Electronic Supplementary Material (ESI) for RSC Advances.

XYZ coordinates, Angstrom:

N,N'-diethyl-N,N'-di(p-hexylphenyl)-1,10-phenantroline-4,7-dichloro-2,9-dicarboxamides

C	-2.359484	2.133315	0.772571
C	-3.425844	3.055628	0.925158
C	-3.197247	4.367385	0.587364
C	-1.930343	4.808575	0.131183
N	-1.143740	2.505412	0.365793
C	-0.908167	3.810357	0.060101
C	0.427293	4.193732	-0.369333
C	-1.636792	6.156880	-0.253478
C	-0.392556	6.509032	-0.694014
C	0.666424	5.546866	-0.767282
N	1.407620	3.248498	-0.372185
C	2.630194	3.578290	-0.796447
C	1.977116	5.838894	-1.220794
C	2.956090	4.875903	-1.263689
Cl	-4.570760	5.554626	0.740796
Cl	2.392664	7.524106	-1.773858
C	-2.640117	0.713540	1.208996
H	-4.374490	2.709550	1.310496
H	-2.425041	6.897005	-0.195783
H	-0.189240	7.529214	-0.994499
C	3.698766	2.522794	-0.921212
H	3.947805	5.072470	-1.646516
N	-2.017017	-0.350238	0.601738
N	3.838077	1.562904	0.052063
O	-3.470232	0.567583	2.143305
O	4.438341	2.572800	-1.936336
C	-2.280257	-1.685160	1.102578
C	-1.252997	-0.270311	-0.679360
C	-2.169002	-0.382632	-1.904975
C	3.171357	1.584772	1.382895
C	2.042830	0.559029	1.513524
C	-3.576624	-2.217175	1.114853
C	-3.788667	-3.522121	1.565343
C	-2.722106	-4.326260	2.004925
C	-1.429753	-3.775024	1.991993
C	-1.208074	-2.467196	1.551449
C	4.768545	0.479885	-0.187600
C	4.506257	-0.467822	-1.185242
C	5.929098	0.362283	0.588296
C	5.397202	-1.522517	-1.398530
C	6.560924	-1.661791	-0.621550
C	6.810492	-0.701135	0.373763
C	-2.957847	-5.757633	2.444587

C	-2.958690	-6.762206	1.264900
C	-3.210671	-8.213867	1.709935
C	-3.219852	-9.215621	0.540161
C	-3.479239	-10.668754	0.979934
C	-3.491589	-11.661138	-0.194074
C	7.501630	-2.832795	-0.827593
C	7.177416	-4.041779	0.083486
C	8.126729	-5.232631	-0.136012
C	7.815731	-6.434800	0.772999
C	8.756499	-7.633003	0.549382
C	8.438907	-8.826848	1.463275
H	-0.537513	-1.097682	-0.665967
H	-0.688196	0.659869	-0.687823
H	-2.748135	-1.312723	-1.884291
H	-1.572323	-0.371540	-2.825006
H	-2.872111	0.458318	-1.947913
H	2.789633	2.590181	1.560993
H	3.949832	1.390906	2.130013
H	1.214867	0.832708	0.856683
H	1.674622	0.540692	2.546628
H	2.398572	-0.447116	1.262262
H	-4.411063	-1.603737	0.798080
H	-4.799256	-3.921984	1.579698
H	-0.591112	-4.369956	2.343165
H	-0.208152	-2.044321	1.567881
H	3.615998	-0.365126	-1.795500
H	6.151368	1.110521	1.342903
H	5.189662	-2.246922	-2.181790
H	7.712362	-0.776654	0.975064
H	-3.920274	-5.829979	2.970468
H	-2.183344	-6.056427	3.164526
H	-1.994751	-6.697567	0.738589
H	-3.727185	-6.460409	0.538005
H	-4.173378	-8.269213	2.242241
H	-2.439756	-8.511590	2.437743
H	-2.256177	-9.163796	0.009393
H	-3.988507	-8.915485	-0.189133
H	-4.441040	-10.718342	1.512602
H	-2.710304	-10.968946	1.707527
H	-4.272864	-11.402023	-0.920416
H	-3.680001	-12.685403	0.149031
H	-2.530086	-11.657464	-0.724091
H	8.536583	-2.514351	-0.638209
H	7.461034	-3.157615	-1.876482
H	6.139183	-4.358020	-0.096884
H	7.222909	-3.722270	1.135488

H	9.165213	-4.907368	0.034533
H	8.074133	-5.549694	-1.189576
H	6.775036	-6.755914	0.608030
H	7.875357	-6.119804	1.826821
H	9.796410	-7.311414	0.712150
H	8.694892	-7.948553	-0.503238
H	8.527382	-8.548203	2.521643
H	9.121000	-9.665417	1.279830
H	7.414646	-9.186279	1.299797

N,N'-diethyl-N,N'-di(p-hexylphenyl)-1,10-phenantroline-4,7-dichloro-2,9-dicarboxamides_H3O+

C	-2.230909	1.393519	0.181902
C	-3.281872	2.303140	0.411546
C	-3.023839	3.655105	0.354979
C	-1.713982	4.121224	0.086237
N	-0.996773	1.802079	-0.028566
C	-0.735811	3.110791	-0.062750
C	0.637324	3.497378	-0.250089
C	-1.331698	5.490507	-0.034866
C	-0.041031	5.840636	-0.279396
C	0.987190	4.853997	-0.381345
N	1.590912	2.531135	-0.274020
C	2.884595	2.802447	-0.442329
C	2.361081	5.137133	-0.596371
C	3.295142	4.121720	-0.629368
Cl	-4.312350	4.775269	0.620935
Cl	2.890793	6.757893	-0.808599
C	-2.345060	-0.124145	0.282714
H	-4.278217	1.957425	0.638046
H	-2.088738	6.254817	0.062890
H	0.227821	6.880807	-0.385711
C	3.817304	1.612285	-0.616874
H	4.339418	4.339424	-0.794383
N	-3.425781	-0.766367	-0.222015
N	4.770451	1.388791	0.311162
O	-1.424279	-0.709501	0.846763
O	3.640646	0.973032	-1.639762
C	-3.515804	-2.194229	-0.009246
C	-4.413204	-0.185871	-1.151398
C	-5.833556	-0.167153	-0.598316
C	4.850946	2.078666	1.613067
C	4.385025	1.223897	2.787303
C	-3.873107	-2.692159	1.237975
C	-3.971296	-4.062894	1.431435
C	-3.721772	-4.963134	0.392545

C	-3.362327	-4.441391	-0.851471
C	-3.255754	-3.071501	-1.055287
C	5.716670	0.321572	0.069019
C	5.375955	-1.001219	0.322981
C	6.982229	0.633208	-0.412369
C	6.306436	-2.006556	0.095345
C	7.585852	-1.716985	-0.384031
C	7.905079	-0.380449	-0.633049
C	-3.863572	-6.449235	0.602937
C	-5.295722	-6.962634	0.377169
C	-5.429409	-8.469472	0.600336
C	-6.850048	-8.994383	0.393319
C	-6.983804	-10.501148	0.621626
C	-8.406450	-11.017804	0.416084
C	8.602450	-2.809401	-0.598409
C	9.445162	-3.108203	0.654102
C	10.488002	-4.202267	0.422321
C	11.335554	-4.509211	1.657707
C	12.382809	-5.599337	1.423537
C	13.227892	-5.901768	2.659746
H	-4.387689	-0.782013	-2.064854
H	-4.086040	0.811666	-1.432378
H	-6.171674	-1.173867	-0.355860
H	-6.513803	0.244898	-1.344563
H	-5.913139	0.438104	0.306027
H	4.256664	2.989039	1.560044
H	5.888004	2.385342	1.754577
H	3.348314	0.910262	2.661268
H	4.462136	1.801702	3.709593
H	5.002632	0.334465	2.897484
H	-4.061644	-2.009707	2.055990
H	-4.243032	-4.440187	2.409530
H	-3.149530	-5.115805	-1.671615
H	-2.955407	-2.691278	-2.023143
H	4.387386	-1.242838	0.689817
H	7.241252	1.662340	-0.626050
H	6.030292	-3.035717	0.289102
H	8.885712	-0.128701	-1.016716
H	-3.552454	-6.701587	1.619889
H	-3.184880	-6.978573	-0.070320
H	-5.610566	-6.711099	-0.640441
H	-5.977494	-6.429725	1.046895
H	-5.099038	-8.713831	1.615882
H	-4.746667	-8.997011	-0.074222
H	-7.181135	-8.753550	-0.623033
H	-7.533438	-8.465912	1.066873

H	-6.651037	-10.741492	1.636493
H	-6.302492	-11.029200	-0.052656
H	-9.105886	-10.532662	1.100099
H	-8.468940	-12.093767	0.586608
H	-8.753116	-10.823488	-0.601617
H	9.269330	-2.528433	-1.416890
H	8.092891	-3.724149	-0.911527
H	8.779774	-3.399532	1.472468
H	9.942646	-2.189211	0.979714
H	11.144999	-3.906009	-0.402071
H	9.984508	-5.117567	0.092361
H	10.679333	-4.809376	2.481800
H	11.837330	-3.593552	1.990021
H	13.037321	-5.298514	0.599596
H	11.881941	-6.514346	1.091681
H	13.767910	-5.014117	2.997361
H	13.965343	-6.679497	2.455958
H	12.605987	-6.243949	3.489906
O	1.289625	-0.075070	0.423123
H	1.314335	1.520586	-0.115088
H	1.597034	-0.744304	-0.196017
H	0.355326	-0.293048	0.626099

2,5,9,12-tetra(n-hexyl)-benzo[f]quinolino-[3,4-b]-[1,7]-naphthyridine-6,8(5H,9H)-dione

H	-6.061204	-2.349100	-1.817603
H	-7.252724	-1.054980	-1.922689
H	-7.508644	-2.400264	-0.812515
C	-6.750539	-1.736436	-1.231788
H	-4.215898	-0.601765	-1.268641
H	-5.397465	0.685787	-1.374441
C	-6.012303	-0.968178	-0.137168
C	-4.937140	-0.025601	-0.679014
H	-5.551613	-1.677902	0.557569
H	-6.732848	-0.392038	0.452541
H	-2.381849	1.107079	-0.705368
H	-3.560883	2.403363	-0.819285
C	-4.192720	0.743586	0.412407
C	-3.113326	1.680026	-0.130743
H	-3.733856	0.030273	1.105456
H	-4.914903	1.319550	1.002973
H	-3.727945	4.464077	0.428282
C	-2.373972	2.411564	0.990477
H	-3.354573	8.822474	-1.468445
H	-4.218950	6.767215	-0.122402
C	-2.908943	5.120698	0.183702
O	0.128060	1.555526	0.661287

N	-1.312316	3.308956	0.512576
C	-3.187531	6.434895	-0.135922
H	-1.885521	1.681189	1.630566
C	-0.044153	2.732054	0.414816
C	-1.590947	4.634146	0.171840
H	-3.061899	2.989127	1.606787
C	-2.174996	7.333976	-0.486812
C	1.059699	3.650301	0.014889
C	-0.553945	5.518031	-0.201678
H	-1.653419	9.218233	-1.352198
C	-2.488237	8.775847	-0.801290
N	2.265617	3.105337	-0.054469
C	-0.879630	6.846259	-0.516386
C	0.812675	5.012832	-0.261808
H	6.705540	2.196304	-1.295797
O	4.751255	1.974742	-0.229895
H	-0.089393	7.524908	-0.807504
C	3.303635	3.859875	-0.384769
H	7.510879	3.649094	-1.870324
C	4.615659	3.157504	-0.469058
C	1.918531	5.793648	-0.592043
C	3.196093	5.241082	-0.656433
H	-3.951338	11.120140	-0.573480
H	1.783403	6.841706	-0.805878
N	5.701974	3.940081	-0.867336
C	6.971187	3.215775	-1.029237
C	4.397689	6.001948	-0.978570
C	5.632034	5.320309	-1.069982
H	3.431594	7.913096	-1.122082
C	4.374355	7.387587	-1.194459
C	-2.776270	9.627774	0.444888
H	-3.610312	9.183836	0.997680
H	-2.257254	11.531667	-0.423382
C	-3.100331	11.085490	0.116244
C	6.783958	6.066229	-1.369711
H	8.892217	1.400822	-0.267717
H	4.456133	9.908911	-2.030062
H	7.744519	5.581282	-1.432390
C	5.507374	8.125150	-1.495628
H	6.153002	9.919510	-2.461617
C	6.717364	7.430046	-1.579852
H	10.722709	-0.068371	-0.031108
H	9.705400	2.865012	-0.782053
C	5.450617	9.621691	-1.677985
H	7.629286	7.966720	-1.812857
H	-4.586809	13.426785	0.328805

