Electronic Supporting Information for

The Polymerisation of Oligo(ethylene glycol methyl ether) Methacrylate from a Multifunctional Poly(ethylene imine) Derived Amide: A Stabiliser for the Synthesis and Dispersion of Magnetite Nanoparticles

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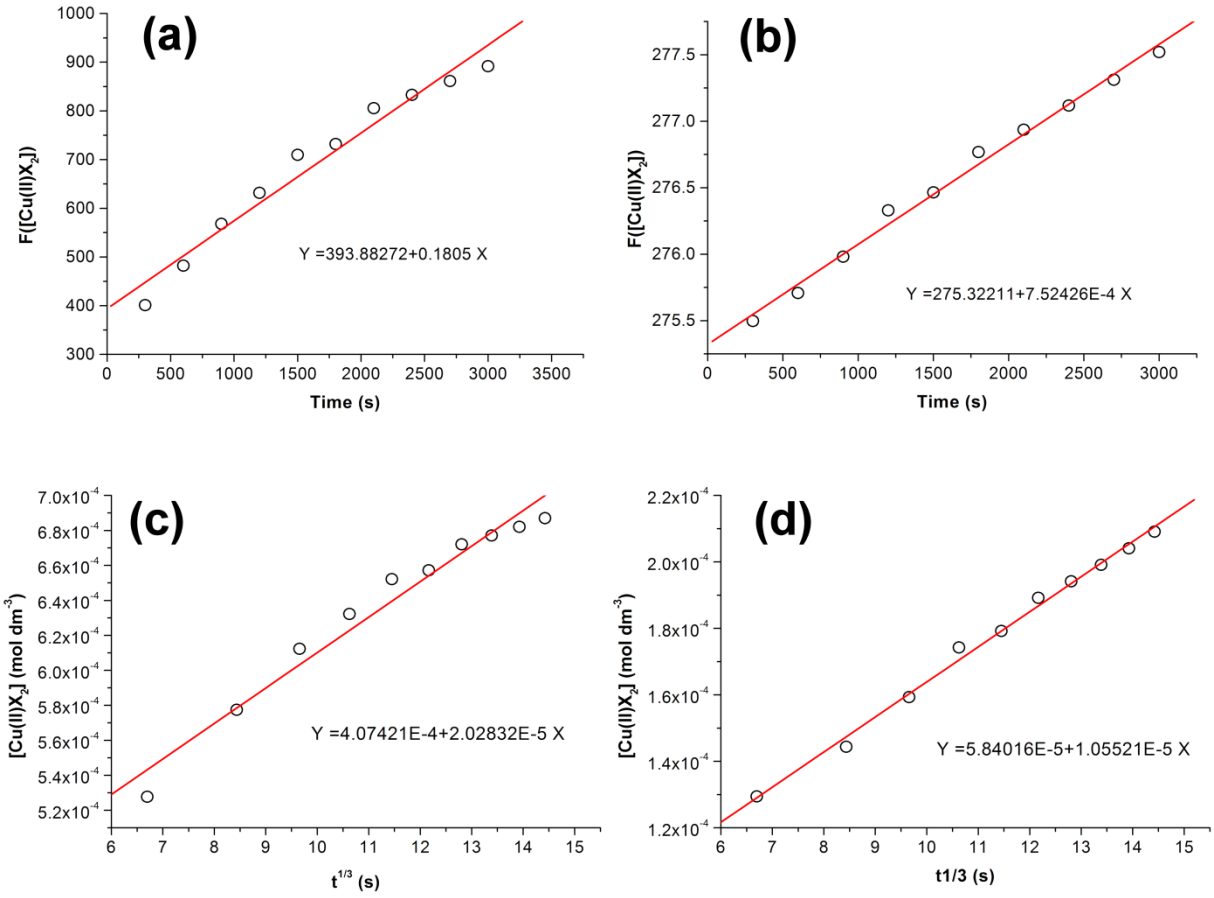

Figure SI 1. (a) and (b) plots of function of Cu(II) concentrations with time for the calculation of K_{ATRP} of MBriP and MBriPA respectively according to Matyjaszewski method; (c) and (d) (a) and (b) plots of Cu(II) concentrations with time for the calculation of K_{ATRP} of MBriP and MBriPA respectively according to Fischer method.

