Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Experimental setup for the study of anions and neutrals

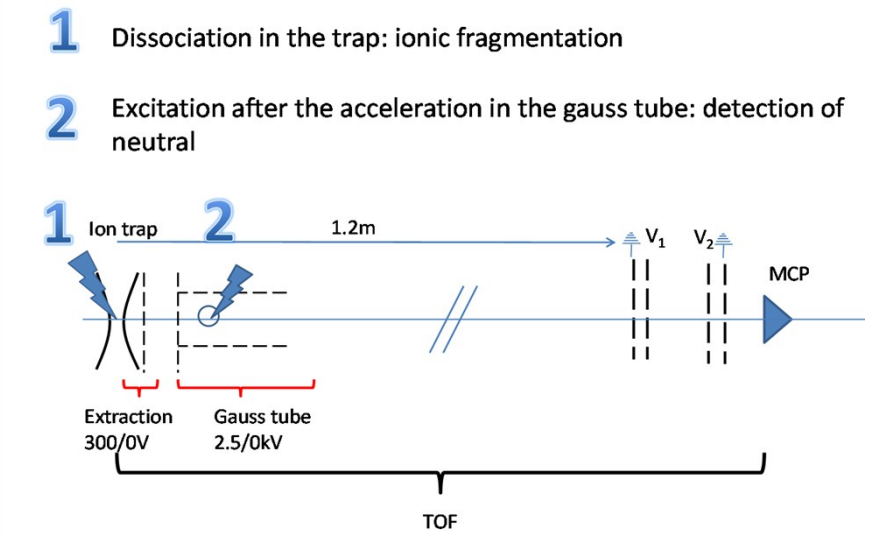


Figure SI-1: Scheme of the experimental setup. The two regions where the laser interacts with the ion packet are 1) in the cold trap, and 2) in the gauss tube.

Symmetrization of the mass peaks

As can be seen in Figure SI-2 panel A, the raw data anion signal, as well as the neutral signal, is not symmetrical, but broadened towards higher times of flight due to electronic ringing in the detector. One way to get rid of this deformation is to subtract a baseline, as in panel B, but we have to estimate the baseline, and the resulting fit is not optimal. Another method is to take the first half of the signal (up to the peak maximum), reverse it, and add the two components, as illustrated in panel C. We then obtain a good fit with a three component function: a Gaussian function for the narrow peak - $C*\exp(-(x^2/l^2))$ - and two combinations of erf functions for the fragments $A*((1-\mathrm{erf}((x-w)/l1))+(1-\mathrm{erf}((-x-w)/l1)))-2*A$, where w represents the half width at half maximum of the function (see panel D).

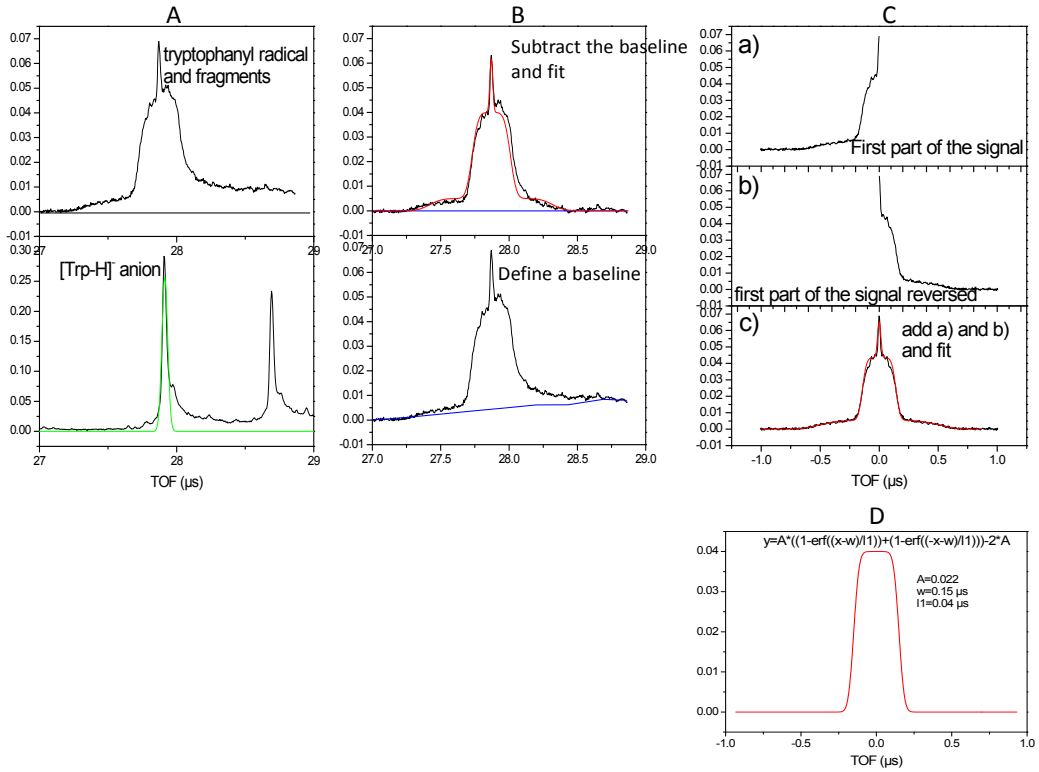


Figure SI-2: panel A, raw time of flight mass spectra as recorded with the MCP detector. Panel B, subtraction of a baseline and fit. Panel C, symmetrization by selecting the first half of the peak, reversing it, and adding the two contributions. Panel D, combination of erf functions to fit the fragment profile of the form A*((1-erf((x-w)/l1))+(1-erf((-x-w)/l1)))-2*A, where w represents the half width at half maximum of the function, l1 the slope of the erf functions.

