

Efficient syntheses of substituted (\pm)-3-oxoisindoline-1-carbonitriles and carboxamides using OSU-6

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Supporting Information

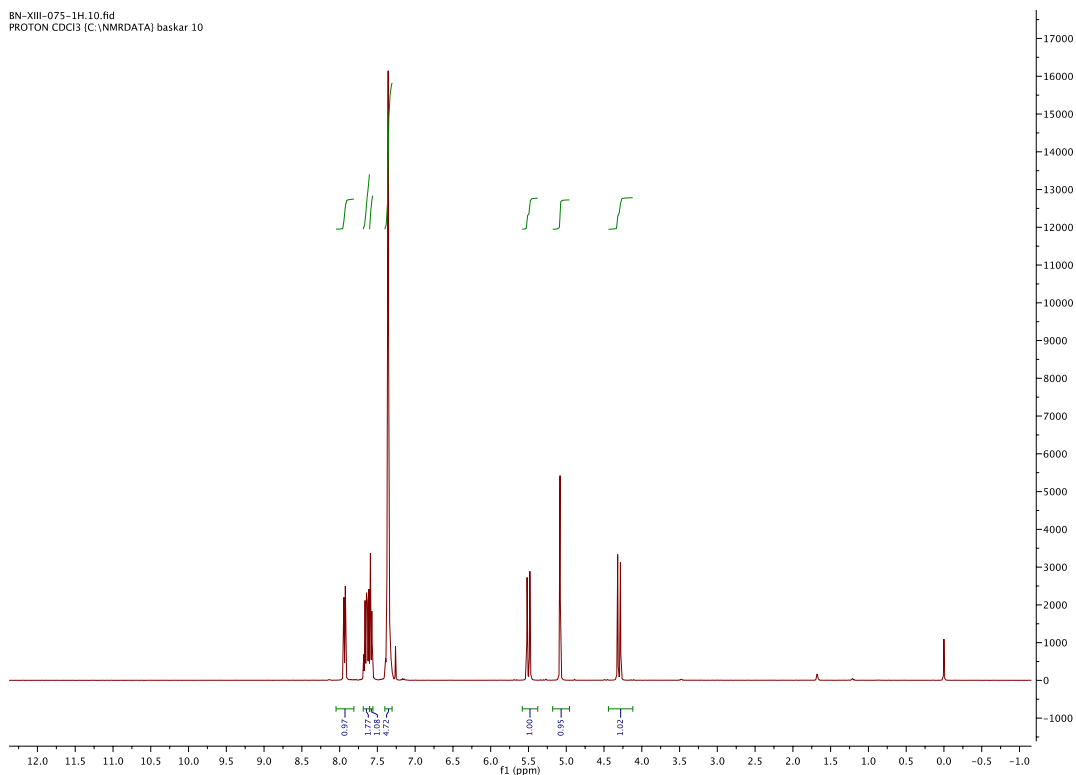
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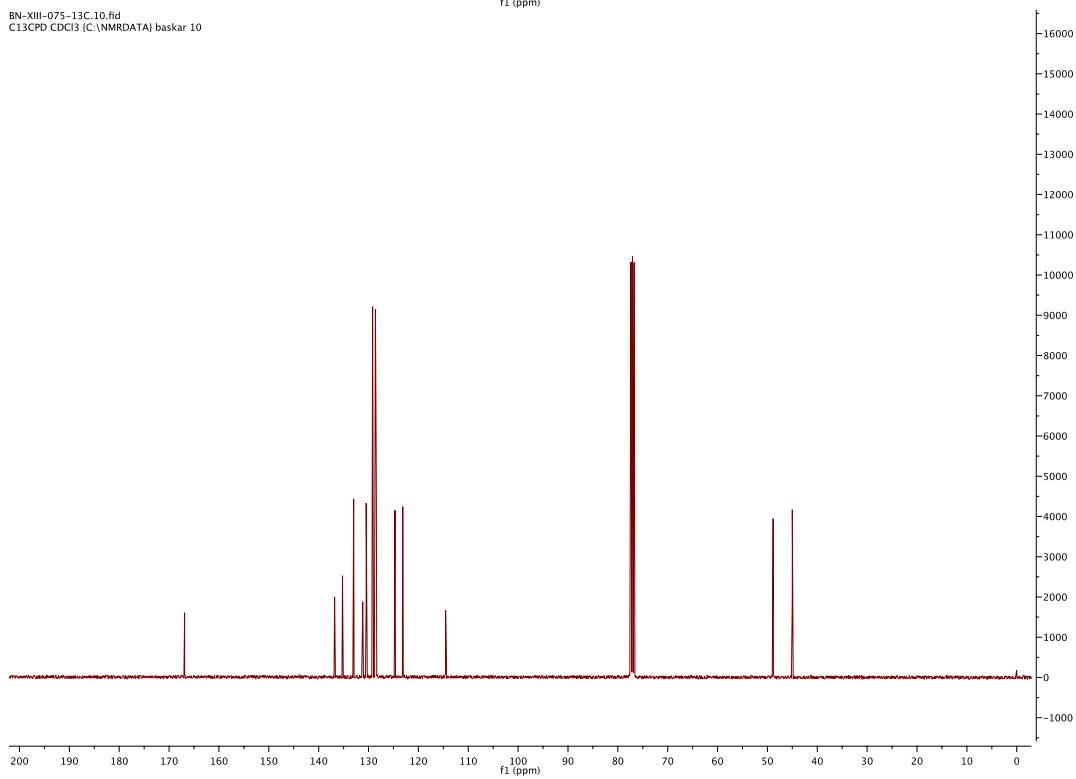
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(±)-2-Benzyl-3-oxoisindoline-1-carbonitrile (3a)

BN-XIII-075-1H.10.fid
PROTON CDCl3 (C:\NMRDATA) baskar 10

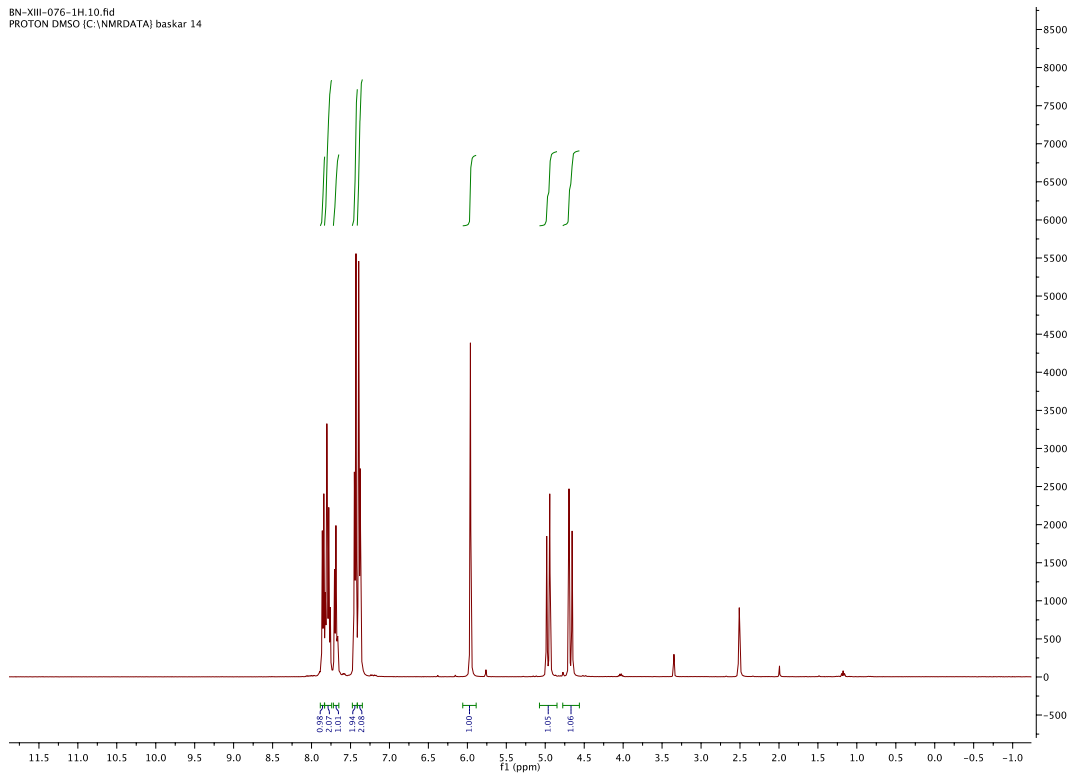


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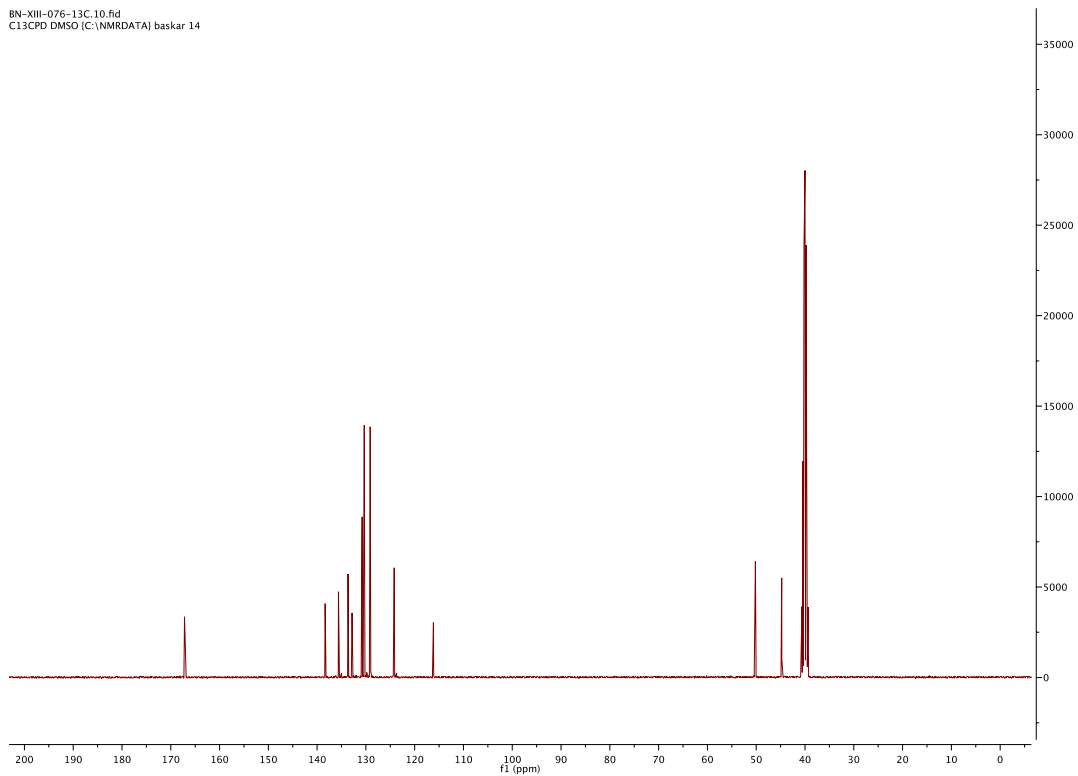


(±)-2-(4-Chlorobenzyl)-3-oxoisindoline-1-carbonitrile (3b)

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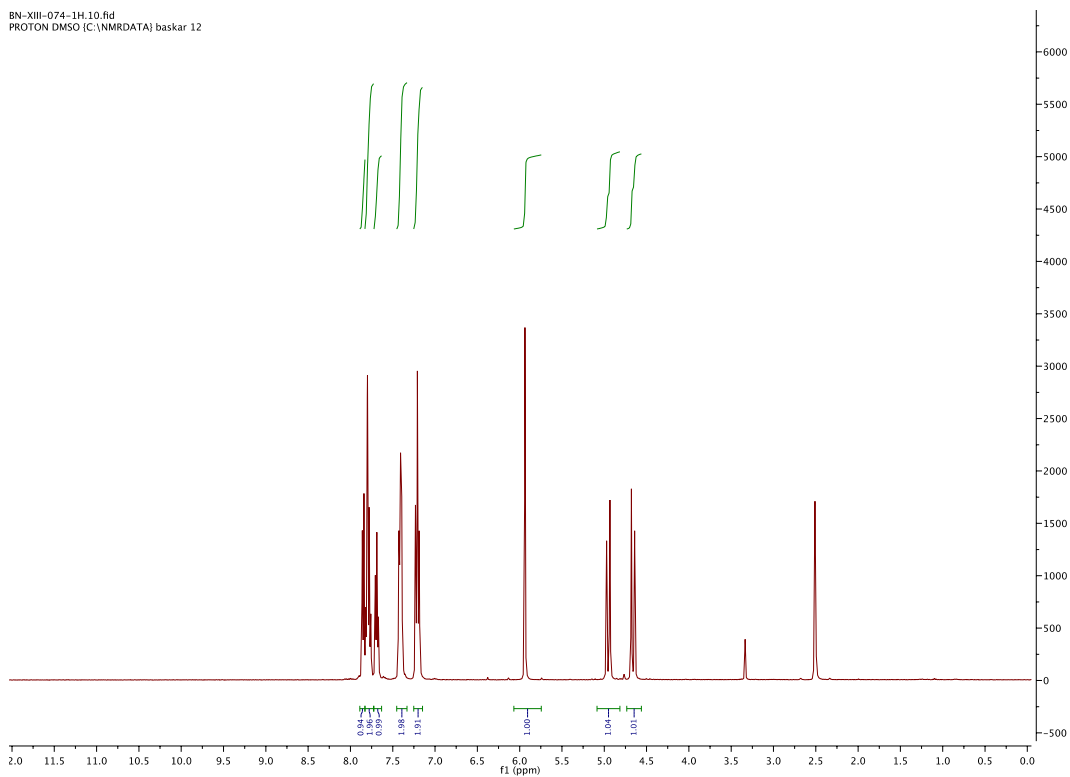


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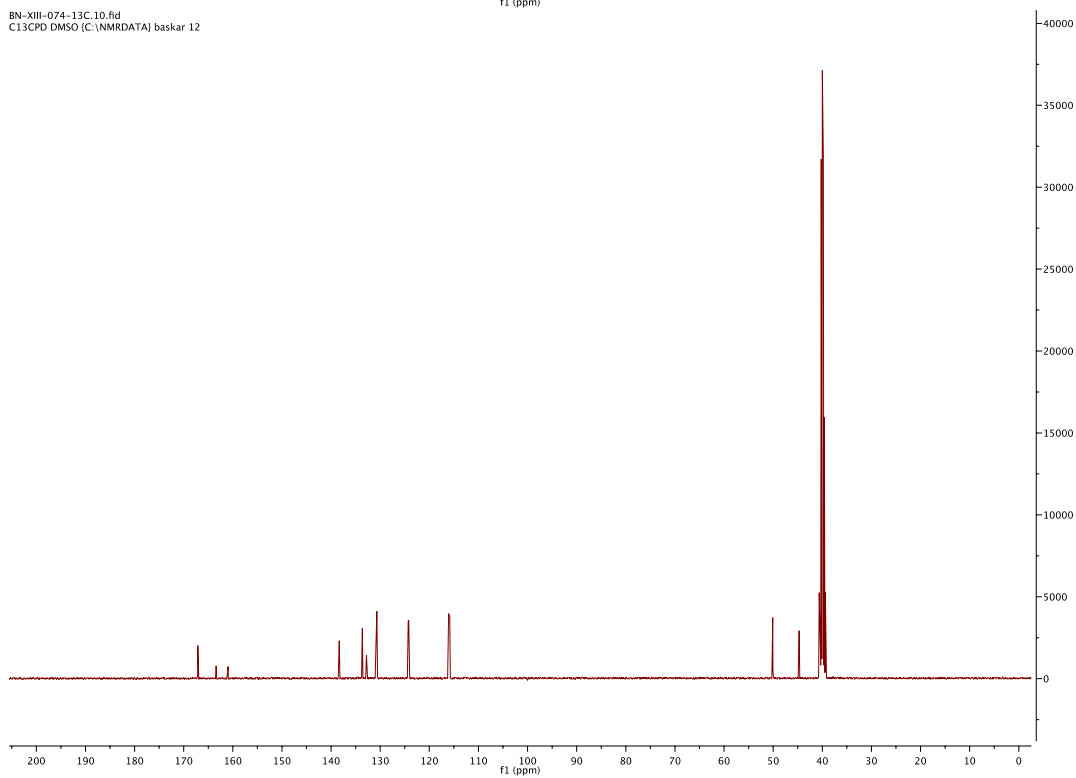


(±)-2-(4-Fluorobenzyl)-3-oxoisindoline-1-carbonitrile (3c)

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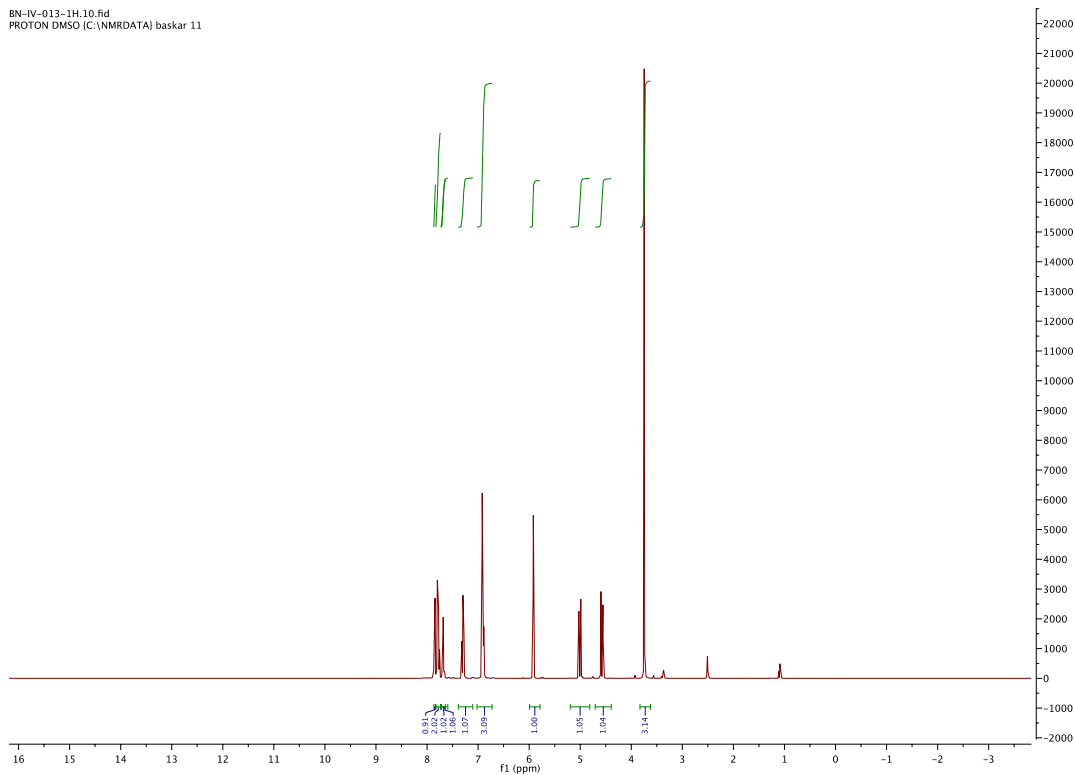


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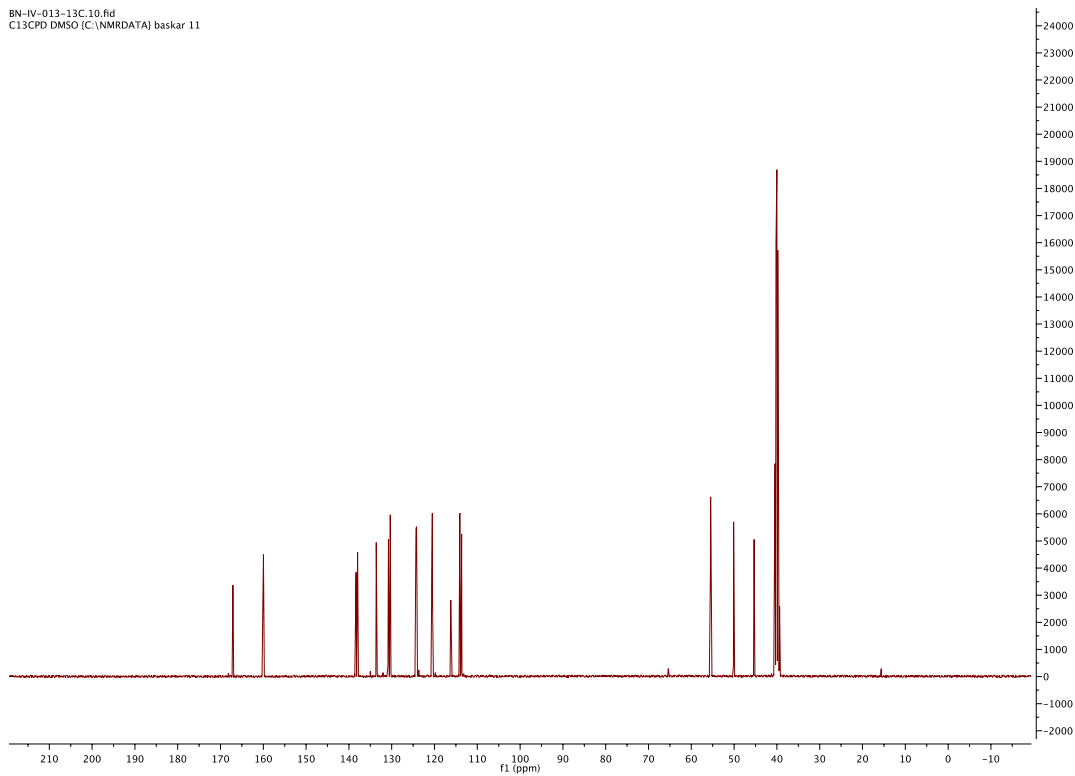


(±)-2-(3-Methoxybenzyl)-3-oxoindoline-1-carbonitrile (3d)

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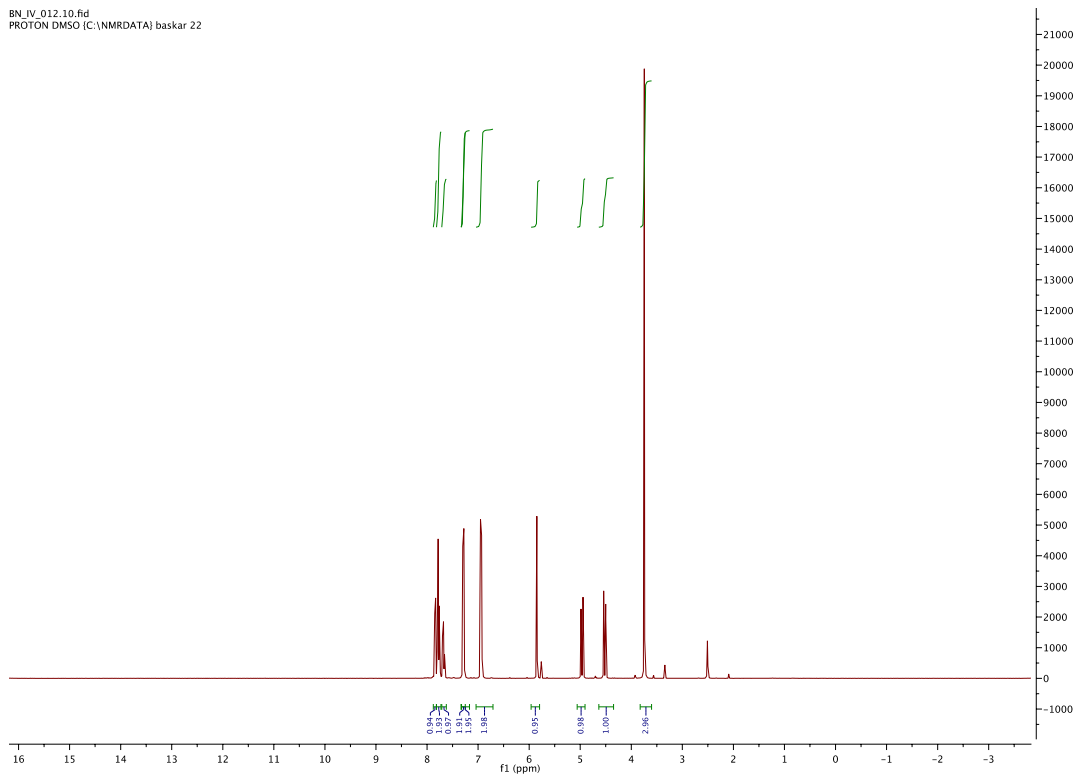


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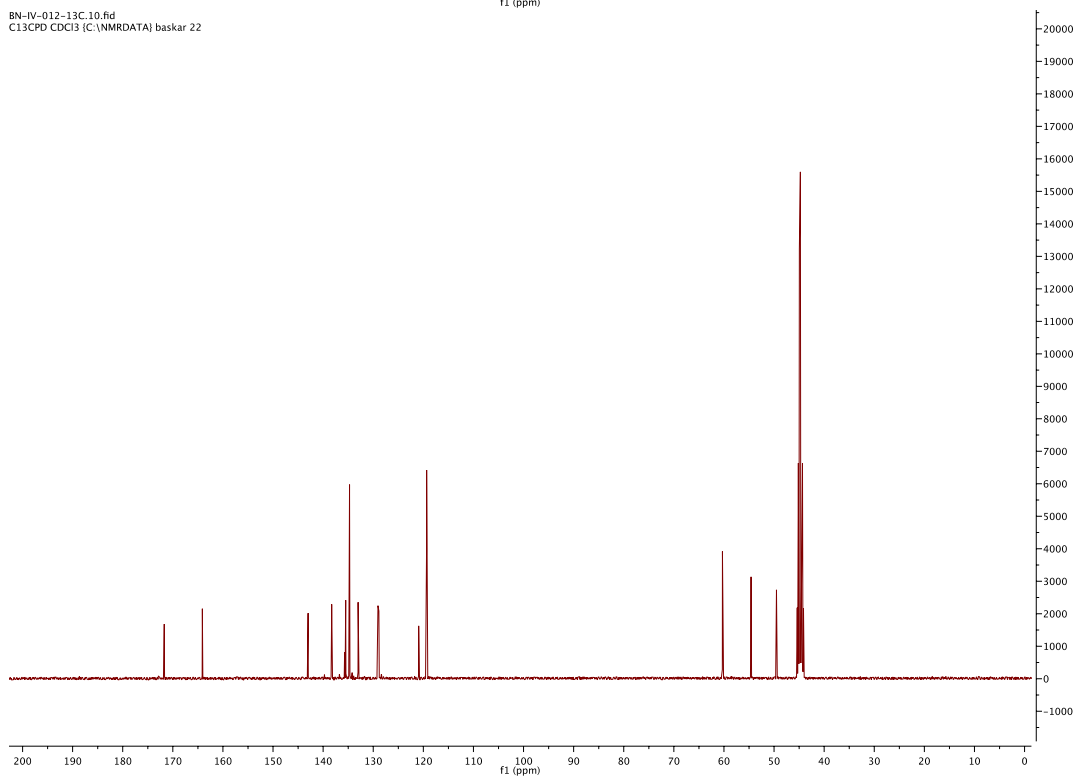


(±)-2-(4-Methoxybenzyl)-3-oxoindoline-1-carbonitrile (3e)

BN-IV_012-10.fid
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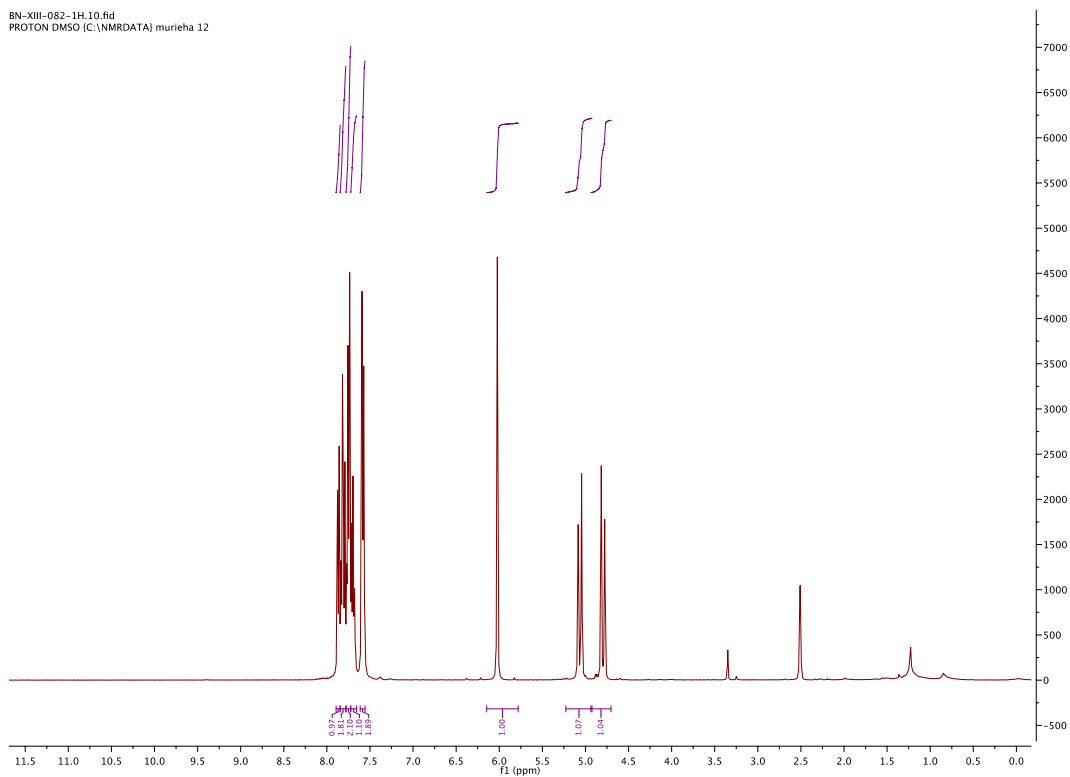


