



*Supplement of*

## **Identification of particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze River**

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This supplementary information document contains three figures and ten tables, totaling 31 pages. Presented in each table are OSs and nitrooxy-OSs with an arbitrary intensity larger than 0.5% of the most abundant one in the same sample.

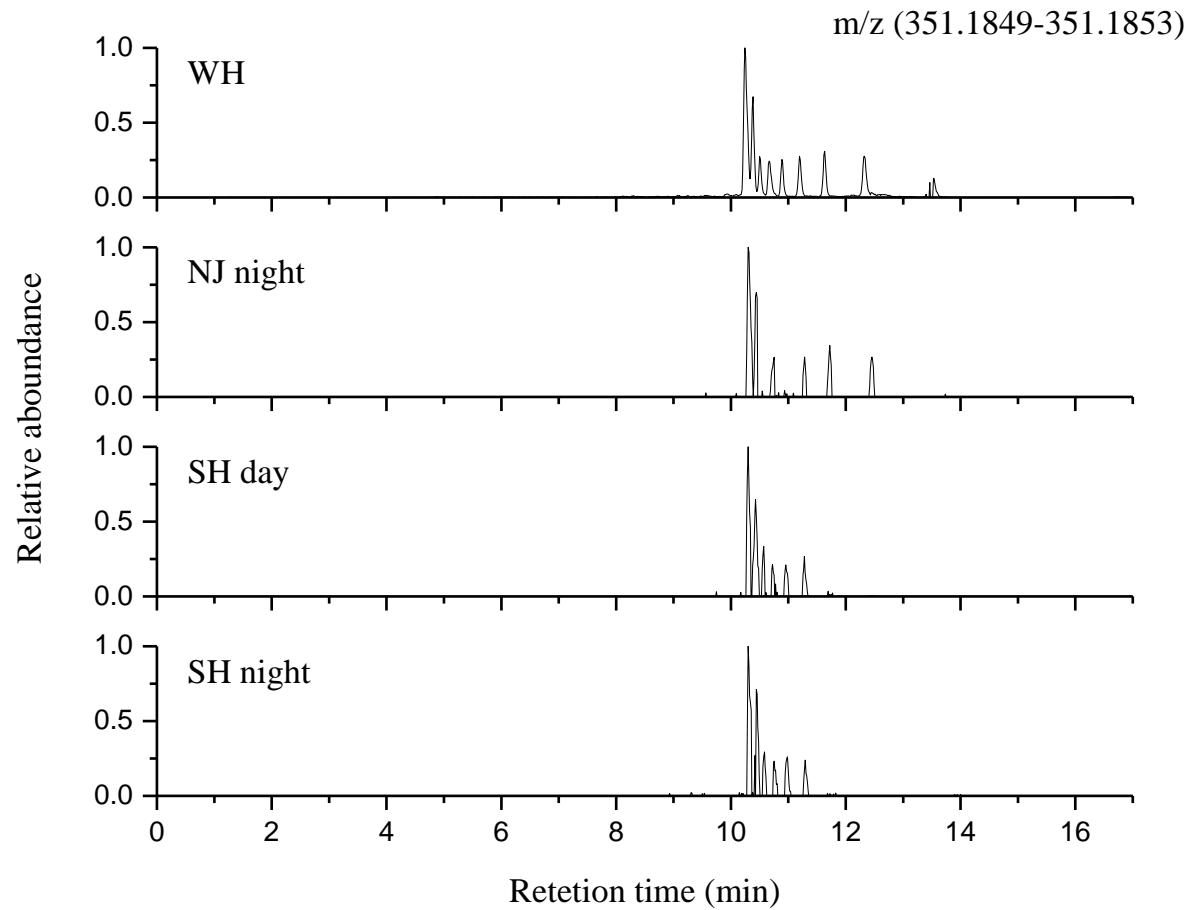
### **Extraction efficiency and repeatability of the extraction protocol – Protocol**

5  $\mu\text{L}$  of a 200  $\mu\text{M}$  solution of methyl sulfate, octyl sulfate, dodecyl sulfate and camphor sulfonic acid, were deposited on quartz filter that was then extracted and analyzed as described in the text. Three replicates were performed. The average chromatographic peak area obtained for each compounds were compared to the average value obtained for three injections of a 1  $\mu\text{M}$  standard solution (1  $\mu\text{M}$  being the theoretical final concentration of the extract) to assess the extraction efficiencies. The repeatabilities were determined as the standard deviation obtained from the injection of the three replicates. Results are given Table S1.

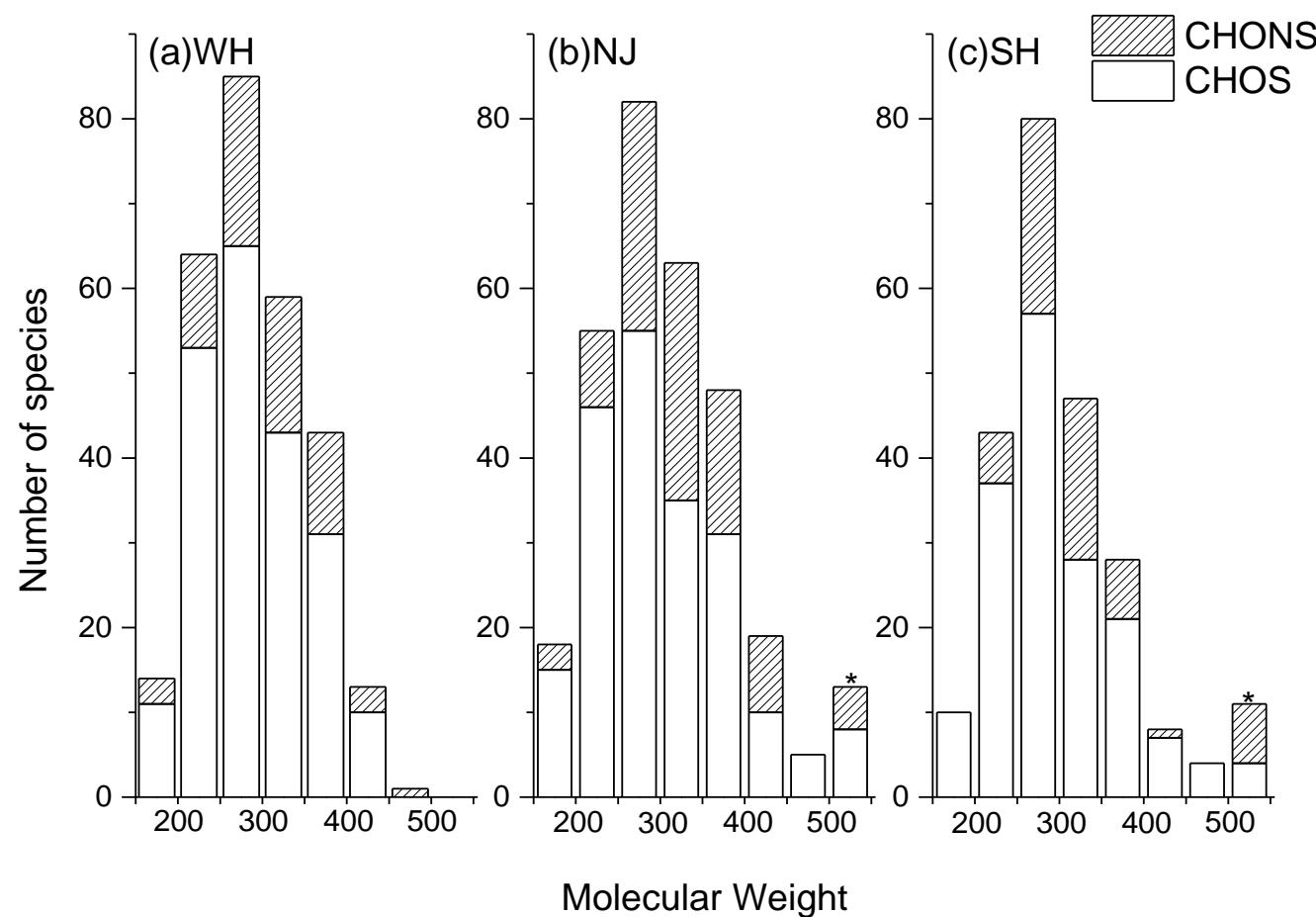
**Figure S1.** LC chromatograms of one OS ( $\text{C}_{16}\text{H}_{32}\text{O}_6\text{S}_1$ ) detected in WH, NJ and SH. WH corresponds to the daily sample collected from 8:30 a.m., Jun. 15 to 8:30 a.m., Jun. 16, 2012; NJ corresponds to the nighttime sample collected from 7:30 p.m., Aug. 29 to 7:30 a.m., Aug. 30, 2012; SH day corresponds to the daytime samples collected from 8:00 a.m. to 8:00 p.m., Jul. 28, 2013; SH night corresponds to the nighttime samples collected from 8:00 p.m., Jul. 28 to 8:00 a.m., Jul. 29, 2013.