Neutral fragment peak analysis

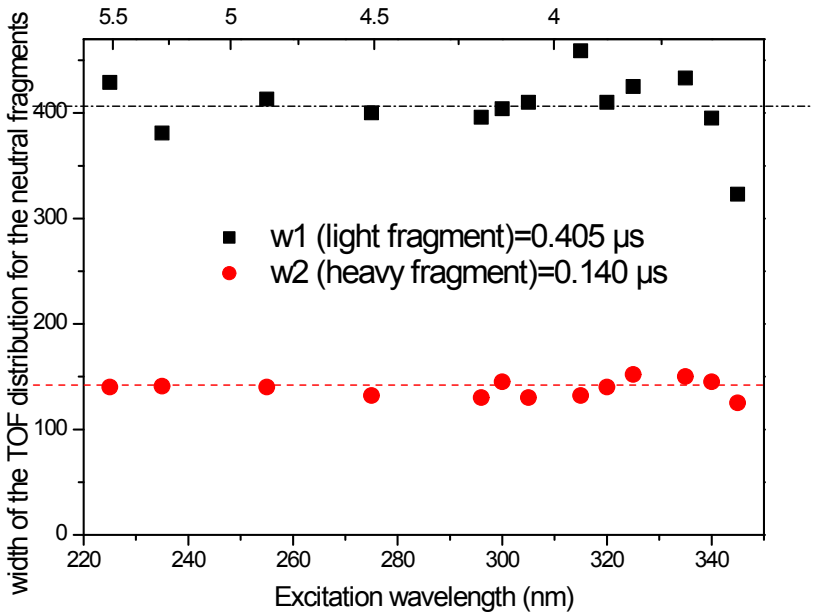


Figure SI-3. Variation of the widths of the fragment peaks as a function of the excitation wavelength for the fragments of the [Phe-H]• radical. The kinetic energy released does not depend on the photon energy.

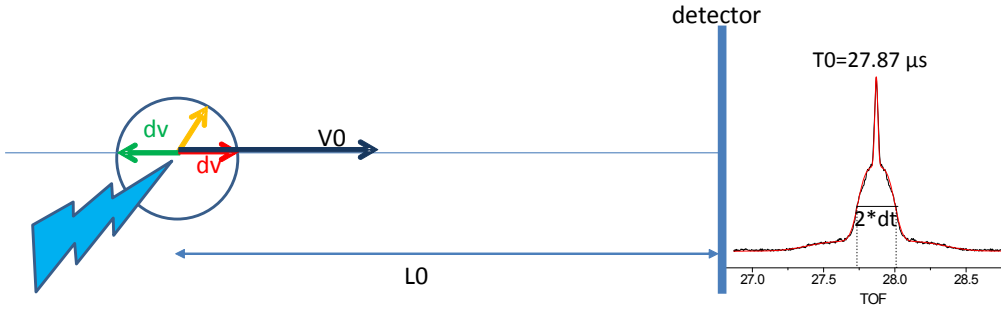


Figure SI-4: Kinetic energy released in the fragmentation process.

A parent ion travelling at velocity V0 will arrive at the detector at time T0= L0/V0. Fragments are created upon interaction with the laser at distance L0, with fragments recoiling from the parent position in a sphere. TOFs lower than T0 correspond to fragments recoiling forward in the direction of the ion beam, and TOFs higher than T0 correspond to fragments recoiling backward.

The distribution of energy in the fragments depends on the fragmentation mechanism. If we assume that the energy released in the fragmentation is monokinetic, a fragment ion has the initial velocity of the parent plus a relative velocity dv due to the fragmentation process. If dv is in the opposite direction to V0, the fragment will arrive later on the detector at time T0+dt, conversely, if dv is in the same direction as V0, the fragment will arrive sooner on the detector at time T0-dt. All the fragments that have an initial velocity in another direction will arrive at times between T0-dt and T+dt.

Under these conditions, the kinetic energy can be deduced from the width of the TOF profile:
*for the intact molecule, V0=L0/T0,
*For the fragment V0-dv=L0/(T0+dt) which becomes dv=V0*dt/T0 (since dt/T0 is small in our case, 0.13/27.9).

Therefore, the relative kinetic energy of fragment m_f is:

$E_{kin}=1/2*m_f*(V0*dt/T0)^2$ or $E_{kin}=1/2*m_f*(L0/T0)^2*(dt/T0)^2$

These TOF spectra are analogous to Doppler profiles measured in optical studies after photolysis of a molecular system. The resulting profile will correspond to the projection of a hollow sphere onto the planar detector, which is a square function that can be modeled as:

A*((1-erf((x-dt)/l1))+(1-erf((-x-dt)/l1)))-2*A,

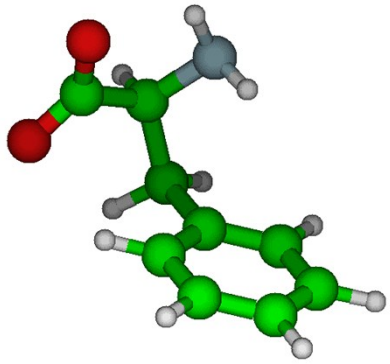
in which A is the height of the "square", and 2*dt is the full width.

If the energy of the fragments is not monokinetic, but corresponds to a distribution around a value $E_{kin,}$ the width of the distribution will be simulated with the l1 parameter.

On the other hand, if the kinetic energy of the fragment can take any value between 0 and E_{kin}^{max}, then the TOF profile should correspond to the projection of a filled sphere onto the detector, which corresponds to a Gaussian function. In this study, attempts to fit our peak profiles with Gaussian functions were not very successful and thus we used erf functions which fitted well.

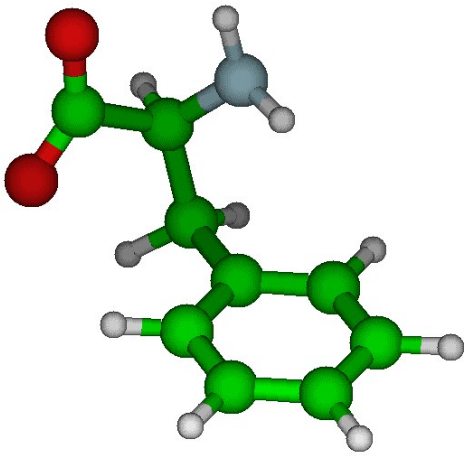
Geometries of deprotonated anion or radical calculated at the DFT/B3LYP/aug-cc-pVTZ level