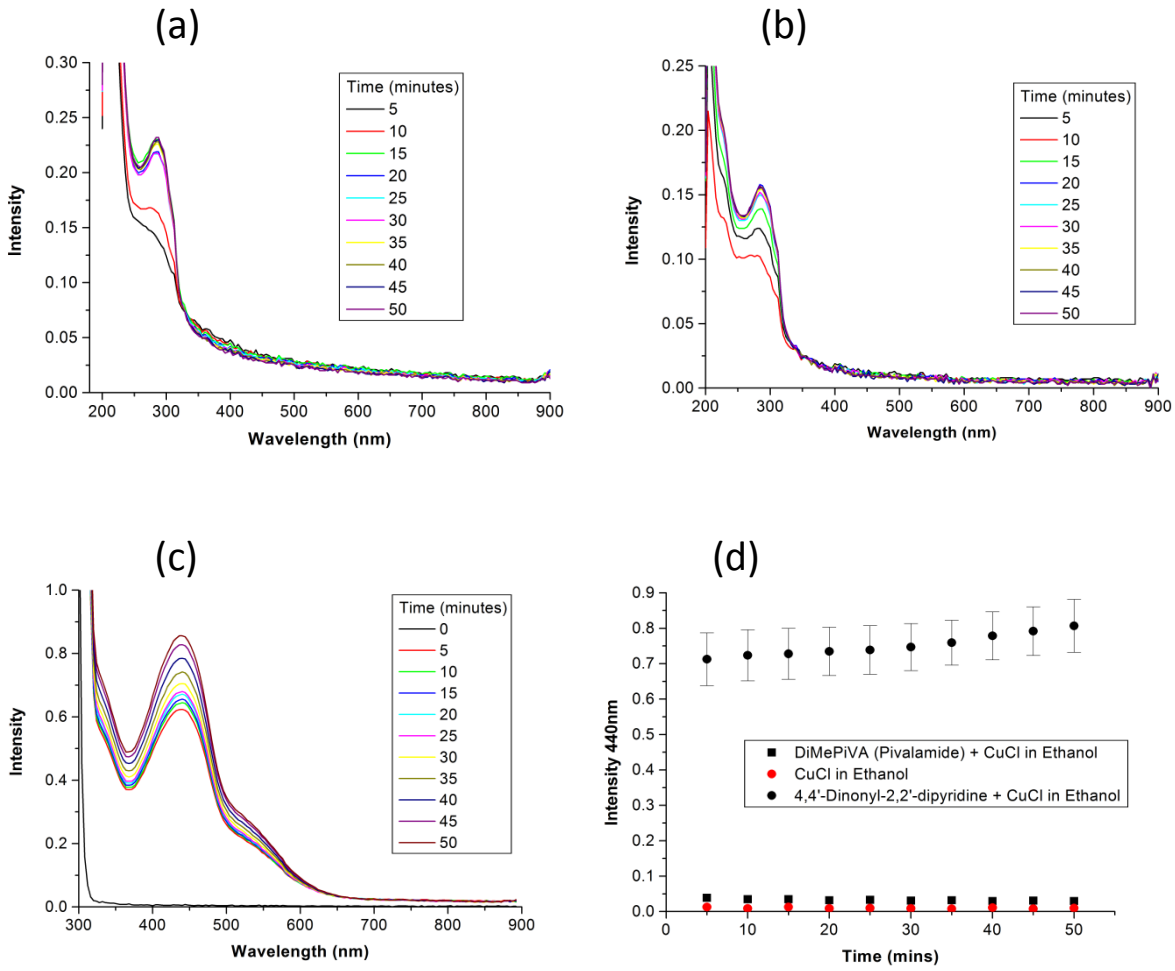

Figure SI 2. UV-vis spectra of (a) Cu(I)Cl in ethanol, (b) DiMePiVA and Cu(I)Cl in ethanol, and (c) Cu(I)Cl and 4,4'-dinonyl-2,2'-dipyridine in ethanol, (d) relative intensities of all 3 solutions at 440 nm. Plots indicate no complexation or solubilisation of Cu(I)Cl as evidenced by the absence of Cu(I) ligand absorption bands.

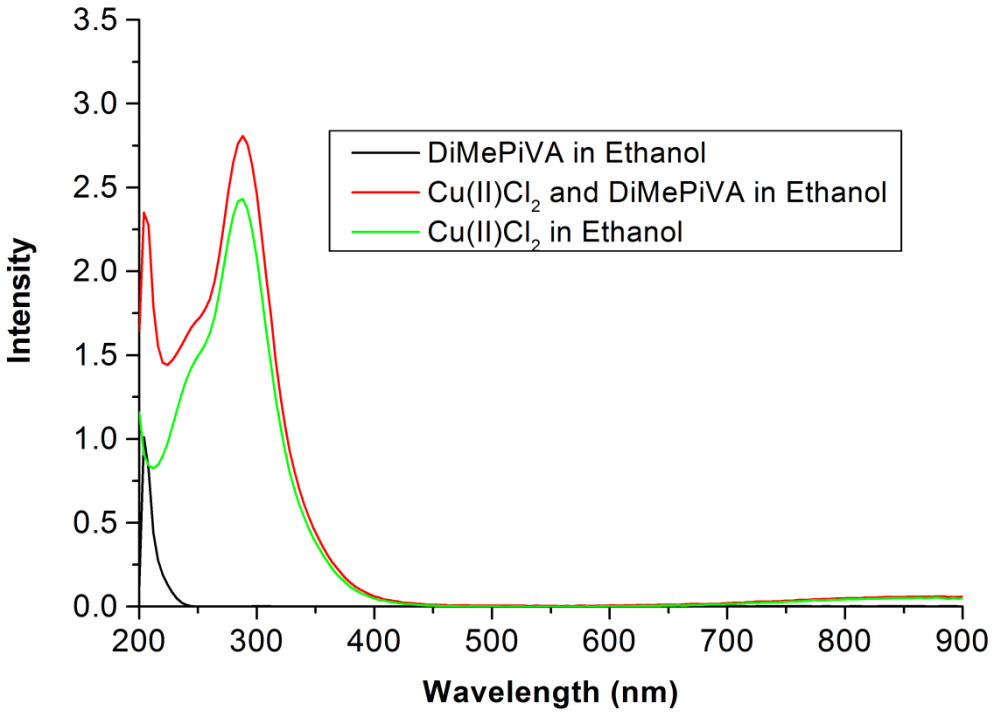

Figure SI 3. UV-vis spectra of DiMePiVA and $Cu(II)Cl_2$ in ethanol. Plots indicate no complexation or solubilisation of $Cu(II)Cl_2$.

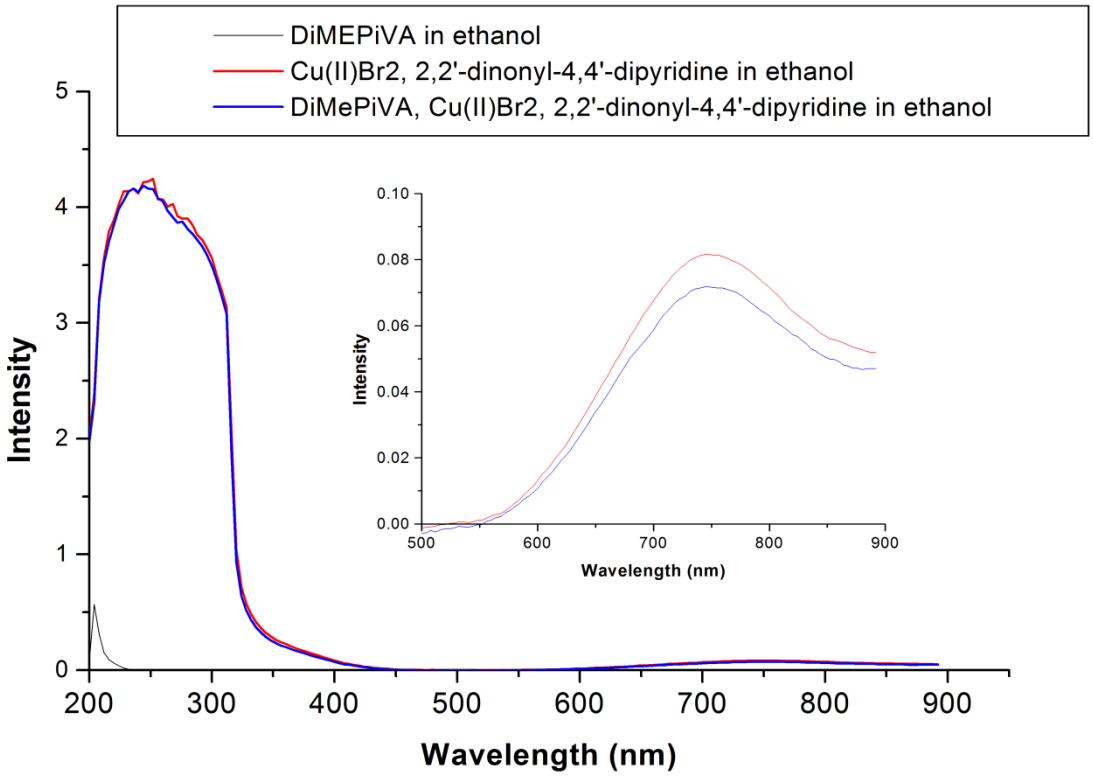

Figure SI 4. UV-vis spectra of DiMePiVA, 2,2'-dinonyl-4,4'-dipyridine and $Cu(II)Br_2$ in ethanol. Plots indicate no complexation or solubilisation of $Cu(II)Br_2$.