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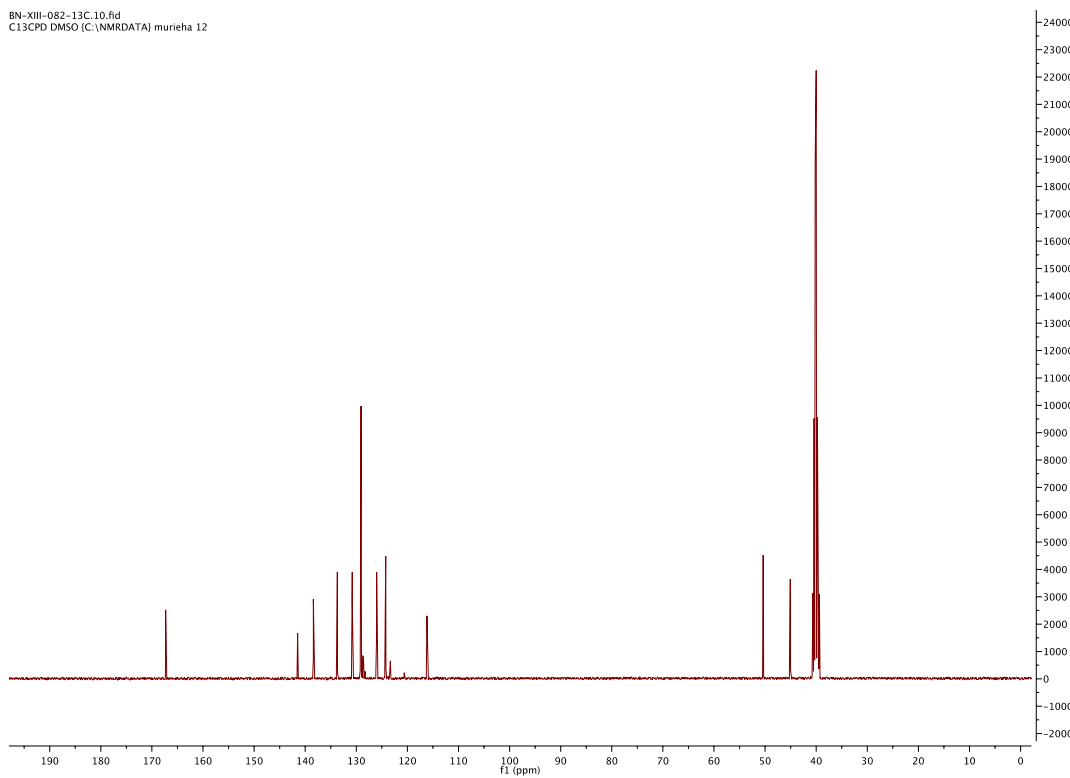


(±)-2-[(4-Trifluoromethyl)benzyl]-3-oxoisindoline-1-carbonitrile (3f)

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PROTON DMSO [C:\NMRDATA] murieha 12

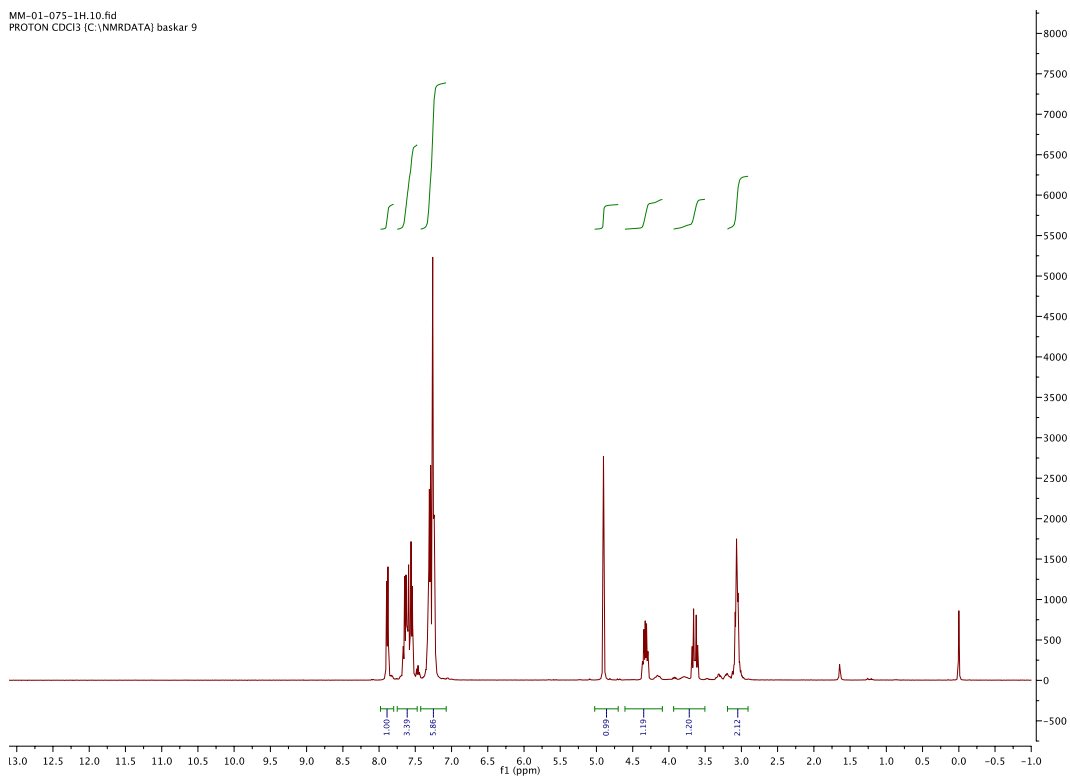


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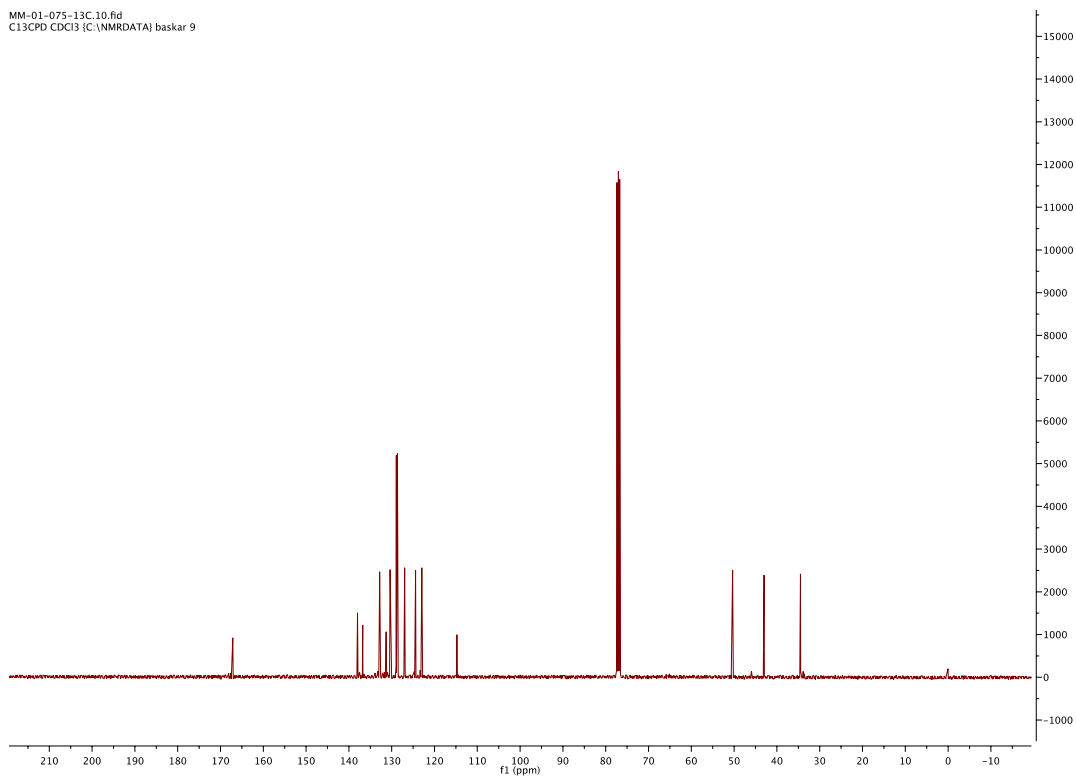


(±)-3-Oxo-2-(2-phenylethyl)isoindoline-1-carbonitrile (3g)

MM-01-075-1H.10.fid
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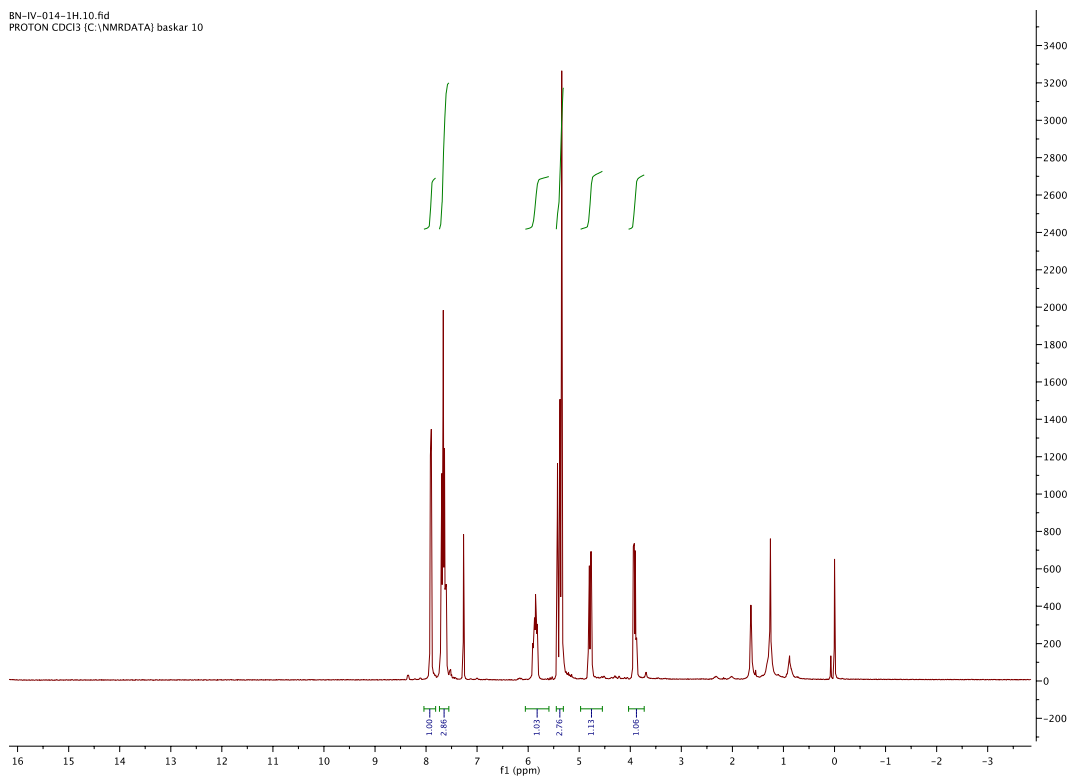


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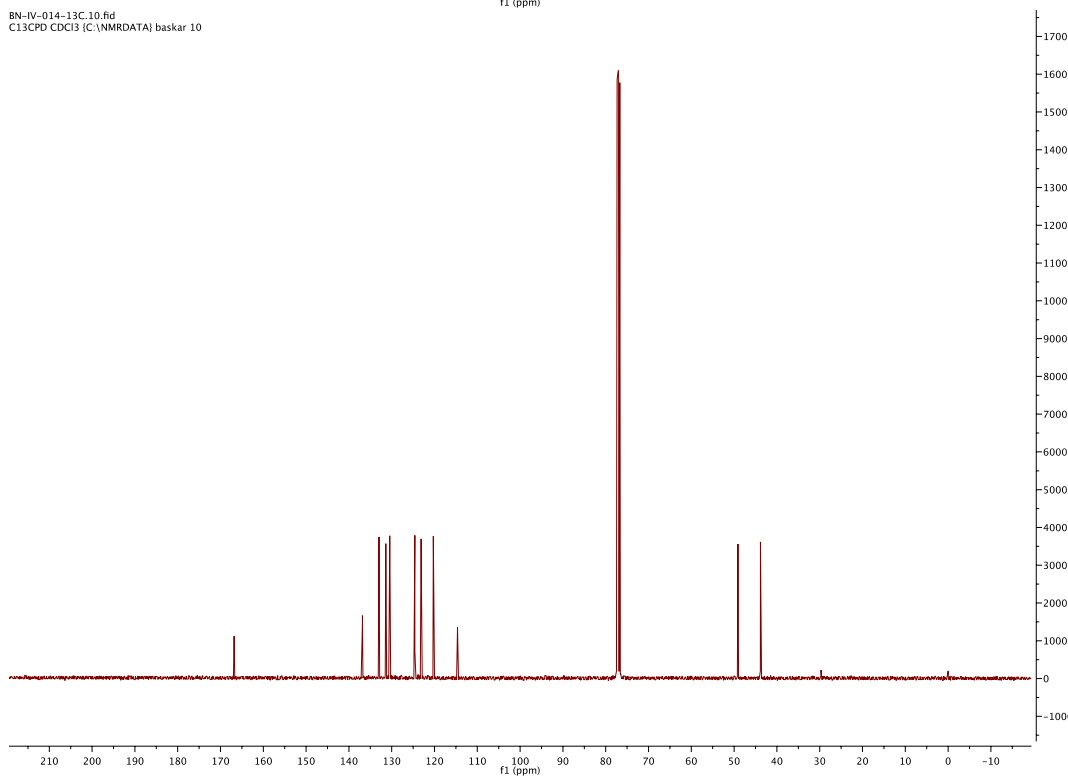


(±)-2-Allyl-3-oxoisindoline-1-carbonitrile (3h)

BN-IV-014-1H.10.fid
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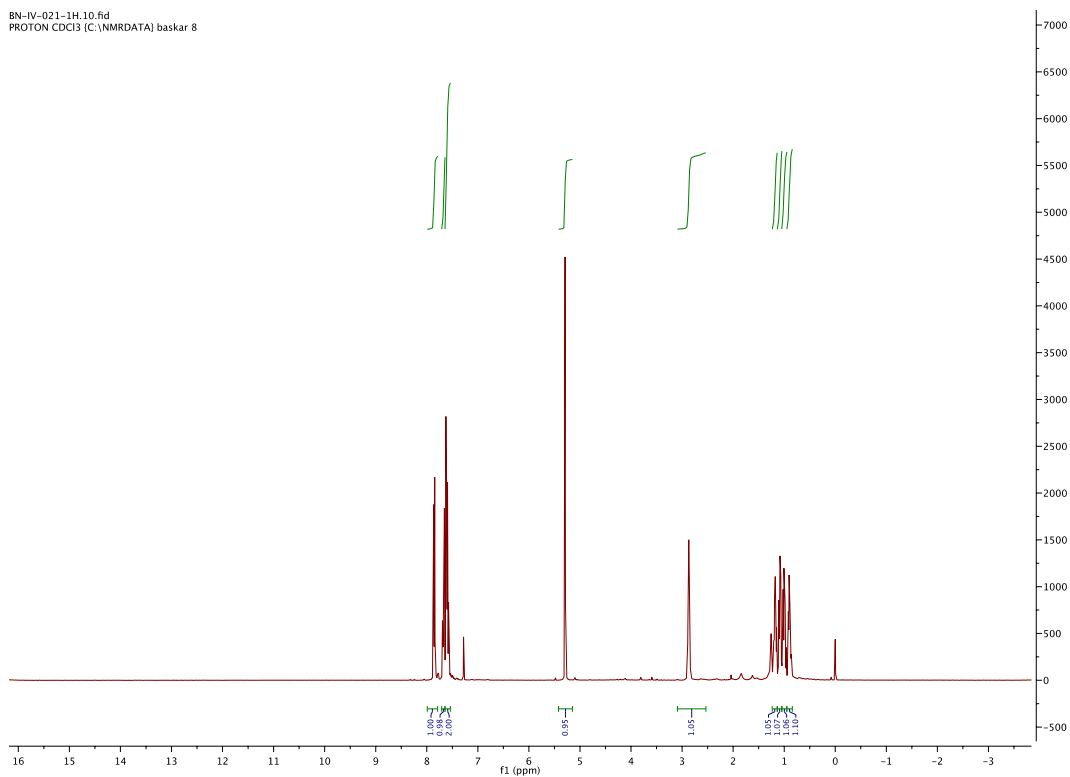


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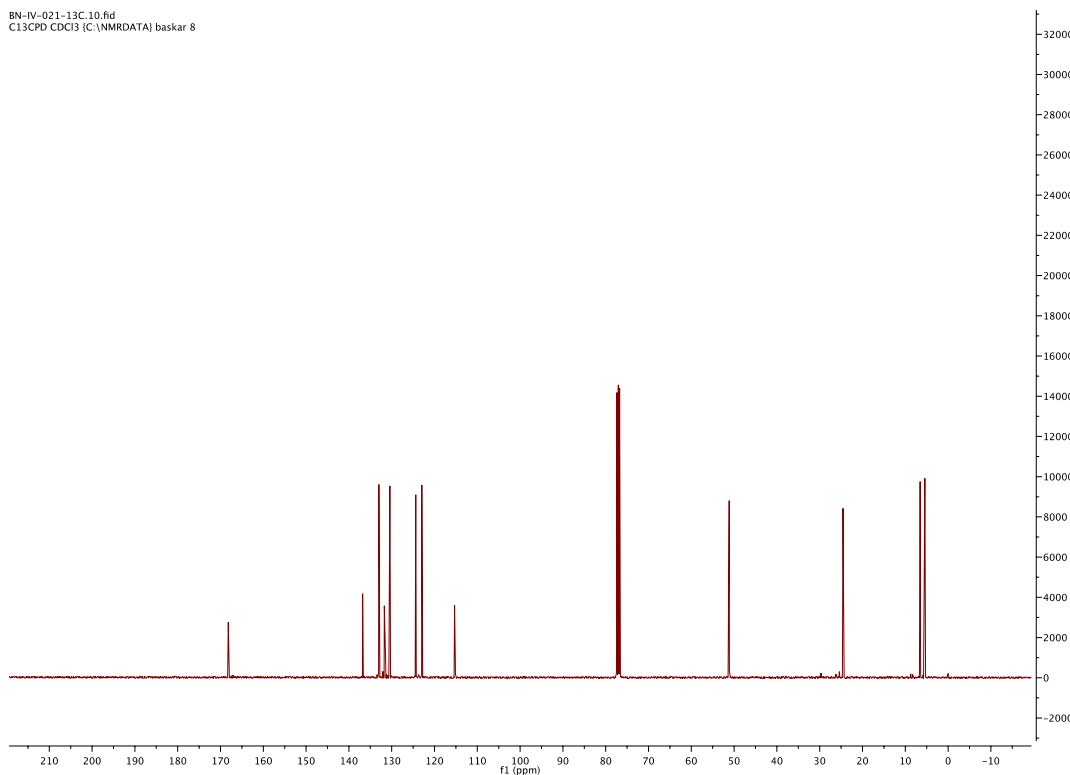


(±)-2-Cyclopropyl-3-oxoisindoline-1-carbonitrile (3i)

BN-IV-021-1H.fid
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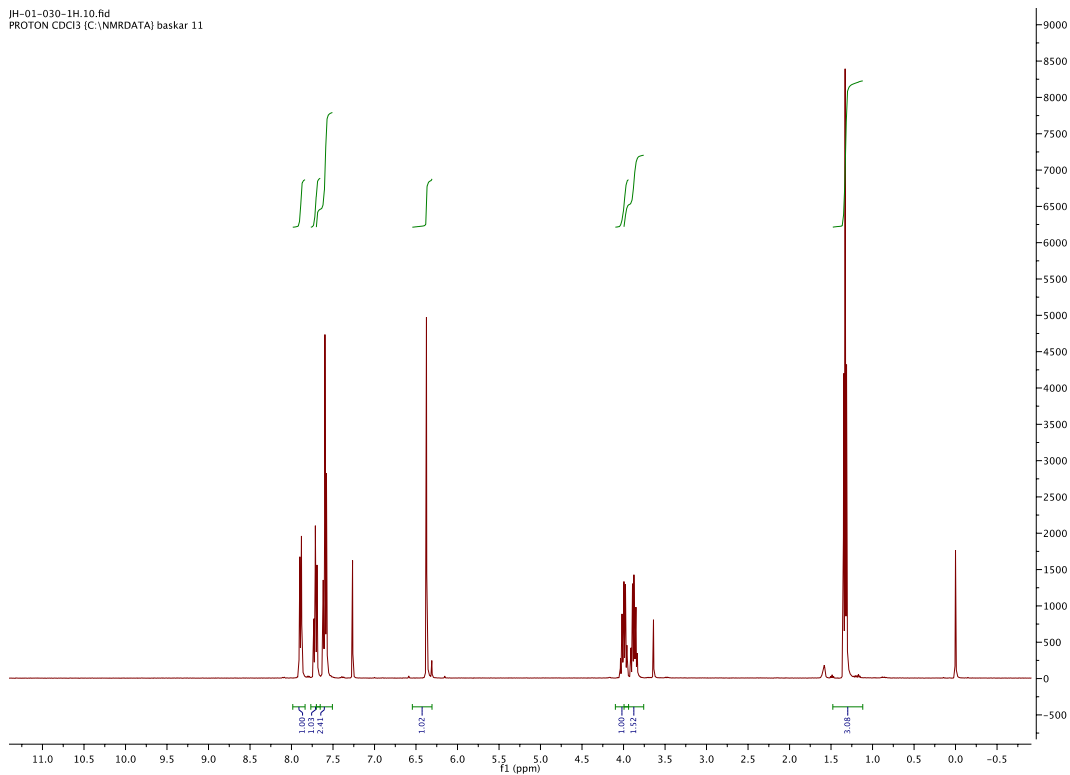


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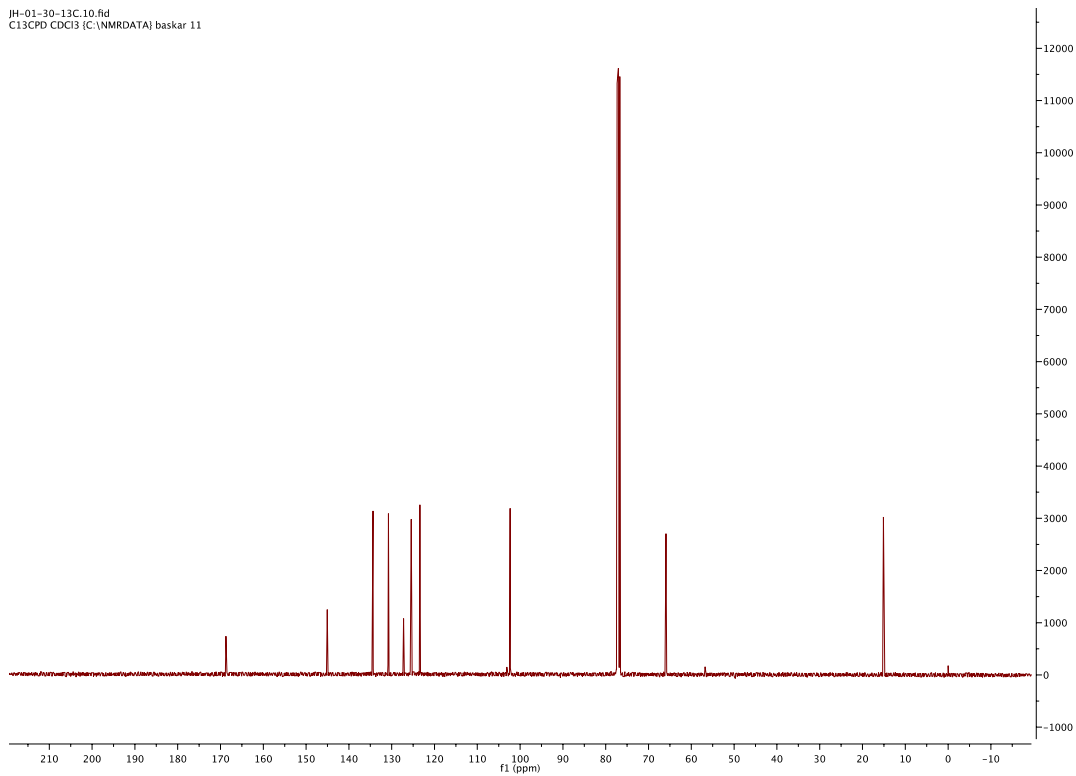


(±)-2-Ethyl-3-oxoisindoline-1-carbonitrile (3j)

JH-01-030-1H.10.fid
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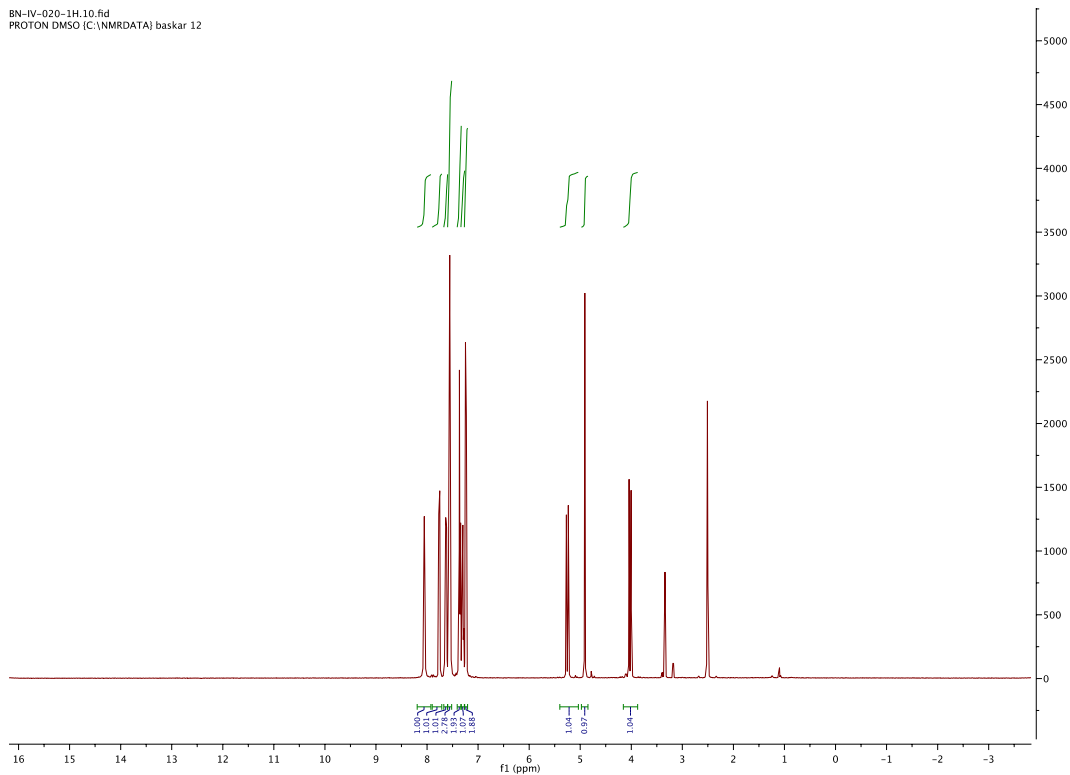


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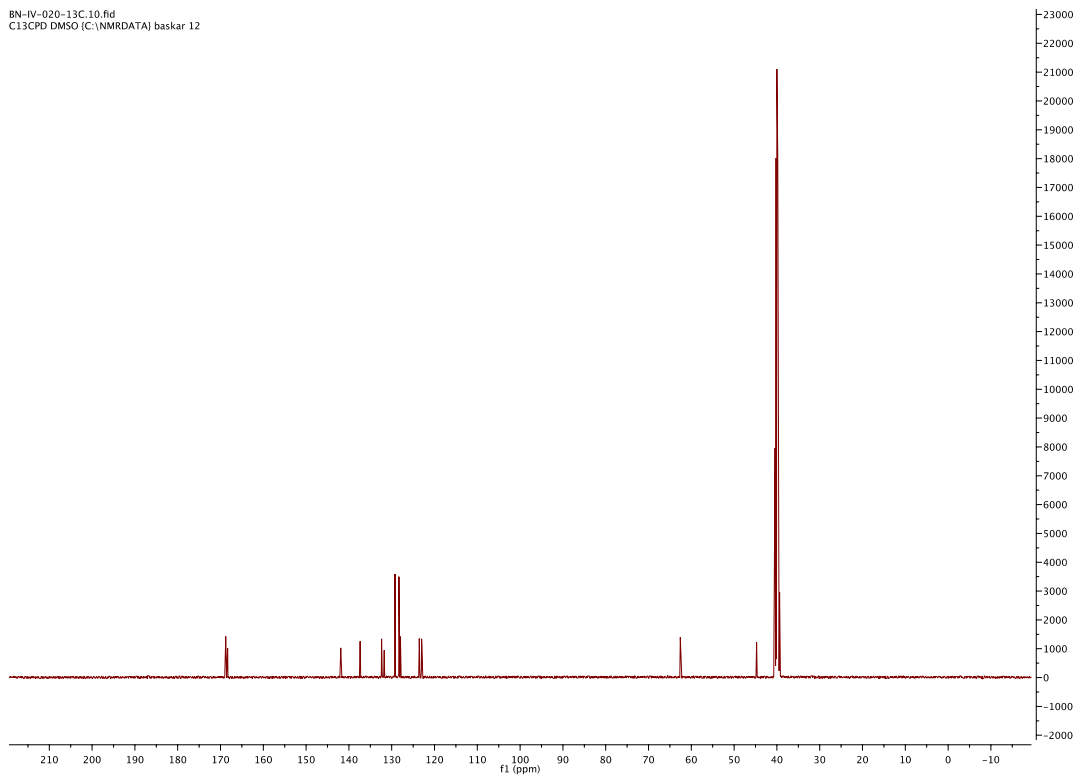


