

SUPPORTING INFORMATION

U.S. FDA Approved Drugs from 2015 - June 2020: A Perspective

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Table S1. Exploration of molecular descriptors to determine chemical spaces for USFDA approved small molecules. The table illustrates the year-wise distribution of median, mean and standard deviation (SD) values for molecular descriptors.

| Drug Category | | MW (g/mol) | | | TPSA (Å ²) | | | nROTB | | | nHBDon | | | nHBAcc | | | AlogP | | |
|-------------------------|------|------------|--------|--------|------------------------|--------|--------|--------|------|------|--------|------|------|--------|------|------|--------|--------|------|
| | | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD |
| Anticancer Drugs | 2015 | 507.67 | 513.66 | 108.80 | 108.40 | 121.03 | 51.30 | 7.5 | 7.6 | 2.98 | 3 | 3.2 | 1.39 | 9 | 8.9 | 3.51 | -1.14 | -0.94 | 1.75 |
| | 2016 | 595.23 | 595.23 | 384.78 | 114.64 | 114.64 | 86.94 | 8.5 | 8.5 | 7.77 | 3 | 3 | 0 | 7.5 | 7.5 | 4.94 | 0.26 | 0.26 | 0.07 |
| | 2017 | 480.22 | 487.65 | 81.14 | 94.61 | 96.74 | 23.28 | 7 | 6.8 | 2.61 | 2 | 1.88 | 0.60 | 9 | 8.55 | 1.81 | -1.45 | -1.29 | 1.83 |
| | 2018 | 440.02 | 460.42 | 70.75 | 92.55 | 101.40 | 22.17 | 5 | 5.9 | 3.26 | 2 | 2.09 | 0.83 | 7 | 7.90 | 1.81 | -0.99 | -1.00 | 1.10 |
| | 2019 | 458.73 | 472.82 | 57.73 | 106.68 | 98.35 | 23.40 | 7.5 | 8.2 | 1.90 | 2.5 | 2.37 | 0.74 | 8 | 7.75 | 1.28 | -0.52 | -0.33 | 0.76 |
| | 2020 | 492.72 | 492.55 | 47.39 | 86.01 | 91.67 | 12.21 | 6.5 | 6.7 | 1.66 | 1.5 | 1.75 | 0.88 | 8.5 | 8.25 | 1.83 | -0.59 | -0.69 | 1.35 |
| Neurological disorders | 2015 | 427.26 | 467.22 | 108.71 | 44.81 | 50.96 | 14.39 | 7 | 9.8 | 5.97 | 1 | 0.8 | 0.44 | 5 | 5.4 | 0.89 | 0.64 | 0.44 | 1.36 |
| | 2016 | 212.15 | 212.15 | NA | 63.4 | 63.4 | NA | 5 | 5 | NA | 1 | 1 | NA | 4 | 4 | NA | -1.90 | -1.90 | NA |
| | 2017 | 309.67 | 302.92 | 100.18 | 51.56 | 52.45 | 19.87 | 5.5 | 5 | 3.16 | 0.5 | 0.75 | 0.95 | 4 | 4.25 | 1.25 | 0.38 | 0.29 | 0.34 |
| | 2018 | 274.17 | 274.17 | 56.638 | 39.57 | 39.57 | 1.25 | 4.5 | 4.5 | 2.12 | 1.5 | 1.5 | 0.70 | 2.5 | 2.5 | 0.70 | 1.44 | 1.44 | 0.11 |
| | 2019 | 377.13 | 354.27 | 101.30 | 74.68 | 62.51 | 30.71 | 5 | 5.33 | 1.93 | 1 | 0.88 | 0.78 | 5 | 5.11 | 2.31 | 0.18 | -0.03 | 0.80 |
| | 2020 | 473.10 | 473.10 | 86.423 | 128.12 | 128.12 | 21.92 | 4 | 4 | 1.41 | 2 | 2 | 0 | 6 | 6 | 4.24 | -0.29 | -0.29 | 2.24 |
| Metabolic disorders | 2015 | 392.29 | 393.17 | 14.65 | 90.56 | 96.45 | 24.49 | 5 | 5.2 | 1.64 | 3 | 2.4 | 1.34 | 5 | 6 | 2.82 | 0.29 | 0.73 | 1.78 |
| | 2017 | 438.67 | 438.67 | 3.59 | 105.43 | 105.43 | 4.49 | 5 | 5 | 1.41 | 2.5 | 2.5 | 2.12 | 7 | 7 | 0 | 0.003 | 0.003 | 0.35 |
| | 2018 | 341.63 | 341.63 | 252.50 | 102.22 | 102.22 | 3.10 | 5 | 5 | 5.65 | 4.5 | 4.5 | 0.70 | 6.5 | 6.5 | 2.12 | -0.74 | -0.74 | 2.39 |
| | 2019 | 428.66 | 428.66 | 129.42 | 92.99 | 92.99 | 26.16 | 7.5 | 7.5 | 2.12 | 2.5 | 2.5 | 2.12 | 7 | 7 | 1.41 | 0.45 | 0.45 | 0.69 |
| | 2020 | 227.08 | 227.08 | NA | 39.39 | 39.39 | NA | 1 | 1 | NA | 1 | 1 | NA | 3 | 3 | NA | -0.72 | -0.72 | NA |
| Respiratory diseases | 2018 | 597.33 | 597.33 | NA | 108.21 | 108.21 | NA | 13 | 13 | NA | 2 | 2 | NA | 9 | 9 | NA | 0.4902 | 0.4902 | NA |
| Anti-infective diseases | 2015 | 631.67 | 610.44 | 142.53 | 173.29 | 176.61 | 49.88 | 13 | 11.5 | 6.45 | 3 | 3 | 0.81 | 11 | 11 | 2.58 | -1.60 | -1.59 | 1.97 |
| | 2017 | 311.62 | 345.13 | 168.06 | 81.82 | 82.33 | 4.12 | 5 | 5.25 | 2.21 | 1 | 1.25 | 0.5 | 5 | 5.25 | 2.21 | 0.13 | 0.13 | 1.51 |
| | 2018 | 564.66 | 556.74 | 99.60 | 149.90 | 153.09 | 69.10 | 6 | 6.62 | 3.77 | 4 | 4.25 | 3.65 | 10.5 | 10 | 3.77 | -0.31 | -1.12 | 3.00 |
| | 2019 | 433.18 | 493.86 | 185.30 | 110.79 | 146.86 | 111.29 | 6 | 7.5 | 5.19 | 2 | 2.5 | 2.64 | 5.5 | 7 | 4.83 | 0.71 | 0.27 | 3.35 |

