*pharmaceuticals*

*Supplementary Materials*

# Identification of a Novel Neuropeptide S Receptor Antagonist Scaffold based on the SHA-68 Core

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**Figure S1.** Compound 3 $^{13}$C-NMR.

**Figure S2.** Compound 3 $^{1}$H-NMR.

**Figure S3.** Compound 2.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-200 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 108 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 8:39:12 PM EST | | |
| Date Processed: | 4/28/2021 2:55:37 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.629 | 19158280 | 100.00 | 3053227 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
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3:05:53 PM America/New_York

**Figure S4.** Compound 3.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-213 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 113 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 11:14:01 PM EST | | |
| Date Processed: | 4/28/2021 2:56:12 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.798 | 14195603 | 100.00 | 2541804 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
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3:06:46 PM America/New_York

**Figure S5.** Compound 4.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-211 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 112 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 10:43:01 PM EST | | |
| Date Processed: | 4/30/2021 4:09:06 PM EST | | |



Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 16.424 | 16777452 | 100.00 | 2641378 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
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4:11:23 PM America/New_York

**Figure S6.** Compound 5.

Empower2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-214 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039214210505 |
| Vial: | 1 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 20.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 5/5/2021 12:48:10 PM EST | | |
| Date Processed: | 5/5/2021 3:36:31 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.895 | 2183496 | 100.00 | 388062 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-05
Date Printed:
5/5/2021
3:36:47 PM America/New_York

**Figure S7.** Compound 6.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-212 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039212210429 |
| Vial: | 46 | Acq. Method Set: | |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 20.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/29/2021 12:01:26 PM EST | | |
| Date Processed: | 4/29/2021 2:20:42 PM EST | | |



Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 3.212 | 8080850 | 100.00 | 704970 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChemMedChem2021-04
Date Printed:
4/30/2021
3:59:59 PM America/New_York

**Figure S8.** Compound 7.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-202 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 109 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 9:10:08 PM EST | | |
| Date Processed: | 4/28/2021 2:55:54 PM EST | | |

**Auto-Scaled Chromatogram**

**Peak Results**

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 13.329 | 676802 | 2.91 | 170590 |
| 2 | 15.742 | 22542429 | 97.09 | 3145532 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:06:18 PM America/New_York

**Figure S9.** Compound 8.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-220 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 114 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 11:44:59 PM EST | | |
| Date Processed: | 4/28/2021 2:56:31 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.477 | 28411387 | 100.00 | 3566894 |

| | |
|---|---|
| Reported by User: walkup | Project Name: MedChem\MedChem2021-04 |
| Report Method: WalkUpReport | Date Printed: |
| Report Method ID: 1018 | 4/28/2021 |
| Page: 1 of 1 | 3:07:15 PM America/New_York |

**Figure S10.** Compound 9.

**Figure S11.** Compound 10.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-233 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 11 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 3:22:05 AM EST | | |
| Date Processed: | 4/28/2021 2:48:39 PM EST | | |



Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.333 | 24465020 | 100.00 | 3042853 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:01:09 PM America/New_York

**Figure S12.** Compound 11.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-224 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 116 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 12:46:53 AM EST | | |
| Date Processed: | 4/24/2021 1:17:06 AM EST | | |

**Auto-Scaled Chromatogram**

**Peak Results**

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 16.049 | 19125876 | 100.00 | 2934973 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
2:41:04 PM America/New_York

**Figure S13.** Compound 12

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-225 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 117 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 1:17:51 AM EST | | |
| Date Processed: | 4/24/2021 1:48:03 AM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.657 | 15401149 | 100.00 | 2888391 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
2:43:46 PM America/New_York

**Figure S14.** Compound 13.

**Figure S15.** Compound 15.

**Figure S16.** Compound 16.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-270 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 106 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 7:37:19 PM EST | | |
| Date Processed: | 4/30/2021 4:11:05 PM EST | | |

**Auto-Scaled Chromatogram**

**Peak Results**

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 16.065 | 15509369 | 100.00 | 2661710 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed: 4/30/2021
4:12:49 PM America/New_York

**Figure S17.** Compound 17.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-231 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 120 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 2:50:49 AM EST | | |
| Date Processed: | 4/28/2021 2:47:59 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 9.468 | 231154 | 1.69 | 56390 |
| 2 | 11.953 | 12998008 | 94.85 | 1868951 |
| 3 | 12.433 | 125353 | 0.91 | -33885 |
| 4 | 12.722 | 349655 | 2.55 | 83931 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:00:30 PM America/New_York