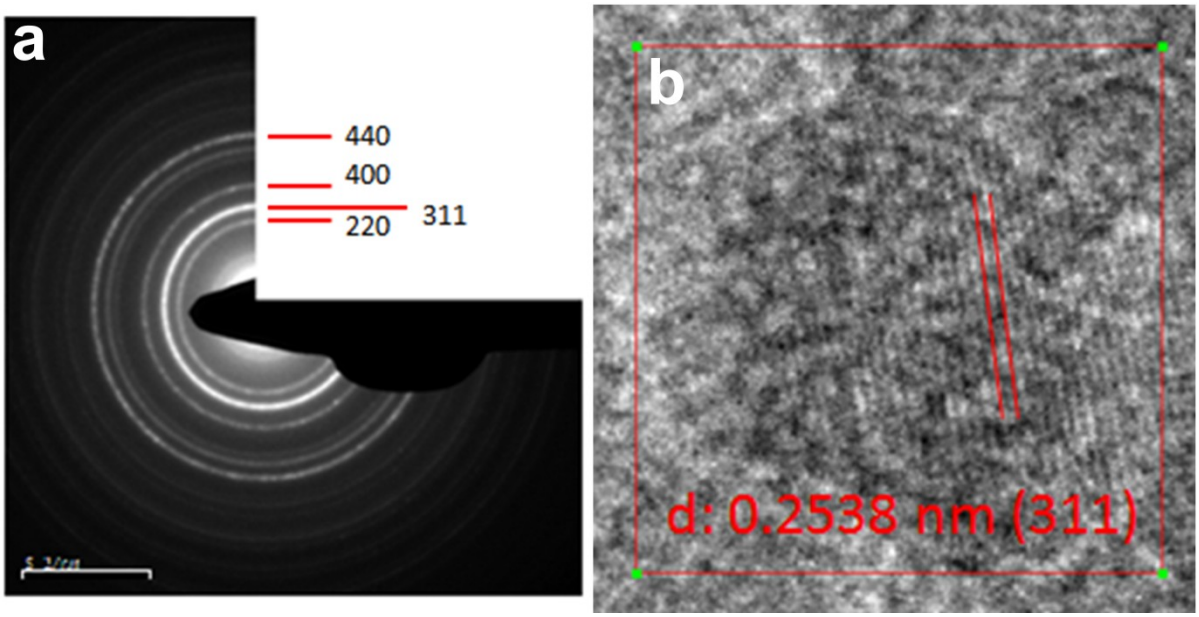

Figure SI 5. (a) X-ray diffraction pattern and (b) high magnification TEM micrograph of PEI-*graft*-POEGMA coated magnetite particles.

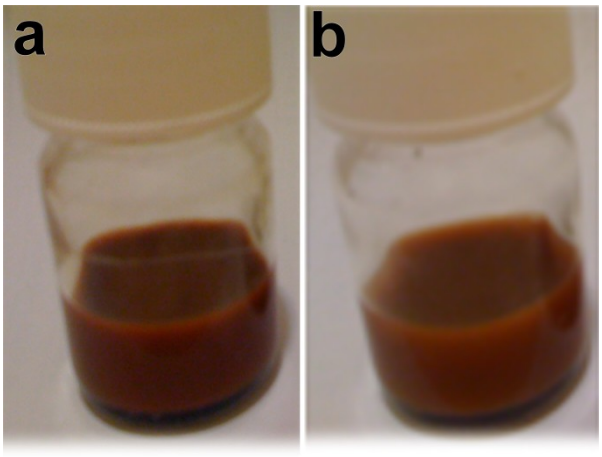

Figure SI 6. (a) Dispersion of PEI-*graft*-POEGMA coated magnetite particles after sonication (b) After 24 hrs.

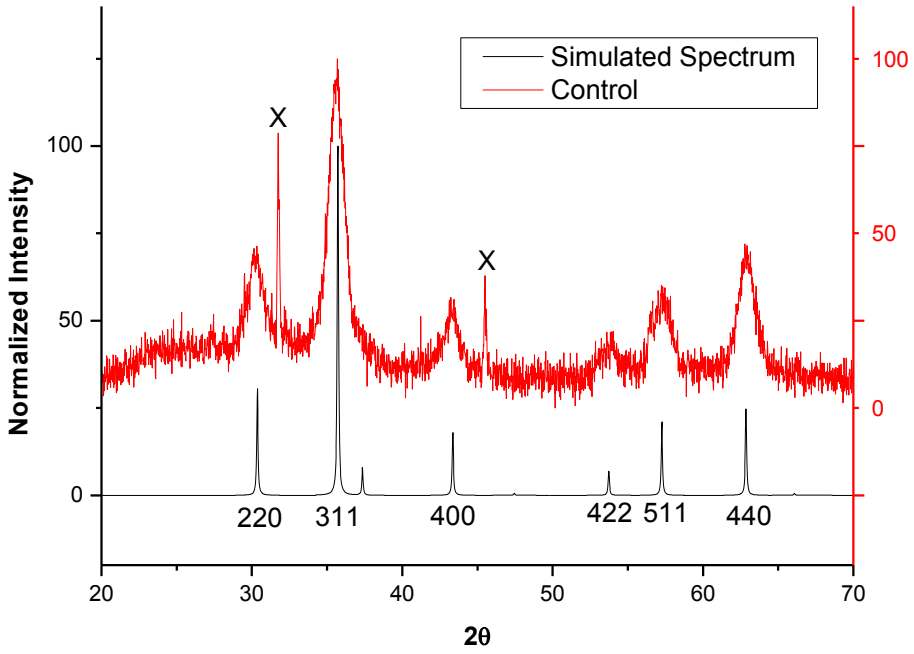

Figure SI 7. X-ray diffraction pattern for bare (no stabiliser) superparamagnetic iron oxide nanoparticles via co-precipitation method (red line) compared simulated pattern of magnetite (black line).

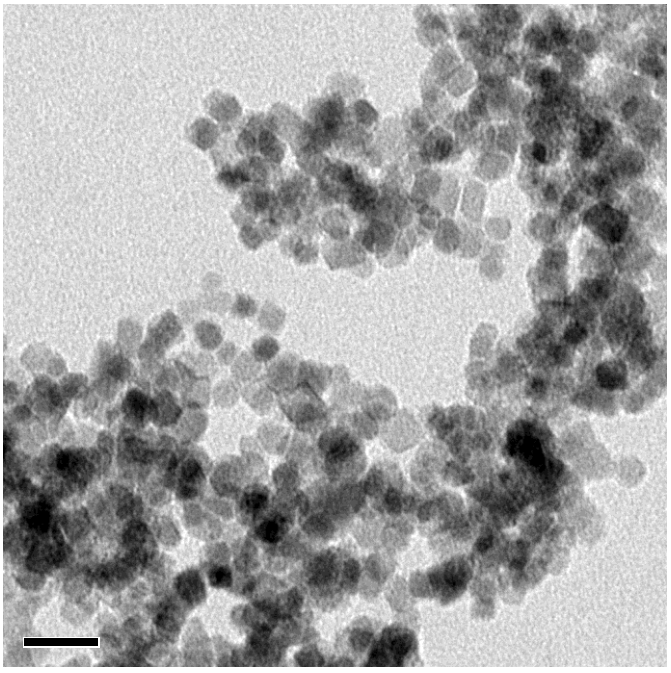

Figure SI 8.TEM micrograph of bare (no stabiliser) superparamagnetic iron oxide nanoparticles via co-precipitation method.

