

## Supporting Information

**Hassane Sadou Yaye<sup>1,2a</sup>, Maher Karoui<sup>1a</sup>, Philippe-Henri Secrétan<sup>1,3</sup>,  
Noureddine Ghermani<sup>4</sup>, Jean-Michel Gillet<sup>5</sup>, Fathi Safta<sup>6</sup>, Najet Yagoubi<sup>1</sup> and  
Bernard Do<sup>1,3\*</sup>**

<sup>1</sup> University of Paris-Sud, Department of Pharmacy, Laboratory "Matériaux et Santé" EA 401, 5 rue Jean Baptiste Clément, 92296 Châtenay-Malabry, France.

<sup>2</sup> Assistance Publique-Hôpitaux de Paris, Groupe Hospitalier Pitié-Salpêtrière, Department of Pharmacy, 47-83 Boulevard de l'Hôpital, 75013 Paris, France.

<sup>3</sup> Assistance Publique-Hôpitaux de Paris, Groupe Hospitalier Henri Mondor, Department of Pharmacy, 1 Avenue du Maréchal de Lattre de Tassigny, 94010 Créteil, France.

<sup>4</sup> University of Paris-Sud, Department of Pharmacy, CNRS UMR 8612 Institut Galien Paris-Sud, LabEx LERMIT, 5, rue Jean Baptiste Clément, 92296 Châtenay-Malabry, France.

<sup>5</sup> University of Paris-Saclay, CNRS UMR 8580, Laboratory "Structures Propriétés et Modélisation des Solides" (SPMS), Grande Voie des Vignes, 92295 Châtenay-Malabry, France.

<sup>6</sup> University of Monastir, Department of Pharmacy, Analytical Chemistry Laboratory, rue Ibn Sina, 5000 Monastir, Tunisia.

<sup>a</sup> The first 2 authors contributed equally to this study and are therefore considered as first authors.

\* Corresponding author. Email: [Bernard.do@u-psud.fr](mailto:Bernard.do@u-psud.fr); Tel: +3362306275.

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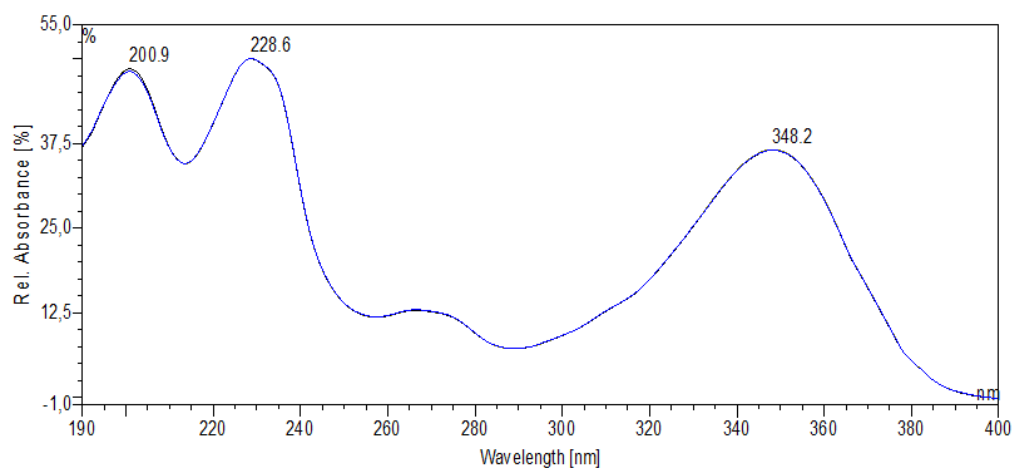


Fig. S1. UV spectrum of 25 µg mL<sup>-1</sup> RALTI in aqueous solution.

