**Table S1** The information on BoxCar scan design.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **BoxCar (50) Scan I** | | | | | | | | | | | | | | |
| **Injection** | Box (m/z low, m/z high) | | | | | | | | | | | | | |
| Inj #1 | (100, 150) | (200, 250) | (300, 350) | (400, 450) | (500, 550) | (600, 650) | (700, 750) | (800, 850) | (900, 950) | (1000, 1050) | (1100, 1150) | (1200, 1250) | (1300, 1350) | (1400, 1450) |
| Inj #2 | (150, 200) | (250, 300) | (350, 400) | (450, 500) | (550, 600) | (650, 700) | (750, 800) | (850, 900) | (950, 1000) | (1050, 1100) | (1150, 1200) | (1250, 1300) | (1350, 1400) | (1450, 1500) |
| **BoxCar (20) Scan II** | | | | | | | | | | | | | | |
| **Injection** | Box (m/z low, m/z high) | | | | | | | | | | | | | |
| Inj #1 | (100, 125) | (200, 225) | (300, 325) | (400, 425) | (500, 525) | (600, 625) | (700, 725) | (800, 825) | (900, 925) | (1000, 1025) | (1100, 1125) | (1200, 1225) | (1300, 1325) | (1400, 1425) |
| Inj #2 | (125, 150) | (225, 250) | (325, 350) | (425, 450) | (525, 550) | (625, 650) | (725, 750) | (825, 850) | (925, 950) | (1025, 1050) | (1125, 1150) | (1225, 1250) | (1325, 1350) | (1425, 1450) |
| Inj #3 | (150, 175) | (250, 275) | (350, 375) | (450, 475) | (550, 575) | (650, 675) | (750, 775) | (850, 875) | (950, 975) | (1050, 1075) | (1150, 1175) | (1250, 1275) | (1350, 1375) | (1450, 1475) |
| Inj #4 | (175, 200) | (275, 300) | (375, 400) | (475, 500) | (575, 600) | (675, 700) | (775, 800) | (875, 900) | (975, 1000) | (1075, 1100) | (1175, 1200) | (1275, 1300) | (1375, 1400) | (1475, 1500) |
| **BoxCar Scan (10) III** | | | | | | | | | | | | | | |
| **Injection** | Box (m/z low, m/z high) | | | | | | | | | | | | | |
| Inj #1 | (100, 110) | (200, 210) | (300, 310) | (400, 410) | (500, 510) | (600, 610) | (700, 710) | (800, 810) | (900, 910) | (1000, 1010) | (1100, 1110) | (1200, 1210) | (1300, 1310) | (1400, 1410) |
| Inj #2 | (110, 120) | (210, 220) | (310, 320) | (410, 420) | (510, 520) | (610, 620) | (710, 720) | (810, 820) | (910, 920) | (1010, 1020) | (1110, 1120) | (1210, 1220) | (1310, 1320) | (1410, 1420) |
| Inj #3 | (120, 130) | (220, 230) | (320, 330) | (420, 430) | (520, 530) | (620, 630) | (720, 730) | (820, 830) | (920, 930) | (1020, 1030) | (1120, 1130) | (1220, 1230) | (1320, 1330) | (1420, 1430) |
| Inj #4 | (130, 140) | (230, 240) | (330, 340) | (430, 440) | (530, 540) | (630, 640) | (730, 740) | (830, 840) | (930, 940) | (1030, 1040) | (1130, 1140) | (1320, 1240) | (1330, 1340) | (1430, 1440) |
| Inj #5 | (140, 150) | (240, 250) | (340, 350) | (440, 450) | (540, 550) | (640, 650) | (740, 750) | (840, 850) | (940, 950) | (1040, 1050) | (1140, 1150) | (1240, 1250) | (1340, 1350) | (1440, 1450) |
| Inj #6 | (150, 160) | (250, 260) | (350, 360) | (450, 460) | (550, 560) | (650, 660) | (750, 760) | (850, 860) | (950, 960) | (1050, 1060) | (1150, 1160) | (1250, 1260) | (1350, 1360) | (1450, 1460) |
| Inj #7 | (160, 170) | (260, 270) | (360, 370) | (460, 470) | (560, 570) | (660, 670) | (760, 770) | (860, 870) | (960, 970) | (1060, 1070) | (1160, 1170) | (1260, 1270) | (1360, 1370) | (1460, 1470) |
| Inj #8 | (170, 180) | (270, 280) | (370, 380) | (470, 480) | (570, 580) | (670, 680) | (770, 780) | (870, 880) | (970, 980) | (1070, 1080) | (1170, 1180) | (1270, 1280) | (1370, 1380) | (1470, 1480) |
| Inj #9 | (180, 190) | (280, 290) | (380, 390) | (480, 490) | (580, 590) | (680, 690) | (780, 790) | (880, 890) | (980, 990) | (1080, 1090) | (1180, 1190) | (1280, 1290) | (1380, 1390) | (1480, 1490) |
| Inj #10 | (190, 200) | (290, 300) | (390, 400) | (490, 500) | (590, 600) | (690, 700) | (790, 800) | (890, 900) | (990, 1000) | (1090, 1100) | (1190, 1200) | (1290, 1300) | (1390, 1400) | (1490, 1500) |



**Figure S1** The distribution of the representative ions acquired from positive (A) and negative (B) ion modes.