**Figure S2.** Number of CHOS and CHONS in the different mass ranges. The bins are 50 Da wide. The last bin with an asterisk symbol includes all species with a molecular weight larger than 500 Da. WH corresponds to the daily sample collected from 8:30 a.m., Jun. 15 to 8:30 a.m., Jun. 16, 2012; NJ corresponds to the daily data, i.e., to the combination of samples collected from 7:30 a.m. to 7:30 p.m., Aug. 29, 2012 and from 7:30 p.m., Aug. 29 to 7:30 a.m., Aug. 30, 2012; SH corresponds to the daily data, i.e., to the combination of samples collected from 8:00 a.m. to 8:00 p.m., Jul. 28, 2013 and from 8:00 p.m., Jul. 28 to 8:00 a.m., Jul. 29, 2013.

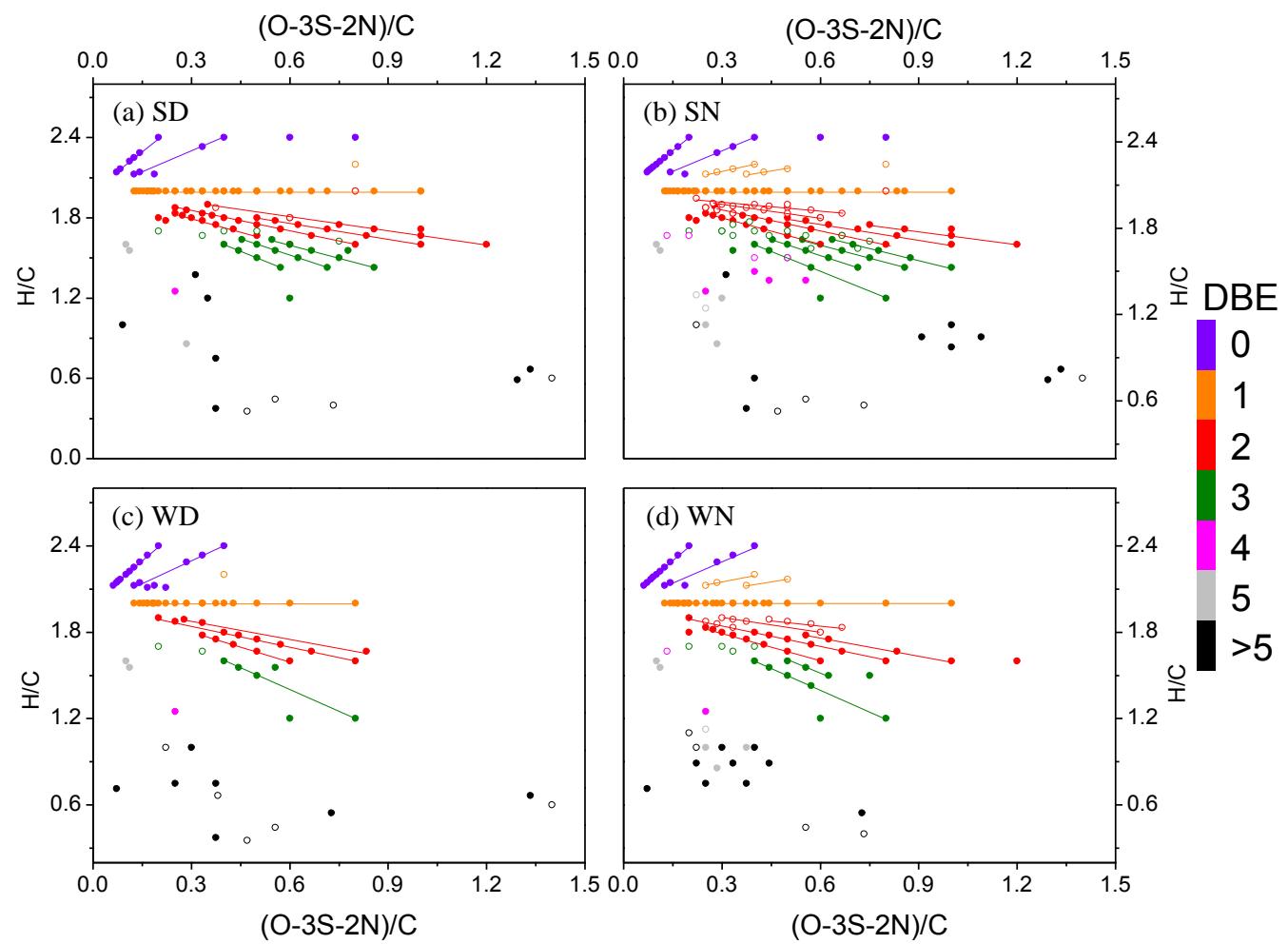
**Figure S3.** (a-d) Van Krevelen diagrams for CHOS and CHONS detected in Shanghai samples. The filled and open circles denote CHOS and CHONS, respectively. SD: summer day; SN: summer night; WD: winter day; WN: winter night. Note that only compounds with a relative abundance greater than or equal to 0.5% of that of  $\text{C}_{10}\text{H}_{17}\text{O}_7\text{N}_1\text{S}_1$  in the SN sample are shown in this figure.



**Figure S1**



**Figure S2**



**Figure S3**

**Table S1 Extraction efficiencies and repeatabilities of the extraction protocol - Results.**

	Standard solution		Filter extract		Ext. Eff.
	Average area	Std. Dev.	Average area	Std. Dev.	
Methyl sulfate	4.6 108	1.6%	3.3 108	5.6%	71.4%
Octyl sulfate	3.2 1011	2.4%	3.0 1011	2.3%	95.0%
Dodecyl sulfate	5.9 1011	2.3%	5.7 1011	3.1%	97.7%
Camphor sulfonic acid	1.3 1011	0.9%	1.2 1011	1.7%	94.0%

**Table S2 Comparisons of average air quality and meteorological conditions (arithmetic mean  $\pm$  standard deviation) between the SH sampling days and the seasonal average.**

time	Air quality <sup>a</sup>						Meteorological conditions <sup>b</sup>		
	PM <sub>2.5</sub> $\mu\text{g m}^{-3}$	PM <sub>10</sub> $\mu\text{g m}^{-3}$	O <sub>3</sub> $\mu\text{g m}^{-3}$	SO <sub>2</sub> $\mu\text{g m}^{-3}$	NO <sub>2</sub> $\mu\text{g m}^{-3}$	CO $\text{mg m}^{-3}$	wind speed $\text{m s}^{-1}$	temperature °C	relative humidity %
28 - 29 Jul, 2013	52.5	75.0	184.5	19.0	38.5	0.69	1.7 $\pm$ 0.8	34.8 $\pm$ 2.2	49.4 $\pm$ 8.3
1 Jun - 31 Aug, 2013	43.4 $\pm$ 24.5	59.9 $\pm$ 26.1	136.0 $\pm$ 58.0	14.6 $\pm$ 5.2	34.0 $\pm$ 11.7	0.67 $\pm$ 0.16	2.5 $\pm$ 1.2	28.7 $\pm$ 5.1	70.1 $\pm$ 16.0
17 - 18 Jan, 2013	77.0	90.5	68.0	32.5	57.5	1.01	2.9 $\pm$ 1.8	0.9 $\pm$ 1.1	58.3 $\pm$ 3.2
26 Dec, 2012 –28 Feb, 2013	78.4 $\pm$ 48.1	84.4 $\pm$ 46.6	72.0 $\pm$ 23.1	27.5 $\pm$ 15.0	54.7 $\pm$ 21.5	0.99 $\pm$ 0.40	2.3 $\pm$ 1.1	5.8 $\pm$ 3.9	71 $\pm$ 16.5

<sup>a</sup>Daily average concentrations and the average air quality in winter only included Jan and Feb.

<sup>b</sup>hourly average concentrations.

**Table S3. A list of OSs in winter in Wuhan**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	4
180.0459	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
182.0252	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	227.0102	C <sub>5</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
182.0616	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	228.0096	C <sub>9</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3
189.9939	C <sub>6</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	3	228.0307	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
192.0095	C <sub>6</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	4	229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
193.9887	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	5	229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	4
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4	230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	6	230.0251	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
196.0772	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	232.0044	C <sub>8</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	7
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	6	232.0772	C <sub>10</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	1
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	234.9790	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	236.0357	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5
204.0096	C <sub>7</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	238.0150	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4
208.0044	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	6	238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
208.0772	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	5	238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	6	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
210.0564	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	7	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	9
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	242.0101	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	242.0464	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
212.0358	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	6	242.0827	C <sub>8</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	243.0053	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
213.9939	C <sub>8</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	244.0044	C <sub>9</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4
216.0096	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	244.0254	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	1
217.9888	C <sub>7</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	5	246.0565	C <sub>10</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	3
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	6	248.0357	C <sub>9</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	4
222.0200	C <sub>7</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5	248.0721	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4
222.0929	C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	6	248.9947	C <sub>7</sub> H <sub>7</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	6
223.9993	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	2	250.0514	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
224.0358	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	5	250.0878	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	5
224.0722	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	6	252.0307	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	252.0671	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	7
225.9786	C <sub>5</sub> H <sub>6</sub> O <sub>8</sub> S <sub>1</sub>	1	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	1
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	5	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3

