Supplementary Material

$^1$H, $^{13}$C NMR, & HRMS Spectra of Representative Compounds

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Spectras of representative compounds

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Table 1: R SQUARED VALUES
**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

**Elements Used:**

C: 18-18  H: 0-300  N: 0-4  O: 1-1

**Sample Name:** 280921_AK-1

**Test Name:** 280921_AK-1 20 (0.435)

**Mass**  | **Calc. Mass**  | **mDa**  | **PPM**  | **DBE**  | **i-FIT**  | **Norm**  | **Conf(%)**  | **Formula**
--- | --- | --- | --- | --- | --- | --- | --- | ---
292.1458 | 292.1450 | 0.8 | 2.7 | 11.5 | 1712.7 | n/a | n/a | C18 H18 N3 O

**Mass Spectrum**

![Mass Spectrum](image)

**Structural Diagram**

![Structural Diagram](image)

**Element:** AK.1
Figure 1. Spectra of compound AK-1
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 19-19 H: 0-300 N: 0-4 O: 1-1 S: 0-1
Sample Name : 280921_AK-2
Test Name
280921_AK-2 21 (0.450)

Minimum: 2.0
Maximum: 300.0 50.0

Mass Calc. Mass mDa FPP DBE i-FIT Norm Conf(%) Formula
338.1333 338.1327 0.6 1.8 11.5 1621.8 n/a n/a C19 H20 N3 O 6

I TRPR
XEVO G2-X3 QTOF

1: TOF MS ES+
2.52e+007

Phytophler 2019-19-18
AK-79
PROTON OCD (C2[3karotopSpin3.2]c) cfl 5

AK.2
Figure 2. Spectras of compound AK-2
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 0 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 18-18 H: 0-300 N: 0-4 O: 1-1 F: 6-6

Sample Name : 280921_AK-3
Test Name : 280921_AK-3 23 (0.497)

[((([O][N])][N])][N]

AK.3
Figure 3. Spectra of compound AK-3
Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass

Elements Used:
C: 20-20 H: 0-300 N: 0-4 O: 1-1

Sample Name: 280921_AK-4
Test Name: 280921_AK-4 22 (0.480)

<table>
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<th>Calc. Mass</th>
<th>mDa</th>
<th>FFM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
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<td>331.1566</td>
<td>331.1559</td>
<td>0.7</td>
<td>2.1</td>
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<td>1853.0</td>
<td>n/a</td>
<td>n/a</td>
<td>C20 H19 N4 O</td>
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Date: 05-2019
AK 72
Figure 4. Spectra of compound AK-4
Figure 5. Spectrums of compound AK-5

<table>
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<th>nDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
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<tbody>
<tr>
<td>308.1405</td>
<td>308.1399</td>
<td>0.6</td>
<td>1.9</td>
<td>11.5</td>
<td>1936.7</td>
<td>n/a</td>
<td>n/a</td>
<td>C18 H18 N3 O2</td>
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</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 19-19 H: 0-300 N: 4-4 O: 0-2
Sample Name: 280021 AK-6
Test Name: 280021 AK-6 32 (0.684)

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<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
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<td>317.1409</td>
<td>317.1402</td>
<td>0.7</td>
<td>2.2</td>
<td>13.5</td>
<td>1843.6</td>
<td>n/a</td>
<td>n/a</td>
<td>C19 H17 N4 O</td>
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</table>

| x-axis | 11.6 | 10.5 | 9.4 | 8.3 | 7.2 | 6.1 | 5.0 | 3.9 | 2.8 | 1.7 | 0.6 |
| y-axis | -20000 | -18000 | -16000 | -14000 | -12000 | -10000 | -8000 | -6000 | -4000 | -2000 | 0 |

AK.6
Figure 6. Spectra of compound AK-6
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM  /  DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 21-21  H: 0-300  N: 0-4  O: 0-4
Simple Name    : 280921_AK-T
Test Name      : 280921_AK-T 27 (0.67b)

Minimum:     2.0
Maximum:     300.0

Mass   Calc. Mass mDa PPM   DBE   i-FIT  Nerr  Conf(%) Formula
382.1770  382.1767  0.3  0.8  11.5  1420.1  n/a  C21 H24 N3 O4

AK.7

1H NMR (CDCl3) [δ ppm]: 6.21 - 7.67
Figure 7. Spectras of compound AK-7
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass. Even Electron Ions
15 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 19-19  H: 0-300  N: 0-4  O: 0-2
Sample Name : 280521_AK-8
Test Name : 280521_AK-8 29 (0.622)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass Da</th>
<th>FFM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
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<tbody>
<tr>
<td>322.1561</td>
<td>322.1556</td>
<td>0.5</td>
<td>1.6</td>
<td>11.5</td>
<td>n/a</td>
<td>n/a</td>
<td>C19 H20 N3 O2</td>
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</table>

