

# EXACT MASS

	Dalton (a.m.u.)
proton	1.00728
neutron	1.00866
electron	0.0005486

# List of possible molecular formulae from a monoisotopic (exact) mass

Molecular formula range: C3-20 H4-20 O0-3 N0-2 ; Cl0-2, Br0-2, S0-2

Mass range: 100 - 200

Unsaturation: 0 - 7

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>5</sub> H <sub>5</sub> Cl	100.00798	C <sub>5</sub> H <sub>12</sub> S	104.06597	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O	110.04801	C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> S	115.99320
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S	100.00952	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	104.08373	C <sub>7</sub> H <sub>10</sub> O	110.07316	C <sub>5</sub> H <sub>5</sub> ClO	116.00289
C <sub>4</sub> H <sub>4</sub> O <sub>3</sub>	100.01604	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O	104.09496	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub>	110.08440	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> OS	116.00443
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	100.02728	C <sub>3</sub> H <sub>4</sub> CINO	104.99814	C <sub>8</sub> H <sub>14</sub>	110.10955	C <sub>4</sub> H <sub>5</sub> CIN <sub>2</sub>	116.01413
C <sub>8</sub> H <sub>4</sub>	100.03130	C <sub>3</sub> H <sub>7</sub> NOS	105.02484	C <sub>5</sub> H <sub>5</sub> NS	111.01427	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	116.02219
C <sub>5</sub> H <sub>8</sub> S	100.03467	C <sub>4</sub> H <sub>8</sub> CIN	105.03453	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub>	111.03203	C <sub>8</sub> H <sub>4</sub> O	116.02621
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	100.05243	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	105.04259	C <sub>6</sub> H <sub>9</sub> NO	111.06841	C <sub>5</sub> H <sub>8</sub> OS	116.02959
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O	100.06366	C <sub>7</sub> H <sub>7</sub> N	105.05785	C <sub>7</sub> H <sub>13</sub> N	111.10480	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub>	116.03745
C <sub>6</sub> H <sub>12</sub> O	100.08882	C <sub>4</sub> H <sub>11</sub> NS	105.06122	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub>	111.98466	C <sub>6</sub> H <sub>9</sub> Cl	116.03928
C <sub>5</sub> H <sub>12</sub> N <sub>2</sub>	100.10005	C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub>	105.07898	C <sub>5</sub> H <sub>4</sub> OS	111.99829	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S	116.04082
C <sub>7</sub> H <sub>16</sub>	100.12520	C <sub>3</sub> H <sub>6</sub> S <sub>2</sub>	105.99109	C <sub>6</sub> H <sub>5</sub> Cl	112.00798	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	116.04734
C <sub>4</sub> H <sub>4</sub> CIN	101.00323	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S	106.00885	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S	112.00952	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	116.05858
C <sub>4</sub> H <sub>7</sub> NS	101.02992	C <sub>4</sub> H <sub>7</sub> ClO	106.01854	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>	112.01604	C <sub>9</sub> H <sub>8</sub>	116.06260
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	101.04768	C <sub>3</sub> H <sub>7</sub> CIN <sub>2</sub>	106.02978	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	112.02728	C <sub>6</sub> H <sub>12</sub> S	116.06597
C <sub>5</sub> H <sub>11</sub> NO	101.08406	C <sub>7</sub> H <sub>6</sub> O	106.04186	C <sub>6</sub> H <sub>8</sub> S	112.03467	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.08373
C <sub>6</sub> H <sub>15</sub> N	101.12045	C <sub>4</sub> H <sub>10</sub> OS	106.04524	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	112.05243	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O	116.09496
C <sub>4</sub> H <sub>6</sub> OS	102.01394	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub>	106.05310	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O	112.06366	C <sub>7</sub> H <sub>16</sub> O	116.12012
C <sub>5</sub> H <sub>7</sub> Cl	102.02363	C <sub>5</sub> H <sub>11</sub> Cl	106.05493	C <sub>7</sub> H <sub>12</sub> O	112.08882	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub>	116.13135
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S	102.02517	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> S	106.05647	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub>	112.10005	C <sub>4</sub> H <sub>4</sub> CINO	116.99814
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	102.03169	C <sub>4</sub> H <sub>10</sub> O <sub>3</sub>	106.06299	C <sub>8</sub> H <sub>16</sub>	112.12520	C <sub>4</sub> H <sub>7</sub> NOS	117.02484
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	102.04293	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	106.07423	C <sub>5</sub> H <sub>4</sub> CIN	113.00323	C <sub>5</sub> H <sub>8</sub> CIN	117.03453
C <sub>8</sub> H <sub>6</sub>	102.04695	C <sub>8</sub> H <sub>10</sub>	106.07825	C <sub>5</sub> H <sub>7</sub> NS	113.02992	C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub>	117.04259
C <sub>5</sub> H <sub>10</sub> S	102.05032	C <sub>3</sub> H <sub>6</sub> CINO	107.01379	C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub>	113.04768	C <sub>8</sub> H <sub>7</sub> N	117.05785
C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.06808	C <sub>6</sub> H <sub>5</sub> NO	107.03711	C <sub>6</sub> H <sub>11</sub> NO	113.08406	C <sub>5</sub> H <sub>11</sub> NS	117.06122
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O	102.07931	C <sub>3</sub> H <sub>9</sub> NOS	107.04049	C <sub>7</sub> H <sub>15</sub> N	113.12045	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	117.07898
C <sub>6</sub> H <sub>14</sub> O	102.10447	C <sub>4</sub> H <sub>10</sub> CIN	107.05018	C <sub>5</sub> H <sub>6</sub> OS	114.01394	C <sub>6</sub> H <sub>15</sub> NO	117.11536
C <sub>5</sub> H <sub>14</sub> N <sub>2</sub>	102.11570	C <sub>3</sub> H <sub>9</sub> NO <sub>3</sub>	107.05824	C <sub>6</sub> H <sub>7</sub> Cl	114.02363	C <sub>4</sub> H <sub>6</sub> S <sub>2</sub>	117.99109
C <sub>3</sub> H <sub>5</sub> NOS	103.00918	C <sub>7</sub> H <sub>9</sub> N	107.07350	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S	114.02517	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> S	118.00885
C <sub>4</sub> H <sub>6</sub> CIN	103.01888	C <sub>3</sub> H <sub>5</sub> ClO <sub>2</sub>	107.99781	C <sub>5</sub> H <sub>6</sub> O <sub>3</sub>	114.03169	C <sub>5</sub> H <sub>7</sub> ClO	118.01854
C <sub>3</sub> H <sub>5</sub> NO <sub>3</sub>	103.02694	C <sub>6</sub> H <sub>4</sub> S	108.00337	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	114.04293	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> OS	118.02008
C <sub>7</sub> H <sub>5</sub> N	103.04220	C <sub>3</sub> H <sub>8</sub> S <sub>2</sub>	108.00674	C <sub>9</sub> H <sub>6</sub>	114.04695	C <sub>4</sub> H <sub>7</sub> CIN <sub>2</sub>	118.02978
C <sub>4</sub> H <sub>9</sub> NS	103.04557	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub>	108.02113	C <sub>6</sub> H <sub>10</sub> S	114.05032	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	118.03784
C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	103.06333	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> S	108.02450	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	114.06808	C <sub>8</sub> H <sub>6</sub> O	118.04186
C <sub>5</sub> H <sub>13</sub> NO	103.09971	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O	108.03236	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O	114.07931	C <sub>5</sub> H <sub>10</sub> OS	118.04524
C <sub>3</sub> H <sub>4</sub> S <sub>2</sub>	103.97544	C <sub>4</sub> H <sub>9</sub> ClO	108.03419	C <sub>7</sub> H <sub>14</sub> O	114.10447	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub>	118.05310
C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> S	103.99320	C <sub>3</sub> H <sub>9</sub> CIN <sub>2</sub>	108.04543	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub>	114.11570	C <sub>6</sub> H <sub>11</sub> Cl	118.05493
C <sub>4</sub> H <sub>5</sub> ClO	104.00289	C <sub>7</sub> H <sub>8</sub> O	108.05751	C <sub>8</sub> H <sub>18</sub>	114.14085	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> S	118.05647
C <sub>3</sub> H <sub>5</sub> CIN <sub>2</sub>	104.01413	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	108.06875	C <sub>4</sub> H <sub>5</sub> NOS	115.00918	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	118.06299
C <sub>7</sub> H <sub>4</sub> O	104.02621	C <sub>8</sub> H <sub>12</sub>	108.09390	C <sub>5</sub> H <sub>6</sub> CIN	115.01888	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	118.07423
C <sub>4</sub> H <sub>8</sub> OS	104.02959	C <sub>3</sub> H <sub>8</sub> CINO	109.02944	C <sub>4</sub> H <sub>5</sub> NO <sub>3</sub>	115.02694	C <sub>9</sub> H <sub>10</sub>	118.07825
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	104.03745	C <sub>6</sub> H <sub>7</sub> NO	109.05276	C <sub>8</sub> H <sub>5</sub> N	115.04220	C <sub>6</sub> H <sub>14</sub> S	118.08162
C <sub>5</sub> H <sub>9</sub> Cl	104.03928	C <sub>7</sub> H <sub>11</sub> N	109.08915	C <sub>5</sub> H <sub>9</sub> NS	115.04557	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	118.09938
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S	104.04082	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub>	109.96901	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	115.06333	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O	118.11061
C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	104.04734	C <sub>3</sub> H <sub>7</sub> ClO <sub>2</sub>	110.01346	C <sub>6</sub> H <sub>13</sub> NO	115.09971	C <sub>3</sub> H <sub>5</sub> NS <sub>2</sub>	118.98634
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	104.05858	C <sub>6</sub> H <sub>6</sub> S	110.01902	C <sub>7</sub> H <sub>17</sub> N	115.13610	C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub> S	119.00410
C <sub>8</sub> H <sub>8</sub>	104.06260	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	110.03678	C <sub>4</sub> H <sub>4</sub> S <sub>2</sub>	115.97544	C <sub>4</sub> H <sub>6</sub> CINO	119.01379

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>7</sub> H <sub>5</sub> NO	119.03711	C <sub>4</sub> H <sub>11</sub> CIN <sub>2</sub>	122.06108	C <sub>3</sub> H <sub>7</sub> Cl <sub>2</sub> N	126.99555	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.09938
C <sub>4</sub> H <sub>9</sub> NOS	119.04049	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	122.06914	C <sub>5</sub> H <sub>5</sub> NOS	127.00918	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O	130.11061
C <sub>5</sub> H <sub>10</sub> CIN	119.05018	C <sub>8</sub> H <sub>10</sub> O	122.07316	C <sub>6</sub> H <sub>6</sub> CIN	127.01888	C <sub>8</sub> H <sub>18</sub> O	130.13577
C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	119.05824	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	122.08440	C <sub>5</sub> H <sub>5</sub> NO <sub>3</sub>	127.02694	C <sub>7</sub> H <sub>18</sub> N <sub>2</sub>	130.14700
C <sub>8</sub> H <sub>9</sub> N	119.07350	C <sub>9</sub> H <sub>14</sub>	122.10955	C <sub>6</sub> H <sub>9</sub> NS	127.04557	C <sub>4</sub> H <sub>5</sub> NS <sub>2</sub>	130.98634
C <sub>5</sub> H <sub>13</sub> NS	119.07687	C <sub>3</sub> H <sub>6</sub> CINO <sub>2</sub>	123.00871	C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub>	127.06333	C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> S	131.00410
C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub>	119.09463	C <sub>6</sub> H <sub>5</sub> NS	123.01427	C <sub>7</sub> H <sub>13</sub> NO	127.09971	C <sub>5</sub> H <sub>6</sub> CINO	131.01379
C <sub>3</sub> H <sub>5</sub> Br	119.95746	C <sub>3</sub> H <sub>9</sub> NS <sub>2</sub>	123.01764	C <sub>8</sub> H <sub>17</sub> N	127.13610	C <sub>8</sub> H <sub>5</sub> NO	131.03711
C <sub>3</sub> H <sub>4</sub> OS <sub>2</sub>	119.97036	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123.03203	C <sub>5</sub> H <sub>4</sub> S <sub>2</sub>	127.97544	C <sub>5</sub> H <sub>9</sub> NOS	131.04049
C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> S	119.98812	C <sub>3</sub> H <sub>9</sub> NO <sub>2</sub> S	123.03540	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> O	127.97957	C <sub>6</sub> H <sub>10</sub> CIN	131.05018
C <sub>4</sub> H <sub>5</sub> ClO <sub>2</sub>	119.99781	C <sub>4</sub> H <sub>10</sub> CINO	123.04509	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub> S	127.99320	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>	131.05824
C <sub>7</sub> H <sub>4</sub> S	120.00337	C <sub>7</sub> H <sub>9</sub> NO	123.06841	C <sub>6</sub> H <sub>5</sub> CIO	128.00289	C <sub>9</sub> H <sub>9</sub> N	131.07350
C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>	120.00674	C <sub>8</sub> H <sub>13</sub> N	123.10480	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> OS	128.00443	C <sub>6</sub> H <sub>13</sub> NS	131.07687
C <sub>3</sub> H <sub>5</sub> CIN <sub>2</sub> O	120.00904	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub>	123.98466	C <sub>5</sub> H <sub>5</sub> CIN <sub>2</sub>	128.01413	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	131.09463
C <sub>7</sub> H <sub>4</sub> O <sub>2</sub>	120.02113	C <sub>3</sub> H <sub>5</sub> CIO <sub>3</sub>	123.99272	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	128.02219	C <sub>7</sub> H <sub>17</sub> NO	131.13101
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S	120.02450	C <sub>6</sub> H <sub>4</sub> OS	123.99829	C <sub>6</sub> H <sub>8</sub> OS	128.02959	C <sub>4</sub> H <sub>5</sub> Br	131.95746
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O	120.03236	C <sub>3</sub> H <sub>8</sub> OS <sub>2</sub>	124.00166	C <sub>7</sub> H <sub>9</sub> Cl	128.03928	C <sub>4</sub> H <sub>4</sub> OS <sub>2</sub>	131.97036
C <sub>5</sub> H <sub>9</sub> CIO	120.03419	C <sub>7</sub> H <sub>5</sub> Cl	124.00798	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> S	128.04082	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	131.98159
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> OS	120.03573	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> S	124.00952	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub>	128.04734	C <sub>4</sub> H <sub>4</sub> O <sub>3</sub> S	131.98812
C <sub>4</sub> H <sub>9</sub> CIN <sub>2</sub>	120.04543	C <sub>6</sub> H <sub>4</sub> O <sub>3</sub>	124.01604	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	128.05858	C <sub>5</sub> H <sub>5</sub> CIO <sub>2</sub>	131.99781
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	120.05349	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> S	124.01942	C <sub>10</sub> H <sub>8</sub>	128.06260	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S	131.99935
C <sub>8</sub> H <sub>8</sub> O	120.05751	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	124.02728	C <sub>7</sub> H <sub>12</sub> S	128.06597	C <sub>8</sub> H <sub>4</sub> S	132.00337
C <sub>5</sub> H <sub>12</sub> OS	120.06089	C <sub>4</sub> H <sub>9</sub> CIO <sub>2</sub>	124.02911	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	128.08373	C <sub>5</sub> H <sub>8</sub> S <sub>2</sub>	132.00674
C <sub>7</sub> H <sub>8</sub> N <sub>2</sub>	120.06875	C <sub>7</sub> H <sub>8</sub> S	124.03467	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O	128.09496	C <sub>4</sub> H <sub>5</sub> CIN <sub>2</sub> O	132.00904
C <sub>6</sub> H <sub>13</sub> Cl	120.07058	C <sub>3</sub> H <sub>9</sub> CIN <sub>2</sub> O	124.04034	C <sub>8</sub> H <sub>16</sub> O	128.12012	C <sub>8</sub> H <sub>4</sub> O <sub>2</sub>	132.02113
C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> S	120.07212	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	124.05243	C <sub>7</sub> H <sub>16</sub> N <sub>2</sub>	128.13135	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> S	132.02450
C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>	120.07864	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O	124.06366	C <sub>9</sub> H <sub>20</sub>	128.15650	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O	132.03236
C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	120.08988	C <sub>8</sub> H <sub>12</sub> O	124.08882	C <sub>5</sub> H <sub>4</sub> CINO	128.99814	C <sub>6</sub> H <sub>9</sub> CIO	132.03419
C <sub>9</sub> H <sub>12</sub>	120.09390	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub>	124.10005	C <sub>5</sub> H <sub>7</sub> NOS	129.02484	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> OS	132.03573
C <sub>3</sub> H <sub>4</sub> CINO <sub>2</sub>	120.99306	C <sub>9</sub> H <sub>16</sub>	124.12520	C <sub>6</sub> H <sub>8</sub> CIN	129.03453	C <sub>5</sub> H <sub>9</sub> CIN <sub>2</sub>	132.04543
C <sub>3</sub> H <sub>7</sub> NS <sub>2</sub>	121.00199	C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub> N	124.97990	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	129.04259	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	132.05349
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	121.01975	C <sub>6</sub> H <sub>4</sub> CIN	125.00323	C <sub>9</sub> H <sub>7</sub> N	129.05785	C <sub>9</sub> H <sub>8</sub> O	132.05751
C <sub>4</sub> H <sub>8</sub> CINO	121.02944	C <sub>3</sub> H <sub>8</sub> CINO <sub>2</sub>	125.02436	C <sub>6</sub> H <sub>11</sub> NS	129.06122	C <sub>6</sub> H <sub>12</sub> OS	132.06089
C <sub>7</sub> H <sub>7</sub> NO	121.05276	C <sub>6</sub> H <sub>7</sub> NS	125.02992	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>	129.07898	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub>	132.06875
C <sub>4</sub> H <sub>11</sub> NOS	121.05614	C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub>	125.04768	C <sub>7</sub> H <sub>15</sub> NO	129.11536	C <sub>7</sub> H <sub>13</sub> Cl	132.07058
C <sub>5</sub> H <sub>12</sub> CIN	121.06583	C <sub>7</sub> H <sub>11</sub> NO	125.08406	C <sub>8</sub> H <sub>19</sub> N	129.15175	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S	132.07212
C <sub>4</sub> H <sub>11</sub> NO <sub>3</sub>	121.07389	C <sub>8</sub> H <sub>15</sub> N	125.12045	C <sub>5</sub> H <sub>6</sub> S <sub>2</sub>	129.99109	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	132.07864
C <sub>8</sub> H <sub>11</sub> N	121.08915	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O	125.96392	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub> S	130.00885	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	132.08988
C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub>	121.96901	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub>	126.00031	C <sub>6</sub> H <sub>7</sub> CIO	130.01854	C <sub>10</sub> H <sub>12</sub>	132.09390
C <sub>3</sub> H <sub>7</sub> Br	121.97311	C <sub>3</sub> H <sub>7</sub> CIO <sub>3</sub>	126.00837	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> OS	130.02008	C <sub>7</sub> H <sub>16</sub> S	132.09727
C <sub>3</sub> H <sub>6</sub> OS <sub>2</sub>	121.98601	C <sub>6</sub> H <sub>6</sub> OS	126.01394	C <sub>5</sub> H <sub>7</sub> CIN <sub>2</sub>	130.02978	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>	132.11503
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> S	122.00377	C <sub>7</sub> H <sub>7</sub> Cl	126.02363	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	130.03784	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> O	132.12626
C <sub>4</sub> H <sub>7</sub> CIO <sub>2</sub>	122.01346	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> S	126.02517	C <sub>9</sub> H <sub>6</sub> O	130.04186	C <sub>3</sub> H <sub>4</sub> BrN	132.95271
C <sub>7</sub> H <sub>6</sub> S	122.01902	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	126.03169	C <sub>6</sub> H <sub>10</sub> OS	130.04524	C <sub>4</sub> H <sub>4</sub> CINO <sub>2</sub>	132.99306
C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	122.02239	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	126.04293	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub>	130.05310	C <sub>4</sub> H <sub>7</sub> NS <sub>2</sub>	133.00199
C <sub>3</sub> H <sub>7</sub> CIN <sub>2</sub> O	122.02469	C <sub>7</sub> H <sub>10</sub> S	126.05032	C <sub>7</sub> H <sub>11</sub> Cl	130.05493	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> S	133.01975
C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122.03678	C <sub>7</sub> H <sub>10</sub> O <sub>2</sub>	126.06808	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> S	130.05647	C <sub>5</sub> H <sub>8</sub> CINO	133.02944
C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S	122.04015	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O	126.07931	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	130.06299	C <sub>8</sub> H <sub>7</sub> NO	133.05276
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	122.04801	C <sub>8</sub> H <sub>14</sub> O	126.10447	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	130.07423	C <sub>5</sub> H <sub>11</sub> NOS	133.05614
C <sub>5</sub> H <sub>11</sub> CIO	122.04984	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub>	126.11570	C <sub>10</sub> H <sub>10</sub>	130.07825	C <sub>6</sub> H <sub>12</sub> CIN	133.06583
C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> OS	122.05138	C <sub>9</sub> H <sub>18</sub>	126.14085	C <sub>7</sub> H <sub>14</sub> S	130.08162	C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub>	133.07389

