



Supporting Information

for

Complexes of resorcin[4]arene with secondary amines: synthesis, solvent influence on “*in-out*” structure, and theoretical calculations of non-covalent interactions

Waldemar Iwanek

Beilstein J. Org. Chem. **2023**, *19*, 1525–1536. [doi:10.3762/bjoc.19.109](https://doi.org/10.3762/bjoc.19.109)

NMR spectra of complexes and coordinates of the optimized complex structures

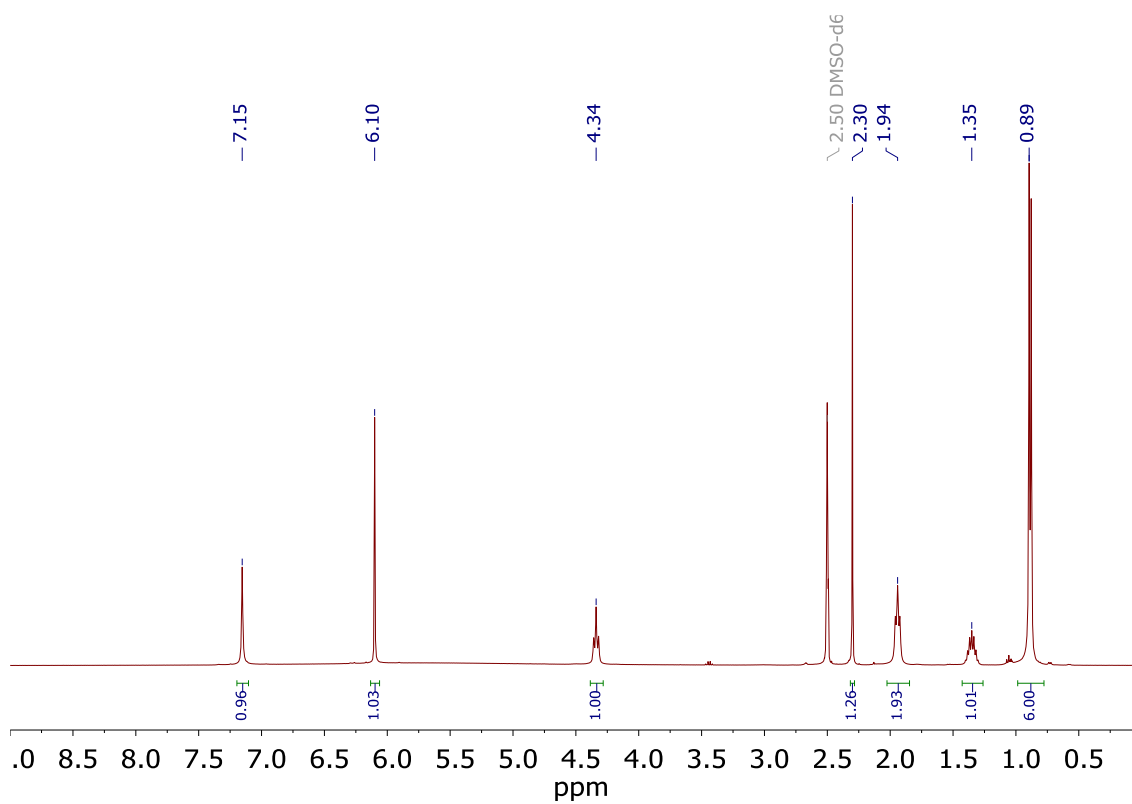
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2. The xyz coordinates of the optimized complex structures calculated by the PBE0-D4/mTZVPP method in CHCl_3 and DMSO.

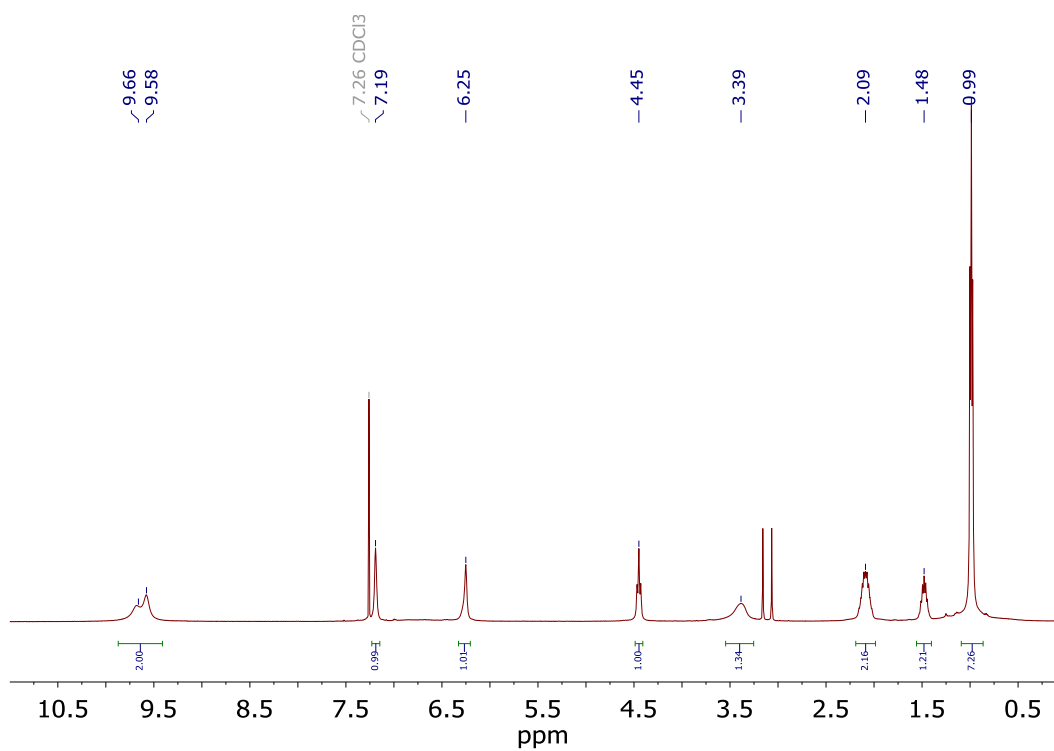
1. NMR spectra of R[4]A complexes with sec-amines