(±)-2-Benzyl-3-oxoisindoline-1-carboxamide (4a)

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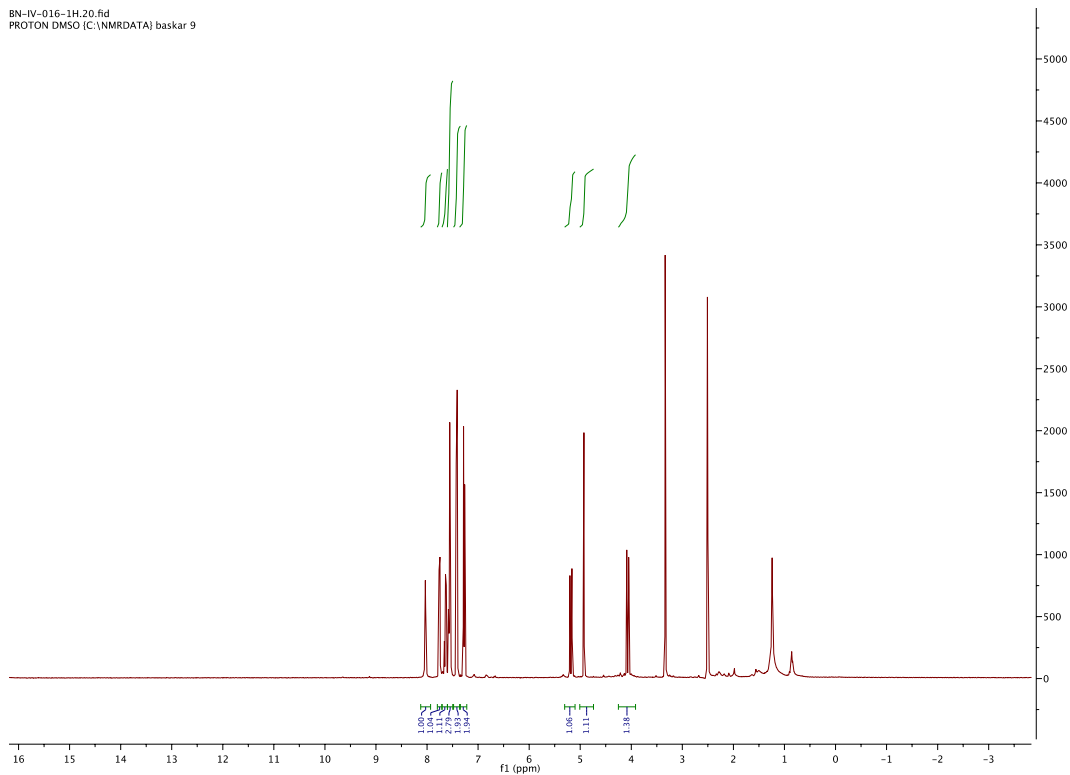


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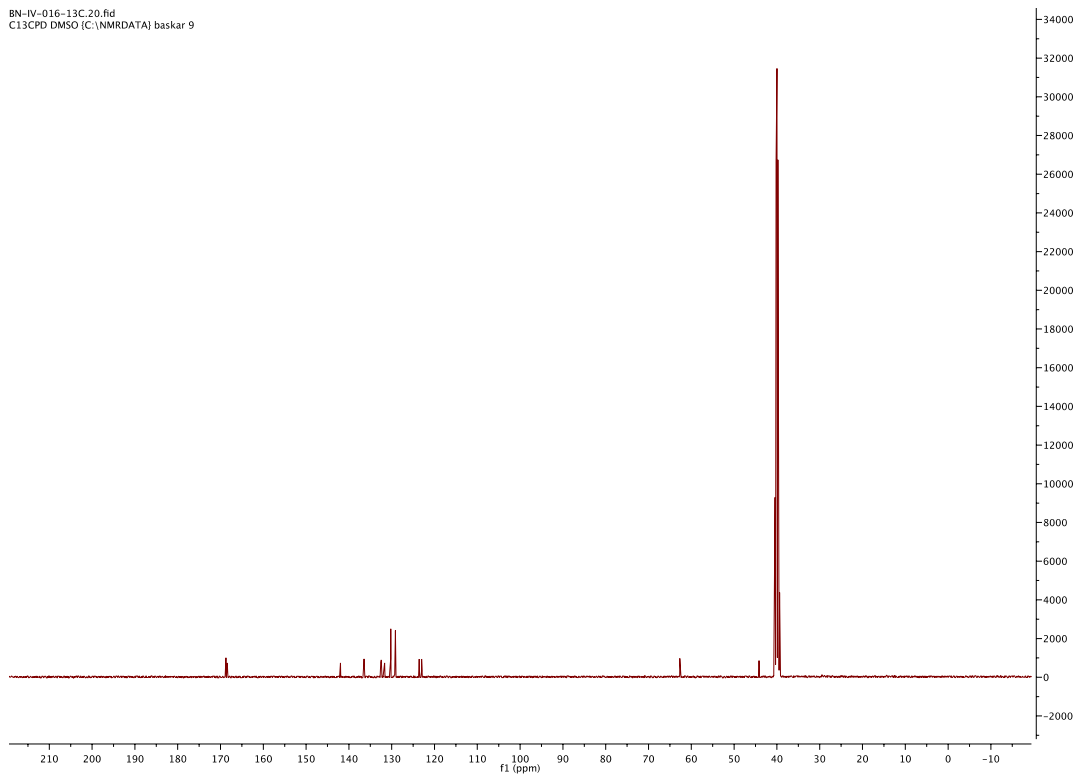


(±)-2-(4-Chlorobenzyl)-3-oxoisindoline-1-carboxamide (4b)

BN-IV-016-1H.20.fid
PROTON DMSO (C:\NMRDATA) baskar 9

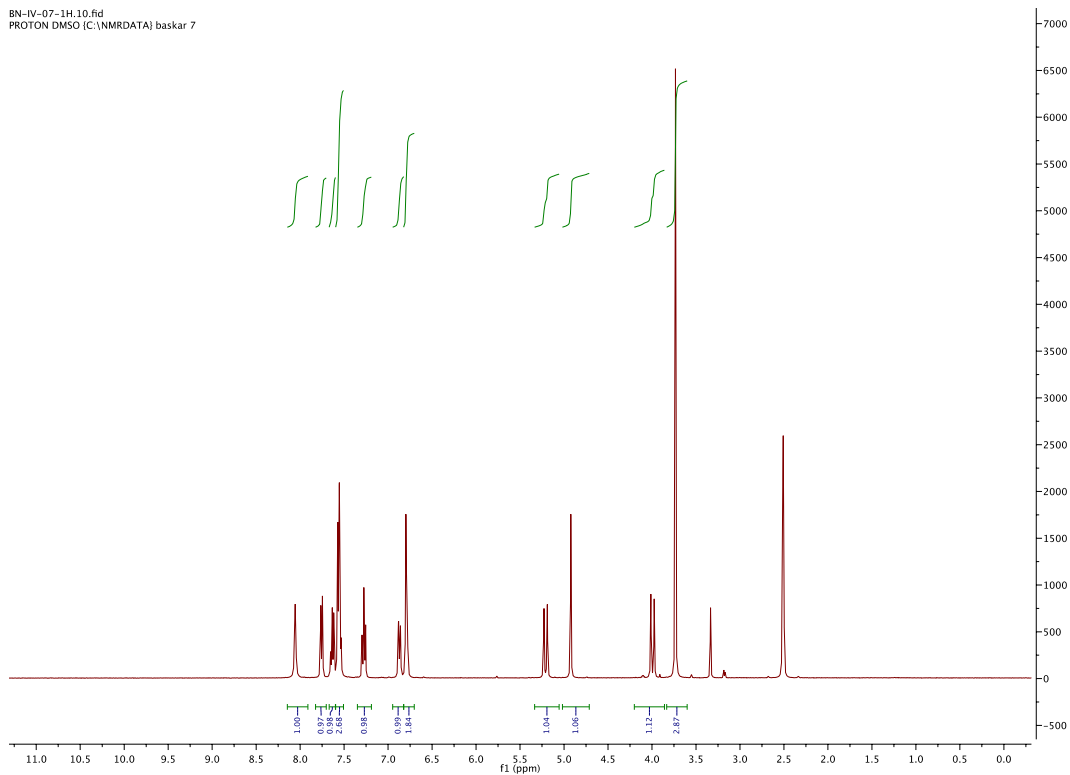


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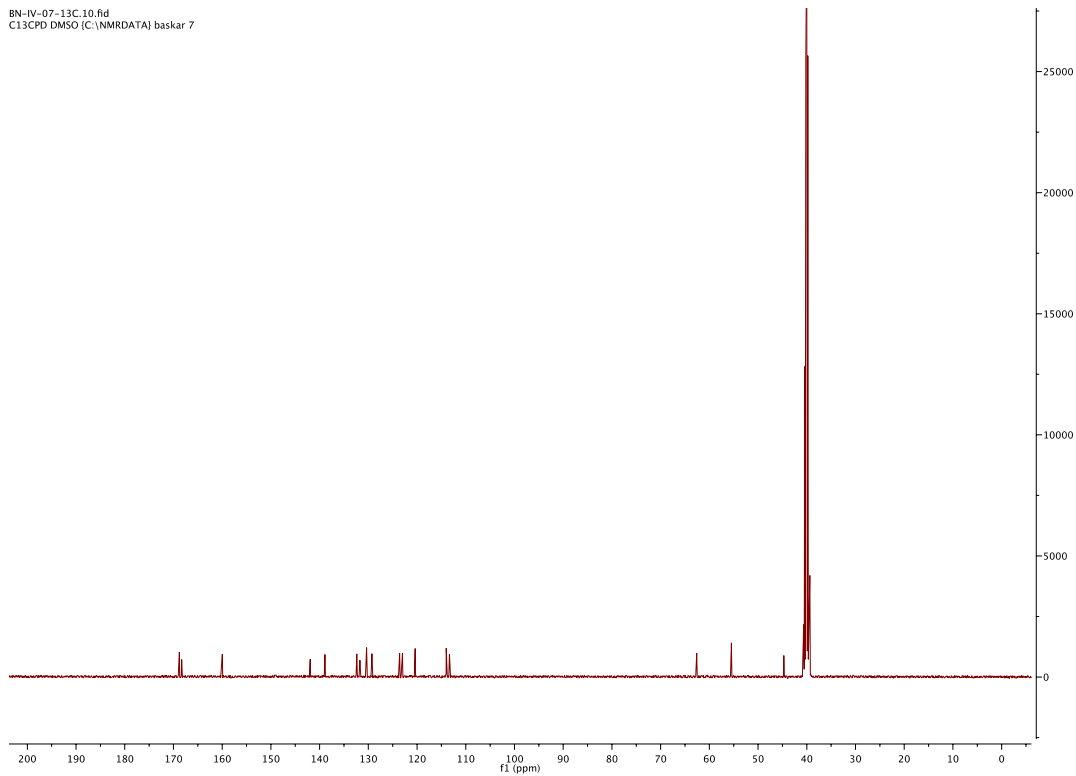


(±)-2-(3-Methoxybenzyl)-3-oxoisindoline-1-carboxamide (4c)

BN-IV-07-1H.10.fid
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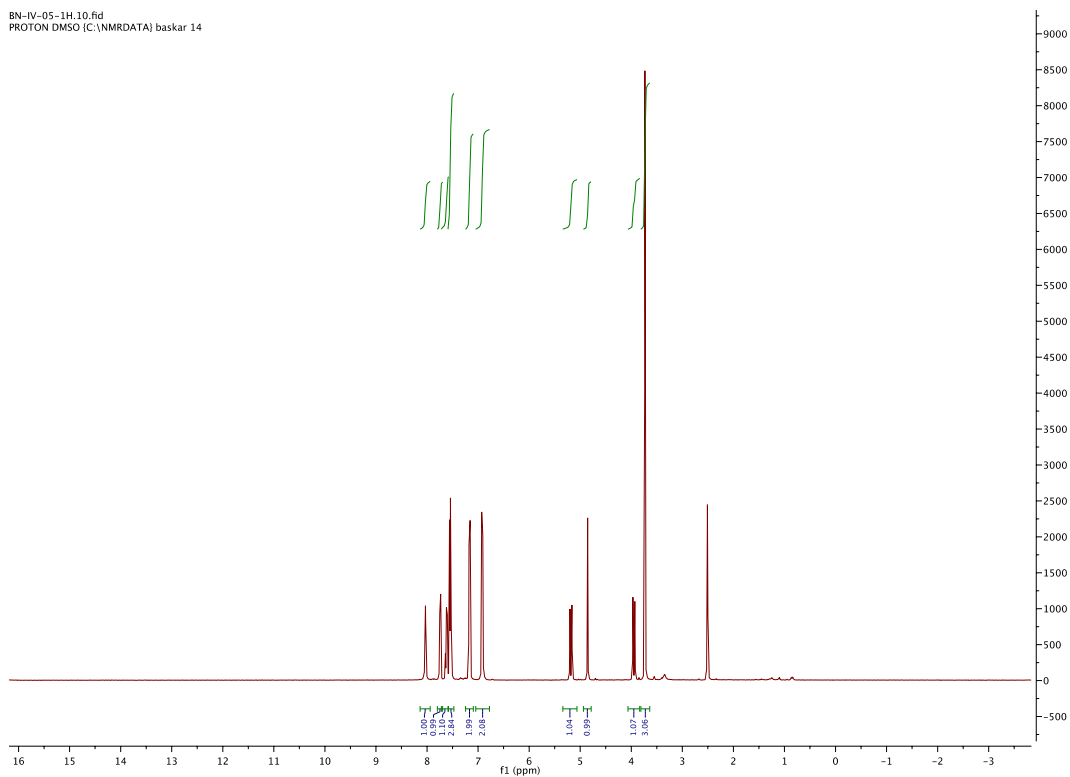


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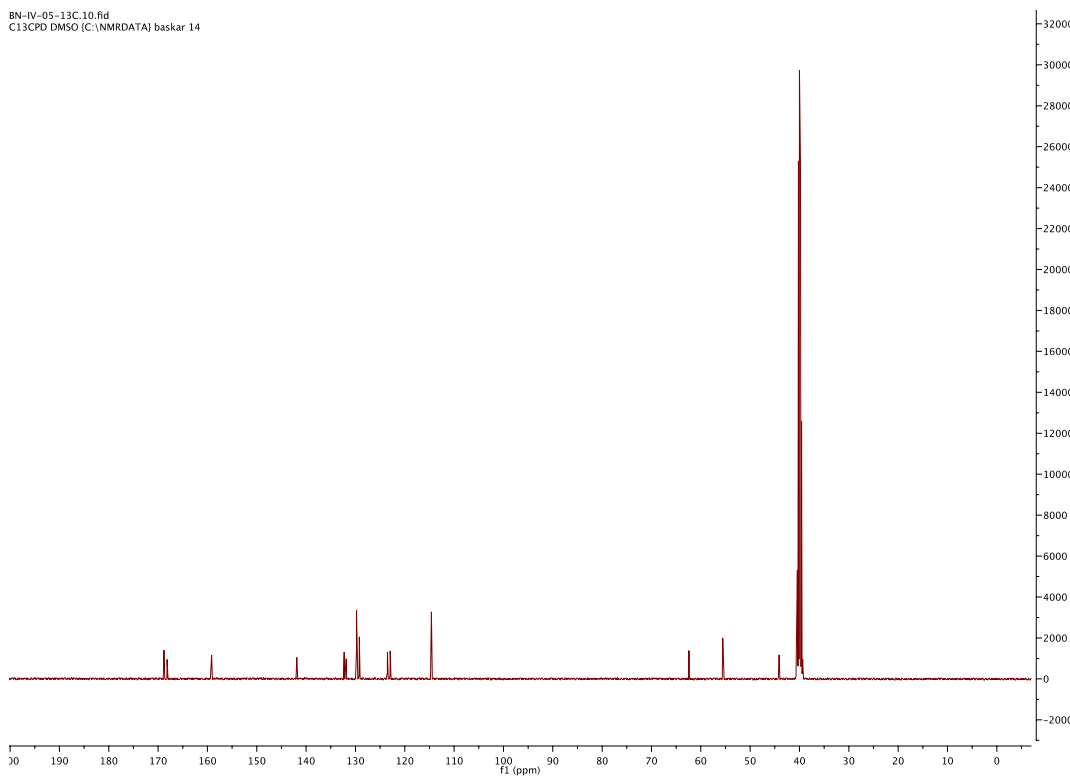


(±)-2-(4-Methoxybenzyl)-3-oxoisindoline-1-carboxamide (4d)

BN-IV-05-1H.10.fid
PROTON DMSO [C:\NMRDATA] baskar 14

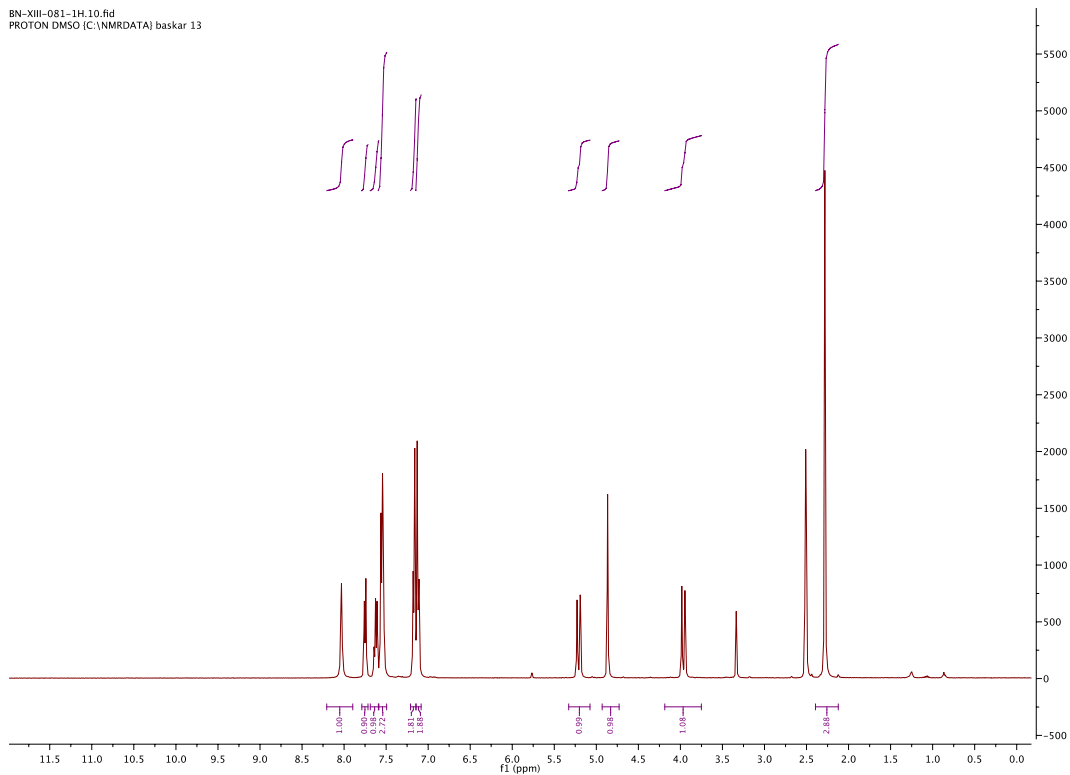


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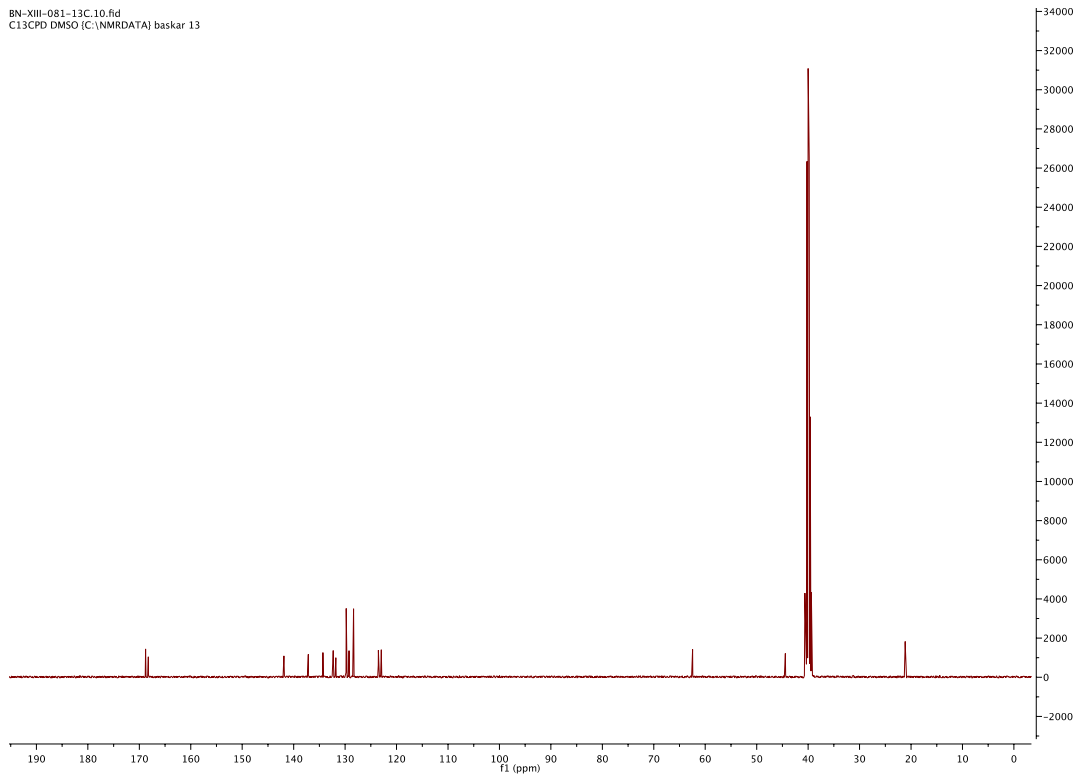


(±)-2-(4-Methylbenzyl)-3-oxoisindoline-1-carboxamide (4e)

BN-XIII-081-1H.10.fid
PROTON DMSO [C:\NMRDATA] baskar 13

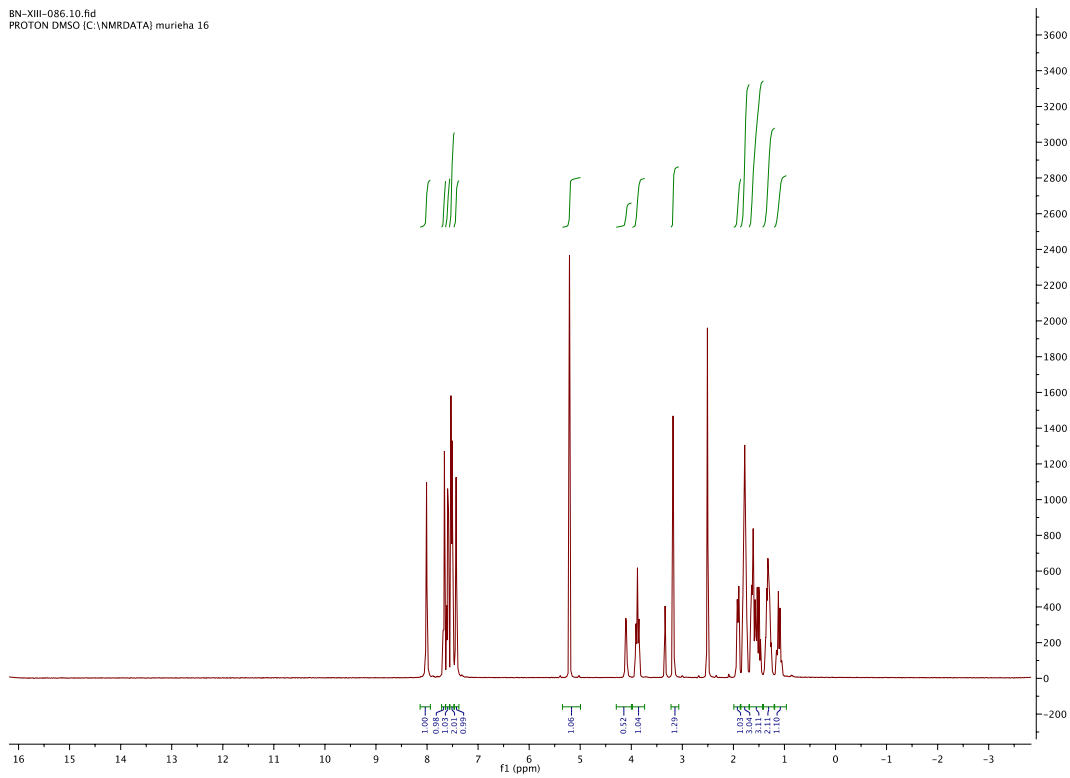


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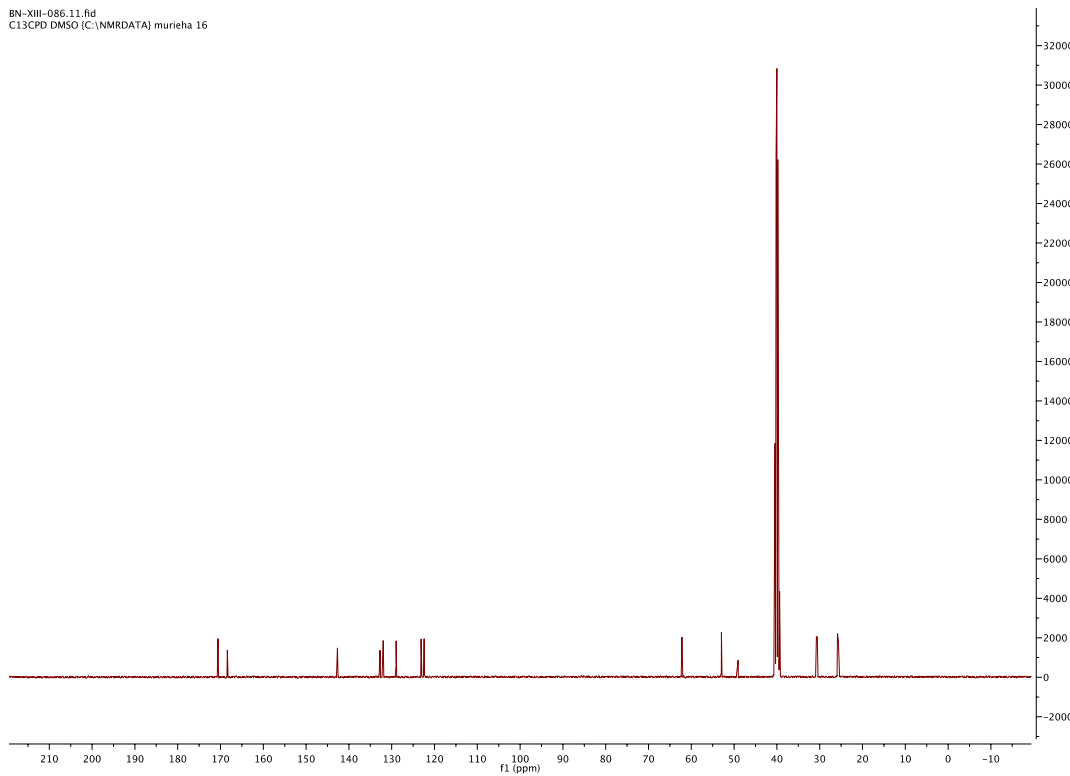


(±)-2-Cyclohexyl-3-oxoisindoline-1-carboxamide (4f)

