Screening of protic ionic liquids with catalytic potential in the transesterification reaction using COSMO-RS and machine learning

Luis Alberto Gallo-García[a,b,c], Pedro J Carvalho[b], Maria Isabel da Silva Nunes[c], Nian Vieira Freire[a], Alessandro Cazonatto Galvao[d], Daniela Helena Pelegrine Guimarães[a], Pedro Felipe Arce[a]*

[a] *Chemical Engineering Department, Engineering School of Lorena, University of São Paulo (USP), 12602-810, Lorena-SP, Brazil*

[b] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal*

[c] *CESAM – Centre for Environmental and Marine Studies, Department of Environment and Planning, University of Aveiro, 3810-193, Aveiro, Portugal*

[d] *Laboratory ApTher - Applied Thermophysics, Department of Food and Chemical Engineering, Santa Catarina State University (UDESC), 89870-000, Pinhalzinho-SC, Brazil*

* Corresponding Author: Pedro Felipe Arce

Email: parce@usp.br

Tel: 55-12-31595326

ORCID:

Luis Alberto. Gallo-García	:	0000-0002-2973-9648
Pedro J Carvalho	:	0000-0002-1943-0006
Maria Isabel da Silva Nunes	:	0000-0002-5456-8123
Nian Vieira Freire	:	0000-0003-1257-4928
Alessandro Cazonatto Galvão	:	0000-0002-8255-4511
Daniela Helena Pelegrine Guimarães	:	0000-0002-4797-1168
Pedro Felipe Arce	:	0000-0002-4687-5297

Table S1. Predictive acidity of ionic liquids using COSMO-RS.

Ionic liquids	Predictive acidity	H_0 (Literature)	Predictive yield FAME (%)	References
[Proline][NO_3]	4.570	2.490	45.000	
[Phenylalanine][NO_3]	4.840	2.770	28.000	
[Alanine][NO_3]	4.970	2.630	20.000	
[Histidine][NO_3]$_2$	6.300	2.480	70.000	[1]
[Serine][NO_3]	6.340	2.620	22.000	
[Glutamic_acid][NO_3]	6.490	2.350	50.000	
[Aspartic_acid][NO_3]	6.790	2.270	90.000	
[Im(N(CH_2)$_3$$SO_3$H)$_2$][$HSO_4$]	1.960	0.850	96.000	
[(CH_3CH_2)$_3$N(CH_2)$_4$$SO_3$H][$HSO_4$]	3.560	1.260	57.000	
[PyN(CH_2)$_4$$SO_3$H][$HSO_4$]	4.080	1.290	55.000	[2]
[MimN(CH_2)$_4$$SO_3$H][$HSO_4$]	4.070	1.310	70.000	
bis[3-(CH_2)$_3$$SO_3$H-1-($CH_2$)2-Im][$HSO_4$]$_2$	5.420	0.910	83.000	

$[C_3(Mim)_2][HSO_4]_2$	2.700	1.510	87.000	
$[C_6(Mim)_2][HSO_4]_2$	2.330	1.560	85.000	[3]
$[C_{12}(Mim)_2][HSO_4]_2$	2.300	1.550	82.000	
$[TEABS][CF_3SO_3]$	2.030	2.593	69.000	
$[TEABS][HSO_4]$	3.380	2.613	68.000	
$[TMEDADBS][CF_3SO_3]_2$	4.150	2.388	83.000	[4]
$[DABCODBS][CF_3SO_3]_2$	4.470	2.528	89.000	
$[TMEDADBS][HSO_4]_2$	6.100	2.370	85.000	
$[DABCODBS][HSO_4]_2$	6.600	2.421	90.000	
$[Ps\text{-}N\text{-}Ch(Me)_2][p\text{-}TSA]$	3.370	-	85.210	
[Ps-mim][p-TSA]	3.800	-	76.550	
$[Ps\text{-}N\text{-}Ch(Me)_2][HSO_4]$	3.850	-	73.600	[5]
$[Ps\text{-}mim][HSO_4]$	4.190	-	56.480	
$[BSMBIM][CF_3SO_3]$	2.340	1.035	47.420	
$[BSMBIM][CH_3SO_3]$	3.610	1.054	45.120	

[BSMBIM][HSO_4]	3.790	1.056	44.850	[6]
[BSMBIM][CF_3CO_2]	3.910	1.121	32.830	
[C_{18}MIM][Br]	1.070	-	81.000	
[C_{16}MIM][Br]	1.070	-	77.500	
[EMIM][Br]	1.090	-	78.000	
[BMIM][CH_3SO_3]	1.280	-	92.000	[7]
[BMIM][Cl]	1.280	-	77.000	
[EMIM][CH_3SO_3]	1.290	-	83.000	
[N_{4444}][L-arginine]	1.460	-	99.000	
[N_{1111}][L-arginine]	2.230	-	97.000	[8]
[Choline][L-arginine]	4.600	-	99.000	
[Choline][OH]	2.740	-	95.000	
[Choline][Imidazolium]	3.570	-	76.900	[9]
[Choline][methoxide]	4.950	-	88.300	
[HMIM][BF_4]	0.830	-	70.100	

[BMIM][BF_4]	0.860	-	68.300	
[HMIM][HSO_4]	2.170	-	81.900	[10]
[BMIM][HSO_4]	2.200	-	89.600	
[HMIM][H_2PO_4]	4.530	-	72.300	
[BMIM][H_2PO_4]	4.530	-	75.000	
([TMEDAPS][HSO_4])$_2$	5.100	1.930	95.000	
TMHDAPS][HSO_4]$_2$	5.360	1.840	96.000	[11]
[TMPDAPS][HSO_4]$_2$	6.290	1.900	95.000	
[BMIM][Cl]	1.280	-	12.000	
[AMIM][OH]	2.740	-	52.000	
[EMIM][OH]	2.880	-	63.000	[12]
[BMIM][OH]	2.920	-	55.000	
[HMIM][OH]	2.950	-	51.000	
[BMIM][OH]	2.920	-	38.500	
[HPMIM][OH]	7.100	-	93.700	[13]

[GLYMIM][OH]	10.950	-	99.900	
[N_{2222}][L-arginine]	1.480	-	98.380	[14]
[BMIM][Imidazolium]	1.690	-	95.000	[15]
[BMIM][HSO_4]	2.200	-	90.000	
[BIM][HSO_4]	3.180	-	79.000	[16]
[MIM][HSO_4]	3.660	-	72.000	
[1-butyl-3-methyl morpholine][Imidazolium]	0.690	2.490	95.800	[17]

Table S2. Interaction energies of ionic liquids calculated with COSMOtherm.

LI	$E_{INT}C$	$E_{MF}C$	$E_{HB}C$	$E_{vdW}C$	$E_{INT}A$	$E_{MF}A$	$E_{HB}A$	$E_{vdW}A$
[Arginine][NO_3]$_2$	-98.56096	14.32222	-77.28783	-39.75520	-42.45692	4.84728	-37.77961	-13.68445
[Proline][NO_3]	-55.41666	13.66454	-43.81542	-25.41227	-46.91384	4.91751	-42.91884	-13.07237
[Phenylalanine][NO_3]	-69.71043	15.30239	-47.08559	-37.27104	-48.65075	6.87127	-46.33647	-13.34541
[Alanine][NO_3]	-55.08274	8.68376	-47.27987	-20.64649	-49.99839	5.88433	-46.75952	-13.28306
[Histidine][NO_3]$_2$	-102.94620	10.87274	-82.14746	-31.81792	-43.89596	5.45473	-40.12708	-13.38347
[Serine][NO_3]	-71.66498	7.56357	-63.27982	-20.10859	-62.92553	4.91459	-59.05019	-12.94979
[Glutamic_acid][NO_3]	-78.14005	12.26646	-67.29554	-27.27083	-63.09425	5.63813	-59.83212	-13.06011
[Aspartic_acid][NO_3]	-75.88304	11.30373	-69.20068	-22.14595	-66.53975	6.39865	-64.29191	-12.80635
[Im(N(CH_2)$_3$$SO_3$H)2][$HSO_4$]	-21.26795	4.71246	-12.38024	-13.63518	-17.95380	1.00283	-15.76350	-4.18735
[(CH_3CH_2)$_3$N(CH2)$_4$$SO_3$H][$HSO_4$]	-40.90570	32.45950	-25.41896	-52.10610	-52.51602	7.30267	-46.33053	-17.64802
[PyN(CH_2)$_4$$SO_3$H][$HSO_4$]	-52.28535	24.82740	-30.03297	-46.42359	-57.81583	5.50361	-49.69221	-17.78710
[MimN(CH_2)$_4$$SO_3$H][$HSO_4$]	-51.12539	26.54269	-30.19591	-47.61865	-57.66932	5.84452	-49.90250	-17.77120