R[4]A:dimethylamine

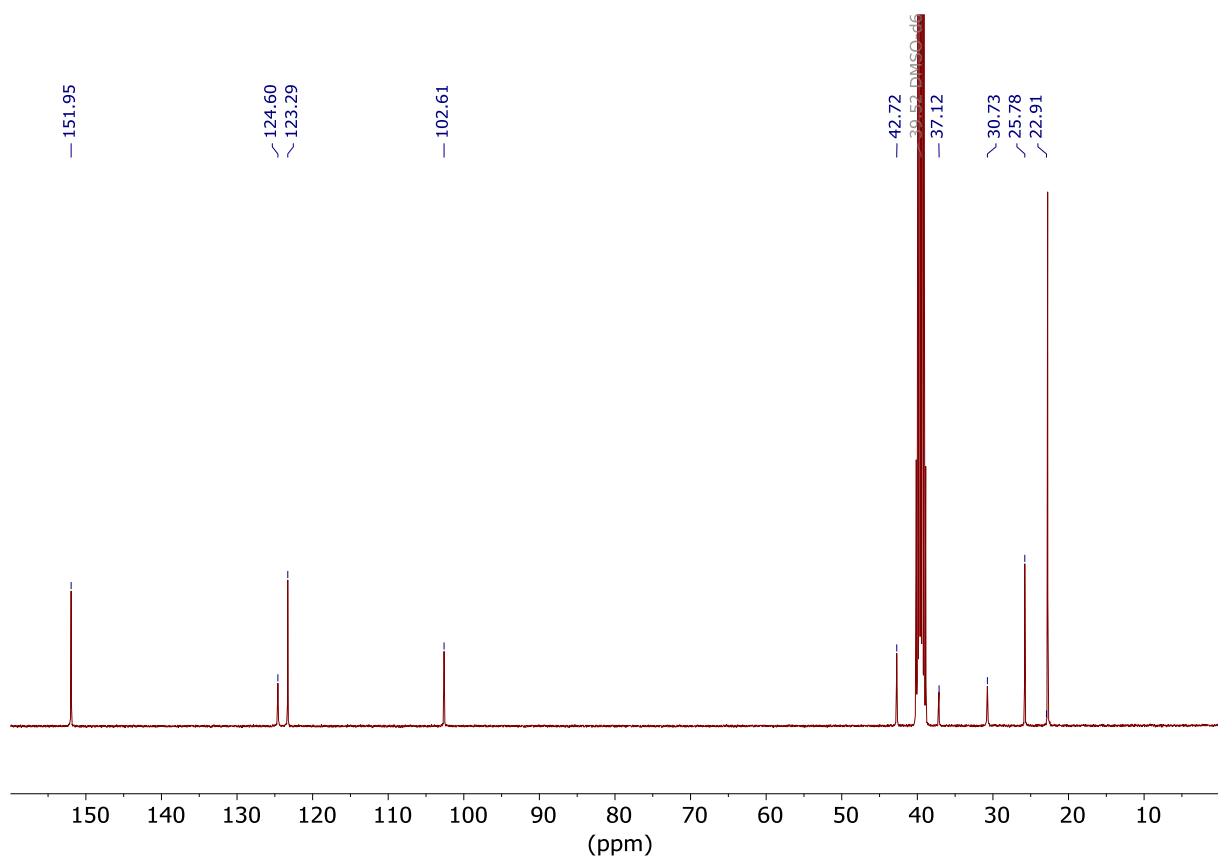
¹H NMR in DMSO



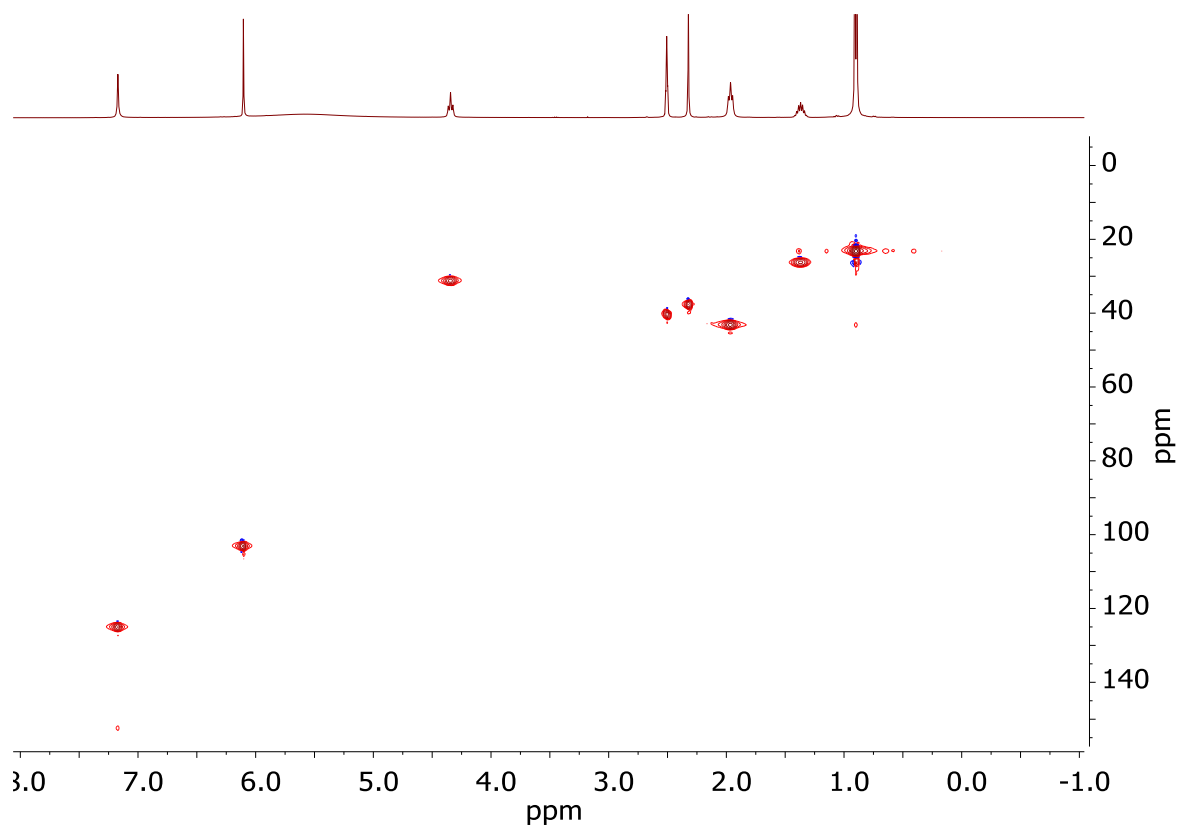
¹H NMR in CDCl₃



^{13}C NMR in $\text{DMSO-}d_6$

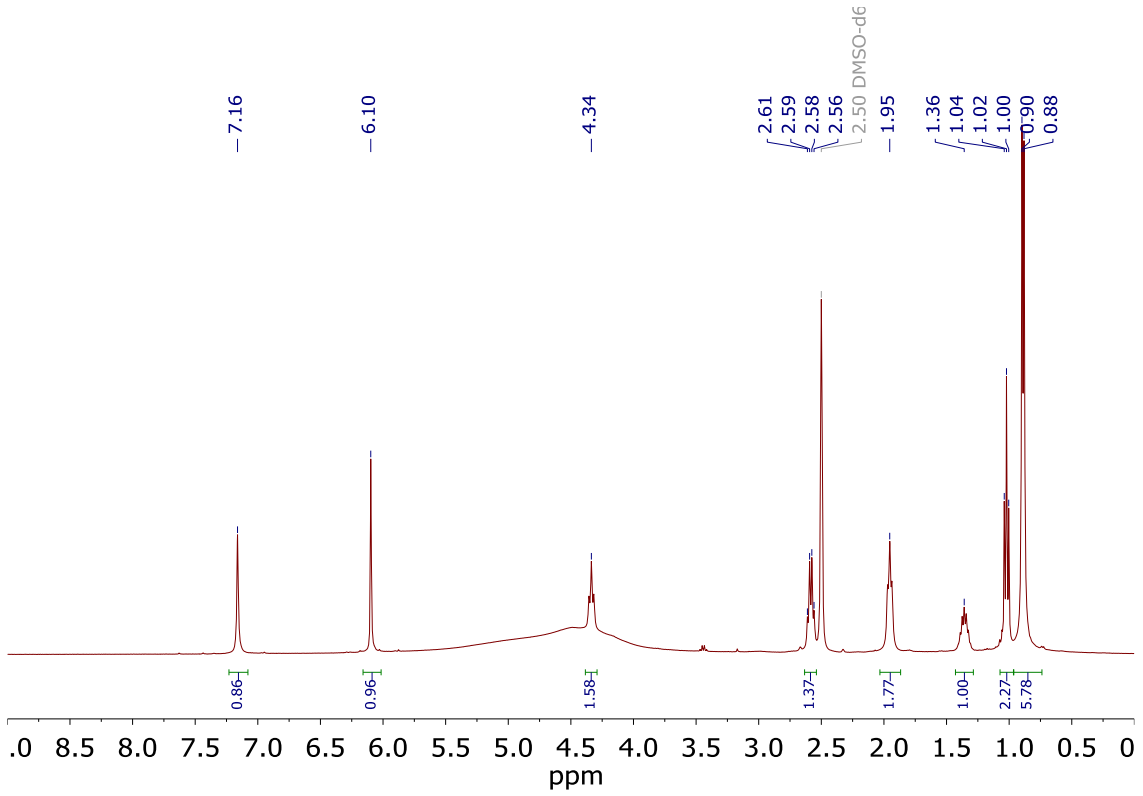


HSQC ^{13}C $\text{DMSO-}d_6$

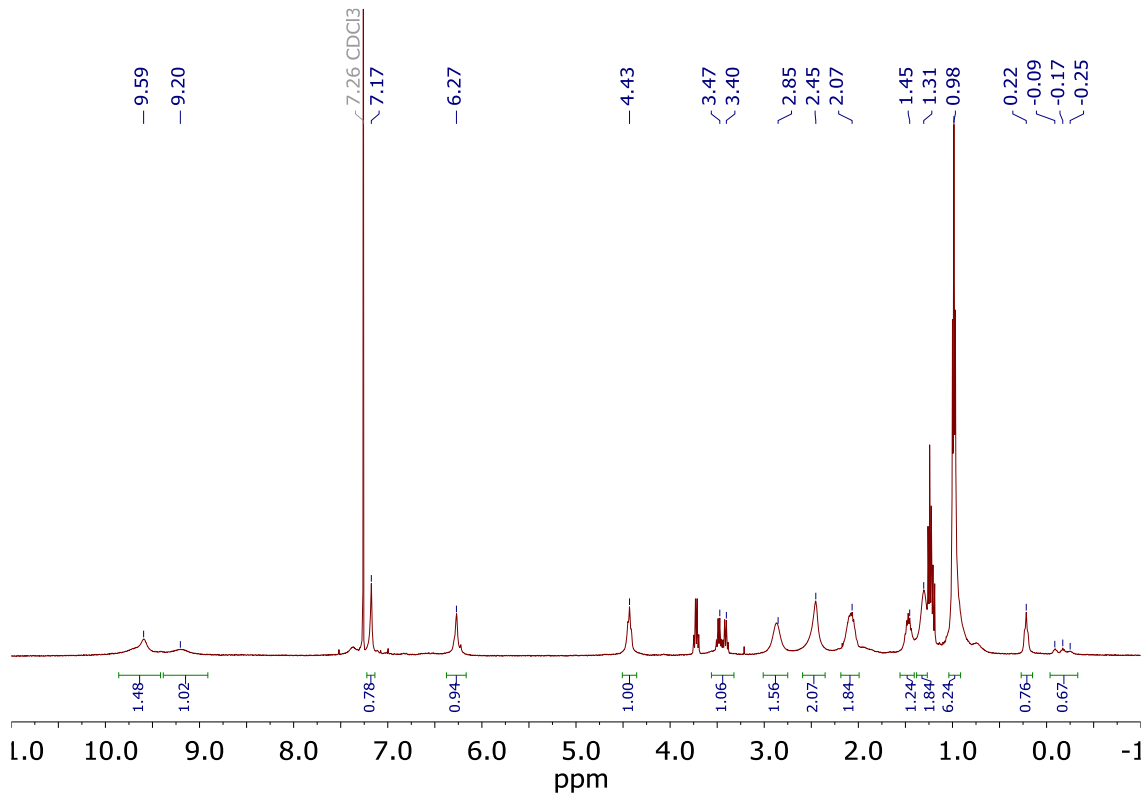


R[4]A:diethylamine

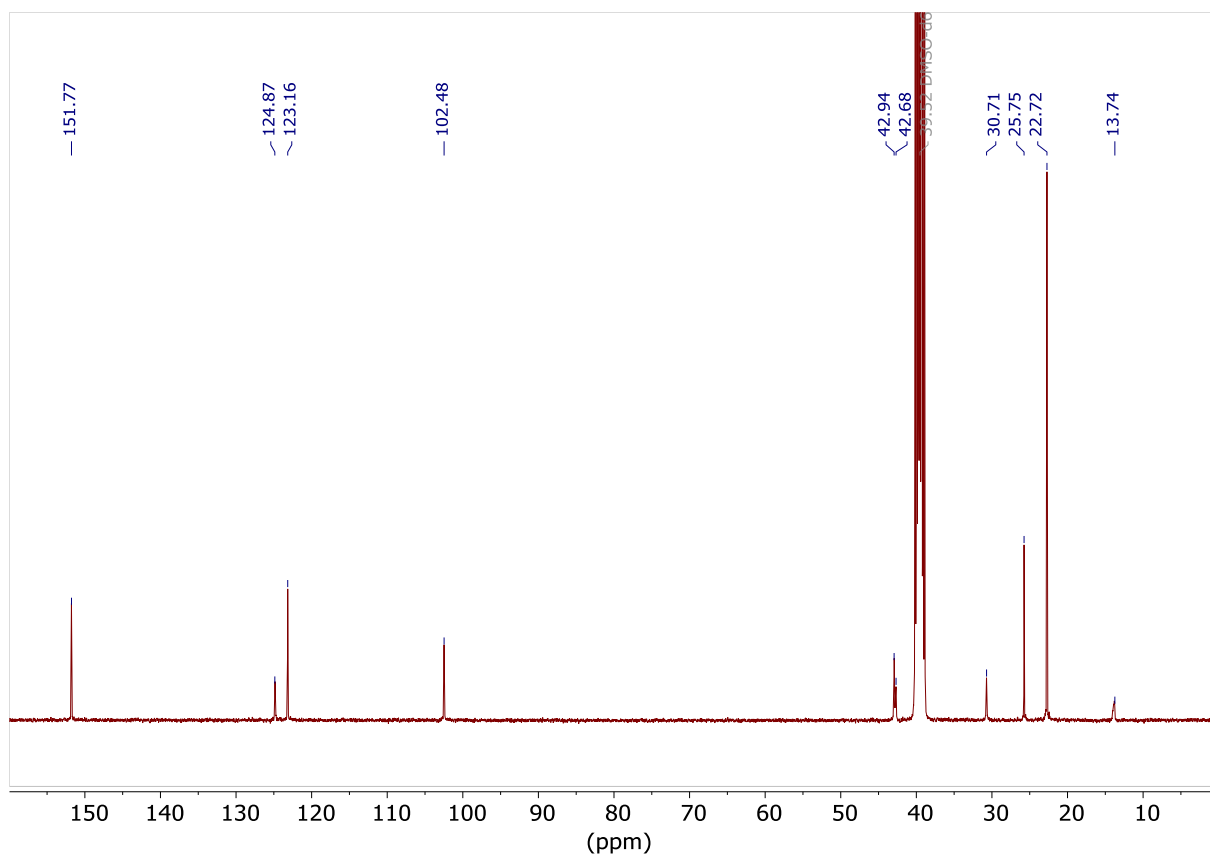
¹H NMR in DMSO



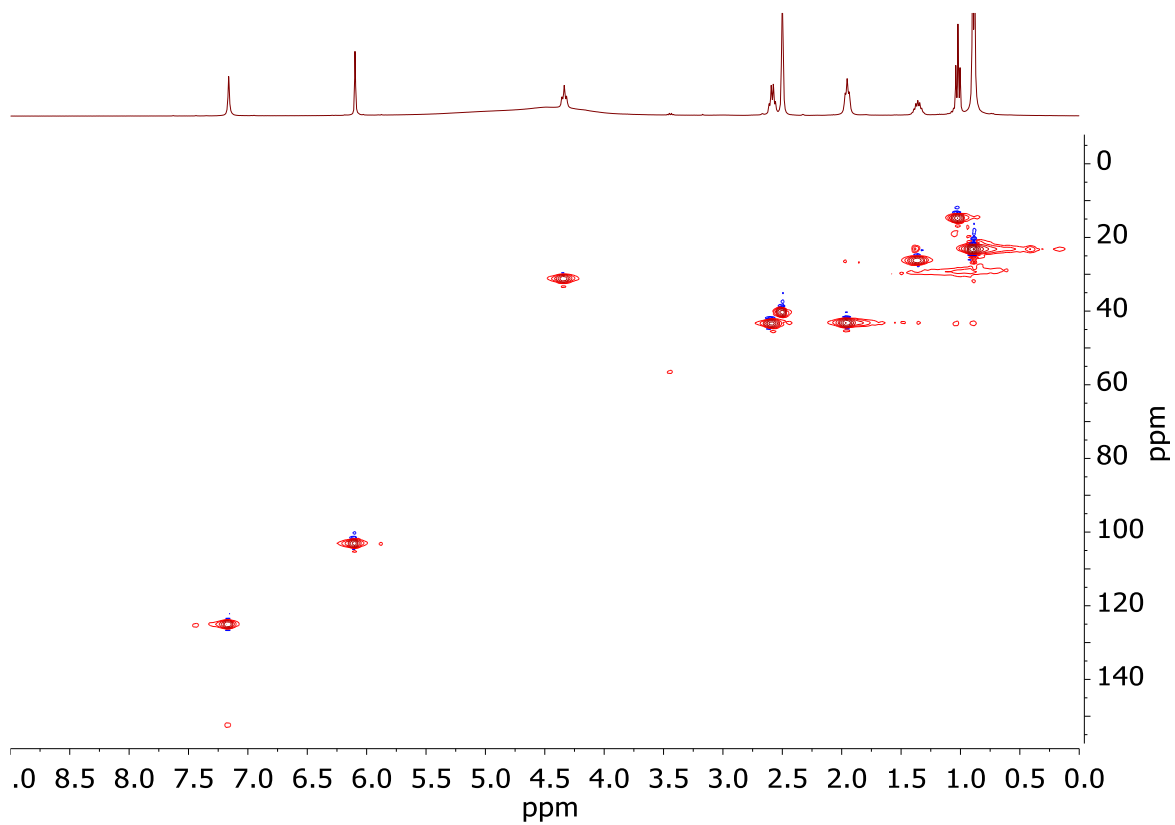
¹H NMR in CDCl₃



^{13}C NMR in $\text{DMSO-}d_6$

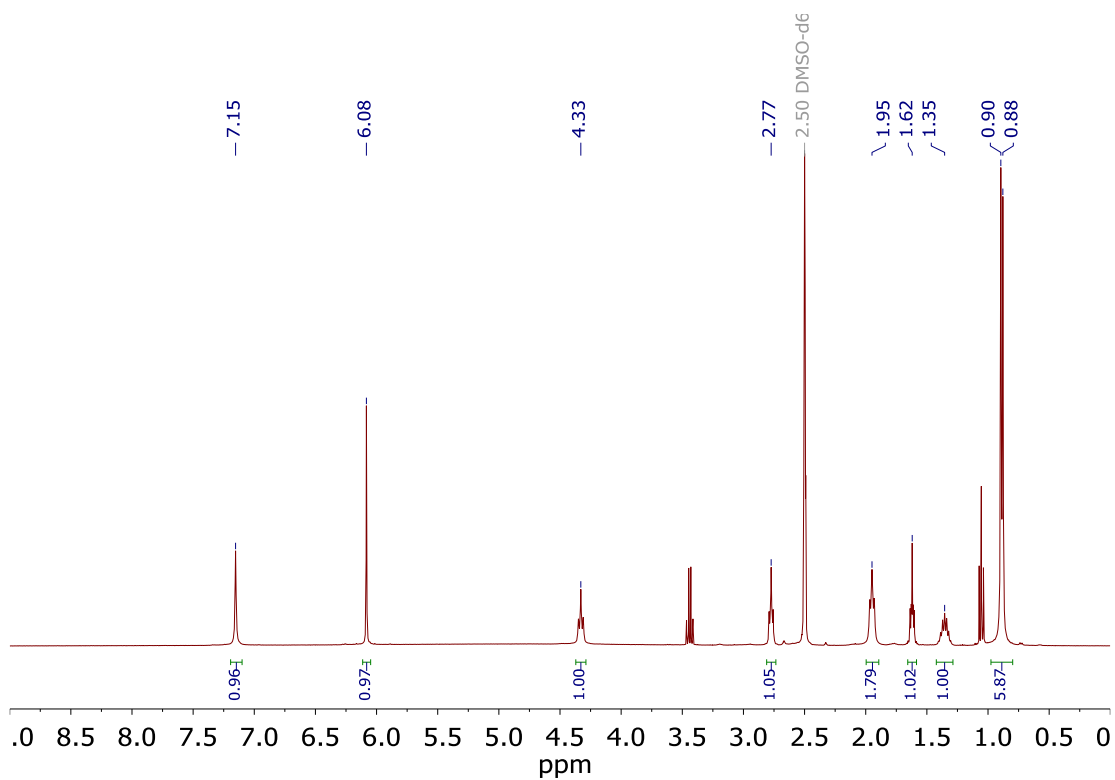


HSQC ^{13}C $\text{DMSO-}d_6$

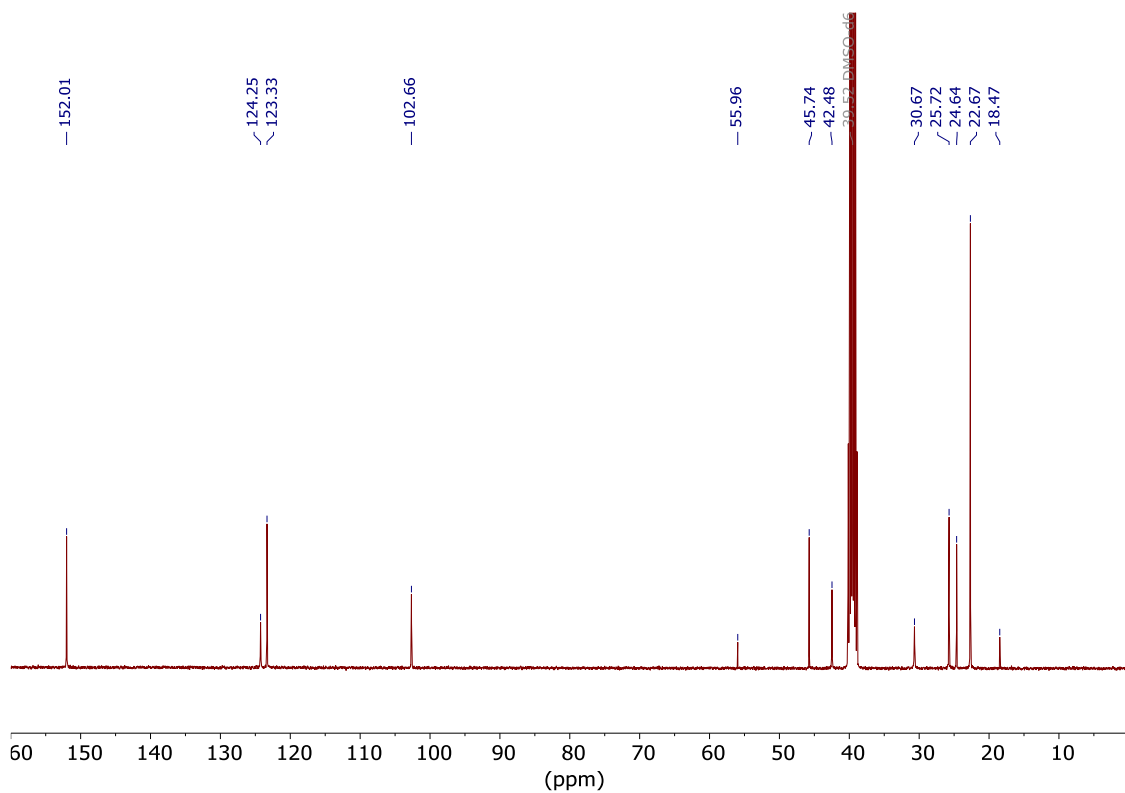


R[4]A:pyrrolidine

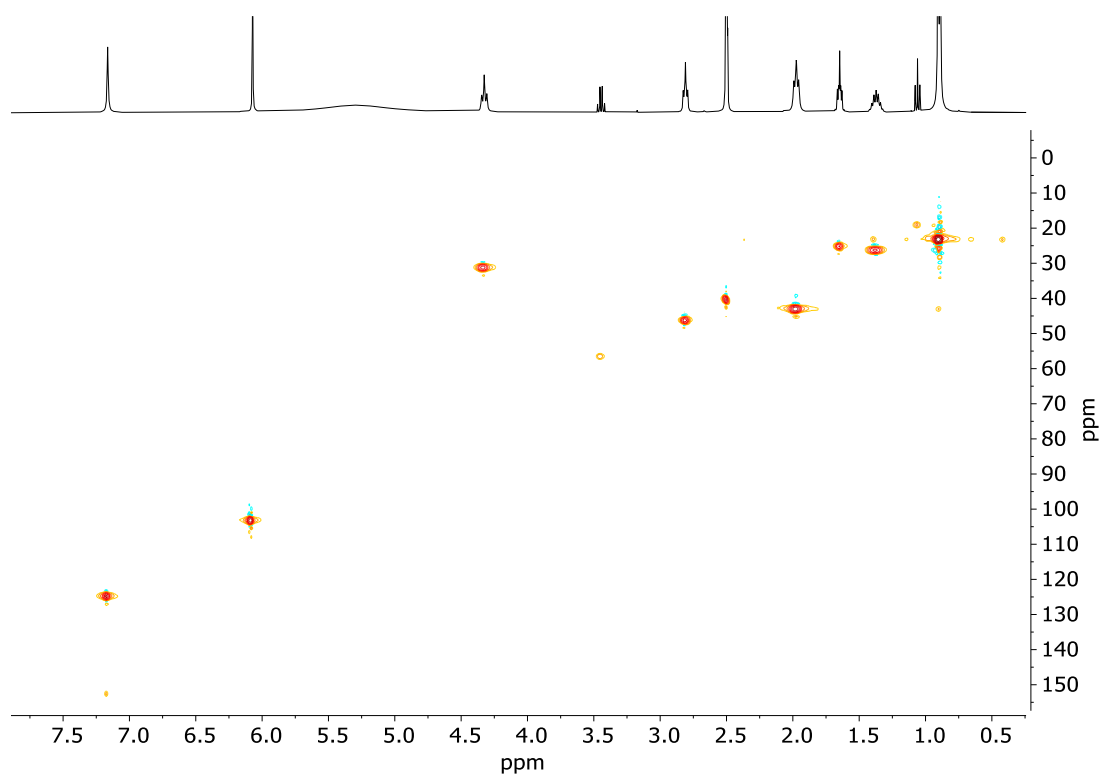
^1H NMR in DMSO



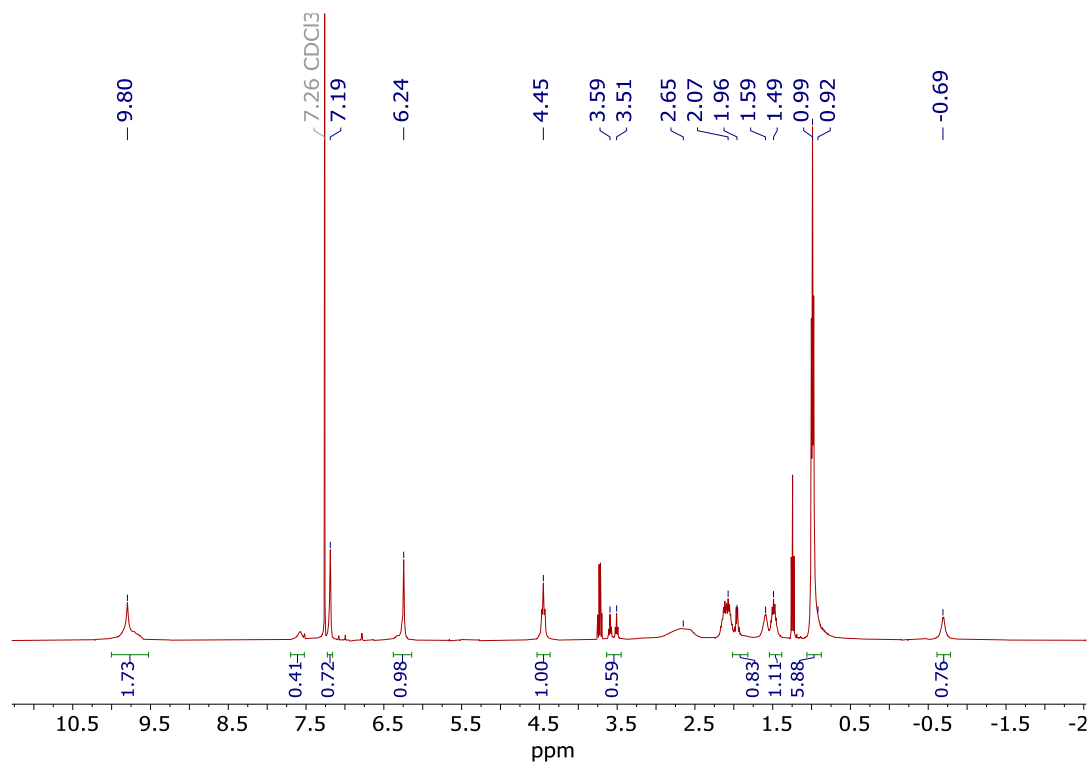
^{13}C NMR DMSO- d_6



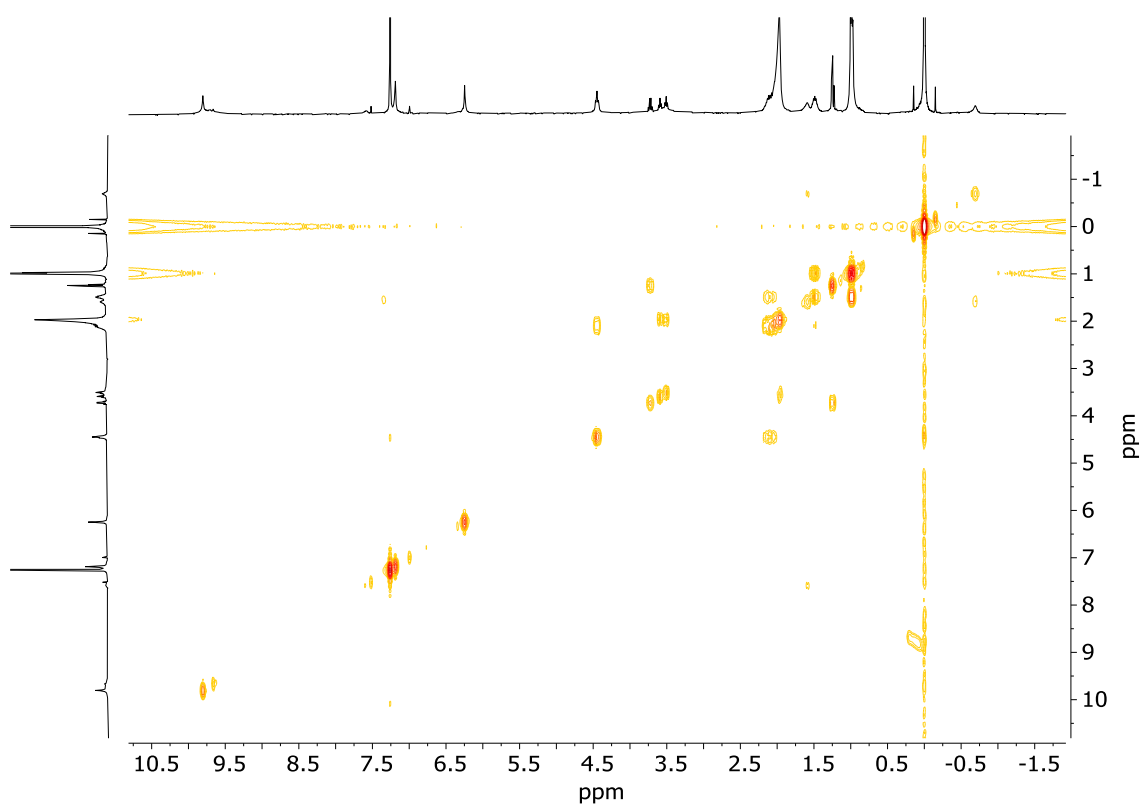
HSQC ^{13}C DMSO- d_6



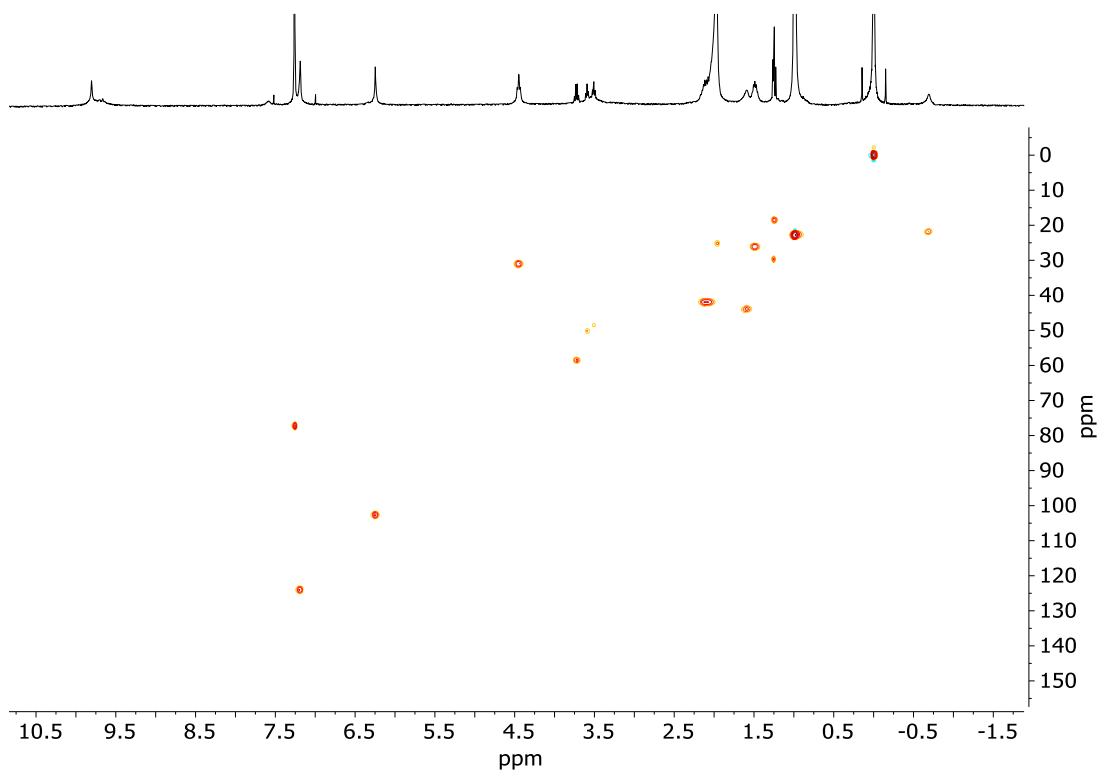
^1H NMR in CDCl_3



COSY $^1\text{H}, ^1\text{H} - \text{CDCl}_3$

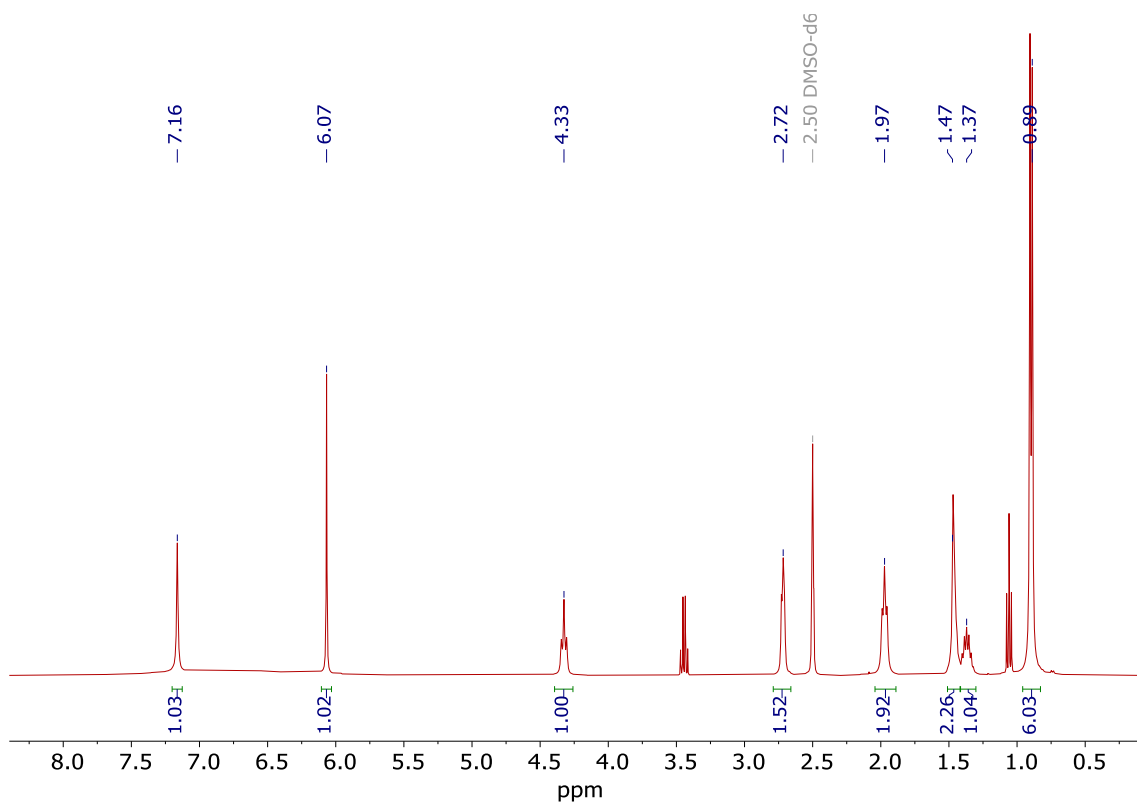


HSQC $^{13}\text{C} - \text{CDCl}_3$

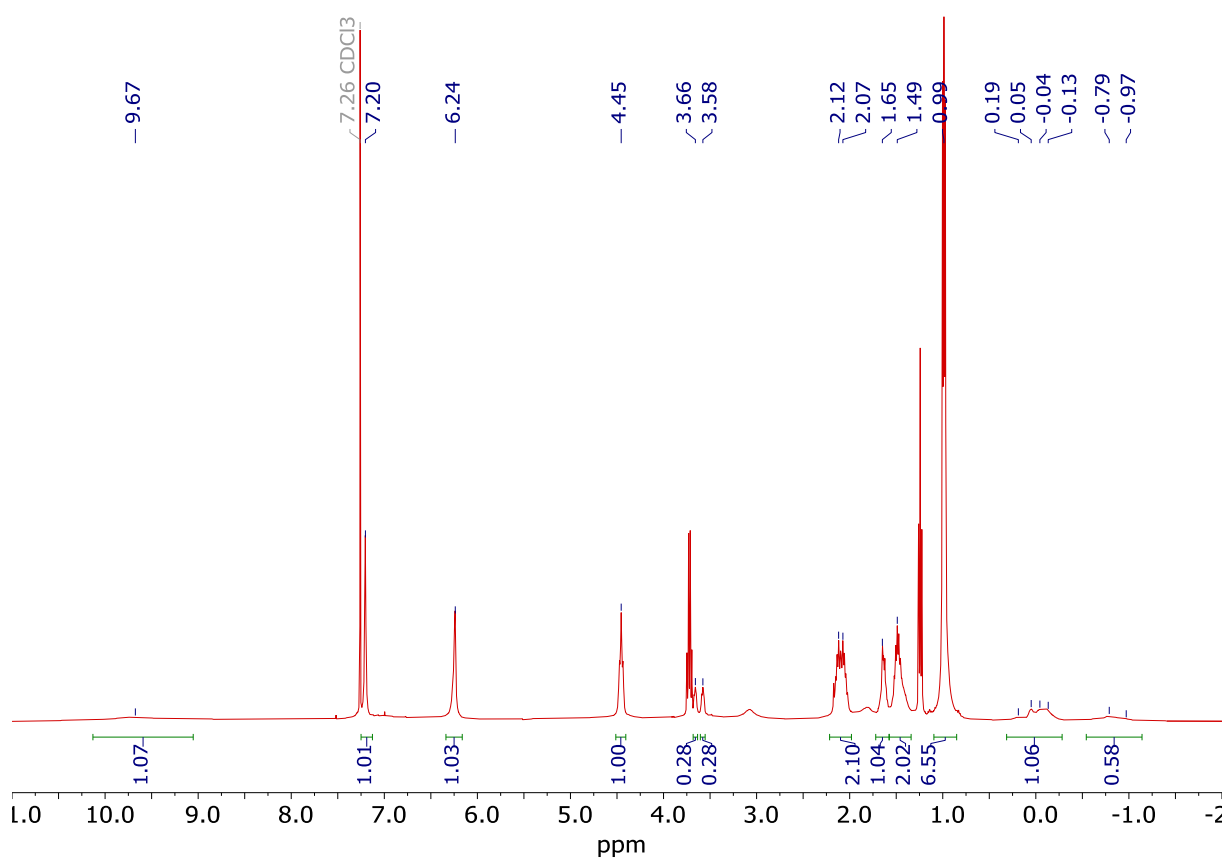


R[4]A:piperidine

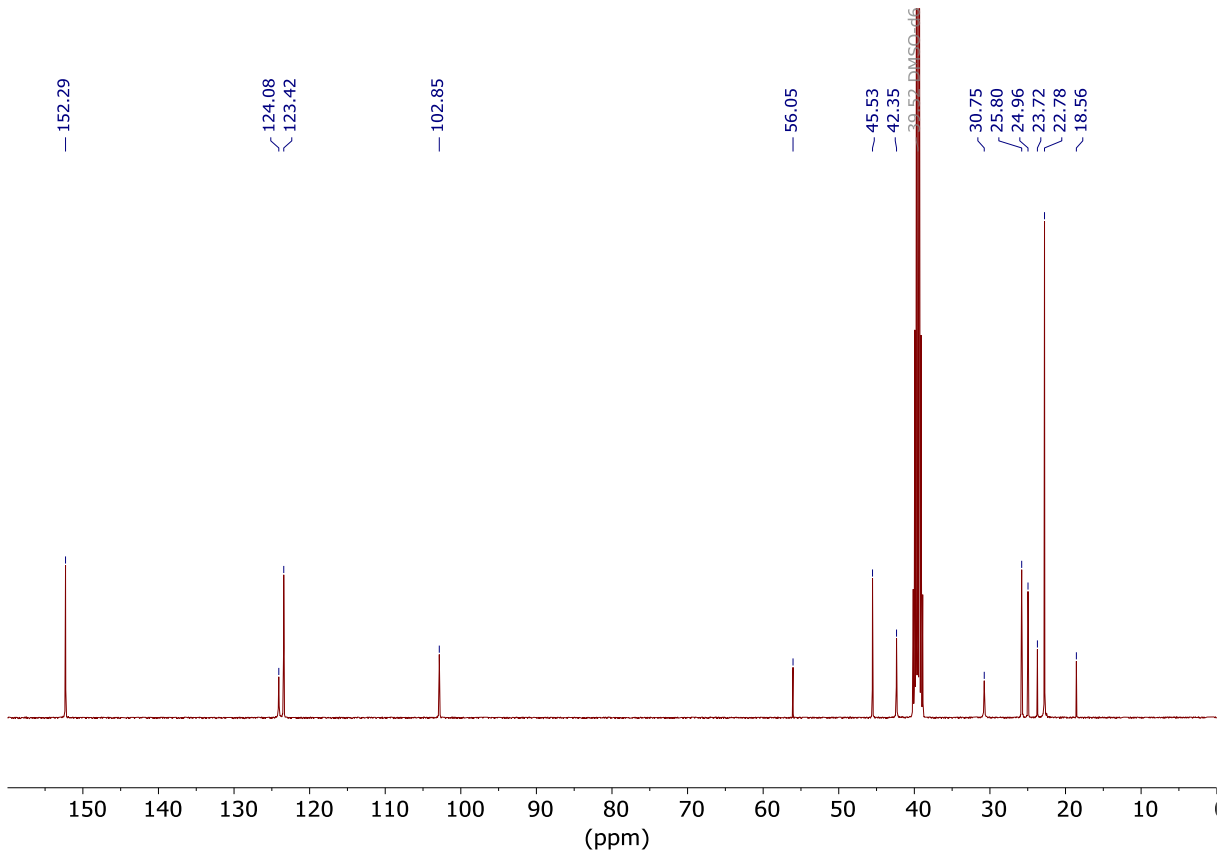
^1H NMR in DMSO



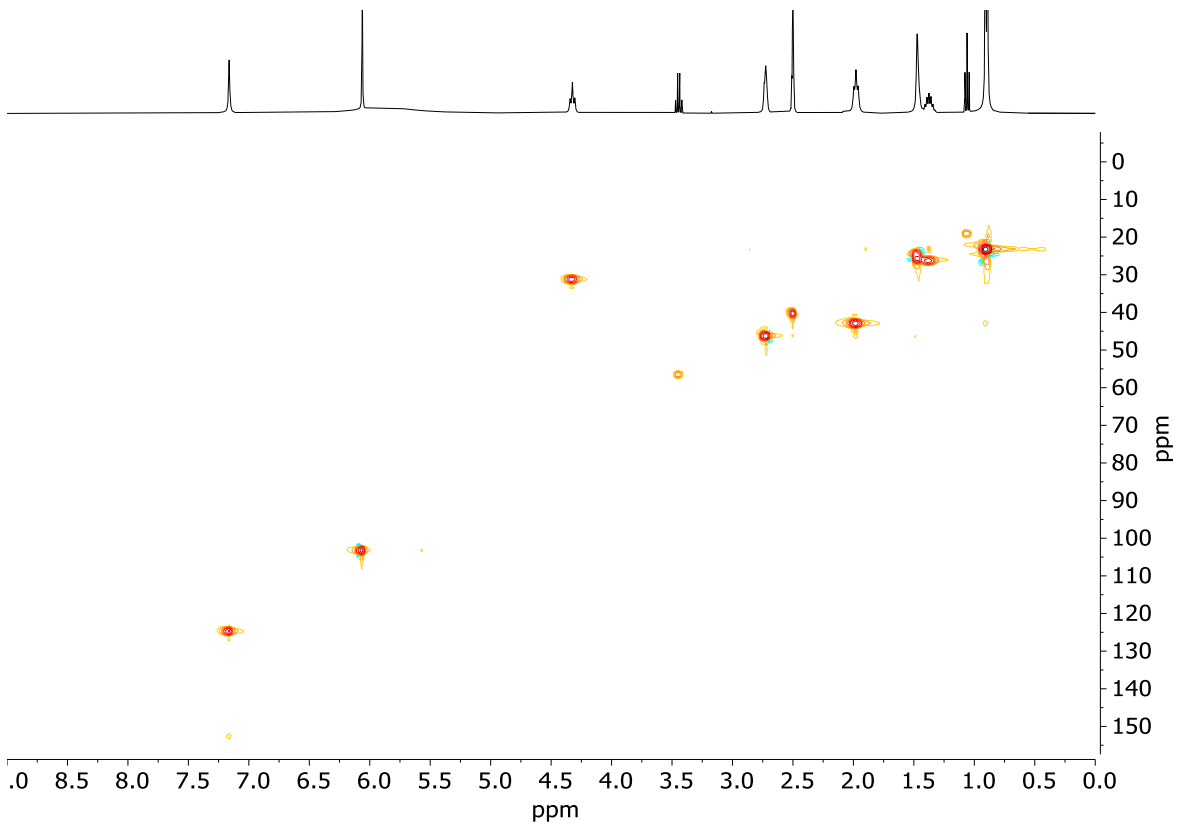
^1H NMR in CDCl_3



^{13}C NMR in $\text{DMSO-}d_6$

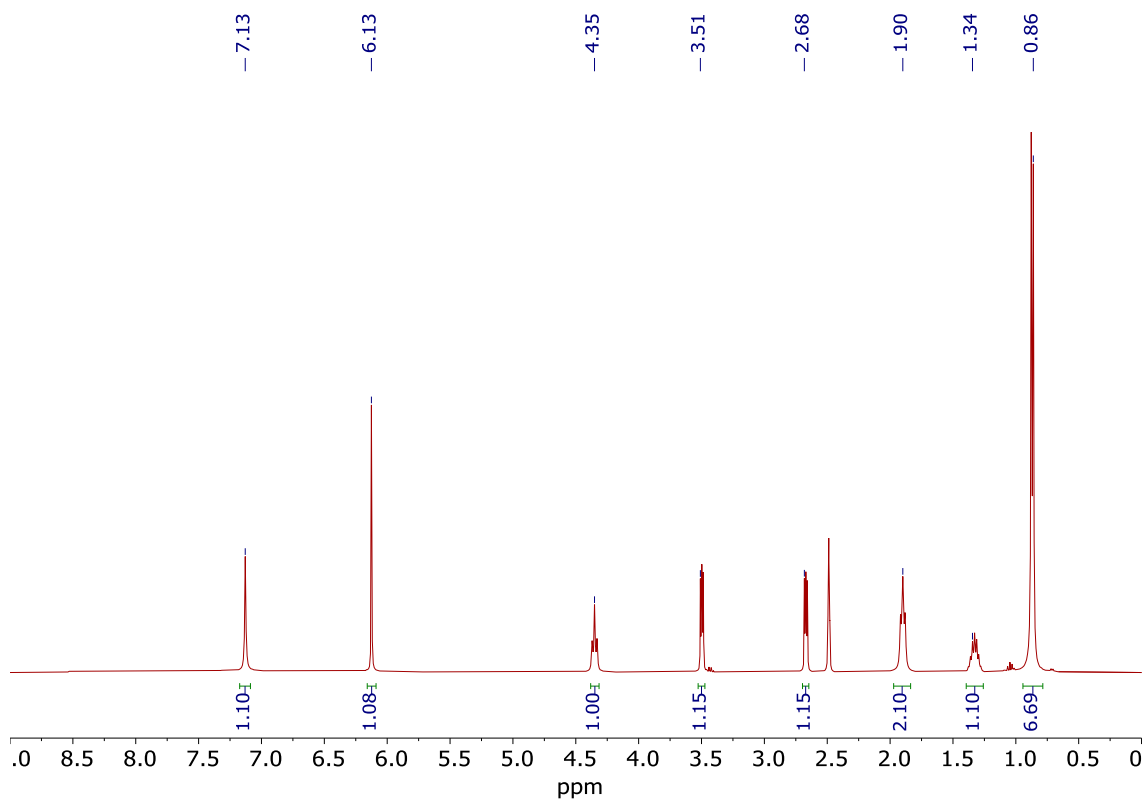


HSQC ^{13}C $\text{DMSO-}d_6$

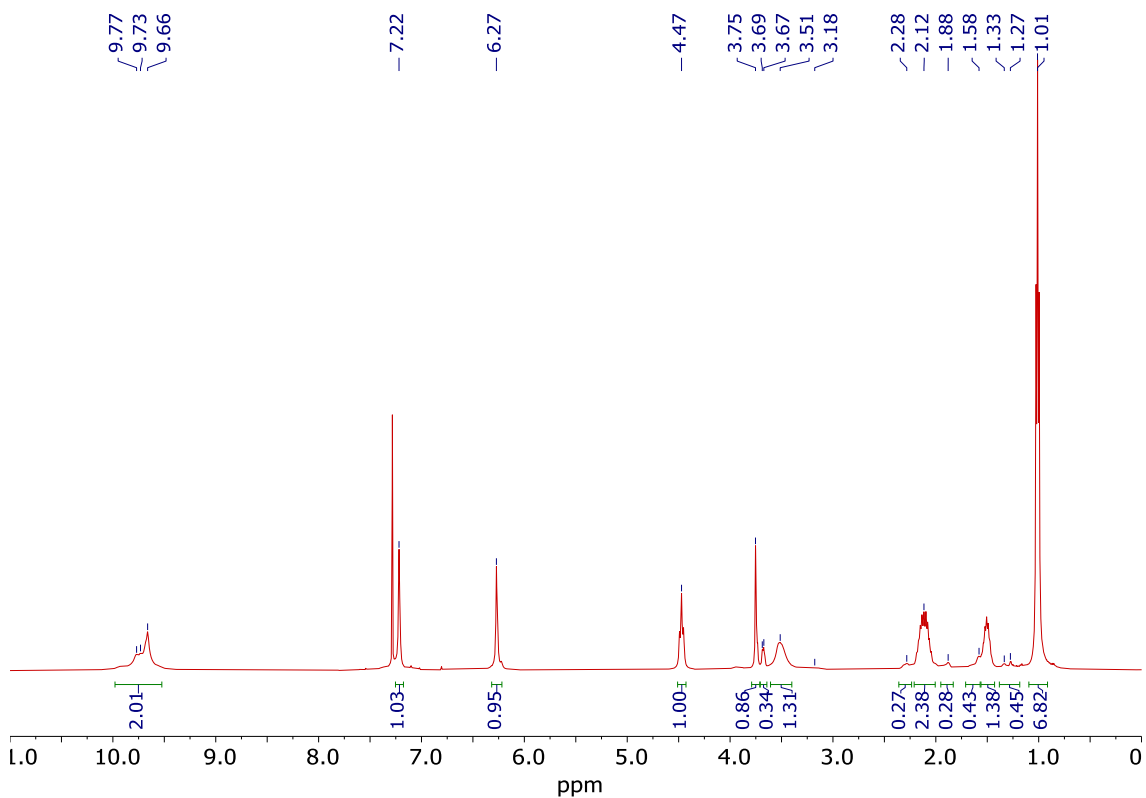


R[4]A:morpholine

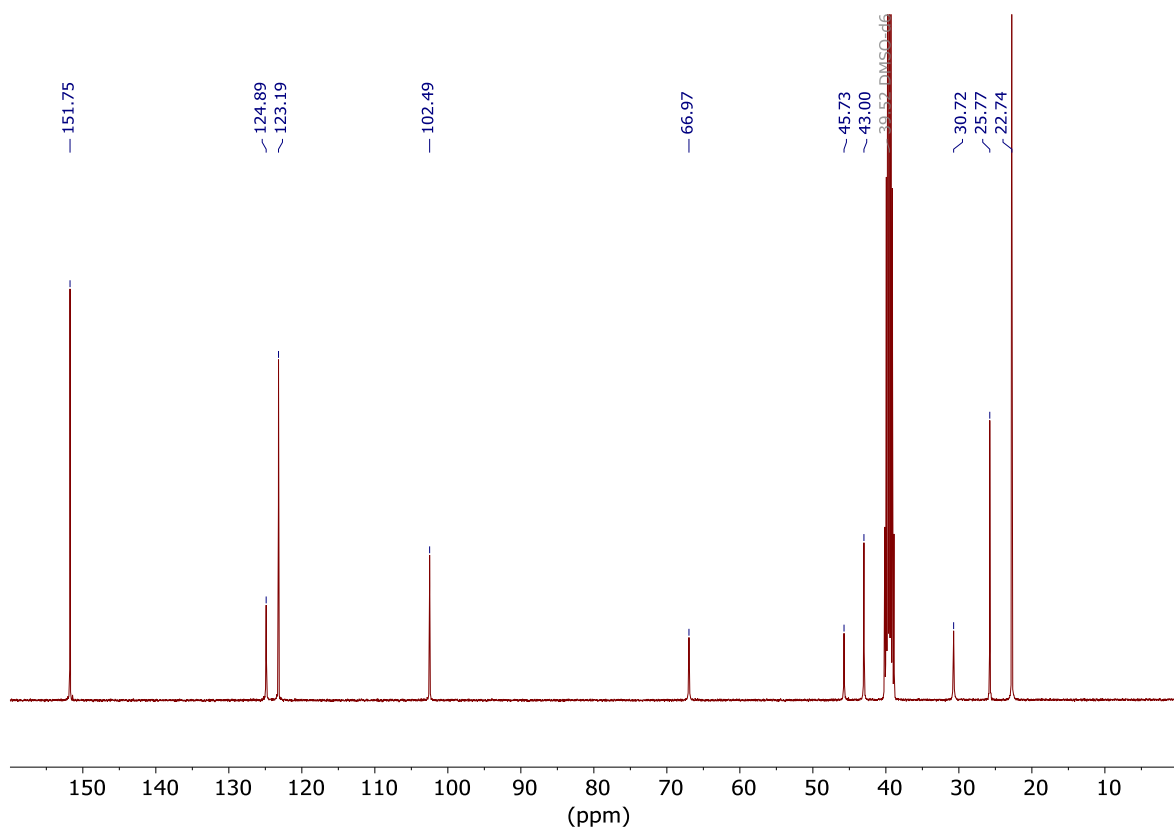
¹H NMR in DMSO



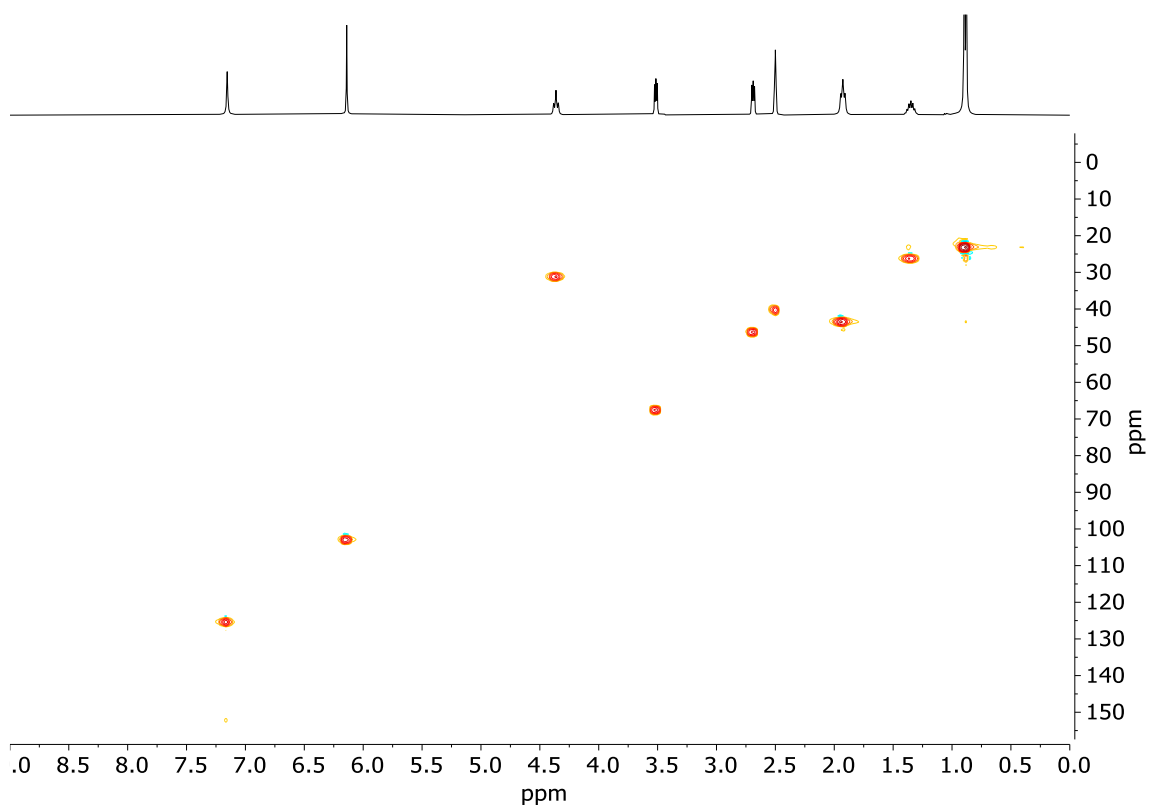
¹H NMR in CDCl₃



^{13}C NMR in $\text{DMSO-}d_6$

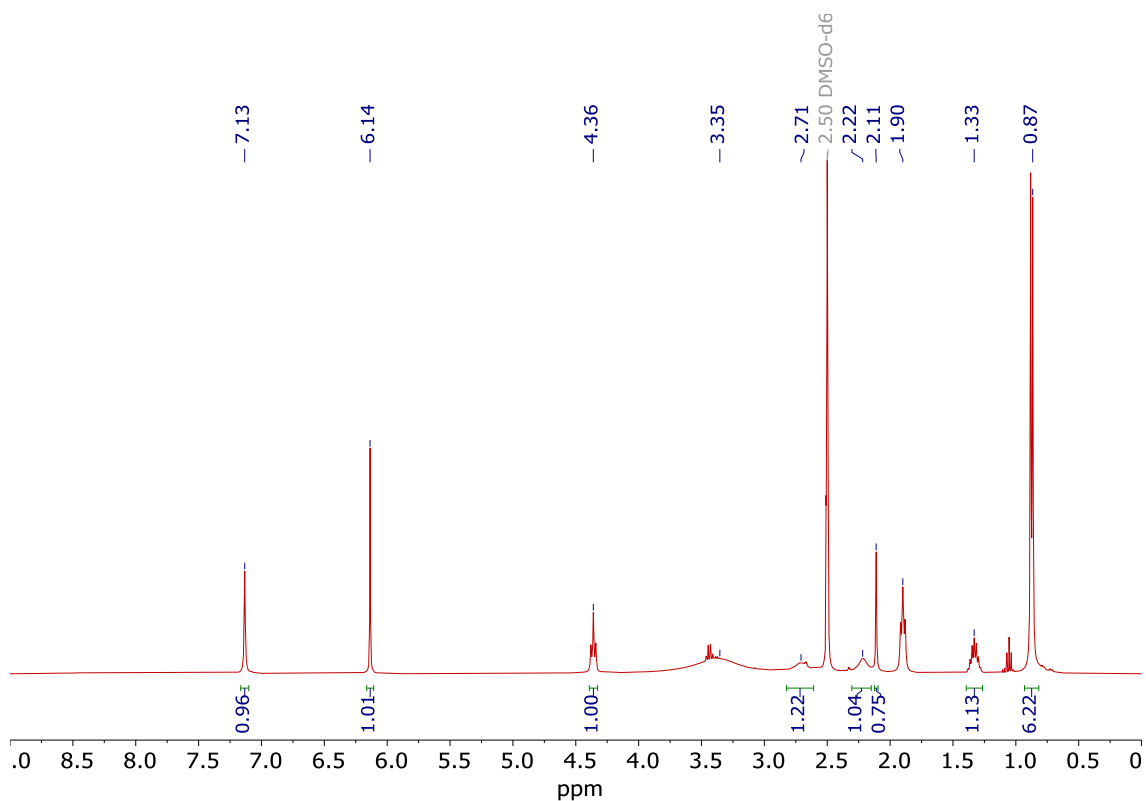


HSQC ^{13}C $\text{DMSO-}d_6$

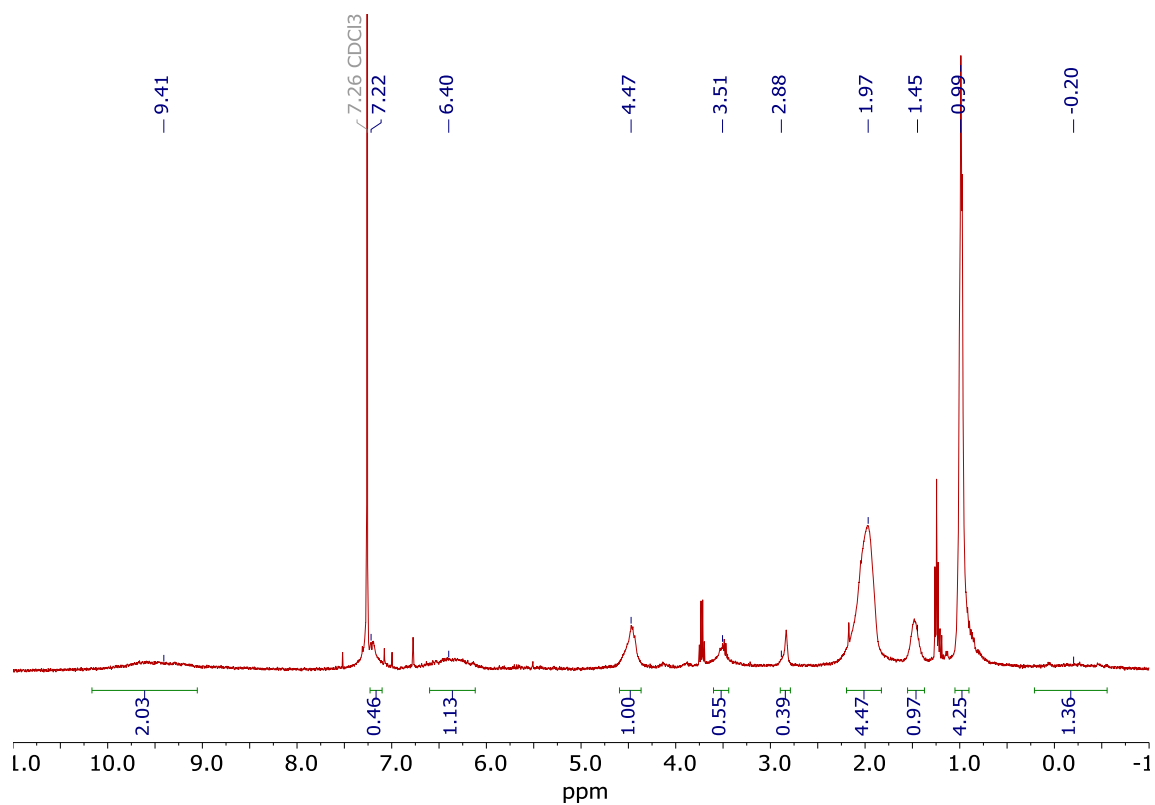


R[4]A:1-methylpiperazine

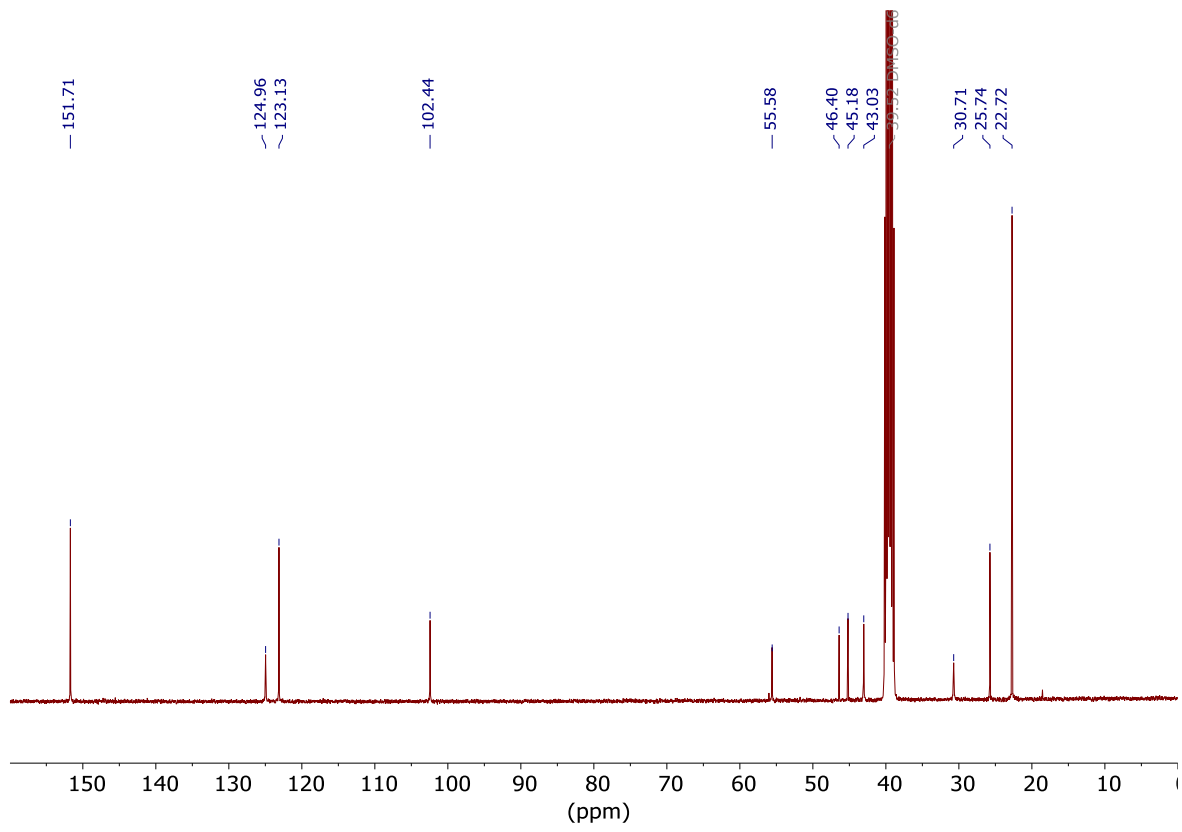
^1H NMR in DMSO



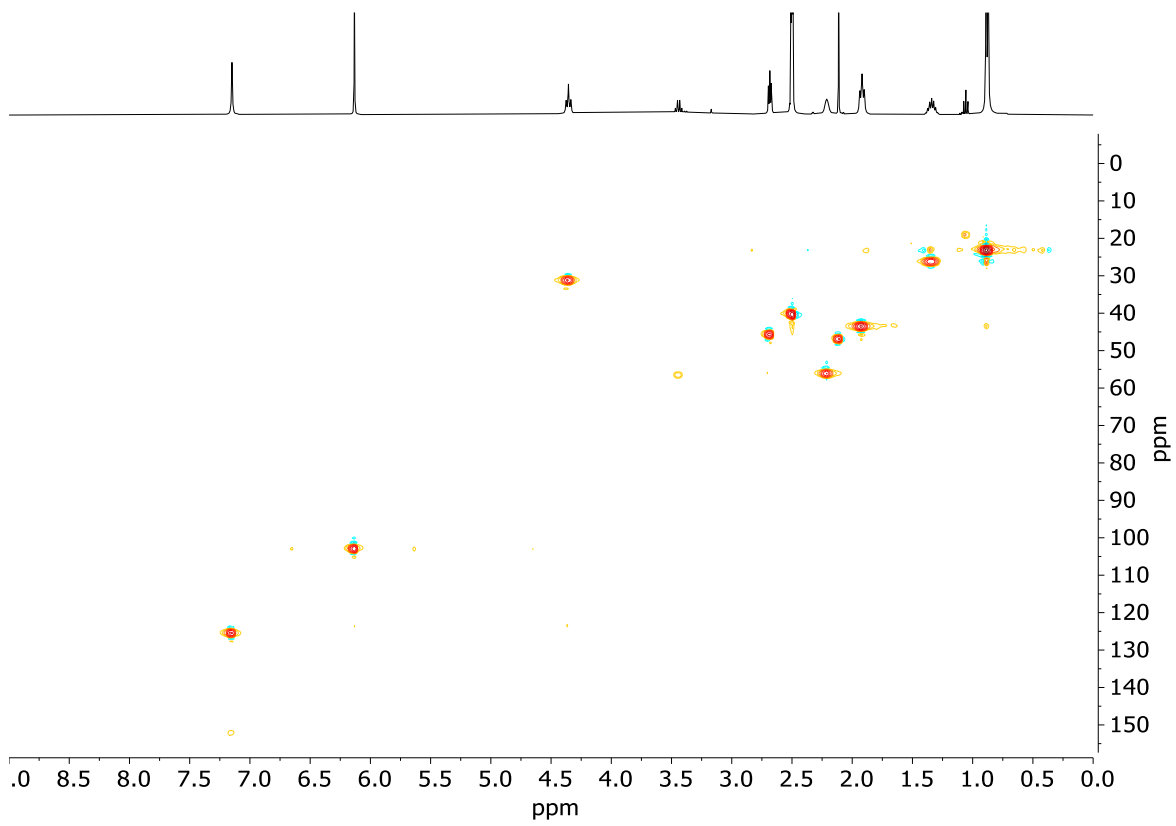
^1H NMR in CDCl_3



¹³C NMR in DMSO

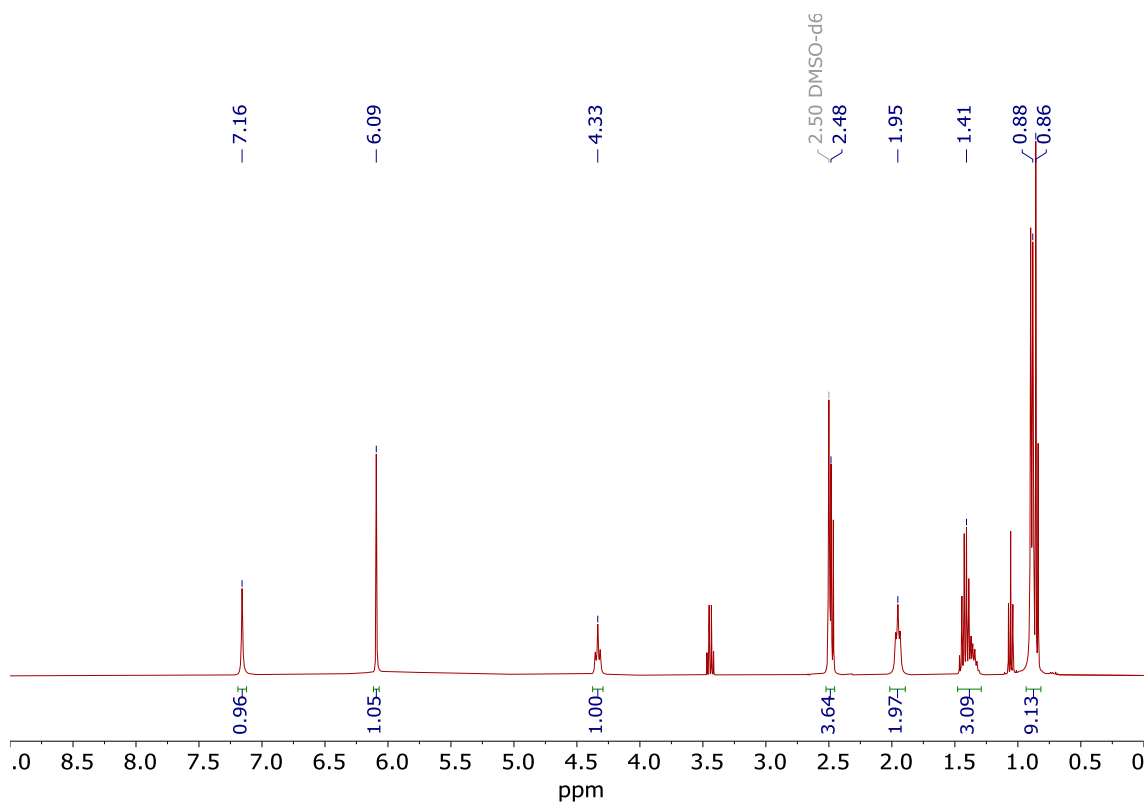


HSQC ¹³C DMSO-d₆

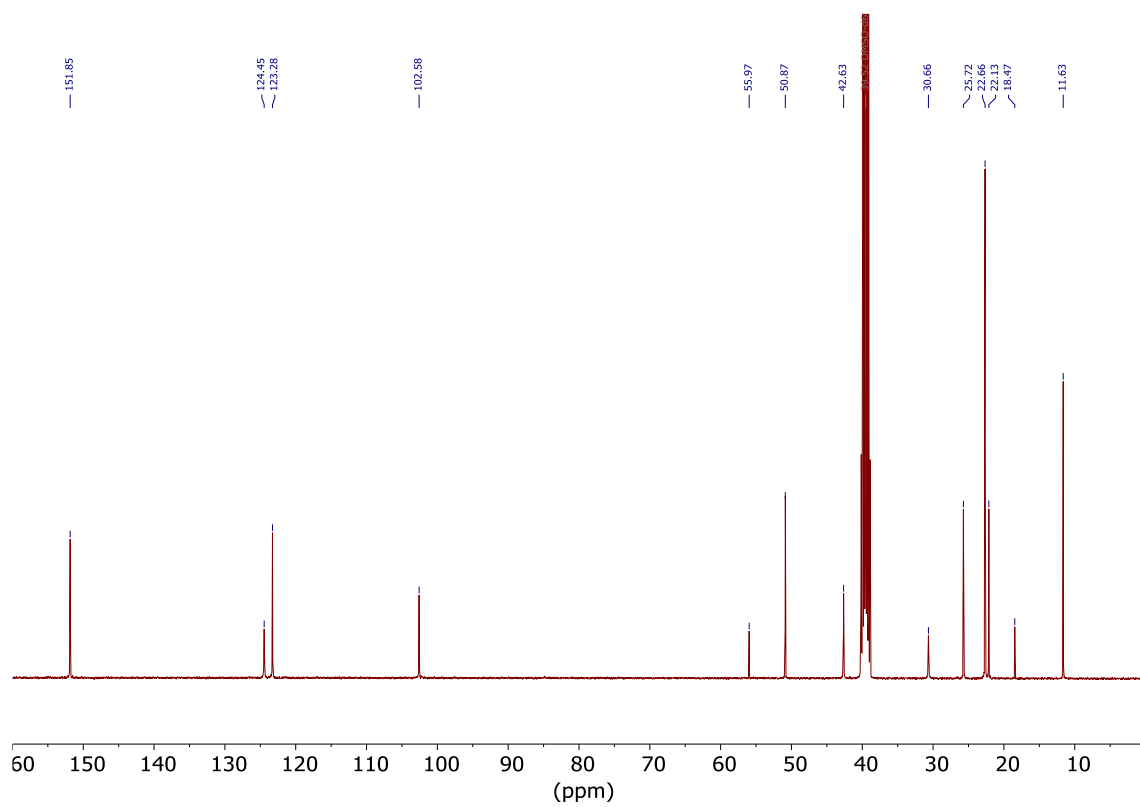


R[4]A:dipropylamine

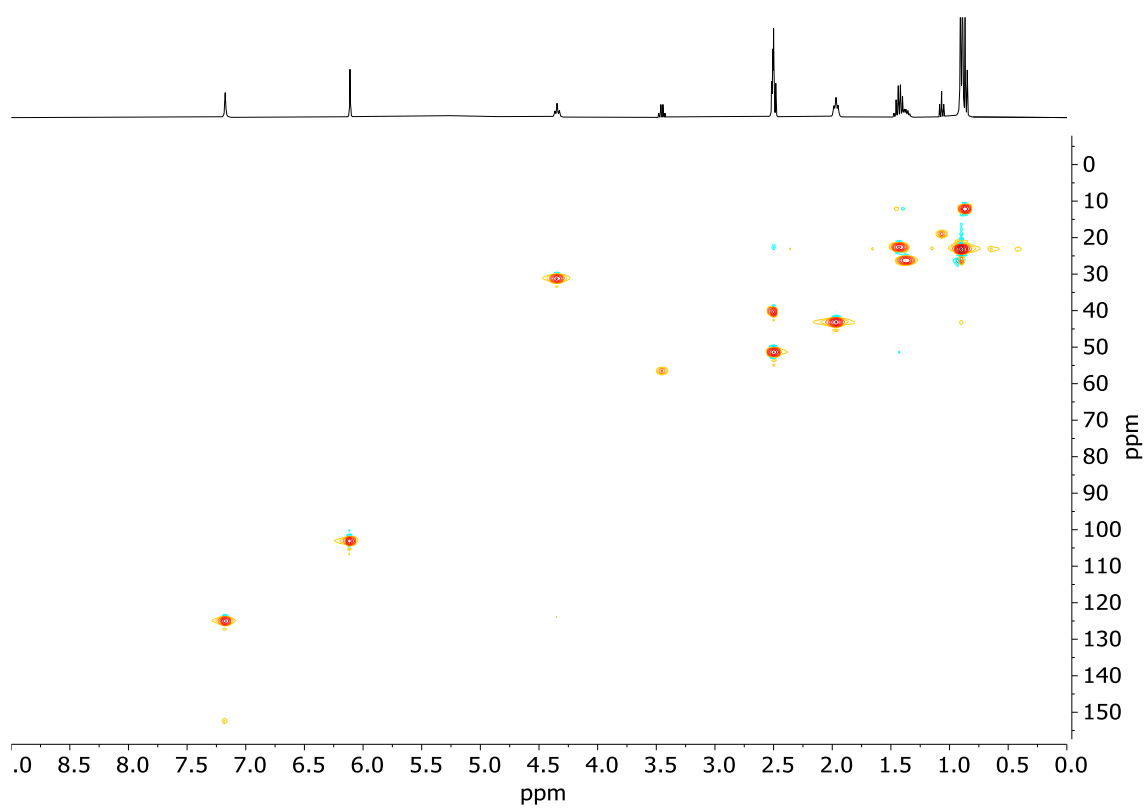
^1H NMR in DMSO



^{13}C NMR in DMSO

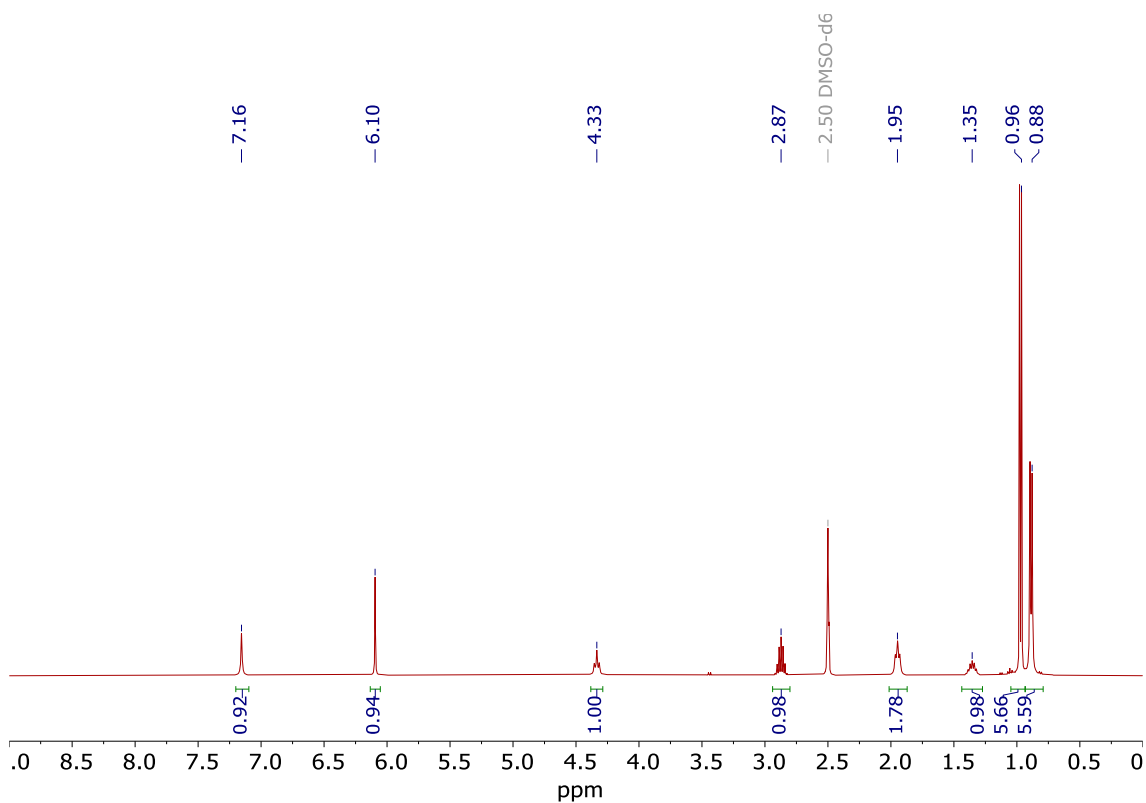


HSQC ^{13}C DMSO- d_6

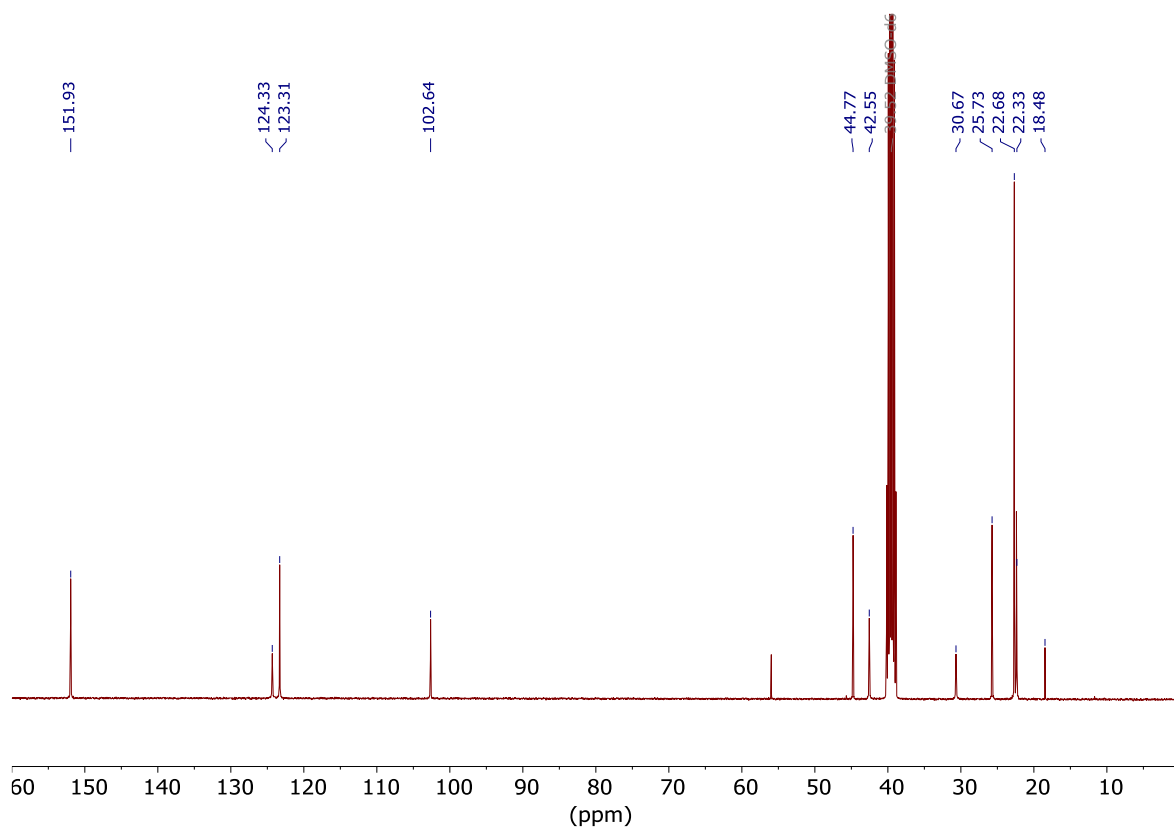


R[4]A:diisopropylamine

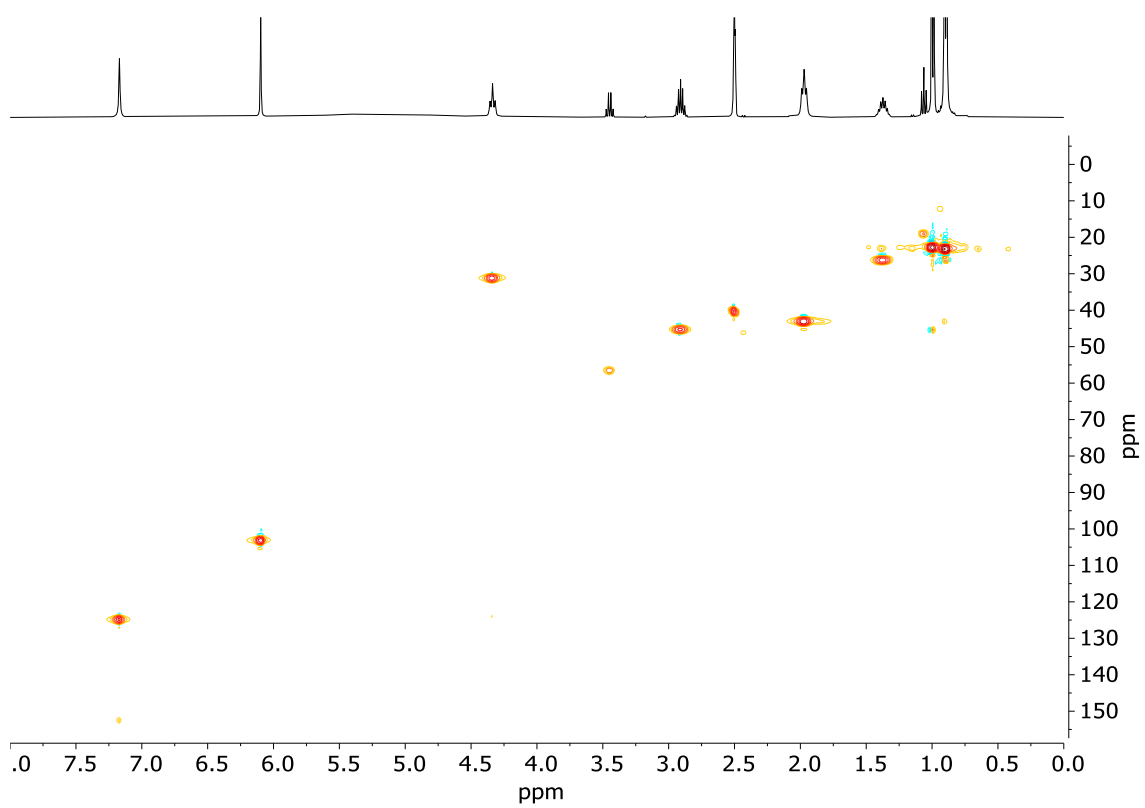
^1H NMR in DMSO



^{13}C NMR in DMSO



HSQC ^{13}C DMSO- d_6



2. The xyz coordinates of the optimized complex structures calculated by the PBE0-D4/mTZVPP method in CHCl₃ and DMSO