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|-------------------------|------|--------|--------|--------|--------|--------|--------|------|------|-------|-----|-----|------|------|------|------|--------|-------|------|
| Autoimmune disorders | 2020 | 384.17 | 384.17 | NA | 100.52 | 100.52 | NA | 5 | 5 | NA | 1 | 1 | NA | 8 | 8 | NA | 0.44 | 0.44 | NA |
| | 2016 | 420.32 | 420.32 | NA | 77.76 | 77.76 | NA | 5 | 5 | NA | 3 | 3 | NA | 4 | 4 | NA | -0.419 | -0.41 | NA |
| | 2018 | 580.14 | 459.72 | 222.38 | 122.52 | 131.04 | 47.68 | 8 | 7.4 | 5.27 | 2 | 2.2 | 1.09 | 9 | 8.6 | 4.33 | -2.430 | -1.13 | 1.98 |
| | 2019 | 448.20 | 448.20 | 96.23 | 67.23 | 67.23 | 7.21 | 8 | 8 | 2.82 | 1.5 | 1.5 | 0.70 | 5 | 5 | 2.82 | 0.0061 | 0.006 | 2.54 |
| | 2020 | 404.18 | 404.18 | NA | 99.23 | 99.23 | NA | 7 | 7 | NA | 2 | 2 | NA | 5 | 5 | NA | -0.363 | -0.36 | NA |
| Cardiovascular diseases | 2015 | 496.21 | 539.56 | 140.44 | 108.81 | 151.10 | 107.78 | 13 | 12.4 | 2.50 | 2 | 2.6 | 2.70 | 8 | 9.8 | 4.43 | 0.2253 | 0.20 | 1.65 |
| | 2017 | 748.33 | 748.33 | 420.29 | 255.71 | 255.71 | 210.48 | 22.5 | 22.5 | 19.09 | 8 | 8 | 7.07 | 16.5 | 16.5 | 12.0 | -3.30 | -3.30 | 6.10 |
| | 2019 | 306.98 | 306.98 | NA | 58.89 | 58.89 | NA | 2 | 2 | NA | 1 | 1 | NA | 4 | 4 | NA | 2.08 | 2.08 | NA |
| | 2020 | 344.25 | 344.25 | NA | 94.83 | 94.83 | NA | 14 | 14 | NA | 3 | 3 | NA | 5 | 5 | NA | -1.34 | -1.34 | NA |

Table S2. Exploration of key descriptors to determine chemical spaces for USFDA approved small drug molecules based on their route of drug administration. The table illustrates the median, mean and standard deviation (SD) values for molecular descriptors employed.

