x 2 inch glass slide and viewing it with the microscope.

3.2 **Field Emission Scanning Electron Micrographs (FESEM)**

The experiments were performed by using a Zeiss supra-55 FESEM. The xerogels of the samples were prepared by dropcasting the hot 1% (w/v) solution of gelator **3a** or **3g** in gelling solvent on a glass slide (2mm x 2mm) and drying them overnight in air inside a vacuum dessicator. The xerogel was then placed on a stub which was then coated with gold by a Quorum -Q150RES sputter coater under vacuum of 5 x 10^{-5} milibar and a current of 20 mA for 2 minutes.

3.4 **Atomic force microscopy (AFM)**

The experiments were performed by using a Bruker Dimension Icon instrument. The samples were prepared by dropcasting a dilute solution of gelator **3a** and **3g** in m-xylene solvent on a
glass slide (2mm x 2mm) and drying them overnight under vacuum inside a dessicator. AFM images of the samples were obtained using Tapping Mode at 1 Hz scanning rate with a silicon cantilever tip (RFESP-MPP-21100-10) at a resonance frequency of 75 kHz and a spring constant of 3 Nm$^{-1}$.

### 3.5 Wide Angle X-ray Diffraction (WXRD)

The xerogels of the sample were prepared by dissolving 3a (100 mg) and 3g (100 mg) in 10 mL of Benzene in a beaker and drying them overnight in a vacuum dessicator. The WXRD diffractogram of the samples were recorded on a ProroAXRD diffractometer. X-rays of wavelength 1.54 Å were used.
**Table S1.** Gelation ability of 3a-g with various solvents.$^a$

<table>
<thead>
<tr>
<th>Compound</th>
<th>Solvent</th>
<th>3a (MGC,$^b$ $T_g$)</th>
<th>3b</th>
<th>3c</th>
<th>3d</th>
<th>3e</th>
<th>3f</th>
<th>3g(MGC,$^b$ $T_g$)</th>
</tr>
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<tr>
<td>Benzene</td>
<td>G, (1.0%, 44-45 °C)</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.7%, 49-50 °C)</td>
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<tr>
<td>Toluene</td>
<td>G, (1.0%, 46-47 °C)</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.5%, 53-54 °C)</td>
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<tr>
<td>α-xylene</td>
<td>G, (0.9%, 47-48 °C)</td>
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<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.5%, 57-58 °C)</td>
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<tr>
<td>m-xylene</td>
<td>G, (0.7%, 48-49 °C)</td>
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<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.5%, 52-53 °C)</td>
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<tr>
<td>p-xylene</td>
<td>G, (0.9%, 46-47 °C)</td>
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<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.5%, 51-52 °C)</td>
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<td>Chlorobenzene</td>
<td>G, (1.0%, 45-46 °C)</td>
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<td>S</td>
<td>S</td>
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<td>S</td>
<td>G, (0.7%, 53-54 °C)</td>
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<td>G, (1.0, 48-49 °C)</td>
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<td>S</td>
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<tr>
<td>Kerosene</td>
<td>G (0.3%, 69-70 °C)</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G (0.3%, 71-72 °C)</td>
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<td>G, (0.3%, 63-64 °C)</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.3%, 61-62 °C)</td>
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<tr>
<td>Diesel</td>
<td>G, (0.3%, 66-67 °C)</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>S</td>
<td>G, (0.3%, 68-69 °C)</td>
<td></td>
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$^a$ G = Gel; S = Solution; I = Insoluble. $^b$ (w/v).
5 Figures and graphs

5.1 Figures of gels at various concentrations

**Figure S1.** Gels from Benzene and 3a at various concentrations of 3a (a) at 1.0% (w/v) (b) at 1.1% (w/v) (c) at 1.2% (w/v) (d) at 1.3% (w/v) (e) at 1.4% (w/v).

**Figure S2.** Gels from toluene and 3a at various concentrations of 3a (a) at 1.0% (w/v) (b) at 1.1% (w/v) (c) at 1.2% (w/v) (d) at 1.3% (w/v) (e) at 1.4% (w/v).
Figure S3. Gels from o-xylene and 3a at various concentrations of 3a (a) at 0.9% (w/v) (b) at 1.0% (w/v) (c) at 1.1% (w/v) (d) at 1.2% (w/v) (e) at 1.3% (w/v).

Figure S4. Gels from m-xylene and 3a at various concentrations of 3a (a) at 0.7% (w/v) (b) at 0.8% (w/v) (c) at 0.9% (w/v) (d) at 1.0% (w/v) (e) at 1.1% (w/v).

Figure S5. Gels from p-xylene and 3a at various concentrations of 3a (a) at 0.9% (w/v) (b) at 1.0% (w/v) (c) at 1.1% (w/v) (d) at 1.2% (w/v) (e) at 1.3% (w/v).