Phenylalanine anion deprotonated on the acidic group



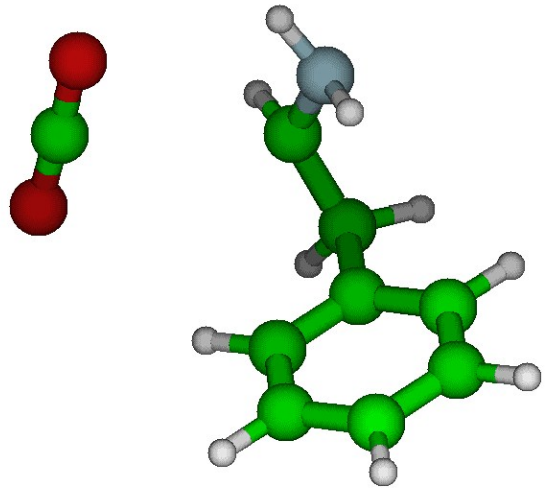
1 c	0.16865091238731	-0.25415226304652	0.25836602724172
2 c	0.41456381453982	0.44948970492088	2.77697528026225
3 c	2.77341038704134	1.12384844586595	3.73025864917984
4 c	4.92861196611267	1.11035955441249	2.20486114397444
5 c	4.65127661420242	0.40601932015652	-0.33256682744145
6 c	2.30000824331672	-0.26811573800071	-1.28720507391389
7 c	7.48587253491187	1.82319214183266	3.25676844904883
8 c	8.49911402170535	4.42170690584230	2.43469350491675
9 c	9.26969693423235	4.54676326724159	-0.44218629418933
10 o	8.87143439177082	6.62351148122967	-1.50607463908593
11 h	-1.66101964217337	-0.77927078938879	-0.49495765025628
12 n	6.81291789894409	6.48639144721865	3.23425380352489
13 o	10.28177356520158	2.59408846802207	-1.32753846628611
14 h	7.17621789691949	7.89780862023176	1.97332836587437
15 h	10.29216824961529	4.66558853561591	3.44649923495727
16 h	7.38566556141583	1.77473789097372	5.32106167240502
17 h	8.88102956512812	0.43863980138080	2.64228774645031
18 h	2.95054261065437	1.67276057903125	5.69550911234131
19 h	6.30954703507718	0.43089801321741	-1.53161826116454
20 h	-1.22553576260103	0.47980879904034	4.00229088004463

Optimized Phenylalanyl Radical with the –C---CO_2bond kept fixed



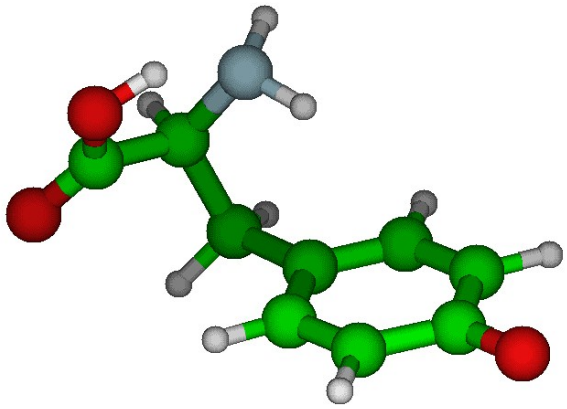
1 c	-6.09090851359800	1.13531954023667	-1.15321827777162
2 c	-5.63380416686941	0.77801489778018	1.40723064735399
3 c	-3.39485552174641	-0.35359782194246	2.19636125248942
4 c	-1.57504461066894	-1.13851978013159	0.44943495917408
5 c	-2.06457006619120	-0.77658704539202	-2.12097317990815
6 c	-4.30110847242929	0.34912371486595	-2.91155708150178
7 c	0.85138164149856	-2.35969605630578	1.34169041202110
8 c	3.11120632514979	-0.56379940929722	1.65592232198492
9 c	4.61101367896291	0.23899742838096	-0.80067137639047
10 o	6.12172172285127	1.94494896331005	-0.45028315947106
11 h	-7.83260254817667	2.00587086150096	-1.77592873527155
12 n	2.50389367912626	1.59391781888687	3.05819975706147
13 o	3.99968591170458	-1.13399226845655	-2.58530151434563
14 h	3.88380164413895	2.91482422992733	3.12705899053461
15 h	4.66713231467567	-1.58797575177256	2.56466815166193
16 h	0.52466940034622	-3.21450301676702	3.19118047753538
17 h	1.41684963166303	-3.85756469042205	0.05549438205285
18 h	-3.07302581920985	-0.66151867356052	4.19514620385332
19 h	-0.68072764848504	-1.37866504556755	-3.49746223408055
20 h	-7.02030086364945	1.36239723196606	2.79183297776067
21 h	-4.65007653962269	0.60609274999538	-4.90984586388169
22 h	0.75284248928950	2.31000809561610	2.78252285105043

Optimized Phenylalanyl Radical with the –C---CO_2 left free



1 c	0.16507534806649	-0.27078463554534	0.21620924081983
2 c	0.19808929064045	0.41330280214110	2.74971363231662
3 c	2.47518830009742	1.01793674400981	3.92425950124909
4 c	4.74798331945495	0.95317485911092	2.59242919206221
5 c	4.68625692837021	0.27466157388837	0.04045143972224
6 c	2.42160649610651	-0.33745048620181	-1.13608297819163
7 c	7.22803514155176	1.62933408864816	3.86415275256727
8 c	8.26877673604632	4.14522734327818	3.09285016458237
9 c	10.12114916478683	5.33090462235400	-2.70353038062186
10 o	9.67054634389591	7.42624855996841	-2.22698137932822
11 h	-1.59828859428247	-0.75217382121331	-0.69931189334066
12 n	6.74375897638459	6.27065773202729	3.37495352712117
13 o	10.60356753368445	3.26212441389759	-3.24980339724940
14 h	7.42060722029110	7.86391774731968	2.57720304223297
15 h	10.27233730638100	4.48463401618785	3.33017575312724
16 h	6.94301671610752	1.55546866677763	5.92339433502590
17 h	8.64094139730366	0.19161564514120	3.42671884368730
18 h	2.48760638724749	1.53289180233159	5.90527559572578
19 h	6.43074493035817	0.22129047147828	-1.02682367303239
20 h	-1.54340701778198	0.47123004332727	3.81983089512267
21 h	2.41624092992967	-0.87528170328793	-3.10900579834480
22 h	4.90050424097583	6.00578255094250	2.95087289530649