Mass: 322.1561, Calc. Mass: 322.1556, FFM: 0.5, DBE: 1.6, i-FIT: 11.5, Norm: n/a, Conf(%): n/a, Formula: C19 H20 N3 O2

AK.8

PROTON COCO (C)/Bruker/Topspin 3.2) 6/3
Figure 8. Spectra of compound AK-8
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 0 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-20  H: 0-300  N: 0-4  O: 0-2

Sample Name: 289021_AK-9  Test Name: 289021_AK-9 13 (0.294)

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula
424.1601 ---

April 05, 2019
AK-71
Figure 9. Spectra of compound AK-9
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-21  H: 0-300  N: 0-4  O: 0-2
Sample Name : 280921_AK-10
Test Name
280921_AK-10 20 (0.435)

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<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
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<td>1567.9</td>
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<td>7.60</td>
<td>C21 H14 N3</td>
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<tr>
<td>308.1515</td>
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<td>-79.5</td>
<td>10.5</td>
<td>1566.7</td>
<td>1.401</td>
<td>24.85</td>
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<tr>
<td>308.0824</td>
<td>58.5</td>
<td>199.8</td>
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<td>24.00</td>
<td>C20 H10 N3 O</td>
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<td>308.2014</td>
<td>-60.5</td>
<td>-196.3</td>
<td>9.5</td>
<td>1567.6</td>
<td>2.309</td>
<td>9.04</td>
<td>C21 H26 N O</td>
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<tr>
<td>308.0712</td>
<td>69.7</td>
<td>226.2</td>
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<td>1568.1</td>
<td>2.629</td>
<td>9.91</td>
<td>C21 H10 N O2</td>
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AK.10

![Chemical Structure Diagram]
Figure 10. Spectra of compound AK-10
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (all results up to 1000 for each mass)
Elements Used:
C: 18-18 H: 0-300 N: 0-4 O: 0-1 Cl: 0-1 F: 0-1

Sample Name: 280921_AK-11
Test Name: 280921_AK-11 22 (0.480)
IITPR

XEVO G2- XS QTOF
1: TOF MS ES+ 1.33e+007

Minimum: 1.5
Maximum: 2.0 300.0 50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf (%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>344.0972</td>
<td>344.0966</td>
<td>0.6</td>
<td>1.7</td>
<td>11.5</td>
<td>1547.3</td>
<td>n/a</td>
<td>n/a</td>
<td>C18 H16 N3 O Cl F</td>
</tr>
</tbody>
</table>

April 05, 2019
AK 93
Figure 11. Spectra of compound AK-11
Elemental Composition Report

Single Mass Analysis
Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 19-19  H: 0-300  N: 0-4  O: 0-1

Sample Name : 280321_AK-12
Test Name : 280321_AK-12 22 (0.480)

Minimum: -1.5
Maximum: 2.0  300.0  50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
306.1614  306.1606  0.8  2.6  11.5  1385.2  n/a  n/a  C19 H20 N3 O
Figure 12. Spectras of compound AK-12
Figure 13. Spectras of compound AK-13
DOCKING

CDK-4- PDB-ID: - 2W96
Coordinates for 2W96 binding site: x = -3.12, y = -3.92, z = 85.1
No docking poses were generated.

BAX- PDB-ID: - 4S0O
Coordinates for 2W96 binding site: x = 11.89, y = 7.0, z = 31.62

<table>
<thead>
<tr>
<th>Sr. No.</th>
<th>Compound</th>
<th>Docking score</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>AK-10</td>
<td>-2.380</td>
</tr>
<tr>
<td>2</td>
<td>AK-3</td>
<td>-1.207</td>
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</tbody>
</table>

Figure 14: Docking pose of AK-3 (A) and AK-10 (B) with BAX- PDB-ID: 4S0O

BCL-XL- PDB-ID: - 6VWC
Coordinates for 2W96 binding site: x = 1.78, y = -4.03, z = 10.8

<table>
<thead>
<tr>
<th>Sr. No.</th>
<th>Compound</th>
<th>Docking score</th>
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<tbody>
<tr>
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<td>AK-3</td>
<td>-7.042</td>
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<tr>
<td>2</td>
<td>AK-10</td>
<td>-6.965</td>
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</tbody>
</table>
Figure 15: Docking pose of AK-3 (A) and AK-10 (B) with BCL-XL - PDB-ID: 6VWC

Table 1: R SQUARED VALUES

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<tr>
<th>Compound</th>
<th>R²</th>
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<td></td>
<td>A549</td>
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<tr>
<td>AK-1</td>
<td>0.9797</td>
</tr>
<tr>
<td>AK-2</td>
<td>1</td>
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<td>AK-3</td>
<td>0.8641</td>
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<td>AK-4</td>
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