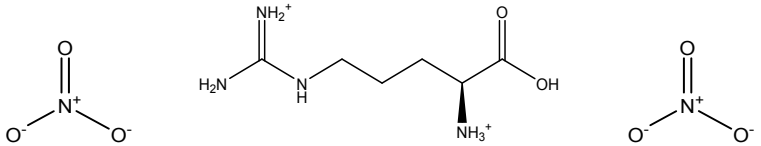
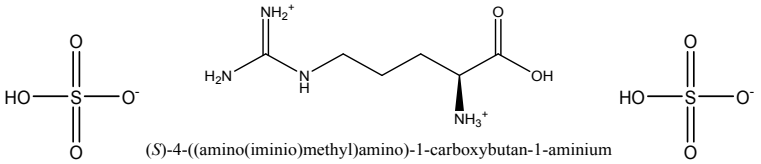
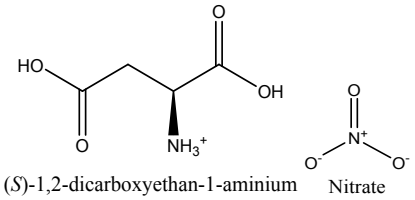
bis[3-$(CH_2)_3SO_3H$-1-$(CH_2)_2$-Im][HSO_4]$_2$	-109.75730	42.29764	-61.95646	-86.23154	-58.98864	4.92760	-50.31628	-17.75981
[C_3(Mim)$_2$][HSO_4]$_2$	-33.02701	46.45159	-22.77878	-52.83291	-43.42723	5.55165	-35.06153	-18.07721
[C_6(Mim)$_2$][HSO_4]$_2$	-35.33720	52.66267	-18.99798	-65.13498	-39.87762	7.38335	-33.38209	-18.03874
[C_{12}(Mim)$_2$] [HSO_4]$_2$	-60.83700	51.95573	-18.14095	-90.78487	-37.89610	8.84036	-32.87676	-18.01956
[TEABS][CF_3SO_3]	-40.05663	25.18358	-19.52776	-49.87232	-26.23891	9.01922	-17.91471	-21.50327
[TEABS][HSO_4]	-38.59621	32.98585	-23.58083	-52.16108	-50.78853	7.33446	-44.59212	-17.69073
[TMEDADBS][CF_3SO_3]$_2$	-100.93000	23.55741	-56.60878	-72.03874	-32.73914	8.97577	-24.29794	-21.57682
[DABCODBS][CF_3SO_3]$_2$	-109.09550	21.43392	-61.28580	-66.98206	-33.81253	9.60059	-25.98476	-21.58822
[TMEDADBS][HSO_4]$_2$	-111.46920	28.97182	-69.55560	-75.04532	-62.22612	3.72656	-52.47619	-17.63635
[DABCODBS][HSO_4]$_2$	-126.09780	20.45348	-75.36742	-64.70334	-64.70334	3.16676	-54.52256	-17.50739
[Ps-N-Ch(Me)$_2$][p-TSA]	-62.38097	26.97313	-35.08771	-53.61019	-53.44761	18.07261	-33.80932	-37.05470
[Ps-mim][p-TSA]	-61.77080	21.49807	-38.77471	-44.64065	-57.97300	17.11030	-37.17179	-37.25531
[Ps-N-Ch(Me)$_2$][HSO_4]	-53.74129	27.19379	-27.64397	-52.63491	-55.19393	6.46627	-48.14632	-17.67374
[Ps-mim][HSO_4]	-52.01732	21.96282	-30.54013	-43.58649	-58.97099	4.94708	-50.27199	-17.80593

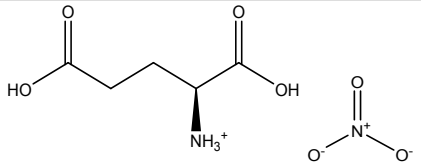
[BSMBIM][CF_3SO_3]	-56.34705	23.98827	-22.71086	-54.56022	-29.02982	9.15437	-20.82653	-21.51751
[BSMBIM][CH_3SO_3]	-63.93378	34.93471	-38.38292	-57.42134	-39.30263	14.42610	-37.39168	-20.49691
[BSMBIM][HSO_4]	-57.76152	29.52397	-27.36421	-56.85705	-54.71959	6.80180	-47.88209	-17.79917
[BSMBIM][CF_3CO_2]	-70.81680	26.20015	-39.25140	-54.70132	-43.32116	8.57443	-37.95198	-18.10347
[C_{18}MIM][Br]	-80.56291	35.63587	-10.70769	-105.63760	-7.58392	16.00905	-10.70769	-14.40536
[C_{16}MIM][Br]	-72.48715	35.20583	-10.81036	-97.02910	-8.05254	15.64577	-10.81036	-14.40803
[EMIM][Br]	-9.24041	39.45337	-12.09875	-36.74151	-13.22607	11.80406	-12.09875	-14.45146
[BMIM][CH3SO3]	-23.62450	30.90695	-13.27066	-41.40727	-12.99002	17.03821	-13.38872	-20.79937
[BMIM][Cl]	-19.01118	40.24745	-14.71679	-44.68832	-10.61063	15.18959	-14.71679	-12.60351
[EMIM][CH_3SO_3]	-14.96397	31.43251	-13.66816	-32.87479	-13.57599	16.85036	-13.78547	-20.80073
[N_{4444}][L-arg]	-35.28315	37.48726	-5.28467	-71.64559	-33.04884	35.92827	-32.29091	-40.84605
[N_{1111}][L-arg]	-5.83677	28.87652	-13.97865	-24.89449	-41.68689	32.39370	-37.31011	-40.93034
[Choline][L-arg]	-37.60796	27.08179	-39.79641	-29.05320	-67.12411	29.11156	-59.57351	-40.82201
[Choline][OH]	-4.49518	71.71268	-39.48149	-36.87285	-9.66243	36.40386	-39.48149	-7.40001
[Choline][Imidazolium]	-35.10824	27.04295	-36.74827	-29.56279	-43.40945	11.27010	-35.43893	-19.38709

[Choline][methoxide]	-33.56255	49.56911	-56.73436	-30.55717	-44.30725	20.10444	-55.53107	-13.04048
[HMIM][BF_4]	-28.82722	23.43183	-5.63686	-46.76867	-8.33276	7.39920	-5.63686	-14.25495
[BMIM][BF_4]	-21.43103	22.50634	-5.83653	-38.24732	-9.66892	6.25857	-5.83653	-14.25083
[HMIM][HSO_4]	-31.44036	26.59257	-8.63712	-49.54229	-37.16954	9.23507	-32.54113	-18.02333
[BMIM][HSO_4]	-23.24003	26.49206	-8.83980	-41.03877	-38.25022	8.43726	-32.81424	-18.03310
[HMIM][H_2PO_4]	-33.22036	30.23913	-13.81642	-49.78954	-80.88169	13.37510	-79.72383	-18.69282
[BMIM][H_2PO_4]	-24.25219	30.89812	-14.02781	-41.26897	-81.55362	12.95622	-79.98437	-18.68533
([TMEDAPS][HSO_4])$_2$	-93.06889	29.92421	-53.97161	-73.18134	-56.92024	4.16809	-47.60843	-17.63976
TMHDAPS][HSO_4]$_2$	-97.56716	44.15163	-61.71076	-84.16788	-58.55604	5.14627	-50.22412	-17.63804
[TMPDAPS][HSO_4]$_2$	25.39176	25.39176	-71.39553	-70.75607	-63.46079	3.57742	-53.63617	-17.56190
[BMIM][Cl]	-19.01118	40.24745	-14.71679	-44.68832	-10.61063	15.18959	-14.71679	-12.60351
[AMIM][OH]	-4.49518	71.71268	-39.48149	-36.87285	-9.66243	36.40386	-39.48149	-7.40001
[EMIM][OH]	-2.95264	71.48309	-40.90439	-33.67781	-11.78147	35.71223	-40.90439	-7.40452
[BMIM][OH]	-15.76608	66.64174	-40.33686	-42.21745	-11.01278	35.92701	-40.33686	-7.41814
[HMIM][OH]	-26.72057	63.90997	-40.03472	-50.74230	-10.65506	35.99228	-40.03472	-7.42783

[BMIM][OH]	-15.76608	66.64174	-40.33686	-42.21745	-11.01278	35.92701	-40.33686	-7.41814
[HPMIM][OH]	-53.99619	70.75699	-85.90515	-38.99451	-57.67545	32.23246	-83.31464	-7.40848
[GLYMIM][OH]	-95.42314	69.63873	-126.64330	-38.56504	-98.85395	30.46311	-122.71950	-7.41274
$[N_{2222}]$[L-Arginine]	-3.67193	35.80782	-5.92363	-37.71598	-34.20756	34.85714	-32.36530	-40.85925
[BMIM][Imidazolium]	-29.17829	29.23707	-16.75135	-41.81048	-23.09192	13.25759	-16.75135	-19.74464
[BMIM][HSO_4]	-23.24003	26.49206	-8.83980	-41.03877	-38.25022	8.43726	-32.81424	-18.03310
[BIM][HSO_4]	-35.85804	17.86058	-18.40895	-35.45614	-47.51322	7.12217	-40.77017	-18.02507
[MIM][HSO_4]	-34.61475	11.30132	-22.38550	-23.67705	-52.97639	5.32094	-44.36371	-18.09349
[1-butyl-3-methyl morpholine][Imidazolium]	-43.76249	10.65951	-29.81536	-24.75313	-34.92910	10.47860	-28.36419	-21.20336

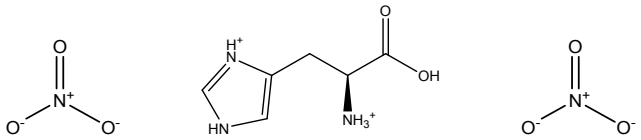
Table S3. Structure of ionic liquids.

Ionic liquids
 [L-arginine][NO_3]$_2$
 [L-arginine][HSO_4]$_2$
 [L-Aspartic acid][NO_3]



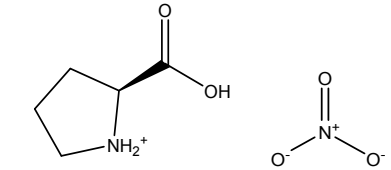
(*S*)-1,3-dicarboxypropan-1-aminium Nitrate

[L-Glutamic acid][NO_3]



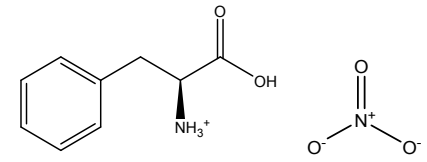
Nitrate (*S*)-4-(2-ammonio-2-carboxyethyl)-1*H*-imidazol-3-ium Nitrate

[L-Histidine][NO_3]$_2$



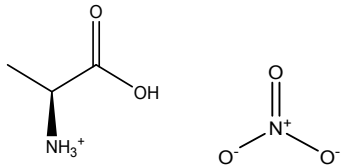
(*S*)-2-carboxypyrrolidin-1-ium Nitrate

[L-Proline][NO_3]



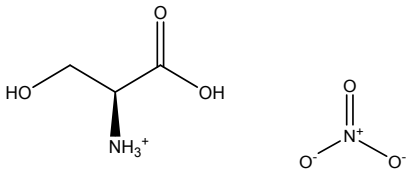
(*S*)-1-carboxy-2-phenylethan-1-aminium Nitrate

[L-Phenylalanine][NO_3]



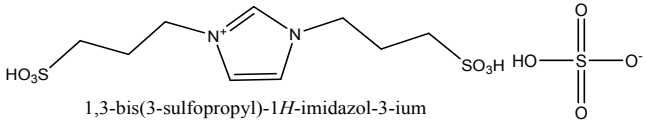
(*S*)-1-carboxyethan-1-aminium Nitrate

[L-Alanine][NO_3]



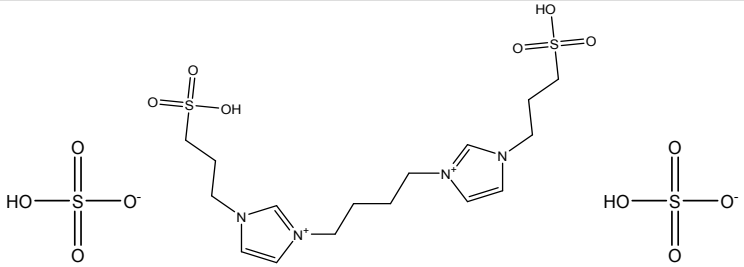
(*S*)-1-carboxy-2-hydroxyethan-1-aminium Nitrate

[L-Serine] [NO_3]

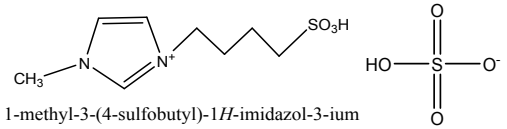


1,3-bis(3-sulfopropyl)-1*H*-imidazol-3-ium

[$Im(N(CH_2)_3SO_3H)_2$][HSO_4]

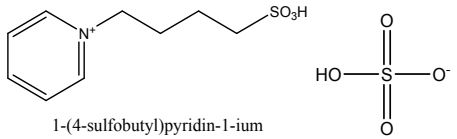


bis[3-$(CH_2)_3SO_3H$-1-$(CH_2)_2$-Im][HSO_4]$_2$.