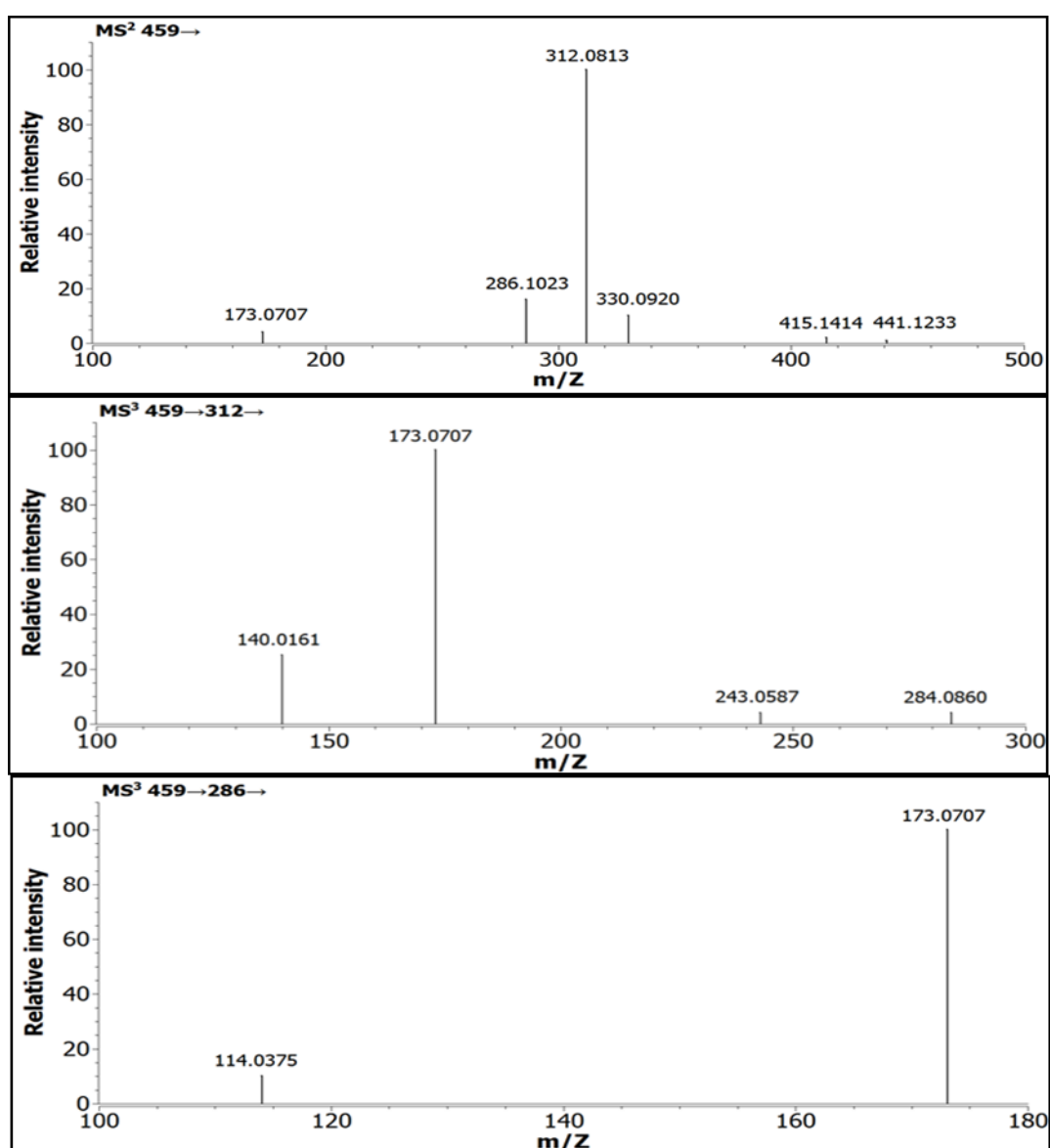


Fig. S2. High-resolution MS<sup>n</sup> mass spectra of protonated RALTI.

