

Supporting Information

Nitrones and Nucleobase-Containing Spiro-Isoxazolidines Derived from Isatin and indanone: Solvent-Free Microwave-Assisted Stereoselective Synthesis and Theoretical Calculations

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^b *Institute of Biocomputation and Physics of Complex Systems (BIFI), Universidad de Zaragoza-CSIC, Zaragoza, Spain*

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^d *Dipartimento di Farmacia e Scienze della Salute e della Nutrizione, Università della Calabria, Rende (CS), Italy*

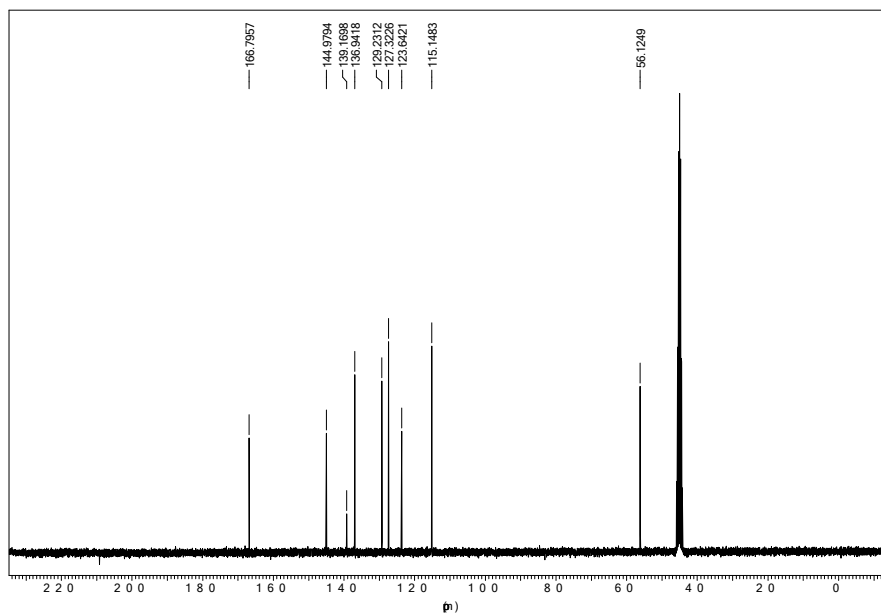
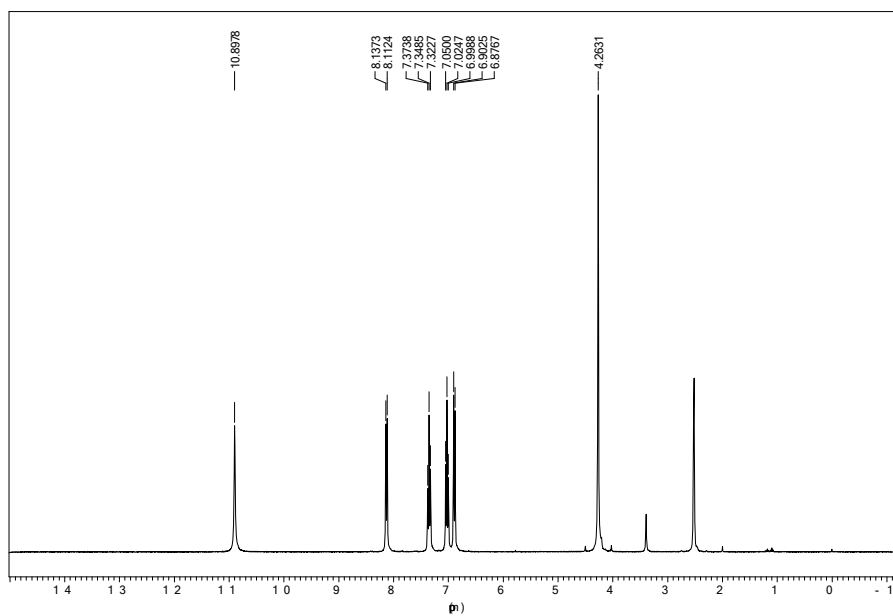
^e *Servicio de Resonancia Magnética Nuclear, CEQMA, Universidad de Zaragoza-CSIC, Zaragoza, Spain*

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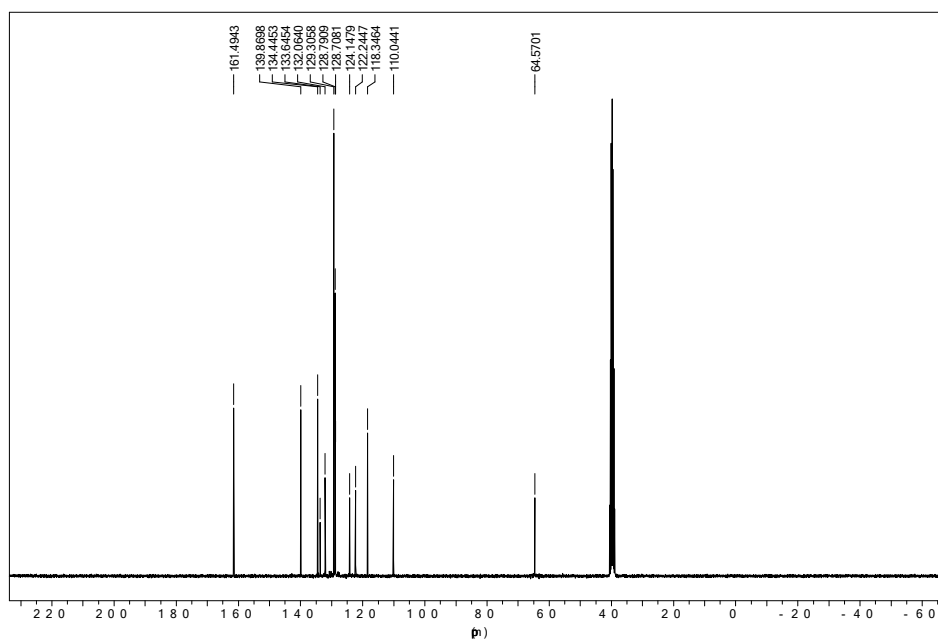
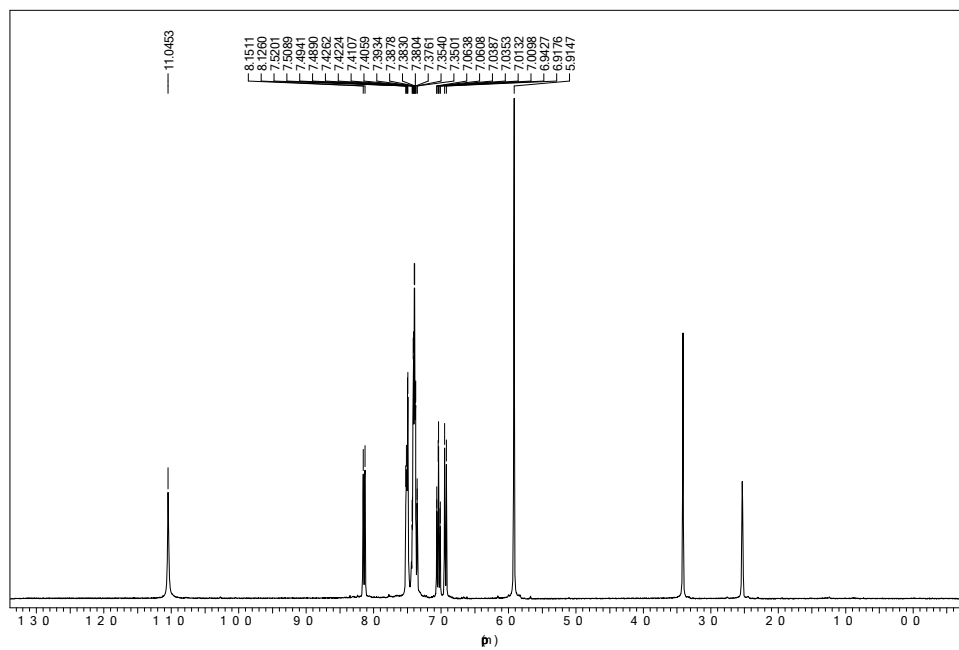
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^1H and ^{13}C NMR spectra of *4a-o* and *5a-i*

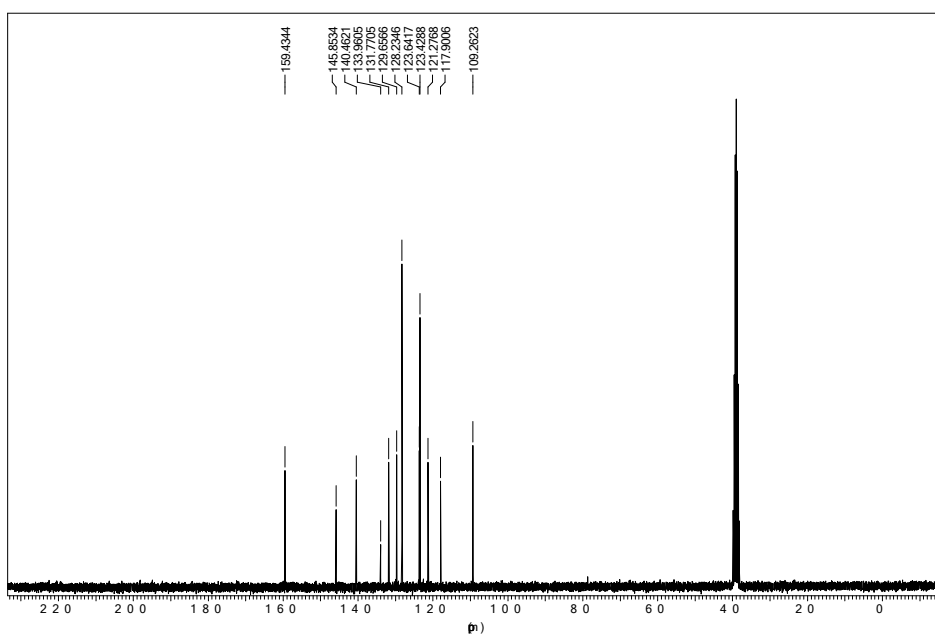
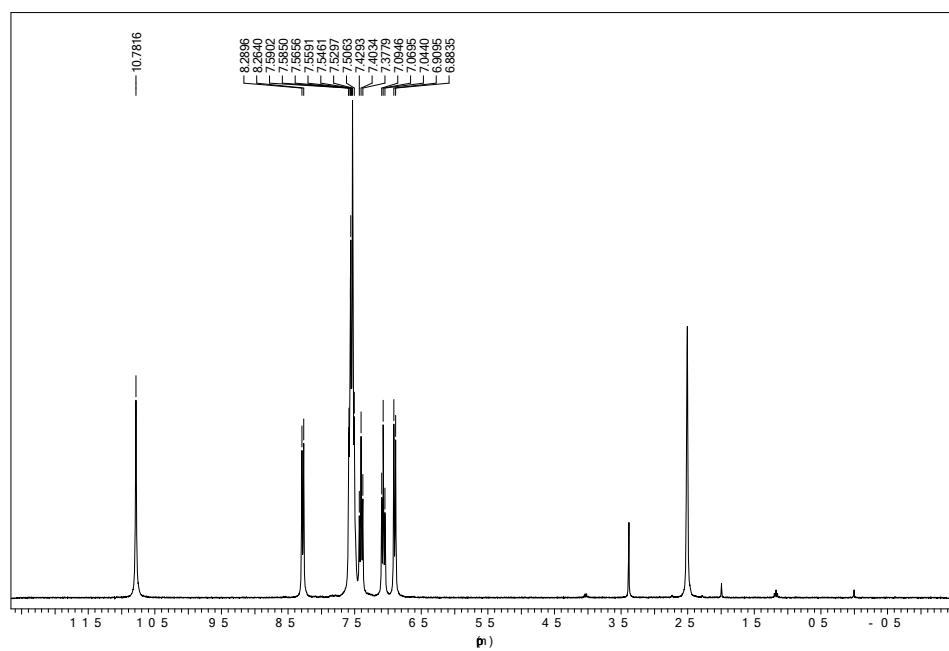
(*E*) *N*-methyl-*C*-isatinylnitrone (**4a**)



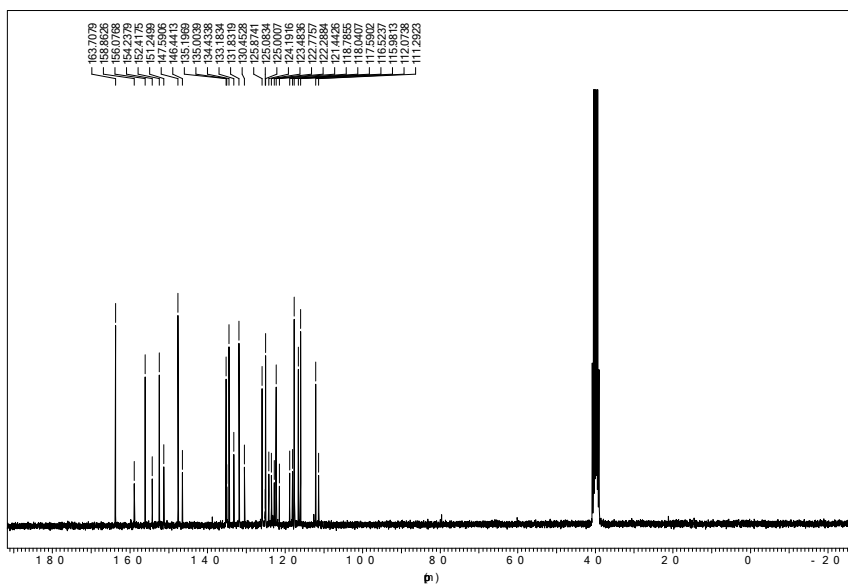
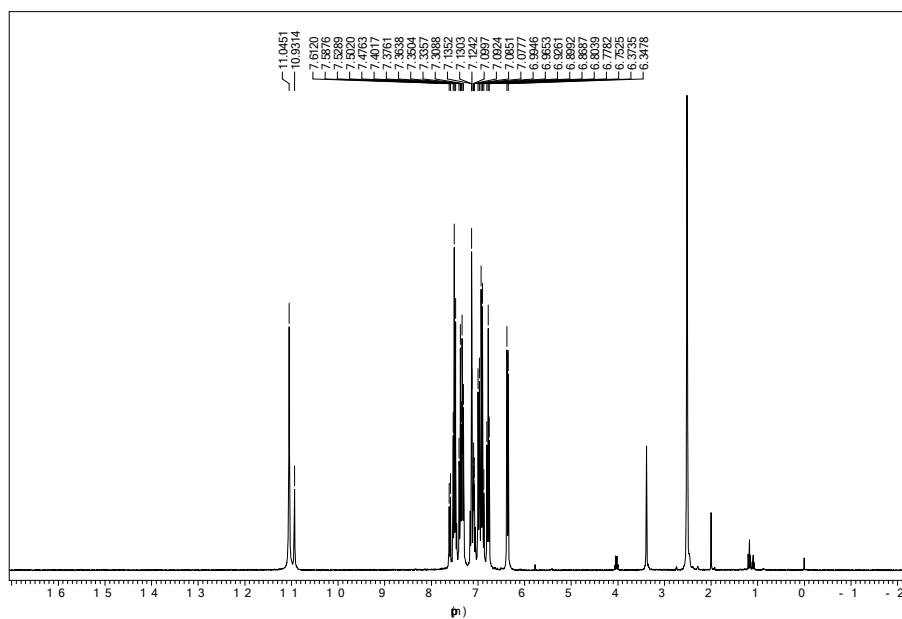
(E) N-benzyl-C-isatinyl nitron (**4b**)



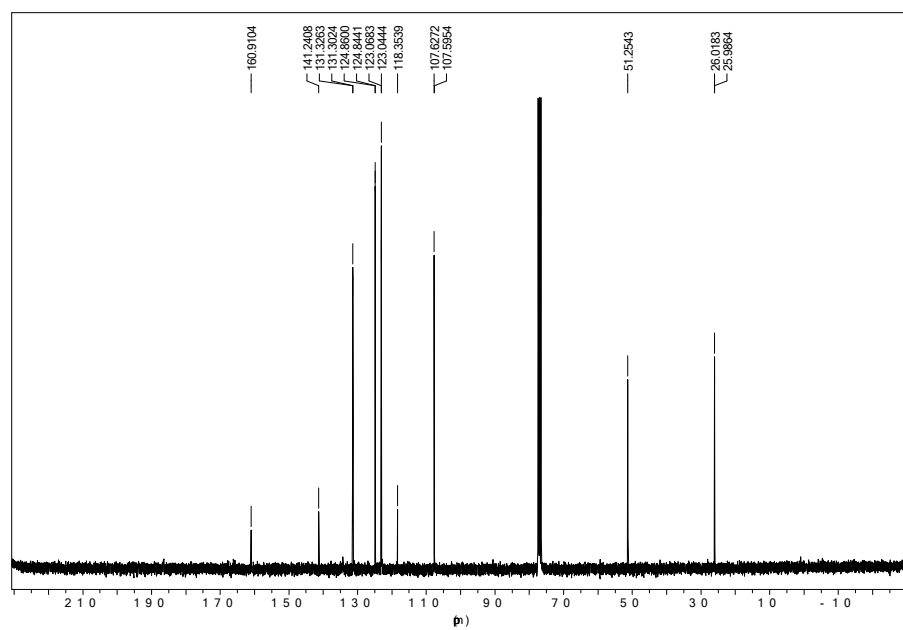
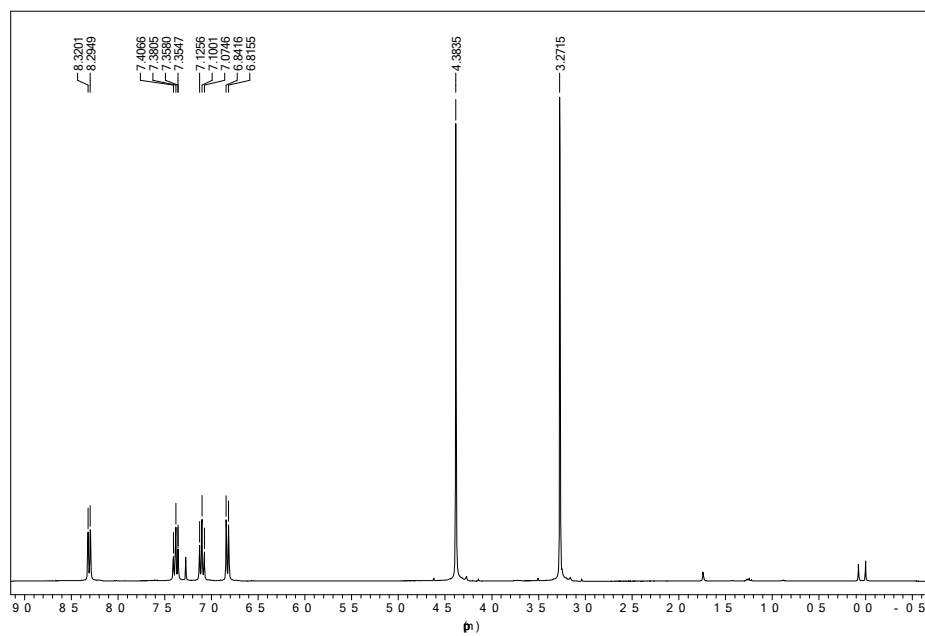
(E) N-phenyl-C-isatinyl nitron (4c)



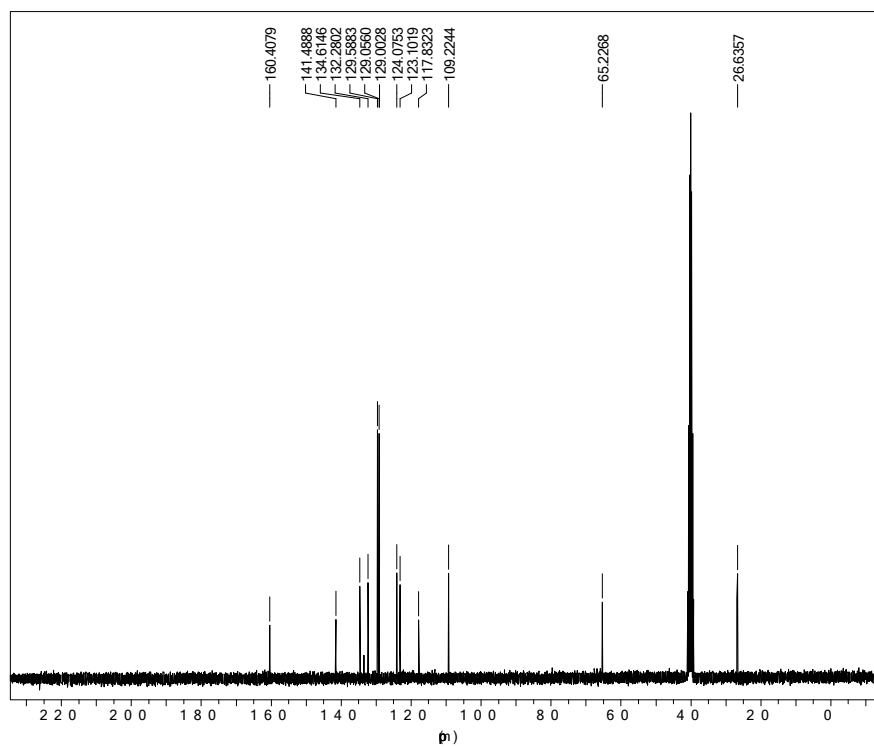
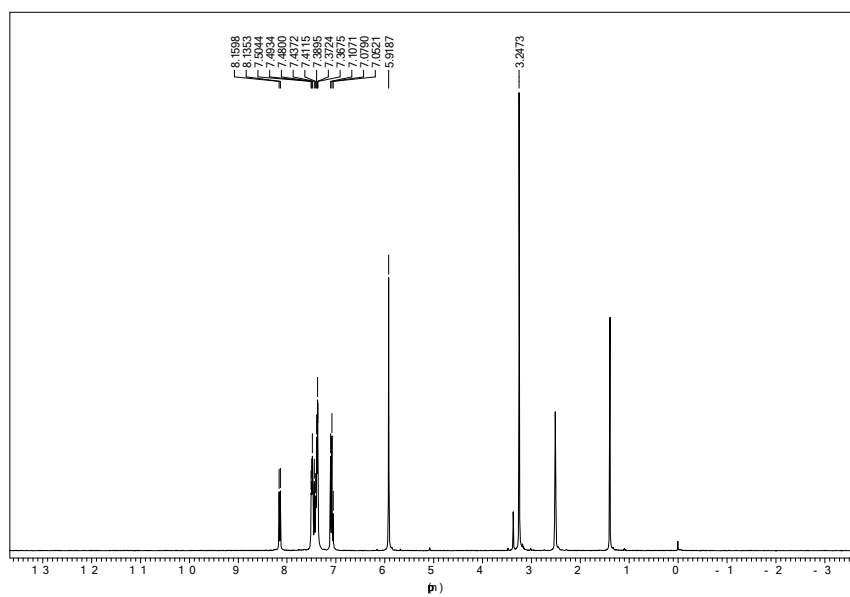
***N*-3-Cl-phenyl-*C*-isatinyl nitrone (4d) (E/Z mixture)**



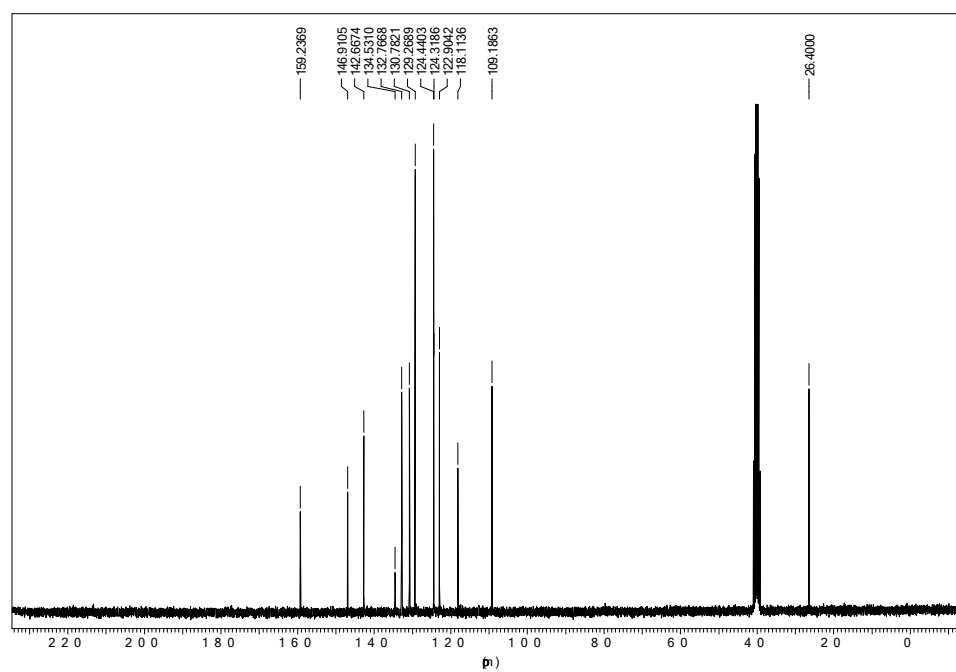
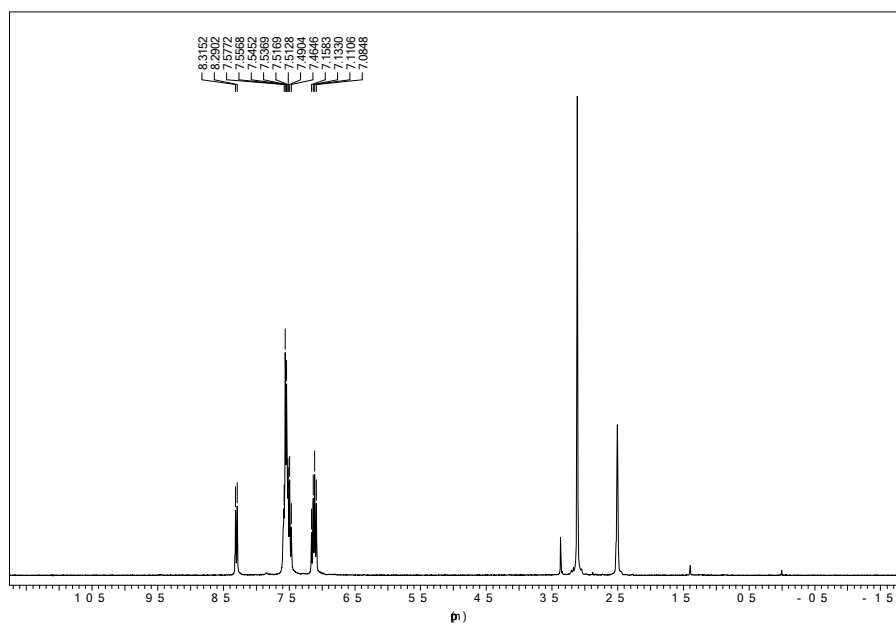
(E) N-methyl-C- (I-methyl)-isatinyI nitronc (4e)



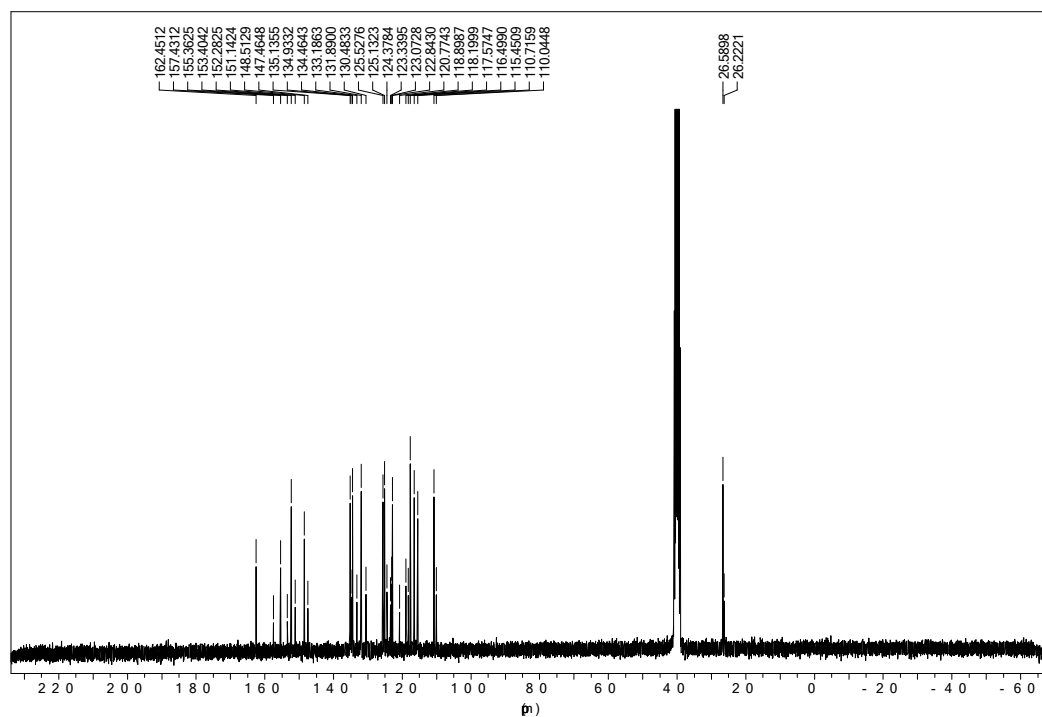
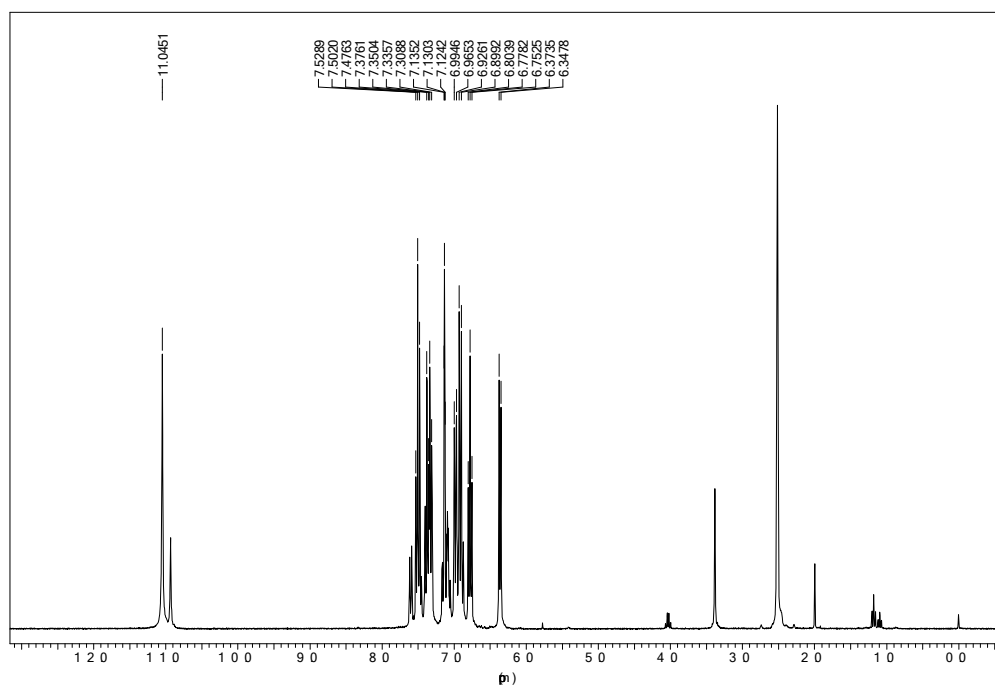
(*E*) N-benzyl-C- (1-methyl)-isatinyl nitron (4f)