Figure S6. Gels from chlorobenzene and 3a at various concentrations of 3a (a) at 1.0% (w/v) (b) at
1.1% (w/v) (c) at 1.2% (w/v) (d) at 1.3% (w/v) (e) at 1.4% (w/v).

**Figure S7.** Gels from ethanol and 3a at various concentrations of 3a (a) at 1.0% (w/v) (b) at 1.1% (w/v) (c) at 1.2% (w/v) (d) at 1.3% (w/v) (e) at 1.4% (w/v).

**Figure S8.** Gels from petrol and 3a at various concentrations of 3a (a) at 0.3% (w/v) (b) at 0.4% (w/v) (c) at 0.5% (w/v) (d) at 0.6% (w/v) (e) at 0.7% (w/v).

**Figure S9.** Gels from diesel and 3a at various concentrations of 3a (a) at 0.3% (w/v) (b) at 0.4% (w/v) (c)
at 0.5% (w/v) (d) at 0.6% (w/v) (e) at 0.7% (w/v).

**Figure S10.** Gels from Crude oil of 3a at minimum gelation concentrations at 0.5% (w/v). (a) 1 ml Crude oil (b) Crude oil gel

**Figure S11.** Gels from benzene and 3g at various concentrations of 3g (a) at 0.7% (w/v) (b) at 0.8% (w/v) (c) at 0.9% (w/v) (d) at 1.0% (w/v) (e) at 1.1% (w/v).

**Figure S12.** Gels from toluene and 3g at various concentrations of 3g (a) at 0.5% (w/v) (b) at 0.6% (w/v) (c) at 0.7% (w/v) (d) at 0.8% (w/v) (e) at 0.9% (w/v).
Figure S13. Gels from o-xylene and 3g at various concentrations of 3g: (a) at 0.5% (w/v) (b) at 0.6% (w/v) (c) at 0.7% (w/v) (d) at 0.8% (w/v) (e) at 0.9% (w/v).

Figure S14. Gels from m-xylene and 3g at various concentrations of 3g: (a) at 0.5% (w/v) (b) at 0.6% (w/v) (c) at 0.7% (w/v) (d) at 0.8% (w/v) (e) at 0.9% (w/v).

Figure S15. Gels from p-xylene and 3g at various concentrations of 3g: (a) at 0.5% (w/v) (b) at 0.6% (w/v) (c) at 0.7% (w/v) (d) at 0.8% (w/v) (e) at 0.9% (w/v).
Figure S16. Gels from chlorobenzene and 3g at various concentrations of 3g (a) at 0.7% (w/v) (b) at 0.8% (w/v) (c) at 0.9% (w/v) (d) at 1.0% (w/v) (e) at 1.1% (w/v).

Figure S17. Gels from petrol and 3g at various concentrations of 3g (a) at 0.3% (w/v) (b) at 0.4% (w/v) (c) at 0.5% (w/v) (d) at 0.6% (w/v) (e) at 0.7% (w/v).

Figure S18. Gels from diesel and 3g at various concentrations of 3g (a) at 0.3% (w/v) (b) at 0.4% (w/v) (c) at 0.5% (w/v) (d) at 0.6% (w/v) (e) at 0.7% (w/v).
Figure S19. Gelation of crude oil with gelator 3g (a) Crude oil (b) Gelled crude oil.

5.2 Tables for variation of Tg with concentration

Figure S20. Variation of $T_g$ with concentration for organogels of 3a.
5.3 Optical microscopy images

Figure S21. Variation of $T_g$ with concentration for organogels of 3g.

Figure S22. Optical microscopy image for (a) 3a in $m$-xylene at 1% (w/v) (b) 3g in $m$-xylene at 1% (w/v) concentration.
5.4 FESEM micrographs

**Figure S23.** FESEM image of xerogel of 3a at 1% (w/v) concentration in benzene.

**Figure S24.** FESEM image of xerogel of 3a at 1% (w/v) concentration in toluene.

**Figure S25.** FESEM image of xerogel of 3a at 1% (w/v) concentration in o-xylene.
Figure S26. FESEM image of xerogel of 3a at 1% (w/v) concentration in m-xylene

Figure S27. FESEM image of xerogel of 3a at 1% (w/v) concentration in p-xylene

Figure S28. FESEM image of xerogel of 3a at 1% (w/v) concentration in chlorobenzene
**Figure S29.** FESEM image of xerogel of 3a at 1% (w/v) concentration in ethanol

**Figure S30.** FESEM image of xerogel of 3a at 1% (w/v) concentration in petrol

**Figure S31.** FESEM image of xerogel of 3a at 1% (w/v) concentration in diesel
Figure S32. FESEM image of xerogel of 3g at 1% (w/v) concentration in benzene