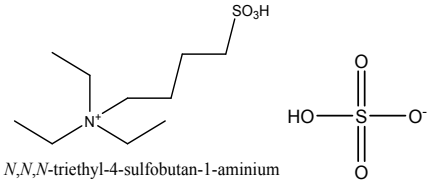
1-methyl-3-(4-sulfobutyl)-1*H*-imidazol-3-ium

[Mim$N(CH_2)_4SO_3H$][HSO_4]



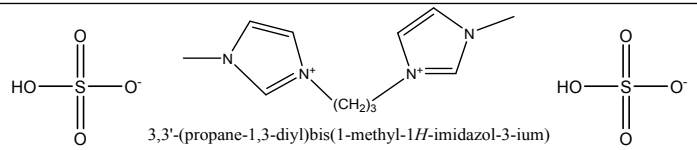
1-(4-sulfobutyl)pyridin-1-ium

[Py$N(CH_2)_4SO_3H$][HSO_4]



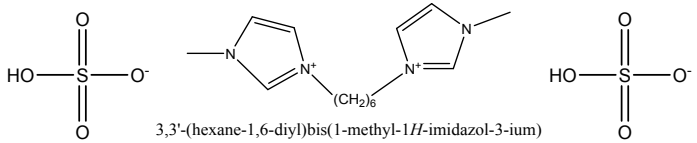
N,*N*,*N*-triethyl-4-sulfobutan-1-aminium

[$(CH_3CH_2)_3N(CH2)_4SO_3H$] [$HSO_4$]



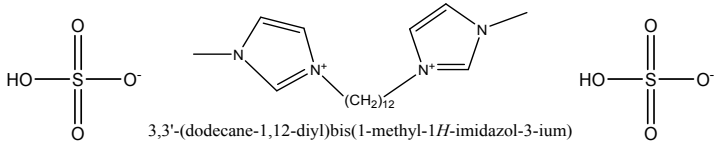
3,3'-(propane-1,3-diyl)bis(1-methyl-1*H*-imidazol-3-ium)

$[C_3(Mim)_2]\ [HSO_4]_2$



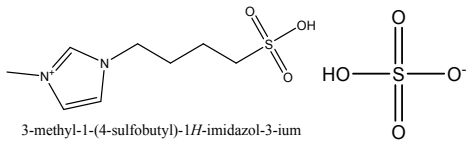
3,3'-(hexane-1,6-diyl)bis(1-methyl-1*H*-imidazol-3-ium)

$[C_6(Mim)_2]\ [HSO_4]_2$



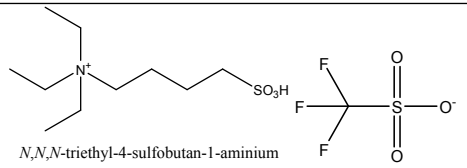
3,3'-(dodecane-1,12-diyl)bis(1-methyl-1*H*-imidazol-3-ium)

$[C_{12}(Mim)_2]\ [HSO_4]_2$



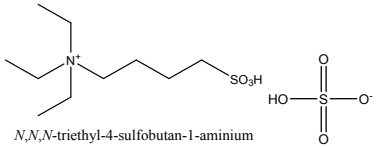
3-methyl-1-(4-sulfobutyl)-1*H*-imidazol-3-ium

1-sulfobutyl-3-methylimidazolium hydrosulfate ($[BHSO_3MIM][HSO_4]$)



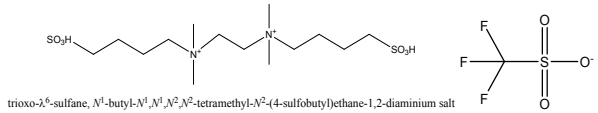
N,*N*,*N*-triethyl-4-sulfobutan-1-aminium

[TEABS][CF_3SO_3]



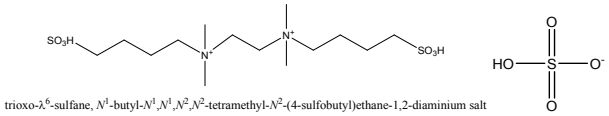
N,*N*,*N*-triethyl-4-sulfobutan-1-aminium

[TEABS] [HSO_4]



trioxo-λ^6-sulfane, N^1-butyl-N^1,N^1,N^2,N^2-tetramethyl-N^2-(4-sulfobutyl)ethane-1,2-diaminium salt

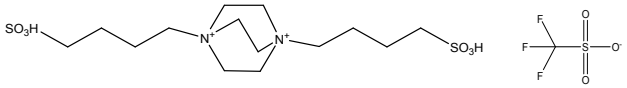
[TMEDADBS][CF_3SO_3]



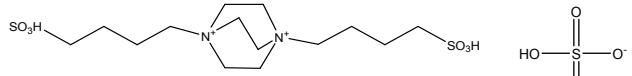
trioxo-λ^6-sulfane, N^1-butyl-N^1,N^1,N^2,N^2-tetramethyl-N^2-(4-sulfobutyl)ethane-1,2-diaminium salt

[TMEDADBS] [HSO_4]

1,4-bis(4-sulfobutyl)-1,4-diazabicyclo[2.2.2]octane-1,4-diium

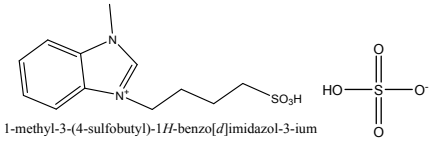


[DABCODBS] [CF_3SO_3]



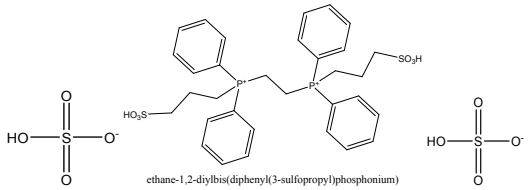
trioxo-λ^6-sulfane, 1-butyl-4-(4-sulfobutyl)-1,4-diazabicyclo[2.2.2]octane-1,4-diium salt

[DABCODBS] [HSO_4]



1-methyl-3-(4-sulfobutyl)-1*H*-benzo[*d*]imidazol-3-ium

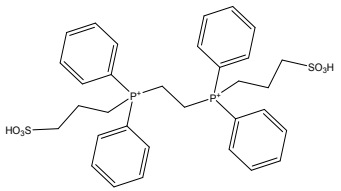
[BSMBIM][HSO_4]



ethane-1,2-diylbis(diphenyl(3-sulfopropyl)phosphonium)

[DPhPE-PS][HSO_4]$_2$

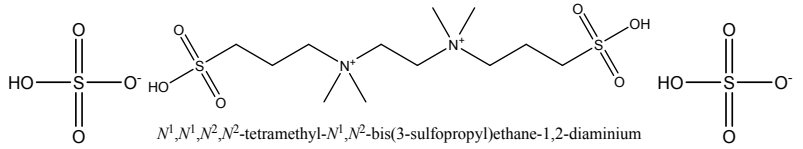
$H_2[PW_{12}0_{40}]^-$



ethane-1,2-diylbis(diphenyl(3-sulfopropyl)phosphonium)

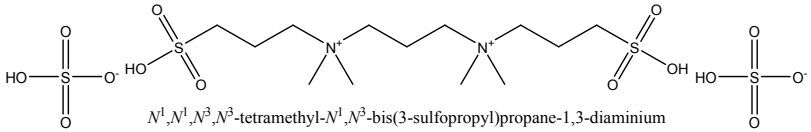
$H_2[PW_{12}0_{40}]^-$

[DPhPE-PS][$PW_{12}O_{40}$]$_2$.



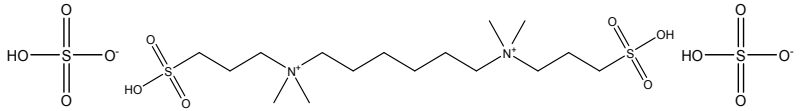
N^1,*N*^{1},*N*^{2},*N*^{2}-tetramethyl-*N*^{1},*N*^{2}-bis(3-sulfopropyl)ethane-1,2-diaminium

$([TMEDAPS][HSO_4])_2$

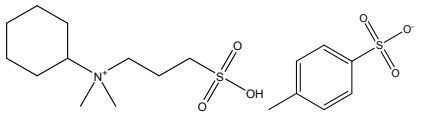


N^1,*N*^{1},*N*^{3},*N*^{3}-tetramethyl-*N*^{1},*N*^{3}-bis(3-sulfopropyl)propane-1,3-diaminium

$[TMPDAPS][HSO_4]_2$

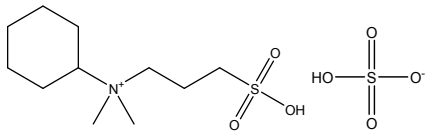


$[TMHDAPS][HSO_4]_2$



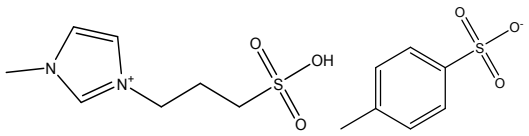
N,*N*-dimethyl-*N*-(3-sulfopropyl)cyclohexanaminium tosylate

$[Ps\text{-}N\text{-}Ch(Me)_2][p\text{-}TSA]$



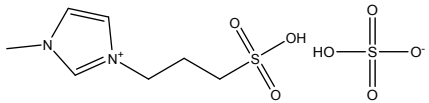
N,*N*-dimethyl-*N*-(3-sulfopropyl)cyclohexanaminium hydrogen sulfate