254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4	284.0205	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	9
254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5	284.0569	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	5
254.0828	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	8	284.0933	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	7
255.0416	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	284.9946	C <sub>10</sub> H <sub>7</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2	285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
256.0620	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	6	287.0315	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1	287.0678	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4
258.0203	C <sub>10</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5	288.0459	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	1
259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	289.0260	C <sub>10</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5
259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3	291.0417	C <sub>10</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
262.0515	C <sub>10</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	5	292.1711	C <sub>14</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	1
263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	294.1143	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	8
264.0670	C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	2	294.1506	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	5
264.1034	C <sub>11</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2	294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	3
266.0252	C <sub>12</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	295.0730	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
266.0463	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	296.0569	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	3
266.0827	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	3	296.1296	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	8
266.1191	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3	297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
266.1555	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	2	297.0885	C <sub>10</sub> H <sub>19</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
268.0256	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	5	298.0301	C <sub>16</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1
268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	298.0361	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	5
268.0985	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	8	298.0727	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	8
269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	298.1241	C <sub>15</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	1
270.0413	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	7	299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
270.0777	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	9	300.1399	C <sub>15</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
271.0366	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7	300.9894	C <sub>10</sub> H <sub>7</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	1
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	301.0471	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	3	302.1190	C <sub>14</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	1
272.0358	C <sub>11</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	3	308.1661	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	6
274.0151	C <sub>10</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	308.2025	C <sub>15</sub> H <sub>32</sub> O <sub>4</sub> S <sub>1</sub>	2
274.0303	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1	310.1092	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	9
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	310.1819	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	6
277.0260	C <sub>9</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	311.0679	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3	312.0519	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	3
280.0620	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	313.0472	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
280.0984	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	7	313.0836	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
280.1348	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	4	315.0629	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
280.1710	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	3	321.0521	C <sub>11</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	1
282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4	322.2180	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	4
282.0778	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	6	324.1611	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	9
282.1141	C <sub>11</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	10	326.0133	C <sub>10</sub> H <sub>14</sub> O <sub>8</sub> S <sub>2</sub>	1

327.0628	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	368.1875	C <sub>16</sub> H <sub>32</sub> O <sub>7</sub> S <sub>1</sub>	8
329.0785	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9	374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2
332.1300	C <sub>15</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	6	376.1925	C <sub>18</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	3
338.1768	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	6	378.2083	C <sub>18</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	4
338.2130	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	5	380.2238	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	8
341.0421	C <sub>10</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3	385.9429	C <sub>9</sub> H <sub>6</sub> O <sub>15</sub> S <sub>1</sub>	1
343.0577	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	5	391.0249	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	4
345.0736	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7	394.2032	C <sub>18</sub> H <sub>34</sub> O <sub>7</sub> S <sub>1</sub>	7
350.1769	C <sub>16</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	7	396.2188	C <sub>18</sub> H <sub>36</sub> O <sub>7</sub> S <sub>1</sub>	4
352.1925	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	9	410.1982	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	5
354.2079	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1	412.1222	C <sub>16</sub> H <sub>28</sub> O <sub>8</sub> S <sub>2</sub>	2
355.0943	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3	413.1726	C <sub>16</sub> H <sub>31</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
363.1358	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5	417.1464	C <sub>18</sub> H <sub>27</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	1
363.9484	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1	425.9192	C <sub>11</sub> H <sub>6</sub> O <sub>14</sub> S <sub>2</sub>	1
366.1717	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	7	441.2037	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
366.2081	C <sub>17</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	8	452.0727	C <sub>27</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	1
368.1512	C <sub>15</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	5	533.9332	C <sub>15</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>1</sub>	1

**Table S4. A list of OSs in summer in Wuhan**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
177.9937	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	2	228.0667	C <sub>7</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	4
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	7	229.9886	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	3
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1
192.0095	C <sub>6</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	230.0251	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	5	232.0044	C <sub>8</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	7
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	232.0407	C <sub>9</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	4
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	6	234.9789	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	236.0357	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	6	236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	238.0149	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	238.0877	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
206.0251	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
208.0043	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	6	239.9942	C <sub>6</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	3
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	8	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	11
210.0563	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	7	240.1034	C <sub>9</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	6
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	242.0252	C <sub>10</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	2
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	7	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	242.0826	C <sub>8</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2	244.0044	C <sub>9</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	6	244.0254	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2
221.9470	C <sub>5</sub> H <sub>2</sub> O <sub>8</sub> S <sub>1</sub>	1	244.0407	C <sub>10</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	5
222.0200	C <sub>7</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5	246.0200	C <sub>9</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5
222.0928	C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	6	248.0721	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4
223.9993	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	2	248.9945	C <sub>7</sub> H <sub>7</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	7
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	4	250.0514	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	7	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	251.9940	C <sub>7</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	5
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	5	252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	5	252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	7
226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	3
227.0102	C <sub>5</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1	254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	5

254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5	277.0259	C <sub>9</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	8	278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
254.1190	C <sub>10</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3	280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4
255.0414	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	280.0982	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	7
256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	3	280.1347	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	6
256.0618	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	7	280.1709	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	4
257.0208	C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5	281.0207	C <sub>8</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1	282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	3
258.0201	C <sub>10</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	4	282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	6
258.0412	C <sub>7</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	1	282.1139	C <sub>11</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	11
259.0000	C <sub>5</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2	282.1503	C <sub>12</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	4
259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	283.0000	C <sub>7</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4
259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3	284.0203	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	9
260.0203	C <sub>6</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	2	284.0566	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	6
260.0357	C <sub>10</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2	284.0932	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	10
261.0157	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4	285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
262.0149	C <sub>9</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	2	285.9997	C <sub>7</sub> H <sub>10</sub> O <sub>10</sub> S <sub>1</sub>	2
263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	286.0360	C <sub>8</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3
264.0306	C <sub>9</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3	287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
264.0670	C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	2	287.0677	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
266.0099	C <sub>8</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	6	288.0153	C <sub>7</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	2
266.0252	C <sub>12</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	288.0307	C <sub>11</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	289.0259	C <sub>10</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
266.0826	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	5	294.0777	C <sub>11</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	2
266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	4	294.1141	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	9
266.1554	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	2	294.1503	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	7
268.0253	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	5	295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	5	296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4
268.0983	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	10	296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	7
268.1347	C <sub>11</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	3	296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	8
269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	296.1660	C <sub>13</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	5
270.0048	C <sub>7</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	2	297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
270.0411	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	8	298.0360	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	5
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	9	298.0724	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	8
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	298.1087	C <sub>11</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	10
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	3	299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
273.0158	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	300.0152	C <sub>8</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	6
274.0150	C <sub>10</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	300.0516	C <sub>9</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	1
274.0303	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1	301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	301.0833	C <sub>9</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
276.0307	C <sub>10</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	7	302.0309	C <sub>8</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2

306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7	338.1404	C <sub>14</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	9
308.0933	C <sub>12</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	2	338.1764	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	9
308.1296	C <sub>13</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	4	338.2130	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	7
308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	6	340.1195	C <sub>13</sub> H <sub>24</sub> O <sub>8</sub> S <sub>1</sub>	9
308.2021	C <sub>15</sub> H <sub>32</sub> O <sub>4</sub> S <sub>1</sub>	3	340.1559	C <sub>14</sub> H <sub>28</sub> O <sub>7</sub> S <sub>1</sub>	8
310.0361	C <sub>10</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	4	341.0421	C <sub>10</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3
310.0726	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	5	341.0784	C <sub>11</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4
310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	11	342.0624	C <sub>11</sub> H <sub>18</sub> O <sub>10</sub> S <sub>1</sub>	3
310.1450	C <sub>13</sub> H <sub>26</sub> O <sub>6</sub> S <sub>1</sub>	12	342.0989	C <sub>12</sub> H <sub>22</sub> O <sub>9</sub> S <sub>1</sub>	2
310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	6	343.0576	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6
311.0677	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7	345.0369	C <sub>9</sub> H <sub>15</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3
312.0518	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	3	345.0733	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7
312.0882	C <sub>11</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	8	348.1246	C <sub>15</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	10
312.1245	C <sub>12</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	4	350.1038	C <sub>14</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	5
313.0470	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6	350.1404	C <sub>15</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	6
313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7	350.1766	C <sub>16</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	7
314.0310	C <sub>9</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2	350.2130	C <sub>17</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	7
314.0675	C <sub>10</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	4	352.1198	C <sub>14</sub> H <sub>24</sub> O <sub>8</sub> S <sub>1</sub>	2
315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9	352.1557	C <sub>15</sub> H <sub>28</sub> O <sub>7</sub> S <sub>1</sub>	5
320.1298	C <sub>14</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	5	352.1922	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	9
322.1090	C <sub>13</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	5	352.2287	C <sub>17</sub> H <sub>36</sub> O <sub>5</sub> S <sub>1</sub>	2
322.1453	C <sub>14</sub> H <sub>26</sub> O <sub>6</sub> S <sub>1</sub>	4	354.0988	C <sub>13</sub> H <sub>22</sub> O <sub>9</sub> S <sub>1</sub>	4
322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	3	354.1353	C <sub>14</sub> H <sub>26</sub> O <sub>8</sub> S <sub>1</sub>	9
322.2179	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	4	354.1718	C <sub>15</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	5
324.0883	C <sub>12</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	4	355.0942	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
324.1245	C <sub>13</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	6	357.0735	C <sub>11</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4
324.1608	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	10	363.1356	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5
324.1971	C <sub>15</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	5	363.9484	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1
326.0675	C <sub>11</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	2	364.1925	C <sub>17</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	3
326.1040	C <sub>12</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	4	364.2286	C <sub>18</sub> H <sub>36</sub> O <sub>5</sub> S <sub>1</sub>	8
326.1403	C <sub>13</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	7	365.1150	C <sub>14</sub> H <sub>23</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
327.0626	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7	366.1716	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	11
328.0467	C <sub>10</sub> H <sub>16</sub> O <sub>10</sub> S <sub>1</sub>	3	366.2078	C <sub>17</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	8
329.0419	C <sub>9</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6	366.2440	C <sub>18</sub> H <sub>38</sub> O <sub>5</sub> S <sub>1</sub>	2
329.0783	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9	368.1144	C <sub>14</sub> H <sub>24</sub> O <sub>9</sub> S <sub>1</sub>	5
331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3	368.1509	C <sub>15</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	6
332.1298	C <sub>15</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	5	368.1873	C <sub>16</sub> H <sub>32</sub> O <sub>7</sub> S <sub>1</sub>	8
336.0882	C <sub>13</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	5	371.1618	C <sub>14</sub> H <sub>29</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
336.1611	C <sub>15</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	5	374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2
336.1974	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	2	377.1149	C <sub>15</sub> H <sub>23</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4
338.1040	C <sub>13</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2	378.2081	C <sub>18</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	4