R[4]A:dimethylamine

CHCl ₃			DMSO				
C	-2.87994689139466	-1.96761078395866	2.51130567321679	C	-0.33578104570439	-3.26241287341443	0.09857154007913
C	-3.33327358405858	-2.82926851771368	1.51636327078323	C	-1.40350241630552	-3.99560909176605	-0.41149632292248
C	-2.49929449591604	-3.77259179376594	0.94240062398050	C	-1.89885862785128	-3.76810435970710	-1.68464847428640
C	-1.17838308186158	-3.88519445759472	1.36297758861142	C	-1.32514125402258	-2.79399999979684	-2.50001922203530
C	-0.68795440218617	-3.05319735806441	2.37769630547510	C	-0.21439119239064	-2.07082623855414	-2.03813935170798
C	-1.55309840341986	-2.09893980876998	2.89697365415763	C	0.22333914526436	-2.30870525771995	-0.74221996206378
O	-4.64382564073060	-2.70875720595452	1.11913957823504	O	-1.95862875422764	-4.95898644041347	-0.39772270365573
O	-0.41978756241288	-4.83472601636849	0.76359196602687	O	-1.85963961018018	-2.60636407558165	-3.72311944189635
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C	3.09015620984582	-1.71249916852219	0.30991505885961	C	-1.85359272265289	1.90836467039123	-3.42179315956524
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C	2.74660628993816	-0.04806505175259	2.03229862387539	C	-0.29445149293151	2.48623543139654	-1.66107256898858
C	1.92112951909823	-0.96753040299550	2.67016716204282	C	0.26859435019211	1.22467823256161	-1.83465913666821
O	2.05614856910418	-3.85612624725390	0.48270902603639	O	-1.74040536093806	-0.19629188559200	-4.50552705608141
C	3.02320135441616	1.31580712910084	2.63847938325711	C	0.25954426981118	3.45196378395765	-0.62926056559139
C	2.03369208816187	2.33323647529195	2.10383477969295	C	-0.42691221065590	3.23084654173533	0.70557676952527
C	2.36693865487050	3.16491762311636	1.03752376713843	C	-1.53451709072523	3.99278108077219	1.07334431359772
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C	0.19378332797785	4.18987753152245	1.07290798777434	C	-1.73286808388044	2.81160942987676	3.15898397872537
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C	0.75787958932818	2.47512686925352	2.63099254126617	C	-0.00906766417586	2.26138734196938	1.60671750086672
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C	-3.34720810110243	2.93464815775053	1.28032133604904	C	-1.73102086514281	-0.76308144594724	4.28918720867339
