Electronic Supplementary Material (ESI) for MedChemComm.

Acetophenone derivatives: novel and potent small molecule inhibitors of Monoamine Oxidase B

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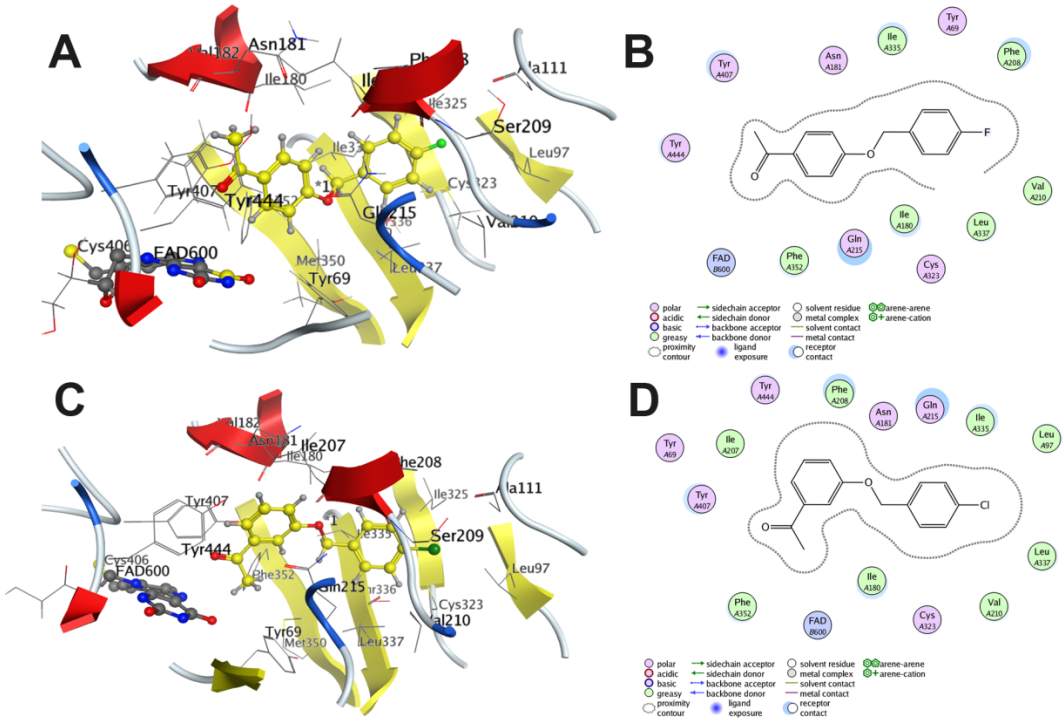
Table S1. Physical properties of compounds **1a-1u** and **2a-2m**.

Compounds	MW [a]	C log P [a]	HBA [a]	HBD [a]	PAS [a]	Log BB [a]
1a	226.27	3.569	2	0	26.3	0.292248
1b	240.3	4.018	2	0	26.3	0.360496
1c	240.3	4.068	2	0	26.3	0.368096
1d	240.3	4.068	2	0	26.3	0.368096
1e	271.27	3.232	4	0	78.11	-0.525764
1f	271.27	3.312	4	0	78.11	-0.513604
1g	271.27	3.312	4	0	78.11	-0.513604
1h	244.26	3.712	3	0	26.3	0.313984
1i	244.26	3.712	3	0	26.3	0.313984
1j	244.26	3.712	3	0	26.3	0.313984
1k	262.25	3.855	4	0	26.3	0.33572
1l	262.25	3.785	4	0	26.3	0.32508
1m	280.24	3.858	5	0	26.3	0.336176
1n	260.72	4.282	3	0	26.3	0.400624
1o	260.72	4.282	3	0	26.3	0.400624
1p	260.72	4.282	3	0	26.3	0.400624
1q	294.27	4.452	5	0	26.3	0.426464
1r	294.27	4.452	5	0	26.3	0.426464
1s	294.27	4.452	5	0	26.3	0.426464
1t	305.17	4.432	3	0	26.3	0.423424
1u	305.17	4.432	3	0	26.3	0.423424
2a	226.27	3.569	2	0	26.3	0.292248
2b	244.26	3.712	3	0	26.3	0.313984
2c	244.26	3.712	3	0	26.3	0.313984
2d	260.72	4.282	3	0	26.3	0.400624
2e	260.72	4.282	3	0	26.3	0.400624
2f	305.17	4.432	3	0	26.3	0.423424
2g	305.17	4.432	3	0	26.3	0.423424
2h	240.3	4.068	2	0	26.3	0.368096
2i	240.3	4.068	2	0	26.3	0.368096
2j	294.27	4.452	5	0	26.3	0.426464
2k	294.27	4.452	5	0	26.3	0.426464
2l	271.27	3.312	4	0	78.11	-0.513604
2m	271.27	3.312	4	0	78.11	-0.513604
Rules	≤450	≤5.0	≤10	≤5	≤90	≥-1.0