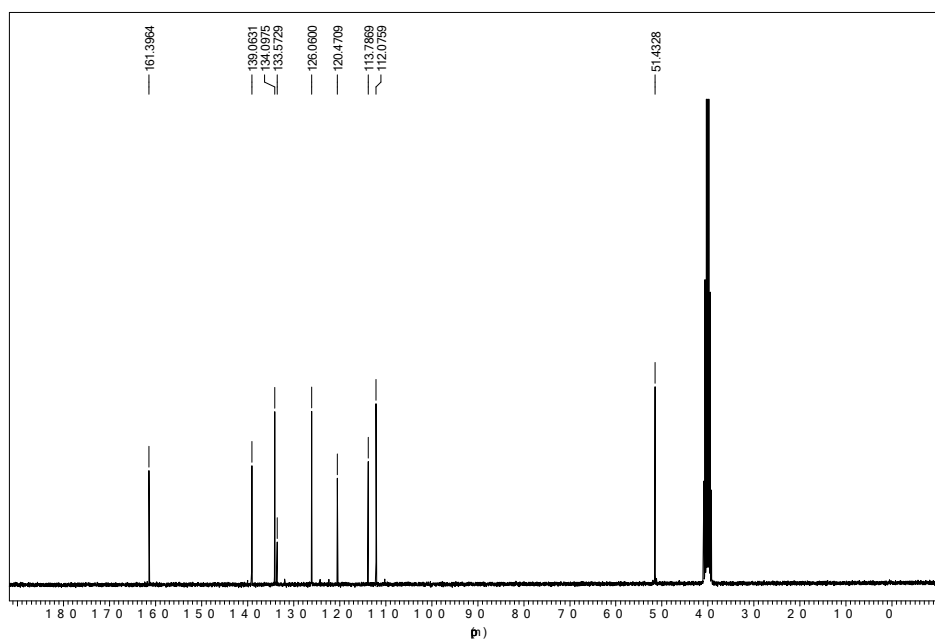
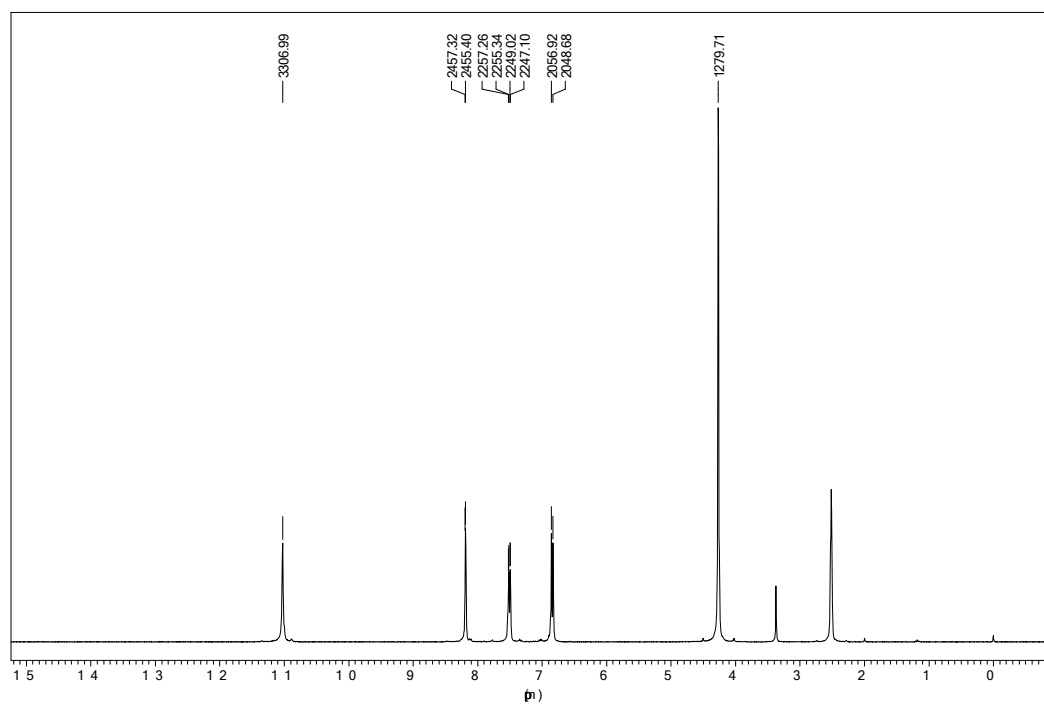
(E) N-phenyl-C- (1-methyl)-isatinyI nitronc (4g)



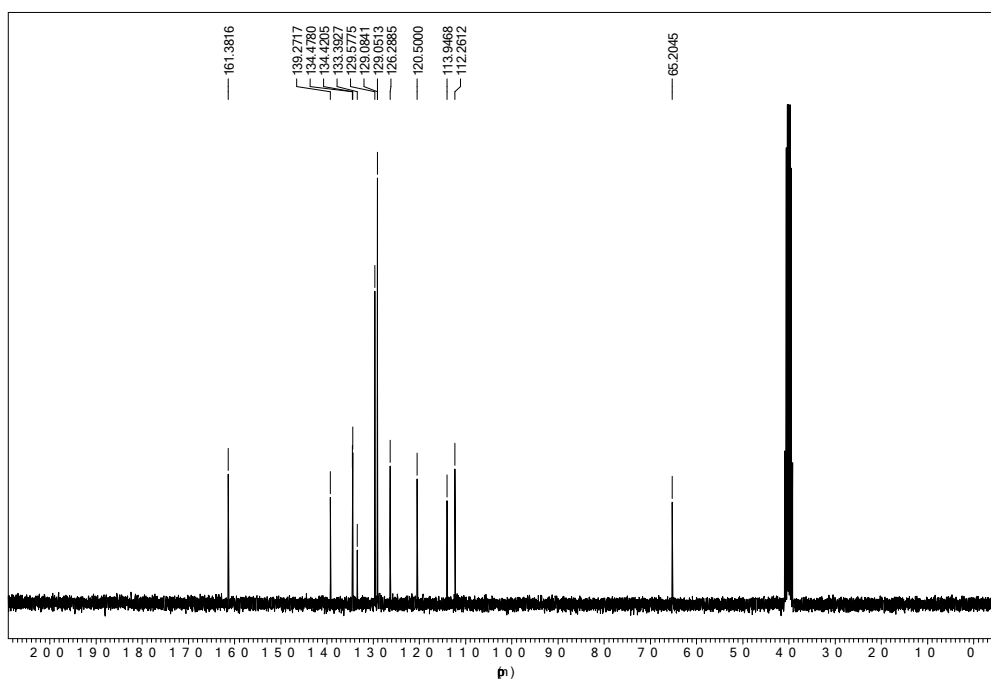
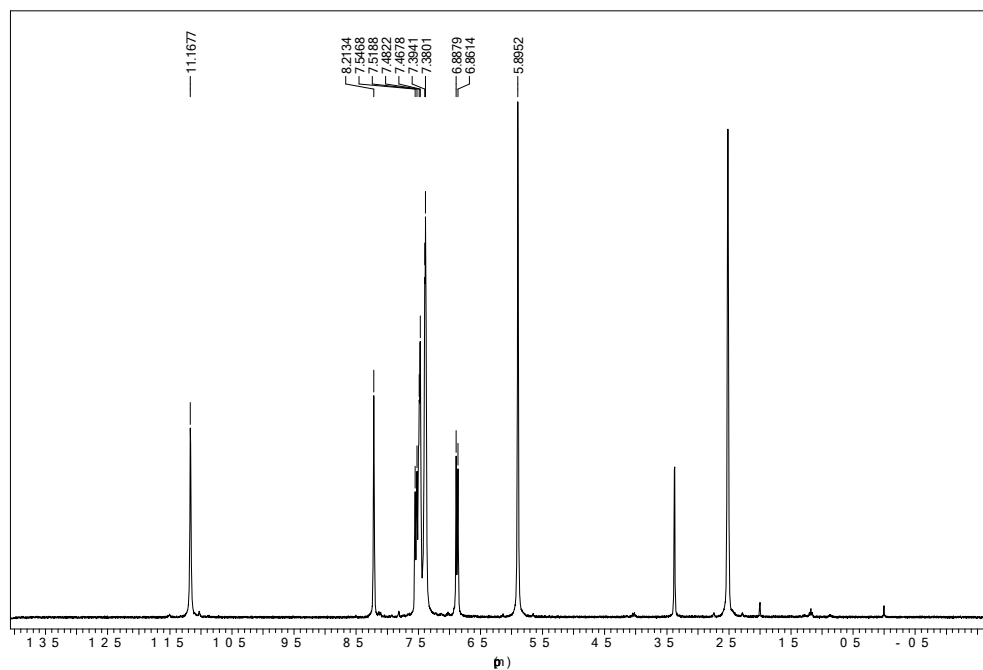
***N*-3-Cl-phenyl -*C*-(*I*-methyl)-isatinylnitrone (4h) (E/Z mixture)**



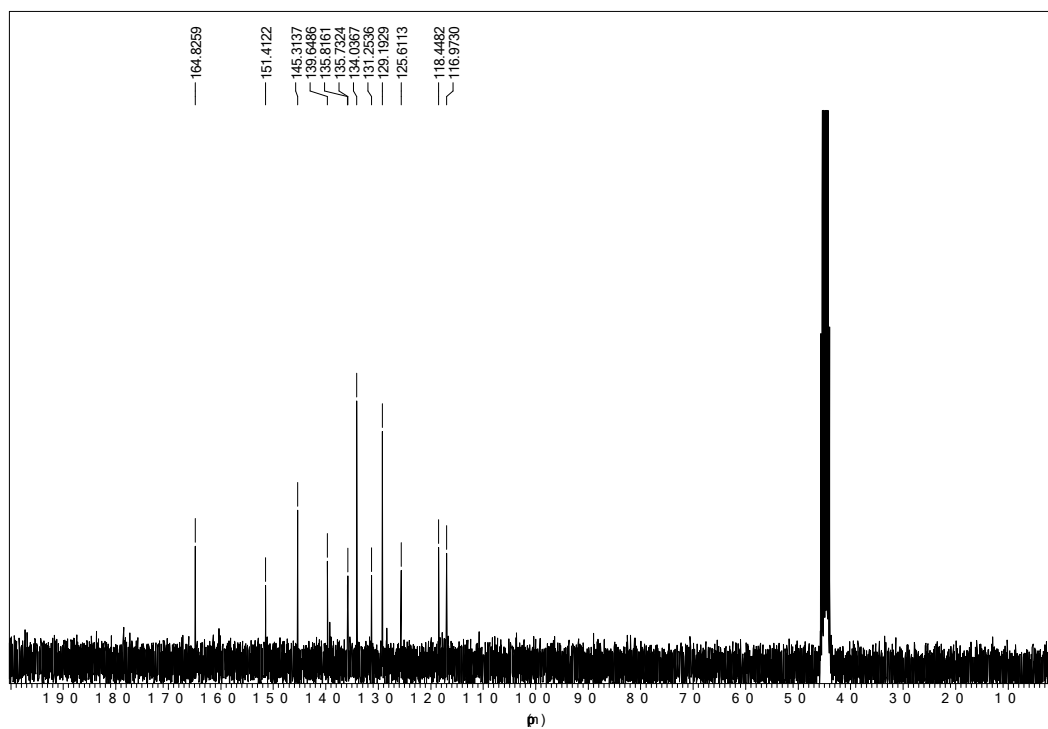
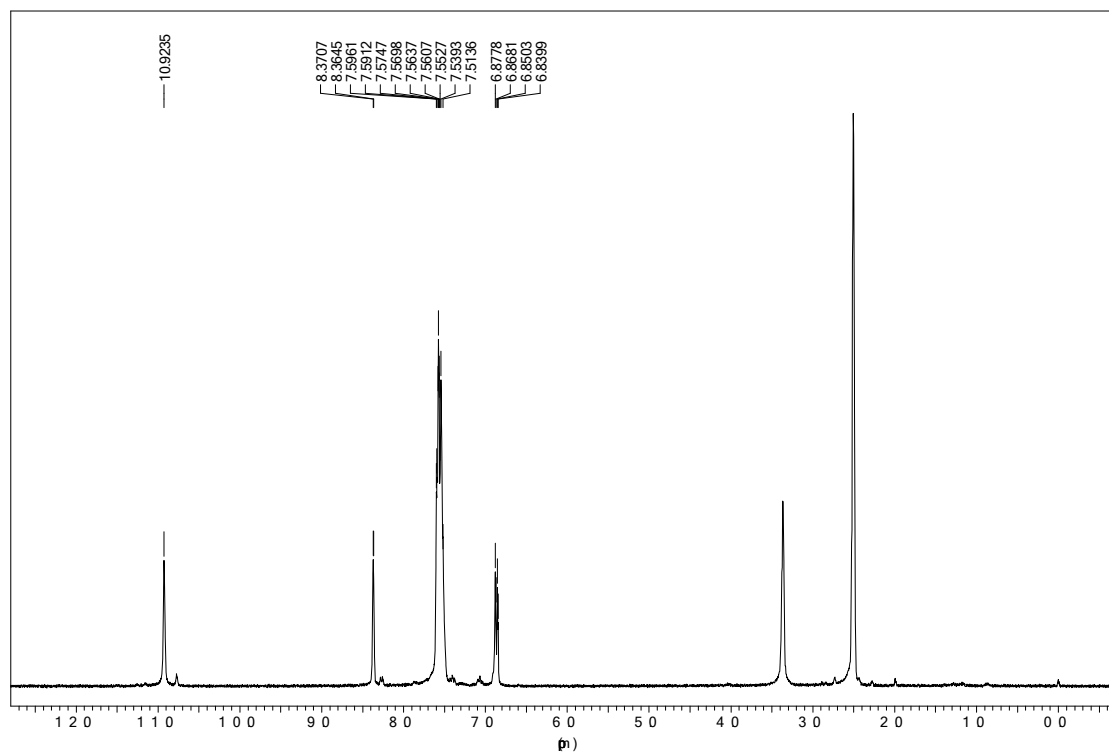
(E) N-methyl-C-(5-Br)-isatinyl nitrone (4i)



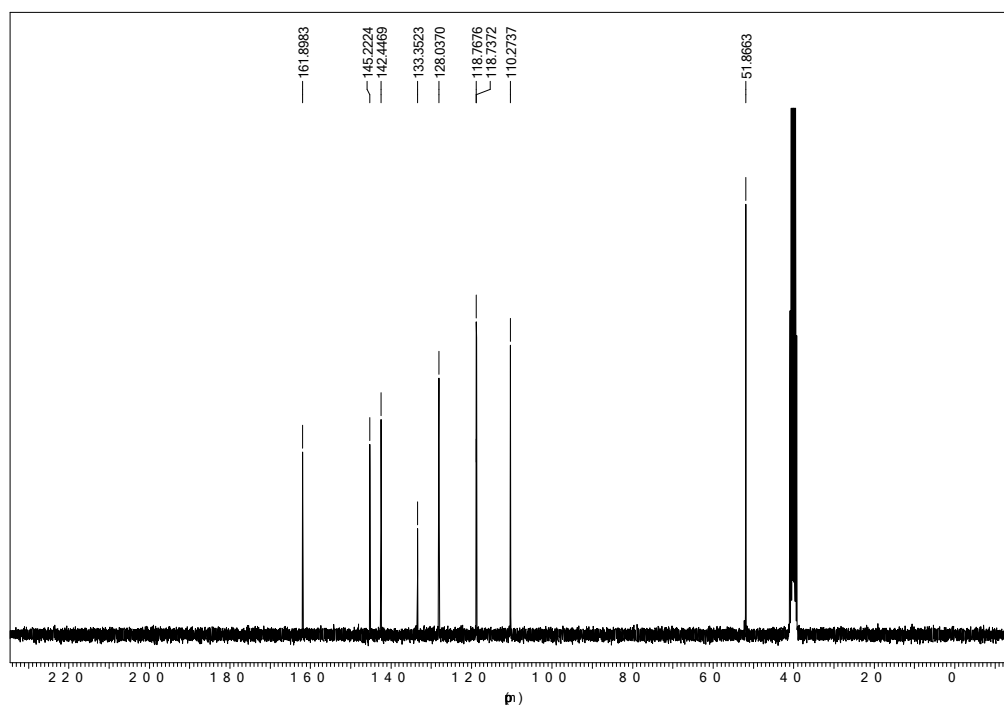
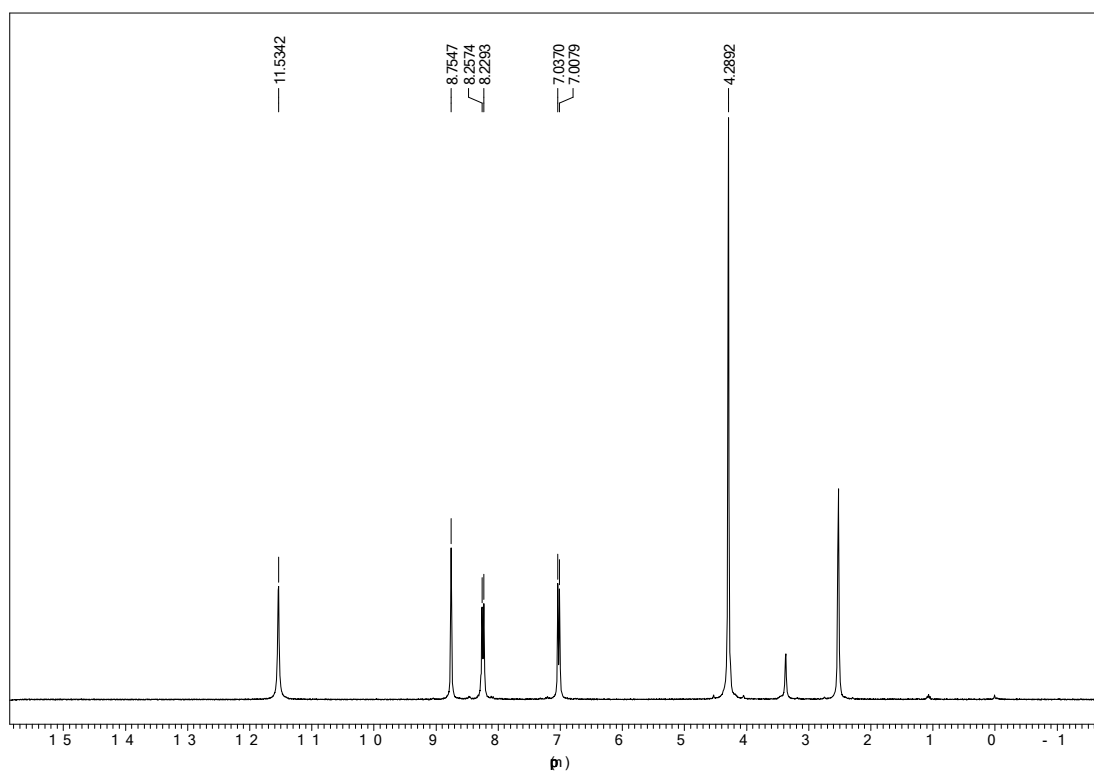
(E) N-benzyl-C-(5-Br)-isatinyl nitron (4j)



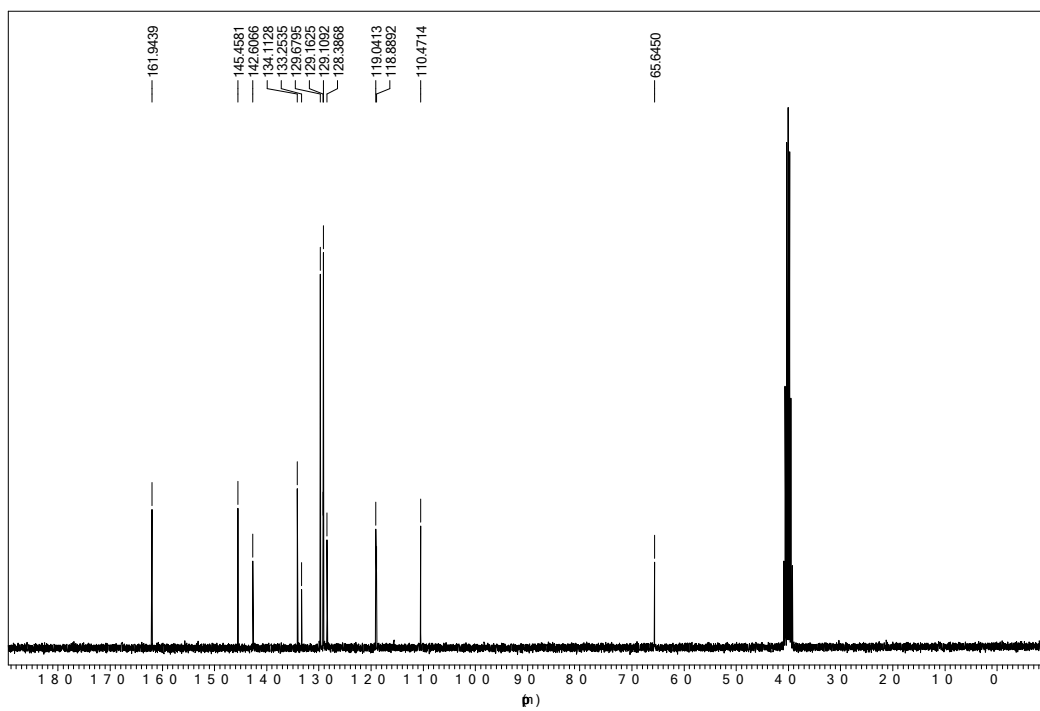
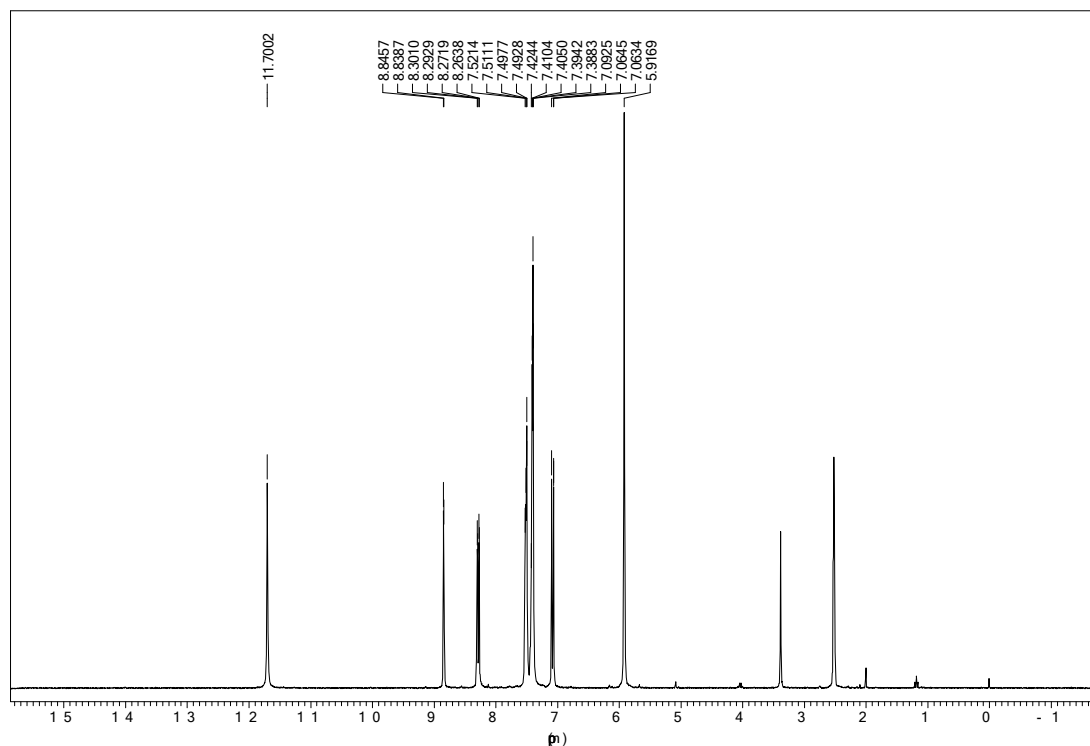
(E) N-phenyl-C-(5-Br)-isatinyl nitron (4k)



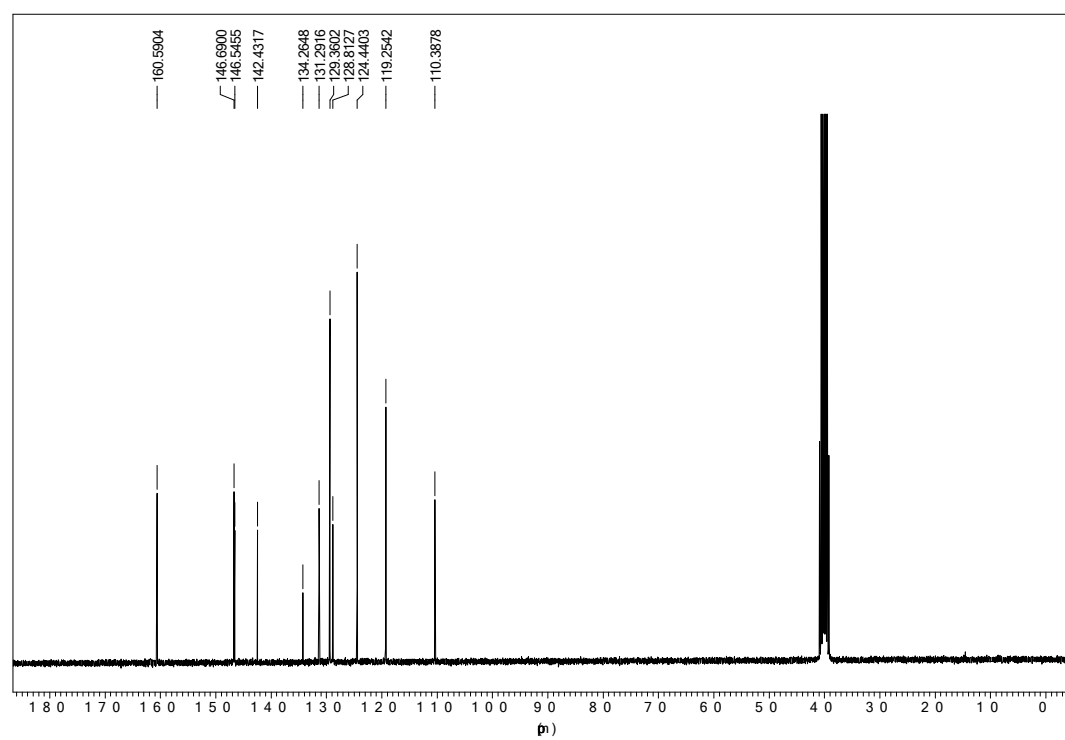
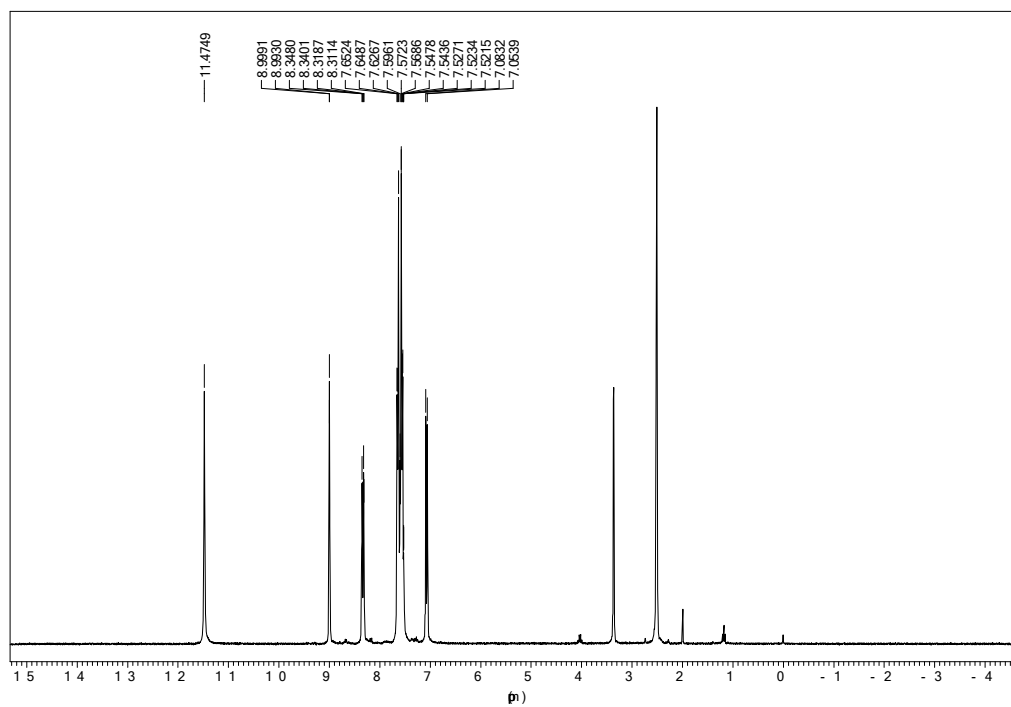
(E) N-methyl-C-(5-NO₂)-isatinyl nitrone (4l)



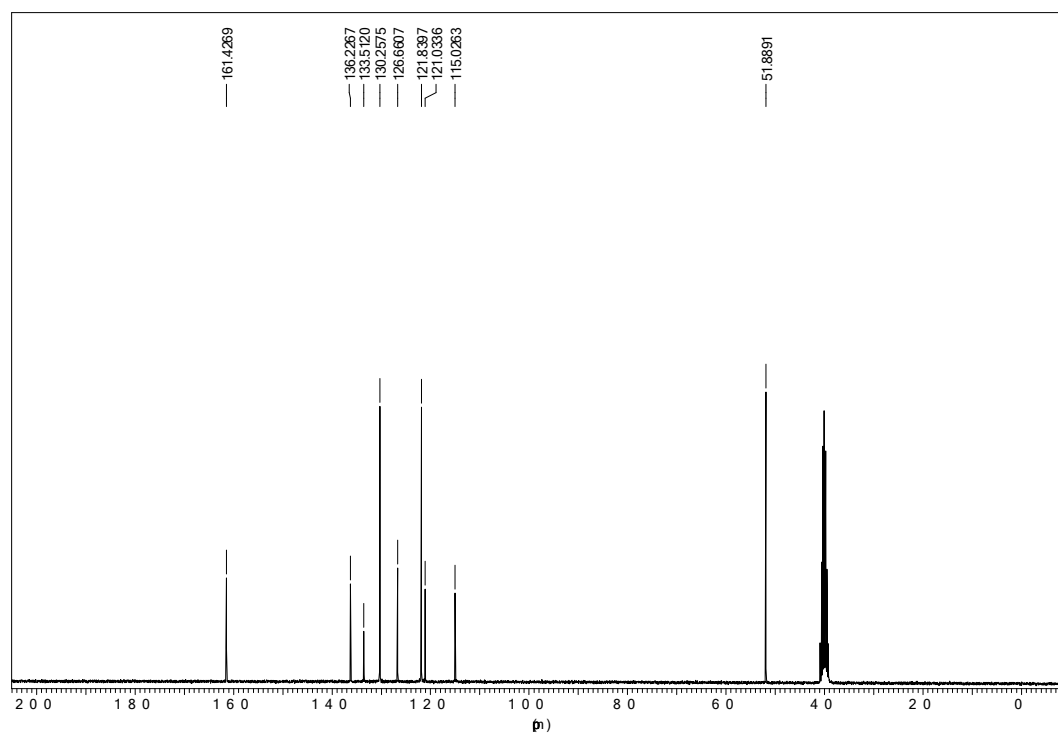
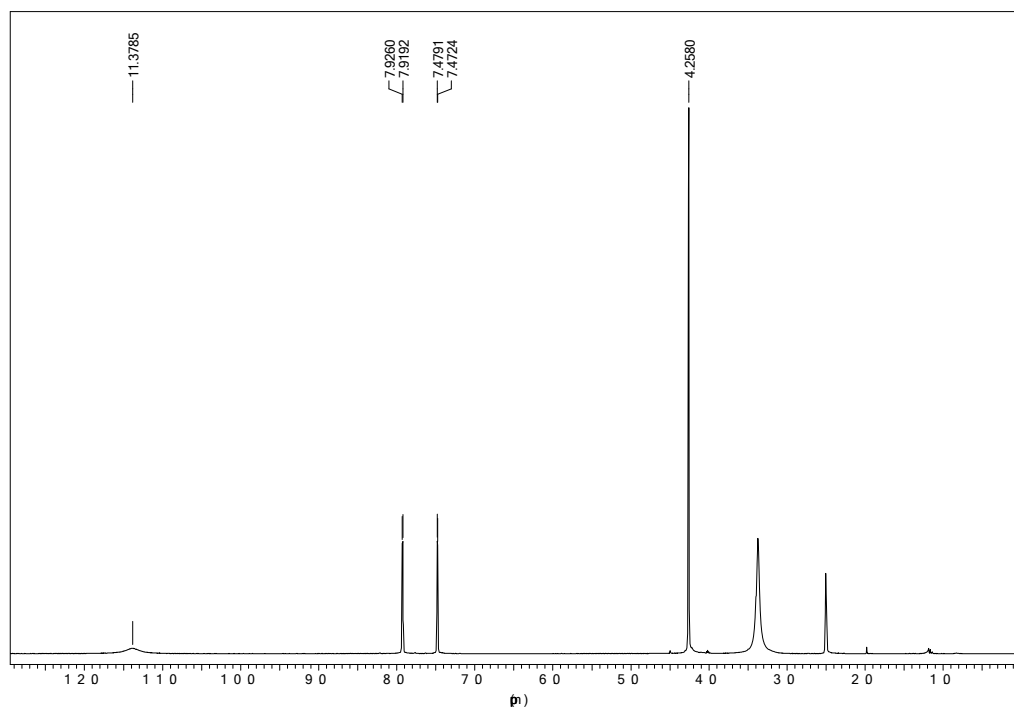
(E) N-benzyl-C-(5-NO₂)-isatinyl nitron (4m)