H	-1.912250	9.583786	1.115705
C	7.830269	3.200276	0.235662
C	9.132367	2.421796	0.041129
H	7.246337	2.746498	1.039637
C	-3.416501	11.933158	1.348393
H	-4.261274	11.487712	1.885952
C	11.229146	0.164437	0.906707
H	-2.894538	13.838012	0.489347
H	8.054482	4.224548	0.547223
C	-3.740416	13.392173	1.022686
H	12.214518	-0.302784	0.868334
H	10.667158	-0.314410	1.712323
H	11.903980	2.127003	0.314738
H	4.734630	12.204364	-0.952136
C	5.773456	10.405732	-0.395489
H	6.433321	12.211036	-1.371730
C	10.003206	2.396748	1.299279
H	-2.567504	11.898354	2.040510
C	11.344637	1.671676	1.138884
H	5.069042	10.111989	0.388850
C	5.726182	11.922373	-0.585988
H	9.439759	1.933034	2.116113
H	6.764360	10.111687	-0.035948
C	-4.062011	14.229805	2.258888
H	4.296248	14.502010	-0.714709
H	-4.923704	13.825059	2.795091
H	10.195784	3.428016	1.611819
H	-4.292805	15.262662	1.993357
H	11.941541	1.844777	2.038910
H	-3.219670	14.246771	2.954809
C	4.702870	14.845218	0.237768
C	6.052820	12.698135	0.692240
H	6.773511	14.494830	-0.258670
H	3.979439	14.591225	1.016826
H	4.769447	15.933629	0.190415
H	5.334836	12.425520	1.473526
C	6.068295	14.223292	0.533865
H	7.032339	12.372867	1.056757
H	6.464709	14.663813	1.452945

2,5,9,12-tetra(n-hexyl)-benzo[f]quinolino-[3,4-b]-[1,7]-naphthyridine-6,8(5H,9H)-dione_H_3O^+

C	0.785233	5.138637	-0.299753
C	1.038562	3.777137	-0.044124
C	1.894793	5.923461	-0.635463
C	3.176105	5.364854	-0.712233
C	3.274071	3.986804	-0.441695

N	2.238179	3.240364	-0.120579
C	-0.009947	2.828487	0.348771
O	0.266108	1.630718	0.575836
C	4.541164	3.249292	-0.498732
O	4.579127	2.025564	-0.242977
N	-1.268732	3.313098	0.469888
C	-1.591089	4.657998	0.169010
C	-0.591859	5.590737	-0.199972
N	5.647757	3.945720	-0.849959
C	4.404281	6.070290	-1.035234
C	5.616694	5.340926	-1.088031
C	-2.921454	5.091172	0.224241
C	-3.251413	6.403063	-0.054171
C	-2.280790	7.350601	-0.403021
C	-0.969073	6.915359	-0.471812
C	4.432563	7.449954	-1.290136
C	5.598019	8.133934	-1.589952
C	6.783393	7.390096	-1.629934
C	6.798404	6.030736	-1.384156
C	-2.308321	2.365603	0.931001
C	-3.049561	1.668622	-0.209687
C	-4.113211	0.703775	0.317654
C	-4.864612	-0.033792	-0.790958
C	-5.925257	-1.001518	-0.264280
C	-6.672102	-1.738387	-1.374001
C	6.911840	3.182326	-0.959774
C	7.738320	3.192970	0.325877
C	9.039934	2.402713	0.172686
C	9.880966	2.396090	1.451699
C	11.222620	1.664153	1.328818
C	11.107094	0.155107	1.111543
C	-2.658945	8.784320	-0.672390
C	-2.933192	9.592112	0.607237
C	-3.337253	11.039540	0.323339
C	-3.628841	11.848117	1.587450
C	-4.040609	13.294480	1.305698
C	5.605162	9.622731	-1.822284
C	5.962230	10.429592	-0.562036
C	5.981718	11.939499	-0.804107
C	6.342273	12.740418	0.449035
C	6.417222	14.257727	0.239578
H	1.761484	6.974654	-0.838524
H	-3.712881	4.402172	0.469065
H	-4.292524	6.697687	-0.009076
H	-0.207721	7.628157	-0.758405
H	3.506206	8.007352	-1.253459

H	7.717798	7.886136	-1.860469
H	7.742586	5.512614	-1.419126
H	-2.991368	2.910065	1.579135
H	-1.796072	1.627313	1.541385
H	-2.323090	1.123420	-0.817488
H	-3.512926	2.411565	-0.864696
H	-3.640458	-0.028075	0.981382
H	-4.831511	1.254284	0.935394
H	-5.339253	0.696839	-1.455449
H	-4.147201	-0.584665	-1.408875
H	-6.641367	-0.449883	0.353060
H	-5.450022	-1.729771	0.400764
H	-7.191020	-1.039343	-2.033742
H	-7.417744	-2.421359	-0.965000
H	-5.987237	-2.326270	-1.989345
H	7.472232	3.583596	-1.801019
H	6.630965	2.164029	-1.211862
H	7.137936	2.762856	1.131466
H	7.962282	4.222436	0.617390
H	8.803215	1.377601	-0.124824
H	9.632258	2.830187	-0.644149
H	10.069492	3.431339	1.752213
H	9.298681	1.945274	2.262652
H	11.797530	1.846656	2.240341
H	11.802758	2.109285	0.514127
H	10.526781	-0.313794	1.910048
H	12.091641	-0.313634	1.102382
H	10.625223	-0.089555	0.163496
H	-3.550662	8.807647	-1.304907
H	-1.863489	9.271002	-1.242645
H	-2.040759	9.574403	1.241065
H	-3.722784	9.098343	1.182239
H	-2.542829	11.532576	-0.247807
H	-4.221988	11.046846	-0.322610
H	-4.421565	11.352678	2.159022
H	-2.743799	11.844322	2.233636
H	-4.924137	13.297338	0.659327
H	-3.247839	13.790052	0.736105
C	-4.335010	14.094683	2.572843
H	4.624835	9.939612	-2.186095
H	6.321379	9.861371	-2.612527
H	6.939215	10.104235	-0.191825
H	5.244913	10.193254	0.230294
H	5.003717	12.252638	-1.180532
H	6.700743	12.169826	-1.597788
H	7.309068	12.388574	0.822480

H	5.615359	12.522085	1.239302
H	7.132106	14.475378	-0.560554
H	6.832127	14.710673	1.143721
C	5.076954	14.922696	-0.076066
H	-5.146320	13.640635	3.146410
H	-4.629226	15.118278	2.337743
H	-3.458325	14.143492	3.223012
H	4.655787	14.568310	-1.018269
H	5.187031	16.005064	-0.157239
H	4.345134	14.722937	0.710892
O	2.550132	0.592707	0.217912
H	1.637030	1.099651	0.382305
H	2.739621	-0.058532	0.902573
H	3.358436	1.260657	0.051577

1-dodecanol

C	-5.679635	-2.588171	-1.512256
C	-4.928638	-2.470251	-0.185030
H	-6.481925	-3.325304	-1.444705
H	-5.022936	-2.893965	-2.327713
H	-6.131120	-1.633350	-1.792789
H	-5.647508	-2.242740	0.606796
C	-3.826709	-1.403337	-0.165596
H	-4.492229	-3.440687	0.074213
H	-3.480925	-1.285057	0.864238
H	-4.257316	-0.437171	-0.454360
C	-2.631619	-1.707541	-1.072878
C	-1.530730	-0.638189	-1.066464
H	-2.981894	-1.832226	-2.100654
H	-2.198605	-2.671925	-0.782105
H	-0.832290	-0.861444	-1.876117
C	-0.758742	-0.522116	0.251415
H	-1.974020	0.334758	-1.309149
H	-1.456682	-0.296407	1.060811
C	0.345128	0.544015	0.257364
H	-0.317879	-1.496006	0.494987
H	-0.085610	1.510920	-0.027980
C	1.535125	0.239212	-0.656773
H	0.700305	0.664304	1.283669
C	2.647804	1.294638	-0.628962
H	1.184850	0.136903	-1.686826
H	1.956310	-0.735181	-0.382073
H	2.217249	2.276730	-0.855358
H	3.351551	1.081329	-1.439985
C	3.426165	1.376101	0.685928
C	4.573122	2.386843	0.635404

H	3.832039	0.385483	0.923259
H	2.760651	1.641264	1.507998
H	4.183706	3.378708	0.385258
H	5.271223	2.114726	-0.162770
C	5.358601	2.495025	1.930324
H	6.217587	3.161566	1.788558
H	5.743467	1.508359	2.218619
O	4.496426	3.008312	2.947920
H	4.979102	3.044972	3.777185

i-dodecane

C	4.665160	5.114045	2.170340
H	5.352876	5.912955	2.455036
H	5.148626	4.169178	2.420765
H	4.547894	5.157038	1.088204
C	3.325013	5.305282	2.917795
C	2.743682	6.650714	2.443566
C	3.689489	5.457786	4.410889
C	2.341346	4.075697	2.638559
C	2.391750	3.685422	1.141704
C	0.810059	4.273897	3.008975
C	2.824263	2.821785	3.404508
C	0.508027	4.663658	4.471502
H	0.414799	3.256524	2.897924
C	-0.026717	5.153698	2.030776
H	0.723684	5.724117	4.623456
H	1.164613	4.117681	5.148402
C	-0.937547	4.395166	4.898956
H	-1.082928	4.654044	5.949646
H	-1.194318	3.339965	4.779522
H	-1.653980	4.978187	4.319694
C	-1.212438	4.423138	1.392616
H	0.593164	5.544862	1.228220
H	-0.396838	6.033512	2.563487
H	-0.874363	3.582437	0.783210
H	-1.782307	5.092134	0.743481
H	-1.898376	4.027788	2.143391
H	2.513889	6.647844	1.378220
H	3.478316	7.441356	2.612454
H	1.838842	6.927302	2.982965
H	2.824262	5.638154	5.042778
H	4.360090	6.312235	4.529664
H	4.214478	4.583220	4.794715
H	2.257939	1.949421	3.071690
H	2.696346	2.900711	4.482370
H	3.877047	2.612335	3.213843

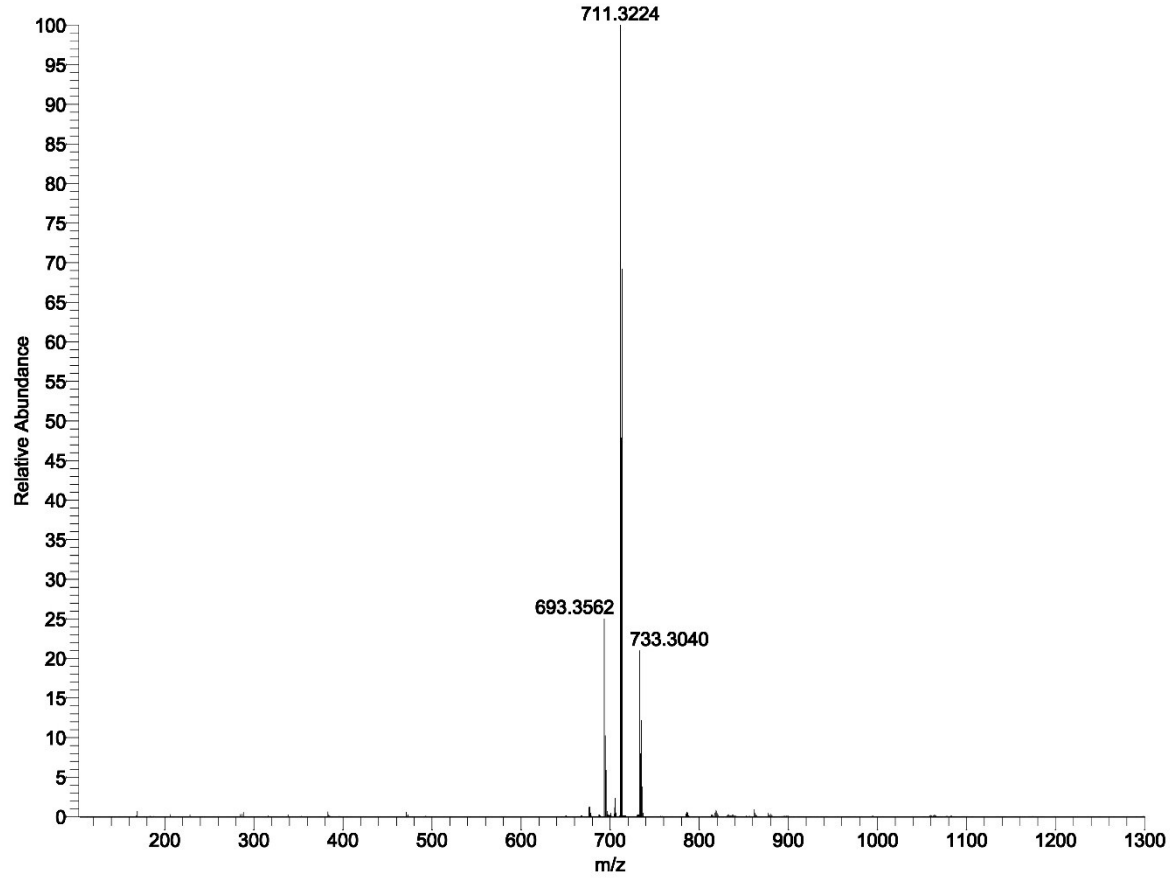
H	3.347296	3.229471	0.884996
H	2.242409	4.528788	0.469121
H	1.616548	2.949255	0.921360