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H	-4.11780259876595	0.15997996820172	4.93066863096848	H	1.87284376289644	-3.23332885955502	2.75340365439308
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H	-5.45044219137359	-1.88788350122417	5.14147110288576	H	1.98897361051841	-5.52070554948596	1.88769394270820
H	4.01478712361768	1.30404509719680	0.30553899093040	H	-1.94042929241513	4.40422219648831	-1.51486850550542
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H	1.42504105153500	-3.96496249395155	6.97396040781825	H	4.70912572881541	-0.75641763590101	-3.08541537880954
H	3.07890466776693	-3.33933994217973	7.00605956501478	H	4.67373069824376	0.68224731423256	-4.11390801710793
H	2.02912668448664	-5.52422505911872	4.93480641096769	H	3.44393736757453	-1.94096899873587	-4.97770979004591
H	2.91360047599817	-4.81380903118214	3.57592923615452	H	1.83939070129494	-1.38617552388484	-5.46324842806266
H	3.67617454884255	-4.91932701394529	5.16197619079015	H	3.26949470482052	-0.45259923512249	-5.91893751190505
H	-3.30787324067583	-1.51760136899405	7.28961617415610	H	4.35500427330149	-3.74531466264181	1.11766631189157
H	-4.77456472136987	-0.54239574106693	7.12330003019045	H	4.00202225705153	-4.33561162056417	2.74824139230991
H	-4.89306325333532	-2.25998232440122	7.53758182787529	H	4.43901864128299	-5.47705133619558	1.46660995719086
H	-3.94932918363361	-3.32266457414763	4.20038494421033	H	1.25520181063536	-5.23879528014851	-0.46786857295628
H	-2.77706364305150	-3.33241193977013	5.48582634865982	H	2.67533685512783	-4.24644212636898	-0.80483840222406
H	-4.36520656136752	-4.01009517962877	5.87448994470006	H	2.86996479957397	-5.95835822442787	-0.39708189726457
H	-1.98352707834668	3.40165112731939	7.08590278927731	H	4.12544681266906	0.30523097562942	4.27369732837154
H	-1.03193321455596	4.86224039166491	6.78283062945403	H	3.87670441433551	1.94979359404225	4.7890529345906
H	-2.74045488754048	4.99282174359907	7.22913267704559	H	4.15887819535007	0.61939867673587	6.01360614424710
H	-4.16008104471293	3.77259129836180	4.00193434587368	H	0.85260234957239	-1.05092765807293	5.62487534380125
H	-3.82913076950025	2.71071721077074	5.37078082473734	H	2.27108725980994	-1.48686825750098	4.67005278969444
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H	2.26083589481013	3.79996569685234	5.02922747498444	H	2.34378988657527	4.16172833284573	2.08841071017239