BN-XIII-086.10.fid
PROTON DMSO (C:\NMRDATA) murieha 16

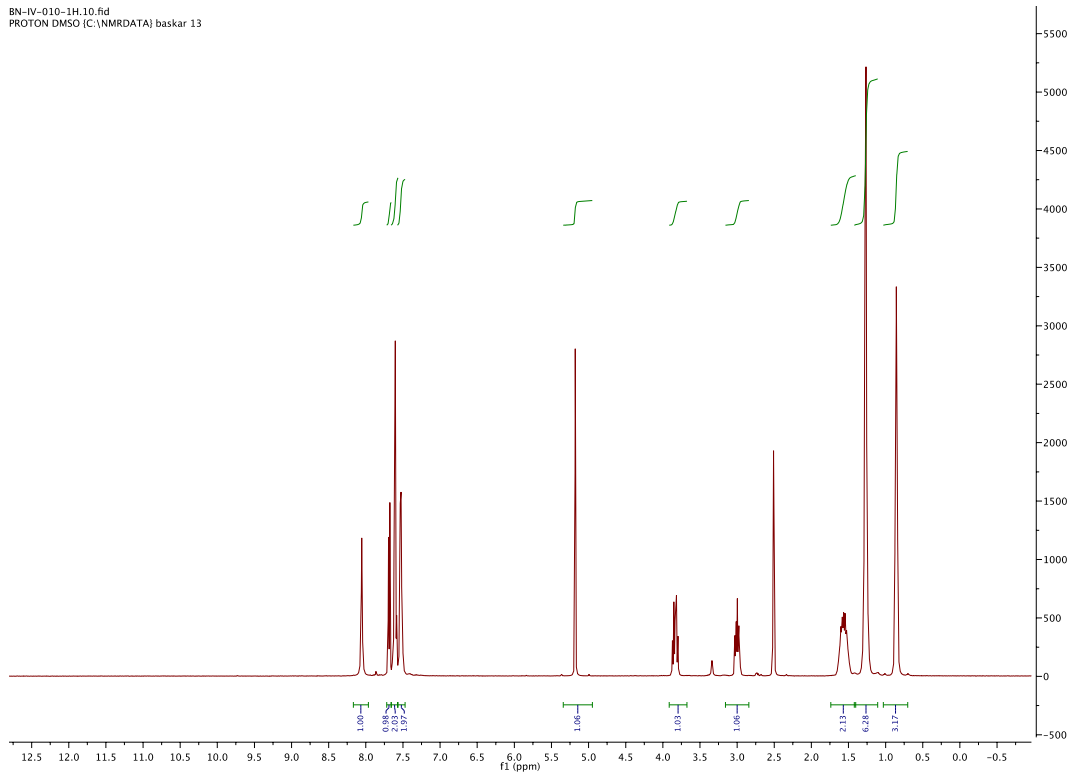


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C13CPD DMSO (C:\NMRDATA) murieha 16

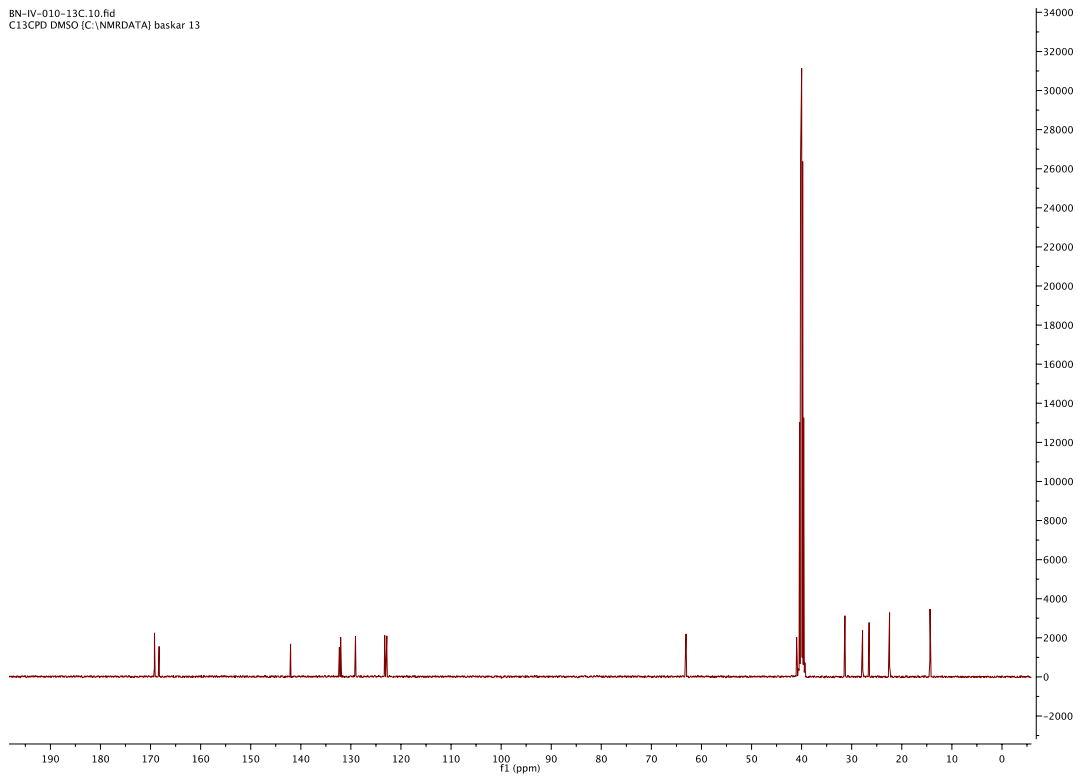


(±)-2-Hexyl-3-oxoisindoline-1-carboxamide (4g)

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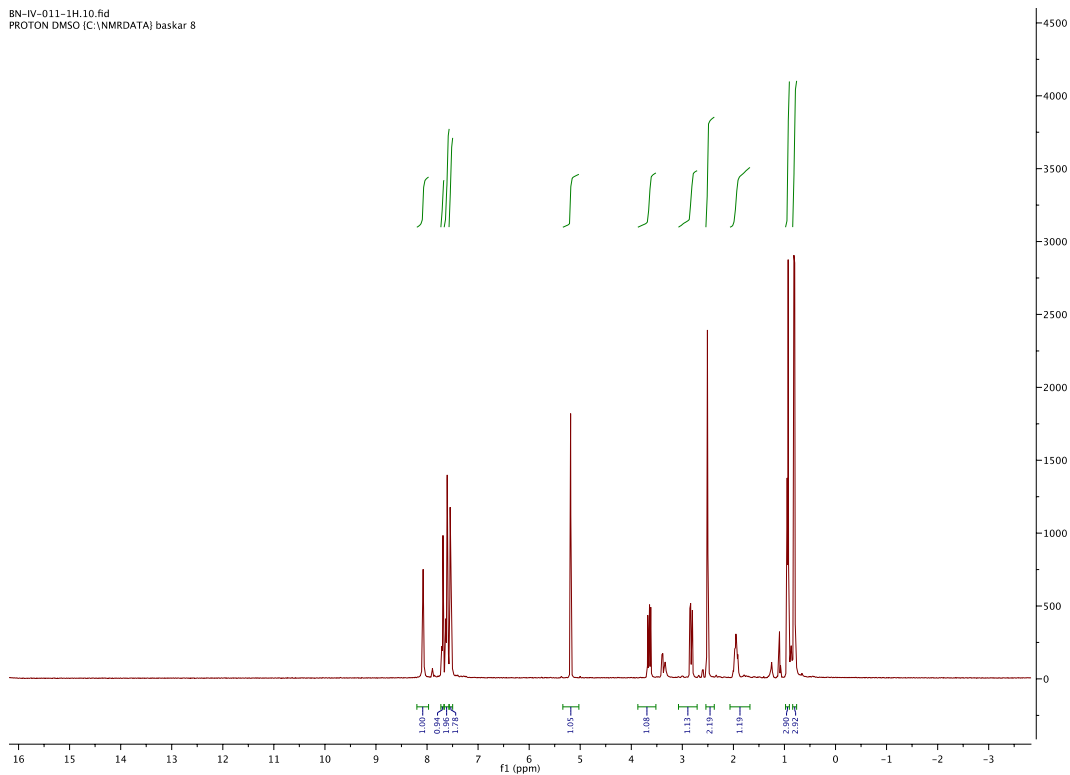


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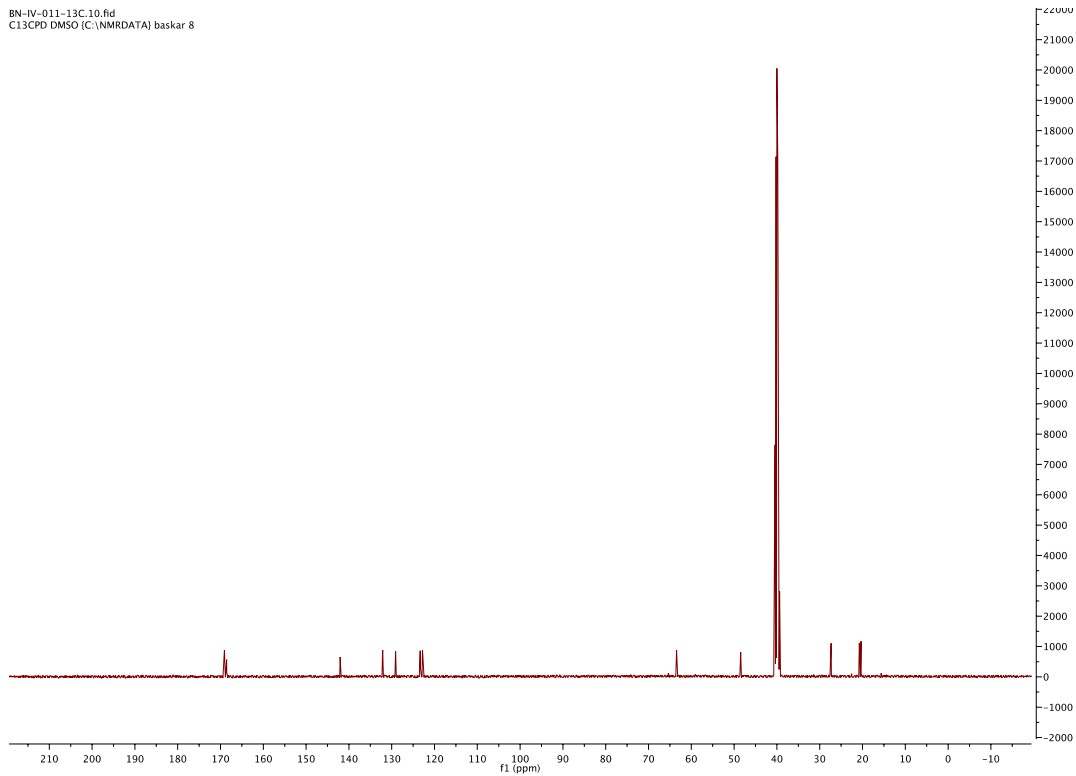


(±)-2-Isobutyl-3-oxoisindoline-1-carboxamide (4h)

BN-IV-011-1H.10.fid
PROTON DMSO (C:\NMRDATA) baskar 8

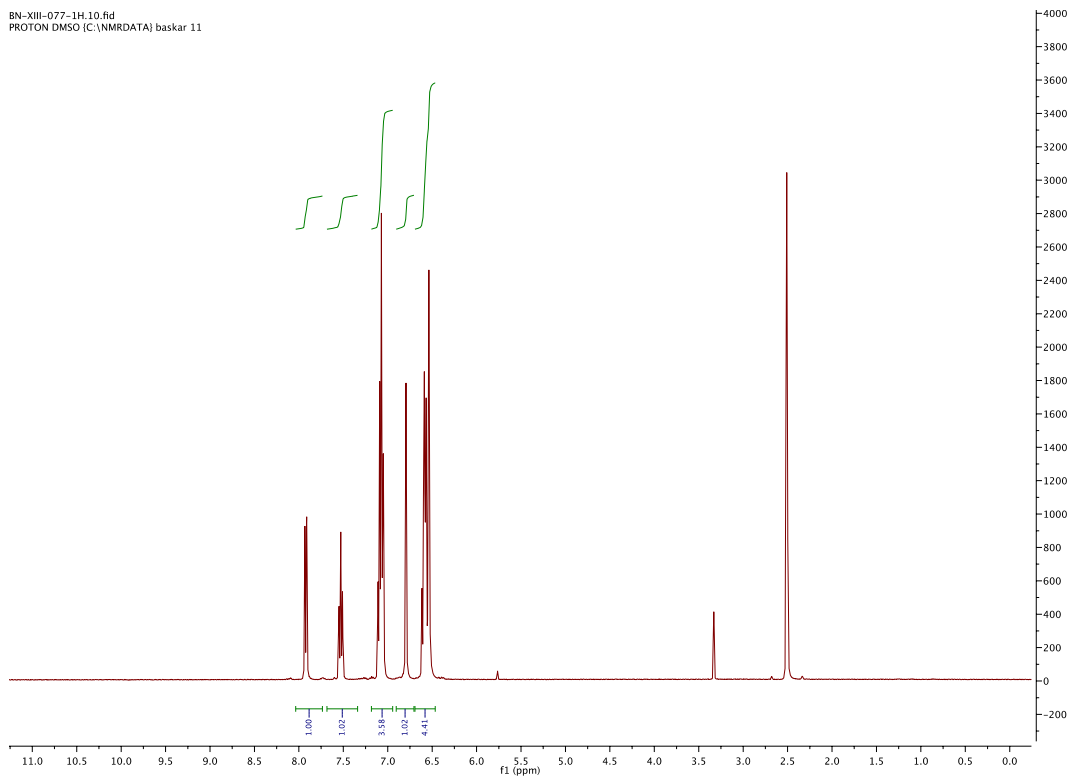


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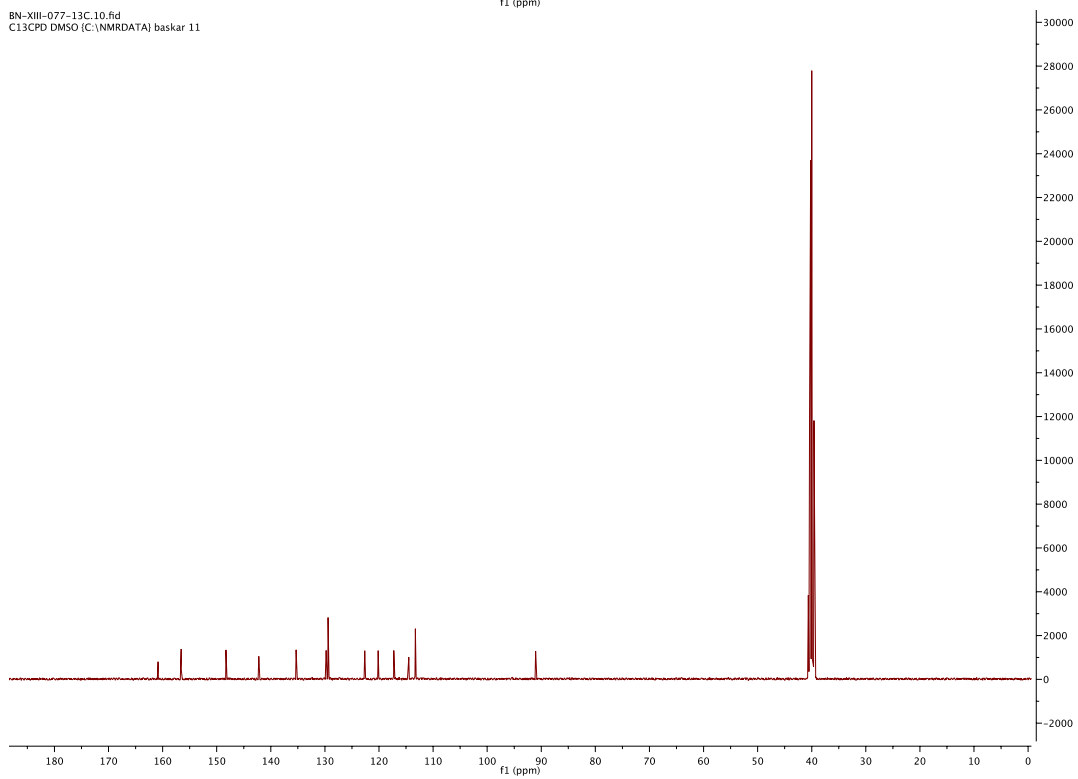


(±)-3-(Phenylamino)isobenzofuran-1(3*H*)-one (6a)

BN-XIII-077-1H.10.fid
PROTON DMSO (C:\NMRDATA) baskar 11

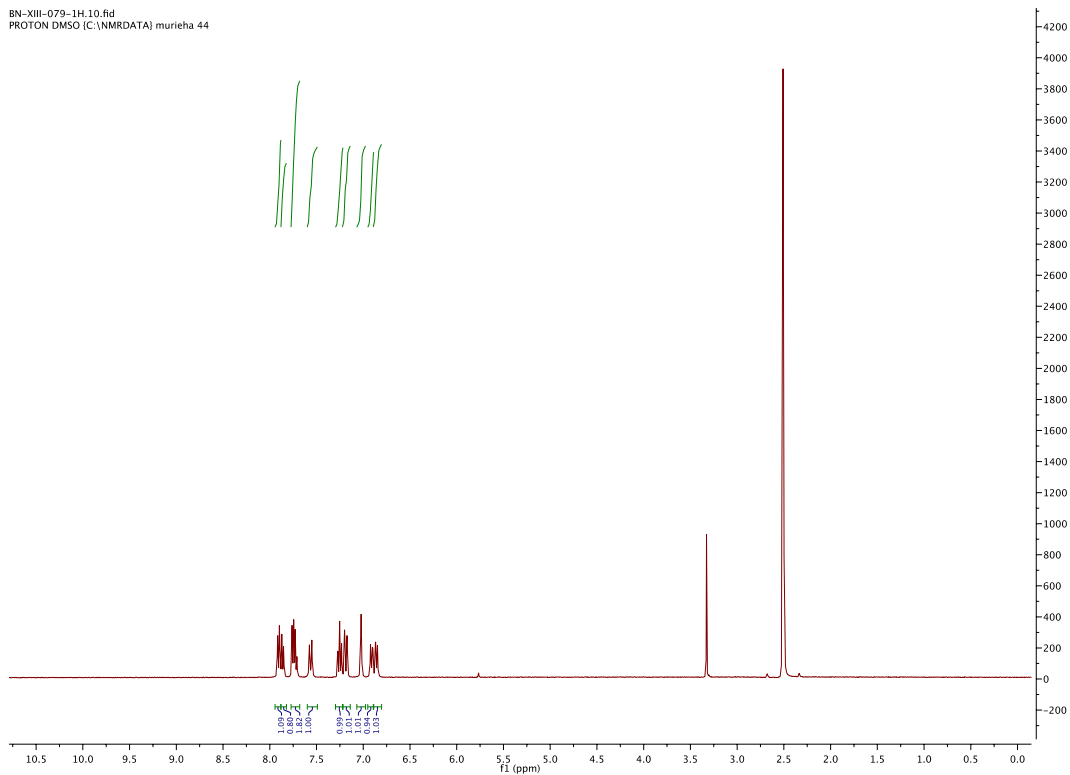


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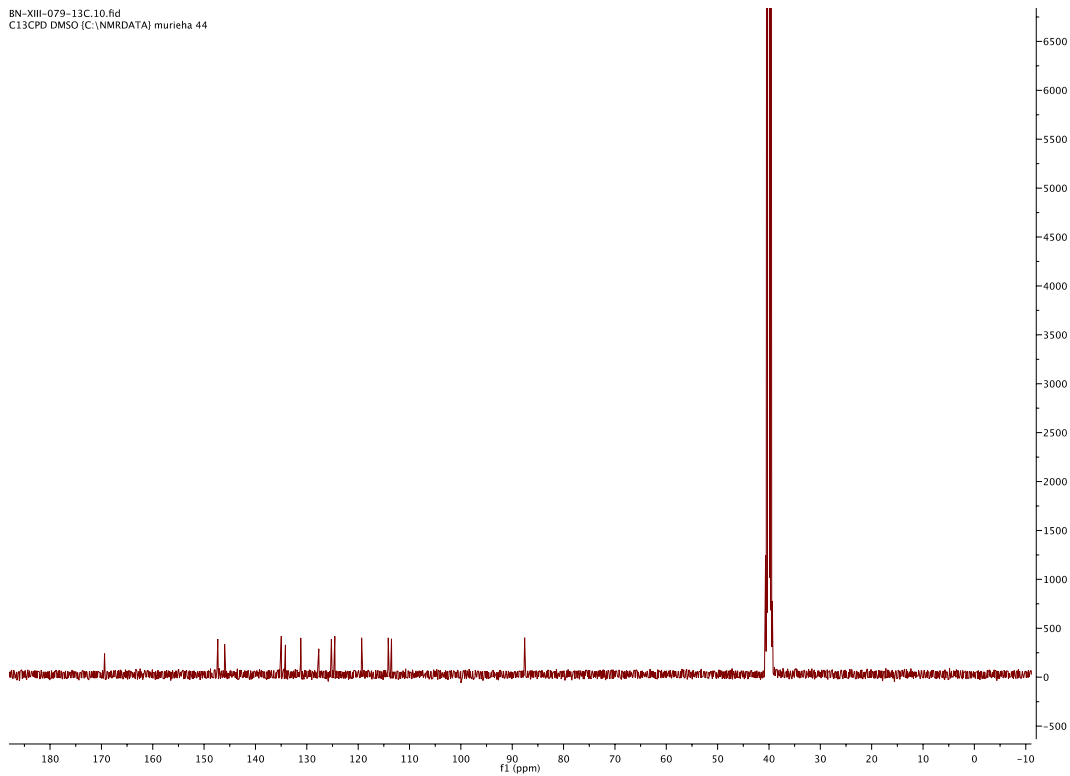


(±)-3-[(3-Chlorophenyl)amino]isobenzofuran-1(3H)-one (6b)

BN-XIII-079-1H.10.fid
PROTON DMSO [C:\NMRDATA] murieha 44

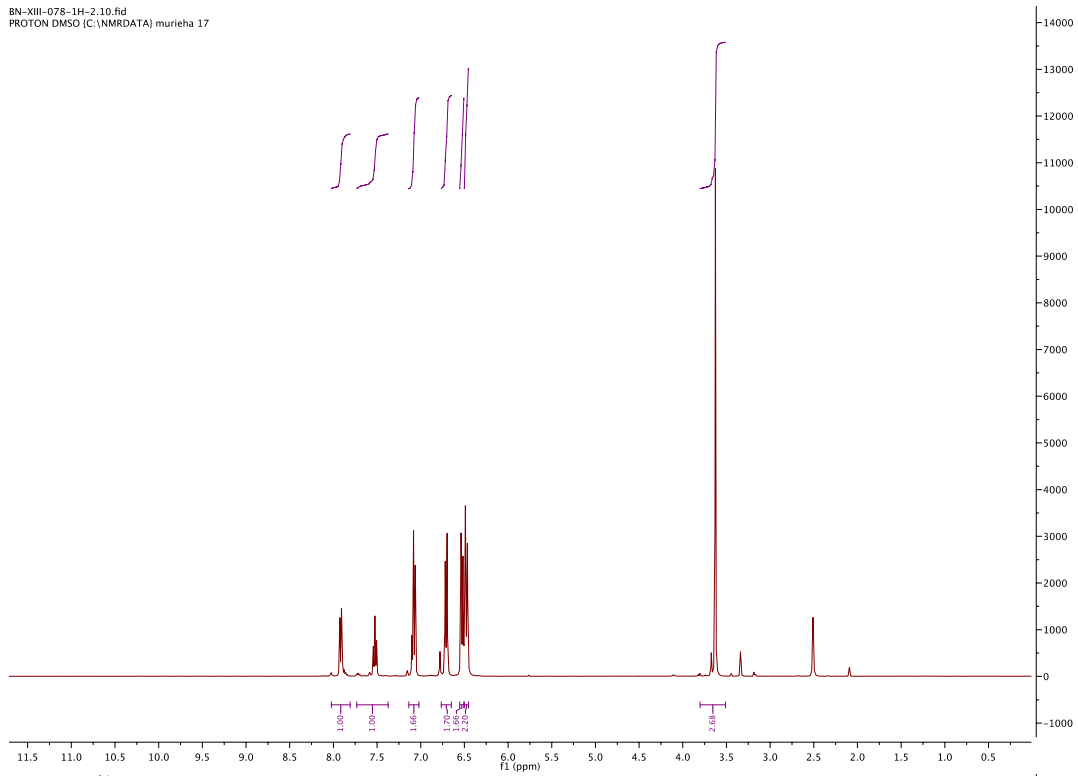


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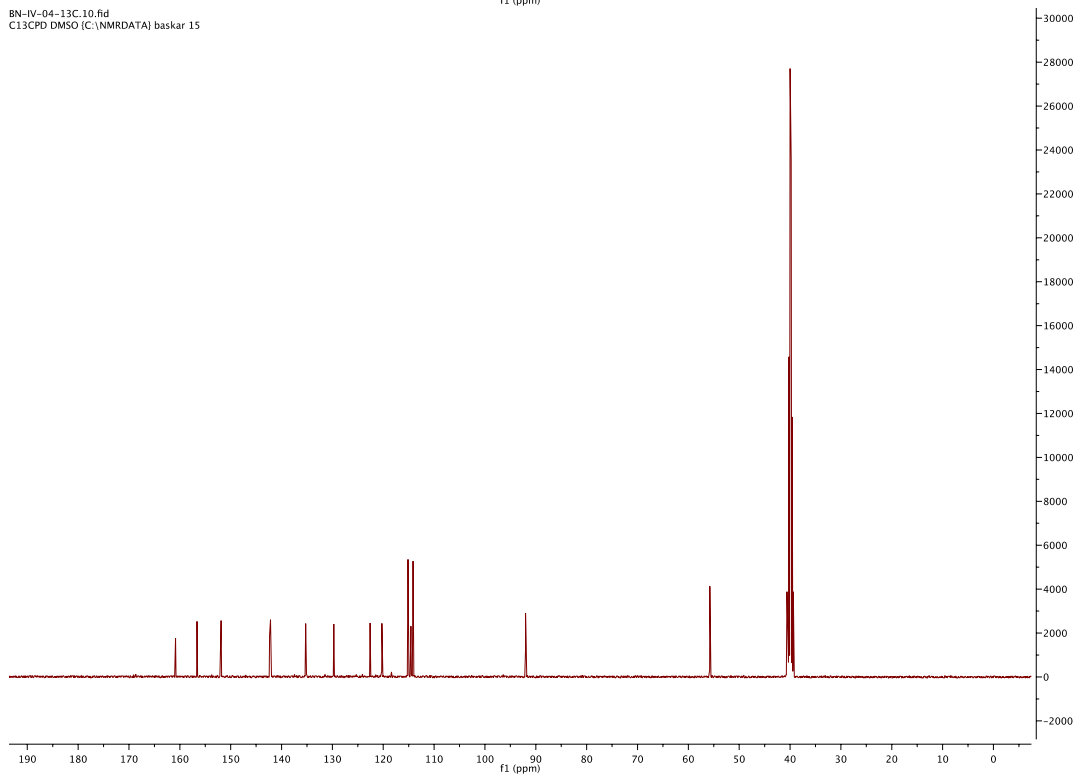


(±)-3-[(4-Methoxyphenyl)amino]isobenzofuran-1(3H)-one (6c)