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>9</sub> H <sub>11</sub> N	133.08915	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S	136.00952	C <sub>8</sub> H <sub>10</sub> S	138.05032	C <sub>8</sub> H <sub>15</sub> NO	141.11536
C <sub>6</sub> H <sub>15</sub> NS	133.09252	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	136.01289	C <sub>4</sub> H <sub>11</sub> ClN <sub>2</sub> O	138.05599	C <sub>9</sub> H <sub>19</sub> N	141.15175
C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub>	133.11028	C <sub>7</sub> H <sub>4</sub> O <sub>3</sub>	136.01604	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	138.06808	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	141.95883
C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub>	133.96901	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> S	136.01942	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O	138.07931	C <sub>6</sub> H <sub>6</sub> S <sub>2</sub>	141.99109
C <sub>4</sub> H <sub>7</sub> Br	133.97311	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	136.02728	C <sub>9</sub> H <sub>14</sub> O	138.10447	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O	141.99522
C <sub>4</sub> H <sub>6</sub> OS <sub>2</sub>	133.98601	C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub>	136.02911	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub>	138.11570	C <sub>3</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub>	142.00645
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	133.99724	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	136.03065	C <sub>10</sub> H <sub>18</sub>	138.14085	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> S	142.00885
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> S	134.00377	C <sub>8</sub> H <sub>8</sub> S	136.03467	C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> N	138.99555	C <sub>7</sub> H <sub>7</sub> ClO	142.01854
C <sub>5</sub> H <sub>7</sub> ClO <sub>2</sub>	134.01346	C <sub>5</sub> H <sub>12</sub> S <sub>2</sub>	136.03804	C <sub>3</sub> H <sub>6</sub> ClNO <sub>3</sub>	139.00362	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> OS	142.02008
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	134.01500	C <sub>4</sub> H <sub>9</sub> ClN <sub>2</sub> O	136.04034	C <sub>6</sub> H <sub>5</sub> NOS	139.00918	C <sub>6</sub> H <sub>7</sub> ClN <sub>2</sub>	142.02978
C <sub>8</sub> H <sub>6</sub> S	134.01902	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	136.05243	C <sub>3</sub> H <sub>9</sub> NOS <sub>2</sub>	139.01256	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	142.03784
C <sub>5</sub> H <sub>10</sub> S <sub>2</sub>	134.02239	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub> S	136.05580	C <sub>7</sub> H <sub>6</sub> CIN	139.01888	C <sub>7</sub> H <sub>10</sub> OS	142.04524
C <sub>4</sub> H <sub>7</sub> ClN <sub>2</sub> O	134.02469	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O	136.06366	C <sub>6</sub> H <sub>5</sub> NO <sub>3</sub>	139.02694	C <sub>8</sub> H <sub>11</sub> Cl	142.05493
C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	134.03678	C <sub>6</sub> H <sub>13</sub> ClO	136.06549	C <sub>3</sub> H <sub>9</sub> NO <sub>3</sub> S	139.03031	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> S	142.05647
C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> S	134.04015	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> OS	136.06703	C <sub>4</sub> H <sub>10</sub> ClNO <sub>2</sub>	139.04001	C <sub>7</sub> H <sub>10</sub> O <sub>3</sub>	142.06299
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O	134.04801	C <sub>5</sub> H <sub>13</sub> ClN <sub>2</sub>	136.07673	C <sub>7</sub> H <sub>9</sub> NS	139.04557	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	142.07423
C <sub>6</sub> H <sub>11</sub> ClO	134.04984	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	136.08479	C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub>	139.06333	C <sub>11</sub> H <sub>10</sub>	142.07825
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> OS	134.05138	C <sub>9</sub> H <sub>12</sub> O	136.08882	C <sub>8</sub> H <sub>13</sub> NO	139.09971	C <sub>8</sub> H <sub>14</sub> S	142.08162
C <sub>5</sub> H <sub>11</sub> ClN <sub>2</sub>	134.06108	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	136.10005	C <sub>9</sub> H <sub>17</sub> N	139.13610	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	142.09938
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	134.06914	C <sub>10</sub> H <sub>16</sub>	136.12520	C <sub>6</sub> H <sub>4</sub> S <sub>2</sub>	139.97544	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O	142.11061
C <sub>9</sub> H <sub>10</sub> O	134.07316	C <sub>4</sub> H <sub>5</sub> Cl <sub>2</sub> N	136.97990	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O	139.97957	C <sub>9</sub> H <sub>18</sub> O	142.13577
C <sub>6</sub> H <sub>14</sub> OS	134.07654	C <sub>3</sub> H <sub>8</sub> BrN	136.98401	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	139.99080	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub>	142.14700
C <sub>8</sub> H <sub>10</sub> N <sub>2</sub>	134.08440	C <sub>3</sub> H <sub>4</sub> ClNO <sub>3</sub>	136.98797	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> S	139.99320	C <sub>5</sub> H <sub>5</sub> NS <sub>2</sub>	142.98634
C <sub>7</sub> H <sub>15</sub> Cl	134.08623	C <sub>3</sub> H <sub>7</sub> NOS <sub>2</sub>	136.99691	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	139.99657	C <sub>3</sub> H <sub>7</sub> Cl <sub>2</sub> NO	142.99047
C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> S	134.08777	C <sub>7</sub> H <sub>4</sub> CIN	137.00323	C <sub>7</sub> H <sub>5</sub> ClO	140.00289	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub> S	143.00410
C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>	134.09429	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> S	137.01466	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> OS	140.00443	C <sub>6</sub> H <sub>6</sub> CINO	143.01379
C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	134.10553	C <sub>4</sub> H <sub>8</sub> ClNO <sub>2</sub>	137.02436	C <sub>6</sub> H <sub>5</sub> ClN <sub>2</sub>	140.01413	C <sub>6</sub> H <sub>9</sub> NOS	143.04049
C <sub>10</sub> H <sub>14</sub>	134.10955	C <sub>7</sub> H <sub>7</sub> NS	137.02992	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub>	140.01596	C <sub>7</sub> H <sub>10</sub> CIN	143.05018
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C <sub>3</sub> H <sub>5</sub> NOS <sub>2</sub>	134.98126	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	137.04768	C <sub>4</sub> H <sub>9</sub> ClO <sub>3</sub>	140.02402	C <sub>10</sub> H <sub>9</sub> N	143.07350
C <sub>3</sub> H <sub>5</sub> NO <sub>3</sub> S	134.99901	C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub> S	137.05105	C <sub>7</sub> H <sub>8</sub> OS	140.02959	C <sub>7</sub> H <sub>13</sub> NS	143.07687
C <sub>4</sub> H <sub>6</sub> ClNO <sub>2</sub>	135.00871	C <sub>5</sub> H <sub>12</sub> ClNO	137.06074	C <sub>3</sub> H <sub>9</sub> ClN <sub>2</sub> O <sub>2</sub>	140.03526	C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub>	143.09463
C <sub>7</sub> H <sub>5</sub> NS	135.01427	C <sub>8</sub> H <sub>11</sub> NO	137.08406	C <sub>8</sub> H <sub>9</sub> Cl	140.03928	C <sub>8</sub> H <sub>17</sub> NO	143.13101
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C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub>	135.03203	C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O	137.96392	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	140.04734	C <sub>5</sub> H <sub>4</sub> OS <sub>2</sub>	143.97036
C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S	135.03540	C <sub>3</sub> H <sub>7</sub> BrO	137.96803	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	140.05858	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	143.97448
C <sub>5</sub> H <sub>10</sub> ClNO	135.04509	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	137.97515	C <sub>8</sub> H <sub>12</sub> S	140.06597	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	143.98159
C <sub>8</sub> H <sub>9</sub> NO	135.06841	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	137.98092	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>	140.08373	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub> S	143.98812
C <sub>5</sub> H <sub>13</sub> NOS	135.07179	C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub>	138.00031	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O	140.09496	C <sub>6</sub> H <sub>5</sub> ClO <sub>2</sub>	143.99781
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C <sub>5</sub> H <sub>13</sub> NO <sub>3</sub>	135.08954	C <sub>7</sub> H <sub>6</sub> OS	138.01394	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub>	140.13135	C <sub>6</sub> H <sub>8</sub> S <sub>2</sub>	144.00674
C <sub>9</sub> H <sub>13</sub> N	135.10480	C <sub>4</sub> H <sub>10</sub> OS <sub>2</sub>	138.01731	C <sub>10</sub> H <sub>20</sub>	140.15650	C <sub>5</sub> H <sub>5</sub> ClN <sub>2</sub> O	144.00904
C <sub>3</sub> H <sub>5</sub> BrO	135.95238	C <sub>3</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>2</sub>	138.01961	C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub> NO	140.97482	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> S	144.02450
C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	135.96527	C <sub>8</sub> H <sub>7</sub> Cl	138.02363	C <sub>6</sub> H <sub>4</sub> CINO	140.99814	C <sub>7</sub> H <sub>9</sub> ClO	144.03419
C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub>	135.98466	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> S	138.02517	C <sub>4</sub> H <sub>9</sub> Cl <sub>2</sub> N	141.01120	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> OS	144.03573
C <sub>4</sub> H <sub>9</sub> Br	135.98876	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	138.02854	C <sub>3</sub> H <sub>8</sub> ClNO <sub>3</sub>	141.01927	C <sub>6</sub> H <sub>9</sub> ClN <sub>2</sub>	144.04543
C <sub>4</sub> H <sub>5</sub> ClO <sub>3</sub>	135.99272	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138.03169	C <sub>6</sub> H <sub>7</sub> NOS	141.02484	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	144.05349
C <sub>7</sub> H <sub>4</sub> OS	135.99829	C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> S	138.03507	C <sub>7</sub> H <sub>8</sub> CIN	141.03453	C <sub>10</sub> H <sub>8</sub> O	144.05751
C <sub>4</sub> H <sub>8</sub> OS <sub>2</sub>	136.00166	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	138.04293	C <sub>6</sub> H <sub>7</sub> NO <sub>3</sub>	141.04259	C <sub>7</sub> H <sub>12</sub> OS	144.06089
C <sub>3</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>2</sub>	136.00396	C <sub>5</sub> H <sub>11</sub> ClO <sub>2</sub>	138.04476	C <sub>7</sub> H <sub>11</sub> NS	141.06122	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub>	144.06875
C <sub>8</sub> H <sub>5</sub> Cl	136.00798	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	138.04630	C <sub>7</sub> H <sub>11</sub> NO <sub>2</sub>	141.07898	C <sub>8</sub> H <sub>13</sub> Cl	144.07058

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S	144.07212	C <sub>4</sub> H <sub>5</sub> NOS <sub>2</sub>	146.98126	C <sub>11</sub> H <sub>16</sub>	148.12520	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>	150.11570
C <sub>7</sub> H <sub>12</sub> O <sub>3</sub>	144.07864	C <sub>4</sub> H <sub>5</sub> NO <sub>3</sub> S	146.99901	C <sub>3</sub> H <sub>4</sub> BrNO	148.94763	C <sub>11</sub> H <sub>18</sub>	150.14085
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	144.08988	C <sub>5</sub> H <sub>6</sub> ClNO <sub>2</sub>	147.00871	C <sub>5</sub> H <sub>5</sub> Cl <sub>2</sub> N	148.97990	C <sub>3</sub> H <sub>6</sub> BrNO	150.96328
C <sub>11</sub> H <sub>12</sub>	144.09390	C <sub>8</sub> H <sub>5</sub> NS	147.01427	C <sub>4</sub> H <sub>8</sub> BrN	148.98401	C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub> S <sub>2</sub>	150.97617
C <sub>8</sub> H <sub>16</sub> S	144.09727	C <sub>5</sub> H <sub>9</sub> NS <sub>2</sub>	147.01764	C <sub>4</sub> H <sub>4</sub> ClNO <sub>3</sub>	148.98797	C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> N	150.99555
C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144.11503	C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub>	147.03203	C <sub>4</sub> H <sub>7</sub> NOS <sub>2</sub>	148.99691	C <sub>4</sub> H <sub>10</sub> BrN	150.99966
C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O	144.12626	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> S	147.03540	C <sub>8</sub> H <sub>4</sub> CIN	149.00323	C <sub>4</sub> H <sub>6</sub> ClNO <sub>3</sub>	151.00362
C <sub>9</sub> H <sub>20</sub> O	144.15142	C <sub>6</sub> H <sub>10</sub> ClNO	147.04509	C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub> S	149.01466	C <sub>7</sub> H <sub>5</sub> NOS	151.00918
C <sub>8</sub> H <sub>20</sub> N <sub>2</sub>	144.16265	C <sub>9</sub> H <sub>9</sub> NO	147.06841	C <sub>5</sub> H <sub>8</sub> ClNO <sub>2</sub>	149.02436	C <sub>4</sub> H <sub>9</sub> NOS <sub>2</sub>	151.01256
C <sub>4</sub> H <sub>4</sub> BrN	144.95271	C <sub>6</sub> H <sub>13</sub> NOS	147.07179	C <sub>8</sub> H <sub>7</sub> NS	149.02992	C <sub>8</sub> H <sub>6</sub> CIN	151.01888
C <sub>5</sub> H <sub>4</sub> ClNO <sub>2</sub>	144.99306	C <sub>7</sub> H <sub>14</sub> CIN	147.08148	C <sub>5</sub> H <sub>11</sub> NS <sub>2</sub>	149.03329	C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub>	151.02694
C <sub>5</sub> H <sub>7</sub> NS <sub>2</sub>	145.00199	C <sub>6</sub> H <sub>13</sub> NO <sub>3</sub>	147.08954	C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub>	149.04768	C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> S	151.03031
C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub> S	145.01975	C <sub>10</sub> H <sub>13</sub> N	147.10480	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	149.05105	C <sub>5</sub> H <sub>10</sub> ClNO <sub>2</sub>	151.04001
C <sub>6</sub> H <sub>8</sub> ClNO	145.02944	C <sub>7</sub> H <sub>17</sub> NS	147.10817	C <sub>6</sub> H <sub>12</sub> ClNO	149.06074	C <sub>8</sub> H <sub>9</sub> NS	151.04557
C <sub>9</sub> H <sub>7</sub> NO	145.05276	C <sub>7</sub> H <sub>17</sub> NO <sub>2</sub>	147.12593	C <sub>9</sub> H <sub>11</sub> NO	149.08406	C <sub>5</sub> H <sub>13</sub> NS <sub>2</sub>	151.04894
C <sub>6</sub> H <sub>11</sub> NOS	145.05614	C <sub>4</sub> H <sub>5</sub> BrO	147.95238	C <sub>6</sub> H <sub>15</sub> NOS	149.08744	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>	151.06333
C <sub>7</sub> H <sub>12</sub> CIN	145.06583	C <sub>3</sub> H <sub>5</sub> BrN <sub>2</sub>	147.96361	C <sub>7</sub> H <sub>16</sub> CIN	149.09713	C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub> S	151.06670
C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub>	145.07389	C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	147.96527	C <sub>6</sub> H <sub>15</sub> NO <sub>3</sub>	149.10519	C <sub>6</sub> H <sub>14</sub> ClNO	151.07639
C <sub>10</sub> H <sub>11</sub> N	145.08915	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> OS <sub>2</sub>	147.97651	C <sub>10</sub> H <sub>15</sub> N	149.12045	C <sub>9</sub> H <sub>13</sub> NO	151.09971
C <sub>7</sub> H <sub>15</sub> NS	145.09252	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub>	147.98466	C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> O	149.96392	C <sub>10</sub> H <sub>17</sub> N	151.13610
C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub>	145.11028	C <sub>5</sub> H <sub>9</sub> Br	147.98876	C <sub>4</sub> H <sub>7</sub> BrO	149.96803	C <sub>3</sub> H <sub>5</sub> BrO <sub>2</sub>	151.94729
C <sub>8</sub> H <sub>19</sub> NO	145.14666	C <sub>5</sub> H <sub>5</sub> ClO <sub>3</sub>	147.99272	C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	149.97515	C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	151.96019
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	145.96901	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S	147.99426	C <sub>3</sub> H <sub>7</sub> BrN <sub>2</sub>	149.97926	C <sub>7</sub> H <sub>4</sub> S <sub>2</sub>	151.97544
C <sub>5</sub> H <sub>7</sub> Br	145.97311	C <sub>8</sub> H <sub>4</sub> OS	147.99829	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	149.98092	C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub> O	151.97957
C <sub>5</sub> H <sub>6</sub> OS <sub>2</sub>	145.98601	C <sub>5</sub> H <sub>8</sub> OS <sub>2</sub>	148.00166	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	149.99216	C <sub>4</sub> H <sub>9</sub> BrO	151.98368
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	145.99724	C <sub>4</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>2</sub>	148.00396	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub>	150.00031	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	151.99080
C <sub>5</sub> H <sub>6</sub> O <sub>3</sub> S	146.00377	C <sub>9</sub> H <sub>5</sub> Cl	148.00798	C <sub>5</sub> H <sub>11</sub> Br	150.00441	C <sub>7</sub> H <sub>4</sub> O <sub>2</sub> S	151.99320
C <sub>6</sub> H <sub>7</sub> ClO <sub>2</sub>	146.01346	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> S	148.00952	C <sub>5</sub> H <sub>7</sub> ClO <sub>3</sub>	150.00837	C <sub>3</sub> H <sub>9</sub> BrN <sub>2</sub>	151.99491
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	146.01500	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	148.01289	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S	150.00991	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	151.99657
C <sub>9</sub> H <sub>6</sub> S	146.01902	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	148.01604	C <sub>8</sub> H <sub>6</sub> OS	150.01394	C <sub>3</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>3</sub>	151.99887
C <sub>6</sub> H <sub>10</sub> S <sub>2</sub>	146.02239	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S	148.01942	C <sub>5</sub> H <sub>10</sub> OS <sub>2</sub>	150.01731	C <sub>8</sub> H <sub>5</sub> ClO	152.00289
C <sub>5</sub> H <sub>7</sub> CIN <sub>2</sub> O	146.02469	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	148.02728	C <sub>4</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>2</sub>	150.01961	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> OS	152.00443
C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	146.03678	C <sub>6</sub> H <sub>9</sub> ClO <sub>2</sub>	148.02911	C <sub>9</sub> H <sub>7</sub> Cl	150.02363	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> OS <sub>2</sub>	152.00781
C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S	146.04015	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	148.03065	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> S	150.02517	C <sub>7</sub> H <sub>5</sub> CIN <sub>2</sub>	152.01413
C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O	146.04801	C <sub>9</sub> H <sub>8</sub> S	148.03467	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	150.02854	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub>	152.01596
C <sub>7</sub> H <sub>11</sub> ClO	146.04984	C <sub>6</sub> H <sub>12</sub> S <sub>2</sub>	148.03804	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	150.03169	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	152.02219
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> OS	146.05138	C <sub>5</sub> H <sub>9</sub> CIN <sub>2</sub> O	148.04034	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> S	150.03507	C <sub>5</sub> H <sub>9</sub> ClO <sub>3</sub>	152.02402
C <sub>6</sub> H <sub>11</sub> CIN <sub>2</sub>	146.06108	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	148.05243	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	150.04293	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S	152.02556
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	146.06914	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> S	148.05580	C <sub>6</sub> H <sub>11</sub> ClO <sub>2</sub>	150.04476	C <sub>8</sub> H <sub>8</sub> OS	152.02959
C <sub>10</sub> H <sub>10</sub> O	146.07316	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O	148.06366	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	150.04630	C <sub>5</sub> H <sub>12</sub> OS <sub>2</sub>	152.03296
C <sub>7</sub> H <sub>14</sub> OS	146.07654	C <sub>7</sub> H <sub>13</sub> ClO	148.06549	C <sub>9</sub> H <sub>10</sub> S	150.05032	C <sub>4</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>2</sub>	152.03526
C <sub>9</sub> H <sub>10</sub> N <sub>2</sub>	146.08440	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> OS	148.06703	C <sub>6</sub> H <sub>14</sub> S <sub>2</sub>	150.05369	C <sub>9</sub> H <sub>9</sub> Cl	152.03928
C <sub>8</sub> H <sub>15</sub> Cl	146.08623	C <sub>6</sub> H <sub>13</sub> CIN <sub>2</sub>	148.07673	C <sub>5</sub> H <sub>11</sub> CIN <sub>2</sub> O	150.05599	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> S	152.04082
C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> S	146.08777	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	148.08479	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	150.06808	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> S <sub>2</sub>	152.04419
C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	146.09429	C <sub>10</sub> H <sub>12</sub> O	148.08882	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> S	150.07145	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	152.04734
C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	146.10553	C <sub>7</sub> H <sub>16</sub> OS	148.09219	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O	150.07931	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> S	152.05072
C <sub>11</sub> H <sub>14</sub>	146.10955	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub>	148.10005	C <sub>7</sub> H <sub>15</sub> ClO	150.08114	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	152.05858
C <sub>8</sub> H <sub>18</sub> S	146.11292	C <sub>8</sub> H <sub>17</sub> Cl	148.10188	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> OS	150.08268	C <sub>6</sub> H <sub>13</sub> ClO <sub>2</sub>	152.06041
C <sub>8</sub> H <sub>18</sub> O <sub>2</sub>	146.13068	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> S	148.10342	C <sub>6</sub> H <sub>15</sub> CIN <sub>2</sub>	150.09238	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S	152.06195
C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> O	146.14191	C <sub>7</sub> H <sub>16</sub> O <sub>3</sub>	148.10994	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	150.10044	C <sub>9</sub> H <sub>12</sub> S	152.06597
C <sub>4</sub> H <sub>6</sub> BrN	146.96836	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	148.12118	C <sub>10</sub> H <sub>14</sub> O	150.10447	C <sub>5</sub> H <sub>13</sub> CIN <sub>2</sub> O	152.07164