H	3.86859428399450	4.52572554148359	5.17935192867922	H	2.65854647306675	5.87443149581373	1.76419282274927
H	-2.86094472229882	-4.42950988444746	0.15727339043780	H	-2.74726208254155	-4.33643046105139	-2.05429911623247
H	3.57321118217118	-1.99854284791499	-0.61724714999057	H	-2.70384670059752	2.18365551343217	-4.03779376125384
H	1.72875637005416	4.70062936244786	-0.32765329887654	H	-3.05864952386177	4.37572183581327	2.54117547940601
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N	1.77053593570723	-3.90613797093559	-2.09198750197819	N	-0.56744485600014	0.25169812575444	-6.73953154900436
C	2.89113234338114	-3.61929549018655	-2.98141918665644	C	-1.15433638281576	1.44726824868314	-7.36870177112661
C	0.62916159722827	-3.02390096089563	-2.32537193455765	C	-0.67084648458717	-0.95952477585697	-7.57139821553222
H	3.24447442545647	-2.60159009865442	-2.80119389673359	H	-2.21580832450595	1.26568515724359	-7.53568992180870
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H	0.92141492362093	-1.99560389105642	-2.09965555780573	H	-1.72581506247899	-1.17067592969183	-7.74513570526767
H	-0.18786143777288	-3.30358375323680	-1.65748782515978	H	-0.21215785298511	-1.79179319161936	-7.03819170454322
H	1.47445526319606	-4.86624199670005	-2.24130916039383	H	0.41300772611376	0.4319282559467	-6.52678026349669
H	3.70977547956113	-4.31166466444912	-2.77699566881905	H	-1.02823071769740	2.29522832910899	-6.69653215710594
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R[4]A:diethylamine

CHCl ₃			DMSO				
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C	-2.27493852485472	-4.16658349704245	1.12490180851704	C	-1.64564928119668	-3.94047146126942	-1.69148778446452
C	-0.95347463305956	-4.20770915045062	1.55334422665447	C	-1.08835698208510	-2.95518961408251	-2.50508743045993
C	-0.47628302372064	-3.26063249744402	2.46700202076469	C	-0.03134905783031	-2.16992555159032	-2.01743037204144
C	-1.34931457986129	-2.25872420543774	2.86821356144011	C	0.37145927234778	-2.36769099226871	-0.70377873329151
O	-4.42562809691485	-1.73275647627316	1.16197876384666	O	-1.72838850996354	-5.09341704734346	0.41263294586721
O	-0.16313013239669	-5.19011358971866	1.05272024395909	O	-1.58548351074687	-2.81271735323339	-3.74933475514357