| Route of drug administration | MW (g/mol) | | | TPSA (Å ²) | | | nROTB | | | nHBDon | | | nHBAcc | | | AlogP | | |
|----------------------------------|------------|--------|--------|------------------------|--------|--------|--------|-------|-------|--------|------|------|--------|-------|------|--------|-------|-------|
| | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD | Median | Mean | SD |
| Oral | 443.72 | 457.13 | 133.22 | 92.67 | 98.94 | 40.92 | 7 | 7.140 | 4.04 | 2 | 2.17 | 1.50 | 7 | 7.26 | 2.84 | -0.03 | -0.21 | 1 |
| Intravenous | 546.09 | 599.3 | 321.83 | 193.73 | 204.83 | 149.53 | 8 | 10.66 | 10.18 | 3 | 4.86 | 4.59 | 12 | 12.13 | 8.45 | -1.87 | -2.71 | -9.17 |
| Both oral and Intravenous | 440.04 | 425.34 | 229.21 | 81.65 | 104.57 | 47.23 | 5 | 7 | 5.43 | 1 | 1.6 | 0.89 | 8 | 7 | 3.60 | -0.33 | -0.29 | -1.90 |
| Topical | 363.15 | 357.82 | 104.18 | 70 | 71.49 | 9.84 | 4 | 4.66 | 3.05 | 2 | 1.66 | 0.57 | 5 | 5 | 1 | 0.353 | 0.68 | -0.61 |
| Ocular | 480.24 | 480.24 | 38.23 | 116.57 | 116.57 | 32.22 | 14 | 14 | 7.07 | 2.5 | 2.5 | 0.70 | 5.5 | 5.5 | 0.70 | 0.268 | 0.26 | -0.90 |
| Inhalation | 597.33 | 597.33 | NA | 108.21 | 108.21 | NA | 13 | 13 | NA | 2 | 2 | NA | 9 | 9 | NA | 0.49 | 0.49 | 0.49 |
| Intramuscular | 659.32 | 659.32 | NA | 62.32 | 62.32 | NA | 20 | 20 | NA | 0 | 0 | NA | 7 | 7 | NA | -1.75 | -1.75 | -1.75 |
| Subcutaneous | 392.29 | 392.29 | NA | 77.76 | 77.76 | NA | 4 | 4 | NA | 3 | 3 | NA | 4 | 4 | NA | 0.29 | 0.29 | 0.29 |

Table S3. Analysis of chemical space parameters for drugs approved by USFDA during year 2015- June 2020

| ID | DB | MW | TopoPSA | nRotB | nHBDdon | nHBAcc | AlogP |
|-----------|--------------------------------|----------|---------|-------|---------|--------|---------|
| Lutathera | Anticancer drugs | 1431.571 | 552.79 | 29 | 14 | 33 | -9.1746 |
| Giapreza | Cardiovascular drugs | 1045.535 | 404.55 | 36 | 13 | 25 | -7.6157 |
| Zemdri | Antiinfective drugs | 592.3432 | 269.29 | 14 | 11 | 16 | -6.9236 |
| Kisqali | Anticancer drugs | 434.2543 | 87.93 | 6 | 2 | 9 | -4.5166 |
| Xerava | Antiinfective drugs | 558.2126 | 193.73 | 6 | 6 | 12 | -4.0147 |
| Ibrance | Anticancer drugs | 447.2383 | 101.76 | 5 | 2 | 9 | -3.7662 |
| Fetroja | Antiinfective drugs | 751.1497 | 306.97 | 15 | 6 | 14 | -3.7039 |
| Avycaz | Antiinfective drugs | 546.0991 | 240.42 | 10 | 3 | 10 | -3.6303 |
| Aliqopa | Anticancer drugs | 480.2234 | 138.73 | 8 | 2 | 12 | -3.5611 |
| Daklinza | Antiinfective drugs | 738.3853 | 166.06 | 17 | 4 | 14 | -2.8834 |
| Firdapse | Drugs for autoimmune disorders | 109.064 | 64.4 | 0 | 2 | 3 | -2.6748 |
| Tavalisse | Drugs for autoimmune disorders | 580.1483 | 194.94 | 10 | 4 | 15 | -2.478 |
| Galafold | Drugs for metabolic disorders | 163.0845 | 92.95 | 1 | 5 | 5 | -2.44 |
| Olumiant | Drugs for autoimmune disorders | 371.1164 | 121.9 | 5 | 1 | 9 | -2.4306 |
| Ayvakit | Anticancer drugs | 498.2404 | 100.78 | 5 | 1 | 10 | -2.4129 |