BN-XIII-078-1H-2.10.fid
PROTON DMSO [C:\NMRDATA] murieha 17

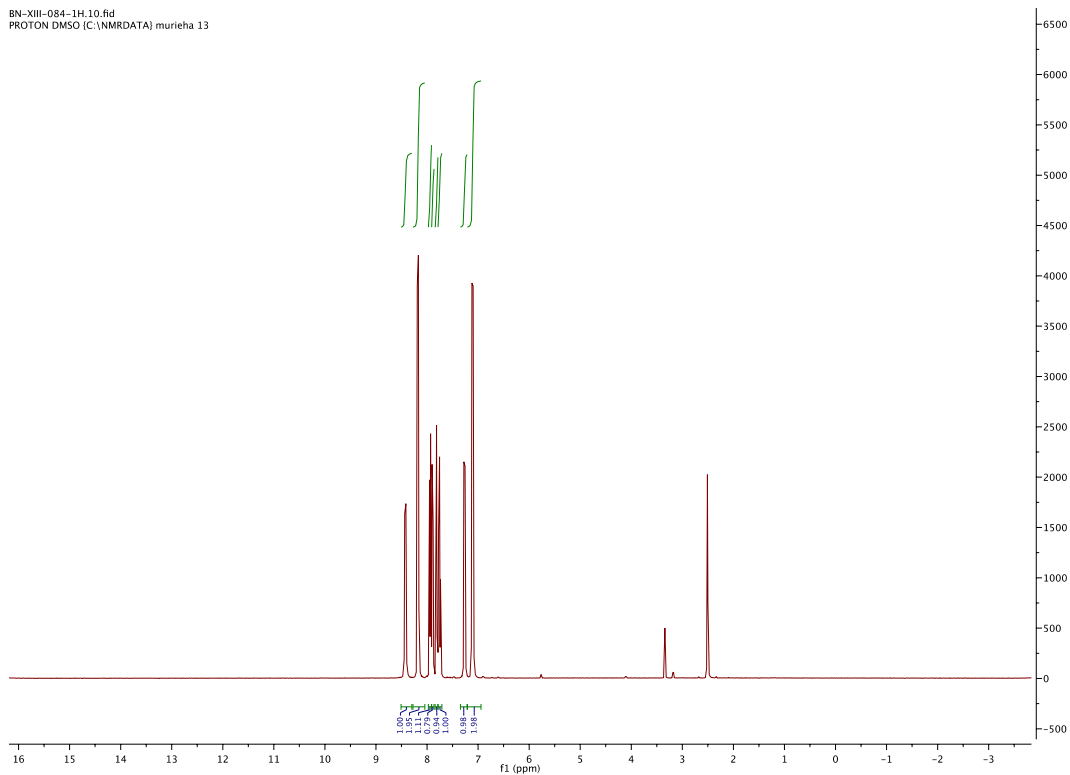


BN-IV-04-13C.10.fid
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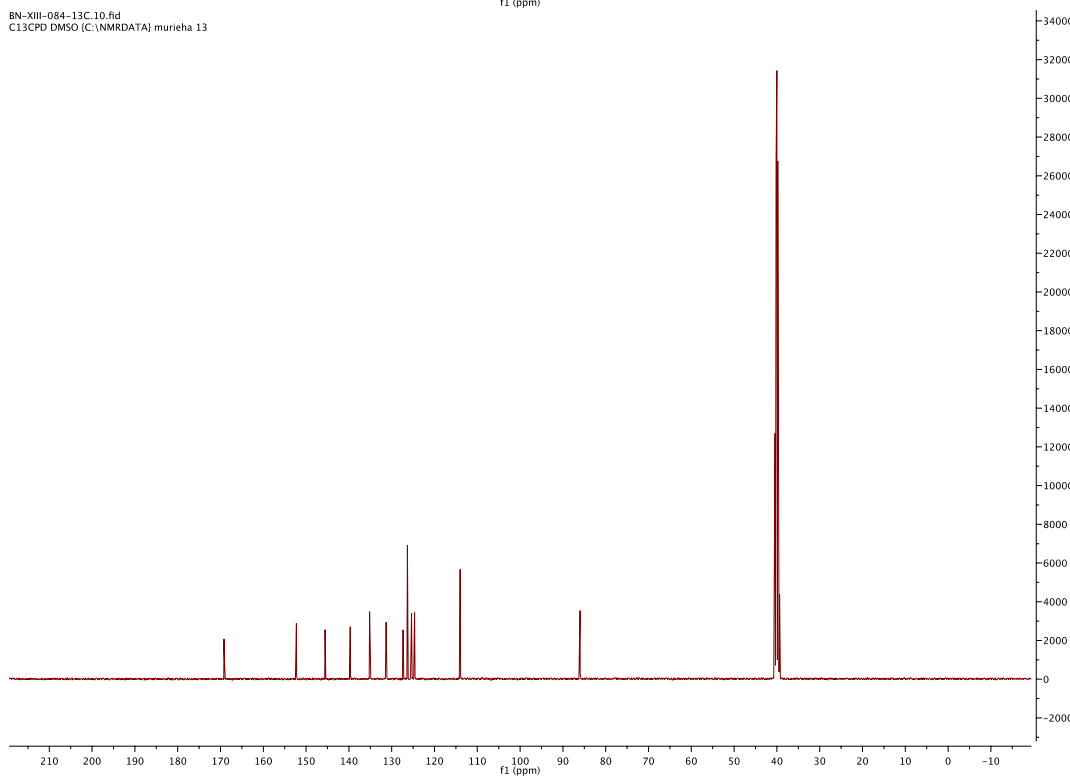


(±)-3-[(4-Nitrophenyl)amino]isobenzofuran-1(3H)-one (6d)

BN-XIII-084-1H.10.fid
PROTON DMSO (C:\NMRDATA) murieha 13

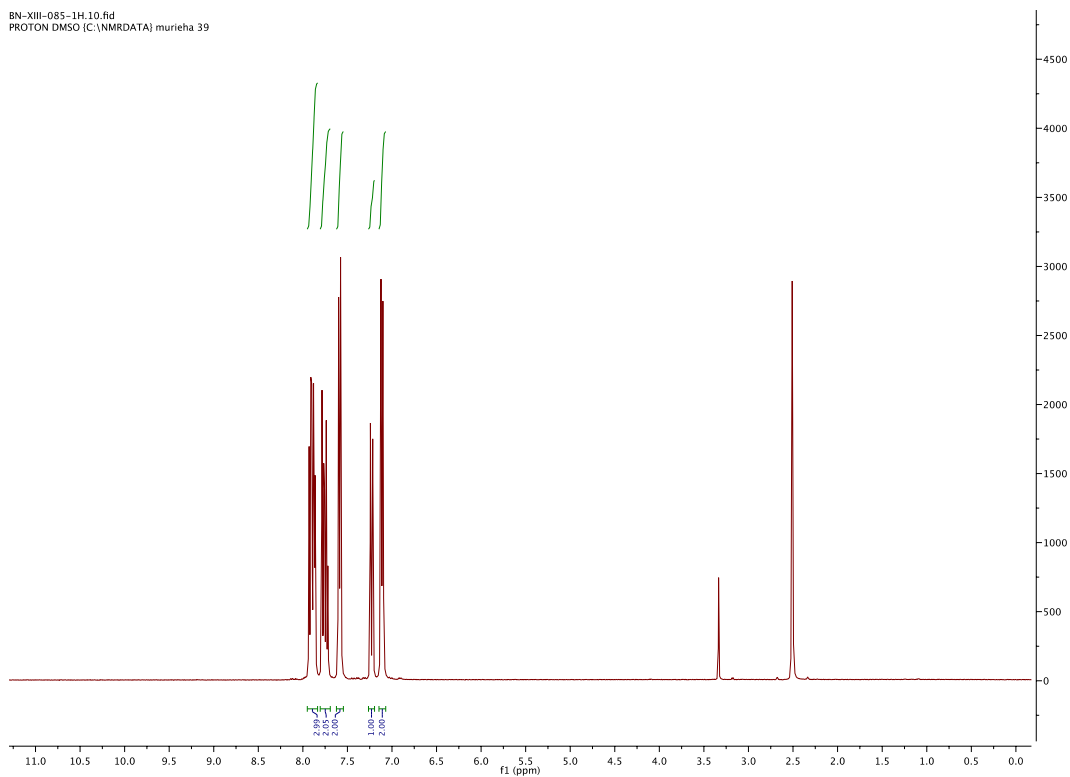


BN-XIII-084-13C.10.fid
C13CPD DMSO (C:\NMRDATA) murieha 13

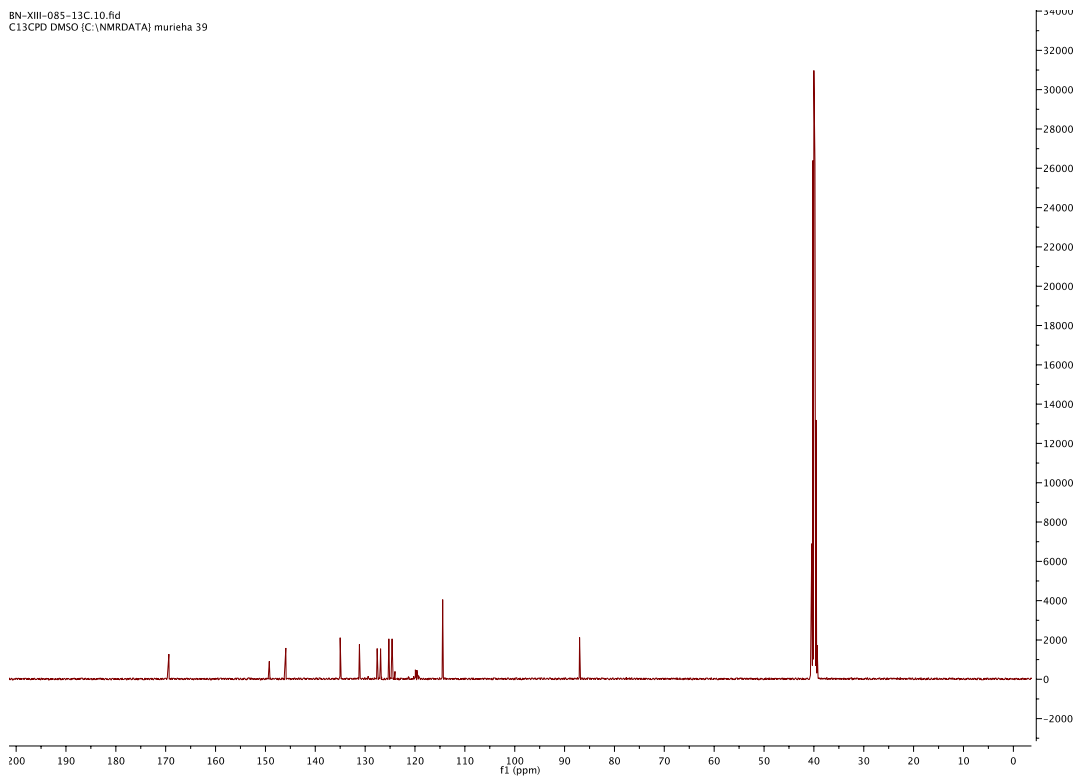


(±)-3-{[4-(Trifluoromethyl)phenyl]amino}isobenzofuran-1(3H)-one (6e)

BN-XIII-085-1H.10.fid
PROTON DMSO (C:\NMRDATA) murieha 39

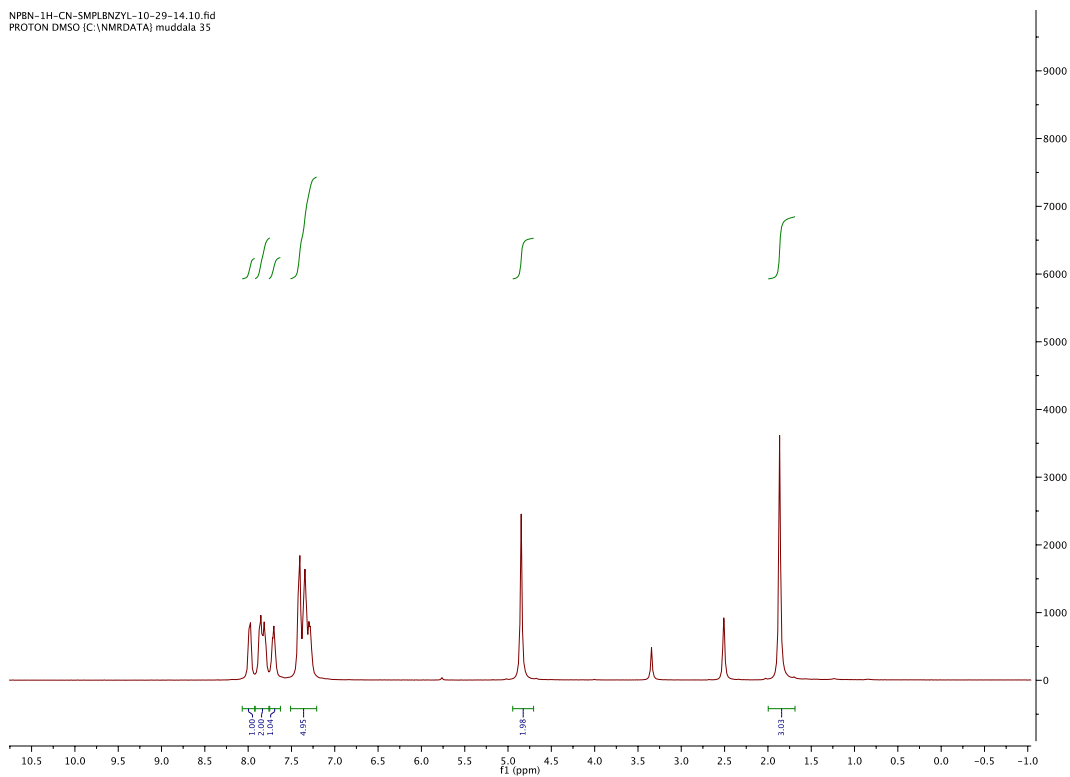


BN-XIII-085-13C.10.fid
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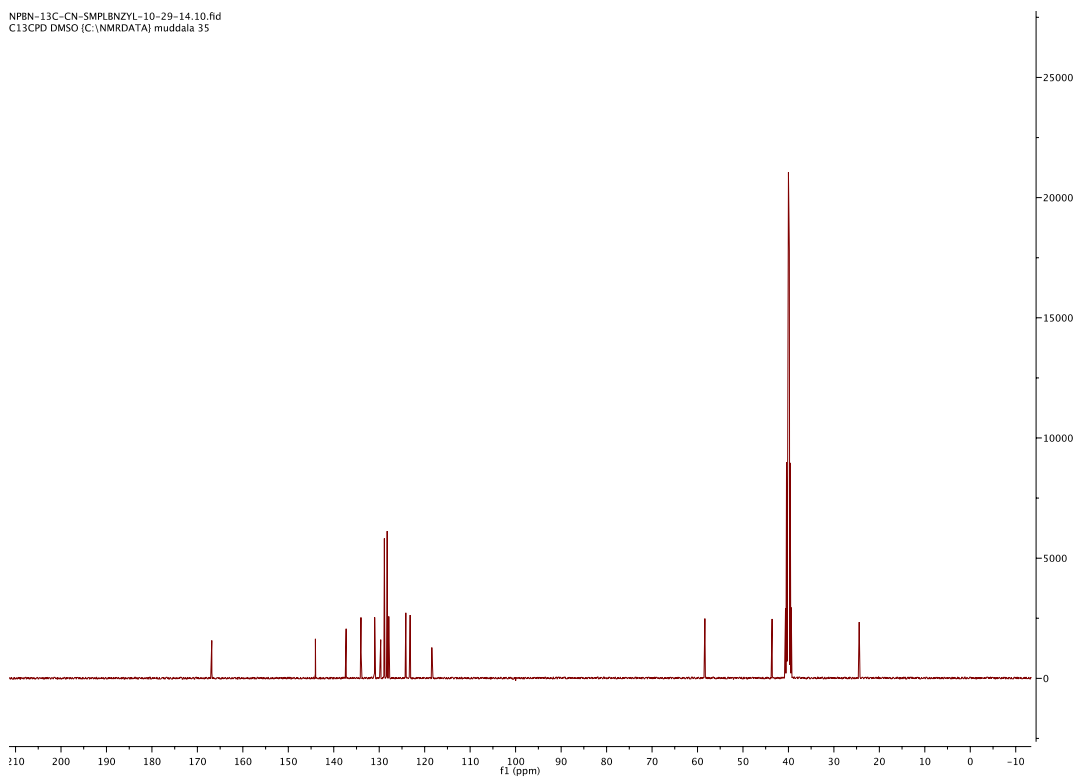


(±)-2-Benzyl-1-methyl-3-oxoisindoline-1-carbonitrile (8a)

NPBN-1H-CN-SMPLBNZYL-10-29-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 35

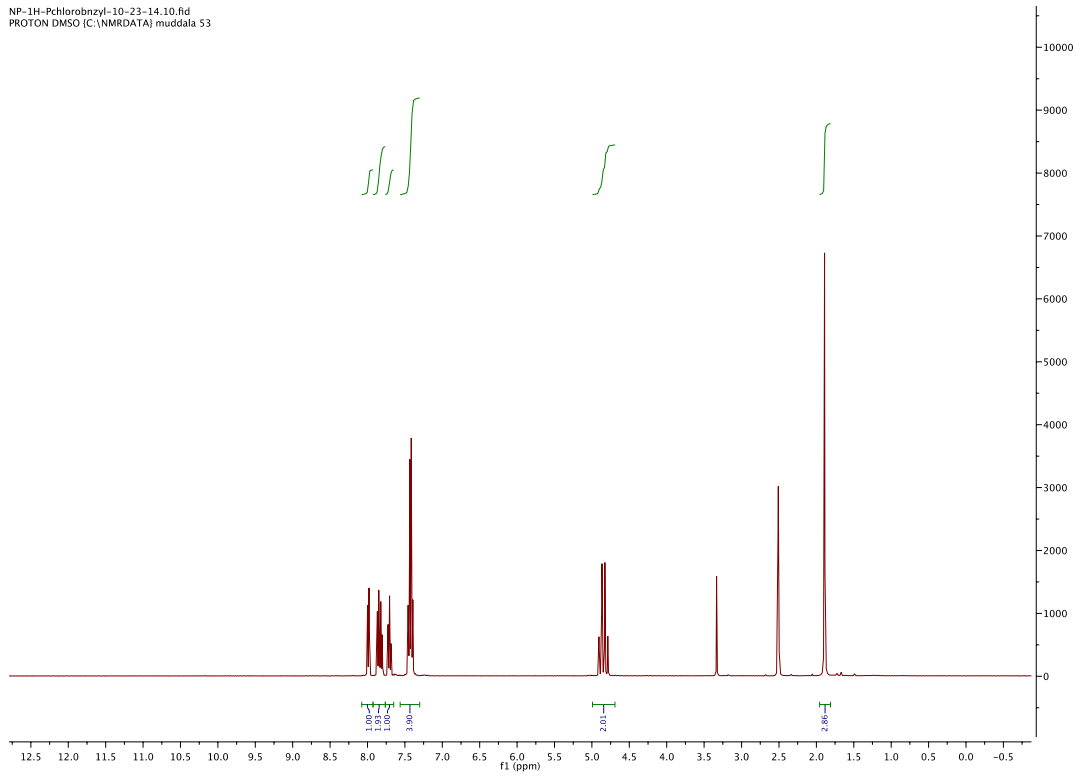


NPBN-13C-CN-SMPLBNZYL-10-29-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 35

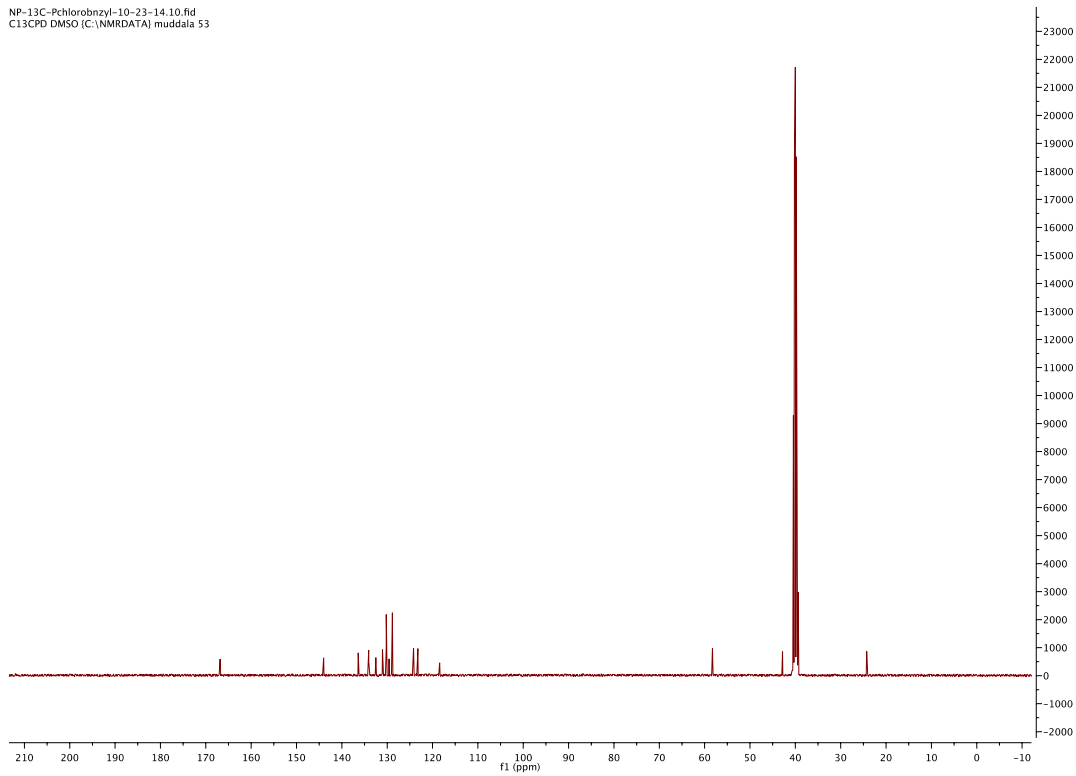


(±)-2-(4-Chlorobenzyl)-1-methyl-3-oxoisindoline-1-carbonitrile (8b)

NP-1H-Pchlorobenzyl-10-23-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 53

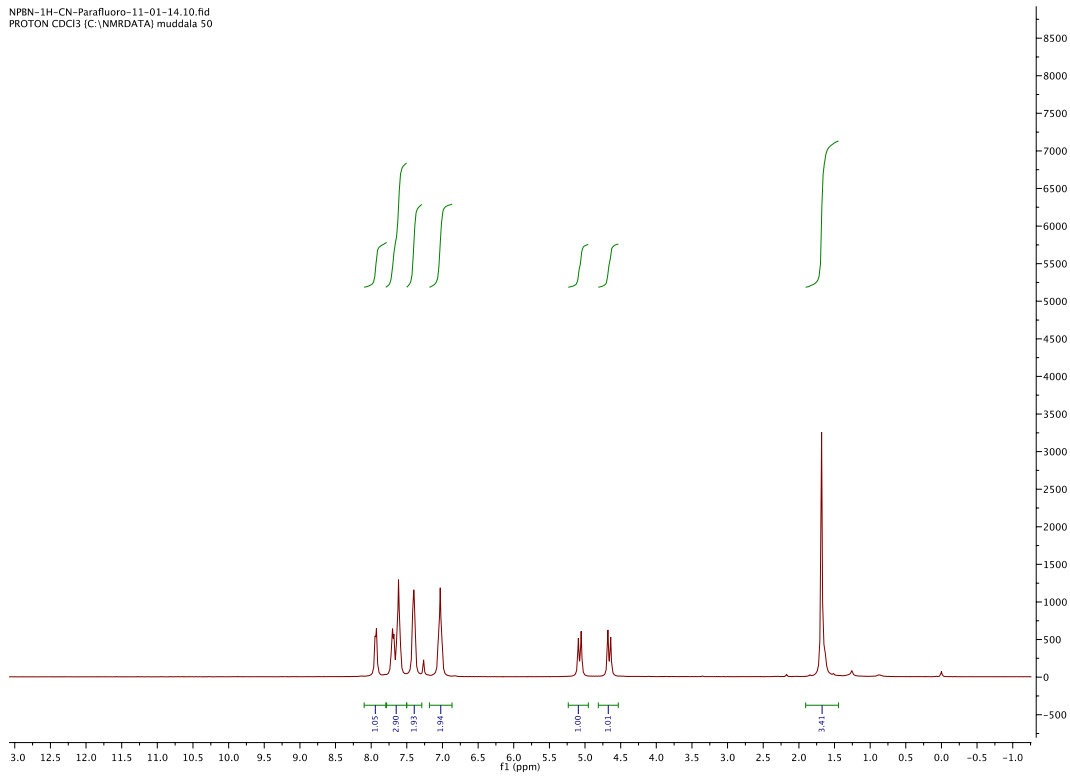


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C13CPD DMSO (C:\NMRDATA) muddala 53

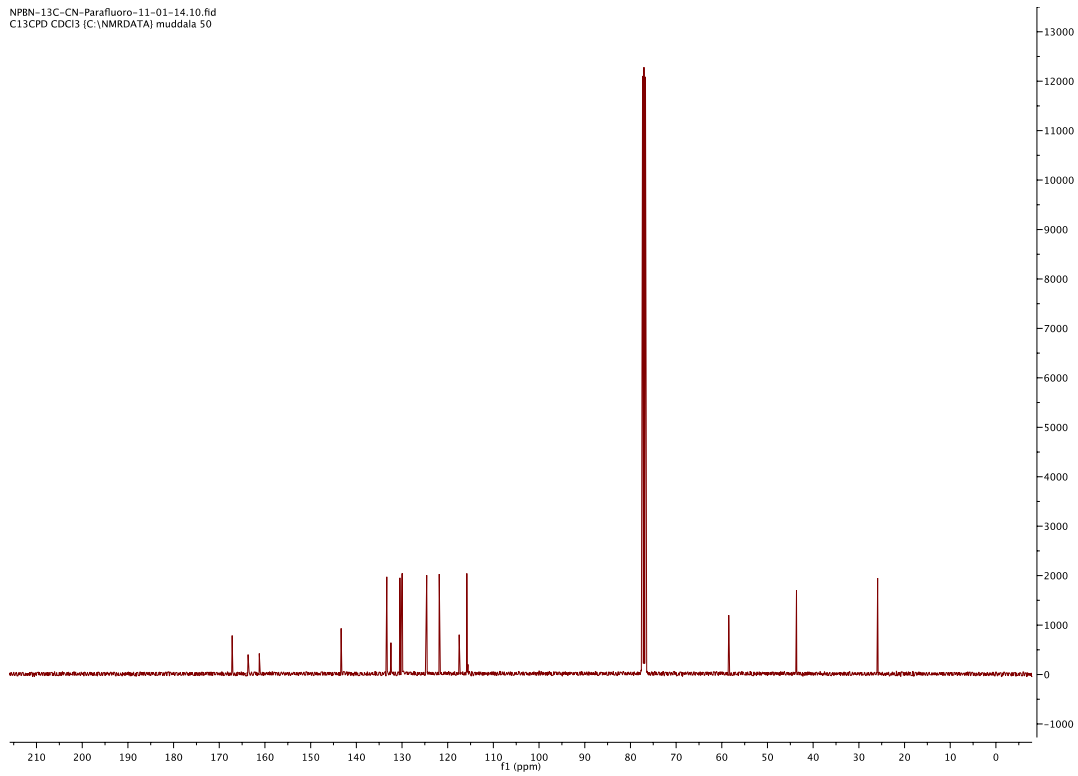


(±)-2-(4-Fluorobenzyl)-1-methyl-3-oxoisindoline-1-carbonitrile (8c)

NPN-1H-CN-Parafuoro-11-01-14.10.fid
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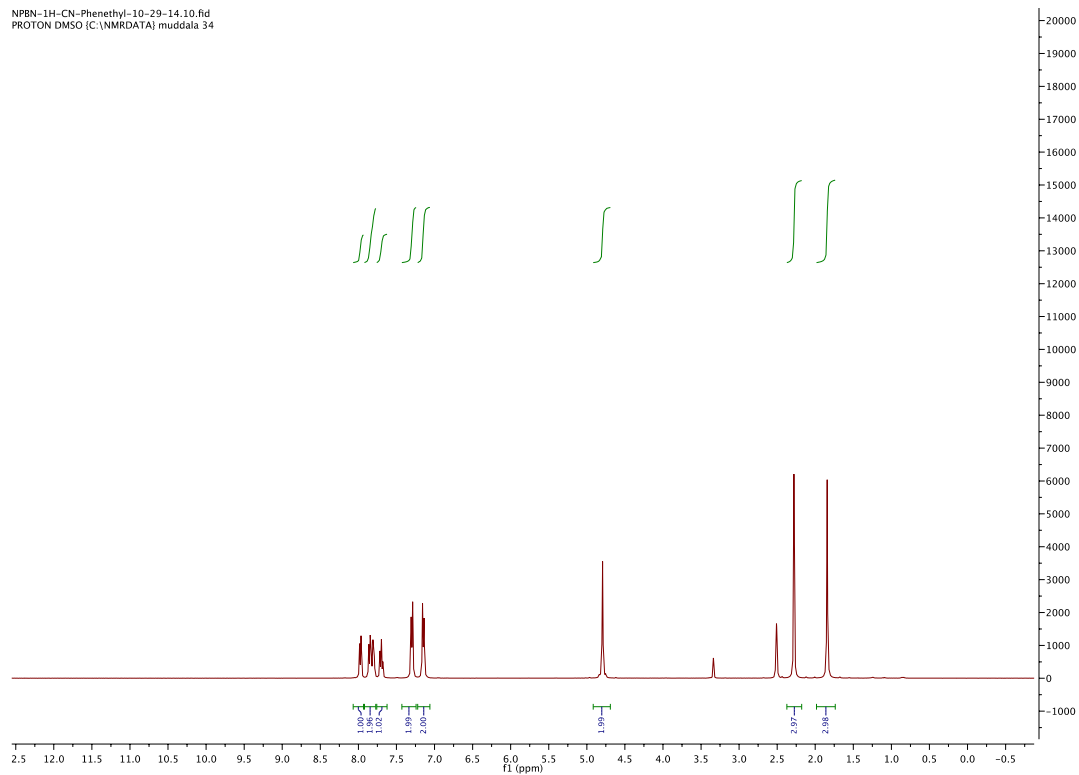