[a] MW: molecular weight; C log P: calculated logarithm of the octanol-water partition coefficient; HBA: hydrogen-bond acceptor atoms; HBD: hydrogen-bond donor atoms; PSA: polar surface area; log BB = 0.0148 × PSA + 0.152 × C log P + 0.130.

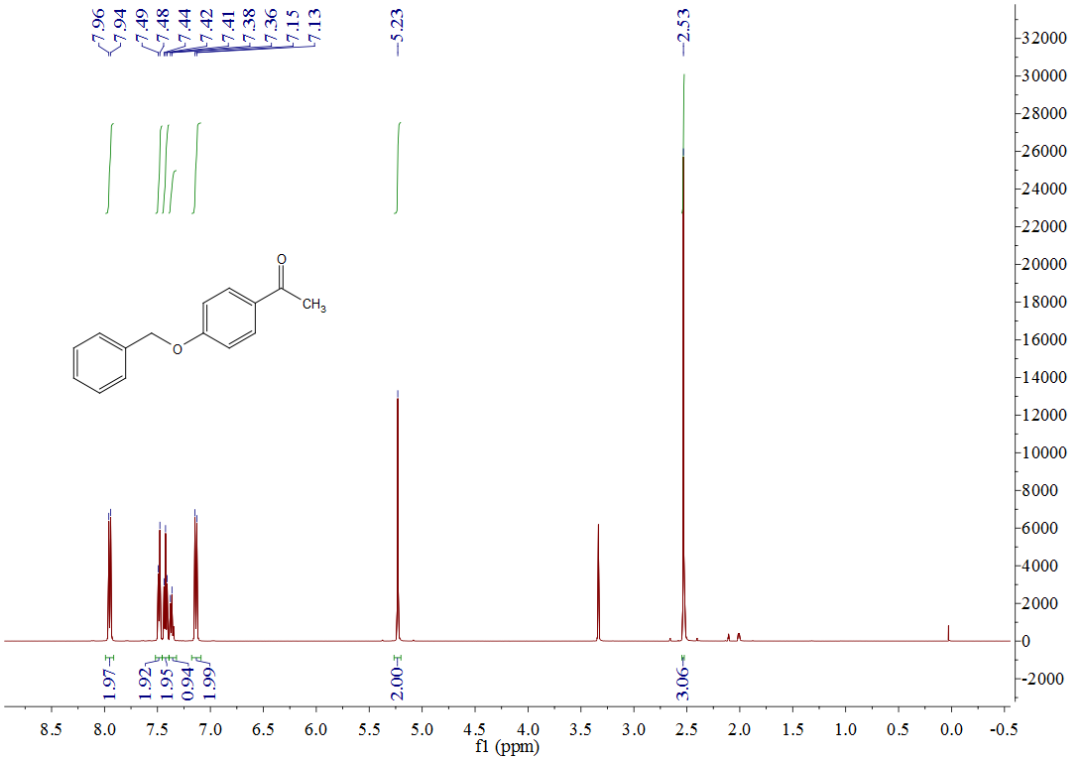
Figure S1. Docking pictures of compounds **1j** and **2e** with MAO-A.