HR-ESI-MS spectra

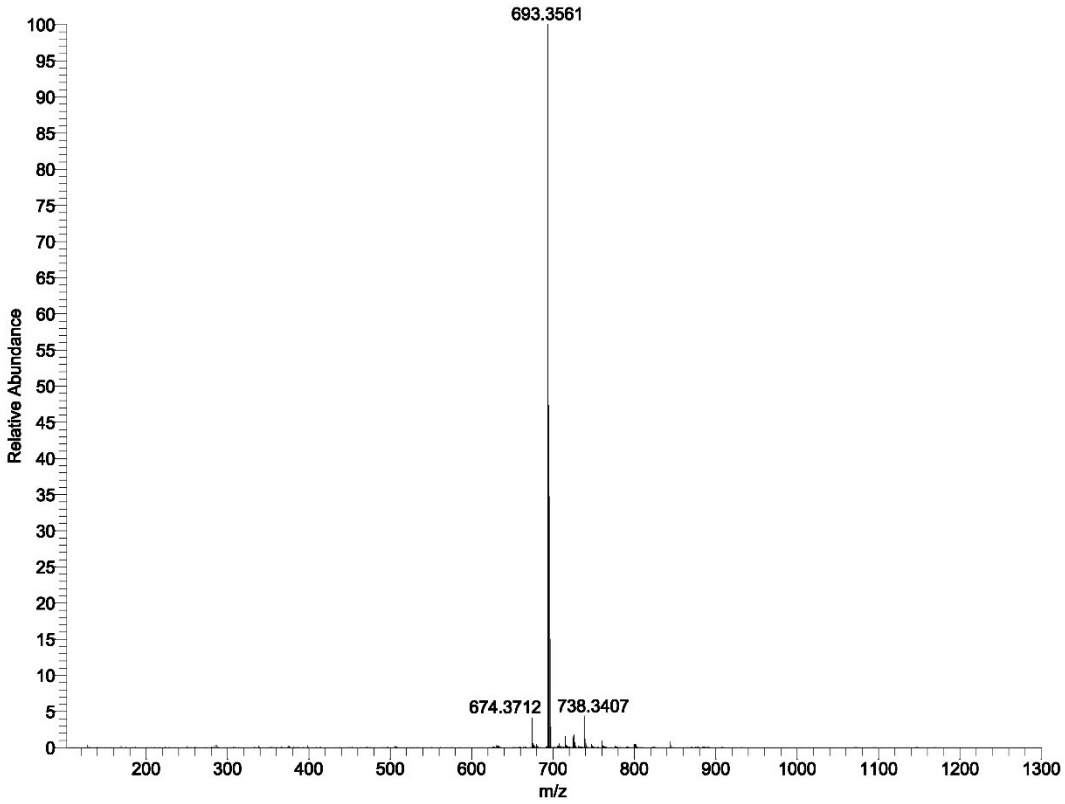
Ageing

N,N'-diethyl-N,N'-di(p-hexylphenyl)-1,10-phenantroline-4,7-dichloro-2,9-dicarboxamides

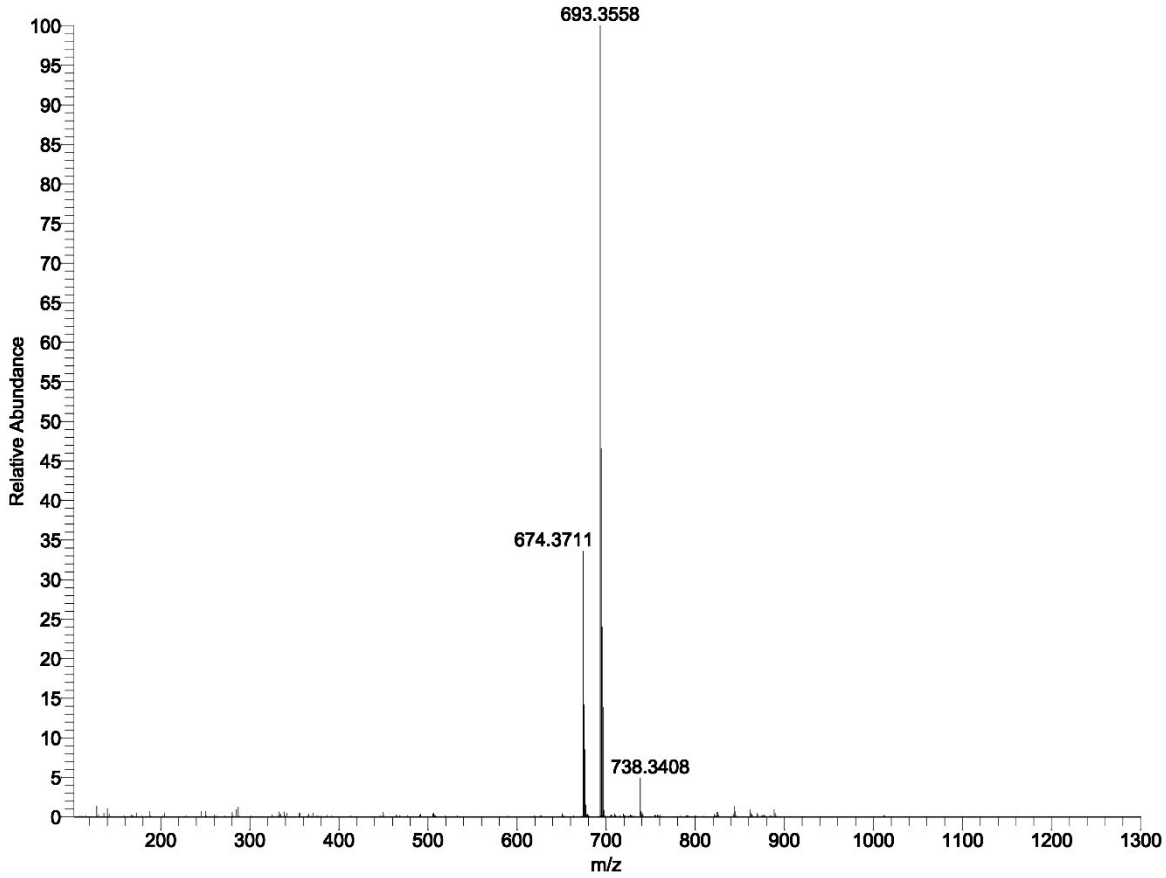
6 months, water



6 months, 1M HNO_3



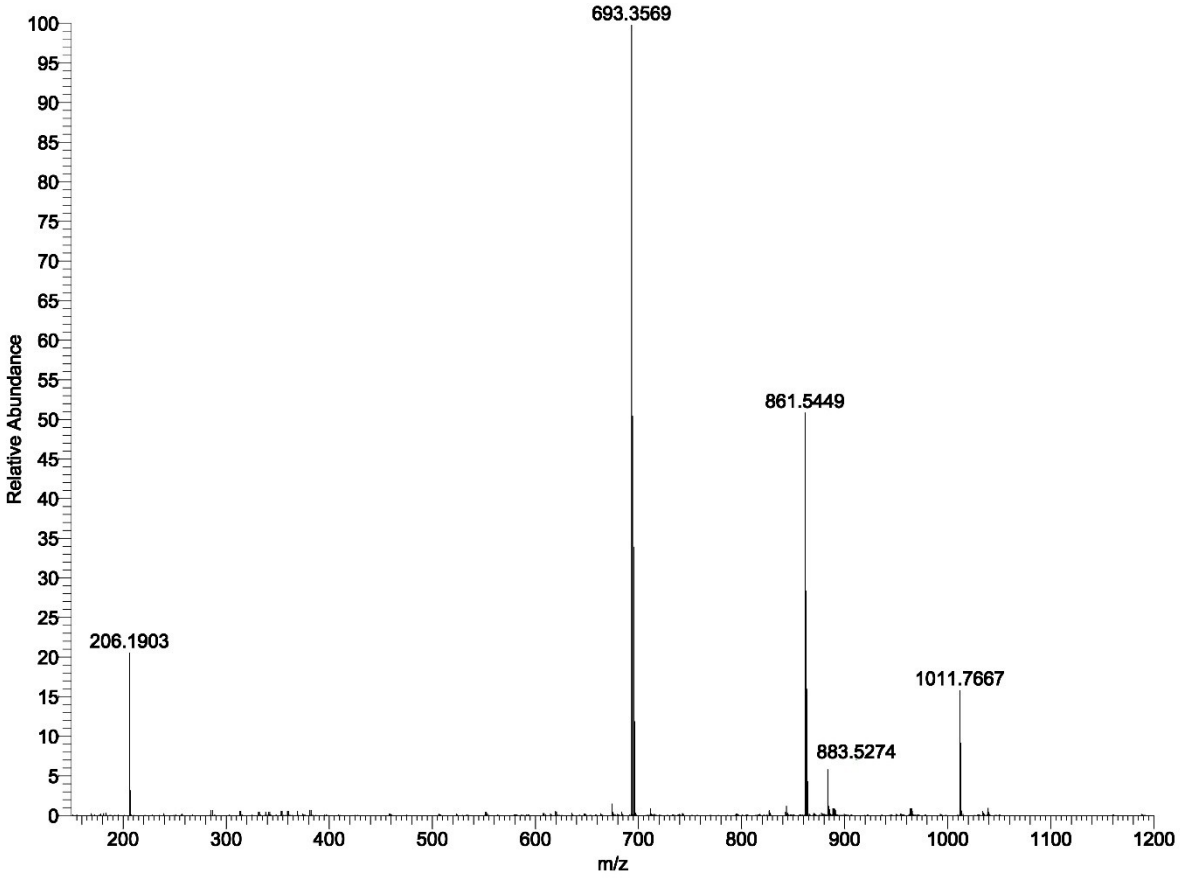
6 months, 6M HNO_3



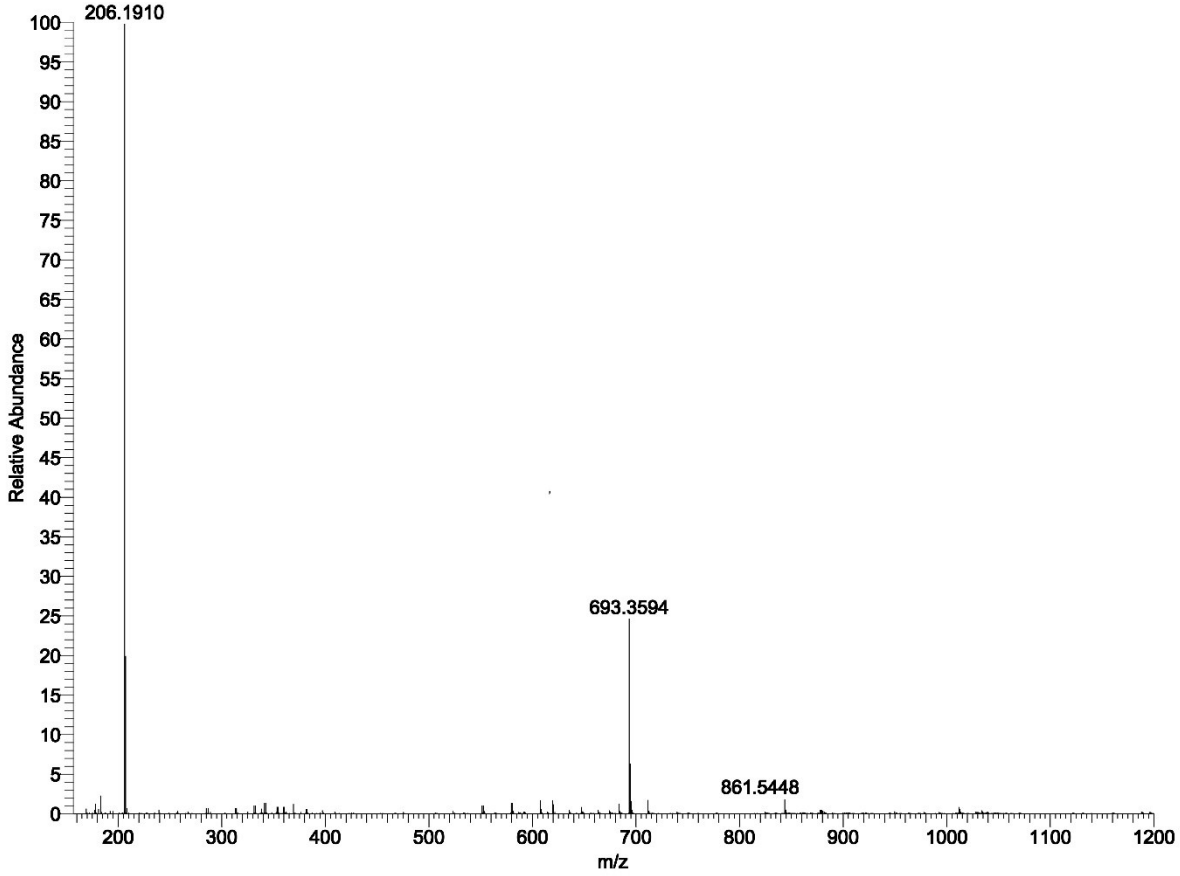
Radiolysis

N,N'-diethyl-N,N'-di(p-hexylphenyl)-1,10-phenantroline-4,7-dichloro-2,9-dicarboxamides