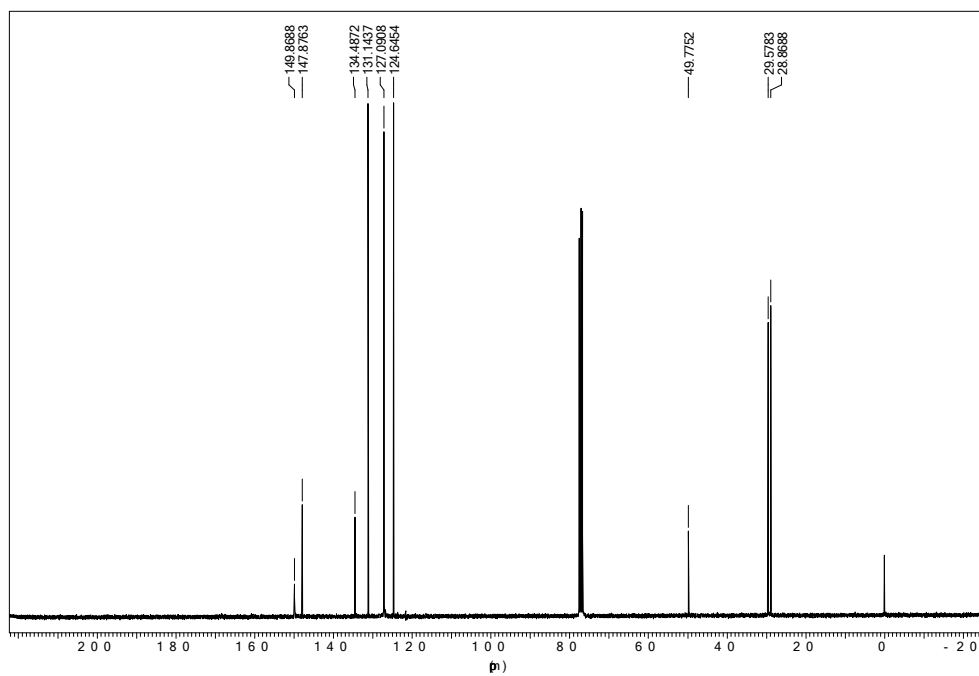
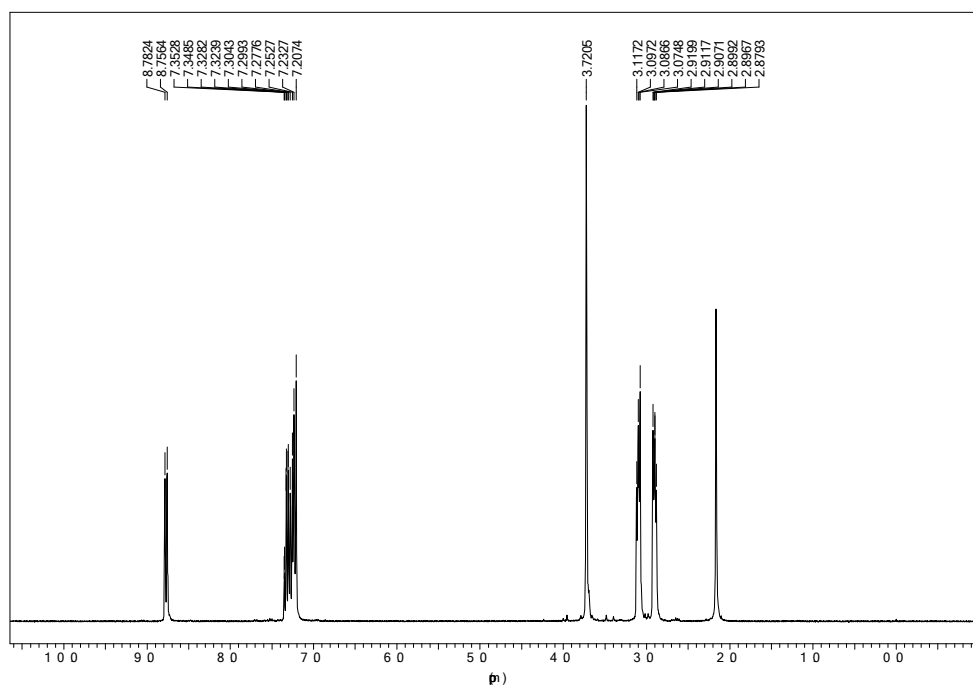
(E) N-phenyl-C-(5-NO₂)-isatinyl nitrone (4n)



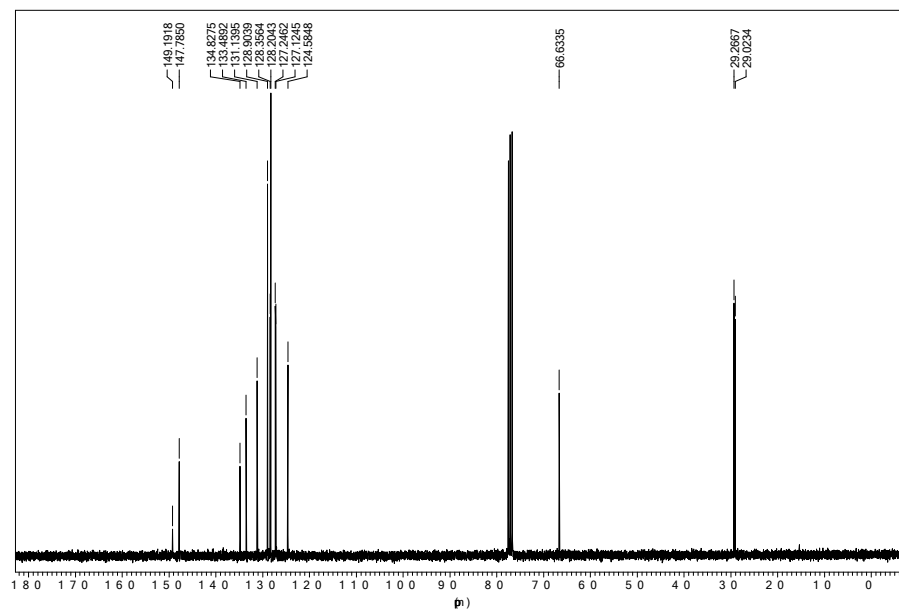
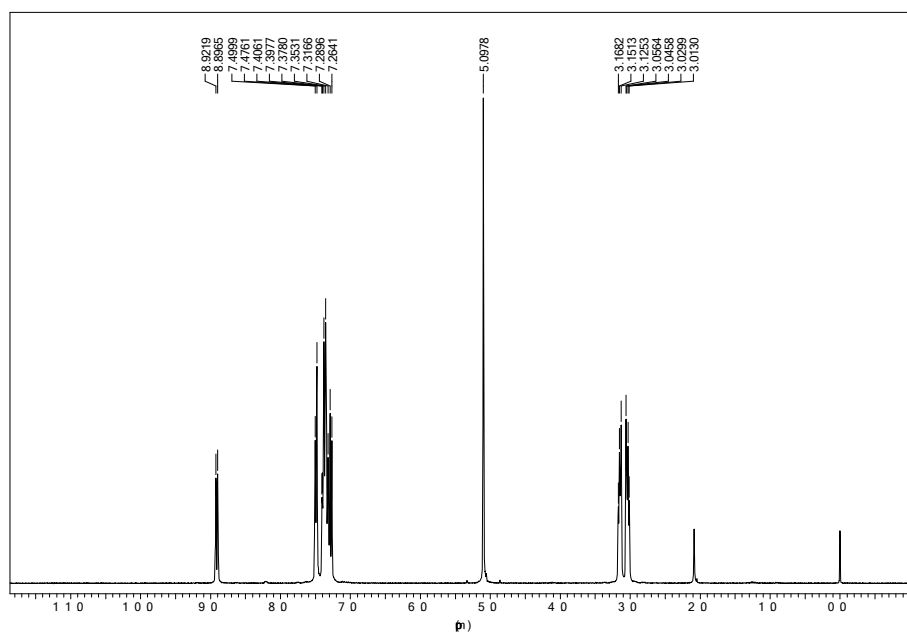
***(E)* N-Methyl-C-(5,7-Cl)-isatinyl nitron 4o**



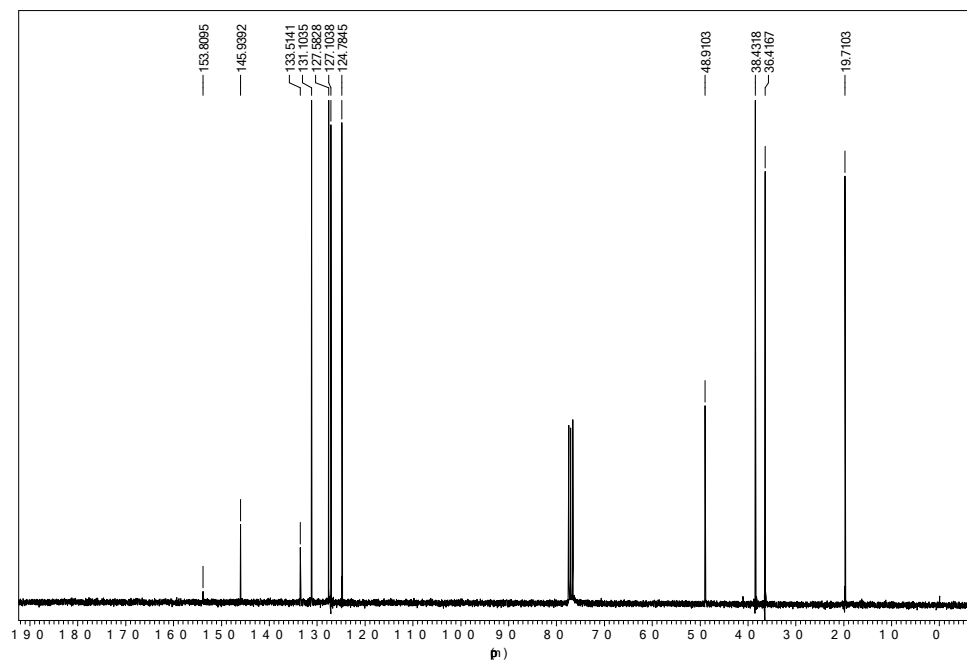
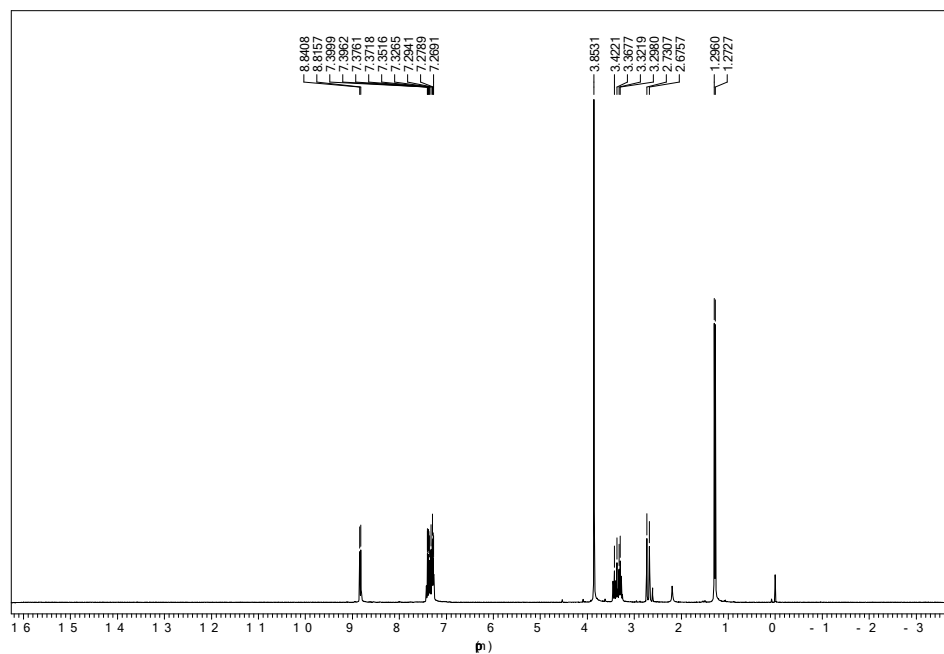
(Z) N-methyl-C-indanoyl nitron (5a)



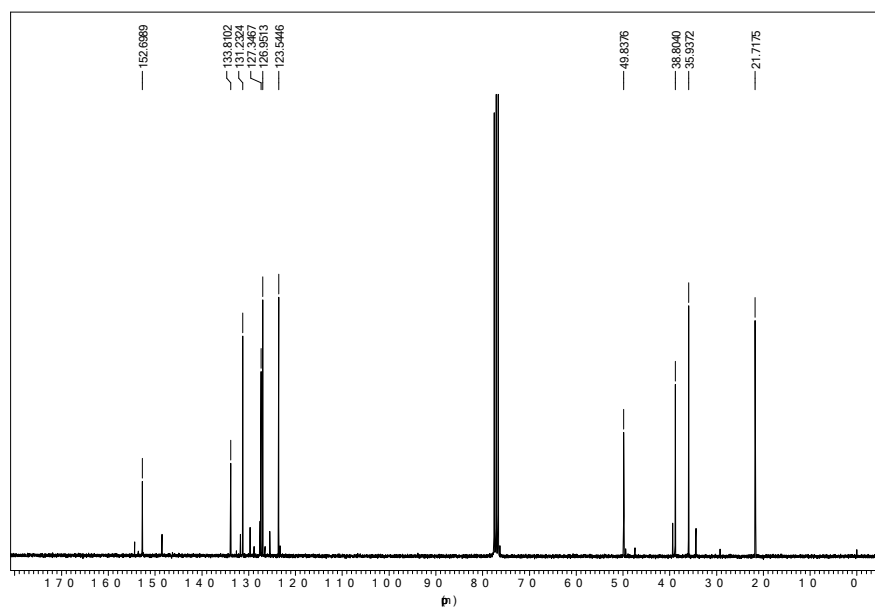
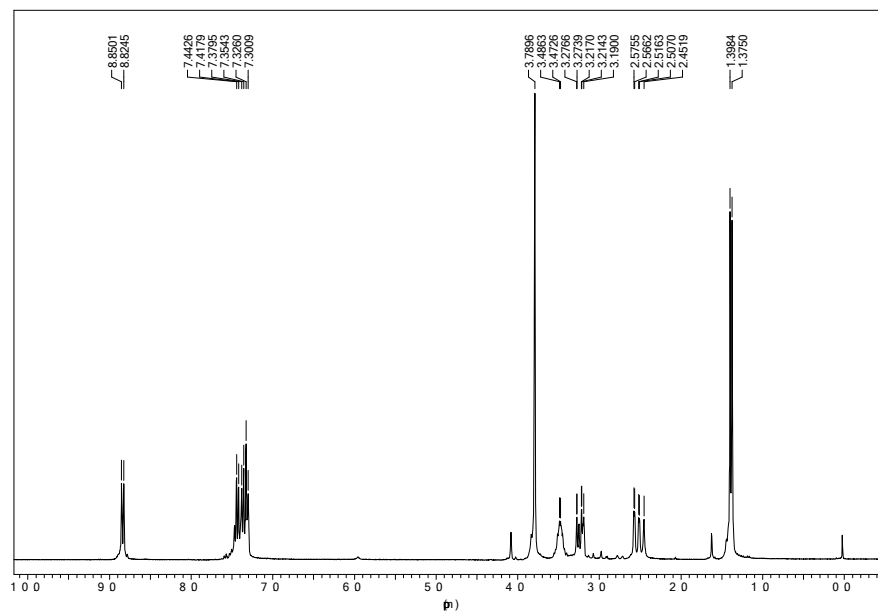
(Z) N-benzyl-C-indanoyl nitron (5b)



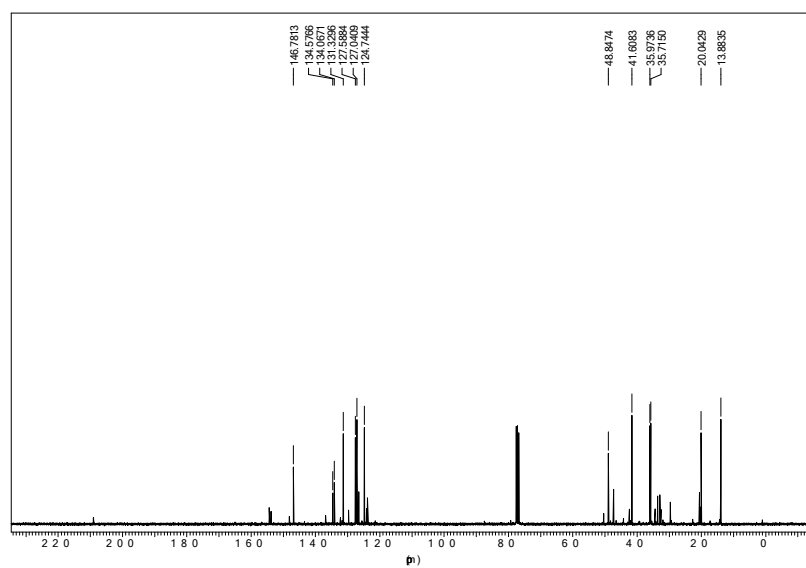
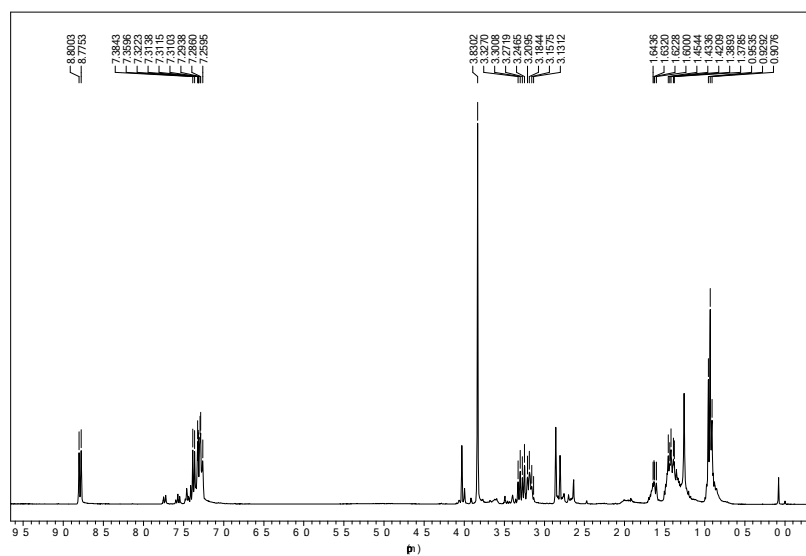
(Z) N-methyl-C-(2-Me)-indanoyl nitron (5c)



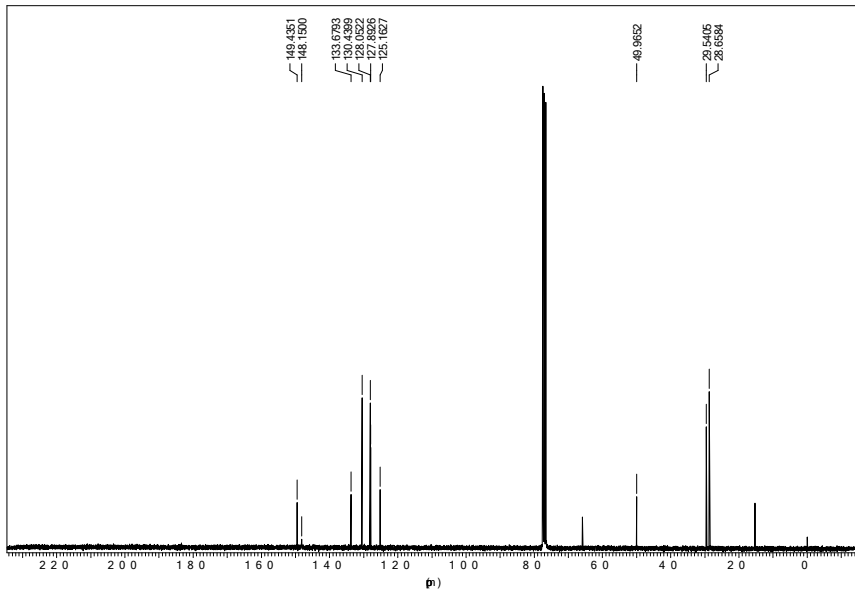
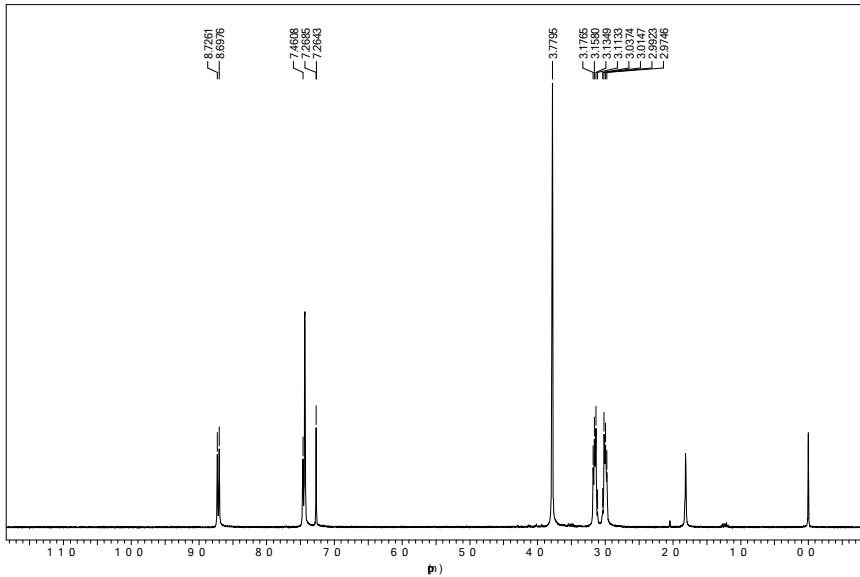
(Z) N-methyl-C-(3-Me)-indanoyl nitronc (5d)



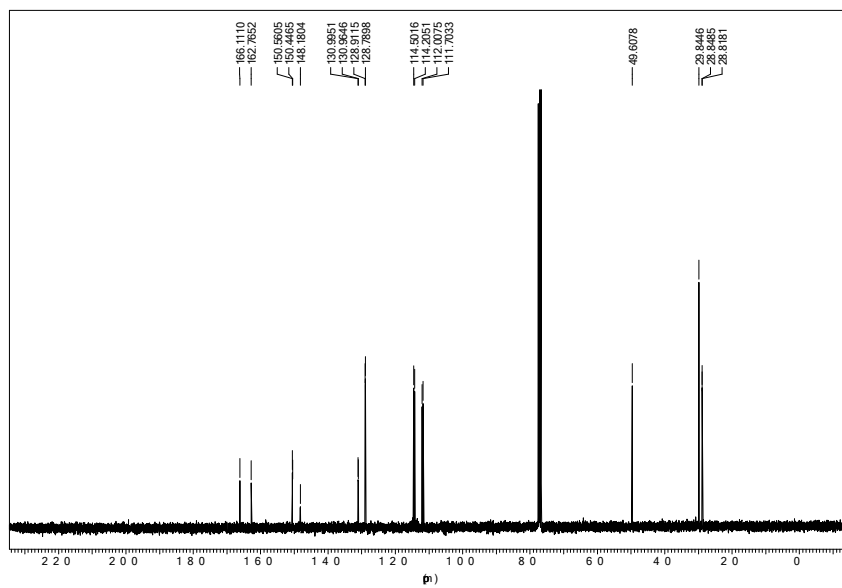
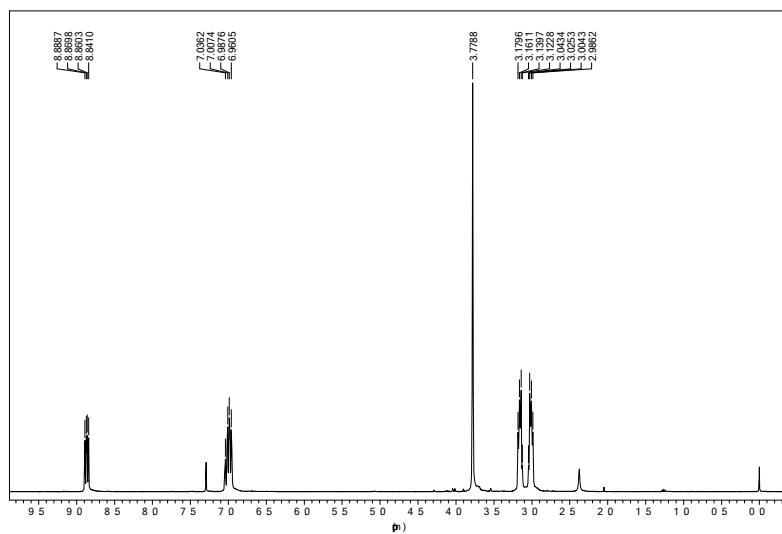
(Z) N-methyl-C-(2-Pr)-indanoyl nitron (5e)



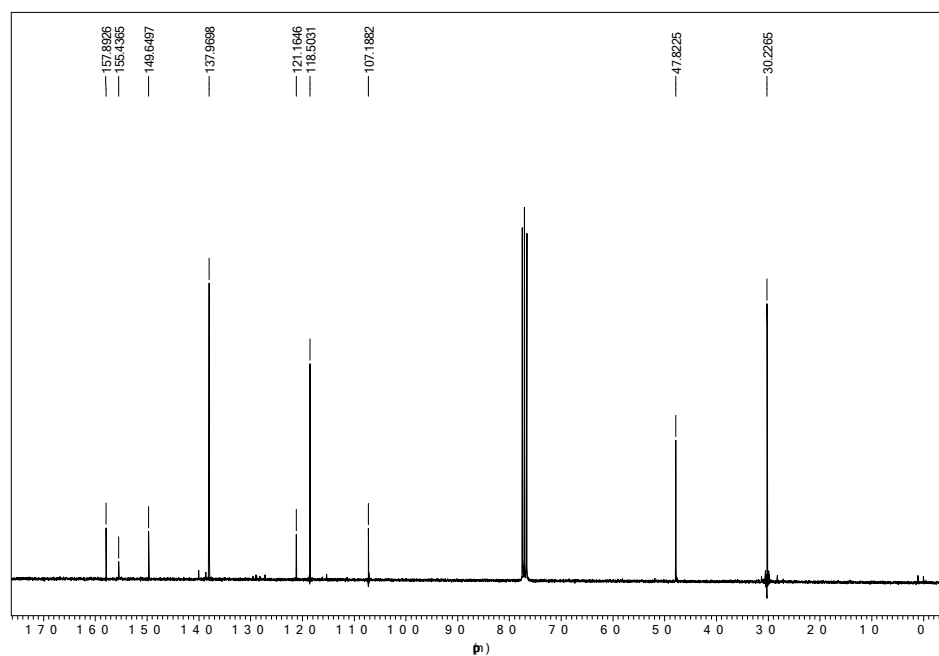
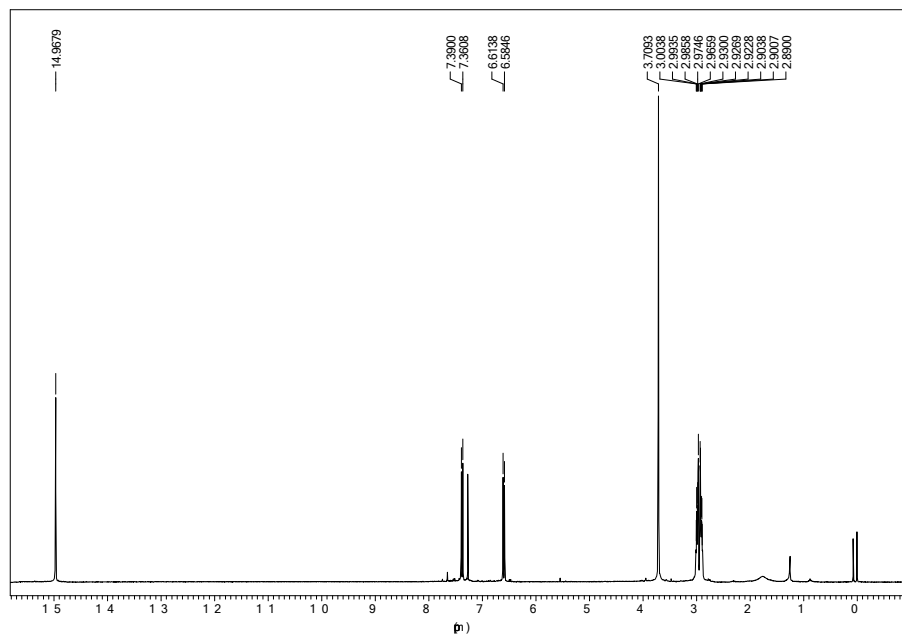
(Z) N-methyl-C-(5-Br)-indanoyl nitron (5f)



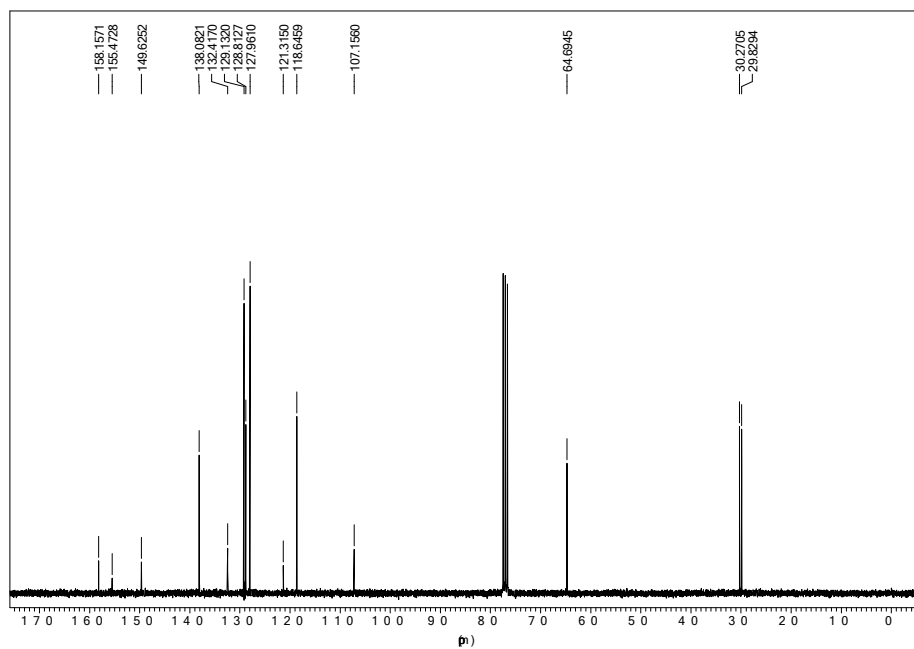
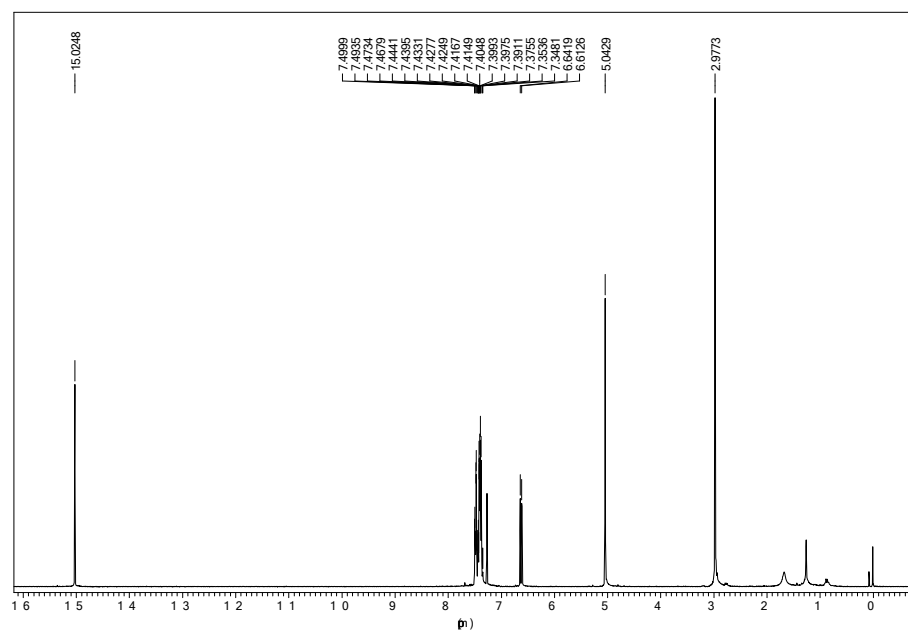
(Z) N-methyl-C-(5-F)-indanoyl nitron (5g)