379.1305	C <sub>15</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	8	408.2188	C <sub>19</sub> H <sub>36</sub> O <sub>7</sub> S <sub>1</sub>	4
380.1511	C <sub>16</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	3	408.2548	C <sub>20</sub> H <sub>40</sub> O <sub>6</sub> S <sub>1</sub>	5
380.1871	C <sub>17</sub> H <sub>32</sub> O <sub>7</sub> S <sub>1</sub>	6	410.1978	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	7
380.2233	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	11	410.2344	C <sub>19</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	3
382.1302	C <sub>15</sub> H <sub>26</sub> O <sub>9</sub> S <sub>1</sub>	4	411.1205	C <sub>15</sub> H <sub>25</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
382.1666	C <sub>16</sub> H <sub>30</sub> O <sub>8</sub> S <sub>1</sub>	3	412.1222	C <sub>16</sub> H <sub>28</sub> O <sub>8</sub> S <sub>2</sub>	2
382.2031	C <sub>17</sub> H <sub>34</sub> O <sub>7</sub> S <sub>1</sub>	4	413.1725	C <sub>16</sub> H <sub>31</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
385.1049	C <sub>13</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6	422.2705	C <sub>21</sub> H <sub>42</sub> O <sub>6</sub> S <sub>1</sub>	3
391.0245	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	3	424.2136	C <sub>19</sub> H <sub>36</sub> O <sub>8</sub> S <sub>1</sub>	6
394.2030	C <sub>18</sub> H <sub>34</sub> O <sub>7</sub> S <sub>1</sub>	10	426.2293	C <sub>19</sub> H <sub>38</sub> O <sub>8</sub> S <sub>1</sub>	8
394.2393	C <sub>19</sub> H <sub>38</sub> O <sub>6</sub> S <sub>1</sub>	4	436.2864	C <sub>22</sub> H <sub>44</sub> O <sub>6</sub> S <sub>1</sub>	4
395.1255	C <sub>15</sub> H <sub>25</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7	440.1724	C <sub>18</sub> H <sub>32</sub> O <sub>10</sub> S <sub>1</sub>	1
396.1823	C <sub>17</sub> H <sub>32</sub> O <sub>8</sub> S <sub>1</sub>	5	441.2037	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
396.2186	C <sub>18</sub> H <sub>36</sub> O <sub>7</sub> S <sub>1</sub>	5	457.1989	C <sub>18</sub> H <sub>35</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2

**Table S5. A list of OSs in summer daytime in Nanjing**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
168.0457	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	2	239.9942	C <sub>6</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	3
180.0094	C <sub>5</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	5	240.0306	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
180.0458	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	2	240.0670	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	4	242.0098	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	7
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	2	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4
194.0250	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	4	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	3	243.0416	C <sub>6</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
196.0406	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	11	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3
198.0199	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	2	252.0669	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6
198.0563	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	3	252.1033	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	4
208.0771	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	4	252.1395	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	5
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	4	254.0098	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	5
210.0564	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	2	254.0461	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	254.0826	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	255.0415	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	3	255.9892	C <sub>6</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
212.0720	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	3	256.0254	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	11
214.0149	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	256.0619	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	1
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	1	256.9844	C <sub>5</sub> H <sub>7</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
218.0250	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	257.0208	C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
222.0563	C <sub>8</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	257.0572	C <sub>7</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
224.0356	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	9	258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	2
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4	259.0000	C <sub>5</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
224.1084	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	261.0156	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
225.9786	C <sub>5</sub> H <sub>6</sub> O <sub>8</sub> S <sub>1</sub>	2	263.0102	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
226.0149	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	2	264.1033	C <sub>11</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2
226.0513	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	3	266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	1
226.0877	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	2	266.0826	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	2
227.9942	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	2	266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	4
228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3	266.1553	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	3
229.0259	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	268.0254	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	14
229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	1	268.0619	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	1
230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1	268.0981	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	5
236.0719	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	3	269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
238.0512	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2	270.0047	C <sub>7</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	5
238.0874	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	5	270.0412	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	1
238.1241	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	6	270.0775	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	1

271.0364	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6	310.0724	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	2
271.0728	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	6	310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	5
272.0204	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	2	310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	2
273.0157	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	1	311.0676	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
274.9950	C <sub>5</sub> H <sub>9</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	1	312.0516	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	2
275.0103	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	312.0882	C <sub>11</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	3
278.0462	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	2	313.0833	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
280.0618	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	3	314.0310	C <sub>9</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	3
280.0983	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	1	315.0626	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5
280.1346	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	3	315.0991	C <sub>10</sub> H <sub>21</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
280.1709	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	6	317.0053	C <sub>7</sub> H <sub>11</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3
282.0411	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	2	320.1295	C <sub>14</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	4
282.0775	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	2	322.1813	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	5
284.0203	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	5	322.2178	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	2
284.0567	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	3	324.0517	C <sub>11</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	4
285.0521	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	324.0880	C <sub>12</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	4
287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4	324.1246	C <sub>13</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	4
289.0107	C <sub>6</sub> H <sub>11</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4	324.1610	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	3
290.1190	C <sub>13</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	1	325.0470	C <sub>10</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
292.1347	C <sub>13</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	3	327.0626	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5
294.1504	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	4	329.0418	C <sub>9</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	5
294.1866	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	6	329.0782	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	331.0211	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	2
296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	2	331.0575	C <sub>9</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	4	336.1246	C <sub>14</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	5
296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	3	336.1972	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	5
297.0519	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4	338.1402	C <sub>14</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	7
297.0884	C <sub>10</sub> H <sub>19</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	338.1766	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	4
298.0359	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	6	340.0830	C <sub>12</sub> H <sub>20</sub> O <sub>9</sub> S <sub>1</sub>	3
299.0675	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	341.0784	C <sub>11</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
300.0152	C <sub>8</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	4	343.0574	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
300.0516	C <sub>9</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	5	345.0731	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4
301.0105	C <sub>7</sub> H <sub>11</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2	348.1246	C <sub>15</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	4
301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3	350.1037	C <sub>14</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	10
301.0832	C <sub>9</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4	350.1767	C <sub>16</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	5
306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	2	350.2128	C <sub>17</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	6
306.1139	C <sub>13</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	2	352.1560	C <sub>15</sub> H <sub>28</sub> O <sub>7</sub> S <sub>1</sub>	1
308.0931	C <sub>12</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	2	352.1919	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	8
308.1296	C <sub>13</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	3	354.2078	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1
308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	4	355.0940	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
308.2021	C <sub>15</sub> H <sub>32</sub> O <sub>4</sub> S <sub>1</sub>	4	355.1304	C <sub>13</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5

357.0734	C <sub>11</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3	384.0731	C <sub>13</sub> H <sub>20</sub> O <sub>11</sub> S <sub>1</sub>	2
359.0527	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	4	385.1047	C <sub>13</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3
363.1354	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5	391.0249	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	1
364.2286	C <sub>18</sub> H <sub>36</sub> O <sub>5</sub> S <sub>1</sub>	7	394.0937	C <sub>15</sub> H <sub>22</sub> O <sub>10</sub> S <sub>1</sub>	3
365.1147	C <sub>14</sub> H <sub>23</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	394.2029	C <sub>18</sub> H <sub>34</sub> O <sub>7</sub> S <sub>1</sub>	6
366.0986	C <sub>14</sub> H <sub>22</sub> O <sub>9</sub> S <sub>1</sub>	5	396.1092	C <sub>15</sub> H <sub>24</sub> O <sub>10</sub> S <sub>1</sub>	4
366.1713	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	7	396.2187	C <sub>18</sub> H <sub>36</sub> O <sub>7</sub> S <sub>1</sub>	2
366.2075	C <sub>17</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	5	398.2341	C <sub>18</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	1
368.1141	C <sub>14</sub> H <sub>24</sub> O <sub>9</sub> S <sub>1</sub>	4	409.1045	C <sub>15</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3
368.1509	C <sub>15</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	1	410.1974	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	3
368.1871	C <sub>16</sub> H <sub>32</sub> O <sub>7</sub> S <sub>1</sub>	4	411.1201	C <sub>15</sub> H <sub>25</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4
374.0634	C <sub>10</sub> H <sub>18</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	5	422.2341	C <sub>20</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	1
374.1040	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2	426.2655	C <sub>20</sub> H <sub>42</sub> O <sub>7</sub> S <sub>1</sub>	1
378.2079	C <sub>18</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	5	441.2036	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
379.1305	C <sub>15</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4	442.2604	C <sub>20</sub> H <sub>42</sub> O <sub>8</sub> S <sub>1</sub>	1
380.2232	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	13	486.2289	C <sub>24</sub> H <sub>38</sub> O <sub>8</sub> S <sub>1</sub>	2
382.0936	C <sub>14</sub> H <sub>22</sub> O <sub>10</sub> S <sub>1</sub>	3	530.3127	C <sub>24</sub> H <sub>50</sub> O <sub>10</sub> S <sub>1</sub>	1
382.2393	C <sub>18</sub> H <sub>38</sub> O <sub>6</sub> S <sub>1</sub>	1			