NPN-13C-CN-Parafuoro-11-01-14.10.fid
C13CPD CDCI3 (C:\NMRDATA) muddala 50

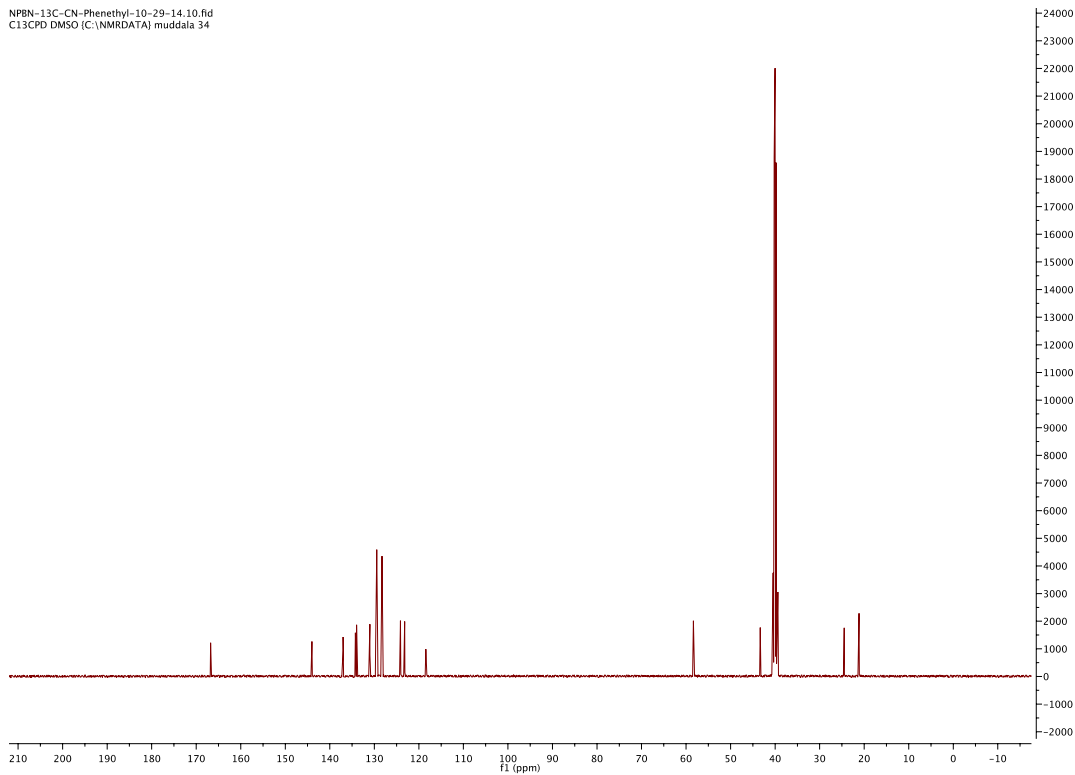


(±)-1-Methyl-2-(4-methylbenzyl)-3-oxoisindoline-1-carbonitrile (8d)

NPBN-1H-CN-Phenethyl-10-29-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 34

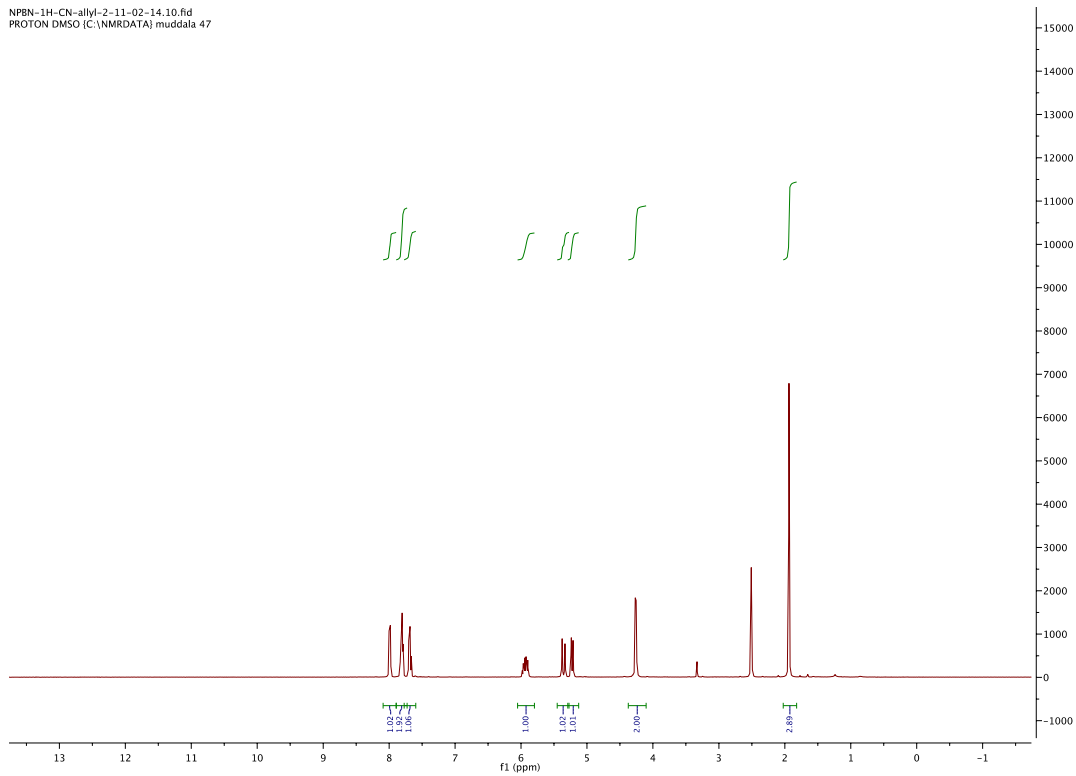


NPBN-13C-CN-Phenethyl-10-29-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 34

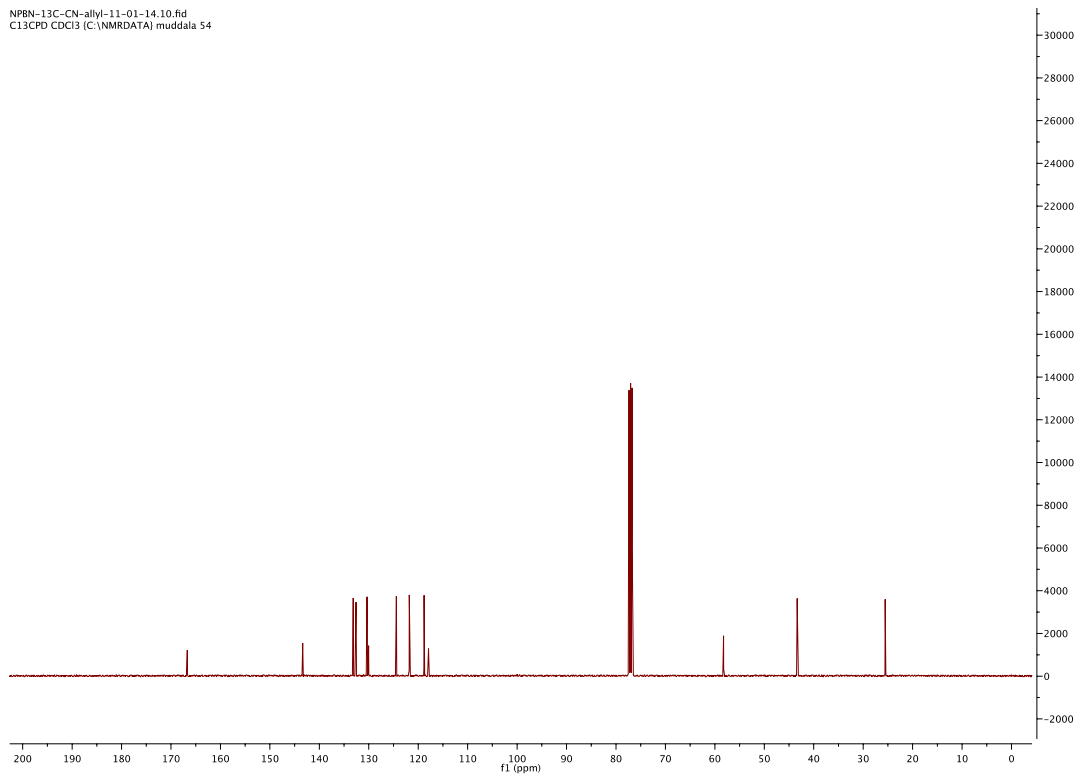


(±)-2-Allyl-1-methyl-3-oxoisindoline-1-carbonitrile (8e)

NPN-1H-CN-allyl-2-11-02-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 47

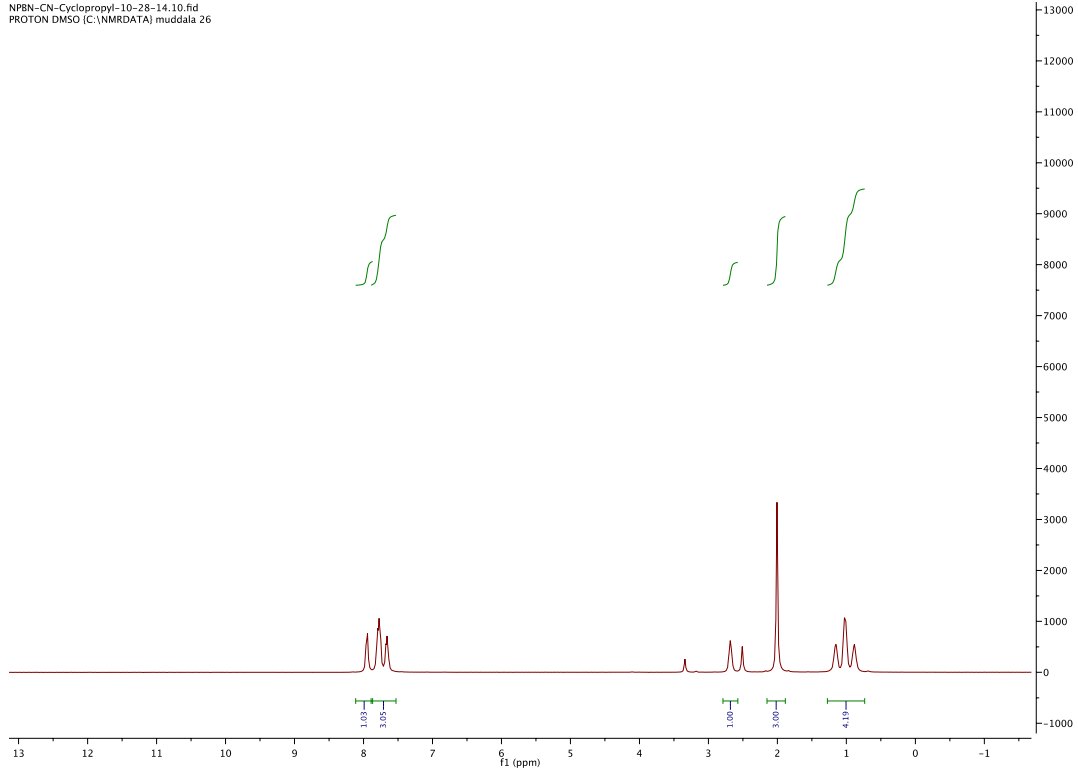


NPN-13C-CN-allyl-11-01-14.10.fid
C13CPD CDCl3 [C:\NMRDATA] muddala 54

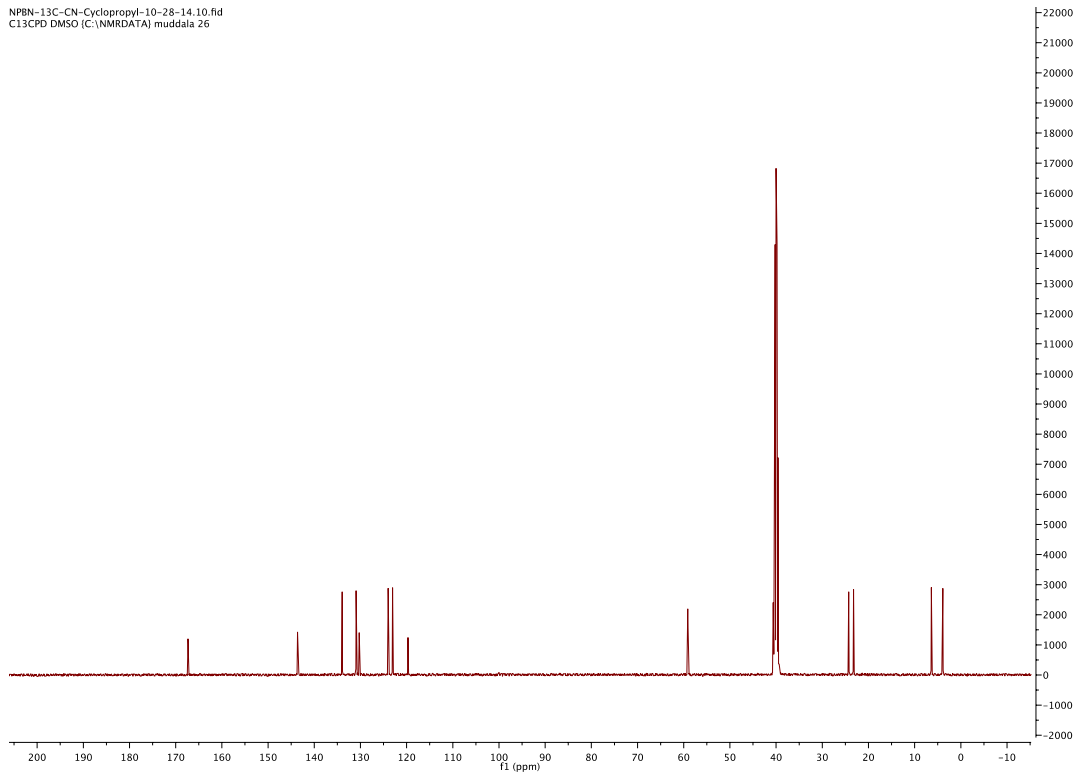


(±)-2-Cyclopropyl-1-methyl-3-oxoisindoline-1-carbonitrile (8f)

NPN-CN-Cyclopropyl-10-28-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 26

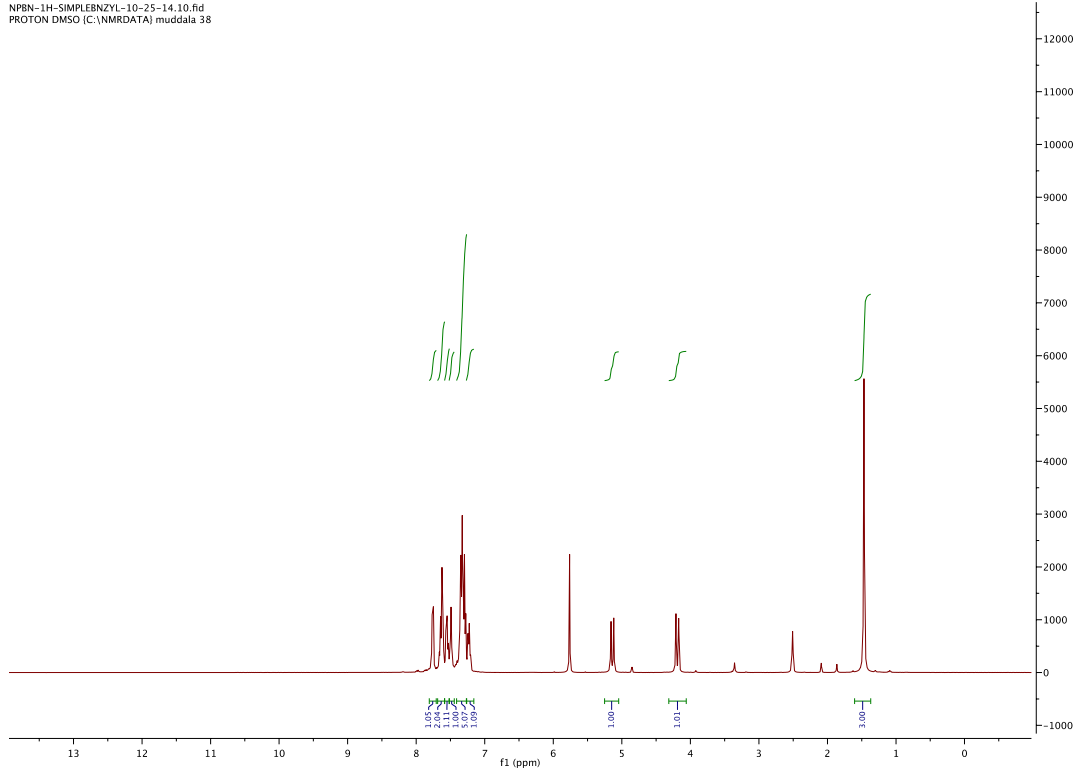


NPN-13C-CN-Cyclopropyl-10-28-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 26

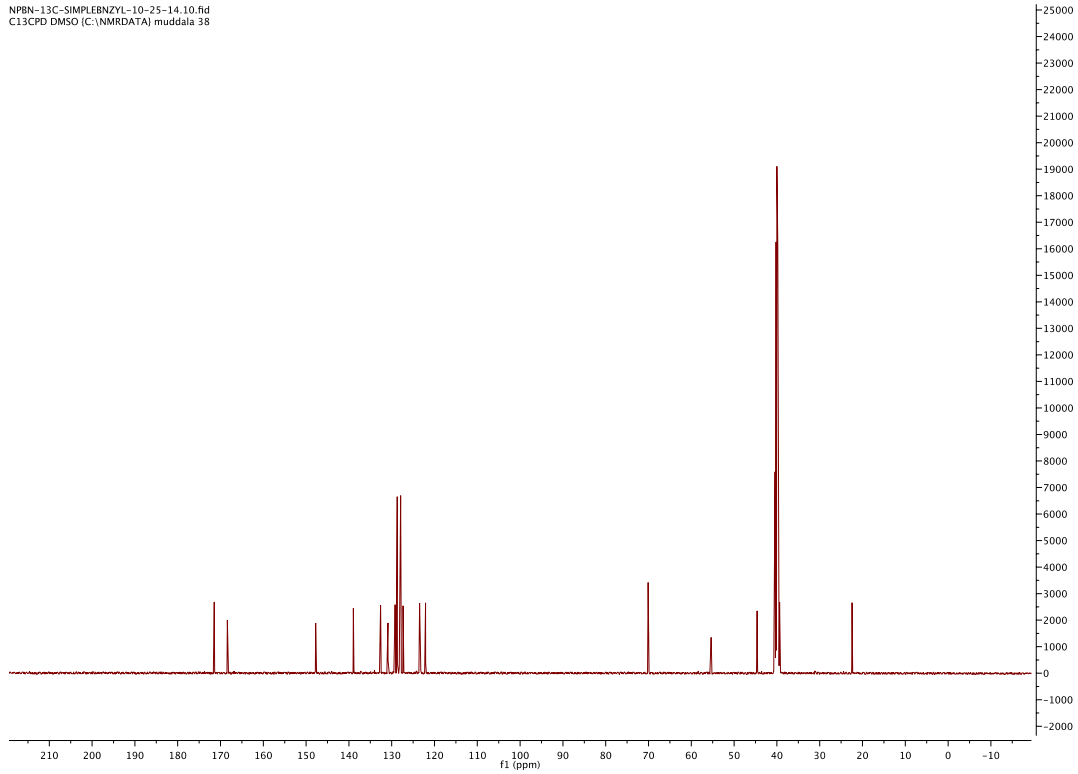


(±)-2-Benzyl-1-methyl-3-oxoisindoline-1-carboxamide (9a)

NPN-1H-SIMPLEBNZYL-10-25-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 38

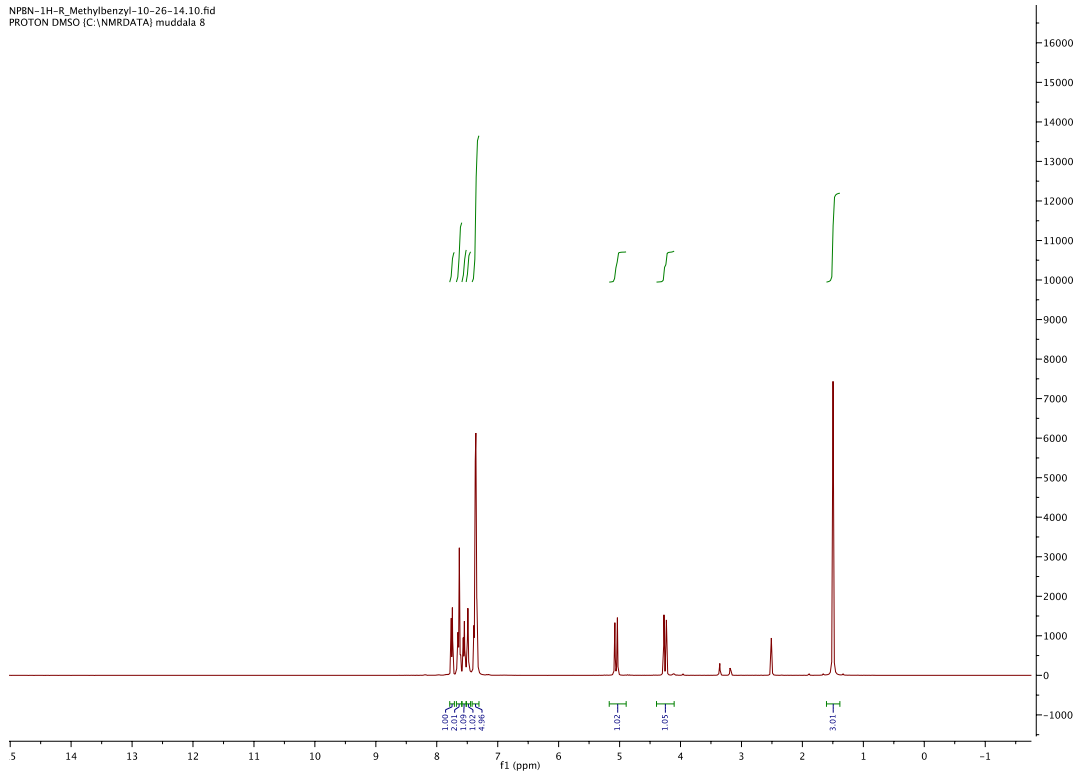


NPN-13C-SIMPLEBNZYL-10-25-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 38

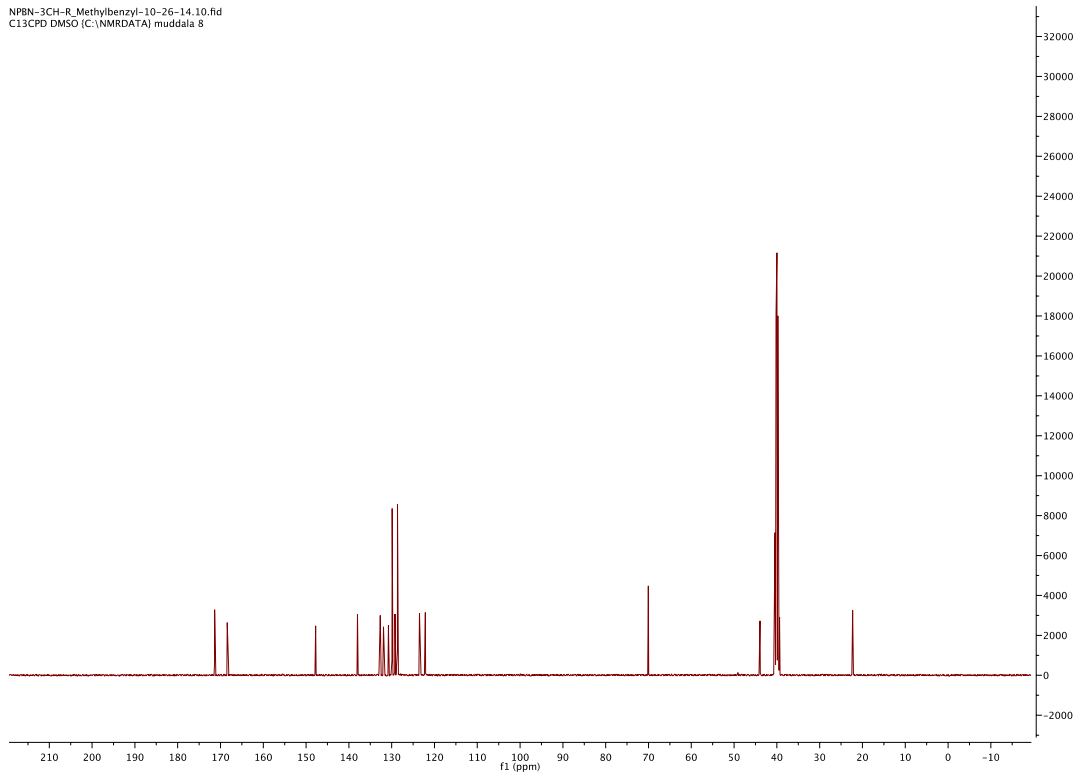


(±)-2-(4-Chlorobenzyl)-1-methyl-3-oxoisindoline-1-carboxamide (9b)

NPN-1H-R_Methylbenzyl-10-26-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 8

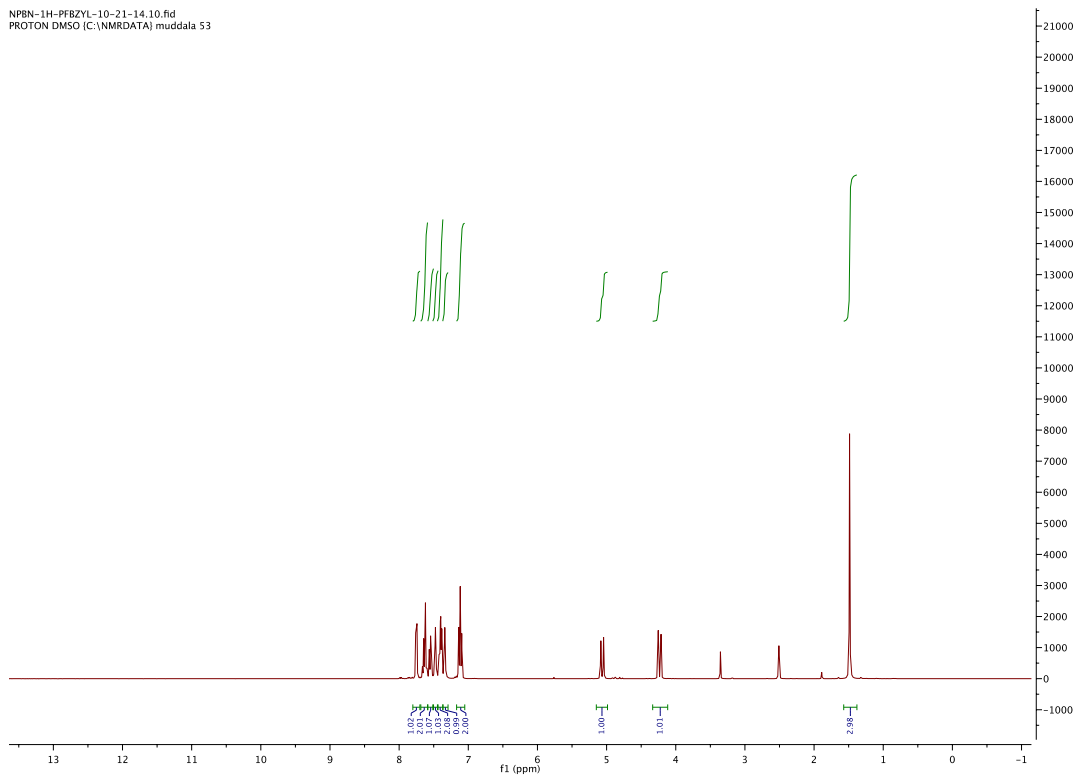


NPN-13C-R_Methylbenzyl-10-26-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 8

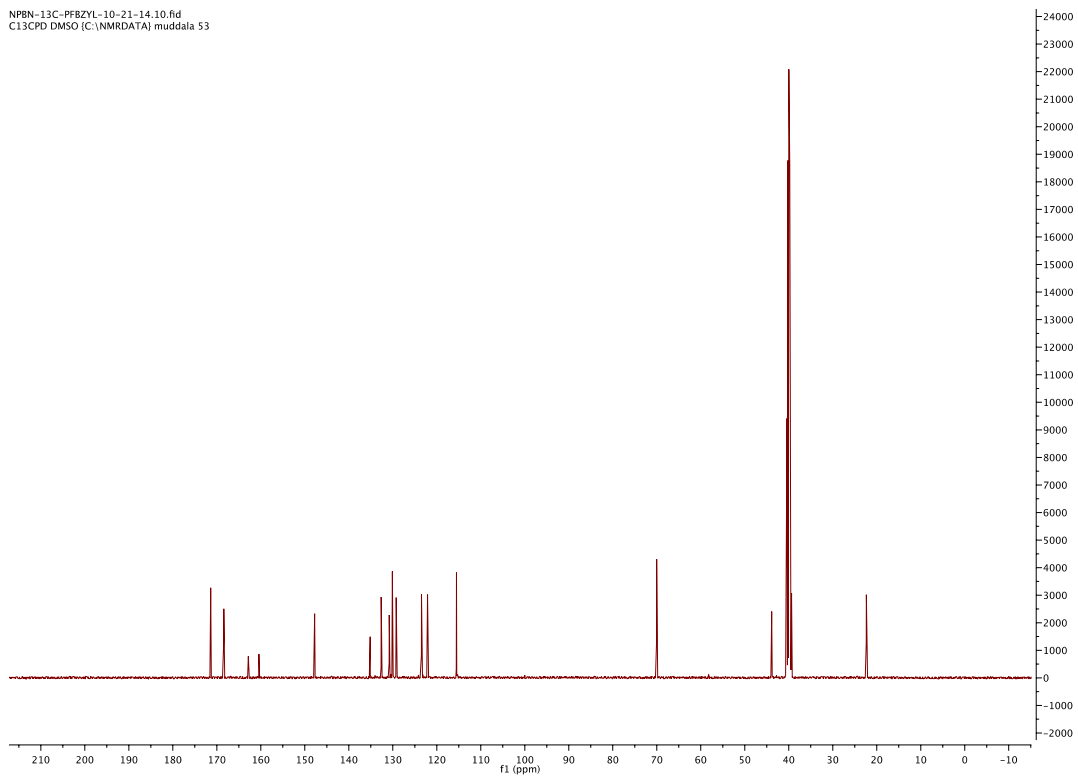


(±)-2-(4-Fluorobenzyl)-1-methyl-3-oxoisindoline-1-carboxamide (9c)