[Ps-N-Ch(Me)$_2$][HSO$_4$]



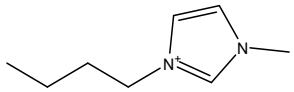
1-methyl-3-(3-sulfopropyl)-1*H*-imidazol-3-ium tosylate

[Ps-mim][p-TSA]



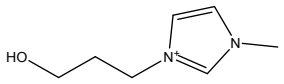
1-methyl-3-(3-sulfopropyl)-1*H*-imidazol-3-ium hydrogen sulfate

[Ps-mim][HSO$_4$]



OH^-
Hydroxide

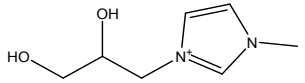
[BMIM][OH]



3-(3-hydroxypropyl)-1-methyl-1*H*-imidazol-3-ium

OH^-
Hydroxide

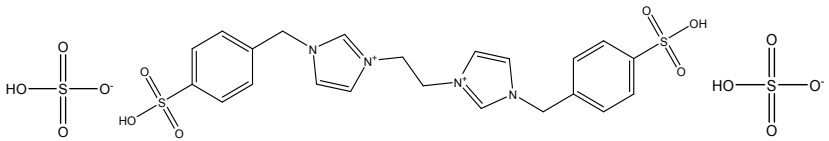
[HPMIM][OH]



3-(2,3-dihydroxypropyl)-1-methyl-1*H*-imidazol-3-ium

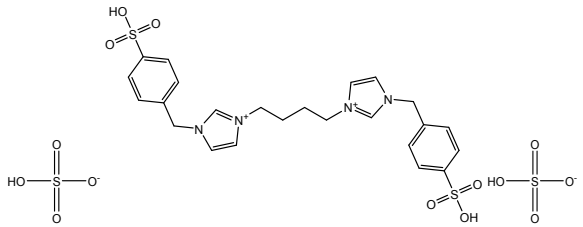
Hydroxide

[GLYMIM][OH]



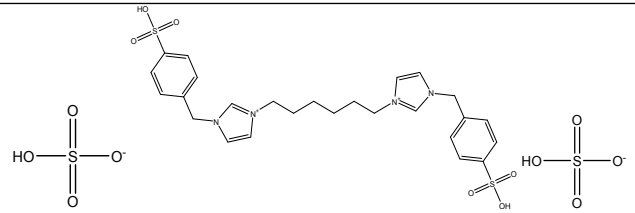
1-(4-sulfobenzyl)-3-(2-(1-(4-sulfobenzyl)-1*H*-imidazol-3-ium-3-yl)ethyl)-1*H*-imidazol-3-ium

[SSIEI][HSO_4]$_2$



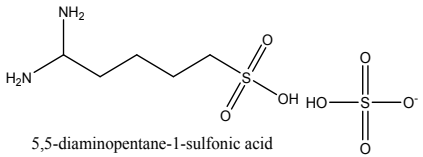
1-(4-sulfobenzyl)-3-(4-(1-(4-sulfobenzyl)-1H-imidazol-3-ium-3-yl)butyl)-1H-imidazol-3-ium

[SSIBI][HSO_4]$_2$

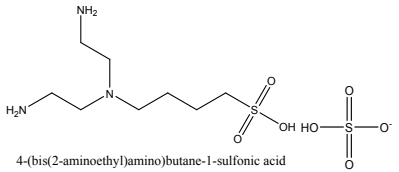


1-(4-sulfobenzyl)-3-(6-(1-(4-sulfobenzyl)-1*H*-imidazol-3-ium-3-yl)hexyl)-1*H*-imidazol-3-ium

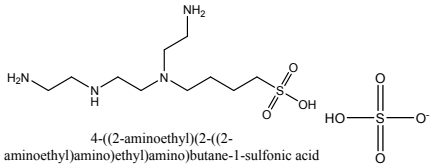
[SSIHI][HSO_4]$_2$



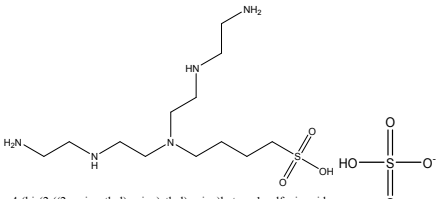
[EDA-PS][HSO_4] EDA-PS =Ethylenediamine-1,3-Propanesultone



[DETA-PS][HSO_4] DETA-PS= diethylenetriamine-1,3-Propanesultone

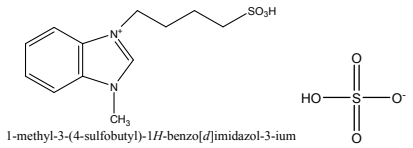


[TETA-PS][HSO_4] TETA-PS = triethylenetetramine-1,3-Propanesultone



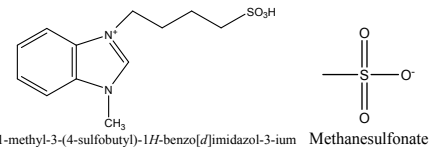
4-(bis(2-((2-aminoethyl)amino)ethyl)amino)butane-1-sulfonic acid

[TEPA-PS][HSO_4] TEPA-PS = tetraethylenepentamine-1,3-Propanesultone



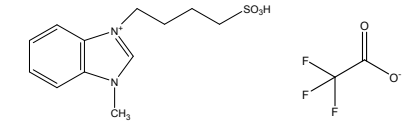
1-methyl-3-(4-sulfobutyl)-1*H*-benzo[*d*]imidazol-3-ium

[BSMBIM][HSO_4]



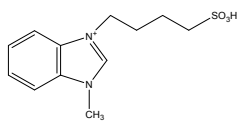
1-methyl-3-(4-sulfobutyl)-1*H*-benzo[*d*]imidazol-3-ium Methanesulfonate

[BSMBIM][CH_3SO_3] methanesulfonate = [CH_3SO_3]

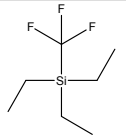


1-methyl-3-(4-sulfobutyl)-1*H*-benzo[*d*]imidazol-3-ium Trifluoroacetate

[BSMBIM][CF_3CO_2] trifluoroacetate = [CF_3CO_2]



1-methyl-3-(4-sulfobutyl)-1*H*-benzo[*d*]imidazol-3-ium



Triethylsilyl trifluoromethane

[BSMBIM][CF_3SO_3]

Table S4. Areas below the sigma profile curve of ILs (CA) calculated in Jupyter Notebook.

IL	A1CA	A2CA	A3CA	A4CA	A5CA
[Arginine][NO_3]$_2$	1.91403	5.35077	6.38800	7.30867	1.41763
[Proline][NO_3]	2.68867	4.61500	10.69067	8.25293	1.41763
[Phenylalanine][NO_3]	2.86317	3.78493	4.67783	7.43087	1.41763
[Alanine][NO_3]	4.79848	7.67457	5.14263	7.25370	1.41763
[Histidine][NO_3]$_2$	2.75044	5.00047	3.72377	8.20347	1.43080
[Serine][NO_3]	1.68778	5.26487	5.63150	10.21493	1.43413
[Glutamic_acid][NO_3]	3.57436	4.26997	4.67513	9.37917	1.41763
[Aspartic_acid][NO_3]	1.14028	14.11253	9.38610	17.01333	0.31623
[Im(N(CH_2)$_3$$SO_3$H)2][$HSO_4$]	0.41217	7.72693	15.98860	12.82367	0.31623
[(CH_3CH_2)$_3$N(CH2)$_4$$SO_3$H][$HSO_4$]	0.65036	10.82817	10.11237	12.63957	0.31623
[PyN(CH_2)$_4$$SO_3$H][$HSO_4$]	0.65018	10.29423	11.23657	12.66180	0.31623
[MimN(CH_2)$_4$$SO_3$H][$HSO_4$]	1.04715	21.08860	16.77930	16.95403	0.31623

bis[3-$(CH_2)_3SO_3H$-1-$(CH_2)_2$-Im][HSO_4]$_2$	0.15777	15.98323	12.05037	8.00050	0.31623
[C_3(Mim)$_2$][HSO_4]$_2$	0.15777	13.62060	20.31647	8.00050	0.31623
[C_6(Mim)$_2$][HSO_4]$_2$	0.15777	13.39123	32.46940	8.04700	0.31623
[C_{12}(Mim)$_2$] [HSO_4]$_2$	0.42353	9.59947	18.88477	11.29710	0.04050
[TEABS][CF_3SO_3]	0.58129	10.30013	13.55080	12.55473	0.31623
[TEABS][HSO_4]	1.01224	22.66407	10.25717	17.09537	0.31623
[TMEDADBS][CF_3SO_3]$_2$	0.85337	22.30667	12.69297	15.79033	0.04050
[DABCODBS][CF_3SO_3]$_2$	1.01224	22.66407	10.25717	17.09537	0.31623
[TMEDADBS][HSO_4]$_2$	1.01224	22.66407	10.25717	17.09537	0.31623
[DABCODBS][HSO_4]$_2$	0.49259	10.74393	19.30963	10.57007	2.26057
[Ps-N-Ch(Me)$_2$][p-TSA]	0.44582	11.02073	17.84107	10.39760	2.26057
[Ps-mim][p-TSA]	0.61328	10.25787	13.89170	12.42667	0.31623
[Ps-N-Ch(Me)$_2$][HSO_4]	0.60358	11.10497	8.64380	12.46710	0.31623
[Ps-mim][HSO_4]	0.49990	10.67270	19.66273	11.48353	0.04050

[BSMBIM][CF_3SO_3]	0.49990	11.39247	16.66210	8.52663	3.27180
[BSMBIM][CH_3SO_3]	0.65767	11.37337	14.32877	12.74117	0.31623
[BSMBIM][HSO_4]	0.49990	10.65793	18.03623	9.32987	1.98310
[BSMBIM][CF_3CO_2]	0.00000	6.16720	41.55643	3.00500	3.06877
[C_{18}MIM][Br]	0.00000	6.25213	37.67797	2.96753	3.06877
[C_{16}MIM][Br]	0.00000	6.62027	9.59160	2.79410	3.06877
[EMIM][Br]	0.00000	7.00960	16.92893	3.78627	3.27180
[BMIM][CH3SO3]	0.00000	6.27507	13.94783	0.02857	5.25273
[BMIM][Cl]	0.00000	7.35480	12.57270	3.78597	3.27180
[EMIM][CH_3SO_3]	0.00000	7.91390	38.91650	4.05227	5.12089
[N_{4444}][L-arg]	0.00000	11.74613	13.40330	4.05090	5.12089
[N_{1111}][L-arg]	0.02953	12.49020	13.99383	5.02620	5.14729
[Choline][L-arg]	0.07909	9.66263	5.39323	1.76768	2.21293
[Choline][OH]	0.02953	8.95540	7.96450	5.65040	2.52282
[Choline][Imidazolium]	0.02953	8.94680	6.84827	3.25170	1.30164