**Table S6. A list of OSs in summer nighttime in Nanjing**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
166.0301	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	7	228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
180.0458	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	2	229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	1
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	230.0251	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	232.0407	C <sub>9</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	4
188.0145	C <sub>7</sub> H <sub>8</sub> O <sub>4</sub> S <sub>1</sub>	3	236.0357	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	4	236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4
194.0250	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3	238.0149	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	3
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	5	238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	3	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	7
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	241.0259	C <sub>6</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
206.0251	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	4	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
208.0043	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6
208.0771	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	243.0417	C <sub>6</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	244.0254	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	1
210.0563	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	5	244.0407	C <sub>10</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	5
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	245.0207	C <sub>5</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	248.0721	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	3
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	6	250.0514	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
223.9993	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	2	254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	5	254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4	254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	255.0415	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	7	256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2
226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	4	256.0618	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4
226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4	256.9845	C <sub>5</sub> H <sub>7</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	1
227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1	257.0209	C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4

258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1	286.0360	C <sub>8</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3
258.0412	C <sub>7</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	1	286.1242	C <sub>14</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	1
259.0000	C <sub>5</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3	287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	287.0677	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4
259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3	288.1399	C <sub>14</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	1
261.0157	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4	289.0259	C <sub>10</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
263.0102	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	294.0412	C <sub>10</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4
264.0306	C <sub>9</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3	294.0777	C <sub>11</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	2
264.0670	C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	2	294.1505	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	4
266.0252	C <sub>12</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	2
266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
266.0827	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	3	296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	3
266.1191	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	2	296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	3
266.1554	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	2	297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
268.0253	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	5	298.0360	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3
268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	5	298.0724	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	5
268.0984	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	6	299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	300.0152	C <sub>8</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	4
270.0048	C <sub>7</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	2	300.0516	C <sub>9</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	1
270.0412	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	6	301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	8	301.0833	C <sub>9</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
271.0364	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7	306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	2	308.0048	C <sub>6</sub> H <sub>12</sub> O <sub>12</sub> S <sub>1</sub>	3
273.0158	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	5
273.0522	C <sub>7</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	309.0521	C <sub>10</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
274.9951	C <sub>5</sub> H <sub>9</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2	310.0361	C <sub>10</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	4
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	310.0726	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	4
277.0259	C <sub>9</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	8
278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3	310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	4
280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	311.0102	C <sub>12</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
280.0983	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	4	311.0677	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
280.1348	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	2	312.0518	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	3
280.1710	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	3	313.0470	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	3	313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	4	314.0310	C <sub>9</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2
284.0204	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	8	314.0675	C <sub>10</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	4
284.0569	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4	315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
284.0932	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	6	322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	1
285.0156	C <sub>7</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2	322.2179	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	2
285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	324.1609	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	5
285.9997	C <sub>7</sub> H <sub>10</sub> O <sub>10</sub> S <sub>1</sub>	2	325.0470	C <sub>10</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3

326.0675	C <sub>11</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	1	384.1972	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1
327.0626	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6	385.1049	C <sub>13</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6
328.0467	C <sub>10</sub> H <sub>16</sub> O <sub>10</sub> S <sub>1</sub>	3	391.0245	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	4
329.0419	C <sub>9</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6	393.1100	C <sub>15</sub> H <sub>23</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	1
329.0783	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	8	395.1255	C <sub>15</sub> H <sub>25</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3	396.2186	C <sub>18</sub> H <sub>36</sub> O <sub>7</sub> S <sub>1</sub>	3
332.1299	C <sub>15</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	4	397.1410	C <sub>15</sub> H <sub>27</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
336.0882	C <sub>13</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	5	409.1048	C <sub>15</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
337.0836	C <sub>12</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	1	410.1981	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	1
338.2130	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	3	411.1205	C <sub>15</sub> H <sub>25</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
341.0421	C <sub>10</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3	413.1362	C <sub>15</sub> H <sub>27</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2
341.0784	C <sub>11</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4	413.9742	C <sub>11</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
342.0624	C <sub>11</sub> H <sub>18</sub> O <sub>10</sub> S <sub>1</sub>	3	425.0998	C <sub>15</sub> H <sub>23</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	2
343.0576	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6	425.9192	C <sub>11</sub> H <sub>6</sub> O <sub>14</sub> S <sub>2</sub>	1
345.0369	C <sub>9</sub> H <sub>15</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3	425.9743	C <sub>12</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
345.0733	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7	427.1154	C <sub>15</sub> H <sub>25</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	1
348.1246	C <sub>15</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	10	438.0108	C <sub>14</sub> H <sub>14</sub> O <sub>14</sub> S <sub>1</sub>	1
350.1404	C <sub>15</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	5	438.1354	C <sub>21</sub> H <sub>26</sub> O <sub>8</sub> S <sub>1</sub>	1
352.1923	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	6	441.2037	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
354.2079	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1	442.0512	C <sub>25</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	1
355.0942	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3	443.1106	C <sub>15</sub> H <sub>25</sub> O <sub>12</sub> N <sub>1</sub> S <sub>1</sub>	1
356.1659	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	1	456.1460	C <sub>21</sub> H <sub>28</sub> O <sub>9</sub> S <sub>1</sub>	1
357.0735	C <sub>11</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4	494.2136	C <sub>29</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	1
363.1357	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	495.9773	C <sub>19</sub> H <sub>12</sub> O <sub>12</sub> S <sub>2</sub>	1
363.9484	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1	499.9235	C <sub>9</sub> H <sub>8</sub> O <sub>22</sub> S <sub>1</sub>	1
364.1196	C <sub>15</sub> H <sub>24</sub> O <sub>8</sub> S <sub>1</sub>	5	525.9679	C <sub>11</sub> H <sub>14</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	1
365.1150	C <sub>14</sub> H <sub>23</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	531.9747	C <sub>13</sub> H <sub>12</sub> O <sub>19</sub> N <sub>2</sub> S <sub>1</sub>	2
366.1715	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	4	533.9332	C <sub>15</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>1</sub>	1
368.1873	C <sub>16</sub> H <sub>32</sub> O <sub>7</sub> S <sub>1</sub>	6	539.9671	C <sub>20</sub> H <sub>12</sub> O <sub>14</sub> S <sub>2</sub>	1
369.1098	C <sub>13</sub> H <sub>23</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2	545.9742	C <sub>22</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2	575.9650	C <sub>14</sub> H <sub>12</sub> O <sub>21</sub> N <sub>2</sub> S <sub>1</sub>	1
376.1924	C <sub>18</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	1	581.9719	C <sub>29</sub> H <sub>10</sub> O <sub>10</sub> S <sub>2</sub>	1
377.1149	C <sub>15</sub> H <sub>23</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4	589.9641	C <sub>23</sub> H <sub>10</sub> O <sub>17</sub> S <sub>1</sub>	1
379.1305	C <sub>15</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	8	631.9687	C <sub>11</sub> H <sub>20</sub> O <sub>26</sub> S <sub>2</sub>	1
380.1652	C <sub>20</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	1	649.9218	C <sub>13</sub> H <sub>14</sub> O <sub>26</sub> S <sub>2</sub>	3
380.2236	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	6	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	1
381.1463	C <sub>15</sub> H <sub>27</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	1
381.9843	C <sub>11</sub> H <sub>10</sub> O <sub>13</sub> S <sub>1</sub>	2	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	1

**Table S7. A list of OSs in winter daytime in Shanghai**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
166.0301	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	7	228.0096	C <sub>9</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	4
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
180.0458	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	2
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	230.0251	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	5	232.0044	C <sub>8</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4
194.0250	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	4	232.0407	C <sub>9</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	4
194.0614	C <sub>7</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	5	234.9789	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4	236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	5	238.0150	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	3
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
208.0043	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	10
208.0771	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	4	240.1034	C <sub>9</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	5
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	241.0259	C <sub>6</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	6	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	2
210.0564	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	7	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	243.9891	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	8	244.0044	C <sub>9</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
213.9939	C <sub>8</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	250.1243	C <sub>11</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	1
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2
222.0928	C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	5	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
223.9993	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	2	254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	4	254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	255.0414	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
225.9786	C <sub>5</sub> H <sub>6</sub> O <sub>8</sub> S <sub>1</sub>	1	256.0619	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	3
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	7	257.0573	C <sub>7</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	5	258.0201	C <sub>10</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5
226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4	259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1	259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3