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	152.08373	C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> NO	154.99047	C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub>	157.07389	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	159.96940
C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O	152.09496	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> S	155.00410	C <sub>11</sub> H <sub>11</sub> N	157.08915	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> OS <sub>2</sub>	159.97651
C <sub>10</sub> H <sub>16</sub> O	152.12012	C <sub>3</sub> H <sub>9</sub> NO <sub>2</sub> S <sub>2</sub>	155.00747	C <sub>8</sub> H <sub>15</sub> NS	157.09252	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub>	159.98466
C <sub>9</sub> H <sub>16</sub> N <sub>2</sub>	152.13135	C <sub>7</sub> H <sub>6</sub> CINO	155.01379	C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub>	157.11028	C <sub>6</sub> H <sub>9</sub> Br	159.98876
C <sub>11</sub> H <sub>20</sub>	152.15650	C <sub>5</sub> H <sub>11</sub> Cl <sub>2</sub> N	155.02685	C <sub>9</sub> H <sub>19</sub> NO	157.14666	C <sub>6</sub> H <sub>5</sub> ClO <sub>3</sub>	159.99272
C <sub>4</sub> H <sub>5</sub> Cl <sub>2</sub> NO	152.97482	C <sub>4</sub> H <sub>10</sub> CINO <sub>3</sub>	155.03492	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>3</sub>	157.95375	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S	159.99426
C <sub>3</sub> H <sub>8</sub> BrNO	152.97893	C <sub>7</sub> H <sub>9</sub> NOS	155.04049	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub>	157.96901	C <sub>6</sub> H <sub>8</sub> OS <sub>2</sub>	160.00166
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S <sub>2</sub>	152.99182	C <sub>8</sub> H <sub>10</sub> CIN	155.05018	C <sub>6</sub> H <sub>7</sub> Br	157.97311	C <sub>5</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>2</sub>	160.00396
C <sub>7</sub> H <sub>4</sub> CINO	152.99814	C <sub>7</sub> H <sub>9</sub> NO <sub>3</sub>	155.05824	C <sub>6</sub> H <sub>6</sub> OS <sub>2</sub>	157.98601	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	160.01289
C <sub>5</sub> H <sub>9</sub> Cl <sub>2</sub> N	153.01120	C <sub>8</sub> H <sub>13</sub> NS	155.07687	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>	157.99013	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> S	160.01942
C <sub>4</sub> H <sub>8</sub> CINO <sub>3</sub>	153.01927	C <sub>8</sub> H <sub>13</sub> NO <sub>2</sub>	155.09463	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	157.99724	C <sub>7</sub> H <sub>9</sub> ClO <sub>2</sub>	160.02911
C <sub>7</sub> H <sub>7</sub> NOS	153.02484	C <sub>9</sub> H <sub>17</sub> NO	155.13101	C <sub>3</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O	158.00137	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	160.03065
C <sub>4</sub> H <sub>11</sub> NOS <sub>2</sub>	153.02821	C <sub>6</sub> H <sub>5</sub> Br	155.95746	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> S	158.00377	C <sub>10</sub> H <sub>8</sub> S	160.03467
C <sub>8</sub> H <sub>8</sub> CIN	153.03453	C <sub>6</sub> H <sub>4</sub> OS <sub>2</sub>	155.97036	C <sub>7</sub> H <sub>7</sub> ClO <sub>2</sub>	158.01346	C <sub>7</sub> H <sub>12</sub> S <sub>2</sub>	160.03804
C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	153.04259	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	155.97448	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	158.01500	C <sub>6</sub> H <sub>9</sub> CIN <sub>2</sub> O	160.04034
C <sub>4</sub> H <sub>11</sub> NO <sub>3</sub> S	153.04596	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	155.98159	C <sub>7</sub> H <sub>10</sub> S <sub>2</sub>	158.02239	C <sub>10</sub> H <sub>8</sub> O <sub>2</sub>	160.05243
C <sub>5</sub> H <sub>12</sub> CINO <sub>2</sub>	153.05566	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O	155.98572	C <sub>6</sub> H <sub>7</sub> CIN <sub>2</sub> O	158.02469	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> S	160.05580
C <sub>8</sub> H <sub>11</sub> NS	153.06122	C <sub>6</sub> H <sub>4</sub> O <sub>3</sub> S	155.98812	C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> S	158.04015	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O	160.06366
C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>	153.07898	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> S <sub>2</sub>	155.99149	C <sub>8</sub> H <sub>11</sub> ClO	158.04984	C <sub>8</sub> H <sub>13</sub> ClO	160.06549
C <sub>9</sub> H <sub>15</sub> NO	153.11536	C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub>	155.99781	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> OS	158.05138	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> OS	160.06703
C <sub>10</sub> H <sub>19</sub> N	153.15175	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S	155.99935	C <sub>7</sub> H <sub>11</sub> CIN <sub>2</sub>	158.06108	C <sub>7</sub> H <sub>13</sub> CIN <sub>2</sub>	160.07673
C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	153.95883	C <sub>7</sub> H <sub>8</sub> S <sub>2</sub>	156.00674	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	158.06914	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	160.08479
C <sub>3</sub> H <sub>7</sub> BrO <sub>2</sub>	153.96294	C <sub>6</sub> H <sub>5</sub> CIN <sub>2</sub> O	156.00904	C <sub>11</sub> H <sub>10</sub> O	158.07316	C <sub>11</sub> H <sub>12</sub> O	160.08882
C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O	153.97007	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> O	156.01087	C <sub>8</sub> H <sub>14</sub> OS	158.07654	C <sub>8</sub> H <sub>16</sub> OS	160.09219
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> S <sub>2</sub>	153.97584	C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub>	156.02210	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub>	158.08440	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub>	160.10005
C <sub>7</sub> H <sub>6</sub> S <sub>2</sub>	153.99109	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> S	156.02450	C <sub>9</sub> H <sub>15</sub> Cl	158.08623	C <sub>9</sub> H <sub>17</sub> Cl	160.10188
C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> O	153.99522	C <sub>3</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>3</sub>	156.03017	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> S	158.08777	C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> S	160.10342
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C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> S	154.00885	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> OS	156.03573	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	158.10553	C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	160.12118
C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S <sub>2</sub>	154.01222	C <sub>7</sub> H <sub>9</sub> CIN <sub>2</sub>	156.04543	C <sub>12</sub> H <sub>14</sub>	158.10955	C <sub>12</sub> H <sub>16</sub>	160.12520
C <sub>3</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>3</sub>	154.01452	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	156.05349	C <sub>9</sub> H <sub>18</sub> S	158.11292	C <sub>9</sub> H <sub>20</sub> S	160.12857
C <sub>8</sub> H <sub>7</sub> ClO	154.01854	C <sub>8</sub> H <sub>12</sub> OS	156.06089	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	158.13068	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub>	160.14633
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> OS	154.02008	C <sub>9</sub> H <sub>13</sub> Cl	156.07058	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> O	158.14191	C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> O	160.15756
C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> OS <sub>2</sub>	154.02346	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> S	156.07212	C <sub>5</sub> H <sub>6</sub> BrN	158.96836	C <sub>4</sub> H <sub>4</sub> BrNO	160.94763
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C <sub>5</sub> H <sub>11</sub> ClO <sub>3</sub>	154.03967	C <sub>9</sub> H <sub>16</sub> S	156.09727	C <sub>6</sub> H <sub>6</sub> CINO <sub>2</sub>	159.00871	C <sub>5</sub> H <sub>7</sub> NOS <sub>2</sub>	160.99691
C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	154.04121	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	156.11503	C <sub>6</sub> H <sub>9</sub> NS <sub>2</sub>	159.01764	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub> S	161.01466
C <sub>8</sub> H <sub>10</sub> OS	154.04524	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O	156.12626	C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> S	159.03540	C <sub>6</sub> H <sub>8</sub> CINO <sub>2</sub>	161.02436
C <sub>4</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>2</sub>	154.05091	C <sub>10</sub> H <sub>20</sub> O	156.15142	C <sub>7</sub> H <sub>10</sub> CINO	159.04509	C <sub>9</sub> H <sub>7</sub> NS	161.02992
C <sub>9</sub> H <sub>11</sub> Cl	154.05493	C <sub>9</sub> H <sub>20</sub> N <sub>2</sub>	156.16265	C <sub>10</sub> H <sub>9</sub> NO	159.06841	C <sub>6</sub> H <sub>11</sub> NS <sub>2</sub>	161.03329
C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> S	154.05647	C <sub>5</sub> H <sub>4</sub> BrN	156.95271	C <sub>7</sub> H <sub>13</sub> NOS	159.07179	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>	161.04768
C <sub>8</sub> H <sub>10</sub> O <sub>3</sub>	154.06299	C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	156.96973	C <sub>8</sub> H <sub>14</sub> CIN	159.08148	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> S	161.05105
C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	154.07423	C <sub>6</sub> H <sub>4</sub> CINO <sub>2</sub>	156.99306	C <sub>7</sub> H <sub>13</sub> NO <sub>3</sub>	159.08954	C <sub>7</sub> H <sub>12</sub> CINO	161.06074
C <sub>9</sub> H <sub>14</sub> S	154.08162	C <sub>6</sub> H <sub>7</sub> NS <sub>2</sub>	157.00199	C <sub>11</sub> H <sub>13</sub> N	159.10480	C <sub>10</sub> H <sub>11</sub> NO	161.08406
C <sub>9</sub> H <sub>14</sub> O <sub>2</sub>	154.09938	C <sub>4</sub> H <sub>9</sub> Cl <sub>2</sub> NO	157.00612	C <sub>8</sub> H <sub>17</sub> NS	159.10817	C <sub>7</sub> H <sub>15</sub> NOS	161.08744
C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O	154.11061	C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> S	157.01975	C <sub>8</sub> H <sub>17</sub> NO <sub>2</sub>	159.12593	C <sub>8</sub> H <sub>16</sub> CIN	161.09713
C <sub>10</sub> H <sub>18</sub> O	154.13577	C <sub>7</sub> H <sub>8</sub> CINO	157.02944	C <sub>5</sub> H <sub>5</sub> BrO	159.95238	C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub>	161.10519
C <sub>9</sub> H <sub>18</sub> N <sub>2</sub>	154.14700	C <sub>7</sub> H <sub>11</sub> NOS	157.05614	C <sub>4</sub> H <sub>5</sub> BrN <sub>2</sub>	159.96361	C <sub>11</sub> H <sub>15</sub> N	161.12045
C <sub>6</sub> H <sub>5</sub> NS <sub>2</sub>	154.98634	C <sub>8</sub> H <sub>12</sub> CIN	157.06583	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	159.96527	C <sub>8</sub> H <sub>19</sub> NS	161.12382

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>8</sub> H <sub>19</sub> NO <sub>2</sub>	161.14158	C <sub>9</sub> H <sub>9</sub> NS	163.04557	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	164.11609	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> S	166.05647
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O	161.96392	C <sub>6</sub> H <sub>13</sub> NS <sub>2</sub>	163.04894	C <sub>11</sub> H <sub>16</sub> O	164.12012	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>	166.05984
C <sub>5</sub> H <sub>7</sub> BrO	161.96803	C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub>	163.06333	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub>	164.13135	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	166.06299
C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	161.97515	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> S	163.06670	C <sub>12</sub> H <sub>20</sub>	164.15650	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> S	166.06637
C <sub>4</sub> H <sub>7</sub> BrN <sub>2</sub>	161.97926	C <sub>7</sub> H <sub>14</sub> CINO	163.07639	C <sub>3</sub> H <sub>4</sub> BrNO <sub>2</sub>	164.94254	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	166.07423
C <sub>5</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	161.98092	C <sub>10</sub> H <sub>13</sub> NO	163.09971	C <sub>5</sub> H <sub>5</sub> Cl <sub>2</sub> NO	164.97482	C <sub>7</sub> H <sub>15</sub> ClO <sub>2</sub>	166.07606
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	161.99216	C <sub>7</sub> H <sub>17</sub> NOS	163.10309	C <sub>4</sub> H <sub>8</sub> BrNO	164.97893	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	166.07760
C <sub>7</sub> H <sub>8</sub> Cl <sub>2</sub>	162.00031	C <sub>8</sub> H <sub>18</sub> CIN	163.11278	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> S <sub>2</sub>	164.99182	C <sub>10</sub> H <sub>14</sub> S	166.08162
C <sub>6</sub> H <sub>11</sub> Br	162.00441	C <sub>7</sub> H <sub>17</sub> NO <sub>3</sub>	163.12084	C <sub>8</sub> H <sub>4</sub> CINO	164.99814	C <sub>6</sub> H <sub>15</sub> CIN <sub>2</sub> O	166.08729
C <sub>6</sub> H <sub>7</sub> ClO <sub>3</sub>	162.00837	C <sub>11</sub> H <sub>17</sub> N	163.13610	C <sub>6</sub> H <sub>9</sub> Cl <sub>2</sub> N	165.01120	C <sub>10</sub> H <sub>14</sub> O <sub>2</sub>	166.09938
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S	162.00991	C <sub>4</sub> H <sub>5</sub> BrO <sub>2</sub>	163.94729	C <sub>5</sub> H <sub>12</sub> BrN	165.01531	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O	166.11061
C <sub>9</sub> H <sub>6</sub> OS	162.01394	C <sub>3</sub> H <sub>5</sub> BrN <sub>2</sub> O	163.95853	C <sub>5</sub> H <sub>8</sub> CINO <sub>3</sub>	165.01927	C <sub>11</sub> H <sub>18</sub> O	166.13577
C <sub>6</sub> H <sub>10</sub> OS <sub>2</sub>	162.01731	C <sub>4</sub> H <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	163.96019	C <sub>8</sub> H <sub>7</sub> NOS	165.02484	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub>	166.14700
C <sub>5</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>2</sub>	162.01961	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	163.97142	C <sub>5</sub> H <sub>11</sub> NOS <sub>2</sub>	165.02821	C <sub>3</sub> H <sub>6</sub> BrNO <sub>2</sub>	166.95819
C <sub>10</sub> H <sub>7</sub> Cl	162.02363	C <sub>8</sub> H <sub>4</sub> S <sub>2</sub>	163.97544	C <sub>9</sub> H <sub>8</sub> CIN	165.03453	C <sub>3</sub> H <sub>5</sub> NO <sub>3</sub> S <sub>2</sub>	166.97109
C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> S	162.02517	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> O	163.97957	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub>	165.04259	C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub>	166.98634
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	162.02854	C <sub>5</sub> H <sub>9</sub> BrO	163.98368	C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub> S	165.04596	C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> NO	166.99047
C <sub>9</sub> H <sub>6</sub> O <sub>3</sub>	162.03169	C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	163.99080	C <sub>6</sub> H <sub>12</sub> CINO <sub>2</sub>	165.05566	C <sub>4</sub> H <sub>10</sub> BrNO	166.99458
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C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	162.04293	C <sub>4</sub> H <sub>9</sub> BrN <sub>2</sub>	163.99491	C <sub>6</sub> H <sub>15</sub> NS <sub>2</sub>	165.06459	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S <sub>2</sub>	167.00747
C <sub>7</sub> H <sub>11</sub> ClO <sub>2</sub>	162.04476	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	163.99657	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	165.07898	C <sub>8</sub> H <sub>6</sub> CINO	167.01379
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	162.04630	C <sub>4</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>3</sub>	163.99887	C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub> S	165.08235	C <sub>6</sub> H <sub>11</sub> Cl <sub>2</sub> N	167.02685
C <sub>10</sub> H <sub>10</sub> S	162.05032	C <sub>9</sub> H <sub>5</sub> ClO	164.00289	C <sub>7</sub> H <sub>16</sub> CINO	165.09204	C <sub>5</sub> H <sub>10</sub> CINO <sub>3</sub>	167.03492
C <sub>7</sub> H <sub>14</sub> S <sub>2</sub>	162.05369	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> OS	164.00443	C <sub>10</sub> H <sub>15</sub> NO	165.11536	C <sub>8</sub> H <sub>9</sub> NOS	167.04049
C <sub>6</sub> H <sub>11</sub> CIN <sub>2</sub> O	162.05599	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> OS <sub>2</sub>	164.00781	C <sub>11</sub> H <sub>19</sub> N	165.15175	C <sub>5</sub> H <sub>13</sub> NOS <sub>2</sub>	167.04386
C <sub>10</sub> H <sub>10</sub> O <sub>2</sub>	162.06808	C <sub>8</sub> H <sub>5</sub> CIN <sub>2</sub>	164.01413	C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	165.95883	C <sub>9</sub> H <sub>10</sub> CIN	167.05018
C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> S	162.07145	C <sub>7</sub> H <sub>10</sub> Cl <sub>2</sub>	164.01596	C <sub>4</sub> H <sub>7</sub> BrO <sub>2</sub>	165.96294	C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub>	167.05824
C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O	162.07931	C <sub>6</sub> H <sub>13</sub> Br	164.02006	C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O	165.97007	C <sub>5</sub> H <sub>13</sub> NO <sub>3</sub> S	167.06161
C <sub>8</sub> H <sub>15</sub> ClO	162.08114	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	164.02219	C <sub>3</sub> H <sub>7</sub> BrN <sub>2</sub> O	165.97418	C <sub>6</sub> H <sub>14</sub> CINO <sub>2</sub>	167.07131
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C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	162.10044	C <sub>9</sub> H <sub>8</sub> OS	164.02959	C <sub>8</sub> H <sub>6</sub> S <sub>2</sub>	165.99109	C <sub>10</sub> H <sub>17</sub> NO	167.13101
C <sub>11</sub> H <sub>14</sub> O	162.10447	C <sub>6</sub> H <sub>12</sub> OS <sub>2</sub>	164.03296	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> O	165.99522	C <sub>3</sub> H <sub>5</sub> BrO <sub>3</sub>	167.94221
C <sub>8</sub> H <sub>18</sub> OS	162.10784	C <sub>5</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>2</sub>	164.03526	C <sub>5</sub> H <sub>11</sub> BrO	165.99933	C <sub>7</sub> H <sub>5</sub> Br	167.95746
C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>	162.11570	C <sub>10</sub> H <sub>9</sub> Cl	164.03928	C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub>	166.00645	C <sub>7</sub> H <sub>4</sub> OS <sub>2</sub>	167.97036
C <sub>9</sub> H <sub>19</sub> Cl	162.11753	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> S	164.04082	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> S	166.00885	C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	167.97448
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C <sub>4</sub> H <sub>6</sub> BrNO	162.96328	C <sub>7</sub> H <sub>13</sub> ClO <sub>2</sub>	164.06041	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> OS	166.02008	C <sub>3</sub> H <sub>9</sub> BrN <sub>2</sub> O	167.98983
C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> S <sub>2</sub>	162.97617	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S	164.06195	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> OS <sub>2</sub>	166.02346	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> S <sub>2</sub>	167.99149
C <sub>6</sub> H <sub>7</sub> Cl <sub>2</sub> N	162.99555	C <sub>10</sub> H <sub>12</sub> S	164.06597	C <sub>8</sub> H <sub>7</sub> CIN <sub>2</sub>	166.02978	C <sub>8</sub> H <sub>5</sub> ClO <sub>2</sub>	167.99781
C <sub>5</sub> H <sub>10</sub> BrN	162.99966	C <sub>7</sub> H <sub>16</sub> S <sub>2</sub>	164.06934	C <sub>7</sub> H <sub>12</sub> Cl <sub>2</sub>	166.03161	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S	167.99935
C <sub>5</sub> H <sub>6</sub> CINO <sub>3</sub>	163.00362	C <sub>6</sub> H <sub>13</sub> CIN <sub>2</sub> O	164.07164	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	166.03784	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	168.00272
C <sub>8</sub> H <sub>5</sub> NOS	163.00918	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	164.08373	C <sub>6</sub> H <sub>11</sub> ClO <sub>3</sub>	166.03967	C <sub>8</sub> H <sub>8</sub> S <sub>2</sub>	168.00674
C <sub>5</sub> H <sub>9</sub> NOS <sub>2</sub>	163.01256	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> S	164.08710	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	166.04121	C <sub>7</sub> H <sub>5</sub> CIN <sub>2</sub> O	168.00904
C <sub>9</sub> H <sub>6</sub> CIN	163.01888	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O	164.09496	C <sub>9</sub> H <sub>10</sub> OS	166.04524	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> O	168.01087
C <sub>8</sub> H <sub>5</sub> NO <sub>3</sub>	163.02694	C <sub>8</sub> H <sub>17</sub> ClO	164.09679	C <sub>6</sub> H <sub>14</sub> OS <sub>2</sub>	166.04861	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub>	168.02210
C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> S	163.03031	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> OS	164.09833	C <sub>5</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>2</sub>	166.05091	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> S	168.02450
C <sub>6</sub> H <sub>10</sub> CINO <sub>2</sub>	163.04001	C <sub>7</sub> H <sub>17</sub> CIN <sub>2</sub>	164.10803	C <sub>10</sub> H <sub>11</sub> Cl	166.05493	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub> S <sub>2</sub>	168.02787

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>4</sub> H <sub>9</sub> ClN <sub>2</sub> O <sub>3</sub>	168.03017	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	170.01837	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub> S	172.01942	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S	174.00991
C <sub>9</sub> H <sub>9</sub> ClO	168.03419	C <sub>8</sub> H <sub>10</sub> S <sub>2</sub>	170.02239	C <sub>8</sub> H <sub>9</sub> ClO <sub>2</sub>	172.02911	C <sub>7</sub> H <sub>10</sub> OS <sub>2</sub>	174.01731
C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> OS	168.03573	C <sub>7</sub> H <sub>7</sub> ClN <sub>2</sub> O	170.02469	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	172.03065	C <sub>6</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>2</sub>	174.01961
C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> OS <sub>2</sub>	168.03911	C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> O	170.02652	C <sub>8</sub> H <sub>12</sub> S <sub>2</sub>	172.03804	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	174.02854
C <sub>8</sub> H <sub>9</sub> ClN <sub>2</sub>	168.04543	C <sub>5</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub>	170.03775	C <sub>7</sub> H <sub>9</sub> ClN <sub>2</sub> O	172.04034	C <sub>7</sub> H <sub>10</sub> O <sub>3</sub> S	174.03507
C <sub>7</sub> H <sub>14</sub> Cl <sub>2</sub>	168.04726	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> S	170.04015	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub> S	172.05580	C <sub>8</sub> H <sub>11</sub> ClO <sub>2</sub>	174.04476
C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	168.05349	C <sub>4</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>3</sub>	170.04582	C <sub>9</sub> H <sub>13</sub> ClO	172.06549	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	174.04630
C <sub>6</sub> H <sub>13</sub> ClO <sub>3</sub>	168.05532	C <sub>9</sub> H <sub>11</sub> ClO	170.04984	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> OS	172.06703	C <sub>11</sub> H <sub>10</sub> S	174.05032
C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S	168.05686	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> OS	170.05138	C <sub>8</sub> H <sub>13</sub> ClN <sub>2</sub>	172.07673	C <sub>8</sub> H <sub>14</sub> S <sub>2</sub>	174.05369
C <sub>9</sub> H <sub>12</sub> OS	168.06089	C <sub>8</sub> H <sub>11</sub> ClN <sub>2</sub>	170.06108	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	172.08479	C <sub>7</sub> H <sub>11</sub> ClN <sub>2</sub> O	174.05599
C <sub>5</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>	168.06656	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	170.06914	C <sub>12</sub> H <sub>12</sub> O	172.08882	C <sub>11</sub> H <sub>10</sub> O <sub>2</sub>	174.06808
C <sub>10</sub> H <sub>13</sub> Cl	168.07058	C <sub>9</sub> H <sub>14</sub> OS	170.07654	C <sub>9</sub> H <sub>16</sub> OS	172.09219	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> S	174.07145
C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> S	168.07212	C <sub>10</sub> H <sub>15</sub> Cl	170.08623	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub>	172.10005	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O	174.07931
C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	168.07864	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> S	170.08777	C <sub>10</sub> H <sub>17</sub> Cl	172.10188	C <sub>9</sub> H <sub>15</sub> ClO	174.08114
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C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>	168.11503	C <sub>13</sub> H <sub>14</sub>	170.10955	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	172.12118	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	174.10044
C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O	168.12626	C <sub>10</sub> H <sub>18</sub> S	170.11292	C <sub>13</sub> H <sub>16</sub>	172.12520	C <sub>12</sub> H <sub>14</sub> O	174.10447
C <sub>11</sub> H <sub>20</sub> O	168.15142	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	170.13068	C <sub>10</sub> H <sub>20</sub> S	172.12857	C <sub>9</sub> H <sub>18</sub> OS	174.10784
C <sub>10</sub> H <sub>20</sub> N <sub>2</sub>	168.16265	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O	170.14191	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	172.14633	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub>	174.11570
C <sub>6</sub> H <sub>4</sub> BrN	168.95271	C <sub>6</sub> H <sub>6</sub> BrN	170.96836	C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O	172.15756	C <sub>10</sub> H <sub>19</sub> Cl	174.11753
C <sub>4</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	168.96973	C <sub>6</sub> H <sub>5</sub> NOS <sub>2</sub>	170.98126	C <sub>5</sub> H <sub>4</sub> BrNO	172.94763	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> S	174.11907
C <sub>3</sub> H <sub>8</sub> BrNO <sub>2</sub>	168.97384	C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>2</sub>	170.98538	C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>3</sub>	172.96465	C <sub>9</sub> H <sub>18</sub> O <sub>3</sub>	174.12559
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C <sub>5</sub> H <sub>12</sub> ClNO <sub>3</sub>	169.05057	C <sub>9</sub> H <sub>14</sub> ClN	171.08148	C <sub>7</sub> H <sub>11</sub> NO <sub>2</sub> S	173.05105	C <sub>6</sub> H <sub>9</sub> NOS <sub>2</sub>	175.01256
C <sub>8</sub> H <sub>11</sub> NOS	169.05614	C <sub>8</sub> H <sub>13</sub> NO <sub>3</sub>	171.08954	C <sub>8</sub> H <sub>12</sub> ClNO	173.06074	C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub> S	175.03031
C <sub>9</sub> H <sub>12</sub> ClN	169.06583	C <sub>12</sub> H <sub>13</sub> N	171.10480	C <sub>11</sub> H <sub>11</sub> NO	173.08406	C <sub>7</sub> H <sub>10</sub> ClNO <sub>2</sub>	175.04001
C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>	169.07389	C <sub>9</sub> H <sub>17</sub> NS	171.10817	C <sub>8</sub> H <sub>15</sub> NOS	173.08744	C <sub>10</sub> H <sub>9</sub> NS	175.04557
C <sub>9</sub> H <sub>15</sub> NS	169.09252	C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub>	171.12593	C <sub>9</sub> H <sub>16</sub> ClN	173.09713	C <sub>7</sub> H <sub>13</sub> NS <sub>2</sub>	175.04894
C <sub>9</sub> H <sub>15</sub> NO <sub>2</sub>	169.11028	C <sub>6</sub> H <sub>5</sub> BrO	171.95238	C <sub>8</sub> H <sub>15</sub> NO <sub>3</sub>	173.10519	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>	175.06333
C <sub>10</sub> H <sub>19</sub> NO	169.14666	C <sub>5</sub> H <sub>5</sub> BrN <sub>2</sub>	171.96361	C <sub>12</sub> H <sub>15</sub> N	173.12045	C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub> S	175.06670
C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>3</sub>	169.95375	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	171.96527	C <sub>9</sub> H <sub>19</sub> NS	173.12382	C <sub>8</sub> H <sub>14</sub> ClNO	175.07639
C <sub>3</sub> H <sub>7</sub> BrO <sub>3</sub>	169.95786	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	171.96940	C <sub>9</sub> H <sub>19</sub> NO <sub>2</sub>	173.14158	C <sub>11</sub> H <sub>13</sub> NO	175.09971
C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	169.96498	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> OS <sub>2</sub>	171.97651	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> O	173.96392	C <sub>8</sub> H <sub>17</sub> NOS	175.10309
C <sub>8</sub> H <sub>4</sub> Cl <sub>2</sub>	169.96901	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	171.98063	C <sub>6</sub> H <sub>7</sub> BrO	173.96803	C <sub>9</sub> H <sub>18</sub> ClN	175.11278
C <sub>7</sub> H <sub>7</sub> Br	169.97311	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub>	171.98466	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	173.97515	C <sub>8</sub> H <sub>17</sub> NO <sub>3</sub>	175.12084
C <sub>7</sub> H <sub>6</sub> OS <sub>2</sub>	169.98601	C <sub>7</sub> H <sub>9</sub> Br	171.98876	C <sub>5</sub> H <sub>7</sub> BrN <sub>2</sub>	173.97926	C <sub>12</sub> H <sub>17</sub> N	175.13610
C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>	169.99013	C <sub>7</sub> H <sub>5</sub> ClO <sub>3</sub>	171.99272	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	173.98092	C <sub>5</sub> H <sub>5</sub> BrO <sub>2</sub>	175.94729
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	169.99724	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S	171.99426	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	173.98505	C <sub>4</sub> H <sub>5</sub> BrN <sub>2</sub> O	175.95853
C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O	170.00137	C <sub>7</sub> H <sub>8</sub> OS <sub>2</sub>	172.00166	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	173.99216	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	175.96019
C <sub>7</sub> H <sub>6</sub> O <sub>3</sub> S	170.00377	C <sub>6</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>2</sub>	172.00396	C <sub>3</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	173.99628	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	175.97142
C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> S <sub>2</sub>	170.00714	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>	172.00578	C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub>	174.00031	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub> O	175.97957
C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub>	170.01346	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	172.01289	C <sub>7</sub> H <sub>11</sub> Br	174.00441	C <sub>6</sub> H <sub>9</sub> BrO	175.98368
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	170.01500	C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O	172.01702	C <sub>7</sub> H <sub>7</sub> ClO <sub>3</sub>	174.00837	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	175.99080



MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>5</sub> H <sub>9</sub> BrN <sub>2</sub>	175.99491	C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub>	177.07898	C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	178.13174	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> OS	180.03573
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	175.99657	C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub> S	177.08235	C <sub>12</sub> H <sub>18</sub> O	178.13577	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> OS <sub>2</sub>	180.03911
C <sub>5</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>3</sub>	175.99887	C <sub>8</sub> H <sub>16</sub> CINO	177.09204	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub>	178.14700	C <sub>9</sub> H <sub>9</sub> CIN <sub>2</sub>	180.04543
C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> OS <sub>2</sub>	176.00781	C <sub>11</sub> H <sub>15</sub> NO	177.11536	C <sub>4</sub> H <sub>6</sub> BrNO <sub>2</sub>	178.95819	C <sub>8</sub> H <sub>14</sub> Cl <sub>2</sub>	180.04726
C <sub>8</sub> H <sub>10</sub> Cl <sub>2</sub>	176.01596	C <sub>8</sub> H <sub>19</sub> NOS	177.11874	C <sub>4</sub> H <sub>5</sub> NO <sub>3</sub> S <sub>2</sub>	178.97109	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	180.05349
C <sub>7</sub> H <sub>13</sub> Br	176.02006	C <sub>9</sub> H <sub>20</sub> CIN	177.12843	C <sub>8</sub> H <sub>5</sub> NS <sub>2</sub>	178.98634	C <sub>7</sub> H <sub>13</sub> ClO <sub>3</sub>	180.05532
C <sub>7</sub> H <sub>9</sub> ClO <sub>3</sub>	176.02402	C <sub>8</sub> H <sub>19</sub> NO <sub>3</sub>	177.13649	C <sub>6</sub> H <sub>7</sub> Cl <sub>2</sub> NO	178.99047	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S	180.05686
C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S	176.02556	C <sub>12</sub> H <sub>19</sub> N	177.15175	C <sub>5</sub> H <sub>10</sub> BrNO	178.99458	C <sub>10</sub> H <sub>12</sub> OS	180.06089
C <sub>10</sub> H <sub>8</sub> OS	176.02959	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	177.95883	C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub> S	179.00410	C <sub>7</sub> H <sub>16</sub> OS <sub>2</sub>	180.06426
C <sub>7</sub> H <sub>12</sub> OS <sub>2</sub>	176.03296	C <sub>5</sub> H <sub>7</sub> BrO <sub>2</sub>	177.96294	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> S <sub>2</sub>	179.00747	C <sub>6</sub> H <sub>13</sub> CIN <sub>2</sub> O <sub>2</sub>	180.06656
C <sub>6</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>2</sub>	176.03526	C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O	177.97007	C <sub>9</sub> H <sub>6</sub> CINO	179.01379	C <sub>11</sub> H <sub>13</sub> Cl	180.07058
C <sub>11</sub> H <sub>9</sub> Cl	176.03928	C <sub>4</sub> H <sub>7</sub> BrN <sub>2</sub> O	177.97418	C <sub>7</sub> H <sub>11</sub> Cl <sub>2</sub> N	179.02685	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> S	180.07212
C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> S	176.04082	C <sub>5</sub> H <sub>6</sub> O <sub>3</sub> S <sub>2</sub>	177.97584	C <sub>6</sub> H <sub>14</sub> BrN	179.03096	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> S <sub>2</sub>	180.07549
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S <sub>2</sub>	176.04419	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	177.98707	C <sub>6</sub> H <sub>10</sub> CINO <sub>3</sub>	179.03492	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	180.07864
C <sub>10</sub> H <sub>8</sub> O <sub>3</sub>	176.04734	C <sub>9</sub> H <sub>6</sub> S <sub>2</sub>	177.99109	C <sub>9</sub> H <sub>9</sub> NOS	179.04049	C <sub>7</sub> H <sub>16</sub> O <sub>3</sub> S	180.08202
C <sub>7</sub> H <sub>12</sub> O <sub>3</sub> S	176.05072	C <sub>7</sub> H <sub>8</sub> Cl <sub>2</sub> O	177.99522	C <sub>6</sub> H <sub>13</sub> NOS <sub>2</sub>	179.04386	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	180.08988
C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	176.05858	C <sub>6</sub> H <sub>11</sub> BrO	177.99933	C <sub>10</sub> H <sub>10</sub> CIN	179.05018	C <sub>8</sub> H <sub>17</sub> ClO <sub>2</sub>	180.09171
C <sub>8</sub> H <sub>13</sub> ClO <sub>2</sub>	176.06041	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub>	178.00645	C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub>	179.05824	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S	180.09325
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S	176.06195	C <sub>9</sub> H <sub>6</sub> O <sub>2</sub> S	178.00885	C <sub>6</sub> H <sub>13</sub> NO <sub>3</sub> S	179.06161	C <sub>11</sub> H <sub>16</sub> S	180.09727
C <sub>11</sub> H <sub>12</sub> S	176.06597	C <sub>5</sub> H <sub>11</sub> BrN <sub>2</sub>	178.01056	C <sub>7</sub> H <sub>14</sub> CINO <sub>2</sub>	179.07131	C <sub>7</sub> H <sub>17</sub> CIN <sub>2</sub> O	180.10294
C <sub>8</sub> H <sub>16</sub> S <sub>2</sub>	176.06934	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S <sub>2</sub>	178.01222	C <sub>10</sub> H <sub>13</sub> NS	179.07687	C <sub>11</sub> H <sub>16</sub> O <sub>2</sub>	180.11503
C <sub>7</sub> H <sub>13</sub> CIN <sub>2</sub> O	176.07164	C <sub>5</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>3</sub>	178.01452	C <sub>7</sub> H <sub>17</sub> NS <sub>2</sub>	179.08024	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O	180.12626
C <sub>11</sub> H <sub>12</sub> O <sub>2</sub>	176.08373	C <sub>10</sub> H <sub>7</sub> ClO	178.01854	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>	179.09463	C <sub>12</sub> H <sub>20</sub> O	180.15142
C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> S	176.08710	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> OS	178.02008	C <sub>7</sub> H <sub>17</sub> NO <sub>2</sub> S	179.09800	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub>	180.16265
C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O	176.09496	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> OS <sub>2</sub>	178.02346	C <sub>8</sub> H <sub>18</sub> CINO	179.10769	C <sub>3</sub> H <sub>4</sub> BrNO <sub>3</sub>	180.93746
C <sub>9</sub> H <sub>17</sub> ClO	176.09679	C <sub>9</sub> H <sub>7</sub> CIN <sub>2</sub>	178.02978	C <sub>11</sub> H <sub>17</sub> NO	179.13101	C <sub>7</sub> H <sub>4</sub> BrN	180.95271
C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> OS	176.09833	C <sub>8</sub> H <sub>12</sub> Cl <sub>2</sub>	178.03161	C <sub>4</sub> H <sub>5</sub> BrO <sub>3</sub>	179.94221	C <sub>5</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	180.96973
C <sub>8</sub> H <sub>17</sub> CIN <sub>2</sub>	176.10803	C <sub>7</sub> H <sub>15</sub> Br	178.03571	C <sub>3</sub> H <sub>5</sub> BrN <sub>2</sub> O <sub>2</sub>	179.95344	C <sub>4</sub> H <sub>8</sub> BrNO <sub>2</sub>	180.97384
C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	176.11609	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	178.03784	C <sub>8</sub> H <sub>5</sub> Br	179.95746	C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub> S <sub>2</sub>	180.98674
C <sub>12</sub> H <sub>16</sub> O	176.12012	C <sub>7</sub> H <sub>11</sub> ClO <sub>3</sub>	178.03967	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	179.96633	C <sub>8</sub> H <sub>4</sub> CINO <sub>2</sub>	180.99306
C <sub>9</sub> H <sub>20</sub> OS	176.12349	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	178.04121	C <sub>8</sub> H <sub>4</sub> OS <sub>2</sub>	179.97036	C <sub>8</sub> H <sub>7</sub> NS <sub>2</sub>	181.00199
C <sub>11</sub> H <sub>16</sub> N <sub>2</sub>	176.13135	C <sub>10</sub> H <sub>10</sub> OS	178.04524	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	179.97448	C <sub>6</sub> H <sub>9</sub> Cl <sub>2</sub> NO	181.00612
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C <sub>9</sub> H <sub>20</sub> O <sub>3</sub>	176.14124	C <sub>6</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>2</sub>	178.05091	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	179.98159	C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub> S	181.01975
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C <sub>13</sub> H <sub>20</sub>	176.15650	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> S	178.05647	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub> S	179.98812	C <sub>9</sub> H <sub>8</sub> CINO	181.02944
C <sub>4</sub> H <sub>4</sub> BrNO <sub>2</sub>	176.94254	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>	178.05984	C <sub>4</sub> H <sub>9</sub> BrN <sub>2</sub> O	179.98983	C <sub>7</sub> H <sub>13</sub> Cl <sub>2</sub> N	181.04250
C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> NO	176.97482	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	178.06299	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S <sub>2</sub>	179.99149	C <sub>6</sub> H <sub>12</sub> CINO <sub>3</sub>	181.05057
C <sub>5</sub> H <sub>8</sub> BrNO	176.97893	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> S	178.06637	C <sub>9</sub> H <sub>5</sub> ClO <sub>2</sub>	179.99781	C <sub>9</sub> H <sub>11</sub> NOS	181.05614
C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub> S <sub>2</sub>	176.99182	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	178.07423	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S	179.99935	C <sub>6</sub> H <sub>15</sub> NOS <sub>2</sub>	181.05951
C <sub>7</sub> H <sub>9</sub> Cl <sub>2</sub> N	177.01120	C <sub>8</sub> H <sub>15</sub> ClO <sub>2</sub>	178.07606	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	180.00272	C <sub>10</sub> H <sub>12</sub> CIN	181.06583
C <sub>6</sub> H <sub>12</sub> BrN	177.01531	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	178.07760	C <sub>9</sub> H <sub>8</sub> S <sub>2</sub>	180.00674	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	181.07389
C <sub>6</sub> H <sub>8</sub> CINO <sub>3</sub>	177.01927	C <sub>11</sub> H <sub>14</sub> S	178.08162	C <sub>8</sub> H <sub>5</sub> CIN <sub>2</sub> O	180.00904	C <sub>6</sub> H <sub>15</sub> NO <sub>3</sub> S	181.07726
C <sub>9</sub> H <sub>7</sub> NOS	177.02484	C <sub>8</sub> H <sub>18</sub> S <sub>2</sub>	178.08499	C <sub>7</sub> H <sub>10</sub> Cl <sub>2</sub> O	180.01087	C <sub>7</sub> H <sub>16</sub> CINO <sub>2</sub>	181.08696
C <sub>6</sub> H <sub>11</sub> NOS <sub>2</sub>	177.02821	C <sub>7</sub> H <sub>15</sub> CIN <sub>2</sub> O	178.08729	C <sub>6</sub> H <sub>13</sub> BrO	180.01498	C <sub>10</sub> H <sub>15</sub> NS	181.09252
C <sub>10</sub> H <sub>8</sub> CIN	177.03453	C <sub>11</sub> H <sub>14</sub> O <sub>2</sub>	178.09938	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub>	180.02210	C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>	181.11028
C <sub>9</sub> H <sub>7</sub> NO <sub>3</sub>	177.04259	C <sub>8</sub> H <sub>18</sub> O <sub>2</sub> S	178.10275	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub> S	180.02450	C <sub>11</sub> H <sub>19</sub> NO	181.14666
C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> S	177.04596	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O	178.11061	C <sub>5</sub> H <sub>13</sub> BrN <sub>2</sub>	180.02621	C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>3</sub>	181.95375
C <sub>7</sub> H <sub>12</sub> CINO <sub>2</sub>	177.05566	C <sub>9</sub> H <sub>19</sub> ClO	178.11244	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> S <sub>2</sub>	180.02787	C <sub>4</sub> H <sub>7</sub> BrO <sub>3</sub>	181.95786
C <sub>10</sub> H <sub>11</sub> NS	177.06122	C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> OS	178.11398	C <sub>5</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>3</sub>	180.03017	C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	181.96498
C <sub>7</sub> H <sub>15</sub> NS <sub>2</sub>	177.06459	C <sub>8</sub> H <sub>19</sub> CIN <sub>2</sub>	178.12368	C <sub>10</sub> H <sub>9</sub> ClO	180.03419	C <sub>9</sub> H <sub>4</sub> Cl <sub>2</sub>	181.96901

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>3</sub> H <sub>7</sub> BrN <sub>2</sub> O <sub>2</sub>	181.96909	C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N	183.05815	C <sub>3</sub> H <sub>8</sub> BrNO <sub>3</sub>	184.96876	C <sub>11</sub> H <sub>19</sub> Cl	186.11753
C <sub>8</sub> H <sub>7</sub> Br	181.97311	C <sub>6</sub> H <sub>14</sub> CINO <sub>3</sub>	183.06622	C <sub>8</sub> H <sub>5</sub> Cl <sub>2</sub> N	184.97990	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> S	186.11907
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	181.98198	C <sub>9</sub> H <sub>13</sub> NOS	183.07179	C <sub>7</sub> H <sub>8</sub> BrN	184.98401	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>	186.12559
C <sub>8</sub> H <sub>6</sub> OS <sub>2</sub>	181.98601	C <sub>10</sub> H <sub>14</sub> CIN	183.08148	C <sub>7</sub> H <sub>4</sub> CINO <sub>3</sub>	184.98797	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	186.13683
C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>	181.99013	C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>	183.08954	C <sub>7</sub> H <sub>7</sub> NOS <sub>2</sub>	184.99691	C <sub>14</sub> H <sub>18</sub>	186.14085
C <sub>5</sub> H <sub>11</sub> BrO <sub>2</sub>	181.99424	C <sub>10</sub> H <sub>17</sub> NS	183.10817	C <sub>5</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>	185.00103	C <sub>6</sub> H <sub>6</sub> BrNO	186.96328
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	181.99724	C <sub>10</sub> H <sub>17</sub> NO <sub>2</sub>	183.12593	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub> S	185.01466	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> S <sub>2</sub>	186.97617
C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O	182.00137	C <sub>7</sub> H <sub>5</sub> BrO	183.95238	C <sub>4</sub> H <sub>11</sub> NO <sub>3</sub> S <sub>2</sub>	185.01804	C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>3</sub>	186.98030
C <sub>8</sub> H <sub>6</sub> O <sub>3</sub> S	182.00377	C <sub>6</sub> H <sub>5</sub> BrN <sub>2</sub>	183.96361	C <sub>8</sub> H <sub>8</sub> CINO <sub>2</sub>	185.02436	C <sub>8</sub> H <sub>7</sub> Cl <sub>2</sub> N	186.99555
C <sub>4</sub> H <sub>11</sub> BrN <sub>2</sub> O	182.00548	C <sub>7</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	183.96527	C <sub>8</sub> H <sub>11</sub> NS <sub>2</sub>	185.03329	C <sub>7</sub> H <sub>10</sub> BrN	186.99966
C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> S <sub>2</sub>	182.00714	C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	183.96940	C <sub>6</sub> H <sub>13</sub> Cl <sub>2</sub> NO	185.03742	C <sub>7</sub> H <sub>6</sub> CINO <sub>3</sub>	187.00362
C <sub>9</sub> H <sub>7</sub> CIO <sub>2</sub>	182.01346	C <sub>4</sub> H <sub>9</sub> BrO <sub>3</sub>	183.97351	C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub> S	185.05105	C <sub>7</sub> H <sub>9</sub> NOS <sub>2</sub>	187.01256
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	182.01500	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> OS <sub>2</sub>	183.97651	C <sub>9</sub> H <sub>12</sub> CINO	185.06074	C <sub>5</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	187.01668
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	182.01837	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	183.98063	C <sub>9</sub> H <sub>15</sub> NOS	185.08744	C <sub>7</sub> H <sub>9</sub> NO <sub>3</sub> S	187.03031
C <sub>9</sub> H <sub>10</sub> S <sub>2</sub>	182.02239	C <sub>9</sub> H <sub>6</sub> Cl <sub>2</sub>	183.98466	C <sub>10</sub> H <sub>16</sub> CIN	185.09713	C <sub>8</sub> H <sub>10</sub> CINO <sub>2</sub>	187.04001
C <sub>8</sub> H <sub>7</sub> CIN <sub>2</sub> O	182.02469	C <sub>3</sub> H <sub>9</sub> BrN <sub>2</sub> O <sub>2</sub>	183.98474	C <sub>9</sub> H <sub>15</sub> NO <sub>3</sub>	185.10519	C <sub>8</sub> H <sub>13</sub> NS <sub>2</sub>	187.04894
C <sub>7</sub> H <sub>12</sub> Cl <sub>2</sub> O	182.02652	C <sub>8</sub> H <sub>9</sub> Br	183.98876	C <sub>13</sub> H <sub>15</sub> N	185.12045	C <sub>8</sub> H <sub>13</sub> NO <sub>2</sub> S	187.06670
C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub>	182.03775	C <sub>8</sub> H <sub>5</sub> CIO <sub>3</sub>	183.99272	C <sub>10</sub> H <sub>19</sub> NS	185.12382	C <sub>9</sub> H <sub>14</sub> CINO	187.07639
C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> S	182.04015	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S	183.99426	C <sub>10</sub> H <sub>19</sub> NO <sub>2</sub>	185.14158	C <sub>12</sub> H <sub>13</sub> NO	187.09971
C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>	182.04352	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	183.99763	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	185.95990	C <sub>9</sub> H <sub>17</sub> NOS	187.10309
C <sub>5</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>3</sub>	182.04582	C <sub>8</sub> H <sub>8</sub> OS <sub>2</sub>	184.00166	C <sub>8</sub> H <sub>4</sub> Cl <sub>2</sub> O	185.96392	C <sub>10</sub> H <sub>18</sub> CIN	187.11278
C <sub>10</sub> H <sub>11</sub> CIO	182.04984	C <sub>7</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>2</sub>	184.00396	C <sub>7</sub> H <sub>7</sub> BrO	185.96803	C <sub>9</sub> H <sub>17</sub> NO <sub>3</sub>	187.12084
C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> OS	182.05138	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>	184.00578	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	185.97515	C <sub>13</sub> H <sub>17</sub> N	187.13610
C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> OS <sub>2</sub>	182.05476	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	184.01289	C <sub>6</sub> H <sub>7</sub> BrN <sub>2</sub>	185.97926	C <sub>6</sub> H <sub>5</sub> BrO <sub>2</sub>	187.94729
C <sub>9</sub> H <sub>11</sub> CIN <sub>2</sub>	182.06108	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O	184.01702	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	185.98092	C <sub>5</sub> H <sub>5</sub> BrN <sub>2</sub> O	187.95853
C <sub>8</sub> H <sub>16</sub> Cl <sub>2</sub>	182.06291	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> S	184.01942	C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	185.98505	C <sub>6</sub> H <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	187.96019
C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	182.06914	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> S <sub>2</sub>	184.02279	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	185.99216	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	187.97142
C <sub>7</sub> H <sub>15</sub> CIO <sub>3</sub>	182.07097	C <sub>9</sub> H <sub>9</sub> CIO <sub>2</sub>	184.02911	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	185.99628	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	187.97555
C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	182.07251	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	184.03065	C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub>	186.00031	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O	187.97957
C <sub>10</sub> H <sub>14</sub> OS	182.07654	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	184.03402	C <sub>8</sub> H <sub>11</sub> Br	186.00441	C <sub>7</sub> H <sub>9</sub> BrO	187.98368
C <sub>6</sub> H <sub>15</sub> CIN <sub>2</sub> O <sub>2</sub>	182.08221	C <sub>9</sub> H <sub>12</sub> S <sub>2</sub>	184.03804	C <sub>8</sub> H <sub>7</sub> CIO <sub>3</sub>	186.00837	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	187.99080
C <sub>11</sub> H <sub>15</sub> Cl	182.08623	C <sub>8</sub> H <sub>9</sub> CIN <sub>2</sub> O	184.04034	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S	186.00991	C <sub>6</sub> H <sub>9</sub> BrN <sub>2</sub>	187.99491
C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> S	182.08777	C <sub>7</sub> H <sub>14</sub> Cl <sub>2</sub> O	184.04217	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	186.01328	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	187.99657
C <sub>10</sub> H <sub>14</sub> O <sub>3</sub>	182.09429	C <sub>6</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub>	184.05340	C <sub>8</sub> H <sub>10</sub> OS <sub>2</sub>	186.01731	C <sub>6</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>3</sub>	187.99887
C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	182.10553	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub> S	184.05580	C <sub>7</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>2</sub>	186.01961	C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>3</sub>	188.00070
C <sub>11</sub> H <sub>18</sub> S	182.11292	C <sub>5</sub> H <sub>13</sub> CIN <sub>2</sub> O <sub>3</sub>	184.06147	C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>2</sub>	186.02143	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> OS <sub>2</sub>	188.00781
C <sub>11</sub> H <sub>18</sub> O <sub>2</sub>	182.13068	C <sub>10</sub> H <sub>13</sub> CIO	184.06549	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	186.02854	C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	188.01193
C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O	182.14191	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> OS	184.06703	C <sub>5</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	186.03267	C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub>	188.01596
C <sub>3</sub> H <sub>6</sub> BrNO <sub>3</sub>	182.95311	C <sub>9</sub> H <sub>13</sub> CIN <sub>2</sub>	184.07673	C <sub>8</sub> H <sub>10</sub> O <sub>3</sub> S	186.03507	C <sub>8</sub> H <sub>13</sub> Br	188.02006
C <sub>7</sub> H <sub>6</sub> BrN	182.96836	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	184.08479	C <sub>9</sub> H <sub>11</sub> CIO <sub>2</sub>	186.04476	C <sub>8</sub> H <sub>9</sub> CIO <sub>3</sub>	188.02402
C <sub>7</sub> H <sub>5</sub> NOS <sub>2</sub>	182.98126	C <sub>10</sub> H <sub>16</sub> OS	184.09219	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	186.04630	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S	188.02556
C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>2</sub>	182.98538	C <sub>11</sub> H <sub>17</sub> Cl	184.10188	C <sub>9</sub> H <sub>14</sub> S <sub>2</sub>	186.05369	C <sub>8</sub> H <sub>12</sub> OS <sub>2</sub>	188.03296
C <sub>4</sub> H <sub>10</sub> BrNO <sub>2</sub>	182.98949	C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> S	184.10342	C <sub>8</sub> H <sub>11</sub> CIN <sub>2</sub> O	186.05599	C <sub>7</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>2</sub>	188.03526
C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> S	182.99901	C <sub>10</sub> H <sub>16</sub> O <sub>3</sub>	184.10994	C <sub>9</sub> H <sub>14</sub> O <sub>2</sub> S	186.07145	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> S <sub>2</sub>	188.04419
C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> S <sub>2</sub>	183.00239	C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	184.12118	C <sub>10</sub> H <sub>15</sub> CIO	186.08114	C <sub>8</sub> H <sub>12</sub> O <sub>3</sub> S	188.05072
C <sub>8</sub> H <sub>6</sub> CINO <sub>2</sub>	183.00871	C <sub>14</sub> H <sub>16</sub>	184.12520	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> OS	186.08268	C <sub>9</sub> H <sub>13</sub> CIO <sub>2</sub>	188.06041
C <sub>8</sub> H <sub>9</sub> NS <sub>2</sub>	183.01764	C <sub>11</sub> H <sub>20</sub> S	184.12857	C <sub>9</sub> H <sub>15</sub> CIN <sub>2</sub>	186.09238	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S	188.06195
C <sub>6</sub> H <sub>11</sub> Cl <sub>2</sub> NO	183.02177	C <sub>11</sub> H <sub>20</sub> O <sub>2</sub>	184.14633	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	186.10044	C <sub>12</sub> H <sub>12</sub> S	188.06597
C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> S	183.03540	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O	184.15756	C <sub>13</sub> H <sub>14</sub> O	186.10447	C <sub>9</sub> H <sub>16</sub> S <sub>2</sub>	188.06934
C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub> S <sub>2</sub>	183.03877	C <sub>6</sub> H <sub>4</sub> BrNO	184.94763	C <sub>10</sub> H <sub>18</sub> OS	186.10784	C <sub>8</sub> H <sub>13</sub> CIN <sub>2</sub> O	188.07164
C <sub>9</sub> H <sub>10</sub> CINO	183.04509	C <sub>4</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>3</sub>	184.96465	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>	186.11570	C <sub>12</sub> H <sub>12</sub> O <sub>2</sub>	188.08373