[Choline][methoxide]	0.00000	6.27707	17.91457	9.05437	0.00000
[HMIM][BF_4]	0.00000	6.27507	13.97253	9.03260	0.00000
[BMIM][BF_4]	0.15777	6.99250	18.53763	8.02257	0.31623
[HMIM][HSO_4]	0.15777	6.99050	14.59560	8.00080	0.31623
[BMIM][HSO_4]	0.09395	7.85477	18.72040	4.00480	3.76377
[HMIM][H_2PO_4]	0.15777	6.99050	14.59560	8.00080	0.31623
[BMIM][H_2PO_4]	1.21963	21.91250	7.32127	16.70727	0.31623
([TMEDAPS][HSO_4])$_2$	1.25243	21.17733	16.09240	16.78023	0.31623
TMHDAPS][HSO_4]$_2$	1.26445	22.72247	8.46960	16.86123	0.31623
[TMPDAPS][HSO_4]$_2$	0.00000	6.27507	13.94783	0.02857	5.25273
[BMIM][Cl]	0.15777	8.13640	10.57343	8.29873	0.31623
[AMIM][OH]	0.04957	7.33610	9.82183	0.79238	2.18653
[EMIM][OH]	0.04957	6.99090	14.17807	0.79268	2.18653
[BMIM][OH]	0.04957	6.99290	18.12010	0.81444	2.18653
[HMIM][OH]	0.04957	6.99090	14.17807	0.79268	2.18653

[BMIM][OH]	0.05536	8.54630	10.25940	1.87361	2.53863
[HPMIM][OH]	0.11243	9.53000	8.76503	2.57628	2.47900
[GLYMIM][OH]	0.00000	9.62683	21.43907	4.05090	5.12089
$[N_{2222}]$[L-Arginine]	0.00000	6.28367	16.74933	4.67540	2.49642
[BMIM][Imidazolium]	0.15777	6.99050	14.59560	8.00080	0.31623
[BMIM][HSO_4]	0.99703	6.46917	11.16000	8.86453	0.31713
[BIM][HSO_4]	1.09375	7.10020	4.69820	8.86013	0.31687

Table S5. Areas below the sigma profile curve of ILs calculated in Jupyter Notebook.

IL	A1C	A2C	A3C	A4C	A5C	A1A	A2A	A3A	A4A	A5A
[Arginine][NO_3]$_2$	1.91403	5.35077	5.76090	1.71860	0.00000	0.00000	0.00000	0.62710	5.59007	1.41763
[Proline][NO_3]	2.68867	4.61500	10.06357	2.66287	0.00000	0.00000	0.00000	0.62710	5.59007	1.41763
[Phenylalanine][NO_3]	2.86317	3.78493	4.05073	1.84080	0.00000	0.00000	0.00000	0.62710	5.59007	1.41763
[Alanine][NO_3]	4.79848	7.67457	4.51553	1.66363	0.00000	0.00000	0.00000	0.62710	5.59007	1.41763
[Histidine][NO_3]$_2$	2.75044	5.00047	3.09667	2.61340	0.01317	0.00000	0.00000	0.62710	5.59007	1.41763
[Serine][NO_3]	1.68778	5.26487	5.00440	4.62487	0.01650	0.00000	0.00000	0.62710	5.59007	1.41763
[Glutamic_acid][NO_3]	3.57436	4.26997	4.04803	3.78910	0.00000	0.00000	0.00000	0.62710	5.59007	1.41763
[Aspartic_acid][NO_3]	0.98252	13.39710	8.73833	9.01283	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[Im(N(CH_2)$_3$$SO_3$H)2][$HSO_4$]	0.25440	7.01150	15.34083	4.82317	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[(CH_3CH_2)$_3$N(CH2)$_4$$SO_3$H][$HSO_4$]	0.49259	10.11273	9.46460	4.63907	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[PyN(CH_2)$_4$$SO_3$H][$HSO_4$]	0.49242	9.57880	10.58880	4.66130	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[MimN(CH_2)$_4$$SO_3$H][$HSO_4$]	0.88938	20.37317	16.13153	8.95353	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623

bis[3-$(CH_2)_3SO_3H$-1-$(CH_2)_2$-										
Im][HSO_4]$_2$	0.00000	15.26780	11.40260	0.00000	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[C_3(Mim)$_2$][HSO_4]$_2$	0.00000	12.90517	19.66870	0.00000	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[C_6(Mim)$_2$][HSO_4]$_2$	0.00000	12.67580	31.82163	0.04650	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[C_{12}(Mim)$_2$] [HSO_4]$_2$	0.42353	9.58470	12.90303	4.55423	0.00000	0.00000	0.01477	5.98173	6.74287	0.04050
[TEABS][CF_3SO_3]	0.42353	9.58470	12.90303	4.55423	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[TEABS][HSO_4]	0.85448	21.94863	9.60940	9.09487	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[TMEDADBS][CF_3SO_3]$_2$	0.85337	22.29190	6.71123	9.04747	0.00000	0.00000	0.01477	5.98173	6.74287	0.04050
[DABCODBS][CF_3SO_3]$_2$	0.85448	21.94863	9.60940	9.09487	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[TMEDADBS][HSO_4]$_2$	0.85448	21.94863	9.60940	9.09487	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[DABCODBS][HSO_4]$_2$	0.49259	10.11273	9.46460	4.63907	0.00000	0.00000	0.63120	9.84503	5.93100	2.26057
[Ps-N-Ch(Me)$_2$][p-TSA]	0.44582	10.38953	7.99603	4.46660	0.00000	0.00000	0.63120	9.84503	5.93100	2.26057
[Ps-mim][p-TSA]	0.45551	9.54243	13.24393	4.42617	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[Ps-N-Ch(Me)$_2$][HSO_4]	0.44582	10.38953	7.99603	4.46660	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[Ps-mim][HSO_4]	0.49990	10.65793	13.68100	4.74067	0.00000	0.00000	0.01477	5.98173	6.74287	0.04050

[BSMBIM][CF_3SO_3]	0.49990	10.65793	13.68100	4.74067	0.00000	0.00000	0.73453	2.98110	3.78597	3.27180
[BSMBIM][CH_3SO_3]	0.49990	10.65793	13.68100	4.74067	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[BSMBIM][HSO_4]	0.49990	10.65793	13.68100	4.74067	0.00000	0.00000	0.00000	4.35523	4.58920	1.98310
[BSMBIM][CF_3CO_2]	0.00000	6.16720	41.55643	0.21090	0.00000	0.00000	0.00000	0.00000	2.79410	3.06877
[C_{18}MIM][Br]	0.00000	6.25213	37.67797	0.17343	0.00000	0.00000	0.00000	0.00000	2.79410	3.06877
[C_{16}MIM][Br]	0.00000	6.62027	9.59160	0.00000	0.00000	0.00000	0.00000	0.00000	2.79410	3.06877
[EMIM][Br]	0.00000	6.27507	13.94783	0.00030	0.00000	0.00000	0.73453	2.98110	3.78597	3.27180
[BMIM][CH3SO3]	0.00000	6.27507	13.94783	0.00030	0.00000	0.00000	0.00000	0.00000	0.02827	5.25273
[BMIM][Cl]	0.00000	6.62027	9.59160	0.00000	0.00000	0.00000	0.73453	2.98110	3.78597	3.27180
[EMIM][CH_3SO_3]	0.00000	4.37050	30.08567	0.00137	0.00000	0.00000	3.54340	8.83083	4.05090	5.12089
[N_{4444}][L-arg]	0.00000	8.20273	4.57247	0.00000	0.00000	0.00000	3.54340	8.83083	4.05090	5.12089
[N_{1111}][L-arg]	0.02953	8.94680	5.16300	0.97530	0.02640	0.00000	3.54340	8.83083	4.05090	5.12089
[Choline][L-arg]	0.02953	8.94680	5.16300	0.97530	0.02640	0.04957	0.71583	0.23023	0.79238	2.18653
[Choline][OH]	0.02953	8.94680	5.16300	0.97530	0.02640	0.00000	0.00860	2.80150	4.67510	2.49642
[Choline][Imidazolium]	0.02953	8.94680	5.16300	0.97530	0.02640	0.00000	0.00000	1.68527	2.27640	1.27524

[Choline][methoxide]	0.00000	6.27707	17.88987	0.02207	0.00000	0.00000	0.00000	0.02470	9.03230	0.00000
[HMIM][BF_4]	0.00000	6.27507	13.94783	0.00030	0.00000	0.00000	0.00000	0.02470	9.03230	0.00000
[BMIM][BF_4]	0.00000	6.27707	17.88987	0.02207	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[HMIM][HSO_4]	0.00000	6.27507	13.94783	0.00030	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[BMIM][HSO_4]	0.00000	6.27707	17.88987	0.02207	0.00000	0.09395	1.57770	0.83053	3.98273	3.76377
[HMIM][H_2PO_4]	0.00000	6.27507	13.94783	0.00030	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[BMIM][H_2PO_4]	1.06187	21.19707	6.67350	8.70677	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
([TMEDAPS][HSO_4])$_2$	1.09467	20.46190	15.44463	8.77973	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
TMHDAPS][HSO_4]$_2$	1.10668	22.00703	7.82183	8.86073	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[TMPDAPS][HSO_4]$_2$	0.00000	6.27507	13.94783	0.00030	0.00000	0.00000	0.00000	0.00000	0.02827	5.25273
[BMIM][Cl]	0.00000	7.42097	9.92567	0.29823	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[AMIM][OH]	0.00000	6.62027	9.59160	0.00000	0.00000	0.04957	0.71583	0.23023	0.79238	2.18653
[EMIM][OH]	0.00000	6.27507	13.94783	0.00030	0.00000	0.04957	0.71583	0.23023	0.79238	2.18653
[BMIM][OH]	0.00000	6.27707	17.88987	0.02207	0.00000	0.04957	0.71583	0.23023	0.79238	2.18653
[HMIM][OH]	0.00000	6.27507	13.94783	0.00030	0.00000	0.04957	0.71583	0.23023	0.79238	2.18653

[BMIM][OH]	0.00579	7.83047	10.02917	1.08123	0.35210	0.04957	0.71583	0.23023	0.79238	2.18653
[HPMIM][OH]	0.06287	8.81417	8.53480	1.78390	0.29247	0.04957	0.71583	0.23023	0.79238	2.18653
[GLYMIM][OH]	0.00000	6.08343	12.60823	0.00000	0.00000	0.00000	3.54340	8.83083	4.05090	5.12089
$[N_{2222}]$[L-Arginine]	0.00000	6.27507	13.94783	0.00030	0.00000	0.00000	0.00860	2.80150	4.67510	2.49642
[BMIM][Imidazolium]	0.00000	6.27507	13.94783	0.00030	0.00000	0.15777	0.71543	0.64777	8.00050	0.31623
[BMIM][HSO_4]	0.83927	5.75373	10.51223	0.86403	0.00090	0.15777	0.71543	0.64777	8.00050	0.31623
[BIM][HSO_4]	0.93598	6.38477	4.05043	0.85963	0.00063	0.15777	0.71543	0.64777	8.00050	0.31623

Table S6. Variance Inflation Factor.