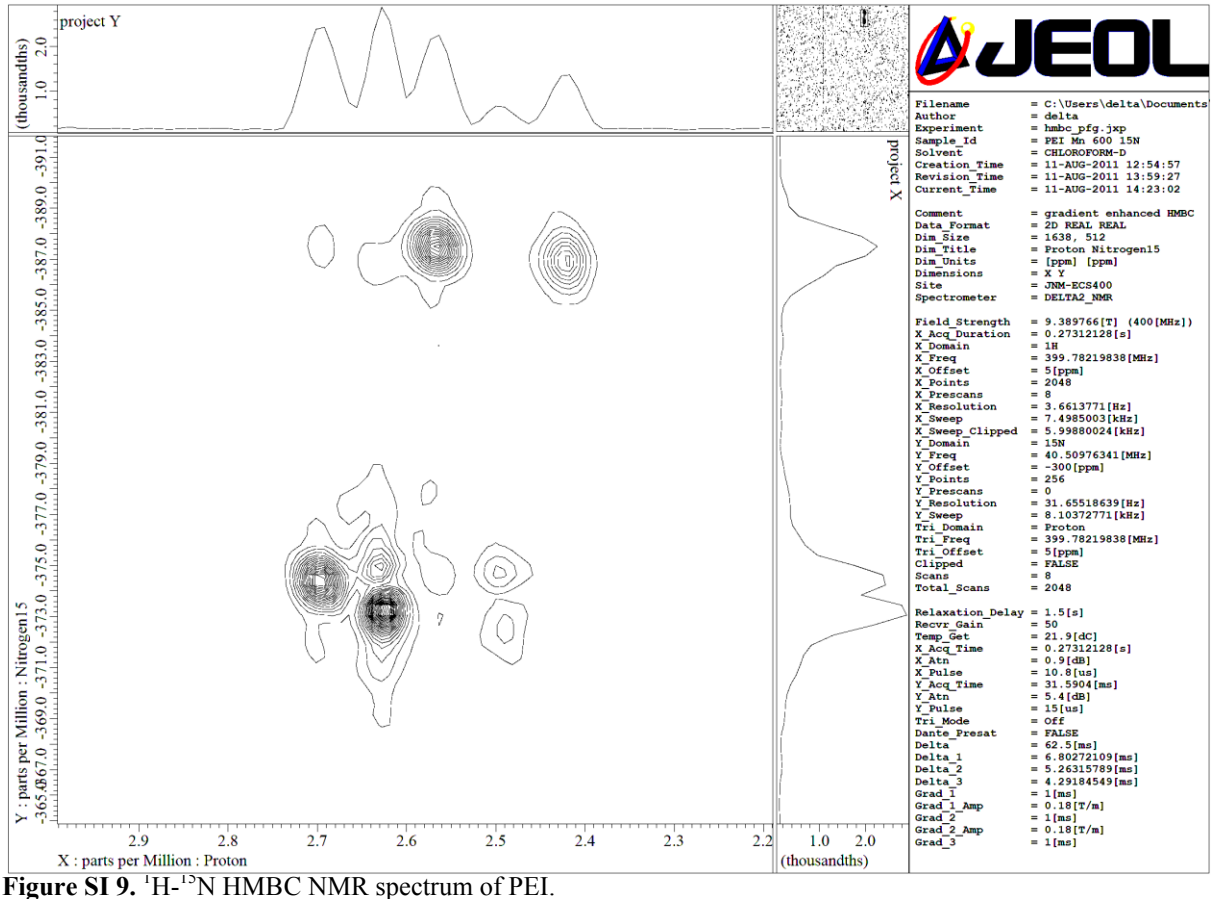

Figure SI 9. ^{1}H-^{15}N HMBC NMR spectrum of PEI.

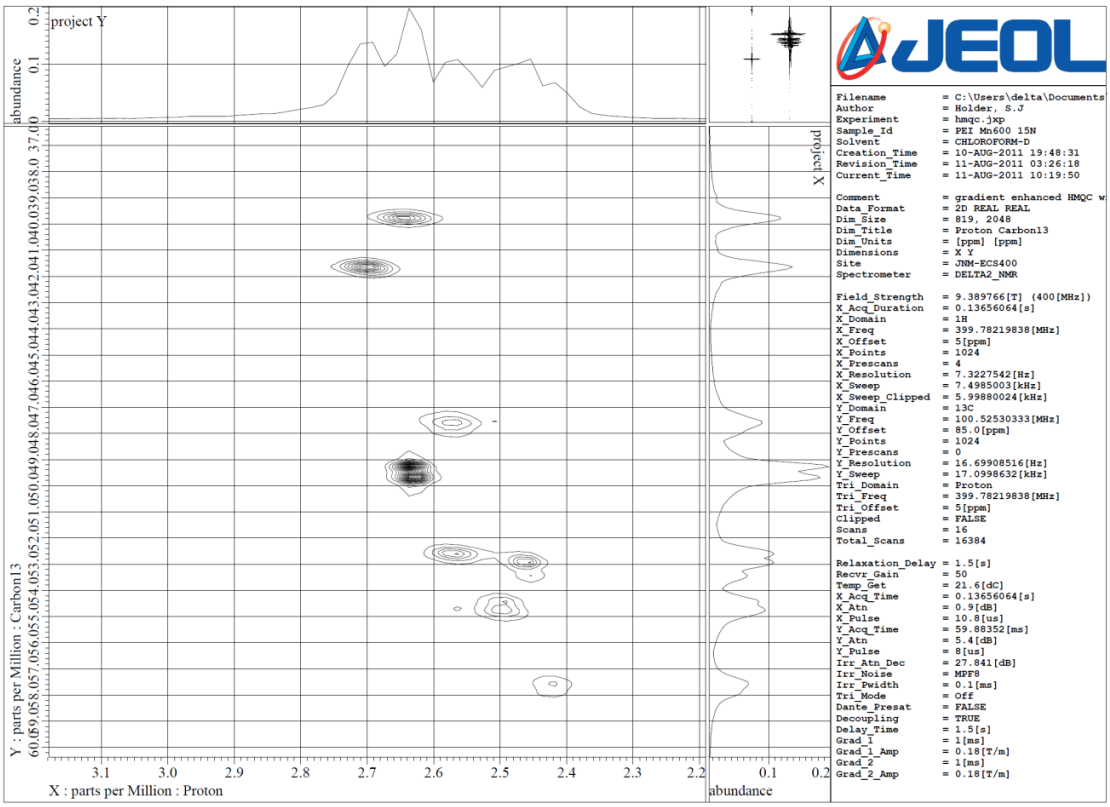

Figure SI 10. ^{1}H-^{13}C HMQC NMR spectrum of PEI.

GAMESS inputs for geometry/energy minimisations for compounds in gas phase.