(Z) N-methyl-C-(4-Br-7-OH)-indanyl nitron 5h

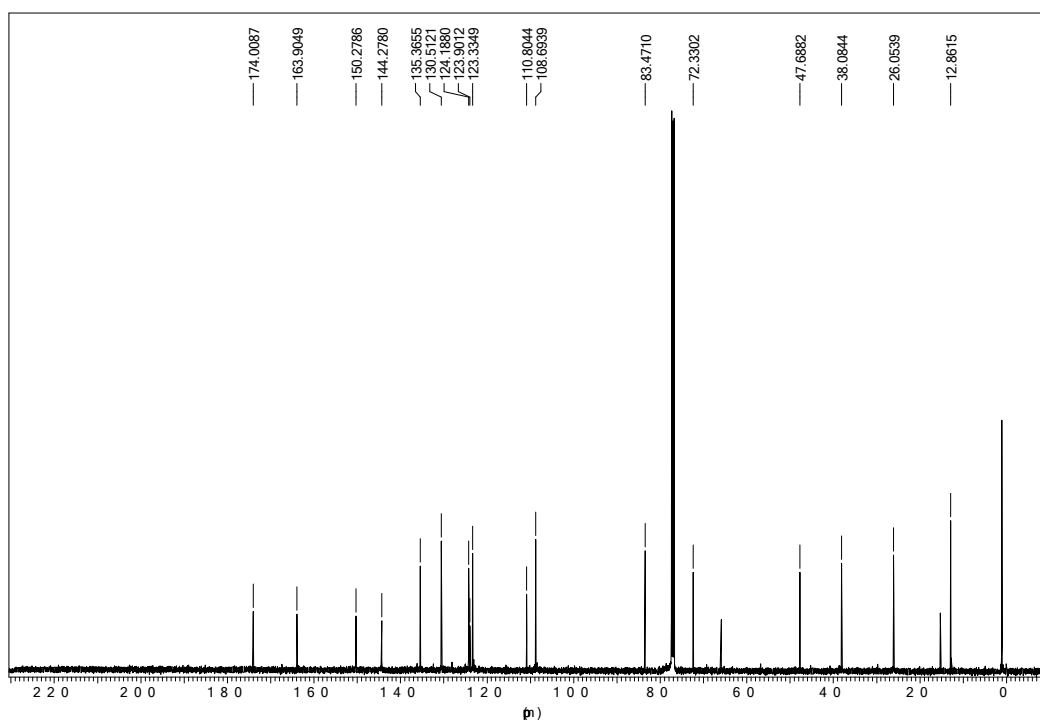
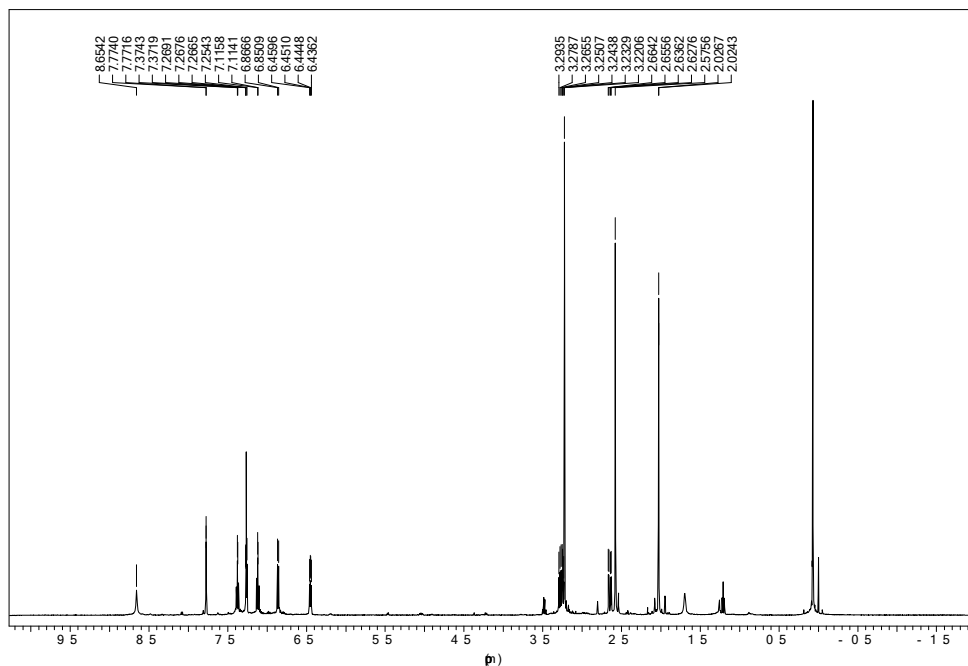


(Z) N-benzyl-C-(4-Br-7-OH)-indanyl nitrone 5i

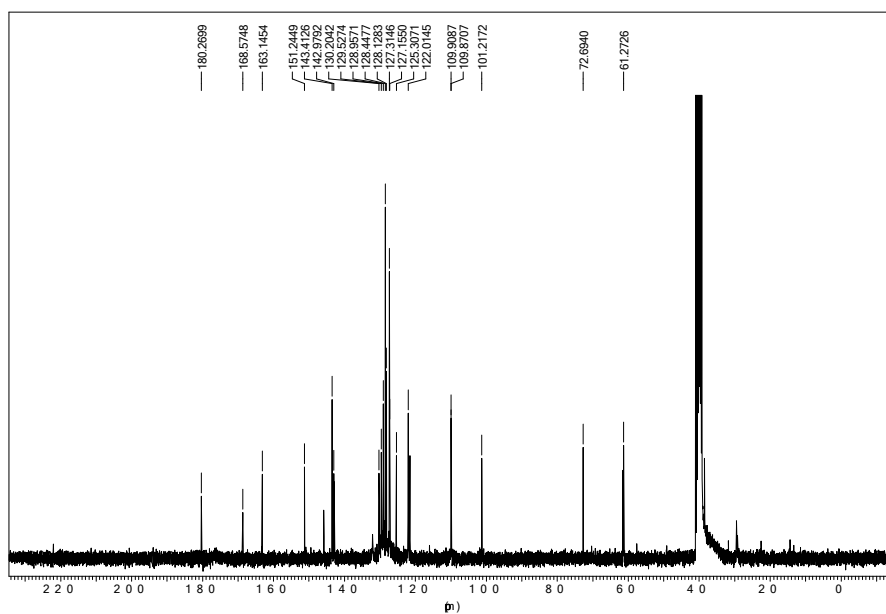
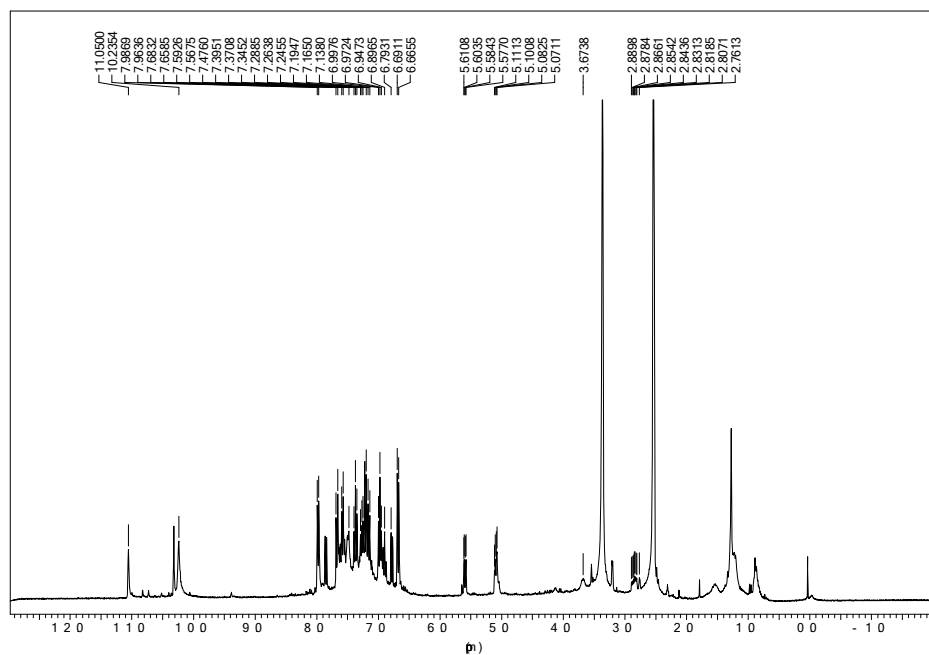


¹H and ¹³C NMR spectra of 7a-h and 8a-b

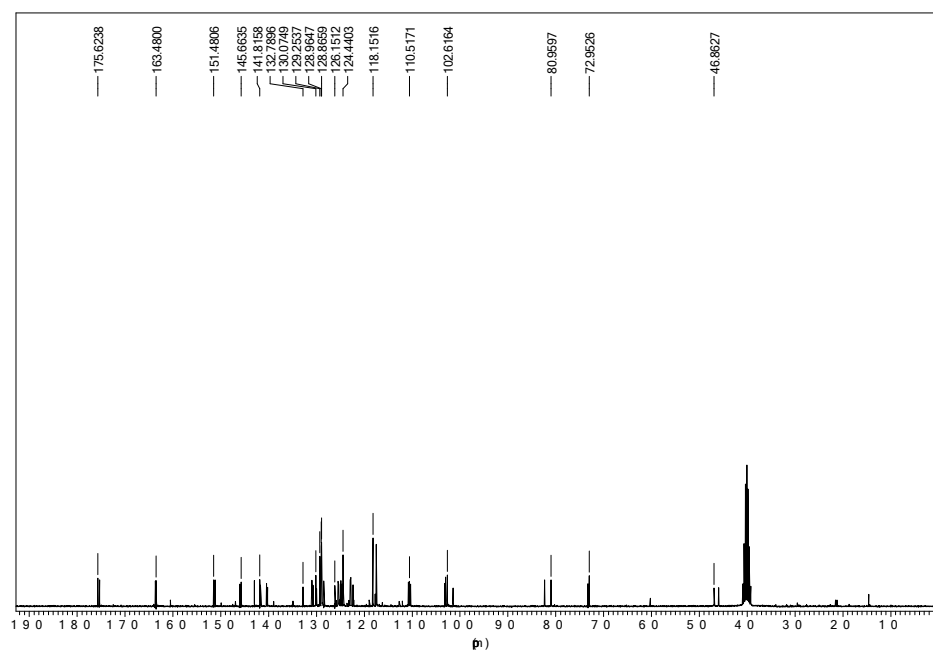
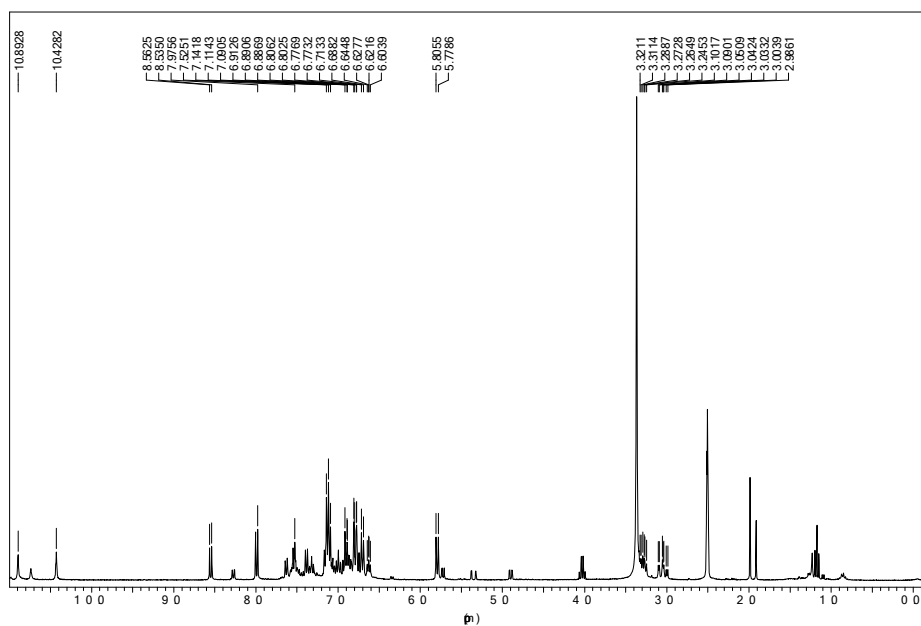
5'-Thyminy-2'-methyl-spiro [indoline-3,3'-isoxazolidine]-1-methyl-2-one (7a)



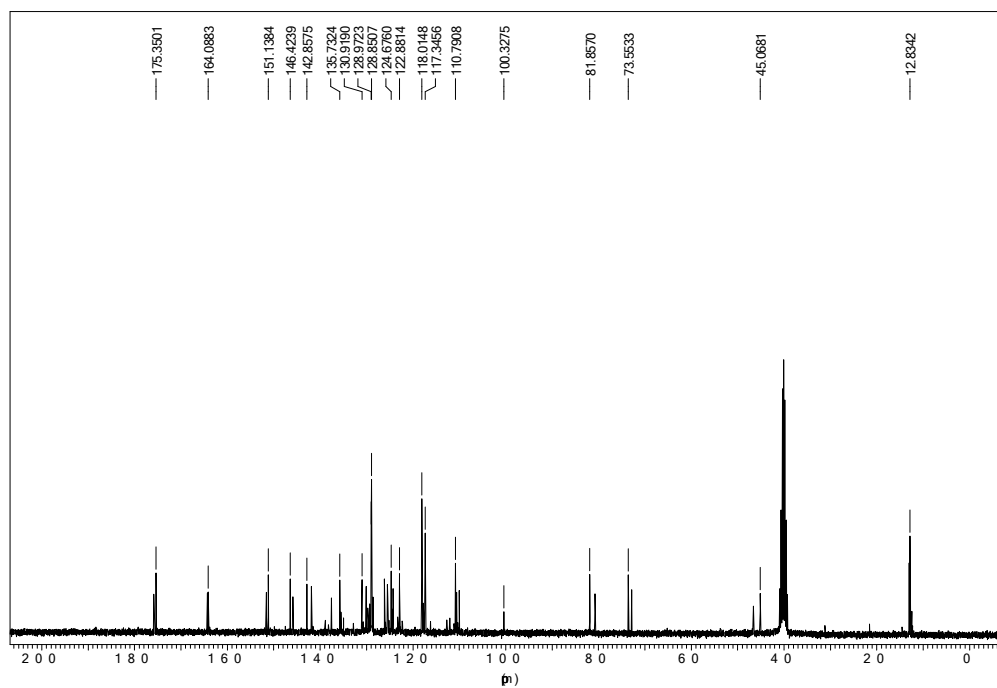
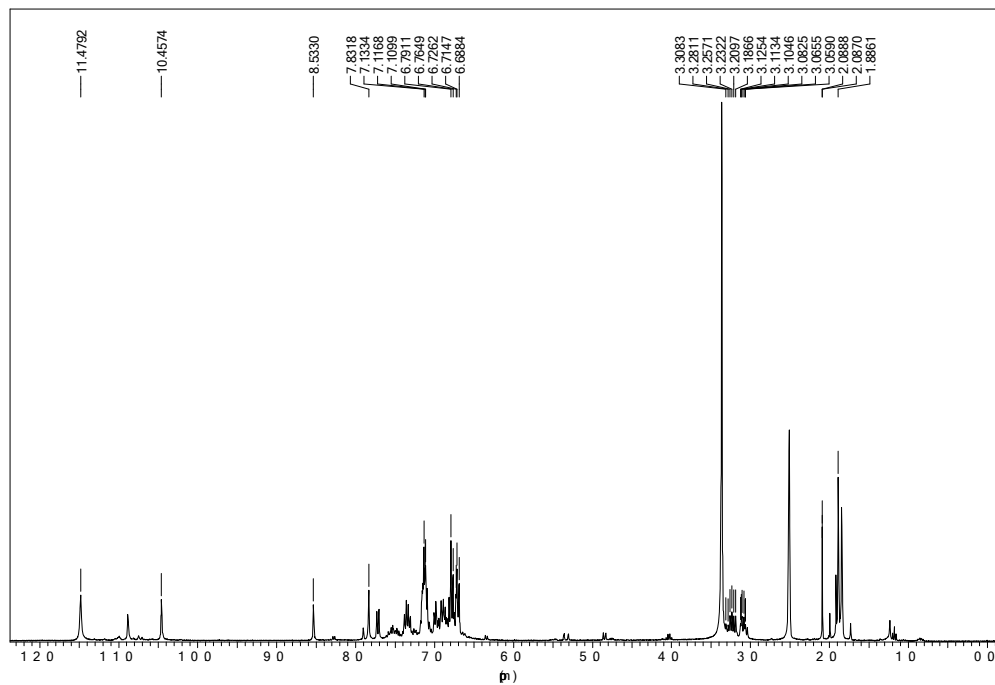
5'-Uracil -2'-benzyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7b)



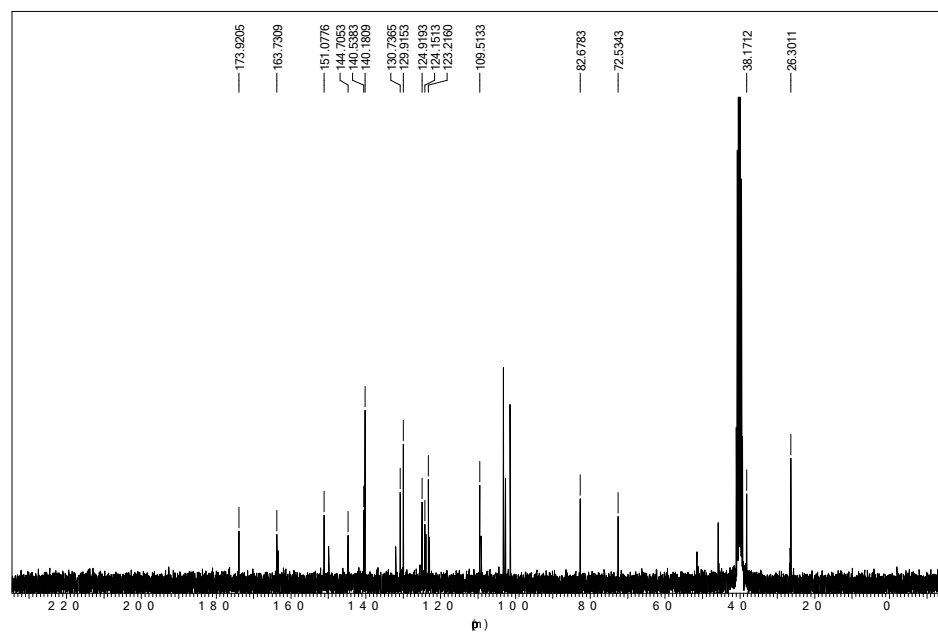
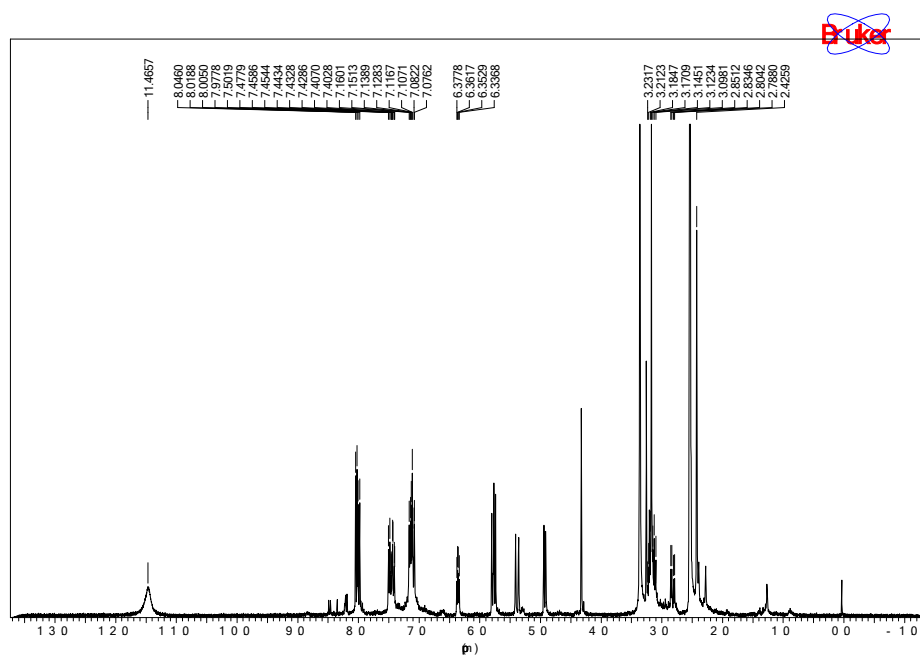
5'-Uracil-2'-phenyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7c)



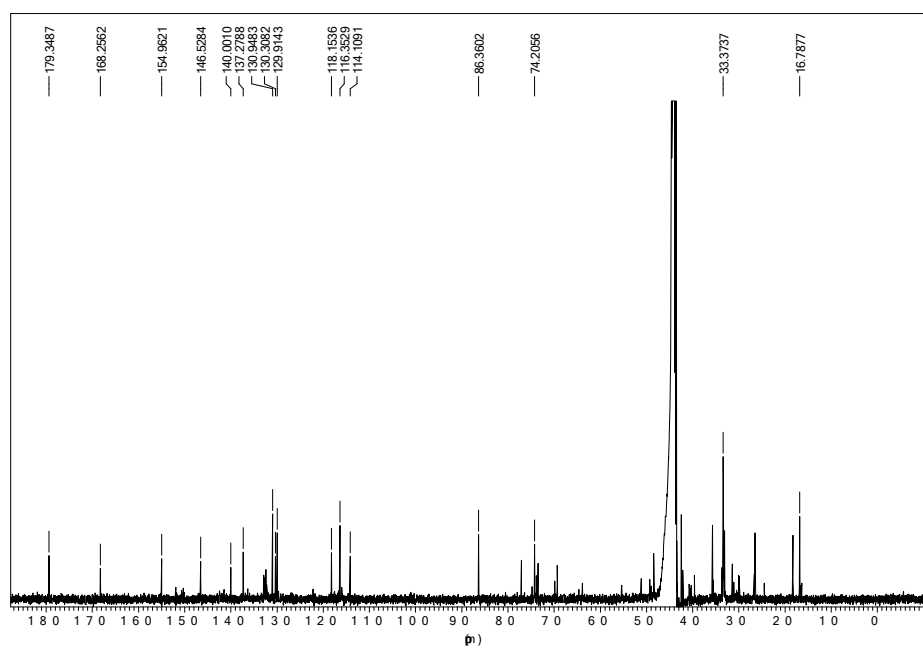
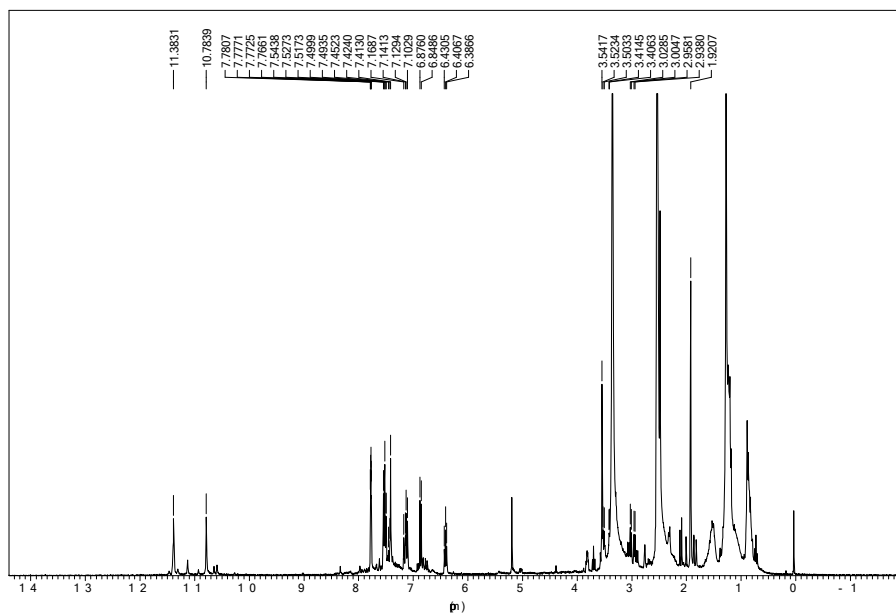
5'-Thyminy-2'-phenyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7d)



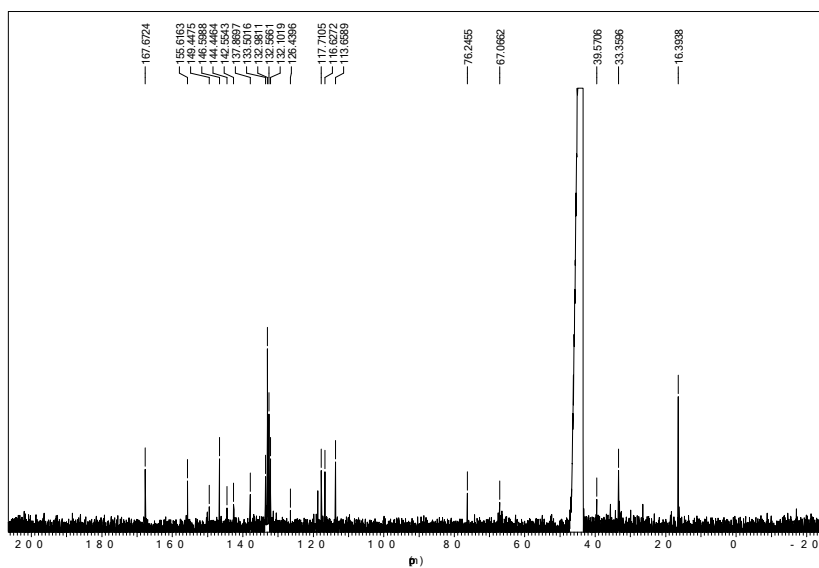
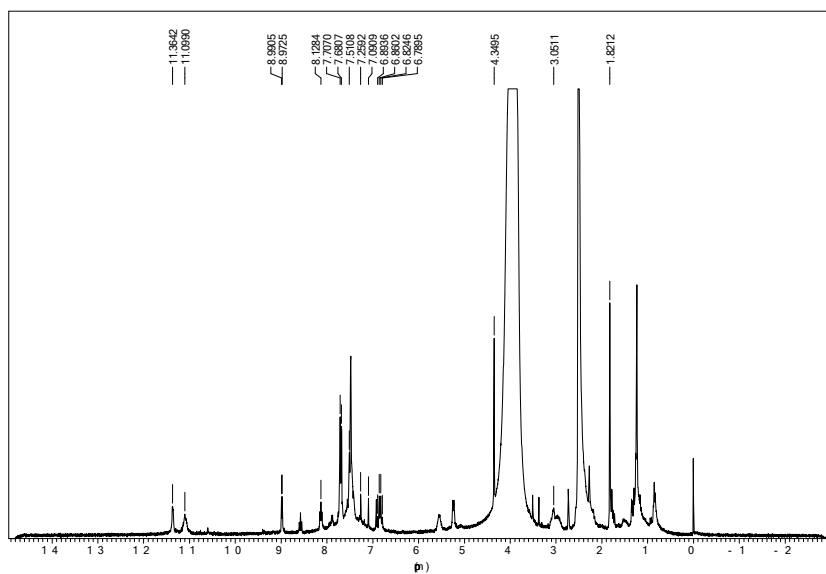
5'-Uracil-2'-methyl-spiro [indoline-3,3'-isoxazolidine]-1methyl-2-one (7e)



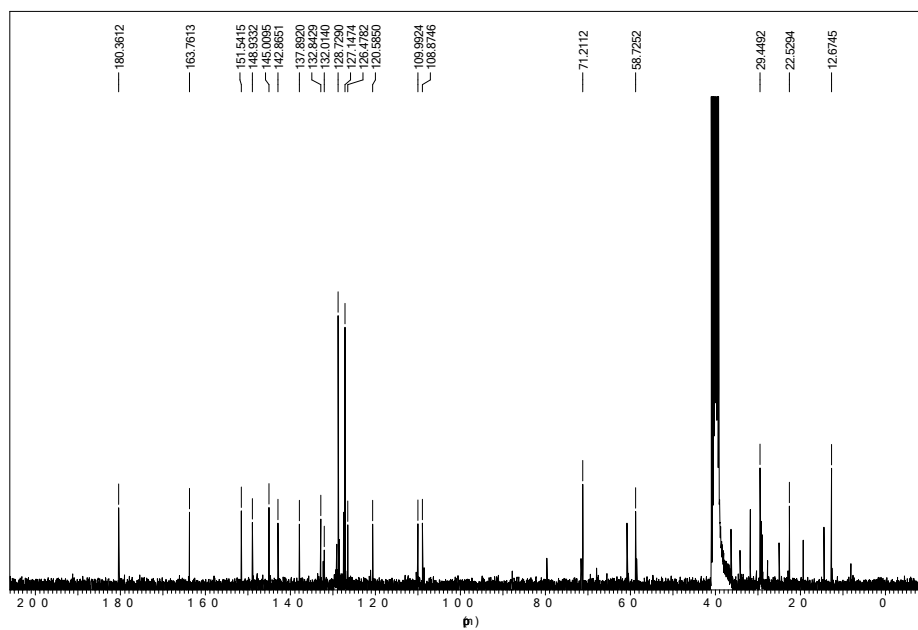
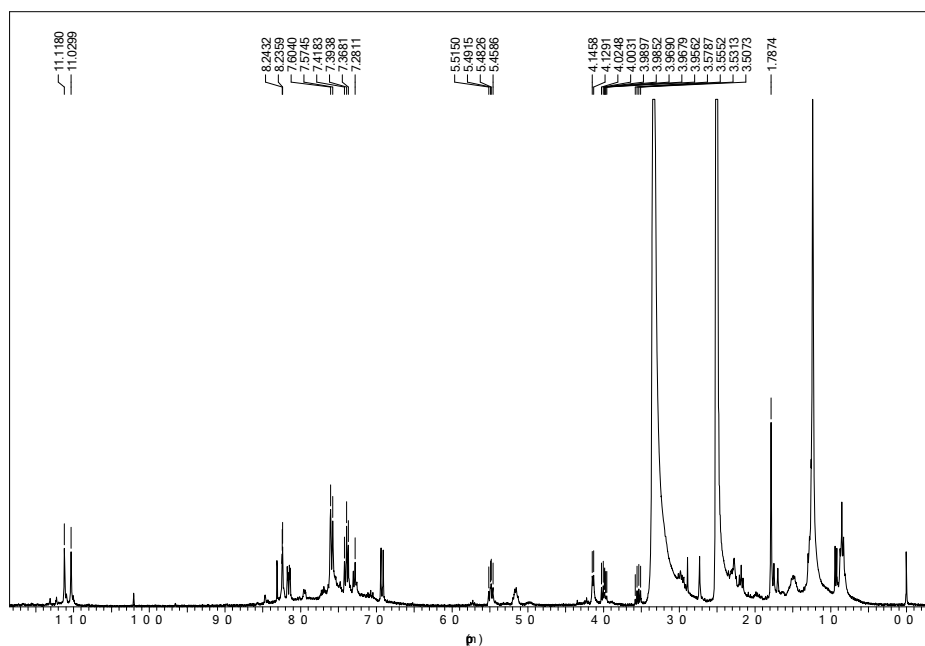
5'-Thyminy-2'-methyl-spiro [5-bromo-indoline-3,3'-isoxazolidine]-2-one (7f)



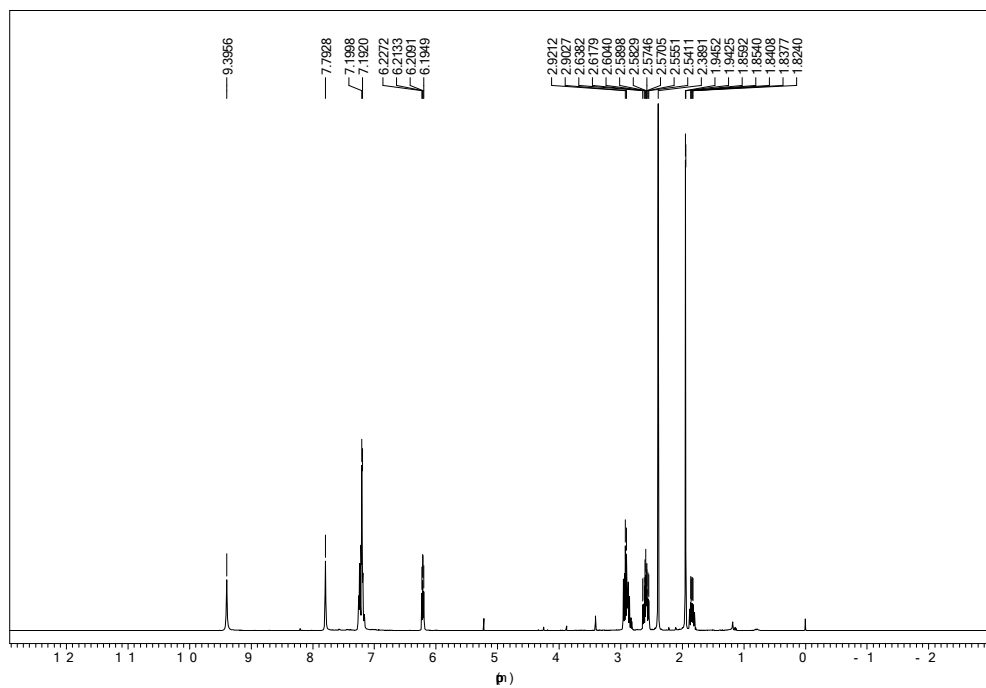
5'-Thyminy-2'-benzyl-spiro [5-bromo-indoline-3,3'-isoxazolidine]-2-one (7g)



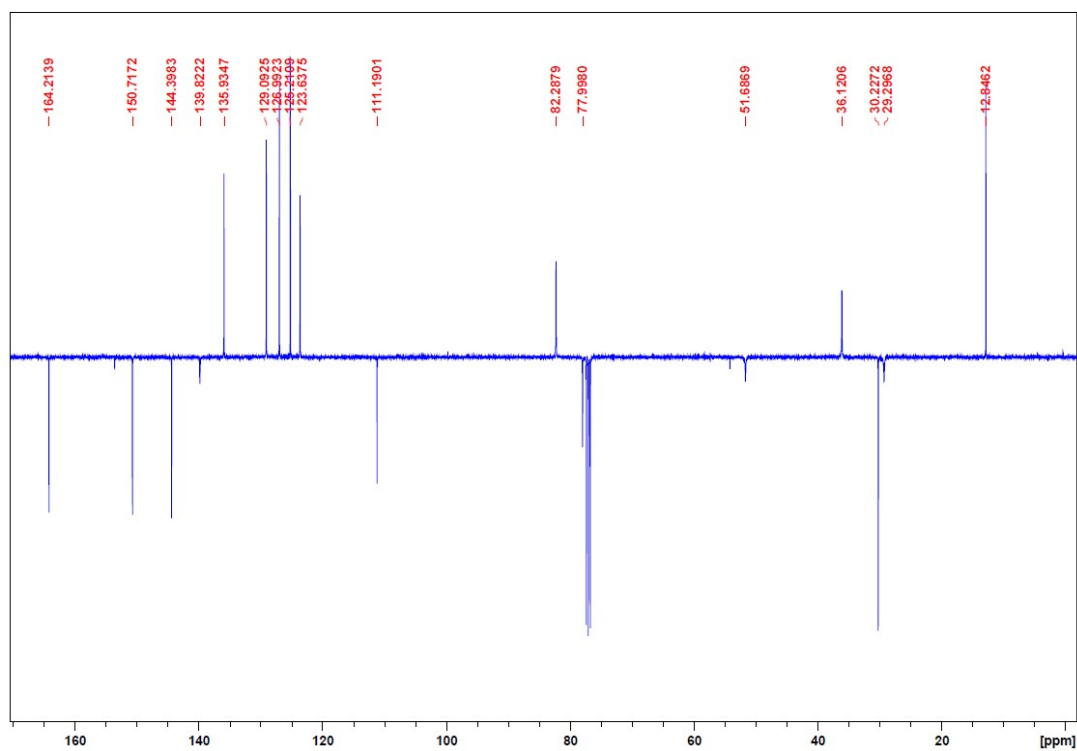
5'-Thyminyl-2'-benzyl-spiro [5-nitro-indoline-3,3'-isoxazolidine]-2-one (7h)