**Figure S18.** Compound 18.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-240 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 14 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 4:54:59 AM EST | | |
| Date Processed: | 4/28/2021 3:02:59 PM EST | | |



Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 12.933 | 17573821 | 100.00 | 3040557 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:08:12 PM America/New_York

**Figure S19.** Compound 19.

Empower2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R0609-241 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | rajwanaR0609241210423 |
| Vial: | 60 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 10:14:06 AM EST | | |
| Date Processed: | 4/23/2021 10:44:19 AM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 14.025 | 463010 | 3.03 | 104944 |
| 2 | 14.206 | 14834915 | 96.97 | 2835618 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/23/2021
10:55:50 AM America/New_York

**Figure S20.** Compound 20.

**Figure S21.** Compound 21.

Empower2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-244 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039 |
| Vial: | 46 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 280.0nm-4.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 280.0 nm at 4.0 |
| Date Acquired: | 4/29/2021 3:52:00 PM EST | | |
| Date Processed: | 4/29/2021 4:22:12 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 16.363 | 5678716 | 100.00 | 1113265 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/30/2021
4:00:54 PM America/New_York

**Figure S22.** Compound 22.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-262 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 102 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 280.0nm-4.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 280.0 nm at 4.0 |
| Date Acquired: | 4/23/2021 5:33:29 PM EST | | |
| Date Processed: | 4/23/2021 6:03:42 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 17.208 | 6614813 | 100.00 | 1245134 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed: 4/28/2021
2:25:14 PM America/New_York

**Figure S23.** Compound 23.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-268 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 104 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 280.0nm-4.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 280.0 nm at 4.0 |
| Date Acquired: | 4/23/2021 6:35:23 PM EST | | |
| Date Processed: | 4/28/2021 2:28:11 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 18.024 | 417386 | 100.00 | 79381 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
2:53:25 PM America/New_York

**Figure S24.** Compound 24.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-242 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 97 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 2:58:40 PM EST | | |
| Date Processed: | 4/28/2021 2:55:20 PM EST | | |



Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 16.846 | 20121130 | 100.00 | 2986796 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed: 4/28/2021
3:05:24 PM America/New_York

**Figure S25.** Compound 25.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-238 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 13 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 4:23:59 AM EST | | |
| Date Processed: | 4/28/2021 2:49:58 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 15.317 | 1320549 | 7.46 | 144081 |
| 2 | 15.878 | 16391937 | 92.54 | 2747838 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:02:27 PM America/New_York

**Figure S26.** Compound 26.

Empower 2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-267 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 103 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/23/2021 6:04:29 PM EST | | |
| Date Processed: | 5/5/2021 3:41:52 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 13.427 | 10732925 | 96.91 | 1436939 |
| 2 | 14.031 | 342438 | 3.09 | 60009 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID:1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
5/5/2021
3:42:08 PM America/New_York

**Figure S27.** Compound 27.

Empower2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-237 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039210423 |
| Vial: | 12 | Acq. Method Set: | MethodSetAB5T95B15Min |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 10.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/24/2021 3:53:01 AM EST | | |
| Date Processed: | 4/28/2021 2:49:21 PM EST | | |

Auto-Scaled Chromatogram

Peak Results

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 13.375 | 1580261 | 5.52 | 223486 |
| 2 | 13.951 | 942261 | 3.29 | 237265 |
| 3 | 14.192 | 26115200 | 91.19 | 3051355 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
Date Printed:
4/28/2021
3:01:52 PM America/New_York

**Figure S28.** Compound 28.

Empower2 software

WalkUpReport

SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Sample Name: | R06039-257 | Acquired By: | walkup |
| Sample Type: | Unknown | Sample Set Name: | RajwanaR06039 |
| Vial: | 48 | Acq. Method Set: | |
| Injection #: | 1 | Processing Method: | 220W280W15MIN |
| Injection Volume: | 20.00 ul | Channel Name: | W2996 220.0nm-2.0 |
| Run Time: | 30.0 Minutes | Proc. Chnl. Descr.: | W2996 PDA 220.0 nm at 2.0 |
| Date Acquired: | 4/29/2021 4:54:02 PM EST | | |
| Date Processed: | 4/30/2021 4:03:53 PM EST | | |

**Auto-Scaled Chromatogram**

**Peak Results**

| | RT | Area | % Area | Height |
|---|---|---|---|---|
| 1 | 3.495 | 7635741 | 100.00 | 591338 |

Reported by User: walkup
Report Method: WalkUpReport
Report Method ID: 1018
Page: 1 of 1

Project Name: MedChem\MedChem2021-04
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**Figure S29.** Compound 29.