Figure S33. FESEM image of xerogel of 3g at 1% (w/v) concentration in toluene

Figure S34. FESEM image of xerogel of 3g at 1% (w/v) concentration in o-xylene
Figure S35. FESEM image of xerogel of 3g at 1% (w/v) concentration in m-xylene

Figure S36. FESEM image of xerogel of 3g at 1% (w/v) concentration in p-xylene

Figure S37. FESEM image of xerogel of 3g at 1% (w/v) concentration chlorobenzene
Figure S38. FESEM image of xerogel of 3g at 1% (w/v) concentration petrol

Figure S39. FESEM image of xerogel of 3g at 1% (w/v) concentration diesel

5.5 AFM images

Figure S40. AFM image of 3a in m-xylene (a) 2-D image (b) 3-D image
**Figure S41.** AFM image of 3g in *m*-xylene (a) 2-D image (b) 3-D image

### 5.6 Rheology

**Figure S42.** (a) DSS curve of 3a gel with benzene at 1% (w/v) at frequency 1 Hz and temperature 25 °C  
(b) DFS curve of 3a gel with benzene at 1% (w/v) at strain 0.001% and temperature 25 °C  
(c) DTS curve of 3a gel with benzene at 1% (w/v) at frequency 1 Hz and temperature 25°C.

**Figure S43.** (a) DSS curve of 3a gel with toluene at 1% (w/v) at frequency 1 Hz and temperature 25 °C  
(b) DFS curve of 3a gel with toluene at 1% (w/v) at strain 0.001% and temperature 25 °C  
(c) DTS curve of 3a gel with toluene at 1% (w/v) at frequency 1 Hz and temperature 25°C.
Figure S44. (a) DSS curve of 3a gel with o-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with o-xylene at 1% (w/v) at strain 0.001% and temperature 25 °C (c) DTS curve of 3a gel with o-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C.

Figure S45. (a) DSS curve of 3a gel with m-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with m-xylene at 1% (w/v) at strain 0.002% and temperature 25 °C (c) DTS curve of 3a gel with m-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C.

Figure S46. (a) DSS curve of 3a gel with p-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with p-xylene at 1% (w/v) at strain 0.001% and temperature 25 °C (c) DTS curve of 3a gel with p-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C.
Figure S47. (a) DSS curve of 3a gel with Chloro-benzene at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with Chloro-benzene at 1% (w/v) at strain 0.001% and temperature 25 °C (c) DTS curve of 3a gel with Chloro-benzene at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S48. (a) DSS curve of 3a gel with Ethanol at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with Ethanol at 1% (w/v) at strain 0.003% and temperature 25 °C (c) DTS curve of 3a gel with Ethanol at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S49. (a) DSS curve of 3a gel with Petrol at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with Petrol at 1% (w/v) at strain 0.002% and temperature 25 °C (c) DTS curve of 3a gel with Petrol at 1% (w/v) at frequency 1 Hz and temperature 25°C.
Figure S50. (a) DSS curve of 3a gel with Diesel at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with Diesel at 1% (w/v) at strain 0.002% and temperature 25 °C (c) DTS curve of 3a gel with Diesel at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S51. (a) DSS curve of 3a gel with Crude oil at 2% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3a gel with Crude oil at 1% (w/v) at strain 0.002% and temperature 25 °C (c) DTS curve of 3a gel with Crude oil at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S52. (a) DSS curve of 3g gel with benzene at 1% (w/v) at frequency 1 Hz and temperature 25 °C (b) DFS curve of 3g gel with benzene at 1% (w/v) at strain 0.001% and temperature 25 °C (c) DTS curve of 3g gel with benzene at 1% (w/v) at frequency 1 Hz and temperature 25°C.
Figure S53. (a) DSS curve of 3g gel with toluene at 1% (w/v) at frequency 1 Hz and temperature 25 °C. (b) DFS curve of 3g gel with toluene at 1% (w/v) at strain 0.001% and temperature 25 °C. (c) DTS curve of 3g gel with toluene at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S54. (a) DSS curve of 3g gel with o-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C. (b) DFS curve of 3g gel with o-xylene at 1% (w/v) at strain 0.002% and temperature 25 °C. (c) DTS curve of 3g gel with o-xylene at 1% (w/v) at frequency 1 Hz and temperature 25°C.

Figure S55. (a) DSS curve of 3g gel with m-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 °C. (b) DFS curve of 3g gel with m-xylene at 1% (w/v) at strain 0.001% and temperature 25 °C. (c) DTS curve of 3g gel with m-xylene at 1% (w/v) at frequency 1 Hz and temperature 25°C.
Figure S56. (a) DSS curve of 3g gel with p-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 ºC (b) DFS curve of 3g gel with p-xylene at 1% (w/v) at strain 0.001% and temperature 25 ºC (c) DTS curve of 3g gel with p-xylene at 1% (w/v) at frequency 1 Hz and temperature 25 ºC.