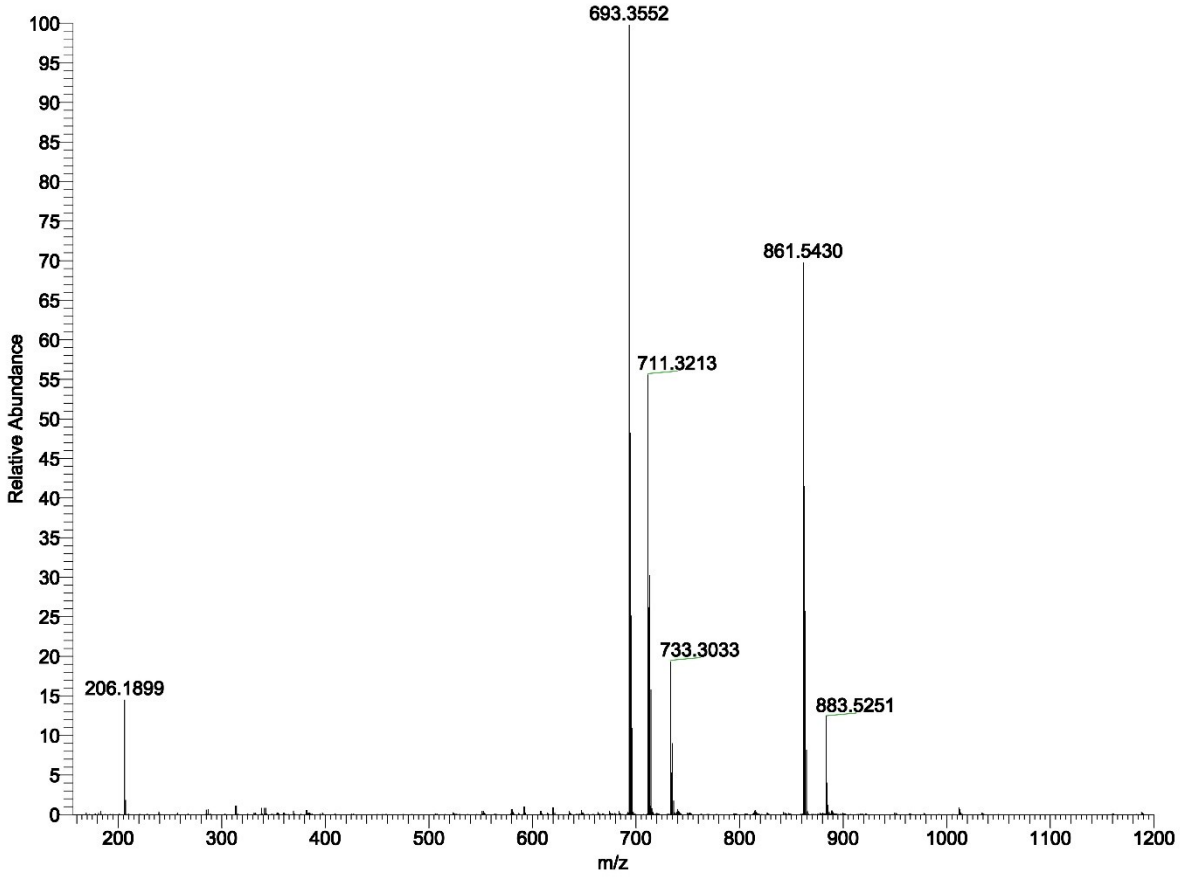
25 kGy, without aqueous phase



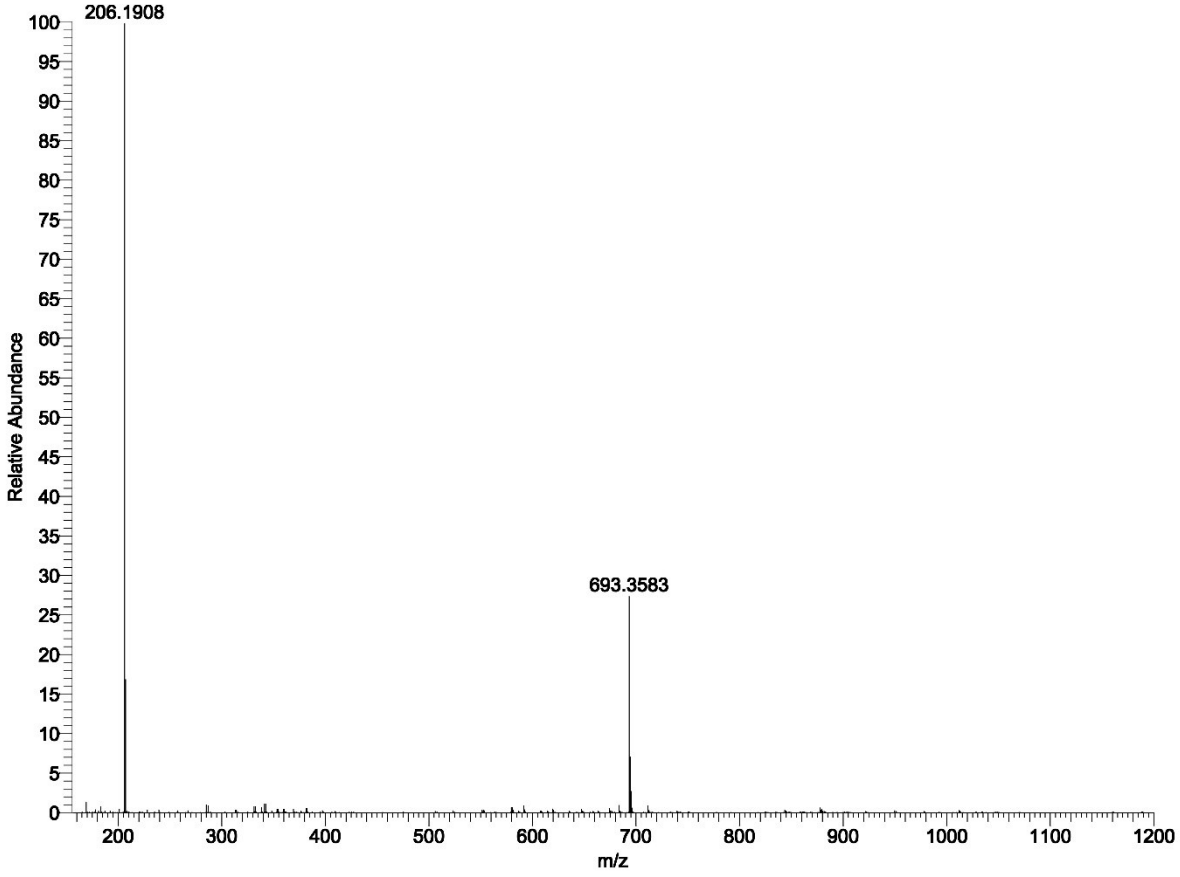
200 kGy, without aqueous phase



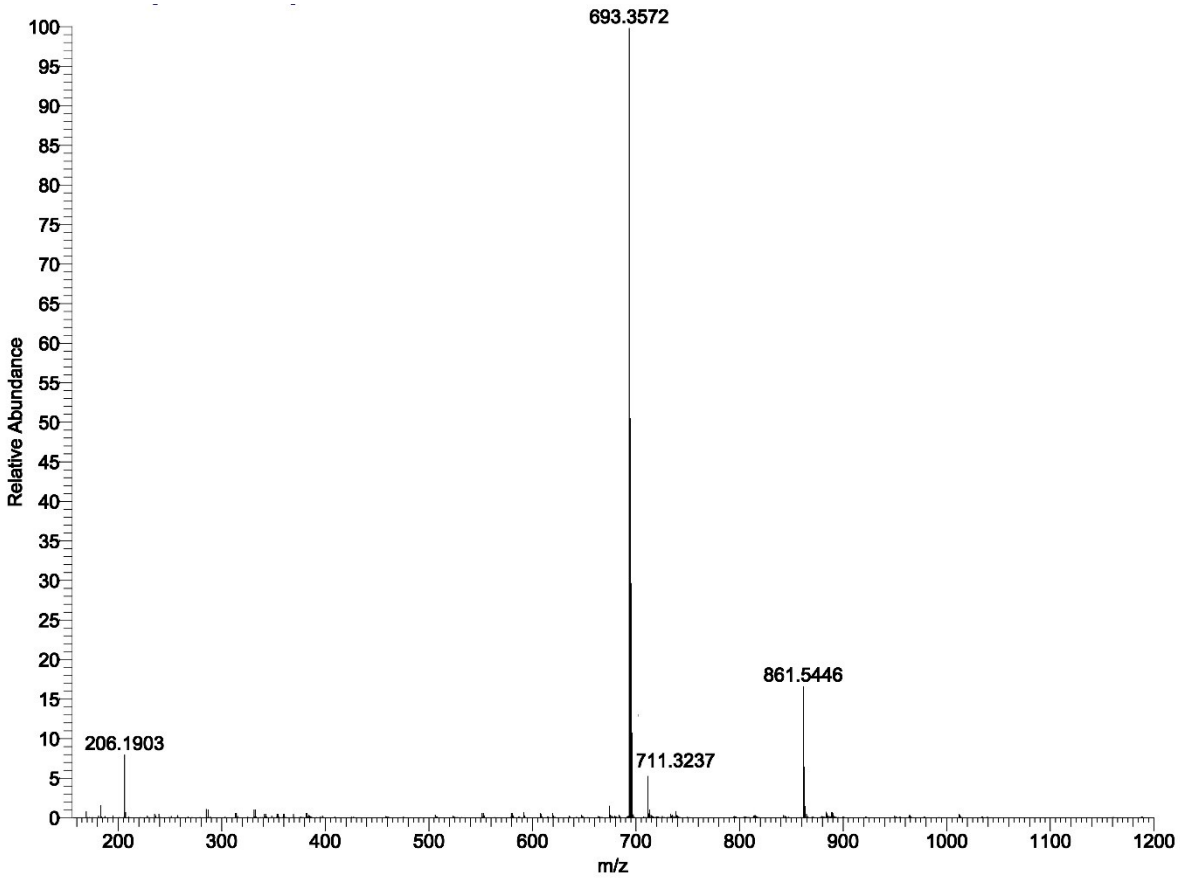
25 kGy, water



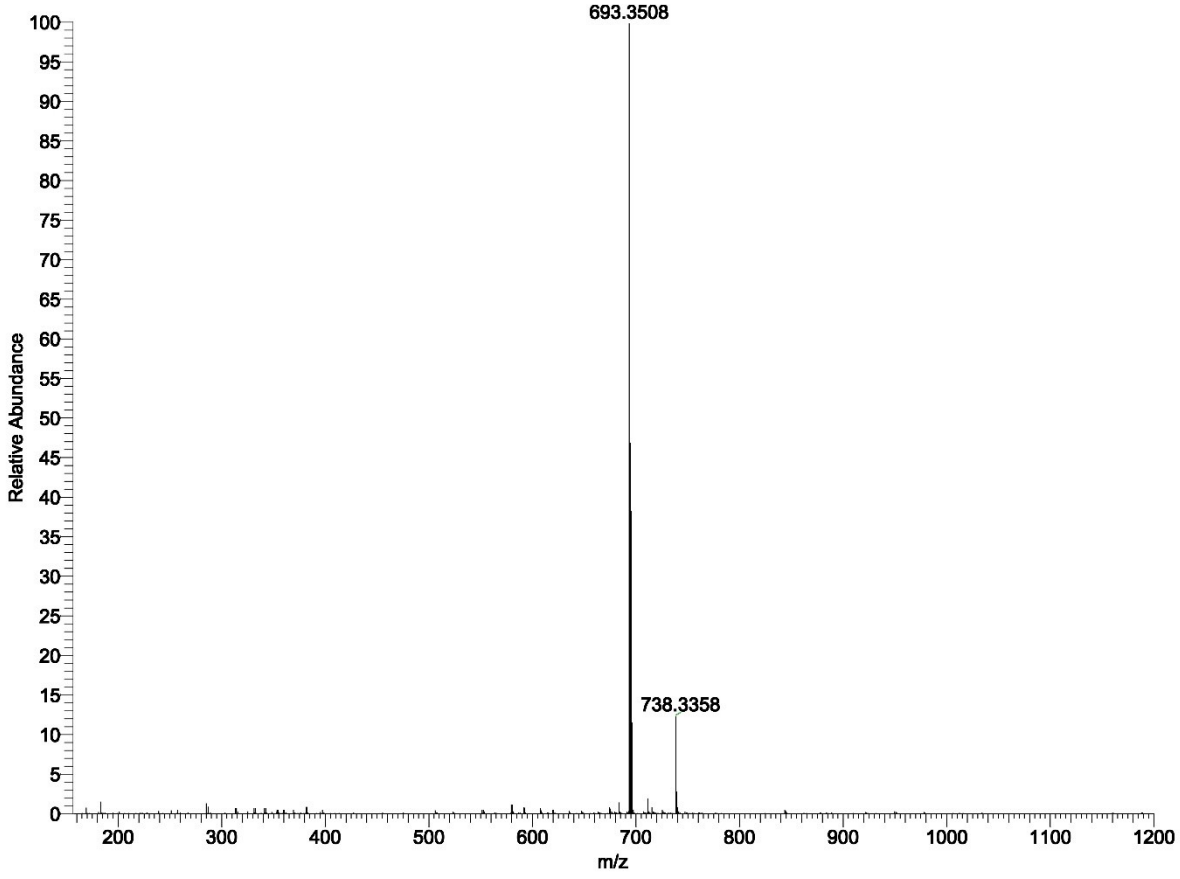
200 kGy, water



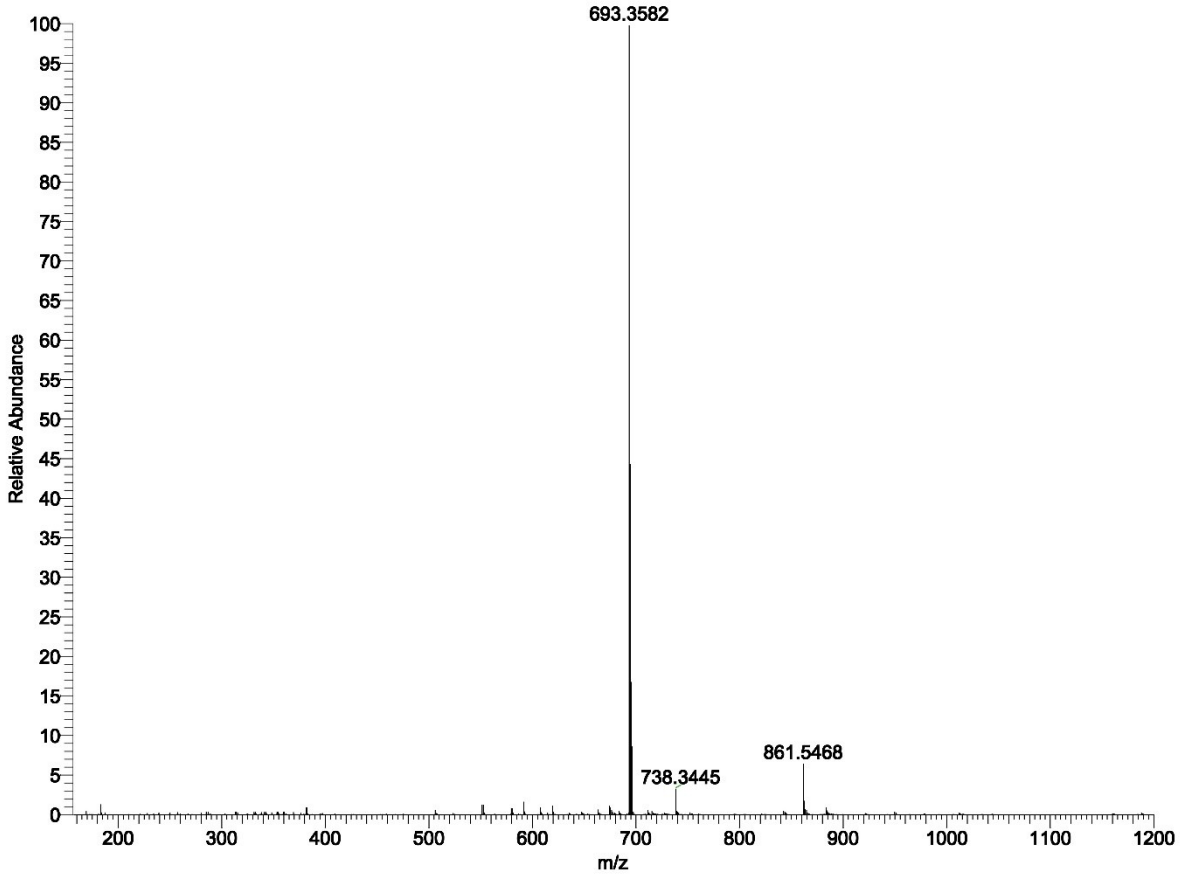