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>9</sub> H <sub>16</sub> O <sub>2</sub> S	188.08710	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	190.04121	C <sub>5</sub> H <sub>9</sub> BrN <sub>2</sub> O	191.98983	C <sub>10</sub> H <sub>8</sub> CINO	193.02944
C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O	188.09496	C <sub>11</sub> H <sub>10</sub> OS	190.04524	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> S <sub>2</sub>	191.99149	C <sub>8</sub> H <sub>13</sub> Cl <sub>2</sub> N	193.04250
C <sub>10</sub> H <sub>17</sub> ClO	188.09679	C <sub>8</sub> H <sub>14</sub> OS <sub>2</sub>	190.04861	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	192.00272	C <sub>7</sub> H <sub>16</sub> BrN	193.04661
C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> OS	188.09833	C <sub>7</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>2</sub>	190.05091	C <sub>10</sub> H <sub>8</sub> S <sub>2</sub>	192.00674	C <sub>7</sub> H <sub>12</sub> CINO <sub>3</sub>	193.05057
C <sub>9</sub> H <sub>17</sub> CIN <sub>2</sub>	188.10803	C <sub>12</sub> H <sub>11</sub> Cl	190.05493	C <sub>8</sub> H <sub>10</sub> Cl <sub>2</sub> O	192.01087	C <sub>10</sub> H <sub>11</sub> NOS	193.05614
C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	188.11609	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> S	190.05647	C <sub>7</sub> H <sub>13</sub> BrO	192.01498	C <sub>7</sub> H <sub>15</sub> NOS <sub>2</sub>	193.05951
C <sub>13</sub> H <sub>16</sub> O	188.12012	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>	190.05984	C <sub>7</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub>	192.02210	C <sub>11</sub> H <sub>12</sub> CIN	193.06583
C <sub>10</sub> H <sub>20</sub> OS	188.12349	C <sub>11</sub> H <sub>10</sub> O <sub>3</sub>	190.06299	C <sub>10</sub> H <sub>8</sub> O <sub>2</sub> S	192.02450	C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>	193.07389
C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>	188.13135	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub> S	190.06637	C <sub>6</sub> H <sub>13</sub> BrN <sub>2</sub>	192.02621	C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub> S	193.07726
C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> S	188.13472	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	190.07423	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> S <sub>2</sub>	192.02787	C <sub>8</sub> H <sub>16</sub> CINO <sub>2</sub>	193.08696
C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>	188.14124	C <sub>9</sub> H <sub>15</sub> ClO <sub>2</sub>	190.07606	C <sub>6</sub> H <sub>9</sub> CIN <sub>2</sub> O <sub>3</sub>	192.03017	C <sub>11</sub> H <sub>15</sub> NS	193.09252
C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	188.15248	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	190.07760	C <sub>11</sub> H <sub>9</sub> ClO	192.03419	C <sub>8</sub> H <sub>19</sub> NS <sub>2</sub>	193.09589
C <sub>14</sub> H <sub>20</sub>	188.15650	C <sub>12</sub> H <sub>14</sub> S	190.08162	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> OS	192.03573	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	193.11028
C <sub>5</sub> H <sub>4</sub> BrNO <sub>2</sub>	188.94254	C <sub>9</sub> H <sub>18</sub> S <sub>2</sub>	190.08499	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> OS <sub>2</sub>	192.03911	C <sub>8</sub> H <sub>19</sub> NO <sub>2</sub> S	193.11365
C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO	188.97482	C <sub>8</sub> H <sub>15</sub> CIN <sub>2</sub> O	190.08729	C <sub>10</sub> H <sub>9</sub> CIN <sub>2</sub>	192.04543	C <sub>9</sub> H <sub>20</sub> CINO	193.12334
C <sub>6</sub> H <sub>8</sub> BrNO	188.97893	C <sub>12</sub> H <sub>14</sub> O <sub>2</sub>	190.09938	C <sub>9</sub> H <sub>14</sub> Cl <sub>2</sub>	192.04726	C <sub>12</sub> H <sub>19</sub> NO	193.14666
C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> S <sub>2</sub>	188.99182	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub> S	190.10275	C <sub>8</sub> H <sub>17</sub> Br	192.05136	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>3</sub>	193.95375
C <sub>4</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>3</sub>	188.99595	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O	190.11061	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	192.05349	C <sub>5</sub> H <sub>7</sub> BrO <sub>3</sub>	193.95786
C <sub>8</sub> H <sub>9</sub> Cl <sub>2</sub> N	189.01120	C <sub>10</sub> H <sub>19</sub> ClO	190.11244	C <sub>8</sub> H <sub>13</sub> ClO <sub>3</sub>	192.05532	C <sub>5</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	193.96498
C <sub>7</sub> H <sub>12</sub> BrN	189.01531	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> OS	190.11398	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S	192.05686	C <sub>4</sub> H <sub>7</sub> BrN <sub>2</sub> O <sub>2</sub>	193.96909
C <sub>7</sub> H <sub>8</sub> CINO <sub>3</sub>	189.01927	C <sub>9</sub> H <sub>19</sub> CIN <sub>2</sub>	190.12368	C <sub>11</sub> H <sub>12</sub> OS	192.06089	C <sub>9</sub> H <sub>7</sub> Br	193.97311
C <sub>7</sub> H <sub>11</sub> NOS <sub>2</sub>	189.02821	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	190.13174	C <sub>8</sub> H <sub>16</sub> OS <sub>2</sub>	192.06426	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	193.98198
C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub> S	189.04596	C <sub>13</sub> H <sub>18</sub> O	190.13577	C <sub>7</sub> H <sub>13</sub> CIN <sub>2</sub> O <sub>2</sub>	192.06656	C <sub>9</sub> H <sub>6</sub> OS <sub>2</sub>	193.98601
C <sub>8</sub> H <sub>12</sub> CINO <sub>2</sub>	189.05566	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub>	190.14700	C <sub>12</sub> H <sub>13</sub> Cl	192.07058	C <sub>7</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>	193.99013
C <sub>11</sub> H <sub>11</sub> NS	189.06122	C <sub>5</sub> H <sub>6</sub> BrNO <sub>2</sub>	190.95819	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> S	192.07212	C <sub>6</sub> H <sub>11</sub> BrO <sub>2</sub>	193.99424
C <sub>8</sub> H <sub>15</sub> NS <sub>2</sub>	189.06459	C <sub>5</sub> H <sub>5</sub> NO <sub>3</sub> S <sub>2</sub>	190.97109	C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> S <sub>2</sub>	192.07549	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub>	193.99724
C <sub>11</sub> H <sub>11</sub> NO <sub>2</sub>	189.07898	C <sub>7</sub> H <sub>7</sub> Cl <sub>2</sub> NO	190.99047	C <sub>11</sub> H <sub>12</sub> O <sub>3</sub>	192.07864	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O	194.00137
C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> S	189.08235	C <sub>6</sub> H <sub>10</sub> BrNO	190.99458	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub> S	192.08202	C <sub>9</sub> H <sub>6</sub> O <sub>3</sub> S	194.00377
C <sub>9</sub> H <sub>16</sub> CINO	189.09204	C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> S <sub>2</sub>	191.00747	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	192.08988	C <sub>5</sub> H <sub>11</sub> BrN <sub>2</sub> O	194.00548
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C <sub>9</sub> H <sub>19</sub> NOS	189.11874	C <sub>7</sub> H <sub>14</sub> BrN	191.03096	C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S	192.09325	C <sub>10</sub> H <sub>7</sub> ClO <sub>2</sub>	194.01346
C <sub>10</sub> H <sub>20</sub> CIN	189.12843	C <sub>7</sub> H <sub>10</sub> CINO <sub>3</sub>	191.03492	C <sub>12</sub> H <sub>16</sub> S	192.09727	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	194.01500
C <sub>9</sub> H <sub>19</sub> NO <sub>3</sub>	189.13649	C <sub>10</sub> H <sub>9</sub> NOS	191.04049	C <sub>9</sub> H <sub>20</sub> S <sub>2</sub>	192.10064	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	194.01837
C <sub>13</sub> H <sub>19</sub> N	189.15175	C <sub>7</sub> H <sub>13</sub> NOS <sub>2</sub>	191.04386	C <sub>8</sub> H <sub>17</sub> CIN <sub>2</sub> O	192.10294	C <sub>10</sub> H <sub>10</sub> S <sub>2</sub>	194.02239
C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	189.95883	C <sub>11</sub> H <sub>10</sub> CIN	191.05018	C <sub>12</sub> H <sub>16</sub> O <sub>2</sub>	192.11503	C <sub>9</sub> H <sub>7</sub> CIN <sub>2</sub> O	194.02469
C <sub>6</sub> H <sub>7</sub> BrO <sub>2</sub>	189.96294	C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub>	191.05824	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> S	192.11840	C <sub>8</sub> H <sub>12</sub> Cl <sub>2</sub> O	194.02652
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C <sub>5</sub> H <sub>7</sub> BrN <sub>2</sub> O	189.97418	C <sub>8</sub> H <sub>14</sub> CINO <sub>2</sub>	191.07131	C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> OS	192.12963	C <sub>7</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub>	194.03775
C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> S <sub>2</sub>	189.97584	C <sub>11</sub> H <sub>13</sub> NS	191.07687	C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	192.14739	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> S	194.04015
C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	189.98707	C <sub>8</sub> H <sub>17</sub> NS <sub>2</sub>	191.08024	C <sub>13</sub> H <sub>20</sub> O	192.15142	C <sub>6</sub> H <sub>15</sub> BrN <sub>2</sub>	194.04186
C <sub>3</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	189.99120	C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub>	191.09463	C <sub>12</sub> H <sub>20</sub> N <sub>2</sub>	192.16265	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>	194.04352
C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> O	189.99522	C <sub>8</sub> H <sub>17</sub> NO <sub>2</sub> S	191.09800	C <sub>4</sub> H <sub>4</sub> BrNO <sub>3</sub>	192.93746	C <sub>6</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>3</sub>	194.04582
C <sub>7</sub> H <sub>11</sub> BrO	189.99933	C <sub>9</sub> H <sub>18</sub> CINO	191.10769	C <sub>8</sub> H <sub>4</sub> BrN	192.95271	C <sub>11</sub> H <sub>11</sub> ClO	194.04984
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C <sub>6</sub> H <sub>11</sub> BrN <sub>2</sub>	190.01056	C <sub>5</sub> H <sub>5</sub> BrO <sub>3</sub>	191.94221	C <sub>5</sub> H <sub>8</sub> BrNO <sub>2</sub>	192.97384	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> OS <sub>2</sub>	194.05476
C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> S <sub>2</sub>	190.01222	C <sub>4</sub> H <sub>5</sub> BrN <sub>2</sub> O <sub>2</sub>	191.95344	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub> S <sub>2</sub>	192.98674	C <sub>10</sub> H <sub>11</sub> CIN <sub>2</sub>	194.06108
C <sub>6</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>3</sub>	190.01452	C <sub>9</sub> H <sub>5</sub> Br	191.95746	C <sub>9</sub> H <sub>7</sub> NS <sub>2</sub>	193.00199	C <sub>9</sub> H <sub>16</sub> Cl <sub>2</sub>	194.06291
C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> OS <sub>2</sub>	190.02346	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	191.96633	C <sub>7</sub> H <sub>9</sub> Cl <sub>2</sub> NO	193.00612	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	194.06914
C <sub>9</sub> H <sub>12</sub> Cl <sub>2</sub>	190.03161	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	191.97448	C <sub>6</sub> H <sub>12</sub> BrNO	193.01023	C <sub>8</sub> H <sub>15</sub> ClO <sub>3</sub>	194.07097
C <sub>8</sub> H <sub>15</sub> Br	190.03571	C <sub>6</sub> H <sub>9</sub> BrO <sub>2</sub>	191.97859	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub> S	193.01975	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	194.07251
C <sub>8</sub> H <sub>11</sub> ClO <sub>3</sub>	190.03967	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O	191.98572	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> S <sub>2</sub>	193.02312	C <sub>11</sub> H <sub>14</sub> OS	194.07654