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ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=OPTIMIZE
SCFTYP=UHF
UNITS=ANGS
DFTTYP=B3LYP
 $END
 $DFT
METHOD=GRID
IDCVER=3
 $END
 $BASIS
DIFFSP=.true.
GBASIS=N31
NDFUNC=1
NGAUSS=6
POLAR=POPN31
 $END
 $SCF
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
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 $STATPT
METHOD=QA
NSTEP=200
OPTTOL=0.0000010
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 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
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[JobTitle]
C1
[MolSpecific]
 $END
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 $SCF
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
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C1
[MolSpecific]
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Cartesian co-ordinates for energy minimised conformations in gas phase.

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O	8.0	-1.07756042	-0.33812642	-0.41660273
C	6.0	-0.05550046	0.52472246	-0.27774563
O	8.0	-0.14723897	1.59865415	0.28034240
C	6.0	1.24303329	-0.00902919	-0.89488298
C	6.0	1.44892025	-1.50446784	-0.66067713
Br	35.0	0.98814297	0.28008035	-2.89010835
C	6.0	2.43667746	0.82718527	-0.44986400
C	6.0	-2.35715485	0.12092806	0.06508701
H	1.0	2.37192988	-1.83339894	-1.14749050
H	1.0	0.61337429	-2.09245801	-1.04338646
H	1.0	1.54001749	-1.68713605	0.41883600
H	1.0	3.34241271	0.48814574	-0.96070725
H	1.0	2.57310772	0.70349187	0.63236749
H	1.0	2.28028083	1.88849902	-0.65081775
H	1.0	-3.05662441	-0.68218446	-0.16917790
H	1.0	-2.63929939	1.04562151	-0.44634074
H	1.0	-2.31523585	0.30013353	1.14328957

MBriP RAD

O	8.0	-1.44454777	0.22000106	-0.33657023
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C	6.0	0.83224243	-1.16775155	-1.18970931
C	6.0	2.10221004	-0.10356264	0.77626425
C	6.0	-2.64208007	0.90885746	0.05506723
H	1.0	1.72429788	-1.00212014	-1.81123984
H	1.0	-0.05937862	-1.05075276	-1.80897176
H	1.0	0.87913322	-2.21981120	-0.86150908
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H	1.0	2.89701176	0.32858002	0.14814790
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MBriPA

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N	7.0	-2.76211667	-1.73810494	0.24134198
C	6.0	-3.42977881	-2.70001960	-0.43010762
O	8.0	-2.86103797	-3.61289001	-1.03138685
C	6.0	-4.97596645	-2.68036175	-0.49463430
C	6.0	-5.40601015	-2.42219305	-1.94161201
C	6.0	-5.53164482	-3.99705601	0.05156265
Br	35.0	-5.79633188	-1.19007421	0.63905358
H	1.0	-0.97982043	-0.96577018	0.99239570
H	1.0	-0.92146105	-2.69887590	0.56310803
H	1.0	-3.28592300	-1.00407898	0.69797802
H	1.0	-5.03978348	-1.45564175	-2.30074430
H	1.0	-4.98148537	-3.21372056	-2.56935978
H	1.0	-6.49665976	-2.43984342	-2.02834606
H	1.0	-6.62219477	-4.01358175	-0.03429276
H	1.0	-5.25899649	-4.14262438	1.10133338
H	1.0	-5.10909653	-4.81923008	-0.53572536

MBriPA RAD

H	1.0	-1.01605022	-2.40194607	-0.47018090
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N	7.0	-2.37493253	-1.10713422	0.45804963
C	6.0	-2.90454721	-0.46135744	-0.63984483
O	8.0	-2.78592682	-0.95328045	-1.77427435
C	6.0	-3.57834601	0.82113338	-0.40470624
C	6.0	-4.15721035	1.55106890	-1.57159531
C	6.0	-3.68731594	1.42645502	0.96545047
H	1.0	-1.30336738	-2.70146036	1.26558387
H	1.0	-2.51884079	-3.18455577	0.04491343
H	1.0	-2.60472298	-0.78566039	1.38671601
H	1.0	-3.65629125	2.52319193	-1.71040928
H	1.0	-4.05334663	0.97116894	-2.49136877
H	1.0	-5.22237873	1.77612388	-1.40484309
H	1.0	-4.17453718	2.40622735	0.92263877
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H	1.0	-4.28317404	0.80092114	1.65085769

MBriPA2

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N	7.0	-2.50596881	-0.66405386	0.22559024
C	6.0	-3.66638732	-1.13060665	0.78550106
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C	6.0	-4.94507694	-0.24735706	0.85764849
C	6.0	-6.04312801	-0.99587458	1.61435509
C	6.0	-4.70495367	1.12582827	1.49160433
Br	35.0	-5.67966986	0.00307149	-1.03177917
H	1.0	-0.43562722	-0.90506595	0.40511739
H	1.0	-1.41376269	-2.20244026	1.15292478
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H	1.0	-6.24073315	-1.97149122	1.16836119
H	1.0	-5.71787930	-1.16052651	2.64768720
H	1.0	-6.96150875	-0.40114272	1.61661148
H	1.0	-5.64793634	1.67606997	1.56672037
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H	1.0	-3.24489713	1.01447403	-0.84753901
H	1.0	-1.87553108	0.18984079	-1.58019972
H	1.0	-1.61917710	1.21293843	-0.14468835

MBriPA2 RAD

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C	6.0	-3.55537534	-1.17959464	0.95984447
O	8.0	-3.56796980	-2.37731957	1.28872323
C	6.0	-4.70215750	-0.31903774	1.28870726
C	6.0	-6.02733755	-0.97507644	1.51383567
C	6.0	-4.56540060	1.12069273	1.68869114
H	1.0	-0.37562144	-0.82626987	0.09963399
H	1.0	-1.13544071	-2.06769109	1.13732219
C	6.0	-2.52490354	0.44677666	-0.63120586
H	1.0	-6.07700920	-1.96372032	1.05050981
H	1.0	-6.21650219	-1.11078250	2.59220028
H	1.0	-6.84312916	-0.34540555	1.12990534
H	1.0	-5.13322115	1.78795433	1.01956177
H	1.0	-3.52610445	1.46073461	1.71011746
H	1.0	-4.99034929	1.26834333	2.69386721
H	1.0	-3.52611041	0.87865698	-0.65541607
H	1.0	-2.31246233	0.04401755	-1.63377440
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MCliP

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C	6.0	0.94705689	0.46331900	-1.50357473
C	6.0	1.04928434	-0.89361542	-2.20183253
Cl	17.0	0.15109867	1.65810919	-2.67817378
C	6.0	2.31062222	1.02491128	-1.11629939
C	6.0	-2.08403230	-0.29741830	0.53438658
H	1.0	1.70148993	-0.81195247	-3.07712626
H	1.0	0.06851675	-1.25377381	-2.51799273
H	1.0	1.48638546	-1.62417281	-1.50861883
H	1.0	2.93350267	1.12534690	-2.00999522
H	1.0	2.80059695	0.33866835	-0.41545692
H	1.0	2.21315765	1.99710310	-0.62909228
H	1.0	-2.93597364	-0.84785694	0.13410036
H	1.0	-2.37599301	0.71652782	0.82260877
H	1.0	-1.65788198	-0.81228542	1.40022194

MCliPA

H	1.0	3.50090337	0.88497353	-0.68796772
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N	7.0	1.49872601	0.55329967	-0.22068821
C	6.0	0.47688338	-0.30167654	0.00181287
O	8.0	0.63263053	-1.51601517	0.13452812
C	6.0	-0.97228557	0.23892130	0.07856617
C	6.0	-1.78533983	-0.35041308	-1.07780933
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H	1.0	3.24532843	-0.21427111	0.69665396
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H	1.0	1.30294776	1.54234254	-0.28838527
H	1.0	-1.36720741	-0.05461854	-2.04522395
H	1.0	-1.75875843	-1.44201195	-1.00142431
H	1.0	-2.82291460	-0.00694189	-1.02250540
H	1.0	-2.60786605	0.23138285	1.49817193
H	1.0	-1.00184584	0.35532510	2.25499511
H	1.0	-1.53726315	-1.19758713	1.57116795

GAMESS inputs for geometry/energy minimisations for compounds in xylene.