25 kGy, 1M HNO_3



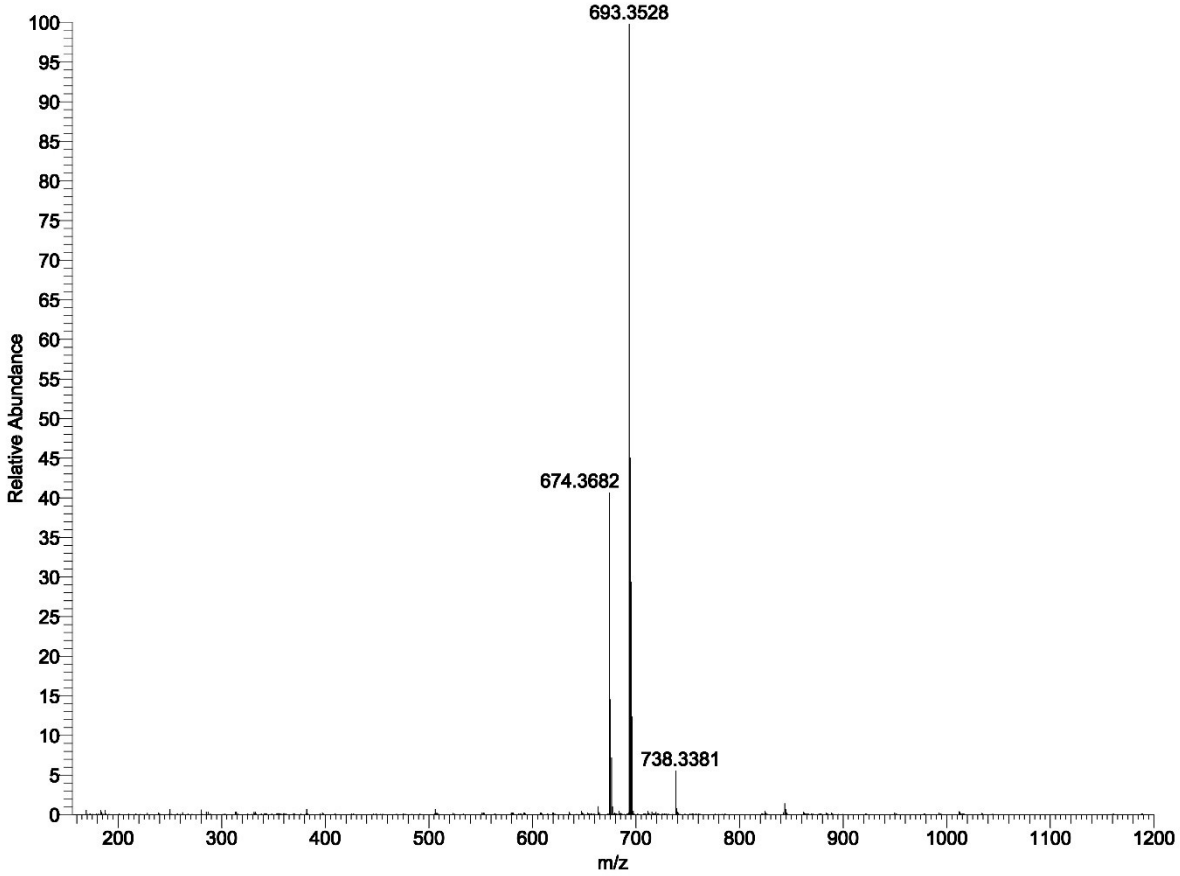
200 kGy, 1M HNO_3



25 kGy, 6M HNO_3



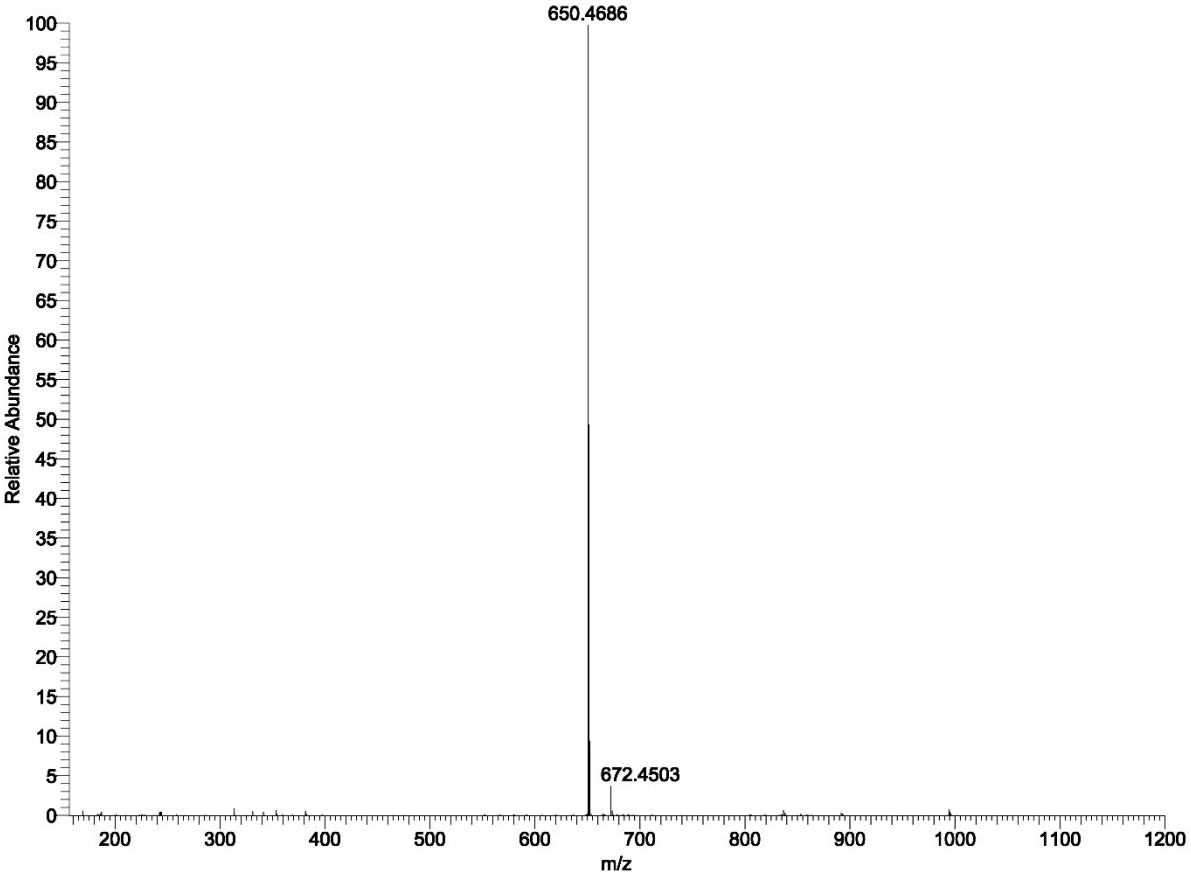
200 kGy, 6M HNO_3



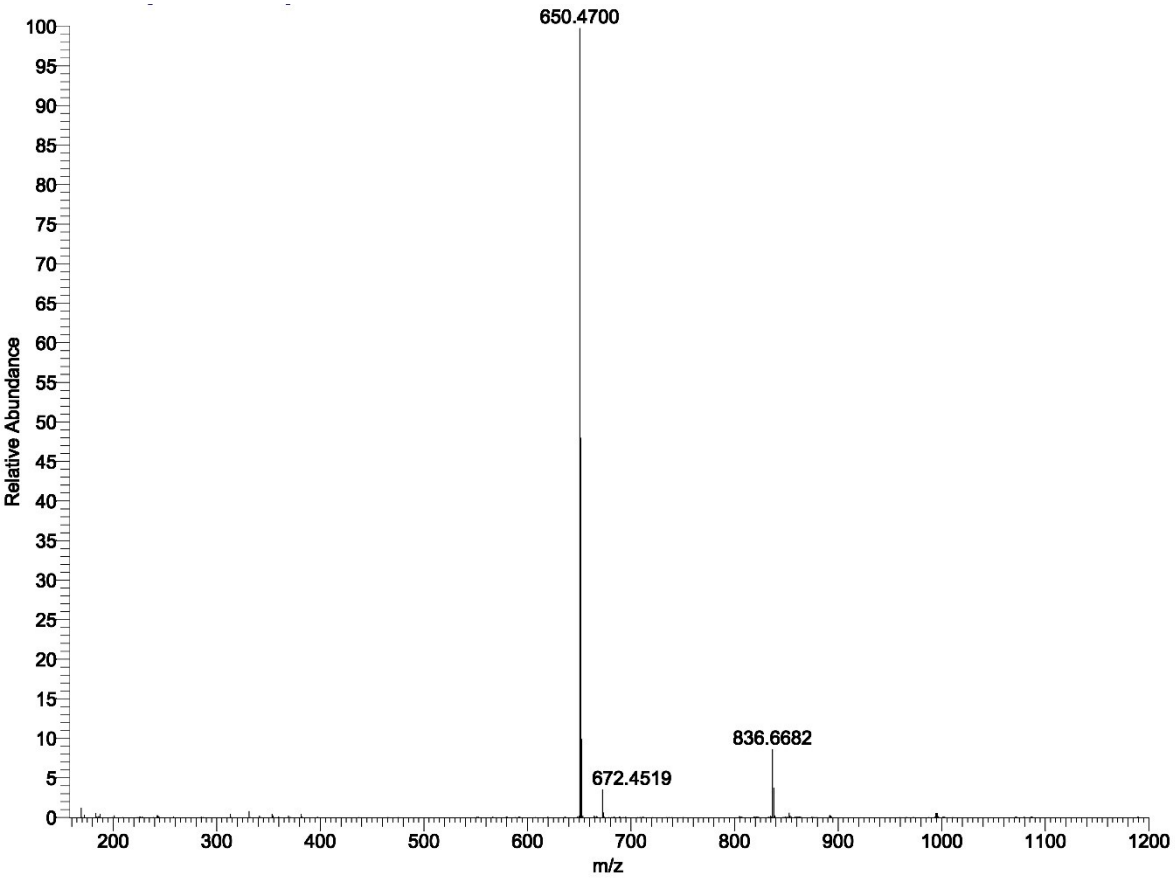
Radiolysis

2,5,9,12-tetra(n-hexyl)-benzo[f]quinolino-[3,4-b]-[1,7]-naphthyridine-6,8(5H,9H)-dione