263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	9
266.0252	C <sub>12</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	5
266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	311.0102	C <sub>12</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
266.0827	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	3	313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3	315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5
266.1555	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	3	322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	1
268.0256	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	4	322.2179	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	3
268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	324.1609	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	4
268.0984	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	6	328.1345	C <sub>16</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	1
269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	2
270.0412	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	6	336.1974	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	7	338.2131	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	5
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	346.0760	C <sub>11</sub> H <sub>22</sub> O <sub>8</sub> S <sub>2</sub>	1
274.0150	C <sub>10</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	352.1923	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	6
274.0303	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1	354.2079	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	2
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	356.1659	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	2
280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	363.1357	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
280.0982	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	5	363.9485	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1
280.1347	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	4	366.1716	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	7
280.1709	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	4	368.1510	C <sub>15</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	2
282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4	380.2236	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	4
282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	5	382.2395	C <sub>18</sub> H <sub>38</sub> O <sub>6</sub> S <sub>1</sub>	1
282.1139	C <sub>11</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	8	384.1972	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1
283.0001	C <sub>7</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2	385.9429	C <sub>9</sub> H <sub>6</sub> O <sub>15</sub> S <sub>1</sub>	1
283.0729	C <sub>9</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	398.2345	C <sub>18</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	1
284.0204	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	6	402.1306	C <sub>13</sub> H <sub>26</sub> O <sub>10</sub> N <sub>2</sub> S <sub>1</sub>	1
284.0569	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4	410.1981	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	1
285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	422.2345	C <sub>20</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	1
287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	425.9192	C <sub>11</sub> H <sub>6</sub> O <sub>14</sub> S <sub>2</sub>	1
287.0677	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4	440.0843	C <sub>12</sub> H <sub>24</sub> O <sub>15</sub> S <sub>1</sub>	1
289.0259	C <sub>10</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	5	440.1724	C <sub>18</sub> H <sub>32</sub> O <sub>10</sub> S <sub>1</sub>	1
294.1141	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	7	442.2607	C <sub>20</sub> H <sub>42</sub> O <sub>8</sub> S <sub>1</sub>	1
294.1505	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	3	453.9304	C <sub>16</sub> H <sub>6</sub> O <sub>12</sub> S <sub>2</sub>	1
294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	3	456.1098	C <sub>20</sub> H <sub>24</sub> O <sub>10</sub> S <sub>1</sub>	1
295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	499.9235	C <sub>9</sub> H <sub>8</sub> O <sub>22</sub> S <sub>1</sub>	1
296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	3	521.9178	C <sub>10</sub> H <sub>6</sub> O <sub>21</sub> N <sub>2</sub> S <sub>1</sub>	1
296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	5	589.9054	C <sub>17</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	2
297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	645.9682	C <sub>21</sub> H <sub>14</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	1
299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	651.8755	C <sub>10</sub> H <sub>8</sub> O <sub>27</sub> N <sub>2</sub> S <sub>2</sub>	1
306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	2
308.1660	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	3			

**Table S8. A list of OSs in winter nighttime in Shanghai**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
166.0301	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	8	225.9785	C <sub>5</sub> H <sub>6</sub> O <sub>8</sub> S <sub>1</sub>	2
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	7
177.9937	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	3	226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	5
180.0458	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	228.0096	C <sub>9</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
188.0146	C <sub>7</sub> H <sub>8</sub> O <sub>4</sub> S <sub>1</sub>	3	228.0667	C <sub>7</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	3
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	5	229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
194.0250	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	4	229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	2
194.0614	C <sub>7</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	230.0251	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	6	232.0044	C <sub>8</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	6
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	232.0407	C <sub>9</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	234.9789	C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	236.0357	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2
200.0146	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub> S <sub>1</sub>	5	236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	238.0150	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
208.0043	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4	238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3
208.0771	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	9
210.0564	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	5	240.1034	C <sub>9</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	6
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	241.0259	C <sub>6</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	3
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	8	242.0251	C <sub>10</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
213.9939	C <sub>8</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	242.0826	C <sub>8</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	243.0416	C <sub>6</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	1	243.9891	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	244.0044	C <sub>9</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4
222.0928	C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	4	244.0255	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	1
223.9993	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	2	244.0407	C <sub>10</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	6
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2	246.0200	C <sub>9</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	6	248.0357	C <sub>9</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	3
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	248.0721	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	3

250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4	275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
250.1243	C <sub>11</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	1	277.0259	C <sub>9</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5	278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6	280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4
252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2	280.0982	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	6
252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3	280.1347	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	4
254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4	280.1710	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	3
254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	3
254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	8	282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	5
255.0415	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	282.1139	C <sub>11</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	8
256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2	283.0000	C <sub>7</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
256.0619	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	283.0729	C <sub>9</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
257.0208	C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5	284.0204	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	7
257.0572	C <sub>7</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	284.0569	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	5
258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1	284.0932	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	7
258.0201	C <sub>10</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5	284.9946	C <sub>10</sub> H <sub>7</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3	287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
261.0157	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4	287.0677	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	288.0459	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	1
266.0099	C <sub>8</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	5	289.0259	C <sub>10</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
266.0252	C <sub>12</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	1	294.0777	C <sub>11</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	2
266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4	294.1141	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	7
266.0827	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	3	294.1505	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	4
266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3	294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	2
266.1555	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	2	295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
268.0253	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	5	296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4
268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	3	296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	5
268.0984	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	9	296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	7
269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
270.0048	C <sub>7</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	2	297.0884	C <sub>10</sub> H <sub>19</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
270.0411	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	8	298.0301	C <sub>16</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	7	298.0360	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	4
271.0365	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6	298.0724	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	6
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	2	301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
272.0357	C <sub>11</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	3	301.0833	C <sub>9</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2
273.0158	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	302.0097	C <sub>11</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
273.0522	C <sub>7</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7
274.0150	C <sub>10</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	308.0934	C <sub>12</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	2
274.0303	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub> S <sub>1</sub>	1	308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	4

310.0726	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	4	343.0576	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3
310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	7	343.1304	C <sub>12</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
310.1453	C <sub>13</sub> H <sub>26</sub> O <sub>6</sub> S <sub>1</sub>	7	345.0733	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6
310.1816	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	7	350.1404	C <sub>15</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	5
311.0102	C <sub>12</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	352.1923	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	6
311.0678	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6	354.2080	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1
312.0518	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	2	355.0942	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
312.0882	C <sub>11</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	5	356.1659	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	2
313.0470	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6	363.1357	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7	363.9485	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1
315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9	366.1716	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	5
315.0992	C <sub>10</sub> H <sub>21</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	1	366.2080	C <sub>17</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	4
321.0157	C <sub>10</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	1	368.1510	C <sub>15</sub> H <sub>28</sub> O <sub>8</sub> S <sub>1</sub>	3
322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	2	374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2
322.2179	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	2	380.2236	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	5
324.1246	C <sub>13</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	3	384.1972	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1
324.1609	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	6	391.0245	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	3
327.0627	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	410.1981	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	1
327.0992	C <sub>11</sub> H <sub>21</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	413.9742	C <sub>11</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
327.1356	C <sub>12</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	422.2342	C <sub>20</sub> H <sub>38</sub> O <sub>7</sub> S <sub>1</sub>	2
329.0783	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	8	425.9192	C <sub>11</sub> H <sub>6</sub> O <sub>14</sub> S <sub>2</sub>	1
331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3	440.0843	C <sub>12</sub> H <sub>24</sub> O <sub>15</sub> S <sub>1</sub>	1
336.1974	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	2	441.2037	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
338.1404	C <sub>14</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	5	484.0526	C <sub>16</sub> H <sub>20</sub> O <sub>15</sub> S <sub>1</sub>	1
338.1767	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	5	499.9235	C <sub>9</sub> H <sub>8</sub> O <sub>22</sub> S <sub>1</sub>	1
338.2130	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	6	533.9332	C <sub>15</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>1</sub>	1
340.1195	C <sub>13</sub> H <sub>24</sub> O <sub>8</sub> S <sub>1</sub>	5	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	1
341.1511	C <sub>13</sub> H <sub>27</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1			

**Table S9. A list of OSs in summer daytime in Shanghai**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	5	238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	9
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	4	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	5
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	4	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	244.0254	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	1
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	248.0721	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	3
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	250.0514	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
208.0043	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	4	251.9940	C <sub>7</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	3
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
210.0563	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	6	252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	5
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	3
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	6	254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5
213.9939	C <sub>8</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	256.0618	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	7
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2	258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3	258.0201	C <sub>10</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	5
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2	258.0412	C <sub>7</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	1
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	4	259.0000	C <sub>5</sub> H <sub>9</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	7	259.9993	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	3
226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	4	261.0157	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4
226.0878	C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4	262.0513	C <sub>10</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	4
227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1	263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5	264.0306	C <sub>9</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3
229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	264.0670	C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	2
229.9887	C <sub>8</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	1	266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4
230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1	266.0826	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	4
236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3
238.0149	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	266.1554	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	2
238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2	268.0253	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	4