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|---------------|-----------------------------------|----------|--------|----|---|----|---------|
| Lonsurf | Anticancer drugs | 574.0957 | 184.39 | 5 | 6 | 13 | -2.2897 |
| Edoxaban | Anticancer drugs | 547.1769 | 160.87 | 10 | 3 | 11 | -2.1505 |
| Savaysa | Cardiovascular drugs | 547.1769 | 160.87 | 10 | 3 | 11 | -2.1505 |
| Tibsovo | Anticancer drugs | 582.1394 | 118.23 | 9 | 1 | 9 | -2.1152 |
| Pemazyre | Anticancer drugs | 487.2031 | 78.87 | 6 | 1 | 9 | -2.0014 |
| Retevmo | Anticancer drugs | 525.2488 | 109.28 | 8 | 1 | 10 | -1.931 |
| Lenvima | Anticancer drugs | 426.1095 | 115.04 | 8 | 3 | 8 | -1.9183 |
| Dayvigo | Neurological drugs | 410.1554 | 75.41 | 7 | 1 | 6 | -1.9081 |
| Briviact | Neurological drugs | 212.1525 | 63.4 | 5 | 1 | 4 | -1.9042 |
| Nurtec ODT | Neurological drugs | 534.2191 | 112.62 | 5 | 2 | 9 | -1.877 |
| Rinvoq | Drugs for autoimmune disorders | 380.1572 | 72.33 | 6 | 2 | 7 | -1.7924 |
| Aristada | Neurological drugs | 659.3257 | 62.32 | 20 | 0 | 7 | -1.755 |
| Alunbrig | Anticancer drugs | 583.2591 | 94.61 | 8 | 2 | 9 | -1.7501 |
| Vitrakvi | Anticancer drugs | 428.1772 | 83.77 | 5 | 2 | 8 | -1.6178 |
| Verzenio | Anticancer drugs | 506.2718 | 71.19 | 7 | 1 | 8 | -1.57 |
| Solosec | Antiinfective drugs | 185.08 | 81.65 | 3 | 1 | 3 | -1.5601 |
| Balversa | Anticancer drugs | 446.243 | 74.05 | 9 | 1 | 8 | -1.5308 |
| Braftovi | Anticancer drugs | 539.1518 | 145.23 | 11 | 3 | 11 | -1.4779 |
| Calquence | Anticancer drugs | 465.1913 | 115.75 | 6 | 2 | 9 | -1.4508 |

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|----------|-------------------------------|----------|--------|----|---|----|---------|
| Cotellic | Anticancer drugs | 531.0631 | 64.6 | 5 | 3 | 5 | -1.3709 |
| Nuzyra | Antiinfective drugs | 556.2897 | 176.66 | 7 | 6 | 11 | -1.3671 |
| Nexletol | Cardiovascular drugs | 344.2563 | 94.83 | 14 | 3 | 5 | -1.3411 |
| Xuriden | Drugs for metabolic disorders | 370.1012 | 137.54 | 8 | 1 | 11 | -1.3162 |
| Xenleta | Antiinfective drugs | 507.3018 | 135.15 | 6 | 3 | 6 | -1.2708 |
| Vizimpro | Anticancer drugs | 469.1681 | 78.32 | 8 | 2 | 7 | -1.196 |
| Mektovi | Anticancer drugs | 440.0296 | 86.19 | 7 | 3 | 5 | -0.9933 |
| Aemcolo | Antiinfective drugs | 697.3098 | 201.31 | 3 | 6 | 13 | -0.9126 |
| Tagrisso | Anticancer drugs | 499.2696 | 84.8 | 11 | 2 | 9 | -0.9104 |
| Talzenna | Anticancer drugs | 380.1197 | 81.45 | 2 | 2 | 7 | -0.8178 |
| Xpovio | Anticancer drugs | 524.257 | 115.8 | 11 | 3 | 9 | -0.7967 |
| Inrebic | Anticancer drugs | 524.257 | 115.8 | 11 | 3 | 9 | -0.7967 |
| Isturisa | Drugs for metabolic disorders | 227.0859 | 39.39 | 1 | 0 | 3 | -0.7267 |
| Tukysa | Anticancer drugs | 480.2022 | 107.56 | 6 | 2 | 10 | -0.6567 |
| Xepi | Antiinfective drugs | 363.1583 | 82 | 4 | 2 | 6 | -0.6178 |
| Ubrelyvy | Neurological drugs | 549.1988 | 103.23 | 6 | 2 | 8 | -0.6111 |
| Lorbrena | Anticancer drugs | 406.1554 | 107.31 | 0 | 1 | 8 | -0.5771 |
| Koselugo | Anticancer drugs | 456 | 86.19 | 7 | 3 | 5 | -0.5344 |
| Cholbam | Drugs for metabolic disorders | 408.2876 | 97.99 | 4 | 4 | 5 | -0.4664 |
| Daurismo | Anticancer drugs | 374.1855 | 92.55 | 5 | 3 | 7 | -0.4552 |
| Corlanor | Cardiovascular drugs | 468.2624 | 60.47 | 10 | 0 | 7 | -0.4254 |