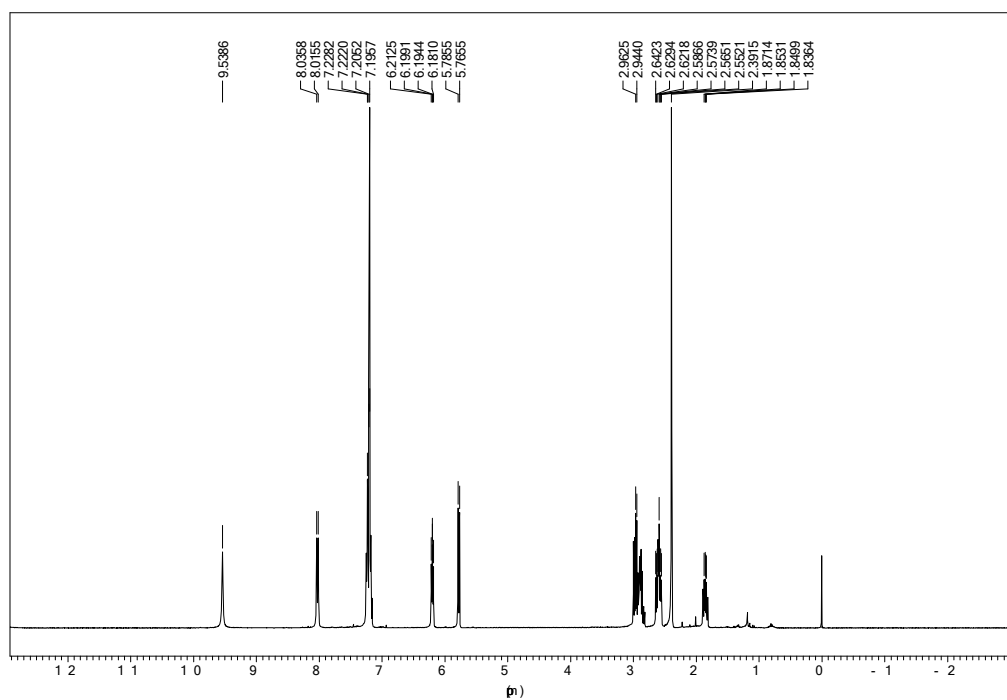
5'-Thyminy-2'-methyl-spiro [indane-3,3'-isoaxazolidine] (8a)



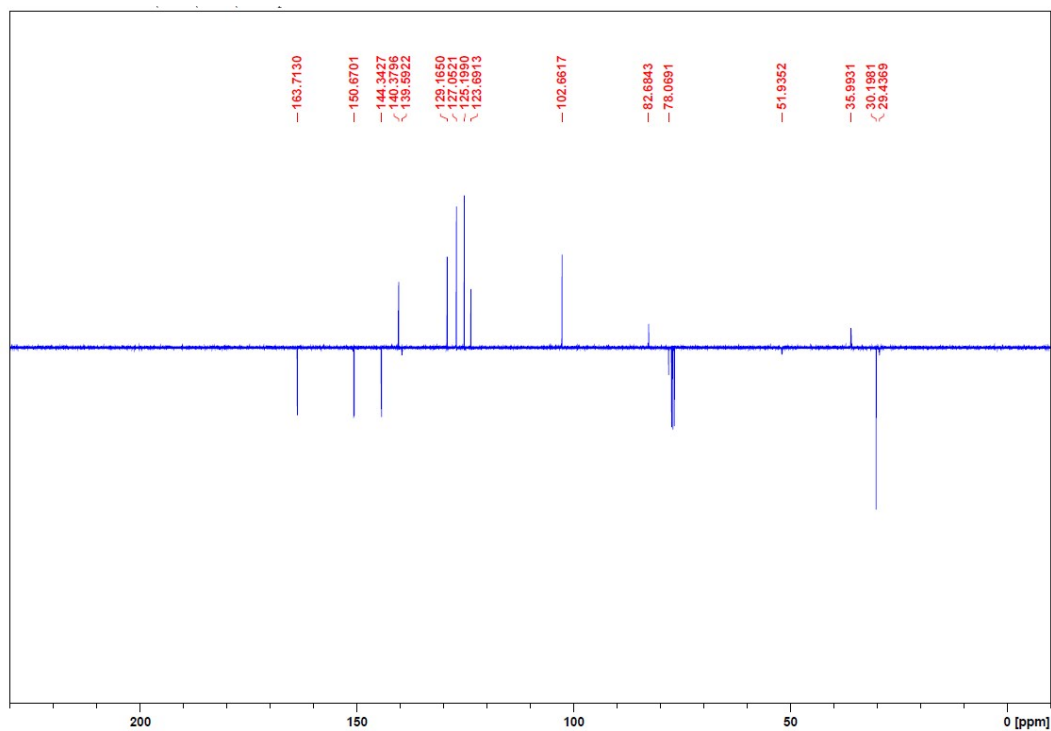
APT C/CH₂↓CH/CH₃↑



5'-Uracil-2'-methyl-spiro [indane-3,3'-isoaxazolidine] (8b)

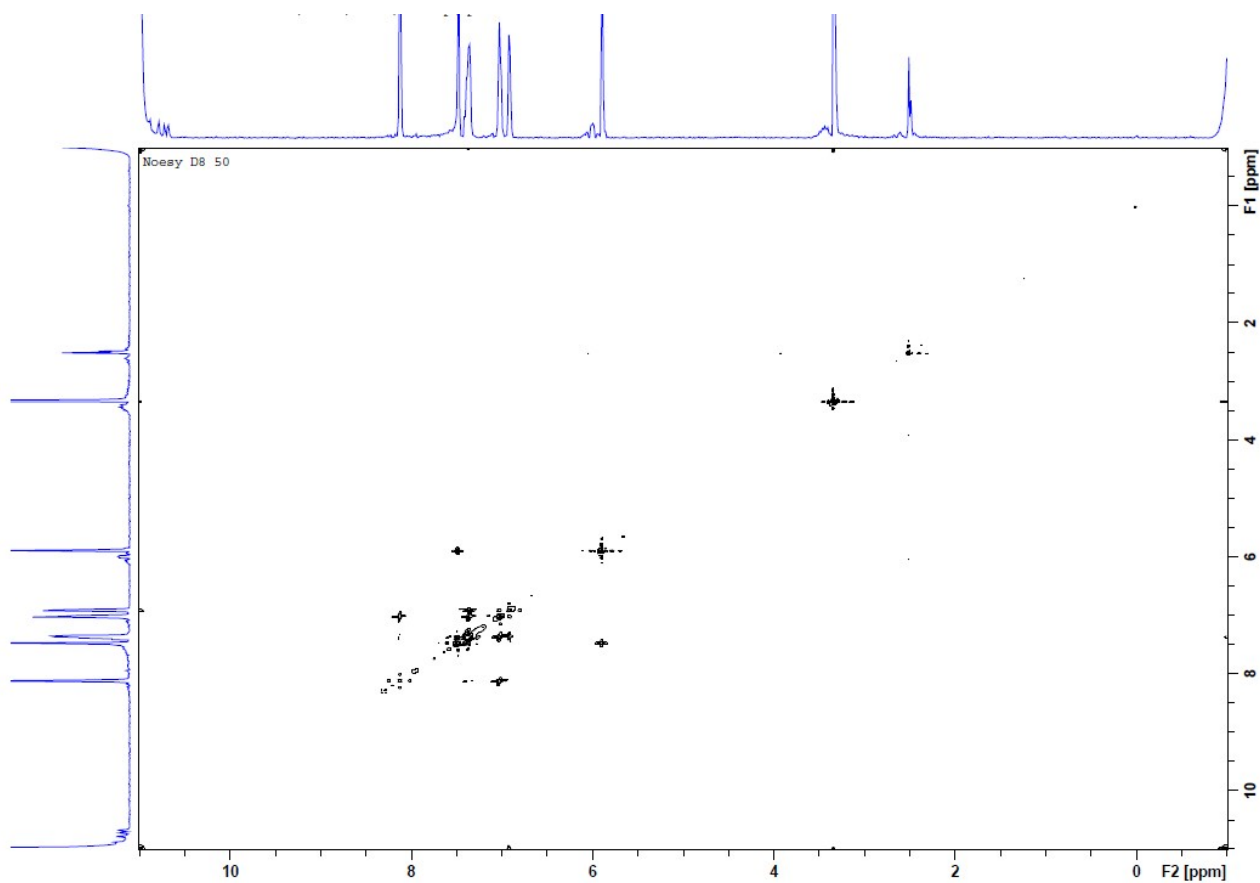


APT CH/CH₃ ↓ C/CH₂ ↑

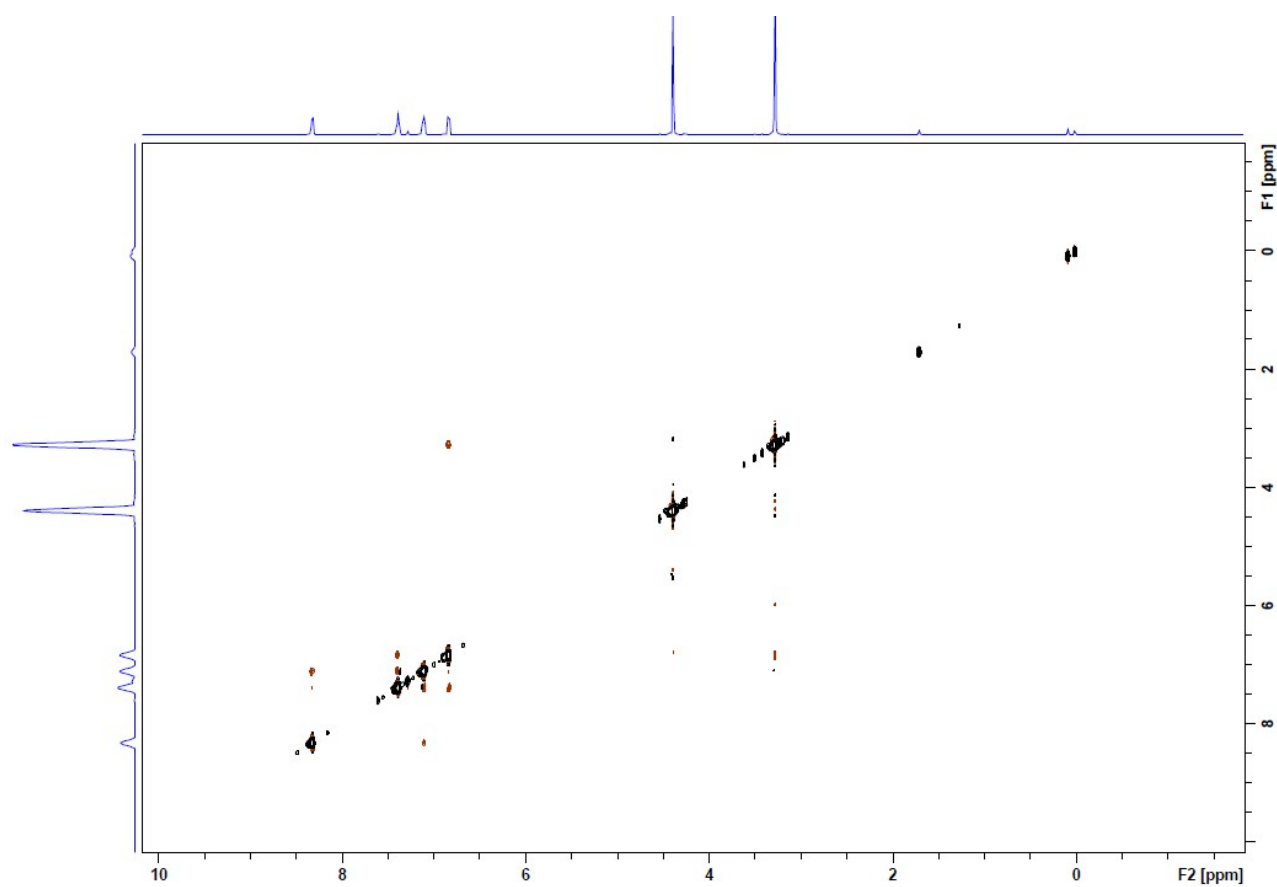


NOESY of 4b, 4e, 5a, 7a and 8b

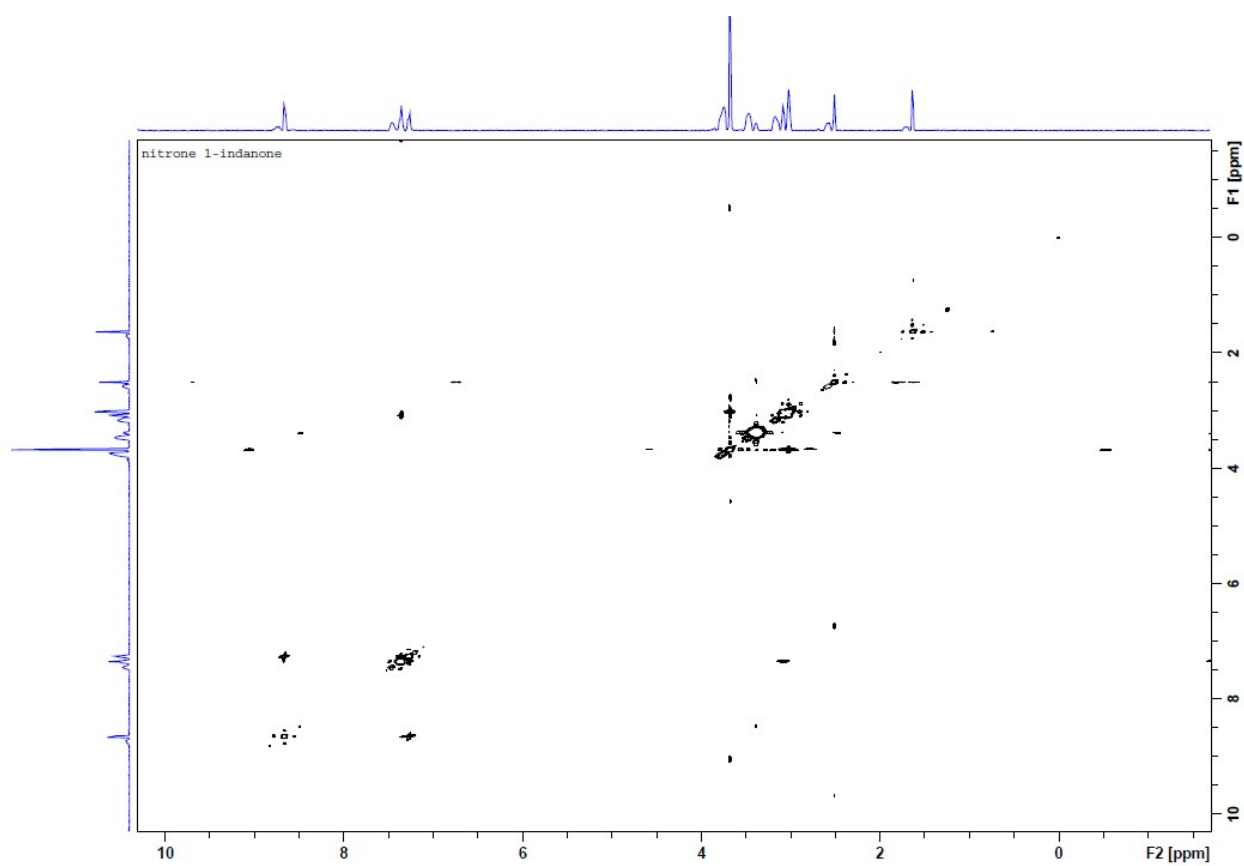
(*E*) *N*-benzyl-*C*-isatinyl nitron (4b)



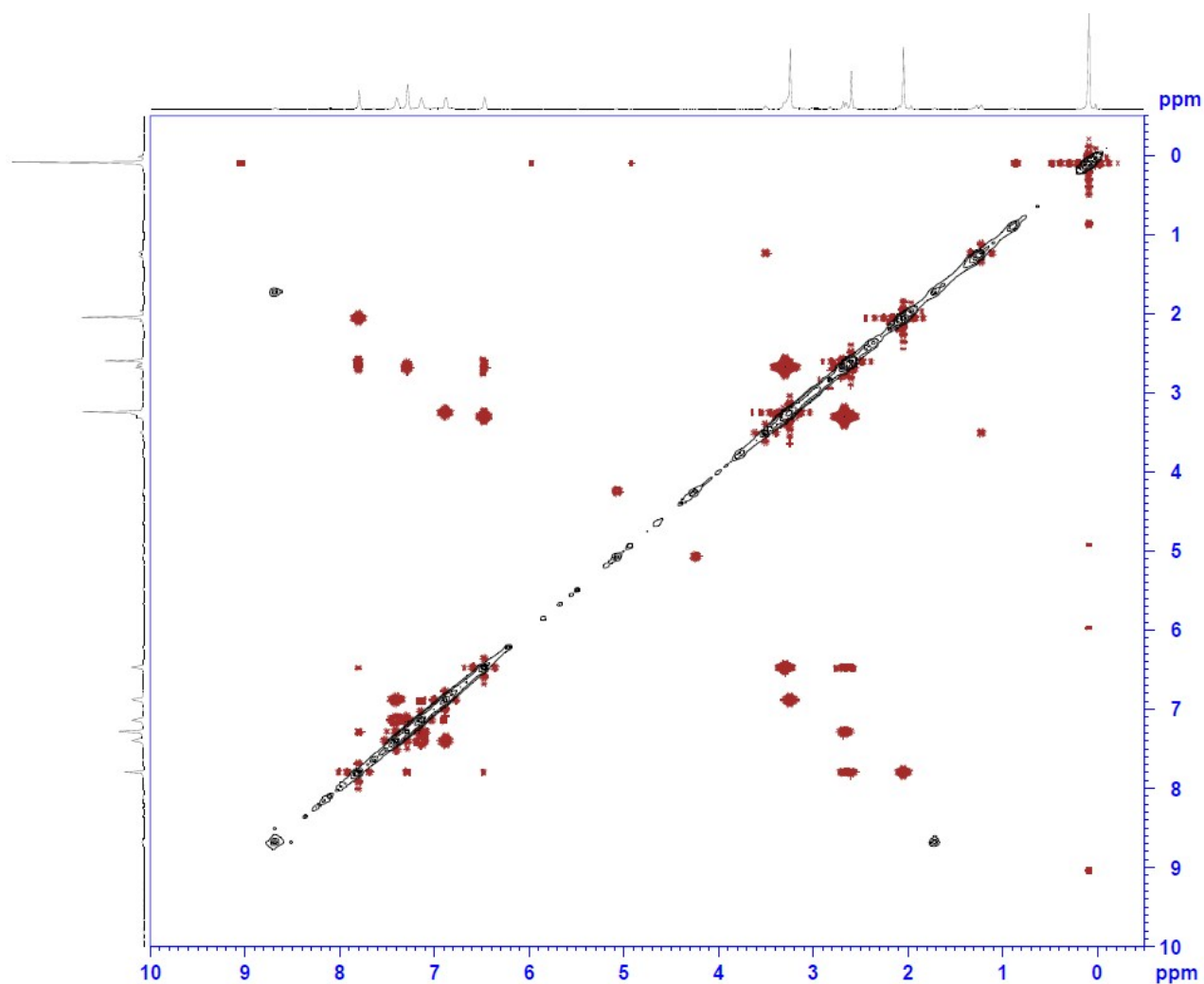
(*E*) N-methyl-C- (1-methyl)-isatinyl nitron (4e)



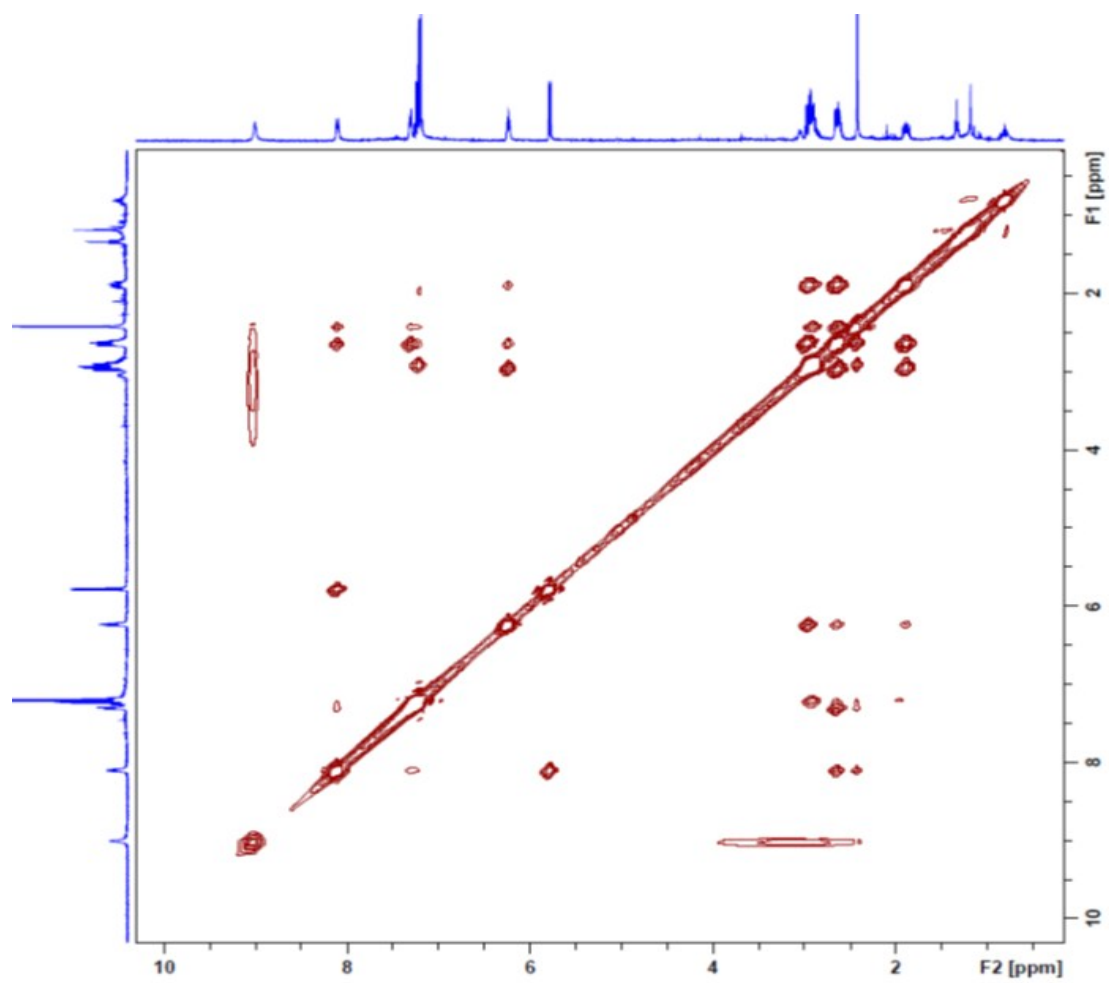
(Z) N-methyl-C-indanoyl nitrone (5a)



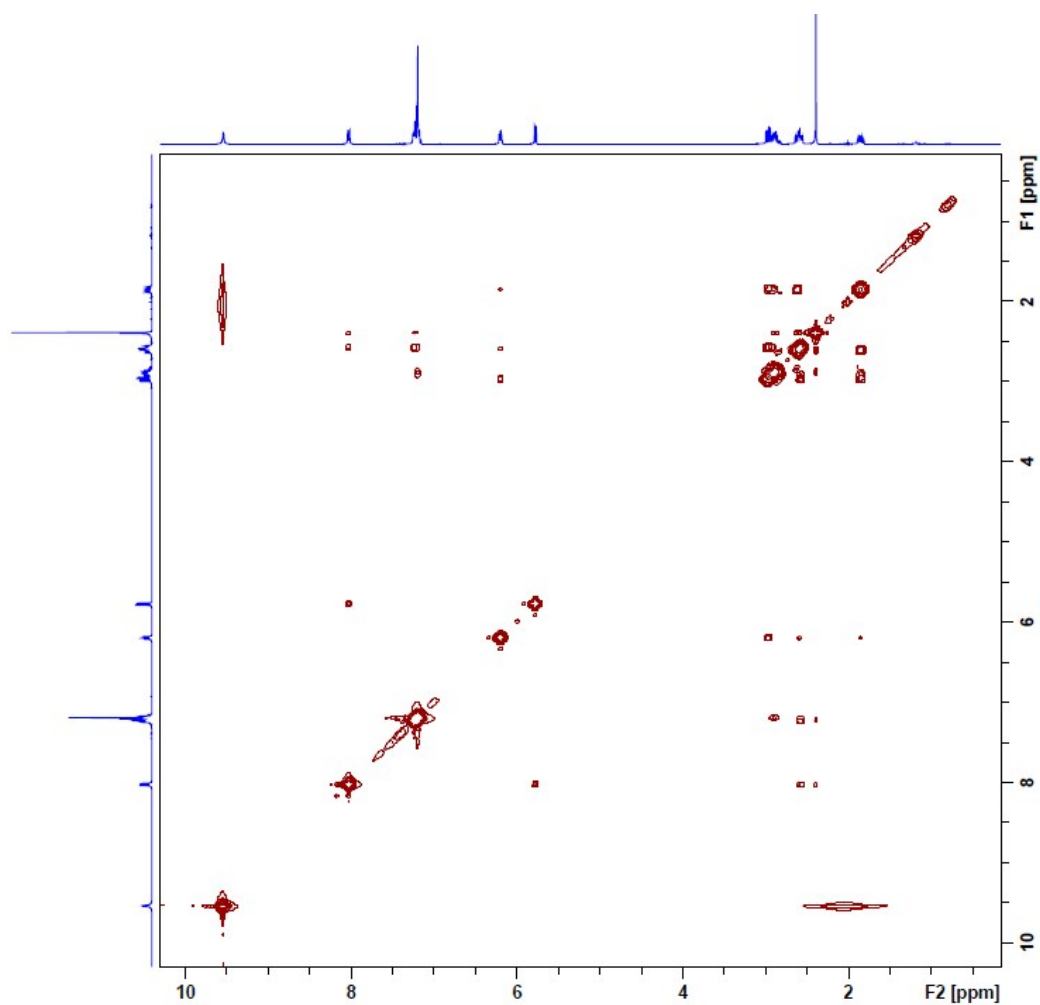
5'-Thyminy1-2'-methyl- spiro [indoline-3,3'-isoxazolidine]-1-methyl-2-one (7a)



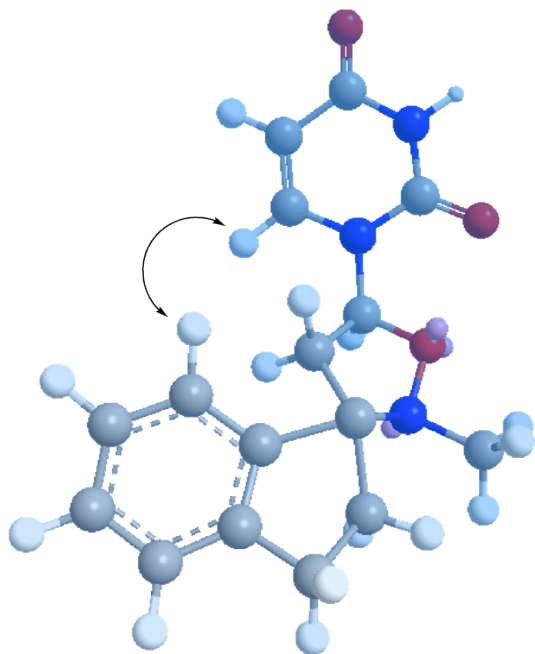
Exo 5'-Uracil-2'-methyl- spiro [indane-3,3'-isoaxazolidine] (8b)



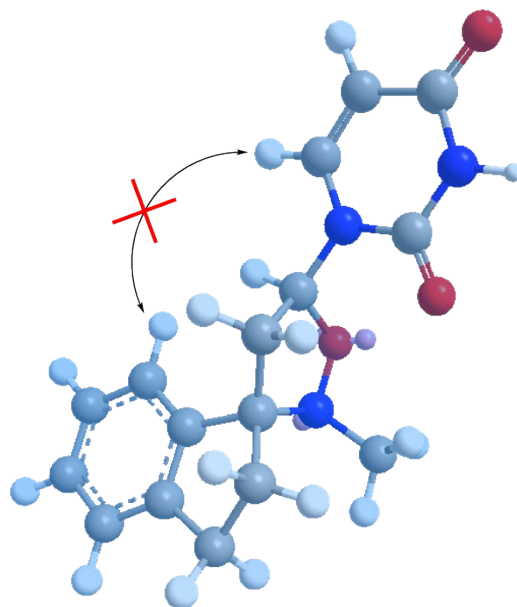
***Endo* 5'-Uracil-2'-methyl- spiro [indane-3,3'-isoaxazolidine] (8b)**



Correlation between H on C-6 of uracil and H on C-4 of aromatic ring for *Exo* 8b (a), absent in *Endo* 8b (b).