Tyrosine anion deprotonated on the phenoxy group



1 n	0.08731893607592	-0.25244351356949	-0.12203400028704
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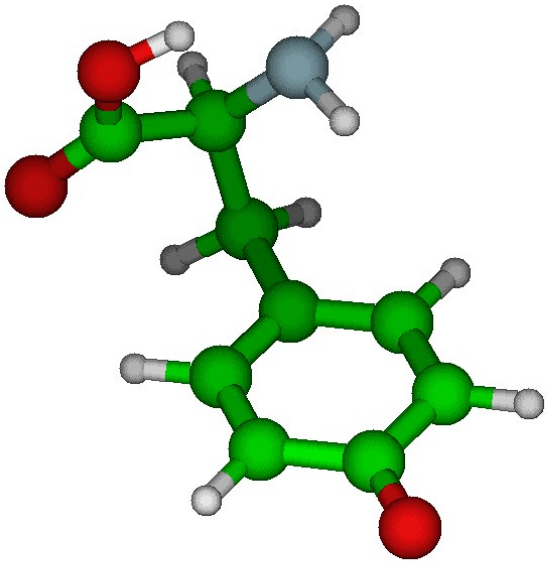
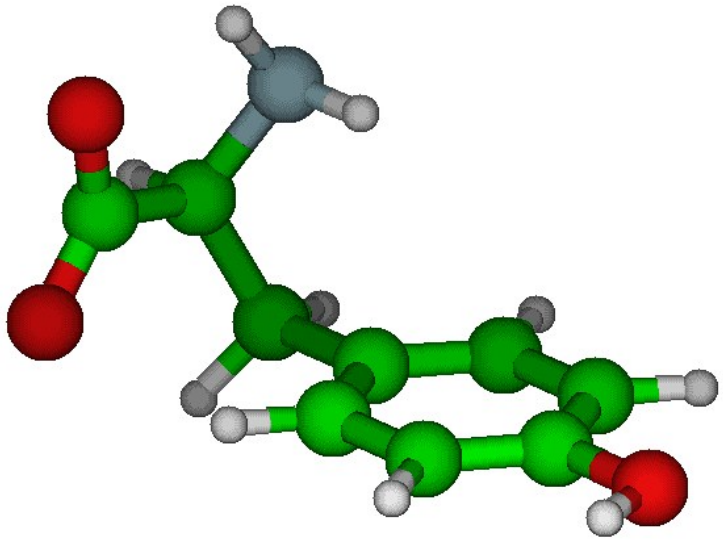
3 c	2.73887415133195	-0.10833062897929	-0.95170642267331
4 h	2.79815835536698	-0.13874521613986	-3.01674106579478
5 c	4.12334012769014	-2.54893195194012	-0.18224548456307
6 o	6.32392124735807	-2.94377724033993	-0.63127003499251
7 c	4.14030760869025	2.31946946684994	-0.02904325539235
8 h	3.69819058575667	3.81919084271027	-1.38016765767281
9 h	6.16270261801547	1.94184986607070	-0.19176800005810
10 c	3.41846153315479	3.18322706025511	2.58217318756225
11 c	1.61319062914294	5.09738025555072	2.94480392965426
12 h	0.81279115706252	6.01934719956391	1.28846470210290
13 c	4.43350799709272	2.09133843757311	4.78311090559494
14 h	5.85445819548094	0.62001768896691	4.59654065102123
15 c	0.84033501177501	5.87729399312862	5.31641028722067
16 h	-0.54282292537020	7.37633114879438	5.51499434272217
17 c	3.69497923922455	2.83473244783240	7.17236084721973
18 h	4.52730883738272	1.95929226997194	8.82775578913408
19 c	1.82772928581537	4.78024903389330	7.60930188260323
20 o	1.13892950667281	5.46474474833142	9.79106026544944
21 o	2.63589452769747	-4.25673137713968	0.94816089675463
22 h	0.96793665248393	-3.41383541792348	1.01026617334631
23 h	-1.11820661652626	0.28780002411562	-1.50074840174992

Tyrosyl radical dehydrogenated on the phenoxy group



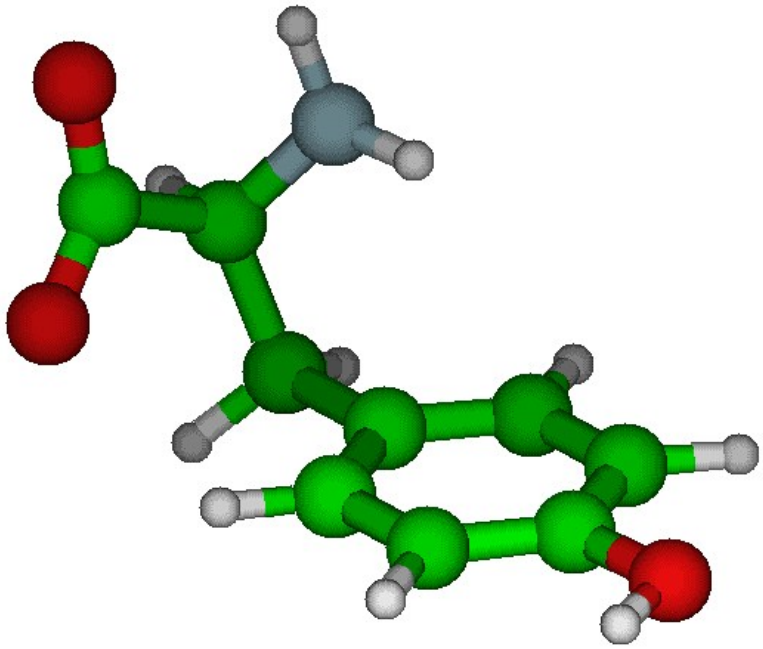
1 n	-2.34470016461140	2.82955649575025	-3.21555965734288
2 h	-2.76913058401107	2.69111512163324	-1.35351916718856
3 c	0.08121694190611	1.63527920292872	-3.81544714334473
4 h	0.81939483004206	2.56406827240692	-5.50542343612384
5 c	-0.34722499160123	-1.11783597195172	-4.65429905057539
6 o	1.34319504875821	-2.61972996561951	-4.88645660712412
7 c	2.16662580144788	1.82841119156115	-1.76703502044393
8 h	2.73141486069690	3.80641901848040	-1.63235659169408
9 h	3.78345841130886	0.75385561375231	-2.45424114559107
10 c	1.38620005546631	0.88690206505149	0.79878919931263
11 c	0.49637266236483	2.59413655620627	2.64624565752756
12 h	0.45837300151722	4.59385035503084	2.20649164579325
13 c	1.50001696220605	-1.71528699422705	1.39761931106822
14 h	2.19840169985107	-3.02003997156457	-0.01289294215441
15 c	-0.28058997269830	1.77742707179292	4.97959692830472
16 h	-0.95929895597406	3.07397962767947	6.40628691216150
17 c	0.74077549221170	-2.58587182442128	3.71356426928432
18 h	0.82343857018192	-4.57155867561253	4.19092881489361
19 c	-0.20665615712536	-0.87882241023186	5.63105241180275
20 o	-0.91765771567179	-1.65292236611434	7.74924818062116
21 o	-2.75279268186007	-1.66859737195631	-5.18998879434182
22 h	-3.71501819818809	-0.12972803128822	-4.80386701253443
23 h	-2.38677697787618	4.67639085244690	-3.69813719655978