**Table S1.** Photoinduced electron and energy transfer reactions and the corresponding evaluating criteria

Reaction	Evaluating criteria for spontaneous reactions
<u>Electron transfer</u>	
I. $\text{RALTI}_{\text{S1/T1}} + {}^3\text{O}_2 \rightarrow \text{RALTI}^{\bullet+} + \text{O}_2^{\bullet-}$	$\Delta G_1 = \text{AEA}({}^3\text{O}_2) + \text{VIE}_{\text{S1/T1}} < 0$
II. $\text{RALTI}_{\text{S1/T1}} + \text{RALTI}_{\text{S0}} \rightarrow \text{RALTI}^{\bullet+} + \text{RALTI}^{\bullet-}$	$\Delta G_2 = \text{VEA}_{\text{S0}} + \text{VIE}_{\text{S1/T1}} < 0$
III. $\text{RALTI}_{\text{S1/T1}} + \text{RALTI}_{\text{S1/T1}} \rightarrow \text{RALTI}^{\bullet+} + \text{RALTI}^{\bullet-}$	$\Delta G_3 = \text{VEA}_{\text{S1/T1}} + \text{VIE}_{\text{S0}} < 0^a$
IV. $\text{RALTI}^{\bullet-} + {}^3\text{O}_2 \rightarrow \text{RALTI}_{\text{S0}} + \text{O}_2^{\bullet-}$	$\Delta G_4 = \text{VEA}_{\text{S1/T1}} + \text{VIE}_{\text{S1/T1}} < 0$
	$\Delta G_5 = \text{AEA}({}^3\text{O}_2) + \text{VIE}_{\text{S0}}(\text{RALTI}^{\bullet-}) < 0^b$
<u>Energy transfer</u>	
VI. $\text{RALTI}_{\text{S1}} + {}^3\text{O}_2({}^3\Sigma_g^-) \rightarrow \text{RALTI}_{\text{T1}} + {}^1\text{O}_2({}^1\Sigma_g^+)$	$E_{\text{S1}} - E_{\text{T1}} > E_{\Sigma}^c$
V. $\text{RALTI}_{\text{S1}} + {}^3\text{O}_2({}^3\Sigma_g^-) \rightarrow \text{RALTI}_{\text{T1}} + {}^1\text{O}_2({}^1\Delta_g)$	$E_{\text{S1}} - E_{\text{T1}} > E_{\Delta}^d$
VII. $\text{RALTI}_{\text{T1}} + {}^3\text{O}_2({}^3\Sigma_g^-) \rightarrow \text{RALTI}_{\text{S0}} + {}^1\text{O}_2({}^1\Sigma_g^+)$	$E_{\text{T1}} > E_{\Sigma}$
VIII. $\text{RALTI}_{\text{T1}} + {}^3\text{O}_2({}^3\Sigma_g^-) \rightarrow \text{RALTI}_{\text{S0}} + {}^1\text{O}_2({}^1\Delta_g)$	$E_{\text{T1}} > E_{\Delta}$
<p><sup>a</sup> <math>\Delta G_2</math> and <math>\Delta G_3</math> are for the electron transfer reactions with RALTI as electron acceptor and donor, respectively. <sup>b</sup> <math>\text{VIE}_{\text{S0}}(\text{RALTI}^{\bullet-}) = -\text{VEA}_{\text{S0}}(\text{RALTI})</math>. <sup>c</sup> <math>E_{\text{S1}}</math> and <math>E_{\text{T1}}</math> are the lowest singlet and triplet excitation energies of RALTI, respectively; <math>E_{\Sigma}</math> is the excitation energy of <math>{}^3\text{O}_2({}^3\Sigma_g^-)</math> to <math>{}^1\text{O}_2({}^1\Sigma_g^+)</math>. <sup>d</sup> <math>E_{\Delta}</math> is the excitation energy of <math>{}^3\text{O}_2({}^3\Sigma_g^-)</math> to <math>{}^1\text{O}_2({}^1\Delta_g)</math>.</p>	

**Table S2.** Relative retention times (rRTs), accurate masses with errors, elemental compositions and MS<sup>n</sup> product ions of raltitrexed and its photoproducts.