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|-----------|--------------------------------|----------|--------|----|---|----|---------|
| Ocaliva | Antiinfective drugs | 420.324 | 77.76 | 5 | 3 | 4 | -0.4199 |
| Zeposia | Cardiovascular drugs | 404.1848 | 99.23 | 7 | 2 | 5 | -0.3631 |
| Baxdela | Antiinfective drugs | 440.0499 | 119.46 | 3 | 3 | 8 | -0.3329 |
| Emflaza | Drugs for metabolic disorders | 441.2151 | 102.26 | 4 | 1 | 7 | -0.2473 |
| Yondelis | Anticancer drugs | 761.2618 | 194.02 | 4 | 4 | 14 | -0.2227 |
| Zejula | Anticancer drugs | 320.1637 | 70.72 | 3 | 2 | 5 | -0.2107 |
| Ingrezza | Neurological drugs | 418.2832 | 74.02 | 8 | 1 | 6 | -0.1778 |
| Reyvow | Neurological drugs | 377.1351 | 61.77 | 5 | 1 | 5 | -0.1266 |
| Oxbryta | Drugs for metabolic disorders | 337.1426 | 74.49 | 6 | 1 | 6 | -0.0392 |
| Idhifa | Anticancer drugs | 473.1399 | 106.09 | 8 | 3 | 8 | -0.0018 |
| Copiktra | Anticancer drugs | 416.1152 | 81.45 | 4 | 2 | 7 | 0.0524 |
| Ninlaro | Anticancer drugs | 516.0874 | 168.33 | 13 | 4 | 11 | 0.0629 |
| Wakix | Neurological drugs | 295.1703 | 12.47 | 8 | 0 | 2 | 0.116 |
| Qinlock | Anticancer drugs | 509.0863 | 85.83 | 7 | 3 | 7 | 0.1786 |
| Nourianz | Neurological drugs | 384.1798 | 74.68 | 6 | 0 | 8 | 0.1819 |
| Doptelet | Drugs for autoimmune disorders | 648.1511 | 151.44 | 8 | 2 | 9 | 0.2084 |
| Rubraca | Anticancer drugs | 323.1434 | 53.16 | 3 | 3 | 4 | 0.2183 |
| Upravi | Cardiovascular drugs | 496.2144 | 108.81 | 13 | 1 | 8 | 0.2253 |
| Steglatro | Drugs for metabolic disorders | 436.1289 | 108.61 | 6 | 4 | 7 | 0.2544 |
| Rexulti | Neurological drugs | 433.1824 | 70.11 | 7 | 1 | 5 | 0.258 |

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|----------------------|-------------------------------|----------|--------|----|---|----|--------|
| Radicava | Neurological drugs | 174.0793 | 32.67 | 1 | 0 | 3 | 0.2609 |
| Tpoxx | Antiinfective drugs | 376.1035 | 66.48 | 4 | 1 | 5 | 0.2772 |
| Kybella | Drugs for metabolic disorders | 392.2927 | 77.76 | 4 | 3 | 4 | 0.2999 |
| Venclexta | Anticancer drugs | 867.3181 | 176.12 | 14 | 3 | 11 | 0.3214 |
| Zulresso | Neurological drugs | 318.2559 | 37.3 | 1 | 1 | 2 | 0.3247 |
| Rozlytrek | Anticancer drugs | 560.2711 | 81.23 | 8 | 3 | 8 | 0.3401 |
| Tabrecta | Anticancer drugs | 412.1448 | 81.78 | 5 | 1 | 7 | 0.3642 |
| Sunosi | Neurological drugs | 194.1055 | 78.34 | 5 | 2 | 4 | 0.3975 |
| Artesunate | Antiinfective drugs | 384.1784 | 100.52 | 5 | 1 | 8 | 0.4477 |
| Caplyta | Neurological drugs | 393.2216 | 26.79 | 5 | 0 | 4 | 0.4702 |
| Cresemba | Antiinfective drugs | 717.2419 | 180.52 | 16 | 2 | 12 | 0.4804 |
| Yupelri | Drugs for respiratory disease | 597.3315 | 108.21 | 13 | 2 | 9 | 0.4902 |
| Nerlynx | Anticancer drugs | 556.199 | 111.34 | 12 | 2 | 9 | 0.5111 |
| Turalio | Anticancer drugs | 417.0968 | 61.14 | 6 | 2 | 5 | 0.5127 |
| Deutetrabe nazine | Neurological drugs | 317.1991 | 38.77 | 4 | 0 | 4 | 0.5182 |
| Krintafel | Antiinfective drugs | 463.2083 | 78.1 | 10 | 2 | 6 | 0.5529 |
| Xadago | Neurological drugs | 302.1431 | 64.35 | 7 | 2 | 4 | 0.5867 |
| Piqray | Anticancer drugs | 441.1446 | 125.45 | 7 | 2 | 7 | 0.6373 |
| Vraylar | Neurological drugs | 426.1953 | 38.82 | 7 | 1 | 5 | 0.646 |
| Farydak | Anticancer drugs | 349.179 | 73.39 | 8 | 4 | 3 | 0.7421 |