268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	298.0724	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	8
268.0983	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	8	299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
270.0048	C <sub>7</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	2	300.0152	C <sub>8</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	4
270.0411	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	8	301.0106	C <sub>7</sub> H <sub>11</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	7	301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
271.0366	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	302.0309	C <sub>8</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	2	308.0933	C <sub>12</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	2
273.0158	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	308.1296	C <sub>13</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	3
274.0362	C <sub>7</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	1	308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	6
274.9951	C <sub>5</sub> H <sub>9</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	2	310.0361	C <sub>10</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	4
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	310.0726	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	5
278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3	310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	11
280.0255	C <sub>9</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2	310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	4
280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	311.0678	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
280.0983	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	5	312.0518	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	3
280.1347	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	5	312.0882	C <sub>11</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	5
280.1710	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	1	313.0470	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4	313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	5	314.0310	C <sub>9</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2
282.1139	C <sub>11</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	7	314.0675	C <sub>10</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	5
284.0203	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	8	315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9
284.0566	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	6	318.0412	C <sub>12</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	2
284.0932	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	9	322.1090	C <sub>13</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	4
285.0158	C <sub>7</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	1	322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	2
285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	322.2179	C <sub>16</sub> H <sub>34</sub> O <sub>4</sub> S <sub>1</sub>	3
285.9997	C <sub>7</sub> H <sub>10</sub> O <sub>10</sub> S <sub>1</sub>	2	324.0883	C <sub>12</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	4
286.0360	C <sub>8</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3	324.1246	C <sub>13</sub> H <sub>24</sub> O <sub>7</sub> S <sub>1</sub>	4
287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7	324.1609	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	6
288.0153	C <sub>7</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	2	326.0675	C <sub>11</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	2
294.0412	C <sub>10</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4	327.0626	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
294.0777	C <sub>11</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	2	327.0992	C <sub>11</sub> H <sub>21</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
294.1141	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	8	328.0467	C <sub>10</sub> H <sub>16</sub> O <sub>10</sub> S <sub>1</sub>	3
294.1505	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	4	329.0419	C <sub>9</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6
294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	3	331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3
295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	336.0882	C <sub>13</sub> H <sub>20</sub> O <sub>8</sub> S <sub>1</sub>	5
296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4	336.1974	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	2
296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	4	338.1404	C <sub>14</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	5
296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	6	338.1767	C <sub>15</sub> H <sub>30</sub> O <sub>6</sub> S <sub>1</sub>	5
297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	338.2130	C <sub>16</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	4
298.0360	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3	341.0421	C <sub>10</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3

342.0624	C <sub>11</sub> H <sub>18</sub> O <sub>10</sub> S <sub>1</sub>	3	385.9429	C <sub>9</sub> H <sub>6</sub> O <sub>15</sub> S <sub>1</sub>	1
343.0576	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7	390.0991	C <sub>16</sub> H <sub>22</sub> O <sub>9</sub> S <sub>1</sub>	1
350.1038	C <sub>14</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	5	398.1194	C <sub>22</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	1
350.1404	C <sub>15</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	5	413.9742	C <sub>11</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
350.2130	C <sub>17</sub> H <sub>34</sub> O <sub>5</sub> S <sub>1</sub>	4	418.1330	C <sub>15</sub> H <sub>30</sub> O <sub>9</sub> S <sub>2</sub>	1
352.0829	C <sub>13</sub> H <sub>20</sub> O <sub>9</sub> S <sub>1</sub>	4	425.9192	C <sub>11</sub> H <sub>6</sub> O <sub>14</sub> S <sub>2</sub>	1
352.1198	C <sub>14</sub> H <sub>24</sub> O <sub>8</sub> S <sub>1</sub>	2	425.9743	C <sub>12</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1
352.1561	C <sub>15</sub> H <sub>28</sub> O <sub>7</sub> S <sub>1</sub>	3	440.0843	C <sub>12</sub> H <sub>24</sub> O <sub>15</sub> S <sub>1</sub>	1
352.1923	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	6	453.9304	C <sub>16</sub> H <sub>6</sub> O <sub>12</sub> S <sub>2</sub>	1
354.0988	C <sub>13</sub> H <sub>22</sub> O <sub>9</sub> S <sub>1</sub>	4	456.1098	C <sub>20</sub> H <sub>24</sub> O <sub>10</sub> S <sub>1</sub>	1
354.2079	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1	484.0526	C <sub>16</sub> H <sub>20</sub> O <sub>15</sub> S <sub>1</sub>	1
356.1659	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	1	499.9235	C <sub>9</sub> H <sub>8</sub> O <sub>22</sub> S <sub>1</sub>	1
361.0684	C <sub>10</sub> H <sub>19</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	2	521.9178	C <sub>10</sub> H <sub>6</sub> O <sub>21</sub> N <sub>2</sub> S <sub>1</sub>	1
363.1357	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1	525.9679	C <sub>11</sub> H <sub>14</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	1
363.9484	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1	531.9747	C <sub>13</sub> H <sub>12</sub> O <sub>19</sub> N <sub>2</sub> S <sub>1</sub>	2
366.1715	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	6	533.9332	C <sub>15</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>1</sub>	1
366.2078	C <sub>17</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	6	539.9671	C <sub>20</sub> H <sub>12</sub> O <sub>14</sub> S <sub>2</sub>	1
368.1144	C <sub>14</sub> H <sub>24</sub> O <sub>9</sub> S <sub>1</sub>	5	550.1753	C <sub>20</sub> H <sub>38</sub> O <sub>13</sub> S <sub>2</sub>	1
369.9841	C <sub>10</sub> H <sub>10</sub> O <sub>13</sub> S <sub>1</sub>	2	589.9054	C <sub>17</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	1
374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2	651.8755	C <sub>10</sub> H <sub>8</sub> O <sub>27</sub> N <sub>2</sub> S <sub>2</sub>	1
380.2236	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	5	696.8671	C <sub>11</sub> H <sub>7</sub> O <sub>32</sub> N <sub>1</sub> S <sub>1</sub>	1
381.9843	C <sub>11</sub> H <sub>10</sub> O <sub>13</sub> S <sub>1</sub>	2	699.9188	C <sub>16</sub> H <sub>12</sub> O <sub>29</sub> S <sub>1</sub>	1
384.1972	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1	725.8798	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	3

**Table S10. A list of OSs in summer nighttime in Shanghai**

Neutral Mass	formula	Number of isomers	Neutral Mass	formula	Number of isomers
168.0458	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> S <sub>1</sub>	3	240.0671	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	9
182.0251	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	6	241.0259	C <sub>6</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
182.0615	C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> S <sub>1</sub>	6	242.0099	C <sub>6</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	5
184.0407	C <sub>5</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	3	242.0463	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4
193.9886	C <sub>5</sub> H <sub>6</sub> O <sub>6</sub> S <sub>1</sub>	4	243.0052	C <sub>5</sub> H <sub>9</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6
196.0043	C <sub>5</sub> H <sub>8</sub> O <sub>6</sub> S <sub>1</sub>	5	243.0416	C <sub>6</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
196.0407	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> S <sub>1</sub>	6	243.9890	C <sub>5</sub> H <sub>8</sub> O <sub>9</sub> S <sub>1</sub>	1
196.0771	C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>1</sub>	3	244.0254	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2
198.0200	C <sub>5</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	7	250.0514	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2
198.0564	C <sub>6</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	4	250.0877	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	4
200.0357	C <sub>5</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	1	252.0306	C <sub>8</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5
201.9938	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub> S <sub>1</sub>	1	252.0670	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S <sub>1</sub>	6
209.9836	C <sub>5</sub> H <sub>6</sub> O <sub>7</sub> S <sub>1</sub>	2	252.1035	C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> S <sub>1</sub>	2
210.0200	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	8	252.1399	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> S <sub>1</sub>	3
210.0563	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> S <sub>1</sub>	7	254.0099	C <sub>7</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	4
210.0928	C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>1</sub>	3	254.0463	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	5
211.9993	C <sub>5</sub> H <sub>8</sub> O <sub>7</sub> S <sub>1</sub>	1	254.0827	C <sub>9</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	6
212.0356	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	6	255.0414	C <sub>7</sub> H <sub>13</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
212.0721	C <sub>7</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	256.0256	C <sub>7</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2
214.0150	C <sub>5</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	1	256.0618	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	7
216.0095	C <sub>8</sub> H <sub>8</sub> O <sub>5</sub> S <sub>1</sub>	3	257.0208	C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
216.0306	C <sub>5</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2	257.0572	C <sub>7</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3
218.0251	C <sub>8</sub> H <sub>10</sub> O <sub>5</sub> S <sub>1</sub>	3	258.0048	C <sub>6</sub> H <sub>10</sub> O <sub>9</sub> S <sub>1</sub>	1
224.0357	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	5	258.0412	C <sub>7</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	1
224.0720	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	6	259.0364	C <sub>6</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3
224.1085	C <sub>9</sub> H <sub>20</sub> O <sub>4</sub> S <sub>1</sub>	4	260.0357	C <sub>10</sub> H <sub>12</sub> O <sub>6</sub> S <sub>1</sub>	2
226.0150	C <sub>6</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	7	261.0157	C <sub>5</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	4
226.0514	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	4	263.0103	C <sub>8</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	1
227.9943	C <sub>5</sub> H <sub>8</sub> O <sub>8</sub> S <sub>1</sub>	1	264.0306	C <sub>9</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	3
228.0306	C <sub>6</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	5	266.0462	C <sub>9</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	4
229.0260	C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	266.0827	C <sub>10</sub> H <sub>18</sub> O <sub>6</sub> S <sub>1</sub>	4
230.0098	C <sub>5</sub> H <sub>10</sub> O <sub>8</sub> S <sub>1</sub>	1	266.1190	C <sub>11</sub> H <sub>22</sub> O <sub>5</sub> S <sub>1</sub>	3
236.0721	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub> S <sub>1</sub>	5	266.1554	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S <sub>1</sub>	3
238.0149	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> S <sub>1</sub>	4	268.0253	C <sub>8</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	5
238.0514	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub> S <sub>1</sub>	2	268.0620	C <sub>9</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	5
238.0878	C <sub>9</sub> H <sub>18</sub> O <sub>5</sub> S <sub>1</sub>	3	268.0983	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	8
238.1242	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S <sub>1</sub>	4	269.0572	C <sub>8</sub> H <sub>15</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2
240.0307	C <sub>7</sub> H <sub>12</sub> O <sub>7</sub> S <sub>1</sub>	2	270.0048	C <sub>7</sub> H <sub>10</sub> O <sub>6</sub> S <sub>1</sub>	2