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C <sub>8</sub> H <sub>18</sub> OS <sub>2</sub>	194.07991	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	195.99763	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> S	197.05105	C <sub>11</sub> H <sub>18</sub> O <sub>3</sub>	198.12559
C <sub>7</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub>	194.08221	C <sub>9</sub> H <sub>8</sub> OS <sub>2</sub>	196.00166	C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub> S <sub>2</sub>	197.05442	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	198.13683
C <sub>12</sub> H <sub>15</sub> Cl	194.08623	C <sub>8</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>2</sub>	196.00396	C <sub>10</sub> H <sub>12</sub> CINO	197.06074	C <sub>15</sub> H <sub>18</sub>	198.14085
C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> S	194.08777	C <sub>7</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>	196.00578	C <sub>8</sub> H <sub>17</sub> Cl <sub>2</sub> N	197.07380	C <sub>7</sub> H <sub>6</sub> BrNO	198.96328
C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> S <sub>2</sub>	194.09114	C <sub>6</sub> H <sub>13</sub> BrO <sub>2</sub>	196.00989	C <sub>7</sub> H <sub>16</sub> CINO <sub>3</sub>	197.08187	C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub> S <sub>2</sub>	198.97617
C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	194.09429	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	196.01289	C <sub>10</sub> H <sub>15</sub> NOS	197.08744	C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>3</sub>	198.98030
C <sub>8</sub> H <sub>18</sub> O <sub>3</sub> S	194.09767	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O	196.01702	C <sub>11</sub> H <sub>16</sub> CIN	197.09713	C <sub>4</sub> H <sub>10</sub> BrNO <sub>3</sub>	198.98441
C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	194.10553	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> S	196.01942	C <sub>10</sub> H <sub>15</sub> NO <sub>3</sub>	197.10519	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N	198.99555
C <sub>9</sub> H <sub>19</sub> ClO <sub>2</sub>	194.10736	C <sub>5</sub> H <sub>13</sub> BrN <sub>2</sub> O	196.02113	C <sub>11</sub> H <sub>19</sub> NS	197.12382	C <sub>8</sub> H <sub>10</sub> BrN	198.99966
C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S	194.10890	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> S <sub>2</sub>	196.02279	C <sub>11</sub> H <sub>19</sub> NO <sub>2</sub>	197.14158	C <sub>8</sub> H <sub>6</sub> CINO <sub>3</sub>	199.00362
C <sub>12</sub> H <sub>18</sub> S	194.11292	C <sub>10</sub> H <sub>9</sub> ClO <sub>2</sub>	196.02911	C <sub>3</sub> H <sub>4</sub> Br <sub>2</sub>	197.86798	C <sub>8</sub> H <sub>9</sub> NOS <sub>2</sub>	199.01256
C <sub>8</sub> H <sub>19</sub> ClN <sub>2</sub> O	194.11859	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	196.03065	C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	197.95990	C <sub>6</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	199.01668
C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>	194.13068	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	196.03402	C <sub>9</sub> H <sub>4</sub> Cl <sub>2</sub> O	197.96392	C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub> S	199.03031
C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O	194.14191	C <sub>10</sub> H <sub>12</sub> S <sub>2</sub>	196.03804	C <sub>3</sub> H <sub>7</sub> BrN <sub>2</sub> O <sub>3</sub>	197.96400	C <sub>5</sub> H <sub>13</sub> NO <sub>3</sub> S <sub>2</sub>	199.03369
C <sub>4</sub> H <sub>6</sub> BrNO <sub>3</sub>	194.95311	C <sub>9</sub> H <sub>9</sub> ClN <sub>2</sub> O	196.04034	C <sub>8</sub> H <sub>7</sub> BrO	197.96803	C <sub>9</sub> H <sub>10</sub> CINO <sub>2</sub>	199.04001
C <sub>8</sub> H <sub>6</sub> BrN	194.96836	C <sub>8</sub> H <sub>14</sub> Cl <sub>2</sub> O	196.04217	C <sub>8</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>2</sub>	197.97515	C <sub>9</sub> H <sub>13</sub> NS <sub>2</sub>	199.04894
C <sub>8</sub> H <sub>5</sub> NOS <sub>2</sub>	194.98126	C <sub>7</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub>	196.05340	C <sub>7</sub> H <sub>7</sub> BrN <sub>2</sub>	197.97926	C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> NO	199.05307
C <sub>6</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>2</sub>	194.98538	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> S	196.05580	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	197.98092	C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub> S	199.06670
C <sub>5</sub> H <sub>10</sub> BrNO <sub>2</sub>	194.98949	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> S <sub>2</sub>	196.05917	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	197.98505	C <sub>10</sub> H <sub>14</sub> CINO	199.07639
C <sub>8</sub> H <sub>5</sub> NO <sub>3</sub> S	194.99901	C <sub>6</sub> H <sub>13</sub> CIN <sub>2</sub> O <sub>3</sub>	196.06147	C <sub>5</sub> H <sub>11</sub> BrO <sub>3</sub>	197.98916	C <sub>10</sub> H <sub>17</sub> NOS	199.10309
C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> S <sub>2</sub>	195.00239	C <sub>11</sub> H <sub>13</sub> ClO	196.06549	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	197.99216	C <sub>11</sub> H <sub>18</sub> CIN	199.11278
C <sub>9</sub> H <sub>6</sub> CINO <sub>2</sub>	195.00871	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> OS	196.06703	C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	197.99628	C <sub>10</sub> H <sub>17</sub> NO <sub>3</sub>	199.12084
C <sub>9</sub> H <sub>9</sub> NS <sub>2</sub>	195.01764	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> OS <sub>2</sub>	196.07041	C <sub>10</sub> H <sub>8</sub> Cl <sub>2</sub>	198.00031	C <sub>14</sub> H <sub>17</sub> N	199.13610
C <sub>7</sub> H <sub>11</sub> Cl <sub>2</sub> NO	195.02177	C <sub>10</sub> H <sub>13</sub> CIN <sub>2</sub>	196.07673	C <sub>4</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>	198.00039	C <sub>3</sub> H <sub>6</sub> Br <sub>2</sub>	199.88363
C <sub>6</sub> H <sub>14</sub> BrNO	195.02588	C <sub>9</sub> H <sub>18</sub> Cl <sub>2</sub>	196.07856	C <sub>9</sub> H <sub>11</sub> Br	198.00441	C <sub>7</sub> H <sub>5</sub> BrO <sub>2</sub>	199.94729
C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> S	195.03540	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	196.08479	C <sub>9</sub> H <sub>7</sub> ClO <sub>3</sub>	198.00837	C <sub>6</sub> H <sub>5</sub> BrN <sub>2</sub> O	199.95853
C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> S <sub>2</sub>	195.03877	C <sub>8</sub> H <sub>17</sub> ClO <sub>3</sub>	196.08662	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> S	198.00991	C <sub>7</sub> H <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	199.96019
C <sub>10</sub> H <sub>10</sub> CINO	195.04509	C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S	196.08816	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	198.01328	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	199.97142
C <sub>8</sub> H <sub>15</sub> Cl <sub>2</sub> N	195.05815	C <sub>11</sub> H <sub>16</sub> OS	196.09219	C <sub>9</sub> H <sub>10</sub> OS <sub>2</sub>	198.01731	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	199.97555
C <sub>7</sub> H <sub>14</sub> CINO <sub>3</sub>	195.06622	C <sub>7</sub> H <sub>17</sub> CIN <sub>2</sub> O <sub>2</sub>	196.09786	C <sub>8</sub> H <sub>7</sub> CIN <sub>2</sub> O <sub>2</sub>	198.01961	C <sub>9</sub> H <sub>6</sub> Cl <sub>2</sub> O	199.97957
C <sub>10</sub> H <sub>13</sub> NOS	195.07179	C <sub>12</sub> H <sub>17</sub> Cl	196.10188	C <sub>7</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>2</sub>	198.02143	C <sub>3</sub> H <sub>9</sub> BrN <sub>2</sub> O <sub>3</sub>	199.97965
C <sub>7</sub> H <sub>17</sub> NOS <sub>2</sub>	195.07516	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> S	196.10342	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	198.02854	C <sub>8</sub> H <sub>9</sub> BrO	199.98368
C <sub>11</sub> H <sub>14</sub> CIN	195.08148	C <sub>11</sub> H <sub>16</sub> O <sub>3</sub>	196.10994	C <sub>6</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	198.03267	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	199.99080
C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>	195.08954	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	196.12118	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> S	198.03507	C <sub>7</sub> H <sub>9</sub> BrN <sub>2</sub>	199.99491
C <sub>7</sub> H <sub>17</sub> NO <sub>3</sub> S	195.09291	C <sub>12</sub> H <sub>20</sub> S	196.12857	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> S <sub>2</sub>	198.03844	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	199.99657
C <sub>8</sub> H <sub>18</sub> CINO <sub>2</sub>	195.10261	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	196.14633	C <sub>10</sub> H <sub>11</sub> ClO <sub>2</sub>	198.04476	C <sub>7</sub> H <sub>5</sub> CIN <sub>2</sub> O <sub>3</sub>	199.99887
C <sub>11</sub> H <sub>17</sub> NS	195.10817	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O	196.15756	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	198.04630		
C <sub>11</sub> H <sub>17</sub> NO <sub>2</sub>	195.12593	C <sub>7</sub> H <sub>4</sub> BrNO	196.94763	C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	198.04967		
C <sub>3</sub> H <sub>5</sub> BrN <sub>2</sub> O <sub>3</sub>	195.94835	C <sub>5</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>3</sub>	196.96465	C <sub>10</sub> H <sub>14</sub> S <sub>2</sub>	198.05369		
C <sub>8</sub> H <sub>5</sub> BrO	195.95238	C <sub>4</sub> H <sub>8</sub> BrNO <sub>3</sub>	196.96876	C <sub>9</sub> H <sub>11</sub> CIN <sub>2</sub> O	198.05599		
C <sub>7</sub> H <sub>5</sub> BrN <sub>2</sub>	195.96361	C <sub>9</sub> H <sub>5</sub> Cl <sub>2</sub> N	196.97990	C <sub>8</sub> H <sub>16</sub> Cl <sub>2</sub> O	198.05782		
C <sub>8</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	195.96527	C <sub>8</sub> H <sub>8</sub> BrN	196.98401	C <sub>7</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub>	198.06905		
C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	195.96940	C <sub>8</sub> H <sub>4</sub> CINO <sub>3</sub>	196.98797	C <sub>10</sub> H <sub>14</sub> O <sub>2</sub> S	198.07145		
C <sub>5</sub> H <sub>9</sub> BrO <sub>3</sub>	195.97351	C <sub>8</sub> H <sub>7</sub> NOS <sub>2</sub>	196.99691	C <sub>6</sub> H <sub>15</sub> CIN <sub>2</sub> O <sub>3</sub>	198.07712		
C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> OS <sub>2</sub>	195.97651	C <sub>6</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>	197.00103	C <sub>11</sub> H <sub>15</sub> ClO	198.08114		
C <sub>5</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	195.98063	C <sub>5</sub> H <sub>12</sub> BrNO <sub>2</sub>	197.00514	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> OS	198.08268		
C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	195.98466	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> S	197.01466	C <sub>10</sub> H <sub>15</sub> CIN <sub>2</sub>	198.09238		
C <sub>4</sub> H <sub>9</sub> BrN <sub>2</sub> O <sub>2</sub>	195.98474	C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub> S <sub>2</sub>	197.01804	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	198.10044		
C <sub>9</sub> H <sub>9</sub> Br	195.98876	C <sub>9</sub> H <sub>8</sub> CINO <sub>2</sub>	197.02436	C <sub>11</sub> H <sub>18</sub> OS	198.10784		
C <sub>9</sub> H <sub>5</sub> ClO <sub>3</sub>	195.99272	C <sub>9</sub> H <sub>11</sub> NS <sub>2</sub>	197.03329	C <sub>12</sub> H <sub>19</sub> Cl	198.11753		
C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S	195.99426	C <sub>7</sub> H <sub>13</sub> Cl <sub>2</sub> NO	197.03742	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> S	198.11907		

# **NATURAL ISOTOPIC ABUNDANCE**

## List of isotopic natural abundance of some elements

Atom	Mass	%	Atom	Mass	%	Atom	Mass	%	Atom	Mass	%
Ag	108.904755	48.161	Fe	53.939613	5.9	Nd	141.90771	27.13	Si	28.976496	4.67
Ag	106.90509	51.839	Ga	70.9247	39.892	Nd	149.92088	5.64	Si	27.976927	92.23
Al	26.981539	100	Ga	68.92558	60.108	Nd	147.91689	5.76	Sm	153.92221	22.7
Ar	39.962383	99.6	Gd	157.9241	24.84	Nd	145.91312	17.19	Sm	151.91972	26.7
Ar	37.96273	0.063	Gd	156.92395	15.65	Nd	144.91257	8.3	Sm	149.91727	7.4
Ar	35.967545	0.337	Gd	155.92212	20.47	Nd	143.91008	23.8	Sm	148.91718	13.8
As	74.92159	100	Gd	154.92262	14.8	Ne	21.991383	9.25	Sm	147.91483	11.3
Au	196.96654	100	Gd	153.92087	2.18	Ne	20.993843	0.27	Sm	146.9149	15
B	11.009305	80.1	Gd	151.91978	0.2	Ne	19.992435	90.48	Sm	143.912	3.1
B	10.012937	19.9	Gd	159.92705	21.86	Ni	61.928345	3.634	Sn	123.90527	5.79
Ba	137.90523	71.7	Ge	75.9214	7.44	Ni	60.931057	1.14	Sn	121.90344	4.63
Ba	136.9058	11.23	Ge	73.92118	35.94	Ni	59.930786	26.223	Sn	119.9022	32.59
Ba	135.90456	7.85	Ge	72.92346	7.72	Ni	57.935345	68.077	Sn	118.90331	8.58
Ba	134.90567	6.593	Ge	71.92208	27.66	Ni	63.927967	0.926	Sn	117.90161	24.22
Ba	133.90448	2.42	Ge	69.92425	21.24	Np	237.0482	100	Sn	116.902954	7.68
Ba	131.90504	0.101	H	2.014	0.015	O	17.99916	0.2	Sn	115.90175	14.53
Ba	129.90628	0.106	H	1.007825	99.985	O	16.99913	0.04	Sn	114.90335	0.36
Be	9.012182	100	He	4.0026	100	O	15.994915	99.76	Sn	113.90279	0.65
Bi	208.98038	100	He	3.01603	1.37e-06	Os	189.95844	26.4	Sn	111.90482	0.97
Br	78.918335	50.69	Hf	173.94005	0.162	Os	188.95813	16.1	Sr	87.90562	82.58
Br	80.91629	49.31	Hf	179.94655	35.1	Os	187.95586	13.3	Sr	86.90888	7
C	13.003355	1.1	Hf	178.94582	13.629	Os	186.95573	1.6	Sr	85.90926	9.86
C	12	98.9	Hf	177.9437	27.297	Os	185.95383	1.58	Sr	83.91343	0.56
Ca	45.95369	0.004	Hf	176.94322	18.606	Os	183.95248	0.02	Ta	180.948	99.998
Ca	43.95548	2.086	Hf	175.9414	5.206	Os	191.96147	41	Ta	179.94746	0.012
Ca	42.958767	0.135	Hg	203.97346	6.87	P	30.973763	100	Tb	158.92534	100
Ca	41.95862	0.647	Hg	201.97061	29.86	Pb	206.97588	22.1	Te	125.90331	18.93
Ca	39.96259	96.941	Hg	200.97028	13.18	Pb	205.97444	24.1	Te	124.904434	7.12
Ca	47.952534	0.187	Hg	199.9683	23.1	Pb	203.97302	1.4	Te	123.902824	4.79
Cd	110.90418	12.8	Hg	198.96825	16.87	Pb	207.97662	52.4	Te	122.904274	0.905
Cd	109.90301	12.49	Hg	197.96674	9.97	Pd	109.90517	11.72	Te	121.90305	2.59
Cd	107.90418	0.89	Hg	195.9658	0.15	Pd	107.90389	26.46	Te	119.904045	0.095
Cd	115.904755	7.49	Ho	164.93031	100	Pd	105.90348	27.33	Te	129.90623	33.87
Cd	113.90336	28.73	I	126.90447	100	Pd	104.90508	22.33	Te	127.904465	31.7
Cd	112.9044	12.22	In	114.90388	95.7	Pd	103.90403	11.14	Th	232.03806	100
Cd	111.902756	24.13	In	112.90406	4.3	Pd	101.90563	1.02	Ti	46.951763	7.3
Ce	141.90924	11.13	Ir	190.96059	37.3	Pr	140.90765	100	Ti	45.95263	8
Ce	139.90543	88.43	Ir	192.96292	62.7	Pt	189.95992	0.01	Ti	49.944794	5.4
Ce	137.90599	0.25	K	40.961826	6.7302	Pt	197.96786	7.2	Ti	48.947872	5.5
Ce	135.90714	0.19	K	39.964	0.0117	Pt	195.96492	25.3	Ti	47.94795	73.8
Cl	36.965904	24.23	K	38.963707	93.2581	Pt	194.96477	33.8	Tl	204.9744	70.476
Cl	34.968853	75.77	Kr	77.9204	0.35	Pt	193.96266	32.9	Tl	202.97232	29.524
Co	58.933197	100	Kr	85.910614	17.3	Pt	191.96101	0.79	Tm	168.93422	100
Cr	53.93888	2.365	Kr	83.91151	57	Rb	86.90919	27.83	V	50.943962	99.75
Cr	52.94065	9.5	Kr	82.91414	11.5	Rb	84.9118	72.17	V	49.947163	0.25
Cr	51.94051	83.79	Kr	81.91348	11.6	Re	186.95575	62.6	W	185.95436	28.6
Cr	49.946045	4.345	Kr	79.91638	2.25	Re	184.95296	37.4	W	183.95093	30.7
Cs	132.90543	100	La	138.90634	99.9088	Rh	102.9055	100	W	182.95023	14.28
Cu	62.939598	69.17	La	137.9071	0.0902	Ru	103.905426	18.6	W	181.9482	26.3
Cu	64.927795	30.83	Li	7.016003	92.5	Ru	101.90435	31.6	W	179.9467	0.12
Dy	157.92441	0.1	Li	6.015121	7.5	Ru	100.90558	17.1	Y	88.905846	100
Dy	155.92528	0.06	Lu	174.94077	97.41	Ru	99.90422	12.6	Yb	173.93886	31.8
Dy	163.92917	28.2	Lu	175.94267	2.59	Ru	98.90594	12.7	Yb	172.9382	16.12
Dy	162.92873	24.9	Mg	25.982594	11.01	Ru	97.90529	1.86	Yb	171.93637	21.9
Dy	161.92679	25.5	Mg	24.985838	10	Ru	95.9076	5.54	Yb	170.93633	14.3
Dy	160.92693	18.9	Mg	23.985043	78.99	S	35.96708	0.02	Yb	169.93475	3.05
Dy	159.92519	2.34	Mn	54.938046	100	S	33.967865	4.21	Yb	167.9339	0.13
Er	169.93546	14.9	Mo	94.90584	15.92	S	32.971455	0.75	Yb	175.94257	12.7
Er	167.93237	26.8	Mo	93.90508	9.25	S	31.97207	95.02	Zn	69.92532	0.6
Er	166.93205	22.95	Mo	91.90681	14.84	Sb	122.90421	42.64	Zn	67.92484	18.8
Er	165.93028	33.6	Mo	99.90748	9.63	Sb	120.903824	57.36	Zn	66.92713	4.1
Er	163.9292	1.61	Mo	97.9054	24.13	Sc	44.95591	100	Zn	65.92603	27.9
Er	161.92877	0.14	Mo	96.90602	9.55	Se	77.917305	23.77	Zn	63.929146	48.6
Eu	152.92122	52.2	Mo	95.90468	16.68	Se	76.919914	7.63	Zr	93.90647	17.38
Eu	150.91985	47.8	N	15.000108	0.37	Se	75.91921	9.36	Zr	91.90504	17.15
F	18.998404	100	N	14.003074	99.63	Se	73.92248	0.89	Zr	90.90565	11.22
Fe	57.933277	0.28	Na	22.989767	100	Se	81.916695	8.74	Zr	89.9047	51.45
Fe	56.935394	2.1	Nb	92.90638	100	Se	79.91652	49.61	Zr	95.90827	2.8
Fe	55.93494	91.72	Nd	142.9098	12.18	Si	29.97377	3.1			

**IR**



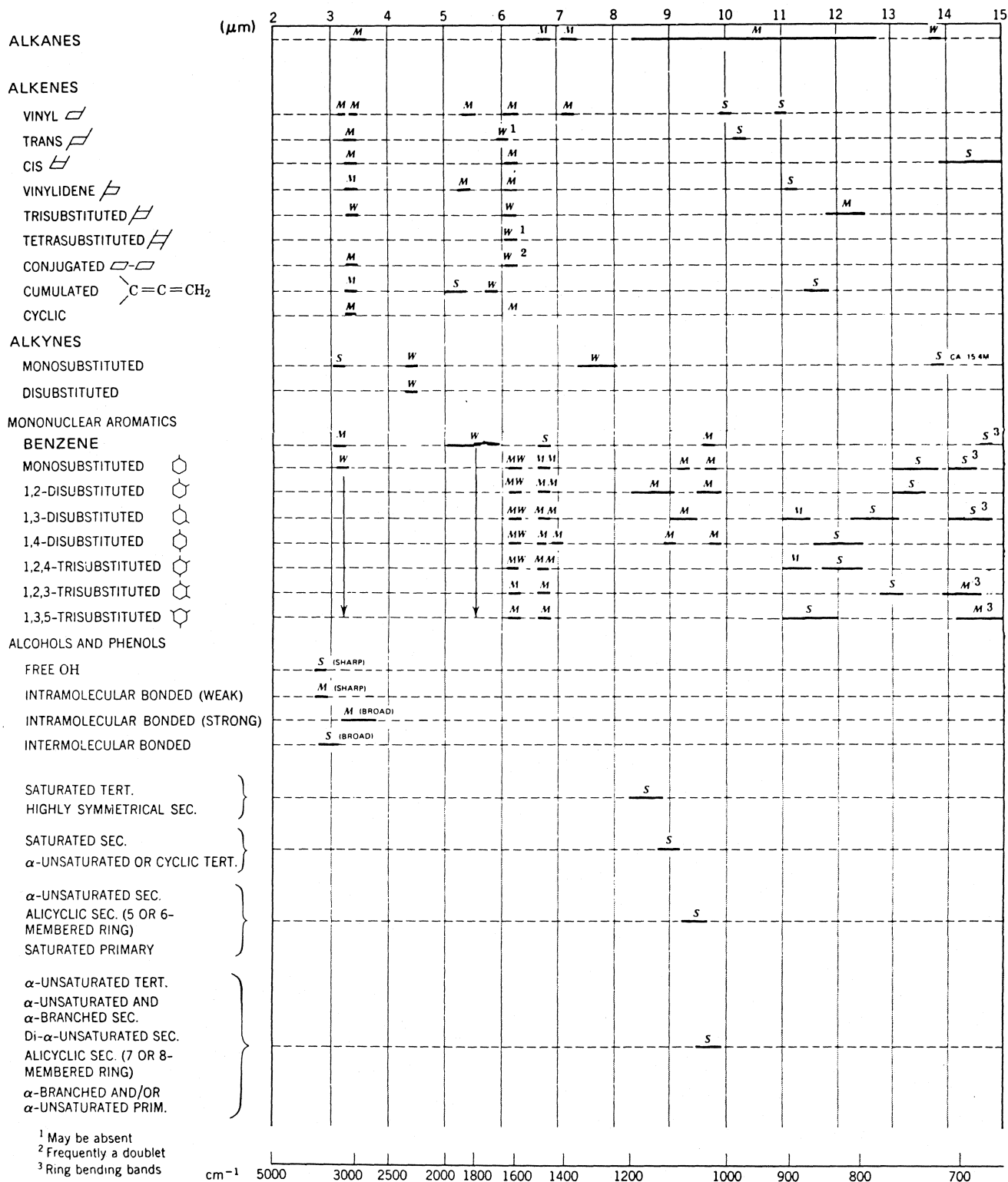


**TABLE 11-4**

Characteristic Infrared Stretching Wavenumber Ranges of Organic Molecules

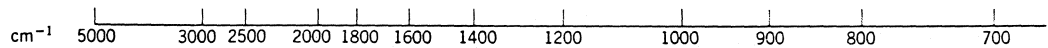
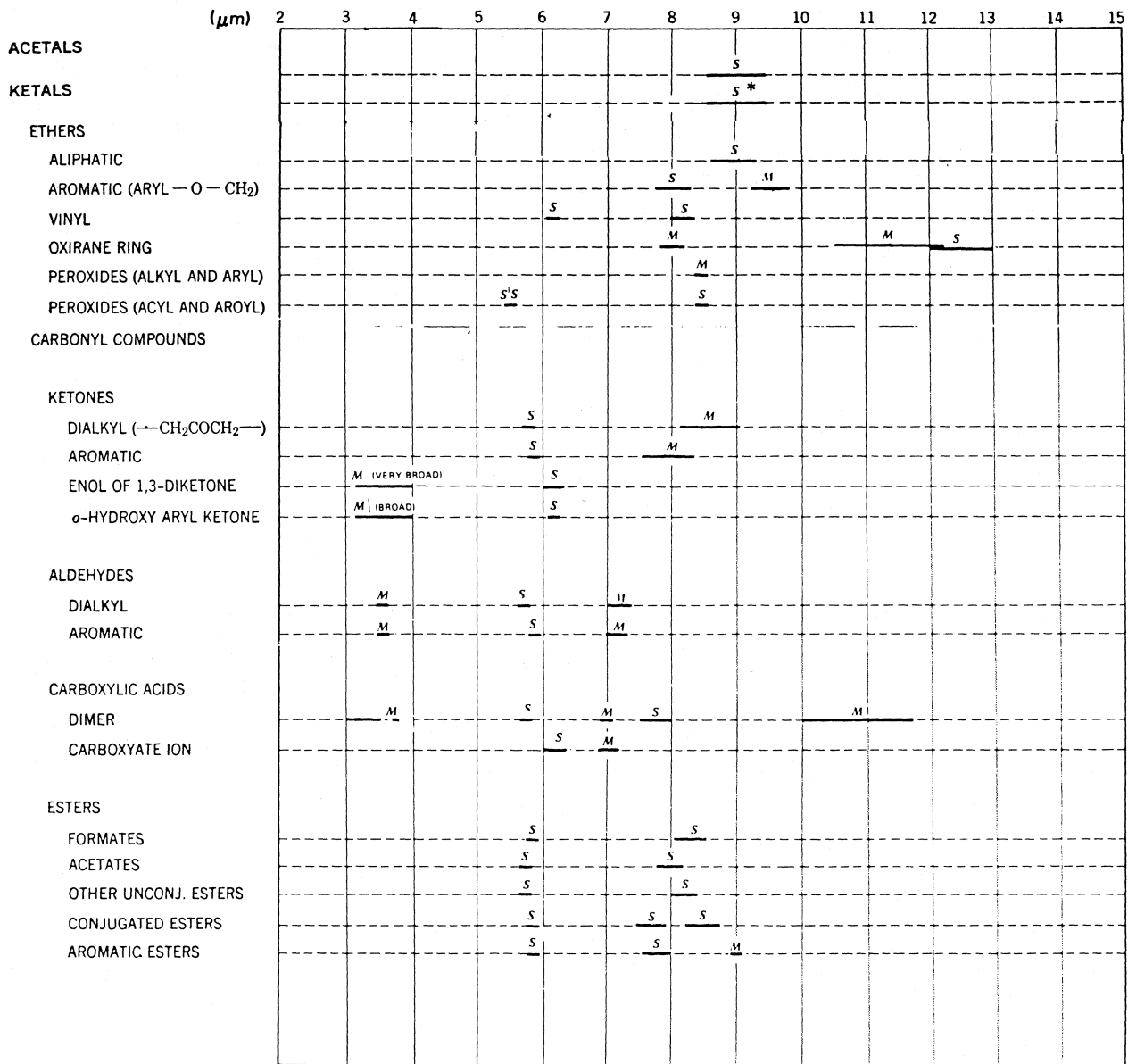
Bond or functional group	$\tilde{\nu}$ (cm <sup>-1</sup> )	Bond or functional group	$\tilde{\nu}$ (cm <sup>-1</sup> )
RO—H (alcohols)	3200–3650	RC≡N (nitriles)	2220–2260
$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCO—H} \end{array}$ (carboxylic acids)	2500–3300	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCH, RCR}' \end{array}$ (aldehydes, ketones)	1690–1750
R <sub>2</sub> N—H (amines)	3250–3500	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOR}' \end{array}$ (esters)	1735–1750
RC≡C—H (alkynes)	3260–3330	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOH} \end{array}$ (carboxylic acids)	1710–1760
$\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array}$ (alkenes)	3050–3150	$\begin{array}{c} \diagdown \\ \text{C}=\text{C} \\ \diagup \end{array}$ (alkenes)	1620–1680
$\begin{array}{c}   \\ \text{—C—H} \\   \end{array}$ (alkanes)	2840–3000	$\begin{array}{c}   \\ \text{RC—OR}' \\   \end{array}$ (alcohols, ethers)	1000–1260
RC≡CH (alkynes)	2100–2260		