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ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
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SCFTYP=UHF
UNITS=ANGS
DFTTYP=B3LYP
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 $DFT
METHOD=GRID
IDCVER=3
 $END
 $BASIS
DIFFSP=.true.
GBASIS=N31
NDFUNC=1
NGAUSS=6
POLAR=POPN31
 $END
 $SCF
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
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METHOD=QA
NSTEP=200
OPTTOL=0.0000010
 $END
 $PCM
IEF=-10
SMD=.true.
SOLVNT=XYLENEMX
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
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[JobTitle]
C1
[MolSpecific]
 $END
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Xylene SMD
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DFTTYP=B3LYP
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 $END
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GBASIS=N31
NDFUNC=1
NGAUSS=6
POLAR=POPN31
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DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
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[JobTitle]
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Cartesian co-ordinates for energy minimised conformations in xylene.

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C	6.0	-0.05775041	0.53645104	-0.29311433
O	8.0	-0.15747947	1.63390326	0.21991122
C	6.0	1.24503303	-0.00556743	-0.89576209
C	6.0	1.44266760	-1.50167608	-0.67002219
Br	35.0	0.99374825	0.30162200	-2.89836931
C	6.0	2.44084096	0.82110262	-0.44261503
C	6.0	-2.35580039	0.11435114	0.07994342
H	1.0	2.37558913	-1.83308983	-1.13644922
H	1.0	0.61624837	-2.09062791	-1.07120979
H	1.0	1.51130903	-1.69302976	0.40976653
H	1.0	3.35132146	0.47765848	-0.94259435
H	1.0	2.57099271	0.69278228	0.64029646
H	1.0	2.30002952	1.88535106	-0.64123154
H	1.0	-3.04606867	-0.70183456	-0.13842310
H	1.0	-2.65309048	1.02252078	-0.45254332
H	1.0	-2.32087231	0.31066382	1.15563166

MBriP RAD

O	8.0	-1.43800831	0.20105682	-0.31512144
C	6.0	-0.33757821	0.47155508	0.44242850
O	8.0	-0.37497613	1.24607730	1.39968038
C	6.0	0.84758061	-0.24133815	-0.00403722
C	6.0	0.82274115	-1.16516399	-1.17940879
C	6.0	2.11829686	-0.08643064	0.76265752
C	6.0	-2.64600873	0.88310039	0.06203127
H	1.0	1.80411458	-1.19668913	-1.67026794
H	1.0	0.06351863	-0.88963675	-1.91693950
H	1.0	0.59924412	-2.19665456	-0.85641140
H	1.0	2.54902816	-1.07147813	0.99891025
H	1.0	1.97664654	0.47282177	1.69089568
H	1.0	2.87523794	0.43924367	0.15740411
H	1.0	-3.40174222	0.55276269	-0.65340346
H	1.0	-2.51420259	1.96850145	0.00111720
H	1.0	-2.94389057	0.61226726	1.08047092

MBriPA

H	1.0	-0.87290174	-1.75030792	-0.76175177
C	6.0	-1.30511582	-1.69635534	0.24341610
N	7.0	-2.76040721	-1.71202528	0.17980926
C	6.0	-3.42801094	-2.73689818	-0.38436565
O	8.0	-2.85698104	-3.70180702	-0.90166485
C	6.0	-4.97361946	-2.70850444	-0.46821409
C	6.0	-5.38602829	-2.36597061	-1.90196407
C	6.0	-5.55338192	-4.04171467	0.00341714
Br	35.0	-5.79191923	-1.27108800	0.74262083
H	1.0	-0.98948675	-0.76641798	0.72221941
H	1.0	-0.92951506	-2.54674840	0.82425034
H	1.0	-3.28193307	-0.97144103	0.62804049
H	1.0	-5.00835848	-1.38634360	-2.21118927
H	1.0	-4.96924353	-3.12725663	-2.57249451
H	1.0	-6.47581387	-2.37005830	-2.00386763
H	1.0	-6.64453173	-4.03373289	-0.07567456
H	1.0	-5.27697182	-4.25727463	1.04025459
H	1.0	-5.15648174	-4.84065247	-0.63154453

MBriPA RAD

H	1.0	-0.98808306	-2.40795016	-0.44117552
C	6.0	-1.77130103	-2.42321634	0.32262009
N	7.0	-2.37117243	-1.10429180	0.44927013
C	6.0	-2.88475657	-0.45261830	-0.64897221
O	8.0	-2.74173617	-0.93157583	-1.79084468
C	6.0	-3.56944346	0.82218438	-0.40985471
C	6.0	-4.17610121	1.54620492	-1.56528556
C	6.0	-3.67347193	1.42626894	0.96004760
H	1.0	-1.32771516	-2.70093107	1.28302956
H	1.0	-2.51057363	-3.18343544	0.03421205
H	1.0	-2.64538932	-0.80580932	1.37479472
H	1.0	-3.68155956	2.51935625	-1.72075570
H	1.0	-4.09806156	0.96857947	-2.48951960
H	1.0	-5.23709965	1.77187538	-1.37348235
H	1.0	-4.11664867	2.42709160	0.91307384
H	1.0	-2.69282985	1.52428532	1.45023191
H	1.0	-4.31094694	0.82828528	1.63315749

MBriPA2

H	1.0	-1.36752462	-2.28819394	-0.49868438
C	6.0	-1.33695781	-1.53760171	0.30309826
N	7.0	-2.50124574	-0.65008670	0.23501328
C	6.0	-3.66384625	-1.12839925	0.76600116
O	8.0	-3.70671153	-2.25354147	1.27487588
C	6.0	-4.94374752	-0.24945098	0.85300487
C	6.0	-6.04332256	-1.00308514	1.59998941
C	6.0	-4.71090603	1.11985397	1.49452078
Br	35.0	-5.67392588	0.00175386	-1.04660070
H	1.0	-0.43049178	-0.93524295	0.19149354
H	1.0	-1.30957031	-2.05682826	1.26251173
C	6.0	-2.29800940	0.53084904	-0.60261297
H	1.0	-6.24537706	-1.97659516	1.15048015
H	1.0	-5.72531843	-1.17177474	2.63549304
H	1.0	-6.96280766	-0.40982446	1.60734904
H	1.0	-5.65569496	1.66593421	1.58158481
H	1.0	-3.99967480	1.75067019	0.96051919
H	1.0	-4.31771183	0.95834136	2.50787997
H	1.0	-3.22467422	1.05496299	-0.81259322
H	1.0	-1.87512767	0.22037461	-1.56711841
H	1.0	-1.59487569	1.22173250	-0.11947543