NPN-1H-PFBZYL-10-21-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 53

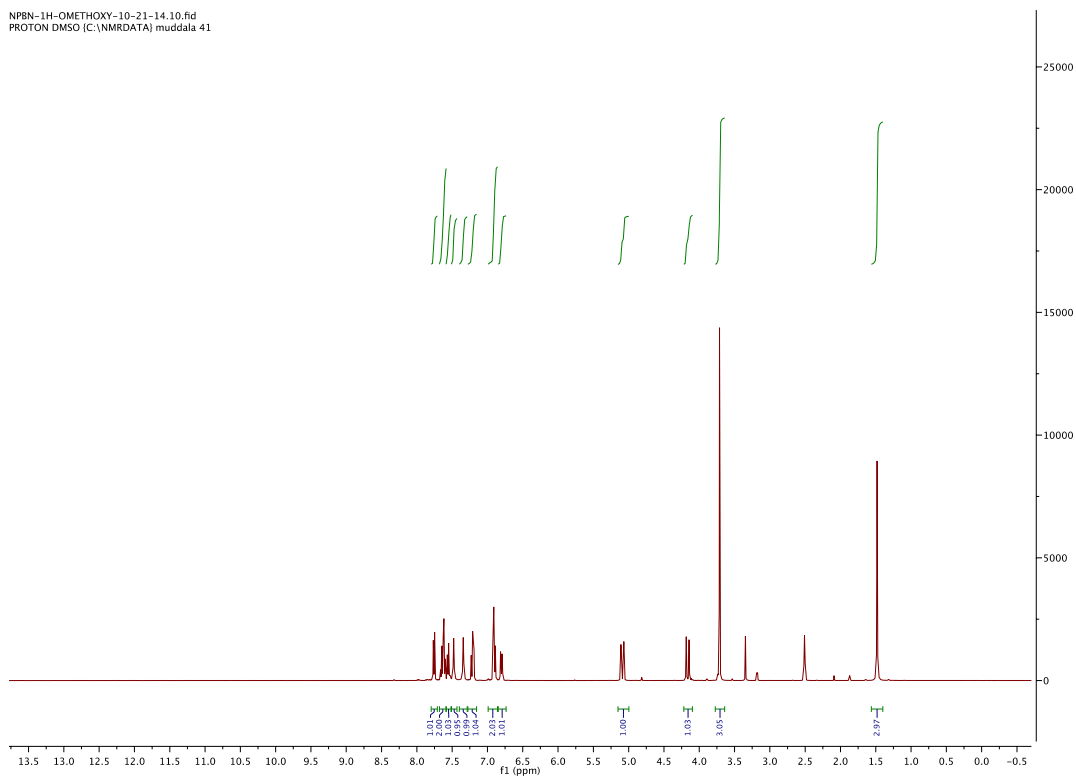


NPN-13C-PFBZYL-10-21-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 53

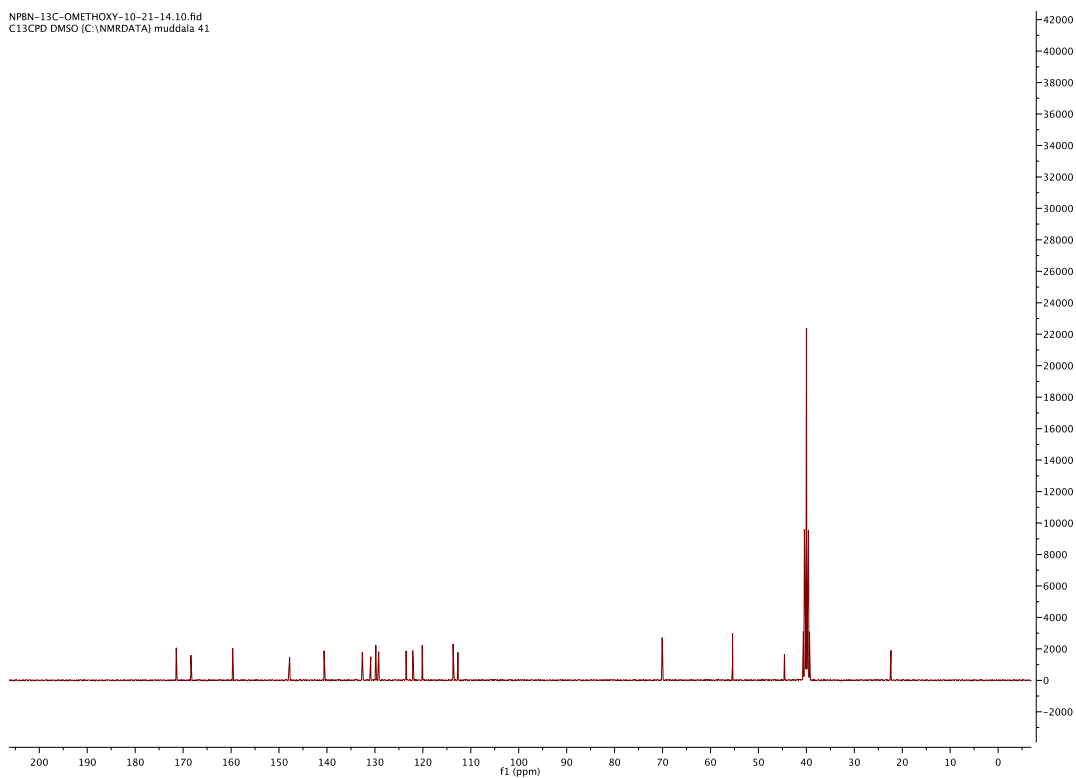


(±)-2-(3-Methoxybenzyl)-1-methyl-3-oxoisindoline-1-carboxamide (9d)

NPN-1H-OMETHOXY-10-21-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 41

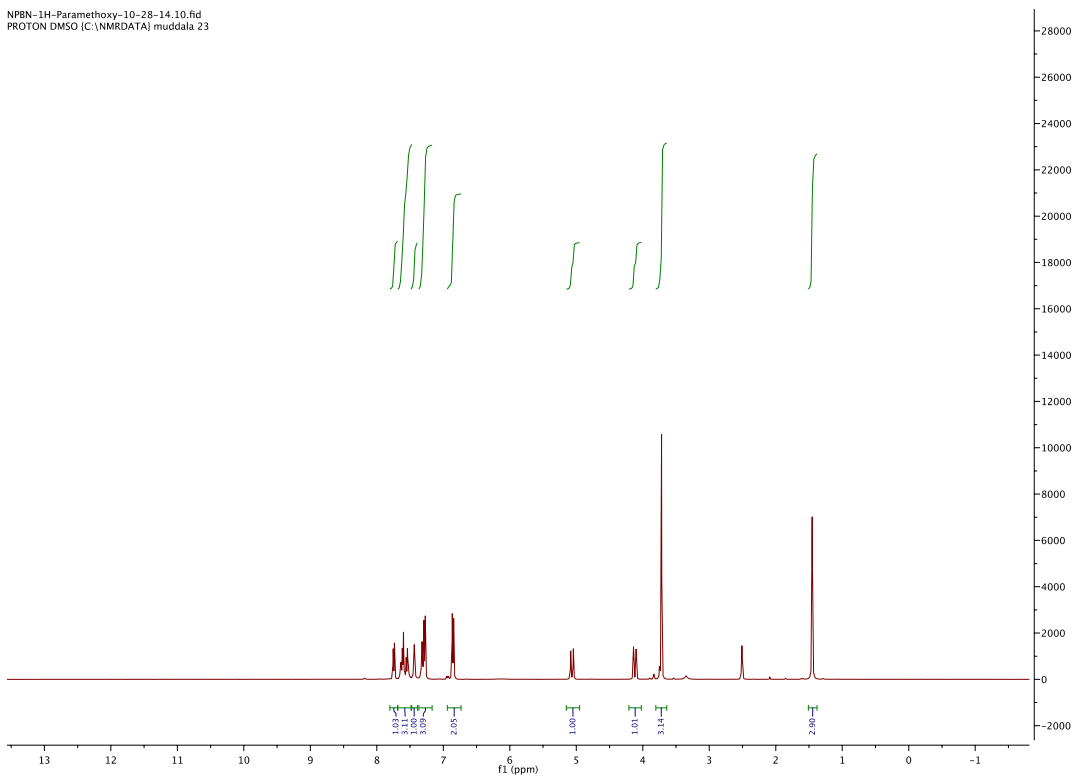


NPN-13C-OMETHOXY-10-21-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 41

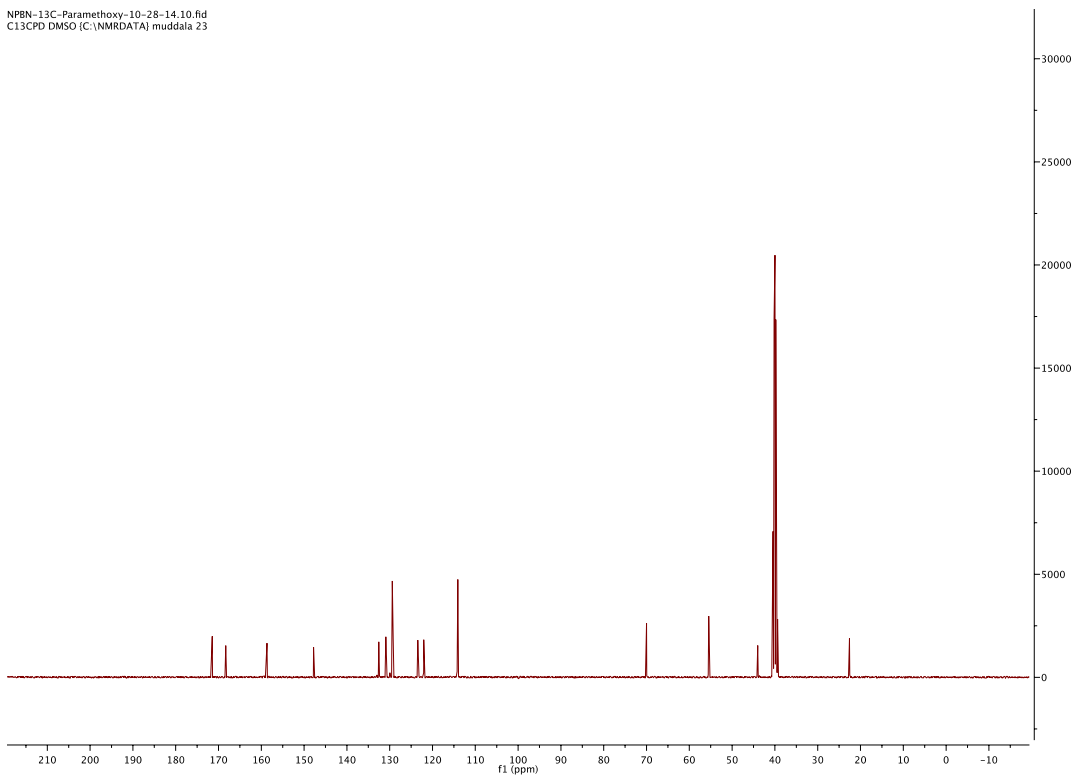


(±)-2-(4-Methoxybenzyl)-1-methyl-3-oxoisindoline-1-carboxamide (9e)

NPN-1H-Paramethoxy-10-28-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 23

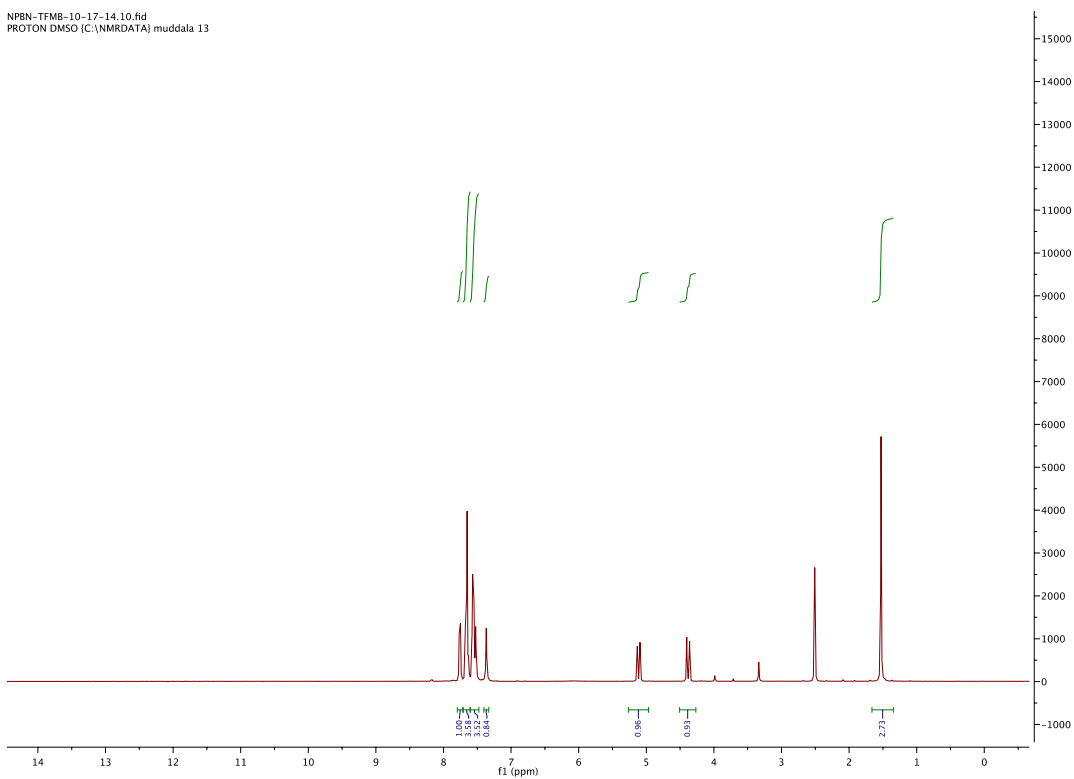


NPN-13C-Paramethoxy-10-28-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 23

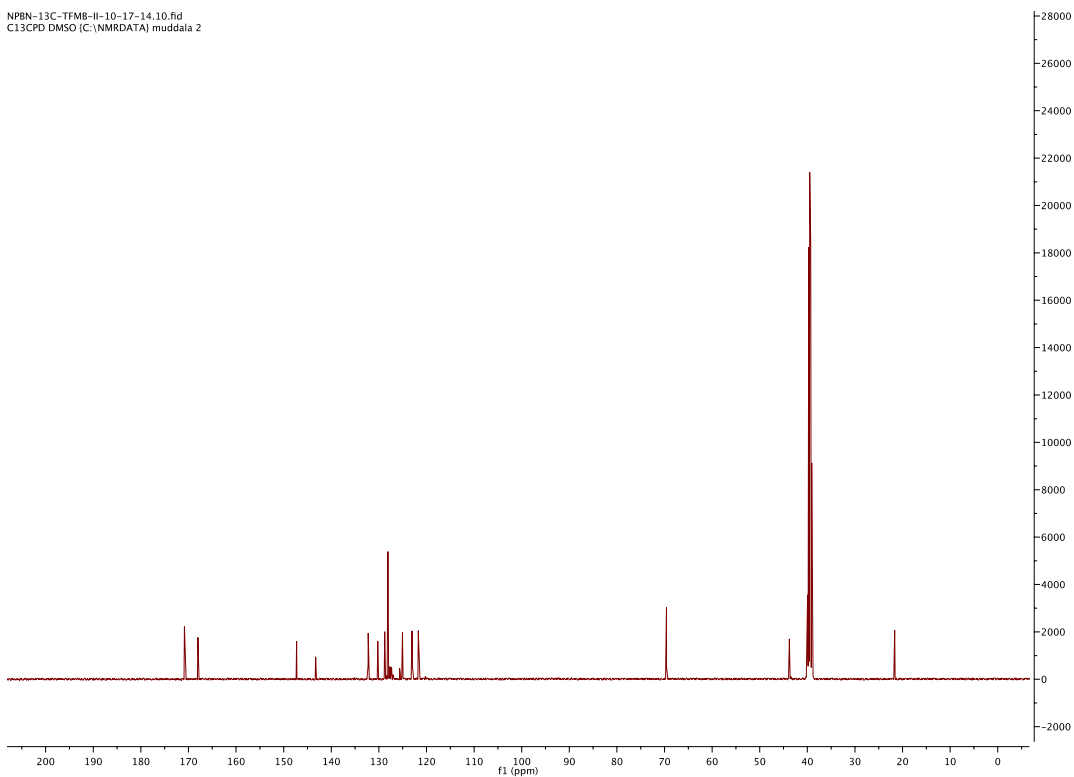


(±)-1-Methyl-3-oxo-2-[4-(trifluoromethyl)benzyl]isoindoline-1-carboxamide (9f)

NPN-TFMB-10-17-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 13

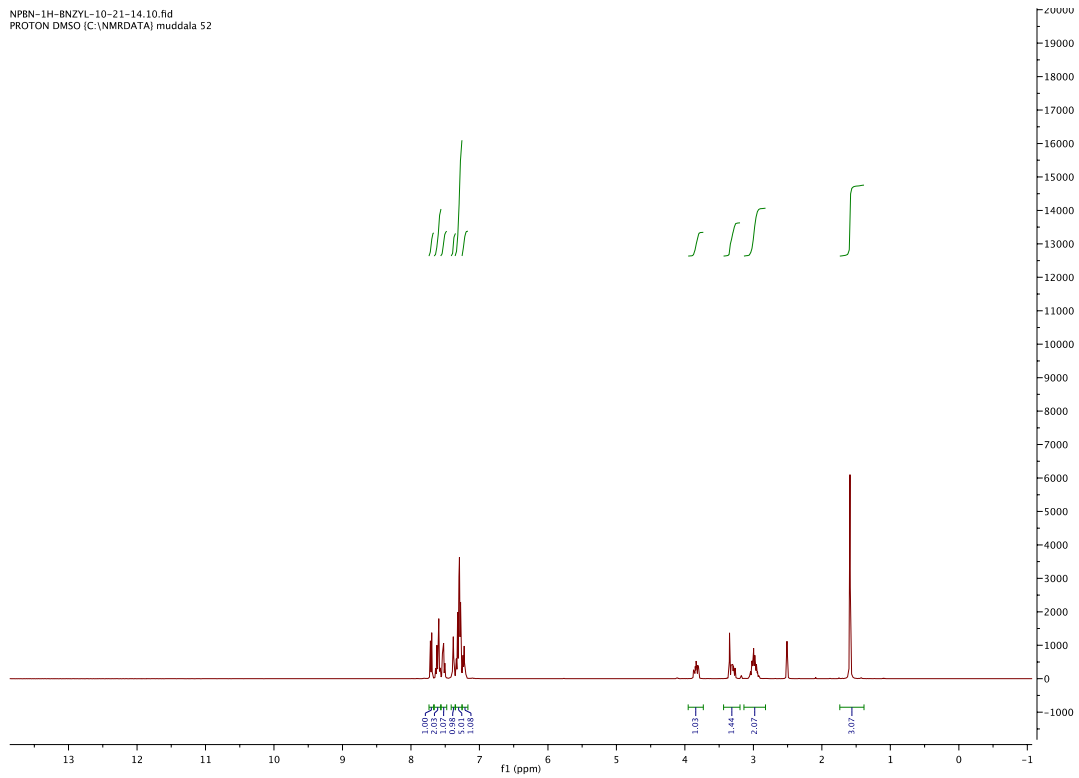


NPN-13C-TFMB-II-10-17-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 2

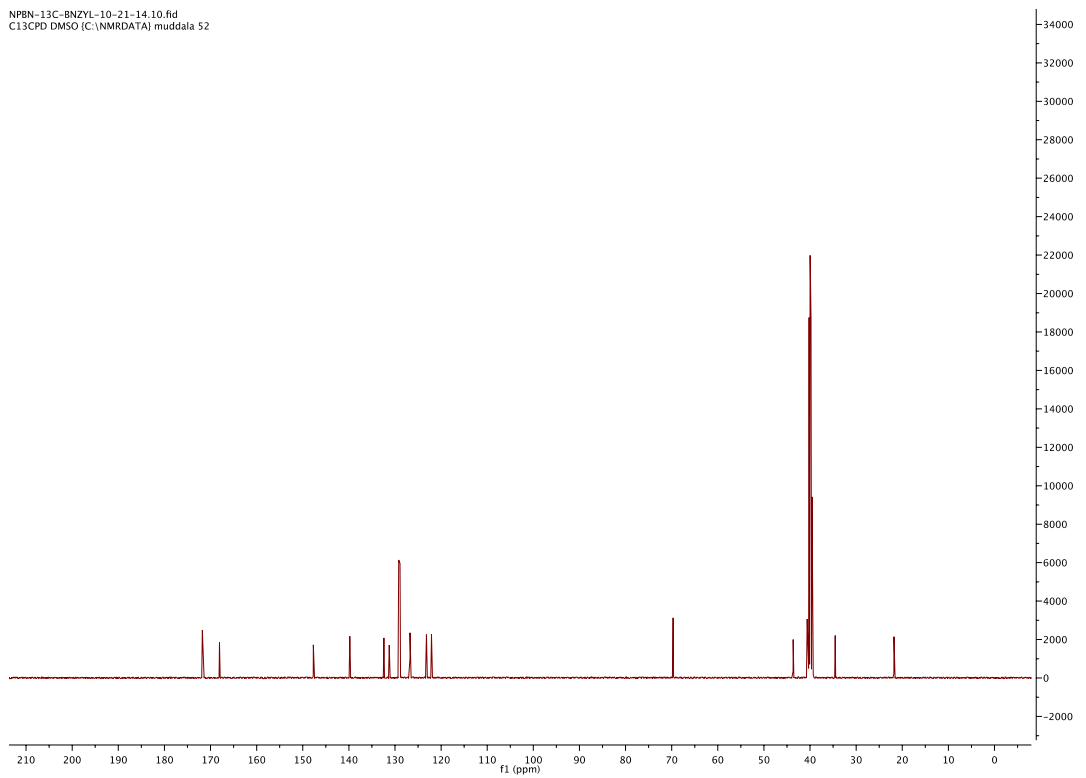


(±)-1-Methyl-3-oxo-2-phenethylisoindoline-1-carboxamide (9g)

NPBN-1H-BNZYL-10-21-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 52

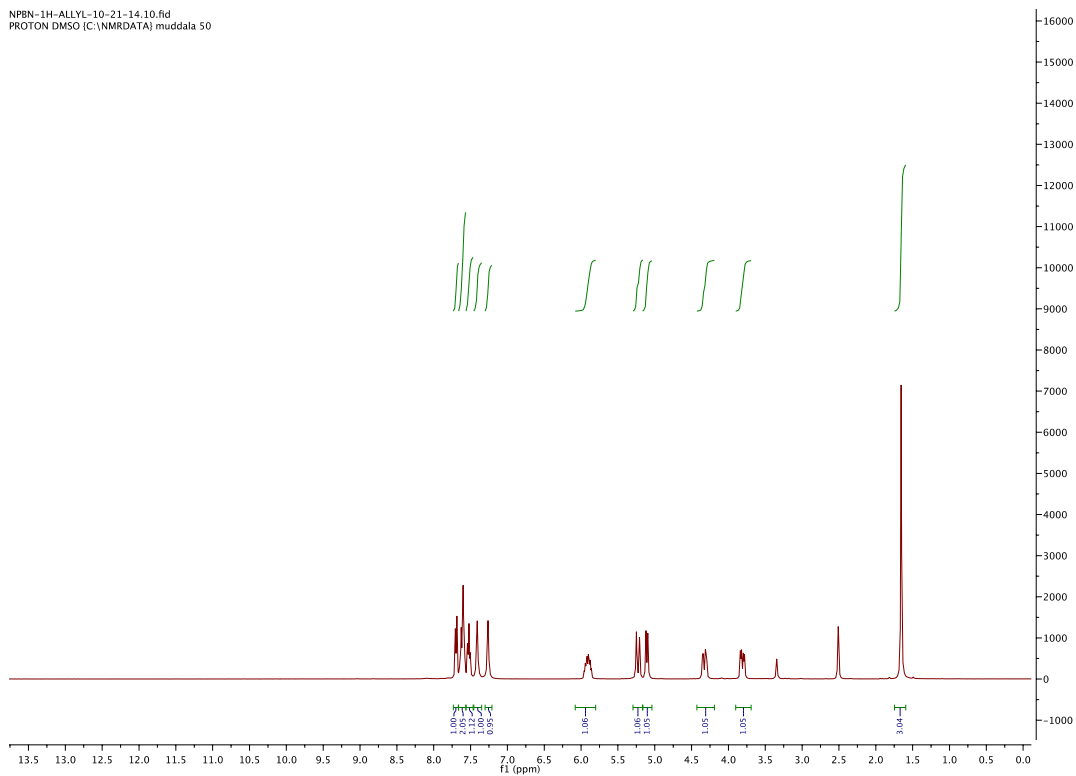


NPBN-13C-BNZYL-10-21-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 52

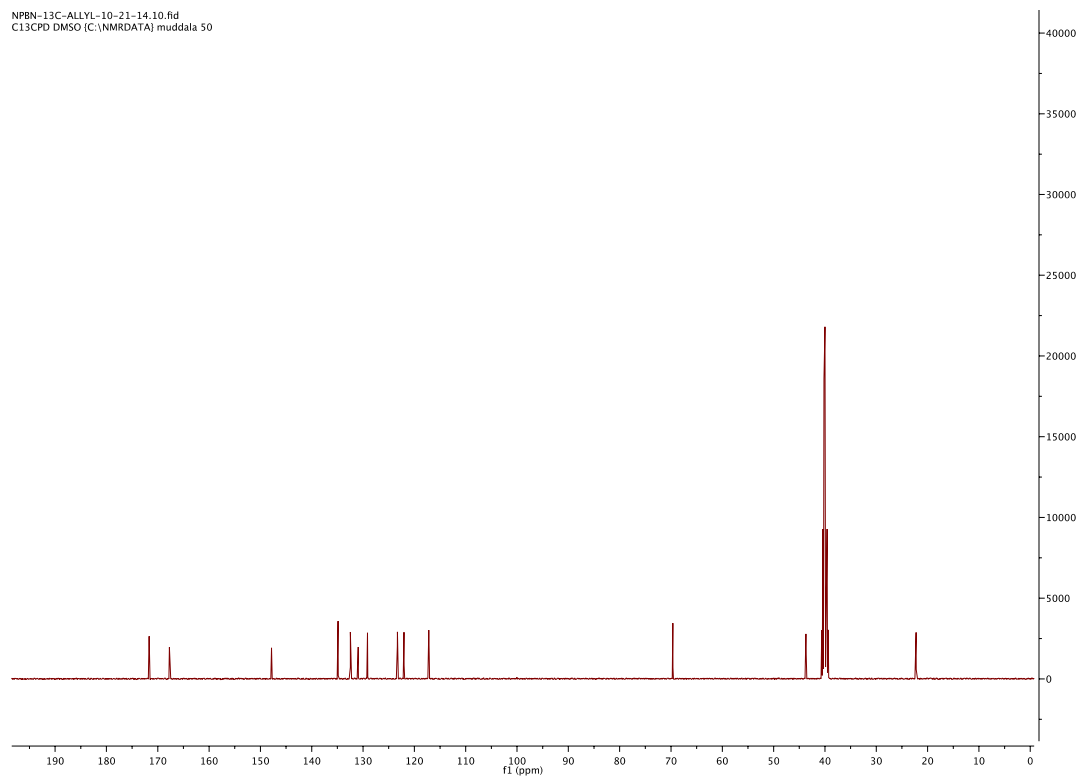


(±)-2-Allyl-1-methyl-3-oxoisindoline-1-carboxamide (9h)