Tyrosine anion deprotonated on the acidic group



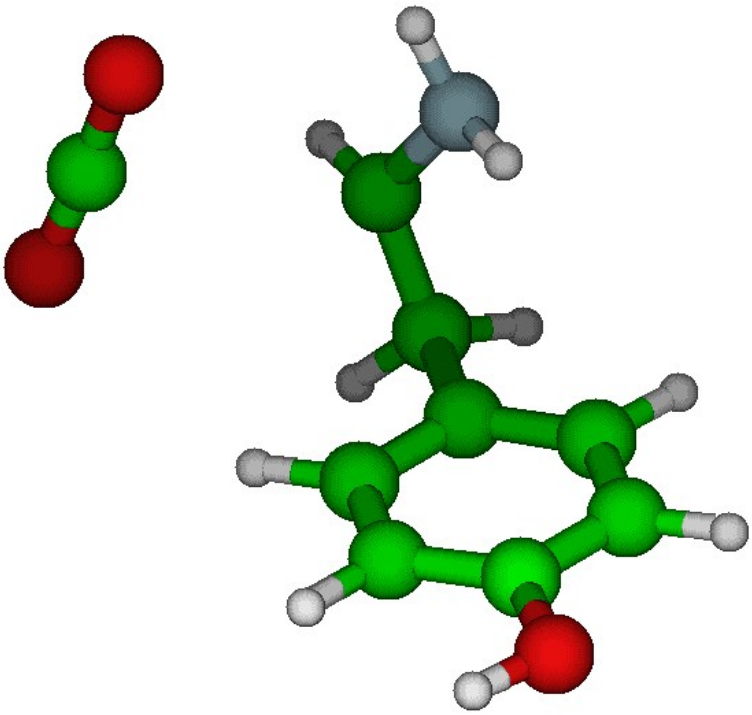
1 n	0.19109204607645	-0.29564895266318	0.24242006035000
2 h	0.29223166938765	0.23861161365828	2.09130489822343
3 c	2.79507994085767	0.00548904675671	-0.69304406881894
4 h	3.76421032396840	-1.80668612366649	-0.41861931681936
5 c	4.41869261276810	1.94553666102485	0.88272378766078
6 o	6.47812685186440	2.60013363346470	-0.09526650207409
7 c	2.85790076271253	0.50541113732678	-3.55577679399181
8 h	1.99523542371758	-1.10247542946640	-4.52826641248435
9 h	4.84552691848086	0.58692260157164	-4.08780687653902
10 c	1.55247361657096	2.89726045097223	-4.41521443280041
11 c	-0.74557684390784	2.82840799409098	-5.70920956881890
12 h	-1.61417892902189	1.01416927656517	-6.09536903590285
13 c	2.61520087172863	5.27346254906997	-3.94347240494668
14 h	4.37947378114326	5.36282383931686	-2.90954135505346
15 c	-1.96021880511330	5.01813487542496	-6.52063846129266
16 h	-3.74295826426822	4.93387029675707	-7.51903076013455
17 c	1.42244414176583	7.47136656667652	-4.73981416086121
18 h	2.27378929612468	9.29522775322143	-4.34206715651789
19 c	-0.86600166603745	7.34949568308305	-6.03021972882701
20 o	-2.11105515543351	9.49279370994813	-6.85582953310133
21 o	3.51611127270609	2.56018875003720	2.98272022074423
22 h	-0.89812420192583	1.06091134846790	-0.57039353411658
23 h	-1.15743366442383	10.94733439432629	-6.32802874293679

Optimized Tyrosyl Radical dehydrogenated on the acidic group with the C--CO_2 bond kept at fixed value



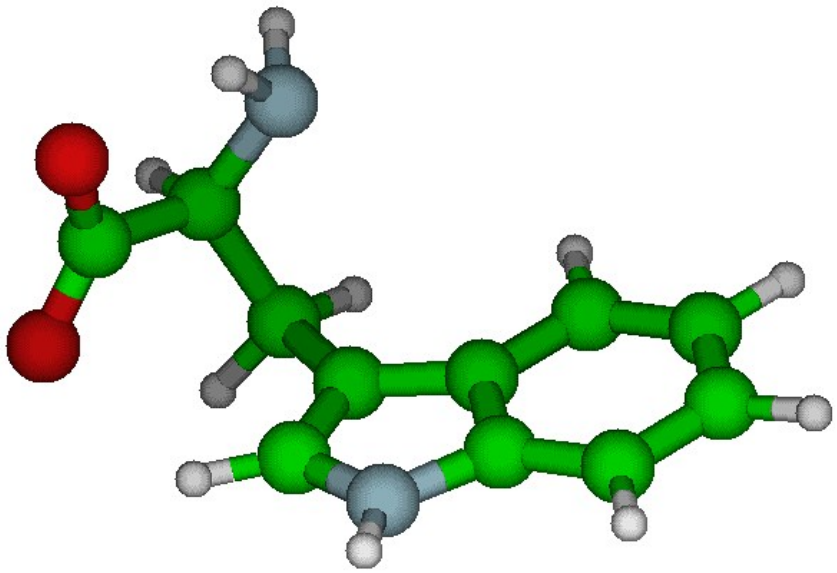
1 n	-2.05703875414633	-2.74433307978794	3.38752064016210
2 h	-3.47893494548639	-2.50709262471879	4.64251416010559
3 c	0.21312061587459	-1.56325869045659	4.05717708813992
4 h	0.98370750500431	-2.42981743534226	5.77524826415005
5 c	-0.36879414145779	1.11308897211048	5.23396987209609
6 o	1.27836535815085	2.64033260033877	4.59868992937803
7 c	2.19956259111908	-1.70063456532078	1.94309230784686
8 h	2.81372366695957	-3.66800836206979	1.84605486620815
9 h	3.81477923357503	-0.57672247698294	2.53352758184692
10 c	1.29801091435380	-0.88603443471875	-0.64296411748194
11 c	0.42894585434069	-2.66751992327122	-2.39071598030860
12 h	0.44347934171269	-4.65439869946006	-1.89508776686574
13 c	1.31066443930996	1.65003979753913	-1.37664722207197
14 h	1.97826414858712	3.06998874232331	-0.06931096368783
15 c	-0.42086076375135	-1.96648246409955	-4.77214379043153
16 h	-1.07956491046827	-3.35992560953260	-6.11312113575636
17 c	0.47028819423504	2.37715645979324	-3.75250876748621
18 h	0.50143293144303	4.35523881452449	-4.28433953432164
19 c	-0.40555234076097	0.57172841636778	-5.45740307497798
20 o	-1.25299889385378	1.17984665544212	-7.81882746580018
21 o	-2.22882610135704	1.14586479964090	6.59744087373616
22 h	-2.58893307848929	-2.55619477688455	1.56062977555740
23 h	-1.14550174058174	2.97833644273237	-8.06973518650852