MBriPA2 RAD

H	1.0	-1.33729112	-2.16909957	-0.61493671
C	6.0	-1.25743806	-1.47092283	0.23255430
N	7.0	-2.44322777	-0.63110787	0.35432193
C	6.0	-3.55627918	-1.18265581	0.96274757
O	8.0	-3.56717229	-2.38038850	1.30887449
C	6.0	-4.70269871	-0.32031310	1.28542697
C	6.0	-6.02677631	-0.97381824	1.52138412
C	6.0	-4.56809902	1.12237847	1.67175758
H	1.0	-0.38421687	-0.82770473	0.07666644
H	1.0	-1.11708939	-2.05524683	1.14373553
C	6.0	-2.52224970	0.44998524	-0.62376451
H	1.0	-6.11138487	-1.93520677	1.00629151
H	1.0	-6.18386650	-1.16808069	2.59640408
H	1.0	-6.84782887	-0.31712189	1.20000184
H	1.0	-5.13261080	1.78544569	0.99591428
H	1.0	-3.53000093	1.46653867	1.69837296
H	1.0	-4.99867821	1.27937806	2.67357755
H	1.0	-3.52921915	0.86583275	-0.67550373
H	1.0	-2.27364969	0.06666996	-1.62494111
H	1.0	-1.81807137	1.25621510	-0.38037819

GAMESS inputs for geometry/energy minimisations for compounds in ethanol.

```
! Minimize (Energy/Geometry) B3LYP/6-31+G(d) Ethanol
SMD
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=OPTIMIZE
SCFTYP=UHF
UNITS=ANGS
DFTTYP=B3LYP
 $END
 $DFT
METHOD=GRID
IDCVER=3
 $END
 $BASIS
DIFFSP=.true.
GBASIS=N31
NDFUNC=1
NGAUSS=6
POLAR=POPN31
 $END
 $SCF
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
METHOD=QA
NSTEP=200
OPTTOL=0.0000010
 $END
 $PCM
IEF=-10
SMD=.true.
 SOLVNT=ETHANOL
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

```
! Minimize (Energy/Geometry) B3LYP/6-31+G(d) Ethanol
SMD
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=2
PLTORB=.TRUE.
RUNTYP=OPTIMIZE
SCFTYP=UHF
UNITS=ANGS
DFTTYP=B3LYP
 $END
 $DFT
METHOD=GRID
IDCVER=3
 $END
 $BASIS
DIFFSP=.true.
GBASIS=N31
NDFUNC=1
NGAUSS=6
POLAR=POPN31
 $END
 $SCF
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
METHOD=QA
NSTEP=200
OPTTOL=0.0000010
 $END
 $PCM
IEF=-10
SMD=.true.
SOLVNT=ETHANOL
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

Cartesian co-ordinates for energy minimised conformations inethanol.

MBriP

O	8.0	-1.04988122	-0.34506541	-0.35106319
C	6.0	-0.06225616	0.55373067	-0.32679364
O	8.0	-0.18521546	1.68733609	0.10745307
C	6.0	1.24897909	0.00288478	-0.90091783
C	6.0	1.42637956	-1.49800932	-0.70133978
Br	35.0	1.03234792	0.35686404	-2.90614152
C	6.0	2.44500637	0.80705559	-0.41106209
C	6.0	-2.34900832	0.10286433	0.10851416
H	1.0	2.36774349	-1.82939804	-1.15051126
H	1.0	0.60573930	-2.07378149	-1.13256907
H	1.0	1.46864235	-1.70982945	0.37572783
H	1.0	3.36277223	0.45596325	-0.89244729
H	1.0	2.55001783	0.65929449	0.67248583
H	1.0	2.32840657	1.87628281	-0.59930032
H	1.0	-3.00113416	-0.76610720	0.01351689
H	1.0	-2.70669937	0.92089039	-0.52368951
H	1.0	-2.29255795	0.42968547	1.15025878

MBriP RAD

O	8.0	-1.44023252	0.19140479	-0.29896376
C	6.0	-0.33128488	0.47922587	0.43411517
O	8.0	-0.35878783	1.28718245	1.37215686
C	6.0	0.84585762	-0.24841367	0.00135016
C	6.0	0.81990349	-1.16944265	-1.17469561
C	6.0	2.11622047	-0.09802408	0.76816225
C	6.0	-2.64933848	0.88868678	0.06097123
H	1.0	1.79854000	-1.18948579	-1.67175567
H	1.0	0.05377649	-0.90176117	-1.90770888
H	1.0	0.61337274	-2.20351791	-0.84850687
H	1.0	2.59474993	-1.07725096	0.91418594
H	1.0	1.96298540	0.37473771	1.74178016
H	1.0	2.83938670	0.51499820	0.20400241
H	1.0	-3.40937471	0.52540964	-0.63331741
H	1.0	-2.51894903	1.96946728	-0.05328164
H	1.0	-2.93682313	0.65677851	1.09151161

MBriPA

H	1.0	-0.86330891	-1.75854182	-0.74827904
C	6.0	-1.30352354	-1.69943798	0.25259516
N	7.0	-2.76048017	-1.71837211	0.17719978
C	6.0	-3.42983341	-2.72819662	-0.39675254
O	8.0	-2.85791802	-3.69211960	-0.93222487
C	6.0	-4.97348738	-2.70625901	-0.47461596
C	6.0	-5.39337730	-2.36772370	-1.90706170
C	6.0	-5.54621124	-4.03903198	0.00661435
Br	35.0	-5.78678703	-1.26852787	0.73962456
H	1.0	-0.99615663	-0.76412714	0.72538328
H	1.0	-0.93193424	-2.54028583	0.84920776
H	1.0	-3.28012371	-0.98232257	0.63585538
H	1.0	-5.01605415	-1.39004421	-2.22334886
H	1.0	-4.98349047	-3.13168430	-2.57898021
H	1.0	-6.48371029	-2.37154818	-2.00310206
H	1.0	-6.63804579	-4.03331423	-0.06228640
H	1.0	-5.25890875	-4.25217390	1.04129779
H	1.0	-5.15735292	-4.84088659	-0.62982863