Compound	MS <sup>n</sup> mode	Best possible elemental formula	Accurate mass m/z	Theoretical mass m/z	Relative error (ppm)	Relative Retention time (raltitrexed's retention time : 16.02 min)
<b>Raltitrexed</b>	<b>Precursor ion</b>	<b>C<sub>21</sub>H<sub>23</sub>N<sub>4</sub>O<sub>6</sub>S<sup>+</sup></b>	<b>459.1330</b>	<b>459.1332</b>	<b>-0.44</b>	<b>1</b>
	MS <sup>2</sup> (459 →)	C <sub>21</sub> H <sub>21</sub> N <sub>4</sub> O <sub>5</sub> S <sup>+</sup>	441.1233	441.1227	1.36	
	MS <sup>2</sup> (459 →)	C <sub>20</sub> H <sub>23</sub> N <sub>4</sub> O <sub>4</sub> S <sup>+</sup>	415.1414	415.1434	-4.81	
	MS <sup>2</sup> (459 →)	C <sub>16</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	330.0920	330.0907	3.94	
	MS <sup>2</sup> (459 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	312.0813	312.0801	3.85	
	MS <sup>2</sup> (459 →)	C <sub>15</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> <sup>+</sup>	286.1023	286.1009	4.89	
	MS <sup>2</sup> (459 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0707	173.0709	-1.16	
	MS <sup>3</sup> (459→312→)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> <sup>+</sup>	284.0860	284.0852	2.82	
	MS <sup>3</sup> (459→312→)	C <sub>13</sub> H <sub>11</sub> N <sub>2</sub> O <sub>3</sub> <sup>+</sup>	243.0592	243.0587	2.06	
	MS <sup>3</sup> (459→312→)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0707	173.0709	-1.16	
	MS <sup>3</sup> (459→312→)	C <sub>6</sub> H <sub>6</sub> NOS <sup>+</sup>	140.0161	140.0164	-2.14	
	MS <sup>3</sup> (459→286→)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0707	173.0709	-1.16	
	MS <sup>3</sup> (459→286→)	C <sub>5</sub> H <sub>8</sub> NS <sup>+</sup>	114.0375	114.0372	2.63	
<b>P-1</b>	<b>Precursor ion</b>	<b>C<sub>11</sub>H<sub>14</sub>N<sub>3</sub>O<sup>+</sup></b>	<b>204.1132</b>	<b>204.1131</b>	<b>0.49</b>	<b>0.167</b>
	MS <sup>2</sup> (204 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0709	173.0709	0.00	
	MS <sup>2</sup> (204 →)	C <sub>8</sub> H <sub>6</sub> NO <sup>+</sup>	132.0446	132.0443	2.27	
<b>P-2</b>	<b>Precursor ion</b>	<b>C<sub>10</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup></b>	<b>191.0817</b>	<b>191.0815</b>	<b>1.05</b>	<b>0.169</b>
	MS <sup>2</sup> (191 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0705	173.0709	-2.31	
	MS <sup>2</sup> (191 →)	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	161.0710	161.0709	0.62	
	MS <sup>2</sup> (191 →)	C <sub>8</sub> H <sub>6</sub> NO <sup>+</sup>	132.0446	132.0443	2.27	
<b>P-3</b>	<b>Precursor ion</b>	<b>C<sub>15</sub>H<sub>16</sub>N<sub>3</sub>O<sub>4</sub><sup>+</sup></b>	<b>302.1144</b>	<b>302.1135</b>	<b>2.98</b>	<b>0.257</b>
	MS <sup>2</sup> (302 →)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> <sup>+</sup>	284.1036	284.1029	2.46	
	MS <sup>2</sup> (302 →)	C <sub>14</sub> H <sub>11</sub> N <sub>2</sub> O <sub>4</sub> <sup>+</sup>	271.0717	271.0713	1.48	
	MS <sup>2</sup> (302 →)	C <sub>14</sub> H <sub>16</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	258.1239	258.1237	0.77	
	MS <sup>2</sup> (302 →)	C <sub>14</sub> H <sub>9</sub> N <sub>2</sub> O <sub>3</sub> <sup>+</sup>	253.0611	253.0607	1.58	
	MS <sup>2</sup> (302 →)	C <sub>13</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	227.0818	227.0815	1.32	
	MS <sup>2</sup> (302 →)	C <sub>10</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	187.0511	187.0520	-4.80	
	MS <sup>2</sup> (302 →)	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	161.0712	161.0709	1.86	
	MS <sup>2</sup> (302 →)	C <sub>6</sub> H <sub>8</sub> NO <sub>3</sub> <sup>+</sup>	142.0501	142.0498	2.11	
	MS <sup>3</sup> (302→284→)	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	256.1086	256.1080	2.34	
<b>P-4</b>	<b>Precursor ion</b>	<b>C<sub>14</sub>H<sub>16</sub>N<sub>3</sub>O<sub>4</sub><sup>+</sup></b>	<b>290.1142</b>	<b>290.1135</b>	<b>2.41</b>	<b>0.288</b>
	MS <sup>2</sup> (290 →)	C <sub>13</sub> H <sub>16</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	246.1241	246.1237	1.63	