	VIF	Variable
0	21.670271	Intercept
1	5.162970	EMFC
2	2.098596	EHBC
3	1.829746	EvdWC
4	4.430978	EMFA
5	2.112332	EHBA
6	2.069352	EvdWA

Table S7. Prediction of FAME using the GBR machine learning model.

Ionic liquids	Predicted FAME yield (%)
[Arginine][HSO_4]$_2$	91.2860
[Aspartic_acid][HSO_4]	91.2860
[Glutamic_acid][HSO_4]	92.1301
[Histidine][HSO_4]$_2$	92.0693
[Proline][HSO_4]	84.6421
[Phenylalanine][HSO_4]	92.1301
[Alanine][HSO_4]	92.3325
[Serine][HSO_4]	91.1207
[Arginine][CF3SO3]$_2$	93.5901
[Aspartic_acid][CF3SO3]	93.5901
[Glutamic_acid][CF3SO3]	94.4342
[Histidine][CF_3SO_3]$_2$	94.2318
[Proline][CF3SO3]	87.0083
[Phenylalanine][CF3SO3]	94.4342
[Alanine][CF3SO3]	94.4950
[Serine][CF3SO3]	93.4248
[Arginine][CH_3SO_3]$_2$	93.9230
[Aspartic_acid][CH_3SO_3]	93.9230

[Glutamic_acid][CH_3SO_3]	94.7672
[Histidine][CH_3SO_3]$_2$	94.5648
[Proline][CH_3SO_3]	86.7686
[Phenylalanine][CH3SO3]	94.7672
[Alanine][CH3SO3]	94.8279
[Serine][CH3SO3]	93.7578
[Arginine][H_2PO_4]$_2$	91.6234
[Aspartic_acid][H2PO4]	91.6234
[Glutamic_acid][H2PO4]	92.4676
[Histidine][H2PO4]2	92.4068
[Proline][H2PO4]	84.4070
[Phenylalanine][H2PO4]	92.4676
[Alanine][H2PO4]	92.6700
[Serine][H2PO4]	91.4581
[Arginine][Phosphotungstic_acid]$_2$	93.9230
[Aspartic_acid][Phosphotungstic_acid]	93.9230
[Glutamic_acid][Phosphotungstic_acid]	94.7672
[Histidine][Phosphotungstic_acid]2	94.5648
[Proline][Phosphotungstic_acid]	86.7686
[Phenylalanine][Phosphotungstic_acid]	94.7672
[Alanine][Phosphotungstic_acid]	94.8279

[Serine][Phosphotungstic_acid]	93.7578
[Butyl-diethanol-ammonium][HSO4]	85.4805
[Butyl-diethanol-ammonium][CF3SO3]	89.7568
[Butyl-diethanol-ammonium][CH3SO3]	89.1349
[Butyl-diethanol-ammonium][H2PO4]	84.8631
[Butyl-diethanol-ammonium][Phosphotungstic_acid]	89.1349
[Butyl-diethanol-ammonium][NO3]	83.1340
[Butyl-trimethyl-ammonium][HSO4]	77.0997
[Butyl-trimethyl-ammonium][CF3SO3]	80.0094
[Butyl-trimethyl-ammonium][CH3SO3]	80.6051
[Butyl-trimethyl-ammonium][H2PO4]	77.6999
[Butyl-trimethyl-ammonium][Phosphotungstic_acid]	80.6051
[Butyl-trimethyl-ammonium][NO3]	75.9708
[Diethanolammonium][HSO4]	89.6138
[Diethanolammonium][CF3SO3]	93.2885
[Diethanolammonium][CH3SO3]	92.6666
[Diethanolammonium][H2PO4]	88.9964
[Diethanolammonium][Phosphotungstic_acid]	92.6666
[Diethanolammonium][NO3]	87.2674
[Dimethylethanolammonium][HSO4]	80.2568
[Dimethylethanolammonium][CF3SO3]	86.5161

[Dimethylethanolammonium][CH3SO3]	85.8942
[Dimethylethanolammonium][H2PO4]	79.6395
[Dimethylethanolammonium][Phosphotungstic_acid]	85.8942
[Dimethylethanolammonium][NO3	77.9104
[Heptyltrimethylammonium][HSO4]	77.0997
[Heptyltrimethylammonium][CF3SO3]	80.0094
[Heptyltrimethylammonium][CH3SO3]	80.6051
[Heptyltrimethylammonium][H2PO4]	77.6999
[Heptyltrimethylammonium][Phosphotungstic_acid]	80.6051
[Heptyltrimethylammonium][NO3]	75.9708
[Tetraethylammonium][HSO4]	77.0997
[Tetraethylammonium][CF3SO3]	80.0094
[Tetraethylammonium][CH3SO3]	80.6051
[Tetraethylammonium][H2PO4]	77.6999
[Tetraethylammonium][Phosphotungstic_acid]	80.6051
[Tetraethylammonium][NO3]	75.9708
[Tetramethylammonium][HSO4]	77.0997
[Tetramethylammonium][CF3SO3]	80.0094
[Tetramethylammonium][CH3SO3]	80.6051
[Tetramethylammonium][H2PO4]	77.6999
[Tetramethylammonium][Phosphotungstic_acid]	80.6051

[Tetramethylammonium][NO3]	75.9708
[Tetrabutylammonium][HSO4]	77.0997
[Tetrabutylammonium][CF3SO3]	80.0094
[Tetrabutylammonium][CH3SO3]	80.6051
[Tetrabutylammonium][H2PO4]	77.6999
[Tetrabutylammonium][Phosphotungstic_acid]	80.6051
[Tetrabutylammonium][NO3]	75.9708
[Tetrapropylammonium][HSO4]	77.0997
[Tetrapropylammonium][CF3SO3]	80.0094
[Tetrapropylammonium][CH3SO3]	80.6051
[Tetrapropylammonium][H2PO4]	77.6999
[Tetrapropylammonium][Phosphotungstic_acid]	80.6051
[Tetrapropylammonium][NO3]	75.9708
[Tributylmethylammonium][HSO4]	77.0997
[Tributylmethylammonium][CF3SO3]	80.0094
[Tributylmethylammonium][CH3SO3]	80.6051
[Tributylmethylammonium][H2PO4]	77.6999
[Tributylmethylammonium][Phosphotungstic_acid]	80.6051
[Tributylmethylammonium][NO3]	75.9708
[Triethylheptylammonium][HSO4]	77.0997
[Triethylheptylammonium][CF3SO3]	80.0094

[Triethylheptylammonium][CH3SO3]	80.6051
[Triethylheptylammonium][H2PO4]	77.6999
[Triethylheptylammonium][Phosphotungstic_acid]	80.6051
[Triethylheptylammonium][NO3]	75.9708
[Triethylpentylammonium][HSO4]	77.0997
[Triethylpentylammonium][CF3SO3]	80.0094
[Triethylpentylammonium][CH3SO3]	80.6051
[Triethylpentylammonium][H2PO4]	77.6999
[Triethylpentylammonium][Phosphotungstic_acid]	80.6051
[Triethylpentylammonium][NO3]	75.9708
[Trimethylethylammonium][HSO4]	77.0997
[Trimethylethylammonium][CF3SO3]	80.0094
[Trimethylethylammonium][CH3SO3]	80.6051
[Trimethylethylammonium][H2PO4]	77.6999
[Trimethylethylammonium][Phosphotungstic_acid]	80.6051
[Trimethylethylammonium][NO3]	75.9708
[Butyl-diethanol-ammonium][Arginine]	91.9329
[Butyl-diethanol-ammonium][Aspartic_acid]	89.1349
[Butyl-diethanol-ammonium][Glutamic_acid]	89.1349
[Butyl-diethanol-ammonium][Histidine]	91.9329
[Butyl-diethanol-ammonium][Proline]	89.1349

[Butyl-diethanol-ammonium][Phenylalanine]	89.1349
[Butyl-diethanol-ammonium][Alanine]	89.1349
[Butyl-diethanol-ammonium][Serine]	89.1349
[Butyl-trimethyl-ammonium][Arginine]	86.0035
[Butyl-trimethyl-ammonium][Aspartic_acid]	80.6051
[Butyl-trimethyl-ammonium][Glutamic_acid]	80.6051
[Butyl-trimethyl-ammonium][Histidine]	86.0035
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[Proline][Butanoate]	86.7686
[Phenylalanine][Butanoate]	94.7672
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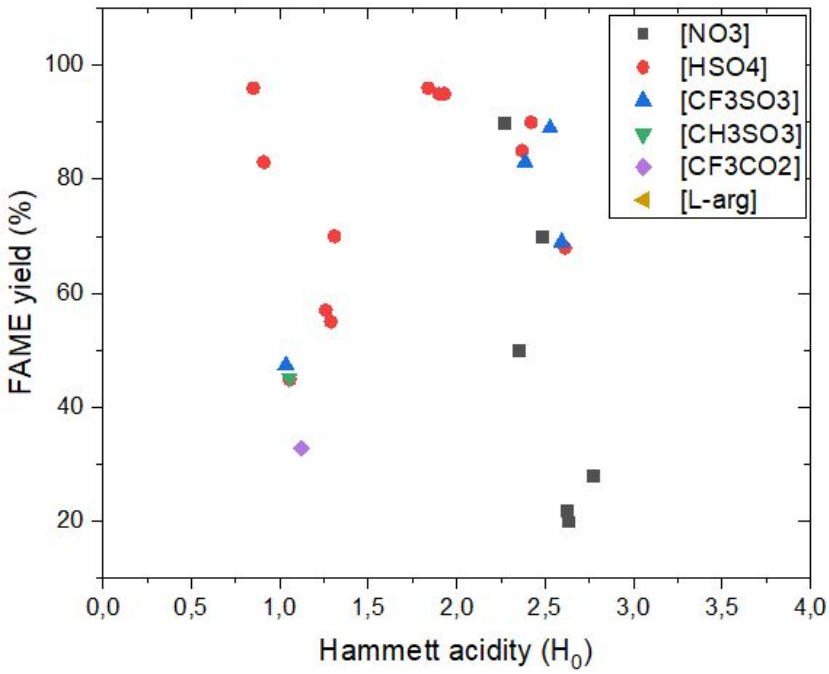


Figure S1. Hammett acidity vs FAME yield: anion analysis.