Optimized Tyrosyl Radical dehydrogenated on the acidic group with the C--CO_2 bond left free



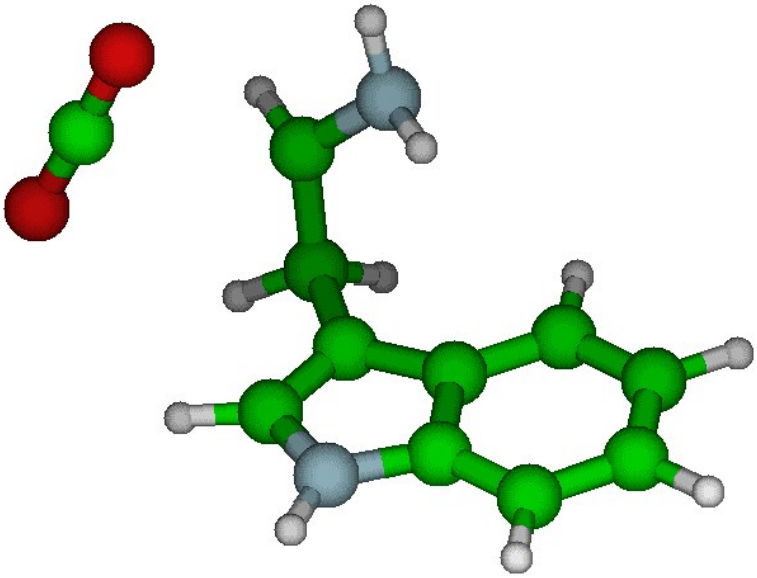
1 n	0.04093495372257	-0.37395502325248	-0.11531545310275
2 h	0.02902241470023	-0.55582469774193	1.78196509187458
3 c	2.41885679827831	-0.36110634498989	-1.23951066032412
4 h	3.74518546449896	-1.71106262230362	-0.45982770019786
5 c	5.60779579336056	3.09498575369787	2.59353018954085
6 o	7.21117763142793	3.49517691180830	1.14961821588335
7 c	2.60730453337436	0.26780888300662	-3.99372554106203
8 h	1.74078795369488	-1.23537988032806	-5.14271124767680
9 h	4.60509272229448	0.29954666180165	-4.50582356237349
10 c	1.38695996054502	2.75881281586243	-4.71528844493003
11 c	-0.98355671547782	2.84515331902129	-5.86716116456968
12 h	-1.95666662371836	1.09407709829207	-6.28926155673692
13 c	2.59593610492285	5.05185317652094	-4.22714819277896
14 h	4.43980411773682	5.04865284369952	-3.34030643652916
15 c	-2.12615510423825	5.12211339483309	-6.50813567653795
16 h	-3.96164098104702	5.16900093817100	-7.40492460015937
17 c	1.48752872329718	7.34269415583679	-4.86739399958062
18 h	2.47186086814726	9.09992764618434	-4.49074510498900
19 c	-0.88522070480108	7.38287382258471	-6.00866459316969
20 o	-2.07437253141718	9.58253072386885	-6.67484987736033
21 o	4.05468545774235	2.74171152837617	4.10407745408026
22 h	-1.13148045871467	1.02075701715046	-0.68965366143361
23 h	-1.02179459913585	11.00239544359054	-6.24718146719995