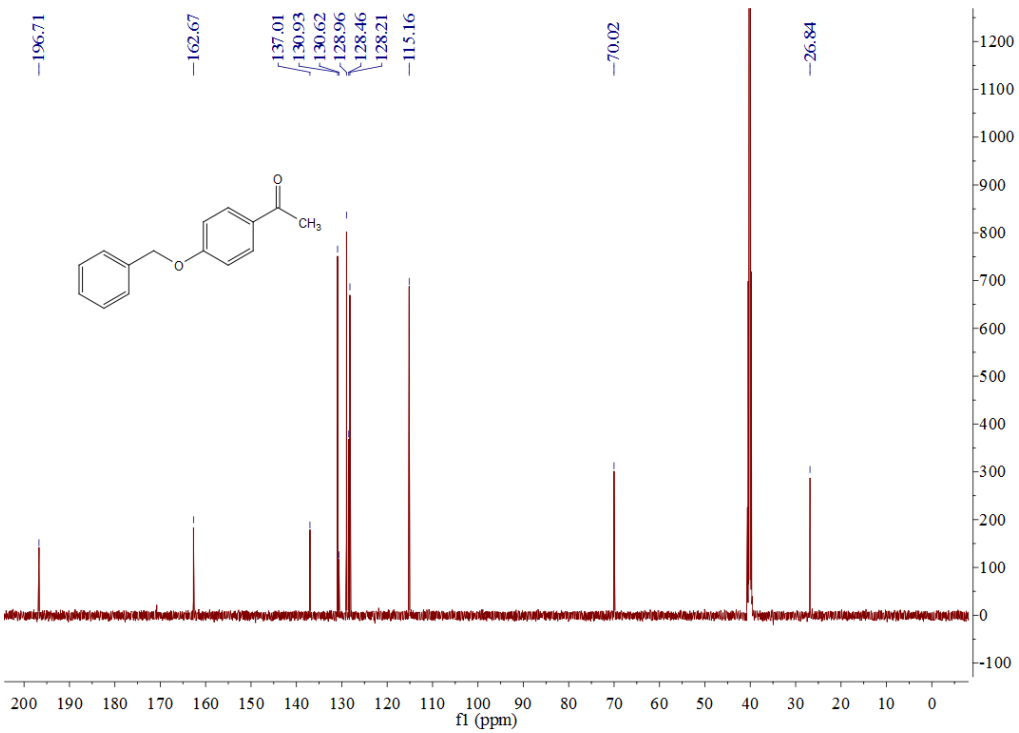
(A) 3D docking model of compound **1j** with MAO-A. Atom colors: yellow-carbon atoms of **1j**, gray-carbon atoms of residues of MAO-A, dark blue-nitrogen atoms, red-oxygen atoms. The dashed lines represent the interactions between the protein and the ligand. (B) 2D schematic diagram of docking model of compound **1j** with MAO-A. (C) 3D docking model of compound **2e** with MAO-A. (D) 2D schematic diagram of docking model of compound **2e** with MAO-A. The figure was prepared using the ligand interactions application in MOE.

Figure S2. The representative ^{1}H NMR, ^{13}C NMR and HRMS (ESI) spectrums of compounds **1a**, **1j**, **2a** and **2e**.

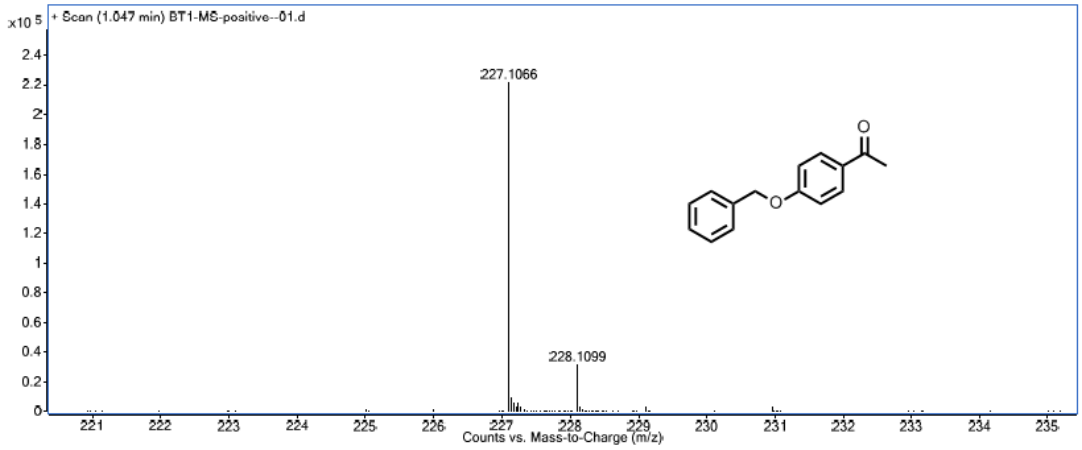
^{1}H NMR spectrum of compound 1a in DMSO