	MS <sup>2</sup> (290 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	189.0662	189.0658	2.12	
	MS <sup>2</sup> (290 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0712	173.0709	1.73	
	MS <sup>3</sup> (290 → 246 →)	C <sub>12</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	215.0820	215.0815	2.32	
	MS <sup>3</sup> (290 → 246 →)	C <sub>11</sub> H <sub>11</sub> N <sub>2</sub> O <sup>+</sup>	187.0872	187.0866	3.21	
	MS <sup>3</sup> (290 → 246 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0712	173.0709	1.73	
	MS <sup>3</sup> (290 → 246 →)	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	161.0717	161.0709	4.97	
<b>P-5</b>	<b>Precursor ion</b>	<b>C<sub>10</sub>H<sub>9</sub>N<sub>2</sub>O<sub>3</sub><sup>+</sup></b>	<b>205.0604</b>	<b>205.0608</b>	<b>-1.95</b>	<b>0.477</b>
	MS <sup>2</sup> (205 →)	C <sub>10</sub> H <sub>6</sub> NO <sub>3</sub> <sup>+</sup>	188.0348	188.0342	3.19	
	MS <sup>2</sup> (205 →)	C <sub>8</sub> H <sub>6</sub> NO <sub>3</sub> <sup>+</sup>	164.0345	164.0342	1.83	
	MS <sup>2</sup> (205 →)	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	161.0714	161.0709	3.10	
	MS <sup>2</sup> (205 →)	C <sub>8</sub> H <sub>4</sub> NO <sub>2</sub> <sup>+</sup>	146.0231	146.0236	-3.42	
<b>P-6</b>	<b>Precursor ion</b>	<b>C<sub>10</sub>H<sub>9</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup></b>	<b>189.0654</b>	<b>189.0658</b>	<b>-2.12</b>	<b>0.667</b>
	MS <sup>2</sup> (189 →)	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	161.0714	161.0709	3.10	
	MS <sup>2</sup> (189 →)	C <sub>8</sub> H <sub>6</sub> NO <sub>2</sub> <sup>+</sup>	148.0397	148.0393	2.70	
<b>P-7</b>	<b>Precursor ion</b>	<b>C<sub>21</sub>H<sub>23</sub>O<sub>8</sub>N<sub>4</sub>S<sup>+</sup></b>	<b>491.1228</b>	<b>491.1231</b>	<b>-0.61</b>	<b>0.692</b>
	MS <sup>2</sup> (491 →)	C <sub>21</sub> H <sub>21</sub> N <sub>4</sub> O <sub>7</sub> S <sup>+</sup>	473.1134	473.1126	1.69	
	MS <sup>2</sup> (491 →)	C <sub>20</sub> H <sub>21</sub> N <sub>4</sub> O <sub>6</sub> S <sup>+</sup>	445.1162	445.1176	-3.15	
	MS <sup>2</sup> (491 →)	C <sub>20</sub> H <sub>19</sub> N <sub>4</sub> O <sub>5</sub> S <sup>+</sup>	427.1084	427.1071	3.04	
	MS <sup>2</sup> (491 →)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	316.0762	316.0750	3.80	
	MS <sup>2</sup> (491 →)	C <sub>11</sub> H <sub>12</sub> N <sub>3</sub> O <sup>+</sup>	202.0975	202.0974	0.49	