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|--------------|--------------------------------|----------|--------|----|---|----|--------|
| Xcopri | Neurological drugs | 267.0523 | 92.64 | 5 | 1 | 7 | 0.8177 |
| Benznidazole | Antiinfective drugs | 260.0909 | 87.84 | 6 | 1 | 4 | 0.888 |
| Rydapt | Anticancer drugs | 570.2267 | 74.35 | 4 | 1 | 8 | 0.9367 |
| Symdeko | Drugs for metabolic disorders | 520.1821 | 111.49 | 9 | 4 | 8 | 0.9419 |
| Trikafta | Drugs for metabolic disorders | 520.1821 | 111.49 | 9 | 4 | 8 | 0.9419 |
| Bevyxxa | Cardiovascular drugs | 451.1411 | 106.88 | 9 | 3 | 8 | 1.0124 |
| Xofluza | Antiinfective drugs | 571.1225 | 123.15 | 6 | 0 | 10 | 1.113 |
| Kengreal | Cardiovascular drugs | 774.9483 | 332.66 | 16 | 7 | 17 | 1.1588 |
| Erleada | Anticancer drugs | 477.0883 | 120.89 | 5 | 1 | 7 | 1.1695 |
| Nuplazid | Neurological drugs | 427.2635 | 44.81 | 10 | 1 | 5 | 1.2168 |
| Ongentys | Neurological drugs | 411.9977 | 143.62 | 3 | 2 | 3 | 1.2918 |
| Epidioloex | Neurological drugs | 314.2246 | 40.46 | 6 | 2 | 2 | 1.3566 |
| Tazverik | Anticancer drugs | 572.3363 | 83.14 | 10 | 2 | 8 | 1.4708 |
| Diacomit | Neurological drugs | 234.1256 | 38.69 | 3 | 1 | 3 | 1.5248 |
| Mulpleta | Drugs for autoimmune disorders | 590.1409 | 122.52 | 14 | 2 | 7 | 1.7042 |
| Mayzent | Cardiovascular drugs | 516.26 | 62.13 | 10 | 1 | 3 | 1.8046 |
| Prevymis | Antiinfective drugs | 572.2047 | 77.84 | 8 | 1 | 8 | 1.824 |
| Addyi | Neurological drugs | 390.1667 | 38.82 | 5 | 1 | 5 | 1.8372 |
| Vyndaqel | Cardiovascular drugs | 306.9803 | 58.89 | 2 | 1 | 4 | 2.0867 |

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|------------|-------------------------------|----------|--------|----|---|---|--------|
| Moxidectin | Antiinfective drugs | 639.3771 | 116.04 | 3 | 2 | 7 | 2.2379 |
| Entresto | Cardiovascular drugs | 411.2046 | 92.7 | 13 | 2 | 6 | 2.239 |
| Orkambi | Drugs for metabolic disorders | 392.21 | 78.43 | 5 | 3 | 5 | 2.3079 |
| Odomzo | Anticancer drugs | 485.1926 | 63.16 | 7 | 1 | 6 | 2.3696 |
| Egaten | Antiinfective drugs | 357.9501 | 58.92 | 3 | 1 | 3 | 2.7063 |
| Zurampic | Drugs for metabolic disorders | 402.999 | 90.56 | 5 | 1 | 5 | 2.849 |
| Pretomanid | Antiinfective drugs | 359.0729 | 86.43 | 6 | 0 | 5 | 3.3662 |