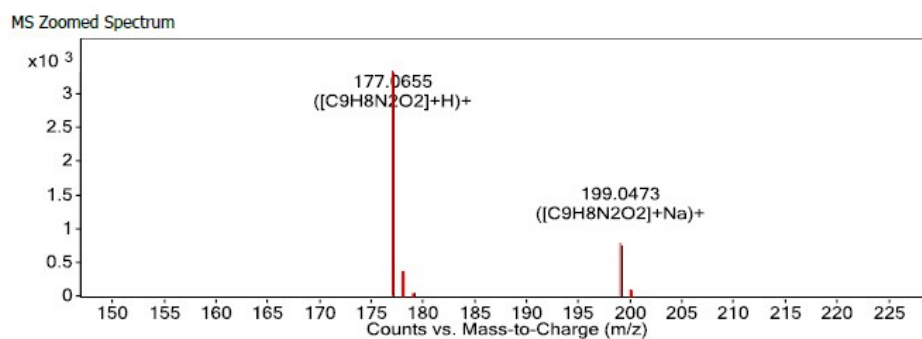
a) *Exo* 8b



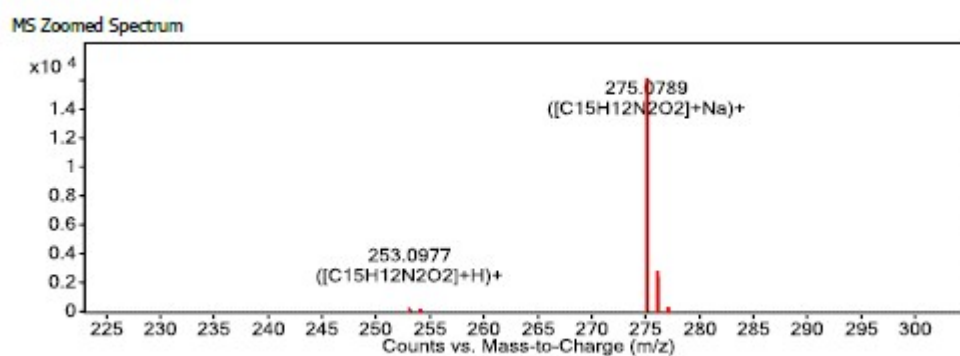
b) *Endo* 8b

ESI(+)-MS spectra of 4a-o, 5a-i, 7a-h and 8a-b

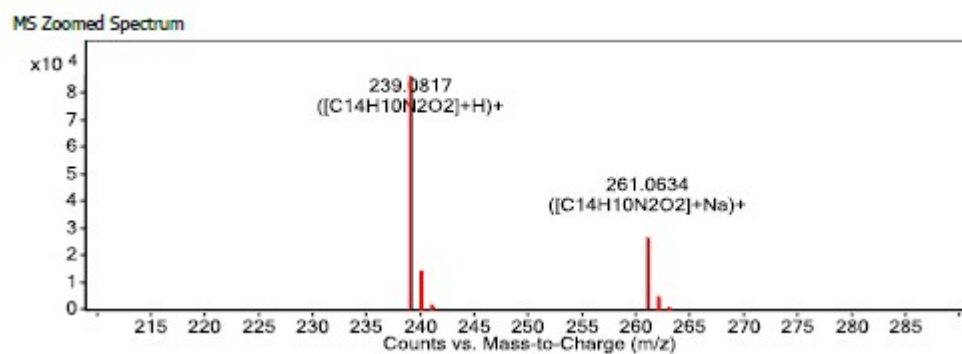
(*E*) *N*-methyl-isatinyl nitrone (4a)



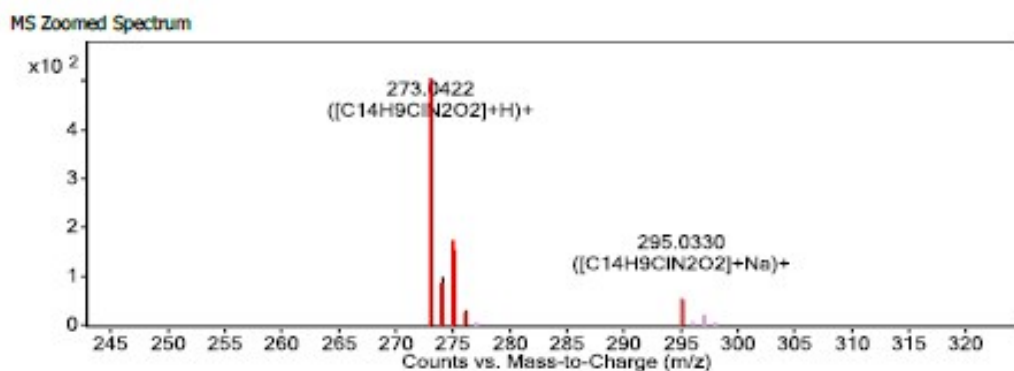
(*E*) *N*-benzyl-isatinyl nitrone (4b)



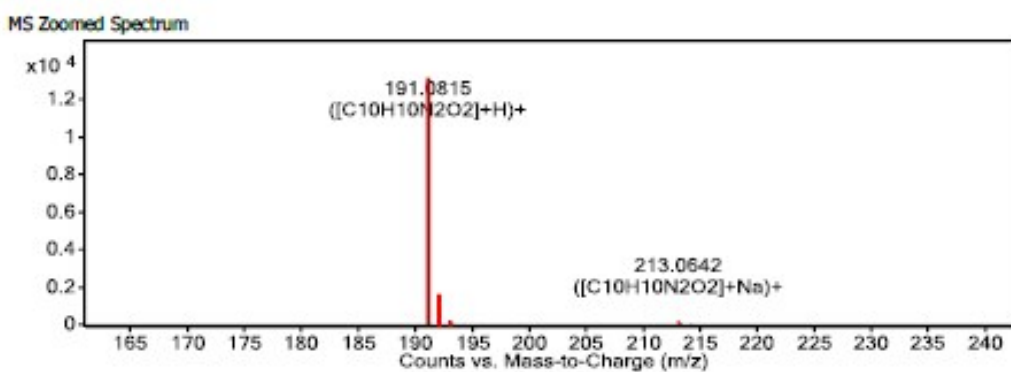
(*E*) *N*-phenyl-isatinyl nitrone (4c)



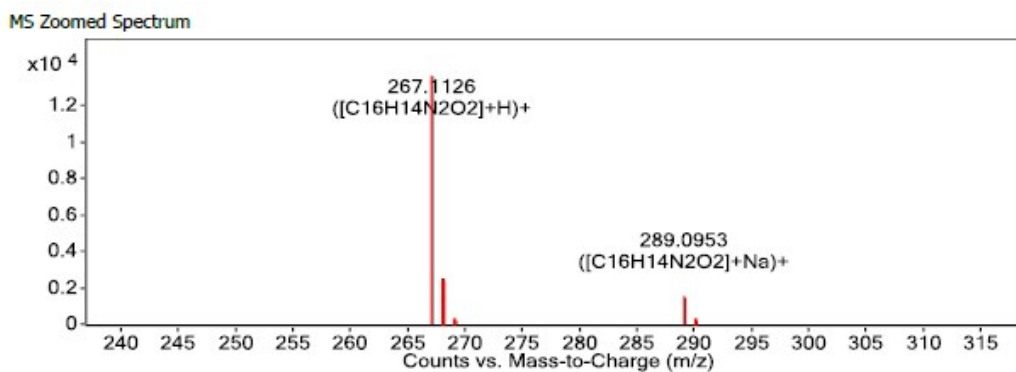
(E) N-3-Cl-phenyl-C-isatinylnitrone (4d)



(E) N-methyl-C- (I-methyl)-isatinylnitrone (4e)

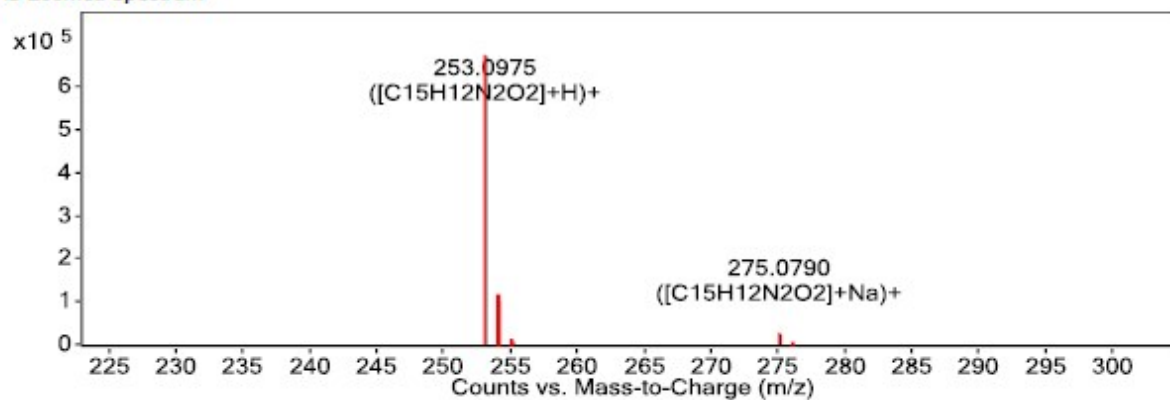


(E) N-benzyl-C- (I-methyl)-isatinylnitrone (4f)



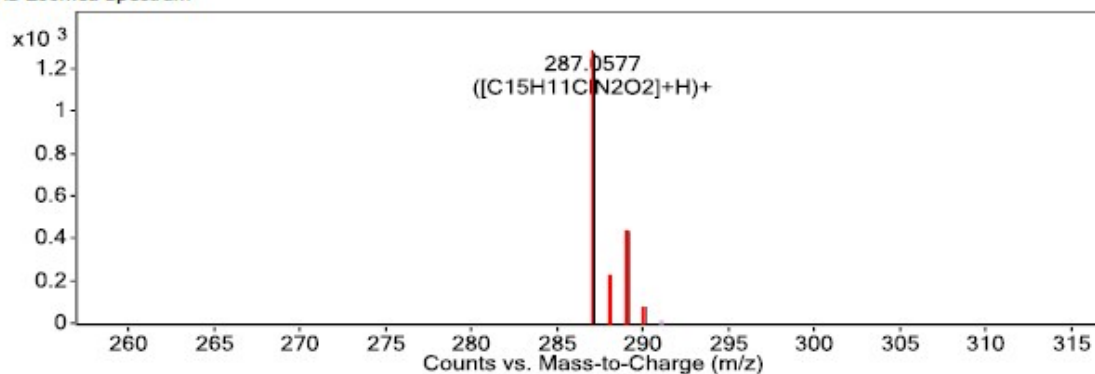
(E) N-phenyl-C- (I-methyl)-isatinylnitrone (4g)

MS Zoomed Spectrum



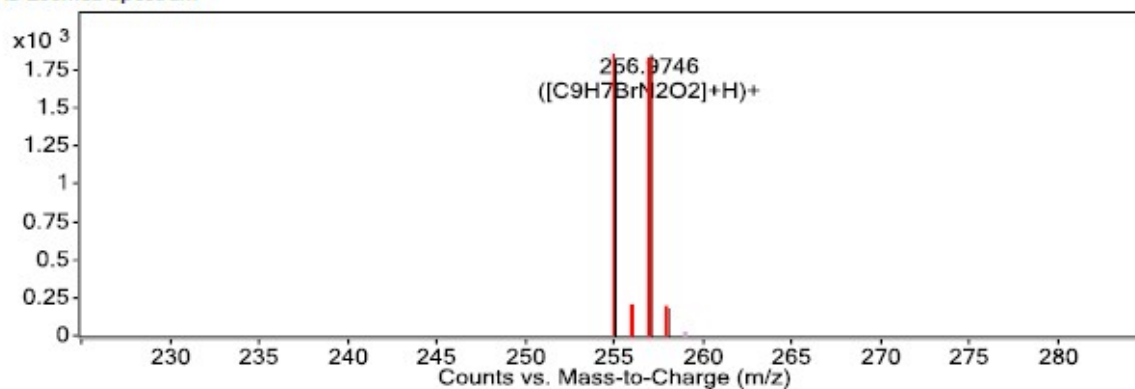
(E) N-3-Cl-phenyl -C-(I-methyl)-isatinylnitrone (4h)

MS Zoomed Spectrum



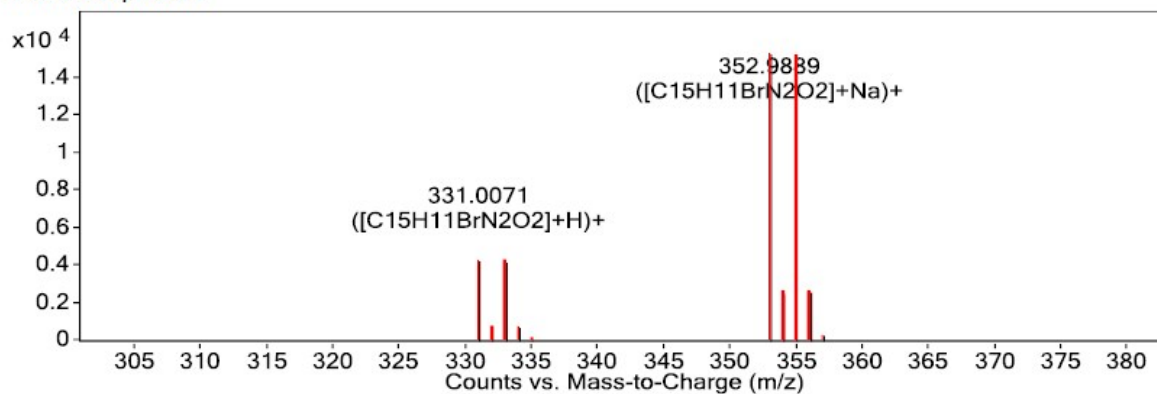
(E) N-methyl-C-(5-Br)-isatinylnitrone (4i)

MS Zoomed Spectrum



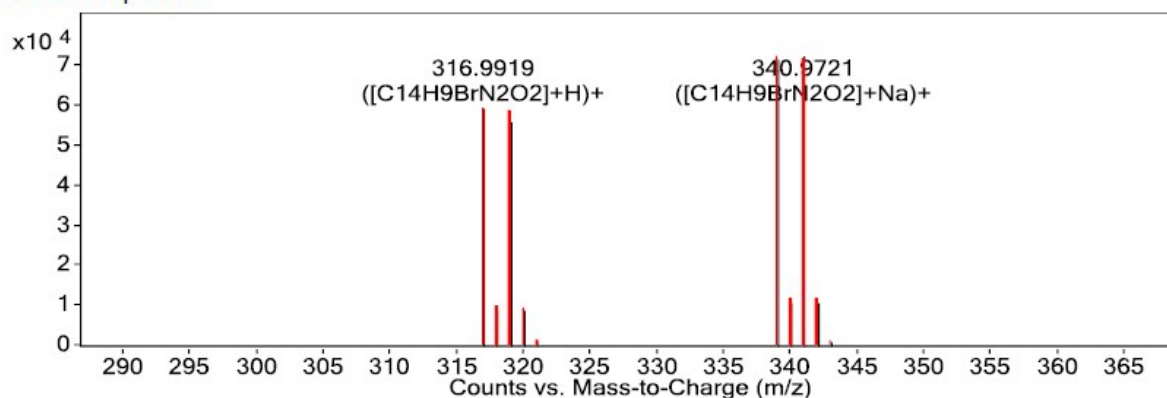
(E) N-benzyl-C-(5-Br)-isatinyl nitrone (4j)

MS Zoomed Spectrum



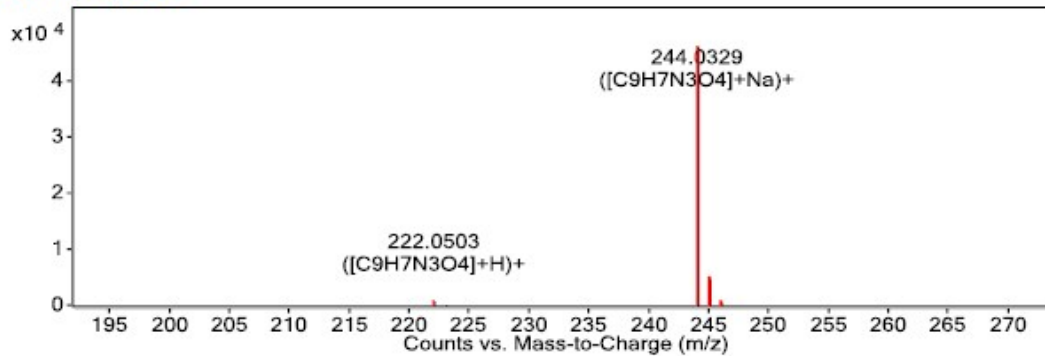
(E) N-phenyl-C-(5-Br)-isatinyl nitrone (4k)

MS Zoomed Spectrum

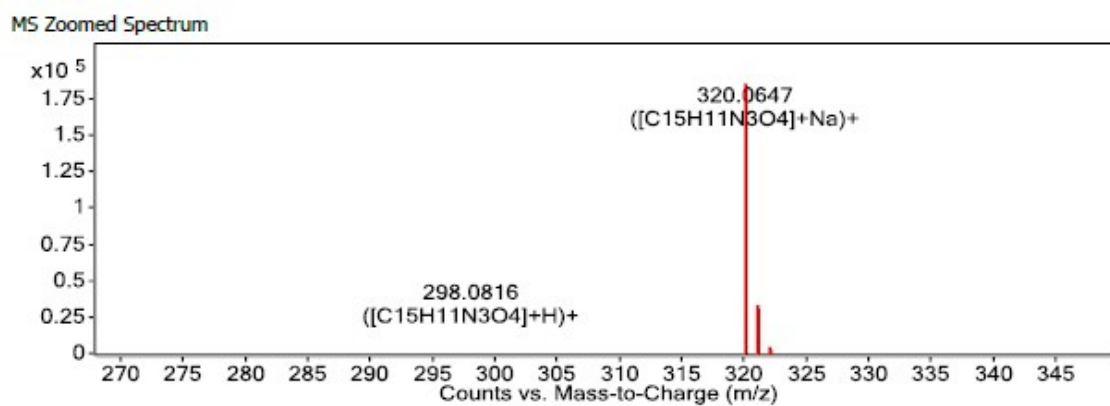


(E) N-methyl-C-(5-NO₂)-isatinyl nitrone (4l)

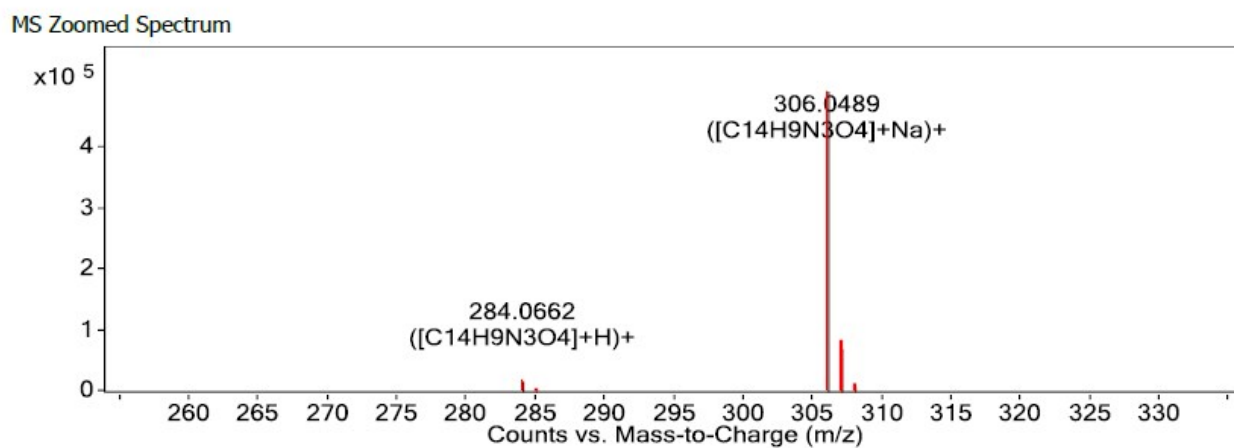
MS Zoomed Spectrum



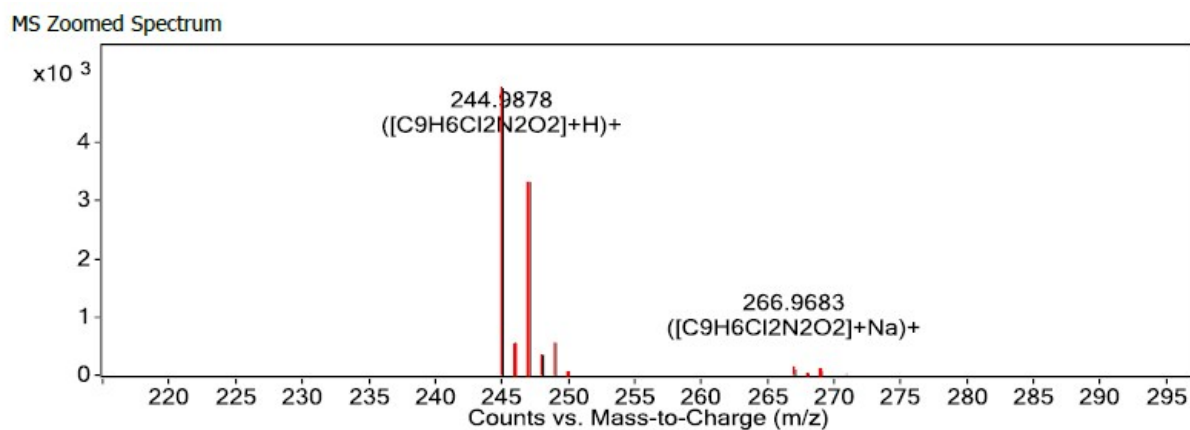
(E) N-benzyl-C-(5-NO₂)-isatinyl nitrone (4m)



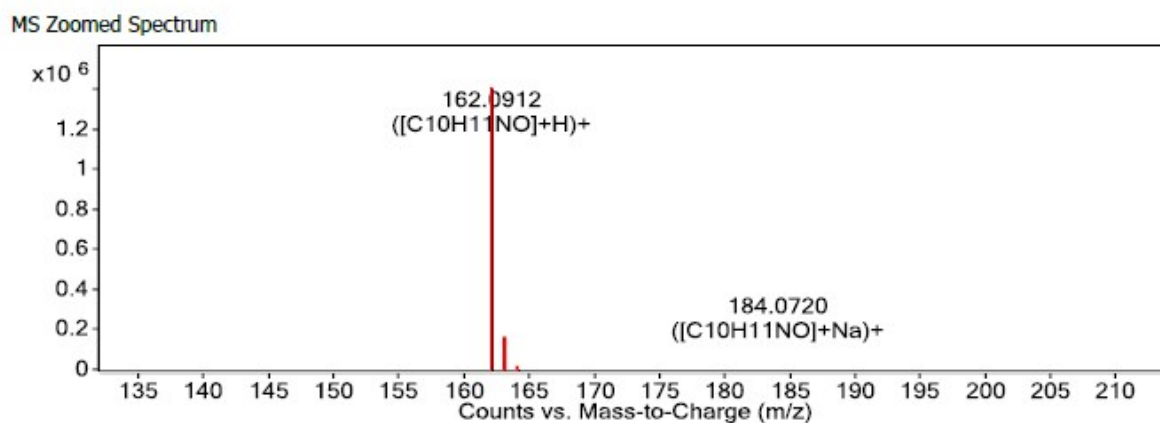
(E) N-phenyl-C-(5-NO₂)-isatinyl nitrone (4n)



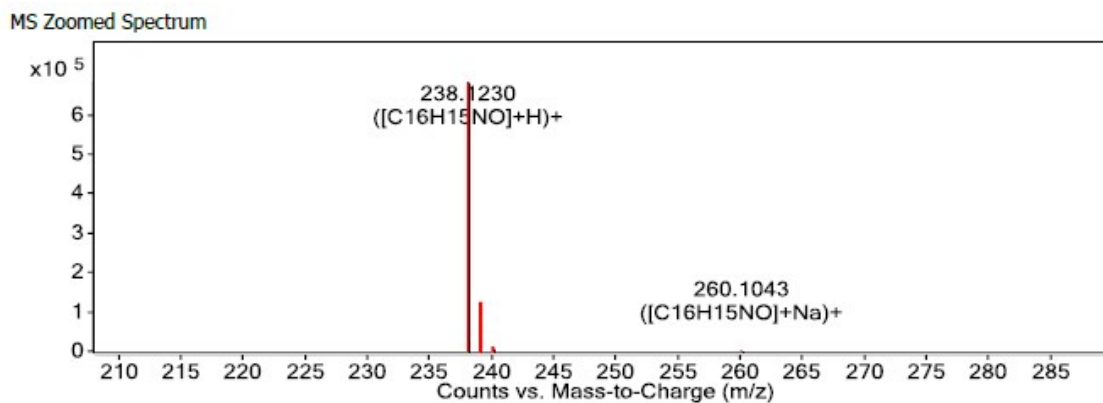
(E) N-Methyl-C-(5,7-Cl)-isatinyl nitrone (4o)



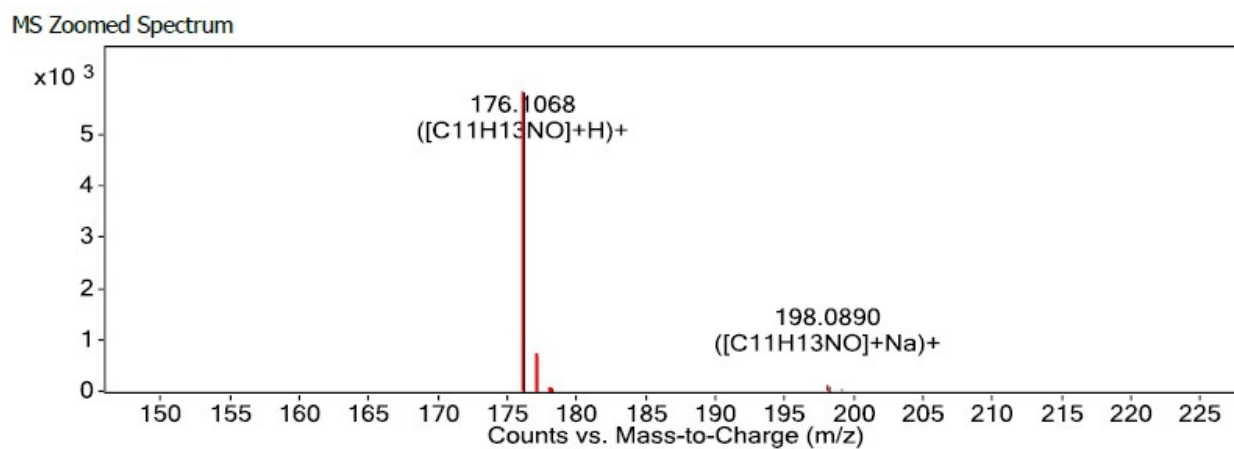
(Z) N-methyl-C-indanoyl nitrone 5a



(Z) N-benzyl-C-indanoyl nitrone (5b)

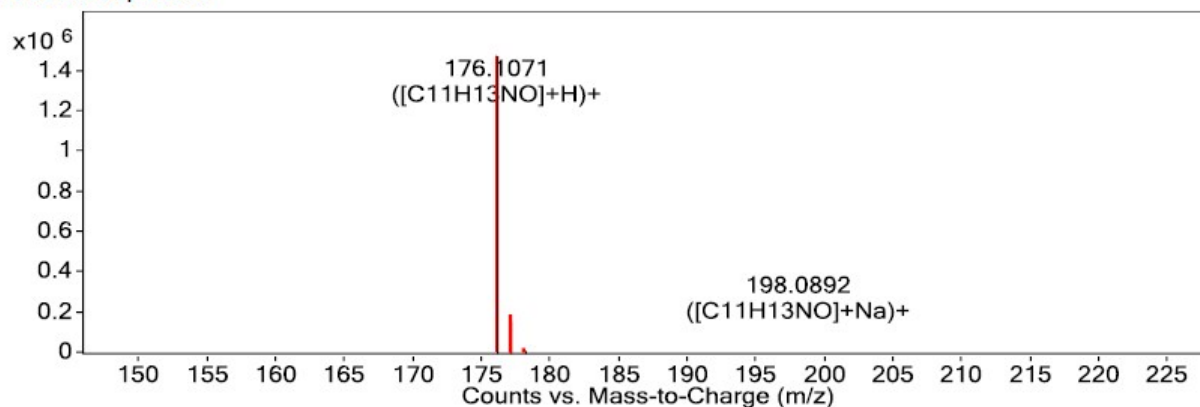


(Z) N-methyl-C-(2-Me)-indanoyl nitrone (5c)



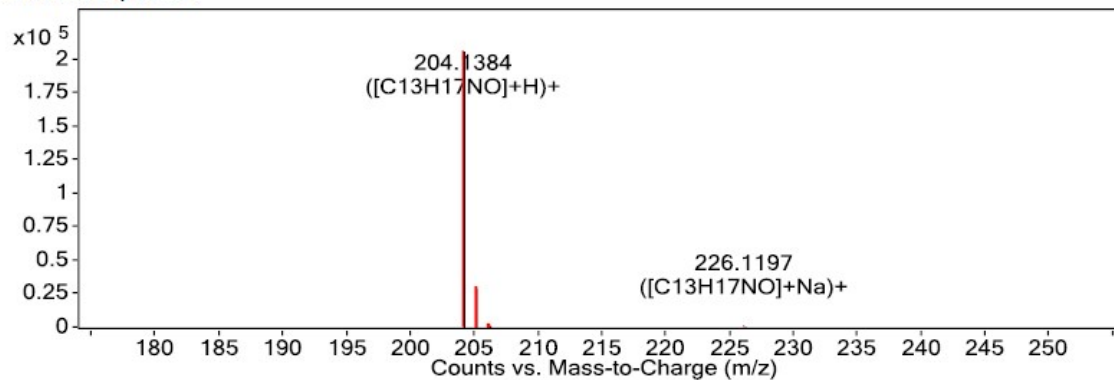
(Z) N-methyl-C-(3-Me)-indanoyl nitron (5d)

MS Zoomed Spectrum



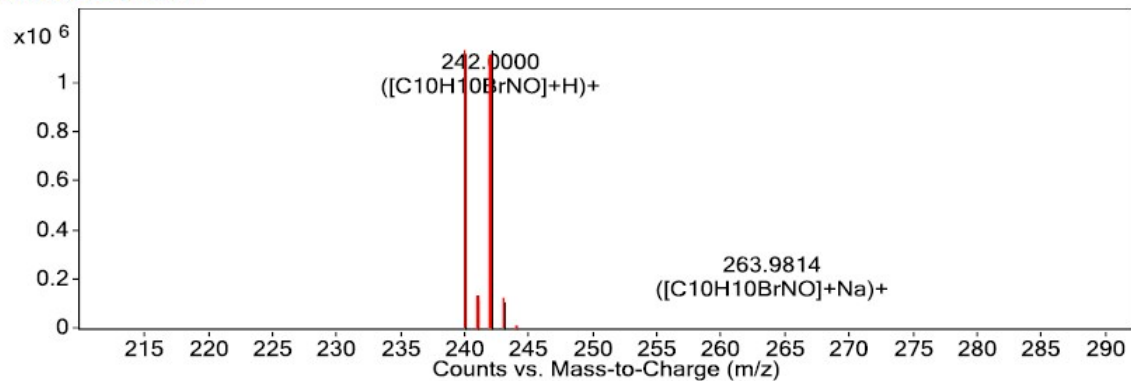
(Z) N-methyl-C-(2-Pr)-indanoyl nitron (5e)

MS Zoomed Spectrum

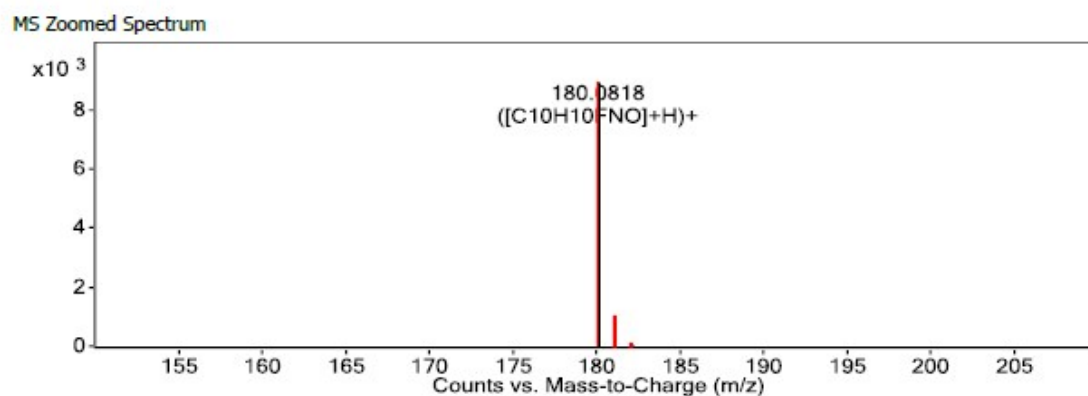


(Z) N-methyl-C-(5-Br)-indanoyl nitron (5f)

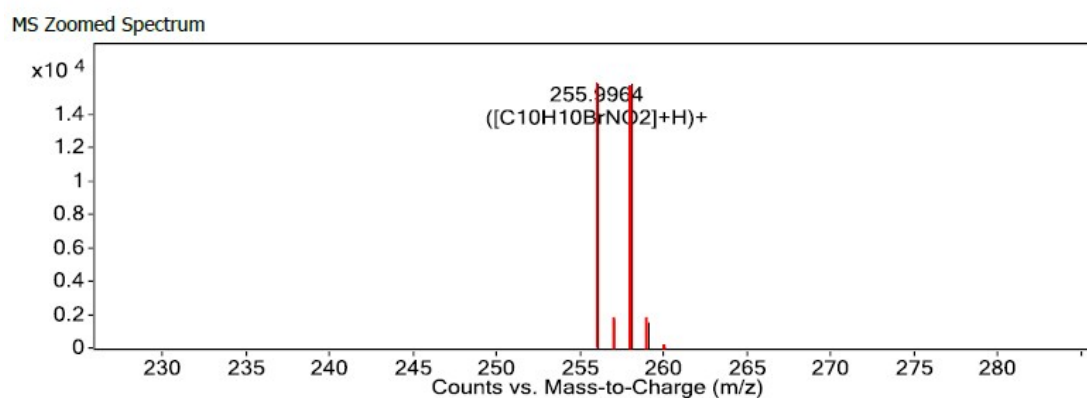
MS Zoomed Spectrum



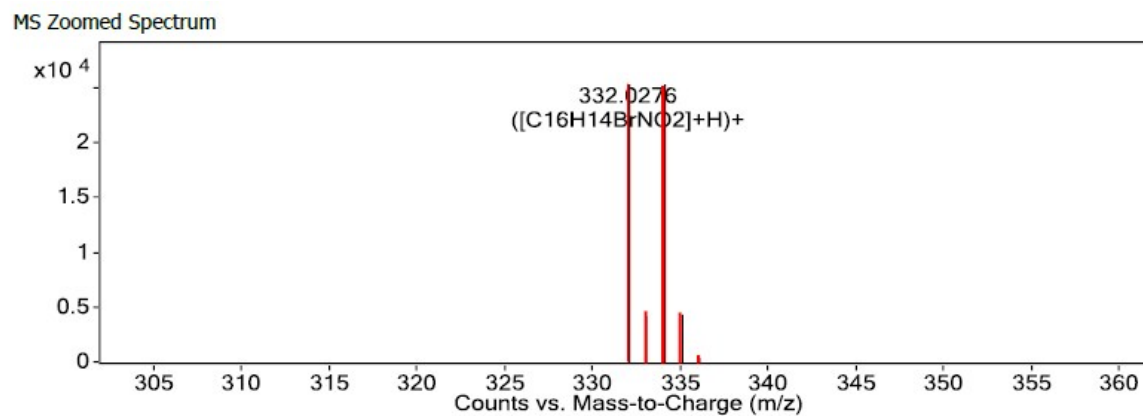
(Z) N-methyl-C-(5-F)-indanoyl nitron (5g)