Tryptophan anion deprotonated on the acidic group



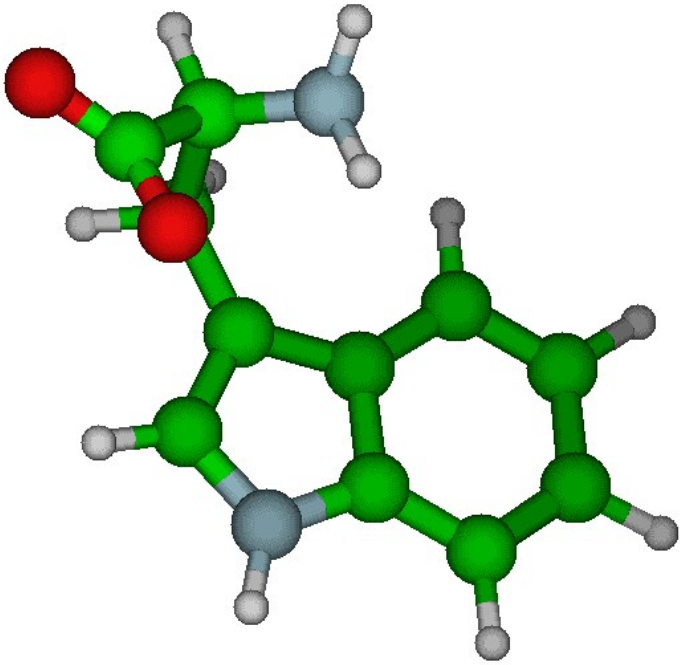
1 n	0.52768610527851	-1.19355049942161	-0.06924010476488
2 h	0.91641871424601	-2.04873592675984	1.61494450056308
3 c	2.98873411503976	-0.27049785513588	-0.97332753753218
4 h	3.56862055192035	-1.30466994579041	-2.67371324642338
5 c	5.14546804414503	-0.77495686950151	1.01645593178419
6 o	4.55117190506973	-2.10348202325628	2.88417900730597
7 c	2.88554205897985	2.54531281466465	-1.73939509108134
8 h	4.69619516738275	2.99822059415026	-2.61622153093111
9 h	1.42096326234976	2.77524867020388	-3.17900251486940
10 c	2.38497954859575	4.35841534939567	0.38749342274723
11 c	3.94621162866067	4.81291351553098	2.39721004498649
12 h	5.73701887065005	3.93896059136119	2.81794018221910
13 c	0.21532234793748	5.95766413598184	0.74458478196846
14 n	2.88282785428328	6.60614239254147	3.97814282862802
15 h	3.61440309588853	7.15349554227851	5.63738500041925
16 c	0.58689255897863	7.34049733298298	3.02157625278755
17 c	-2.01570460558809	6.36921268222554	-0.62103542438360
18 h	-2.37034156272606	5.32738246002502	-2.34473822730669
19 c	-1.17910233314498	9.07172704825381	3.92401313126157
20 h	-0.86422116690819	10.09969335460260	5.66717327740275
21 c	-3.77592479867278	8.09340497283245	0.26749528832563
22 h	-5.50562732931782	8.40758696733402	-0.78040651028961
23 c	-3.36504313789008	9.43545236338114	2.52231476011997
24 h	-4.77525053700531	10.76471190906054	3.17851439880090
25 o	7.23822738315491	0.21683234409946	0.51563881189657
26 h	-0.14802828955308	-2.55056942777157	-1.23506607202346

Optimized tryptophanyl Radical dehydrogenated on the acidic group with the C--CO_2 bond left free



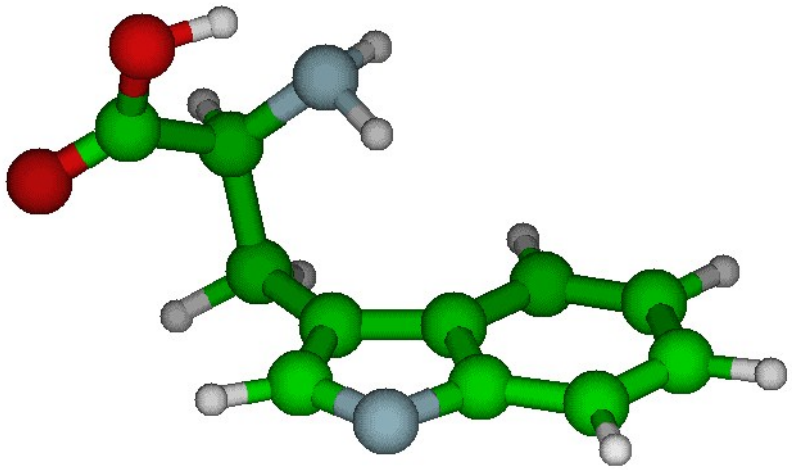
1 n	-4.06556346565252	-2.63977960970772	1.15341218768968
2 h	-3.19520318189824	-1.12283663498732	1.94400408167724
3 c	-2.76868940459854	-3.75091138491116	-0.86231006550992
4 h	-3.60726229589053	-5.50645970163668	-1.55274845779715
5 c	1.53860824549740	-7.20610002022106	1.61718073935416
6 o	0.27548378485659	-7.34514619716112	3.42274183691075
7 c	-1.51727086177122	-2.04508022775211	-2.76985294059102
8 h	-0.43585187774907	-3.24196820466873	-4.07806211853112
9 h	-2.96225730967751	-1.07394658417539	-3.94060857905076
10 c	0.21257264830673	-0.06572187335156	-1.66122215373202
11 c	2.78995458297811	-0.26383425669578	-1.36849482035894
12 h	4.04067730637719	-1.81305911361585	-1.86224543709999
13 c	-0.47525974721533	2.40184966565661	-0.70353358788974
14 n	3.74243839438288	1.92000846770549	-0.28306817263797
15 h	5.58148975946991	2.24704352356353	0.09171313971783
16 c	1.78775702518153	3.59453531091486	0.14206999840834
17 c	-2.77703336864379	3.73235646021349	-0.50184731366333
18 h	-4.54165286543969	2.87324679241408	-1.12890206172359
19 c	1.80687029578146	6.03445224014749	1.17182746086466
20 h	3.55621319960811	6.92092617820954	1.80626210231110
21 c	-2.76649523781500	6.15747092800691	0.51824779747366
22 h	-4.53513006712033	7.20272709859845	0.68108629719110
23 c	-0.49739084925814	7.29739066954193	1.34874449957369
24 h	-0.54933488413149	9.19956448264943	2.14016078121323
25 o	2.87994593865503	-7.14083581638826	-0.13690164653521
26 h	-4.69630015194929	-3.85708249202693	2.48954042361946

Optimized Tryptophanyl Radical dehydrogenated on the acidic group with the C--CO_2 bond kept at a fixed value