C	0.93604261215575	-3.33452801844322	3.01234775238997	C	0.63371458628902	-1.13253265526870	-2.89955979550967
C	1.84168288945990	-2.33989495708357	2.31992278533894	C	-0.07473119578374	0.19954500284212	-2.78019834701748
C	2.37260907588807	-2.64091327519235	1.06348000511973	C	-1.18184862011498	0.47038620415137	-3.61176266363365
C	3.20101007558944	-1.73275647627316	0.42048130682298	C	-1.83520058338400	1.69886620917174	-3.46679401072829
C	3.48055822117007	-0.49508798998296	0.98534023596451	C	-1.42005664768560	2.64122595945093	-2.53421908715717
C	2.94960408800872	-0.15331003263125	2.23435931255065	C	-0.31481781574647	2.39253244327376	-1.71386905870267
C	2.14057521000524	-1.09623300728052	2.85996964482152	C	0.31088789523904	1.15717477445466	-1.85688433727011
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C	3.22611749180166	1.20222532120043	2.85958999014187	C	0.18151589793961	3.40462922019430	-0.69806310118999
C	2.31594071507587	2.23879089186258	2.22642413998741	C	-0.51929403000682	3.18409654712977	0.62957113522157
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C	1.94011411883407	4.01131579906971	0.61764160848118	C	-2.32246112980159	3.70533590406598	2.16139265869358
C	0.60665684333688	4.09811762633789	0.99873035329678	C	-1.85380156482724	2.75902444216223	3.06623413386217
C	0.11302760866967	3.28814513771127	2.02668508549401	C	-0.69922359198308	2.02113865125016	2.78097810623169
C	0.98009810959273	2.35590580389725	2.58337667703963	C	-0.08833469062113	2.23914199379192	1.55078751206607
O	4.10373290931307	3.00645458405950	0.88116428730868	O	-2.09250572442721	4.86246212590104	0.07362943091400
O	-0.15906040303307	5.01378312085947	0.34786447910084	O	-2.55450303285252	2.63258102424373	4.22345961927446
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C	-3.89257599129212	0.41146240827736	0.89106218890074	C	-1.65600617247198	-2.93266313955036	3.12466332708624
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O	-4.72412375021051	-0.47073163285154	0.28272200916032	O	-2.22391029348833	-4.15724223695619	2.96895192304114
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C	-3.83227999662479	3.68362394146017	4.43677601325848	C	1.85545147899843	-0.72244064622262	5.52308844657845
C	3.94678240517645	2.00156600201734	6.60286597281062	C	3.84707023132115	4.63681956123615	-0.18604226718554