NPN-1H-ALLYL-10-21-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 50

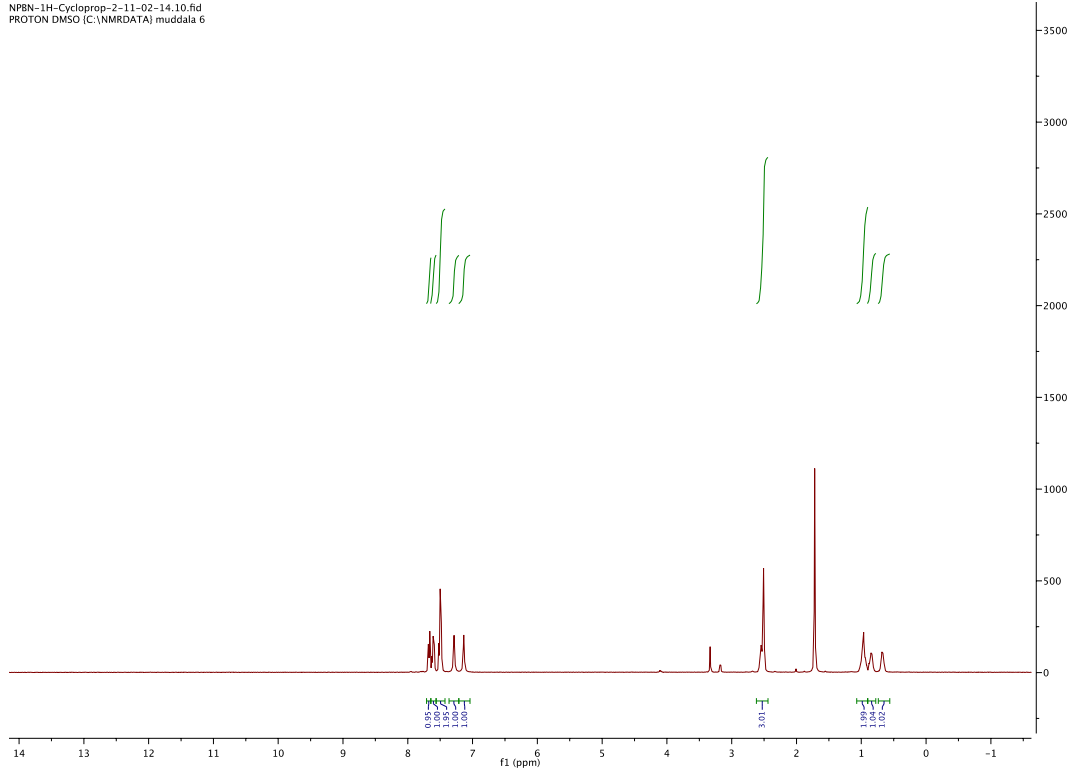


NPN-13C-ALLYL-10-21-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 50

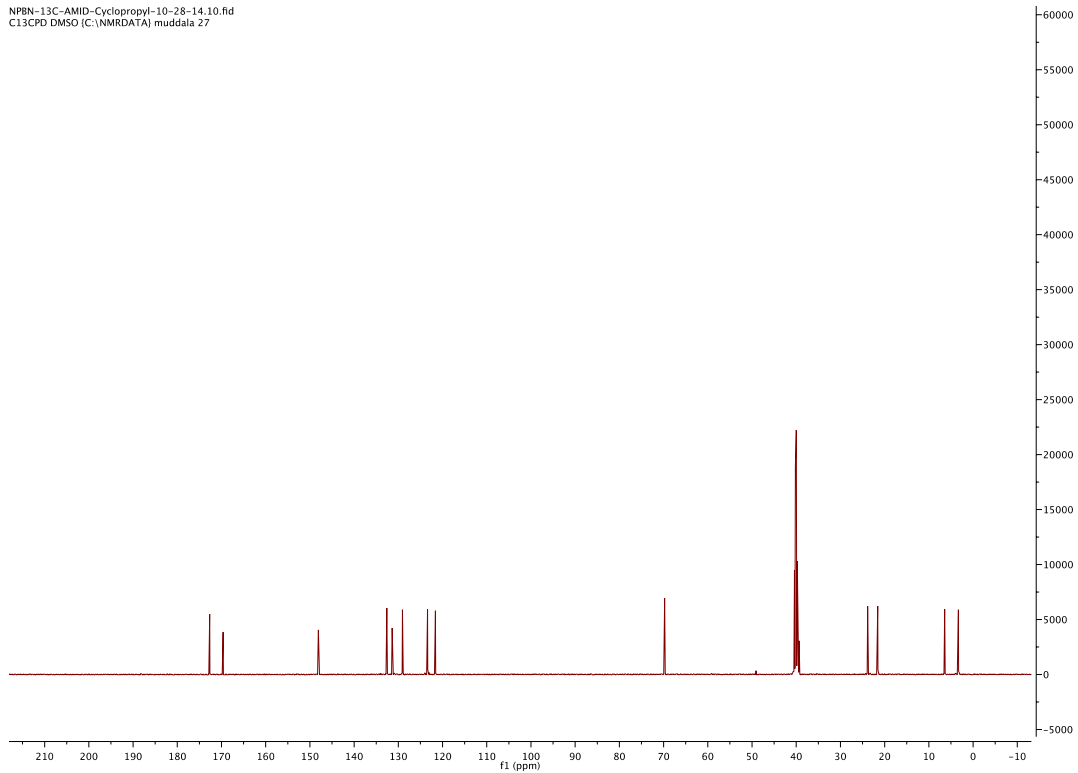


(±)-2-Cyclopropyl-1-methyl-3-oxoisindoline-1-carboxamide (9i)

NPN-1H-Cycloprop-2-11-02-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 6

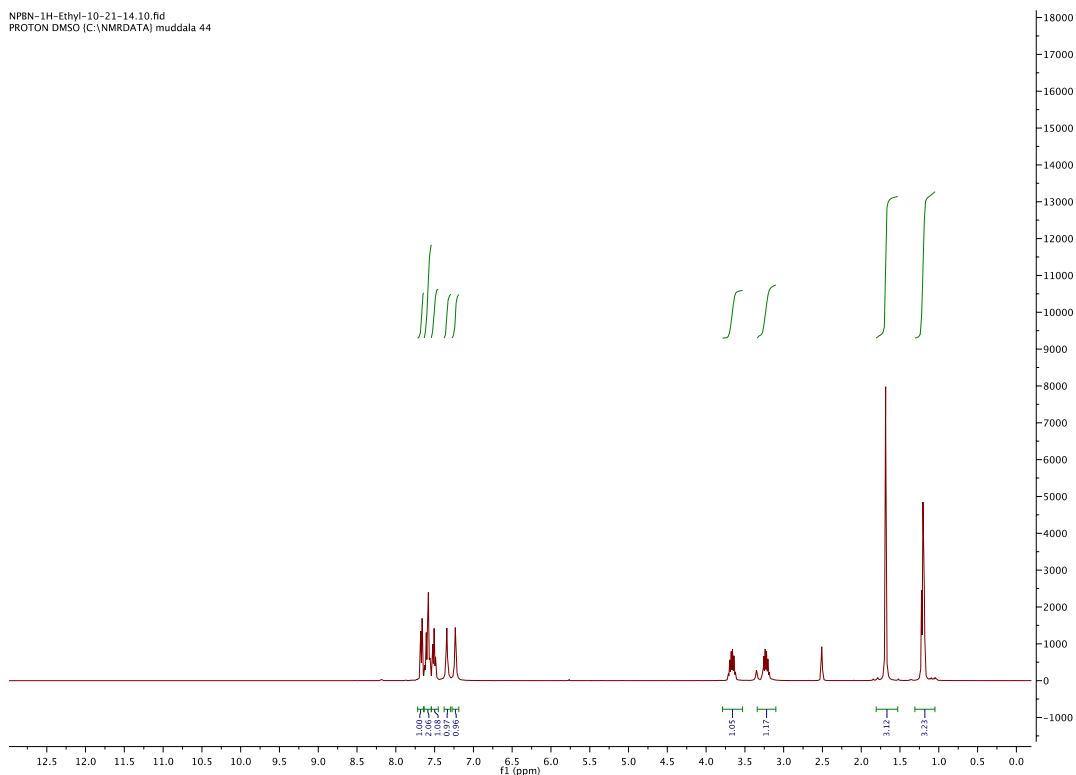


NPN-13C-AMID-Cyclopropyl-10-28-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 27

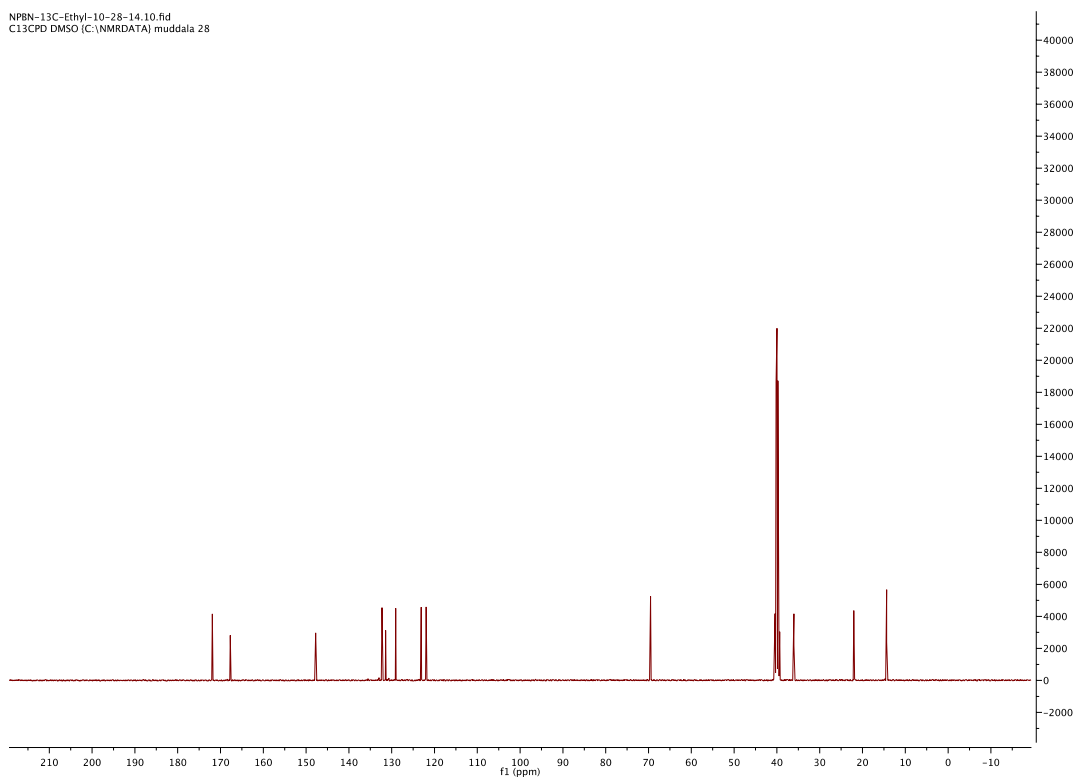


(±)-2-Ethyl-1-methyl-3-oxoisindoline-1-carboxamide (9j)

NPN-1H-Ethyl-10-21-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 44

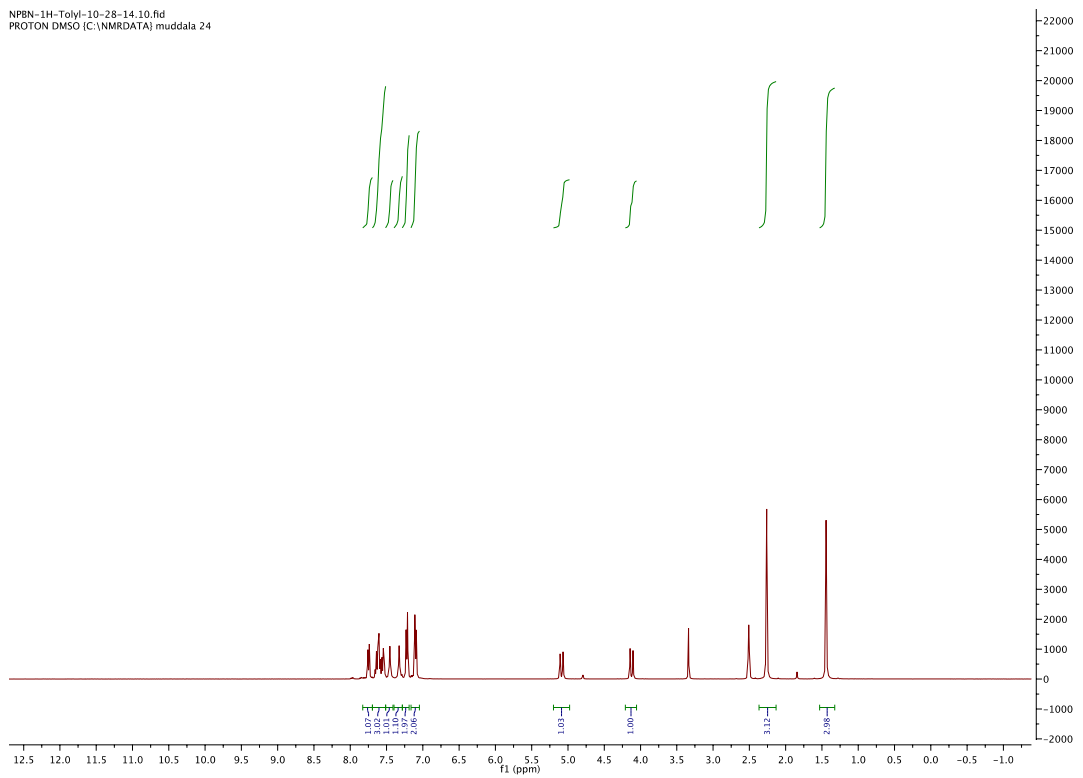


NPN-13C-Ethyl-10-28-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 28

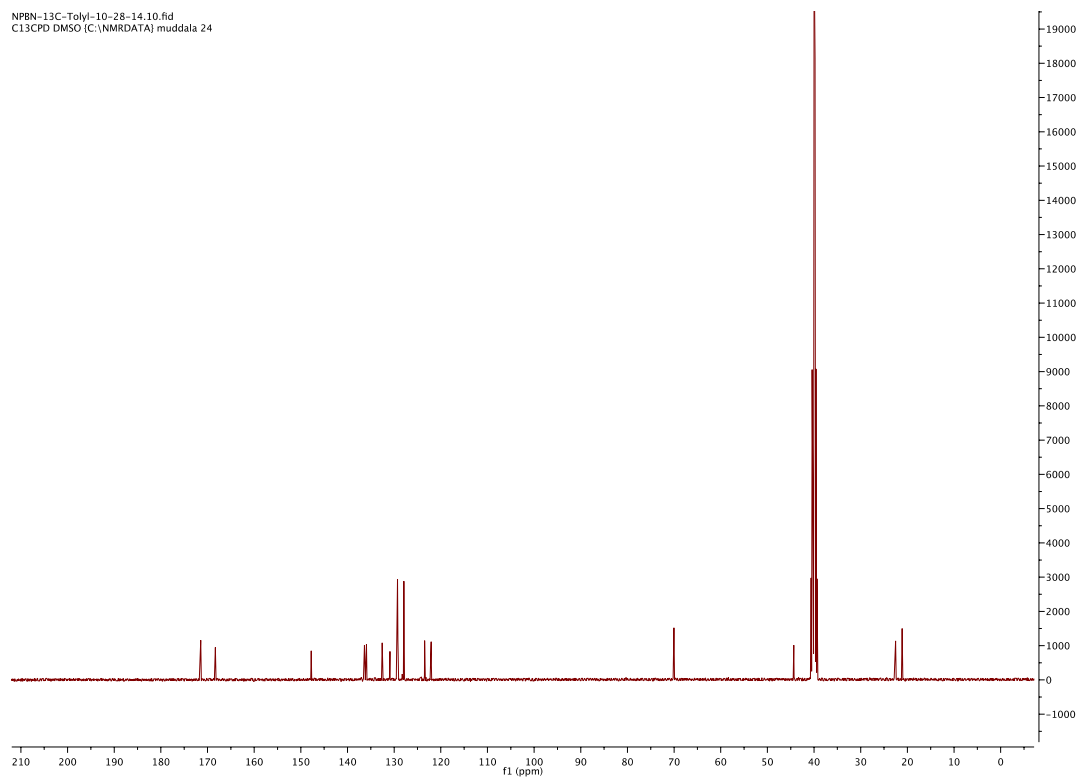


(±)-1-Methyl-2-(4-methylbenzyl)-3-oxoisindoline-1-carboxamide (9k)

NPB-1H-Tolyl-10-28-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 24

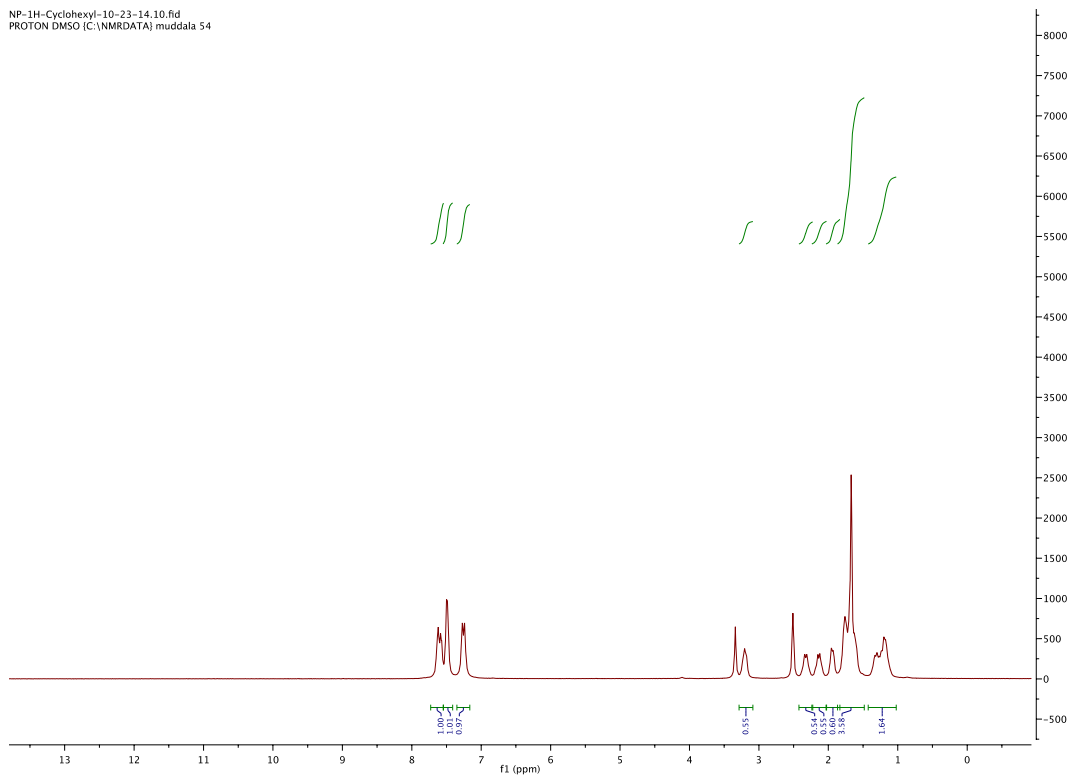


NPB-13C-Tolyl-10-28-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 24

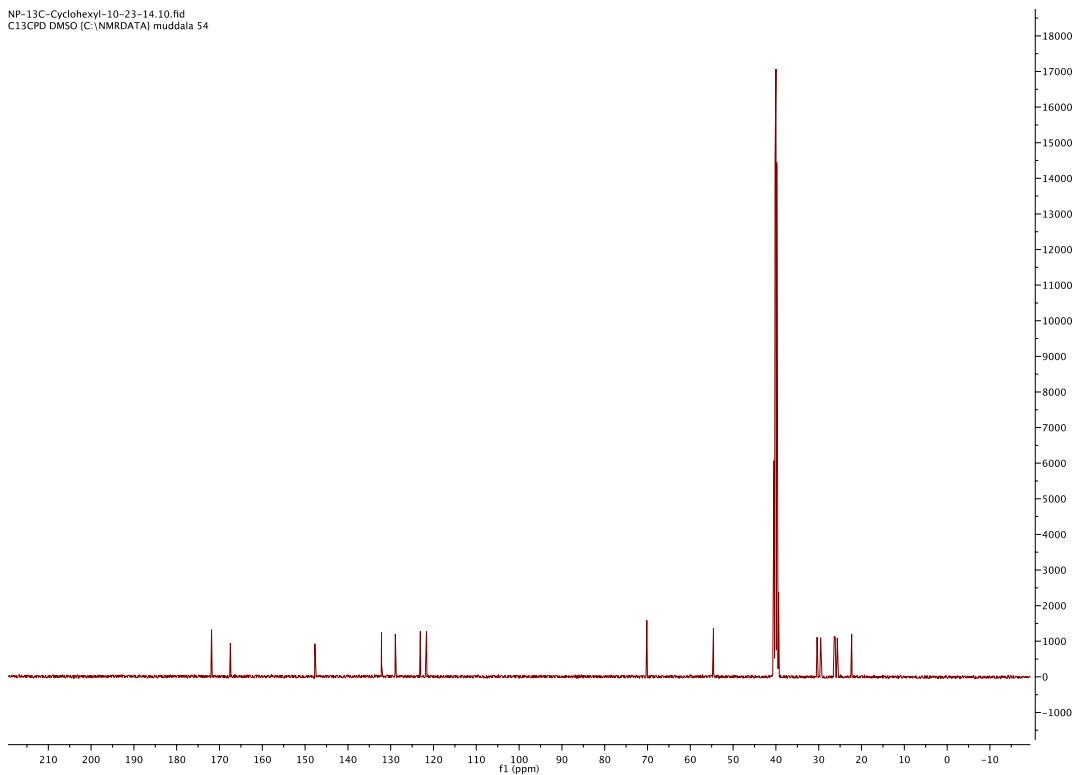


(±)-2-Cyclohexyl-1-methyl-3-oxoisindoline-1-carboxamide (9I)

NP-1H-Cyclohexyl-10-23-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 54

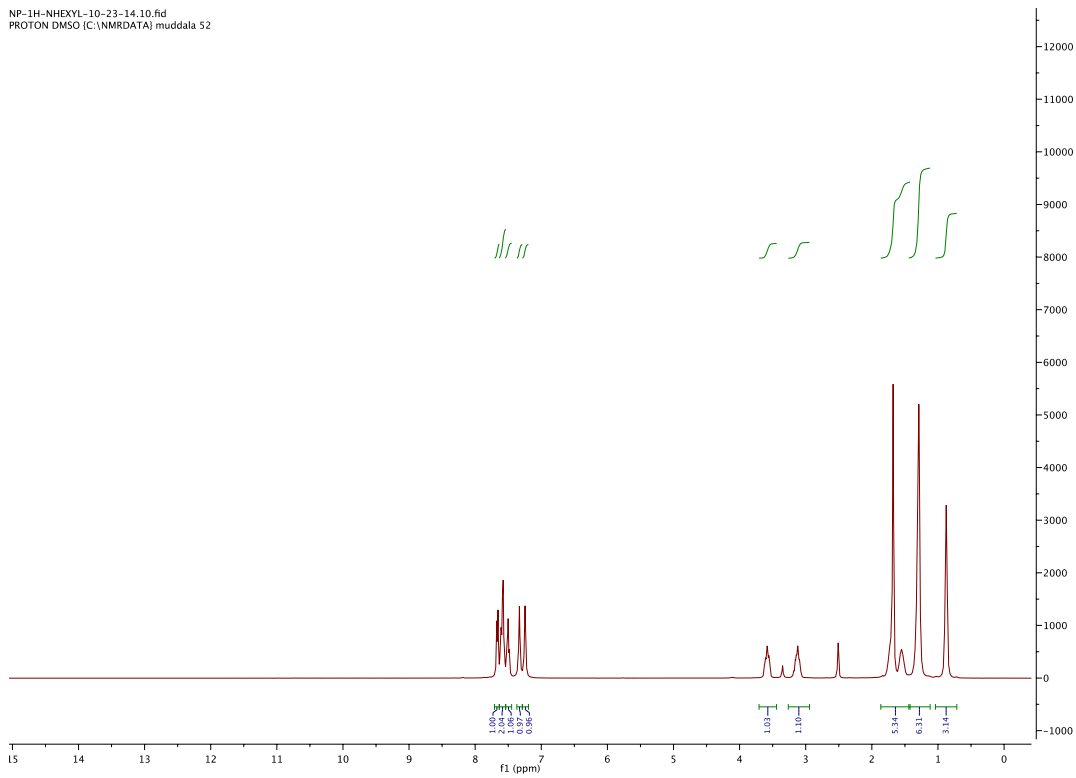


NP-13C-Cyclohexyl-10-23-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 54

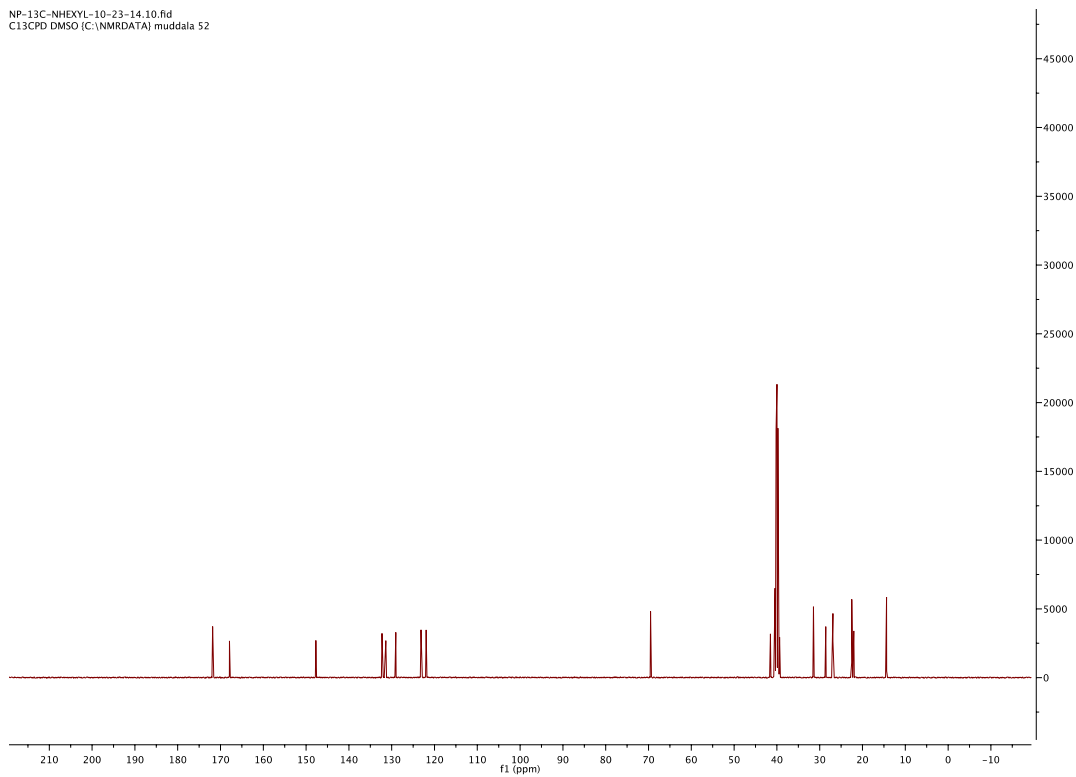


(±)-2-Hexyl-1-methyl-3-oxoisindoline-1-carboxamide (9m)

NP-1H-NHEXYL-10-23-14.10.fid
PROTON DMSO [C:\NMRDATA] muddala 52

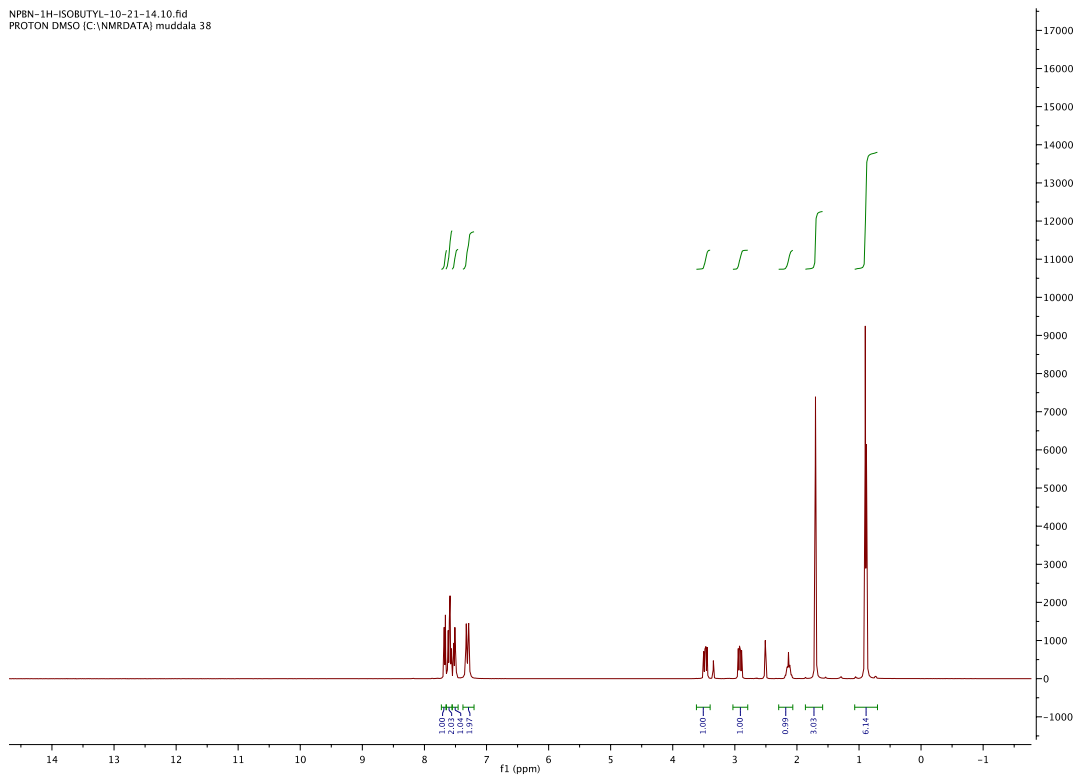


NP-13C-NHEXYL-10-23-14.10.fid
C13CPD DMSO [C:\NMRDATA] muddala 52



(±)-2-Isobutyl-1-methyl-3-oxoisindoline-1-carboxamide (9n)

NPN-1H-ISOBUTYL-10-21-14.10.fid
PROTON DMSO (C:\NMRDATA) muddala 38



NPN-13C-ISOBUTYL-10-21-14.10.fid
C13CPD DMSO (C:\NMRDATA) muddala 38