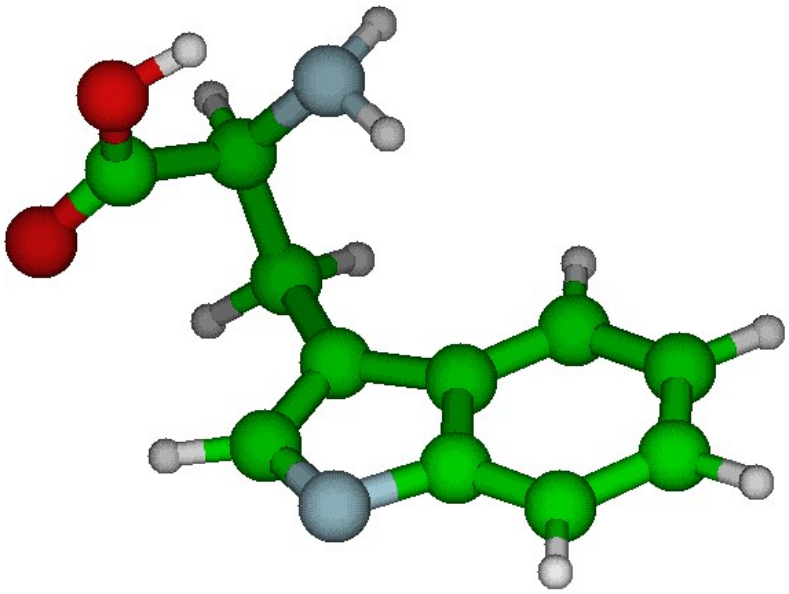
1 n	-3.58842970896621	-2.74249664435268	1.35811565870386
2 h	-2.44539440061223	-1.85529098003560	2.60953582251437
3 c	-2.29254611192938	-4.05476174639724	-0.55577480682781
4 h	-3.61322059308870	-5.24691821588126	-1.57436658373128
5 c	-0.17154237913709	-5.80954012327845	0.57549754554472
6 o	1.18254291895562	-4.80607031372513	2.16190080645818
7 c	-0.92829031857737	-2.30575540687949	-2.51885482397093
8 h	0.21430717987383	-3.52896798274878	-3.71702918123189
9 h	-2.45255891396254	-1.55681749044022	-3.69357717478170
10 c	0.59773375512295	-0.19098416209867	-1.48434355210613
11 c	3.17609202912268	-0.16865308855296	-1.16514666940217
12 h	4.52671740138320	-1.64357814139366	-1.54029862760306
13 c	-0.29470784348326	2.23165663468269	-0.62010487654204
14 n	3.93018064627486	2.09477729015143	-0.16918718089928
15 h	5.71877862539254	2.54827742251113	0.27211175950195
16 c	1.84489997418823	3.61963072656770	0.19599887048805
17 c	-2.68170459780957	3.36732845701551	-0.46644726983835
18 h	-4.35273969359930	2.35896751764944	-1.07230336851011
19 c	1.66422492293332	6.06329257596236	1.14716379410727
20 h	3.31864770801493	7.09723043732196	1.76166601448458
21 c	-2.87261125382053	5.79949522705204	0.48442563446587
22 h	-4.70622650829633	6.69387643875188	0.61358892777636
23 c	-0.72464230239234	7.13356283235478	1.28294422315113
24 h	-0.93404283804720	9.03055819896934	2.01399884496711
25 o	-0.30409240667403	-7.91289683843504	-0.44083128325068
26 h	-4.99006107812565	-3.70711619557046	2.2185099324286

Tryptophan anion deprotonated on the indolic nitrogen



1 c	-0.07941896584551	0.52590159833412	-0.22265335494369
2 c	-0.08941086880027	0.37973245035178	2.39542639791044
3 c	2.19260286484681	0.01163667105852	3.68831520099709
4 c	4.52467396078646	-0.22262087246027	2.28688977900201
5 c	4.47930315488693	-0.05476125545532	-0.36529773833003
6 c	2.19434517703601	0.31665800738041	-1.59674426468076
7 n	2.59941748445347	-0.16516624853155	6.22788333182100
8 c	5.11835188306881	-0.50717935022860	6.45818438410848
9 c	6.43399444809020	-0.56725732240663	4.15561491145816
10 c	9.20272315274548	-0.93982191018166	3.72044664224005
11 c	10.02754776421784	-3.75683469299002	3.46132530039619
12 c	10.63141921002831	-4.96953794350959	6.03661853850604
13 o	12.03947231520036	-4.04443526819702	7.57314363871864
14 n	8.18757384259374	-5.35466611041025	2.11648728645525
15 o	9.52963897438716	-7.22285410510592	6.38278302996619
16 h	8.54465299380642	-7.47005756531810	4.81008617075896
17 h	11.82654130482936	-3.82244741807580	2.44658957323946
18 h	10.33078462945607	-0.11740383616996	5.23951049522276
19 h	9.76622826215042	0.02132950561312	1.97674415889866
20 h	5.96298694096284	-0.69744109633055	8.31613150544534
21 h	6.20934661781077	-0.19691816989463	-1.46224183968230
22 h	-1.83596549817119	0.55171634372428	3.45337801762145
23 h	2.15092543241407	0.45275678333189	-3.64088455493205
24 h	-1.83877608084616	0.80826449078692	-1.23366663295184
25 h	8.61379514509236	-5.50150994294147	0.26050953297007
26 h	6.46180989902599	-4.50345321311901	2.23807550616149

Optimized tryptophanyl radical dehydrogenated on the indolic nitrogen



1 c	-0.14399216436251	0.50842154945102	-0.03919824937705
2 c	-0.03644979401436	0.40604404446206	2.61505809977940
3 c	2.28497868838626	0.06805471471604	3.73214240663618
4 c	4.51666560917663	-0.18716386060441	2.25443289327512
5 c	4.38599467816391	-0.06662086541039	-0.37714590284834
6 c	2.02628342959385	0.28287745588797	-1.50808380181139
7 n	2.84144790251473	-0.07284018741020	6.33392495058272
8 c	5.29055565996058	-0.40878203941865	6.47685147373494
9 c	6.51841579489535	-0.51241921855531	4.03989812913207
10 c	9.25177901517835	-0.93569607577472	3.53072872122946
11 c	10.04195752275183	-3.76000916688435	3.52470373134565
12 c	9.93776527435273	-4.88199655331522	6.21713853419435
13 o	10.56326474983761	-3.71719359897828	8.06481755622048
14 n	8.68923072831393	-5.40571571205835	1.75755347419808
15 o	9.17157770726546	-7.28713216542875	6.29958431545107
16 h	8.74364343778301	-7.73389736635430	4.55038909174738
17 h	12.04365864402009	-3.82416854960775	3.02288193166393
18 h	10.38747372436138	-0.00366180101754	4.97627856121609
19 h	9.76531771088272	-0.13175729078688	1.70183711788302
20 h	6.24451362584703	-0.58959235463069	8.27467902677772
21 h	6.06498663124129	-0.22068529535211	-1.53717552426497
22 h	-1.72495055581636	0.59112054525973	3.75101735954676
23 h	1.88341189006844	0.38616858980368	-3.54384736451026
24 h	-1.95122561908683	0.77597276491767	-0.95641006798322
25 h	9.51943405243206	-5.46530911272303	0.03954000996904
26 h	6.86882570047961	-4.86038892093263	1.52105854258898