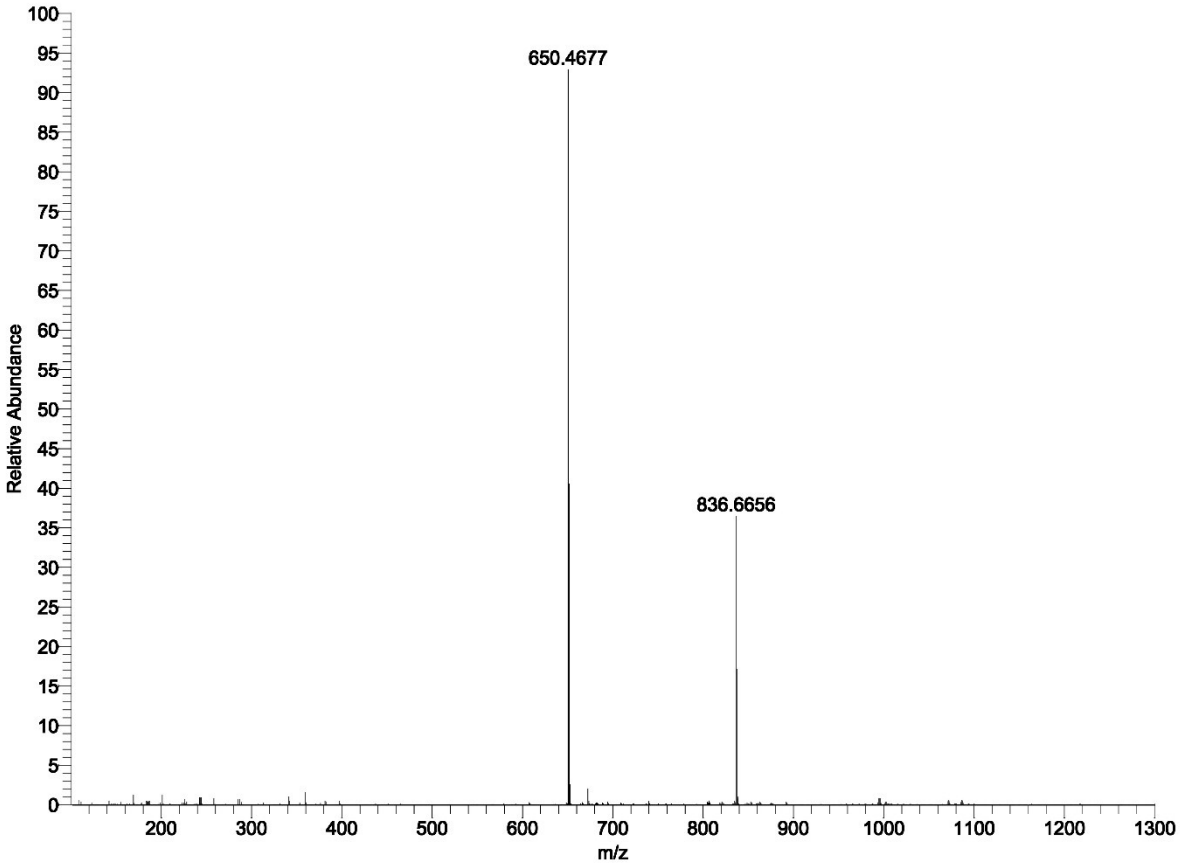
100 кGy, without aqueous phase



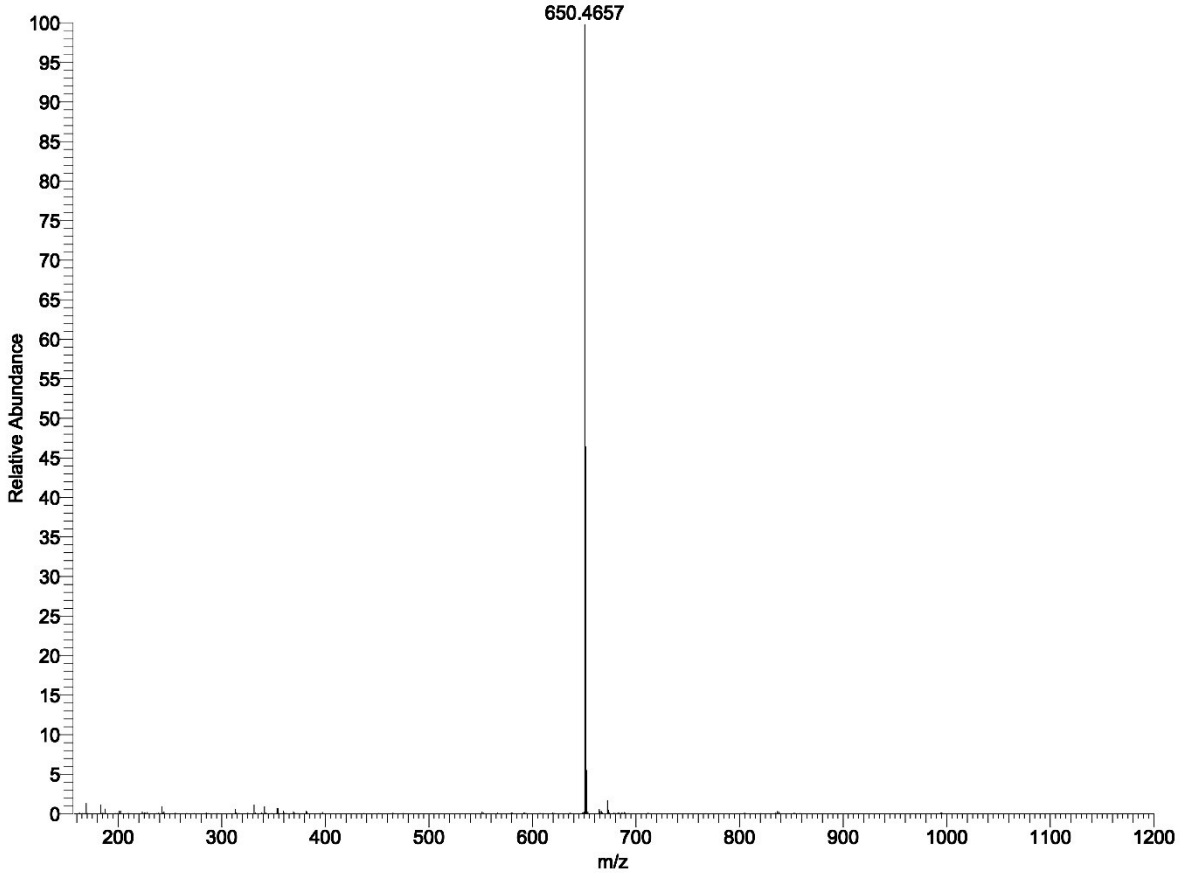
200 кGy, without aqueous phase



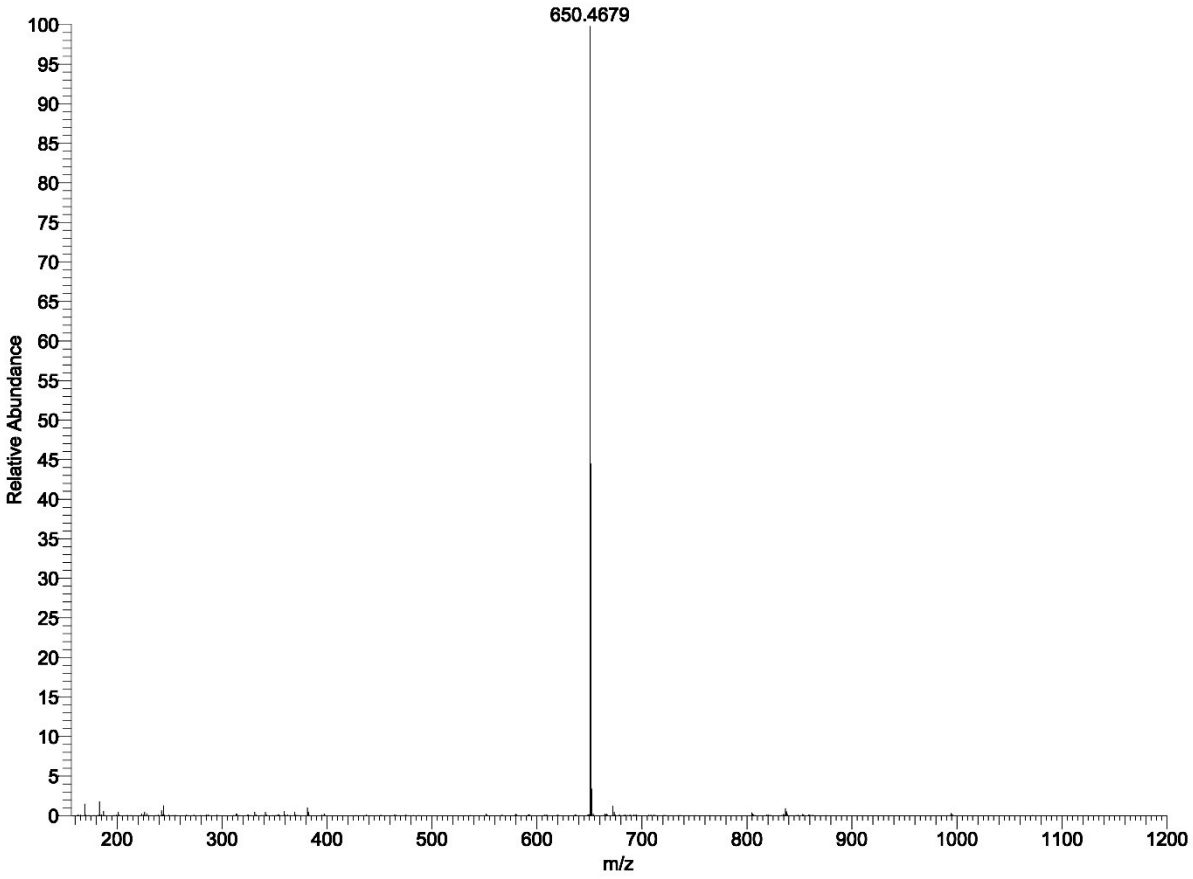
300 кGy, without aqueous phase



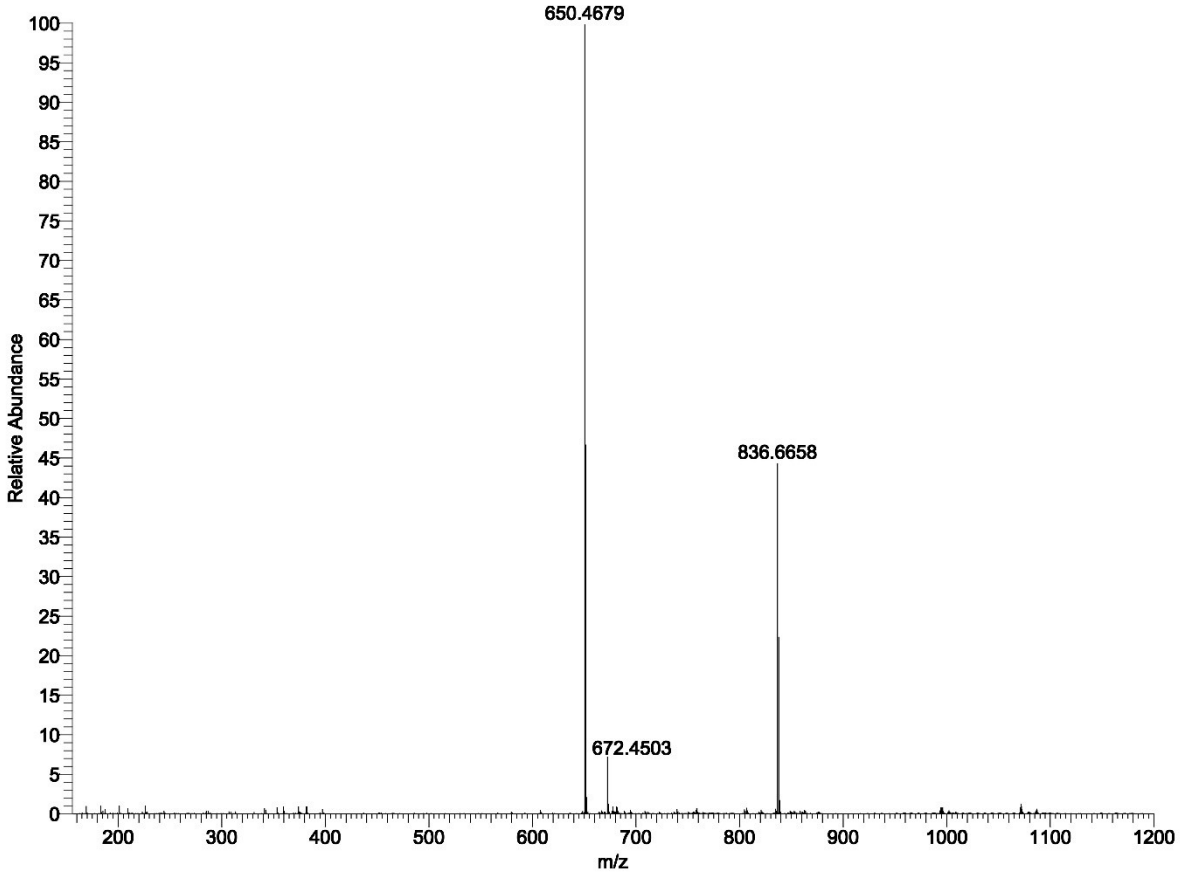