	MS <sup>2</sup> (491 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0706	173.0709	-1.73	
	MS <sup>3</sup> (491 → 473 →)	C <sub>20</sub> H <sub>21</sub> N <sub>4</sub> O <sub>6</sub> S <sup>+</sup>	445.1182	445.1176	1.35	
	MS <sup>3</sup> (491 → 473 →)	C <sub>20</sub> H <sub>19</sub> N <sub>4</sub> O <sub>5</sub> S <sup>+</sup>	427.1079	427.1070	2.11	
	MS <sup>3</sup> (491 → 473 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>4</sub> S <sup>+</sup>	344.0699	344.0699	0.00	
	MS <sup>3</sup> (491 → 473 →)	C <sub>16</sub> H <sub>12</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	326.0617	326.0594	-0.30	
	MS <sup>3</sup> (491 → 473 →)	C <sub>15</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	266.0928	266.0924	1.50	
	MS <sup>3</sup> (491 → 473 →)	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub> O <sup>+</sup>	240.1134	240.1131	1.25	
	MS <sup>3</sup> (491 → 473 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0706	173.0709	-1.73	
	MS <sup>3</sup> (491 → 316 →)	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	256.1086	256.1080	2.34	
<b>P-8</b>	<b>Precursor ion</b>	<b>C<sub>22</sub>H<sub>23</sub>N<sub>2</sub>O<sub>6</sub>S<sup>+</sup></b>	<b>471.1321</b>	<b>471.1323</b>	<b>-0.42</b>	<b>0.840</b>
	MS <sup>2</sup> (471 →)	C <sub>17</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	342.0918	342.0907	3.22	
	MS <sup>2</sup> (471 →)	C <sub>17</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	324.0814	324.0801	4.01	
	MS <sup>2</sup> (471 →)	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>5</sub> S <sup>+</sup>	299.0707	299.0696	3.68	
	MS <sup>3</sup> (471 → 342 →)	C <sub>16</sub> H <sub>16</sub> N <sub>3</sub> OS <sup>+</sup>	298.1018	298.1008	3.35	
<b>P-9</b>	<b>Precursor ion</b>	<b>C<sub>42</sub>H<sub>44</sub>N<sub>8</sub>O<sub>12</sub>S<sub>2</sub><sup>2+</sup></b>	<b>458.1250</b>	<b>458.1255</b>	<b>-1.09</b>	<b>0.843</b>
	MS <sup>2</sup> (458 →)	C <sub>32</sub> H <sub>35</sub> N <sub>6</sub> O <sub>11</sub> S <sub>2</sub> <sup>+</sup>	743.1833	743.1799	4.57	
	MS <sup>2</sup> (458 →)	C <sub>37</sub> H <sub>37</sub> N <sub>7</sub> O <sub>9</sub> S <sub>2</sub> <sup>2+</sup>	393.6040	393.6042	-0.41	
	MS <sup>2</sup> (458 →)	C <sub>36</sub> H <sub>37</sub> N <sub>7</sub> O <sub>7</sub> S <sub>2</sub> <sup>2+</sup>	371.6105	371.6093	3.36	
	MS <sup>3</sup> (458 → 743 →)	C <sub>27</sub> H <sub>26</sub> N <sub>5</sub> O <sub>7</sub> S <sub>2</sub> <sup>+</sup>	596.1290	596.1268	3.69	