^{13}C NMR spectrum of compound 1a in DMSO



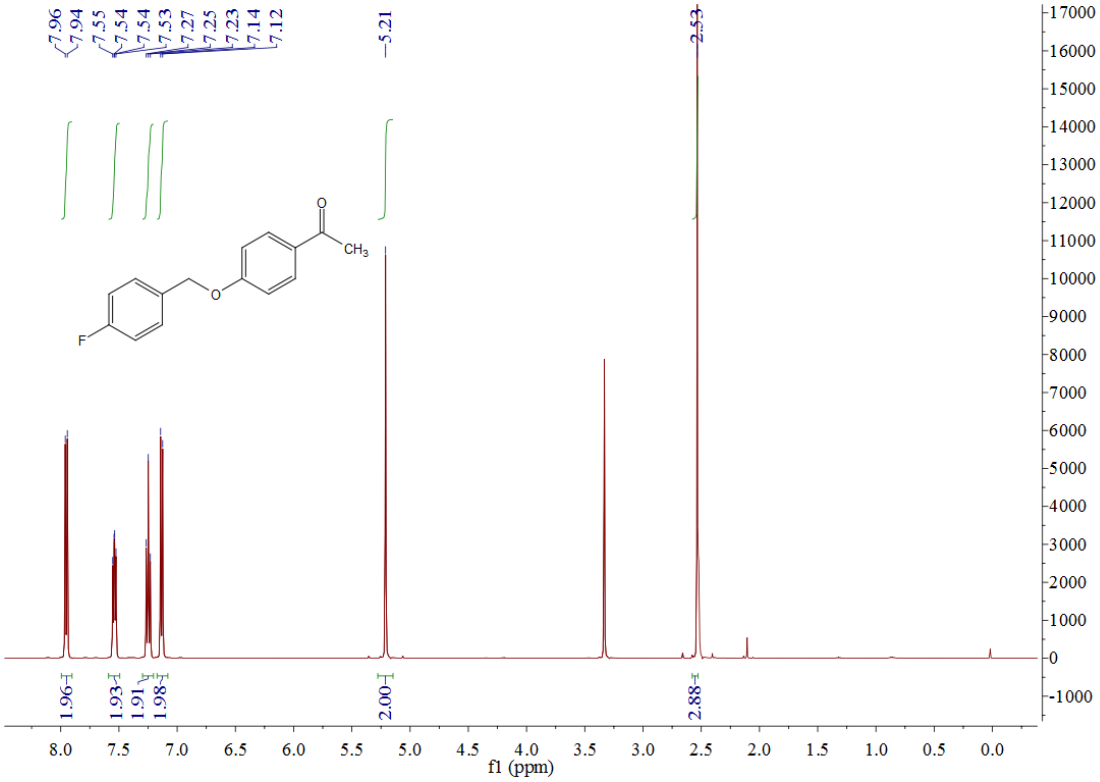
HRMS (ESI) spectrum of compound 1a



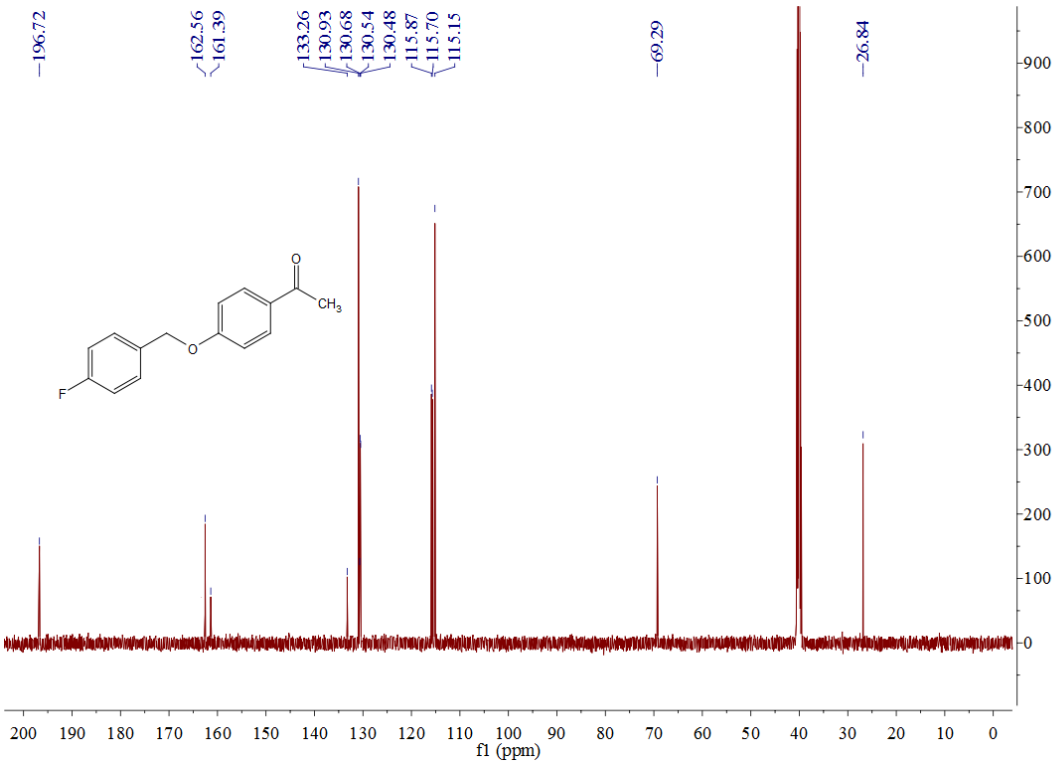
Elemental Composition Calculator

Target m/z:	227.1066	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C15H15O2		227.1067		0.41	

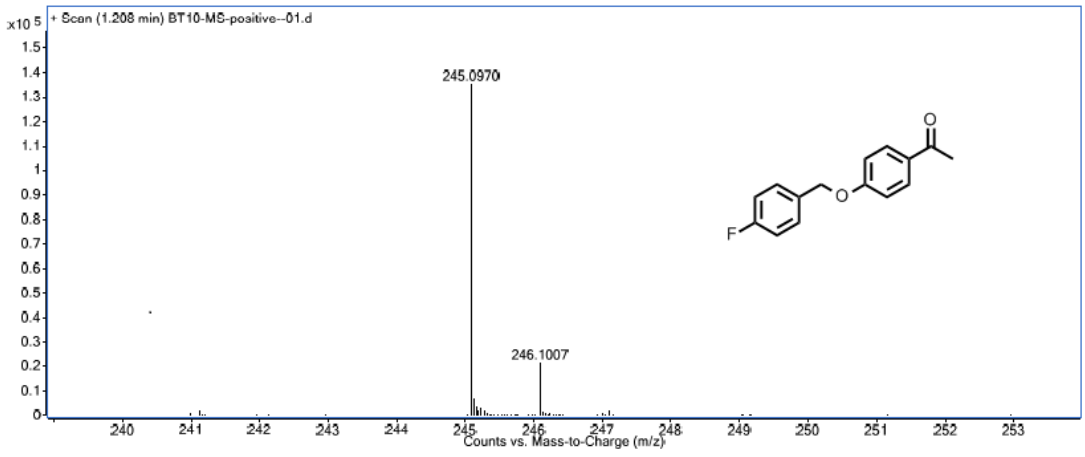
^{1}H NMR spectrum of compound 1j in DMSO