MBriPA RAD

H	1.0	-0.95650291	-2.39748192	-0.40575680
C	6.0	-1.77194250	-2.42516518	0.32268405
N	7.0	-2.38899493	-1.11191738	0.44291082
C	6.0	-2.86364579	-0.43971589	-0.64999098
O	8.0	-2.67553020	-0.89864260	-1.80567575
C	6.0	-3.55949402	0.82439059	-0.41254529
C	6.0	-4.19692469	1.53527308	-1.55882943
C	6.0	-3.65751147	1.43173182	0.95531416
H	1.0	-1.36637700	-2.70929313	1.29736972
H	1.0	-2.49611259	-3.18697286	0.00308938
H	1.0	-2.68128014	-0.82311529	1.36708605
H	1.0	-3.70571065	2.50591135	-1.73905218
H	1.0	-4.15360641	0.95138162	-2.48142886
H	1.0	-5.24975872	1.76681483	-1.33295679
H	1.0	-4.05658007	2.45062947	0.90021622
H	1.0	-2.68295741	1.48764157	1.46235657
H	1.0	-4.33396053	0.86283308	1.61575615

MBriPA2

H	1.0	-1.37011027	-2.28096247	-0.53013092
C	6.0	-1.34054673	-1.54865265	0.28786007
N	7.0	-2.50709176	-0.65908784	0.23429024
C	6.0	-3.66554260	-1.13215840	0.75788474
O	8.0	-3.71709633	-2.27508211	1.24614573
C	6.0	-4.94298267	-0.25427699	0.85376358
C	6.0	-6.03931618	-0.99658203	1.61600161
C	6.0	-4.71309137	1.12439311	1.47471106
Br	35.0	-5.67383575	-0.04696793	-1.05397177
H	1.0	-0.43431687	-0.94427025	0.18974024
H	1.0	-1.31047809	-2.08289838	1.23871374
C	6.0	-2.29399109	0.54294294	-0.57600778
H	1.0	-6.24502230	-1.97856104	1.18629742
H	1.0	-5.72161531	-1.13988805	2.65568471
H	1.0	-6.95894432	-0.40345851	1.61553693
H	1.0	-5.66215658	1.66143918	1.57122350
H	1.0	-4.01666021	1.75911129	0.92687863
H	1.0	-4.30360699	0.97734618	2.48388743
H	1.0	-3.22013807	1.05533350	-0.81536621
H	1.0	-1.83182275	0.24975540	-1.52713263
H	1.0	-1.61915636	1.23637307	-0.05928031

MBriPA2 RAD

H	1.0	-1.35560393	-2.19831276	-0.64047426
C	6.0	-1.26792943	-1.49630392	0.20189592
N	7.0	-2.45775175	-0.65971136	0.33072007
C	6.0	-3.54967546	-1.17933393	0.97668976
O	8.0	-3.55038977	-2.37733984	1.36130238
C	6.0	-4.69776964	-0.32161990	1.29339278
C	6.0	-6.02005434	-0.97810853	1.53297400
C	6.0	-4.57549047	1.12852168	1.65271497
H	1.0	-0.40047583	-0.85033005	0.02916148
H	1.0	-1.10807109	-2.06980658	1.11660624
C	6.0	-2.51677918	0.46770626	-0.59924346
H	1.0	-6.10046005	-1.94736755	1.03144503
H	1.0	-6.18534470	-1.15204382	2.61038089
H	1.0	-6.84000206	-0.32834619	1.19518709
H	1.0	-5.13109732	1.77497315	0.95405209
H	1.0	-3.54094839	1.48147810	1.69320583
H	1.0	-5.02644730	1.30082572	2.64275169
H	1.0	-3.53130722	0.85659295	-0.69146931
H	1.0	-2.20467806	0.13067485	-1.59745598
H	1.0	-1.84757245	1.27862883	-0.28533024

GAMESS inputs for single point energy minimisations for compounds.

```
! Compute Properties U BMK/aug-cc-pVTZ
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=ENERGY
SCFTYP=UHF
UNITS=ANGS
ISPHER=1
DFTTYP=BMK
QMTTOL= 1.0E-05
ICUT=11
 $END
 $DFT
METHOD=GRID
NRAD=125
IDCVER=3
DCSR=1.931
DCS6=1.0
DCS8=2.168
 $END
 $BASIS
GBASIS=ACCT
 $END
 $SCF
DAMP=.true.
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
NSTEP=200
OPTTOL=0.000010
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

```
! Compute Properties U BMK/aug-cc-pVTZ
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=ENERGY
SCFTYP=UHF
UNITS=ANGS
ISPHER=1
DFTTYP=BMK
QMTTOL= 1.0E-05
ICUT=11
 $END
 $DFT
METHOD=GRID
NRAD=125
IDCVER=3
DCSR=1.931
DCS6=1.0
DCS8=2.168
 $END
 $BASIS
GBASIS=ACCT
 $END
 $SCF
DAMP=.true.
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
NSTEP=200
OPTTOL=0.000010
 $END
 $PCM
IEF=-10
SMD=.true.
SOLVNT=XYLENEMX
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

```
! Compute Properties U BMK/aug-cc-pVTZ
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=ENERGY
SCFTYP=UHF
UNITS=ANGS
ISPHER=1
DFTTYP=BMK
QMTTOL= 1.0E-05
ICUT=11
 $END
 $DFT
METHOD=GRID
NRAD=125
IDCVER=3
DCSR=1.931
DCS6=1.0
DCS8=2.168
 $END
 $BASIS
GBASIS=ACCT
 $END
 $SCF
DAMP=.true.
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
NSTEP=200
OPTTOL=0.000010
 $END
 $PCM
IEF=-10
SMD=.true.
SOLVNT=ETHANOL
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

```
! Compute Properties M06-2X D3/aug-cc-pVTZ
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=200
MULT=1
PLTORB=.TRUE.
RUNTYP=ENERGY
SCFTYP=UHF
UNITS=ANGS
ISPHER=1
DFTTYP=M06-2X
QMTTOL= 1.0E-06
ICUT=11
 $END
 $DFT
METHOD=GRID
NRAD=250
IDCVER=3
DCSR=1.619
DCS6=1.0
DCS8=0.00
 $END
 $BASIS
GBASIS=ACCT
 $END
 $SCF
DAMP=.true.
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
NSTEP=200
OPTTOL=0.000010
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=150
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```

```
! Compute Properties U B2GP-PLYP/aug-cc-pVTZ D3
 $CONTRL
COORD=UNIQUE
ICHARG=0
MAXIT=50
MULT=1
PLTORB=.TRUE.
RUNTYP=ENERGY
SCFTYP=UHF
UNITS=ANGS
ISPHER=1
DFTTYP=B2PLYP
QMTTOL=5.0E-06
ICUT=11
 $END
 $DFT
CHF=0.65
CMP2=0.36
DC=.true.
IDCVER=3
DCSR=1.586
DCS6=0.56
DCS8=0.760
METHOD=GRID
NRAD=125
 $END
 $BASIS
GBASIS=ACCT
 $END
 $SCF
DAMP=.true.
DIIS=.true.
DIRSCF=.true.
EXTRAP=.true.
NPREO(1)=1,9999,1,9999
SOSCF=.false.
 $END
 $STATPT
NSTEP=50
OPTTOL=0.0000100
 $END
 $GUESS
GUESS=HUCKEL
 $END
 $SYSTEM
MWORDS=100
MEMDDI=900
 $END
 $DATA
[JobTitle]
C1
[MolSpecific]
 $END
```