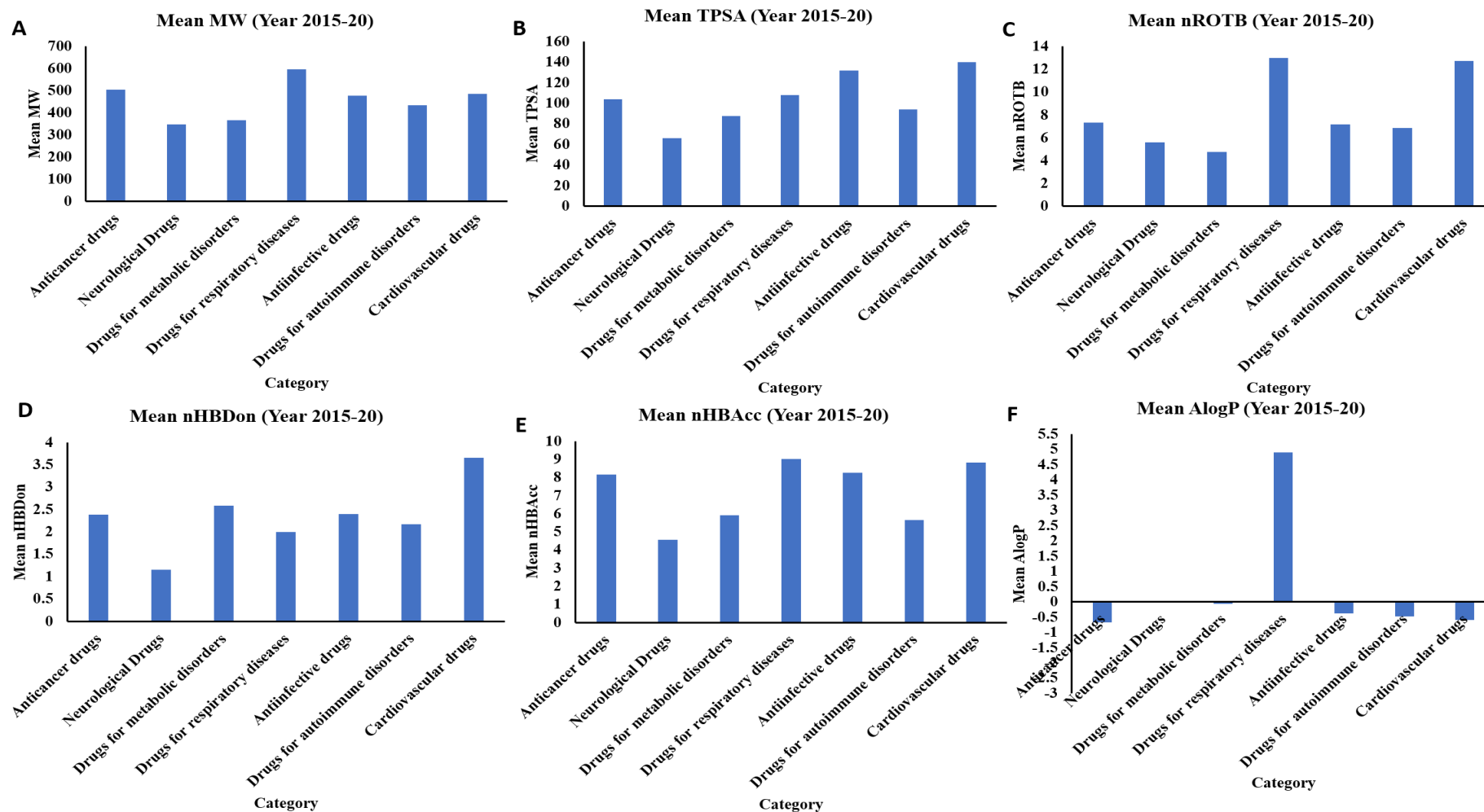


Figure S1. Year-wise graphical illustration portrays key descriptor (A-F) parameters for studying chemical space for approved drugs (2015-June 2020).