100 кGy, water



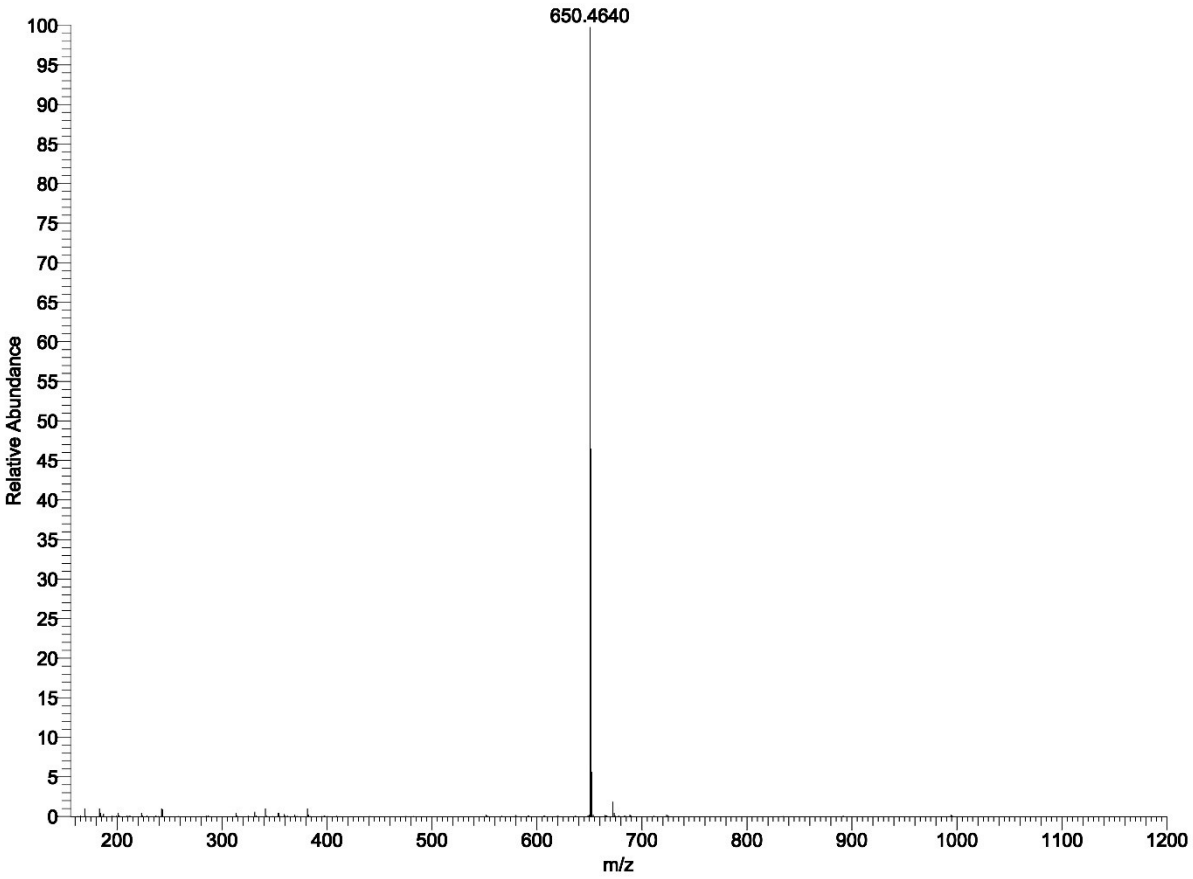
200 кGy, water



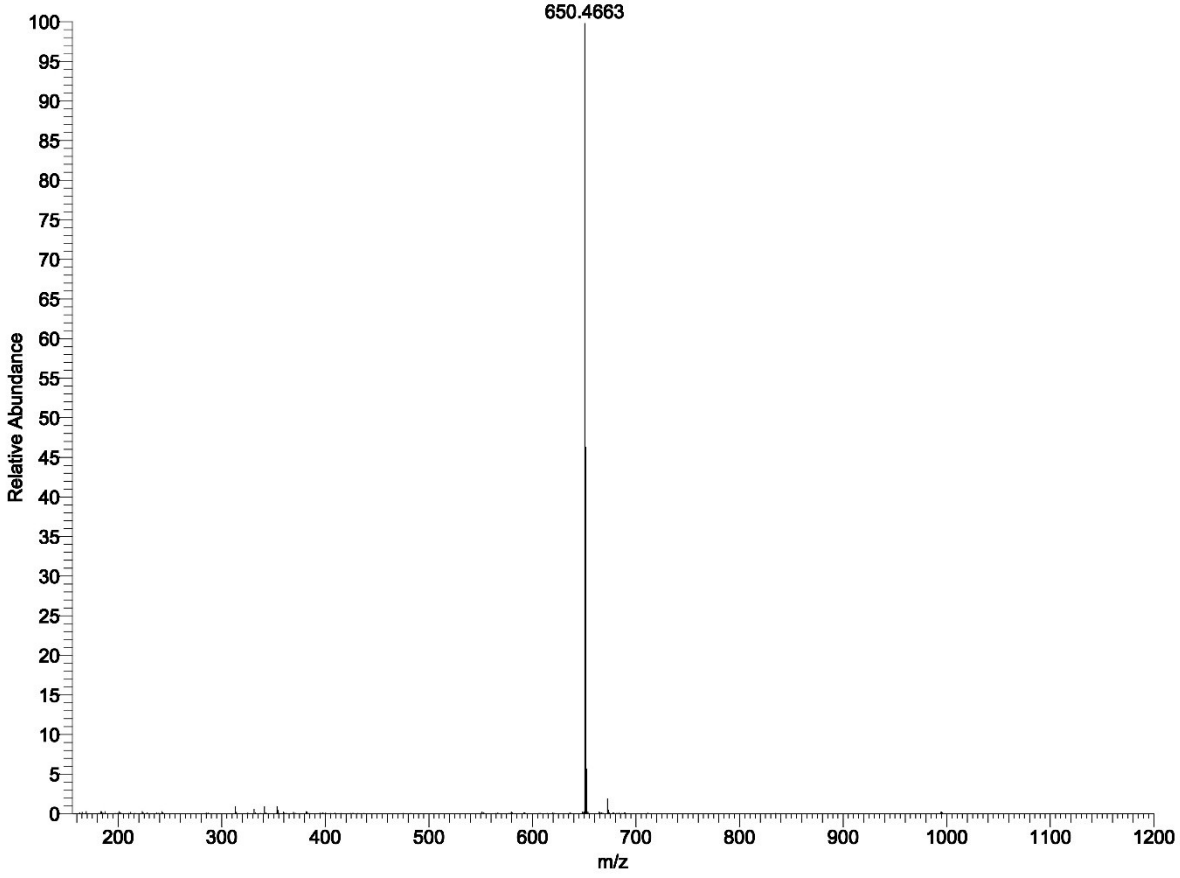
300 кGy, water



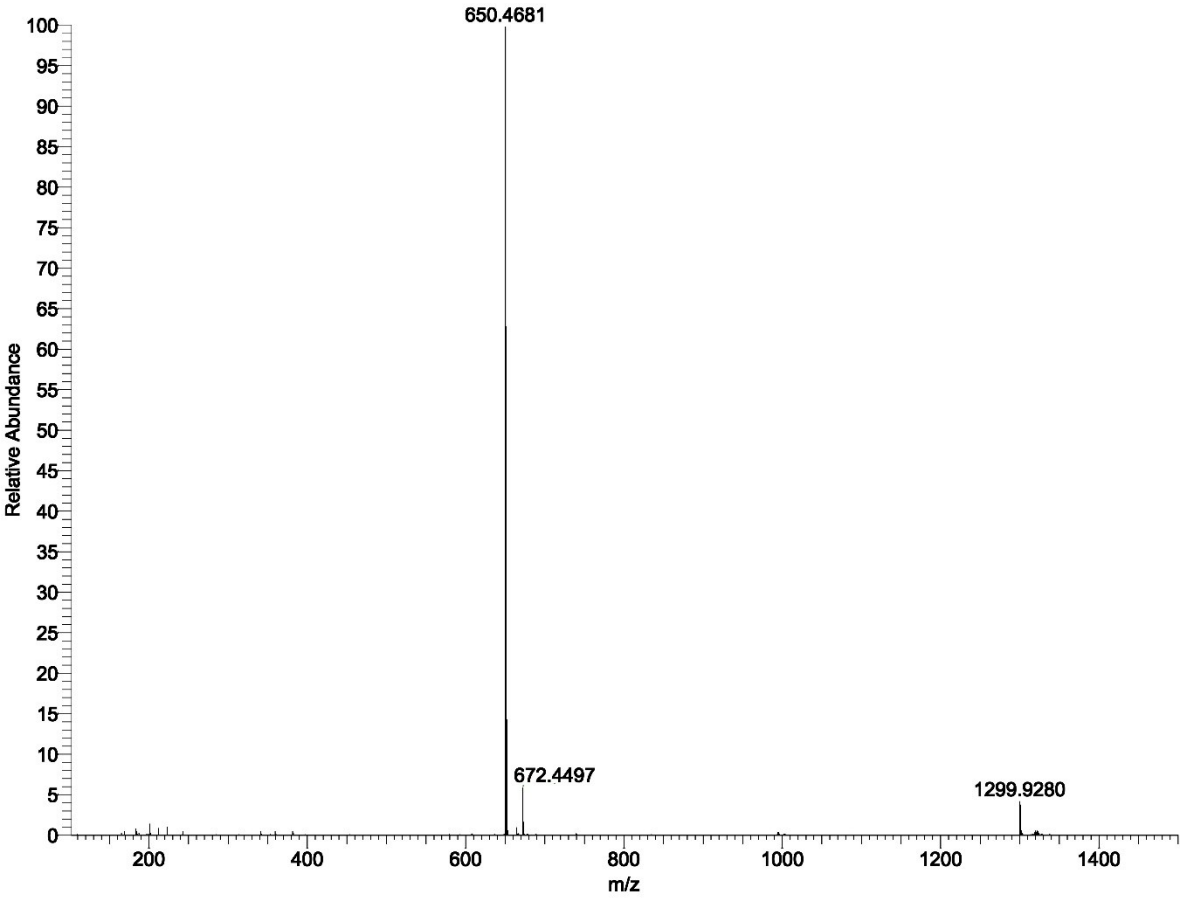
100 кGy, 1 M HNO_3



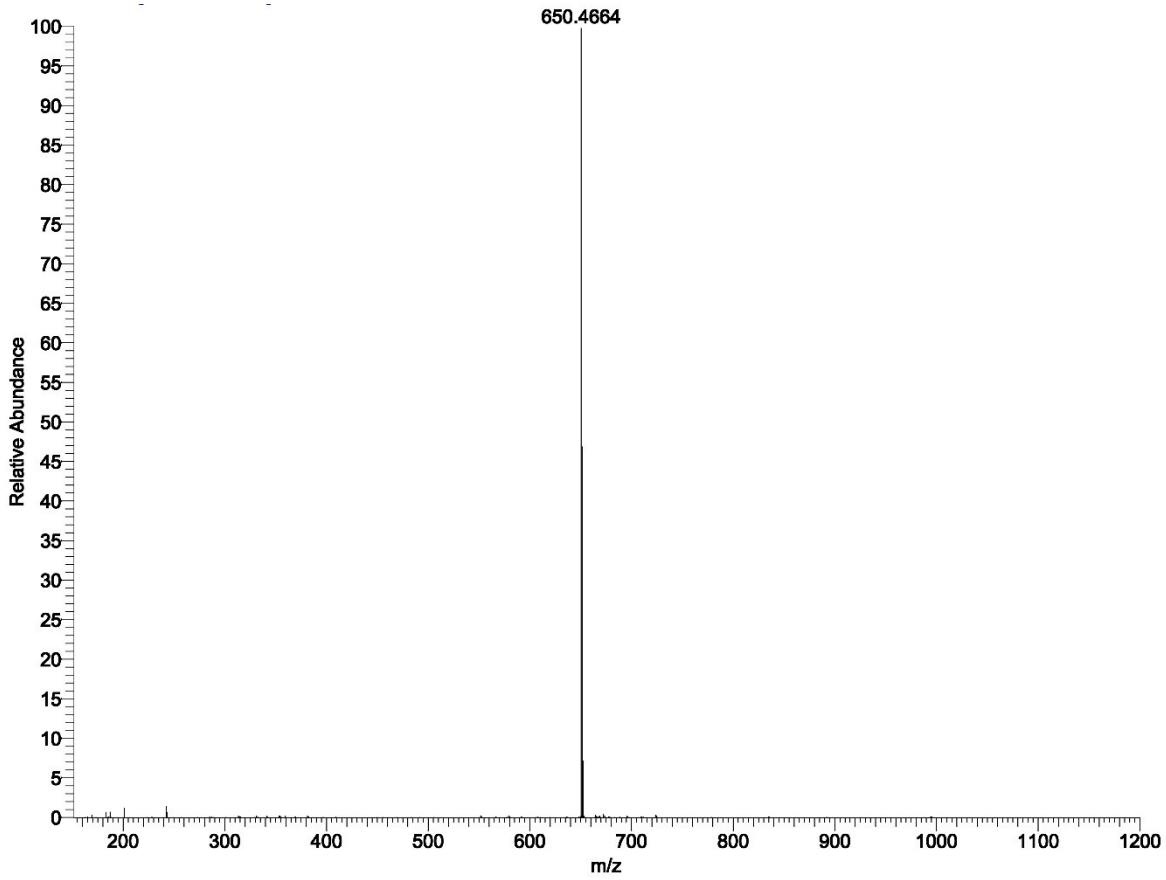