270.0412	C <sub>8</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	7	301.0468	C <sub>8</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
270.0776	C <sub>9</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	9	306.0007	C <sub>5</sub> H <sub>10</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	7
271.0365	C <sub>7</sub> H <sub>13</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6	308.1659	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	6
271.0729	C <sub>8</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4	310.0726	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	5
272.0205	C <sub>7</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	3	310.1088	C <sub>12</sub> H <sub>22</sub> O <sub>7</sub> S <sub>1</sub>	10
273.0158	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	5	310.1815	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	3
273.0522	C <sub>7</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	311.0678	C <sub>10</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5
274.0362	C <sub>7</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	1	312.0518	C <sub>10</sub> H <sub>16</sub> O <sub>9</sub> S <sub>1</sub>	3
275.0104	C <sub>9</sub> H <sub>9</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	2	313.0470	C <sub>9</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	6
277.0259	C <sub>9</sub> H <sub>11</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	313.0834	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	7
278.0463	C <sub>10</sub> H <sub>14</sub> O <sub>7</sub> S <sub>1</sub>	3	314.0310	C <sub>9</sub> H <sub>14</sub> O <sub>10</sub> S <sub>1</sub>	2
280.0255	C <sub>9</sub> H <sub>12</sub> O <sub>8</sub> S <sub>1</sub>	2	314.0675	C <sub>10</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	4
280.0619	C <sub>10</sub> H <sub>16</sub> O <sub>7</sub> S <sub>1</sub>	4	315.0627	C <sub>9</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9
280.0982	C <sub>11</sub> H <sub>20</sub> O <sub>6</sub> S <sub>1</sub>	6	322.1817	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S <sub>1</sub>	2
280.1347	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S <sub>1</sub>	4	324.1609	C <sub>14</sub> H <sub>28</sub> O <sub>6</sub> S <sub>1</sub>	6
280.1710	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> S <sub>1</sub>	2	325.0470	C <sub>10</sub> H <sub>15</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
282.0412	C <sub>9</sub> H <sub>14</sub> O <sub>8</sub> S <sub>1</sub>	4	326.0675	C <sub>11</sub> H <sub>18</sub> O <sub>9</sub> S <sub>1</sub>	2
282.0776	C <sub>10</sub> H <sub>18</sub> O <sub>7</sub> S <sub>1</sub>	5	327.0626	C <sub>10</sub> H <sub>17</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7
284.0203	C <sub>8</sub> H <sub>12</sub> O <sub>9</sub> S <sub>1</sub>	8	327.0992	C <sub>11</sub> H <sub>21</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	4
284.0569	C <sub>9</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	5	328.0467	C <sub>10</sub> H <sub>16</sub> O <sub>10</sub> S <sub>1</sub>	3
284.0932	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	7	329.0419	C <sub>9</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6
285.0156	C <sub>7</sub> H <sub>11</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2	329.0783	C <sub>10</sub> H <sub>19</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	9
285.0522	C <sub>8</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	331.0213	C <sub>8</sub> H <sub>13</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3
285.9997	C <sub>7</sub> H <sub>10</sub> O <sub>10</sub> S <sub>1</sub>	2	336.1974	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	2
286.0360	C <sub>8</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3	338.1404	C <sub>14</sub> H <sub>26</sub> O <sub>7</sub> S <sub>1</sub>	6
287.0313	C <sub>7</sub> H <sub>13</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	7	341.0421	C <sub>10</sub> H <sub>15</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	3
287.0677	C <sub>8</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	5	342.0624	C <sub>11</sub> H <sub>18</sub> O <sub>10</sub> S <sub>1</sub>	3
288.0153	C <sub>7</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	2	343.0576	C <sub>10</sub> H <sub>17</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7
294.1141	C <sub>12</sub> H <sub>22</sub> O <sub>6</sub> S <sub>1</sub>	8	345.0369	C <sub>9</sub> H <sub>15</sub> O <sub>11</sub> N <sub>1</sub> S <sub>1</sub>	3
294.1505	C <sub>13</sub> H <sub>26</sub> O <sub>5</sub> S <sub>1</sub>	3	345.0733	C <sub>10</sub> H <sub>19</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	7
294.1868	C <sub>14</sub> H <sub>30</sub> O <sub>4</sub> S <sub>1</sub>	4	352.1923	C <sub>16</sub> H <sub>32</sub> O <sub>6</sub> S <sub>1</sub>	6
295.0729	C <sub>10</sub> H <sub>17</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	3	354.2079	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S <sub>1</sub>	1
296.0567	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub> S <sub>1</sub>	4	355.0942	C <sub>12</sub> H <sub>21</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	3
296.0931	C <sub>11</sub> H <sub>20</sub> O <sub>7</sub> S <sub>1</sub>	6	356.1659	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub> S <sub>1</sub>	1
296.1295	C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> S <sub>1</sub>	6	363.1357	C <sub>15</sub> H <sub>25</sub> O <sub>7</sub> N <sub>1</sub> S <sub>1</sub>	4
297.0520	C <sub>9</sub> H <sub>15</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	2	363.9484	C <sub>9</sub> H <sub>4</sub> O <sub>12</sub> N <sub>2</sub> S <sub>1</sub>	1
298.0360	C <sub>9</sub> H <sub>14</sub> O <sub>9</sub> S <sub>1</sub>	3	366.1715	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> S <sub>1</sub>	6
298.0724	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> S <sub>1</sub>	8	369.9841	C <sub>10</sub> H <sub>10</sub> O <sub>13</sub> S <sub>1</sub>	2
299.0677	C <sub>9</sub> H <sub>17</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	3	374.1041	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub> S <sub>1</sub>	2
300.0152	C <sub>8</sub> H <sub>12</sub> O <sub>10</sub> S <sub>1</sub>	6	379.1305	C <sub>15</sub> H <sub>25</sub> O <sub>8</sub> N <sub>1</sub> S <sub>1</sub>	6
301.0106	C <sub>7</sub> H <sub>11</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	4	380.2236	C <sub>18</sub> H <sub>36</sub> O <sub>6</sub> S <sub>1</sub>	4

381.9843	C <sub>11</sub> H <sub>10</sub> O <sub>13</sub> S <sub>1</sub>	2	441.2037	C <sub>18</sub> H <sub>35</sub> O <sub>9</sub> N <sub>1</sub> S <sub>1</sub>	2
384.1972	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub> S <sub>1</sub>	1	453.9304	C <sub>16</sub> H <sub>6</sub> O <sub>12</sub> S <sub>2</sub>	1
385.1049	C <sub>13</sub> H <sub>23</sub> O <sub>10</sub> N <sub>1</sub> S <sub>1</sub>	6	521.9178	C <sub>10</sub> H <sub>6</sub> O <sub>21</sub> N <sub>2</sub> S <sub>1</sub>	1
385.9429	C <sub>9</sub> H <sub>6</sub> O <sub>15</sub> S <sub>1</sub>	1	533.9332	C <sub>15</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>1</sub>	1
391.0245	C <sub>10</sub> H <sub>17</sub> O <sub>11</sub> N <sub>1</sub> S <sub>2</sub>	3	539.9671	C <sub>20</sub> H <sub>12</sub> O <sub>14</sub> S <sub>2</sub>	1
410.1981	C <sub>18</sub> H <sub>34</sub> O <sub>8</sub> S <sub>1</sub>	1	589.9054	C <sub>17</sub> H <sub>6</sub> O <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	1
413.9742	C <sub>11</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1	725.8800	C <sub>17</sub> H <sub>10</sub> O <sub>28</sub> S <sub>2</sub>	2
425.9743	C <sub>12</sub> H <sub>10</sub> O <sub>15</sub> S <sub>1</sub>	1			