(Z) N-methyl-C-(4-Br-7-OH)-indanyl nitron 5h

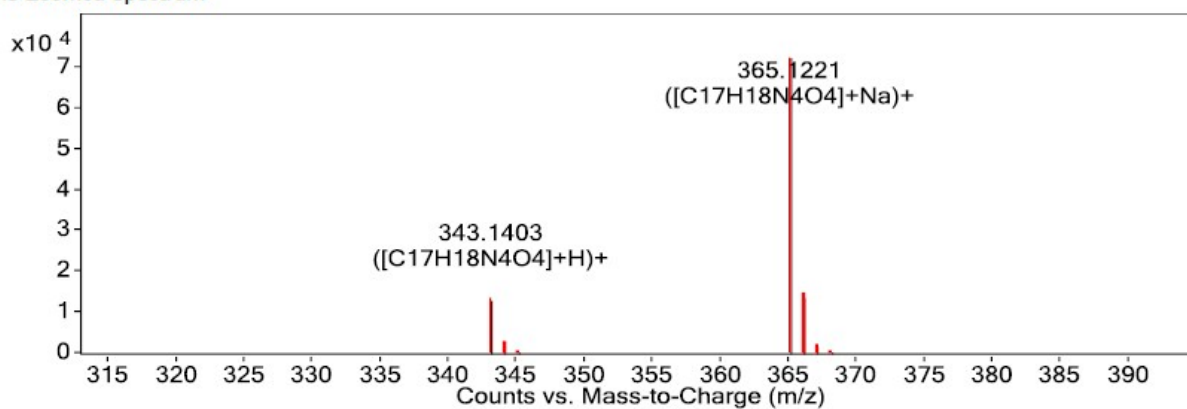


(Z) N-benzyl-C-(4-Br-7-OH)-indanyl nitron 5i



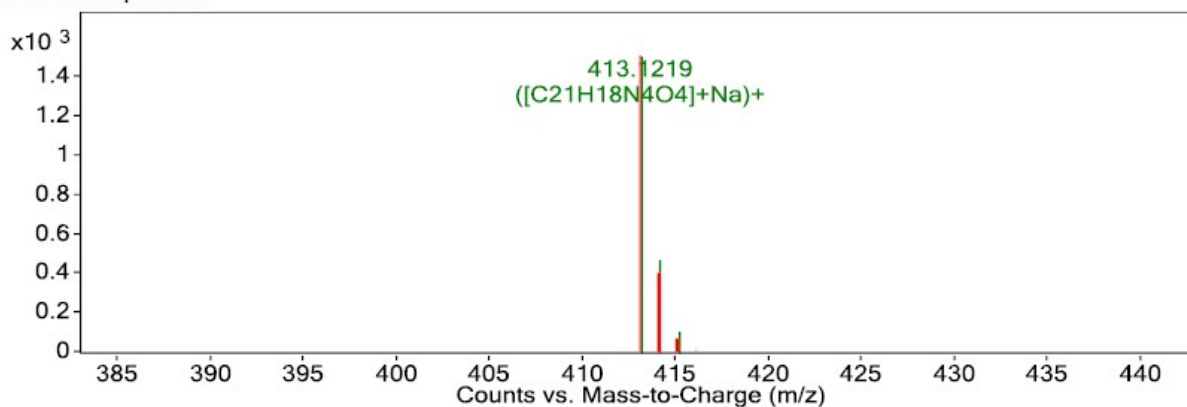
5'-Thyminy-2'-methyl-spiro [indoline-3,3'-isoxazolidine]-1-methyl-2-one (7a)

MS Zoomed Spectrum



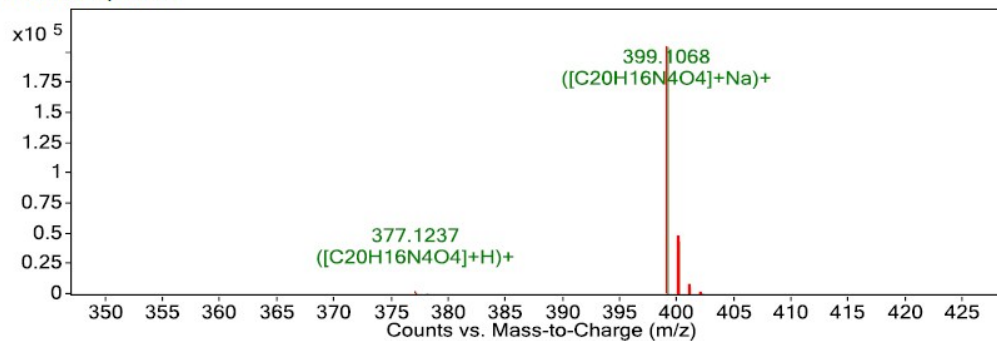
5'-Uracil -2'-benzyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7b)

MS Zoomed Spectrum



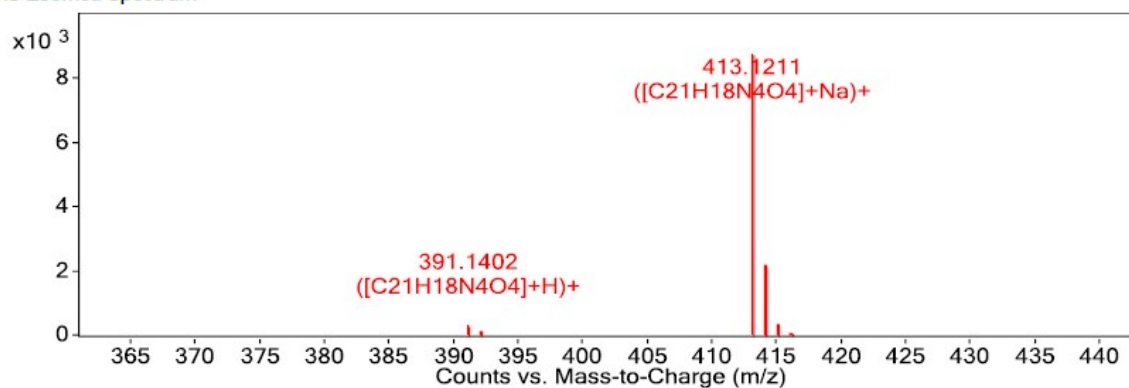
5'-Uracil-2'-phenyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7c)

MS Zoomed Spectrum



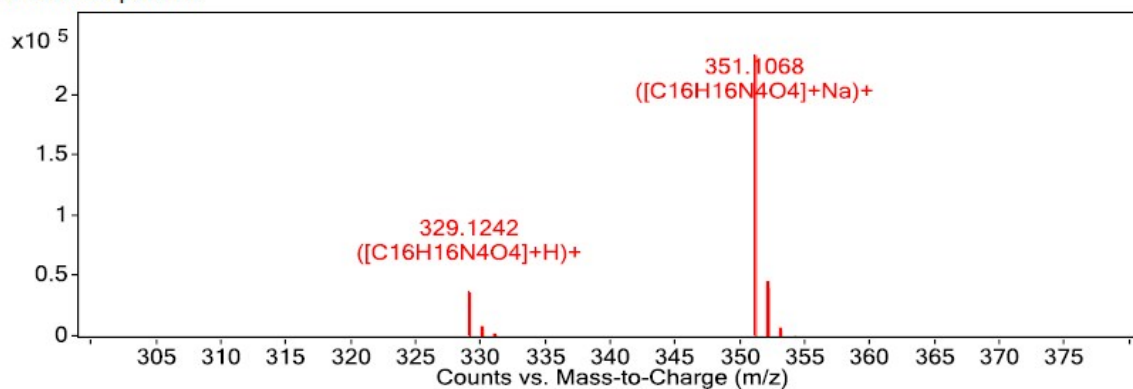
5'-Thyminy-2'-phenyl-spiro [indoline-3,3'-isoxazolidine]-2-one (7d)

MS Zoomed Spectrum



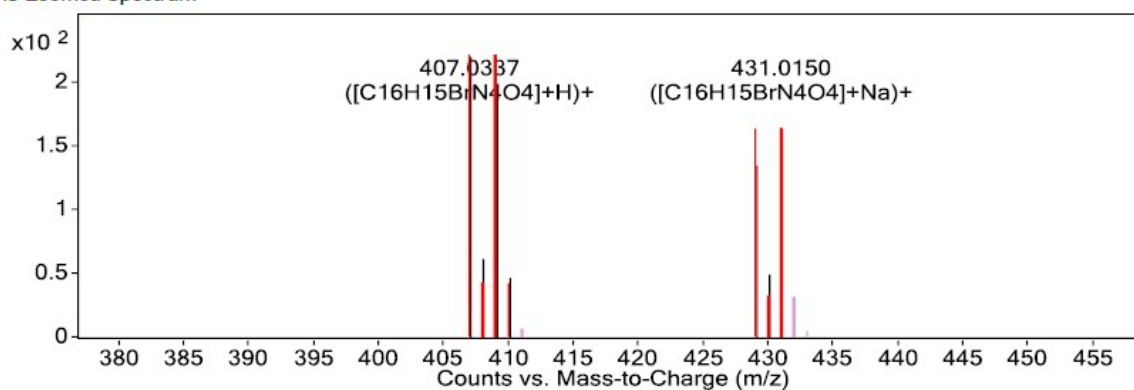
5'-Uracil-2'-methyl-spiro [indoline-3,3'-isoxazolidine]-1methyl-2-one (7e)

MS Zoomed Spectrum

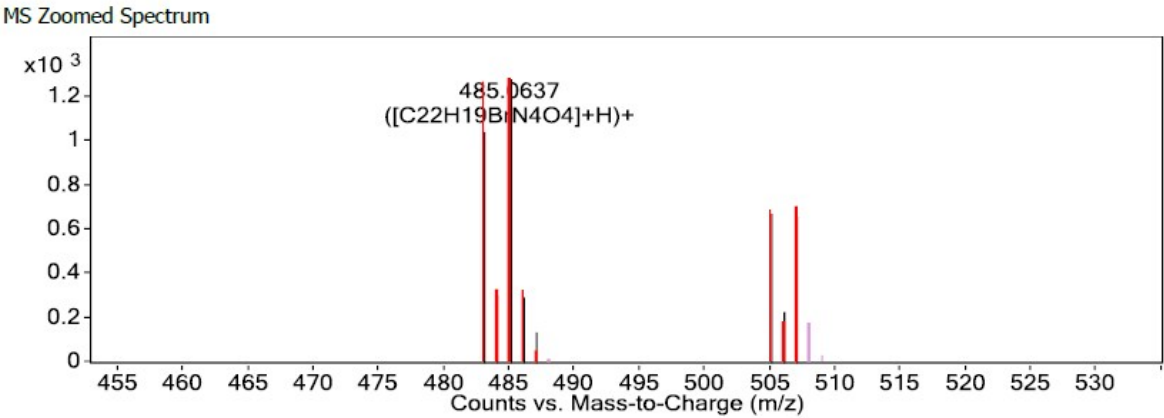


5'-Thyminy-2'-methyl-spiro [5-bromo-indoline-3,3'-isoxazolidine]-2-one (7f)

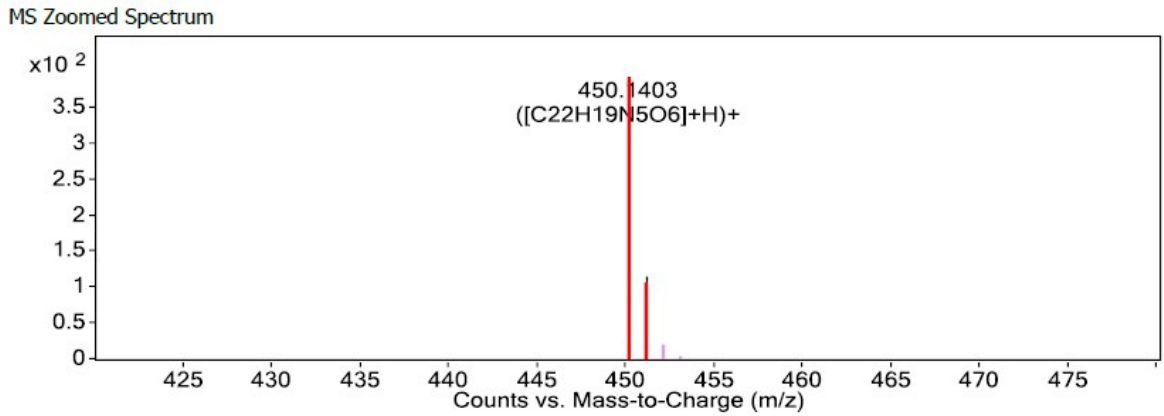
MS Zoomed Spectrum



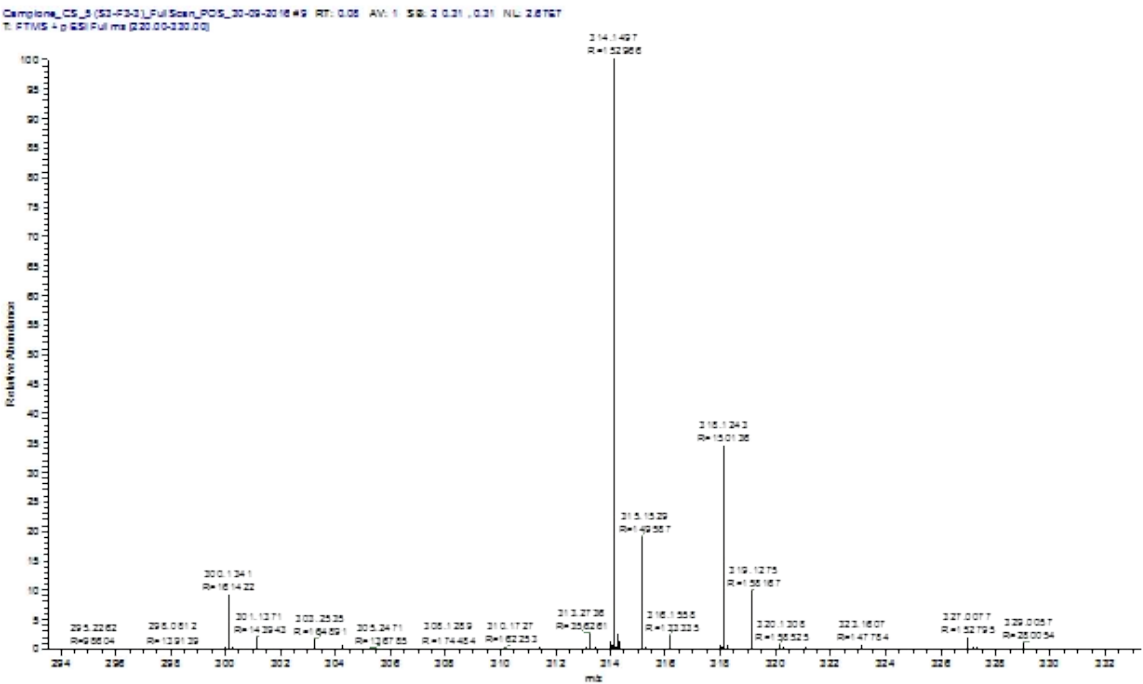
5'-Thyminy-2'-benzyl-spiro [5-bromo-indoline-3,3'-isoxazolidine]-2-one (7g)



5'-Thyminy-2'-benzyl-spiro [5-nitro-indoline-3,3'-isoxazolidine]-2-one (7h)

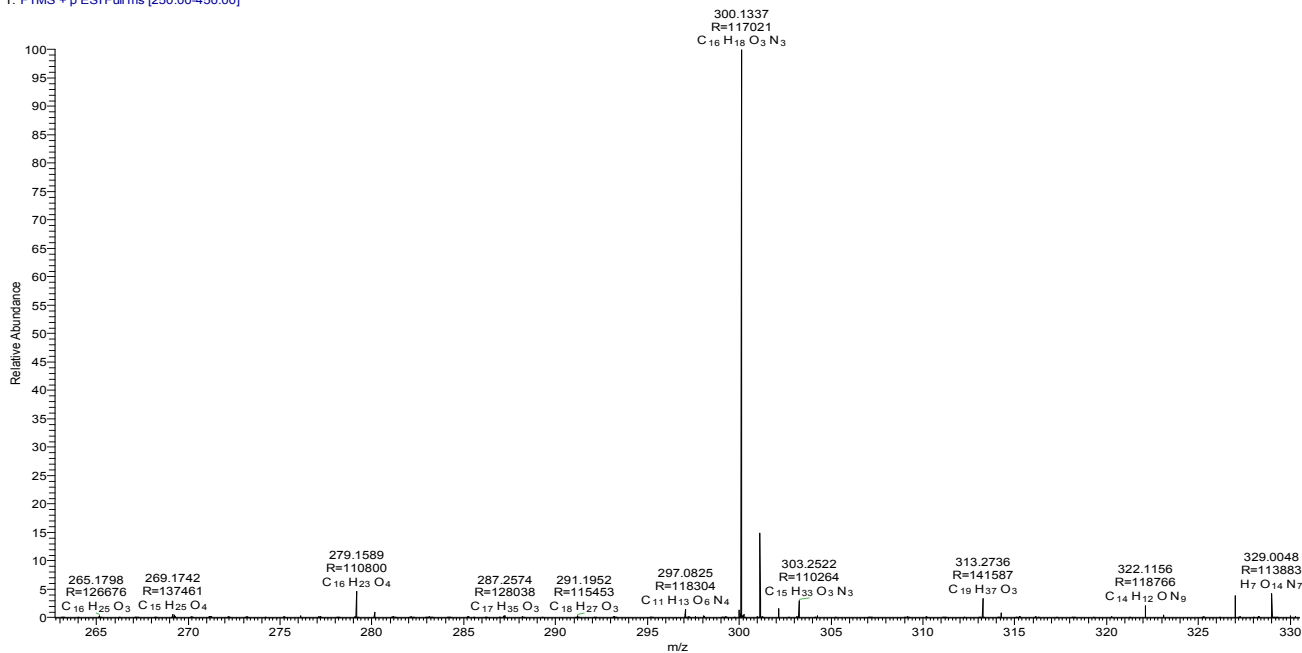


5'-Thyminy-2'-methyl-spiro [indane-3,3'-isoxazolidine] (8a)



5'-Uracil-2'-methyl- spiro [indane-3,3'-isoaxazolidine] (8b)

Campione_CS_1_principale(S4-F2b-3)_FullScan_30-09-16 #36 RT: 0.34 AV: 1 SB: 11 0.54-0.62, 0.88 NL: 1.18E7
T: FTMS + p ESI Full ms [250.00-450.00]



Theoretical Calculations

All of the calculations were performed using the Gaussian09 program.¹ Molecular geometries were optimized with the B3LYP functional² using added D3 version of Grimme's dispersion³ with Becke-Johnson damping⁴ in conjunction with Def2SVP basis set a double- ζ quality set with polarization functions on both hydrogens as well as non-hydrogen atoms.⁵ This combination of functional and basis has been recently used successfully⁶ particularly because the Grimme-D3 dispersion corrections have been specifically parametrized for Ahlrichs' basis sets. Analytical second derivatives of the energy were calculated to classify the nature of the minima, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies.

Reactivity Indices

The electronic chemical potential μ , that is the negative of electronegativity χ , is associated with the charge transfer ability of the system in its ground state geometry and is the index pointing to the direction of the electronic flux during the cycloaddition. It can be approximated, using Koopmans' theorem, to the half value of the sum of the one-electron energies of HOMO and LUMO orbitals (Eq. 1).¹

$$\mu = \frac{\varepsilon_{\text{HOMO}} + \varepsilon_{\text{LUMO}}}{2} \quad (1)$$

The chemical hardness η (approximated to be the difference between LUMO and HOMO energies) is a measure of the stability of a system, the system having the maximum hardness being the most stable (Eq. 2).²

$$\eta = \varepsilon_{\text{HOMO}} - \varepsilon_{\text{LUMO}} \quad (2)$$

The chemical softness parameter S is strictly related to the chemical hardness and it is due to the inverse of 2η (Eq. 3).³

$$S = \frac{1}{2\eta} \quad (3)$$

¹ (a) Pearson, R. G. *J. Chem. Ed.* **1987**, *64*, 561–567. (b) Parr, R. G.; von Szentpály, L.; Liu, S. *J. Am. Chem. Soc.* **1999**, *121*, 1922–1924.

² Domingo, L. R.; Aurell, M. J.; Perez, P.; Contreras, R. *Tetrahedron* **2002**, *58*, 4417–4423.

The global electrophilicity power ω is a useful descriptor of reactivity that allows a quantitative classification of the global electrophilic character of a molecule,³ and it is extremely useful for evaluating both Diels-Alder reactions⁴ and 1,3-dipolar cycloaddition reactions.⁵ The ω index measures the stabilization in energy when the system acquires an additional electronic charge ΔN from the environment and it is defined as illustrated in Eq. 4.⁶

$$\omega = \frac{\mu^2}{2\eta} \quad (4)$$

The maximum amount of electronic charge that the electrophile system may accept is given by:

$$\Delta N_{\max} = -\frac{\mu}{\eta} \quad (5)$$

³ Chattaraj, P. K.; Sarkar, U.; Roy, D. R. *Chem. Rev.* **2006**, *106*, 2065-2091.

⁴ (a) Chandra, A. K.; Nguyen, M. T. *J. Phys. Chem. A* **1998**, *102*, 6181-6185. (b) Chandra, A. K.; Nguyen, M. T. *J. Comput. Chem.* **1998**, *19*, 195-202. (c) Nguyen, T. L.; De Proft, F.; Chandra, A. K.; Uchimaru, T.; Nguyen, M. T.; Geerlings, P. *J. Org. Chem.* **2001**, *66*, 6096-6103. (d) Sengupta, D.; Chandra, A. K.; Nguyen, M. T. *J. Org. Chem.* **1997**, *62*, 6404-6406. (e) Damoun, S.; Van de Woude, G.; Mendez, F.; Geerlings, P. *J. Phys. Chem. A* **1997**, *101*, 886-893.

⁵ (a) Parr, R. G.; Pearson, R. G. *J. Am. Chem. Soc.* **1983**, *105*, 7512-7516. (b) Parr, R. G.; Yang, W. In *Density Functional Theory of Atoms and Molecules*; Oxford University, New York, 1989.

⁶ Perez, P.; Domingo, L. R.; Aurell, M. J.; Contreras, R. *Tetrahedron* **2003**, *59*, 3117-3125.

Table S1. Calculated (B3LYP-D3BJ/def2SVP) absolute energies (hartrees) of hydroxylamines **1a-h**

	E ₀	G
1a	-170.831800	-170.856995
1b	-401.663482	-401.697409
1c	-362.407258	-362.438264
1d	-821.887369	-821.920554
1e	-476.816677	-476.851397
1f	-566.761050	-566.796116
1g	-1035.986147	-1036.030943
1h	-858.205142	-858.242438
1i	-837.943001	-837.986422

Table S2. Calculated (B3LYP-D3BJ/def2SVP) absolute energies (hartrees) of ketones **2a-k**

	E ₀	G
2a	-512.612135	-512.645056
2b	-551.874436	-551.909245
2c	-3085.892123	-3085.928301
2d	-716.960109	-716.997196
2e	-611.780175	-611.814329
2f	-627.027817	-627.064097
2g	-849.400063	-849.440167
2h	-909.248800	-909.286713
2i	-740.286602	-740.326443
2j	-3085.893544	-3085.929692
2k	-716.957737	-716.994951

Table S3. Calculated (B3LYP-D3BJ/def2SVP) absolute energies (hartrees) of ketones **3a-o**

	E ₀	G
3a	-422.592006	-422.624855
3b	-461.857110	-461.891515
3c	-461.856218	-461.891239
3d	-540.381406	-540.420124
3e	-2995.874151	-2995.910267
3f	-521.760373	-521.794436
3g	-461.859289	-461.892840
3h	-561.026211	-561.060984
3i	-576.273753	-576.310638
3j	-759.380596	-759.417464
3k	-626.939844	-626.976975
3l	-537.006034	-537.042206
3m	-521.749455	-521.783194
3n	-819.234663	-819.272436
3o	-666.207730	-666.245644
3p	-748.191259	-747.962896

Table S1. Calculated (B3LYP-D3BJ/def2SVP) reactivity indices

	HOMO	LUMO	μ	η	ω	μ (eV)	η (eV)	ω (eV)	N (eV)
1a	-0.23462	0.05814	-0.0882	0.2928	0.0133	-2.40	7.97	0.36	4.78
1b	-0.23775	-0.01351	-0.1256	0.2242	0.0352	-3.42	6.10	0.96	4.69
1c	-0.21083	-0.00549	-0.1082	0.2053	0.0285	-2.94	5.59	0.78	5.43
1d	-0.21973	-0.01606	-0.1179	0.2037	0.0341	-3.21	5.54	0.93	5.18
1e	-0.23371	0.05973	-0.0892	0.2743	0.0135	-2.38	7.89	0.38	4.81
1f	-0.19350	-0.00684	-0.1002	0.1867	0.0269	-2.73	5.08	0.73	5.90
1g	-0.23941	-0.07976	-0.1596	0.1597	0.0798	-4.34	4.34	2.17	4.65
1h	-0.24104	-0.05289	-0.1470	0.1882	0.0574	-4.00	5.12	1.56	4.60
1i	-0.24357	-0.03613	-0.1399	0.2074	0.0471	-3.81	5.64	1.28	4.54
2a	-0.24758	-0.10323	-0.1754	0.1444	0.1066	-4.77	3.93	2.90	4.43
2b	-0.24069	-0.10142	-0.1711	0.1393	0.1050	-4.65	3.79	2.86	4.61
2c	-0.24571	-0.11208	-0.1789	0.1336	0.1197	-4.87	3.64	3.26	4.48
2d	-0.27356	-0.12618	-0.1999	0.1474	0.1355	-5.44	4.01	3.69	3.72
2e	-0.25447	-0.10569	-0.1801	0.1488	0.1090	-4.90	4.05	2.97	4.24
2f	-0.24017	-0.09217	-0.1662	0.1480	0.0933	-4.52	4.03	2.54	4.63
2g	-0.26389	-0.11692	-0.1904	0.1470	0.1233	-5.18	4.00	3.36	3.98
2h	-0.26432	-0.12211	-0.1932	0.1422	0.1313	-5.26	3.87	3.57	3.97
2i	-0.25906	-0.10967	-0.1844	0.1494	0.1138	-5.02	4.07	3.10	4.11
2j	-0.25423	-0.11018	-0.1822	0.1441	0.1152	-4.96	3.92	3.14	4.25
2k	-0.2708	-0.13673	-0.2038	0.1341	0.1548	-5.54	3.65	4.21	3.79
3a	-0.24658	-0.05999	-0.1533	0.1866	0.0630	-4.17	5.08	1.71	4.45
3b	-0.24539	-0.06035	-0.1529	0.1850	0.0631	-4.16	5.04	1.72	4.49
3c	-0.24544	-0.05994	-0.1527	0.1855	0.0628	-4.15	5.05	1.71	4.48
3d	-0.24495	-0.06003	-0.1525	0.1849	0.0629	-4.15	5.03	1.71	4.50
3e	-0.25333	-0.0692	-0.1613	0.1841	0.0706	-4.39	5.01	1.92	4.27
3f	-0.2508	-0.06159	-0.1562	0.1892	0.0645	-4.25	5.15	1.54	4.34
3g	-0.23462	0.05814	-0.0882	0.2928	0.0133	-2.40	7.97	0.36	4.78
3h	-0.24681	-0.05989	-0.1534	0.1869	0.0629	-4.17	5.09	1.71	4.45
3i	-0.25267	-0.06828	-0.1605	0.1844	0.0698	-4.37	5.02	1.90	4.29
3j	-0.23329	-0.04896	-0.1411	0.1843	0.0540	-3.84	5.02	1.47	4.82
3k	-0.25847	-0.0745	-0.1665	0.1840	0.0753	-4.53	5.01	2.05	4.13
3l	-0.26706	-0.1117	-0.1894	0.1554	0.1154	-5.15	4.23	3.14	3.90
3m	-0.23607	-0.04971	-0.1429	0.1864	0.0548	-3.89	5.07	1.49	4.74
3n	-0.25445	-0.07353	-0.1640	0.1809	0.0743	-4.46	4.92	2.02	4.24
3o	-0.26668	-0.07873	-0.1727	0.1880	0.0793	-4.70	5.11	2.16	3.91
3p	-0.26685	-0.10979	-0.1883	0.1571	0.1129	-5.12	4.27	3.07	3.90
3q	-0.23462	0.05814	-0.0882	0.2928	0.0133	-2.40	7.97	0.36	4.78

Cartesian Coordinates

C1a

0 1

N	-0.2548389798	0.5466371153	-0.0194744923
H	0.1041519106	-0.4103661017	0.0025996889
O	0.3090075739	1.1491546703	1.1491811897
H	-0.4698862274	1.4611699449	1.6293250865
C	0.2951753202	1.2179591544	-1.1842037994
H	-0.0259224811	0.6658611497	-2.0826221568
H	-0.1092460846	2.2403663364	-1.2474625429
H	1.4011535983	1.2845901406	-1.1791120437

1b

0 1

N	-0.4011070236	0.7258409872	-0.0422558702
H	-0.4357452146	-0.2888794339	0.0845250112
O	0.2266411013	1.2155453358	1.1419971203
H	-0.4264582106	1.8337895668	1.4968569497
C	0.4742645439	1.0119545944	-1.1765497200
H	0.5073950014	2.1093968453	-1.2937994187
H	1.5149857815	0.6807707558	-0.9944645034
C	-0.0680463948	0.3651577791	-2.4298349466
C	0.7622896658	-0.3898934633	-3.2684599652
C	-1.4204702151	0.5155865485	-2.7762958992
C	0.2602496013	-0.9716997413	-4.4364005373
H	1.8148893984	-0.5224340913	-3.0036661641
C	-1.9254885576	-0.0699013192	-3.9382180596
H	-2.0741024837	1.0891792350	-2.1159876134
C	-1.0856922203	-0.8134644551	-4.7740509908
H	0.9225312226	-1.5549251406	-5.0809634126
H	-2.9804522422	0.0550782271	-4.1950817099
H	-1.4810983137	-1.2702938900	-5.6845614702

1c

0 1

N	0.2928286231	0.5228564518	0.0525060074
H	1.1753648173	0.2689238673	0.4947084865
O	-0.5060333321	1.1454349433	1.0313129968
H	-1.2752993500	0.5628114677	1.1044406798
C	0.4807235797	1.2899844749	-1.1107295876
C	-0.4531392916	2.2560725501	-1.5150134171
C	1.5981163650	1.0286982025	-1.9240354277
C	-0.2695016721	2.9393622238	-2.7185612389
H	-1.3054970399	2.4694294855	-0.8712306705
C	1.7664561380	1.7154250841	-3.1252444274

H	2.3311392794	0.2792931139	-1.6118438191
C	0.8344549888	2.6755641625	-3.5335495551
H	-1.0020574547	3.6927809965	-3.0196436353
H	2.6398536167	1.5007147848	-3.7462685444
H	0.9711284225	3.2142513314	-4.4735198577

1d

0 1

N	0.3002300750	0.5392044010	0.0588994711
H	1.1793684874	0.2997223564	0.5154608580
O	-0.5290999878	1.1487852858	1.0165536033
H	-1.2873410057	0.5504146003	1.0817699251
C	0.4875265696	1.2935932608	-1.1092097109
C	-0.4545274098	2.2494452324	-1.5158873434
C	1.6080058055	1.0313948130	-1.9190375910
C	-0.2650344531	2.9168443855	-2.7263034810
H	-1.3108678579	2.4728569894	-0.8838706320
C	1.7690073855	1.7122986569	-3.1233501931
H	2.3447758336	0.2885851494	-1.6028113954
C	0.8358599987	2.6636853762	-3.5467737423
H	2.6418452938	1.5022795302	-3.7462326010
H	0.9563397539	3.2022033869	-4.4866856765
Cl	-1.4453942986	4.1105162957	-3.2218209507

1e

0 1

N	0.3400292201	0.5512197847	0.1246548820
H	1.2571145536	0.1810725532	0.3729808361
O	-0.0918865463	1.3380855941	1.2165048476
H	-0.8970180304	0.8908379144	1.5123856450
C	0.3850417813	1.2637793176	-1.0938609836
C	-0.4974480117	2.3243434920	-1.3588420663
C	1.2733701217	0.8618747075	-2.0986185407
C	-0.4895048090	2.9526299337	-2.5990090917
H	-1.1757137789	2.6572396112	-0.5739625855
C	1.2772976368	1.4860409655	-3.3501360542
H	1.9729316030	0.0427254729	-1.9087211853
C	0.3917252204	2.5403384065	-3.6106944744
H	1.9828563504	1.1433759058	-4.1066217065
H	-1.1673094041	3.7817916877	-2.8110629228
O	0.3189511499	3.2168638193	-4.7909149478
C	1.1839123180	2.8463129208	-5.8347194218
H	0.9596161022	3.5081783760	-6.6821705177
H	2.2467006297	2.9720561439	-5.5558092211
H	1.0267306731	1.7978593532	-6.1496485309

1f

0 1

N	0.2881595652	0.5373140033	0.0401271694
H	1.1435470780	0.2266846780	0.4980780336
O	-0.5663725837	1.0967130489	0.9965626101
H	-1.3203244376	0.4890123023	1.0281797308
C	0.4957638089	1.3067484101	-1.0991503961
C	-0.4333217168	2.2831442149	-1.5070799229
C	1.6327508305	1.0516655193	-1.8960430968
C	-0.2328266242	2.9818945419	-2.6913668966
H	-1.2966191586	2.4890633373	-0.8766675438
C	1.8296205158	1.7476430308	-3.0795679924
H	2.3579282779	0.2974151785	-1.5803477496
C	0.8927650661	2.7089177331	-3.4714147035
H	2.6993681564	1.5671765440	-3.7100374385
H	-0.9349527494	3.7445767405	-3.0263542436
N	1.1006577908	3.4465633109	-4.7194457919
O	2.1002957248	3.1851081043	-5.3739844138
O	0.2626216959	4.2795818719	-5.0341638142