	MS <sup>3</sup> (458 →743→)	C <sub>22</sub> H <sub>19</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub> <sup>+</sup>	467.0838	467.0842	-0.85	
	MS <sup>3</sup> (458 →743→)	C <sub>21</sub> H <sub>19</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub> <sup>+</sup>	423.0956	423.0944	2.84	
	MS <sup>3</sup> (458 →743→)	C <sub>16</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	310.0660	310.0645	4.93	
	MS <sup>3</sup> (458 →371→)	C <sub>36</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> S <sub>2</sub> <sup>2+</sup>	362.6044	362.6040	1.21	
	MS <sup>3</sup> (458 →371→)	C <sub>31</sub> H <sub>28</sub> N <sub>6</sub> O <sub>3</sub> S <sub>2</sub> <sup>2+</sup>	298.0837	298.0827	3.46	
	MS <sup>3</sup> (458 →371→)	C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> OS <sup>++</sup>	285.0944	285.0930	4.81	
	MS <sup>3</sup> (458 →371→)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0713	173.0709	2.08	
<b>P-10</b>	<b>Precursor ion</b>	<b>C<sub>20</sub>H<sub>23</sub>O<sub>5</sub>N<sub>4</sub>S<sup>+</sup></b>	<b>431.1380</b>	<b>431.1384</b>	<b>-0.93</b>	<b>0.848</b>
	MS <sup>2</sup> (431 →)	C <sub>20</sub> H <sub>21</sub> N <sub>4</sub> O <sub>4</sub> S <sup>+</sup>	413.1271	413.1278	-1.69	
	MS <sup>2</sup> (431 →)	C <sub>20</sub> H <sub>21</sub> N <sub>4</sub> O <sub>5</sub> <sup>+</sup>	397.1518	397.1507	2.77	
	MS <sup>2</sup> (431 →)	C <sub>16</sub> H <sub>16</sub> O <sub>3</sub> N <sub>3</sub> S <sup>+</sup>	330.0914	330.0906	2.42	
	MS <sup>2</sup> (431 →)	C <sub>15</sub> H <sub>16</sub> O <sub>2</sub> N <sub>3</sub> S <sup>+</sup>	302.0969	302.0958	3.64	
	MS <sup>3</sup> (431 →330→)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	312.0809	312.0801	2.56	
	MS <sup>3</sup> (431 →330→)	C <sub>15</sub> H <sub>16</sub> O <sub>2</sub> N <sub>3</sub> S <sup>+</sup>	302.0966	302.0958	2.65	
	MS <sup>3</sup> (431 →330→)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> <sup>+</sup>	296.1035	296.1030	1.68	
	MS <sup>3</sup> (431 →302→)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> OS <sup>+</sup>	284.0857	284.0852	1.76	
	MS <sup>3</sup> (431 →302→)	C <sub>14</sub> H <sub>11</sub> O <sub>2</sub> N <sub>2</sub> S <sup>+</sup>	271.0536	271.0536	0.00	
	MS <sup>3</sup> (431 →302→)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	268.1079	268.1081	-0.75	
	MS <sup>3</sup> (431 →302→)	C <sub>13</sub> H <sub>11</sub> N <sub>2</sub> OS <sup>+</sup>	243.0587	243.0586	0.41	
	MS <sup>3</sup> (431 →302→)	C <sub>13</sub> H <sub>11</sub> N <sub>2</sub> O <sup>+</sup>	211.0866	211.0865	0.47	
	MS <sup>3</sup> (431 →302→)	C <sub>11</sub> H <sub>12</sub> ON <sub>3</sub> <sup>+</sup>	202.0982	202.0975	3.46	
	MS <sup>3</sup> (431 →302→)	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> N <sub>2</sub> <sup>+</sup>	189.0665	189.0659	3.17	
MS <sup>3</sup> (431 →302→)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0710	173.0709	0.58		
<b>P-11</b>	<b>Precursor ion</b>	<b>C<sub>20</sub>H<sub>21</sub>O<sub>6</sub>N<sub>4</sub>S<sup>+</sup></b>	<b>445.1174</b>	<b>445.1176</b>	<b>-0.45</b>	<b>0.864</b>
	MS <sup>2</sup> (445 →)	C <sub>20</sub> H <sub>19</sub> N <sub>4</sub> O <sub>5</sub> S <sup>+</sup>	427.1083	427.1071	2.81	
	MS <sup>2</sup> (445 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>4</sub> S <sup>+</sup>	344.0709	344.0699	2.91	
	MS <sup>2</sup> (445 →)	C <sub>15</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	316.0761	316.0750	3.48	
	MS <sup>2</sup> (445 →)	C <sub>11</sub> H <sub>12</sub> N <sub>3</sub> O <sup>+</sup>	202.0984	202.0975	4.45	
	MS <sup>3</sup> (445 →427→)	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub> O <sup>+</sup>	240.1134	240.1131	1.25	
	MS <sup>3</sup> (445 →316→)	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	256.1086	256.1081	1.95	
<b>P-12</b>	<b>Precursor ion</b>	<b>C<sub>21</sub>H<sub>23</sub>O<sub>7</sub>N<sub>4</sub>S<sup>+</sup></b>	<b>475.1275</b>	<b>475.1282</b>	<b>-1.47</b>	<b>0.895</b>
	MS <sup>2</sup> (475 →)	C <sub>19</sub> H <sub>20</sub> N <sub>3</sub> O <sub>7</sub> <sup>+</sup>	402.1306	402.1296	2.49	
	MS <sup>2</sup> (475 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	328.0760	328.0750	3.05	
	MS <sup>2</sup> (475 →)	C <sub>16</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	310.0658	310.0645	4.19	
	MS <sup>2</sup> (475 →)	C <sub>11</sub> H <sub>15</sub> N <sub>2</sub> O <sub>5</sub> S <sup>+</sup>	287.0710	287.0696	4.88	
	MS <sup>2</sup> (475 →)	C <sub>11</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	218.0919	218.0924	-2.29	
	MS <sup>2</sup> (475 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	189.0667	189.0658	4.76	
	MS <sup>2</sup> (475 →)	C <sub>6</sub> H <sub>6</sub> NOS <sup>+</sup>	140.0171	140.0165	4.29	
<b>P-13</b>	<b>Precursor ion</b>	<b>C<sub>21</sub>H<sub>23</sub>O<sub>7</sub>N<sub>4</sub>S<sup>+</sup></b>	<b>475.1278</b>	<b>475.1282</b>	<b>-0.84</b>	<b>0.958</b>