# appendix c CHARACTERISTIC GROUP ABSORPTIONS

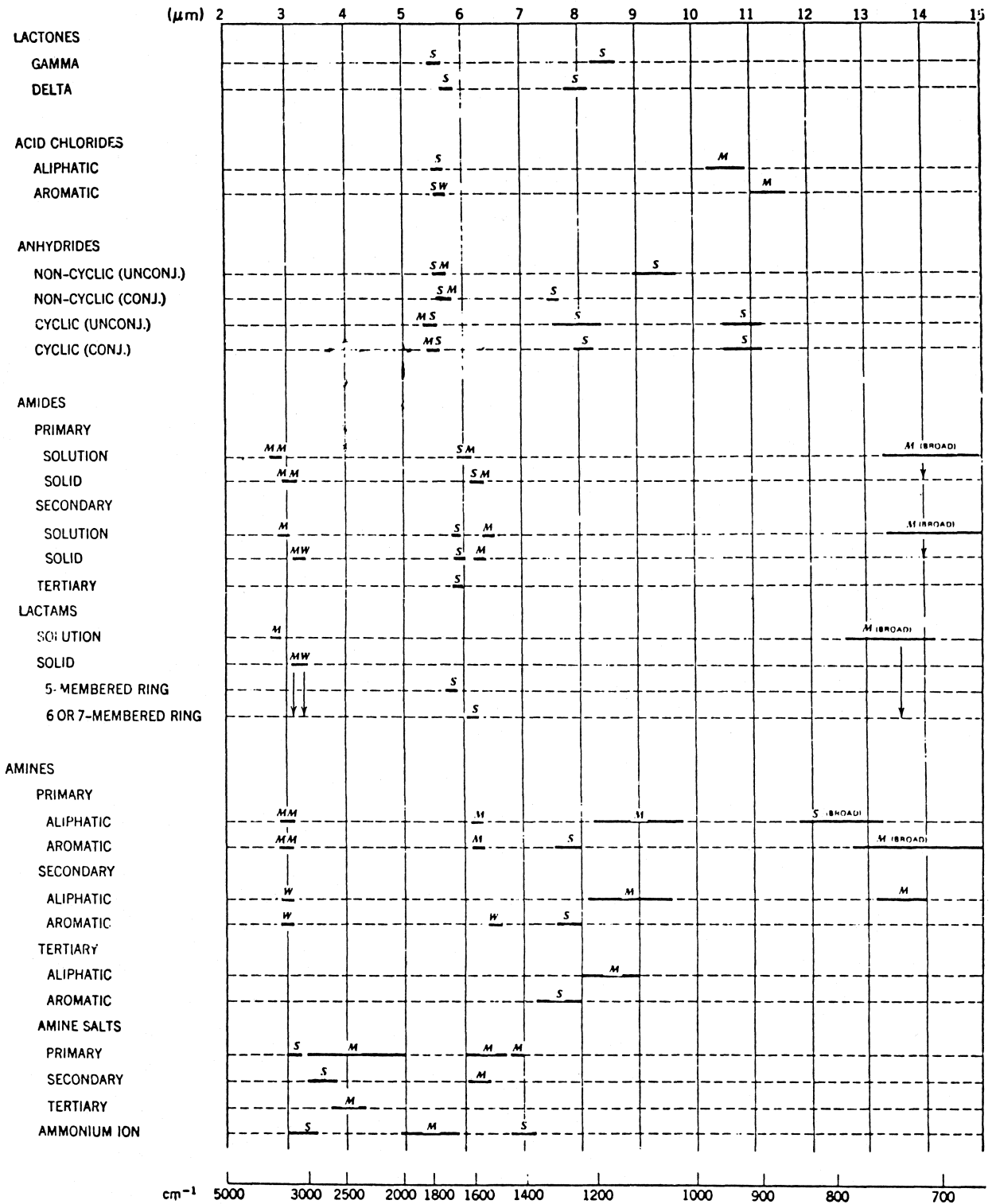


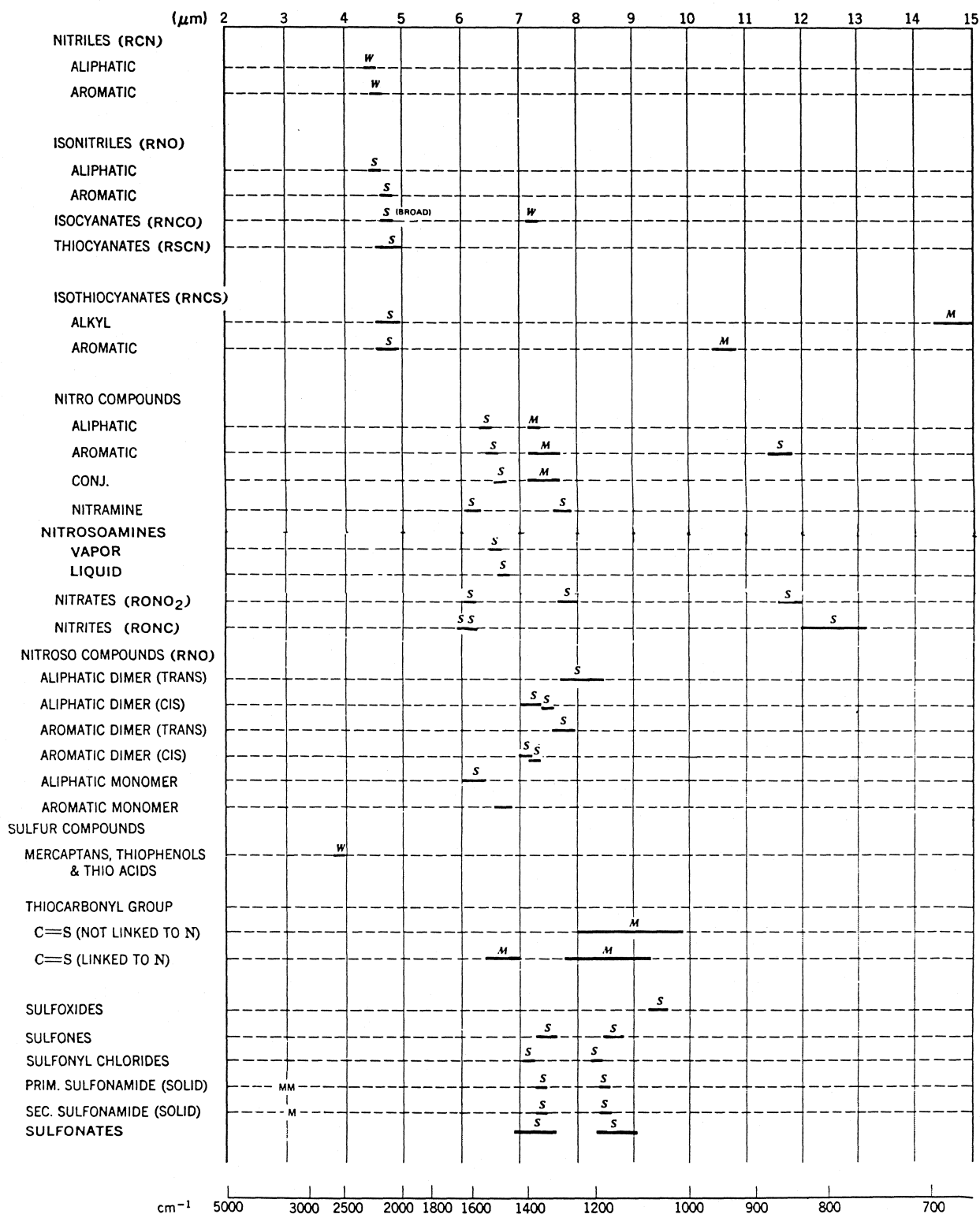
<sup>1</sup> May be absent  
<sup>2</sup> Frequently a doublet  
<sup>3</sup> Ring bending bands

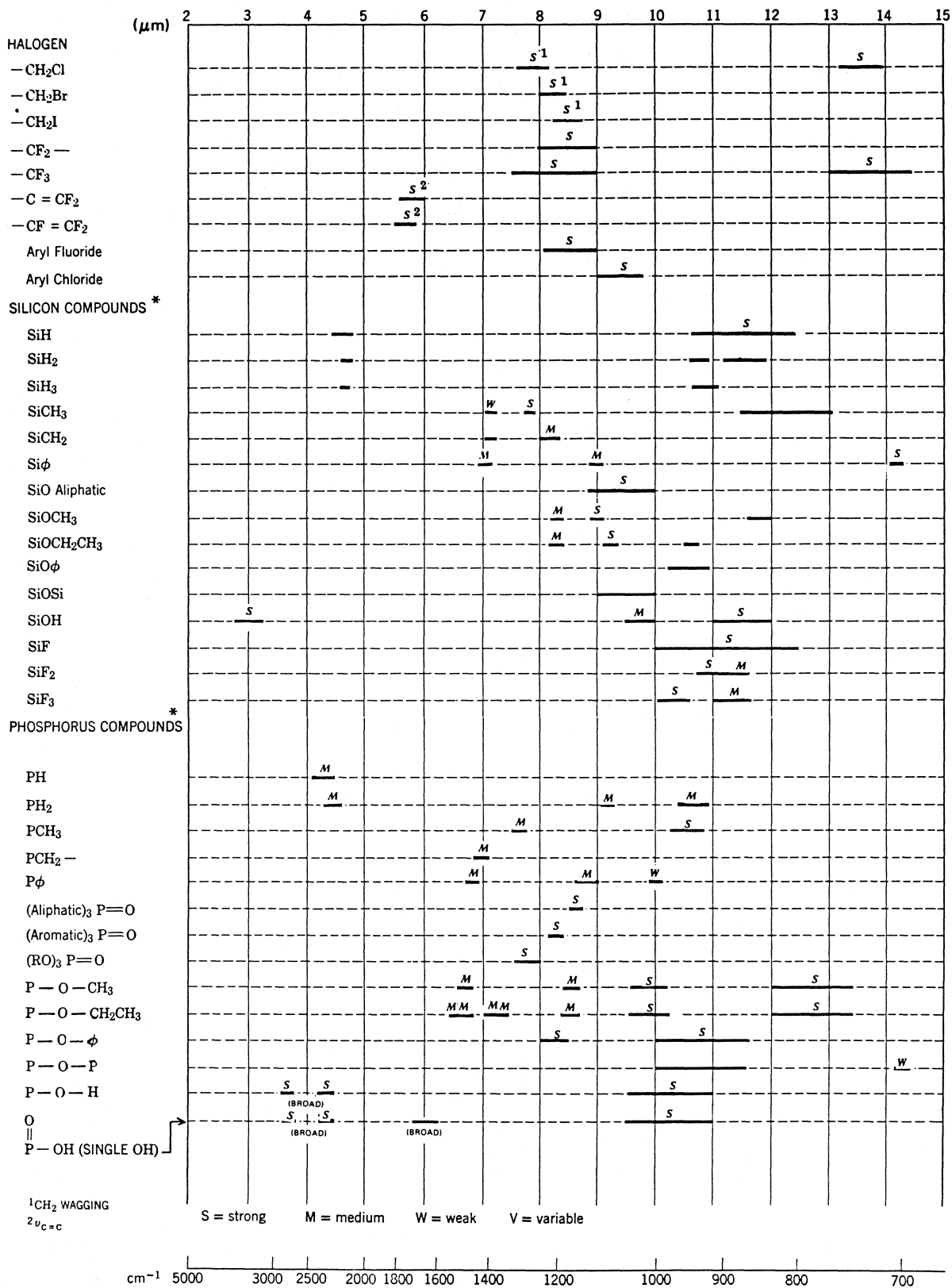
Characteristic group frequencies. The position of narrow absorption ranges is covered by a single letter indicating an average intensity. Broader absorption regions are indicated by a heavy bar. For example, a monosubstituted mononuclear aromatic may have four bands between 6 and 7  $\mu\text{m}$ , three of medium intensity, and one weak.



\*Three bands, sometimes a fourth band for ketals and a fifth band for acetals.





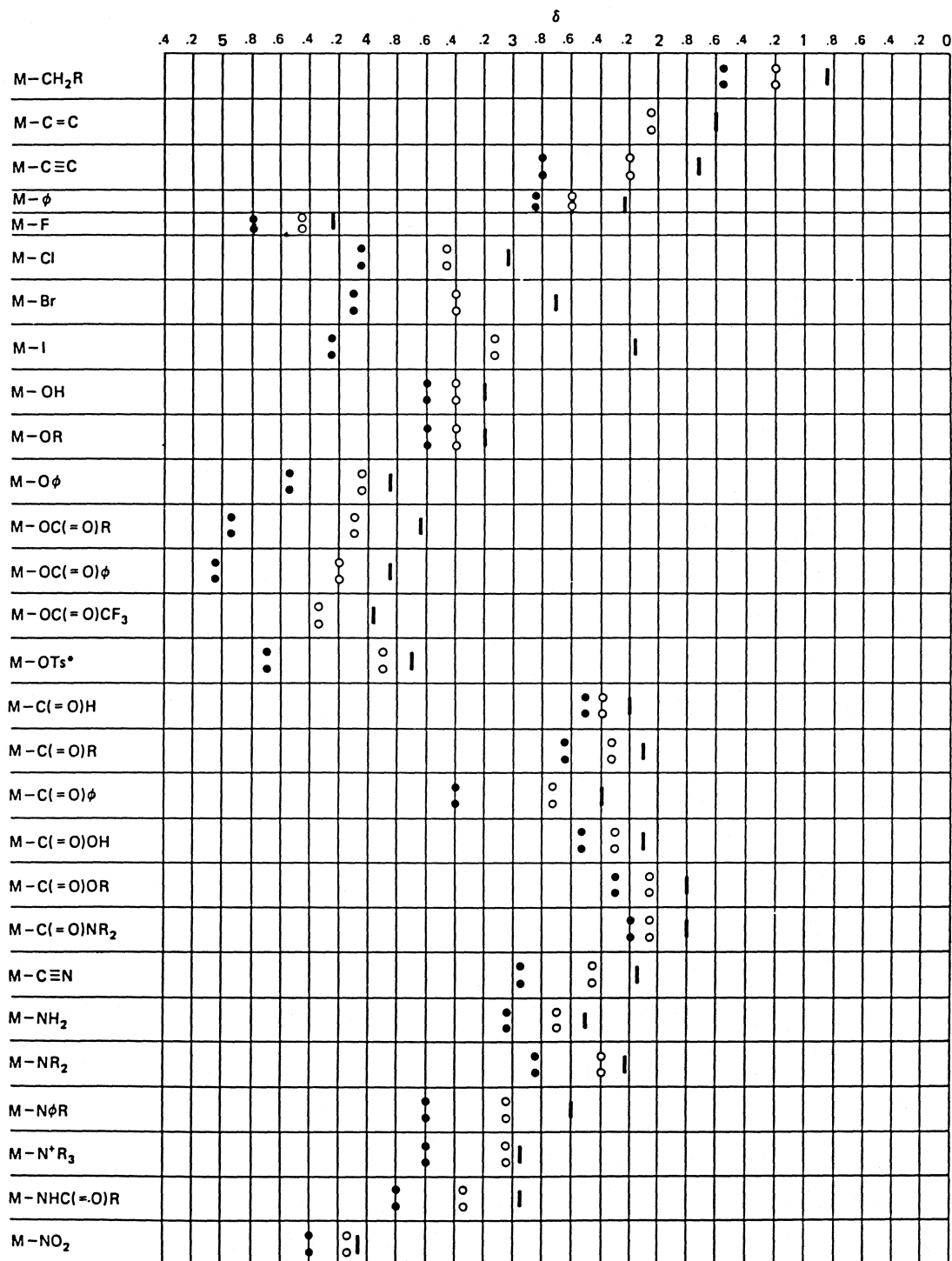


\*Tables relating to these absorptions are found in Appendix E.

**NMR**

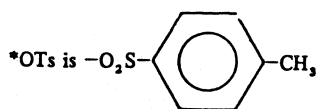
CHART 1. CHEMICAL SHIFTS OF PROTONS ON A CARBON  
 ATOM ADJACENT ( $\alpha$  - POSITION) TO A FUNCTIONAL  
 GROUP IN ALIPHATIC COMPOUNDS (M-Y).

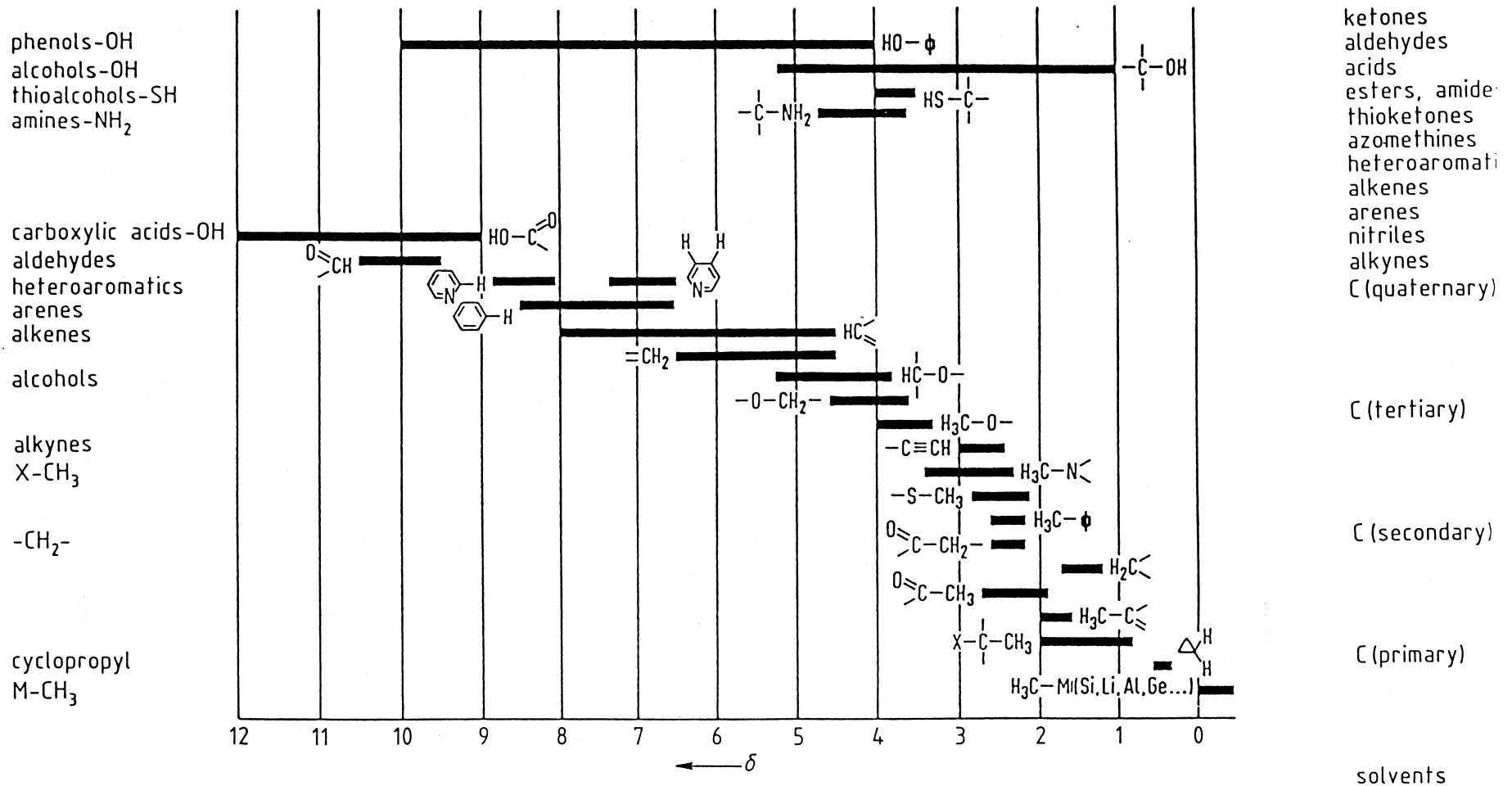
- I M = methyl
- o M = methylene
- M = methine





	.4	.2	5	.8	.6	.4	.2	4	.8	.6	.4	.2	3	.8	.6	.4	.2	2	.8	.6	.4	.2	1	.8	.6	.4	.2	0	
M-N=C				•									○																
M-N=C=O													○																
M-O-C≡N					○																								
M N=C=S								•		○																			
M-S-C≡N													•		○														
M-O-N=O				○																									
M-SH													•		○														
M-SR													•		○														
M-Sφ																													
M-SSR															○														
M-SOR													○																
M-SO <sub>2</sub> R													○																
M-SO <sub>3</sub> R																													
M-PR <sub>2</sub>																													
M-P <sup>+</sup> Cl <sub>3</sub>													○																
M-P(=O)R <sub>2</sub>																													
M-P(=S)R <sub>2</sub>															○														





**Figure 2-1.**  
Chemical shifts of  $^1\text{H}$  nuclei in organic compounds.

**Figure 2-2.**  
Chemical sh

## 2.1.1 Influence of the Charge Density on the Shielding

# <sup>1</sup>H-NMR

## SUBSTITUTED ALKANES

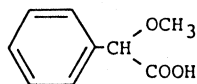
### Estimation of the Chemical Shift in Polysubstituted Alkanes

( $\delta$  in ppm relative to TMS)

$$\delta_{\text{CH}_2\text{R}_1\text{R}_2} = 1.25 + \sum_1^2 Z_i \quad \delta_{\text{CHR}_1\text{R}_2\text{R}_3} = 1.50 + \sum_1^3 Z_i$$

Substituent	$Z_i$
-alkyl	0.0
<b>C</b> -C=C-	0.8
-C≡C-	0.9
-phenyl	1.3
<b>H</b> -Cl	2.0
<b>A</b> -Br	1.9
<b>L</b> -I	1.4
-OH	1.7
-O-alkyl	1.5
<b>O</b> -O-phenyl	2.3
-OCO-alkyl	2.7
-OCO-phenyl	2.9
-NH <sub>2</sub>	1.0
<b>N</b> -N-alkyl <sub>2</sub>	1.0
-NO <sub>2</sub>	3.0
<b>S</b> -S-alkyl	1.0
-CHO	1.2
<b>O</b> -CO-alkyl	1.2
<b>H</b> -COOH	0.8
<b>C</b> -COO-alkyl	0.7
<b>\</b> -CN	1.2

Example:



base value:	1.5
-O-alkyl	1.5
-COOH	0.8
-phenyl	1.3
estimated:	5.1
determined:	4.8

# <sup>1</sup>H-NMR

## SUBSTITUTED ALKANES

### Estimation of the <sup>1</sup>H-Chemical Shift of Methylene Groups R<sub>1</sub>CH<sub>2</sub>R<sub>2</sub>

( $\delta$  in ppm relative to TMS); see H.M. Bell, L.K. Berry, E.A. Madigan, Org. Magn. Res. 22, 693 (1984).

$$\delta_{\text{CH}_2\text{R}_1\text{R}_2} = 0.23 + Z_{\text{R}_1} + Z_{\text{R}_2}$$

Substituent R	$Z_R$
-alkyl	see p. H17
-C=C-	1.33
-C≡CH	1.52
<b>C</b> -C≡Calkyl	1.52
-C≡Cphenyl	1.77
-phenyl	1.85
<b>H</b> -F	3.15
<b>A</b> -Cl	2.48
<b>L</b> -Br	2.29
-OH	2.46
-Oalkyl	2.27
<b>O</b> -Ophenyl	2.89
-OCOalkyl	2.98
-OCOPhenyl	3.23
-NH <sub>2</sub>	1.69
-NHalkyl	1.60
-N(alkyl) <sub>2</sub>	1.41
-NHphenyl <sup>2</sup>	2.15
<b>N</b> -N(alkyl)phenyl	2.39
-NH <sub>3</sub> <sup>+</sup>	2.31
-NH <sub>2</sub> <sup>+</sup> alkyl	2.31
-NH <sup>+</sup> (alkyl) <sub>2</sub>	2.46
-N <sup>+</sup> (alkyl) <sub>3</sub>	2.56
-NHCOalkyl	2.23
-N(alkyl)COalkyl	2.23
-NHCOPhenyl	2.33
-SH	1.63
<b>S</b> -Salkyl	1.63
-Sphenyl	1.92
-COalkyl	1.58
-COPhenyl	2.08
<b>O</b> -COOH	1.49
<b>H</b> -COOalkyl	1.49
<b>C</b> -COOPhenyl	1.74
<b>\</b> -CONH <sub>2</sub>	1.39
-CON(alkyl) <sub>2</sub>	1.39
-CONHphenyl	1.59
-C≡N	1.73

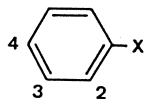
a) for CD<sub>3</sub>SOCD<sub>3</sub> or CD<sub>3</sub>SOCD<sub>3</sub>/CDCl<sub>3</sub> as solvent 0.2-0.3 ppm lower values must be used.

b) for CDCl as solvent 0.3-0.5 ppm higher values must be used.