^{13}C NMR spectrum of compound 1j in DMSO



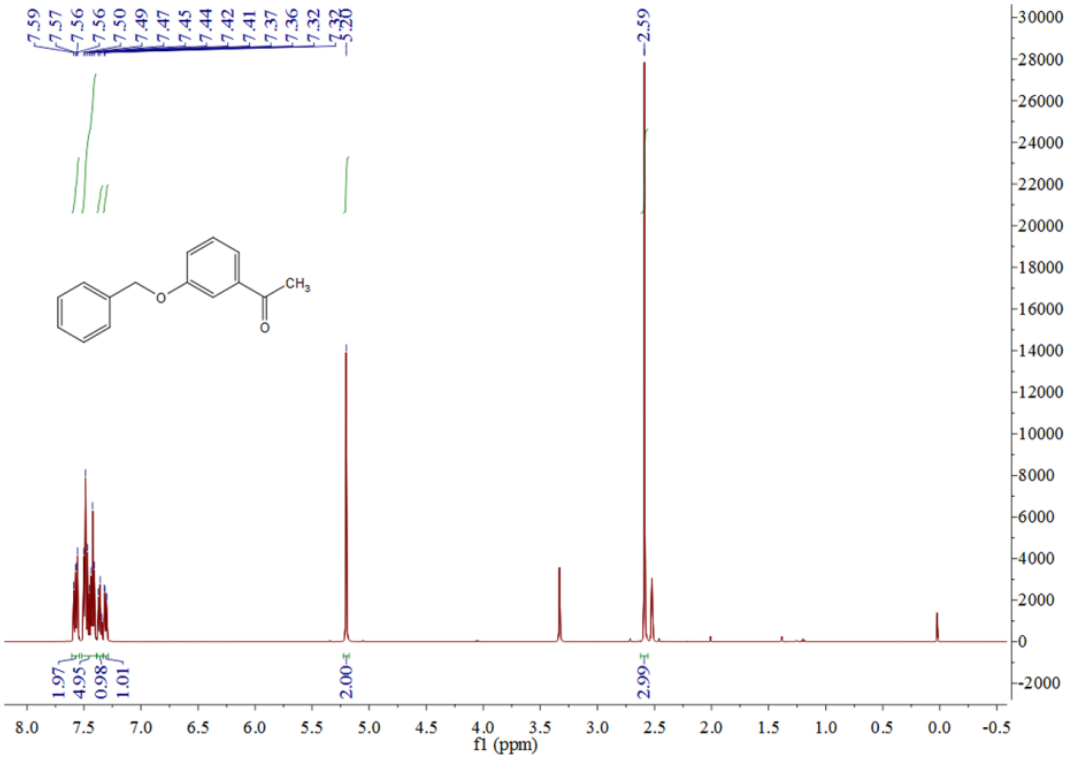
HRMS (ESI) spectrum of compound 1j



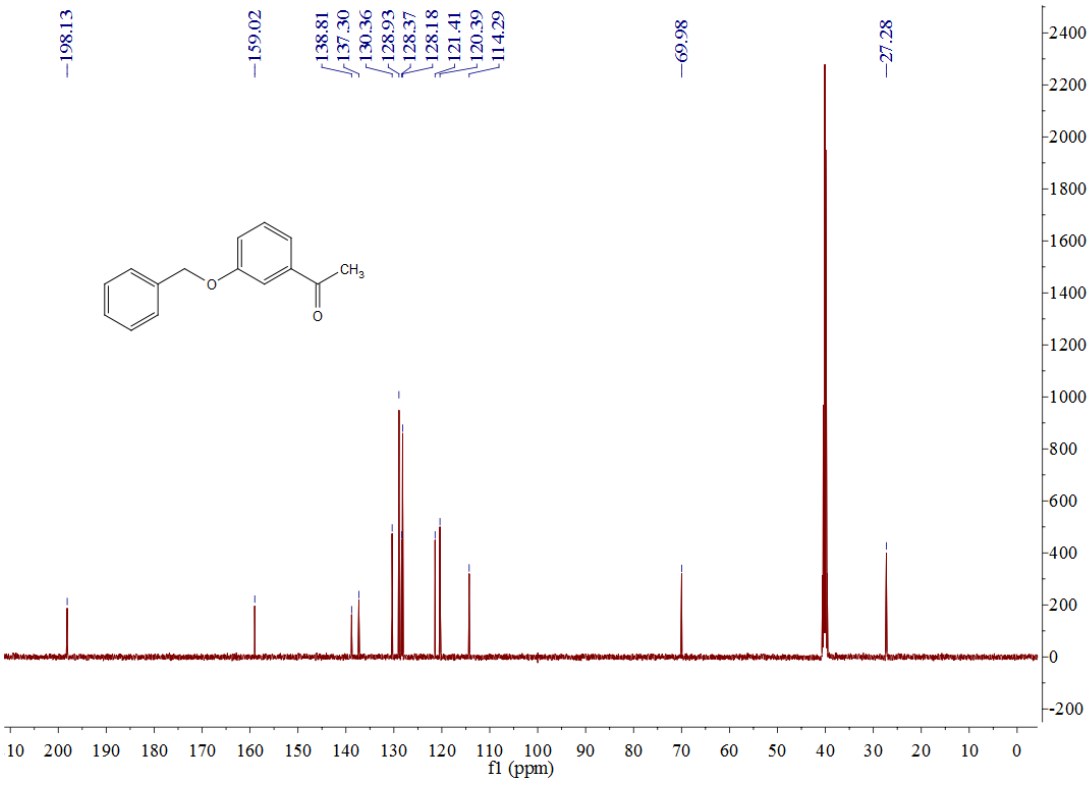
Elemental Composition Calculator

Target m/z:	245.0970	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); F (0-5)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C15H14FO2		245.0972		0.83	