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H	-4.59710530835747	-3.77987668965137	0.50159821357826	H	-2.46081204490567	-5.52981901219300	-0.03877127415298
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H	2.12203276084391	1.14746535416531	4.73791482900894	H	2.08117392588267	2.58482466953444	0.00067747131656
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R[4]A:pyrrolidine

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C	1.91700246539228	-2.37850936145881	2.33729998247060	C	-0.26931722734352	0.08499496885491	-2.78755664451598
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R[4]A:piperidine

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R[4]A:morpholine

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C	1.01282904382304	-1.48702234833770	-4.61199617345696	N	-2.27949028903520	0.73851193546321	-6.64811771215190
N	1.84222159713529	-2.67634747601815	-4.85294197413790	C	-1.98525841273801	-0.30513901163212	-7.65803816253649
C	1.1218447753591	-3.61955607934119	-5.71415901565728	C	-1.37378520583147	1.90155629392309	-6.80812973364698
C	-0.19494917919852	-3.97984504384539	-5.06000404033894	C	-0.52357813323278	-0.68477488113249	-7.55907714622049
O	-0.98642721463766	-2.82844874762399	-4.81802668083737	H	-2.21690391293286	0.09479177143053	-8.64825179050493
C	-0.29583692425255	-1.91089364094473	-3.98366678884003	C	0.05901731244712	1.42144359840355	-6.74488555465582
H	0.81038997285072	-0.95803208229135	-5.55390050655867	H	-3.24771578279693	1.04122133571486	-6.73605401980267
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H	2.69706779613208	-2.39076692312184	-5.31969281520689	H	-2.62453304296008	-1.16677131756404	-7.45758638974829
H	1.72689136022342	-4.52069853394909	-5.84566117745714	H	-1.58034277317524	2.61096645034991	-6.00571849866481
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H	-0.00724160015550	-4.50704850973103	-4.11543923526255	H	0.73406449082850	2.25760297810421	-6.93217015760431
H	-0.77667655031409	-4.63177040415340	-5.71469669978422	O	0.31258904323313	0.44461632589700	-7.73995002201776
H	-0.11378257562276	-2.36568432148456	-3.00047189304806	H	-0.27700999021017	-1.39957524502388	-8.34531542415367
H	-0.95119456094812	-1.04779052810413	-3.85115749936850	H	0.28035722159441	1.01145089546566	-5.74956331653304