# <sup>1</sup>H-NMR

BENZENE, SUBSTITUENT EFFECTS

Effect of a Substituent on the Chemical Shift of the Ring-Protons  
in Benzene ( $\delta$  in ppm relative to TMS)



$$\delta_{H_i} = 7.26 + Z_i$$

Substituent X	Z <sub>2</sub>	Z <sub>3</sub>	Z <sub>4</sub>
-H	0	0	0
-CH <sub>3</sub>	-0.20	-0.12	-0.22
-CH <sub>2</sub> CH <sub>3</sub>	-0.14	-0.06	-0.17
-CH(CH <sub>3</sub> ) <sub>2</sub>	-0.13	-0.08	-0.18
-C(CH <sub>3</sub> ) <sub>3</sub>	0.02	-0.08	-0.21
-CH <sub>2</sub> Cl	0.00	0.00	0.00
-CF <sub>3</sub>	0.32	0.14	0.20
<b>C</b> -CCl <sub>3</sub>	0.64	0.13	0.10
-CH <sub>2</sub> OH	-0.07	-0.07	-0.07
-CH=CH <sub>2</sub>	0.06	-0.03	-0.10
-CH=CH-phenyl	0.15	-0.01	-0.16
-C≡CH	0.15	-0.02	-0.01
-C≡C-phenyl	0.19	0.02	0.00
-phenyl	0.37	0.20	0.10
<b>H</b> -F	-0.26	0.00	-0.20
<b>A</b> -Cl	0.03	-0.02	-0.09
<b>L</b> -Br	0.18	-0.08	-0.04
-I	0.39	-0.21	0.00
-OH	-0.56	-0.12	-0.45
-OCH <sub>3</sub>	-0.48	-0.09	-0.44
-OCH <sub>2</sub> CH <sub>3</sub>	-0.46	-0.10	-0.43
<b>O</b> -O-phenyl	-0.29	-0.05	-0.23
-OCOCH <sub>3</sub>	-0.25	0.03	-0.13
-OCO-phenyl	-0.09	0.09	-0.08
-OSO <sub>2</sub> CH <sub>3</sub>	-0.05	0.07	-0.01

# <sup>1</sup>H-NMR

BENZENE, SUBSTITUENT EFFECTS

Substituent X	Z <sub>2</sub>	Z <sub>3</sub>	Z <sub>4</sub>
-NH <sub>2</sub>	-0.75	-0.25	-0.65
-NHCH <sub>3</sub>	-0.80	-0.22	-0.68
-N(CH <sub>3</sub> ) <sub>2</sub>	-0.66	-0.18	-0.67
-N <sup>+</sup> (CH <sub>3</sub> ) <sub>3</sub> I <sup>-</sup>	0.69	0.36	0.31
<b>N</b> -NHCOCH <sub>3</sub>	0.12	-0.07	-0.28
-N(CH <sub>3</sub> )COCH <sub>3</sub>	-0.16	0.05	-0.02
-NHNH <sub>2</sub>	-0.60	-0.08	-0.55
-N=N-phenyl	0.67	0.20	0.20
-NO	0.58	0.31	0.37
-NO <sub>2</sub>	0.95	0.26	0.38
-SH	-0.08	-0.16	-0.22
-SCH <sub>3</sub>	-0.08	-0.10	-0.24
<b>S</b> -S-phenyl	0.06	-0.09	-0.15
-SO <sub>3</sub> CH <sub>3</sub>	0.60	0.26	0.33
-SO <sub>2</sub> Cl	0.76	0.35	0.45
-CHO	0.56	0.22	0.29
-COCH <sub>3</sub>	0.62	0.14	0.21
-COCH <sub>2</sub> CH <sub>3</sub>	0.63	0.13	0.20
-COC(CH <sub>3</sub> ) <sub>3</sub>	0.44	0.05	0.05
<b>O</b> -CO-phenyl	0.47	0.13	0.22
-COOH	0.85	0.18	0.27
-COOCH <sub>3</sub>	0.71	0.11	0.21
-COOCH(CH <sub>3</sub> ) <sub>2</sub>	0.70	0.09	0.19
-COO-phenyl	0.90	0.17	0.27
-CONH <sub>2</sub>	0.61	0.10	0.17
-COCl	0.84	0.22	0.36
-COBr	0.80	0.21	0.37
-CH=N-phenyl	~0.6	~0.2	~0.2
-CN	0.36	0.18	0.28
-Si(CH <sub>3</sub> ) <sub>3</sub>	0.22	-0.02	-0.02
-PO(OCH <sub>3</sub> ) <sub>2</sub>	0.48	0.16	0.24

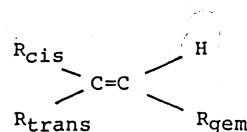
# <sup>1</sup>H-NMR

## ALKENES, ADDITIVITY RULE

### The Chemical Shift of Protons at a Double Bond

( $\delta$  in ppm relative to TMS)

$$\delta_{C=CH} = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$$



Substituent R	Z <sub>gem</sub>	Z <sub>cis</sub>	Z <sub>trans</sub>
-H	0	0	0
-alkyl	0.45	-0.22	-0.28
-alkyl ring <sup>1)</sup>	0.69	-0.25	-0.28
-CH <sub>2</sub> -aromatic	1.05	-0.29	-0.32
-CH <sub>2</sub> X, X: F, Cl, Br	0.70	0.11	-0.04
-CHF <sub>2</sub>	0.66	0.32	0.21
-CF <sub>3</sub>	0.66	0.61	0.32
<b>C</b> -CH <sub>2</sub> O	0.64	-0.01	-0.02
-CH <sub>2</sub> N	0.58	-0.10	-0.08
-CH <sub>2</sub> S	0.71	-0.13	-0.22
-CH <sub>2</sub> CO, CH <sub>2</sub> CN	0.69	-0.08	-0.06
-C=C isolated	1.00	-0.09	-0.23
-C=C conjugated <sup>2)</sup>	1.24	0.02	-0.05
-C≡C	0.47	0.38	0.12
-aromatic free rotation	1.38	0.36	-0.07
-aromatic fixed <sup>3)</sup>	1.60	-	-0.05
-aromatic o-substituted	1.65	0.19	0.09
<b>H</b> -F	1.54	-0.40	-1.02
-Cl	1.08	0.18	0.13
<b>A</b> -Br	1.07	0.45	0.55
<b>L</b> -I	1.14	0.81	0.88

- 1) The increment for "alkyl ring" is to be used if the substituent and the double bond are part of a cyclic structure.
- 2) The increment "C=C conjugated" is to be used if either the double bond or the C=C substituent is conjugated to other substituents.
- 3) The increment "aromatic, fixed" is to be used if the double bond conjugated to an aromatic ring is part of a fused ring (such as in 1,2-dihydronaphthalene).

# <sup>1</sup>H-NMR

## ALKENES, ADDITIVITY RULE

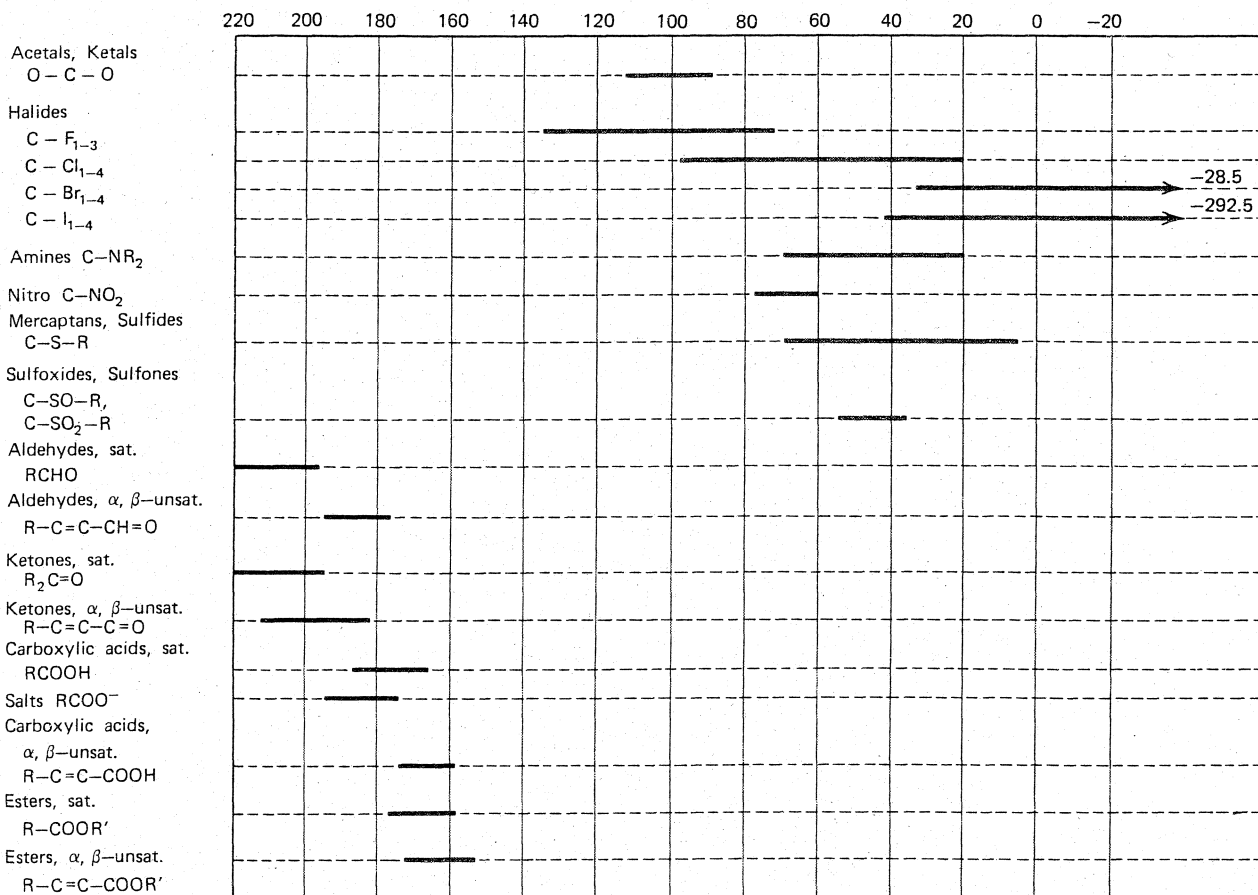
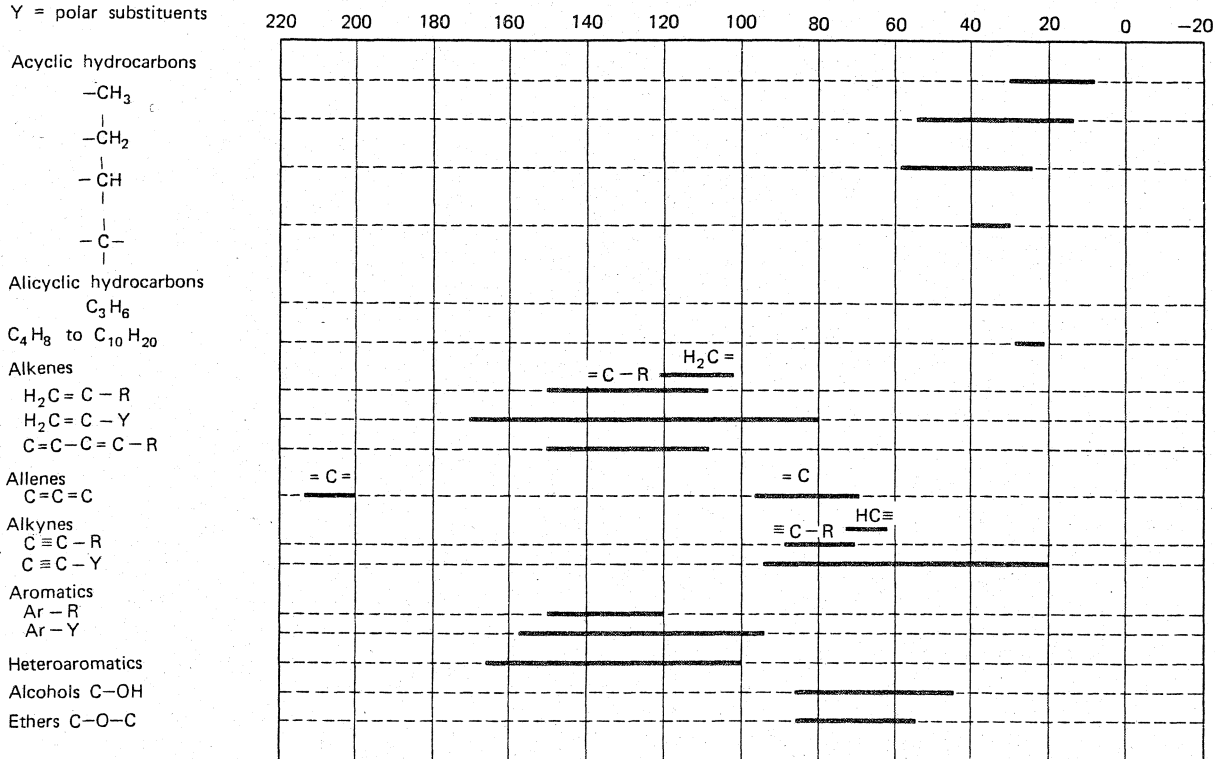
Substituent R	Z <sub>gem</sub>	Z <sub>cis</sub>	Z <sub>trans</sub>
<b>O</b> -OR, R aliphatic	1.22	-1.07	-1.21
-OR, R unsaturated	1.21	-0.60	-1.00
-OCOR	2.11	-0.35	-0.64
-NH <sub>2</sub>	0.80	-1.26	-1.21
-NHR, R aliphatic	0.80	-1.26	-1.21
-NR <sub>2</sub> , R aliphatic	0.80	-1.26	-1.21
<b>N</b> -NHR, R unsaturated	1.17	-0.53	-0.99
-NRR', R unsaturated, } R' any substituent	1.17	-0.53	-0.99
-NCOR	2.08	-0.57	-0.72
-N=N-phenyl	2.39	1.11	0.67
-NO <sub>2</sub>	1.87	1.30	0.62
-SR	1.11	-0.29	-0.13
-SOR	1.27	0.67	0.41
<b>S</b> -SO <sub>2</sub> R	1.55	1.16	0.93
-SCOR	1.41	0.06	0.02
-SCN	0.94	0.45	0.41
-SF <sub>5</sub>	1.68	0.61	0.49
-CHO	1.02	0.95	1.17
-CO isolated	1.10	1.12	0.87
-CO conjugated <sup>1)</sup>	1.06	0.91	0.74
<b>O=C</b> -COOH isolated	0.97	1.41	0.71
-COOH conjugated <sup>1)</sup>	0.80	0.98	0.32
-COOR isolated	0.80	1.18	0.55
-COOR conjugated <sup>1)</sup>	0.78	1.01	0.46
-CONR <sub>2</sub>	1.37	0.98	0.46
-COCl	1.11	1.46	1.01
-CN	0.27	0.75	0.55
-PO(OCH <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	0.66	0.88	0.67
-OPO(OCH <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	1.33	-0.34	-0.66

- 1) The increment "conjugated" is to be used if either the double bond or the substituent is conjugated to additional substituents.

# appendix c. <sup>13</sup>C correlation chart for chemical classes.

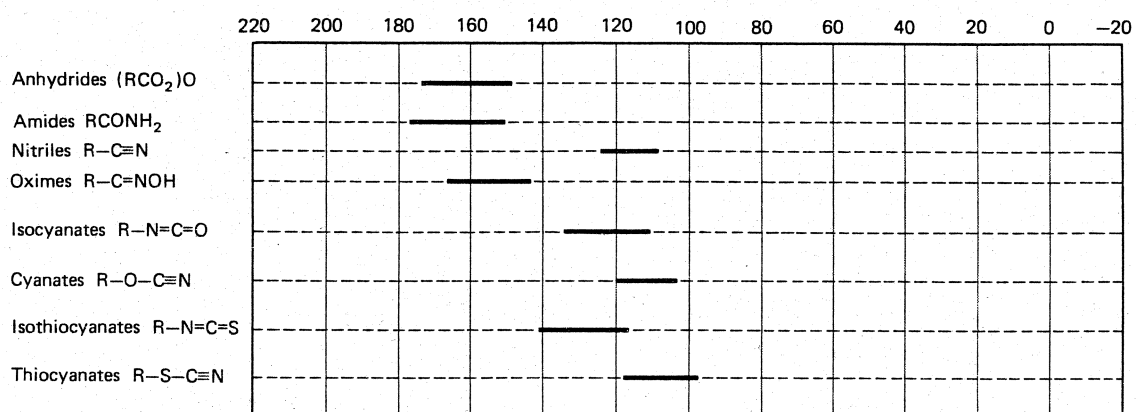
R = H or alkyl substituents  
Y = polar substituents

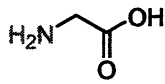
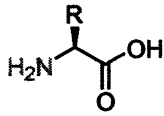
<sup>13</sup>C Correlation Chart for Chemical Classes



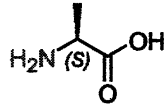
Continued on next page

appendix c (continued)

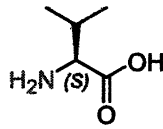




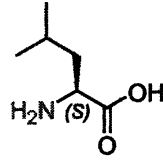
Glycine  
Gly  
G



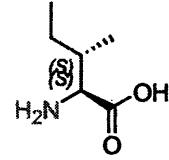
Alanine  
Ala  
A



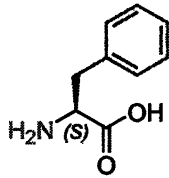
Valine  
Val  
V



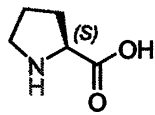
Leucine  
Leu  
L



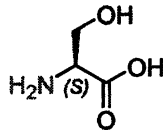
Isoleucine  
Ile  
I



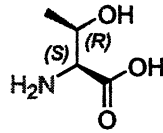
Phenylalanine  
Phe  
F



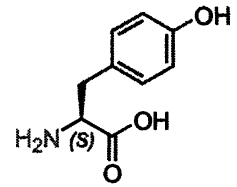
Proline  
Pro  
P



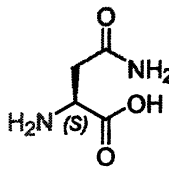
Serine  
Ser  
S



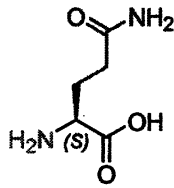
Threonine  
Thr  
T



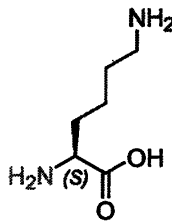
Tyrosine  
Tyr  
Y



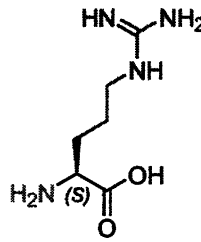
Asparagine  
Asn  
N



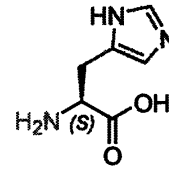
Glutamine  
Gln  
Q



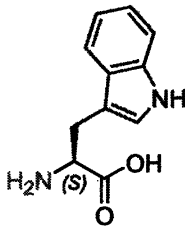
Lysine  
Lys  
K



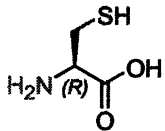
Arginine  
Arg  
R



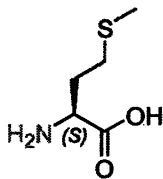
Histidine  
His  
H



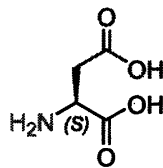
Tryptophan  
Trp  
W



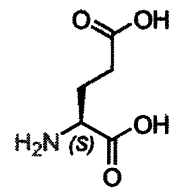
Cysteine  
Cys  
C



Methionine  
Met  
M



Aspartic acid  
Asp  
D



Glutamic acid  
Glu  
E