Figure S57. (a) DSS curve of 3g gel with chlorobenzene at 1% (w/v) at frequency 1 Hz and temperature 25 ºC (b) DFS curve of 3g gel with chlorobenzene at 1% (w/v) at strain 0.001% and temperature 25 ºC (c) DTS curve of 3g gel with chlorobenzene at 1% (w/v) at frequency 1 Hz and temperature 25 ºC.

Figure S58. (a) DSS curve of 3g gel with petrol at 1% (w/v) at frequency 1 Hz and temperature 25 ºC (b) DFS curve of 3g gel with petrol at 1% (w/v) at strain 0.001% and temperature 25 ºC (c) DTS curve of 3g gel with petrol at 1% (w/v) at frequency 1 Hz and temperature 25 ºC.
Figure S59. (a) DSS curve of 3g gel with diesel at 1% (w/v) at frequency 1 Hz and temperature 25 °C. (b) DFS curve of 3g gel with diesel at 1% (w/v) at strain 0.002% and temperature 25 °C. (c) DTS curve of 3g gel with diesel at 1% (w/v) at frequency 1 Hz and temperature 25 °C.

Figure S60. (a) DSS curve of 3g gel with crude oil at 1% (w/v) at frequency 1 Hz and temperature 25 °C. (b) DFS curve of 3g gel with crude oil at 1% (w/v) at strain 0.001% and temperature 25 °C. (c) DTS curve of 3g gel with crude oil at 1% (w/v) at frequency 1 Hz and temperature 25 °C.

Figure S61. Curves for thixotropic experiment for the meta-xylene gel at 1% (w/v) concentration for (a) 3a and (b) 3g.
5.7 PSOG of petrol, diesel and crude-oil

Figure S62. PSOG of petrol and recovery of congealed petrol using gelator 3a. (a) Water (b) Biphasic mixture of petrol and water (c) congealed petrol layer (d) separated congealed petrol layer (e) transfer of congealed petrol into a flask (f) residual water after removal of congealed petrol (g) distillation set-up for recovery of petrol (h) petrol distillate (i) residual organogelator.
Figure S63. Phase selective gelation of diesel using 3a in diesel (a) 4 ml of water. (b) Biphasic mixture of water and diesel (c) Congealed diesel layer (d) separated congealed diesel layer (e) transfer of congealed diesel gel into a flask (f) residue water after removal of congealed diesel (g) distillation set-up for recovery of diesel (h) diesel distillate (i) residual organogelator.
Figure S64. Phase selective gelation of petrol using $3g$ in petrol (a) 4 ml of water. (b) Biphasic mixture of water and diesel (c) Congealed petrol layer (d) separated congealed petrol layer (e) transfer of congealed petrol gel into a flask (f) residue water after removal of congealed petrol (g) distillation set-up for recovery of petrol (h) petrol distillate (i) residual organogelator.
Figure S6. Phase selective gelation of diesel using 3g in diesel (a) 4 ml of water. (b) Biphasic mixture of water and diesel. (c) Congealed diesel layer (d) separated congealed diesel layer (e) transfer of congealed diesel gel into a dish. (f) residue water after removal of congealed diesel (g) distillation set-up for recovery of diesel. (h) diesel distillate (i) residual organogelator.
Figure S66. Phase selective gelation of crude oil using 3g (a) Water (b) Biphasic mixture of water and crude-oil (c) congealed crude-oil layer after addition of gelator (d) floating congealed crude-oil layer (e) removed congealed crude-oil (f) residual water
6 Spectra of 3a-3g

Figure S67. $^1$H NMR spectra of 3a in CDCl$_3$. 
Figure S68. $^{13}$C NMR spectra of 3a in CDCl$_3$. 

3a
Figure S69. $^1$H NMR spectra of 3b in CDCl$_3$. 
Figure S70. $^{13}$C NMR spectra of 3b in CDCl$_3$. 
Figure S71. $^1$H NMR spectra of 3c in CDCl$_3$. 

(3c)
Figure S7. $^{13}$C NMR spectra of 3c in CDCl$_3$. 
Figure S73. $^1$H NMR spectra of 3d in CDCl$_3$. 
Figure S7. $^{13}$C NMR spectra of 3d in CDCl$_3$. 
Figure S7. $^1$H NMR spectra of 3e in CDCl$_3$. 

![Figure S7](image-url)
Figure S7. $^{13}$C NMR spectra of 3e in CDCl$_3$. 
Figure S7. $^1$H NMR spectra of 3f in CDCl$_3$. 
Figure S78. $^{13}$C NMR spectra of 3f in CDCl$_3$. 
Figure S79. $^1$H NMR spectra of 3g in CDCl$_3$. 
Figure S80. $^{13}$C NMR spectra of 3g in CDCl$_3$. 