200 кGy, 1 M HNO_3



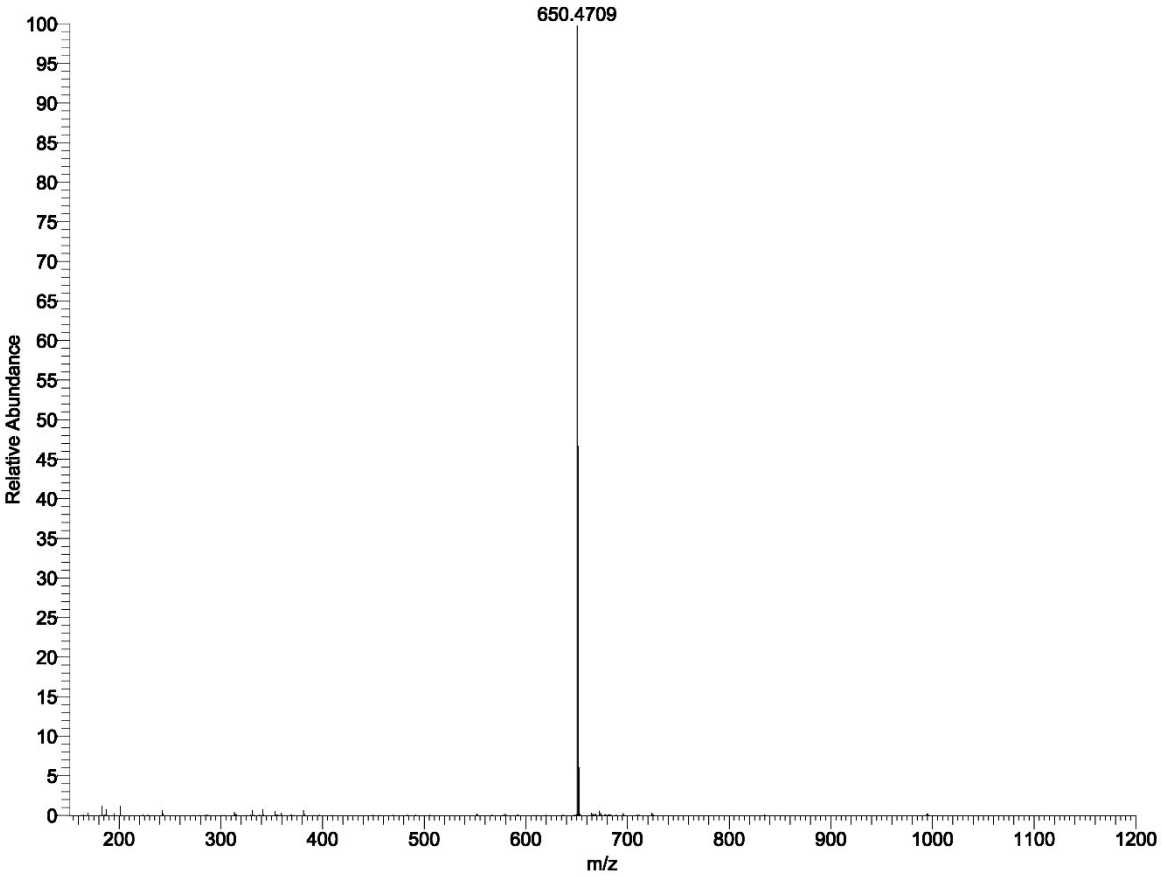
300 кGy, 1 M HNO_3



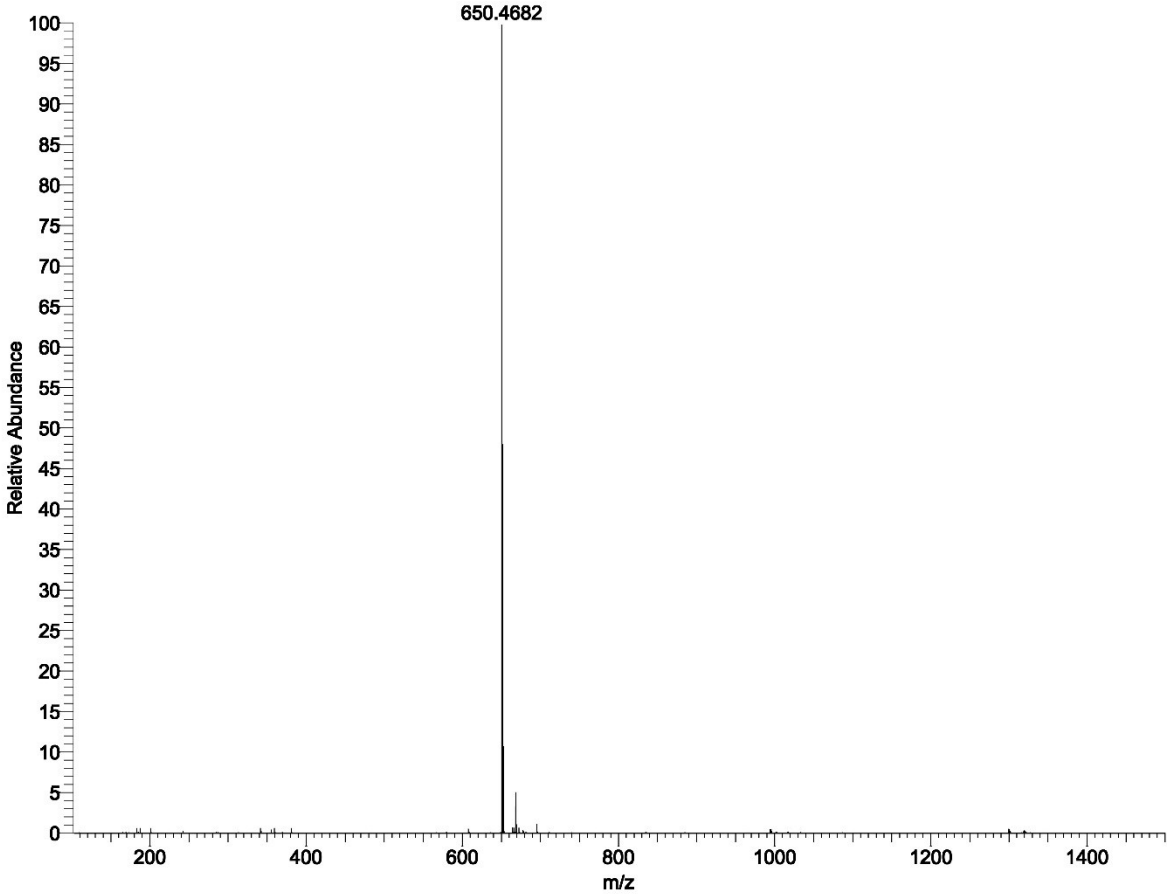
100 кGy, 6 M HNO_3



200 кGy, 6 M HNO_3



300 кGy, 6 M HNO_3



Fragmentation of peak with m/z = 836.66