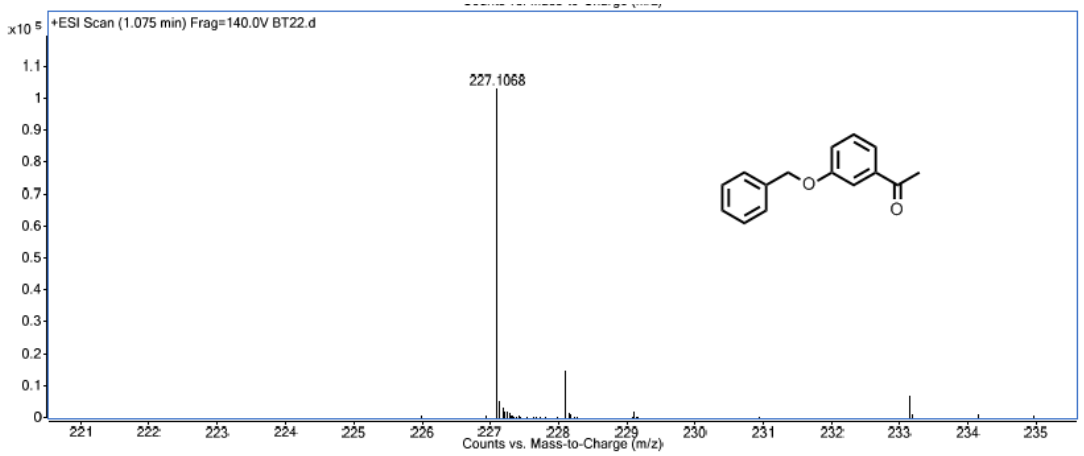
^{1}H NMR spectrum of compound 2a in DMSO