R[4]A:N-methylpiperazine

CHCl ₃			DMSO				
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C	-3.11894624877130	-3.21487344252896	1.55922699863926	C	-1.18592541257472	-4.15429930429338	-0.34854681482190
C	-2.27190609689501	-4.21038545887636	1.10570197363280	C	-1.68390763659346	-4.00384065757604	-1.63153161126692
C	-0.95321740494680	-4.25170860717849	1.54264428370126	C	-1.18293586063838	-3.00806132698438	-2.46442374466738
C	-0.48213010280800	-3.30612345363639	2.46007187831730	C	-0.15723766711468	-2.16751776693749	-2.01378814803400
C	-1.35942792241121	-2.30886401708951	2.86293465533992	C	0.28538627735160	-2.33433242266568	-0.70732583846457
O	-4.42324401583216	-3.14465334283887	1.13239876471813	O	-1.66393785514182	-5.13732768296273	0.48258560187857
O	-0.15852219531265	-5.23225399027711	1.04428176902225	O	-1.71224301013567	-2.92288047288805	-3.70972332594182
C	0.92461798118818	-3.38794700334267	3.01420291583988	C	0.46035541620969	-1.12174271838157	-2.91911924787180
C	1.86369736199840	-2.41485600387079	2.33513247917215	C	-0.24038588871012	0.21258943909093	-2.76110460040780
C	2.46634755361933	-2.75380530829415	1.12245373001815	C	-1.34422323520440	0.52595101738349	-3.56182027800903
C	3.39606532896200	-1.90687914892557	0.54169275751610	C	-2.00126863366294	1.73955997196469	-3.40262574030789
C	3.66629554346160	-0.65979041088877	1.09020264434195	C	-1.56694855408475	2.66721731244088	-2.46338472971718
C	3.02352888278457	-0.25428231808462	2.26460280711981	C	-0.45621778896294	2.39124556067868	-1.65896615663924
C	2.14983294993821	-1.16075378852872	2.85786361835071	C	0.15699582368691	1.15346440833783	-1.82167811778360
O	2.11315460722800	-3.90177972492341	0.47213393323065	O	-1.78003597269465	-0.37619373363631	-4.47445764166912
C	3.24145292286199	1.13139760885734	2.84649538471990	C	0.06401754132508	3.39076012534860	-0.64194826178485
C	2.31186671678126	2.10875694114832	2.14736526325358	C	-0.61051839882365	3.16006197064714	0.69747847138020
C	2.75262745081103	2.87802061816306	1.07243924426598	C	-1.75100978748061	3.87641305542344	1.05631643831142
C	1.89548610765405	3.71204824340823	0.37773609497064	C	-2.39612200051388	3.65249073675521	2.25968255493545
C	0.56678161785301	3.82869070871291	0.76806700994778	C	-1.89779758991910	2.71248411760751	3.15501525665771
C	0.0990833538931	3.12998280145144	1.88582657184073	C	-0.73253647092767	1.99912384377286	2.85296790578575
C	0.98138662679571	2.25863134947763	2.51441339865637	C	-0.14668928082521	2.22531469578402	1.61257655238559
O	4.07695943541357	2.77863831046283	0.71832259774892	O	-2.21548135366058	4.81867620045773	0.17290364950975
O	-0.20975985386286	4.66691488745863	0.03465669517167	O	-2.58063152424657	2.56659183883264	4.32060421019837
C	-1.30088769278264	3.35197031506231	0.24076327082203	O	-0.10207533695477	1.04246757056265	3.84998312710796
C	-2.26315131683336	2.30215116553347	1.91381211469193	C	-0.60149224218949	-0.37090064896236	3.62182282865771
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C	-3.85849739585980	1.56672202237555	0.24358739454821	C	-2.20163391592356	-2.12636696508508	4.10437891701957
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C	-3.61182667323875	-1.13926692633126	2.92010539690813	C	0.31759381187003	-3.47298400146768	1.56874764375215
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C	3.85428189643814	2.31256451048248	5.06816599640658	C	2.22529734420609	4.69783730523159	-0.06386312669214
C	-2.4388994459832	4.31024514434020	4.55281054978772	C	2.09849699380926	0.76292389251563	5.18501874707545
C	-4.31627580288563	-1.89655076667012	5.29444665887635	C	2.66628041814417	-4.53568827454295	1.323536807101237
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C	-3.80932779596756	3.67666134951604	4.34496759068525	C	1.92552874916584	-0.71137794964907	5.53012939903257
C	3.85503050956706	2.07741732371099	6.57502804864156	C	3.74273110766827	4.59970381295694	-0.17726804783324
C	3.25731682206292	3.67895433348236	4.7524222329790	C	1.83090683060176	5.05525568660243	1.36401271259706
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H	-4.59105500901223	-3.82452723947722	0.46984560288907	H	-2.38335702047338	-5.61635348148014	0.05371226073080
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C	-0.55980215811311	-1.89020552784022	-1.05421167509589	C	-0.59662608518423	2.28174097775350	-6.83375978292714
H	-0.57446870510877	-4.02977051781516	-1.22883483459060	H	-3.30948564994601	0.37326807017023	-6.97577704976751
H	1.45441064094053	-4.10630924281798	-2.47342905372659	H	-2.35664172838805	2.26783447691579	-8.05963181896019
H	-0.70411777200145	-3.192063943338534	-2.77481724981261	H	-1.70051169141220	-1.30987864023435	-7.49259507686868
H	2.83708671496568	-2.17207227917043	-2.73760818248524	H	-2.66673759628408	2.57651850980733	-6.33933006417525
N	-0.08325810304711	-0.72772076480859	-1.78828753762544	H	0.23786292846176	-0.22832546626092	-6.46187585824221
H	1.68332484986784	0.02703839429929	-2.59384003144912	H	-0.40704361590047	3.33852122730617	-7.04212715496927
H	1.88127415109811	-0.75019849496586	-1.01433147417036	N	0.21678664159698	1.47139430137649	-7.72693877449460
H	-0.13015868909584	-1.92472688213042	-0.03739512124031	H	0.55953961953489	-0.53390859728249	-8.17909032013805
H	-1.64566608142505	-1.81727818658303	-0.94319390147468	H	-0.32615808252658	2.09719405647792	-5.77720659270895
C	-0.40813866346446	0.48821472165797	-1.06857423732799	C	1.62324446346404	1.77151756094140	-7.55056239522980
H	0.07530355762802	0.52667811393112	-0.07617405342547	H	1.96694655733993	1.57659215032935	-6.51991134038768
H	-1.48850049236987	0.55809594976767	-0.92231614907203	H	1.80732851305891	2.82445876694932	-7.77907889256488
H	-0.07647145167211	1.35922201855253	-1.64029005975517	H	2.22003071049791	1.15893063765740	-8.23103461094546

R[4]A:dipropylamine

R[4]A:diisopropylamine

DMSO			DMSO				
C	-0.54894533414278	-3.83697226838031	0.45577138441533	C	0.24680831404755	-3.28813363794180	-0.19395472925174
C	-0.75463221619290	-4.60350145729316	-0.68720678772490	C	-0.85971055596321	-4.06973279831546	0.12356839544253
C	0.27637887266291	-5.31635401444718	-1.27688634803883	C	-1.44201038793705	-4.02534331290871	1.37988922834128
C	1.55614673569532	-5.28969132080194	-0.72579108294016	C	-0.92268973818218	-3.19077344395668	2.36841978700290
C	1.79352235479081	-4.55691259242647	0.44812272677284	C	0.21306415378043	-2.41185982715558	2.09396935510054
C	0.73583736133708	-3.83354955577959	0.98342821631841	C	0.74320019492683	-2.46911336116035	0.81211207929671
O	-2.02163019888835	-4.62295846203446	-1.22000696300858	O	-1.36397465844066	-4.88709427589395	-0.86117855692010
O	2.51911733975550	-6.00112987022362	-1.34745667972981	O	-1.53417837761500	-3.18372623304008	3.56968529217181
C	3.16047276286229	-4.56506387542456	1.10658144793110	C	0.83204555759930	-1.53795058168802	3.16924434297727
C	4.03302285954120	-3.45014983548159	0.56817753943854	C	0.22071054049069	-0.15223015058456	3.16067432744450
C	4.79695395007653	-3.67477645726177	-0.59719823000116	C	-0.96814957824520	0.08103800676264	3.88760127762487
C	5.57612036465789	-2.62293114256076	-1.09400205914966	C	-1.53003746013274	1.36339651952003	3.84399771417659
C	5.60945697994659	-1.38299213769916	-0.46726167557398	C	-0.94361384332213	2.39236296169507	3.11663583444469
C	4.87928198566691	-1.15388302042371	0.70201637084461	C	0.24485153364993	2.18209962618212	2.41190024558803
C	4.09176614381346	-2.20338776161852	1.16928917545512	C	0.77786102307150	0.89548763357717	2.44669128952419
O	4.77102536744348	-4.85037597217965	-1.21320594098026	O	-1.53880774083693	-0.88550429364258	4.59078026344940
C	4.92328178015810	0.17887875967805	1.42769005581398	C	0.92165004628295	3.29045220525175	1.62362962828567
C	3.82645664053607	1.08609497712735	0.90239601403651	C	0.39558888056427	3.29886658902716	0.20049945063012
C	4.08355572477249	2.01585046092249	-0.10119648454923	C	-0.65065505619102	4.13681728810707	-0.17404465349194
C	3.07991496898563	2.81105232281552	-0.62893975640012	C	-1.17428868391018	4.11398733992790	-1.45606439840830
C	1.77425023391266	2.70506029753844	-0.15287276741161	C	-0.65041260933629	3.25047940366966	-2.41684389155676
C	1.48501808122944	1.80741107491848	0.88566081120315	C	0.43228398149420	2.42069028910074	-2.08739162275537
C	2.51696423510639	1.00765810390929	1.35977505932514	C	0.89917632174190	2.45288298968226	-0.77994106156573
O	5.37650190811709	2.11614268607897	-0.55944361975945	O	-1.15574453053746	4.98994001406697	0.77993829822556
O	0.83676811594468	3.50129836404659	-0.70592653460793	O	-1.20461277742542	3.27107112248994	-3.64601247953120
C	0.09205940413750	1.72919101993184	1.48429200773710	C	1.07928057227783	1.52750559773057	-3.13201734256508
C	-0.74403178674989	0.69615499558413	0.75555548260902	C	0.40734824695667	0.16986194245340	-3.15351350557429
C	-1.45863179405044	1.08747312331824	-0.39842734711060	C	-0.73515792909419	-0.101011463827440	-3.96588128560722
C	-2.23283397780175	0.12823196112671	-1.06062289906466	C	-1.35873499510598	-1.26400448786964	-3.96330688211989
C	-2.29683453890661	-1.18709155118217	-0.61622783775956	C	-0.87602885867704	-2.31563321993219	-3.19299421151957
C	-1.59900188855834	-1.58890949084961	0.52607958634150	C	0.26692604786617	-2.15932647649946	-2.40581678468624
O	-0.82041677850315	-0.62443180125099	1.16339874505251	C	0.85793734180807	-0.89701748942790	-2.39659128501433
O	-1.39599912611168	2.33354015548978	-0.84954118869850	O	-1.20312456542621	0.98241129905800	-4.70704330884632
O	-3.08434294489430	-2.03718788537061	-1.34245932792968	O	-1.56677300630153	-3.49309887848642	-3.27153031384819
C	-1.67114301126848	-3.01099361995754	1.05452976538472	C	0.84247632973763	-3.30241371997103	-1.58809073014004
C	3.06520624911298	-4.57889341031669	2.63345584352509	C	2.36044154313218	-1.53138500018391	3.10165978658560
C	4.92405883273517	0.00668025040421	2.95347642857660	C	2.45117573842004	3.22084037846120	1.72994941562861
C	0.14170254761361	1.58389223755861	3.01103967374735	C	2.60683187306017	1.50142798973380	-2.99432935166826
C	-1.73787631811826	-3.05288571305676	2.58742115530145	C	2.37715737672784	-3.31352711584692	-1.61829531721519
C	4.39418988130090	-4.80538285442969	3.35272424819678	C	3.04779194908675	-0.84791885775637	4.28327559811865
C	5.53638358506351	1.16406008648841	3.74281492060938	C	3.19783619075963	4.52425808333178	1.44384551388107
C	-1.09701134418740	2.08006358470297	3.76014078624009	C	3.37258440611241	1.18215891363984	-4.27979412924295
C	-2.36099713283221	-4.31441357016393	3.18614970666972	C	3.03822478898899	-4.65894693213729	-1.31731862649218
O	6.40127173240170	-0.43069513747337	-1.04429424857389	O	-1.57854189885780	3.60205910996590	3.15375888755193
C	4.23052401000203	-4.54742456366536	4.84575533557621	C	4.53634730375775	-0.68780908011264	3.99719255706440
C	4.94157303883677	-6.20653550302310	3.10981067827696	C	2.83183004967314	-1.60603426828711	5.58771019041458
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C	-1.58761172444015	-5.59262445136390	2.88482045233825	C	2.77936116214942	-5.17750945002017	0.09256821216348
C	-0.78571673071265	2.18026513277263	5.24996393812063	C	4.86499661426105	1.39711509748442	-4.05146362425693
C	-2.33520710607985	1.21901798034477	3.54372354413280	C	3.12312694953593	-0.22029740648676	-4.82136732043403
C	5.65607178467845	0.76834298794473	5.21086248395617	C	4.67575020246553	4.33964771069855	1.77285799316651
C	4.76902562157024	2.47430415879035	3.61355171902503	C	3.04178562008661	5.03146581931887	0.01466169141754
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H	-2.03127091804016	-5.14037650470962	-2.03426144756408	H	-2.16845163534829	-5.32200449726434	-0.55360936116235
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H	5.50579674321528	-0.89479886257174	3.17994195805155	H	2.69122322929986	2.91948379239834	2.75673211425421
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H	-2.34337964191010	-2.19779261230409	2.91040548201361	H	2.68388552297861	-3.01171012804362	-2.62692221494737
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H	0.09956657715835	-5.89419772411695	-2.18047474694136	H	-2.31684774088892	-4.63095848361944	1.60295410627343
H	6.14806514574243	-2.76395607505031	-2.00671468102053	H	-2.45755023152686	1.55756690867212	4.37534388268371
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H	-2.77821734898857	0.41108824245985	-1.95704674540196	H	-2.25435336659401	-1.41938788123912	-4.55784639883514
N	-3.51379723771508	3.59986717075679	-1.53885147824531	N	-2.36528203661099	0.58526405028060	-6.98734920925885
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C	-3.54769326766767	3.63773002574058	-3.01858602816186	C	-3.86370452120151	0.56839355248363	-6.88742148582399
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H	-3.73708916450134	2.61490086629436	-3.35788635867106	H	-4.15729559120715	-0.48063342888255	-6.99204872536063
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H	-3.48614636236290	5.01144106189675	-5.41571024896516	H	-1.86268170323342	1.62271422087828	6.80073324882086
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H	-4.85896815831128	4.83559324129088	1.25763765569992	C	-4.45491649280993	-0.85093271312632	5.91005216510134
H	-3.14821806297840	4.40001667175555	1.10000553192411	C	-1.82839410760231	1.20093798998183	8.90696137008237
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C	8.10767102137763	-5.33501745185295	-1.11777459812594	H	0.51866669655388	1.44573469086779	7.52977655185475
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H	8.19744825786209	-4.26095959366419	-1.29904647388770	H	-3.78214486866937	-0.67423656906924	9.31095213406345
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