1g

0 1

N	0.2768942295	0.5866830638	0.0835503713
H	1.1376750858	0.3617532155	0.5806190502
O	-0.6200703120	1.1680440599	0.9910450590
H	-1.3523681775	0.5357113605	1.0378254417
C	0.4867017319	1.3315168716	-1.0808022293
C	-0.4549077636	2.2648058502	-1.5346181315
C	1.6398008677	1.0880245392	-1.8479916009
C	-0.2458333014	2.9277141314	-2.7461141533
H	-1.3335806214	2.4740164483	-0.9279872377
C	1.8325397609	1.7638727148	-3.0499960425
H	2.3816018107	0.3629717491	-1.5081773052
C	0.8917510233	2.6882378339	-3.5167152055
H	1.0460752508	3.2117152596	-4.4591073035
C	3.1034244452	1.5461278547	-3.8333473743
C	-1.3063562084	3.8789575318	-3.2439463468
F	4.0267158216	2.4799707636	-3.5373147725
F	2.8876093665	1.6130272423	-5.1572029978
F	3.6564431958	0.3488965365	-3.5708417533
F	-2.3066501055	3.2168418905	-3.8561739828
F	-1.8593208809	4.5772777950	-2.2372304116
F	-0.8155322691	4.7607927276	-4.1294764835

1h

0 1

N	0.1524278262	0.4311173161	-0.0100993183
H	0.9636709290	-0.1347240648	0.2328769701
O	-0.1596387493	1.2128094655	1.1307820315
H	-1.1008543402	1.0375076517	1.2754911816
C	0.4074512288	1.2182996374	-1.1400318883
C	-0.5333132206	2.1550465954	-1.5952043535
C	1.5844212783	1.0598127680	-1.8841903435
C	-0.3030604194	2.9048084879	-2.7478548999
C	1.8132869160	1.7803722776	-3.0561585626
C	0.8711087670	2.7180875219	-3.4842978357
F	2.5029486031	0.1817043022	-1.4613597002
F	2.9349694356	1.6004817718	-3.7460847254
F	1.0835282763	3.4226352820	-4.5908396315
F	-1.2067427244	3.7875091777	-3.1609221269
F	-1.6785979565	2.3218998096	-0.9320724474

2a

0 1

C	-1.2187343546	0.8815503226	-0.0502351836
C	-0.3923398324	-0.2631679208	-0.0175124273
C	-0.9341769894	-1.5353954806	0.1484334753
C	-2.3208207411	-1.6615204762	0.2831614258
C	-3.1330789721	-0.5193792982	0.2494230039
C	-2.5991107081	0.7674264292	0.0828251018
H	-0.2732023045	-2.4047131649	0.1703205873
H	-2.7740569375	-2.6457855671	0.4145666966
H	-4.2150685231	-0.6297685907	0.3556602040
H	-3.2476573340	1.6453647042	0.0590368096
C	1.0023266639	0.1848660688	-0.1827714131
O	2.0302931669	-0.4428905111	-0.2158255087
C	0.9084057991	1.7485680074	-0.3193071179
O	1.8088060938	2.5317729530	-0.4717657103
N	-0.4456185798	2.0338170682	-0.2255882132
H	-0.8127312871	2.9766988563	-0.2803505002

2b

0 1

C	-1.1972002909	0.8535044401	0.0973805670
C	-0.3889479980	-0.2972391150	-0.0355392929
C	-0.9393192610	-1.5736043471	0.0288529495
C	-2.3192927298	-1.6994432640	0.2292887364
C	-3.1137201456	-0.5528610000	0.3601344081
C	-2.5702851670	0.7404614674	0.2969731000
H	-0.2921844269	-2.4471777697	-0.0769649802
H	-2.7795026274	-2.6877272714	0.2841333385
H	-4.1896652795	-0.6636415339	0.5162525387
H	-3.2070349449	1.6198298240	0.4013487064

C	0.9990199940	0.1558482527	-0.2329918780
O	2.0158505978	-0.4717594374	-0.3898104599
C	0.9143691894	1.7210086207	-0.2007561100
O	1.8158350677	2.5118613440	-0.3227065106
N	-0.4278395958	2.0199650137	-0.0004666763
C	-0.9433087794	3.3650142996	0.0920397013
H	-0.0946360674	4.0519726175	-0.0235413416
H	-1.6810056933	3.5635837359	-0.7029924189
H	-1.4214015918	3.5411487529	1.0698469025

2c

0 1

C	0.8967766469	-0.6168248671	0.0000001281
C	1.3318010207	0.7256334562	0.0000005798
C	0.4280240541	1.7838929658	0.0000007265
C	-0.9362623269	1.4770075033	0.0000003897
C	-1.3740651011	0.1450500662	-0.0000000551
C	-0.4617512307	-0.9191889231	-0.0000001893
H	0.7862203879	2.8144750170	0.0000010660
H	-0.8182511888	-1.9509379734	-0.0000005348
C	2.8084383638	0.7196073139	0.0000008270
O	3.5950207151	1.6308189540	0.0000012641
C	3.2017458362	-0.8028732275	0.0000003789
O	4.3060142847	-1.2784362873	0.0000002870
N	1.9927205397	-1.4840002928	0.0000000861
H	1.9330579107	-2.4956234082	-0.0000004612
Br	-2.2203991872	2.8826147456	0.0000005392
H	-2.4447402451	-0.0648675727	-0.0000002889

2d

0 1

C	0.8944243368	-0.6111682409	0.0000002781
C	1.3336721788	0.7348386018	0.0000009921
C	0.4302108426	1.7879355493	0.0000015165
C	-0.9288062467	1.4634993566	0.0000012254
C	-1.3775419604	0.1371817385	0.0000005243
C	-0.4663880690	-0.9213307365	0.0000000524
H	0.7566745071	2.8276981100	0.0000020480
H	-0.8149134843	-1.9553935624	-0.0000004554
C	2.8111293232	0.7257482223	0.0000011546
O	3.5993210199	1.6341207426	0.0000018840
C	3.1991054969	-0.7962470279	0.0000000866
O	4.2970844410	-1.2811347366	-0.0000006418
N	1.9820559448	-1.4755217039	0.0000000292
H	1.9197544543	-2.4876101935	-0.0000015513
H	-2.4521276535	-0.0440722097	0.0000003765
N	-1.9234530158	2.5488093127	0.0000017561

O	-3.1026225059	2.2333087737	0.0000015715
O	-1.5024050199	3.6936440238	0.0000023334

2e

0 1

C	-1.2194218581	0.8825431575	-0.0486656702
C	-0.3908541277	-0.2632147988	-0.0175768060
C	-0.9368363999	-1.5344279974	0.1493160084
C	-2.3198811829	-1.6686486129	0.2866968604
C	-3.1124019183	-0.5168312300	0.2517899831
C	-2.5988302561	0.7750680471	0.0859136397
H	-0.2792128802	-2.4060301560	0.1704980562
H	-2.8005052621	-2.6383609531	0.4198014399
H	-3.2719483018	1.6326938959	0.0674246527
C	1.0008925592	0.1826166012	-0.1845603288
O	2.0298486688	-0.4439849419	-0.2195852777
C	0.9064275305	1.7461019485	-0.3206169149
O	1.8032635991	2.5314380699	-0.4742891492
N	-0.4505293276	2.0327719349	-0.2245089708
H	-0.8178712297	2.9757300114	-0.2785404030
F	-4.4335070933	-0.6489957761	0.3833841004

2f

0 1

C	-1.1712126527	0.9581610797	-0.1138887325
C	-0.3802791010	-0.2172062456	-0.0891062663
C	-0.9885300616	-1.4681588817	-0.1185956381
C	-2.3812261309	-1.5604548008	-0.1726966119
C	-3.1563111003	-0.3819227536	-0.1968507074
C	-2.5515837522	0.8956121136	-0.1673699388
H	-0.3693826044	-2.3679187038	-0.0991001574
H	-2.8568299586	-2.5392514085	-0.1957616880
H	-3.1871710833	1.7814637830	-0.1875654985
C	1.0293893797	0.1826702154	-0.0328646205
O	2.0395919984	-0.4771108397	0.0028657275
C	0.9973700261	1.7546191770	-0.0265024843
O	1.9291435329	2.5146540126	0.0130514623
N	-0.3502733142	2.0871183804	-0.0767947529
H	-0.6792207032	3.0454554654	-0.0848742719
O	-4.5016231729	-0.3725297290	-0.2486362061
C	-5.2109508387	-1.5950728356	-0.2818239290
H	-5.0200886406	-2.1988489945	0.6220121873
H	-6.2759004369	-1.3334483016	-0.3215667920
H	-4.9509410156	-2.1902132226	-1.1740666113

2g

0 1

C	-1.2128114336	0.8807929390	-0.0155142006
C	-0.3911329446	-0.2678525210	-0.0495694242
C	-0.9267296768	-1.5408841464	0.1012393026
C	-2.3085062170	-1.6644721911	0.2910852046
C	-3.1208136973	-0.5198344860	0.3211590382
C	-2.5887599384	0.7650341830	0.1693582686
H	-0.2762374838	-2.4163150010	0.0652009168
H	-3.2370336282	1.6426792882	0.1918756605
C	0.9987609160	0.1797035035	-0.2657432096
O	2.0187692915	-0.4518761821	-0.3626788583
C	0.9043123384	1.7459450663	-0.3535404847
O	1.7968853814	2.5321252328	-0.5231533509
N	-0.4469502566	2.0317159420	-0.1917022383
H	-0.8129214713	2.9768907399	-0.2052304702
H	-4.1970247157	-0.6381559819	0.4596544175
C	-2.9236484200	-3.0209492398	0.5149395309
F	-2.2036852075	-3.9942916807	-0.0660602795
F	-3.0044959241	-3.3188374943	1.8260138698
F	-4.1739589623	-3.0858865805	0.0230223368

2h

0 1

C	-1.2088460253	0.8742451175	-0.0485833928
C	-0.3813918928	-0.2710967315	-0.0171778370
C	-0.9355571465	-1.5376084362	0.1512353255
C	-2.3234776695	-1.6643959920	0.2893369334
C	-3.1331360104	-0.5214866526	0.2565371359
C	-2.5831155245	0.7589970768	0.0871991024
C	1.0136083624	0.1890356977	-0.1869834533
O	2.0475846215	-0.4216986496	-0.2241766334
C	0.9015818404	1.7525564408	-0.3224459449
O	1.7961289547	2.5379116401	-0.4770039299
N	-0.4563626259	2.0308977046	-0.2248098965
H	-0.8460446685	2.9649382187	-0.2763768388
F	-0.1839422861	-2.6239299807	0.1840441240
F	-2.8829400835	-2.8588219379	0.4515169426
F	-4.4427903677	-0.6524319605	0.3879045674
F	-3.3776215883	1.8314756446	0.0595801652

2i

0 1

C	-1.3715647402	0.8167991499	0.1485542049
C	-0.4629904824	-0.2257792205	-0.1224367145
C	-0.8406478596	-1.5654647820	-0.0326947271
C	-2.1528475224	-1.8640774626	0.3353796094

C	-3.0518462630	-0.8223334026	0.6036461647
C	-2.6850034096	0.5285813793	0.5171148032
C	0.8308606496	0.3579606083	-0.4816282268
O	1.8755935822	-0.1618594186	-0.7844619060
C	0.6244709682	1.9022473510	-0.4031829960
O	1.4482759064	2.7383120636	-0.6258683858
N	-0.7386687943	2.0859754591	-0.0144524765
H	-0.1074068646	-2.3448346521	-0.2505901623
H	-2.4817960160	-2.9019557707	0.4152138882
H	-4.0780584865	-1.0637282751	0.8913996873
H	-3.3924003446	1.3252394966	0.7279117058
C	-1.4053395051	3.3045639416	0.1902456792
O	-2.5646992912	3.3819882360	0.5199390270
O	-0.6022597685	4.3396194698	-0.0241227645
C	-1.1848372014	5.6309136736	0.1576840303
H	-1.5433907713	5.7536285499	1.1902949727
H	-0.3861354567	6.3492423360	-0.0595237350
H	-2.0311156190	5.7757789594	-0.5298706676

2j

0 1

C	-1.2194863646	0.8807174944	-0.0453257588
C	-0.3913819009	-0.2636878461	-0.0180172098
C	-0.9368208212	-1.5333676499	0.1502837969
C	-2.3207221570	-1.6674244850	0.2930597031
C	-3.1237021803	-0.5181526045	0.2629344454
C	-2.5989672663	0.7731442963	0.0945956221
H	-0.2812940406	-2.4068227270	0.1689135787
H	-2.7793812990	-2.6471202033	0.4264839397
H	-3.2531529236	1.6450079610	0.0759864004
C	1.0013214516	0.1837739751	-0.1904749612
O	2.0289354402	-0.4440705333	-0.2295242510
C	0.9052967265	1.7468772030	-0.3253342775
O	1.8020439749	2.5319259419	-0.4821369072
N	-0.4508136515	2.0321711398	-0.2237796854
H	-0.8189556043	2.9749785719	-0.2758951331
Br	-5.0034921333	-0.7074297434	0.4575319166

2k

0 1

C	-1.2239244401	0.8835465025	-0.0333911763
C	-0.4000795429	-0.2649090793	-0.0131408365
C	-0.9346243704	-1.5371901324	0.1618696327
C	-2.3176776418	-1.6719367053	0.3202505148
C	-3.1058803462	-0.5194152599	0.2958600974
C	-2.6009343291	0.7741443550	0.1219827078
H	-0.2746251100	-2.4068951793	0.1733958846

H	-2.7966358809	-2.6392266941	0.4609620543
H	-3.2789027658	1.6258942348	0.1140169765
C	0.9965386969	0.1850730326	-0.2023481951
O	2.0178506436	-0.4486922650	-0.2509201345
C	0.8999055556	1.7469184645	-0.3378150360
O	1.7965058388	2.5286571955	-0.5052389625
N	-0.4552754673	2.0321545524	-0.2215478176
H	-0.8240748275	2.9751907152	-0.2706132015
N	-4.5738906926	-0.6658849834	0.4642879312
O	-5.2429774395	0.3531203217	0.4396994582
O	-5.0117238508	-1.7922366857	0.6155871023

3a

0 1

C	-1.2179587858	0.9473899890	-0.0000300250
C	-0.3957724302	-0.1853909411	-0.0000190008
C	-0.9213790141	-1.4812792038	0.0000450041
C	-2.3066223873	-1.6325578447	0.0001093796
C	-3.1396383828	-0.5001358387	0.0001061590
C	-2.6064591047	0.7923620919	0.0000350655
C	-0.4036620675	2.2253416836	-0.0001442788
C	1.0670888132	1.7542743989	-0.0000111341
H	-0.2442637392	-2.3382500224	0.0000474559
H	-2.7517062446	-2.6299603426	0.0001651121
H	-4.2241873942	-0.6339483310	0.0001597504
H	-3.2679973404	1.6623107226	0.0000293732
H	-0.6438095779	2.8406163006	-0.8823130969
H	1.6318563940	2.0942871280	0.8818661124
C	1.0333165073	0.2174963506	-0.0000795871
H	1.6321045759	2.0944140669	-0.8816763189
H	-0.6439155668	2.8408852852	0.8818055534
O	1.9957021050	-0.5160833829	-0.0001547441

3b

0 1

C	-1.2622507517	0.9239080475	-0.0511932081
C	-0.4313618564	-0.2039012217	-0.0649685395
C	-0.9448721046	-1.5024035613	0.0102896154
C	-2.3256868705	-1.6619781393	0.1148145756
C	-3.1661485091	-0.5354303442	0.1378118276
C	-2.6456034991	0.7599516091	0.0533487338
C	-0.4595008967	2.1993396300	-0.1894972014
C	1.0188420701	1.7542115125	-0.0891718953
H	-0.2630797450	-2.3557056506	-0.0099512280
H	-2.7610431080	-2.6617749401	0.1811247076
H	-4.2468665891	-0.6758927769	0.2218684733
H	-3.3134119402	1.6252549842	0.0672240259

H	-0.6608128830	2.6668083936	-1.1694231214
H	1.3894364534	1.9686041618	0.9305639132
C	0.9867282630	0.2154558755	-0.1760846728
H	-0.7354282807	2.9442970395	0.5736768129
O	1.9539527764	-0.5015749328	-0.3079977066
C	1.9810137657	2.3729062717	-1.0982028039
H	2.0793941767	3.4590397913	-0.9475292861
H	2.9747039343	1.9115925576	-0.9999160690
H	1.6307125046	2.2007408323	-2.1291683633

3c

0 1

C	-1.2097640587	0.9283462513	-0.0206425824
C	-0.3932185113	-0.2076653954	0.0263734399
C	-0.9236196361	-1.5013782533	0.0501559167
C	-2.3093789518	-1.6480703733	0.0217429013
C	-3.1374094885	-0.5132599356	-0.0279055933
C	-2.5986454439	0.7771753653	-0.0496895461
C	-0.3953445686	2.2132168331	-0.0304995908
C	1.0734341093	1.7218206422	-0.0496464315
H	-0.2498790738	-2.3604276873	0.0885674479
H	-2.7584141515	-2.6438817142	0.0379547603
H	-4.2225099929	-0.6430490047	-0.0491236448
H	-3.2590742762	1.6471323639	-0.0859030222
H	1.6858025808	2.1252197944	0.7712929967
C	1.0364092904	0.1906013269	0.0441669951
H	-0.5915936112	2.7518718497	0.9136425614
O	1.9954266133	-0.5449617231	0.1122619058
C	-0.7529598085	3.1440981877	-1.1935522219
H	-1.8104937963	3.4485173157	-1.1555057587
H	-0.1391874283	4.0582042472	-1.1678669811
H	-0.5813118879	2.6425116157	-2.1597198982
H	1.5882912618	1.9947882237	-0.9860159941

3d

0 1

C	-1.3567594706	0.8734409887	-0.1122912063
C	-0.4700440486	-0.2064567468	-0.0146618540
C	-0.9196044651	-1.5224351984	0.1326500626
C	-2.2936789293	-1.7483849991	0.1939083500
C	-3.1905290686	-0.6696082768	0.1041788513
C	-2.7332486803	0.6429606324	-0.0508035280
C	-0.6159931635	2.1785478603	-0.3060106907
C	0.8795933394	1.8190646007	-0.1380642014
H	-0.1949930468	-2.3371514030	0.1998687229
H	-2.6801306353	-2.7632038468	0.3135835065
H	-4.2653355799	-0.8617494013	0.1553963507

H	-3.4440425826	1.4702237700	-0.1237745544
H	1.2205653811	2.1414874885	0.8638378284
C	0.9280549633	0.2795704337	-0.0985859881
H	-0.9552503521	2.9508935646	0.4020258368
O	1.9350992332	-0.3930958389	-0.1297111260
H	-0.8120727343	2.5758732898	-1.3174926004
C	1.8363380987	2.4018207062	-1.1778155156
H	2.8171533919	1.9158618271	-1.0441682040
H	1.4873311947	2.1141164863	-2.1868645490
C	1.9887178376	3.9210636994	-1.0995953766
H	1.0000042274	4.4002795025	-1.2148046278
H	2.3389029119	4.1946637984	-0.0878295383
C	2.9505244256	4.4792498366	-2.1470638579
H	3.0519481707	5.5728304086	-2.0643052474
H	3.9555262511	4.0394343957	-2.0373168424
H	2.6025091801	4.2519258511	-3.1684453709

3e

0 1

C	-1.2175851017	0.9454328732	0.0025272212
C	-0.3946955146	-0.1861670464	0.0018460544
C	-0.9246549140	-1.4798909654	0.0004372882
C	-2.3079654398	-1.6376245582	-0.0002951660
C	-3.1289919364	-0.4964284884	0.0003985611
C	-2.6060899385	0.8001028886	0.0018042670
C	-0.4044278065	2.2241904125	0.0040272875
C	1.0665140160	1.7532412703	0.0042878318
H	-0.2532003831	-2.3412521536	-0.0000633557
H	-3.2723956946	1.6641308241	0.0023088156
H	1.6302841292	2.0931205801	0.8867453010
C	1.0339995173	0.2165463148	0.0028277781
H	-0.6467532313	2.8375446001	0.8866496063
O	1.9949511684	-0.5182332868	0.0025443055
H	-0.6459370004	2.8390783893	-0.8777517766
H	1.6311477806	2.0947941573	-0.8769689323
Br	-5.0186137230	-0.7285340742	-0.0006154197
H	-2.7614452478	-2.6292976373	-0.0013931674

3f

0 1

C	-1.2179046429	0.9465978878	0.0025122650
C	-0.3940297142	-0.1857242000	0.0018659598
C	-0.9233360005	-1.4811030207	0.0004407239
C	-2.3057475556	-1.6386273051	-0.0003511264
C	-3.1173110141	-0.4955838613	0.0003073577
C	-2.6057595384	0.8010836160	0.0017283136
C	-0.4041301459	2.2241943988	0.0040711397

C	1.0665593801	1.7530496248	0.0042629272
H	-0.2496861849	-2.3405432662	-0.0000257623
H	-3.2904877522	1.6510678776	0.0021817282
H	1.6304506345	2.0928123715	0.8866627397
C	1.0330959428	0.2159120403	0.0028939227
H	-0.6466730023	2.8375997775	0.8866904656
O	1.9953340427	-0.5178471563	0.0026998145
H	-0.6459156298	2.8392881256	-0.8775793753
H	1.6311570504	2.0943508394	-0.8770920934
F	-4.4450602192	-0.6608086556	-0.0004676906
H	-2.7800642204	-2.6211382241	-0.0014683099

3g

0 1

C	-3.6508171680	-3.0270043521	0.2595455448
C	-3.0293898188	-1.6658344743	0.2868697294
C	-3.8050047940	-0.5051083541	0.4970507697
H	-1.0827106900	-2.4873565429	-0.0673491040
C	-1.6412775196	-1.5636114446	0.0949757320
C	-3.1577088669	0.7384771040	0.5094684488
C	-1.7783535054	0.8321248752	0.3234898417
C	-1.0135144576	-0.3230924655	0.1153343993
H	-3.7481627557	1.6458919698	0.6628578767
H	-1.2955334036	1.8125680295	0.3349285941
H	0.0662847123	-0.2482914450	-0.0322604075
C	-5.1470906660	-3.1014740020	0.5195823841
H	-5.2719423593	-3.2219705797	1.6129931428
H	-5.5230650250	-4.0247073693	0.0554106379
C	-5.8918438328	-1.8501005691	0.0547531517
H	-6.9647724677	-1.9333774627	0.2882729544
H	-5.8102284777	-1.7587362938	-1.0424199038
C	-5.2975234935	-0.6048255706	0.7132712516
H	-5.4980609785	-0.6418934296	1.8012855467
H	-5.7879813983	0.3102834821	0.3455806667
O	-2.9900831740	-4.0277718054	0.0589361128

3h

0 1

C	-3.6495030616	-3.0269842752	0.2580353480
C	-3.0287948358	-1.6631050544	0.2863117689
C	-3.8054834736	-0.5038367848	0.4971738882
H	-1.0629087242	-2.4817727431	-0.0723488302
C	-1.6412974074	-1.5718182382	0.0925123860
C	-3.1552878551	0.7390101972	0.5094596599
C	-1.7774673437	0.8380457202	0.3233316543
C	-1.0354755258	-0.3267451247	0.1168374618
H	-3.7410568185	1.6489477535	0.6633275680

H	-1.2666878775	1.8027480178	0.3291404823
C	-5.1443994323	-3.1014460080	0.5198858200
H	-5.2672367761	-3.2215736408	1.6135785039
H	-5.5207053471	-4.0249757200	0.0567443809
C	-5.8904059161	-1.8503499972	0.0555746130
H	-6.9628309953	-1.9355230988	0.2900911751
H	-5.8097118054	-1.7589108206	-1.0416056120
C	-5.2979261179	-0.6040098202	0.7140249545
H	-5.5009943110	-0.6399198670	1.8015536300
H	-5.7891100143	0.3095023108	0.3435118609
O	-2.9849405621	-4.0236353083	0.0553162190
F	0.2891692107	-0.2281586380	-0.0637198323

3i

0 1

C	-3.6707888093	-3.0289807291	0.2377233718
C	-3.0848982774	-1.6765315308	0.4483680183
C	-3.8946049438	-0.5338439014	0.6576139301
H	-1.0936608650	-2.4369780231	0.2672902297
C	-1.6894558816	-1.5373047588	0.4336738849
C	-3.2830236976	0.7037571786	0.8431078000
C	-1.8845004586	0.8320835322	0.8315105496
C	-1.0787890812	-0.3031115033	0.6245104779
H	-3.8779810258	1.6063676669	0.9977120583
C	-5.1881594130	-3.1327894109	0.2983832820
H	-5.4485798899	-3.3559796266	1.3508951361
H	-5.4875918516	-4.0104053260	-0.2928203503
C	-5.8905957683	-1.8481812818	-0.1412504923
H	-6.9826187312	-1.9563369034	-0.0477122608
H	-5.6790520345	-1.6588307607	-1.2081048794
C	-5.4001407557	-0.6627720185	0.6909519838
H	-5.7203620812	-0.8028867088	1.7410793069
H	-5.8623984825	0.2782989479	0.3542400488
O	-2.9769481273	-4.0108954481	0.0444695276
H	0.0079094782	-0.2284758237	0.6089790797
O	-1.4031377398	2.0803294601	1.0211371658
C	-0.0077682668	2.2910807814	1.0138482660
H	0.4424457463	2.0109208508	0.0452261291
H	0.1462636682	3.3647457449	1.1828376133
H	0.4950520197	1.7246767022	1.8174357632

3j

0 1

C	-1.2134575827	0.9433653539	0.0531571135
C	-0.3944151498	-0.1843281501	-0.0601578149
C	-0.9156378973	-1.4800917693	-0.0920798410
C	-2.2978356643	-1.6326187361	-0.0069112564

C	-3.1335079255	-0.5042558766	0.1051550926
C	-2.6004595045	0.7837654359	0.1365442231
C	-0.4009764842	2.2210073979	0.0637897134
C	1.0667859550	1.7561846884	-0.0585970452
H	-0.2470082962	-2.3371716560	-0.1840994646
H	-4.2147381444	-0.6463744392	0.1631902655
H	-3.2620944922	1.6490709874	0.2222913433
H	1.6886722674	2.0521677409	0.8007137558
C	1.0340608307	0.2220577361	-0.1371290548
H	-0.5840909595	2.7894238750	0.9902312768
O	1.9898110031	-0.5107771889	-0.2413060167
H	-0.7020844572	2.8791745778	-0.7675185392
H	1.5718301381	2.1449231023	-0.9566567489
C	-2.9275883707	-3.0020750136	-0.0022810395
F	-3.4082609884	-3.3167692977	1.2161103523
F	-2.0563768998	-3.9613320434	-0.3484560916
F	-3.9666637978	-3.0678827846	-0.8560859434

3k

0 1

C	-1.2192153357	0.9511202189	0.0025668753
C	-0.4015374963	-0.1856271163	0.0019140414
C	-0.9253830567	-1.4819100332	0.0005685779
C	-2.3085080799	-1.6399677881	-0.0001427778
C	-3.1155728909	-0.4942440483	0.0005203173
C	-2.6067171589	0.8047042377	0.0018638787
C	-0.4025144600	2.2266625183	0.0040230326
C	1.0675010120	1.7525033458	0.0041798881
H	-0.2501982435	-2.3401193504	0.0001007461
H	-3.2939133168	1.6503494291	0.0023161230
H	1.6327516789	2.0918296954	0.8862917350
C	1.0330359448	0.2177185376	0.0028566691
H	-0.6438302216	2.8408226050	0.8864998392
O	1.9870760347	-0.5237562635	0.0026205973
H	-0.6431393309	2.8424015501	-0.8775412542
H	1.6334126210	2.0933258053	-0.8769315700
H	-2.7838777932	-2.6197849861	-0.0011939912
N	-4.5876031472	-0.6701846779	-0.0002450325
O	-5.2736983551	0.3382049648	0.0003466964
O	-5.0178765546	-1.8108720141	-0.0014162416

3l

0 1

C	-1.1513054564	1.0580583307	-0.0998646038
C	-0.3700455535	-0.1079971445	-0.1219760436
C	-0.9497248759	-1.3590219513	-0.3420472451
C	-2.3254652779	-1.4471352290	-0.5424079353

C	-3.1137614041	-0.2746635517	-0.5205538474
C	-2.5234809193	0.9839430339	-0.2981674447
C	-0.2980002483	2.2844785919	0.1553491791
C	1.1412929720	1.7411990135	0.2939550521
H	-0.3189817519	-2.2510286974	-0.3543787393
H	-3.1670253973	1.8659527879	-0.2887259901
H	1.5925852209	1.9535499422	1.2759255080
C	1.0530971714	0.2155388071	0.1112562379
H	-0.6351100352	2.8104580449	1.0634364741
O	1.9843064048	-0.5588066403	0.1536817479
H	-0.3945698049	3.0045590913	-0.6735526968
H	1.8330584097	2.1475963433	-0.4605814840
H	-2.7842109052	-2.4200220445	-0.7146511544
O	-4.4525724602	-0.2689901301	-0.7053197297
C	-5.1299344783	-1.4854200777	-0.9350556984
H	-5.0190730700	-2.1818065420	-0.0852469439
H	-6.1915549656	-1.2327037471	-1.0538322157
H	-4.7741579750	-1.9841761611	-1.8537965867

3m

0 1

C	-1.2144549540	0.9467764682	-0.0255608049
C	-0.3928648924	-0.1903053626	-0.0628307333
C	-0.9213926394	-1.4844147571	-0.0365081855
C	-2.3050643685	-1.6309304999	0.0489139945
C	-3.1332768645	-0.4967309693	0.1024003412
C	-2.5989096164	0.7957365378	0.0654437687
C	-0.3987100776	2.2170307413	-0.1287962749
C	1.0431739930	1.7466876504	0.1178569948
H	-0.2499532035	-2.3451139499	-0.0760834509
H	-3.2572536927	1.6673498367	0.1001565419
H	1.3322933842	1.8991271154	1.1748153494
C	1.0283837262	0.2197418067	-0.1341485816
H	-0.7312639096	3.0013216277	0.5674333109
O	2.0005789755	-0.4691912632	-0.3275903712
H	-0.4535849960	2.6337752242	-1.1489050597
H	-2.7518538247	-2.6272975662	0.0784355125
H	-4.2160716243	-0.6279929471	0.1714394119
F	1.9650063848	2.3858451969	-0.6726582939

3n

0 1

C	-1.2047840919	0.9338796123	0.0024977626
C	-0.3793637693	-0.1996279348	0.0018998893
C	-0.9230533245	-1.4856721232	0.0005276920
C	-2.3121157172	-1.6311324820	-0.0002506242
C	-3.1386290859	-0.4977028648	0.0003464318

C	-2.5841395283	0.7865407856	0.0017233358
C	-0.4102526753	2.2195068136	0.0039957461
C	1.0605855644	1.7582761223	0.0042389985
H	1.6213780057	2.1019168064	0.8867831137
C	1.0525479814	0.2207292968	0.0029342563
H	-0.6632782082	2.8285906762	0.8859188078
O	2.0251150164	-0.4917302206	0.0027963861
H	-0.6625005347	2.8301752644	-0.8770531366
H	1.6221270654	2.1034037139	-0.8772489083
F	-0.1646872877	-2.5720437284	-0.0000626167
F	-2.8669703479	-2.8382623917	-0.0015617057
F	-4.4548549715	-0.6572322953	-0.0004102330
F	-3.3949577613	1.8473381593	0.0022662445

3o

0 1

C	-3.6497678888	-3.0236734256	0.2582170157
C	-3.0279337962	-1.6561989940	0.2813098240
C	-3.8085333780	-0.4983122476	0.4903636748
H	-1.0808627296	-2.4800376708	-0.0744712208
C	-1.6402118893	-1.5569916263	0.0866441029
C	-3.1693701329	0.7471202340	0.5004468653
C	-1.7929253312	0.8141727712	0.3101669806
C	-1.0066007828	-0.3210546155	0.1016966622
H	-3.7276898978	1.6710279300	0.6497027092
C	-5.1416008330	-3.0997634188	0.5288130679
H	-5.2580328007	-3.2120145460	1.6240348790
H	-5.5193305372	-4.0269458190	0.0745447918
C	-5.8909206756	-1.8524794284	0.0586959124
H	-6.9619732329	-1.9373555611	0.2976658343
H	-5.8153442304	-1.7679351219	-1.0393011320
C	-5.3003386695	-0.6000535861	0.7072443101
H	-5.4970356396	-0.6272569262	1.7958512022
H	-5.7914105730	0.3112010057	0.3324999512
O	-2.9805780369	-4.0152336992	0.0513871706
H	0.0670194455	-0.2121201334	-0.0441620561
N	-1.1400010278	2.1431302118	0.3227503644
O	0.0679049798	2.1760948007	0.1598653597
O	-1.8514394319	3.1188796164	0.4959709906