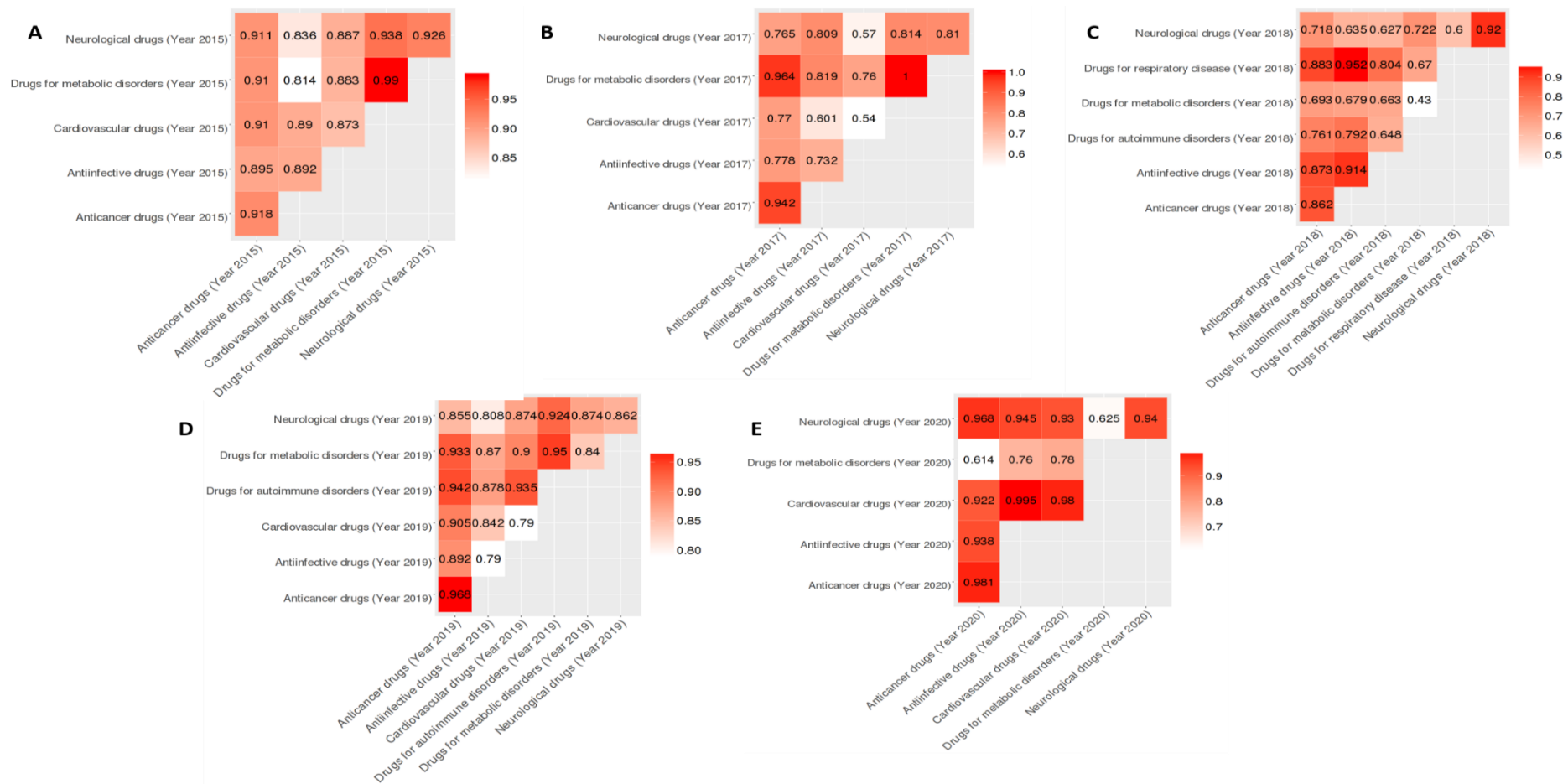


Figure S2. Tanimoto coefficient analysis of drugs approved in (A) 2015, (B) 2017, (C) 2018, (D) 2019 and (E) until June 2020.

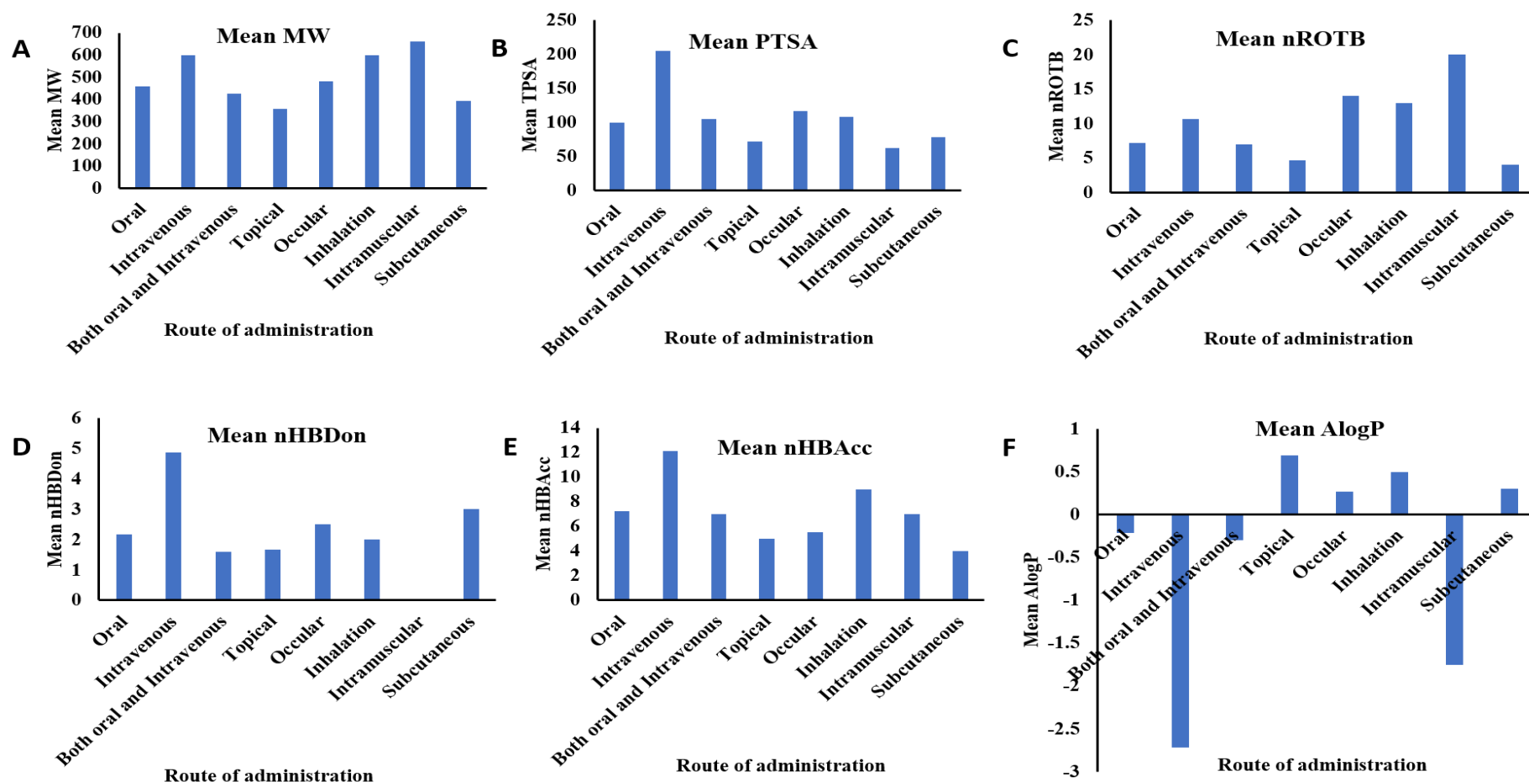


Figure S3. Graphical illustration portraying mean values of key descriptor (A-F) parameters employed for studying chemical space based on drug administration routes for approved drugs (2015-June 2020).