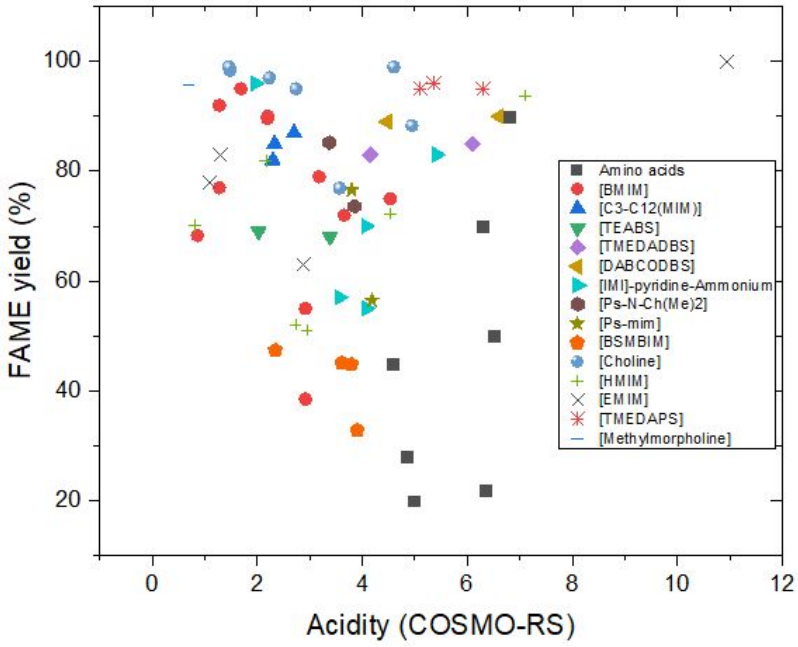


Figure S2. Analysis of cation acidity of ionic liquids vs. FAME yield.

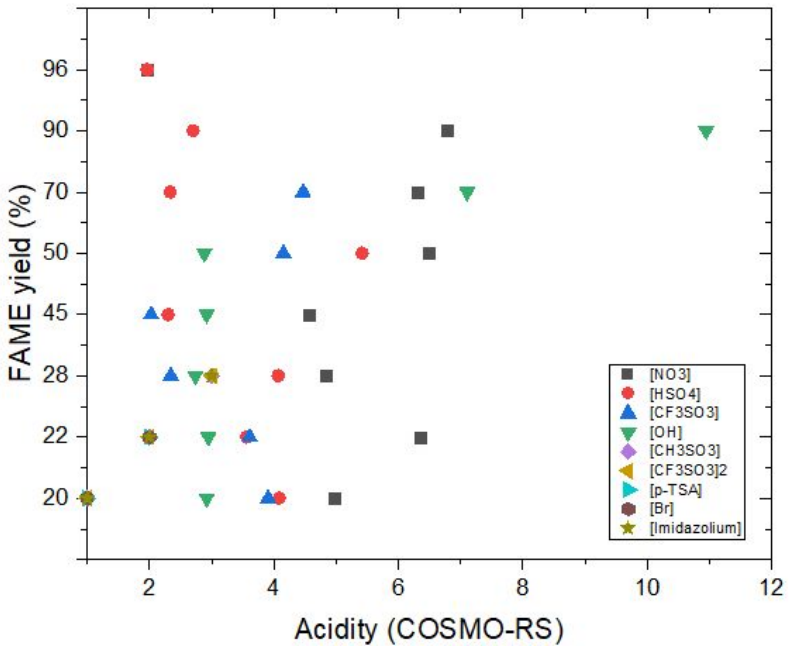


Figure S3. Analysis of anion acidity of ionic liquids vs. yield.

Characterization of ILs

The ^{1}H and ^{13}C nuclear magnetic resonances of the ionic liquids [L-arginine][Acetate], [L-arginine][NO_3], and [L-arginine][HSO_3] are shown in Figures S4, S5, and S6.

The ^{1}H NMR of [L-arginine][Acetate] in D_2O shows: δ: 1.60 (m, 4H, CH_2CH_2); 1.84 (s, 3H, CH_3); 3.16 (t, 4H, CH_2 and NH_2); 3.69 (t, 2H, NH_2). The ^{13}C NMR (D_2O, 75.47 MHz, [ppm]) displays the following peaks: 23.21; 23.79; 27.45; 40.37; 54.16; 156.67; 174.33; 181.30. The IL was obtained as a white solid.

The ^{1}H NMR and ^{13}C NMR spectra of [L-arginine][NO_3] are shown in Figure S5. The IL was obtained as a white solid. The ^{1}H NMR [L-arginine][NO_3] in D_2O shows the following peaks: δ: 1.63 (m, 4H, CH_2CH_2); 1.81 (m, 4H, CH_3); 3.17 (t, 4H, CH_2 and NH_2); 3.66 (t, 2H, NH_2). The ^{13}C NMR (D_2O, 75.47 MHz, [ppm]) shows peaks at 24.07; 28.15; 40.16; 54.36; 156.69; 175.21.

The ^{1}H NMR [L-arginine][HSO_3] in D_2O shows the following peaks: δ: 1.66 (m, 4H, CH_2CH_2); 1.99 (m, 4H, CH_2); 3.21 (t, 4H, NH_2); 4.04 (t, 2H, NH_2). The ^{13}C NMR (D_2O, 75.47 MHz, [ppm]) shows peaks at 23.66; 26.77; 40.03; 52.69; 156.75; 172.24. The IL was obtained as a white solid.

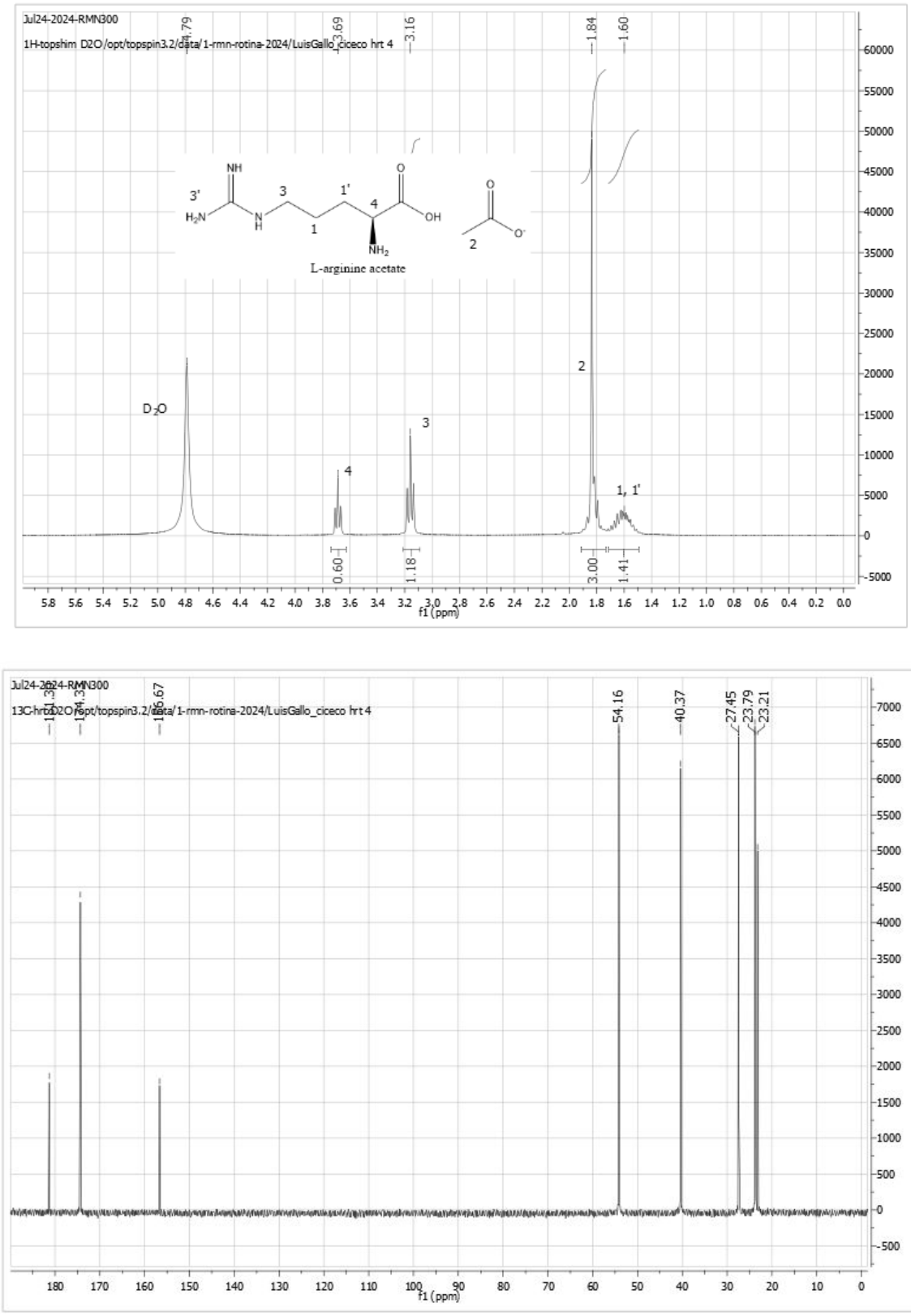
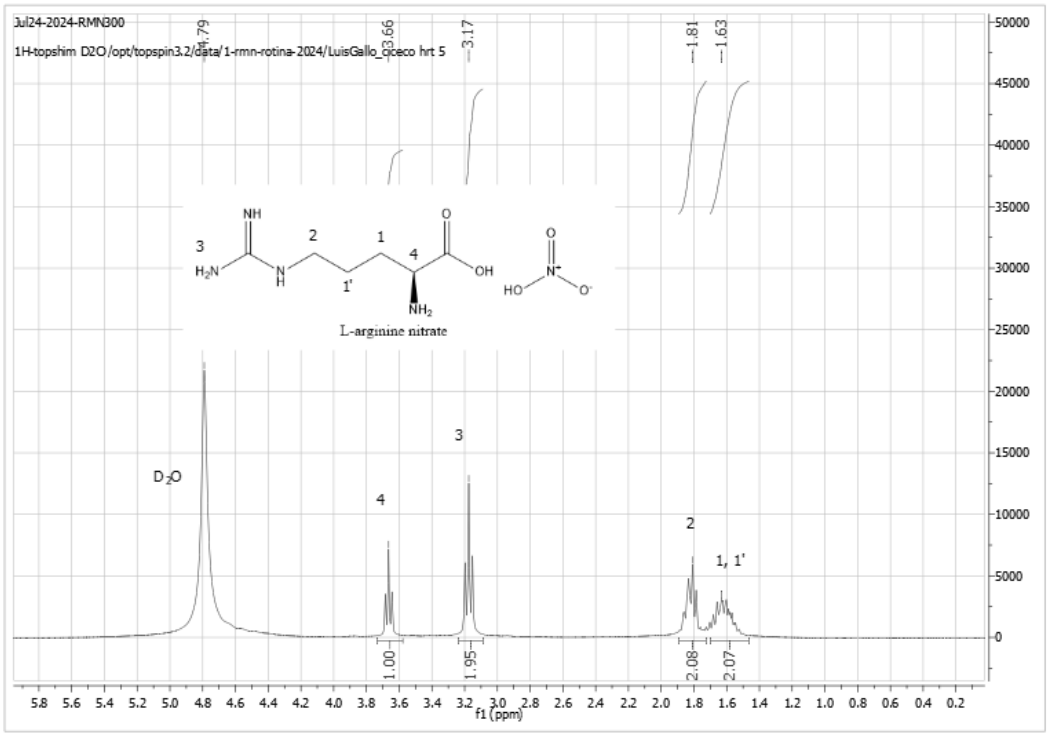