^{13}C NMR spectrum of compound 2a in DMSO



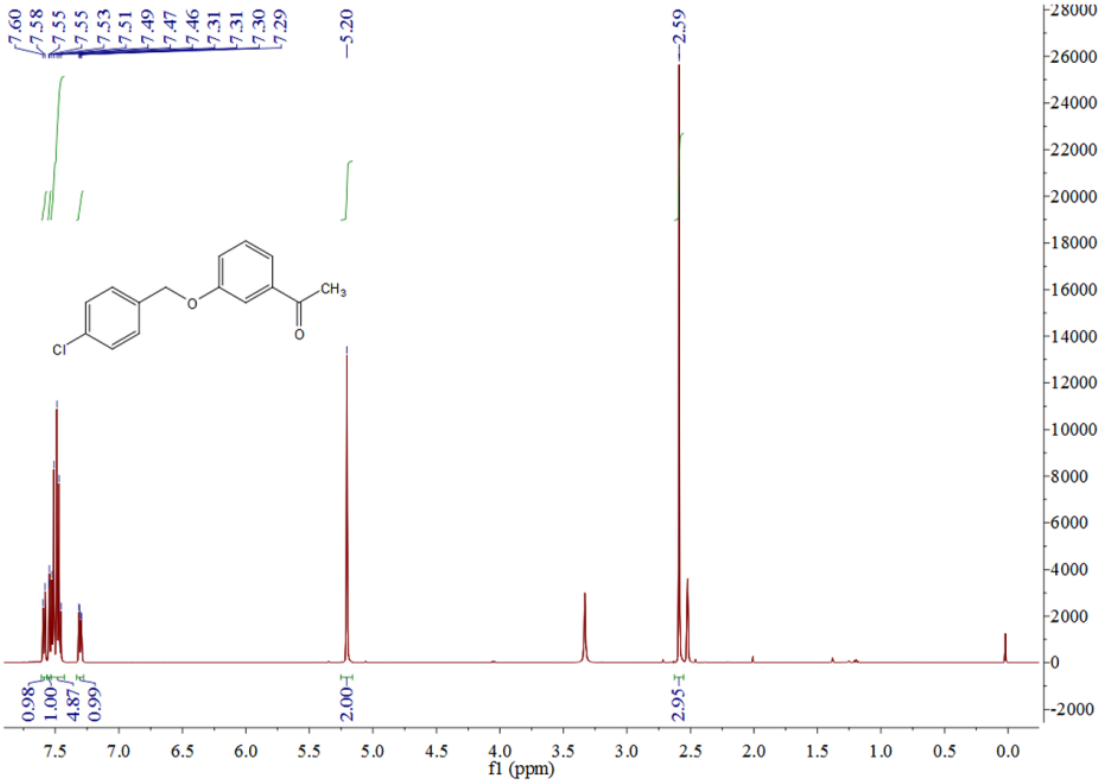
HRMS (ESI) spectrum of compound 2a



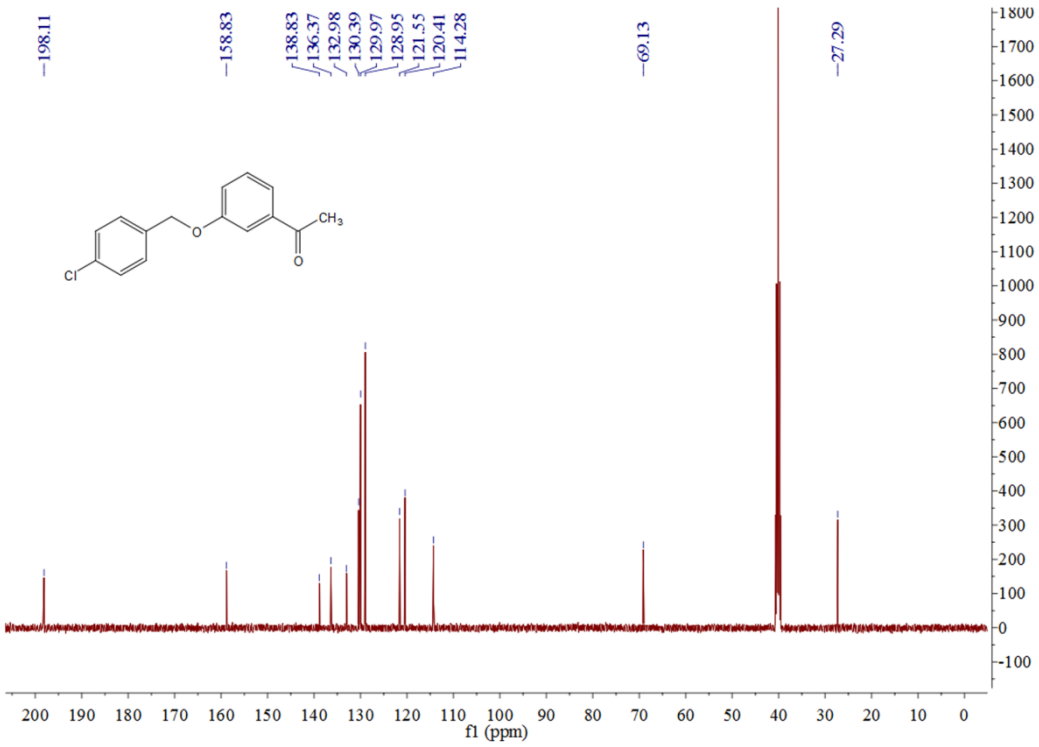
Elemental Composition Calculator

Target m/z:	227.1068	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Cl (0-5)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C15H15O2		227.1067		-0.67	

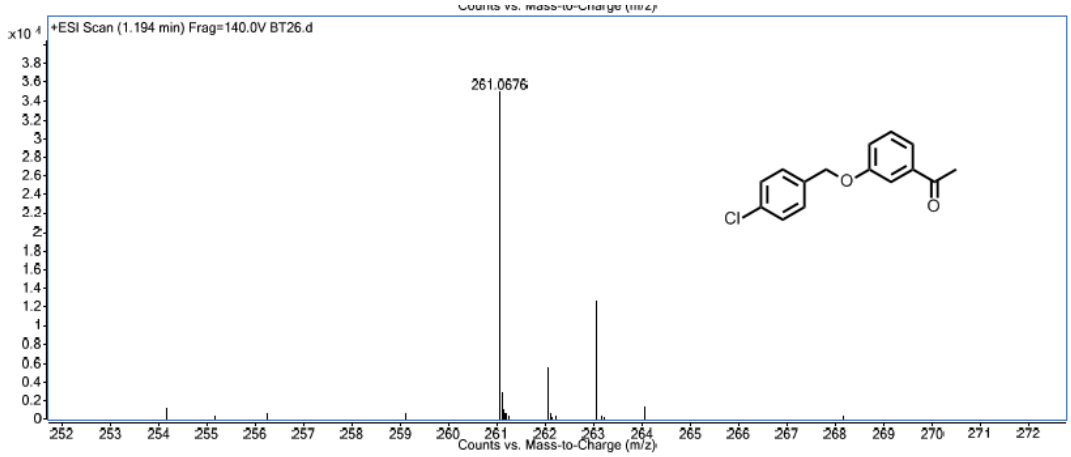
^{1}H NMR spectrum of compound 2e in DMSO



^{13}C NMR spectrum of compound 2e in DMSO



HRMS (ESI) spectrum of compound 2e



Elemental Composition Calculator

Target m/z:	261.0676	**Result type:**	Positive ions	**Species:**	$[M+H]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Cl (0-5)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C15H14ClO2		261.0677		0.5	