	MS <sup>2</sup> (475 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	328.0758	328.0750	2.44	
	MS <sup>2</sup> (475 →)	C <sub>16</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	310.0652	310.0645	2.26	
	MS <sup>2</sup> (475 →)	C <sub>11</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	218.0919	218.0924	-2.29	
	MS <sup>2</sup> (475 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0703	173.0709	-3.47	
<b>P-14</b>	<b>Precursor ion</b>	<b>C<sub>20</sub>H<sub>21</sub>N<sub>4</sub>O<sub>5</sub>S<sup>+</sup></b>	<b>429.1222</b>	<b>429.1227</b>	<b>-1.17</b>	<b>1.099</b>
	MS <sup>2</sup> (429 →)	C <sub>16</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	330.0914	330.0906	2.42	
	MS <sup>2</sup> (429 →)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	312.0803	312.0801	0.64	
	MS <sup>2</sup> (429 →)	C <sub>15</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> S <sup>+</sup>	286.1003	286.1008	-1.75	
	MS <sup>2</sup> (429 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0704	173.0709	-2.88	
<b>P-15</b>	<b>Precursor ion</b>	<b>C<sub>43</sub>H<sub>46</sub>N<sub>8</sub>O<sub>12</sub>S<sub>2</sub><sup>2+</sup></b>	<b>465.1329</b>	<b>465.1333</b>	<b>-0.82</b>	<b>1.542</b>
	MS <sup>2</sup> (465 →)	C <sub>38</sub> H <sub>36</sub> N <sub>7</sub> O <sub>8</sub> S <sub>2</sub> <sup>+</sup>	782.2074	782.2061	1.62	
	MS <sup>2</sup> (465 →)	C <sub>33</sub> H <sub>37</sub> N <sub>6</sub> O <sub>11</sub> S <sub>2</sub> <sup>+</sup>	757.1971	757.1956	1.98	
	MS <sup>2</sup> (465 →)	C <sub>22</sub> H <sub>23</sub> N <sub>4</sub> O <sub>6</sub> S <sup>+</sup>	471.1348	471.1333	3.23	
	MS <sup>2</sup> (465 →)	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> O <sup>+</sup>	173.0713	173.0709	2.08	
	MS <sup>2</sup> (465 →)	C <sub>5</sub> H <sub>10</sub> NO <sub>4</sub> <sup>+</sup>	148.0610	148.0604	3.85	
	MS <sup>3</sup> (465 →757→)	C <sub>22</sub> H <sub>23</sub> N <sub>4</sub> O <sub>6</sub> S <sup>+</sup>	471.1354	471.1333	4.50	
	MS <sup>3</sup> (465 →757→)	C <sub>21</sub> H <sub>23</sub> N <sub>4</sub> O <sub>6</sub> S <sup>+</sup>	459.1348	459.1333	3.31	
	MS <sup>3</sup> (465 →757→)	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub> S <sup>+</sup>	312.0801	312.0801	-0.06	