Figure S4. ^{1}H and ^{13}C RMN Ionic liquid [L-arginine][Acetate].



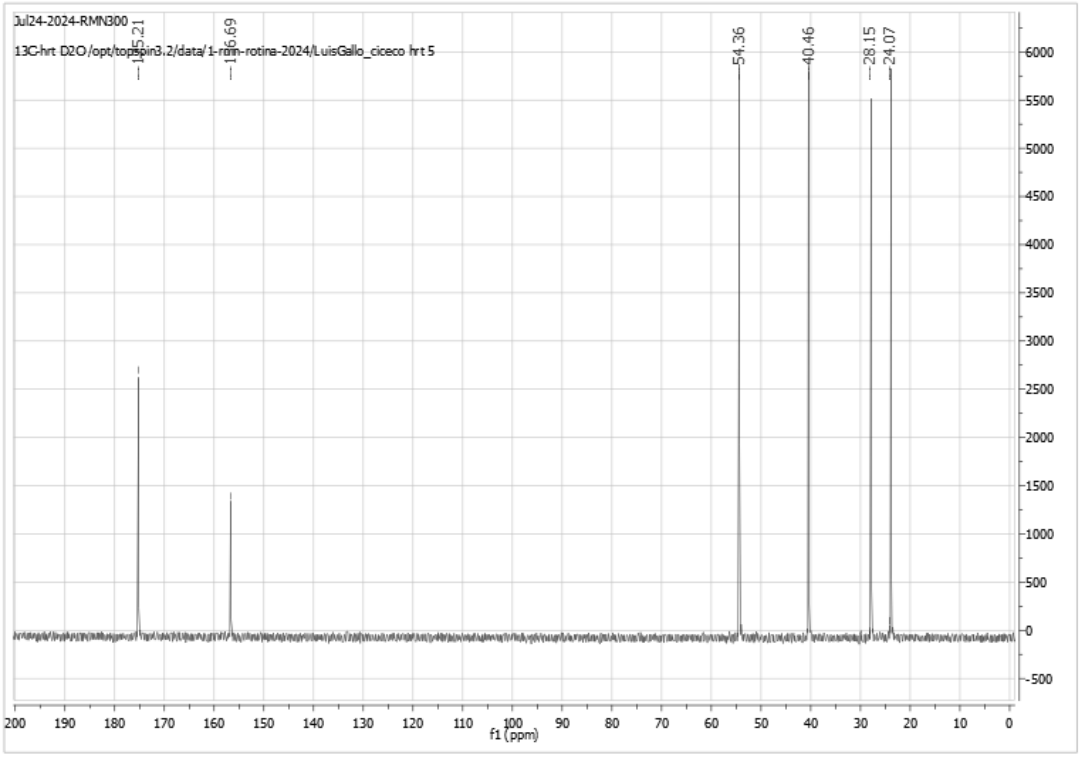
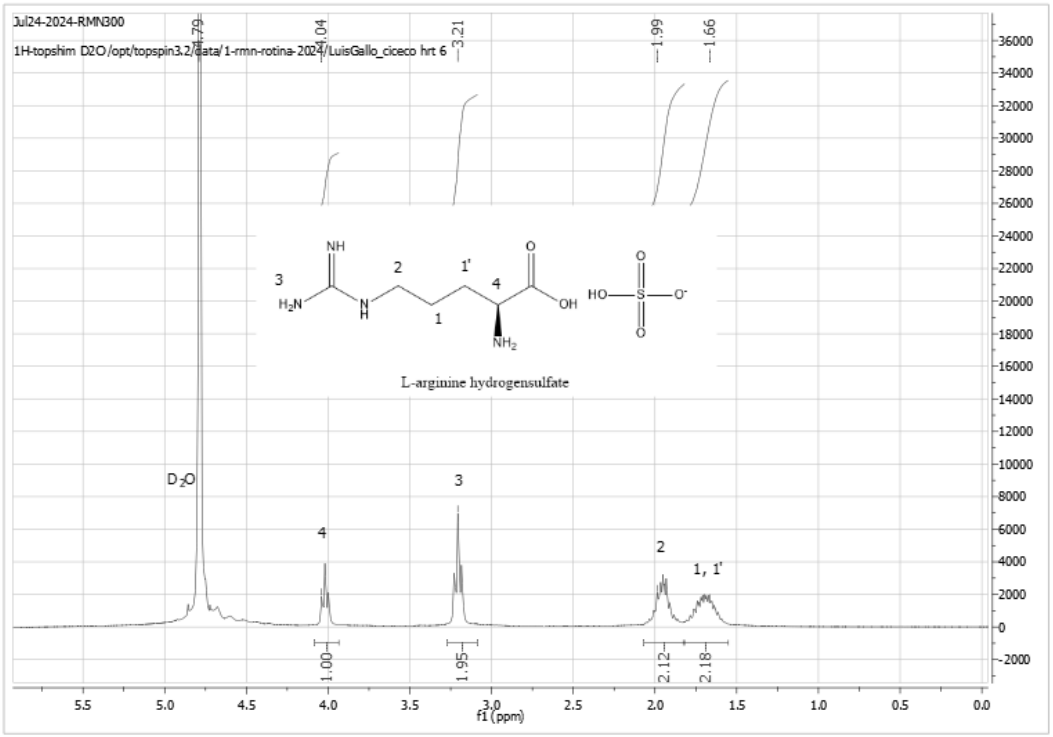


Figure S5. ^{1}H and ^{13}C RMN Ionic liquid [L-arginine][NO_3].



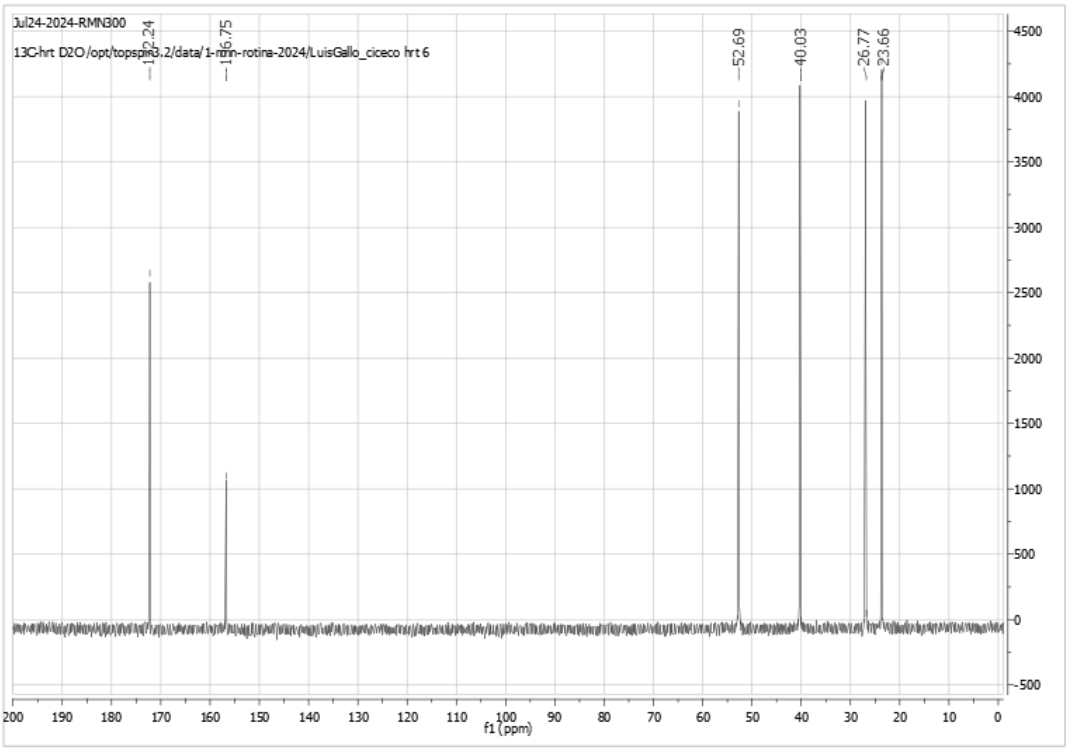


Figure S6. ^{1}H and ^{13}C RMN Ionic liquid [L-arginine][HSO_3].

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